Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Enantioselective Organocatalytic Michael Addition of Isorhodanines to α, β-Unsaturated Aldehydes

Supporting Information

Contents:

Preparation of substrates

To a solution of thiazolidine-2,4-dione (0.61 g, 5.2 mmol, 1.0 equiv) in dry toluene (12.0 mL) was added Lawesson's reagent (2.2 g, 5.2 mmol, 1.0 equiv). The reaction mixture was refluxed for 2 h and cooled to room temperature. The solid was filtered off and crystallized from acetone to afford isorhodanine (0.64 g, 98% yield) as a yellow crystal. ^{1}H NMR (600 MHz, DMSO-d_6, TMS): δ = 13.58 (s, 1H), 4.67 (s, 2H); MS (ESI) m/z: 134.24 $[M+H]^+$.

To a solution of isorhodanine (0.60 g, 4.5 mmol, 1.0 equiv) in DMF (10.0 mL) was added NaH (0.19 g, 4.9 mmol, 1.1 equiv) and the mixture was stirred for 0.5 h at 0 °C. Then, iodomethane (0.75 g, 4.5 mmol, 1.0 equiv) was added and the reaction mixture was stirred for 1 h. Water (30.0 mL) was added to the reaction mixture and extracted by ethyl acetate (15.0 mL × 3). The organic layer was dried over Na_2SO_4, and concentrated to give the crude product, which was further purified by column chromatography to yield the desired substrate **2a**. The synthetic method for substrates **2b-k** was similar to the synthesis of substrate **2a**. For substrate **2l**, 2 equivalent of iodomethane was used.

4-(Methylthio)thiazol-2(3*H*)-one (2a). ^{1}H NMR (600 MHz, DMSO-d_6, TMS): δ = 11.63 (s, 1H), 6.26 (s, 1H), 2.41 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$, TMS): δ = 174.47, 126.31, 103.30, 17.08; HRMS (ESI) calcd for $C_4H_6NO_2S_2$ $[M+H]^+$ = 148.2186, found 147.9435.

4-(Ethylthio)thiazol-2(3*H*)-one (2b). ^{1}H NMR (600 MHz, DMSO-d_6, TMS): δ = 11.60 (s, 1H), 6.46-6.47 (m, 1H), 2.85 (dd, J = 7.0, 14.6 Hz, 2H), 1.19 (t, J = 7.5 Hz, 3H); ^{13}C NMR (150 MHz, DMSO-d_6, TMS): δ = 172.69, 124.85, 105.00, 27.64, 14.75; HRMS (ESI) calcd for $C_5H_8NOS_2$ $[M+H]^+$ = 162.2452, found 162.2563.

4-((Naphthalen-2-ylmethyl)thio)thiazol-2(3*H*)-one (2c). ^{1}H NMR (600 MHz, $CDCl_3$, TMS): δ = 9.67 (s, 1H), 7.82-7.84 (m, 2H), 7.78-7.80 (m, 1H), 7.62 (s, 1H), 7.48-7.50 (m, 2H), 7.40 (dd, J = 1.8, 8.4 Hz, 1H), 6.03 (s, 1H), 4.13 (s, 2H); ^{13}C NMR (150 MHz, DMSO-d_6, TMS) δ = 133.52, 132.74, 132.19, 128.17,

127.25, 127.21, 126.10, 108.81, 39.72, 29.20; HRMS (ESI) calcd for $C_{14}H_{12}NOS_2$ $[M+H]^+$ = 274.0282, found 274.0364.

4-((3-Fluorobenzyl)thio)thiazol-2(3*H*)-one (2d). ^{1}H NMR (600 MHz,$CDCl_3$, TMS): δ = 10.34 (s, 1H), 7.23-7.30 (m, 1H), 6.30-7.00 (m, 3H), 6.08 (s, 1H), 3.97 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$, TMS): δ = 174.87, 164.48, 161.21, 139.22, 139.12, 130.23, 130.12, 24.56, 124.52, 123.86, 115.91, 115.62, 114.83, 114.55, 109.22, 39.11, 39.08; HRMS (ESI) calcd for $C_{10}H_7FNOS_2$ $[M-H]^-$ = 241.3050, found 241.2135.

4-((2-Methylbenzyl)thio)thiazol-2(3*H*)-one (2e). ^{1}H NMR (600 MHz, DMSO-d_6, TMS): δ = 11.69 (s, 1H), 7.14-7.18 (m, 2H), 7.08-7.13 (m, 2H), 6.29 (d, J = 1.7 Hz, 1H), 4.09 (s, 2H), 2.32 (s, 3H); ^{13}C NMR (150 MHz, DMSO-d_6, TMS): δ = 172.58, 136.94, 135.02, 130.82, 130.16, 128.11, 126.34, 124.53, 106.59, 36.44, 19.14; HRMS (ESI) calcd for $C_{11}H_{12}NOS_2$ $[M+H]^+$ = 238.3411, found 238.4163.

4-((4-Methylbenzyl)thio)thiazol-2(3*H*)-one (2f). ^{1}H NMR (300 MHz, DMSO-d_6, TMS): δ = 11.68 (s, 1H), 7.11 (s, 4H), 6.27 (d, J = 1.8 Hz, 1H), 4.05 (s, 2H), 2.26 (s, 3H); ^{13}C NMR (75 MHz, DMSO-d_6, TMS): δ = 172.62, 136.93, 134.31, 129.50, 129.16, 124.63, 105.83, 37.54, 21.18; HRMS (ESI) calcd for $C_{11}H_{12}NOS_2$ $[M+H]^+$ = 238.3411, found 238.6234.

4-((2-Nitrobenzyl)thio)thiazol-2(3*H*)-one (2g). ^{1}H NMR (500 MHz, DMSO-d_6, TMS): δ = 11.65 (s, 1H), 8.04 (dd, J = 1.1, 8.1 Hz, 1H), 7.68 (td, J = 1.2, 7.5, 15.2 Hz, 1H), 7.55 (td, J = 1.3, 8.2, 15.5 Hz, 1H), 7.38 (dd, J = 1.2, 7.7 Hz, 1H), 6.27 (d, J = 1.6 Hz, 1H), 4.35 (s, 2H), ^{13}C NMR (125 MHz, DMSO-d_6, TMS) δ = 172.45, 148.32, 134.16, 132.89, 132.63, 129.50, 125.65, 123.35, 108.64, 35.53; HRMS (ESI) calcd for $C_{10}H_7N_2O_3S_2$ $[M-H]^-$ = 268.3121, found 268.1252.

4-((4-Nitrobenzyl)thio)thiazol-2(3*H*)-one (2h). ^{1}H NMR (500 MHz, DMSO-d_6, TMS): δ = 11.69 (s, 1H), 8.19 (d, J = 9.1 Hz, 2H), 7.49 (d, J = 9.1 Hz, 2H), 6.30 (d, J = 0.9 Hz, 1H), 4.22 (s, 2H); ^{13}C NMR (125 MHz, DMSO-d_6,

TMS): δ = 172.51, 147.07, 145.90, 130.51, 124.09, 123.46, 107.53, 37.05; HRMS (ESI) calcd for $C_{10}H_7N_2O_3S_2$ $[M-H]^-$ = 268.3121, found 268.3347.

4-(((2-Oxo-2,3-dihydrothiazol-4-yl)thio)methyl)benzonitrile (2i). ^{1}H NMR (300 MHz, DMSO-d_6, TMS): δ = 11.73 (s, 1H), 7.81 (d, J = 8.1 Hz, 2H), 7.42 (d, J = 8.2 Hz, 2H), 6.32 (d, J = 1.3 Hz, 1H), 4.18 (s, 2H); ^{13}C NMR (75 MHz, DMSO-d_6, TMS): δ = 171.53, 143.66, 132.85, 130.21, 123.54, 110.42, 107.36, 37.32; HRMS (ESI) calcd for $C_{11}H_9N_2OS_2$ $[M+H]^-$ = 249.3240, found 249.3312.

4-((4-(Tert-butyl)benzyl)thio)thiazol-2(3*H*)-one (2j). ^{1}H NMR (300 MHz, DMSO-d_6, TMS): δ = 11.69 (s, 1H), 7.33 (d, J = 8.3 Hz, 2H), 7.17 (d, J = 8.3 Hz, 2H), 6.31 (d, J = 1.6 Hz, 1H), 4.10 (s, 2H), 1.24 (s, 9H); ^{13}C NMR (75 MHz, DMSO-d_6, TMS): δ = 172.63, 150.18, 134.24, 128.96, 125.71, 124.89, 105.28, 37.38, 34.69, 31.56; HRMS (ESI) calcd for $C_{14}H_{18}NOS_2$ $[M+H]^+$ = 280.4209, found 280.3562.

2-((2-Oxo-2,3-dihydrothiazol-4-yl)thio)acetonitrile (2k). ^{1}H NMR (600 MHz, DMSO-d_6, TMS): δ = 11.73 (s, 1H), 6.80 (s, 1H), 4.06 (s, 1H); ^{13}C NMR (150 MHz, DMSO-d_6, TMS): δ = 175.5, 138.16, 125.39, 110.46, 41.33; HRMS (ESI) calcd for $C_5H_3N_2OS_2$ $[M-H]^-$ = 171.2281, found 171.2131.

3-Methyl-4-(methylthio)thiazol-2(3*H*)-one (2l). ^{1}H NMR (600 MHz, $CDCl_3$, TMS): δ = 7.27 (s, 1H), 6.04 (s, 1H), 3.33 (s,3H), 2.36 (s, 3H); HRMS (ESI) calcd for $C_5H_8NOS_2$ $[M+H]^+$ = 161.2452, found 161.3362.

X-ray structure of 3a

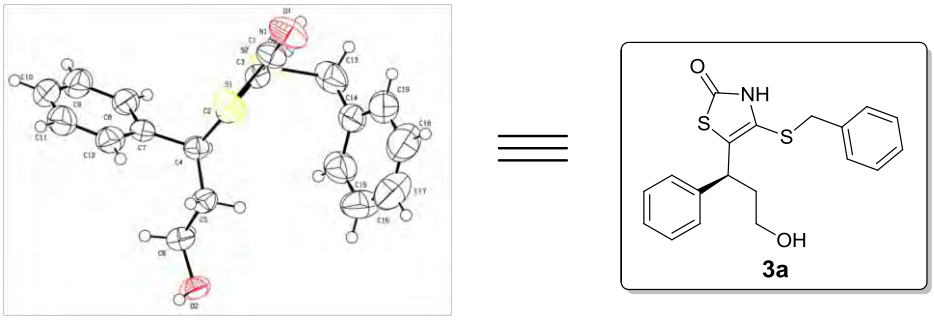


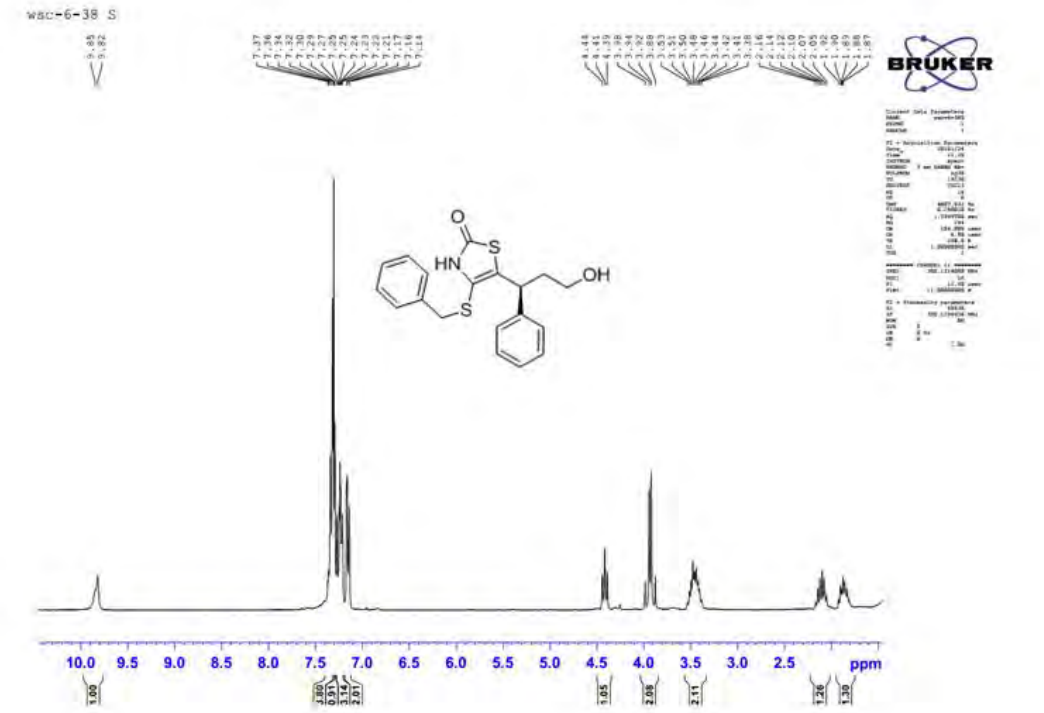
Table 1. Crystal data and structure refinement for **3a**.

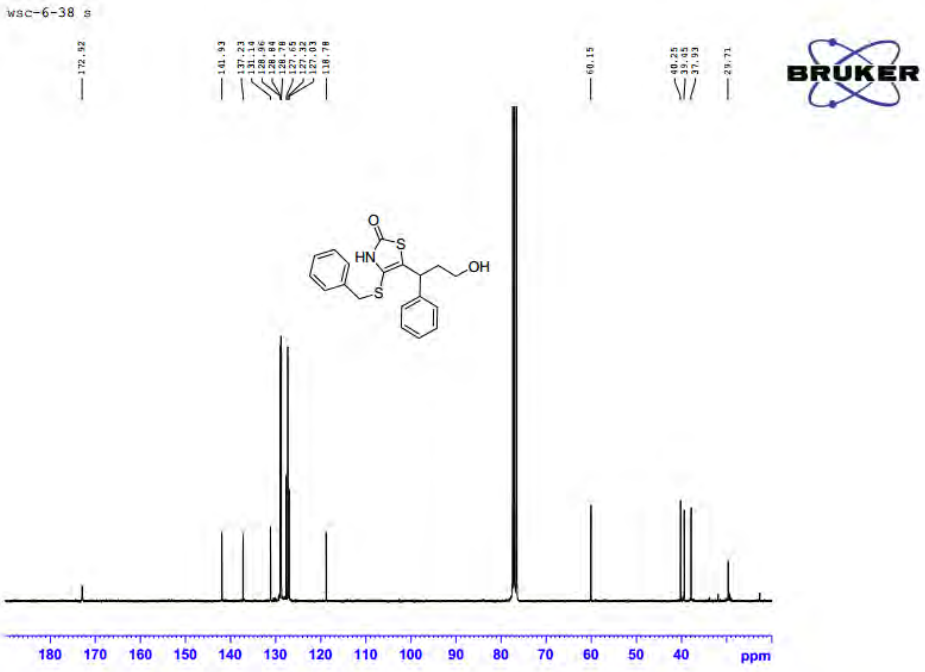
Identification code	mo_21229a
Empirical formula	C19H19NO2S2
Formula weight	357.47
Temperature	296(2) K
Wavelength	0.71073 Å
Crystal system, space group	Orthorhombic, P2(1)2(1)2(1)
Unit cell dimensions	a = 10.8460(13) Å alpha = 90 deg.
	b = 11.5153(15) Å beta = 90 deg.
	c = 14.8533(18) Å gamma = 90 deg.
Volume	1855.1(4) $Å^3$
Z, Calculated density	4, 1.280 Mg/m^3
Absorption coefficient	0.297 mm^{-1}
F(000)	752
Crystal size	0.12 x 0.11 x 0.09 mm
Theta range for data collection	2.24 to 27.48 deg.
Limiting indices	-14<=h<=14, -14<=k<=14, -19<=l<=16
Reflections collected / unique	13700 / 4244 [R(int) = 0.0388]
Completeness to theta = 27.48	99.6 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9737 and 0.9652
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4244 / 1 / 225

Goodness-of-fit on F^2	0.750
Final R indices [I>2sigma(I)]	R1 = 0.0395, wR2 = 0.1071
R indices (all data)	R1 = 0.0775, wR2 = 0.1408
Absolute structure parameter	0.00(12)
Largest diff. peak and hole	0.185 and -0.149 e. $Å^{-3}$

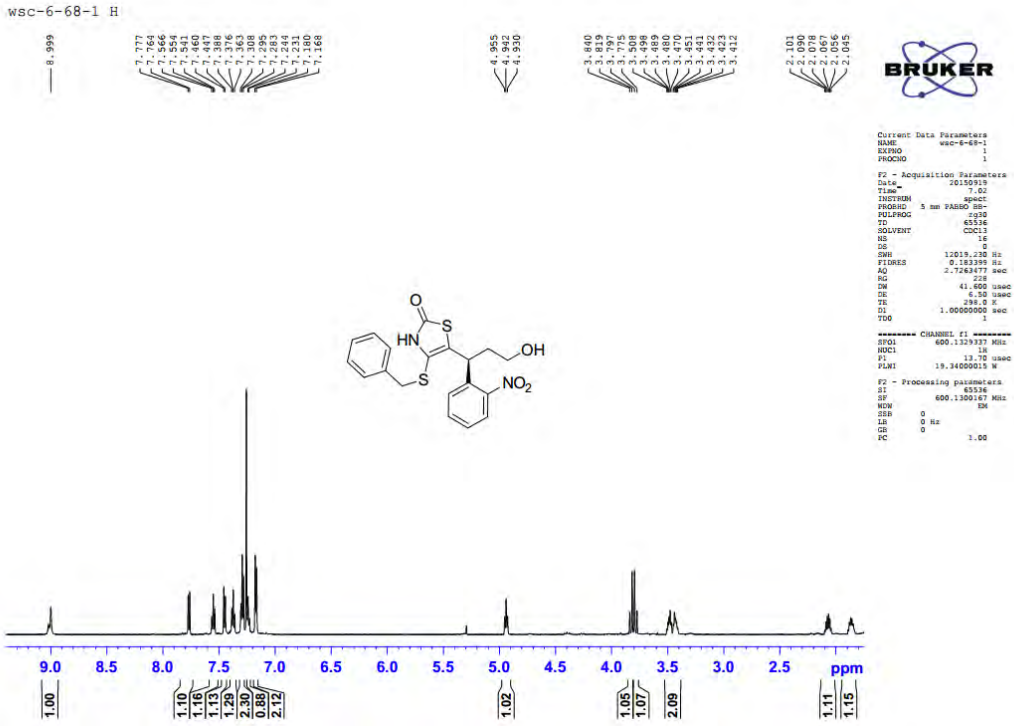
NMR Spectra

Compound **3a**





Compound **3b**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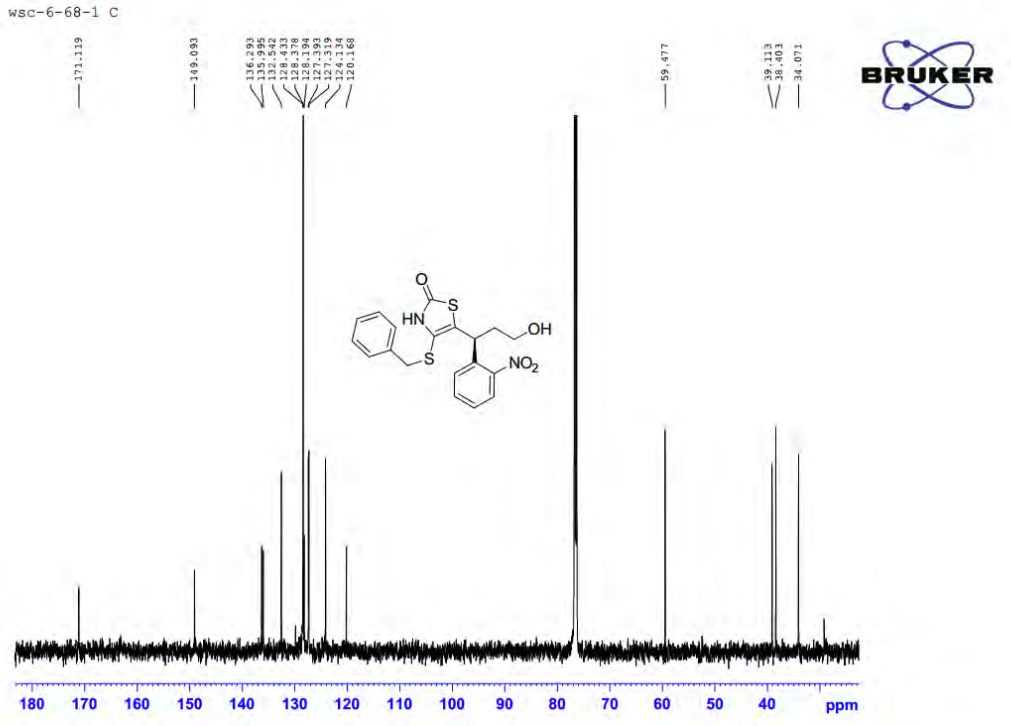
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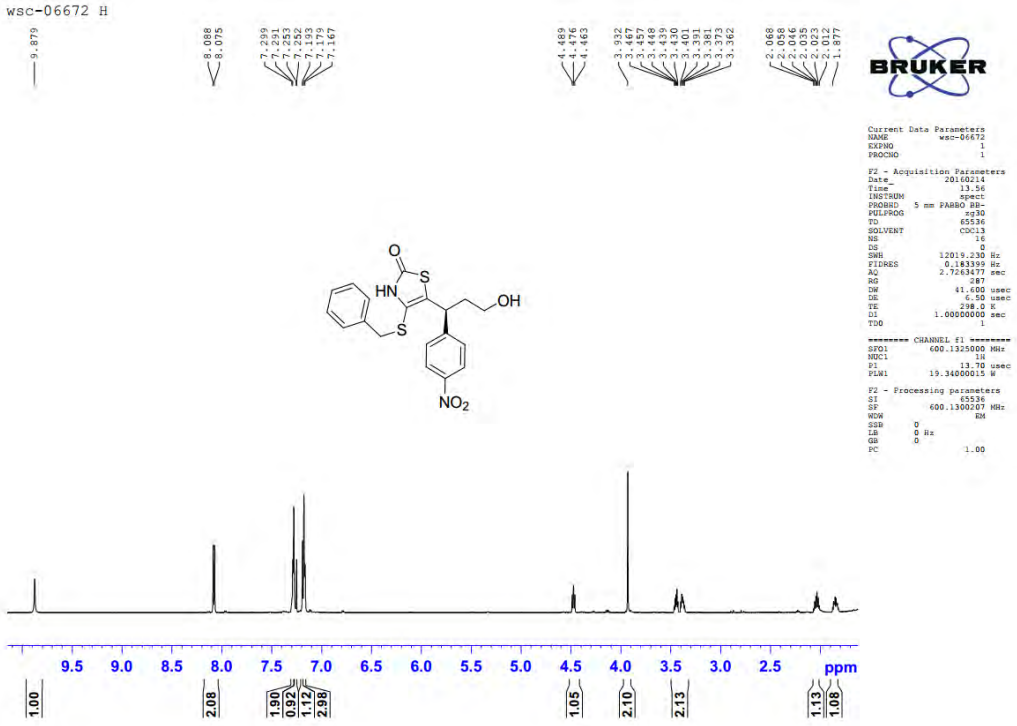
Compound **3c**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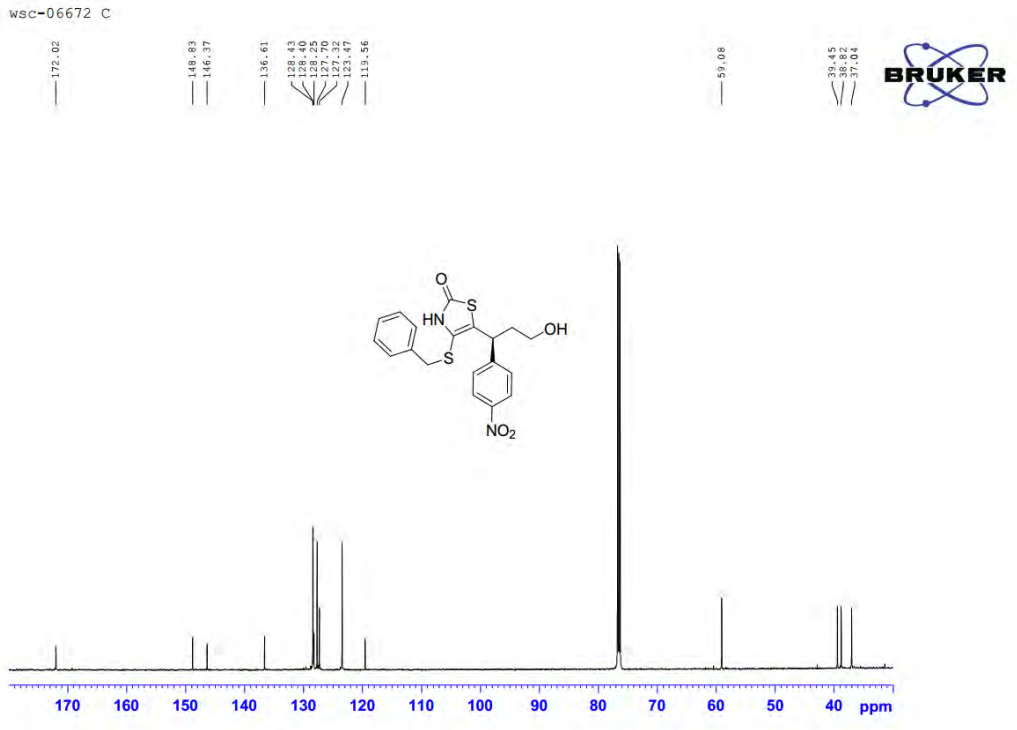
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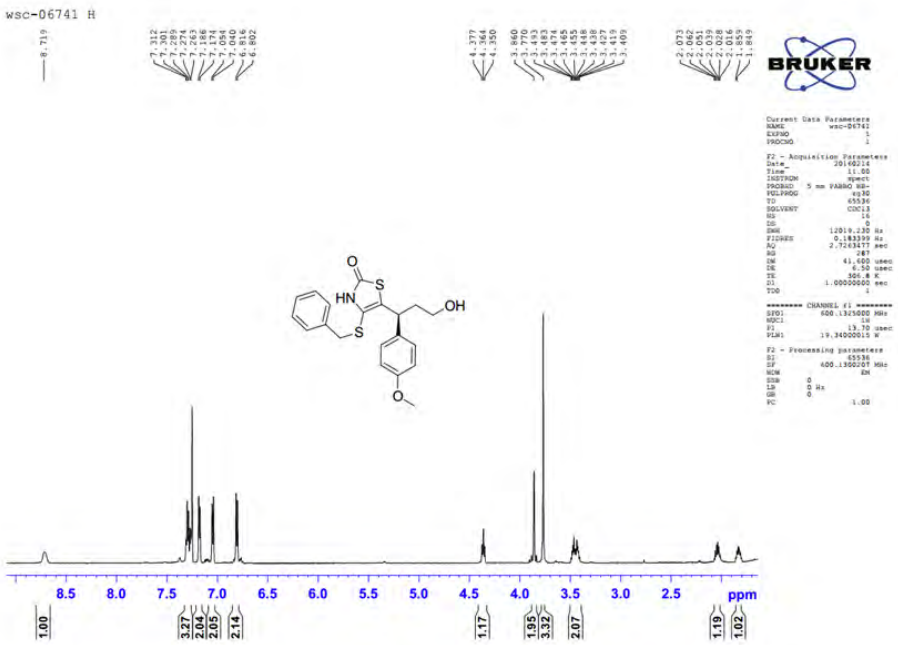
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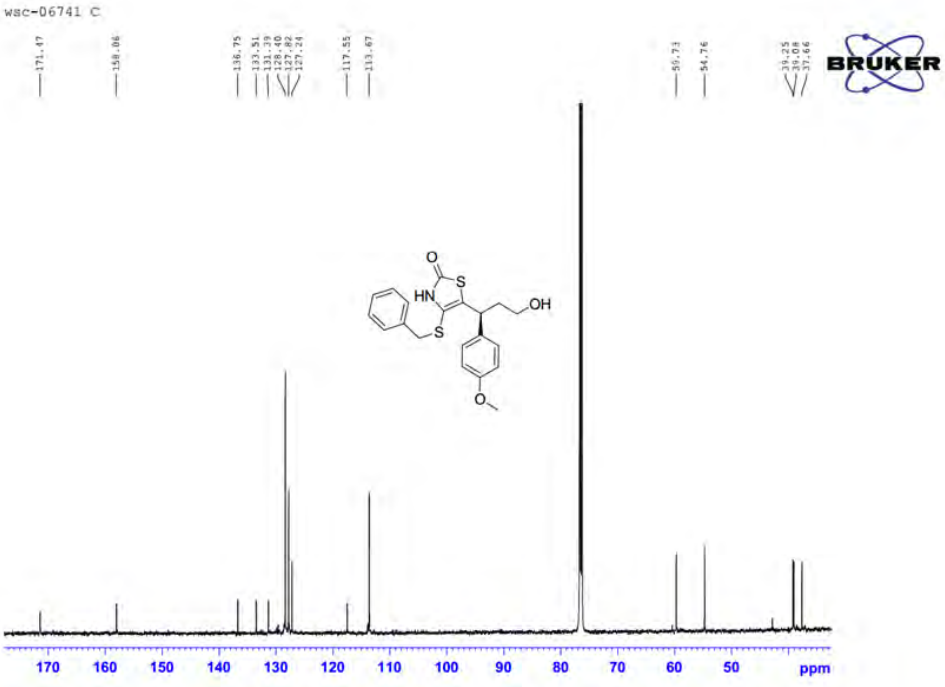
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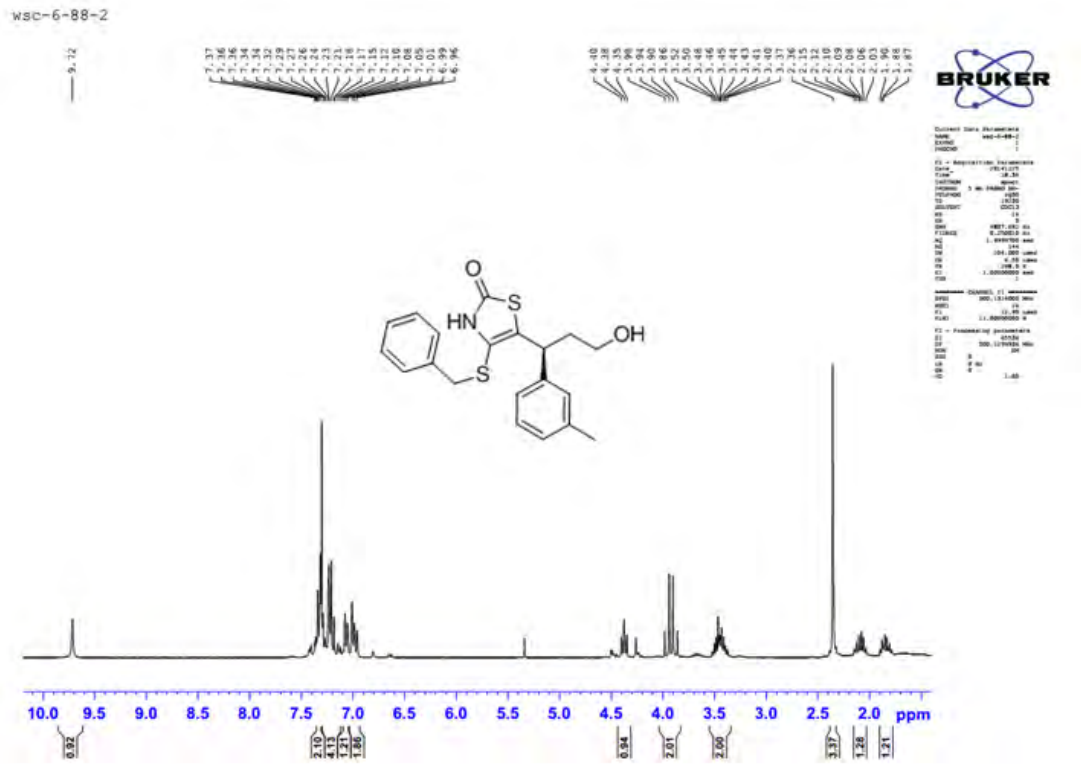
Compound **3e**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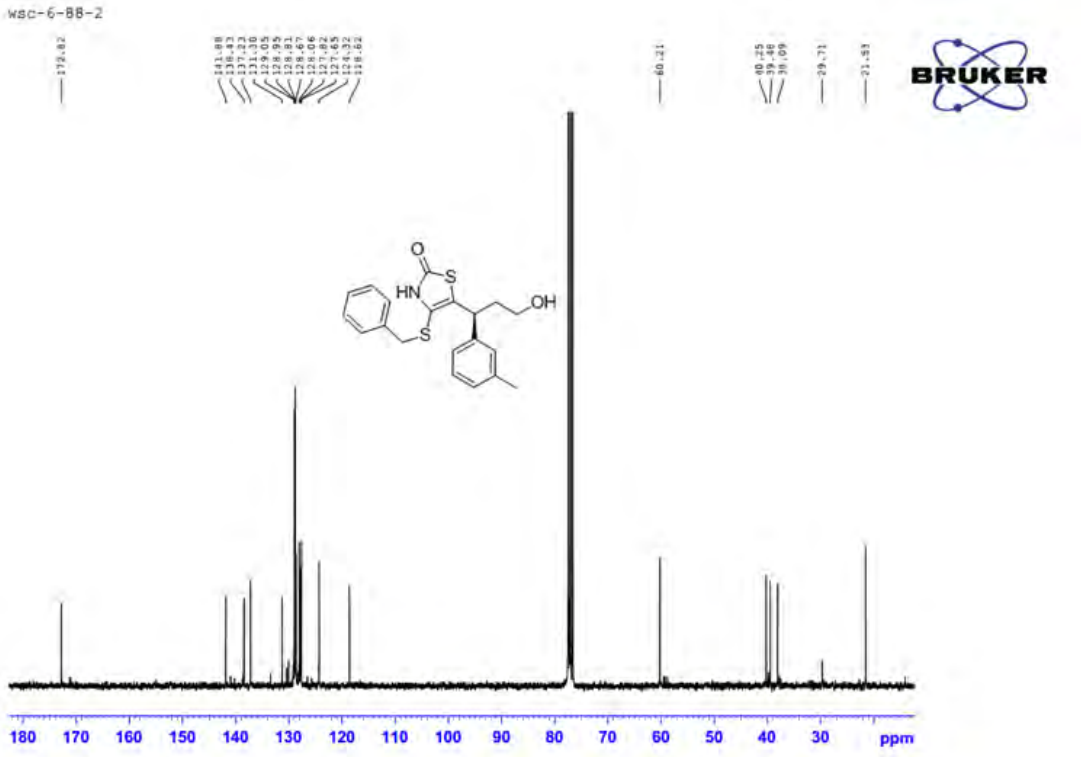
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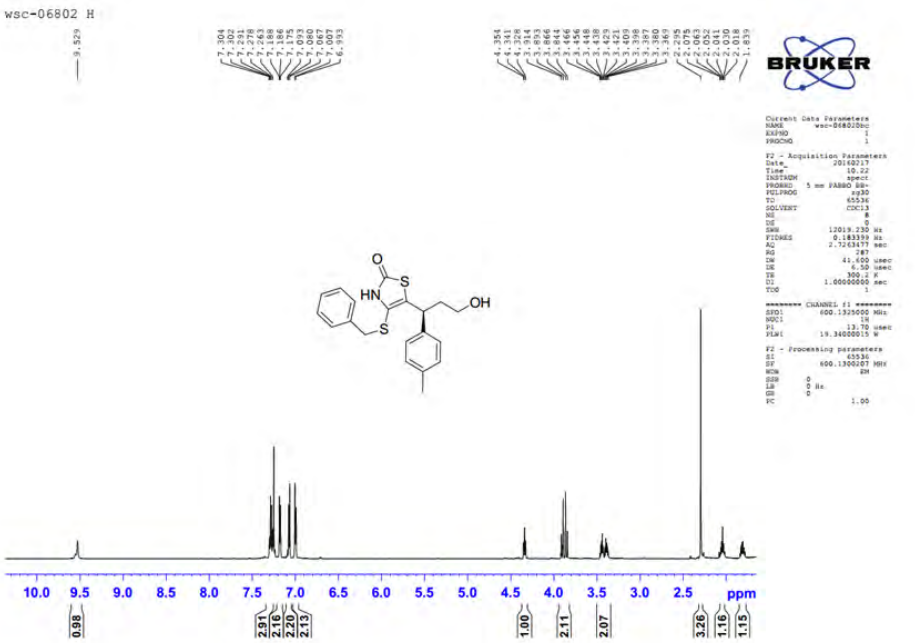
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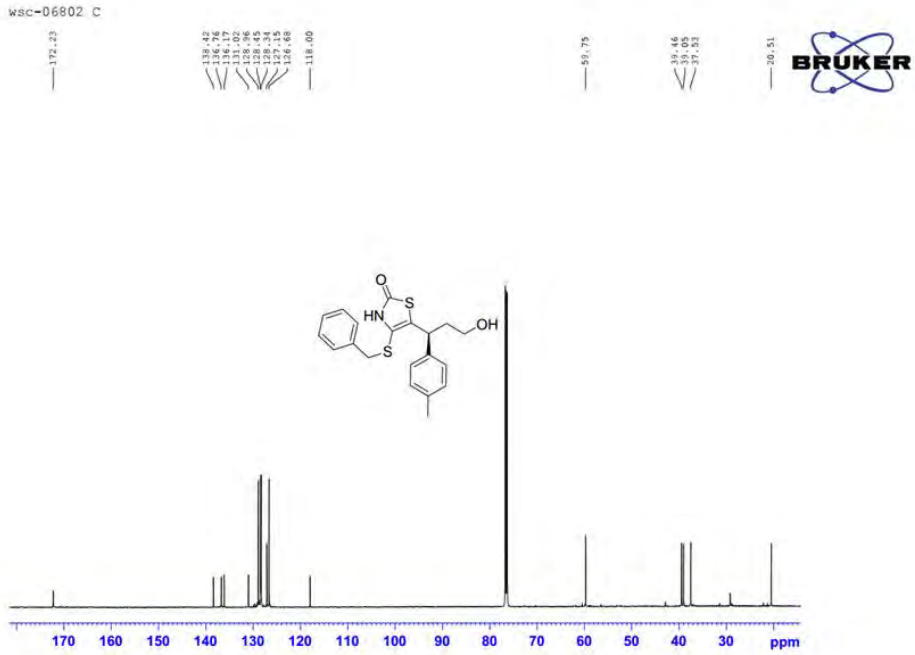
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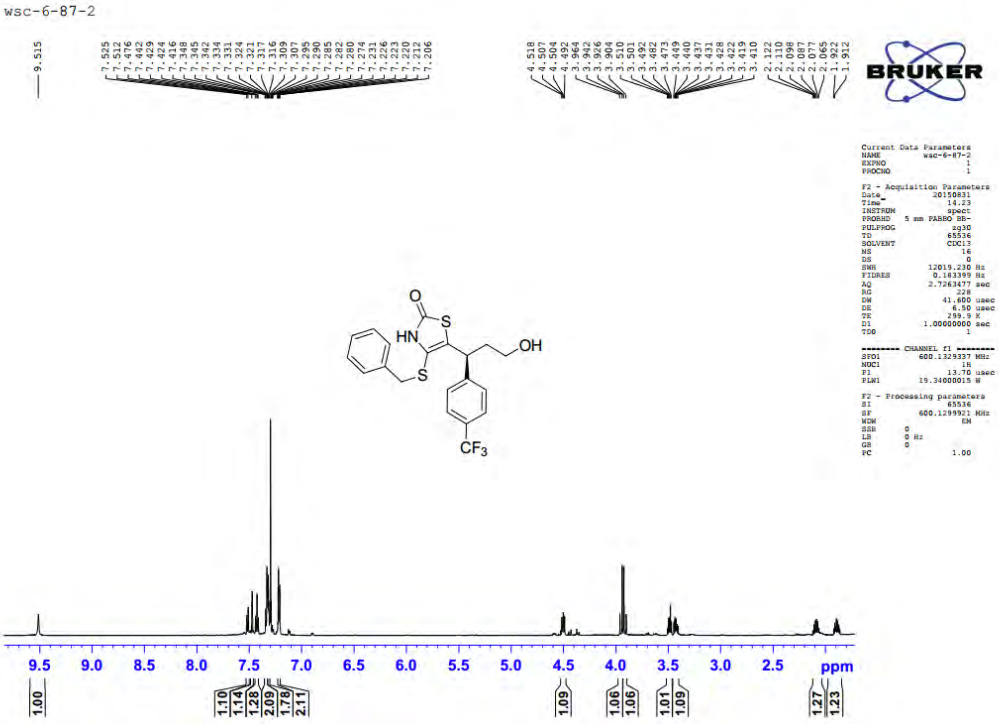
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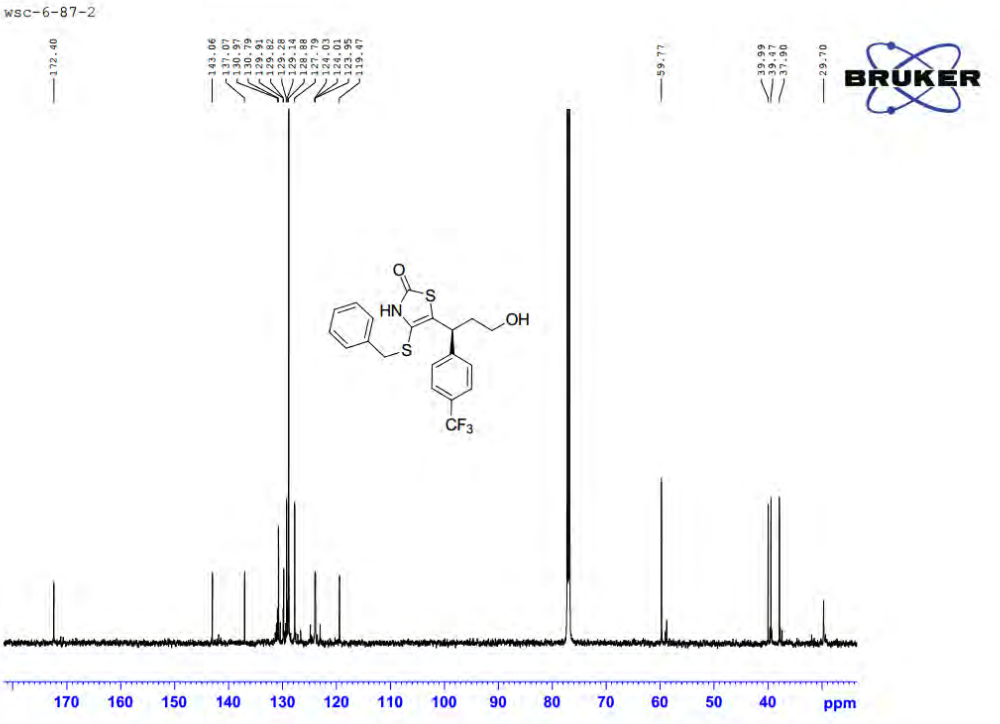
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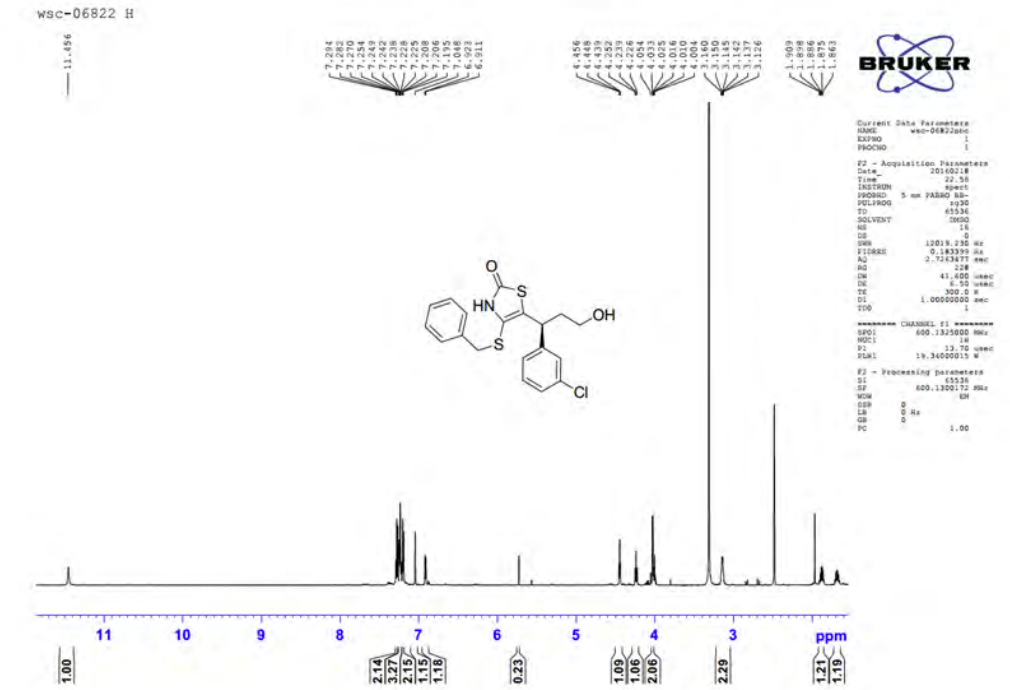
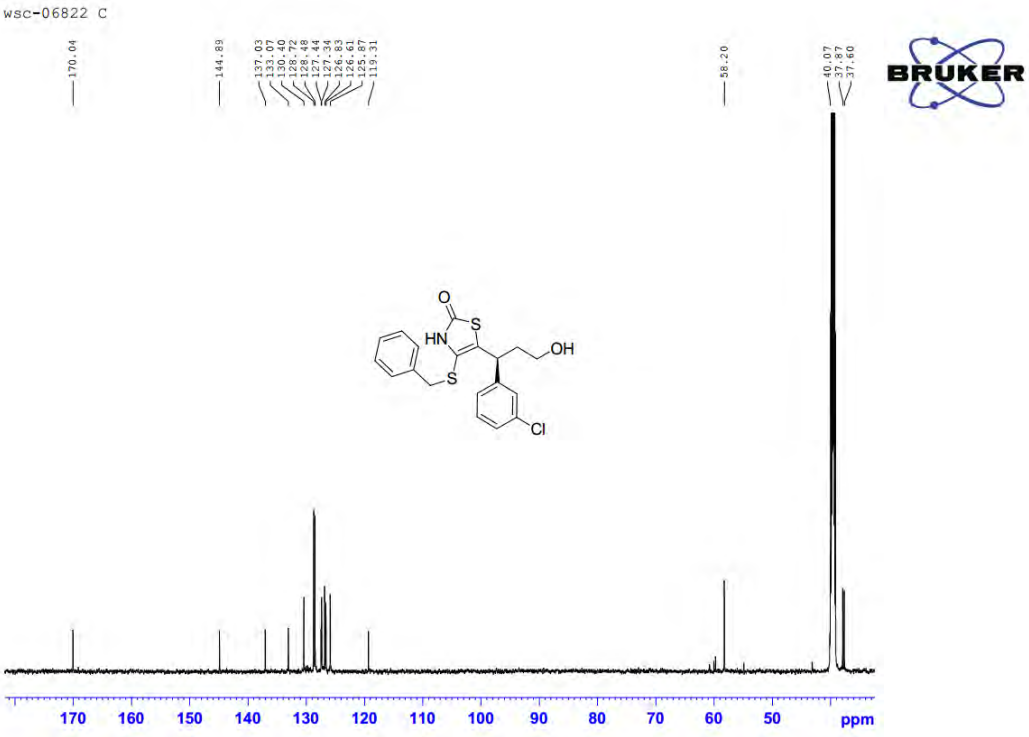
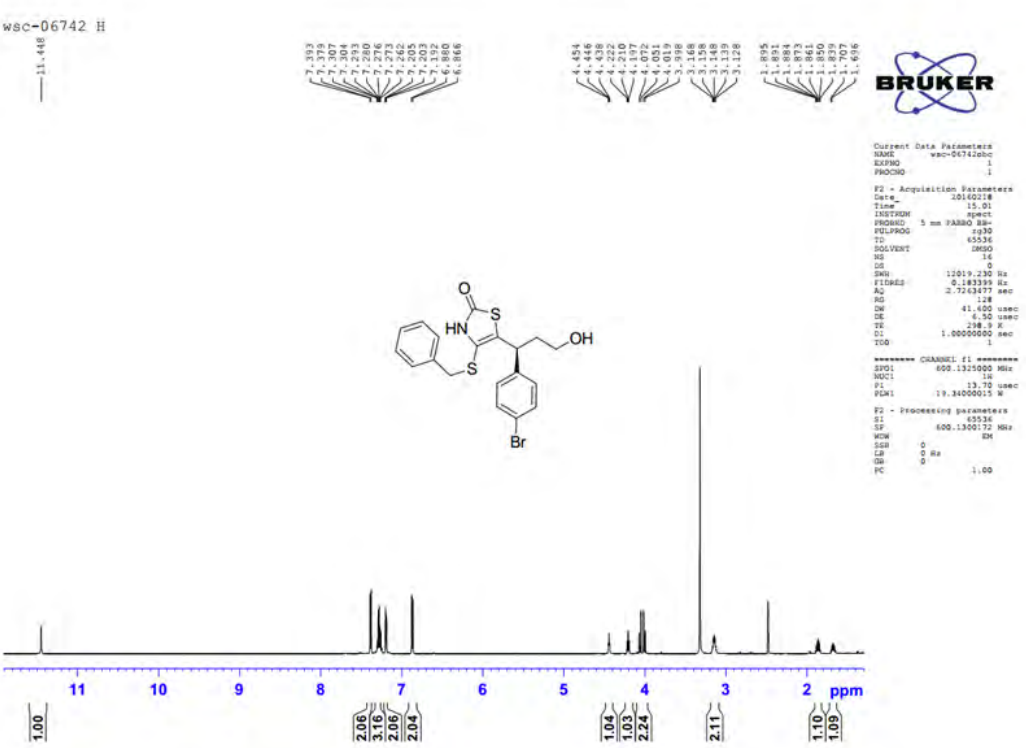




