Figure S 1
Viable geometries of trimeric acylphloroglucinols in which no phenol OH is replaced by other functions.

The geometries are characterized by three factors: the mutual orientations of the monomers, the conformer type of each monomer, and the mutual orientations of the methylene bridges.

It is selected to orient the first monomer on the left with the acyl chain 'up', i.e., the ring is oriented in such a way that the acyl group is in its upper part. The orientations of the next monomers are identified as 'up' or 'down' with reference to the orientation of the first monomer.

The conformer types of the individual monomers are determined by the position of the first IHB and the orientations of relevant OHs, and are denoted according to the criteria outlined in the caption of fig. 3: a conformer is *d* if the first IHB is of the H15···O14 type and *s* if it is of the H17···O14 type; in d-r and s-w conformers, H16 is oriented towards the side of the first IHB, and in d-w and s-r conformers it is oriented to the other side.

The combinations of monomers' orientations and conformers' geometries are denoted by numbers, written after the acronym denoting the molecule (table S2). Their numbering is based on the conformers' energy-increasing sequence in the DFT/B3LYP/6-31+G(d,p) results for T1.

The two possible mutual orientations of the convex sides of the methylene bridges give origin to outstretched-type geometries if they are oriented in opposite ways, and to half-bowl-shaped geometries if they are oriented in the same way; the latter is denoted by adding the letter *y* to the number denoting the conformer. Both options are shown for each combination of monomers' geometries, to provide complete illustration.

1   1-y
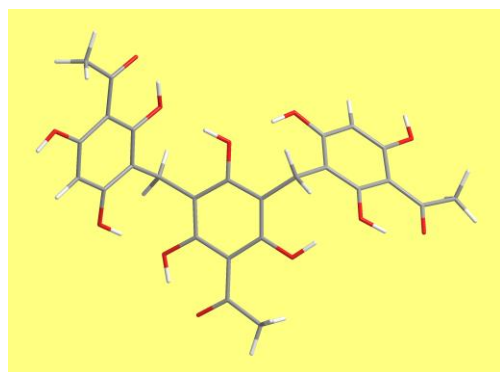
orientation of acyl groups: up—down—down
monomers' conformer types: d-r—s-w—s-w
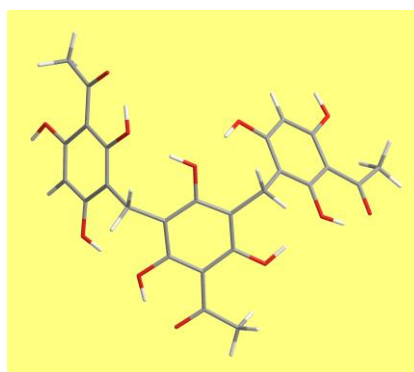
2

2-y

orientation of acyl groups: up—down—up

monomers' conformer types: d-r—s-w—d-r

3

3-y

orientation of acyl groups: up—up—up

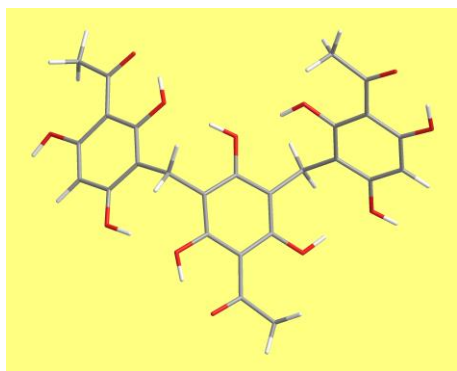monomers' conformer types: d-r—d-r—d-r

4

4-y

orientation of acyl groups: up—down—down

monomers' conformer types: d-r-u—s-w—s-w

5

5-y

orientation of acyl groups: up—down—up
monomers' conformer types: d-r-u—s-w—d-r

6

6-y

orientation of acyl groups: up—down—down
monomers' conformer types: s-w—d-r—d-r

7

7-y

orientation of acyl groups: up—up—up
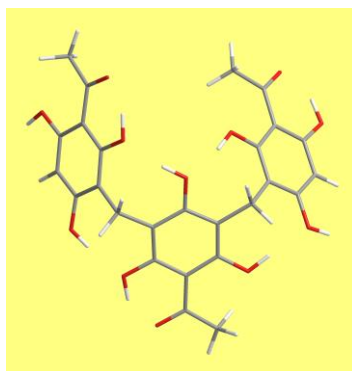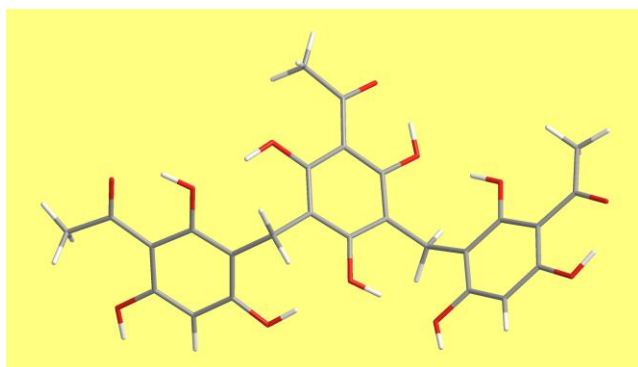monomers' conformer types: d-r-u—d-r—d-r

8

8-y
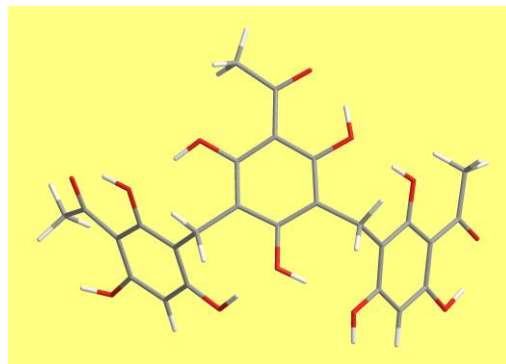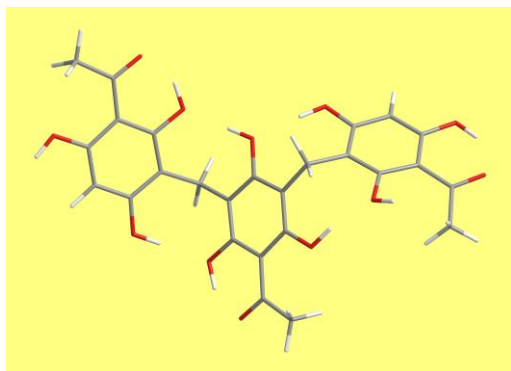
orientation of acyl groups: up—down—down
monomers' conformer types: d-r—s-w—d-r-u

9

9-y

orientation of acyl groups: up—down—down
monomers' conformer types: d-r-u—d-r—s-w-u

10

10-y
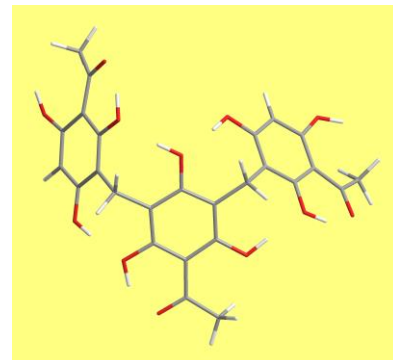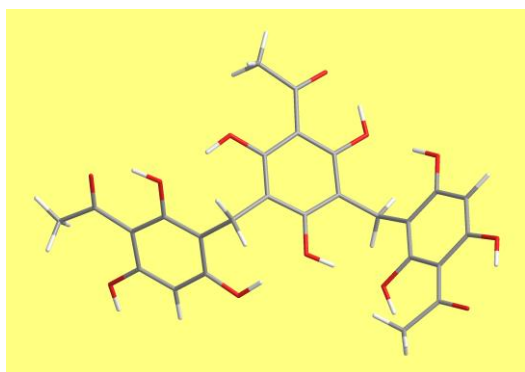
orientation of acyl groups: up—up—down
monomers' conformer types: d-r—d-r—d-w-u
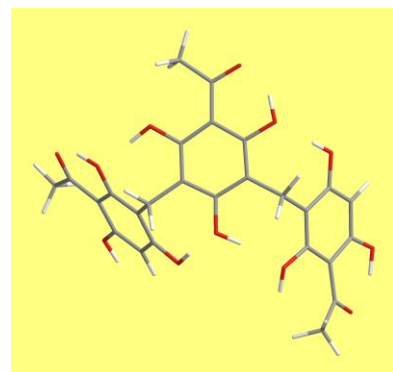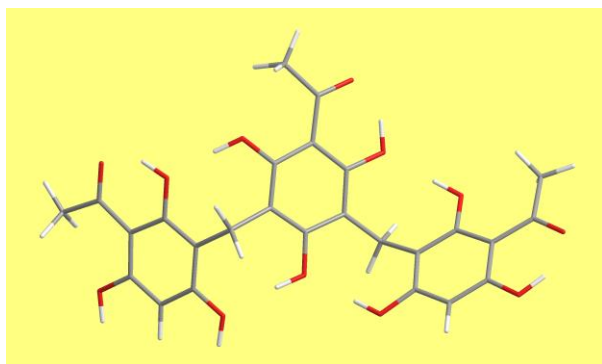
11

orientation of acyl groups: up—up—up
monomers' conformer types: d-w—d-w—d-w
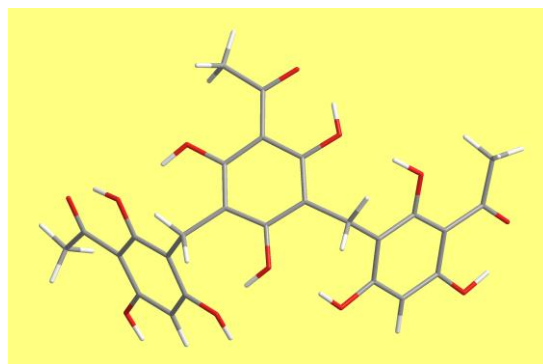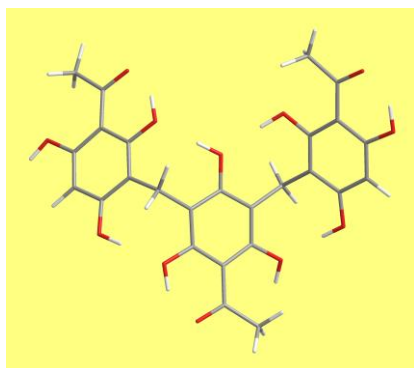
12

orientation of acyl groups: up—down—up
monomers' conformer types: d-r—s-w-u—d-w
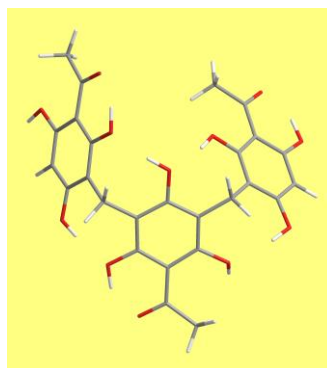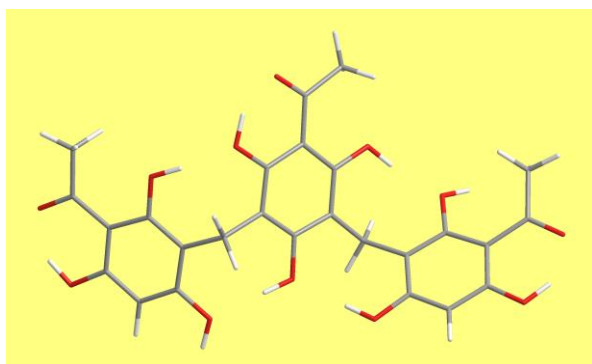
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orientation of acyl groups: up—up—up
monomers' conformer types: s-w—s-w—d-w-u
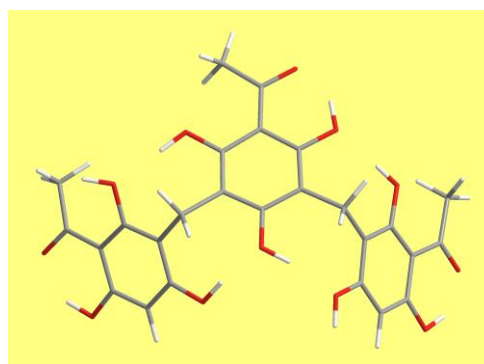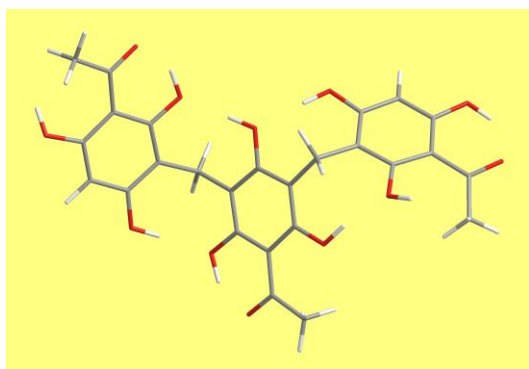
14

orientation of acyl groups: up—down—down

monomers' conformer types: d-r-u—s-w—d-w-u
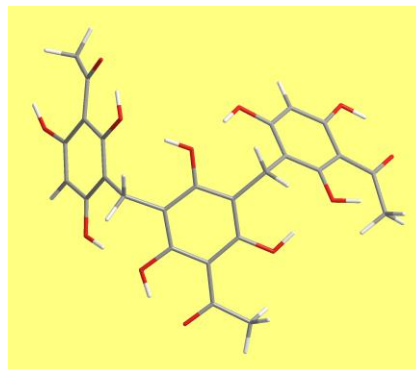
14-y
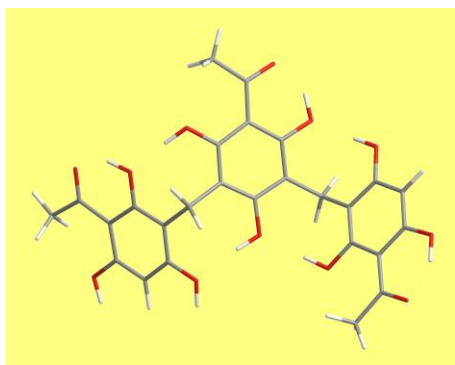
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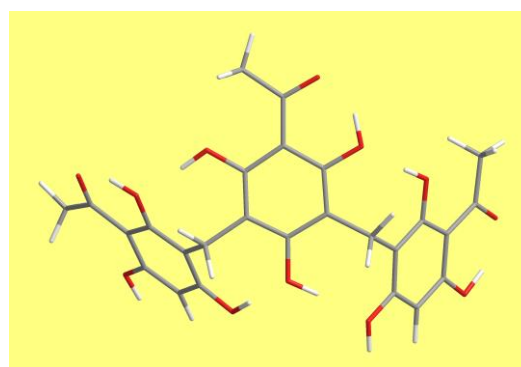orientation of acyl groups: up—up—down

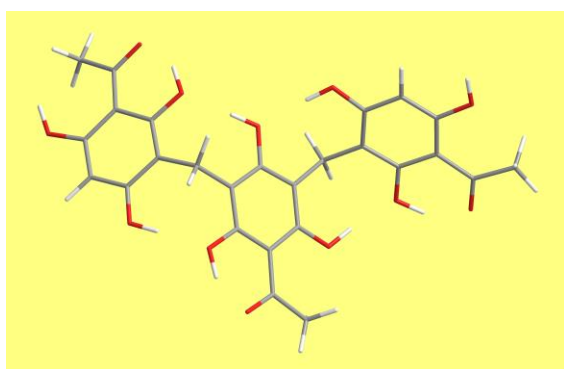monomers' conformer types: d-w—d-w—d-w
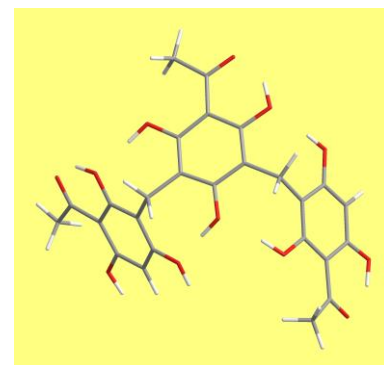
15-y
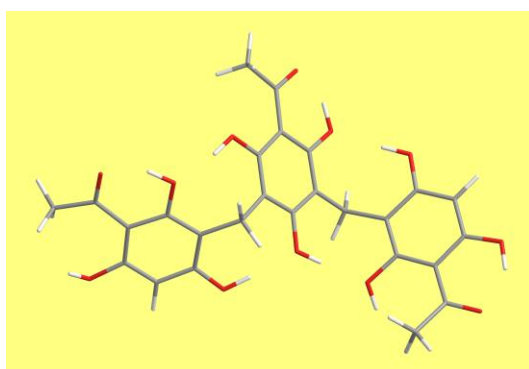
16

orientation of acyl groups: up—up—down

monomers' conformer types: d-r-u—d-r—d-r-u
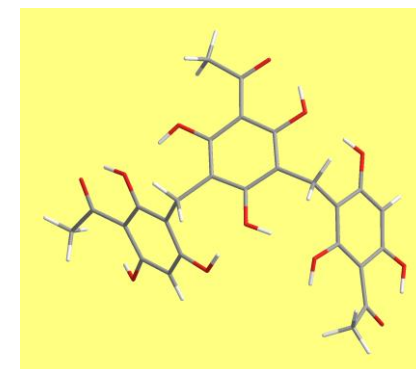
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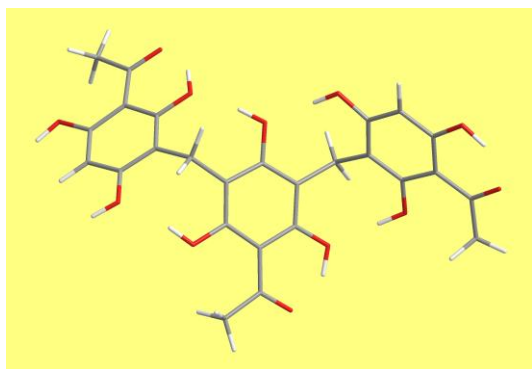
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17-y

orientation of acyl groups: up—down—down
monomers' conformer types: d-w—d-w—d-w

18

18-y
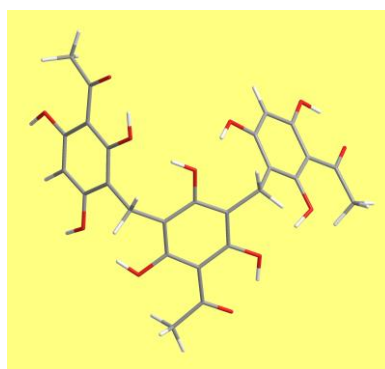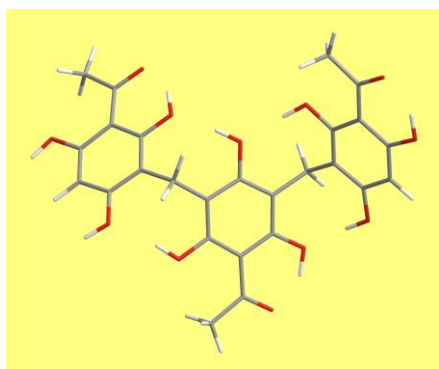
orientation of acyl groups: up—down—up
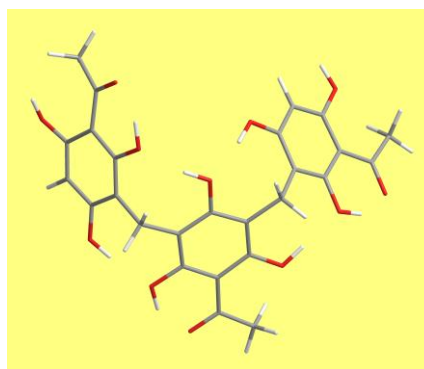monomers' conformer types: d-w—d-r—d-w
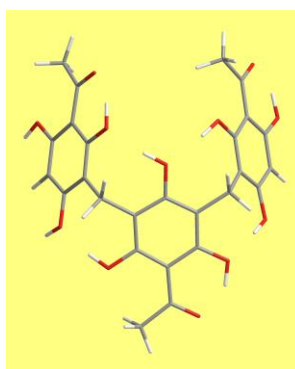
19

19-y

orientation of acyl groups: up—up—up
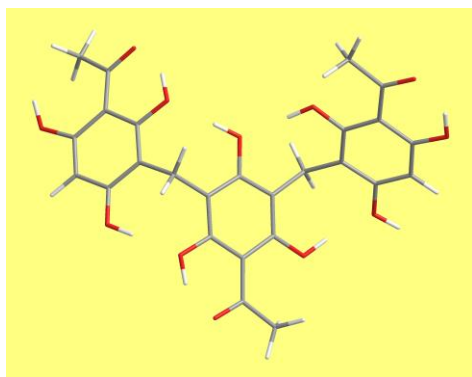monomers' conformer types: d-w-u—d-w—d-w

20

orientation of acyl groups: up—down—down

monomers' conformer types: d-w-u—d-w—d-w

20-y

21

orientation of acyl groups: up—up—down

monomers' conformer types: d-w-u—d-w—d-w

21-y

22

orientation of acyl groups: up—down—up

monomers' conformer types: d-w-u—d-w—d-w

22-y

23

orientation of acyl groups: up—down—up
monomers' conformer types: d-r-u—s-w-u—d-w

23-y

24

orientation of acyl groups: up—down—down
monomers' conformer types: d-r-u—s-w-u—d-w
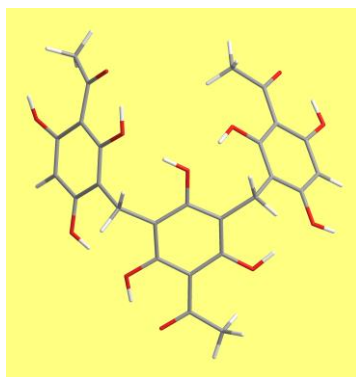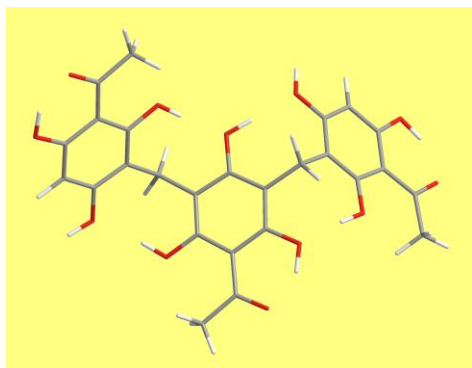

24-y

25

25-y

orientation of acyl groups: up—down—down
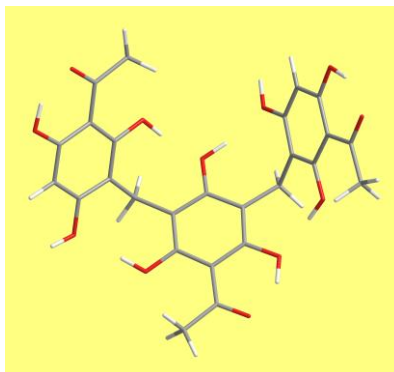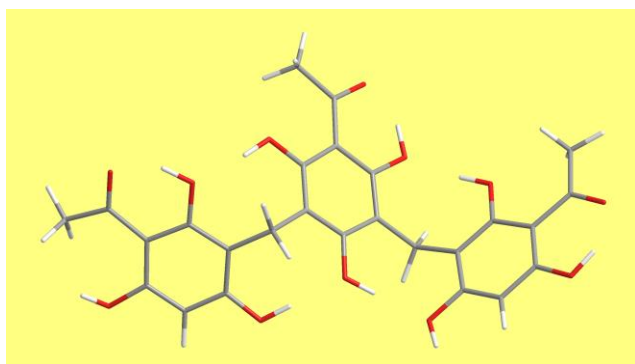monomers' conformer types: s-w-u—d-w—d-w

26

26-y

orientation of acyl groups: up—up—down

monomers' conformer types: s-w—d-w-u—d-w

27

27-y

orientation of acyl groups: up—up—up

monomers' conformer types: s-w-u—d-w—d-w

28

28-y

orientation of acyl groups: up—down—up

monomers' conformer types: s-w-u—d-w—d-w

29   29-y
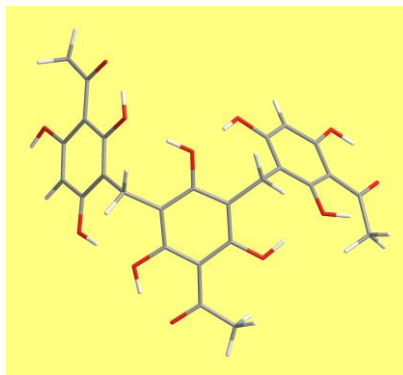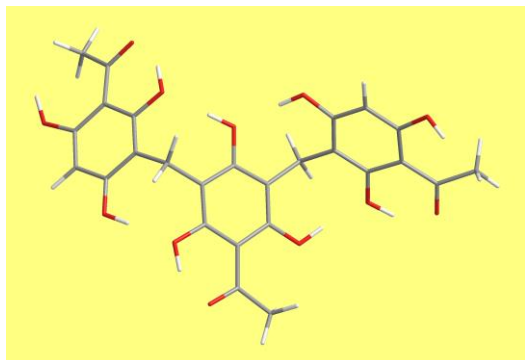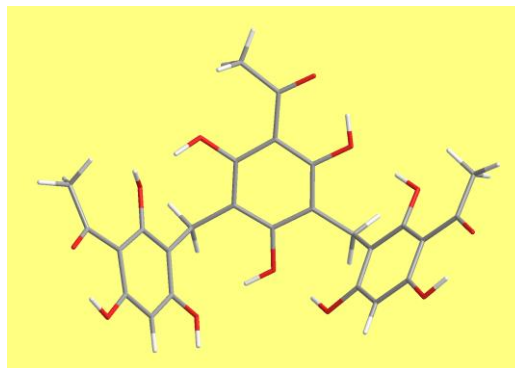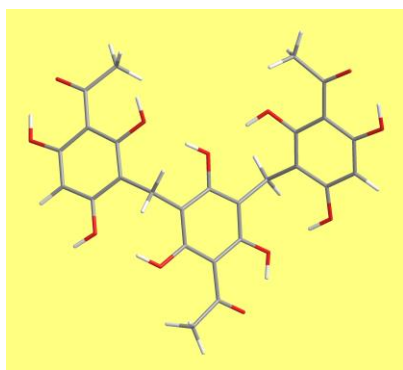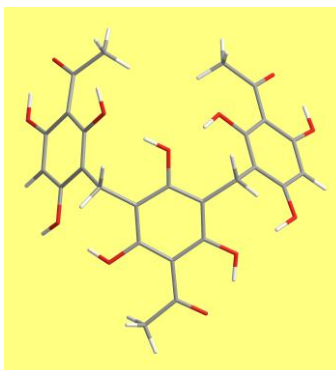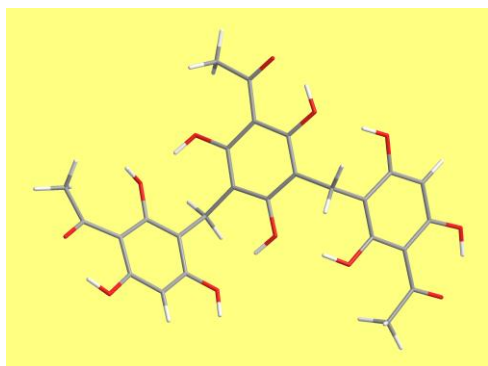
orientation of acyl groups: up—up—down
monomers' conformer types: s-w-u—d-w—d-w
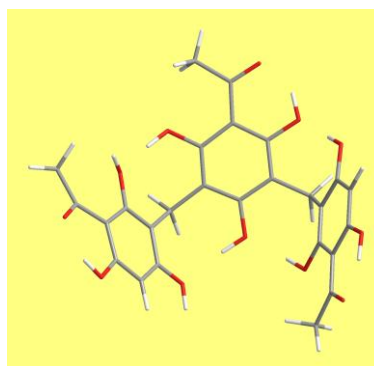
Figure S 2
Geometries of the conformers of the calculated trimeric acylphloroglucinols in which no OH is replaced by a different function
The conformers are visualized showing pairs of outstretched-shaped and half-bowl-shaped corresponding conformers. The acronym identifying the conformer is reported on the left under each image; the meaning of the numbers and letters used to build the acronyms is explained in section 3.1 and in table S2, and visualised in fig. S1. The conformers of structure T1 are not reported because they are shown in figure S1.
The relative energy values (kcal/mol, DFT/B3LYP/6-31+G(d,p) results) are reported centrally or centre-right under the conformers' images.

Structure T7
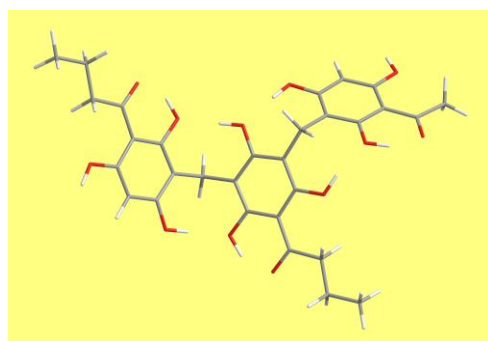
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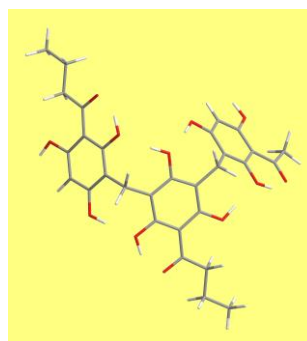
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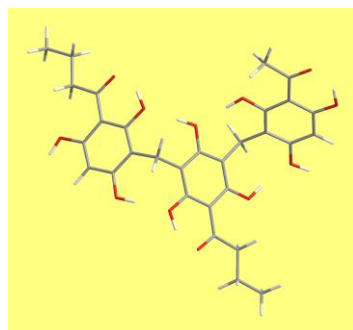
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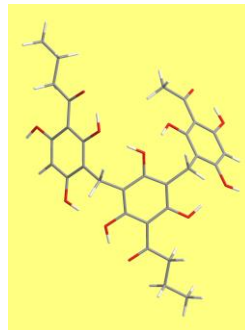
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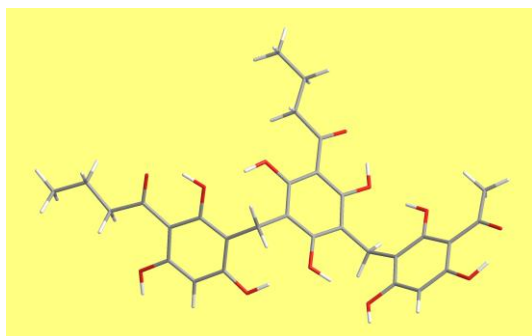
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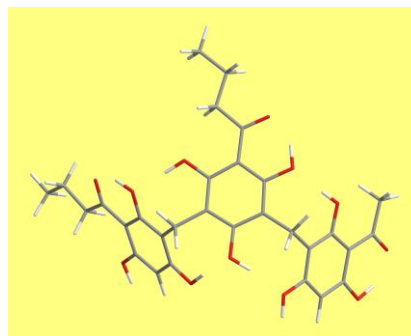
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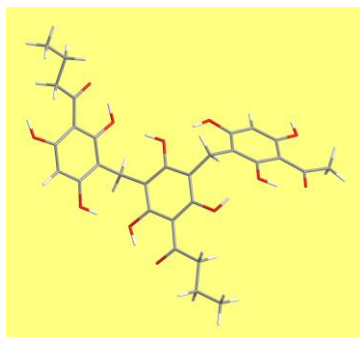
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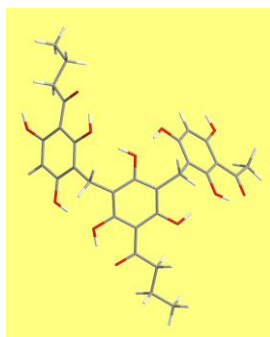
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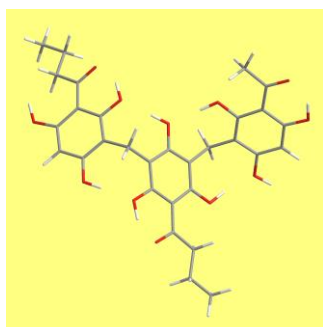
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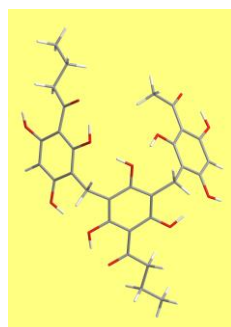
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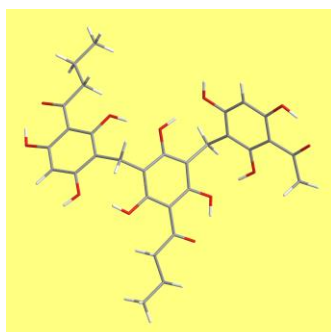
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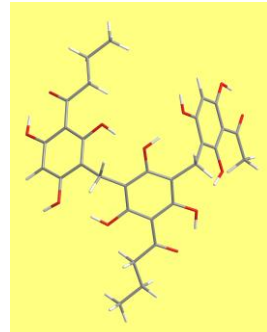
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Structure T9
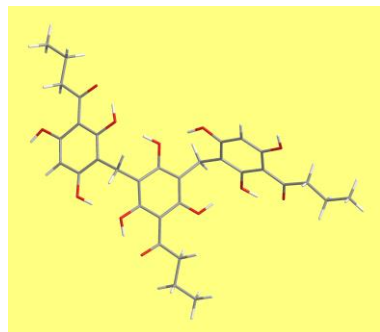
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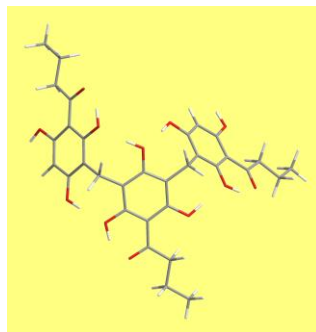
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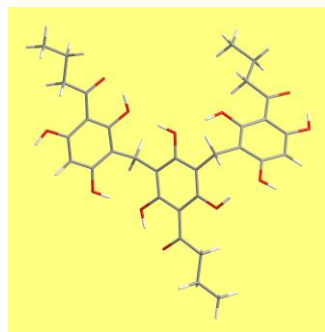
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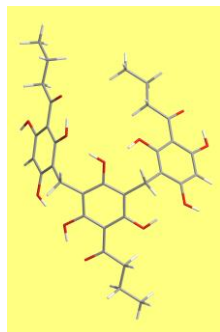
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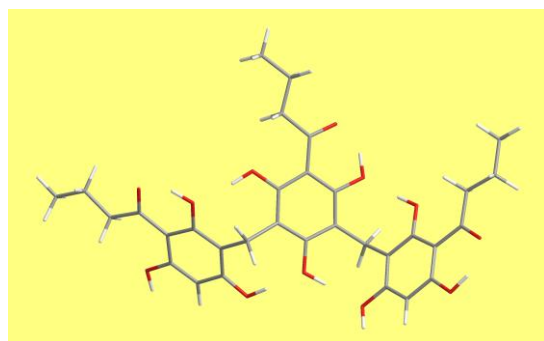
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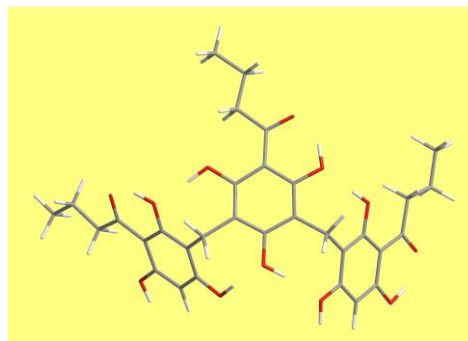
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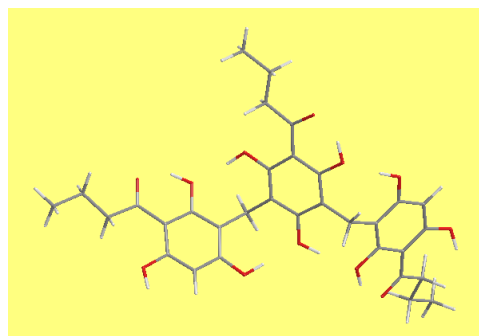
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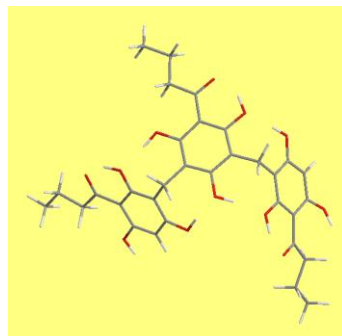
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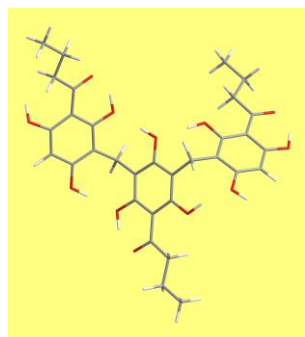
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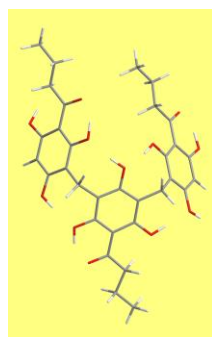
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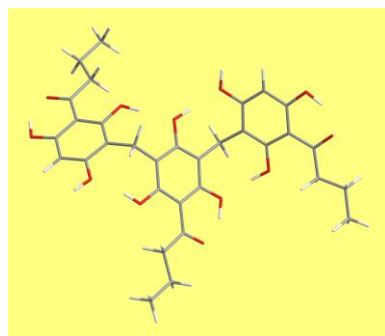
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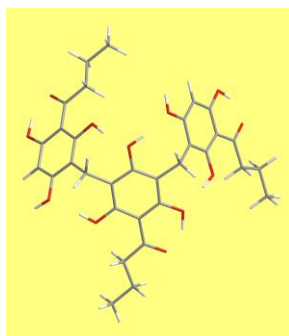
6-y   7.503

Structure T9-M5,5′
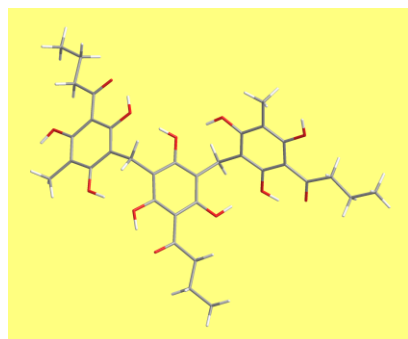
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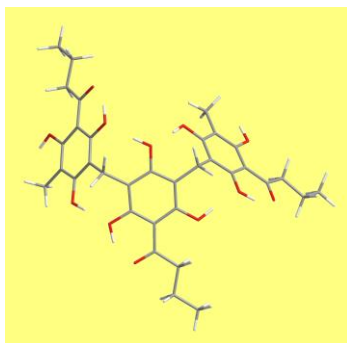
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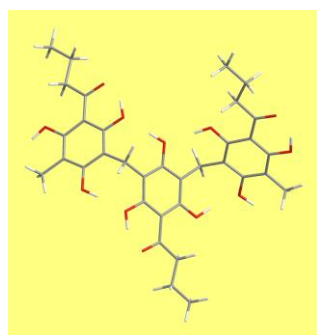
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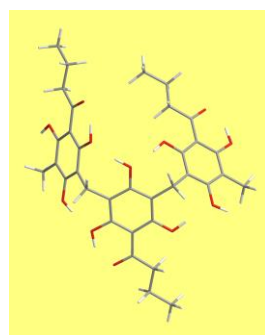
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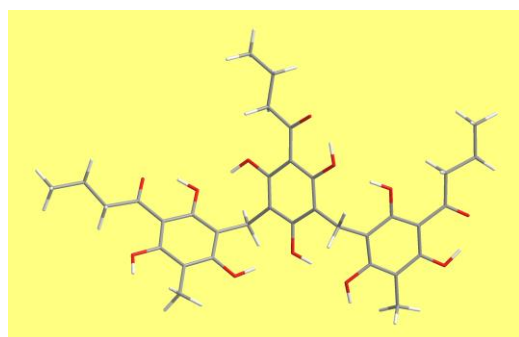
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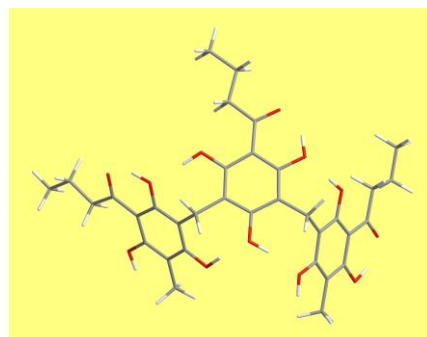
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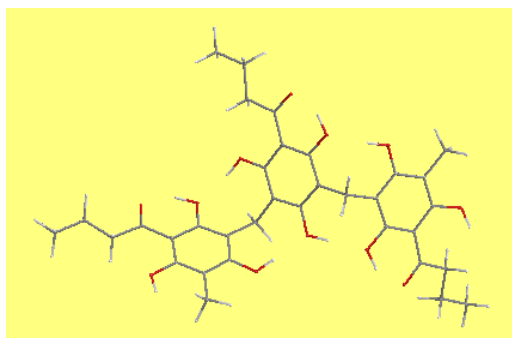
4   3.654
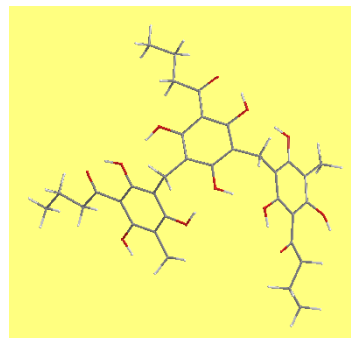
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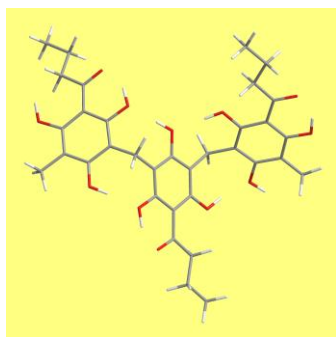
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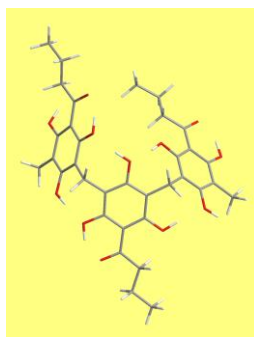
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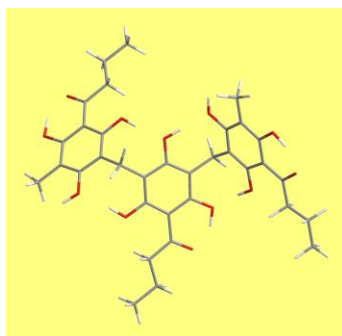
6   6.240
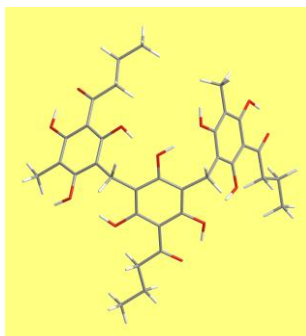
6-y   6.358

Structure T10
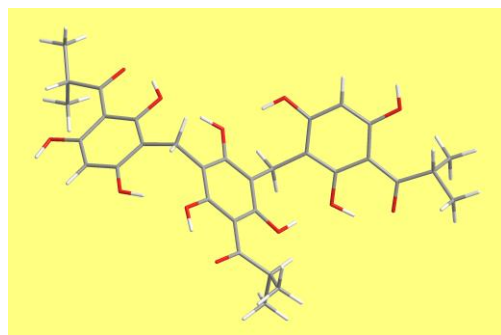
1   0.000
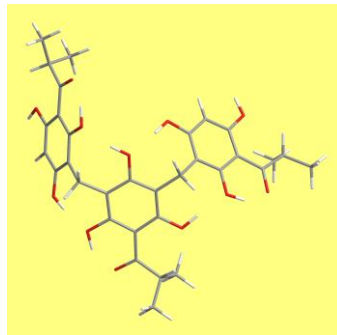
1-y   0.275
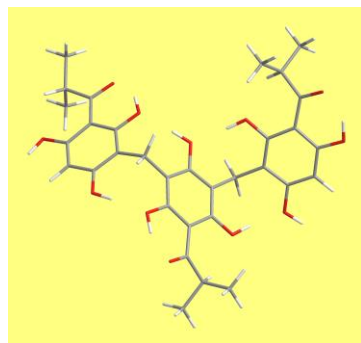
2   3.831
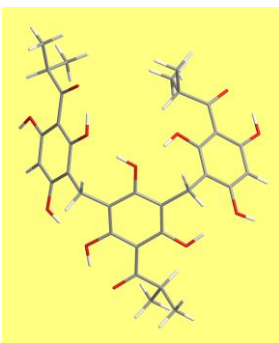
2-y   3.744
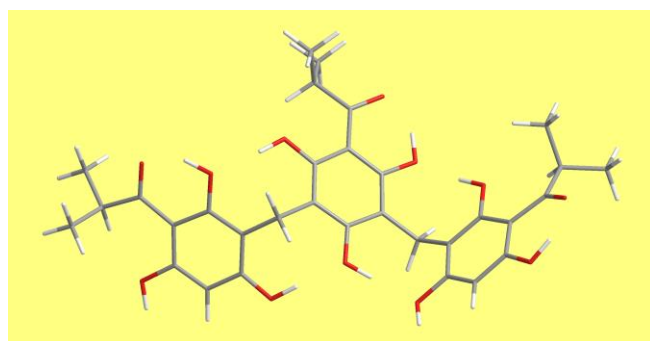
3   4.030

3-y   3.987
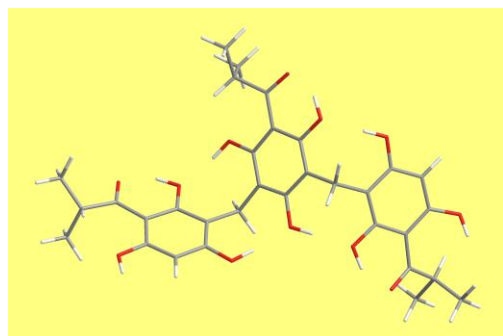
4   3.784
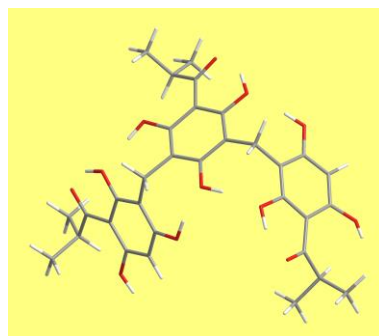
4-y   4.303
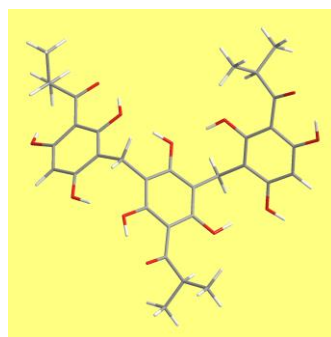
5   7.720
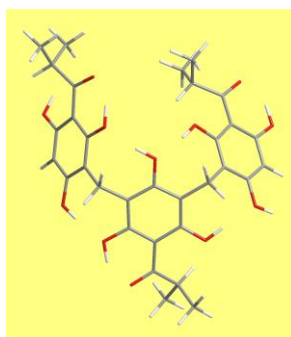
5-y   7.582
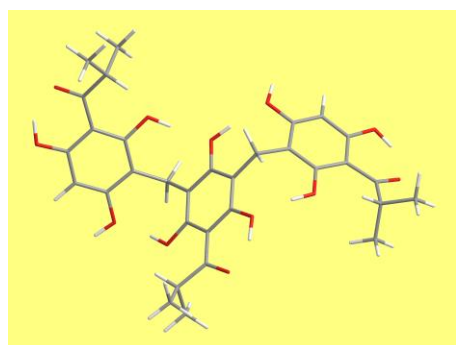
6   7.942
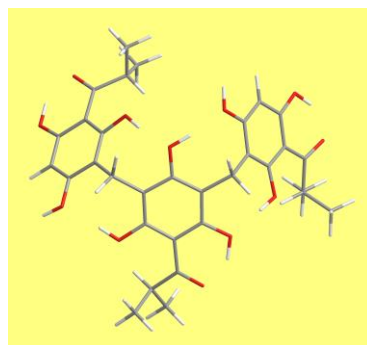
6-y   8.169

Figure S3
Illustration of the outcome of the reversal of the conformer-types of the two outer monomers in trimeric acylphloroglucinols
The figure considers a trimeric acylphloroglucinol with R ≠ R″, in which the OHs at C6 and C2″ are replaced by OCH$_3$ groups, and shows the two possibilities (I and II) with outstretched geometry. Conformers of this type have very close energies in the HF results, and identical energies in the DFT results. For this reason, only one of them is reported for each molecule in tables and figures (along with the corresponding half-bowl-shaped conformer).

a)   The two possibilities with outstretched geometry

I

II

| orientation of acyl groups: | up—up—down | up—down—down |
| monomers' conformer types: | d-r—d-r—s-w | d-r—s-w—s-w |
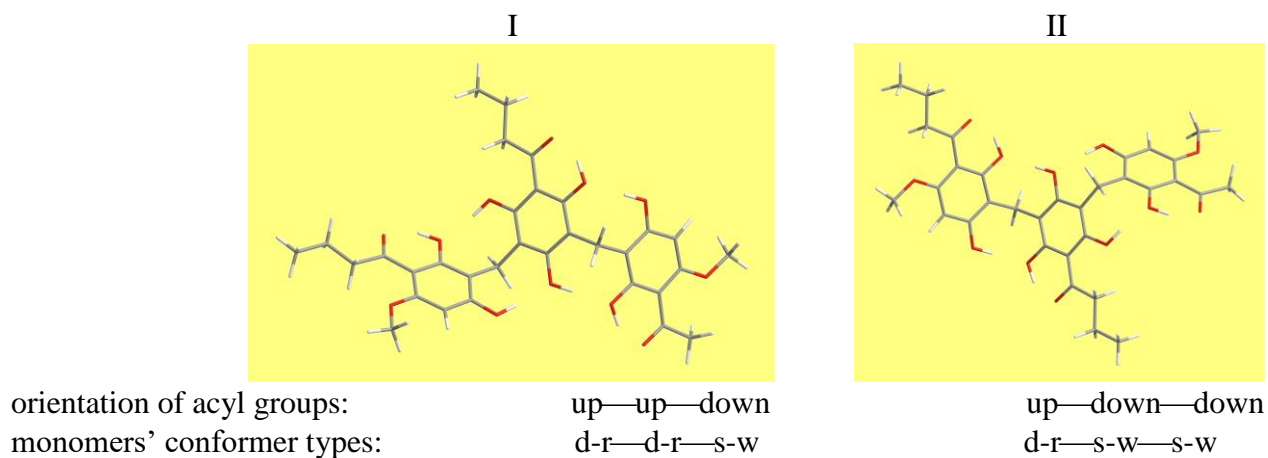
b)   Conformer II seen from two different perspectives

II-a

II-b
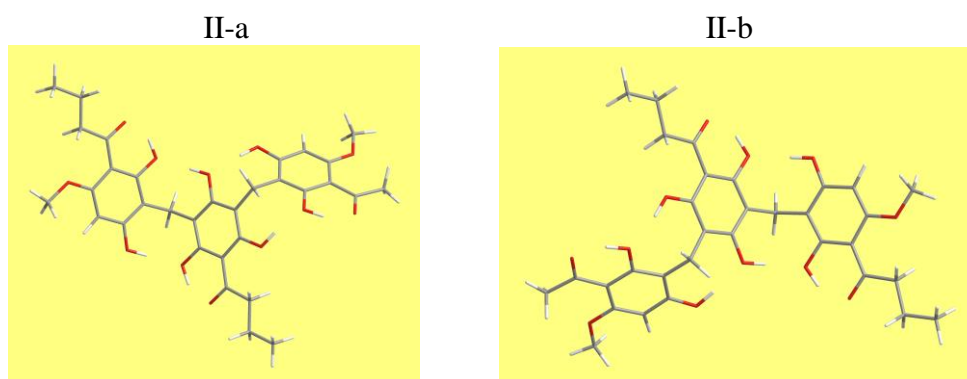
Image II-a shows conformer II from the same perspective as in part (a). Image II-b shows it from a rotated perspective which reverses the roles of the first and third conformer; within this perspective, the orientation of the monomers and the monomers' conformer-types are the same as for conformer I.

Figure S 4
Geometries of the conformers of the calculated trimeric acylphloroglucinols in which one or more OH groups are replaced by OCH₃ groups, and no other substitutions occur

The conformers are visualized showing pairs of outstretched-shaped and half-bowl-shaped corresponding conformers. The acronym identifying the conformer is reported on the left under each image; the meaning of the numbers and letters used to build the acronyms is explained in section 3.2 and in table S2.

The relative energy values (kcal/mol, DFT/B3LYP/6-31+G(d,p) results) are reported centrally or centre-right under the conformers' images.

Structure T3-ET6,2″
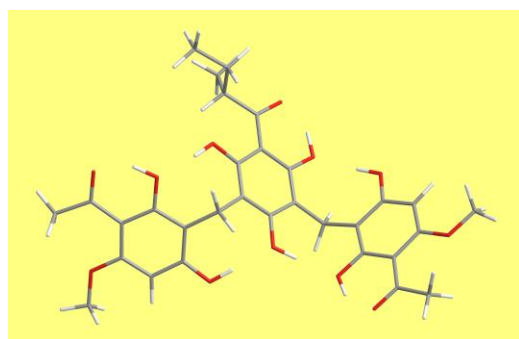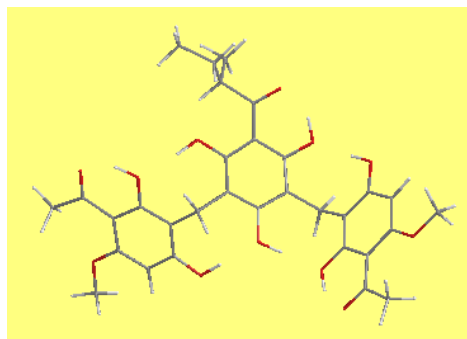
1 0.000	1-y 0.485

Structure T3- M5,3″-ET6,2″
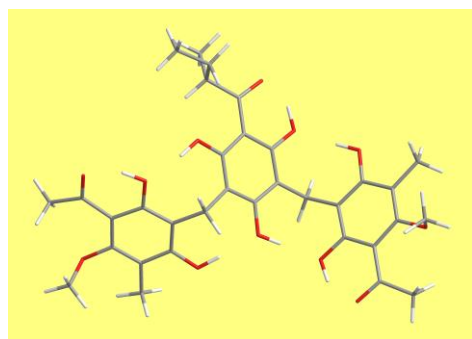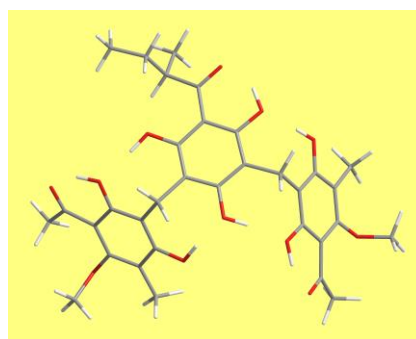
1 0.000	1-y 0.028

Structure T6-M5,3″-ET6,4″
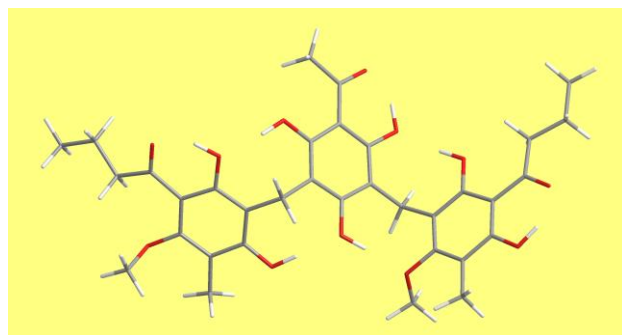
1   0.000
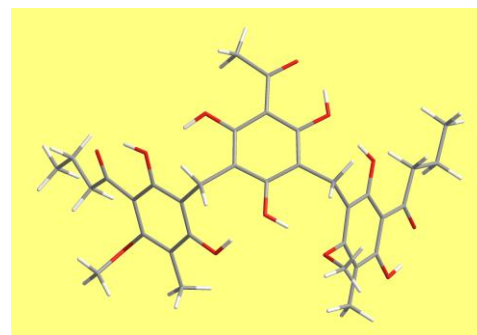
1-y-out-out   0.141
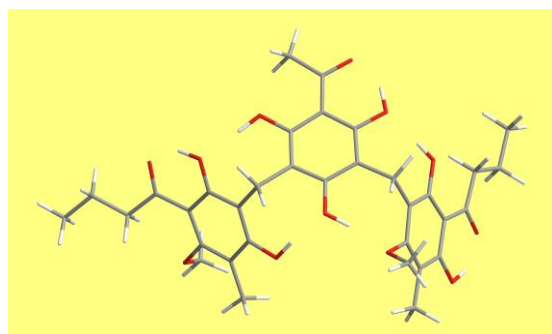
1-y-in-out   0.190
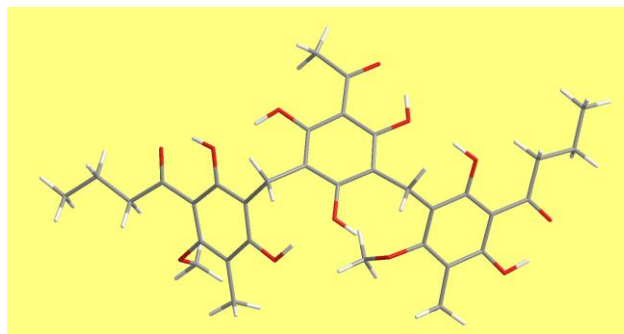
1-y-in-in   4.737

Structure T7-ET6,2″
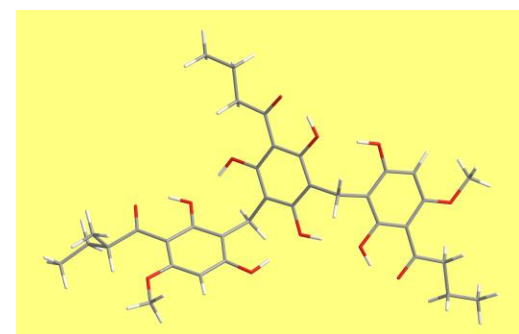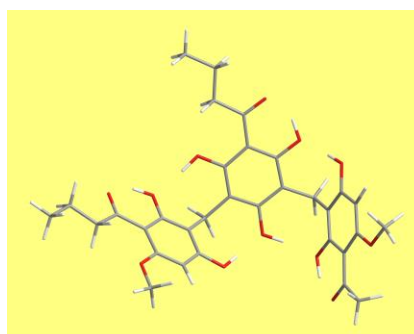
1   0.000

1-y   0.347

Structure T7- M5,3″-ET6,2″
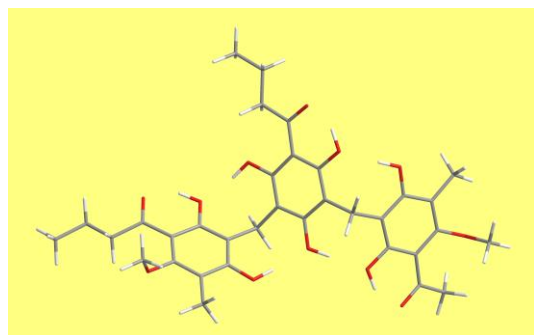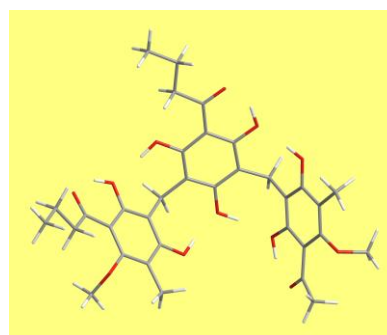
1   0.000

1-y   0.288

'

Structure T9-ET6,2″
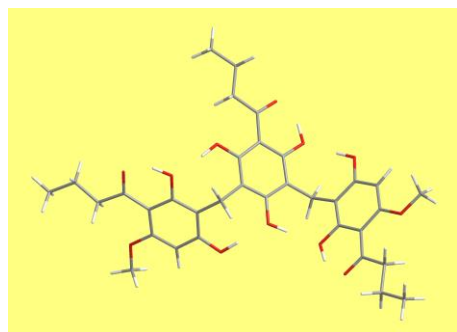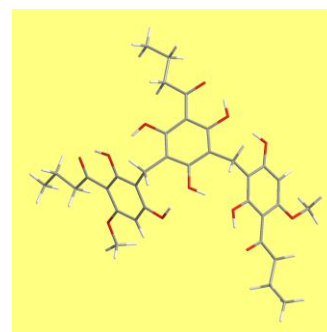
1   0.000

1-y   0.346

Structure T9-M5,3″-ET6,2″
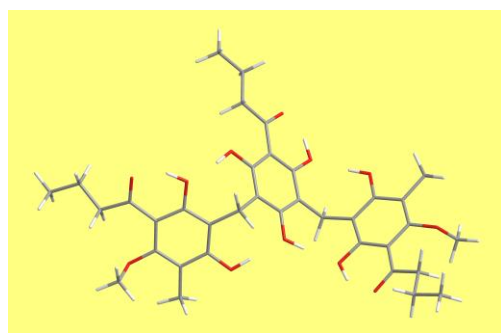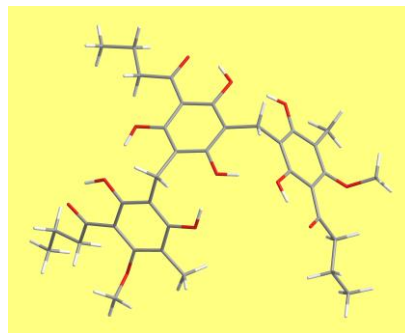
1   0.000

1-y   0.279

Structure T9-M5,3″-ET4,2″
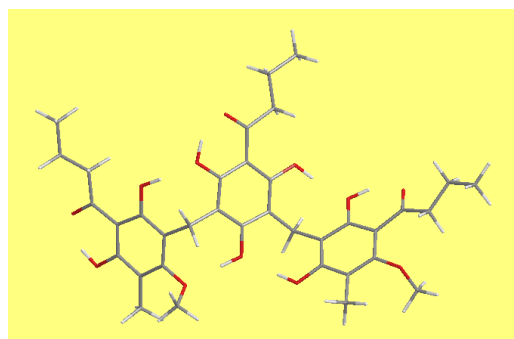
1   0.000
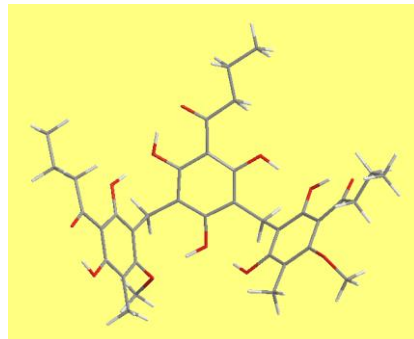
1-y   0.2097
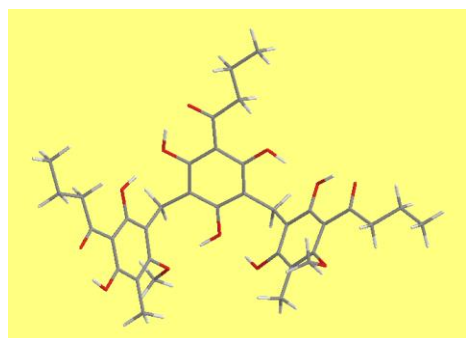
1-y-in-out   0.2184
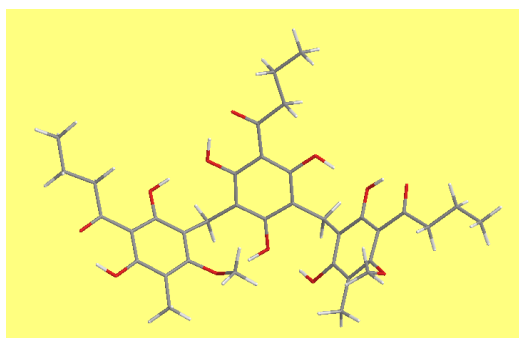
1-y-in-in   3.2935

Structure T10-ET6,2″
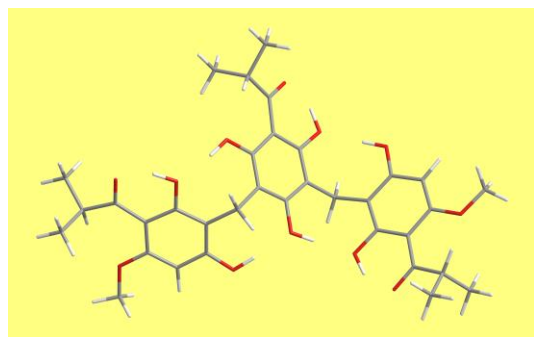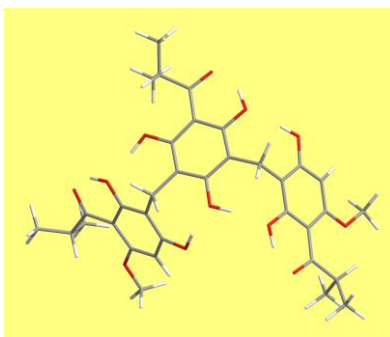
1   0.0000

1-y   0.303

Structure T10-M5,3″-ET6,2″
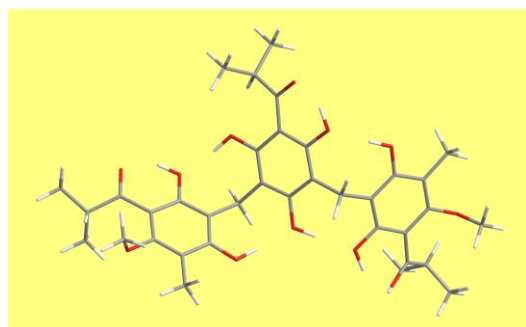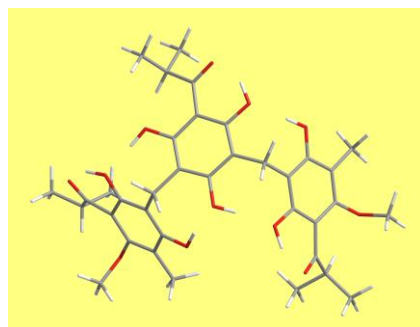
| 1 | 0.018 | 1-y | 0.569 |

Structure T10-M5,3″-ET6,2″,6″
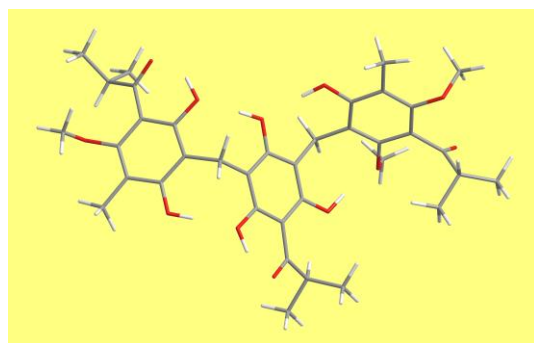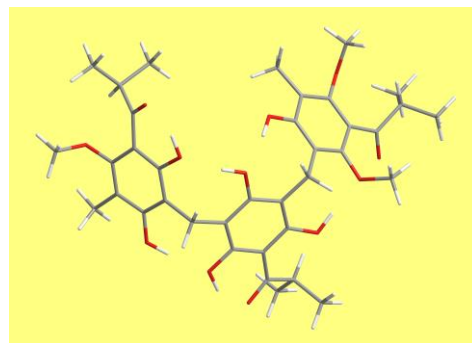
| 1 | 0.000 | 1-y | 0.728 |

Structure T11-ET6,2″
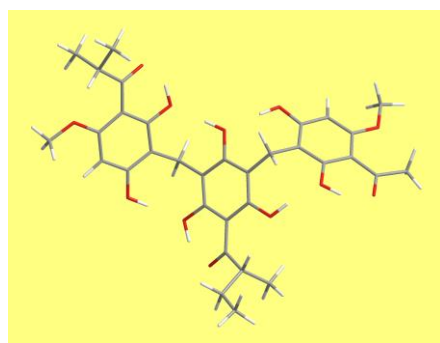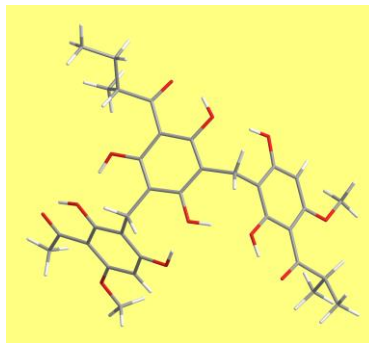
| 1 | 0.000 | 1-y | 0.388 |

Structure T11- M5,3″-ET6,2″
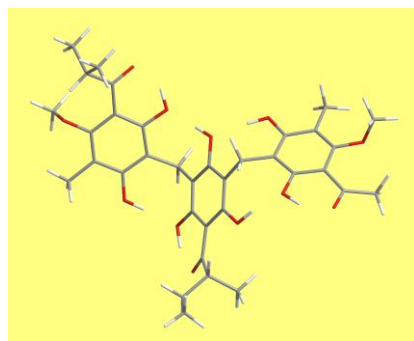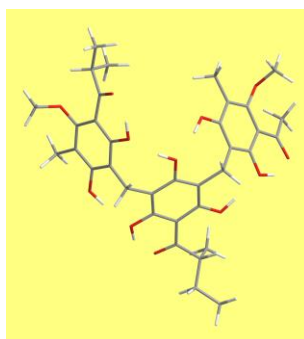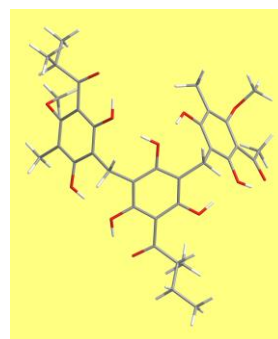
| 1 | 0.000 | 1-y | 0.003 | 1-y-in-out | 0.508 |

Structure T13-ET6,2″
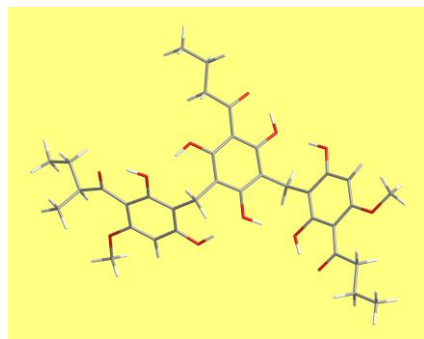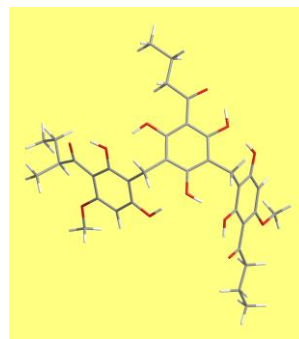
| 1 | 0.000 | 1-y | 0.355 |

Structure T13- M5,3″-ET6,2″
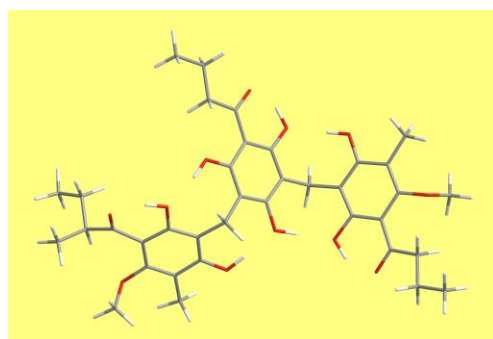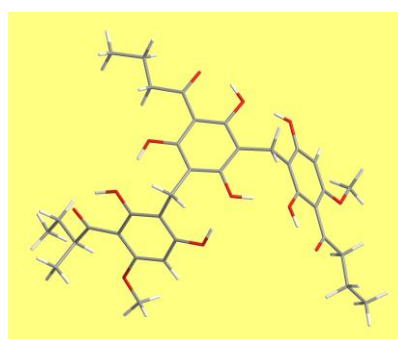
| 1 | 0.000 | 1-y | 0.281 |

Structure T14-ET6,2″
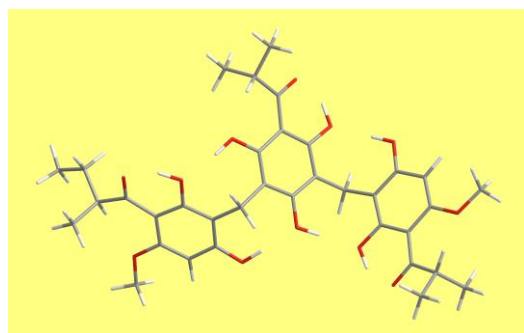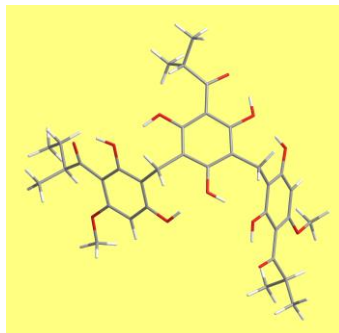
1 0.000	1-y 0.614

