

Supplementary material for the article:

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Supplementary Material - II

Benzothiazole carbamates and amides as antiproliferative species

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[#]Serbian Academy of Sciences and Arts, Knez Mihailova 35, 11158 Belgrade, Serbia

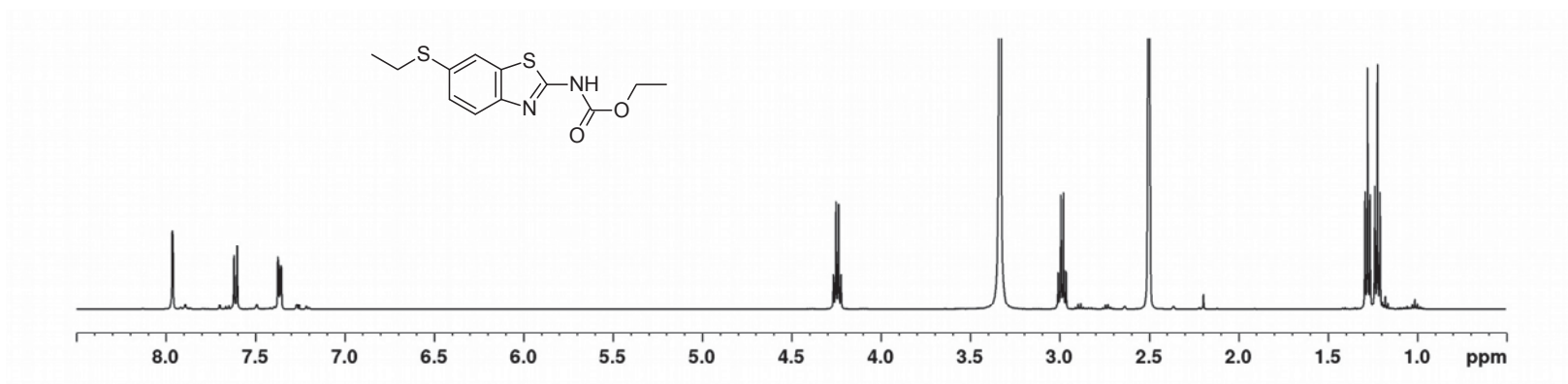
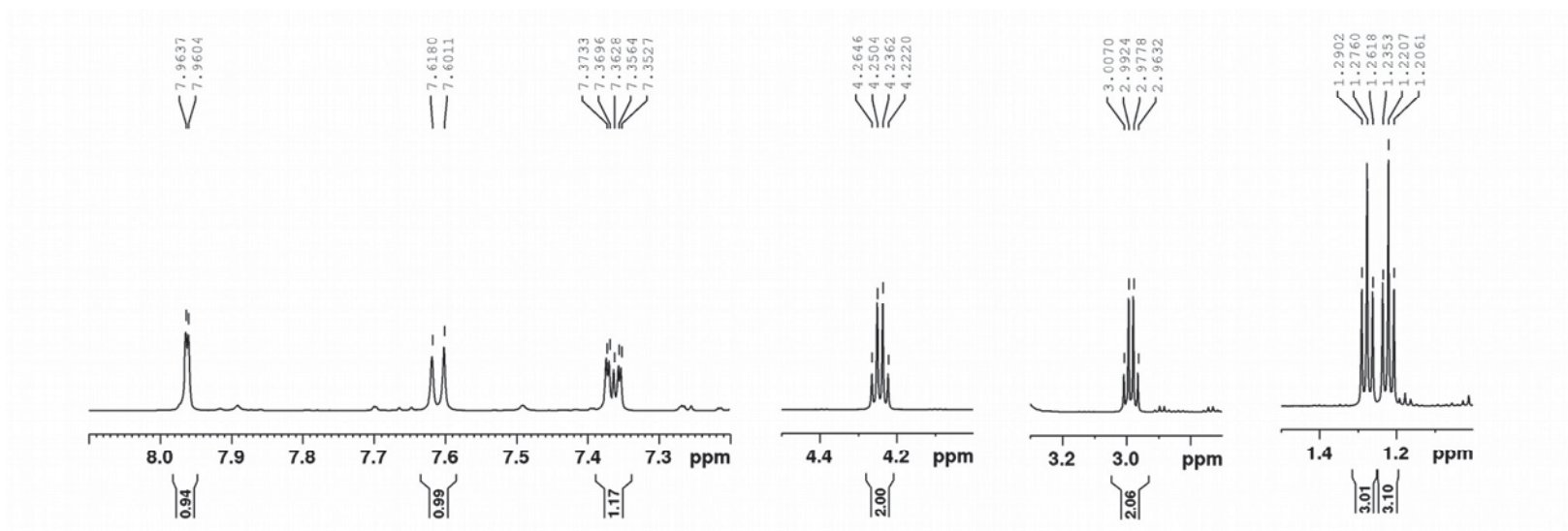
[◇] University of Belgrade – Faculty of Chemistry, Studentski trg 16, P.O. Box 51, 11158 Belgrade, Serbia

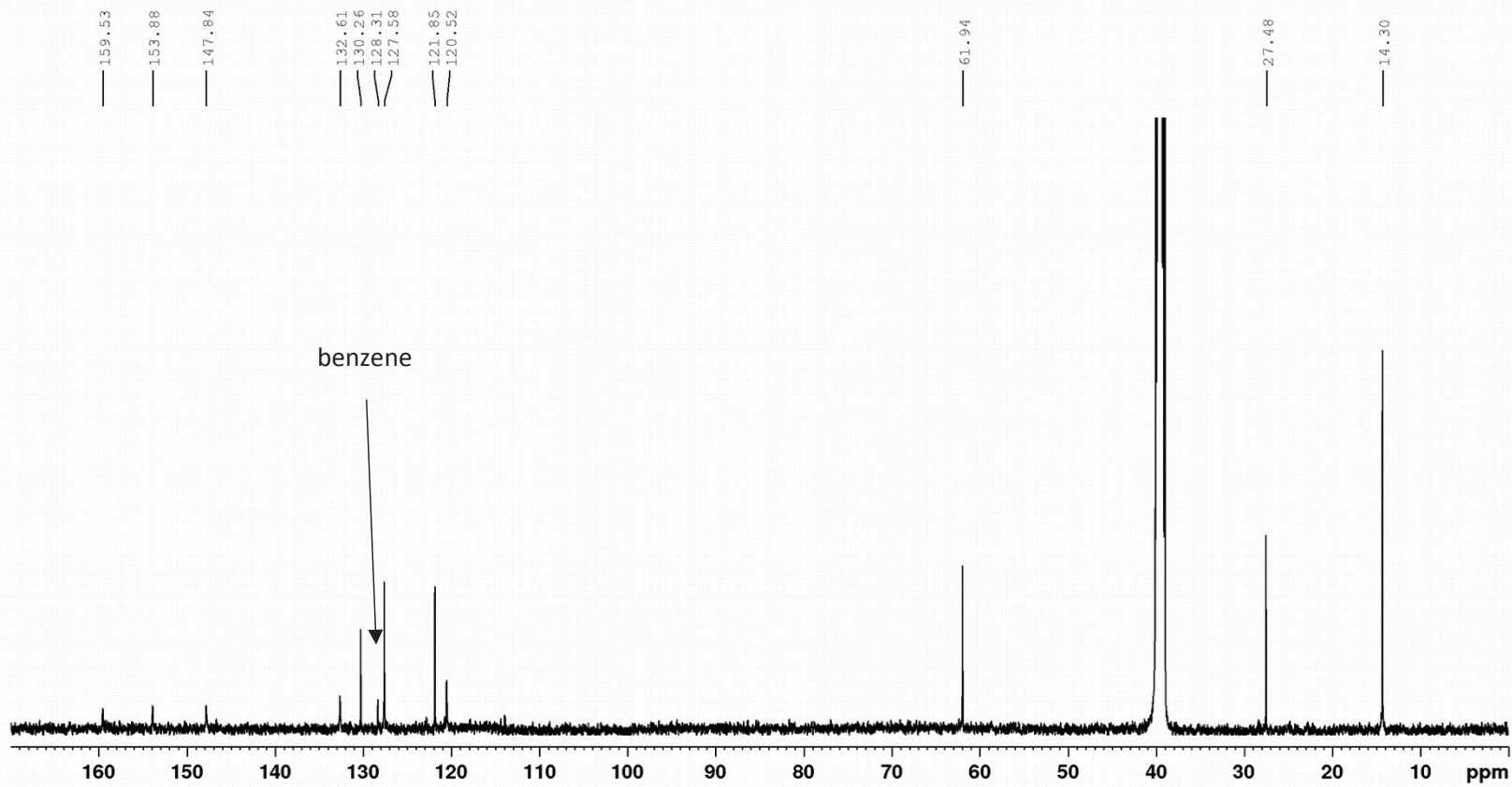
[⊥]Institute for Oncology and Radiology of Serbia, Pasterova 14, 11000 Belgrade, Serbia

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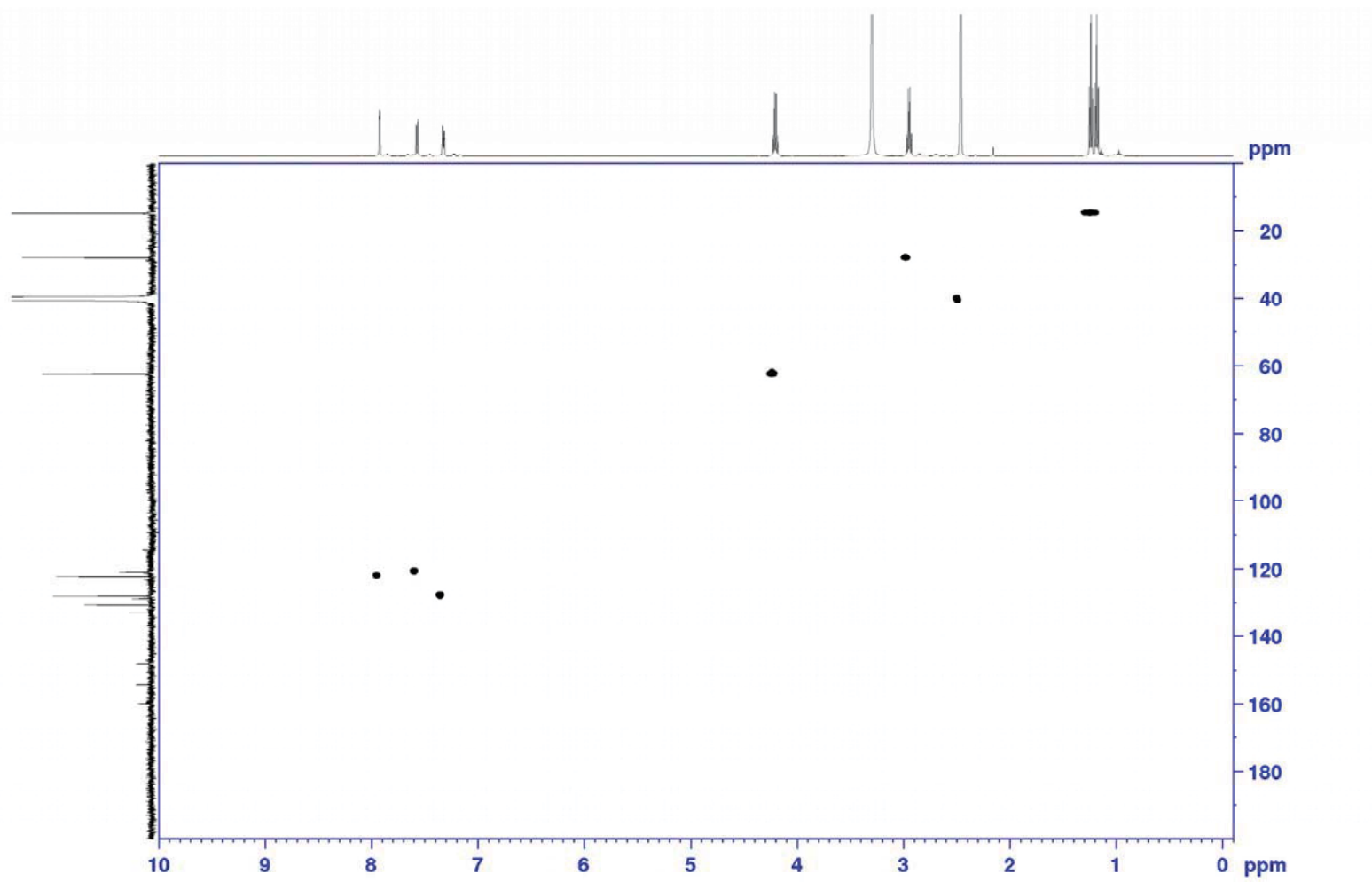
NMR spectra of synthesized compounds	II – S3
HPLC analyses for purity	II – S30

Ethyl [6-(ethylsulfanyl)-1,3-benzothiazol-2-yl]carbamate (24).

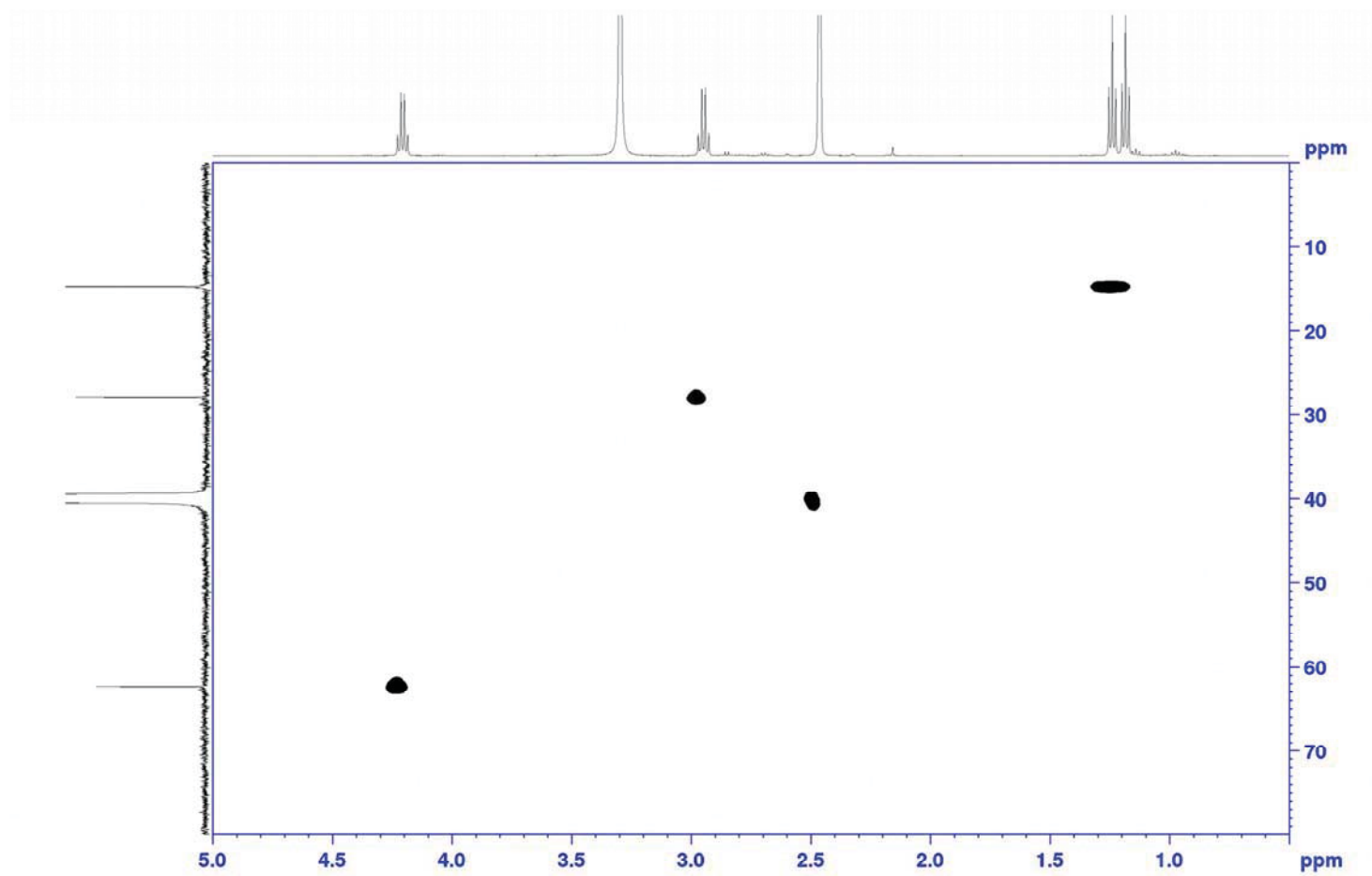




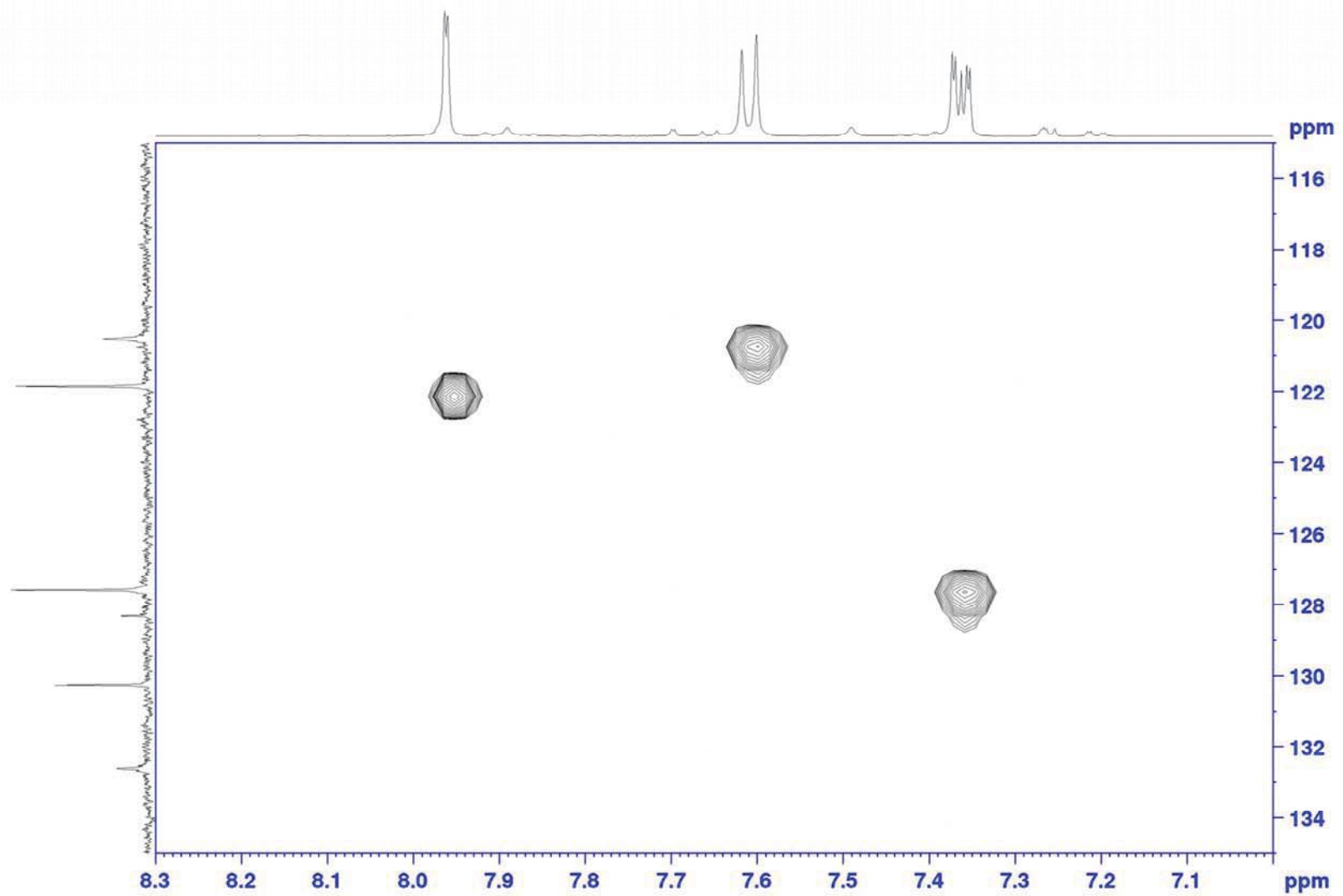
HSQC spectrum



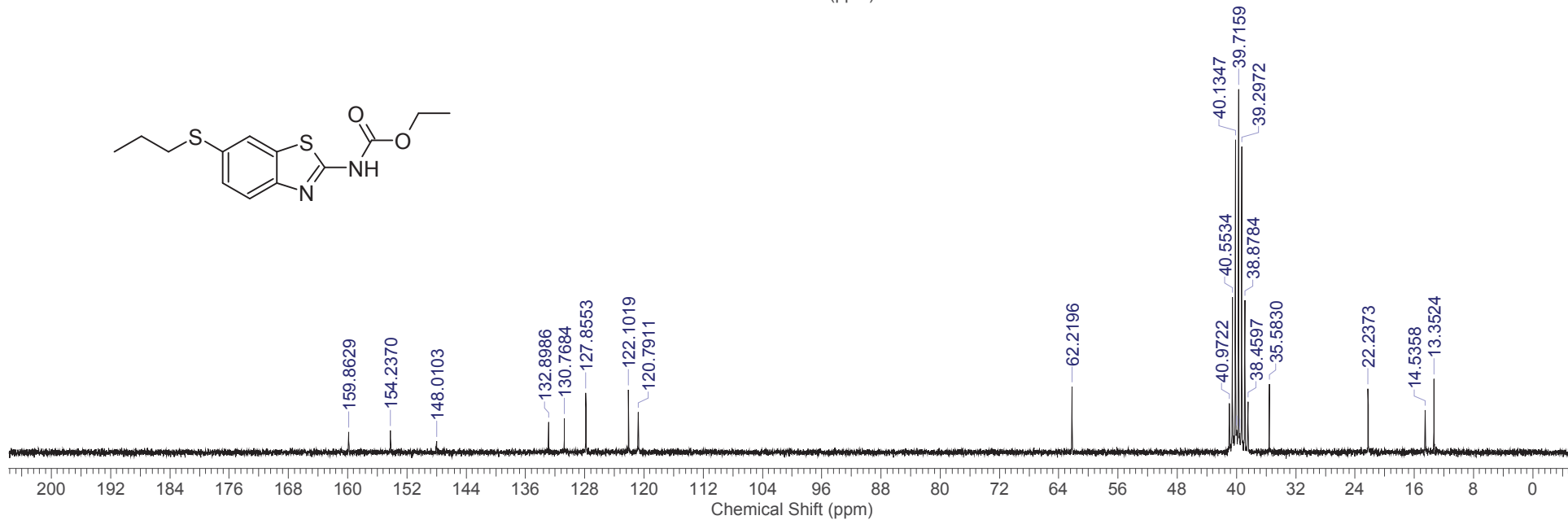
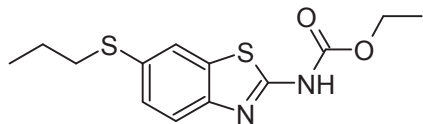
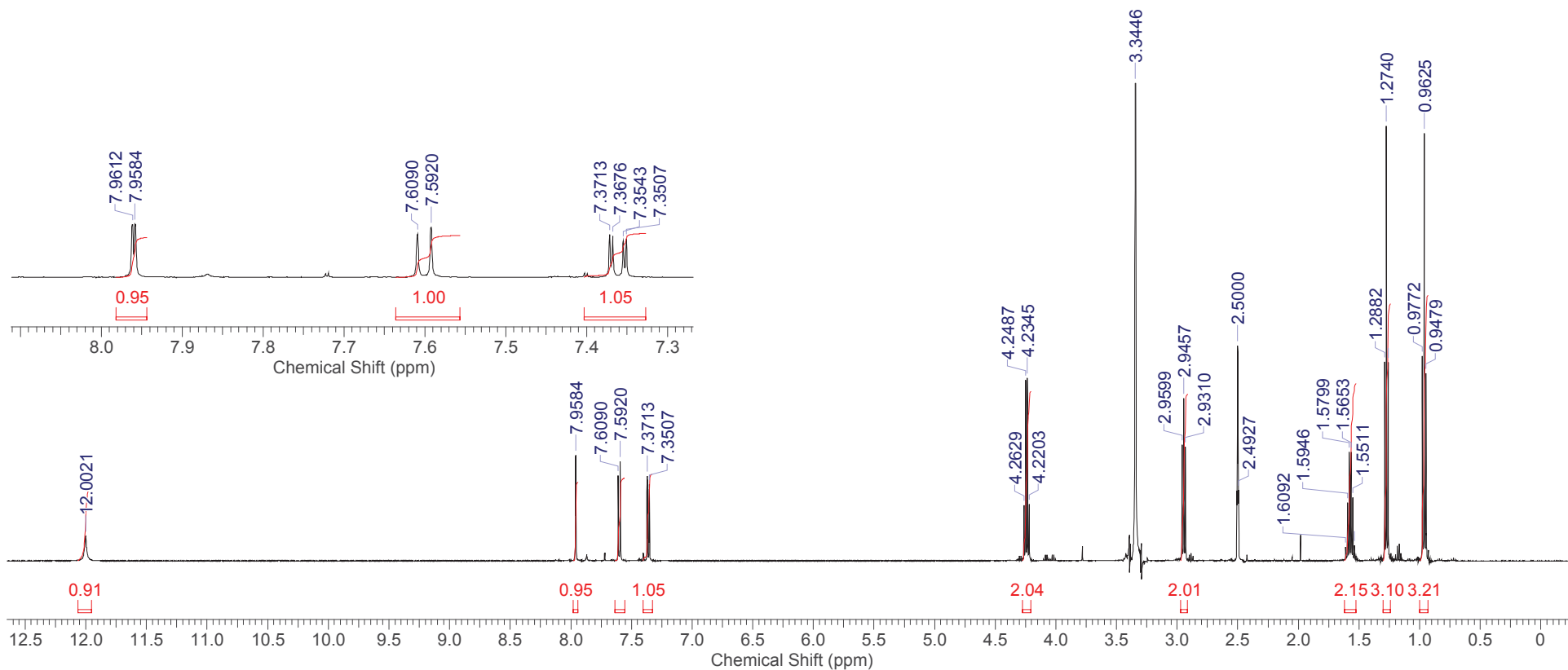
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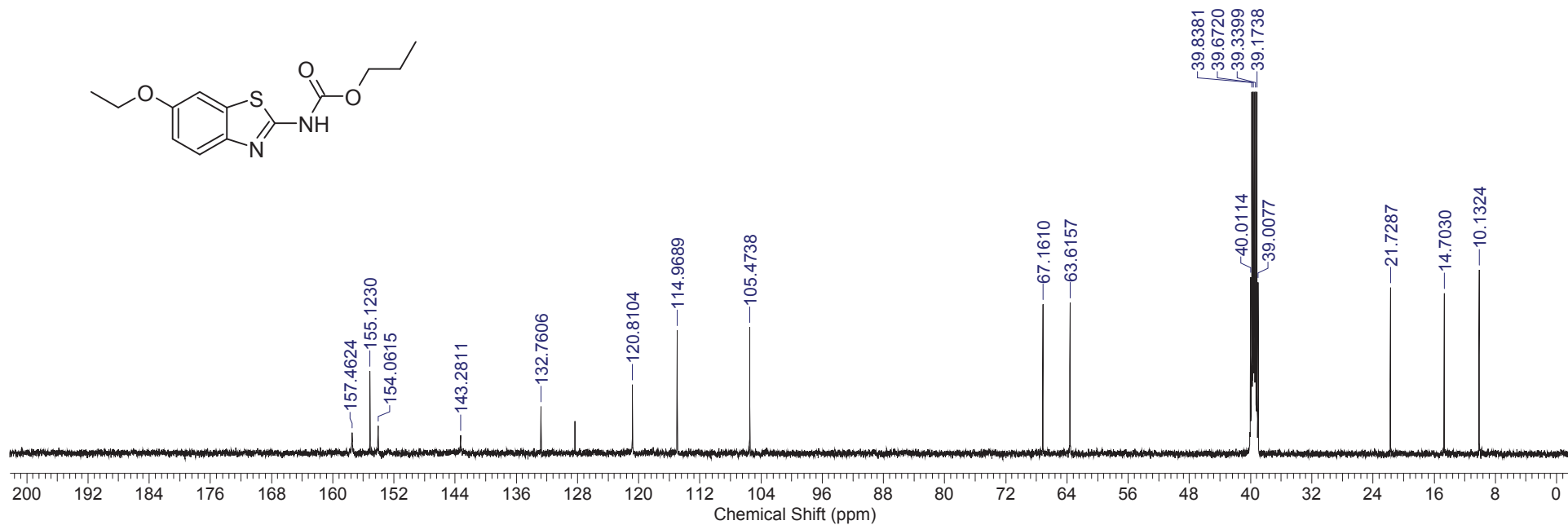
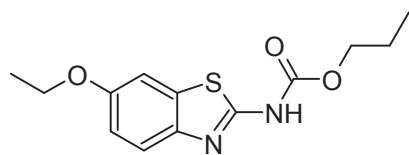
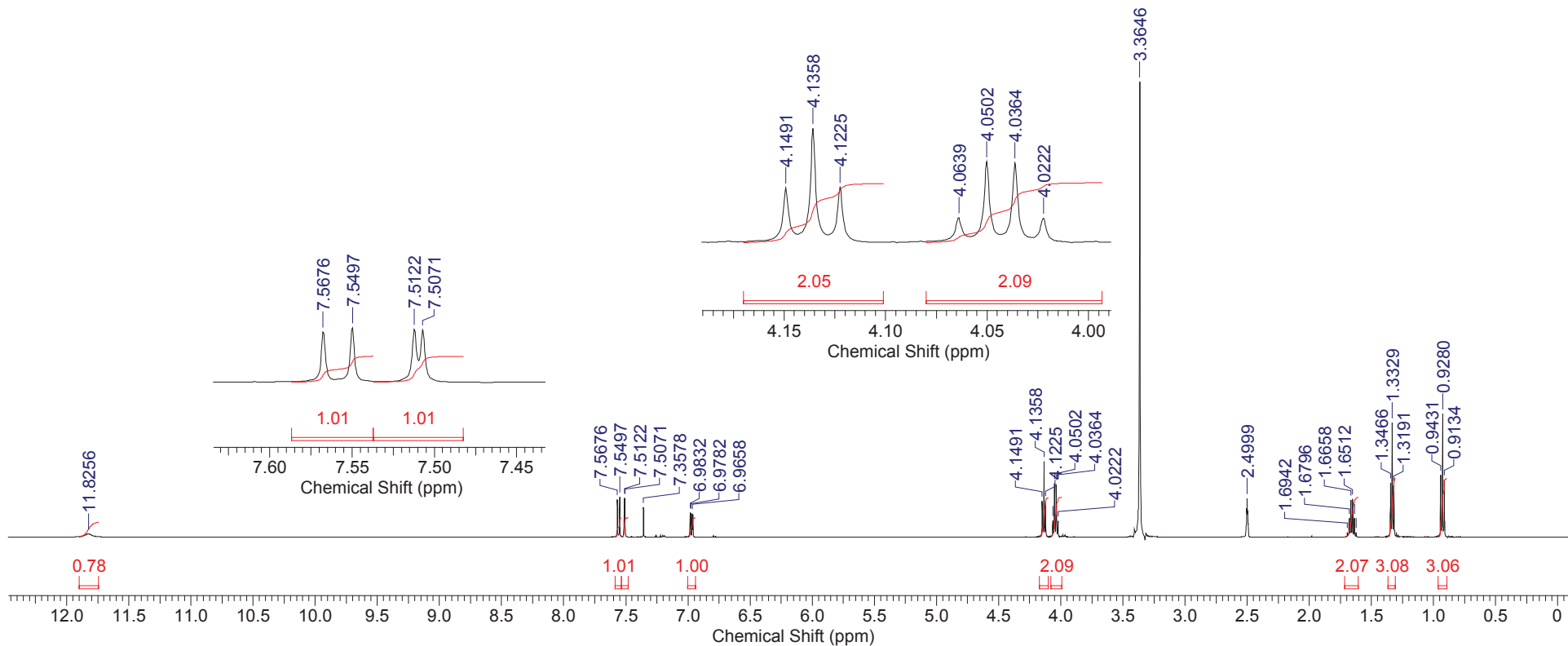
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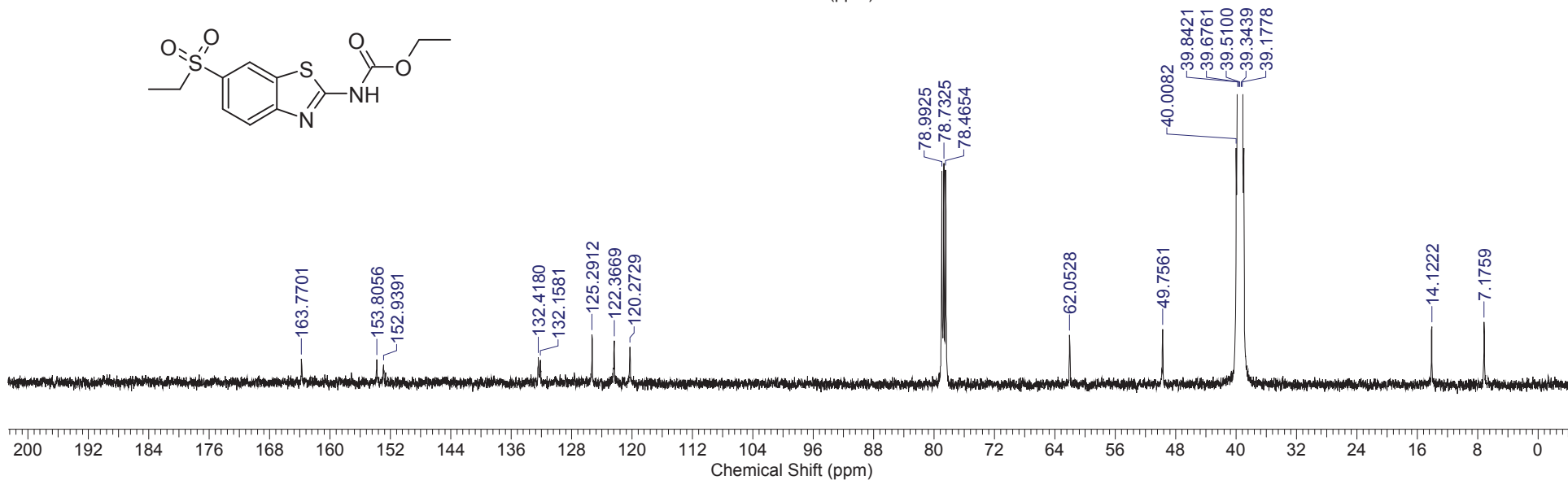
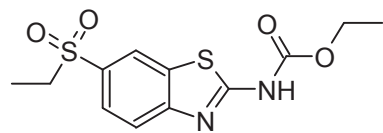
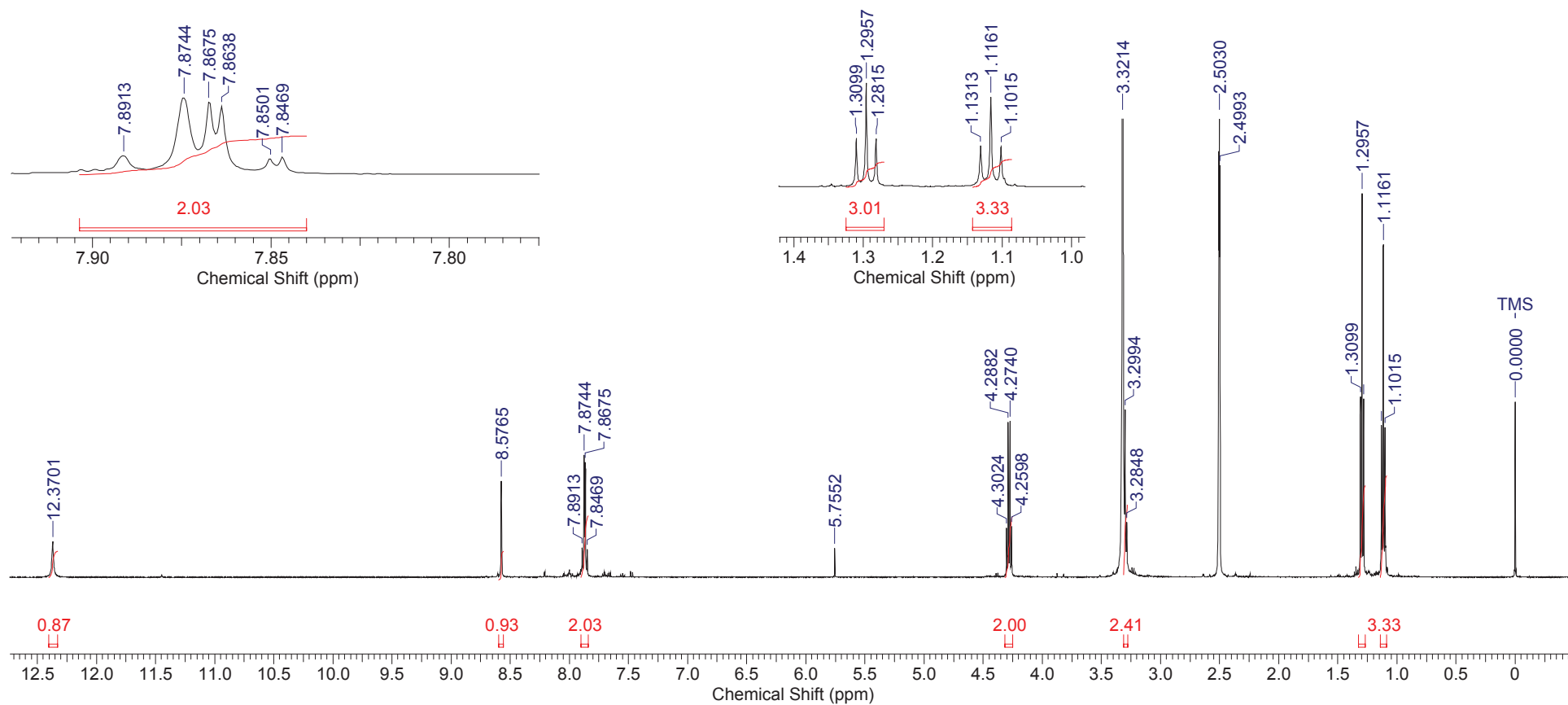
Ethyl [6-(propylsulfanyl)-1,3-benzothiazol-2-yl]carbamate (25)



