Electronic Supplementary Material (ESI) for RSC Advances.

Bimetallic titanium complex catalyzed enantioselective oxidation of thioethers using aqueous H_2O_2 as terminal oxidant

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1. Characterization data and of the sulfoxides

Methyl phenyl sulfoxide[1]: Colourless oil; Yield: 89%; ee: 91%; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.66-7.64 (m, 2H), 7.53-7.48 (m, 3H), 2.71 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 145.1, 130.5, 128.9, 123.0, 43.3 ppm; The enantiomeric excess was determined by HPLC analysis. HPLC condition: Daicel Chiralcel OD column, 80:20 Hex/IPA, 0.5 ml/min, 30 ^{o}C, 254 nm; t_r (***R***) = 13.8 min, t_r (***S***) = 15.8 min.

4-Methylphenyl methyl sulfoxide[1]: White solid; Yield: 86%; ee: 94%; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.54 (d, *J* = 8.0 Hz, 2H), 7.32 (d, *J* = 8 Hz, 2H), 2.70 (s, 3H), 2.41 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 142.1, 141.2, 129.7, 123.3, 43.6, 21.1 ppm; The enantiomeric excess was determined by HPLC analysis. HPLC condition: Daicel Chiralcel OD column, 94:06 Hex/IPA, 0.5 ml/min, 30 ^{o}C, 254 nm; t_r (***R***) = 32.2 min, t_r (***S***) = 35.8 min.

4-Methoxyphenyl methyl sulfoxide[1]: Yellow oil; Yield: 84%; ee: 82%; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.45 (d, *J* = 7.8 Hz, 1H), 6.88 (d, *J* = 7.6 Hz, 1H), 3.70 (s, 3H), 2.56 (s, 3H) ppm; ^{13}C NMR (50 MHz, $CDCl_3$): δ = 161.5, 136.0, 125.0, 114.4, 55.1, 43.4 ppm; The enantiomeric excess was determined by HPLC analysis. HPLC condition: Daicel Chiralcel OD column, 90:10 Hex/IPA, 0.7 ml/min, 30 ^{o}C, 254 nm; t_r (***R***) = 21.7 min, t_r (***S***) = 23.3 min.

4-Fluorophenyl methyl sulfoxide[2]: Colourless oil; Yield: 84%; ee: 84%; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.69-7.66 (m, 2H), 7.25-7.22 (m, 2H), 2.73 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 165.0, 163.0, 140.8, 125.7, 125.6, 116.5, 116.3, 43.8 ppm; The enantiomeric excess was determined by HPLC analysis. HPLC condition: Daicel Chiralcel OD column, 92:08 Hex/IPA, 0.4 ml/min, 30 ^{o}C, 254 nm; t_r (***R***) = 32.3 min, t_r (***S***) = 34.7 min.

4-Chlorophenyl methyl sulfoxide[1]: Colourless oil; Yield: 81%; ee: 91%; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.61 (d, *J* = 8.5 Hz, 2H), 7.51 (d, *J* = 8.5 Hz, 2H), 2.73 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 143.8, 136.7, 129.2, 124.6, 43.6 ppm; The enantiomeric excess was determined by HPLC analysis. HPLC condition: Daicel Chiralcel OB column, 80:20 Hex/IPA, 0.7 ml/min, 30 ^{o}C, 254 nm; t_r (***R***) = 11.5 min, t_r (***S***) = 16.9 min.

4-Bromophenyl methyl sulfoxide[1]: White solid; Yield: 83%; ee: 95%; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.67 (d, *J* = 8.5 Hz, 2H), 7.53 (d, *J* = 8.5 Hz, 2H), 2.73 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 144.7, 132.5, 125.4, 125.1, 43.8 ppm; The enantiomeric excess was determined by HPLC analysis. HPLC condition: Daicel Chiralcel OB column, 80:20 Hex/IPA, 0.5 ml/min, 30 ^{o}C, 254 nm; t_r (***R***) = 17.6 min, t_r (***S***) = 24.3 min.

4-Nitrophenyl methyl sulfoxide[1]: White solid; Yield: 64%; ee: 99%; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 8.40 (d, *J* = 8.5 Hz, 2H), 7.86 (d, *J* = 8.5 Hz, 2H), 2.82 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 153.1, 149.4, 124.6, 124.4, 43.8 ppm; The enantiomeric excess was determined by HPLC analysis. HPLC condition: Daicel Chiralcel OJ column, 65:35 Hex/IPA, 0.5 ml/min, 30 ^{o}C, 254 nm; t_r (***R***) = 22.3 min, t_r (***S***) = 25.8 min.

3-Chlorophenyl methyl sulfoxide[3]: Colourless oil; Yield: 79%; ee: 91%; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.67 (s, 1H), 7.52-7.49 (m, 1H), 7.48-7.46 (m, 2H), 2.75 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 147.5, 135.4, 130.9, 130.4, 123.3, 121.4, 43.7 ppm; The enantiomeric excess was determined by HPLC analysis. HPLC condition: Daicel Chiralcel OB column, 90:10 Hex/IPA, 1.0 ml/min, 30 ^{o}C, 254 nm; t_r (***R***) = 12.5 min, t_r (***S***) = 18.9 min.

3-Bromophenyl methyl sulfoxide[4]: Colorless oil; Yield: 80%; ee: 85%; ^{1}H NMR (200 MHz, $CDCl_3$): δ = 7.82 (s, 1H), 7.65-7.53 (m, 2H), 7.47-7.32 (m, 1H), 2.75 (s, 3H) ppm; ^{13}C NMR (50

MHz, $CDCl_3$): δ = 147.9, 134.1, 130.8, 126.4, 123.5, 122.1, 44.0 ppm; The enantiomeric excess was determined by HPLC analysis. HPLC condition: Daicel Chiralcel OB column, 80:20 Hex/IPA, 1.0 ml/min, 30 °C, 254 nm; t_r (***R***) = 8.9 min, t_r (***S***) = 13.6 min.

Ethyl phenyl sulfoxide[1]: Colourless oil; Yield: 84%; ee: 78%; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.62-7.60 (m, 2H), 7.54-7.49 (m, 3H), 2.95-2.87 (m, 1H), 2.81-2.74 (m, 1H), 1.20 (t, *J* = 7.5, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 143.0, 130.8, 129.0, 124.0, 50.1, 5.8 ppm; The enantiomeric excess was determined by HPLC analysis. HPLC condition: Daicel Chiralcel OD column, 90:10 Hex/IPA, 0.5 ml/min, 30 °C, 254 nm; t_r (***R***) = 19.4 min, t_r (***S***) = 23.3 min.

Benzyl phenyl sulfoxide[1]: White solid; Yield: 81%; ee: 79%; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.46-7.37 (m, 5H), 7.29-7.23 (m, 3H), 6.98 (m, 2H), 4.12 (d, *J* = 12.5 Hz, 1H), 4.00 (d, *J* = 12.5 Hz, 1H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 142.6, 131.2, 130.3, 129.1, 128.8, 128.4, 128.2, 124.4, 63.5 ppm; The enantiomeric excess was determined by HPLC analysis. HPLC condition: Daicel Chiralcel OD column, 90:10 Hex/IPA, 0.5 ml/min, 30 °C, 254 nm; t_r (***R***) = 24.1 min, t_r (***S***) = 28.8 min.

(+)-trans-(1*S*,2*S*)-2-Phenyl-1,3-dithiane 1-oxide[5]: White solid; Yield: 93%; ee: 84%; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.43-7.37 (m, 5H), 4.55 (s, 1H), 3.57-3.56 (m, 1H), 2.90-2.84 (m, 1H), 2.78-2.72 (m, 1H), 2.68-2.65 (m, 1H), 2.62-2.49 (m, 1H), 2.40-2.31 (m, 1H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 133.3, 129.3, 129.0, 128.7, 69.6, 54.7, 31.3, 29.4 ppm; The enantiomeric excess was determined by HPLC analysis. HPLC condition: Daicel Chiralcel OD column, 70:30 Hex/IPA, 0.7 ml/min, 30 °C, 254 nm; t_r (***minor***) = 13.3 min, t_r (***major***) = 26.4 min.

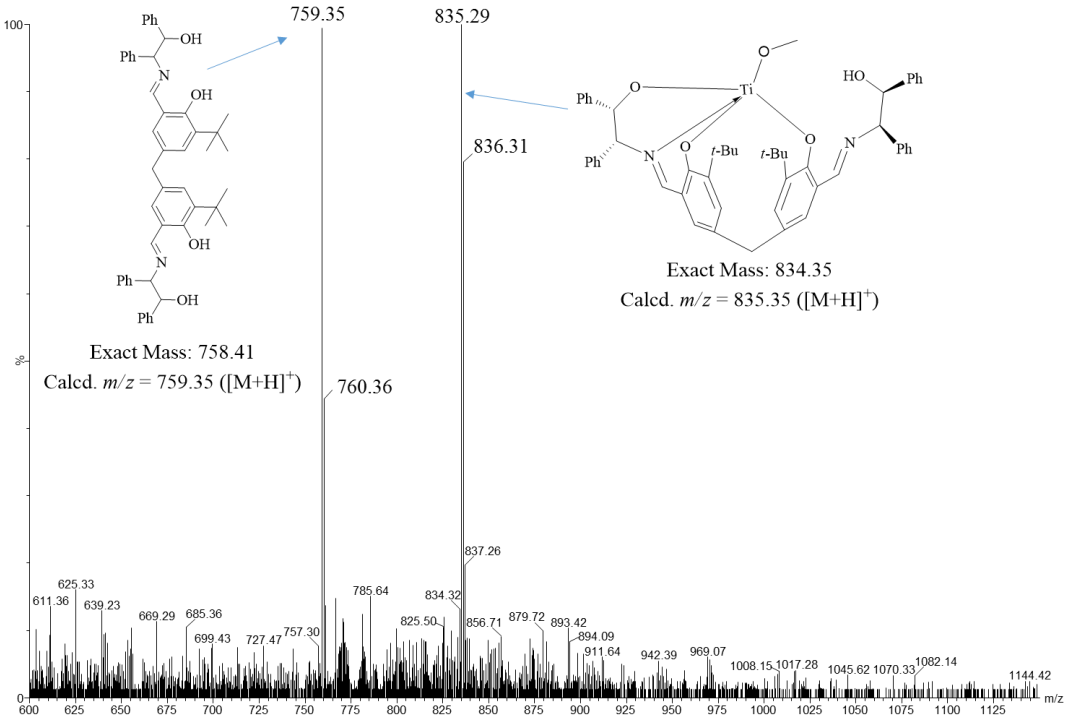
(+)-trans-2-(4-Methylphenyl)-1,3-dithiane 1-oxide[5]: White solid; Yield: 94%; ee: 78%; ^{1}H NMR (200 MHz, $CDCl_3$): δ = 7.31 (d, *J* = 8Hz 2H), 7.20 (d, *J* = 8Hz, 2H), 4.54 (s, 1H), 3.59-

3.53 (m, 1H), 2.96-2.62 (m, 3H), 2.58-2.43 (m, 2H), 2.34 (s, 3H) ppm; ^{13}C NMR (50 MHz, $CDCl_3$): δ = 139.3, 130.2, 129.8, 128.5, 69.4, 31.4, 29.5, 21.2 ppm; The enantiomeric excess was determined by HPLC analysis. HPLC condition: Daicel Chiralcel OD column, 70:30 Hex/IPA, 0.7 ml/min, 30 ^{o}C, 254 nm; t_r (***minor***) = 12.9 min, t_r (***major***) = 22.9 min.

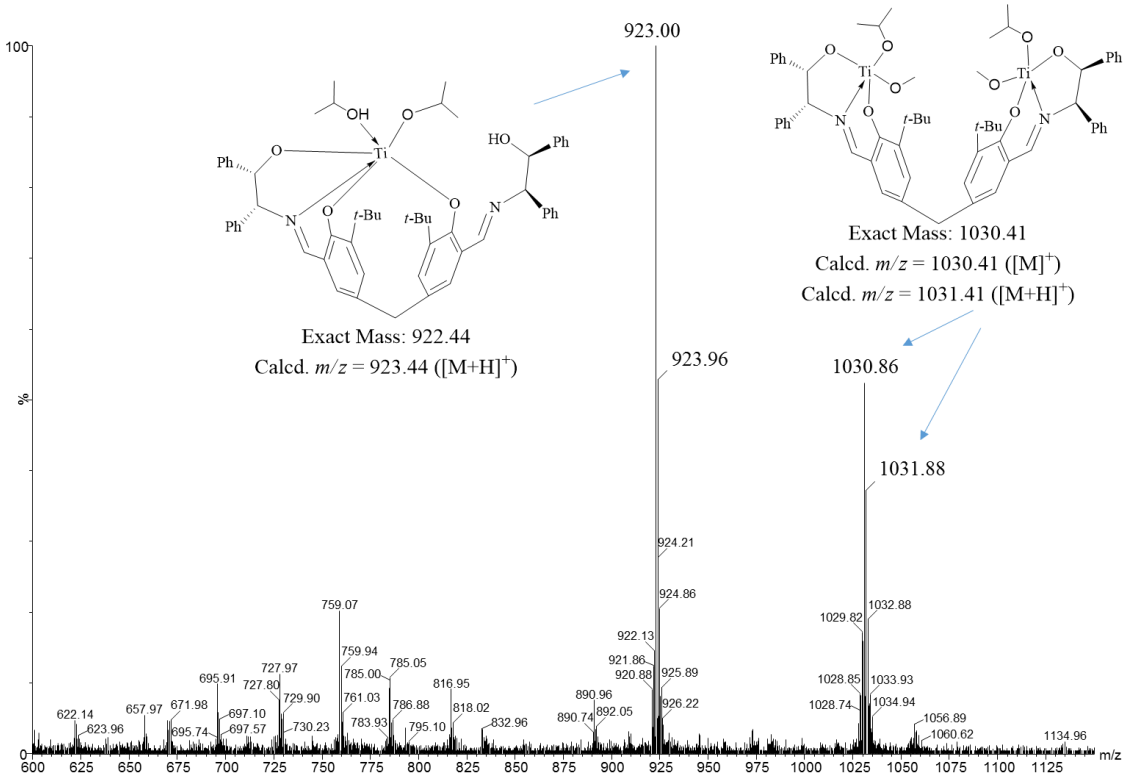
(+)-trans-2-(4-Chlorophenyl)-1,3-dithiane 1-Oxide[5]: White solid; Yield: 94%; ee: 95%; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.36 (d, *J* = 5Hz, 4H), 4.53 (s, 1H), 3.58-3.56 (m, 1H), 2.90-2.85 (m, 1H), 2.79-2.73 (m, 1H), 2.70-2.67 (m, 1H), 2.54-2.51 (m, 1H), 2.40-2.32 (m, 1H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 135.3, 131.8, 130.0, 129.3, 68.8, 54.7, 31.3, 29.4 ppm; The enantiomeric excess was determined by HPLC analysis. HPLC condition: Daicel Chiralcel OD column, 70:30 Hex/IPA, 0.7 ml/min, 30 ^{o}C, 254 nm; t_r (***minor***) = 14.1 min, t_r (***major***) = 33.9 min.

(+)-trans-2-(2-Fluorophenyl)-1,3-dithiane 1-oxide[5]: White solid; Yield: 92%; ee: 84%; ^{1}H NMR (200 MHz, $CDCl_3$): δ = 7.36-7.29 (m, 2H), 7.05-6.97 (m, 2H), 4.48 (s, 1H), 3.51-3.45 (m, 1H), 2.87-2.62 (m, 3H), 2.49-2.23 (m, 2H) ppm; ^{13}C NMR (50 MHz, $CDCl_3$): δ = 165.5, 160.6, 130.5, 130.4, 129.2, 129.1, 116.2, 115.8, 68.6, 54.6, 31.3, 29.4 ppm; The enantiomeric excess was determined by HPLC analysis. HPLC condition: Daicel Chiralcel OD column, 70:30 Hex/IPA, 0.7 ml/min, 30 ^{o}C, 254 nm; t_r (***minor***) = 12.9 min, t_r (***major***) = 33.6 min.

2. (a) ESI-MS analysis of *in situ* generated **L1**-Ti complex at **L1**:Ti =1:1.