Structure T14- M5,3″-ET6,2″
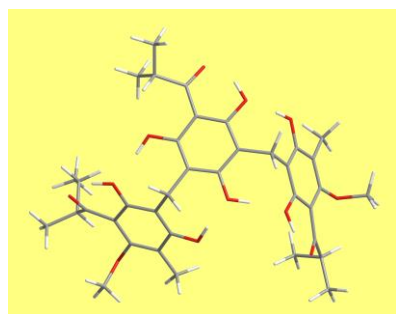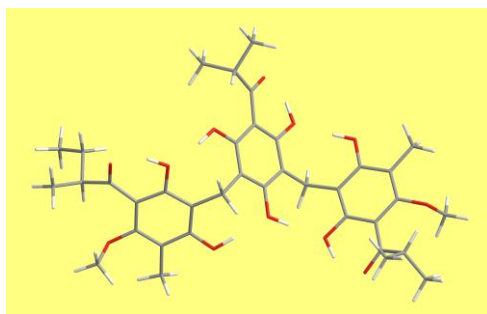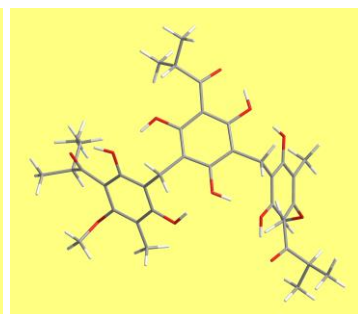
1-y 0.000	1 0.011	1-y-in-out 0.517

Figure S 5
Viable geometries of trimeric acylphloroglucinols in which an inward OH *ortho* to the acyl group is replaced by a keto O
The table shows the independent numbering of the conformers of molecules of this type.
The conformers are visualized showing pairs of outstretched-shaped and half-bowl-shaped corresponding conformers. The acronym identifying the conformer is reported on the left under each image, and the explanation of the characterising geometry features is provided underneath.

a) **Structures in which the OH at C6″ is replaced by a keto O**
The conformers of structure T7-KT6″-M5,3″,3″ are utilized for illustration.
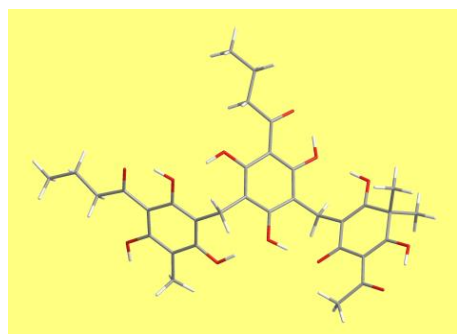
1   1-y
orientation of acyl groups: up—up—down
monomers' conformer types: d-r— d-r—d-w
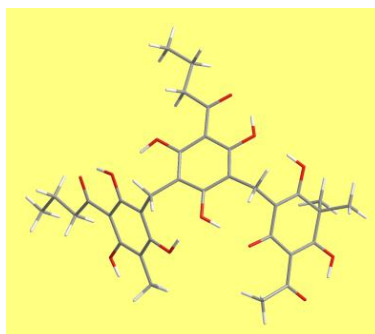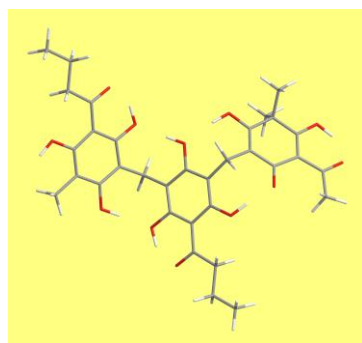
2   2-y
orientation of acyl groups: up—down—down
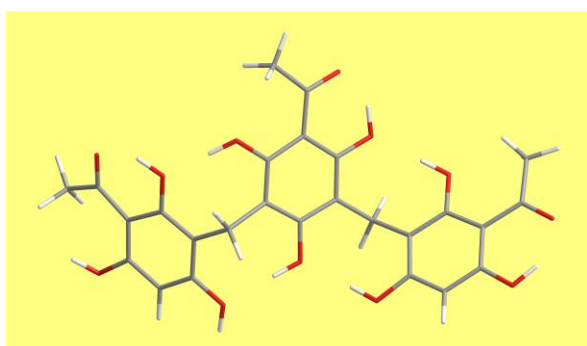monomers' conformer types: d-r—s-w—d-w

3
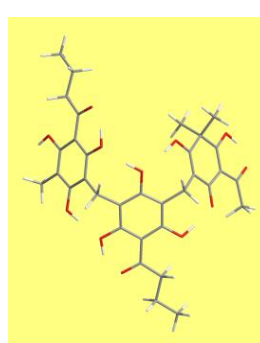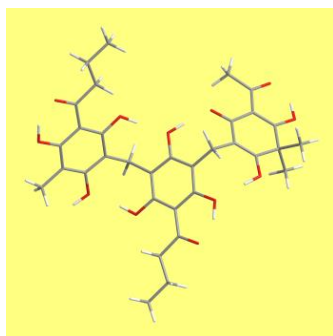
orientation of acyl groups: up—down—up
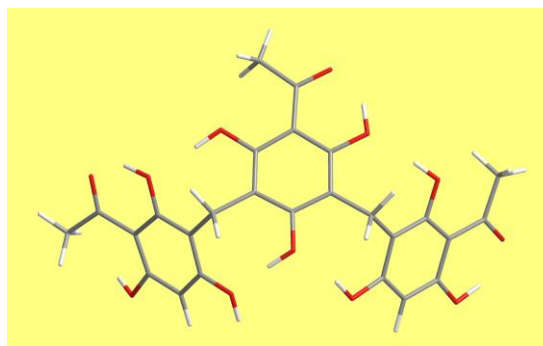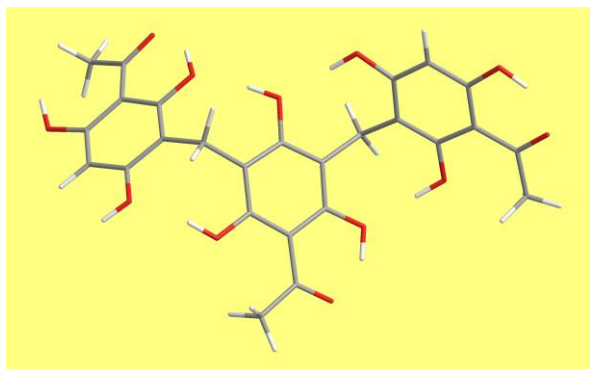monomers' conformer types: s-w—d-r—d-w

3-y

4

orientation of acyl groups: up—up—up
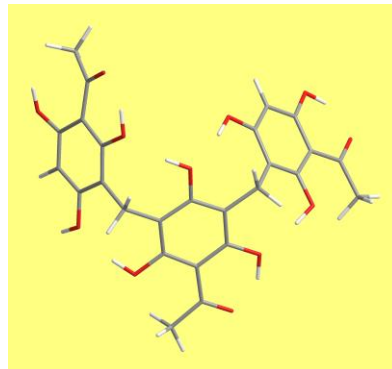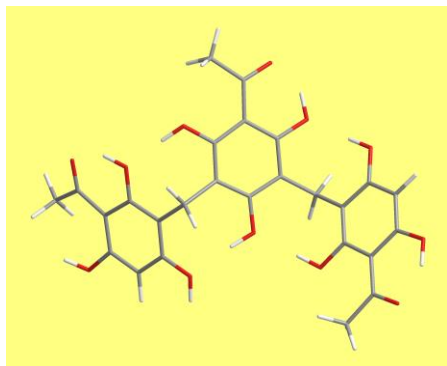monomers' conformer types: s-w—s-w—d-w
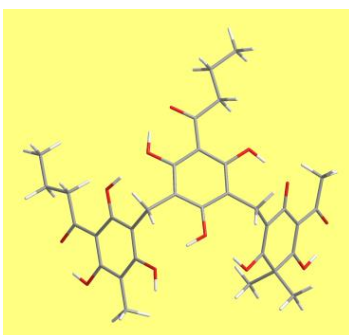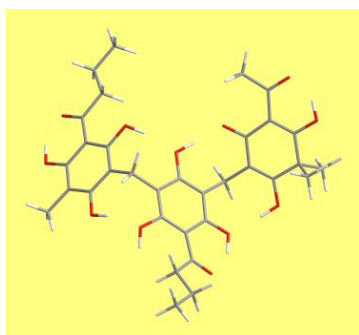
4-y

5

orientation of acyl groups: up—down—up
monomers' conformer types: s-r— d-r-u—d-w
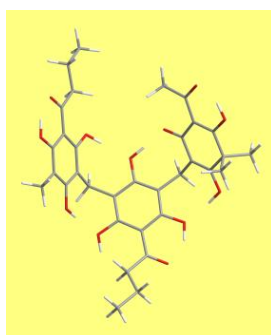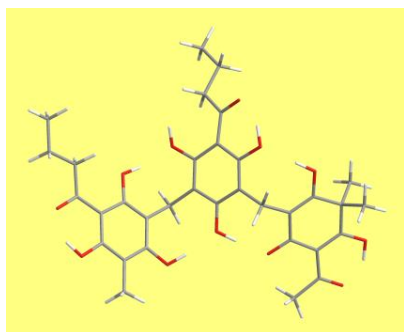
5-y

6

6-y

orientation of acyl groups: up—up—down

monomers' conformer types: s-r—d-r-u—d-w

7

7-y

orientation of acyl groups: up—up—up

monomers' conformer types: s-r—s-r—d-r

8

8-y

orientation of acyl groups: up—down—down
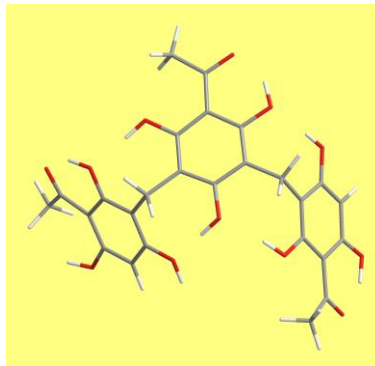
monomers' conformer types: s-r—s-r—d-r

9   9-y
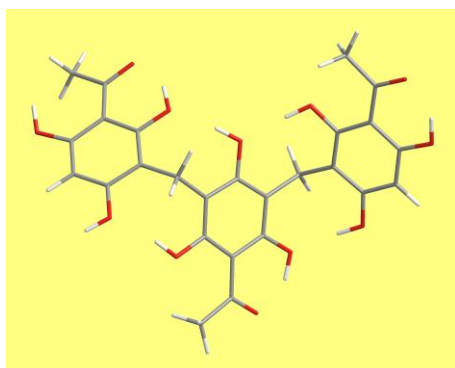
orientation of acyl groups: up—up—down

monomers' conformer types: s-r— s-r—d-r

10   10-y
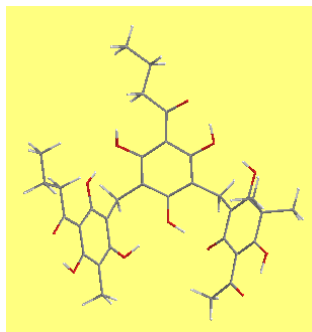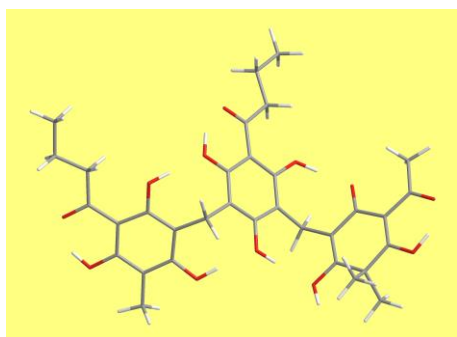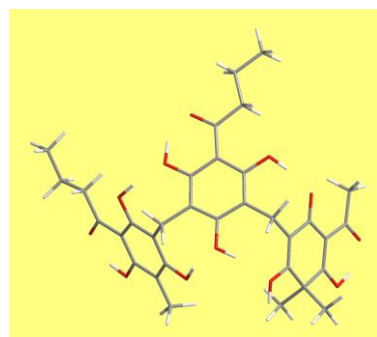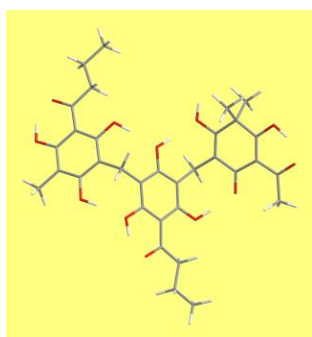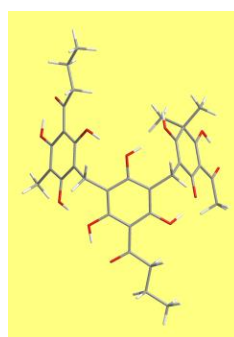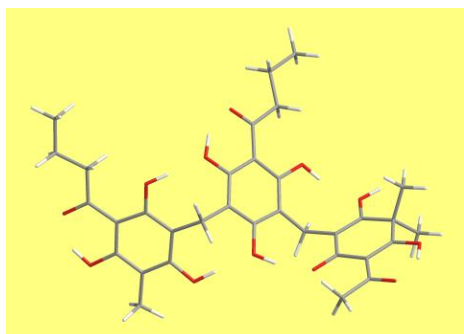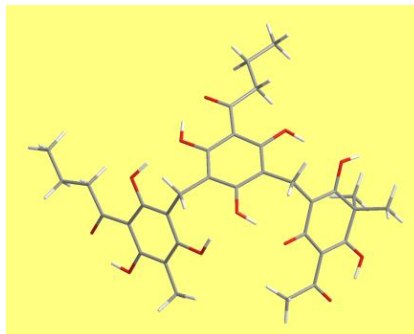
orientation of acyl groups: up—down—up

monomers' conformer types: s-r—s-r—d-r
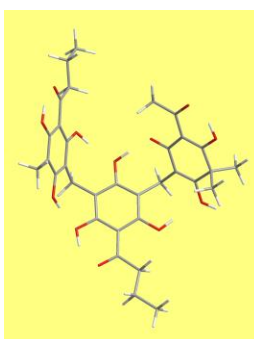
b)   Structures in which the OH at C2 is replaced by a keto O
The conformers of structure T8-KT2-M5,5,3″ are utilized for illustration.
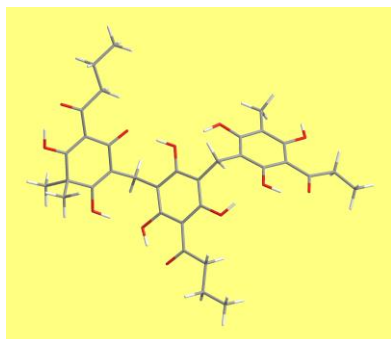
1   1-y
orientation of acyl groups: up—down—down
monomers' conformer types: s-r—s-w—s-w
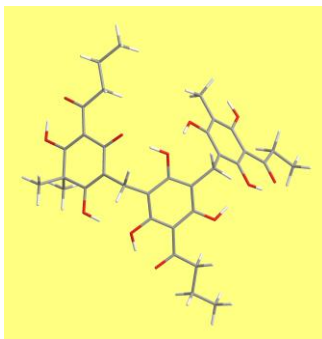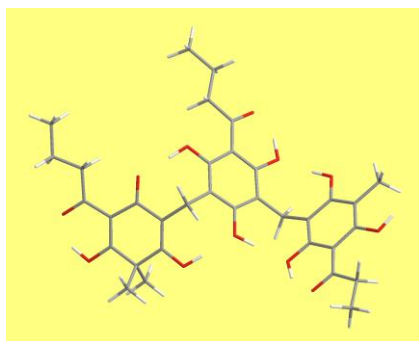
2   2-y
orientation of acyl groups: up—up—down
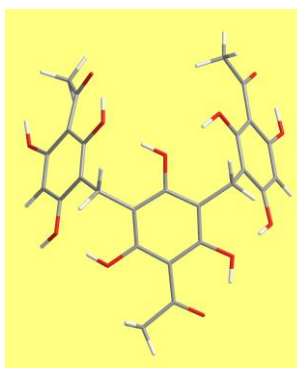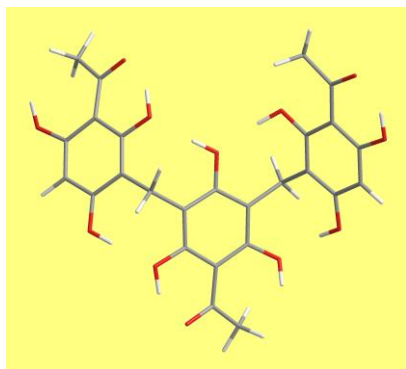monomers' conformer types: s-r— d-r—s-w
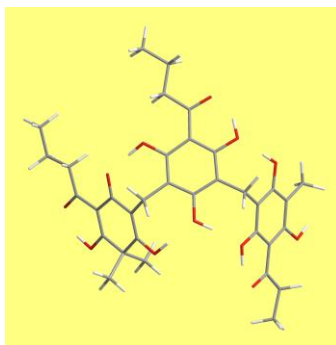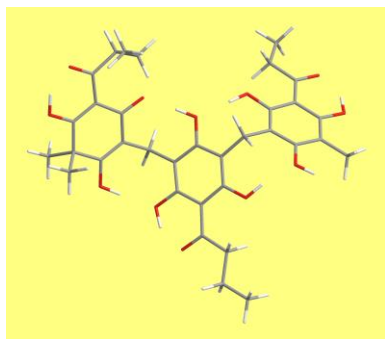
3   3-y
orientation of acyl groups: up—down—up
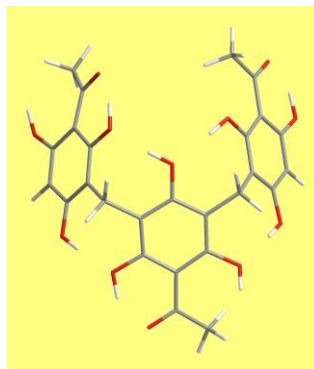monomers' conformer types: s-r—s-w—d-r

4

4-y
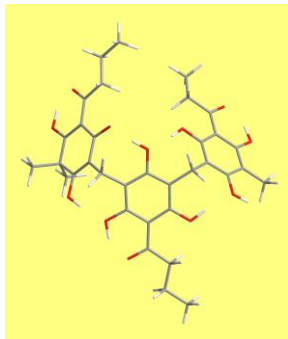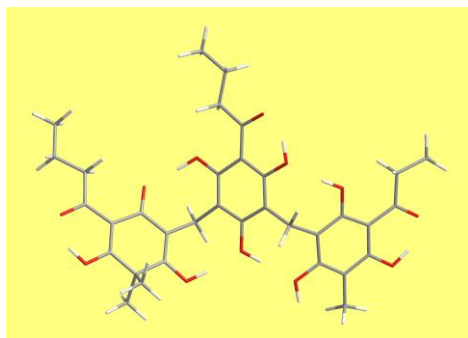
orientation of acyl groups: up—up—up
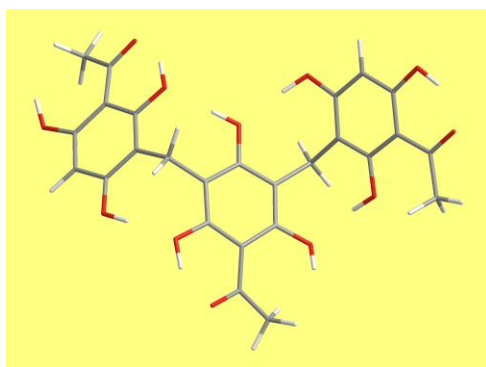monomers' conformer types: s-r—d-r—d-r
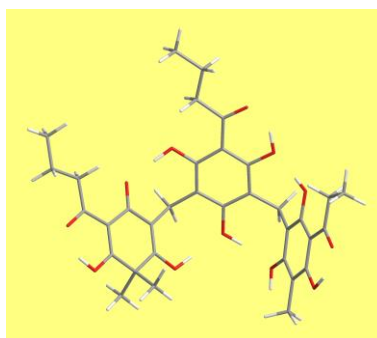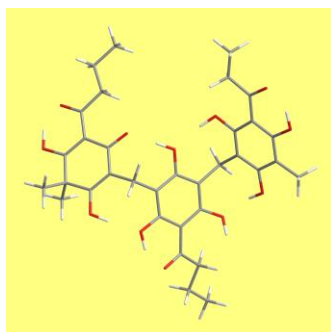
5

5-y

orientation of acyl groups: up—down—up
monomers' conformer types: s-r—s-w-u—d-w

6

6-y

orientation of acyl groups: up—down—down
monomers' conformer types: s-r—s-w-u—d-w

7

7-y

orientation of acyl groups: up—up—up
monomers' conformer types: s-w—d-w—d-w

8

8-y

orientation of acyl groups: up—up—down
monomers' conformer types: s-w—d-w—d-w

9

9-y
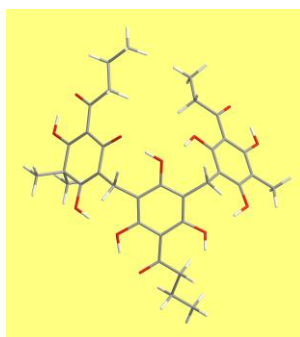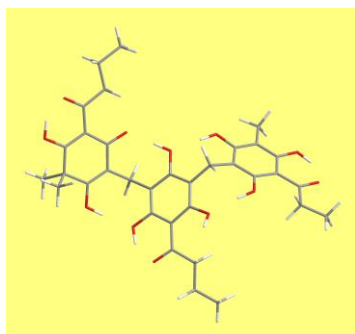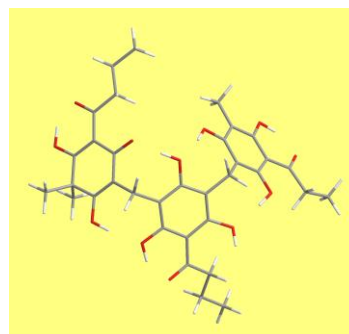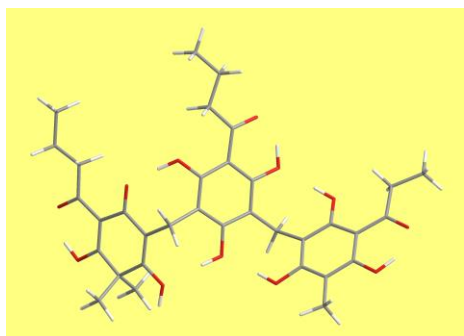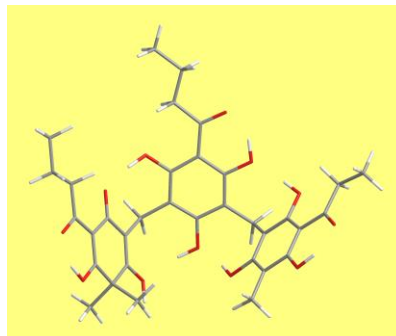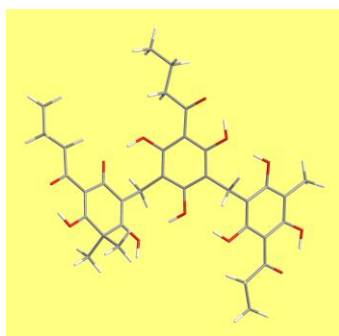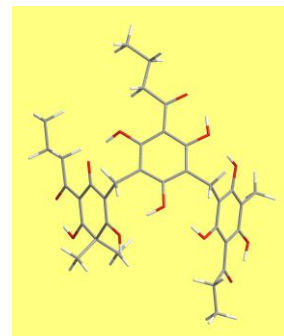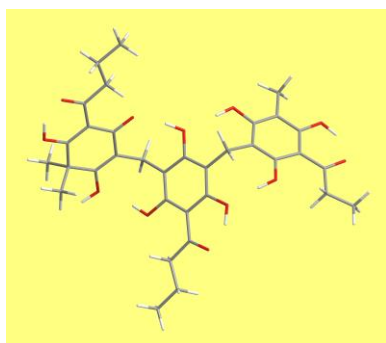
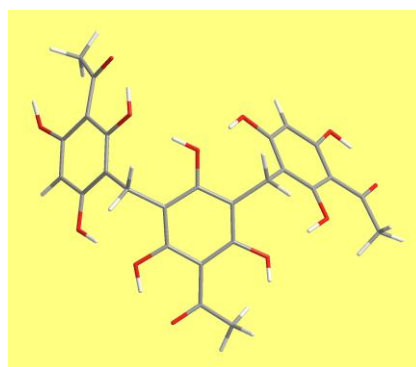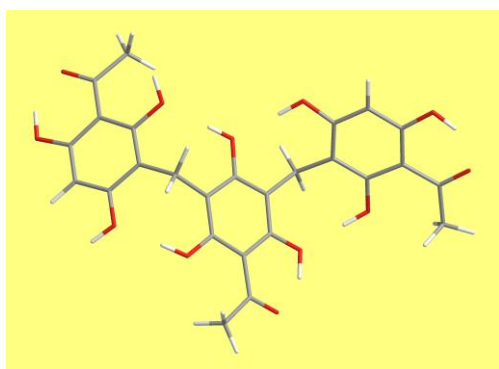orientation of acyl groups: up—down—down
monomers' conformer types: s-w— s-r—s-r
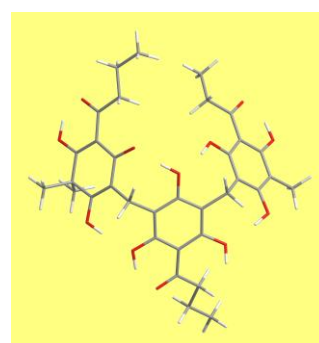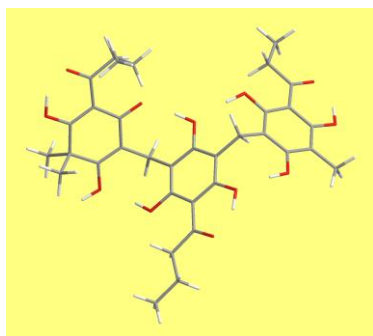
10

10-y
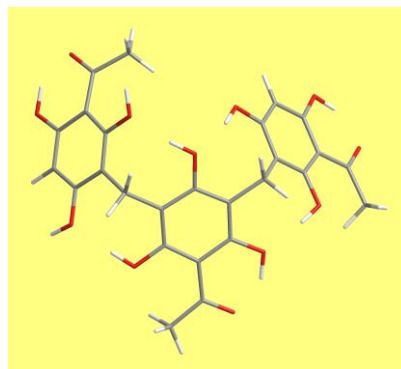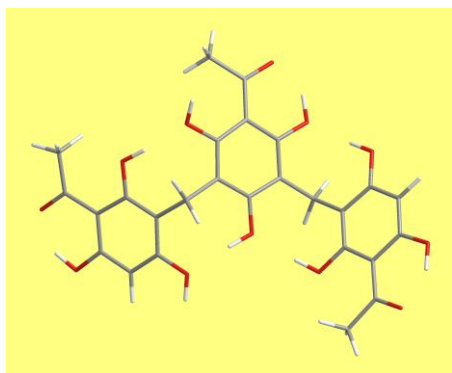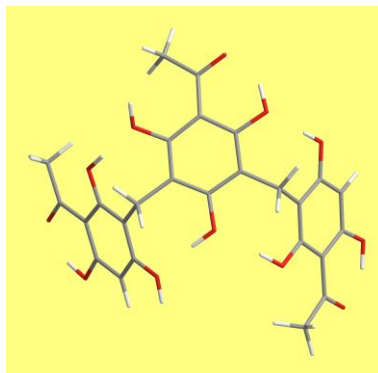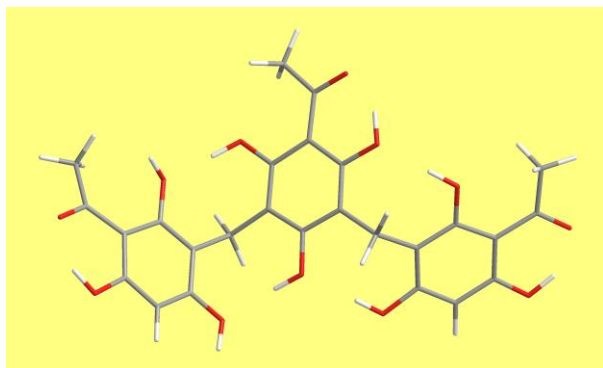
orientation of acyl groups: up—down—up

monomers' conformer types: s-w—d-w—d-w
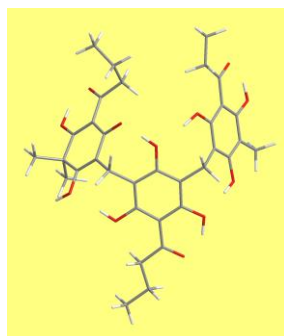
Figure S 6
Geometries and relative energies of the conformers of the calculated trimeric acylphloroglucinols in which one or two inward OHs *ortho* to the acyl group are replaced by keto O

The conformers are visualized showing pairs of outstretched-shaped and half-bowl-shaped corresponding conformers. The acronym identifying the conformer is reported on the left under each image; the meaning of the numbers and letters used to build the acronyms is explained in section 3.1 and table S2 and illustrated in figure S5.

The relative energy values (kcal/mol, DFT/B3LYP/6-31+G(d,p) results) are reported centrally or centre-right under the conformers' images.

a)   **Structures in which the OH at C2 or C6″ is replaced by a keto O and no other OHs are replaced by other functions**

Structure T7-KT6″-M5,3″,3″
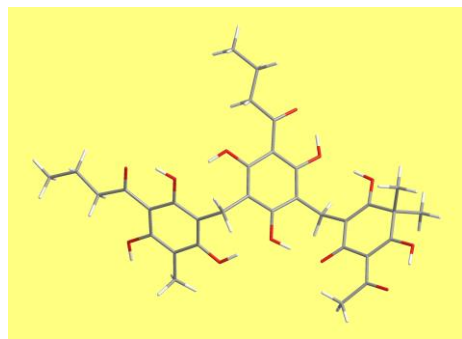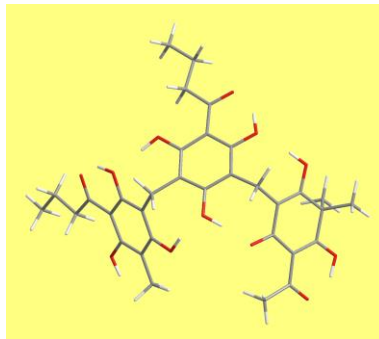
1   0.000

1-y   0.287
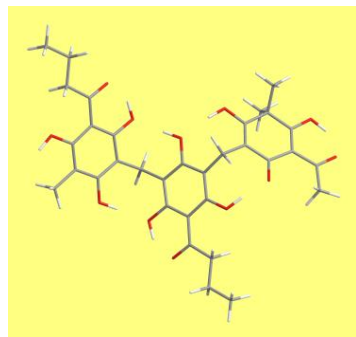
2   0.610
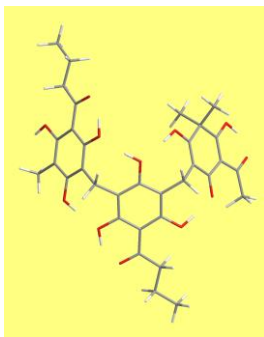
2-y   0.898
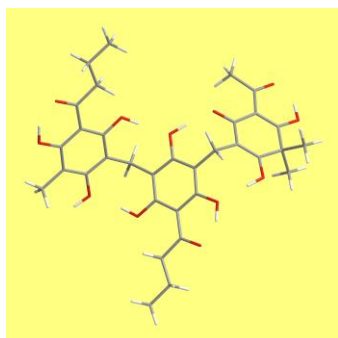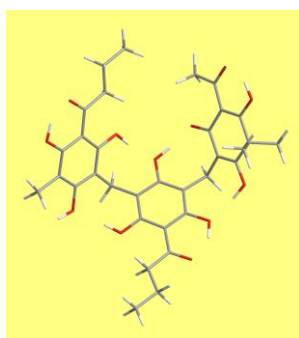
3   2.011   3-y   3.226
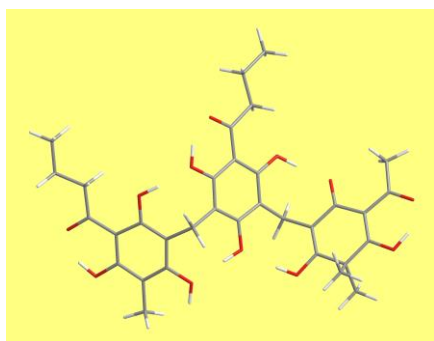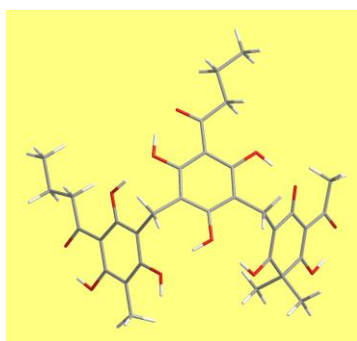
4   4.168   4-y   4.311
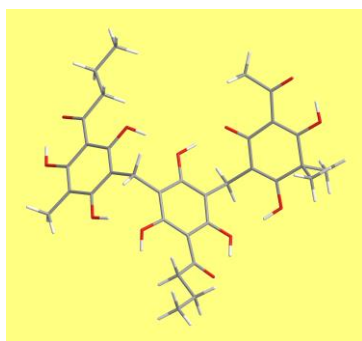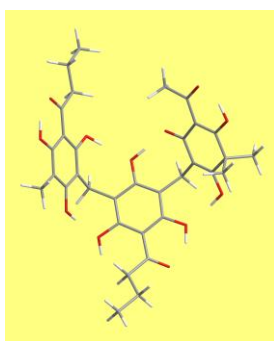
5   10.602   5-y   10.510
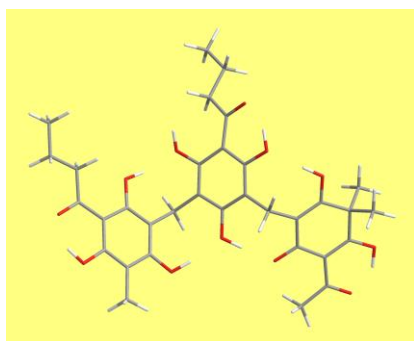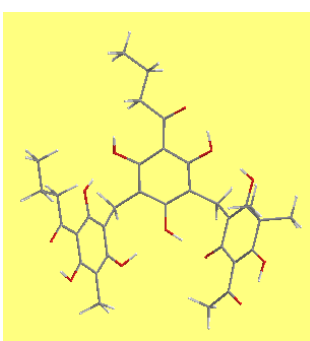
6   10.196   6-y   10.249
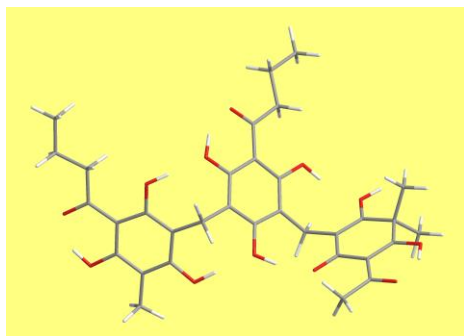
7   15.573
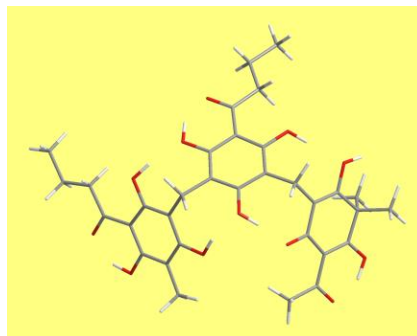
7-y   14.387
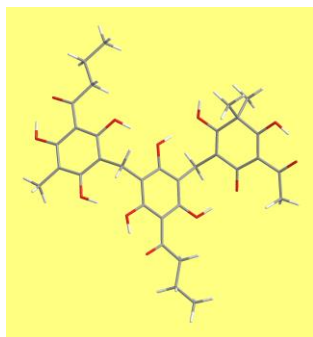
8   15.982
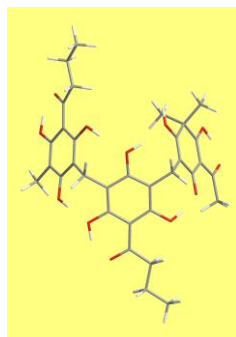
8-y   15.114
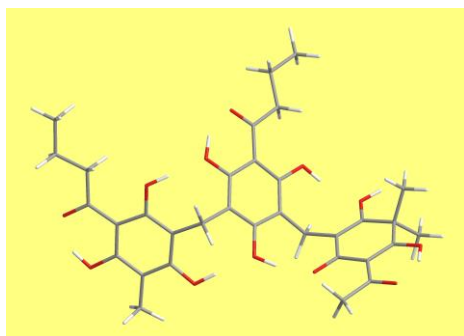
9   15.595
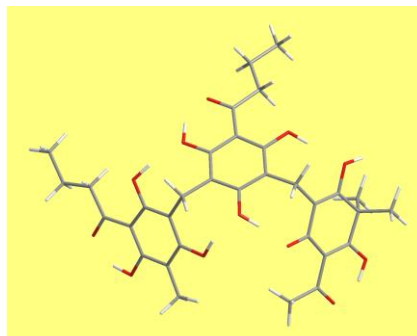
9-y   15.141
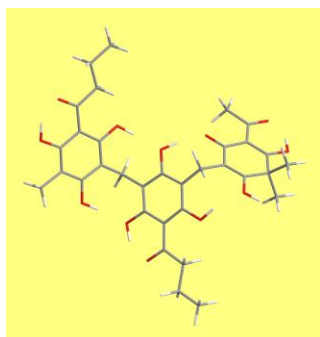
10   15.732
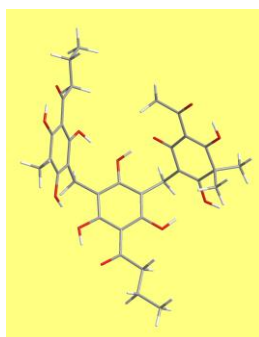
10-y   15.474

Structure T8-KT6″-M5,3″,3″
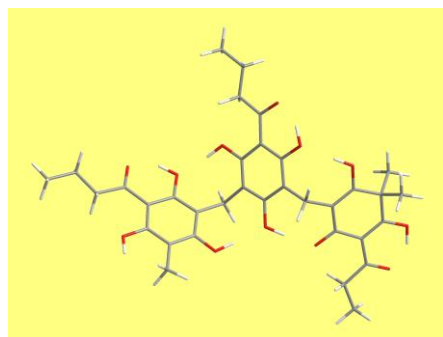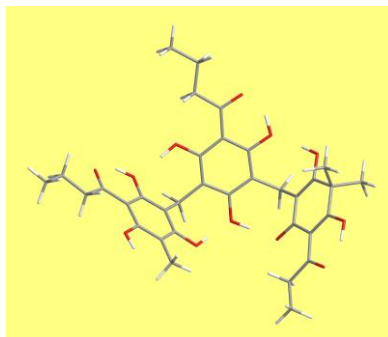
1   0.000

1-y   0.249
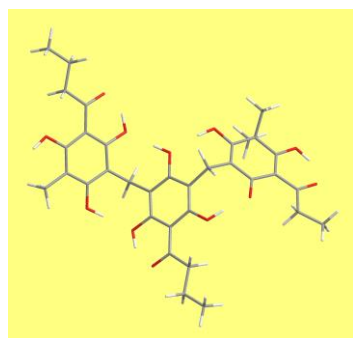
2   0.574
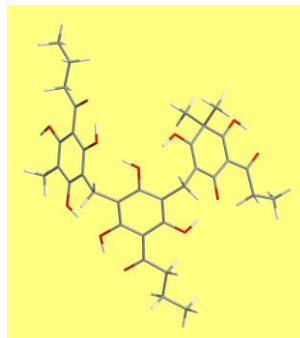
2-y   0.860
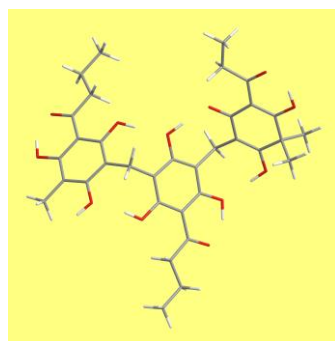
3   2.856
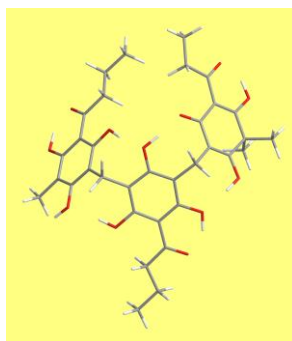
3-y   3.242
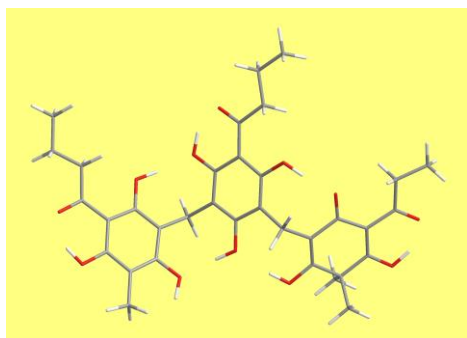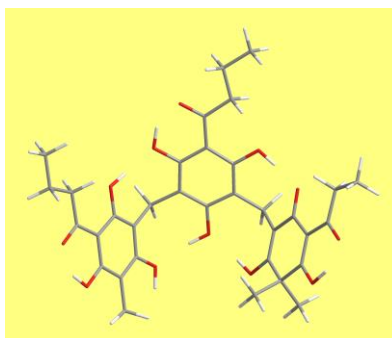
4   4.108   4-y   4.252
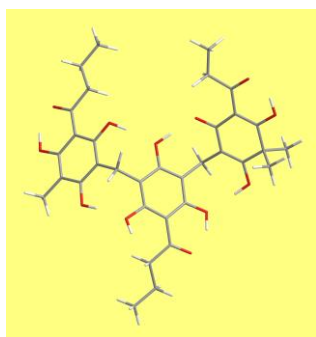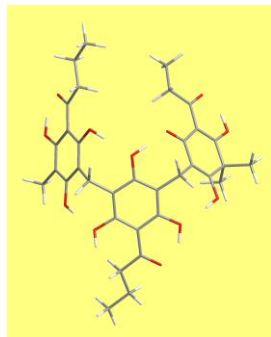
5   10.508   5-y   10.400
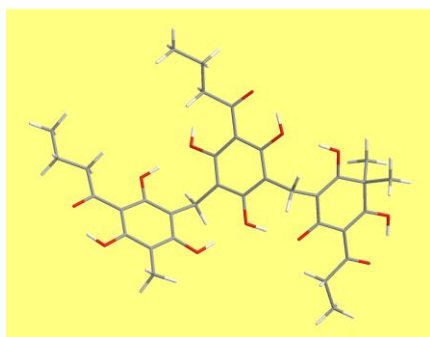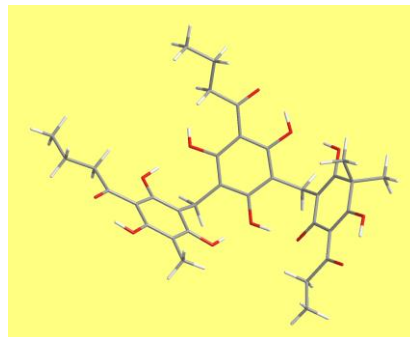
6   10.086   6-y   10.179
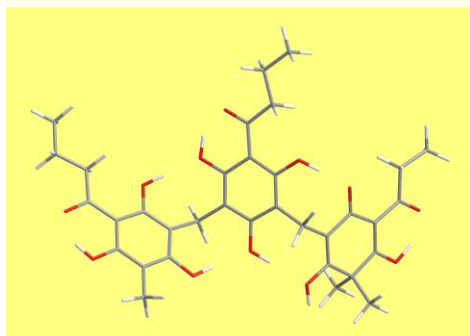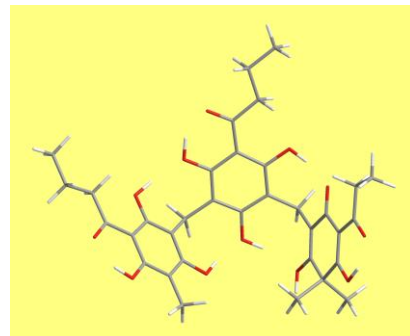
7   15.428   7-y   14.203
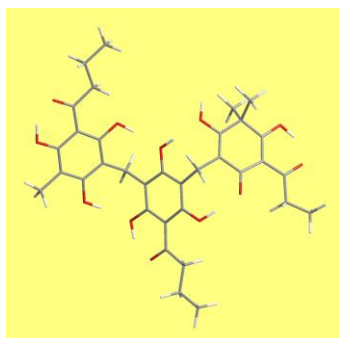
8   15.791
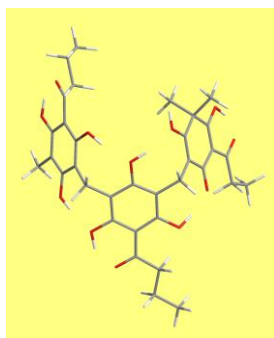
8-y   14.931
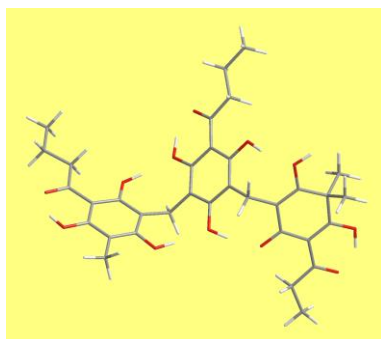
9   15.386
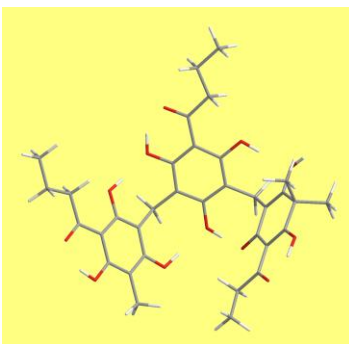
9-y   14.931
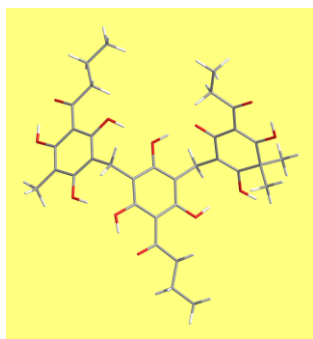
10   15.552
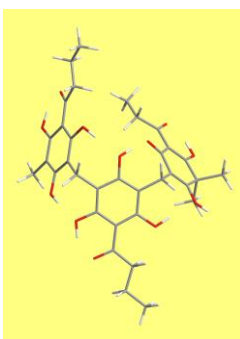
10-y   15.319

Structure T8-KT2-M5,5,3″
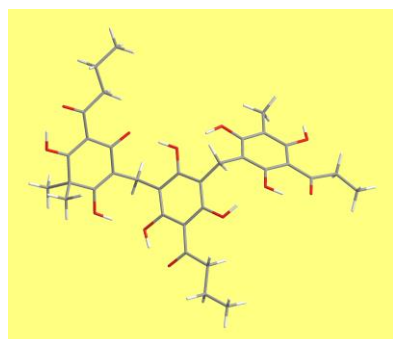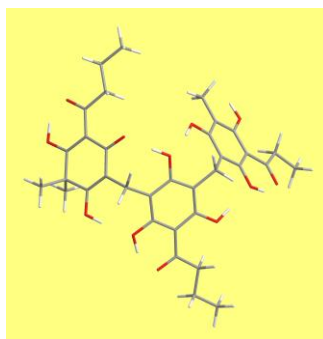
1   0.000

1-y   0.274
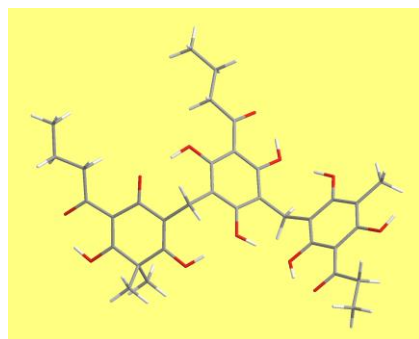
2   0.538
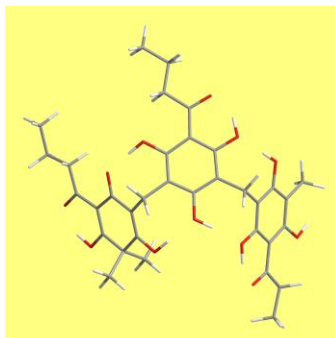
2-y   0.834
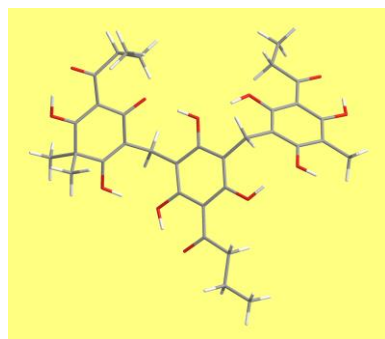
3   4.401
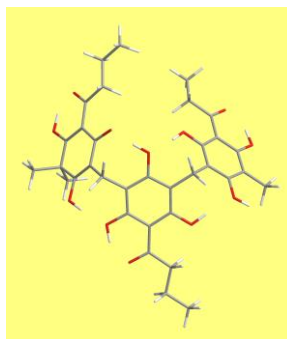
3-y   2.1883
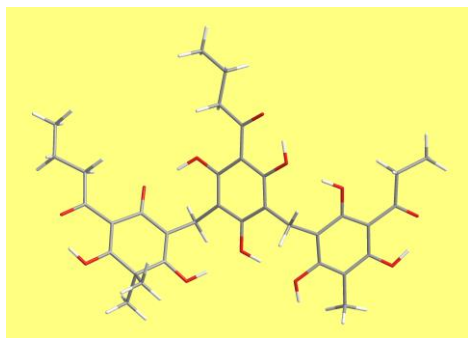
4   4.039
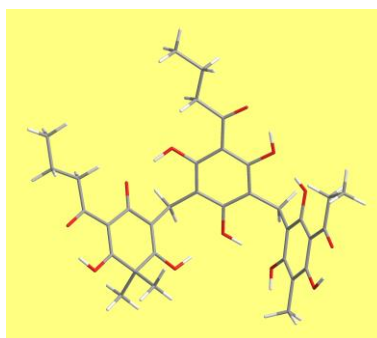
4-y   4.135
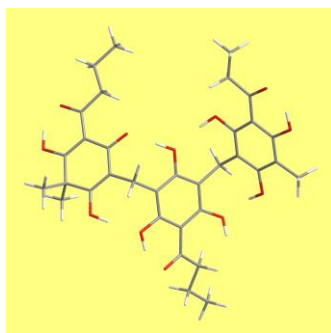
5   10.056
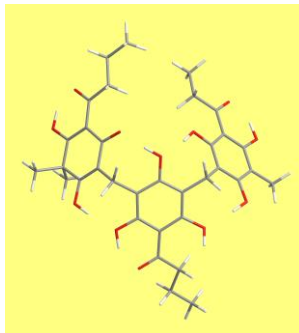
5-y   10.165
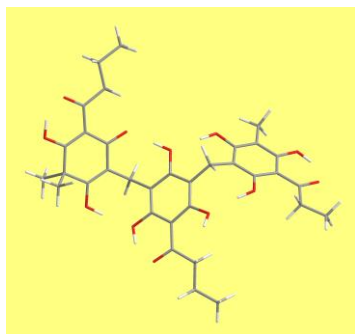
6   10.460
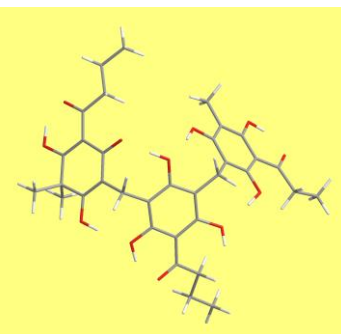
6-y   10.399
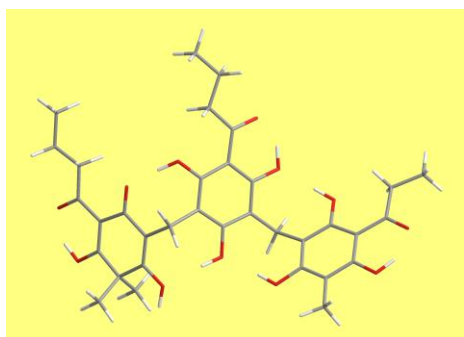
7   15.317
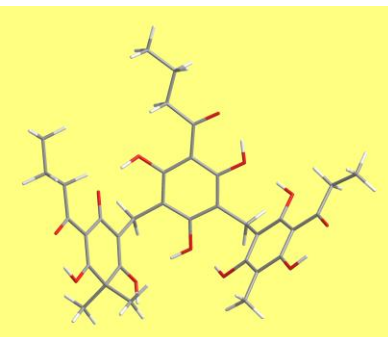
7-y   14.173
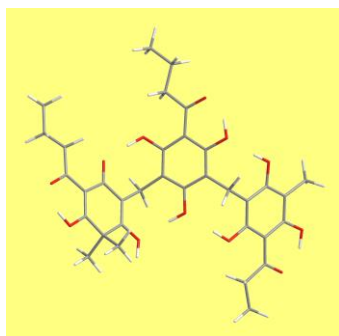
8   15.770
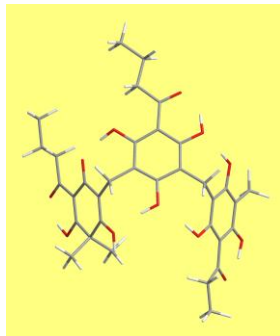
8-y   14.875
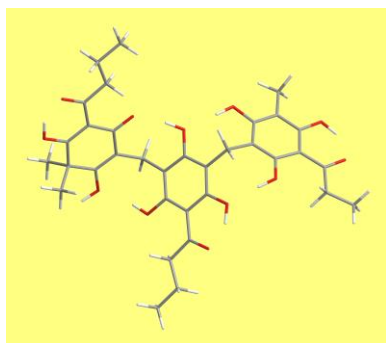
9   15.770
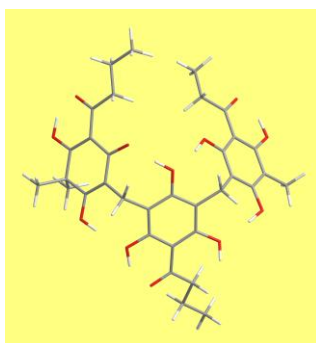
9-y   14.875
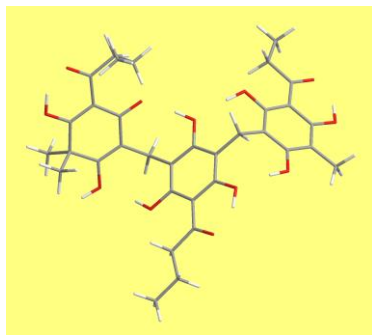
10   16.749
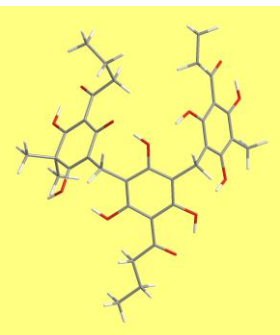
10-y   16.453

Structure T9-KT6″-M5,3″,3″
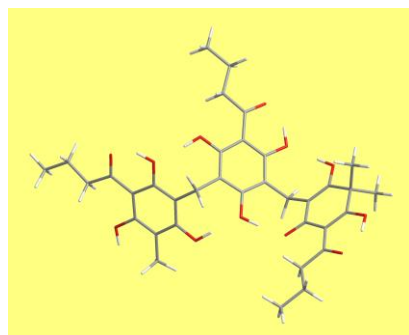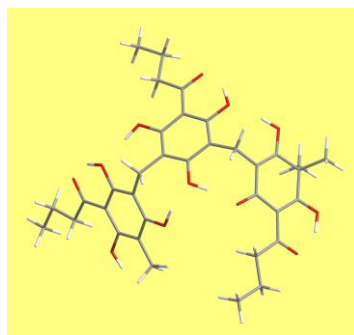
1   0.000

1-y   0.266
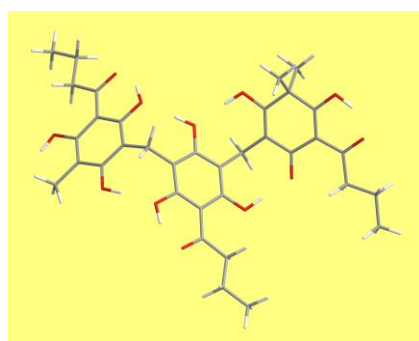
2   0.544
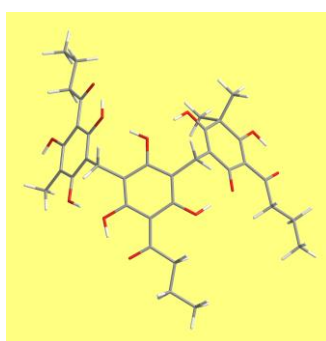
2-y   0.868
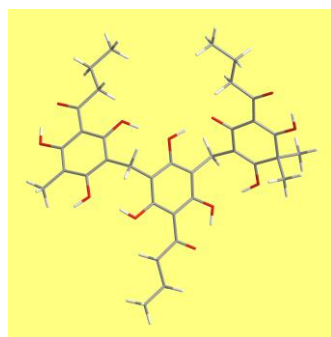
3   2.853
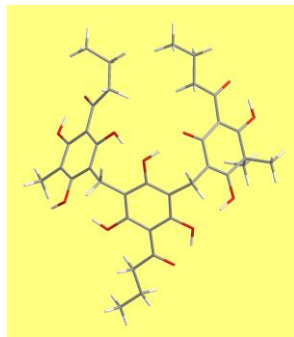
3-y   4.268
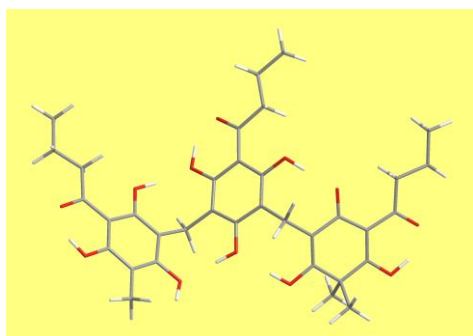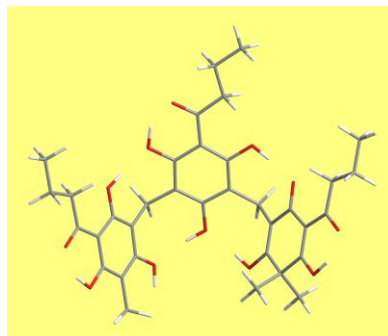
4   4.070   4-y   4.210
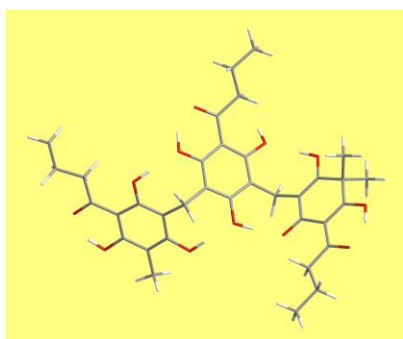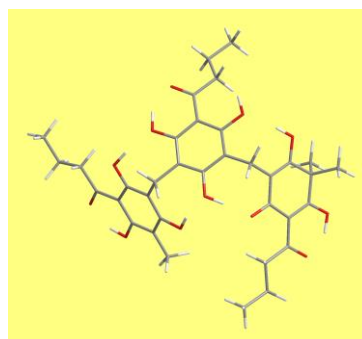
5   11.948   5-y   11.730
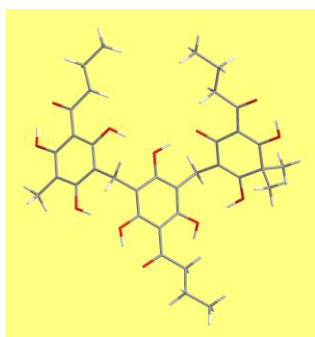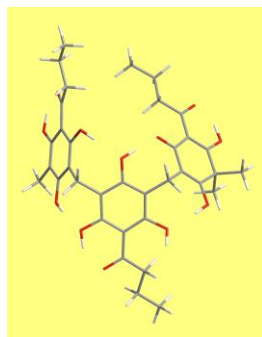
6   11.914   6-y   12.251
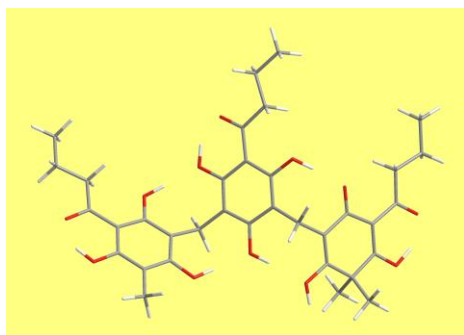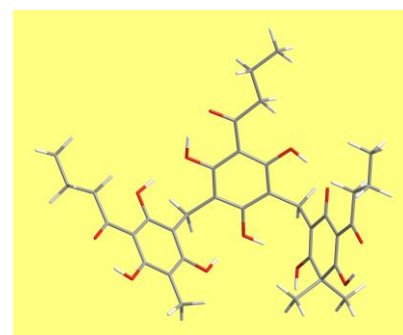
7   15.391   7-y   14.162
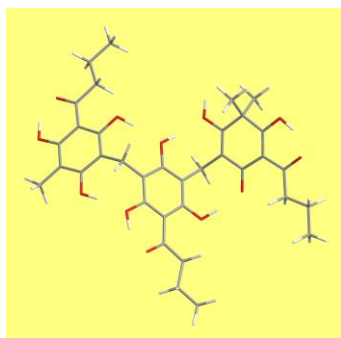
8   15.794
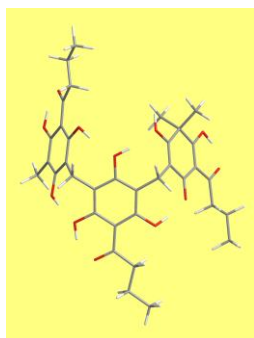
8-y   14.899
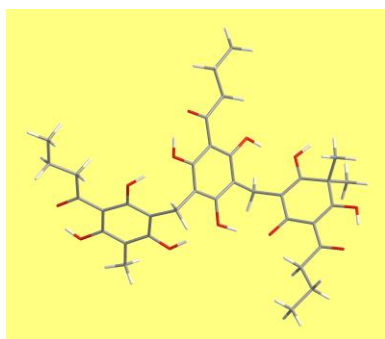
9   15.349
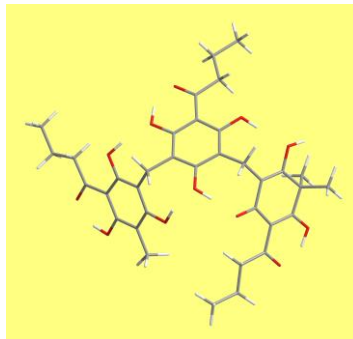
9-y   14.865
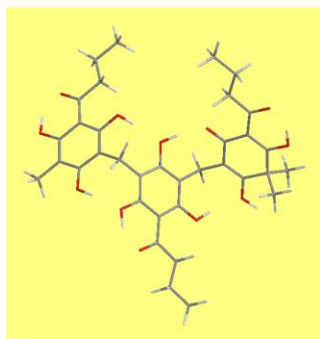
10   15.465
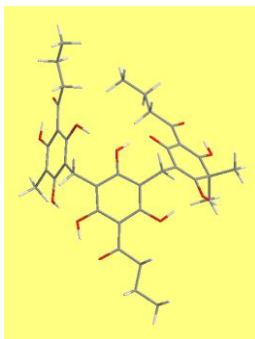
10-y   15.949

Structure T12-KT6″-M5,3″,3″
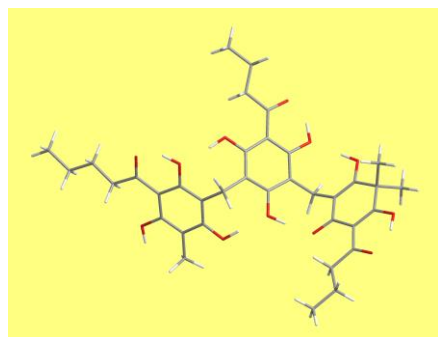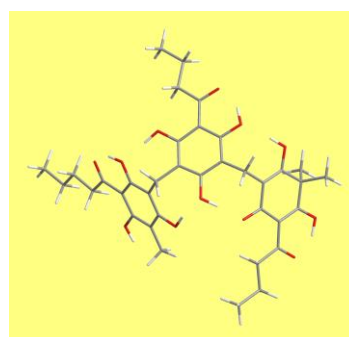
1   0.000

1-y   0.267
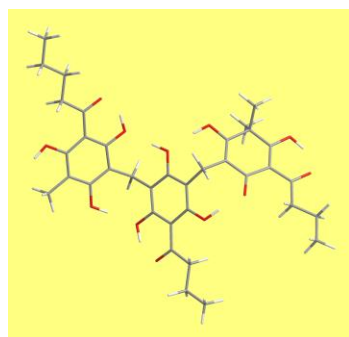
2   0.581
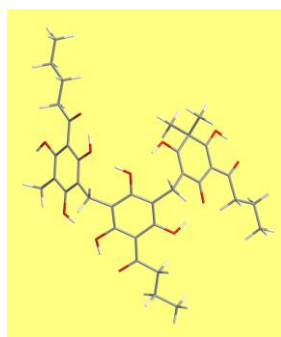
2-y   0.869
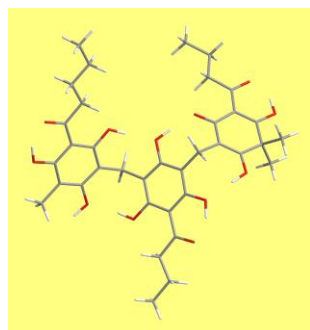
3   2.865
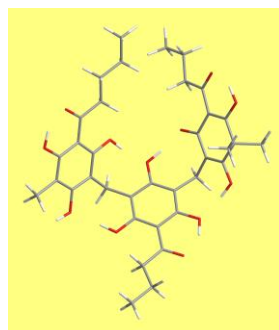
3-y   3.260
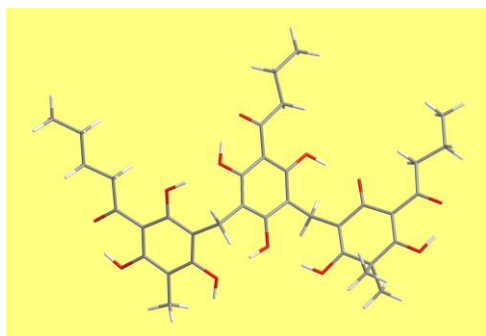
4   4.079
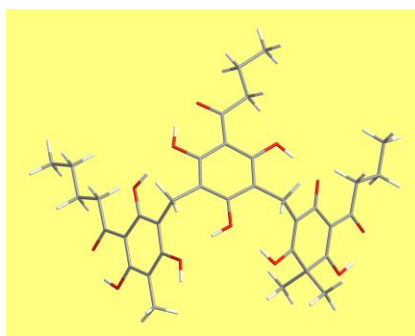
4-y   4.255
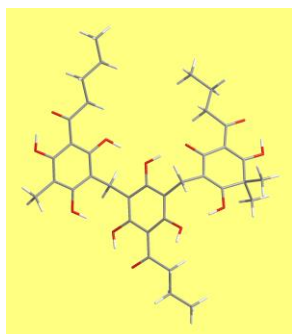
5   11.971
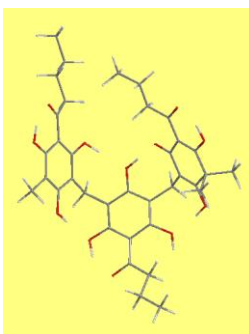
5-y   11.793
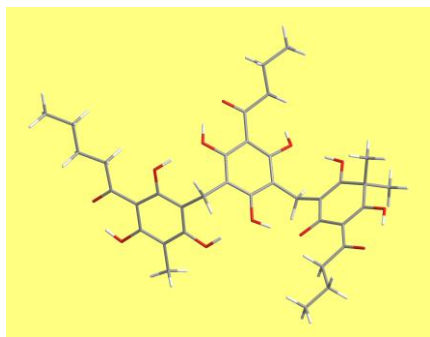
6   11.947
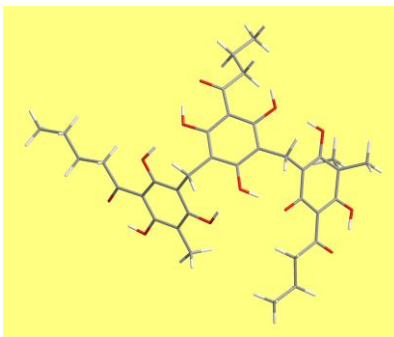
6-y   12.262
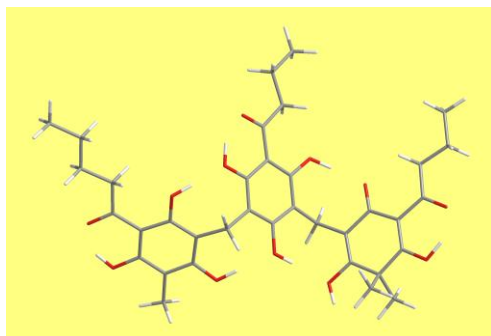
7   15.415
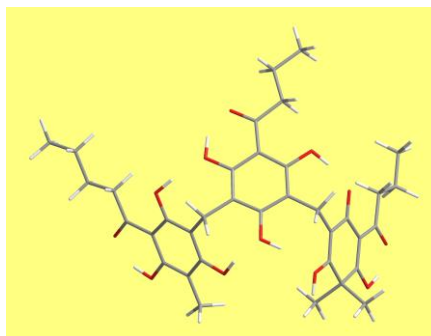
7-y   14.205
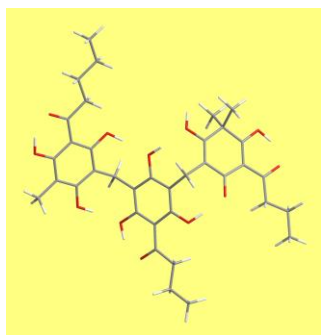
8   15.813
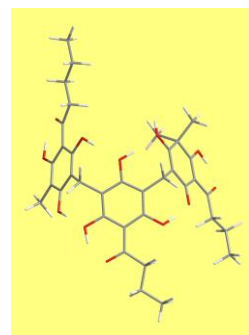
8-y   14.916
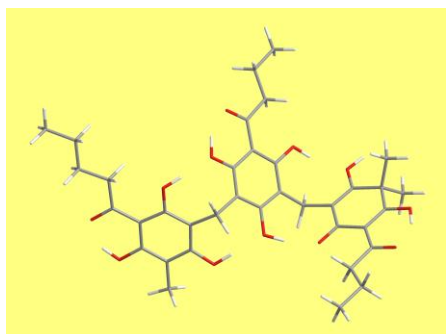
9   15.371
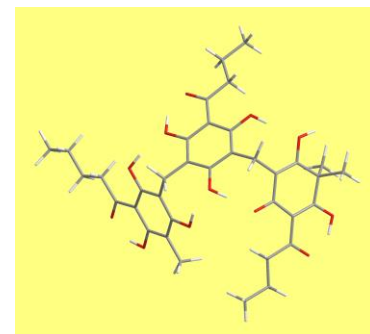
9-y   14.928
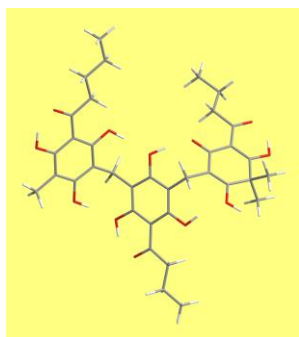
10   15.549
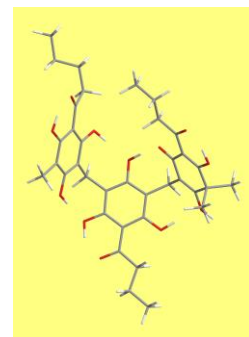
10-y   15.831

Structure T12-KT2-M5,5,3″
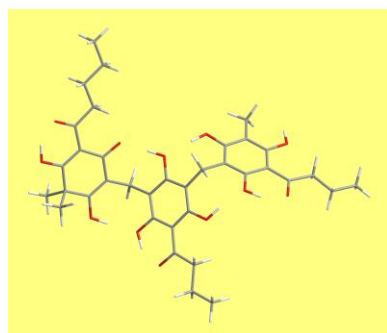
1   0.000
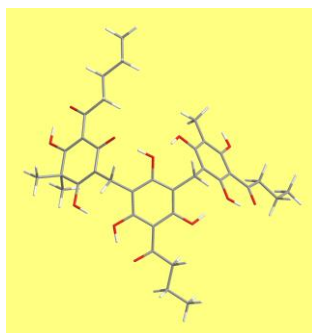
1-y   0.272
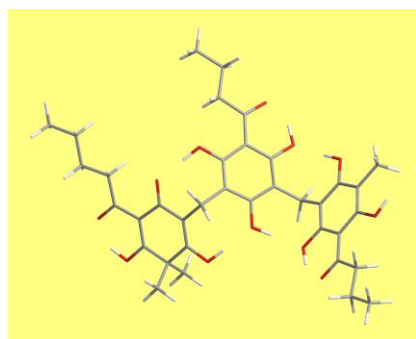
2   0.575
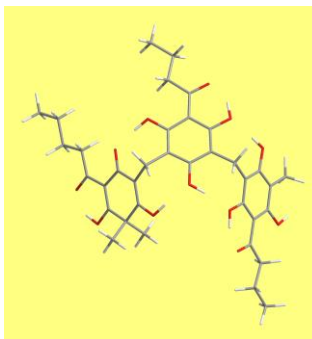
2-a-y   0.865
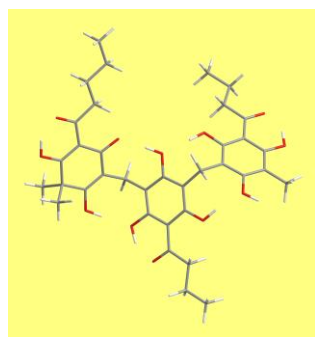
3   2.851
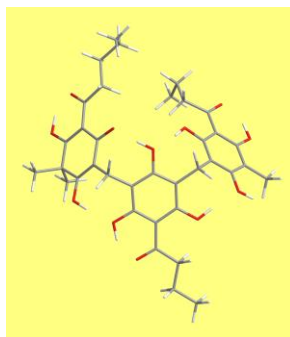
3-y   4.590
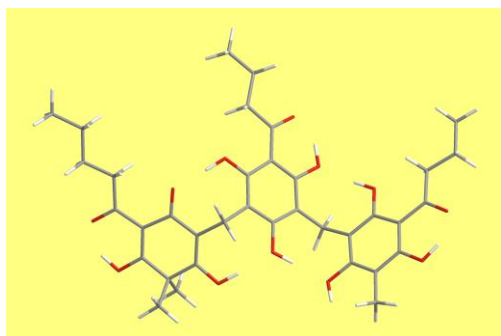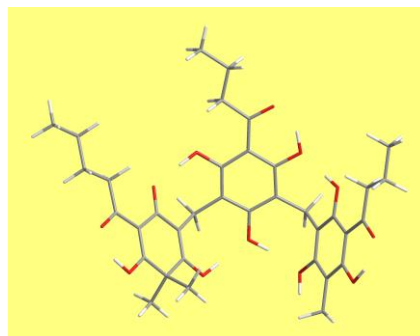
4   4.107   4-y   4.238
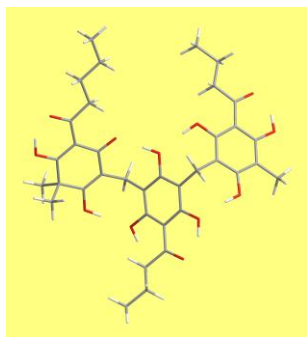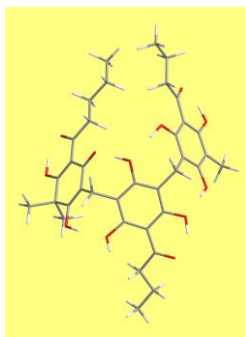
5   11.904   5-y   12.232
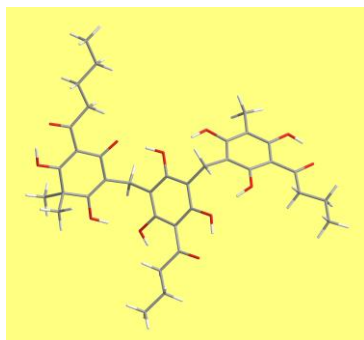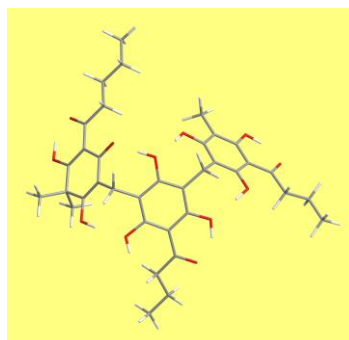
6   11.926   6y   11.904
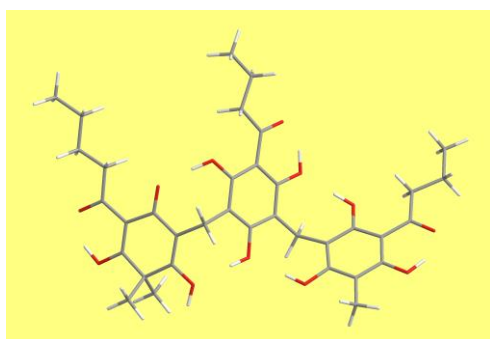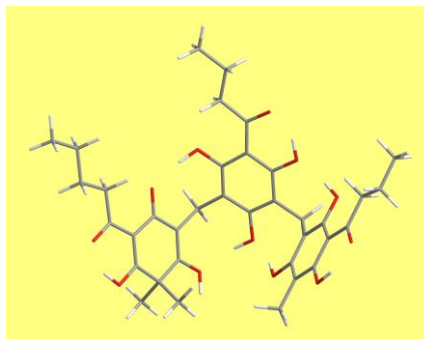
7   15.360   7-y   14.154
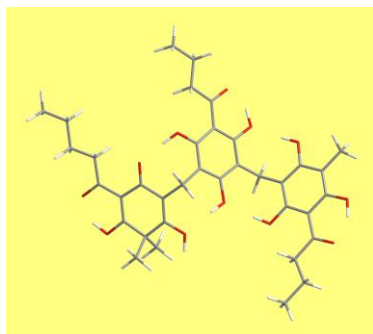
8   15.761
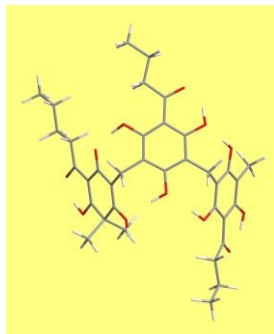
8-y   14.876
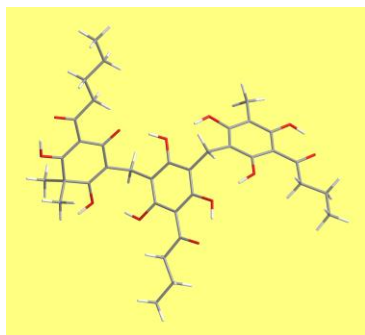
9   13.534
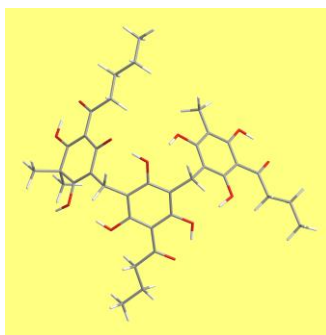
9-y   12.856
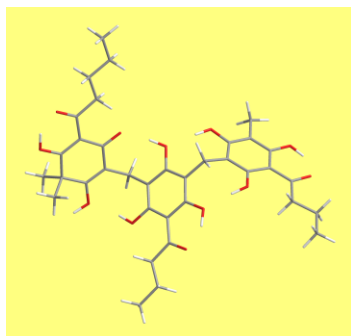
10   15.439
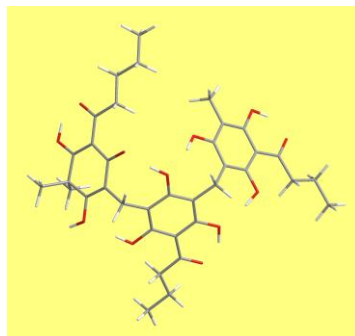
10-y   15.507

b) Structures in which the OH at C6″ is replaced by a keto O and one or more other OHs are replaced by OCH₃ groups

Structure T5-KT6″-M3″,3″-ET4
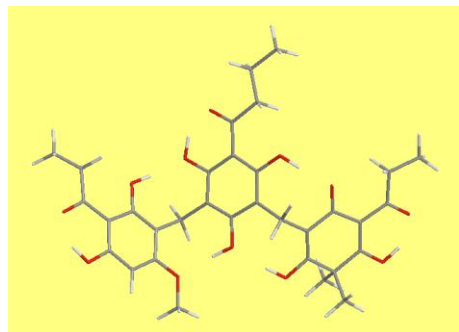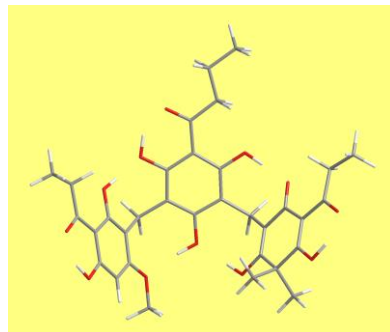
| 1 | 0.000 | 1-y | 0.086 |

Structure T9-KT6″-M3″,3″-ET4
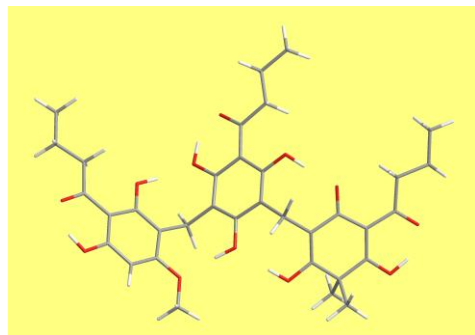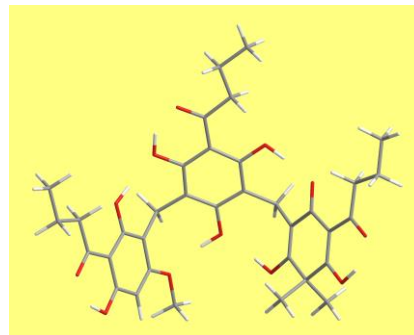
| 1 | 0.000 | 1-y | 0.085 |

Structure T9-KT6″-M5,3″,3″-ET6
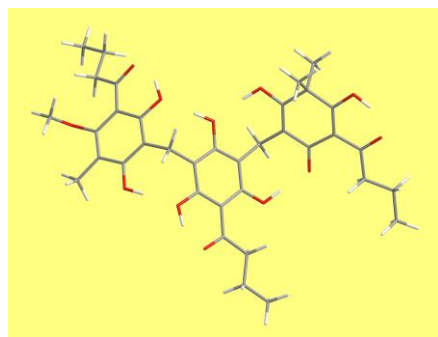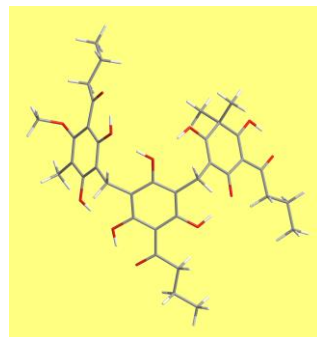
1   0.000

1-y   0.530
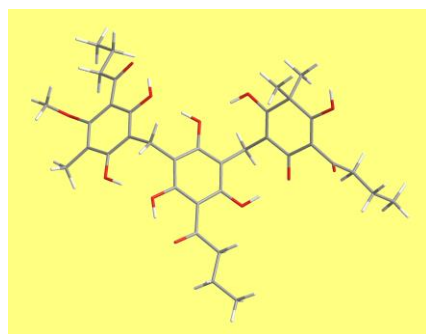
40[a]   18.045
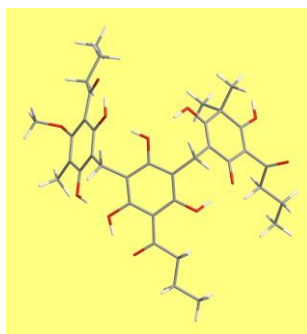
40-y   18.364

[a] Number given arbitrarily to high energy conformers in which one of the first IHBs is not present.

