

Supplementary Material – II

Antimalarials with benzothiophene moieties as aminoquinoline partners

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jelena.srbljanovic@imi.bg.ac.rs (J.S.); olgicadj@imi.bg.ac.rs (O.DjDj.)

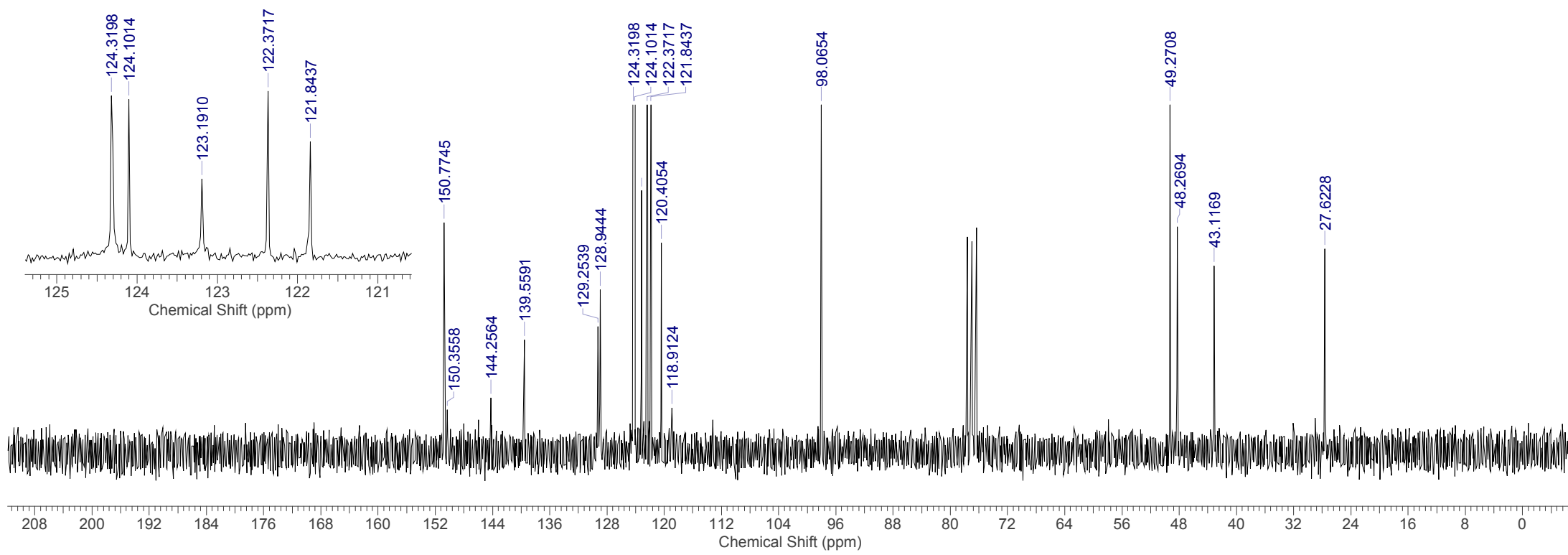
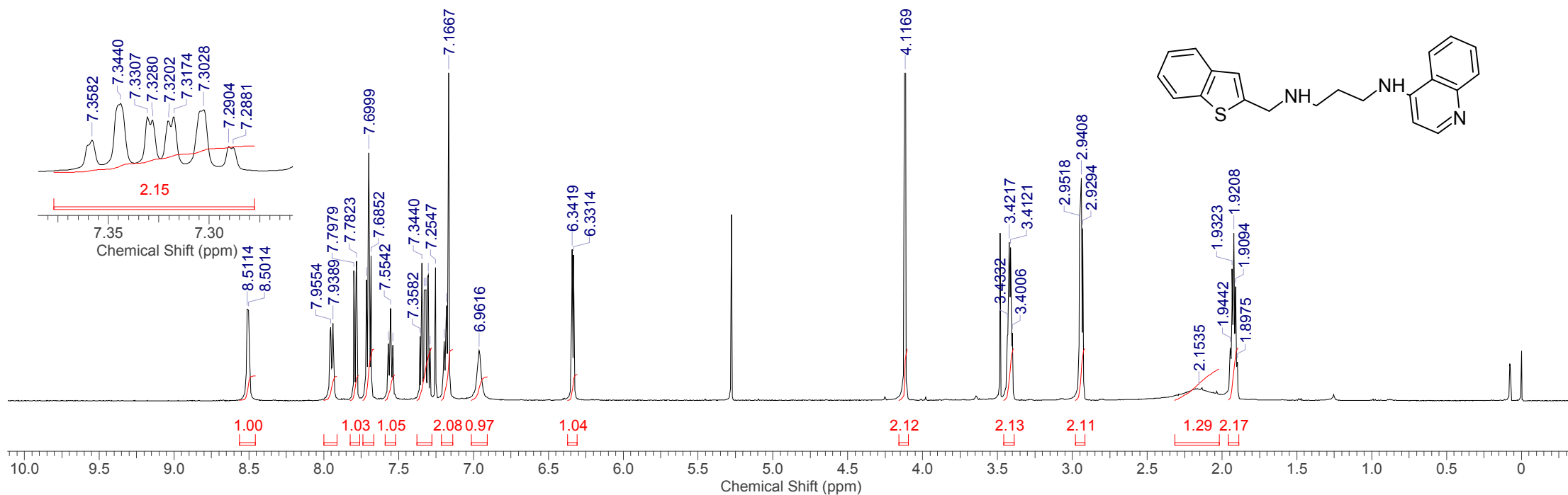
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* Correspondence: bsolaja@chem.bg.ac.rs; Tel.: +381-11-263-86-06

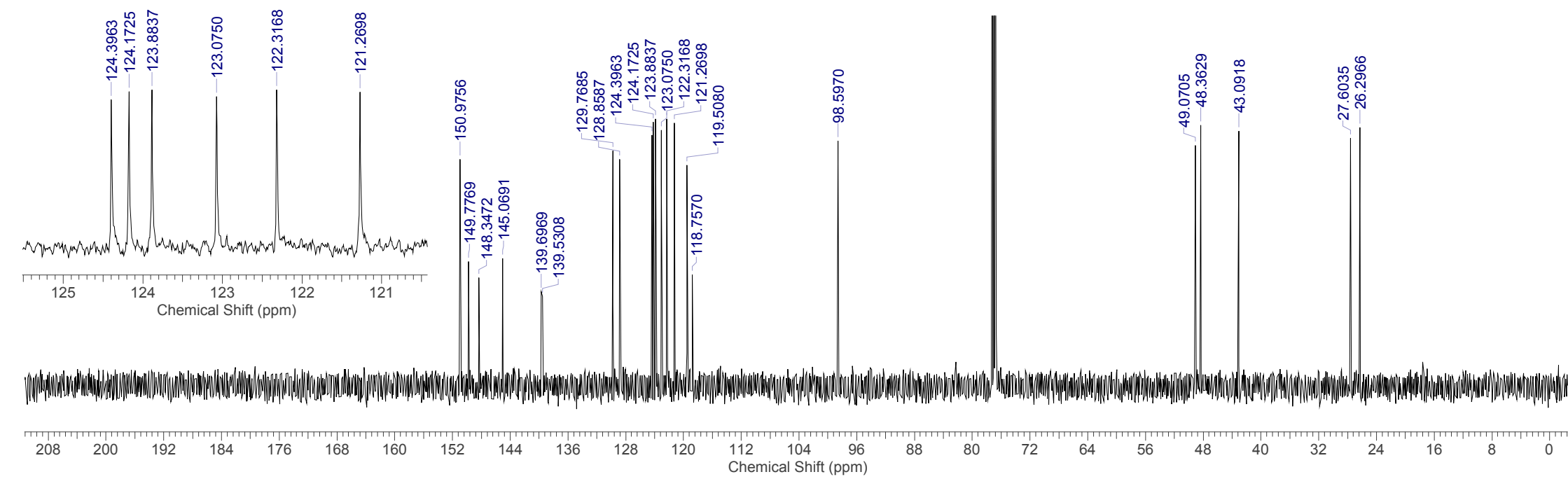
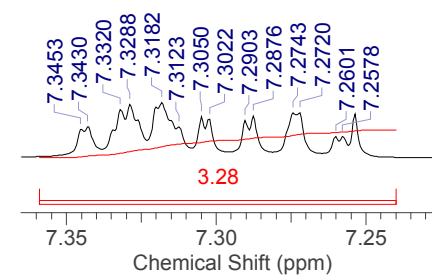
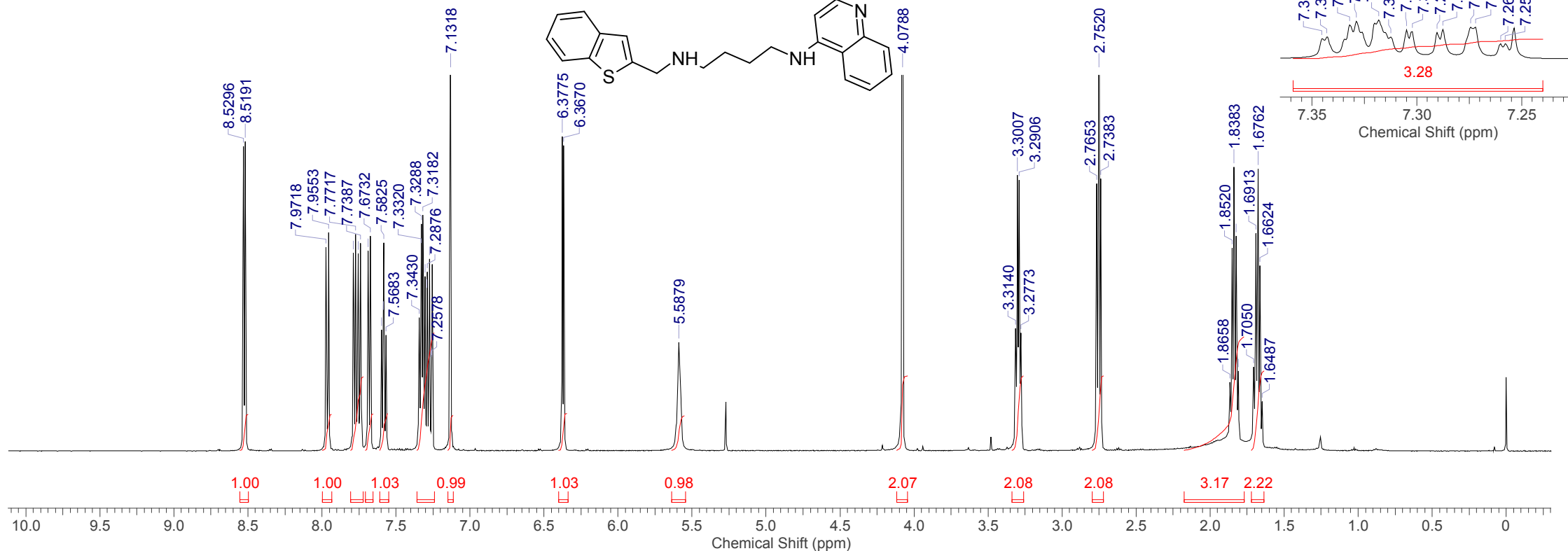
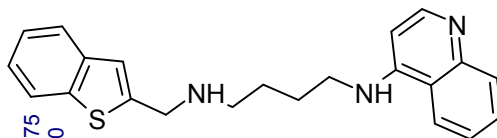
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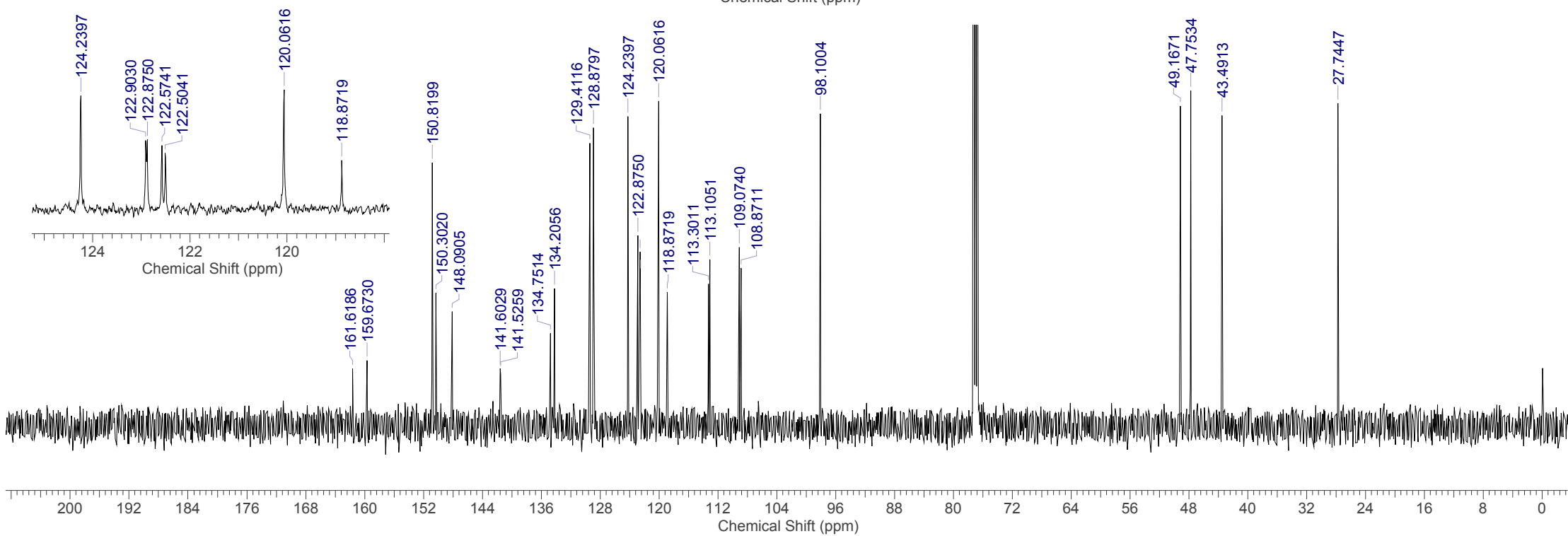
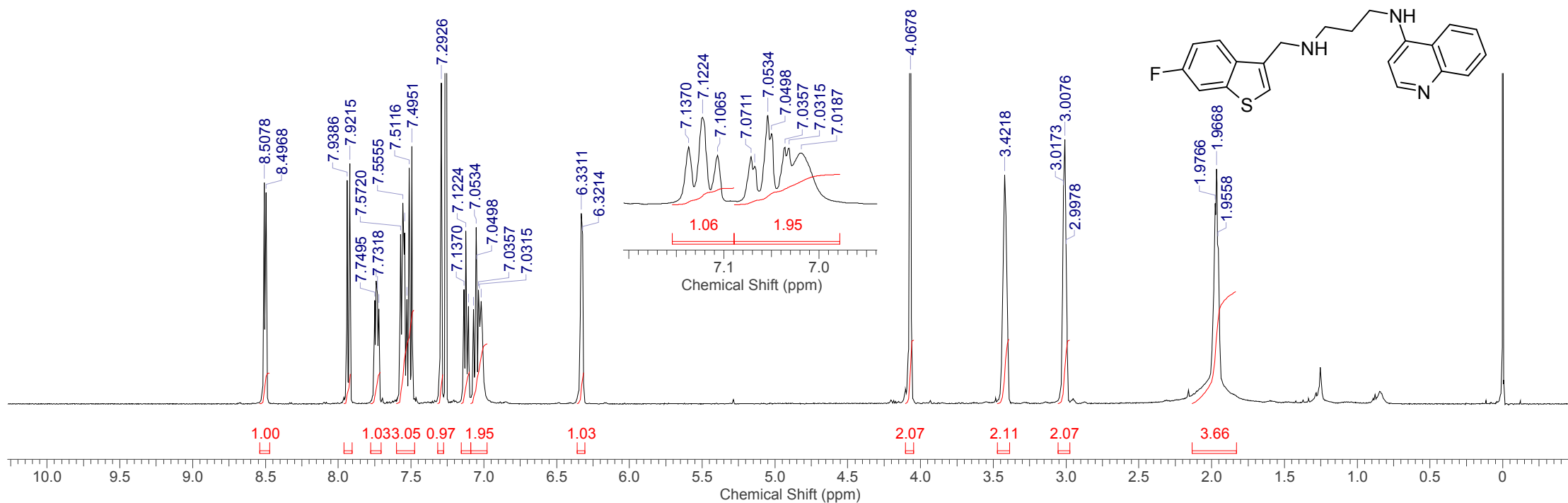
***N*-(1-benzothien-2-ylmethyl)-*N'*-quinolin-4-ylpropane-1,3-diamine (8)**



