Supporting Information

Structure Guided Design, Synthesis, and Biological Evaluation of Novel Benzosuberene Analogues as Inhibitors of Tubulin Polymerization

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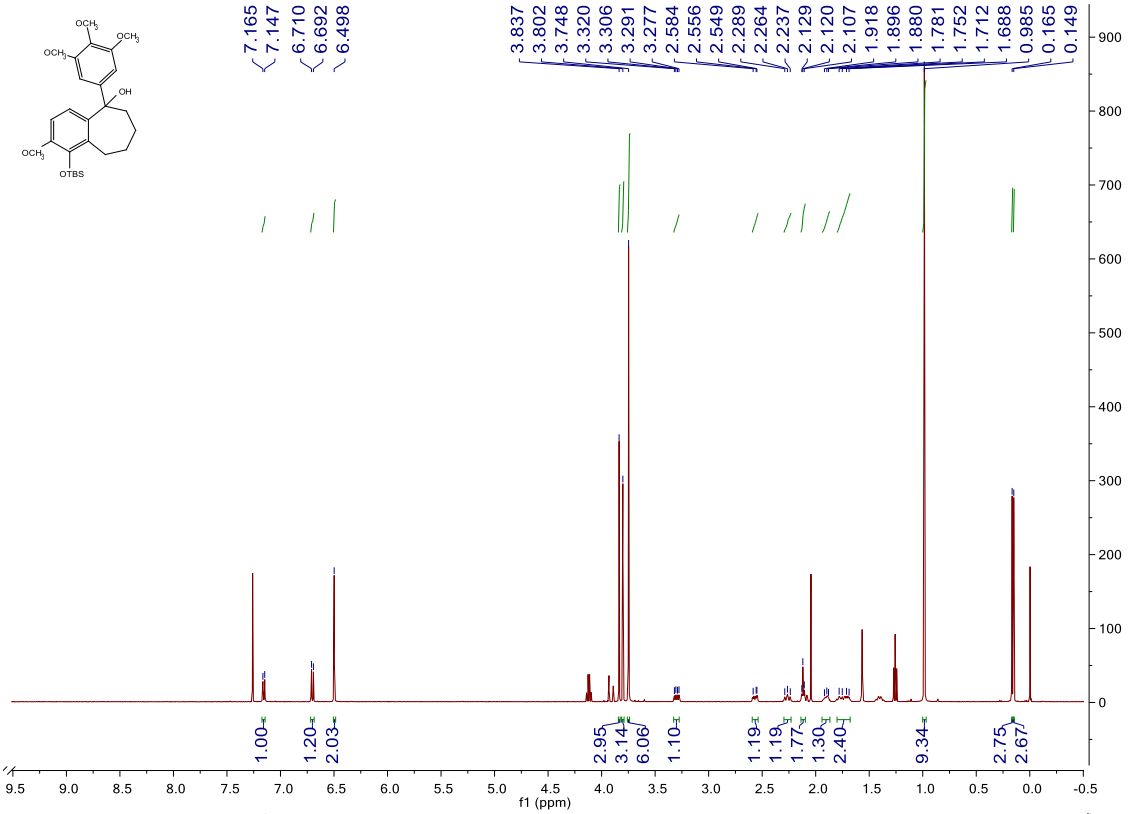
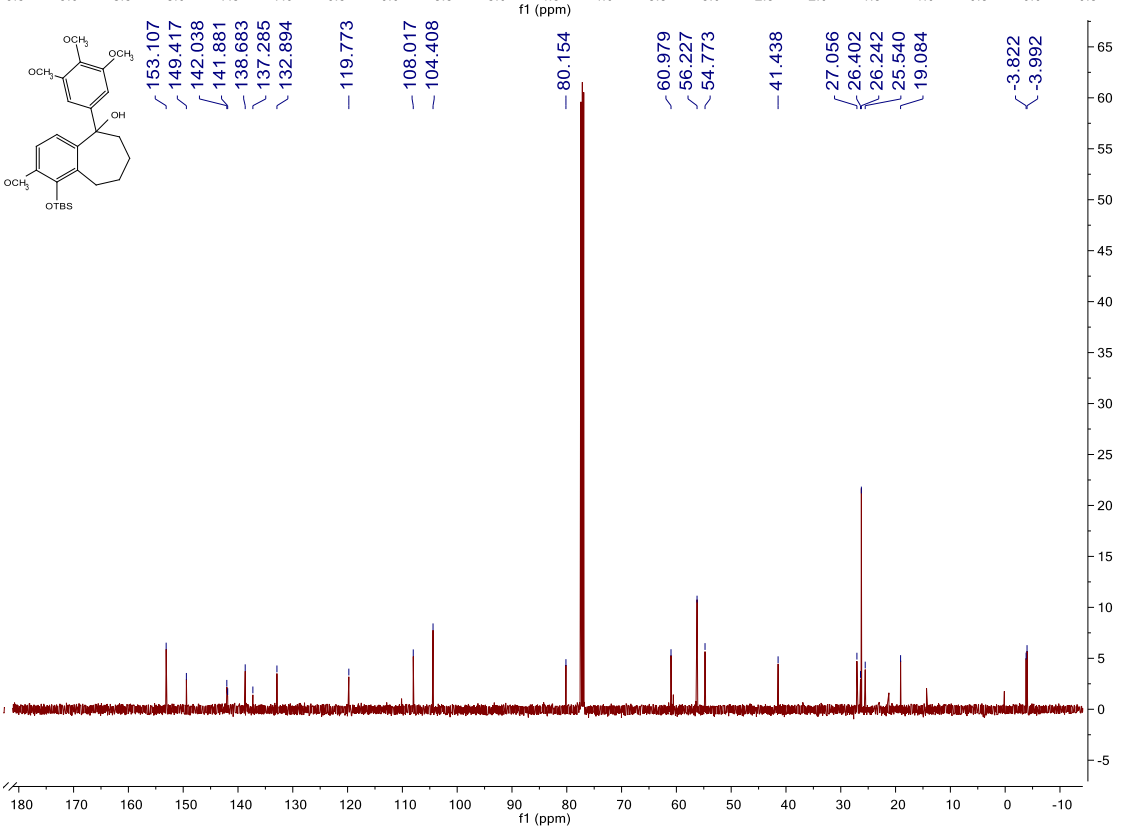
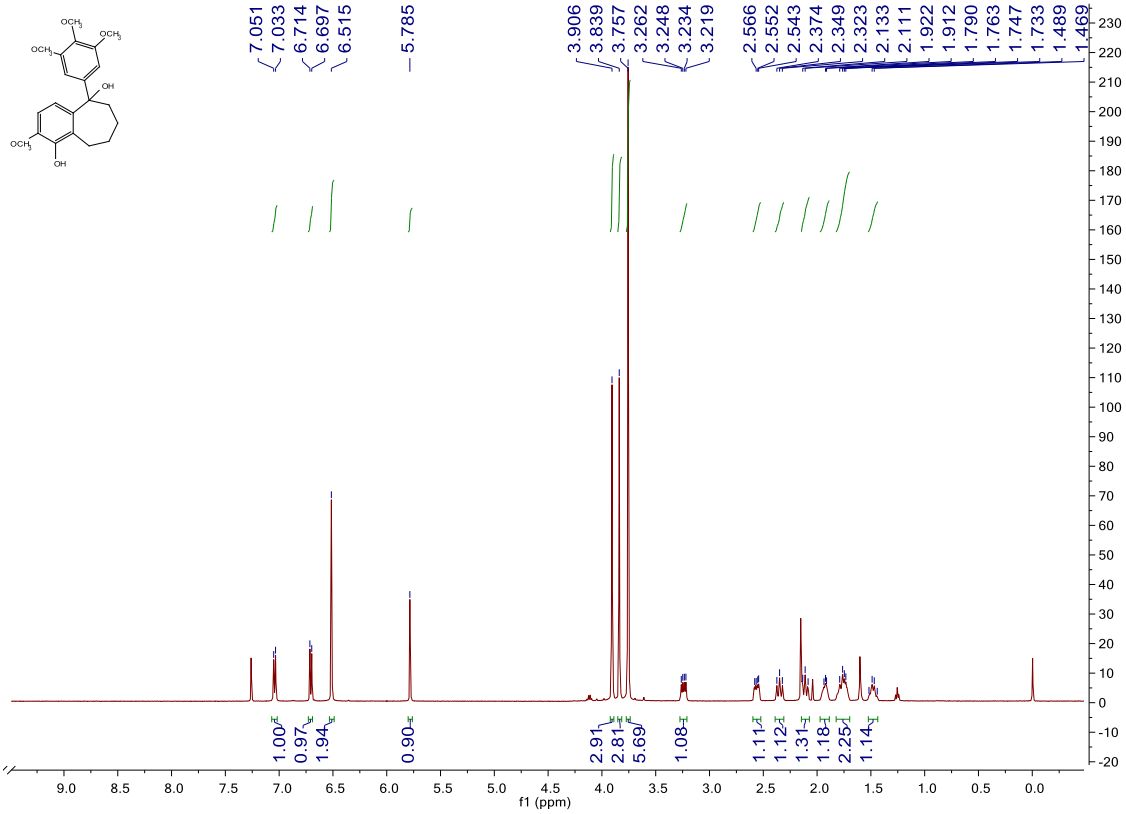
Supporting Information Table of Contents

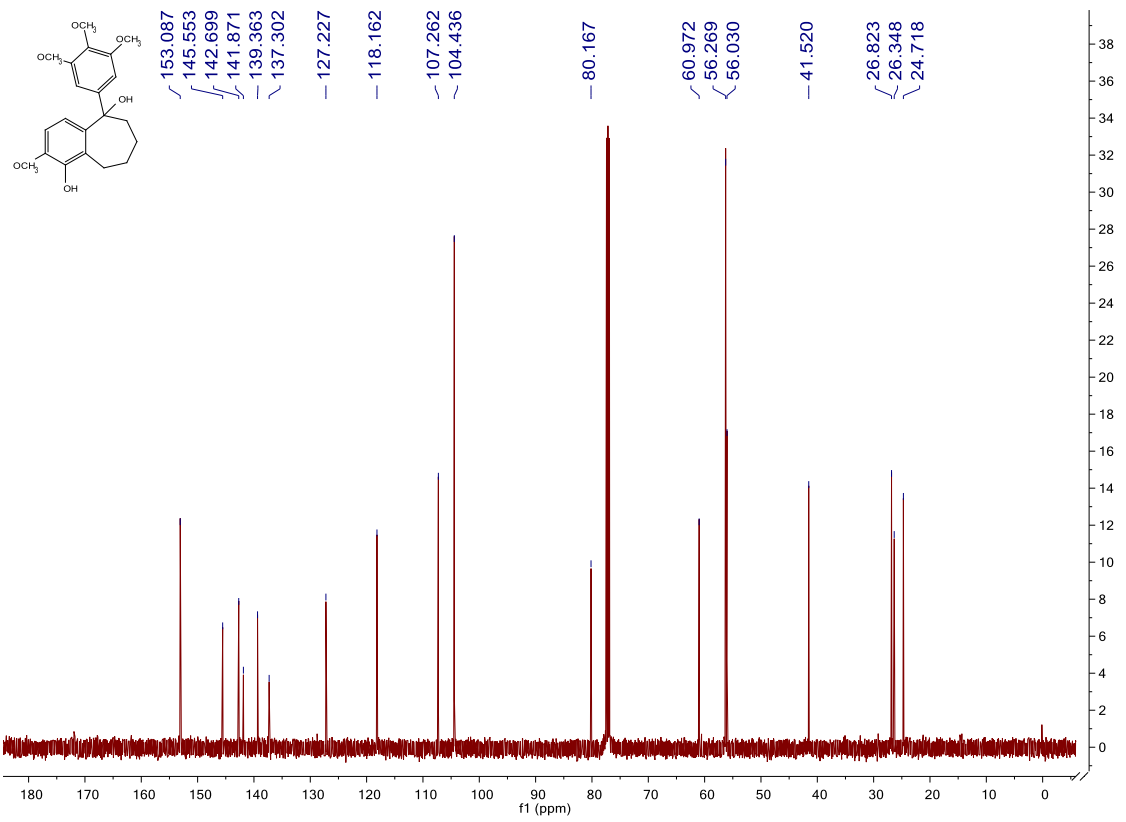
2. 1-((Tert-butyldimethylsilyl)oxy)-2-methoxy-5-(3,4,5-trimethoxyphenyl)-6,7,8,9-tetrahydro-5H-benzo[7]annulen-5-ol





3. 2-Methoxy-5-(3,4,5-trimethoxyphenyl)-6,7,8,9-tetrahydro-5H-benzo[7]annulene-1,5-diol





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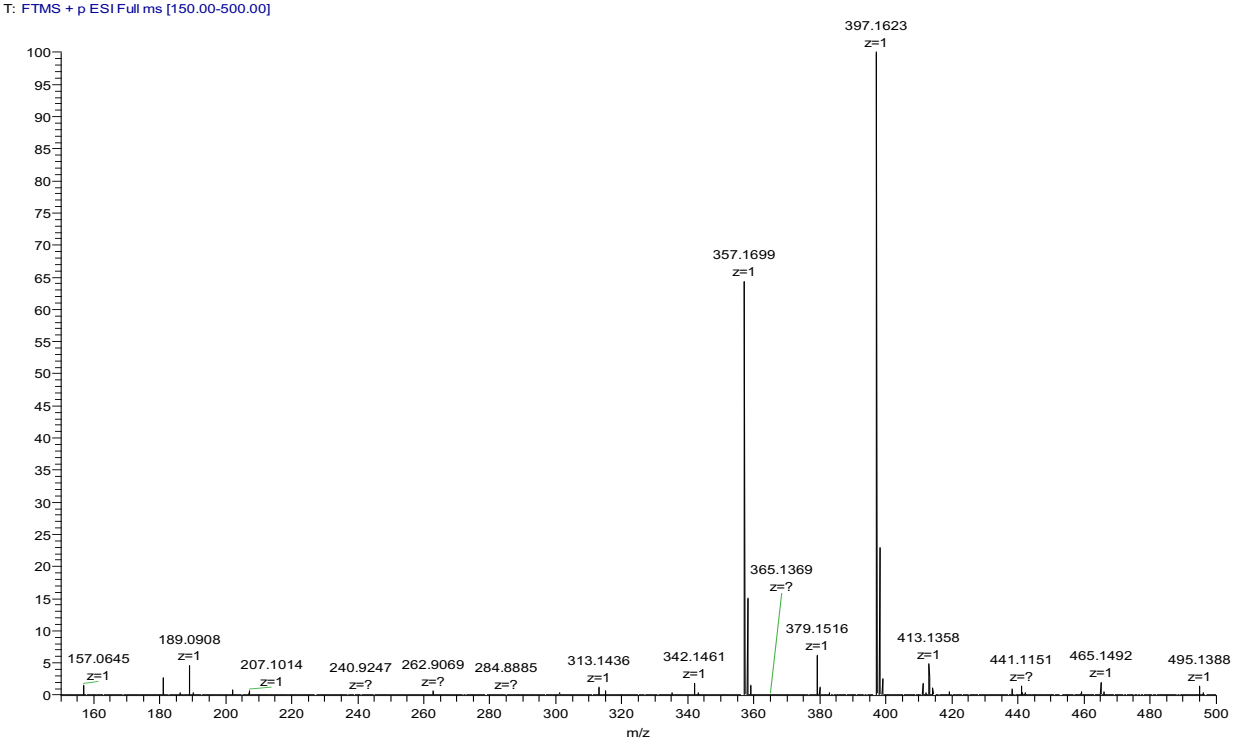
T: FTMS + p ESI Full ms [150.00-500.00]



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Sample Name: KGP423_Concentrated

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Sample Operator : SYSTEM
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                                             Inj Volume : No inj
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Last changed    : 12/2/2015 12:37:42 PM by Eric Lin
Analysis Method : C:\CHEM32\1\METHODS\RT-ACNWASH 2.M
Last changed    : 7/9/2015 2:27:22 PM by Blake
Method Info     : General Column Wash Method

