Article

Intramolecular Hydrogen Bond, Hirshfeld Analysis, AIM; DFT Studies of Pyran-2,4-dione Derivatives

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X-Ray single crystal determination of 1

The crystal of **1** was immersed in cryo-oil, mounted in a loop, and measured at a temperature of 120 K. The X-ray diffraction data was collected on a Rigaku Oxford Diffraction Supernova diffractometer using Cu Kα radiation. The *CrysAlisPro* [1] software package was used for cell refinement and data reduction. A multi-scan absorption correction (*CrysAlisPro* [2]) was applied to the intensities before structure solution. The structure was solved by intrinsic phasing (*SHELXT*) method. Structural refinement was carried out using *SHELXL* [3] software with *SHELXLE* [4] graphical user interface. The NH hydrogen atom was located from the difference Fourier map and refined isotropically. All other hydrogen atoms were positioned geometrically and constrained to ride on their parent atoms, with C-H = 0.95 Å and U_{iso} = 1.2· U_{eq} (parent atom). The topology analyses of molecular packing were performed using Crystal Explorer 17.5 program [5].

References

1. Rikagu Oxford Diffraction, *CrysAlisPro*, Agilent Technologies inc., **2018,** Yarnton, Oxfordshire, England.
2. Sheldrick, G.M. *Acta Cryst.* **2015,** *C71*, 3-8.
3. Hübschle, C. B.; Sheldrick, G.M.; Dittrich, B. *J. Appl. Cryst.* **2011**, *44*, 1281-1284.
4. Sheldrick, G. M. SADABS - Bruker Nonius scaling and absorption correction -, Bruker AXS, Inc.: Madison, Wisconsin, USA, 2012.

5. Turner, M. J.; McKinnon, J. J.; Wolff, S. K.; Grimwood, D. J.; Spackman, P. R.; Jayatilaka, D.; Spackman, M. A. Crystal Explorer17 (2017) University of Western Australia. http://hirshfeldsurface.net

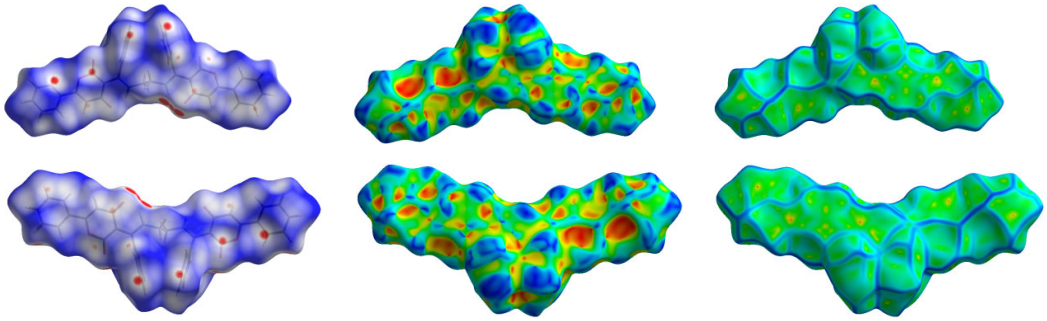


Fig. S1 Hirshfeld surfaces of **1**.

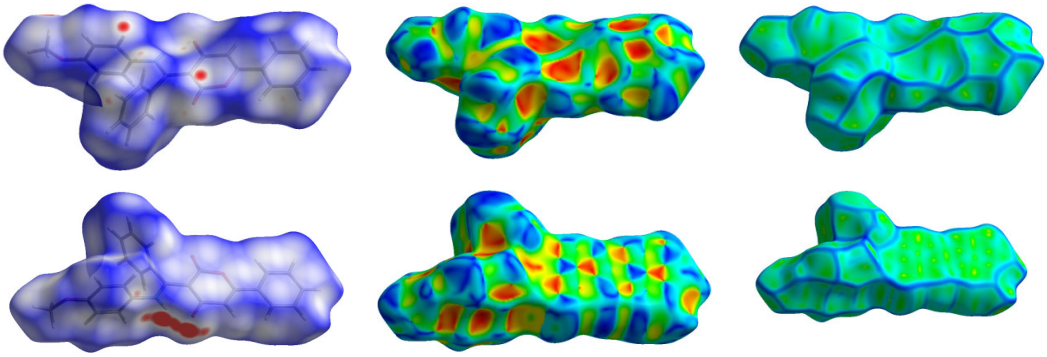
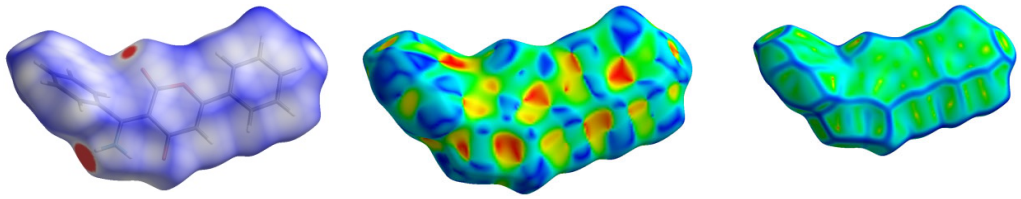
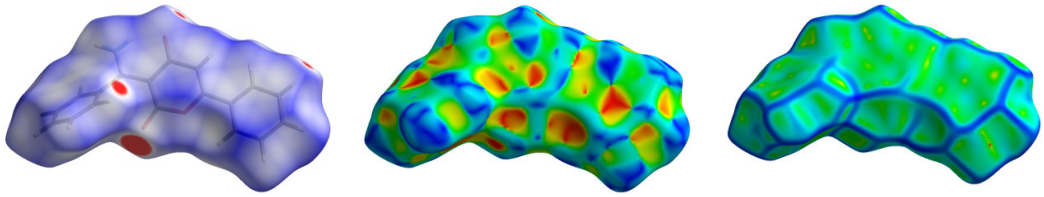


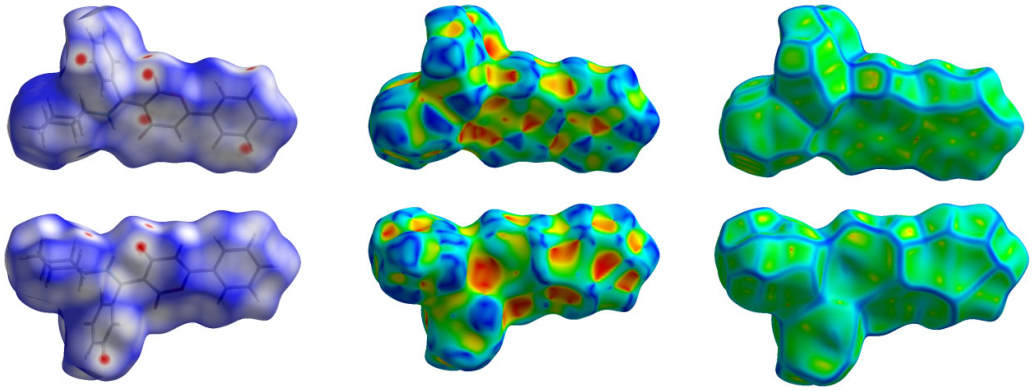
Fig. S2 Hirshfeld surfaces of **2**.