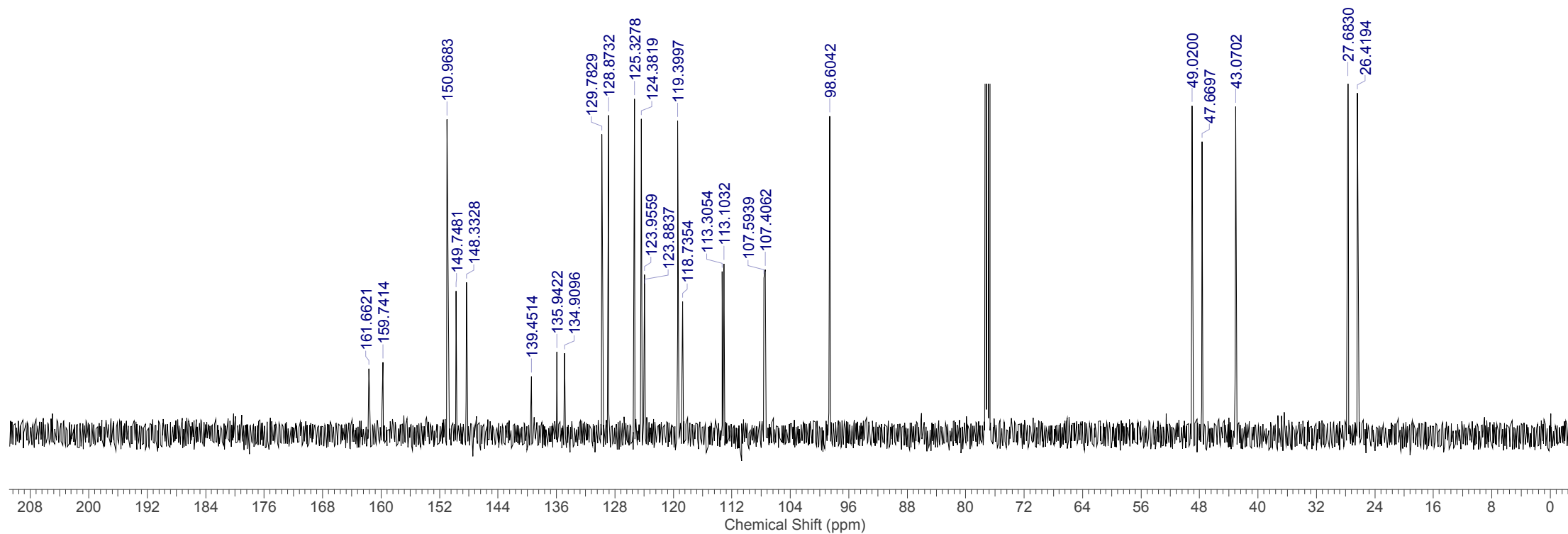
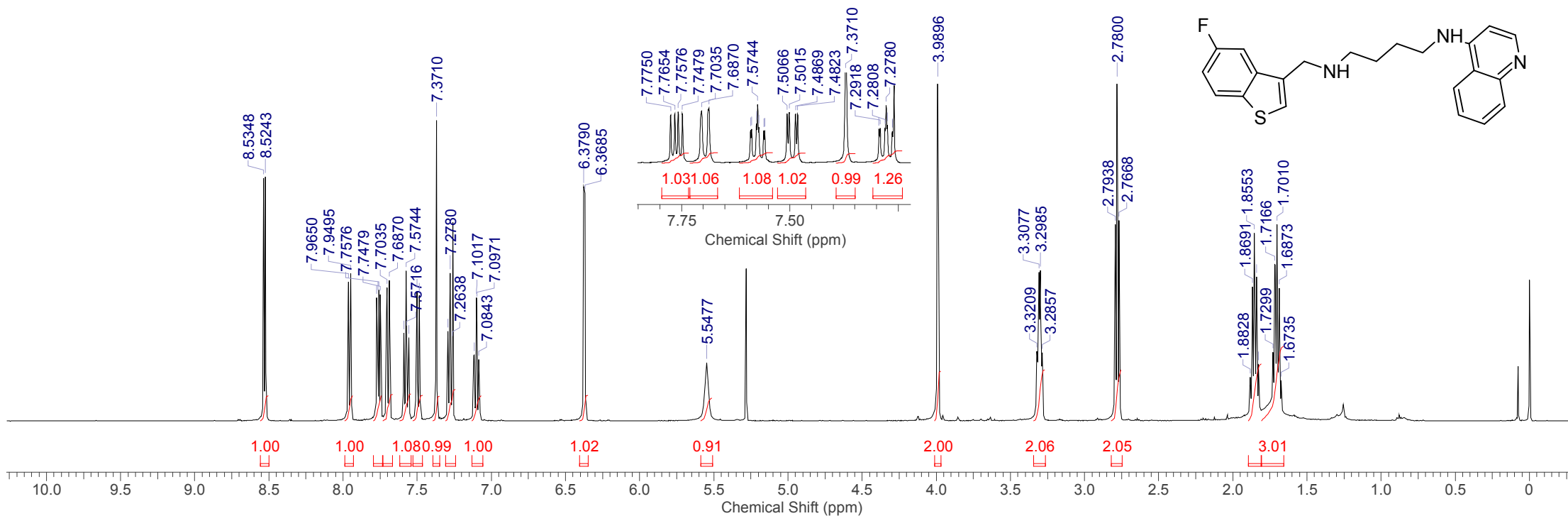
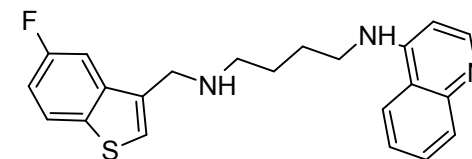
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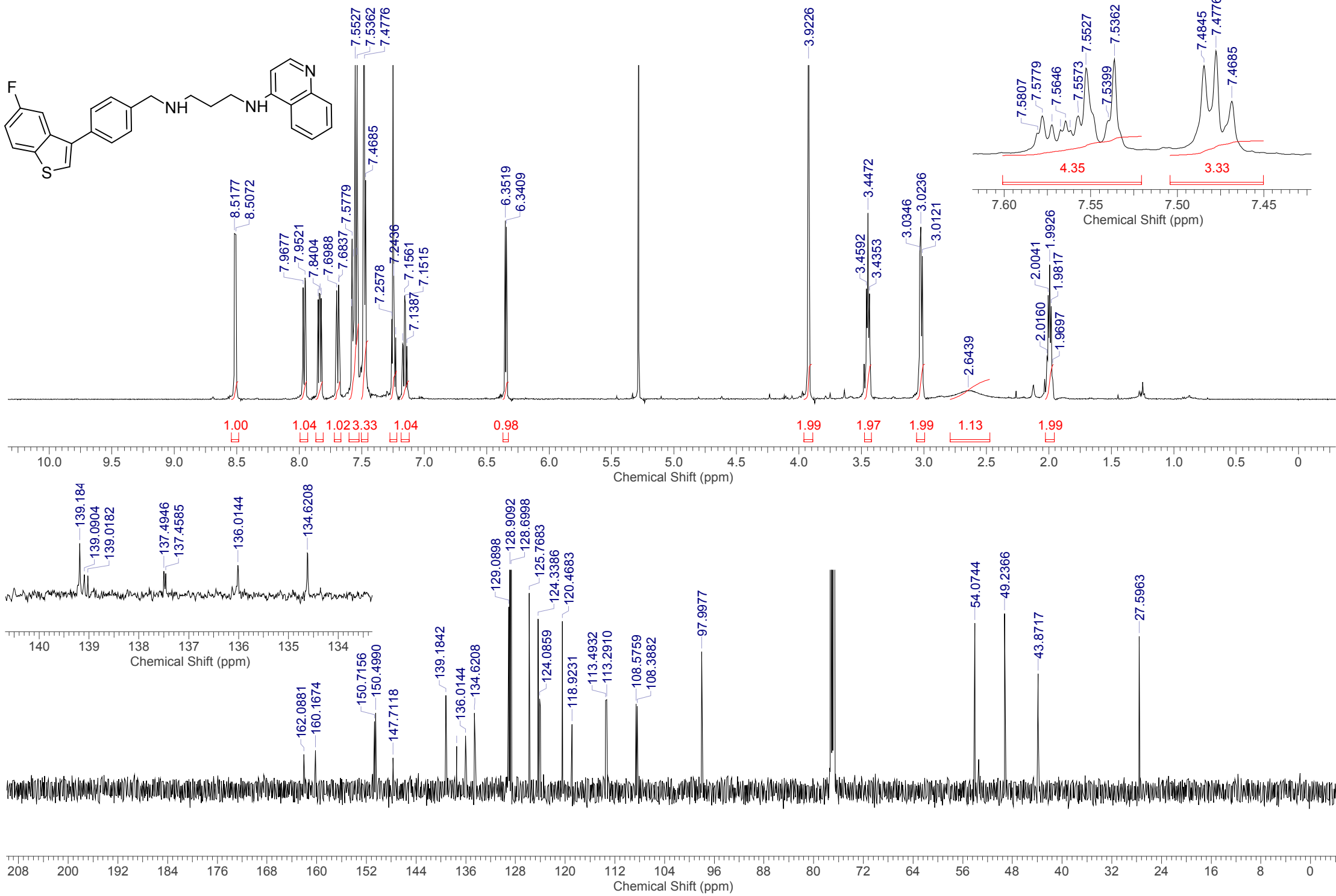
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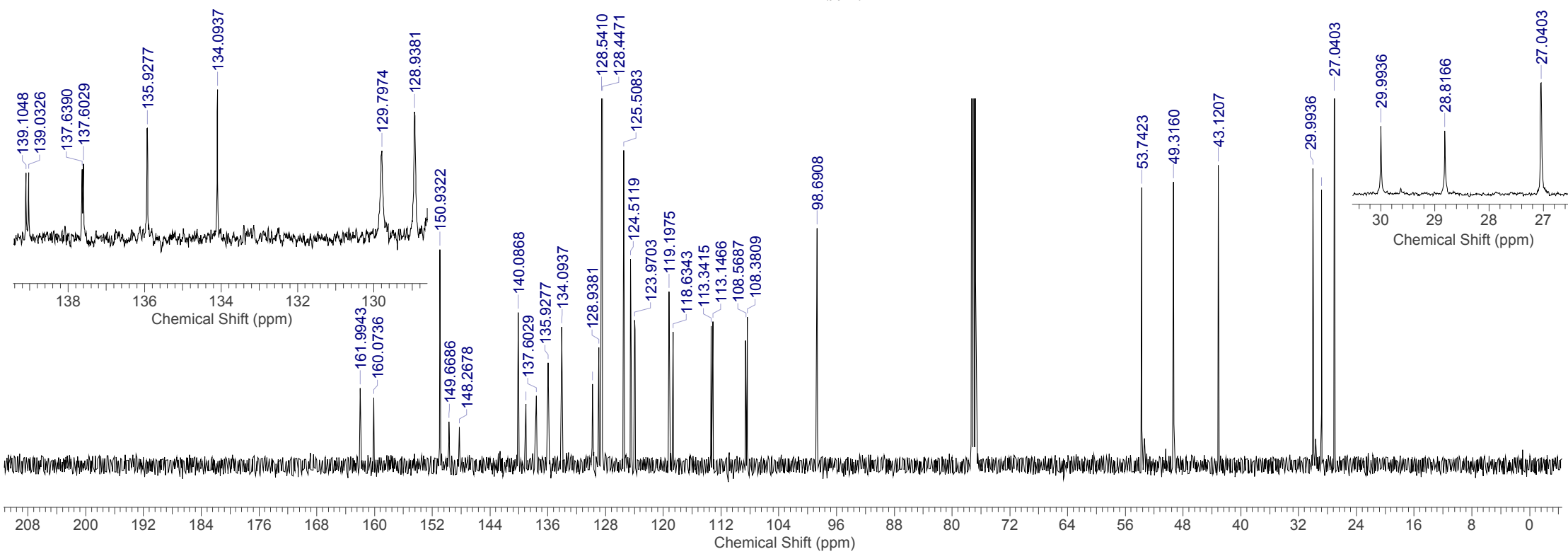
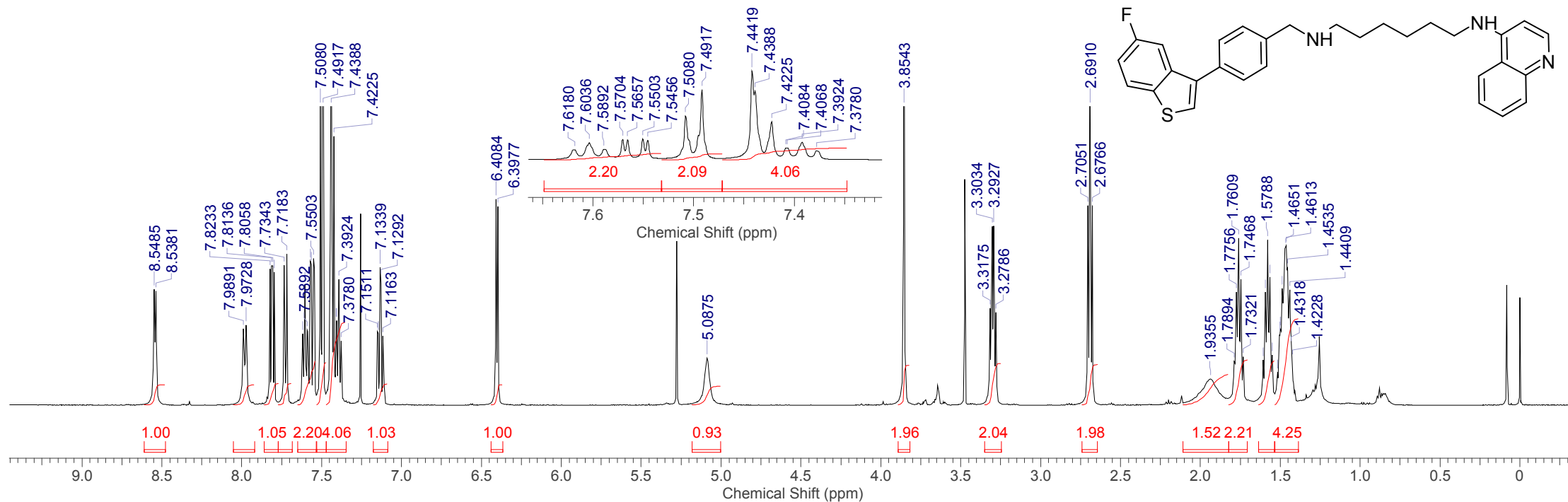
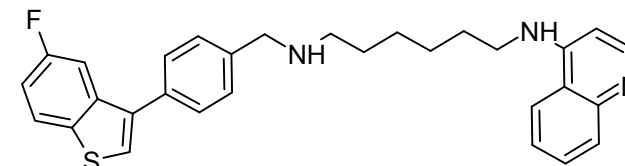
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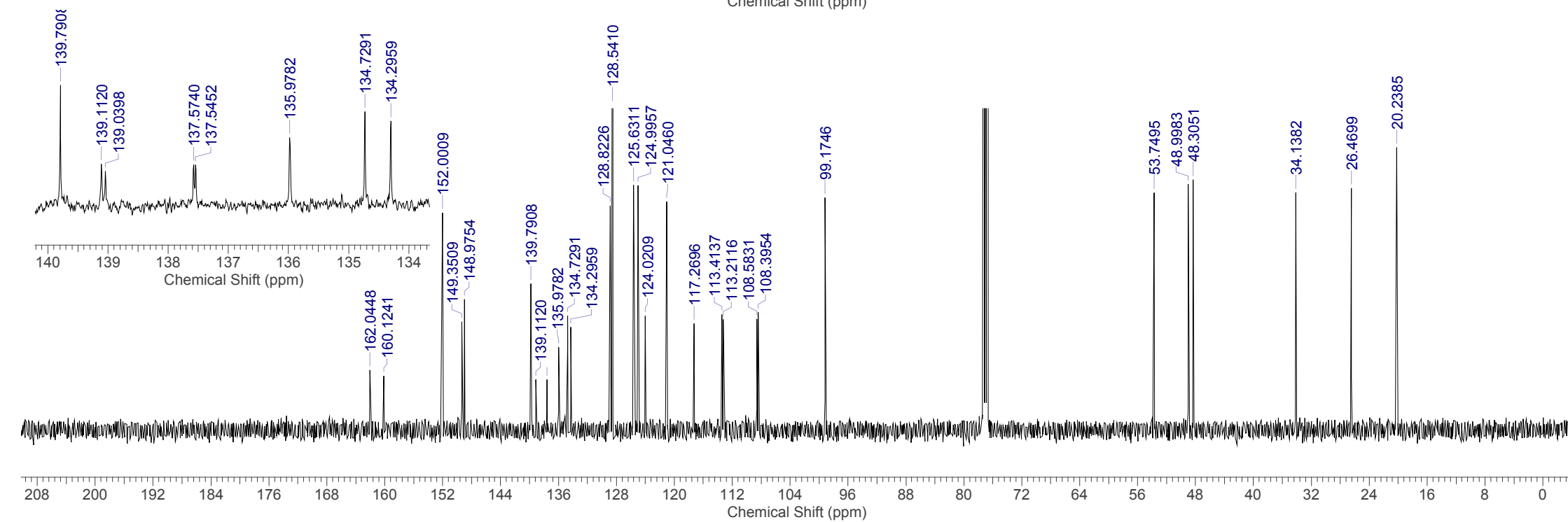
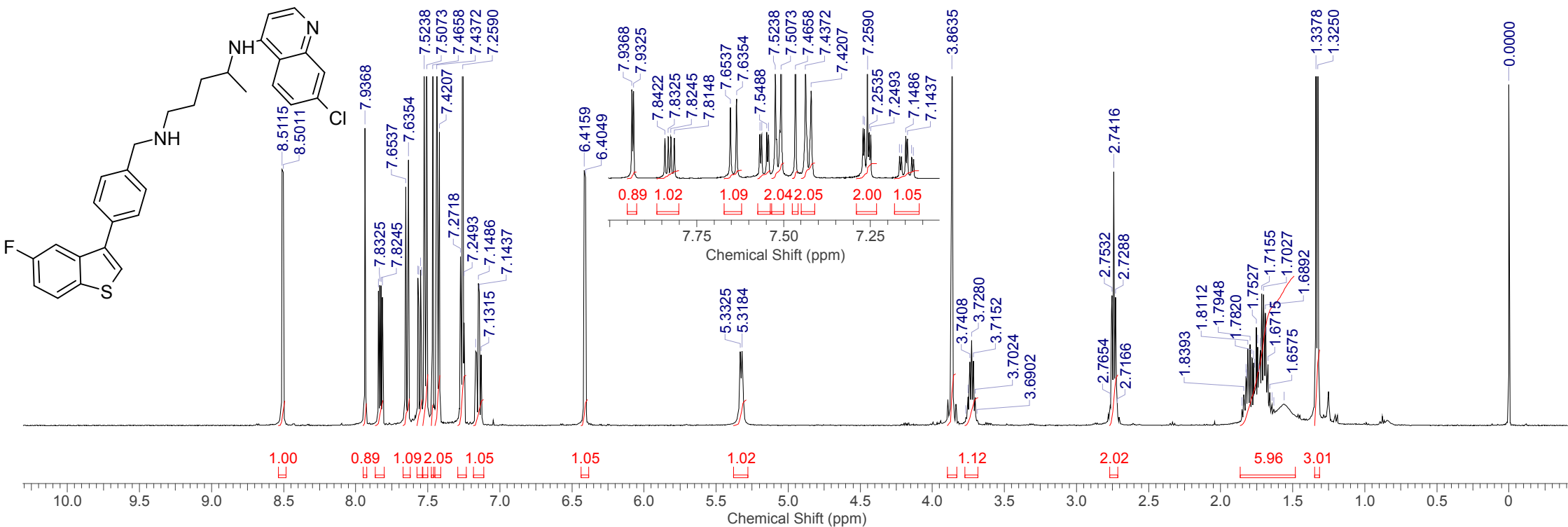
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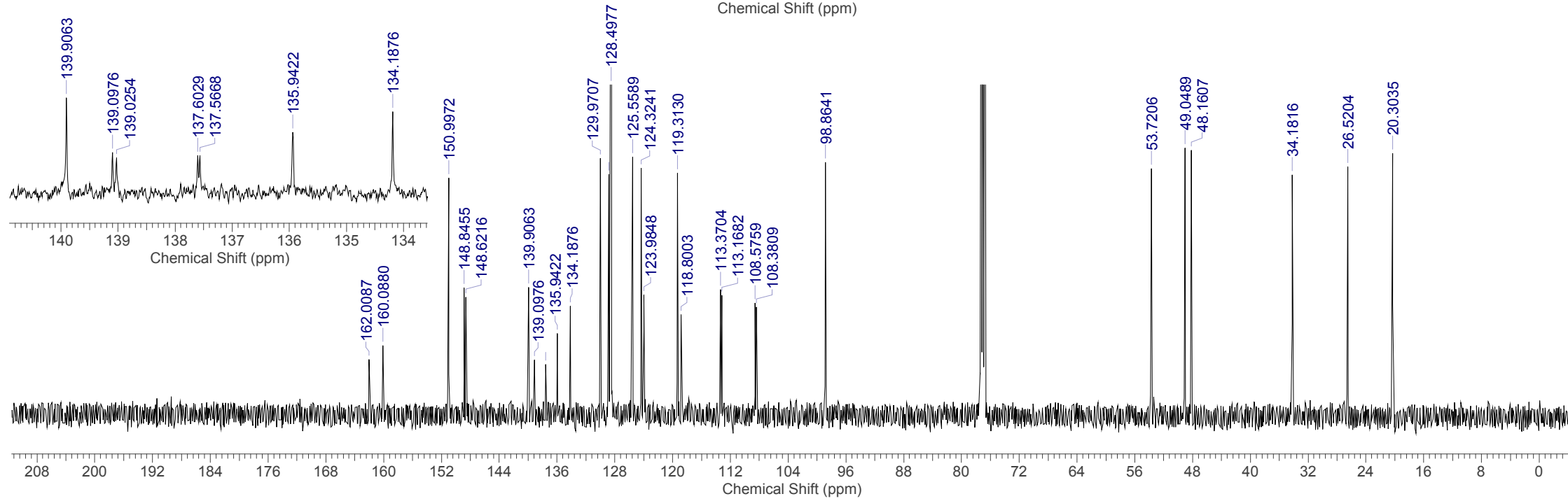
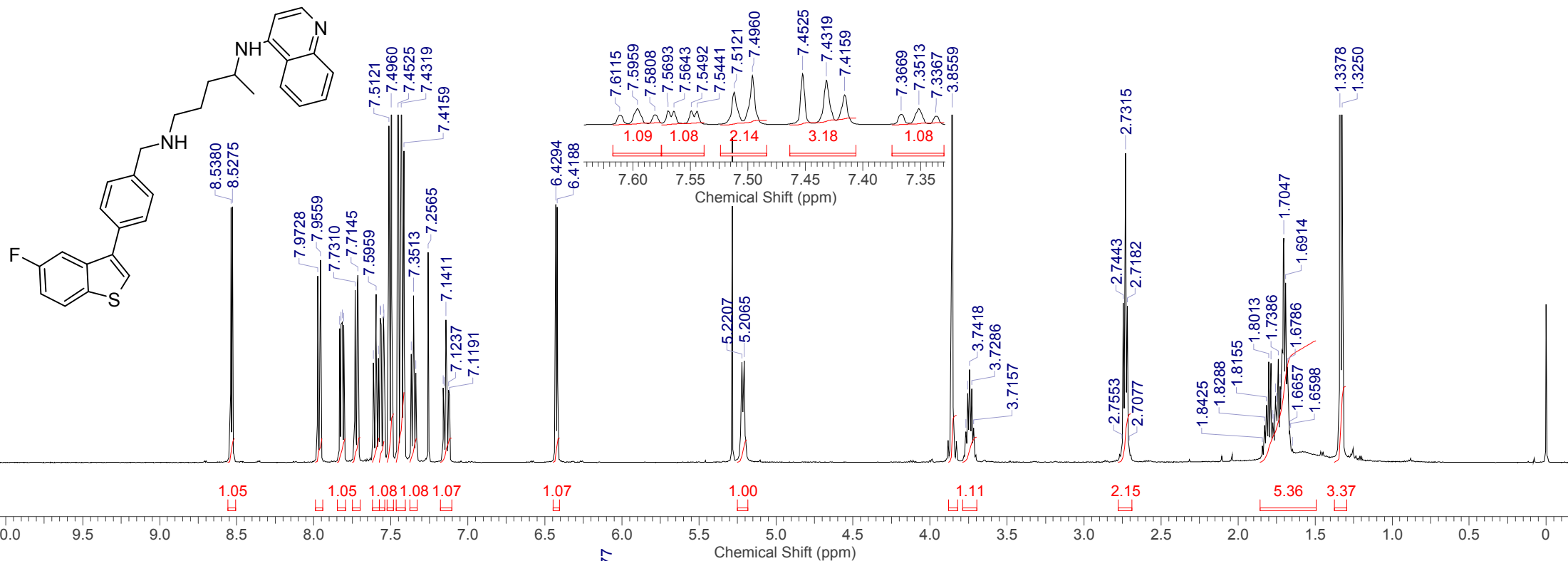
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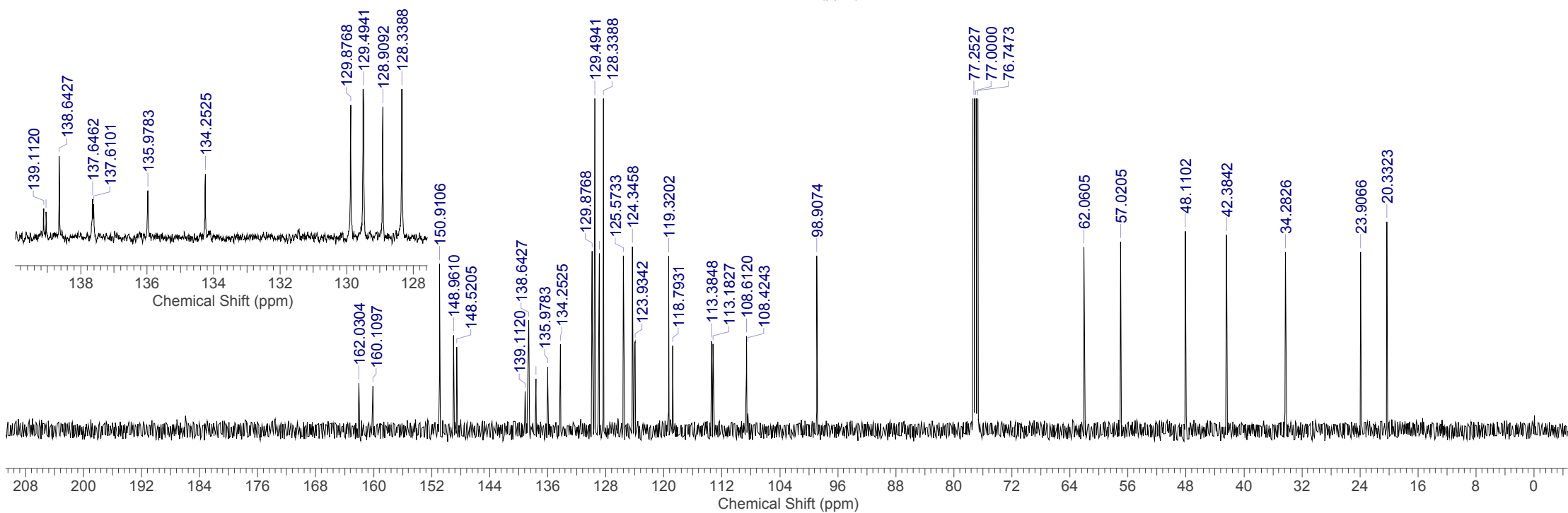
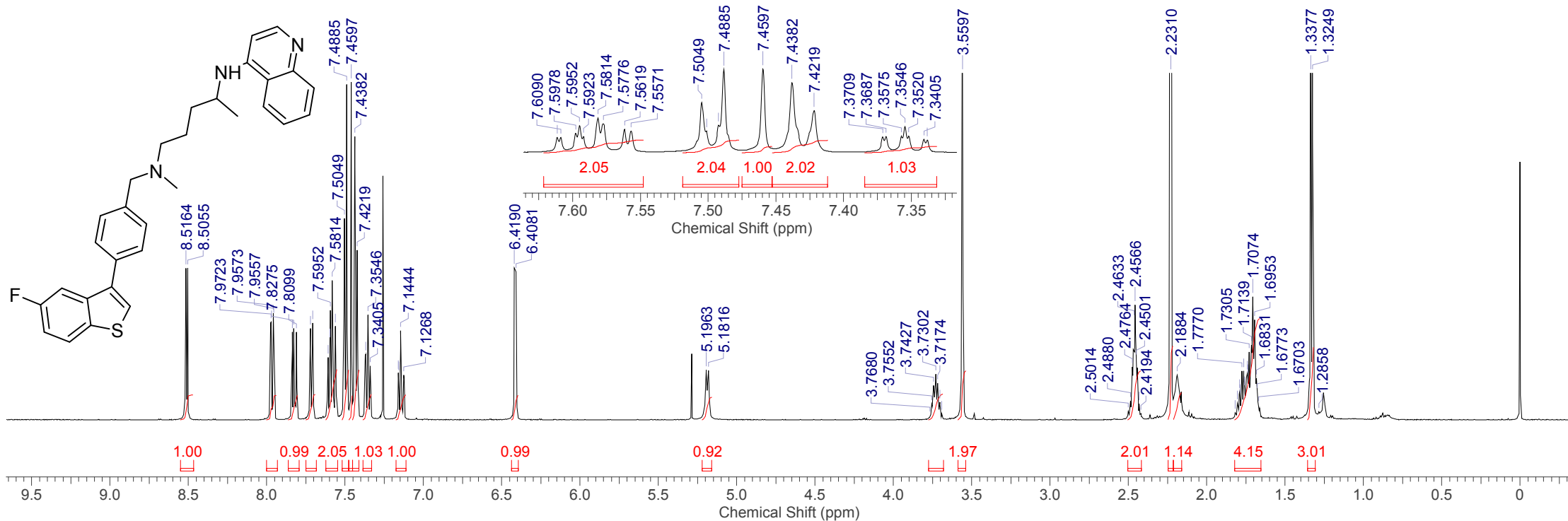
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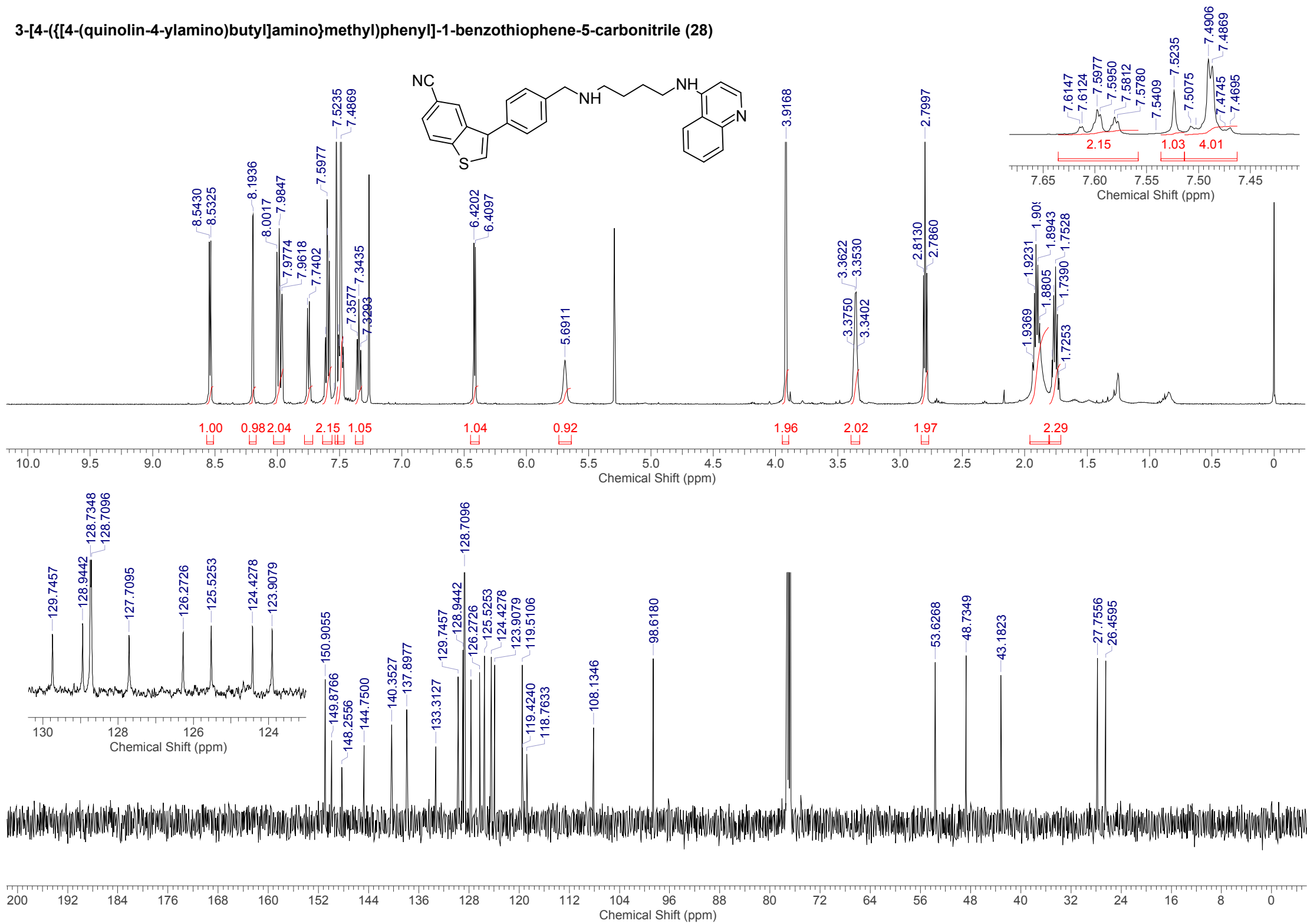
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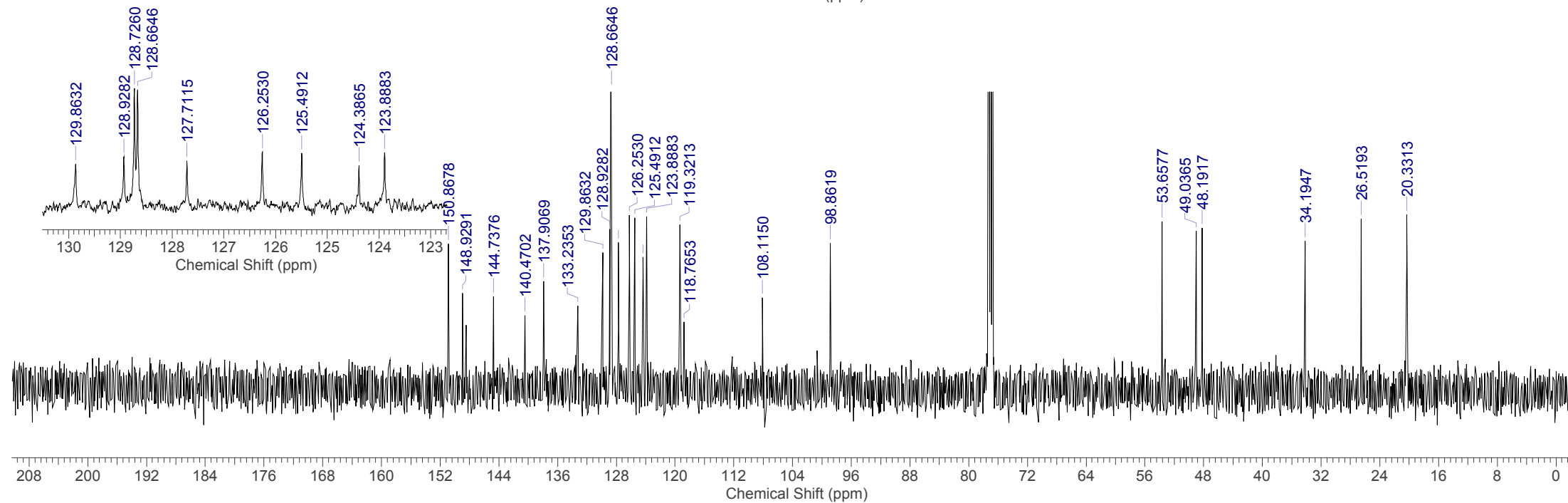
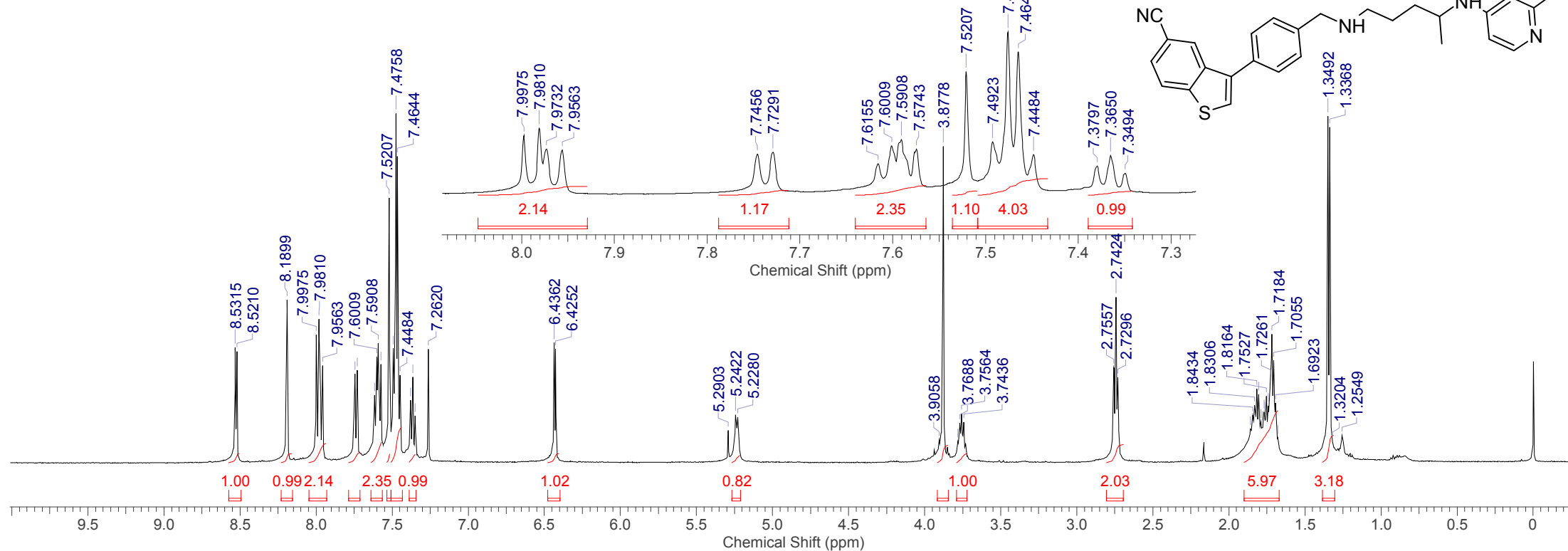
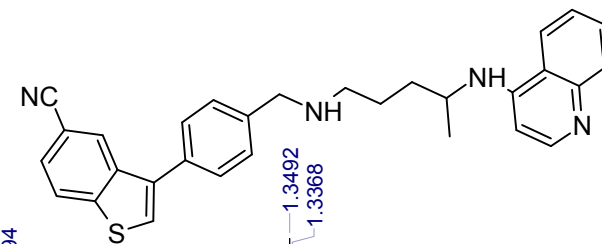
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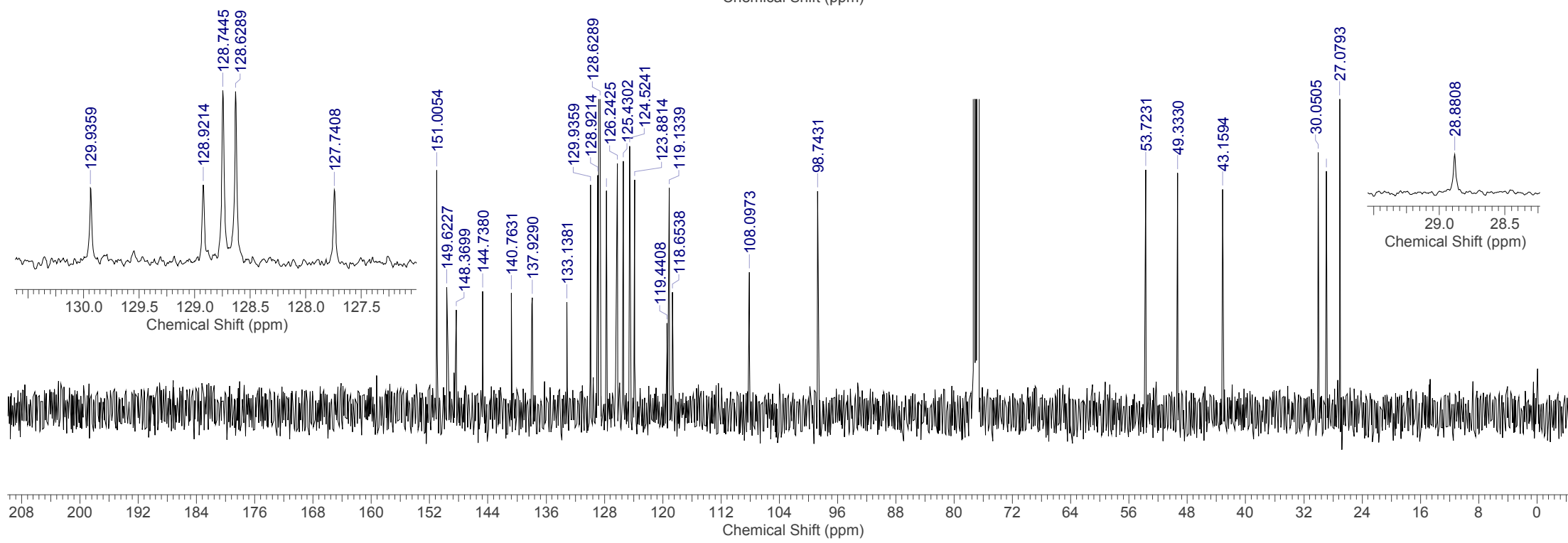
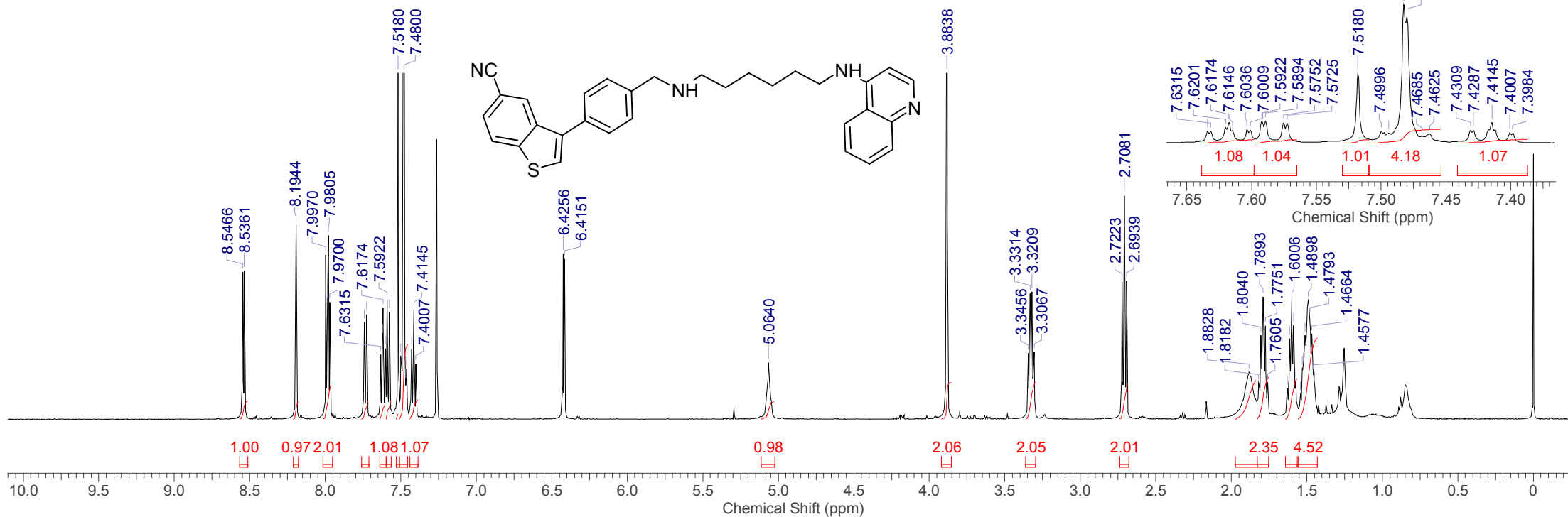
3-[4-({[4-(quinolin-4-ylamino)butyl]amino}methyl)phenyl]-1-benzothiophene-5-carbonitrile (28)



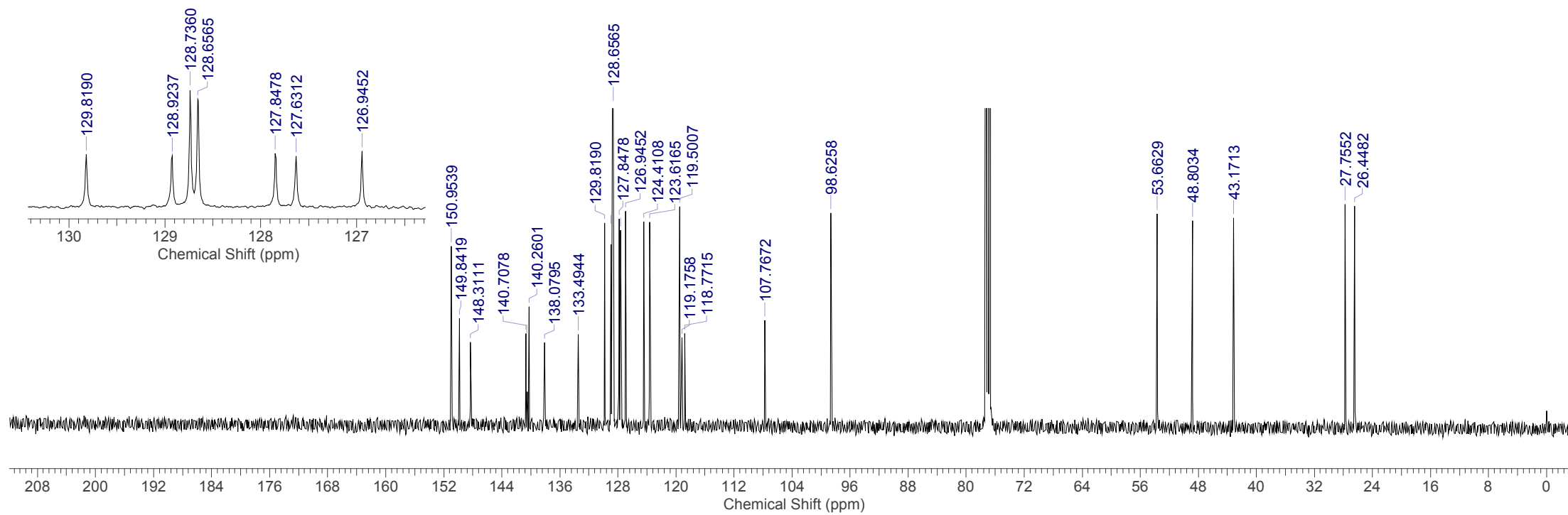
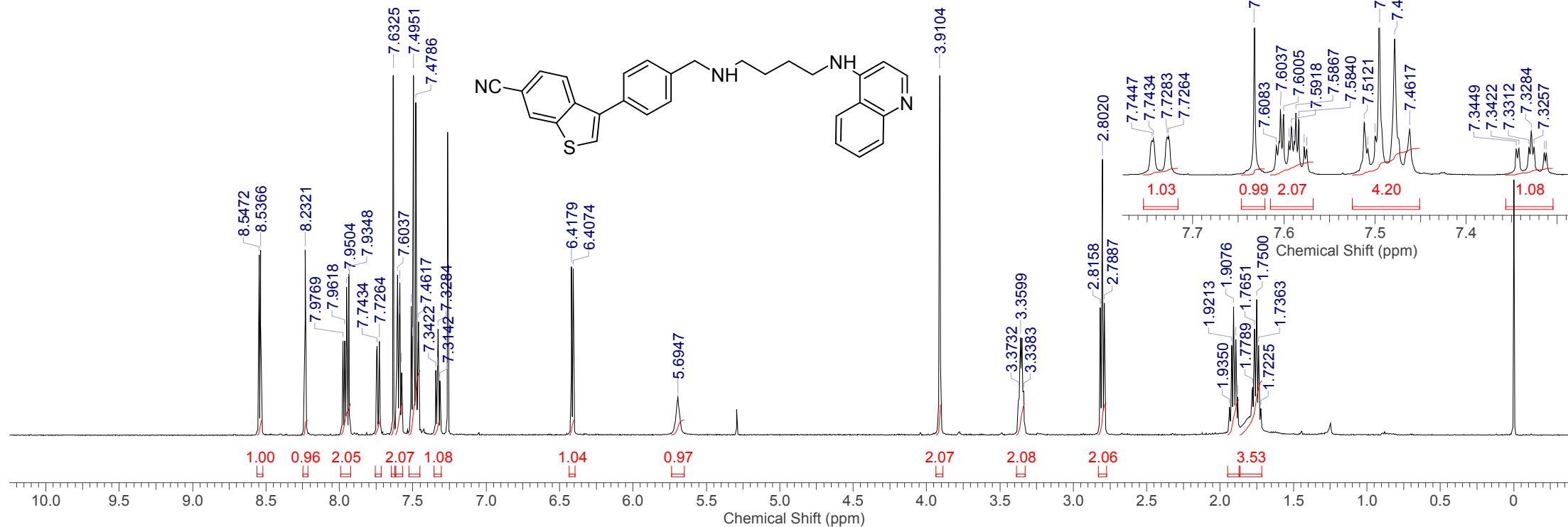
3-[4-({[4-(quinolin-4-ylamino)pentyl]amino}methyl)phenyl]-1-benzothiophene-5-carbonitrile (29)