Compound **3i**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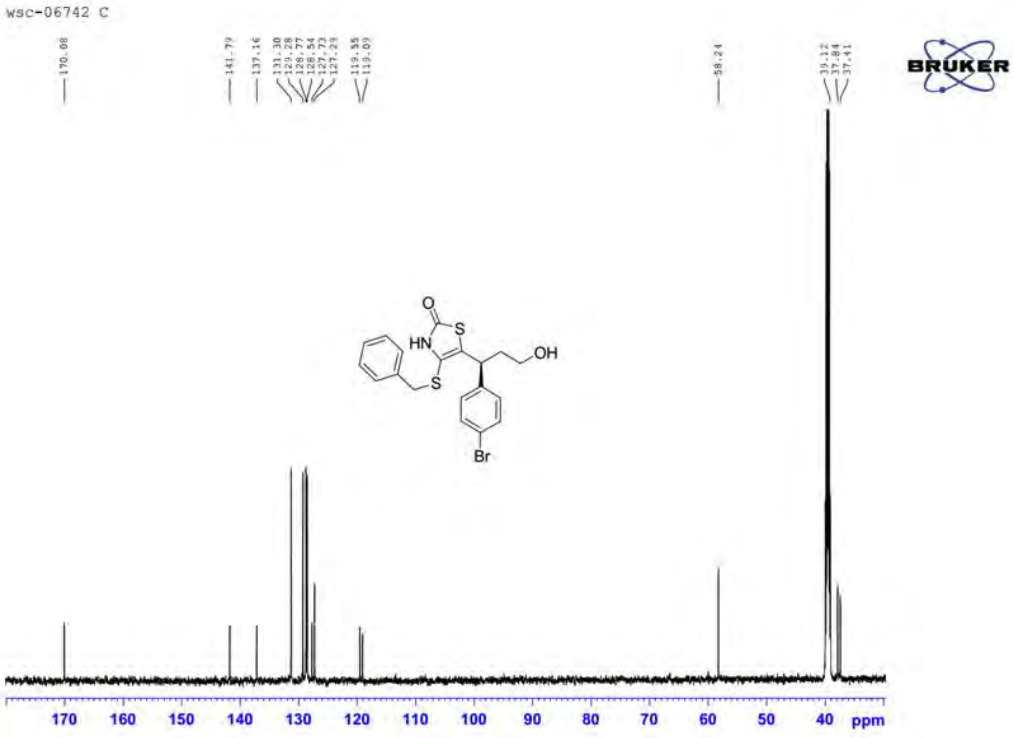
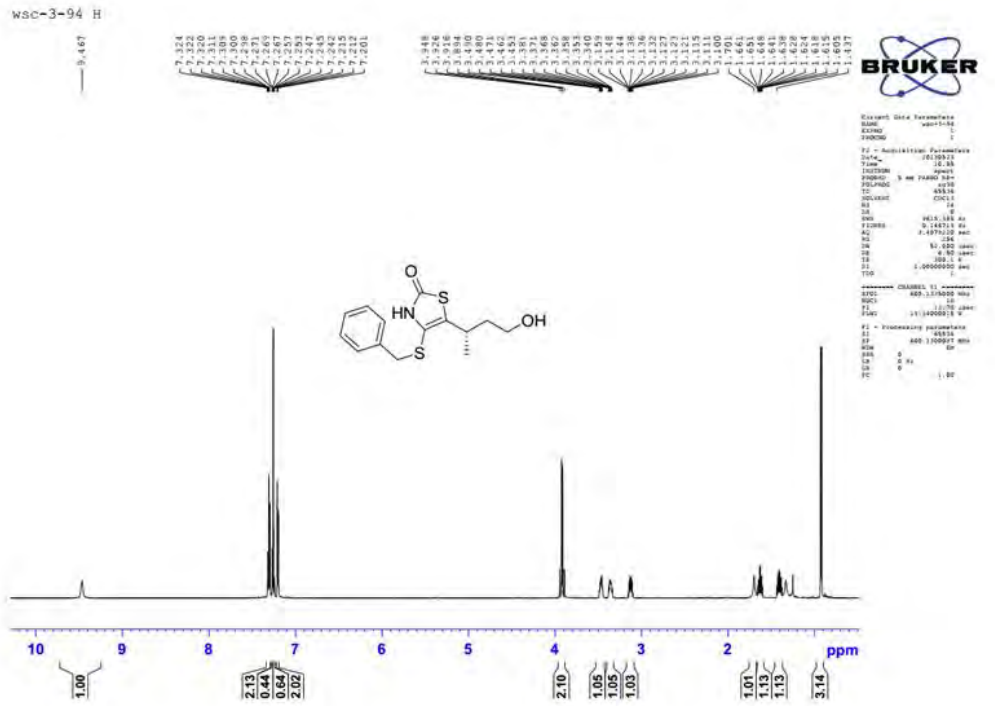
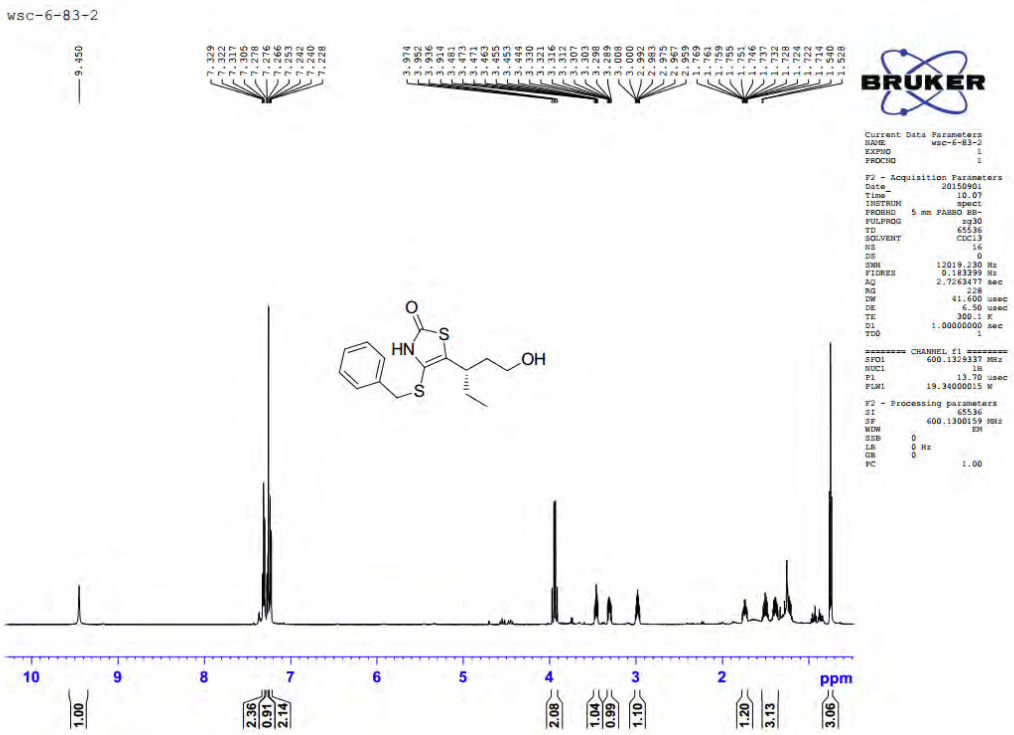
2
ppm

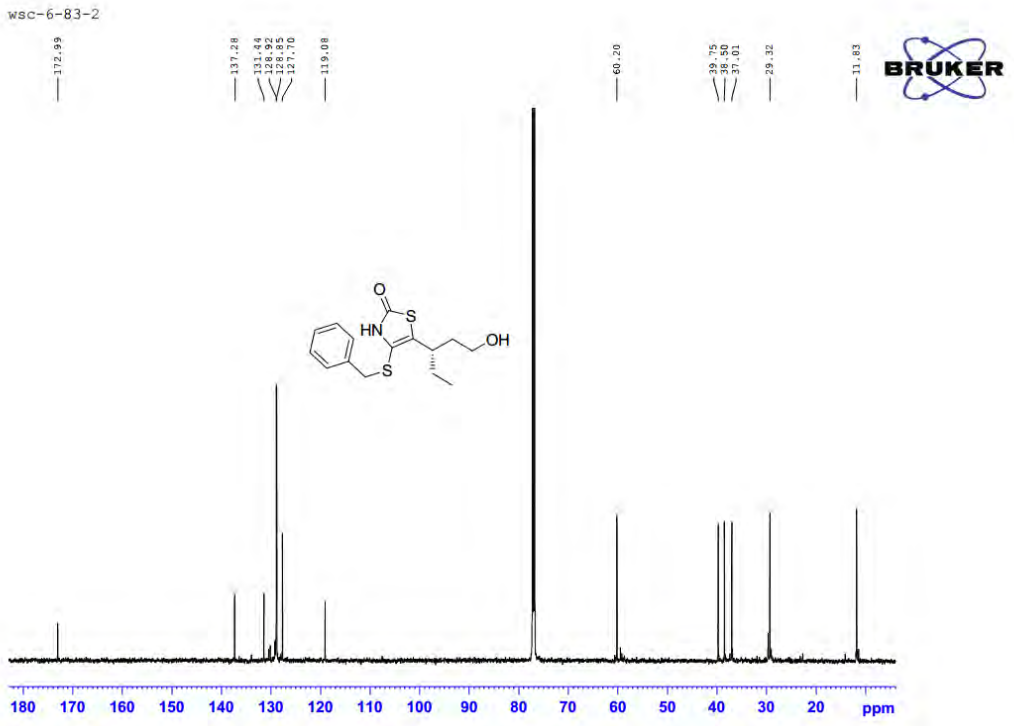

wsc-06742 C
BRUKER
HN
S
O
OH
Br
170
160
150
140
130
120
110
100
90
80
70
60
50
40
ppm

Compound **3j**

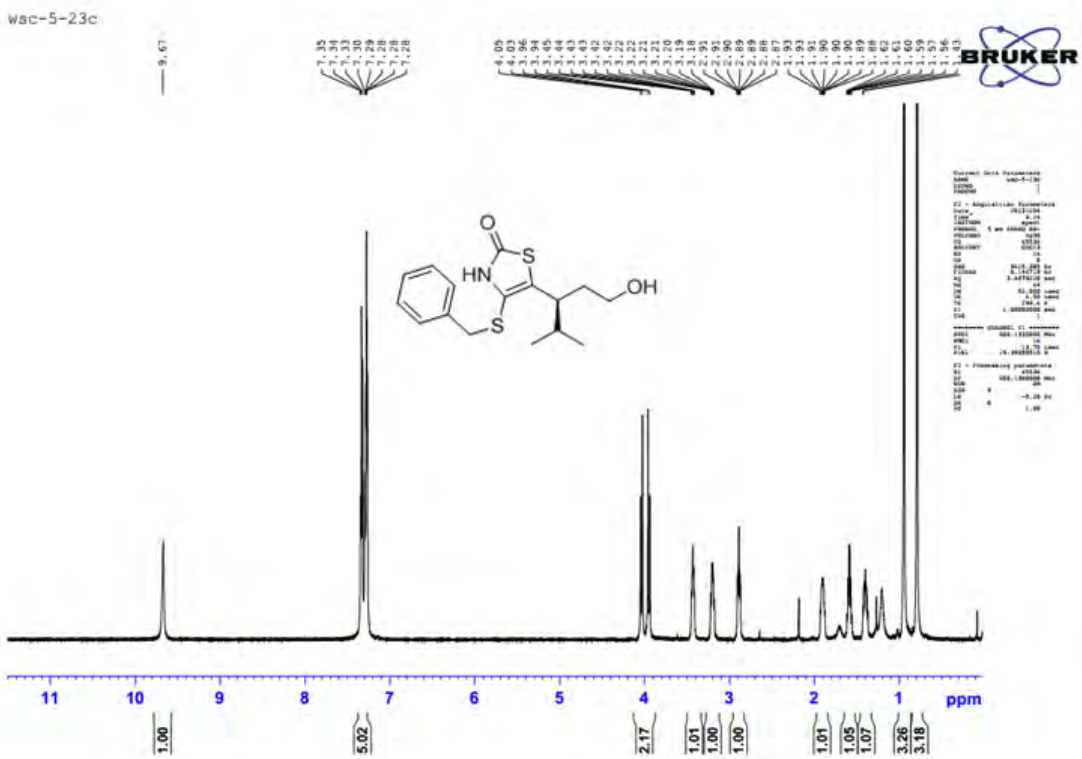

wsc-3-94 H
BRUKER
HN
O
S
S
OH
10
9
8
7
6
5
4
3
2
ppm
1.00
2.13
0.44
0.64
2.02
2.10
1.05
1.05
1.03
1.01
1.13
1.13
3.14

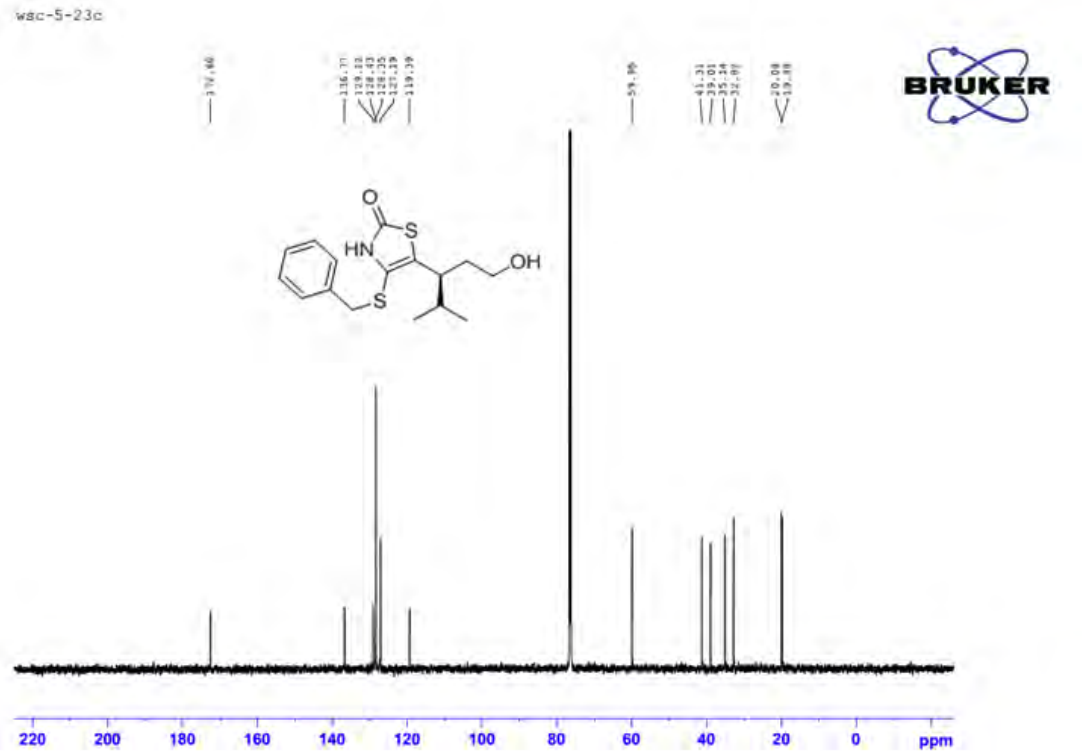
Compound **3k**


wsc-6-83-2
BRUKER
HN
O
S
S
OH
10
9
8
7
6
5
4
3
2
ppm

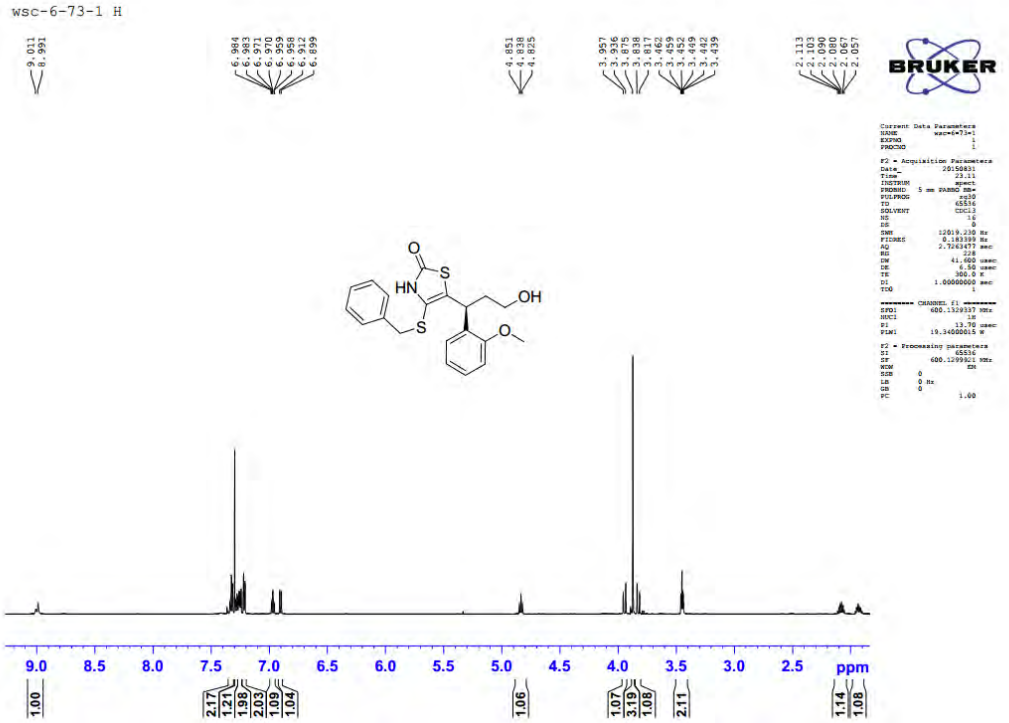

wsc-6-83-2
BRUKER
HN
O
S
S
OH
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

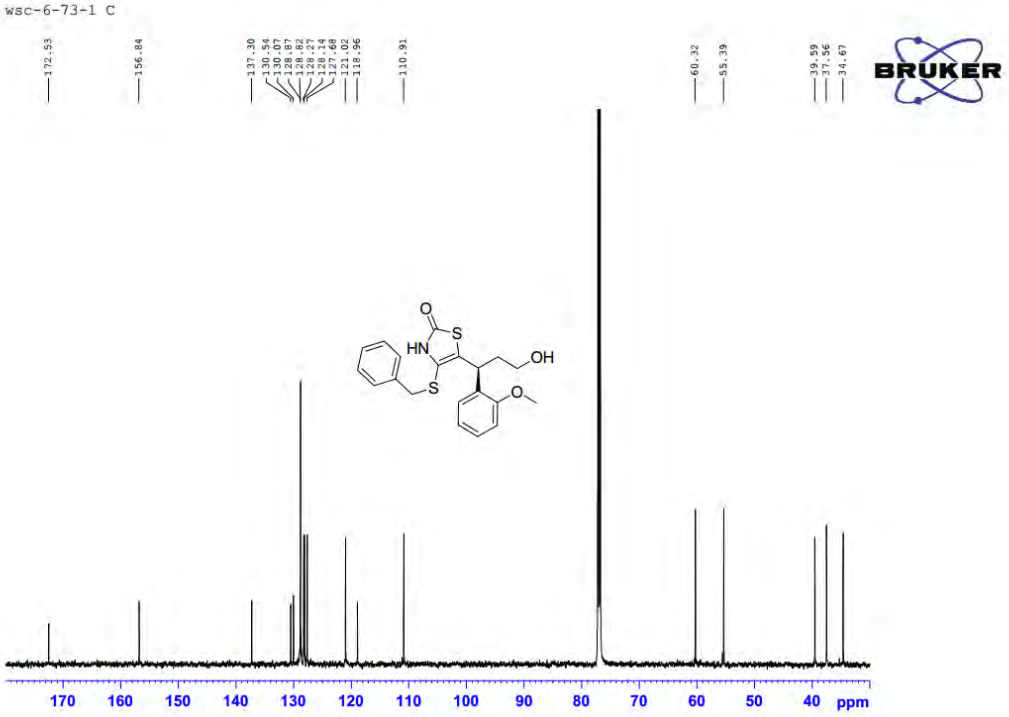
Compound **3l**


wsc-5-23c
BRUKER
HN
O
S
S
OH
11
10
9
8
7
6
5
4
3
2
1
ppm
1.00
5.02
2.17
1.01
1.00
1.00
1.01
1.05
1.07
3.26
3.18

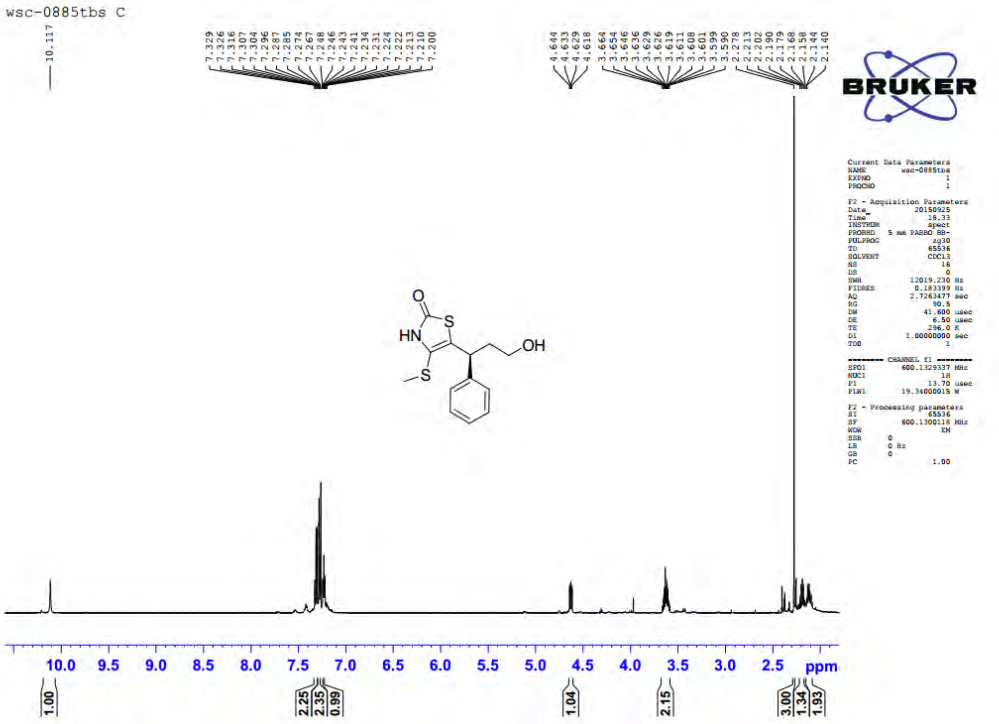

wsc-5-23c
BRUKER
HN
O
S
S
OH
220
200
180
160
140
120
100
80
60
40
20
0
ppm

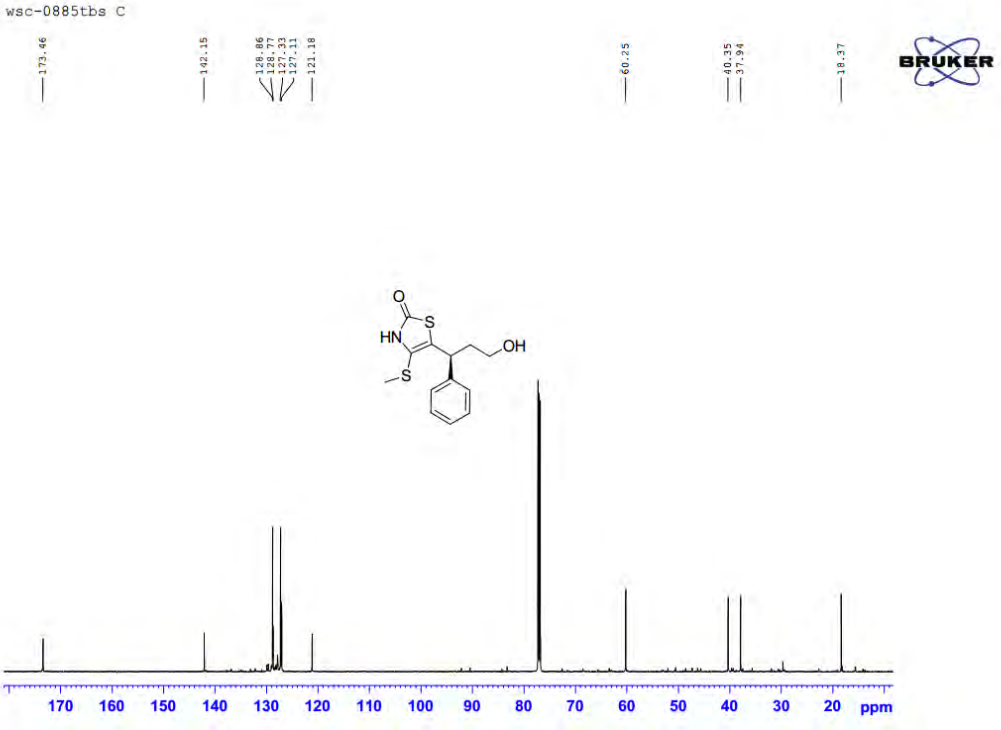
Compound **3m**


wsc-6-73-1 H
9.011
8.991
6.984
6.983
6.971
6.970
6.959
6.958
6.912
6.899
4.851
4.838
4.825
3.957
3.936
3.875
3.838
3.817
3.466
3.459
3.452
3.449
3.442
3.439
2.113
2.103
2.090
2.080
2.067
2.057
BRUKER
O
S
HN
S
OH
O
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
ppm
1.00
2.17
1.21
1.98
2.03
1.09
1.04
1.06
1.07
3.19
1.08
2.11
1.14
1.08