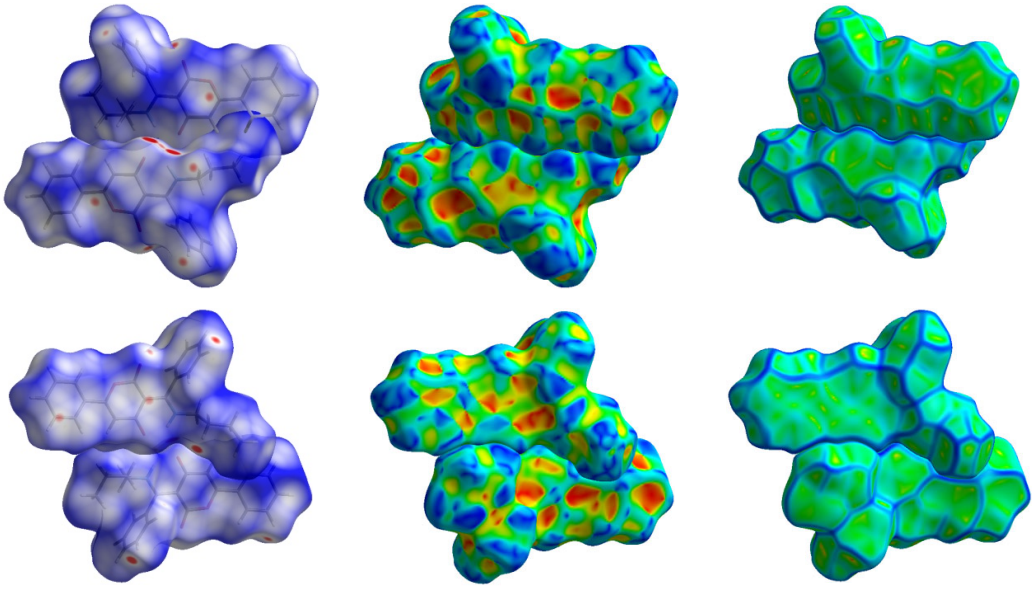
d_{norm} **Shape index** **Curvedness**

Fig. S3 Hirshfeld surfaces of **3**.



d_{norm} **Shape index** **Curvedness**

Fig. S4 Hirshfeld surfaces of **4**.



d_{norm} **Shape index** **Curvedness**

Fig. S5 Hirshfeld surfaces of **5**.

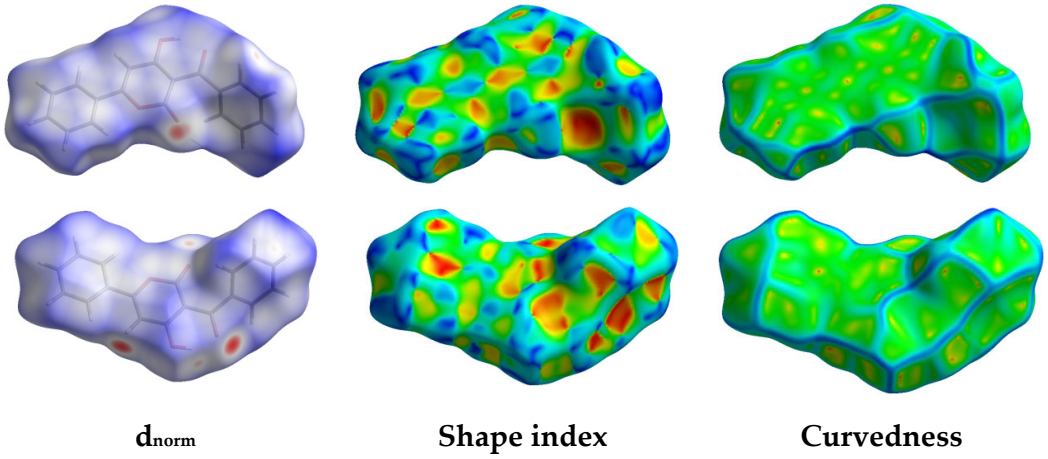


Fig. S6 Hirshfeld surfaces for one molecular unit of **6**.

Table S1 Crystal data and structure refinement for **1**.

Contact	1
empirical formula	$C_{38}H_{28}N_2O_6$
fw	608.62
temp (K)	120(2)
λ(Å)	0.71073
cryst syst	Monoclinic
space group	C2/c
a (Å)	14.0869(4)
b (Å)	20.9041(5)
c (Å)	10.1444(2)
β (deg)	99.687(2)
V (Å^3)	2944.67(12)
Z	4
ρ_{calc} (Mg/m^3)	1.373
μ(Mo Kα) (mm^{-1})	0.094
No. reflns.	12328
Unique reflns.	3657
GOOF (F^2)	1.040
R_{int}	0.0204
R1[a] ($I \geq 2\sigma$)	0.0453
wR2[b] ($I \geq 2\sigma$)	0.1136
CCDC No.	2068753

Table S2 Bond lengths (Å) and angles (°) for **1**.

Bond	**Length/Å**	**Bond**	**Length/Å**
O1-C9	1.2524(18)	C7-C8	1.329(2)
O2-C11	1.2079(19)	C8-C9	1.444(2)
O3-C7	1.3573(19)	C9-C10	1.439(2)
O3-C11	1.4069(17)	C10-C12	1.4290(19)
N1-C12	1.3239(18)	C10-C11	1.445(2)
N1-C19	1.4668(17)	C12-C13	1.489(2)
C1-C6	1.391(2)	C13-C18	1.389(2)
C1-C2	1.393(2)	C13-C14	1.391(2)
C2-C3	1.380(3)	C14-C15	1.383(2)
C3-C4	1.370(3)	C15-C16	1.372(2)
C4-C5	1.389(2)	C16-C17	1.376(2)
C5-C6	1.393(2)	C17-C18	1.389(2)
C6-C7	1.478(2)	C19-C19[1]	1.531(3)
Bonds	**Angle/°**	**Bonds**	**Angle/°**
C7-O3-C11	123.04(12)	C12-C10-C11	119.08(14)
C12-N1-C19	126.22(14)	C9-C10-C11	119.73(13)
C6-C1-C2	120.32(16)	O2-C11-O3	114.04(13)
C3-C2-C1	119.97(18)	O2-C11-C10	128.89(14)
C4-C3-C2	120.13(16)	O3-C11-C10	117.05(14)
C3-C4-C5	120.48(16)	N1-C12-C10	119.86(14)
C4-C5-C6	120.19(16)	N1-C12-C13	117.53(12)
C1-C6-C5	118.87(14)	C10-C12-C13	122.60(12)
C1-C6-C7	120.87(14)	C18-C13-C14	119.27(15)
C5-C6-C7	120.24(15)	C18-C13-C12	120.87(13)
C8-C7-O3	121.01(14)	C14-C13-C12	119.85(13)
C8-C7-C6	126.35(15)	C15-C14-C13	120.31(15)
O3-C7-C6	112.61(13)	C16-C15-C14	120.21(16)
C7-C8-C9	122.15(16)	C15-C16-C17	119.99(16)
O1-C9-C10	123.21(13)	C16-C17-C18	120.57(15)
O1-C9-C8	119.85(15)	C17-C18-C13	119.64(15)
C10-C9-C8	116.94(13)	N1-C19-C19[1]	111.66(15)
C12-C10-C9	121.19(13)		

Symm. Code. [1]1-X,+Y,5/2-Z

Table S3 The calculated geometric parameters of **1**[a].