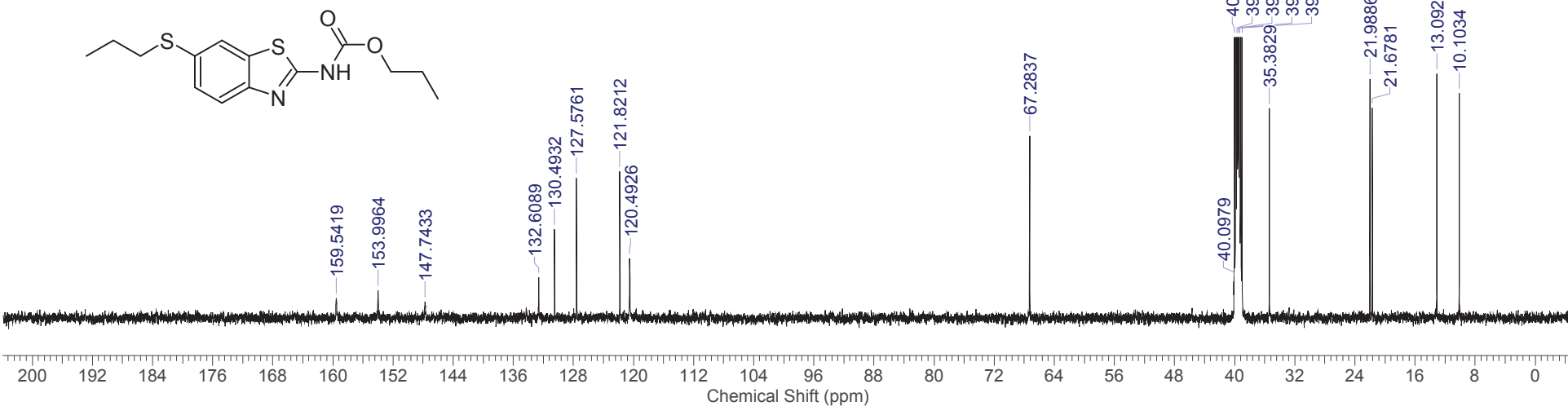
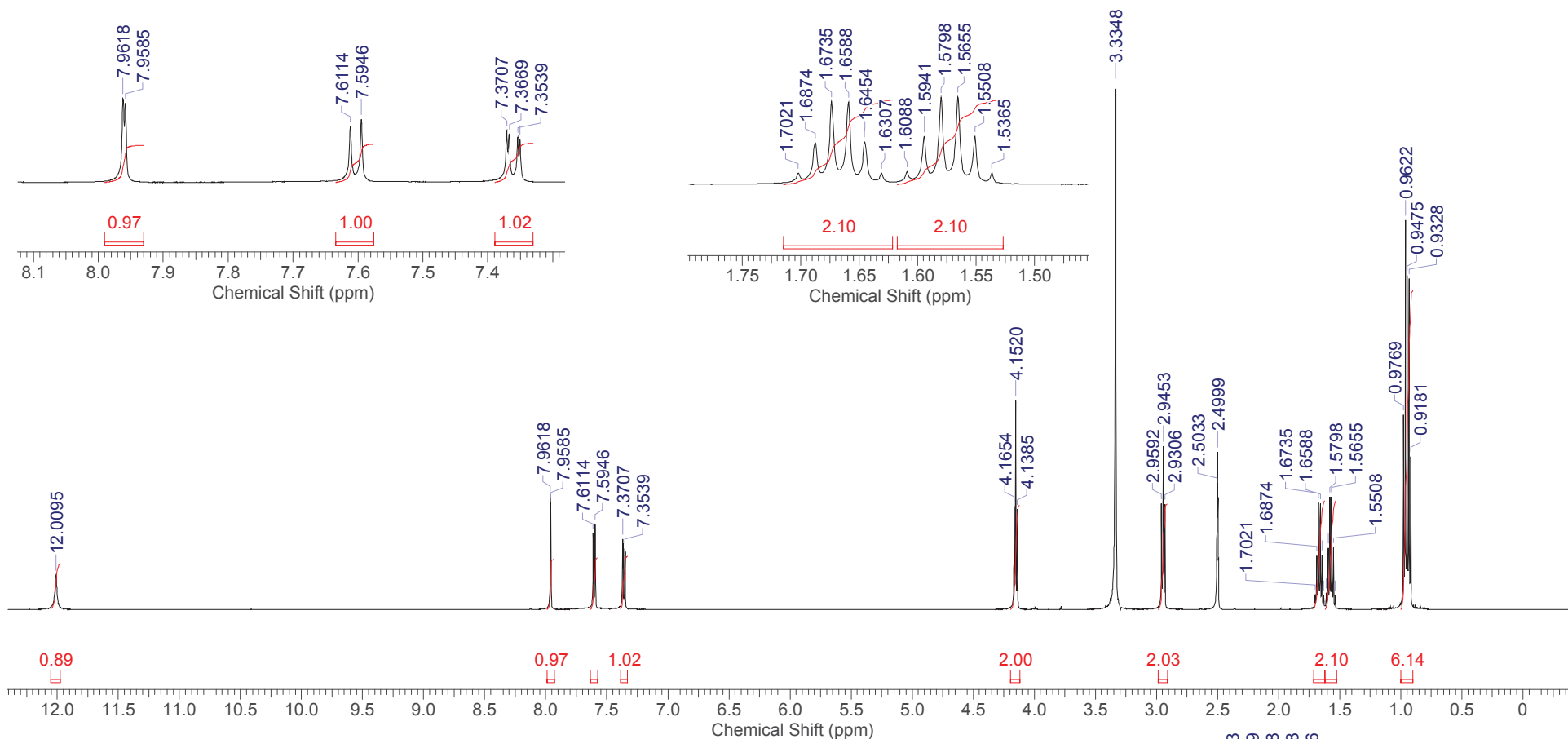
Propyl (6-ethoxy-1,3-benzothiazol-2-yl)carbamate (26)



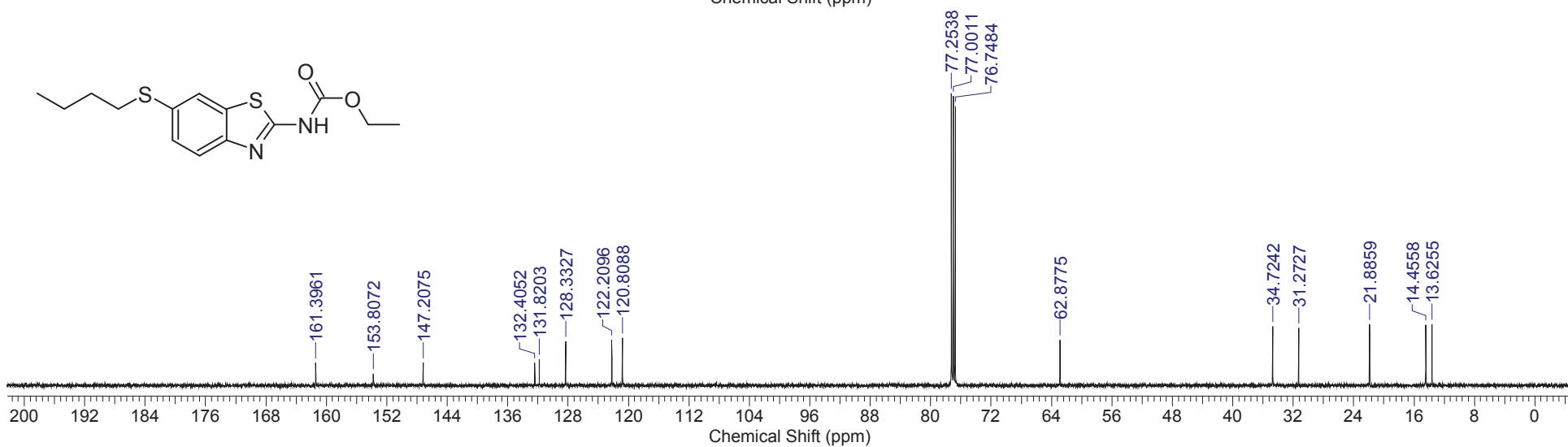
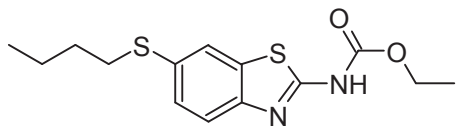
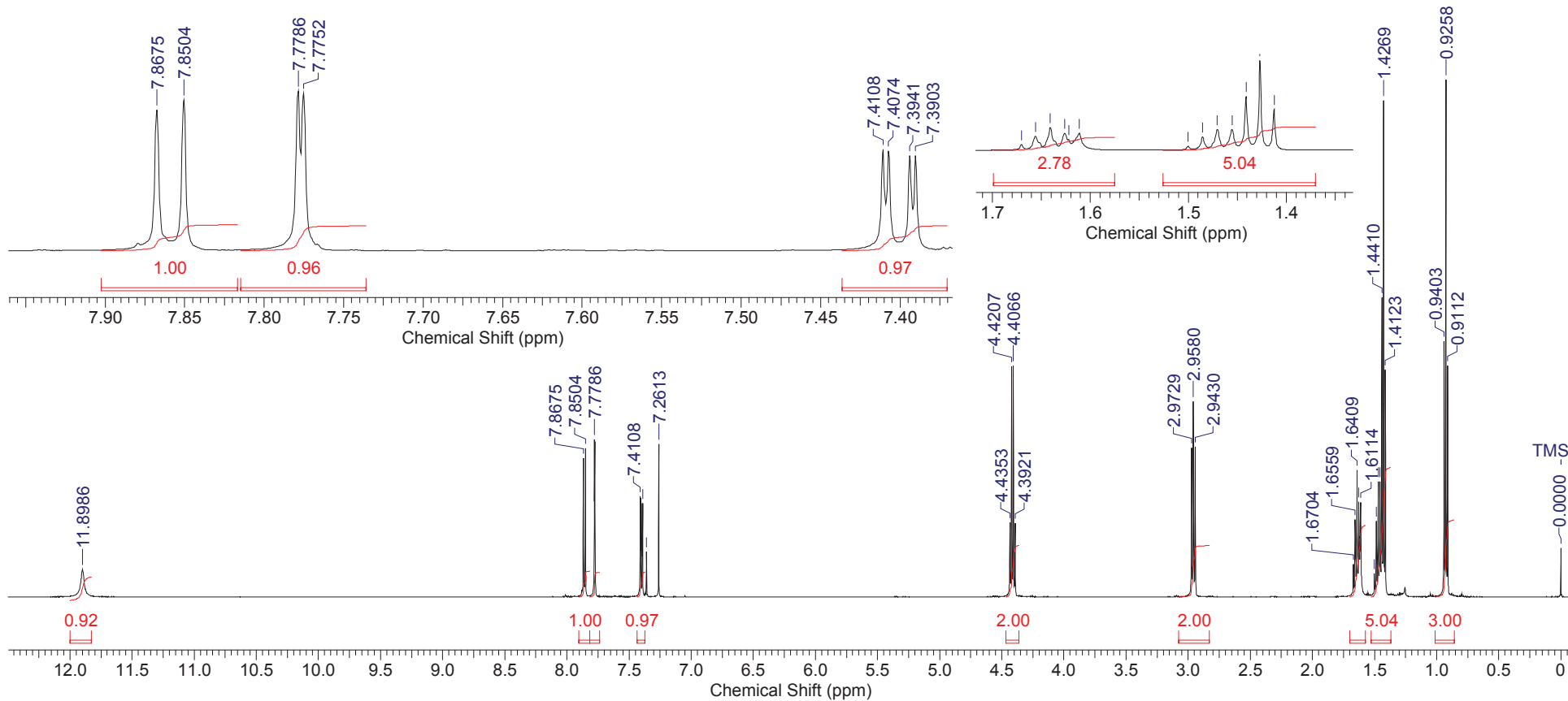
Ethyl [6-(ethanesulfonyl)-1,3-benzothiazol-2-yl]carbamate (27)



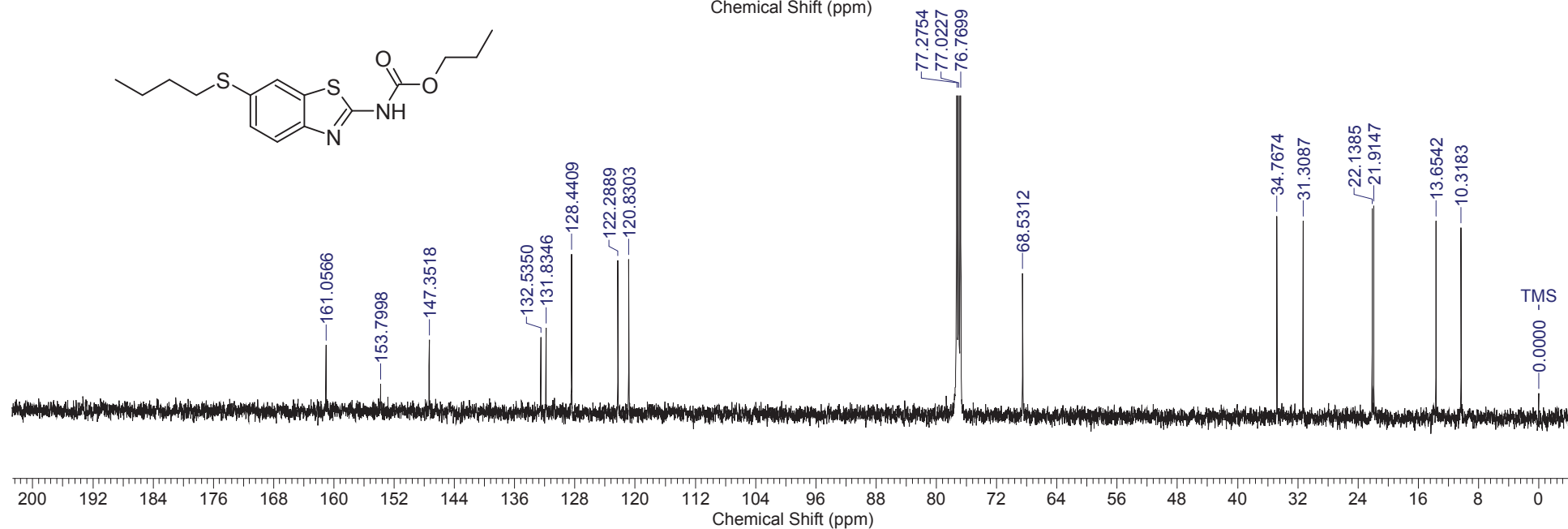
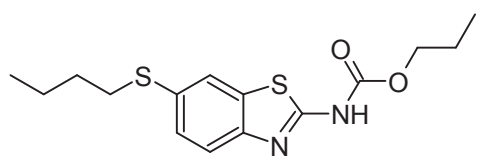
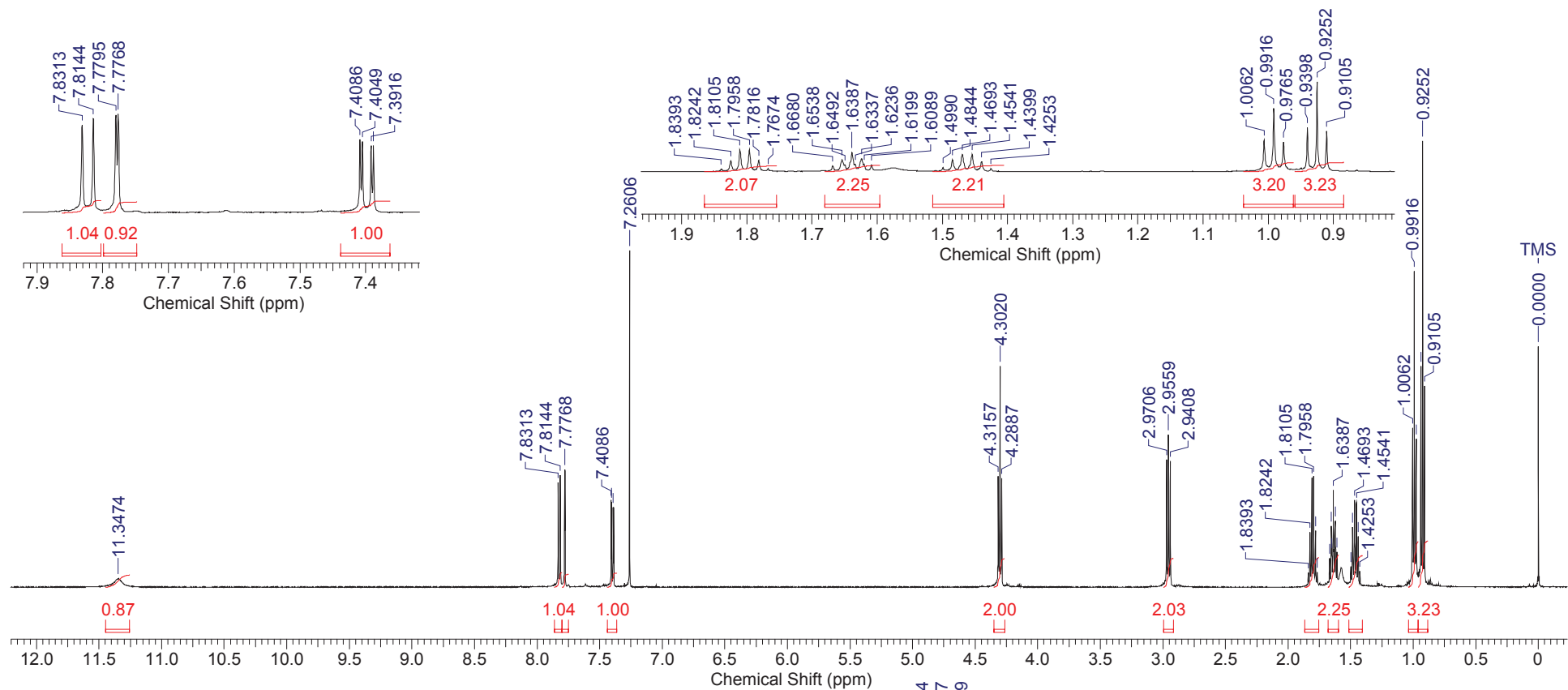
Propyl [6-(propylsulfanyl)-1,3-benzothiazol-2-yl]carbamate (28)



