

Supplementary data for the article:

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Supporting Information – II

New Steroidal 4-Aminoquinolines Antagonize Botulinum Neurotoxin Serotype A in Mouse Embryonic Stem Cell Derived Motor Neurons in Post-intoxication Model

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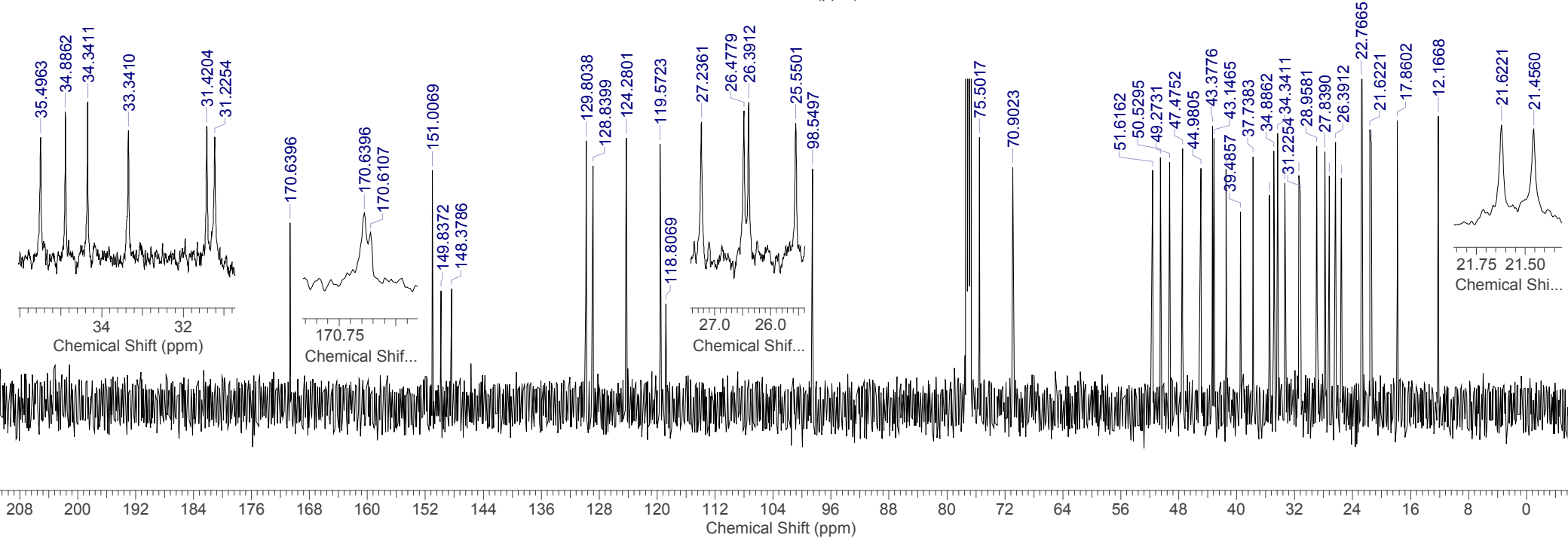
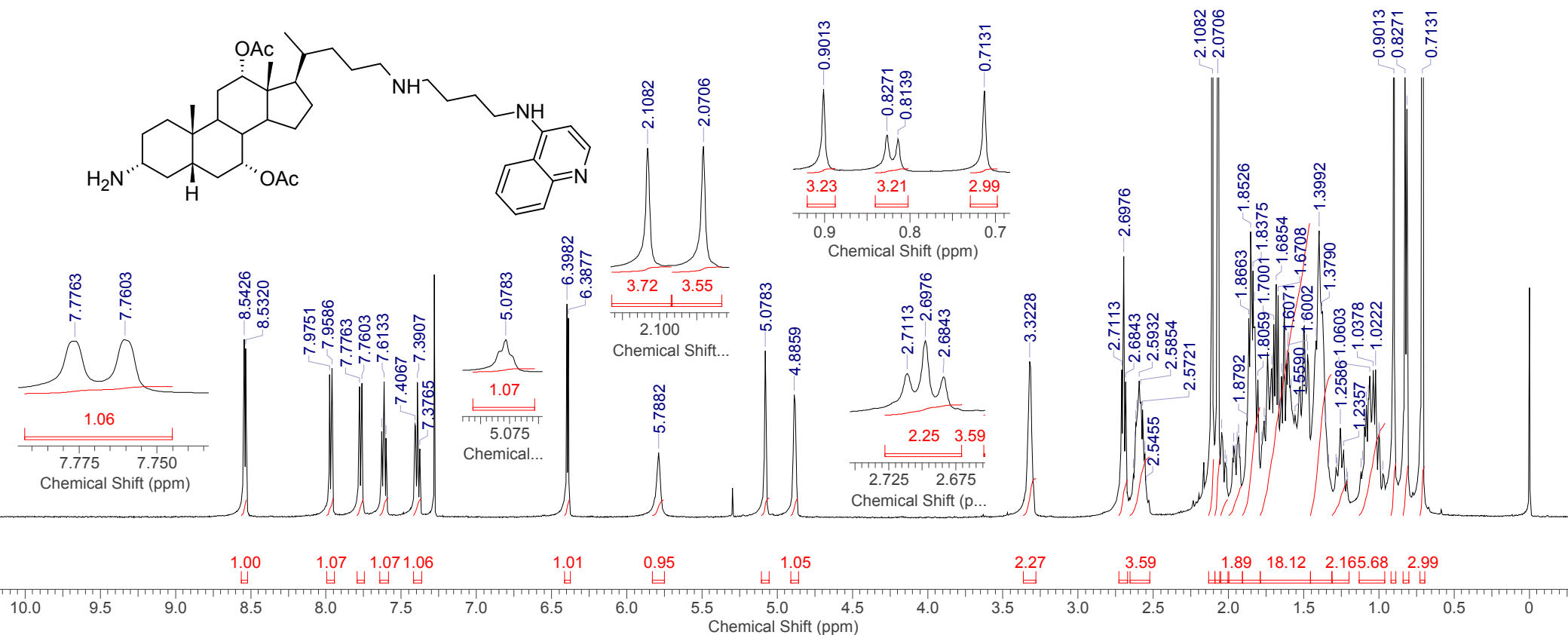
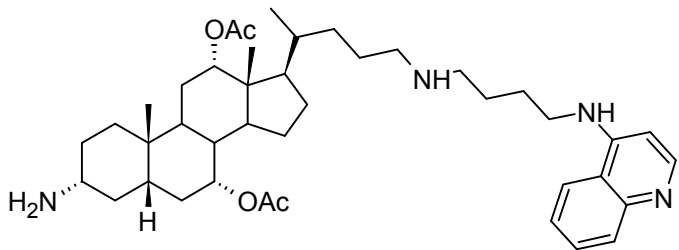
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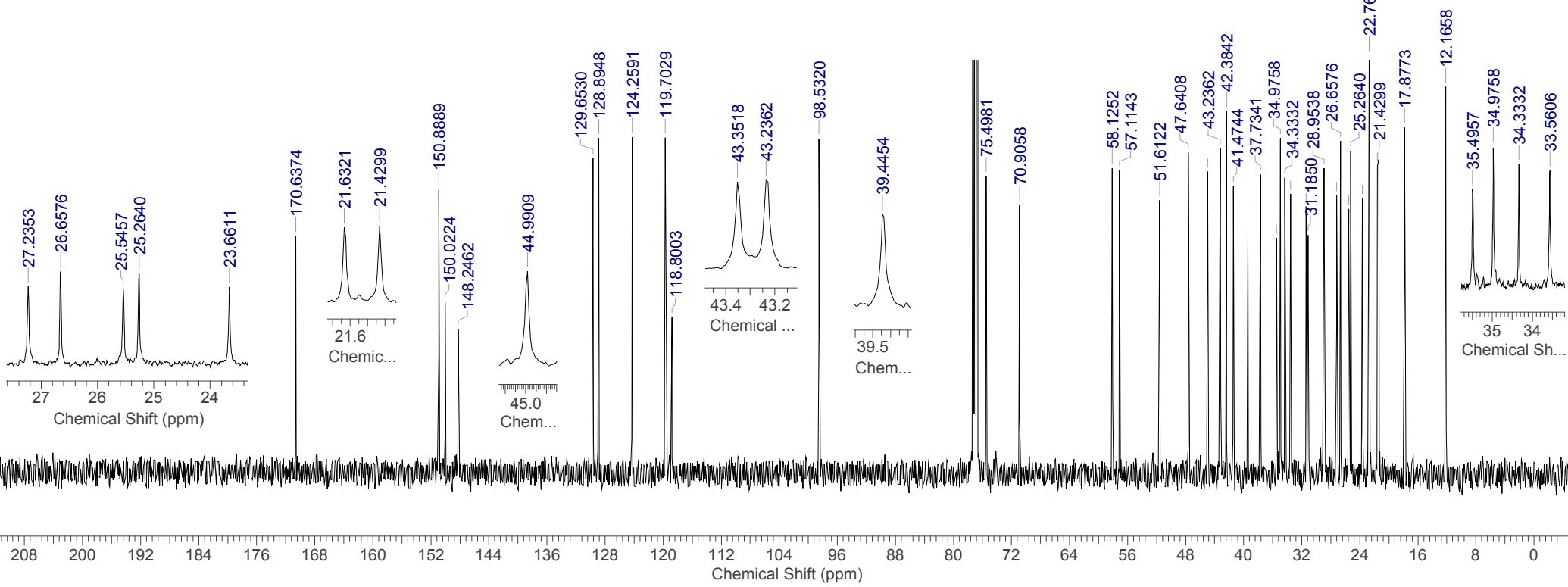
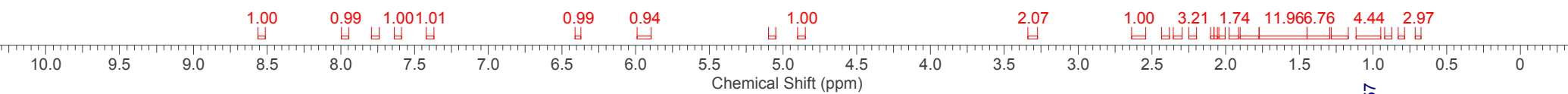
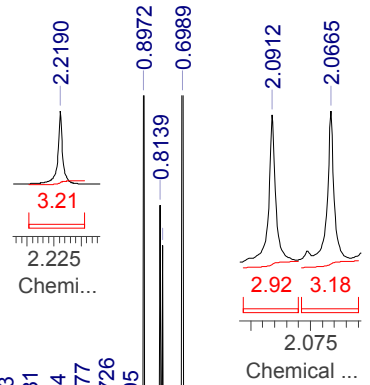
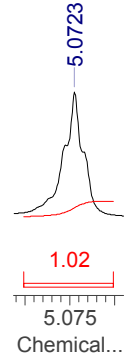
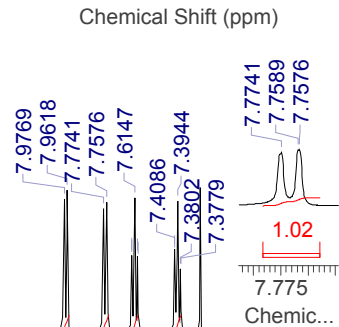
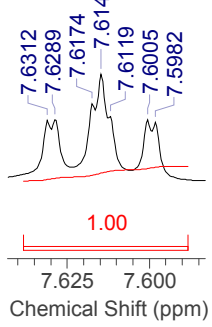
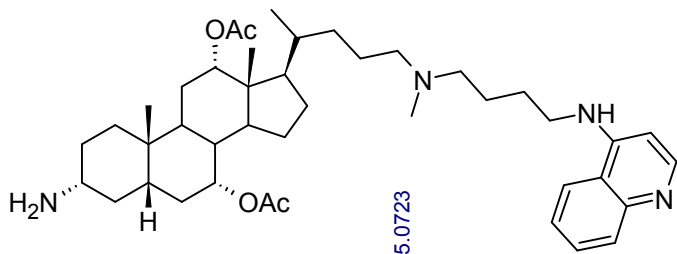
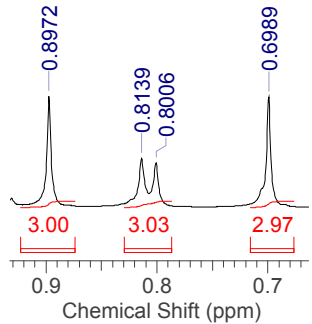
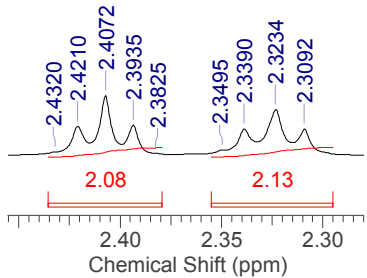
NMR spectra of synthesized compounds	II-S3-II-S48
HPLC analyses for purity	II-S49-II-S99

NMR spectra of synthesized compounds

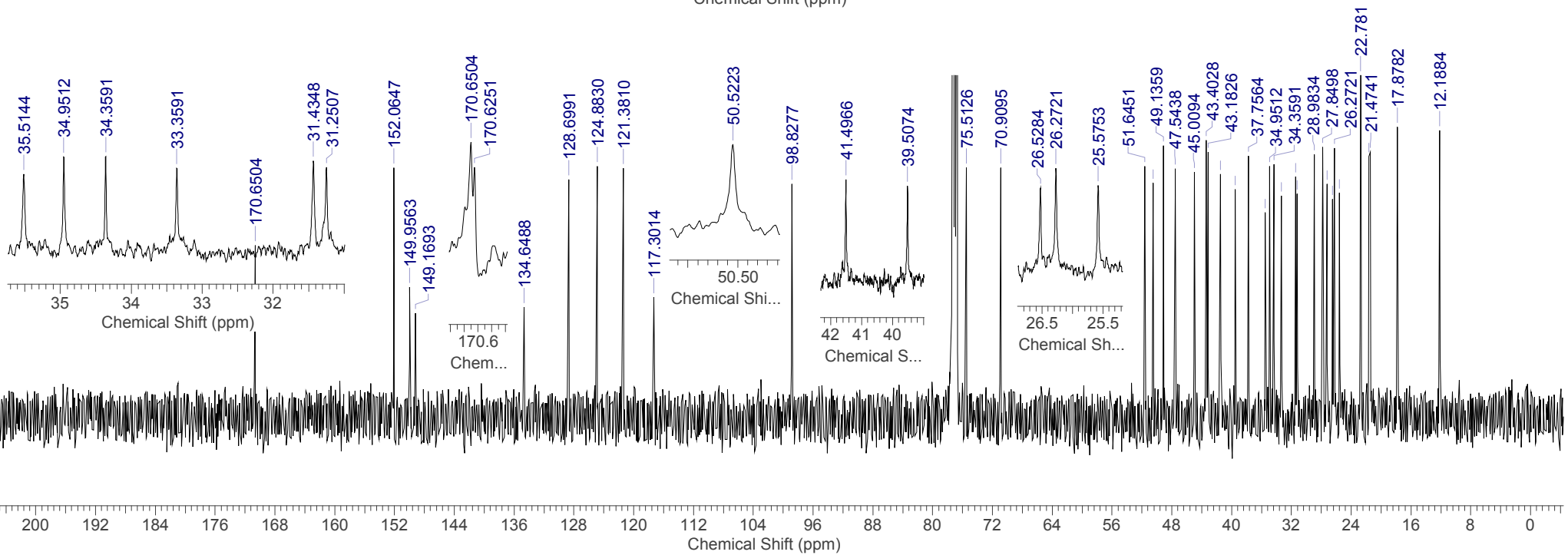
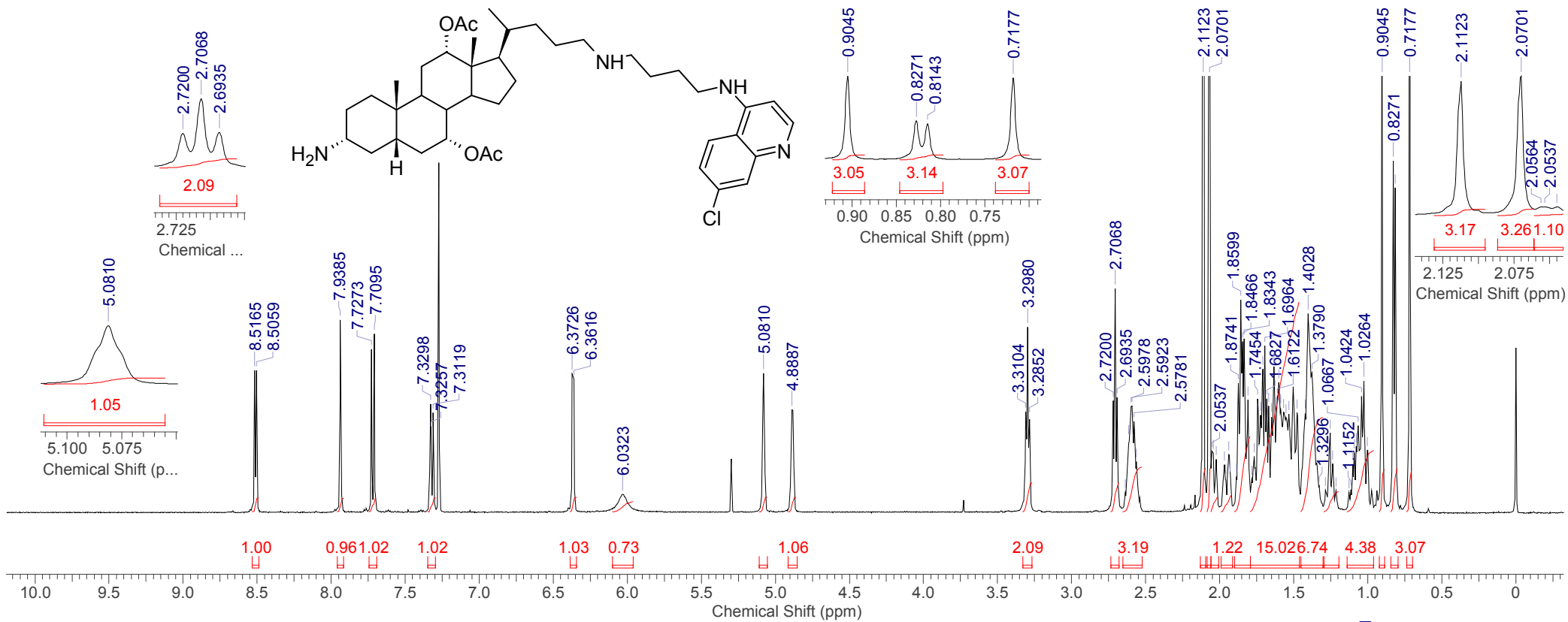
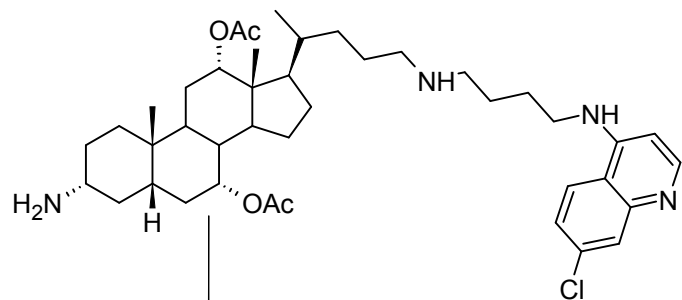
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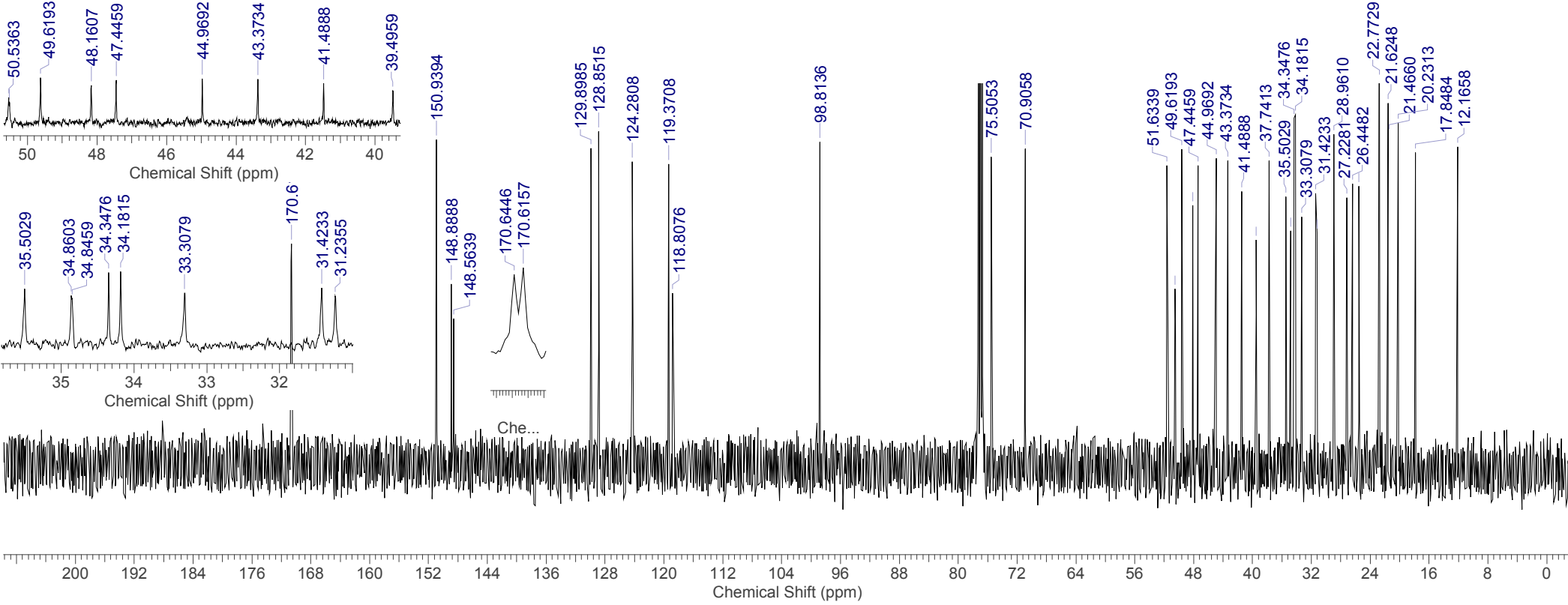
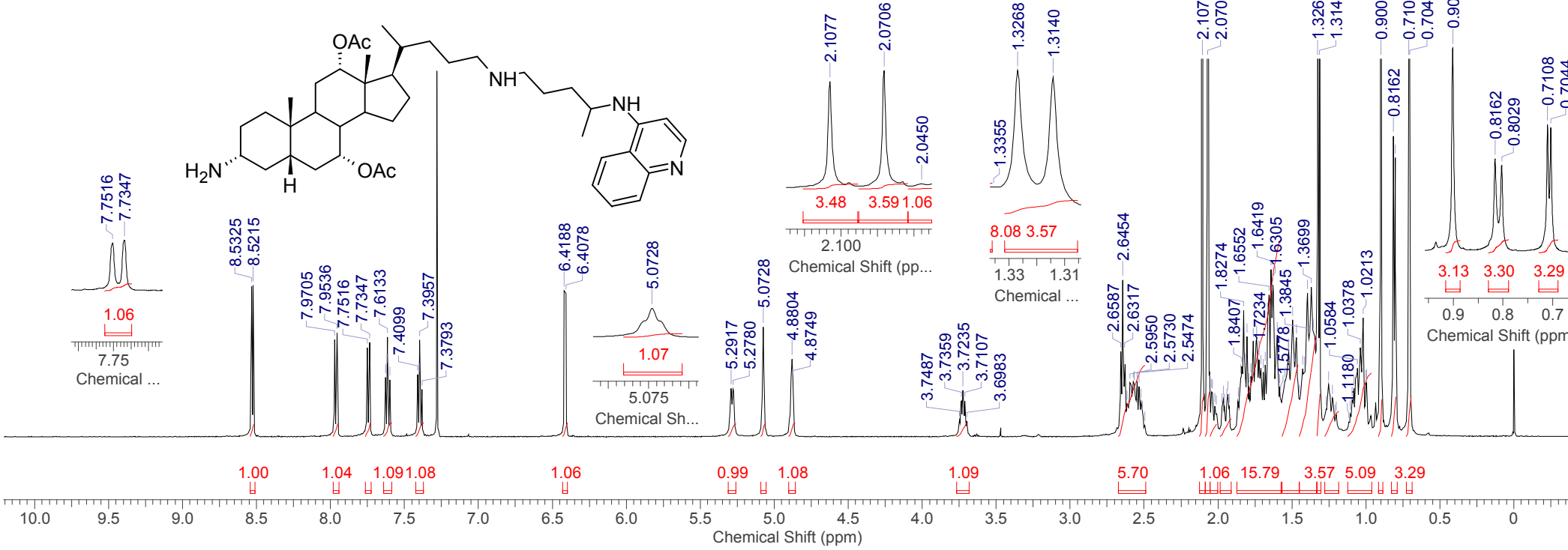
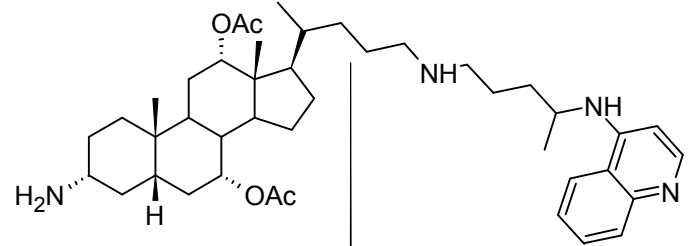
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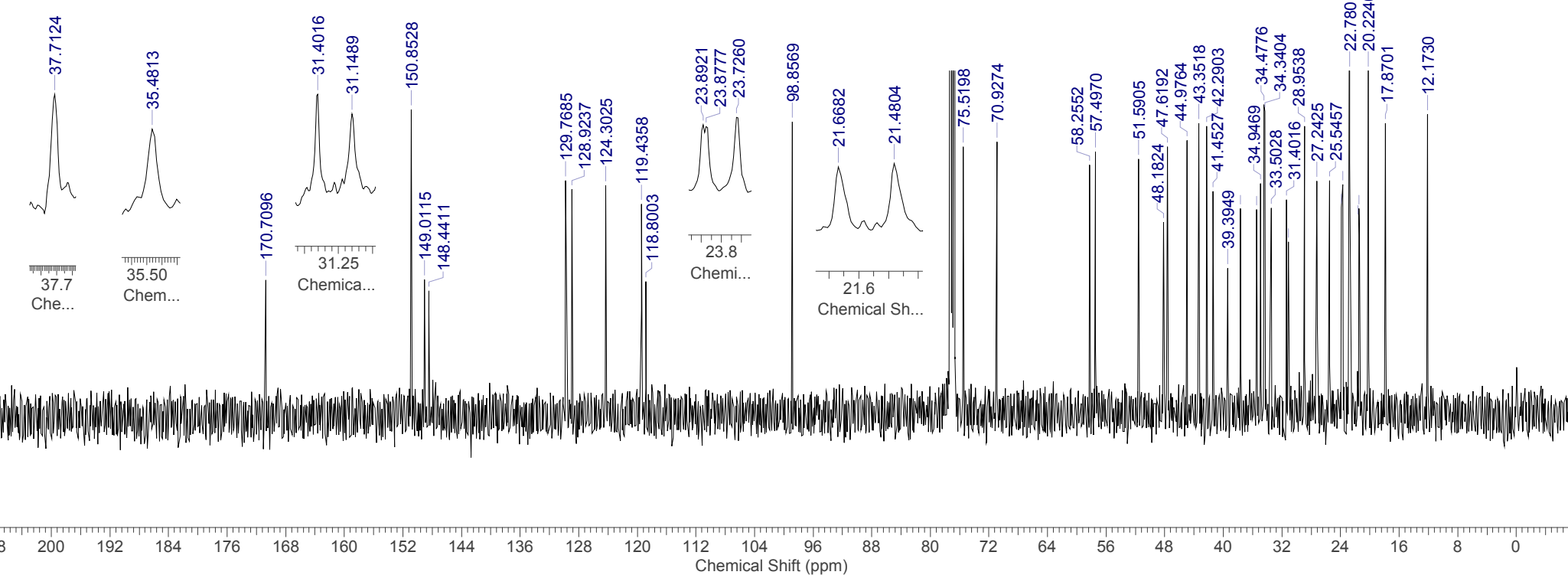
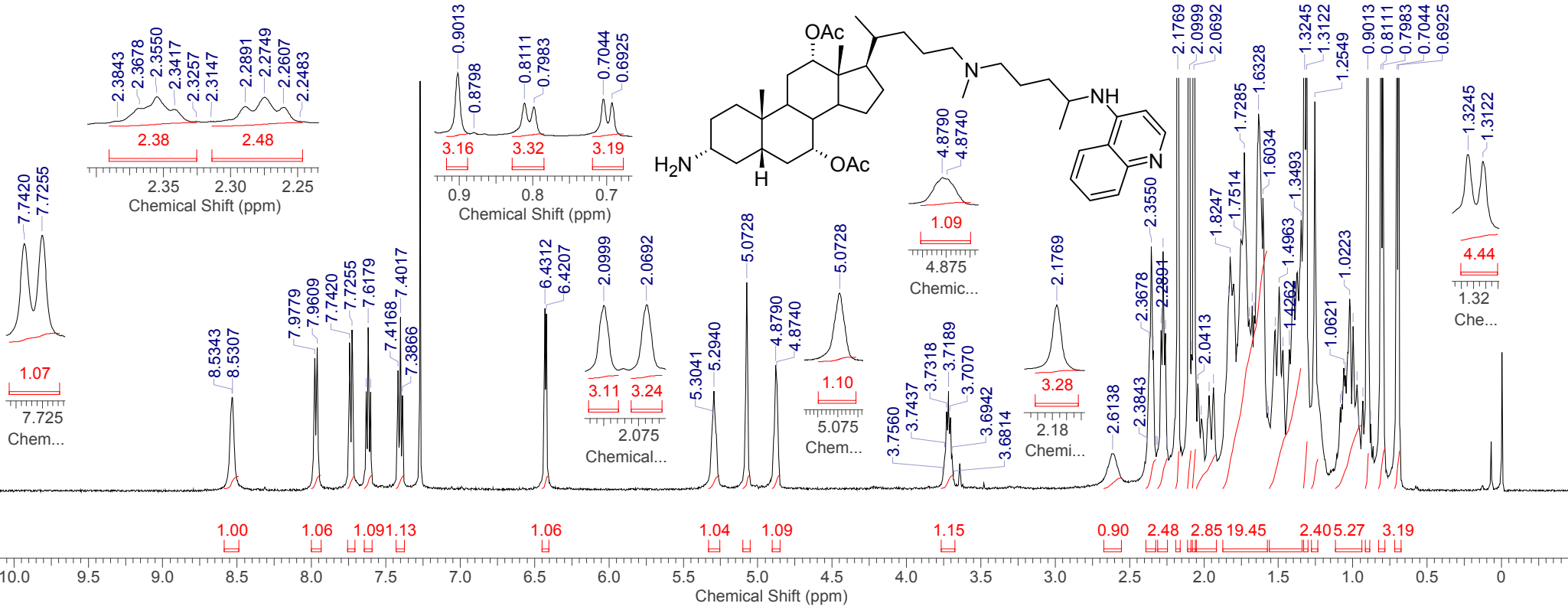
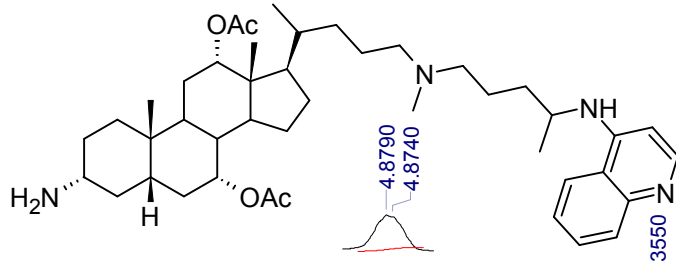
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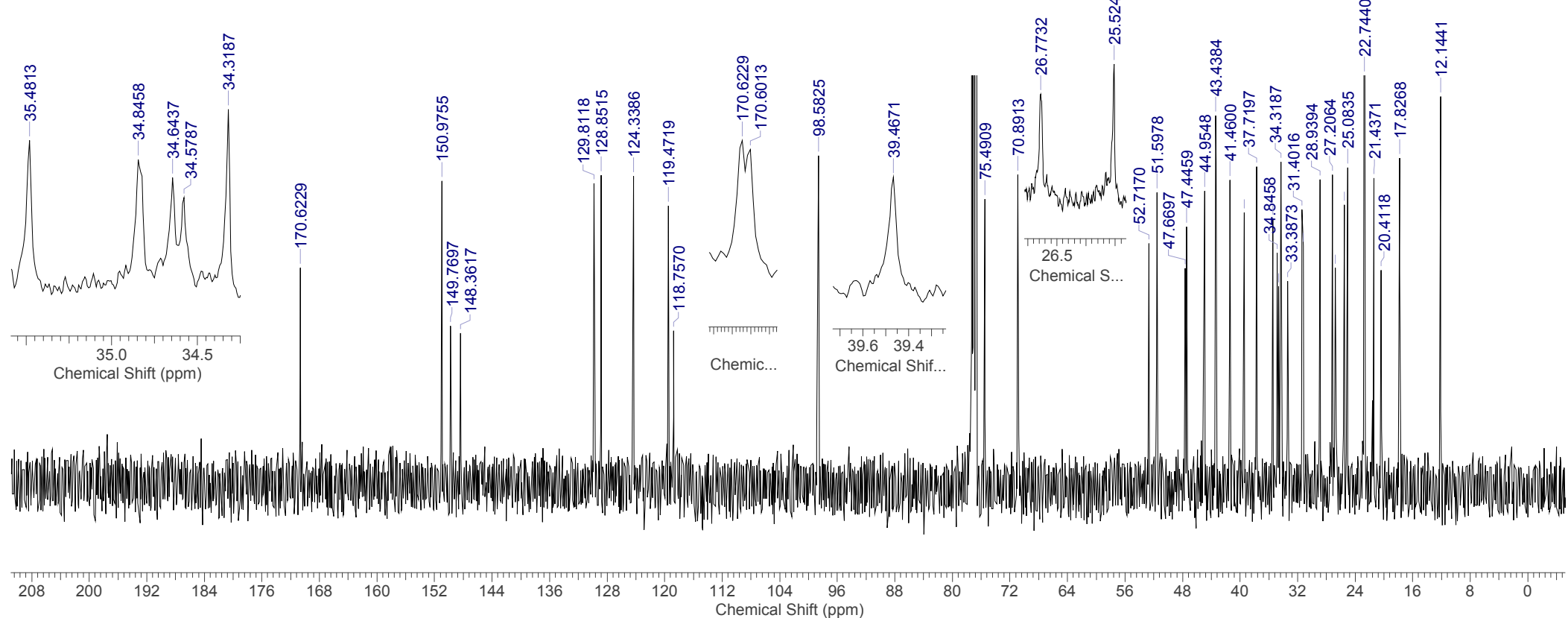
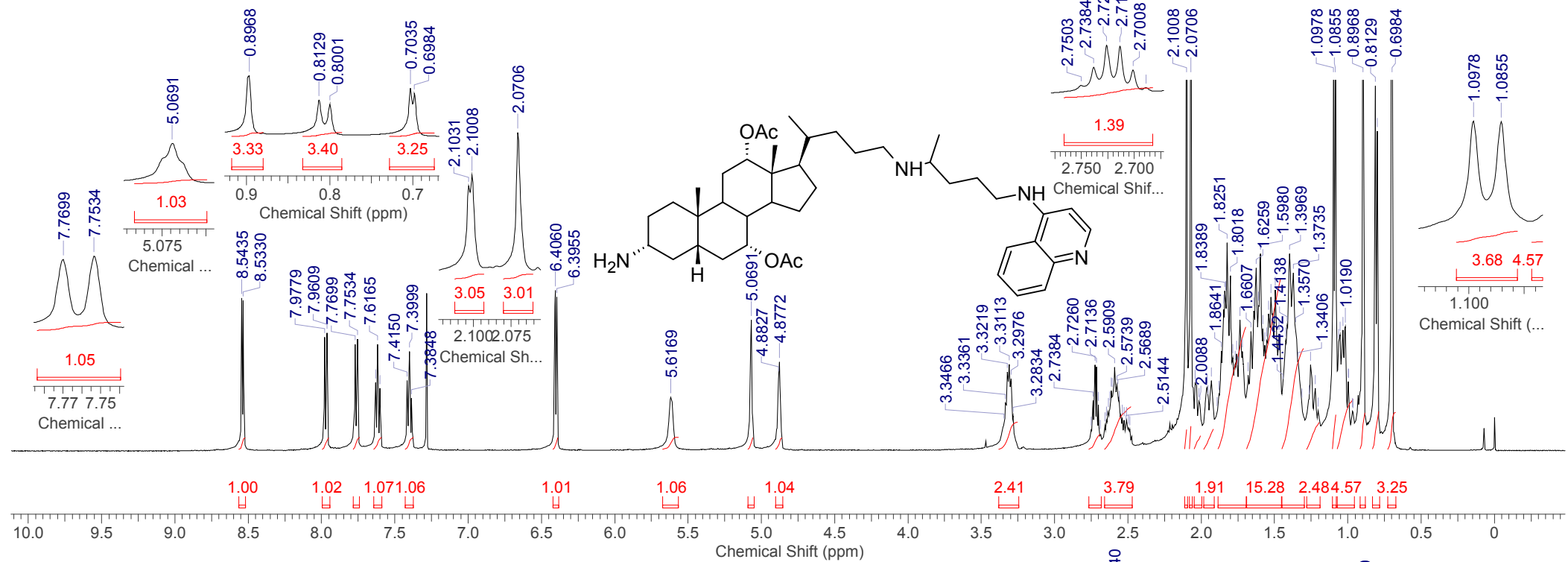
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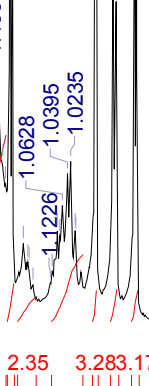
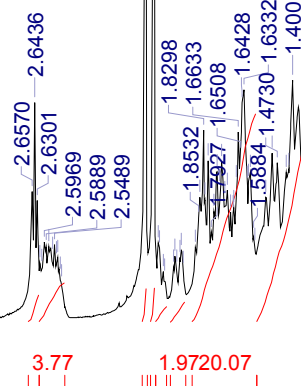
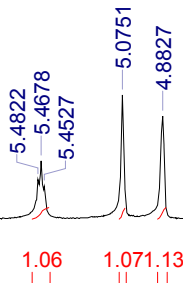
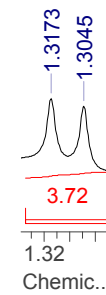
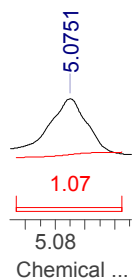
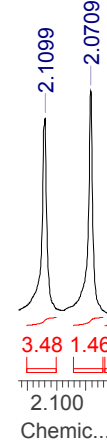
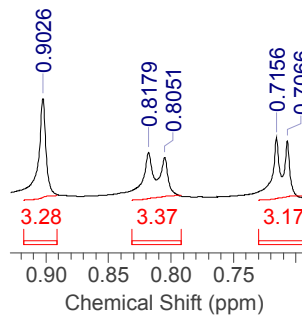
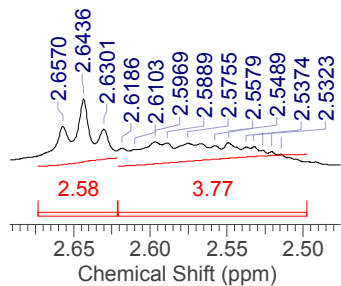
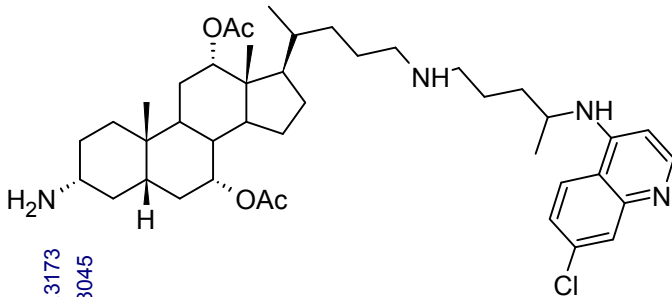
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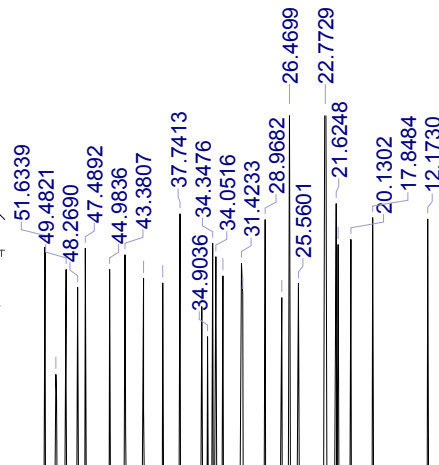
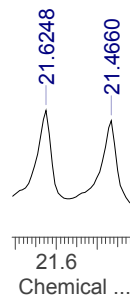
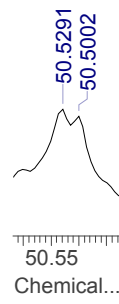
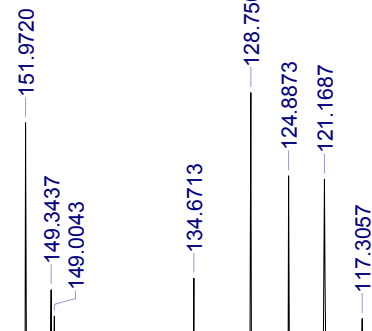
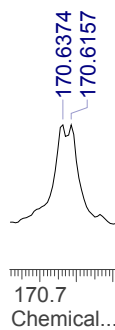
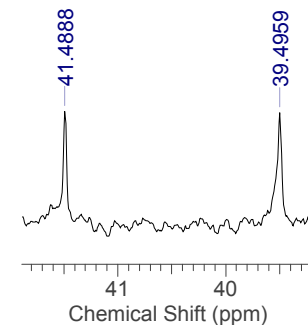
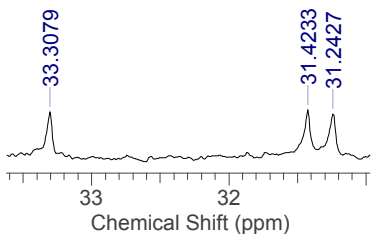
(3a,5b,7a,12a)-3-Amino-24-[[1-methyl-4-(quinolin-4-ylamino)butyl]amino]cholane-7,12-diyl diacetate (19)



(3a,5b,7a,12a)-3-Amino-24-({4-[(7-chloroquinolin-4-yl)amino]pentyl}amino)cholane-7,12-diyl diacetate (20)

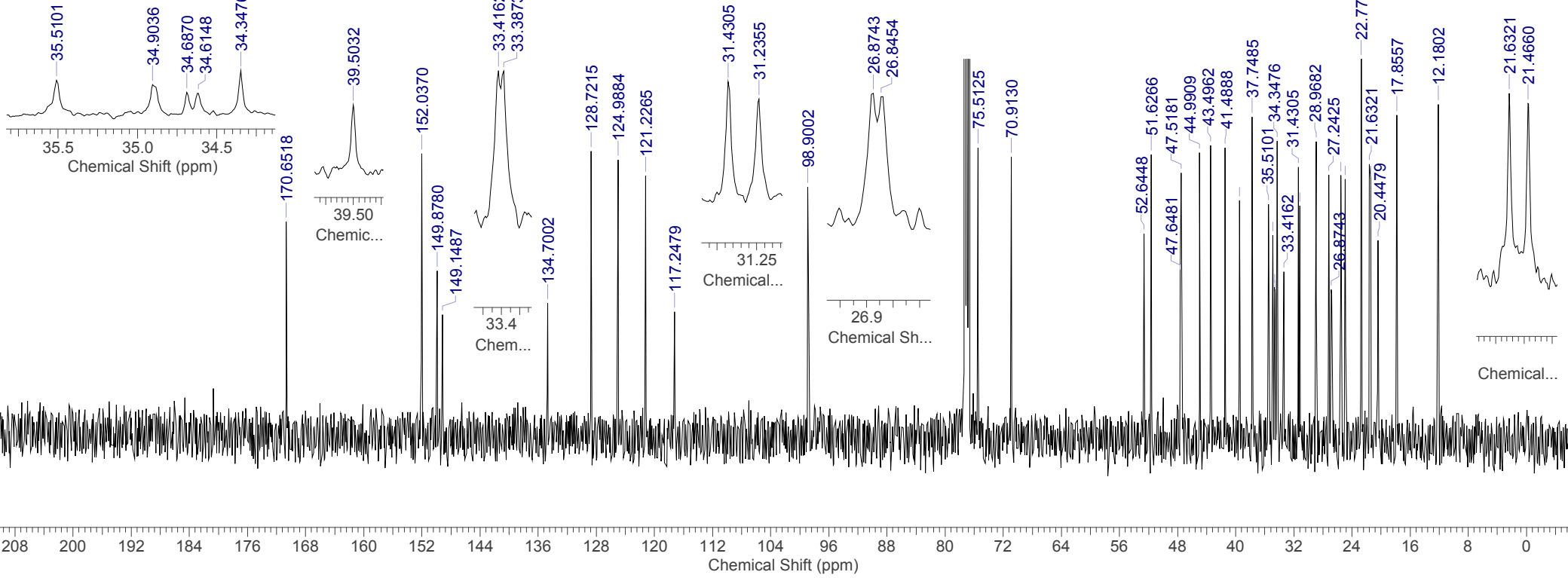
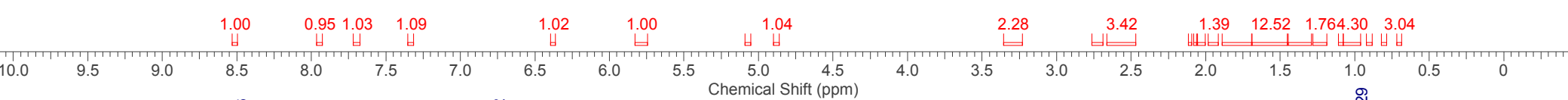
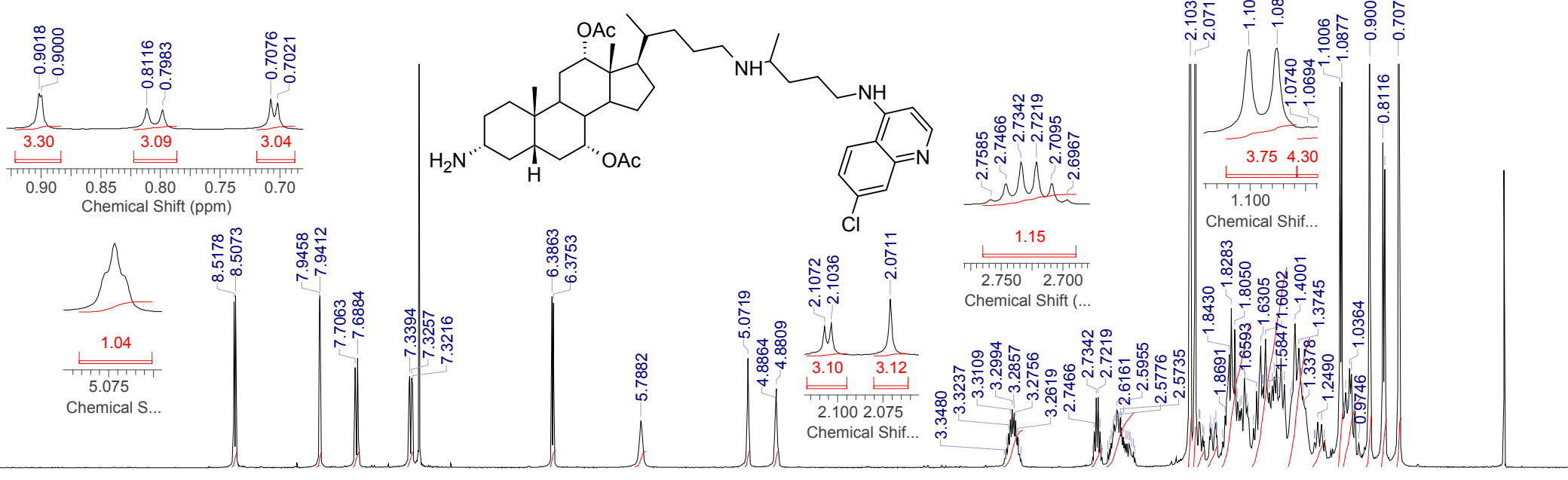


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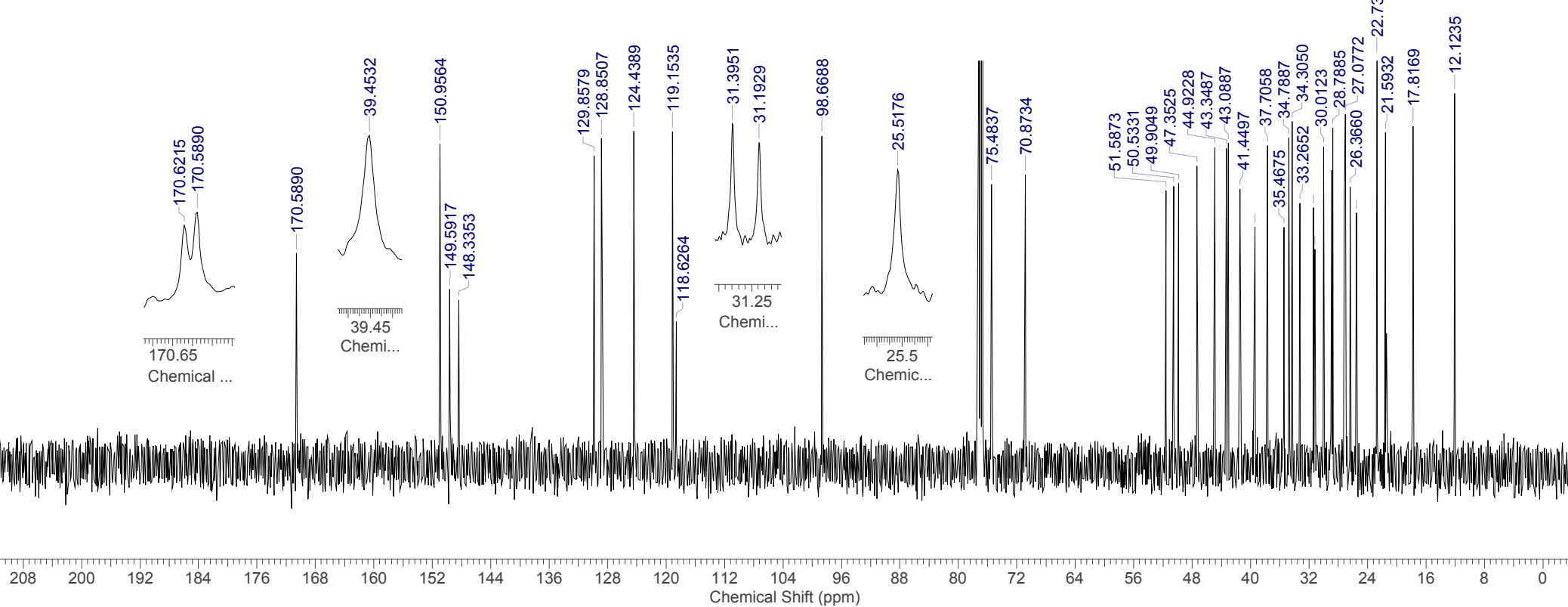
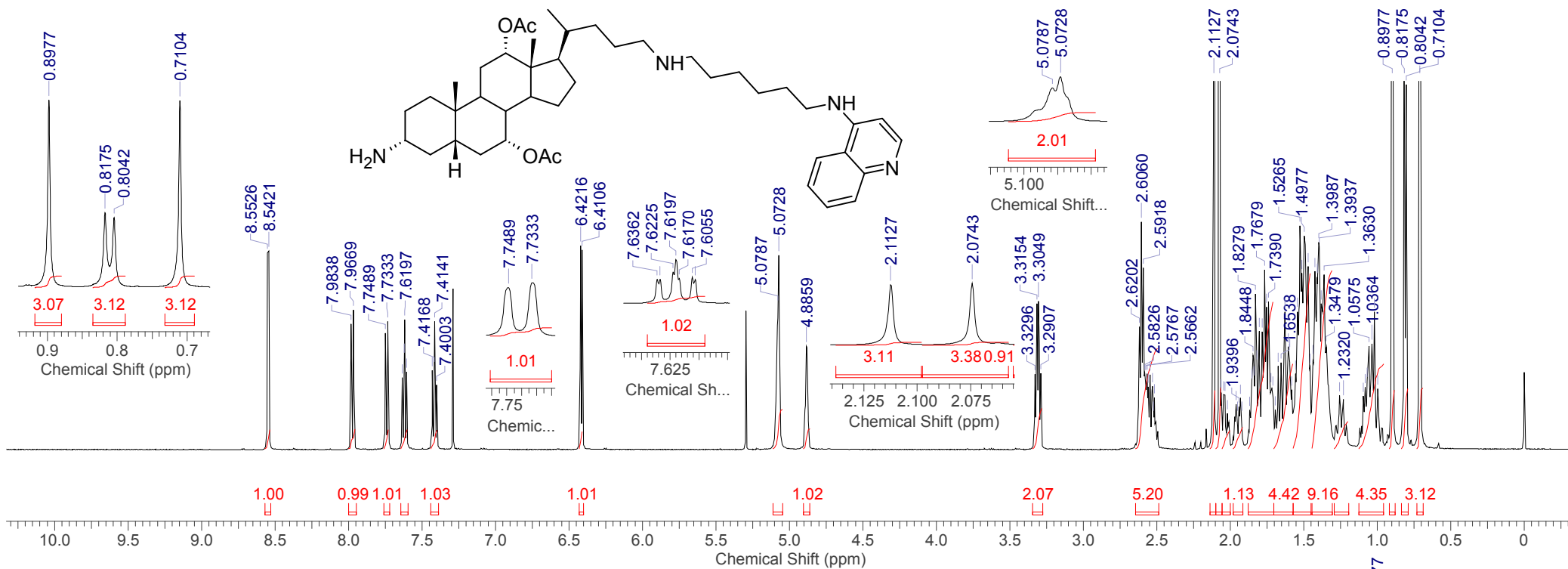