parameter	Calc	Exp
R(1-18)	1.359	1.37
R(1-19)	1.412	1.403
R(2-19)	1.209	1.208
R(3-6)	1.608	1.663
R(3-21)	1.258	1.259
R(4-41)	1.363	1.373
R(4-42)	1.42	1.441
R(5-24)	1.34	1.33
R(5-36)	1.419	1.433
R(7-9)	1.391	1.379
R(7-17)	1.406	1.397
R(9-11)	1.397	1.387
R(11-13)	1.395	1.382
R(13-15)	1.393	1.376
R(15-17)	1.405	1.394
R(17-18)	1.475	1.464
R(18-22)	1.354	1.341
R(19-20)	1.457	1.438
R(20-21)	1.463	1.449
R(20-24)	1.42	1.418
R(21-22)	1.448	1.431
R(24-25)	1.493	1.493
R(25-26)	1.401	1.37
R(25-34)	1.399	1.361
R(26-28)	1.392	1.384
R(28-30)	1.397	1.365
R(30-32)	1.395	1.361
R(32-34)	1.395	1.384
R(36-37)	1.398	1.371
R(36-48)	1.405	1.366
R(37-39)	1.396	1.39
R(39-41)	1.4	1.376
R(41-46)	1.403	1.376
R(46-48)	1.386	1.385
R(35-37)	1.397	1.381

R(37-39)	1.392	1.383
R(41-42)	1.555	1.549
R(43-46)	1.519	1.496
R(50-51)	1.404	1.382
R(50-59)	1.406	1.392
R(51-53)	1.396	1.39
R(53-55)	1.393	1.379
R(55-57)	1.397	1.381
R(57-59)	1.391	1.387
R(61-62)	1.477	1.478
R(63-66)	1.52	1.512
A(18-1-19)	123.8	122.8
A(1-18-17)	112.5	112.4
A(1-18-22)	121.2	120.8
A(1-19-2)	114.8	113.9
A(1-19-20)	116.3	117.8
A(2-19-20)	128.9	128.3
A(6-3-21)	101.1	104.2
A(3-6-5)	145.6	139.1
A(3-21-20)	123.2	122.2
A(3-21-22)	119.7	119.7
A(41-4-42)	118.3	116.5
A(4-41-39)	124.8	124.7
A(4-41-46)	115.8	116
A(4-42-43)	111.6	109.5
A(4-42-44)	106	109.5
A(4-42-45)	111.6	109.4
A(24-5-36)	131.4	125.9
A(5-24-20)	118	119.6
A(5-24-25)	118.7	115.6
A(24-5-6)	110.8	113.8
A(5-36-37)	124.3	120
A(5-36-48)	116.7	120.6
A(36-5-6)	117.5	120.3
A(8-7-9)	119.4	119.7
A(8-7-17)	120	119.8
A(9-7-17)	120.5	120.6
A(7-9-10)	119.6	119.6
A(7-9-11)	120.2	120.9
A(7-17-15)	118.9	117.8
A(7-17-18)	121.1	120.8
A(10-9-11)	120.1	119.6
A(9-11-12)	120.1	120.5
A(9-11-13)	119.7	118.9
A(12-11-13)	120.2	120.6
A(11-13-14)	120.1	119.8

A(11-13-15)	120.3	120.4
A(14-13-15)	119.6	119.8
A(13-15-16)	120.5	119.3
A(13-15-17)	120.4	121.4
A(16-15-17)	119.2	119.3
A(15-17-18)	120.1	121.4
A(17-18-22)	126.3	126.8
A(18-22-21)	121.3	121.7
A(18-22-23)	121.7	119.1
A(19-20-21)	119.5	118.9
A(19-20-24)	120	120.1
A(21-20-24)	120.5	120.9
A(20-21-22)	117.1	118
A(20-24-25)	123.3	124.8
A(21-22-23)	117	119.2
A(24-25-26)	120.6	119.1
A(24-25-34)	119.8	122.1
A(26-25-34)	119.6	118.6
A(25-26-27)	119.6	119.8
A(25-26-28)	120.1	120.4
A(25-34-32)	120.1	120.9
A(25-34-35)	119.7	119.6
A(27-26-28)	120.2	119.8
A(26-28-29)	119.7	119.7
A(26-28-30)	120.2	120.7
A(29-28-30)	120.1	119.6
A(28-30-31)	120.1	120.6
A(28-30-32)	119.8	118.8
A(31-30-32)	120.1	120.6
A(30-32-33)	120.2	119.7
A(30-32-34)	120.2	120.5
A(33-32-34)	119.7	119.7
A(32-34-35)	120.1	119.5
A(37-36-48)	118.9	119.2
A(36-37-38)	120.3	119.6
A(36-37-39)	120.6	120.8
A(36-48-46)	120.8	120.6
A(36-48-49)	119.3	119.7
A(38-37-39)	119.2	119.5
A(37-39-40)	118.8	120.2
A(37-39-41)	120.2	119.7
A(40-39-41)	121	120.2
A(39-41-46)	119.4	119.3
A(41-46-47)	118.7	119.9
A(41-46-48)	120.2	120.3
A(43-42-44)	109.2	109.5

A(43-42-45)	109.1	109.5
A(44-42-45)	109.2	109.5
A(47-46-48)	121.1	119.9
A(46-48-49)	119.9	119.7

[a]Atom numbering refer to **Fig. 9**

Table S4 The calculated geometric parameters of **2**[a].

Parameter	**Calc**	**Exp**
R(1-19)	1.254	1.263
R(1-35)	1.694	1.729
R(2-21)	1.21	1.217
R(3-22)	1.335	1.318
R(4-16)	1.36	1.367
R(4-21)	1.409	1.391
R(5-7)	1.393	1.379
R(5-15)	1.405	1.395
R(7-9)	1.395	1.381
R(9-11)	1.397	1.386
R(11-13)	1.391	1.391
R(13-15)	1.406	1.397
R(15-16)	1.475	1.471
R(16-17)	1.353	1.321
R(17-19)	1.45	1.445
R(19-20)	1.467	1.45
R(20-21)	1.456	1.439
R(20-22)	1.412	1.424
R(22-23)	1.491	1.49
R(23-24)	1.402	1.394
R(23-32)	1.402	1.394
R(24-26)	1.395	1.385
R(26-28)	1.394	1.383
R(28-30)	1.398	1.393
R(30-32)	1.391	1.388
A(19-1-35)	103.4	101.4
A(1-19-17)	119.8	119.1
A(1-19-20)	123.5	123.6
A(1-35-3)	137.9	139.9
A(2-21-4)	114.9	114.4
A(2-21-20)	128.7	127.8
A(22-3-34)	119.4	122.5
A(22-3-35)	115.6	115.5

A(3-22-20)	119.4	119.1
A(3-22-23)	114.5	114.3
A(34-3-35)	123.8	121.7
A(16-4-21)	123.8	123.2
A(4-16-15)	112.4	112.6
A(4-16-17)	121.3	120.9
A(4-21-20)	116.4	117.8
A(6-5-7)	120.4	119.8
A(6-5-15)	119.2	119.8
A(7-5-15)	120.4	120.4
A(5-7-8)	119.6	119.7
A(5-7-9)	120.3	120.6
A(5-15-13)	118.8	118.7
A(5-15-16)	120.1	120.9
A(8-7-9)	120.1	119.7
A(7-9-10)	120.2	120
A(7-9-11)	119.7	120
A(10-9-11)	120.1	120
A(9-11-12)	120.1	120.2
A(9-11-13)	120.2	119.6
A(12-11-13)	119.6	120.2
A(11-13-14)	119.4	119.6
A(11-13-15)	120.5	120.8
A(14-13-15)	120.1	119.6
A(13-15-16)	121.1	120.4
A(15-16-17)	126.3	126.6
A(16-17-18)	121.6	119
A(16-17-19)	121.5	121.9
A(18-17-19)	116.9	119.1
A(17-19-20)	116.6	117.3
A(19-20-21)	119.9	118.8
A(19-20-22)	119.8	120.1
A(21-20-22)	120.2	121.1
A(20-22-23)	126	126.6
A(22-23-24)	119.2	119.3
A(22-23-32)	121.2	121
A(24-23-32)	119.4	119.4
A(23-24-25)	119.6	119.9
A(23-24-26)	120.3	120.2
A(23-32-30)	120.1	120.2
A(23-32-33)	119.7	119.9
A(25-24-26)	120.1	119.9
A(24-26-27)	119.7	119.9
A(24-26-28)	120	120.2
A(27-26-28)	120.3	119.9
A(26-28-29)	120.1	119.9

A(26-28-30)	119.9	120.1
A(29-28-30)	120	120
A(28-30-31)	120.1	120.1
A(28-30-32)	120.3	119.9
A(31-30-32)	119.6	120.1
A(30-32-33)	120.2	119.9
A(28-30-32)	120.3	118.8
A(31-30-32)	119.6	120.6
A(30-32-33)	120.2	119.7

[a]Atom numbering refer to **Fig. 9**

Table S5 The calculated geometric parameters of **3**[a].