Structure T2-KT2,6″-M5,5,3″,3″
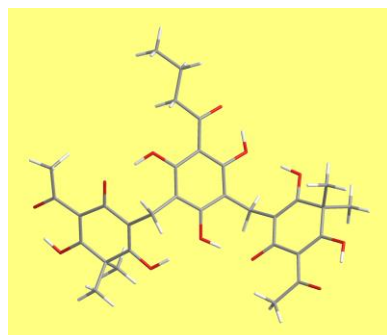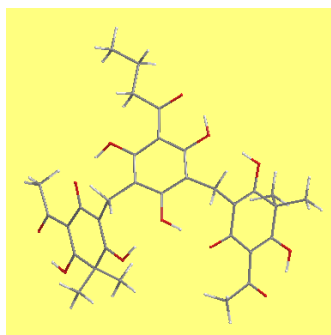
1   0.000

1-y   0.385

Structure T4-KT2,6″-M5,5,3″,3″
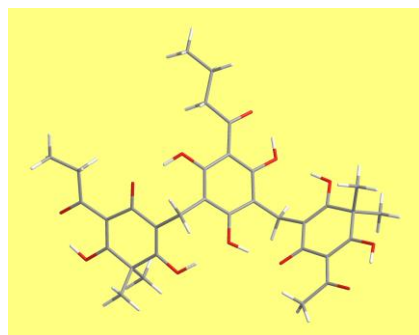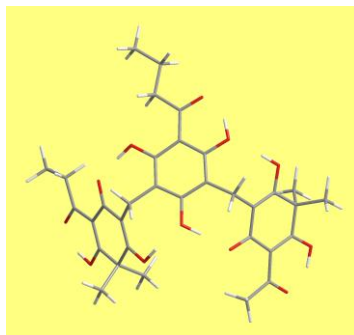
1   0.000

1-y   0.383

Structure T5-KT2,6″-M5,5,3″,3″
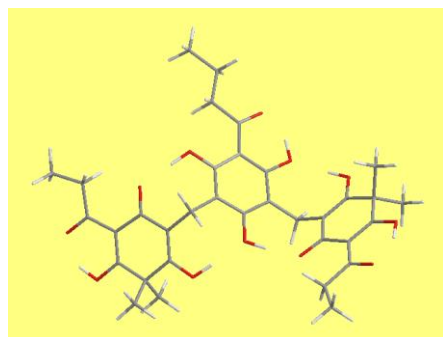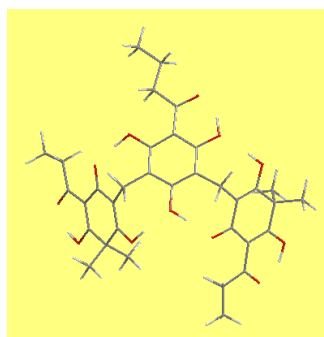
1	0.000	1-y	0.370

Structure T7-KT2,6″-M5,5,3″,3″
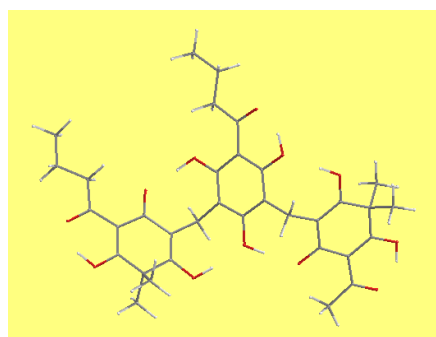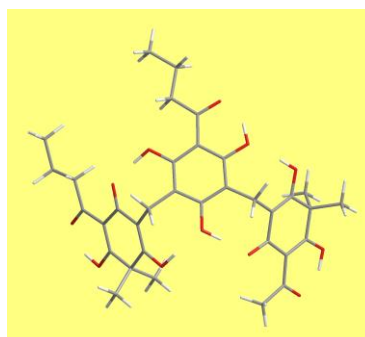
1	0.000	1-y	0.384

Structure T8-KT2,6″-M5,5,3″,3″
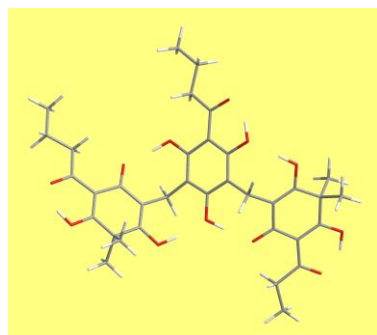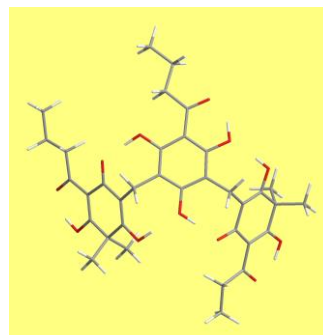
1	0.000	1-y	0.373

Structure T9-KT2,6″-M5,5,3″,3″
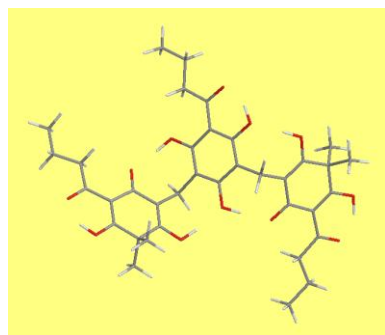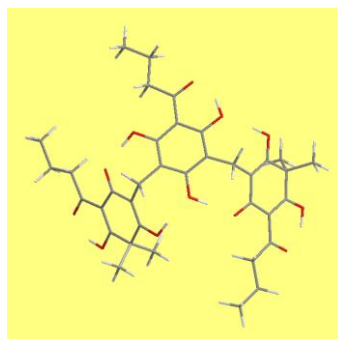
1   0.000

1-y   0.380

Structure T10-KT2,6″-M5,5,3″,3″
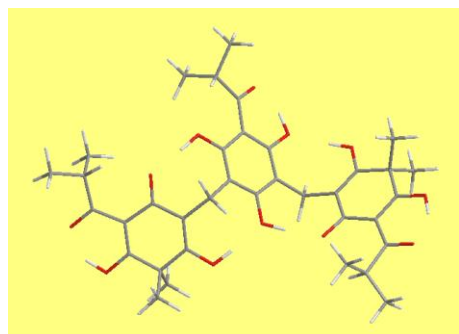
1   0.000
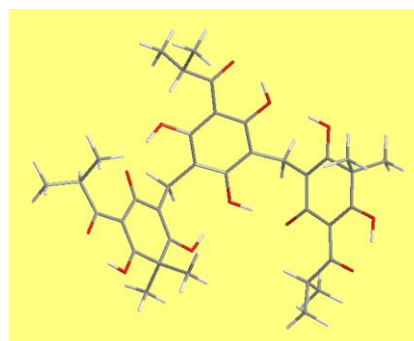
1-y   0.587

Figure S 7
Visualization of relevant trends of the lowering effect of Grimme's correction on the estimation of the energy of the conformers of the calculated trimeric acylphloroglucinols.
The values of this effect (kcal/mol, reported in table S6) pertain to the vertical axis of the graphs.

a) **Molecules in which no OH group is replaced by other functions.**
In this case, the numbers on the horizontal axis denote the pairs of conformers, as indicated in table S6. For each pair, the blue line refers to the outstretched-shape conformer and the brown line to the half-bowl-shaped conformer.

a) 1) **conformers of the T1 molecule**
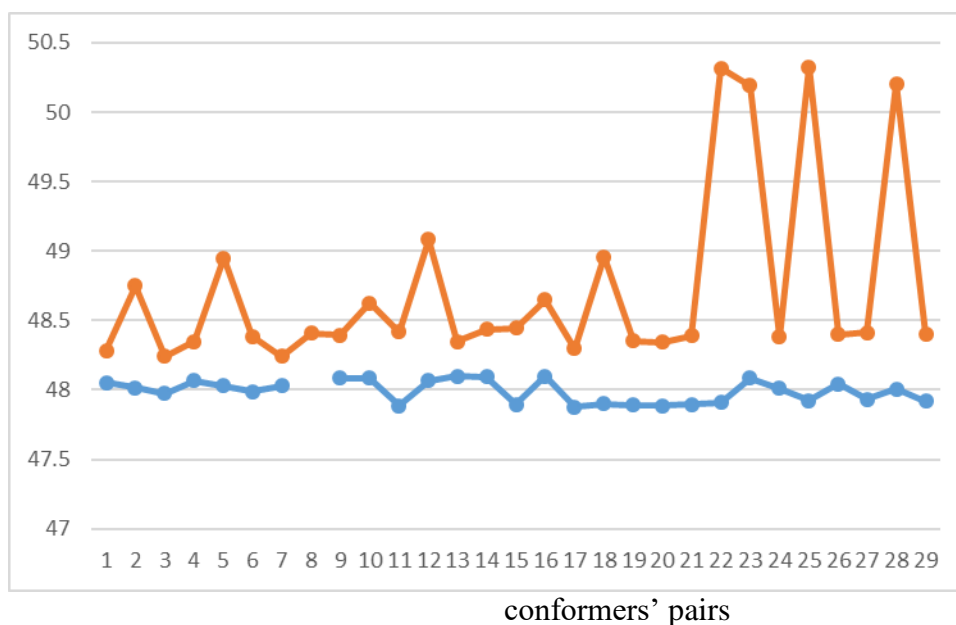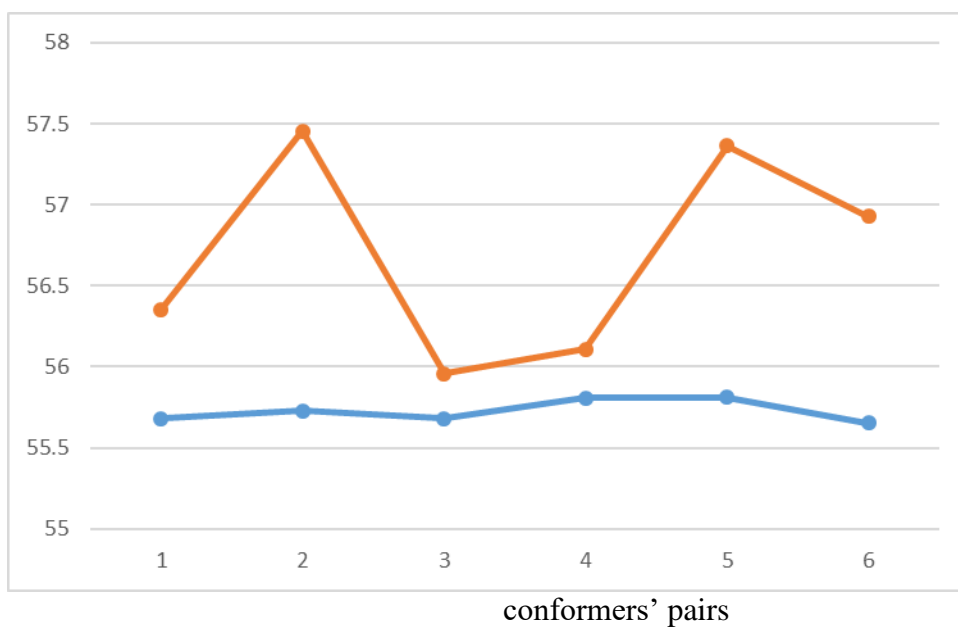
conformers' pairs

a)   2)   conformers of the T7 molecule

conformers' pairs

a)   3)   conformers of the T9 molecule

conformers' pairs

a)   4)   conformers of the T9- M5,3″ molecule
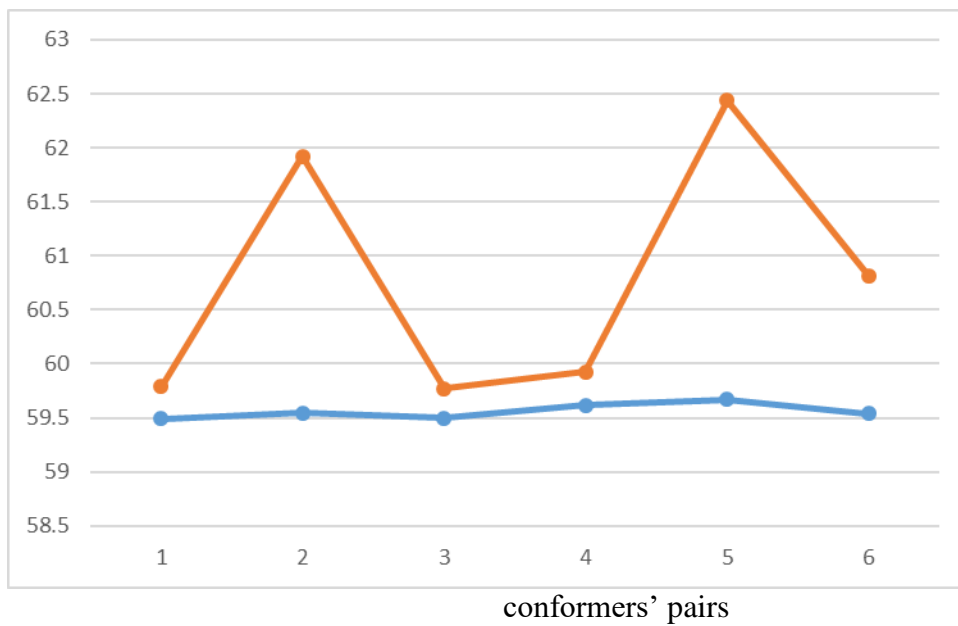
conformers' pairs

a)   5)   conformers of the T10 molecule
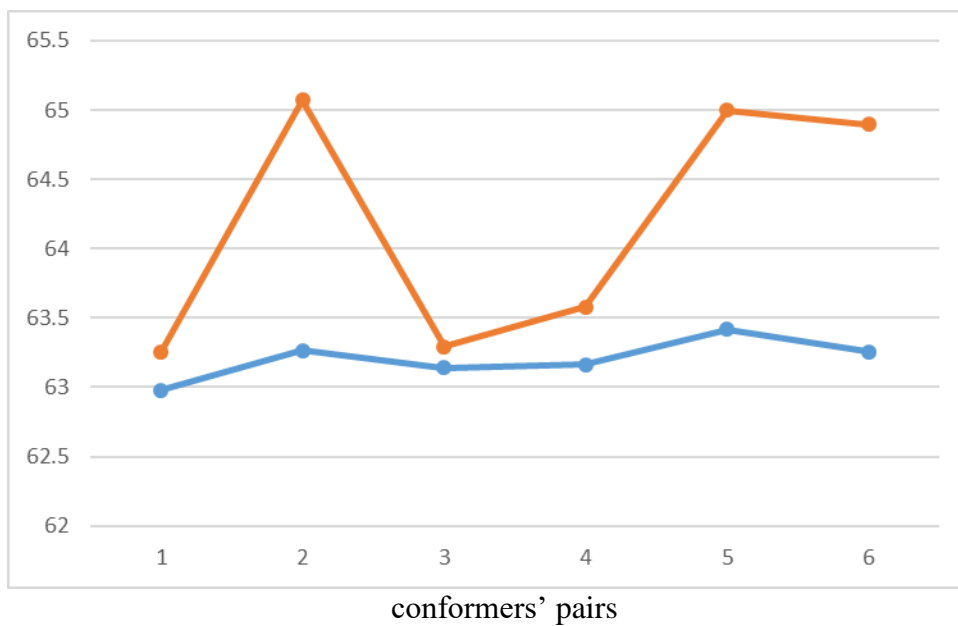
conformers' pairs

b) **Molecules in which an OH group ortho to the acyl group is replaced by a keto O in one of the outer monomers**

In this case, the numbers on the horizontal axis denote the pairs of conformers, as indicated in table S6. For each pair, the blue line refers to the outstretched-shape conformer and the brown line to the half-bowl-shaped conformer.

b) **1)** **conformers of the T7-KT6″-M5,3″,3″ molecule**

conformers' pairs

b) **2)** **conformers of the T8-KT6″-M5,3″,3″ molecule**

conformers' pairs

b) 3) conformers of the T8-KT2-M5,5,3″ molecule

conformers' pairs

b) 4) conformers of the T9-KT6″-M5,3″,3″ molecule

conformers' pairs

b)   5)   conformers of the T12-KT2-M5,5,3″ molecule

conformers' pairs

b)   6)   conformers of the T12-KT6″-M5,3″,3″ molecule

conformers' pairs

c) **Molecules in which the inward OH group ortho to the acyl group is replaced by a keto O in each of the outer monomers**

In this case, there is only one pair of conformers or each molecule. The numbers on the horizontal axis denote the molecules as indicated in the table below. For each molecule, the blue line refers to the outstretched-shape conformer and the brown line to the half-bowl-shaped conformer.

molecule	number denoting it on the x axis	molecule	number denoting it on the x axis
T2-KT2,6″-M5,5,3″,3″	1	T8-KT2,6″-M5,5,3″,3″	5
T4-KT2,6″-M5,5,3″,3″	2	T9-KT2,6″-M5,5,3″,3″	6
T5-KT2,6″- M5,5,3″,3″	3	T10-KT2,6″-M5,5,3″,3″	7
T7-KT2,6″-M5,5,3″,3″	4		

molecules (denoted by numbers)

d) **Molecules in which the OH groups at C6 and at C2″ are replaced by OCH₃ ether groups**

In this case, there is only one pair of conformers or each molecule. The numbers on the horizontal axis denote the molecules as indicated in the table below. For each molecule, the blue line refers to the outstretched-shape conformer and the brown line to the half-bowl-shaped conformer.

molecule	number denoting it on the x axis	molecule	number denoting it on the x axis
T3-ET6,2″	1	T10-M5,3″-ET6,2″	8
T3-M5,3″-ET6,2″	2	T11-ET6,2″	9
T7-ET6,2″	3	T11-M5,3″-ET6,2″	10
T7-M5,3″-ET6,2″	4	T13-ET6,2″	11
T9-ET6,2″	5	T13-M5,3″-ET6,2″	12
T9-M5,3″-ET6,2″	6	T14-ET6,2″	13
T10-ET6,2″	7	T14-M5,3″-ET6,2″	14

molecules (denoted by numbers)

e) **Trend in terms of the molecular formulas**
The diagram considers the smallest value of the dispersion-related energy decrease among the calculated T-ACPL molecules having the same molecular formula (table S 7). The numbers on the horizontal axis correspond to the molecular formulas as indicated in the table below. For each selection, the blue line refers to the outstretched-shape conformer and the brown line to the half-bowl-shaped conformer.

number on the x axis	molecular formula	molecular mass (a.m.u)	number on the x axis	molecular formula	molecular mass (a.m.u)
1	$C_{26}H_{24}O_{12}$	528	6	$C_{34}H_{40}O_{12}$	640
2	$C_{30}H_{32}O_{12}$	584	7	$C_{35}H_{42}O_{12}$	654
3	$C_{31}H_{34}O_{12}$	598	8	$C_{36}H_{44}O_{12}$	668
4	$C_{32}H_{36}O_{12}$	612	9	$C_{37}H_{46}O_{12}$	682
5	$C_{33}H_{38}O_{12}$	626			

molecular formulas   (represented by numbers)

Visualization of relevant trends of the effect of Grimme's correction on the estimation of the ZPE correction for the conformers of selected trimeric acylphloroglucinols.
The values of the ZPE correction (kcal/mol, reported in table S9) pertain to the vertical axis of the graphs.

━●━   DFT/B3LYP/6-31+G(d,p) results for conformers with outstretched geometry

━●━   DFT/B3LYP/6-31+G(d,p) results for conformers with half-bowl-shaped geometry

━●━   DFT/B3LYP/6-31+G(d,p)-D3 results for conformers with outstretched geometry

━●━   DFT/B3LYP/6-31+G(d,p)-D3 results for conformers with half-bowl-shaped geometry

a)   **Molecules in which no OH group is replaced by other functions.**
In this case, the numbers on the horizontal axis denote the conformers' pairs.

a)   **1)**   **conformers of the T1 molecule**
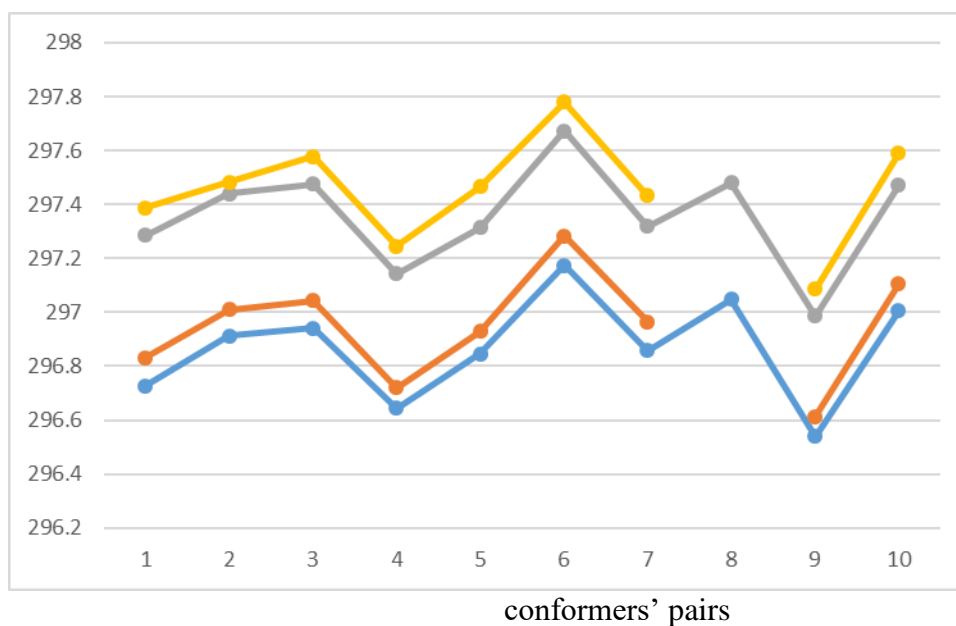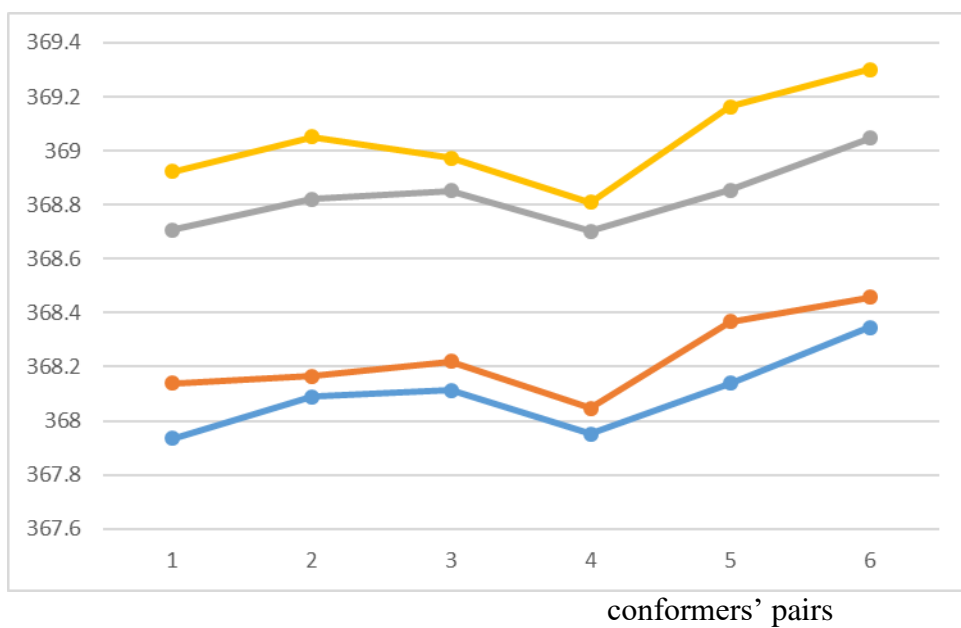
conformers' pairs

a) **2)** **conformers of the T7 molecule**

conformers' pairs

a) **3)** **conformers of the T9 molecule**

conformers' pairs

a) 4) conformers of the T9- M5,3″ molecule

conformers' pairs
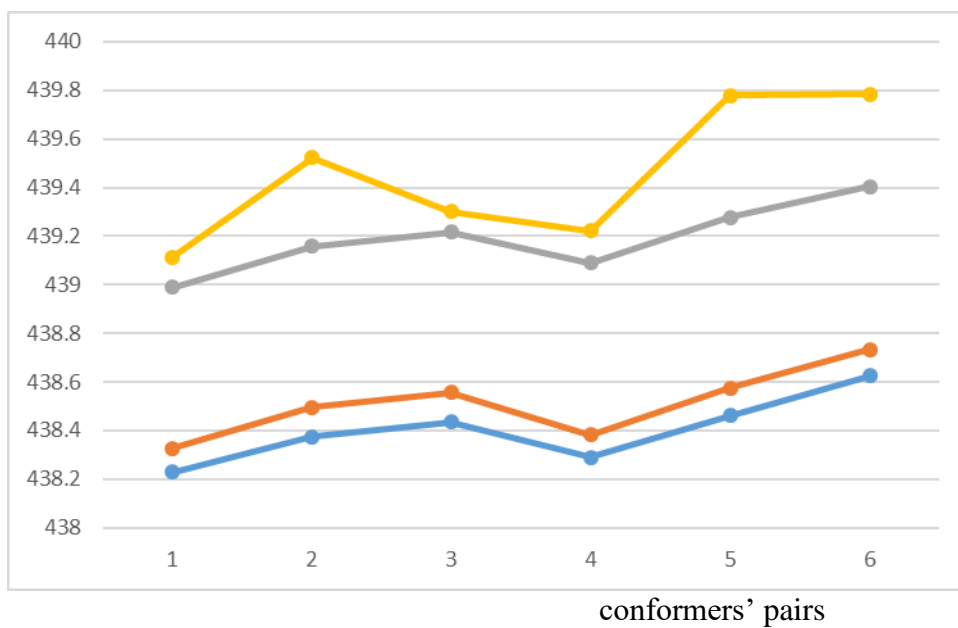
a) 5) conformers of the T10 molecule
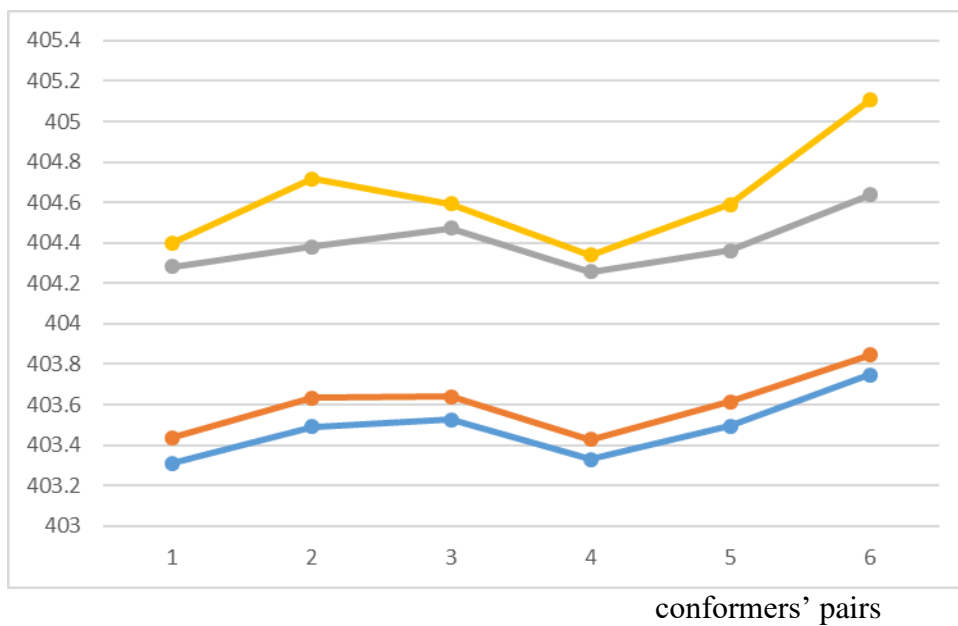
conformers' pairs

b) **Molecules in which the inward OH group ortho to the acyl group is replaced by a keto O in one of the outer monomers**

In this case, the numbers on the horizontal axis denote the pairs of conformers.

b) **1)** **conformers of the T7-KT6″-M5,3″,3″ molecule**

conformers' pairs

b) **2)** **conformers of the T8-KT6″-M5,3″,3″ molecule**

conformers' pairs

b)   3)   conformers of the T8-KT2-M5,5,3″ molecule

conformers' pairs

b)   4)   conformers of the T9-KT6″-M5,3″,3″ molecule

conformers' pairs

b) 5) conformers of the T12-KT2-M5,5,3″ molecule

conformers' pairs

b) 6) conformers of the T12-KT6″-M5,3″,3″ molecule

conformers' pairs

c) **Molecules in which the inward OH group ortho to the acyl group is replaced by a keto O in each of the outer monomers**

In this case, there is only one pair of conformers for each molecule. The numbers on the horizontal axis denote the molecules as indicated in the table below.

molecule	number denoting it on the x axis	molecule	number denoting it on the x axis
T2-KT2,6″-M5,5,3″,3″	1	T8-KT2,6″-M5,5,3″,3″	5
T4-KT2,6″-M5,5,3″,3″	2	T9-KT2,6″-M5,5,3″,3″	6
T5-KT2,6″- M5,5,3″,3″	3	T10-KT2,6″-M5,5,3″,3″	7
T7-KT2,6″-M5,5,3″,3″	4		

molecules (denoted by numbers)

d) **Molecules in which the OH groups at C6 and at C2″ are replaced by OCH₃ ether groups**

In this case, there is only one pair of conformers for each molecule. The numbers on the horizontal axis denote the molecules as indicated in the table below.

molecule	number denoting it on the x axis	molecule	number denoting it on the x axis
T3-ET6,2″	1	T10-M5,3″-ET6,2″	8
T3-M5,3″-ET6,2″	2	T11-ET6,2″	9
T7-ET6,2″	3	T11-M5,3″-ET6,2″	10
T7-M5,3″-ET6,2″	4	T13-ET6,2″	11
T9-ET6,2″	5	T13-M5,3″-ET6,2″	12
T9-M5,3″-ET6,2″	6	T14-ET6,2″	13
T10-ET6,2″	7	T14-M5,3″-ET6,2″	14

molecules (denoted by numbers)

e)   **Trend in terms of the molecular formulas**
The diagram considers the smallest value of the dispersion-related energy decrease among the molecules having the same molecular formula (table S 7). The numbers on the horizontal axis correspond to the molecular formulas as indicated in the table below. For each formula, the blue line refers to the DFT results and the brown line to the DFT-D3 results.

number on the x axis	molecular formula	molecular mass (a.m.u)	number on the x axis	molecular formula	molecular mass (a.m.u)
1	$C_{26}H_{24}O_{12}$	528	6	$C_{34}H_{40}O_{12}$	640
2	$C_{30}H_{32}O_{12}$	584	7	$C_{35}H_{42}O_{12}$	654
3	$C_{31}H_{34}O_{12}$	598	8	$C_{36}H_{44}O_{12}$	668
4	$C_{32}H_{36}O_{12}$	612	9	$C_{37}H_{46}O_{12}$	682
5	$C_{33}H_{38}O_{12}$	626			

molecular formulas   (represented by numbers)

Figure S 9. Comparisons of the lengths of corresponding intramolecular hydrogen bonds (IHBs) in the DFT/B3LYP/6-31+G(d,p) results without and with the Grimme's correction, for selected trimeric acylphloroglucinol molecules.

The conformers of the lowest energy pair (1 and 1-y) are considered for each selected molecule. The molecules are grouped according to the presence of the same set of IHBs in the lowest energy conformers.

The molecules and the two conformers considered are denoted by numbers, as indicated in specific tables for each group of molecules. The length of the IHBs (Å) is the quantity on the vertical axis of the diagrams.

The blue line refers to the results without Grimme's correction and the brown line refers to the results with the Grimme's correction.

Different IHBs are considered individually, in separate diagrams. The titles of the diagrams also recall whether the given IHB is a 'first IHB' or an intermonomer IHB (IMHB).

a) **Comparison of the length of the same IHB in different conformers of the T1 molecule**

The conformers in which the given IHB is present are denoted by numbers on the x axis, as indicated in the tables provided under the name of each IHB. The other IHBs present in the conformer are also reported in the table as information on the molecular context.

a) 1) **H15···O14 first IHB**

number on x axis	conformer	other IHBs in the conformer
1	1	H17′····O14′, H17″····O14″, H16′····O8, H16····O12′,
2	1-y	H16″····O10′, H15′····O12″
3	2	H17′····O14′, H15″····O14″, H16′····O8, H16····O12′,
4	2-y	H17″····O10′, H15′····O10″
5	3	H15′····O14′, H15″····O14″, H17′····O8, H16····O10′,
6	3-y	H17″····O8′, H16′····O10″
7	4	H17′····O14′, H17″····O14″, H10′····O8, H16····O12′,
8	4-y	H16″····O10′, H15′····O12″
9	5	H17′····O14′ , H15″····O14″, H16′····O8, H16····O12′,
10	5-y	H16″····O10′, H15′····O10″
11	7	H15′····O14′, H15″····O14″, H17′····O8, H16····O10′,
12	7-y	H17″····O8′, H16′····O10″
13	9	H17′····O14′, H17″····O14″, H16′····O8, H16····O12′,

14	9-y	H16″····O10′, H15′····O12″
15	10	H15′····O14′, H15″····O14″, H17′····O8, H16····O10′,
16	10-y	H17″····O8′, H16′····O12″
17	11	H15′····O14′, H15″····O14″, H17′····O8, H16′····O10,
18	11-y	H17″····O8′, H16″····O10′
19	12	H17′····O14′, H15″····O14″, H16′····O8, H16····O12′,
20	12-y	H17″····O10′, H16″····O8′
21	15	H15′····O14′, H15″····O14″, H17′····O8, H16····O10′,
22	15-y	H16″····O8′, H17″····O10′
23	16	H15′····O14′, H15″····O14″, H17′····O8, H16····O10′,
24	16-y	H16″····O8′, H17′····O10″′
25	18	H15′····O14′ , H15″····O14″, H16′····O8, H17′····O10,
26	18-y	H17″····O10′, H16″····O8′
27	19	H15′····O14′, H15″····O14″, H17′····O8, H16′····O10,
28	19-y	H17″····O8′, H16″····O10′
29	21	H15′····O14′ , H15″····O14″, H17′····O8, H16′····O10,
30	21-y	H16″····O8′, H17′····O10″
31	22	H15′····O14′ , H15″····O14″, H16′····O8, H17′····O10,
32	22-y	H17″····O10′, H16″····O8′
33	23	H17′····O14′ , H15″····O14, H16′····O8″, H16····O12′,
34	23-y	H17″····O10′, H16″····O8′
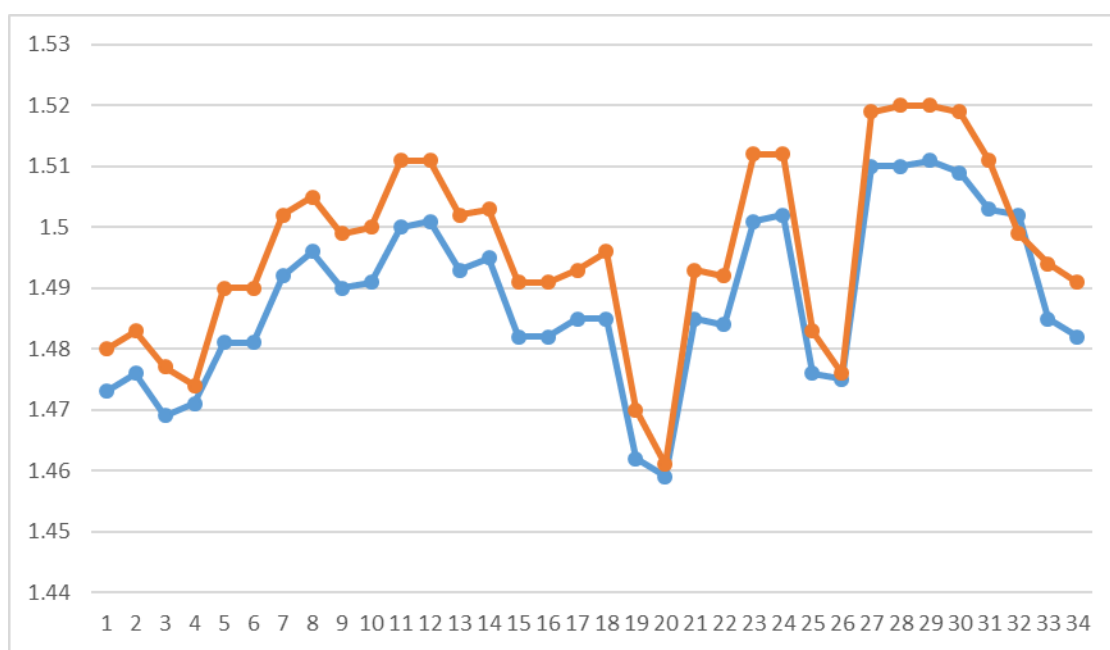
conformers, denoted by numbers

a) 2) H16′····O8 IMHB

number on x axis	conformer	other IHBs in the conformer
1	1	H15····O14, H17′····O14′, H17″····O14″, H16····O12′,
2	1-y	H16″····O10′, H15′····O12″
3	2	H15····O14, H17′····O14′, H15″····O14″, H16····O12′,
4	2-y	H17″····O10′, H15′····O10″
5	5	H15····O14, H17′····O14′ , H15″····O14″, H16····O12′,
6	5-y	H16″····O10′, H15′····O10″
7	9	H15····O14, H17′····O14′, H17″····O14″, H16····O12′,
8	9-y	H16″····O10′, H15′····O12″
9	12	H15····O14, H17′····O14′, H15″····O14″, H16····O12′,
10	12-y	H17″····O10′, H16″····O8′
11	14	H17····O14, H15′····O14′, H17″····O14″, H16····O12′,
12	14-y	H16″····O10′, H15′····O12″
13	17	H17····O14, H17′····O14′, H17″····O14″, H17′····O10,
14	17-y	H16″····O10′, H17″····O8′
15	18	H15····O14, H15′····O14′ , H15″····O14″, H17′····O10,
16	18-y	H17″····O10′, H16″····O8′
17	20	H17····O14, H17′····O14′, H17″····O14″, H17′····O10,
18	20-y	H16″····O10′, H17″····O8′
19	22	H15····O14, H15′····O14′ , H15″····O14″, H16′····O8,
20	22-y	H17′····O10, H17″····O10′, H16″····O8′
21	23	H15····O14, H17′····O14′ , H15″····O14, H16′····O8″,
22	23-y	H16····O12′, H17″····O10′, H16″····O8′
23	25	H17····O14, H15′····O14′, H15″····O14″, H17′····O10,
24	25-y	H16″····O10′, H17″····O8′
25	28	H17····O14, H15′····O14′, H15″····O14″, H17′····O10,
26	28-y	H16″····O8′, H17′····O10″
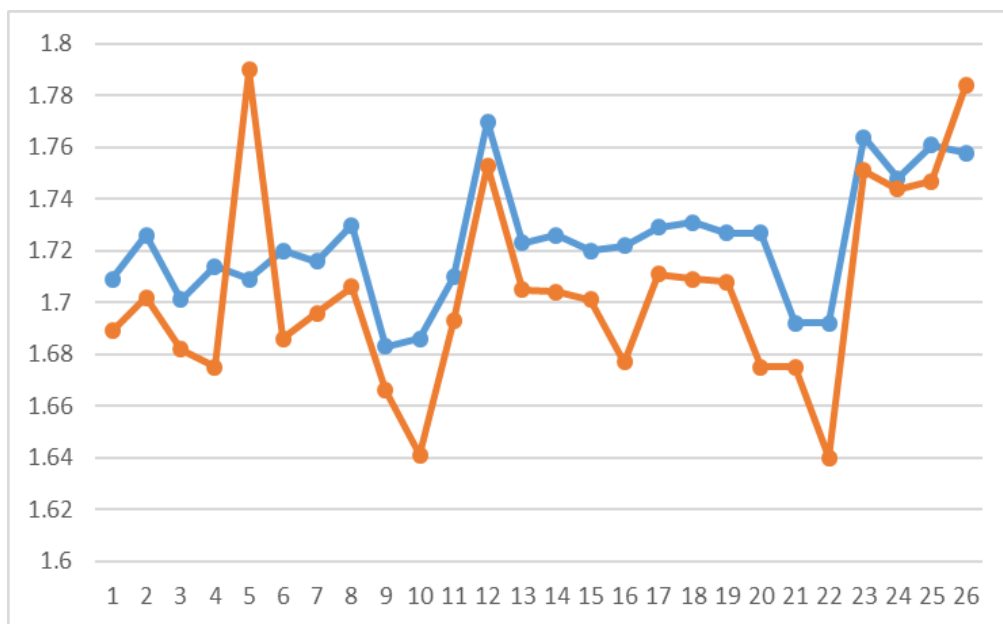
conformers, denoted by numbers

a)   3)   **H16····O12′ IMHB**

number on x axis	conformer	other IHBs in the conformer
1	1	H15····O14, H17′····O14′, H17″····O14″, H16′····O8,
2	1-y	H16″····O10′, H15′····O12″
3	2	H15····O14, H17′····O14′, H15″····O14″, H16′····O8,
4	2-y	H17″····O10′, H15′····O10″
5	4	H15····O14, H17′····O14′, H17″····O14″, H10′····O8,
6	4-y	H16″····O10′, H15′····O12″
7	5	H15····O14, H17′····O14′ , H15″····O14″, H16′····O8,
8	5-y	H16″····O10′, H15′····O10″
9	9	H15····O14, H17′····O14′, H17″····O14″, H16′····O8,
10	9-y	H16″····O10′, H15′····O12″
11	12	H15····O14, H17′····O14′, H15″····O14″, H16′····O8,
12	12-y	H17″····O10′, H16″····O8′
13	14	H17····O14, H15′····O14′, H17″····O14″, H16′····O8,
14	14-y	H16″····O10′, H15′····O12″
15	23	H15····O14, H17′····O14′ , H15″····O14, H16′····O8″,
16	23-y	H17″····O10′, H16″····O8′

conformers, denoted by numbers

b) **Molecules whose lowest energy conformer contains the following IHBs: H15····O14, H17′····O14′, H17″····O14″, H16′····O8, H16····O12′, H16″····O10′, H15′····O12″.**

The molecules and the conformers of their lowest energy pair are denoted by numbers of the x axis, according to the following table:

molecule	conformer	number on x axis	molecule	conformer	number on x axis
T1	1	1	T10	1	9
	1-y	2		1-y	10
T7	1	3	T10-M5,3″-ET6,2″,6″	1	11
	1-y	4		1-y	12
T9	1	5	T11-ET6,2″	1	13
	1-y	6		1-y	14
T9-M5,3″	1	7	T11-M5,3″-ET6,2″	1	15
	1-y	8		1-y	16

b) **1)** **length of the H15····O14 first IHB**
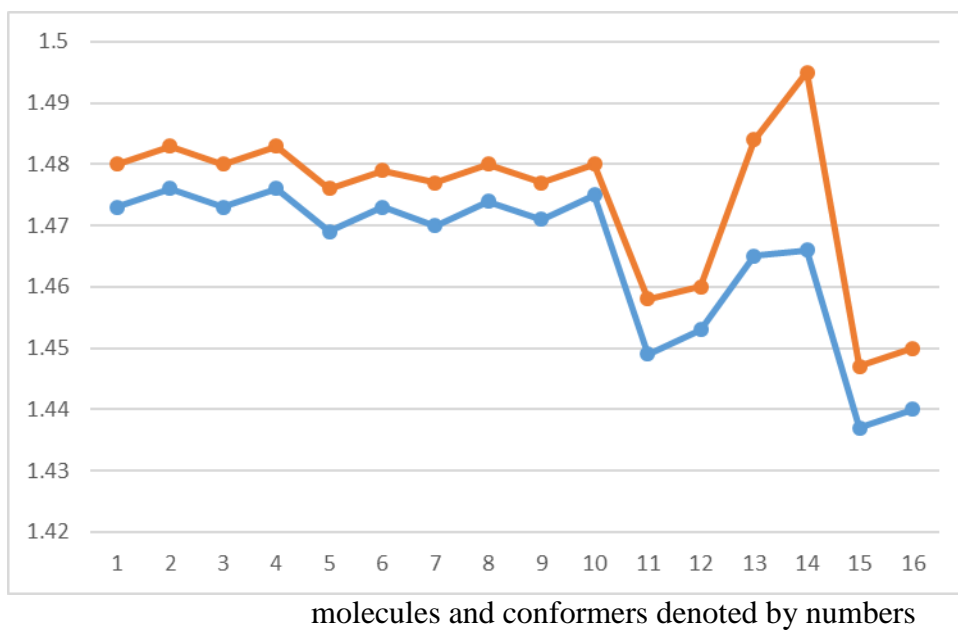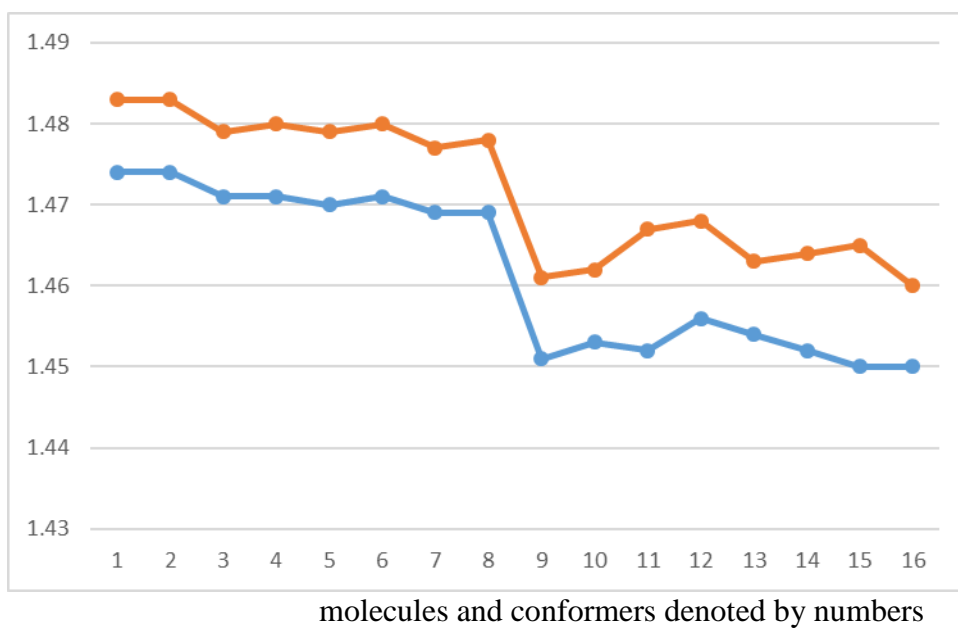
molecules and conformers denoted by numbers

b) **2)** **length of the H17′····O14′ first IHB**

molecules and conformers denoted by numbers

b)   3)   length of the H17″····O14′ first IHB

molecules and conformers denoted by numbers

b)   4)   length of the H16′····O8 IMHB

molecules and conformers denoted by numbers

b) 5) length of the H16····O12′ IMHB

molecules and conformers denoted by numbers

b) 6) length of the H16″····O10′ IMHB

molecules and conformers denoted by numbers
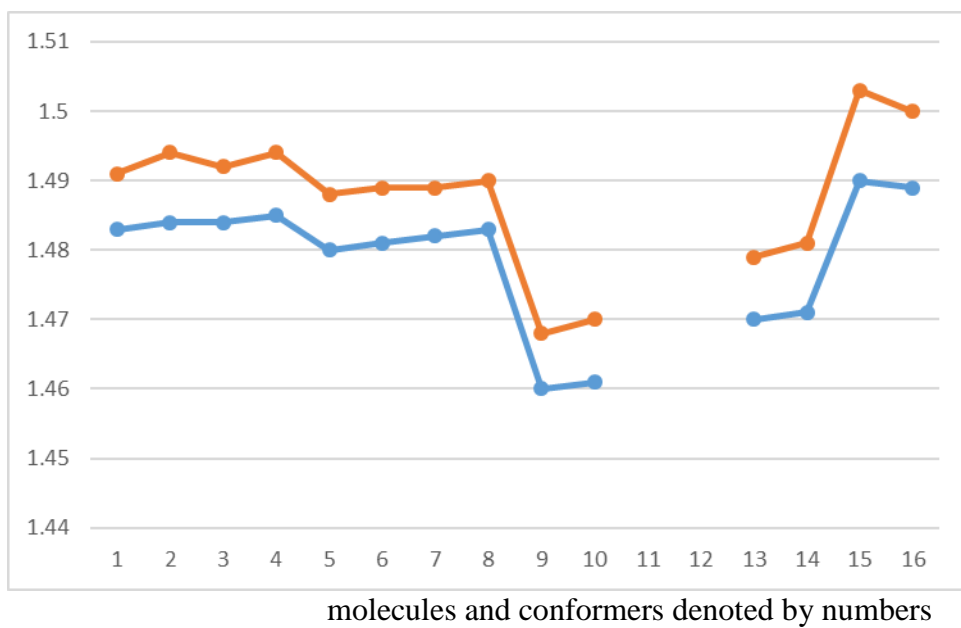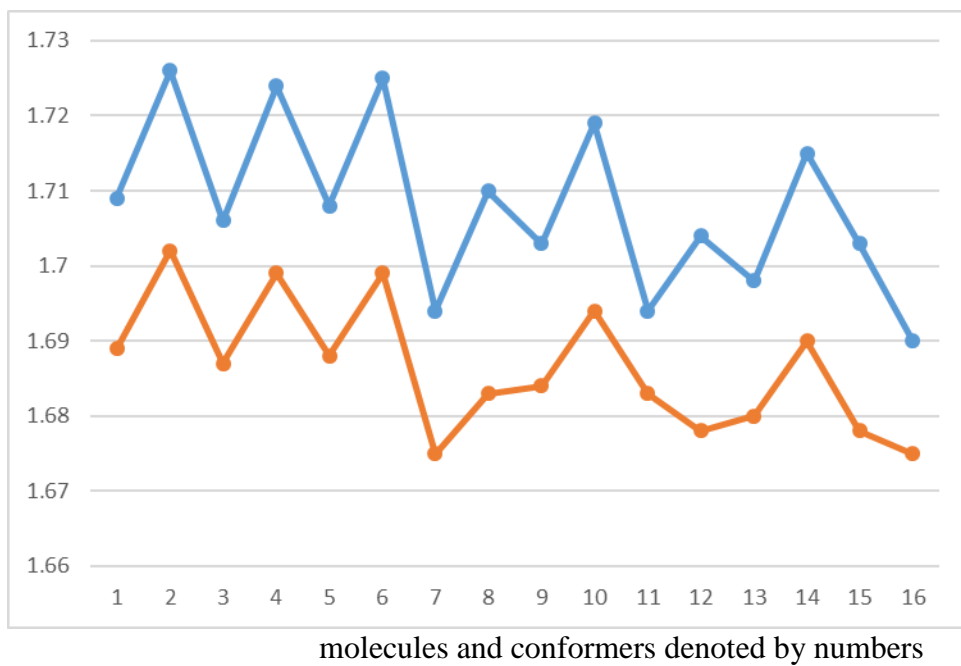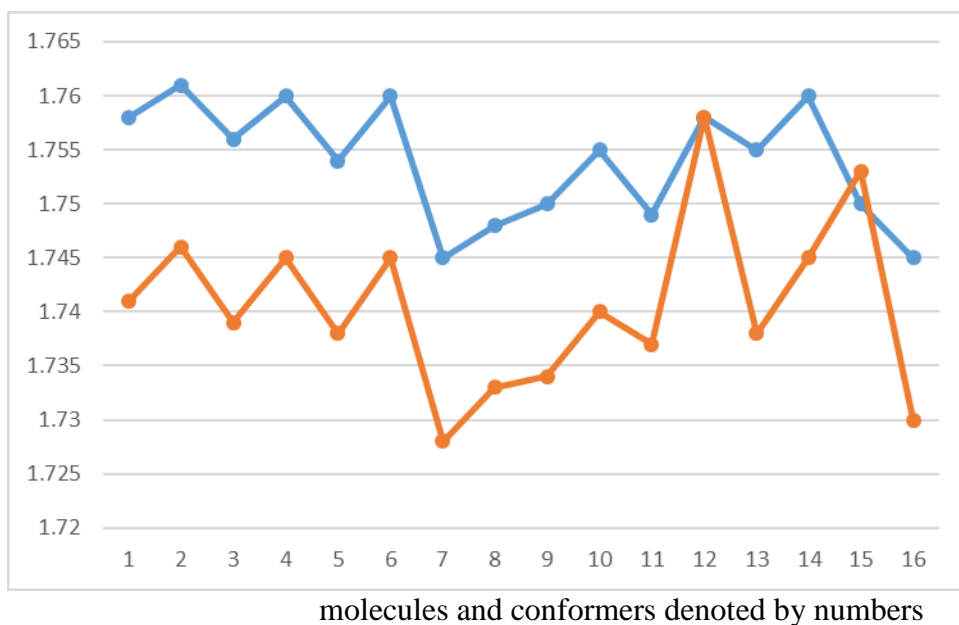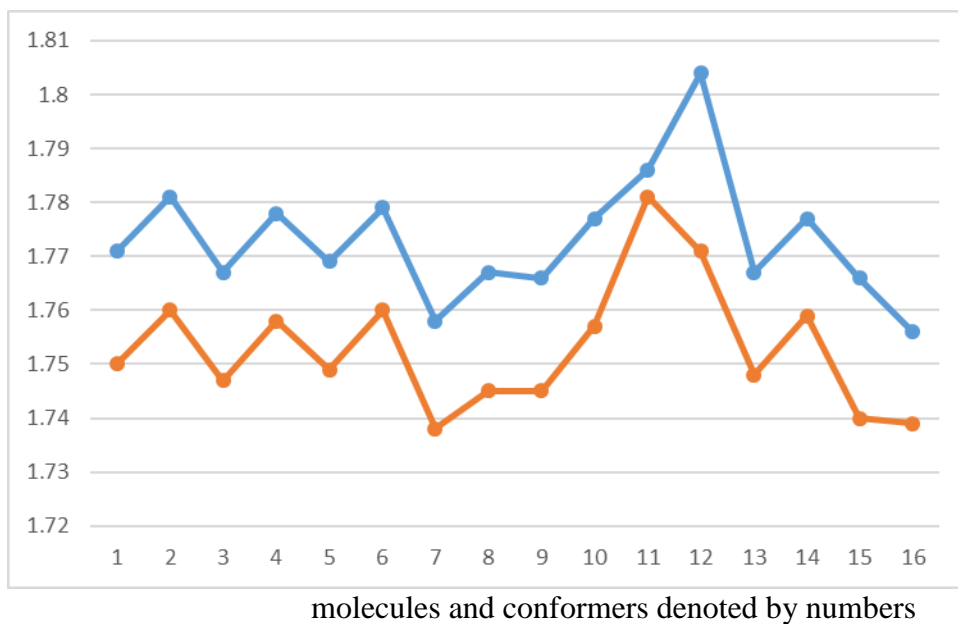
b) **7)** **length of the H15′···· O12″ IMHB**

molecules and conformers denoted by numbers
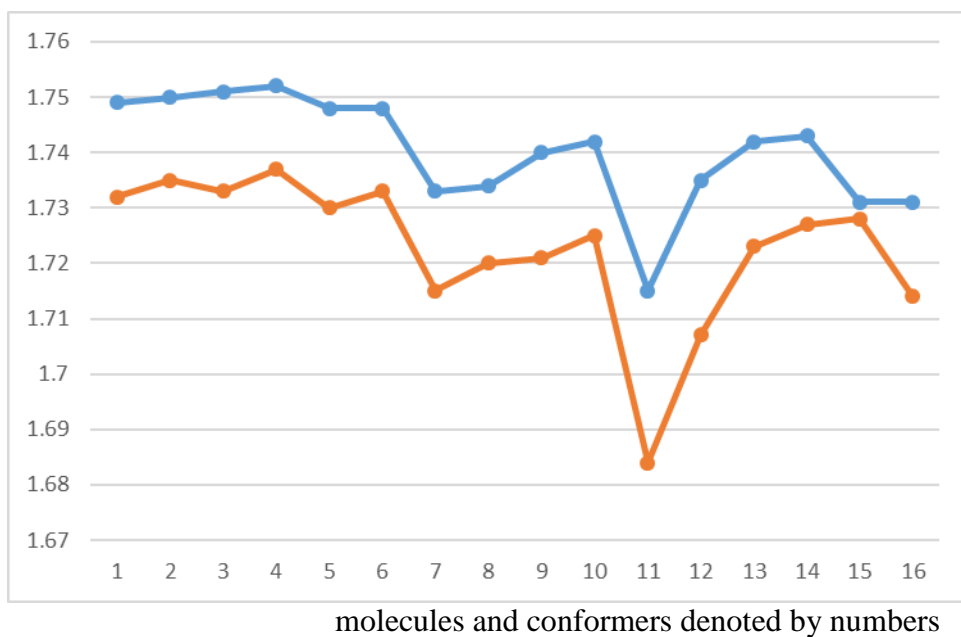
c) **Molecules in which the OH at C6″ is replaced by a keto O. The lowest energy conformer pair contain the following IHBs:** **H15····O14,** **H15′····O14′, H15″····O14″, H17′····O8, H16····O10′, H16″····O8′, H16′····O12″.**
The molecules and the conformers of their lowest energy pair are denoted by numbers on the x axis, according to the following table:

molecule	conformer	number on x axis
T7-KT6″-M5,3″,3″	1	1
	1-y	2
T8-KT6″-M5,3″,3″	1	3
	1-y	4
T9-KT6″-M5,3″,3″	1	5
	1-y	6
T12-KT6″-M5,3″,3″	1	7
	1-y	8

c) 1) length of the H15····O14 first IHB
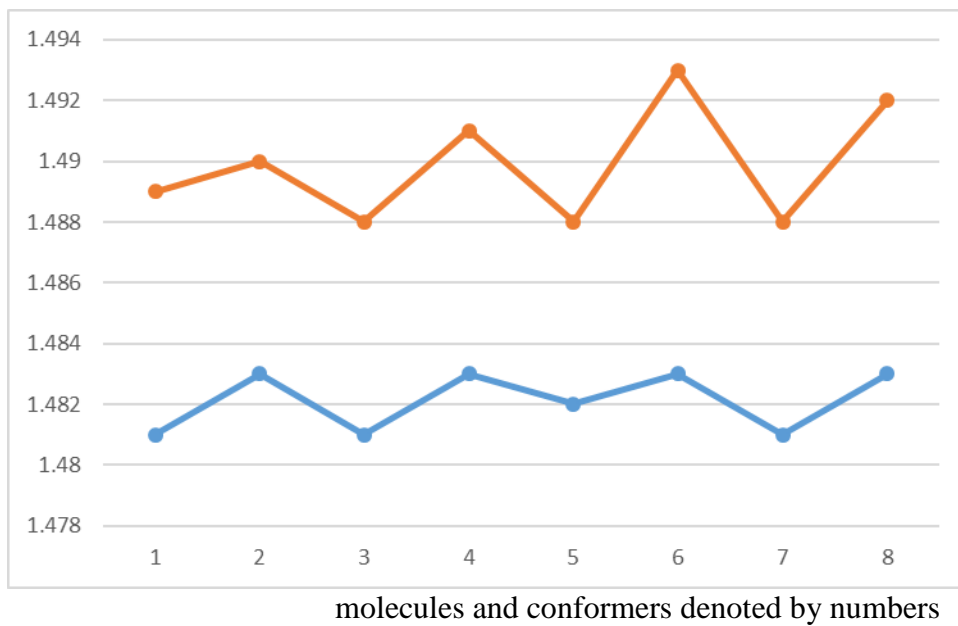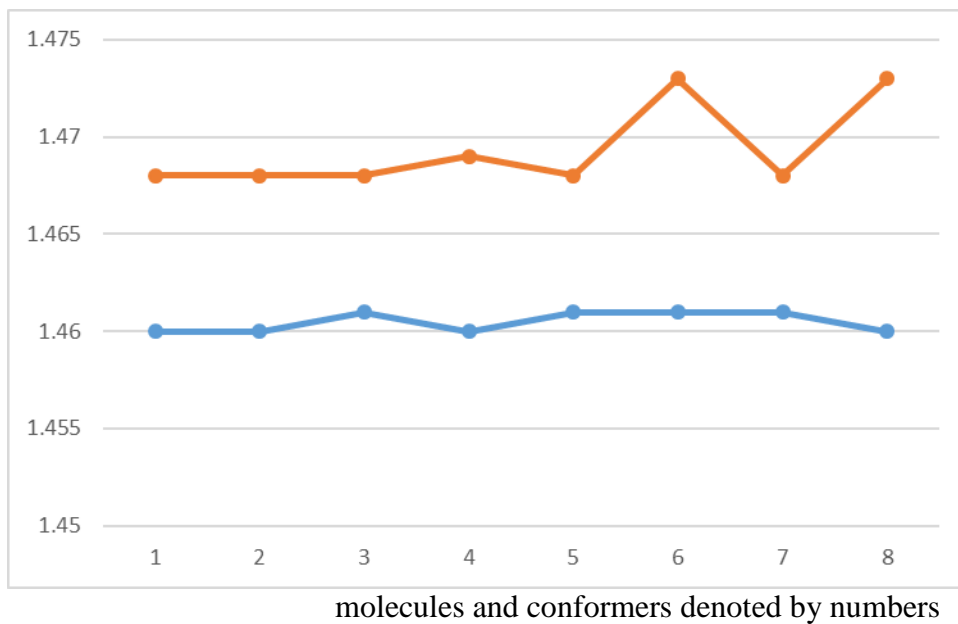
molecules and conformers denoted by numbers

c) 2) length of the H15′····O14′ first IHB

molecules and conformers denoted by numbers

c) 3) length of the H15″····O14″ first IHB

molecules and conformers denoted by numbers

c) 4) length of the H17′····O8 IMHB

molecules and conformers denoted by numbers

c) **5)** **length of the H16····O10′ IMHB**

molecules and conformers denoted by numbers

c) **6)** **length of the H16″····O8′ IMHB**

molecules and conformers denoted by numbers

c)   7)   length of the H16′····O12″ IMHB

molecules and conformers denoted by numbers
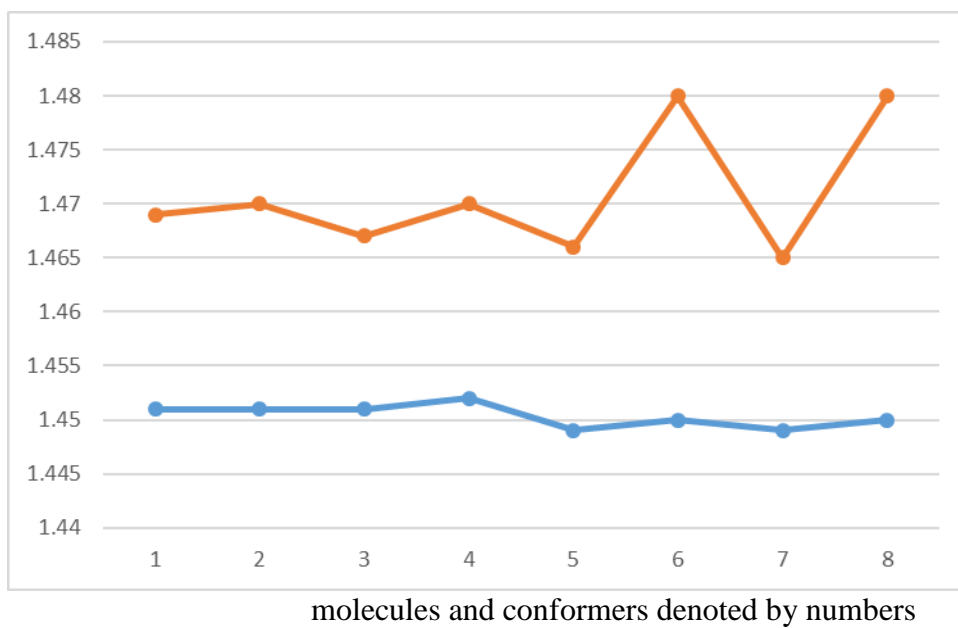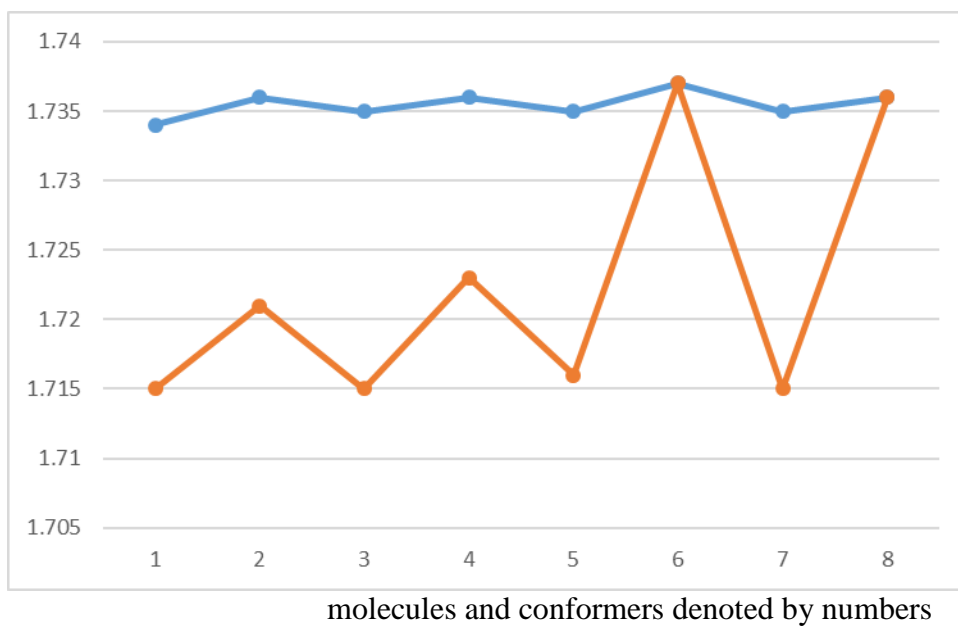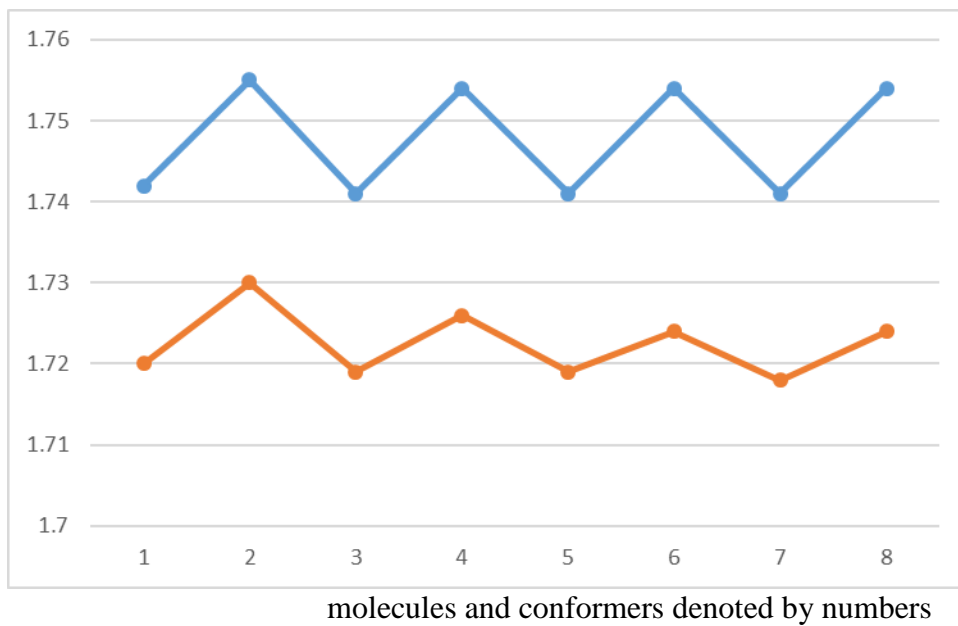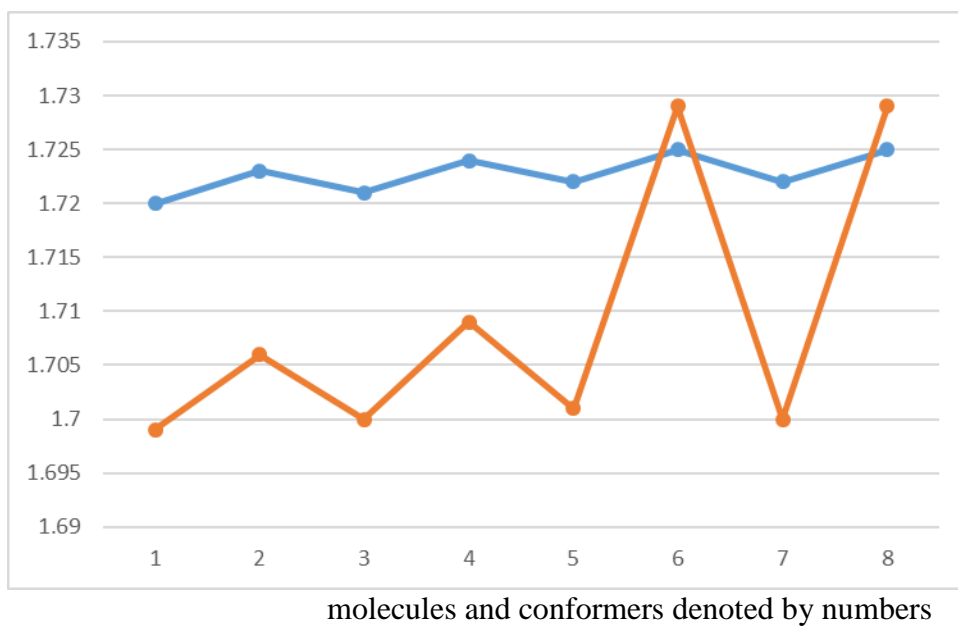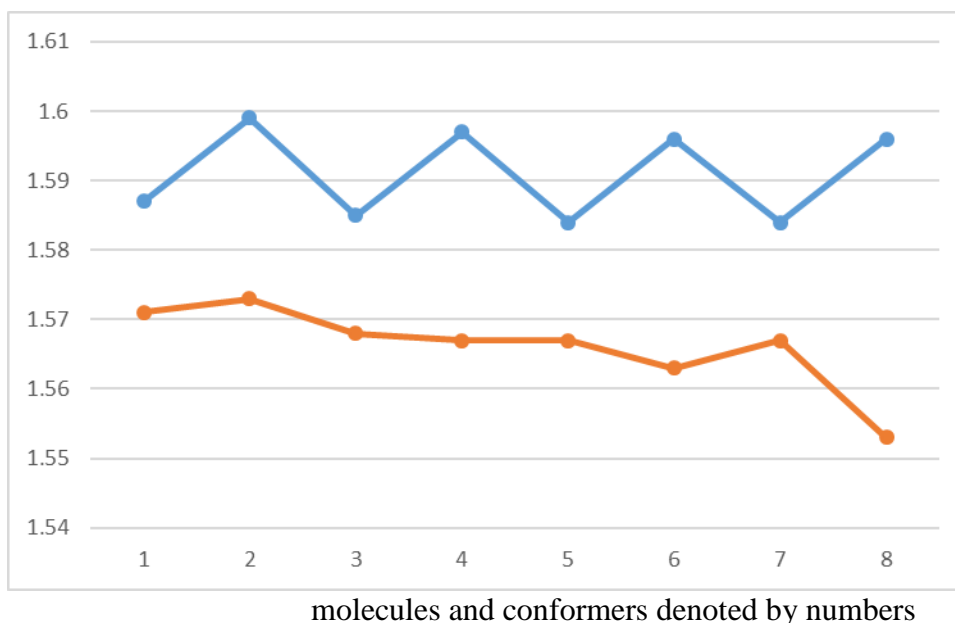
d)   Molecules in which the OHs at C2 and C6″ are replaced by keto O. The lowest energy conformer pair contain the following IHBs: H15····O14,   H15′····O14′, H15″····O14″, H17′····O8, H16····O10′, H16″····O8′, H16′····O12″.