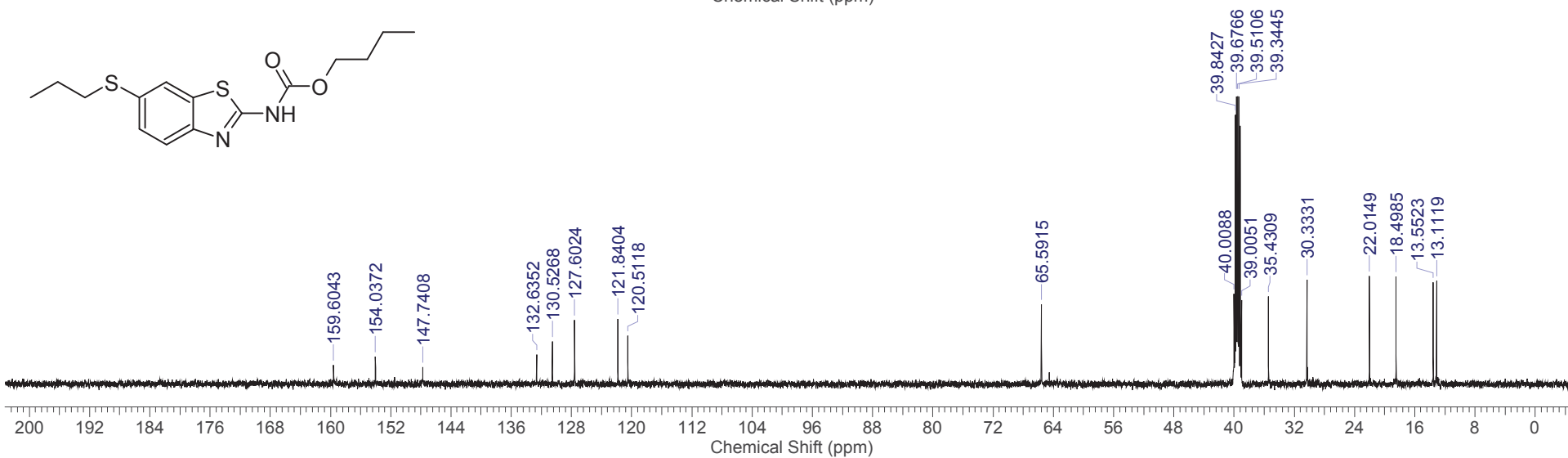
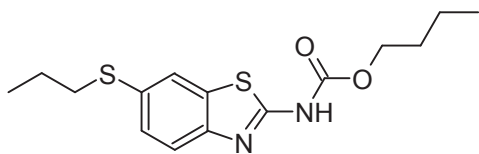
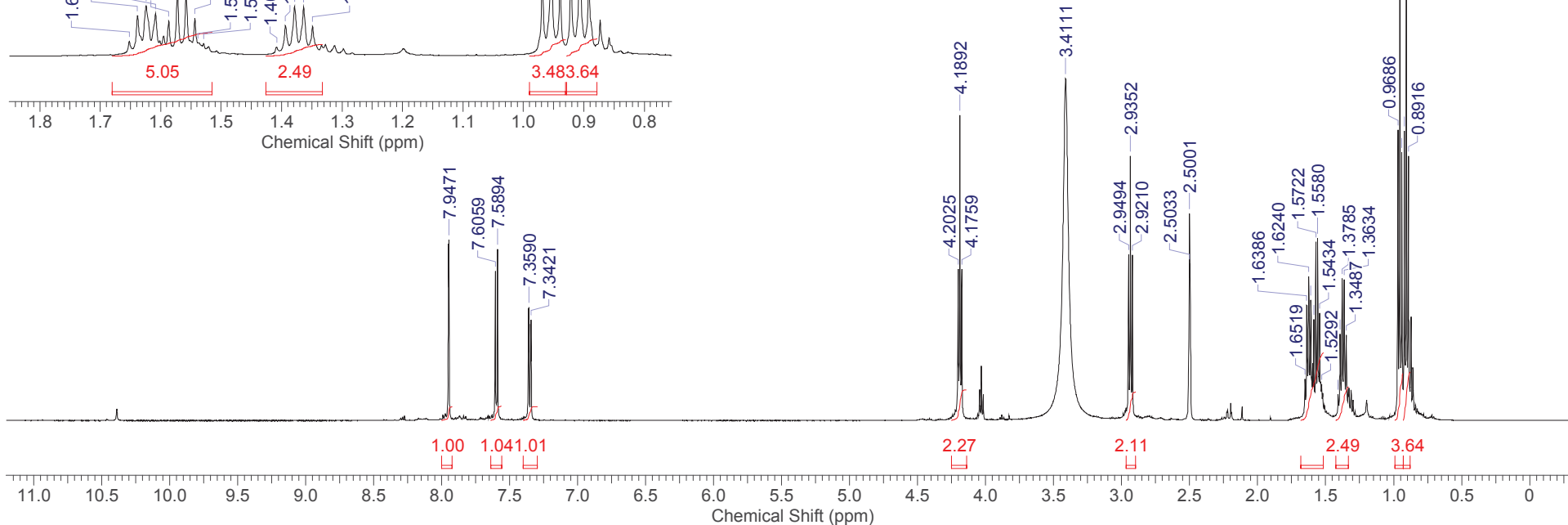
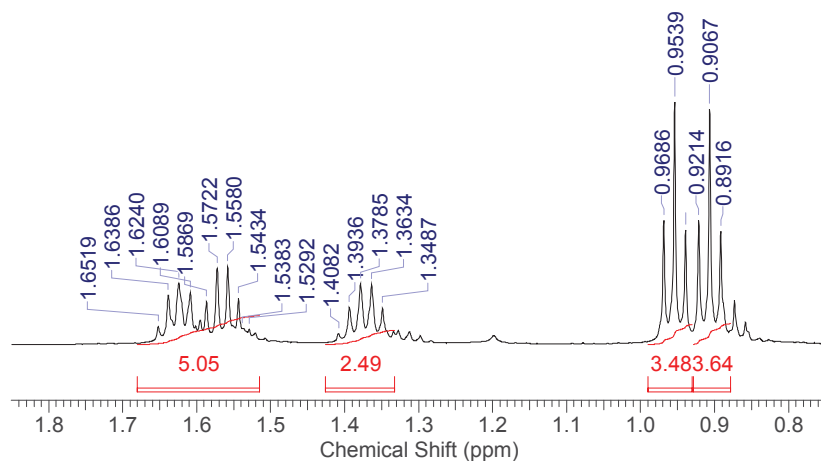
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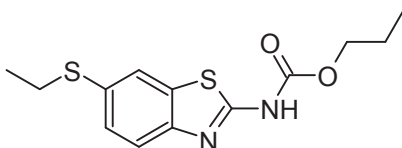
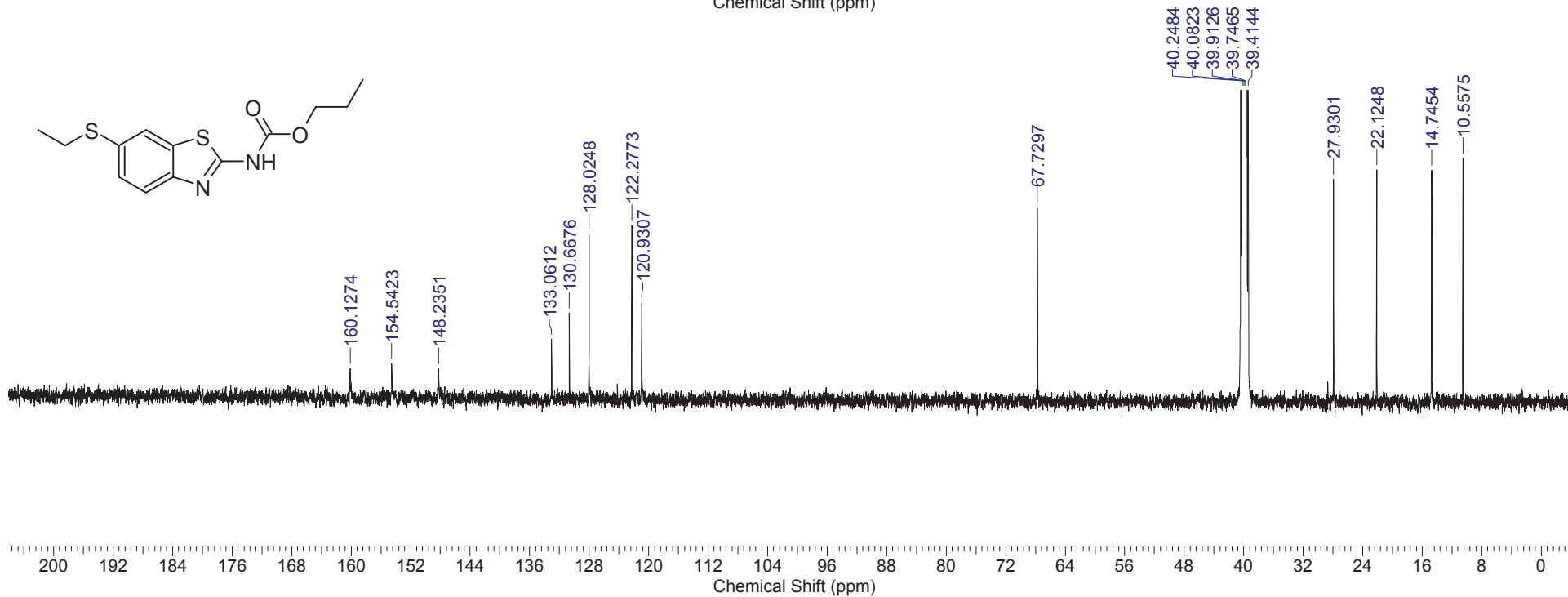
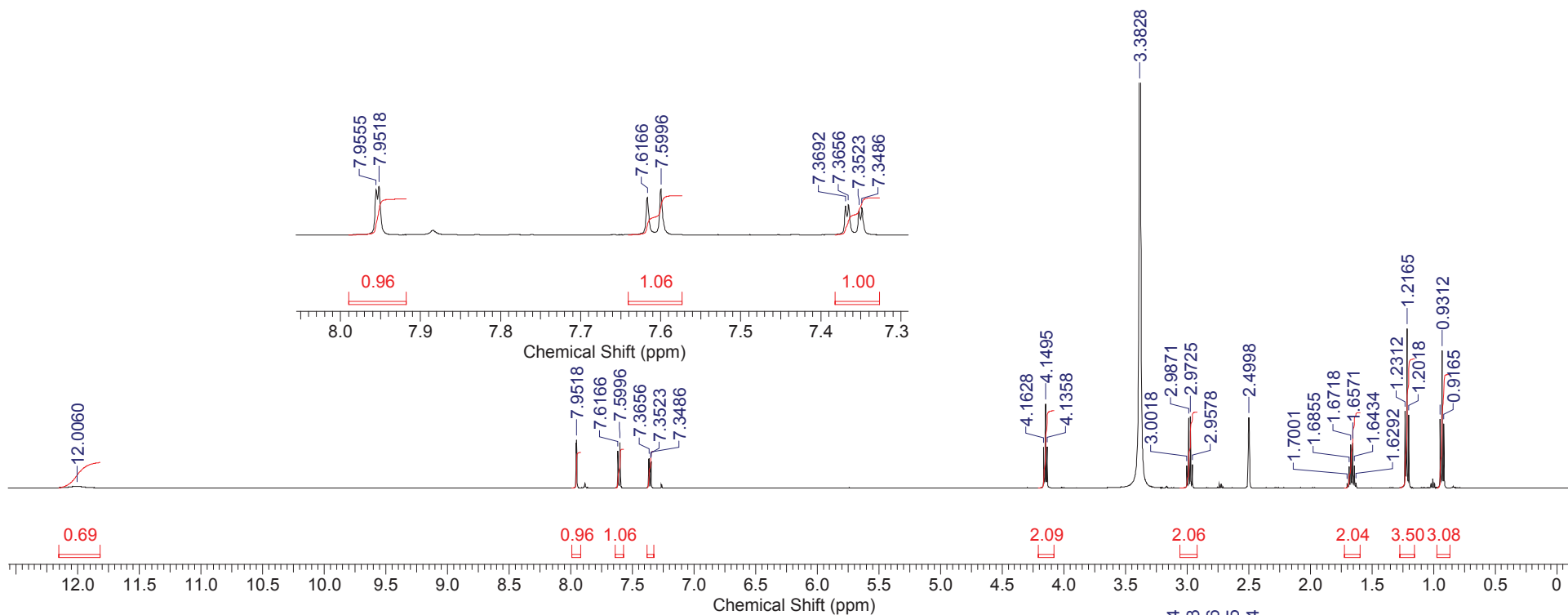
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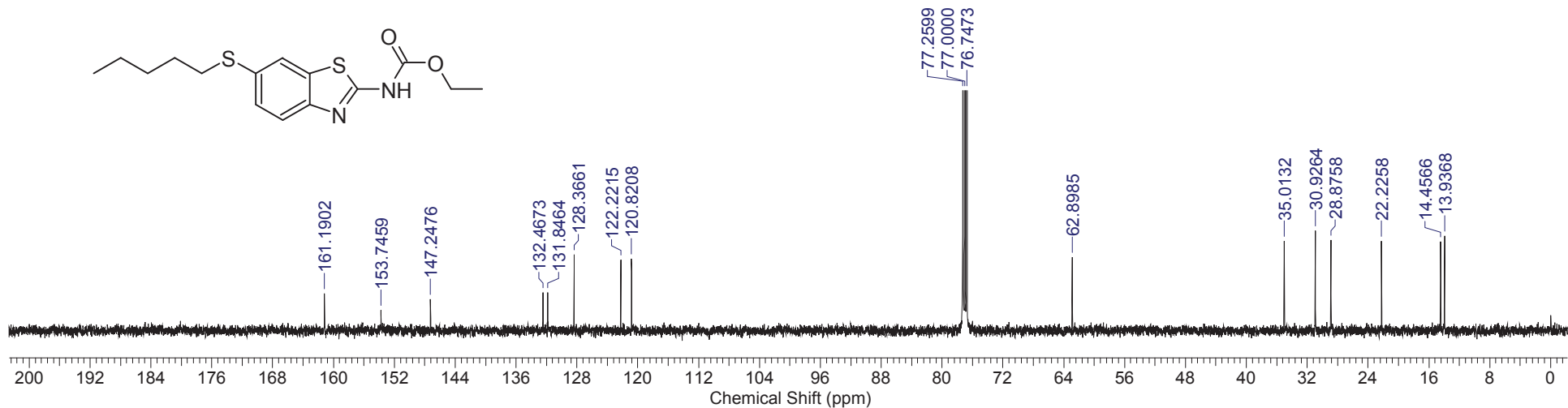
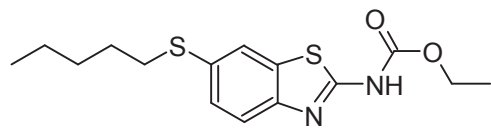
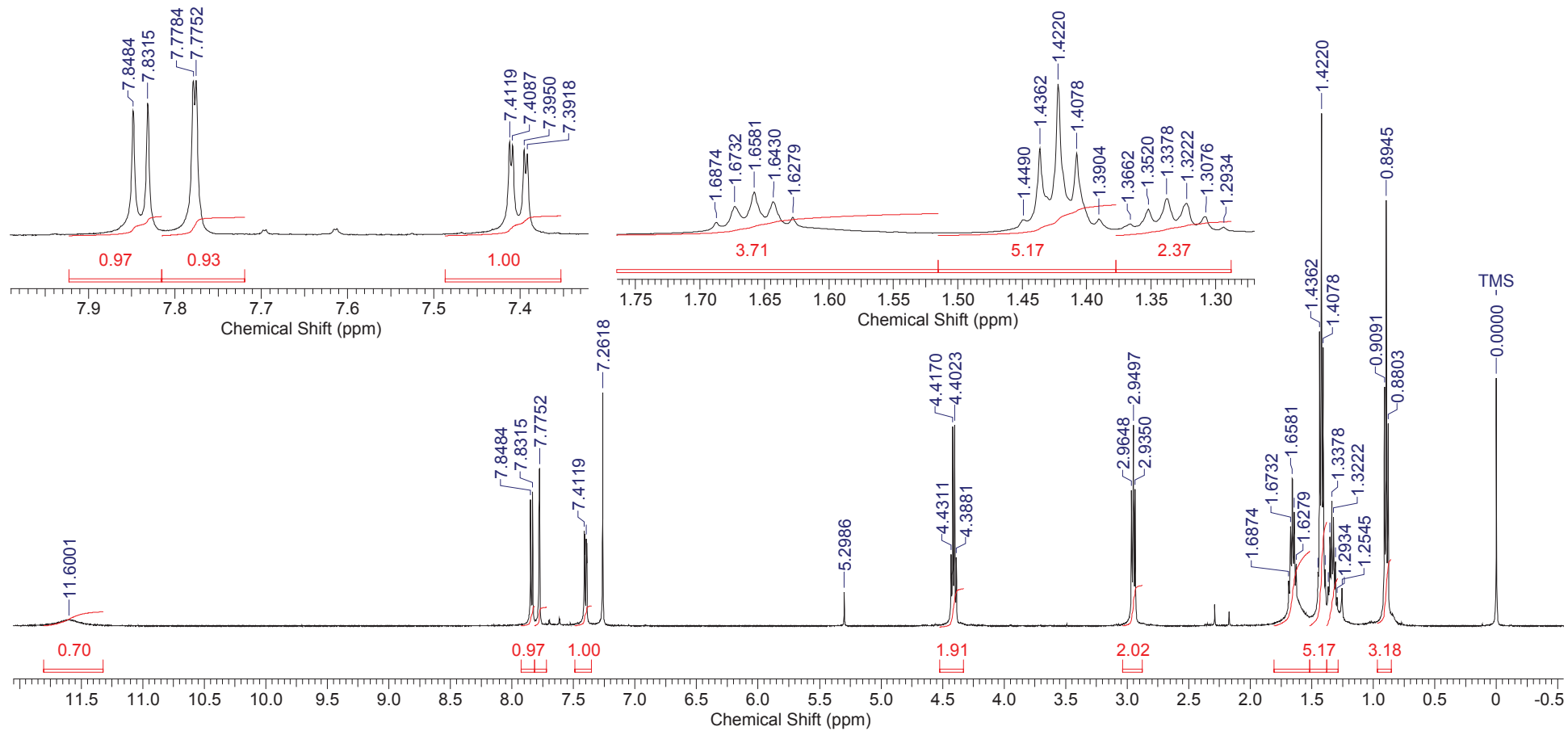
Butyl [6-(propylsulfanyl)-1,3-benzothiazol-2-yl]carbamate (31)



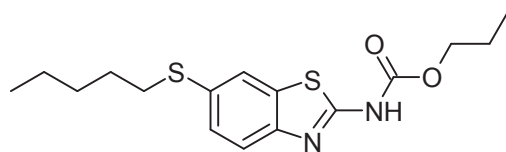
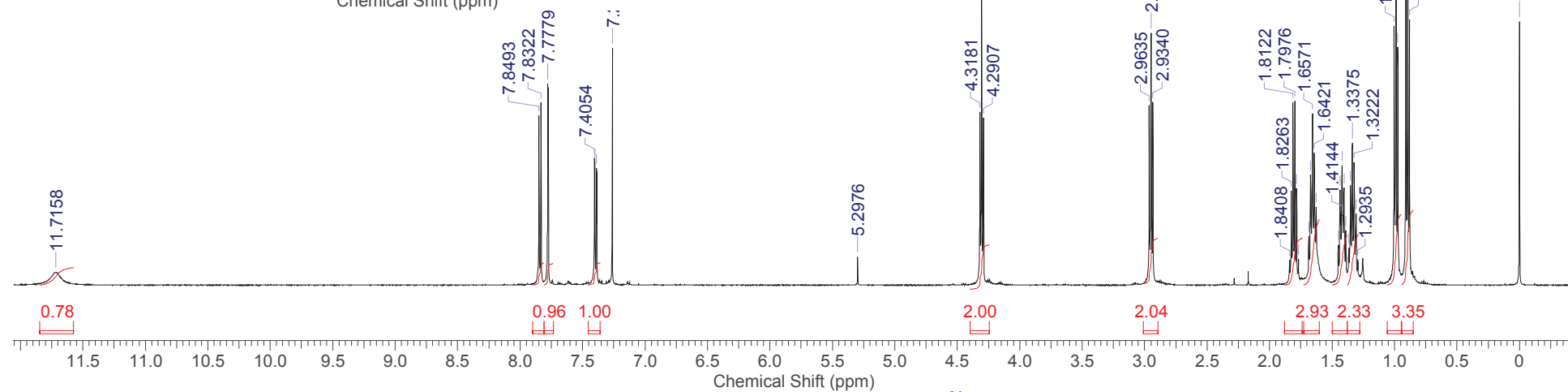
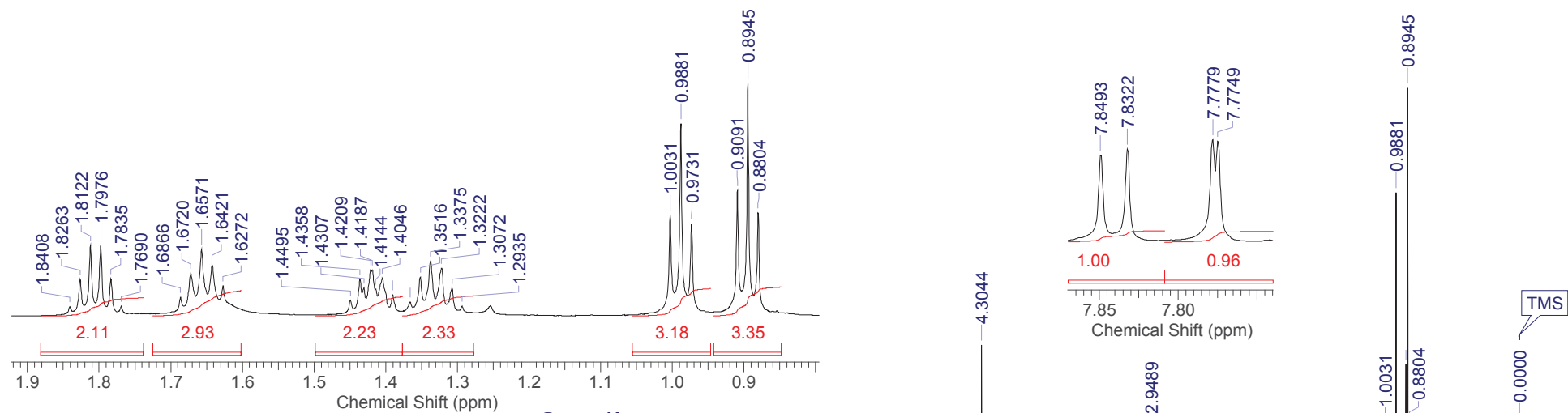
Propyl [6-(ethylsulfanyl)-1,3-benzothiazol-2-yl]carbamate (32)



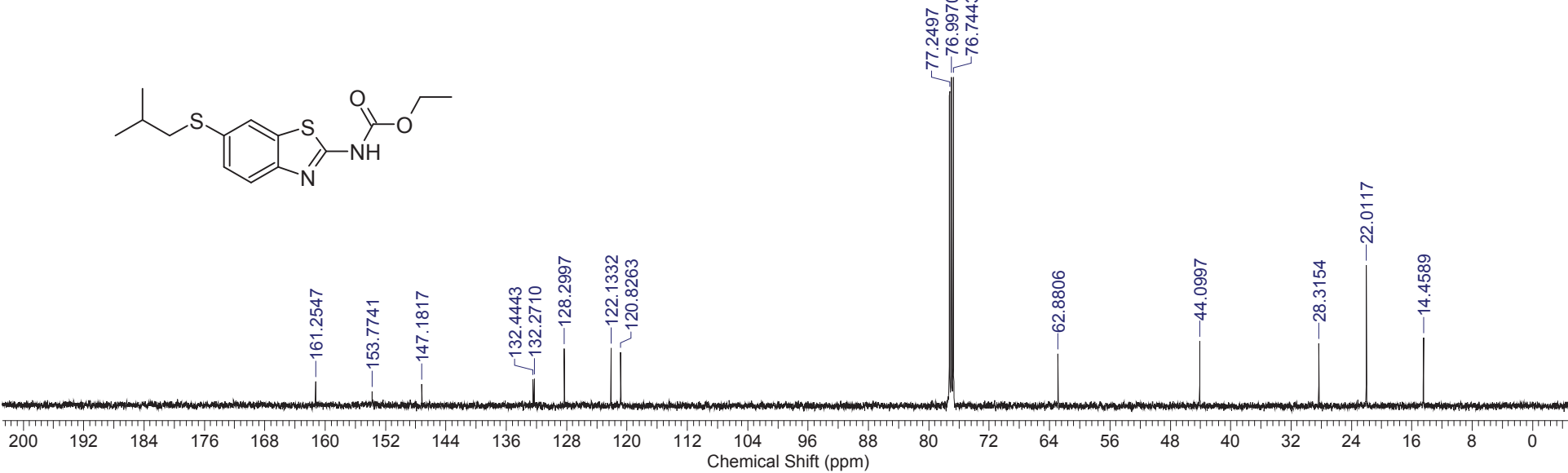
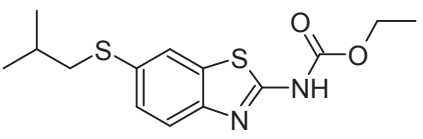
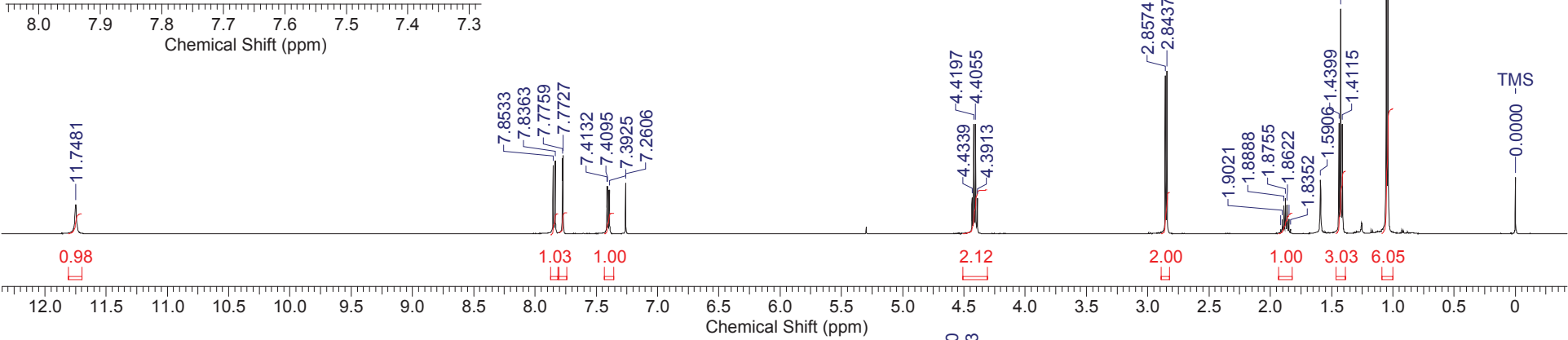
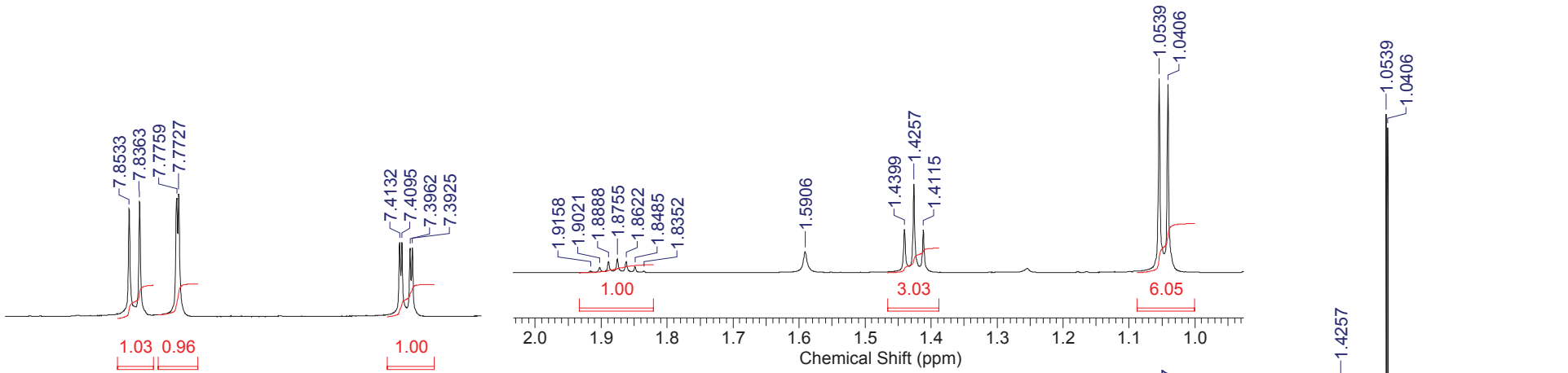
Ethyl [6-(pentylsulfanyl)-1,3-benzothiazol-2-yl]carbamate (33)



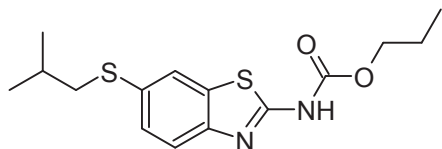
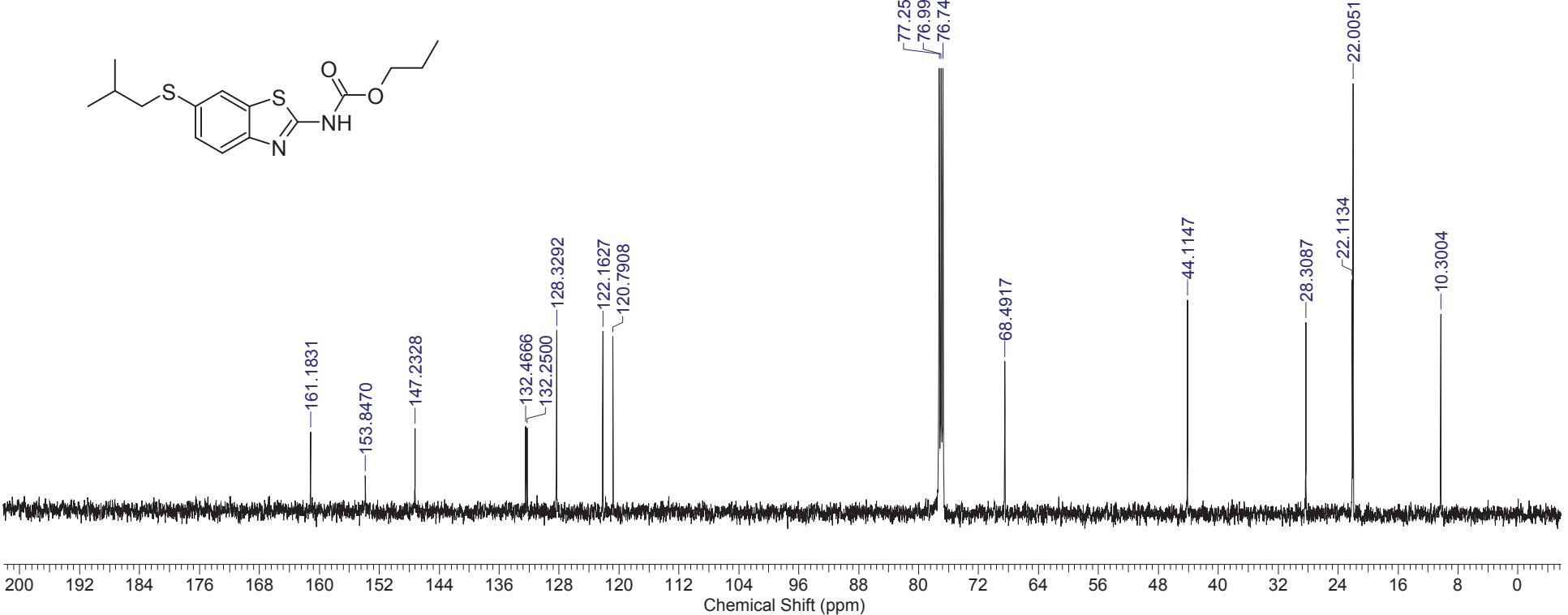
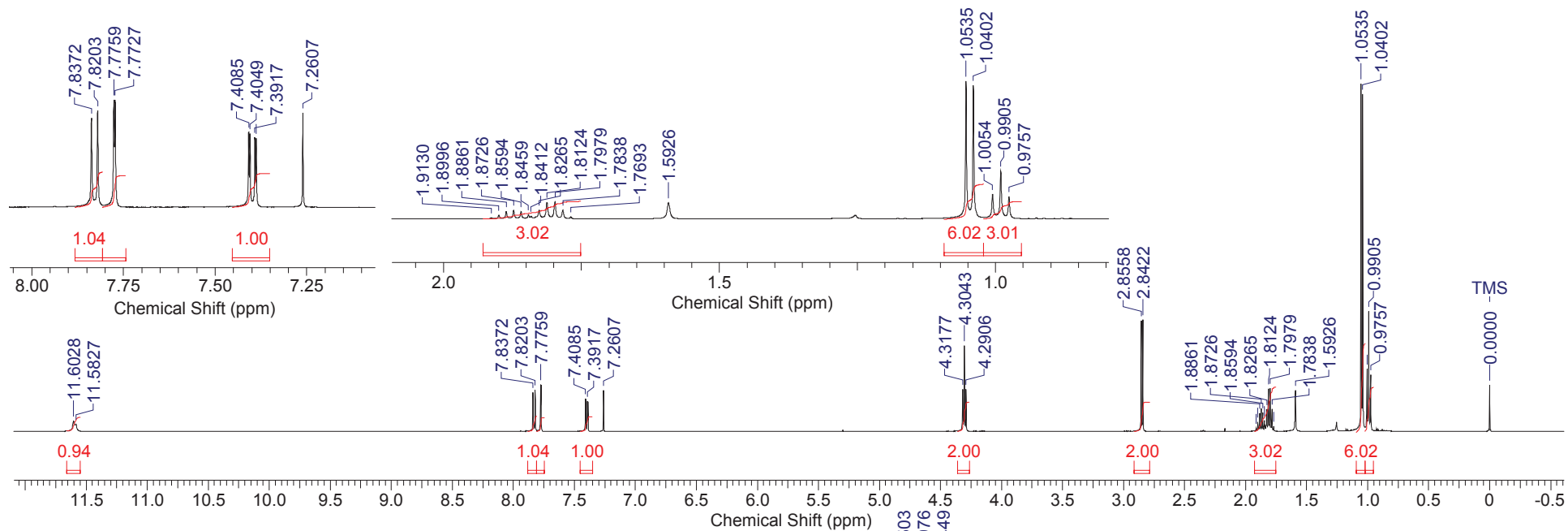
Propyl [6-(pentylsulfanyl)-1,3-benzothiazol-2-yl]carbamate (34)