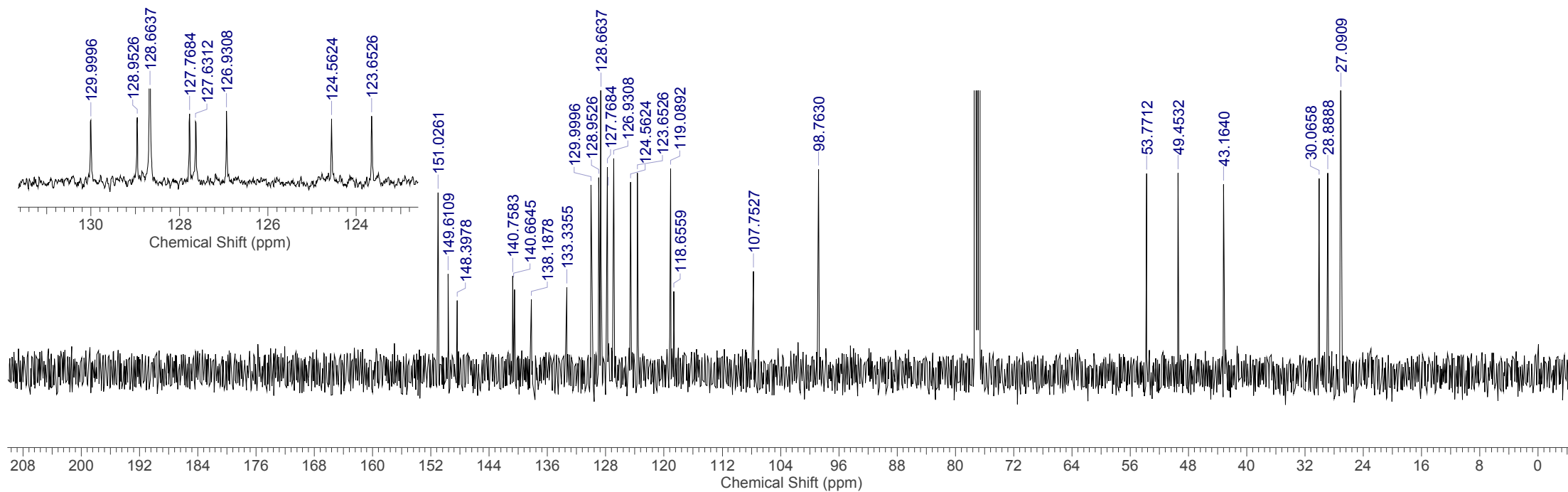
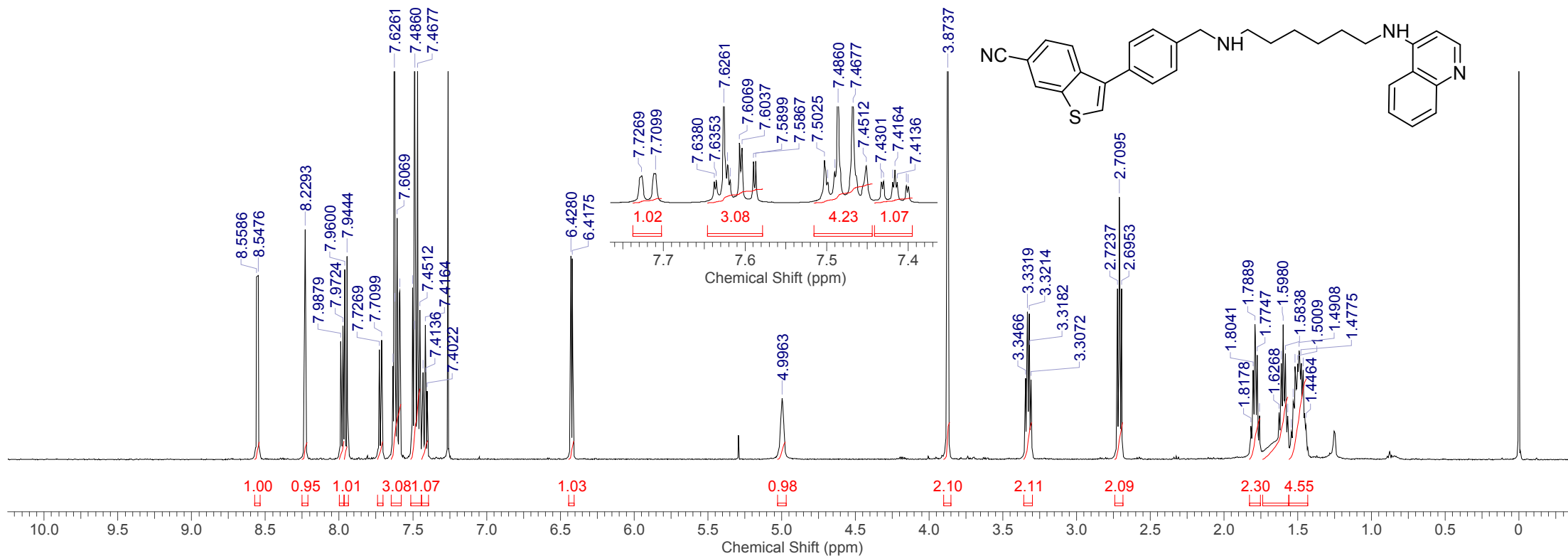
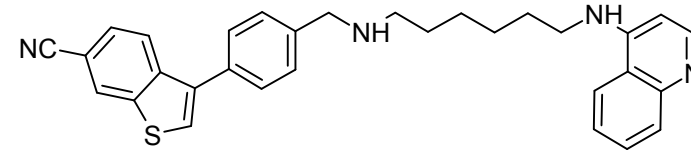
3-[4-({[6-(quinolin-4-ylamino)hexyl]amino}methyl)phenyl]-1-benzothiophene-5-carbonitrile (30)



3-[4-([4-(quinolin-4-ylamino)butyl]amino)methyl]phenyl]-1-benzothiophene-6-carbonitrile (31)

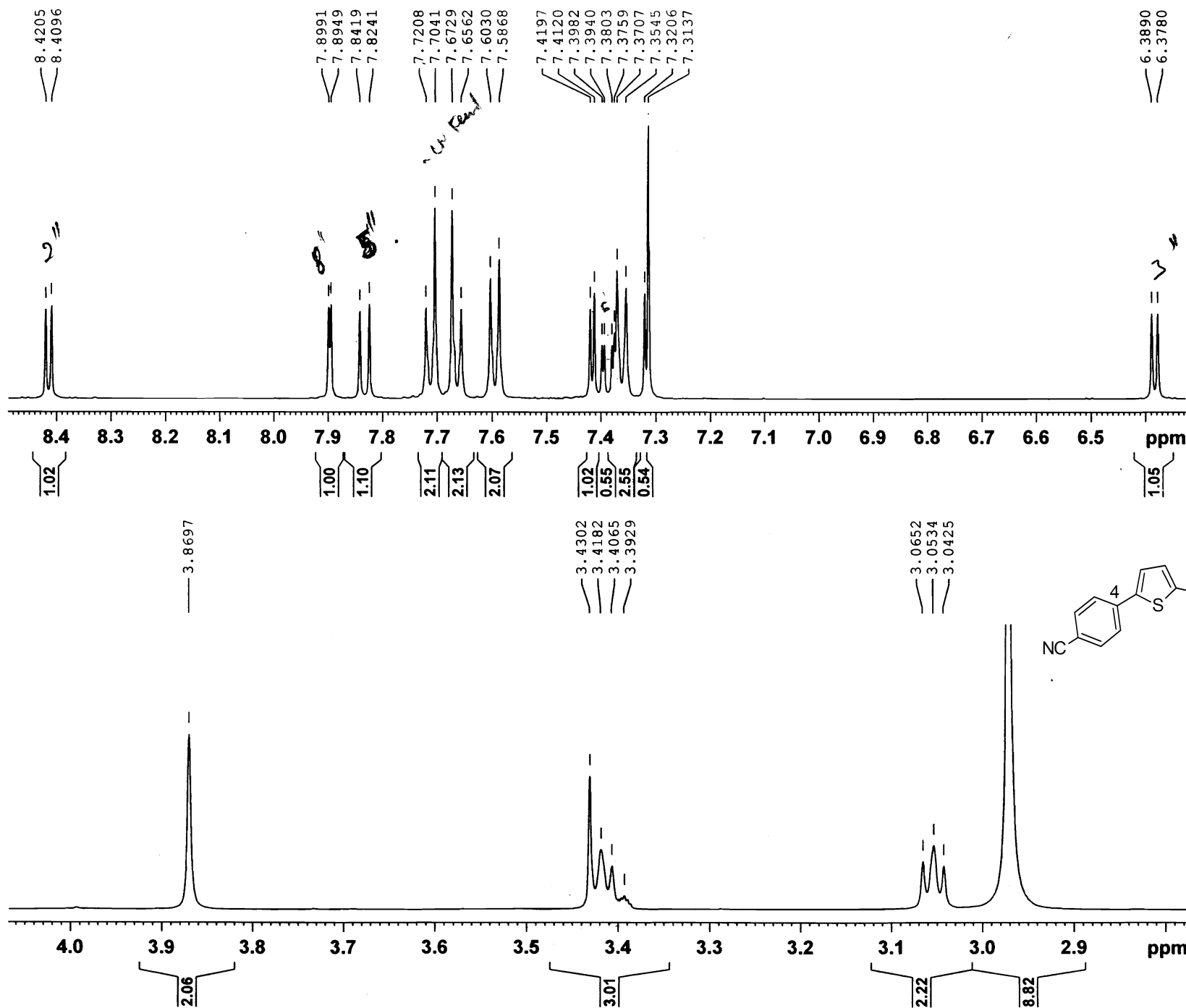


3-[4-({[6-(quinolin-4-ylamino)hexyl]amino}methyl)phenyl]-1-benzothiophene-6-carbonitrile (32)



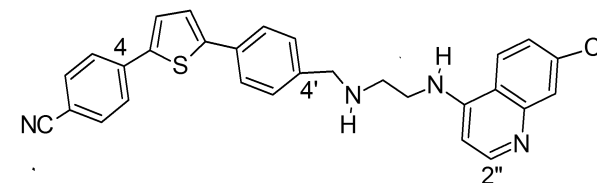
4-(5-{4-[(2-{(7-chloroquinolin-4-yl)amino}ethyl)amino)methyl]phenyl}-2-thienyl)benzonitrile (37)

11/14/6 SA AQ2

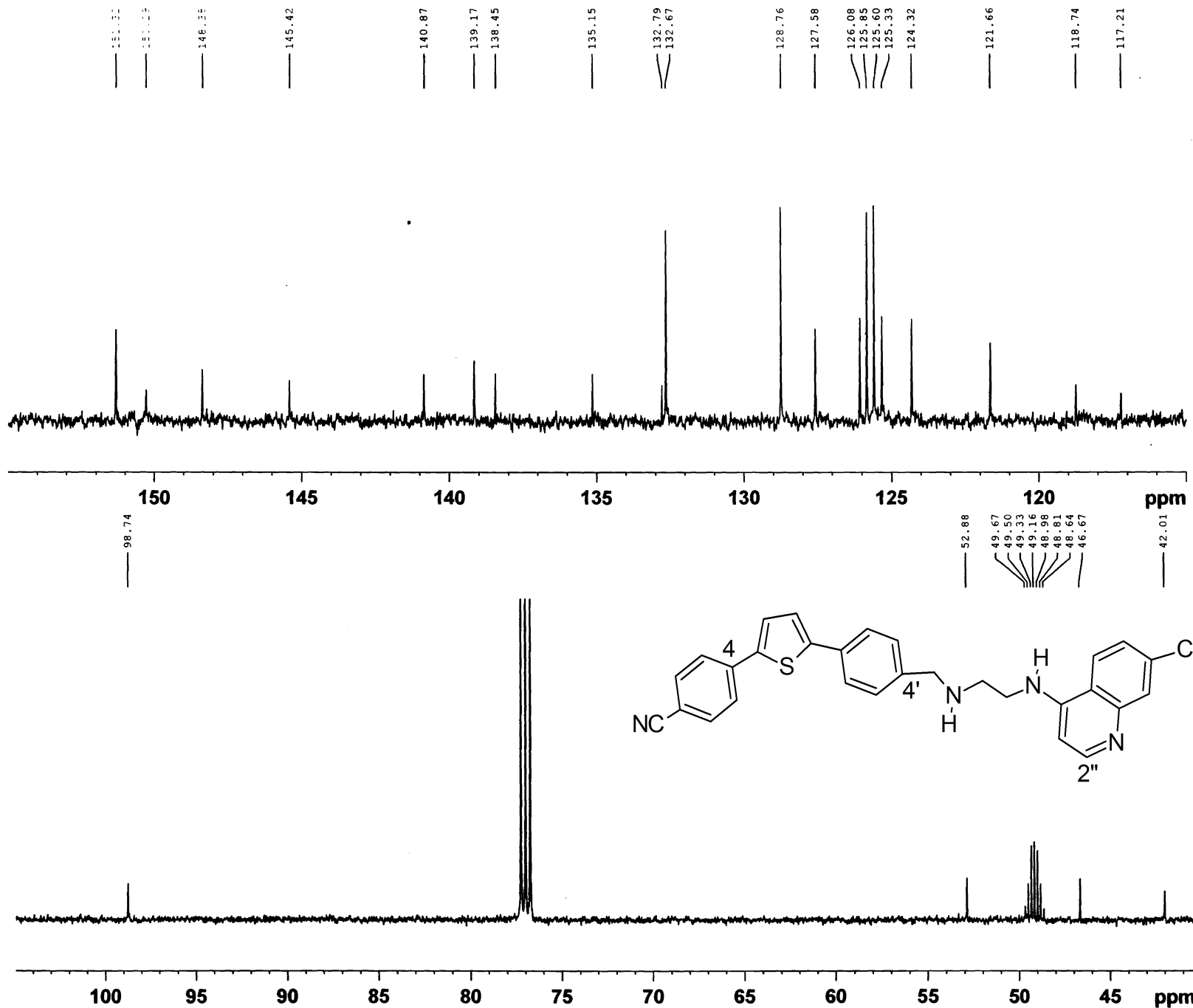


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 RG 575
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 DE 6.50 usec
 TE 298.0 K
 D1 2.00000000 sec
 TDO 1

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 P1 9.35 usec
 PL1 0.00 dB
 PL1W 27.37956238 W
 SFO1 500.2625923 MHz
 SI 16384
 SF 500.2599881 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



4-{5-[4-[(2-[(7-chloroquinolin-4-yl)amino]ethyl)amino)methyl]phenyl]-2-thienyl}benzonitrile (37)

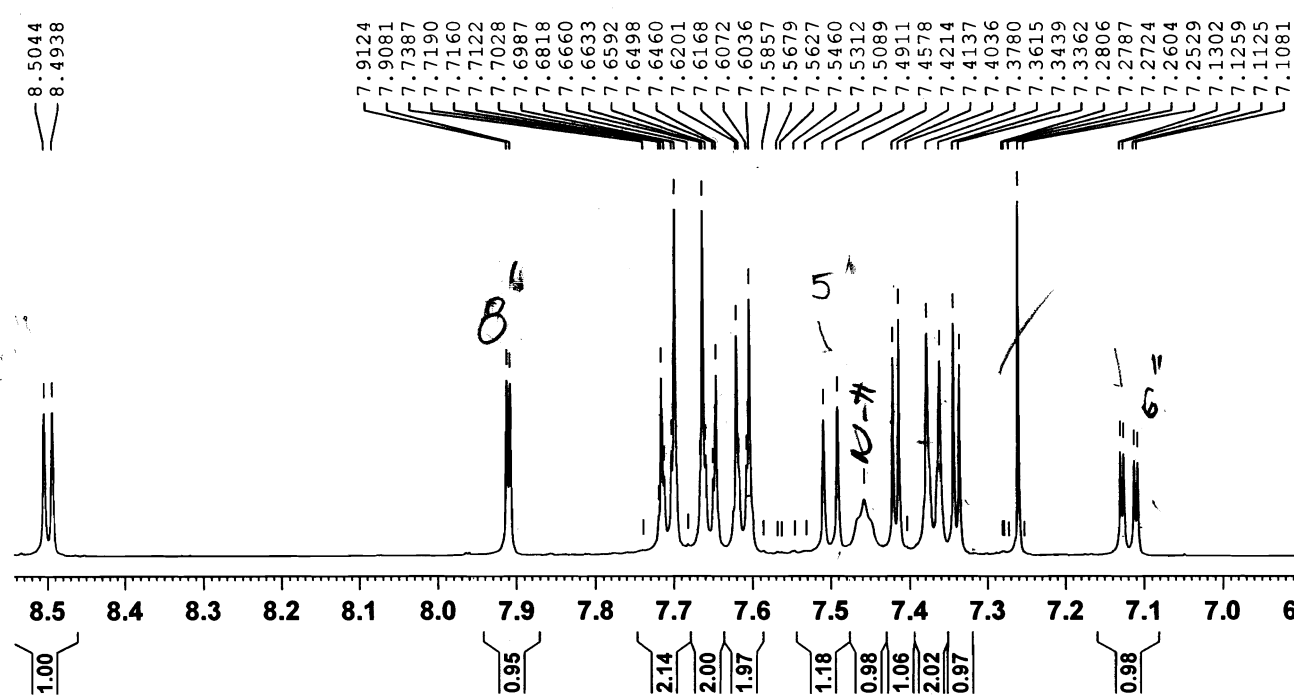


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 SOLVENT CDC13
 NS 625
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 FIDRES 0.908261 Hz
 AQ 0.5505524 sec
 RG 1290
 DW 16.800 usec
 DE 6.50 usec
 TE 298.1 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
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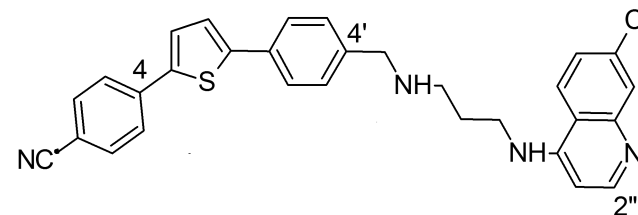
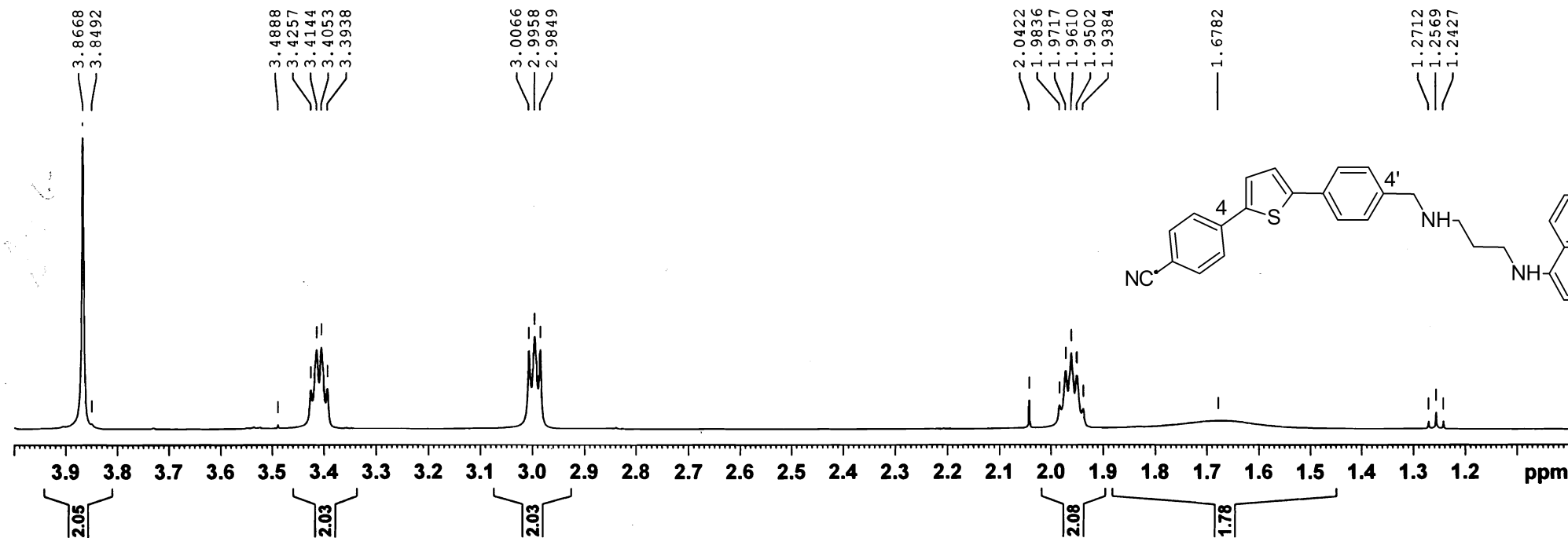
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 PL12 18.40 dB
 PL13 18.40 dB
 PL2W 20.76952171 W
 PL12W 0.39575511 W
 PL13W 0.39575511 W
 SFO2 500.2620010 MHz
 SI 32768
 SF 125.7904878 MHz
 WDW EM
 SSB 0
 LB 1.50 Hz
 GB 0
 PC 1.40

4-(5-{4-[[{3-[(7-chloroquinolin-4-yl)amino]propyl}amino)methyl]phenyl}-2-thienyl)benzonitrile (38)

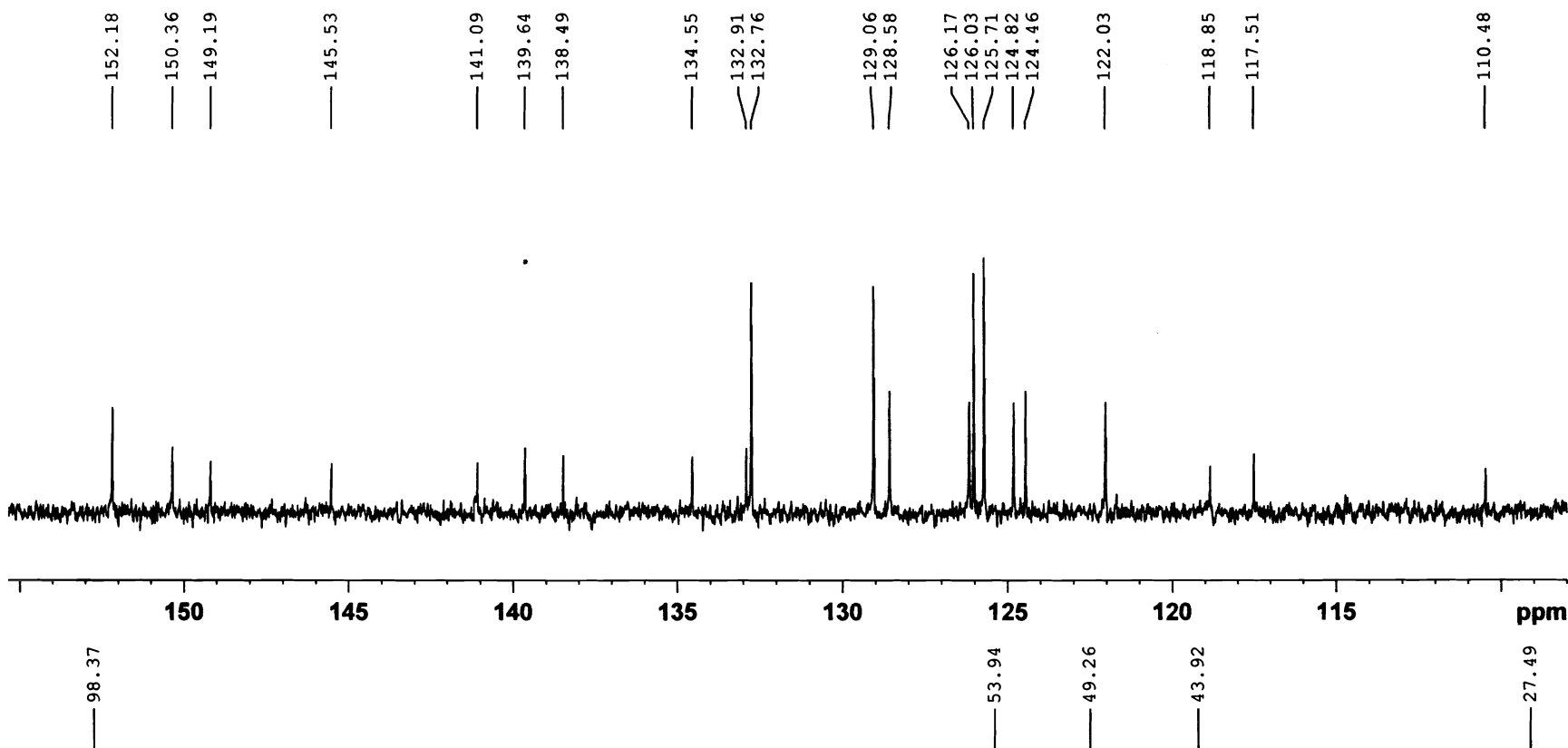


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 NS 16
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 SWH 6487.889 Hz
 FIDRES 0.197995 Hz
 AQ 2.5253706 sec
 RG 322
 DW 77.067 use
 DE 6.50 use
 TE 298.0 K
 D1 2.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.35 use
 PL1 0.00 dB
 PL1W 27.37956238 W
 SFO1 500.2627938 MHz
 SI 32768
 SF 500.2600143 MHz
 WDW EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.00



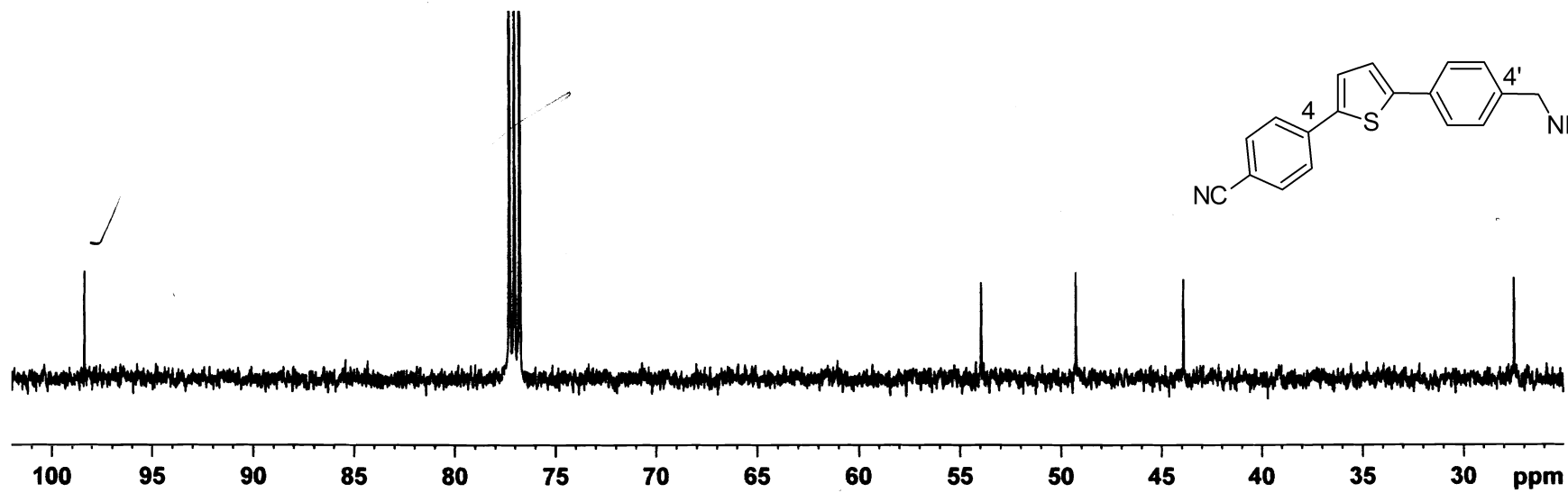
4-(5-{4-[(3-[(7-chloroquinolin-4-yl)amino]propyl)amino)methyl]phenyl}-2-thienyl)benzonitrile (38)



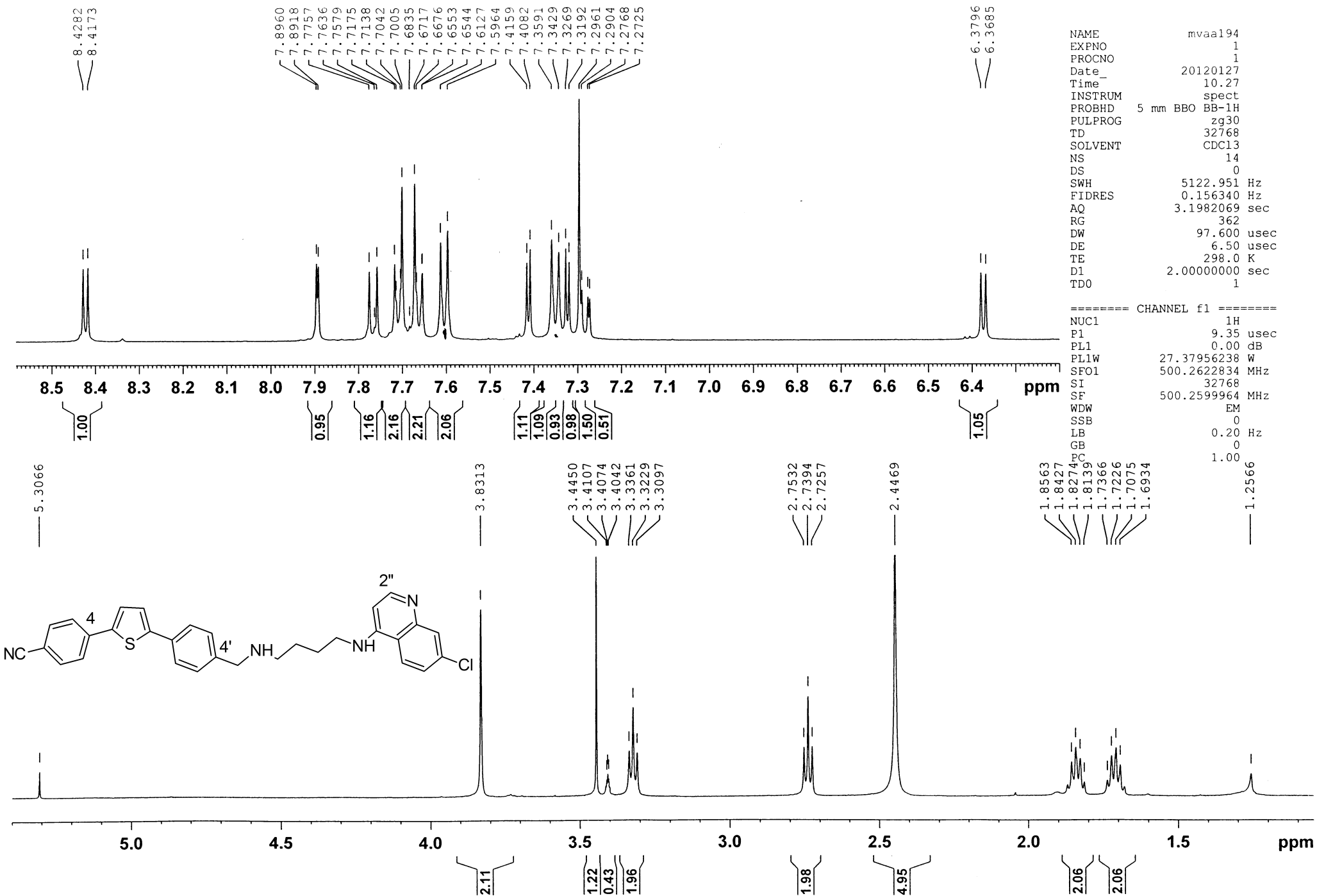
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TD 32768
SOLVENT CDCl3
NS 148
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 0.5505524 sec
RG 1030
DW 16.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 11.50 usec
PL1 3.00 dB
PL1W 32.22848892 W
SFO1 125.8043140 MHz

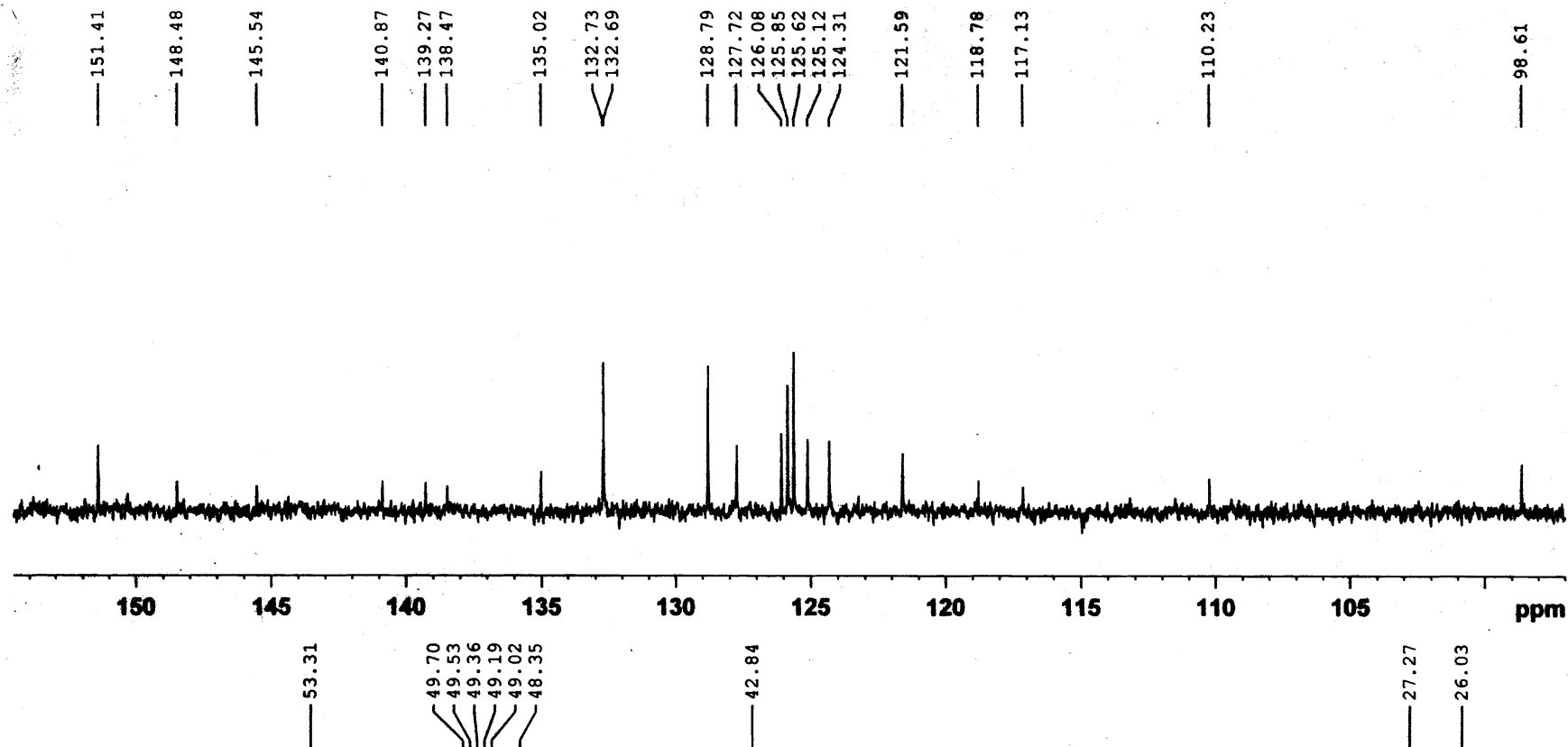
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NUC2 1H
PCPD2 80.00 usec
PL2 1.20 dB
PL12 18.40 dB
PL13 18.40 dB
PL2W 20.76952171 W
PL12W 0.39575511 W
PL13W 0.39575511 W
SFO2 500.2621871 MHz
SI 32768
SF 125.7904800 MHz
WDW EM
SSB 0
LB 1.50 Hz
GB 0
PC 1.40