The molecules and the conformers of their lowest energy pair are denoted by numbers on the x axis, according to the following table:

molecule	conformer	number on x axis
T2-KT2,6″-M5,5,3″,3″	1	1
	1-y	2
T4-KT2,6″-M5,5,3″,3″	1	3
	1-y	4
T5-KT2,6″-M5,5,3″,3″	1	5
	1-y	6
T7-KT2,6″-M5,5,3″,3″	1	7
	1-y	8
T8-KT2,6″-M5,5,3″,3″	1	9
	1-y	10
T9-KT2,6″-M5,5,3″,3″	1	11
	1-y	12
T10-KT2,6″-M5,5,3″,3″	1	13
	1-y	14

d)   1)   length of the H15····O14 first IHB
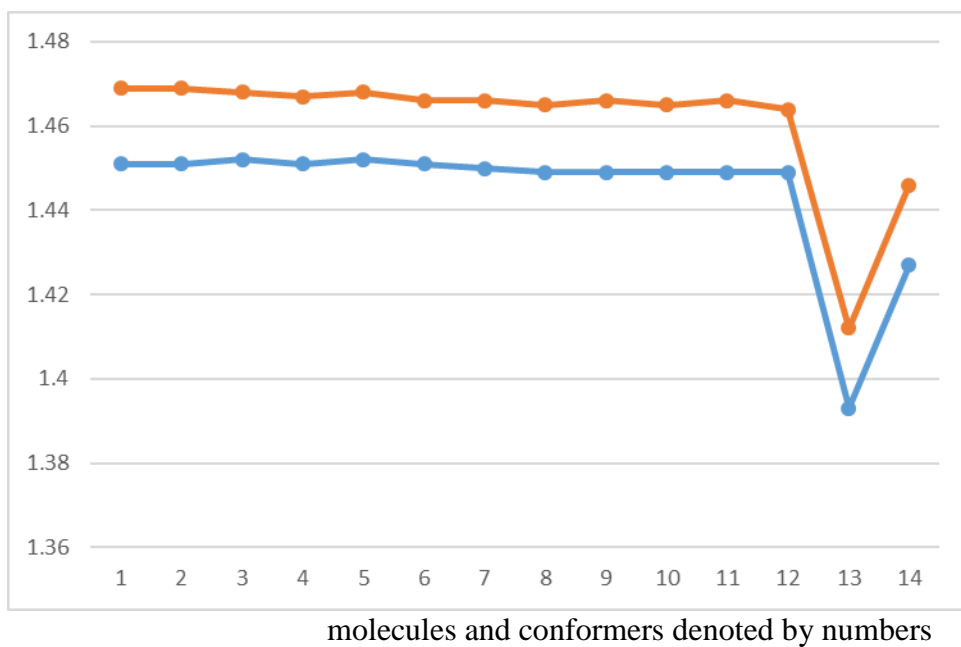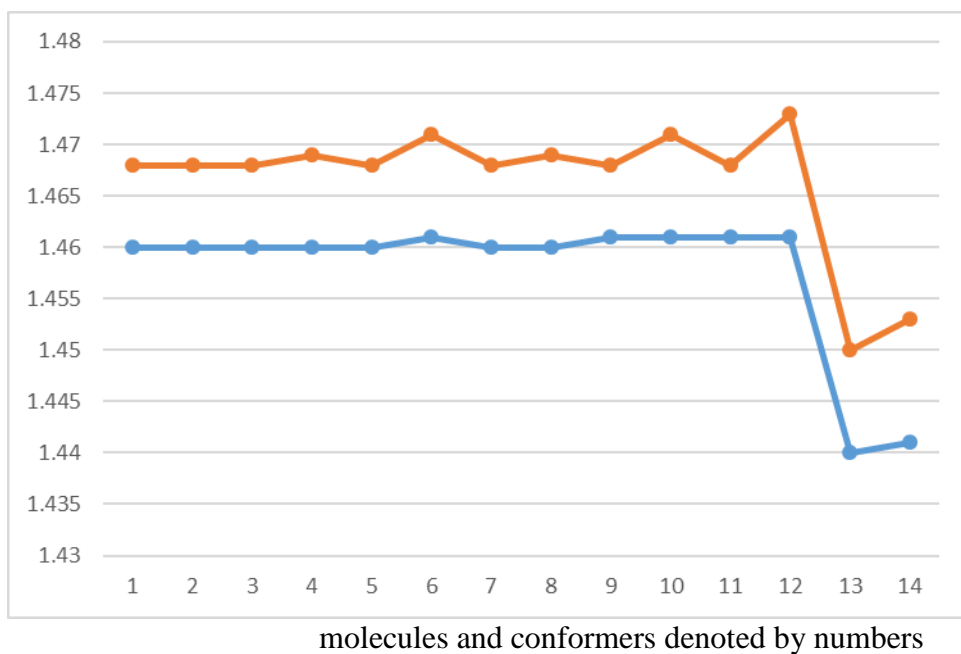
molecules and conformers denoted by numbers

d)   2)   length of the H15′····O14′ first IHB

molecules and conformers denoted by numbers

d) **3)** **length of the H15″····O14″ first IHB**

molecules and conformers denoted by numbers

d) **4)** **length of the H17′····O8 IMHB**

molecules and conformers denoted by numbers

d) 5) length of the H16····O10′ IMHB

molecules and conformers denoted by numbers

d) 6) length of the H16″····O8′ IMHB

molecules and conformers denoted by numbers

d) **7)** **length of the H16′····O12″ IMHB**

molecules and conformers denoted by numbers
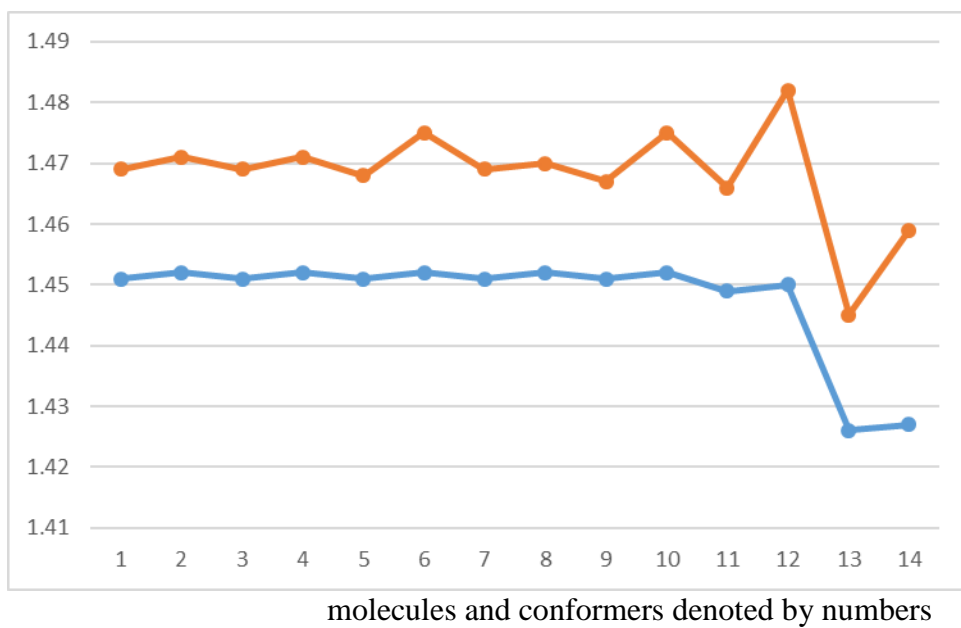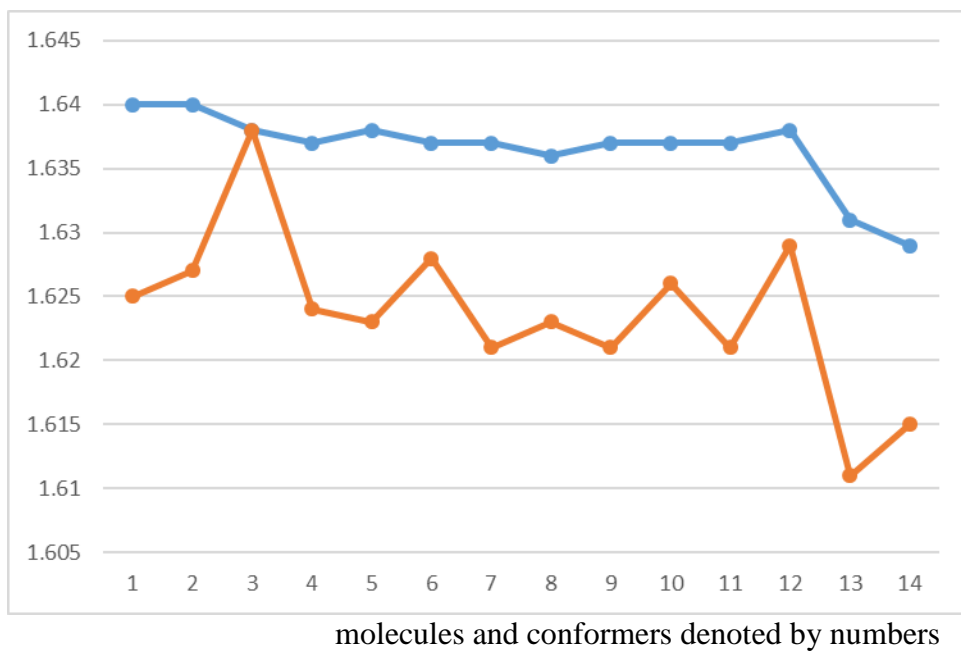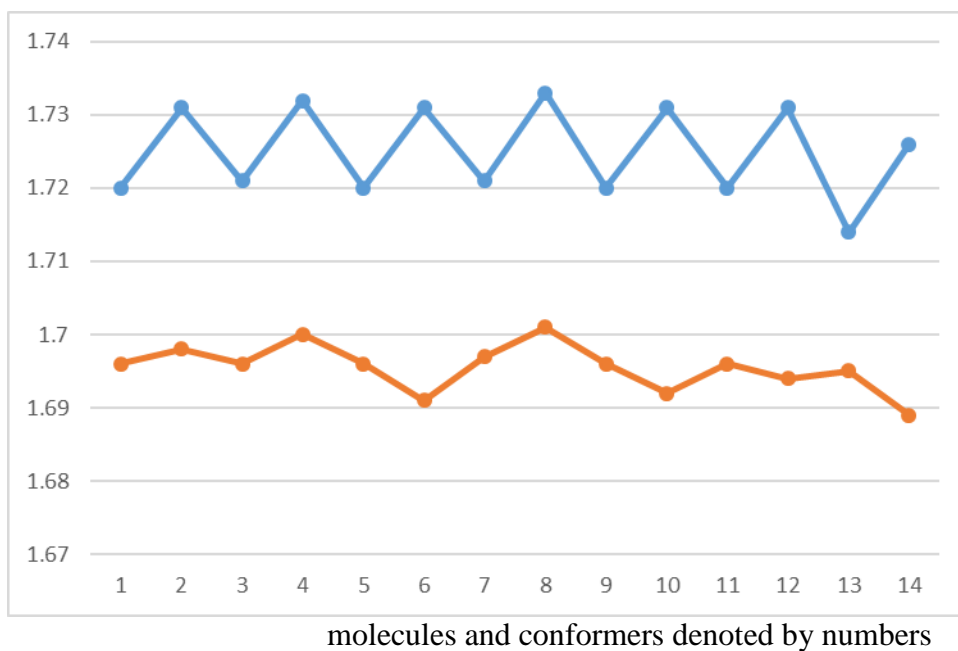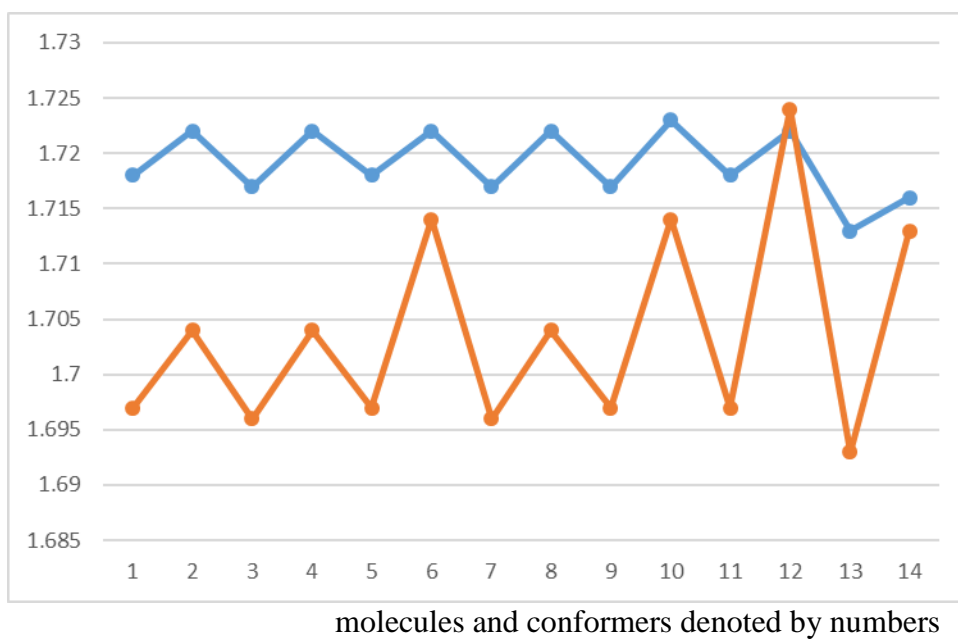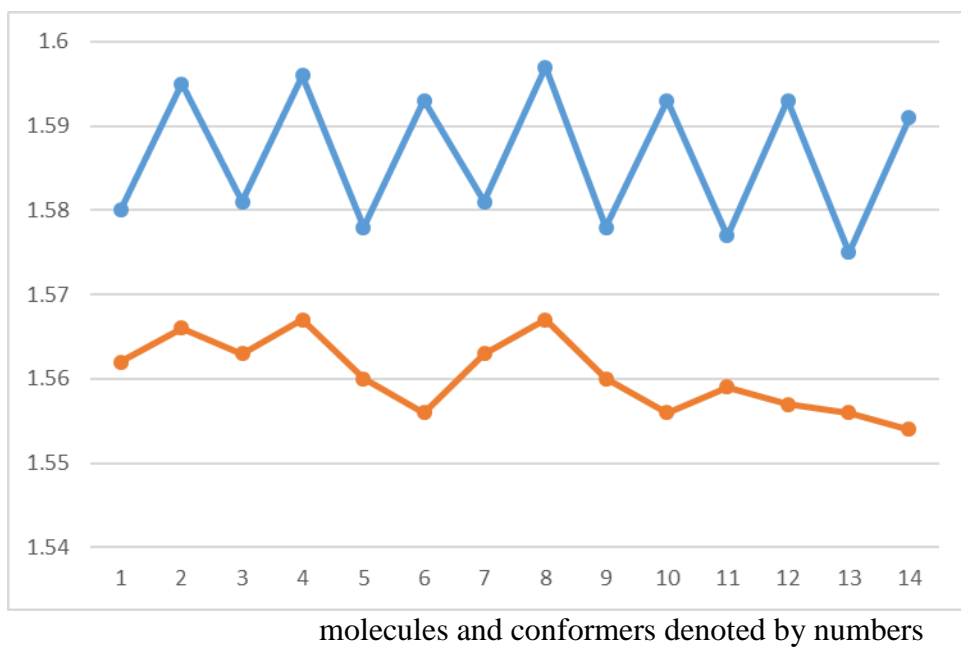
Figure S 10

C−H···O intramolecular hydrogen bonds in trimeric acylphloroglucinols.

The T4-KT2,6″-M5,5,3″,3″-1 conformer is selected as an example for illustration purposes.

The C−H···O intramolecular hydrogen bonds (IHBs) are indicated by blue segments. The molecule is viewed from different sides, to highlight all the C−H···O IHBs present.
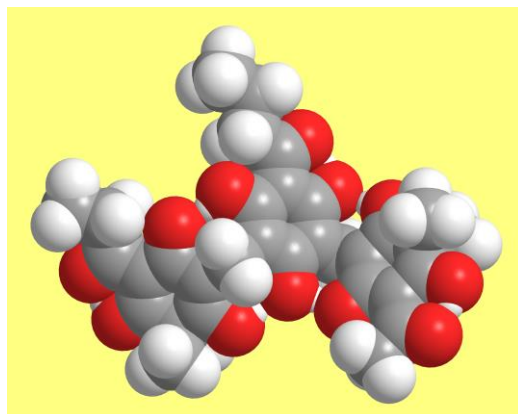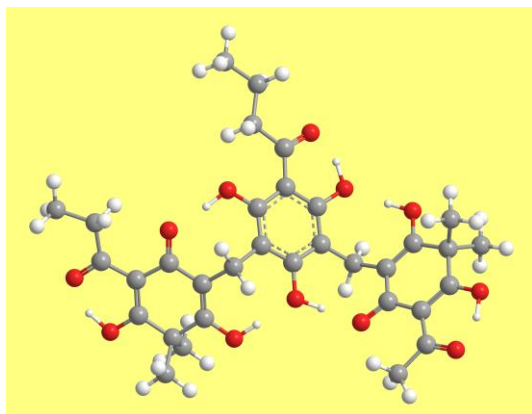
Molecular structure of T4-KT2,6″-M5,5,3″,3″ shown through the geometry of its lowest energy conformer.
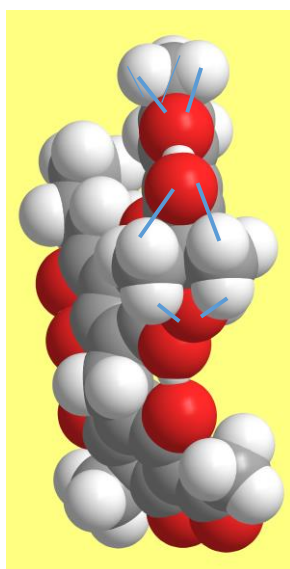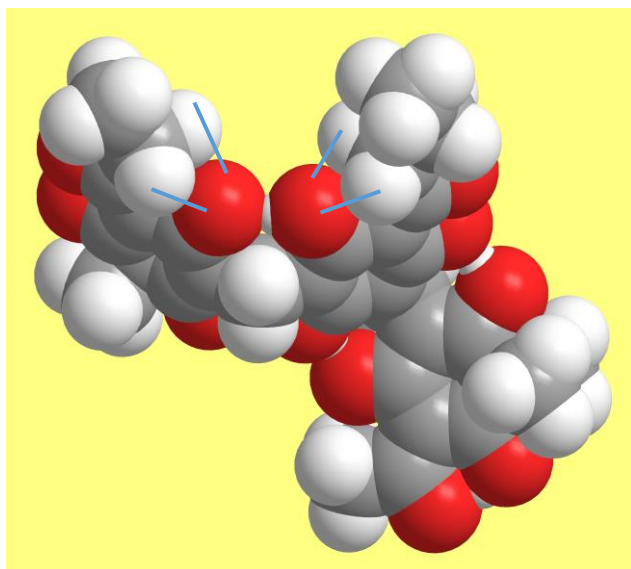
(a)   (b)

a)   View from the outer side of the first monomer.
        The H atoms attached to the second C atom of the R chain act as donors to O14 (H19$_a$····O14 and H19$_b$····O14). One H atom from each of the methyl groups at C5 acts as donor to O12 (H11$_a$····O12 and H11$_b$····O12); another H atom from each of the methyl groups at C5 acts as donor to O10 (H11$_c$····O10 and H11$_d$····O10).
b)   View of the part between the first and the second monomer in the upper rim.

The H atoms attached to the first C atom of the R chain act as donors to O8 (H13$_a$····O8 and H13$_b$····O8). The H atoms attached to the first C atom of the R′ chain act as donors to O12′ (H13$_a$′····O12′ and H13$_b$′····O12′).
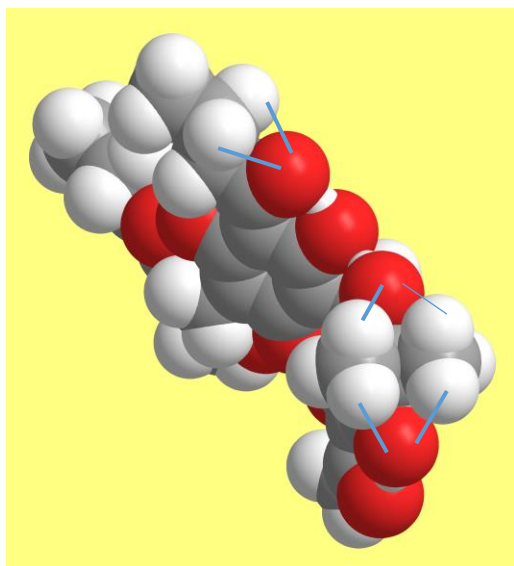
(c)
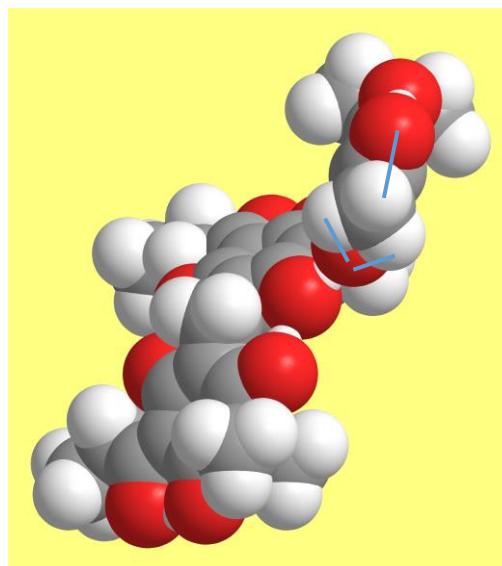
(d)

c)   View of the part between the second and the third monomer in the upper rim.
     The H atoms attached to the second C atom of the R′ chain act as donors to O14′ (H19$_a$′····O14′ and H19$_b$′····O14′). One H atom from each of the methyl groups at C5″ acts as donor to O10″ (H9$_c$″····O10″ and H9$_d$″····O10″). Another H atom from each of the methyl groups at C5″ acts as donor to O8″ (H9$_a$″····O8″ and H9$_b$″····O8″).
d)   View from the outer side of the third monomer, towards the bottom rim.
     One of the H atoms attached to the first C atom of the R″ chain acts as donor to O14 (H13$_a$″····O14″), the other two act as donors to O12″ (H13$_b$″····O12″ and H13$_c$″····O12″).

Table S 1
Common names, natural occurrence and medicinal properties of the naturally occurring trimeric acylphloroglucinols considered in this study

Acronym denoting the molecule in this work	Common name	Natural occurrence	Medicinal properties
T2-KT2,6″-M5,5,3″,3″	filixic acid ABA	*Dryopteris* species	against influenza
T3-M5,3″-ET6,2″	agrimol E	*Agrimonia pilosa*	
T4-KT2,6″-M5,5,3″,3″	filixic acid ABP	*Dryopteris* species	
T5-KT6″-M3″,3″-ET6	trisdesaspidin BPB	*Dryopteris subimpressa*	
T5-KT2,6″-M5,5,3″,3″	filixic acid PBP	*Dryopteris* species	
T6-M5,5′-ET6,4′	triaemulin BAB (trisaspidinol BAB)	*Dryopteris aemula, Dryopteris inequalis, Dryopteris erythrosora*	
T7-M5,3″-ET6,2″	agrimol F	*Agrimonia pilosa*	antimicrobial, antimalarial
T7-KT6″-M5,3″,3″	trisflavaspidic acid ABB	*Dryopteris austriaca, Dryopteris villarii, Dryopteris aitoniana*	
T7-KT2,6″-M5,5,3″,3″	filixic acid ABB	*Dryopteris* species	nematocidal, antihelmintic
T8-KT6″-M5,3″,3″	trisparaspidin PBB	*Dryopteris remota*	
T8-KT2-M5,5,3″	trisparaspidin BBP	*Dryopteris remota*	
T8-KT2,6″-M5,5,3″,3″	filixic acid PBB	*Dryopteris* species	
T9-M5,5′	trisabbreviatin BBB	*Dryopteris abbreviata*	
T9-M5,3″-ET6,2″	agrimol C	*Agrimonia pilosa*	antimicrobial, antimalarial
T9-M5,3″-ET6,4″	triaemulin ABB (trisaspidinol ABB)	*Dryopteris aemula, Dryopteris inequalis, Dryopteris erythrosora*	
T9-KT6″-M5,3″,3″	trisflavaspidic acid BBB (trisparaspidin BBB)	*Dryopteris austriaca, Dryopteris villarii, Dryopteris aitoniana*	
T9-KT6″-M5,3″,3″-ET6	triaspidin	*Dryopteris austriaca,*	
T9-KT6″-M3″,3″-ET4	trisdesaspidin BBB	*Dryopteris austriaca, Dryopteris caucasica,*	

T9-KT2,6″-M5,5,3″,3″	filixic acid BBB	*Dryopteris* species	
T10-KT2,6″-M5,5, 3″,3″	japonicin D	*Hypericum japonicum* *Agrimonia pilosa*	antimicrobial, antimalarial
T10-M5,3″-ET6,2″,6″	protokosin	*Hagenia abyssinica*	antihelmintic, anticancer
T10-KT2,6″-M5,5, 3″,3″	japonicin D	*Hypericum japonicum*	
T11-M5,3″-ET6,2″	agrimol D	*Agrimonia pilosa*	
T12-KT2-M5,5,3″	trisparaspidin VBB	*Dryopteris remota*	
T12-KT6″-M5,3″,3″	trisparaspidin BBV	*Dryopteris remota*	
T13-M5,3″-ET6,2″	agrimol B	*Agrimonia pilosa*	anticancer
T14-M5,3″-ET6,2″	agrimol A	*Agrimonia pilosa*	

Table S 2
Molecular formulas of the calculated trimeric acylphloroglucinols

acronym denoting the molecular structure	formula	acronym denoting the molecular structure	formula
T1	$C_{26}H_{24}O_{12}$	T9-M5,3″-ET6,2″	$C_{36}H_{44}O_{12}$
T2-KT2,6″-M5,5,3″,3″	$C_{32}H_{36}O_{12}$	T9-M5,3″-ET6,4″	$C_{36}H_{44}O_{12}$
T3-ET6,2″	$C_{31}H_{34}O_{12}$	T9-KT6″-M5,3″,3″	$C_{35}H_{42}O_{12}$
T3-M5,3″-ET6,2″	$C_{33}H_{38}O_{12}$	T9-KT6″-M3″,3″-ET4	$C_{35}H_{42}O_{12}$
T4-KT2,6″-M5,5,3″,3″	$C_{33}H_{38}O_{12}$	T9-KT6″-M5,3″,3″-ET6	$C_{36}H_{44}O_{12}$
T5-KT6″-M3″,3″-ET4	$C_{33}H_{38}O_{12}$	T9-KT2,6″-M5,5,3″,3″	$C_{36}H_{44}O_{12}$
T5-KT2,6″-M5,5,3″,3″	$C_{34}H_{40}O_{12}$	T10	$C_{32}H_{36}O_{12}$
T6-M5,3″-ET6,4″	$C_{34}H_{40}O_{12}$	T10-ET6,2″	$C_{34}H_{40}O_{12}$
T7	$C_{30}H_{32}O_{12}$	T10-M5,3″-ET6,2″	$C_{36}H_{44}O_{12}$
T7-ET6,2″	$C_{32}H_{36}O_{12}$	T10-M5,3″-ET6,2″,6″	$C_{37}H_{46}O_{12}$
T7-M5,3″-ET6,2″	$C_{34}H_{40}O_{12}$	T10-KT2,6″-M5,5,3″,3″	$C_{36}H_{44}O_{12}$
T7-KT6″-M5,3″,3″	$C_{33}H_{38}O_{12}$	T11-ET6,2″	$C_{33}H_{38}O_{12}$
T7-KT2,6″-M5,5,3″,3″	$C_{34}H_{40}O_{12}$	T11-M5,3″-ET6,2″	$C_{35}H_{42}O_{12}$
T8-KT6″-M5,3″,3″	$C_{34}H_{40}O_{12}$	T12-KT2-M5,5,3″	$C_{36}H_{44}O_{12}$
T8-KT2-M5,5,3″	$C_{34}H_{40}O_{12}$	T12-KT6″-M5,3″,3″	$C_{36}H_{44}O_{12}$
T8-KT2,6″-M5,5,3″,3″	$C_{35}H_{42}O_{12}$	T13-ET6,2″	$C_{35}H_{42}O_{12}$
T9	$C_{32}H_{36}O_{12}$	T13-M5,3″-ET6,2″	$C_{37}H_{46}O_{12}$
T9-M5,3″	$C_{34}H_{40}O_{12}$	T14-ET6,2″	$C_{35}H_{42}O_{12}$
T9-ET6,2″	$C_{34}H_{40}O_{12}$	T14-M5,3″-ET6,2″	$C_{37}H_{46}O_{12}$

Table S 3
Viable combinations of monomers' conformer types in trimeric acylphloroglucinols.
Each combination corresponds to a viable conformer for trimeric acylphloroglucinols (T-ACPL).
Monomer combinations are considered viable if they enable the formation of two hydrogen
bonds between each pair of monomers, on either side of the methylene bridge joining them.
The combinations of monomers' geometries differ by the mutual orientations of the monomers
(identified in terms of positions of the acyl chains with respect to each other), by the geometries
of the individual monomers and by the mutual orientations of the methylene bridges.
The mutual positions of the acyl chains are conventionally indicated as *up* or *down*, starting from
the monomer conventionally taken as 'first monomer', whose orientation is taken as *up*. For T-
ACPLs with different R chains in the outer monomers (R ≠ R″), the 'first monomer' is taken as
the outer monomer with the longer R.
The conformers of individual monomers are denoted with the same symbols utilized in the study
of monomeric acylphloroglucinols [4−6] and summarized in figure 3.
The T-ACPL conformers are numbered on the basis of their most recurrent positions in the
increasing relative energy sequence.
The mutual orientations of the two methylene bridges give origin to outstretched-shaped
geometries if they are oriented in opposite ways and to half-bowl-shaped geometries if they are
oriented in the same way; the latter are identified by adding the letter *y* to the number denoting
the conformer. Since the other geometry aspects (conformations of individual monomers and
mutual orientations of the acyl chains) are the same for such pairs of conformers, the table reports
only the conformers' numbers and the geometry aspects corresponding to each number. Both
shapes corresponding to each number are shown in figures S1, S2, S4, S5 and S6.

a) **Combinations when no phenol OH is replaced by other functions**
The geometries are illustrated in figure S1.

number denoting the conformer	conformations of individual monomers			mutual orientations of the acyl chains		
	first monomer	second monomer	third monomer	first monomer	second monomer	third monomer
1	d-r	s-w	s-w	up	down	down
2	d-r	s-w	d-r	up	down	up
3	d-r	d-r	d-r	up	up	up
4	d-r-u	s-w	s-w	up	down	down
5	d-r-u	s-w	d-r	up	down	up
6	s-w	d-r	d-r	up	down	down
7	d-r-u	d-r	d-r	up	up	up
8	d-r	s-w	d-r-u	up	down	down
9	d-r-u	s-w	s-w-u	up	down	down
10	d-r	d-r	d-w-u	up	up	down

11	d-w	d-w	d-w	up	up	up
12	d-r	s-w-u	d-w	up	down	up
13	s-w	s-w	d-w-u	up	up	up
14	d-r-u	s-w	d-w-u	up	down	down
15	d-w	d-w	d-w	up	up	down
16	d-r-u	d-r	d-r-u	up	up	down
17	d-w	d-w	d-w	up	down	down
18	d-w	d-r	d-w	up	down	up
19	d-w-u	d-w	d-w	up	up	up
20	d-w-u	d-w	d-w	up	down	down
21	d-w-u	d-w	d-w	up	up	down
22	d-w-u	d-w	d-w	up	down	up
23	d-r-u	s-w-u	d-w	up	down	up
24	d-r-u	s-w-u	d-w	up	down	down
25	s-w-u	d-w	d-w	up	down	down
26	s-w	d-w-u	d-w	up	up	down
27	s-w-u	d-w	d-w	up	up	up
28	s-w-u	d-w	d-w	up	down	up
29	s-w-u	d-w	d-w	up	up	down

b)   Combination when the OH at C6 and C2″ are replaced by OCH₃ functions

One combination is viable and is numbered as 1. (additional explanation in fig. S3).

number denoting the conformer	conformations of individual monomers			mutual orientations of the acyl chains		
	first monomer	second monomer	third monomer	first monomer	second monomer	third monomer
1	d-r	d-r	s-w	up	up	down

c) **Combination when the OH at C6 and C4″ are replaced by OCH₃ functions**
One combination is viable and is numbered as 1. Different geometries of the bowl-shaped conformer (1-y) arise according to whether the OCH₃ groups are oriented towards the concave (inner) or the convex (outer) side of the bowl.

number denoting the conformer	conformations of individual monomers			mutual orientations of the acyl chains		
	first monomer	second monomer	third monomer	first monomer	second monomer	third monomer
1	d-r	d-r	d-r	up	up	up

d) **Combinations when the OH at C6″ is replaced by a keto O.**
The conformers' numbering is independent of the one shown in table (a), because different (and fewer) combinations of monomeric conformers are possible, due to the presence of the keto O at C6″, i.e., in a position concerned with the first IHB and with the intermonomer H-bonds. The combinations are shown in fig. S5.

number denoting the conformer	conformations of individual monomers			mutual orientations of the acyl chains		
	first monomer	second monomer	third monomer	first monomer	second monomer	third monomer
1	d-r	d-r	d-w	up	up	down
2	d-r	s-w	d-w	up	down	down
3	s-w	d-r	d-w	up	down	up
4	s-w	s-w	d-w	up	up	up
5	s-r	d-r-u	d-w	up	down	up
6	s-r	d-r-u	d-w	up	up	down
7	s-r	s-r	d-r	up	up	up
8	s-r	s-r	d-r	up	down	down
9	s-r	s-r	d-r	up	up	down
10	s-r	s-r	d-r	up	down	up

e) **Combinations when the OH at C2 is replaced by a keto O.**
Similarly to case (d), the conformers' numbering is independent of the one shown in table (a) because different (and fewer) combinations of monomeric conformers are possible, due to the presence of the keto O at C2, i.e., in a position concerned with the first IHB and with an intermonomer H-bond. They mostly reflect situations symmetric to those included in table (d). The geometries are illustrated in fig. S5.

number denoting the conformer	conformations of individual monomers			mutual orientations of the acyl chains		
	first monomer	second monomer	third monomer	first monomer	second monomer	third monomer
1	s-r	s-w	s-w	up	down	down
2	s-r	d-r	s-w	up	up	down
3	s-r	s-w	d-r	up	down	up
4	s-r	d-r	d-r	up	up	up
5	s-r	s-w-u	d-w	up	down	up
6	s-r	s-w-u	d-w	up	down	down
7	s-w	d-w	d-w	up	up	up
8	s-w	d-w	d-w	up	up	down
9	s-r	s-w	d-r	up	down	up
10	s-w	d-w	d-w	up	down	up

f) **Combination when the OHs at C2 and C6″ are both replaced by keto O**
One combination is viable and is numbered as 1.

number denoting the conformer	conformations of individual monomers			mutual orientations of the acyl chains		
	first monomer	second monomer	third monomer	first monomer	second monomer	third monomer
1	s-r	d-r	d-w	up	up	down

g) **Combination when the OH at C6″ is replaced by a keto O and the OH at C4 is replaced by a CH₃O group.**

One combination is viable and is numbered as 1.

number denoting the conformer	conformations of individual monomers			mutual orientations of the acyl chains		
	first monomer	second monomer	third monomer	first monomer	second monomer	third monomer
1	s-w	s-w	d-w	up	up	up

Table S 4

Relative energies of the calculated conformers of trimeric acylphloroglucinols.

The table reports the HF/6-31G(d,p), HF/6-31+G(d,p), DFT/B3LYP/6-31+G(d,p), and DFT/B3LYP/6-31+G(d,p) with the Grimme' corrections results, respectively denoted as HF, HF+, DFT and DFT-D3 in the column headings.

For each molecule, the conformers are listed in order of increasing relative energy in the DFT/B3LYP/6-31+G(d,p) results.

Two different tables are presented, respectively grouping the molecules according to their acyl groups or according to their other substituents.

a)   The molecules are grouped according to their acyl groups

conformers	relative energy (kcal/mol)			
	HF	HF+	DFT	DFT-D3
structure T1				
1	0.000	0.000	0.000	0.000
1-y	0.282	0.285	0.325	0.093
2	2.477	2.470	3.432	2.844
2-y	2.580	2.530	3.545	3.469
3	2.630	2.657	3.766	3.843
3-y	2.667	2.711	3.794	3.604
4	5.220	5.358	3.858	3.843
4-y	5.462	5.591	4.166	3.868
5	7.686	7.821	7.281	7.301
6	5.223	5.218	7.366	7.429
5-y	7.792	7.874	7.375	6.480
7	7.688	7.793	7.424	7.447
7-y	7.755	7.884	7.450	7.257
8	8.154	8.151		
8-y	8.336	8.339	7.465	7.106
6-y	5.367	5.389	7.496	7.160
9	10.381	10.585	7.585	7.554
10-y	8.918	8.920	7.717	7.141
10	8.434	8.486	7.768	7.737
9-y	10.506	10.714	7.813	7.471
11-y	8.532	8.502	10.381	10.015
12-y	10.926	10.961	10.598	9.566
12	10.962	10.859	10.685	10.669
13	10.690	10.712	11.006	10.959
13-y	10.801	10.864	11.053	10.755
14	13.323	13.458	11.073	11.030

14-y	13.425	13.544	11.180	10.795
15-y	9.342	9.356	11.278	10.884
16-y	13.990	14.076	11.310	10.712
16	13.449	13.578	11.386	11.339
11	9.563	9.450	11.571	11.737
17-y	9.677	9.597	11.608	11.360
18-y	9.879	9.597	11.869	10.961
17	10.079	9.871	11.946	12.121
15	10.143	10.097	12.100	12.258
19-y	12.557	12.671	13.131	12.831
18	10.344	10.192	12.199	12.348
20-y	13.093	13.126	13.777	13.483
21-y	13.317	13.438	13.946	13.608
22-y	13.367	13.448	14.074	11.810
19	13.391	13.395	14.119	14.279
23-y	15.782	15.825	14.276	12.134
20	13.708	13.661	14.304	14.469
23	16.071	16.286	14.432	14.399
22	14.010	14.019	14.594	14.734
21	13.935	13.998	14.610	14.765
24-y	16.354	16.419	14.757	14.425
24	16.734	16.827	14.827	14.867
25-y	14.307	14.452	15.447	13.171
26	14.864	14.843	15.983	15.991
27-y	15.334	15.491	16.033	15.671
26-y	14.965	14.960	16.049	15.701
25	15.285	15.304	16.507	16.633
28-y	15.581	15.333	16.598	14.442
29	16.280	16.467	16.809	16.942
29-y	15.958	16.225	16.831	16.482
28	15.876	15.961	17.100	17.146
27	15.756	15.880	17.246	17.363
structure T2-KT2,6″-M5,5,3″,3″				
1	0.000	0.000	0.000	0.172
1-y	0.391	0.392	0.385	0.000
structure T3-ET6,2″				
1	0.158	0.000	0.000	0.154
1-y	0.000	0.200	0.485	0.000
structure T3-M5,3″-ET6,2″				
1	0.030	0.015	0.000	0.329
1-y	0.000	0.000	0.028	0.000

structure T4-KT2,6″-M5,5,3″,3″				
1	0.000	0.000	0.000	0.177
1-y	0.389	0.389	0.383	0.000
structure T5-KT2,6″-M5,5,3″,3″				
1	0.000	0.000	0.000	0.330
1-y	0.387	0.384	0.370	0.000
structure T5-KT6″-M3″,3″-ET2″				
1	0.000	0.004	0.000	0.454
1-y	0.017	0.000	0.086	0.000
structure T6-M5,3″-ET6,4″				
3	0.000	0.000	0.000	0.195
3-y-out-out	0.209	0.195	0.141	0.000
3-y-in-out	0.220	0.184	0.190	0.030
3-y-in-in	3.310	4.231	4.737	2.823
structure T7				
1	0.000	0.000	0.000	0.000
1-y	0.280	0.285	1.007	0.331
2	2.439	2.460	3.467	3.419
2-y	2.534	2.500	3.626	1.852
4	4.997	5.106	3.636	3.509
3	2.600	2.621	3.837	3.834
3-y	2.636	2.671	3.863	3.584
4-y	5.235	5.337	3.946	3.516
5	7.419	7.551	7.001	6.867
5-y	7.491	7.580	7.121	5.435
6	5.299	5.270	7.372	7.317
6-y	5.220	5.317	7.448	6.199
structure T7-ET6,2″				
1	0.000	0.000	0.000	0.000
1-y	0.296	0.307	0.347	0.046
structure T7-M5,3″-ET6,2″				
1	0.000	0.000	0.000	0.188
1-y	0.201	0.181	0.279	0.000
structure T7-KT6″-M5,3″,3″				
1	0.000	0.000	0.000	0.219
1-y	0.260	0.306	0.287	0.000
2	0.433	0.498	0.610	0.816
2-y	0.623	0.664	0.898	0.612

3	2.003	2.007	2.911	3.077
3-y	2.276	2.282	3.226	1.275
4	2.884	2.968	4.168	4.373
4-y	2.950	3.054	4.311	4.088
5	10.137	10.104	10.196	10.216
5-y	9.896	9.828	10.249	8.521
6	10.570	10.582	10.510	9.925
6-y	10.662	10.644	10.602	10.698
7-y	12.073	11.902	14.387	12.814
7	13.251	13.016	15.573	15.611
8-y	12.948	12.698	15.114	12.780
9-y	13.161	13.044	15.141	13.766
10-y	13.341	13.085	15.474	13.043
9	13.594	13.282	15.595	15.707
10	13.698	13.426	15.732	15.777
8	13.743	13.556	15.982	15.980
structure T7-KT2,6″-M5,5,3″,3″				
1	0.000	0.000	0.000	0.140
1-y	0.390	0.391	0.384	0.000
structure T8-KT6″-M5,3″,3″				
1	0.000	0.000	0.000	0.324
1-y	0.268	0.307	0.249	0.000
2	0.436	0.502	0.574	0.882
2-y	0.627	0.668	0.860	0.694
3	1.998	1.996	2.856	3.118
3-y	2.281	2.267	3.242	0.981
4	2.878	2.956	4.108	4.418
4-y	2.941	3.039	4.252	4.127
5	10.092	9.962	10.086	10.186
5-y	9.844	9.765	10.179	7.885
6-y	10.423	10.375	10.400	9.517
6	10.644	10.548	10.508	10.705
7-y	11.986	11.836	14.203	12.742
9-y	13.288	12.964	14.931	13.121
8-y	12.858	12.584	14.931	12.718
10-y	13.132	12.922	15.319	11.967
9	13.479	13.183	15.386	15.595
7	13.163	12.939	15.428	15.518
10	13.585	13.296	15.552	15.657
8	13.653	13.438	15.791	15.885
structure T8-KT2-M5,5,3″				
1	0.000	0.000	0.000	0.670

1-y	0.262	0.305	0.274	0.000
2	0.440	0.460	0.538	1.232
2-y	0.630	0.665	0.834	1.049
3-y	3.807	3.784	3.060	1.272
4	2.188	2.155	4.039	4.727
3	3.571	3.584	4.041	3.568
4-y	2.923	2.932	4.135	4.427
5	10.090	9.981	10.056	10.571
5-y	10.291	9.742	10.165	8.747
6-y	10.372	10.321	10.399	9.376
6	10.635	10.442	10.460	11.078
7-y	11.970	11.731	14.173	13.017
9-y	13.031	12.867	14.803	13.004
8-y	12.841	12.564	14.875	13.816
9	13.453	13.075	15.279	15.894
7	13.130	12.824	15.317	15.848
8	13.667	13.462	15.770	16.282
10-y	14.872	14.603	16.453	12.839
10	15.169	14.859	16.749	16.064
structure T8-KT2,6″-M5,5,3″,3″				
1	0.000	0.000	0.000	0.336
1-y	0.387	0.422	0.373	0.000
structure T9				
1	0.000	0.000	0.000	0.000
1-y	0.275	0.280	0.319	0.020
2	2.509	2.516	3.452	3.401
4	4.994	5.103	3.632	3.506
2-y	2.599	2.581	3.655	1.229
3	2.672	2.708	3.810	3.805
3-y	2.710	2.763	3.836	3.555
4-y	5.228	5.328	3.933	3.501
5	7.487	7.605	7.067	6.888
5-y	7.553	7.631	7.252	4.307
6	5.859	5.349	7.419	7.370
6-y	5.360	5.391	7.503	6.181
structure T9-M5,3″				
1	0.000	0.000	0.000	0.134
1-y	0.225	0.216	0.266	0.000
2	1.998	2.028	2.866	2.936
2-y	2.073	2.029	3.067	0.657
3	2.247	2.251	3.323	3.437
3-y	2.269	2.309	3.356	3.084

4	4.626	4.738	3.654	3.687
4-y	4.837	4.935	3.934	3.564
6	4.282	4.292	6.240	6.287
6-y	4.323	4.365	6.358	4.689
5	6.598	6.707	6.479	6.446
5-y	6.656	6.658	6.687	3.754
structure T9-ET6,2″				
1	0.000	0.000	0.000	0.000
1-y	0.293	0.299	0.346	0.025
structure T9-M5,3″-ET6,2″				
1	0.000	0.000	0.000	0.195
1-y	0.199	0.176	0.279	0.000
structure T9-M5,3″-ET6,4″				
3	0.000	0.000	0.000	0.150
3-y	0.210	0.195	0.186	0.000
3-y-in-out	0.218	0.183		0.030
3-y-in-in	3.294	4.216	4.738	2.773
structure T9-KT6″-M5,3″,3″				
1	0.000	0.000	0.000	0.672
1-y	0.261	0.352	0.266	0.000
2	0.439	0.545	0.544	1.196
2-y	0.630	0.711	0.868	1.040
3	1.996	2.035	2.853	3.452
4	2.878	2.995	4.070	4.725
4-y	2.941	3.037	4.210	4.431
3-y	2.756	2.854	4.268	1.817
6-y	11.266	11.341	11.730	10.476
5	11.424	11.406	11.914	12.378
6	11.485	11.467	11.948	12.575
5-y	11.265	11.238	12.251	9.837
7-y	11.961	11.806	14.162	13.040
9-y	12.961	12.968	14.865	13.019
8-y	12.831	12.594	14.899	12.981
9	13.451	13.194	15.349	15.900
7	13.136	12.950	15.391	15.858
10	13.555	13.338	15.465	15.931
8	13.645	13.484	15.794	16.220
10-y	12.933	12.893	15.949	13.576
structure T9-KT6″-M3″,3″-ET2″				
1	0.000	0.004	0.000	0.457

1-y	0.017	0.000	0.085	0.000
structure T9-KT6″-M5,3″,3′-ET2″				
1	0.000	0.000	0.000	0.000
1-y	0.182	0.157	0.530	0.043
structure T9-KT2,6″-M5,5,3″,3′				
1	0.000	0.000	0.000	0.962
1-y	0.383	0.387	0.380	0.000
structure T10				
1	0.000	0.067	0.000	0.001
1-y	0.380	0.447	0.275	0.000
2-y	2.414	2.441	3.744	1.651
4	4.492	4.658	3.784	3.600
2	2.564	2.594	3.831	3.544
3-y	2.577	2.627	3.987	3.671
3	2.748	2.752	4.030	3.870
4-y	4.572	4.744	4.303	3.702
5-y	6.996	7.071	7.582	5.565
5	7.152	7.296	7.720	7.283
6-y	5.204	5.140	7.926	6.011
6	5.304	5.316	7.942	7.667
structure T10-ET6,2″				
1	0.000	0.000	0.000	0.000
1-y	0.568	0.547	0.303	0.032
structure T10-M5,3″-ET6,2″				
1	0.030	0.026	0.000	0.000
1-y	0.000	0.000	0.569	0.089
structure T10-M5,3″-ET6,2″,6″				
1	0.000	0.000	0.000	0.000
1-y	6.983	6.809	0.728	0.486
structure T10-KT2,6″-M5,5,3″,3′				
1-y	0.549	0.000	0.000	0.000
1	0.000	4.410	3.800	4.632
structure T11-ET6,2″				
1	0.080	0.000	0.000	0.000
1-y	0.000	0.511	0.388	0.062
structure T11-M5,3″-ET6,2″				
1	0.000	0.000	0.000	0.000

1-y	0.566	0.514	0.508	0.007

structure T12-KT2-M5,5,3″

1	0.000	0.000	0.000	0.930
1-y	0.263	0.307	0.272	0.000
2	0.439	0.497	0.575	1.485
2-y	0.629	0.663	0.865	1.280
3	1.994	1.987	2.851	3.699
4	2.876	2.945	4.107	5.018
4-y	2.939	3.030	4.238	4.677
3-y	3.656	3.734	4.590	0.880
6-y	11.255	11.276	11.699	10.453
5	11.413	11.338	11.904	12.599
6	11.475	11.402	11.926	12.812
5-y	11.250	11.135	12.232	9.894
7-y	11.947	11.739	14.154	13.262
9-y	12.940	12.882	14.872	12.956
8-y	12.816	12.569	14.876	13.248
9	13.430	13.120	15.309	16.150
7	13.120	12.882	15.360	16.083
10	13.534	13.265	15.439	16.155
10-y	12.856	12.731	15.507	11.633
8	13.609	13.416	15.761	16.440

structure T12-KT6″-M5,3″,3″

1	0.000	0.000	0.000	0.688
1-y	0.261	0.306	0.267	0.000
2	0.438	0.462	0.581	1.250
2-y	0.629	0.629	0.869	1.041
3	2.003	1.961	2.865	3.469
3-y	2.279	2.181	3.260	0.155
4	2.882	2.961	4.079	4.746
4-y	2.944	2.965	4.255	4.456
6-y	11.277	11.275	11.793	10.531
5	11.437	11.341	11.947	12.386
6	11.497	11.404	11.971	12.612
5-y	11.591	11.626	12.262	9.136
7-y	11.970	11.787	14.205	13.062
8-y	12.842	12.523	14.916	12.548
9-y	12.971	12.903	14.928	13.042
9	13.461	13.130	15.371	15.937
7	13.145	12.883	15.415	15.899
10	13.569	13.279	15.549	15.966
8	13.640	13.428	15.813	16.254
10-y	13.262	13.294	15.831	12.683

structure T13-ET6,2″				
1	0.000	0.000	0.000	0.000
1-y	0.295	0.300	0.355	0.023
structure T13-M5,3″-ET6,2″				
1	0.000	0.000	0.000	0.203
1-y	0.200	0.180	0.281	0.000
structure T14-ET6,2″				
1	0.000	0.000	0.000	0.000
1-y	0.502	0.482	0.614	0.513
structure T14-M5,3″-ET6,2″				
1	0.000	0.000	0.000	0.027
1-y	0.551	0.502	0.505	0.000

b)   The molecules are grouped according to their other substituents

conformers	relative energy (kcal/mol)			
	HF	HF+	DFT	DFT-D3
structure T1				
1	0.000	0.000	0.000	0.000
1-y	0.282	0.285	0.325	0.093
2	2.477	2.470	3.432	2.844
2-y	2.580	2.530	3.545	3.469
3	2.630	2.657	3.766	3.843
3-y	2.667	2.711	3.794	3.604
4	5.220	5.358	3.858	3.843
4-y	5.462	5.591	4.166	3.868
5	7.686	7.821	7.281	7.301
6	5.223	5.218	7.366	7.429
5-y	7.792	7.874	7.375	6.480

7	7.688	7.793	7.424	7.447
7-y	7.755	7.884	7.450	7.257
8	8.154	8.151		
8-y	8.336	8.339	7.465	7.106
6-y	5.367	5.389	7.496	7.160
9	10.381	10.585	7.585	7.554
10-y	8.918	8.920	7.717	7.141
10	8.434	8.486	7.768	7.737
9-y	10.506	10.714	7.813	7.471
11-y	8.532	8.502	10.381	10.015
12-y	10.926	10.961	10.598	9.566
12	10.962	10.859	10.685	10.669
13	10.690	10.712	11.006	10.959
13-y	10.801	10.864	11.053	10.755
14	13.323	13.458	11.073	11.030
14-y	13.425	13.544	11.180	10.795
15-y	9.342	9.356	11.278	10.884
16-y	13.990	14.076	11.310	10.712
16	13.449	13.578	11.386	11.339
11	9.563	9.450	11.571	11.737
17-y	9.677	9.597	11.608	11.360
18-y	9.879	9.597	11.869	10.961
17	10.079	9.871	11.946	12.121
15	10.143	10.097	12.100	12.258
19-y	12.557	12.671	13.131	12.831
18	10.344	10.192	12.199	12.348
20-y	13.093	13.126	13.777	13.483
21-y	13.317	13.438	13.946	13.608
22-y	13.367	13.448	14.074	11.810
19	13.391	13.395	14.119	14.279
23-y	15.782	15.825	14.276	12.134
20	13.708	13.661	14.304	14.469
23	16.071	16.286	14.432	14.399
22	14.010	14.019	14.594	14.734
21	13.935	13.998	14.610	14.765
24-y	16.354	16.419	14.757	14.425
24	16.734	16.827	14.827	14.867
25-y	14.307	14.452	15.447	13.171
26	14.864	14.843	15.983	15.991
27-y	15.334	15.491	16.033	15.671
26-y	14.965	14.960	16.049	15.701
25	15.285	15.304	16.507	16.633
28-y	15.581	15.333	16.598	14.442
29	16.280	16.467	16.809	16.942
29-y	15.958	16.225	16.831	16.482

28	15.876	15.961	17.100	17.146
27	15.756	15.880	17.246	17.363
structure T7				
1	0.000	0.000	0.000	0.000
1-y	0.280	0.285	1.007	0.331
2	2.439	2.460	3.467	3.419
2-y	2.534	2.500	3.626	1.852
4	4.997	5.106	3.636	3.509
3	2.600	2.621	3.837	3.834
3-y	2.636	2.671	3.863	3.584
4-y	5.235	5.337	3.946	3.516
5	7.419	7.551	7.001	6.867
5-y	7.491	7.580	7.121	5.435
6	5.299	5.270	7.372	7.317
6-y	5.220	5.317	7.448	6.199
structure T9				
1	0.000	0.000	0.000	0.000
1-y	0.275	0.280	0.319	0.020
2	2.509	2.516	3.452	3.401
4	4.994	5.103	3.632	3.506
2-y	2.599	2.581	3.655	1.229
3	2.672	2.708	3.810	3.805
3-y	2.710	2.763	3.836	3.555
4-y	5.228	5.328	3.933	3.501
5	7.487	7.605	7.067	6.888
5-y	7.553	7.631	7.252	4.307
6	5.859	5.349	7.419	7.370
6-y	5.360	5.391	7.503	6.181
structure T10				
1	0.000	0.067	0.000	0.001
1-y	0.380	0.447	0.275	0.000
2-y	2.414	2.441	3.744	1.651
4	4.492	4.658	3.784	3.600
2	2.564	2.594	3.831	3.544
3-y	2.577	2.627	3.987	3.671
3	2.748	2.752	4.030	3.870
4-y	4.572	4.744	4.303	3.702
5-y	6.996	7.071	7.582	5.565
5	7.152	7.296	7.720	7.283
6-y	5.204	5.140	7.926	6.011
6	5.304	5.316	7.942	7.667
////////////////	////////////////	////////////////	////////////////	////////////////

	structure T9-M5,3″			
1	0.000	0.000	0.000	0.134
1-y	0.225	0.216	0.266	0.000
2	1.998	2.028	2.866	2.936
2-y	2.073	2.029	3.067	0.657
3	2.247	2.251	3.323	3.437
3-y	2.269	2.309	3.356	3.084
4	4.626	4.738	3.654	3.687
4-y	4.837	4.935	3.934	3.564
6	4.282	4.292	6.240	6.287
6-y	4.323	4.365	6.358	4.689
5	6.598	6.707	6.479	6.446
5-y	6.656	6.658	6.687	3.754
////////////////////	////////////////////	////////////////////	////////////////////	////////////////////
	structure T3-ET6,2″			
1	0.158	0.000	0.000	0.154
1-y	0.000	0.200	0.485	0.000
	structure T7-ET6,2″			
1	0.000	0.000	0.000	0.000
1-y	0.296	0.307	0.347	0.046
	structure T9-ET6,2″			
1	0.000	0.000	0.000	0.000
1-y	0.293	0.299	0.346	0.025
	structure T10-ET6,2″			
1	0.000	0.000	0.000	0.000
1-y	0.568	0.547	0.303	0.032
	structure T11-ET6,2″			
1	0.080	0.000	0.000	0.000
1-y	0.000	0.511	0.388	0.062
	structure T13-ET6,2″			
1	0.000	0.000	0.000	0.000
1-y	0.295	0.300	0.355	0.023
	structure T14-ET6,2″			
1	0.000	0.000	0.000	0.000
1-y	0.502	0.482	0.614	0.513
////////////////////	////////////////////	////////////////////	////////////////////	////////////////////
	structure T3-M5,3″-ET6,2″			

1	0.030	0.015	0.000	0.329
1-y	0.000	0.000	0.028	0.000
structure T7-M5,3″-ET6,2″				
1	0.000	0.000	0.000	0.188
1-y	0.201	0.181	0.279	0.000
structure T9-M5,3″-ET6,2″				
1	0.000	0.000	0.000	0.195
1-y	0.199	0.176	0.279	0.000
structure T10-M5,3″-ET6,2″				
1	0.030	0.026	0.000	0.000
1-y	0.000	0.000	0.569	0.089
structure T11-M5,3″-ET6,2″				
1	0.000	0.000	0.000	0.000
1-y	0.566	0.514	0.508	0.007
structure T13-M5,3″-ET6,2″				
1	0.000	0.000	0.000	0.203
1-y	0.200	0.180	0.281	0.000
structure T14-M5,3″-ET6,2″				
1	0.000	0.000	0.000	0.027
1-y	0.551	0.502	0.505	0.000
structure T10-M5,3″-ET6,2″,6″				
1	0.000	0.000	0.000	0.000
1-y	6.983	6.809	0.728	0.486
///////////////	///////////////	///////////////	///////////////	///////////////
structure T6-M5,3″-ET6,4″				
3	0.000	0.000	0.000	0.195
3-y-out-out	0.209	0.195	0.141	0.000
3-y-in-out	0.220	0.184	0.190	0.030
3-y-in-in	3.310	4.231	4.737	2.823
///////////////	///////////////	///////////////	///////////////	///////////////
structure T7-KT6″-M5,3″,3″				
1	0.000	0.000	0.000	0.219
1-y	0.260	0.306	0.287	0.000
2	0.433	0.498	0.610	0.816
2-y	0.623	0.664	0.898	0.612
3	2.003	2.007	2.911	3.077
3-y	2.276	2.282	3.226	1.275

4	2.884	2.968	4.168	4.373
4-y	2.950	3.054	4.311	4.088
5	10.137	10.104	10.196	10.216
5-y	9.896	9.828	10.249	8.521
6	10.570	10.582	10.510	9.925
6-y	10.662	10.644	10.602	10.698
7-y	12.073	11.902	14.387	12.814
7	13.251	13.016	15.573	15.611
8-y	12.948	12.698	15.114	12.780
9-y	13.161	13.044	15.141	13.766
10-y	13.341	13.085	15.474	13.043
9	13.594	13.282	15.595	15.707
10	13.698	13.426	15.732	15.777
8	13.743	13.556	15.982	15.980
structure T8-KT6″-M5,3″,3″				
1	0.000	0.000	0.000	0.324
1-y	0.268	0.307	0.249	0.000
2	0.436	0.502	0.574	0.882
2-y	0.627	0.668	0.860	0.694
3	1.998	1.996	2.856	3.118
3-y	2.281	2.267	3.242	0.981
4	2.878	2.956	4.108	4.418
4-y	2.941	3.039	4.252	4.127
5	10.092	9.962	10.086	10.186
5-y	9.844	9.765	10.179	7.885
6-y	10.423	10.375	10.400	9.517
6	10.644	10.548	10.508	10.705
7-y	11.986	11.836	14.203	12.742
9-y	13.288	12.964	14.931	13.121
8-y	12.858	12.584	14.931	12.718
10-y	13.132	12.922	15.319	11.967
9	13.479	13.183	15.386	15.595
7	13.163	12.939	15.428	15.518
10	13.585	13.296	15.552	15.657
8	13.653	13.438	15.791	15.885
structure T9-KT6″-M5,3″,3″				
1	0.000	0.000	0.000	0.672
1-y	0.261	0.352	0.266	0.000
2	0.439	0.545	0.544	1.196
2-y	0.630	0.711	0.868	1.040
3	1.996	2.035	2.853	3.452
4	2.878	2.995	4.070	4.725
4-y	2.941	3.037	4.210	4.431

3-y	2.756	2.854	4.268	1.817
6-y	11.266	11.341	11.730	10.476
5	11.424	11.406	11.914	12.378
6	11.485	11.467	11.948	12.575
5-y	11.265	11.238	12.251	9.837
7-y	11.961	11.806	14.162	13.040
9-y	12.961	12.968	14.865	13.019
8-y	12.831	12.594	14.899	12.981
9	13.451	13.194	15.349	15.900
7	13.136	12.950	15.391	15.858
10	13.555	13.338	15.465	15.931
8	13.645	13.484	15.794	16.220
10-y	12.933	12.893	15.949	13.576
structure T12-KT6″-M5,3″,3″				
1	0.000	0.000	0.000	0.688
1-y	0.261	0.306	0.267	0.000
2	0.438	0.462	0.581	1.250
2-y	0.629	0.629	0.869	1.041
3	2.003	1.961	2.865	3.469
3-y	2.279	2.181	3.260	0.155
4	2.882	2.961	4.079	4.746
4-y	2.944	2.965	4.255	4.456
6-y	11.277	11.275	11.793	10.531
5	11.437	11.341	11.947	12.386
6	11.497	11.404	11.971	12.612
5-y	11.591	11.626	12.262	9.136
7-y	11.970	11.787	14.205	13.062
8-y	12.842	12.523	14.916	12.548
9-y	12.971	12.903	14.928	13.042
9	13.461	13.130	15.371	15.937
7	13.145	12.883	15.415	15.899
10	13.569	13.279	15.549	15.966
8	13.640	13.428	15.813	16.254
10-y	13.262	13.294	15.831	12.683
structure T8-KT2-M5,5,3″				
1	0.000	0.000	0.000	0.670
1-y	0.262	0.305	0.274	0.000
2	0.440	0.460	0.538	1.232
2-y	0.630	0.665	0.834	1.049
3-y	3.807	3.784	3.060	1.272
4	2.188	2.155	4.039	4.727
3	3.571	3.584	4.041	3.568
4-y	2.923	2.932	4.135	4.427

5	10.090	9.981	10.056	10.571
5-y	10.291	9.742	10.165	8.747
6-y	10.372	10.321	10.399	9.376
6	10.635	10.442	10.460	11.078
7-y	11.970	11.731	14.173	13.017
9-y	13.031	12.867	14.803	13.004
8-y	12.841	12.564	14.875	13.816
9	13.453	13.075	15.279	15.894
7	13.130	12.824	15.317	15.848
8	13.667	13.462	15.770	16.282
10-y	14.872	14.603	16.453	12.839
10	15.169	14.859	16.749	16.064
structure T12-KT2-M5,5,3″				
1	0.000	0.000	0.000	0.930
1-y	0.263	0.307	0.272	0.000
2	0.439	0.497	0.575	1.485
2-y	0.629	0.663	0.865	1.280
3	1.994	1.987	2.851	3.699
4	2.876	2.945	4.107	5.018
4-y	2.939	3.030	4.238	4.677
3-y	3.656	3.734	4.590	0.880
6-y	11.255	11.276	11.699	10.453
5	11.413	11.338	11.904	12.599
6	11.475	11.402	11.926	12.812
5-y	11.250	11.135	12.232	9.894
7-y	11.947	11.739	14.154	13.262
9-y	12.940	12.882	14.872	12.956
8-y	12.816	12.569	14.876	13.248
9	13.430	13.120	15.309	16.150
7	13.120	12.882	15.360	16.083
10	13.534	13.265	15.439	16.155
10-y	12.856	12.731	15.507	11.633
8	13.609	13.416	15.761	16.440
/////////////////	/////////////////	/////////////////	/////////////////	/////////////////
structure T2-KT2,6″-M5,5,3″,3″				
1	0.000	0.000	0.000	0.172
1-y	0.391	0.392	0.385	0.000
structure T4-KT2,6″-M5,5,3″,3″				
1	0.000	0.000	0.000	0.177
1-y	0.389	0.389	0.383	0.000
structure T5-KT2,6″-M5,5,3″,3″				