Chemical Shift (ppm)

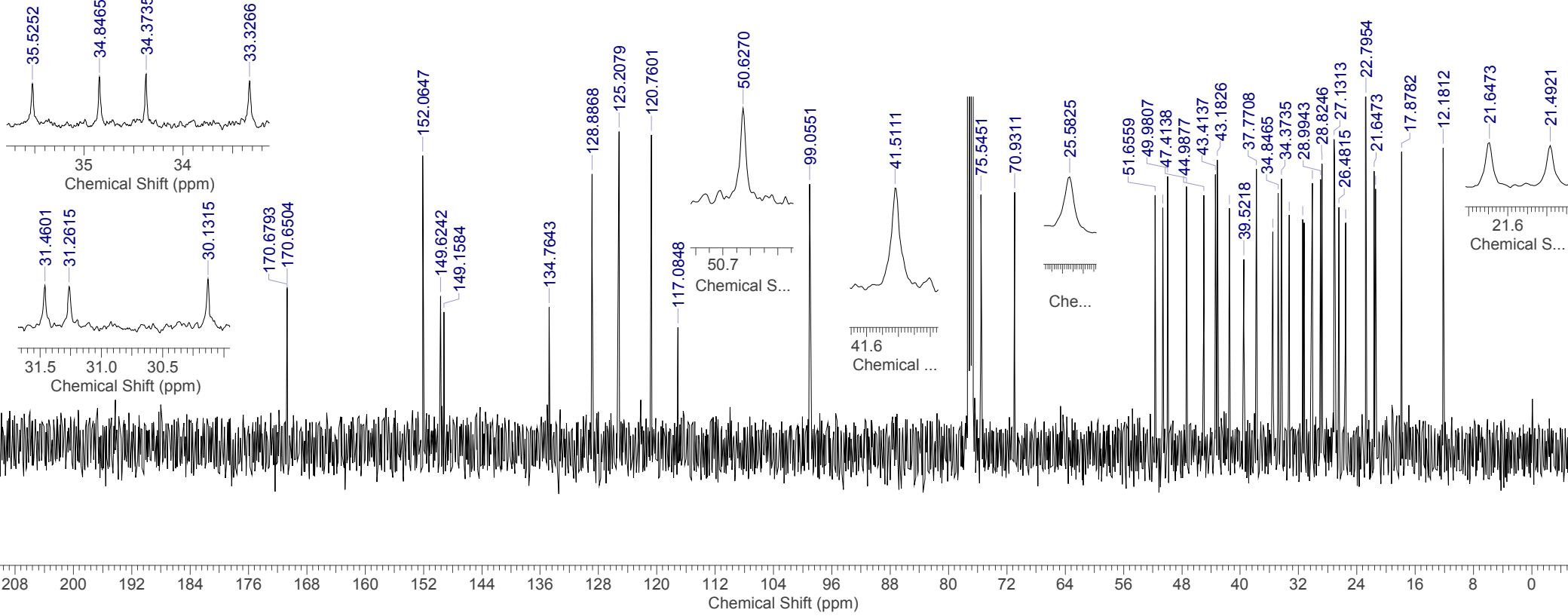
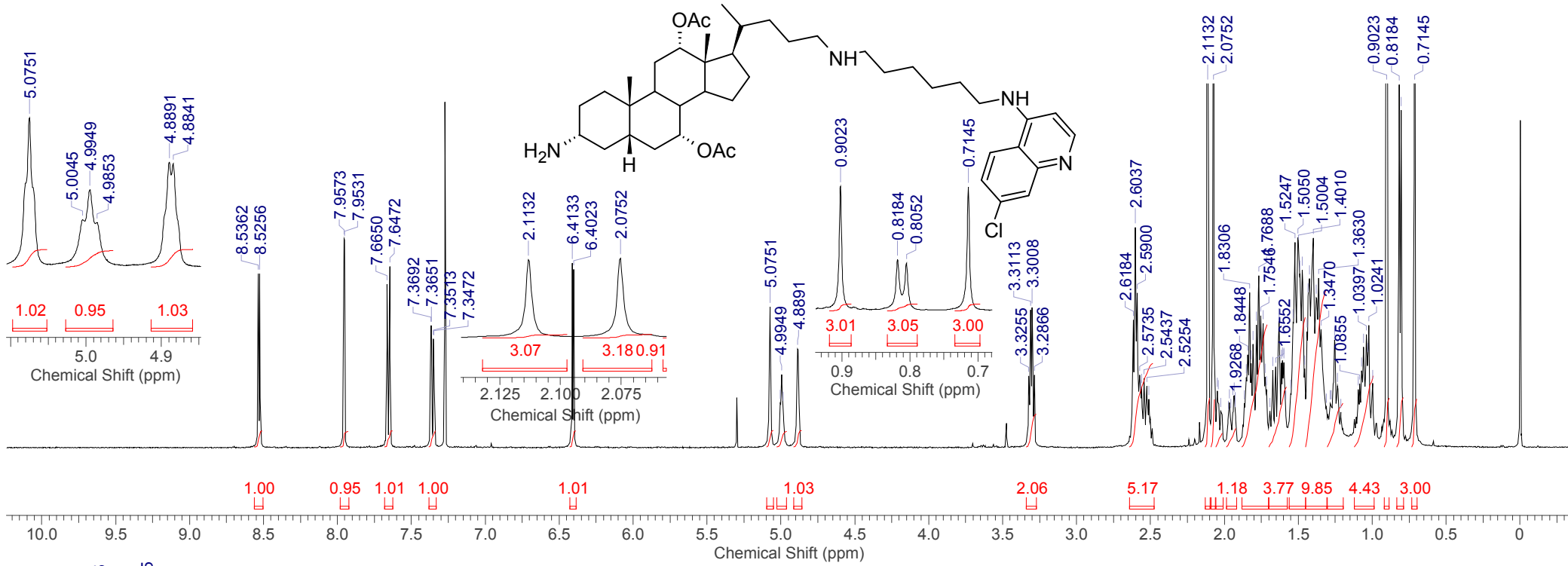
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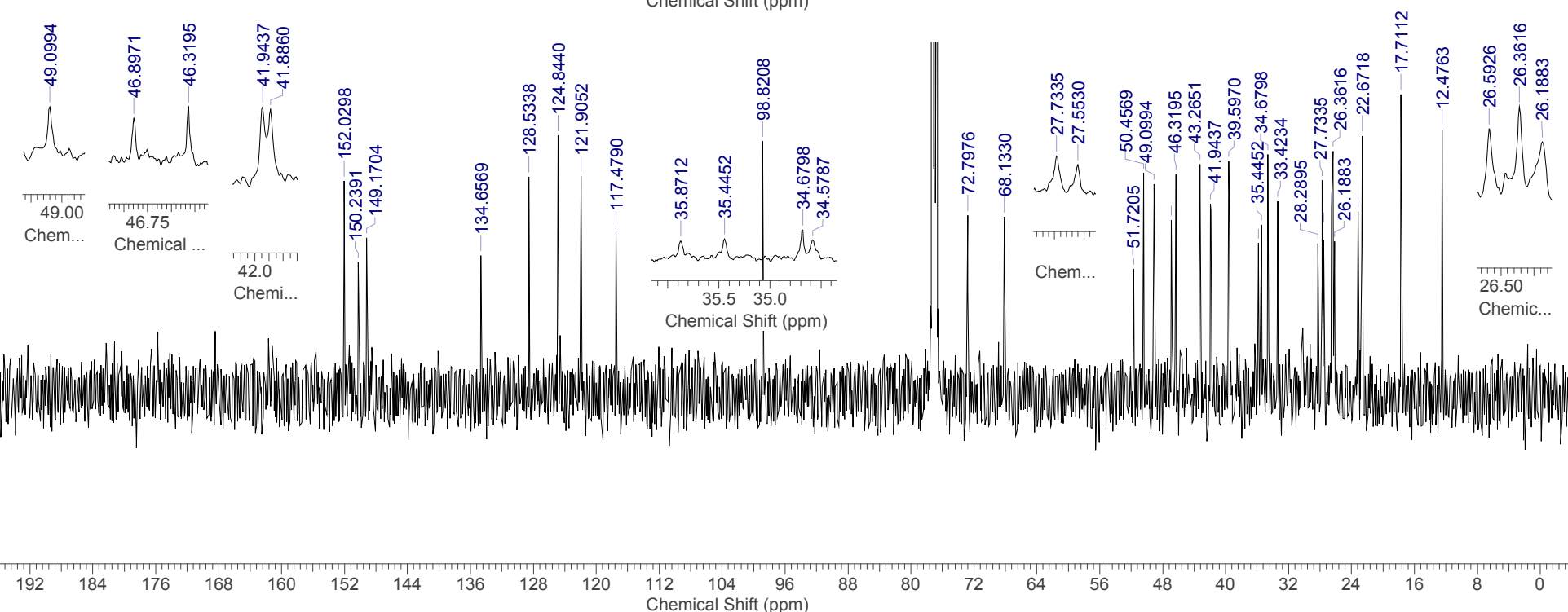
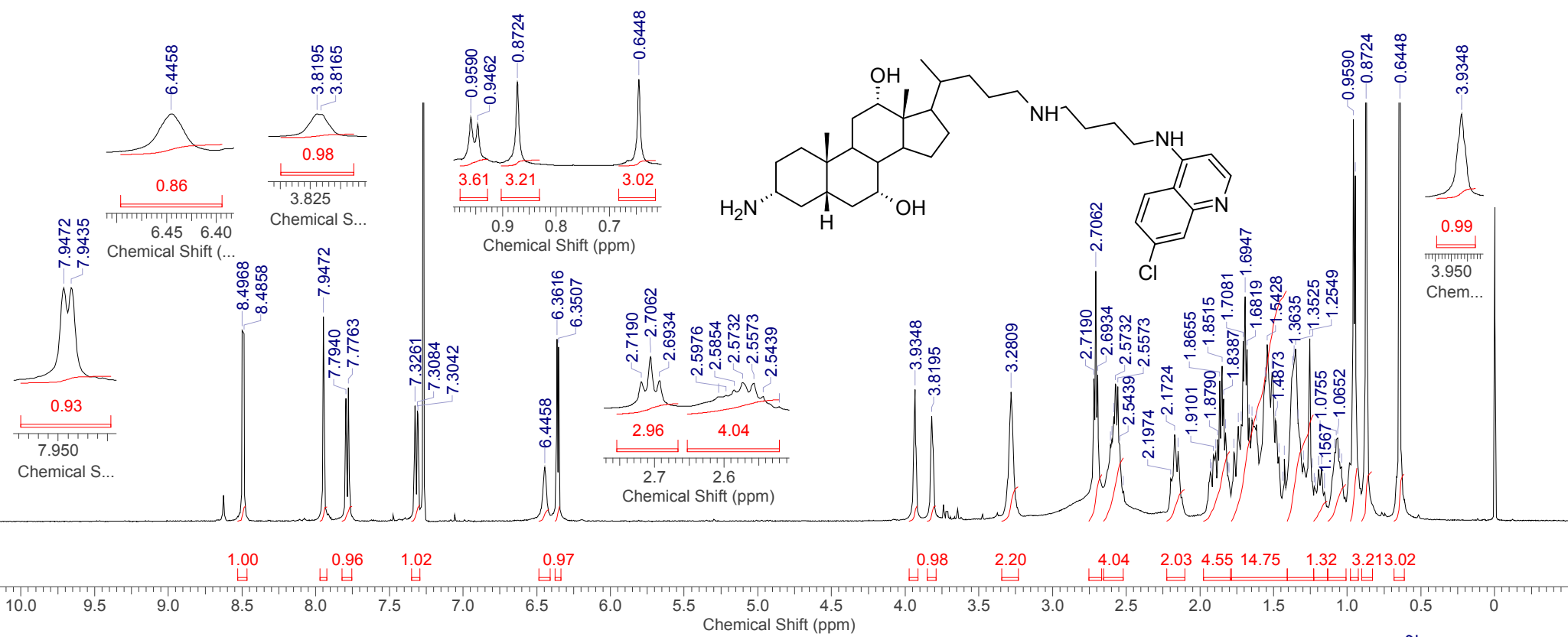
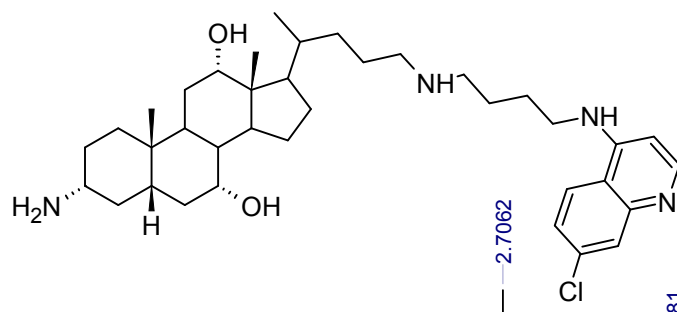
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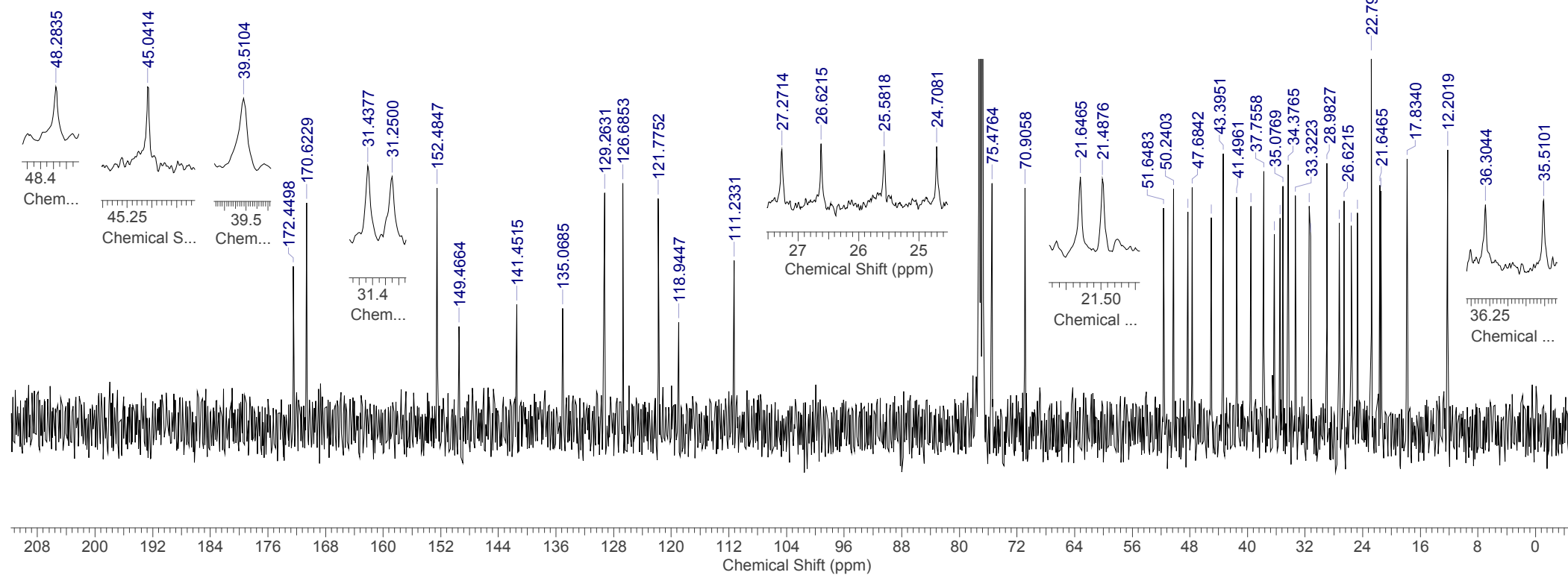
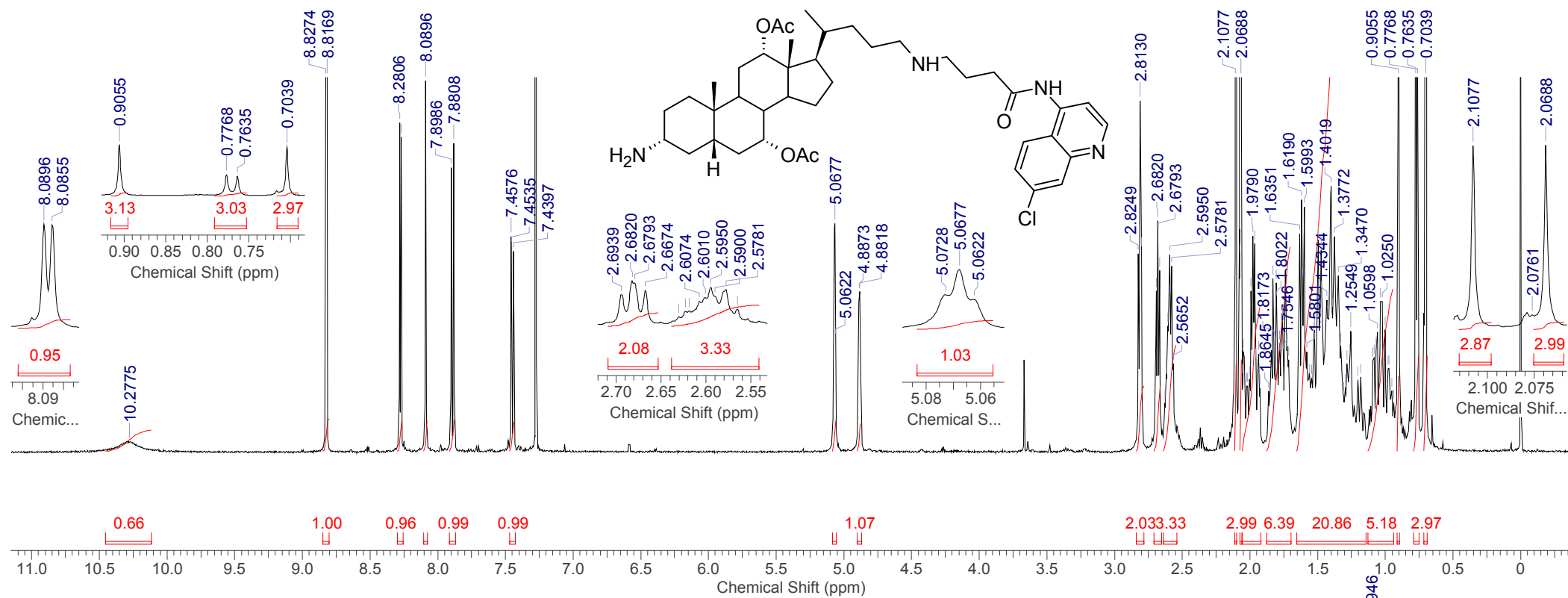
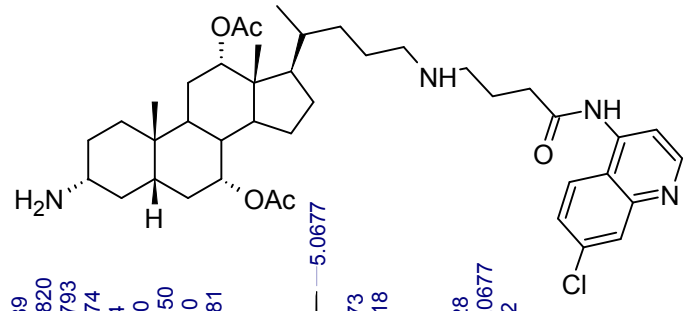
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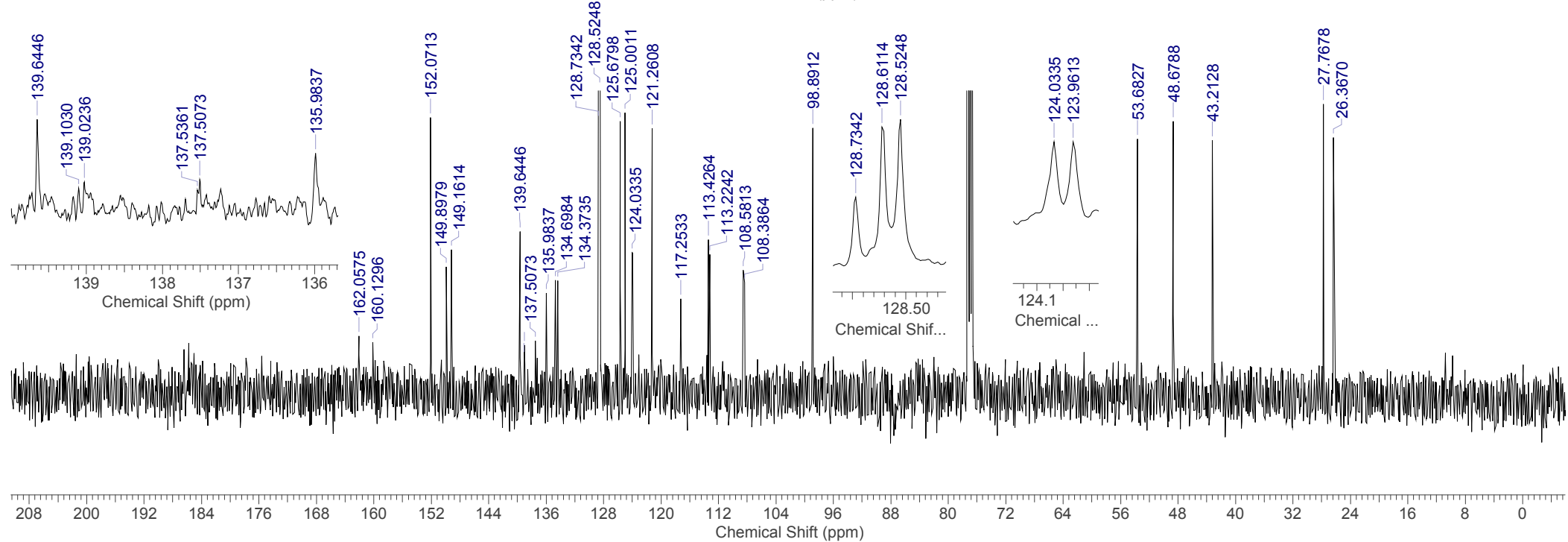
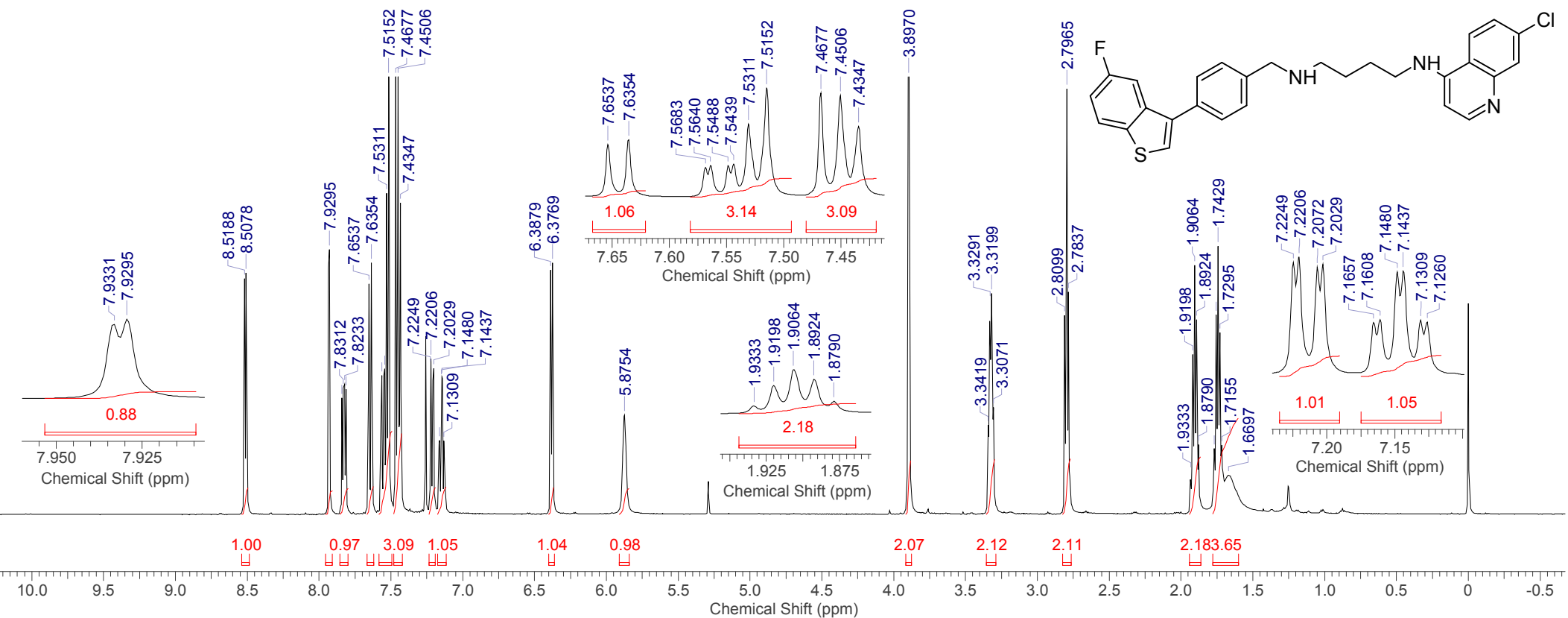
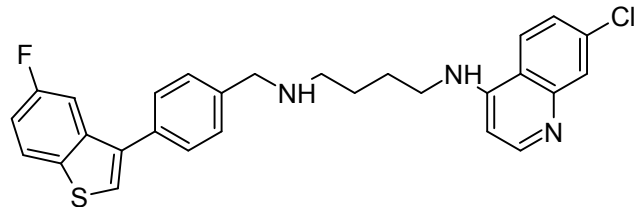
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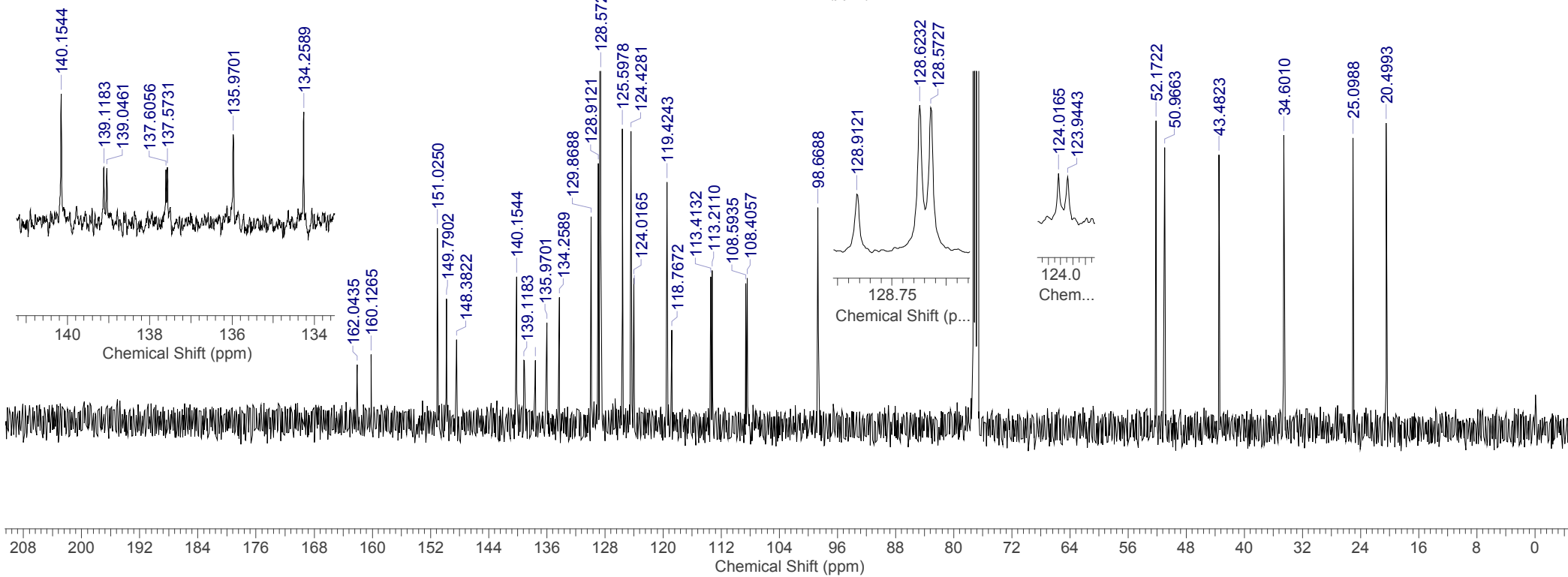
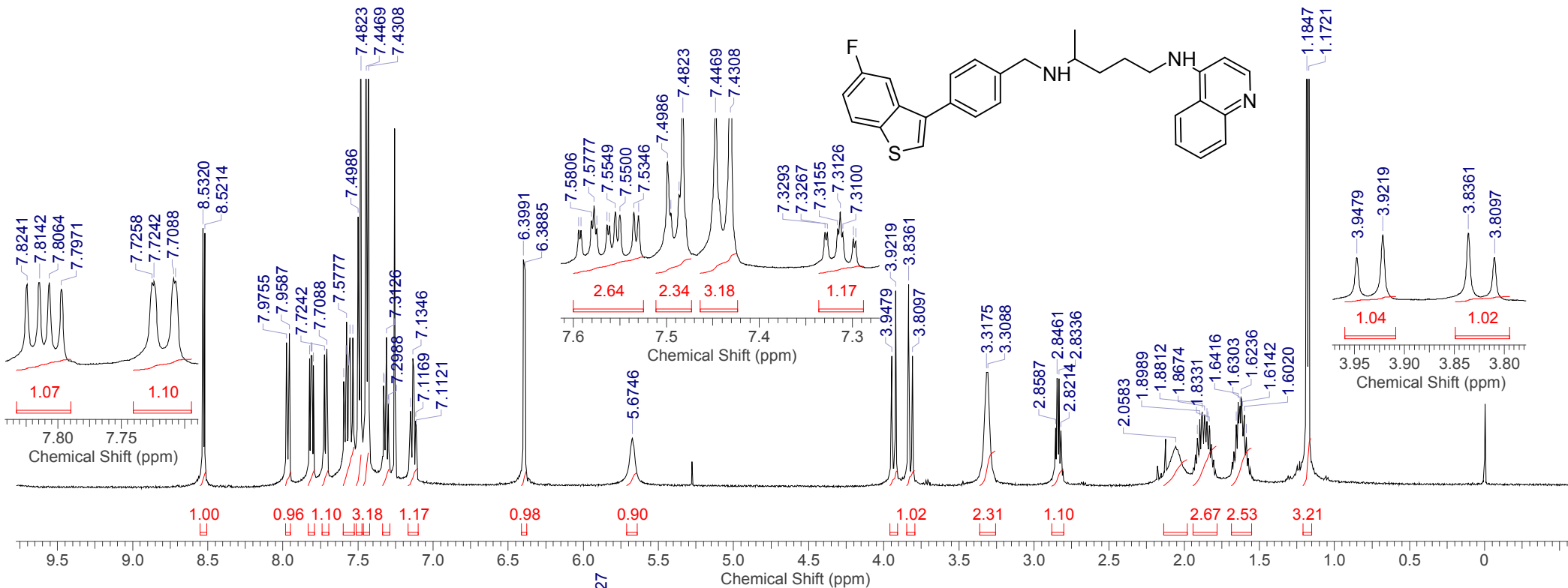
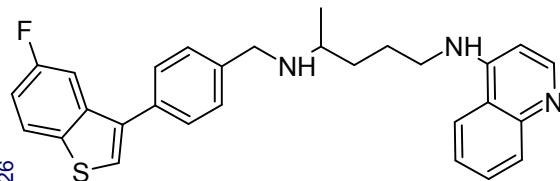
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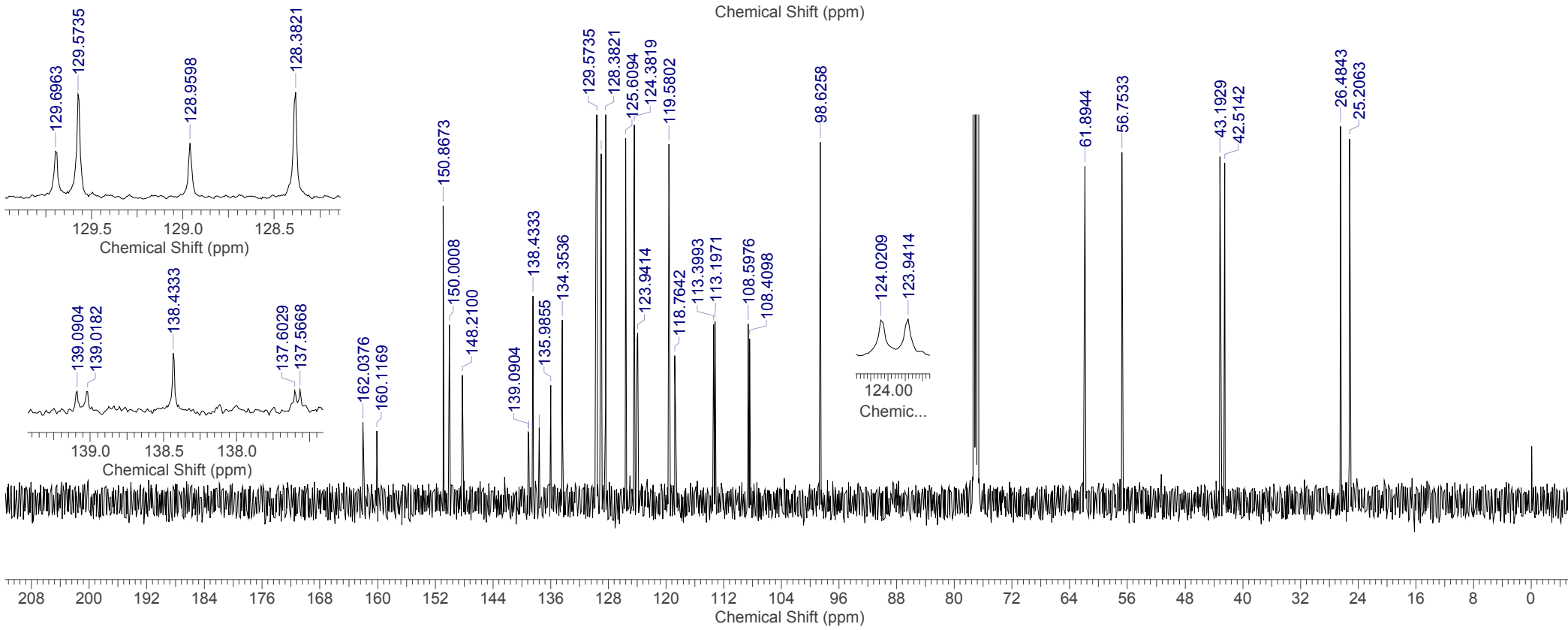
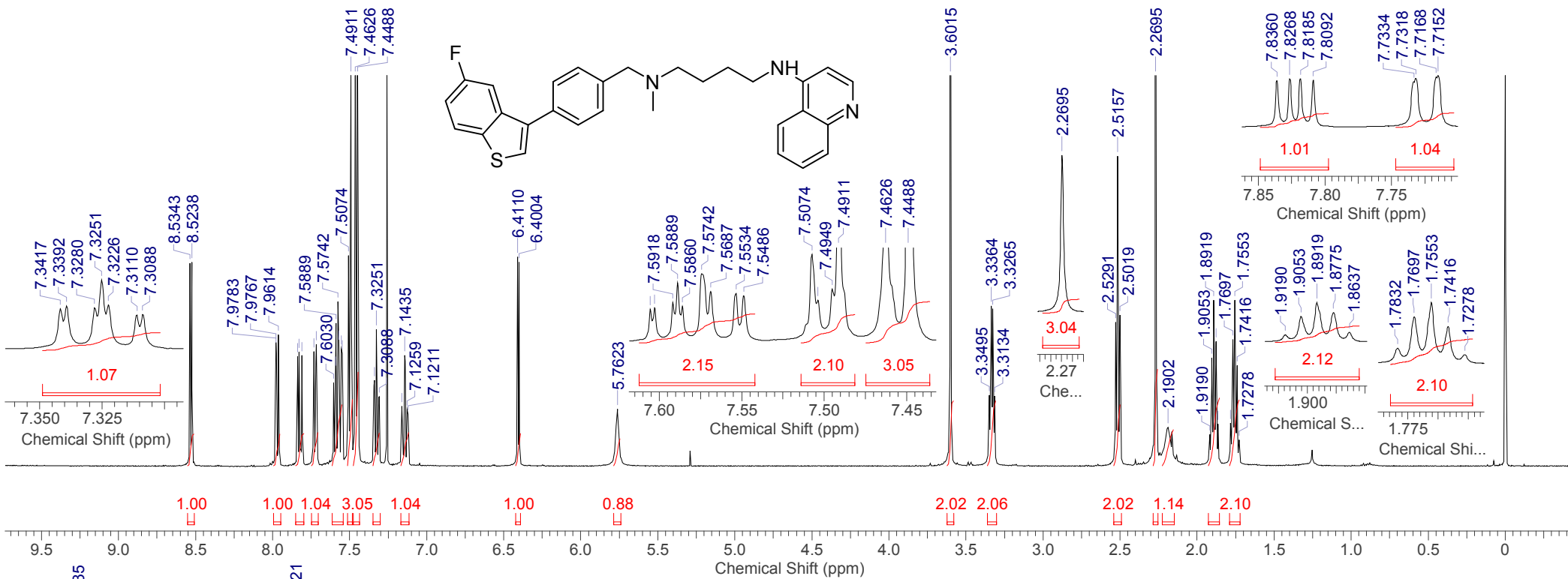
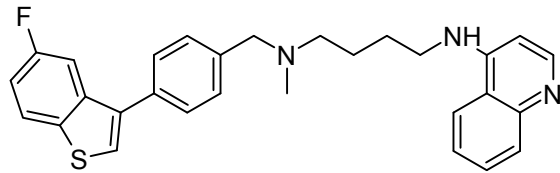
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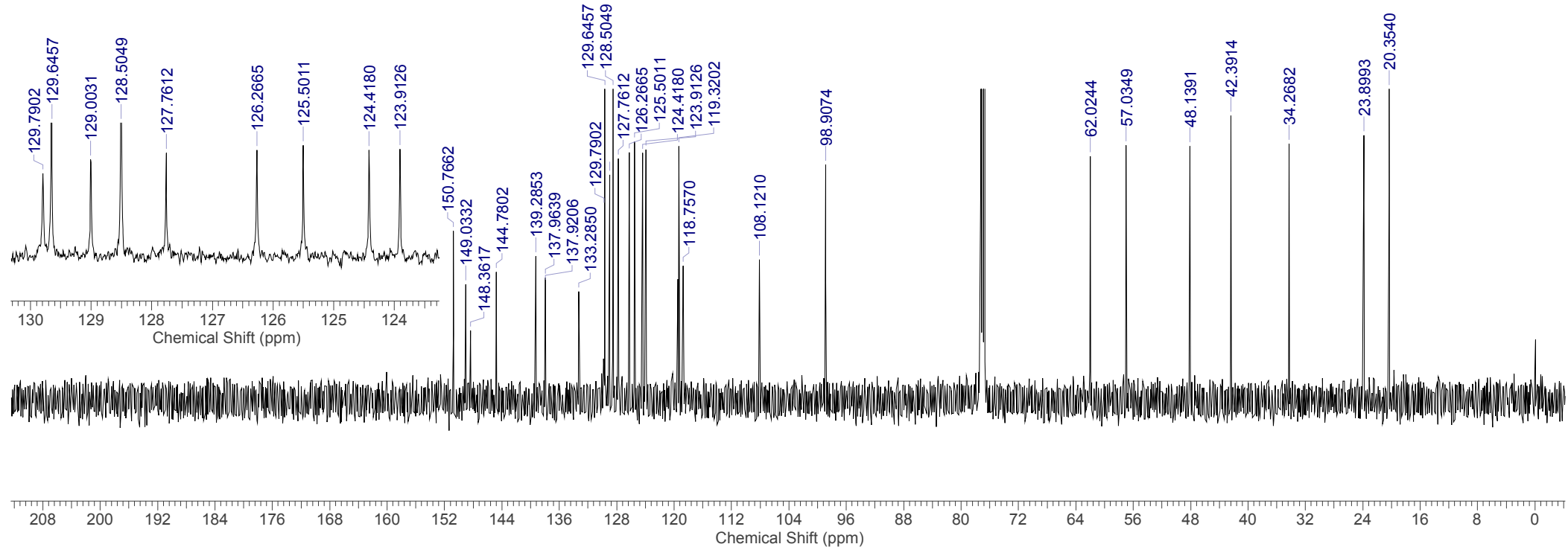
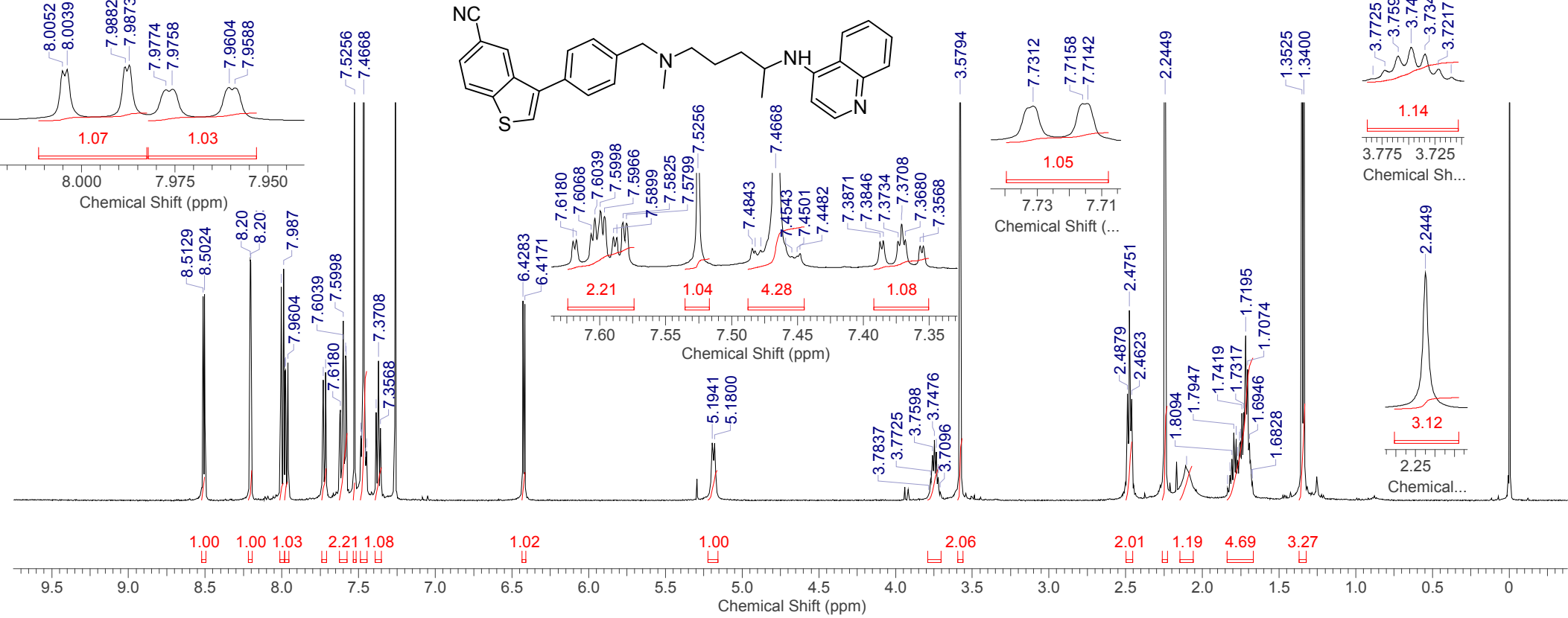
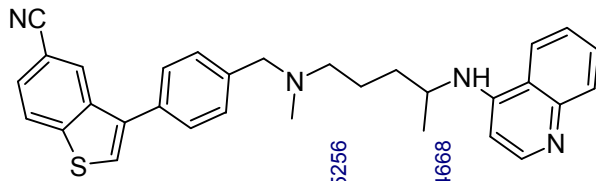
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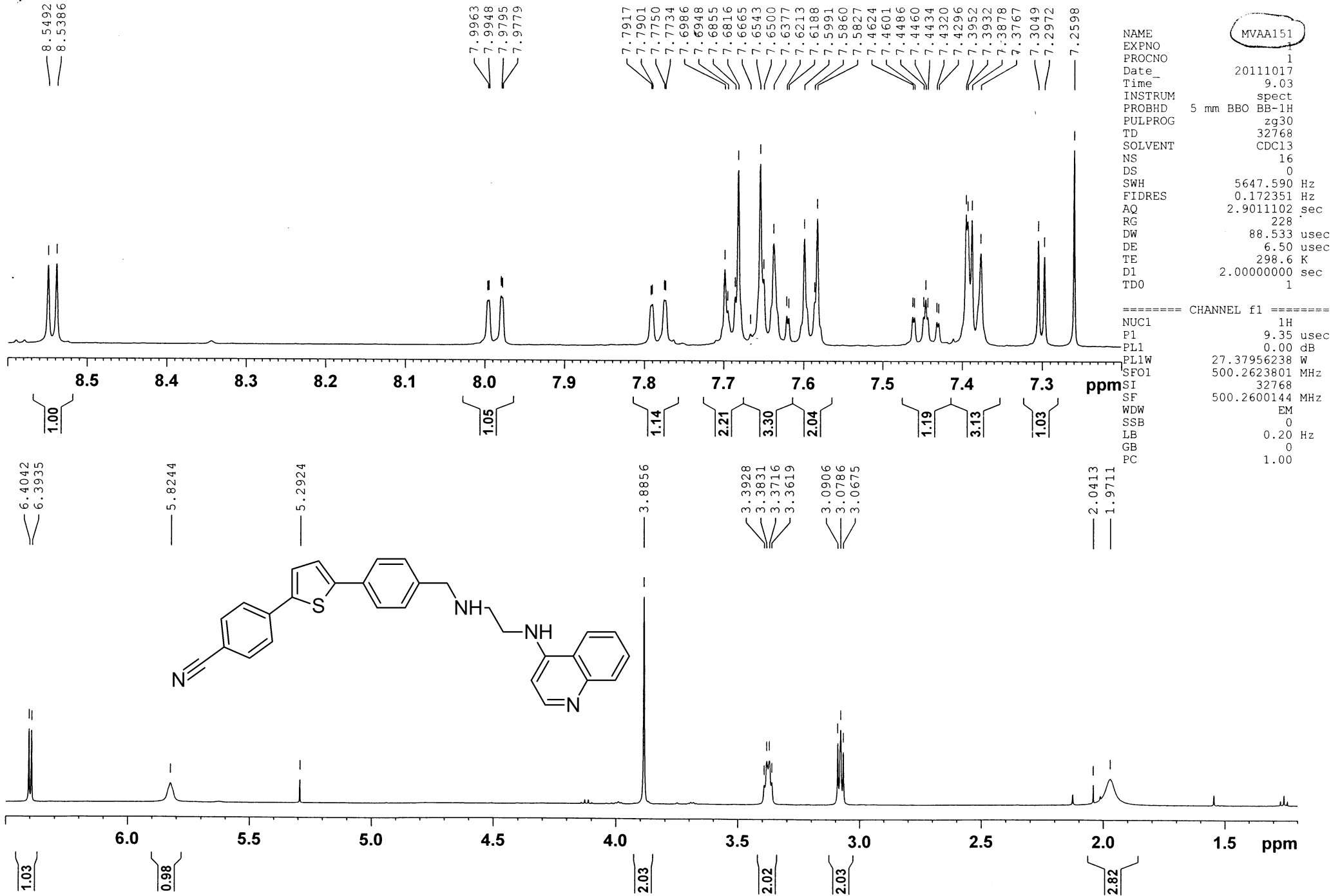
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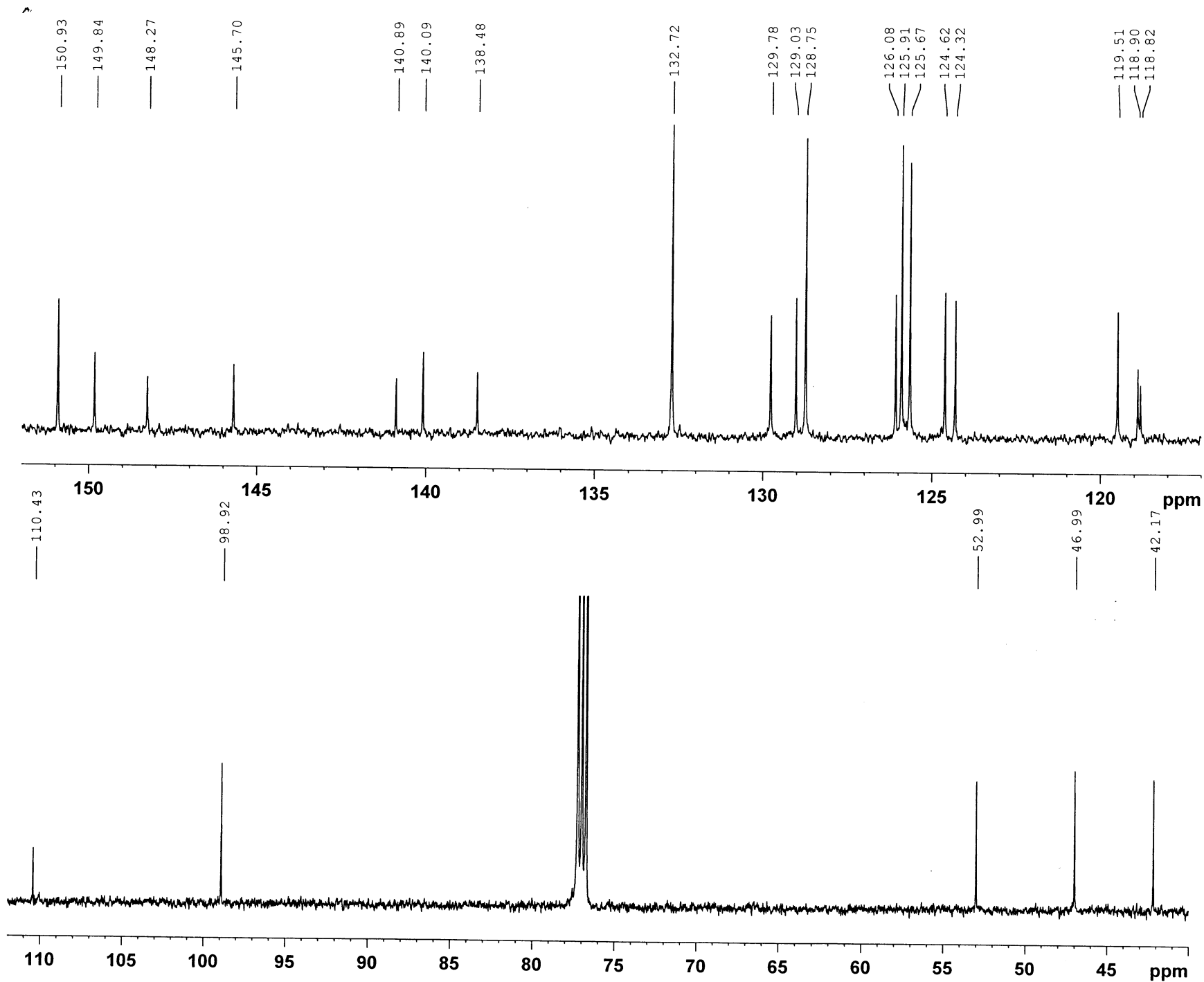


3-[4-((methyl[4-(quinolin-4-ylamino)pentyl]amino)methyl)phenyl]-1-benzothiophene-5-carbonitrile (38)



4-{5-[4-({[2-(quinolin-4-ylamino)ethyl]amino}methyl)phenyl]-2-thienyl}benzonitrile (42)