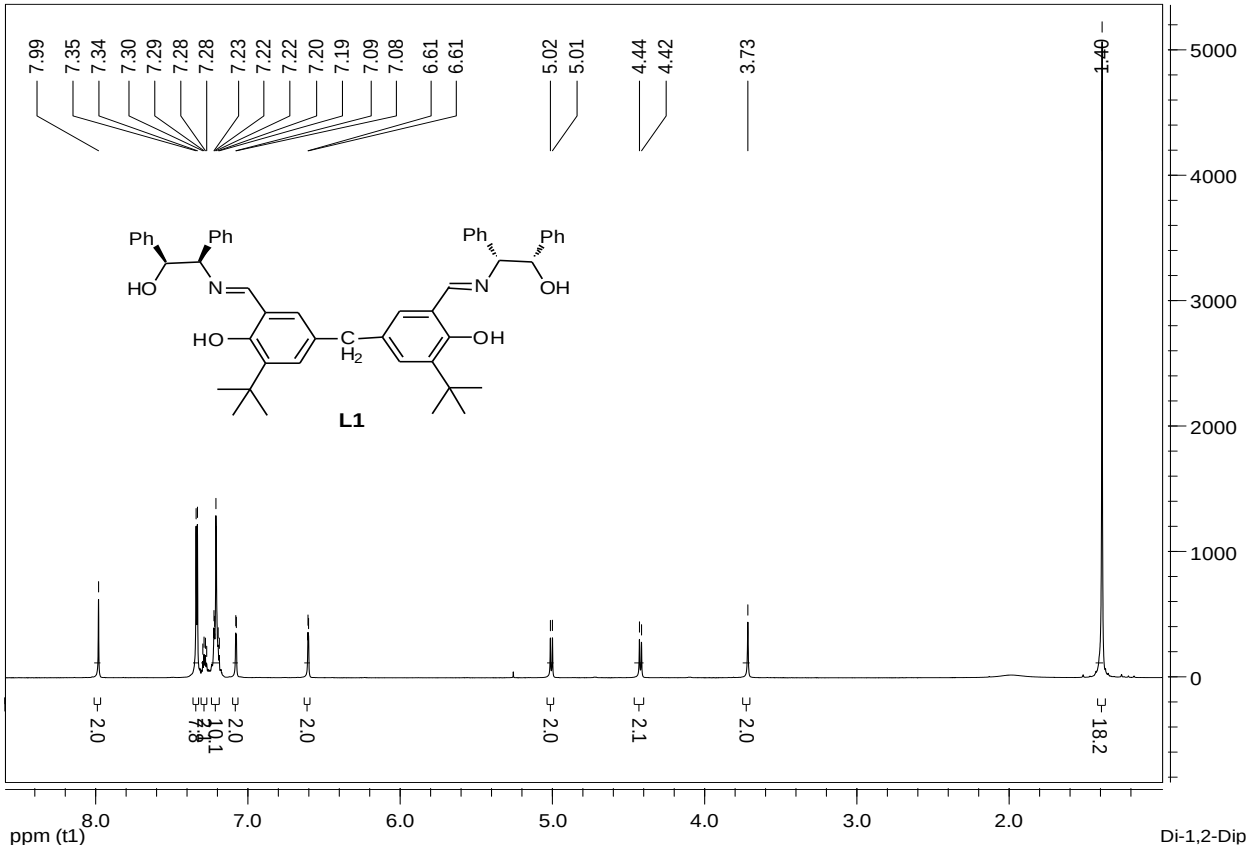


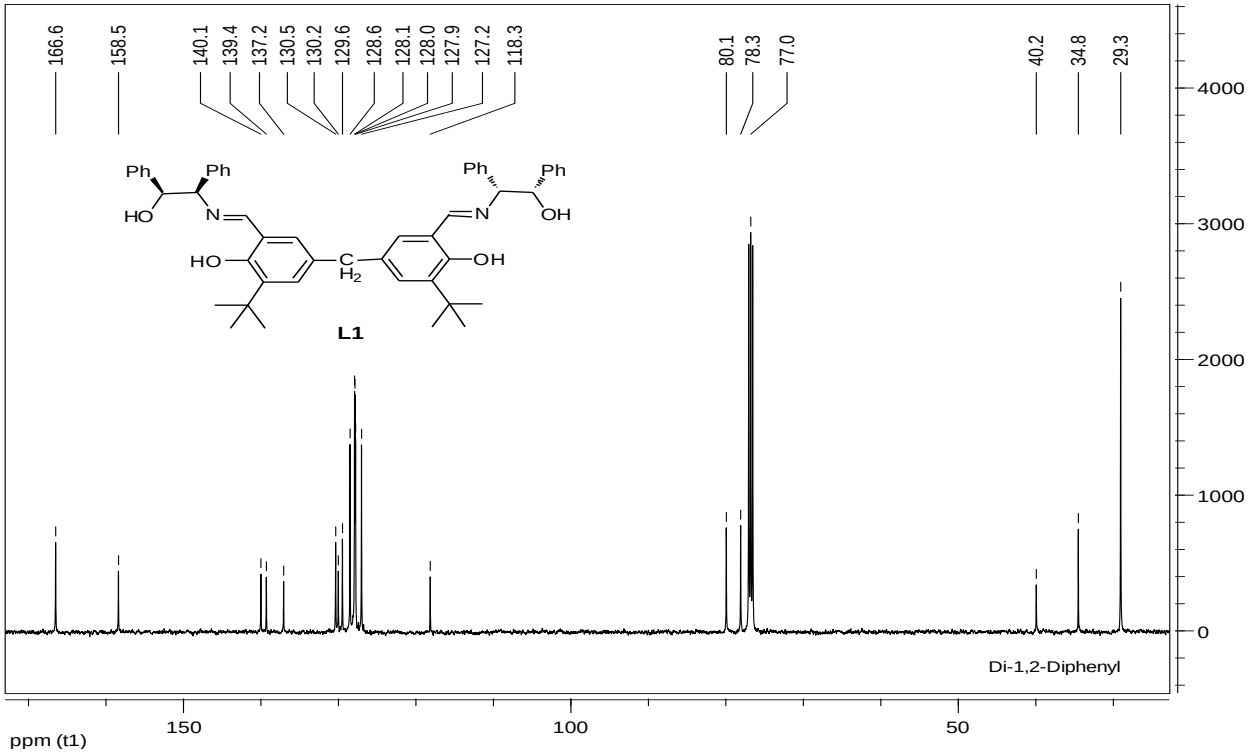
(b) ESI-MS analysis of *in situ* generated **L1**-Ti complex at **L1**:Ti =1:2.



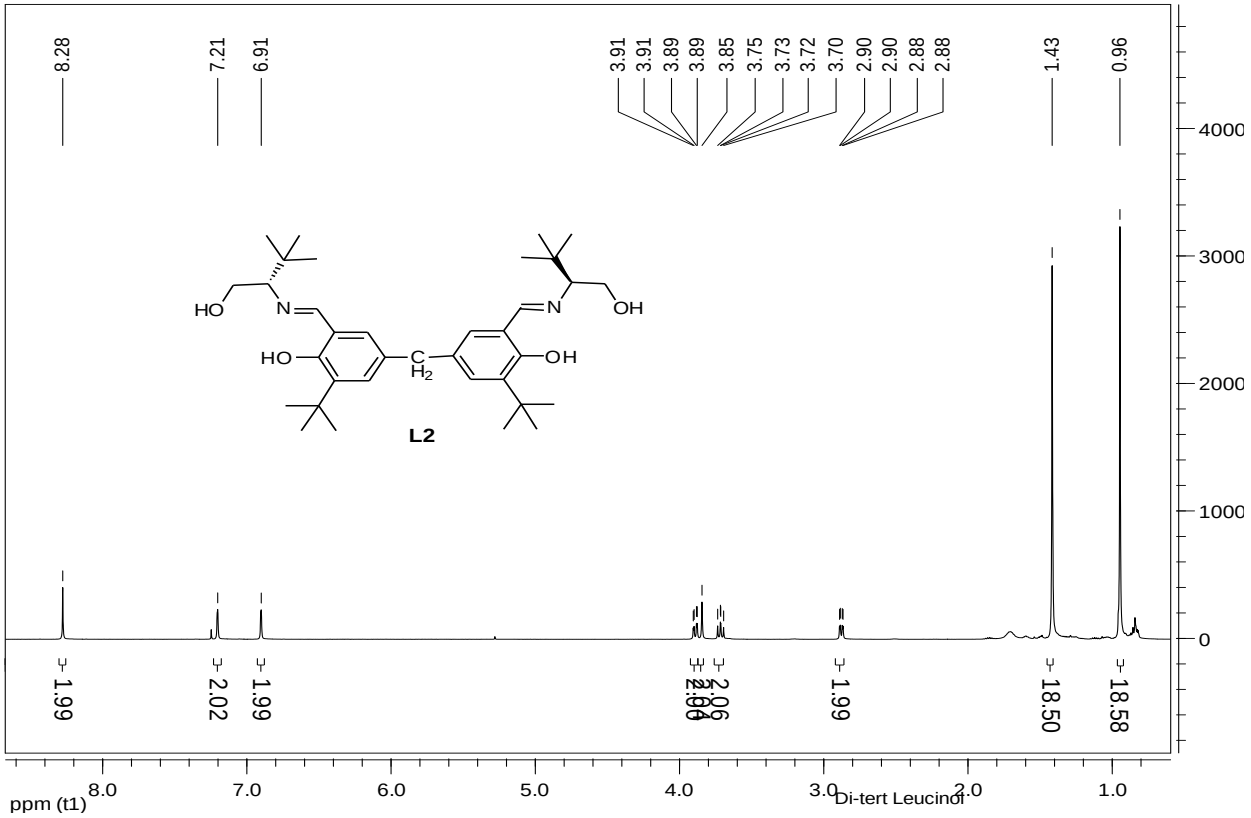
3. ^{1}H and ^{13}C NMR spectra of dimeric ligands (L1-L7)

Ligand L1





Ligand L2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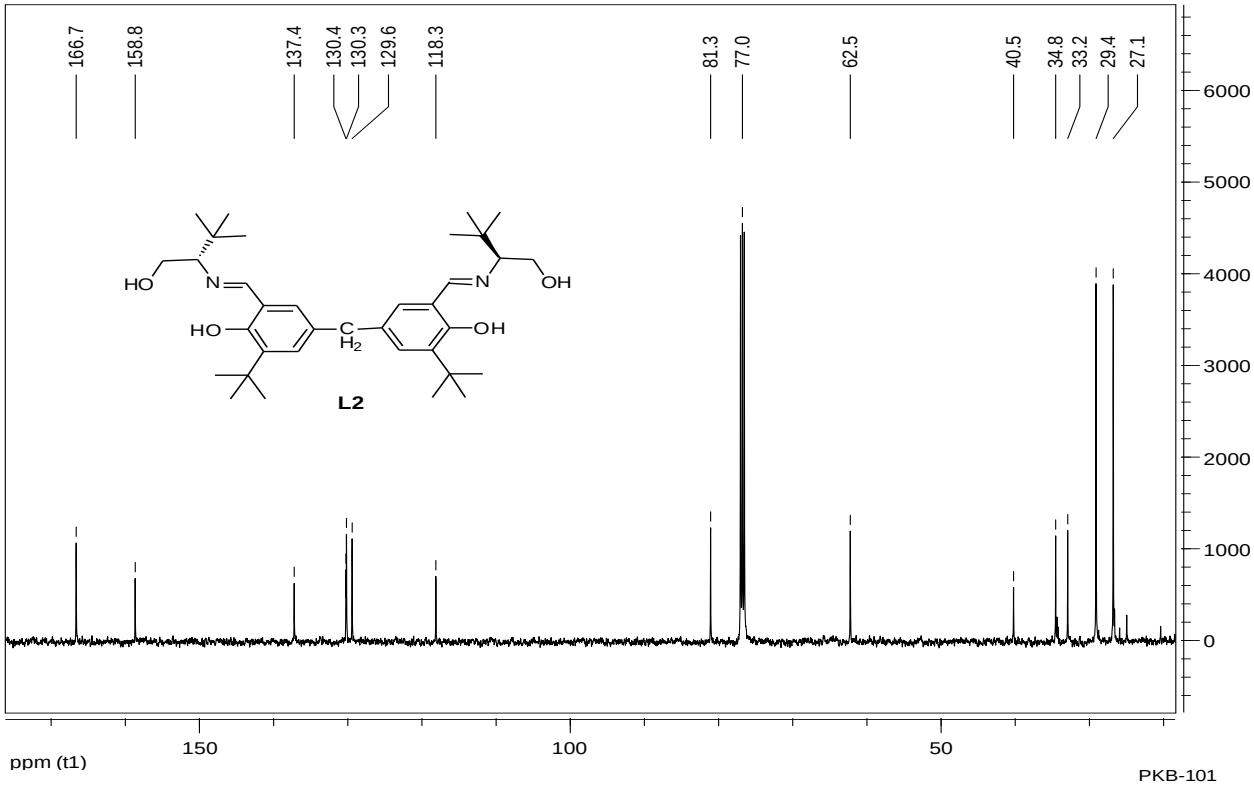
6.91
3.91
3.91
3.89
3.89
3.85
3.75
3.73
3.72
3.70
2.90
2.90
2.88
2.88
1.43
0.96
HO
N
OH
HO
C
H2
OH
L2
1.99
2.02
1.99
1.96
1.99
18.50
18.58
ppm (t1)
Di-tert Leucinol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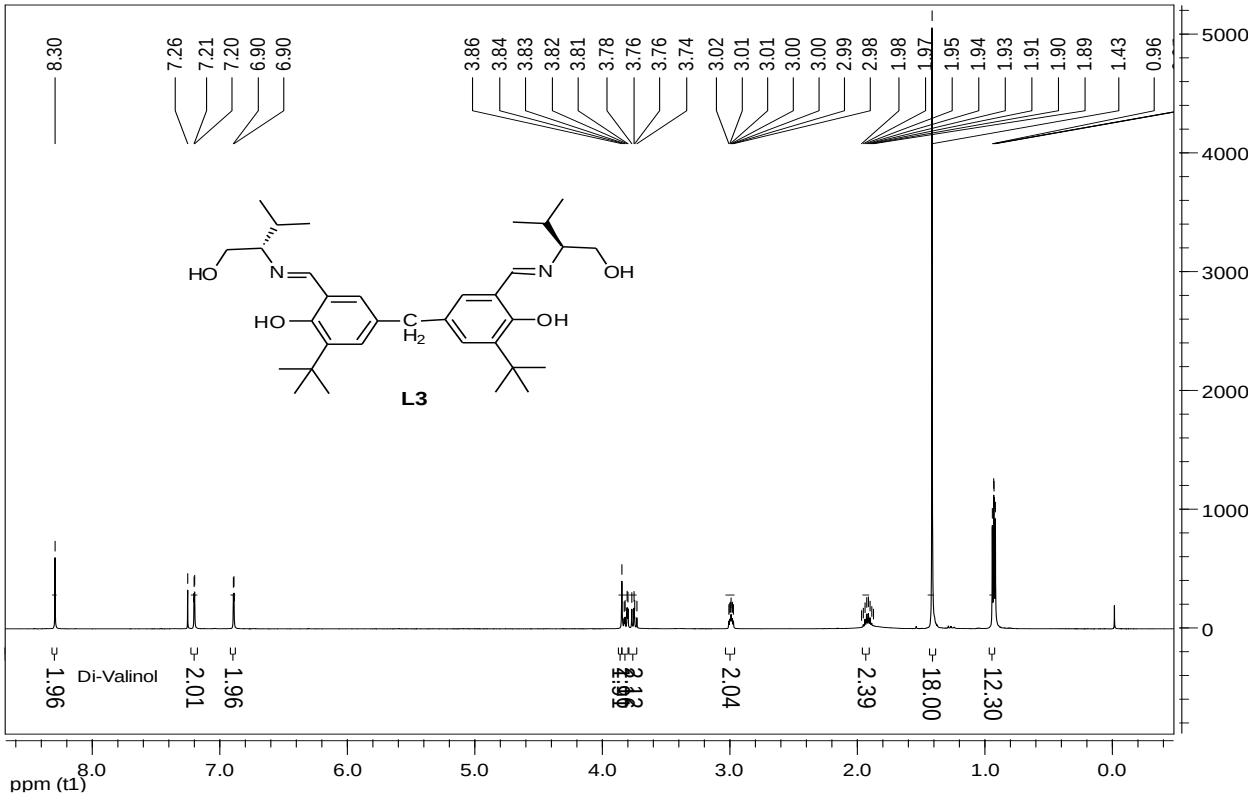
158.8
137.4
130.4
130.3
129.6
118.3
81.3
77.0
62.5
40.5
34.8
33.2
29.4
27.1
HO
N
OH
HO
C
H2
OH
L2
ppm (t1)
PKB-101