4-(5-{4-[[{4-[(7-chloroquinolin-4-yl)amino]butyl}amino)methyl]phenyl}-2-thienyl)benzonitrile (39)



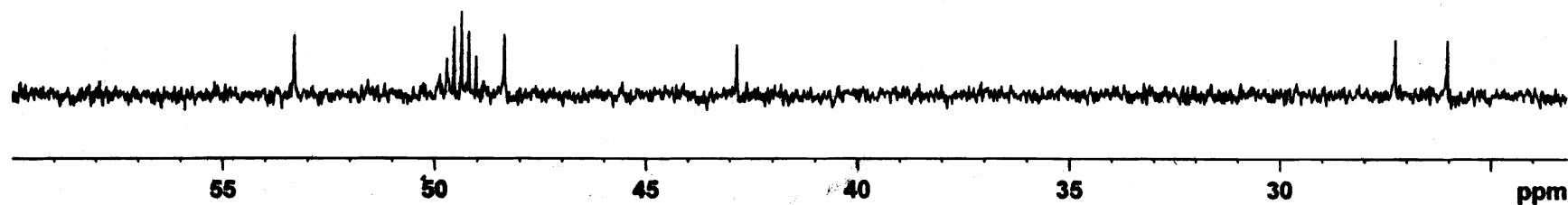
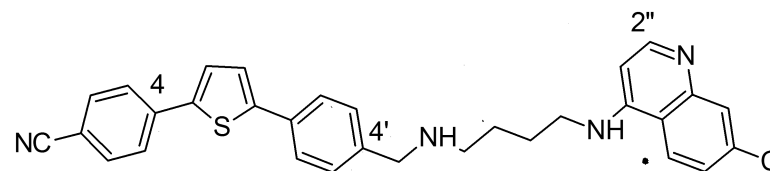
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NAME mvaal194
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 PULPROG zgpg30
 TD 32768
 SOLVENT CDCl3
 NS 221
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.908261 Hz
 AQ 0.5505524 sec
 RG 1030
 DM 16.800 usec
 DE 6.50 usec
 TE 298.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

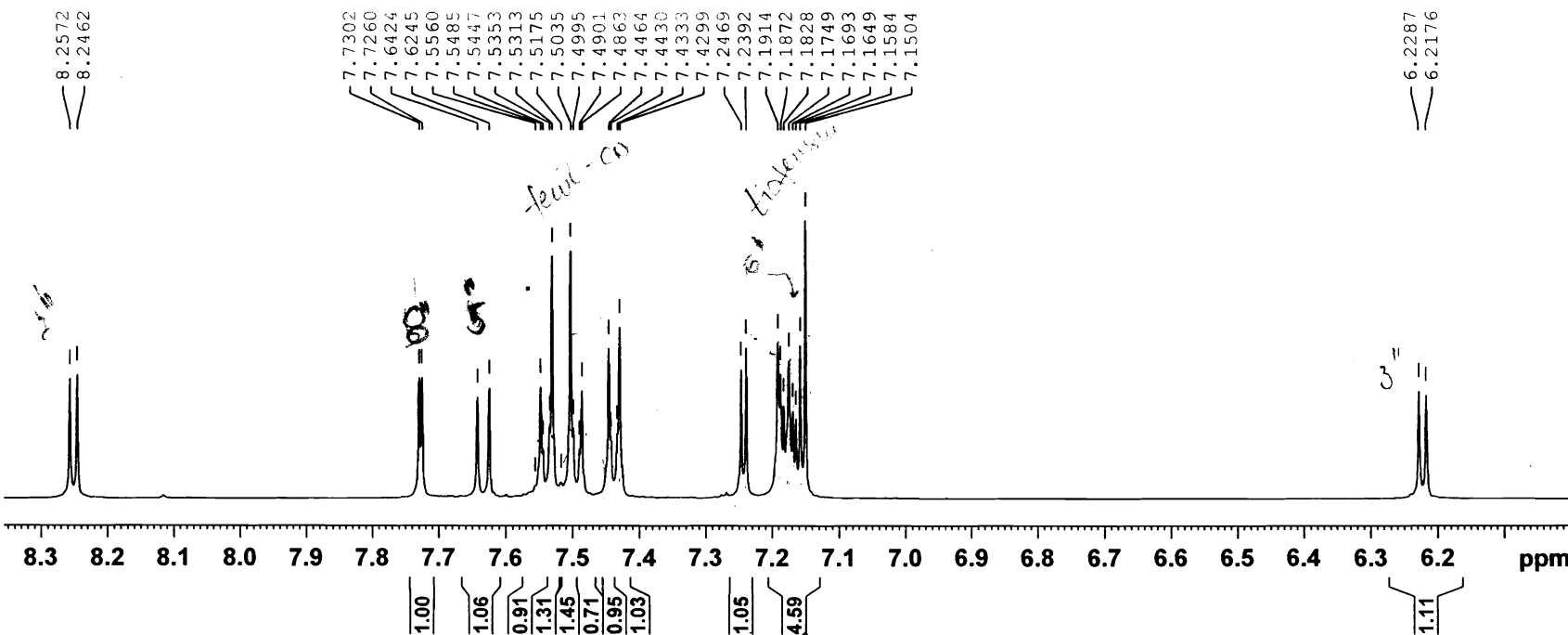
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 P1 11.50 usec
 PL1 3.00 dB
 PL1W 32.22848892 W
 SFO1 125.8043140 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 1.20 dB
 PL12 18.40 dB
 PL13 18.40 dB
 PL2W 20.76952171 W
 PL12W 0.39575511 W
 PL13W 0.39575511 W
 SFO2 500.2619175 MHz
 SI 32768
 SF 125.7904862 MHz
 WDW EM
 SSB 0
 LB 1.50 Hz
 GB 0
 PC 1.40



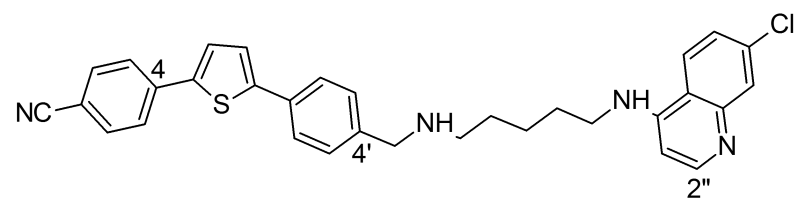
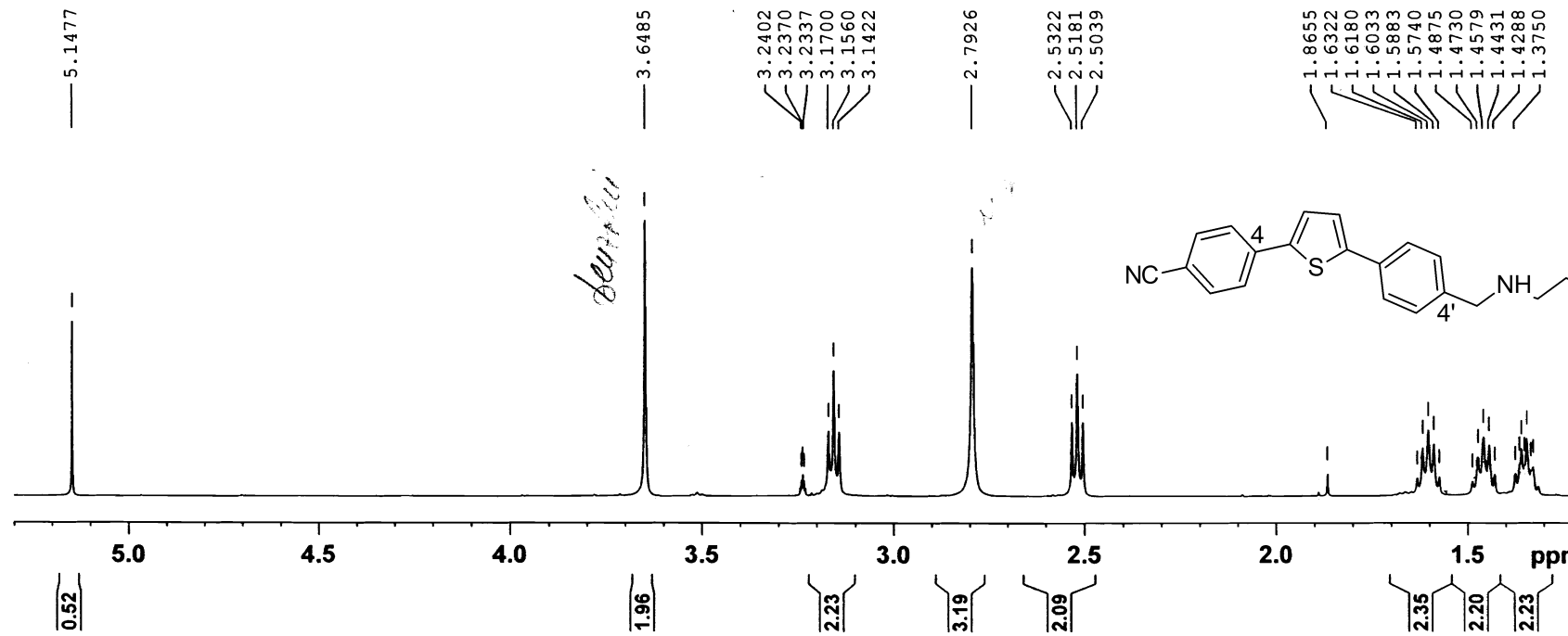
4-(5-[(7-chloroquinolin-4-yl)amino]pentyl)amino)methyl]phenyl)-2-thienyl)benzonitrile (40)

MVA151 SA AQS



NAME MVA208
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PROCNO 1
Date 20120312
Time 10.00
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 5555.556 Hz
FIDRES 0.169542 Hz
AQ 2.9491701 sec
RG 322
DW 90.000 usec
DE 6.50 usec
TE 298.0 K
D1 2.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 9.35 usec
PL1 0.00 dB
PL1W 27.37956238 W
SFO1 500.2623221 MHz
SI 32768
SF 500.2600689 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 1.00



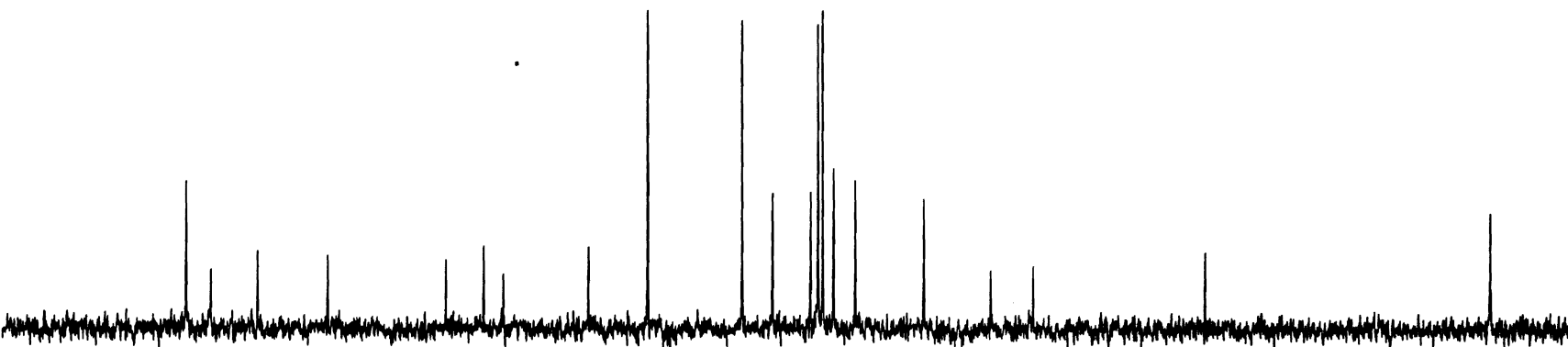
4-(5-[[4-[[[(7-chloroquinolin-4-yl)amino]pentyl]amino)methyl]phenyl]-2-thienyl)benzonitrile (40)

NAME MVAA208
EXPNO 2
PROCNO 1
Date_ 20120312
Time 10.04
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDC13
NS 100
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 0.5505524 sec
RG 1030
DW 16.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 11.50 usec
PL1 3.00 dB
PL1W 32.22848892 W
SFO1 125.8030560 MHz

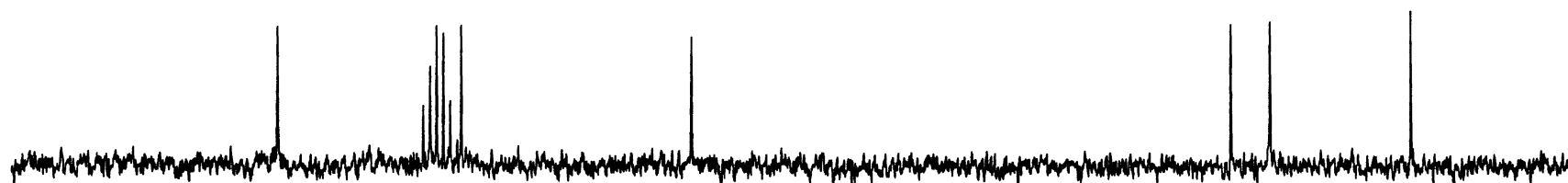
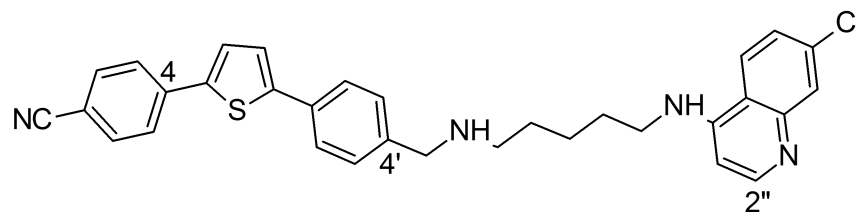
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.20 dB
PL12 18.40 dB
PL13 18.40 dB
PL2W 20.76952171 W
PL12W 0.39575511 W
PL13W 0.39575511 W
SFO2 500.2621271 MHz
SI 32768
SF 125.7904891 MHz
WDW EM
SSB 0
LB 1.50 Hz
GB 0
PC 1.40

151.22
150.22
148.32
145.52
140.76
139.23
138.45
135.02
132.64
128.82
127.58
126.06
125.76
125.56
125.13
124.25
121.49
118.75
117.03
110.12
98.60



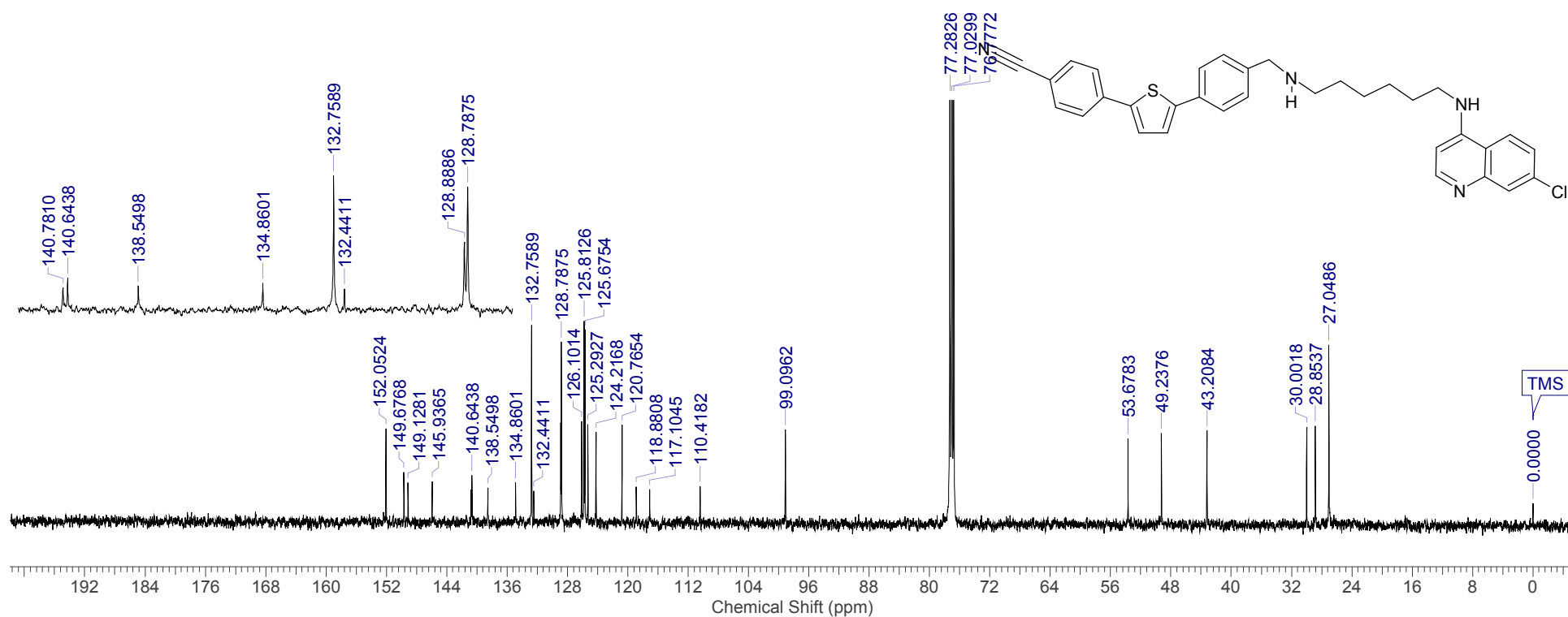
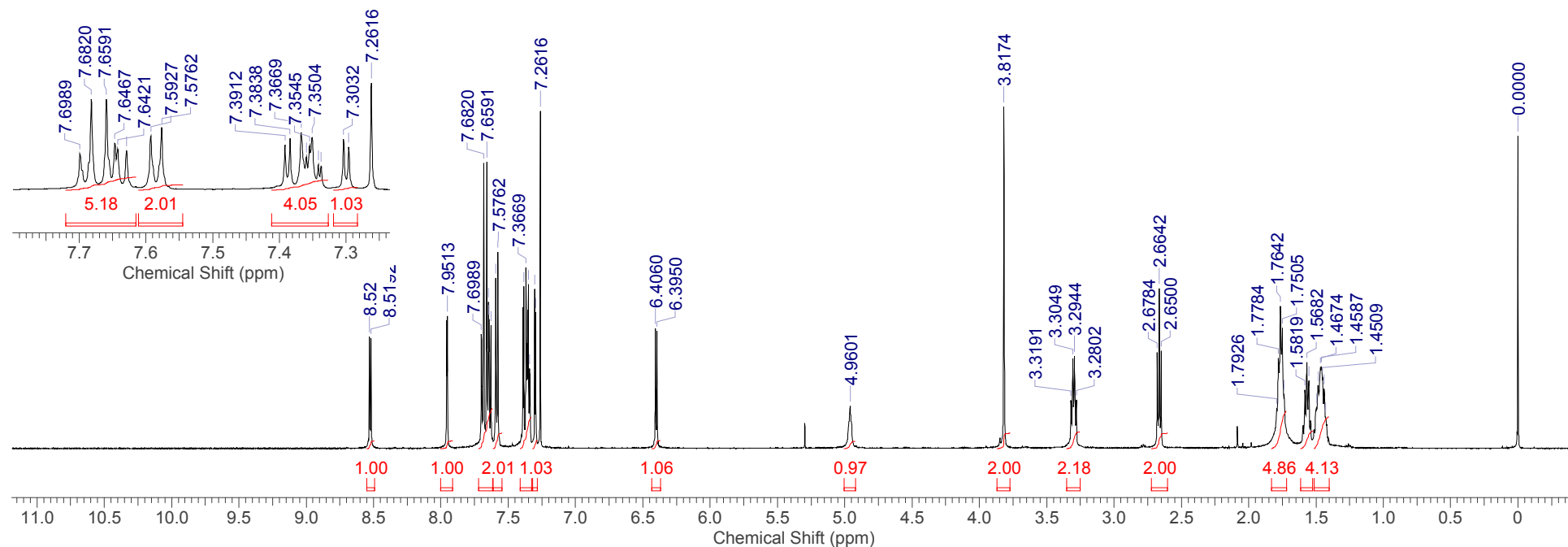
155 150 145 140 135 130 125 120 115 110 105 100 ppm

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49.50
49.33
49.16
48.99
48.82
48.54
42.73
29.08
28.09
24.53

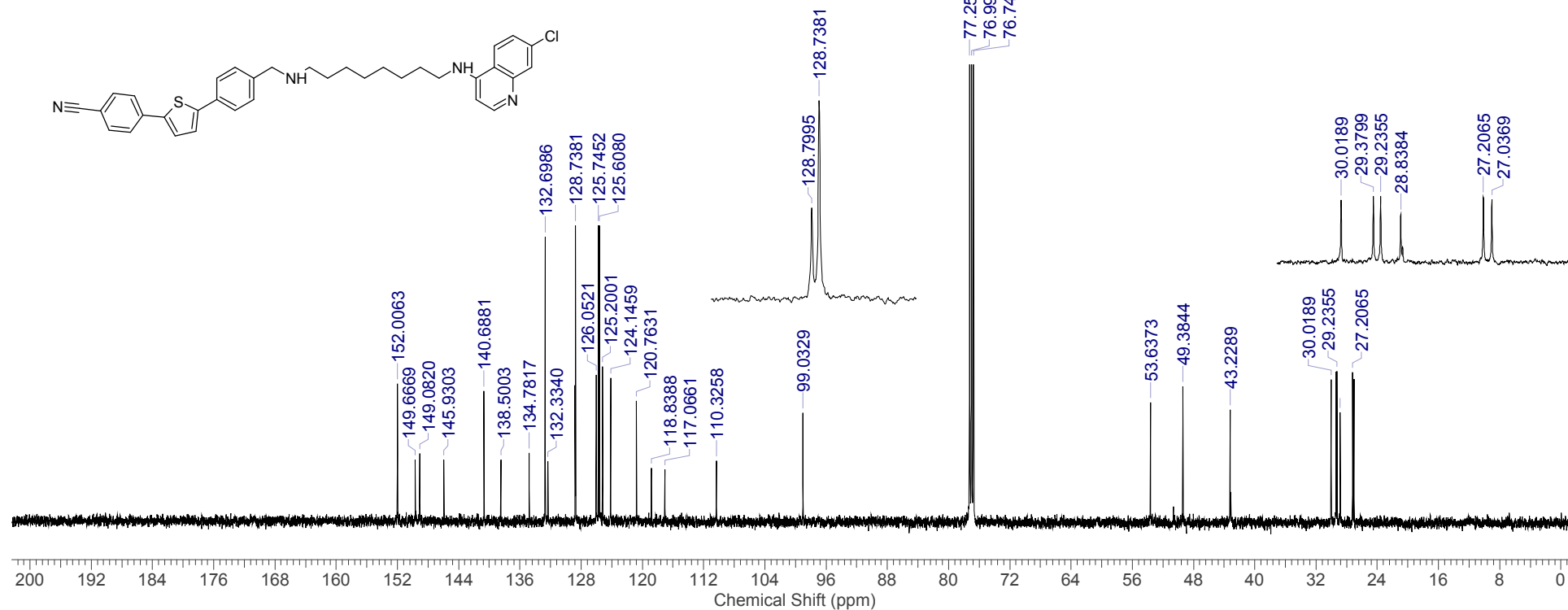
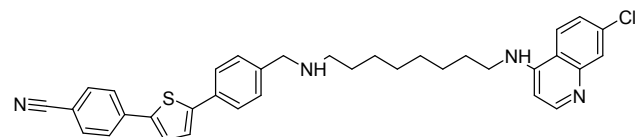
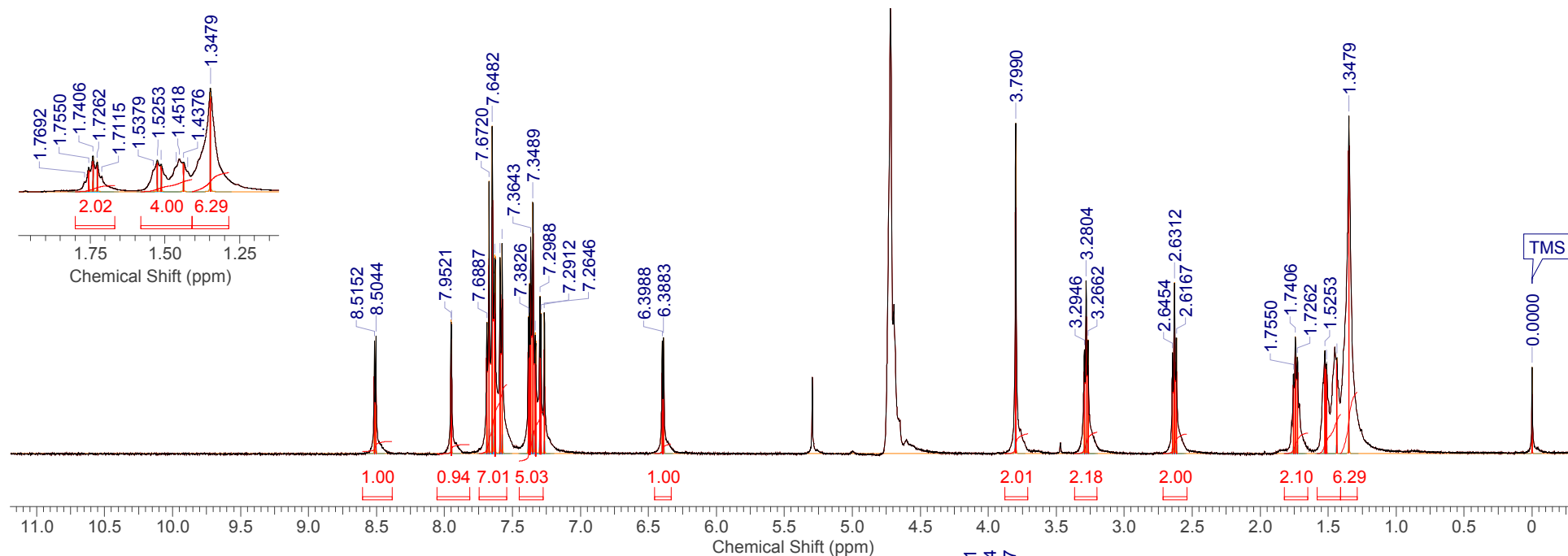


55 50 45 40 35 30 25 ppm

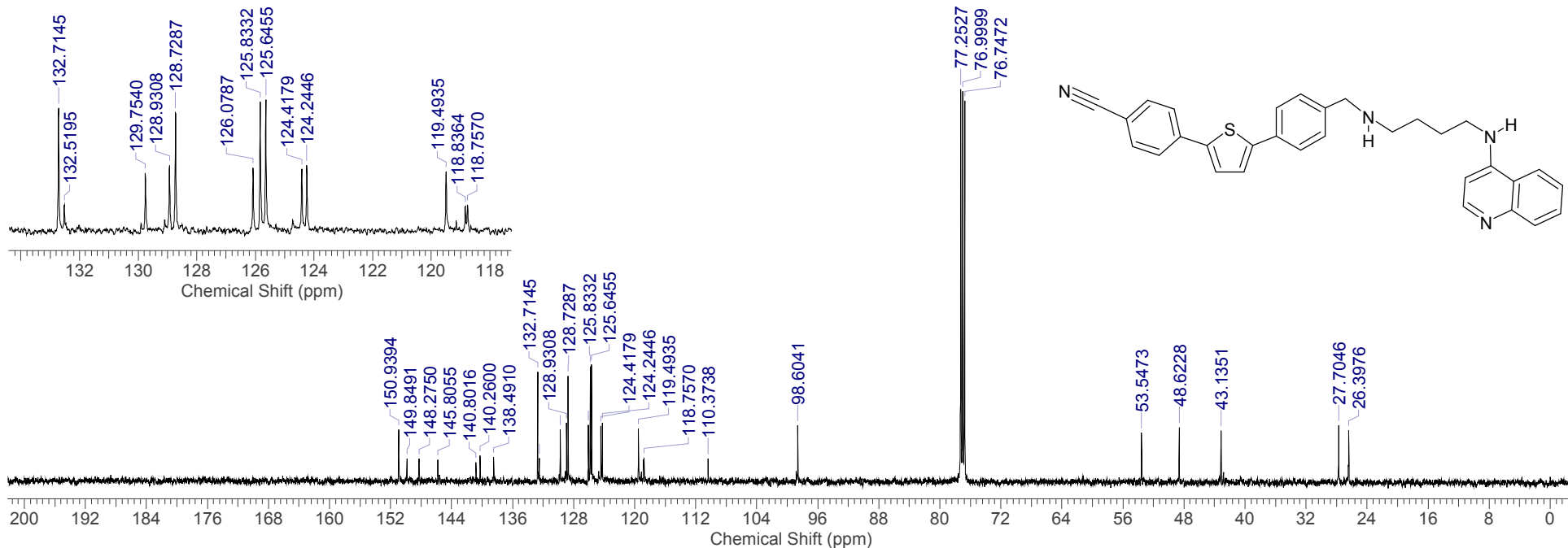
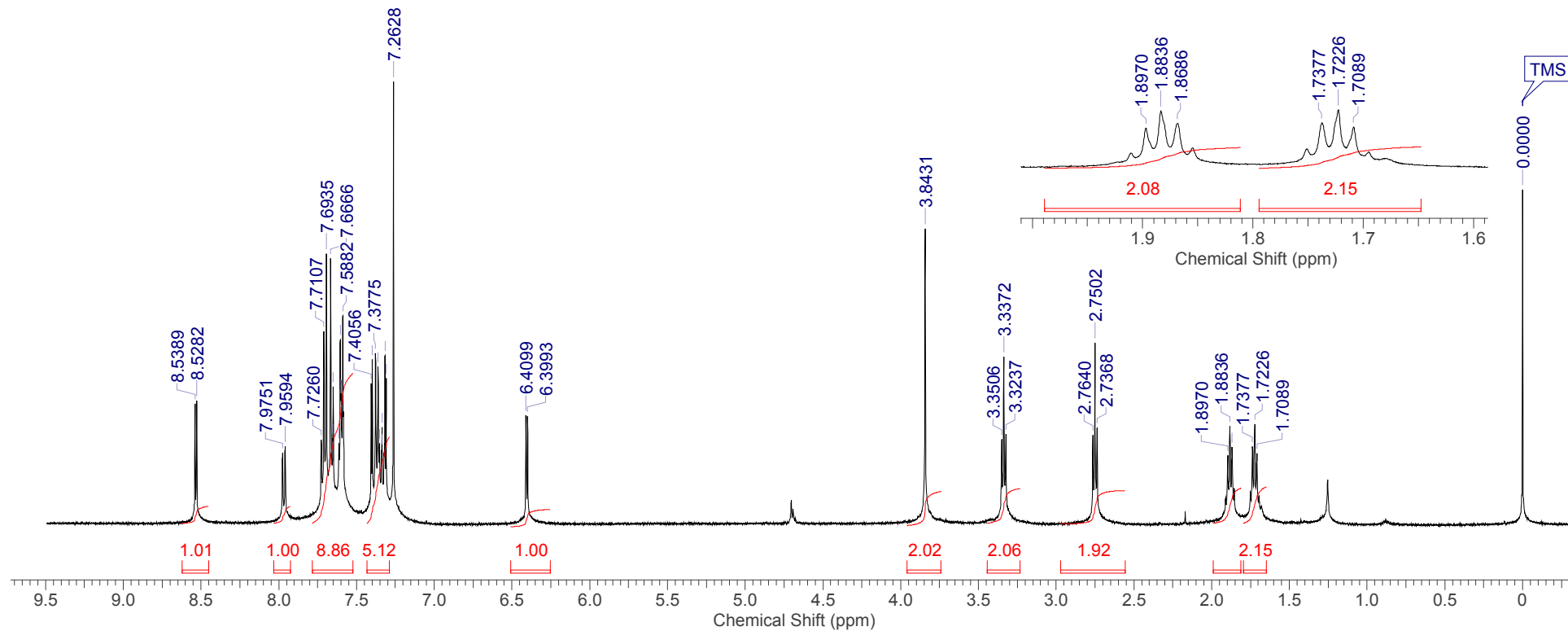
4-(5-{4-[(6-{(7-chloroquinolin-4-yl)amino)hexyl]amino)methyl]phenyl}-2-thienyl)benzonitrile (41)