Sample Info     : 20180228

Additional Info : Peak(s) manually integrated
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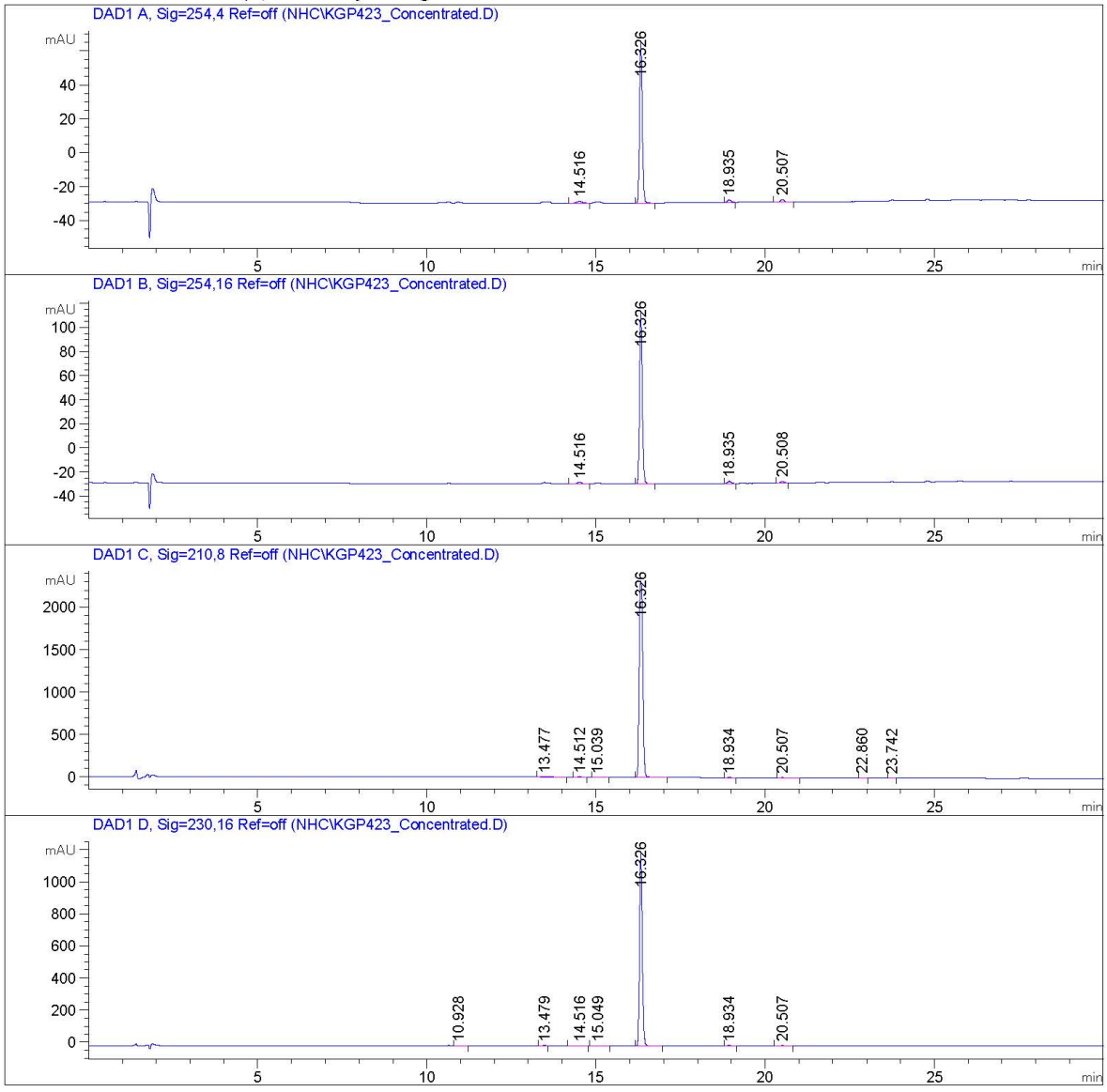

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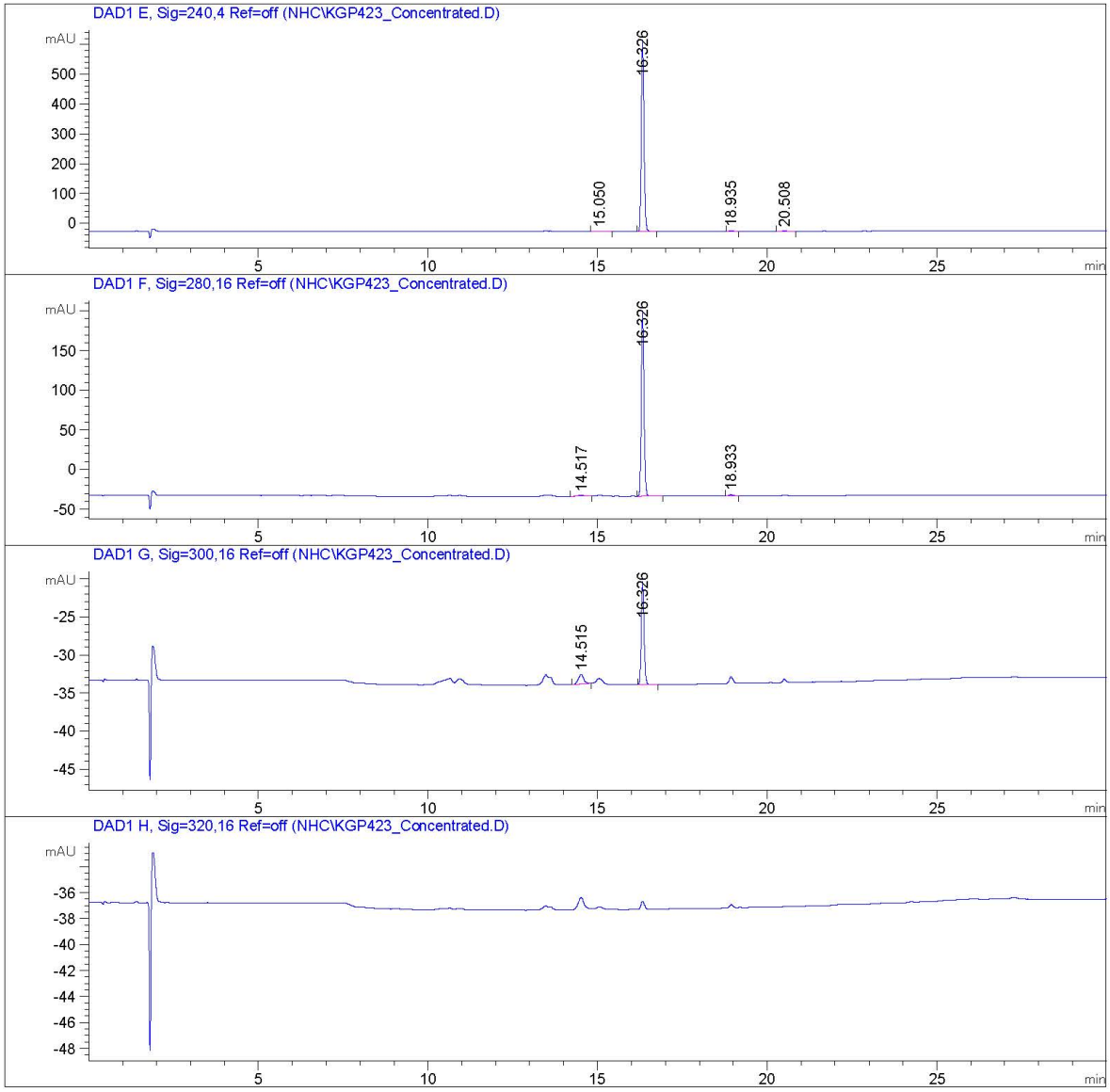

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Area Percent Report

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Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Data File C:\Chem32\1\Data\NHC\KGP423_Concentrated.D
Sample Name: KGP423_Concentrated

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.516	BB	0.1778	12.18939	1.06303	2.0882
2	16.326	BB	0.0890	549.49310	95.70014	94.1337
3	18.935	BB	0.1072	11.11266	1.59757	1.9037
4	20.507	BB	0.1137	10.94184	1.45591	1.8744
Totals :				583.73699	99.81665	

Signal 2: DAD1 B, Sig=254,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.516	BB	0.1777	11.84406	1.03376	1.3883
2	16.326	BB	0.0887	819.88495	143.44756	96.1059
3	18.935	BB	0.1082	12.16774	1.72736	1.4263
4	20.508	BB	0.1051	9.20869	1.35873	1.0794
Totals :				853.10544	147.56741	

Signal 3: DAD1 C, Sig=210,8 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.477	BB	0.2327	39.49652	2.36664	0.2233
2	14.512	BB	0.1700	14.40840	1.33437	0.0815
3	15.039	BB	0.1902	13.94672	1.17727	0.0788
4	16.326	BB	0.1244	1.75529e4	2316.53833	99.2274
5	18.934	BB	0.1035	24.18566	3.64064	0.1367
6	20.507	BB	0.1167	30.13945	3.87693	0.1704
7	22.860	BB	0.0957	7.71542	1.22161	0.0436
8	23.742	BB	0.0942	6.77223	1.12567	0.0383
Totals :				1.76896e4	2331.28146	

Signal 4: DAD1 D, Sig=230,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.928	BB	0.2032	12.69255	1.06344	0.1792
2	13.479	BB	0.1326	9.38471	1.15774	0.1325
3	14.516	BB	0.1772	12.57849	1.11851	0.1776
4	15.049	BB	0.2010	16.94126	1.36305	0.2392
5	16.326	BB	0.0892	6985.17969	1213.45679	98.6394

Data File C:\Chem32\1\Data\NHC\KGP423_Concentrated.D
Sample Name: KGP423_Concentrated

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
6	18.934	BB	0.1110	26.36960	3.62025	0.3724
7	20.507	BB	0.1126	18.38573	2.47801	0.2596
Totals :				7081.53202	1224.25779	

Signal 5: DAD1 E, Sig=240,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.050	BB	0.2001	14.74686	1.16207	0.3973
2	16.326	BB	0.0884	3665.24316	644.11462	98.7488
3	18.935	BB	0.1071	19.65609	2.76107	0.5296
4	20.508	BB	0.1164	12.03636	1.55380	0.3243
Totals :				3711.68247	649.59157	

Signal 6: DAD1 F, Sig=280,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.517	BB	0.1784	12.28676	1.05104	0.9112
2	16.326	BB	0.0881	1323.39343	233.58379	98.1393
3	18.933	BB	0.1149	12.80499	1.68103	0.9496
Totals :				1348.48518	236.31586	

Signal 7: DAD1 G, Sig=300,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.515	BB	0.1796	14.69596	1.26399	15.6681
2	16.326	BB	0.0902	79.09951	13.52710	84.3319
Totals :				93.79547	14.79109	

Signal 8: DAD1 H, Sig=320,16 Ref=off

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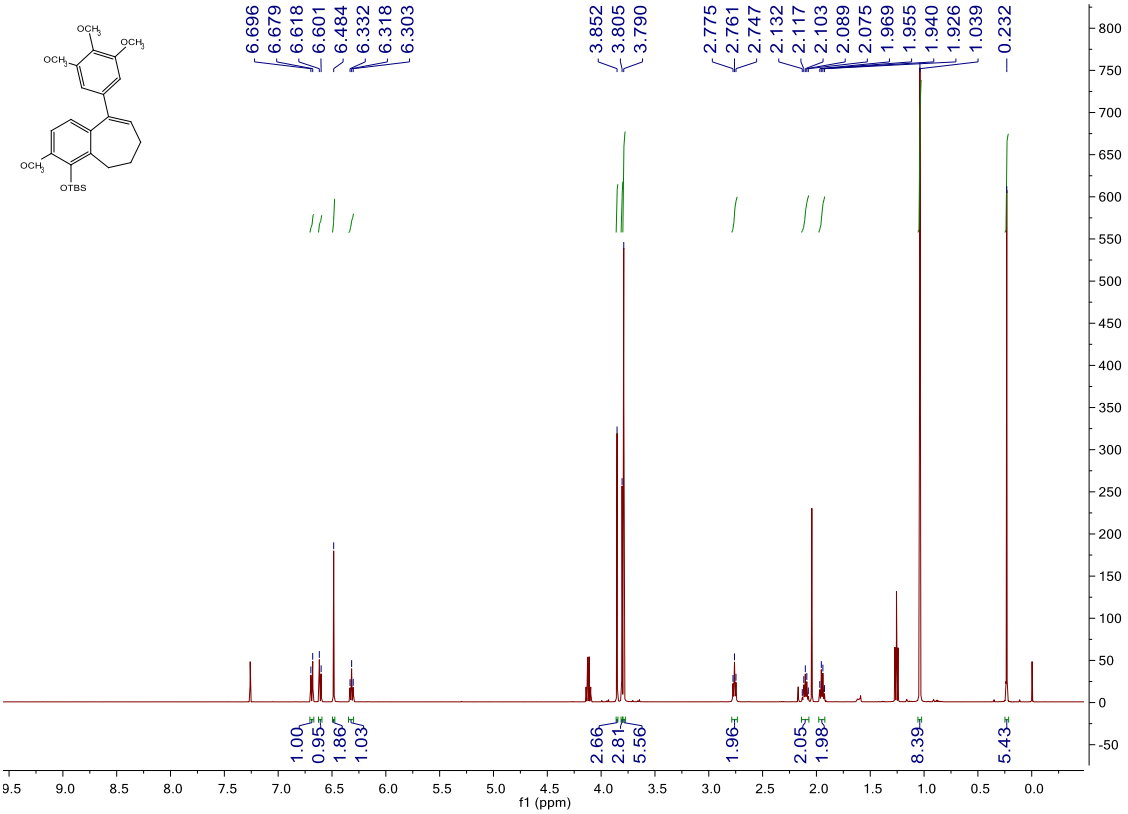
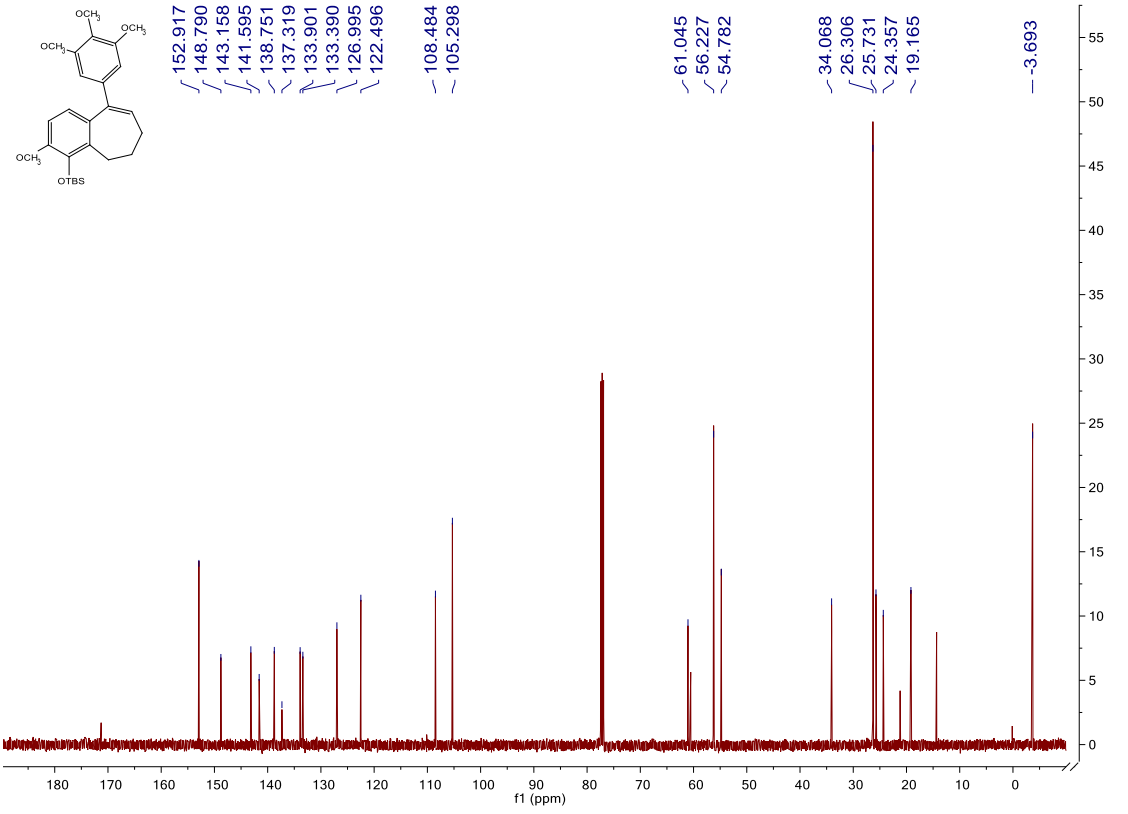
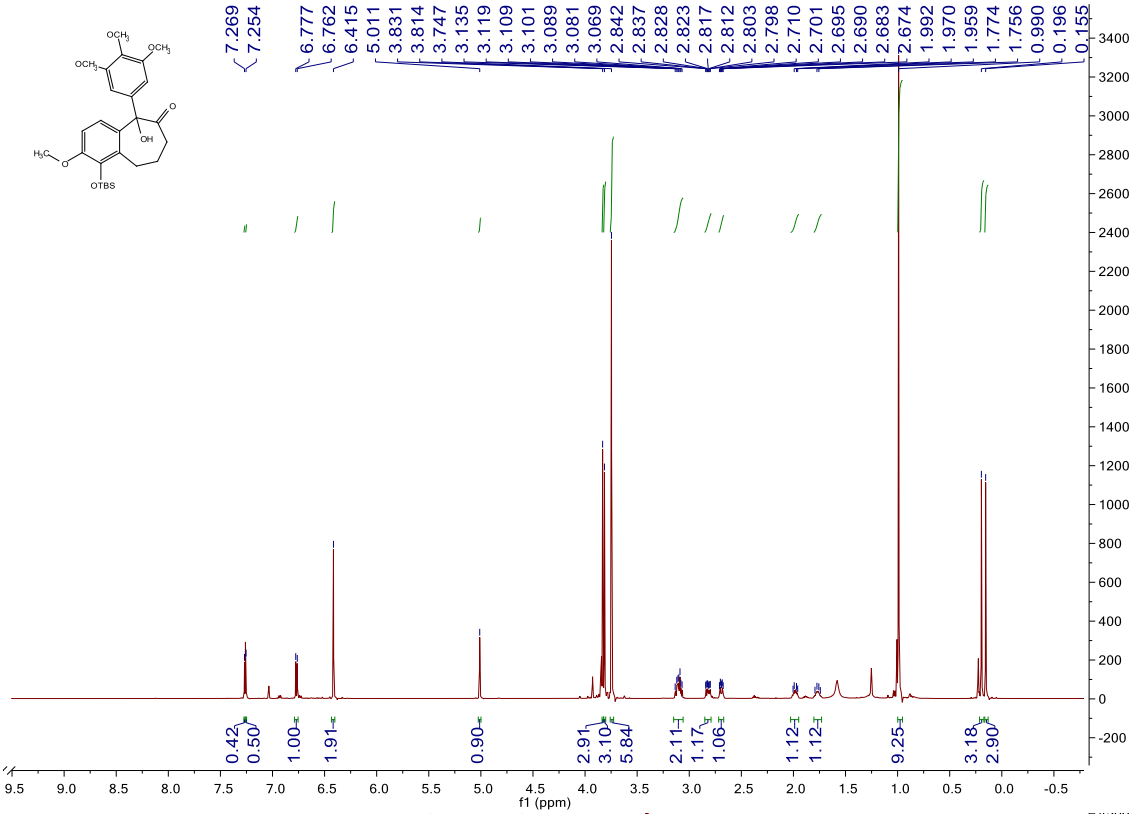
*** End of Report ***