Ligand L3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7.20
6.90
6.90
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3.82
3.81
3.78
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3.76
3.74
3.02
3.01
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3.00
3.00
2.99
2.98
1.98
1.97
1.95
1.94
1.93
1.91
1.90
1.89
1.43
0.96
HO
N
OH
HO
C
H2
OH
L3
Di-Valinol
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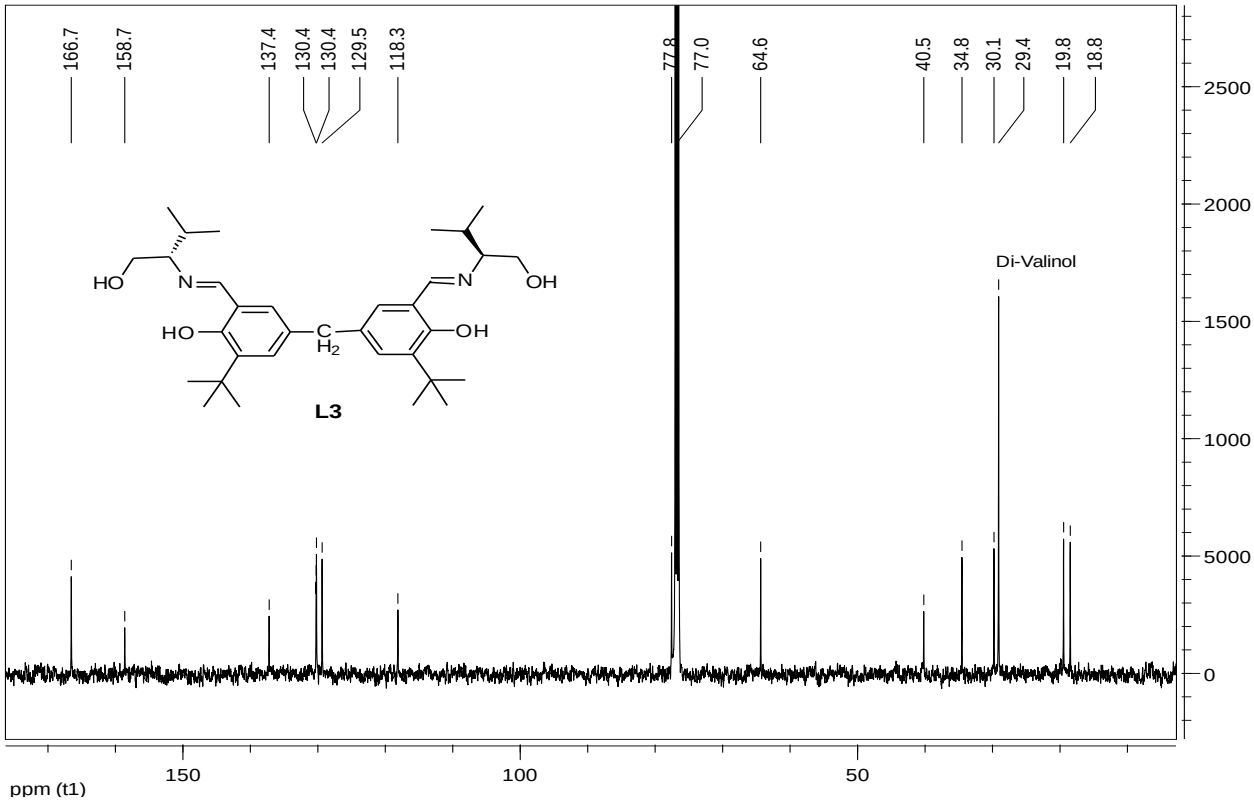
1.96
2.04
2.39
18.00
12.30
ppm (t1)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130.4
129.5
118.3
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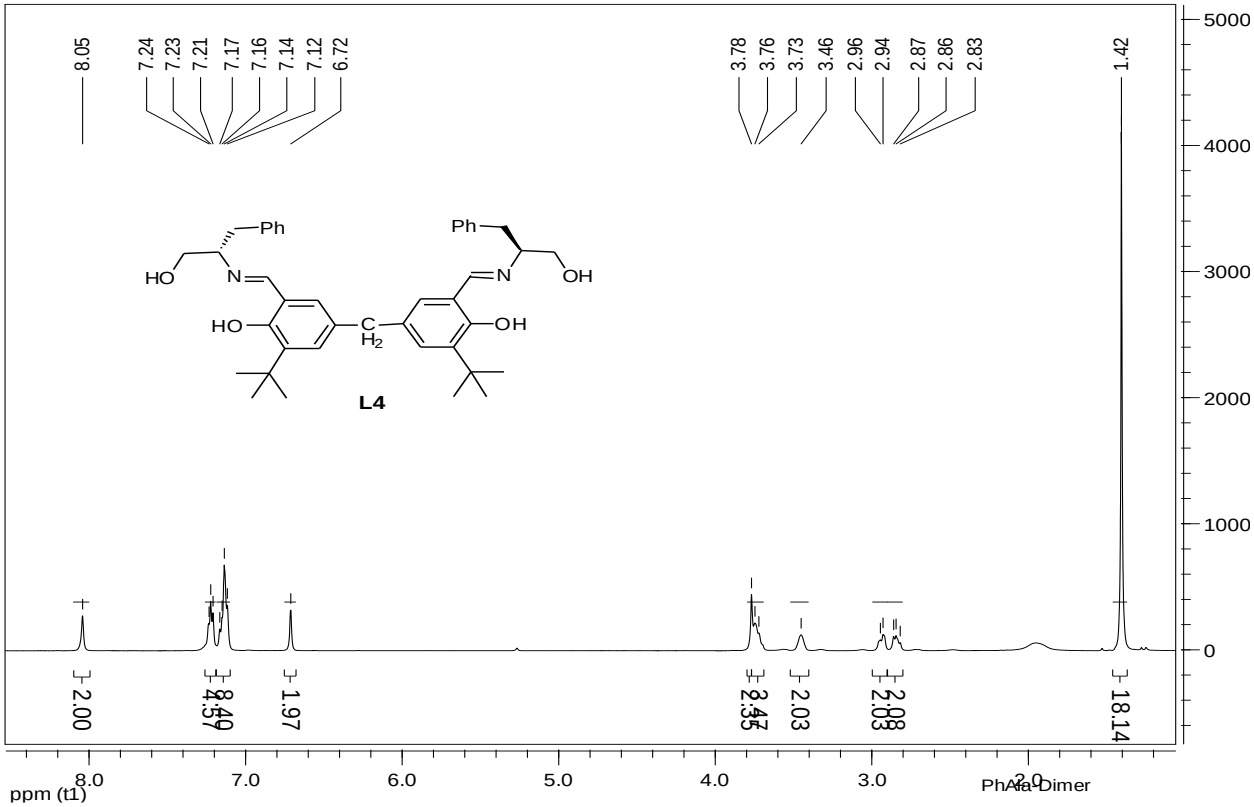
77.0
64.6
40.5
34.8
30.1
29.4
19.8
18.8
HO
N
OH
HO
C
H2
OH
L3
Di-Valinol
ppm (t1)

Ligand L4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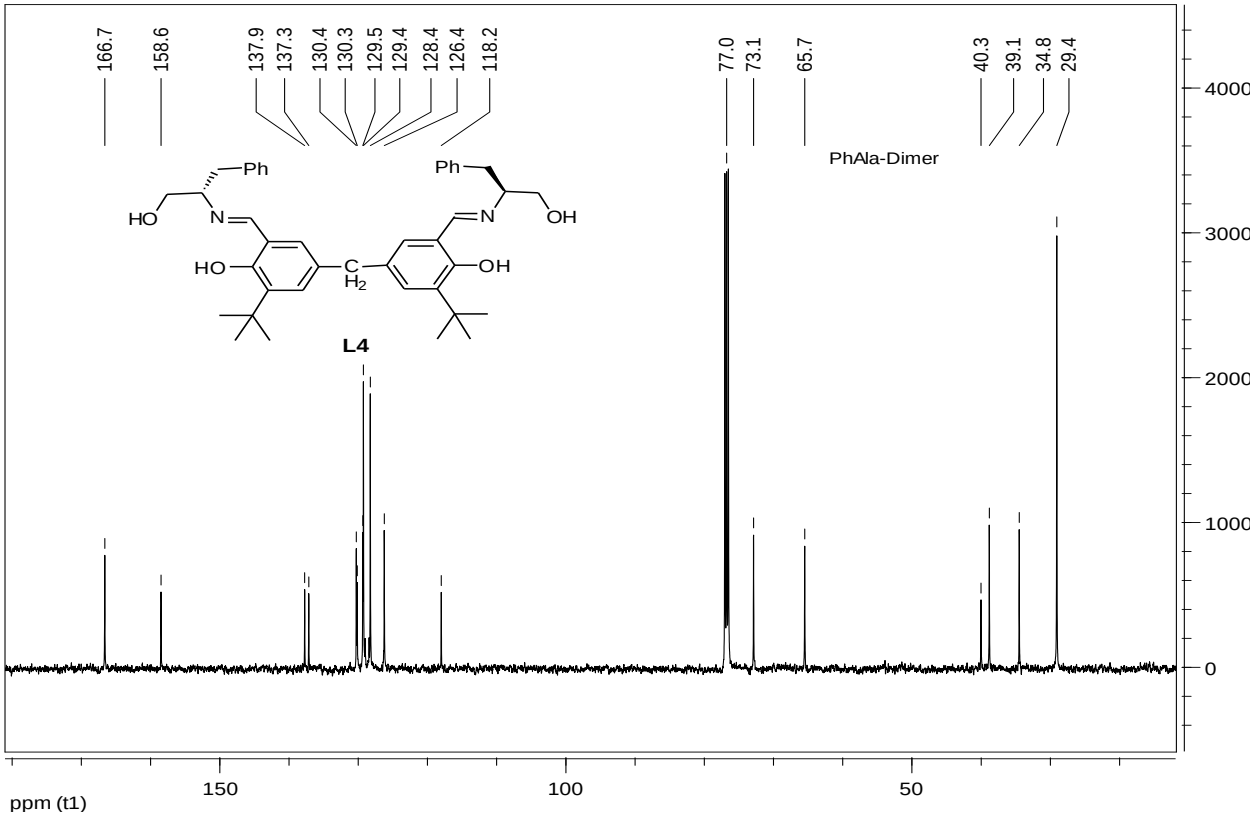
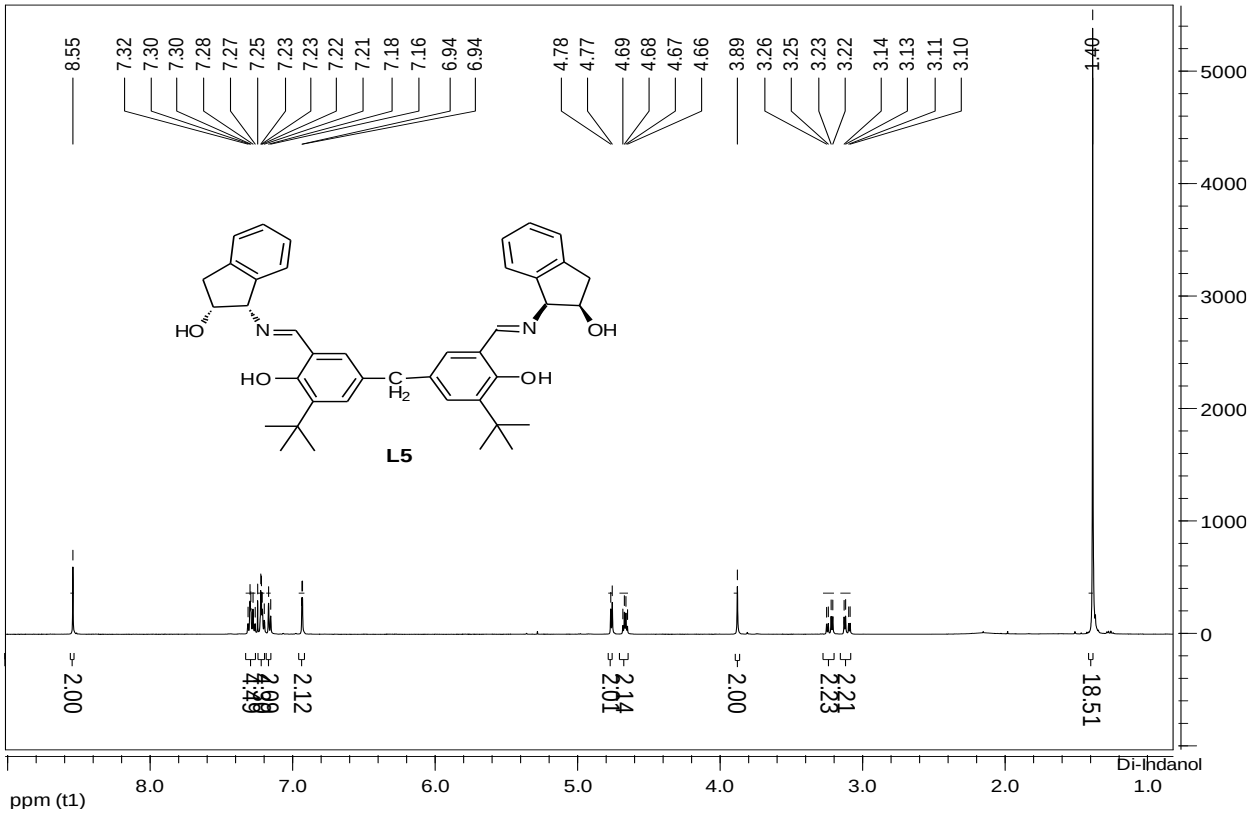
7.23
7.21
7.17
7.16
7.14
7.12
6.72
3.78
3.76
3.73
3.46
2.96
2.94
2.87
2.86
2.83
1.42
Ph
HO
N
OH
HO
C
H2
OH
L4
2.00
4.57
1.97
2.03
2.08
18.14
ppm (t1)
PhAla-Dimer


166.7
158.6
137.9
137.3
130.4
130.3
129.5
129.4
128.4
126.4
118.2
77.0
73.1
65.7
40.3
39.1
34.8
29.4
PhAla-Dimer
Ph
HO
N
OH
HO
C
H2
OH
L4
ppm (t1)

Ligand L5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7.30
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7.27
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7.23
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7.22
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4.66
3.89
3.26
3.25
3.23
3.22
3.14
3.13
3.11
3.10
1.40
HO
N
OH
HO
C
H2
OH
L5
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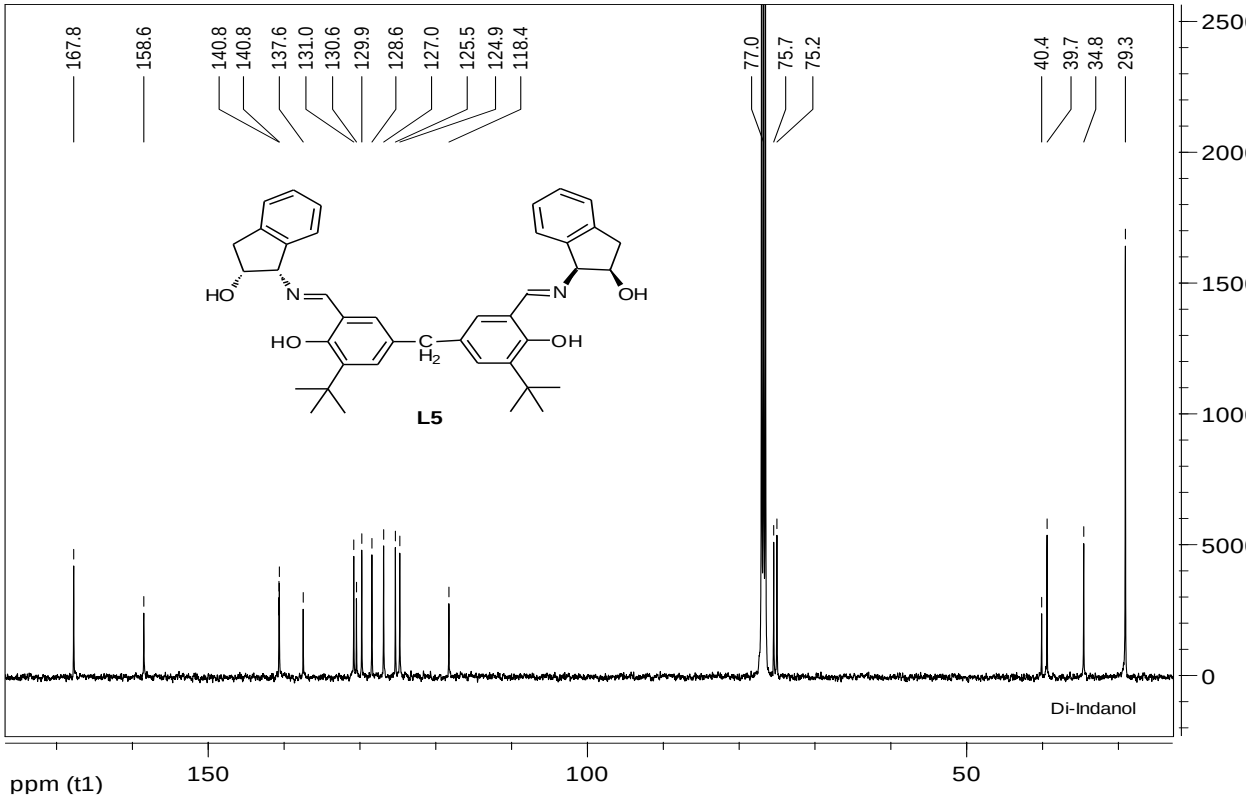
2.12
2.14
2.00
2.21
18.51
Di-Indanol
ppm (t1)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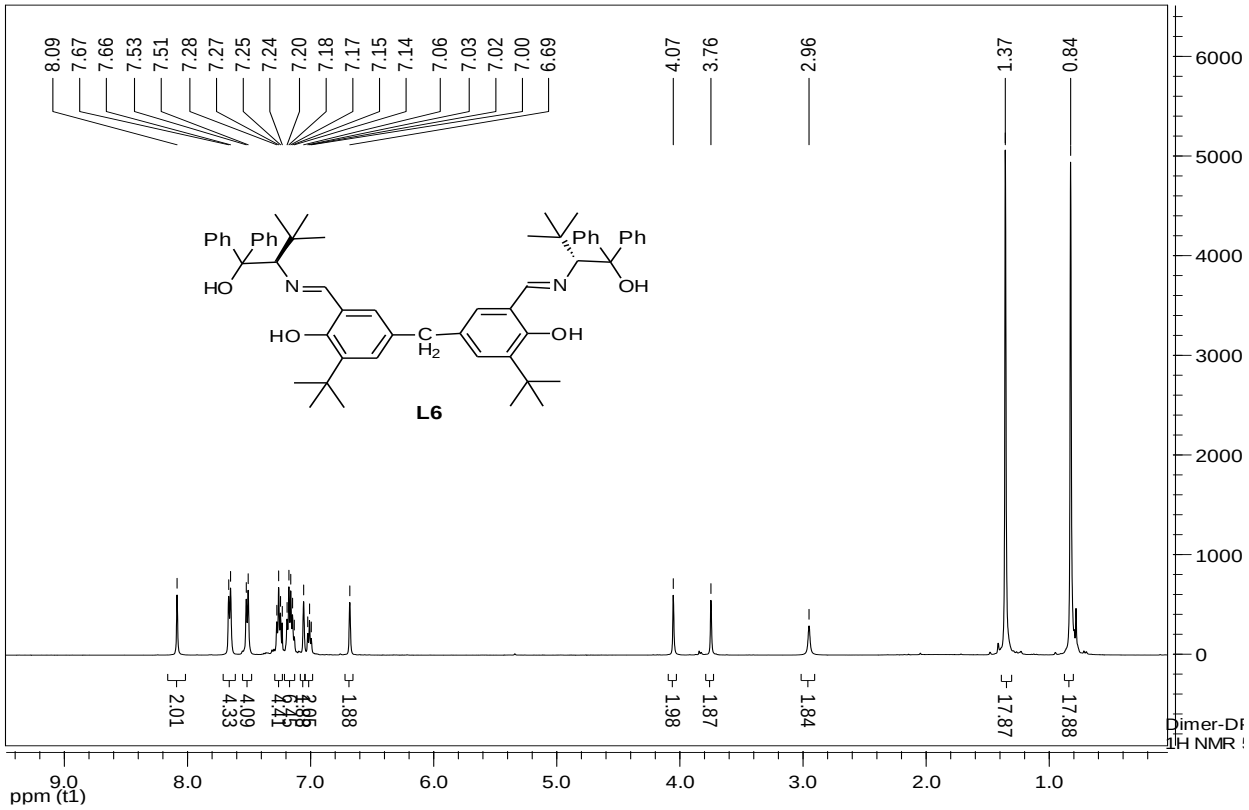
158.6
140.8
140.8
137.6
131.0
130.6
129.9
128.6
127.0
125.5
124.9
118.4
77.0
75.7
75.2
40.4
39.7
34.8
29.3
HO
N
OH
HO
C
H2
OH
L5
Di-Indanol
ppm (t1)