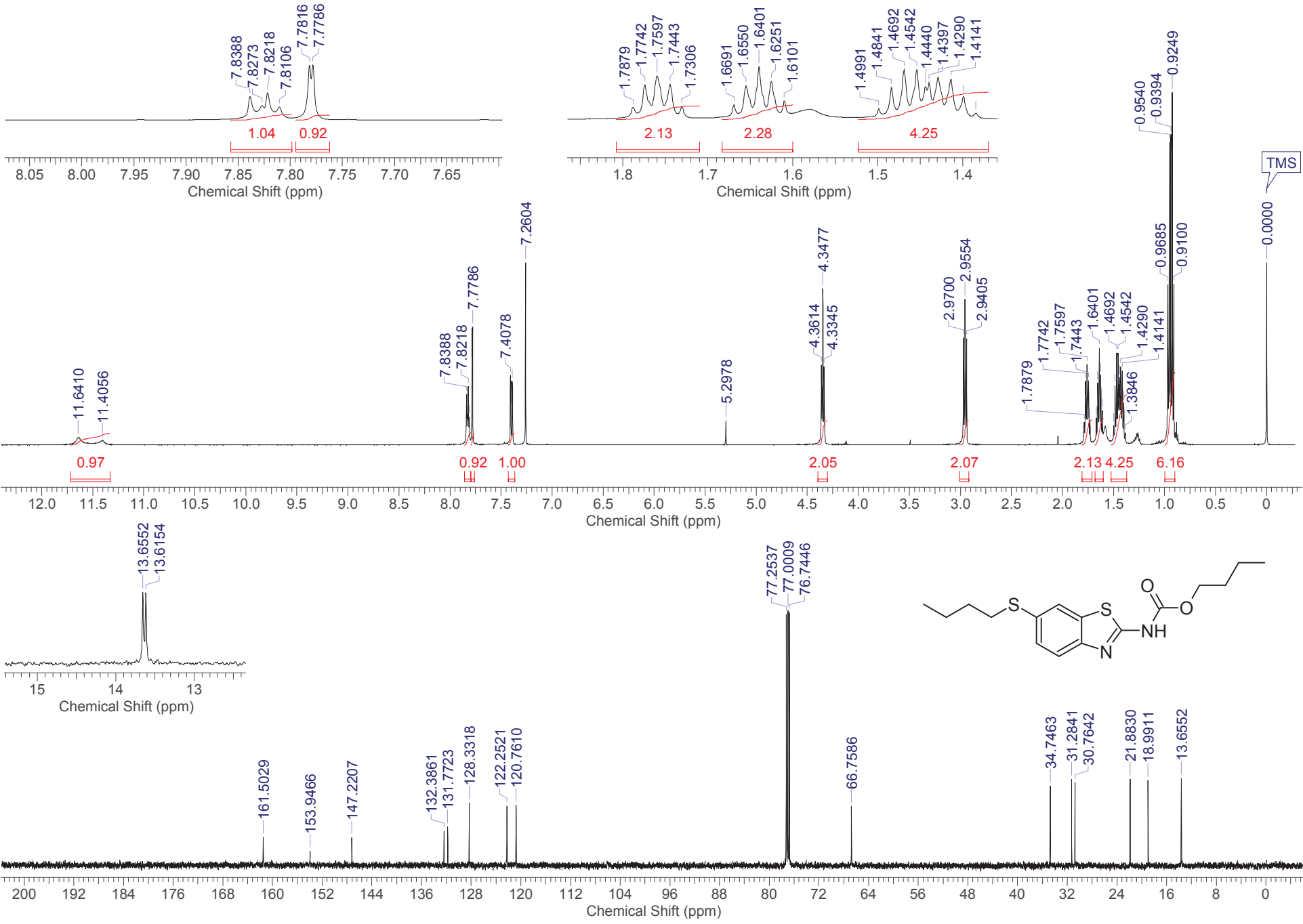
Ethyl {6-[(2-methylpropyl)sulfanyl]-1,3-benzothiazol-2-yl}carbamate (35)



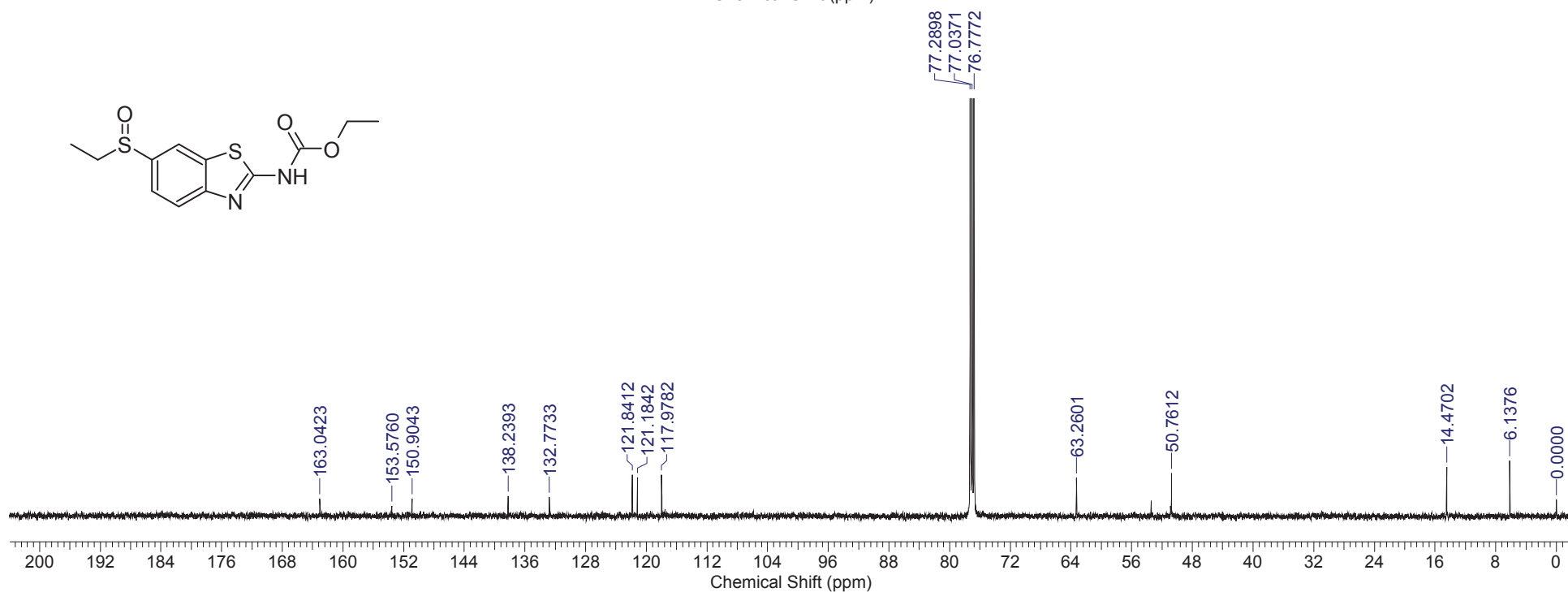
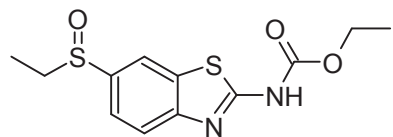
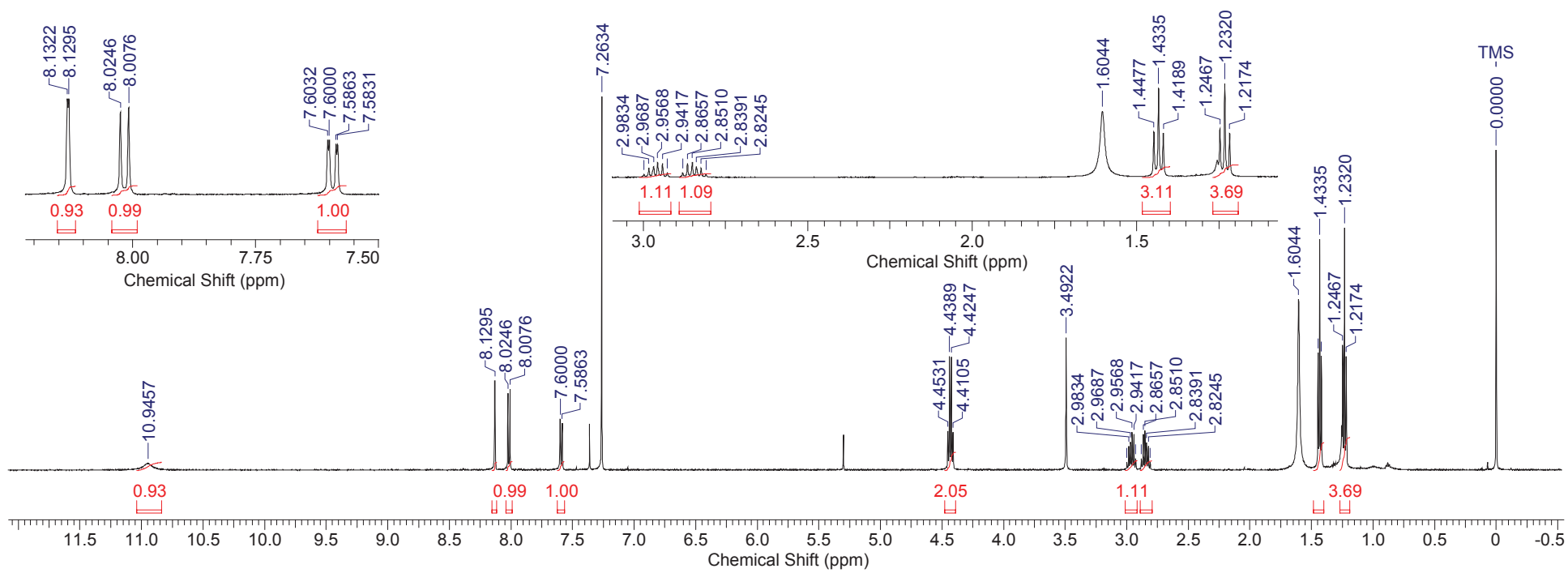
Propyl {6-[(2-methylpropyl)sulfanyl]-1,3-benzothiazol-2-yl}carbamate (36)



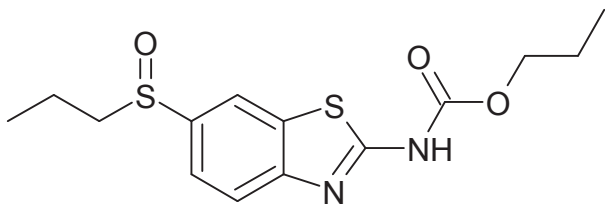
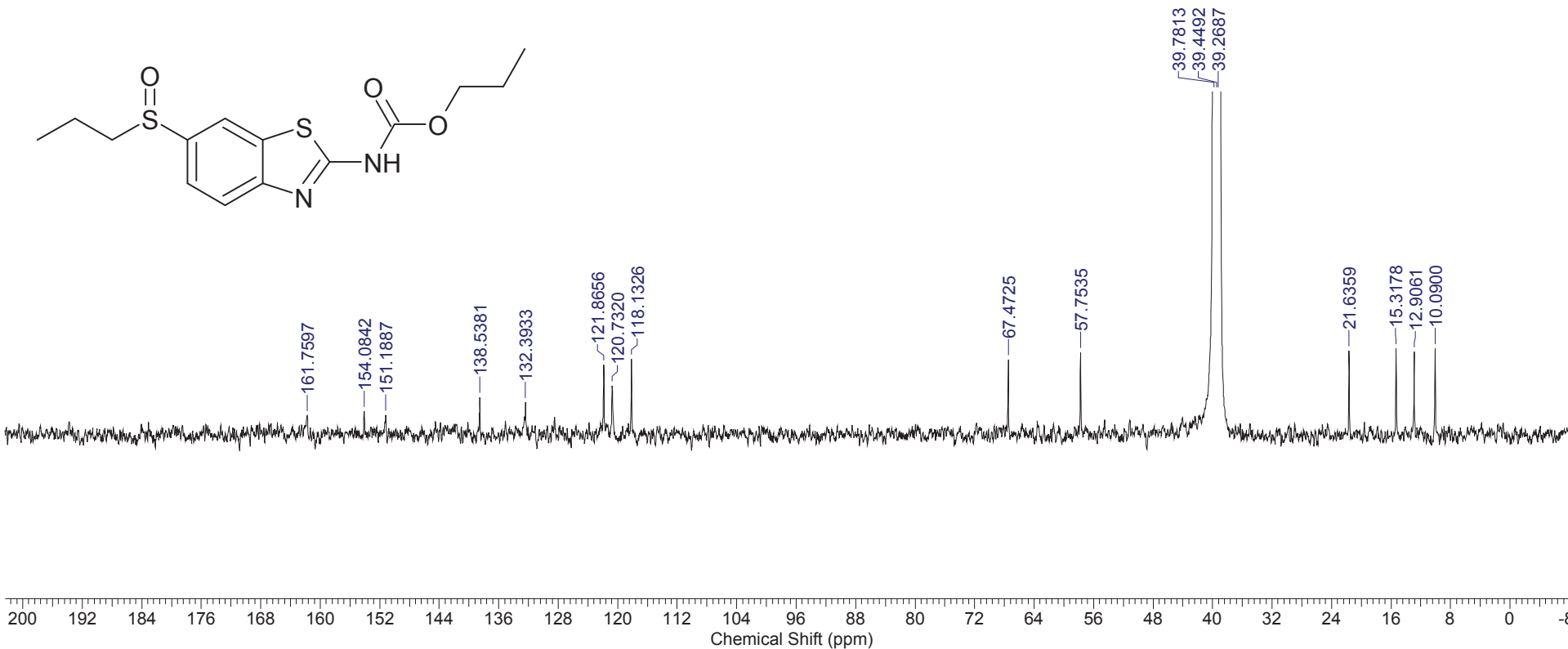
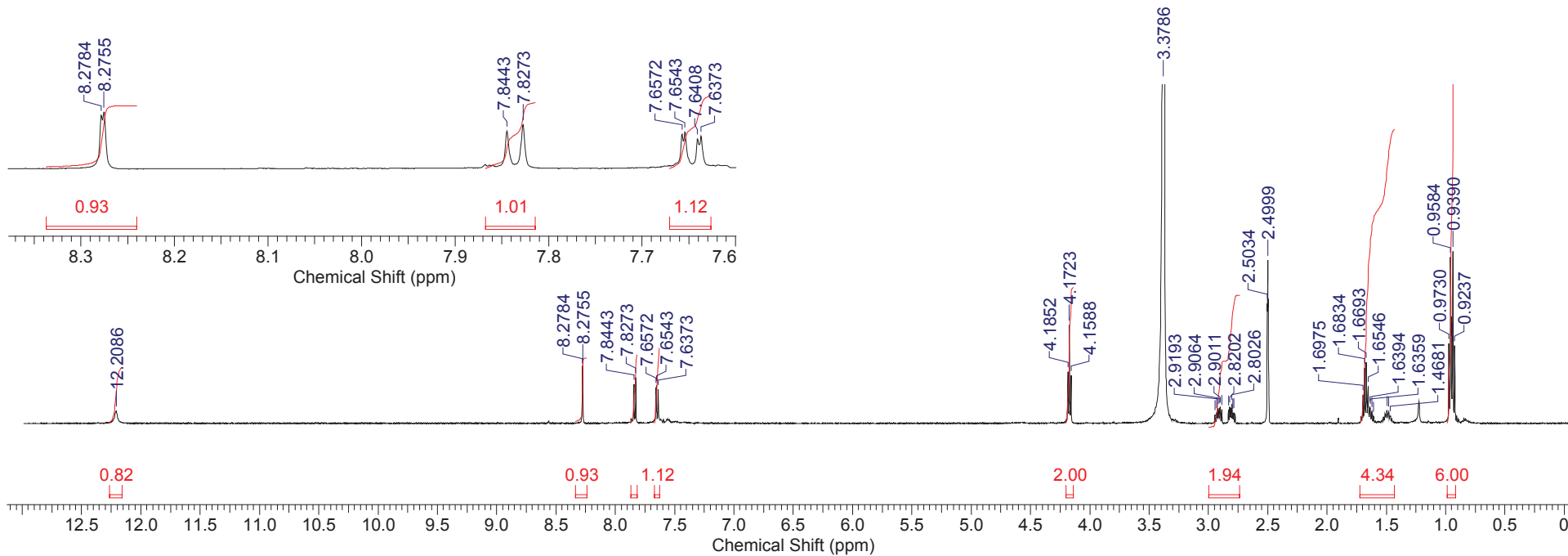
Butyl [6-(butylsulfanyl)-1,3-benzothiazol-2-yl]carbamate (37)



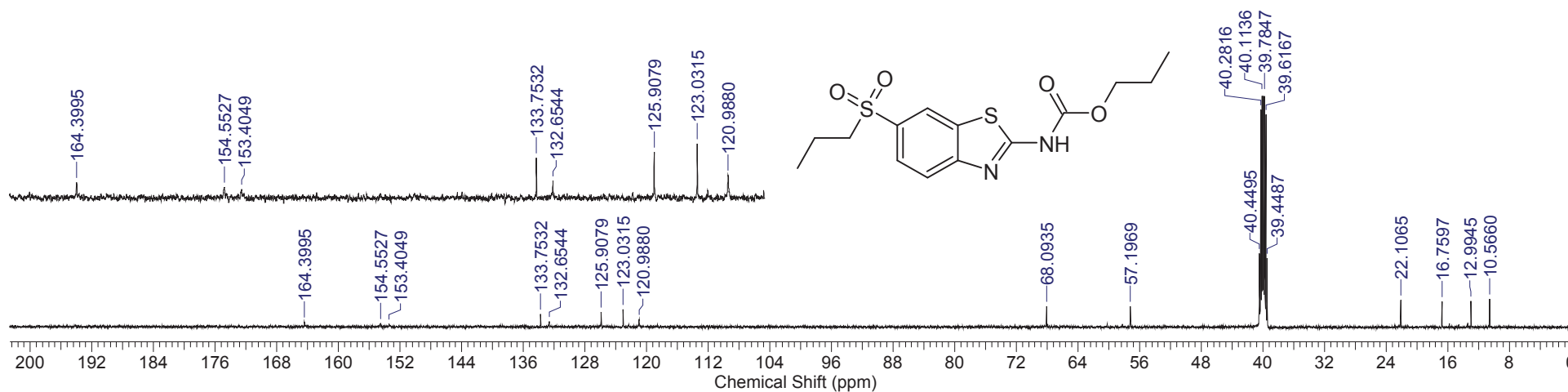
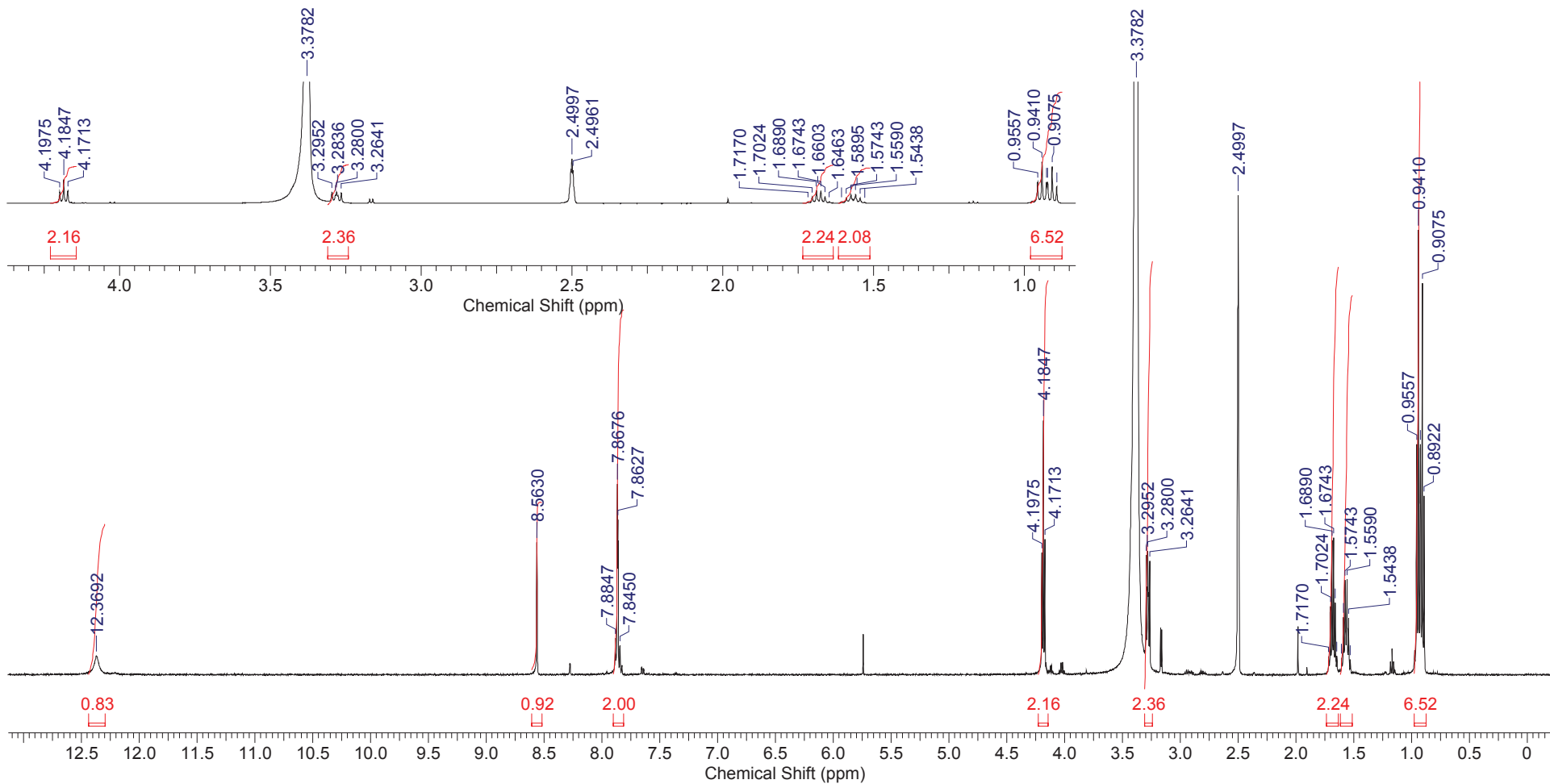
Ethyl [6-(ethanesulfinyl)-1,3-benzothiazol-2-yl]carbamate (38)