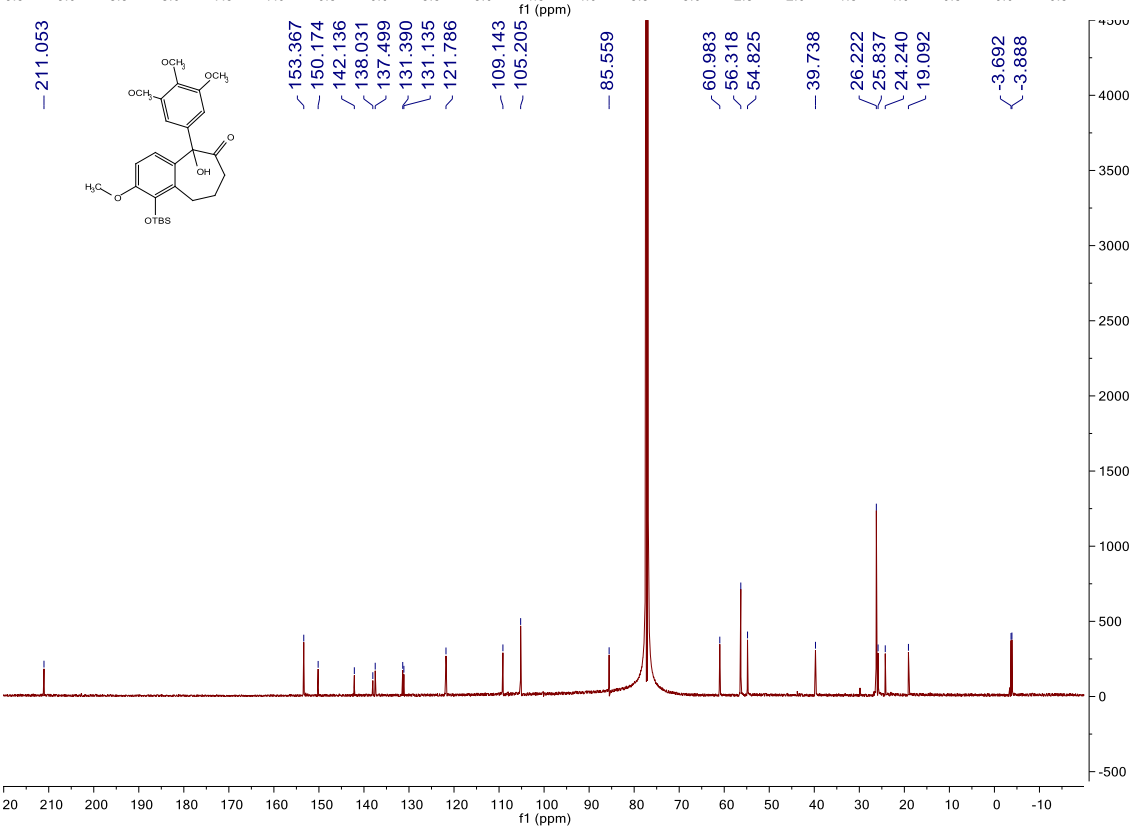
4. Tert-butyl((3-methoxy-9-(3,4,5-trimethoxyphenyl)-6,7-dihydro-5H-benzo[7]annulen-4-yl)oxy)dimethylsilane





5. 1-((tert-butyldimethylsilyl)oxy)-5-hydroxy-2-methoxy-5-(3,4,5-trimethoxyphenyl)-5,7,8,9-tetrahydro-6H-benzo[7]annulen-6-one





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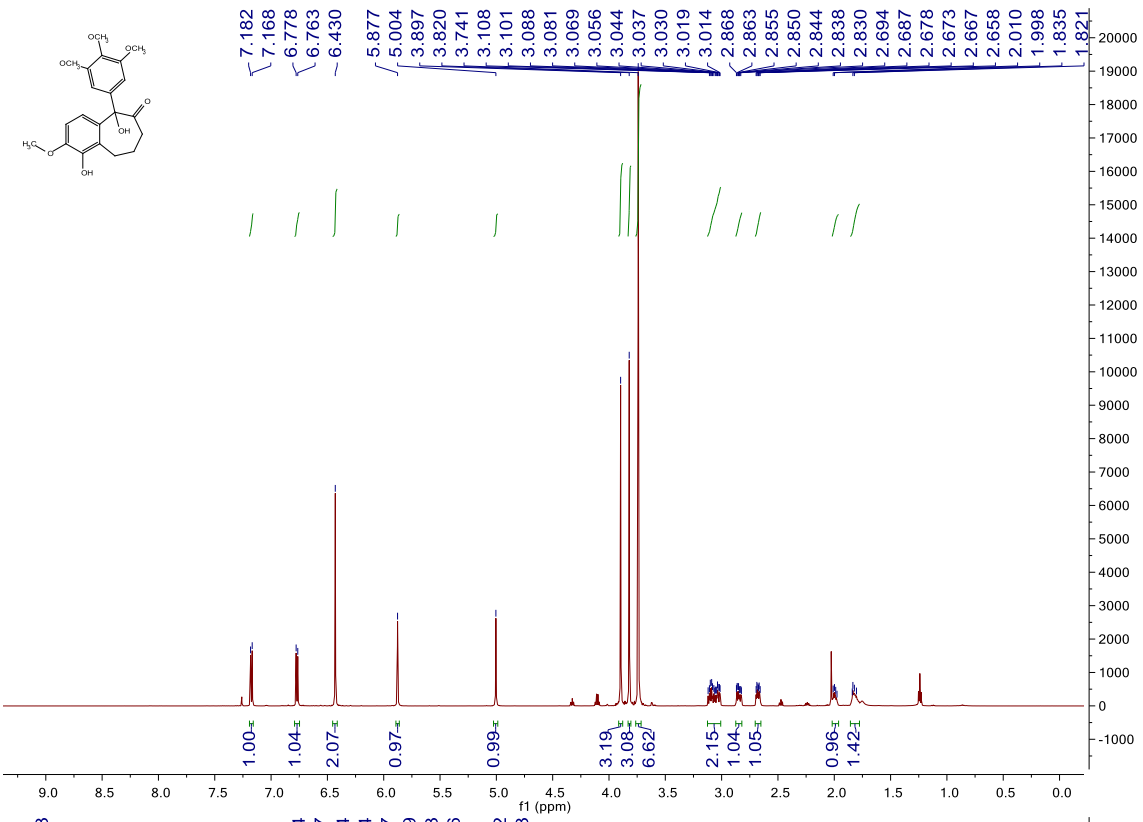

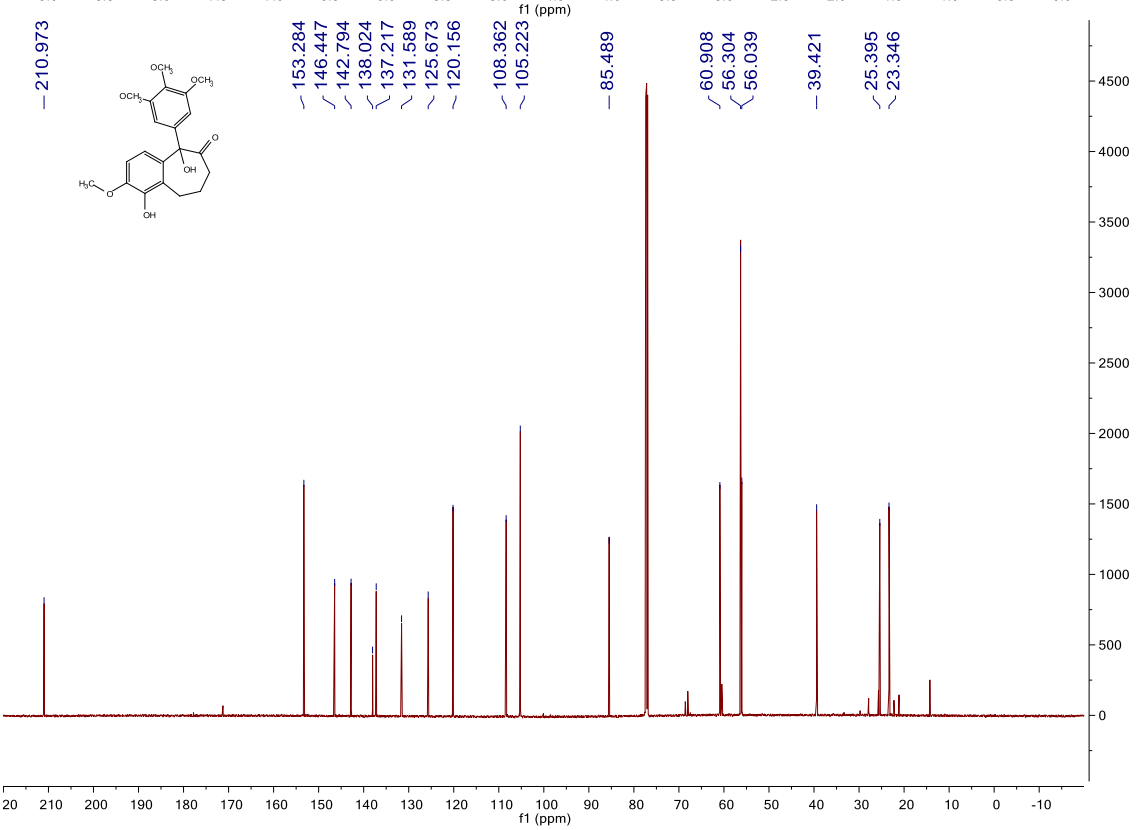

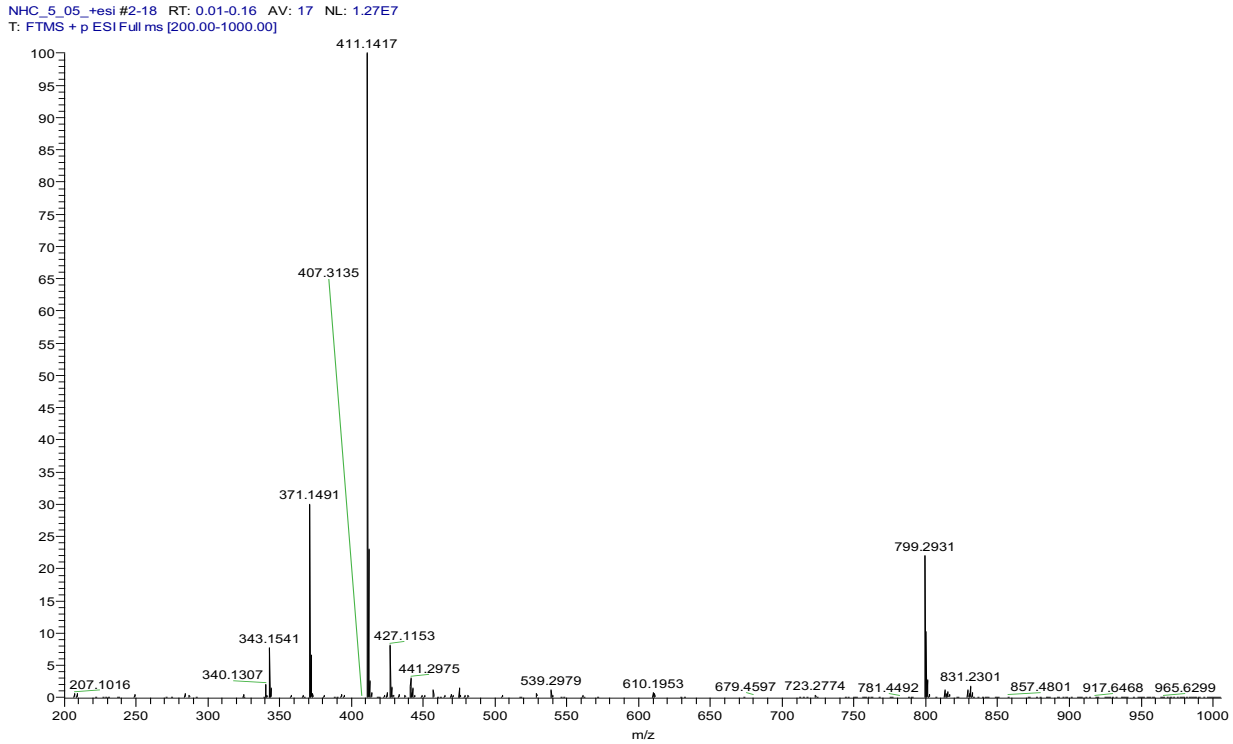
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799.2931
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441.2975
340.1307
207.1016
539.2979
610.1953
679.4597
723.2774
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857.4801
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Data File C:\Chem32\1\Data\NHC\NHC_5_18_sample.D
Sample Name: NHC_5_18_sample

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Sample Operator  : SYSTEM
Acq. Instrument  : 1200 HPLC                    Location :   1
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Last changed     : 12/2/2015 12:37:42 PM by Eric Lin
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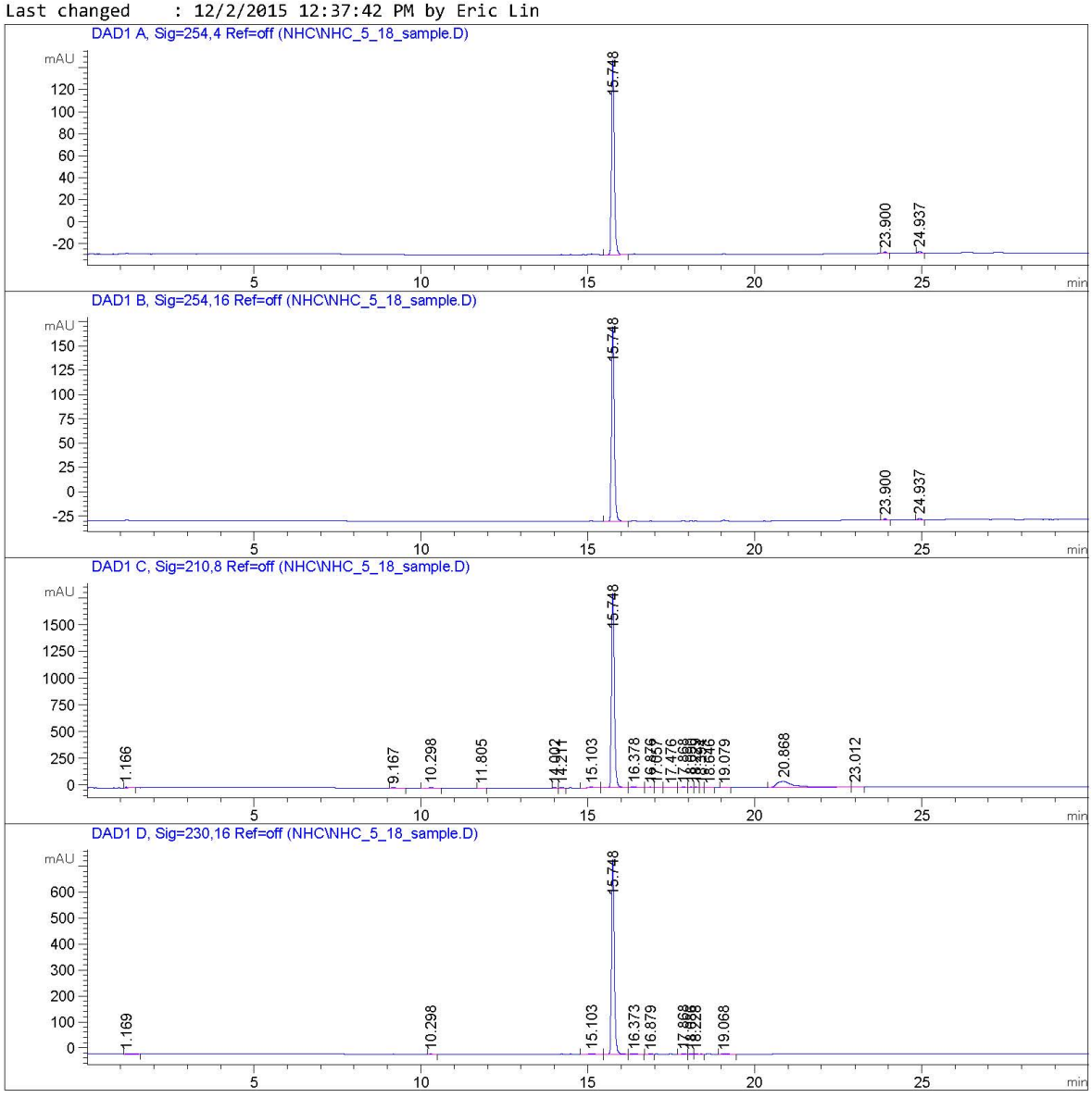