Parameter	Calc	Exp
R(1-17)	1.359	1.364
R(1-22)	1.412	1.406
R(2-22)	1.21	1.207
R(3-5)	1.653	1.787
R(3-20)	1.257	1.25
R(4-23)	1.331	1.315
R(4-35)	1.462	1.472
R(6-8)	1.391	1.389
R(6-16)	1.406	1.394
R(8-10)	1.397	1.383
R(10-12)	1.395	1.383
R(12-14)	1.393	1.386
R(14-16)	1.405	1.394
R(16-17)	1.476	1.479
R(17-18)	1.354	1.331
R(18-20)	1.45	1.447
R(20-21)	1.461	1.446
R(21-22)	1.454	1.44
R(21-23)	1.42	1.423
R(23-24)	1.499	1.496
R(24-25)	1.4	1.387
R(24-33)	1.399	1.389
R(25-27)	1.394	1.389
R(27-29)	1.396	1.381
R(29-31)	1.396	1.382
R(31-33)	1.394	1.386
R(35-37)	1.541	1.521
R(35-49)	1.54	1.52
R(37-40)	1.536	1.523
R(40-43)	1.535	1.512
R(43-46)	1.535	1.515
R(46-49)	1.536	1.531

A(17-1-22)	123.9	122.7
A(1-17-16)	112.4	111.8
A(1-17-18)	121.2	121.4
A(1-22-2)	114.8	114.4
A(1-22-21)	116.4	116.8
A(2-22-21)	128.8	128.9
A(5-3-20)	101.8	100.4
A(3-5-4)	143.3	141.3
A(3-20-18)	119.7	120.2
A(3-20-21)	123.4	123.6
A(5-4-23)	111.9	114.2
A(5-4-35)	119.4	118.6
A(23-4-35)	128.7	127
A(4-23-21)	119.3	119.9
A(4-23-24)	117.5	117.3
A(4-35-36)	108	108.7
A(4-35-37)	110	110.5
A(4-35-49)	109.9	108.7
A(7-6-8)	119.3	119.9
A(7-6-16)	120.1	120
A(8-6-16)	120.6	120.1
A(6-8-9)	119.6	119.9
A(6-8-10)	120.3	120.3
A(6-16-14)	118.8	119.1
A(6-16-17)	121.2	120.2
A(9-8-10)	120.1	119.9
A(8-10-11)	120.1	120
A(8-10-12)	119.6	120.1
A(11-10-12)	120.2	120
A(10-12-13)	120.1	120
A(10-12-14)	120.3	120
A(13-12-14)	119.5	120
A(12-14-15)	120.4	119.7
A(12-14-16)	120.4	120.5
A(15-14-16)	119.1	119.7
A(14-16-17)	120	120.7
A(16-17-18)	126.3	126.8
A(17-18-19)	121.7	119
A(17-18-20)	121.4	122.1
A(19-18-20)	116.8	119
A(18-20-21)	116.9	116.2
A(20-21-22)	120.1	120.3
A(20-21-23)	120.3	120.3
A(22-21-23)	119.6	119.3
A(21-23-24)	123.2	122.7
A(23-24-25)	120.2	119

A(23-24-33)	120.1	120.8
A(25-24-33)	119.6	120.1
A(24-25-26)	119.7	120.1
A(24-25-27)	120.1	119.8
A(24-33-31)	120.1	119.9
A(24-33-34)	119.7	120
A(26-25-27)	120.2	120.1
A(25-27-28)	119.7	120.1
A(25-27-29)	120.2	119.8
A(28-27-29)	120.1	120.1
A(27-29-30)	120.1	119.7
A(27-29-31)	119.8	120.6
A(30-29-31)	120.1	119.7
A(29-31-32)	120.1	120.1
A(29-31-33)	120.2	119.8
A(32-31-33)	119.7	120.1
A(31-33-34)	120.2	120
A(36-35-37)	108.8	108.7
A(36-35-49)	108.8	108.7
A(37-35-49)	111.2	111.6
A(35-37-38)	109.3	109.5
A(35-37-39)	108.8	109.5
A(35-37-40)	111.5	110.8
A(35-49-46)	111.5	110.6
A(35-49-50)	108.8	109.5
A(35-49-51)	109.3	109.5
A(38-37-39)	106.7	108.1
A(38-37-40)	110.7	109.5
A(39-37-40)	109.7	109.5
A(37-40-41)	109.6	109.5
A(37-40-42)	109.2	109.5
A(37-40-43)	111.6	110.9
A(41-40-42)	106.4	108.1
A(41-40-43)	110.5	109.5
A(42-40-43)	109.3	109.5
A(40-43-44)	110.2	109.3
A(40-43-45)	109.3	109.3
A(40-43-46)	111.2	111.4
A(44-43-45)	106.5	108
A(44-43-46)	110.2	109.4
A(45-43-46)	109.3	109.4
A(43-46-47)	109.3	109.4
A(43-46-48)	110.5	109.3
A(43-46-49)	111.6	111.5
A(47-46-48)	106.4	108
A(47-46-49)	109.3	109.3

A(48-46-49)	109.6	109.3
A(46-49-50)	109.6	109.5
A(46-49-51)	110.7	109.5
A(50-49-51)	106.7	108.1

[a]Atom numbering refer to **Fig. 9**

Table S6 The calculated geometric parameters of **4**[a].

Parameter	Calc	Exp
R(1-19)	1.257	1.253
R(2-21)	1.21	1.203
R(3-16)	1.359	1.362
R(3-21)	1.411	1.406
R(4-22)	1.332	1.318
R(4-34)	1.458	1.466
R(5-7)	1.391	1.388
R(5-15)	1.406	1.398
R(7-9)	1.397	1.39
R(9-11)	1.395	1.381
R(11-13)	1.393	1.384
R(13-15)	1.405	1.398
R(15-16)	1.476	1.471
R(16-17)	1.354	1.338
R(17-19)	1.45	1.445
R(19-20)	1.461	1.445
R(20-21)	1.454	1.449
R(20-22)	1.419	1.428
R(22-23)	1.499	1.495
R(23-24)	1.4	1.391
R(23-32)	1.399	1.387
R(24-26)	1.394	1.39
R(26-28)	1.396	1.385
R(28-30)	1.395	1.383
R(30-32)	1.394	1.387
R(34-37)	1.537	1.525
R(37-40)	1.537	1.524
R(40-43)	1.533	1.512
A(1-19-17)	119.7	119.6
A(1-19-20)	123.3	123.3
A(2-21-3)	114.8	114.5
A(2-21-20)	128.8	128.7
A(16-3-21)	123.9	123.2
A(3-16-15)	112.4	112.9
A(3-16-17)	121.2	121.1
A(3-21-20)	116.4	116.8
A(22-4-34)	127.9	126.1