1	0.000	0.000	0.000	0.330
1-y	0.387	0.384	0.370	0.000

structure T7-KT2,6″-M5,5,3″,3″

1	0.000	0.000	0.000	0.140
1-y	0.390	0.391	0.384	0.000

structure T8-KT2,6″-M5,5,3″,3″

1	0.000	0.000	0.000	0.336
1-y	0.387	0.422	0.373	0.000

structure T9-KT2,6″-M5,5,3″,3″

1	0.000	0.000	0.000	0.962
1-y	0.383	0.387	0.380	0.000

structure T10-KT2,6″-M5,5,3″,3″

1-y	0.549	0.000	0.000	0.000
1	0.000	4.410	3.800	4.632
///////////////////	///////////////////	///////////////////	///////////////////	///////////////////

structure T5-KT6″-M3″,3″-ET2″

1	0.000	0.004	0.000	0.454
1-y	0.017	0.000	0.086	0.000

structure T9-KT6″-M3″,3″-ET2″

1	0.000	0.004	0.000	0.457
1-y	0.017	0.000	0.085	0.000

structure T9-KT6″-M5,3″,3″-ET2″

1	0.000	0.000	0.000	0.000
1-y	0.182	0.157	0.530	0.043

Table S 5
Energy difference between corresponding conformers with outstretched and half-bowl-shaped geometries, in the calculated trimeric acylphloroglucinols
The table reports the differences in the HF/6-31G(d,p), HF/6-31+G(d,p), DFT/B3LYP/6-31+G(d,p), and DFT/B3LYP/6-31+G(d,p) with the Grimme' corrections results, respectively denoted as HF, HF+, DFT and DFT-D3 in the column headings. The differences are taken as «energy of the conformer with bowl-shaped geometry minus energy of the conformer with outstretched geometry ». To facilitate comparisons of different bowl-shaped geometry-types, the values for conformers with up—down—up orientations of the monomers are highlighted in yellow and the values for conformers with up—up—up orientations of the monomers are highlighted in blue (the values for up—down—down conformers are not highlighted).

molecule	conformer	energy difference between half-bowl-shaped and outstretched-shaped conformers (kcal/mol)			
		HF	HF+	DFT	DFT-D3
T1	1	0.282	0.285	0.325	0.093
	2	0.103	0.060	0.113	0.625
	3	0.037	0.054	0.028	-0.239
	4	0.242	0.233	0.308	0.025
	5	0.106	0.053	0.094	-0.821
	6	0.144	0.171	0.130	-0.269
	7	0.067	0.091	0.026	-0.190
	8	0.182	0.188		
	9	0.125	0.129	0.228	-0.083
	10	0.484	0.434	-0.051	-0.596
	11	-1.031	-0.948	-1.190	-1.722
	12	-0.036	0.102	-0.087	-1.103
	13	0.111	0.152	0.047	-0.204
	14	0.102	0.086	0.107	-0.235
	15	-0.801	-0.741	-0.822	-1.374
	16	0.541	0.498	-0.076	-0.627
	17	-0.402	-0.274	-0.338	-0.761
	18	-0.465	-0.595	-0.330	-1.387
	19	-0.834	-0.724	-0.988	-1.448
	20	-0.615	-0.535	-0.527	-0.986
	21	-0.618	-0.560	-0.664	-1.157
	22	-0.643	-0.571	-0.520	-2.924
	23	-0.289	-0.461	-0.156	-2.265
	24	-0.380	-0.408	-0.070	-0.442
	25	-0.978	-0.852	-1.060	-3.462
	26	0.101	0.117	0.066	-0.290
	27	-0.422	-0.389	-1.213	-1.692
	28	-0.295	-0.628	-0.502	-2.704

	29	-0.322	-0.242	0.022	-0.460
T2-KT2,6″-M5,5,3″,3″	1	0.391	0.392	0.385	-0.172
T3-ET6,2″	1	-0.158	0.200	0.485	-0.154
T3-M5,3″-ET6,2″	1	-0.030	-0.015	0.028	-0.329
T4-KT2,6″-M5,5,3″,3″	1	0.389	0.389	0.383	-0.177
T5-KT6″-M3″,3″-ET4	1	0.387	0.384	0.370	-0.330
T5-KT2,6″-M5,5,3″,3″	1	0.017	-0.004	0.086	-0.454
T6-M5,3″-ET6,4″	1	0.209	0.195	0.141	-0.195
	1-y-in-out	0.220	0.184	0.190	0.165
	1-y-in-in	3.310	4.231	4.737	2.628
T7	1	0.280	0.285	1.007	0.331
	2	0.095	0.040	0.159	-1.567
	3	0.036	0.050	0.026	-0.250
	4	0.238	0.231	0.310	0.007
	5	0.072	0.029	0.120	-1.432
	6	-0.079	0.047	0.076	-1.118
T7-ET6,2″	1	0.296	0.307	0.347	0.046
T7-M5,3″-ET6,2″	1	0.201	0.181	0.279	-0.188
T7-KT6″-M5,3″,3″	1	0.260	0.306	0.287	-0.219
	2	0.190	0.166	0.288	-0.204
	3	0.273	0.275	0.315	-3.077
	4	0.066	0.086	0.143	-0.285
	5	-0.241	-0.276	0.053	-1.695
	6	0.092	0.062	0.092	0.773
	7	-1.178	-1.114	-1.186	-2.797
	8	-0.795	-0.858	-0.868	-3.200
	9	-0.433	-0.238	-0.454	-1.941
	10	-0.357	-0.341	-0.258	-2.734
T7-KT2,6″-M5,5,3″,3″	1	0.390	0.391	0.384	-0.140
T8-KT6″-M5,3″,3″	1	0.268	0.307	0.249	-0.324
	2	0.191	0.166	0.286	-0.188

	3	0.283	0.271	0.386	-2.137
	4	0.063	0.083	0.144	-0.291
	5	-0.248	-0.197	0.093	-2.301
	6	-0.221	-0.173	-0.108	-1.188
	7	-1.177	-1.103	-1.225	-2.776
	8	-0.795	-0.854	-0.860	-3.167
	9	-0.191	-0.219	-0.455	-2.474
	10	-0.453	-0.374	-0.233	-3.690
T8-KT2-M5,5,3″	1	0.262	0.305	0.274	-0.670
	2	0.190	0.205	0.296	-0.183
	3	0.236	0.200	-0.981	-2.296
	4	0.735	0.777	0.096	-0.300
	5	0.201	-0.239	0.109	-1.824
	6	-0.263	-0.121	-0.061	-1.702
	7	-1.160	-1.093	-1.144	-2.831
	8	-0.826	-0.898	-0.895	-2.466
	9	-0.422	-0.208	-0.476	-2.890
	10	-0.297	-0.256	-0.296	-3.225
T8-KT2,6″-M5,5,3″,3″	1	0.387	0.422	0.373	-0.336
T9	1	0.275	0.280	0.319	0.020
	2	0.090	0.065	0.203	-2.172
	3	0.038	0.055	0.026	-0.250
	4	0.234	0.225	0.301	-0.005
	5	0.066	0.026	0.185	-2.581
	6	-0.499	0.042	0.084	-1.189
T9-M5,3″	1	0.225	0.216	0.266	-0.134
	2	0.075	0.001	0.201	-2.279
	3	0.022	0.058	0.033	-0.353
	4	0.211	0.197	0.280	-0.123
	5	0.058	-0.049	0.208	-2.692
	6	0.041	0.073	0.118	-1.598
T9-ET6,2″	1	0.293	0.299	0.346	0.025
T9-M5,3″-ET6,2″	1	0.199	0.176	0.279	-0.195
T9-M5,3″-ET6,4″	1	0.210	0.195	0.186	-0.150
	1-y-in-out	0.218	0.183		-0.180
	1-y-in-in	3.294	4.216	4.738	2.798

T9-KT6″-M5,3″,3″	1	0.261	0.352	0.266	-0.672
	2	0.191	0.166	0.324	-0.156
	3	0.760	0.819	1.415	-1.635
	4	0.063	0.042	0.140	-0.294
	5	-0.159	-0.168	0.337	-2.541
	6	-0.219	-0.126	-0.218	-2.099
	7	-1.175	-1.144	-1.229	-2.818
	8	-0.814	-0.890	-0.895	-3.239
	9	-0.490	-0.226	-0.484	-2.881
	10	-0.622	-0.445	0.484	-2.355
T9-KT6″-M3″,3″-ET2″	1	-0.017	-0.004	0.085	-0.457
T9-KT6″-M5,3″,3″-ET2″	1	0.182	0.157	0.530	0.043
T9-KT2,6″-M5,5,3″,3″	1	0.383	0.387	0.380	-0.962
T10	1	0.380	0.380	0.275	-0.001
	2	-0.150	-0.153	-0.087	-1.893
	3	-0.171	-0.125	-0.043	-0.199
	4	0.080	0.086	0.519	0.102
	5	-0.156	-0.225	-0.138	-1.718
	6	-0.100	-0.176	-0.016	-1.656
T10-ET6,2″	1	0.568	0.547	0.303	0.032
T10-M5,3″-ET6,2″	1	-0.030	-0.026	0.569	0.089
T10-M5,3″-ET6,2″,6″	1	6.983	6.809	0.728	0.486
T10-KT2,6″-M5,5,3″,3″	1	-0.549	4.410	3.800	4.632
T11-ET6,2″	1	-0.080	0.511	0.388	0.062
T11-M5,3″-ET6,2″	1	0.566	0.514	0.508	0.007
T12-KT2-M5,5,3″	1	0.263	0.307	0.272	-0.930
	2	0.190	0.166	0.290	-0.205
	3	1.662	1.747	1.739	-2.819
	4	0.063	0.085	0.131	-0.341
	5	-0.163	-0.203	0.328	-2.705
	6	-0.220	-0.126	-0.227	-2.359
	7	-1.173	-1.143	-1.206	-2.821
	8	-0.793	-0.847	-0.885	-3.192

	9	-0.490	-0.238	-0.437	-3.194
	10	-0.678	-0.534	0.068	-4.522
T12-KT6″-M5,3″,3″	1	0.261	0.306	0.267	-0.688
	2	0.191	0.167	0.288	-0.209
	3	0.276	0.220	0.395	-3.314
	4	0.062	0.004	0.176	-0.290
	5	0.154	0.285	0.315	-3.250
	6	-0.220	-0.129	-0.178	-2.081
	7	-1.175	-1.096	-1.210	-2.837
	8	-0.798	-0.905	-0.897	-3.706
	9	-0.490	-0.227	-0.443	-2.895
	10	-0.307	0.015	0.282	-3.283
T13-ET6,2″	1	0.295	0.300	0.355	0.023
T13-M5,3″-ET6,2″	1	0.200	0.180	0.281	-0.203
T14-ET6,2″	1	0.502	0.482	0.614	0.513
T14-M5,3″-ET6,2″	1	0.551	0.502	0.505	-0.027

Table S 6
Lowering effect of Grimme's correction on the estimation of the energy of the conformers of the calculated trimeric acylphloroglucinols
The table reports the difference in the estimations of the conformers' energies, taken as «energy in the DFT/B3LYP/6-31+G(d,p) result without Grimme's correction minus energy in the DFT/B3LYP/6-31+G(d,p) result comprising Grimme's correction».

molecule	conformer	energy difference (kcal/mol)	conformer	energy difference (kcal/mol)
T1	1	48.051	1-y	48.283
	2	48.014	2-y	48.752
	3	47.975	3-y	48.241
	4	48.066	4-y	48.349
	5	48.031	5-y	48.947
	6	47.988	6-y	48.387
	7	48.028	7-y	48.244
	8		8-y	48.410
	9	48.083	9-y	48.393
	10	48.083	10-y	48.627
	11	47.886	11-y	48.417
	12	48.068	12-y	49.083
	13	48.098	13-y	48.349
	14	48.094	14-y	48.436
	15	47.894	15-y	48.446
	16	48.098	16-y	48.649
	17	47.876	17-y	48.299
	18	47.902	18-y	48.960
	19	47.891	19-y	48.352
	20	47.886	20-y	48.346
	21	47.897	21-y	48.389
	22	47.911	22-y	50.316
	23	48.085	23-y	50.193
	24	48.011	24-y	48.383
	25	47.925	25-y	50.327
	26	48.043	26-y	48.400
	27	47.934	27-y	48.413
	28	48.005	28-y	50.207
	29	47.918	29-y	48.400
T2-KT2,6″-M5,5,3″,3″	1	65.490	1-y	66.047
T3-ET6,2″	1	59.732	1-y	60.371

T3-M5,3″-ET6,2″	1	66.952	1-y	67.309
T4-KT2,6″-M5,5,3″,3″	1	67.499	1-y	68.058
T5-KT2,6″- M5,5,3″,3″	1	69.510	1-y	70.211
T5-KT6″-M3″,3″-ET2″	1	65.224	1-y	65.763
T6-M5,3″-ET6,4″	3	67.429	3-y	67.765
			3-y-in-out	67.784
			3-y-in-in	69.537
T6-KT2,6″-M5,5,3″,3″	1	69.510	1-y	70.211
T7	1	55.679	1-y	56.355
	2	55.727	2-y	57.453
	3	55.682	3-y	55.958
	4	55.806	4-y	56.110
	5	55.813	5-y	57.365
	6	55.654	6-y	56.928
T7-ET6,2″	1	59.927	1-y	60.228
T7-M5,3″-ET6,2″	1	67.154	1-y	67.621
T7-KT6″-M5,3″,3″	1	64.831	1-y	65.337
	2	64.845	2-y	65.336
	3	64.884	3-y	67.001
	4	64.844	4-y	65.274
	5	65.030	5-y	66.778
	6	64.955	6-y	65.635
	7	65.012	7-y	66.622
	8	65.052	8-y	67.383
	9	64.938	9-y	66.424
	10	65.005	10-y	67.481
T7-KT2,6″-M5,5,3″,3″	1	69.362	1-y	69.886
T8-KT6″-M5,3″,3″	1	66.841	1-y	67.414
	2	66.857	2-y	67.332
	3	66.905	3-y	69.427
	4	66.856	4-y	67.291
	5	67.066	5-y	69.459

	6	66.968	6-y	68.048
	7	67.075	7-y	68.627
	8	67.071	8-y	69.378
	9	66.957	9-y	68.976
	10	67.060	10-y	70.518
T8-KT2-M5,5,3″	1	66.914	1-y	67.858
	2	66.890	2-y	67.369
	3	68.058	3-y	69.372
	4	66.896	4-y	67.293
	5	67.070	5-y	69.002
	6	66.966	6-y	68.607
	7	67.054	7-y	68.740
	8	67.072	8-y	68.643
	9	66.969	9-y	69.383
	10	68.270	10-y	71.199
T8-KT2,6″-M5,5,3″,3″	1	71.377	1-y	72.086
T9	1	59.491	1-y	59.790
	2	59.543	2-y	61.918
	3	59.496	3-y	59.772
	4	59.618	4-y	59.923
	5	59.670	5-y	62.437
	6	59.540	6-y	60.814
T9-M5,3″	1	64.208	1-y	64.608
	2	64.273	2-y	66.752
	3	64.228	3-y	64.614
	4	64.309	4-y	64.712
	5	64.375	5-y	67.275
	6	64.295	6-y	66.012
T9-ET6,2″	1	63.799	1-y	64.120
T9-M5,3″-ET6,2″	1	71.097		71.571
T9-M5,3″-ET6,4″	1	71.306	1-y	71.642
			1-y-in-in	73.420
T9-KT6″-M5,3″,3″	1	68.703	1-y	69.641
	2	68.722	2-y	69.203
	3	68.776	3-y	71.825
	4	68.720	4-y	69.153
	5	68.748	5-y	70.629

	6	68.911	6-y	71.789
	7	68.908	7-y	70.496
	8	68.948	8-y	71.293
	9	68.823	9-y	71.221
	10	68.909	10-y	71.748
T9-KT6″-M3″,3″-ET4	1	68.909	1-y	69.451
T9-KT6″-M5,3″,3″-ET6	1	72.160	1-y	72.647
	40	72.300	40-y	72.966
T9-KT2,6″-M5,5,3″,3″	1	73.243	1-y	74.585
T10	1	62.978	1-y	63.254
	2	63.267	2-y	65.072
	3	63.140	3-y	63.294
	4	63.163	4-y	63.580
	5	63.416	5-y	64.996
	6	63.254	6-y	64.894
T10-ET6,2″	1	67.535	1-y	67.806
T10-M5,3″-ET6,2″	1	74.617	1-y	75.096
T10-M5,3″-ET6,2″,6″	1	79.163	1-y	79.405
T10-KT2,6″-M5,5,3″,3″	1	78.129	1-y	77.298
T11-ET6,2″	1	64.653	1-y	64.979
T11-M5,3″-ET6,2″	1	71.589	1-y	72.640
T12-KT2-M5,5,3″	1	70.461	1-y	71.663
	2	70.481	2-y	70.976
	3	70.543	3-y	75.101
	4	70.480	4-y	70.953
	5	70.696	5-y	73.730
	6	70.505	6-y	72.637
	7	70.668	7-y	72.282
	8	70.712	8-y	73.019
	9	70.550	9-y	73.306
	10	70.676	10-y	75.266
T12-KT6″-M5,3″,3″	1	70.456	1-y	71.411

	2	70.476	2-y	70.972
	3	70.541	3-y	74.250
	4	70.478	4-y	70.944
	5	70.705	5-y	74.270
	6	70.503	6-y	72.407
	7	70.660	7-y	72.287
	8	70.703	8-y	73.512
	9	70.578	9-y	73.030
	10	70.727	10-y	74.292
T13-ET6,2″	1	67.228	1-y	67.560
T13-M5,3″-ET6,2″	1	74.863	1-y	75.348
T14-ET6,2″	1	70.107	1-y	70.209
T14-M5,3″-ET6,2″	1	77.128	1-y	77.305
			1-y-in-out	77.661

Table S 7
Ranges of the lowering effect of Grimme's correction on the estimation of the energy of the conformers of the calculated trimeric acylphloroglucinols, grouping the molecules according to their formulas
The lowering (table S6) is evaluated as «energy in the DFT/B3LYP/6-31+G(d,p) result minus energy in the DFT/B3LYP/6-31+G(d,p)/D-3 result». When only one conformers-pair is present for a given molecule, the value for each conformer is reported, and the two values are separated by a comma.

molecular formula	molecule	energy difference range (kcal/mol)	
		outstretched geometry	half-bowl geometry
$C_{26}H_{24}O_{12}$	T1	47.89 – 48.09	48.24 – 50.33
$C_{30}H_{32}O_{12}$	T7	55.68 – 55.81	55.96 – 57.45
$C_{31}H_{34}O_{12}$	T3-ET6,2″	59.73	60.37
$C_{32}H_{36}O_{12}$	T2-KT2,6″-M5,5,3″,3″	65.49	66.05
	T7-ET6,2″	59.93	60.23
	T9	59.49 – 59.67	59.77 – 62.44
	T10	62.98 – 63.42	63.25 – 65.07
$C_{33}H_{38}O_{12}$	T3-M5,3″-ET6,2″	66.95	67.31
	T4-KT2,6″-M5,5,3″,3″	67.50	68.06
	T5-KT6″-M3″,3″-ET4	65.22	65.76
	T7-KT6″-M5,3″,3″	64.83 – 65.05	65.27 – 67.48
	T11-ET6,2″	64.65	64.98
$C_{34}H_{40}O_{12}$	T5-KT2,6″-M5,5,3″,3″	69.51	70.21
	T6-M5,3″-ET6,4″	67.43	67.77 – 69.54
	T7-M5,3″-ET6,2″	67.15	67.62
	T7-KT2,6″-M5,5,3″,3″	69.36	69.89
	T8-KT6″-M5,3″,3″	66.84 – 67.08	67.33 – 70.52
	T8-KT2-M5,5,3″	66.89 – 68.27	67.29 – 71.20
	T9-M5,3″	64.21 – 64.38	64.61 – 67.28
	T9-ET6,2″	63.80	64.12
	T10-ET6,2″	67.54	67.81
$C_{35}H_{42}O_{12}$	T8-KT2,6″-M5,5,3″,3″	71.38	72.09
	T9-KT6″-M5,3″,3″	68.70 – 68.95	69.15 – 71.83
	T9-KT6″-M3″,3″-ET4	68.91	69.45
	T11-M5,3″-ET6,2″	71.59	72.64
	T13-ET6,2″	67.23	67.56
	T14-ET6,2″	70.11	70.21
$C_{36}H_{44}O_{12}$	T9-M5,3″-ET6,2″	71.10	71.57
	T9-M5,3″-ET6,4″	71.31	71.64 – 73.42
	T9-KT6″-M5,3″,3″-ET6	72.16	72.65

	T9-KT2,6″-M5,5,3″,3″	73.24	74.59
	T10-M5,3″-ET6,2″	74.62	75.10
	T10-KT2,6″-M5,5,3″,3″	78.13	77.30
	T12-KT2-M5,5,3″	70.46 – 70.71	70.95 – 75.27
	T12-KT6″-M5,3″,3″	70.46 – 70.73	70.94 – 74.29
$C_{37}H_{46}O_{12}$	T10-M5,3″-ET6,2″,6″	79.16	79.41
	T13-M5,3″-ET6,2″	74.86	75.35
	T14-M5,3″-ET6,2″	77.13	77.31 – 77.66

Table S 8

Relative energies non-corrected (ΔE, kcal/mol) and corrected for ZPE (ΔE_corr, kcal/mol) and relative free energies (sum of electronic and thermal free energies, ΔG, kcal/mol) in the HF results of representative conformers of the calculated trimeric acylphloroglucinols.
For each molecule, the conformers are listed in order of increasing relative energy in the DFT/B3LYP/6-31+G(d,p) results.

conformers	HF/6-31G(d,p)			HF/6-31+G(d,p)		
	ΔE	ΔE_corr	ΔG	ΔE	ΔE_corr	ΔG
structure T1						
1	0.000	0.000	0.000	0.000	0.000	0.000
1-y	0.282	0.358	0.385	0.285	0.348	0.388
2	2.477	2.460	2.183	2.470	2.420	2.100
2-y	2.580	2.641	2.363	2.530	2.542	2.284
3	2.630	2.613	2.312	2.657	2.609	2.277
3-y	2.667	2.730	2.466	2.711	2.728	2.422
4	5.220	5.070	5.005	5.358	5.163	5.078
4-y	5.462	5.383	5.374	5.591	5.457	5.429
5	7.686	7.524	7.187	7.821	7.582	7.162
6	5.223	5.202	4.644	5.218	5.122	4.477
5-y	7.792	7.709	7.329	7.874	7.703	7.334
7	7.688	7.540	7.194	7.793	7.570	7.165
7-y	7.755	7.692	7.319	7.884	7.733	7.327
8	8.154	7.875	7.608	8.151	7.846	7.614
8-y	8.336	8.127	7.948	8.339	8.090	7.941
6-y	5.367	5.429	4.973	5.389	5.363	4.832
9	10.381	10.079	9.952	10.585	10.202	10.024
10-y	8.918	8.980	8.869	8.920	8.903	8.709
10	8.434	8.154	7.889	8.486	8.170	7.930
9-y	10.506	10.297	10.252	10.714	10.408	10.304
11-y	8.532	8.371	7.405	8.502	8.306	6.515
12-y	10.926	10.592	10.152	10.961	10.562	10.176
12	10.962	10.572	9.938	10.859	10.423	9.773
13	10.690	10.420	9.888	10.712	10.382	9.847
13-y	10.801	10.624	10.041	10.864	10.621	10.082
15-y	9.342	9.109	8.356	9.356	9.033	8.059
11	9.563	9.298	8.437	9.450	9.127	8.094
17-y	9.677	9.414	8.693	9.597	9.238	8.314
18-y	9.879	9.615	8.751	9.597	9.239	8.308
17	10.079	9.726	8.745	9.871	9.490	8.417
15	10.143	9.887	8.907	10.097	9.776	8.469

structure T2-KT2,6″-M5,5,3″,3″						
1	0.000	0.000	0.000	0.000	0.000	0.000
1-y	0.391	0.479	0.429	0.392	0.467	0.418
structure T3-ET6,2″						
1	0.158	0.000	0.000	0.000	0.000	0.000
1-y	0.000	0.255	0.354	0.200	0.247	0.315
structure T3-M5,3″-ET6,2″						
1	0.030	0.000	0.000	0.015	0.000	0.000
1-y	0.000	0.032	0.129	0.000	0.017	0.087
structure T4-KT2,6″-M5,5,3″,3″						
1	0.000	0.000	0.000	0.000	0.000	0.000
1-y	0.389	0.478	0.426	0.389	0.466	0.415
structure T5-KT2,6″-M5,5,3″,3″						
1	0.000	0.000	0.000	0.000	0.000	0.000
1-y	0.387	0.473	0.426	0.384	0.454	0.391
structure T5-KT6″-M3″,3″-ET4						
1	0.000	0.000	0.000	0.004	0.000	0.000
1-y	0.017	0.055	0.082	0.000	0.018	0.039
structure T6-M5,3″-ET6,4″						
3	0.000	0.000	0.000	0.000	0.000	0.000
3-y-out-out	0.209	0.278	0.293	0.195	0.243	0.238
3-y-in-out	0.220	0.294	0.374	0.184	0.235	0.304
3-y-in-in	3.310	3.757	4.630	4.231	4.499	5.003
structure T7						
1	0.000	0.000	0.000	0.000	0.000	0.000
1-y	0.280	0.355	0.387	0.285	0.345	0.375
2	2.439	2.424	2.150	2.460	2.420	2.117
2-y	2.534	2.599	2.330	2.500	2.526	2.298
4	4.997	4.945	4.848	5.106	5.031	4.906
3	2.600	2.585	2.287	2.621	2.573	2.237
3-y	2.636	2.700	2.435	2.671	2.689	2.374
4-y	5.235	5.254	5.216	5.337	5.319	5.242
5	7.419	7.356	6.983	7.551	7.442	6.992
5-y	7.491	7.512	7.145	7.580	7.537	7.144
6	5.299	5.179	4.571	5.270	5.152	4.408
6-y	5.220	5.345	4.876	5.317	5.268	4.737
structure T7-ET6,2″						

1	0.000	0.000	0.000	0.000	0.000	0.000
1-y	0.296	0.370	0.400	0.307	0.365	0.387
structure T7-M5,3″-ET6,2″						
1	0.000	0.000	0.000	0.000	0.000	0.000
1-y	0.201	0.275	0.328	0.181	0.234	0.283
structure T7-KT6″-M5,3″,3″						
1	0.000	0.000	0.000	0.000	0.000	0.000
1-y	0.260	0.395	0.386	0.306	0.423	0.422
2	0.433	0.481	0.419	0.498	0.525	0.415
2-y	0.623	0.728	0.668	0.664	0.722	0.575
3	2.003	1.955	1.550	2.007	1.979	1.552
3-y	2.276	2.378	2.265	2.282	2.388	2.322
4	2.884	2.880	2.381	2.968	2.954	2.338
4-y	2.950	2.994	2.586	3.054	3.070	2.529
5	10.137	10.125	9.563	10.104	10.031	9.211
5-y	9.896	9.664	9.027	9.828	9.534	8.769
6	10.570	10.611	10.281	10.582	10.540	10.029
6-y	10.662	10.670	10.267	10.644	10.579	10.029
7-y	12.073	11.691	10.630	11.902	11.487	10.227
7	13.251	12.789	11.792	13.016	12.491	11.275
8-y	12.948	12.521	11.549	12.698	12.184	11.162
9-y	13.161	12.792	11.990	13.044	12.631	11.406
10-y	13.341	12.915	12.043	13.085	12.595	11.640
9	13.594	13.048	11.678	13.282	12.721	11.276
10	13.698	13.213	12.102	13.426	12.903	11.492
8	13.743	13.298	12.208	13.556	13.033	11.566
structure T7-KT2,6″-M5,5,3″,3″						
1	0.000	0.000	0.000	0.000	0.000	0.000
1-y	0.390	0.479	0.421	0.391	0.467	0.420
structure T8-KT6″-M5,3″,3″						
1	0.000	0.000	0.000	0.000	0.000	0.000
1-y	0.268	0.400	0.388	0.307	0.420	0.419
2	0.436	0.483	0.420	0.502	0.528	0.426
2-y	0.627	0.730	0.676	0.668	0.727	0.577
3	1.998	1.950	1.547	1.996	1.968	1.544
3-y	2.281	2.395	2.727	2.267	2.378	2.603
4	2.878	2.873	2.374	2.956	2.943	2.365
4-y	2.941	2.986	2.576	3.039	3.058	2.508
5	10.092	9.825	9.015	9.962	9.664	8.712
5-y	9.844	9.617	9.344	9.765	9.463	8.880
6-y	10.423	10.308	9.470	10.375	10.182	9.148

6	10.644	10.359	8.757	10.548	10.225	8.523
7-y	11.986	11.614	10.564	11.836	11.431	10.178
9-y	13.288	12.835	11.429	12.964	12.518	11.342
8-y	12.858	12.440	11.473	12.584	12.078	11.054
10-y	13.132	12.729	12.748	12.922	12.432	11.523
9	13.479	12.952	11.782	13.183	12.644	11.274
7	13.163	12.710	11.724	12.939	12.426	11.211
10	13.585	13.120	12.039	13.296	12.780	11.341
8	13.653	13.213	12.117	13.438	12.921	11.455
structure T8-KT2-M5,5,3″						
1	0.000	0.000	0.000	0.000	0.000	0.000
1-y	0.262	0.393	0.382	0.305	0.415	0.451
2	0.440	0.486	0.417	0.460	0.480	0.404
2-y	0.630	0.733	0.673	0.665	0.724	0.599
3-y	3.807	4.263	4.081	3.784	4.201	3.931
4	2.188	2.857	2.388	2.155	2.920	2.432
3	3.571	3.900	3.492	3.584	3.903	3.475
4-y	2.923	2.969	2.588	2.932	2.945	2.496
5	10.090	10.087	9.566	9.981	9.920	9.269
5-y	10.291	10.200	9.900	9.742	9.447	8.830
6-y	10.372	10.268	9.577	10.321	10.137	9.240
6	10.635	10.363	9.034	10.442	10.129	8.844
7-y	11.970	11.599	10.601	11.731	11.335	10.243
9-y	13.031	12.665	12.013	12.867	12.480	11.502
8-y	12.841	12.423	11.433	12.564	12.051	10.949
9	13.453	12.925	11.560	13.075	12.536	11.180
7	13.130	12.676	11.670	12.824	12.321	11.180
8	13.667	13.220	12.102	13.462	12.959	11.594
10-y	14.872	14.840	14.064	14.603	14.470	13.494
10	15.169	15.068	13.970	14.859	14.691	13.347
structure T8-KT2,6″-M5,5,3″,3″						
1	0.000	0.000	0.000	0.000	0.000	0.000
1-y	0.387	0.474	0.420	0.422	0.496	0.430
structure T9						
1	0.000	0.000	0.000	0.000	0.000	0.000
1-y	0.275	0.350	0.383	0.280	0.337	0.363
2	2.509	2.471	2.141	2.516	2.437	2.034
4	4.994	4.944	4.842	5.103	5.028	4.906
2-y	2.599	2.636	2.546	2.581	2.576	2.654
3	2.672	2.635	2.275	2.708	2.636	2.226
3-y	2.710	2.753	2.422	2.763	2.755	2.356
4-y	5.228	5.247	5.203	5.328	5.309	5.227

5	7.487	7.400	6.970	7.605	7.453	6.912
5-y	7.553	7.534	7.140	7.631	7.541	7.339
6	5.859	5.223	4.552	5.349	5.206	4.386
6-y	5.360	5.385	4.853	5.391	5.316	4.698
structure T9-M5,3″						
1	0.000	0.000	0.000	0.000	0.000	0.000
1-y	0.225	0.307	0.350	0.216	0.282	0.318
2	1.998	1.956	1.610	2.028	2.008	1.620
2-y	2.073	2.109	2.166	2.029	2.083	2.235
3	2.247	2.201	1.805	2.251	2.215	1.761
3-y	2.269	2.303	1.963	2.309	2.345	1.926
4	4.626	4.547	4.187	4.738	4.658	4.252
4-y	4.837	4.827	4.511	4.935	4.909	4.548
6	4.282	4.206	3.471	4.292	4.234	3.379
6-y	4.323	4.337	3.876	4.365	4.391	3.881
5	6.598	6.480	5.784	6.707	6.602	5.837
5-y	6.656	6.594	6.052	6.658	6.622	6.268
structure T9-ET6,2″						
1	0.000	0.000	0.000	0.000	0.000	0.000
1-y	0.293	0.366	0.396	0.299	0.360	0.385
structure T9-M5,3″-ET6,2″						
1	0.000	0.000	0.000	0.000	0.000	0.000
1-y	0.199	0.272	0.326	0.176	0.230	0.272
structure T9-M5,3″-ET6,4″						
3	0.000	0.000	0.000	0.000	0.000	0.000
3-y	0.210	0.277	0.294	0.195	0.242	0.238
3-y-in-out	0.218	0.292	0.374	0.183	0.232	0.287
3-y-in-in	3.294	3.742	4.616	4.216	4.479	4.963
structure T9-KT6″-M5,3″,3″						
1	0.000	0.000	0.000	0.000	0.000	0.000
1-y	0.261	0.393	0.383	0.352	0.469	0.474
2	0.439	0.486	0.417	0.545	0.577	0.467
2-y	0.630	0.734	0.669	0.711	0.777	0.620
3	1.996	1.948	1.547	2.035	2.017	1.593
4	2.878	2.873	2.370	2.995	2.991	2.407
4-y	2.941	2.986	2.570	3.037	3.060	2.506
3-y	2.756	2.989	3.396	2.854	3.063	3.332
6-y	11.266	11.154	10.498	11.341	11.136	10.106
5	11.424	11.222	10.404	11.406	11.132	10.001
6	11.485	11.220	10.329	11.467	11.139	9.888

5-y	11.265	11.157	11.775	11.238	10.998	10.787
7-y	11.961	11.593	10.546	11.806	11.404	10.152
9-y	12.961	12.632	12.167	12.968	12.587	11.616
8-y	12.831	12.418	11.448	12.594	12.099	11.058
9	13.451	12.930	11.762	13.194	12.661	11.269
7	13.136	12.688	11.703	12.950	12.449	11.227
10	13.555	13.095	12.015	13.338	12.841	11.397
8	13.645	13.190	12.096	13.484	12.989	11.546
10-y	12.933	12.580	12.964	12.893	12.447	12.157
structure T9-KT6″-M3″,3″-ET4						
1	0.000	0.000	0.000	0.004	0.000	0.000
1-y	0.017	0.056	0.076	0.000	0.018	0.028
structure T9-KT6″-M5,3″,3″-ET6						
1	0.000	0.000	0.000	0.000	0.000	0.000
1-y	0.182	0.242	0.238	0.157	0.191	0.140
40	15.882	14.676	13.854	14.894	13.621	12.727
40-y	15.645	14.972	14.110	14.679	13.870	12.895
structure T9-KT2,6″-M5,5,3″,3″						
1	0.000	0.000	0.000	0.000	0.000	0.000
1-y	0.383	0.466	0.441	0.387	0.457	0.418
structure T10						
1	0.000	0.000	0.000	0.067	0.000	0.000
1-y	0.380	0.436	0.244	0.447	0.444	0.345
2-y	2.414	2.462	2.849	2.441	2.354	2.589
4	4.492	4.430	4.554	4.658	4.450	4.549
2	2.564	2.535	2.499	2.594	2.453	2.423
3-y	2.577	2.637	2.690	2.627	2.535	2.575
3	2.748	2.728	2.621	2.752	2.625	2.582
4-y	4.572	4.583	4.845	4.744	4.589	4.802
5-y	6.996	6.968	7.092	7.071	6.846	7.058
5	7.152	7.073	7.195	7.296	7.038	7.159
6-y	5.204	5.234	5.401	5.140	4.948	5.104
6	5.304	5.262	5.243	5.316	5.109	5.156
structure T10-ET6,2″						
1	0.000	0.000	0.000	0.000	0.000	0.000
1-y	0.568	0.621	0.134	0.547	0.637	0.358
structure T10-M5,3″-ET6,2″						
1	0.030	0.000	0.000	0.026	0.005	0.000
1-y	0.000	0.021	0.063	0.000	0.000	0.046

structure T10-M5,3″-ET6,2″,6″						
1	0.000	0.000	0.000	0.000	0.000	0.000
1-y	6.983	7.388	7.750	6.809	7.163	7.562
structure T10-KT2,6″-M5,5,3″,3″						
1-y	0.549	0.256	0.628	0.000	4.357	4.534
1	0.000	0.000	0.000	4.410	0.000	0.000
structure T11-ET6,2″						
1	0.080	0.000	0.000	0.000	0.000	0.000
1-y	0.000	0.583	0.348	0.511	0.594	0.476
structure T11-M5,3″-ET6,2″						
1	0.000	0.000	0.000	0.000	0.000	0.000
1-y	0.214	0.272	0.624	0.357	0.412	0.692
1-y-out-in	0.566	0.654	0.624	0.514	0.622	0.689
structure T12-KT2-M5,5,3″						
1	0.000	0.000	0.000	0.000	0.000	0.000
1-y	0.263	0.395	0.380	0.307	0.417	0.417
2	0.439	0.486	0.413	0.497	0.527	0.435
2-y	0.629	0.734	0.668	0.663	0.727	0.585
3	1.994	1.947	1.544	1.987	1.965	1.557
4	2.876	2.872	2.369	2.945	2.938	2.372
4-y	2.939	2.985	2.567	3.030	3.053	2.509
3-y	3.656	3.993	4.519	3.734	4.049	4.379
6-y	11.255	11.145	10.498	11.276	11.067	10.029
5	11.413	11.212	10.382	11.338	11.063	9.962
6	11.475	11.212	10.318	11.402	11.076	9.831
5-y	11.250	11.126	11.582	11.135	10.894	10.807
7-y	11.947	11.582	10.531	11.739	11.338	10.092
9-y	12.940	12.610	12.137	12.882	12.492	11.529
8-y	12.816	12.406	11.436	12.569	12.078	11.056
9	13.430	12.911	11.738	13.120	12.587	11.206
7	13.120	12.675	11.686	12.882	12.382	11.182
10	13.534	13.077	11.995	13.265	12.767	11.337
10-y	12.856	12.478	12.280	12.731	12.267	11.915
8	13.609	13.177	12.080	13.416	12.920	11.487
structure T12-KT6″-M5,3″,3″						
1	0.000	0.000	0.000	0.000	0.000	0.000
1-y	0.261	0.394	0.382	0.306	0.417	0.404
2	0.438	0.485	0.416	0.462	0.483	0.374
2-y	0.629	0.734	0.668	0.629	0.683	0.523

3	2.003	1.954	1.548	1.961	1.930	1.497
3-y	2.279	2.389	2.885	2.181	2.287	2.691
4	2.882	2.877	2.369	2.961	2.949	2.359
4-y	2.944	2.989	2.567	2.965	2.969	2.348
6-y	11.277	11.164	10.497	11.275	11.057	10.019
5	11.437	11.234	10.398	11.341	11.047	9.842
6	11.497	11.230	10.329	11.404	11.060	9.733
5-y	11.591	11.637	12.438	11.626	11.505	11.421
7-y	11.970	11.601	10.548	11.787	11.373	10.088
8-y	12.842	12.429	11.448	12.523	12.021	11.000
9-y	12.971	12.640	12.166	12.903	12.502	11.492
9	13.461	12.938	11.765	13.130	12.584	11.170
7	13.145	12.696	11.708	12.883	12.369	11.151
10	13.569	13.106	12.021	13.279	12.765	11.295
8	13.640	13.203	12.100	13.428	12.916	11.444
10-y	13.262	13.069	13.602	13.294	12.969	12.812
structure T13-ET6,2″						
1	0.000	0.000	0.000	0.000	0.000	0.000
1-y	0.295	0.368	0.390	0.300	0.361	0.373
structure T13-M5,3″-ET6,2″						
1	0.000	0.000	0.000	0.000	0.000	0.000
1-y	0.200	0.272	0.309	0.180	0.231	0.279
structure T14-ET6,2″						
1	0.000	0.000	0.000	0.000	0.000	0.000
1-y	0.502	0.558	0.195	0.482	0.456	0.404
structure T14-M5,3″-ET6,2″						
1	0.000	0.000	0.000	0.000	0.000	0.000
1-y	0.195	0.246	0.494	0.337	0.381	0.577
1-y-out-in	0.551	0.636	0.516	0.502	0.601	0.611

Table S 9

Relative energies non-corrected (ΔE, kcal/mol) and corrected for ZPE (ΔE$_{corr}$, kcal/mol) and relative free energies (sum of electronic and thermal free energies, ΔG, kcal/mol) in the DFT results (without and with dispersion correction) of representative conformers of the calculated trimeric acylphloroglucinols.

For each molecule, the conformers are listed in order of increasing relative energy in the DFT/B3LYP/6-31+G(d,p) results.

conformers	DFT/B3LYP/6-31+G(d,p)			DFT/B3LYP/6-31+G(d,p)-D3		
	ΔE	ΔE$_{corr}$	ΔG	ΔE	ΔE$_{corr}$	ΔG
structure T1						
1	0.000	0.000	0.000	0.000	0.000	0.000
1-y	0.325	0.429	0.402	0.093	0.196	0.154
2	3.432	3.617	3.415	2.844	3.624	3.368
2-y	3.545	3.828	3.609	3.469	3.042	2.018
3	3.766	3.980	3.790	3.843	4.033	3.771
3-y	3.794	4.109	3.927	3.604	3.899	3.636
4	3.858	3.775	3.394	3.843	3.700	3.282
4-y	4.166	4.159	3.680	3.868	3.827	3.392
5	7.281	7.400	6.843	7.301	7.329	6.669
6	7.366	7.811	7.390	7.429	7.818	7.318
5-y	7.375	7.577	7.095	6.480	6.659	6.616
7	7.424	7.555	6.963	7.447	7.481	6.751
7-y	7.450	7.688	7.095	7.257	7.405	6.649
8-y	7.465	7.785	7.449	7.106	7.302	6.768
6-y	7.496	8.052	7.682	7.160	7.654	7.113
9	7.585	7.396	6.573	7.554	7.255	6.375
10-y	7.717	8.094	7.736	7.141	7.447	6.984
10	7.768	8.047	7.708	7.737	7.922	7.438
9-y	7.813	7.698	6.791	7.471	7.270	6.394
17-y	11.608	11.825	10.899	11.360	11.573	10.505
17	11.946	12.064	11.163	12.121	12.270	11.288
structure T2-KT2,6″-M5,5,3″,3″						
1	0.000	0.000	0.000	0.172	0.097	0.409
1-y	0.385	0.485	0.518	0.000	0.000	0.000
structure T3-ET6,2″						
1	0.000	0.000	0.000	0.154	0.065	0.215
1-y	0.485	0.592	0.508	0.000	0.000	0.000

structure T3-M5,3″-ET6,2″						
1	0.000	0.000	0.000	0.329	0.215	0.198
1-y	0.028	0.145	0.174	0.000	0.000	0.000
structure T4-KT2,6″-M5,5,3″,3″						
1	0.000	0.000	0.000	0.177	0.096	0.368
1-y	0.383	0.476	0.521	0.000	0.000	0.000
structure T5-KT2,6″-M5,5,3″,3″						
1	0.000	0.000	0.000	0.330	0.221	0.338
1-y	0.370	0.467	0.418	0.000	0.000	0.000
structure T5-KT6″-M3″,3″-ET4						
1	0.000	0.000	0.000	0.454	0.387	0.562
1-y	0.086	0.168	0.207	0.000	0.000	0.000
structure T6-M5,3″-ET6,4″						
3	0.000	0.000	0.000	0.195	0.089	0.132
3-y	0.141	0.188	0.081	0.000	0.000	0.000
3-y-in-out	0.190	0.274	0.236	0.030	0.013	0.003
3-y-in-in	4.737	5.106	5.417	2.823	3.224	3.818
structure T7						
1	0.000	0.000	0.000	0.000	0.000	0.000
1-y	1.007	1.212	1.320	0.331	0.549	0.673
2	3.467	3.622	3.419	3.419	3.535	3.293
2-y	3.626	3.857	3.650	1.852	2.198	2.775
4	3.636	3.654	3.325	3.509	3.507	3.105
3	3.837	4.017	3.809	3.834	3.980	3.697
3-y	3.863	4.148	3.953	3.584	3.850	3.564
4-y	3.946	4.059	3.647	3.516	3.618	3.185
5	7.001	7.206	6.615	6.867	7.017	6.370
5-y	7.121	15.274	17.526	5.435	5.893	6.728
6	7.372	7.782	7.381	7.317	7.658	7.152
6-y	7.448	7.971	7.658	6.199	6.795	7.429
structure T7-ET6,2″						
1	0.000	0.000	0.000	0.000	0.000	0.000
1-y	0.347	0.462	0.441	0.046	0.152	0.138
structure T7-M5,3″-ET6,2″						
1	0.000	0.000	0.000	0.188	0.074	0.096
1-y	0.279	0.377	0.366	0.000	0.000	0.000
structure T7-KT6″-M5,3″,3″						

1	0.000	0.000	0.000	0.219	0.110	0.329
1-y	0.287	0.403	0.421	0.000	0.000	0.000
2	0.610	0.666	0.619	0.816	0.777	0.971
2-y	0.898	1.072	1.012	0.612	0.667	0.662
3	2.911	3.067	2.802	3.077	3.125	3.045
3-y	3.226	3.513	3.311	1.275	1.679	2.835
4	4.168	4.418	4.068	4.373	4.548	4.424
4-y	4.311	4.652	4.349	4.088	4.369	4.214
structure T7-KT2,6″-M5,5,3″,3″						
1	0.000	0.000	0.000	0.140	0.060	0.314
1-y	0.384	0.459	0.401	0.000	0.000	0.000
structure T8-KT6″-M5,3″,3″						
1	0.000	0.000	0.000	0.324	0.201	0.431
1-y	0.249	0.379	0.429	0.000	0.000	0.000
2	0.574	0.648	0.619	0.882	0.849	1.135
2-y	0.860	1.039	0.980	0.694	0.739	0.747
3	2.856	3.025	2.820	3.118	3.178	3.247
3-y	3.242	3.554	3.465	0.981	1.429	2.912
4	4.108	4.382	4.107	4.418	4.598	4.594
4-y	4.252	4.602	4.308	4.127	4.408	4.315
structure T8-KT2-M5,5,3″						
1	0.000	0.000	0.000	0.670	0.418	0.131
1-y	0.274	0.375	0.356	0.000	0.000	0.000
2	0.538	0.604	0.573	1.232	1.062	0.745
2-y	0.834	1.005	0.926	1.049	0.956	0.491
3-y	3.060	3.340	3.154	1.272	1.659	2.646
4	4.039	4.285	3.930	4.727	4.732	4.085
3	4.041	4.420	4.128	3.568	3.749	3.222
4-y	4.135	4.479	4.186	4.427	4.554	3.921
structure T8-KT2,6″-M5,5,3″,3″						
1	0.000	0.000	0.000	0.336	0.221	0.257
1-y	0.373	0.474	0.451	0.000	0.000	0.000
structure T9						
1	0.000	0.000	0.538	0.000	0.000	0.000
1-y	0.319	0.468	3.415	0.020	0.139	0.145
2	3.452	3.611	3.268	3.401	3.534	3.306
4	3.632	3.648	3.729	3.506	3.510	3.120
2-y	3.655	3.901	3.815	1.229	1.728	3.186
3	3.810	3.997	3.926	3.805	3.975	3.734
3-y	3.836	4.132	3.746	3.555	3.823	3.572

4-y	3.933	4.080	6.672	3.501	3.623	3.247
5	7.067	7.234	6.884	6.888	7.013	6.379
5-y	7.252	7.481	7.438	4.307	4.912	6.265
6	7.419	7.806	7.624	7.370	7.698	7.230
6-y	7.503	7.984	0.538	6.181	6.760	7.478
structure T9-M5,3″						
1	0.000	0.000	0.000	0.134	0.010	0.065
1-y	0.266	0.364	0.308	0.000	0.000	0.000
2	2.866	3.012	2.763	2.936	2.981	2.807
2-y	3.067	3.333	3.184	0.657	1.067	2.277
3	3.323	3.528	3.287	3.437	3.539	3.367
3-y	3.356	3.683	3.473	3.084	3.272	3.016
4	3.654	3.713	3.098	3.687	3.663	3.176
4-y	3.934	4.087	3.367	3.564	3.673	3.172
6	6.240	6.637	6.153	6.287	6.576	6.151
6-y	6.358	6.862	6.426	4.689	5.360	6.510
5	6.479	6.710	5.882	6.446	6.610	5.932
5-y	6.687	7.032	6.325	3.754	4.419	5.732
structure T9-ET6,2″						
1	0.000	0.000	0.000	0.000	0.000	0.000
1-y	0.346	0.438	0.396	0.025	0.147	0.124
structure T9-M5,3″-ET6,2″						
1	0.000	0.000	0.000	0.195	0.095	0.204
1-y	0.279	0.375	0.351	0.000	0.000	0.000
structure T9-M5,3″-ET6,4″						
3	0.000	0.000	0.000	0.150	0.075	0.167
3-y	0.186	0.252	0.216	0.000	0.000	0.000
3-y-in-out		2.895	4.922	0.030	3.200	3.832
3-y-in-in	4.738	5.099	5.395	2.773	3.200	3.832
structure T9-KT6″-M5,3″,3″						
1	0.000	0.000	0.000	0.672	0.429	0.307
1-y	0.266	0.377	0.395	0.000	0.000	0.000
2	0.544	0.599	0.526	1.196	1.026	0.900
2-y	0.868	1.032	0.963	1.040	0.964	0.629
3	2.853	3.006	2.767	3.452	3.358	2.946
4	4.070	4.336	4.035	4.725	4.768	4.361
4-y	4.210	4.549	4.245	4.431	4.565	4.079
3-y	4.268	4.598	4.935	1.817	2.275	4.004
structure T9-KT6″-M3″,3″-ET4						

1	0.000	0.000	0.000	0.457	0.406	0.616
1-y	0.085	0.147	0.130	0.000	0.000	0.000

<div align="center">

structure T9-KT6″-M5,3″,3″-ET6

</div>

1	0.000	0.000	0.000	0.000	0.000	0.070
1-y	0.530	0.644	0.616	0.043	0.137	0.000
40	18.045	17.560	16.211	17.905	17.301	16.046
40-y	18.364	18.019	16.699	17.558	17.027	15.380

<div align="center">

structure T9-KT2,6″-M5,5,3″,3″

</div>

1	0.000	0.000	0.000	0.962	0.685	0.000
1-y	0.380	0.478	0.557	0.000	0.000	0.434

<div align="center">

structure T10

</div>

1	0.000	0.000	0.000	0.001	0.000	0.000
1-y	0.275	0.402	0.365	0.000	0.118	0.028
2-y	3.744	4.067	3.961	1.651	2.083	2.999
4	3.784	3.802	3.742	3.600	3.574	3.382
2	3.831	4.010	3.724	3.544	3.641	3.104
3-y	3.987	4.314	4.015	3.671	3.981	3.552
3	4.030	4.246	4.005	3.870	4.059	3.725
4-y	4.303	4.419	4.305	3.702	3.758	3.397
5-y	7.582	7.885	7.482	5.565	5.873	6.204
5	7.720	7.902	7.474	7.283	7.363	6.652
6-y	7.926	8.459	7.792	6.011	6.834	8.325
6	7.942	8.379	7.724	7.667	8.021	7.140

<div align="center">

structure T10-ET6,2″

</div>

1	0.000	0.000	0.000	0.000	0.000	0.000
1-y	0.303	0.400	0.323	0.032	0.173	0.242

<div align="center">

structure T10-M5,3″-ET6,2″

</div>

1	0.000	16.847	31.825	0.000	0.000	0.309
1-y	0.569	0.000	0.000	0.089	0.128	0.000

<div align="center">

structure T10-M5,3″-ET6,2″,6″

</div>

1	0.000	0.000	0.000	0.000	0.000	0.170
1-y	0.728	0.789	0.798	0.486	0.446	0.000

<div align="center">

structure T10-KT2,6″-M5,5,3″,3″

</div>

1-y	0.000	0.000	0.000	0.000	0.000	0.000
1	3.800	3.560	3.500	4.632	4.222	3.159

<div align="center">

structure T11-ET6,2″

</div>

1	0.000	0.000	0.000	0.000	0.000	0.000
1-y	0.388	0.420	0.419	0.062	0.185	0.142

structure T11-M5,3″-ET6,2″						
1	0.000	0.000	0.000	1.048	0.931	0.181
1-y	0.003	0.136	0.720	0.000	0.000	0.000
1-y-out-in	0.508	0.576	0.354	1.054	1.012	0.011
structure T12-KT2-M5,5,3″						
1	0.000	0.000	0.000	0.930	0.490	0.000
1-y	0.272	0.375	0.280	0.000	0.000	0.630
2	0.575	0.654	0.634	1.485	1.144	0.670
2-y	0.865	1.052	1.027	1.280	1.040	0.430
3	2.851	3.011	2.754	3.699	3.431	2.635
4	4.107	4.371	4.062	5.018	4.867	4.046
4-y	4.238	4.617	4.370	4.677	4.622	3.837
3-y	4.590	5.052	5.092	0.880	1.322	2.455
structure T12-KT6″-M5,3″,3″						
1	0.000	0.000	0.000	0.688	0.409	0.061
1-y	0.267	0.369	0.356	0.000	0.000	0.000
2	0.581	0.621	0.537	1.250	1.028	0.631
2-y	0.869	1.042	1.022	1.041	0.899	0.298
3	2.865	3.016	2.774	3.469	3.340	2.720
3-y	3.260	3.590	3.781	0.155	0.555	1.653
4	4.079	4.342	4.062	4.746	4.755	4.128
4-y	4.255	4.614	4.359	4.456	4.534	3.827
structure T13-ET6,2″						
1	0.000	0.000	0.000	0.000	0.000	0.000
1-y	0.355	0.428	0.230	0.023	0.151	0.166
structure T13-M5,3″-ET6,2″						
1	0.000	0.000	0.000	0.203	0.090	0.189
1-y	0.281	0.358	0.287	0.000	0.000	0.000
structure T14-ET6,2″						
1	0.000	0.000	0.000	0.000	0.000	0.000
1-y	0.614	0.656	0.695	0.513	0.567	0.513
structure T14-M5,3″-ET6,2″						
1-y	0.000	0.150	0.000	0.000	0.000	0.178
1	0.011	0.000	0.834	0.188	0.247	0.000
1-y-out-in	0.517	0.583	0.410	0.161	0.330	0.134

Table S 10
ZPE correction for representative conformers of the calculated trimeric acylphloroglucinols.
Results from HF/6-31G(d,p), HF/6-31+G(d,p), DFT/B3LYP/6-31+G(d,p), and DFT/B3LYP/6-31+G(d,p) with the Grimme' correction calculations, respectively denoted as HF, HF+, DFT and DFT-D3 in the column headings.
For each molecule, the conformers are listed in order of increasing relative energy in the DFT/B3LYP/6-31+G(d,p) results.

conformers	ZPE correction (kcal/mol)			
	HF	HF+	DFT	DFT-D3
structure T1				
1	322.204	321.460	296.728	297.286
1-y	322.279	321.524	296.832	297.388
2	322.187	321.411	296.913	297.441
2-y	322.265	321.473	297.011	297.483
3	322.187	321.413	296.942	297.476
3-y	322.267	321.478	297.043	297.579
4	322.053	321.266	296.645	297.142
4-y	322.125	321.327	296.721	297.244
5	322.042	321.221	296.847	297.314
6	322.184	321.365	297.173	297.674
5-y	322.122	321.289	296.929	297.465
7	322.056	321.237	296.859	297.319
7-y	322.141	321.310	296.965	297.433
8	321.926	321.155		
8-y	321.995	321.212	297.048	297.481
6-y	322.265	321.434	297.284	297.779
9	321.902	321.078	296.539	296.987
10-y	322.265	321.443	297.106	297.590
10	321.923	321.145	297.006	297.470
9-y	321.995	321.156	296.614	297.085
17-y	321.941	321.102	296.945	297.498
17	321.851	321.080	296.846	297.434
structure T2-KT2,6″-M5,5,3″,3″				
1	435.164	434.133	401.568	402.846
1-y	435.252	434.208	401.669	402.921
structure T3-ET6,2″				
1	417.095	416.147	385.569	386.428
1-y	417.170	416.195	385.676	386.515

structure T3-M5,3″-ET6,2″				
1	453.754	452.786	419.908	421.007
1-y	453.815	452.818	420.024	421.121
structure T4-KT2,6″-M5,5,3″,3″				
1	454.165	453.097	419.421	420.716
1-y	454.253	453.174	419.513	420.796
structure T5-KT2,6″-M5,5,3″,3″				
1	473.165	472.064	437.270	438.570
1-y	473.251	472.135	437.367	438.679
structure T5-KT6″-M3″,3″-ET4				
1	454.630	453.582	420.675	421.702
1-y	454.667	453.604	420.756	421.769
structure T6-M5,3″-ET6,4″				
3	472.681	471.667	438.003	439.034
3-y	472.750	471.715	438.048	439.140
3-y-in-out	472.755	471.717	438.087	439.123
3-y-in-in	473.128	471.934	438.372	439.541
structure T7				
1	398.132	397.245	367.934	368.706
1-y	398.207	397.305	368.139	368.924
2	398.117	397.205	368.089	368.822
2-y	398.197	397.271	368.165	369.052
4	398.082	397.170	367.952	368.702
3	398.117	397.198	368.114	368.851
3-y	398.197	397.263	368.219	368.972
4-y	398.152	397.228	368.047	368.808
5	398.069	397.137	368.139	368.855
5-y	398.154	397.203	368.367	369.163
6	398.092	397.127	368.345	369.047
6-y	398.179	397.197	368.457	369.302
structure T7-ET6,2″				
1	436.014	435.054	403.409	404.251
1-y	436.088	435.112	403.524	404.358
structure T7-M5,3″-ET6,2″				
1	472.674	471.692	437.762	438.837
1-y	472.748	471.745	437.859	438.951
structure T7-KT6″-M5,3″,3″				

1	454.125	453.105	419.873	420.882
1-y	454.260	453.223	419.989	420.991
2	454.173	453.132	419.929	420.953
2-y	454.230	453.164	420.046	421.047
3	454.077	453.077	420.029	421.039
3-y	454.227	453.211	420.160	421.395
4	454.121	453.091	420.123	421.166
4-y	454.169	453.122	420.213	421.273
structure T7-KT2,6″-M5,5,3″,3″				
1	473.124	472.016	437.192	438.547
1-y	473.213	472.092	437.267	438.628
structure T8-KT6″-M5,3″,3″				
1	473.125	472.070	437.705	438.734
1-y	473.258	472.183	437.836	438.857
2	473.173	472.097	437.779	438.824
2-y	473.230	472.129	437.883	438.902
3	473.077	472.043	437.873	438.917
3-y	473.240	472.182	438.016	439.305
4	473.121	472.057	437.979	439.037
4-y	473.170	472.089	438.055	439.139
structure T8-KT2-M5,5,3″				
1	473.129	472.079	437.722	438.756
1-y	473.260	472.190	437.824	439.008
2	473.174	472.099	437.788	438.837
2-y	473.232	472.138	437.893	438.915
3-y	473.585	472.497	438.003	439.396
4	473.124	472.072	437.968	439.012
3	473.457	472.398	438.100	439.190
4-y	473.174	472.092	438.066	439.135
structure T8-KT2,6″-M5,5,3″,3″				
1	492.124	490.981	455.026	456.404
1-y	492.211	491.055	455.126	456.519
structure T9				
1	436.108	435.152	403.557	404.419
1-y	436.183	435.209	403.707	404.537
2	436.069	435.073	403.717	404.553
4	436.058	435.078	403.574	404.423
2-y	436.144	435.147	403.803	404.918
3	436.070	435.080	403.745	404.589
3-y	436.151	435.145	403.854	404.687

4-y	436.126	435.134	403.704	404.540
5	436.021	435.000	403.724	404.544
5-y	436.089	435.062	403.786	405.024
6	436.045	435.009	403.944	404.746
6-y	436.133	435.077	404.039	404.998
structure T9-M5,3″				
1	473.148	472.099	438.230	438.990
1-y	473.230	472.165	438.327	439.113
2	473.106	472.079	438.375	439.158
2-y	473.184	472.154	438.496	439.524
3	473.102	472.063	438.434	439.216
3-y	473.181	472.135	438.557	439.302
4	473.068	472.019	438.289	439.089
4-y	473.139	472.073	438.382	439.222
6	473.072	472.042	438.626	439.403
6-y	473.162	472.125	438.734	439.785
5	473.031	471.995	438.461	439.278
5-y	473.085	472.064	438.575	439.778
structure T9-ET6,2″				
1	473.973	472.946	439.039	439.966
1-y	474.045	473.007	439.131	440.088
structure T9-M5,3″-ET6,2″				
1	510.647	509.586	473.370	474.544
1-y	510.721	509.639	473.467	474.645
structure T9-M5,3″-ET6,4″				
3	510.630	509.544	473.584	474.721
3-y	510.697	509.590	473.650	474.796
3-y-in-out	510.703	509.594	473.785	475.223
3-y-in-in	511.078	509.806	473.946	475.223
structure T9-KT6″-M5,3″,3″				
1	492.084	490.986	455.483	456.586
1-y	492.216	491.102	455.593	456.829
2	492.130	491.018	455.539	456.659
2-y	492.188	491.053	455.646	456.754
3	492.036	490.968	455.636	456.735
4	492.080	490.982	455.749	456.872
4-y	492.130	491.009	455.823	456.962
3-y	492.318	491.196	455.814	457.287
structure T9-KT6″-M3″,3″-ET4				

1	492.545	491.417	456.196	457.376
1-y	492.584	491.439	456.258	457.428

structure T9-KT6″-M5,3″,3″-ET6				
1	510.881	509.763	473.109	474.441
1-y	510.942	509.796	473.223	474.535
40	509.913	508.704	472.623	473.836
40-y	509.972	508.740	472.763	473.910

structure T9-KT2,6″-M5,5,3″,3″				
1	511.082	509.904	472.783	474.242
1-y	511.166	509.975	472.881	474.519

structure T10				
1	436.010	435.015	403.311	404.282
1-y	436.066	435.079	403.437	404.401
2-y	436.058	434.996	403.634	404.716
4	435.949	434.875	403.330	404.258
2	435.981	434.942	403.490	404.381
3-y	436.071	434.990	403.638	404.593
3	435.991	434.956	403.527	404.473
4-y	436.021	434.928	403.427	404.339
5-y	435.987	434.857	403.614	404.591
5	435.931	434.824	403.493	404.362
6-y	436.040	434.891	403.844	405.105
6	435.968	434.875	403.748	404.637

structure T10-ET6,2″				
1	473.892	472.783	438.754	439.768
1-y	473.944	472.873	438.852	439.910

structure T10-M5,3″-ET6,2″				
1	510.407	509.244	474.508	474.338
1-y	510.457	509.266	473.091	474.377

structure T10-M5,3″-ET6,2″,6″				
1	528.253	527.041	490.001	491.302
1-y	528.658	527.396	490.062	491.262

structure T10-KT2,6″-M5,5,3″,3″				
1-y	511.165	509.801	472.618	474.347
1	511.033	509.854	472.377	473.937

structure T11-ET6,2″				
1	454.961	453.907	420.995	421.990
1-y	455.022	453.990	421.120	422.113

structure T11-M5,3″-ET6,2″				
1	491.535	490.451	455.281	456.527
1-y	491.592	490.507	455.414	456.643
1-y-out-in	491.624	490.560	455.349	456.601
structure T12-KT2-M5,5,3″				
1	511.073	509.935	473.256	474.419
1-y	511.205	510.044	473.359	474.859
2	511.120	509.964	473.335	474.518
2-y	511.178	509.998	473.444	474.620
3	511.026	509.912	473.415	474.591
4	511.069	509.927	473.520	474.708
4-y	511.119	509.958	473.635	474.805
3-y	511.410	510.250	473.718	475.301
structure T12-KT6″-M5,3″,3″				
1	511.073	509.942	473.270	474.443
1-y	511.206	510.054	473.372	474.722
2	511.121	509.964	473.310	474.500
2-y	511.178	509.997	473.444	474.580
3	511.025	509.911	473.421	474.593
3-y	511.184	510.049	473.600	475.123
4	511.070	509.930	473.532	474.731
4-y	511.119	509.945	473.629	474.800
structure T13-ET6,2″				
1	492.940	491.854	456.742	457.760
1-y	493.014	491.916	456.815	457.888
structure T13-M5,3″-ET6,2″				
1	529.520	528.401	491.116	492.424
1-y	529.592	528.453	491.192	492.538
structure T14-ET6,2″				
1	492.890	491.849	456.582	457.701
1-y	492.945	491.823	456.623	457.754
structure T14-M5,3″-ET6,2″				
1	529.382	528.201	490.839	492.194
1-y	529.434	528.245	491.001	492.145
1-y-out-in	529.467	528.299	490.917	492.315

Table S 11
Ranges of the ZPE correction for the conformers of the calculated trimeric acylphloroglucinols, grouping the molecules according to their formulas.
Since the difference between conformers with outstretched geometry and corresponding conformers with half-bowl-shaped geometry is marginal with respect to the value of the ZPE correction, the distinction between the two conformer types has been neglected for molecules with many conformers. When only one conformers-pair is present for a given molecule, the value for each conformer is reported, and the two values are separated by a comma.

molecular formula	molecule	range of ZPE correction (kcal/mol)	
		DFT results	DFT-D3 results
$C_{26}H_{24}O_{12}$	T1	296.54–297.28	296.99–297.78
$C_{30}H_{32}O_{12}$	T7	367.93–368.46	368.70–369.30
$C_{31}H_{34}O_{12}$	T3-ET6,2″	385.57 , 385.68	386.43 , 386.52
$C_{32}H_{36}O_{12}$	T2-KT2,6″-M5,5,3″,3″	401.57 , 401.67	402.85 , 402.92
	T7-ET6,2″	403.41 , 403.52	404.25 , 404.36
	T9	403.56–404.04	404.42–405.02
	T10	403.31–403.84	404.26–405.11
$C_{33}H_{38}O_{12}$	T3-M5,3″-ET6,2″	419.91 , 420.02	421.01 , 421.12
	T4-KT2,6″-M5,5,3″,3″	419.42 , 419.51	420.72 , 420.80
	T5-KT6″-M3″,3″-ET4	420.68, 420.76	421.70, 421.77
	T7-KT6″-M5,3″,3″	419.87–420.21	420.88–421.27
	T11-ET6,2″	421.00, 421.12	421.99, 422.11
$C_{34}H_{40}O_{12}$	T5-KT2,6″-M5,5,3″,3″	437.27, 437.37	438.57, 438.68
	T6-M5,3″-ET6,4″	438.00, 438.37	439.03, 439.54
	T7-M5,3″-ET6,2″	437.76, 437.86	438.84, 438.95
	T7-KT2,6″-M5,5,3″,3″	437.19, 437.27	438.55, 438.63
	T8-KT6″-M5,3″,3″	437.71–438.06	438.73–439.31
	T8-KT2-M5,5,3″	437.72–438.10	438.76–439.30
	T9-M5,3″	438.23–438.73	438.99–439.79
	T9-ET6,2″	439.04, 439.13	439.97, 440.09
	T10-ET6,2″	438.75, 438.85	439.77, 439.91
$C_{35}H_{42}O_{12}$	T8-KT2,6″-M5,5,3″,3″	455.03, 455.13	456.40, 456.52
	T9-KT6″-M5,3″,3″	455.48–455.82	456.59–457.29
	T9-KT6″-M3″,3″-ET4	456.20, 456.26	457.43, 457.38
	T11-M5,3″-ET6,2″	455.28, 455.41	456.53, 456.64
	T13-ET6,2″	456.74, 456.82	457.76, 457.89
	T14-ET6,2″	456.58, 456.62	457.70, 457.75
$C_{36}H_{44}O_{12}$	T9-M5,3″-ET6,2″	473.37, 473.47	474.54, 474.65
	T9-M5,3″-ET6,4″	473.58, 473.95	474.72, 475.22

	T9-KT6″-M5,3″,3″-ET6	473.11, 473.22	474.44, 474.54
	T9-KT2,6″-M5,5,3″,3″	472.78, 472.88	474.24, 474.52
	T10-M5,3″-ET6,2″	474.51, 473.09	474.34, 474.38
	T10-KT2,6″-M5,5,3″,3″	472.62, 472.38	474.35, 473.94
	T12-KT2-M5,5,3″	473.26, 473.72	474.42, 475.30
	T12-KT6″-M5,3″,3″	473.27, 473.63	474.44, 474.80
$C_{37}H_{46}O_{12}$	T10-M5,3″-ET6,2″,6″	490.00, 490.06	491.30, 491.26
	T13-M5,3″-ET6,2″	491.12, 491.19	492.42, 492.54
	T14-M5,3″-ET6,2″	490.84, 491.00	492.19, 492.15

Table S 12
Bond lengths of the intramolecular hydrogen bonds in the calculated trimeric acylphloroglucinols
HF/6-31G(d,p), HF/6-31+G(d,p), DFT/B3LYP//6-31+G(d,p) without Grimme's correction and DFT/B3LYP/6-31+G(d,p) with Grimme's correction results in vacuo, respectively denoted as HF, HF+, DFT and DFT-D3 in the columns' headings. Conformers of the same pair (outstretched and half-bowl-shaped) are listed one after the other to facilitate their comparison; the pairs are listed in order of increasing relative energy in the DFT/B3LYP/6-31+G(d,p) results.
The IHBs of a given conformer are listed "reading" the molecular geometry from left to right. The IHBs for which O14 (or O14′ or O14″) is the acceptor are the first IHBs in the corresponding monomers, and are listed first. The IHBs between monomers (IMHBs) are listed considering them in the following order: above the methylene bridge between the first and the second monomer; below the methylene bridge between the first and the second monomer; above the methylene bridge between the second and the third monomer; below the methylene bridge between the second and the third monomer. The atom numbering is shown in fig. 2.