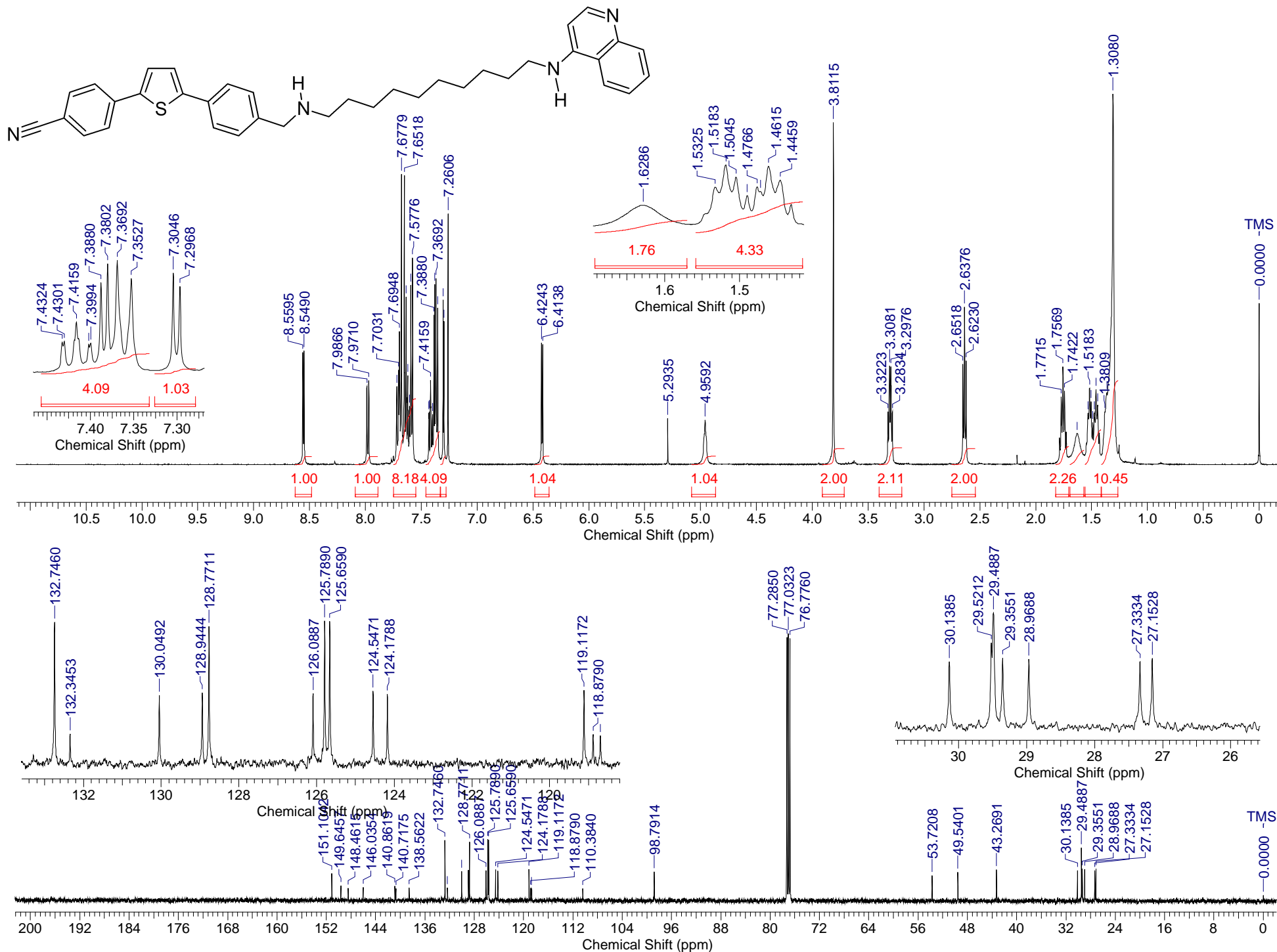


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 SOLVENT CDCl3
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 FIDRES 0.605507 Hz
 AQ 0.8258036 sec
 RG 1820
 DW 16.800 usec
 DE 6.50 usec
 TE 298.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
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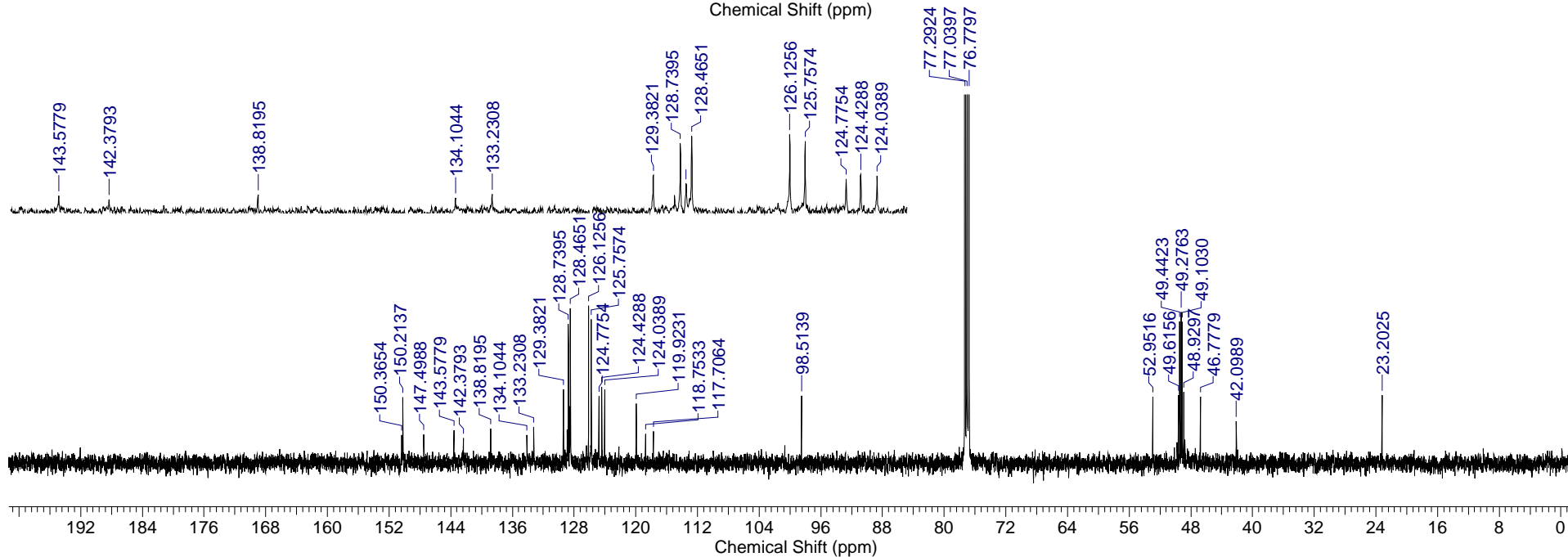
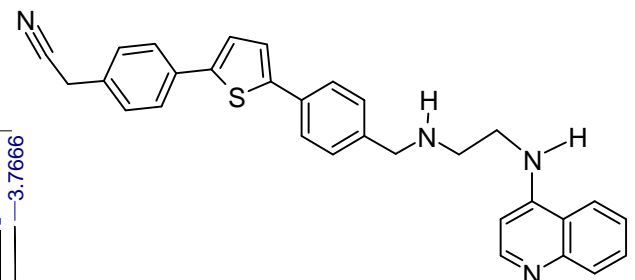
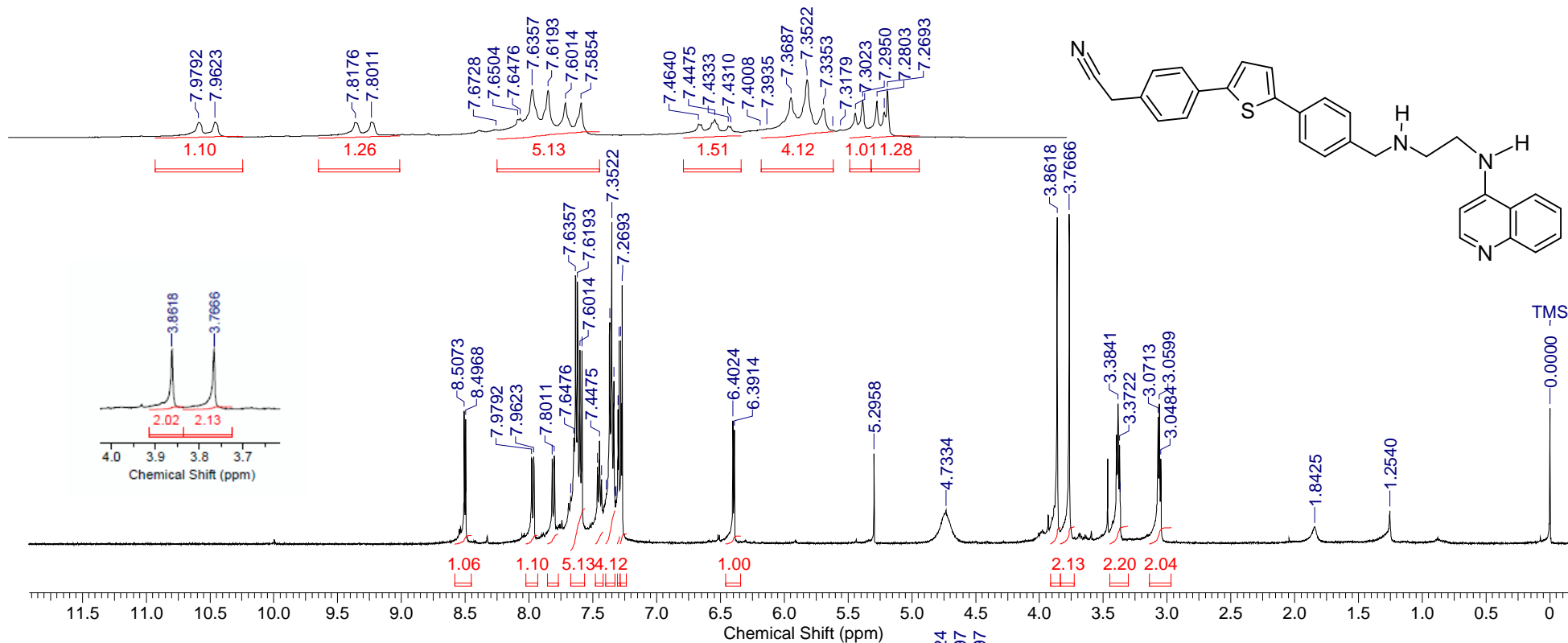
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 PL13 18.40 dB
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 PL12W 0.39575511 W
 PL13W 0.39575511 W
 SFO2 500.2634038 MHz
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 WDW EM
 SSB 0
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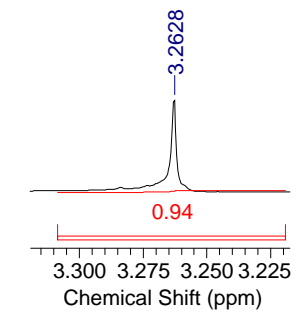
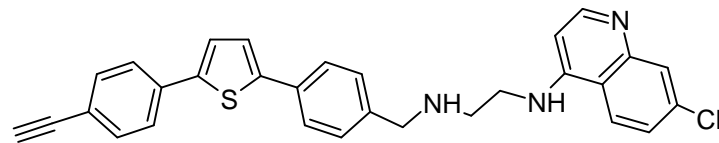
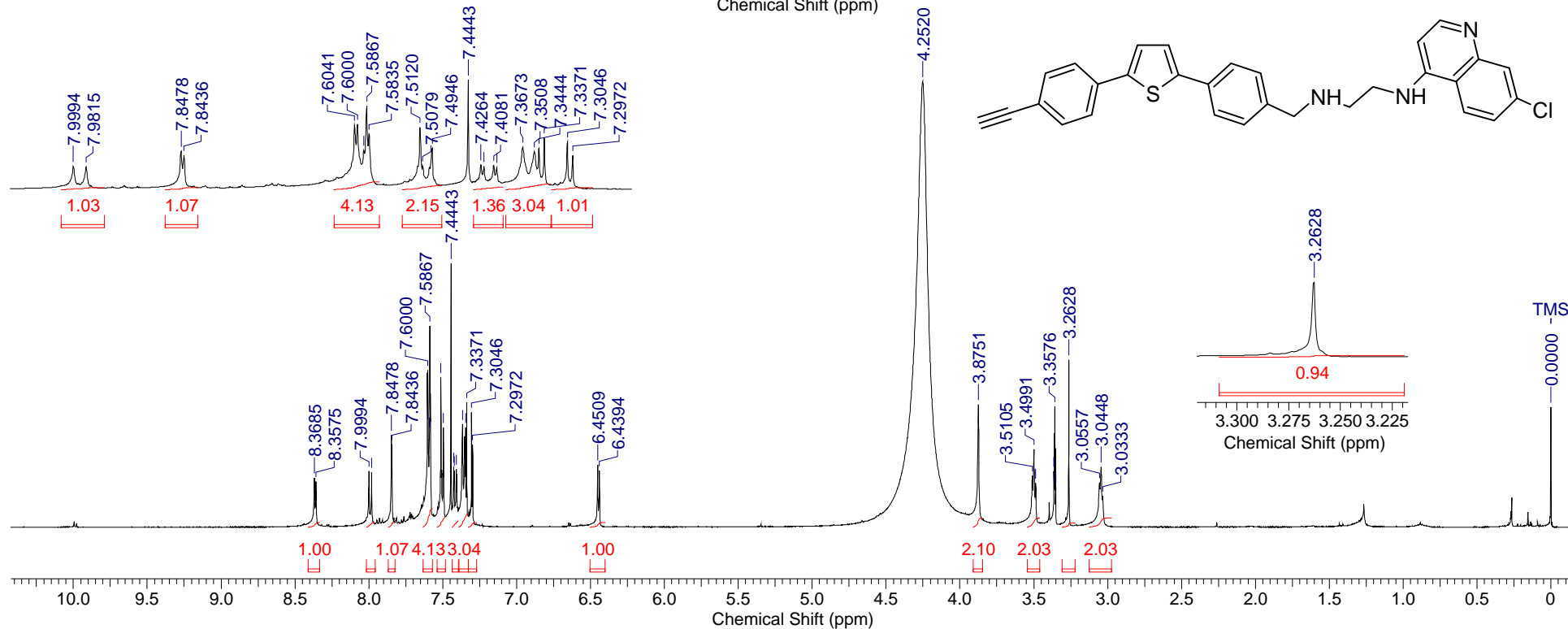
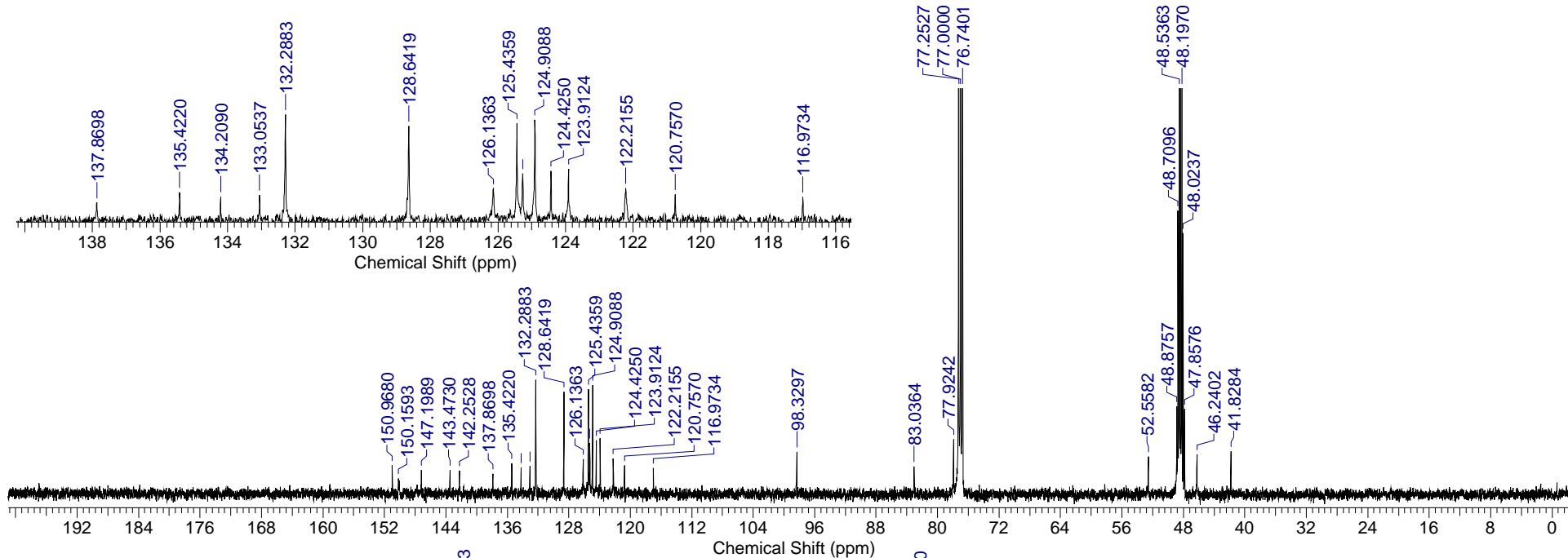


4-{5-[4-({[2-(quinolin-4-ylamino)ethyl]amino)methyl]phenyl]-2-thienyl}phenyl)acetonitrile

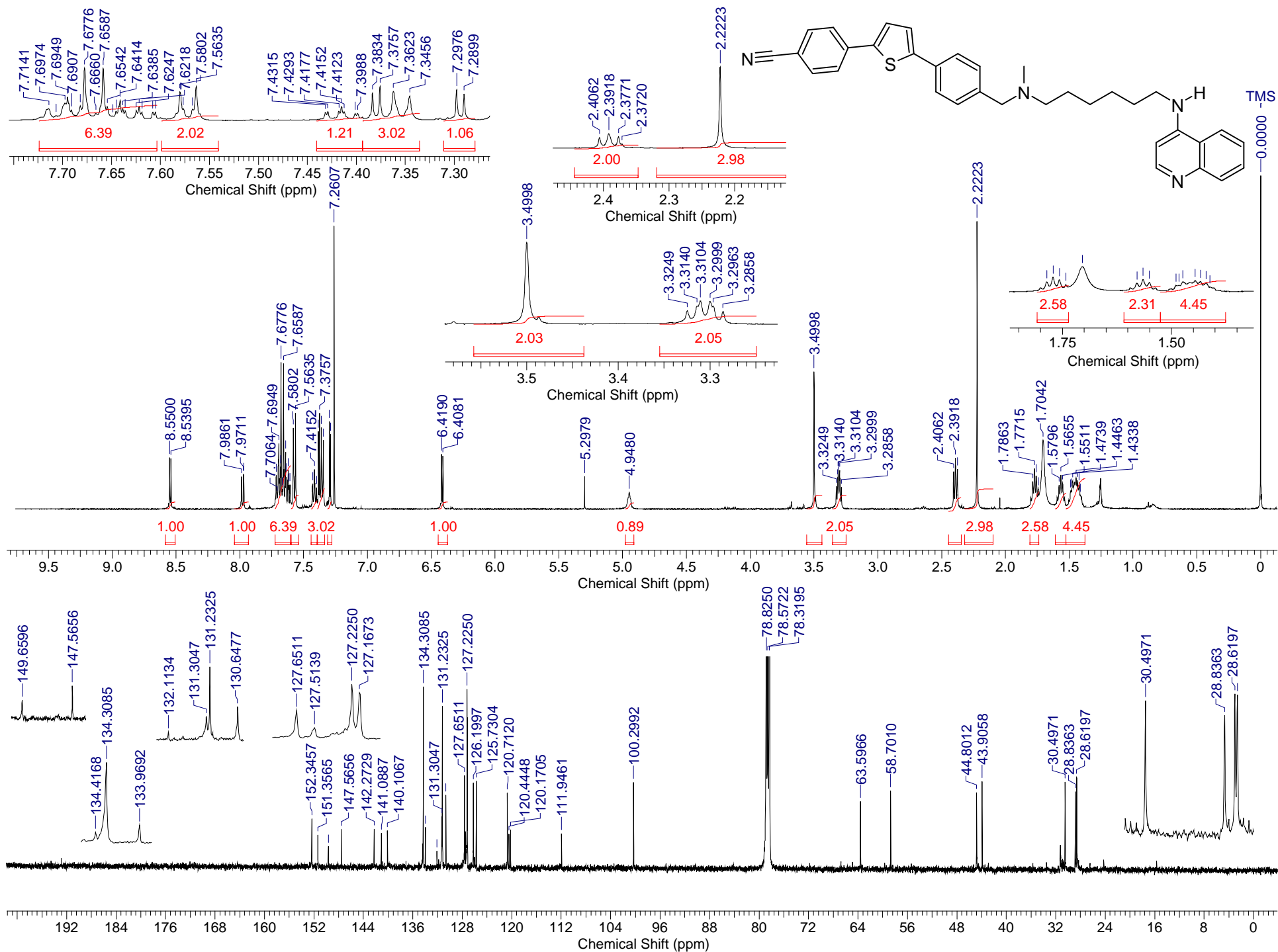
(44)



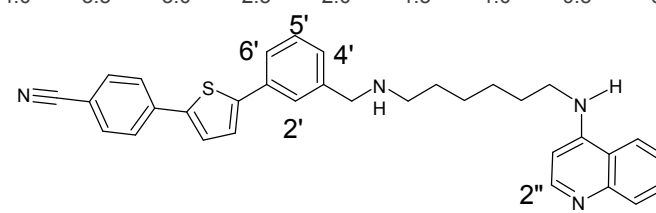
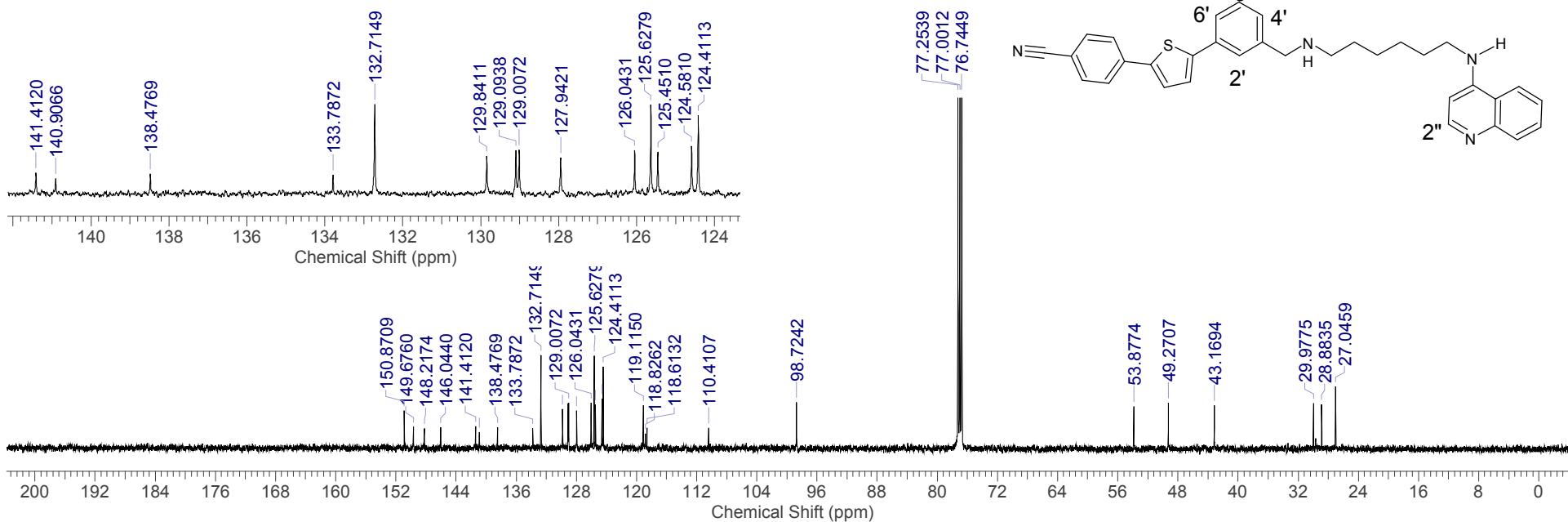
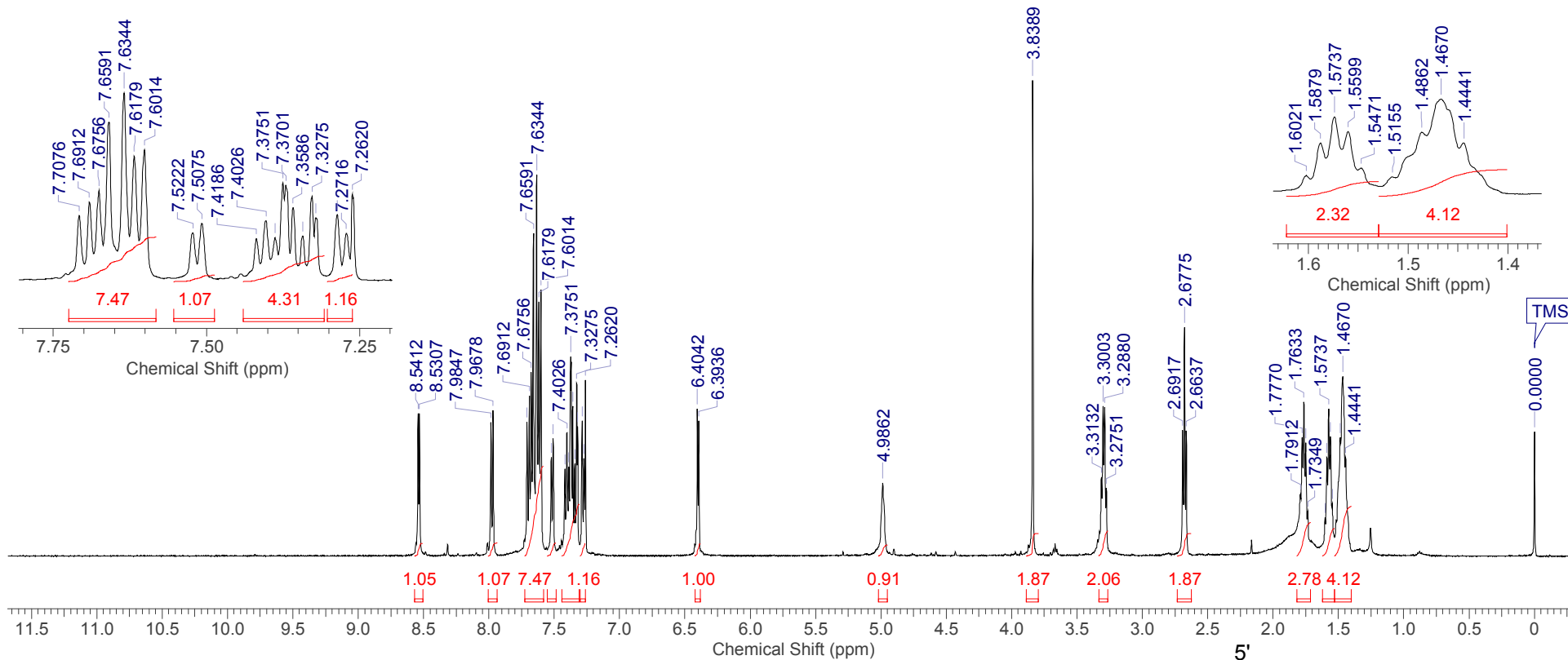
***N*-(7-chloroquinolin-4-yl)-*N*'-{4-[5-(4-ethynylphenyl)-2-thienyl]benzyl}ethane-1,2-diamine (47)**



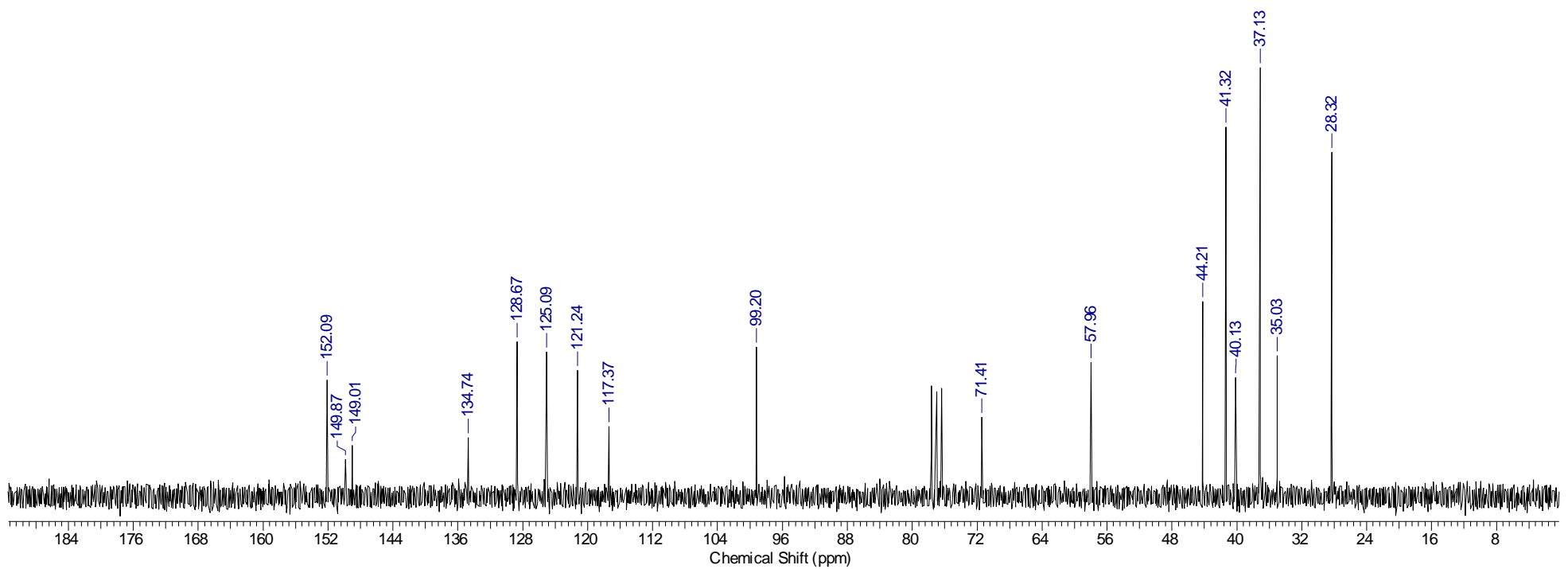
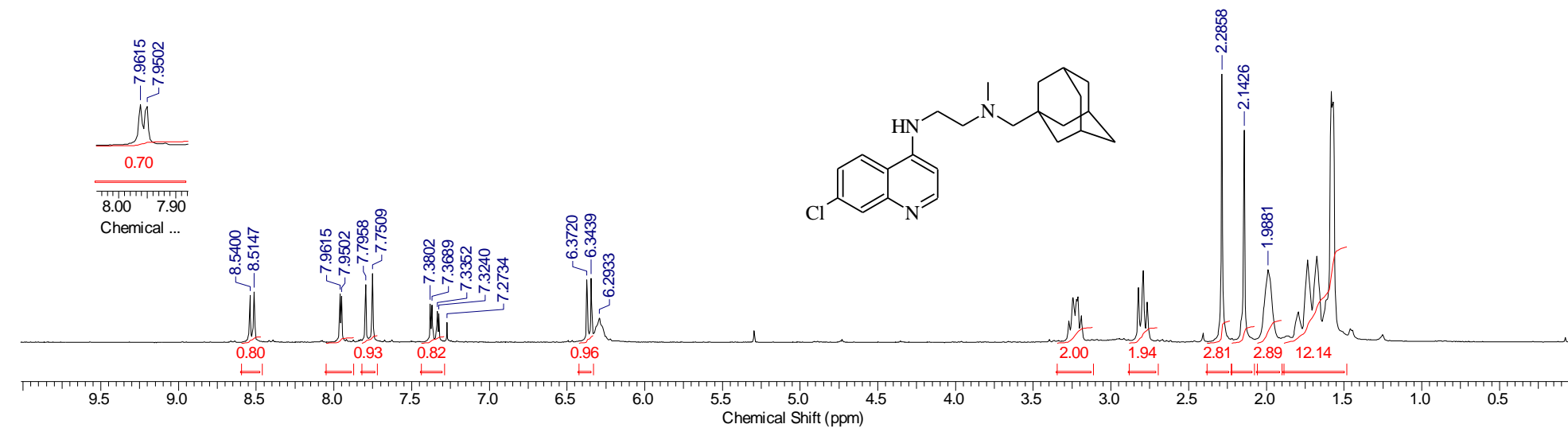
4-{5-[4-((methyl)[6-(quinolin-4-ylamino)hexyl]amino)methyl]phenyl]-2-thienyl}benzonitrile (48)



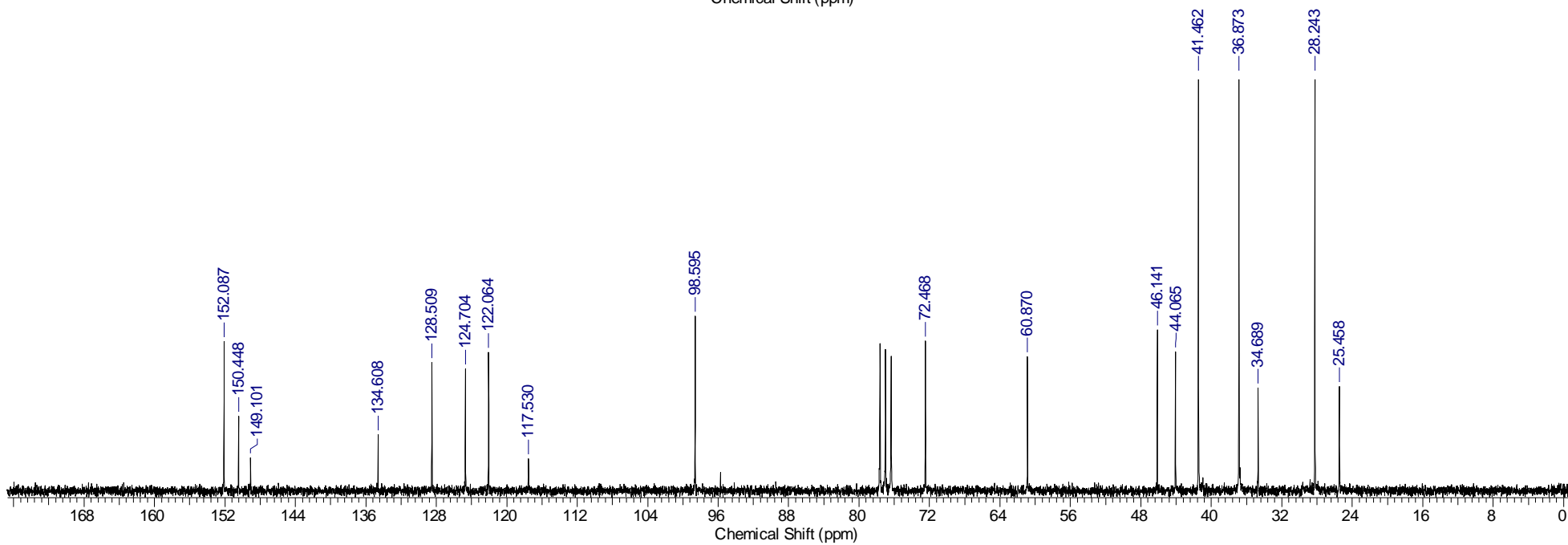
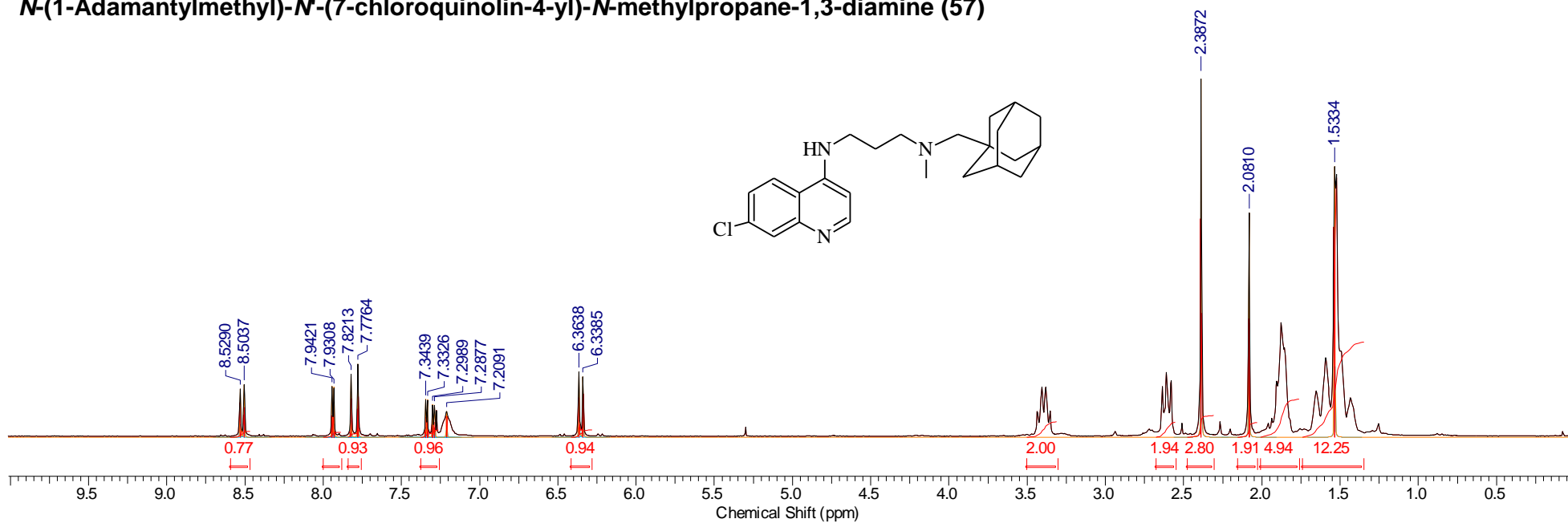
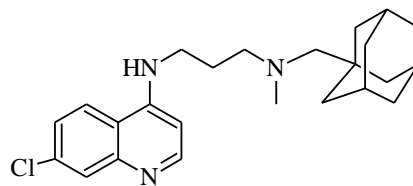
4-{5-[3-({[6-(quinolin-4-ylamino)hexyl]amino)methyl}phenyl]-2-thienyl}benzonitrile (50)



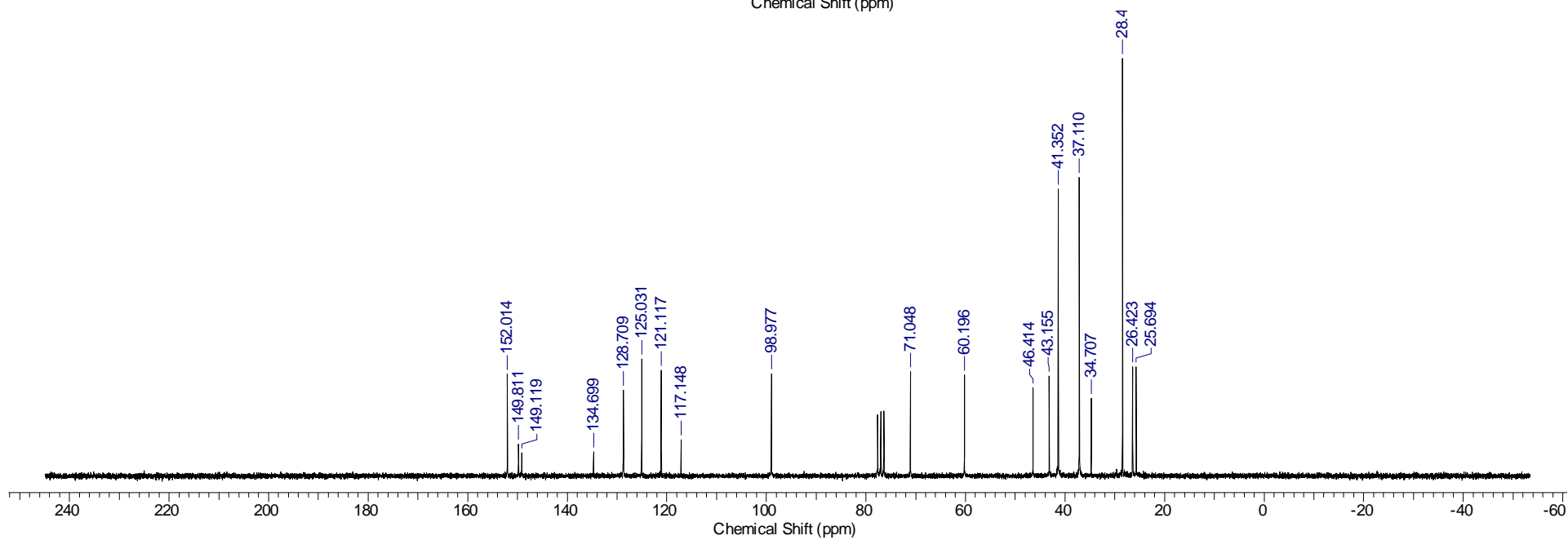
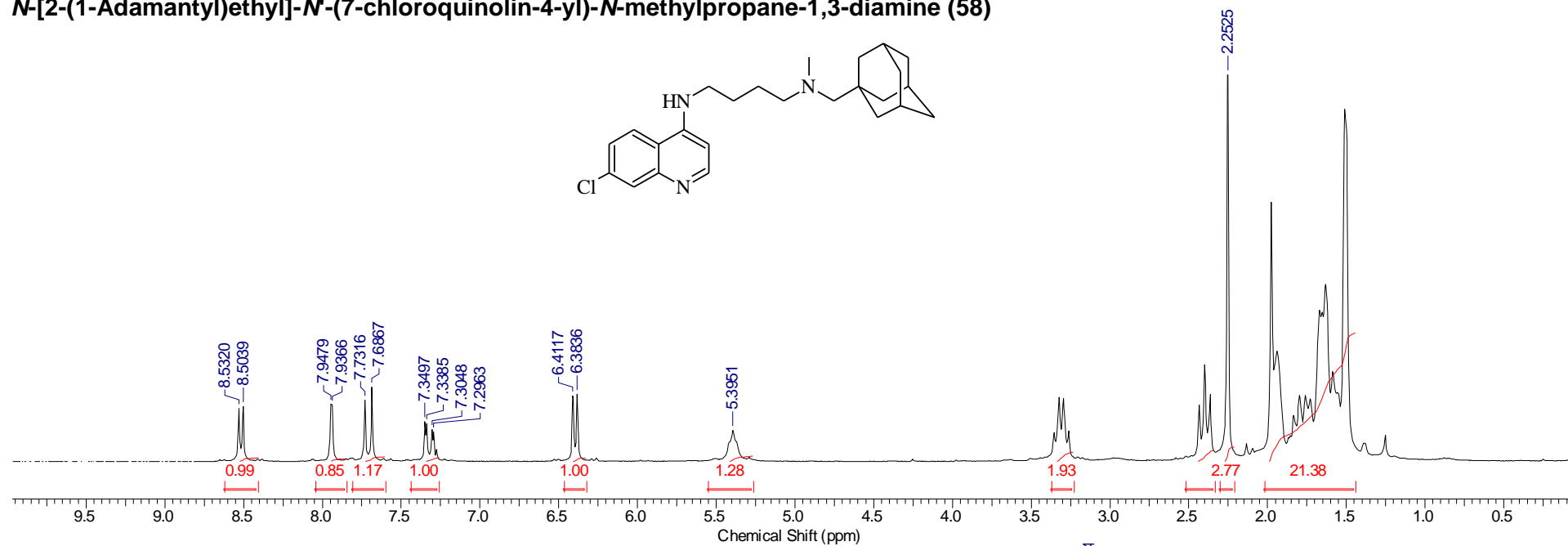
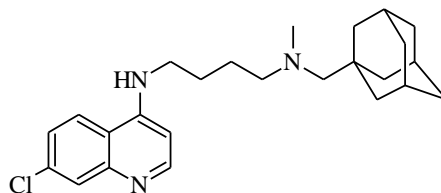
***N*-(1-Adamantylmethyl)-*N*-(7-chloroquinolin-4-yl)-*N*-methylethane-1,2-diamine (56)**



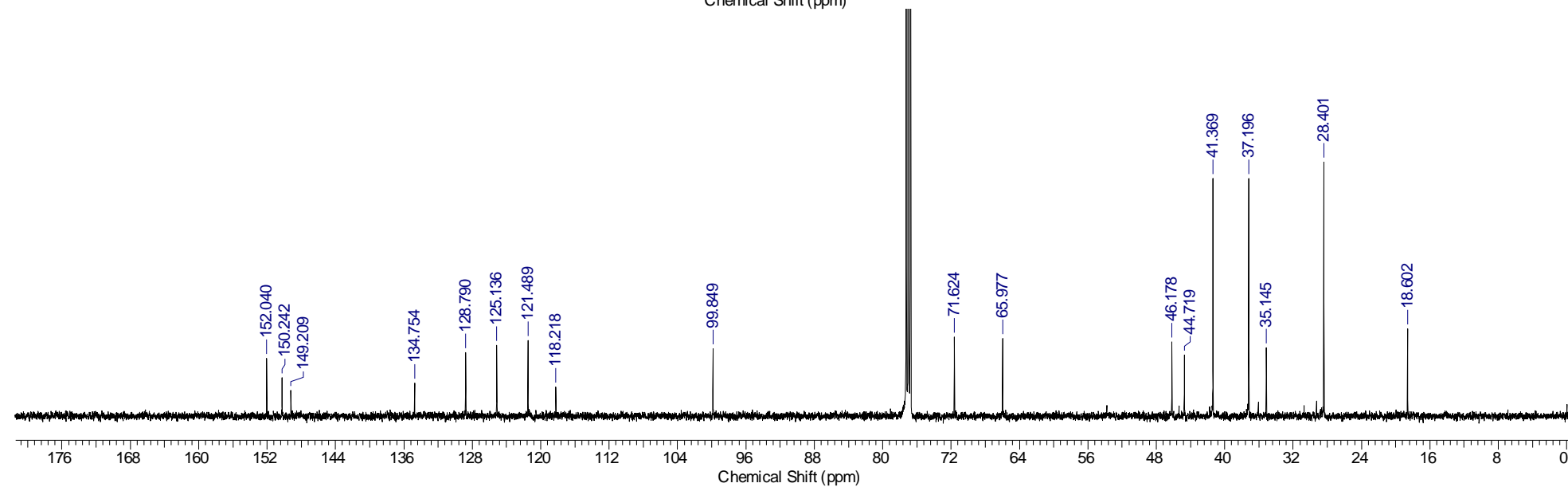
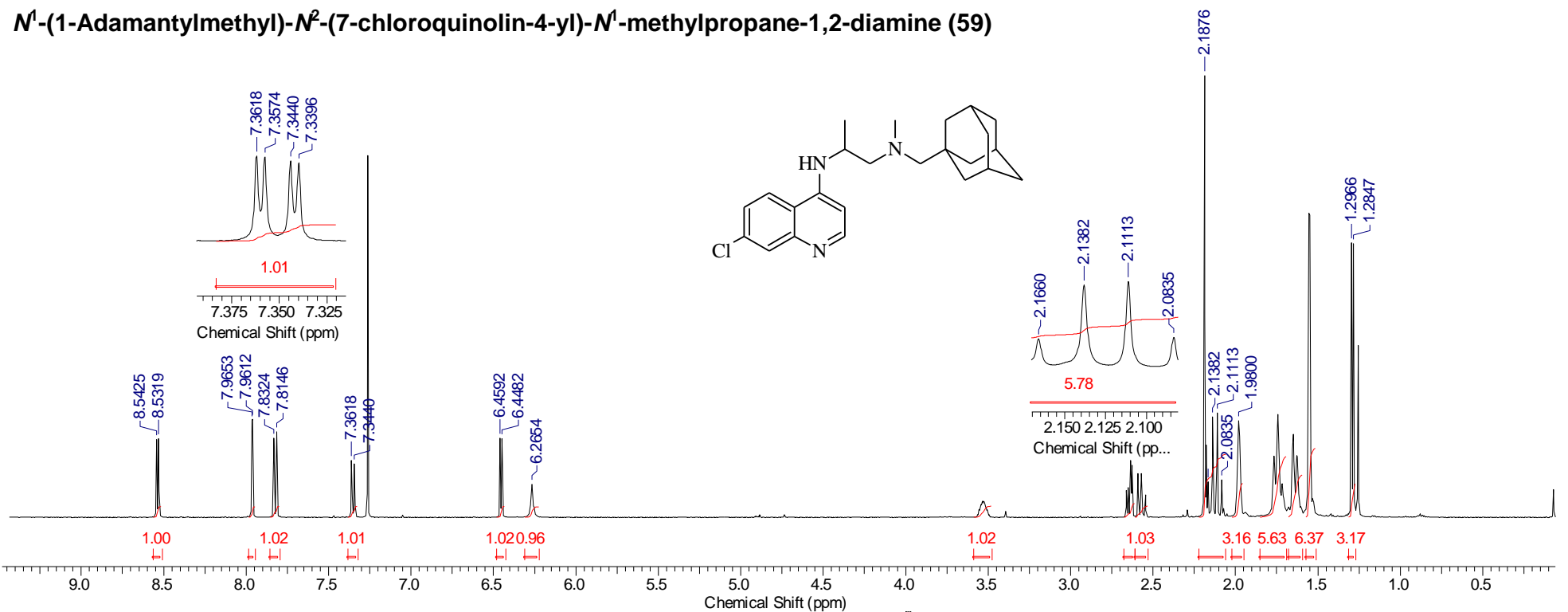
***N*-(1-Adamantylmethyl)-*N*-(7-chloroquinolin-4-yl)-*N*-methylpropane-1,3-diamine (57)**



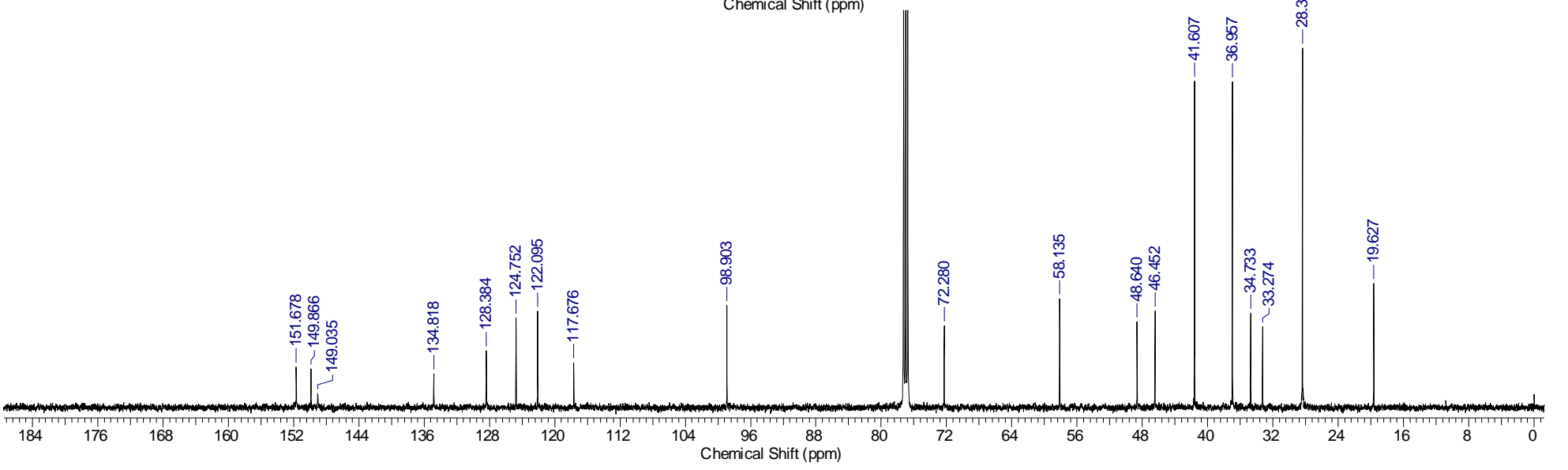
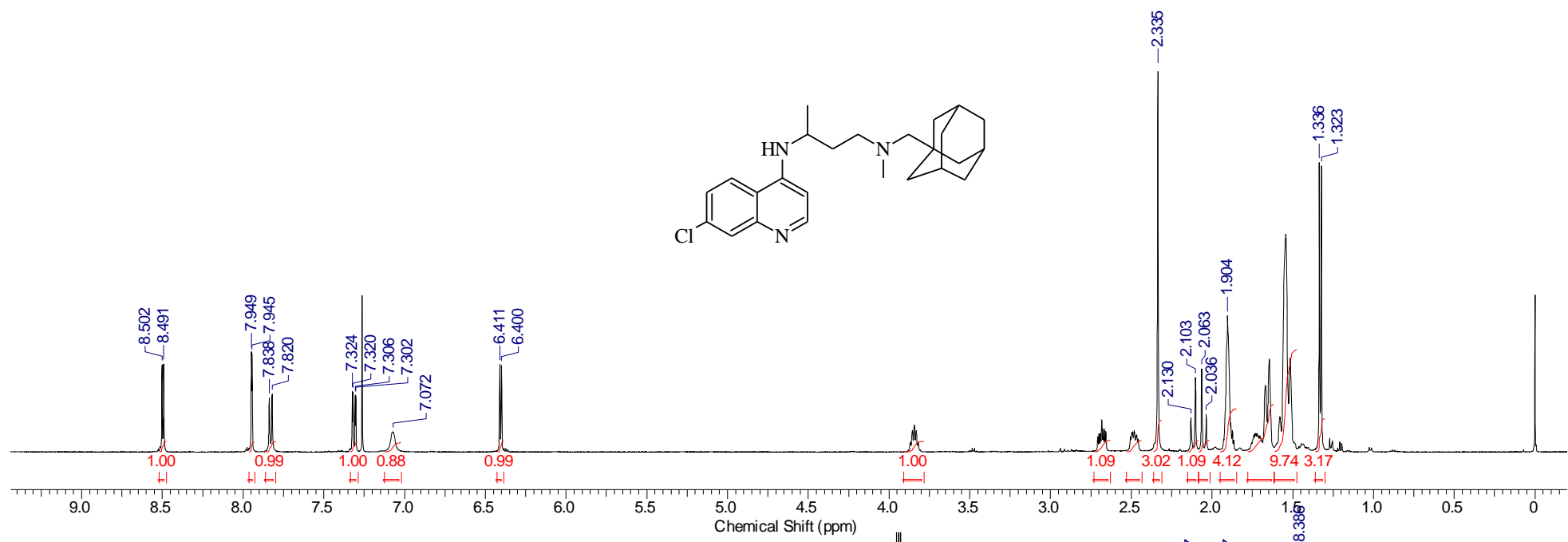
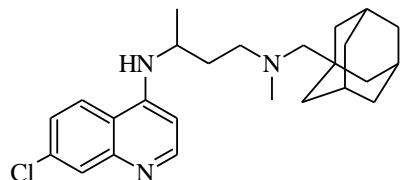
***N*-[2-(1-Adamanty)ethyl]-*N'*-(7-chloroquinolin-4-yl)-*N*-methylpropane-1,3-diamine (58)**