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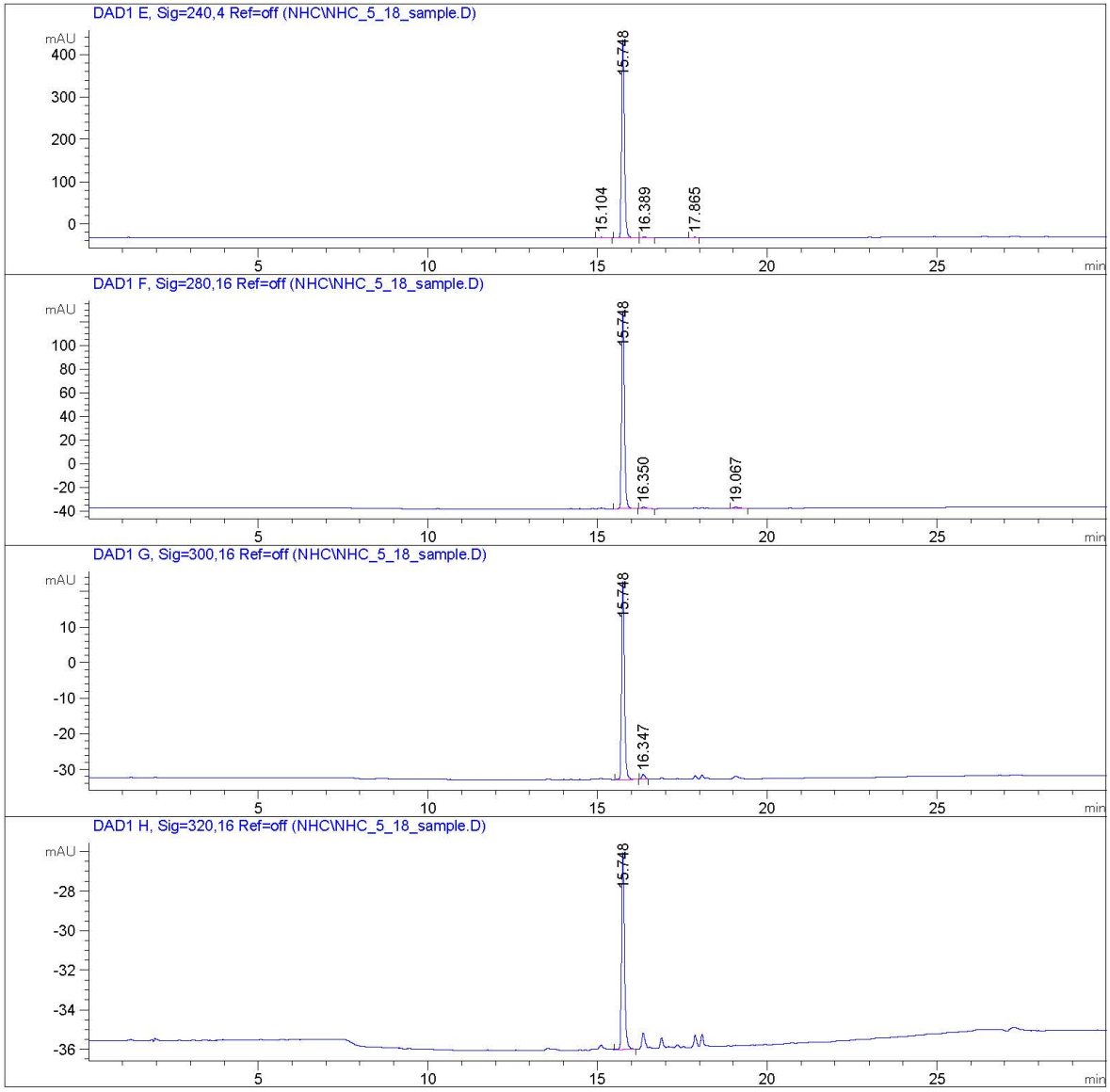
Sample Name: NHC_5_18_sample



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Area Percent Report

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Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Data File C:\Chem32\1\Data\NHC\NHC_5_18_sample.D
Sample Name: NHC_5_18_sample

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.748	BB	0.0855	997.10504	177.72156	98.4605
2	23.900	BB	0.0910	7.08494	1.19758	0.6996
3	24.937	BB	0.0886	8.50512	1.49063	0.8398
Totals :				1012.69510	180.40977	

Signal 2: DAD1 B, Sig=254,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.748	BB	0.0854	1126.68262	201.02759	98.7568
2	23.900	BB	0.0910	6.48629	1.09726	0.5685
3	24.937	BB	0.0885	7.69665	1.35074	0.6746
Totals :				1140.86556	203.47559	

Signal 3: DAD1 C, Sig=210,8 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.166	BB	0.0835	47.85056	7.80683	0.3566
2	9.167	BB	0.1063	13.97762	1.93481	0.1042
3	10.298	BV	0.0906	33.77399	5.42592	0.2517
4	11.805	BB	0.0789	7.71623	1.47941	0.0575
5	14.002	VB	0.0815	9.81697	1.86147	0.0732
6	14.211	BB	0.0787	13.73305	2.72825	0.1024
7	15.103	BB	0.1282	63.81578	7.14180	0.4756
8	15.748	BV	0.0926	1.07524e4	1827.57117	80.1394
9	16.378	VB	0.1544	92.25219	9.24782	0.6876
10	16.876	BV	0.1043	24.89547	3.52923	0.1856
11	17.057	VV	0.0904	10.56320	1.80182	0.0787
12	17.476	VB	0.1387	17.91890	1.79144	0.1336
13	17.868	BV	0.0974	35.46511	5.64002	0.2643
14	18.090	VV	0.1016	24.55433	3.69338	0.1830
15	18.229	VV	0.0948	21.80468	3.39961	0.1625
16	18.394	VV	0.1012	9.44995	1.35756	0.0704
17	18.646	VB	0.1419	19.23294	1.84058	0.1433
18	19.079	BV	0.1797	16.48769	1.43897	0.1229
19	20.868	BV	0.5854	2181.10962	54.44286	16.2562
20	23.012	VB	0.1443	20.28592	1.93512	0.1512
Totals :				1.34171e4	1946.06806	

Data File C:\Chem32\1\Data\NHC\NHC_5_18_sample.D
Sample Name: NHC_5_18_sample

Signal 4: DAD1 D, Sig=230,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.169	BB	0.0999	10.99118	1.49301	0.2517
2	10.298	BB	0.0763	7.57351	1.51456	0.1735
3	15.103	BB	0.1373	27.71015	2.85272	0.6347
4	15.748	BB	0.0854	4229.88135	754.78497	96.8779
5	16.373	BB	0.1419	30.43041	3.41769	0.6970
6	16.879	BV	0.1020	10.01752	1.46037	0.2294
7	17.868	BV	0.0959	13.96439	2.26496	0.3198
8	18.086	VV	0.0952	10.92282	1.74124	0.2502
9	18.228	VB	0.1007	7.61600	1.10094	0.1744
10	19.068	BB	0.1620	17.09307	1.58321	0.3915
Totals :				4366.20038	772.21368	

Signal 5: DAD1 E, Sig=240,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.104	BB	0.1199	12.98084	1.57981	0.4875
2	15.748	BB	0.0852	2626.94897	469.82678	98.6648
3	16.389	BB	0.1377	14.91375	1.74472	0.5601
4	17.865	BV	0.0941	7.65627	1.23852	0.2876
Totals :				2662.49984	474.38983	

Signal 6: DAD1 F, Sig=280,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.748	BB	0.0851	937.63831	168.07391	97.4011
2	16.350	BB	0.1267	11.80592	1.51851	1.2264
3	19.067	BB	0.1521	13.21233	1.28328	1.3725
Totals :				962.65655	170.87570	

Signal 7: DAD1 G, Sig=300,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.748	BB	0.0856	313.61978	55.81817	97.2840
2	16.347	BB	0.0971	8.75556	1.36054	2.7160
Totals :				322.37534	57.17871	

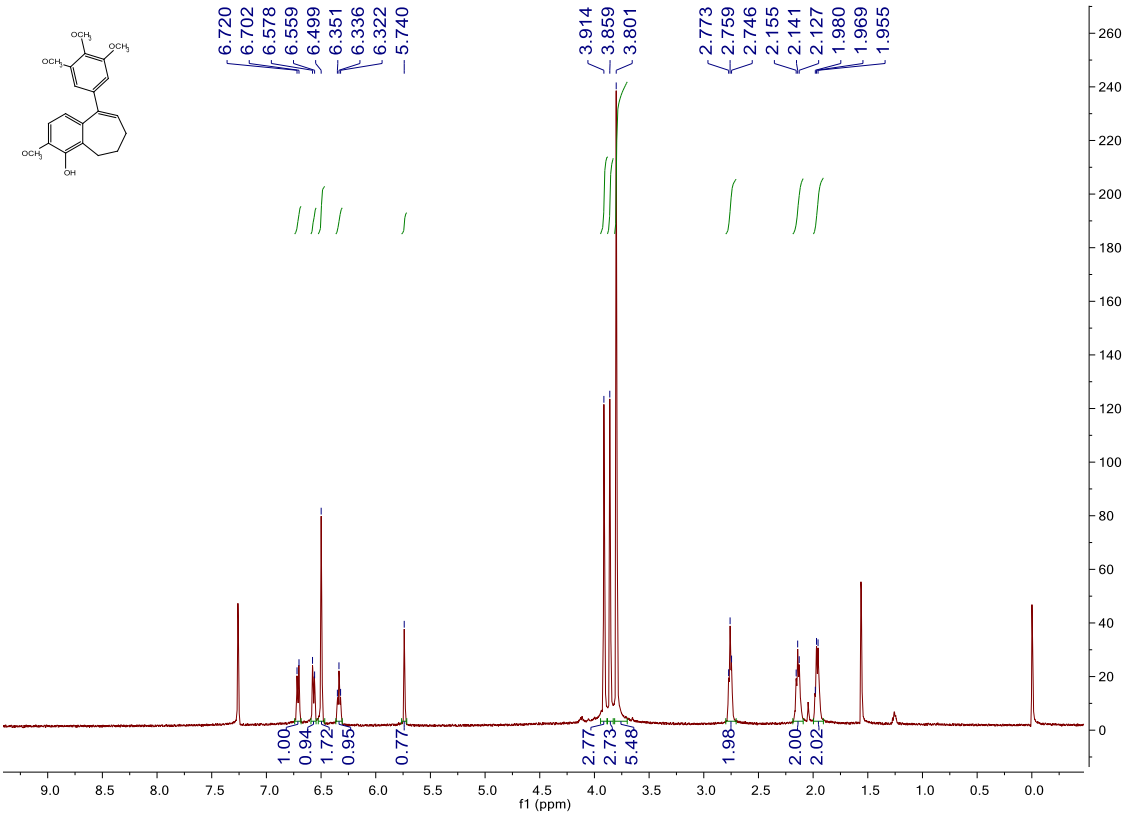
Data File C:\Chem32\1\Data\NHC\NHC_5_18_sample.D
Sample Name: NHC_5_18_sample

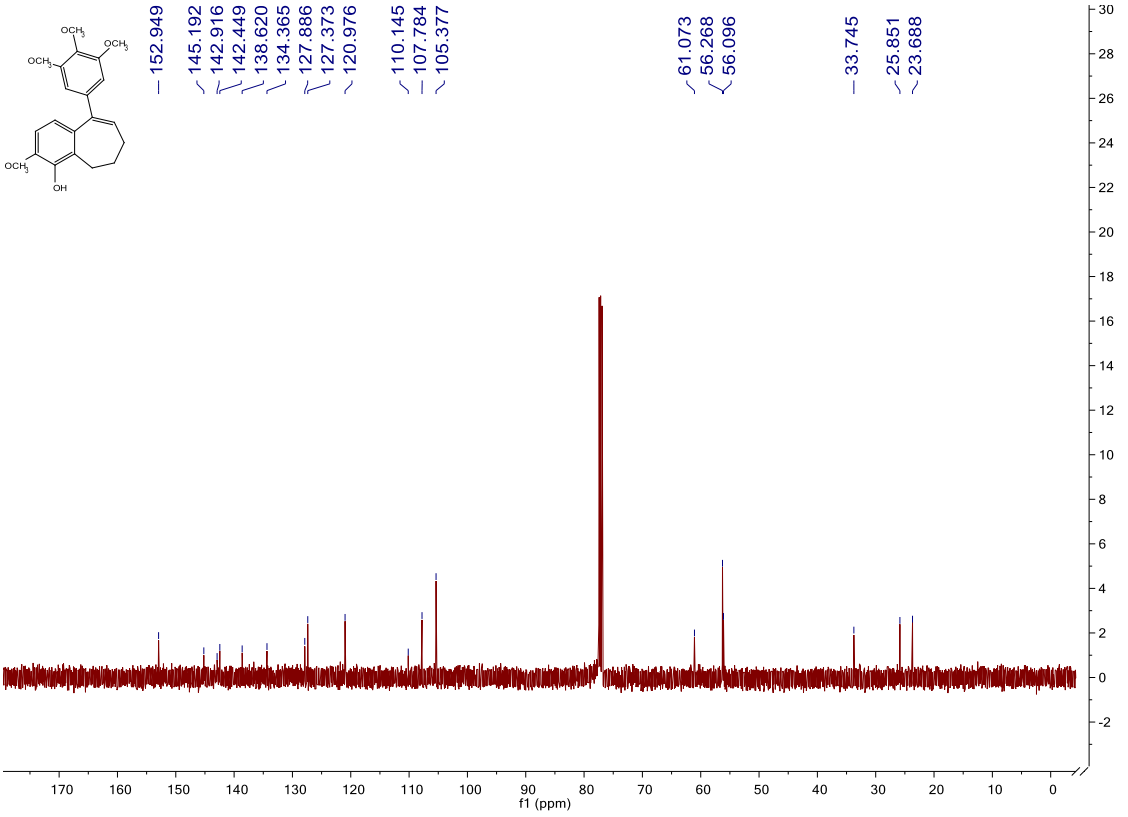
Signal 8: DAD1 H, Sig=320,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.748	BB	0.0873	57.64566	9.99286	100.0000
Totals :				57.64566	9.99286	