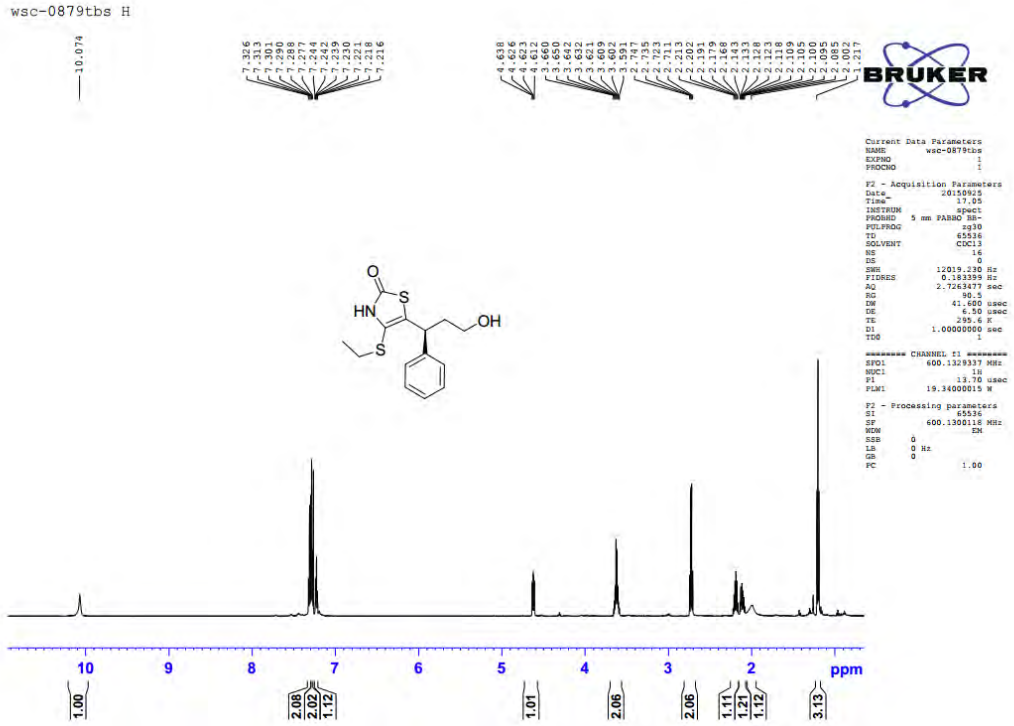

wsc-6-73-1 C
172.53
156.84
137.30
130.54
130.07
128.87
128.82
128.77
128.14
127.68
121.02
118.96
110.91
60.32
55.39
39.59
37.56
34.67
BRUKER
O
S
HN
S
OH
O
170
160
150
140
130
120
110
100
90
80
70
60
50
40
ppm

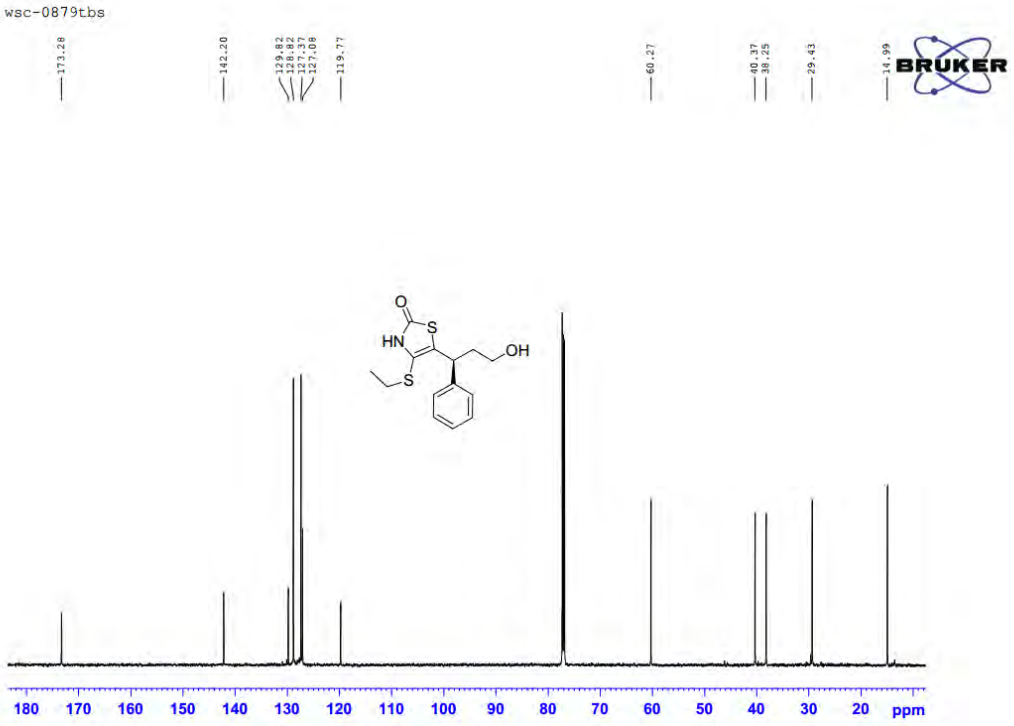
Compound **4a**


wsc-0885tbs C
10.117
7.329
7.326
7.316
7.307
7.304
7.296
7.287
7.285
7.274
7.267
7.248
7.246
7.243
7.241
7.234
7.231
7.224
7.222
7.213
7.210
7.200
4.644
4.633
4.629
4.618
3.654
3.654
3.646
3.636
3.629
3.626
3.619
3.611
3.608
3.601
3.598
3.590
2.278
2.213
2.202
2.196
2.179
2.168
2.158
2.144
2.140
BRUKER
Current Data Parameters
NAME wsc-0885tbs
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150925
Time 18.33
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 90.5
DW 41.600 usec
DE 6.50 usec
TE 296.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 600.1329337 MHz
NUC1 1H
P1 13.70 usec
PLW1 19.34000015 W
F2 - Processing parameters
SI 65536
SF 600.1300118 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00
O
S
HN
S
OH
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 ppm
1.00
2.25
2.35
0.99
1.04
2.15
3.00
1.34
1.93

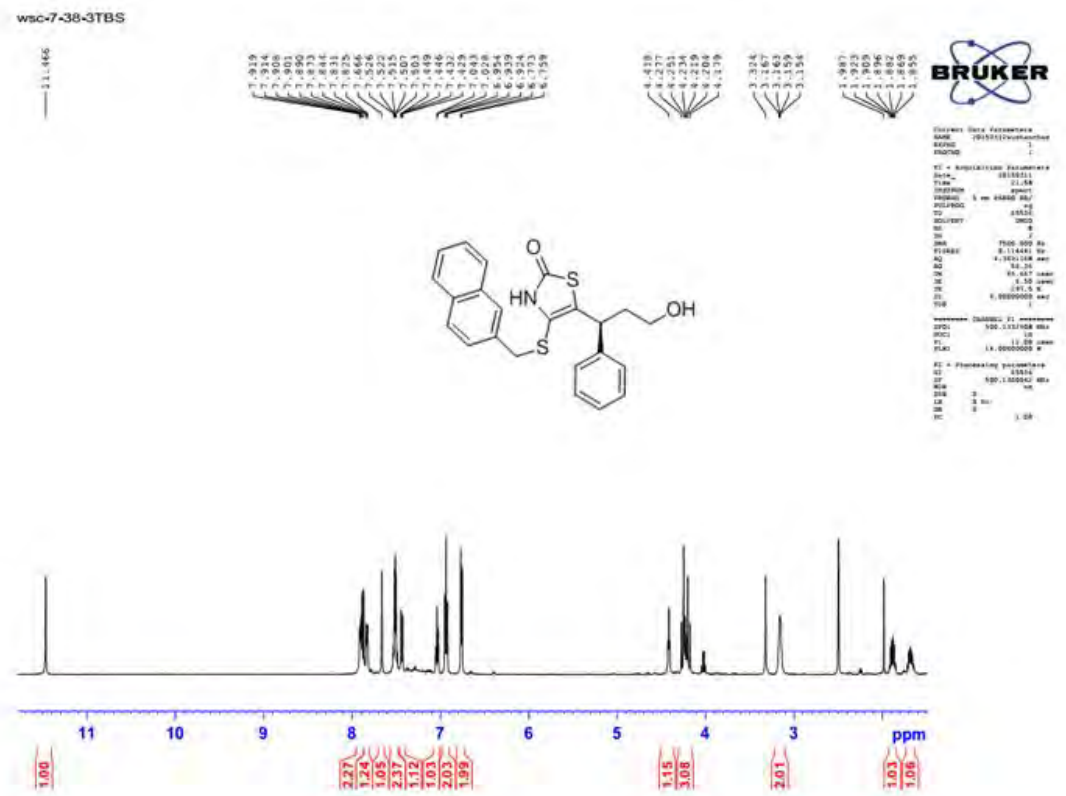

wsc-0885tbs C
173.46
142.15
128.86
128.77
127.33
127.11
121.18
60.25
40.35
37.94
18.37
BRUKER
O
S
HN
S
OH
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

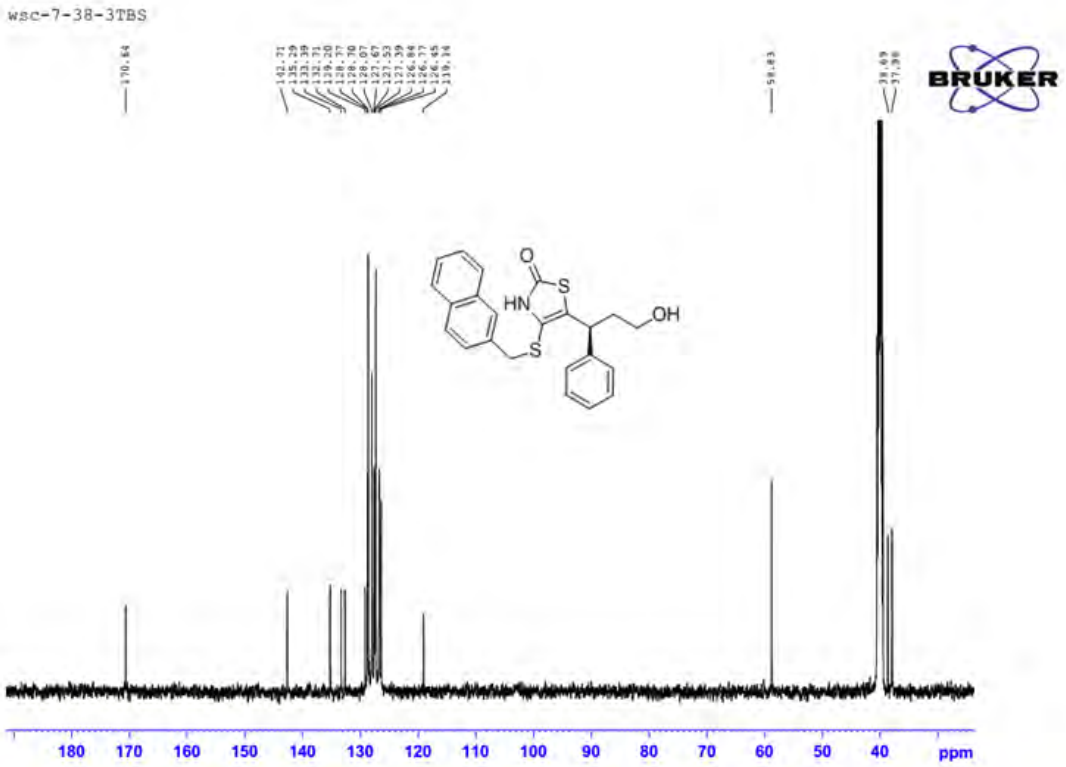
Compound **4b**


wsc-0879tbs H
10.074
7.326
7.313
7.301
7.290
7.288
7.277
7.244
7.242
7.239
7.230
7.221
7.218
7.216
4.638
4.626
4.623
4.622
3.660
3.650
3.642
3.632
3.631
3.609
3.602
3.591
2.737
2.735
2.723
2.711
2.213
2.202
2.191
2.179
2.168
2.143
2.133
2.128
2.123
2.118
2.109
2.105
2.100
2.095
2.085
2.002
1.217
BRUKER
Current Data Parameters
NAME wsc-0879tbs
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150925
Time 17.05
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 90.5
DW 41.600 usec
DE 6.50 usec
TE 295.6 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 600.1329337 MHz
NUC1 1H
P1 13.70 usec
PLW1 19.34000015 W
F2 - Processing parameters
SI 65536
SF 600.1300118 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00
O
HN
S
S
OH
10
9
8
7
6
5
4
3
2
ppm
1.00
2.08
2.02
1.12
1.01
2.06
2.06
1.11
1.21
1.12
3.13

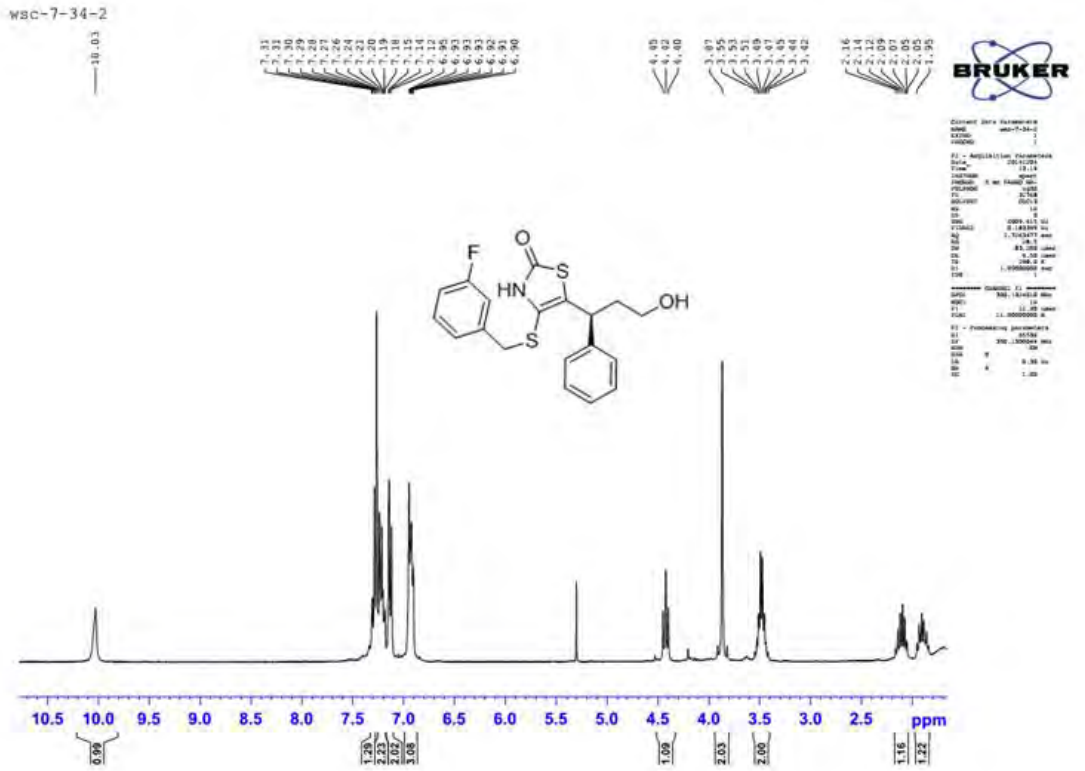

wsc-0879tbs
173.28
142.20
129.82
128.82
127.37
127.08
119.77
60.27
40.37
38.25
29.43
14.99
BRUKER
O
HN
S
S
OH
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

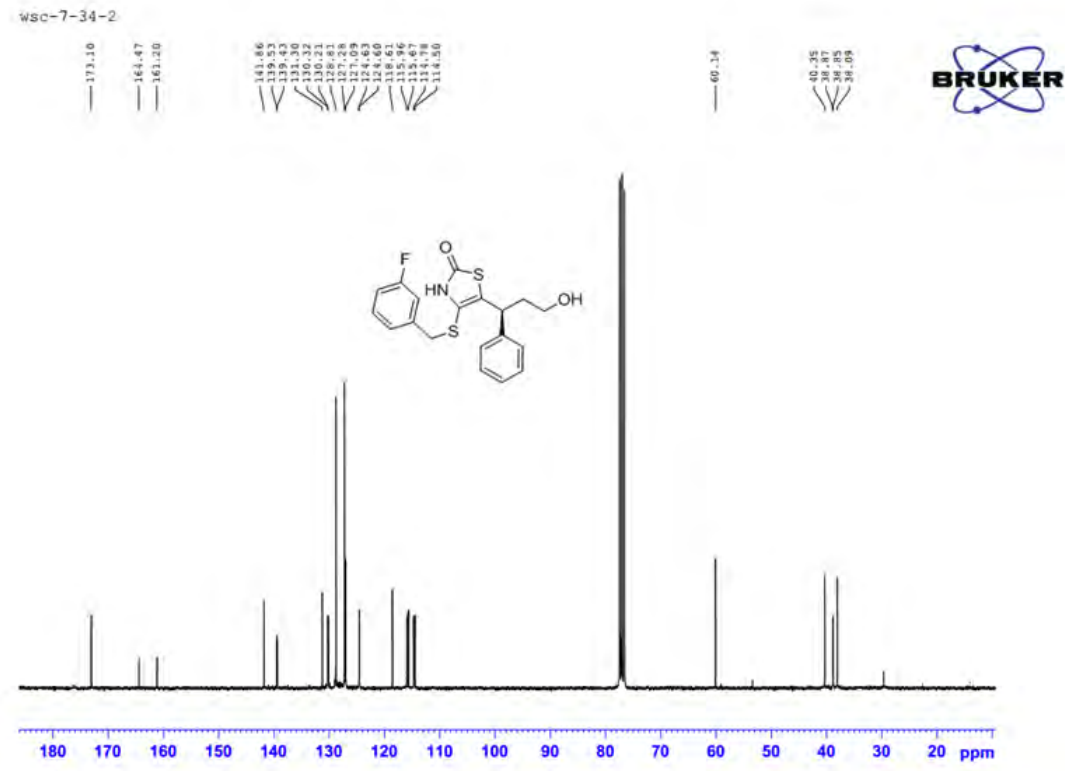
Compound **4c**


wsc-7-38-3TBS
BRUKER
O
S
HN
OH
S
11
10
9
8
7
6
5
4
3
ppm

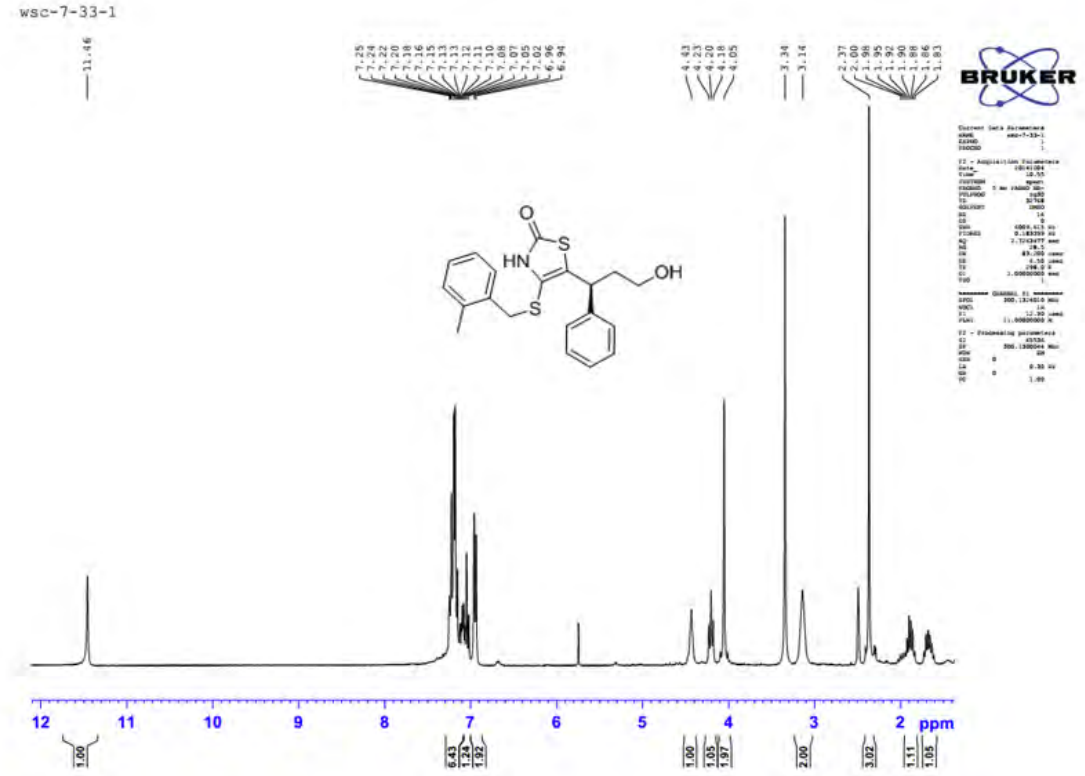

wsc-7-38-3TBS
BRUKER
O
S
HN
OH
S
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
ppm

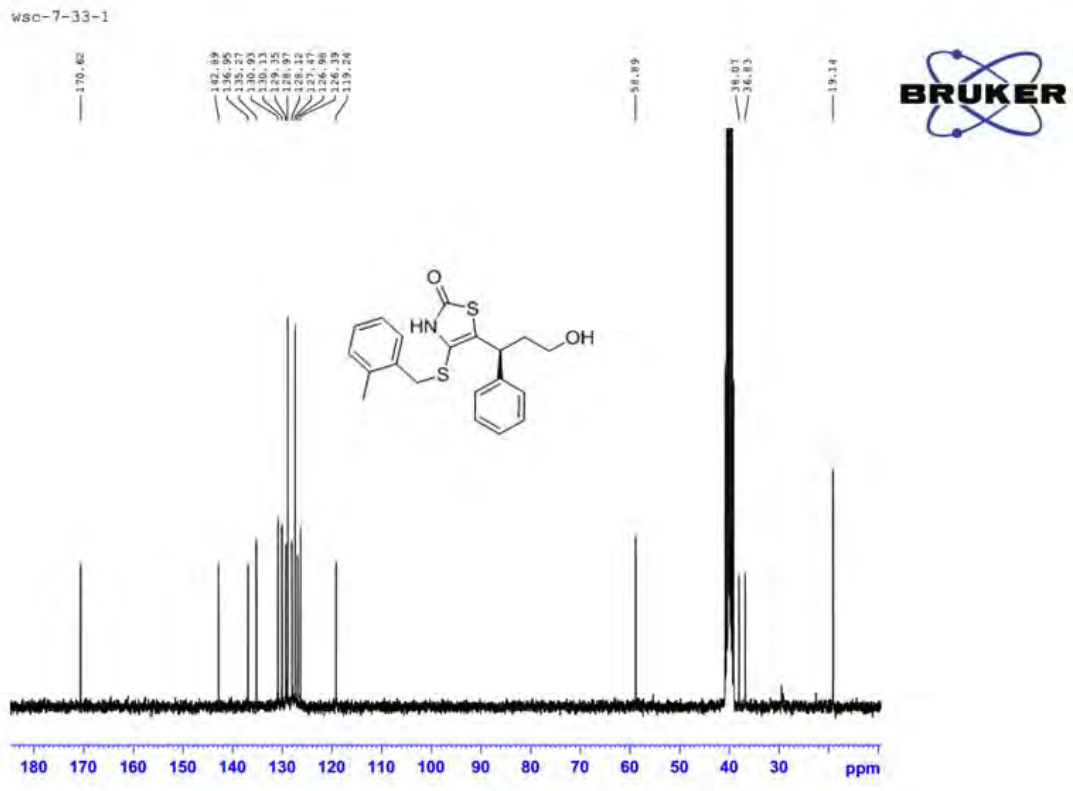
Compound **4d**


wsc-7-34-2
BRUKER
F
O
HN
S
S
OH
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 ppm

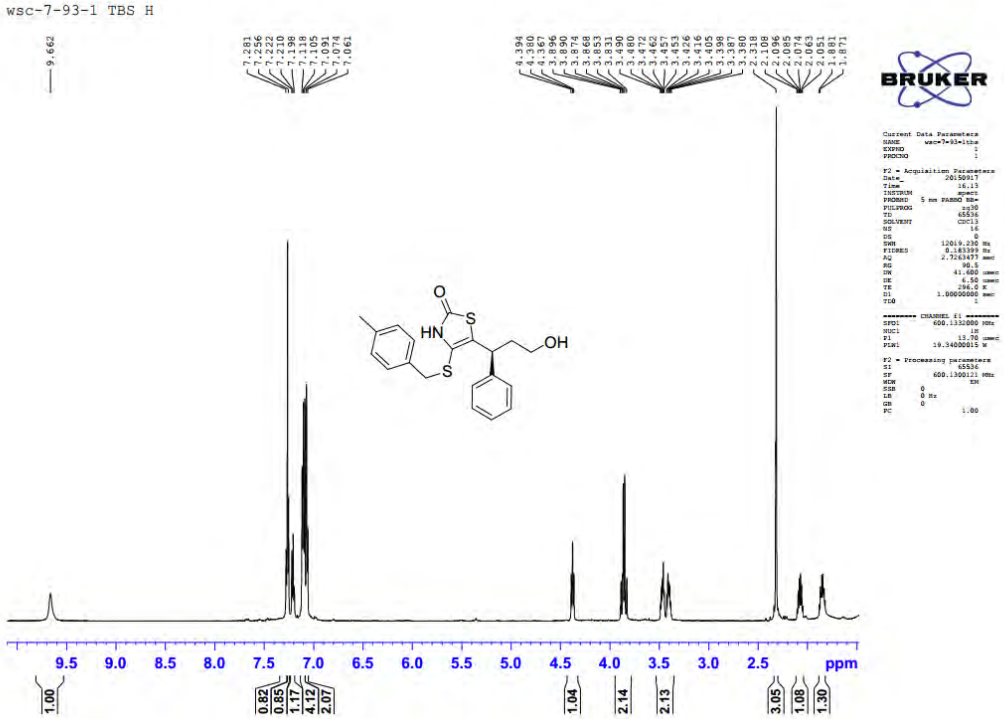

wsc-7-34-2
BRUKER
F
O
HN
S
S
OH
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

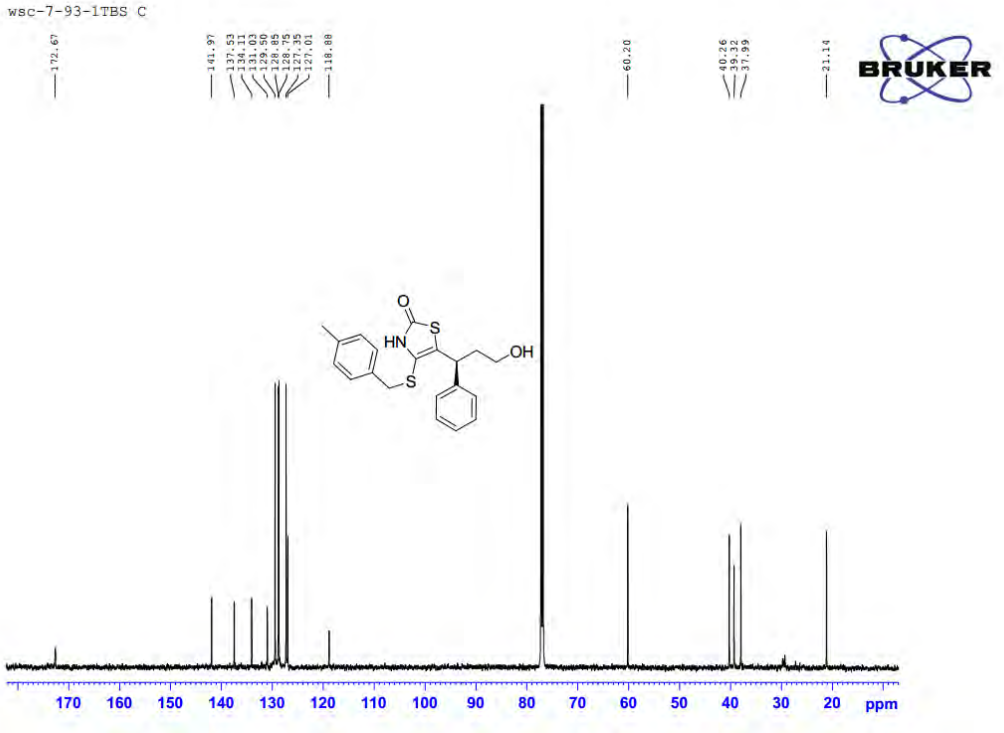
Compound **4e**


wsc-7-33-1
BRUKER
O
S
HN
S
OH
12
11
10
9
8
7
6
5
4
3
2
ppm

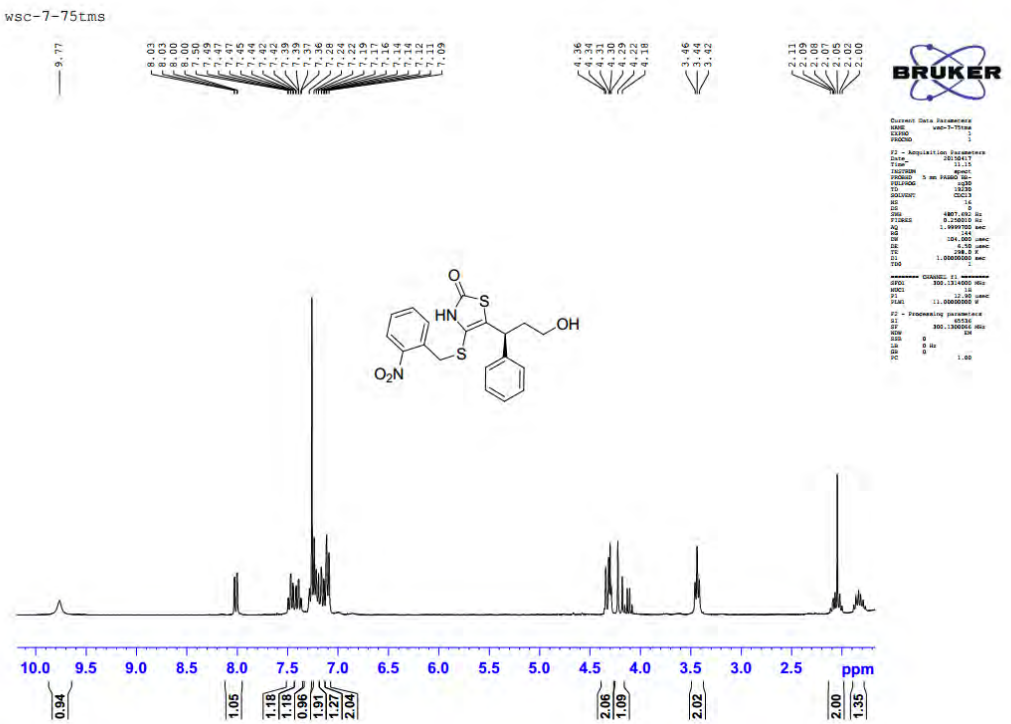

wsc-7-33-1
BRUKER
O
S
HN
S
OH
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
ppm

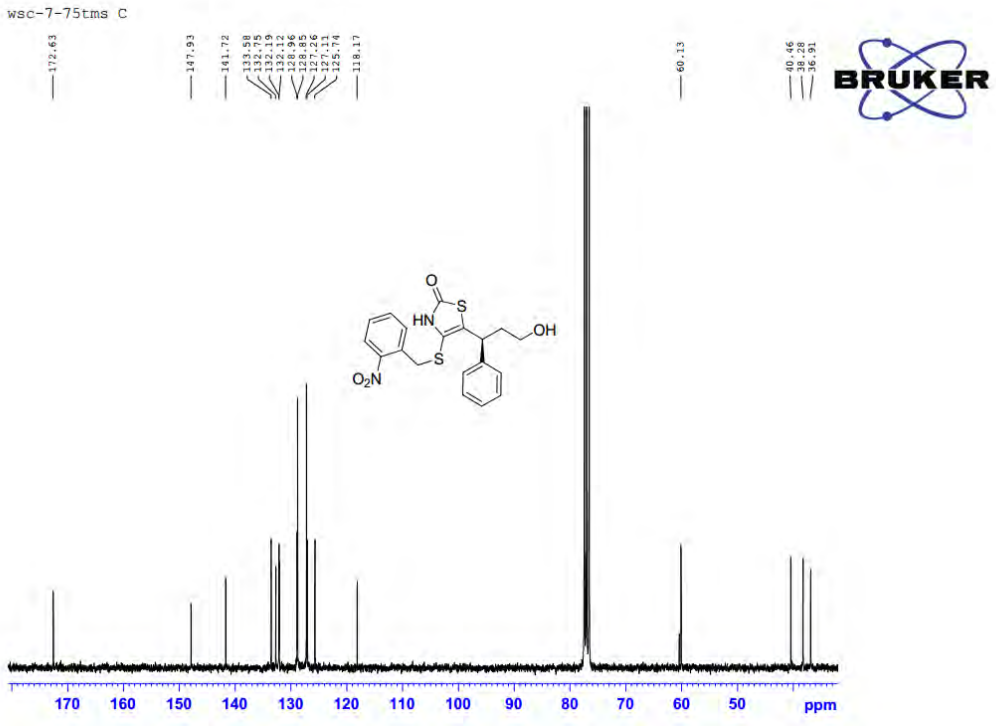
Compound **4f**


wsc-7-93-1 TBS H
9.662
7.281
7.256
7.222
7.210
7.198
7.118
7.105
7.091
7.074
7.061
4.394
4.380
4.367
3.896
3.890
3.874
3.868
3.853
3.831
3.490
3.480
3.472
3.462
3.457
3.453
3.426
3.416
3.405
3.398
3.387
3.380
2.318
2.108
2.096
2.085
2.074
2.063
2.051
1.881
1.871
BRUKER
Current Data Parameters
NAME wsc-7-93-1tbs
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150917
Time 16.13
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7263497 sec
RG 90.5
DW 41.600 usec
DE 6.50 usec
TE 296.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 600.1332000 MHz
NUC1 1H
P1 13.70 usec
PLW1 19.54000615 W
F2 - Processing parameters
SI 65536
SF 600.1300121 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00
O
S
HN
S
OH
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 ppm
1.00
0.82
0.85
1.17
4.12
2.07
1.04
2.14
2.13
3.05
1.08
1.30

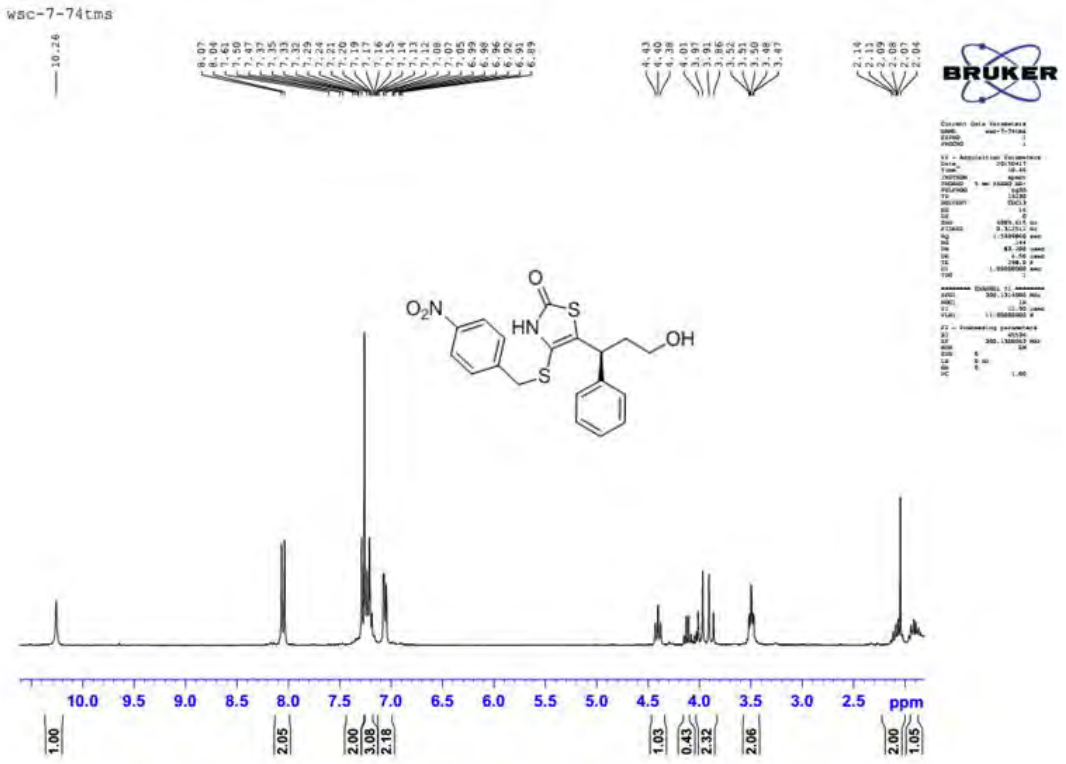

wsc-7-93-1TBS C
172.67
141.97
137.53
136.11
131.03
129.50
128.85
128.75
127.35
127.01
118.88
60.20
40.26
39.32
37.99
21.14
BRUKER
O
S
HN
S
OH
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