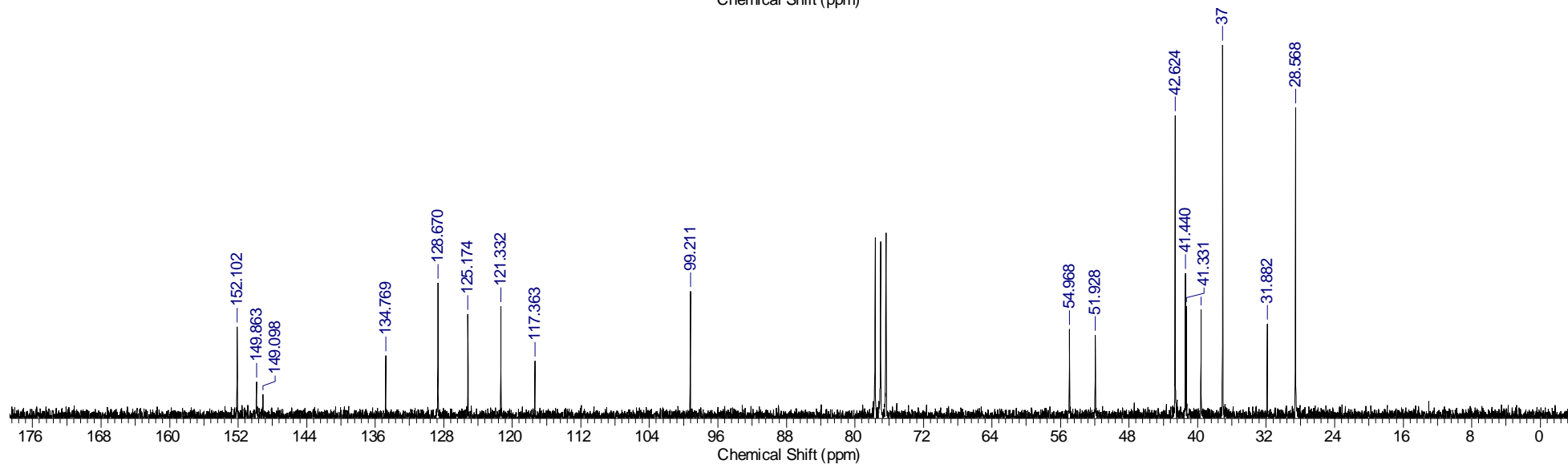
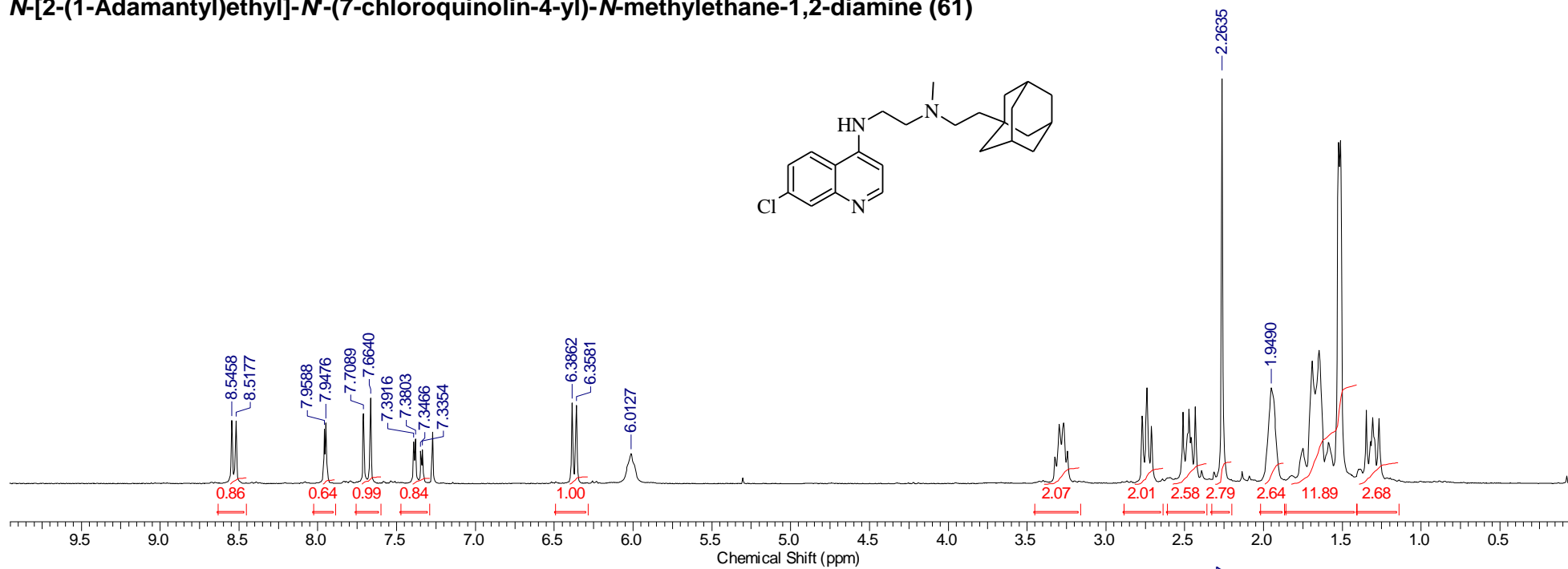
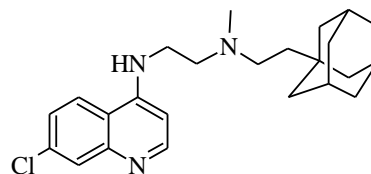
***N*¹-(1-Adamantylmethyl)-*N*²-(7-chloroquinolin-4-yl)-*N*¹-methylpropane-1,2-diamine (59)**



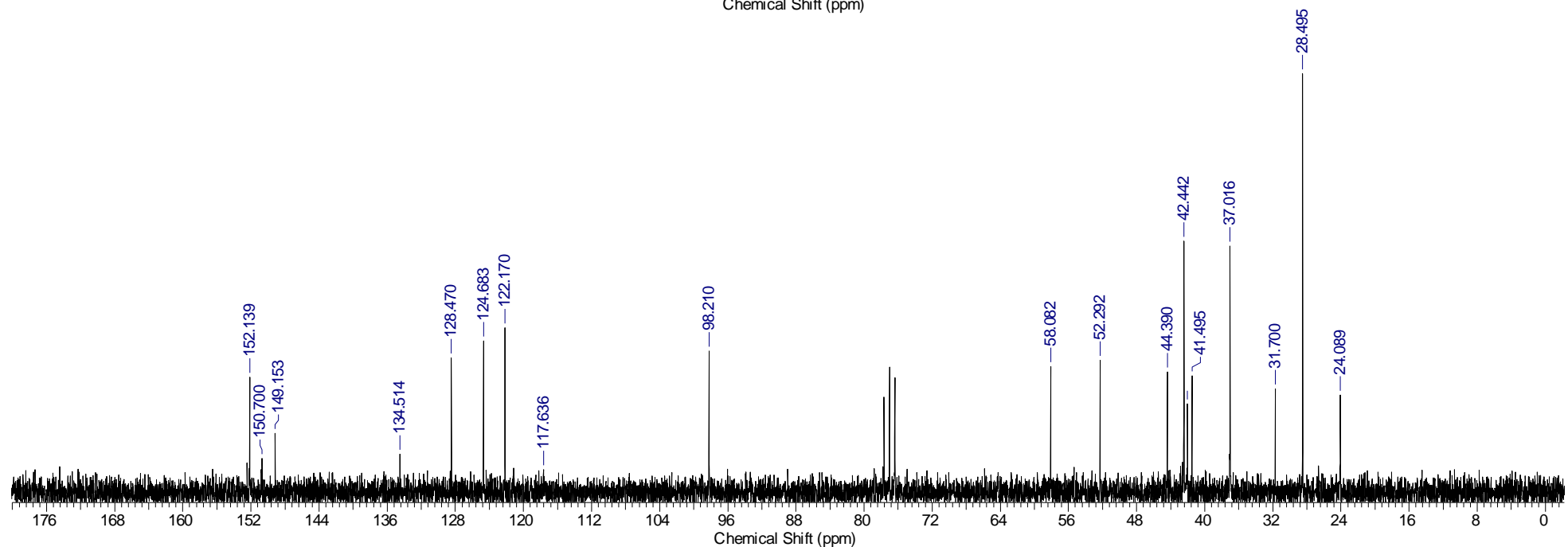
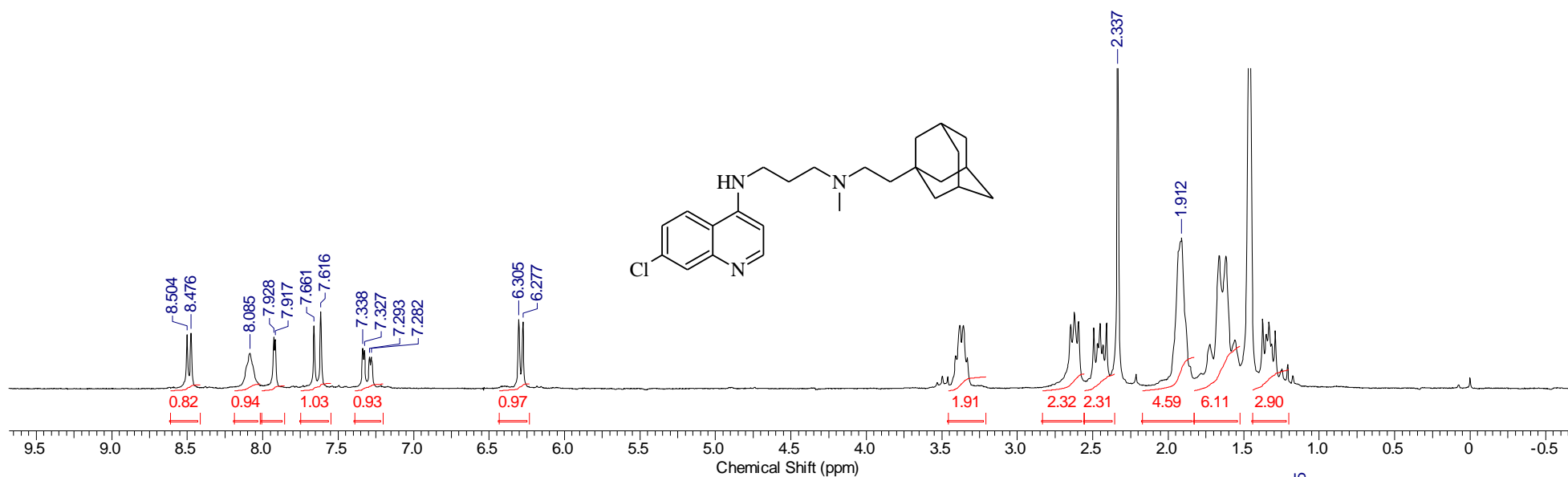
***N*¹-(1-Adamantylmethyl)-*N*³-(7-chloroquinolin-4-yl)-*N*¹-methylbutane-1,3-diamine (60)**



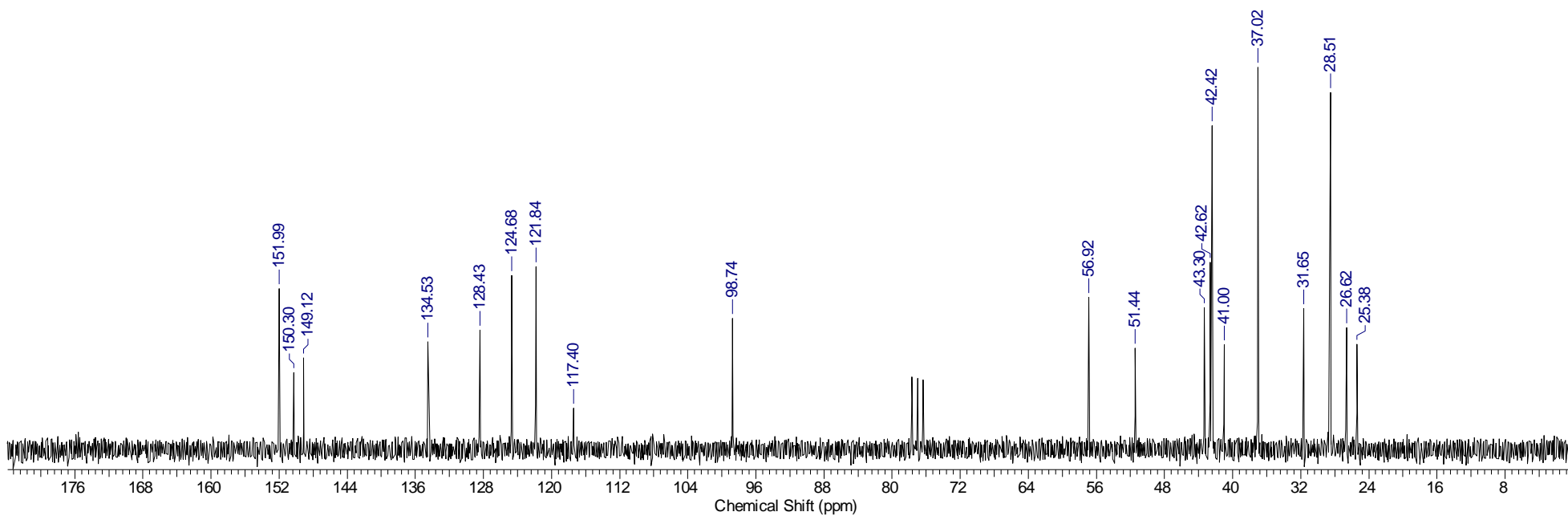
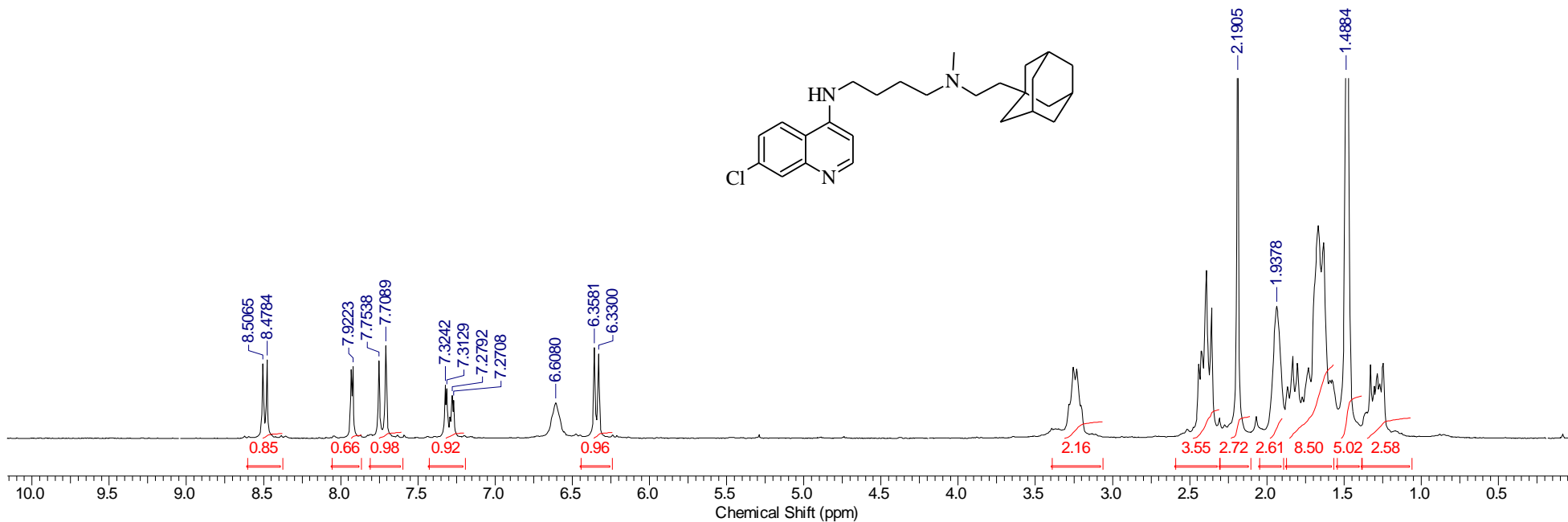
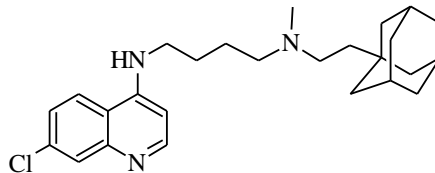
***N*-[2-(1-Adamanty)ethyl]-*N*-(7-chloroquinolin-4-yl)-*N*-methylethane-1,2-diamine (61)**



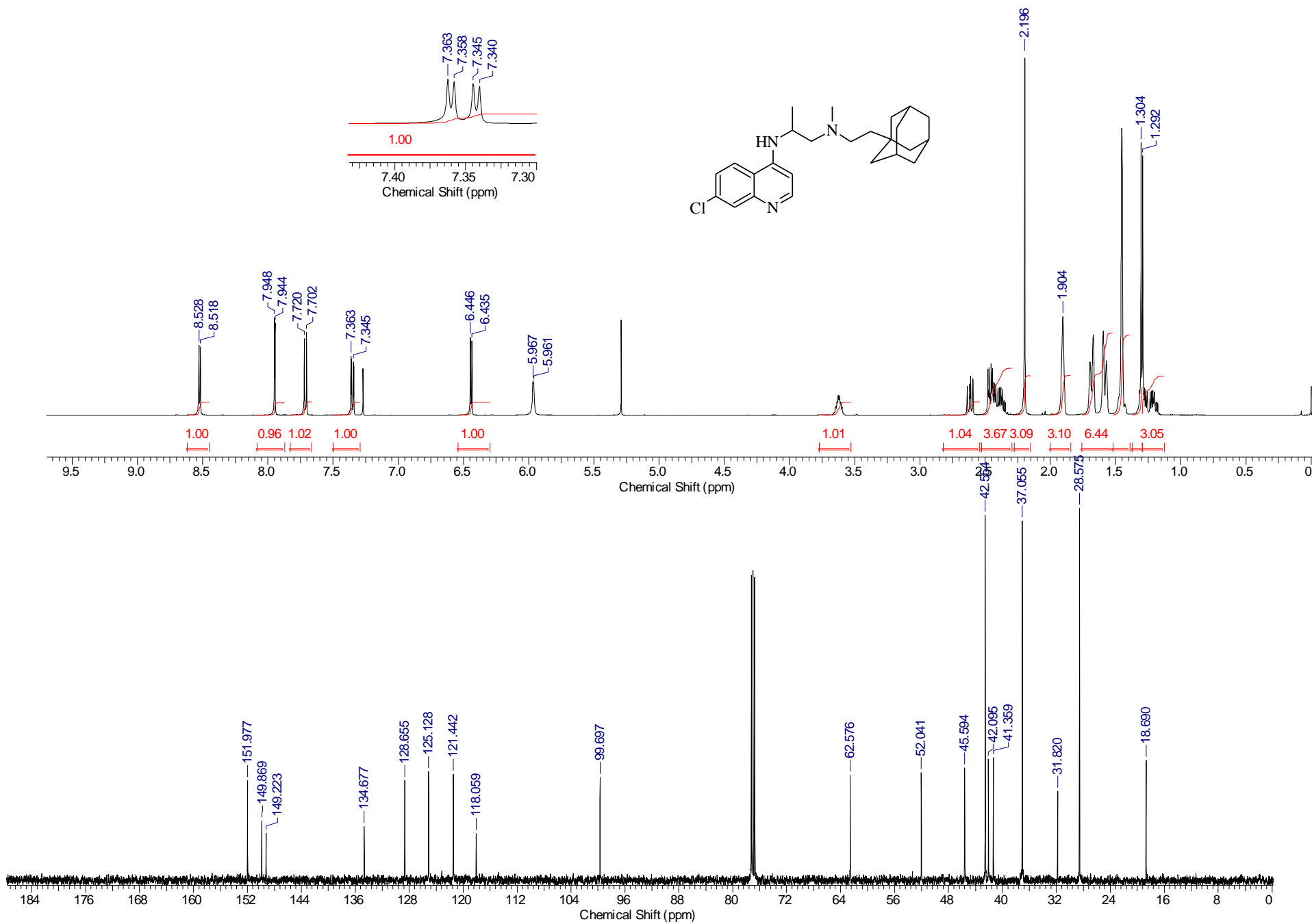
***N*-[2-(1-Adamanty)ethyl]-*N*-(7-chloroquinolin-4-yl)-*N*-methylpropane-1,3-diamine (62)**



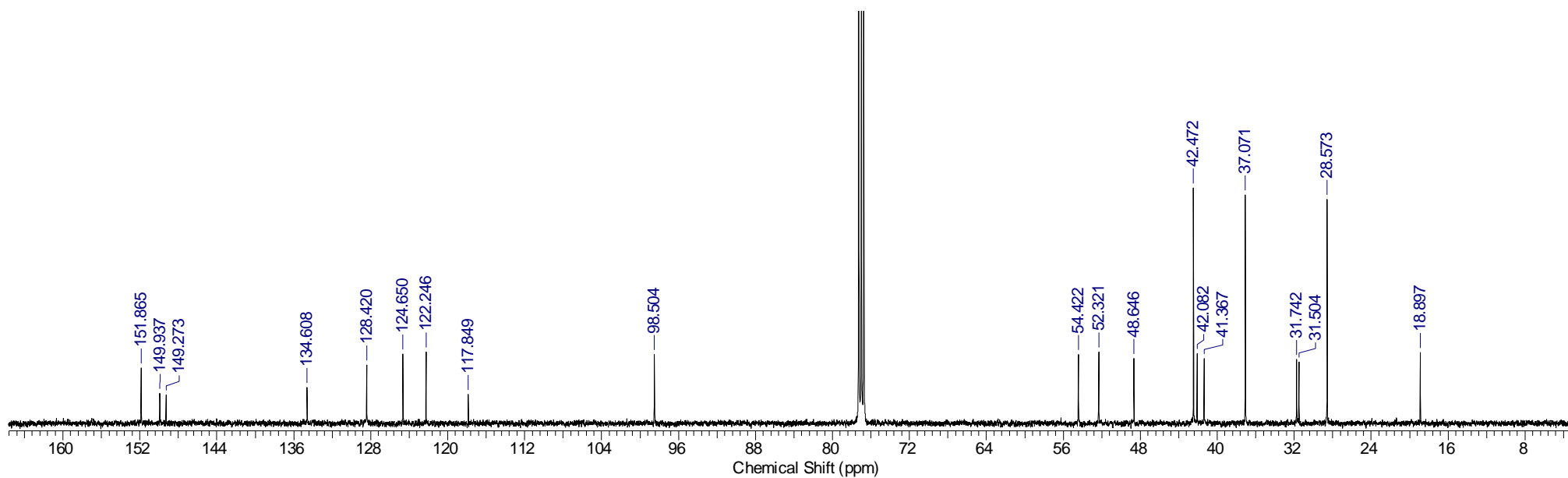
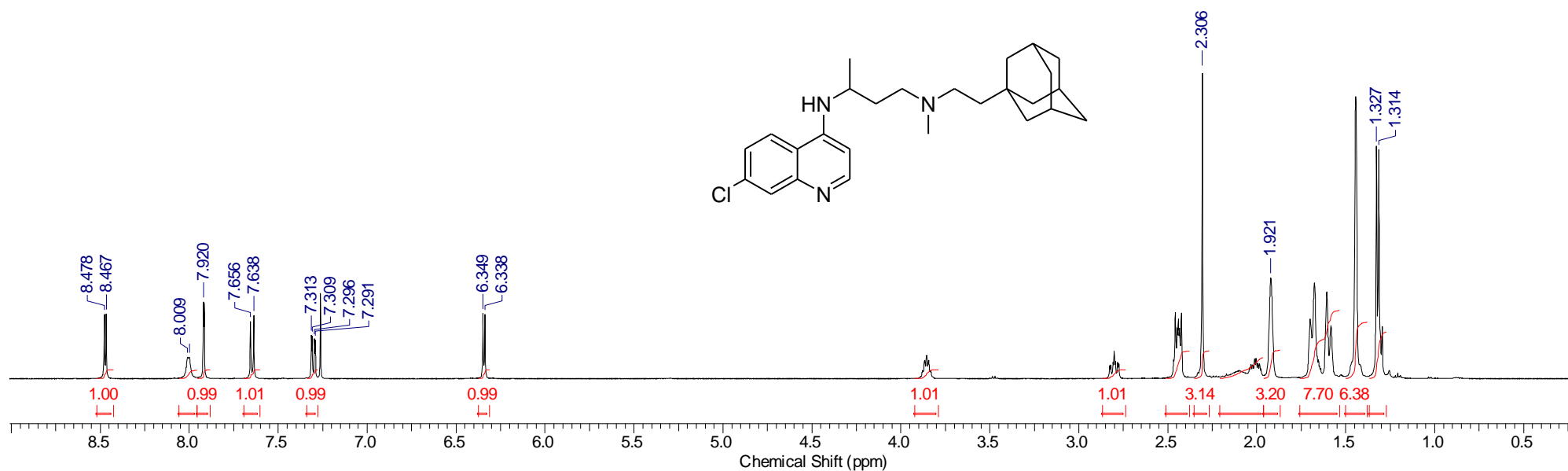
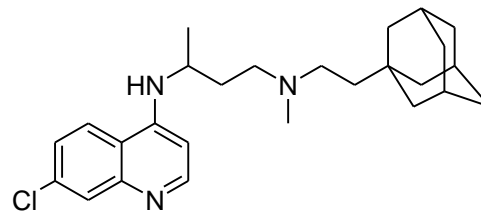
***N*-[2-(1-Adamanty)ethyl]-*N*-(7-chloroquinolin-4-yl)-*N*-methylbutane-1,4-diamine (63)**



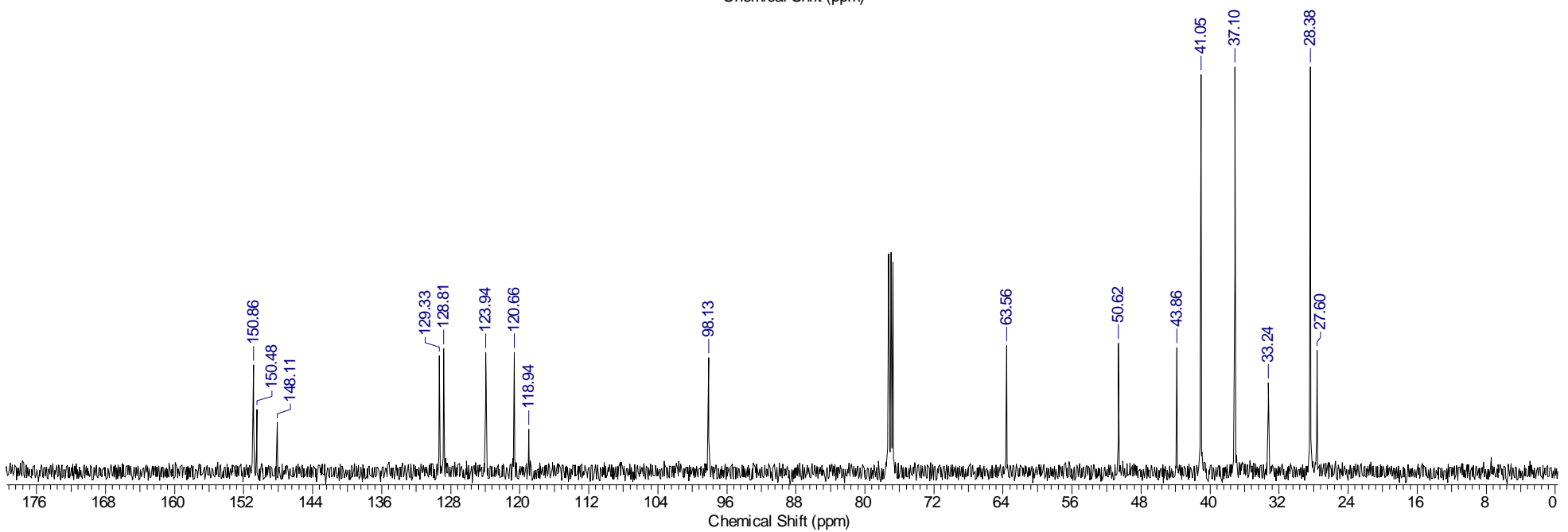
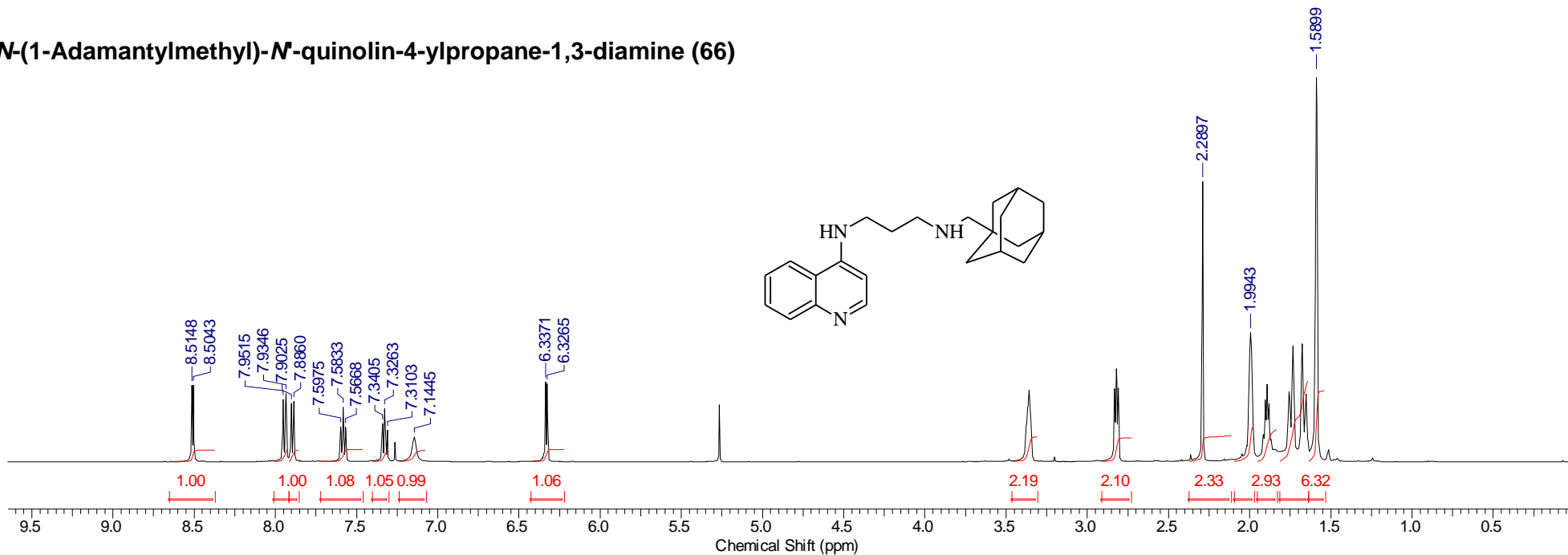
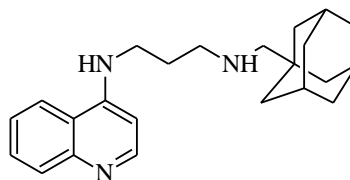
***N'*-[2-(1-Adamantyl)ethyl]-*N*'-(7-chloroquinolin-4-yl)-*N*'-methylpropane-1,2-diamine (64)**



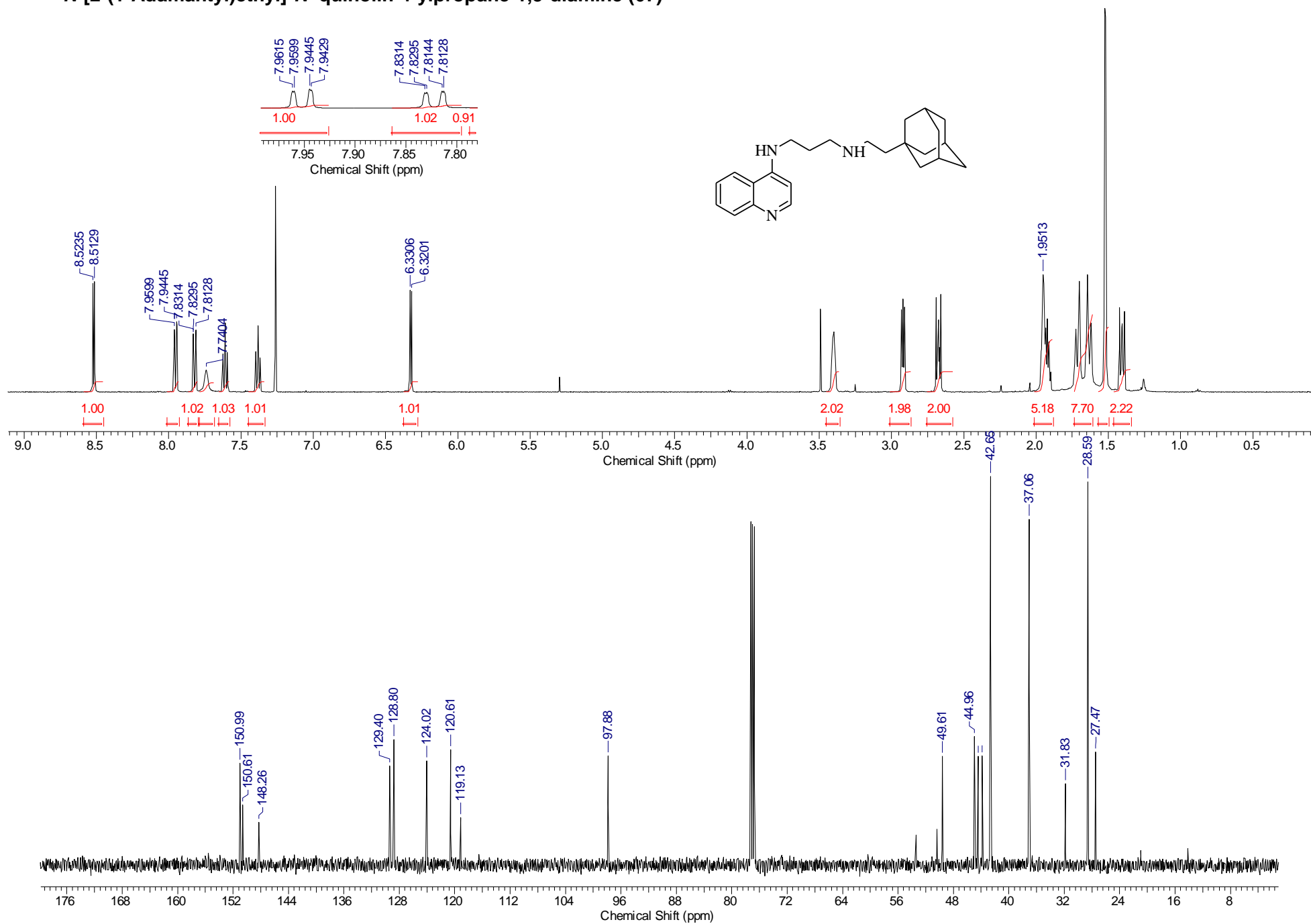
***N*¹-[2-(1-Adamantyl)ethyl]-*N*³-(7-chloroquinolin-4-yl)-*N*¹-methylbutane-1,3-diamine (65)**



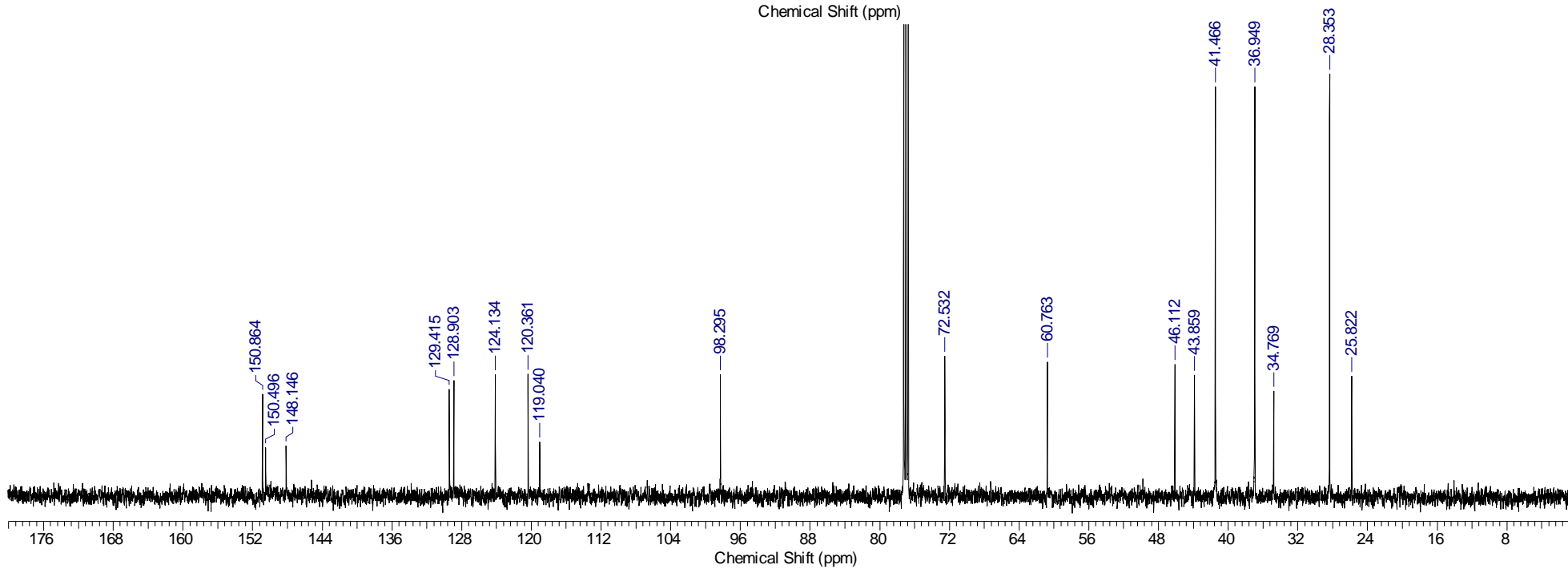
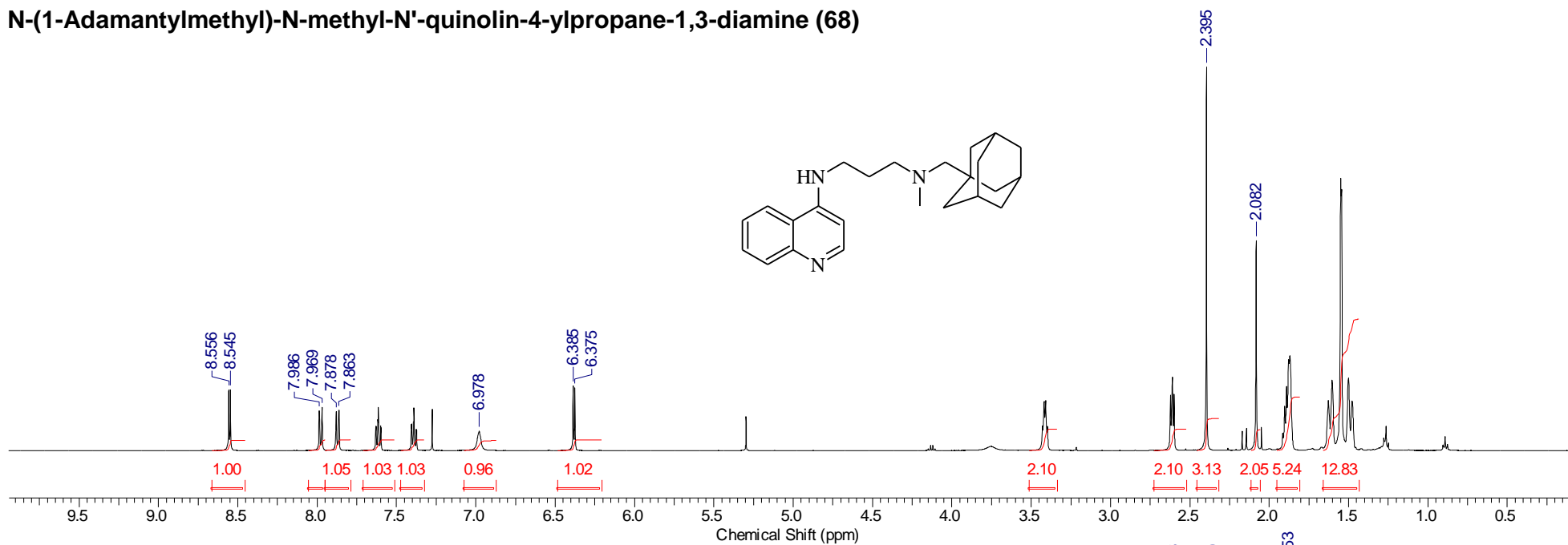
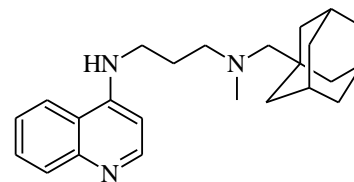
***N*-(1-Adamantylmethyl)-*N'*-quinolin-4-ylpropane-1,3-diamine (66)**



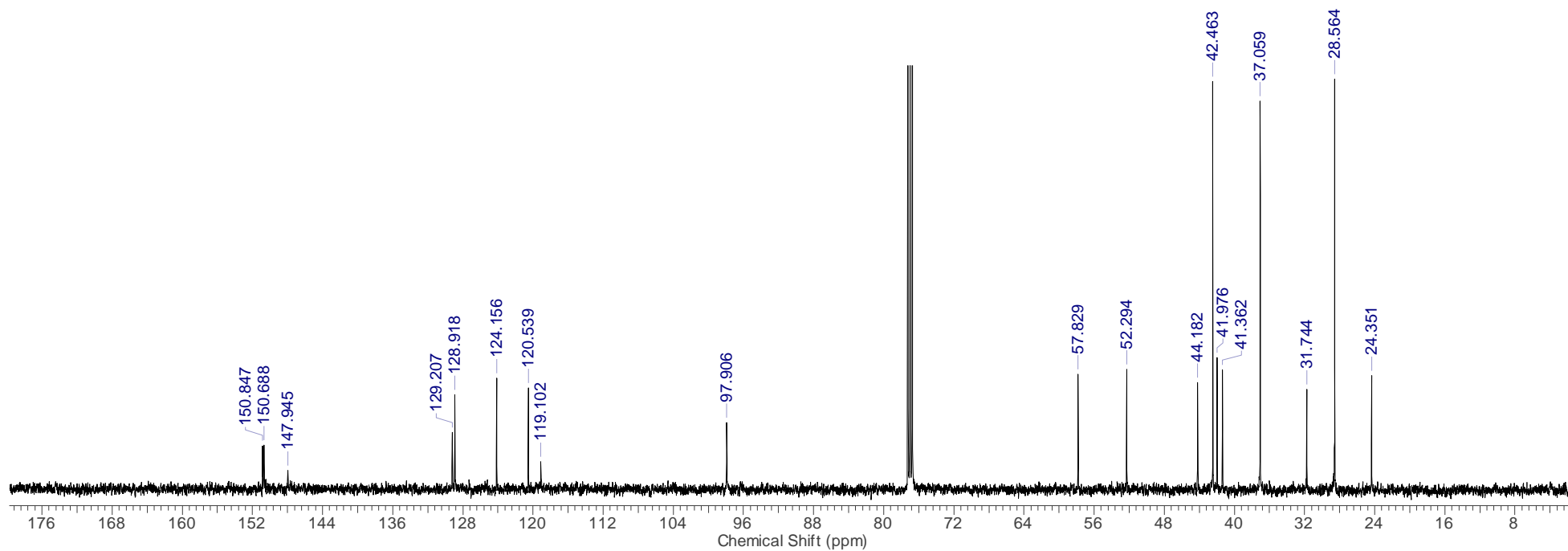
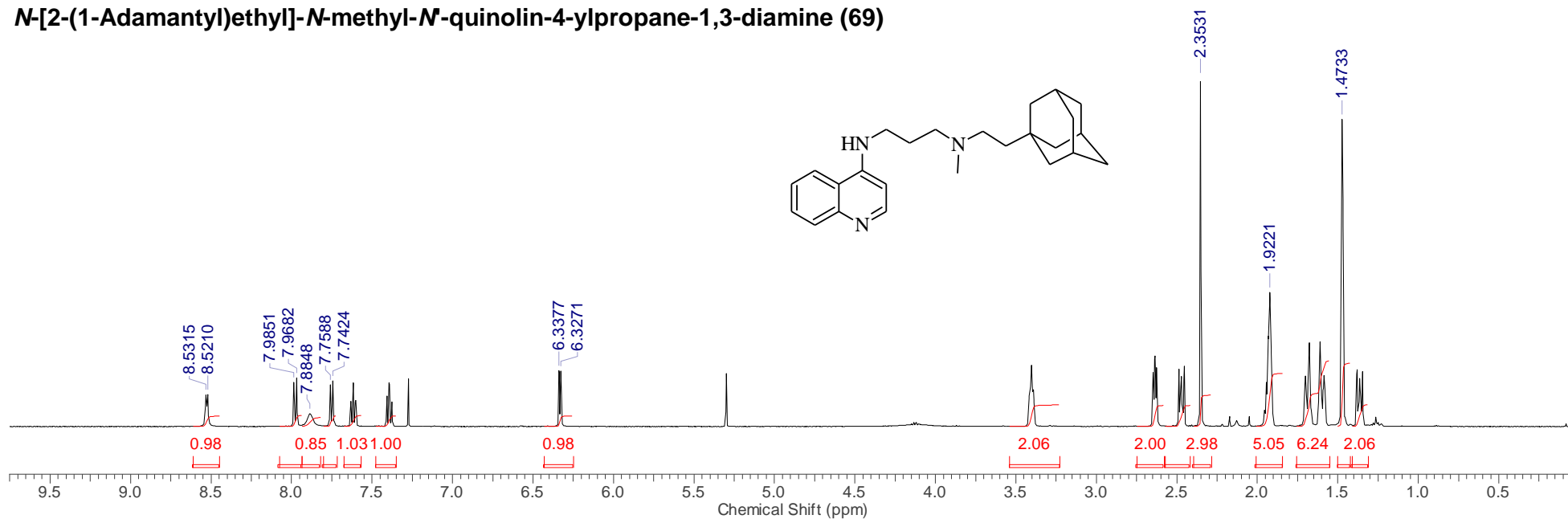
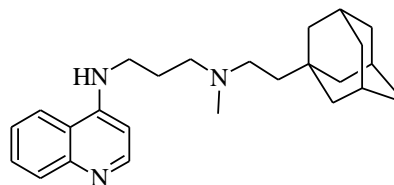
N-[2-(1-Adamantyl)ethyl]-*N'*-quinolin-4-ylpropane-1,3-diamine (67)



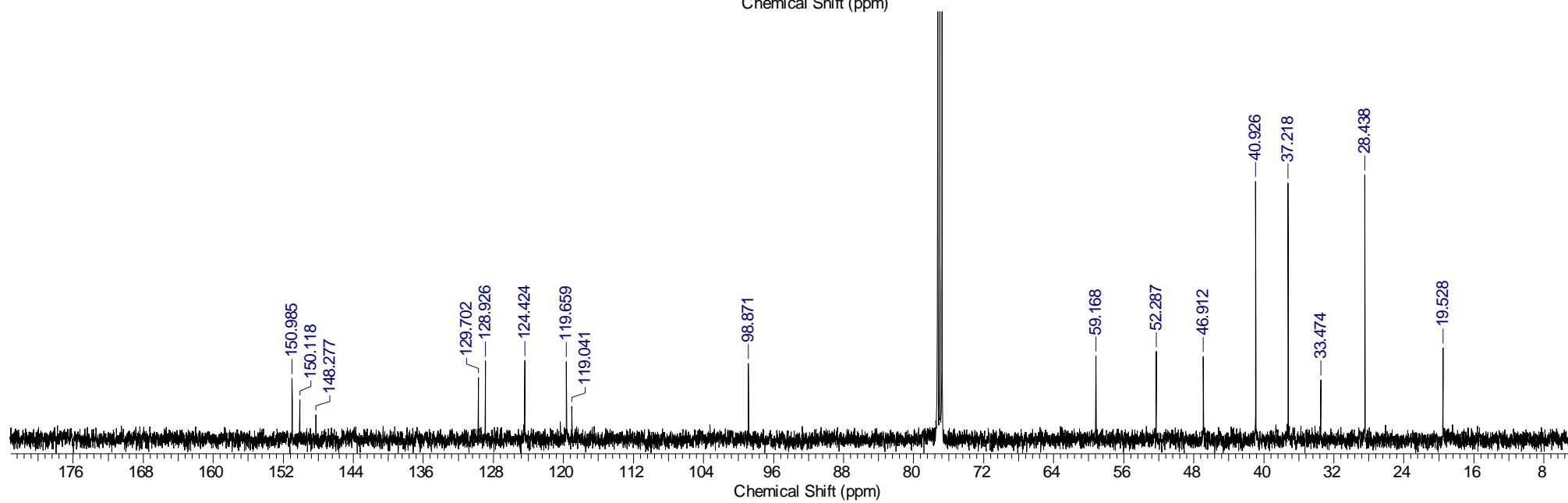
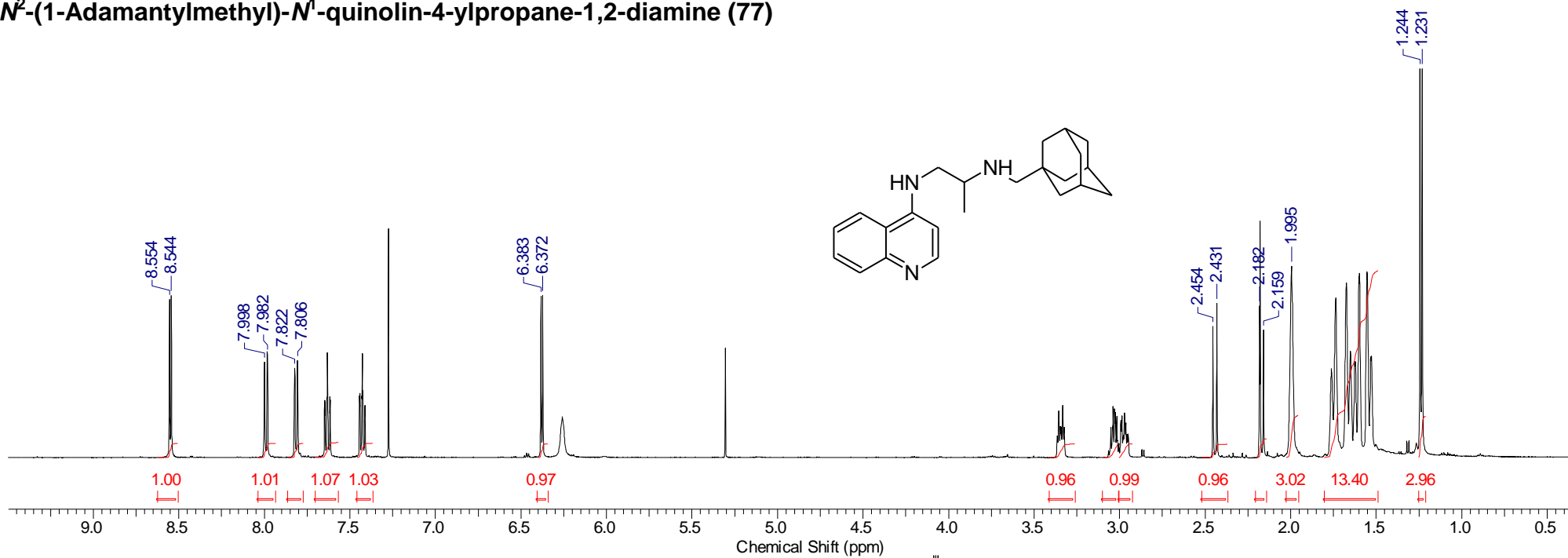
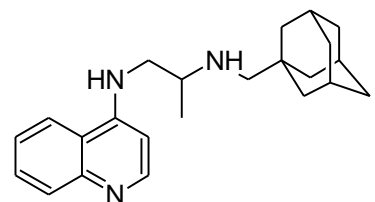
N-(1-Adamantylmethyl)-N-methyl-N'-quinolin-4-ylpropane-1,3-diamine (68)