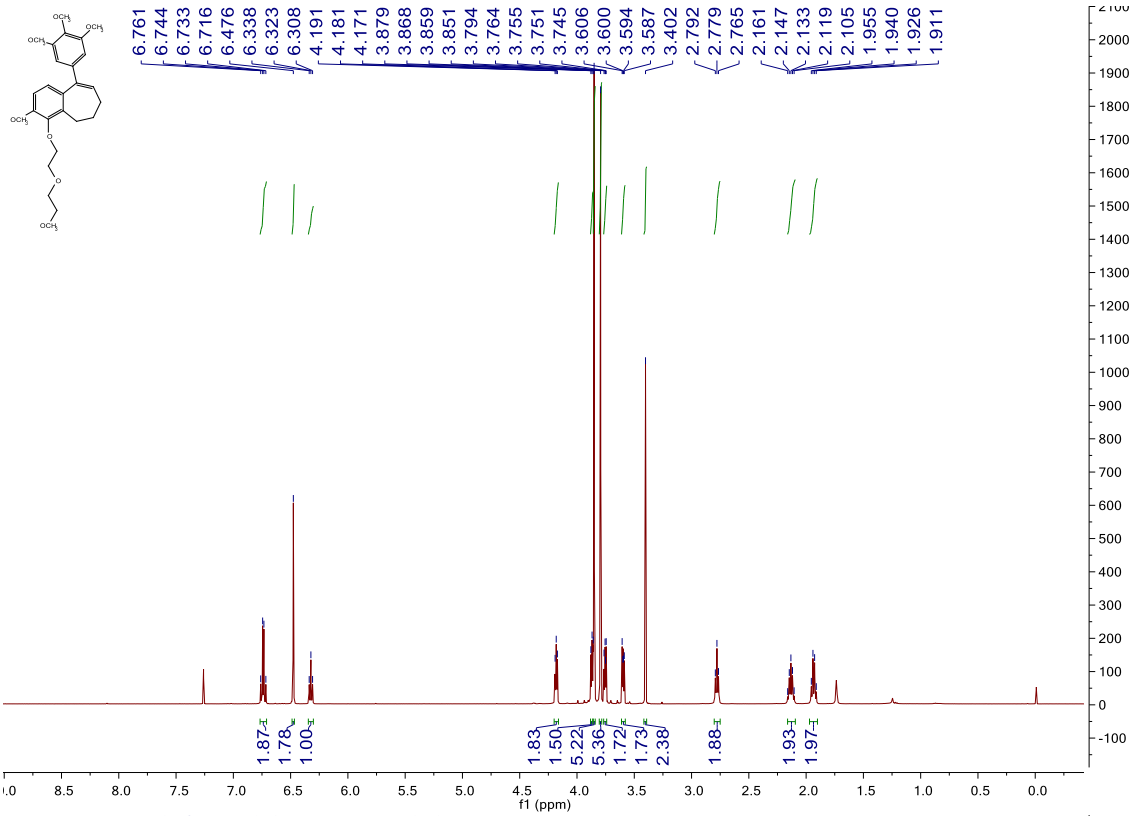
*** End of Report ***

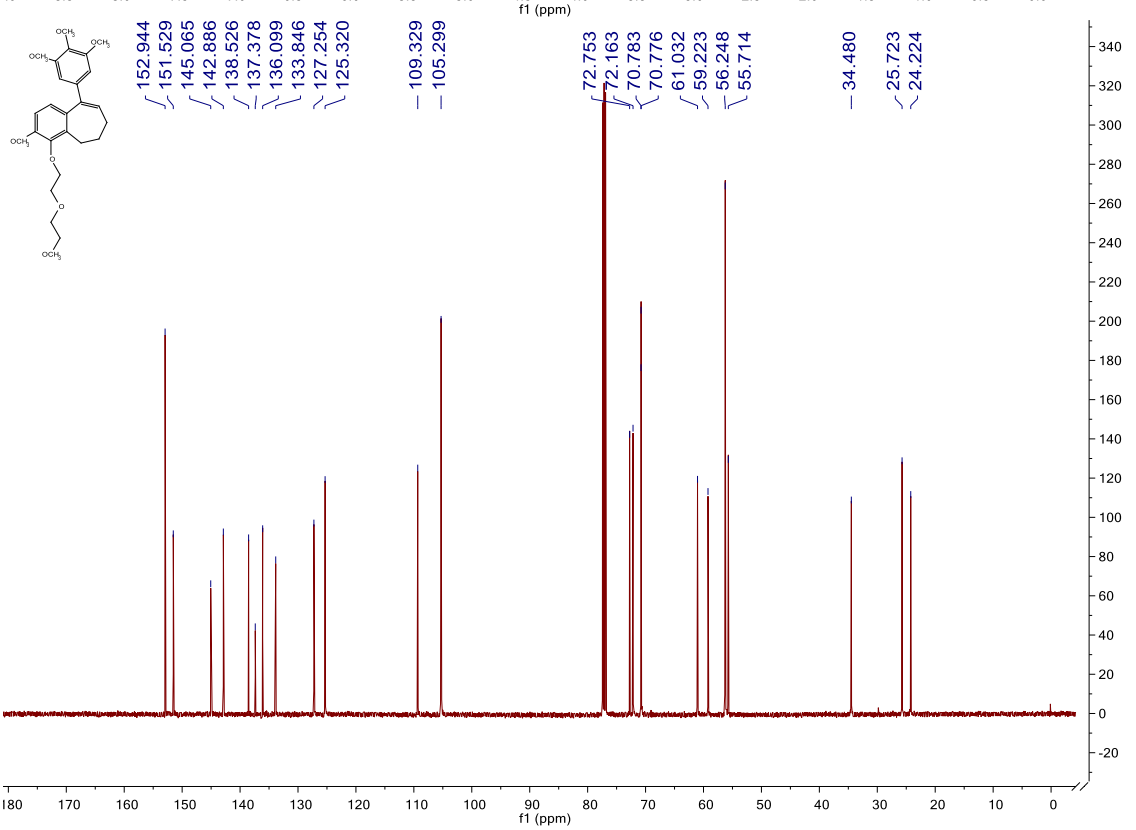
7. 3-Methoxy-9-(3,4,5-trimethoxyphenyl)-6,7-dihydro-5H-benzo[7]annulen-4-ol





8. 3-Methoxy-4-(2-(2-methoxyethoxy) ethoxy)-9-(3,4,5-trimethoxyphenyl)-6,7-dihydro-5H-benzo[7]annulene





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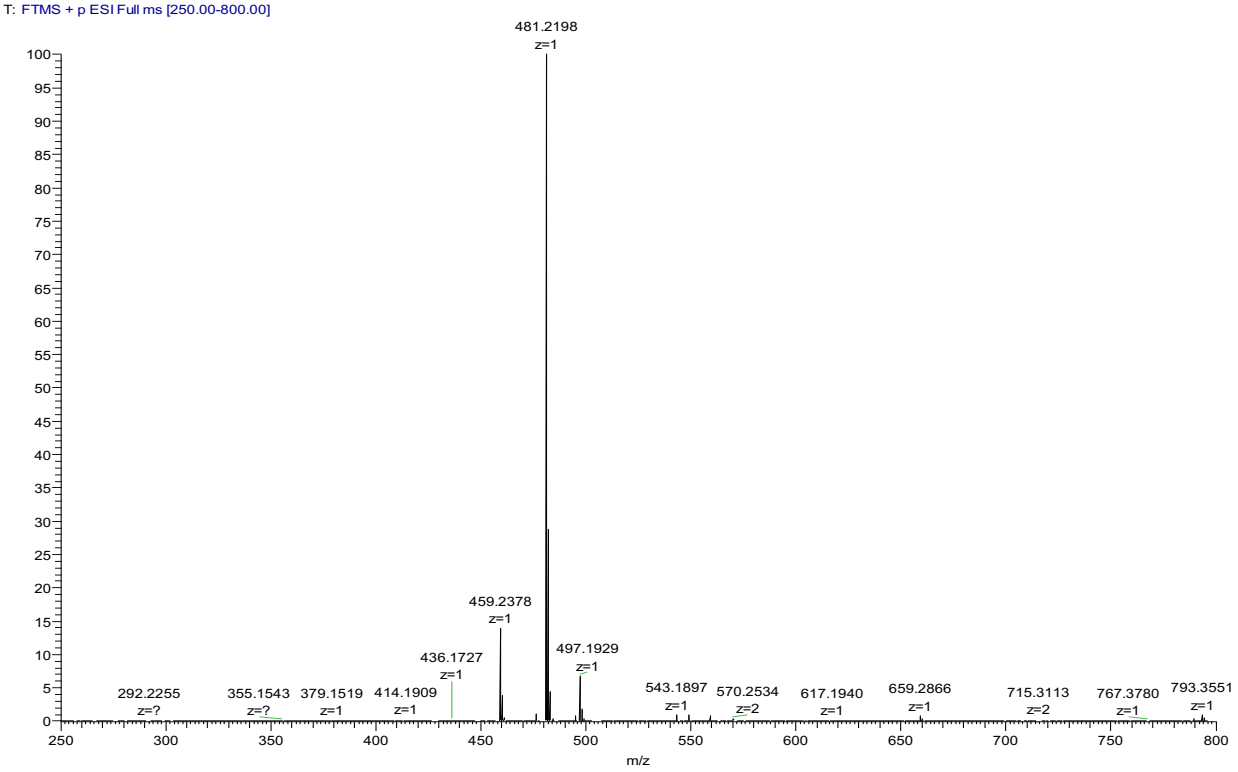

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Sample Operator : SYSTEM
Acq. Instrument : 1200 HPLC                    Location :   1
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                                              Inj Volume : No inj
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Analysis Method : C:\CHEM32\1\METHODS\RT-ACNWASH 2.M
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Method Info     : General Column Wash Method

Sample Info     : 20180228

Additional Info : Peak(s) manually integrated
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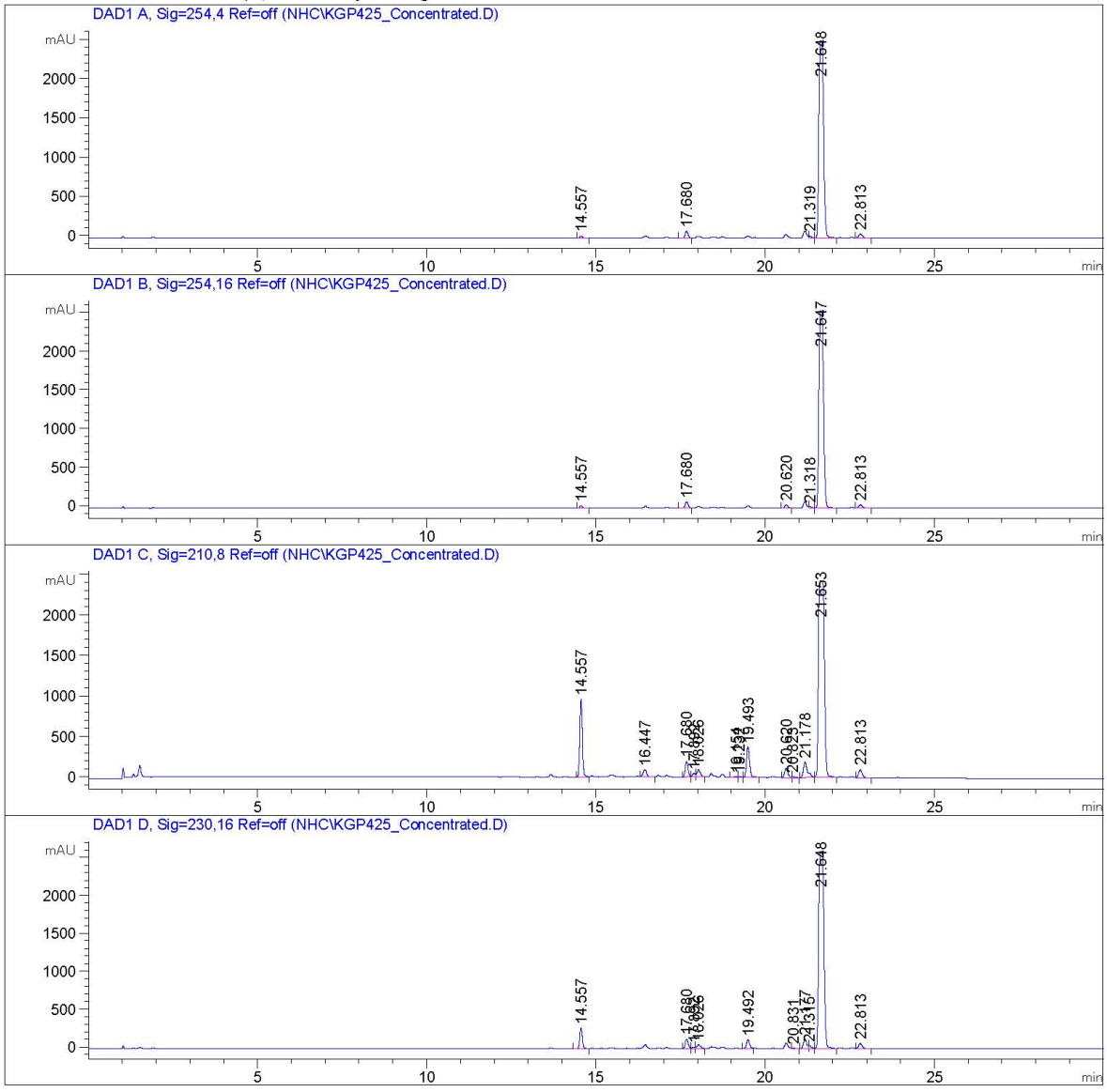
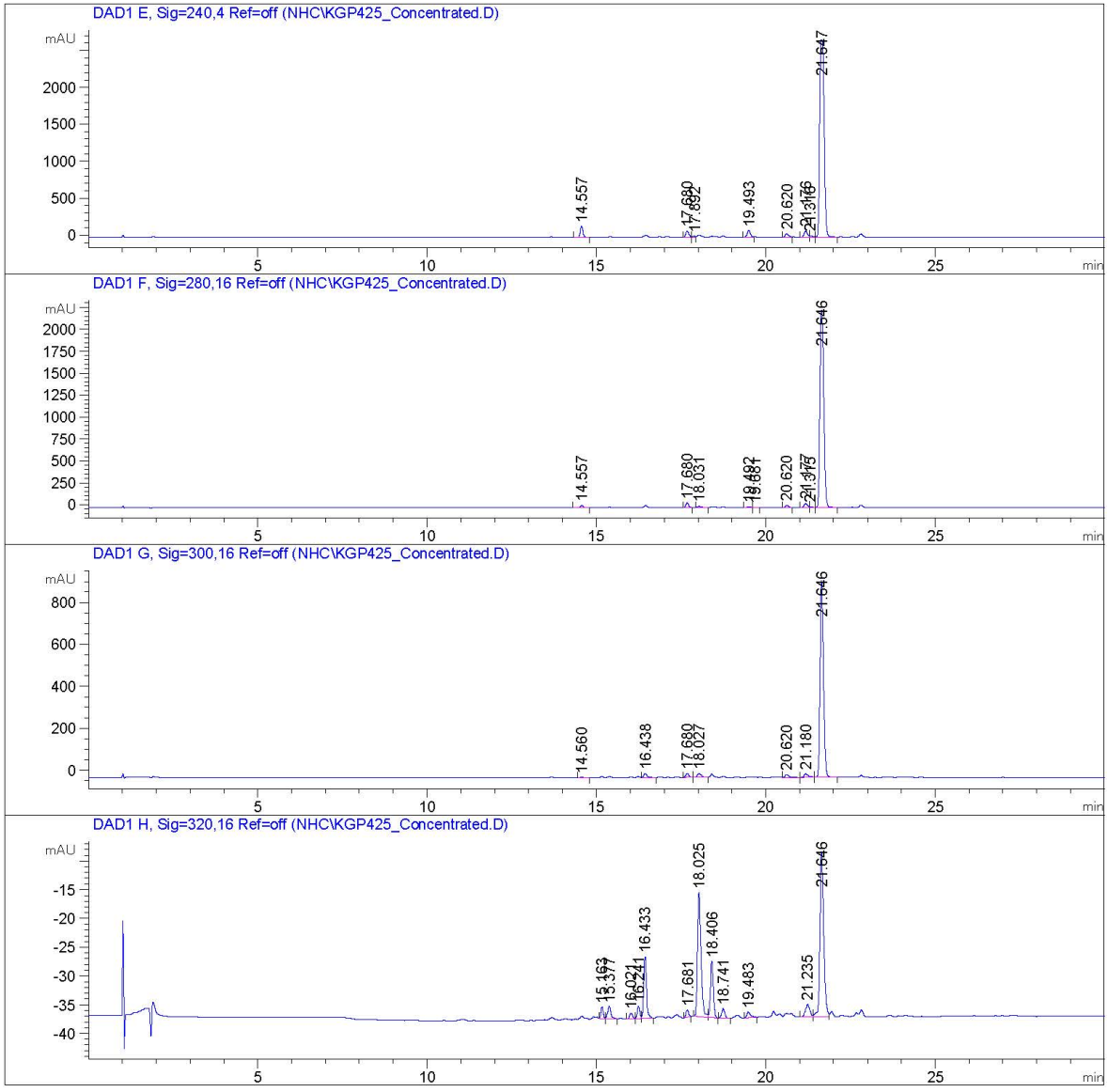


Data File C:\Chem32\1\Data\NHC\KGP425_Concentrated.D
Sample Name: KGP425_Concentrated



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Area Percent Report

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Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Data File C:\Chem32\1\Data\NHC\KGP425_Concentrated.D
Sample Name: KGP425_Concentrated

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.557	BV	0.0823	118.86156	22.25858	0.4708
2	17.680	BV	0.0892	490.85931	85.26562	1.9441
3	21.319	VV	0.0847	118.80322	20.79025	0.4705
4	21.648	VV	0.1564	2.42181e4	2513.18140	95.9184
5	22.813	VB	0.1041	302.01974	45.12530	1.1962
Totals :				2.52486e4	2686.62115	

Signal 2: DAD1 B, Sig=254,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.557	BV	0.0820	175.41304	33.01146	0.6943
2	17.680	BV	0.0891	466.62897	81.11676	1.8470
3	20.620	BV	0.0996	252.97607	39.05746	1.0013
4	21.318	VV	0.0856	115.58350	19.96070	0.4575
5	21.647	VV	0.1537	2.39580e4	2547.32373	94.8324
6	22.813	VB	0.1059	294.92889	43.04778	1.1674
Totals :				2.52636e4	2763.51789	

Signal 3: DAD1 C, Sig=210,8 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.557	BV	0.0843	5126.17432	960.03735	12.0626
2	16.447	VB	0.1174	672.09033	87.72803	1.5815
3	17.680	BB	0.0865	1067.51355	193.13002	2.5120
4	17.892	BV	0.0797	215.70448	42.13689	0.5076
5	18.026	VV	0.1079	627.46326	87.27602	1.4765
6	19.154	BV	0.1083	72.89687	9.41314	0.1715
7	19.232	VV	0.0910	54.21881	8.90705	0.1276
8	19.493	VV	0.1006	2496.98657	380.27234	5.8758
9	20.620	VV	0.1052	773.66321	111.09237	1.8205
10	20.823	VB	0.0938	51.07826	8.30413	0.1202
11	21.178	BV	0.1216	1603.45532	191.76048	3.7732
12	21.653	VB	0.1959	2.90408e4	2421.63306	68.3371
13	22.813	VB	0.1061	694.33698	101.09408	1.6339
Totals :				4.24964e4	4602.78496	