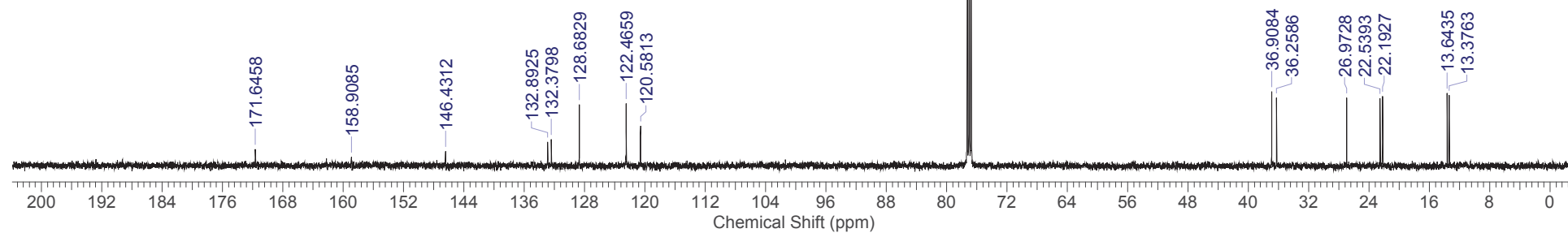
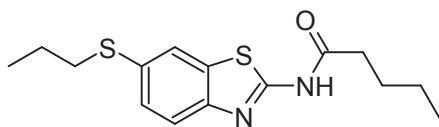
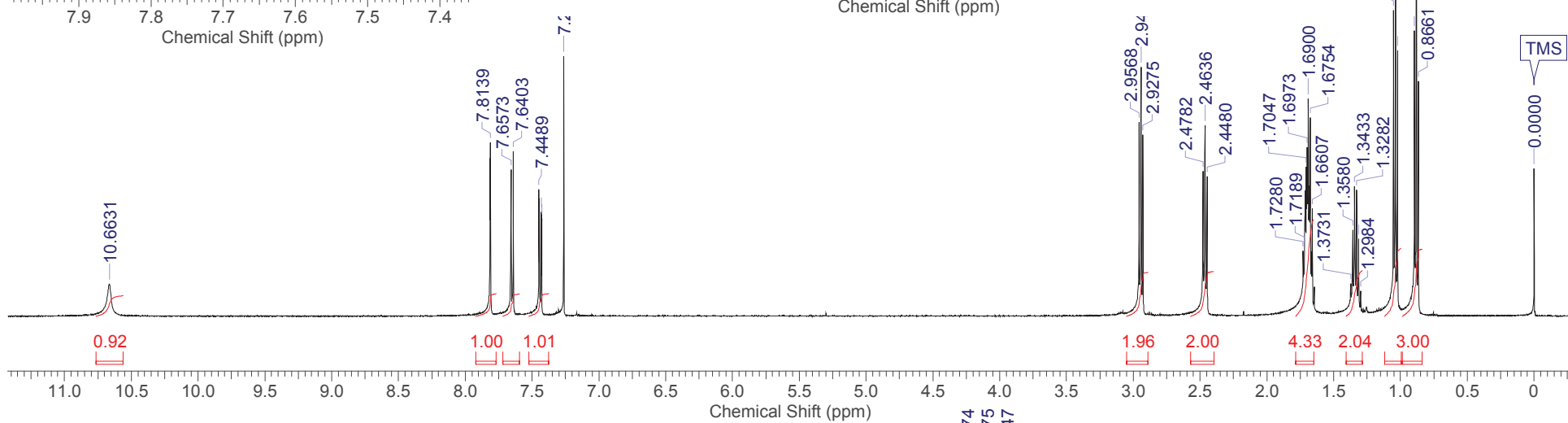
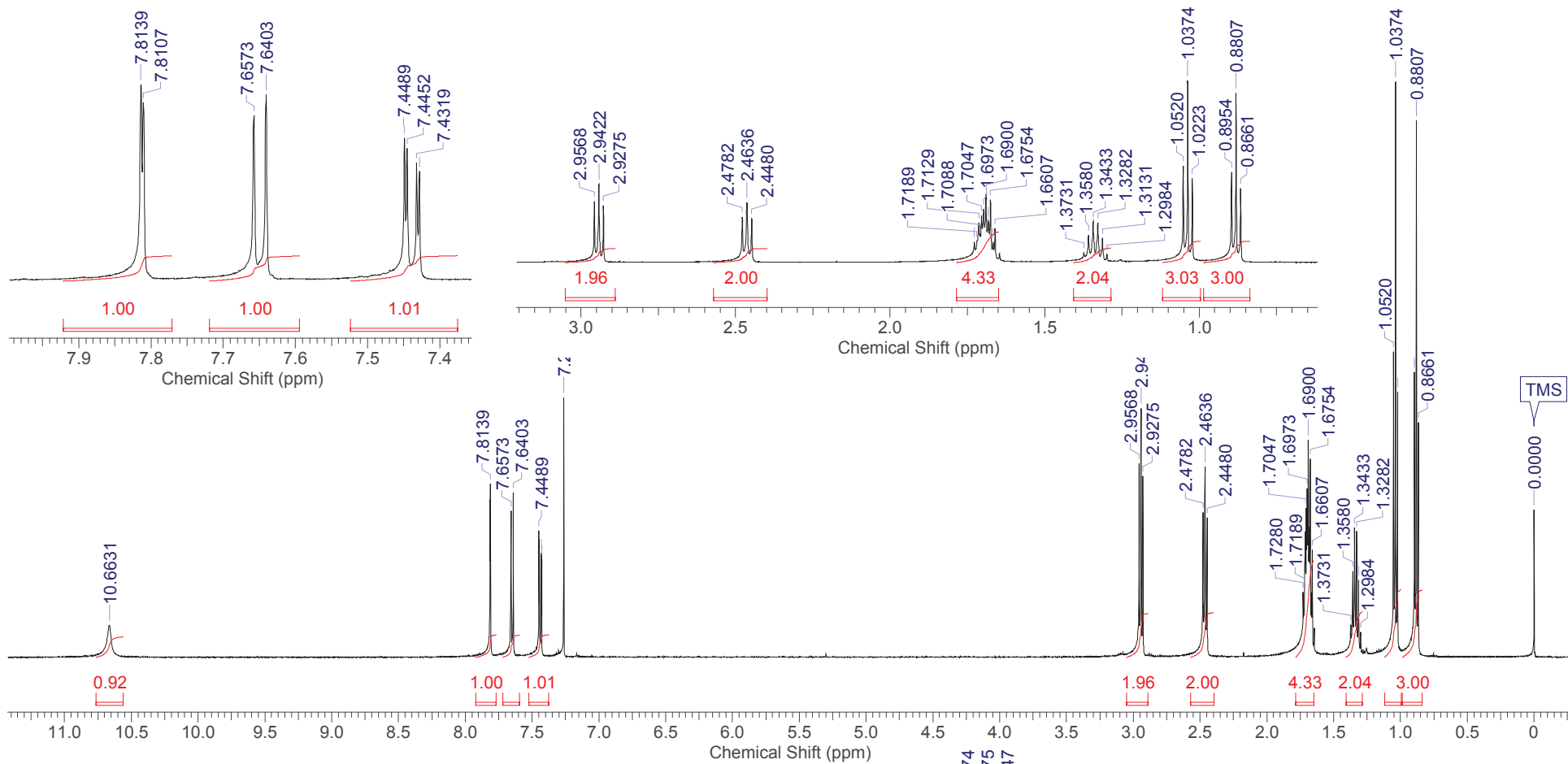
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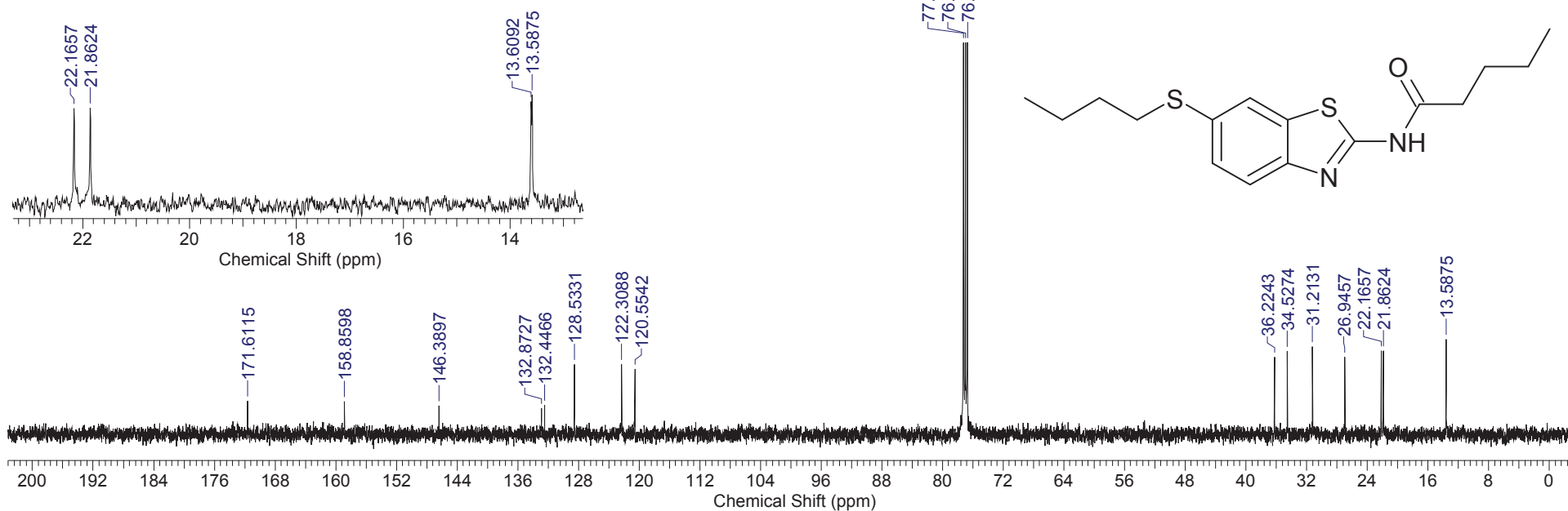
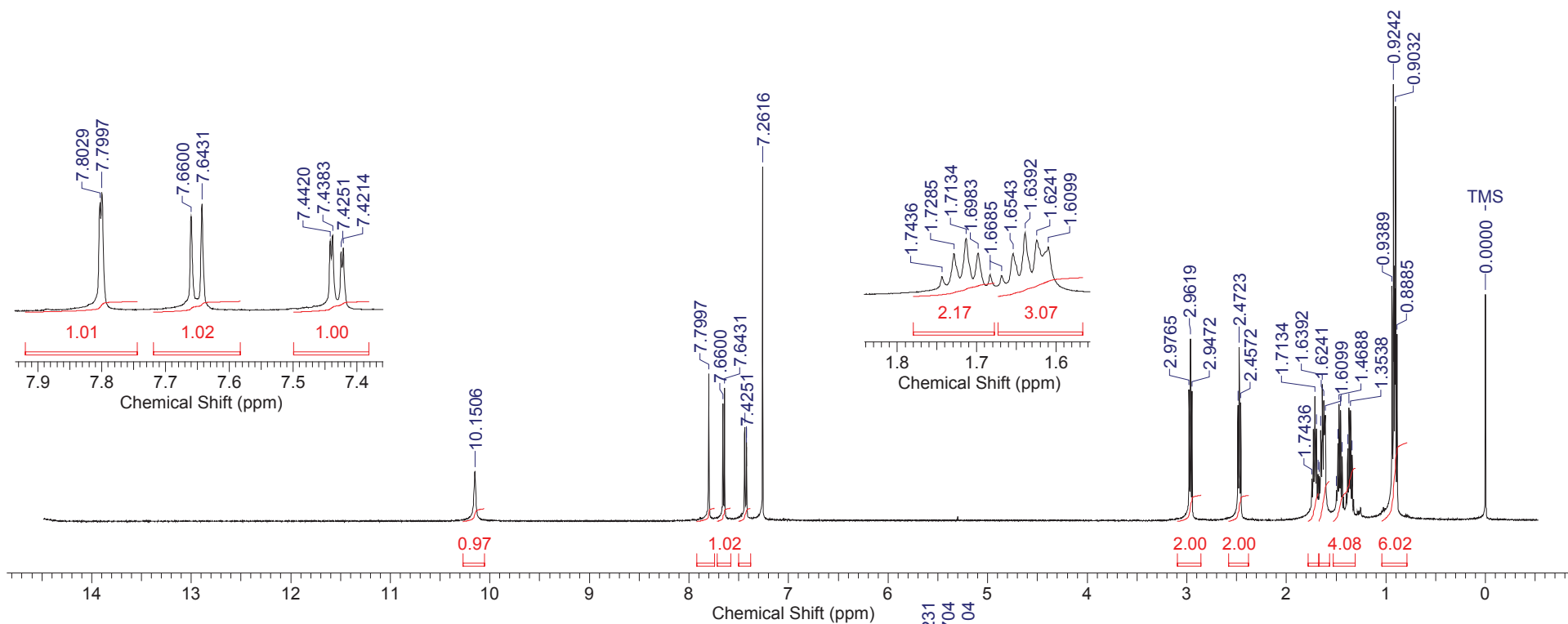
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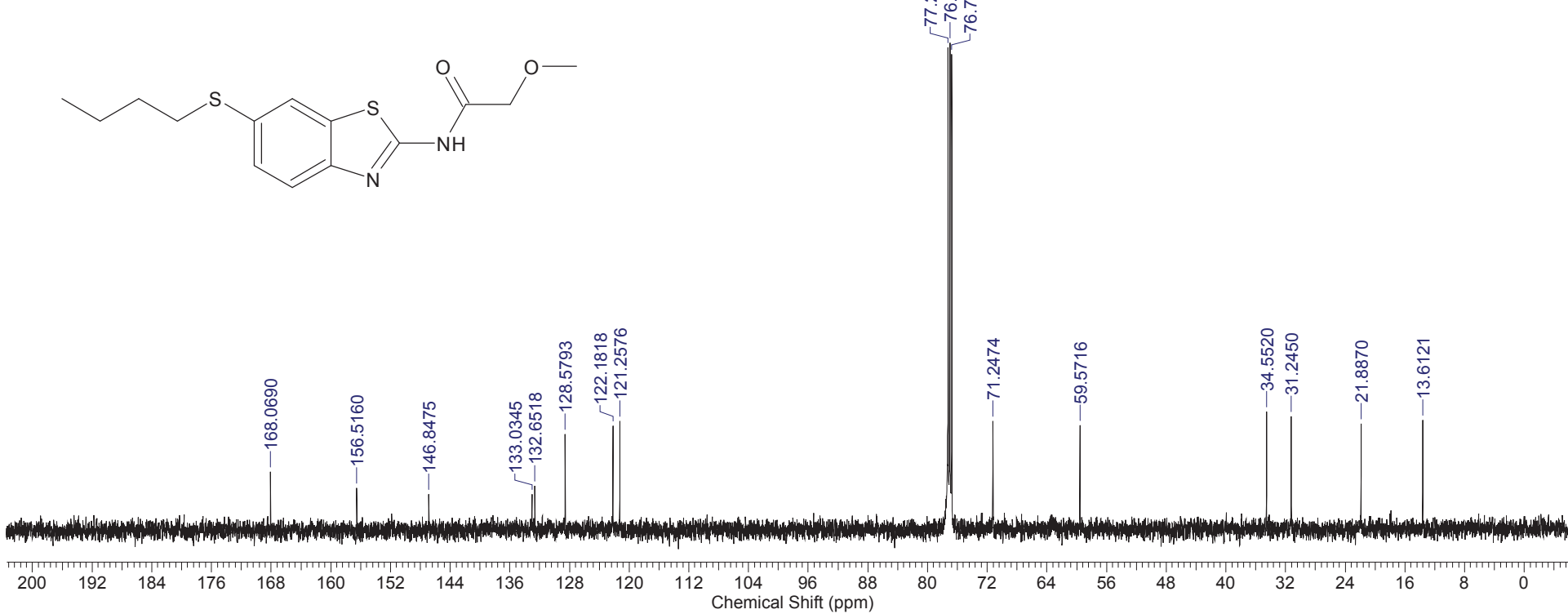
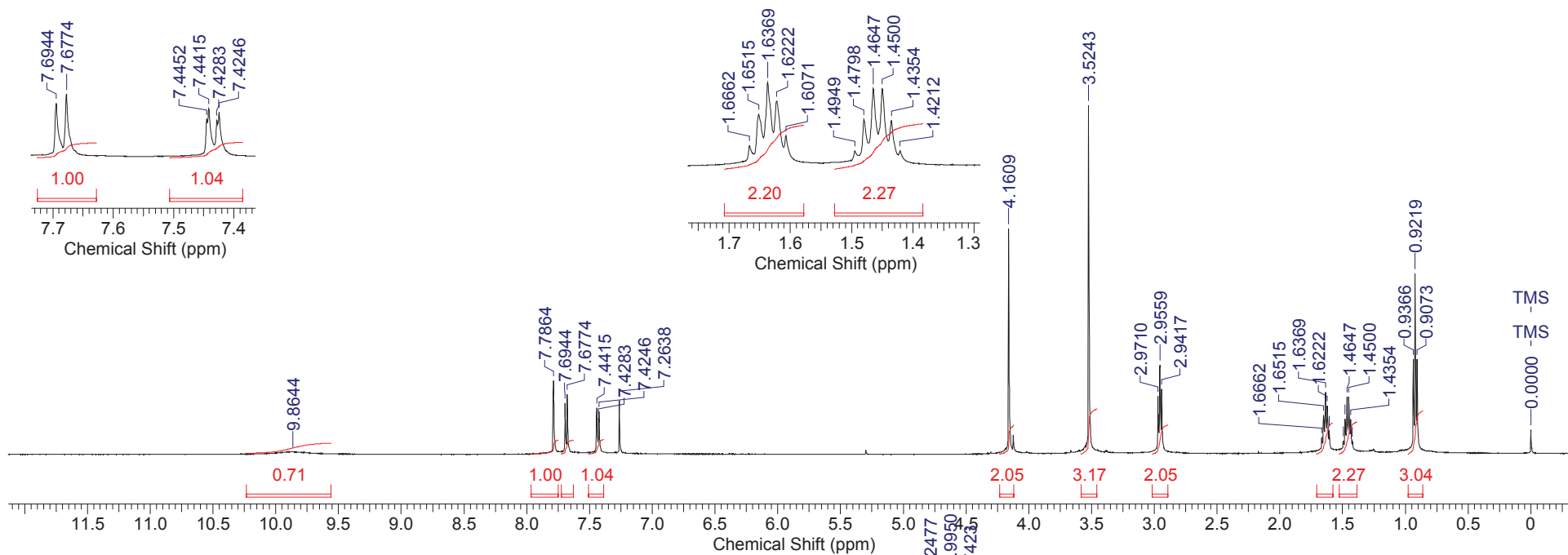
N-[6-(propylsulfanyl)-1,3-benzothiazol-2-yl]pentanamide (41)



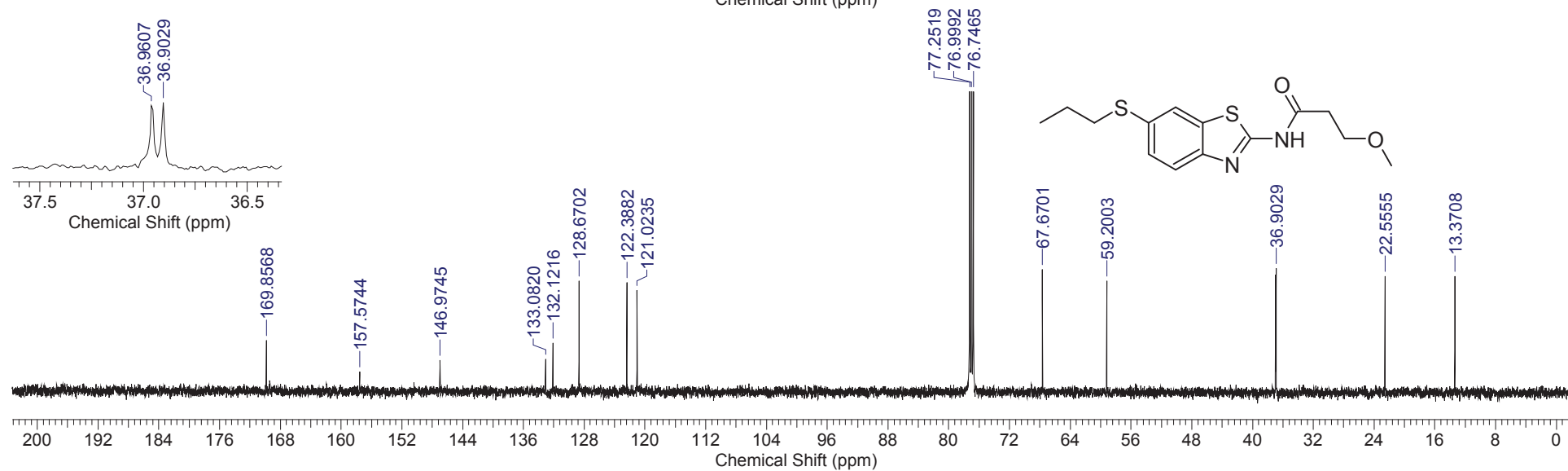
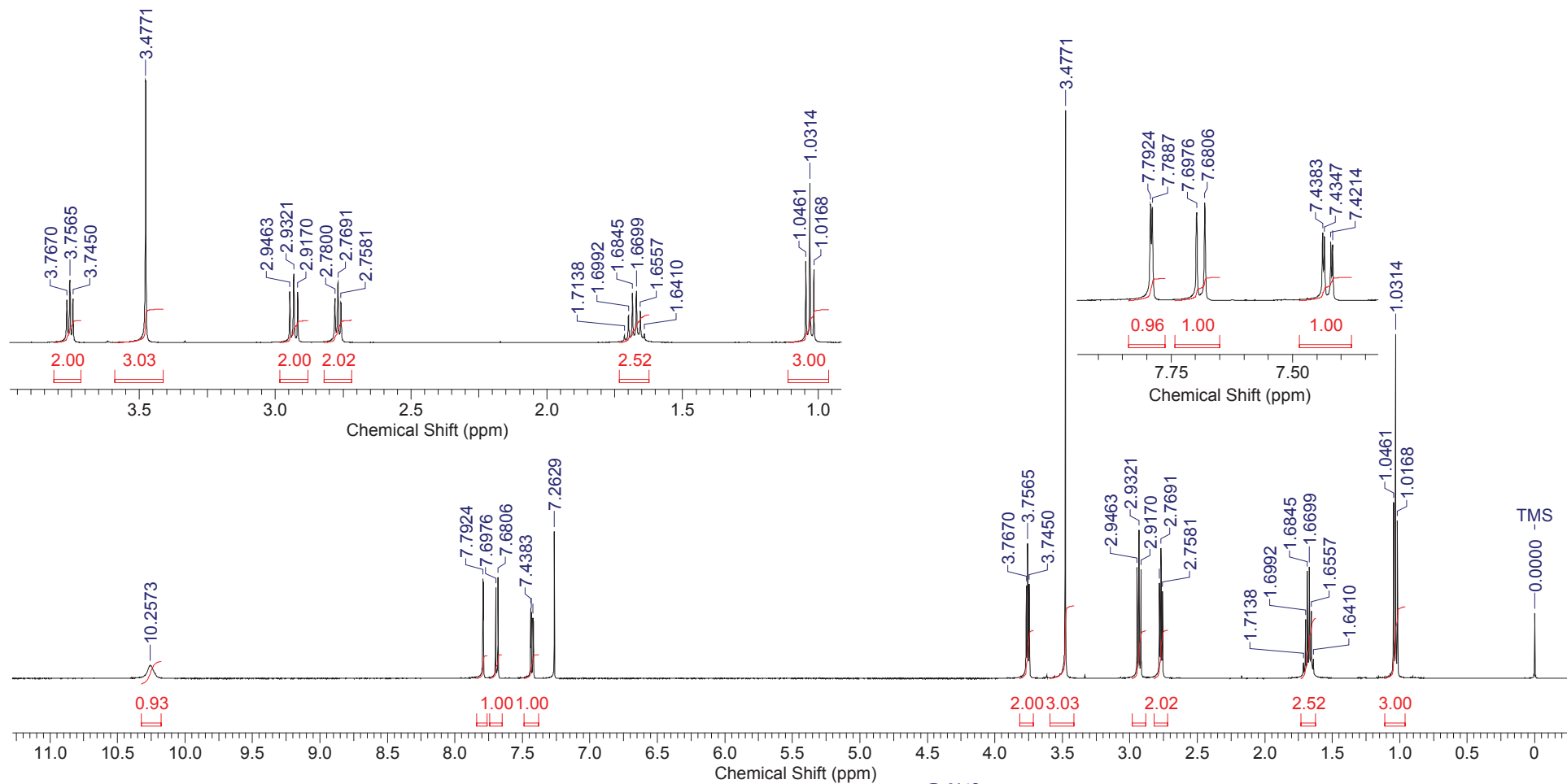
***N*-[6-(butylsulfanyl)-1,3-benzothiazol-2-yl]-3-methoxypropanamide (42)**



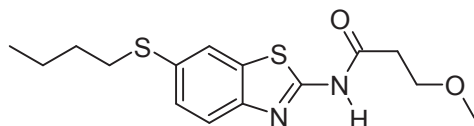
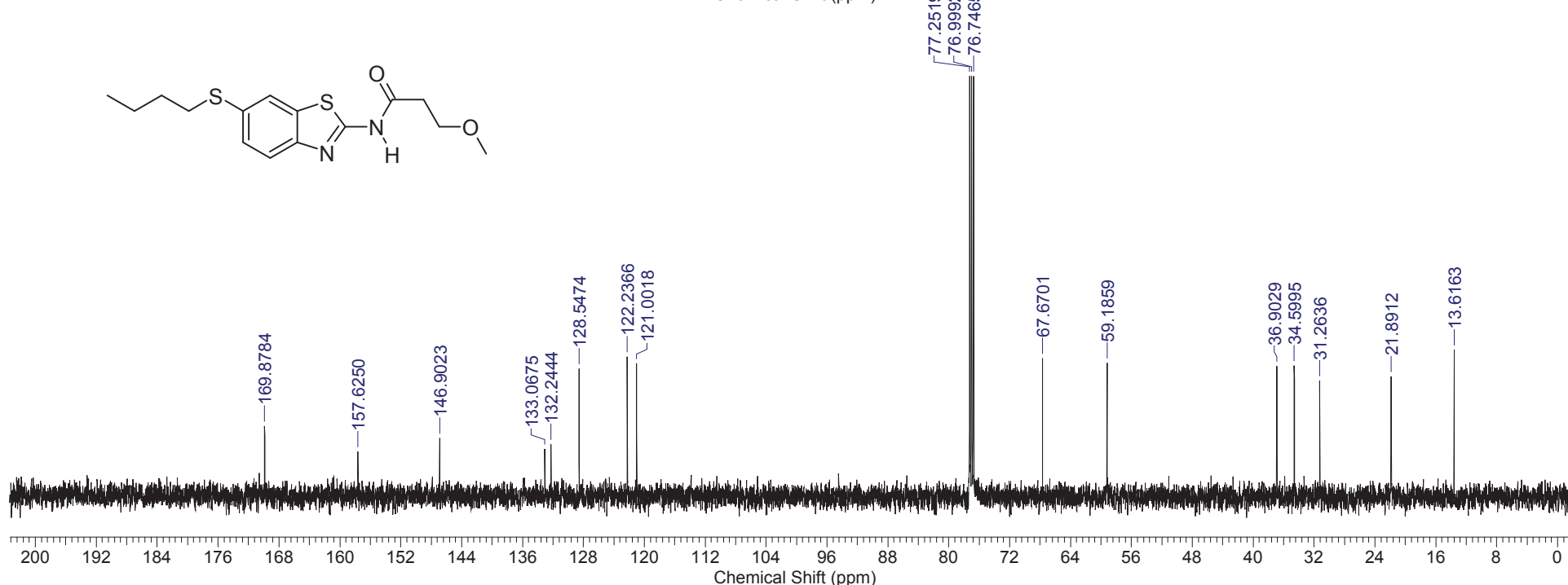
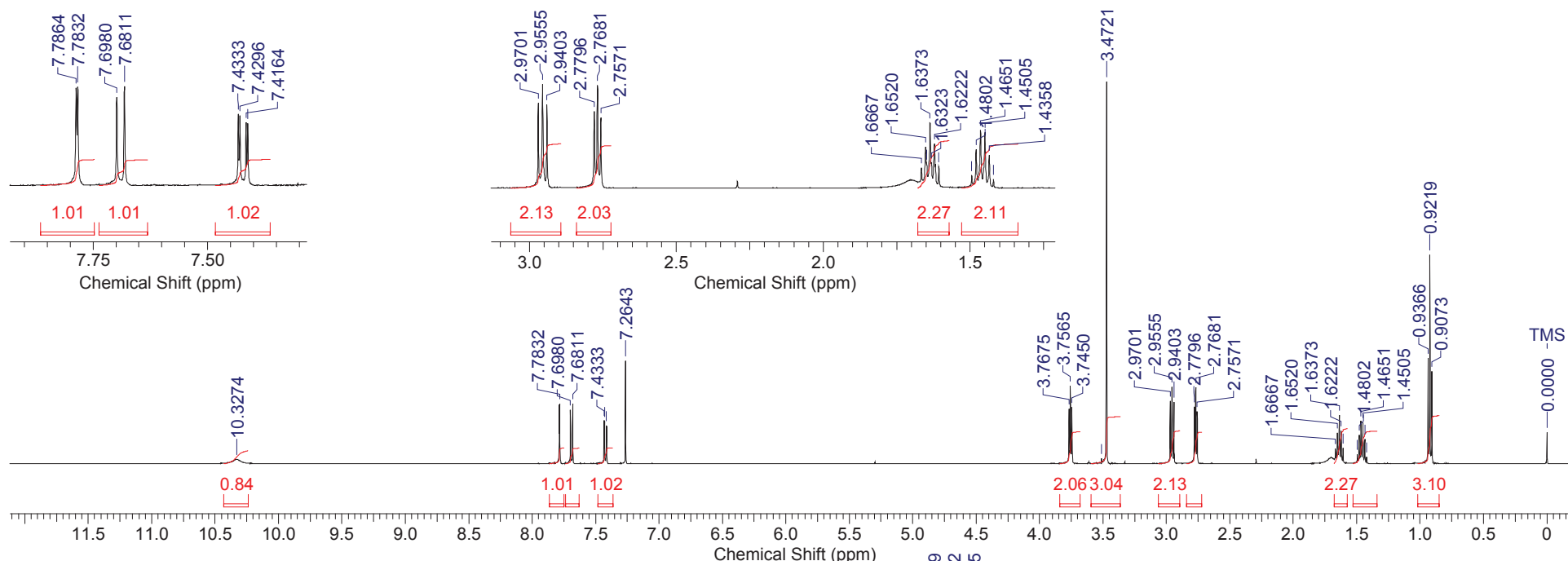
***N*-[6-(butylsulfanyl)-1,3-benzothiazol-2-yl]-2-methoxyacetamide (43)**



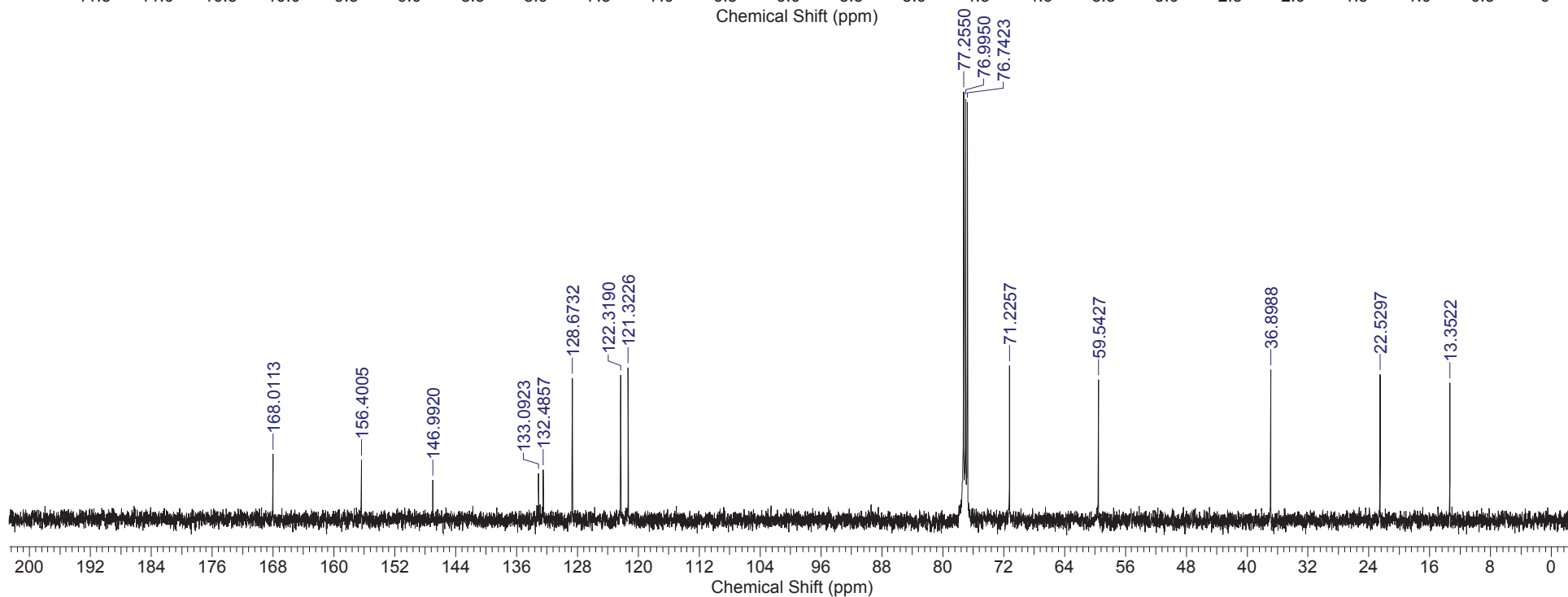
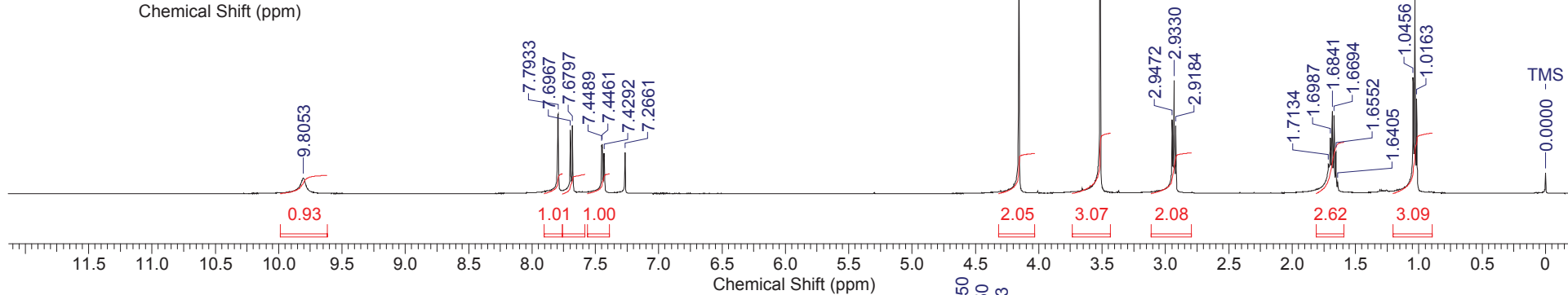
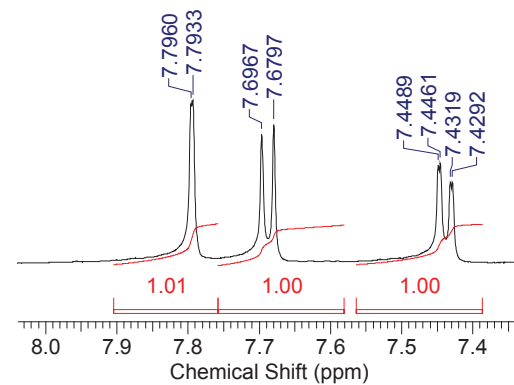
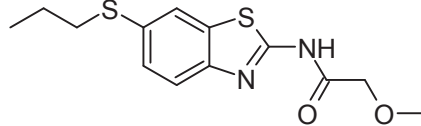
3-Methoxy-N-[6-(propylsulfanyl)-1,3-benzothiazol-2-yl]propanamide (44)