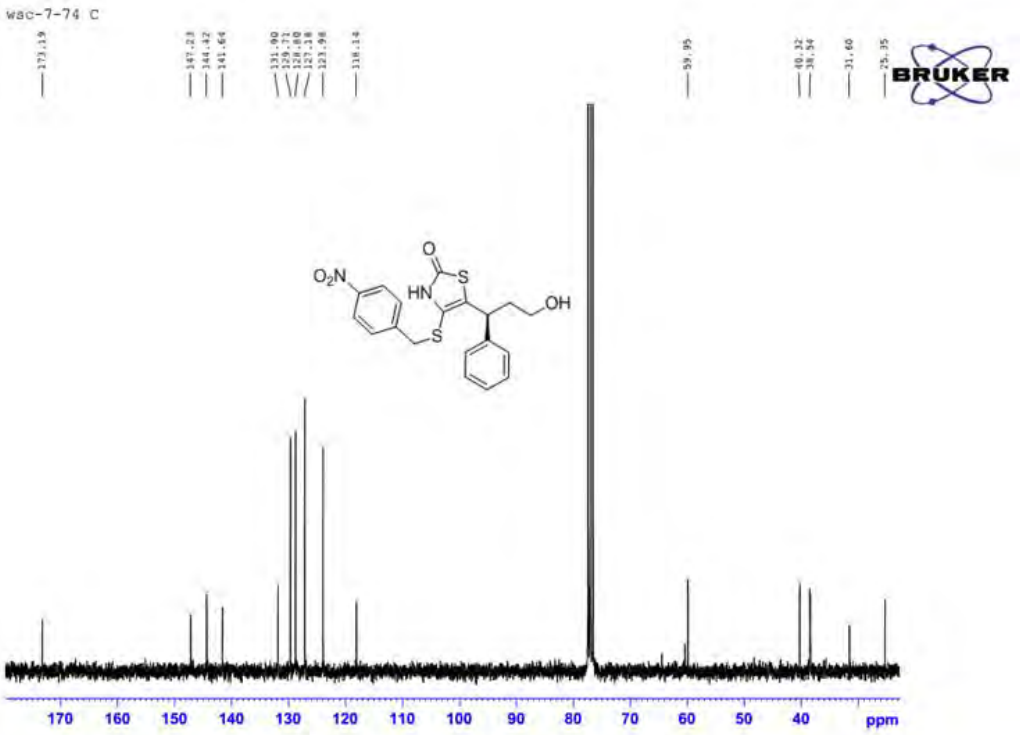
Compound **4g**


wsc-7-75tms
9.77
8.03
8.03
8.00
8.00
7.50
7.49
7.47
7.47
7.45
7.44
7.42
7.42
7.39
7.39
7.37
7.36
7.28
7.24
7.22
7.19
7.17
7.16
7.14
7.14
7.12
7.11
7.09
4.36
4.34
4.31
4.30
4.29
4.27
4.18
3.46
3.44
3.42
2.11
2.09
2.08
2.07
2.05
2.02
2.00
BRUKER
O
S
HN
OH
S
O2N
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
ppm
0.94
1.05
1.18
1.18
0.96
1.91
1.27
2.04
2.06
1.09
2.02
2.00
1.35

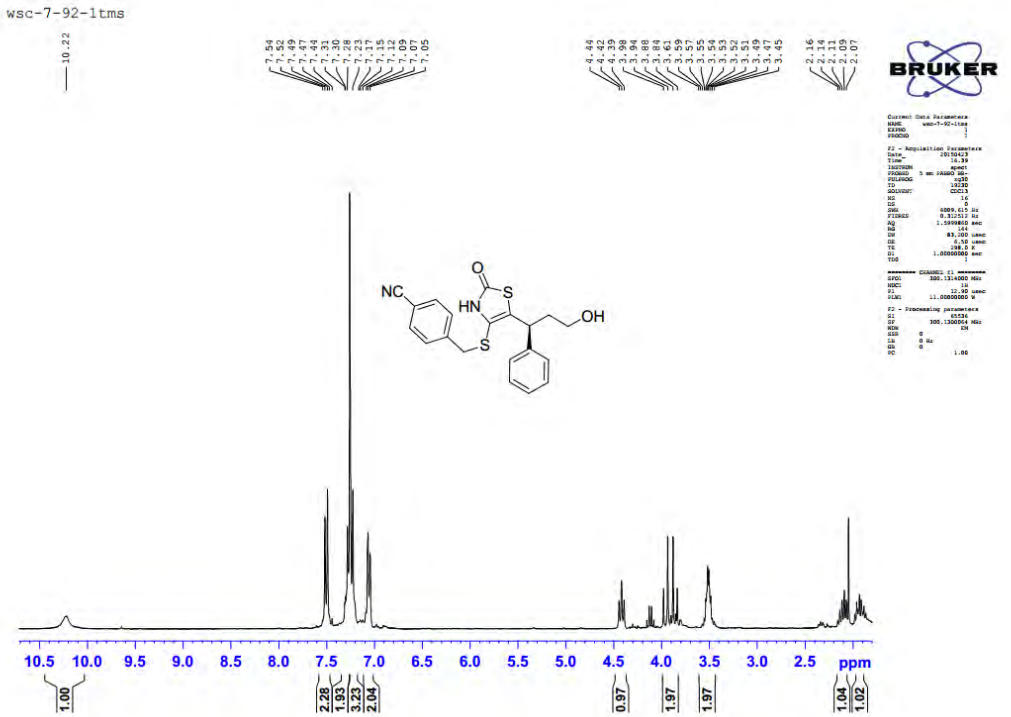

wsc-7-75tms C
172.63
147.93
141.72
133.58
132.75
132.29
132.12
128.96
128.85
127.66
127.11
125.74
118.17
60.13
40.46
38.20
36.91
BRUKER
O
S
HN
OH
S
O2N
170
160
150
140
130
120
110
100
90
80
70
60
50
ppm

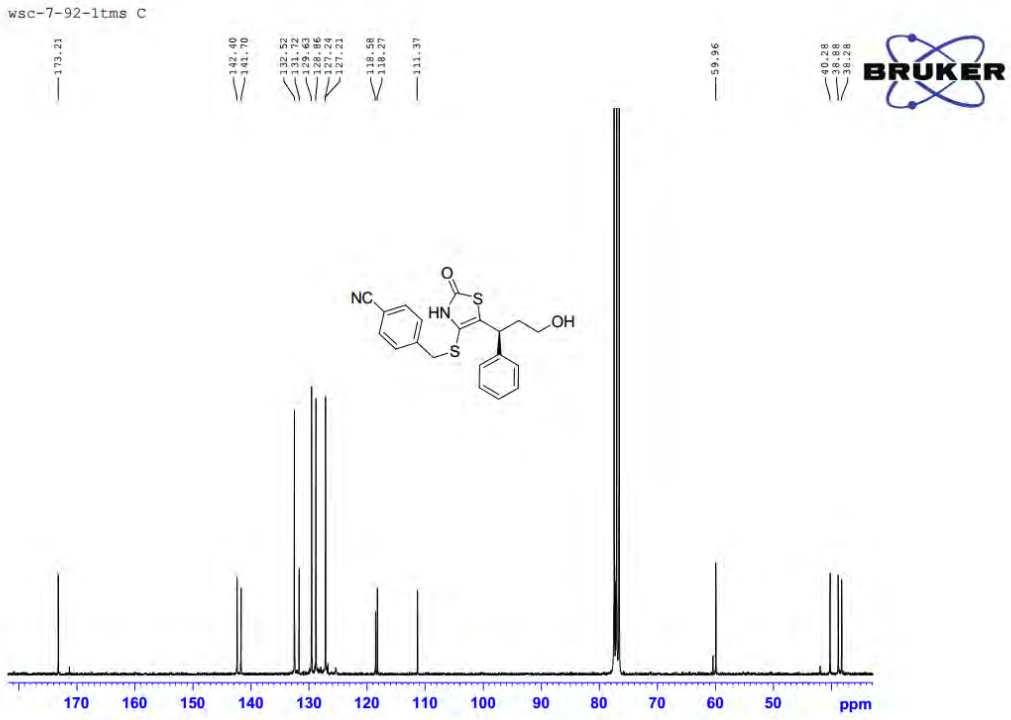
Compound **4h**


wsc-7-74tms
BRUKER
O2N
HN
S
OH
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 ppm
1.00 2.05 2.00 3.08 2.18 1.03 0.43 2.32 2.06 2.00 1.05

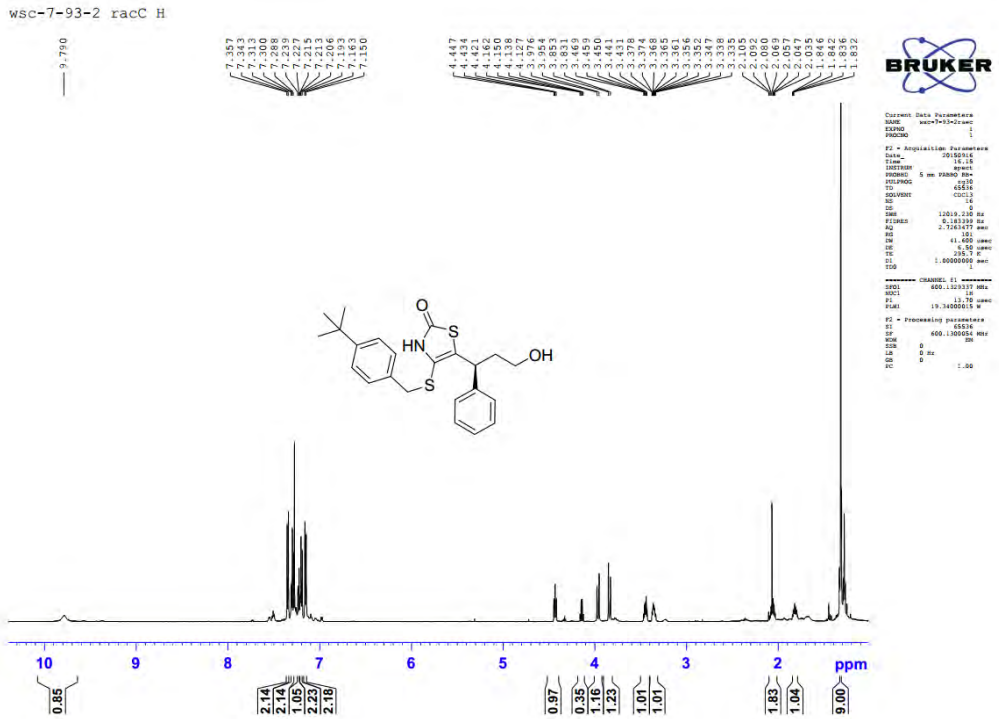

wsc-7-74 C
BRUKER
O2N
HN
S
OH
170 160 150 140 130 120 110 100 90 80 70 60 50 40 ppm

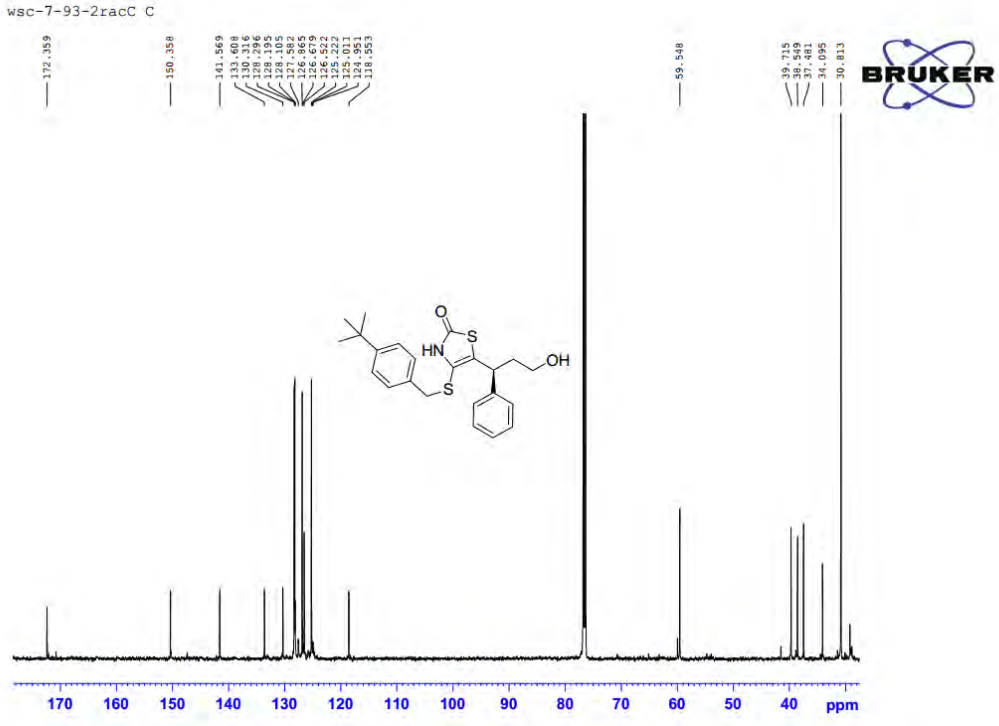
Compound **4i**


wsc-7-92-1tms
10.22
7.54
7.52
7.49
7.47
7.44
7.31
7.30
7.28
7.23
7.17
7.15
7.12
7.09
7.07
7.05
4.44
4.42
4.39
3.98
3.94
3.88
3.84
3.61
3.59
3.57
3.55
3.54
3.53
3.52
3.51
3.49
3.47
3.45
2.16
2.14
2.11
2.09
2.07
BRUKER
NC
HN
O
S
S
OH
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 ppm
1.00
2.28
1.93
3.23
2.04
0.97
1.97
1.97
1.04
1.02

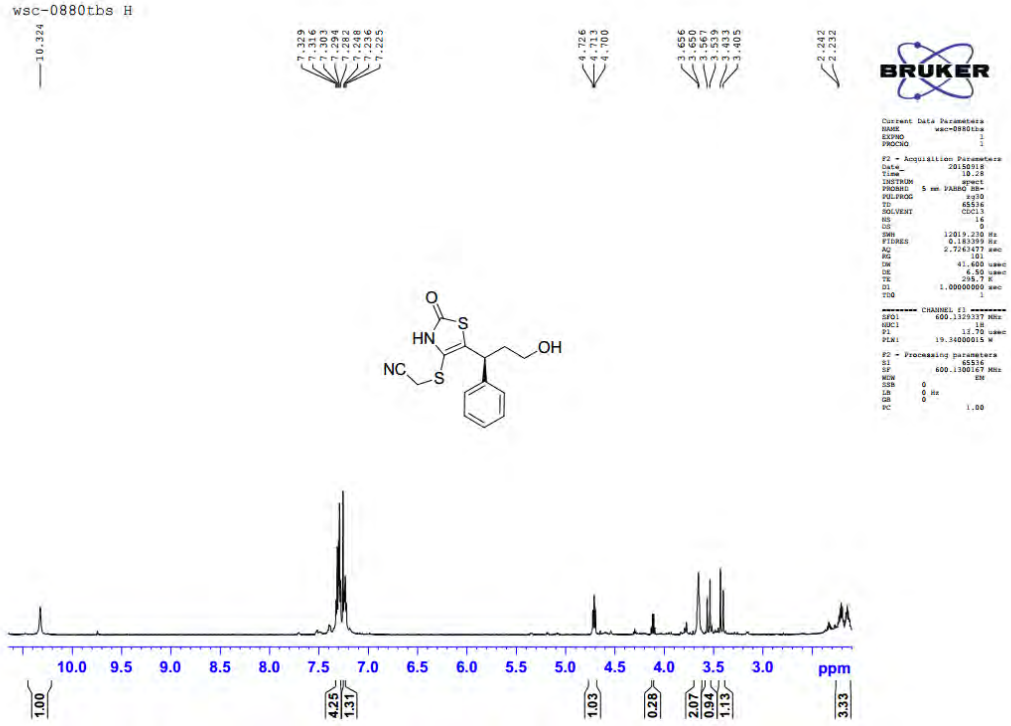

wsc-7-92-1tms C
173.21
142.40
141.70
132.52
131.72
129.63
128.86
127.24
127.21
118.58
118.27
111.37
59.96
40.28
38.88
38.28
BRUKER
NC
HN
O
S
S
OH
170 160 150 140 130 120 110 100 90 80 70 60 50 ppm

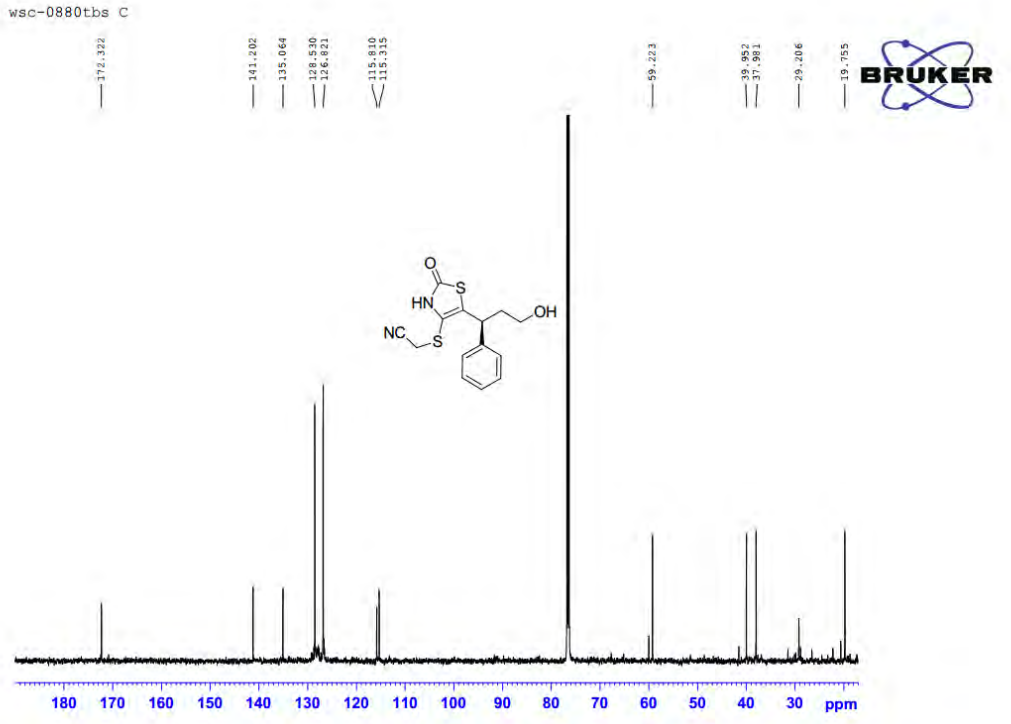
Compound **4j**


wsc-7-93-2 racC H
9.790
7.357
7.348
7.313
7.300
7.288
7.239
7.227
7.215
7.213
7.206
7.193
7.165
7.150
4.447
4.438
4.421
4.162
4.150
4.139
4.127
3.976
3.954
3.853
3.831
3.469
3.459
3.450
3.441
3.381
3.378
3.374
3.368
3.365
3.361
3.356
3.352
3.347
3.338
3.335
2.105
2.092
2.080
2.069
2.057
2.047
2.035
1.846
1.842
1.836
1.832
BRUKER
HN
O
S
S
OH
10
9
8
7
6
5
4
3
2
ppm
0.85
2.14
2.14
1.05
2.23
2.18
0.97
0.35
1.16
1.23
1.01
1.01
1.83
1.04
9.00

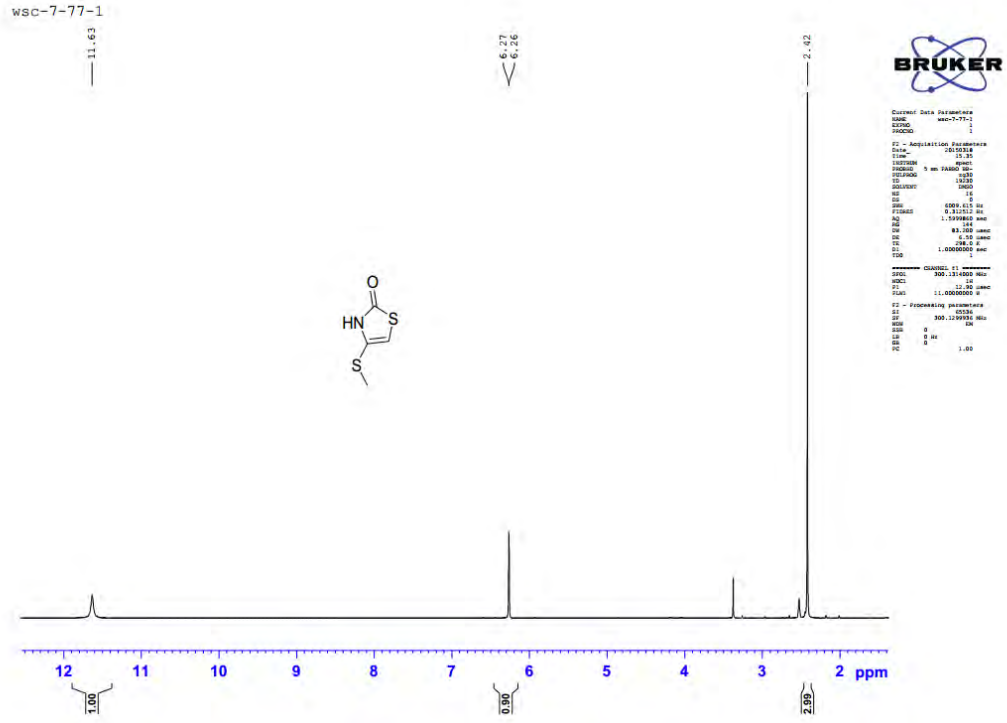

wsc-7-93-2racC C
172.359
150.358
141.569
133.608
130.316
129.196
128.595
128.105
127.582
126.865
126.659
126.522
125.222
125.011
124.951
118.593
59.548
39.715
38.549
37.481
34.095
30.813
BRUKER
HN
O
S
S
OH
170
160
150
140
130
120
110
100
90
80
70
60
50
40
ppm

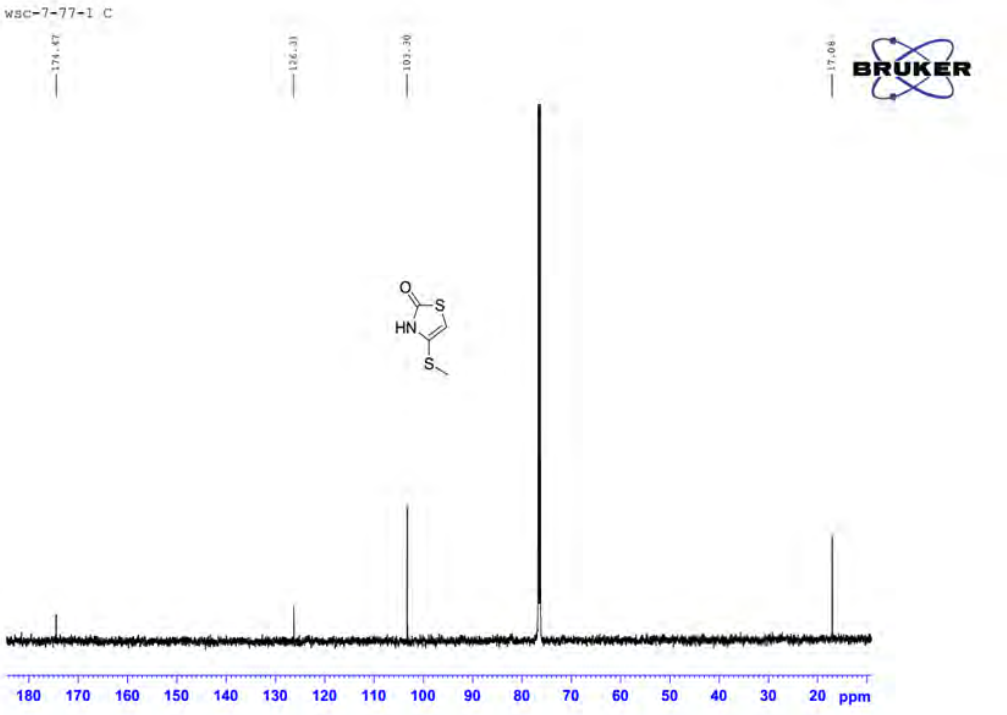
Compound **4k**


wsc-0880tbs H
10.324
7.329
7.316
7.303
7.294
7.282
7.248
7.236
7.225
4.726
4.713
4.700
3.656
3.650
3.557
3.539
3.433
3.405
2.242
2.232
BRUKER
HN
S
O
NC
S
OH
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
ppm
1.00
4.25
1.31
1.03
0.28
2.07
0.94
1.13
3.33

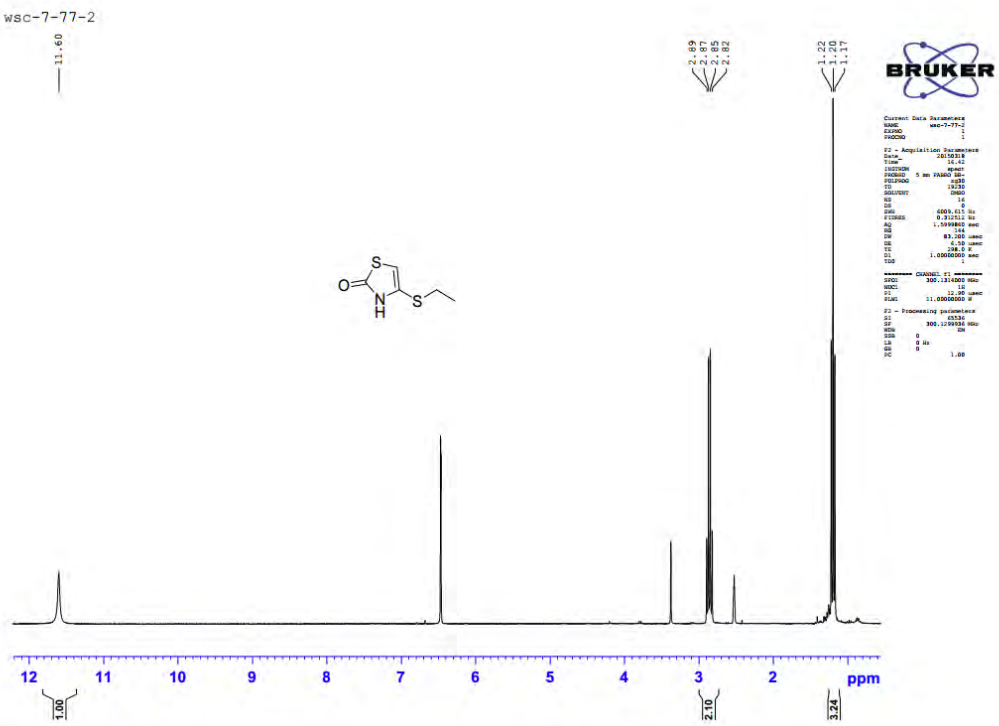

wsc-0880tbs C
172.322
141.202
135.064
128.530
126.821
115.810
115.315
59.223
39.952
37.981
29.206
19.755
BRUKER
HN
S
O
NC
S
OH
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
ppm

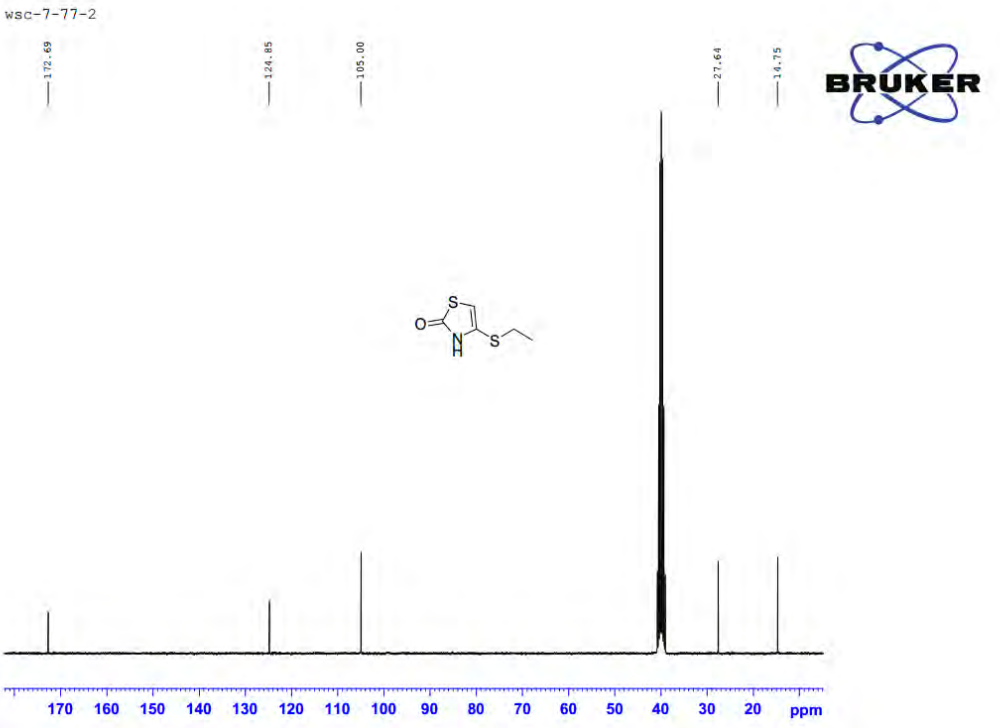
Compound 2a


wsc-7-77-1
11.63
6.27
6.26
2.42
BRUKER
HN
O
S
S
12
11
10
9
8
7
6
5
4
3
2 ppm
1.00
0.90
2.99

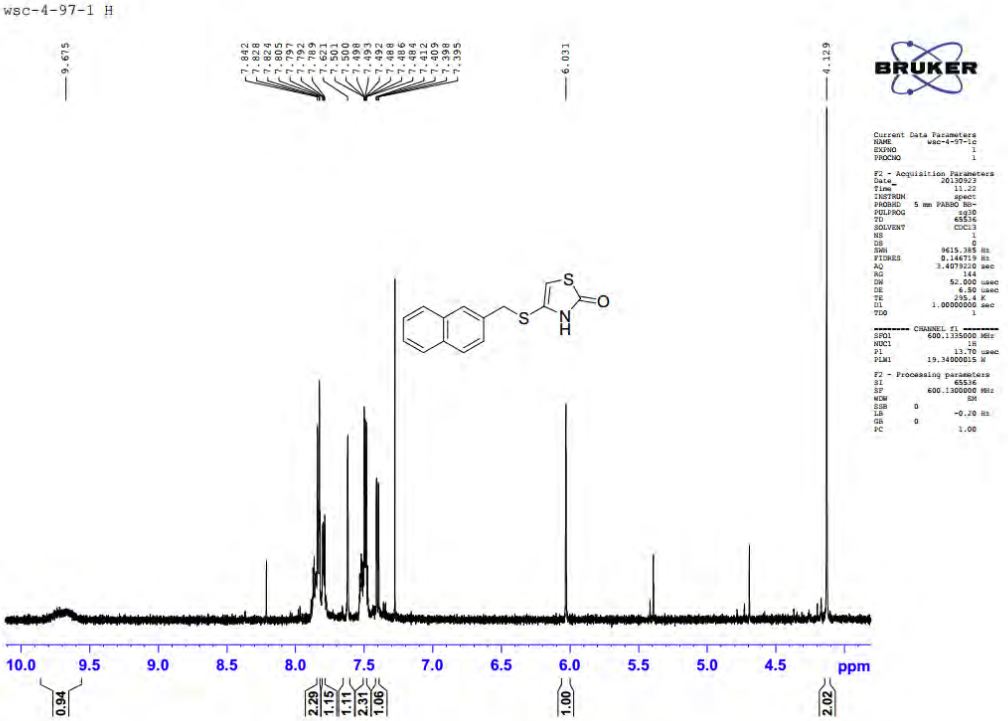

wsc-7-77-1 C
174.47
126.31
103.30
17.08
BRUKER
HN
O
S
S
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20 ppm

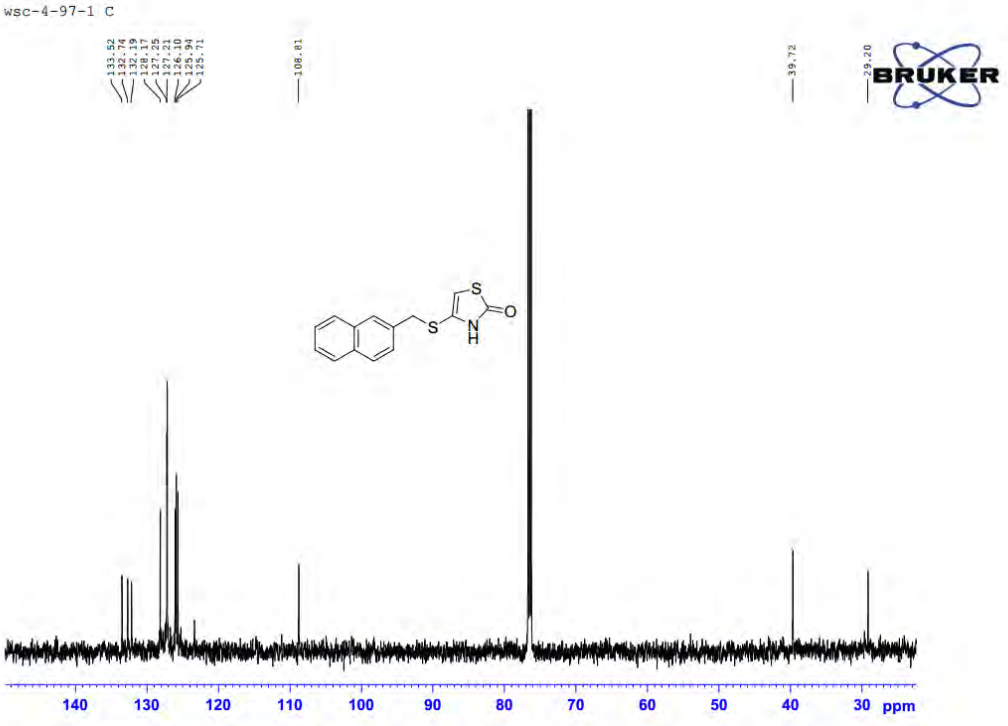
Compound 2b


wsc-7-77-2
11.60
2.89
2.87
2.85
2.82
1.22
1.20
1.17
BRUKER
12
11
10
9
8
7
6
5
4
3
2
ppm
1.00
2.10
3.24

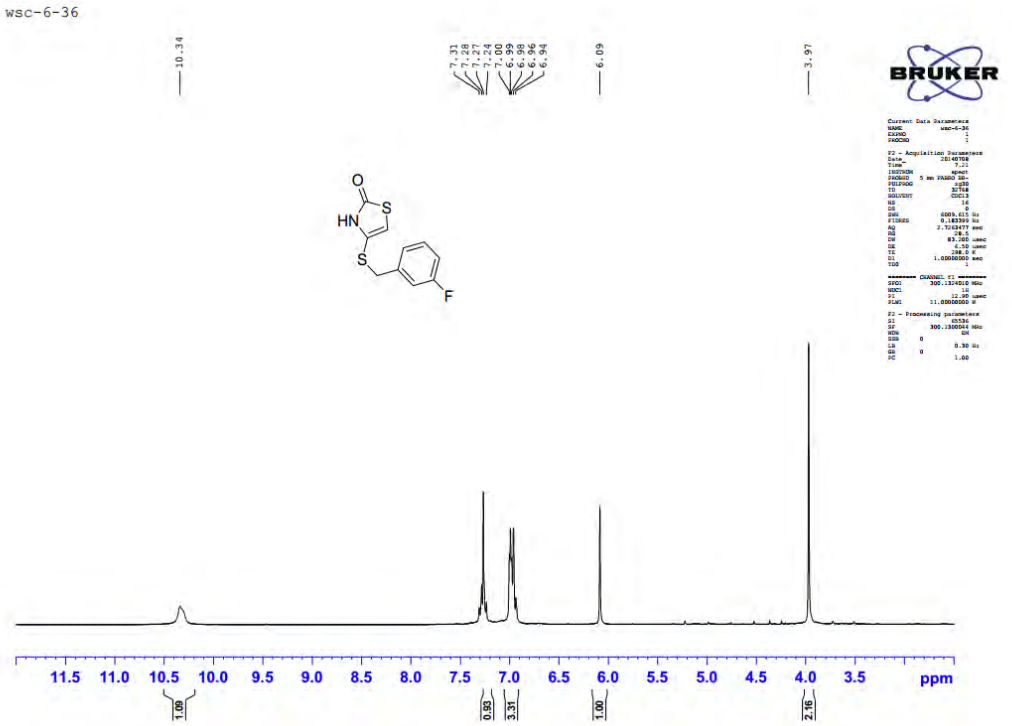

wsc-7-77-2
172.69
124.85
105.00
27.64
14.75
BRUKER
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