Data File C:\Chem32\1\Data\NHC\KGP425_Concentrated.D
Sample Name: KGP425_Concentrated

Signal 4: DAD1 D, Sig=230,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.557	BV	0.0818	1434.35364	270.67902	4.4262
2	17.680	BV	0.0883	715.41840	125.79987	2.2077
3	17.892	VV	0.0798	85.76254	16.17930	0.2646
4	18.026	VB	0.1060	331.48679	46.01447	1.0229
5	19.492	BV	0.0987	749.68884	117.13616	2.3134
6	20.831	VB	0.0994	31.53558	4.75552	0.0973
7	21.177	BV	0.1025	838.00244	124.61800	2.5859
8	21.315	VV	0.0828	180.34955	32.48801	0.5565
9	21.648	VV	0.1736	2.75846e4	2602.97729	85.1217
10	22.813	VB	0.1050	454.86087	67.19091	1.4036
Totals :				3.24061e4	3407.83856	

Signal 5: DAD1 E, Sig=240,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.557	BV	0.0820	777.21985	146.28734	2.8433
2	17.680	BB	0.0870	443.48972	79.54295	1.6224
3	17.892	BV	0.0741	41.77242	8.68438	0.1528
4	19.493	BV	0.0983	559.97467	87.88669	2.0486
5	20.620	BV	0.1005	284.78500	43.45454	1.0418
6	21.176	BV	0.1018	522.82568	78.39069	1.9127
7	21.316	VV	0.0847	117.19544	20.48845	0.4287
8	21.647	VV	0.1493	2.45879e4	2672.75610	89.9497
Totals :				2.73351e4	3137.49114	

Signal 6: DAD1 F, Sig=280,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.557	BB	0.0832	145.26443	26.81715	0.7533
2	17.680	BB	0.0876	298.43884	53.05305	1.5477
3	18.031	VB	0.1294	108.40925	13.84524	0.5622
4	19.492	BV	0.1014	68.71871	10.63372	0.3564
5	19.681	VB	0.0961	9.85323	1.55113	0.0511
6	20.620	VV	0.1022	184.61534	27.53001	0.9574
7	21.177	BV	0.1020	321.54666	48.06583	1.6675
8	21.315	VV	0.0823	68.22184	12.37105	0.3538
9	21.646	VB	0.1277	1.80780e4	2250.99805	93.7507
Totals :				1.92831e4	2444.86521	

Data File C:\Chem32\1\Data\NHC\KGP425_Concentrated.D
Sample Name: KGP425_Concentrated

Signal 7: DAD1 G, Sig=300,16 Ref=off

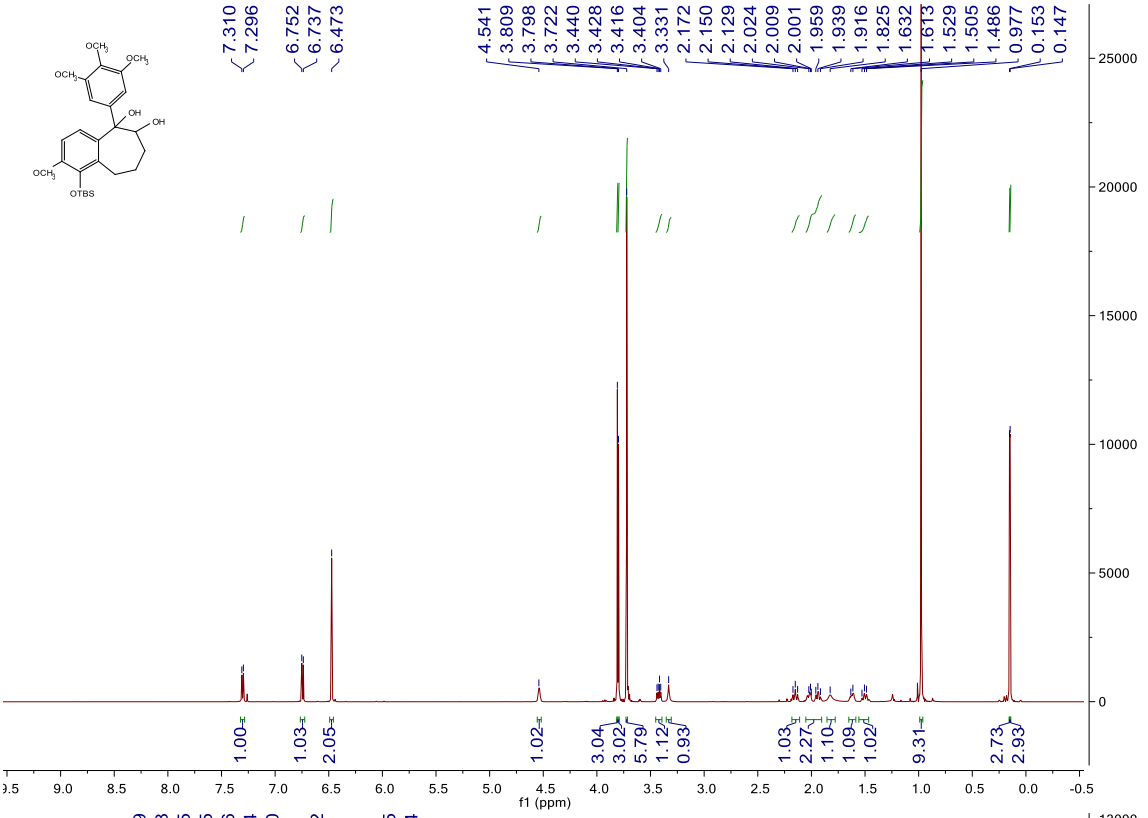
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.560	BB	0.1121	9.52692	1.23345	0.1306
2	16.438	VV	0.0964	122.05368	19.13903	1.6736
3	17.680	BB	0.0878	107.45611	19.05733	1.4734
4	18.027	BV	0.1122	148.10034	19.16150	2.0307
5	20.620	VB	0.1110	96.67720	12.95937	1.3256
6	21.180	BV	0.1285	141.55328	16.11868	1.9410
7	21.646	VV	0.1110	6667.56348	936.89960	91.4250
Totals :				7292.93101	1024.56897	

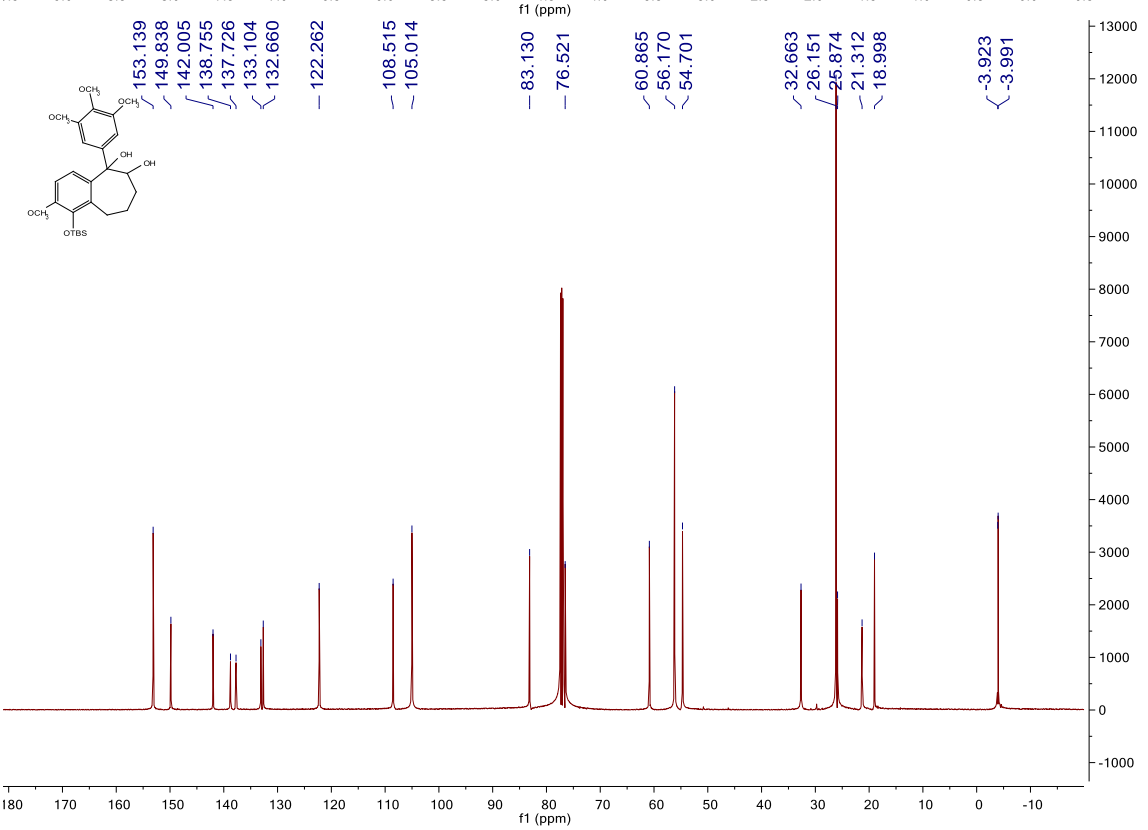
Signal 8: DAD1 H, Sig=320,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.163	BV	0.0767	9.68951	1.99357	1.6498
2	15.377	VB	0.1018	14.73561	2.15531	2.5090
3	16.021	BV	0.0919	6.27725	1.01919	1.0688
4	16.241	VV	0.0823	11.66878	2.18467	1.9868
5	16.433	VB	0.0878	60.74028	10.76672	10.3421
6	17.681	BB	0.0832	6.50484	1.23932	1.1076
7	18.025	BV	0.1051	153.84769	21.60467	26.1953
8	18.406	VB	0.0922	58.86423	9.77991	10.0227
9	18.741	BB	0.0978	10.26478	1.62227	1.7478
10	19.483	BB	0.1199	8.38881	1.02103	1.4283
11	21.235	BV	0.1326	19.49195	2.17432	3.3188
12	21.646	VV	0.1198	226.83722	28.82724	38.6230
Totals :				587.31093	84.38821	

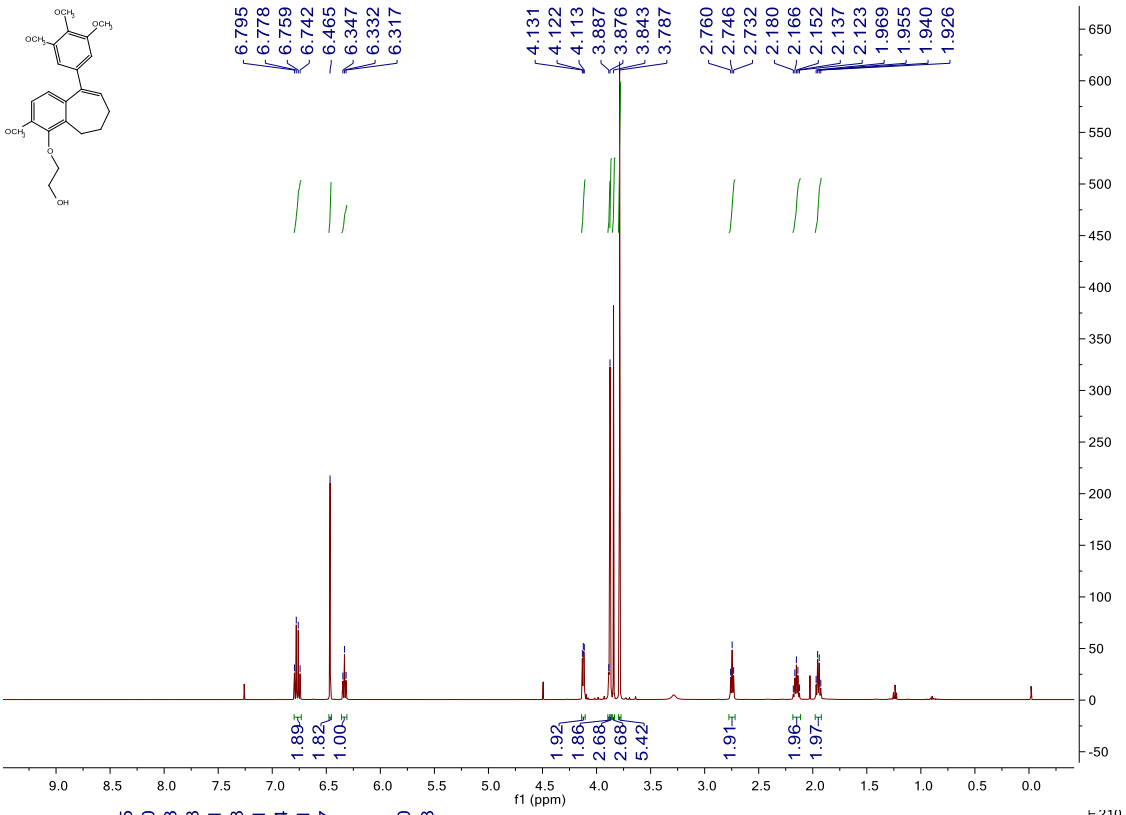
*** End of Report ***

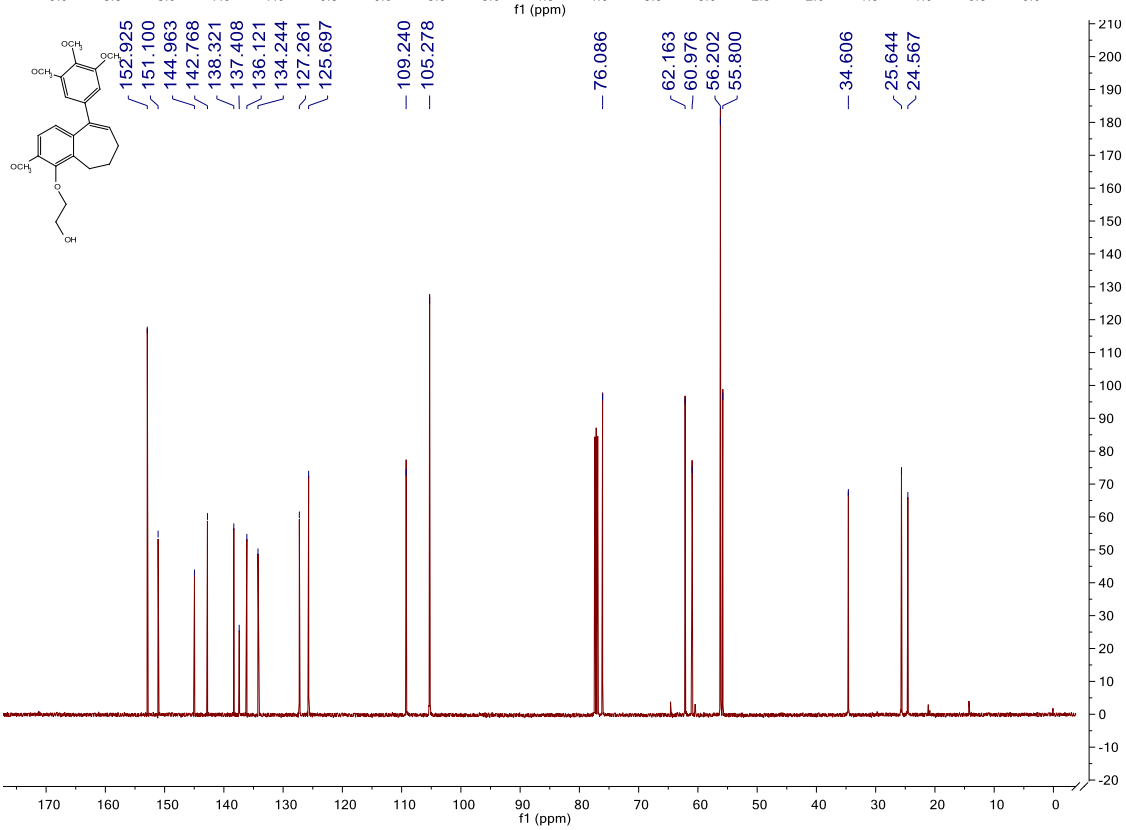
10. 1-((tert-butyldimethylsilyl)oxy)-2-methoxy-5-(3,4,5-trimethoxyphenyl)-6,7,8,9-tetrahydro-5H-benzo[7]annulene-5,6-diol