A(22-4-47)	112	115.6
A(4-22-20)	119.3	120.2
A(4-22-23)	117.3	116.8
A(34-4-47)	120	118.1
A(4-34-35)	109.1	109.3
A(4-34-36)	107.4	109.3
A(4-34-37)	112	111.5
A(6-5-7)	119.3	119.9
A(6-5-15)	120.1	119.9
A(7-5-15)	120.6	120.2
A(5-7-8)	119.6	120
A(5-7-9)	120.3	120
A(5-15-13)	118.8	119
A(5-15-16)	121.2	120.5
A(8-7-9)	120.1	120
A(7-9-10)	120.1	119.9
A(7-9-11)	119.6	120.1
A(10-9-11)	120.2	120
A(9-11-12)	120.1	119.9
A(9-11-13)	120.3	120.1
A(12-11-13)	119.5	119.9
A(11-13-14)	120.4	119.7
A(11-13-15)	120.4	120.5
A(14-13-15)	119.1	119.7
A(13-15-16)	120	120.5
A(15-16-17)	126.4	126
A(16-17-18)	121.8	119.1
A(16-17-19)	121.4	121.8
A(18-17-19)	116.8	119.1
A(17-19-20)	116.9	117
A(19-20-21)	120.1	119.9
A(19-20-22)	120.3	120.4
A(21-20-22)	119.5	119.7
A(20-22-23)	123.3	123
A(22-23-24)	120.2	120.7
A(22-23-32)	120.1	119.4
A(24-23-32)	119.6	119.7
A(23-24-25)	119.7	120.1
A(23-24-26)	120.1	119.9
A(23-32-30)	120.1	120.2
A(23-32-33)	119.7	119.9
A(25-24-26)	120.2	120.1
A(24-26-27)	119.7	120
A(24-26-28)	120.2	120.1
A(27-26-28)	120.1	120
A(26-28-29)	120.1	119.9

A(26-28-30)	119.8	120.1
A(29-28-30)	120.1	119.9
A(28-30-31)	120.1	120
A(28-30-32)	120.2	120
A(31-30-32)	119.7	120
A(30-32-33)	120.2	119.9
A(35-34-36)	107.5	108
A(35-34-37)	111	109.3
A(36-34-37)	109.6	109.3
A(34-37-38)	108.6	109
A(34-37-39)	108.6	109
A(34-37-40)	113.5	112.7
A(38-37-39)	106.5	107.8
A(38-37-40)	109.9	109.1
A(39-37-40)	109.4	109
A(37-40-41)	108.1	109
A(37-40-42)	109.2	109
A(37-40-43)	114.5	113.1
A(41-40-42)	105.9	107.8
A(41-40-43)	109.1	109
A(42-40-43)	109.6	109
A(40-43-44)	112.2	109.5
A(40-43-45)	110.9	109.5
A(40-43-46)	111.1	109.5
A(44-43-45)	107.2	109.5
A(44-43-46)	107.5	109.5
A(45-43-46)	107.7	109.5

[a]Atom numbering refer to **Fig. 9**

Table S7 The calculated geometric parameters of **5**[a].

Parameter	Calc	Exp
R(1-19)	1.258	1.252
R(2-21)	1.209	1.208
R(3-16)	1.359	1.357
R(3-21)	1.41	1.407
R(4-22)	1.336	1.324
R(4-34)	1.452	1.467
R(5-7)	1.391	1.393
R(5-15)	1.406	1.391
R(7-9)	1.397	1.38
R(9-11)	1.395	1.37
R(11-13)	1.393	1.389
R(13-15)	1.405	1.393
R(15-16)	1.475	1.478
R(16-17)	1.354	1.329
R(17-19)	1.448	1.444
R(19-20)	1.463	1.439
R(20-21)	1.456	1.445
R(20-22)	1.416	1.429
R(22-23)	1.497	1.489
R(23-24)	1.4	1.391
R(23-32)	1.399	1.389
R(24-26)	1.394	1.383
R(26-28)	1.396	1.372
R(28-30)	1.395	1.376
R(30-32)	1.394	1.389
R(34-71)	1.543	1.531
R(38-56)	1.258	1.252
R(39-58)	1.209	1.208
R(40-53)	1.359	1.357
R(40-58)	1.41	1.407
R(41-59)	1.336	1.324
R(41-71)	1.452	1.467
R(42-44)	1.391	1.393
R(42-52)	1.406	1.391
R(44-46)	1.397	1.38
R(46-48)	1.395	1.37
R(48-50)	1.393	1.389
R(50-52)	1.405	1.393
R(52-53)	1.475	1.478
R(53-54)	1.354	1.329
R(54-56)	1.448	1.444
R(56-57)	1.463	1.439
R(57-58)	1.456	1.445
R(57-59)	1.416	1.429

R(59-60)	1.497	1.489
R(60-61)	1.4	1.391
R(60-69)	1.399	1.389
R(61-63)	1.394	1.383
R(63-65)	1.396	1.372
R(65-67)	1.395	1.376
R(67-69)	1.394	1.389
A(1-19-17)	119.8	119.8
A(1-19-20)	123.2	123.2
A(2-21-3)	114.9	114
A(2-21-20)	128.7	128.9
A(16-3-21)	123.9	123
A(3-16-15)	112.4	112.6
A(3-16-17)	121.2	121
A(3-21-20)	116.3	117.1
A(22-4-34)	127.9	126.2
A(22-4-37)	111.7	115.6
A(4-22-20)	119	119.9
A(4-22-23)	117.5	117.5
A(34-4-37)	120.2	118.1
A(4-34-35)	110.2	109.3
A(4-34-36)	108.8	109.3
A(4-34-71)	110.7	111.7
A(6-5-7)	119.3	119.8
A(6-5-15)	120.2	119.8
A(7-5-15)	120.5	120.3
A(5-7-8)	119.6	120
A(5-7-9)	120.3	120
A(5-15-13)	118.8	118.9
A(5-15-16)	121.2	120.9
A(8-7-9)	120.1	120
A(7-9-10)	120.1	119.9
A(7-9-11)	119.6	120.1
A(10-9-11)	120.2	119.9
A(9-11-12)	120.1	119.8
A(9-11-13)	120.3	120.5
A(12-11-13)	119.5	119.8
A(11-13-14)	120.4	119.9
A(11-13-15)	120.4	120.2
A(14-13-15)	119.2	119.9
A(13-15-16)	120	120.2
A(15-16-17)	126.4	126.3
A(16-17-18)	121.7	118.9
A(16-17-19)	121.4	122.1
A(18-17-19)	116.9	118.9
A(17-19-20)	117	116.9

A(19-20-21)	120	119.7
A(19-20-22)	120.4	121.2
A(21-20-22)	119.6	119.1
A(20-22-23)	123.5	122.6
A(22-23-24)	120	119.9
A(22-23-32)	120.2	120.9
A(24-23-32)	119.7	119.3
A(23-24-25)	119.8	119.8
A(23-24-26)	120.1	120.3
A(23-32-30)	120	119.6
A(23-32-33)	119.9	120.2
A(25-24-26)	120.2	119.8
A(24-26-27)	119.7	119.9
A(24-26-28)	120.2	120.2
A(27-26-28)	120.2	119.9
A(26-28-29)	120.1	120
A(26-28-30)	119.8	120
A(29-28-30)	120.1	120
A(28-30-31)	120.2	119.7
A(28-30-32)	120.2	120.6
A(31-30-32)	119.6	119.7
A(30-32-33)	120.1	120.2
A(35-34-36)	107.8	108
A(35-34-71)	110.1	109.3
A(36-34-71)	109.3	109.3
A(34-71-41)	110.7	111.7
A(34-71-72)	110.1	109.3
A(34-71-73)	109.3	109.3
A(38-56-54)	119.8	119.8
A(38-56-57)	123.2	123.2
A(39-58-40)	114.9	114
A(39-58-57)	128.7	128.9
A(53-40-58)	123.9	123
A(40-53-52)	112.4	112.6
A(40-53-54)	121.2	121
A(40-58-57)	116.3	117.1
A(59-41-71)	127.9	126.2
A(59-41-74)	111.7	115.6
A(41-59-57)	119	119.9
A(41-59-60)	117.5	117.5
A(71-41-74)	120.2	118.1
A(41-71-72)	110.2	109.3
A(41-71-73)	108.8	109.3
A(43-42-44)	119.3	119.8
A(43-42-52)	120.2	119.8
A(44-42-52)	120.5	120.3