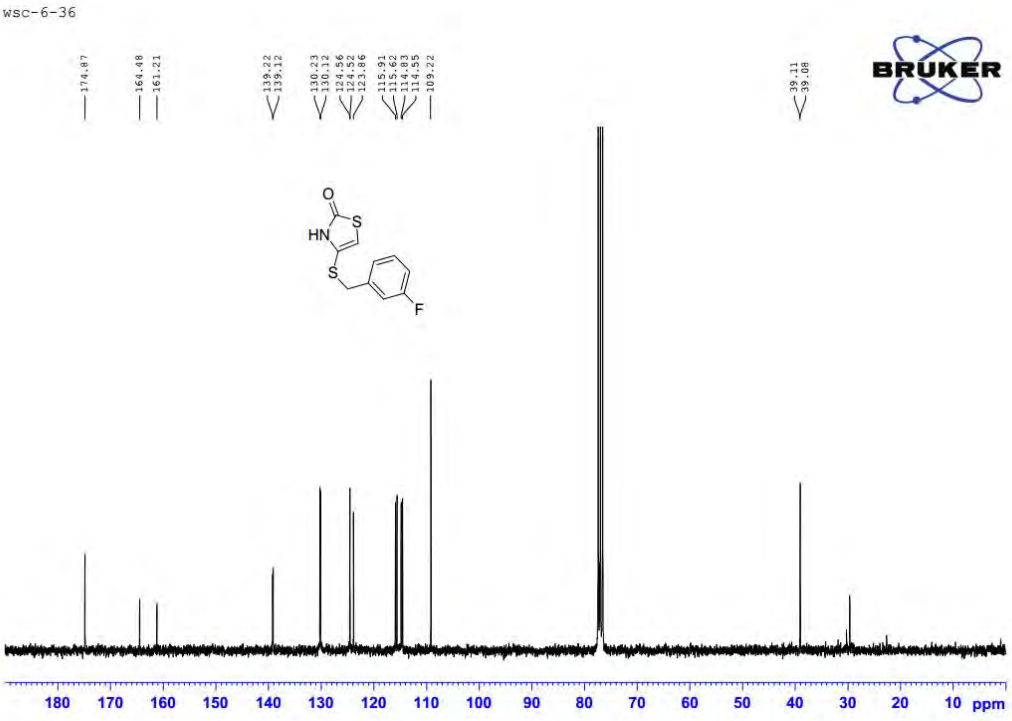
Compound 2c


wsc-4-97-1 H
9.675
7.842
7.828
7.826
7.805
7.797
7.792
7.789
7.671
7.501
7.500
7.498
7.493
7.488
7.486
7.484
7.412
7.409
7.398
7.395
6.031
4.129
BRUKER
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
ppm
0.94
2.29
1.15
1.11
2.31
1.06
1.00
2.02

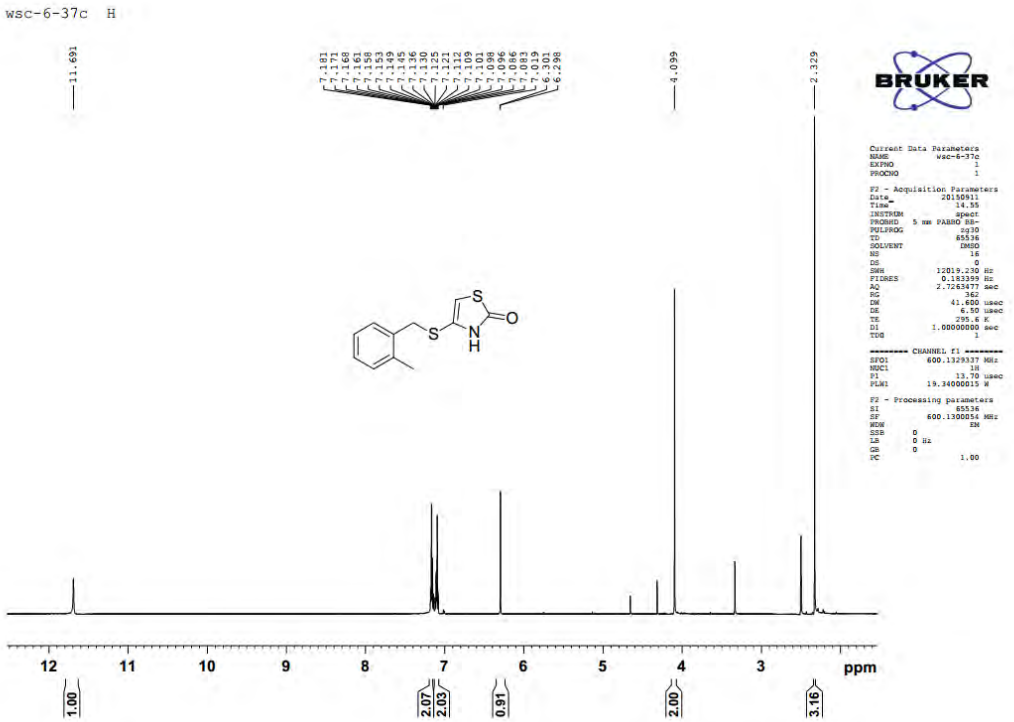

wsc-4-97-1 C
133.52
132.74
132.19
128.17
127.25
127.21
126.10
125.94
125.71
108.81
39.72
29.20
BRUKER
140
130
120
110
100
90
80
70
60
50
40
30
ppm

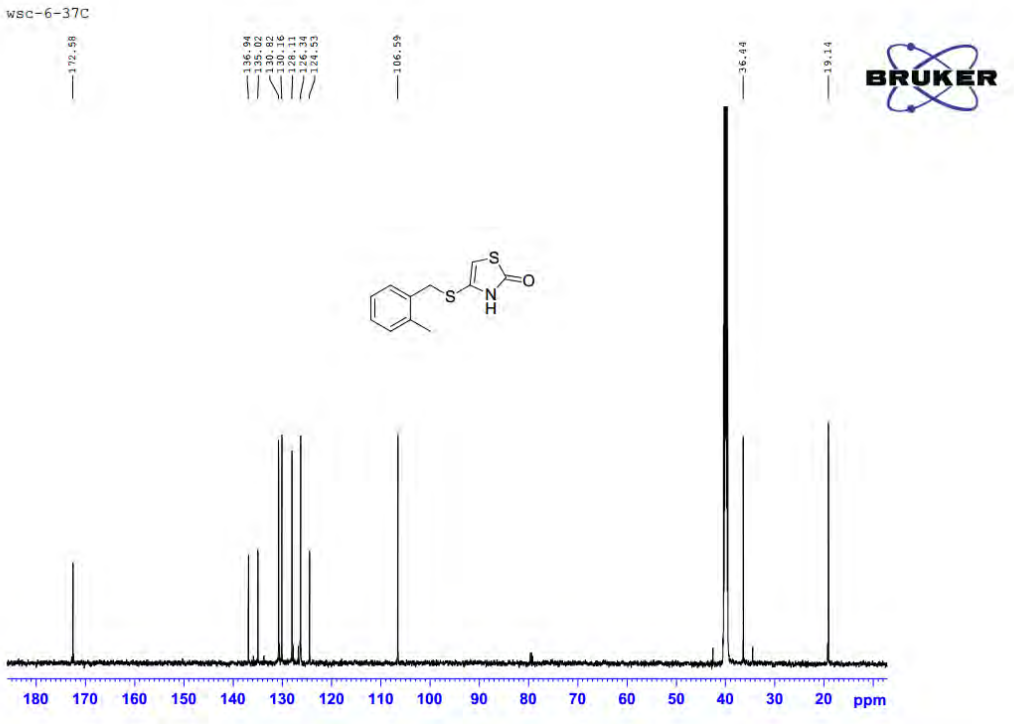
Compound 2d


wsc-6-36
10.34
7.31
7.28
7.27
7.24
7.00
6.99
6.98
6.96
6.94
6.09
3.97
BRUKER
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 ppm
1.09
0.93
3.31
1.00
2.16

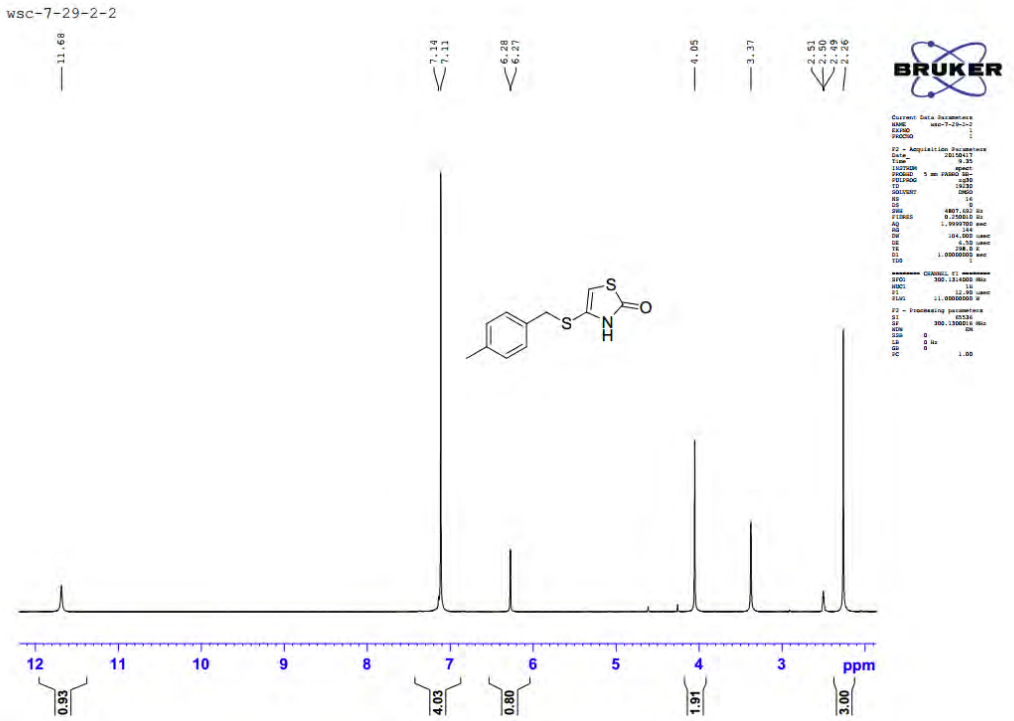

wsc-6-36
174.87
164.48
161.21
139.22
139.12
130.23
130.12
124.56
124.52
123.86
115.91
115.62
114.83
114.55
109.22
39.11
39.08
BRUKER
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

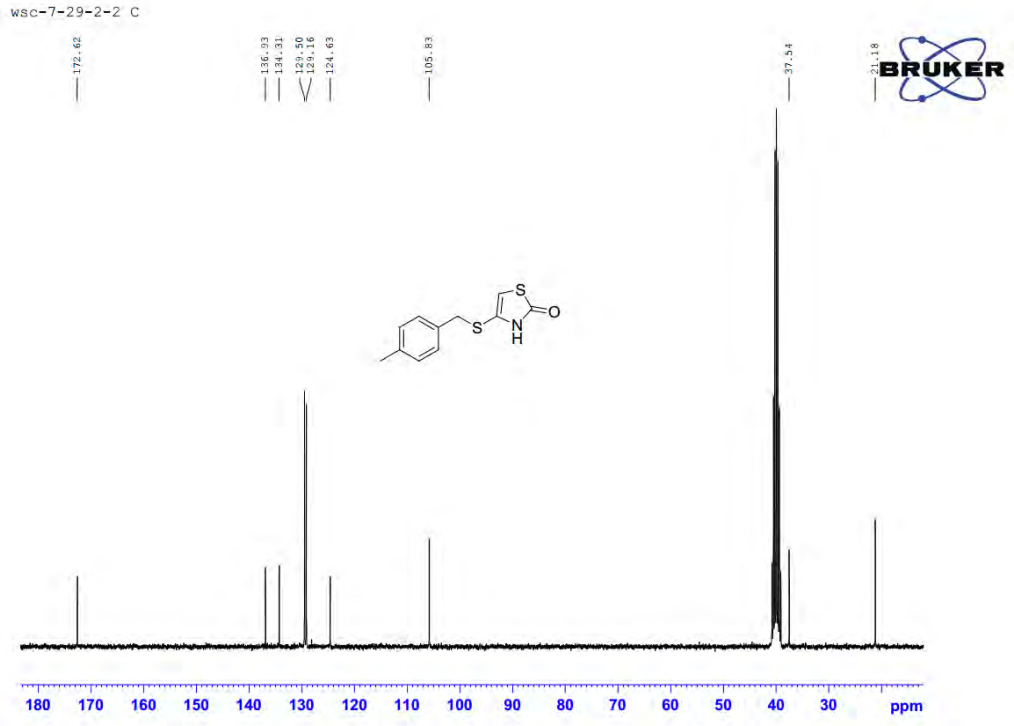
Compound 2e


wsc-6-37c H
11.691
7.181
7.171
7.168
7.161
7.156
7.153
7.149
7.145
7.136
7.130
7.125
7.121
7.112
7.109
7.101
7.098
7.096
7.086
7.083
7.079
7.039
6.301
6.298
4.099
2.329
BRUKER
Current Data Parameters
NAME wsc-6-37c
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150911
Time 14.55
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 0
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 362
DW 41.600 usec
DE 6.50 usec
TE 295.6 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 600.1329337 MHz
NUC1 1H
P1 13.70 usec
PLW1 19.34000015 W
F2 - Processing parameters
SI 65536
SF 600.1300054 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00
S
O
N
H
S
12
11
10
9
8
7
6
5
4
3
ppm
1.00
2.07
2.03
0.91
2.00
3.16

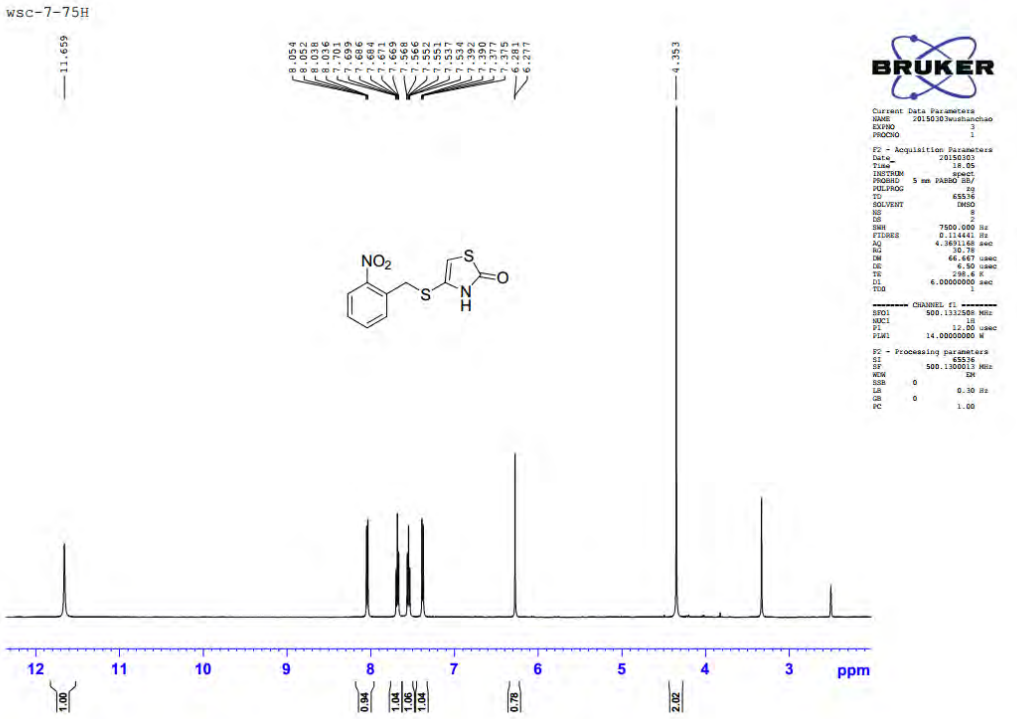

wsc-6-37c
172.58
136.94
135.02
131.82
130.16
128.11
126.34
124.53
106.59
36.44
19.14
BRUKER
S
O
N
H
S
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

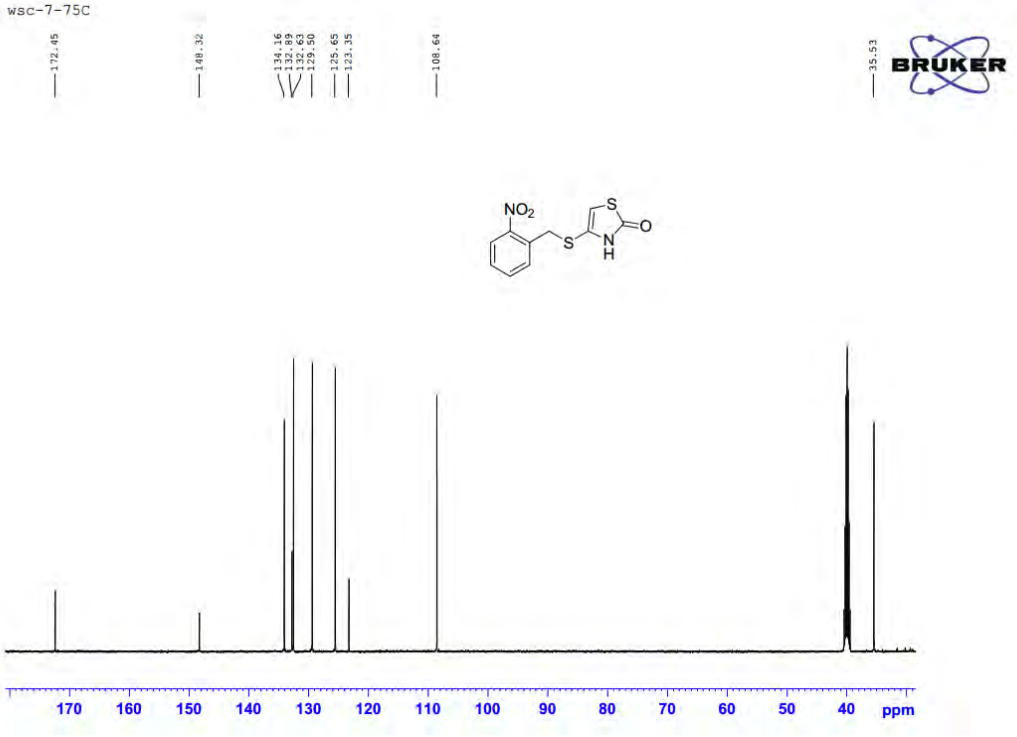
Compound 2f


wsc-7-29-2-2
11.68
7.14
7.11
6.28
6.27
4.05
3.37
2.51
2.50
2.49
2.46
BRUKER
S
O
N
H
S
12
11
10
9
8
7
6
5
4
3
ppm
0.93
4.03
0.80
1.91
3.00

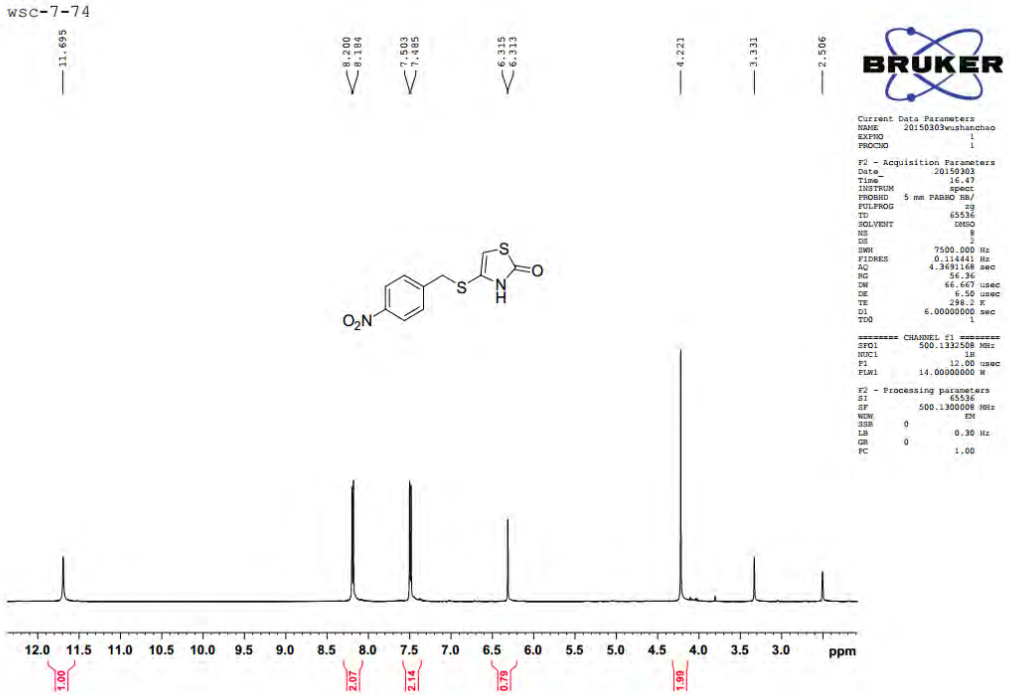

wsc-7-29-2-2 C
172.62
136.03
134.31
129.50
129.16
124.63
105.83
37.54
21.18
BRUKER
S
O
N
H
S
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
ppm

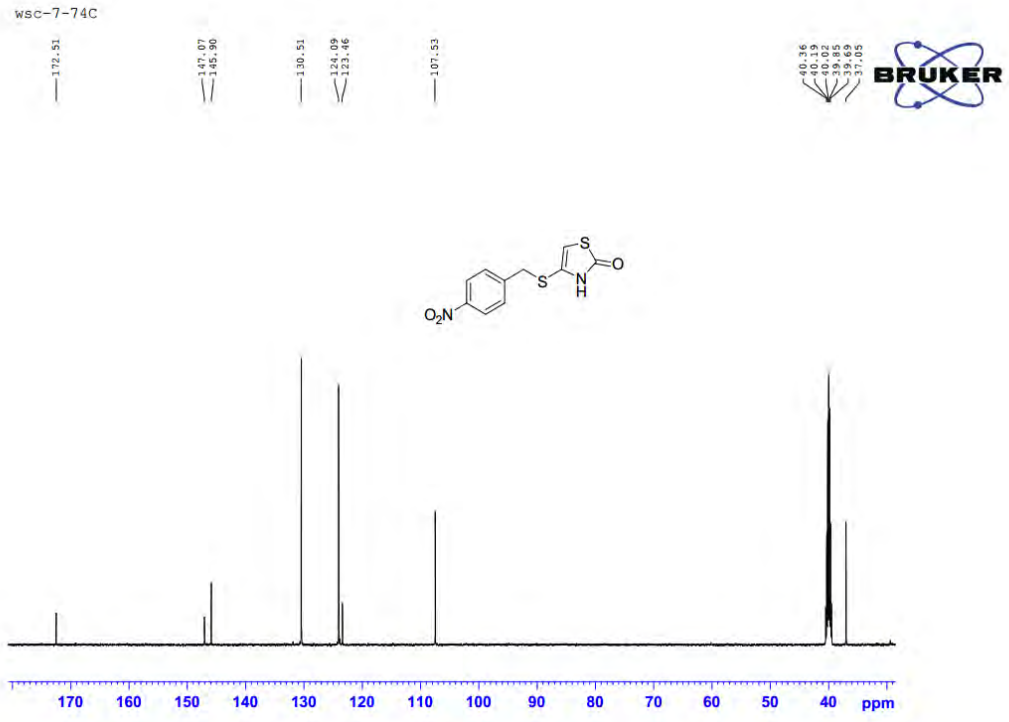
Compound 2g


wsc-7-75H
11.659
8.054
8.052
8.038
8.036
8.016
8.013
7.699
7.686
7.684
7.671
7.669
7.568
7.566
7.552
7.550
7.537
7.534
7.392
7.390
7.377
7.375
6.281
6.277
4.353
BRUKER
NO2
S
O
N
H
12
11
10
9
8
7
6
5
4
3
ppm
1.00
0.94
1.04
1.00
1.04
0.78
2.02

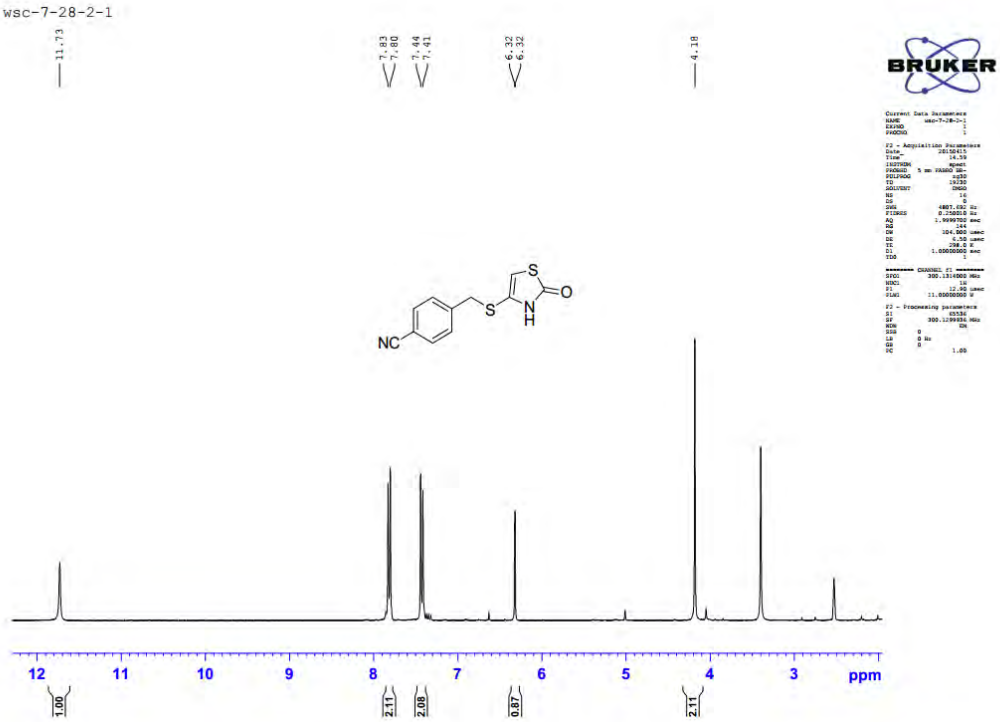

wsc-7-75C
172.45
148.32
134.16
132.89
132.63
129.50
125.65
123.35
108.64
35.53
BRUKER
NO2
S
O
N
H
170
160
150
140
130
120
110
100
90
80
70
60
50
40
ppm

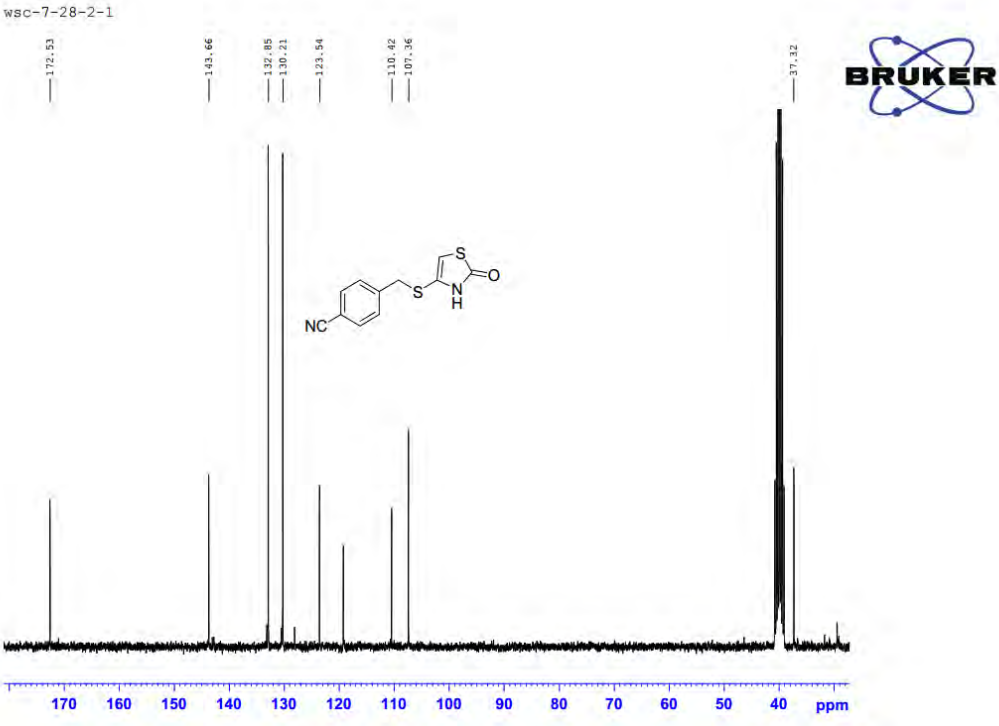
Compound 2h


wsc-7-74
11.695
8.200
8.184
7.503
7.485
6.315
6.313
4.221
3.331
2.506
BRUKER
Current Data Parameters
NAME 20150303wushanchao
EXPNO 1
PROCNO 1
F1 - Acquisition Parameters
Date_ 20150303
Time 16.47
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg
TD 65536
SOLVENT DMSO
NS 8
DS 2
SWH 7500.000 Hz
FIDRES 0.114441 Hz
AQ 4.3691168 sec
RG 56.36
DW 66.667 usec
DE 6.50 usec
TE 298.2 K
D1 6.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 500.1332508 MHz
NUC1 1H
P1 12.00 usec
PLW1 14.00000000 W
F2 - Processing parameters
SI 65536
SF 500.1300008 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
S
O
N
H
O2N
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 ppm
1.00
2.07
2.14
0.79
1.99

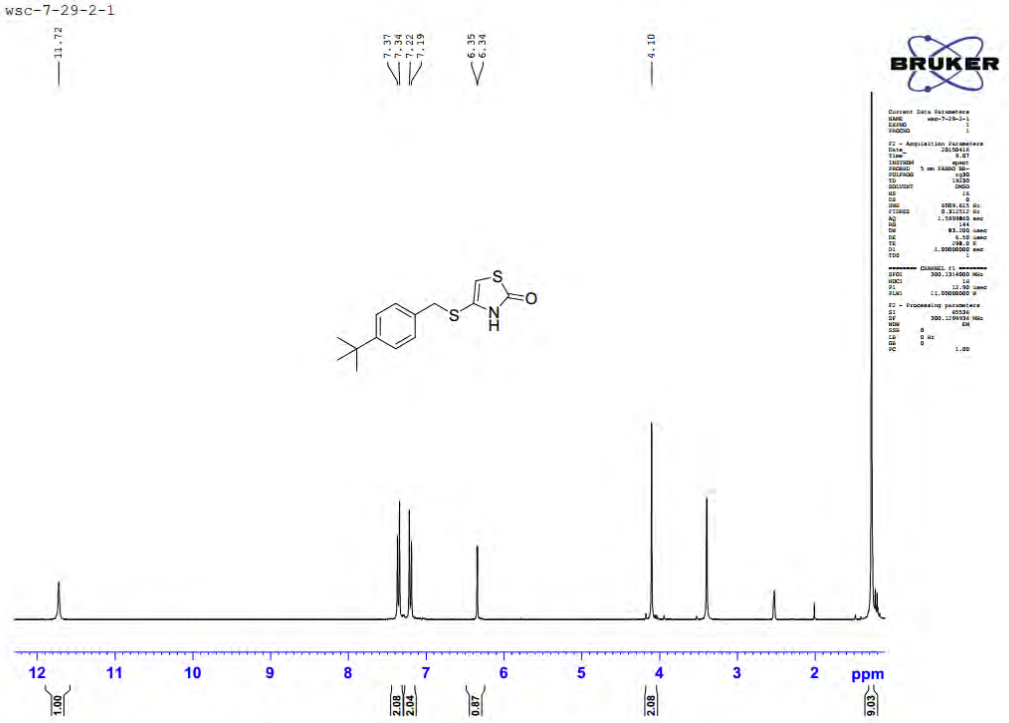

wsc-7-74C
172.51
147.07
145.90
130.51
124.09
123.46
107.53
40.36
40.19
40.02
39.85
39.69
37.05
BRUKER
S
O
N
H
O2N
170 160 150 140 130 120 110 100 90 80 70 60 50 40 ppm

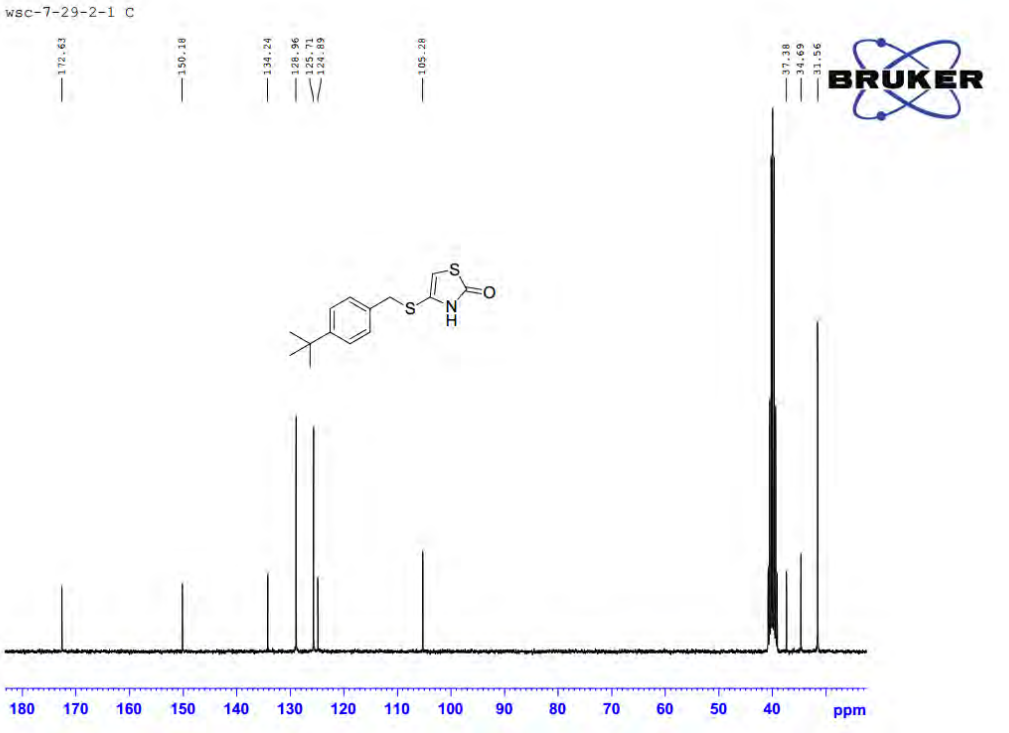
Compound 2i


wsc-7-28-2-1
11.73
7.83
7.80
7.44
7.41
6.32
6.32
4.18
BRUKER
S
O
N
H
S
NC
12
11
10
9
8
7
6
5
4
3
ppm
1.00
2.11
2.08
0.87
2.11

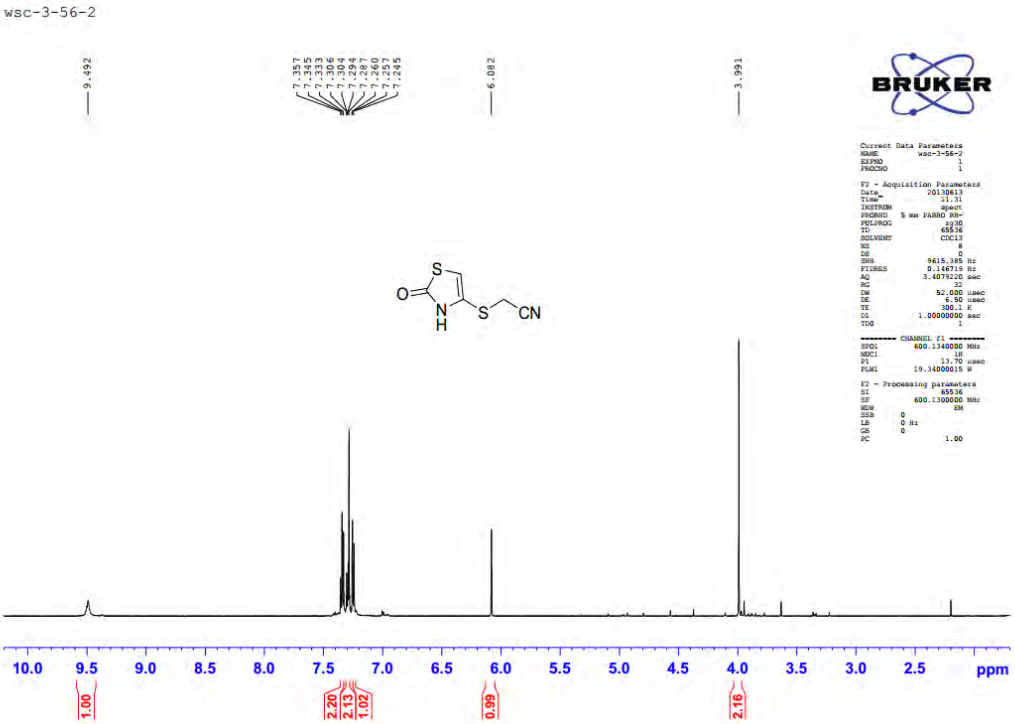

wsc-7-28-2-1
172.53
143.66
132.85
130.21
123.54
110.42
107.36
37.32
BRUKER
S
O
N
H
S
NC
170
160
150
140
130
120
110
100
90
80
70
60
50
40
ppm

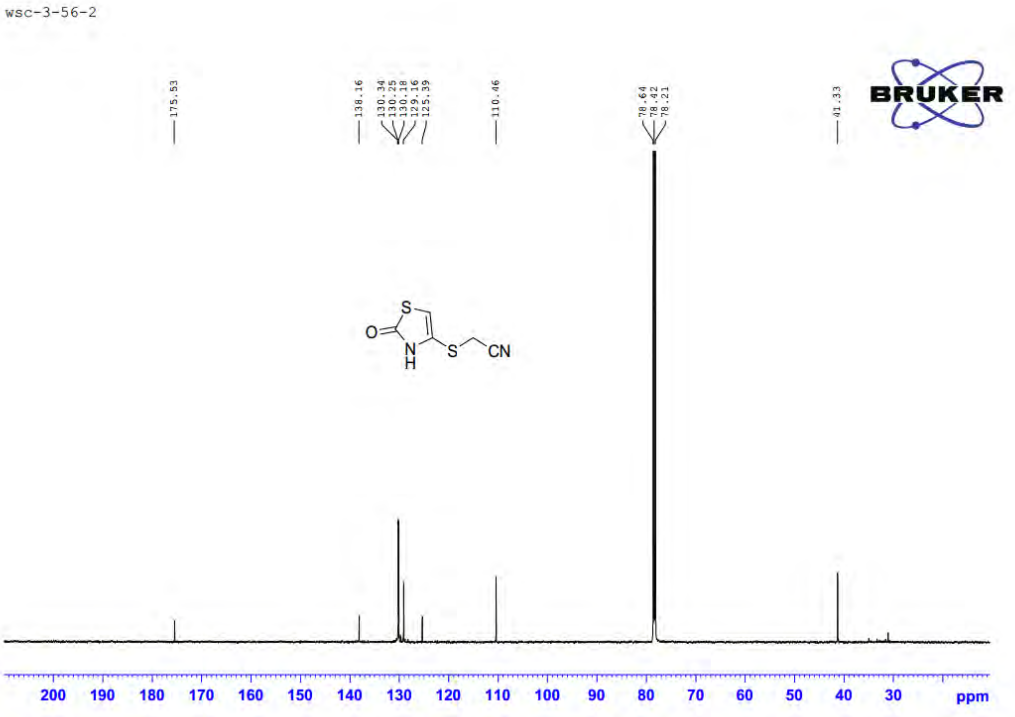
Compound 2j


wsc-7-29-2-1
11.72
7.37
7.34
7.22
7.19
6.35
6.34
4.10
BRUKER
12
11
10
9
8
7
6
5
4
3
2
ppm
1.00
2.08
2.04
0.87
2.08
9.03