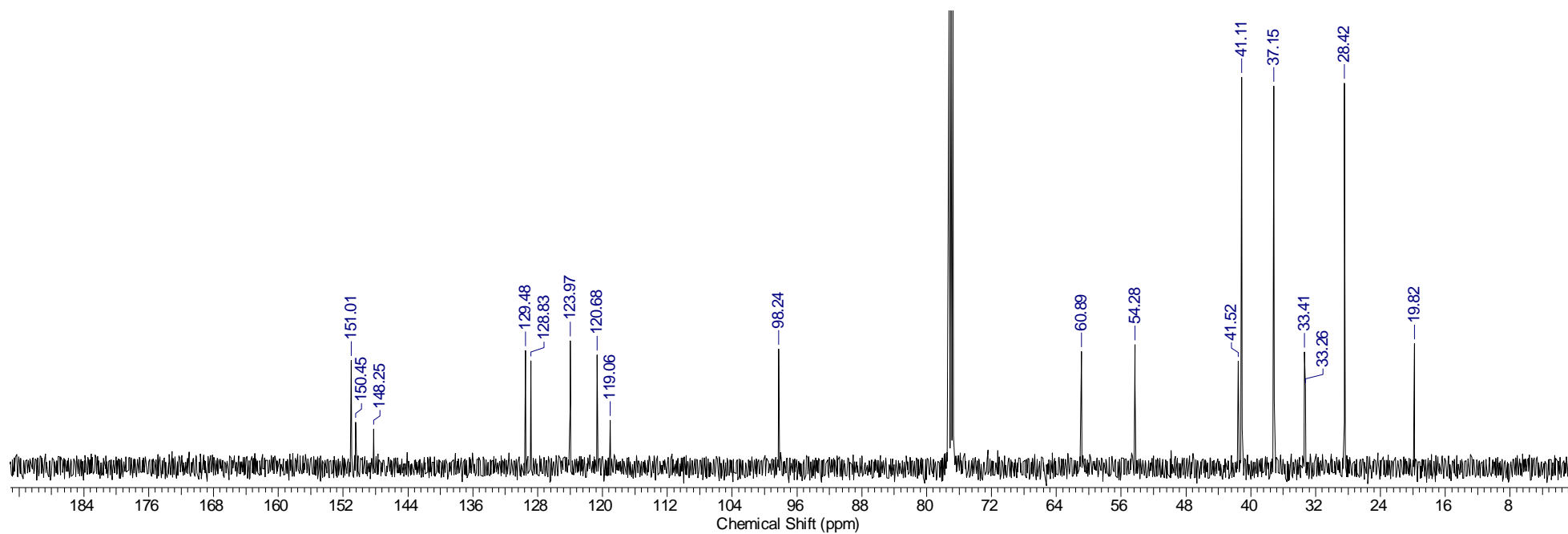
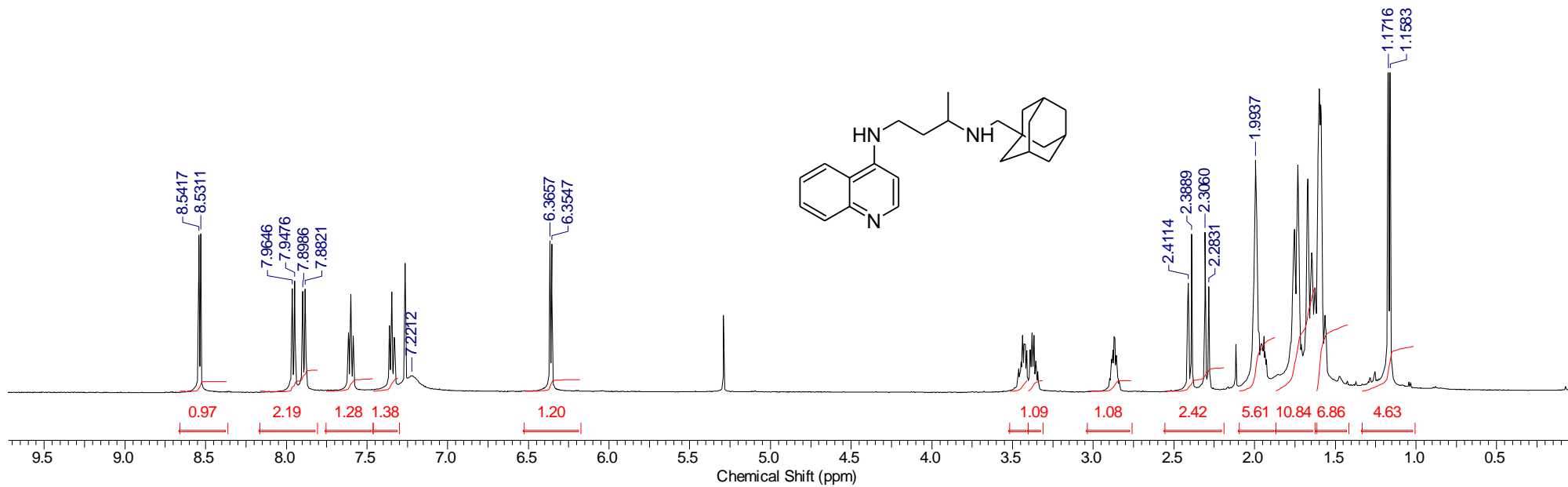
***N*-[2-(1-Adamanty)ethyl]-*N*-methyl-*N*-quinolin-4-ylpropane-1,3-diamine (69)**



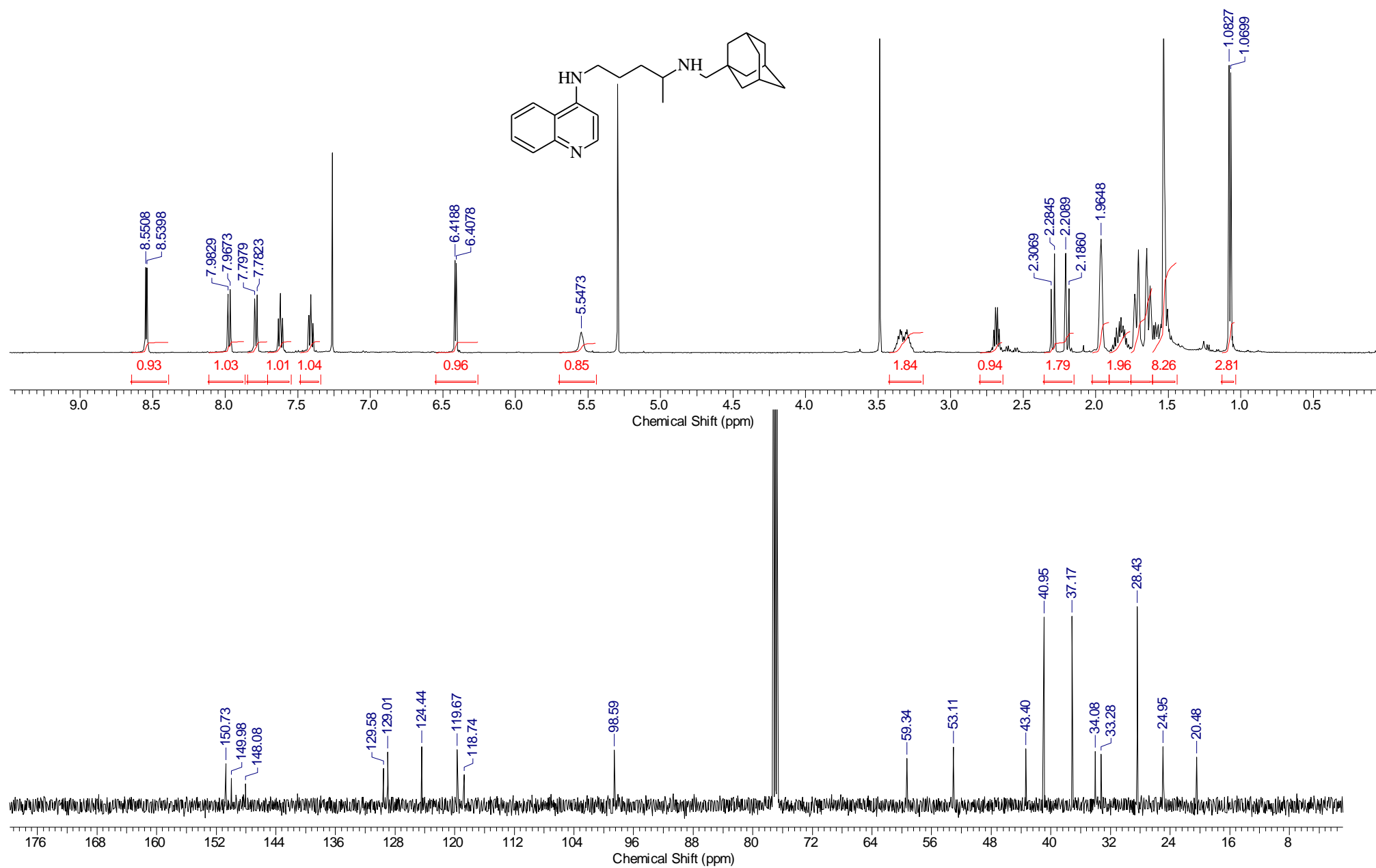
***N*²-(1-Adamantylmethyl)-*N*¹-quinolin-4-ylpropane-1,2-diamine (77)**



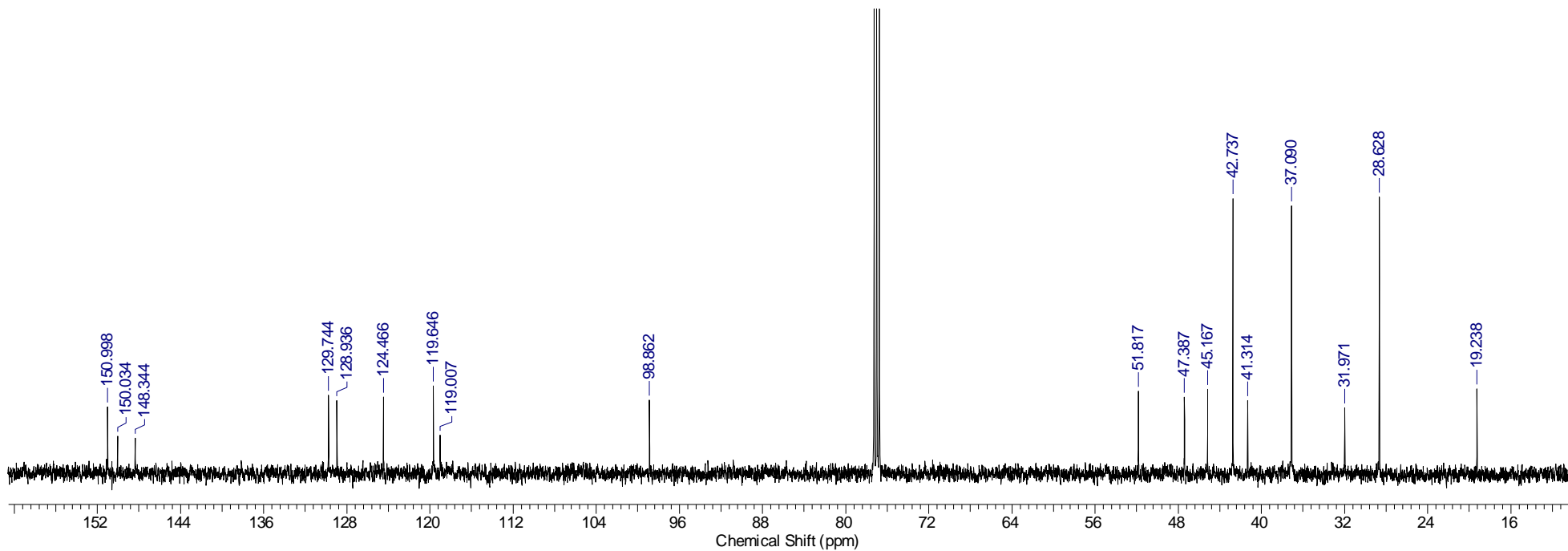
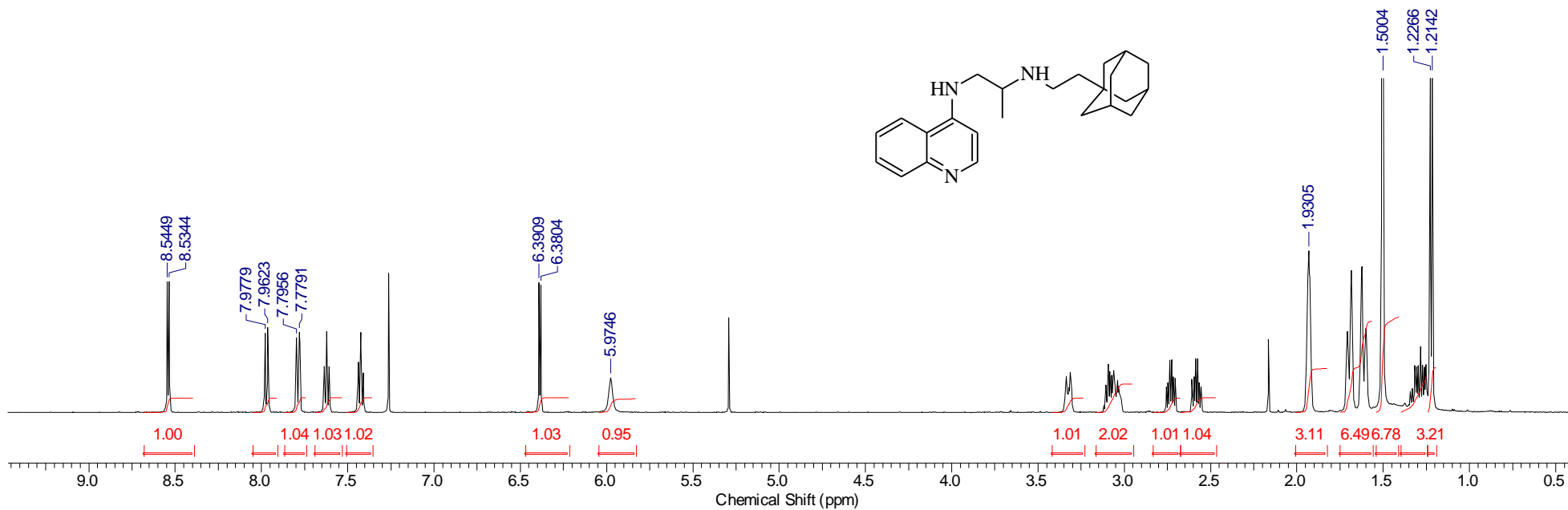
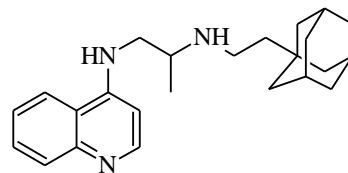
***N*³-(1-Adamantylmethyl)-*N*¹-quinolin-4-ylbutane-1,3-diamine (78)**



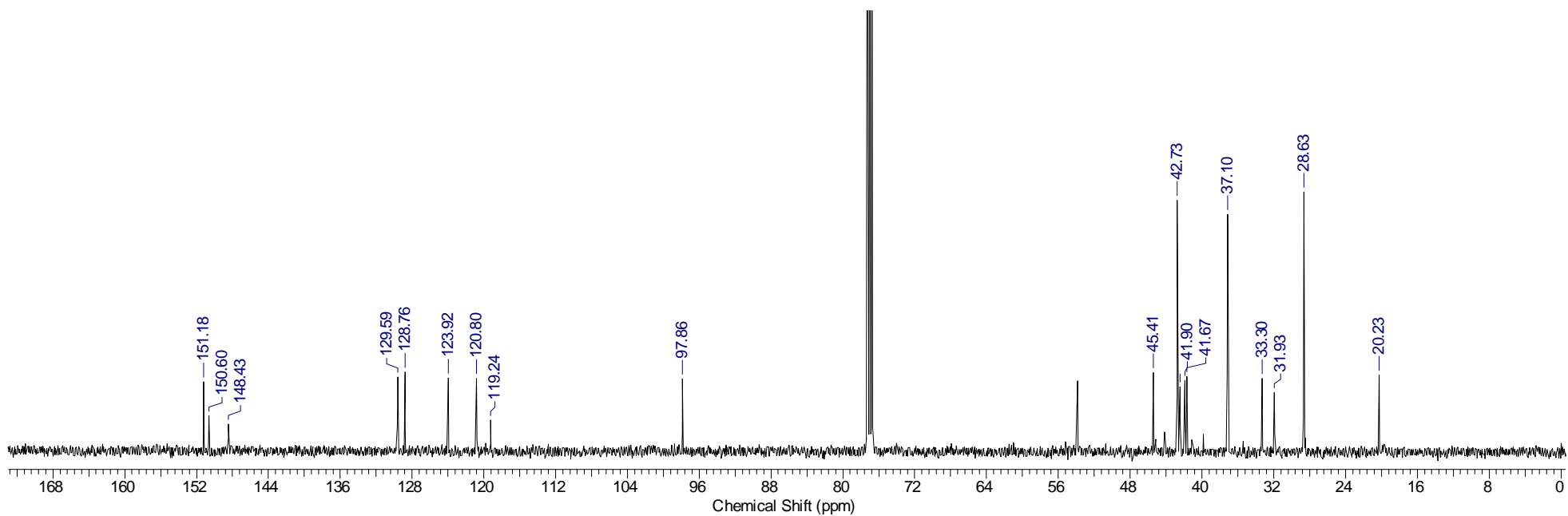
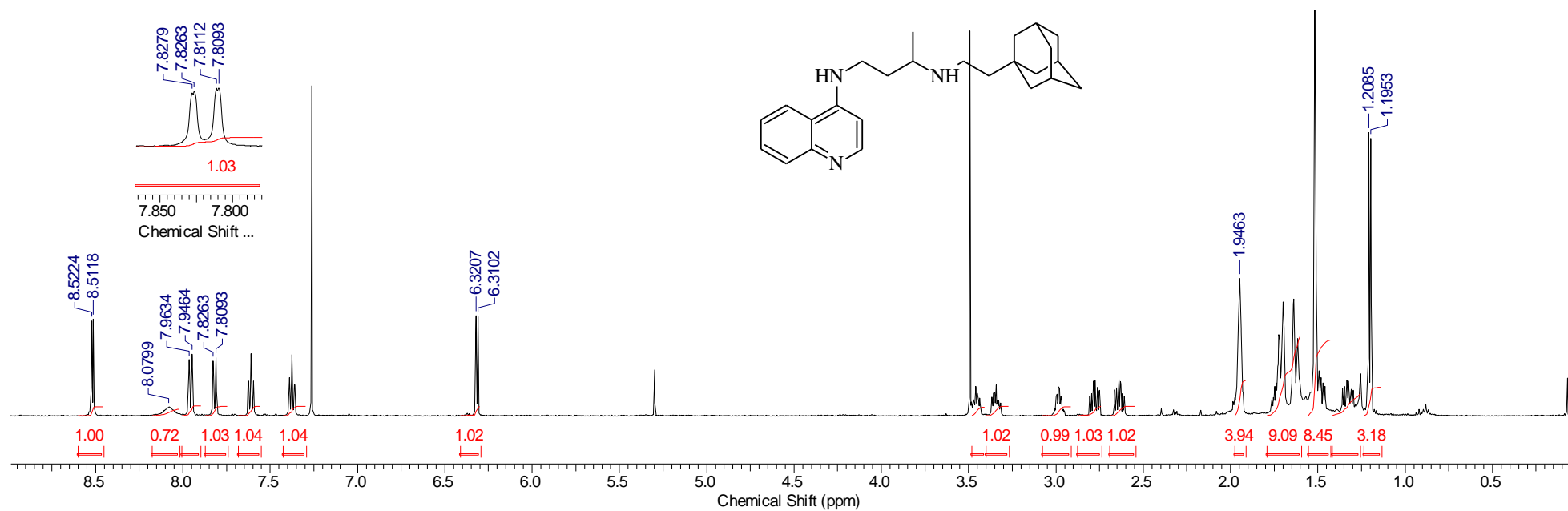
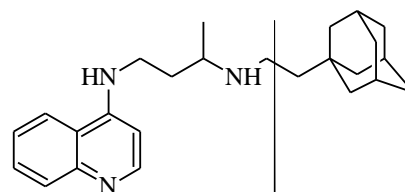
***N*⁴-(1-adamantylmethyl)-*N*¹-quinolin-4-ylpentane-1,4-diamine (79)**



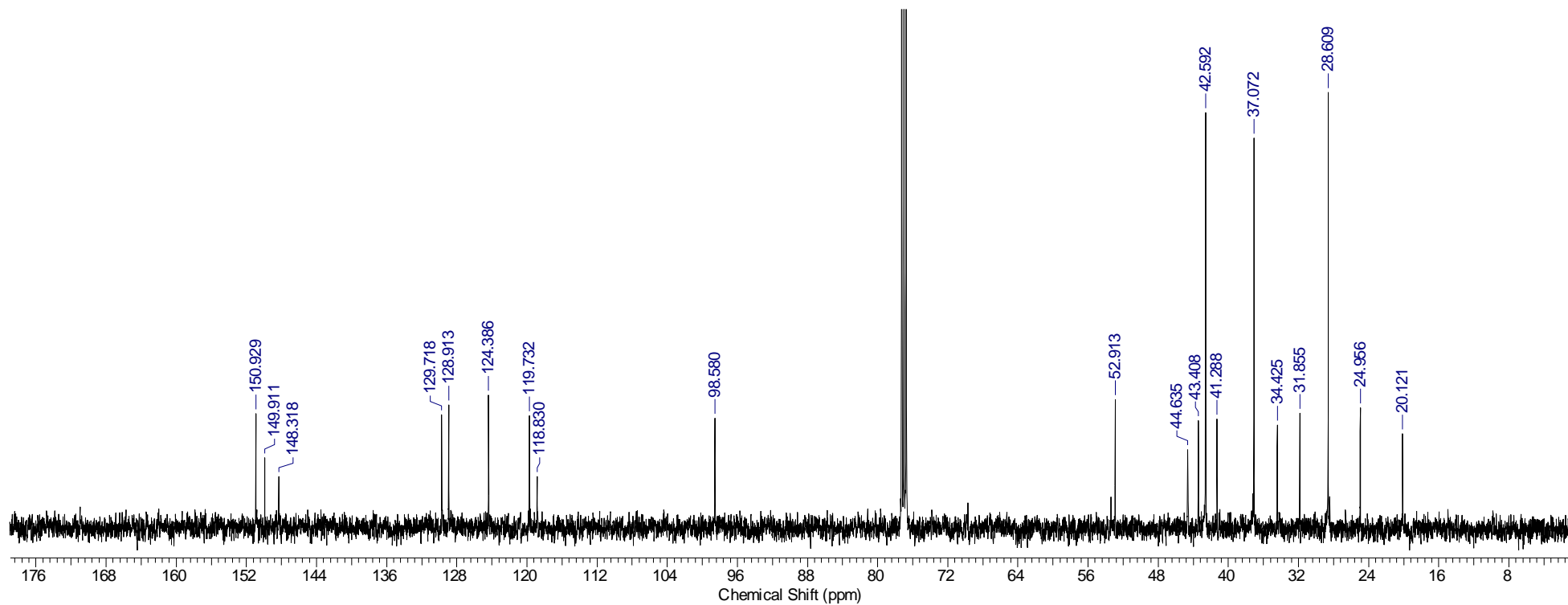
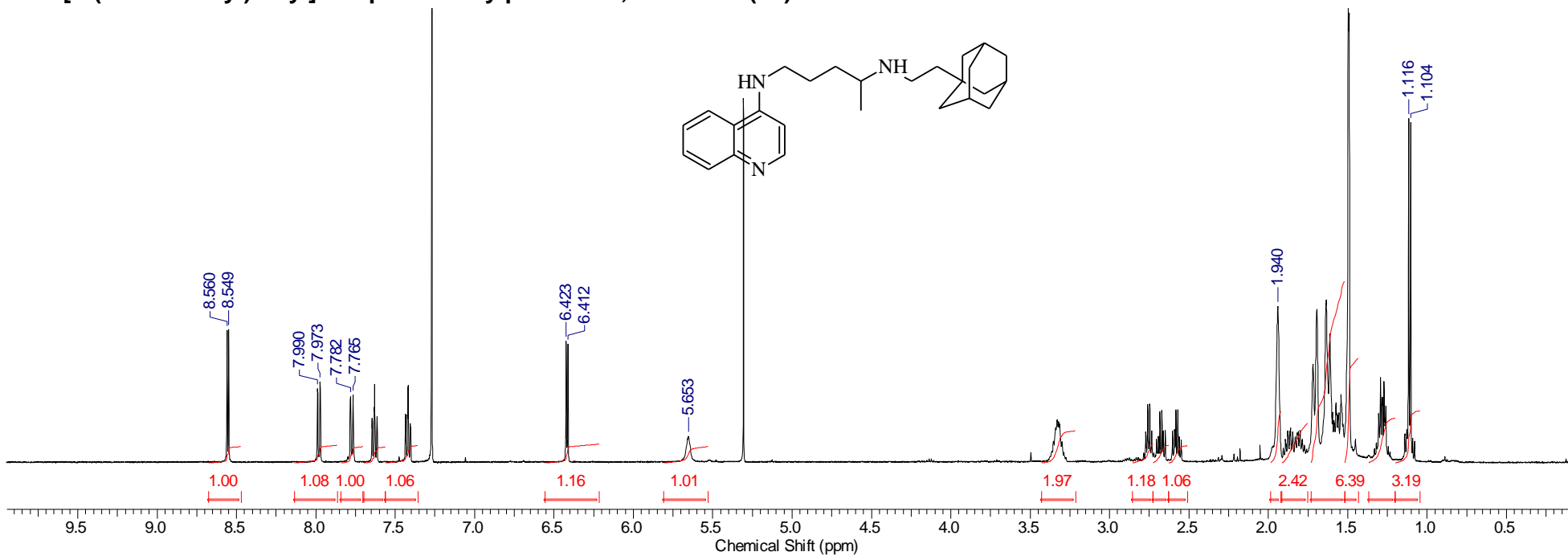
N^2 -[2-(1-Adamantyl)ethyl]- N^1 -quinolin-4-ylpropane-1,2-diamine (80)



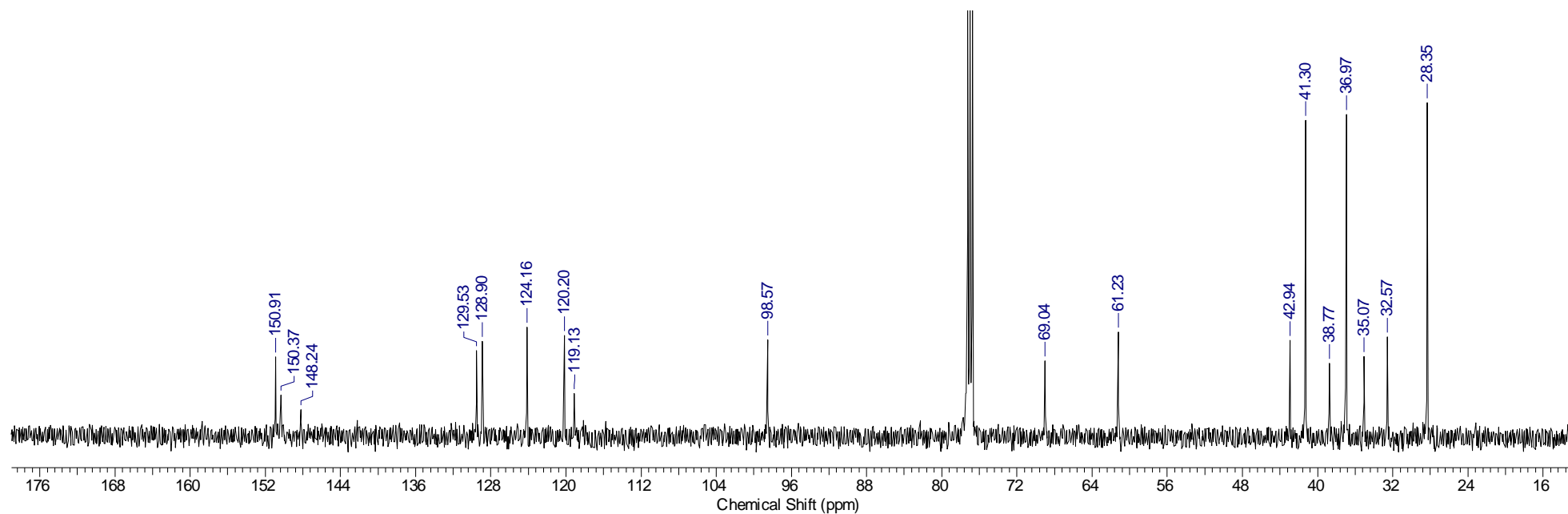
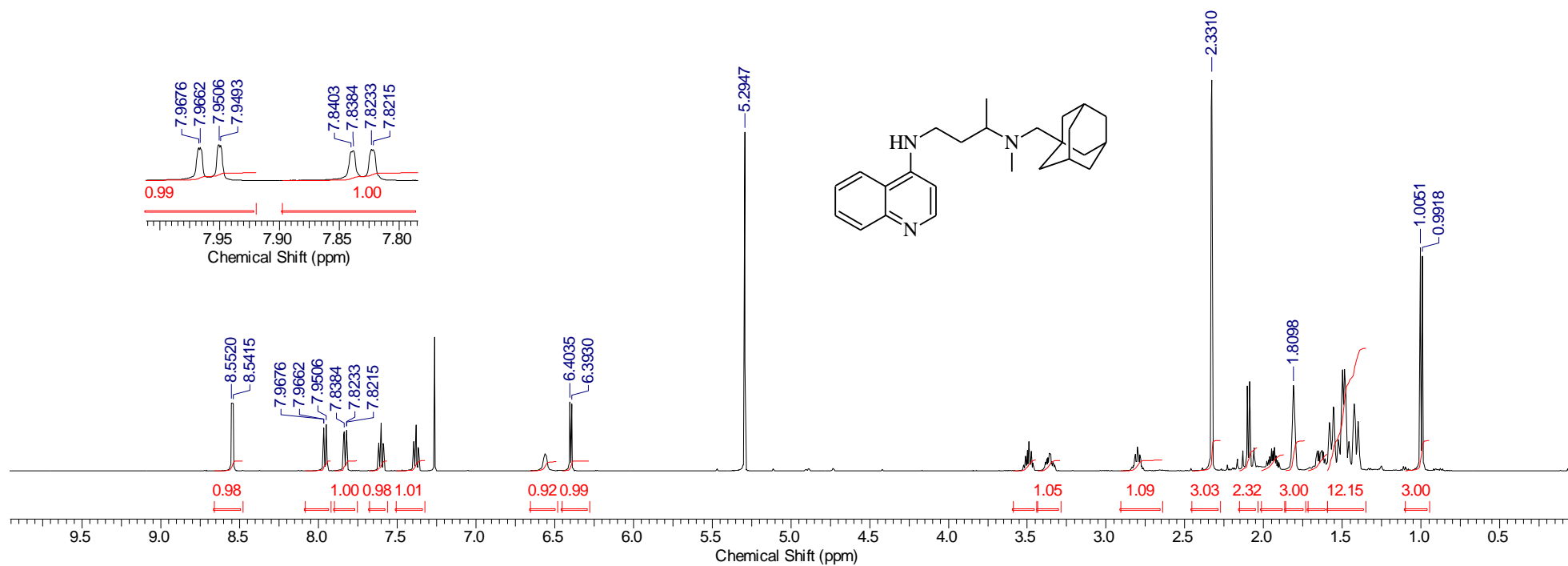
***N*³-[2-(1-adamantyl)ethyl]-*N*¹-quinolin-4-ylbutane-1,3-diamine (81)**



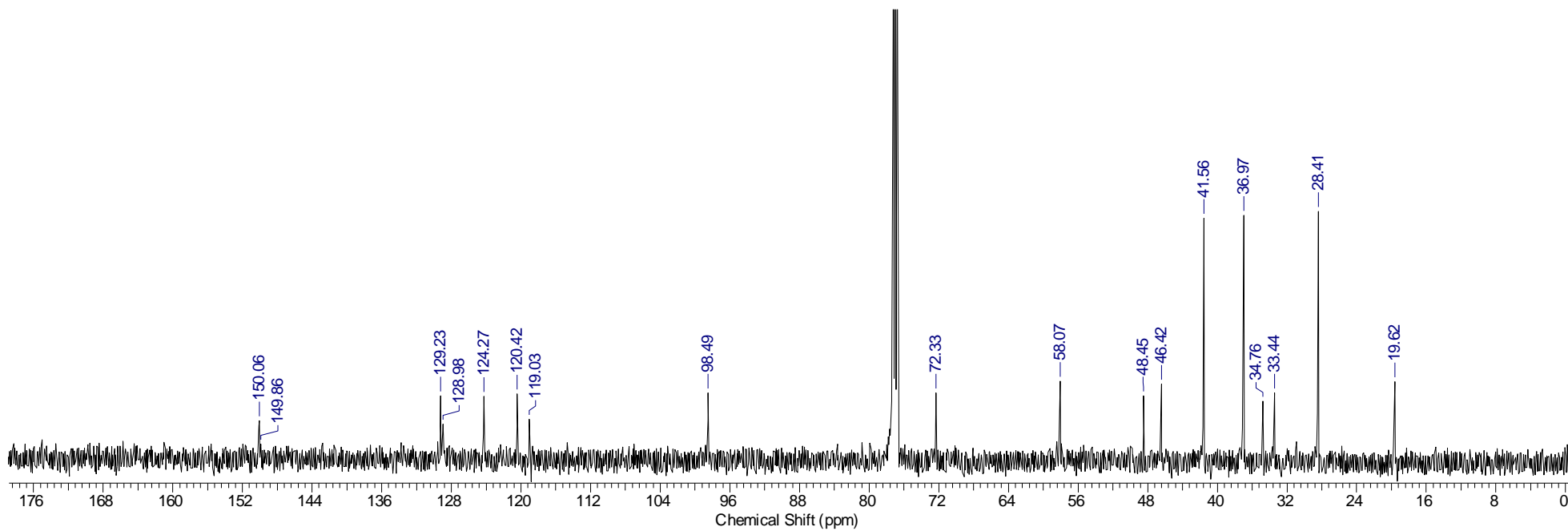
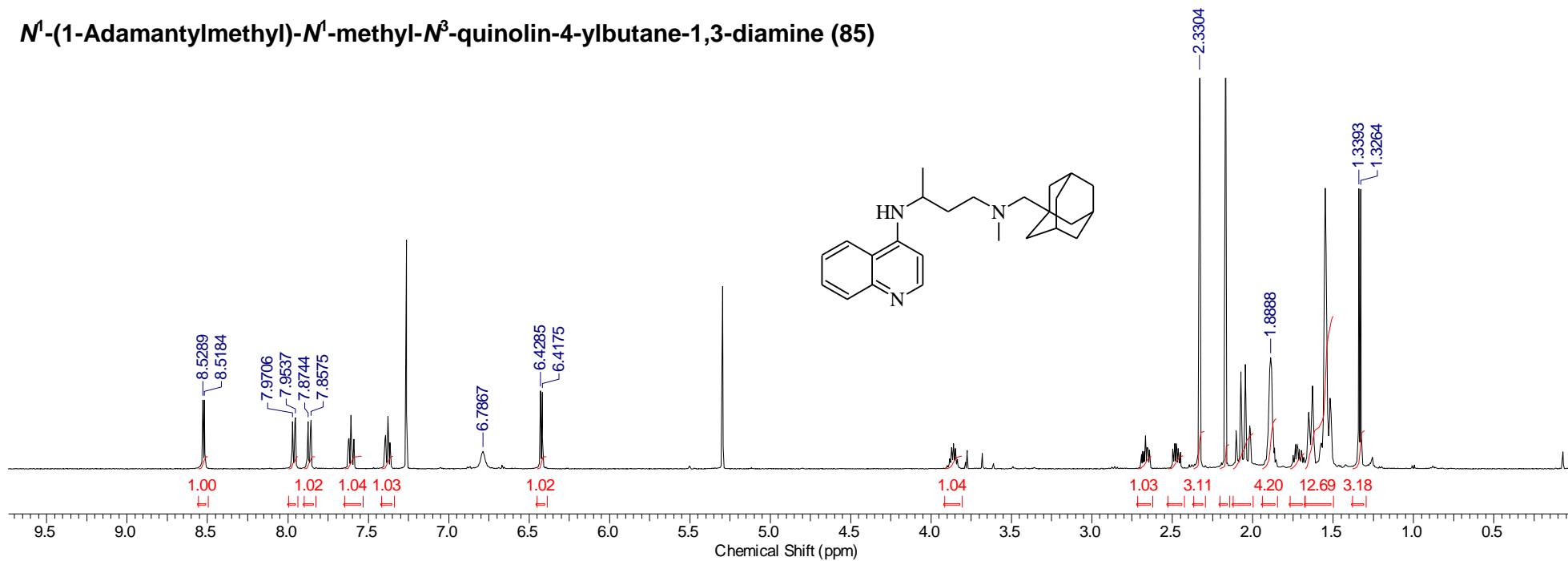
***N*⁴-[2-(1-adamantyl)ethyl]-*N*¹-quinolin-4-ylpentane-1,4-diamine (82)**



***N*³-(1-adamantylmethyl)-*N*³-methyl-*N*¹-quinolin-4-ylbutane-1,3-diamine (84)**



***N*¹-(1-Adamantylmethyl)-*N*¹-methyl-*N*³-quinolin-4-ylbutane-1,3-diamine (85)**

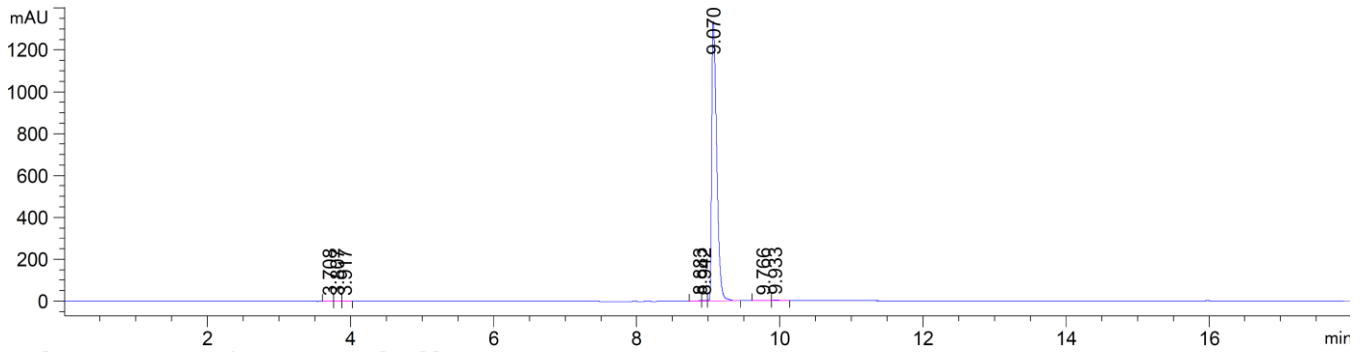


HPLC analyses for purity

Compound: 14

Method A

DAD1 B, Sig=330,4 Ref=off (JELENA\SEKV 18 JELENA 2014-04-10 12-20-35\TEST0000002.D)



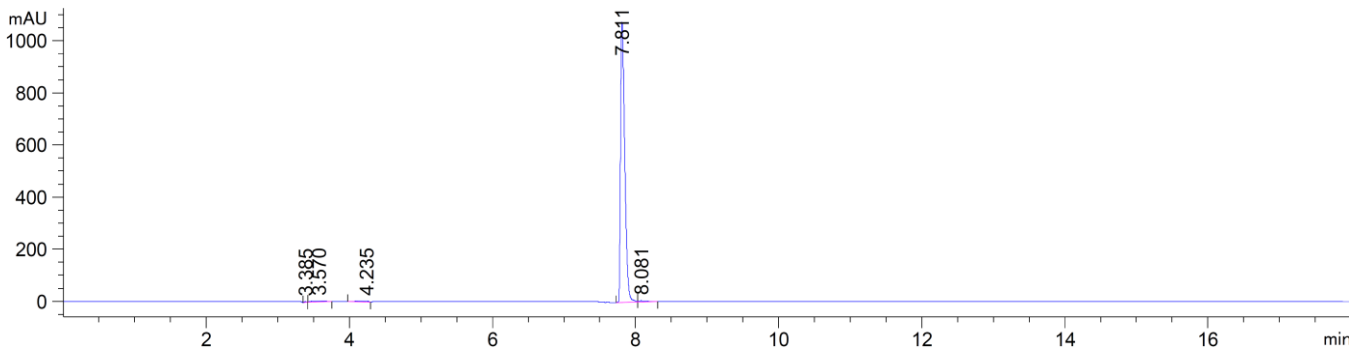
Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.708	BV	0.0683	9.40774	1.73411	0.1440
2	3.807	VV	0.0696	9.65636	1.65443	0.1478
3	3.917	VB	0.0544	6.36903	1.47369	0.0975
4	8.883	BV	0.0454	8.81655	2.75342	0.1350
5	8.942	VV	0.0569	13.24519	3.26217	0.2028
6	9.070	VB	0.0758	6454.85107	1337.75061	98.8286
7	9.766	BV	0.0960	9.31904	1.15040	0.1427
8	9.933	VB	0.0840	19.69601	2.85515	0.3016

Totals : 6531.36100 1352.63399

Method B

DAD1 B, Sig=330,4 Ref=off (JELENA\SEKV 18 JELENA 2014-04-09 11-05-47\TEST0000002.D)



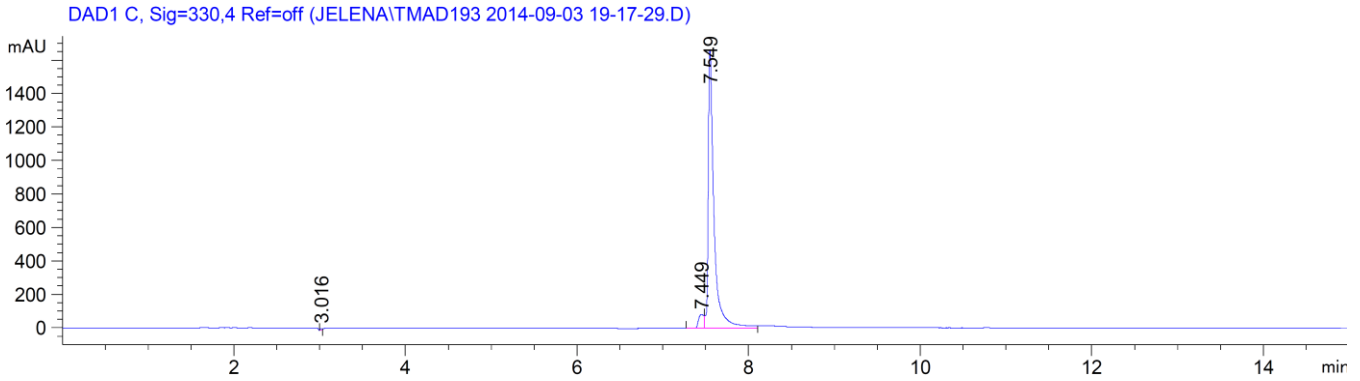
Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.385	BV	0.0358	5.57718	2.47196	0.1229
2	3.570	VB	0.1637	55.97943	4.03917	1.2331
3	4.235	BB	0.1272	42.55352	3.96612	0.9374
4	7.811	BV	0.0627	4401.26318	1075.80005	96.9492
5	8.081	VB	0.0965	34.38691	4.53239	0.7575

Totals : 4539.76022 1090.80968

Compound: 15

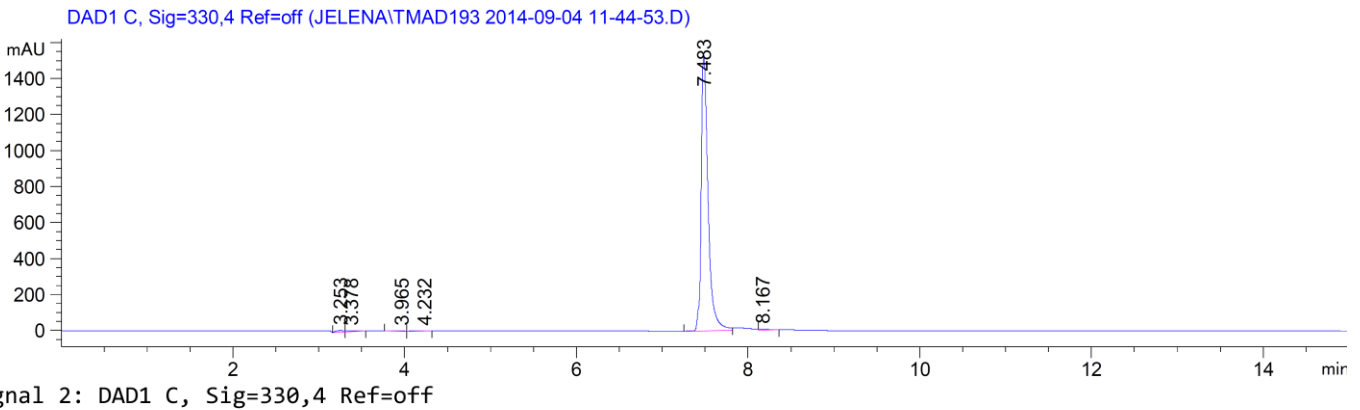
Method A



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.016	BV	0.0268	16.98758	10.00137	0.2085
2	7.449	BV	0.0647	341.71597	81.93553	4.1942
3	7.549	VV	0.0667	7788.62061	1662.34448	95.5973

Totals : 8147.32416 1754.28138

Method B

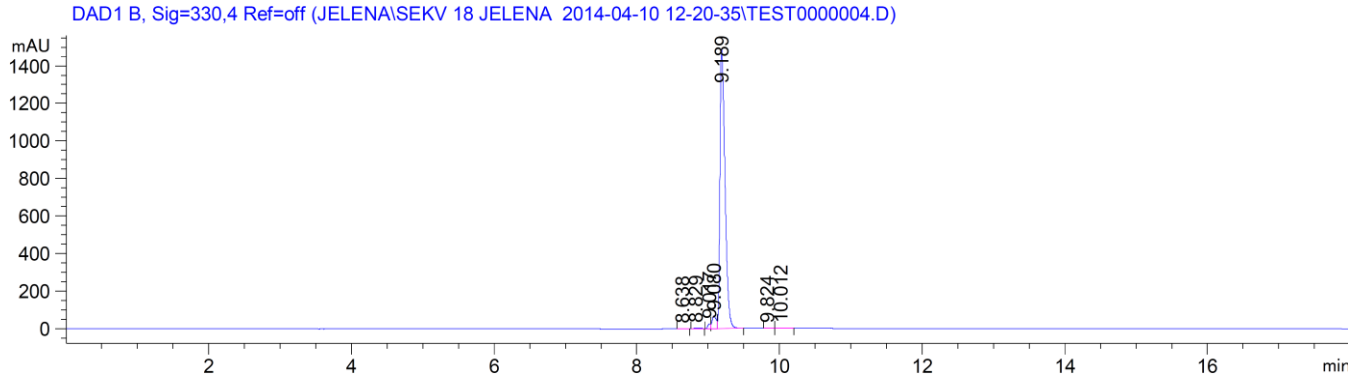


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.253	BV	0.0851	56.65427	8.79670	0.6430
2	3.378	VB	0.1165	51.31584	5.23096	0.5824
3	3.965	BB	0.1046	34.00576	3.86528	0.3859
4	4.232	BB	0.2730	28.43819	1.22422	0.3228
5	7.483	BV	0.0848	8591.60547	1546.04041	97.5092
6	8.167	VB	0.0908	49.05535	6.62785	0.5567

Totals : 8811.07488 1571.78541

Compound: 16

Method A

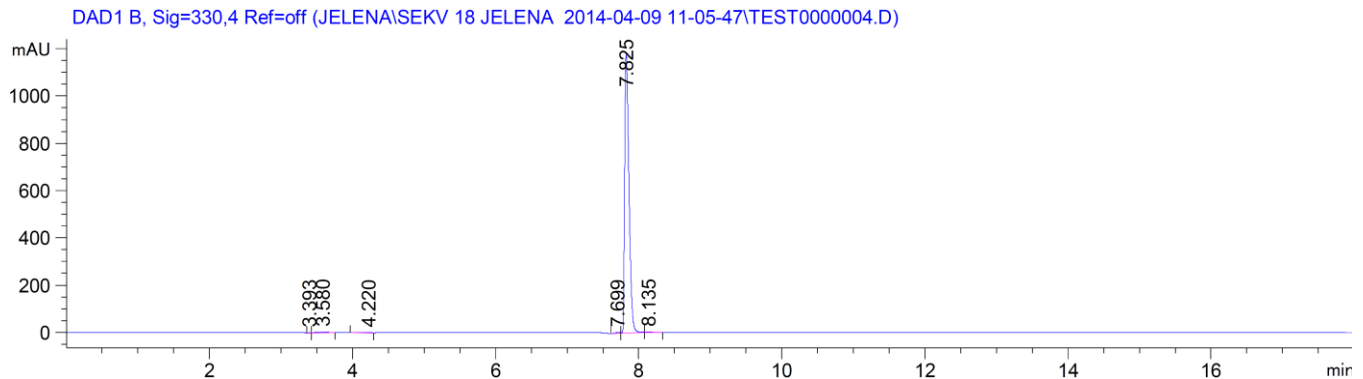


Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.638	VB	0.0762	7.97347	1.26152	0.1037
2	8.829	BB	0.0704	20.42958	4.00926	0.2657
3	9.017	BV	0.0387	61.83350	25.09577	0.8042
4	9.080	VV	0.0603	274.32880	66.97717	3.5677
5	9.189	VB	0.0778	7306.54639	1486.42981	95.0236
6	9.824	VV	0.0650	5.62031	1.04156	0.0731
7	10.012	VB	0.0923	12.45910	1.60075	0.1620

Totals : 7689.19115 1586.41584

Method B



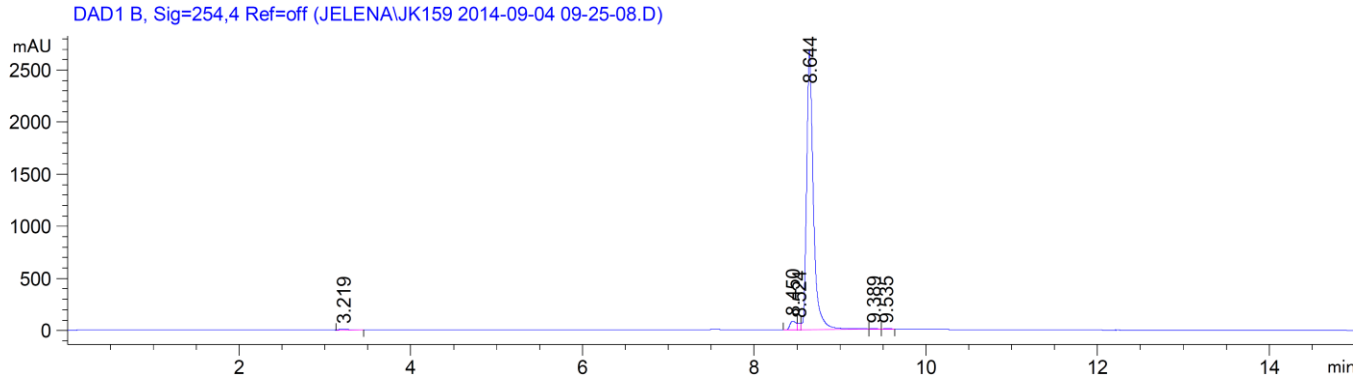
Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.393	BV	0.0360	5.61560	2.57091	0.1101
2	3.580	VB	0.1580	52.42299	3.90883	1.0279
3	4.220	BB	0.1364	42.56967	3.69513	0.8347
4	7.699	BV	0.0548	14.41591	3.55524	0.2827
5	7.825	VV	0.0648	4960.58545	1185.06458	97.2618
6	8.135	VB	0.0950	24.63265	3.13938	0.4830

Totals : 5100.24226 1201.93408

Compound: 17

Method A

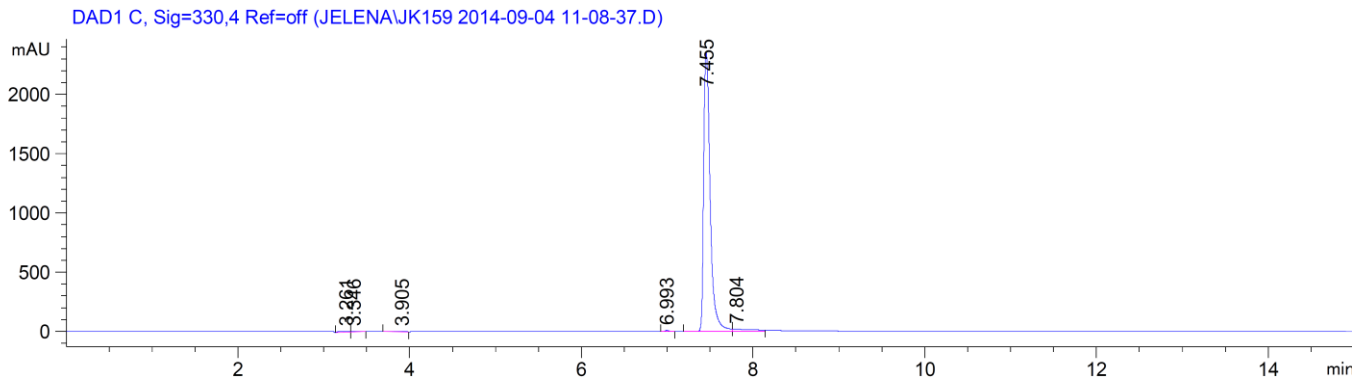


Signal 1: DAD1 B, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.219	BB	0.1171	81.14095	8.22102	0.5328
2	8.450	BV	0.0822	407.93576	78.37833	2.6784
3	8.524	VV	0.0347	144.53949	60.94197	0.9490
4	8.644	VB	0.0794	1.45842e4	2685.00610	95.7569
5	9.389	BB	0.0541	5.99054	1.61990	0.0393
6	9.535	BB	0.0612	6.63049	1.46749	0.0435