Ligand L6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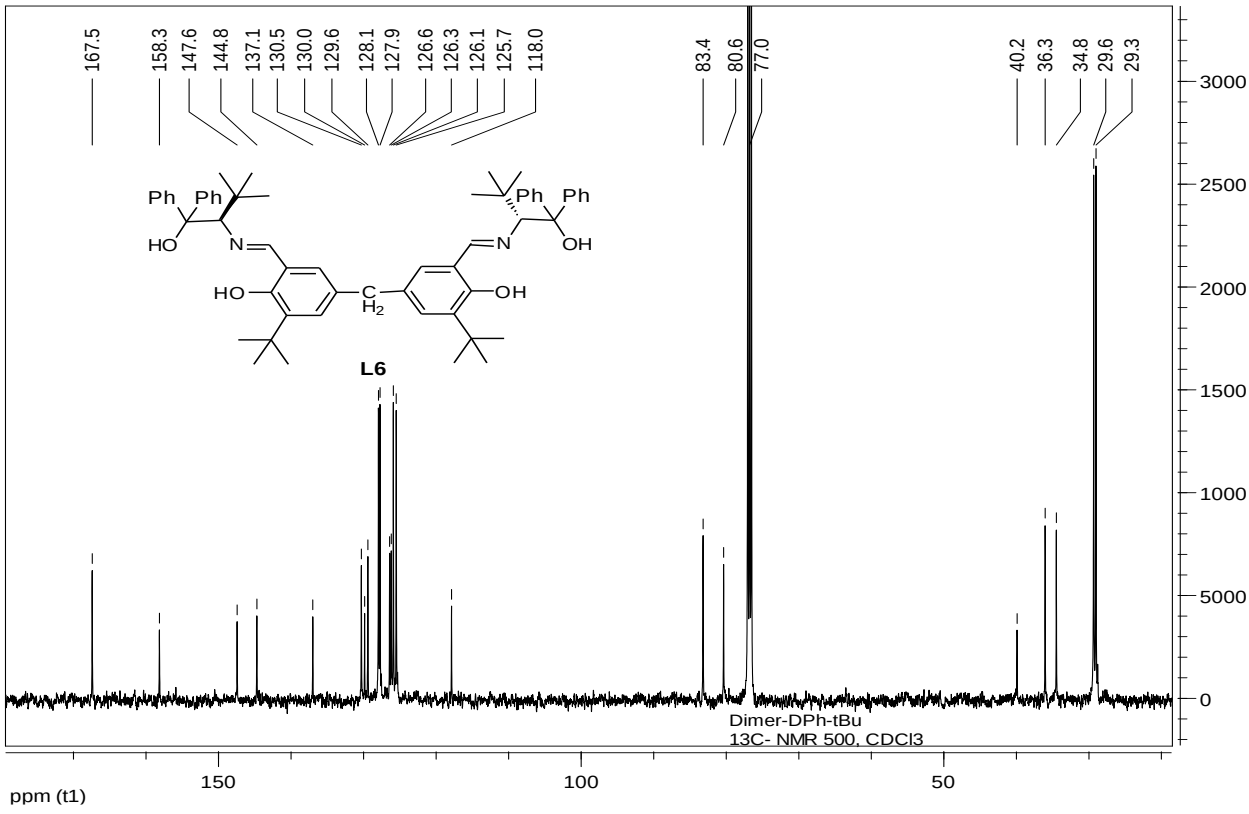
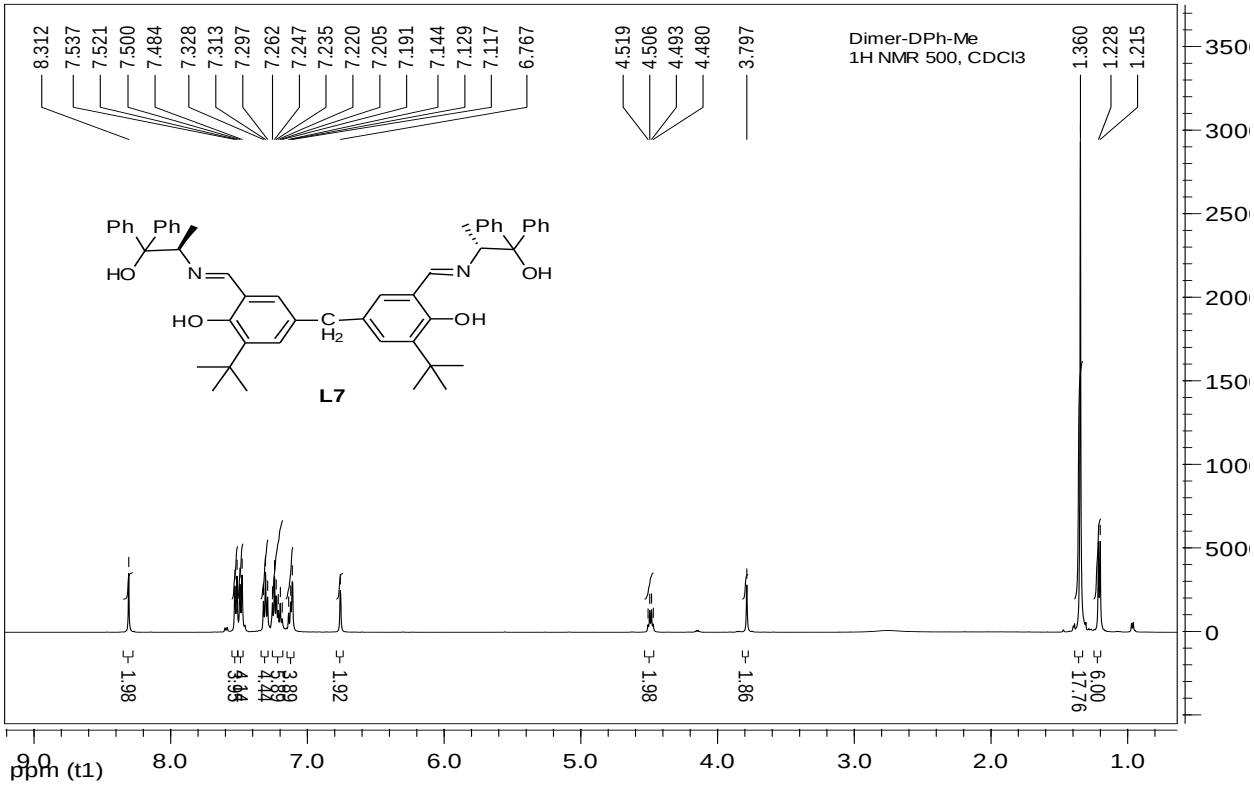
7.66
7.53
7.51
7.28
7.27
7.25
7.24
7.20
7.18
7.17
7.15
7.14
7.06
7.03
7.02
7.00
6.69
4.07
3.76
2.96
1.37
0.84
L6
2.01
4.33
4.09
1.88
1.98
1.87
1.84
17.87
17.88
ppm (t1)


167.5
158.3
147.6
144.8
137.1
130.5
130.0
129.6
128.1
127.9
126.6
126.3
126.1
125.7
118.0
83.4
80.6
77.0
40.2
36.3
34.8
29.6
29.3
L6
Dimer-DPh-tBu
13C- NMR 500, CDCl3
ppm (t1)

Ligand L7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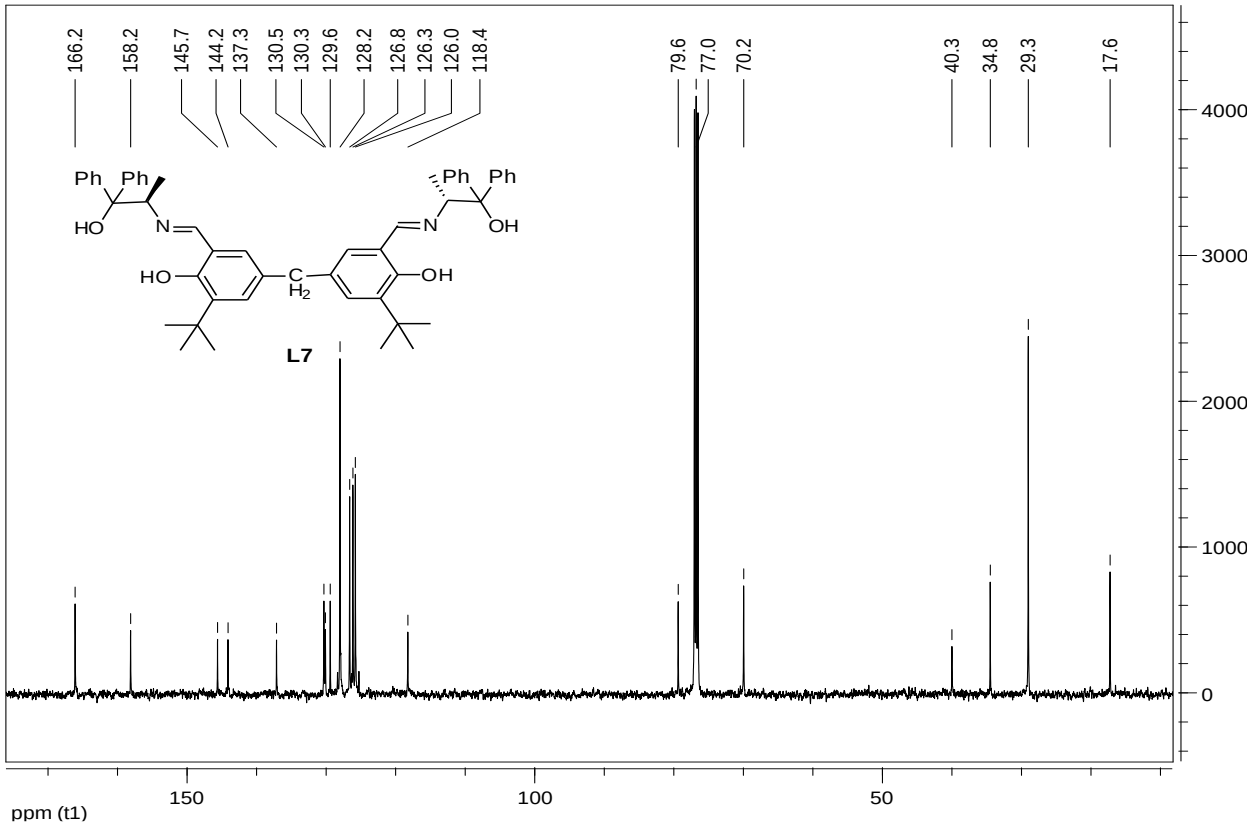
7.500
7.484
7.328
7.313
7.297
7.262
7.247
7.235
7.220
7.205
7.191
7.144
7.129
7.117
6.767
4.519
4.506
4.493
4.480
3.797
1.360
1.228
1.215
Dimer-DPh-Me
1H NMR 500, CDCl3
L7
1.98
3.96
4.14
1.92
1.98
1.86
17.76
6.00
ppm (t1)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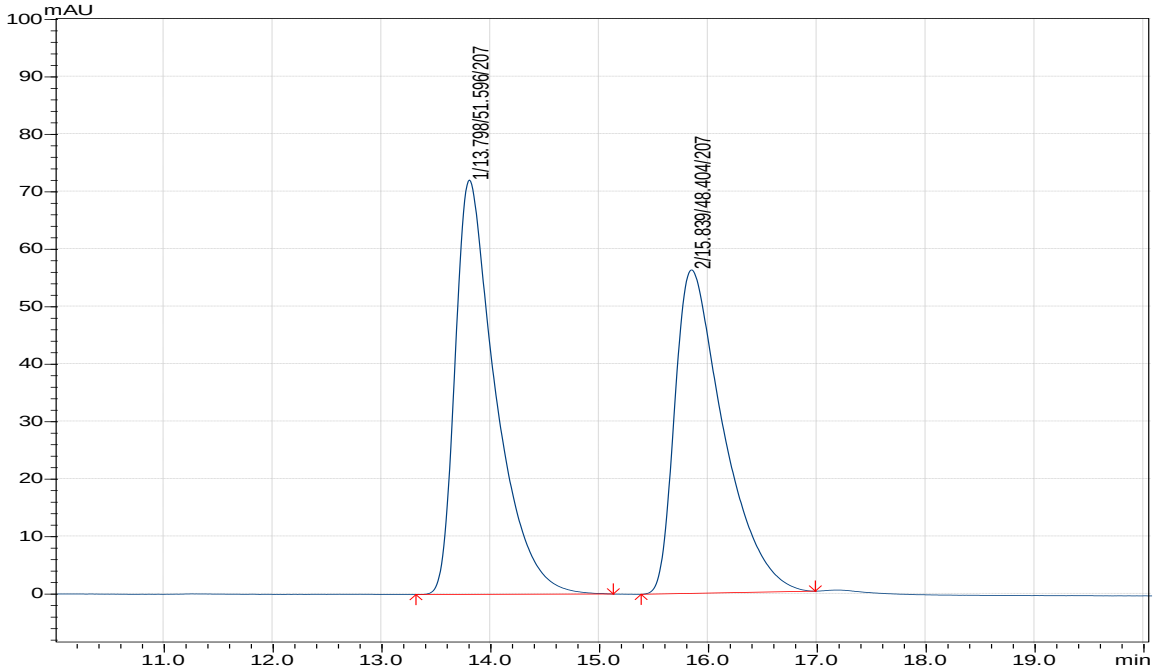
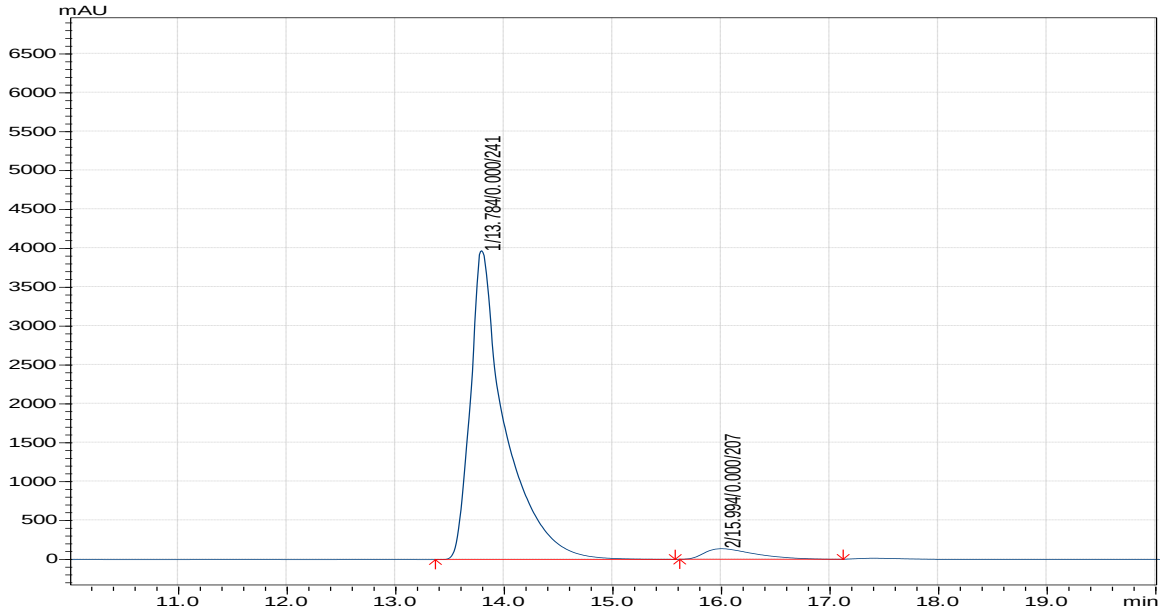
144.2
137.3
130.5
130.3
129.6
128.2
126.8
126.3
126.0
118.4
79.6
77.0
70.2
40.3
34.8
29.3
17.6
L7
ppm (t1)

4. HPLC chromatogram of racemic and chiral sulfoxides

Phenyl methyl sulfoxide

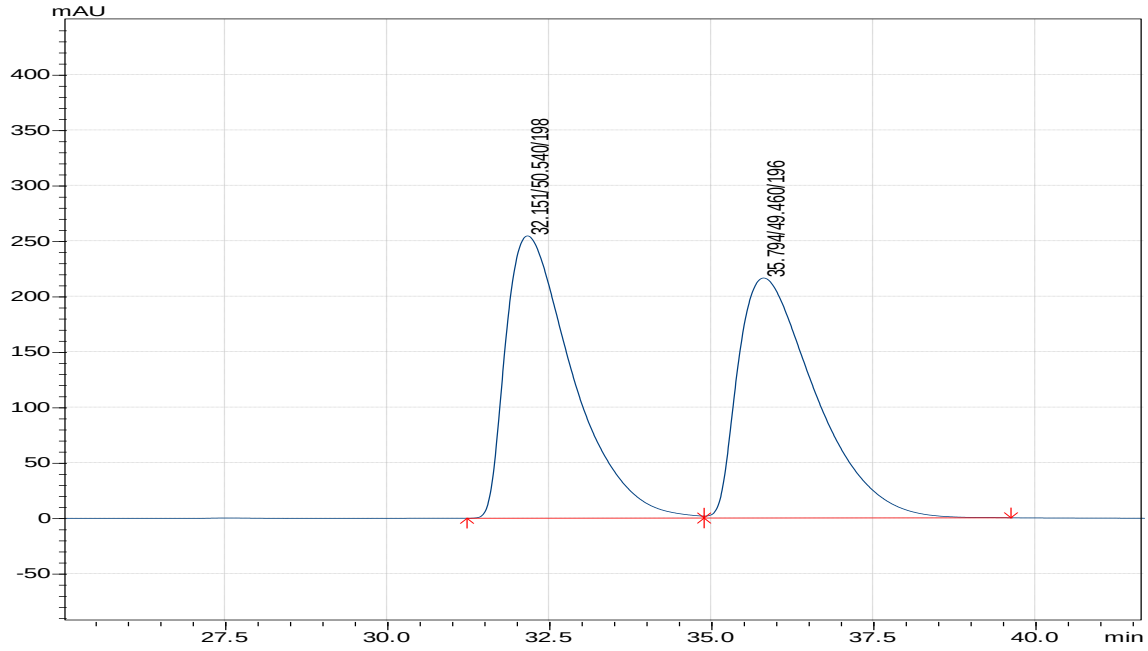


Ret. Time	Area	Peak Start	Peak End	Area%
13.798	1864485	13.312	15.125	51.5957
15.839	1749161	15.381	16.981	48.4043