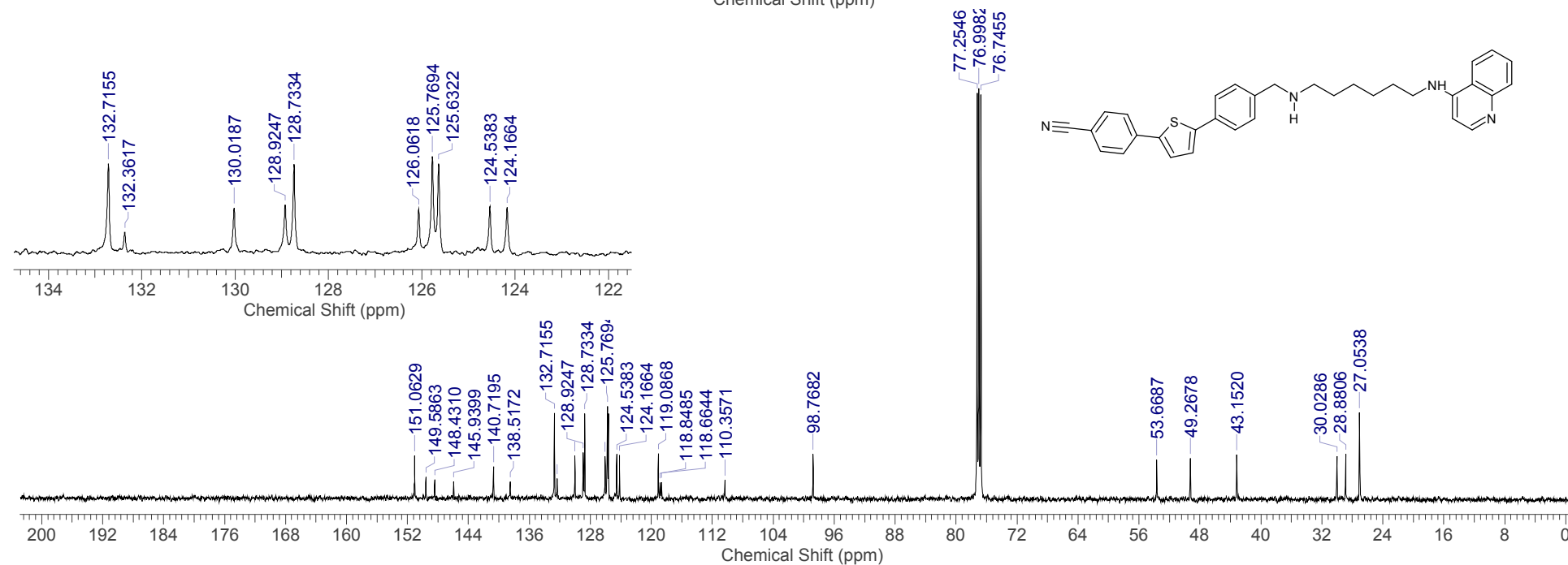
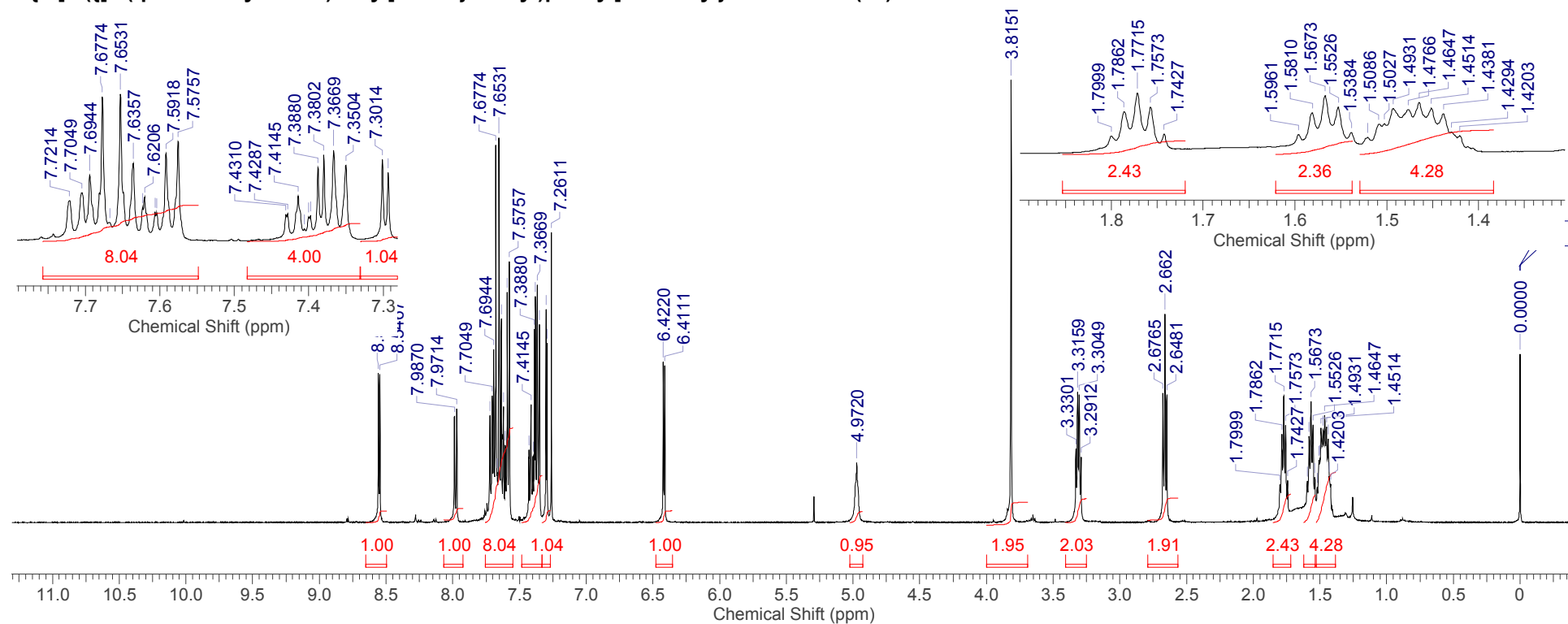
4-(5-{4-[(8-[(7-chloroquinolin-4-yl)amino]octyl)amino)methyl]phenyl}-2-thienyl)benzonitrile (42)



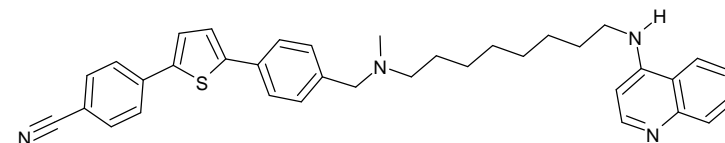
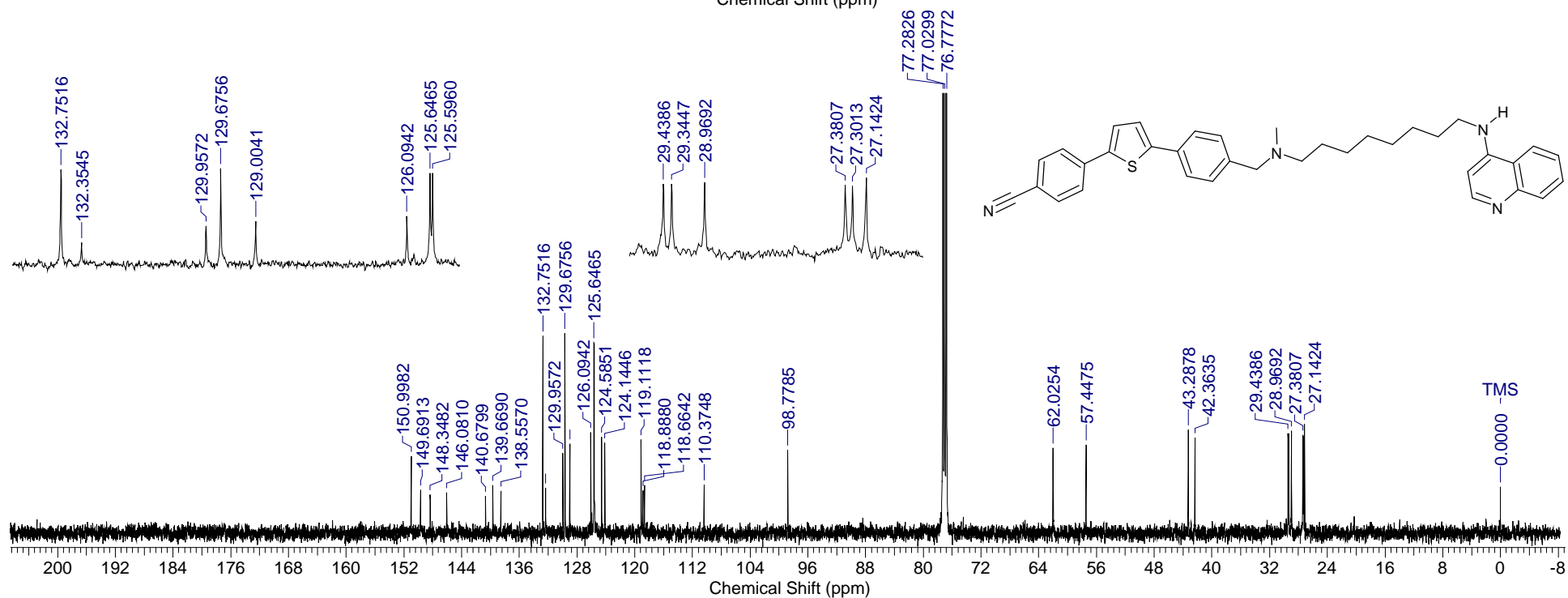
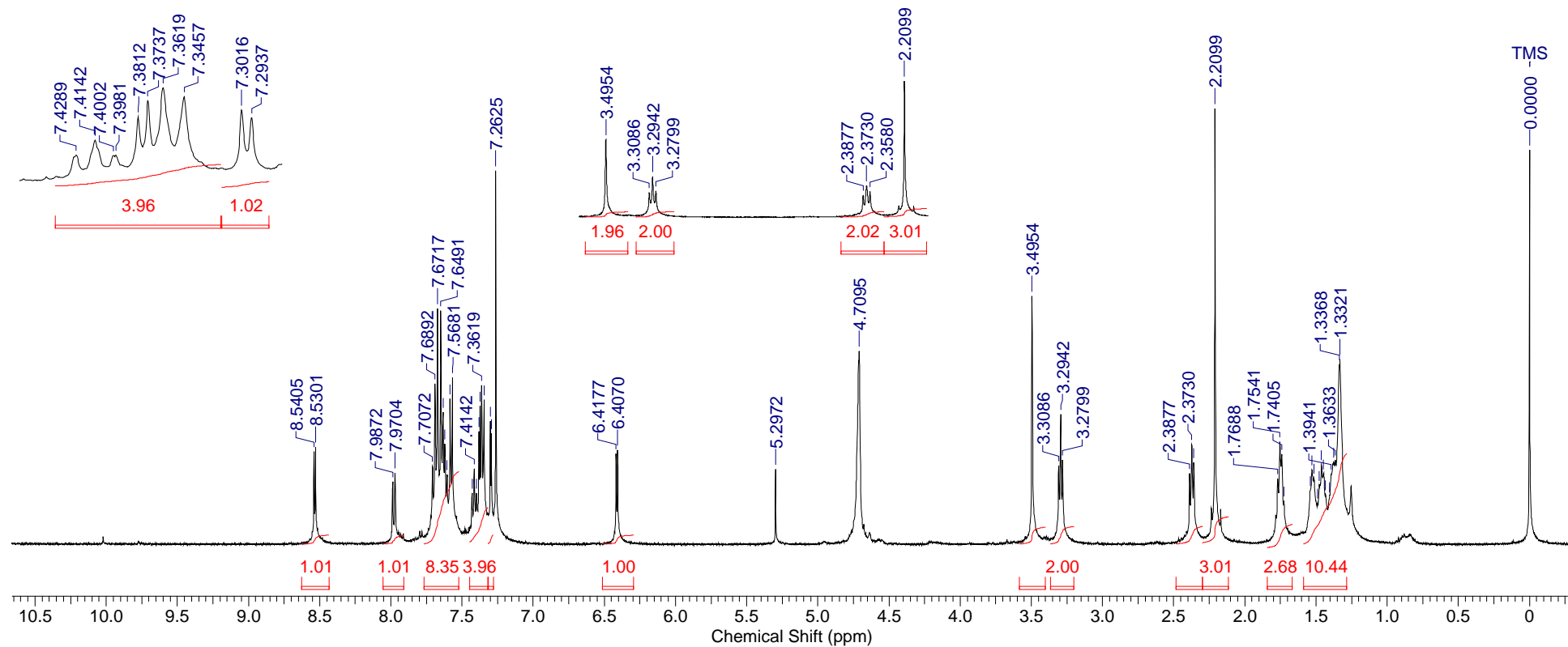
4-{5-[4-({[4-(quinolin-4-ylamino)butyl]amino}methyl)phenyl]-2-thienyl}benzonitrile (43)



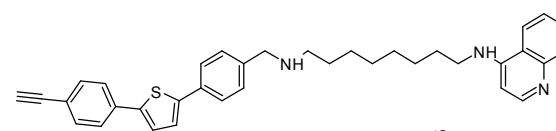
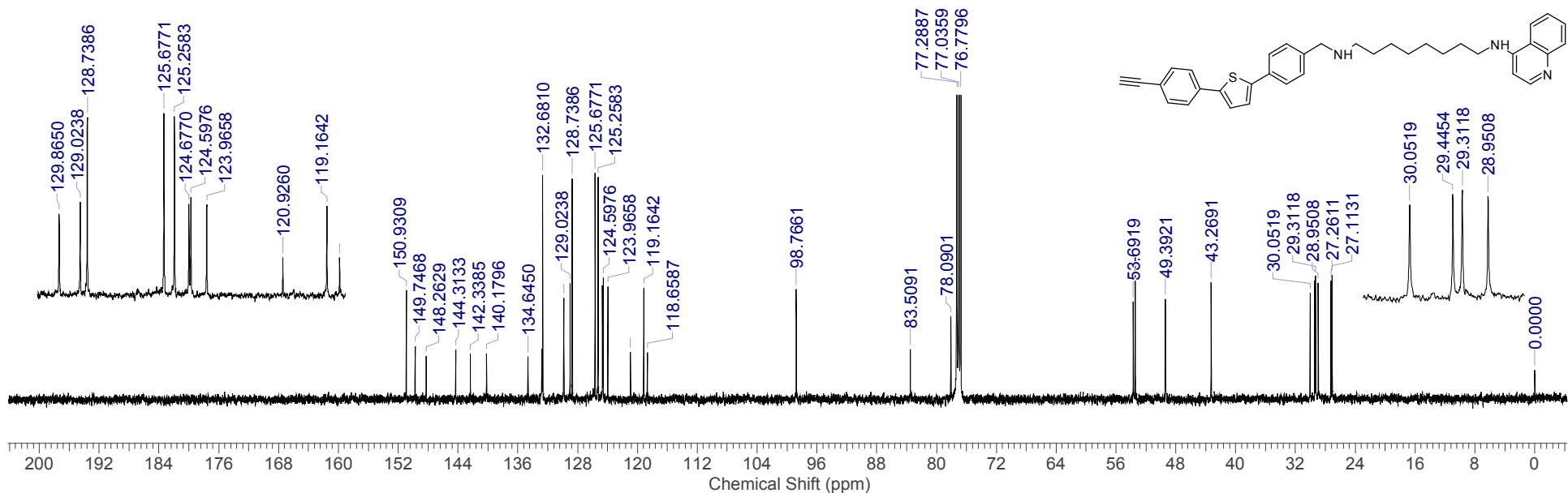
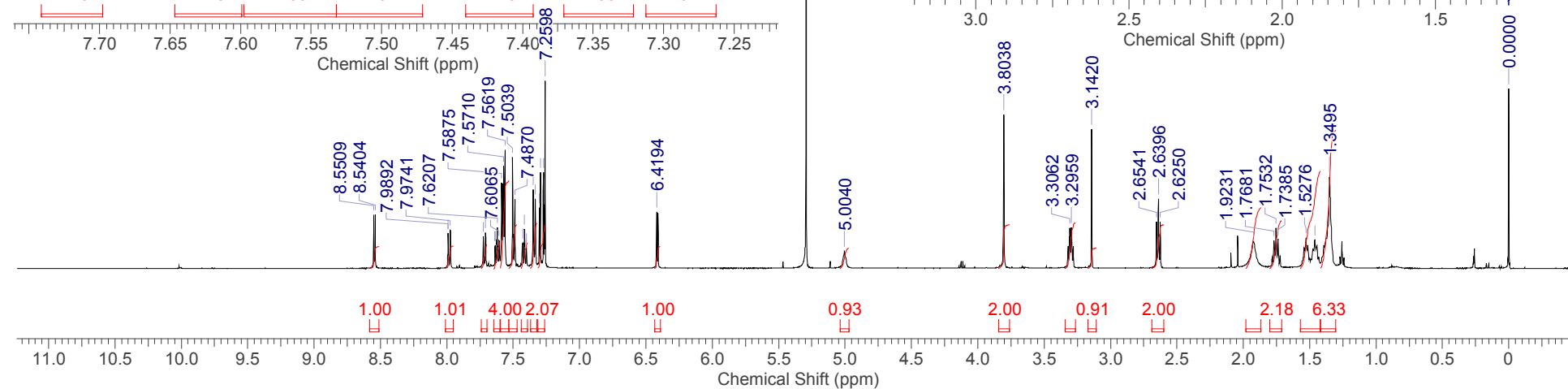
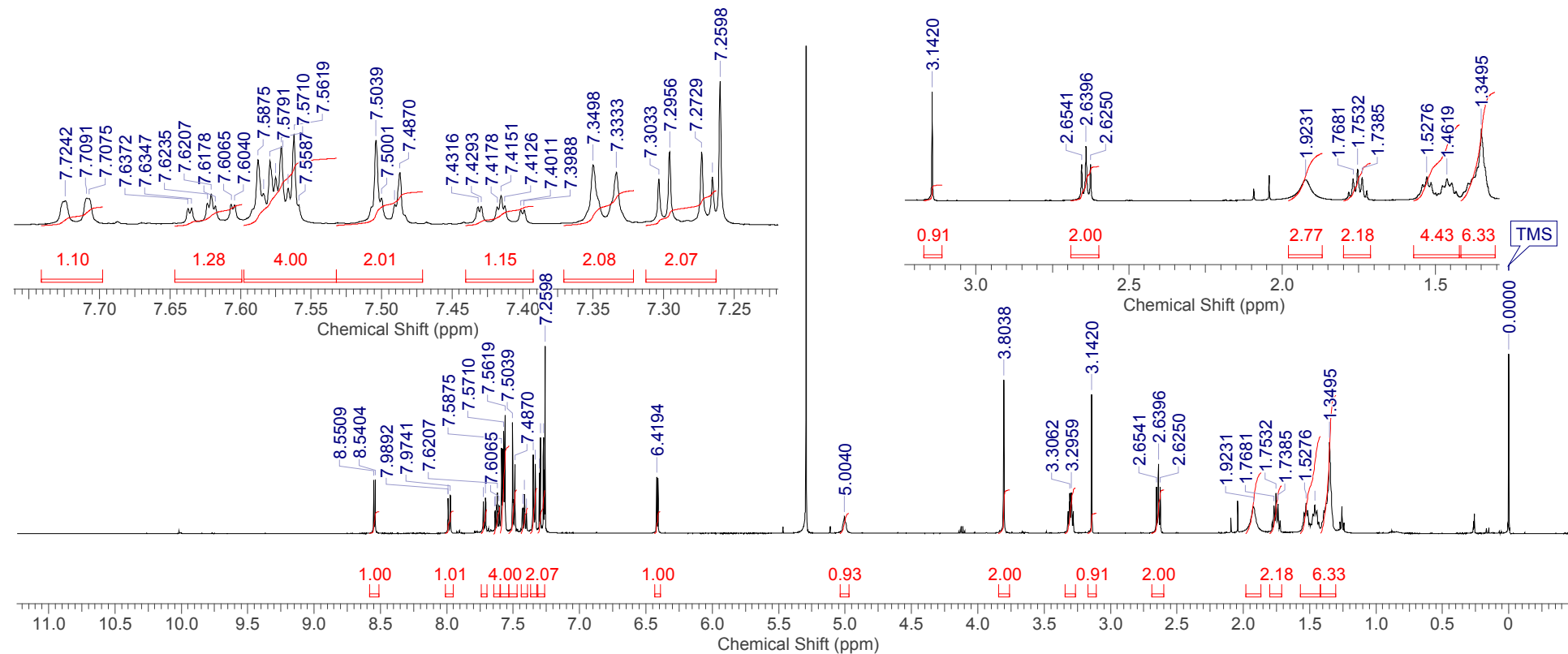
4-{5-[4-({[6-(quinolin-4-ylamino)hexyl]amino)methyl}phenyl]-2-thienyl}benzonitrile (44)



4-{5-[4-({methyl}[8-(quinolin-4-ylamino)octyl]amino)methyl]phenyl]-2-thienyl}benzonitrile (46)

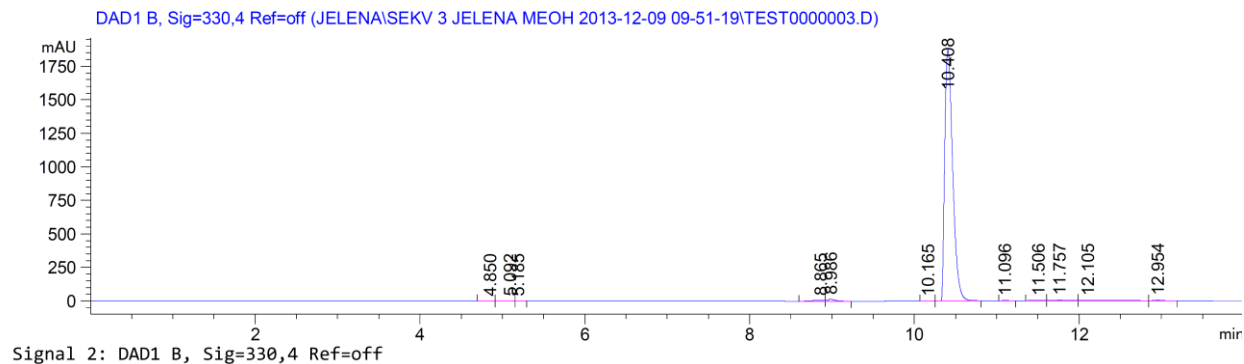


N-{4-[5-(4-ethynylphenyl)-2-thienyl]benzyl}-N'-quinolin-4-yl-octane-1,8-diamine (52)



Compound: 8

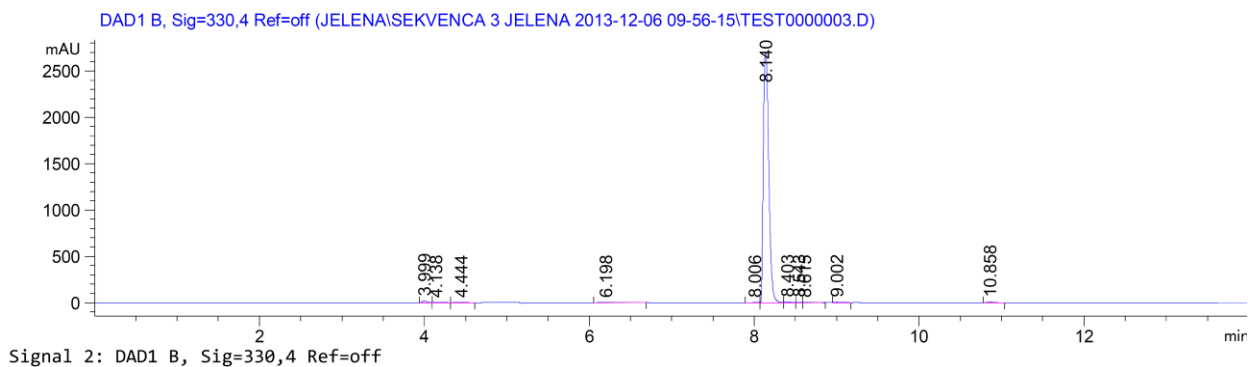
Method A



| Peak # | RetTime [min] | Type | Width [min] | Area [mAU*s] | Height [mAU] | Area % |
|--------|---------------|------|-------------|--------------|--------------|---------|
| 1 | 4.850 | BV | 0.1185 | 12.05899 | 1.20222 | 0.0931 |
| 2 | 5.092 | VV | 0.1232 | 22.98553 | 2.21302 | 0.1774 |
| 3 | 5.185 | VB | 0.0602 | 6.02563 | 1.29629 | 0.0465 |
| 4 | 8.865 | BV | 0.1306 | 68.79704 | 6.28988 | 0.5310 |
| 5 | 8.986 | VB | 0.0933 | 89.84259 | 14.59206 | 0.6934 |
| 6 | 10.165 | BV | 0.0758 | 12.86007 | 2.44710 | 0.0992 |
| 7 | 10.408 | VV | 0.1058 | 1.25434e4 | 1869.86841 | 96.8059 |
| 8 | 11.096 | BB | 0.0682 | 6.48302 | 1.14317 | 0.0500 |
| 9 | 11.506 | BV | 0.0907 | 28.83651 | 4.11794 | 0.2226 |
| 10 | 11.757 | VV | 0.1681 | 64.71497 | 4.54664 | 0.4994 |
| 11 | 12.105 | VV | 0.3068 | 72.90954 | 2.79494 | 0.5627 |
| 12 | 12.954 | VB | 0.0869 | 28.35678 | 4.83394 | 0.2188 |

Totals : 1.29573e4 1915.34562

Method B

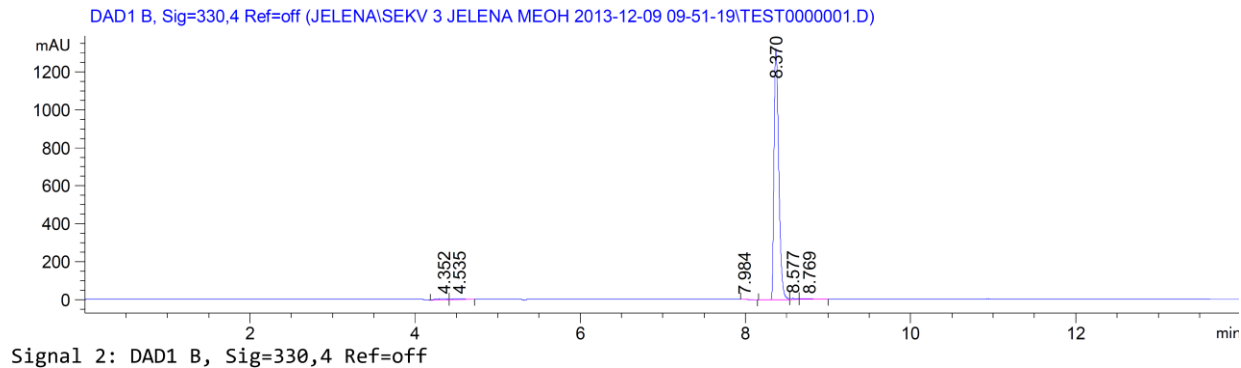


| Peak # | RetTime [min] | Type | Width [min] | Area [mAU*s] | Height [mAU] | Area % |
|--------|---------------|------|-------------|--------------|--------------|---------|
| 1 | 3.999 | BV | 0.0671 | 94.15331 | 21.30407 | 0.7341 |
| 2 | 4.138 | VV | 0.1166 | 43.08921 | 4.46536 | 0.3359 |
| 3 | 4.444 | VB | 0.1275 | 31.27032 | 2.96527 | 0.2438 |
| 4 | 6.198 | BB | 0.1530 | 58.01780 | 4.58770 | 0.4523 |
| 5 | 8.006 | BV | 0.0632 | 27.83480 | 6.21669 | 0.2170 |
| 6 | 8.140 | VV | 0.0724 | 1.23704e4 | 2704.55054 | 96.4456 |
| 7 | 8.403 | VV | 0.0893 | 71.28415 | 11.26316 | 0.5558 |
| 8 | 8.543 | VV | 0.0624 | 30.18333 | 6.91841 | 0.2353 |
| 9 | 8.615 | VB | 0.0775 | 33.58511 | 5.59406 | 0.2618 |
| 10 | 9.002 | VV | 0.0662 | 28.54764 | 6.14638 | 0.2226 |
| 11 | 10.858 | BB | 0.0665 | 37.93799 | 8.85370 | 0.2958 |

Totals : 1.28263e4 2782.86534

Compound: 9

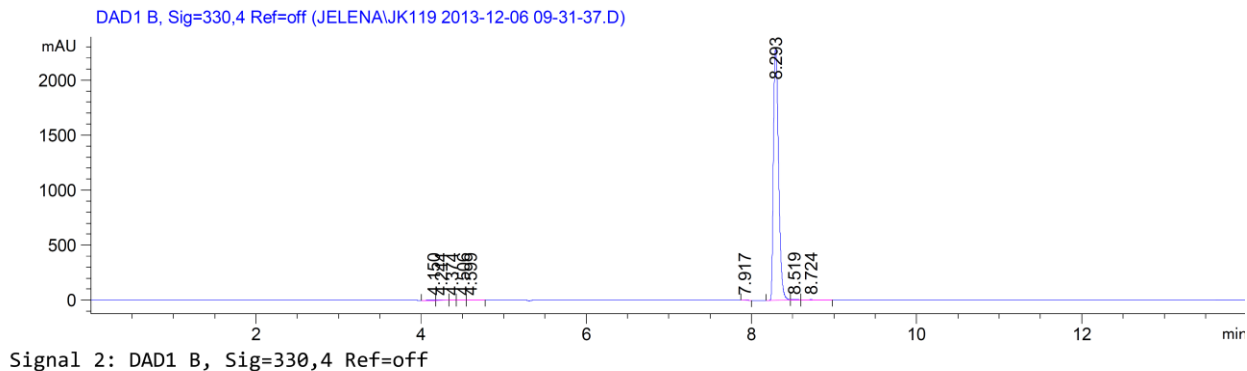
Method A



| Peak # | RetTime [min] | Type | Width [min] | Area [mAU*s] | Height [mAU] | Area % |
|--------|---------------|------|-------------|--------------|--------------|---------|
| 1 | 4.352 | BV | 0.1243 | 57.48040 | 5.46058 | 1.0512 |
| 2 | 4.535 | VB | 0.1316 | 52.48553 | 4.72408 | 0.9598 |
| 3 | 7.984 | BB | 0.0690 | 8.03986 | 1.61602 | 0.1470 |
| 4 | 8.370 | BV | 0.0616 | 5289.68652 | 1325.03345 | 96.7339 |
| 5 | 8.577 | VV | 0.0726 | 30.47131 | 5.58997 | 0.5572 |
| 6 | 8.769 | VB | 0.1543 | 30.12488 | 2.33077 | 0.5509 |

Totals : 5468.28849 1344.75486

Method B

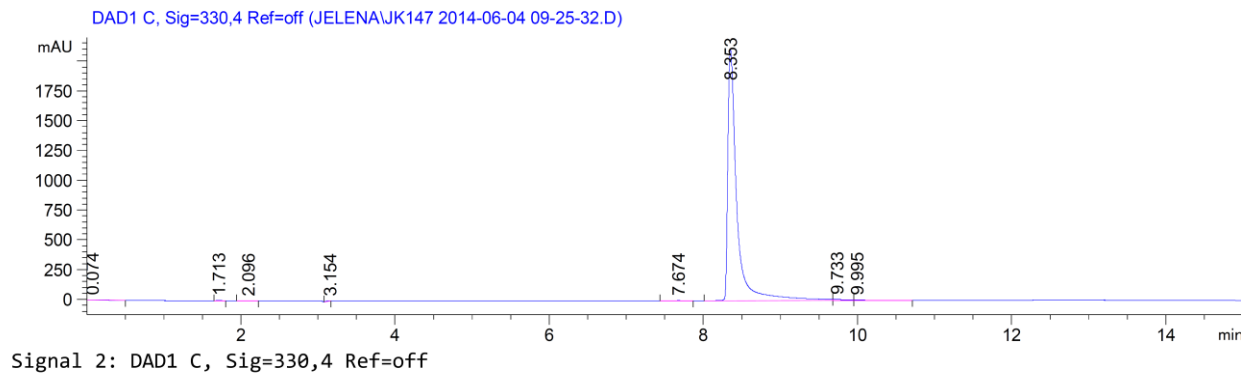


| Peak # | RetTime [min] | Type | Width [min] | Area [mAU*s] | Height [mAU] | Area % |
|--------|---------------|------|-------------|--------------|--------------|---------|
| 1 | 4.150 | BV | 0.0873 | 45.32769 | 6.16115 | 0.4460 |
| 2 | 4.244 | VV | 0.0958 | 43.91695 | 5.61102 | 0.4321 |
| 3 | 4.374 | VB | 0.0496 | 7.37839 | 2.04480 | 0.0726 |
| 4 | 4.506 | BV | 0.0527 | 6.91900 | 1.57619 | 0.0681 |
| 5 | 4.599 | VB | 0.0947 | 14.64486 | 1.99405 | 0.1441 |
| 6 | 7.917 | BB | 0.0474 | 10.53126 | 3.41979 | 0.1036 |
| 7 | 8.293 | BV | 0.0683 | 9942.72656 | 2281.36108 | 97.8319 |
| 8 | 8.519 | VV | 0.0791 | 49.58509 | 9.02305 | 0.4879 |
| 9 | 8.724 | VB | 0.1409 | 42.04624 | 3.62201 | 0.4137 |