A(42-44-45)	119.6	120
A(42-44-46)	120.3	120
A(42-52-50)	118.8	118.9
A(42-52-53)	121.2	120.9
A(45-44-46)	120.1	120
A(44-46-47)	120.1	119.9
A(44-46-48)	119.6	120.1
A(47-46-48)	120.2	119.9
A(46-48-49)	120.1	119.8
A(46-48-50)	120.3	120.5
A(49-48-50)	119.5	119.8
A(48-50-51)	120.4	119.9
A(48-50-52)	120.4	120.2
A(51-50-52)	119.2	119.9
A(50-52-53)	120	120.2
A(52-53-54)	126.4	126.3
A(53-54-55)	121.7	118.9
A(53-54-56)	121.4	122.1
A(55-54-56)	116.9	118.9
A(54-56-57)	117	116.9
A(56-57-58)	120	119.7
A(56-57-59)	120.4	121.2
A(58-57-59)	119.6	119.1
A(57-59-60)	123.5	122.6
A(59-60-61)	120	119.9
A(59-60-69)	120.2	120.9
A(61-60-69)	119.7	119.3
A(60-61-62)	119.8	119.8
A(60-61-63)	120.1	120.3
A(60-69-67)	120	119.6
A(60-69-70)	119.9	120.2
A(62-61-63)	120.2	119.8
A(61-63-64)	119.7	119.9
A(61-63-65)	120.2	120.2
A(64-63-65)	120.2	119.9
A(63-65-66)	120.1	120
A(63-65-67)	119.8	120
A(66-65-67)	120.1	120
A(65-67-68)	120.2	119.7
A(65-67-69)	120.2	120.6
A(68-67-69)	119.6	119.7
A(67-69-70)	120.1	120.2
A(72-71-73)	107.8	108

[a]Atom numbering refer to **Fig. 9**

Table S8 The calculated geometric parameters of **6**[a].

Parameter	Calc	Exp
R(1-20)	1.315	1.32
R(3-22)	1.198	1.206
R(4-17)	1.344	1.36
R(4-22)	1.432	1.401
R(5-23)	1.249	1.247
R(6-8)	1.39	1.389
R(6-16)	1.403	1.394
R(8-10)	1.393	1.388
R(10-12)	1.395	1.383
R(12-14)	1.388	1.39
R(14-16)	1.404	1.403
R(16-17)	1.472	1.467
R(17-18)	1.36	1.345
R(18-20)	1.42	1.419
R(20-21)	1.413	1.402
R(21-22)	1.449	1.444
R(21-23)	1.466	1.459
R(23-24)	1.491	1.488
R(24-25)	1.401	1.4
R(24-33)	1.399	1.393
R(25-27)	1.389	1.383
R(27-29)	1.394	1.384
R(29-31)	1.394	1.391
R(31-33)	1.39	1.387
A(2-1-20)	105.5	109.5
A(1-2-5)	150.3	146.8
A(1-20-18)	116.5	116.2
A(1-20-21)	122.3	122.3
A(2-5-23)	103.9	102.3
A(3-22-4)	114.7	114.3
A(3-22-21)	130	129
A(17-4-22)	124.4	123.6
A(4-17-16)	113.3	112.4
A(4-17-18)	120.6	120.7
A(17-4-7)	88.8	86.6
A(4-22-21)	115.3	116.7
A(22-4-7)	145.1	149.8
A(5-23-21)	119	119.3
A(5-23-24)	116.7	116.7
A(7-6-8)	120.5	119.8
A(7-6-16)	119.2	119.9
A(6-7-4)	97.4	100.4

A(8-6-16)	120.3	120.3
A(6-8-9)	119.6	119.8
A(6-8-10)	120.3	120.4
A(6-16-14)	119	119.1
A(6-16-17)	119.9	120.7
A(9-8-10)	120.1	119.8
A(8-10-11)	120.2	120.2
A(8-10-12)	119.8	119.7
A(11-10-12)	120.1	120.2
A(10-12-13)	120.1	119.7
A(10-12-14)	120.2	120.6
A(13-12-14)	119.7	119.7
A(12-14-15)	119.2	120
A(12-14-16)	120.4	120
A(15-14-16)	120.3	120
A(14-16-17)	121.2	120.2
A(16-17-18)	126.1	126.9
A(17-18-19)	122.3	120.3
A(17-18-20)	119.4	119.3
A(19-18-20)	118.3	120.4
A(18-20-21)	121.2	121.4
A(20-21-22)	118.5	118
A(20-21-23)	118.1	119.1
A(22-21-23)	123.2	122.7
A(21-23-24)	124.3	124
A(23-24-25)	117.5	117.3
A(23-24-33)	122.9	122.8
A(25-24-33)	119.3	119.7
A(24-25-26)	118.9	119.8
A(24-25-27)	120.4	120.3
A(24-33-31)	120.2	119.4
A(24-33-34)	120.3	120.3
A(26-25-27)	120.7	119.8
A(25-27-28)	119.9	120
A(25-27-29)	119.9	119.9
A(28-27-29)	120.2	120.1
A(27-29-30)	120.1	120.1
A(27-29-31)	119.9	119.8
A(30-29-31)	120	120.1
A(29-31-32)	120.1	119.6
A(29-31-33)	120.2	120.8
A(32-31-33)	119.7	119.6
A(31-33-34)	119.5	120.3

[a]Atom numbering refer to **Fig. 9**

Table S9 Natural charges (NC) at the different atomic sites in the studied molecules[a].