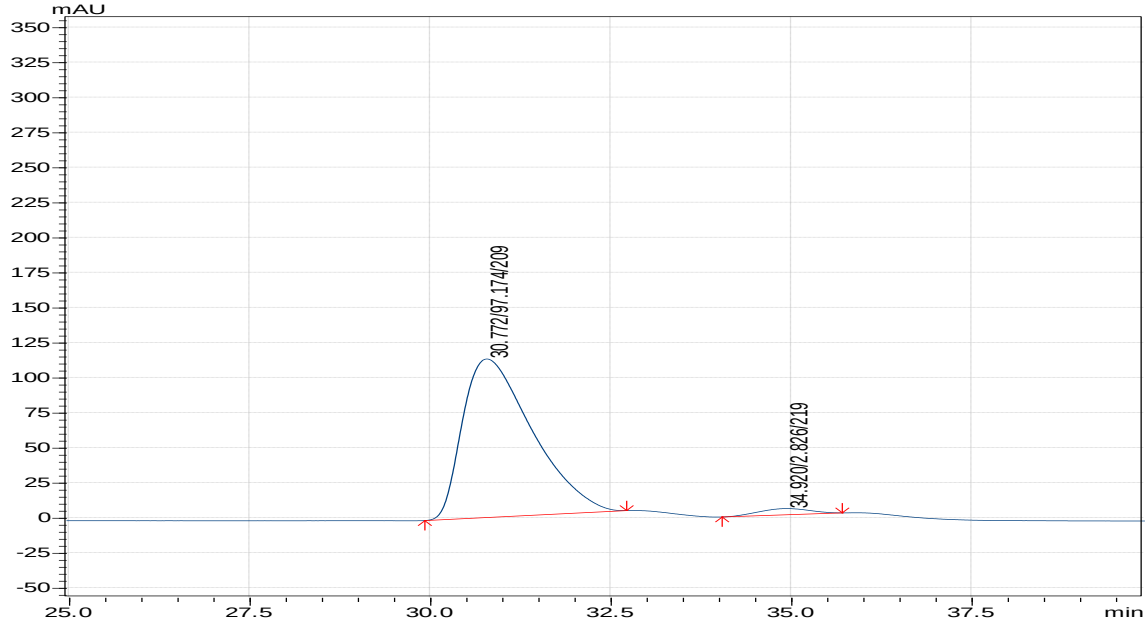


Ret. Time	Area	Peak Start	Peak End	Area%
13.835	101215329	13.365	17.120	95.2059
15.994	5096672	15.573	17.120	4.7941

4-Methylphenyl methyl sulfoxide

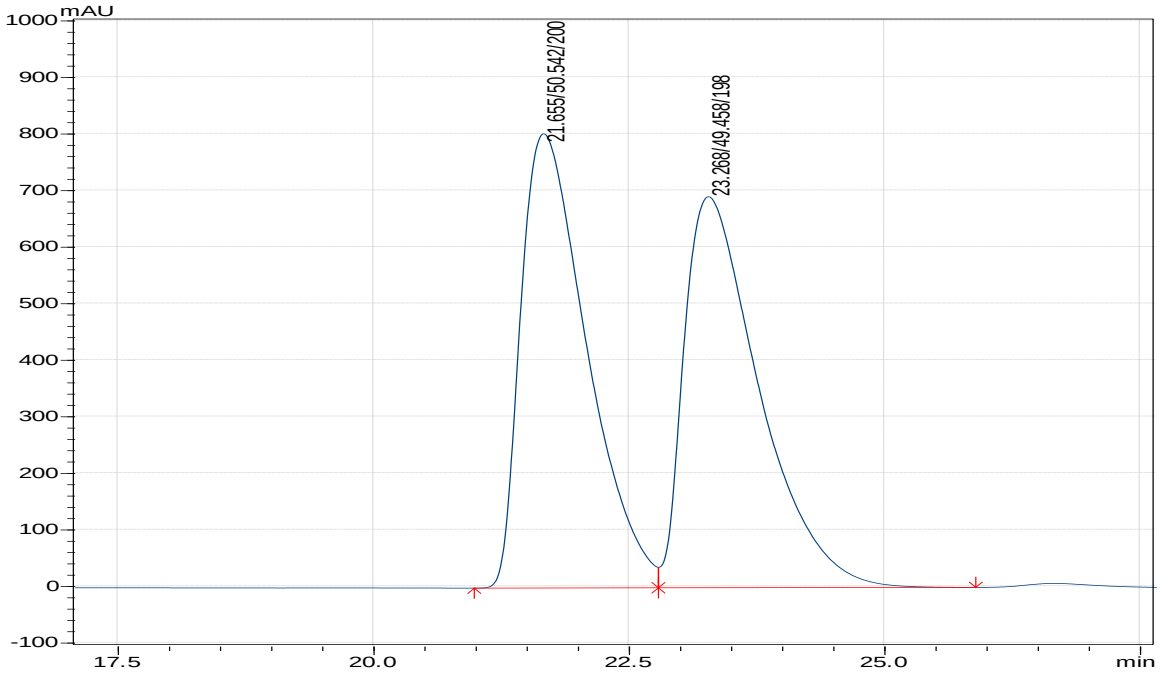


Ret. Time	Area	Peak Start	Peak End	Area%
32.151	18389022	31.221	34.880	50.5395
35.794	17996409	34.880	39.616	49.4605

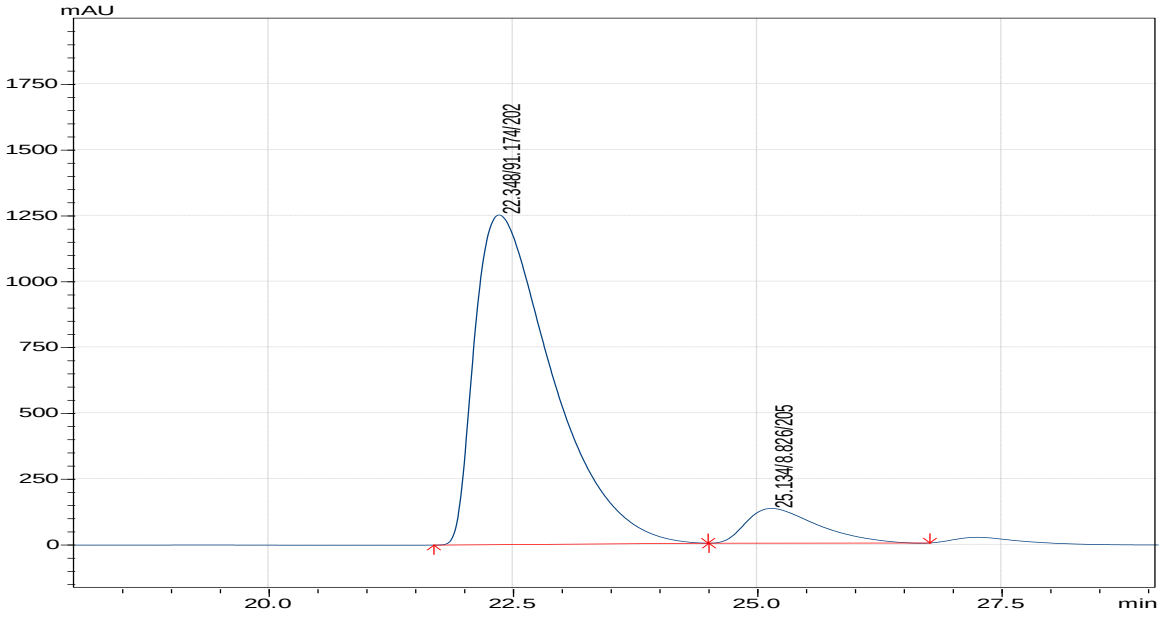


Ret. Time	Area	Peak Start	Peak End	Area%
30.772	7594068	29.920	32.715	97.1741
34.920	220838	34.037	35.701	2.8259

4-Methoxyphenyl methyl sulfoxide

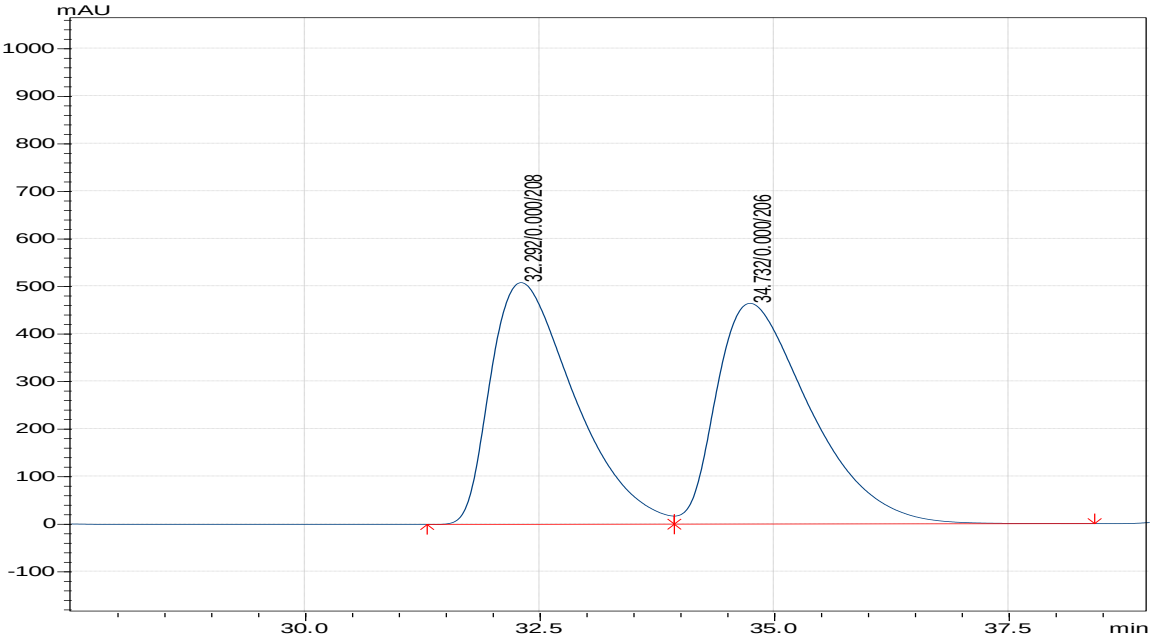


Ret. Time	Area	Peak Start	Peak End	Area%
21.655	36059168	20.981	22.784	50.5422
23.268	35285457	22.784	25.888	49.4578

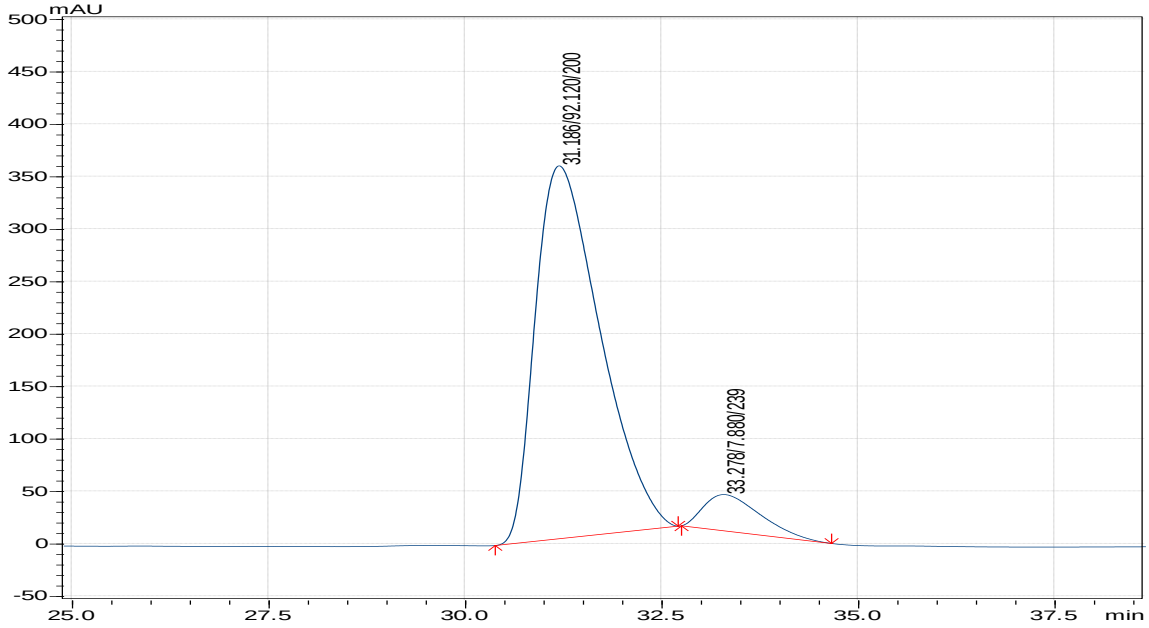


Ret. Time	Area	Peak Start	Peak End	Area%
22.348	69131198	21.685	24.491	91.1735
25.134	6692584	24.501	26.763	8.8265

4-Fluorophenyl methyl sulfoxide

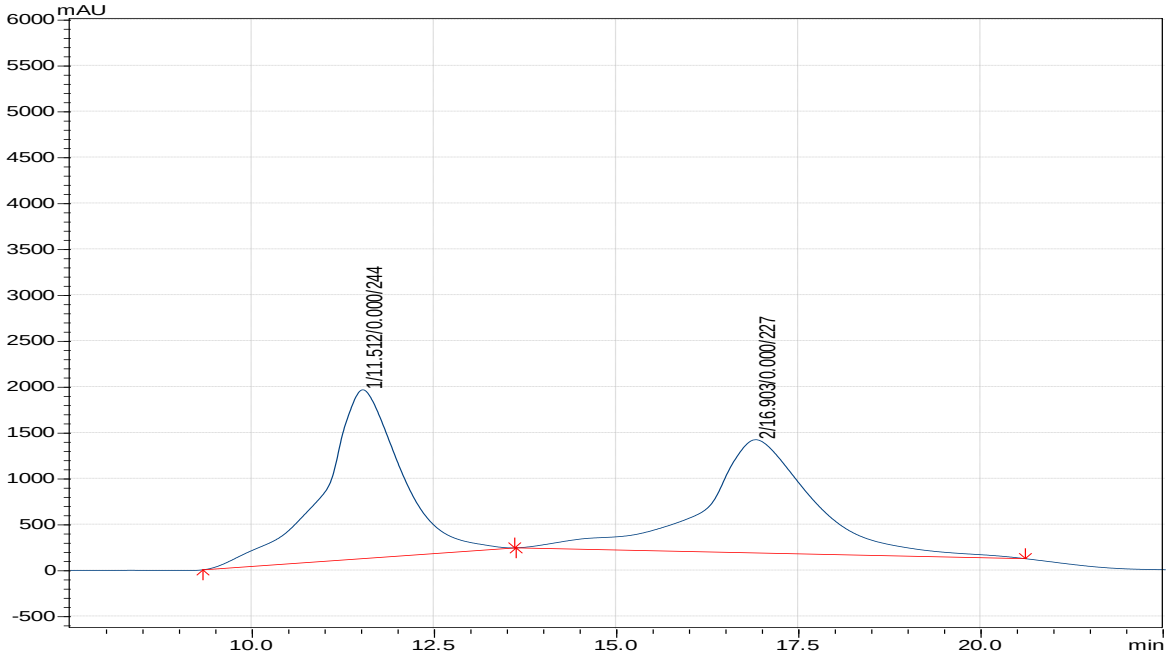


Ret. Time	Area	Peak Start	Peak End	Area%
32.292	31637611	31.296	33.931	49.4862
34.732	32294609	33.931	38.411	50.5138

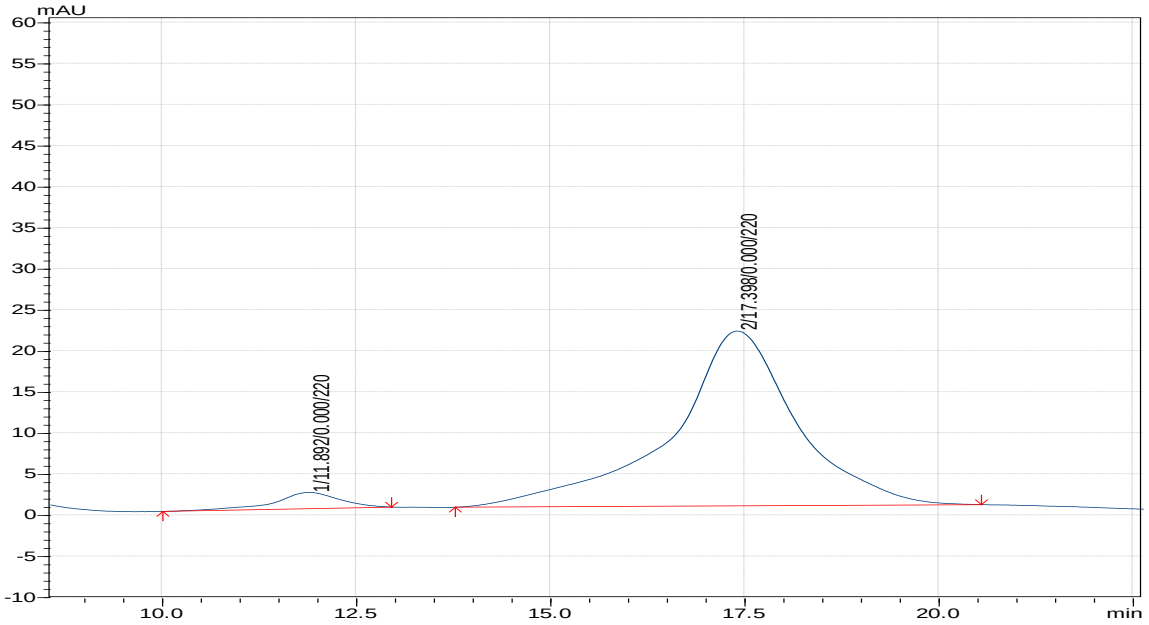


Ret. Time	Area	Peak Start	Peak End	Area%
31.186	20408120	30.379	32.704	92.1199
33.278	1745743	32.747	34.656	7.8801