Totals : 1.52304e4 2835.63481

Method B



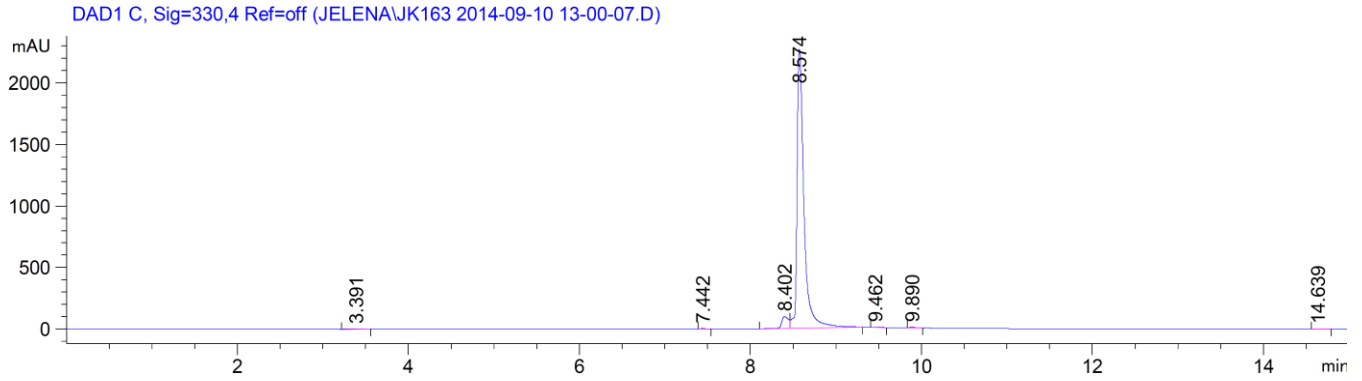
Signal 2: DAD1 C, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.261	BV	0.1102	67.23597	7.60437	0.5175
2	3.346	VB	0.0762	30.45018	4.75817	0.2344
3	3.905	BB	0.1322	48.58632	4.35253	0.3739
4	6.993	BV	0.0453	34.35384	11.36862	0.2644
5	7.455	BV	0.0818	1.24510e4	2351.23096	95.8282
6	7.804	VV	0.1969	361.42252	21.69092	2.7817

Totals : 1.29930e4 2401.00557

Compound: 18

Method A

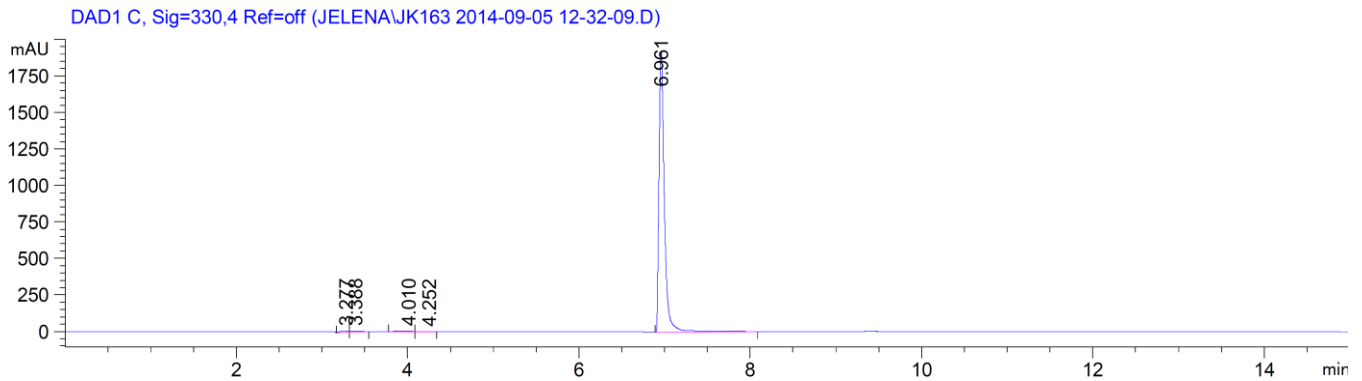


Signal 2: DAD1 C, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.391	BB	0.1413	37.95834	3.17984	0.2851
2	7.442	BV	0.0517	15.78314	4.52560	0.1186
3	8.402	BV	0.0883	534.52533	94.09093	4.0151
4	8.574	VB	0.0828	1.26817e4	2265.07031	95.2590
5	9.462	BB	0.0721	8.21736	1.35786	0.0617
6	9.890	BB	0.0628	28.27421	6.62160	0.2124
7	14.639	BB	0.0634	6.41093	1.22868	0.0482

Totals : 1.33129e4 2376.07483

Method B



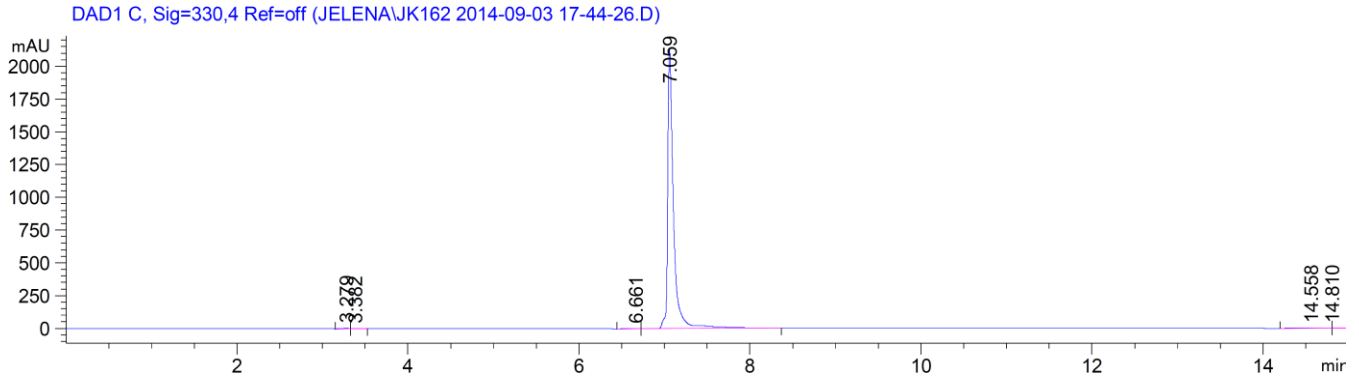
Signal 2: DAD1 C, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.277	BV	0.0895	59.69650	8.44700	0.6884
2	3.388	VB	0.1070	45.97728	5.10913	0.5302
3	4.010	BB	0.1318	39.39859	3.52658	0.4544
4	4.252	BB	0.1962	21.10557	1.26817	0.2434
5	6.961	BB	0.0668	8505.12402	1914.43054	98.0836

Totals : 8671.30197 1932.78142

Compound: 19

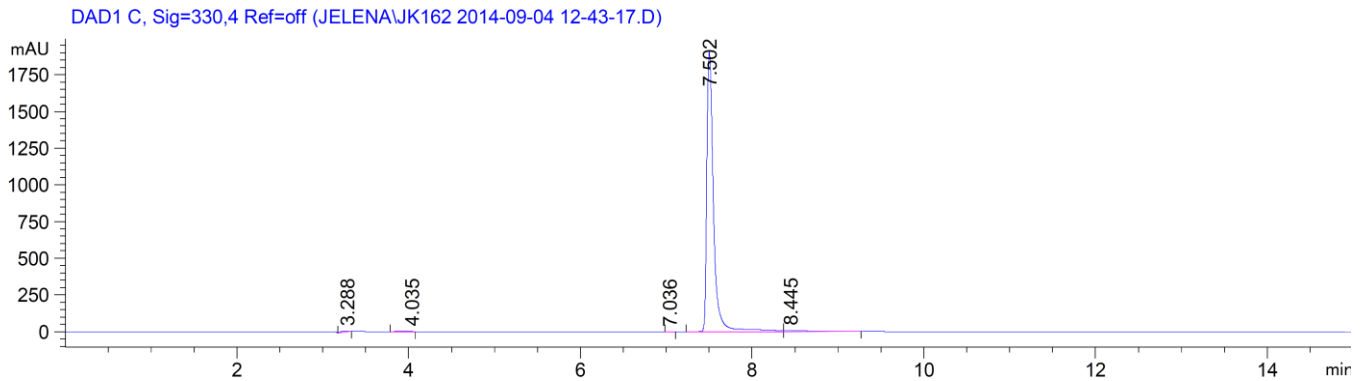
Method A



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.279	BV	0.1011	36.36034	4.32375	0.3534
2	3.382	VB	0.0834	17.71332	2.57012	0.1721
3	6.661	BV	0.0753	14.56192	2.34890	0.1415
4	7.059	VB	0.0681	1.01580e4	2129.95996	98.7188
5	14.558	BV	0.2424	55.45602	2.69702	0.5389
6	14.810	VBA	0.0732	7.74142	1.26788	0.0752

Totals : 1.02898e4 2143.16763

Method B

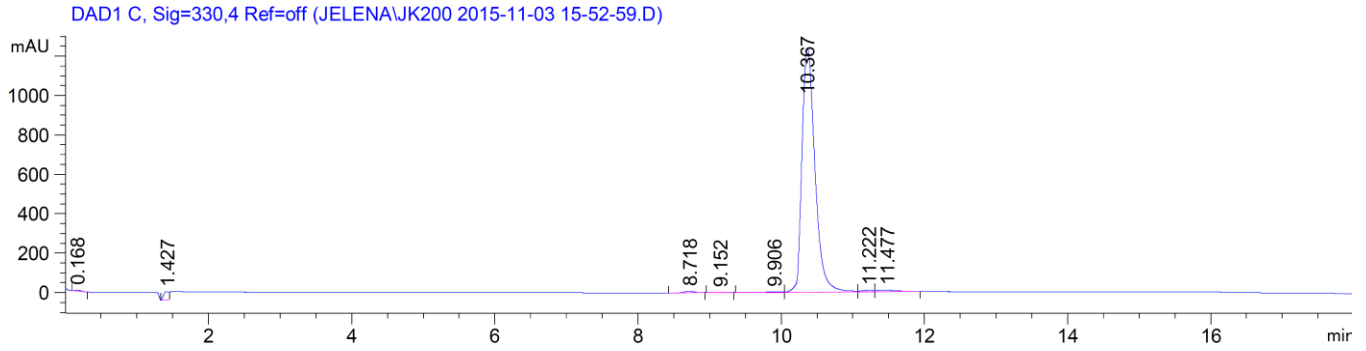


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.288	BB	0.1058	34.19210	3.84354	0.3183
2	4.035	BB	0.1237	36.30308	3.70989	0.3379
3	7.036	BB	0.0473	5.62679	1.69380	0.0524
4	7.502	VV	0.0839	1.04984e4	1902.81714	97.7234
5	8.445	VB	0.2658	168.45518	7.43581	1.5681

Totals : 1.07429e4 1919.50019

Compound: 20

Method C

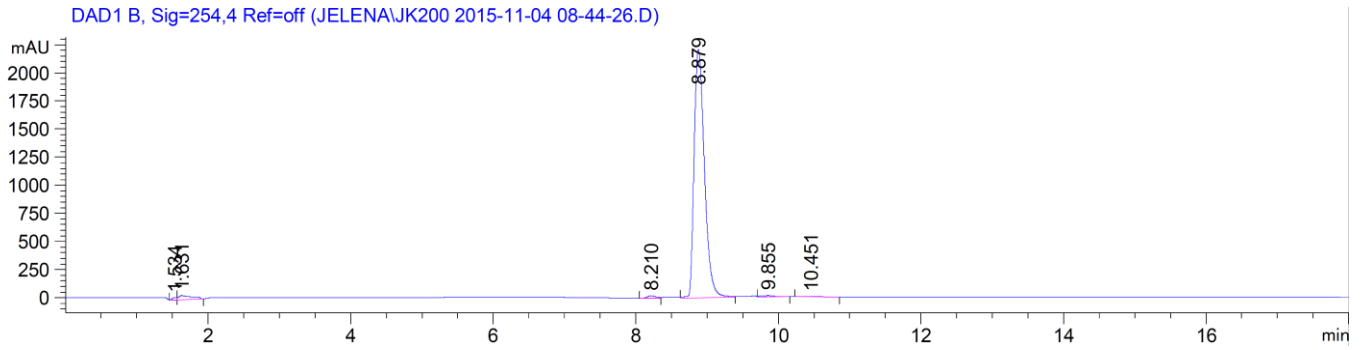


Signal 3: DAD1 C, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	0.168	BB	0.0738	36.41005	7.03952	0.2236
2	1.427	BV	0.0696	216.50752	39.71888	1.3297
3	8.718	BB	0.1333	92.16120	8.24878	0.5660
4	9.152	BB	0.1283	27.33589	2.51506	0.1679
5	9.906	BV	0.1967	61.14628	3.65421	0.3755
6	10.367	VV	0.1966	1.56095e4	1237.73877	95.8674
7	11.222	VV	0.1405	89.59920	7.63243	0.5503
8	11.477	VB	0.2345	149.72250	7.53071	0.9195

Totals : 1.62823e4 1314.07837

Method D



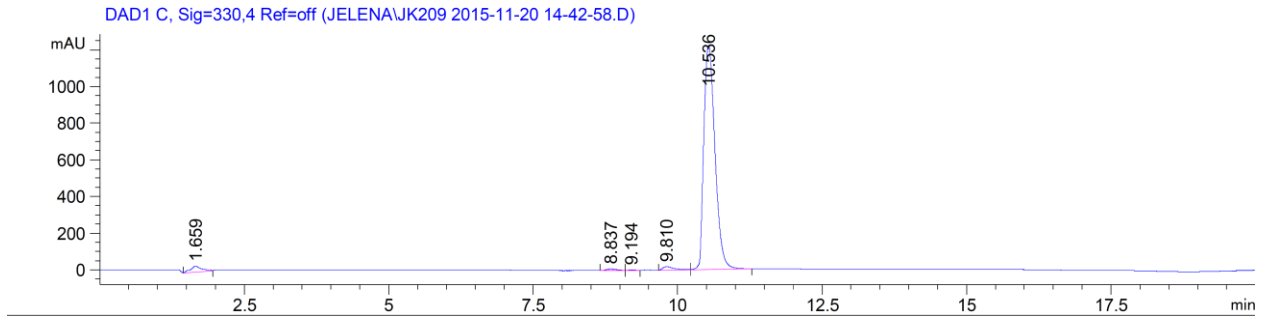
Signal 1: DAD1 B, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.534	BV	0.0610	84.68669	21.97379	0.3643
2	1.631	VB	0.1817	516.76556	37.17271	2.2231
3	8.210	BV	0.1296	192.43353	21.78019	0.8278
4	8.879	VV	0.1550	2.22303e4	2206.92749	95.6349
5	9.855	VB	0.1657	165.88641	12.50860	0.7136
6	10.451	BB	0.1518	54.89505	4.31757	0.2362

Totals : 2.32450e4 2304.68034

Compound: 21

Method C

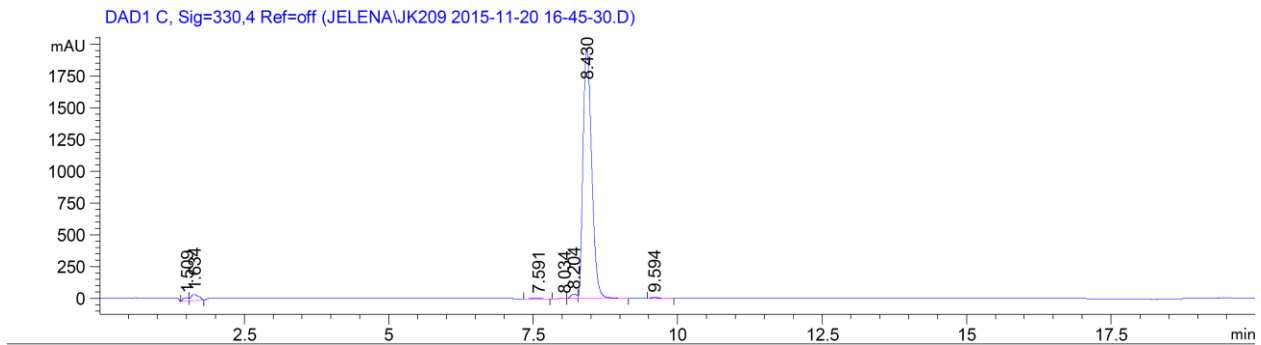


Signal 3: DAD1 C, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.659	BV	0.1808	430.99899	32.17452	2.5070
2	8.837	BV	0.1491	104.39903	8.36470	0.6073
3	9.194	VB	0.1126	13.77882	1.45364	0.0801
4	9.810	BV	0.1677	244.15356	17.78471	1.4202
5	10.536	VV	0.2115	1.63984e4	1222.19775	95.3854

Totals : 1.71918e4 1281.97531

Method D



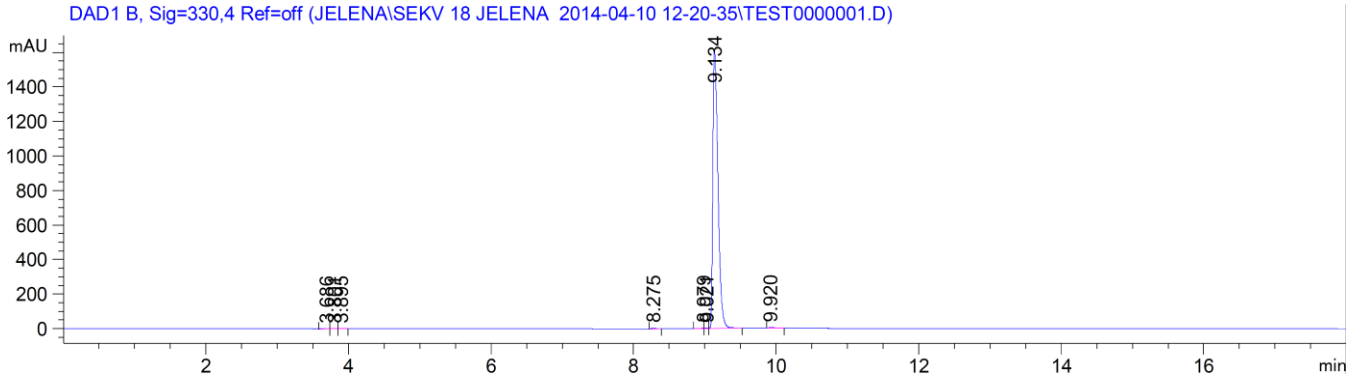
Signal 2: DAD1 C, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.509	BV	0.0877	166.60329	25.17060	0.7751
2	1.634	VB	0.1311	448.48056	48.64172	2.0865
3	7.591	BB	0.1454	62.28218	5.17511	0.2898
4	8.034	BB	0.0840	9.91510	1.41976	0.0461
5	8.204	BV	0.1140	232.28119	32.66100	1.0806
6	8.430	VB	0.1639	2.04986e4	1961.60852	95.3648
7	9.594	BB	0.1052	76.75870	9.03016	0.3571

Totals : 2.14949e4 2083.70685

Compound: 22

Method A

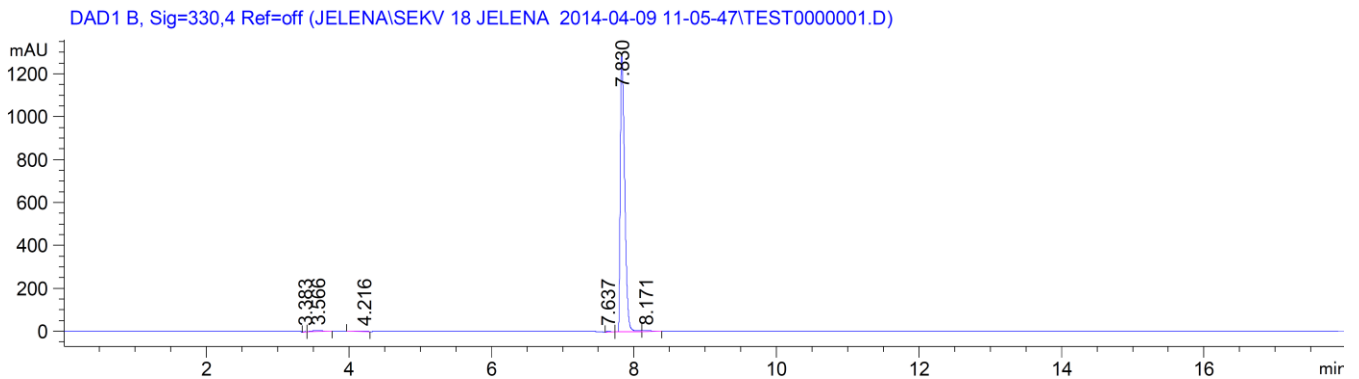


Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.686	BV	0.0709	9.52379	1.72594	0.1168
2	3.801	VV	0.0701	9.52884	1.63341	0.1168
3	3.895	VB	0.0585	6.16523	1.45285	0.0756
4	8.275	BV	0.0665	23.78122	5.28091	0.2915
5	8.979	BV	0.0474	10.52549	3.12000	0.1290
6	9.021	VV	0.0482	12.68996	3.87195	0.1556
7	9.134	VB	0.0782	8064.33154	1616.49988	98.8644
8	9.920	BB	0.0827	20.41698	3.25447	0.2503

Totals : 8156.96305 1636.83942

Method B



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

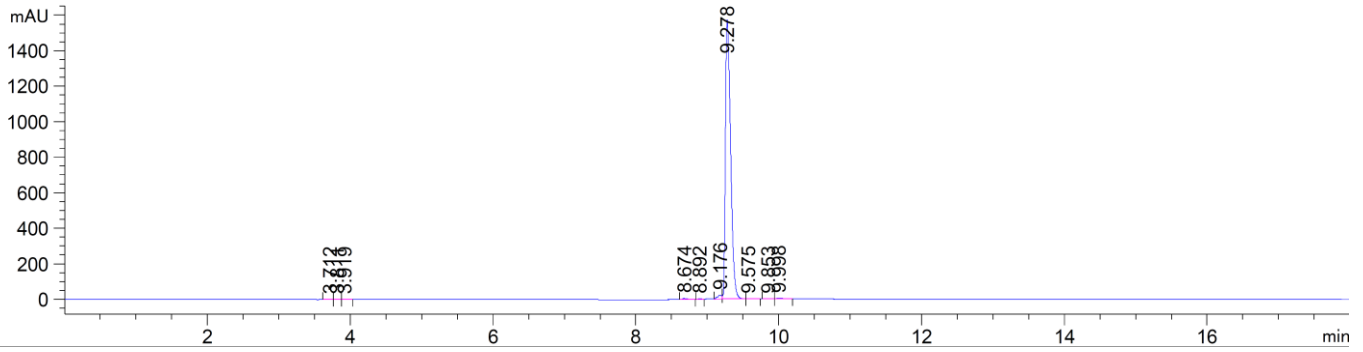
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.383	BV	0.0390	7.11713	2.91155	0.1241
2	3.566	VB	0.1674	59.29624	4.16895	1.0340
3	4.216	BB	0.1384	42.96358	3.66179	0.7492
4	7.637	BV	0.0562	18.84275	4.86638	0.3286
5	7.830	VV	0.0681	5573.74561	1297.70300	97.1971
6	8.171	VB	0.0970	32.51299	4.23630	0.5670

Totals : 5734.47829 1317.54796

Compound: 23

Method A

DAD1 B, Sig=330,4 Ref=off (JELENA\SEKV 18 JELENA 2014-04-10 12-20-35\TEST0000003.D)



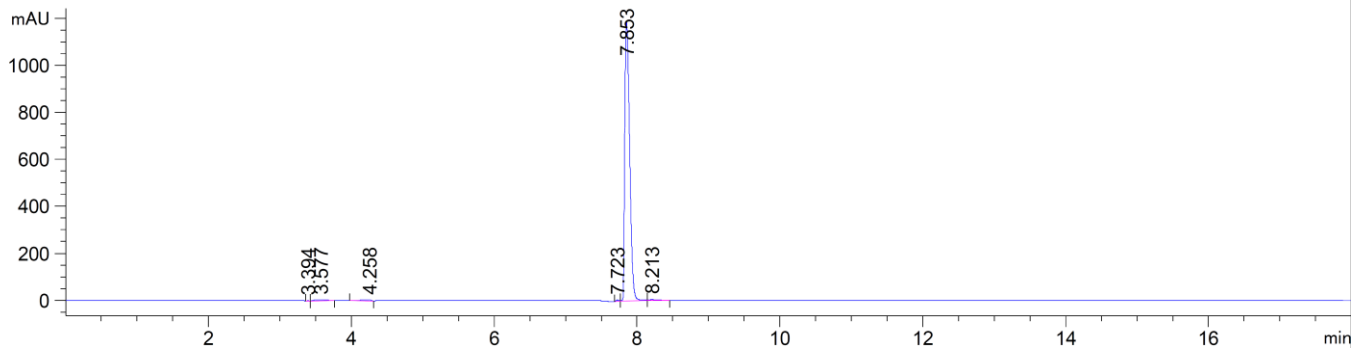
Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.712	BV	0.0654	9.48127	1.75726	0.1168
2	3.811	VV	0.0693	9.51207	1.63705	0.1171
3	3.919	VB	0.0613	6.75664	1.47896	0.0832
4	8.674	BB	0.0639	28.71559	6.32705	0.3536
5	8.892	BB	0.0539	7.33160	1.94932	0.0903
6	9.176	VV	0.0620	96.76475	22.37342	1.1917
7	9.278	VB	0.0798	7922.89893	1571.63757	97.5737
8	9.575	BB	0.0547	5.45337	1.22994	0.0672
9	9.853	BV	0.0718	7.10174	1.19643	0.0875
10	9.998	VB	0.0885	25.89958	3.84734	0.3190

Totals : 8119.91554 1613.43433

Method B

DAD1 B, Sig=330,4 Ref=off (JELENA\SEKV 18 JELENA 2014-04-09 11-05-47\TEST0000003.D)



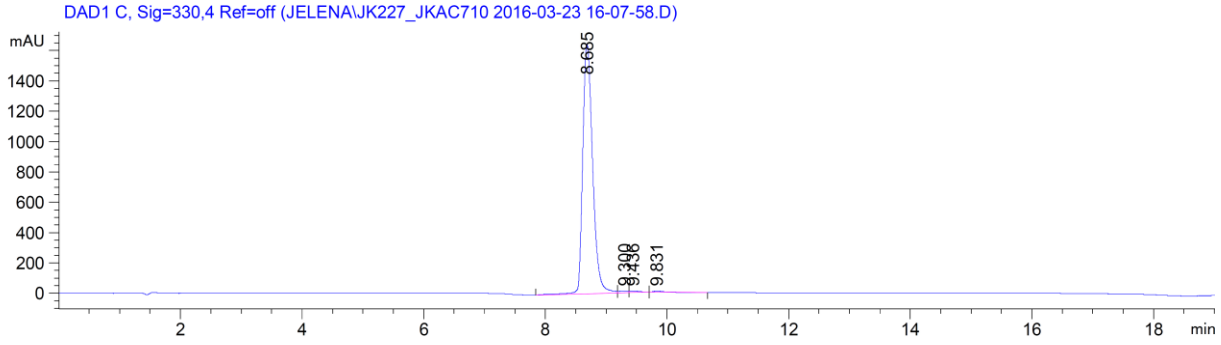
Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.394	BV	0.0359	5.55919	2.45466	0.0959
2	3.577	VB	0.1616	55.47598	4.04361	0.9566
3	4.258	BB	0.1335	43.76991	3.98935	0.7547
4	7.723	BV	0.0477	16.97182	5.46966	0.2926
5	7.853	VV	0.0764	5637.01172	1186.92810	97.1998
6	8.213	VB	0.1076	40.61673	4.71184	0.7004

Totals : 5799.40534 1207.59722

Compound: 24

Method C

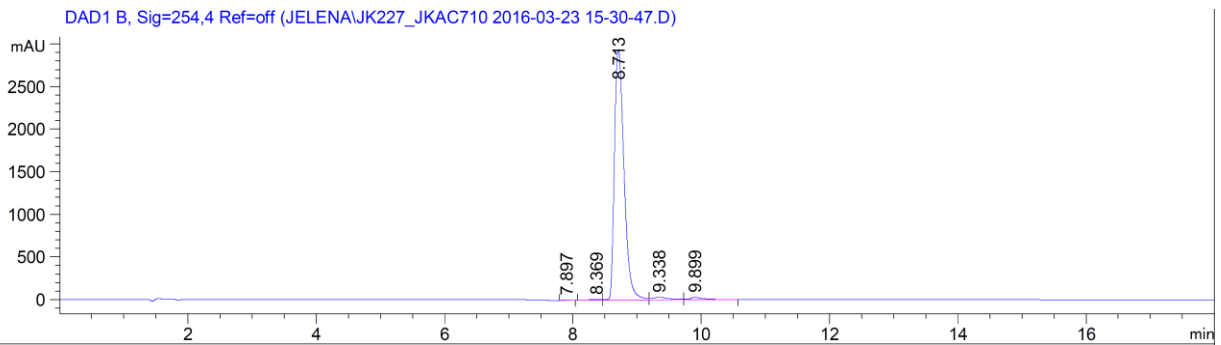


Signal 2: DAD1 C, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.685	BV	0.1717	1.85830e4	1645.56714	97.9043
2	9.300	VV	0.1223	140.00540	13.51863	0.7376
3	9.436	VB	0.1342	134.76904	11.93530	0.7100
4	9.831	BB	0.1615	123.01369	9.05701	0.6481

Totals : 1.89808e4 1680.07808

Method D



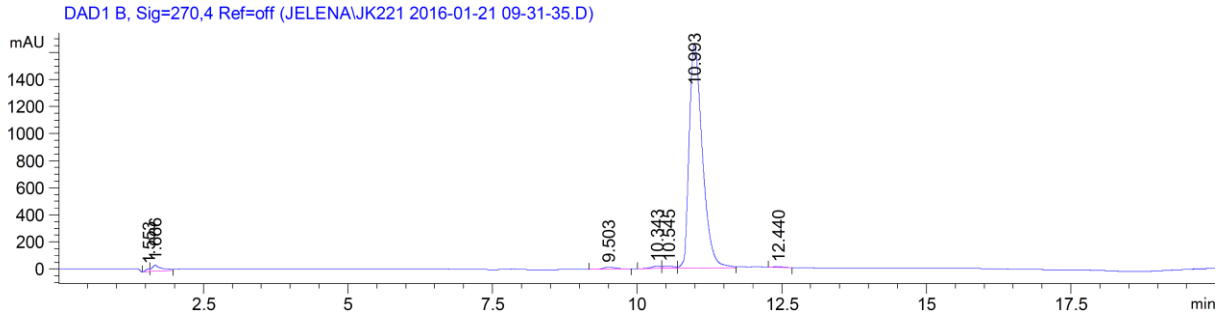
Signal 1: DAD1 B, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.897	BB	0.0910	26.33291	3.98946	0.0836
2	8.369	BV	0.1343	99.15839	8.91244	0.3149
3	8.713	VV	0.1236	3.04286e4	2942.62183	96.6320
4	9.338	VV	0.2245	524.28052	27.48666	1.6650
5	9.899	VB	0.1888	410.78421	28.30616	1.3045

Totals : 3.14892e4 3011.31654

Compound: 30

Method C

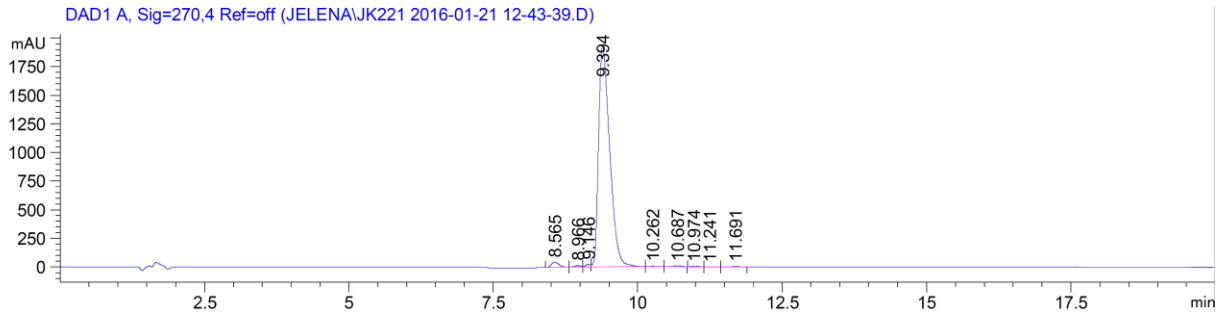


Signal 2: DAD1 B, Sig=270,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.553	BV	0.0701	88.81815	19.50127	0.3222
2	1.666	VV	0.1566	513.96075	44.04816	1.8645
3	9.503	BB	0.1715	213.78432	14.79861	0.7756
4	10.343	BV	0.1396	199.40753	17.54875	0.7234
5	10.545	VV	0.1620	239.91306	17.59921	0.8704
6	10.993	VV	0.2370	2.62515e4	1655.29199	95.2346
7	12.440	BB	0.1407	57.71477	4.85525	0.2094

Totals : 2.75651e4 1773.64324

Method D



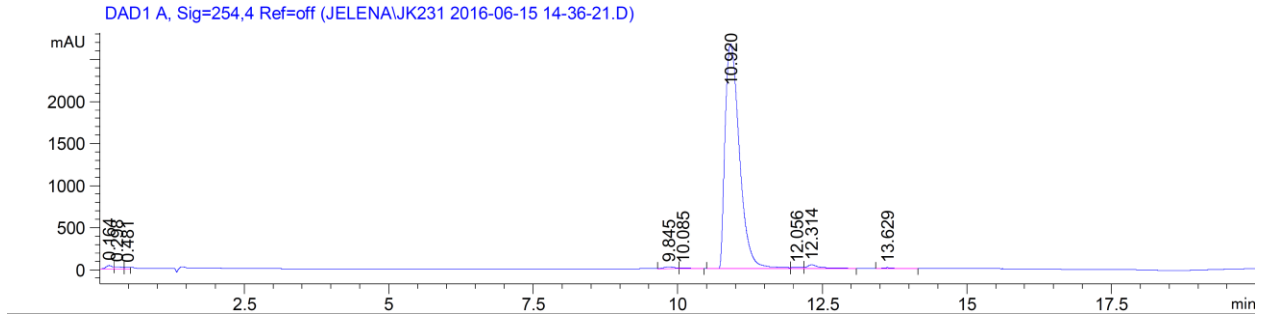
Signal 1: DAD1 A, Sig=270,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.565	BB	0.1386	410.05853	45.93987	1.5396
2	8.966	BV	0.1184	100.17350	12.50869	0.3761
3	9.146	VV	0.0970	132.47423	21.03988	0.4974
4	9.394	VV	0.1809	2.57852e4	1935.43262	96.8112
5	10.262	VB	0.1176	42.14872	4.48732	0.1582
6	10.687	BB	0.1347	78.95959	7.38892	0.2965
7	10.974	BV	0.1024	41.78683	4.90339	0.1569
8	11.241	VB	0.1019	9.56739	1.11742	0.0359
9	11.691	BB	0.1145	34.14515	3.57372	0.1282

Totals : 2.66346e4 2036.39182

Compound: 33

Method C

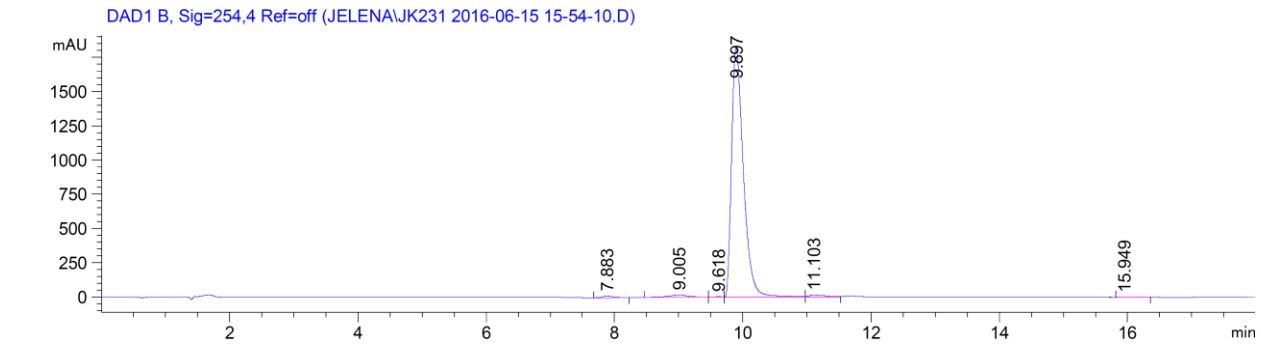


Signal 1: DAD1 A, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	0.164	BV	0.1051	289.40579	39.42096	0.6059
2	0.298	VV	0.1133	209.25114	22.85293	0.4381
3	0.481	VV	0.0827	93.06570	15.91664	0.1948
4	9.845	VV	0.1607	288.00705	21.30806	0.6030
5	10.085	VB	0.1507	114.53904	9.04484	0.2398
6	10.920	BV	0.2040	4.59235e4	2666.02124	96.1488
7	12.056	VV	0.1476	144.96884	11.73332	0.3035
8	12.314	VB	0.1881	567.36078	42.00801	1.1879
9	13.629	BB	0.1623	132.84119	9.69860	0.2781

Totals : 4.77629e4 2838.00460

Method D



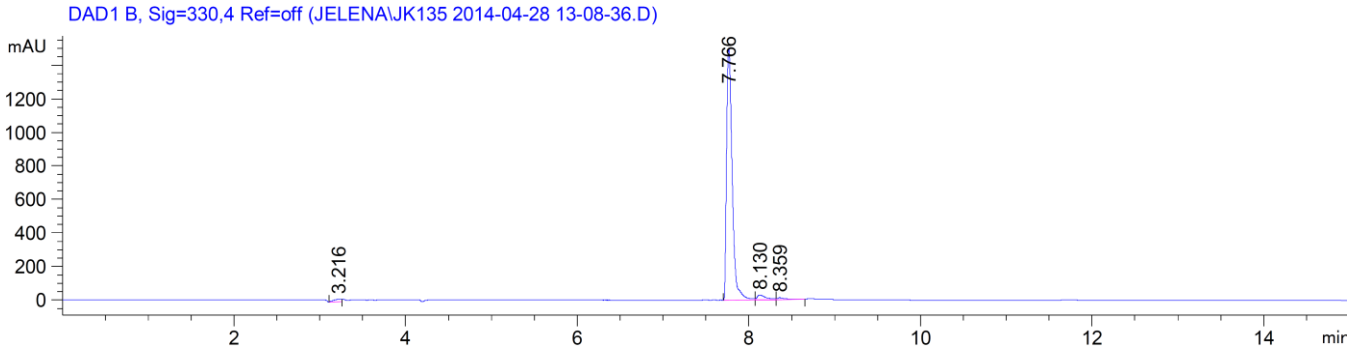
Signal 1: DAD1 B, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.883	BB	0.1400	138.50456	11.79684	0.5723
2	9.005	BV	0.2569	387.96310	18.07590	1.6031
3	9.618	VV	0.1518	46.02542	3.60939	0.1902
4	9.897	VV	0.1829	2.33294e4	1821.22021	96.3992
5	11.103	VV	0.2126	257.63907	14.30849	1.0646
6	15.949	BB	0.1682	41.28741	2.96914	0.1706

Totals : 2.42008e4 1871.97998

Compound: 34

Method A

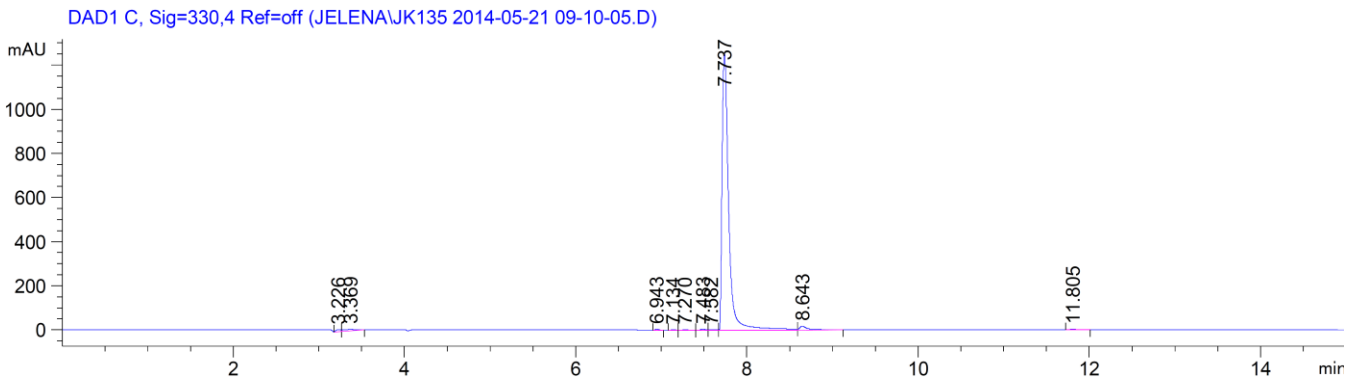


Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.216	BV	0.0810	87.92660	13.06701	1.2246
2	7.766	BV	0.0711	6823.75732	1499.98523	95.0389
3	8.130	VV	0.1018	199.70891	28.32542	2.7815
4	8.359	VB	0.0884	68.56588	10.60477	0.9550

Totals : 7179.95871 1551.98244

Method B



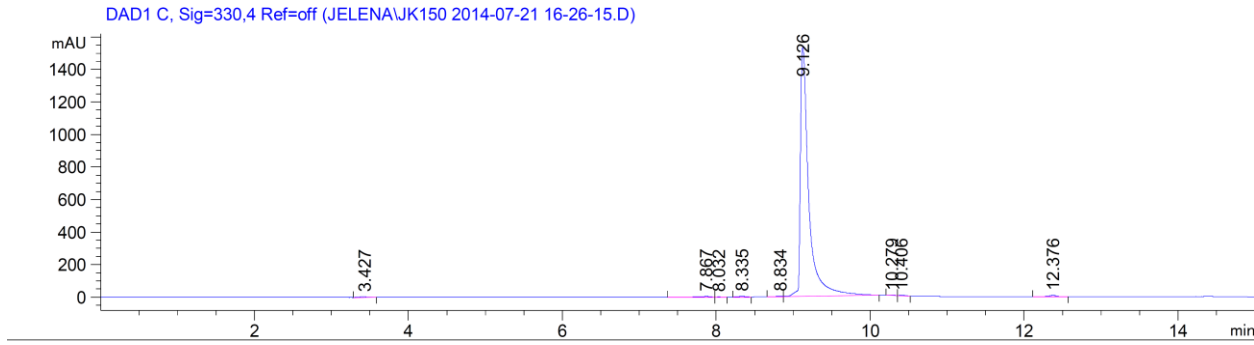
Signal 2: DAD1 C, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.226	BV	0.0548	35.15579	9.80435	0.4984
2	3.369	VB	0.1312	73.14174	6.55420	1.0370
3	6.943	BB	0.0414	17.26729	6.22013	0.2448
4	7.134	BV	0.0456	9.76850	3.19895	0.1385
5	7.270	VB	0.0724	7.17090	1.27984	0.1017
6	7.483	BV	0.0515	17.39144	5.20212	0.2466
7	7.582	VV	0.0767	13.29390	2.06362	0.1885
8	7.737	VV	0.0814	6712.64795	1256.00952	95.1724
9	8.643	VV	0.1102	145.48645	17.45539	2.0627
10	11.805	BB	0.0651	21.82069	5.13137	0.3094

Totals : 7053.14465 1312.91948

Compound: 37

Method A

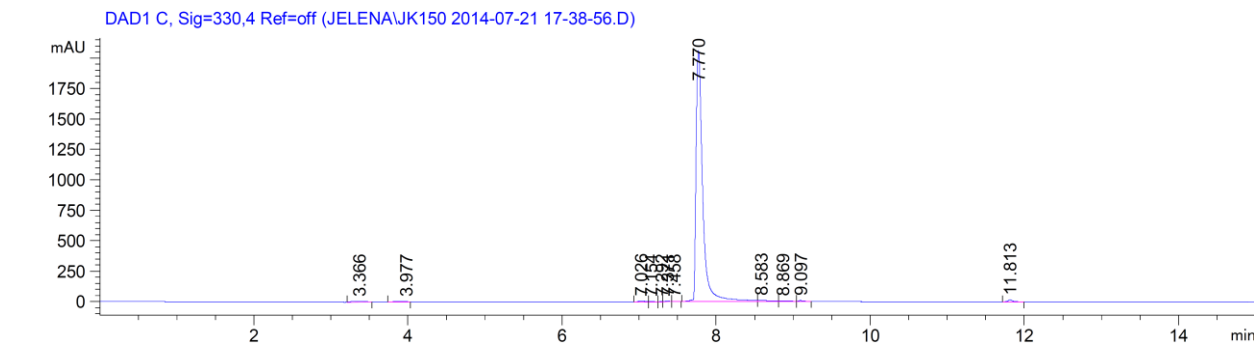


Signal 2: DAD1 C, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.427	BB	0.1285	33.07053	3.03737	0.2783
2	7.867	BV	0.1197	60.01989	6.56467	0.5052
3	8.032	VB	0.0576	6.64809	1.47501	0.0560
4	8.335	VB	0.0811	38.33893	6.66965	0.3227
5	8.834	VB	0.0778	14.76404	2.24266	0.1243
6	9.126	VV	0.1102	1.16280e4	1537.87415	97.8678
7	10.279	BB	0.0614	12.81295	3.05589	0.1078
8	10.406	BB	0.0627	23.25148	5.51174	0.1957
9	12.376	BB	0.0912	64.43293	9.55082	0.5423

Totals : 1.18813e4 1575.98196

Method B



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

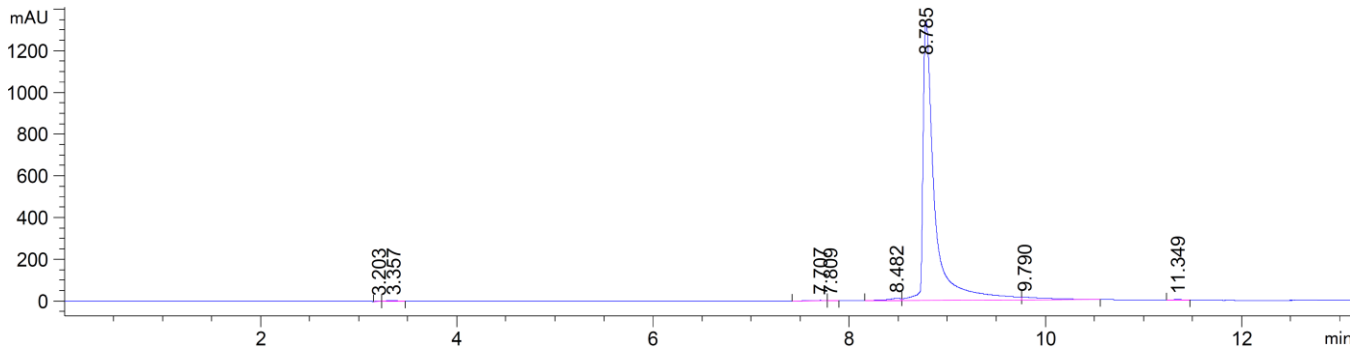
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.366	VB	0.1526	58.74958	4.56747	0.4606
2	3.977	BB	0.1137	40.61127	4.29967	0.3184
3	7.026	BV	0.0884	50.32940	8.70890	0.3946
4	7.154	VB	0.0497	19.23182	5.58518	0.1508
5	7.292	BV	0.0379	6.75184	2.63889	0.0529
6	7.371	VV	0.0642	28.36860	6.40606	0.2224
7	7.458	VB	0.0575	15.97623	3.35714	0.1253
8	7.770	BV	0.0913	1.23352e4	2061.28857	96.7095
9	8.583	VV	0.1346	82.94082	7.49524	0.6503
10	8.869	VB	0.0803	29.79179	4.87203	0.2336
11	9.097	BB	0.0642	24.39027	5.78289	0.1912
12	11.813	BB	0.0637	62.56354	14.53671	0.4905

Totals : 1.27549e4 2129.53876

Compound: 38

Method A

DAD1 C, Sig=330,4 Ref=off (JELENAJK151 2014-07-21 14-57-58.D)



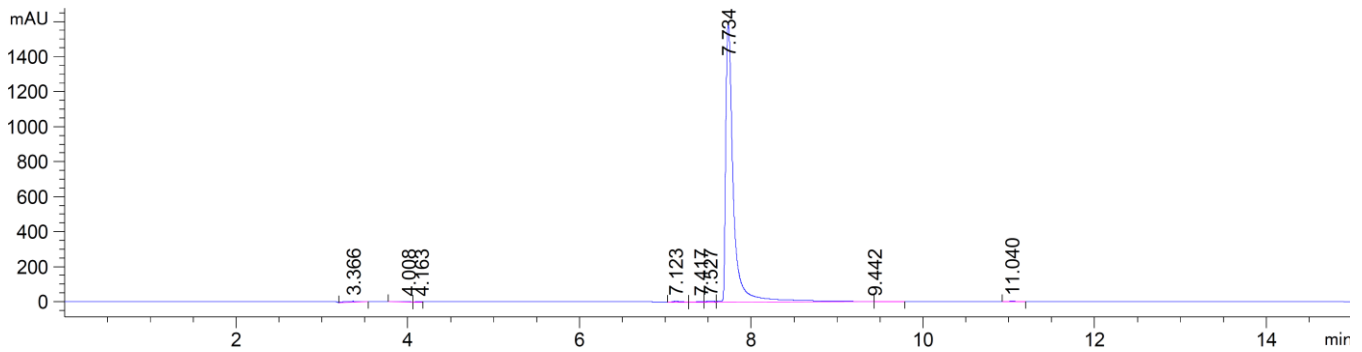
Signal 2: DAD1 C, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.203	BV	0.0475	8.11539	2.59359	0.0717
2	3.357	VB	0.1079	23.35480	2.61102	0.2065
3	7.707	BV	0.1144	26.94110	2.80796	0.2382
4	7.809	VB	0.0482	5.83131	1.63308	0.0515
5	8.482	BV	0.1058	85.74706	10.28364	0.7580
6	8.785	VV	0.1176	1.09163e4	1338.68799	96.5008
7	9.790	VB	0.2079	226.09036	12.81158	1.9986
8	11.349	BB	0.0678	19.75787	4.05670	0.1747

Totals : 1.13122e4 1375.48555

Method B

DAD1 C, Sig=330,4 Ref=off (JELENAJK151 2014-07-21 18-05-17.D)



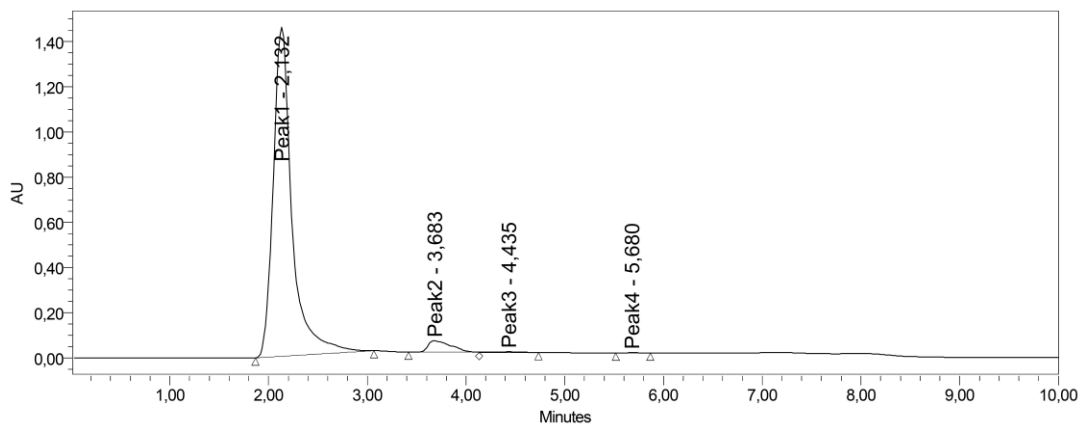
Signal 2: DAD1 C, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.366	BB	0.1576	64.22700	4.81634	0.6323
2	4.008	BB	0.1189	33.18065	3.57252	0.3267
3	4.163	BV	0.0832	11.41506	1.67070	0.1124
4	7.123	BB	0.0738	28.68355	5.50434	0.2824
5	7.417	BV	0.0537	9.00908	2.09229	0.0887
6	7.527	VV	0.0789	35.58220	5.77728	0.3503
7	7.734	VV	0.0930	9944.02051	1599.12415	97.9005
8	9.442	VB	0.1194	10.92408	1.08994	0.1075
9	11.040	BV	0.0602	20.22775	4.89613	0.1991

Totals : 1.01573e4 1628.54369

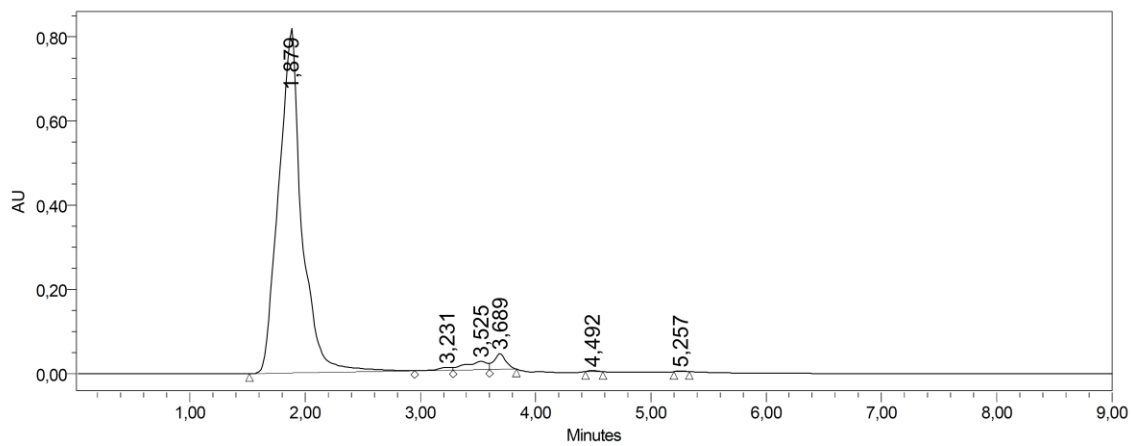
Compound: 42

Method G



	Peak Name	RT	Area	% Area	Height
1	Peak1	2,132	19221293	95,55	1455564
2	Peak2	3,683	822849	4,09	50738
3	Peak3	4,435	57611	0,29	3144
4	Peak4	5,680	14638	0,07	1722