Atom	NC	Atom	NC	Atom	NC	Atom	NC	Atom	NC	Atom	NC
1		**2**		**3**		**4**		**5**		**6**	
O1	-0.5242	O1	-0.6413	O1	-0.5250	O1	-0.6479	O1	-0.6465	O1	-0.6328
O2	-0.5773	O2	-0.5803	O2	-0.5821	O2	-0.5815	O2	-0.5770	H2	0.4938
O3	-0.6433	N3	-0.7580	O3	-0.6487	O3	-0.5249	O3	-0.5238	O3	-0.5632
O4	-0.5169	O4	-0.5247	N4	-0.5493	N4	-0.5496	N4	-0.5636	O4	-0.5303
N5	-0.5486	C5	-0.2009	H5	0.4650	C5	-0.2025	C5	-0.2017	O5	-0.6296
H6	0.4726	H6	0.2632	C6	-0.2030	H6	0.2405	H6	0.2408	C6	-0.1574
C7	-0.2030	C7	-0.2345	H7	0.2406	C7	-0.2370	C7	-0.2366	H7	0.2268
H8	0.2416	H8	0.2445	C8	-0.2371	H8	0.2432	H8	0.2441	C8	-0.1916
C9	-0.2367	C9	-0.2226	H9	0.2431	C9	-0.2236	C9	-0.2217	H9	0.2074
H10	0.2436	H10	0.2424	C10	-0.2240	H10	0.2419	H10	0.2427	C10	-0.1743
C11	-0.2230	C11	-0.2366	H11	0.2417	C11	-0.2347	C11	-0.2344	H11	0.2051
H12	0.2422	H12	0.2438	C12	-0.2347	H12	0.2440	H12	0.2448	C12	-0.1940
C13	-0.2346	C13	-0.2026	H13	0.2439	C13	-0.2016	C13	-0.2004	H13	0.2065
H14	0.2444	H14	0.2415	C14	-0.2017	H14	0.2636	H14	0.2637	C14	-0.1642
C15	-0.2009	C15	-0.1040	H15	0.2634	C15	-0.1032	C15	-0.1050	H15	0.2042
H16	0.2632	C16	0.3867	C16	-0.1028	C16	0.3865	C16	0.3900	C16	-0.1083
C17	-0.1038	C17	-0.3731	C17	0.3861	C17	-0.3712	C17	-0.3730	C17	0.4327
C18	0.3883	H18	0.2571	C18	-0.3713	H18	0.2552	H18	0.2568	C18	-0.3532
C19	0.7922	C19	0.4914	H19	0.2551	C19	0.4869	C19	0.4882	H19	0.2324
C20	-0.3503	C20	-0.3618	C20	0.4863	C20	-0.3579	C20	-0.3546	C20	0.4787
C21	0.4854	C21	0.7948	C21	-0.3581	C21	0.7934	C21	0.7954	C21	-0.3808
C22	-0.3731	C22	0.3436	C22	0.7929	C22	0.3496	C22	0.3514	C22	0.7901
H23	0.2572	C23	-0.0896	C23	0.3525	C23	-0.0877	C23	-0.0935	C23	0.5637
C24	0.3468	C24	-0.2260	C24	-0.0876	C24	-0.2127	C24	-0.2131	C24	-0.1223
C25	-0.0921	H25	0.2460	C25	-0.2122	H25	0.2468	H25	0.2474	C25	-0.1521
C26	-0.2039	C26	-0.2337	H26	0.2456	C26	-0.2272	C26	-0.2267	H26	0.2158
H27	0.2486	H27	0.2445	C27	-0.2273	H27	0.2436	H27	0.2452	C27	-0.2019
C28	-0.2309	C28	-0.2226	H28	0.2432	C28	-0.2332	C28	-0.2322	H28	0.2034
H29	0.2439	H29	0.2435	C29	-0.2338	H29	0.2422	H29	0.2434	C29	-0.1740
C30	-0.2288	C30	-0.2305	H30	0.2419	C30	-0.2269	C30	-0.2275	H30	0.2015
H31	0.2417	H31	0.2459	C31	-0.2270	H31	0.2433	H31	0.2433	C31	-0.1995
C32	-0.2296	C32	-0.1836	H32	0.2432	C32	-0.2126	C32	-0.2083	H32	0.2039
H33	0.2435	H33	0.2522	C33	-0.2114	H33	0.2455	H33	0.2479	C33	-0.1469
C34	-0.2053	H34	0.4231	H34	0.2458	C34	-0.2713	C34	-0.2778	H34	0.2103
H35	0.2479	H35	0.4620	C35	-0.0649	H35	0.2491	H35	0.2565		
C36	0.1107			H36	0.2554	H36	0.2407	H36	0.2483		
C37	-0.2230			C37	-0.4733	C37	-0.4726	H37	0.4674		
H38	0.2549			H38	0.2485	H38	0.2361	O38	-0.6465		
C39	-0.3132			H39	0.2369	H39	0.2443	O39	-0.5770		
H40	0.2458			C40	-0.4677	C40	-0.4667	O40	-0.5238		
C41	0.3203			H41	0.2481	H41	0.2436	N41	-0.5636		

C42	-0.3290	H42	0.2315	H42	0.2319	C42	-0.2017
H43	0.2070	C43	-0.4680	C43	-0.6919	H43	0.2408
H44	0.2342	H44	0.2451	H44	0.2280	C44	-0.2366
H45	0.2071	H45	0.2310	H45	0.2399	H45	0.2441
C46	-0.2677	C46	-0.4676	H46	0.2316	C46	-0.2217
H47	0.2549	H47	0.2314	H47	0.4671	H47	0.2427
C48	-0.2298	H48	0.2481			C48	-0.2344
H49	0.2508	C49	-0.4733			H49	0.2448
		H50	0.2369			C50	-0.2004
		H51	0.2485			H51	0.2637
						C52	-0.1050
						C53	0.3900
						C54	-0.3730
						H55	0.2568
						C56	0.4882
						C57	-0.3546
						C58	0.7954
						C59	0.3514
						C60	-0.0935
						C61	-0.2131
						H62	0.2474
						C63	-0.2267
						H64	0.2452
						C65	-0.2322
						H66	0.2434
						C67	-0.2275
						H68	0.2433
						C69	-0.2083
						H70	0.2479
						C71	-0.2778
						H72	0.2565
						H73	0.2483
						H74	0.4674

[a]Atom numbering refer to **Fig. 9**

Table S10 The calculated and experimental NMR chemical shifts of **1**[a].

Atom	Calc.	Exp.	Atom	Calc.	Exp.
C 7	114.215	127.12	H 6	15.657	15.43
C 9	116.623	129.5	H 8	8.231	7.93
C 11	119.272	128.55	H 10	7.934	7.55
C 13	116.68	129.5	H 12	7.95	7.55
C 15	114.631	127.12	H 14	7.92	7.55
C 17	119.766	129.88	H 16	8.358	7.93
C 18	151.174	172.86	H 23	6.668	6.79
C 19	148.81	160.57	H 27	7.981	7.36
C 20	91.754	97.53	H 29	7.955	7.31
C 21	170.596	184.49	H 31	7.903	7.31
C 22	94.268	104.59	H 33	7.773	7.31
C 24	159.015	158.36	H 35	7.464	7.36
C 25	122.989	131.98	H 38	6.734	6.94
C 26	117.932	128.24	H 40	6.721	6.79
C 28	116.398	129.55	H 43	3.777	3.69
C 30	117.306	131.22	H 44	4.191	3.69
C 32	116.38	129.55	H 45	3.821	3.69
C 34	114.679	128.24	H 47	7.189	6.79
C 36	117.796	129.56	H 49	7.535	6.94
C 37	115.023	126.35			
C 39	98.26	114.53			
C 41	144.671	133.4			
C 42	45.758	55.75			
C 46	105.506	114.53			
C 48	113.663	126.35			

[a]Atom numbering refer to **Fig. 9**

Table S11 The calculated and experimental NMR chemical shifts of **2**[a].

Atom	Calc.	Exp.	Atom	Calc.	Exp.
C 5	114.666	126.21	H 6	8.368	7.98
C 7	116.649	128.47	H 8	7.913	7.48
C 9	119.281	130.49	H 10	7.94	7.48
C 11	116.561	128.47	H 12	7.935	7.48
C 13	114.169	126.21	H 14	8.228	7.89
C 15	119.928	131.47	H 18	6.612	6.61
C 16	151.185	175.72	H 25	7.863	7.55
C 17	94.561	105.17	H 27	7.998	7.44
C 19	170.563	183.9	H 29	8.004	7.44
C 20	90.233	95.8	H 31	7.849	7.44
C 21	149.468	162.14	H 33	7.885	7.55
C 22	162.827	159.85	H 34	5.995	10
C 23	126.34	136.7	H 35	12.928	12.25
C 24	113.911	127.76			
C 26	116.794	129.49			
C 28	118.679	131.71			
C 30	115.488	129.49			
C 32	117.007	127.76			

[a]Atom numbering refer to **Fig. 9**

Table S12 The calculated and experimental NMR chemical shifts of **3**[a].