N-[6-(butylsulfanyl)-1,3-benzothiazol-2-yl]-3-methoxypropanamide (45)

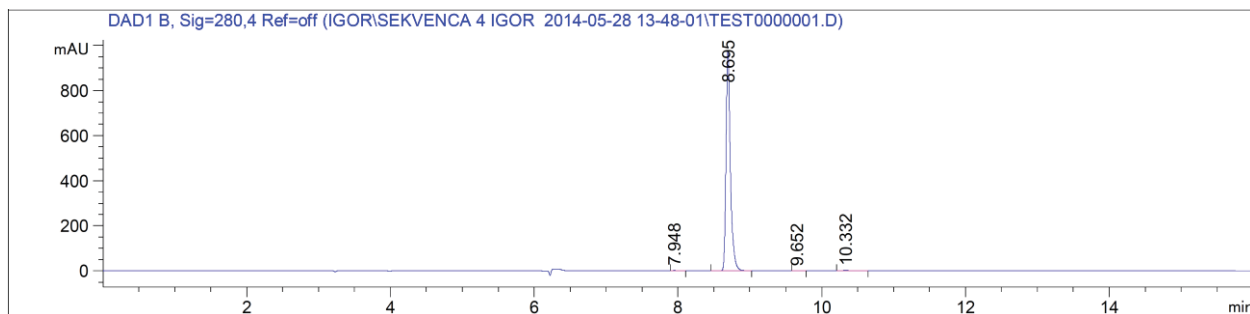


2-Methoxy-N-[6-(propylsulfanyl)-1,3-benzothiazol-2-yl]acetamide (46)



Compound 24

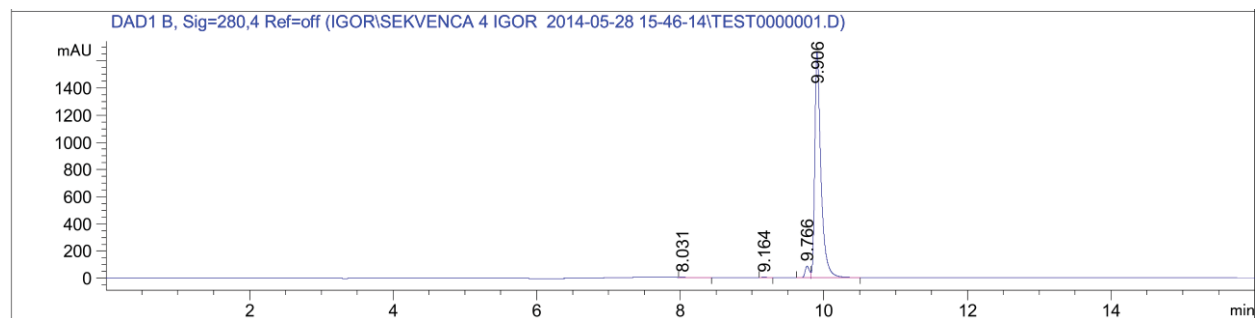
Method A



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.948	VB	0.0617	7.96617	1.83315	0.1917
2	8.695	BV	0.0629	4126.12646	974.99304	99.2674
3	9.652	VB	0.0695	6.04993	1.22706	0.1456
4	10.332	BB	0.0802	16.43694	3.00826	0.3954

Totals : 4156.57950 981.06152

Method B

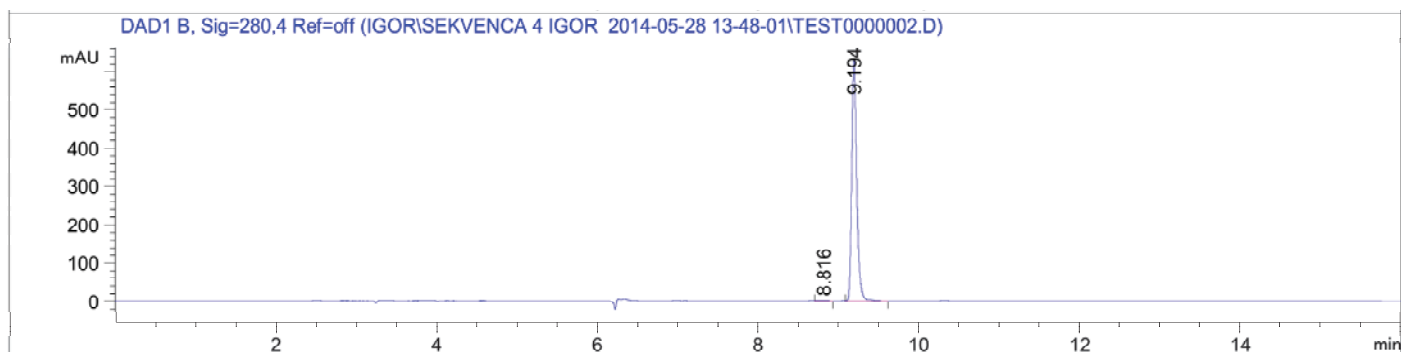


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.031	BB	0.0718	6.55642	1.12026	0.0634
2	9.164	VB	0.0681	21.51386	4.68658	0.2080
3	9.766	VV	0.0649	355.59402	84.86288	3.4376
4	9.906	VV	0.0886	9960.69824	1658.69763	96.2911

Totals : 1.03444e4 1749.36736

Compound 25

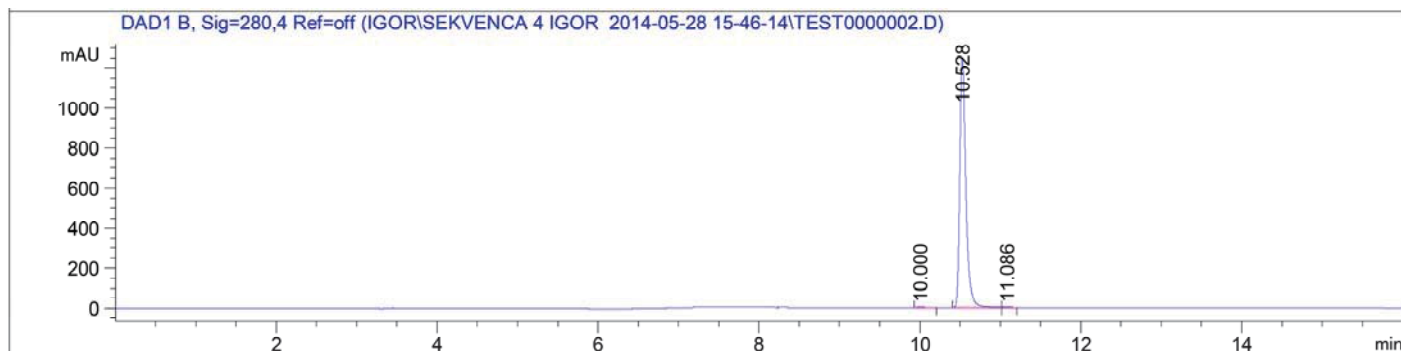
Method A



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.816	VB	0.0717	8.93553	1.70391	0.3236
2	9.194	VB	0.0663	2752.14233	631.74182	99.6764

Totals : 2761.07786 633.44573

Method B

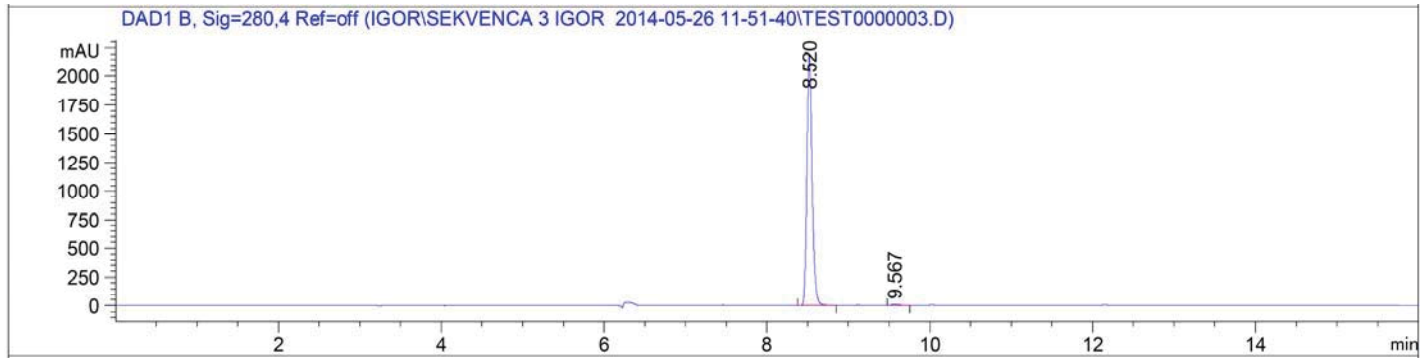


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.000	VB	0.0717	18.14887	3.70130	0.2753
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3	11.086	VV	0.0739	18.49010	3.48700	0.2805

Totals : 6592.45098 1259.54743

Compound 26

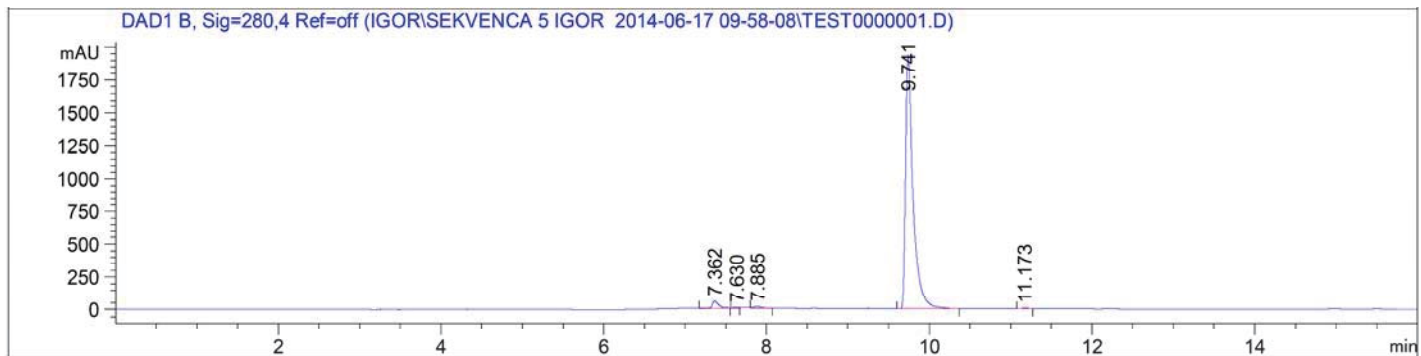
Method A



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.520	BV	0.0666	9746.07520	2203.58862	99.4835
2	9.567	VB	0.0724	50.60378	10.10886	0.5165

Totals : 9796.67897 2213.69748

Method B

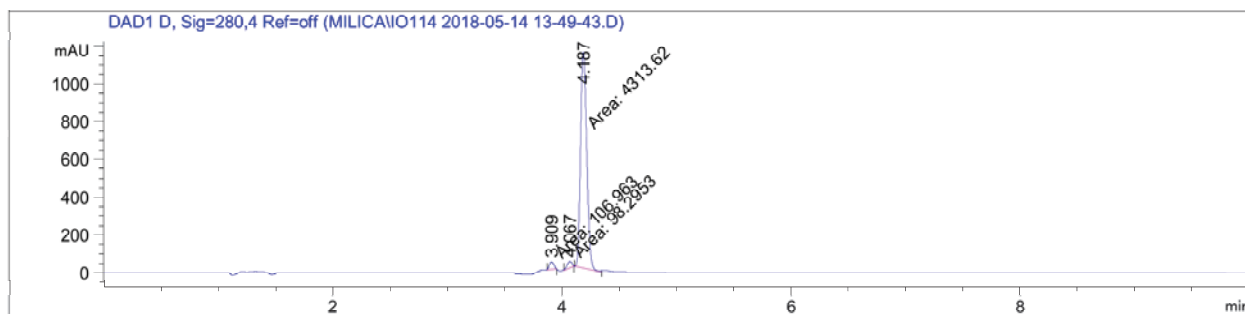


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.362	VB	0.0838	302.88644	54.09494	2.3456
2	7.630	BV	0.0585	6.52400	1.35821	0.0505
3	7.885	VB	0.0850	72.29404	12.88054	0.5599
4	9.741	BB	0.0933	1.24853e4	1935.00427	96.6898
5	11.173	BV	0.0779	45.73245	8.68949	0.3542

Totals : 1.29127e4 2012.02745

Compound 27

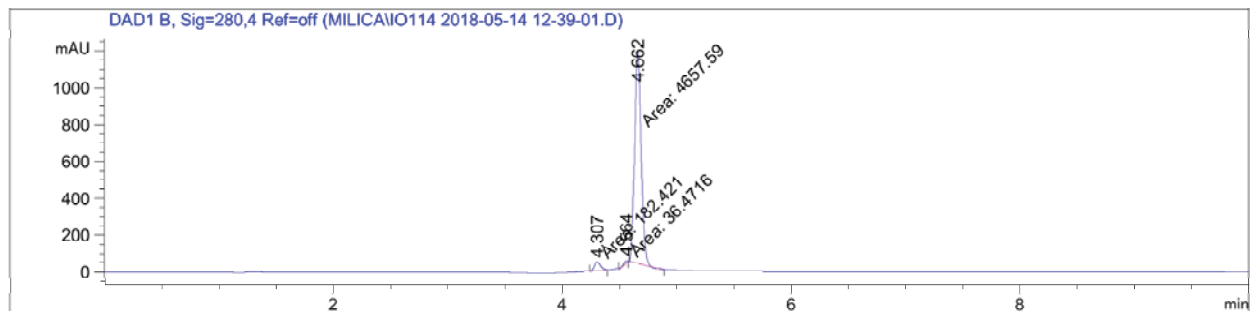
Method D



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.909	MM T	0.0459	106.96311	38.84392	2.3670
2	4.067	MM T	0.0484	98.29530	33.84376	2.1752
3	4.187	MM T	0.0629	4313.61621	1142.71313	95.4578

Totals : 4518.87462 1215.40081

Method I

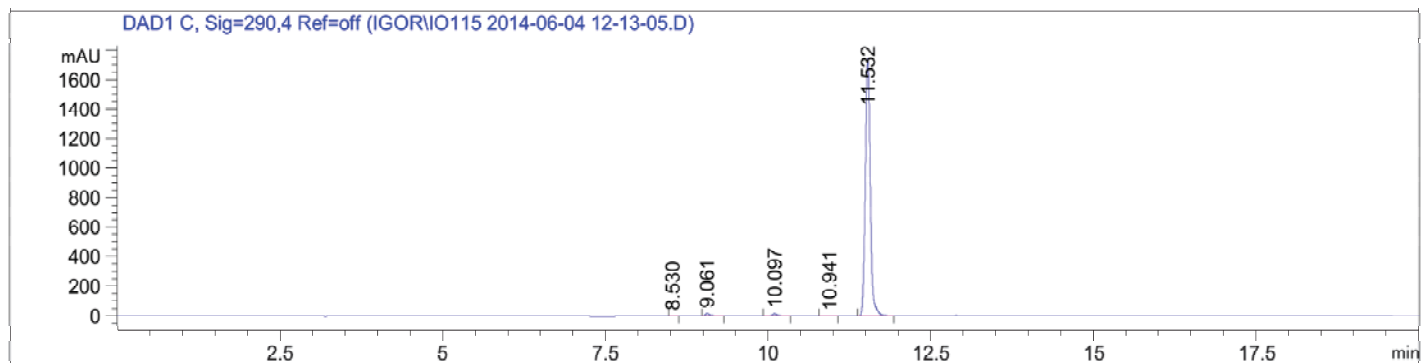


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.307	MM	0.0662	182.42131	45.94308	3.7408
2	4.564	MM	0.0420	36.47161	14.45628	0.7479
3	4.662	MM	0.0670	4657.58984	1158.74329	95.5113

Totals : 4876.48277 1219.14265

Compound 28

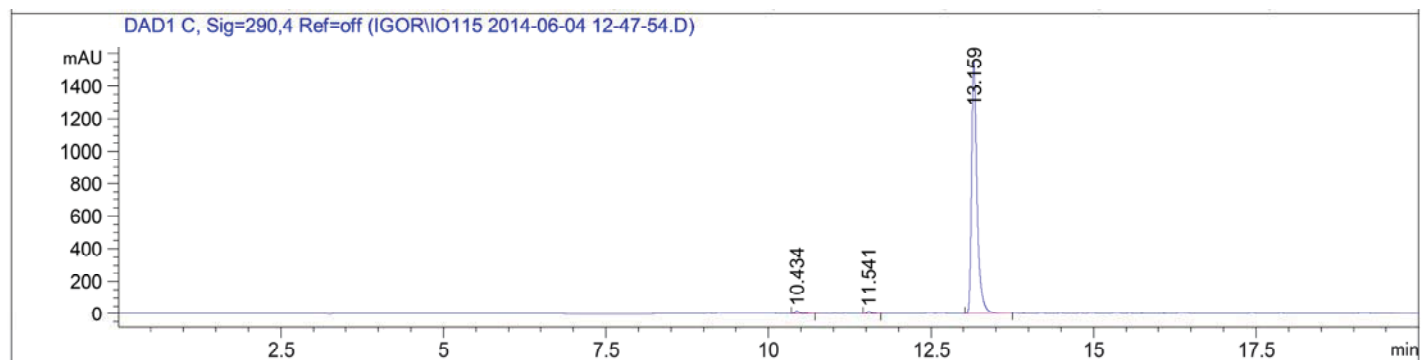
Method A



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.530	BB	0.0607	5.36399	1.15433	0.0570
2	9.061	BB	0.0712	76.62478	15.75676	0.8136
3	10.097	BB	0.0689	74.93712	15.64029	0.7957
4	10.941	BB	0.0937	9.76336	1.26288	0.1037
5	11.532	BB	0.0814	9250.86523	1742.87146	98.2300

Totals : 9417.55448 1776.68572

Method B

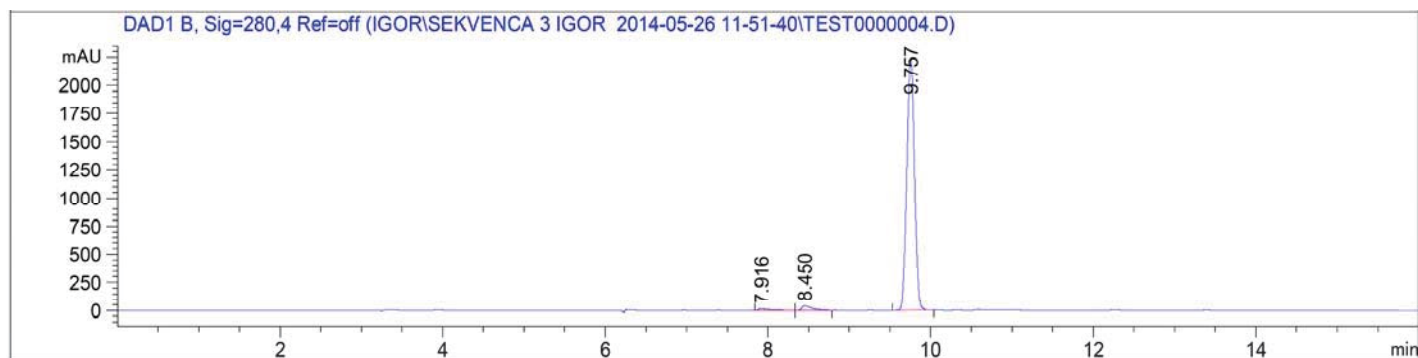


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.434	BB	0.0724	76.64764	15.58902	0.8304
2	11.541	BB	0.0692	59.26611	12.88552	0.6421
3	13.159	BB	0.0876	9093.89160	1557.28979	98.5274

Totals : 9229.80535 1585.76434

Compound 29

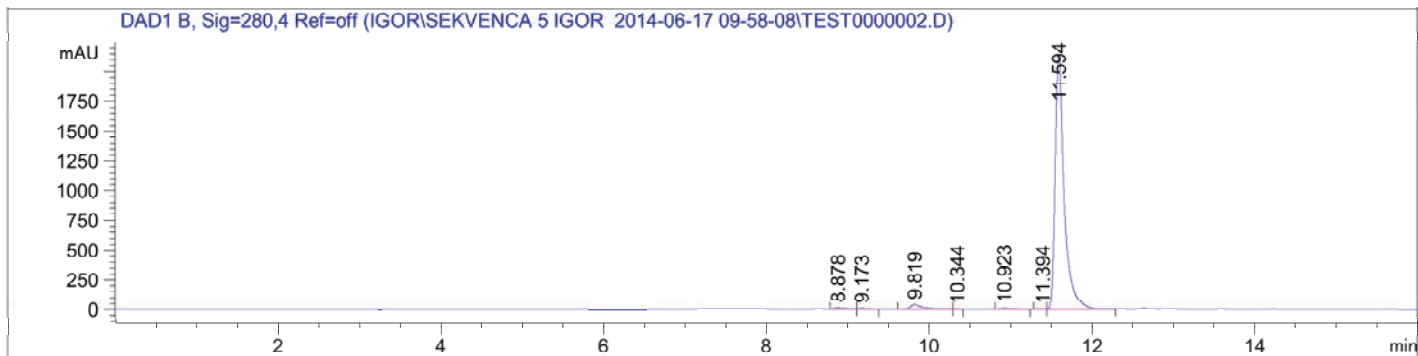
Method A



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.916	BB	0.1105	117.37466	14.04834	0.7710
2	8.450	BV	0.1094	326.26669	40.54747	2.1433
3	9.757	BB	0.1021	1.47793e4	2236.46240	97.0857

Totals : 1.52230e4 2291.05822

Method B

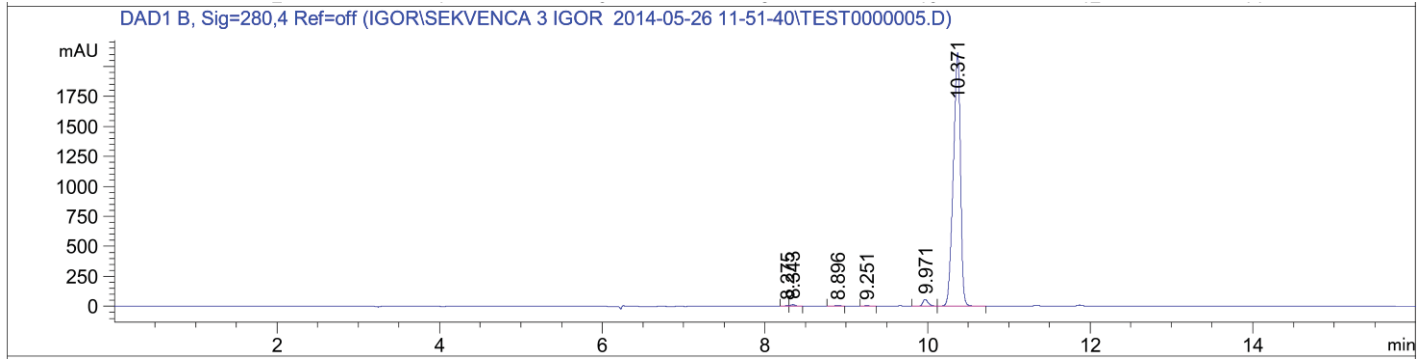


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.878	VV	0.1371	113.55533	11.26979	0.6620
2	9.173	VB	0.0824	46.79509	8.03767	0.2728
3	9.819	BV	0.1457	419.87234	39.27106	2.4478
4	10.344	VV	0.0739	5.74360	1.00211	0.0335
5	10.923	BB	0.1006	55.58533	7.89578	0.3241
6	11.394	BV	0.0692	21.35677	4.10480	0.1245
7	11.594	VV	0.1140	1.64902e4	2136.43848	96.1353

Totals : 1.71531e4 2208.01969

Compound 30

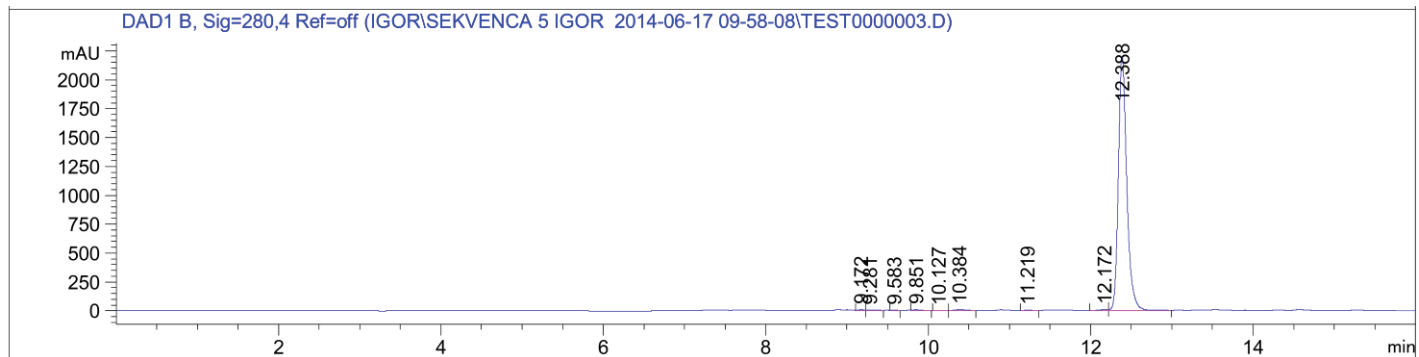
Method A



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.275	BV	0.0469	20.01075	6.49592	0.1492
2	8.343	VB	0.0614	61.09449	14.56748	0.4555
3	8.896	BV	0.0789	46.91047	8.49947	0.3497
4	9.251	BB	0.0642	28.99215	6.74384	0.2161
5	9.971	BV	0.0716	277.29309	58.21828	2.0673
6	10.371	VB	0.0947	1.29791e4	2111.64697	96.7622

Totals : 1.34134e4 2206.17197

Method B

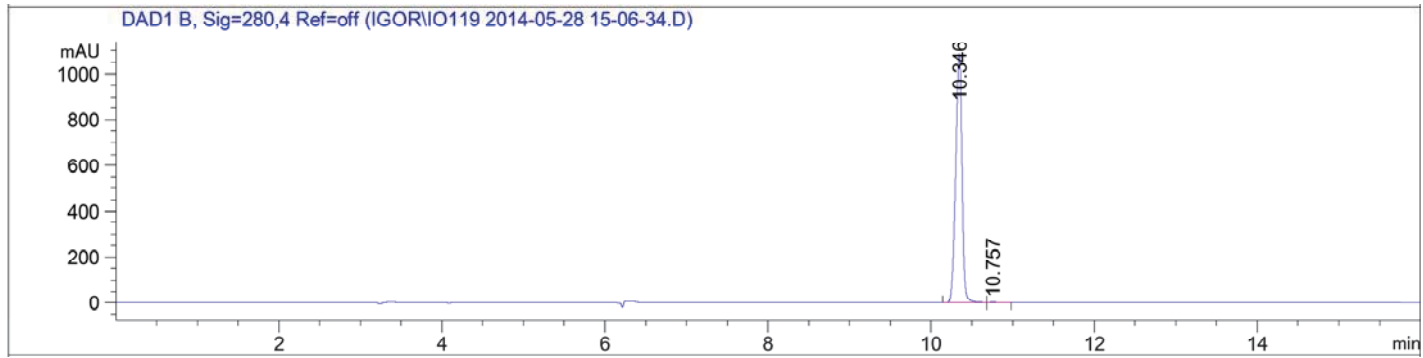


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.172	BV	0.0627	26.83034	6.49291	0.1670
2	9.281	VB	0.0854	26.67105	3.94525	0.1660
3	9.583	VB	0.0545	6.04534	1.68033	0.0376
4	9.851	VB	0.0745	34.98310	6.91304	0.2177
5	10.127	BV	0.0719	5.13864	1.04408	0.0320
6	10.384	VB	0.1162	65.84212	7.98751	0.4098
7	11.219	BV	0.0867	10.56188	1.69414	0.0657
8	12.172	BV	0.0823	52.63279	9.54319	0.3276
9	12.388	VV	0.1093	1.58389e4	2204.41016	98.5766