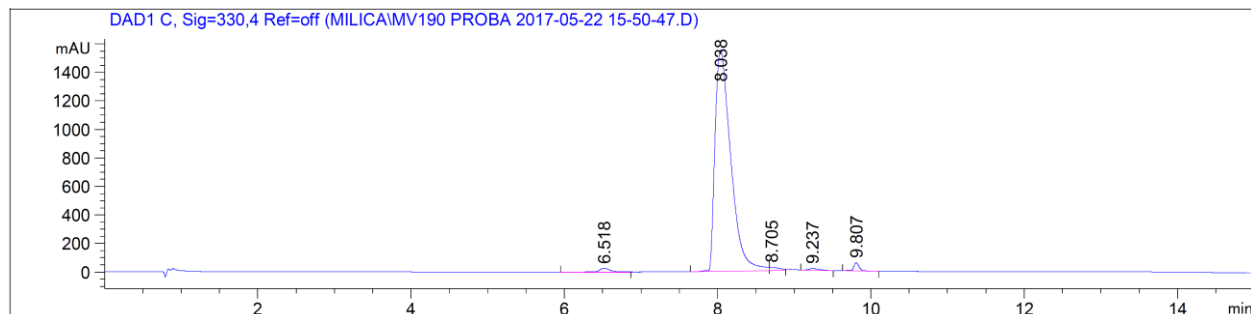
Method H



	RT	Area	% Area	Height
1	1,879	11371351	95,01	817435
2	3,231	58996	0,49	7141
3	3,525	256173	2,14	19622
4	3,689	264374	2,21	36869
5	4,492	10230	0,09	1937
6	5,257	7266	0,06	1516

Compound: 43

Method C

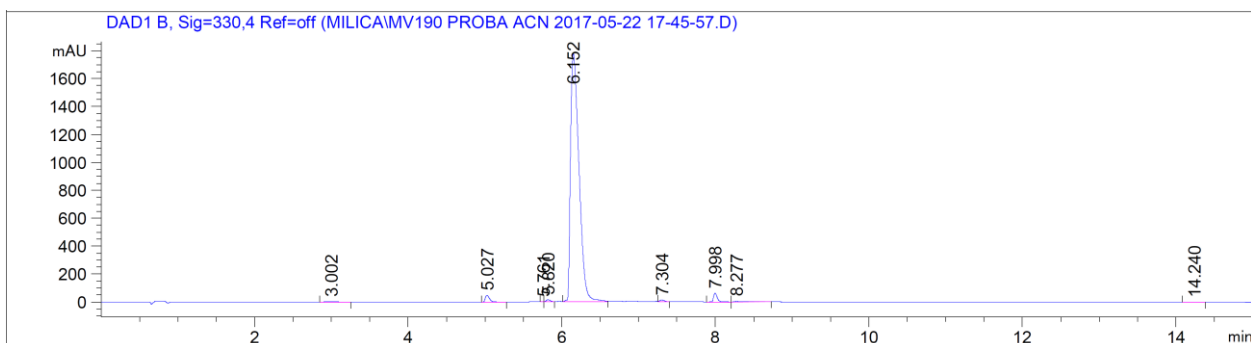


Signal 3: DAD1 C, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.518	BV	0.1385	258.23196	25.30854	1.1241
2	8.038	BV	0.1975	2.21153e4	1549.88318	96.2724
3	8.705	VV	0.1059	192.60329	21.72797	0.8384
4	9.237	BB	0.1163	114.89076	13.16687	0.5001
5	9.807	VB	0.0765	290.57172	57.91777	1.2649

Totals : 2.29716e4 1668.00434

Method D



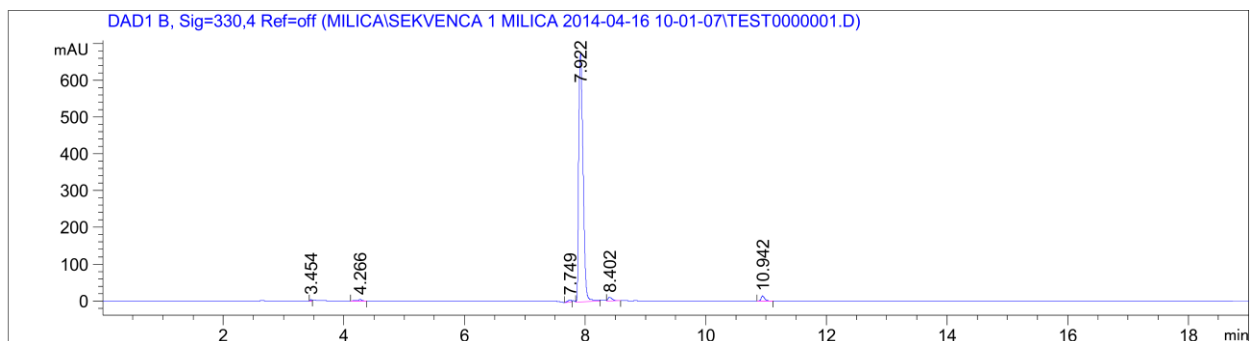
Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.002	BB	0.1168	21.08238	2.16106	0.1496
2	5.027	BV	0.0603	192.46234	48.99674	1.3657
3	5.761	BV	0.0252	2.62834	1.35268	0.0186
4	5.820	VV	0.0586	50.54870	13.83813	0.3587
5	6.152	BV	0.1115	1.35283e4	1772.43787	95.9933
6	7.304	VB	0.0662	46.55672	11.03887	0.3304
7	7.998	BB	0.0525	207.95050	62.17960	1.4756
8	8.277	BB	0.1144	37.45362	4.37204	0.2658
9	14.240	BB	0.1042	5.98101	6.86411e-1	0.0424

Totals : 1.40930e4 1917.06340

Compound: 44

Method B

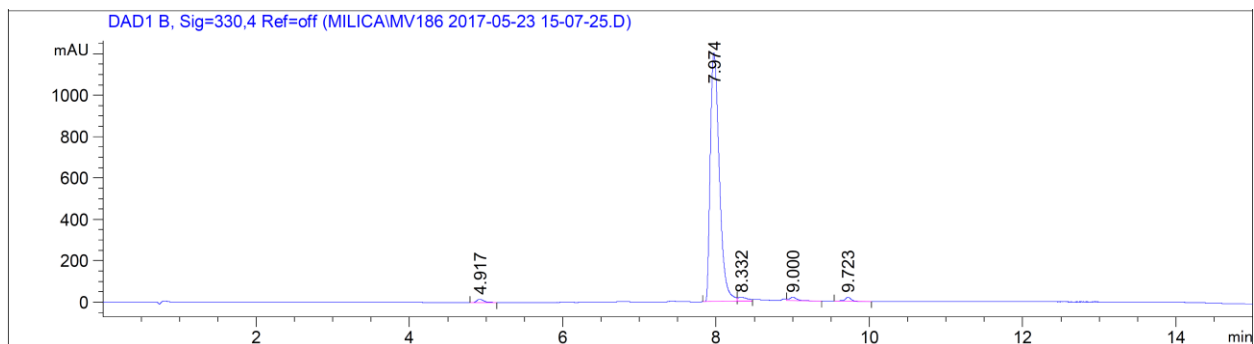


Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.454	BV	0.0274	6.60746	3.60233	0.1856
2	4.266	BB	0.0507	15.78087	4.46554	0.4434
3	7.749	BV	0.0560	25.58624	6.86114	0.7188
4	7.922	VV	0.0826	3407.48193	678.12067	95.7329
5	8.402	VB	0.0705	50.60367	10.35993	1.4217
6	10.942	BB	0.0583	53.30160	13.43398	1.4975

Totals : 3559.36177 716.84358

Method C



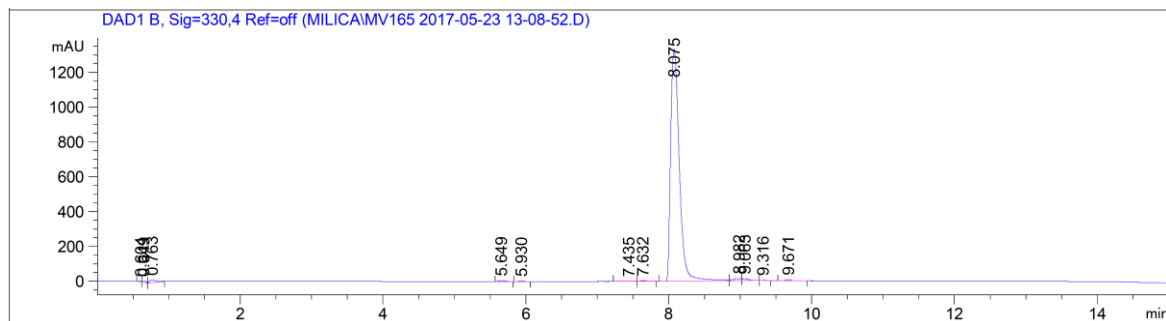
Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.917	BV	0.0894	93.04006	15.53817	0.8992
2	7.974	BV	0.1287	9854.13281	1200.95142	95.2415
3	8.332	VV	0.1169	157.76595	17.72366	1.5248
4	9.000	VB	0.1014	122.02502	16.48204	1.1794
5	9.723	BB	0.0854	119.50657	20.07878	1.1550

Totals : 1.03465e4 1270.77407

Compound: 47

Method C

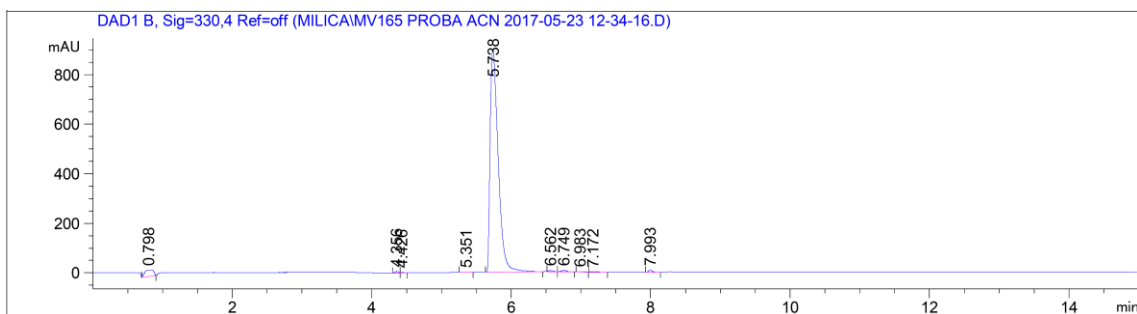


Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	0.604	BV	0.0369	10.12167	3.33901	0.0878
2	0.649	VB	0.0466	24.82949	6.35785	0.2154
3	0.763	BV	0.1019	99.96941	13.35211	0.8673
4	5.649	BV	0.0869	37.05835	6.18813	0.3215
5	5.930	VV	0.0762	11.30739	1.80295	0.0981
6	7.435	BV	0.0970	10.26521	1.25375	0.0891
7	7.632	VB	0.0907	16.59370	2.19417	0.1440
8	8.075	BV	0.1310	1.11192e4	1330.32166	96.4631
9	8.982	VV	0.0998	88.77036	10.64480	0.7701
10	9.063	VB	0.0828	65.05870	10.79022	0.5644
11	9.316	BB	0.0593	5.16457	1.08929	0.0448
12	9.671	BB	0.0789	38.55864	7.09417	0.3345

Totals : 1.15269e4 1394.42811

Method D



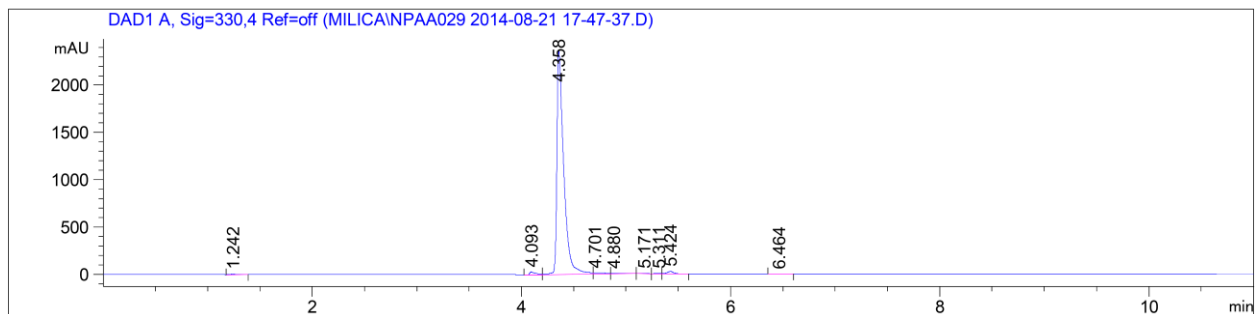
Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	0.798	BV	0.1158	219.50848	25.28385	2.8924
2	4.356	BV	0.0562	22.84946	6.24789	0.3011
3	4.426	VB	0.0447	8.67736	2.45756	0.1143
4	5.351	BV	0.0653	8.54845	1.65322	0.1126
5	5.738	BB	0.1234	7233.08691	898.34271	95.3081
6	6.562	VB	0.0702	24.15495	4.96893	0.3183
7	6.749	BB	0.0692	32.18052	6.67924	0.4240
8	6.983	BB	0.0457	6.91161	1.88980	0.0911
9	7.172	BB	0.0614	6.41924	1.25092	0.0846
10	7.993	BB	0.0526	26.82496	7.89762	0.3535

Totals : 7589.16196 956.67174

Compound: 48

Method E

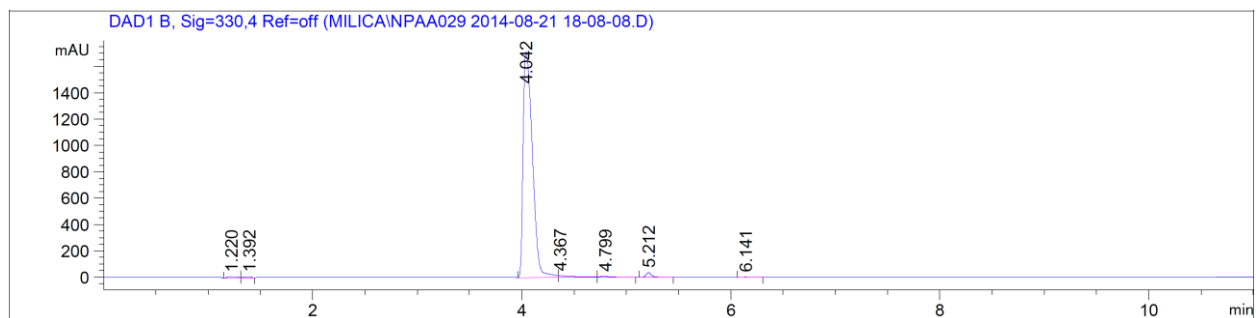


Signal 1: DAD1 A, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.242	BB	0.0898	32.85369	5.15835	0.2919
2	4.093	BV	0.0588	134.35452	30.82844	1.1936
3	4.358	VV	0.0650	1.07826e4	2372.80054	95.7928
4	4.701	VV	0.0858	111.43839	15.60658	0.9900
5	4.880	VB	0.0880	53.39765	7.78917	0.4744
6	5.171	BB	0.0492	12.03496	3.58144	0.1069
7	5.311	BV	0.0514	14.59159	4.27087	0.1296
8	5.424	VB	0.0622	107.45930	24.99597	0.9547
9	6.464	BB	0.0544	7.43452	1.67094	0.0660

Totals : 1.12562e4 2466.70231

Method F



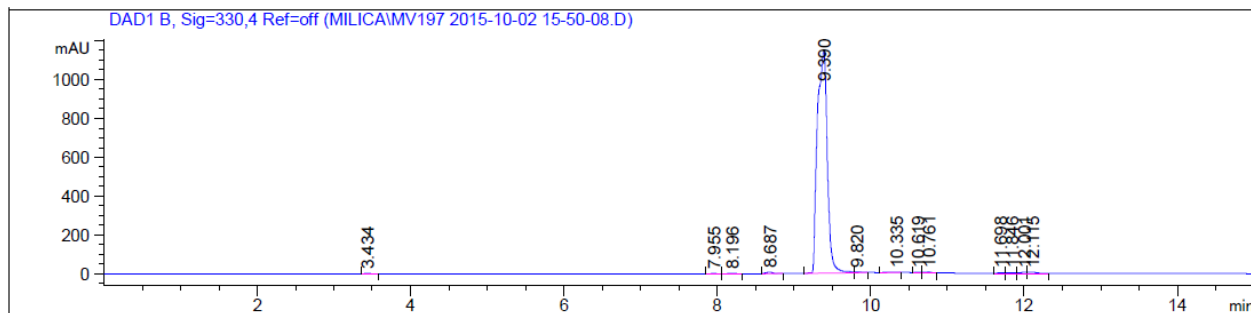
Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.220	BV	0.1038	78.67262	10.89240	0.7144
2	1.392	VB	0.0818	44.73525	7.31524	0.4062
3	4.042	BV	0.1003	1.05393e4	1712.82336	95.7090
4	4.367	VV	0.1354	162.70767	14.89914	1.4776
5	4.799	VB	0.0960	60.16482	8.41006	0.5464
6	5.212	BB	0.0533	118.60275	33.87966	1.0770
7	6.141	BB	0.0598	7.63817	1.70321	0.0694

Totals : 1.10119e4 1789.92307

Compound 50

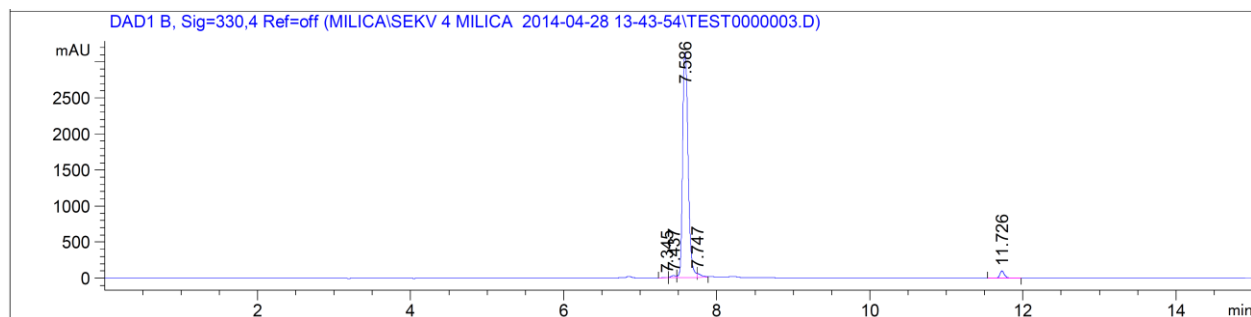
Method A



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.434	BB	0.0726	6.89827	1.13186	0.0657
2	7.955	BB	0.0561	9.48502	2.02770	0.0903
3	8.196	BV	0.0707	15.66721	2.91605	0.1491
4	8.687	BB	0.0834	41.24639	6.59805	0.3926
5	9.390	BV	0.1233	1.02596e4	1147.25659	97.6608
6	9.820	VB	0.0669	26.07065	4.68870	0.2482
7	10.335	BV	0.0900	10.27740	1.36961	0.0978
8	10.619	BV	0.0690	15.91878	2.79346	0.1515
9	10.761	VB	0.0790	27.74316	4.76242	0.2641
10	11.698	BV	0.0710	8.84721	1.50760	0.0842
11	11.846	VV	0.0841	17.17547	2.54982	0.1635
12	12.001	VV	0.0788	27.74920	4.24248	0.2641
13	12.115	VB	0.1003	38.66140	4.63414	0.3680

Totals : 1.05054e4 1186.47848

Method B

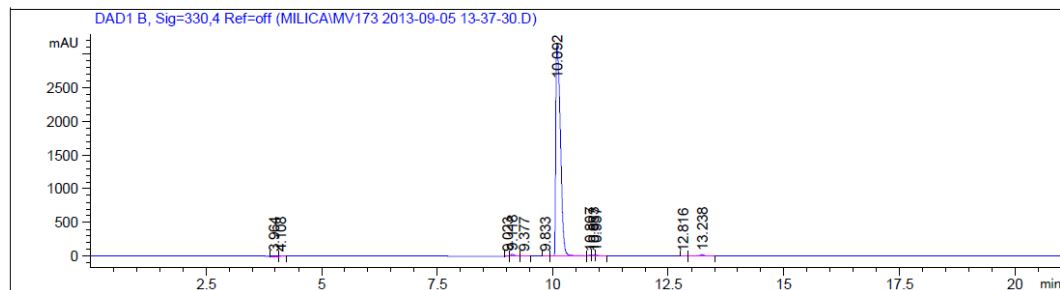


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.345	BB	0.0530	13.48670	3.49808	0.0824
2	7.437	BV	0.0730	114.41154	25.92632	0.6993
3	7.586	VV	0.0767	1.55805e4	3121.62939	95.2299
4	7.747	VV	0.0607	236.20111	53.79499	1.4437
5	11.726	BB	0.0631	416.33008	99.84488	2.5447

Totals : 1.63609e4 3304.69367

Compound: 93

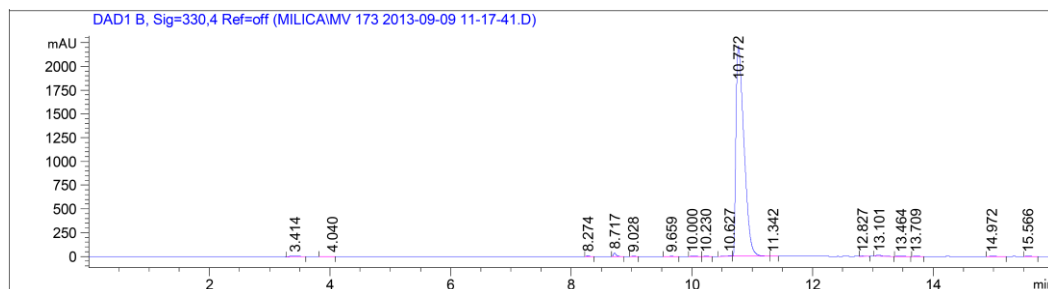
Method A



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.964	BV	0.0924	19.55329	2.57985	0.0872
2	4.108	VB	0.0749	8.68331	1.48206	0.0387
3	9.023	BV	0.0606	21.85141	5.47642	0.0974
4	9.118	VB	0.0695	143.28685	28.81312	0.6387
5	9.377	BB	0.0778	18.69127	3.26687	0.0833
6	9.833	BV	0.0622	15.27885	3.34955	0.0681
7	10.092	VB	0.0906	2.18653e4	3125.15137	97.4654
8	10.807	BV	0.0556	40.61069	10.86071	0.1810
9	10.883	VV	0.0507	52.67857	14.92841	0.2348
10	10.937	VB	0.0681	65.78538	13.54881	0.2932
11	12.816	VB	0.0649	8.01962	1.78522	0.0357
12	13.238	BB	0.1197	174.16573	19.97355	0.7763

Totals : 2.24339e4 3231.21595

Method B



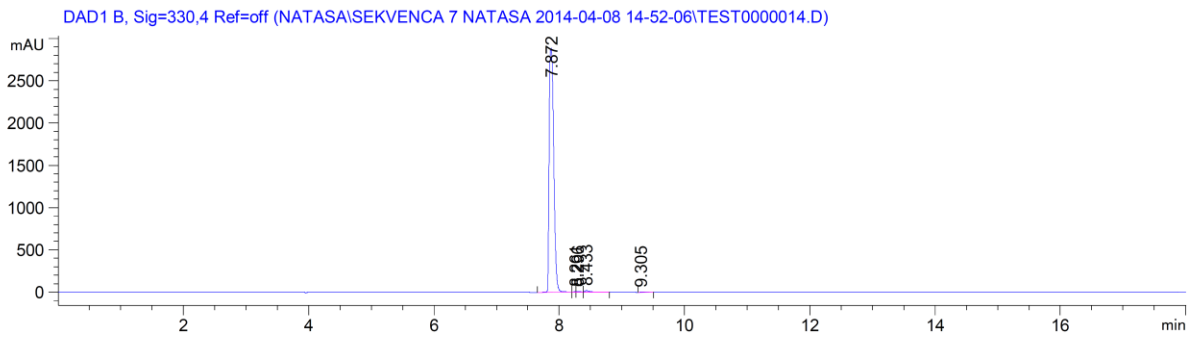
Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.414	BB	0.1508	57.76731	4.53033	0.2772
2	4.040	BB	0.1116	29.02518	3.34897	0.1393
3	8.274	BB	0.0440	21.39058	7.56075	0.1027
4	8.717	BB	0.0470	112.42612	36.38964	0.5395
5	9.028	BV	0.0524	13.47235	3.84515	0.0647
6	9.659	BV	0.0672	10.25847	2.02086	0.0492
7	10.000	BV	0.0717	23.33257	4.51842	0.1120
8	10.230	VB	0.0535	16.14855	4.59056	0.0775
9	10.627	BV	0.0674	42.24029	9.14999	0.2027
10	10.772	VV	0.1390	2.03690e4	2210.80518	97.7534
11	11.342	VB	0.0704	5.90208	1.14035	0.0283
12	12.827	VB	0.0581	18.86507	4.82801	0.0905
13	13.101	VB	0.1032	86.10670	13.10270	0.4132
14	13.464	BB	0.0871	6.57275	1.02831	0.0315
15	13.709	BB	0.0569	5.84986	1.47227	0.0281
16	14.972	BB	0.0628	10.86918	2.51900	0.0522
17	15.566	BB	0.0606	7.90032	2.00084	0.0379

Totals : 2.08372e4 2312.85134

Compound: 56

Method A

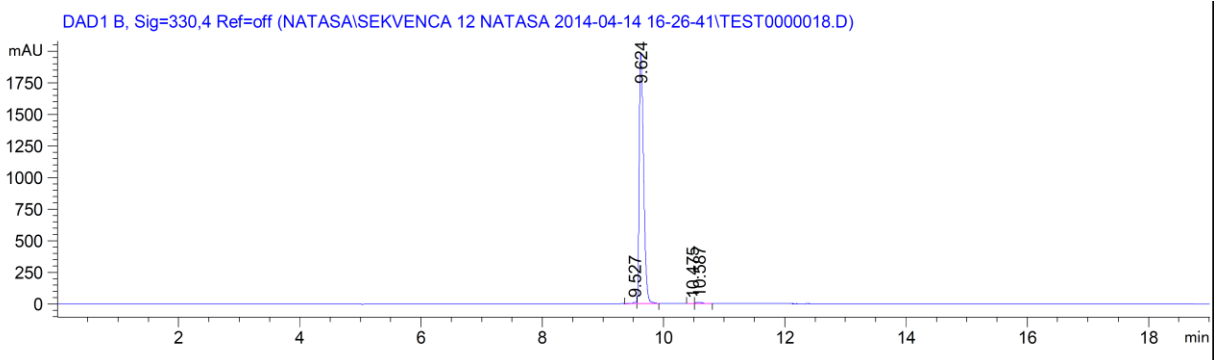


Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.872	BV	0.0625	1.47453e4	2891.94897	98.4870
2	8.261	VV	0.0474	21.99726	5.65454	0.1469
3	8.296	VV	0.0768	35.56199	5.65894	0.2375
4	8.433	VB	0.0811	118.53759	19.86254	0.7917
5	9.305	BB	0.0906	50.43294	7.29904	0.3369

Totals : 1.49718e4 2930.42403

Method B



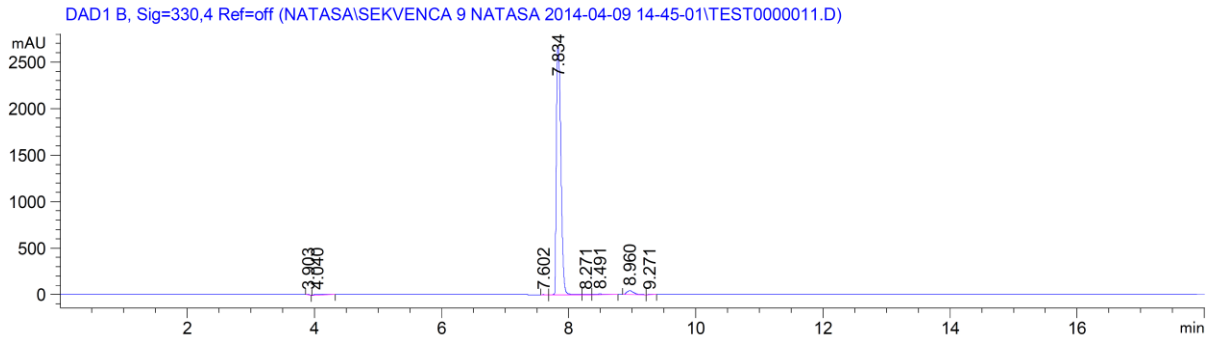
Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.527	BV	0.0618	35.00754	9.11107	0.3476
2	9.624	VB	0.0797	9959.46973	1979.45459	98.8795
3	10.475	BB	0.0485	7.00063	1.99130	0.0695
4	10.587	BV	0.0948	70.85368	10.49114	0.7034

Totals : 1.00723e4 2001.04810

Compound: 57

Method A

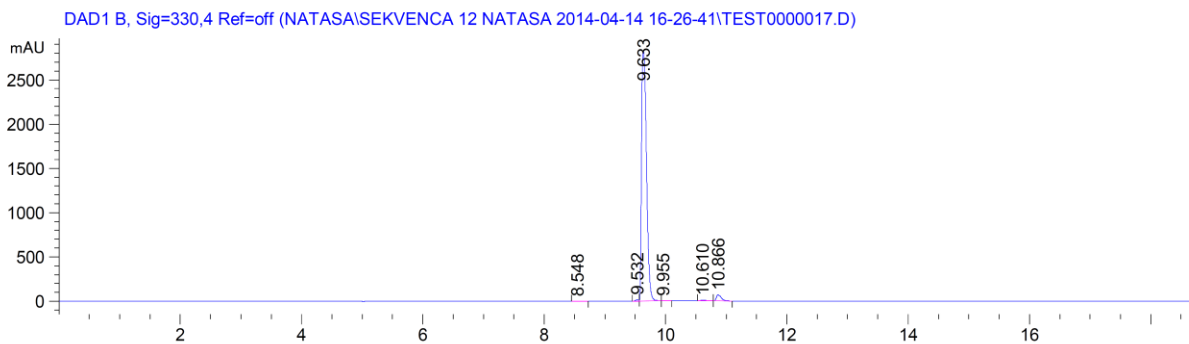


Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.903	BB	0.0459	12.32677	3.24069	0.0898
2	4.040	BB	0.1458	85.17356	6.98080	0.6206
3	7.602	BB	0.0497	13.86869	4.23228	0.1010
4	7.834	BV	0.0790	1.31924e4	2675.45679	96.1224
5	8.271	VV	0.1009	28.63622	3.39643	0.2086
6	8.491	VB	0.1088	62.24164	7.57909	0.4535
7	8.960	BB	0.1072	321.92850	42.57342	2.3456
8	9.271	BB	0.0617	8.01683	1.80907	0.0584

Totals : 1.37246e4 2745.26855

Method B



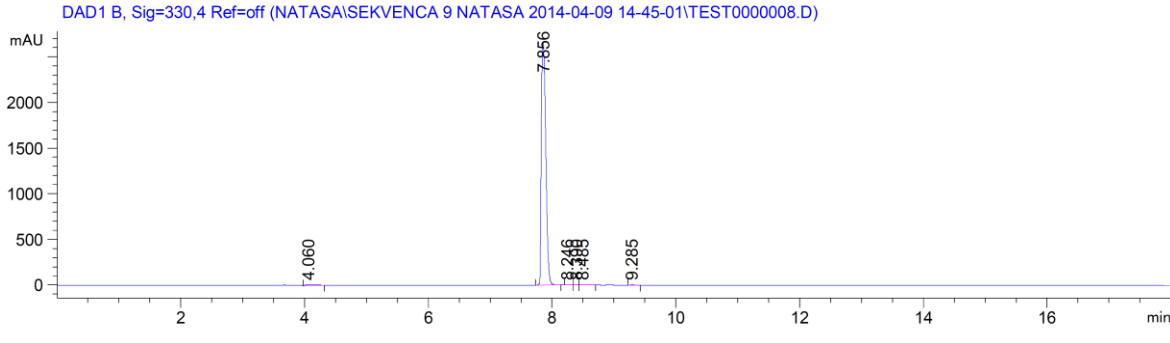
Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.548	BB	0.0821	23.07074	4.16508	0.1393
2	9.532	BV	0.0555	48.24945	13.08779	0.2913
3	9.633	VV	0.0762	1.60418e4	2826.84668	96.8639
4	9.955	VB	0.0611	14.30501	3.02871	0.0864
5	10.610	BV	0.0883	60.83349	9.54838	0.3673
6	10.866	VB	0.0881	372.92511	66.83367	2.2518

Totals : 1.65612e4 2923.51031

Compound: 58

Method A

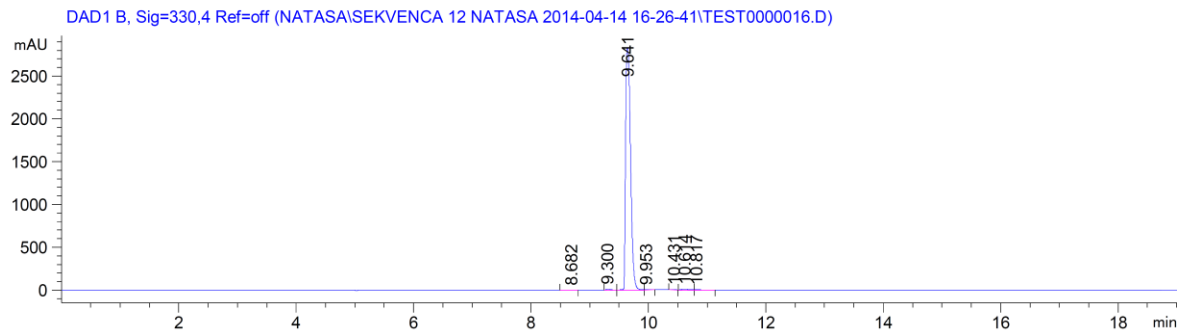


Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.060	BB	0.1379	74.10491	6.36350	0.5465
2	7.856	BB	0.0816	1.34324e4	2652.45581	99.0571
3	8.246	VB	0.0584	9.46721	2.33126	0.0698
4	8.390	BV	0.0500	5.58801	1.48101	0.0412
5	8.485	VB	0.0686	23.19528	4.73565	0.1711
6	9.285	BB	0.0757	15.51103	2.95529	0.1144

Totals : 1.35603e4 2670.32253

Method B



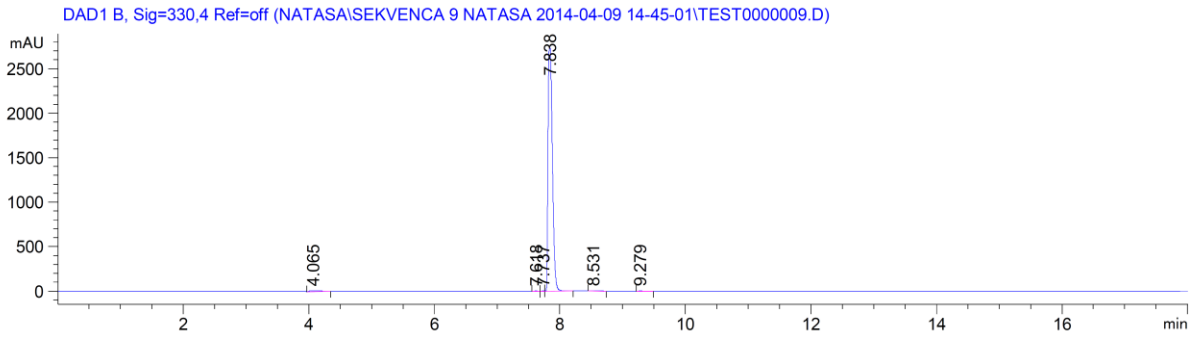
Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.682	BB	0.0686	6.65815	1.15691	0.0396
2	9.300	BV	0.0717	69.98252	14.39190	0.4167
3	9.641	VV	0.0793	1.65763e4	2829.87646	98.7034
4	9.953	VB	0.0695	14.49203	2.58252	0.0863
5	10.431	BB	0.0826	9.82574	1.41421	0.0585
6	10.614	BV	0.0966	96.13948	12.95786	0.5725
7	10.817	VB	0.0893	20.65772	2.89228	0.1230

Totals : 1.67940e4 2865.27215

Compound: 59

Method A

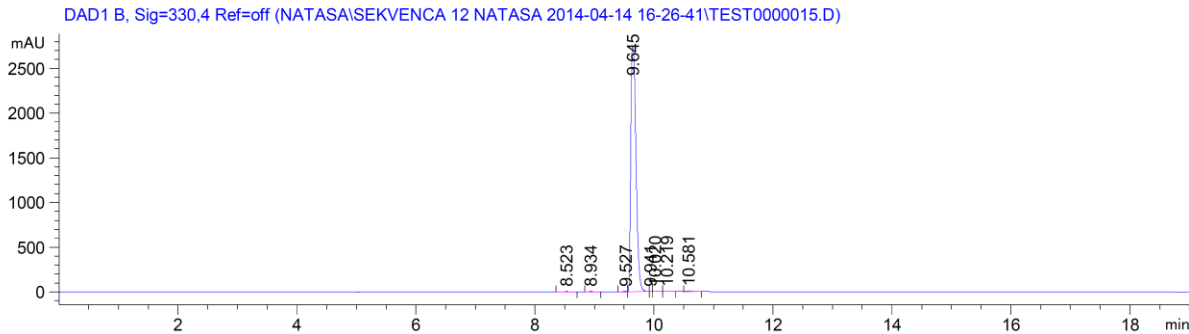


Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.065	BB	0.1473	79.03783	6.32624	0.5855
2	7.618	BB	0.0491	18.53803	5.52894	0.1373
3	7.737	BV	0.0390	14.48638	5.72939	0.1073
4	7.838	VB	0.0769	1.33464e4	2759.09253	98.8605
5	8.531	VB	0.0817	20.59265	3.37490	0.1525
6	9.279	BB	0.0922	21.17863	3.17831	0.1569

Totals : 1.35002e4 2783.23031

Method B



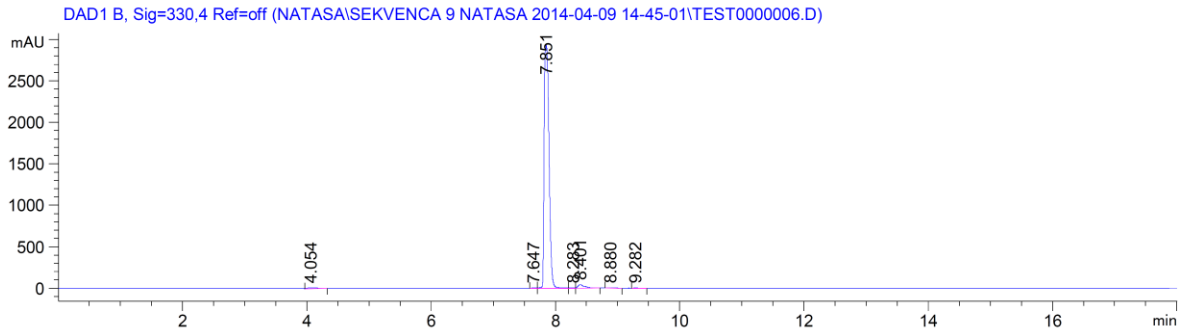
Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.523	BB	0.0991	37.97367	5.14786	0.2250
2	8.934	BB	0.0810	27.61630	4.56706	0.1637
3	9.527	BV	0.0558	16.62083	3.60095	0.0985
4	9.645	VV	0.0835	1.67129e4	2747.22168	99.0405
5	9.941	VV	0.0360	5.85439	2.13217	0.0347
6	10.020	VB	0.0730	13.45216	2.34239	0.0797
7	10.219	BB	0.0823	8.07627	1.16616	0.0479
8	10.581	BB	0.0840	52.31254	8.47235	0.3100

Totals : 1.68748e4 2774.65063

Compound: 60

Method A

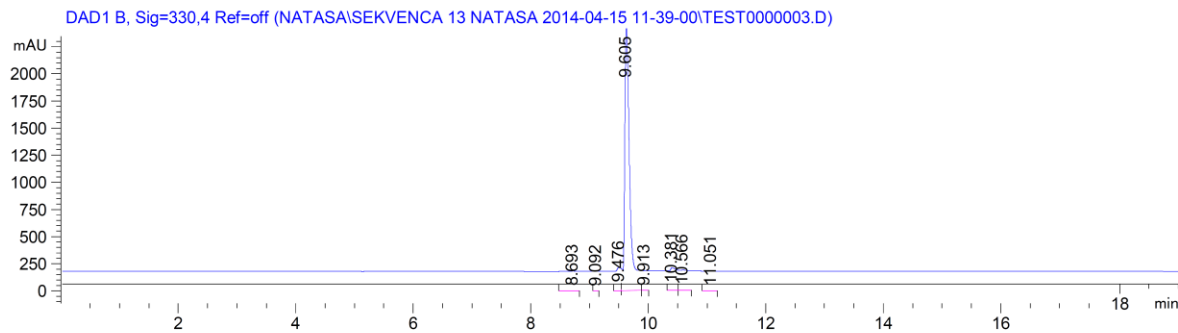


Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.054	BB	0.1400	76.77130	6.46633	0.4639
2	7.647	BV	0.0669	44.85147	10.38683	0.2710
3	7.851	VV	0.0662	1.60190e4	2932.14624	96.7991
4	8.283	VV	0.0783	40.24760	6.72498	0.2432
5	8.401	VB	0.1067	326.38083	43.40168	1.9722
6	8.880	VB	0.0913	19.27374	2.54714	0.1165
7	9.282	BV	0.1031	22.18926	2.84248	0.1341

Totals : 1.65487e4 3004.51569

Method B



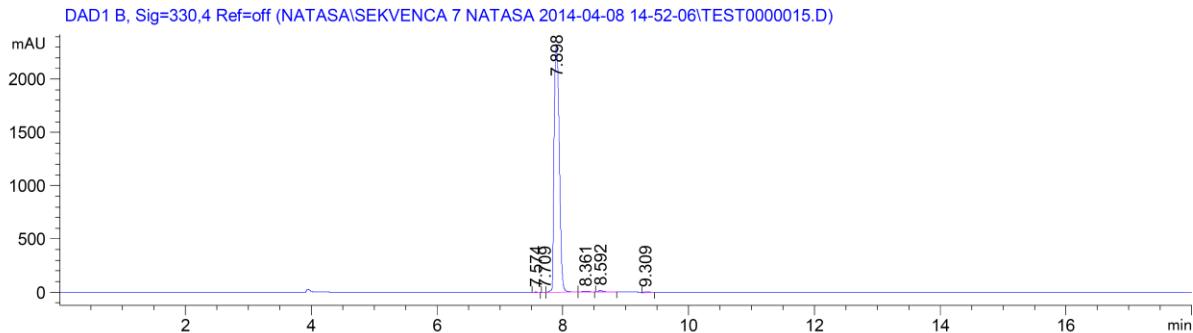
Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.693	BV	0.0844	26.97740	4.25877	0.2377
2	9.092	BV	0.0499	6.48211	1.87371	0.0571
3	9.476	BV	0.0724	156.76759	34.54624	1.3810
4	9.605	VV	0.0761	1.09312e4	2232.33496	96.2982
5	9.913	VB	0.0539	8.17391	2.03334	0.0720
6	10.381	VB	0.0745	152.74124	28.27456	1.3456
7	10.566	VB	0.0892	55.31636	9.12635	0.4873
8	11.051	BV	0.0742	13.74273	2.53779	0.1211

Totals : 1.13514e4 2314.98574

Compound: 61

Method A

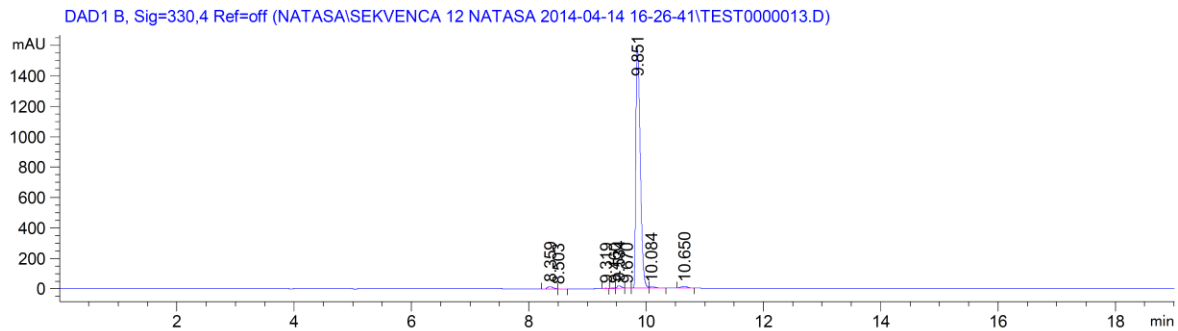


Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.574	BB	0.0498	10.98274	3.06618	0.0818
2	7.709	BV	0.0402	5.32185	2.02105	0.0396
3	7.898	VV	0.0962	1.32699e4	2305.23462	98.8599
4	8.361	VB	0.0972	42.86095	5.63544	0.3193
5	8.592	BB	0.0725	62.80040	12.84540	0.4679
6	9.309	BB	0.0763	31.07413	5.63554	0.2315

Totals : 1.34230e4 2334.43824

Method B



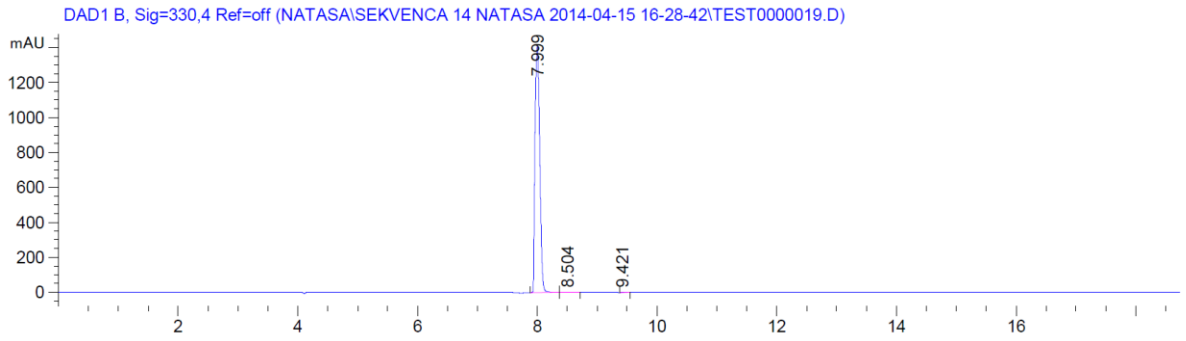
Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.359	BV	0.1030	104.23132	15.10967	1.2048
2	8.503	VB	0.0492	5.21808	1.27504	0.0603
3	9.319	BB	0.0596	5.54395	1.16362	0.0641
4	9.460	BV	0.0497	9.49700	2.65749	0.1098
5	9.534	VV	0.0810	78.42601	15.63771	0.9066
6	9.670	VB	0.0554	9.83352	2.39261	0.1137
7	9.851	BV	0.0825	8289.27051	1585.12732	95.8183
8	10.084	VB	0.0902	56.78719	8.16040	0.6564
9	10.650	BB	0.1050	92.22041	11.76338	1.0660

Totals : 8651.02799 1643.28723

Compound: 62

Method A

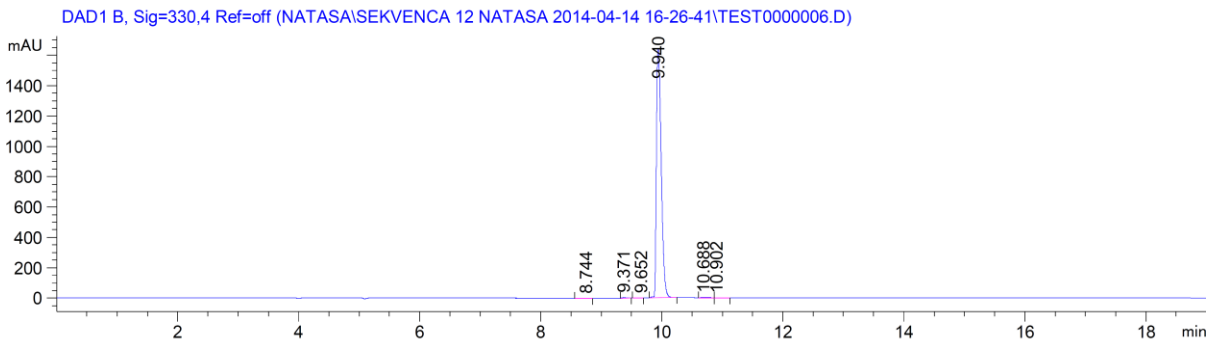


Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.999	BB	0.0948	7959.89844	1411.25439	99.7428
2	8.504	BV	0.1111	12.08869	1.32941	0.1515
3	9.421	BB	0.0634	8.43619	1.82545	0.1057

Totals : 7980.42332 1414.40926

Method B



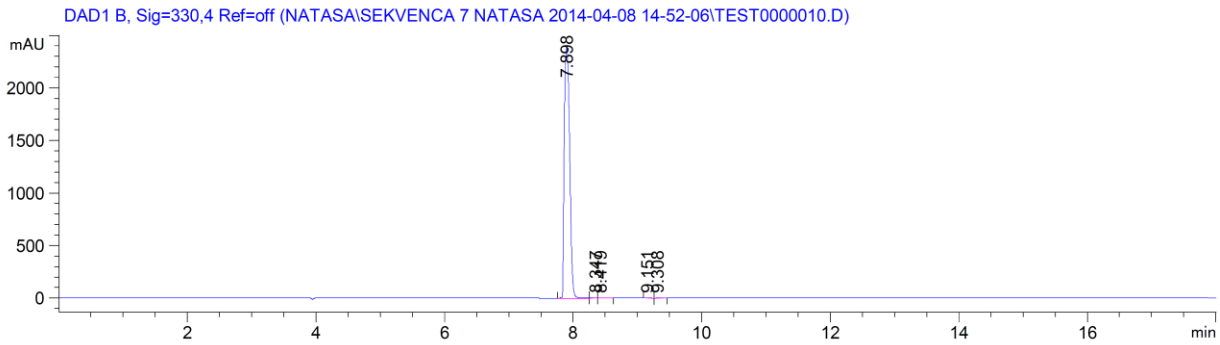
Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.744	BB	0.0772	6.65576	1.04623	0.0729
2	9.371	BB	0.0672	18.59013	3.96670	0.2037
3	9.652	BV	0.0729	7.48154	1.23095	0.0820
4	9.940	VB	0.0872	9039.47949	1641.97095	99.0386
5	10.688	BV	0.1202	42.40695	4.44773	0.4646
6	10.902	VV	0.1087	12.61870	1.39959	0.1383

Totals : 9127.23257 1654.06214

Compound: 63

Method A

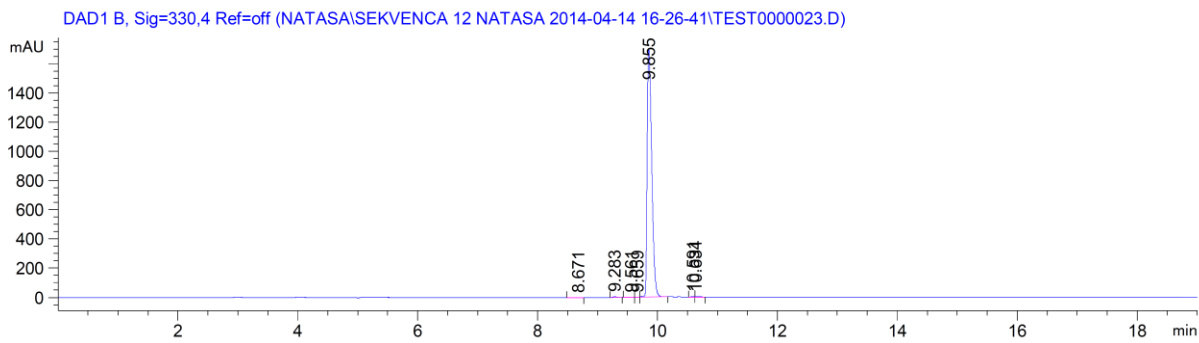


Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.898	BV	0.0978	1.39827e4	2388.04785	99.3732
2	8.347	VV	0.0874	20.41422	2.82323	0.1451
3	8.419	VV	0.1030	29.67100	3.60416	0.2109
4	9.151	BB	0.1113	14.39959	1.53654	0.1023
5	9.308	BB	0.0737	23.71076	4.30790	0.1685