4-Chlorophenyl methyl sulfoxide

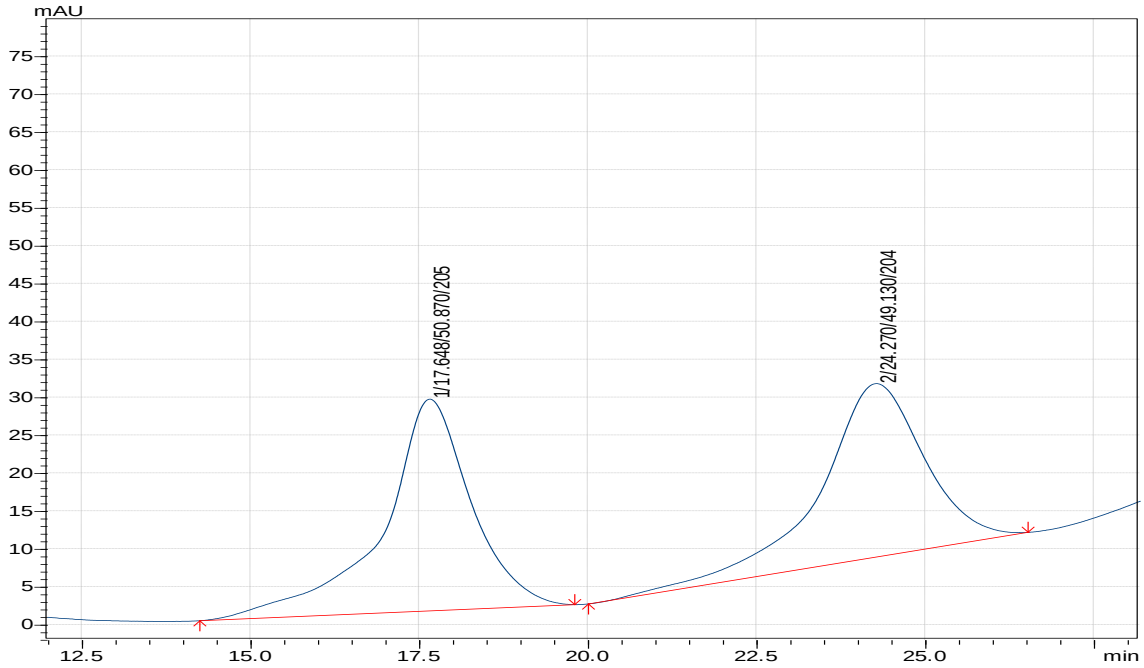


Ret. Time	Area	Peak Start	Peak End	Area%
11.512	137217214	9.323	13.600	51.0558
16.903	131541922	13.621	20.608	48.9442

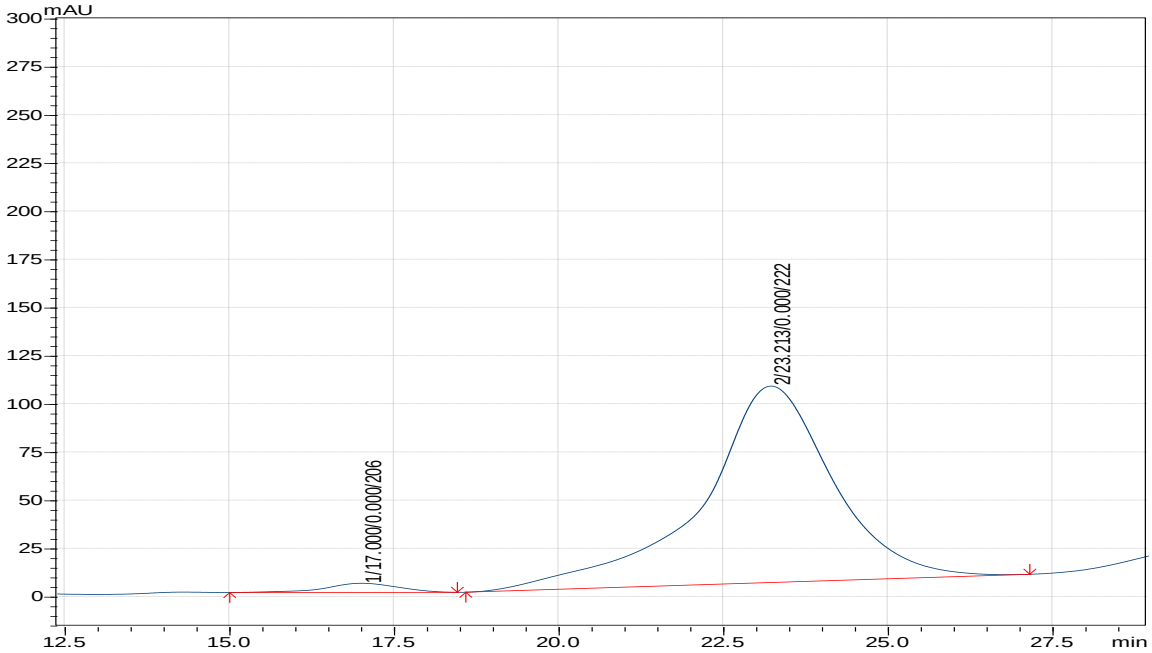


Ret. Time	Area	Peak Start	Peak End	Area%
11.892	115325	10.005	12.949	4.6079
17.398	2387451	13.771	20.544	95.3921

4-Bromophenyl methyl sulfoxide

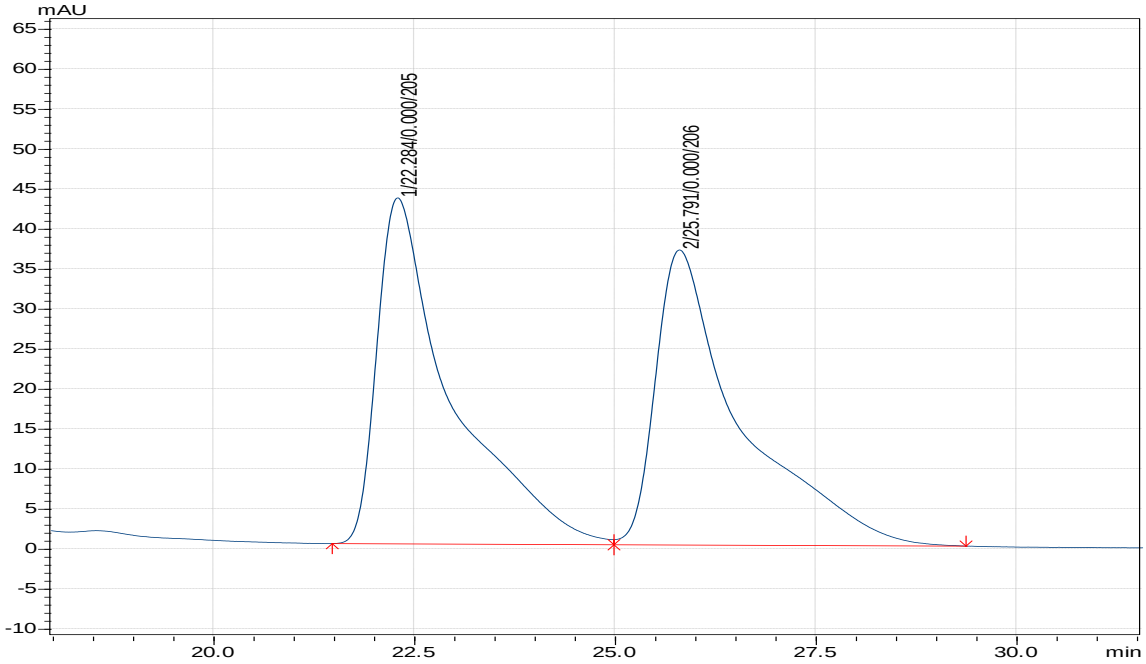


Ret. Time	Area	Peak Start	Peak End	Area%
17.648	2543207	14.240	19.797	50.8699
24.270	2456222	20.000	26.517	49.1301

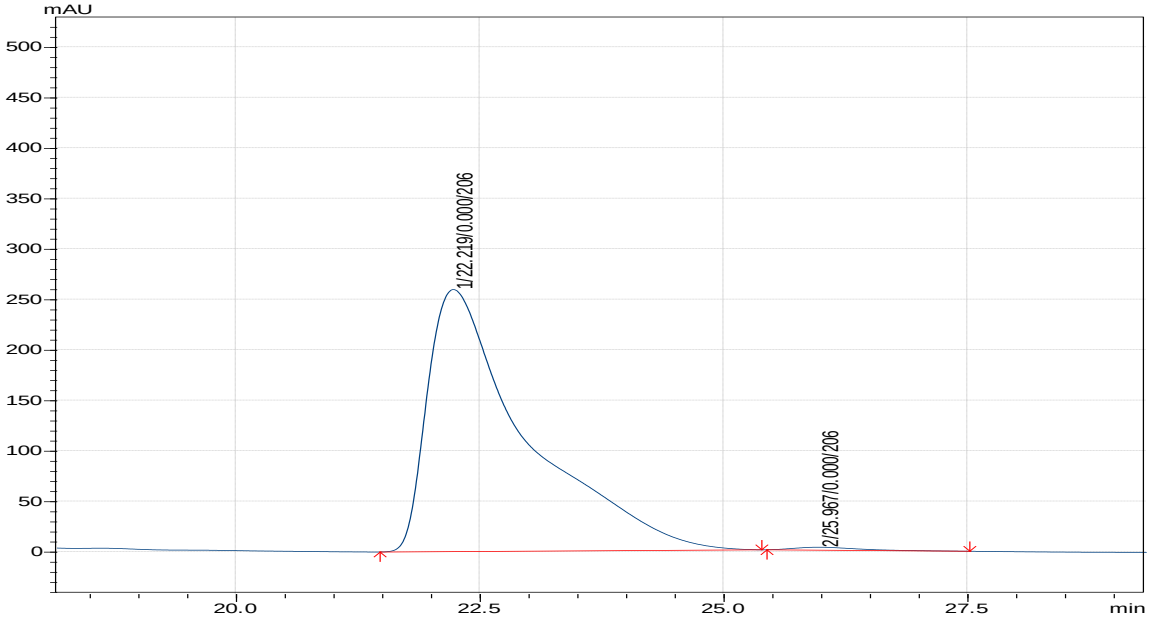


Ret. Time	Area	Peak Start	Peak End	Area%
17.000	364499	14.997	18.453	2.5191
23.213	14104768	18.581	27.147	97.4809

4-Nitrophenyl methyl sulfoxide

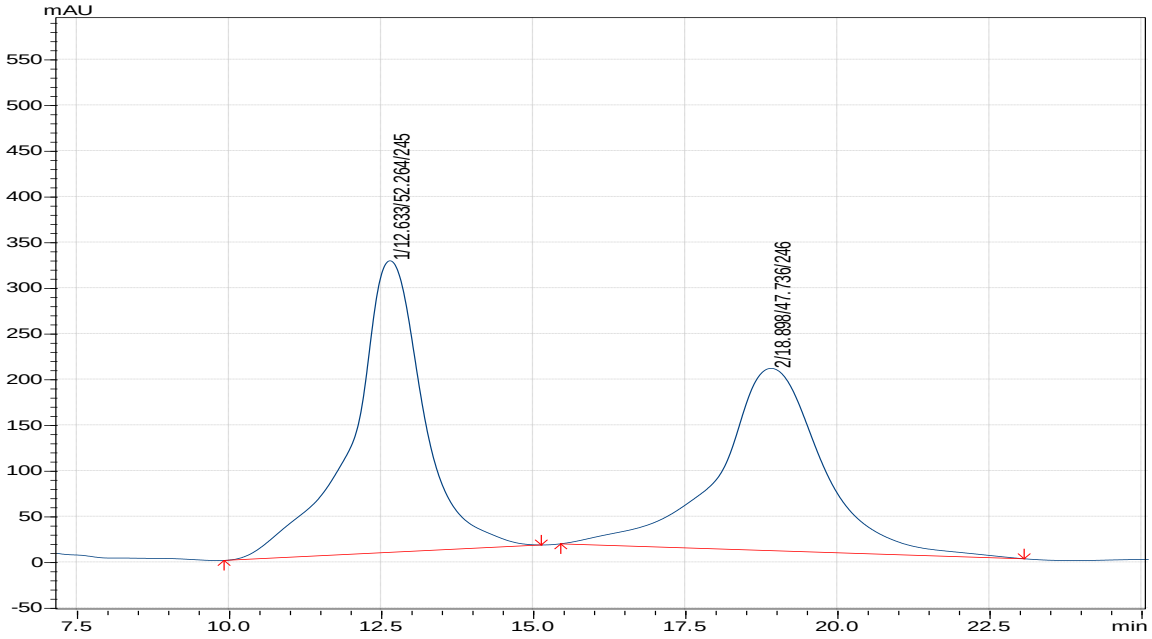


Ret. Time	Area	Peak Start	Peak End	Area%
22.284	2792446	21.472	24.981	50.7877
25.791	2705822	24.981	29.365	49.2123

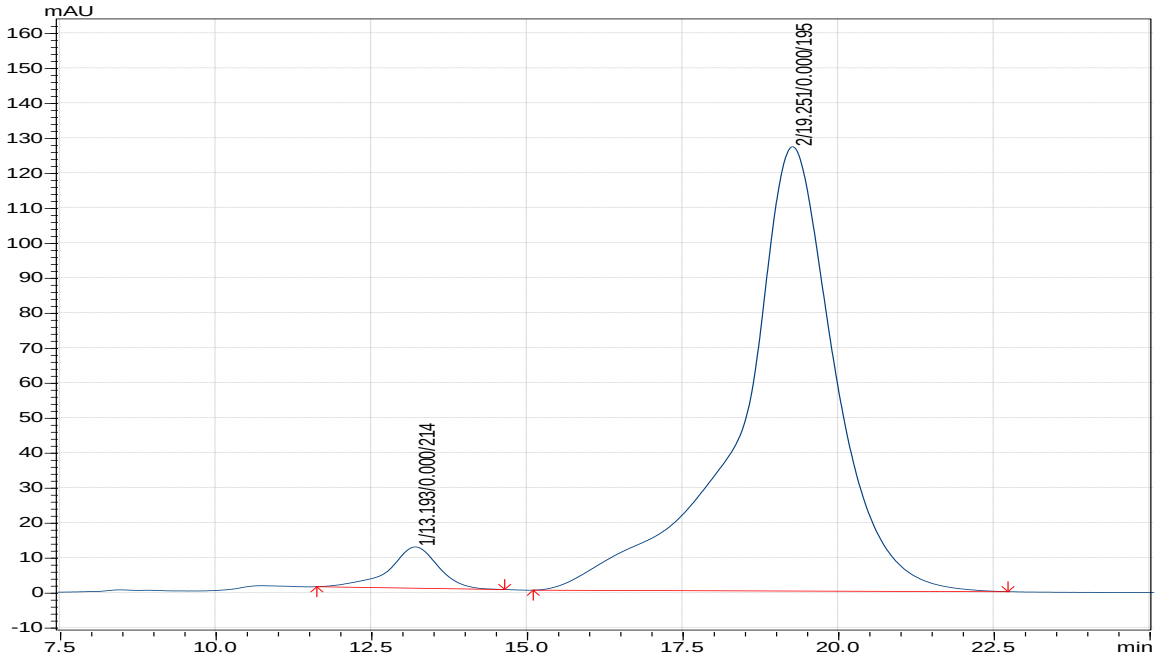


Ret. Time	Area	Peak Start	Peak End	Area%
22.219	18248354	21.472	25.387	99.2883
25.967	130800	25.440	27.520	0.7117