Totals : 1.60676e4 2243.71059

Compound 31

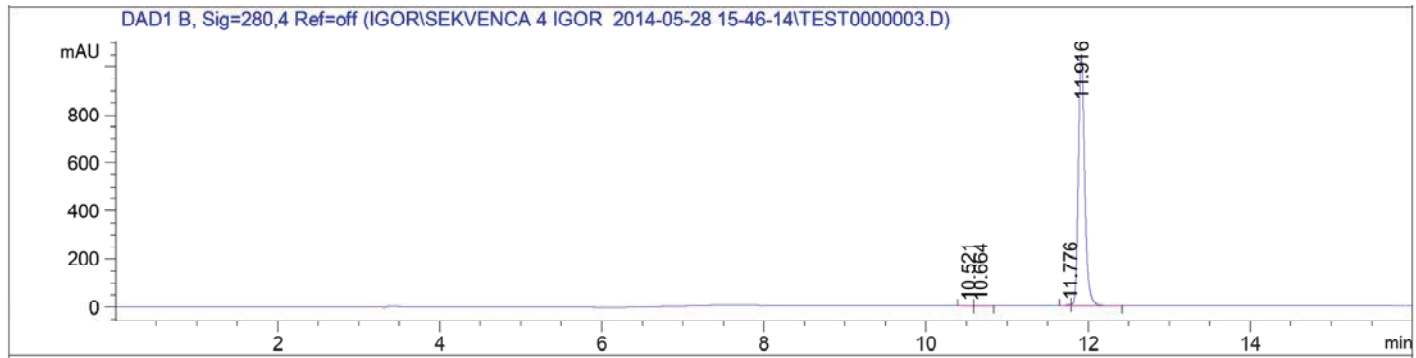
Method A



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.346	BV	0.0829	5861.91455	1088.05420	99.7836
2	10.757	VB	0.0885	12.71138	1.71536	0.2164

Totals : 5874.62593 1089.76956

Method B

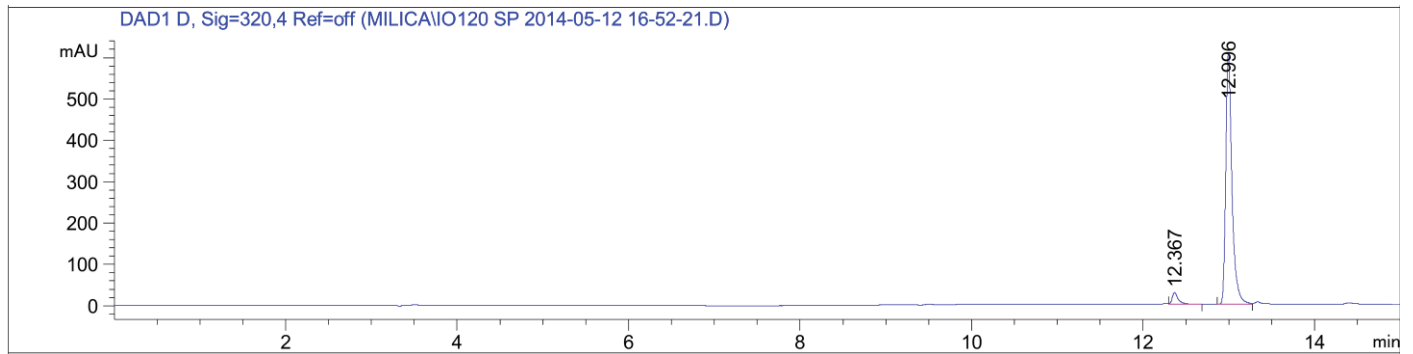


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.521	BV	0.0701	6.13881	1.05153	0.1061
2	10.664	VB	0.0988	9.43180	1.13715	0.1630
3	11.776	VV	0.0558	21.61969	5.50936	0.3735
4	11.916	VB	0.0833	5750.59912	1051.05920	99.3574

Totals : 5787.78942 1058.75725

Compound 32

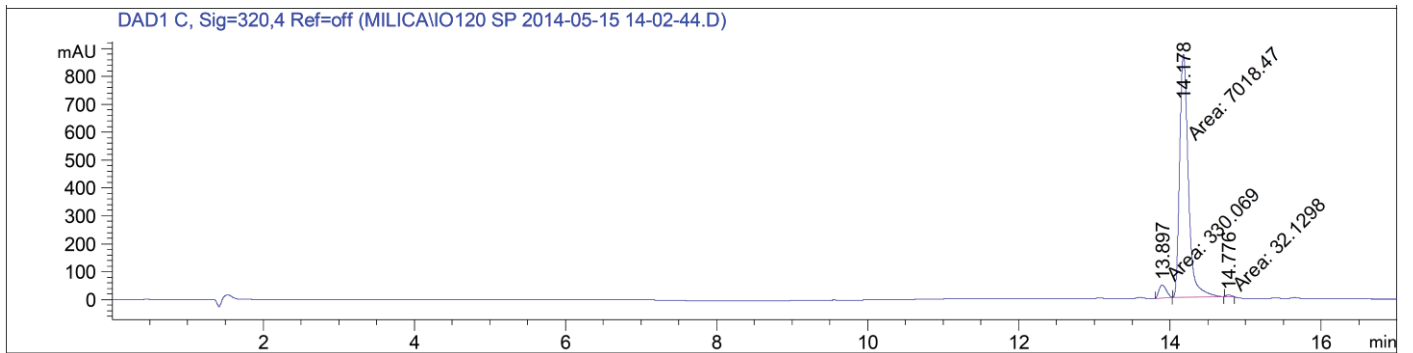
Method B



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.367	VB	0.0720	139.65514	28.32107	4.3899
2	12.996	BV	0.0750	3041.64331	606.90167	95.6101

Totals : 3181.29845 635.22274

Method C

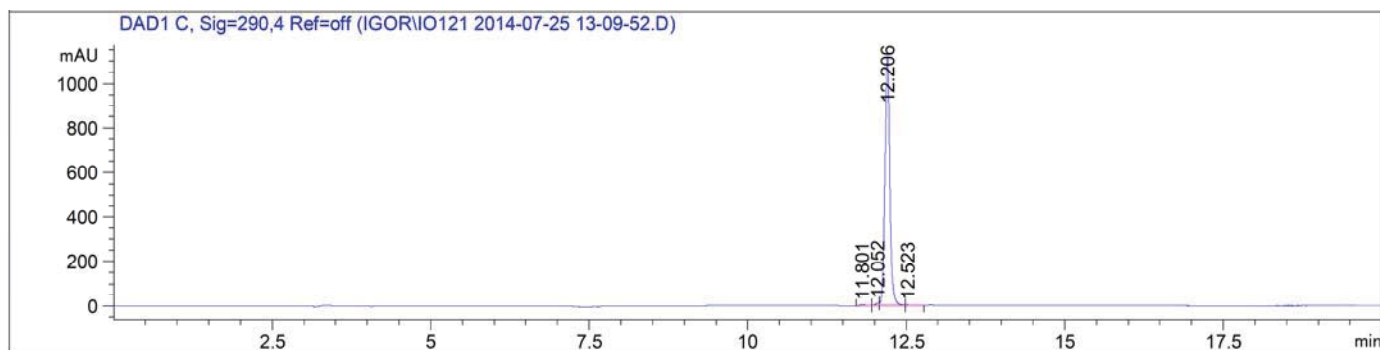


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.897	MM	0.1154	330.06851	47.66168	4.4721
2	14.178	MM	0.1340	7018.47363	872.82043	95.0926
3	14.776	MM	0.0867	32.12980	6.17982	0.4353

Totals : 7380.67194 926.66194

Compound 33

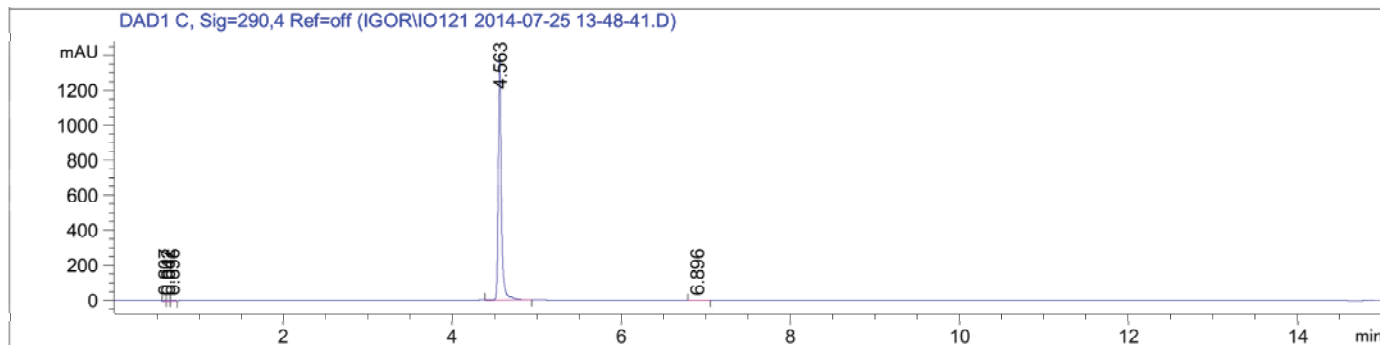
Method A



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.801	BV	0.0846	29.78626	4.85110	0.4858
2	12.052	VV	0.0574	45.10627	11.98949	0.7357
3	12.206	VV	0.0817	6040.41748	1115.09985	98.5224
4	12.523	VB	0.0858	15.70028	2.23816	0.2561

Totals : 6131.01029 1134.17860

Method D

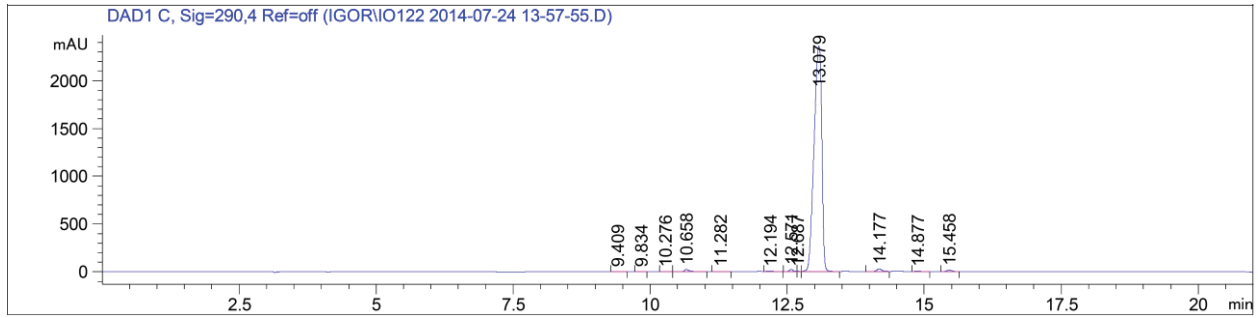


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	0.607	BV	0.0283	12.19010	6.99654	0.3359
2	0.642	VV	0.0405	19.72140	6.85805	0.5435
3	0.696	VB	0.0488	23.11195	5.70254	0.6369
4	4.563	VV	0.0376	3566.35620	1404.19775	98.2808
5	6.896	BB	0.0638	7.36203	1.42480	0.2029

Totals : 3628.74168 1425.17969

Compound 34

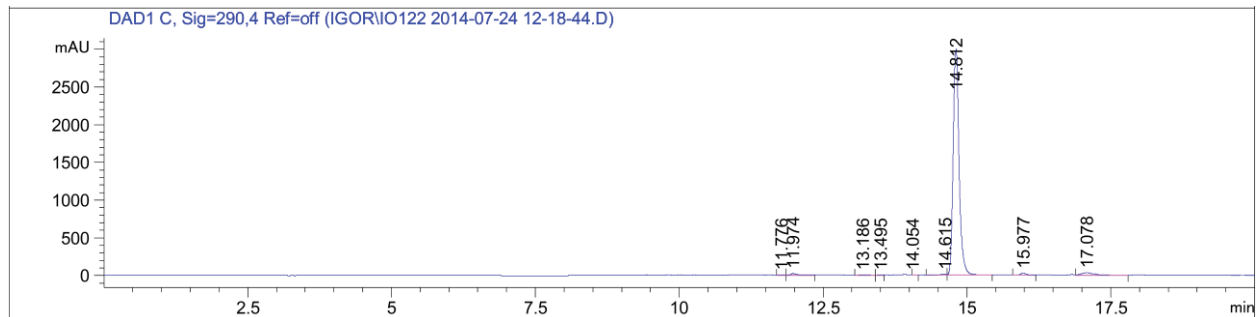
Method A



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.409	VB	0.0840	19.47042	3.07080	0.0812
2	9.834	BV	0.0691	11.49738	2.38935	0.0479
3	10.276	VB	0.0750	8.30582	1.32655	0.0346
4	10.658	BB	0.0942	162.55806	24.24324	0.6779
5	11.282	BB	0.0691	18.37643	3.42572	0.0766
6	12.194	VB	0.1075	53.07141	6.09947	0.2213
7	12.571	BV	0.0807	120.73660	22.64286	0.5035
8	12.687	VV	0.0502	12.25862	3.60272	0.0511
9	13.079	VB	0.1554	2.32185e4	2358.20410	96.8208
10	14.177	BV	0.0987	194.94652	29.08063	0.8129
11	14.877	VB	0.1015	53.42120	7.89237	0.2228
12	15.458	BV	0.1068	107.74665	15.66364	0.4493

Totals : 2.39809e4 2477.64144

Method B

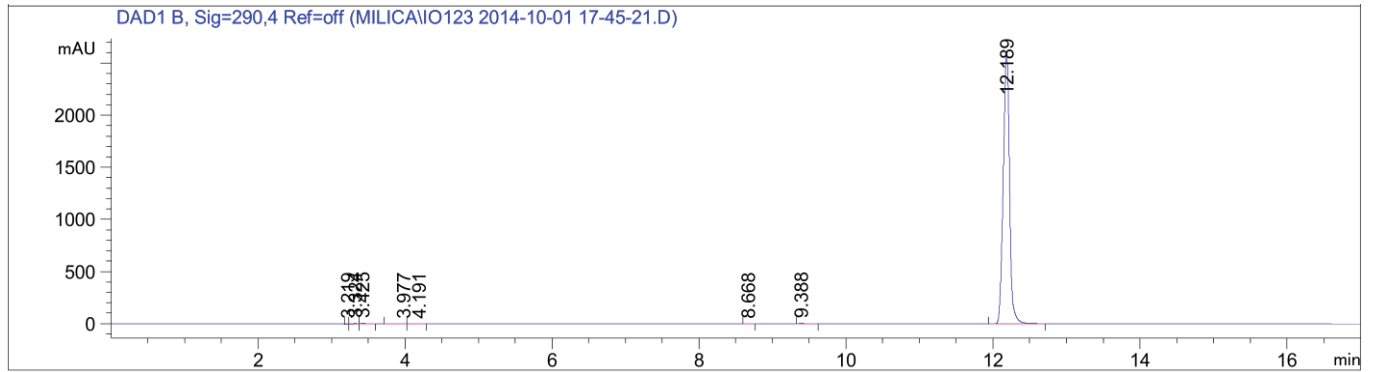


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.776	BV	0.0660	16.79807	3.69528	0.0747
2	11.974	VV	0.1120	172.34093	21.84600	0.7663
3	13.186	BB	0.0845	41.58721	7.18818	0.1849
4	13.495	BV	0.0691	12.87956	2.75376	0.0573
5	14.054	VB	0.0463	5.26249	1.44126	0.0234
6	14.615	BV	0.1003	78.20777	10.45106	0.3477
7	14.812	VB	0.1088	2.14802e4	2990.36816	95.5112
8	15.977	BV	0.0990	183.48778	27.81453	0.8159
9	17.078	VB	0.2225	498.94922	31.54800	2.2186

Totals : 2.24898e4 3097.10623

Compound 35

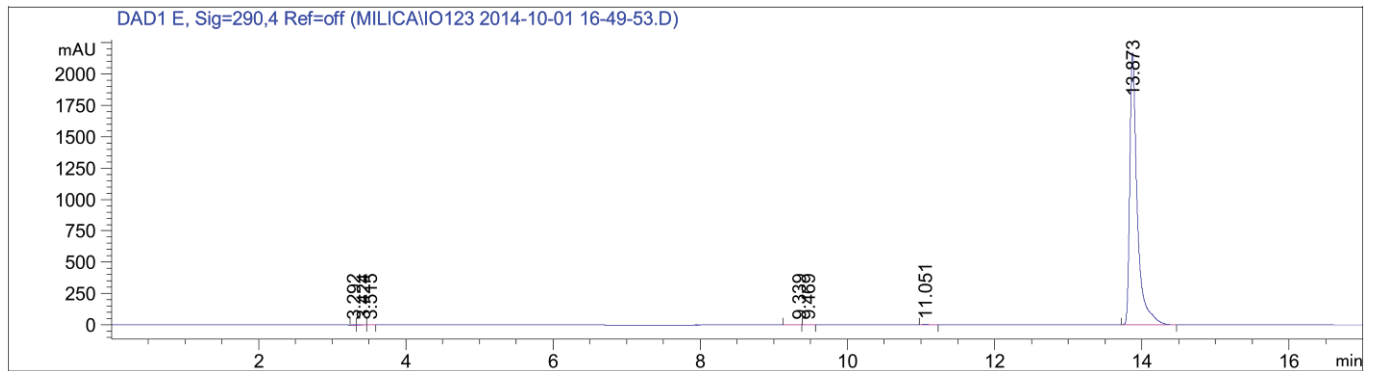
Method E



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.219	BV	0.0314	7.65493	3.65935	0.0491
2	3.324	VV	0.0848	34.13437	5.08736	0.2189
3	3.425	VB	0.0804	30.14030	4.66214	0.1933
4	3.977	BB	0.1157	39.34331	4.05623	0.2523
5	4.191	BB	0.1892	23.04424	1.43270	0.1478
6	8.668	BB	0.0646	8.63142	1.60764	0.0553
7	9.388	BV	0.0672	12.93848	2.42714	0.0830
8	12.189	BV	0.0916	1.54390e4	2606.72510	99.0004

Totals : 1.55949e4 2629.65766

Method F

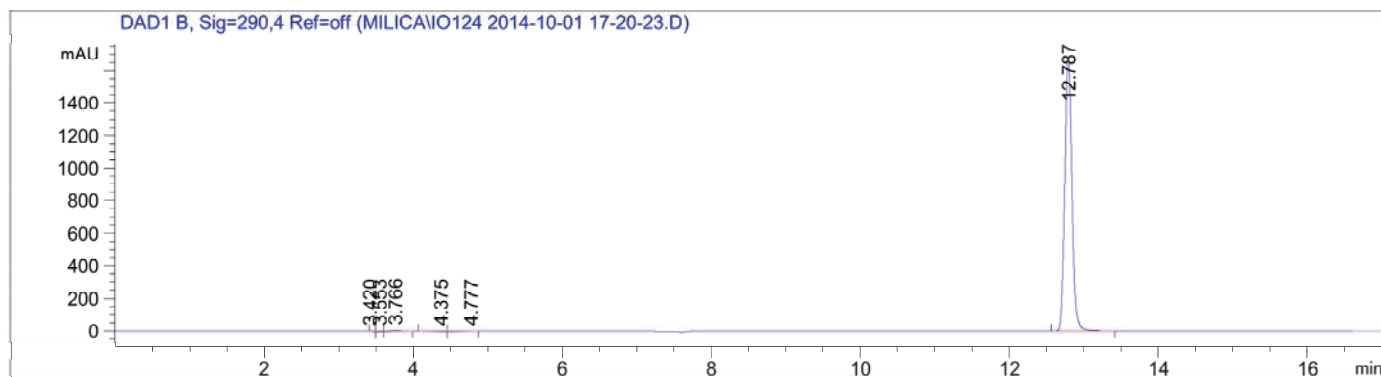


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.292	BV	0.0478	7.82498	2.51184	0.0510
2	3.424	VV	0.0758	13.51953	2.24448	0.0882
3	3.515	VV	0.0608	8.29779	1.80008	0.0541
4	9.339	BB	0.0868	11.69108	1.61725	0.0762
5	9.469	BB	0.0823	14.29541	2.09060	0.0932
6	11.051	BB	0.0623	7.85966	1.57350	0.0513
7	13.873	BB	0.1028	1.52714e4	2165.27759	99.5860

Totals : 1.53349e4 2177.11533

Compound 36

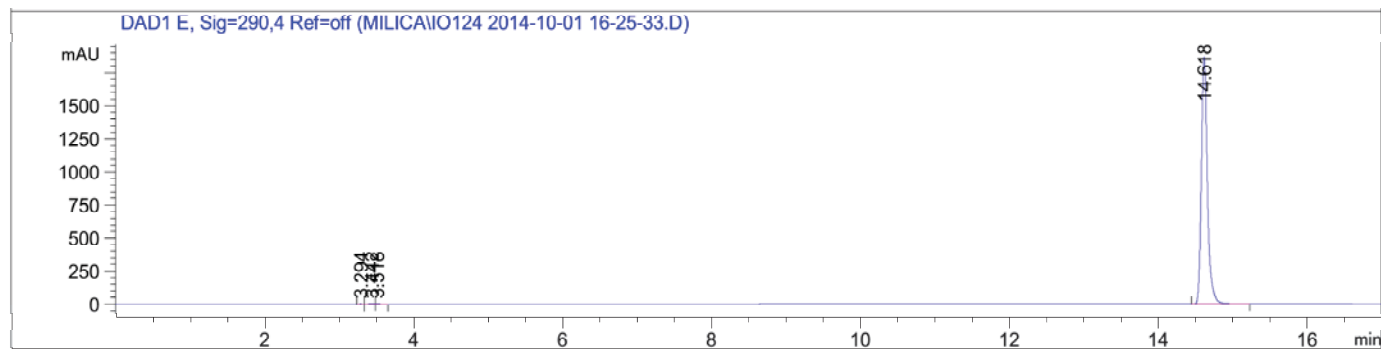
Method E



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.420	VB	0.0786	12.21035	1.85874	0.1070
2	3.553	BV	0.0646	19.17599	4.13624	0.1680
3	3.766	VB	0.1613	68.36065	5.02084	0.5988
4	4.375	VB	0.1621	63.53466	4.62847	0.5566
5	4.777	BV	0.4361	55.92376	1.50302	0.4899
6	12.787	BB	0.1028	1.11964e4	1680.02893	98.0798

Totals : 1.14156e4 1697.17624

Method F

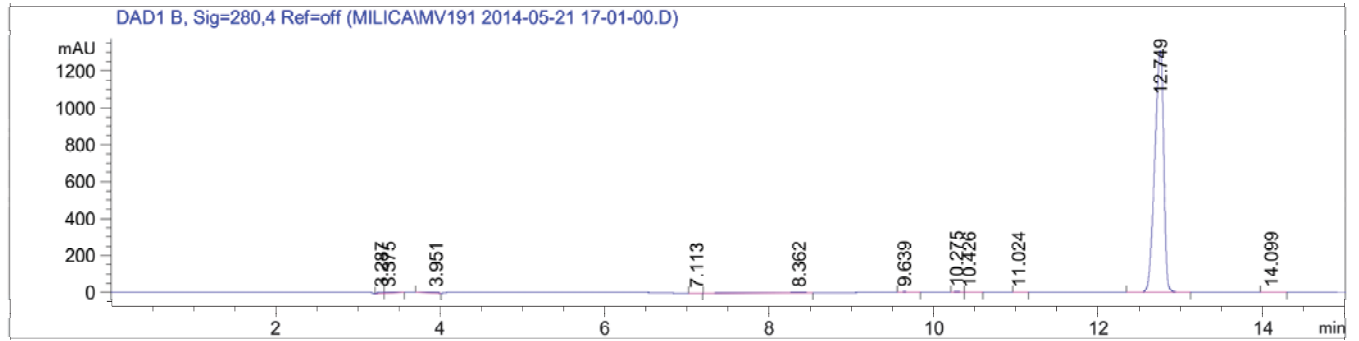


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.294	BB	0.0467	8.27530	2.56027	0.0783
2	3.442	BV	0.0689	12.08097	2.25774	0.1144
3	3.518	VB	0.0553	6.70089	1.49616	0.0634
4	14.618	BB	0.0852	1.05351e4	1871.61548	99.7438

Totals : 1.05622e4 1877.92965

Compound 37

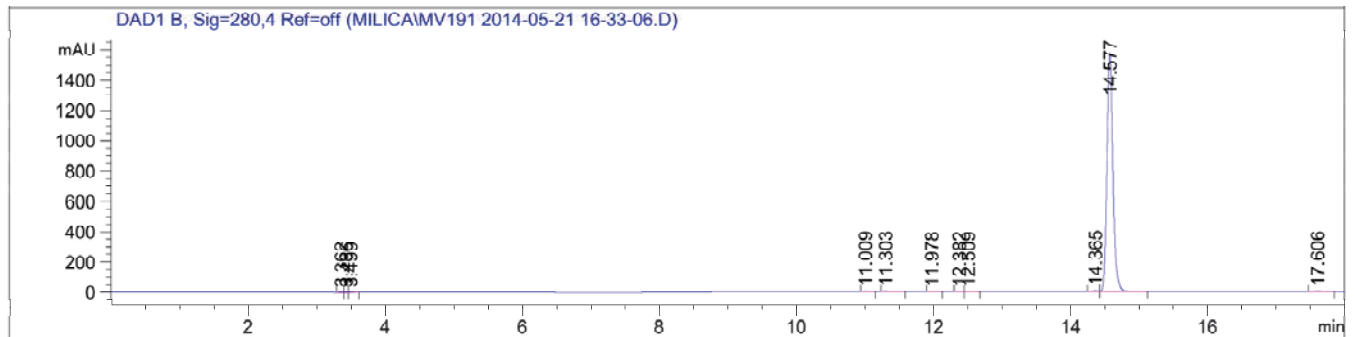
Method E



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.287	BV	0.0623	40.15187	7.70153	0.3912
2	3.375	VB	0.1063	51.78588	6.14679	0.5045
3	3.951	BB	0.1232	50.10155	4.80382	0.4881
4	7.113	BB	0.0830	11.90904	1.73623	0.1160
5	8.362	BB	1.1541	189.36116	1.91762	1.8449
6	9.639	BB	0.0652	16.38812	3.59243	0.1597
7	10.275	BV	0.0634	23.85492	5.30796	0.2324
8	10.426	VB	0.0609	12.14924	2.70593	0.1184
9	11.024	VB	0.0650	7.06059	1.49822	0.0688
10	12.749	BB	0.1177	9845.56738	1310.09668	95.9247
11	14.099	VB	0.1063	15.51829	1.73565	0.1512

Totals : 1.02638e4 1347.24285

Method F

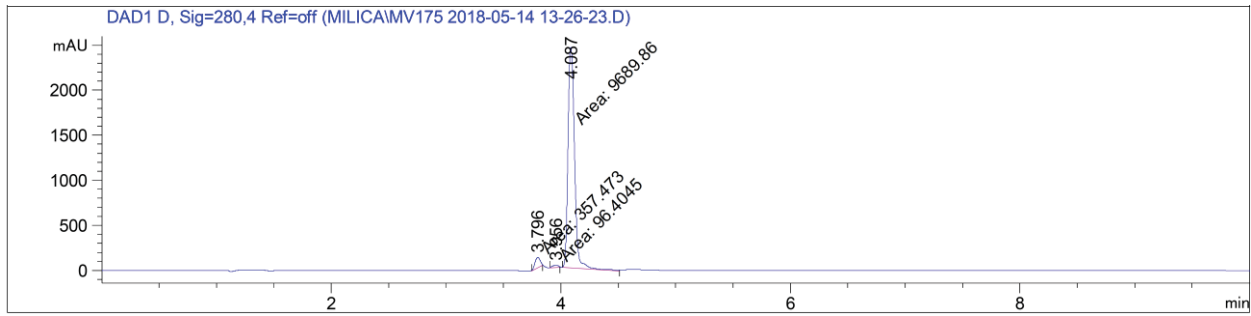


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.362	BV	0.0629	14.71013	3.30369	0.1506
2	3.436	VV	0.0480	9.40157	2.38329	0.0963
3	3.499	VD	0.0615	9.22804	1.80908	0.0945
4	11.009	VV	0.0709	17.31799	3.40314	0.1773
5	11.303	VB	0.0829	24.05853	4.16197	0.2463
6	11.978	BB	0.0608	8.98777	1.94900	0.0920
7	12.382	BV	0.0639	7.01079	1.46200	0.0718
8	12.509	VB	0.0688	8.21085	1.43460	0.0841
9	14.365	BV	0.0814	40.17031	7.45145	0.4113
10	14.577	VB	0.0921	9596.25293	1584.67627	98.2547
11	17.606	BB	0.1110	31.36051	3.38744	0.3211

Totals : 9766.71023 1615.50354

Compound 38

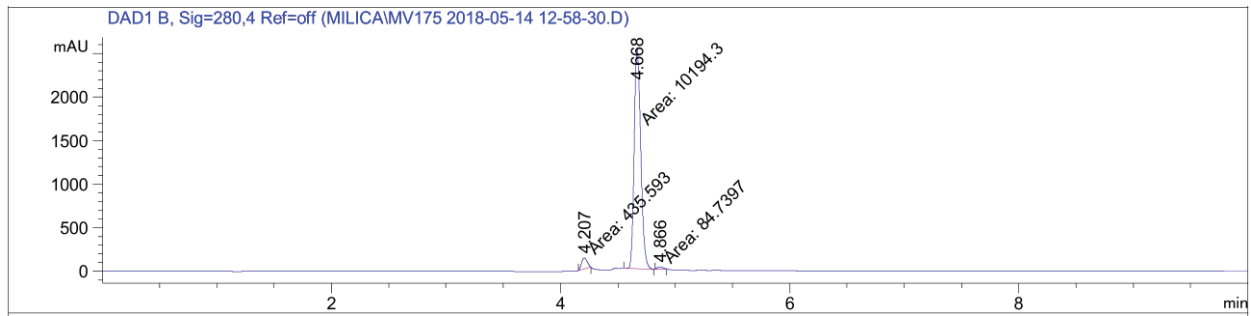
Method D



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.796	MM	0.0520	357.47327	114.65036	3.5241
2	3.956	MM	0.0609	96.40455	26.38447	0.9504
3	4.087	PM	0.0660	9689.86426	2446.78760	95.5255