Conformer	IHB considered	Length of given H-bond (Å)			
		HF	HF+	DFT	DFT-D3
structure T1					
1	H15····O14	1.626	1.631	1.473	1.480
	H17′····O14′	1.622	1.627	1.474	1.483
	H17″····O14″	1.632	1.637	1.483	1.491
	H16′····O8	1.815	1.822	1.709	1.689
	H16····O12′	1.851	1.855	1.758	1.741
	H16″····O10′	1.857	1.866	1.771	1.750
	H15′····O12″	1.847	1.854	1.749	1.732
1-y	H15····O14	1.630	1.634	1.476	1.483
	H17′····O14′	1.624	1.629	1.474	1.483
	H17″····O14″	1.632	1.637	1.484	1.494
	H16′····O8	1.837	1.846	1.726	1.702
	H16····O12′	1.863	1.868	1.761	1.746
	H16″····O10′	1.847	1.879	1.781	1.760
	H15′····O12″	1.870	1.855	1.750	1.735
2	H15····O14	1.624	1.629	1.469	1.477
	H17′····O14′	1.625	1.629	1.478	1.487
	H15″····O14″	1.691	1.696	1.557	1.568
	H16′····O8	1.857	1.818	1.701	1.682
	H16····O12′	1.811	1.861	1.766	1.749
	H17″····O10′	1.885	1.858	1.758	1.737
	H15′····O10″	1.849	1.897	1.801	1.788

2-y	H15····O14	1.626	1.631	1.471	1.474
	H17′····O14′	1.627	1.632	1.478	1.490
	H15″····O14″	1.691	1.697	1.557	1.573
	H16′····O8	1.828	1.837	1.714	1.675
	H16····O12′	1.867	1.872	1.770	1.761
	H17″····O10′	1.860	1.871	1.767	1.727
	H15′····O10″	1.889	1.903	1.805	1.810
3	H15····O14	1.631	1.636	1.481	1.490
	H15′····O14′	1.621	1.627	1.470	1.480
	H15″····O14″	1.690	1.696	1.556	1.567
	H17′····O8	1.846	1.853	1.746	1.730
	H16····O10′	1.861	1.870	1.780	1.760
	H17″····O8′	1.836	1.843	1.742	1.726
	H16′····O10″	1.852	1.865	1.769	1.753
3-y	H15····O14	1.631	1.636	1.481	1.490
	H15′····O14′	1.632	1.629	1.471	1.481
	H15″····O14″	1.690	1.696	1.556	1.567
	H17′····O8	1.844	1.851	1.747	1.732
	H16····O10′	1.865	1.874	1.782	1.762
	H17″····O8′	1.849	1.855	1.747	1.731
	H16′····O10″	1.870	1.884	1.780	1.760
4	H15····O14	1.650	1.656	1.492	1.502
	H17′····O14′	1.623	1.628	1.475	1.483
	H17″····O14″	1.632	1.637	1.483	1.492
	H10′····O8	1.819	1.828	1.716	1.697
	H16····O12′	1.852	1.858	1.759	1.742
	H16″····O10′	1.858	1.867	1.771	1.751
	H15′····O12″	1.848	1.855	1.750	1.733
4-y	H15····O14	1.650	1.661	1.496	1.505
	H17′····O14′	1.625	1.631	1.475	1.484
	H17″····O14″	1.633	1.638	1.484	1.494
	H10′····O8	1.842	1.852	1.733	1.709
	H16····O12′	1.867	1.873	1.764	1.749
	H16″····O10′	1.871	1.880	1.781	1.762
	H15′····O12″	1.850	1.858	1.751	1.737
5	H15····O14	1.648	1.653	1.490	1.499
	H17′····O14′	1.625	1.630	1.479	1.488
	H15″····O14″	1.691	1.697	1.557	1.568
	H16′····O8	1.816	1.824	1.709	1.790
	H16····O12′	1.859	1.864	1.768	1.751
	H16″····O10′	1.850	1.859	1.758	1.738
	H15′····O10″	1.886	1.898	1.802	1.788

5-y	H15⋯O14	1.649	1.656	1.491	1.500
	H17′⋯O14′	1.628	1.633	1.479	1.496
	H15″⋯O14″	1.693	1.699	1.559	1.584
	H16′⋯O8	1.831	1.841	1.720	1.686
	H16⋯O12′	1.868	1.875	1.771	1.779
	H16″⋯O10′	1.858	1.870	1.765	1.724
	H15′⋯O10″	1.889	1.905	1.805	1.837
6	H17⋯O14	1.692	1.698	1.559	1.570
	H15′⋯O14′	1.624	1.629	1.475	1.485
	H15″⋯O14″	1.690	1.696	1.556	1.567
	H15⋯O10′	1.857	1.866	1.770	1.750
	H17′⋯O10	1.887	1.898	1.800	1.788
	H16′⋯O10″	1.851	1.863	1.764	1.749
	H17″⋯O8′	1.843	1.850	1.751	1.735
6-y	H17⋯O14	1.694	1.700	1.561	1.572
	H15′⋯O14′	1.626	1.632	1.476	1.487
	H15″⋯O14″	1.691	1.696	1.556	1.567
	H15⋯O10′	1.866	1.877	1.777	1.756
	H17′⋯O10	1.890	1.902	1.806	1.800
	H16′⋯O10″	1.867	1.882	1.774	1.754
	H17″⋯O8′	1.854	1.861	1.754	1.742
7	H15⋯O14	1.654	1.661	1.500	1.511
	H15′⋯O14′	1.622	1.627	1.472	1.481
	H15″⋯O14″	1.690	1.696	1.556	1.567
	H17′⋯O8	1.850	1.857	1.753	1.736
	H16⋯O10′	1.863	1.871	1.780	1.761
	H17″⋯O8′	1.840	1.846	1.744	1.728
	H16′⋯O10″	1.853	1.866	1.769	1.753
7-y	H15⋯O14	1.654	1.660	1.501	1.511
	H15′⋯O14′	1.623	1.629	1.473	1.482
	H15″⋯O14″	1.691	1.696	1.556	1.568
	H17′⋯O8	1.846	1.854	1.753	1.738
	H16⋯O10′	1.863	1.873	1.780	1.761
	H17″⋯O8′	1.845	1.853	1.747	1.731
	H16′⋯O10″	1.862	1.878	1.775	1.755
8	H17⋯O14	1.626	1.631		
	H15′⋯O14′	1.625	1.631		
	H17″⋯O14″	1.742	1.651		
	H16′⋯O8	1.811	1.819		
	H16⋯O10′	1.856	1.861		
	H16″⋯O10′	1.857	1.867		
	H15′⋯O12″	1.876	1.889		

8-y	H17····O14	1.627	1.632	1.541	1.577
	H15′····O14′	1.629	1.634	1.482	1.489
	H17″····O14″	1.640	1.649	1.596	1.609
	H16′····O8	1.831	1.839	1.714	1.690
	H16····O10′	1.874	1.879	1.776	1.761
	H16″····O10′	1.872	1.882	1.784	1.769
	H15′····O12″	1.882	1.895	1.801	1.789
9	H15····O14	1.650	1.656	1.493	1.502
	H17′····O14′	1.624	1.629	1.476	1.485
	H17″····O14″	1.652	1.659	1.502	1.512
	H16′····O8	1.820	1.827	1.716	1.696
	H16····O12′	1.855	1.859	1.761	1.744
	H16″····O10′	1.863	1.871	1.773	1.752
	H15′····O12″	1.855	1.862	1.756	1.740
9-y	H15····O14	1.654	1.661	1.495	1.503
	H17′····O14′	1.626	1.632	1.477	1.487
	H17″····O14″	1.656	1.662	1.503	1.514
	H16′····O8	1.840	1.849	1.730	1.706
	H16····O12′	1.871	1.876	1.768	1.754
	H16″····O10′	1.872	1.881	1.782	1.762
	H15′····O12″	1.855	1.863	1.759	1.745
10	H15····O14	1.632	1.636	1.482	1.491
	H15′····O14′	1.622	1.628	1.474	1.485
	H15″····O14″	1.742	1.751	1.598	1.612
	H17′····O8	1.847	1.855	1.749	1.732
	H16····O10′	1.861	1.869	1.779	1.758
	H17″····O8′	1.849	1.857	1.757	1.746
	H16′····O12″	1.844	1.857	1.763	1.744
10-y	H15····O14	1.631	1.636	1.482	1.491
	H15′····O14′	1.628	1.623	1.475	1.486
	H15″····O14″	1.739	1.743	1.598	1.633
	H17′····O8	1.846	1.854	1.752	1.741
	H16····O10′	1.861	1.869	1.776	1.746
	H17″····O8′	1.875	1.881	1.762	1.757
	H16′····O12″	1.884	1.888	1.769	1.733
11	H15····O14	1.633	1.635	1.485	1.493
	H15′····O14′	1.630	1.633	1.485	1.494
	H15″····O14″	1.697	1.703	1.566	1.578
	H17′····O8	1.859	1.858	1.764	1.747
	H16′····O10	1.899	1.896	1.813	1.798
	H17″····O8′	1.836	1.838	1.757	1.738
	H16″····O10′	1.874	1.873	1.809	1.788

11-y	H15····O14	1.640	1.634	1.485	1.496
	H15′····O14′	1.629	1.634	1.486	1.495
	H15″····O14″	1.695	1.700	1.564	1.575
	H17′····O8	1.879	1.841	1.763	1.751
	H16····O10′	1.883	1.868	1.797	1.770
	H17″····O8′	1.852	1.843	1.765	1.749
	H16′····O10″	1.885	1.872	1.808	1.786
12	H15····O14	1.622	1.626	1.462	1.470
	H17′····O14′	1.666	1.675	1.510	1.521
	H15″····O14″	1.699	1.703	1.568	1.580
	H16′····O8	1.805	1.812	1.683	1.666
	H16····O12′	1.876	1.881	1.794	1.776
	H17″····O10′	1.857	1.865	1.781	1.762
	H16″····O8′	1.904	1.905	1.827	1.819
12-y	H15····O14	1.623	1.628	1.459	1.461
	H17′····O14′	1.660	1.670	1.513	1.527
	H15″····O14″	1.697	1.703	1.568	1.579
	H16′····O8	1.820	1.829	1.686	1.641
	H16····O12′	1.886	1.893	1.803	1.804
	H17″····O10′	1.927	1.925	1.787	1.758
	H16″····O8′	1.998	2.000	1.828	1.846
13	H17····O14	1.690	1.696	1.556	1.567
	H17′····O14′	1.625	1.630	1.478	1.488
	H15″····O14″	1.741	1.750	1.596	1.611
	H15····O12′	1.846	1.852	1.754	1.737
	H16′····O10	1.851	1.864	1.765	1.751
	H15′····O12″	1.874	1.887	1.794	1.778
	H16″····O10′	1.859	1.869	1.779	1.763
13-y	H17····O14	1.691	1.697	1.557	1.568
	H17′····O14′	1.626	1.632	1.478	1.488
	H15″····O14″	1.742	1.751	1.596	1.611
	H15····O12′	1.847	1.855	1.754	1.736
	H16′····O10	1.854	1.869	1.765	1.746
	H15′····O12″	1.870	1.885	1.795	1.780
	H16″····O10′	1.858	1.869	1.778	1.763
14	H17····O14	1.650	1.656	1.492	1.501
	H15′····O14′	1.626	1.631	1.481	1.491
	H17″····O14″	1.642	1.651	1.596	1.611
	H16′····O8	1.816	1.825	1.710	1.693
	H16····O12′	1.859	1.864	1.770	1.753
	H16″····O10′	1.857	1.867	1.772	1.756
	H15′····O12″	1.876	1.889	1.798	1.781

14-y	H17····O14	1.641	1.660	1.491	1.499
	H15′····O14′	1.630	1.635	1.483	1.493
	H17″····O14″	1.652	1.750	1.596	1.609
	H16′····O8	1.834	1.843	1.720	1.697
	H16····O12′	1.876	1.882	1.778	1.763
	H16″····O10′	1.869	1.878	1.781	1.767
	H15′····O12″	1.881	1.894	1.801	1.789
15	H15····O14	1.632	1.635	1.485	1.493
	H15′····O14′	1.637	1.640	1.490	1.500
	H15″····O14″	1.703	1.708	1.574	1.587
	H17′····O8	1.855	1.853	1.763	1.745
	H16····O10′	1.897	1.892	1.810	1.793
	H16″····O8′	1.866	1.859	1.774	1.760
	H17″····O10′	1.853	1.854	1.796	1.771
15-y	H15····O14	1.638	1.640	1.484	1.492
	H15′····O14′	1.642	1.646	1.491	1.500
	H15″····O14″	1.712	1.723	1.578	1.593
	H17′····O8	1.867	1.860	1.760	1.745
	H16····O10′	1.879	1.879	1.804	1.774
	H16″····O8′	1.918	1.915	1.780	1.768
	H17″····O10′	1.909	1.912	1.800	1.768
16	H15····O14	1.654	1.661	1.501	1.512
	H15′····O14′	1.623	1.629	1.496	1.486
	H15″····O14″	1.741	1.751	1.597	1.612
	H17′····O8	1.851	1.859	1.755	1.739
	H16····O10′	1.862	1.869	1.778	1.758
	H16″····O8′	1.852	1.859	1.760	1.749
	H17′····O10″	1.845	1.858	1.763	1.743
16-y	H15····O14	1.650	1.657	1.502	1.512
	H15′····O14′	1.628	1.633	1.477	1.488
	H15″····O14″	1.737	1.741	1.597	1.623
	H17′····O8	1.849	1.857	1.758	1.747
	H16····O10′	1.859	1.868	1.774	1.743
	H16″····O8′	1.871	1.877	1.762	1.757
	H17′····O10″	1.876	1.881	1.763	1.727
17	H17····O14	1.630	1.698	1.478	1.486
	H17′····O14′	1.633	1.633	1.493	1.501
	H17″····O14″	1.698	1.630	1.568	1.579
	H16′····O8	1.832	1.833	1.723	1.705
	H17′····O10	1.821	1.823	1.851	1.830
	H16″····O10′	1.879	1.882	1.812	1.790
	H17″····O8′	1.843	1.847	1.764	1.746

17-y	H17····O14	1.638	1.642	1.478	1.485
	H17′····O14′	1.636	1.638	1.493	1.502
	H17″····O14″	1.697	1.702	1.566	1.578
	H16′····O8	1.858	1.857	1.726	1.704
	H17′····O10	1.922	1.829	1.844	1.827
	H16″····O10′	1.901	1.900	1.821	1.801
	H17″····O8′	1.854	1.854	1.764	1.748
18	H15····O14	1.628	1.631	1.476	1.483
	H15′····O14′	1.639	1.643	1.498	1.508
	H15″····O14″	1.700	1.704	1.571	1.583
	H16′····O8	1.831	1.830	1.720	1.701
	H17′····O10	1.926	1.925	1.853	1.833
	H17″····O10′	1.851	1.855	1.794	1.768
	H16″····O8′	1.868	1.865	1.782	1.769
18-y	H15····O14	1.633	1.642	1.475	1.476
	H15′····O14′	1.645	1.638	1.500	1.514
	H15″····O14″	1.700	1.701	1.571	1.583
	H16′····O8	1.838	1.857	1.722	1.677
	H17′····O10	1.913	1.929	1.846	1.842
	H17″····O10′	1.882	1.900	1.805	1.768
	H16″····O8′	1.898	1.854	1.787	1.791
19	H15····O14	1.661	1.666	1.510	1.519
	H15′····O14′	1.630	1.634	1.486	1.495
	H15″····O14″	1.698	1.703	1.567	1.579
	H17′····O8	1.857	1.857	1.770	1.752
	H16′····O10	1.889	1.886	1.806	1.791
	H17″····O8′	1.838	1.840	1.758	1.739
	H16″····O10′	1.877	1.875	1.810	1.790
19-y	H15····O14	1.662	1.660	1.510	1.520
	H15′····O14′	1.630	1.634	1.488	1.496
	H15″····O14″	1.695	1.700	1.565	1.576
	H17′····O8	1.874	1.847	1.768	1.753
	H16′····O10	1.874	1.862	1.794	1.768
	H17″····O8′	1.849	1.843	1.765	1.748
	H16″····O10′	1.886	1.876	1.811	1.791
20	H17····O14	1.660	1.664	1.505	1.514
	H17′····O14′	1.632	1.635	1.491	1.500
	H17″····O14″	1.698	1.703	1.568	1.579
	H16′····O8	1.829	1.831	1.729	1.711
	H17′····O10	1.906	1.910	1.844	1.823
	H16″····O10′	1.877	1.880	1.811	1.790
	H17″····O8′	1.842	1.845	1.763	1.744

20-y	H17····O14	1.671	1.677	1.505	1.513
	H17′····O14′	1.635	1.637	1.492	1.501
	H17″····O14″	1.696	1.701	1.566	1.577
	H16′····O8	1.855	1.854	1.731	1.709
	H17′····O10	1.913	1.921	1.840	1.822
	H16″····O10′	1.894	1.894	1.818	1.798
	H17″····O8′	1.852	1.852	1.764	1.748
21	H15····O14	1.661	1.665	1.511	1.520
	H15′····O14′	1.637	1.640	1.491	1.501
	H15″····O14″	1.702	1.707	1.574	1.586
	H17′····O8	1.854	1.851	1.769	1.751
	H16′····O10	1.887	1.880	1.803	1.786
	H16″····O8′	1.865	1.859	1.775	1.761
	H17′····O10″	1.853	1.854	1.797	1.772
21-y	H15····O14	1.667	1.670	1.509	1.519
	H15′····O14′	1.642	1.647	1.492	1.501
	H15″····O14″	1.709	1.719	1.577	1.590
	H17′····O8	1.867	1.860	1.766	1.750
	H16′····O10	1.874	1.875	1.801	1.773
	H16″····O8′	1.914	1.908	1.780	1.767
	H17′····O10″	1.906	1.909	1.803	1.773
22	H15····O14	1.658	1.661	1.503	1.511
	H15′····O14′	1.638	1.641	1.497	1.507
	H15″····O14″	1.700	1.705	1.572	1.584
	H16′····O8	1.830	1.829	1.727	1.708
	H17′····O10	1.915	1.914	1.846	1.825
	H17″····O10′	1.849	1.854	1.794	1.768
	H16″····O8′	1.867	1.864	1.781	1.768
22-y	H15····O14	1.662	1.669	1.502	1.499
	H15′····O14′	1.644	1.647	1.498	1.532
	H15″····O14″	1.701	1.710	1.573	1.584
	H16′····O8	1.833	1.834	1.727	1.675
	H17′····O10	1.903	1.906	1.841	1.859
	H17″····O10′	1.881	1.891	1.803	1.749
	H16″····O8′	1.901	1.898	1.787	1.884
23	H15····O14	1.646	1.652	1.485	1.494
	H17′····O14′	1.668	1.676	1.512	1.523
	H15″····O14″	1.699	1.704	1.569	1.581
	H16′····O8	1.812	1.819	1.692	1.675
	H16····O12′	1.881	1.885	1.796	1.779
	H17″····O10′	1.857	1.865	1.781	1.762
	H16″····O8′	1.905	1.906	1.826	1.819

23-y	H15⋯O14	1.644	1.651	1.482	1.491
	H17′⋯O14′	1.676	1.685	1.514	1.541
	H15″⋯O14″	1.699	1.704	1.570	1.580
	H16′⋯O8	1.804	1.816	1.692	1.640
	H16⋯O12′	1.888	1.893	1.803	1.833
	H17″⋯O10′	1.872	1.881	1.786	1.843
	H16″⋯O8′	1.926	1.925	1.829	1.944
24	H17⋯O14	1.649	1.655	1.487	1.496
	H15′⋯O14′	1.674	1.680	1.514	1.524
	H17″⋯O14″	1.702	1.708	1.573	1.584
	H16′⋯O8	1.813	1.821	1.692	1.675
	H16⋯O12′	1.879	1.884	1.797	1.780
	H16″⋯O10′	1.895	1.903	1.788	1.770
	H17″⋯O8′	1.919	1.914	1.810	1.794
24-y	H17⋯O14	1.650	1.658	1.484	1.492
	H15′⋯O14′	1.679	1.689	1.517	1.529
	H17″⋯O14″	1.700	1.706	1.571	1.582
	H15⋯O12′	1.818	1.828	1.695	1.671
	H16⋯O10′	1.895	1.902	1.810	1.794
	H16″⋯O8′	1.883	1.887	1.792	1.777
	H16′⋯O12″	1.880	1.886	1.808	1.798
25	H17⋯O14	1.736	1.745	1.588	1.602
	H15′⋯O14′	1.632	1.636	1.489	1.498
	H15″⋯O14″	1.697	1.703	1.566	1.578
	H16′⋯O8	1.864	1.863	1.764	1.751
	H17′⋯O10	1.887	1.893	1.813	1.801
	H16″⋯O10′	1.878	1.875	1.807	1.786
	H17″⋯O8′	1.842	1.843	1.762	1.743
25-y	H17⋯O14	1.748	1.751	1.588	1.589
	H15′⋯O14′	1.633	1.636	1.490	1.499
	H15″⋯O14″	1.696	1.701	1.565	1.578
	H16′⋯O8	1.826	1.836	1.748	1.744
	H17′⋯O10	1.878	1.878	1.816	1.879
	H16″⋯O10′	1.875	1.875	1.805	1.830
	H17″⋯O8′	1.857	1.852	1.771	1.769
26	H17⋯O14	1.694	1.699	1.561	1.573
	H15′⋯O14′	1.682	1.689	1.529	1.541
	H15″⋯O14″	1.701	1.706	1.572	1.584
	H15⋯O12′	1.887	1.898	1.820	1.805
	H16′⋯O10	1.844	1.856	1.752	1.743
	H16″⋯O8′	1.897	1.891	1.799	1.787
	H17″⋯O10′	1.873	1.878	1.803	1.780

26-y	H17····O14	1.695	1.701	1.562	1.587
	H15′····O14′	1.694	1.702	1.529	1.540
	H15″····O14″	1.703	1.707	1.574	1.574
	H15····O12′	1.881	1.899	1.820	1.778
	H16′····O10	1.833	1.853	1.750	1.787
	H16″····O8′	1.907	1.895	1.799	1.734
	H17″····O10′	1.888	1.887	1.807	1.808
27	H17····O14	1.736	1.746	1.590	1.579
	H15′····O14′	1.637	1.641	1.490	1.499
	H15″····O14″	1.698	1.703	1.567	1.603
	H17′····O8	1.926	1.921	1.798	1.744
	H16′····O10	1.900	1.892	1.770	1.791
	H17″····O8′	1.846	1.848	1.763	1.778
	H16″····O10′	1.886	1.883	1.812	1.755
27-y	H17····O14	1.737	1.746	1.590	1.577
	H15′····O14′	1.635	1.637	1.492	1.500
	H15″····O14″	1.697	1.702	1.565	1.604
	H17′····O8	1.911	1.905	1.805	1.752
	H16′····O10	1.884	1.877	1.767	1.798
	H17″····O8′	1.847	1.848	1.769	1.802
	H16″····O10′	1.883	1.881	1.815	1.754
28	H17····O14	1.736	1.746	1.588	1.603
	H15′····O14′	1.640	1.644	1.493	1.504
	H15″····O14″	1.703	1.708	1.575	1.587
	H16′····O8	1.865	1.862	1.761	1.747
	H17′····O10	1.885	1.888	1.812	1.801
	H16″····O8′	1.858	1.860	1.794	1.768
	H17′····O10″	1.872	1.866	1.778	1.765
28-y	H17····O14	1.740	1.749	1.587	1.595
	H15′····O14′	1.637	1.650	1.494	1.523
	H15″····O14″	1.703	1.726	1.578	1.596
	H16′····O8	1.866	1.867	1.758	1.784
	H17′····O10	1.887	1.912	1.807	1.899
	H16″····O8′	1.867	1.918	1.801	1.738
	H17′····O10″	1.865	1.923	1.783	1.857
29	H17····O14	1.736	1.745	1.589	1.589
	H15′····O14′	1.645	1.651	1.496	1.496
	H15″····O14″	1.702	1.707	1.574	1.574
	H17′····O8	1.925	1.918	1.799	1.799
	H16′····O10	1.903	1.893	1.770	1.770
	H16″····O8′	1.874	1.866	1.781	1.781
	H17′····O10″	1.864	1.864	1.799	1.799

29-y	H17····O14	1.735	1.745	1.590	1.605
	H15′····O14′	1.643	1.646	1.496	1.606
	H15″····O14″	1.703	1.708	1.576	1.590
	H17′····O8	1.920	1.919	1.798	1.787
	H16′····O10	1.899	1.897	1.770	1.748
	H16″····O8′	1.888	1.880	1.784	1.771
	H17′····O10″	1.879	1.881	1.806	1.779

structure T2-KT2,6″-M5,5,3″,3″

1	H17····O14	1.637	1.643	1.451	1.469
	H15′····O14′	1.610	1.612	1.460	1.468
	H15″····O14″	1.637	1.643	1.451	1.469
	H17′····O8	1.745	1.749	1.640	1.625
	H16····O10′	1.831	1.836	1.720	1.696
	H16″····O8′	1.841	1.845	1.718	1.697
	H16′····O12″	1.709	1.711	1.580	1.562
1-y	H17····O14	1.637	1.643	1.451	1.469
	H15′····O14′	1.612	1.613	1.460	1.468
	H15″····O14″	1.638	1.644	1.452	1.471
	H17′····O8	1.747	1.748	1.640	1.627
	H16····O10′	1.853	1.858	1.731	1.698
	H16″····O8′	1.844	1.848	1.722	1.704
	H16′····O12″	1.723	1.727	1.595	1.566

structure T3-ET6,2″

1	H15····O14	1.620	1.625	1.469	1.478
	H15′····O14′	1.620	1.630	1.452	1.464
	H17″····O14″	1.615	1.620	1.459	1.468
	H17′····O8	1.845	1.550	1.742	1.723
	H16····O10′	1.861	1.870	1.770	1.750
	H16″····O8′	1.853	1.857	1.754	1.737
	H16′····O12″	1.813	1.813	1.705	1.786
1-y	H15····O14	1.621	1.626	1.470	1.478
	H15′····O14′	1.636	1.646	1.452	1.470
	H17″····O14″	1.618	1.623	1.463	1.471
	H17′····O8	1.846	1.857	1.743	1.721
	H16····O10′	1.873	1.883	1.777	1.764
	H16″····O8′	1.864	1.869	1.759	1.742
	H16′····O12″	1.834	1.844	1.722	1.697

structure T3-M5,3″-ET6,2″

1	H15····O14	1.659	1.668	1.488	1.499
	H15′····O14′	1.624	1.634	1.451	1.462
	H17″····O14″	1.649	1.658	1.479	1.491
	H17′····O8	1.835	1.646	1.731	1.771
	H16····O10′	1.854	1.866	1.760	1.741
	H16″····O8′	1.853	1.858	1.752	1.735
	H16′····O12″	1.810	1.818	1.700	1.682
1-y	H15····O14	1.660	1.669	1.488	1.501
	H15′····O14′	1.636	1.646	1.450	1.462
	H17″····O14″	1.657	1.667	1.481	1.492
	H17′····O8	1.837	1.849	1.733	1.719
	H16····O10′	1.865	1.876	1.770	1.750
	H16″····O8′	1.857	1.865	1.749	1.736
	H16′····O12″	1.821	1.831	1.708	1.686

structure T4-KT2,6″-M5,5,3″,3″

1	H17····O14	1.632	1.635	1.452	1.468
	H15′····O14′	1.610	1.612	1.460	1.468
	H15″····O14″	1.637	1.643	1.451	1.469
	H17′····O8	1.743	1.746	1.638	1.638
	H16····O10′	1.831	1.836	1.721	1.696
	H16″····O8′	1.841	1.845	1.717	1.696
	H16′····O12″	1.709	1.711	1.581	1.563
1-y	H17····O14	1.631	1.635	1.451	1.467
	H15′····O14′	1.612	1.613	1.460	1.469
	H15″····O14″	1.639	1.644	1.452	1.471
	H17′····O8	1.745	1.747	1.637	1.624
	H16····O10′	1.853	1.858	1.732	1.700
	H16″····O8′	1.844	1.844	1.722	1.704
	H16′····O12″	1.723	1.727	1.596	1.567

structure T5-KT6″-M3″,3″-ET4

1	H17····O14	1.685	1.689	1.553	1.564
	H17′····O14′	1.616	1.619	1.470	1.479
	H15″····O14″	1.631	1.634	1.449	1.466
	H15····O12′	1.838	1.845	1.742	1.727
	H16′····O10	1.827	1.834	1.733	1.702
	H15′····O12″	1.741	1.744	1.636	1.622
	H16″····O10′	1.844	1.851	1.747	1.720
1-y	H17····O14	1.685	1.688	1.553	1.563
	H17′····O14′	1.619	1.622	1.471	1.481

	H15″····O14″	1.631	1.634	1.449	1.466
	H15····O12′	1.831	1.867	1.753	1.736
	H16′····O10	1.851	1.860	1.751	1.705
	H15′····O12″	1.742	1.744	1.635	1.624
	H16″····O10′	1.854	1.860	1.752	1.715

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structure T5-KT2,6″-M5,5,3″,3″

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1	H17····O14	1.632	1.635	1.452	1.468
	H15′····O14′	1.610	1.612	1.460	1.468
	H15″····O14″	1.631	1.635	1.451	1.468
	H17′····O8	1.743	1.747	1.638	1.623
	H16····O10′	1.830	1.835	1.720	1.696
	H16″····O8′	1.840	1.845	1.718	1.697
	H16′····O12″	1.707	1.709	1.578	1.560
1-y	H17····O14	1.631	1.635	1.451	1.466
	H15′····O14′	1.612	1.613	1.461	1.471
	H15″····O14″	1.632	1.636	1.452	1.475
	H17′····O8	1.745	1.747	1.637	1.628
	H16····O10′	1.853	1.857	1.731	1.691
	H16″····O8′	1.844	1.848	1.722	1.714
	H16′····O12″	1.721	1.725	1.593	1.556

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structure T6-M5,3″-ET6,4″

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1	H15····O14	1.658	1.665	1.491	1.495
	H15′····O14′	1.624	1.629	1.490	1.482
	H15″····O14″	1.673	1.682	1.563	1.556
	H17′····O8	1.830	1.838	1.704	1.715
	H16····O10′	1.850	1.860	1.754	1.739
	H17″····O8′	1.853	1.862	1.780	1.736
	H16′····O10″	1.804	1.807	1.818	1.660
1-y	H15····O14	1.657	1.664	1.484	1.495
	H15′····O14′	1.626	1.631	1.474	1.484
	H15″····O14″	1.673	1.682	1.546	1.556
	H17′····O8	1.826	1.834	1.727	1.715
	H16····O10′	1.866	1.875	1.778	1.756
	H17″····O8′	1.868	1.875	1.761	1.743
	H16′····O10″	1.821	1.823	1.698	1.668
1-y-in-out	H15····O14	1.654	1.660	1.485	1.496
	H15′····O14′	1.618	1.630	1.475	1.484
	H15″····O14″	1.674	1.684	1.546	1.557
	H17′····O8	1.837	1.842	1.736	1.722

	H16····O10′	1.874	1.883	1.786	1.762
	H17″····O8′	1.864	1.875	1.761	1.742
	H16′····O10″	1.822	1.823	1.699	1.668
1-y-in-in	H15····O14	1.651	1.657	1.484	1.492
	H15′····O14′	1.622	1.633	1.474	1.489
	H15″····O14″	1.687	1.692	1.549	1.562
	H17′····O8	1.819	1.824	1.732	1.711
	H16····O10′	1.876	1.885	1.795	1.764
	H17″····O8′	1.895	1.904	1.771	1.779
	H16′····O10″	1.990	2.909	1.837	1.823

<div align="center">**structure T7**</div>

1	H15····O14	1.619	1.621	1.469	1.476
	H17′····O14′	1.615	1.617	1.471	1.479
	H17″····O14″	1.632	1.637	1.484	1.492
	H16′····O8	1.813	1.820	1.706	1.687
	H16····O12′	1.849	1.853	1.756	1.739
	H16″····O10′	1.855	1.863	1.767	1.747
	H15′····O12″	1.848	1.855	1.751	1.733
1-y	H15····O14	1.622	1.625	1.473	1.479
	H17′····O14′	1.618	1.620	1.471	1.480
	H17″····O14″	1.633	1.638	1.485	1.494
	H16′····O8	1.835	1.843	1.724	1.699
	H16····O12′	1.862	1.866	1.760	1.745
	H16″····O10′	1.868	1.877	1.778	1.758
	H15′····O12″	1.838	1.858	1.752	1.737
2	H15····O14	1.617	1.619	1.466	1.473
	H17′····O14′	1.617	1.619	1.475	1.483
	H15″····O14″	1.691	1.696	1.557	1.568
	H16′····O8	1.809	1.816	1.698	1.679
	H16····O12′	1.855	1.859	1.764	1.747
	H17″····O10′	1.848	1.857	1.754	1.734
	H15′····O10″	1.886	1.899	1.804	1.789
2-y	H15····O14	1.619	1.622	1.468	1.478
	H17′····O14′	1.620	1.623	1.475	1.484
	H15″····O14″	1.691	1.697	1.558	1.566
	H16′····O8	1.825	1.834	1.712	1.676
	H16····O12′	1.865	1.870	1.768	1.750
	H17″····O10′	1.859	1.869	1.764	1.713
	H15′····O10″	1.891	1.906	1.807	1.789
3	H15····O14	1.624	1.627	1.478	1.486
	H15′····O14′	1.614	1.617	1.467	1.475

	H15″····O14″	1.691	1.696	1.556	1.567
	H17′····O8	1.844	1.851	1.744	1.727
	H16····O10′	1.861	1.869	1.779	1.760
	H17″····O8′	1.834	1.840	1.738	1.722
	H16′····O10″	1.853	1.866	1.771	1.755
3-y	H15····O14	1.624	1.627	1.478	1.486
	H15′····O14′	1.616	1.619	1.468	1.476
	H15″····O14″	1.690	1.696	1.556	1.567
	H17′····O8	1.842	1.849	1.745	1.729
	H16····O10′	1.864	1.873	1.781	1.762
	H17″····O8′	1.846	1.851	1.743	1.727
	H16′····O10″	1.871	1.885	1.781	1.762
4	H15····O14	1.642	1.647	1.489	1.498
	H17′····O14′	1.616	1.619	1.472	1.480
	H17″····O14″	1.633	1.637	1.484	1.493
	H10′····O8	1.817	1.825	1.712	1.693
	H16····O12′	1.852	1.857	1.758	1.742
	H16″····O10′	1.856	1.864	1.768	1.747
	H15′····O12″	1.849	1.857	1.753	1.734
4-y	H15····O14	1.646	1.652	1.493	1.501
	H17′····O14′	1.619	1.622	1.472	1.481
	H17″····O14″	1.634	1.639	1.485	1.495
	H10′····O8	1.839	1.848	1.729	1.705
	H16····O12′	1.867	1.872	1.763	1.749
	H16″····O10′	1.869	1.878	1.778	1.758
	H15′····O12″	1.852	1.860	1.754	1.739
5	H15····O14	1.640	1.644	1.486	1.495
	H17′····O14′	1.619	1.621	1.476	1.485
	H15″····O14″	1.691	1.697	1.556	1.568
	H16′····O8	1.814	1.821	1.704	1.687
	H16····O12′	1.859	1.863	1.766	1.750
	H16″····O10′	1.848	1.857	1.754	1.734
	H15′····O10″	1.888	1.900	1.804	1.790
5-y	H15····O14	1.642	1.646	1.491	1.506
	H17′····O14′	1.622	1.625	1.479	1.541
	H15″····O14″	1.693	1.699	1.559	1.646
	H16′····O8	1.827	1.838	1.720	2.125
	H16····O12′	1.868	1.874	1.771	1.454
	H16″····O10′	1.855	1.868	1.765	1.780
	H15′····O10″	1.891	1.908	1.805	1.801
6	H17····O14	1.686	1.689	1.554	1.565
	H15′····O14′	1.617	1.619	1.471	1.480

	H15″····O14″	1.691	1.696	1.556	1.567
	H15····O10′	1.857	1.867	1.768	1.748
	H16′····O10	1.887	1.899	1.800	1.788
	H16′····O10″	1.852	1.866	1.766	1.751
	H17″····O10′	1.841	1.847	1.747	1.732
6-y	H17····O14	1.689	1.693	1.556	1.576
	H15′····O14′	1.619	1.622	1.471	1.490
	H15″····O14″	1.691	1.696	1.557	1.567
	H15····O10′	1.863	1.875	1.776	1.756
	H16′····O10	1.892	1.905	1.807	1.839
	H16′····O10″	1.866	1.882	1.776	1.770
	H17″····O10′	1.851	1.857	1.750	1.770

structure T7-ET6,2″

1	H15····O14	1.614	1.610	1.467	1.476
	H15′····O14′	1.616	1.618	1.472	1.480
	H17″····O14″	1.615	1.625	1.459	1.469
	H16′····O8	1.841	1.817	1.742	1.725
	H16····O12′	1.860	1.857	1.773	1.753
	H16″····O10′	1.851	1.866	1.757	1.740
	H15′····O12″	1.813	1.852	1.707	1.688
1-y	H15····O14	1.614	1.617	1.468	1.477
	H15′····O14′	1.618	1.621	1.472	1.481
	H17″····O14″	1.618	1.623	1.463	1.471
	H16′····O8	1.842	1.850	1.742	1.728
	H16····O12′	1.873	1.882	1.784	1.764
	H16″····O10′	1.863	1.868	1.762	1.747
	H15′····O12″	1.835	1.844	1.725	1.699

structure T7-M5,3″-ET6,2″

1	H15····O14	1.656	1.663	1.487	1.498
	H15′····O14′	1.615	1.618	1.469	1.477
	H17″····O14″	1.654	1.662	1.478	1.490
	H16′····O8	1.843	1.849	1.739	1.723
	H16····O12′	1.862	1.871	1.771	1.750
	H16″····O10′	1.844	1.850	1.748	1.732
	H15′····O12″	1.803	1.811	1.696	1.679
1-y	H15····O14	1.659	1.666	1.486	1.498
	H15′····O14′	1.617	1.620	1.469	1.478
	H17″····O14″	1.658	1.667	1.482	1.492
	H16′····O8	1.834	1.842	1.731	1.720

	H16····O12′	1.865	1.875	1.773	1.752
	H16″····O10′	1.858	1.864	1.753	1.740
	H15′····O12″	1.823	1.832	1.712	1.688
structure T7-KT6″-M5,3″,3″					
1	H15····O14	1.624	1.628	1.481	1.489
	H15′····O14′	1.610	1.612	1.460	1.468
	H15″····O14″	1.637	1.642	1.451	1.469
	H17′····O8	1.827	1.836	1.734	1.715
	H16····O10′	1.829	1.840	1.742	1.720
	H16″····O8′	1.844	1.848	1.720	1.699
	H16′····O12″	1.713	1.717	1.587	1.571
1-y	H15····O14	1.626	1.629	1.483	1.490
	H15′····O14′	1.611	1.613	1.460	1.468
	H15″····O14″	1.638	1.643	1.451	1.470
	H17′····O8	1.834	1.840	1.736	1.721
	H16····O10′	1.851	1.860	1.755	1.730
	H16″····O8′	1.844	1.849	1.723	1.706
	H16′····O12″	1.723	1.730	1.599	1.573
2	H15····O14	1.617	1.620	1.468	1.474
	H17′····O14′	1.614	1.638	1.469	1.477
	H15″····O14″	1.637	1.643	1.449	1.466
	H16′····O8	1.796	1.802	1.688	1.667
	H16····O12′	1.831	1.838	1.741	1.724
	H16″····O10′	1.843	1.850	1.738	1.714
	H16′····O12″	1.741	1.745	1.634	1.619
2-y	H15····O14	1.617	1.624	1.473	1.477
	H17′····O14′	1.614	1.619	1.470	1.479
	H15″····O14″	1.637	1.642	1.449	1.465
	H16′····O8	1.796	1.826	1.706	1.676
	H16····O12′	1.831	1.852	1.747	1.731
	H16″····O10′	1.843	1.866	1.745	1.716
	H16′····O12″	1.741	1.746	1.634	1.620
3	H17····O14	1.654	1.657	1.529	1.538
	H15′····O14′	1.613	1.615	1.465	1.472
	H15″····O14″	1.637	1.642	1.449	1.468
	H15····O10′	1.827	1.840	1.739	1.715
	H17′····O10	1.863	1.879	1.790	1.773
	H16′····O12″	1.708	1.712	1.579	1.563
	H16″····O8′	1.849	1.854	1.729	1.708
3-y	H17····O14	1.653	1.657	1.529	1.562
	H15′····O14′	1.615	1.617	1.465	1.477

	H15″····O14″	1.638	1.644	1.449	1.468
	H15····O10′	1.872	1.878	1.739	1.751
	H17′····O10	1.882	1.892	1.790	1.841
	H16′····O12″	1.722	1.727	1.579	1.568
	H16″····O8′	1.847	1.852	1.729	1.724
4	H17····O14	1.654	1.657	1.528	1.537
	H17′····O14′	1.613	1.616	1.468	1.477
	H15″····O14″	1.637	1.652	1.449	1.468
	H15····O12′	1.827	1.837	1.739	1.722
	H17′····O10	1.835	1.847	1.752	1.734
	H15′····O12″	1.740	1.744	1.635	1.621
	H16″····O10′	1.845	1.852	1.748	1.725
4-y	H17····O14	1.653	1.656	1.527	1.536
	H17′····O14′	1.618	1.620	1.470	1.480
	H15″····O14″	1.637	1.642	1.449	1.467
	H15····O12′	1.853	1.861	1.749	1.737
	H17′····O10	1.865	1.878	1.772	1.751
	H15′····O12″	1.742	1.745	1.637	1.624
	H16″····O10′	1.857	1.863	1.752	1.723
5	H17····O14	1.677	1.678	1.543	1.554
	H15′····O14′	1.657	1.659	1.497	1.507
	H15″····O14″	1.636	1.641	1.446	1.464
	H15····O10′	1.852	1.857	1.761	1.743
	H16····O12′	1.930	1.923	1.832	1.827
	H16′····O12″	1.696	1.698	1.559	1.544
	H16″····O8′	1.868	1.872	1.759	1.738
5-y	H17····O14	1.678	1.682	1.545	1.562
	H15′····O14′	1.663	1.667	1.499	1.509
	H15″····O14″	1.675	1.640	1.444	1.461
	H15····O10′	1.872	1.874	1.775	1.756
	H16····O12′	1.937	1.937	1.834	1.860
	H16′····O12″	1.698	1.702	1.564	1.535
	H16″····O8′	1.872	1.877	1.762	1.745
6	H17····O14	1.682	1.687	1.554	1.566
	H15′····O14′	1.659	1.661	1.498	1.508
	H15″····O14″	1.665	1.641	1.446	1.464
	H15····O12′	1.921	1.915	1.814	1.802
	H16····O10′	1.869	1.874	1.766	1.751
	H16″····O8′	1.869	1.870	1.760	1.738
	H16′····O12″	1.698	1.700	1.560	1.546
6-y	H17····O14	1.681	1.685	1.554	1.565
	H15′····O14′	1.653	1.655	1.501	1.513

	H15″····O14″	1.634	1.639	1.443	1.462
	H15····O12′	1.943	1.935	1.810	1.811
	H16····O10′	1.898	1.903	1.771	1.753
	H16″····O8′	1.879	1.883	1.770	1.756
	H16′····O12″	1.697	1.702	1.559	1.529
7	H17····O14	1.666	1.670	1.541	1.552
	H17′····O14′	1.623	1.625	1.481	1.490
	H15″····O14″	1.632	1.637	1.427	1.447
	H15····O12′	1.840	1.841	1.753	1.734
	H16····O10′	1.883	1.881	1.807	1.788
	H15′····O12″	1.795	1.796	1.679	1.673
	H16″····O10′	1.949	1.947	1.859	1.844
7-y	H17····O14	1.663	1.664	1.539	1.556
	H17′····O14′	1.626	1.625	1.482	1.495
	H15″····O14″	1.632	1.637	1.429	1.451
	H15····O12′	1.859	1.852	1.762	1.750
	H16····O10′	1.885	1.880	1.807	1.761
	H15′····O12″	1.798	1.791	1.673	1.672
	H16″····O10′	1.938	1.934	1.838	1.801
8	H17····O14	1.671	1.674	1.551	1.561
	H17′····O14′	1.632	1.634	1.486	1.496
	H15″····O14″	1.632	1.637	1.427	1.447
	H15····O10′	1.858	1.861	1.794	1.769
	H16····O12′	1.868	1.862	1.767	1.755
	H16′····O10″	1.947	1.944	1.856	1.839
	H15′····O12″	1.794	1.794	1.679	1.673
8-y	H17····O14	1.681	1.699	1.554	1.595
	H17′····O14′	1.635	1.637	1.487	1.504
	H15″····O14″	1.633	1.637	1.428	1.450
	H15····O10′	1.889	1.901	1.798	1.767
	H16····O12′	1.902	1.907	1.773	1.801
	H16′····O10″	1.932	1.932	1.842	1.796
	H15′····O12″	1.788	1.790	1.673	1.661
9	H17····O14	1.676	1.678	1.543	1.553
	H17′····O14′	1.627	1.629	1.492	1.501
	H15″····O14″	1.630	1.635	1.422	1.443
	H15····O12′	1.835	1.840	1.767	1.750
	H16····O10′	1.860	1.865	1.797	1.776
	H15′····O10″	1.979	1.979	1.903	1.883
	H16′····O12″	1.767	1.767	1.633	1.626
9-y	H17····O14	1.676	1.677	1.550	1.552
	H17′····O14′	1.629	1.631	1.491	1.501

	H15″····O14″	1.634	1.636	1.417	1.441
	H15····O12′	1.860	1.850	1.761	1.760
	H16····O10′	1.911	1.898	1.801	1.799
	H15′····O10″	1.968	1.961	1.894	1.902
	H16′····O12″	1.750	1.756	1.627	1.605
10	H17····O14	1.678	1.680	1.547	1.557
	H17′····O14′	1.636	1.637	1.498	1.509
	H15″····O14″	1.630	1.635	1.422	1.443
	H15····O10′	1.842	1.846	1.782	1.758
	H16····O12′	1.969	1.967	1.787	1.778
	H16′····O12″	1.763	1.762	1.631	1.621
	H15′····O10″	1.981	1.981	1.905	1.884
10-y	H17····O14	1.681	1.690	1.550	1.563
	H17′····O14′	1.641	1.645	1.499	1.521
	H15″····O14″	1.629	1.635	1.417	1.435
	H15····O10′	1.889	1.891	1.795	1.787
	H16····O12′	1.915	1.912	1.791	1.841
	H16′····O12″	1.757	1.759	1.631	1.605
	H15′····O10″	1.974	1.977	1.897	1.933
structure T7-KT2,6″-M5,5,3″,3″					
1	H17····O14	1.630	1.633	1.450	1.466
	H15′····O14′	1.610	1.622	1.460	1.468
	H15″····O14″	1.637	1.643	1.451	1.469
	H17′····O8	1.743	1.746	1.637	1.621
	H16····O10′	1.831	1.836	1.721	1.697
	H16″····O8′	1.840	1.845	1.717	1.696
	H16′····O12″	1.708	1.711	1.581	1.563
1-y	H17····O14	1.630	1.633	1.449	1.465
	H15′····O14′	1.612	1.613	1.460	1.469
	H15″····O14″	1.639	1.644	1.452	1.470
	H17′····O8	1.744	1.746	1.636	1.623
	H16····O10′	1.853	1.858	1.733	1.701
	H16″····O8′	1.844	1.848	1.722	1.704
	H16′····O12″	1.723	1.728	1.597	1.567
structure T8-KT6″-M5,3″,3″					
1	H15····O14	1.625	1.628	1.481	1.488
	H15′····O14′	1.610	1.612	1.461	1.468
	H15″····O14″	1.631	1.635	1.451	1.467
	H17′····O8	1.827	1.836	1.735	1.715

	H16····O10′	1.829	1.839	1.741	1.719
	H16″····O8′	1.843	1.848	1.721	1.700
	H16′····O12″	1.711	1.715	1.585	1.568
1-y	H15····O14	1.626	1.630	1.483	1.491
	H15′····O14′	1.611	1.613	1.460	1.469
	H15″····O14″	1.632	1.635	1.452	1.470
	H17′····O8	1.835	1.840	1.736	1.723
	H16····O10′	1.851	1.859	1.754	1.726
	H16″····O8′	1.847	1.850	1.724	1.709
	H16′····O12″	1.722	1.728	1.597	1.567
2	H15····O14	1.617	1.620	1.468	1.474
	H17′····O14′	1.614	1.616	1.469	1.477
	H15″····O14″	1.631	1.635	1.451	1.468
	H16′····O8	1.796	1.803	1.688	1.667
	H16····O12′	1.831	1.838	1.741	1.724
	H16″····O10′	1.842	1.849	1.738	1.714
	H16′····O12″	1.739	1.742	1.635	1.620
2-y	H15····O14	1.621	1.621	1.473	1.477
	H17′····O14′	1.617	1.619	1.470	1.479
	H15″····O14″	1.631	1.634	1.451	1.467
	H16′····O8	1.818	1.826	1.706	1.675
	H16····O12′	1.845	1.852	1.747	1.731
	H16″····O10′	1.860	1.866	1.745	1.715
	H16′····O12″	1.743	1.744	1.635	1.621
3	H17····O14	1.654	1.658	1.529	1.538
	H15′····O14′	1.613	1.615	1.466	1.473
	H15″····O14″	1.631	1.634	1.450	1.466
	H15····O10′	1.827	1.839	1.737	1.714
	H17′····O10	1.863	1.879	1.791	1.774
	H16′····O12″	1.706	1.710	1.576	1.559
	H16″····O8′	1.849	1.854	1.730	1.705
3-y	H17····O14	1.655	1.659	1.529	1.547
	H15′····O14′	1.615	1.617	1.466	1.476
	H15″····O14″	1.634	1.638	1.452	1.466
	H15····O10′	1.876	1.879	1.766	1.737
	H17′····O10	1.887	1.894	1.795	1.812
	H16′····O12″	1.722	1.726	1.593	1.566
	H16″····O8′	1.846	1.851	1.732	1.718
4	H17····O14	1.654	1.657	1.528	1.537
	H17′····O14′	1.613	1.616	1.468	1.477
	H15″····O14″	1.631	1.634	1.450	1.466
	H15····O12′	1.827	1.836	1.738	1.722

	H17′····O10	1.835	1.848	1.753	1.735
	H15′····O12″	1.738	1.742	1.633	1.619
	H16″····O10′	1.844	1.852	1.749	1.726
4-y	H17····O14	1.653	1.656	1.527	1.536
	H17′····O14′	1.618	1.620	1.470	1.480
	H15″····O14″	1.631	1.634	1.449	1.466
	H15····O12′	1.852	1.860	1.748	1.737
	H17′····O10	1.864	1.878	1.773	1.751
	H15′····O12″	1.740	1.743	1.634	1.621
	H16″····O10′	1.856	1.862	1.753	1.724
5	H17····O14	1.677	1.679	1.543	1.554
	H15′····O14′	1.655	1.660	1.497	1.507
	H15″····O14″	1.629	1.633	1.446	1.463
	H15····O10′	1.844	1.848	1.763	1.743
	H16····O12′	1.910	1.912	1.832	1.828
	H16′····O12″	1.695	1.697	1.557	1.541
	H16″····O8′	1.869	1.873	1.759	1.738
5-y	H17····O14	1.679	1.684	1.545	1.558
	H15′····O14′	1.663	1.667	1.499	1.510
	H15″····O14″	1.628	1.631	1.444	1.460
	H15····O10′	1.874	1.874	1.776	1.753
	H16····O12′	1.940	1.939	1.834	1.859
	H16′····O12″	1.697	1.699	1.562	1.526
	H16″····O8′	1.872	1.878	1.762	1.752
6	H17····O14	1.678	1.680	1.554	1.566
	H15′····O14′	1.657	1.664	1.499	1.509
	H15″····O14″	1.629	1.633	1.446	1.462
	H15····O12′	1.863	1.871	1.814	1.802
	H16····O10′	1.844	1.848	1.766	1.751
	H16″····O8′	1.872	1.876	1.761	1.739
	H16′····O12″	1.696	1.699	1.557	1.543
6-y	H17····O14	1.679	1.683	1.554	1.566
	H15′····O14′	1.665	1.672	1.501	1.515
	H15″····O14″	1.629	1.632	1.443	1.466
	H15····O12′	1.886	1.889	1.811	1.844
	H16····O10′	1.881	1.881	1.771	1.766
	H16″····O8′	1.878	1.879	1.770	1.771
	H16′····O12″	1.697	1.703	1.556	1.518
7	H17····O14	1.667	1.670	1.541	1.552
	H17′····O14′	1.623	1.625	1.481	1.490
	H15″····O14″	1.626	1.629	1.427	1.445
	H15····O12′	1.839	1.841	1.752	1.734

	H16····O10′	1.883	1.881	1.807	1.789
	H15′····O12″	1.794	1.794	1.677	1.670
	H16″····O10′	1.948	1.946	1.857	1.842
7-y	H17····O14	1.663	1.664	1.539	1.556
	H17′····O14′	1.625	1.625	1.482	1.495
	H15″····O14″	1.626	1.629	1.429	1.449
	H15····O12′	1.859	1.852	1.762	1.750
	H16····O10′	1.884	1.880	1.807	1.761
	H15′····O12″	1.797	1.790	1.671	1.670
	H16″····O10′	1.938	1.933	1.836	1.801
8	H17····O14	1.671	1.674	1.550	1.561
	H17′····O14′	1.632	1.634	1.486	1.497
	H15″····O14″	1.625	1.629	1.427	1.445
	H15····O10′	1.858	1.860	1.794	1.768
	H16····O12′	1.868	1.862	1.767	1.755
	H16′····O10″	1.946	1.943	1.854	1.837
	H15′····O12″	1.793	1.792	1.677	1.670
8-y	H17····O14	1.681	1.699	1.553	1.595
	H17′····O14′	1.635	1.636	1.487	1.504
	H15″····O14″	1.626	1.629	1.428	1.449
	H15····O10′	1.888	1.900	1.798	1.767
	H16····O12′	1.901	1.906	1.773	1.802
	H16′····O10″	1.931	1.932	1.842	1.795
	H15′····O12″	1.787	1.788	1.670	1.658
9	H17····O14	1.666	1.669	1.543	1.553
	H17′····O14′	1.628	1.630	1.493	1.501
	H15″····O14″	1.624	1.627	1.422	1.441
	H15····O12′	1.842	1.846	1.767	1.749
	H16····O10′	1.870	1.871	1.796	1.775
	H15′····O10″	1.978	1.978	1.902	1.883
	H16′····O12″	1.767	1.766	1.631	1.624
9-y	H17····O14	1.662	1.676	1.550	1.551
	H17′····O14′	1.636	1.638	1.491	1.501
	H15″····O14″	1.623	1.627	1.417	1.439
	H15····O12′	1.872	1.874	1.761	1.759
	H16····O10′	1.895	1.892	1.801	1.797
	H15′····O10″	1.969	1.973	1.894	1.901
	H16′····O12″	1.753	1.754	1.627	1.602
10	H17····O14	1.668	1.670	1.547	1.557
	H17′····O14′	1.636	1.638	1.498	1.509
	H15″····O14″	1.624	1.627	1.422	1.440
	H15····O10′	1.847	1.851	1.781	1.757

	H16····O12′	1.875	1.873	1.787	1.778
	H16′····O12″	1.763	1.760	1.628	1.617
	H15′····O10″	1.979	1.979	1.903	1.883
10-y	H17····O14	1.688	1.685	1.551	1.567
	H17′····O14′	1.643	1.644	1.500	1.521
	H15″····O14″	1.633	1.628	1.416	1.431
	H15····O10′	1.897	1.894	1.795	1.772
	H16····O12′	1.944	1.918	1.794	1.841
	H16′····O12″	1.749	1.757	1.630	1.612
	H15′····O10″	2.005	1.983	1.894	1.947

structure T8-KT2-M5,5,3″

1	H17····O14	1.630	1.634	1.449	1.466
	H17′····O14′	1.610	1.614	1.460	1.468
	H17″····O14″	1.626	1.630	1.484	1.490
	H16′····O8	1.711	1.715	1.584	1.567
	H16····O12′	1.843	1.848	1.721	1.701
	H16″····O10′	1.829	1.838	1.741	1.718
	H16′····O12″	1.828	1.835	1.736	1.716
1-y	H17····O14	1.631	1.634	1.450	1.480
	H17′····O14′	1.611	1.613	1.460	1.473
	H17″····O14″	1.627	1.631	1.485	1.494
	H16′····O8	1.721	1.727	1.596	1.563
	H16····O12′	1.848	1.849	1.724	1.729
	H16″····O10′	1.850	1.860	1.754	1.724
	H16′····O12″	1.835	1.841	1.738	1.737
2	H17····O14	1.630	1.633	1.449	1.466
	H15′····O14′	1.614	1.616	1.469	1.478
	H17″····O14″	1.618	1.622	1.470	1.476
	H17′····O8	1.739	1.742	1.634	1.618
	H16····O10′	1.842	1.849	1.738	1.715
	H16″····O8′	1.831	1.838	1.741	1.724
	H16′····O12″	1.797	1.803	1.688	1.668
2-y	H17····O14	1.630	1.633	1.449	1.465
	H15′····O14′	1.617	1.619	1.469	1.479
	H17″····O14″	1.622	1.626	1.474	1.479
	H17′····O8	1.742	1.744	1.633	1.619
	H16····O10′	1.860	1.866	1.746	1.716
	H16″····O8′	1.845	1.851	1.746	1.730
	H16′····O12″	1.818	1.827	1.707	1.677
3	H17····O14	1.618	1.623	1.426	1.447
	H17′····O14′	1.613	1.615	1.465	1.472

	H15″····O14″	1.655	1.658	1.530	1.539
	H16′····O8	1.706	1.710	1.575	1.556
	H15····O12′	1.846	1.853	1.727	1.708
	H17″····O10′	1.827	1.839	1.738	1.714
	H15′····O10″	1.863	1.878	1.790	1.772
3-y	H17····O14	1.618	1.627	1.449	1.470
	H17′····O14′	1.614	1.616	1.466	1.481
	H15″····O14″	1.656	1.660	1.532	1.556
	H16′····O8	1.718	1.720	1.589	1.563
	H15····O12′	1.848	1.852	1.733	1.737
	H17″····O10′	1.854	1.862	1.758	1.746
	H15′····O10″	1.877	1.887	1.796	1.843
4	H17····O14	1.630	1.633	1.447	1.464
	H15′····O14′	1.613	1.616	1.467	1.477
	H15″····O14″	1.655	1.658	1.529	1.537
	H17′····O8	1.738	1.741	1.633	1.618
	H16····O10′	1.844	1.852	1.749	1.726
	H17″····O8′	1.827	1.836	1.738	1.722
	H16′····O10″	1.835	1.848	1.753	1.735
4-y	H17····O14	1.630	1.633	1.447	1.464
	H15′····O14′	1.617	1.620	1.470	1.480
	H15″····O14″	1.654	1.657	1.529	1.538
	H17′····O8	1.740	1.742	1.634	1.620
	H16····O10′	1.856	1.863	1.753	1.725
	H17″····O8′	1.852	1.860	1.748	1.737
	H16′····O10″	1.865	1.879	1.773	1.751
5	H17····O14	1.628	1.632	1.444	1.461
	H17′····O14′	1.657	1.660	1.497	1.507
	H15″····O14″	1.678	1.680	1.544	1.555
	H16′····O8	1.694	1.695	1.556	1.540
	H16····O12′	1.867	1.872	1.759	1.739
	H17″····O10′	1.852	1.856	1.762	1.743
	H16″····O8′	1.930	1.923	1.832	1.828
5-y	H17····O14	1.629	1.628	1.444	1.458
	H17′····O14′	1.664	1.667	1.499	1.510
	H15″····O14″	1.677	1.695	1.545	1.560
	H16′····O8	1.701	1.703	1.564	1.533
	H16····O12′	1.868	1.875	1.763	1.747
	H17″····O10′	1.866	1.885	1.773	1.758
	H16″····O8′	1.889	1.948	1.825	1.839
6	H17····O14	1.628	1.631	1.443	1.460
	H17′····O14′	1.667	1.665	1.499	1.509

	H15″····O14″	1.679	1.681	1.555	1.566
	H15····O12′	1.696	1.700	1.556	1.541
	H16····O10′	1.872	1.876	1.761	1.739
	H16″····O8′	1.847	1.853	1.765	1.750
	H16′····O12″	1.865	1.875	1.813	1.803
6-y	H17····O14	1.629	1.630	1.441	1.467
	H17′····O14′	1.666	1.672	1.501	1.518
	H15″····O14″	1.680	1.680	1.555	1.557
	H17′····O8	1.696	1.702	1.556	1.527
	H16····O12′	1.881	1.883	1.771	1.782
	H16″····O10′	1.880	1.882	1.769	1.781
	H17″····O8′	1.886	1.890	1.803	1.799
7	H17····O14	1.624	1.627	1.424	1.443
	H15′····O14′	1.623	1.624	1.481	1.490
	H15″····O14″	1.677	1.679	1.543	1.552
	H17′····O8	1.794	1.794	1.676	1.667
	H16′····O10	1.948	1.946	1.856	1.844
	H17″····O8′	1.835	1.837	1.752	1.734
	H16″····O10′	1.879	1.877	1.808	1.789
7-y	H17····O14	1.625	1.627	1.426	1.447
	H15′····O14′	1.625	1.624	1.482	1.495
	H15″····O14″	1.676	1.677	1.549	1.557
	H17′····O8	1.797	1.790	1.670	1.669
	H16′····O10	1.938	1.934	1.835	1.802
	H17″····O8′	1.855	1.847	1.757	1.750
	H16″····O10′	1.883	1.877	1.802	1.760
8	H17····O14	1.624	1.626	1.424	1.443
	H15′····O14′	1.632	1.634	1.486	1.496
	H15″····O14″	1.682	1.684	1.550	1.561
	H17′····O8	1.792	1.791	1.675	1.668
	H16′····O10	1.947	1.944	1.853	1.839
	H17″····O8′	1.865	1.858	1.766	1.755
	H16″····O10′	1.856	1.858	1.794	1.770
8-y	H17····O14	1.625	1.627	1.425	1.445
	H15′····O14′	1.635	1.637	1.487	1.497
	H15″····O14″	1.690	1.702	1.555	1.570
	H17′····O8	1.786	1.788	1.670	1.668
	H16′····O10	1.932	1.933	1.842	1.823
	H17″····O8′	1.899	1.902	1.774	1.762
	H16″····O10′	1.886	1.897	1.798	1.763
9	H17····O14	1.622	1.625	1.419	1.438
	H17′····O14′	1.627	1.629	1.499	1.501

	H15″····O14″	1.677	1.679	1.544	1.554
	H16′····O8	1.766	1.766	1.630	1.621
	H17′····O10	1.978	1.978	1.902	1.883
	H16″····O10′	1.859	1.865	1.796	1.774
	H17″····O8′	1.835	1.840	1.767	1.750
9-y	H17····O14	1.622	1.624	1.413	1.439
	H17′····O14′	1.629	1.631	1.491	1.500
	H15″····O14″	1.677	1.678	1.551	1.551
	H16′····O8	1.748	1.753	1.624	1.604
	H17′····O10	1.852	1.951	1.890	1.894
	H16″····O10′	1.915	1.902	1.801	1.805
	H17″····O8′	1.860	1.850	1.760	1.756
10	H17····O14	1.612	1.620	1.392	1.423
	H15′····O14′	1.636	1.638	1.498	1.509
	H15″····O14″	1.679	1.681	1.548	1.558
	H16′····O8	1.763	1.762	1.627	1.617
	H17′····O10	1.981	1.982	1.901	1.894
	H17″····O10′	1.842	1.846	1.781	1.758
	H16″····O8′	1.869	1.867	1.787	1.778
10-y	H17····O14	1.608	1.612	1.387	1.399
	H15′····O14′	1.642	1.645	1.498	1.526
	H15″····O14″	1.682	1.690	1.551	1.569
	H16′····O8	1.758	1.757	1.627	1.612
	H17′····O10	1.972	1.976	1.892	1.949
	H17″····O10′	1.888	1.891	1.792	1.811
	H16″····O8′	1.914	1.913	1.787	1.880
structure T8-KT2,6″-M5,5,3″,3″					
1	H17····O14	1.630	1.633	1.449	1.466
	H15′····O14′	1.610	1.612	1.461	1.468
	H15″····O14″	1.631	1.635	1.451	1.467
	H17′····O8	1.743	1.743	1.637	1.621
	H16····O10′	1.830	1.835	1.720	1.696
	H16″····O8′	1.840	1.844	1.717	1.697
	H16′····O12″	1.707	1.709	1.578	1.560
1-y	H17····O14	1.630	1.633	1.449	1.465
	H15′····O14′	1.612	1.613	1.461	1.471
	H15″····O14″	1.633	1.636	1.452	1.475
	H17′····O8	1.745	1.746	1.637	1.626
	H16····O10′	1.853	1.857	1.731	1.692
	H16″····O8′	1.844	1.848	1.723	1.714
	H16′····O12″	1.721	1.725	1.593	1.556

		structure T9			
1	H15····O14	1.619	1.622	1.470	1.477
	H17′····O14′	1.615	1.618	1.470	1.479
	H17″····O14″	1.625	1.628	1.480	1.488
	H16′····O8	1.813	1.820	1.708	1.688
	H16····O12′	1.849	1.853	1.754	1.738
	H16″····O10′	1.856	1.864	1.769	1.749
	H15′····O12″	1.845	1.852	1.748	1.730
1-y	H15····O14	1.623	1.625	1.474	1.480
	H17′····O14′	1.618	1.620	1.471	1.480
	H17″····O14″	1.626	1.629	1.481	1.489
	H16′····O8	1.836	1.844	1.725	1.699
	H16····O12′	1.861	1.866	1.760	1.745
	H16″····O10′	1.869	1.878	1.779	1.760
	H15′····O12″	1.846	1.854	1.748	1.733
2	H15····O14	1.618	1.620	1.466	1.473
	H17′····O14′	1.617	1.619	1.475	1.484
	H15″····O14″	1.684	1.687	1.553	1.562
	H16′····O8	1.810	1.817	1.699	1.680
	H16····O12′	1.855	1.859	1.764	1.748
	H17″····O10′	1.849	1.859	1.755	1.733
	H15′····O10″	1.886	1.898	1.802	1.788
2-y	H15····O14	1.620	1.622	1.469	1.472
	H17′····O14′	1.621	1.624	1.474	1.484
	H15″····O14″	1.686	1.692	1.553	1.568
	H16′····O8	1.830	1.839	1.715	1.658
	H16····O12′	1.867	1.873	1.764	1.748
	H17″····O10′	1.872	1.883	1.764	1.693
	H15′····O10″	1.899	1.914	1.799	1.782
3	H15····O14	1.624	1.627	1.478	1.486
	H15′····O14′	1.614	1.617	1.468	1.477
	H15″····O14″	1.683	1.687	1.551	1.561
	H17′····O8	1.844	1.851	1.744	1.727
	H16····O10′	1.861	1.869	1.778	1.759
	H17″····O8′	1.834	1.841	1.739	1.723
	H16′····O10″	1.851	1.865	1.768	1.754
3-y	H15····O14	1.624	1.627	1.478	1.487
	H15′····O14′	1.617	1.620	1.468	1.477
	H15″····O14″	1.683	1.686	1.551	1.562
	H17′····O8	1.842	1.849	1.745	1.729
	H16····O10′	1.864	1.873	1.780	1.762

	H17″····O8′	1.846	1.853	1.744	1.729
	H16′····O10″	1.869	1.884	1.779	1.760
4	H15····O14	1.642	1.647	1.489	1.498
	H17′····O14′	1.616	1.619	1.472	1.480
	H17″····O14″	1.625	1.628	1.481	1.488
	H10′····O8	1.817	1.825	1.713	1.695
	H16····O12′	1.852	1.857	1.757	1.741
	H16″····O10′	1.856	1.865	1.769	1.749
	H15′····O12″	1.846	1.854	1.749	1.731
4-y	H15····O14	1.646	1.652	1.492	1.501
	H17′····O14′	1.619	1.622	1.472	1.481
	H17″····O14″	1.626	1.629	1.482	1.490
	H10′····O8	1.840	1.849	1.730	1.706
	H16····O12′	1.867	1.872	1.763	1.749
	H16″····O10′	1.870	1.879	1.779	1.760
	H15′····O12″	1.849	1.857	1.750	1.735
5	H15····O14	1.640	1.645	1.486	1.495
	H17′····O14′	1.619	1.621	1.476	1.485
	H15″····O14″	1.684	1.688	1.552	1.563
	H16′····O8	1.814	1.823	1.705	1.687
	H16····O12′	1.859	1.863	1.767	1.751
	H16″····O10′	1.849	1.860	1.755	1.734
	H15′····O10″	1.887	1.900	1.802	1.789
5-y	H15····O14	1.637	1.640	1.488	1.499
	H17′····O14′	1.620	1.626	1.476	1.489
	H15″····O14″	1.688	1.701	1.554	1.593
	H16′····O8	1.819	1.841	1.720	1.694
	H16····O12′	1.862	1.882	1.768	1.768
	H17″····O10′	1.830	1.877	1.764	1.744
	H15′····O10″	1.876	1.921	1.802	1.851
6	H17····O14	1.686	1.689	1.554	1.565
	H15′····O14′	1.617	1.620	1.472	1.481
	H15″····O14″	1.683	1.687	1.551	1.562
	H15····O10′	1.856	1.866	1.767	1.747
	H16′····O10	1.887	1.899	1.800	1.788
	H16′····O10″	1.851	1.864	1.763	1.749
	H17″····O10′	1.842	1.848	1.748	1.732
6-y	H17····O14	1.689	1.693	1.556	1.576
	H15′····O14′	1.620	1.623	1.472	1.491
	H15″····O14″	1.684	1.687	1.552	1.561
	H15····O10′	1.863	1.875	1.775	1.756
	H16′····O10	1.892	1.905	1.806	1.740

	H16′····O10″	1.865	1.881	1.773	1.770
	H17″····O10′	1.852	1.859	1.752	1.771
structure T9-M5,3″					
1	H15····O14	1.620	1.623	1.471	1.477
	H17′····O14′	1.614	1.617	1.469	1.477
	H17″····O14″	1.626	1.629	1.482	1.489
	H16′····O8	1.802	1.809	1.694	1.675
	H16····O12′	1.838	1.845	1.745	1.728
	H16″····O10′	1.847	1.857	1.758	1.738
	H15′····O12″	1.833	1.840	1.733	1.715
1-y	H15····O14	1.623	1.626	1.475	1.480
	H17′····O14′	1.616	1.619	1.469	1.478
	H17″····O14″	1.626	1.630	1.483	1.490
	H16′····O8	1.821	1.829	1.710	1.683
	H16····O12′	1.849	1.856	1.748	1.733
	H16″····O10′	1.858	1.868	1.767	1.745
	H15′····O12″	1.835	1.842	1.734	1.720
2	H15····O14	1.618	1.621	1.468	1.474
	H17′····O14′	1.617	1.620	1.474	1.483
	H15″····O14″	1.654	1.658	1.528	1.538
	H16′····O8	1.798	1.805	1.686	1.668
	H16····O12′	1.844	1.850	1.754	1.737
	H17″····O10′	1.850	1.861	1.757	1.736
	H15′····O10″	1.874	1.885	1.790	1.776
2-y	H15····O14	1.621	1.624	1.474	1.449
	H17′····O14′	1.621	1.624	1.483	1.465
	H15″····O14″	1.658	1.664	1.538	1.551
	H16′····O8	1.819	1.827	1.668	1.653
	H16····O12′	1.859	1.865	1.737	1.745
	H17″····O10′	1.873	1.883	1.736	1.705
	H15′····O10″	1.888	1.899	1.776	1.793
3	H15····O14	1.625	1.629	1.468	1.474
	H15′····O14′	1.614	1.617	1.474	1.483
	H15″····O14″	1.654	1.657	1.528	1.538
	H17′····O8	1.834	1.841	1.686	1.668
	H16····O10′	1.853	1.864	1.754	1.737
	H17″····O8′	1.835	1.844	1.757	1.736
	H16′····O10″	1.840	1.853	1.790	1.776
3-y	H15····O14	1.625	1.629	1.471	1.479
	H15′····O14′	1.617	1.620	1.474	1.487
	H15″····O14″	1.653	1.656	1.529	1.547

	H17′····O8	1.842	1.841	1.703	1.681
	H16····O10′	1.864	1.869	1.756	1.752
	H17″····O8′	1.846	1.857	1.768	1.752
	H16′····O10″	1.869	1.872	1.787	1.812
4	H15····O14	1.652	1.658	1.490	1.499
	H17′····O14′	1.616	1.619	1.471	1.479
	H17″····O14″	1.626	1.629	1.482	1.489
	H10′····O8	1.807	1.814	1.700	1.682
	H16····O12′	1.844	1.850	1.749	1.733
	H16″····O10′	1.848	1.858	1.758	1.738
	H15′····O12″	1.835	1.842	1.734	1.717
4-y	H15····O14	1.655	1.662	1.493	1.502
	H17′····O14′	1.618	1.622	1.472	1.481
	H17″····O14″	1.627	1.630	1.483	1.491
	H10′····O8	1.827	1.835	1.716	1.690
	H16····O12′	1.857	1.863	1.754	1.740
	H16″····O10′	1.860	1.870	1.768	1.745
	H15′····O12″	1.838	1.845	1.736	1.722
5	H15····O14	1.650	1.656	1.487	1.497
	H17′····O14′	1.619	1.622	1.476	1.485
	H15″····O14″	1.655	1.659	1.529	1.538
	H16′····O8	1.804	1.811	1.692	1.675
	H16····O12′	1.850	1.856	1.759	1.743
	H17″····O10′	1.850	1.861	1.757	1.736
	H15′····O10″	1.875	1.886	1.791	1.777
5-y	H15····O14	1.644	1.649	1.490	1.501
	H17′····O14′	1.623	1.626	1.476	1.489
	H15″····O14″	1.673	1.676	1.531	1.568
	H16′····O8	1.822	1.832	1.708	1.682
	H16····O12′	1.873	1.879	1.762	1.761
	H17″····O10′	1.862	1.877	1.767	1.746
	H15′····O10″	1.899	1.907	1.891	1.836
6	H17····O14	1.657	1.661	1.530	1.540
	H15′····O14′	1.617	1.621	1.473	1.483
	H15″····O14″	1.654	1.657	1.528	1.537
	H15····O10′	1.857	1.868	1.769	1.749
	H17′····O10	1.875	1.886	1.789	1.776
	H16′····O10″	1.839	1.852	1.753	1.738
	H17″····O10′	1.843	1.851	1.751	1.736
6-y	H17····O14	1.658	1.666	1.532	1.550
	H15′····O14′	1.620	1.624	1.474	1.494
	H15″····O14″	1.654	1.658	1.528	1.537