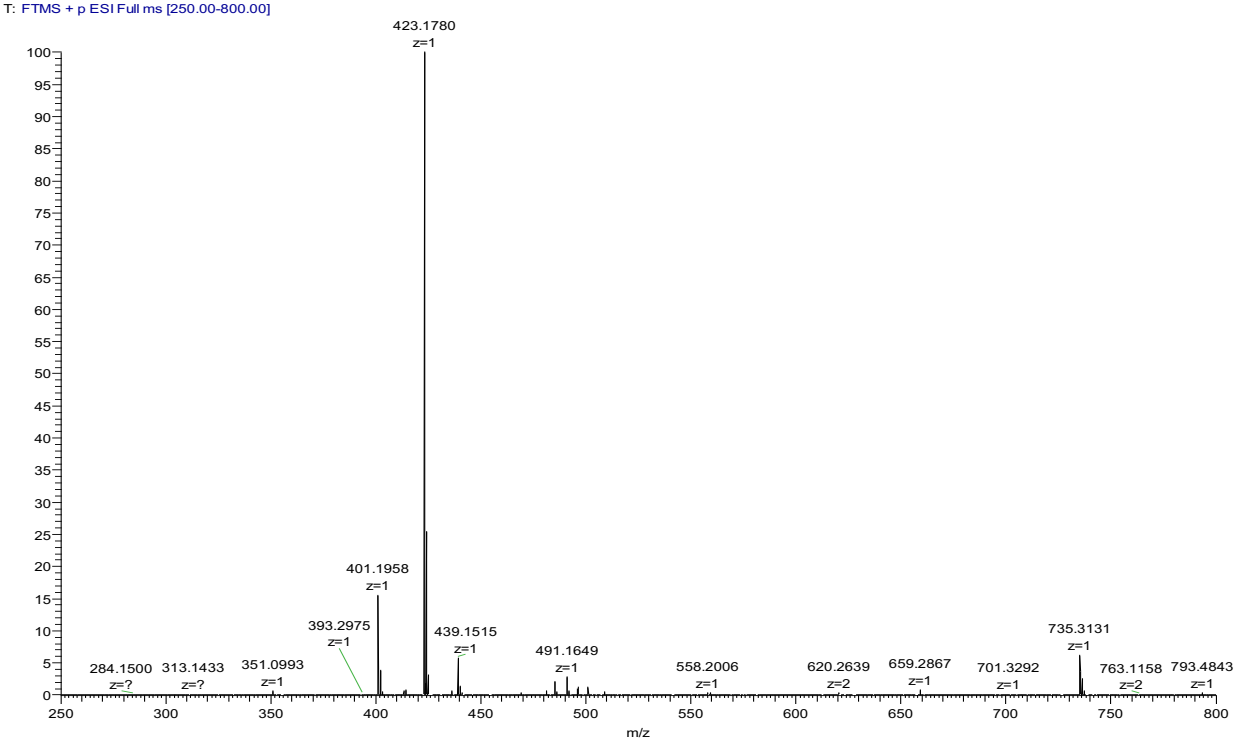


11. 2-((3-Methoxy-9-(3,4,5-trimethoxyphenyl)-6,7-dihydro-5H-benzo [7] annulen-4-yl) oxy)ethan-1-ol





NHC_1_141_03Sept2014 #500 RT: 4.38 AV: 1 NL: 1.79E7
T: FTMS + p ESI Full ms [250.00-800.00]



Data File C:\CHEM32\1\DATA\HAICHAN NIU\KGP426_RUN00001.D
Sample Name: KGP426

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Acq. Instrument : Instrument 1                    Location :   -
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Acq. Method     : C:\CHEM32\1\METHODS\MASTERMETHOD.M
Last changed    : 9/3/2014 6:06:43 PM by Haichan Niu
Analysis Method : C:\CHEM32\1\DATA\HAICHAN NIU\KGP426_RUN00001.D\DA.M (MASTERMETHOD.M)
Last changed    : 9/3/2014 7:09:19 PM by Haichan Niu
Sample Info     : KGP426
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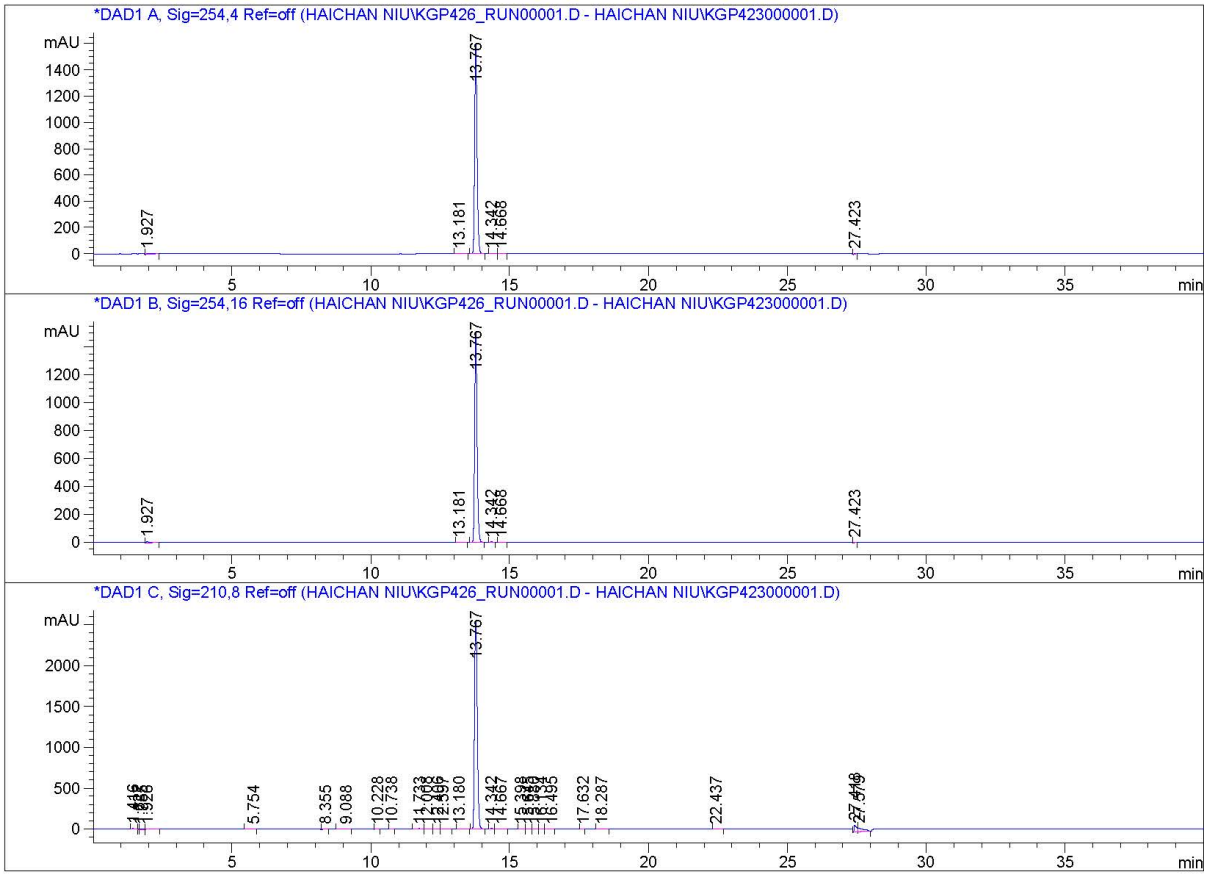
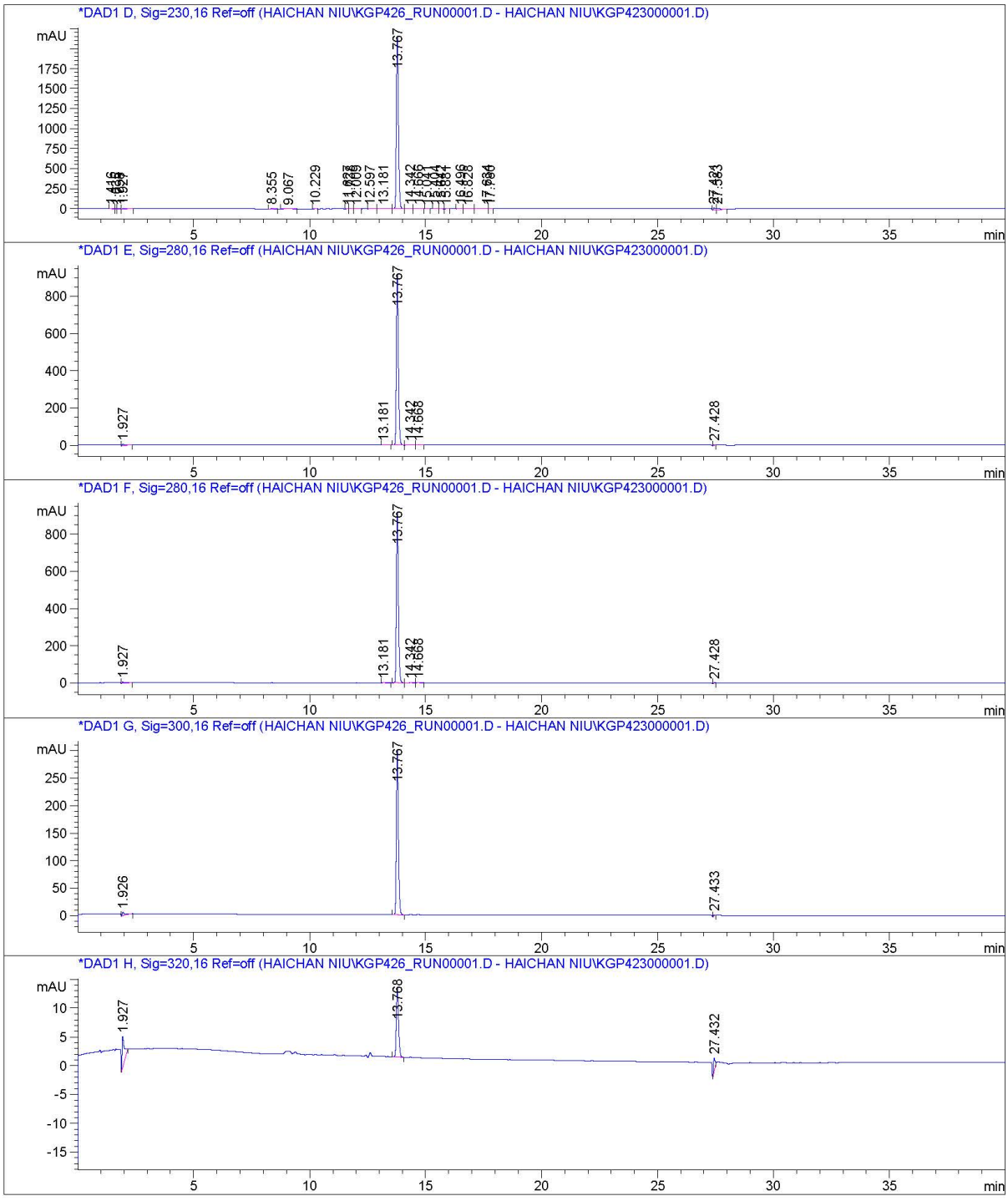


Data File C:\CHEM32\1\DATA\HAICHAN NIU\KGP426_RUN00001.D
Sample Name: KGP426



Data File C:\CHEM32\1\DATA\HAICHAN NIU\KGP426_RUN00001.D
Sample Name: KGP426

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Area Percent Report
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Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.927	BB	0.1399	119.08279	11.21637	1.2223
2	13.181	BB	0.0907	15.13886	2.57139	0.1554
3	13.767	BB	0.0917	9554.34863	1600.01831	98.0718
4	14.342	BV	0.0924	15.24520	2.52756	0.1565
5	14.668	VB	0.0911	10.52975	1.77820	0.1081
6	27.423	BB	0.0724	27.84886	5.97433	0.2859
Totals :				9742.19410	1624.08617	

Signal 2: DAD1 B, Sig=254,16 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.927	BB	0.1399	116.74947	10.99203	1.2738
2	13.181	BB	0.0899	13.98029	2.40313	0.1525
3	13.767	BB	0.0916	8982.48633	1506.09546	98.0063
4	14.342	BB	0.0898	14.18266	2.43999	0.1547
5	14.668	BB	0.0894	10.05478	1.74013	0.1097
6	27.423	BB	0.0707	27.76368	5.92610	0.3029
Totals :				9165.21722	1529.59684	

Signal 3: DAD1 C, Sig=210,8 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.416	BV	0.0834	65.84866	11.07412	0.3348
2	1.627	VV	0.0580	17.29334	4.38142	0.0879
3	1.755	VB	0.1483	68.88960	6.57415	0.3502

Data File C:\CHEM32\1\DATA\HAICHAN NIU\KGP426_RUN00001.D
Sample Name: KGP426

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
4	1.926	BB	0.1418	139.05045	12.89657	0.7069
5	5.754	BB	0.1811	17.70824	1.29856	0.0900
6	8.355	BB	0.1001	39.84661	5.66208	0.2026
7	9.088	BB	0.2386	39.77609	2.36085	0.2022
8	10.228	BB	0.0984	16.11083	2.39876	0.0819
9	10.738	BB	0.0795	5.32537	1.04401	0.0271
10	11.733	BV	0.1327	73.00882	7.56023	0.3712
11	12.008	VV	0.1427	27.33658	2.64206	0.1390
12	12.406	VB	0.1362	13.80634	1.48814	0.0702
13	12.597	BB	0.1172	28.09263	3.44285	0.1428
14	13.180	VB	0.0942	37.12927	5.99732	0.1888
15	13.767	BB	0.1105	1.75956e4	2550.63257	89.4515
16	14.342	BV	0.0915	42.31578	7.10271	0.2151
17	14.667	VB	0.1060	40.25458	5.59206	0.2046
18	15.398	BV	0.1493	13.49356	1.23675	0.0686
19	15.645	VB	0.1455	22.55037	2.16622	0.1146
20	15.880	BV	0.1142	20.79329	2.62974	0.1057
21	16.134	VB	0.1260	11.85367	1.44059	0.0603
22	16.495	BB	0.1390	10.29406	1.06285	0.0523
23	17.632	BV	0.1006	6.64764	1.06805	0.0338
24	18.287	VB	0.1628	16.01570	1.27240	0.0814
25	22.437	BB	0.0952	6.90384	1.07153	0.0351
26	27.418	BV	0.0927	606.74664	89.93950	3.0845
27	27.579	VB	0.1775	687.85321	49.07451	3.4969
Totals :				1.96706e4	2783.11060	

Signal 4: DAD1 D, Sig=230,16 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.416	BV	0.1653	37.19662	2.86874	0.2580
2	1.635	VV	0.0652	22.79852	4.81536	0.1581
3	1.798	VB	0.1576	68.77133	7.18661	0.4770
4	1.927	BB	0.1435	139.15787	12.73060	0.9651
5	8.355	BB	0.1186	40.33474	4.67800	0.2797
6	9.067	BB	0.2603	28.87039	1.40194	0.2002
7	10.229	BB	0.0984	12.34820	1.79232	0.0856
8	11.627	BV	0.0863	11.15424	1.96349	0.0774
9	11.738	VB	0.0937	15.51431	2.45737	0.1076
10	12.009	BB	0.1116	11.38201	1.48170	0.0789
11	12.597	BV	0.1349	18.07800	1.86829	0.1254
12	13.181	VV	0.1324	39.49321	4.17227	0.2739
13	13.767	VV	0.0964	1.33474e4	2152.10620	92.5726
14	14.342	VV	0.1229	45.72311	5.28717	0.3171
15	14.666	VB	0.1413	37.98609	3.71501	0.2635

Data File C:\CHEM32\1\DATA\HAICHAN NIU\KGP426_RUN00001.D
Sample Name: KGP426

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
16	15.041	BB	0.0977	7.02311	1.11142	0.0487
17	15.404	BV	0.1193	18.64751	2.23519	0.1293
18	15.642	VB	0.1470	17.07045	1.61935	0.1184
19	15.881	BB	0.0921	9.88751	1.64665	0.0686
20	16.496	BV	0.1112	21.94571	2.93456	0.1522
21	16.828	VB	0.1681	15.91745	1.34426	0.1104
22	17.634	BV	0.1519	24.40948	2.29782	0.1693
23	17.780	VB	0.0980	11.49500	1.76567	0.0797
24	27.421	BV	0.0966	199.37985	28.85666	1.3828
25	27.583	VB	0.1811	216.32021	15.28291	1.5003
Totals :				1.44183e4	2267.61955	

Signal 5: DAD1 E, Sig=280,16 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.927	BB	0.1375	88.82256	8.52890	1.5777
2	13.181	BB	0.0876	8.21066	1.45974	0.1458
3	13.767	BB	0.0915	5475.32520	918.99084	97.2568
4	14.342	BV	0.1586	27.22835	2.32613	0.4837
5	14.668	VB	0.1104	13.70090	1.80886	0.2434
6	27.428	BB	0.0691	16.47407	3.61662	0.2926
Totals :				5629.76173	936.73110	

Signal 6: DAD1 F, Sig=280,16 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.927	BB	0.1375	88.82256	8.52890	1.5777
2	13.181	BB	0.0876	8.21066	1.45974	0.1458
3	13.767	BB	0.0915	5475.32520	918.99084	97.2568
4	14.342	BV	0.1586	27.22835	2.32613	0.4837
5	14.668	VB	0.1104	13.70090	1.80886	0.2434
6	27.428	BB	0.0691	16.47407	3.61662	0.2926
Totals :				5629.76173	936.73110	

Data File C:\CHEM32\1\DATA\HAICHAN NIU\KGP426_RUN00001.D
Sample Name: KGP426

Signal 7: DAD1 G, Sig=300,16 Ref=off
Signal has been modified after loading from rawdata file!