Totals : 1.01437e4 2587.82242

Method I

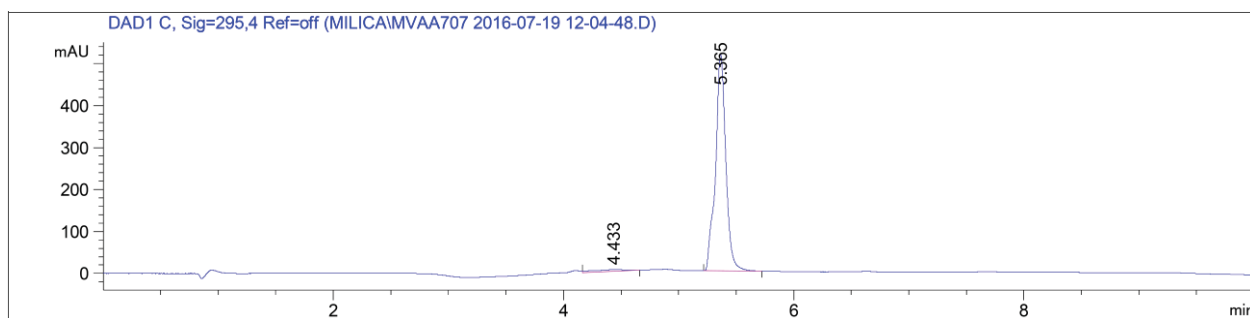


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.207	MM	0.0567	435.59323	127.98046	4.0654
2	4.668	MM	0.0671	1.01943e4	2533.91016	95.1437
3	4.866	MM	0.0596	84.73974	23.69610	0.7909

Totals : 1.07146e4 2685.58672

Compound 39

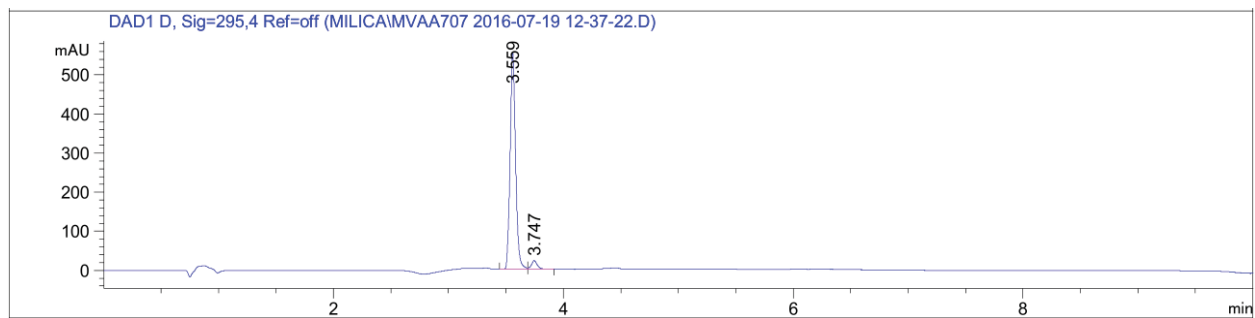
Method G



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.433	VB	0.2505	83.26959	3.90222	2.5051
2	5.365	BB	0.0920	3240.73975	518.19855	97.4949

Totals : 3324.00934 522.10077

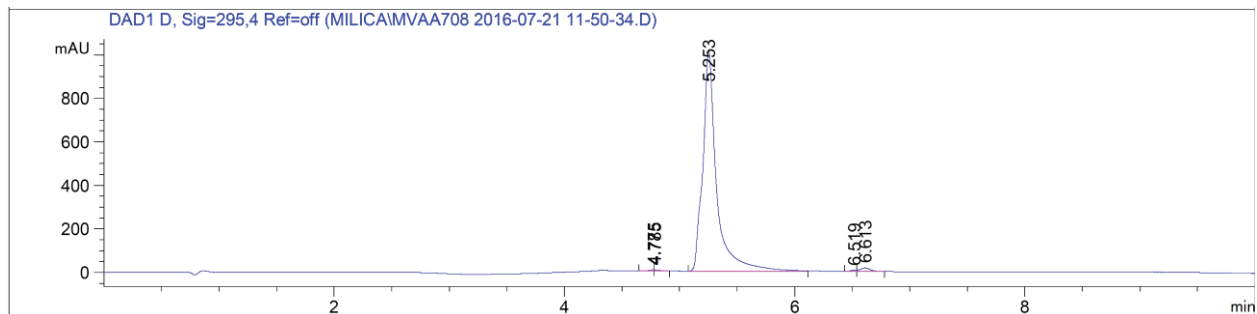
Method H



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.559	BV	0.0489	1826.13672	554.94464	96.0285
2	3.747	VB	0.0502	75.52365	21.89476	3.9715

Totals : 1901.66037 576.83940

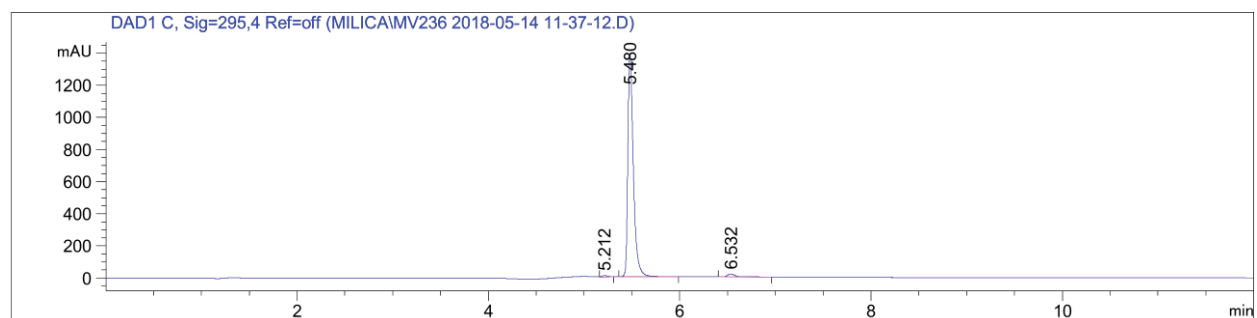
Compound 40
Method G



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.775	BV	0.0404	14.61637	4.44512	0.1699
2	4.785	VV	0.0443	15.74085	4.39078	0.1829
3	5.253	BV	0.1151	8451.55859	1015.08490	98.2119
4	6.519	BV	0.0419	20.98508	6.28678	0.2439
5	6.613	VV	0.0791	102.53422	16.71825	1.1915

Totals : 8605.43512 1046.92583

Method I

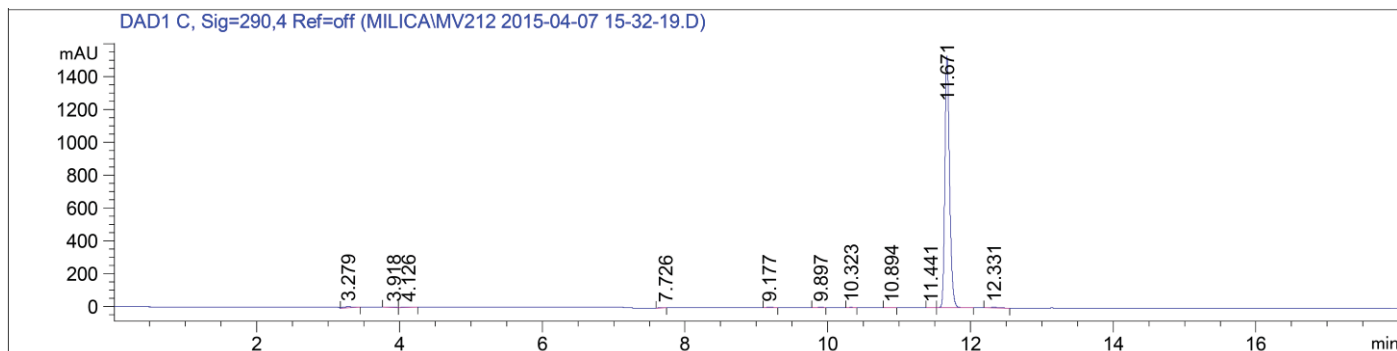


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.212	VB	0.0620	35.60748	8.38787	0.6258
2	5.480	BB	0.0606	5557.19482	1390.95215	97.6714
3	6.532	BB	0.0789	96.88428	18.26054	1.7028

Totals : 5689.68659 1417.60056

Compound 41

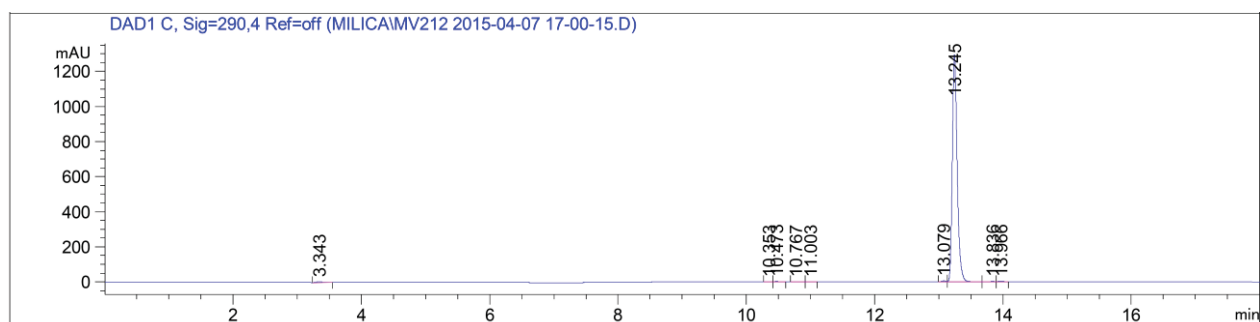
Method A



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.279	BB	0.1228	67.11901	6.45766	0.9223
2	3.918	BB	0.0902	26.12159	3.49566	0.3589
3	4.126	BB	0.1556	20.93233	1.58501	0.2876
4	7.726	BV	0.1221	11.71166	1.15708	0.1609
5	9.177	BB	0.0613	18.43113	4.31395	0.2533
6	9.897	BV	0.0588	11.11961	2.74531	0.1528
7	10.323	BB	0.0467	5.87741	1.60479	0.0808
8	10.894	BV	0.0690	5.80585	1.00335	0.0798
9	11.441	BV	0.0573	5.26474	1.13108	0.0723
10	11.671	VV	0.0701	7062.45605	1538.20361	97.0477
11	12.331	BB	0.1051	42.46464	5.49843	0.5835

Totals : 7277.30403 1567.19594

Method B

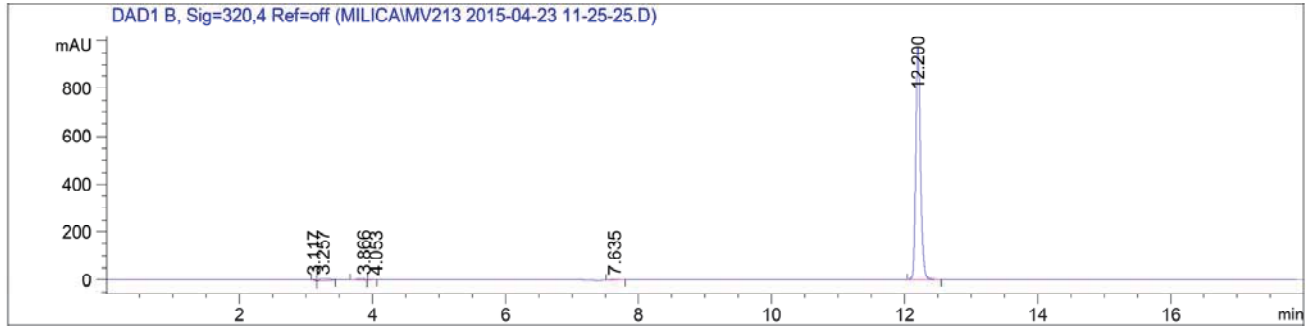


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.343	BB	0.1286	40.60603	3.74068	0.5851
2	10.353	BV	0.0579	6.48895	1.37935	0.0935
3	10.473	VB	0.0635	13.11559	2.78097	0.1890
4	10.767	BB	0.0550	6.69636	1.53055	0.0965
5	11.003	BV	0.0697	11.09414	2.24258	0.1599
6	13.079	VV	0.0652	25.40370	5.42055	0.3660
7	13.245	VB	0.0798	6802.09521	1294.56787	98.0107
8	13.836	BV	0.0738	12.20678	2.01039	0.1759
9	13.966	VV	0.0673	22.44621	4.41838	0.3234

Totals : 6940.15297 1318.09131

Compound 42

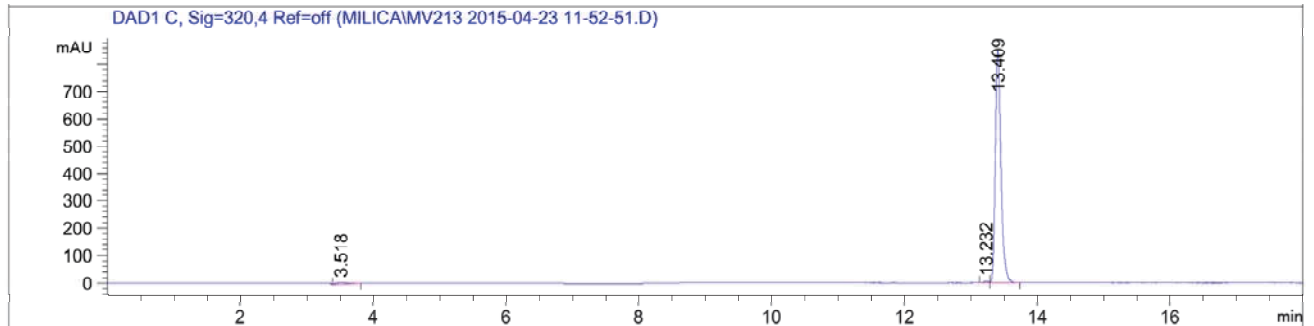
Method A



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.117	BB	0.0396	11.01781	3.37442	0.2216
2	3.257	BV	0.1288	85.84302	7.86738	1.7262
3	3.866	BB	0.0968	31.02504	3.86013	0.6239
4	4.053	BV	0.1171	14.04269	1.41689	0.2824
5	7.635	BB	0.1104	21.43383	2.30721	0.4310
6	12.200	BV	0.0751	4809.63574	973.71350	96.7150

Totals : 4972.99812 992.53953

Method B

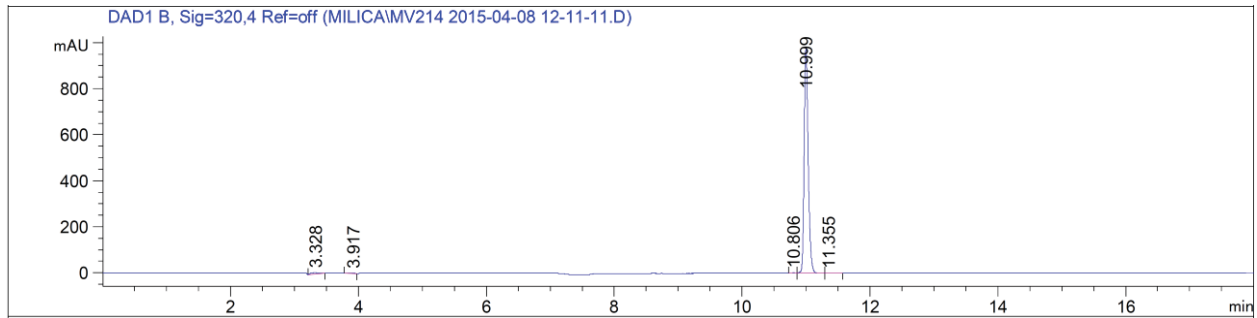


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.518	BB	0.1701	61.19653	4.31202	1.2009
2	13.232	VV	0.0652	31.47390	6.30860	0.6176
3	13.409	VV	0.0894	5003.37939	853.18292	98.1815

Totals : 5096.04982 863.80354

Compound 43

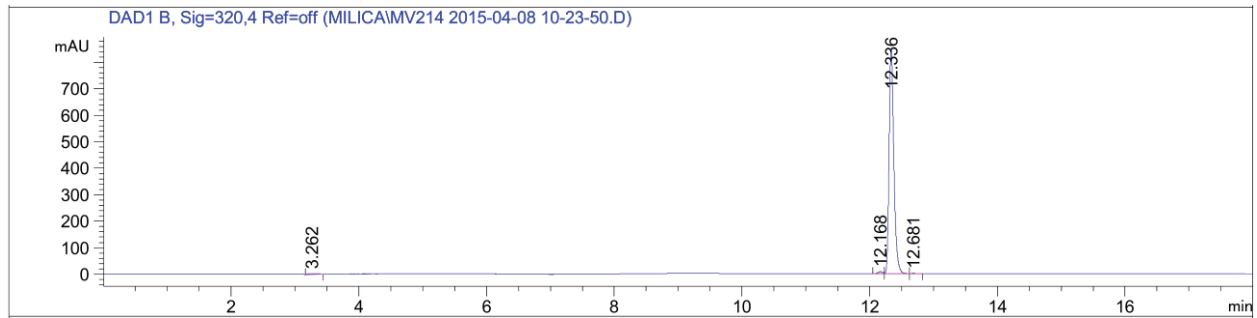
Method A



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.328	BB	0.1266	55.46625	5.19279	1.2645
2	3.917	BB	0.0761	15.86447	2.53360	0.3617
3	10.806	BV	0.0522	8.53832	2.22694	0.1946
4	10.999	VV	0.0666	4299.64014	980.83057	98.0194
5	11.355	VB	0.0736	7.01186	1.16684	0.1599

Totals : 4386.52104 991.95075

Method B

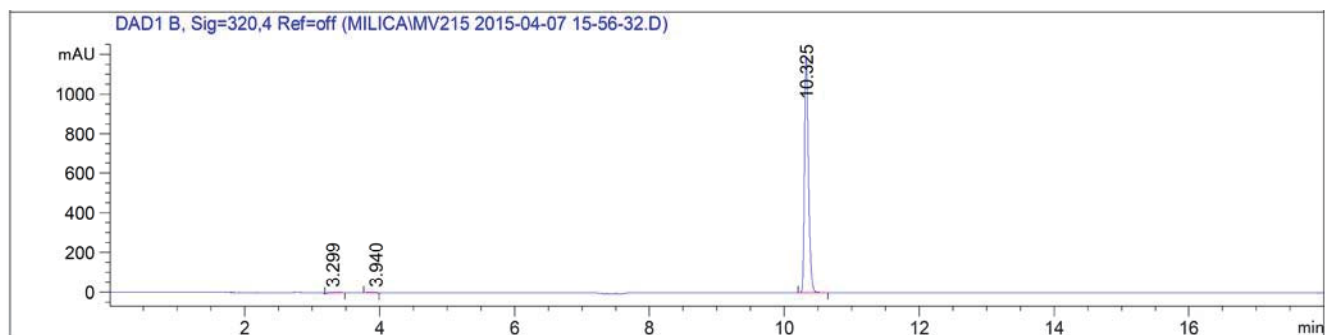


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.262	BB	0.1150	28.57027	2.95096	0.6412
2	12.168	BV	0.0759	37.86645	7.31183	0.8498
3	12.336	VV	0.0781	4383.45068	851.49292	98.3746
4	12.681	VB	0.0706	5.99057	1.04871	0.1344

Totals : 4455.87797 862.80442

Compound 44

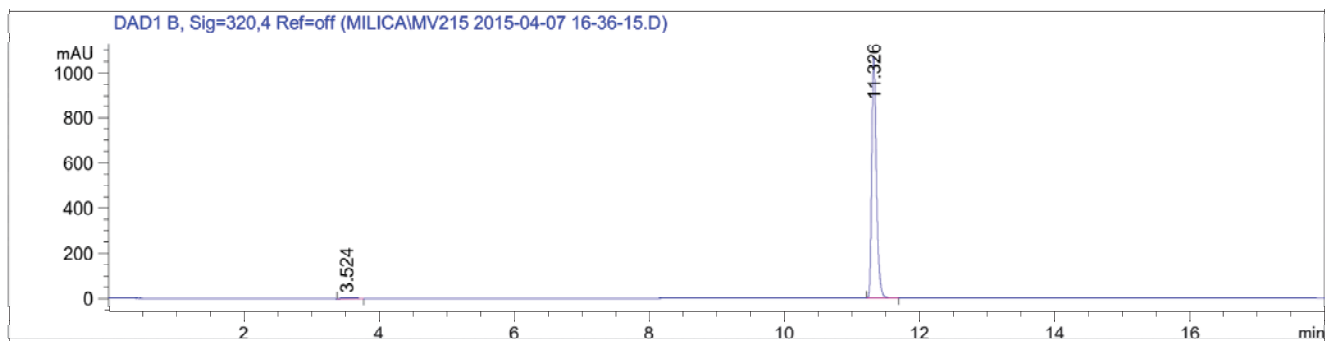
Method A



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.299	BB	0.1317	70.83684	6.44690	1.4166
2	3.940	BB	0.0904	24.75158	3.30314	0.4950
3	10.325	BB	0.0625	4904.98096	1193.25317	98.0884

Totals : 5000.56937 1203.00321

Method B

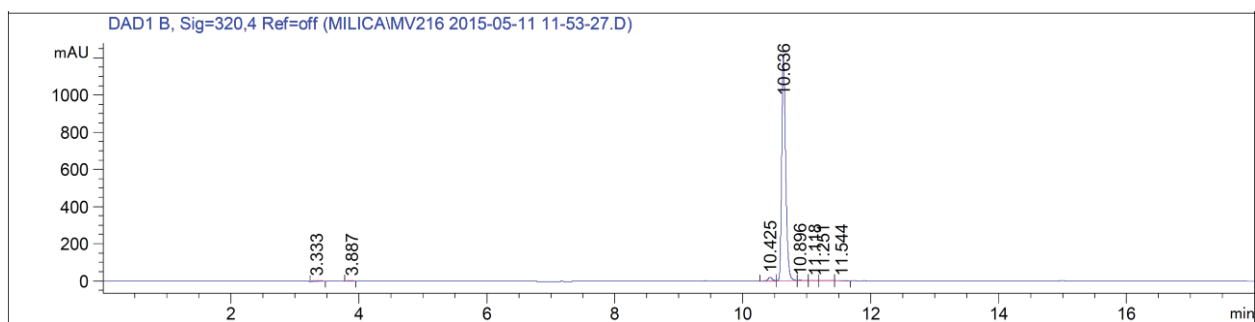


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.524	BB	0.1682	51.74959	3.62096	0.9970
2	11.326	VB	0.0728	5138.71777	1074.81470	99.0030

Totals : 5190.46737 1078.43565

Compound 45

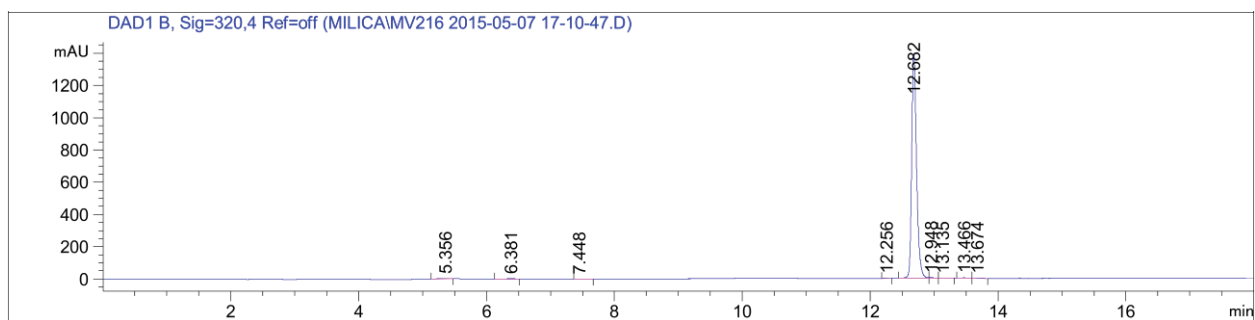
Method A



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.333	BB	0.1049	33.33364	3.76026	0.6157
2	3.887	BB	0.0664	8.45819	1.53256	0.1562
3	10.425	BV	0.0663	86.26466	19.61872	1.5934
4	10.636	VV	0.0652	5239.45166	1218.53650	96.7793
5	10.896	VB	0.0654	14.69987	3.03991	0.2715
6	11.118	BV	0.0565	8.38341	2.10221	0.1549
7	11.251	VB	0.0753	12.34537	2.43086	0.2280
8	11.544	BV	0.0917	10.87887	1.59247	0.2009

Totals : 5413.81568 1252.61350

Method B

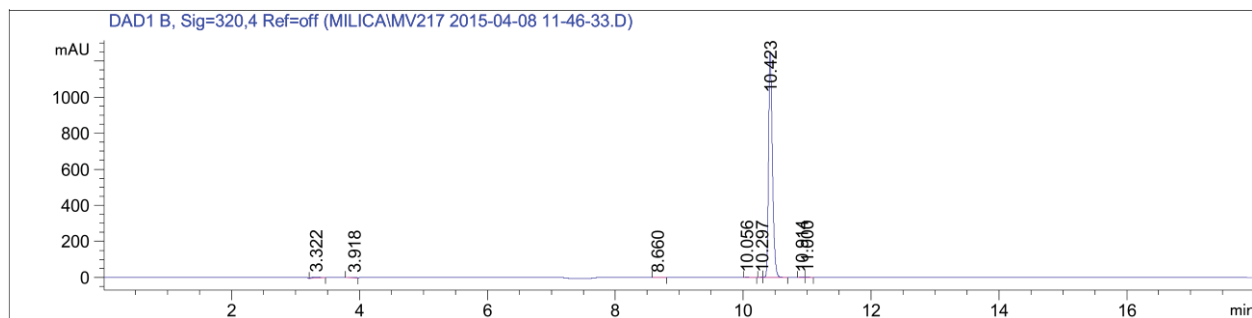


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.356	BB	0.1390	28.71872	2.44515	0.3842
2	6.381	BB	0.1209	26.31177	2.56992	0.3520
3	7.448	BB	0.1161	10.40156	1.05934	0.1392
4	12.256	BB	0.0565	8.84902	1.98496	0.1184
5	12.682	VV	0.0800	7347.05078	1394.32532	98.3001
6	12.948	VB	0.0602	15.74981	3.13033	0.2107
7	13.135	BB	0.0735	10.14757	1.64478	0.1358
8	13.466	BB	0.0826	20.40070	3.08569	0.2730
9	13.674	BB	0.0628	6.47551	1.24197	0.0866

Totals : 7474.10545 1411.48746

Compound 46

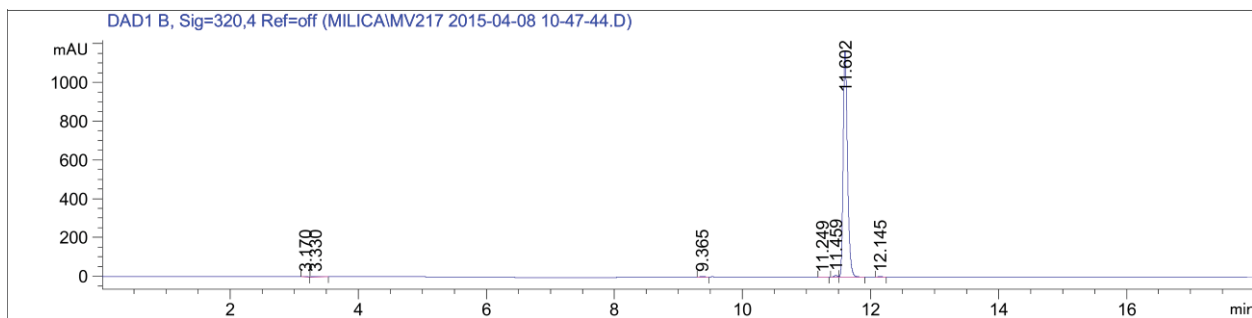
Method A



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.322	BB	0.1232	53.99484	5.22028	1.0018
2	3.918	BB	0.0809	16.78581	2.51314	0.3114
3	8.660	BB	0.0578	6.88864	1.59675	0.1278
4	10.056	VB	0.0634	12.67232	2.76709	0.2351
5	10.297	BV	0.0386	6.96599	2.57150	0.1292
6	10.423	VB	0.0641	5271.83545	1252.44641	97.8144
7	10.914	BV	0.0571	11.90407	3.01535	0.2209
8	11.000	VB	0.0543	8.58386	1.91585	0.1593

Totals : 5389.63097 1272.04637

Method B



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.170	BB	0.0746	8.63786	1.40733	0.1552
2	3.330	BB	0.1182	30.48904	3.07342	0.5479
3	9.365	BV	0.0639	5.61612	1.05864	0.1009
4	11.249	VB	0.0580	5.54772	1.19822	0.0997
5	11.459	BV	0.0635	31.97576	7.68591	0.5746
6	11.602	VB	0.0718	5470.48926	1165.11768	98.3023
7	12.145	BB	0.0581	12.20765	2.78685	0.2194

Totals : 5564.96340 1182.32805