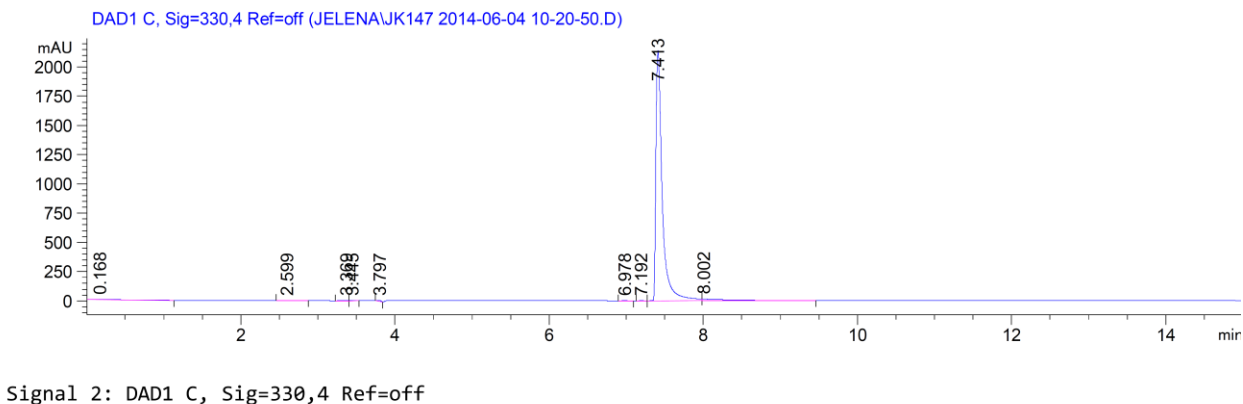
Totals : 1.01631e4 2314.81313

Compound: 12

Method A

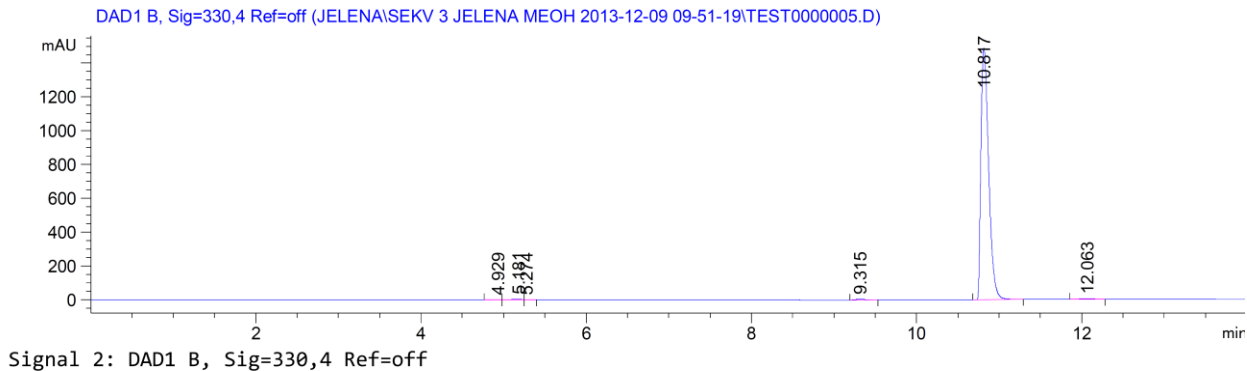


Method B

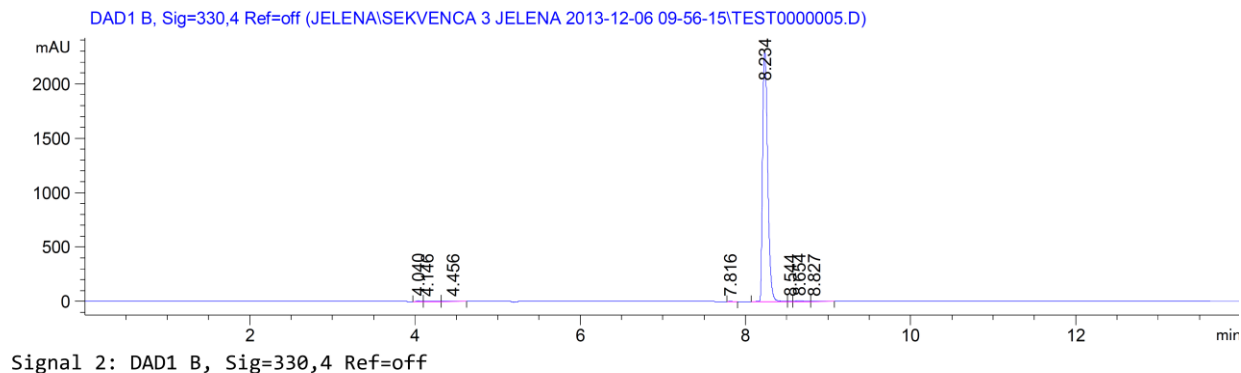


Compound: 13

Method A

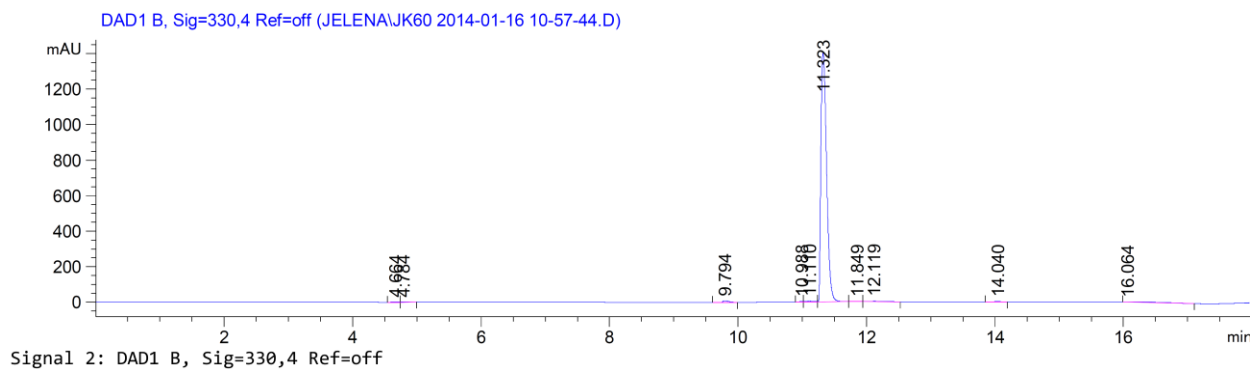


Method B

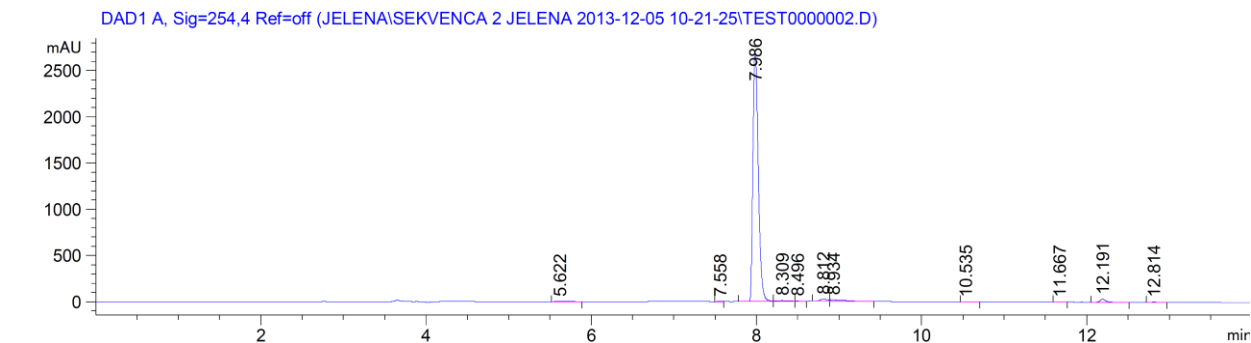


Compound: 23

Method A



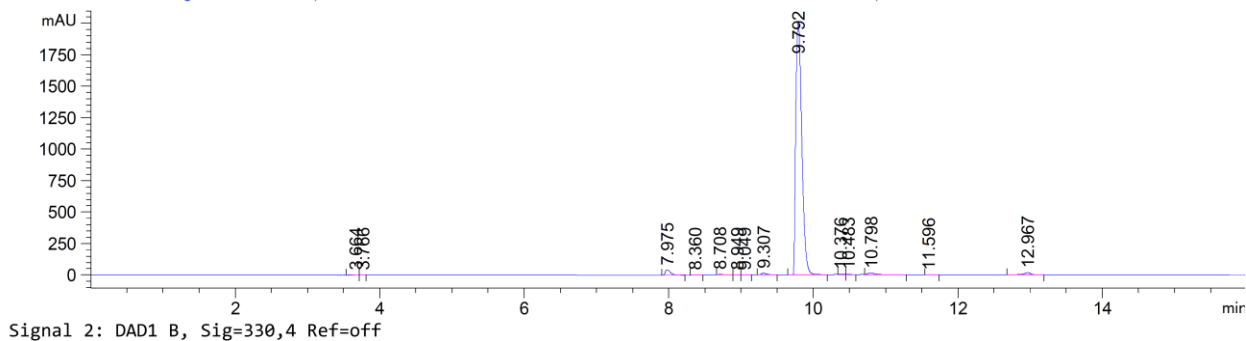
Method B



Compound: 24

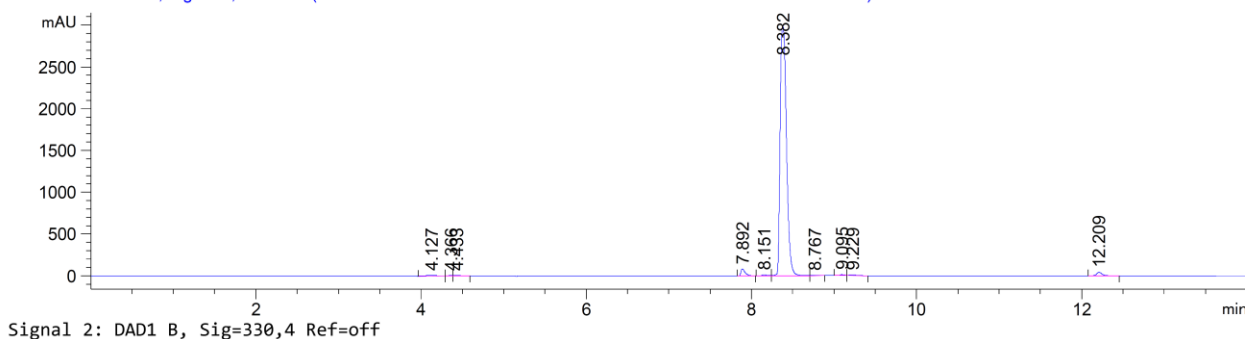
Method A

DAD1 B, Sig=330,4 Ref=off (JELENA\SEKV 7 JELENA MEOH 2014-01-15 13-34-19\TEST0000001.D)



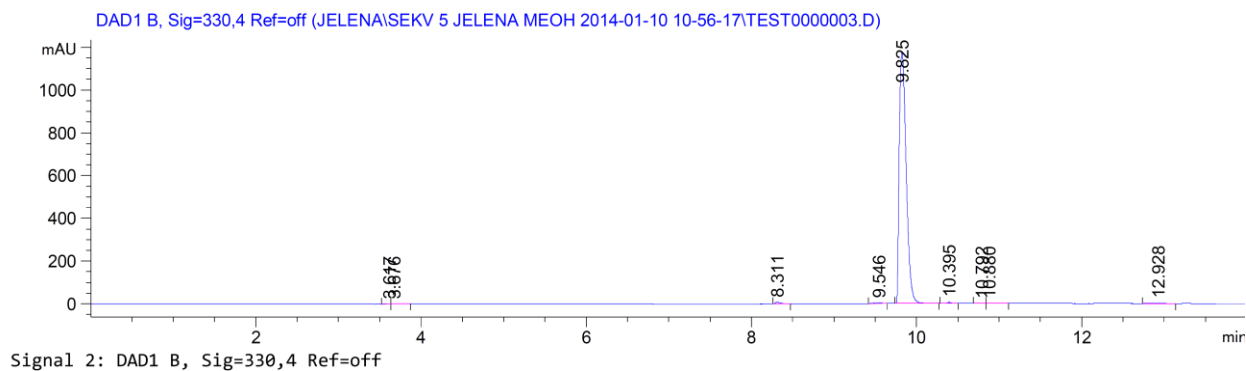
Method B

DAD1 B, Sig=330,4 Ref=off (JELENA\SEKVENCA 3 JELENA 2013-12-06 09-56-15\TEST0000006.D)



Compound: 25

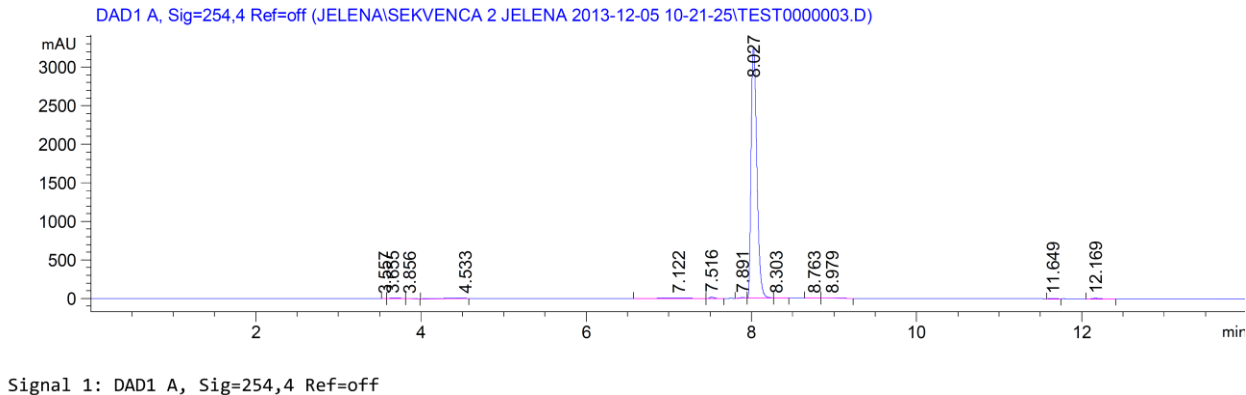
Method A



| Peak # | RetTime [min] | Type | Width [min] | Area [mAU*s] | Height [mAU] | Area % |
|--------|---------------|------|-------------|--------------|--------------|---------|
| 1 | 3.617 | BV | 0.0505 | 9.37448 | 2.25364 | 0.1340 |
| 2 | 3.676 | VB | 0.0847 | 14.90127 | 2.23736 | 0.2131 |
| 3 | 8.311 | VB | 0.0742 | 39.13313 | 8.04708 | 0.5596 |
| 4 | 9.546 | BB | 0.0928 | 29.24839 | 4.00034 | 0.4182 |
| 5 | 9.825 | BB | 0.0931 | 6851.14600 | 1174.38684 | 97.9665 |
| 6 | 10.395 | BB | 0.0227 | 13.68492 | 7.53647 | 0.1957 |
| 7 | 10.792 | VV | 0.0836 | 9.87055 | 1.40295 | 0.1411 |
| 8 | 10.880 | VB | 0.0773 | 9.74870 | 1.57217 | 0.1394 |
| 9 | 12.928 | BB | 0.0831 | 16.24894 | 2.61204 | 0.2323 |

Totals : 6993.35639 1204.04889

Method B



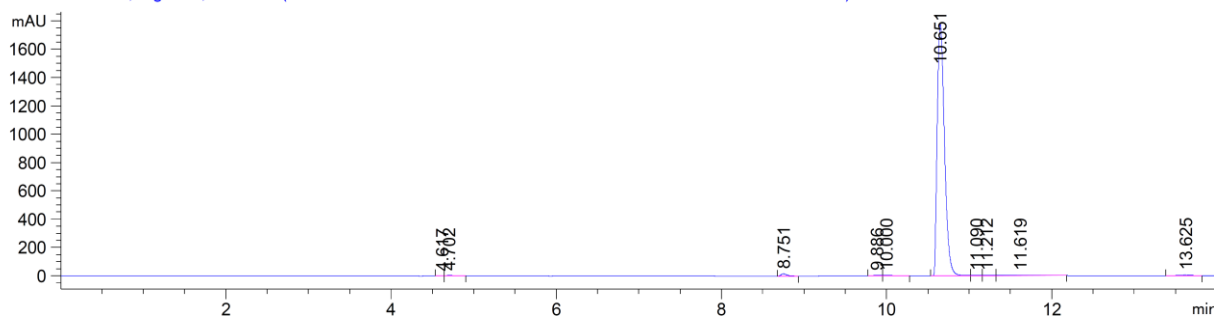
| Peak # | RetTime [min] | Type | Width [min] | Area [mAU*s] | Height [mAU] | Area % |
|--------|---------------|------|-------------|--------------|--------------|---------|
| 1 | 3.557 | BV | 0.0368 | 7.45170 | 3.07264 | 0.0453 |
| 2 | 3.655 | VV | 0.1398 | 77.40693 | 7.00958 | 0.4704 |
| 3 | 3.856 | VB | 0.0833 | 31.95885 | 5.22805 | 0.1942 |
| 4 | 4.533 | BB | 0.3180 | 214.98785 | 8.12900 | 1.3066 |
| 5 | 7.122 | BB | 0.2686 | 92.61446 | 4.06795 | 0.5629 |
| 6 | 7.516 | BB | 0.0513 | 54.86071 | 16.51079 | 0.3334 |
| 7 | 7.891 | BV | 0.0584 | 36.18497 | 9.19101 | 0.2199 |
| 8 | 8.027 | VV | 0.0676 | 1.58162e4 | 3257.52295 | 96.1242 |
| 9 | 8.303 | VB | 0.0713 | 26.08952 | 5.17310 | 0.1586 |
| 10 | 8.763 | BV | 0.0728 | 9.52312 | 1.67680 | 0.0579 |
| 11 | 8.979 | VB | 0.1424 | 40.52629 | 3.51855 | 0.2463 |
| 12 | 11.649 | BV | 0.0633 | 9.24310 | 2.14548 | 0.0562 |
| 13 | 12.169 | BB | 0.0674 | 36.87713 | 8.28553 | 0.2241 |

Totals : 1.64539e4 3331.53142

Compound: 26

Method A

DAD1 B, Sig=330,4 Ref=off (JELENA\SEKV 3 JELENA MEOH 2013-12-09 09-51-19\TEST0000002.D)



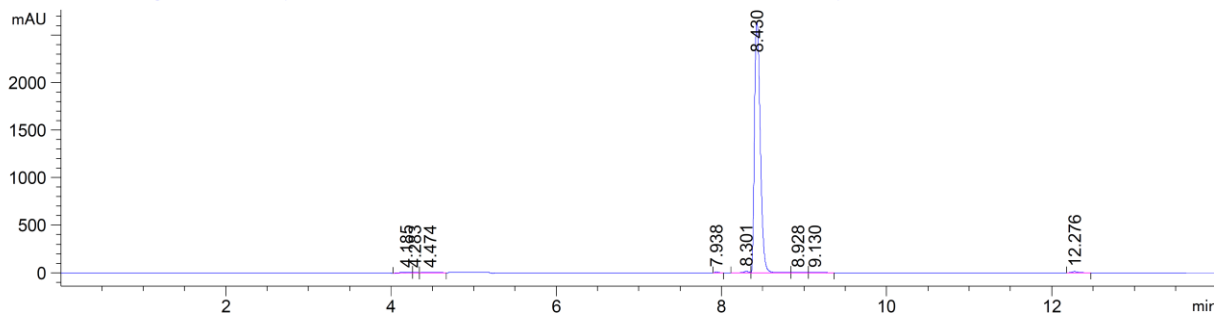
Signal 2: DAD1 B, Sig=330,4 Ref=off

| Peak # | RetTime [min] | Type | Width [min] | Area [mAU*s] | Height [mAU] | Area % |
|--------|---------------|------|-------------|--------------|--------------|---------|
| 1 | 4.617 | BV | 0.0554 | 7.51402 | 1.87047 | 0.0675 |
| 2 | 4.702 | VB | 0.0986 | 21.65252 | 2.60144 | 0.1946 |
| 3 | 8.751 | BB | 0.0759 | 79.05142 | 15.65897 | 0.7105 |
| 4 | 9.886 | BV | 0.0829 | 29.91393 | 5.21826 | 0.2689 |
| 5 | 10.000 | VB | 0.0964 | 30.30073 | 4.18722 | 0.2723 |
| 6 | 10.651 | BV | 0.0972 | 1.08238e4 | 1774.77820 | 97.2785 |
| 7 | 11.090 | VV | 0.0813 | 17.35509 | 2.58638 | 0.1560 |
| 8 | 11.212 | VV | 0.0998 | 16.42139 | 1.95930 | 0.1476 |
| 9 | 11.619 | VB | 0.2318 | 64.19098 | 3.25205 | 0.5769 |
| 10 | 13.625 | BB | 0.0865 | 36.40666 | 5.98266 | 0.3272 |

Totals : 1.11266e4 1818.09495

Method B

DAD1 B, Sig=330,4 Ref=off (JELENA\SEKVENCA 3 JELENA 2013-12-06 09-56-15\TEST0000002.D)



Signal 2: DAD1 B, Sig=330,4 Ref=off

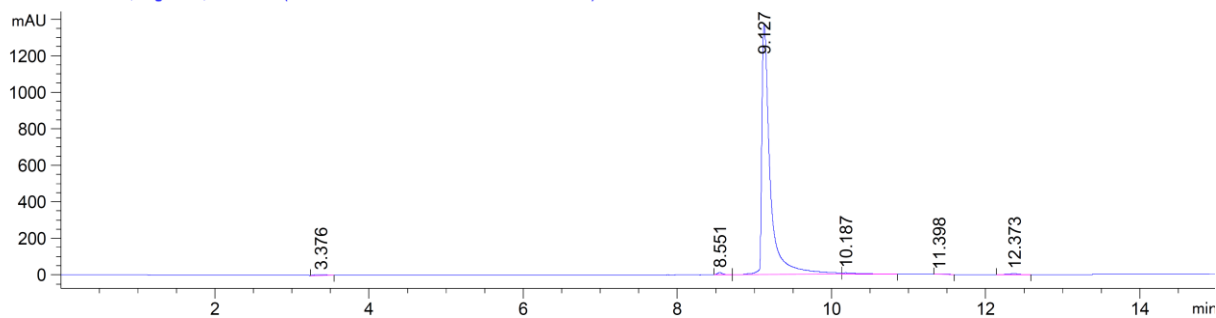
| Peak # | RetTime [min] | Type | Width [min] | Area [mAU*s] | Height [mAU] | Area % |
|--------|---------------|------|-------------|--------------|--------------|---------|
| 1 | 4.185 | BV | 0.1262 | 72.88445 | 6.92958 | 0.5492 |
| 2 | 4.283 | VV | 0.0562 | 23.05473 | 5.05257 | 0.1737 |
| 3 | 4.474 | VB | 0.1468 | 55.43713 | 4.48294 | 0.4177 |
| 4 | 7.938 | BV | 0.0474 | 39.08035 | 12.89380 | 0.2945 |
| 5 | 8.301 | BV | 0.0724 | 81.92766 | 16.95385 | 0.6173 |
| 6 | 8.430 | VV | 0.0770 | 1.28938e4 | 2638.54663 | 97.1565 |
| 7 | 8.928 | VV | 0.1118 | 24.42923 | 2.61844 | 0.1841 |
| 8 | 9.130 | VB | 0.0905 | 25.61717 | 3.66795 | 0.1930 |
| 9 | 12.276 | BB | 0.0679 | 54.92933 | 12.23009 | 0.4139 |

Totals : 1.32711e4 2703.37585

Compound: 27

Method A

DAD1 C, Sig=330,4 Ref=off (JELENA\JK149 2014-07-21 16-44-33.D)



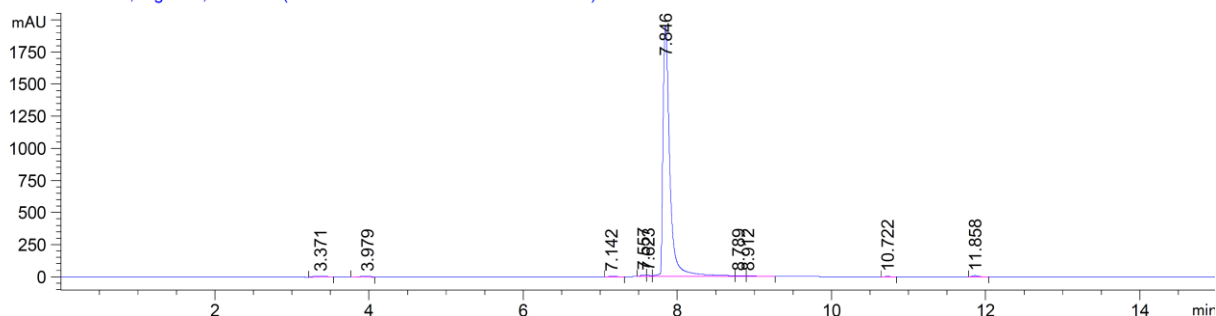
Signal 2: DAD1 C, Sig=330,4 Ref=off

| Peak # | RetTime [min] | Type | Width [min] | Area [mAU*s] | Height [mAU] | Area % |
|--------|---------------|------|-------------|--------------|--------------|---------|
| 1 | 3.376 | BB | 0.1286 | 37.46206 | 3.46634 | 0.3481 |
| 2 | 8.551 | VB | 0.0662 | 58.72265 | 12.74624 | 0.5457 |
| 3 | 9.127 | BV | 0.1110 | 1.04794e4 | 1373.59509 | 97.3772 |
| 4 | 10.187 | VB | 0.2017 | 143.71709 | 8.41833 | 1.3355 |
| 5 | 11.398 | BB | 0.0582 | 5.11887 | 1.07167 | 0.0476 |
| 6 | 12.373 | BB | 0.0892 | 37.23857 | 5.66381 | 0.3460 |

Totals : 1.07616e4 1404.96148

Method B

DAD1 C, Sig=330,4 Ref=off (JELENA\JK149 2014-07-21 17-19-34.D)



Signal 2: DAD1 C, Sig=330,4 Ref=off

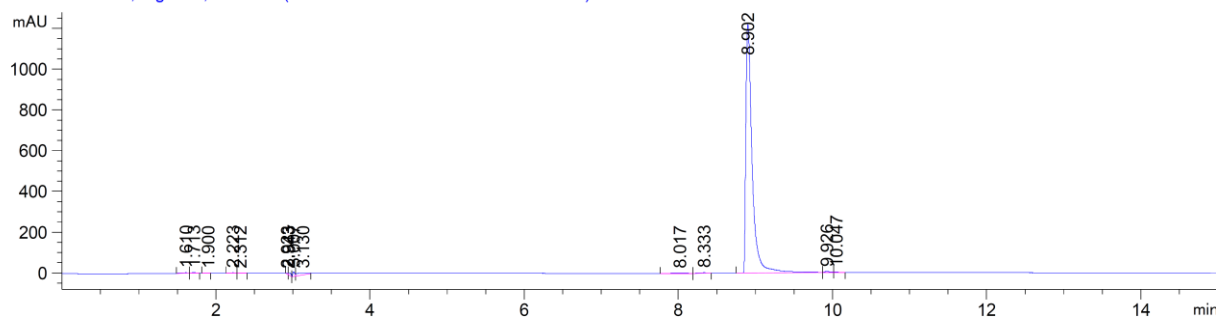
| Peak # | RetTime [min] | Type | Width [min] | Area [mAU*s] | Height [mAU] | Area % |
|--------|---------------|------|-------------|--------------|--------------|---------|
| 1 | 3.371 | BB | 0.1493 | 54.54555 | 4.33396 | 0.4380 |
| 2 | 3.979 | BB | 0.1362 | 43.53336 | 3.76921 | 0.3496 |
| 3 | 7.142 | BB | 0.0835 | 33.94343 | 5.61969 | 0.2726 |
| 4 | 7.557 | BV | 0.0688 | 53.47674 | 12.15959 | 0.4294 |
| 5 | 7.623 | VV | 0.0534 | 34.94339 | 8.98462 | 0.2806 |
| 6 | 7.846 | VV | 0.0937 | 1.21029e4 | 1956.65942 | 97.1804 |
| 7 | 8.789 | VV | 0.0937 | 44.77769 | 6.28099 | 0.3595 |
| 8 | 8.912 | VB | 0.1204 | 41.32400 | 4.14327 | 0.3318 |
| 9 | 10.722 | BB | 0.0551 | 5.33902 | 1.28228 | 0.0429 |
| 10 | 11.858 | VB | 0.0663 | 39.26548 | 8.93423 | 0.3153 |

Totals : 1.24540e4 2012.16725

Compound: 28

Method A

DAD1 C, Sig=330,4 Ref=off (JELENA\KB11 2014-05-14 16-33-57.D)



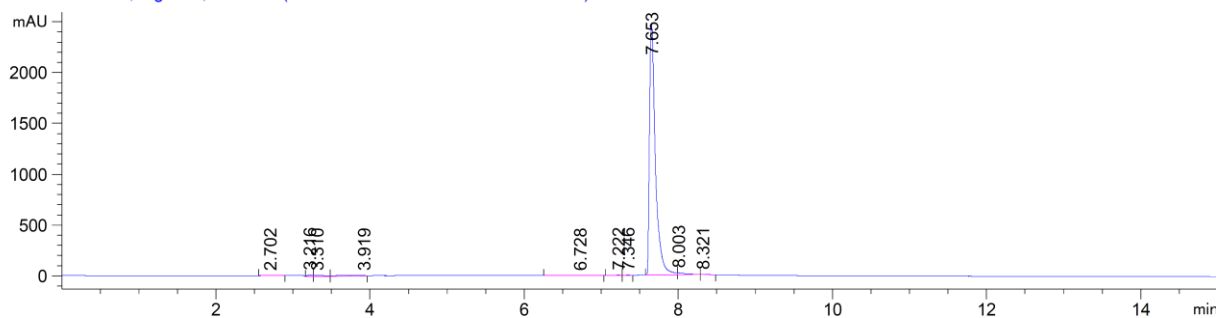
Signal 2: DAD1 C, Sig=330,4 Ref=off

| Peak # | RetTime [min] | Type | Width [min] | Area [mAU*s] | Height [mAU] | Area % |
|--------|---------------|------|-------------|--------------|--------------|---------|
| 1 | 1.610 | BB | 0.0779 | 15.70328 | 2.58483 | 0.2156 |
| 2 | 1.713 | BV | 0.0513 | 12.59033 | 3.04276 | 0.1729 |
| 3 | 1.900 | VV | 0.0643 | 9.27365 | 1.76377 | 0.1274 |
| 4 | 2.223 | VV | 0.0677 | 10.39338 | 1.99806 | 0.1427 |
| 5 | 2.312 | VV | 0.0659 | 6.52515 | 1.27125 | 0.0896 |
| 6 | 2.923 | BV | 0.0229 | 5.54642 | 3.41748 | 0.0762 |
| 7 | 2.943 | VB | 0.0422 | 26.24262 | 7.53159 | 0.3604 |
| 8 | 3.007 | BV | 0.0277 | 38.72638 | 21.87623 | 0.5318 |
| 9 | 3.130 | VV | 0.1229 | 91.16618 | 8.79532 | 1.2520 |
| 10 | 8.017 | VB | 0.1427 | 16.69414 | 1.37970 | 0.2293 |
| 11 | 8.333 | BB | 0.0752 | 16.95468 | 2.87798 | 0.2328 |
| 12 | 8.902 | BV | 0.0855 | 6996.87158 | 1219.09692 | 96.0861 |
| 13 | 9.926 | VV | 0.0699 | 27.38257 | 5.37854 | 0.3760 |
| 14 | 10.047 | VV | 0.0694 | 7.80772 | 1.44832 | 0.1072 |

Totals : 7281.87809 1282.46276

Method B

DAD1 B, Sig=254,4 Ref=off (JELENA\KB11 2014-05-16 13-31-27.D)



Signal 1: DAD1 B, Sig=254,4 Ref=off

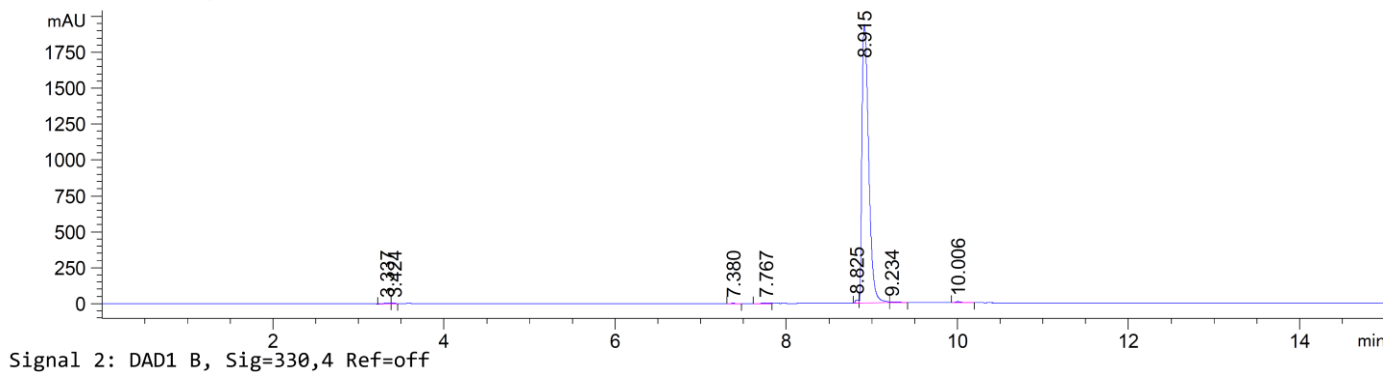
| Peak # | RetTime [min] | Type | Width [min] | Area [mAU*s] | Height [mAU] | Area % |
|--------|---------------|------|-------------|--------------|--------------|---------|
| 1 | 2.702 | BB | 0.1061 | 9.49930 | 1.05988 | 0.0688 |
| 2 | 3.216 | BV | 0.0634 | 49.92383 | 12.14818 | 0.3614 |
| 3 | 3.310 | VV | 0.1107 | 77.92776 | 8.47815 | 0.5642 |
| 4 | 3.919 | VB | 0.2681 | 172.10172 | 7.76571 | 1.2460 |
| 5 | 6.728 | BB | 0.2594 | 59.97980 | 2.72341 | 0.4342 |
| 6 | 7.222 | BV | 0.0990 | 23.79228 | 3.05056 | 0.1722 |
| 7 | 7.346 | VB | 0.0686 | 10.72035 | 1.96540 | 0.0776 |
| 8 | 7.653 | BV | 0.0813 | 1.32674e4 | 2464.38770 | 96.0514 |
| 9 | 8.003 | VB | 0.1029 | 128.24153 | 16.54515 | 0.9284 |
| 10 | 8.321 | BB | 0.0638 | 13.22463 | 2.89726 | 0.0957 |

Totals : 1.38128e4 2521.02139

Compound: 29

Method A

DAD1 B, Sig=330,4 Ref=off (JELENA\KB09 2014-05-06 15-21-55.D)