	H15····O10′	1.868	1.882	1.778	1.780
	H17′····O10	1.879	1.893	1.795	1.834
	H16′····O10″	1.854	1.870	1.763	1.764
	H17″····O10′	1.853	1.863	1.755	1.783

structure T9-ET6,2″

1	H15····O14	1.614	1.616	1.467	1.476
	H15′····O14′	1.616	1.618	1.472	1.481
	H17″····O14″	1.608	1.610	1.457	1.465
	H17′····O8	1.841	1.849	1.742	1.725
	H16····O10′	1.859	1.867	1.772	1.751
	H16″····O8′	1.852	1.857	1.759	1.742
	H16′····O12″	1.811	1.818	1.704	1.685
1-y	H15····O14	1.614	1.617	1.468	1.478
	H15′····O14′	1.618	1.621	1.473	1.481
	H17″····O14″	1.611	1.614	1.461	1.468
	H17′····O8	1.843	1.850	1.743	1.729
	H16····O10′	1.872	1.881	1.783	1.762
	H16″····O8′	1.865	1.869	1.764	1.749
	H16′····O12″	1.833	1.841	1.720	1.695

structure T9-M5,3″-ET6,2″

1	H15····O14	1.658	1.665	1.486	1.496
	H15′····O14′	1.614	1.617	1.469	1.478
	H17″····O14″	1.652	1.659	1.475	1.485
	H17′····O8	1.832	1.840	1.731	1.716
	H16····O10′	1.851	1.861	1.760	1.742
	H16″····O8′	1.844	1.850	1.748	1.733
	H16′····O12″	1.800	1.807	1.691	1.675
1-y	H15····O14	1.659	1.667	1.486	1.498
	H15′····O14′	1.617	1.620	1.470	1.479
	H17″····O14″	1.657	1.665	1.478	1.488
	H17′····O8	1.835	1.843	1.732	1.722
	H16····O10′	1.864	1.874	1.771	1.750
	H16″····O8′	1.859	1.866	1.754	1.742
	H16′····O12″	1.820	1.829	1.707	1.682

structure T9-M5,3″-ET6,4″

1	H15····O14	1.658	1.665	1.485	1.496
	H15′····O14′	1.616	1.619	1.470	1.478
	H15″····O14″	1.673	1.682	1.546	1.557

	H17′····O8	1.830	1.839	1.731	1.716
	H16····O10′	1.848	1.858	1.760	1.738
	H17″····O8′	1.850	1.859	1.752	1.732
	H16′····O10″	1.805	1.808	1.689	1.661
1-y	H15····O14	1.657	1.664	1.485	1.496
	H15′····O14′	1.618	1.621	1.471	1.479
	H15″····O14″	1.673	1.682	1.546	1.557
	H17′····O8	1.827	1.835	1.729	1.716
	H16····O10′	1.865	1.874	1.775	1.754
	H17″····O8′	1.865	1.871	1.757	1.739
	H16′····O10″	1.822	1.823	1.699	1.668
1-y-out-in	H15····O14	1.654	1.661	1.483	1.492
	H15′····O14′	1.618	1.621	1.471	1.484
	H15″····O14″	1.674	1.684	1.549	1.563
	H17′····O8	1.837	1.843	1.724	1.704
	H16····O10′	1.874	1.882	1.781	1.752
	H17″····O8′	1.864	1.871	1.769	1.776
	H16′····O10″	1.822	1.824	1.836	1.820
1-y-in-in	H15····O14	1.651	1.658	1.484	1.492
	H15′····O14′	1.622	1.624	1.470	1.484
	H15″····O14″	1.687	1.692	1.549	1.563
	H17′····O8	1.819	1.825	1.733	1.710
	H16····O10′	1.876	1.884	1.792	1.762
	H17″····O8′	1.895	1.901	1.767	1.774
	H16′····O10″	1.990	2.010	1.838	1.825
structure T9-KT6″-M5,3″,3″					
1	H15····O14	1.625	1.628	1.482	1.488
	H15′····O14′	1.610	1.612	1.461	1.468
	H15″····O14″	1.630	1.633	1.449	1.466
	H17′····O8	1.827	1.837	1.735	1.716
	H16····O10′	1.829	1.839	1.741	1.719
	H16″····O8′	1.843	1.848	1.722	1.701
	H16′····O12″	1.711	1.714	1.584	1.567
1-y	H15····O14	1.626	1.630	1.483	1.493
	H15′····O14′	1.611	1.613	1.461	1.473
	H15″····O14″	1.631	1.634	1.450	1.480
	H17′····O8	1.835	1.840	1.737	1.737
	H16····O10′	1.850	1.860	1.754	1.724
	H16″····O8′	1.849	1.849	1.725	1.729
	H16′····O12″	1.721	1.727	1.596	1.563
2	H15····O14	1.617	1.620	1.468	1.474

	H17′⋯O14′	1.614	1.616	1.469	1.477
	H15″⋯O14″	1.630	1.633	1.449	1.466
	H16′⋯O8	1.796	1.803	1.688	1.667
	H16⋯O12′	1.831	1.838	1.741	1.724
	H16″⋯O10′	1.842	1.833	1.738	1.714
	H16′⋯O12″	1.739	1.742	1.634	1.619
2-y	H15⋯O14	1.621	1.624	1.473	1.477
	H17′⋯O14′	1.617	1.619	1.470	1.479
	H15″⋯O14″	1.630	1.633	1.449	1.465
	H16′⋯O8	1.818	1.826	1.706	1.676
	H16⋯O12′	1.845	1.852	1.747	1.731
	H16″⋯O10′	1.860	1.866	1.745	1.716
	H16′⋯O12″	1.742	1.744	1.634	1.620
3	H17⋯O14	1.655	1.658	1.529	1.538
	H15′⋯O14′	1.613	1.615	1.466	1.473
	H15″⋯O14″	1.630	1.633	1.448	1.465
	H15⋯O10′	1.827	1.839	1.737	1.711
	H17′⋯O10	1.863	1.878	1.789	1.771
	H16′⋯O12″	1.706	1.709	1.575	1.557
	H16″⋯O8′	1.848	1.854	1.730	1.709
3-y	H17⋯O14	1.665	1.674	1.535	1.551
	H15′⋯O14′	1.615	1.617	1.464	1.473
	H15″⋯O14″	1.631	1.634	1.444	1.462
	H15⋯O10′	1.862	1.865	1.745	1.711
	H17′⋯O10	1.881	1.889	1.770	1.757
	H16′⋯O12″	1.718	1.721	1.594	1.562
	H16″⋯O8′	1.848	1.853	1.725	1.712
4	H17⋯O14	1.654	1.657	1.528	1.537
	H17′⋯O14′	1.613	1.616	1.468	1.477
	H15″⋯O14″	1.630	1.633	1.447	1.464
	H15⋯O12′	1.827	1.836	1.738	1.721
	H17′⋯O10	1.835	1.848	1.753	1.735
	H15′⋯O12″	1.738	1.741	1.632	1.618
	H16″⋯O10′	1.844	1.852	1.749	1.726
4-y	H17⋯O14	1.653	1.656	1.528	1.536
	H17′⋯O14′	1.617	1.620	1.470	1.480
	H15″⋯O14″	1.630	1.633	1.447	1.464
	H15⋯O12′	1.852	1.860	1.748	1.736
	H17′⋯O10	1.864	1.878	1.772	1.750
	H15′⋯O12″	1.740	1.742	1.633	1.620
	H16″⋯O10′	1.856	1.862	1.754	1.724
5	H17⋯O14	1.666	1.668	1.545	1.556

	H15′····O14′	1.681	1.688	1.528	1.542
	H15″····O14″	1.627	1.630	1.440	1.459
	H15····O10′	1.856	1.859	1.780	1.754
	H16····O12′	1.898	1.896	1.804	1.800
	H16′····O12″	1.693	1.696	1.561	1.546
	H16″····O8′	1.891	1.898	1.798	1.776
5-y	H17····O14	1.694	1.694	1.544	1.571
	H15′····O14′	1.695	1.704	1.526	1.536
	H15″····O14″	1.627	1.627	1.446	1.457
	H15····O10′	1.901	1.901	1.803	1.771
	H16····O12′	1.956	1.935	1.785	1.786
	H16′····O12″	1.700	1.703	1.581	1.553
	H16″····O8′	1.912	1.904	1.805	1.791
6	H17····O14	1.666	1.667	1.544	1.554
	H15′····O14′	1.672	1.678	1.523	1.535
	H15″····O14″	1.627	1.630	1.440	1.458
	H15····O12′	1.867	1.866	1.785	1.767
	H16····O10′	1.885	1.880	1.793	1.771
	H16″····O8′	1.893	1.900	1.800	1.776
	H16′····O12″	1.700	1.701	1.564	1.551
6-y	H17····O14	1.664	1.667	1.543	1.552
	H15′····O14′	1.679	1.687	1.522	1.533
	H15″····O14″	1.631	1.630	1.437	1.464
	H15····O12′	1.872	1.870	1.780	1.772
	H16····O10′	1.899	1.898	1.802	1.778
	H16″····O8′	1.909	1.907	1.809	1.823
	H16′····O12″	1.695	1.703	1.564	1.538
7	H17····O14	1.667	1.669	1.541	1.552
	H17′····O14′	1.623	1.625	1.481	1.490
	H15″····O14″	1.624	1.627	1.424	1.443
	H15····O12′	1.839	1.841	1.752	1.734
	H16····O10′	1.883	1.881	1.808	1.790
	H15′····O12″	1.794	1.793	1.676	1.668
	H16″····O10′	1.948	1.946	1.856	1.843
7-y	H17····O14	1.663	1.664	1.539	1.556
	H17′····O14′	1.626	1.625	1.483	1.495
	H15″····O14″	1.625	1.627	1.426	1.447
	H15····O12′	1.859	1.851	1.761	1.750
	H16····O10′	1.885	1.880	1.808	1.761
	H15′····O12″	1.797	1.790	1.671	1.669
	H16″····O10′	1.938	1.934	1.836	1.801
8	H17····O14	1.671	1.674	1.550	1.561

	H17′····O14′	1.632	1.634	1.486	1.497
	H15″····O14″	1.624	1.627	1.424	1.443
	H15····O10′	1.858	1.860	1.794	1.769
	H16····O12′	1.868	1.861	1.767	1.755
	H16′····O10″	1.946	1.944	1.853	1.838
	H15′····O12″	1.792	1.792	1.676	1.669
8-y	H17····O14	1.681	1.699	1.553	1.595
	H17′····O14′	1.635	1.637	1.487	1.504
	H15″····O14″	1.625	1.627	1.425	1.446
	H15····O10′	1.888	1.899	1.798	1.768
	H16····O12′	1.901	1.905	1.773	1.801
	H16′····O10″	1.931	1.932	1.841	1.795
	H15′····O12″	1.786	1.788	1.670	1.657
9	H17····O14	1.666	1.669	1.543	1.553
	H17′····O14′	1.628	1.629	1.493	1.501
	H15″····O14″	1.622	1.625	1.419	1.438
	H15····O12′	1.842	1.846	1.767	1.750
	H16····O10′	1.870	1.871	1.796	1.774
	H15′····O10″	1.977	1.978	1.902	1.884
	H16′····O12″	1.767	1.766	1.630	1.621
9-y	H17····O14	1.664	1.665	1.541	1.550
	H17′····O14′	1.629	1.632	1.491	1.500
	H15″····O14″	1.624	1.625	1.413	1.438
	H15····O12′	1.863	1.856	1.763	1.755
	H16····O10′	1.916	1.907	1.809	1.805
	H15′····O10″	1.956	1.954	1.889	1.893
	H16′····O12″	1.746	1.751	1.624	1.605
10	H17····O14	1.668	1.669	1.547	1.557
	H17′····O14′	1.636	1.638	1.498	1.509
	H15″····O14″	1.622	1.625	1.419	1.438
	H15····O10′	1.846	1.851	1.781	1.757
	H16····O12′	1.875	1.873	1.787	1.779
	H16′····O12″	1.762	1.760	1.627	1.616
	H15′····O10″	1.979	1.979	1.903	1.884
10-y	H17····O14	1.690	1.692	1.545	1.574
	H17′····O14′	1.642	1.645	1.493	1.503
	H15″····O14″	1.617	1.621	1.425	1.438
	H15····O10′	1.900	1.901	1.813	1.790
	H16····O12′	1.932	1.920	1.764	1.771
	H16′····O12″	1.760	1.762	1.637	1.608
	H15′····O10″	1.995	1.973	1.862	1.946

structure T9-KT6″-M3″,3″-ET4					
1	H17····O14	1.685	1.688	1.552	1.562
	H17′····O14′	1.616	1.619	1.470	1.479
	H15″····O14″	1.630	1.633	1.447	1.464
	H15····O12′	1.838	1.845	1.742	1.727
	H16′····O10	1.827	1.834	1.733	1.702
	H15′····O12″	1.740	1.744	1.635	1.621
	H16″····O10′	1.844	1.851	1.747	1.720
1-y	H17····O14	1.684	1.687	1.552	1.562
	H17′····O14′	1.619	1.622	1.472	1.481
	H15″····O14″	1.630	1.633	1.447	1.464
	H15····O12′	1.861	1.867	1.753	1.737
	H16′····O10	1.850	1.860	1.751	1.706
	H15′····O12″	1.741	1.744	1.635	1.623
	H16″····O10′	1.854	1.860	1.752	1.716
structure T9-KT6″-M5,3″,3″-ET6					
1	H15····O14	1.648	1.655	1.471	1.481
	H17′····O14′	1.614	1.616	1.469	1.478
	H15″····O14″	1.630	1.633	1.449	1.466
	H16′····O8	1.795	1.802	1.686	1.668
	H16····O12′	1.837	1.844	1.744	1.728
	H16″····O10′	1.842	1.849	1.738	1.714
	H15′····O12″	1.739	1.742	1.635	1.619
1-y	H15····O14	1.652	1.658	1.478	1.486
	H17′····O14′	1.617	1.619	1.471	1.481
	H15″····O14″	1.630	1.633	1.448	1.465
	H16′····O8	1.818	1.826	1.712	1.684
	H16····O12′	1.852	1.859	1.749	1.743
	H16″····O10′	1.860	1.865	1.746	1.717
	H15′····O12″	1.742	1.744	1.635	1.621
structure T9-KT2,6″-M5,5,3″,3″					
1	H17····O14	1.630	1.633	1.449	1.466
	H15′····O14′	1.610	1.612	1.461	1.468
	H15″····O14″	1.630	1.633	1.449	1.466
	H17′····O8	1.743	1.746	1.637	1.621
	H16····O10′	1.830	1.835	1.720	1.696
	H16″····O8′	1.840	1.845	1.718	1.697
	H16′····O12″	1.707	1.709	1.577	1.559
1-y	H17····O14	1.630	1.633	1.449	1.464

	H15′····O14′	1.612	1.613	1.461	1.473
	H15‴····O14″	1.631	1.635	1.450	1.482
	H17′····O8	1.745	1.746	1.638	1.629
	H16····O10′	1.853	1.857	1.731	1.694
	H16″····O8′	1.844	1.848	1.722	1.724
	H16′····O12″	1.721	1.725	1.593	1.557
structure T10					
1	H15····O14	1.602	1.605	1.449	1.458
	H17′····O14′	1.623	1.635	1.451	1.461
	H17″····O14″	1.612	1.612	1.460	1.468
	H16′····O8	1.812	1.819	1.703	1.684
	H16····O12′	1.850	1.855	1.750	1.734
	H16″····O10′	1.857	1.867	1.766	1.745
	H15′····O12″	1.844	1.854	1.740	1.721
1-y	H15····O14	1.605	1.608	1.453	1.460
	H17′····O14′	1.612	1.626	1.453	1.462
	H17″····O14″	1.608	1.612	1.461	1.470
	H16′····O8	1.834	1.843	1.719	1.694
	H16····O12′	1.861	1.867	1.755	1.740
	H16″····O10′	1.865	1.874	1.777	1.757
	H15′····O12″	1.839	1.846	1.742	1.725
2	H15····O14	1.600	1.603	1.446	1.454
	H17′····O14′	1.636	1.648	1.456	1.466
	H15″····O14″	1.709	1.728	1.535	1.549
	H16′····O8	1.807	1.814	1.694	1.675
	H16····O12′	1.855	1.860	1.760	1.745
	H17″····O10′	1.837	1.846	1.749	1.728
	H15′····O10″	1.873	1.885	1.795	1.784
2-y	H15····O14	1.604	1.608	1.448	1.449
	H17′····O14′	1.646	1.658	1.457	1.465
	H15″····O14″	1.718	1.725	1.535	1.551
	H16′····O8	1.821	1.833	1.707	1.653
	H16····O12′	1.863	1.868	1.763	1.745
	H17″····O10′	1.858	1.873	1.761	1.705
	H15′····O10″	1.895	1.908	1.801	1.793
3	H15····O14	1.611	1.615	1.458	1.466
	H15′····O14′	1.622	1.633	1.448	1.458
	H15″····O14″	1.705	1.723	1.535	1.548
	H17′····O8	1.843	1.853	1.737	1.718
	H16····O10′	1.861	1.870	1.776	1.757
	H17″····O8′	1.833	1.841	1.732	1.714

	H16′⋯O10″	1.850	1.863	1.764	1.752
3-y	H15⋯O14	1.611	1.615	1.458	1.467
	H15′⋯O14′	1.638	1.649	1.449	1.458
	H15″⋯O14″	1.716	1.731	1.534	1.544
	H17′⋯O8	1.841	1.852	1.739	1.721
	H16⋯O10′	1.865	1.875	1.779	1.759
	H17″⋯O8′	1.847	1.858	1.737	1.720
	H16′⋯O10″	1.868	1.885	1.777	1.758
4	H15⋯O14	1.666	1.675	1.487	1.495
	H17′⋯O14′	1.625	1.636	1.452	1.462
	H17″⋯O14″	1.612	1.617	1.460	1.468
	H10′⋯O8	1.819	1.828	1.712	1.693
	H16⋯O12′	1.854	1.860	1.753	1.737
	H16″⋯O10′	1.857	1.867	1.767	1.746
	H15′⋯O12″	1.844	1.855	1.741	1.722
4-y	H15⋯O14	1.672	1.682	1.489	1.496
	H17′⋯O14′	1.643	1.655	1.454	1.467
	H17″⋯O14″	1.613	1.617	1.462	1.471
	H10′⋯O8	1.841	1.851	1.731	1.706
	H16⋯O12′	1.869	1.876	1.761	1.745
	H16″⋯O10′	1.870	1.880	1.776	1.759
	H15′⋯O12″	1.849	1.859	1.743	1.726
5	H15⋯O14	1.660	1.666	1.482	1.490
	H17′⋯O14′	1.640	1.653	1.458	1.467
	H15″⋯O14″	1.710	1.729	1.536	1.549
	H16′⋯O8	1.819	1.827	1.705	1.687
	H16⋯O12′	1.861	1.867	1.765	1.749
	H17″⋯O10′	1.838	1.848	1.750	1.730
	H15′⋯O10″	1.873	1.886	1.796	1.785
5-y	H15⋯O14	1.659	1.669	1.485	1.479
	H17′⋯O14′	1.650	1.662	1.459	1.467
	H15″⋯O14″	1.718	1.726	1.537	1.556
	H16′⋯O8	1.828	1.842	1.717	1.660
	H16⋯O12′	1.879	1.876	1.768	1.749
	H17″⋯O10′	1.848	1.869	1.759	1.691
	H15′⋯O10″	1.892	1.908	1.803	1.790
6	H17⋯O14	1.622	1.639	1.538	1.547
	H15′⋯O14′	1.631	1.643	1.453	1.462
	H15″⋯O14″	1.707	1.725	1.535	1.548
	H15⋯O10′	1.859	1.875	1.764	1.741
	H16′⋯O10	1.891	1.910	1.796	1.781
	H16′⋯O10″	1.848	1.862	1.758	1.746

	H17″····O10′	1.841	1.849	1.741	1.723
6-y	H17····O14	1.626	1.646	1.539	1.606
	H15′····O14′	1.644	1.656	1.453	1.485
	H15″····O14″	1.717	1.732	1.536	1.559
	H15····O10′	1.870	1.884	1.769	1.794
	H16′····O10	1.898	1.917	1.796	1.885
	H16′····O10″	1.866	1.885	1.768	1.809
	H17″····O10′	1.854	1.867	1.745	1.810
structure T10-ET6,2″					
1	H15····O14	1.617	1.626	1.447	1.457
	H15′····O14′	1.633	1.646	1.454	1.464
	H17″····O14″	1.611	1.618	1.436	1.446
	H17′····O8	1.835	1.844	1.735	1.716
	H16····O10′	1.854	1.863	1.767	1.748
	H16″····O8′	1.853	1.859	1.755	1.738
	H16′····O12″	1.810	1.818	1.698	1.680
1-y	H15····O14	1.608	1.617	1.448	1.458
	H15′····O14′	1.613	1.627	1.454	1.463
	H17″····O14″	1.600	1.607	1.440	1.449
	H17′····O8	1.837	1.845	1.737	1.721
	H16····O10′	1.869	1.879	1.780	1.759
	H16″····O8′	1.865	1.871	1.759	1.744
	H16′····O12″	1.833	1.842	1.715	1.690
structure T10-M5,3″-ET6,2″					
1	H15····O14	1.653	1.657	1.473	1.487
	H15′····O14′	1.633	1.644	1.452	1.461
	H17″····O14″	1.702	1.717	1.464	1.481
	H17′····O8	1.838	1.843	1.733	1.717
	H16····O10′	1.859	1.867	1.767	1.748
	H16″····O8′	1.847	1.854	1.746	1.731
	H16′····O12″	1.803	1.812	1.691	1.675
1-y	H15····O14	1.659	1.665	1.475	1.490
	H15′····O14′	1.643	1.653	1.453	1.466
	H17″····O14″	1.709	1.724	1.467	1.477
	H17′····O8	1.834	1.845	1.736	1.724
	H16····O10′	1.865	1.877	1.778	1.758
	H16″····O8′	1.862	1.870	1.757	1.742
	H16′····O12″	1.823	1.832	1.713	1.688
structure T10-M5,3″-ET6,2″,6″					

1	H15⋯O14	1.702	1.717	1.565	1.484
	H17′⋯O14′	1.637	1.649	1.452	1.467
	H16′⋯O8	1.805	1.814	1.694	1.683
	H16⋯O12′	1.849	1.857	1.749	1.737
	H16″⋯O10′	1.884	1.891	1.786	1.781
	H15′⋯O12″	1.837	1.837	1.715	1.684
1-y	H15⋯O14	1.708	1.723	1.566	1.495
	H17′⋯O14′	1.649	1.663	1.456	1.468
	H16′⋯O8	1.822	1.832	1.704	1.678
	H16⋯O12′	1.861	1.869	1.758	1.758
	H16″⋯O10′	1.877	1.894	1.804	1.771
	H15′⋯O12″	1.812	1.821	1.735	1.707

structure T10-KT2,6″-M5,5,3″,3″

1	H17⋯O14	1.665	1.661	1.393	1.412
	H15′⋯O14′	1.610	1.617	1.440	1.450
	H15″⋯O14″	1.611	1.614	1.426	1.445
	H17′⋯O8	1.739	1.746	1.631	1.611
	H16⋯O10′	1.826	1.833	1.714	1.695
	H16″⋯O8′	1.841	1.846	1.713	1.693
	H16′⋯O12″	1.708	1.709	1.575	1.556
1-y	H17⋯O14	1.615	1.619	1.427	1.446
	H15′⋯O14′	1.627	1.632	1.441	1.453
	H15″⋯O14″	1.620	1.615	1.427	1.459
	H17′⋯O8	1.740	1.745	1.629	1.615
	H16⋯O10′	1.846	1.851	1.726	1.689
	H16″⋯O8′	1.841	1.853	1.716	1.713
	H16′⋯O12″	1.720	1.727	1.591	1.554

structure T11-ET6,2″

1	H15⋯O14	1.599	1.618	1.437	1.447
	H17′⋯O14′	1.635	1.658	1.454	1.463
	H17″⋯O14″	1.621	1.624	1.470	1.479
	H16′⋯O8	1.812	1.818	1.698	1.680
	H16⋯O12′	1.855	1.860	1.755	1.738
	H16″⋯O10′	1.860	1.862	1.767	1.748
	H15′⋯O12″	1.845	1.847	1.742	1.723
1-y	H15⋯O14	1.600	1.607	1.440	1.450
	H17′⋯O14′	1.626	1.644	1.452	1.464
	H17″⋯O14″	1.621	1.625	1.471	1.481
	H16′⋯O8	1.834	1.843	1.715	1.690

	H16⋯O12′	1.867	1.873	1.760	1.745
	H16″⋯O10′	1.867	1.876	1.777	1.759
	H15′⋯O12″	1.838	1.847	1.743	1.727

structure T11-M5,3″-ET6,2″

1-y	H15⋯O14	1.658	1.664	1.463	1.484
	H17′⋯O14′	1.627	1.646	1.450	1.465
	H17″⋯O14″	1.660	1.669	1.490	1.503
	H16′⋯O8	1.821	1.830	1.703	1.678
	H16⋯O12′	1.865	1.873	1.750	1.753
	H16″⋯O10′	1.859	1.869	1.766	1.740
	H15′⋯O12″	1.832	1.841	1.731	1.728
1	H15⋯O14	1.701	1.717	1.463	1.481
	H17′⋯O14′	1.640	1.657	1.450	1.460
	H17″⋯O14″	1.659	1.669	1.489	1.500
	H16′⋯O8	1.802	1.811	1.690	1.675
	H16⋯O12′	1.846	1.854	1.745	1.730
	H16″⋯O10′	1.846	1.856	1.756	1.739
	H15′⋯O12″	1.829	1.839	1.731	1.714
1-y-out-in	H15⋯O14	1.695	1.709	1.465	1.477
	H17′⋯O14′	1.629	1.648	1.451	1.464
	H17″⋯O14″	1.660	1.669	1.490	1.502
	H16′⋯O8	1.838	1.847	1.711	1.686
	H16⋯O12′	1.872	1.879	1.757	1.743
	H16″⋯O10′	1.860	1.871	1.766	1.746
	H15′⋯O12″	1.830	1.840	1.733	1.720

structure T12-KT2-M5,5,3″

1	H17⋯O14	1.629	1.632	1.448	1.465
	H17′⋯O14′	1.610	1.612	1.461	1.468
	H17″⋯O14″	1.624	1.628	1.482	1.488
	H16′⋯O8	1.710	1.714	1.584	1.567
	H16⋯O12′	1.843	1.848	1.721	1.701
	H16″⋯O10′	1.829	1.839	1.741	1.718
	H16′⋯O12″	1.827	1.837	1.735	1.715
1-y	H17⋯O14	1.631	1.633	1.449	1.484
	H17′⋯O14′	1.611	1.613	1.460	1.475
	H17″⋯O14″	1.626	1.629	1.483	1.493
	H16′⋯O8	1.721	1.727	1.597	1.567
	H16⋯O12′	1.849	1.849	1.724	1.735
	H16″⋯O10′	1.850	1.859	1.754	1.729

		1.835	1.840	1.736	1.741
2	H17····O14	1.630	1.633	1.448	1.465
	H15′····O14′	1.614	1.616	1.469	1.478
	H17″····O14″	1.617	1.620	1.468	1.474
	H17′····O8	1.739	1.741	1.634	1.618
	H16····O10′	1.842	1.849	1.738	1.714
	H16″····O8′	1.831	1.838	1.742	1.725
	H16′····O12″	1.797	1.803	1.688	1.667
2-y	H17····O14	1.630	1.632	1.448	1.464
	H15′····O14′	1.617	1.619	1.470	1.479
	H17″····O14″	1.621	1.624	1.473	1.477
	H17′····O8	1.742	1.743	1.633	1.619
	H16····O10′	1.860	1.866	1.746	1.715
	H16″····O8′	1.845	1.852	1.746	1.731
	H16′····O12″	1.818	1.826	1.707	1.676
3	H17····O14	1.629	1.632	1.447	1.465
	H17′····O14′	1.613	1.615	1.466	1.473
	H15″····O14″	1.655	1.658	1.529	1.538
	H16′····O8	1.705	1.709	1.575	1.557
	H15····O12′	1.849	1.854	1.731	1.710
	H17″····O10′	1.826	1.839	1.737	1.711
	H15′····O10″	1.863	1.878	1.790	1.772
3-y	H17····O14	1.629	1.632	1.447	1.468
	H17′····O14′	1.615	1.617	1.466	1.482
	H15″····O14″	1.670	1.680	1.531	1.554
	H16′····O8	1.718	1.721	1.588	1.565
	H15····O12′	1.848	1.853	1.734	1.736
	H17″····O10′	1.863	1.868	1.759	1.736
	H15′····O10″	1.883	1.893	1.799	1.832
4	H17····O14	1.629	1.632	1.447	1.464
	H15′····O14′	1.613	1.616	1.467	1.477
	H15″····O14″	1.654	1.657	1.528	1.536
	H17′····O8	1.738	1.741	1.632	1.617
	H16····O10′	1.844	1.852	1.749	1.726
	H17″····O8′	1.827	1.836	1.738	1.722
	H16′····O10″	1.835	1.848	1.753	1.735
4-y	H17····O14	1.629	1.632	1.446	1.463
	H15′····O14′	1.617	1.620	1.470	1.480
	H15″····O14″	1.653	1.656	1.527	1.536
	H17′····O8	1.740	1.742	1.633	1.620
	H16····O10′	1.856	1.862	1.753	1.725
	H17″····O8′	1.852	1.860	1.748	1.736

	H16′····O10″	1.864	1.878	1.772	1.749
5	H17····O14	1.627	1.630	1.439	1.458
	H17′····O14′	1.680	1.688	1.528	1.543
	H15″····O14″	1.666	1.668	1.545	1.557
	H16′····O8	1.693	1.694	1.561	1.545
	H16····O12′	1.892	1.898	1.798	1.777
	H17″····O10′	1.856	1.860	1.780	1.755
	H16″····O8′	1.898	1.898	1.804	1.804
5-y	H17····O14	1.626	1.626	1.445	1.456
	H17′····O14′	1.695	1.703	1.526	1.536
	H15″····O14″	1.694	1.694	1.545	1.571
	H16′····O8	1.701	1.703	1.581	1.552
	H16····O12′	1.911	1.905	1.803	1.790
	H17″····O10′	1.901	1.901	1.804	1.772
	H16″····O8′	1.956	1.935	1.788	1.785
6	H17····O14	1.627	1.630	1.439	1.457
	H17′····O14′	1.672	1.678	1.523	1.534
	H15″····O14″	1.666	1.667	1.544	1.554
	H16′····O8	1.699	1.701	1.563	1.550
	H16····O12′	1.893	1.901	1.800	1.776
	H16″····O10′	1.885	1.880	1.794	1.772
	H17″····O8′	1.867	1.866	1.784	1.766
6-y	H17····O14	1.630	1.629	1.436	1.467
	H17′····O14′	1.679	1.687	1.522	1.532
	H15″····O14″	1.664	1.667	1.543	1.552
	H16′····O8	1.695	1.703	1.563	1.539
	H16····O12′	1.910	1.907	1.810	1.823
	H16″····O10′	1.899	1.898	1.803	1.781
	H17″····O8′	1.872	1.870	1.780	1.770
7	H17····O14	1.624	1.626	1.423	1.442
	H15′····O14′	1.623	1.625	1.481	1.490
	H15″····O14″	1.666	1.670	1.541	1.551
	H17′····O8	1.794	1.793	1.675	1.667
	H16′····O10	1.948	1.946	1.856	1.844
	H17″····O8′	1.839	1.841	1.752	1.734
	H16″····O10′	1.883	1.881	1.808	1.789
7-y	H17····O14	1.624	1.627	1.426	1.446
	H15′····O14′	1.626	1.625	1.483	1.495
	H15″····O14″	1.663	1.664	1.539	1.556
	H17′····O8	1.797	1.789	1.670	1.669
	H16′····O10	1.938	1.934	1.834	1.801
	H17″····O8′	1.859	1.851	1.762	1.749

	H16″····O10′	1.885	1.880	1.806	1.761
8	H17····O14	1.624	1.626	1.423	1.442
	H15′····O14′	1.632	1.634	1.486	1.497
	H15″····O14″	1.671	1.674	1.550	1.561
	H17′····O8	1.792	1.791	1.676	1.669
	H16′····O10	1.946	1.943	1.853	1.839
	H17″····O8′	1.868	1.861	1.766	1.755
	H16″····O10′	1.858	1.860	1.794	1.769
8-y	H17····O14	1.624	1.627	1.425	1.446
	H15′····O14′	1.635	1.637	1.487	1.504
	H15″····O14″	1.681	1.698	1.554	1.595
	H17′····O8	1.786	1.788	1.670	1.656
	H16′····O10	1.931	1.932	1.840	1.795
	H17″····O8′	1.901	1.905	1.773	1.799
	H16″····O10′	1.888	1.900	1.798	1.765
9	H17····O14	1.622	1.624	1.418	1.437
	H17′····O14′	1.628	1.629	1.493	1.501
	H15″····O14″	1.666	1.669	1.543	1.553
	H16′····O8	1.866	1.765	1.630	1.621
	H16····O12′	1.877	1.878	1.902	1.883
	H17″····O10′	1.869	1.860	1.796	1.774
	H15′····O10″	1.842	1.845	1.767	1.749
9-y	H17····O14	1.623	1.624	1.412	1.400
	H17′····O14′	1.629	1.632	1.491	1.499
	H15″····O14″	1.664	1.665	1.541	1.501
	H16′····O8	1.746	1.751	1.624	1.605
	H16····O12′	1.856	1.854	1.889	1.896
	H17″····O10′	1.917	1.907	1.808	1.809
	H15′····O10″	1.863	1.856	1.763	1.753
10	H17····O14	1.622	1.624	1.417	1.438
	H15′····O14′	1.636	1.638	1.498	1.509
	H15″····O14″	1.668	1.669	1.547	1.557
	H16′····O8	1.762	1.759	1.627	1.615
	H17′····O10	1.979	1.979	1.902	1.882
	H17″····O10′	1.846	1.851	1.781	1.756
	H16″····O8′	1.875	1.873	1.787	1.779
10-y	H17····O14	1.622	1.624	1.408	1.445
	H15′····O14′	1.642	1.646	1.502	1.517
	H15″····O14″	1.686	1.690	1.556	1.559
	H16′····O8	1.767	1.767	1.640	1.625
	H17′····O10	1.989	1.985	1.898	1.947
	H17″····O10′	1.902	1.901	1.804	1.785

	H16″····O8′	1.932	1.922	1.807	1.815
structure T12-KT6″-M5,3″,3″					
1	H15····O14	1.624	1.628	1.481	1.488
	H15′····O14′	1.610	1.612	1.461	1.468
	H15″····O14″	1.630	1.633	1.449	1.465
	H17′····O8	1.827	1.836	1.735	1.715
	H16····O10′	1.829	1.839	1.741	1.718
	H16″····O8′	1.843	1.848	1.722	1.700
	H16′····O12″	1.711	1.714	1.584	1.567
1-y	H15····O14	1.626	1.629	1.483	1.492
	H15′····O14′	1.611	1.613	1.460	1.473
	H15″····O14″	1.631	1.634	1.450	1.480
	H17′····O8	1.834	1.840	1.736	1.736
	H16····O10′	1.851	1.859	1.754	1.724
	H16″····O8′	1.848	1.849	1.725	1.729
	H16′····O12″	1.721	1.727	1.596	1.553
2	H15····O14	1.616	1.620	1.467	1.473
	H17′····O14′	1.614	1.616	1.469	1.478
	H15″····O14″	1.630	1.633	1.449	1.466
	H16′····O8	1.796	1.802	1.687	1.666
	H16····O12′	1.831	1.838	1.742	1.725
	H16″····O10′	1.842	1.849	1.737	1.714
	H16′····O12″	1.739	1.742	1.635	1.619
2-y	H15····O14	1.620	1.624	1.472	1.476
	H17′····O14′	1.617	1.619	1.470	1.479
	H15″····O14″	1.630	1.633	1.449	1.465
	H16′····O8	1.818	1.826	1.706	1.674
	H16····O12′	1.845	1.852	1.747	1.731
	H16″····O10′	1.860	1.866	1.746	1.715
	H16′····O12″	1.742	1.744	1.634	1.620
3	H17····O14	1.654	1.658	1.529	1.538
	H15′····O14′	1.613	1.615	1.466	1.473
	H15″····O14″	1.630	1.633	1.447	1.465
	H15····O10′	1.827	1.839	1.737	1.711
	H17′····O10	1.863	1.879	1.790	1.772
	H16′····O12″	1.706	1.710	1.575	1.557
	H16″····O8′	1.848	1.854	1.730	1.710
3-y	H17····O14	1.656	1.666	1.528	1.552
	H15′····O14′	1.615	1.617	1.467	1.476
	H15″····O14″	1.635	1.638	1.451	1.464
	H15····O10′	1.878	1.882	1.774	1.737

	H17′····O10	1.891	1.901	1.801	1.816
	H16′····O12″	1.722	1.725	1.594	1.566
	H16″····O8′	1.847	1.852	1.734	1.717
4	H17····O14	1.654	1.658	1.527	1.536
	H17′····O14′	1.613	1.616	1.468	1.477
	H15″····O14″	1.630	1.633	1.447	1.464
	H15····O12′	1.827	1.837	1.739	1.722
	H17′····O10	1.835	1.848	1.753	1.736
	H15′····O12″	1.738	1.741	1.632	1.617
	H16″····O10′	1.844	1.852	1.749	1.726
4-y	H17····O14	1.653	1.656	1.527	1.536
	H17′····O14′	1.618	1.620	1.470	1.480
	H15″····O14″	1.630	1.633	1.447	1.464
	H15····O12′	1.852	1.860	1.748	1.737
	H17′····O10	1.864	1.878	1.772	1.750
	H15′····O12″	1.740	1.742	1.634	1.620
	H16″····O10′	1.856	1.862	1.753	1.725
5	H17····O14	1.666	1.667	1.545	1.557
	H15′····O14′	1.680	1.689	1.528	1.543
	H15″····O14″	1.627	1.630	1.440	1.459
	H15····O10′	1.856	1.859	1.780	1.754
	H16····O12′	1.898	1.897	1.804	1.803
	H16′····O12″	1.694	1.695	1.561	1.546
	H16″····O8′	1.891	1.898	1.799	1.778
5-y	H17····O14	1.704	1.705	1.544	1.577
	H15′····O14′	1.695	1.703	1.525	1.537
	H15″····O14″	1.627	1.627	1.446	1.456
	H15····O10′	1.899	1.897	1.802	1.772
	H16····O12′	1.957	1.934	1.786	1.790
	H16′····O12″	1.698	1.701	1.580	1.555
	H16″····O8′	1.912	1.905	1.805	1.790
6	H17····O14	1.665	1.667	1.544	1.554
	H15′····O14′	1.672	1.678	1.523	1.535
	H15″····O14″	1.627	1.631	1.440	1.457
	H15····O12′	1.868	1.866	1.784	1.766
	H16····O10′	1.885	1.880	1.794	1.772
	H16″····O8′	1.893	1.900	1.800	1.776
	H16′····O12″	1.700	1.701	1.564	1.551
6-y	H17····O14	1.664	1.666	1.542	1.551
	H15′····O14′	1.679	1.687	1.522	1.533
	H15″····O14″	1.631	1.630	1.437	1.464
	H15····O12′	1.872	1.870	1.781	1.772

	H16····O10′	1.899	1.898	1.801	1.778
	H16″····O8′	1.909	1.907	1.810	1.822
	H16′····O12″	1.695	1.704	1.564	1.538
7	H17····O14	1.666	1.670	1.541	1.551
	H17′····O14′	1.623	1.625	1.481	1.490
	H15″····O14″	1.624	1.627	1.424	1.443
	H15····O12′	1.839	1.841	1.752	1.734
	H16····O10′	1.883	1.881	1.807	1.789
	H15′····O12″	1.794	1.794	1.677	1.669
	H16″····O10′	1.948	1.946	1.856	1.843
7-y	H17····O14	1.663	1.664	1.538	1.555
	H17′····O14′	1.626	1.625	1.483	1.495
	H15″····O14″	1.625	1.627	1.426	1.447
	H15····O12′	1.859	1.852	1.762	1.749
	H16····O10′	1.885	1.880	1.807	1.761
	H15′····O12″	1.797	1.790	1.670	1.669
	H16″····O10′	1.938	1.934	1.836	1.801
8	H17····O14	1.671	1.674	1.550	1.561
	H17′····O14′	1.632	1.634	1.486	1.497
	H15″····O14″	1.624	1.627	1.424	1.443
	H15····O10′	1.858	1.860	1.794	1.768
	H16····O12′	1.868	1.861	1.766	1.755
	H16′····O10″	1.946	1.943	1.853	1.838
	H15′····O12″	1.792	1.792	1.676	1.668
8-y	H17····O14	1.681	1.700	1.553	1.601
	H17′····O14′	1.635	1.637	1.487	1.504
	H15″····O14″	1.625	1.627	1.425	1.447
	H15····O10′	1.888	1.900	1.796	1.769
	H16····O12′	1.901	1.906	1.772	1.804
	H16′····O10″	1.931	1.932	1.840	1.797
	H15′····O12″	1.787	1.788	1.670	1.655
9	H17····O14	1.666	1.669	1.543	1.553
	H17′····O14′	1.628	1.630	1.493	1.501
	H15″····O14″	1.622	1.625	1.419	1.438
	H15····O12′	1.842	1.846	1.767	1.749
	H16····O10′	1.870	1.870	1.795	1.774
	H15′····O10″	1.977	1.978	1.902	1.883
	H16′····O12″	1.767	1.765	1.630	1.622
9-y	H17····O14	1.663	1.665	1.540	1.550
	H17′····O14′	1.629	1.632	1.491	1.500
	H15″····O14″	1.624	1.625	1.413	1.438
	H15····O12′	1.863	1.856	1.763	1.755

	H16····O10′	1.917	1.907	1.809	1.804
	H15′····O10″	1.956	1.953	1.889	1.894
	H16′····O12″	1.746	1.751	1.623	1.604
10	H17····O14	1.668	1.669	1.547	1.557
	H17′····O14′	1.636	1.638	1.498	1.509
	H15″····O14″	1.622	1.625	1.419	1.438
	H15····O10′	1.847	1.852	1.781	1.756
	H16····O12′	1.875	1.873	1.787	1.778
	H16′····O12″	1.762	1.760	1.628	1.616
	H15′····O10″	1.980	1.979	1.903	1.884
10-y	H17····O14	1.700	1.706	1.556	1.568
	H17′····O14′	1.642	1.645	1.499	1.516
	H15″····O14″	1.617	1.621	1.411	1.425
	H15····O10′	1.898	1.899	1.799	1.772
	H16····O12′	1.931	1.920	1.791	1.815
	H16′····O12″	1.757	1.759	1.632	1.612
	H15′····O10″	1.969	1.971	1.882	1.900

structure T13-ET6,2″

1	H15····O14	1.625	1.637	1.448	1.458
	H15′····O14′	1.616	1.618	1.472	1.481
	H17″····O14″	1.608	1.610	1.457	1.465
	H17′····O8	1.841	1.850	1.740	1.722
	H16····O10′	1.858	1.868	1.770	1.750
	H16″····O8′	1.852	1.857	1.759	1.742
	H16′····O12″	1.811	1.818	1.703	1.684
1-y	H15····O14	1.625	1.638	1.448	1.459
	H15′····O14′	1.618	1.621	1.473	1.482
	H17″····O14″	1.611	1.614	1.461	1.468
	H17′····O8	1.842	1.851	1.740	1.725
	H16····O10′	1.871	1.881	1.781	1.761
	H16″····O8′	1.864	1.870	1.764	1.749
	H16′····O12″	1.832	1.841	1.720	1.695

structure T13-M5,3″-ET6,2″

1	H15····O14	1.709	1.728	1.470	1.483
	H15′····O14′	1.614	1.617	1.469	1.478
	H17″····O14″	1.652	1.659	1.475	1.485
	H17′····O8	1.835	1.844	1.728	1.713
	H16····O10′	1.852	1.863	1.760	1.742
	H16″····O8′	1.844	1.850	1.748	1.733

	H16′····O12″	1.799	1.807	1.691	1.675
1-y	H15····O14	1.710	1.729	1.471	1.485
	H15′····O14′	1.618	1.621	1.470	1.480
	H17″····O14″	1.657	1.665	1.479	1.488
	H17′····O8	1.837	1.848	1.729	1.719
	H16····O10′	1.864	1.876	1.771	1.750
	H16″····O8′	1.860	1.867	1.753	1.742
	H16′····O12″	1.820	1.829	1.707	1.683

structure T14-ET6,2″

1	H15····O14	1.725	1.717	1.445	1.458
	H15′····O14′	1.633	1.647	1.453	1.463
	H17″····O14″	1.712	1.605	1.436	1.446
	H17′····O8	1.835	1.852	1.735	1.717
	H16····O10′	1.855	1.872	1.770	1.749
	H16″····O8′	1.853	1.859	1.755	1.738
	H16′····O12″	1.810	1.819	1.699	1.680
1-y	H15····O14	1.725	1.637	1.447	1.458
	H15′····O14′	1.616	1.631	1.454	1.467
	H17″····O14″	1.600	1.607	1.440	1.468
	H17′····O8	1.834	1.845	1.735	1.720
	H16····O10′	1.867	1.878	1.778	1.760
	H16″····O8′	1.865	1.872	1.759	1.746
	H16′····O12″	1.833	1.843	1.716	1.690

structure T14-M5,3″-ET6,2″

1-y	H15····O14	1.710	1.729	1.470	1.492
	H15′····O14′	1.619	1.634	1.451	1.468
	H17″····O14″	1.658	1.664	1.464	1.485
	H17′····O8	1.832	1.842	1.725	1.728
	H16····O10′	1.861	1.872	1.768	1.748
	H16″····O8′	1.865	1.872	1.750	1.755
	H16′····O12″	1.820	1.829	1.703	1.677
1	H15····O14	1.709	1.727	1.469	1.487
	H15′····O14′	1.635	1.647	1.451	1.464
	H17″····O14″	1.701	1.717	1.464	1.482
	H17′····O8	1.829	1.839	1.723	1.709
	H16····O10′	1.848	1.859	1.758	1.743
	H16″····O8′	1.845	1.854	1.745	1.732
	H16′····O12″	1.801	1.811	1.691	1.676
1-y-out-in	H15····O14	1.710	1.728	1.470	1.485

	H15′····O14′	1.621	1.636	1.453	1.466
	H17″····O14″	1.695	1.709	1.467	1.477
	H17′····O8	1.830	1.841	1.725	1.714
	H16····O10′	1.862	1.874	1.768	1.750
	H16″····O8′	1.871	1.878	1.757	1.744
	H16′····O12″	1.838	1.847	1.712	1.687

Table S 13
Effect of the inclusion of Grimme's dispersion correction on the estimation of the length of the intramolecular hydrogen bonds in the calculated trimeric acylphloroglucinols
The table reports the difference in the estimations of the length of the IHBs, taken as «length in the DFT/B3LYP/6-31+G(d,p) result comprising Grimme's correction minus length in the DFT/B3LYP/6-31+G(d,p) result without Grimme's correction»; consequently, a negative value indicates length shortening and a positive value indicates length increase, caused by the Grimme's correction.

molecule	conformer	hydrogen bond	IHB length difference	
			conformer with outstretched geometry	conformer with half-bowl-shaped geometry
T1	1	H15····O14	0.007	0.007
		H17′····O14′	0.009	0.009
		H17″····O14″	0.008	0.010
		H16′····O8	-0.020	-0.024
		H16····O12′	-0.017	-0.015
		H16″····O10′	-0.021	-0.021
		H15′····O12″	-0.017	-0.015
	2	H15····O14	0.008	0.003
		H17′····O14′	0.009	0.012
		H15″····O14″	0.011	0.016
		H16′····O8	-0.019	-0.039
		H16····O12′	-0.017	-0.009
		H17″····O10′	-0.021	-0.040
		H15′····O10″	-0.013	0.005
	3	H15····O14	0.009	0.009
		H15′····O14′	0.010	0.010
		H15″····O14″	0.011	0.011
		H17′····O8	-0.016	-0.015
		H16····O10′	-0.020	-0.020
		H17″····O8′	-0.016	-0.016
		H16′····O10″	-0.016	-0.020
	4	H15····O14	0.010	0.009
		H17′····O14′	0.008	0.009
		H17″····O14″	0.009	0.010
		H10′····O8	-0.019	-0.024
		H16····O12′	-0.017	-0.015

		H16″····O10′	-0.020	-0.019
		H15′····O12″	-0.017	-0.014
	5	H15····O14	0.009	0.009
		H17′····O14′	0.009	0.017
		H15″····O14″	0.011	0.025
		H16′····O8	0.081	-0.034
		H16····O12′	-0.017	0.008
		H16″····O10′	-0.020	-0.041
		H15′····O10″	-0.014	0.032
	6	H17····O14	0.011	0.011
		H15′····O14′	0.010	0.011
		H15″····O14″	0.011	0.011
		H15····O10′	-0.020	-0.021
		H17′····O10	-0.012	-0.006
		H16′····O10″	-0.015	-0.020
		H17″····O8′	-0.016	-0.012
	7	H15····O14	0.011	0.010
		H15′····O14′	0.009	0.009
		H15″····O14″	0.011	0.012
		H17′····O8	-0.017	-0.015
		H16····O10′	-0.019	-0.019
		H17″····O8′	-0.016	-0.016
		H16′····O10″	-0.016	-0.020
	8	H17····O14		0.036
		H15′····O14′		0.007
		H17″····O14″		0.013
		H16′····O8		-0.024
		H16····O10′		-0.015
		H16″····O10′		-0.015
		H15′····O12″		-0.012
	9	H15····O14	0.009	1.493
		H17′····O14′	0.009	1.476
		H17″····O14″	0.010	1.502
		H16′····O8	-0.020	1.716
		H16····O12′	-0.017	1.761
		H16″····O10′	-0.021	1.773
		H15′····O12″	-0.016	1.756
	10	H15····O14	0.009	0.009
		H15′····O14′	0.011	0.011
		H15″····O14″	0.014	0.035
		H17′····O8	-0.017	-0.011
		H16····O10′	-0.021	-0.030

		H17″····O8′	-0.011	-0.005
		H16′····O12″	-0.019	-0.036
	11	H15····O14	0.008	0.011
		H15′····O14′	0.009	0.009
		H15″····O14″	0.012	0.011
		H17′····O8	-0.017	-0.012
		H16′····O10	-0.015	-0.027
		H17″····O8′	-0.019	-0.016
		H16″····O10′	-0.021	-0.022
	12	H15····O14	0.008	0.002
		H17′····O14′	0.011	0.014
		H15″····O14″	0.012	0.011
		H16′····O8	-0.017	-0.045
		H16····O12′	-0.018	0.001
		H17″····O10′	-0.019	-0.029
		H16″····O8′	-0.008	0.018
	13	H17····O14	0.011	0.011
		H17′····O14′	0.010	0.010
		H15″····O14″	0.015	0.015
		H15····O12′	-0.017	-0.018
		H16′····O10	-0.014	-0.019
		H15′····O12″	-0.016	-0.015
		H16″····O10′	-0.016	-0.015
	14	H17····O14	0.009	0.008
		H15′····O14′	0.010	0.010
		H17″····O14″	0.015	0.013
		H16′····O8	-0.017	-0.023
		H16····O12′	-0.017	-0.015
		H16″····O10′	-0.016	-0.014
		H15′····O12″	-0.017	-0.012
	15	H15····O14	0.008	0.008
		H15′····O14′	0.010	0.009
		H15″····O14″	0.013	0.015
		H17′····O8	-0.018	-0.015
		H16····O10′	-0.017	-0.030
		H16″····O8′	-0.014	-0.012
		H17″····O10′	-0.025	-0.032
	16	H15····O14	0.011	0.010
		H15′····O14′	-0.010	0.011
		H15″····O14″	0.015	0.026
		H17′····O8	-0.016	-0.011
		H16····O10′	-0.020	-0.031

		H16″····O8′	-0.011	-0.005
		H17′····O10″	-0.020	-0.036
	17	H17····O14	0.008	0.007
		H17′····O14′	0.008	0.009
		H17″····O14″	0.011	0.012
		H16′····O8	-0.018	-0.022
		H17′····O10	-0.021	-0.017
		H16″····O10′	-0.022	-0.020
		H17″····O8′	-0.018	-0.016
	18	H15····O14	0.007	0.001
		H15′····O14′	0.010	0.014
		H15″····O14″	0.012	0.012
		H16′····O8	-0.019	-0.045
		H17′····O10	-0.020	-0.004
		H17″····O10′	-0.026	-0.037
		H16″····O8′	-0.013	0.004
	19	H15····O14	0.009	0.010
		H15′····O14′	0.009	0.008
		H15″····O14″	0.012	0.011
		H17′····O8	-0.018	-0.015
		H16′····O10	-0.015	-0.026
		H17″····O8′	-0.019	-0.017
		H16″····O10′	-0.020	-0.020
	20	H17····O14	0.009	0.008
		H17′····O14′	0.009	0.009
		H17″····O14″	0.011	0.011
		H16′····O8	-0.018	-0.022
		H17′····O10	-0.021	-0.018
		H16″····O10′	-0.021	-0.020
		H17″····O8′	-0.019	-0.016
	21	H15····O14	0.009	0.010
		H15′····O14′	0.010	0.009
		H15″····O14″	0.012	0.013
		H17′····O8	-0.018	-0.016
		H16′····O10	-0.017	-0.028
		H16″····O8′	-0.014	-0.013
		H17′····O10″	-0.025	-0.030
	22	H15····O14	0.008	-0.003
		H15′····O14′	0.010	0.034
		H15″····O14″	0.012	0.011
		H16′····O8	-0.019	-0.052
		H17′····O10	-0.021	0.018

		H17″····O10′	-0.026	-0.054
		H16″····O8′	-0.013	0.097
	23	H15····O14	0.009	0.009
		H17′····O14′	0.011	0.027
		H15″····O14″	0.012	0.010
		H16′····O8	-0.017	-0.052
		H16····O12′	-0.017	0.030
		H17″····O10′	-0.019	0.057
		H16″····O8′	-0.007	0.115
	24	H17····O14	0.009	0.008
		H15′····O14′	0.010	0.012
		H17″····O14″	0.011	0.011
		H16′····O8	-0.017	-0.024
		H16····O12′	-0.017	-0.016
		H16″····O10′	-0.018	-0.015
		H17″····O8′	-0.016	-0.010
	25	H17····O14	0.014	0.001
		H15′····O14′	0.009	0.009
		H15″····O14″	0.012	0.013
		H16′····O8	-0.013	-0.004
		H17′····O10	-0.012	0.063
		H16″····O10′	-0.021	0.025
		H17″····O8′	-0.019	-0.002
	26	H17····O14	0.012	0.025
		H15′····O14′	0.012	0.011
		H15″····O14″	0.012	0.000
		H15····O12′	-0.015	-0.042
		H16′····O10	-0.009	0.037
		H16″····O8′	-0.012	-0.065
		H17″····O10′	-0.023	0.001
	27	H17····O14	-0.011	-0.013
		H15′····O14′	0.009	0.008
		H15″····O14″	0.036	0.039
		H17′····O8	-0.054	-0.053
		H16′····O10	0.021	0.031
		H17″····O8′	0.015	0.033
		H16″····O10′	-0.057	-0.061
	28	H17····O14	0.015	0.008
		H15′····O14′	0.011	0.029
		H15″····O14″	0.012	0.018
		H16′····O8	-0.014	0.026
		H17′····O10	-0.011	0.092

		H16″····O8′	-0.026	-0.063
		H17′····O10″	-0.013	0.074
	29	H17····O14		0.015
		H15′····O14′		0.110
		H15″····O14″		0.014
		H17′····O8		-0.011
		H16′····O10		-0.022
		H16″····O8′		-0.013
		H17′····O10″		-0.027
T2-KT2,6″-M5,5,3″,3″	1	H17····O14	0.018	0.018
		H15′····O14′	0.008	0.008
		H15″····O14″	0.018	0.019
		H17′····O8	-0.015	-0.013
		H16····O10′	-0.024	-0.033
		H16″····O8′	-0.021	-0.018
		H16′····O12″	-0.018	-0.029
		H15····O14	0.009	0.008
T3-ET6,2″	1	H15′····O14′	0.012	0.018
		H17″····O14″	0.009	0.008
		H17′····O8	-0.019	-0.022
		H16····O10′	-0.020	-0.013
		H16″····O8′	-0.017	-0.017
		H16′····O12″	0.081	-0.025
T3-M5,3″-ET6,2″	1	H15····O14	0.011	0.013
		H15′····O14′	0.011	0.012
		H17″····O14″	0.012	0.011
		H17′····O8	0.040	-0.014
		H16····O10′	-0.019	-0.020
		H16″····O8′	-0.017	-0.013
		H16′····O12″	-0.018	-0.022
T4-KT2,6″-M5,5,3″,3″	1	H17····O14	0.016	0.016
		H15′····O14′	0.008	0.009
		H15″····O14″	0.018	0.019
		H17′····O8	0.000	-0.013
		H16····O10′	-0.025	-0.032
		H16″····O8′	-0.021	-0.018
		H16′····O12″	-0.018	-0.029
T5-KT6″-M3″,3′-ET4	1	H17····O14	0.011	0.010

		H17′⋯O14′	0.009	0.010
		H15″⋯O14″	0.017	0.017
		H15⋯O12′	-0.015	-0.017
		H16′⋯O10	-0.031	-0.046
		H15′⋯O12″	-0.014	-0.011
		H16″⋯O10′	-0.027	-0.037
T5-KT2,6″-M5,5,3″,3″	1	H17⋯O14	0.016	0.015
		H15′⋯O14′	0.008	0.010
		H15″⋯O14″	0.017	0.023
		H17′⋯O8	-0.015	-0.009
		H16⋯O10′	-0.024	-0.040
		H16″⋯O8′	-0.021	-0.008
		H16′⋯O12″	-0.018	-0.037
T6-M5,3″-ET6,4″	1	H15⋯O14	0.004	0.011
		H15′⋯O14′	-0.008	0.010
		H15″⋯O14″	-0.007	0.010
		H17′⋯O8	0.011	-0.012
		H16⋯O10′	-0.015	-0.022
		H17″⋯O8′	-0.044	-0.018
		H16′⋯O10″	-0.158	-0.030
	1-y-in-out	H15⋯O14		0.011
		H15′⋯O14′		0.009
		H15″⋯O14″		0.011
		H17′⋯O8		-0.014
		H16⋯O10′		-0.024
		H17″⋯O8′		-0.019
		H16′⋯O10″		-0.031
	1-y-in-in	H15⋯O14		0.008
		H15′⋯O14′		0.015
		H15″⋯O14″		0.013
		H17′⋯O8		-0.021
		H16⋯O10′		-0.031
		H17″⋯O8′		0.008
		H16′⋯O10″		-0.014
T7	1	H15⋯O14	0.007	0.006
		H17′⋯O14′	0.008	0.009
		H17″⋯O14″	0.008	0.009
		H16′⋯O8	-0.019	-0.025
		H16⋯O12′	-0.017	-0.015

		H16″····O10′	-0.020	-0.020
		H15′····O12″	-0.018	-0.015
	2	H15····O14	0.007	0.010
		H17′····O14′	0.008	0.009
		H15″····O14″	0.011	0.008
		H16′····O8	-0.019	-0.036
		H16····O12′	-0.017	-0.018
		H17″····O10′	-0.020	-0.051
		H15′····O10″	-0.015	-0.018
	3	H15····O14	0.008	0.008
		H15′····O14′	0.008	0.008
		H15″····O14″	0.011	0.011
		H17′····O8	-0.017	-0.016
		H16····O10′	-0.019	-0.019
		H17″····O8′	-0.016	-0.016
		H16′····O10″	-0.016	-0.019
	4	H15····O14	0.009	0.008
		H17′····O14′	0.008	0.009
		H17″····O14″	0.009	0.010
		H10′····O8	-0.019	-0.024
		H16····O12′	-0.016	-0.014
		H16″····O10′	-0.021	-0.020
		H15′····O12″	-0.019	-0.015
	5	H15····O14	0.009	0.015
		H17′····O14′	0.009	0.062
		H15″····O14″	0.012	0.087
		H16′····O8	-0.017	0.405
		H16····O12′	-0.016	-0.317
		H16″····O10′	-0.020	0.015
		H15′····O10″	-0.014	-0.004
	6	H17····O14	0.011	0.020
		H15′····O14′	0.009	0.019
		H15″····O14″	0.011	0.010
		H15····O10′	-0.020	-0.020
		H16′····O10	-0.012	0.032
		H16′····O10″	-0.015	-0.006
		H17″····O10′	-0.015	0.020
T7-ET6,2″	1	H15····O14	0.009	0.009
		H15′····O14′	0.008	0.009
		H17″····O14″	0.010	0.008
		H16′····O8	-0.017	-0.014

		H16····O12′	-0.020	-0.020
		H16″····O10′	-0.017	-0.015
		H15′····O12″	-0.019	-0.026
T7-M5,3″-ET6,2″	1	H15····O14	0.011	0.012
		H15′····O14′	0.008	0.009
		H17″····O14″	0.012	0.010
		H16′····O8	-0.016	-0.011
		H16····O12′	-0.021	-0.021
		H16″····O10′	-0.016	-0.013
		H15′····O12″	-0.017	-0.024
T7-KT6″-M5,3″,3″	1	H15····O14	0.008	0.007
		H15′····O14′	0.008	0.008
		H15″····O14″	0.018	0.019
		H17′····O8	-0.019	-0.015
		H16····O10′	-0.022	-0.025
		H16″····O8′	-0.021	-0.017
		H16′····O12″	-0.016	-0.026
	2	H15····O14	0.006	0.004
		H17′····O14′	0.008	0.009
		H15″····O14″	0.017	0.016
		H16′····O8	-0.021	-0.030
		H16····O12′	-0.017	-0.016
		H16″····O10′	-0.024	-0.029
		H16′····O12″	-0.015	-0.014
	3	H17····O14	0.009	0.033
		H15′····O14′	0.007	0.012
		H15″····O14″	0.019	0.019
		H15····O10′	-0.024	0.012
		H17′····O10	-0.017	0.051
		H16′····O12″	-0.016	-0.011
		H16″····O8′	-0.021	-0.005
	4	H17····O14	0.009	0.009
		H17′····O14′	0.009	0.010
		H15″····O14″	0.019	0.018
		H15····O12′	-0.017	-0.012
		H17′····O10	-0.018	-0.021
		H15′····O12″	-0.014	-0.013
		H16″····O10′	-0.023	-0.029
	5	H17····O14	0.011	0.017
		H15′····O14′	0.010	0.010

		H15″····O14″	0.018	0.017
		H15····O10′	-0.018	-0.019
		H16····O12′	-0.005	0.026
		H16′····O12″	-0.015	-0.029
		H16″····O8′	-0.021	-0.017
	6	H17····O14	0.012	0.011
		H15′····O14′	0.010	0.012
		H15″····O14″	0.018	0.019
		H15····O12′	-0.012	0.001
		H16····O10′	-0.015	-0.018
		H16″····O8′	-0.022	-0.014
		H16′····O12″	-0.014	-0.030
	7	H17····O14	0.011	0.017
		H17′····O14′	0.009	0.013
		H15″····O14″	0.020	0.022
		H15····O12′	-0.019	-0.012
		H16····O10′	-0.019	-0.046
		H15′····O12″	-0.006	-0.001
		H16″····O10′	-0.015	-0.037
	8	H17····O14	0.010	0.041
		H17′····O14′	0.010	0.017
		H15″····O14″	0.020	0.022
		H15····O10′	-0.025	-0.031
		H16····O12′	-0.012	0.028
		H16′····O10″	-0.017	-0.046
		H15′····O12″	-0.006	-0.012
	9	H17····O14	0.010	0.002
		H17′····O14′	0.009	0.010
		H15″····O14″	0.021	0.024
		H15····O12′	-0.017	-0.001
		H16····O10′	-0.021	-0.002
		H15′····O10″	-0.020	0.008
		H16′····O12″	-0.007	-0.022
	10	H17····O14	0.010	0.013
		H17′····O14′	0.011	0.022
		H15″····O14″	0.021	0.018
		H15····O10′	-0.024	-0.008
		H16····O12′	-0.009	0.050
		H16′····O12″	-0.010	-0.026
		H15′····O10″	-0.021	0.036
T7-KT2,6″-M5,5,3″,3″	1	H17····O14	0.016	0.016

		H15′····O14′	0.008	0.009
		H15″····O14″	0.018	0.018
		H17′····O8	-0.016	-0.013
		H16····O10′	-0.024	-0.032
		H16″····O8′	-0.021	-0.018
		H16′····O12″	-0.018	-0.030
T8-KT6″-M5,3″,3″	1	H15····O14	0.007	0.008
		H15′····O14′	0.007	0.009
		H15″····O14″	0.016	0.018
		H17′····O8	-0.020	-0.013
		H16····O10′	-0.022	-0.028
		H16″····O8′	-0.021	-0.015
		H16′····O12″	-0.017	-0.030
	2	H15····O14	0.006	0.004
		H17′····O14′	0.008	0.009
		H15″····O14″	0.017	0.016
		H16′····O8	-0.021	-0.031
		H16····O12′	-0.017	-0.016
		H16″····O10′	-0.024	-0.030
		H16′····O12″	-0.015	-0.014
	3	H17····O14	0.009	0.018
		H15′····O14′	0.007	0.010
		H15″····O14″	0.016	0.014
		H15····O10′	-0.023	-0.029
		H17′····O10	-0.017	0.017
		H16′····O12″	-0.017	-0.027
		H16″····O8′	-0.025	-0.014
	4	H17····O14	0.009	0.009
		H17′····O14′	0.009	0.010
		H15″····O14″	0.016	0.017
		H15····O12′	-0.016	-0.011
		H17′····O10	-0.018	-0.022
		H15′····O12″	-0.014	-0.013
		H16″····O10′	-0.023	-0.029
	5	H17····O14	0.011	0.013
		H15′····O14′	0.010	0.011
		H15″····O14″	0.017	0.016
		H15····O10′	-0.020	-0.023
		H16····O12′	-0.004	0.025
		H16′····O12″	-0.016	-0.036
		H16″····O8′	-0.021	-0.010

	6	H17⋯O14	0.012	0.012
		H15′⋯O14′	0.010	0.014
		H15″⋯O14″	0.016	0.023
		H15⋯O12′	-0.012	0.033
		H16⋯O10′	-0.015	-0.005
		H16″⋯O8′	-0.022	0.001
		H16′⋯O12″	-0.014	-0.038
	7	H17⋯O14	0.011	0.017
		H17′⋯O14′	0.009	0.013
		H15″⋯O14″	0.018	0.020
		H15⋯O12′	-0.018	-0.012
		H16⋯O10′	-0.018	-0.046
		H15′⋯O12″	-0.007	-0.001
		H16″⋯O10′	-0.015	-0.035
	8	H17⋯O14	0.011	0.042
		H17′⋯O14′	0.011	0.017
		H15″⋯O14″	0.018	0.021
		H15⋯O10′	-0.026	-0.031
		H16⋯O12′	-0.012	0.029
		H16′⋯O10″	-0.017	-0.047
		H15′⋯O12″	-0.007	-0.012
	9	H17⋯O14	0.010	0.001
		H17′⋯O14′	0.008	0.010
		H15″⋯O14″	0.019	0.022
		H15⋯O12′	-0.018	-0.002
		H16⋯O10′	-0.021	-0.004
		H15′⋯O10″	-0.019	0.007
		H16′⋯O12″	-0.007	-0.025
	10	H17⋯O14	0.010	0.016
		H17′⋯O14′	0.011	0.021
		H15″⋯O14″	0.018	0.015
		H15⋯O10′	-0.024	-0.023
		H16⋯O12′	-0.009	0.047
		H16′⋯O12″	-0.011	-0.018
		H15′⋯O10″	-0.020	0.053
T8-KT2-M5,5,3″	1	H17⋯O14	0.017	0.030
		H17′⋯O14′	0.008	0.013
		H17″⋯O14″	0.006	0.009
		H16′⋯O8	-0.017	-0.033
		H16⋯O12′	-0.020	0.005
		H16″⋯O10′	-0.023	-0.030

		H16′····O12″	-0.020	-0.001
	2	H17····O14	0.017	0.016
		H15′····O14′	0.009	0.010
		H17″····O14″	0.006	0.005
		H17′····O8	-0.016	-0.014
		H16····O10′	-0.023	-0.030
		H16″····O8′	-0.017	-0.016
		H16′····O12″	-0.020	-0.030
	3	H17····O14	0.021	0.021
		H17′····O14′	0.007	0.015
		H15″····O14″	0.009	0.024
		H16′····O8	-0.019	-0.026
		H15····O12′	-0.019	0.004
		H17″····O10′	-0.024	-0.012
		H15′····O10″	-0.018	0.047
	4	H17····O14	0.017	0.017
		H15′····O14′	0.010	0.010
		H15″····O14″	0.008	0.009
		H17′····O8	-0.015	-0.014
		H16····O10′	-0.023	-0.028
		H17″····O8′	-0.016	-0.011
		H16′····O10″	-0.018	-0.022
	5	H17····O14	0.017	0.014
		H17′····O14′	0.010	0.011
		H15″····O14″	0.011	0.015
		H16′····O8	-0.016	-0.031
		H16····O12′	-0.020	-0.016
		H17″····O10′	-0.019	-0.015
		H16″····O8′	-0.004	0.014
	6	H17····O14	0.017	0.026
		H17′····O14′	0.010	0.017
		H15″····O14″	0.011	0.002
		H15····O12′	-0.015	-0.029
		H16····O10′	-0.022	0.011
		H16″····O8′	-0.015	0.012
		H16′····O12″	-0.010	-0.004
	7	H17····O14	0.019	0.021
		H15′····O14′	0.009	0.013
		H15″····O14″	0.009	0.008
		H17′····O8	-0.009	-0.001
		H16′····O10	-0.012	-0.033
		H17″····O8′	-0.018	-0.007

		H16″····O10′	-0.019	-0.042
	8	H17····O14	0.019	0.020
		H15′····O14′	0.010	0.010
		H15″····O14″	0.011	0.015
		H17′····O8	-0.007	-0.002
		H16′····O10	-0.014	-0.019
		H17″····O8′	-0.011	-0.012
		H16″····O10′	-0.024	-0.035
	9	H17····O14	0.019	0.026
		H17′····O14′	0.002	0.009
		H15″····O14″	0.010	0.000
		H16′····O8	-0.009	-0.020
		H17′····O10	-0.019	0.004
		H16″····O10′	-0.022	0.004
		H17″····O8′	-0.017	-0.004
	10	H17····O14	0.031	0.012
		H15′····O14′	0.011	0.028
		H15″····O14″	0.010	0.018
		H16′····O8	-0.010	-0.015
		H17′····O10	-0.007	0.057
		H17″····O10′	-0.023	0.019
		H16″····O8′	-0.009	0.093
T8-KT2,6″-M5,5,3″,3″	1	H17····O14	0.017	0.016
		H15′····O14′	0.007	0.010
		H15″····O14″	0.016	0.023
		H17′····O8	-0.016	-0.011
		H16····O10′	-0.024	-0.039
		H16″····O8′	-0.020	-0.009
		H16′····O12″	-0.018	-0.037
T9	1	H15····O14	0.007	0.006
		H17′····O14′	0.009	0.009
		H17″····O14″	0.008	0.008
		H16′····O8	-0.020	-0.026
		H16····O12′	-0.016	-0.015
		H16″····O10′	-0.020	-0.019
		H15′····O12″	-0.018	-0.015
	2	H15····O14	0.007	0.003
		H17′····O14′	0.009	0.010
		H15″····O14″	0.009	0.015
		H16′····O8	-0.019	-0.057

		H16····O12′	-0.016	-0.016
		H17″····O10′	-0.022	-0.071
		H15′····O10″	-0.014	-0.017
	3	H15····O14	0.008	0.009
		H15′····O14′	0.009	0.009
		H15″····O14″	0.010	0.011
		H17′····O8	-0.017	-0.016
		H16····O10′	-0.019	-0.018
		H17″····O8′	-0.016	-0.015
		H16′····O10″	-0.014	-0.019
	4	H15····O14	0.009	0.009
		H17′····O14′	0.008	0.009
		H17″····O14″	0.007	0.008
		H10′····O8	-0.018	-0.024
		H16····O12′	-0.016	-0.014
		H16″····O10′	-0.020	-0.019
		H15′····O12″	-0.018	-0.015
	5	H15····O14	0.009	0.011
		H17′····O14′	0.009	0.013
		H15″····O14″	0.011	0.039
		H16′····O8	-0.018	-0.026
		H16····O12′	-0.016	0.000
		H16″····O10′	-0.021	-0.020
		H15′····O10″	-0.013	0.049
	6	H17····O14	0.011	0.020
		H15′····O14′	0.009	0.019
		H15″····O14″	0.011	0.009
		H15····O10′	-0.020	-0.019
		H16′····O10	-0.012	-0.066
		H16′····O10″	-0.014	-0.003
		H17″····O10′	-0.016	0.019
T9-M5,3″	1	H15····O14	0.006	0.005
		H17′····O14′	0.008	0.009
		H17″····O14″	0.007	0.007
		H16′····O8	-0.019	-0.027
		H16····O12′	-0.017	-0.015
		H16″····O10′	-0.020	-0.022
		H15′····O12″	-0.018	-0.014
	2	H15····O14	0.006	-0.025
		H17′····O14′	0.009	-0.018
		H15″····O14″	0.010	0.013

		H16′····O8	-0.018	-0.015
		H16····O12′	-0.017	0.008
		H17″····O10′	-0.021	-0.031
		H15′····O10″	-0.014	0.017
	3	H15····O14	0.006	0.008
		H15′····O14′	0.009	0.013
		H15″····O14″	0.010	0.018
		H17′····O8	-0.018	-0.022
		H16····O10′	-0.017	-0.004
		H17″····O8′	-0.021	-0.016
		H16′····O10″	-0.014	0.025
	4	H15····O14	0.009	0.009
		H17′····O14′	0.008	0.009
		H17″····O14″	0.007	0.008
		H10′····O8	-0.018	-0.026
		H16····O12′	-0.016	-0.014
		H16″····O10′	-0.020	-0.023
		H15′····O12″	-0.017	-0.014
	5	H15····O14	0.010	0.011
		H17′····O14′	0.009	0.013
		H15″····O14″	0.009	0.037
		H16′····O8	-0.017	-0.026
		H16····O12′	-0.016	-0.001
		H17″····O10′	-0.021	-0.021
		H15′····O10″	-0.014	-0.055
	6	H17····O14	0.010	0.018
		H15′····O14′	0.010	0.020
		H15″····O14″	0.009	0.009
		H15····O10′	-0.020	0.002
		H17′····O10	-0.013	0.039
		H16′····O10″	-0.015	0.001
		H17″····O10′	-0.015	0.028
T9-ET6,2″	1	H15····O14	0.009	0.010
		H15′····O14′	0.009	0.008
		H17″····O14″	0.008	0.007
		H17′····O8	-0.017	-0.014
		H16····O10′	-0.021	-0.021
		H16″····O8′	-0.017	-0.015
		H16′····O12″	-0.019	-0.025
T9-M5,3″-ET6,2″	1	H15····O14	0.010	0.012