3-Chlorophenyl methyl sulfoxide

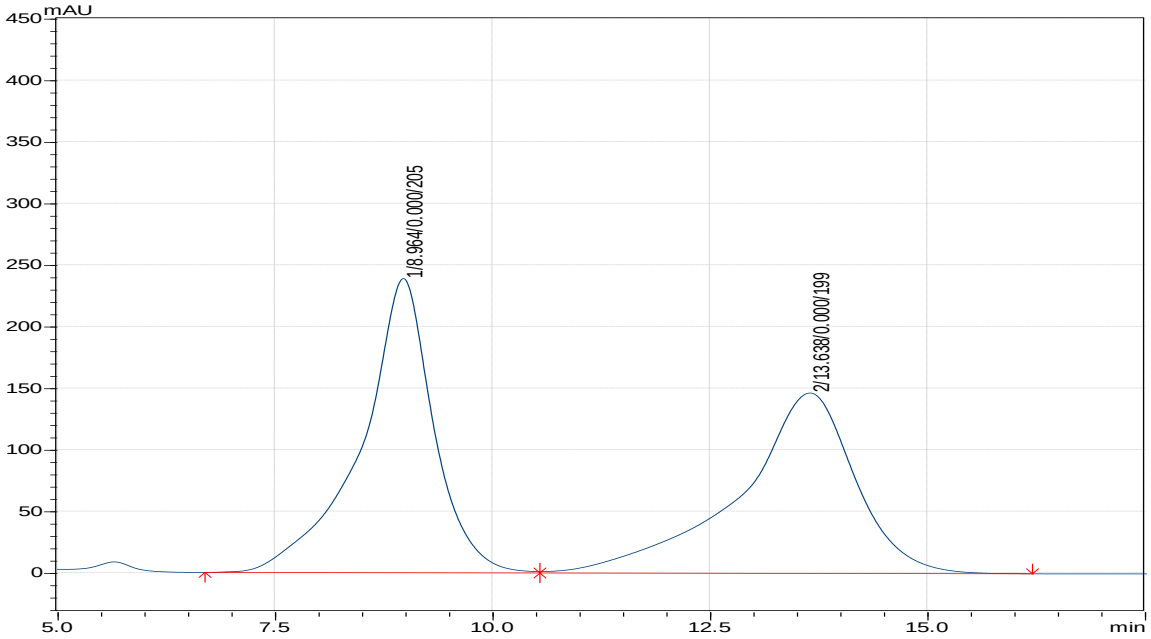


Ret. Time	Area	Peak Start	Peak End	Area%
12.633	26021813	9.909	15.125	52.2636
18.898	23767762	15.445	23.061	47.7364

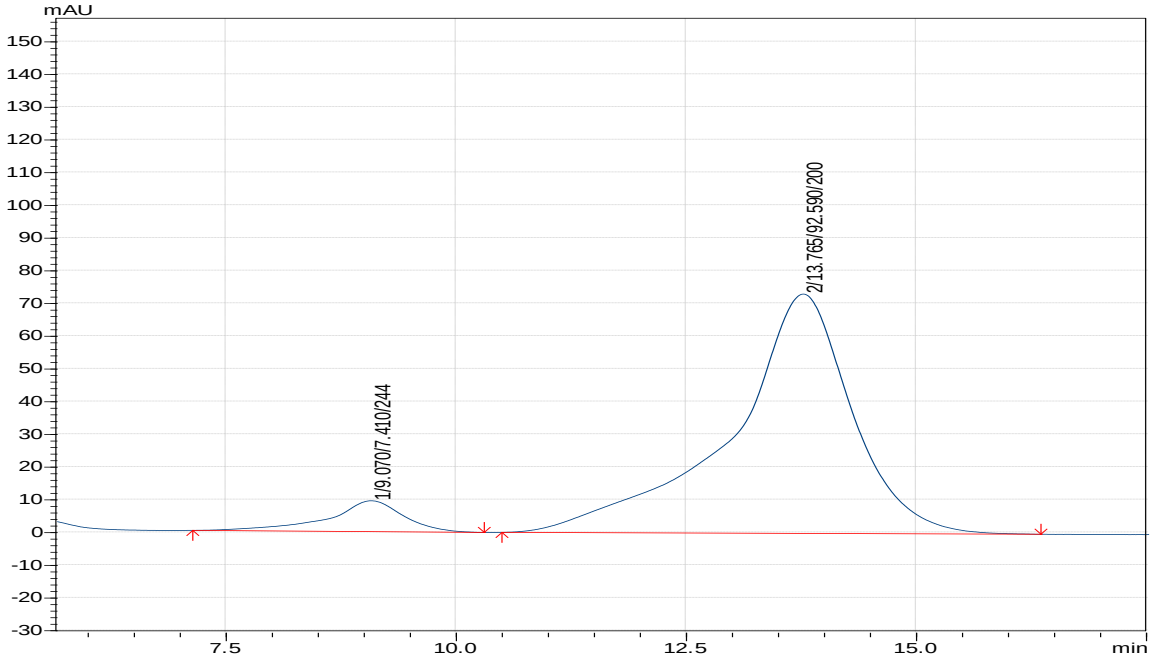


Ret. Time	Area	Peak Start	Peak End	Area%
13.193	647804	11.616	14.635	4.5745
19.251	13513369	15.093	22.720	95.4255

3-Bromophenyl methyl sulfoxide

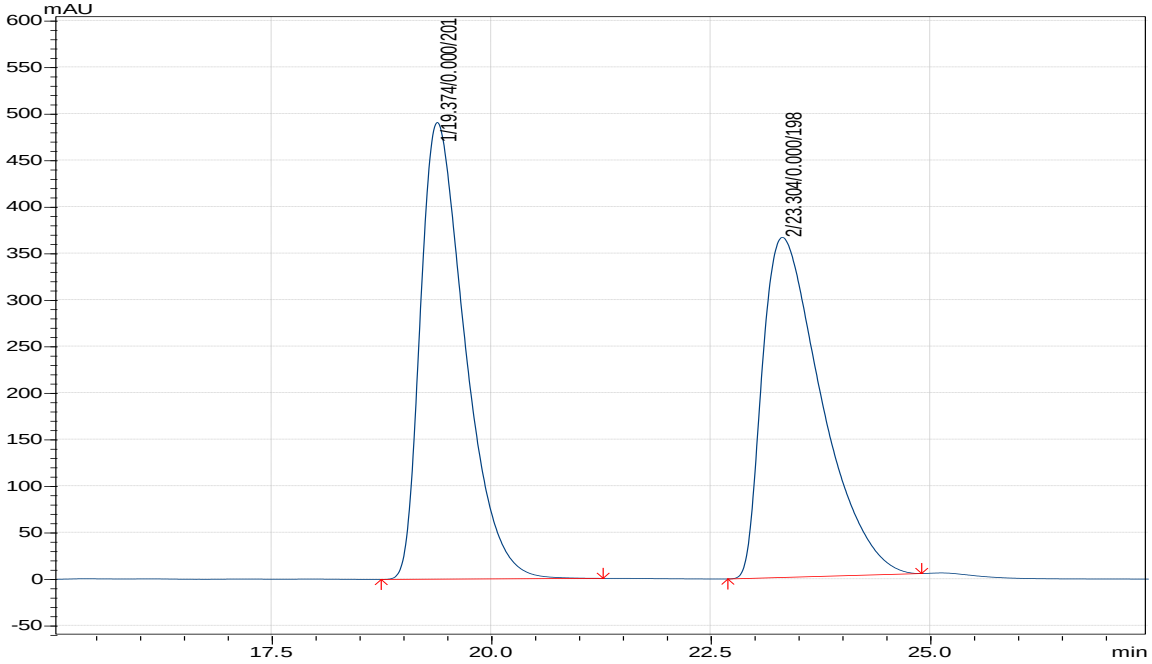


Ret. Time	Area	Peak Start	Peak End	Area%
8.964	13780885	6.688	10.539	50.4502
13.638	13534941	10.539	16.203	49.5498

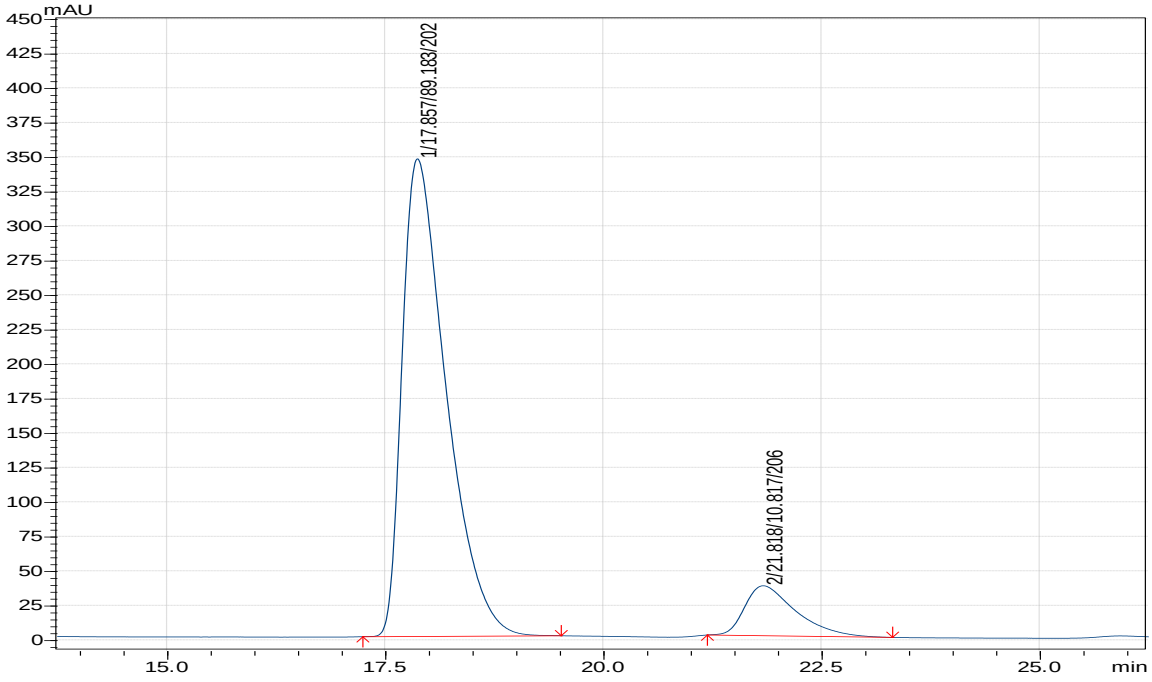


Ret. Time	Area	Peak Start	Peak End	Area%
9.070	533372	7.136	10.304	7.4104
13.765	6664206	10.496	16.352	92.5896

Ethyl phenyl sulfoxide

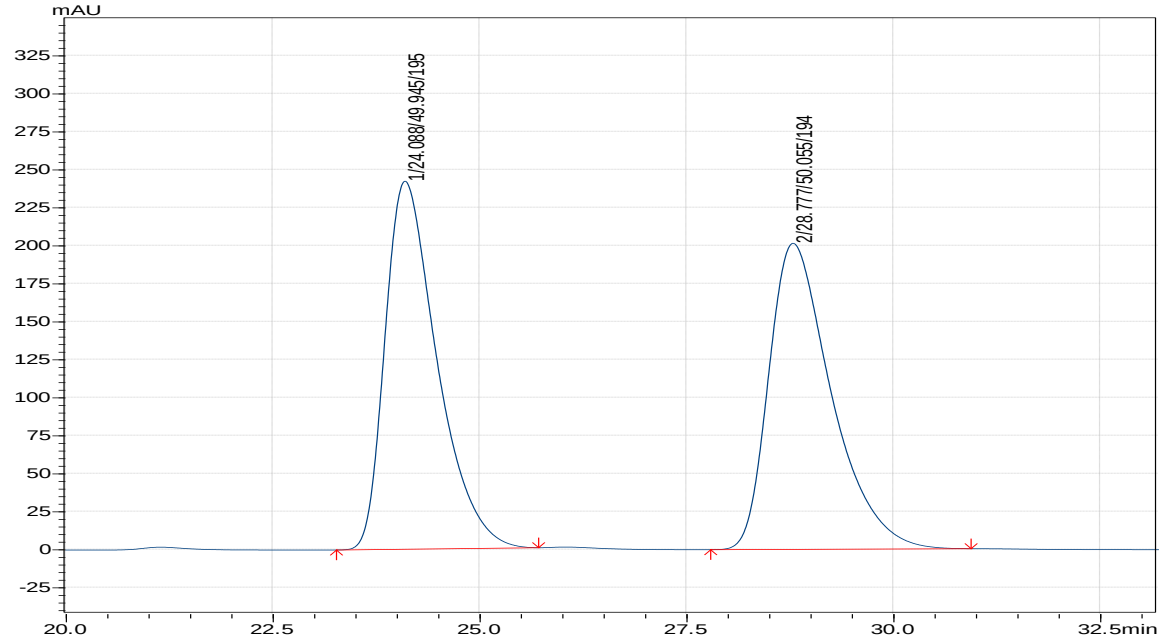


Ret. Time	Area	Peak Start	Peak End	Area%
19.374	17333087	18.741	21.269	50.3180
23.304	17114006	22.688	24.896	49.6820

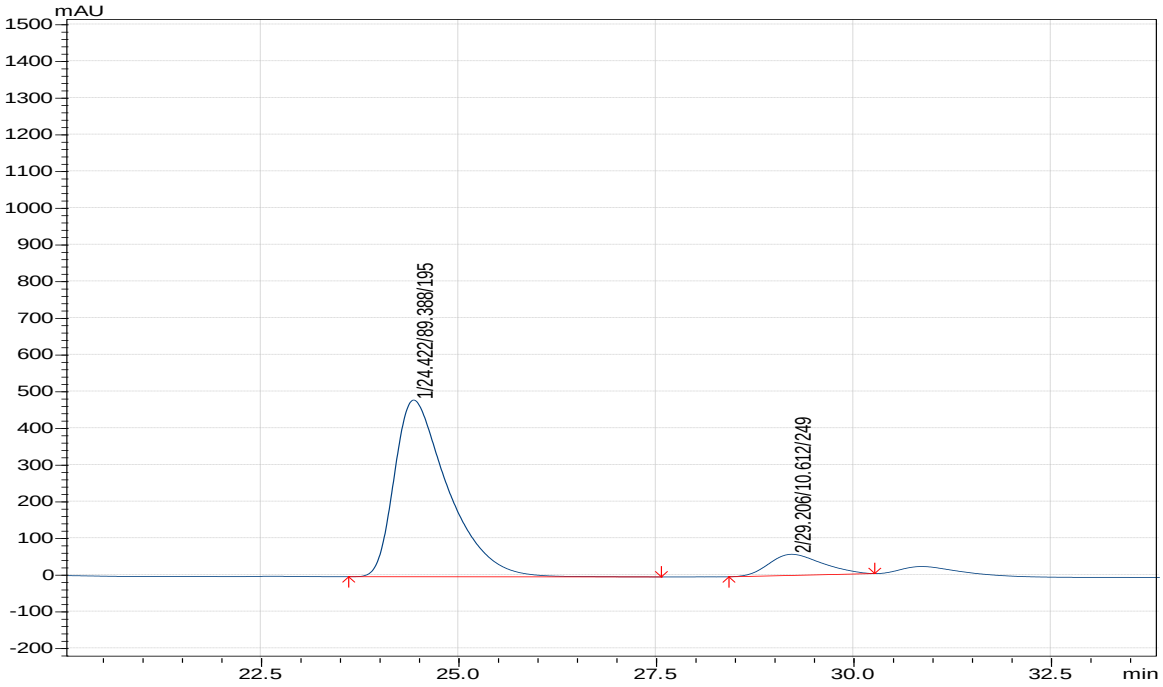


Ret. Time	Area	Peak Start	Peak End	Area%
17.857	12123714	17.237	19.509	89.1831
21.818	1470476	21.184	23.307	10.8169

Benzyl phenyl sulfoxide

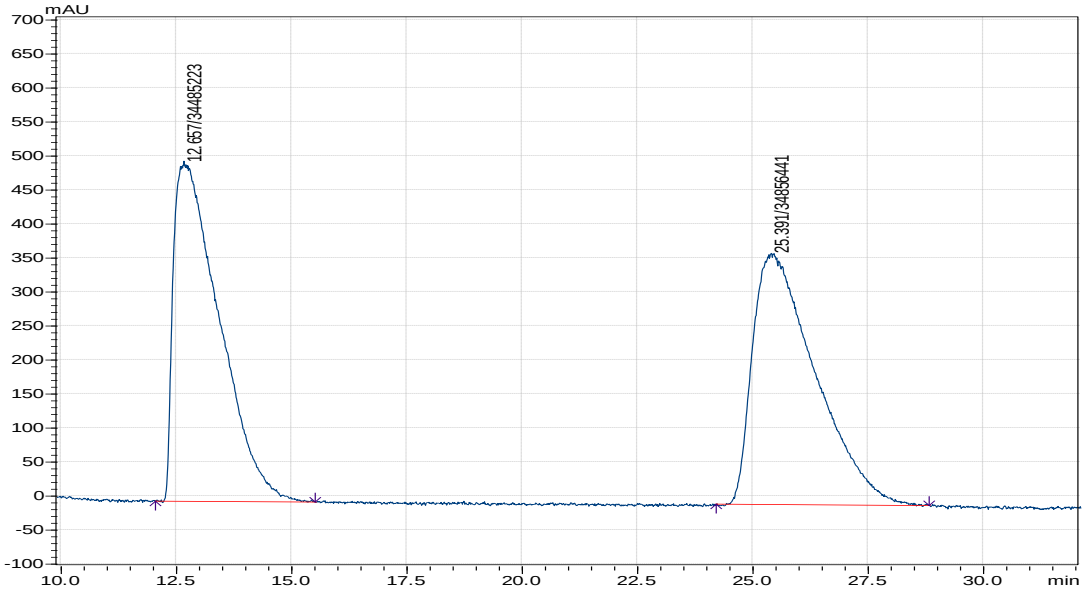


Ret. Time	Area	Peak Start	Peak End	Area%
24.088	10564866	23.264	25.707	49.9445
28.777	10588329	27.787	30.933	50.0555