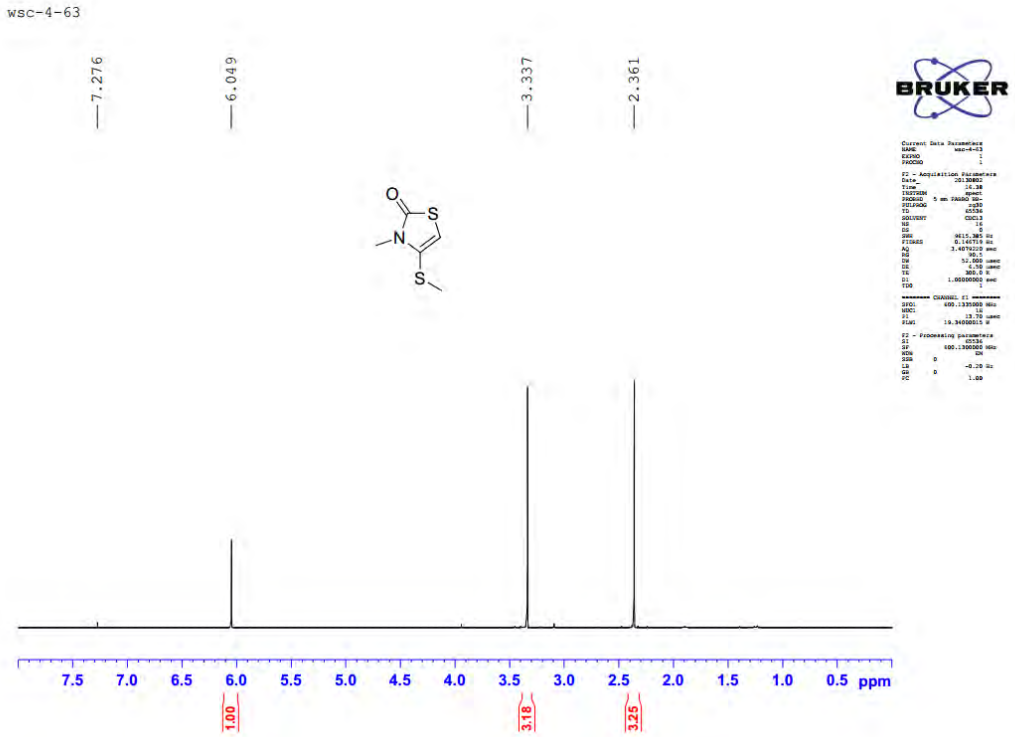

wsc-7-29-2-1 C
172.63
150.18
134.24
128.96
125.71
124.89
105.28
37.38
34.69
31.56
BRUKER
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
ppm

Compound 2k


wsc-3-56-2
9.492
7.357
7.355
7.333
7.331
7.306
7.304
7.294
7.287
7.260
7.257
7.245
6.082
3.991
BRUKER
Current Data Parameters
NAME wsc-3-56-2
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130613
Time 11.31
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 9615.385 Hz
FIDRES 0.146719 Hz
AQ 3.4079220 sec
RG 32
DW 52.000 usec
DE 6.50 usec
TE 300.1 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
SFO1 600.1340000 MHz
NUC1 1H
P1 13.70 usec
PLW1 19.34000015 W
F2 - Processing parameters
SI 65536
SF 600.1300000 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00
O
S
N
H
S
CN
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
ppm
1.00
2.20
2.13
1.02
0.99
2.16

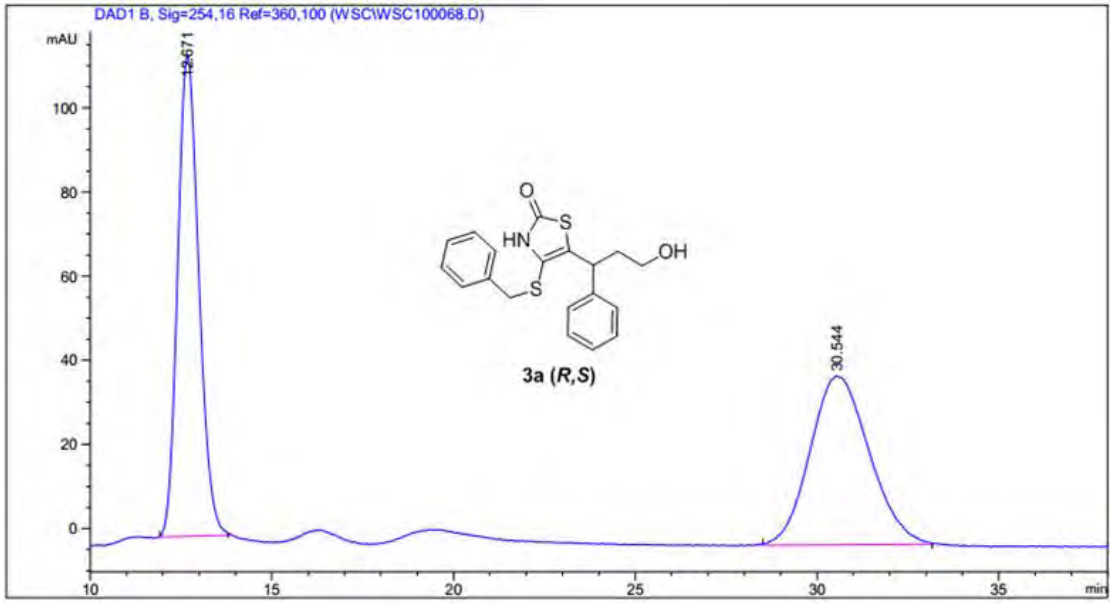

wsc-3-56-2
175.53
138.16
130.34
130.25
130.18
129.16
125.39
110.46
78.64
78.42
78.21
41.33
BRUKER
O
S
N
H
S
CN
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
ppm

Compound 2l

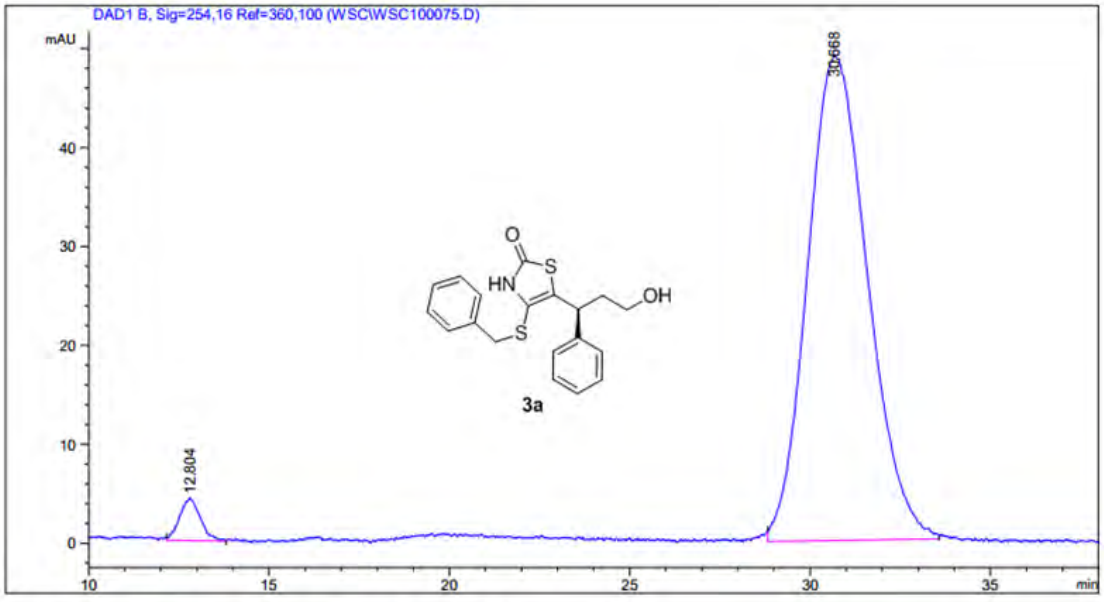

wsc-4-63
7.276
6.049
3.337
2.361
BRUKER
O
S
N
S
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
1.00
3.18
3.25

HPLC Chromatograms

Compound **3a**

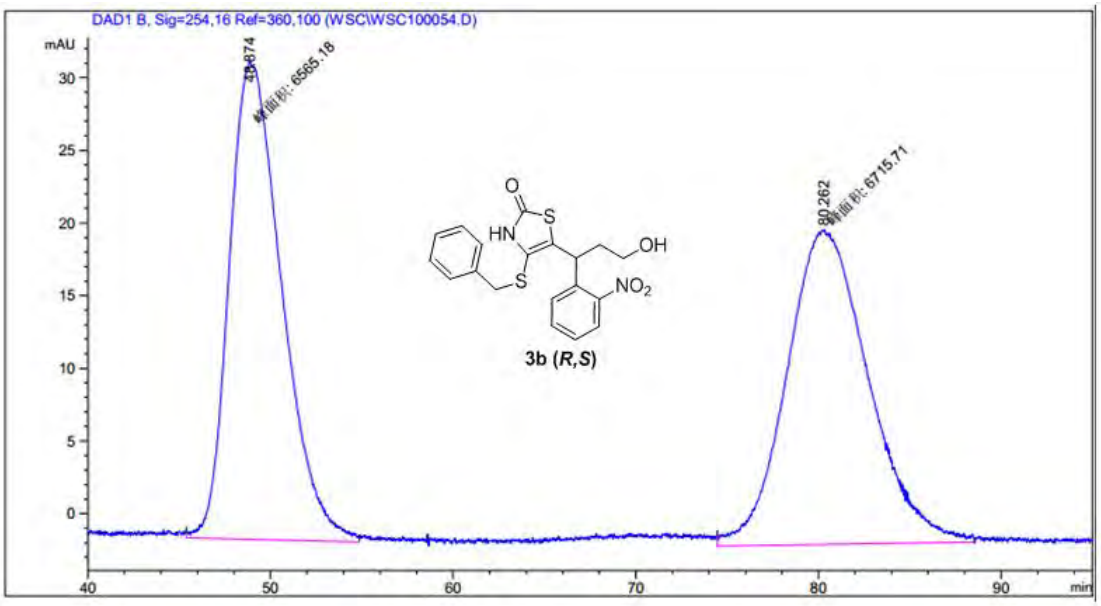


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	12.671	BB	0.5948	4626.54932	114.15897	50.3558
2	30.544	BV	1.3492	4561.16406	40.21619	49.6442

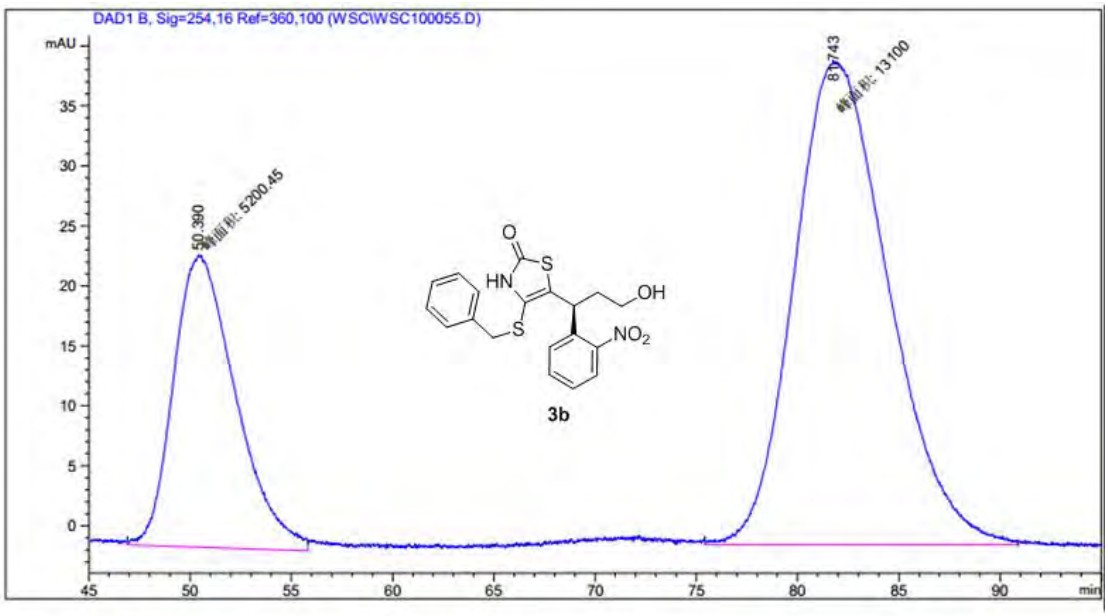


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	12.804	VV	0.4752	170.28683	4.30800	2.9199
2	30.668	BV	1.3610	5661.68506	48.96551	97.0801

Compound **3b**

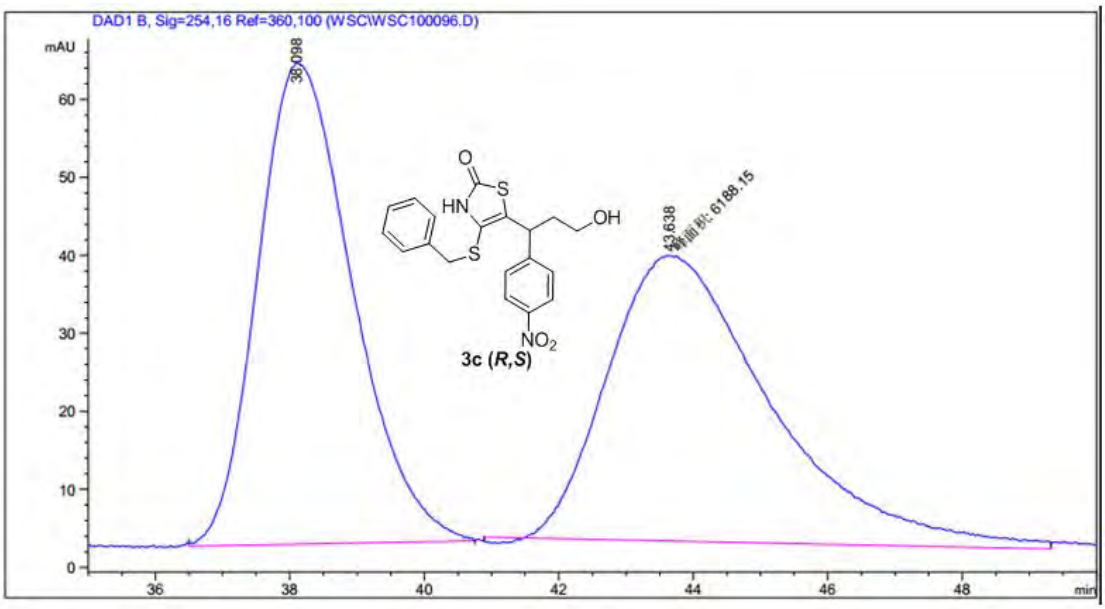


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	48.874	MM	3.3244	6565.18408	32.91372	49.4333
2	80.262	MM	5.1700	6715.70654	21.64964	50.5667

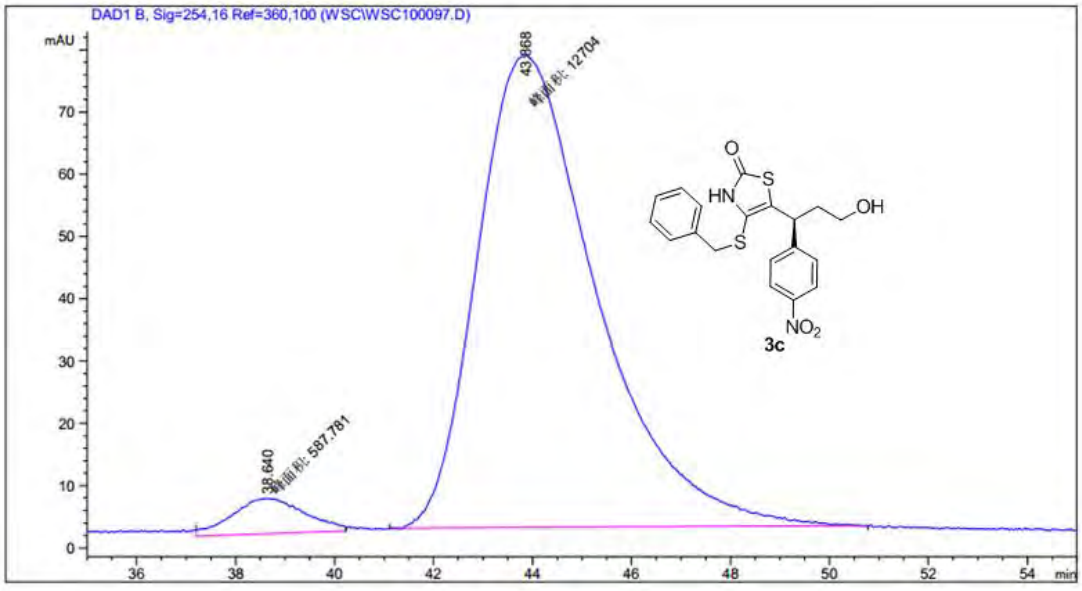


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	50.390	MM	3.5563	5200.44531	24.37207	28.4171
2	81.743	MM	5.4020	1.31000e4	40.41737	71.5829

Compound **3c**

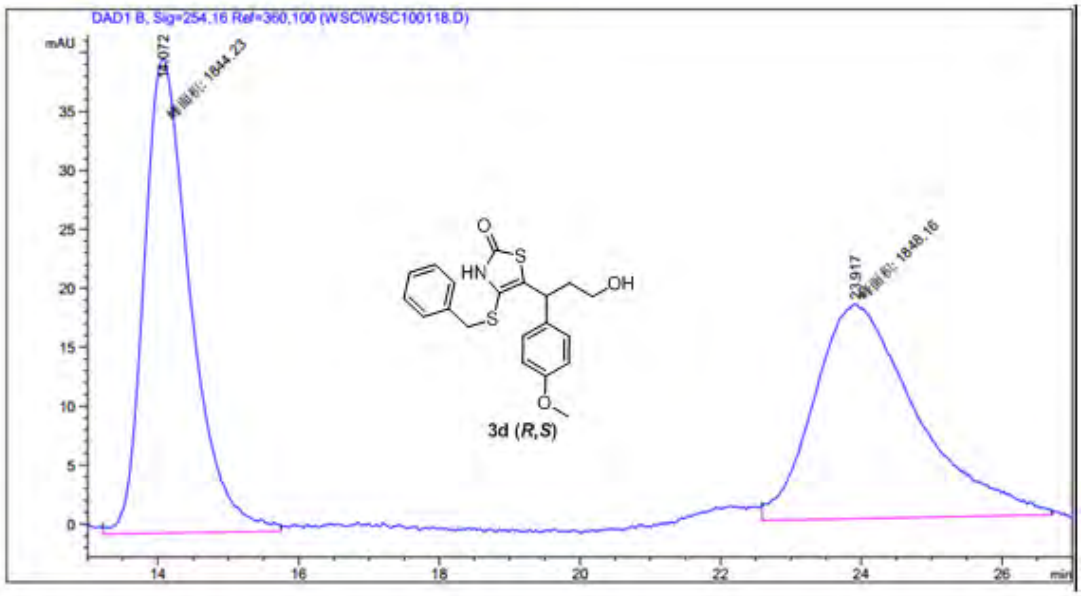


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	38.098	VB	1.1529	6045.41553	61.81981	49.4166
2	43.638	MM	2.8161	6188.14893	36.62403	50.5834

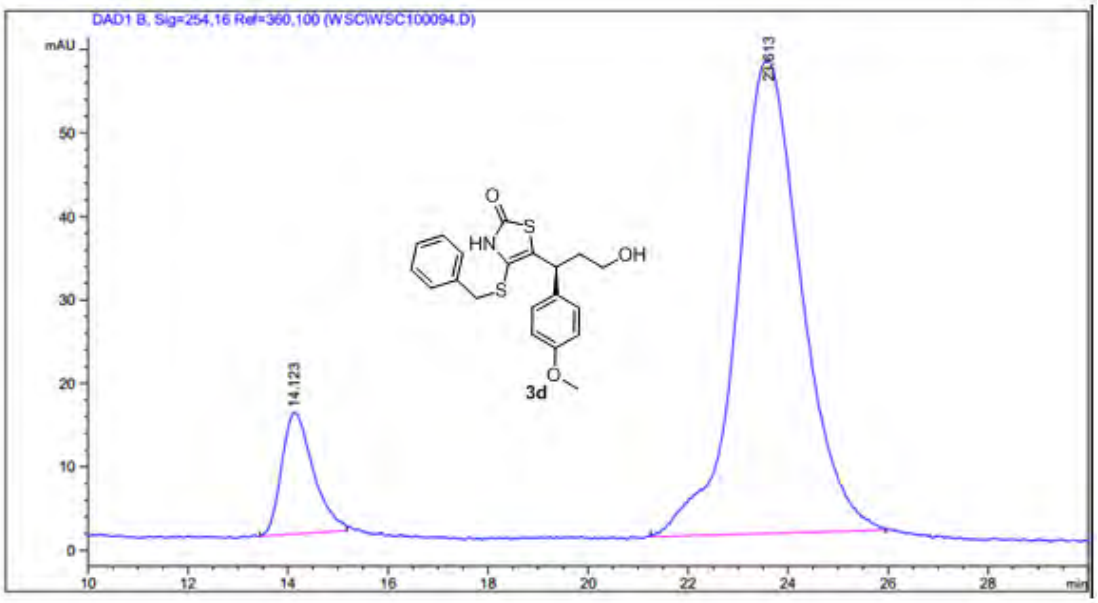


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	38.640	MM	1.6935	587.78149	5.78481	4.4221
2	43.868	MM	2.7935	1.27040e4	75.79579	95.5779

Compound **3d**

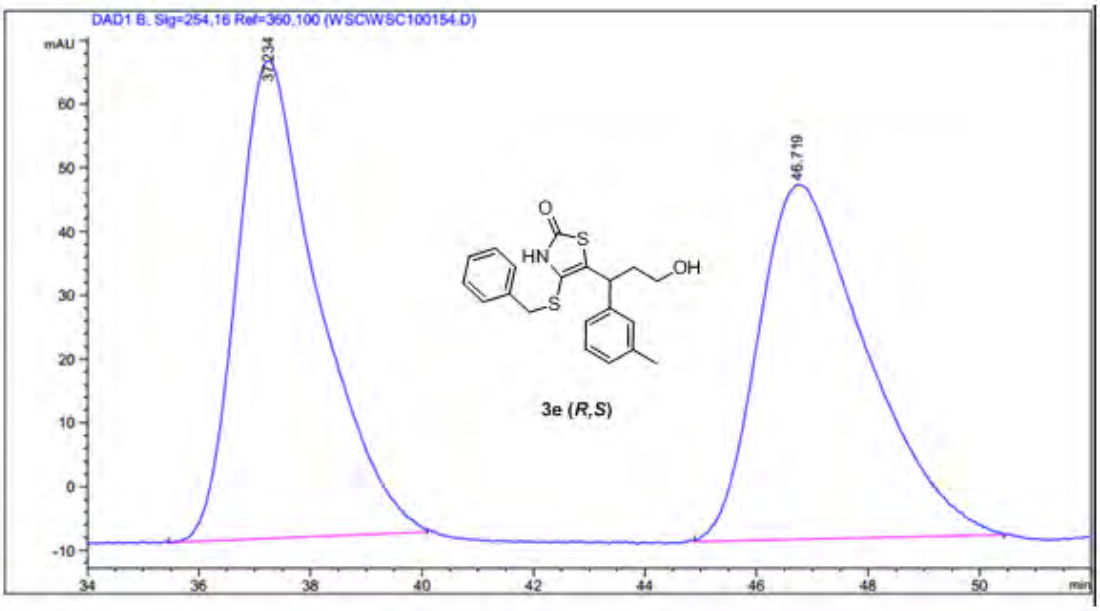


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	14.072	MM	0.7629	1844.22522	40.28852	49.9468
2	23.917	MM	1.6890	1848.15613	18.23667	50.0532

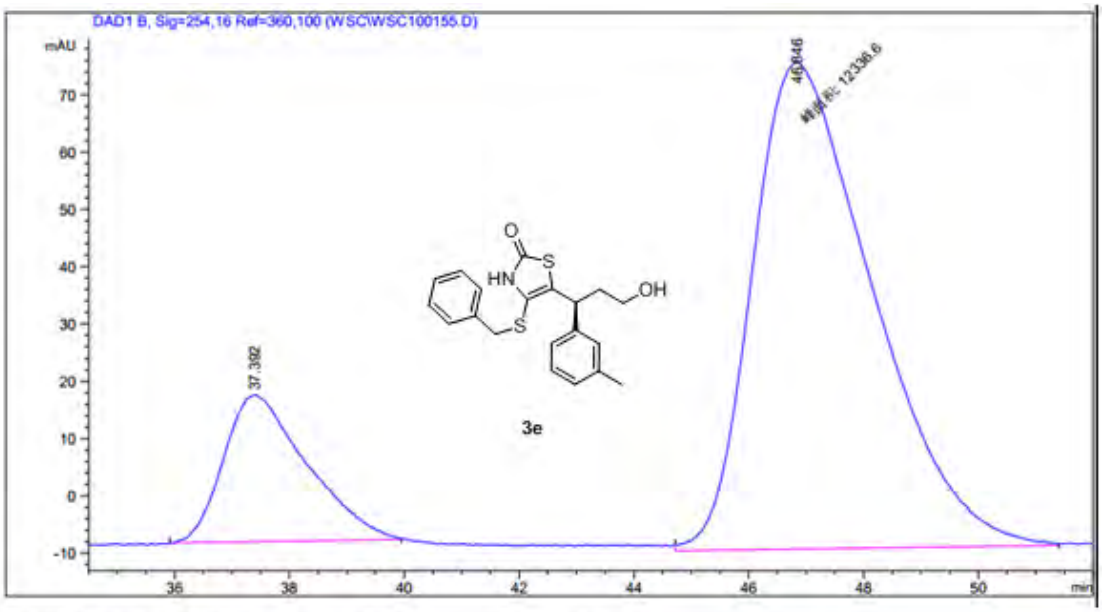


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	14.123	BV	0.5345	641.27637	14.65426	11.2180
2	23.613	BB	1.0572	5075.22021	56.64805	88.7820

Compound **3e**

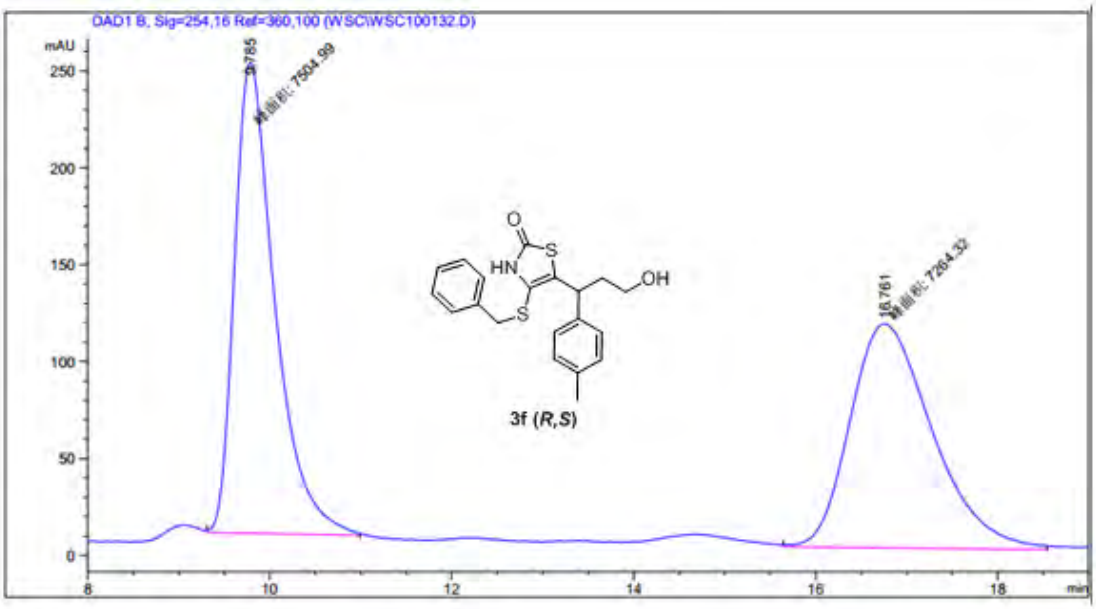


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	37.234	VB	1.1925	7608.27490	74.93673	50.2634
2	46.719	BB	1.5886	7528.52344	55.71075	49.7366

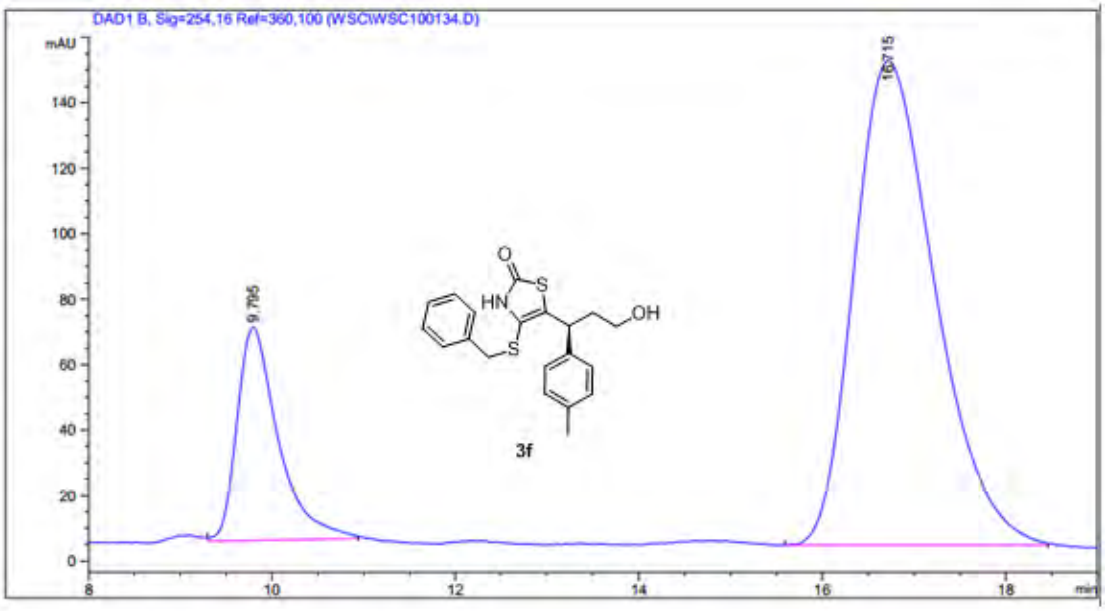


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	37.392	BB	1.1881	2587.67114	25.71184	17.3386
2	46.846	MM	2.4219	1.23366e4	84.89500	82.6614

Compound **3f**

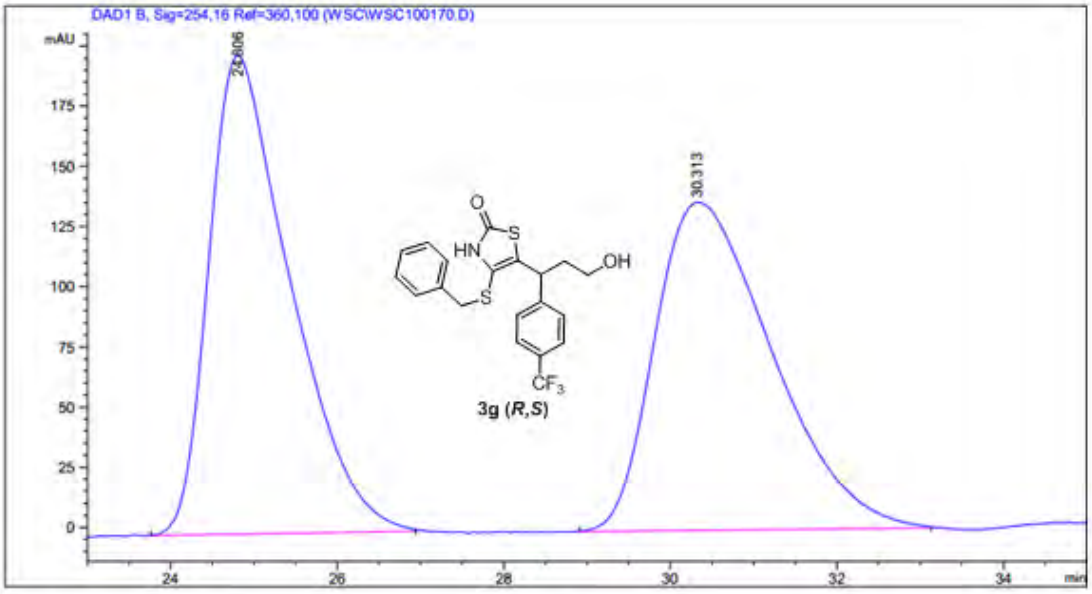


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	9.785	MM	0.5149	7504.99414	242.93436	50.8148
2	16.761	MM	1.0460	7264.31592	115.75166	49.1852

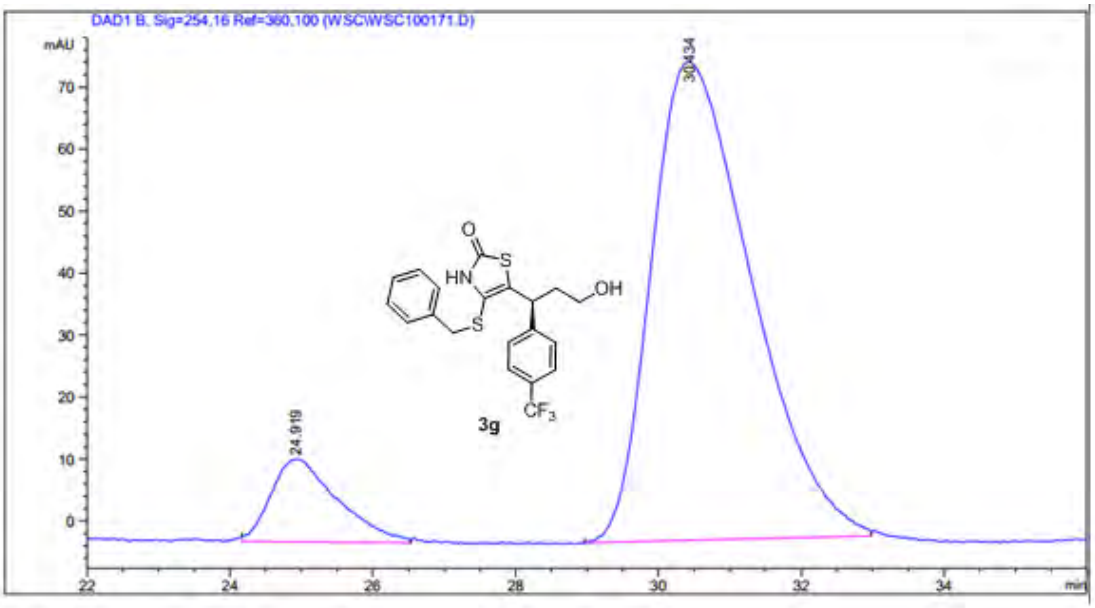


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	9.795	VB	0.4571	2040.72229	65.21947	18.3677
2	16.715	VB	0.8329	9069.68848	148.00372	81.6323

Compound **3g**

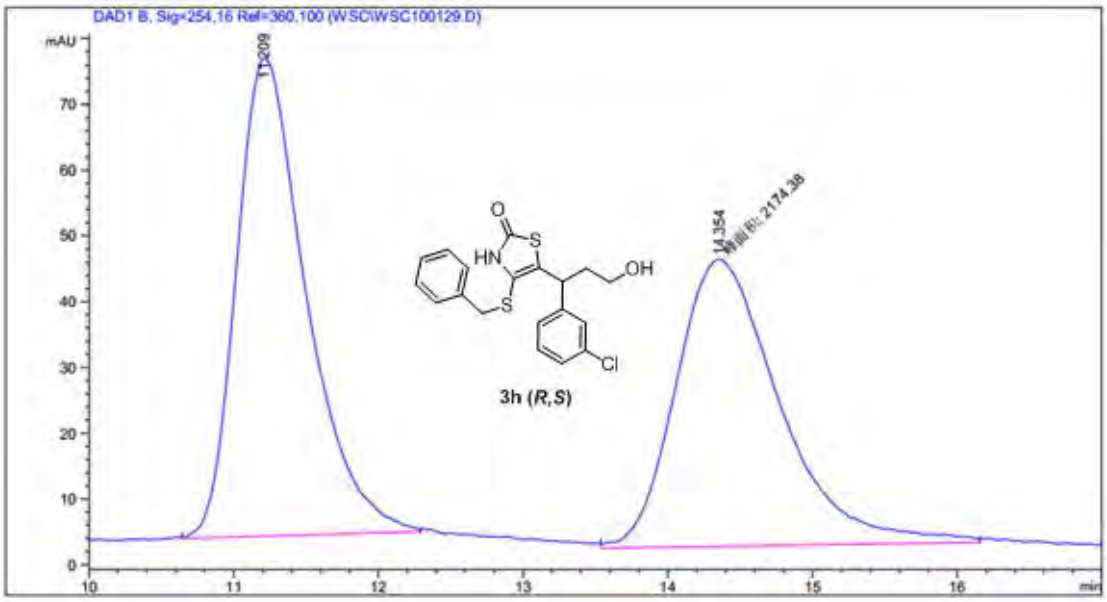


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	24.806	VB	0.9254	1.35236e4	198.85147	50.3401
2	30.313	BB	1.1524	1.33409e4	136.47954	49.6599