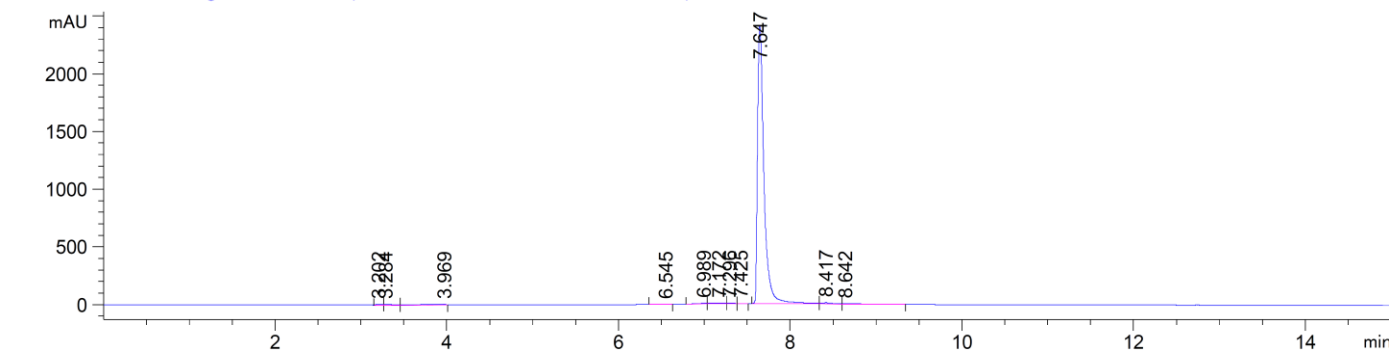


| Peak # | RetTime [min] | Type | Width [min] | Area [mAU*s] | Height [mAU] | Area % |
|--------|---------------|------|-------------|--------------|--------------|---------|
| 1 | 3.337 | BV | 0.0872 | 25.04193 | 3.62127 | 0.2336 |
| 2 | 3.424 | VB | 0.0548 | 5.00681 | 1.12849 | 0.0467 |
| 3 | 7.380 | BB | 0.0482 | 5.18607 | 1.32440 | 0.0484 |
| 4 | 7.767 | BV | 0.0729 | 10.99308 | 1.82142 | 0.1026 |
| 5 | 8.825 | BV | 0.0401 | 59.87083 | 23.63365 | 0.5586 |
| 6 | 8.915 | VV | 0.0853 | 1.05243e4 | 1941.10217 | 98.1950 |
| 7 | 9.234 | VB | 0.0827 | 45.85837 | 6.83856 | 0.4279 |
| 8 | 10.006 | VB | 0.0749 | 41.49577 | 8.01592 | 0.3872 |

Totals : 1.07178e4 1987.48589

Method B

DAD1 B, Sig=254,4 Ref=off (JELENA\KB09 2014-05-16 12-52-58.D)



Signal 1: DAD1 B, Sig=254,4 Ref=off

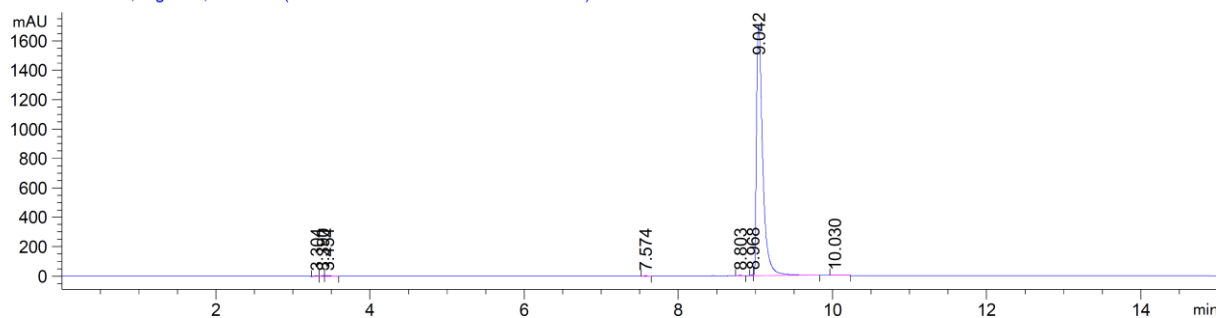
| Peak # | RetTime [min] | Type | Width [min] | Area [mAU*s] | Height [mAU] | Area % |
|--------|---------------|------|-------------|--------------|--------------|---------|
| 1 | 3.202 | BV | 0.0764 | 52.98580 | 10.40431 | 0.4002 |
| 2 | 3.284 | VV | 0.0877 | 55.00214 | 7.53007 | 0.4154 |
| 3 | 3.969 | VB | 0.2957 | 170.33707 | 6.94471 | 1.2864 |
| 4 | 6.545 | BB | 0.0887 | 11.36586 | 1.54739 | 0.0858 |
| 5 | 6.989 | BV | 0.0933 | 48.44630 | 6.94798 | 0.3659 |
| 6 | 7.172 | VV | 0.1366 | 101.32356 | 9.08473 | 0.7652 |
| 7 | 7.296 | VV | 0.0696 | 33.77491 | 6.14939 | 0.2551 |
| 8 | 7.425 | VB | 0.0690 | 13.18127 | 2.36600 | 0.0995 |
| 9 | 7.647 | BV | 0.0795 | 1.25998e4 | 2410.41748 | 95.1541 |
| 10 | 8.417 | VV | 0.1227 | 99.51318 | 10.87686 | 0.7515 |
| 11 | 8.642 | VB | 0.1922 | 55.73877 | 3.40944 | 0.4209 |

Totals : 1.32414e4 2475.67835

Compound: 30

Method A

DAD1 C, Sig=330,4 Ref=off (JELENA\KB10 2014-05-14 15-58-23.D)



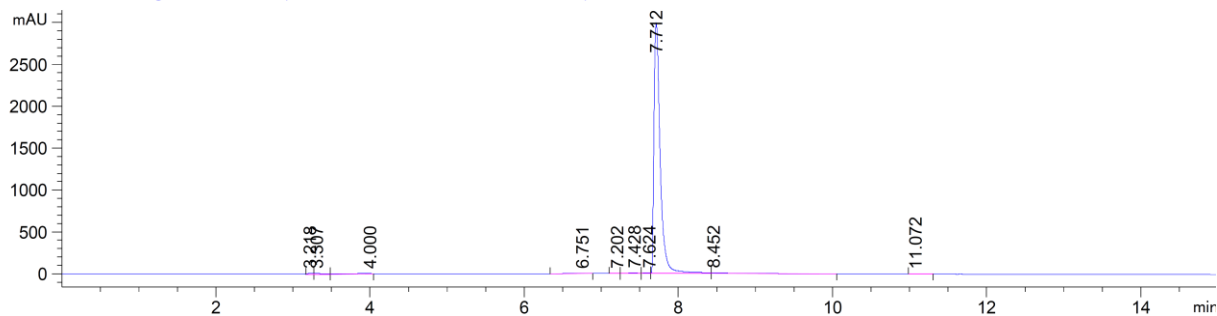
Signal 2: DAD1 C, Sig=330,4 Ref=off

| Peak # | RetTime [min] | Type | Width [min] | Area [mAU*s] | Height [mAU] | Area % |
|--------|---------------|------|-------------|--------------|--------------|---------|
| 1 | 3.304 | BV | 0.0493 | 16.06239 | 4.23136 | 0.1669 |
| 2 | 3.390 | VV | 0.0467 | 11.89283 | 3.13706 | 0.1236 |
| 3 | 3.454 | VB | 0.0773 | 18.19798 | 2.84010 | 0.1891 |
| 4 | 7.574 | BV | 0.0485 | 7.66518 | 2.35465 | 0.0796 |
| 5 | 8.803 | BV | 0.0545 | 13.79927 | 3.88356 | 0.1434 |
| 6 | 8.968 | BV | 0.0280 | 11.70945 | 6.65575 | 0.1217 |
| 7 | 9.042 | VV | 0.0842 | 9537.06250 | 1706.78528 | 99.0906 |
| 8 | 10.030 | BB | 0.0879 | 8.19428 | 1.11260 | 0.0851 |

Totals : 9624.58387 1731.00036

Method B

DAD1 B, Sig=254,4 Ref=off (JELENA\KB10 2014-05-16 13-13-48.D)



Signal 1: DAD1 B, Sig=254,4 Ref=off

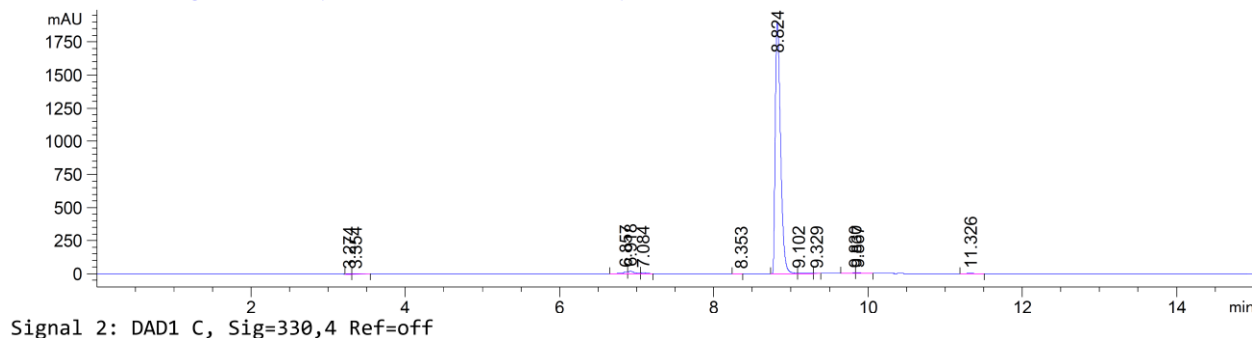
| Peak # | RetTime [min] | Type | Width [min] | Area [mAU*s] | Height [mAU] | Area % |
|--------|---------------|------|-------------|--------------|--------------|---------|
| 1 | 3.218 | BV | 0.0672 | 52.70157 | 11.89874 | 0.3043 |
| 2 | 3.307 | VV | 0.0993 | 67.16257 | 8.21857 | 0.3879 |
| 3 | 4.000 | VB | 0.3056 | 162.46524 | 6.37006 | 0.9382 |
| 4 | 6.751 | BV | 0.2007 | 23.72937 | 1.38993 | 0.1370 |
| 5 | 7.202 | BV | 0.0586 | 6.79644 | 1.42566 | 0.0392 |
| 6 | 7.428 | VB | 0.1261 | 28.87228 | 2.75825 | 0.1667 |
| 7 | 7.624 | BV | 0.0659 | 21.37490 | 4.42103 | 0.1234 |
| 8 | 7.712 | VV | 0.0848 | 1.67501e4 | 2992.34570 | 96.7285 |
| 9 | 8.452 | VB | 0.2838 | 192.19623 | 8.02754 | 1.1099 |
| 10 | 11.072 | BV | 0.0648 | 11.21800 | 2.41173 | 0.0648 |

Totals : 1.73166e4 3039.26721

Compound: 31

Method A

DAD1 C, Sig=330,4 Ref=off (JELENA\KB18 2014-12-19 11-59-28.D)

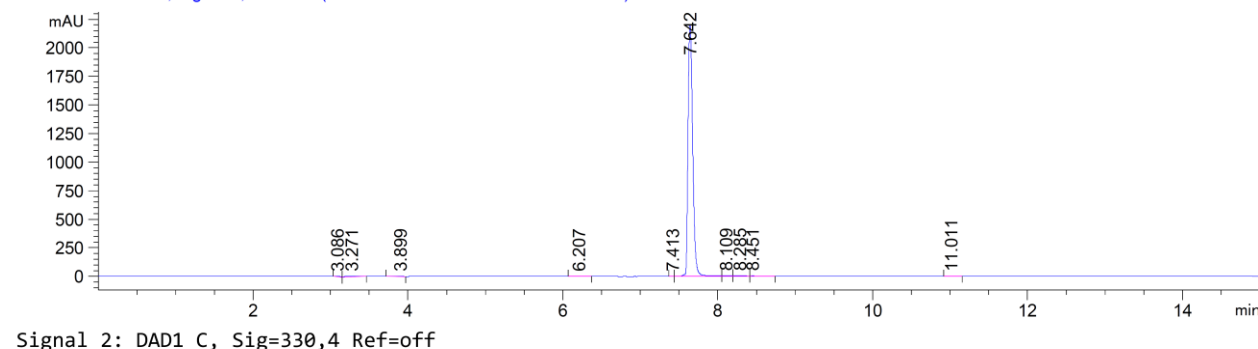


| Peak # | RetTime [min] | Type | Width [min] | Area [mAU*s] | Height [mAU] | Area % |
|--------|---------------|------|-------------|--------------|--------------|---------|
| 1 | 3.274 | BV | 0.0493 | 10.80486 | 2.91279 | 0.1149 |
| 2 | 3.354 | VB | 0.0990 | 24.59103 | 2.94322 | 0.2615 |
| 3 | 6.857 | BV | 0.0663 | 60.44729 | 12.41429 | 0.6428 |
| 4 | 6.918 | VV | 0.0740 | 97.95042 | 18.87545 | 1.0416 |
| 5 | 7.084 | VB | 0.0541 | 30.88347 | 8.35320 | 0.3284 |
| 6 | 8.353 | BV | 0.0611 | 5.07837 | 1.01095 | 0.0540 |
| 7 | 8.824 | BV | 0.0744 | 9083.40430 | 1897.02832 | 96.5961 |
| 8 | 9.102 | VV | 0.0853 | 18.90624 | 2.69666 | 0.2011 |
| 9 | 9.329 | VV | 0.0601 | 5.40396 | 1.09434 | 0.0575 |
| 10 | 9.830 | BV | 0.0487 | 21.79220 | 6.03165 | 0.2317 |
| 11 | 9.867 | VB | 0.0637 | 30.03695 | 6.71436 | 0.3194 |
| 12 | 11.326 | BB | 0.0685 | 14.19316 | 2.73837 | 0.1509 |

Totals : 9403.49227 1962.81359

Method B

DAD1 C, Sig=330,4 Ref=off (JELENA\KB18 2014-12-19 13-30-42.D)

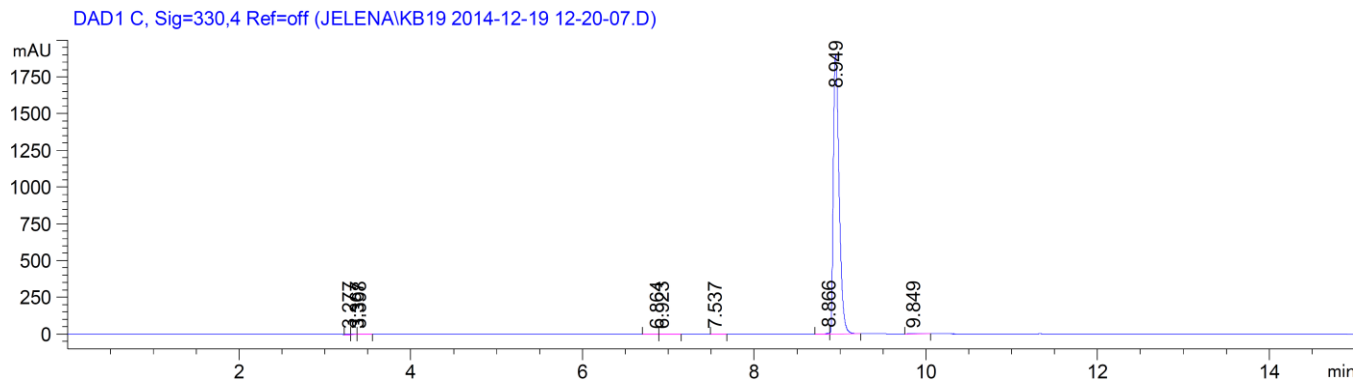


| Peak # | RetTime [min] | Type | Width [min] | Area [mAU*s] | Height [mAU] | Area % |
|--------|---------------|------|-------------|--------------|--------------|---------|
| 1 | 3.086 | BB | 0.0644 | 15.37207 | 2.87526 | 0.1604 |
| 2 | 3.271 | BB | 0.1461 | 71.78635 | 5.91384 | 0.7489 |
| 3 | 3.899 | BB | 0.1071 | 35.31371 | 3.90318 | 0.3684 |
| 4 | 6.207 | BB | 0.0936 | 11.34405 | 1.45344 | 0.1183 |
| 5 | 7.413 | BV | 0.0405 | 5.69019 | 2.01068 | 0.0594 |
| 6 | 7.642 | VV | 0.0663 | 9308.26074 | 2204.40454 | 97.1037 |
| 7 | 8.109 | VV | 0.0847 | 43.05571 | 7.00236 | 0.4492 |
| 8 | 8.285 | VV | 0.1146 | 58.04589 | 6.35468 | 0.6055 |
| 9 | 8.451 | VB | 0.0865 | 22.64468 | 3.36756 | 0.2362 |
| 10 | 11.011 | VV | 0.0601 | 14.38130 | 3.56447 | 0.1500 |

Totals : 9585.89468 2240.85000

Compound: 32

Method A

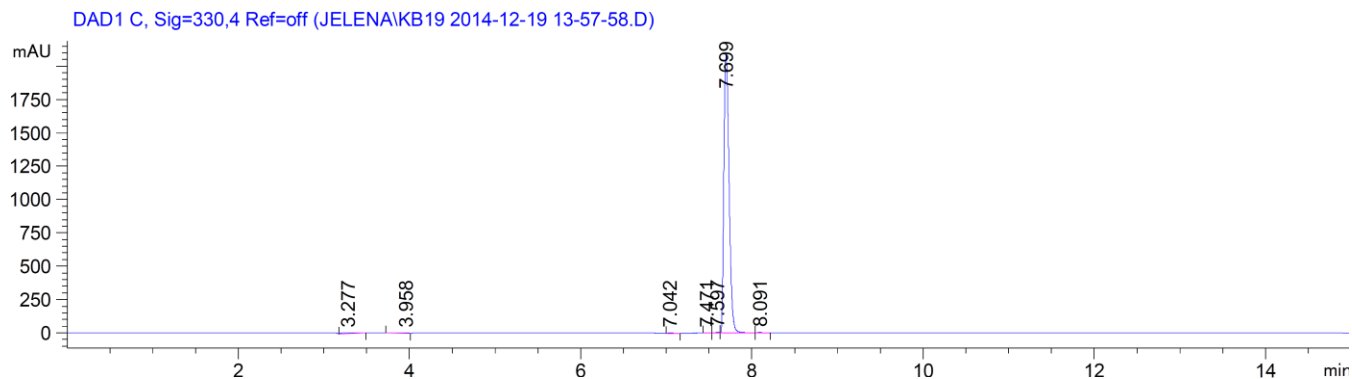


Signal 2: DAD1 C, Sig=330,4 Ref=off

| Peak # | RetTime [min] | Type | Width [min] | Area [mAU*s] | Height [mAU] | Area % |
|--------|---------------|------|-------------|--------------|--------------|---------|
| 1 | 3.277 | BV | 0.0440 | 11.43471 | 3.17432 | 0.1267 |
| 2 | 3.367 | VV | 0.0518 | 11.68167 | 2.71204 | 0.1294 |
| 3 | 3.398 | VB | 0.0707 | 14.61853 | 2.46387 | 0.1619 |
| 4 | 6.864 | BV | 0.0727 | 9.55289 | 1.58673 | 0.1058 |
| 5 | 6.923 | VV | 0.0863 | 12.87940 | 1.95542 | 0.1427 |
| 6 | 7.537 | BB | 0.0501 | 8.28078 | 2.40734 | 0.0917 |
| 7 | 8.866 | BV | 0.0401 | 17.60524 | 7.04945 | 0.1950 |
| 8 | 8.949 | VV | 0.0727 | 8931.37207 | 1904.48181 | 98.9348 |
| 9 | 9.849 | BB | 0.0682 | 10.10827 | 1.92651 | 0.1120 |

Totals : 9027.53357 1927.75751

Method B



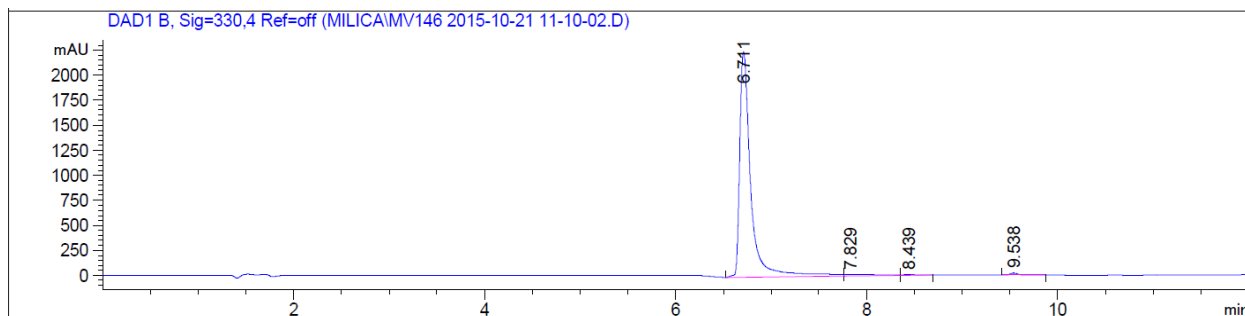
Signal 2: DAD1 C, Sig=330,4 Ref=off

| Peak # | RetTime [min] | Type | Width [min] | Area [mAU*s] | Height [mAU] | Area % |
|--------|---------------|------|-------------|--------------|--------------|---------|
| 1 | 3.277 | BB | 0.1383 | 77.06673 | 6.57384 | 0.8579 |
| 2 | 3.958 | VB | 0.1217 | 37.16552 | 3.65288 | 0.4137 |
| 3 | 7.042 | BB | 0.0436 | 7.98812 | 2.69098 | 0.0889 |
| 4 | 7.471 | VB | 0.0455 | 5.80909 | 1.90782 | 0.0647 |
| 5 | 7.597 | BV | 0.0583 | 14.32890 | 3.57426 | 0.1595 |
| 6 | 7.699 | VV | 0.0669 | 8829.40625 | 2084.87109 | 98.2832 |
| 7 | 8.091 | VB | 0.0631 | 11.87412 | 2.53636 | 0.1322 |

Totals : 8983.63873 2105.80724

Compound: 37

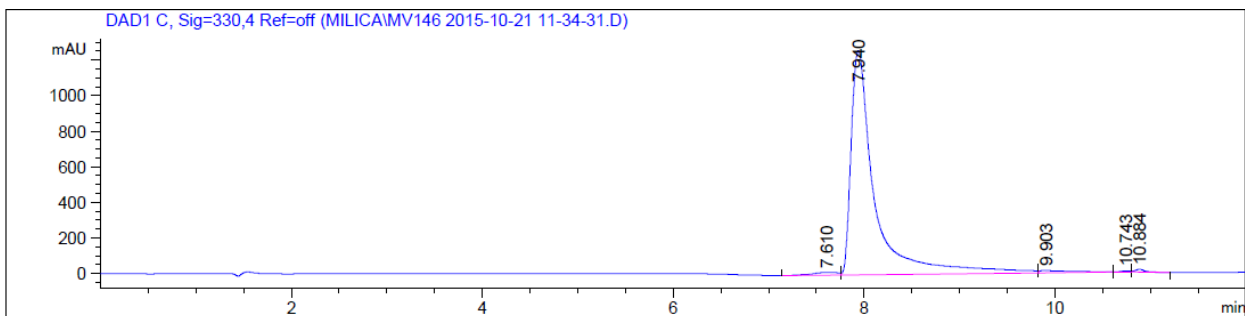
Method E



| Peak # | RetTime [min] | Type | Width [min] | Area [mAU*s] | Height [mAU] | Area % |
|--------|---------------|------|-------------|--------------|--------------|---------|
| 1 | 6.711 | BV | 0.1195 | 1.82389e4 | 2252.57471 | 96.6559 |
| 2 | 7.829 | VV | 0.2625 | 397.60565 | 17.98081 | 2.1071 |
| 3 | 8.439 | VB | 0.1208 | 99.11401 | 11.24984 | 0.5252 |
| 4 | 9.538 | BB | 0.0940 | 134.30275 | 20.89571 | 0.7117 |

Totals : 1.88699e4 2302.70107

Method F

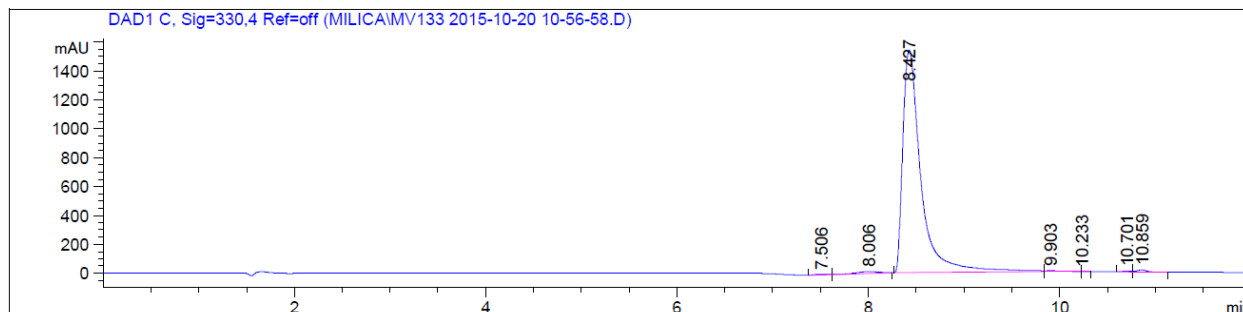


| Peak # | RetTime [min] | Type | Width [min] | Area [mAU*s] | Height [mAU] | Area % |
|--------|---------------|------|-------------|--------------|--------------|---------|
| 1 | 7.610 | BV | 0.2310 | 294.36676 | 14.99576 | 1.3172 |
| 2 | 7.940 | VV | 0.2484 | 2.16302e4 | 1259.08069 | 96.7885 |
| 3 | 9.903 | VB | 0.2489 | 268.31442 | 12.70510 | 1.2006 |
| 4 | 10.743 | BV | 0.0781 | 43.19379 | 6.75414 | 0.1933 |
| 5 | 10.884 | VB | 0.1038 | 111.83592 | 15.94952 | 0.5004 |

Totals : 2.23479e4 1309.48521

Compound: 38

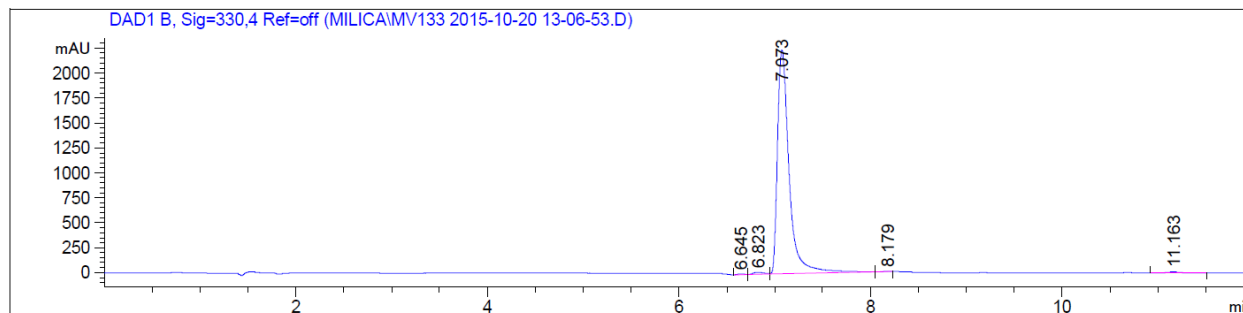
Method C



| Peak # | RetTime [min] | Type | Width [min] | Area [mAU*s] | Height [mAU] | Area % |
|--------|---------------|------|-------------|--------------|--------------|----------|
| 1 | 7.506 | BV | 0.1035 | 50.68055 | 5.88504 | 0.2439 |
| 2 | 8.006 | VB | 0.1723 | 195.34010 | 13.86675 | 0.9399 |
| 3 | 8.427 | BV | 0.1985 | 2.03127e4 | 1538.38354 | 97.7393 |
| 4 | 9.903 | VB | 0.1387 | 80.54507 | 6.87300 | 0.3876 |
| 5 | 10.233 | BB | 0.0317 | 4.16970e-1 | 1.72298e-1 | 2.006e-3 |
| 6 | 10.701 | BV | 0.0792 | 39.33719 | 6.58619 | 0.1893 |
| 7 | 10.859 | VB | 0.1012 | 103.50700 | 14.16939 | 0.4980 |

Totals : 2.07825e4 1585.93621

Method D

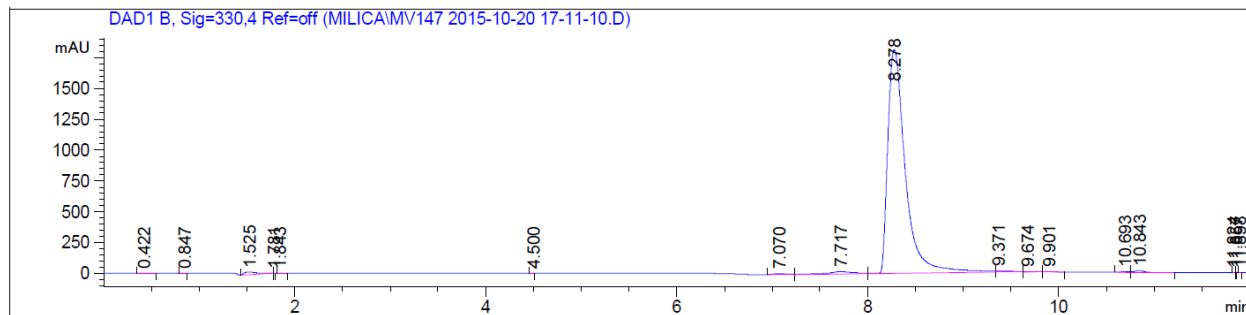


| Peak # | RetTime [min] | Type | Width [min] | Area [mAU*s] | Height [mAU] | Area % |
|--------|---------------|------|-------------|--------------|--------------|---------|
| 1 | 6.645 | BV | 0.0760 | 45.04110 | 8.68723 | 0.2325 |
| 2 | 6.823 | VV | 0.1168 | 178.07773 | 22.88065 | 0.9191 |
| 3 | 7.073 | VV | 0.1138 | 1.90274e4 | 2247.26343 | 98.2077 |
| 4 | 8.179 | VB | 0.1417 | 14.16832 | 1.17885 | 0.0731 |
| 5 | 11.163 | BV | 0.1225 | 109.96989 | 10.87646 | 0.5676 |

Totals : 1.93747e4 2290.88661

Compound: 39

Method C

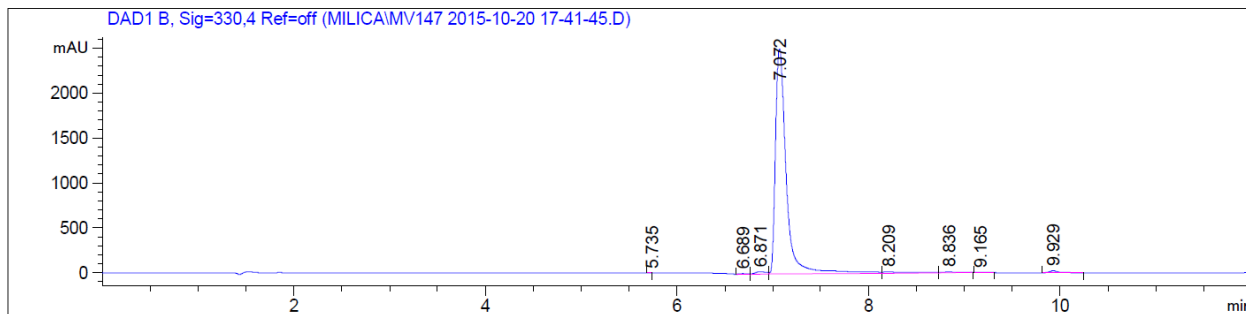


| Peak # | RetTime [min] | Type | Width [min] | Area [mAU*s] | Height [mAU] | Area % |
|--------|---------------|------|-------------|--------------|--------------|----------|
| 1 | 0.422 | BB | 0.0611 | 2.82612 | 5.53636e-1 | 0.0117 |
| 2 | 0.847 | BV | 0.0332 | 2.96316e-1 | 1.09217e-1 | 1.224e-3 |
| 3 | 1.525 | BV | 0.1431 | 210.84047 | 21.09748 | 0.8713 |
| 4 | 1.781 | VB | 9.10e-3 | 2.87732e-1 | 4.41475e-1 | 1.189e-3 |
| 5 | 1.843 | BB | 0.0523 | 1.02715 | 2.35891e-1 | 4.245e-3 |
| 6 | 4.500 | BB | 0.0206 | 1.37211e-1 | 8.59659e-2 | 5.670e-4 |
| 7 | 7.070 | BV | 0.1274 | 78.65191 | 8.23348 | 0.3250 |
| 8 | 7.717 | VV | 0.2327 | 376.93610 | 19.83461 | 1.5576 |
| 9 | 8.278 | VV | 0.1921 | 2.32117e4 | 1815.73730 | 95.9184 |
| 10 | 9.371 | VV | 0.1484 | 126.86670 | 10.10944 | 0.5243 |
| 11 | 9.674 | VB | 0.0869 | 24.97002 | 3.41009 | 0.1032 |
| 12 | 9.901 | BB | 0.0726 | 14.11047 | 2.34950 | 0.0583 |
| 13 | 10.693 | BV | 0.0754 | 40.38631 | 6.93634 | 0.1669 |
| 14 | 10.843 | VB | 0.1015 | 108.59284 | 15.07354 | 0.4487 |
| 15 | 11.824 | BB | 0.0111 | 1.02296 | 1.31299 | 4.227e-3 |
| 16 | 11.857 | BB | 5.50e-3 | 1.64866e-1 | 4.80579e-1 | 6.813e-4 |