Atom	Calc.	Exp.	Atom	Calc.	Exp.
C 6	113.851	126.21	H 5	14.195	14.17
C 8	116.538	129.49	H 7	8.178	7.86
C 10	118.974	129.61	H 9	7.895	7.51
C 12	116.583	129.49	H 11	7.906	7.35
C 14	114.391	126.21	H 13	7.881	7.51
C 16	119.967	131.38	H 15	8.293	7.86
C 17	150.761	173.37	H 19	6.583	6.63
C 18	94.564	104.77	H 26	7.678	7.54
C 20	170.361	184.32	H 28	7.981	7.51
C 21	90.949	96.34	H 30	7.958	7.37
C 22	148.953	161.39	H 32	7.972	7.51
C 23	161.762	160.14	H 34	7.652	7.54
C 24	124.843	133.69	H 36	3.174	3.17
C 25	113.4	128.96	H 38	1.974	1.64
C 27	116.331	126.44	H 39	1.669	1.73
C 29	116.104	131.76	H 41	1.857	1.45
C 31	116.339	126.44	H 42	1.361	1.11
C 33	113.322	128.96	H 44	1.671	1.11
C 35	47.85	53.67	H 45	1.484	1.45
C 37	27.014	32.7	H 47	1.376	1.45
C 40	19.054	24.89	H 48	1.864	1.26
C 43	19.117	23.72	H 50	1.681	1.73
C 46	19.045	23.72	H 51	2	1.64
C 49	27	32.7			

[a]Atom numbering refer to **Fig. 9**

Table S13 The calculated and experimental NMR chemical shifts of **4**[a].

Atom	Calc.	Exp.	Atom	Calc.	Exp.
C 5	113.498	125.82	H 6	8.157	7.82
C 7	116.131	128.79	H 8	7.826	7.44
C 9	118.576	129.45	H 10	7.825	7.44
C 11	116.472	128.79	H 12	7.836	7.44
C 13	114.677	125.82	H 14	8.378	7.82
C 15	119.99	131.36	H 18	6.579	6.45
C 16	150.475	174.94	H 25	7.586	7.52
C 17	94.205	104.44	H 27	7.935	7.26
C 19	170.391	185.05	H 29	7.892	7.52
C 20	91.372	96.8	H 31	7.935	7.26
C 21	148.089	162.12	H 33	7.628	7.52
C 22	162.726	160.94	H 35	3.35	3.2
C 23	124.188	133.43	H 36	3.018	3.2
C 24	113.652	126.01	H 38	1.576	1.59
C 26	116.237	128.88	H 39	1.942	1.59
C 28	116.009	131.12	H 41	1.725	1.37
C 30	116.225	128.88	H 42	1.516	1.37
C 32	113.223	126.01	H 44	0.739	0.9
C 34	36.935	45.19	H 45	1.039	0.9
C 37	26.495	31.77	H 46	0.561	0.9
C 40	15.306	20	H 47	14.346	14.12
C 43	5.675	13.57			

[a]Atom numbering refer to **Fig. 9**

Table S14 The calculated and experimental NMR chemical shifts of **5**[a].

Atom	Calc.	Exp.	Atom	Calc.	Exp.
C 5	113.693	125.8	H 6	8.1	7.82
C 7	116.178	126.12	H 8	7.822	7.47
C 9	118.779	129.75	H 10	7.852	7.47
C 11	116.504	126.12	H 12	7.833	7.47
C 13	114.839	125.8	H 14	8.338	7.82
C 15	119.466	131.39	H 18	6.528	6.49
C 16	150.821	176.03	H 25	7.525	7.07
C 17	93.766	104.23	H 27	7.932	7.47
C 19	170.544	185.33	H 29	7.957	7.47
C 20	91.778	97.64	H 31	7.91	7.47
C 21	147.745	161.57	H 33	7.04	7.07
C 22	163.292	161.52	H 35	3.068	3.39
C 23	123.178	132.6	H 36	3.36	3.39
C 24	113.633	129.75	H 37	14.313	14.34
C 26	116.285	128.85	H 43	8.1	7.82
C 28	116.332	131.14	H 45	7.822	7.47
C 30	116.776	128.85	H 47	7.852	7.47
C 32	113.397	129.75	H 49	7.833	7.47
C 34	37.035	44.65	H 51	8.338	7.82
C 42	113.693	125.8	H 55	6.528	6.49
C 44	116.178	126.12	H 62	7.525	7.07
C 46	118.779	129.75	H 64	7.932	7.47
C 48	116.504	126.12	H 66	7.957	7.47
C 50	114.839	125.8	H 68	7.91	7.47
C 52	119.466	131.39	H 70	7.04	7.07
C 53	150.821	176.03	H 72	3.068	3.39
C 54	93.766	104.23	H 73	3.36	3.39
C 56	170.544	185.33	H 74	14.313	14.34
C 57	91.778	97.64			
C 58	147.745	161.57			
C 59	163.292	161.52			
C 60	123.178	132.6			
C 61	113.633	129.75			
C 63	116.285	128.85			
C 65	116.332	131.14			
C 67	116.776	128.85			
C 69	113.397	129.75			
C 71	37.035	44.65			

[a]Atom numbering refer to **Fig. 9**

Table S15 The calculated and experimental NMR chemical shifts of **6**[a].

Atom	Calc.	Exp.	Atom	Calc.	Exp.
C 6	115.825	126.03	H 2	16.931	-
C 8	117.07	129.05	H 7	8.525	7.92
C 10	121.279	130.97	H 9	7.987	7.63
C 12	116.993	129.05	H 11	8.047	7.53
C 14	115.24	126.03	H 13	7.997	7.63
C 16	118.656	132.22	H 15	8.322	7.92
C 17	156.712	161.22	H 19	6.914	6.92
C 18	87.52	102.58	H 26	8.163	7.89
C 20	167.603	170.91	H 28	7.96	7.53
C 21	91.641	98.47	H 30	8.008	7.66
C 22	147.438	161.83	H 32	7.787	7.53
C 23	187.808	193.4	H 34	8.1	7.89
C 24	127.118	137.72			
C 25	117.171	129.34			
C 27	115.759	129.76			
C 29	120.149	133.76			
C 31	114.296	129.76			
C 33	117.863	129.34			

[a]Atom numbering refer to **Fig. 9**

Table S16 Calculated energies and thermodynamic parameters for the suggested isomers of the studied pyran-2,4-dione[a].

Parameter	1(A)	1(B)	2(A)	2(B)	3(A)	3(B)	5[b]	6(A)	6(B)
E	-2025.8269	-2025.8129	-1319.7818	-1319.7760	-1208.8964	-1208.8883	-1131.4663	-994.3045	-994.0749
ZPVE	0.5752	0.5711	0.3821	0.3804	0.4200	0.4175	0.3829	0.2555	0.2565
E_{tot}	-2025.2517	-2025.2418	-1319.3997	-1319.3956	-1208.4764	-1208.4708	-1131.0835	-994.0489	-993.8184
ΔE	-6.2317		-2.5890		-3.5193		-0.0006	-144.6943	
H	-2025.2134	-2025.2035	-1319.3740	-1319.3699	-1208.4519	-1208.4463	-1131.0593	-994.0309	-993.8004
ΔG	-2025.3291	-2025.3188	-1319.4577	-1319.4531	-1208.5337	-1208.5290	-1131.1402	-994.0960	-993.8652
G	-6.4307		-2.8583		-2.9568		-0.0144	-144.8091	
S	243.5410	242.6320	176.1590	175.1160	172.2040	174.0650	170.2430	137.0620	136.5440

[a] All values in A.U except ΔE and ΔG are in kcal/mole while S in Cal/Mol.K

[b] Geomerty optimization of **5(B)** returned to the same optimized structure of **5(A)**