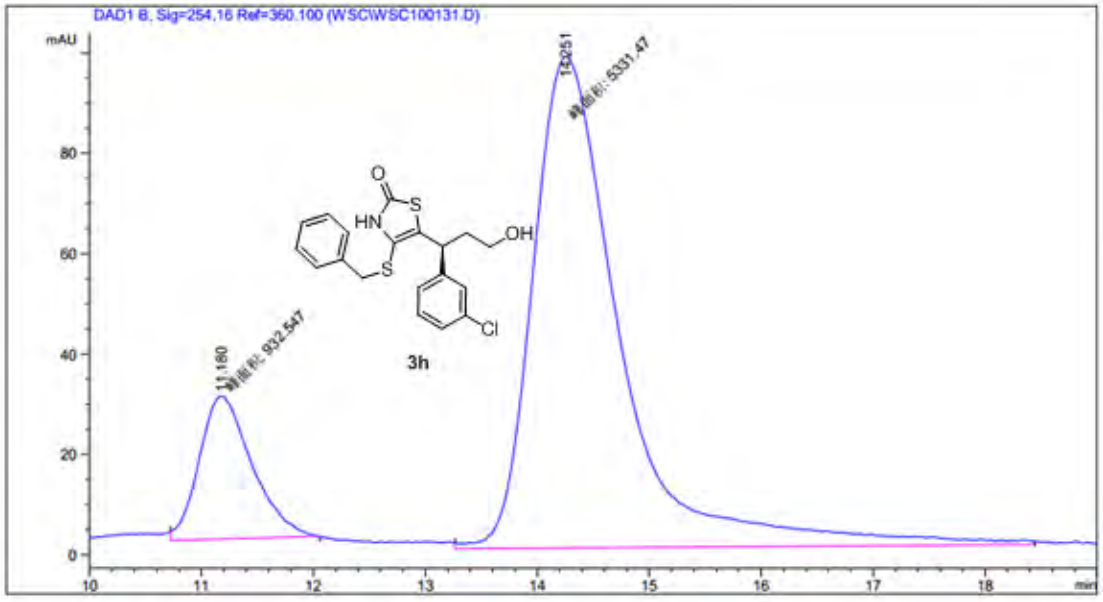


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	24.919	BV	0.7639	871.51251	13.38046	10.3764
2	30.434	BV	1.1444	7527.47900	77.28152	89.6236

Compound **3h**

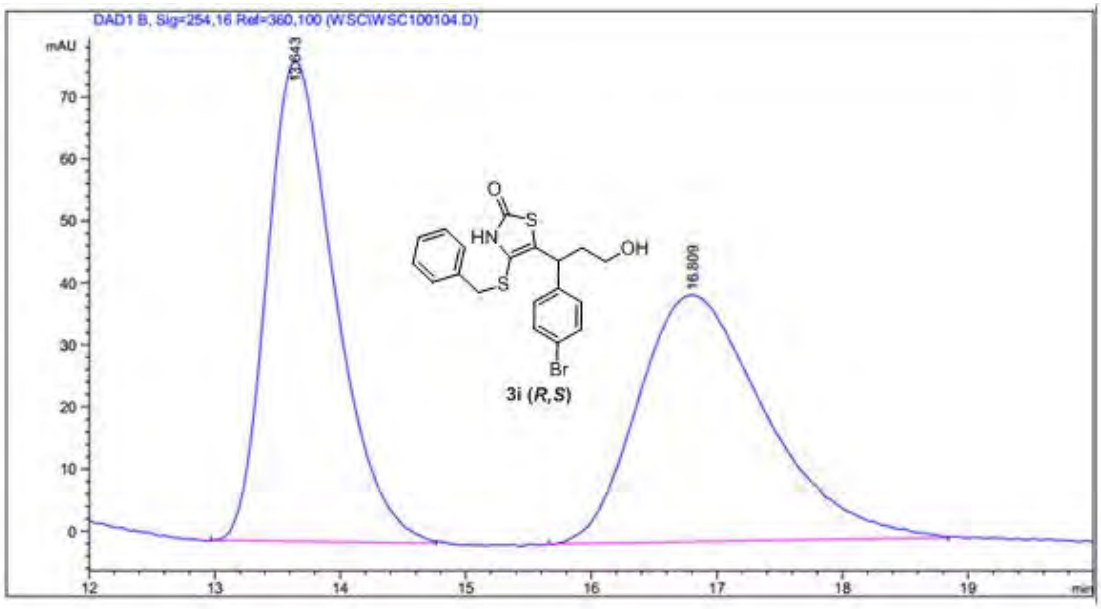


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	11.209	VB	0.4944	2434.26050	72.74574	52.8195
2	14.354	MM	0.8302	2174.38159	43.64977	47.1805

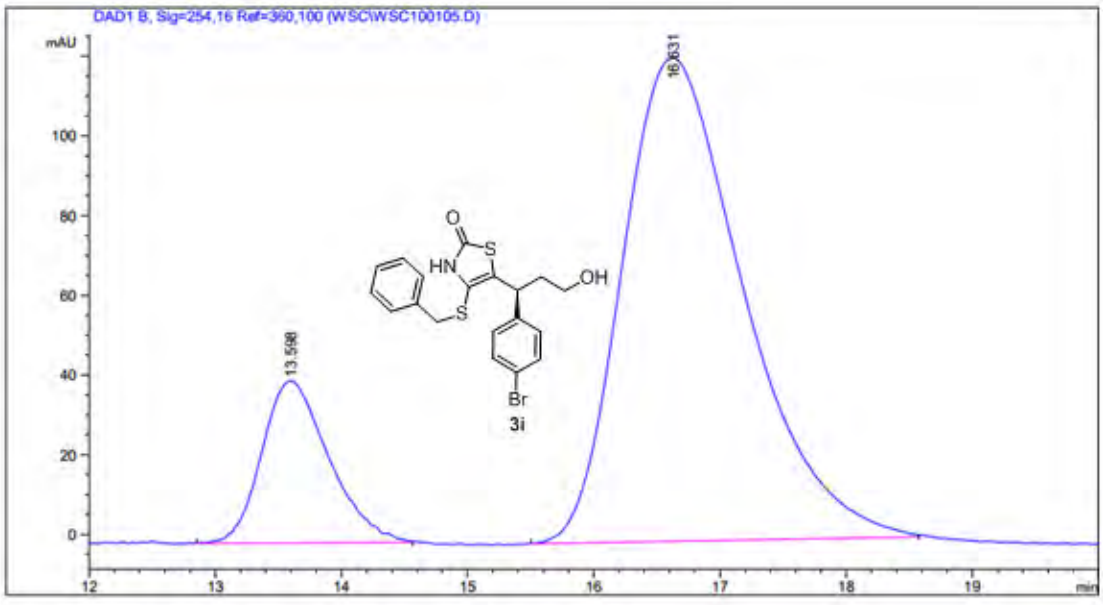


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	11.180	MM	0.5456	932.54651	28.48897	14.8874
2	14.251	MM	0.9073	5331.47217	97.93398	85.1126

Compound **3i**

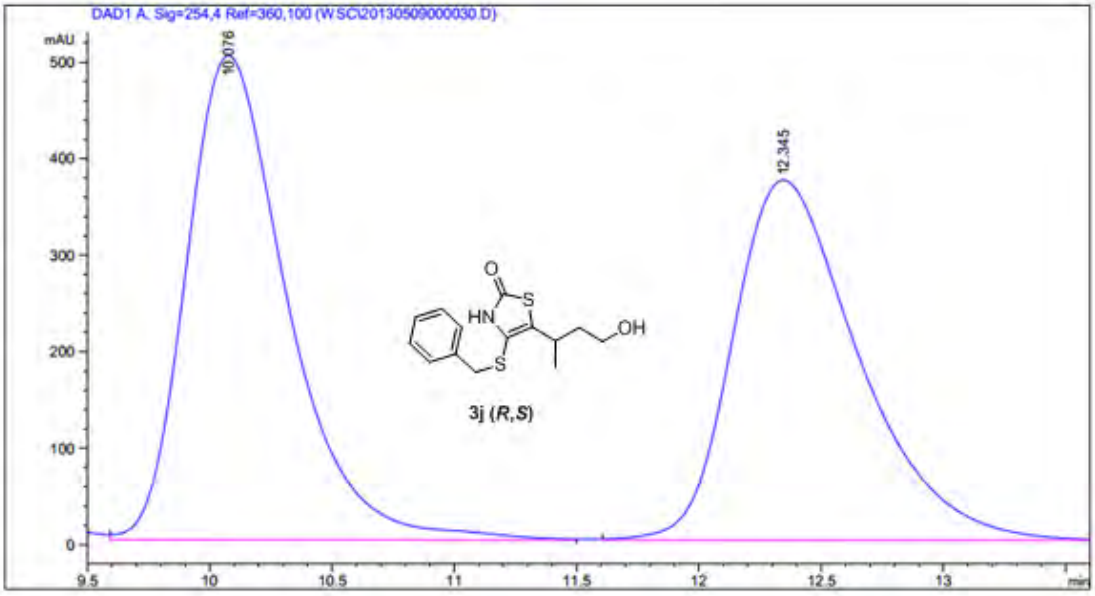


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	13.643	BB	0.5509	2911.69214	77.39071	50.9336
2	16.809	BB	0.8402	2804.95508	39.79921	49.0664

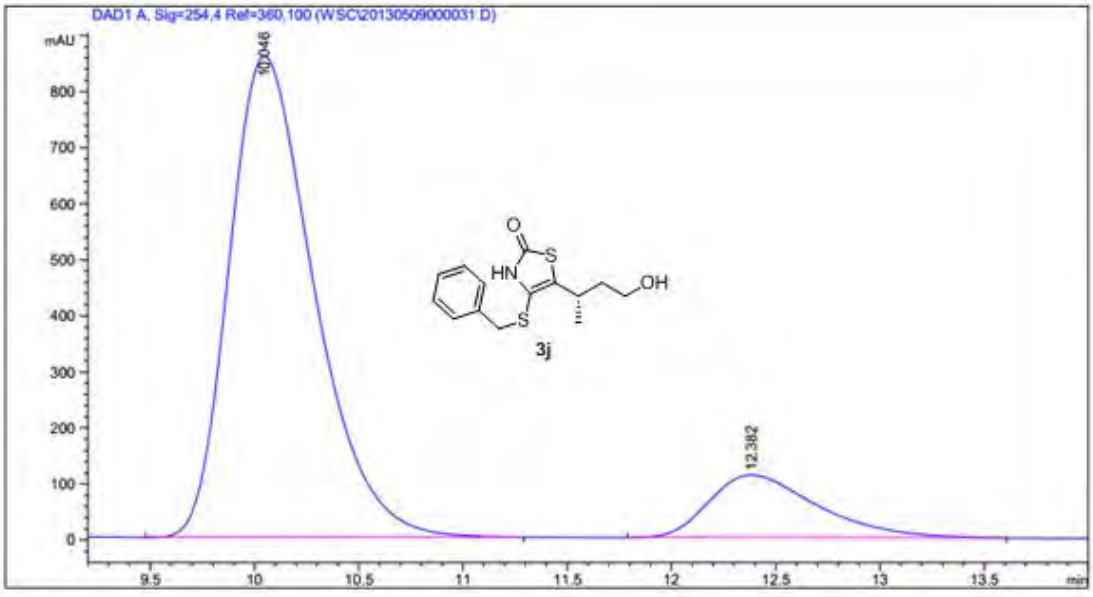


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	13.598	BB	0.4681	1506.86169	40.68762	15.7365
2	16.631	BB	0.8402	8068.71436	121.28095	84.2635

Compound **3j**

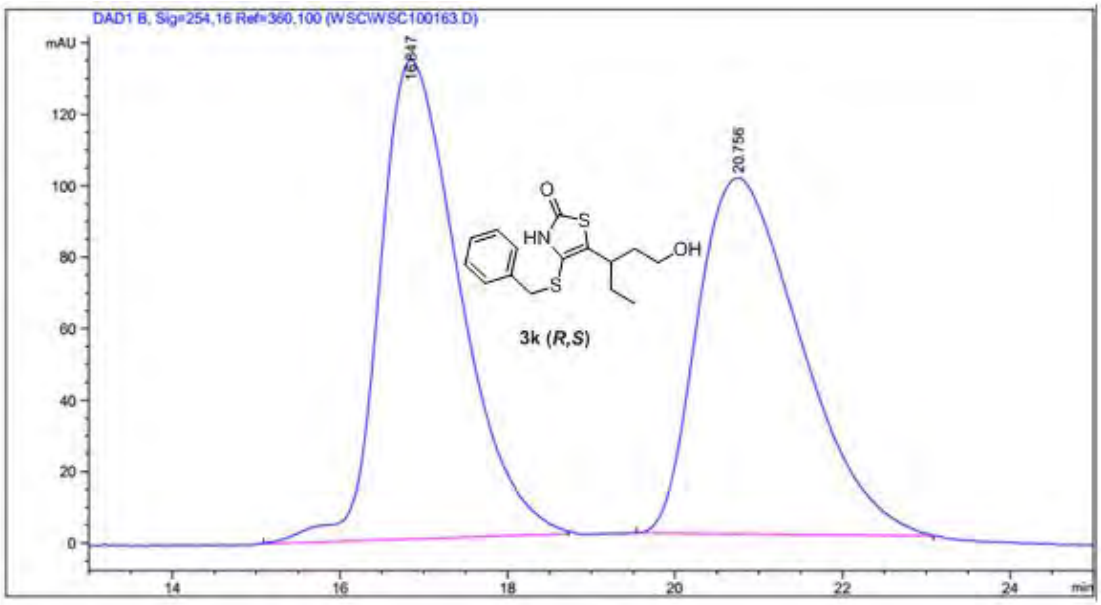


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	10.076	VB	0.4369	1.44162e4	502.17563	51.9112
2	12.345	BB	0.5433	1.33547e4	373.33865	48.0888

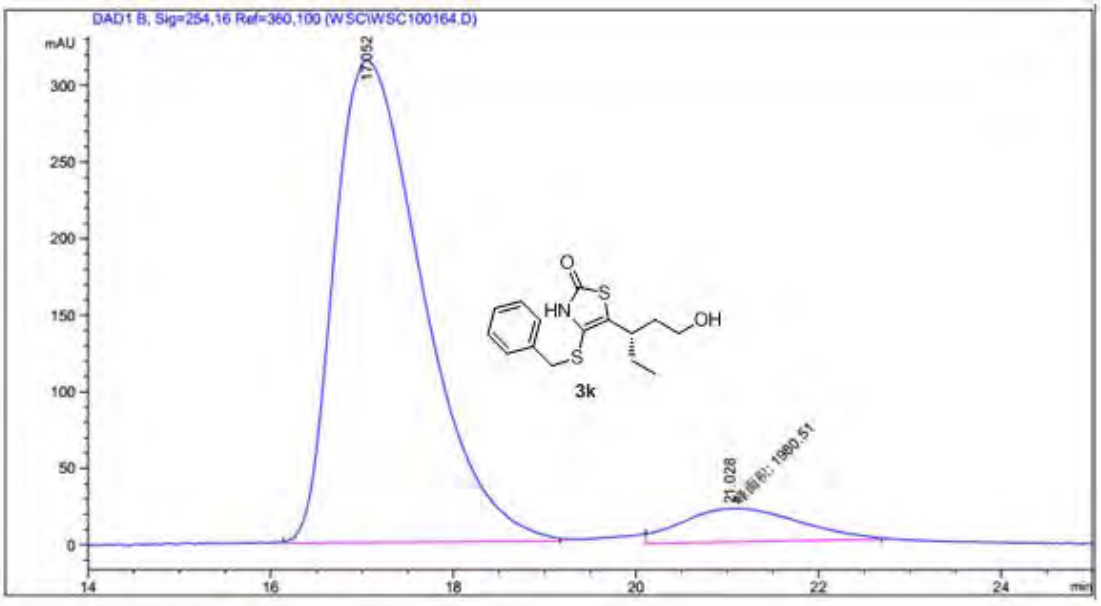


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	10.046	VB	0.4363	2.43076e4	858.52917	85.6889
2	12.382	BB	0.5500	4059.66724	111.71126	14.3111

Compound **3k**

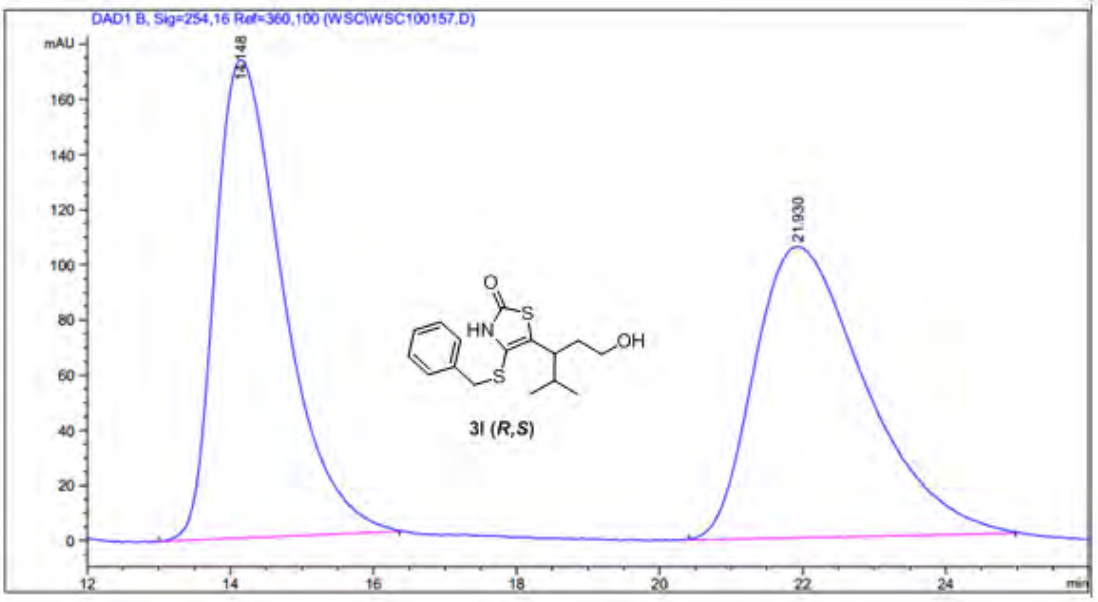


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	16.847	BB	0.8383	8876.90332	134.10666	50.9042
2	20.756	BB	1.0145	8561.54590	99.83149	49.0958

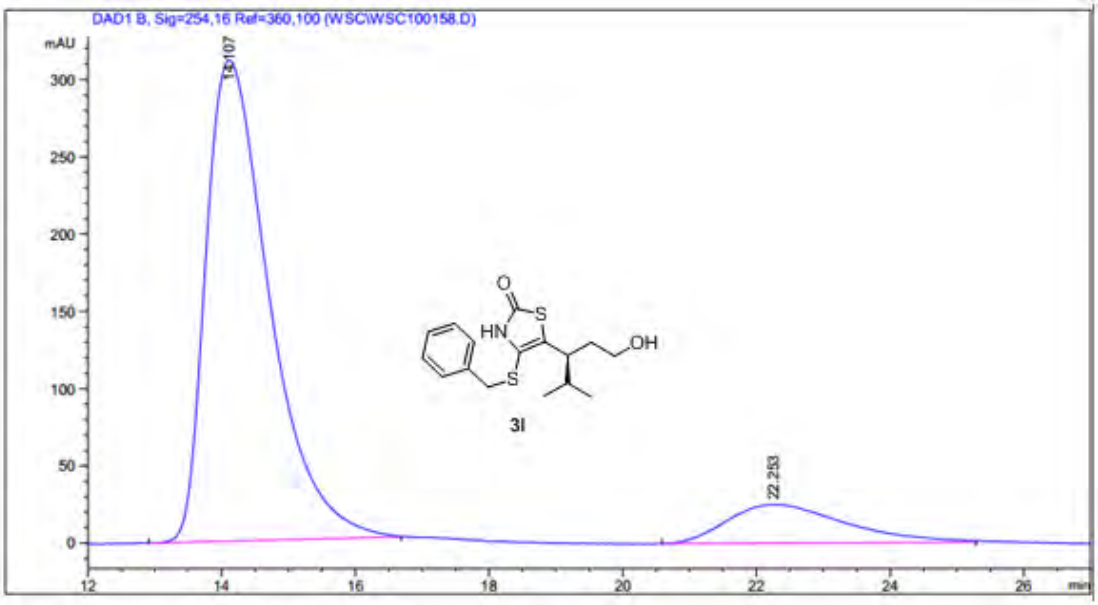


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	17.052	VV	0.8576	2.11436e4	314.78485	91.4353
2	21.028	MM	1.4923	1980.50562	22.11930	8.5647

Compound **3l**

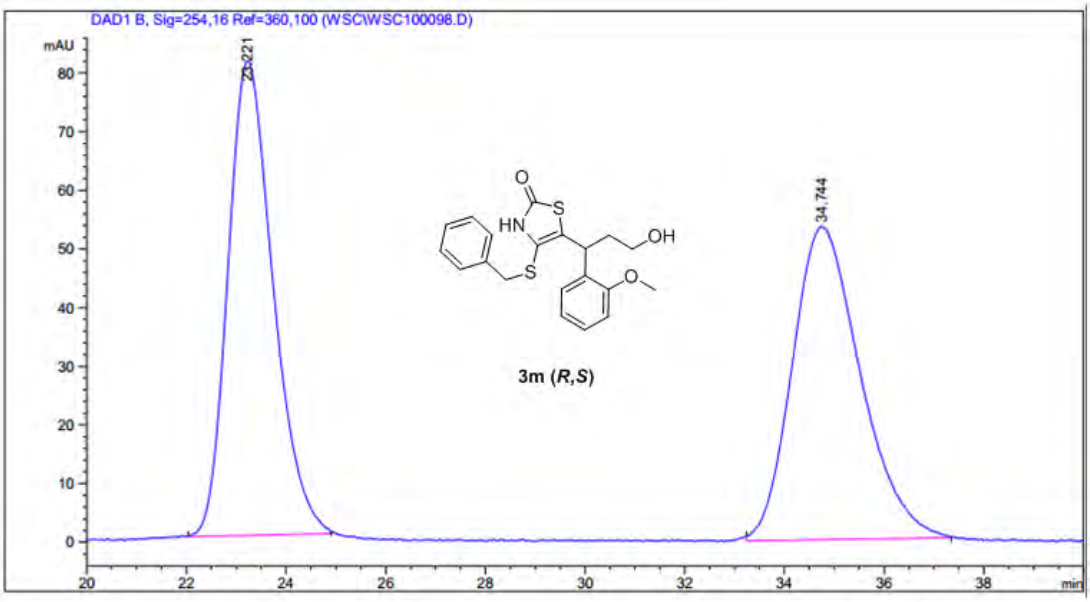


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	14.148	BB	0.9314	1.14966e4	173.41560	50.2124
2	21.930	VB	1.2713	1.13993e4	105.61131	49.7876

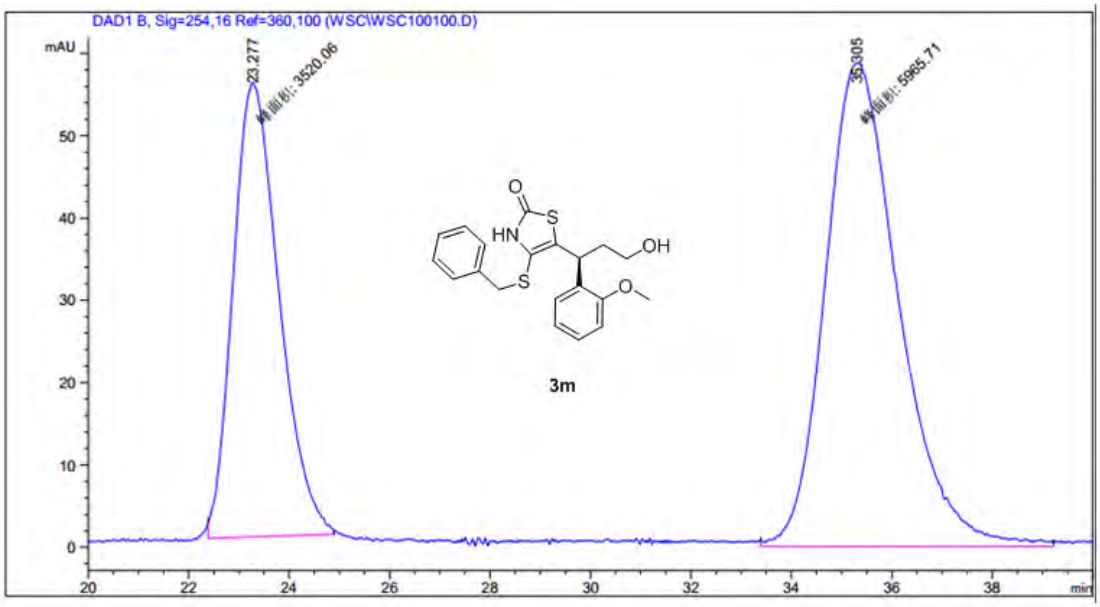


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	14.107	VB	0.7910	2.05794e4	311.40244	86.7886
2	22.253	VV	1.4618	3132.68750	25.14039	13.2114

Compound **3m**

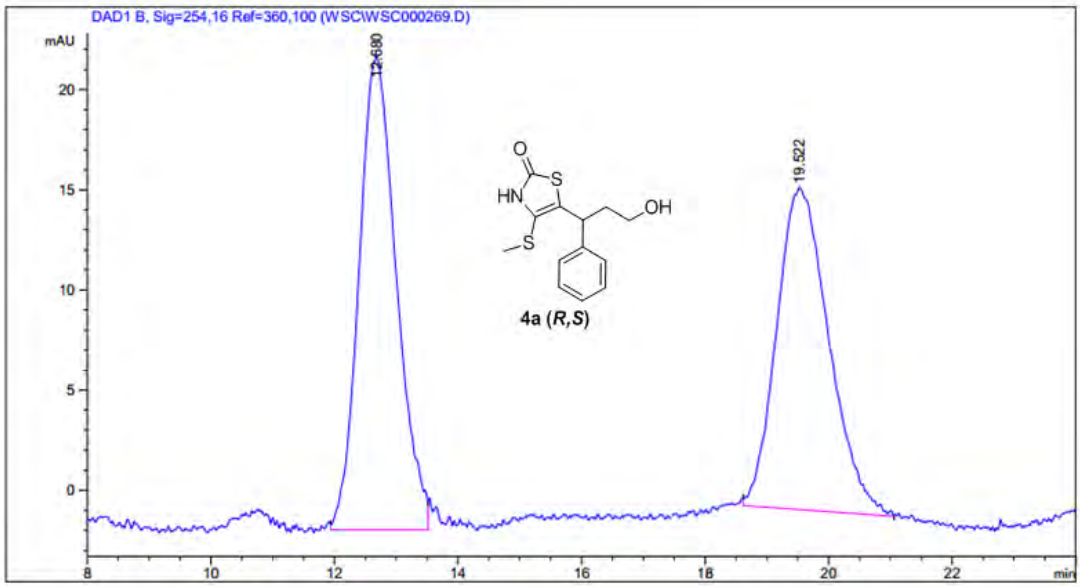


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	23.221	BB	0.7480	5094.18604	80.96675	50.1226
2	34.744	BB	1.1144	5069.27002	53.45415	49.8774

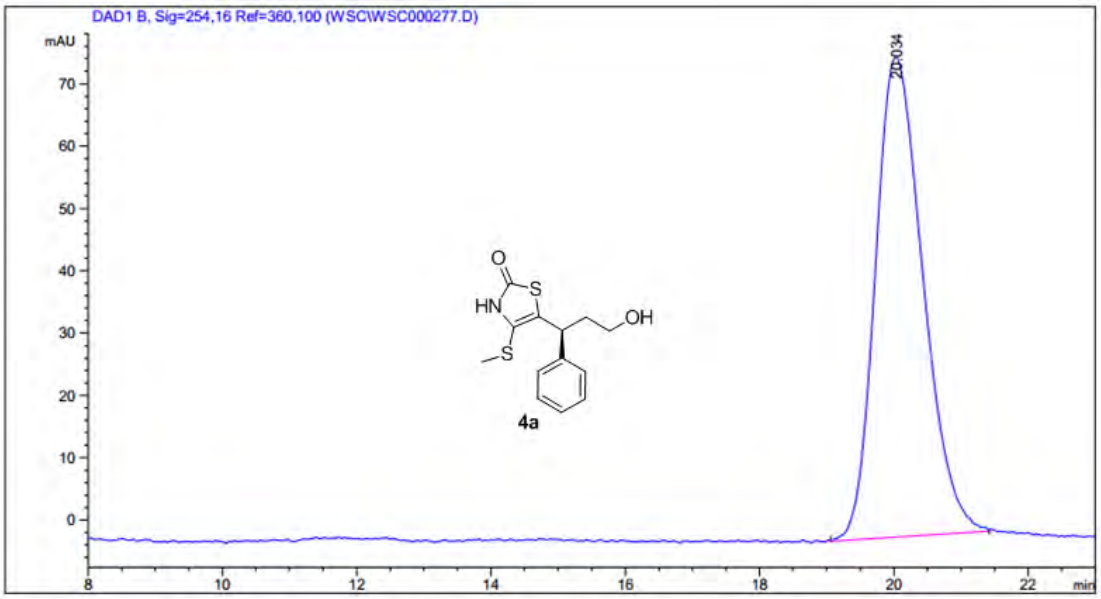


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	23.277	MM	1.0618	3520.06494	55.25493	37.1089
2	35.305	MM	1.6898	5965.70703	58.84169	62.8911

Compound **4a**

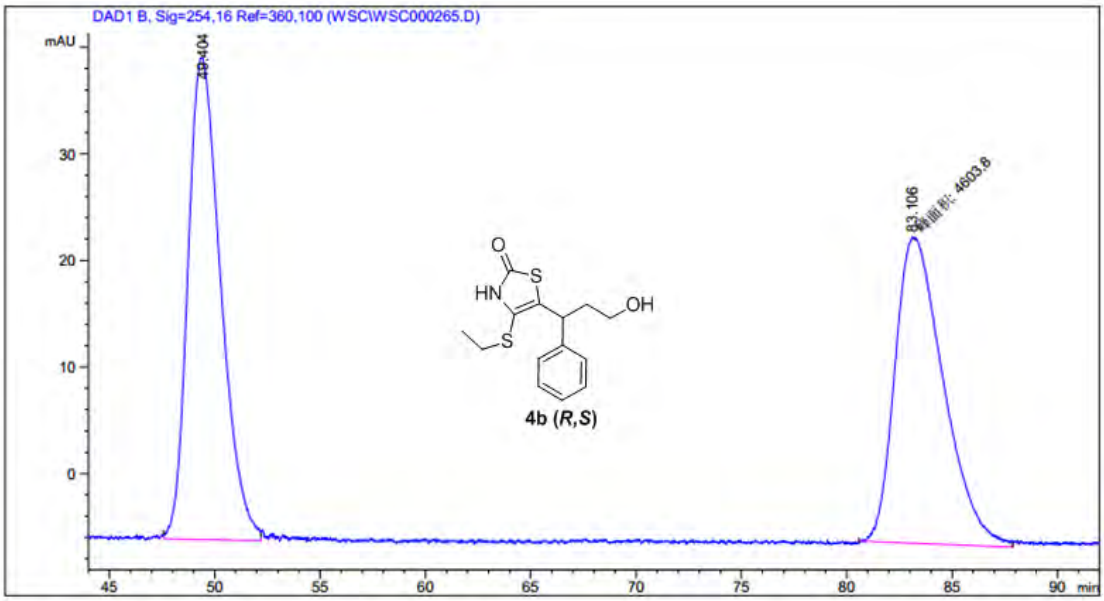


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	12.680	VV	0.5036	992.46179	23.64822	51.3336
2	19.522	BB	0.6944	940.89471	16.08619	48.6664

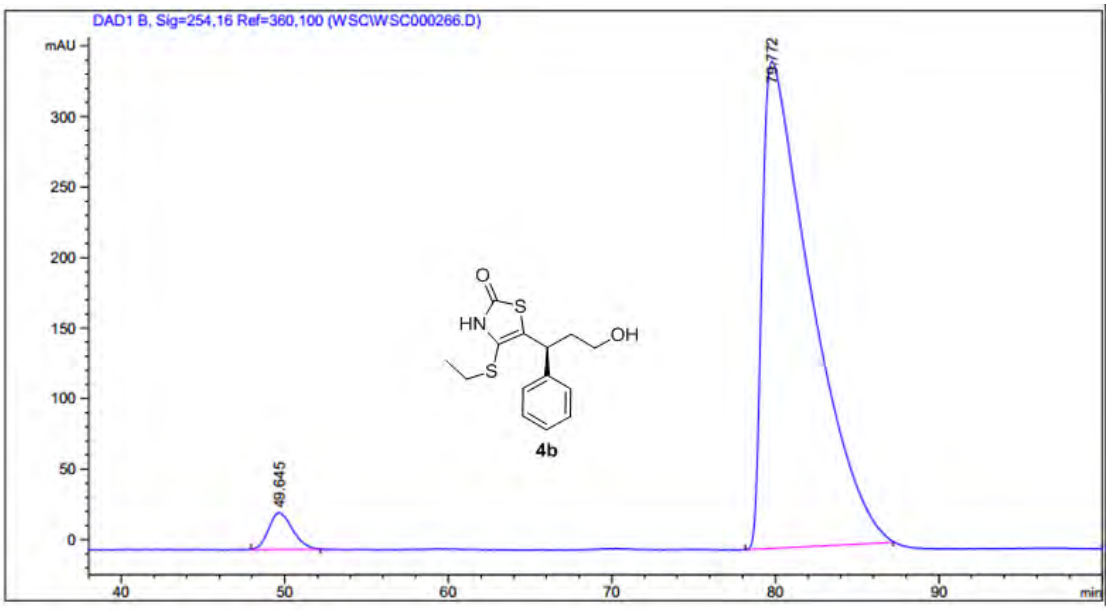


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	20.034	VB	0.6690	3797.41260	77.04863	100.0000

Compound **4b**

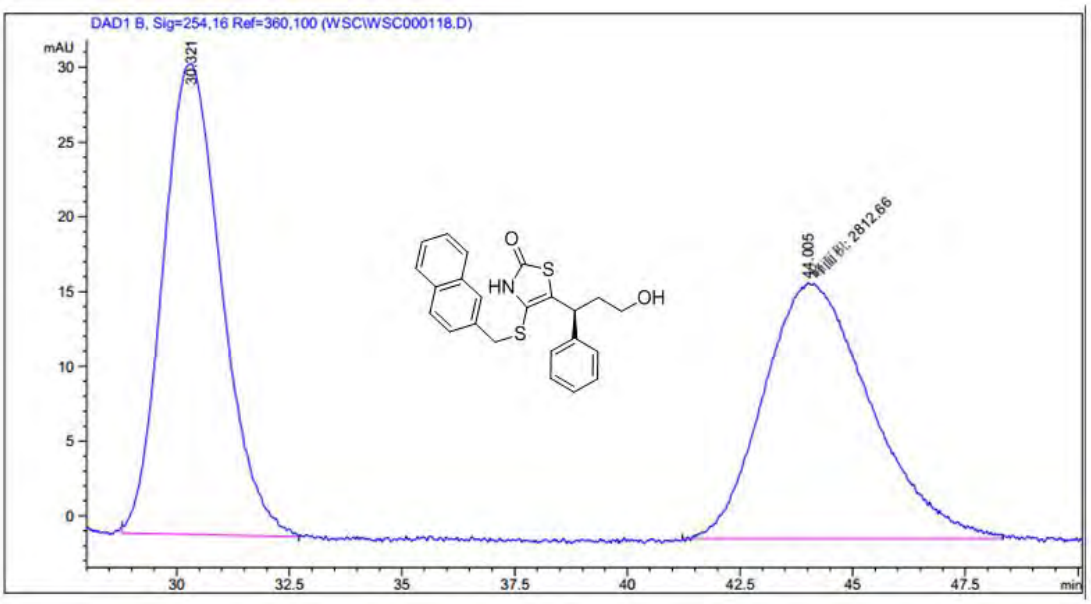


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	49.404	BB	1.2774	4902.64941	45.27115	51.5718
2	83.106	MM	2.6645	4603.79639	28.79763	48.4282