17 11.898 BB 8.09e-3 6.00064e-1 1.25231 2.480e-3

Totals : 2.41994e4 1907.25384

Method D

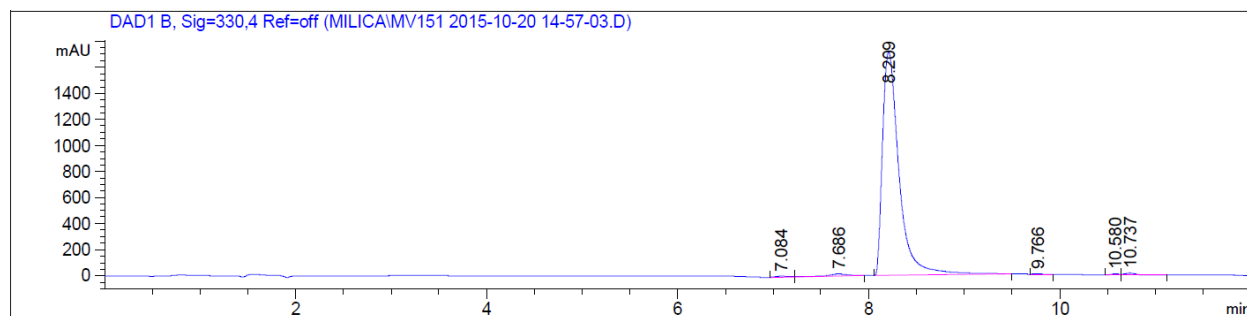


| Peak # | RetTime [min] | Type | Width [min] | Area [mAU*s] | Height [mAU] | Area % |
|--------|---------------|------|-------------|--------------|--------------|----------|
| 1 | 5.735 | BB | 0.0240 | 1.07254e-1 | 5.57080e-2 | 5.243e-4 |
| 2 | 6.689 | BV | 0.0761 | 35.09261 | 6.81063 | 0.1716 |
| 3 | 6.871 | VV | 0.1151 | 208.44798 | 26.55494 | 1.0190 |
| 4 | 7.072 | VV | 0.1089 | 1.97024e4 | 2500.60498 | 96.3184 |
| 5 | 8.209 | VV | 0.2473 | 301.50256 | 14.45508 | 1.4739 |
| 6 | 8.836 | VB | 0.1063 | 83.81390 | 10.47714 | 0.4097 |
| 7 | 9.165 | BB | 0.0662 | 1.79404 | 3.28806e-1 | 8.770e-3 |
| 8 | 9.929 | BB | 0.0911 | 122.33539 | 20.34780 | 0.5981 |

Totals : 2.04555e4 2579.63507

Compound: 40

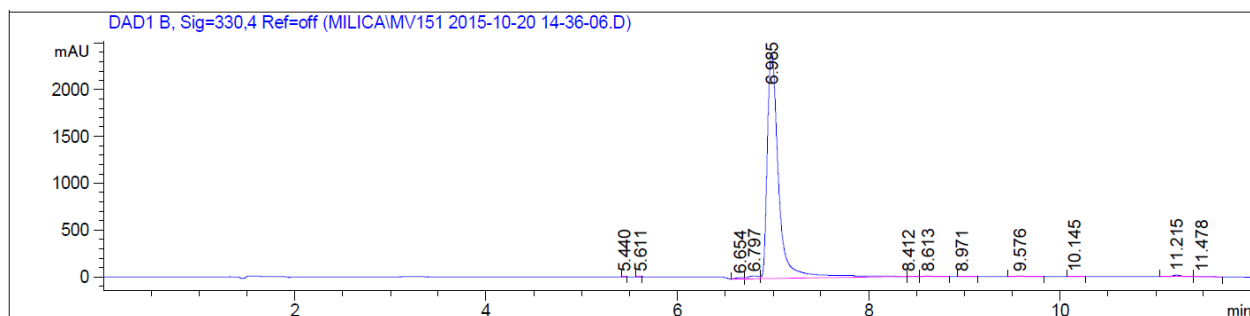
Method C



| Peak # | RetTime [min] | Type | Width [min] | Area [mAU*s] | Height [mAU] | Area % |
|--------|---------------|------|-------------|--------------|--------------|---------|
| 1 | 7.084 | BV | 0.1096 | 62.42950 | 7.50396 | 0.2966 |
| 2 | 7.686 | VB | 0.1675 | 196.83829 | 15.10379 | 0.9353 |
| 3 | 8.209 | BB | 0.1824 | 2.06286e4 | 1714.65063 | 98.0206 |
| 4 | 9.766 | BB | 0.0717 | 13.48948 | 2.27542 | 0.0641 |
| 5 | 10.580 | BV | 0.0724 | 39.16399 | 6.53230 | 0.1861 |
| 6 | 10.737 | VB | 0.1066 | 104.63895 | 14.10237 | 0.4972 |

Totals : 2.10452e4 1760.16847

Method D

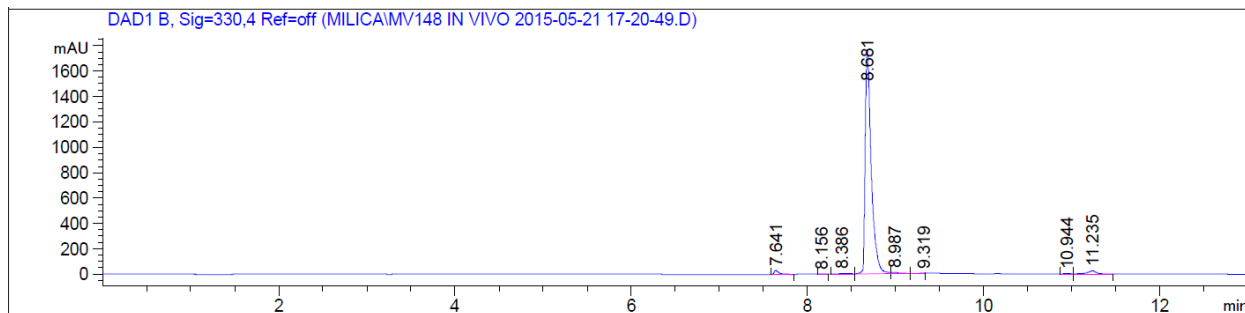


| Peak # | RetTime [min] | Type | Width [min] | Area [mAU*s] | Height [mAU] | Area % |
|--------|---------------|------|-------------|--------------|--------------|----------|
| 1 | 5.440 | BB | 0.0218 | 1.00664e-1 | 5.79854e-2 | 4.883e-4 |
| 2 | 5.611 | BB | 0.0220 | 1.14201e-1 | 6.50129e-2 | 5.540e-4 |
| 3 | 6.654 | BV | 0.0846 | 87.79340 | 15.84885 | 0.4259 |
| 4 | 6.797 | VV | 0.1108 | 249.82582 | 32.44704 | 1.2119 |
| 5 | 6.985 | VV | 0.1246 | 2.00783e4 | 2411.83472 | 97.4014 |
| 6 | 8.412 | VB | 0.0573 | 12.32068 | 2.66933 | 0.0598 |
| 7 | 8.613 | BB | 0.0702 | 16.85452 | 2.90565 | 0.0818 |
| 8 | 8.971 | BB | 0.0790 | 2.19960 | 3.31078e-1 | 0.0107 |
| 9 | 9.576 | BB | 0.0835 | 41.53010 | 7.01789 | 0.2015 |
| 10 | 10.145 | BB | 0.0679 | 1.91939 | 3.42590e-1 | 9.311e-3 |
| 11 | 11.215 | BV | 0.0941 | 113.18070 | 17.94900 | 0.5490 |
| 12 | 11.478 | VB | 0.0929 | 9.82690 | 1.30380 | 0.0477 |

Totals : 2.06140e4 2492.77293

Compound: 41

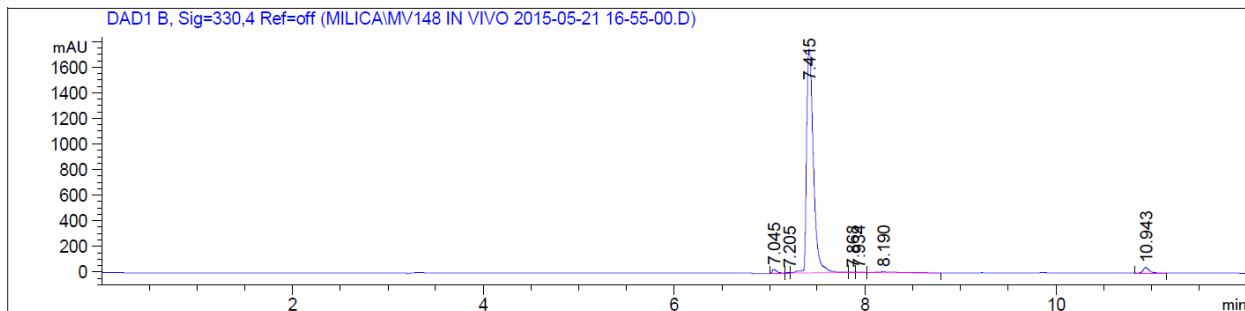
Method A



| Peak # | RetTime [min] | Type | Width [min] | Area [mAU*s] | Height [mAU] | Area % |
|--------|---------------|------|-------------|--------------|--------------|---------|
| 1 | 7.641 | BB | 0.0501 | 108.00912 | 31.43413 | 1.2242 |
| 2 | 8.156 | BB | 0.0447 | 7.95650 | 2.36894 | 0.0902 |
| 3 | 8.386 | BB | 0.0794 | 23.89058 | 3.93031 | 0.2708 |
| 4 | 8.681 | BV | 0.0716 | 8400.87695 | 1764.00928 | 95.2194 |
| 5 | 8.987 | VB | 0.0910 | 65.83261 | 10.30554 | 0.7462 |
| 6 | 9.319 | BV | 0.0675 | 17.72163 | 3.39033 | 0.2009 |
| 7 | 10.944 | VV | 0.0625 | 19.06977 | 3.70876 | 0.2161 |
| 8 | 11.235 | VB | 0.1043 | 179.29144 | 24.67681 | 2.0322 |

Totals : 8822.64861 1843.82410

Method B

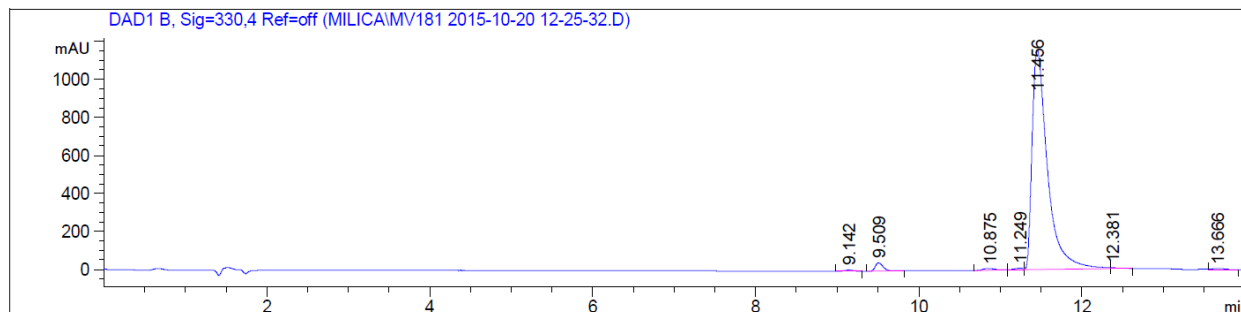


| Peak # | RetTime [min] | Type | Width [min] | Area [mAU*s] | Height [mAU] | Area % |
|--------|---------------|------|-------------|--------------|--------------|---------|
| 1 | 7.045 | BB | 0.0501 | 93.71075 | 29.83362 | 1.0323 |
| 2 | 7.205 | BV | 0.0317 | 6.64790 | 2.70537 | 0.0732 |
| 3 | 7.415 | VV | 0.0774 | 8691.20410 | 1751.03418 | 95.7429 |
| 4 | 7.868 | VV | 0.0573 | 15.86938 | 3.61076 | 0.1748 |
| 5 | 7.934 | VB | 0.0522 | 14.12953 | 3.57062 | 0.1557 |
| 6 | 8.190 | BB | 0.1407 | 69.97594 | 6.39396 | 0.7709 |
| 7 | 10.943 | BV | 0.0652 | 186.11200 | 42.81100 | 2.0502 |

Totals : 9077.64961 1839.95951

Compound: 42

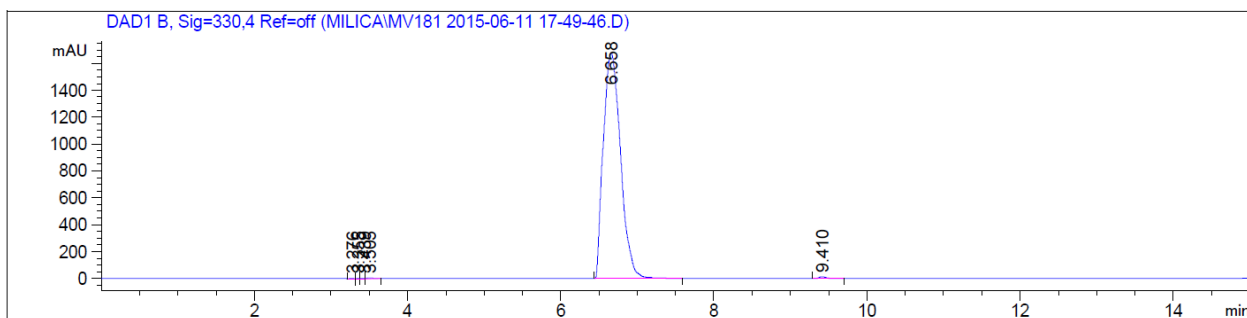
Method D



| Peak # | RetTime [min] | Type | Width [min] | Area [mAU*s] | Height [mAU] | Area % |
|--------|---------------|------|-------------|--------------|--------------|---------|
| 1 | 9.142 | BB | 0.0884 | 40.84436 | 6.54013 | 0.2585 |
| 2 | 9.509 | BB | 0.1027 | 281.94089 | 42.63459 | 1.7841 |
| 3 | 10.875 | BB | 0.1335 | 88.58769 | 8.10531 | 0.5606 |
| 4 | 11.249 | BV | 0.0864 | 51.77385 | 7.37327 | 0.3276 |
| 5 | 11.456 | VV | 0.1951 | 1.52084e4 | 1155.23315 | 96.2378 |
| 6 | 12.381 | VV | 0.1265 | 59.23616 | 5.57472 | 0.3748 |
| 7 | 13.666 | VB | 0.1326 | 72.15301 | 6.42168 | 0.4566 |

Totals : 1.58030e4 1231.88284

Method G

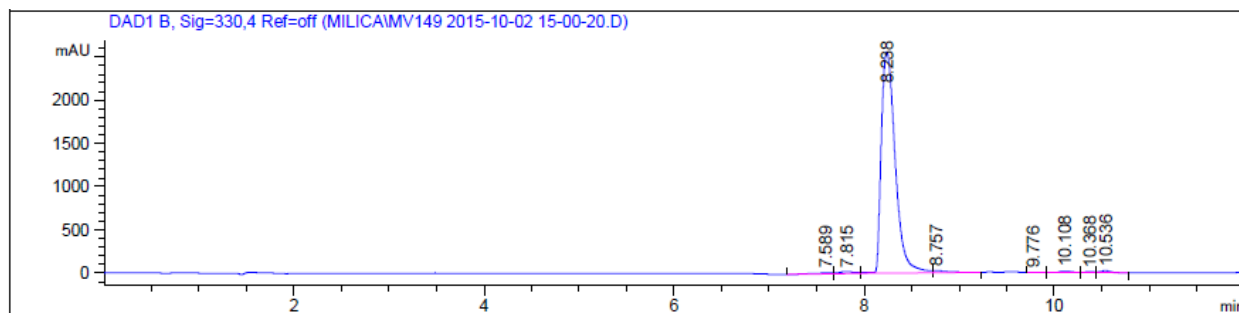


| Peak # | RetTime [min] | Type | Width [min] | Area [mAU*s] | Height [mAU] | Area % |
|--------|---------------|------|-------------|--------------|--------------|---------|
| 1 | 3.276 | BB | 0.0565 | 16.32383 | 4.95032 | 0.0619 |
| 2 | 3.355 | BV | 0.0352 | 7.34878 | 3.20923 | 0.0279 |
| 3 | 3.439 | VV | 0.0529 | 16.47764 | 4.18833 | 0.0625 |
| 4 | 3.505 | VB | 0.0779 | 29.29096 | 4.47131 | 0.1111 |
| 5 | 6.658 | BB | 0.2200 | 2.62094e4 | 1680.20728 | 99.4388 |
| 6 | 9.410 | BB | 0.0876 | 78.48502 | 13.65381 | 0.2978 |

Totals : 2.63574e4 1710.68028

Compound: 43

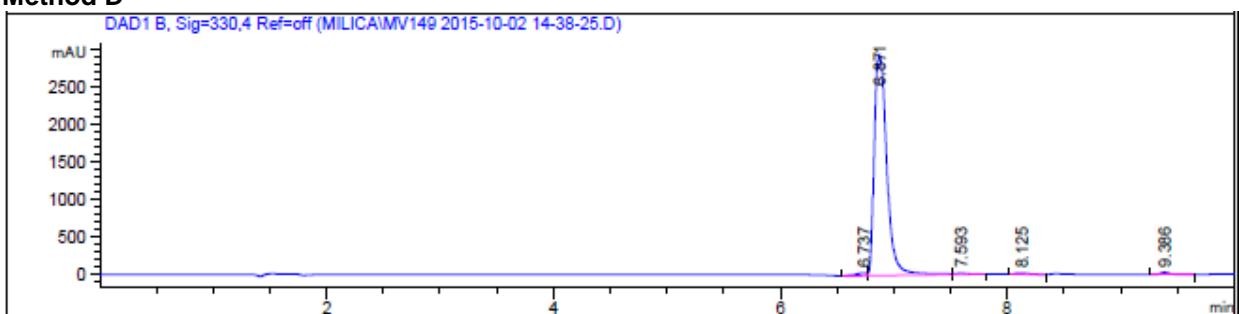
Method C



| Peak # | RetTime [min] | Type | Width [min] | Area [mAU*s] | Height [mAU] | Area % |
|--------|---------------|------|-------------|--------------|--------------|---------|
| 1 | 7.589 | BV | 0.1793 | 157.24036 | 10.37813 | 0.5796 |
| 2 | 7.815 | VV | 0.1532 | 260.49203 | 21.51618 | 0.9601 |
| 3 | 8.238 | VV | 0.1220 | 2.61074e4 | 2558.75122 | 96.2292 |
| 4 | 8.757 | VB | 0.1324 | 259.51468 | 23.12087 | 0.9565 |
| 5 | 9.776 | VB | 0.0797 | 16.24070 | 2.52059 | 0.0599 |
| 6 | 10.108 | BB | 0.1147 | 128.51112 | 16.34383 | 0.4737 |
| 7 | 10.368 | BV | 0.0879 | 49.34284 | 8.17360 | 0.1819 |
| 8 | 10.536 | VB | 0.1040 | 151.68288 | 21.44783 | 0.5591 |

Totals : 2.71304e4 2662.25225

Method D

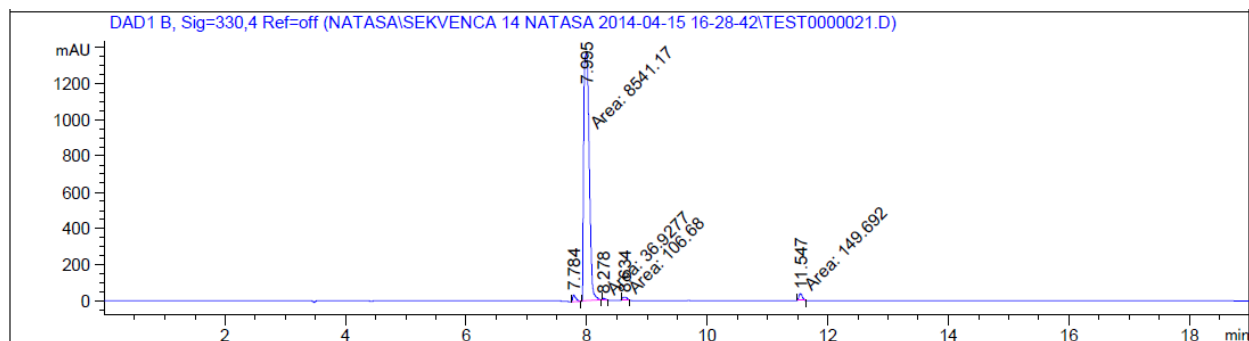


| Peak # | RetTime [min] | Type | Width [min] | Area [mAU*s] | Height [mAU] | Area % |
|--------|---------------|------|-------------|--------------|--------------|---------|
| 1 | 6.737 | BV | 0.0964 | 243.48349 | 37.20078 | 1.0436 |
| 2 | 6.871 | VV | 0.0929 | 2.26023e4 | 2934.04883 | 96.8746 |
| 3 | 7.593 | VB | 0.1159 | 150.26065 | 17.89824 | 0.6440 |
| 4 | 8.125 | BB | 0.1069 | 146.13326 | 20.19939 | 0.6263 |
| 5 | 9.386 | BV | 0.0844 | 189.32347 | 34.30740 | 0.8115 |

Totals : 2.33315e4 3043.65464

Compound: 44

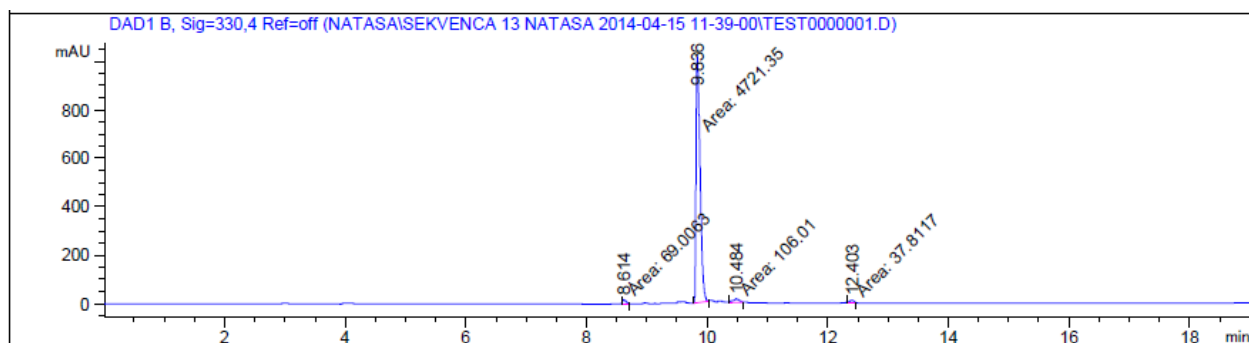
Method A



| Peak # | RetTime [min] | Type | Width [min] | Area [mAU*s] | Height [mAU] | Area % |
|--------|---------------|------|-------------|--------------|--------------|---------|
| 1 | 7.784 | BB | 0.0549 | 137.49791 | 36.94980 | 1.5325 |
| 2 | 7.995 | MM | 0.1044 | 8541.16699 | 1363.20300 | 95.1984 |
| 3 | 8.278 | MM | 0.0676 | 36.92768 | 9.09978 | 0.4116 |
| 4 | 8.634 | MM | 0.0909 | 106.68042 | 19.57051 | 1.1890 |
| 5 | 11.547 | MM | 0.0657 | 149.69228 | 37.99706 | 1.6684 |

Totals : 8971.96528 1466.82016

Method B

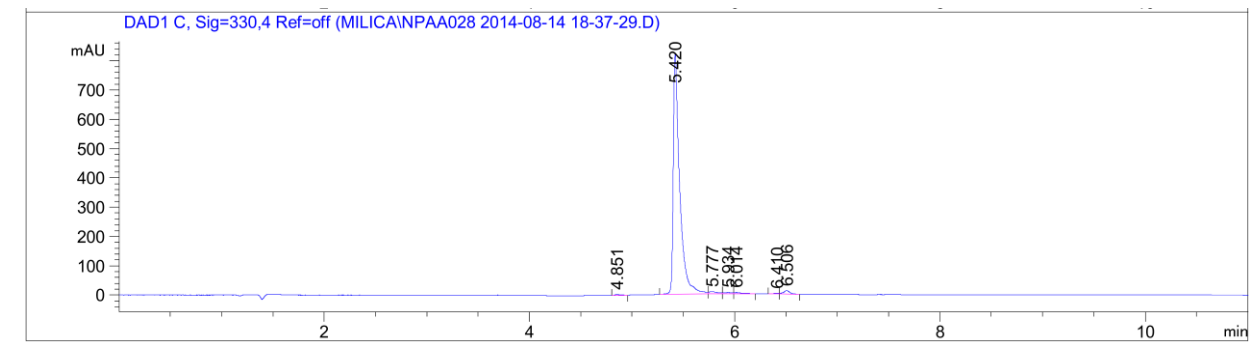


| Peak # | RetTime [min] | Type | Width [min] | Area [mAU*s] | Height [mAU] | Area % |
|--------|---------------|------|-------------|--------------|--------------|---------|
| 1 | 8.614 | MM | 0.0698 | 69.00631 | 16.48519 | 1.3985 |
| 2 | 9.836 | MM | 0.0770 | 4721.34766 | 1021.60065 | 95.6867 |
| 3 | 10.484 | MM | 0.1201 | 106.00954 | 14.70533 | 2.1485 |
| 4 | 12.403 | MM | 0.0679 | 37.81166 | 9.28764 | 0.7663 |

Totals : 4934.17516 1062.07880

Compound: 46

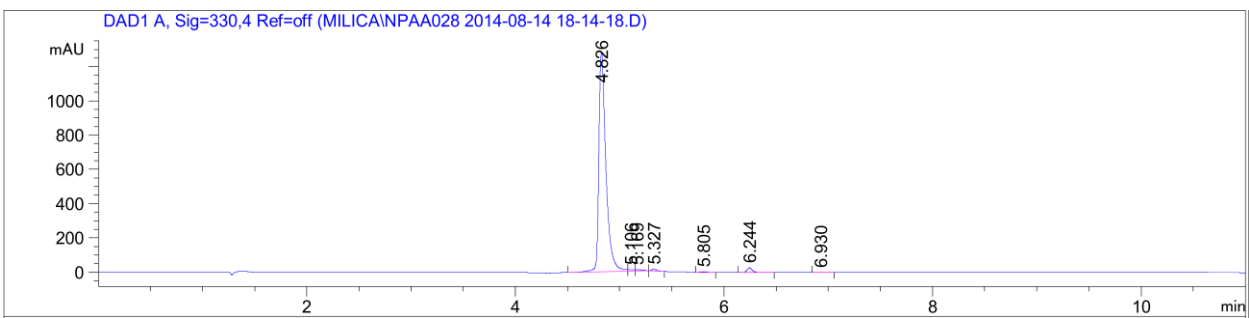
Method I



| Peak # | RetTime [min] | Type | Width [min] | Area [mAU*s] | Height [mAU] | Area % |
|--------|---------------|------|-------------|--------------|--------------|---------|
| 1 | 4.851 | BB | 0.0531 | 11.55937 | 3.20699 | 0.3092 |
| 2 | 5.420 | BV | 0.0611 | 3560.69458 | 821.58832 | 95.2354 |
| 3 | 5.777 | VV | 0.0796 | 51.85744 | 8.28047 | 1.3870 |
| 4 | 5.934 | VV | 0.0744 | 28.90337 | 4.86178 | 0.7731 |
| 5 | 6.014 | VB | 0.0706 | 25.86342 | 4.70832 | 0.6918 |
| 6 | 6.410 | BV | 0.0422 | 9.21101 | 2.64298 | 0.2464 |
| 7 | 6.506 | VB | 0.0626 | 50.74789 | 11.81134 | 1.3573 |

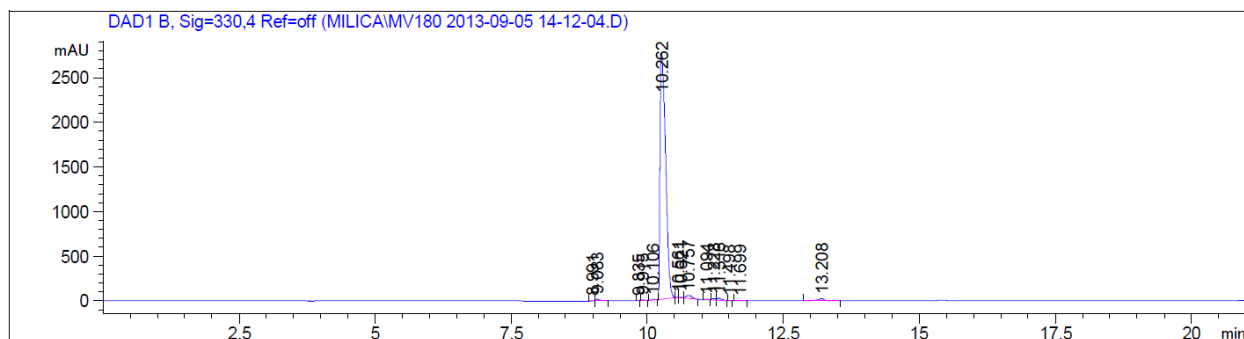
Totals : 3738.83708 857.10019

Method H



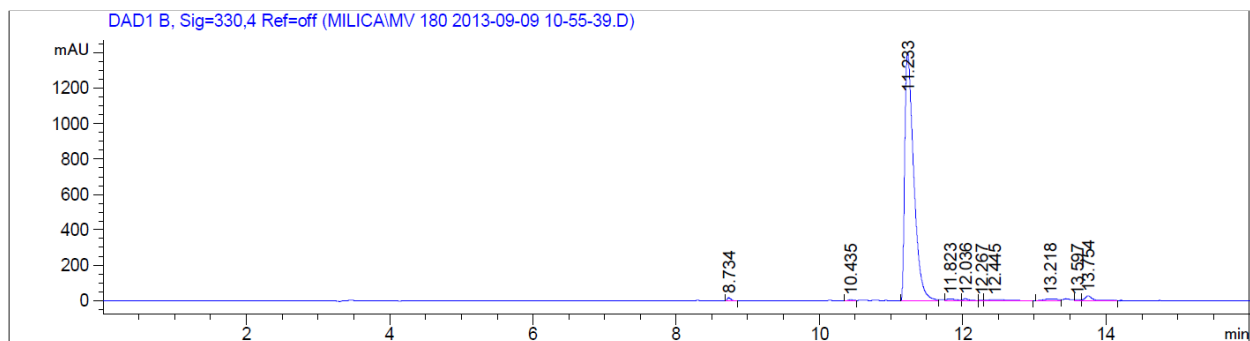
| Peak # | RetTime [min] | Type | Width [min] | Area [mAU*s] | Height [mAU] | Area % |
|--------|---------------|------|-------------|--------------|--------------|---------|
| 1 | 4.826 | BV | 0.0704 | 6058.60107 | 1287.40662 | 96.5369 |
| 2 | 5.106 | VV | 0.0529 | 37.04706 | 9.40642 | 0.5903 |
| 3 | 5.169 | VB | 0.0597 | 33.36654 | 7.67828 | 0.5317 |
| 4 | 5.327 | BB | 0.0535 | 34.47512 | 9.93727 | 0.5493 |
| 5 | 5.805 | BB | 0.0698 | 11.68613 | 2.42034 | 0.1862 |
| 6 | 6.244 | BB | 0.0532 | 94.46011 | 26.75001 | 1.5051 |
| 7 | 6.930 | BB | 0.0577 | 6.30531 | 1.52711 | 0.1005 |

Totals : 6275.94134 1345.12604

Compound: 52**Method A**

| Peak # | RetTime [min] | Type | Width [min] | Area [mAU*s] | Height [mAU] | Area % |
|--------|---------------|------|-------------|--------------|--------------|----------|
| 1 | 8.991 | BV | 0.0582 | 19.20522 | 4.90571 | 0.0934 |
| 2 | 9.083 | VV | 0.0714 | 116.13204 | 22.98373 | 0.5646 |
| 3 | 9.835 | BB | 0.0425 | 4.62732 | 1.79770 | 0.0225 |
| 4 | 9.915 | BB | 0.0548 | 23.58116 | 6.28665 | 0.1146 |
| 5 | 10.106 | BB | 0.0674 | 52.62742 | 11.61486 | 0.2559 |
| 6 | 10.262 | BB | 0.0970 | 1.96133e4 | 2758.01270 | 95.3572 |
| 7 | 10.561 | BV | 0.0388 | 20.52732 | 8.47703 | 0.0998 |
| 8 | 10.621 | VB | 0.0609 | 40.19218 | 9.69200 | 0.1954 |
| 9 | 10.757 | BB | 0.1171 | 245.83640 | 34.52837 | 1.1952 |
| 10 | 11.094 | BB | 0.0684 | 29.20466 | 7.04172 | 0.1420 |
| 11 | 11.228 | BV | 0.0688 | 64.26157 | 15.21992 | 0.3124 |
| 12 | 11.316 | VB | 0.0799 | 124.99713 | 22.99112 | 0.6077 |
| 13 | 11.498 | BB | 0.0396 | 1.01013 | 3.78477e-1 | 4.911e-3 |
| 14 | 11.699 | BB | 0.0980 | 6.47267 | 7.94974e-1 | 0.0315 |
| 15 | 13.208 | BB | 0.1227 | 206.26627 | 23.21161 | 1.0028 |

Totals : 2.05683e4 2927.93657

Method B

| Peak # | RetTime [min] | Type | Width [min] | Area [mAU*s] | Height [mAU] | Area % |
|--------|---------------|------|-------------|--------------|--------------|---------|
| 1 | 8.734 | BB | 0.0510 | 59.07262 | 17.68832 | 0.4644 |
| 2 | 10.435 | BV | 0.0698 | 26.55964 | 5.60821 | 0.2088 |
| 3 | 11.233 | BV | 0.1304 | 1.21063e4 | 1399.71387 | 95.1654 |
| 4 | 11.823 | VV | 0.1312 | 79.11050 | 8.72864 | 0.6219 |
| 5 | 12.036 | VB | 0.0730 | 48.03447 | 9.75311 | 0.3776 |
| 6 | 12.267 | BV | 0.0489 | 3.74937 | 1.20084 | 0.0295 |
| 7 | 12.445 | VB | 0.1986 | 94.13501 | 6.09839 | 0.7400 |
| 8 | 13.218 | BV | 0.1745 | 111.99912 | 7.59500 | 0.8804 |
| 9 | 13.597 | VV | 0.0710 | 23.11556 | 4.49778 | 0.1817 |
| 10 | 13.754 | VB | 0.0932 | 169.25041 | 26.26011 | 1.3304 |

Totals : 1.27213e4 1487.14425