Totals : 1.40709e4 2400.31968

Method B



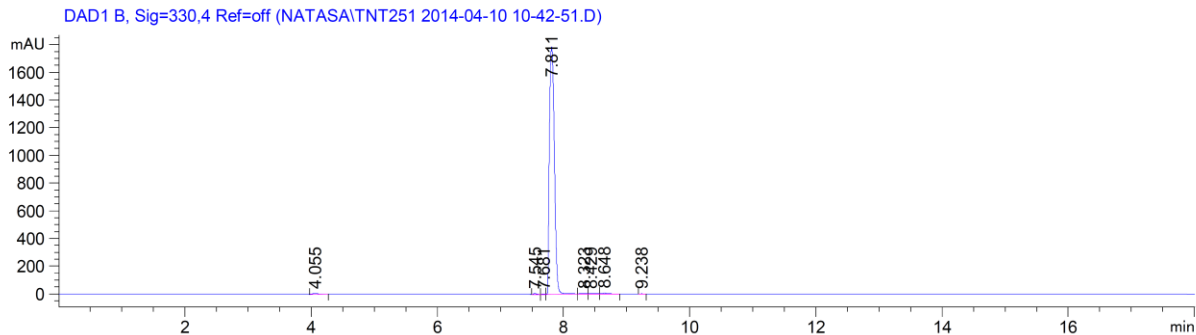
Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.671	BV	0.0692	5.82516	1.01896	0.0642
2	9.283	BB	0.0616	19.24336	4.26434	0.2122
3	9.561	BV	0.0754	10.55903	1.81409	0.1164
4	9.659	VV	0.0537	6.58439	1.51605	0.0726
5	9.855	VB	0.0835	8993.75488	1692.99585	99.1683
6	10.591	BV	0.0505	16.15318	3.92707	0.1781
7	10.634	VB	0.0650	17.06612	3.16131	0.1882

Totals : 9069.18612 1708.69768

Compound: 64

Method A

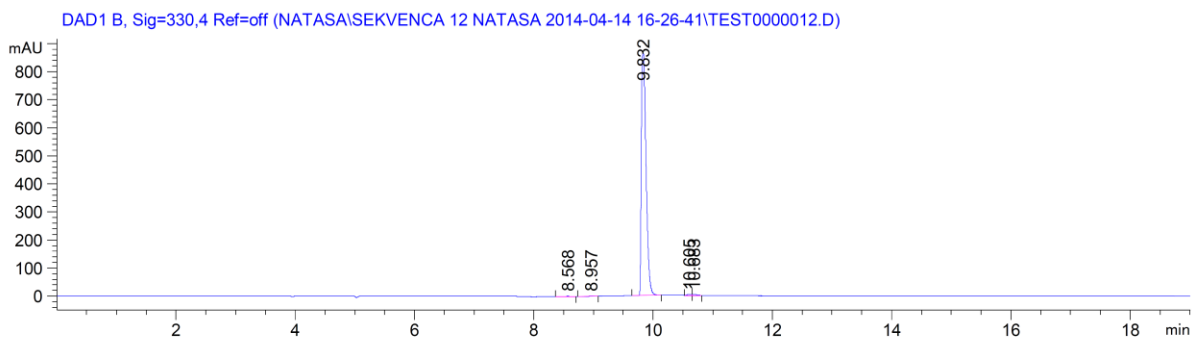


Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.055	BB	0.1110	32.50327	3.46317	0.3243
2	7.545	BB	0.0482	18.24575	5.50040	0.1820
3	7.681	BV	0.0502	12.96887	4.06920	0.1294
4	7.811	VV	0.0918	9842.99902	1785.11328	98.1982
5	8.323	VV	0.0985	38.11309	4.86005	0.3802
6	8.429	VV	0.0969	33.09087	4.46943	0.3301
7	8.648	VB	0.0846	39.62548	6.27882	0.3953
8	9.238	BB	0.0507	6.05605	1.67524	0.0604

Totals : 1.00236e4 1815.42959

Method B



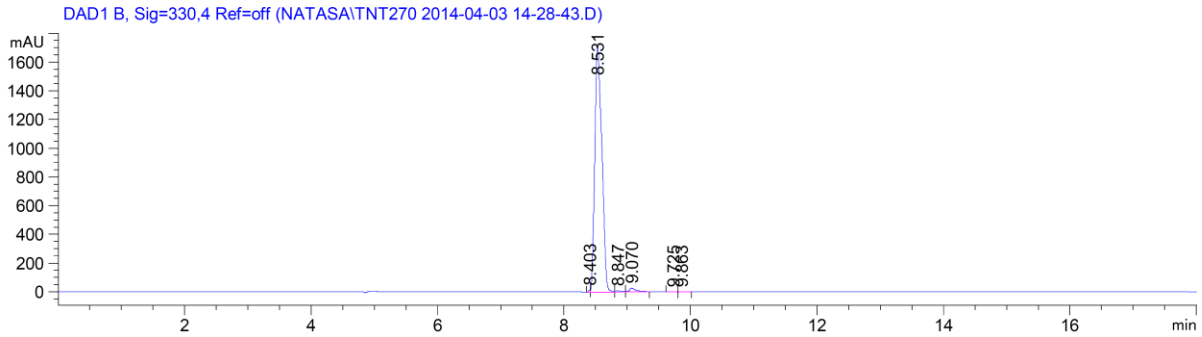
Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.568	BB	0.1087	11.91639	1.29686	0.2479
2	8.957	BB	0.0716	6.97890	1.18674	0.1452
3	9.832	BB	0.0851	4750.17725	870.98187	98.8290
4	10.605	BV	0.0605	18.65528	3.81929	0.3881
5	10.683	VV	0.0720	18.73139	3.28471	0.3897

Totals : 4806.45921 880.56948

Compound: 65

Method A

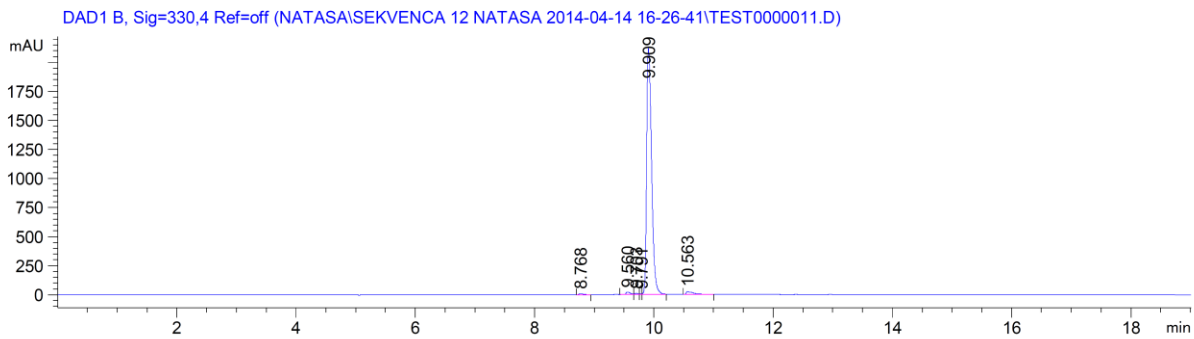


Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.403	BV	0.0357	32.00726	14.81597	0.2341
2	8.531	VV	0.1096	1.33674e4	1721.92603	97.7733
3	8.847	VV	0.1064	63.93130	7.81992	0.4676
4	9.070	VB	0.0988	181.56046	25.57087	1.3280
5	9.725	BB	0.0787	11.55519	1.78175	0.0845
6	9.863	BB	0.0720	15.37577	2.61743	0.1125

Totals : 1.36718e4 1774.53195

Method B



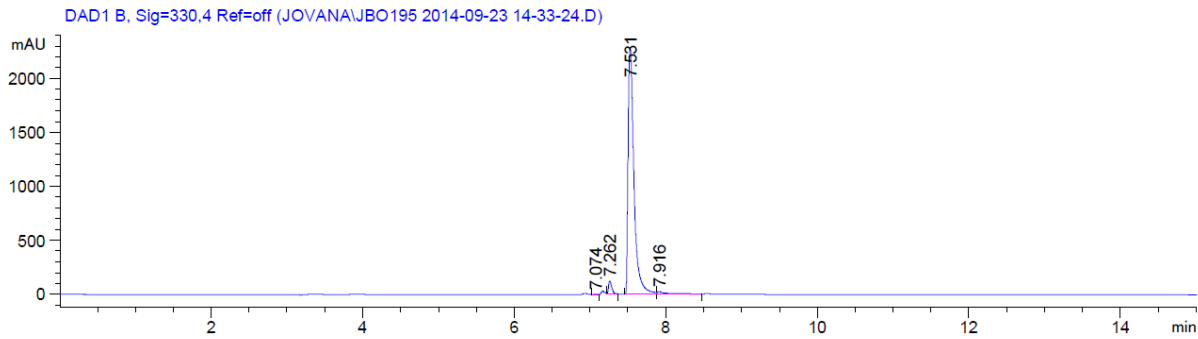
Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.768	VB	0.0851	53.79874	9.56847	0.4287
2	9.560	BV	0.0775	103.28182	20.24667	0.8230
3	9.703	VV	0.0764	40.86622	8.16027	0.3257
4	9.791	VV	0.0340	14.84075	6.53435	0.1183
5	9.909	VB	0.0905	1.21448e4	2113.74512	96.7805
6	10.563	VB	0.1018	191.21921	24.31145	1.5238

Totals : 1.25488e4 2182.56632

Compound: 66

Method A

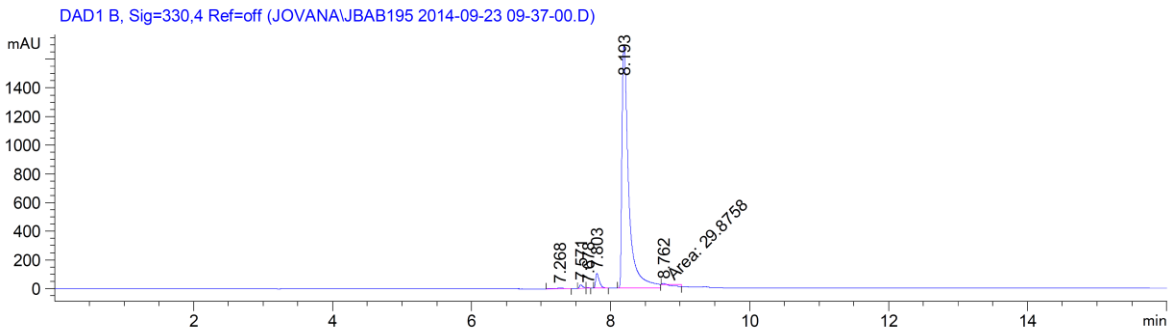


Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.074	VB	0.0452	6.01910	1.99216	0.0468
2	7.262	VB	0.0456	362.23334	122.08355	2.8188
3	7.531	BV	0.0828	1.22974e4	2284.25537	95.6962
4	7.916	VB	0.1092	184.79945	22.40215	1.4381

Totals : 1.28504e4 2430.73323

Method B



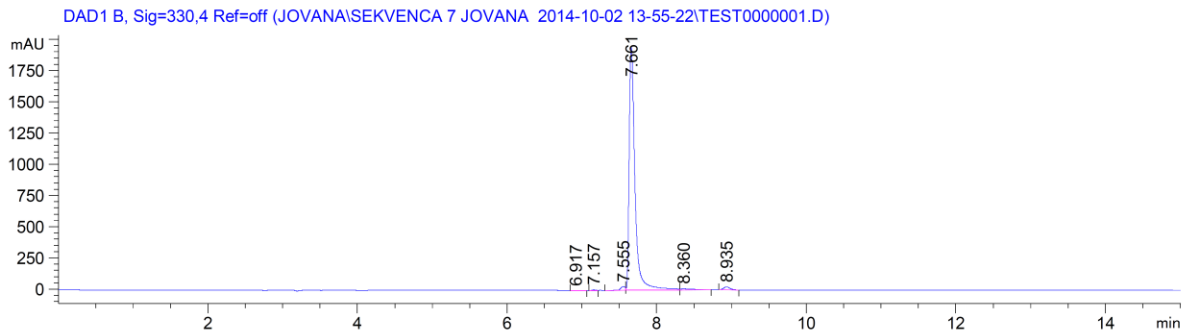
Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.268	BV	0.1212	34.11822	3.36895	0.2850
2	7.571	BV	0.0505	83.76450	25.69889	0.6998
3	7.678	VV	0.0416	10.64213	3.81388	0.0889
4	7.803	BB	0.0544	368.76785	101.43283	3.0808
5	8.193	BV	0.1003	1.14427e4	1683.90186	95.5959
6	8.762	MM	0.0533	29.87580	9.34106	0.2496

Totals : 1.19699e4 1827.55746

Compound: 67

Method A

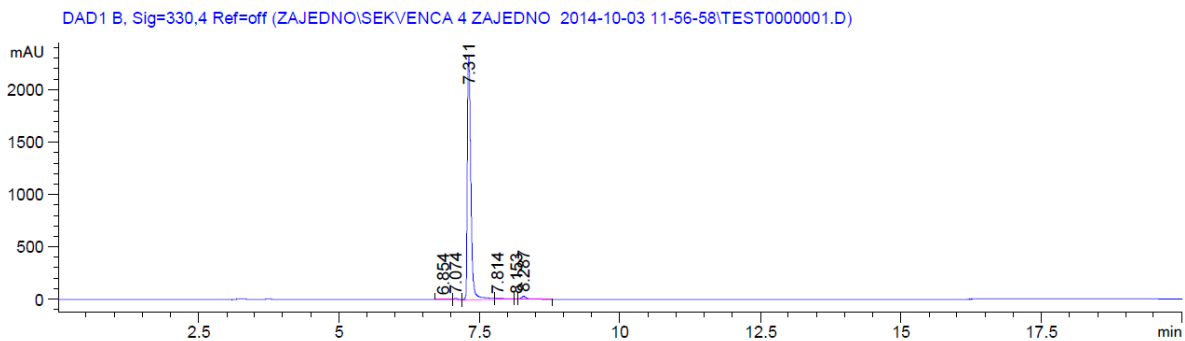


Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.917	BB	0.0834	7.28937	1.22485	0.0667
2	7.157	BV	0.0534	20.64882	6.10660	0.1889
3	7.555	BV	0.0662	127.04780	30.73298	1.1624
4	7.661	VV	0.0814	1.05456e4	1941.02527	96.4855
5	8.360	VB	0.1399	91.25397	8.87714	0.8349
6	8.935	VB	0.0900	137.88000	23.66191	1.2615

Totals : 1.09297e4 2011.62875

Method B



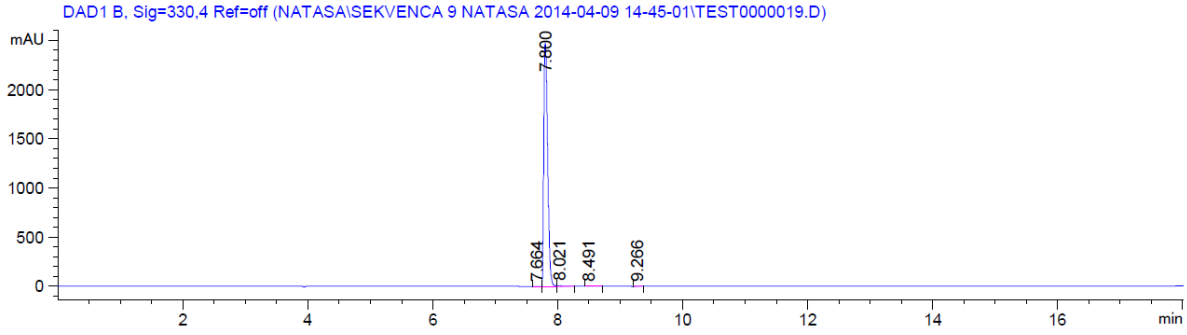
Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.854	BV	0.1336	27.77994	2.52115	0.2588
2	7.074	VB	0.0682	57.12652	11.55568	0.5323
3	7.311	BV	0.0680	1.02242e4	2337.05688	95.2645
4	7.814	VV	0.1762	177.59578	12.69522	1.6548
5	8.153	VV	0.0524	28.15751	6.39338	0.2624
6	8.287	VB	0.1108	217.56828	28.27698	2.0272

Totals : 1.07324e4 2398.49931

Compound: 68

Method A

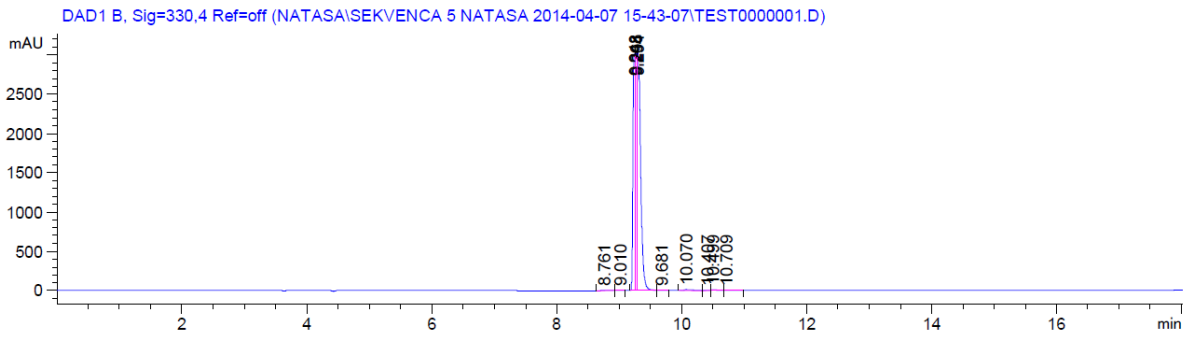


Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.664	BV	0.0593	10.76119	2.49458	0.0990
2	7.800	VV	0.0692	1.07836e4	2481.38989	99.2399
3	8.021	VB	0.0886	52.75755	7.78067	0.4855
4	8.491	BB	0.0587	9.81622	2.32569	0.0903
5	9.266	BB	0.0631	9.26213	2.07373	0.0852

Totals : 1.08862e4 2496.06456

Method B



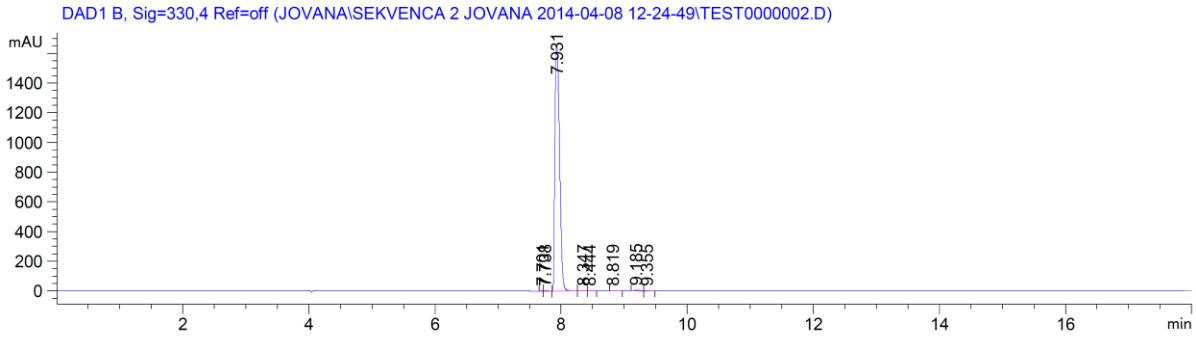
Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.761	BV	0.0946	19.05150	2.55077	0.0774
2	9.010	VB	0.0682	7.01805	1.23590	0.0285
3	9.248	BV	0.0297	6764.55176	3016.98877	27.4790
4	9.268	VV	0.0233	5699.56543	3045.93115	23.1528
5	9.294	VB	0.0462	1.18809e4	3102.94507	48.2629
6	9.681	BB	0.0669	13.16222	2.38397	0.0535
7	10.070	BB	0.1300	115.71299	11.48639	0.4701
8	10.407	BV	0.0705	31.74297	6.22313	0.1289
9	10.499	VV	0.0931	65.87598	9.30566	0.2676
10	10.709	VB	0.1154	19.51246	1.99891	0.0793

Totals : 2.46171e4 9201.04973

Compound: 69

Method A

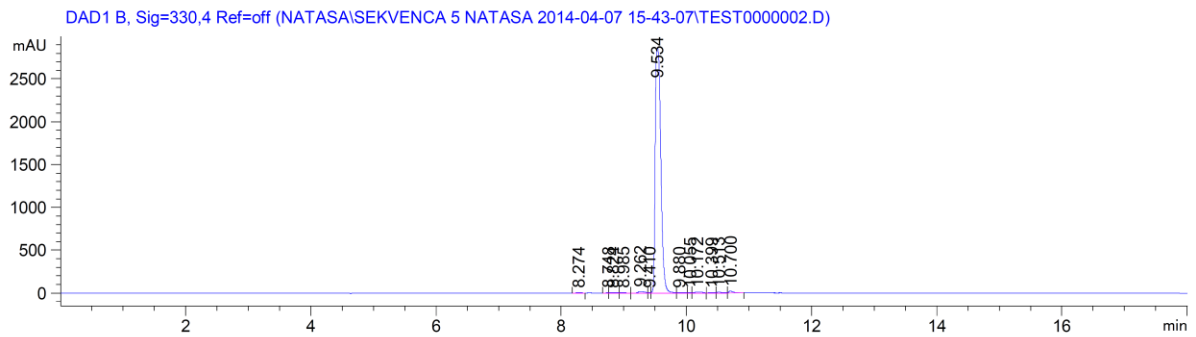


Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.701	BV	0.0447	13.64141	4.71799	0.1583
2	7.738	VB	0.0607	21.09239	4.58670	0.2447
3	7.931	BB	0.0838	8505.27539	1659.32520	98.6688
4	8.347	BV	0.0746	13.74878	2.19445	0.1595
5	8.444	VV	0.0616	9.41721	1.95742	0.1092
6	8.819	BB	0.0575	10.00354	2.40503	0.1161
7	9.185	BB	0.0841	37.60665	6.44058	0.4363
8	9.355	BB	0.0605	9.23786	2.03373	0.1072

Totals : 8620.02324 1683.66109

Method B



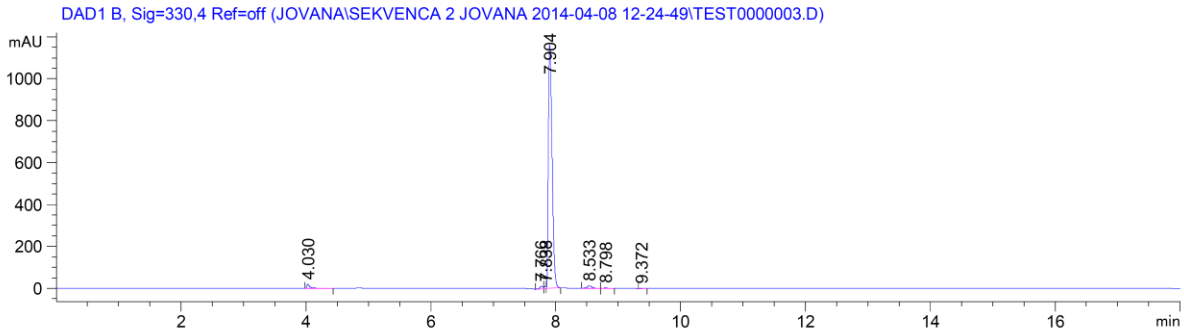
Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.274	BV	0.0817	40.39205	7.69858	0.2205
2	8.748	BV	0.0436	8.25339	2.56424	0.0451
3	8.824	VV	0.0934	23.71711	3.12892	0.1295
4	8.985	VB	0.0802	15.04890	2.23064	0.0822
5	9.262	BV	0.0940	125.29450	18.26360	0.6840
6	9.410	VV	0.0408	17.48903	6.03940	0.0955
7	9.534	VV	0.0759	1.77261e4	2854.50610	96.7743
8	9.880	VV	0.1088	46.52859	5.18057	0.2540
9	10.055	VV	0.0528	20.19332	4.63429	0.1102
10	10.172	VB	0.1224	96.72375	10.31441	0.5281
11	10.399	BV	0.0902	38.41697	6.08354	0.2097
12	10.513	VV	0.0783	56.83020	9.56385	0.3103
13	10.700	VB	0.0669	101.95574	21.67052	0.5566

Totals : 1.83169e4 2951.87866

Compound: 77

Method A

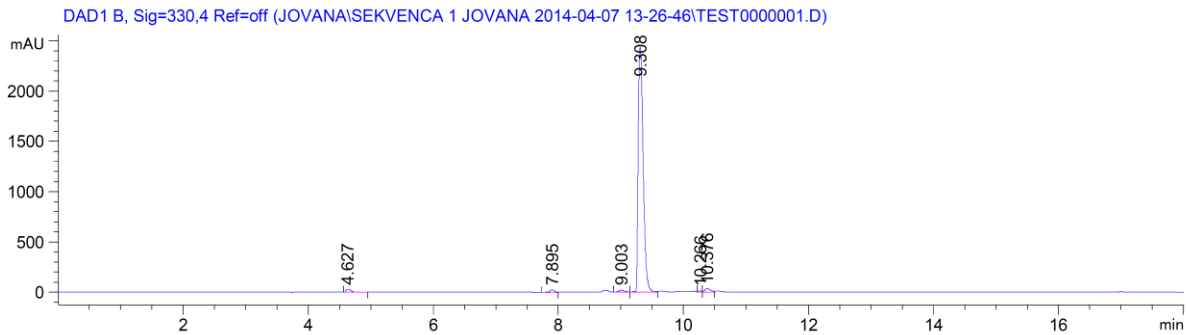


Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.030	BB	0.0529	75.79887	20.60040	1.5039
2	7.766	BV	0.0538	42.28081	11.81159	0.8389
3	7.838	VV	0.0334	22.95304	10.15565	0.4554
4	7.904	VB	0.0659	4816.41211	1161.66919	95.5579
5	8.533	VB	0.0726	64.75261	12.77581	1.2847
6	8.798	BB	0.0669	11.79976	2.55207	0.2341
7	9.372	BB	0.0627	6.31140	1.48253	0.1252

Totals : 5040.30861 1221.04724

Method B



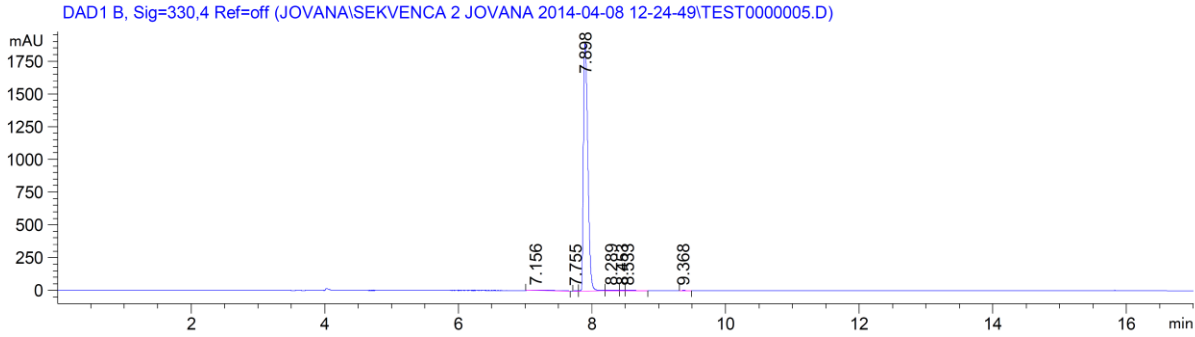
Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.627	BB	0.0893	163.87030	29.28165	1.1589
2	7.895	BV	0.0771	122.72604	24.24271	0.8679
3	9.003	VV	0.1013	122.46661	18.37394	0.8661
4	9.308	VV	0.0876	1.34946e4	2435.65234	95.4309
5	10.266	VV	0.0592	27.63266	6.23845	0.1954
6	10.376	VV	0.0955	209.40958	33.00070	1.4809

Totals : 1.41407e4 2546.78980

Compound: 78

Method A

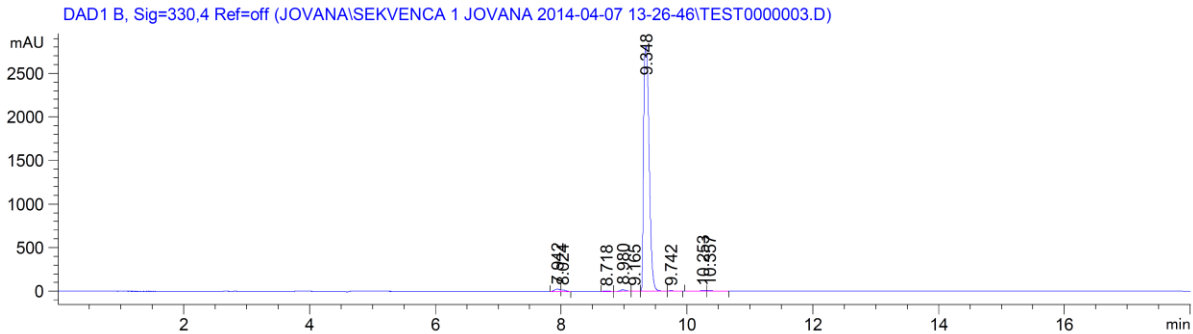


Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.156	BB	0.3858	91.26053	2.77042	1.0340
2	7.755	BV	0.0493	6.75948	2.11363	0.0766
3	7.898	VV	0.0729	8632.54102	1886.03760	97.8049
4	8.289	VV	0.1202	49.92935	5.36075	0.5657
5	8.453	VV	0.0667	15.84448	3.28776	0.1795
6	8.533	VB	0.1086	24.77403	2.97737	0.2807
7	9.368	BB	0.0600	5.17747	1.05109	0.0587

Totals : 8826.28635 1903.59862

Method B



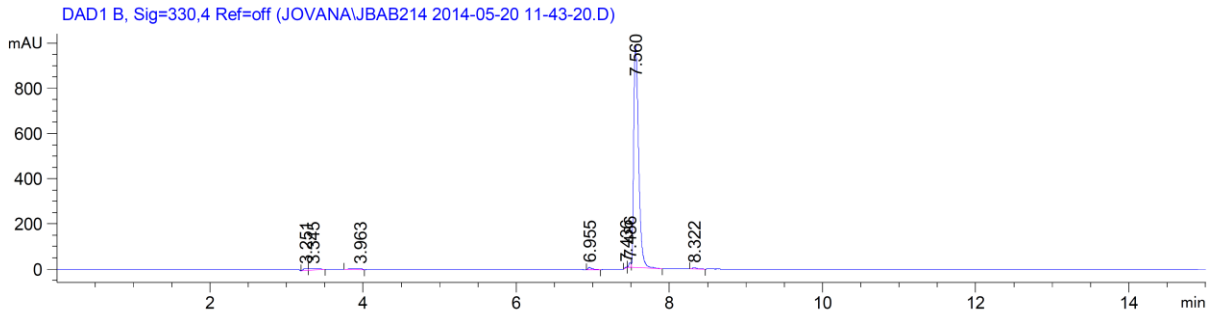
Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.942	BV	0.1004	162.71336	26.96584	0.9199
2	8.024	VV	0.0653	84.80319	18.90702	0.4794
3	8.718	BB	0.0754	13.90129	2.19571	0.0786
4	8.980	BV	0.0867	104.05499	17.92520	0.5883
5	9.165	VV	0.0810	29.02152	5.41988	0.1641
6	9.348	VV	0.0736	1.71820e4	2817.60156	97.1395
7	9.742	VB	0.0755	30.22661	5.46753	0.1709
8	10.253	BV	0.0808	37.31247	5.52375	0.2109
9	10.357	VB	0.0985	43.92458	6.06149	0.2483

Totals : 1.76879e4 2906.06798

Compound: 79

Method A

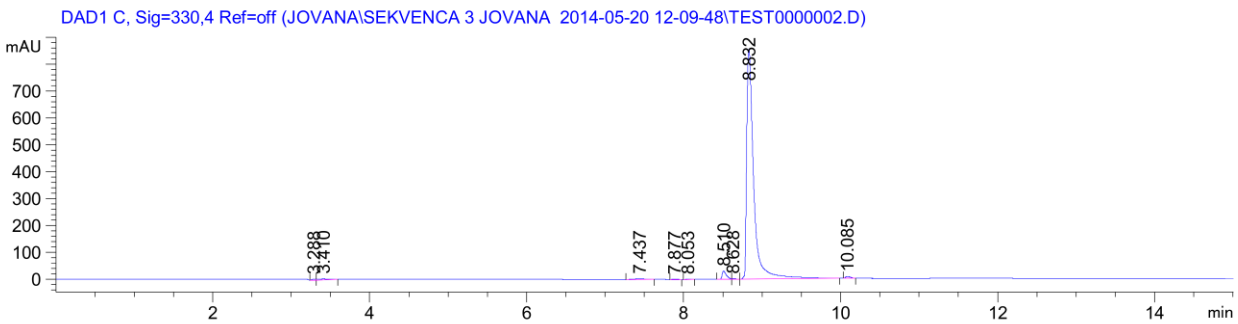


Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.251	BV	0.0665	34.51298	7.97590	0.7566
2	3.345	VB	0.1006	50.06040	5.92239	1.0974
3	3.963	BB	0.1056	30.52218	3.40578	0.6691
4	6.955	BB	0.0528	35.34972	9.86435	0.7749
5	7.436	BB	0.0289	7.02193	4.01750	0.1539
6	7.486	BV	0.0321	40.06248	20.19895	0.8782
7	7.560	VB	0.0684	4340.98877	985.48102	95.1587
8	8.322	BB	0.0620	23.32165	5.92072	0.5112

Totals : 4561.84010 1042.78661

Method B



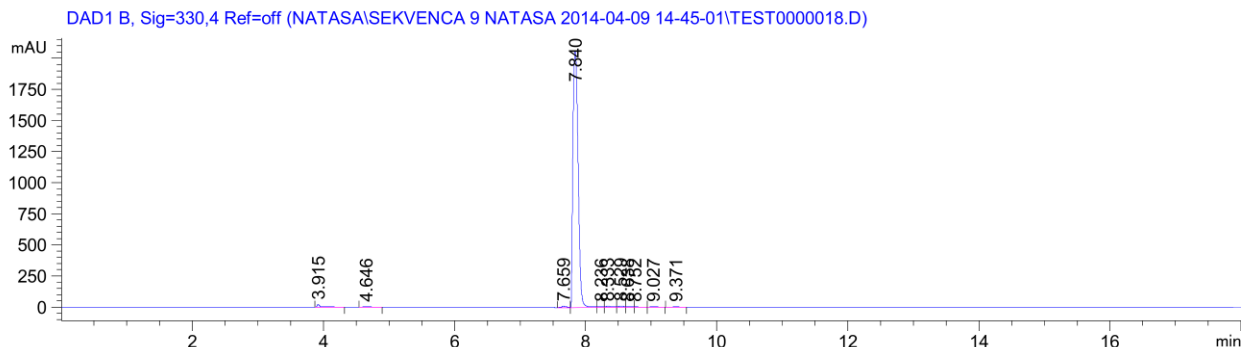
Signal 3: DAD1 C, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.288	BV	0.0489	11.79173	3.78122	0.2134
2	3.410	VB	0.1180	33.03009	3.33760	0.5977
3	7.437	BB	0.1007	31.92348	3.83071	0.5777
4	7.877	BB	0.0480	5.41210	1.57917	0.0979
5	8.053	BV	0.0565	5.53127	1.40251	0.1001
6	8.510	BV	0.0549	114.02178	30.65328	2.0632
7	8.628	VV	0.0467	7.66824	2.25515	0.1388
8	8.832	VB	0.0925	5286.91455	856.47974	95.6678
9	10.085	BV	0.0678	30.03268	6.75808	0.5434

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
Totals :				5526.32593	910.07746	

Compound: 80

Method A

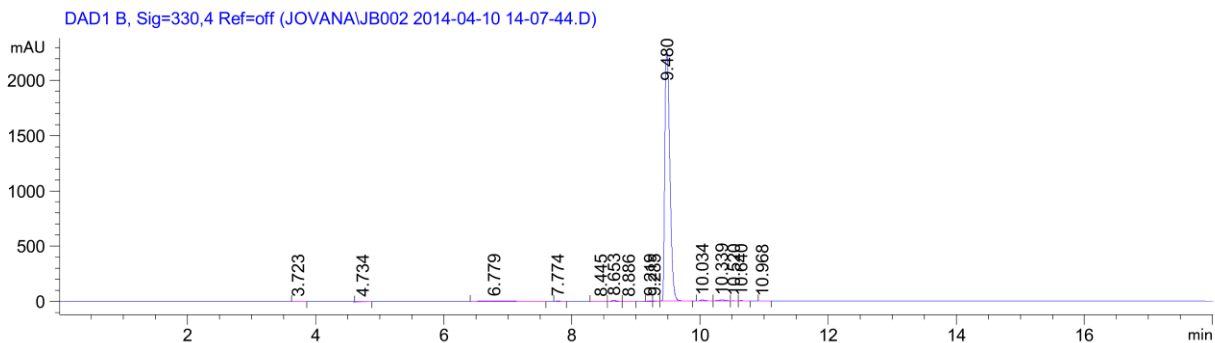


Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.915	BB	0.0496	73.44587	21.35410	0.6299
2	4.646	BB	0.1110	11.15434	1.18859	0.0957
3	7.659	BV	0.0687	53.74442	11.15018	0.4609
4	7.840	VV	0.0904	1.13059e4	2064.86304	96.9644
5	8.236	VV	0.0785	28.29338	4.28767	0.2427
6	8.333	VV	0.0923	63.53181	9.11991	0.5449
7	8.529	VV	0.0775	52.08415	8.93610	0.4467
8	8.638	VV	0.0723	28.73580	5.38145	0.2465
9	8.752	VB	0.0617	8.00376	1.57731	0.0686
10	9.027	BB	0.0800	20.17866	3.46115	0.1731
11	9.371	BB	0.1056	14.77293	1.65597	0.1267

Totals : 1.16599e4 2132.97547

Method B



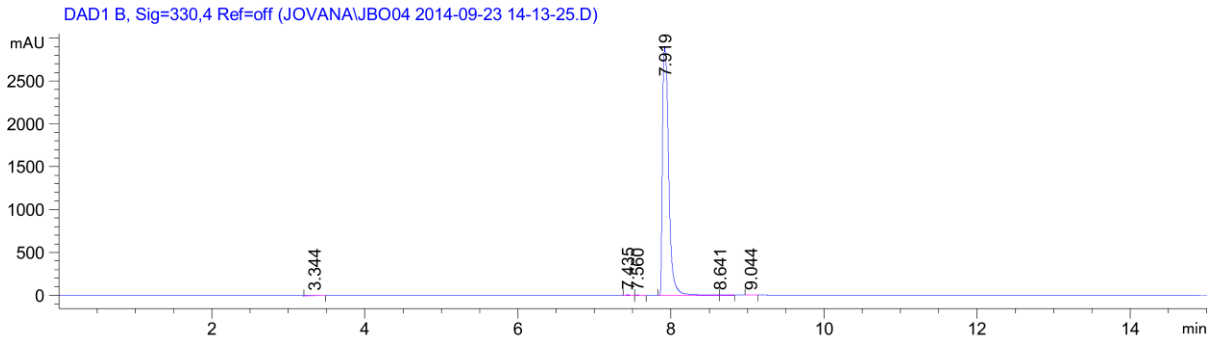
Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.723	BB	0.1068	12.18498	1.35710	0.0947
2	4.734	BB	0.1445	36.00034	2.93739	0.2797
3	6.779	BB	0.4379	136.24687	3.64254	1.0584
4	7.774	BB	0.0644	23.75512	5.61118	0.1845
5	8.445	BV	0.0714	6.70405	1.14292	0.0521
6	8.653	VV	0.0734	48.15835	10.14406	0.3741
7	8.886	VB	0.0648	5.42541	1.01658	0.0421
8	9.219	BV	0.0584	16.19058	3.71369	0.1258
9	9.285	VV	0.0581	13.30906	2.97789	0.1034
10	9.480	VB	0.0862	1.24090e4	2271.90967	96.3937
11	10.034	BV	0.0854	52.23092	7.97832	0.4057
12	10.339	VV	0.1073	80.86919	10.06125	0.6282
13	10.520	VB	0.0615	9.74291	2.18694	0.0757
14	10.640	BB	0.0649	13.51318	3.06635	0.1050
15	10.968	BB	0.0661	9.91450	2.19919	0.0770

Totals : 1.28732e4 2329.94506

Compound: 81

Method A

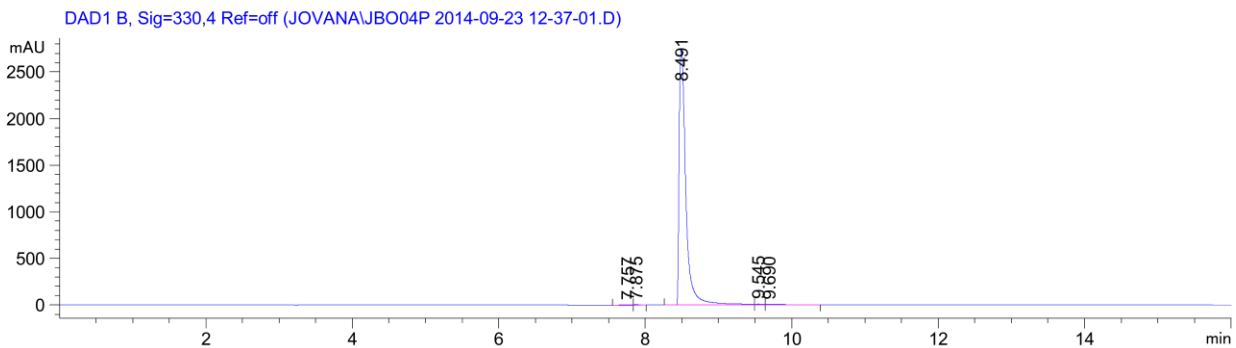


Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.344	BB	0.1500	48.44423	3.80598	0.2897
2	7.435	BB	0.0513	37.27672	11.20887	0.2229
3	7.560	BB	0.0408	20.88432	7.90868	0.1249
4	7.919	VV	0.0690	1.65873e4	2912.21582	99.1954
5	8.641	VV	0.0937	22.03576	2.78979	0.1318
6	9.044	BB	0.0526	5.90192	1.38880	0.0353

Totals : 1.67219e4 2939.31794

Method B



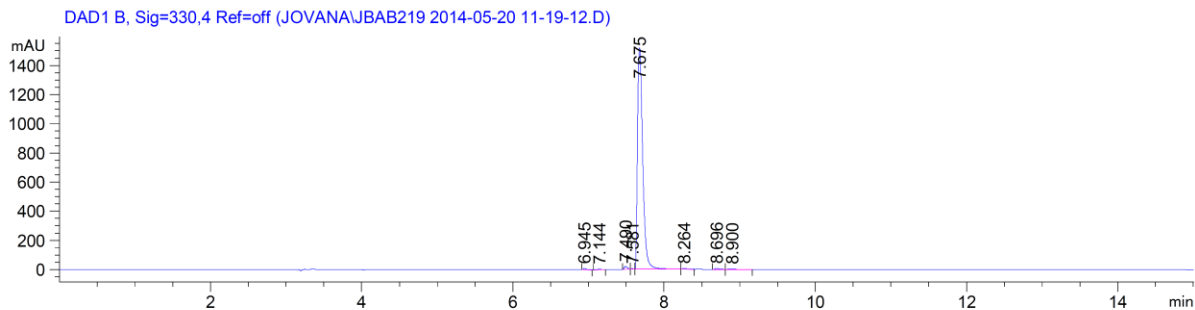
Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.757	BV	0.0915	39.64389	5.40691	0.2216
2	7.875	VB	0.0501	27.98556	8.13536	0.1565
3	8.491	BV	0.0854	1.76395e4	2729.84692	98.6211
4	9.545	VV	0.1009	67.96310	8.97417	0.3800
5	9.690	VB	0.1992	111.04637	6.60233	0.6209

Totals : 1.78862e4 2758.96570

Compound: 82

Method A

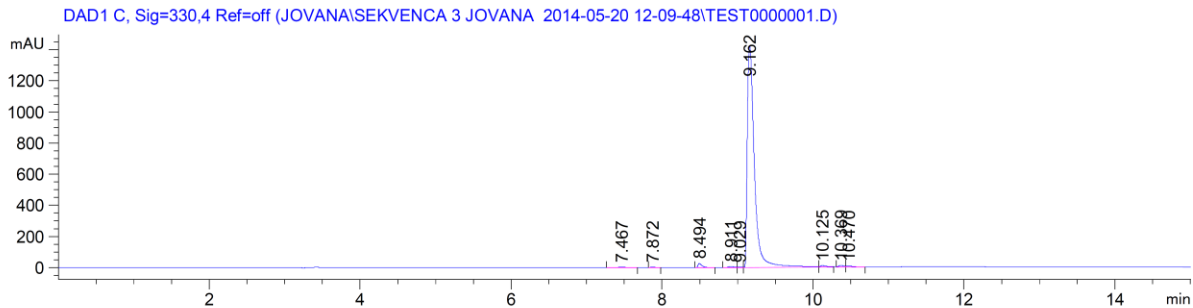


Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.945	BB	0.0445	25.40839	8.71191	0.3405
2	7.144	BB	0.0443	12.88218	4.51760	0.1726
3	7.490	BB	0.0462	58.48474	20.24730	0.7837
4	7.581	BV	0.0364	6.94268	3.06349	0.0930
5	7.675	VV	0.0749	7282.45020	1520.34558	97.5804
6	8.264	VB	0.0600	25.62524	6.17003	0.3434
7	8.696	BV	0.0686	28.11806	6.06860	0.3768
8	8.900	VB	0.0849	23.11784	4.00400	0.3098

Totals : 7463.02933 1573.12853

Method B



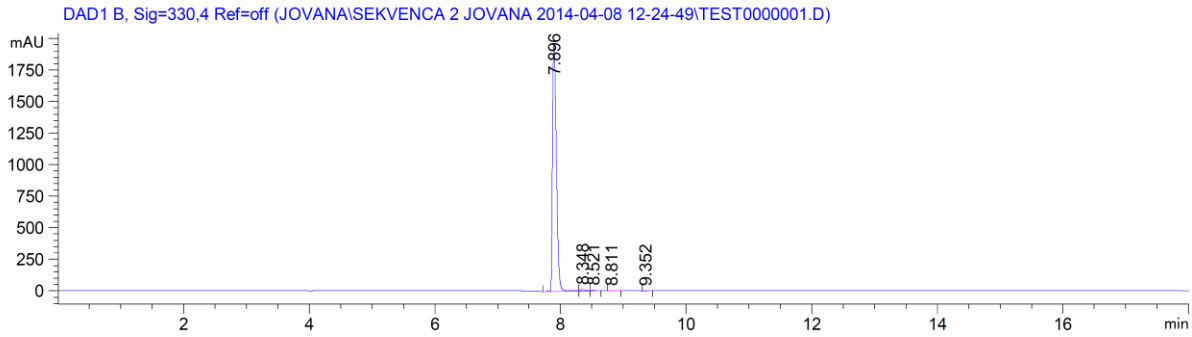
Signal 3: DAD1 C, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.467	BB	0.1191	35.26105	3.68767	0.3643
2	7.872	BB	0.0519	18.53819	5.42384	0.1915
3	8.494	BB	0.0551	94.72851	25.35965	0.9788
4	8.911	BV	0.0644	30.60301	6.74595	0.3162
5	9.029	VV	0.0491	6.23119	1.62870	0.0644
6	9.162	VV	0.1004	9335.27051	1425.76025	96.4552
7	10.125	VV	0.0902	65.13804	9.59330	0.6730
8	10.369	VV	0.0734	48.98382	9.69941	0.5061
9	10.470	VB	0.0899	43.59158	7.22386	0.4504

Totals : 9678.34589 1495.12265

Compound: 84

Method A

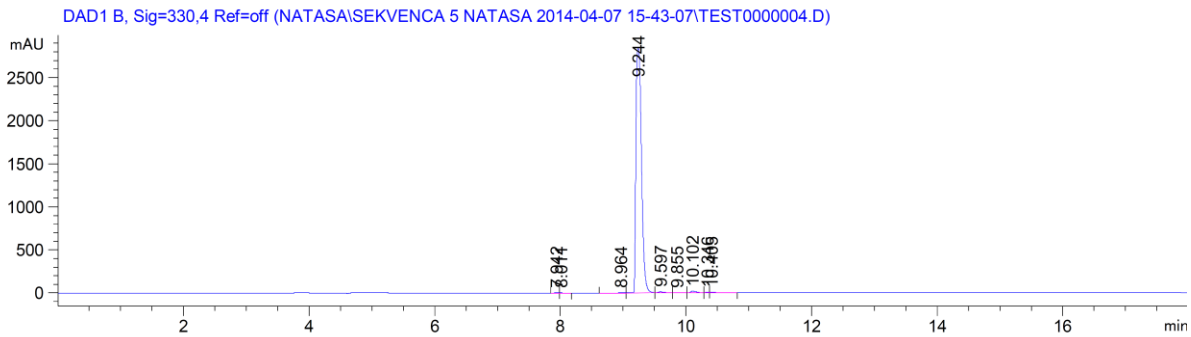


Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.896	BV	0.0683	8401.05957	1950.32312	98.7377
2	8.348	VV	0.0744	65.25713	12.01343	0.7670
3	8.521	VB	0.0690	23.88355	4.80159	0.2807
4	8.811	BB	0.0612	13.20165	3.06863	0.1552
5	9.352	BB	0.0580	5.06253	1.07373	0.0595

Totals : 8508.46443 1971.28049

Method B



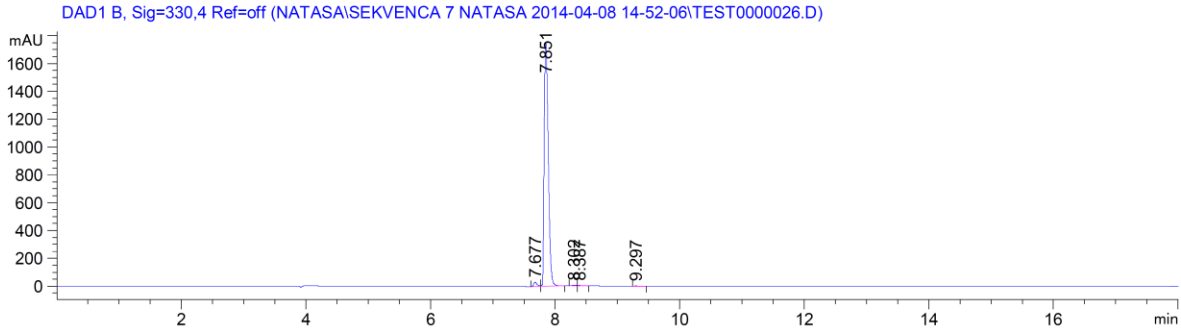
Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.942	BV	0.0666	15.28754	2.82477	0.0861
2	8.011	VB	0.0549	10.16619	2.35343	0.0573
3	8.964	BV	0.0931	16.50475	2.14800	0.0929
4	9.244	VV	0.0735	1.73645e4	2852.34985	97.7883
5	9.597	VV	0.1030	102.36688	13.05850	0.5765
6	9.855	VV	0.1185	26.68129	2.66090	0.1503
7	10.102	VB	0.1021	126.00954	18.83002	0.7096
8	10.346	BV	0.0602	35.32540	9.43586	0.1989
9	10.405	VB	0.0853	60.39959	9.80894	0.3401

Totals : 1.77572e4 2913.47028

Compound: 85

Method A

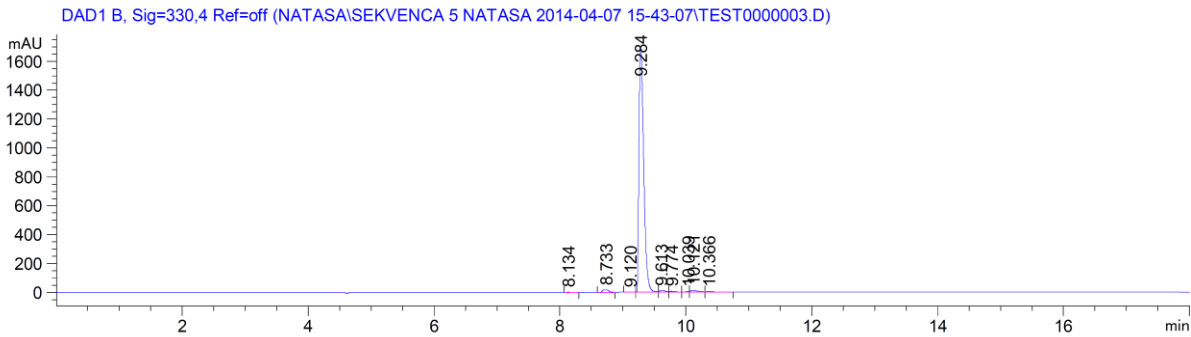


Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.677	BV	0.0621	125.31008	30.73862	1.5370
2	7.851	VB	0.0728	7973.41992	1746.19397	97.7970
3	8.302	VV	0.0637	23.67207	5.49968	0.2903
4	8.387	VB	0.0610	15.28493	3.30129	0.1875
5	9.297	BB	0.0831	15.34058	2.44906	0.1882

Totals : 8153.02758 1788.18262

Method B



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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.134	VB	0.0814	18.67857	2.72858	0.2015
2	8.733	BB	0.0925	127.87912	18.64092	1.3793
3	9.120	VB	0.0841	17.71707	2.54785	0.1911
4	9.284	BV	0.0824	8873.37988	1699.55615	95.7092
5	9.613	VV	0.0752	67.15372	12.38801	0.7243
6	9.774	VB	0.0722	27.64497	5.10566	0.2982
7	10.039	BV	0.0428	12.84184	4.64301	0.1385
8	10.121	VV	0.0995	91.73752	12.30178	0.9895
9	10.366	VB	0.0995	34.15339	4.68503	0.3684

Totals : 9271.18608 1762.59700