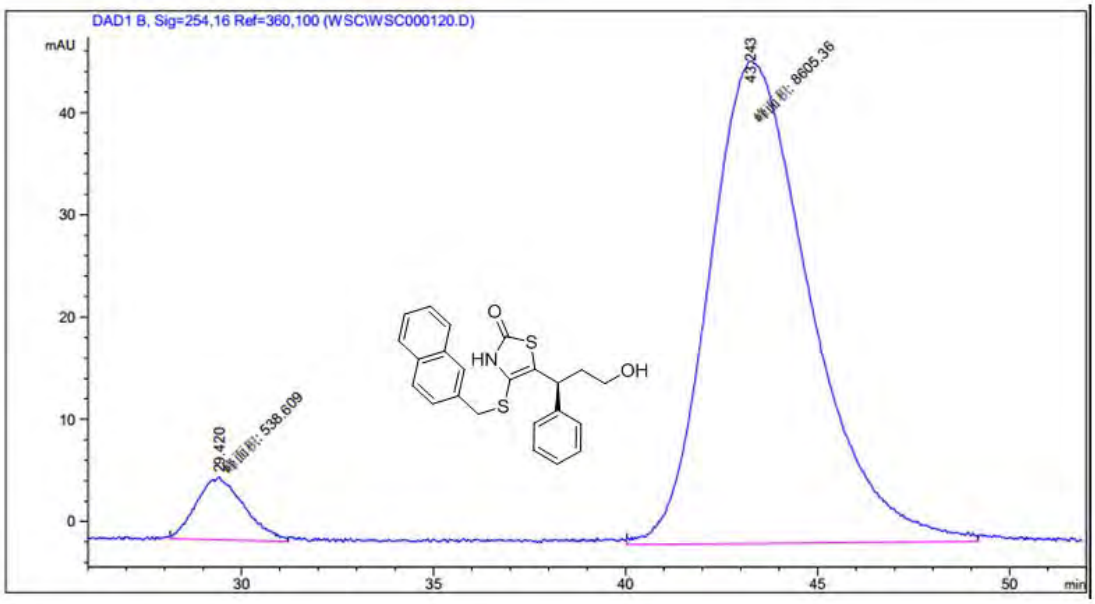


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	49.645	BB	1.2104	2706.55225	26.30501	3.6266
2	79.772	VB	2.4360	7.19234e4	345.30569	96.3734

Compound **4c**

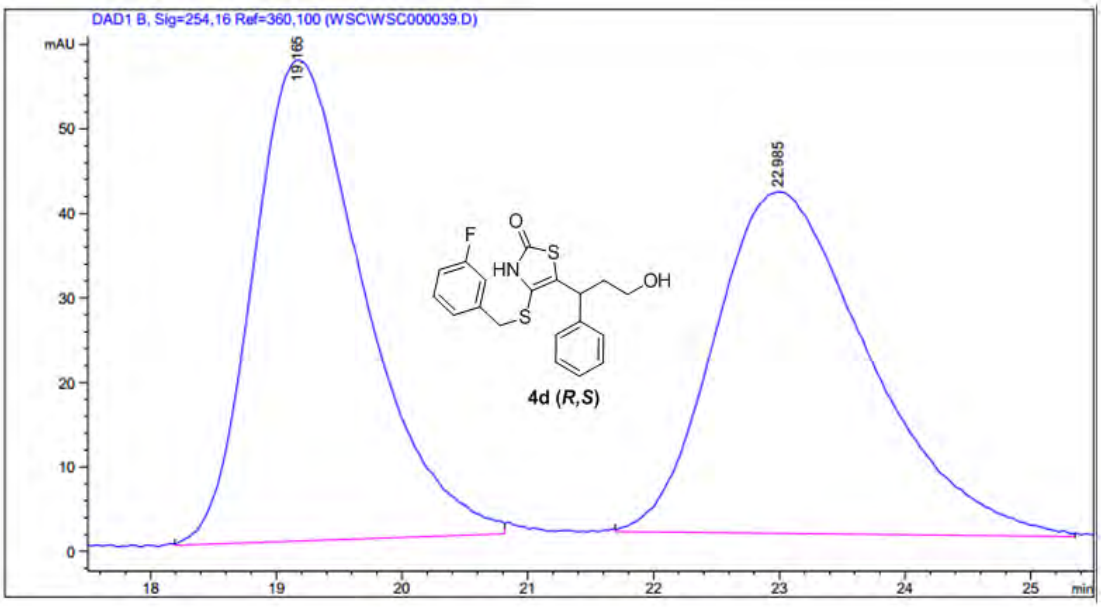


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	30.321	BV	1.0687	2848.20654	31.50510	50.3140
2	44.005	MM	2.7377	2812.65625	17.12284	49.6860

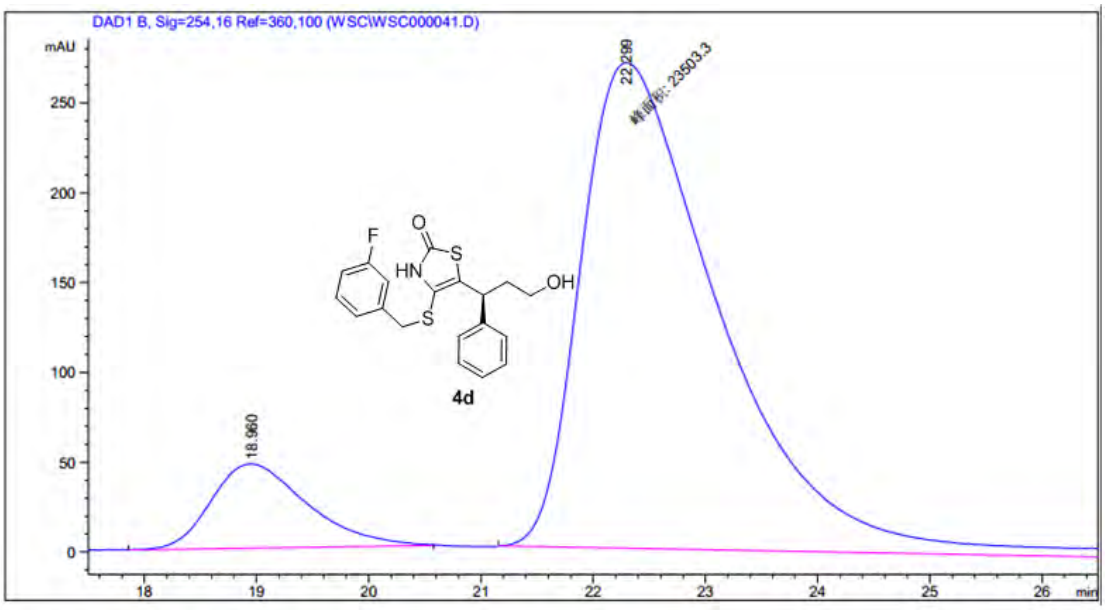


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	29.420	MM	1.4491	538.60901	6.19460	5.8903
2	43.243	MM	3.0394	8605.35742	47.18848	94.1097

Compound **4d**

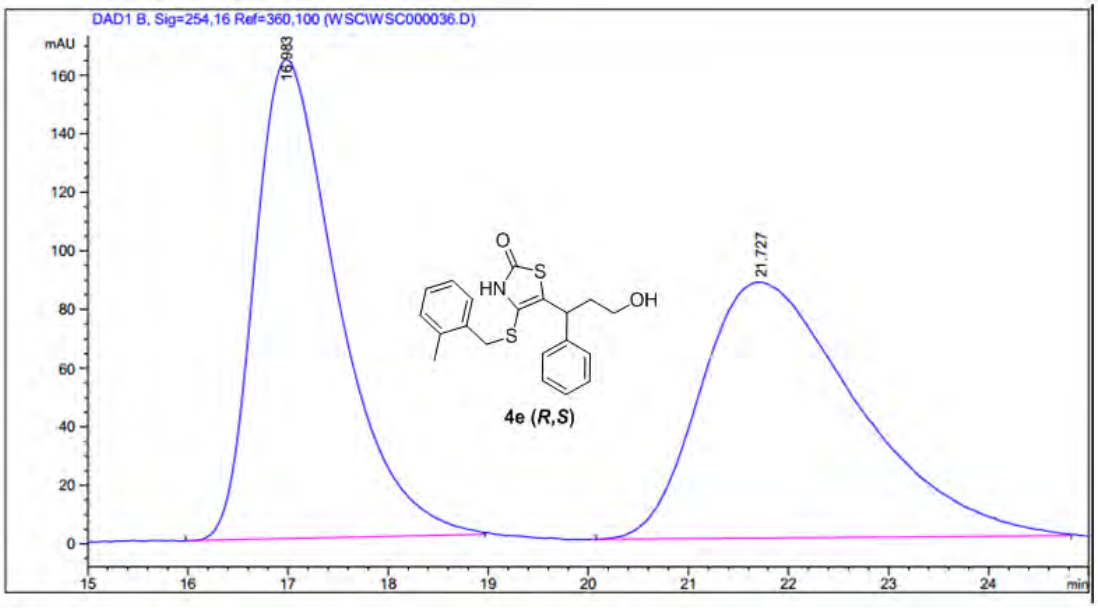


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	19.165	BV	0.7230	3490.79370	56.95990	50.2250
2	22.985	BB	1.0036	3459.51440	40.45906	49.7750

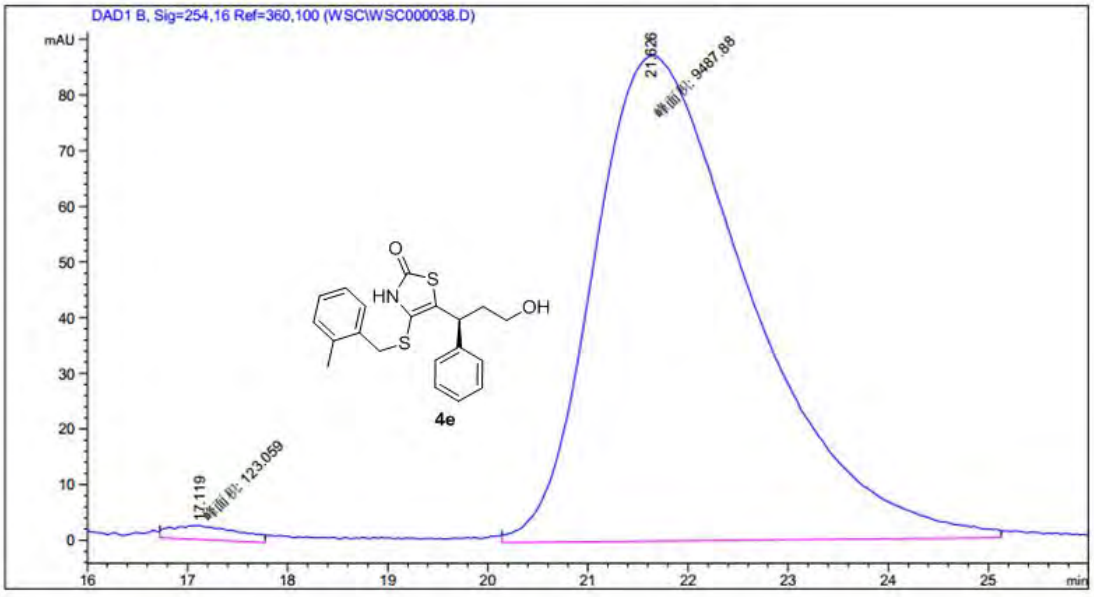


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	18.960	VB	0.7112	2807.10547	46.97192	10.6692
2	22.299	MM	1.4483	2.35033e4	270.46353	89.3308

Compound **4e**

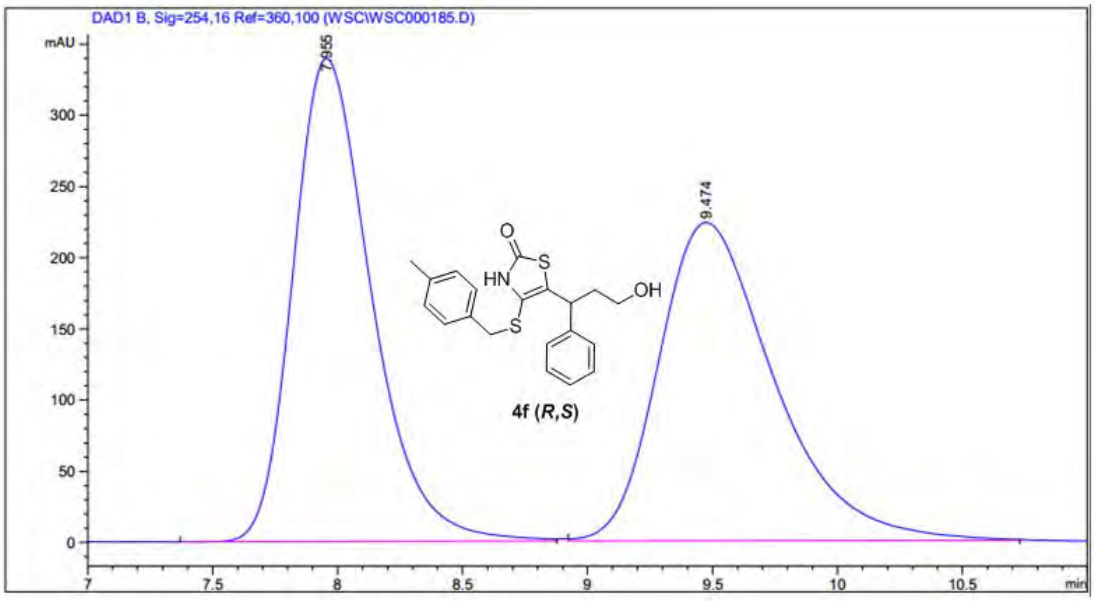


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	16.983	BB	0.8013	9441.83203	163.59357	49.7607
2	21.727	VB	1.2854	9532.62598	87.47350	50.2393

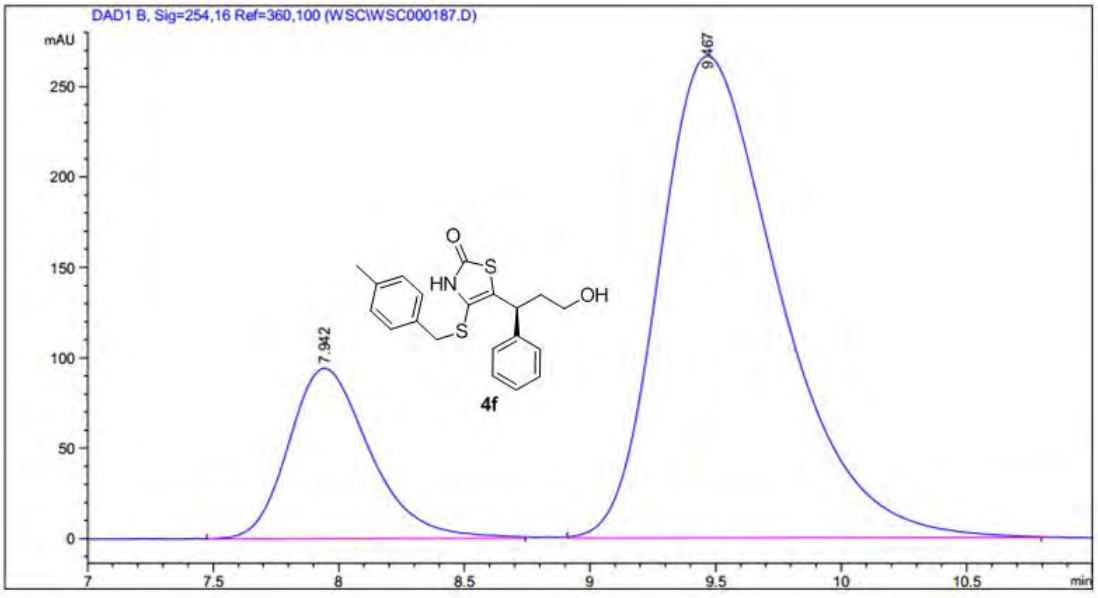


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	17.119	MM	0.7973	123.05882	2.57247	1.2804
2	21.626	MM	1.8133	9487.87988	87.20606	98.7196

Compound **4f**

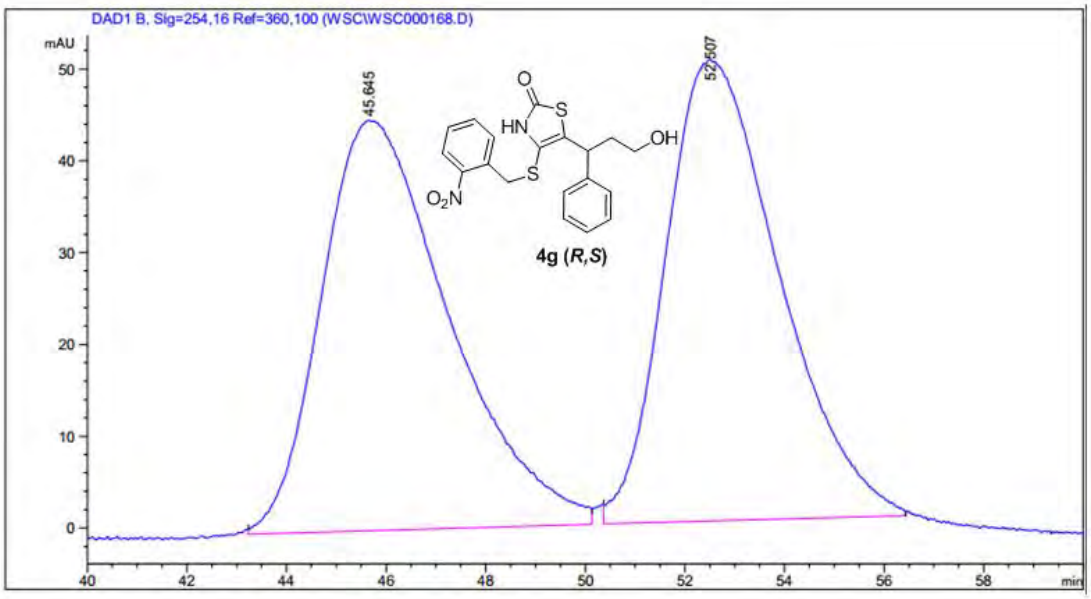


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	7.955	BB	0.3326	7408.60352	339.42798	50.6982
2	9.474	BB	0.4897	7204.55811	223.72467	49.3018

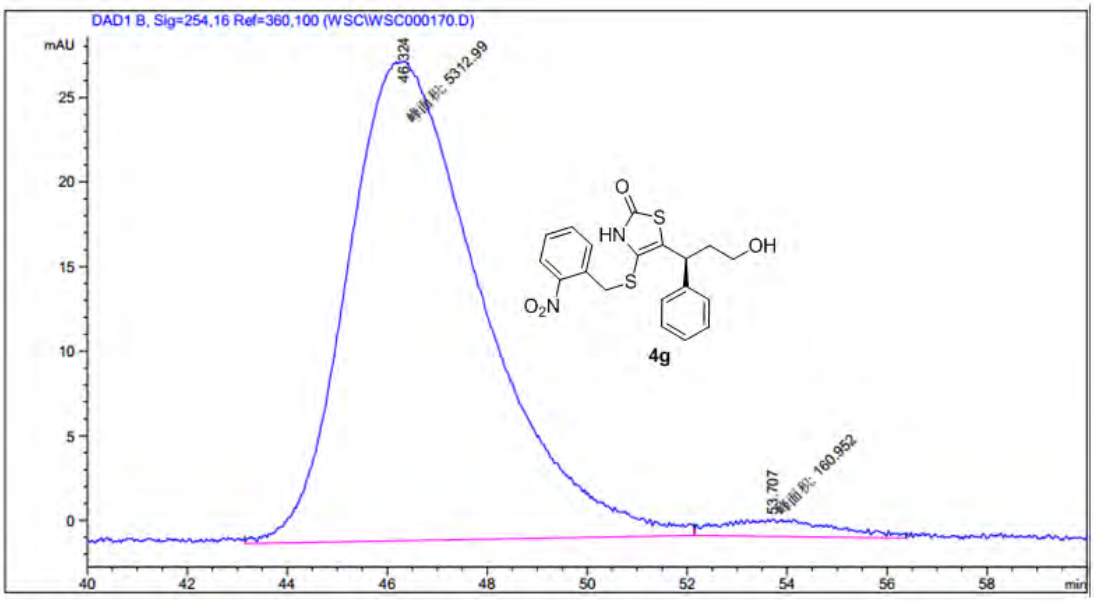


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	7.942	VB	0.3504	2143.40698	94.57014	19.4946
2	9.467	BB	0.4930	8851.44434	266.82669	80.5054

Compound **4g**

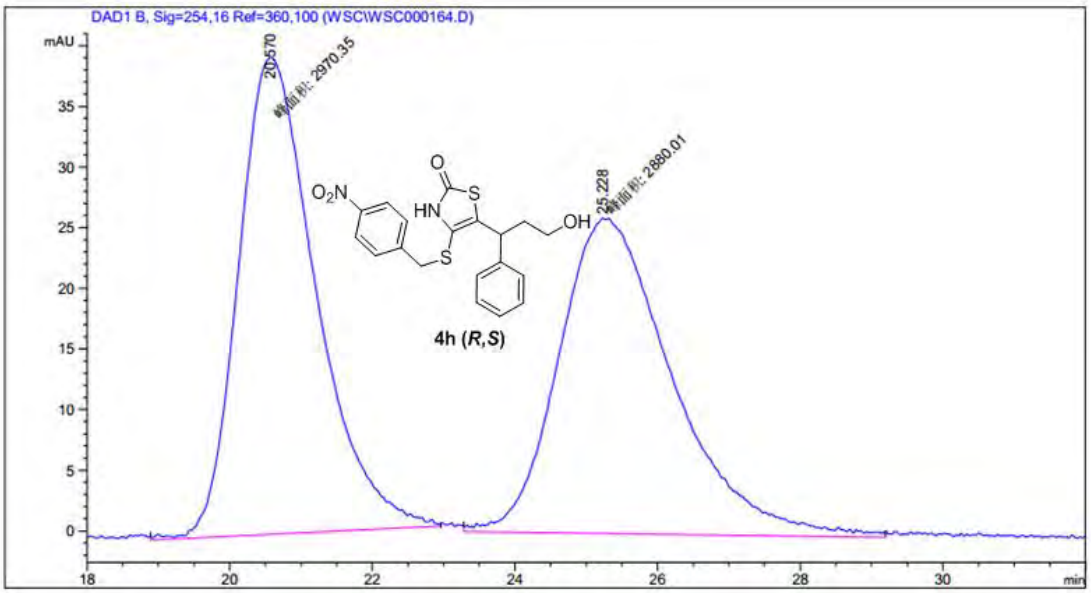


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	45.645	BV	2.0854	7957.32715	44.73222	49.9691
2	52.507	BV	1.8565	7967.17920	50.33953	50.0309

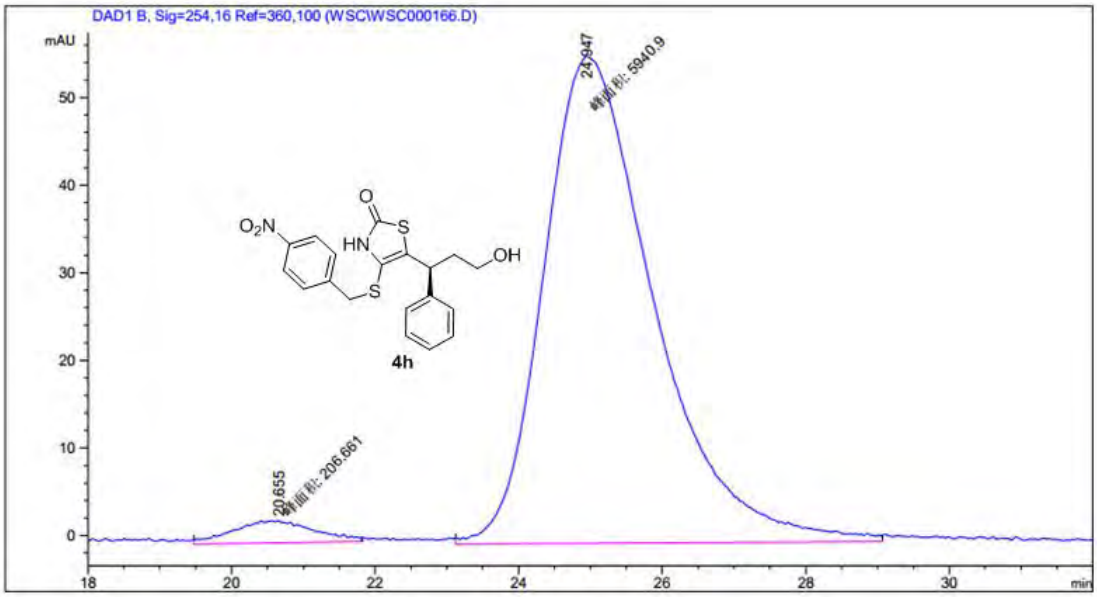


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	46.324	MM	3.1210	5312.98730	28.37249	97.0597
2	53.707	MM	2.5692	160.95164	1.04410	2.9403

Compound **4h**

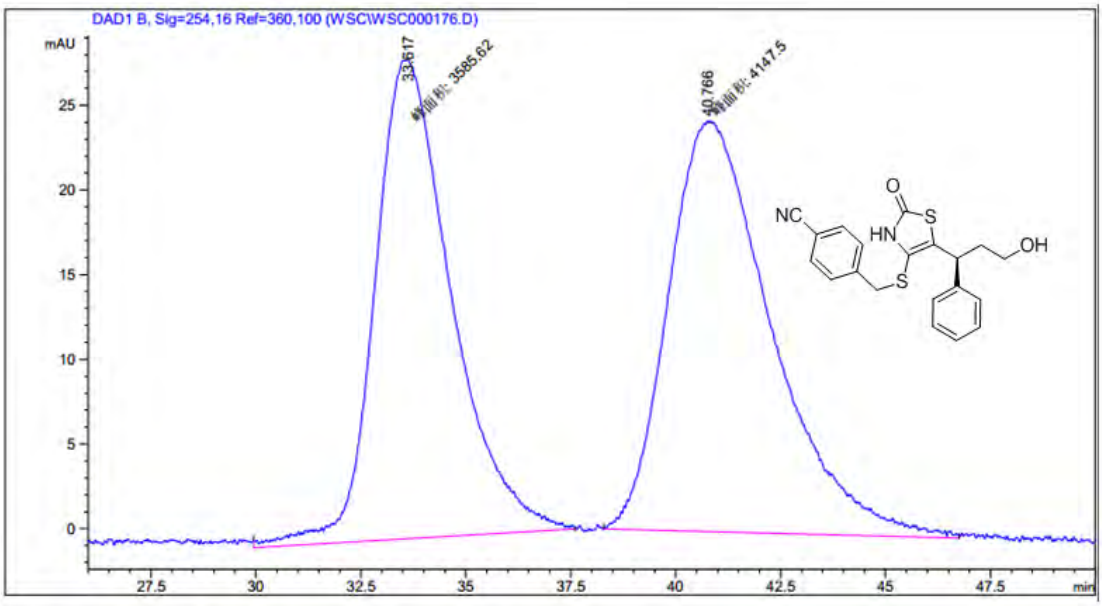


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	20.570	MM	1.2581	2970.34863	39.35086	50.7721
2	25.228	MM	1.8457	2880.01221	26.00658	49.2279

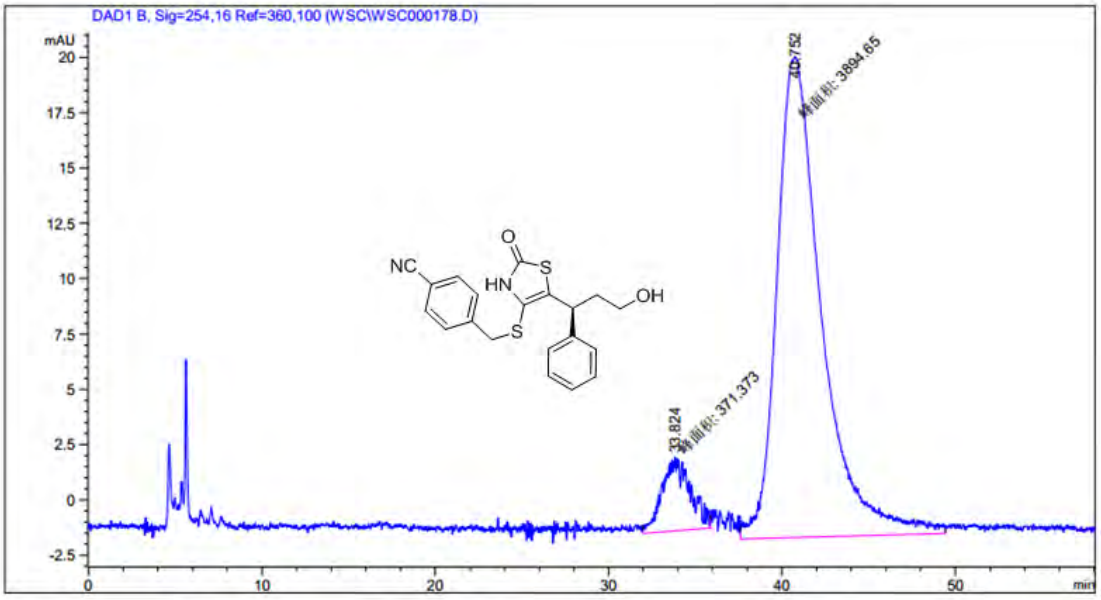


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	20.655	MM	1.3343	206.66110	2.58135	3.3617
2	24.947	MM	1.7804	5940.89502	55.61456	96.6383

Compound **4i**

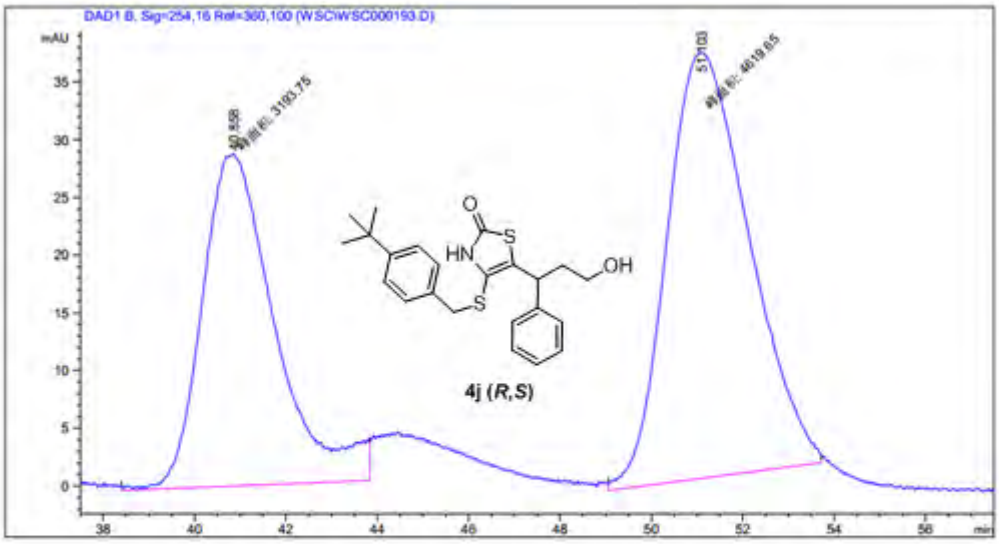


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	33.617	MM	2.1123	3585.62183	28.29177	46.3671
2	40.766	MM	2.8487	4147.49512	24.26541	53.6329

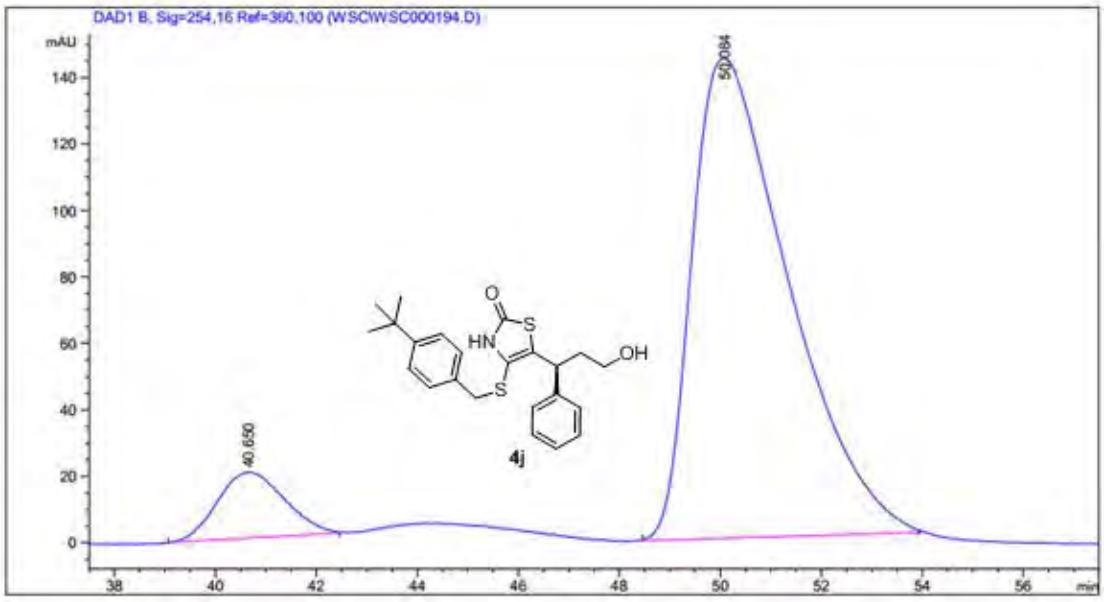


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	33.824	MM	1.8518	371.37302	3.34247	8.7054
2	40.752	MM	2.9837	3894.64893	21.75503	91.2946

Compound **4j**

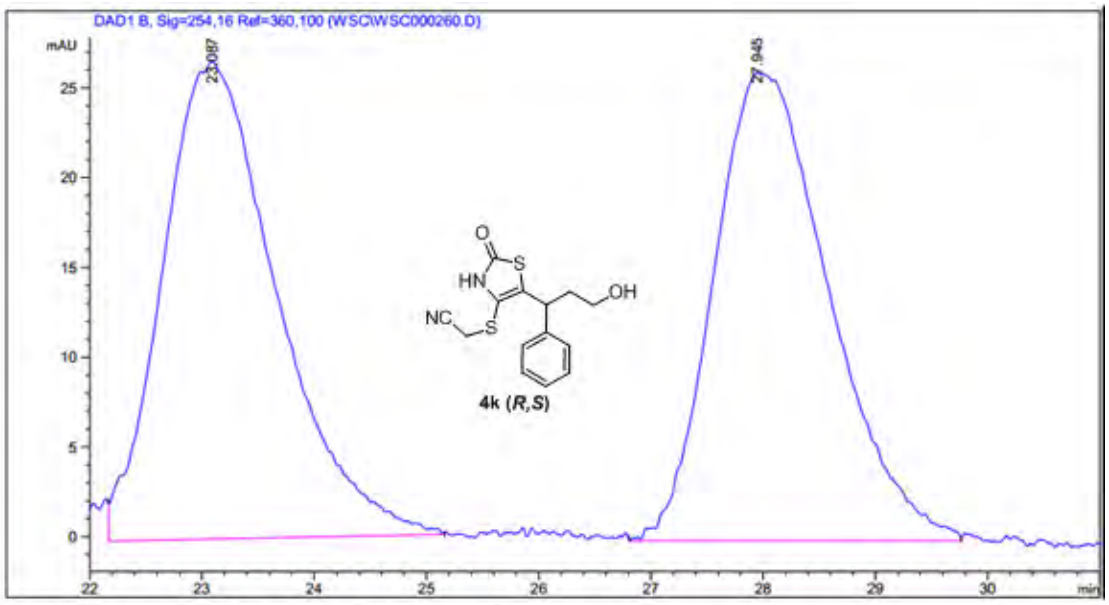


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	40.858	MM	1.8491	3193.74658	28.78666	40.8753
2	51.103	MM	2.0859	4619.65039	36.91171	59.1247

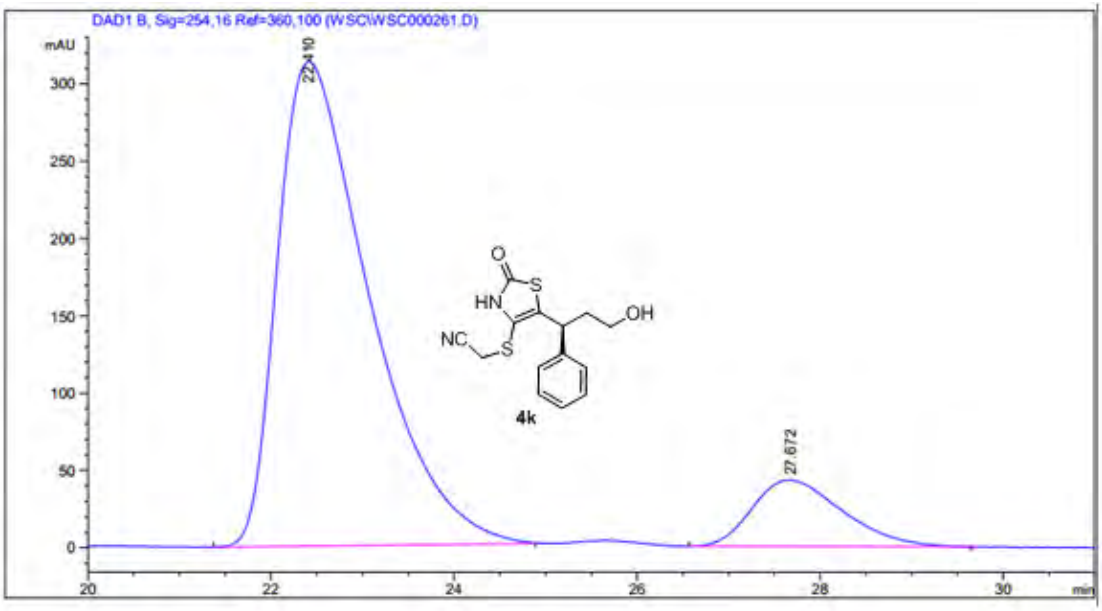


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	40.650	BV	1.0843	1833.70996	19.87615	8.7158
2	50.084	BB	1.5623	1.92052e4	144.52811	91.2842

Compound **4k**



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	23.087	VB	0.8477	1879.15466	26.61428	50.3096
2	27.945	VV	0.8362	1856.02893	26.08264	49.6904



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	22.410	BB	0.9229	2.18551e4	313.67584	88.0837
2	27.672	BB	0.8133	2956.64868	43.15457	11.9163