		H15′····O14′	0.009	0.009
		H17″····O14″	0.010	0.010
		H17′····O8	-0.015	-0.010
		H16····O10′	-0.018	-0.021
		H16″····O8′	-0.015	-0.012
		H16′····O12″	-0.016	-0.025
T9-M5,3″-ET6,4″	1	H15····O14	0.011	0.011
		H15′····O14′	0.008	0.008
		H15″····O14″	0.011	0.011
		H17′····O8	-0.015	-0.013
		H16····O10′	-0.022	-0.021
		H17″····O8′	-0.020	-0.018
		H16′····O10″	-0.028	-0.031
	1-y-out-in	H15····O14		0.009
		H15′····O14′		0.013
		H15″····O14″		0.014
		H17′····O8		-0.020
		H16····O10′		-0.029
		H17″····O8′		0.007
		H16′····O10″		-0.016
	1-y-in-in	H15····O14		0.008
		H15′····O14′		0.014
		H15″····O14″		0.014
		H17′····O8		-0.023
		H16····O10′		-0.030
		H17″····O8′		0.007
		H16′····O10″		-0.013
T9-KT6″-M5,3″,3″	1	H15····O14	0.006	0.010
		H15′····O14′	0.007	0.012
		H15″····O14″	0.017	0.030
		H17′····O8	-0.019	0.000
		H16····O10′	-0.022	-0.030
		H16″····O8′	-0.021	0.004
		H16′····O12″	-0.017	-0.033
	2	H15····O14	0.006	0.004
		H17′····O14′	0.008	0.009
		H15″····O14″	0.017	0.016
		H16′····O8	-0.021	-0.030
		H16····O12′	-0.017	-0.016
		H16″····O10′	-0.024	-0.029

		H16′⋯O12″	-0.015	-0.014
	3	H17⋯O14	0.009	0.016
		H15′⋯O14′	0.007	0.009
		H15″⋯O14″	0.017	0.018
		H15⋯O10′	-0.026	-0.034
		H17′⋯O10	-0.018	-0.013
		H16′⋯O12″	-0.018	-0.032
		H16″⋯O8′	-0.021	-0.013
	4	H17⋯O14	0.009	0.008
		H17′⋯O14′	0.009	0.010
		H15″⋯O14″	0.017	0.017
		H15⋯O12′	-0.017	-0.012
		H17′⋯O10	-0.018	-0.022
		H15′⋯O12″	-0.014	-0.013
		H16″⋯O10′	-0.023	-0.030
	5	H17⋯O14	0.011	0.027
		H15′⋯O14′	0.014	0.010
		H15″⋯O14″	0.019	0.011
		H15⋯O10′	-0.026	-0.032
		H16⋯O12′	-0.004	0.001
		H16′⋯O12″	-0.015	-0.028
		H16″⋯O8′	-0.022	-0.014
	6	H17⋯O14	0.010	0.009
		H15′⋯O14′	0.012	0.011
		H15″⋯O14″	0.018	0.027
		H15⋯O12′	-0.018	-0.008
		H16⋯O10′	-0.022	-0.024
		H16″⋯O8′	-0.024	0.014
		H16′⋯O12″	-0.013	-0.026
	7	H17⋯O14	0.011	0.017
		H17′⋯O14′	0.009	0.012
		H15″⋯O14″	0.019	0.021
		H15⋯O12′	-0.018	-0.011
		H16⋯O10′	-0.018	-0.047
		H15′⋯O12″	-0.008	-0.002
		H16″⋯O10′	-0.013	-0.035
	8	H17⋯O14	0.011	0.042
		H17′⋯O14′	0.011	0.017
		H15″⋯O14″	0.019	0.021
		H15⋯O10′	-0.025	-0.030
		H16⋯O12′	-0.012	0.028
		H16′⋯O10″	-0.015	-0.046

		H15′····O12″	-0.007	-0.013
	9	H17····O14	0.010	0.009
		H17′····O14′	0.008	0.009
		H15″····O14″	0.019	0.025
		H15····O12′	-0.017	-0.008
		H16····O10′	-0.022	-0.004
		H15′····O10″	-0.018	0.004
		H16′····O12″	-0.009	-0.019
	10	H17····O14	0.010	0.029
		H17′····O14′	0.011	0.010
		H15″····O14″	0.019	0.013
		H15····O10′	-0.024	-0.023
		H16····O12′	-0.008	0.007
		H16′····O12″	-0.011	-0.029
		H15′····O10″	-0.019	0.084
T9-KT6″-M3″,3″-ET4	1	H17····O14	0.010	0.010
		H17′····O14′	0.009	0.009
		H15″····O14″	0.017	0.017
		H15····O12′	-0.015	-0.016
		H16′····O10	-0.031	-0.045
		H15′····O12″	-0.014	-0.012
		H16″····O10′	-0.027	-0.036
T9-KT6″-M5,3″,3″-ET6	1	H15····O14	0.010	0.008
		H17′····O14′	0.009	0.010
		H15″····O14″	0.017	0.017
		H16′····O8	-0.018	-0.028
		H16····O12′	-0.016	-0.006
		H16″····O10′	-0.024	-0.029
		H15′····O12″	-0.016	-0.014
T9-KT2,6″-M5,5,3″,3″	1	H17····O14	0.017	0.015
		H15′····O14′	0.007	0.012
		H15″····O14″	0.017	0.032
		H17′····O8	-0.016	-0.009
		H16····O10′	-0.024	-0.037
		H16″····O8′	-0.021	0.002
		H16′····O12″	-0.018	-0.036
T10	1	H15····O14	0.009	0.007
		H17′····O14′	0.010	0.009

		H17″····O14″	0.008	0.009
		H16′····O8	-0.019	-0.025
		H16····O12′	-0.016	-0.015
		H16″····O10′	-0.021	-0.020
		H15′····O12″	-0.019	-0.017
	2	H15····O14	0.008	0.001
		H17′····O14′	0.010	0.008
		H15″····O14″	0.014	0.016
		H16′····O8	-0.019	-0.054
		H16····O12′	-0.015	-0.018
		H17″····O10′	-0.021	-0.056
		H15′····O10″	-0.011	-0.008
	3	H15····O14	0.008	0.009
		H15′····O14′	0.010	0.009
		H15″····O14″	0.013	0.010
		H17′····O8	-0.019	-0.018
		H16····O10′	-0.019	-0.020
		H17″····O8′	-0.018	-0.017
		H16′····O10″	-0.012	-0.019
	4	H15····O14	0.008	0.007
		H17′····O14′	0.010	0.013
		H17″····O14″	0.008	0.009
		H10′····O8	-0.019	-0.025
		H16····O12′	-0.016	-0.016
		H16″····O10′	-0.021	-0.017
		H15′····O12″	-0.019	-0.017
	5	H15····O14	0.008	-0.006
		H17′····O14′	0.009	0.008
		H15″····O14″	0.013	0.019
		H16′····O8	-0.018	-0.057
		H16····O12′	-0.016	-0.019
		H17″····O10′	-0.020	-0.068
		H15′····O10″	-0.011	-0.013
	6	H17····O14	0.009	0.067
		H15′····O14′	0.009	0.032
		H15″····O14″	0.013	0.023
		H15····O10′	-0.023	0.025
		H16′····O10	-0.015	0.089
		H16′····O10″	-0.012	0.041
		H17″····O10′	-0.018	0.065
T10-ET6,2″	1	H15····O14	0.010	0.010

		H15′····O14′	0.010	0.009
		H17″····O14″	0.010	0.009
		H17′····O8	-0.019	-0.016
		H16····O10′	-0.019	-0.021
		H16″····O8′	-0.017	-0.015
		H16′····O12″	-0.018	-0.025
T10-M5,3″-ET6,2″	1	H15····O14	0.014	0.015
		H15′····O14′	0.009	0.013
		H17″····O14″	0.017	0.010
		H17′····O8	-0.016	-0.012
		H16····O10′	-0.019	-0.020
		H16″····O8′	-0.015	-0.015
		H16′····O12″	-0.016	-0.025
T10-M5,3″-ET6,2″,6″	1	H15····O14	-0.081	-0.071
		H17′····O14′	0.015	0.012
		H16′····O8	-0.011	-0.026
		H16····O12′	-0.012	0.000
		H16″····O10′	-0.005	-0.033
		H15′····O12″	-0.031	-0.028
T10-KT2,6″-M5,5,3″,3″	1	H17····O14	0.019	0.019
		H15′····O14′	0.010	0.012
		H15″····O14″	0.019	0.032
		H17′····O8	-0.020	-0.014
		H16····O10′	-0.019	-0.037
		H16″····O8′	-0.020	-0.003
		H16′····O12″	-0.019	-0.037
T11-ET6,2″	1	H15····O14	0.010	0.010
		H17′····O14′	0.009	0.012
		H17″····O14″	0.009	0.010
		H16′····O8	-0.018	-0.025
		H16····O12′	-0.017	-0.015
		H16″····O10′	-0.019	-0.018
		H15′····O12″	-0.019	-0.016
T11-M5,3″-ET6,2″	1	H15····O14	0.021	0.018
		H17′····O14′	0.015	0.010
		H17″····O14″	0.013	0.011
		H16′····O8	-0.025	-0.015
		H16····O12′	0.003	-0.015

		H16″····O10′	-0.026	-0.017
		H15′····O12″	-0.003	-0.017
	1-y-out-in	H15····O14		0.012
		H17′····O14′		0.013
		H17″····O14″		0.012
		H16′····O8		-0.025
		H16····O12′		-0.014
		H16″····O10′		-0.020
		H15′····O12″		-0.013
T12-KT2-M5,5,3″	1	H17····O14	0.017	0.035
		H17′····O14′	0.007	0.015
		H17″····O14″	0.006	0.010
		H16′····O8	-0.017	-0.030
		H16····O12′	-0.020	0.011
		H16″····O10′	-0.023	-0.025
		H16′····O12″	-0.020	0.005
	2	H17····O14	0.017	0.016
		H15′····O14′	0.009	0.009
		H17″····O14″	0.006	0.004
		H17′····O8	-0.016	-0.014
		H16····O10′	-0.024	-0.031
		H16″····O8′	-0.017	-0.015
		H16′····O12″	-0.021	-0.031
	3	H17····O14	0.018	0.021
		H17′····O14′	0.007	0.016
		H15″····O14″	0.009	0.023
		H16′····O8	-0.018	-0.023
		H15····O12′	-0.021	0.002
		H17″····O10′	-0.026	-0.023
		H15′····O10″	-0.018	0.033
	4	H17····O14	0.017	0.017
		H15′····O14′	0.010	0.010
		H15″····O14″	0.008	0.009
		H17′····O8	-0.015	-0.013
		H16····O10′	-0.023	-0.028
		H17″····O8′	-0.016	-0.012
		H16′····O10″	-0.018	-0.023
	5	H17····O14	0.019	0.011
		H17′····O14′	0.015	0.010
		H15″····O14″	0.012	0.026
		H16′····O8	-0.016	-0.029

		H16⋯O12′	-0.021	-0.013
		H17″⋯O10′	-0.025	-0.032
		H16″⋯O8′	0.000	-0.003
	6	H17⋯O14	0.018	0.031
		H17′⋯O14′	0.011	0.010
		H15″⋯O14″	0.010	0.009
		H16′⋯O8	-0.013	-0.024
		H16⋯O12′	-0.024	0.013
		H16″⋯O10′	-0.022	-0.022
		H17″⋯O8′	-0.018	-0.010
	7	H17⋯O14	0.019	0.020
		H15′⋯O14′	0.009	0.012
		H15″⋯O14″	0.010	0.017
		H17′⋯O8	-0.008	-0.001
		H16′⋯O10	-0.012	-0.033
		H17″⋯O8′	-0.018	-0.013
		H16″⋯O10′	-0.019	-0.045
	8	H17⋯O14	0.019	0.021
		H15′⋯O14′	0.011	0.017
		H15″⋯O14″	0.011	0.041
		H17′⋯O8	-0.007	-0.014
		H16′⋯O10	-0.014	-0.045
		H17″⋯O8′	-0.011	0.026
		H16″⋯O10′	-0.025	-0.033
	9	H17⋯O14	0.019	-0.012
		H17′⋯O14′	0.008	0.008
		H15″⋯O14″	0.010	-0.040
		H16′⋯O8	-0.009	-0.019
		H16⋯O12′	-0.019	0.007
		H17″⋯O10′	-0.022	0.001
		H15′⋯O10″	-0.018	-0.010
	10	H17⋯O14	0.021	0.037
		H15′⋯O14′	0.011	0.015
		H15″⋯O14″	0.010	0.003
		H16′⋯O8	-0.012	-0.015
		H17′⋯O10	-0.020	0.049
		H17″⋯O10′	-0.025	-0.019
		H16″⋯O8′	-0.008	0.008
T12-KT6″-M5,3″,3″	1	H15⋯O14	0.007	0.009
		H15′⋯O14′	0.007	0.013
		H15″⋯O14″	0.016	0.030

		H17′⋯O8	-0.020	0.000
		H16⋯O10′	-0.023	-0.030
		H16″⋯O8′	-0.022	0.004
		H16′⋯O12″	-0.017	-0.043
	2	H15⋯O14	0.006	0.004
		H17′⋯O14′	0.009	0.009
		H15″⋯O14″	0.017	0.016
		H16′⋯O8	-0.021	-0.032
		H16⋯O12′	-0.017	-0.016
		H16″⋯O10′	-0.023	-0.031
		H16′⋯O12″	-0.016	-0.014
	3	H17⋯O14	0.009	0.024
		H15′⋯O14′	0.007	0.009
		H15″⋯O14″	0.018	0.013
		H15⋯O10′	-0.026	-0.037
		H17′⋯O10	-0.018	0.015
		H16′⋯O12″	-0.018	-0.028
		H16″⋯O8′	-0.020	-0.017
	4	H17⋯O14	0.009	0.009
		H17′⋯O14′	0.009	0.010
		H15″⋯O14″	0.017	0.017
		H15⋯O12′	-0.017	-0.011
		H17′⋯O10	-0.017	-0.022
		H15′⋯O12″	-0.015	-0.014
		H16″⋯O10′	-0.023	-0.028
	5	H17⋯O14	0.012	0.033
		H15′⋯O14′	0.015	0.012
		H15″⋯O14″	0.019	0.010
		H15⋯O10′	-0.026	-0.030
		H16⋯O12′	-0.001	0.004
		H16′⋯O12″	-0.015	-0.025
		H16″⋯O8′	-0.021	-0.015
	6	H17⋯O14	0.010	0.009
		H15′⋯O14′	0.012	0.011
		H15″⋯O14″	0.017	0.027
		H15⋯O12′	-0.018	-0.009
		H16⋯O10′	-0.022	-0.023
		H16″⋯O8′	-0.024	0.012
		H16′⋯O12″	-0.013	-0.026
	7	H17⋯O14	0.010	0.017
		H17′⋯O14′	0.009	0.012
		H15″⋯O14″	0.019	0.021

		H15⋯O12′	-0.018	-0.013
		H16⋯O10′	-0.018	-0.046
		H15′⋯O12″	-0.008	-0.001
		H16″⋯O10′	-0.013	-0.035
	8	H17⋯O14	0.011	0.048
		H17′⋯O14′	0.011	0.017
		H15″⋯O14″	0.019	0.022
		H15⋯O10′	-0.026	-0.027
		H16⋯O12′	-0.011	0.032
		H16′⋯O10″	-0.015	-0.043
		H15′⋯O12″	-0.008	-0.015
	9	H17⋯O14	0.010	0.010
		H17′⋯O14′	0.008	0.009
		H15″⋯O14″	0.019	0.025
		H15⋯O12′	-0.018	-0.008
		H16⋯O10′	-0.021	-0.005
		H15′⋯O10″	-0.019	0.005
		H16′⋯O12″	-0.008	-0.019
	10	H17⋯O14	0.010	0.012
		H17′⋯O14′	0.011	0.017
		H15″⋯O14″	0.019	0.014
		H15⋯O10′	-0.025	-0.027
		H16⋯O12′	-0.009	0.024
		H16′⋯O12″	-0.012	-0.020
		H15′⋯O10″	-0.019	0.018
T13-ET6,2″	1	H15⋯O14	0.010	0.011
		H15′⋯O14′	0.009	0.009
		H17″⋯O14″	0.008	0.007
		H17′⋯O8	-0.018	-0.015
		H16⋯O10′	-0.020	-0.020
		H16″⋯O8′	-0.017	-0.015
		H16′⋯O12″	-0.019	-0.025
T13-M5,3″-ET6,2″	1	H15⋯O14	0.013	0.014
		H15′⋯O14′	0.009	0.010
		H17″⋯O14″	0.010	0.009
		H17′⋯O8	-0.015	-0.010
		H16⋯O10′	-0.018	-0.021
		H16″⋯O8′	-0.015	-0.011
		H16′⋯O12″	-0.016	-0.024

T14-ET6,2″	1	H15····O14	0.013	0.011
		H15′····O14′	0.010	0.013
		H17″····O14″	0.010	0.028
		H17′····O8	-0.018	-0.015
		H16····O10′	-0.021	-0.018
		H16″····O8′	-0.017	-0.013
		H16′····O12″	-0.019	-0.026
T14-M5,3″-ET6,2″	1	H15····O14	0.022	0.018
		H15′····O14′	0.017	0.013
		H17″····O14″	0.021	0.018
		H17′····O8	0.003	-0.014
		H16····O10′	-0.020	-0.015
		H16″····O8′	0.005	-0.013
		H16′····O12″	-0.026	-0.015
	1-y-out-in	H15····O14		0.015
		H15′····O14′		0.013
		H17″····O14″		0.010
		H17′····O8		-0.011
		H16····O10′		-0.018
		H16″····O8′		-0.013
		H16′····O12″		-0.025

Table S 14

Bond lengths of the C−H····O intramolecular hydrogen bonds in selected trimeric acylphloroglucinols

DFT/B3LYP/6-31+G(d,p) without Grimme's correction and DFT/B3LYP/6-31+G(d,p) with Grimme's correction results in vacuo, respectively denoted as DFT and DFT-D3 in the columns' headings. The conformers-pair numbered as 1 is considered for each of the selected molecules.

IHB considered	Length of given IHB (Å)			
	outstretched conformer		bowl-shaped conformer	
	DFT	DFT-D3	DFT	DFT-D3
structure T1				
H13$_a$····O14	2.416	2.421	2.416	2.421
H13$_b$····O12	2.496	2.483	2.499	2.481
H13$_c$····O12	2.497	2.481	2.496	2.484
H13$_a$′····O14′	2.406	2.412	2.406	2.411
H13$_b$′····O12′	2.467	2.460	2.470	2.457
H13$_c$′····O12′	2.476	2.454	2.474	2.458
H13$_a$″····O14″	2.415	2.421	2.415	2.421
H13$_a$″····O14″	2.496	2.479	2.496	2.480
H13$_a$″····O14″	2.494	2.482	2.495	2.481
structure T4-KT2,6″-M5,5,3″,3″				
H19$_a$····O14	2.701	2.690	2.700	2.704
H19$_b$····O14	2.719	2.703	2.719	2.690
H11$_a$····O12	2.572	2.565	2.537	2.529
H11$_b$····O12	2.534	2.526	2.570	2.565
H11$_c$····O10	2.551	2.540	2.519	2.509
H11$_d$····O10	2.515	2.507	2.556	2.540
H13$_a$····O8	2.458	2.448	2.460	2.449
H13$_b$····O8	2.466	2.451	2.465	2.450
H19$_a$′····O14′	2.654	2.651	2.653	2.648
H19$_b$′····O14′	2.661	2.648	2.662	2.651
H13$_a$′····O12′	2.418	2.409	2.418	2.408
H13$_b$′····O12′	2.420	2.410	2.421	2.411
H13$_a$″····O14″	2.426	2.433	2.427	2.427
H13$_b$″····O12″	2.514	2.511	2.519	2.497
H13$_c$″····O12″	2.537	2.497	2.533	2.500
H9$_a$″····O8″	2.538	2.528	2.541	2.538

H9$_b$″····O8″	2.581	2.574	2.578	2.563
H9$_c$″····O10″	2.519	2.509	2.522	2.521
H9$_d$″····O10″	2.553	2.543	2.552	2.533
structure T7				
H19$_a$····O14	2.662	2.652	2.662	2.548
H19$_b$····O14	2.664	2.654	2.663	2.582
H13$_a$····O12	2.439	2.429	2.439	2.486
H13$_b$····O12	2.438	2.428	2.438	2.370
H19$_a$′····O14′	2.653	2.646	2.649	2.641
H19$_b$′····O14′	2.658	2.648	2.660	2.652
H13$_a$′····O12′	2.410	2.402	2.410	2.404
H13$_b$′····O12′	2.414	2.405	2.414	2.405
H13$_a$″····O14″	2.653	2.421	2.415	2.421
H13$_b$″····O8″	2.658	2.481	2.496	2.482
H13$_c$″····O8″	2.493	2.483	2.494	2.483
structure T9				
H19$_a$····O14	2.661	2.652	2.662	2.652
H19$_b$····O14	2.664	2.655	2.663	2.654
H13$_a$····O12	2.439	2.430	2.439	2.430
H13$_b$····O12	2.438	2.430	2.438	2.430
H19$_a$′····O14′	2.657	2.646	2.660	2.651
H19$_b$′····O14′	2.653	2.648	2.650	2.642
H13$_a$′····O12′	2.411	2.402	2.411	2.402
H13$_b$′····O12′	2.414	2.405	2.415	2.405
H19$_a$″····O14″	2.664	2.654	2.664	2.655
H19$_b$″····O14″	2.661	2.652	2.661	2.652
H13$_a$″····O8″	2.436	2.428	2.437	2.427
H13$_b$″····O8″	2.437	2.429	2.437	2.429
structure T9-M5,3″				
H19$_a$····O14	2.662	2.656	2.661	2.653
H19$_b$····O14	2.657	2.647	2.658	2.646
H13$_a$····O12	2.427	2.420	2.429	2.421
H13$_b$····O12	2.430	2.421	2.428	2.419
H11$_a$····O10	2.298	2.304	2.297	2.303
H19$_a$′····O14′	2.656	2.646	2.650	2.643
H19$_b$′····O14′	2.653	2.646	2.659	2.650
H13$_a$′····O12′	2.411	2.402	2.409	2.402
H13$_b$′····O12′	2.413	2.404	2.415	2.404

H19$_a$″····O14″	2.656	2.647	2.661	2.652
H19$_b$″····O14″	2.661	2.652	2.657	2.647
H13$_a$″····O8″	2.428	2.419	2.428	2.419
H13$_b$″····O8″	2.426	2.417	2.427	2.418
H9$_a$″····O10″	2.294	2.301	2.298	2.303

Table S 15
HOMO-LUMO energy difference of selected calculated conformers of trimeric acylphloroglucinols
The table reports the HF/6-31G(d,p), HF/6-31+G(d,p), DFT/B3LYP/6-31+G(d,p), and DFT/B3LYP/6-31+G(d,p) with the Grimme' correction results, respectively denoted as HF, HF+, DFT and DFT-D3 in the column headings.
For each molecule, the conformers are listed in order of increasing relative energy in the DFT/B3LYP/6-31+G(d,p) results.

conformers	HOMO-LUMO energy difference (kcal/mol)			
	HF	HF+	DFT	DFT-D3
structure T1				
1	252.76	231.47	97.46	97.22
1-y	252.77	230.44	97.55	97.28
2	251.83	228.80	96.71	96.36
2-y	251.89	228.63	96.98	95.88
3	251.46	227.27	95.83	95.73
3-y	251.02	227.45	95.48	95.39
4	247.68	231.46	93.05	92.91
4-y	247.80	230.14	93.17	92.99
5	247.09	228.95	92.61	92.34
6	251.66	225.83	96.80	96.67
5-y	413.30	228.87	93.10	92.37
7	246.13	227.85	91.11	91.08
7-y	245.44	228.54	90.49	90.42
8	251.94	229.35	0.00	0.00
8-y	251.13	228.78	98.17	97.99
6-y	250.96	226.65	96.14	96.00
9	248.33	232.71	93.43	93.30
10-y	250.90	228.24	97.14	96.82
10	251.05	227.57	97.63	97.51
9-y	247.81	232.28	93.06	93.03
17-y	226.19	201.12	67.01	67.76
17	221.75	197.92	63.37	63.10
structure T2-KT2,6″-M5,5,3″,3″				
1	246.65	231.24	89.87	89.72
1-y	246.45	230.76	89.62	89.20
structure T3-ET6,2″				
1	251.89	231.95	96.91	96.74
1-y	251.93	231.17	96.89	96.60

structure T3-M5,3″-ET6,2″				
1	250.93	233.07	96.12	96.01
1-y	251.02	232.98	96.20	95.96
structure T4-KT2,6″-M5,5,3″,3″				
1	246.57	231.13	89.77	89.60
1-y	246.38	230.63	89.51	89.09
structure T5-KT2,6″-M5,5,3″,3″				
1	246.91	230.89	90.32	90.11
1-y	246.72	230.31	90.10	89.41
structure T5-KT6″-M3″,3″-ET4				
1	244.40	225.48	88.52	88.43
1-y	244.66	225.96	88.65	88.57
structure T6-M5,3″-ET6,4″				
3	244.13	223.91	91.65	91.70
3-y	244.52	223.76	92.04	92.16
3-y-in-out	244.91	224.04	92.55	92.68
3-y-in-in	241.10	222.97	88.59	88.14
structure T7				
1	252.97	230.89	97.06	96.84
1-y	252.67	229.94	97.26	96.99
2	251.69	228.78	96.24	95.91
2-y	252.49	228.47	96.54	94.79
4	248.41	230.73	94.06	93.87
3	252.06	227.01	95.37	95.26
3-y	251.62	227.10	95.04	94.93
4-y	248.50	229.03	94.18	93.94
5	248.12	228.82	94.06	93.74
5-y	248.42	228.61	94.56	94.02
6	252.19	226.02	97.84	97.61
6-y	251.42	226.96	97.14	96.82
structure T7-ET6,2″				
1	252.39	231.93	96.86	96.64
1-y	252.12	231.09	96.98	96.67
structure T7-M5,3″-ET6,2″				
1	251.13	233.17	96.70	96.57
1-y	250.82	232.78	96.42	96.35
structure T7-KT6″-M5,3″,3″				

1	245.81	229.71	89.95	89.66
1-y	245.86	228.48	89.93	89.47
2	247.62	229.77	91.27	91.25
2-y	247.33	229.02	90.81	90.84
3	242.63	225.38	86.68	86.28
3-y	243.60	226.10	87.93	87.56
4	243.17	222.64	87.00	86.89
4-y	243.24	222.91	86.93	87.04

structure T7-KT2,6″-M5,5,3″,3″

1	246.53	230.68	89.71	89.56
1-y	246.35	230.28	89.49	89.05

structure T8-KT6″-M5,3″,3″

1	246.17	229.66	90.56	90.20
1-y	246.20	228.26	90.53	89.94
2	247.97	229.71	91.87	91.80
2-y	247.67	228.91	91.45	91.40
3	243.04	225.41	87.34	86.90
3-y	244.06	226.14	88.67	87.95
4	243.57	222.71	87.68	87.52
4-y	243.62	222.94	87.59	87.66

structure T8-KT2-M5,5,3″

1	246.28	229.74	90.69	90.32
1-y	246.31	228.43	90.66	90.12
2	248.07	229.59	91.97	91.88
2-y	247.78	228.63	91.54	91.49
3-y	243.54	225.93	88.65	88.13
4	243.71	222.87	87.88	87.69
3	242.80	225.06	87.15	86.77
4-y	243.78	222.95	87.77	87.82

structure T8-KT2,6″-M5,5,3″,3″

1	246.87	230.75	90.30	90.09
1-y	246.69	230.23	90.07	89.37

structure T9

1	253.04	231.09	98.05	97.75
1-y	253.06	229.93	98.14	97.80
2	252.21	228.58	97.34	96.94
4	248.27	230.97	93.91	93.72
2-y	252.42	228.55	97.75	95.21
3	251.84	226.89	96.48	96.30
3-y	251.39	226.91	96.12	95.96

4-y	248.39	229.04	94.02	93.79
5	247.88	228.56	93.61	93.30
5-y	247.94	228.61	94.29	94.24
6	252.06	225.90	97.52	97.31
6-y	251.31	226.82	96.87	96.69
structure T9-M5,3″				
1	252.61	229.11	97.99	97.64
1-y	252.43	227.92	97.83	97.33
2	249.79	226.17	95.24	94.88
2-y	250.21	226.29	95.76	95.41
3	249.67	223.85	94.85	94.70
3-y	249.40	223.00	94.65	94.60
4	247.40	229.26	93.56	93.34
4-y	247.19	226.39	93.40	93.06
6	249.44	223.36	94.99	94.87
6-y	248.76	224.22	94.38	94.68
5	245.28	226.07	91.52	91.26
5-y	245.96	226.50	92.53	92.55
structure T9-ET6,2″				
1	252.45	232.17	97.82	97.53
1-y	252.40	231.51	97.85	97.50
structure T9-M5,3″-ET6,2″				
1	251.36	233.04	96.74	96.51
1-y	251.44	232.62	97.02	96.64
structure T9-M5,3″-ET6,4″				
3	244.16	223.63	91.64	91.67
3-y	244.58	223.59	92.07	92.14
3-y-in-out	244.98	223.86	0.00	92.66
3-y-in-in	241.16	222.90	88.61	88.13
structure T9-KT6″-M5,3″,3″				
1	246.24	229.69	90.62	90.26
1-y	246.27	228.46	90.61	90.09
2	248.04	229.70	91.94	91.85
2-y	247.74	228.83	91.51	91.44
3	243.13	225.54	87.46	88.25
4	243.66	222.80	91.51	87.62
4-y	243.71	222.90	87.70	87.74
3-y	244.28	226.14	88.77	86.95
structure T9-KT6″-M3″,3″-ET4				

1	244.43	225.36	88.57	88.45
1-y	244.68	225.80	88.71	88.60
structure T9-KT6″-M5,3″,3″-ET6				
1	248.61	231.34	92.31	92.26
1-y	248.44	231.22	91.63	91.54
structure T9-KT2,6″-M5,5,3″,3″				
1	246.94	230.92	90.35	90.14
1-y	246.75	230.60	90.14	89.43
structure T10				
1	251.38	230.10	96.33	96.27
1-y	251.25	228.46	96.39	96.23
2-y	250.63	228.01	96.03	94.94
4	246.60	230.05	92.80	92.69
2	250.70	228.85	95.71	95.49
3-y	249.90	226.98	94.30	94.30
3	250.19	227.12	94.62	94.57
4-y	246.64	227.77	92.92	92.76
5-y	246.12	228.18	93.10	92.16
5	246.04	229.02	92.55	92.30
6-y	250.29	226.38	95.11	95.11
6	250.75	226.73	95.78	95.68
structure T10-ET6,2″				
1	250.90	231.31	96.07	95.98
1-y	250.60	230.04	96.13	95.98
structure T10-M5,3″-ET6,2″				
1	250.99	232.21	94.83	95.00
1-y	251.09	232.33	95.07	94.93
structure T10-M5,3″-ET6,2″,6″				
1	250.68	231.17	95.78	95.70
1-y	251.64	231.21	96.57	96.34
structure T10-KT2,6″-M5,5,3″,3″				
1-y	247.00	230.65	90.36	89.37
1	247.11	230.62	90.64	90.47
structure T11-ET6,2″				
1	251.02	231.51	96.21	96.13
1-y	250.90	230.26	96.25	96.40
structure T11-M5,3″-ET6,2″				

1	250.97	232.76	94.87	95.02
1-y	250.80	232.79	95.94	95.64
1-y-out-in	250.73	232.09	95.27	95.14

structure T12-KT2-M5,5,3″

1	246.30	229.56	90.70	90.34
1-y	246.32	228.29	90.69	90.25
2	248.08	229.62	92.01	91.91
2-y	407.92	228.76	91.56	91.51
3	243.20	225.40	87.52	87.02
4	243.72	222.78	87.87	87.69
4-y	243.77	222.91	87.76	87.79
3-y	244.28	226.08	88.87	88.35

structure T12-KT6″-M5,3″,3″

1	246.22	229.68	90.60	90.24
1-y	246.25	228.61	90.59	90.05
2	248.01	229.46	91.94	91.84
2-y	247.71	228.62	91.48	91.42
3	243.08	225.31	87.41	86.90
3-y	244.06	226.21	88.77	87.95
4	243.63	222.65	87.68	87.58
4-y	243.69	222.69	87.76	87.72

structure T13-ET6,2″

1	251.86	231.93	97.14	97.15
1-y	251.41	231.26	96.67	96.69

structure T13-M5,3″-ET6,2″

1	251.54	233.28	96.57	96.41
1-y	251.50	232.96	96.35	96.35

structure T14-ET6,2″

1	-0.30251	0.09737	-0.30838	0.06011
1-y	-0.30197	0.09757	-0.30801	0.05913

structure T14-M5,3″-ET6,2″

1	251.16	232.80	94.72	94.85
1-y	251.34	232.86	95.78	95.09
1-y-out-in	251.21	232.32	95.16	94.99

Table S 16
Dipole moment of the calculated conformers of trimeric acylphloroglucinols
The table reports the HF/6-31G(d,p), HF/6-31+G(d,p), DFT/B3LYP/6-31+G(d,p), and DFT/B3LYP/6-31+G(d,p) with the Grimme' correction results, respectively denoted as HF, HF+, DFT and DFT-D3 in the column headings.
For each molecule, the conformers are listed in order of increasing relative energy in the DFT/B3LYP/6-31+G(d,p) results.

conformers	dipole moment (debye)			
	HF	HF+	DFT	DFT-D3
structure T1				
1	2.5513	2.6417	2.8462	2.7634
1-y	5.1004	5.1456	5.2126	5.3679
2	5.5914	5.7435	5.8600	5.9867
2-y	1.9269	1.9857	2.3392	1.8843
3	7.4533	7.6551	7.9817	7.9639
3-y	5.4965	5.6080	6.0743	5.8185
4	5.0273	5.1430	5.3400	5.2266
4-y	6.0469	6.1649	6.5604	6.5229
5	4.4844	4.7046	4.9252	5.0350
6	3.0801	3.0490	3.2908	3.2355
5-y	1.8412	2.0225	1.4459	1.8463
7	7.1630	7.3587	7.7992	7.7267
7-y	6.1018	6.2216	6.4344	6.2145
8	6.1765	6.2716		
8-y	2.5565	2.6265	2.6377	2.4603
6-y	6.4138	6.6943	6.6479	6.8416
9	3.0803	3.3621	3.8353	3.7577
10-y	6.7104	6.9026	7.2999	6.8746
10	8.6421	8.8568	9.0546	8.9750
9-y	4.6136	4.7448	5.1556	5.1778
17-y	15.8604	16.0138	17.9541	17.0390
17	20.9513	21.0477	22.0386	22.0221
structure T2-KT2,6″-M5,5,3″,3″				
1	1.8875	1.8654	1.6726	1.7032
1-y	1.7859	1.7704	1.5460	1.5462
structure T3-ET6,2″				
1	2.8804	2.9385	3.1457	3.0491
1-y	6.4596	6.6329	6.5106	6.8887

structure T3-M5,3″-ET6,2″				
1	3.6304	3.5826	3.7202	3.6872
1-y	4.5412	4.7332	4.5044	4.6872
structure T4-KT2,6″-M5,5,3″,3″				
1	1.7759	1.6925	1.4550	1.4827
1-y	1.6895	1.6041	1.3561	1.3581
structure T5-KT2,6″-M5,5,3″,3″				
1	1.9010	1.8643	1.7137	1.7357
1-y	1.8253	1.7796	1.6134	1.5285
structure T5-KT6″-M3″,3″-ET4				
1	6.0287	6.0681	6.1751	6.1557
1-y	5.8237	5.9249	5.9234	5.8088
structure T6-M5,3″-ET6,4″				
3	7.2728	7.5604	7.8690	7.8233
3-y	5.6033	5.7610	6.3346	6.0706
3-y-in-out	3.5091	3.7851	4.1896	3.8734
3-y-in-in	6.5077	6.8289	6.7901	6.3041
structure T7				
1	2.5914	2.6787	2.2270	2.1459
1-y	4.8559	4.8224	4.8755	5.0466
2	5.4660	5.7489	5.7088	5.8258
2-y	1.9610	2.0419	2.5118	2.3210
4	5.2307	5.3404	5.5986	5.4872
3	7.2445	7.4288	7.4139	7.4176
3-y	5.2664	5.3508	5.5286	5.2889
4-y	6.2898	6.4115	6.7889	6.7639
5	4.7039	4.9387	5.1202	5.2553
5-y	1.8253	2.0280	1.5547	2.1315
6	3.0364	3.0113	3.2991	3.2302
6-y	6.1932	6.4183	6.4648	6.7747
structure T7-ET6,2″				
1	3.0163	3.1683	2.7889	2.6781
1-y	6.2722	6.4578	6.2419	6.4709
structure T7-M5,3″-ET6,2″				
1	3.5896	3.6876	3.8735	3.8035
1-y	4.5115	4.7305	4.7835	4.9747
structure T7-KT6″-M5,3″,3″				

1	2.6831	2.7757	2.9590	2.9379
1-y	2.8726	2.8281	3.1293	3.1656
2	3.5574	3.7190	3.5704	3.6328
2-y	3.4897	3.5331	3.4595	3.5346
3	3.7757	3.8144	3.8546	3.9335
3-y	3.4156	3.5846	3.4933	3.3801
4	5.3194	5.3143	5.3507	5.3654
4-y	5.2220	5.2973	5.2242	5.1405

structure T7-KT2,6″-M5,5,3″,3″

1	1.7414	1.6451	1.4039	1.4262
1-y	1.6634	1.5617	1.3155	1.3280

structure T8-KT6″-M5,3″,3″

1	2.7044	2.8133	3.0749	3.0332
1-y	3.0096	3.0129	3.3633	3.3875
2	3.4157	3.5173	3.3193	3.3782
2-y	3.4685	3.4747	3.3656	3.4735
3	3.7568	3.7702	3.7778	3.8716
3-y	3.2747	3.3987	3.2435	3.1859
4	5.3821	5.3876	5.4637	5.4755
4-y	5.2009	5.2623	5.2420	5.1257

structure T8-KT2-M5,5,3″

1	2.7847	2.9168	3.1927	3.1415
1-y	3.1405	3.1904	3.5235	3.4555
2	3.3434	3.4206	3.2221	3.2763
2-y	3.4685	3.4726	3.3389	3.4782
3-y	3.5058	3.6803	3.2663	3.1524
4	5.4673	5.5127	5.5914	5.5948
3	3.8679	3.9491	3.9361	4.0859
4-y	5.2318	5.3163	5.3224	5.1805

structure T8-KT2,6″-M5,5,3″,3″

1	1.8656	1.8167	1.6591	1.6802
1-y	1.8013	1.7418	1.5815	1.5075

structure T9

1	2.3829	2.4149	2.5909	2.5052
1-y	4.9068	4.9242	5.0409	5.2028
2	5.3527	5.4385	5.6085	5.7285
4	5.0643	5.1433	5.3905	5.2732
2-y	1.7570	1.7752	2.1573	2.3315
3	7.0525	7.1395	7.4798	7.4711
3-y	5.1633	5.1548	5.6072	5.3375

4-y	6.1221	6.2288	6.6267	6.6074
5	4.5356	4.7237	4.9233	5.0410
5-y	1.3227	1.9139	1.5635	1.9341
6	2.8975	2.7969	3.0602	3.0092
6-y	5.9697	6.1171	6.1324	6.4555

structure T9-M5,3″

1	2.4698	2.5209	2.7576	2.6748
1-y	5.1269	5.2388	5.2994	5.5131
2	5.3192	5.4375	5.5646	5.7100
2-y	1.8629	1.9082	2.3859	1.8860
3	7.1788	7.3607	7.6546	7.6692
3-y	5.3612	5.4347	5.9250	5.6225
4	5.0937	5.2021	5.5072	5.4002
4-y	6.3196	6.5125	6.9136	6.9218
6	3.1136	3.1058	3.3618	3.3254
6-y	5.7239	5.8558	5.8395	6.1828
5	4.4438	4.6373	4.8031	4.9631
5-y	1.3249	1.4202	0.9641	1.3684

structure T9-ET6,2″

1	2.8079	2.8927	3.1296	3.0132
1-y	6.1128	6.2687	6.3705	6.5726

structure T9-M5,3″-ET6,2″

1	3.3566	3.4011	3.5800	3.5146
1-y	4.3106	4.4931	4.5778	4.7852

structure T9-M5,3″-ET6,4″

3	7.1058	7.3463	7.6207	7.5844
3-y	5.4059	5.4964	6.0489	5.7844
3-y-in-out	3.3061	3.5146		3.5556
3-y-in-in	6.3589	6.6403	6.5753	6.1040

structure T9-KT6″-M5,3″,3″

1	2.7076	2.8119	3.1080	3.0593
1-y	3.0701	3.1012	3.4468	3.3823
2	3.3523	3.4330	3.2308	3.2878
2-y	3.4769	3.4852	3.3569	3.4889
3	3.7614	3.7833	3.7621	3.8599
4	5.4288	5.4554	5.5297	5.5410
4-y	5.1992	5.2657	5.2651	5.1252
3-y	3.2424	3.3196	3.2041	3.1475

structure T9-KT6″-M3″,3″-ET4

1	6.0422	6.0787	6.1806	6.1618
1-y	5.7840	5.8648	5.8699	5.7398

structure T9-KT6″-M5,3″,3″-ET6

1	4.0658	4.1080	3.7776	3.8173
1-y	4.1021	4.1110	3.6909	3.7205
40	7.7307	7.8532	7.3360	7.3157
40-y	8.1416	8.3018	7.8680	7.9244

structure T9-KT2,6″-M5,5,3″,3″

1	1.9329	1.9093	1.7675	1.7813
1-y	1.8697	1.8385	1.6849	1.5052

structure T10

1	2.5022	2.5617	2.7249	2.6407
1-y	4.8677	4.8102	5.1284	5.2795
2-y	2.3219	2.3323	2.2276	2.1811
4	5.1753	5.2219	5.3229	5.2299
2	5.8747	6.0752	5.7702	5.8172
3-y	5.6260	5.6498	5.9185	5.6470
3	7.5176	7.6691	7.7496	7.7314
4-y	6.4000	6.5064	6.5783	6.6759
5-y	0.8494	1.1628	1.3628	0.9937
5	5.2458	5.4814	4.9730	4.9752
6-y	5.2978	5.3715	6.3318	7.1612
6	2.3196	2.2063	3.1378	3.2693

structure T10-ET6,2″

1	2.7721	2.8127	3.3035	3.1880
1-y	5.9992	6.0389	6.4585	6.6501

structure T10-M5,3″-ET6,2″

1	2.2411	2.2872	2.9374	2.7917
1-y	4.5768	4.8348	5.5627	5.6345

structure T10-M5,3″-ET6,2″,6″

1	3.1573	3.1593	2.7850	2.5970
1-y	5.1896	5.3569	1.3655	1.1635

structure T10-KT2,6″-M5,5,3″,3″

1-y	1.9571	1.8520	1.6694	1.5179
1	1.8588	2.0155	1.7676	1.7818

structure T11-ET6,2″

1	2.9376	3.0799	3.3594	3.2322
1-y	5.9793	6.0395	6.5217	6.6060

structure T11-M5,3″-ET6,2″				
1	3.5136	3.5739	3.7767	3.6428
1-y	4.3242	4.4706	4.7303	5.1908
1-y-out-in	4.8213	4.8486	5.3764	5.5930
structure T12-KT2-M5,5,3″				
1	2.7316	2.8509	3.1443	3.0973
1-y	3.0387	3.0615	3.4242	3.2768
2	3.3607	3.4464	3.2494	3.3082
2-y	3.4399	3.4334	3.3045	3.4369
3	3.7264	3.7355	3.7149	3.8148
4	5.3864	5.3942	5.4726	5.4809
4-y	5.1842	5.2446	5.2450	5.1135
3-y	3.2537	3.3319	3.1629	3.0077
structure T12-KT6″-M5,3″,3″				
1	2.7483	2.8751	3.1669	3.1185
1-y	3.1107	3.1635	3.5078	3.4440
2	3.3892	3.4822	3.2991	3.3555
2-y	3.5145	3.5348	3.4076	3.5479
3	3.7909	3.8200	3.8102	3.9100
3-y	3.2271	3.3550	3.1787	3.1521
4	5.4341	5.4604	5.5453	5.5561
4-y	5.2011	5.2657	5.2736	5.1394
structure T13-ET6,2″				
1	2.7021	2.7050	3.1695	3.0706
1-y	6.1272	6.2555	6.3914	6.6110
structure T13-M5,3″-ET6,2″				
1	2.9010	2.9096	3.5500	3.5107
1-y	3.9920	4.1642	4.6798	4.9061
structure T14-ET6,2″				
1	2.6585	3.0673	3.1161	2.9667
1-y	5.9438	5.9725	6.4840	6.8332
structure T14-M5,3″-ET6,2″				
1	2.8734	2.8679	3.5609	3.4544
1-y	3.8958	4.0201	4.7634	4.9207
1-y-out-in	4.4714	4.4830	5.5016	5.7417

Table S 17
Dipole moment estimation difference between corresponding conformers with outstretched and half-bowl-shaped geometries, in the calculated trimeric acylphloroglucinols

The table reports the differences in the HF/6-31G(d,p), HF/6-31+G(d,p), DFT/B3LYP/6-31+G(d,p), and DFT/B3LYP/6-31+G(d,p) with the Grimme' corrections results, respectively denoted as HF, HF+, DFT and DFT-D3 in the column headings. The differences are taken as «dipole moment of the conformer with bowl-shaped geometry minus dipole moment of the conformer with outstretched geometry». To facilitate comparisons of different bowl-shaped geometry-types, the values for conformers with up—down—up orientations of the monomers are highlighted in yellow and the values for conformers with up—up—up orientations of the monomers are highlighted in blue (the values for up—down—down conformers are not highlighted).

molecule	conformer	energy difference between half-bowl-shaped and outstretched-shaped conformers (kcal/mol)			
		HF	HF+	DFT	DFT-D3
T1	1	2.549	2.504	2.366	2.605
	2	-3.665	-3.758	-3.521	-4.102
	3	-1.957	-2.047	-1.907	-2.145
	4	1.020	1.022	1.220	1.296
	5	-2.643	-2.682	-3.479	-3.189
	6	3.334	3.645	3.357	3.606
	7	-1.061	-1.137	-1.365	-1.512
	8	-3.620	-3.645		
	9	1.533	1.383	1.320	1.420
	10	-1.932	-1.954	-1.755	-2.100
	17	-5.091	-5.034	-4.085	-4.983
T2-KT2,6″-M5,5,3″,3″	1	-0.102	-0.095	-0.127	-0.157
T3-ET6,2″	1	3.579	3.694	3.365	3.840
T3-M5,3″-ET6,2″	1	0.911	1.151	0.784	1.000
T4-KT2,6″-M5,5,3″,3″	1	-0.086	-0.088	-0.099	-0.125
T5-KT6″-M3″,3″-ET4	1	-0.205	-0.143	-0.252	-0.347
T5-KT2,6″-M5,5,3″,3″	1	-0.076	-0.085	-0.100	-0.207
T6-M5,3″-ET6,4″	1	-1.670	-1.799	-1.534	-1.753

T7	1	2.265	2.144	2.649	2.901
	2	-3.505	-3.707	-3.197	-3.505
	3	-1.978	-2.078	-1.885	-2.129
	4	1.059	1.071	1.190	1.277
	5	-2.879	-2.911	-3.566	-3.124
	6	3.157	3.407	3.166	3.545
T7-ET6,2″	1	3.256	3.290	3.453	3.793
T7-M5,3″-ET6,2″	1	0.922	1.043	0.910	1.171
T7-KT6″-M5,3″,3″	1	0.190	0.052	0.170	0.228
	2	-0.068	-0.186	-0.111	-0.098
	3	-0.360	-0.230	-0.361	-0.553
	4	-0.097	-0.017	-0.127	-0.225
T7-KT2,6″-M5,5,3″,3″	1	-0.078	-0.083	-0.088	-0.098
T8-KT6″-M5,3″,3″	1	0.305	0.200	0.288	0.354
	2	0.053	-0.043	0.046	0.095
	3	-0.482	-0.372	-0.534	-0.686
	4	-0.181	-0.125	-0.222	-0.350
T8-KT2-M5,5,3″	1	0.356	0.274	0.331	0.314
	2	0.125	0.052	0.117	0.202
	3	-0.362	-0.269	-0.670	-0.934
	4	-0.236	-0.196	-0.269	-0.414
T8-KT2,6″-M5,5,3″,3″	1	-0.064	-0.075	-0.078	-0.173
T9	1	2.524	2.509	2.450	2.698
	2	-3.596	-3.663	-3.451	-3.397
	3	-1.889	-1.985	-1.873	-2.134
	4	1.058	1.086	1.236	1.334
	5	-3.213	-2.810	-3.360	-3.107
	6	3.072	3.320	3.072	3.446
T9-M5,3″	1	2.657	2.718	2.542	2.838
	2	-3.456	-3.529	-3.179	-3.824
	3	-1.818	-1.926	-1.730	-2.047
	4	1.226	1.310	1.406	1.522
	5	-3.119	-3.217	-3.839	-3.595
	6	2.610	2.750	2.478	2.857

T9-ET6,2″	1	3.305	3.376	3.241	3.559
T9-M5,3″-ET6,2″	1	0.954	1.092	0.998	1.271
T9-M5,3″-ET6,4″	1	-1.700	-1.850	-1.572	-1.800
T9-KT6″-M5,3″,3″	1	0.363	0.289	0.339	0.323
	2	0.125	0.052	0.126	0.201
	3	-0.519	-0.464	-0.558	-0.712
	4	-0.230	-0.190	-0.265	-0.416
T9-KT6″-M3″,3″-ET4	1	-0.258	-0.214	-0.311	-0.422
T9-KT6″-M5,3″,3″-ET6	1	0.036	0.003	-0.087	-0.097
T9-KT2,6″-M5,5,3″,3″	1	-0.063	-0.071	-0.083	-0.276
T10	1	2.366	2.249	2.404	2.639
	2	-3.553	-3.743	-3.543	-3.636
	3	-1.892	-2.019	-1.831	-2.084
	4	1.225	1.285	1.255	1.446
	5	-4.396	-4.319	-3.610	-3.982
	6	2.978	3.165	3.194	3.892
T10-ET6,2″	1	3.227	3.226	3.155	3.462
T10-M5,3″-ET6,2″	1	2.336	2.548	2.625	2.843
T10-M5,3″-ET6,2″,6″	1	2.032	2.198	-1.420	-1.434
T10-KT2,6″-M5,5,3″,3″	1	-0.098	0.164	0.098	0.264
T11-ET6,2″	1	3.042	2.960	3.162	3.374
T11-M5,3″-ET6,2″	1	0.811	0.897	0.954	1.548
T12-KT2-M5,5,3″	1	0.307	0.211	0.280	0.180
	2	0.079	-0.013	0.055	0.129
	3	-0.473	-0.404	-0.552	-0.807
	4	-0.202	-0.150	-0.228	-0.367
T12-KT6″-M5,3″,3″	1	0.362	0.288	0.341	0.326
	2	0.125	0.053	0.109	0.192
	3	-0.564	-0.465	-0.632	-0.758

	4	-0.233	-0.195	-0.272	-0.417
T13-ET6,2″	1	3.425	3.551	3.222	3.540
T13-M5,3″-ET6,2″	1	1.091	1.255	1.130	1.395
T14-ET6,2″	1	3.285	2.905	3.368	3.867
T14-M5,3″-ET6,2″	1	1.022	1.152	1.203	1.466

Table S 18
Effect of the inclusion of the Grimme's correction on the estimation of the dipole moment of the conformers of the calculated trimeric acylphloroglucinols
The table reports the difference in the estimations of the conformers' dipole moments, taken as «dipole moment in the DFT/B3LYP/6-31+G(d,p) result comprising Grimme's correction minus dipole moment in the DFT/B3LYP/6-31+G(d,p) result without Grimme's correction».
Two different tables are presented, respectively grouping the molecules according to their acyl groups or according to their other substituents.

a)   The molecules are grouped according to their acyl groups

molecule	conformer	dipole moment difference (debye)	conformer	dipole moment difference (debye)
T1	1	-0.083	1-y	0.155
	2	0.127	2-y	-0.455
	3	-0.018	3-y	-0.256
	4	-0.113	4-y	-0.037
	5	0.110	5-y	0.400
	6	-0.055	6-y	0.194
	7	-0.072	7-y	-0.220
	8		8-y	-0.177
	9	-0.078	9-y	0.022
	10	-0.080	10-y	-0.425
	17	-0.017	17-y	-0.915
T2-KT2,6″-M5,5,3″,3″	1	0.031	1-y	0.000
T3-ET6,2″	1	-0.097	1-y	0.378
T3-M5,3″-ET6,2″	1	-0.033	1-y	0.183
T4-KT2,6″-M5,5,3″,3″	1	0.028	1-y	0.002
T5-KT2,6″- M5,5,3″,3″	1	0.022	1-y	-0.085
T5-KT6″-M3″,3″-ET4	1	-0.019	1-y	-0.115
T6-M5,3″-ET6,4″	3	-0.046	3-y	-0.264
			3-y-in-out	-0.316
			3-y-in-in	-0.486
T7	1	-0.081	1-y	0.171

	2	0.117	2-y	-0.191
	3	0.004	3-y	-0.240
	4	-0.111	4-y	-0.025
	5	0.135	5-y	0.577
	6	-0.069	6-y	0.310
T7-ET6,2″	1	-0.111	1-y	0.229
T7-M5,3″-ET6,2″	1	-0.070	1-y	0.191
T7-KT6″-M5,3″,3″	1	-0.021	1-y	0.036
	2	0.062	2-y	0.075
	3	0.079	3-y	-0.113
	4	0.015	4-y	-0.084
T7-KT2,6″-M5,5,3″,3″	1	0.022	1-y	0.013
T8-KT6″-M5,3″,3″	1	-0.042	1-y	0.024
	2	0.059	2-y	0.108
	3	0.094	3-y	-0.058
	4	0.012	4-y	-0.116
T8-KT2-M5,5,3″	1	-0.051	1-y	-0.068
	2	0.054	2-y	0.139
	3	0.150	3-y	-0.114
	4	0.003	4-y	-0.142
T8-KT2,6″-M5,5,3″,3″	1	0.021	1-y	-0.074
T9	1	-0.086	1-y	0.162
	2	0.120	2-y	0.174
	3	-0.009	3-y	-0.270
	4	-0.117	4-y	-0.019
	5	0.118	5-y	0.371
	6	-0.051	6-y	0.323
T9-M5,3″	1	-0.083	1-y	0.214
	2	0.145	2-y	-0.500
	3	0.015	3-y	-0.303
	4	-0.107	4-y	0.008
	5	0.160	5-y	0.404
	6	-0.036	6-y	0.343
T9-ET6,2″	1	-0.116	1-y	0.202

T9-M5,3″-ET6,2″	1	-0.065	1-y	0.207
T9-M5,3″-ET6,4″	1	-0.036	3-y	-0.265
			3-y-in-in	-0.471
T9-KT6″-M5,3″,3″	1	-0.049	1-y	-0.065
	2	0.057	2-y	0.132
	3	0.098	3-y	-0.057
	4	0.011	4-y	-0.140
T9-KT6″-M3″,3″-ET4	1	-0.019	1-y	-0.130
T9-KT6″-M5,3″,3″-ET6	1	0.040	1-y	0.030
	40	-0.020	40-y	0.056
T9-KT2,6″-M5,5,3″,3″	1	0.014	1-y	-0.180
T10	1	-0.084	1-y	0.151
	2	0.047	2-y	-0.047
	3	-0.018	3-y	-0.272
	4	-0.093	4-y	0.098
	5	0.002	5-y	-0.369
	6	0.132	6-y	0.829
T10-ET6,2″	1	-0.116	1-y	0.192
T10-M5,3″-ET6,2″	1	-0.146	1-y	0.072
T10-M5,3″-ET6,2″,6″	1	-0.188	1-y	-0.202
T10-KT2,6″-M5,5,3″,3″	1	0.014	1-y	-0.152
T11-ET6,2″	1	-0.127	1-y	0.084
T11-M5,3″-ET6,2″	1	-0.134	1-y	0.461
			1-y-out-in	0.217
T12-KT2-M5,5,3″	1	-0.047	1-y	-0.147
	2	0.059	2-y	0.132
	3	0.100	3-y	-0.155
	4	0.008	4-y	-0.132
T12-KT6″-M5,3″,3″	1	-0.048	1-y	-0.064
	2	0.056	2-y	0.140

	3	0.100	3-y	-0.027
	4	0.011	4-y	-0.134
T13-ET6,2″	1	-0.099	1-y	0.220
T13-M5,3″-ET6,2″	1	-0.039	1-y	0.226
T14-ET6,2″	1	-0.149	1-y	0.349
T14-M5,3″-ET6,2″	1	-0.107	1-y	0.157
			1-y-out-in	0.240

b) **The molecules are grouped according to their other substituents**

molecule	conformer	dipole moment difference (debye)	conformer	dipole moment difference (debye)
T1	1	-0.083	1-y	0.155
	2	0.127	2-y	-0.455
	3	-0.018	3-y	-0.256
	4	-0.113	4-y	-0.037
	5	0.110	5-y	0.400
	6	-0.055	6-y	0.194
	7	-0.072	7-y	-0.220
	8	0.000	8-y	-0.177
	9	-0.078	9-y	0.022
	10	-0.080	10-y	-0.425
	17	-0.017	17-y	-0.915
T7	1	-0.081	1-y	0.171
	2	0.117	2-y	-0.191
	3	0.004	3-y	-0.240

	4	-0.111	4-y	-0.025
	5	0.135	5-y	0.577
	6	-0.069	6-y	0.310
T9	1	-0.086	1-y	0.162
	2	0.120	2-y	0.174
	3	-0.009	3-y	-0.270
	4	-0.117	4-y	-0.019
	5	0.118	5-y	0.371
	6	-0.051	6-y	0.323
T10	1	-0.084	1-y	0.151
	2	0.047	2-y	-0.047
	3	-0.018	3-y	-0.272
	4	-0.093	4-y	0.098
	5	0.002	5-y	-0.369
	6	0.132	6-y	0.829
/////////////////	/////////////////	/////////////////	/////////////////	/////////////////
T9-M5,3″	1	-0.083	1-y	0.214
	2	0.145	2-y	-0.500
	3	0.015	3-y	-0.303
	4	-0.107	4-y	0.008
	5	0.160	5-y	0.404
	6	-0.036	6-y	0.343
/////////////////	/////////////////	/////////////////	/////////////////	/////////////////
T3-ET6,2″	1	-0.097	1-y	0.378
T7-ET6,2″	1	-0.111	1-y	0.229
T9-ET6,2″	1	-0.116	1-y	0.202
T10-ET6,2″	1	-0.116	1-y	0.192
T11-ET6,2″	1	-0.127	1-y	0.084
T13-ET6,2″	1	-0.099	1-y	0.220
T14-ET6,2″	1	-0.149	1-y	0.349
/////////////////	/////////////////	/////////////////	/////////////////	/////////////////

T3-M5,3″-ET6,2″	1	-0.033	1-y	0.183
T7-M5,3″-ET6,2″	1	-0.070	1-y	0.191
T9-M5,3″-ET6,2″	1	-0.065	1-y	0.207
T10-M5,3″-ET6,2″	1	-0.146	1-y	0.072
T11-M5,3″-ET6,2″	1	-0.134	1-y	0.461
			1-y-out-in	0.217
T13-M5,3″-ET6,2″	1	-0.039	1-y	0.226
T14-M5,3″-ET6,2″	1	-0.107	1-y	0.157
			1-y-out-in	0.240
T10-M5,3″-ET6,2″,6″	1	-0.188	1-y	-0.202
///////////////////	///////////////	////////////////	////////////////	////////////////
T7-KT6″-M5,3″,3″	1	-0.021	1-y	0.036
	2	0.062	2-y	0.075
	3	0.079	3-y	-0.113
	4	0.015	4-y	-0.084
T8-KT6″-M5,3″,3″	1	-0.042	1-y	0.024
	2	0.059	2-y	0.108
	3	0.094	3-y	-0.058
	4	0.012	4-y	-0.116
T9-KT6″-M5,3″,3″	1	-0.049	1-y	-0.065
	2	0.057	2-y	0.132
	3	0.098	3-y	-0.057
	4	0.011	4-y	-0.140
T12-KT6″-M5,3″,3″	1	-0.048	1-y	-0.064
	2	0.056	2-y	0.140
	3	0.100	3-y	-0.027
	4	0.011	4-y	-0.134
T8-KT2-M5,5,3″	1	-0.051	1-y	-0.068
	2	0.054	2-y	0.139
	3	0.150	3-y	-0.114
	4	0.003	4-y	-0.142

T12-KT2-M5,5,3″	1	-0.047	1-y	-0.147
	2	0.059	2-y	0.132
	3	0.100	3-y	-0.155
	4	0.008	4-y	-0.132
///////////////////	///////////////	///////////////	///////////////	///////////////
T2-KT2,6″-M5,5,3″,3″	1	0.031	1-y	0.000
T4-KT2,6″-M5,5,3″,3″	1	0.028	1-y	0.002
T5-KT2,6″- M5,5,3″,3″	1	0.022	1-y	-0.085
T7-KT2,6″-M5,5,3″,3″	1	0.022	1-y	0.013
T8-KT2,6″-M5,5,3″,3″	1	0.021	1-y	-0.074
T9-KT2,6″-M5,5,3″,3″	1	0.014	1-y	-0.180
T10-KT2,6″-M5,5,3″,3″	1	0.014	1-y	-0.152
///////////////////	///////////////	///////////////	///////////////	///////////////
T6-M5,3″-ET6,4″	3	-0.046	3-y	-0.264
			3-y-in-out	-0.316
			3-y-in-in	-0.486
T9-M5,3″-ET6,4″	1	-0.036	3-y	-0.265
			3-y-in-in	-0.471
T5-KT6″-M3″,3″-ET4	1	-0.019	1-y	-0.115
T9-KT6″-M3″,3″-ET4	1	-0.019	1-y	-0.130
T9-KT6″-M5,3″,3″-ET6	1	0.040	1-y	0.030
	40	-0.020	40-y	0.056

Table S 19
Information from the obtained MP2 results for trimeric acylphloroglucinols
MP2 denotes the MP2/6-31G(d,p) results in the column headings, and MP2+ denotes the MP2/6-31+G(d,p) results.

a) **Relative energies**

Molecule	Conformer	Relative energy (kcal/mol)	
		MP2	**MP2+**
T1	1-y	0.000	_ a _
	1	0.234	
	2-y	1.661	
	2	3.215	
	3-y	3.084	
	3	3.558	
	4-y	3.862	
	4	4.154	
T2-KT2,6″-M5,5,3″,3″	1-y	0.000	0.000
	1	0.870	1.855
T7-KT6″-M5,3″,3″	1-y	0.000	
	1	0.966	

[a] It would not be realistic to use the available data to calculate the MP2+ relative energies for T1, because the expected lowest energy conformer (3-y) did not converge.

b) **Energy difference between the MP2 energy value and the HF energy value reported in the same output**

Molecule	Conformer	Energy difference (kcal/mol)	
		MP2	**MP2+**
T1	1-y	3531.714	3591.292
	1	3530.424	3585.707
	2	3535.242	
	2-y	3529.600	3583.559
	3	3530.507	
	3-y	3529.176	
	4	3532.956	3587.038
	4-y	3531.525	3584.217

T2-KT2,6″-M5,5,3″,3″	1-y	4087.584	4152.266
	1	4083.626	4141.335
T3-M5,3″-ET6,2″	1-y	4183.543	
T7-KT6″-M5,3″,3″	1-y	4180.956	
	1	4175.585	

c)   Hydrogen bond lengths

Molecule	Conformer	H-bond	H-bond length (Å)	
			MP2	MP2+
T1	1-y	H15····O14	1.531	
		H17′····O14′	1.533	
		H17″····O14″	1.543	
		H16′····O8	1.691	
		H16····O12′	1.746	
		H16″····O10′	1.749	
		H15′····O12″	1.739	
	1	H15····O14	1.532	1.528
		H17′····O14′	1.532	1.533
		H17″····O14″	1.541	1.538
		H16′····O8	1.691	1.678
		H16····O12′	1.746	1.738
		H16″····O10′	1.749	1.742
		H15′····O12″	1.739	1.727
	2-y	H15····O14	1.525	1.532
		H17′····O14′	1.540	1.545
		H15″····O14″	1.561	1.648
		H16′····O8	1.667	1.701
		H16····O12′	1.759	1.782
		H17″····O10′	1.723	1.735
		H15′····O10″	1.822	1.837

	2	H15····O14	1.530	
		H17′····O14′	1.536	
		H15″····O14″	1.608	
		H16′····O8	1.683	
		H16····O12′	1.750	
		H17″····O10′	1.747	
		H15′····O10″	1.793	
	3-y	H15····O14	1.540	
		H15′····O14′	1.531	
		H15″····O14″	1.607	
		H17′····O8	1.733	
		H16····O10′	1.748	
		H17″····O8′	1.733	
		H16′····O10″	1.739	
	3	H15····O14	1.540	
		H15′····O14′	1.532	
		H15″····O14″	1.607	
		H17′····O8	1.731	
		H16····O10′	1.755	
		H17″····O8′	1.740	
		H16′····O10″	1.747	
	4-y	H15····O14	1.555	1.570
		H17′····O14′	1.534	1.536
		H17″····O14″	1.543	1.542
		H10′····O8	1.700	1.705
		H16····O12′	1.752	1.770
		H16″····O10′	1.751	1.742
		H15′····O12″	1.741	1.739
	4	H15····O14	1.555	1.561
		H17′····O14′	1.533	1.536
		H17″····O14″	1.542	1.540
		H10′····O8	1.697	1.694
		H16····O12′	1.745	1.748
		H16″····O10′	1.751	1.751
		H15′····O12″	1.736	1.737
T2-KT2,6″-M5,5,3″,3″	1-y	H17····O14	1.522	1.512
		H15′····O14′	1.515	1.534
		H15″····O14″	1.525	1.517
		H17′····O8	1.596	1.641
		H16····O10′	1.718	1.730
		H16″····O8′	1.684	1.675

		H16′····O12″	1.667	1.669
	1	H17····O14	1.514	1.514
		H15′····O14′	1.522	1.522
		H15″····O14″	1.514	1.513
		H17′····O8	1.595	1.587
		H16····O10′	1.697	1.692
		H16″····O8′	1.691	1.687
		H16′····O12″	1.652	1.652
T3-M5,3″-ET6,2″	1-y	H15····O14	1.553	
		H15′····O14′	1.514	
		H17″····O14″	1.544	
		H17′····O8	1.725	
		H16····O10′	1.737	
		H16″····O8′	1.740	
		H16′····O12″	1.629	
T7-KT6″-M5,3″,3″	1-y	H15····O14	1.523	
		H15′····O14′	1.534	
		H15″····O14″	1.513	
		H17′····O8	1.640	
		H16····O10′	1.730	
		H16″····O8′	1.691	
		H16′····O12″	1.666	
	1	H15····O14	1.526	
		H15′····O14′	1.530	
		H15″····O14″	1.514	
		H17′····O8	1.664	
		H16····O10′	1.725	
		H16″····O8′	1.704	
		H16′····O12″	1.656	

d) **Comparison of the estimation of the hydrogen bond lengths with the results of the other methods**

Conf-ormer	H-bond	H-bond length (Å)				
		HF	HF+	DFT	DFT-D3	MP2
T1						
1	H15····O14	1.626	1.631	1.473	1.480	1.532
	H17′····O14′	1.622	1.627	1.474	1.483	1.532
	H17″····O14″	1.632	1.637	1.483	1.491	1.541
	H16′····O8	1.815	1.822	1.709	1.689	1.691
	H16····O12′	1.851	1.855	1.758	1.741	1.746
	H16″····O10′	1.857	1.866	1.771	1.750	1.749
	H15′····O12″	1.847	1.854	1.749	1.732	1.739
1-y	H15····O14	1.630	1.634	1.476	1.483	1.531
	H17′····O14′	1.624	1.629	1.474	1.483	1.533
	H17″····O14″	1.632	1.637	1.484	1.494	1.543
	H16′····O8	1.837	1.846	1.726	1.702	1.691
	H16····O12′	1.863	1.868	1.761	1.746	1.746
	H16″····O10′	1.847	1.879	1.781	1.760	1.749
	H15′····O12″	1.870	1.855	1.750	1.735	1.739
2	H15····O14	1.624	1.629	1.469	1.477	1.530
	H17′····O14′	1.625	1.629	1.478	1.487	1.536
	H15″····O14″	1.691	1.696	1.557	1.568	1.608
	H16′····O8	1.857	1.818	1.701	1.682	1.683
	H16····O12′	1.811	1.861	1.766	1.749	1.750
	H17″····O10′	1.885	1.858	1.758	1.737	1.747
	H15′····O10″	1.849	1.897	1.801	1.788	1.793
2-y	H15····O14	1.626	1.631	1.471	1.474	1.525
	H17′····O14′	1.627	1.632	1.478	1.490	1.540
	H15″····O14″	1.691	1.697	1.557	1.573	1.561
	H16′····O8	1.828	1.837	1.714	1.675	1.667
	H16····O12′	1.867	1.872	1.770	1.761	1.759
	H17″····O10′	1.860	1.871	1.767	1.727	1.723
	H15′····O10″	1.889	1.903	1.805	1.810	1.822
3	H15····O14	1.631	1.636	1.481	1.490	1.540
	H15′····O14′	1.621	1.627	1.470	1.480	1.532
	H15″····O14″	1.690	1.696	1.556	1.567	1.607
	H17′····O8	1.846	1.853	1.746	1.730	1.731
	H16····O10′	1.861	1.870	1.780	1.760	1.755
	H17″····O8′	1.836	1.843	1.742	1.726	1.740

	H16′····O10″	1.852	1.865	1.769	1.753	1.747
3-y	H15····O14	1.631	1.636	1.481	1.490	1.540
	H15′····O14′	1.632	1.629	1.471	1.481	1.531
	H15″····O14″	1.690	1.696	1.556	1.567	1.607
	H17′····O8	1.844	1.851	1.747	1.732	1.733
	H16····O10′	1.865	1.874	1.782	1.762	1.748
	H17″····O8′	1.849	1.855	1.747	1.731	1.733
	H16′····O10″	1.870	1.884	1.780	1.760	1.739
4	H15····O14	1.650	1.656	1.492	1.502	1.555
	H17′····O14′	1.623	1.628	1.475	1.483	1.533
	H17″····O14″	1.632	1.637	1.483	1.492	1.542
	H10′····O8	1.819	1.828	1.716	1.697	1.697
	H16····O12′	1.852	1.858	1.759	1.742	1.745
	H16″····O10′	1.858	1.867	1.771	1.751	1.751
	H15′····O12″	1.848	1.855	1.750	1.733	1.736
4-y	H15····O14	1.650	1.661	1.496	1.505	1.555
	H17′····O14′	1.625	1.631	1.475	1.484	1.534
	H17″····O14″	1.633	1.638	1.484	1.494	1.543
	H10′····O8	1.842	1.852	1.733	1.709	1.700
	H16····O12′	1.867	1.873	1.764	1.749	1.752
	H16″····O10′	1.871	1.880	1.781	1.762	1.751
	H15′····O12″	1.850	1.858	1.751	1.737	1.741
T2-KT2,6″-M5,5,3″,3″						
1	H17····O14	1.637	1.643	1.451	1.469	1.514
	H15′····O14′	1.610	1.612	1.460	1.468	1.522
	H15″····O14″	1.637	1.643	1.451	1.469	1.514
	H17′····O8	1.745	1.749	1.640	1.625	1.595
	H16····O10′	1.831	1.836	1.720	1.696	1.697
	H16″····O8′	1.841	1.845	1.718	1.697	1.691
	H16′····O12″	1.709	1.711	1.580	1.562	1.652
1-y	H17····O14	1.637	1.643	1.451	1.469	1.522
	H15′····O14′	1.612	1.613	1.460	1.468	1.515
	H15″····O14″	1.638	1.644	1.452	1.471	1.525
	H17′····O8	1.747	1.748	1.640	1.627	1.596
	H16····O10′	1.853	1.858	1.731	1.698	1.718
	H16″····O8′	1.844	1.848	1.722	1.704	1.684
	H16′····O12″	1.723	1.727	1.595	1.566	1.667
T3-M5,3″-ET6,2″						
1-y	H15····O14	1.660	1.669	1.488	1.501	1.553
	H15′····O14′	1.636	1.646	1.450	1.462	1.514
	H17″····O14″	1.657	1.667	1.481	1.492	1.544

	H17′····O8	1.837	1.849	1.733	1.719	1.725
	H16····O10′	1.865	1.876	1.770	1.750	1.737
	H16″····O8′	1.857	1.865	1.749	1.736	1.740
	H16′····O12″	1.821	1.831	1.708	1.686	1.629
T7-KT6″-M5,3″,3″						
1	H15····O14	1.624	1.628	1.481	1.489	1.526
	H15′····O14′	1.610	1.612	1.460	1.468	1.530
	H15″····O14″	1.637	1.642	1.451	1.469	1.514
	H17′····O8	1.827	1.836	1.734	1.715	1.664
	H16····O10′	1.829	1.840	1.742	1.720	1.725
	H16″····O8′	1.844	1.848	1.720	1.699	1.704
	H16′····O12″	1.713	1.717	1.587	1.571	1.656
1-y	H15····O14	1.626	1.629	1.483	1.490	1.523
	H15′····O14′	1.611	1.613	1.460	1.468	1.534
	H15″····O14″	1.638	1.643	1.451	1.470	1.513
	H17′····O8	1.834	1.840	1.736	1.721	1.640
	H16····O10′	1.851	1.860	1.755	1.730	1.730
	H16″····O8′	1.844	1.849	1.723	1.706	1.691
	H16′····O12″	1.723	1.730	1.599	1.573	1.666