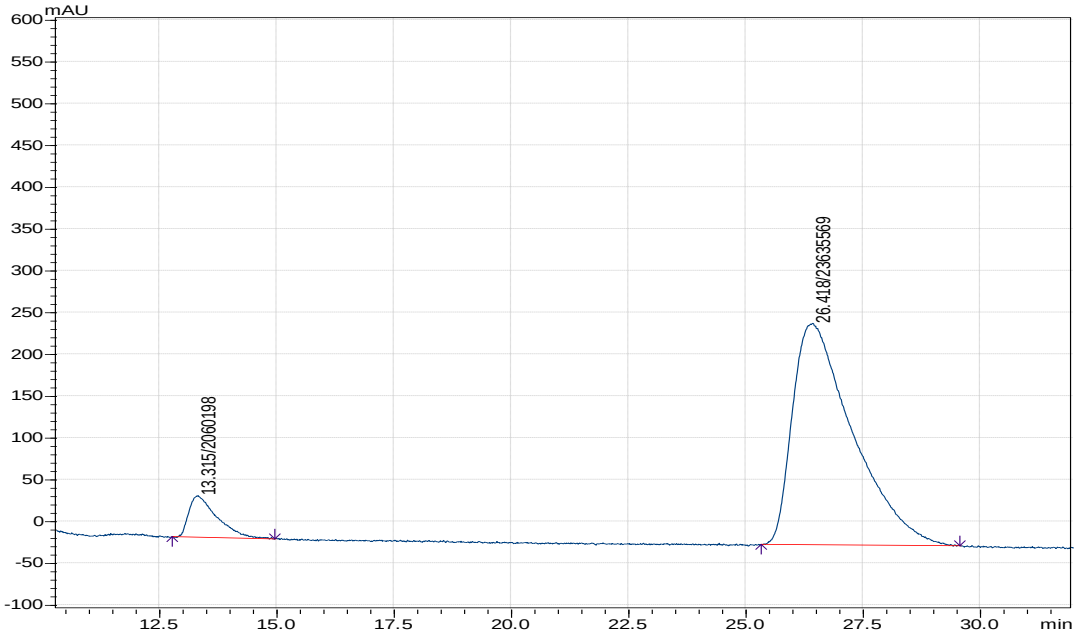


Ret. Time	Area	Peak Start	Peak End	Area%
24.422	22748110	23.605	27.563	89.3881
29.206	2700577	28.416	30.261	10.6119

(+)-trans-(1*S*,2*S*)-2-Phenyl-1,3-dithiane 1-oxide

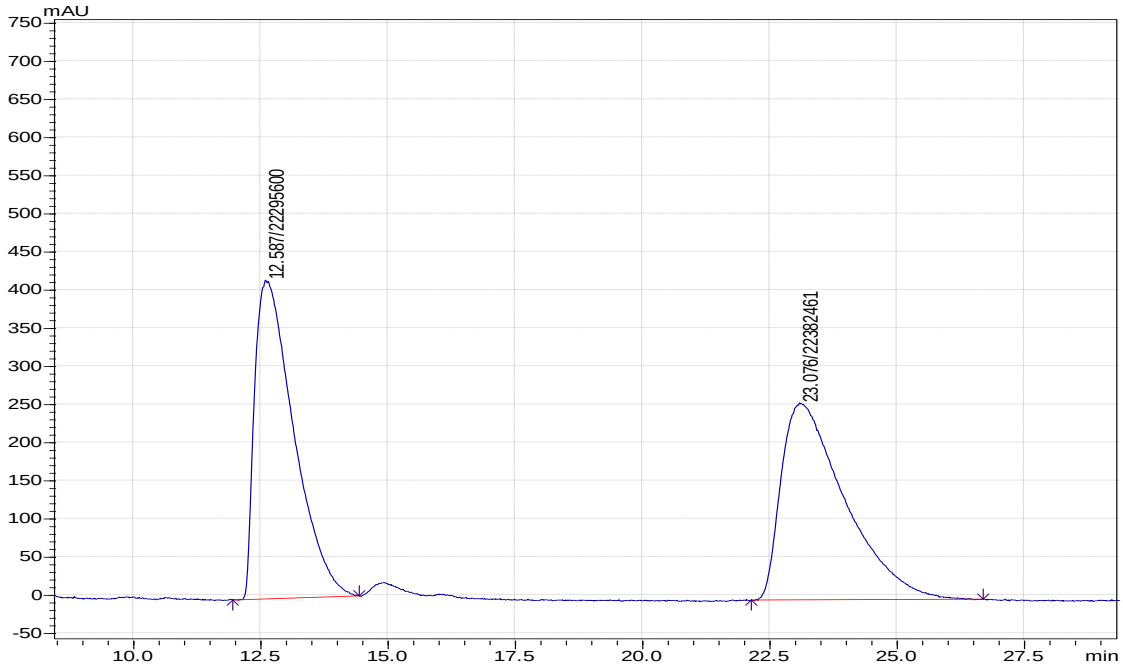


Ret. Time	Area	Peak Start	Peak End	Area%
12.657	34485223	12.043	15.509	49.7323
25.391	34856441	24.203	28.821	50.2677

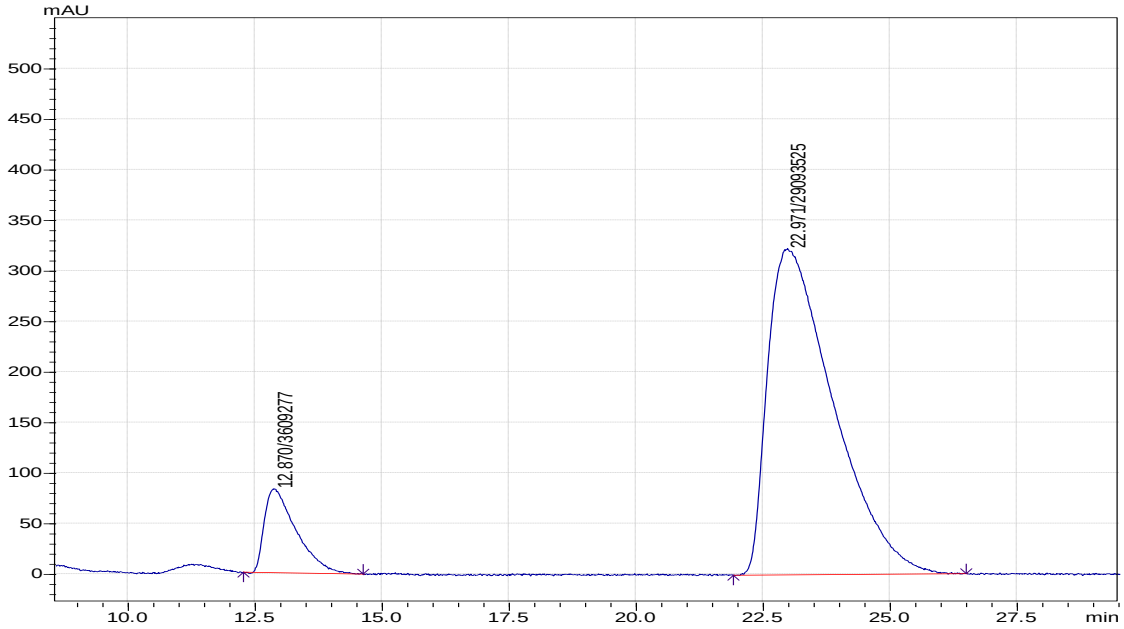


Ret. Time	Area	Peak Start	Peak End	Area%
13.315	2060198	12.768	14.955	8.0177
26.418	23635569	25.323	29.557	91.9823

(+)-trans-2-(4-Methylphenyl)-1,3-dithiane 1-oxide

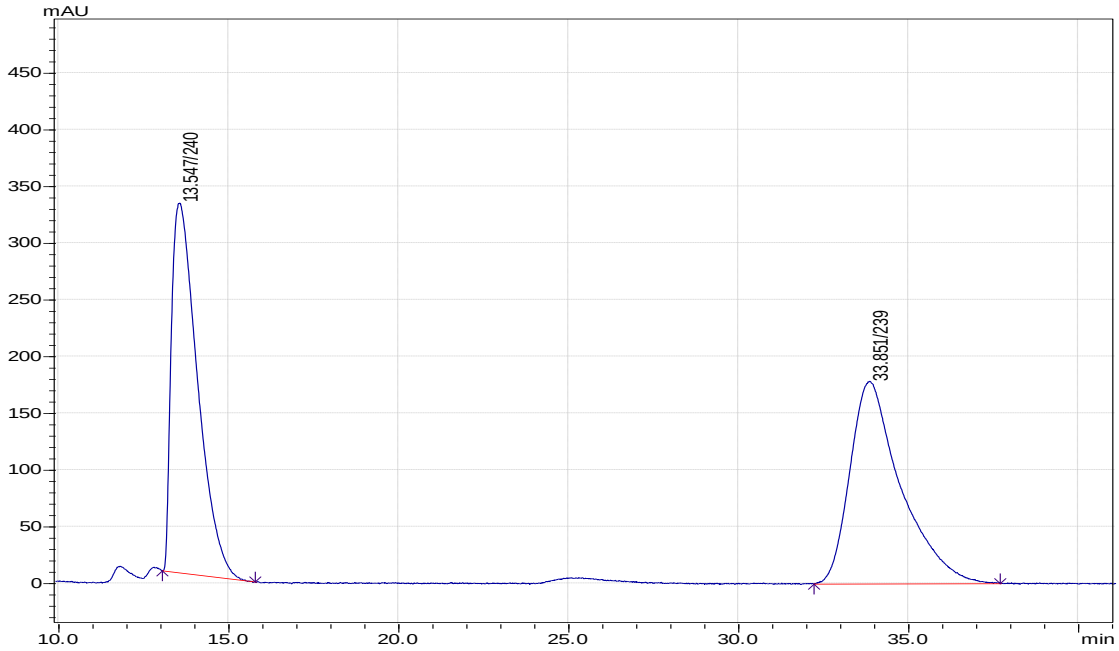


Ret. Time	Area	Peak Start	Peak End	Area%
12.587	22295600	11.947	14.432	49.9028
23.076	22382461	22.133	26.688	50.0972

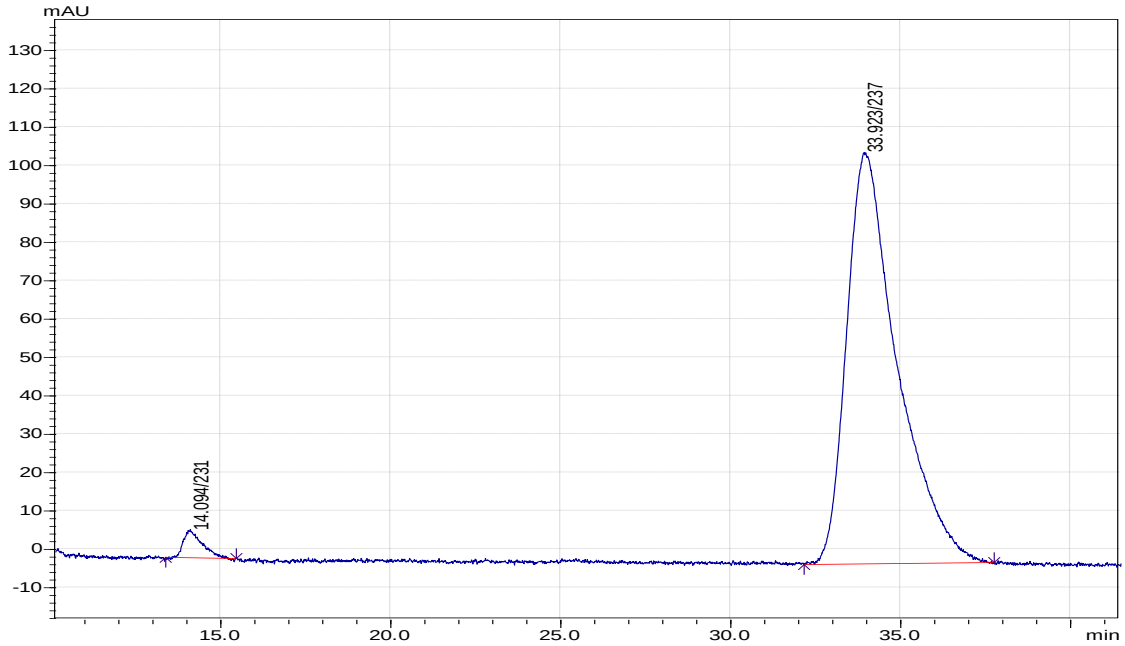


Ret. Time	Area	Peak Start	Peak End	Area%
12.870	3609277	12.267	14.624	11.0366
22.971	29093525	21.909	26.496	88.9634

(+)-trans-2-(4-Chlorophenyl)-1,3-dithiane 1-Oxide

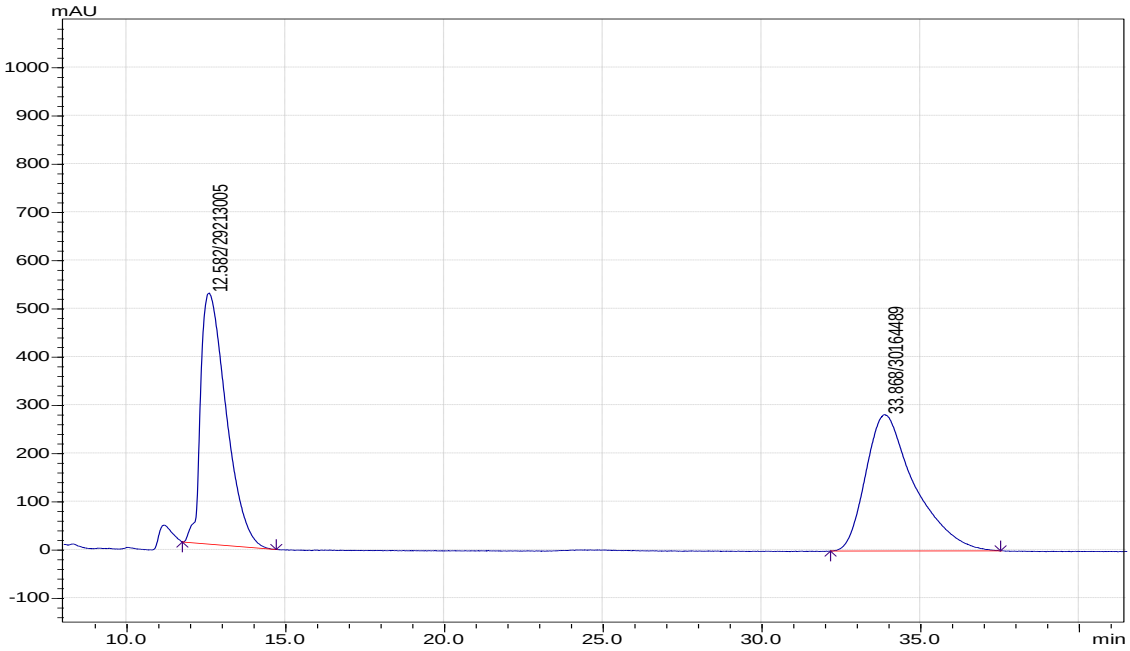


Ret. Time	Area	Peak Start	Peak End	Area%
13.547	17428268	13.045	15.776	48.3763
33.851	18598214	32.213	37.696	51.6237

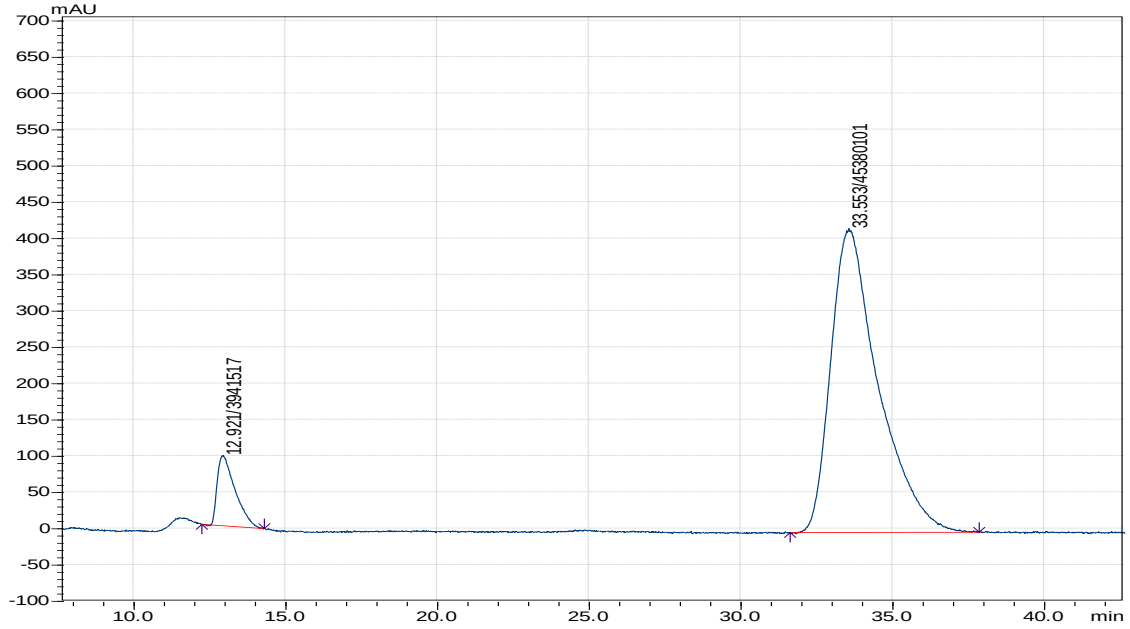


Ret. Time	Area	Peak Start	Peak End	Area%
14.094	269884	13.376	15.456	2.3737
33.923	11100093	32.160	37.749	97.6263

(+)-trans-2-(2-Fluorophenyl)-1,3-dithiane 1-oxide



Ret. Time	Area	Peak Start	Peak End	Area%
12.582	29213005	11.744	14.699	49.1988
33.868	30164489	32.160	37.515	50.8012



Ret. Time	Area	Peak Start	Peak End	Area%
12.921	3941517	12.235	14.293	7.9915
33.553	45380101	31.616	37.845	92.0085

5. Notes and references

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2 J. Sun, C. Zhu, Z. Dai, M. Yang, Y. Pan, H. Hu, *J. Org. Chem*. 2004, **69**, 8500-8503.

3 S. Liaoa, B. List, *Adv. Synth. Catal*., 2012, **354**, 2363-2367.

4 T. Yamaguchi, K. Matsumoto, B. Saito, T. Katsuki, *Angew. Chem. Int. Ed*., 2007, **46**, 4729-4731.

5 Z. M. Liu, H. Zhao, M. Q. Li, Y. B. Lan, Q. B. Yao, J. C. Tao and X. W. Wang, *Adv. Synth. Catal*., 2012, **354**, 1012-1022.