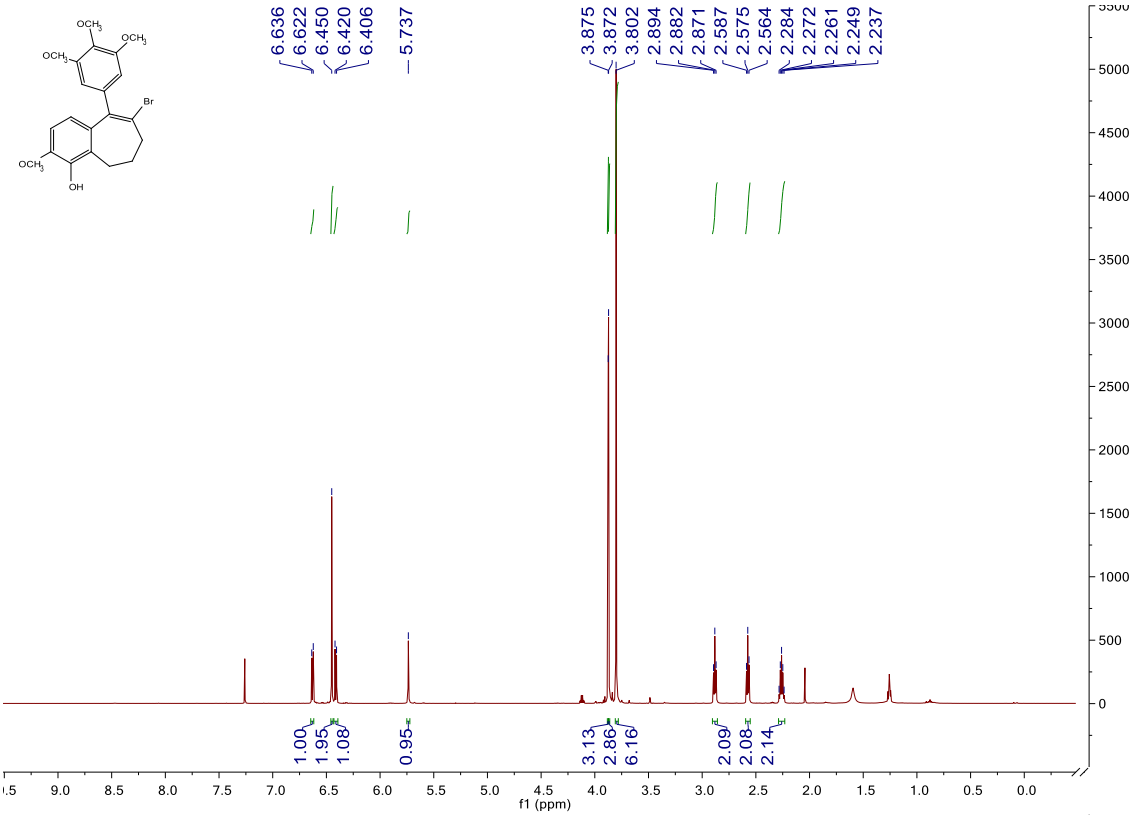
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.926	BB	0.1434	71.31882	6.53171	3.7804
2	13.767	BB	0.0920	1802.34485	300.41882	95.5382
3	27.433	BB	0.0723	12.85422	2.76376	0.6814
Totals :				1886.51788	309.71429	

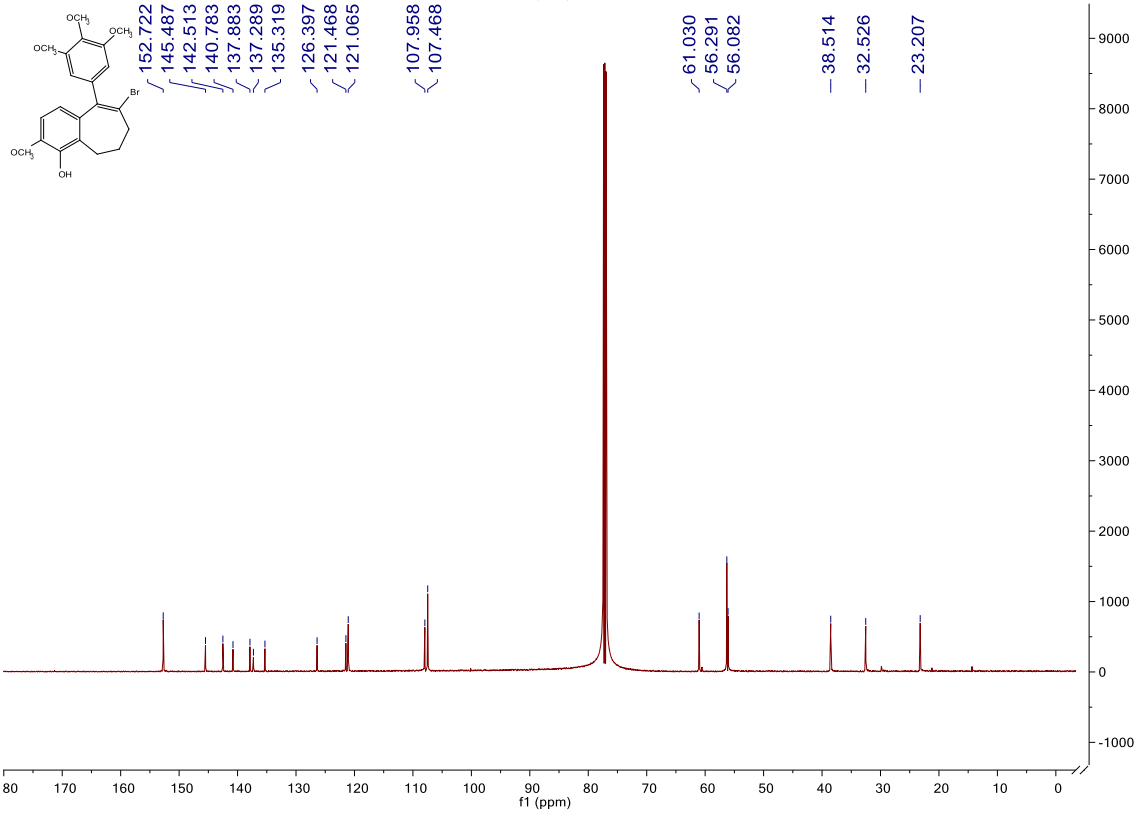
Signal 8: DAD1 H, Sig=320,16 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.927	BB	0.0977	38.60722	5.51177	29.5498
2	13.768	BB	0.1017	80.45616	12.08332	61.5808
3	27.432	BB	0.0735	11.58810	2.43776	8.8695
Totals :				130.65147	20.03285	

*** End of Report ***

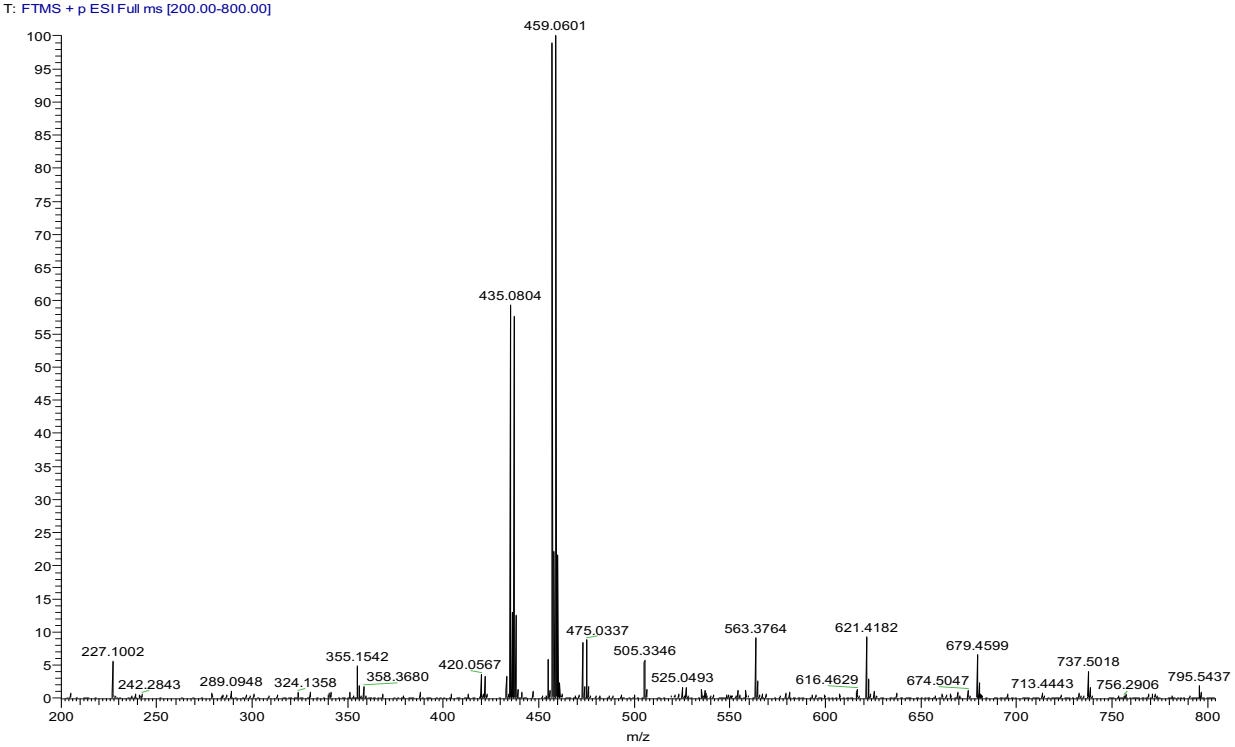
13. 8-bromo-3-methoxy-9-(3,4,5-trimethoxyphenyl)-6,7-dihydro-5H-benzo[7]annulen-4-ol





C:\Xcalibur\...\NHC_5_41_+ESI 9/29/2... ...42:27 AM

NHC_5_41_+ESI #2-19 RT: 0.01-0.15 AV: 18 NL: 1.79E7
T: FTMS + p ESI Full ms [200.00-800.00]



Data File C:\Chem32\1\Data\NHC\NHC_5_45_sample.D
Sample Name: NHC_5_45_sample

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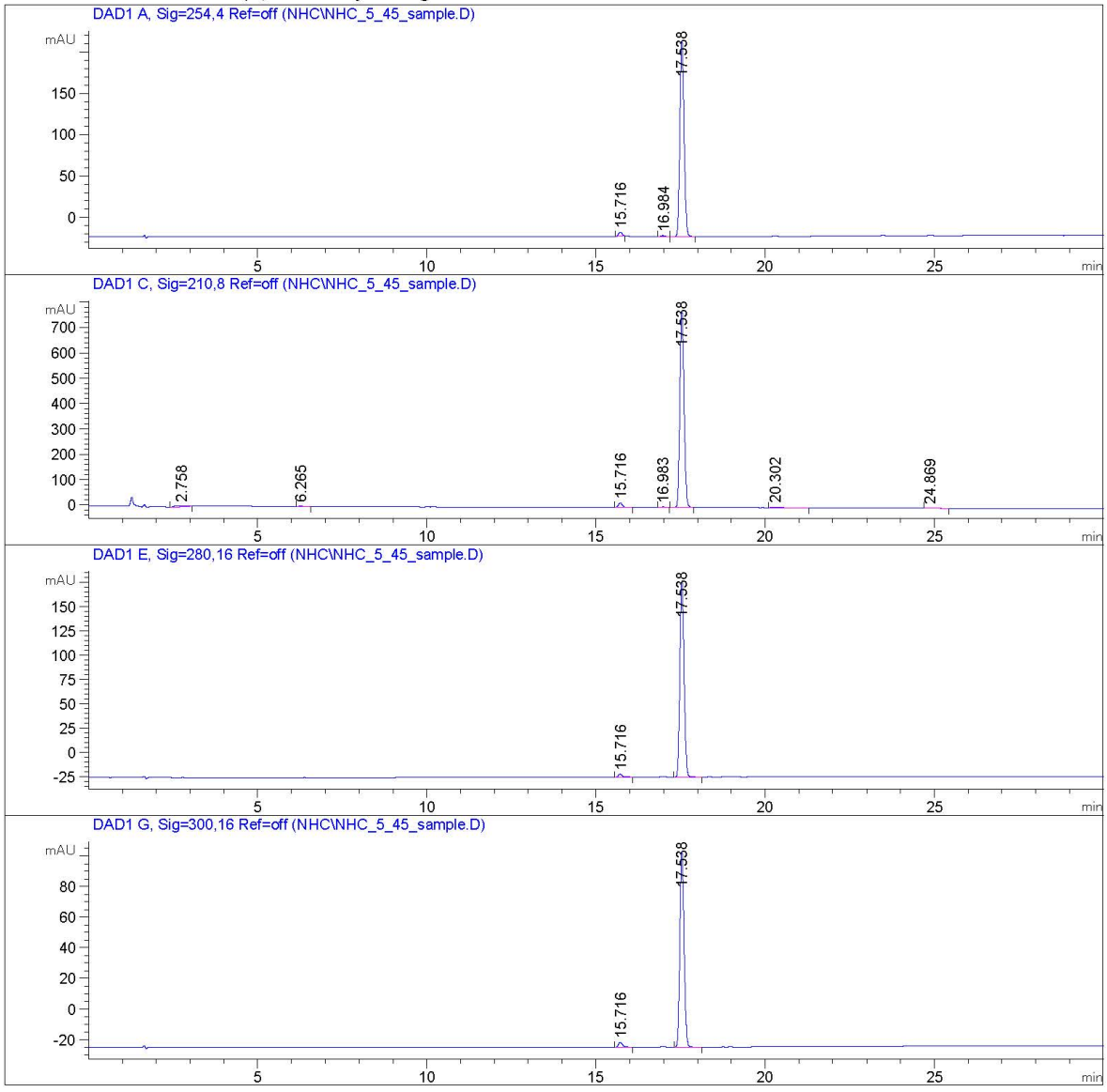
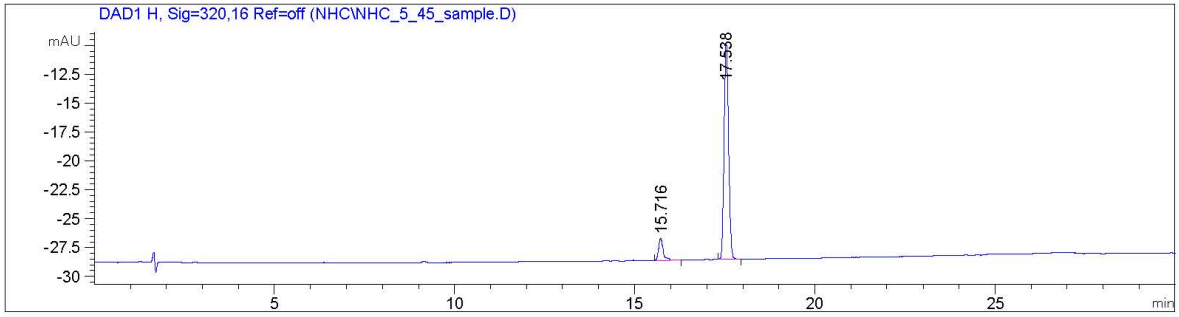
==========================================================================
Acq. Operator   : SYSTEM
Sample Operator : SYSTEM
Acq. Instrument : 1200 HPLC                    Location :   1
Injection Date  : 10/4/2017 10:52:59 AM
                                             Inj Volume : No inj
Acq. Method     : C:\CHEM32\1\METHODS\GRAD 2 30-90 ACN.M
Last changed    : 4/2/2014 4:04:33 PM by ERICA P
Analysis Method : C:\CHEM32\1\METHODS\RT-ACNWASH 2.M
Last changed    : 7/9/2015 2:27:22 PM by Blake
Method Info     : General Column Wash Method

Sample Info     : sample

Additional Info : Peak(s) manually integrated
```



Data File C:\Chem32\1\Data\NHC\NHC_5_45_sample.D
Sample Name: NHC_5_45_sample



==========

Area Percent Report

==========

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.716	BB	0.1128	35.66437	5.02612	1.7540
2	16.984	BB	0.1245	8.29816	1.02467	0.4081
3	17.538	BB	0.1301	1989.40491	236.56825	97.8379
Totals :				2033.36744	242.61904	

Signal 2: DAD1 C, Sig=210,8 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.758	BB	0.3239	69.77796	2.67886	1.0142
2	6.265	BB	0.1188	11.20396	1.37936	0.1628
3	15.716	BB	0.1295	146.68288	17.20089	2.1320
4	16.983	BB	0.1244	23.06185	2.91277	0.3352
5	17.538	BV	0.1306	6568.02832	777.53577	95.4654
6	20.302	BB	0.2160	45.81881	3.18187	0.6660
7	24.869	VB	0.1590	15.43766	1.39669	0.2244
Totals :				6880.01143	806.28621	

Data File C:\Chem32\1\Data\NHC\NHC_5_45_sample.D
Sample Name: NHC_5_45_sample

Signal 3: DAD1 E, Sig=280,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.716	BB	0.1294	26.30809	3.08786	1.5247
2	17.538	BB	0.1301	1699.19666	202.04190	98.4753
Totals :				1725.50475	205.12976	

Signal 4: DAD1 G, Sig=300,16 Ref=off

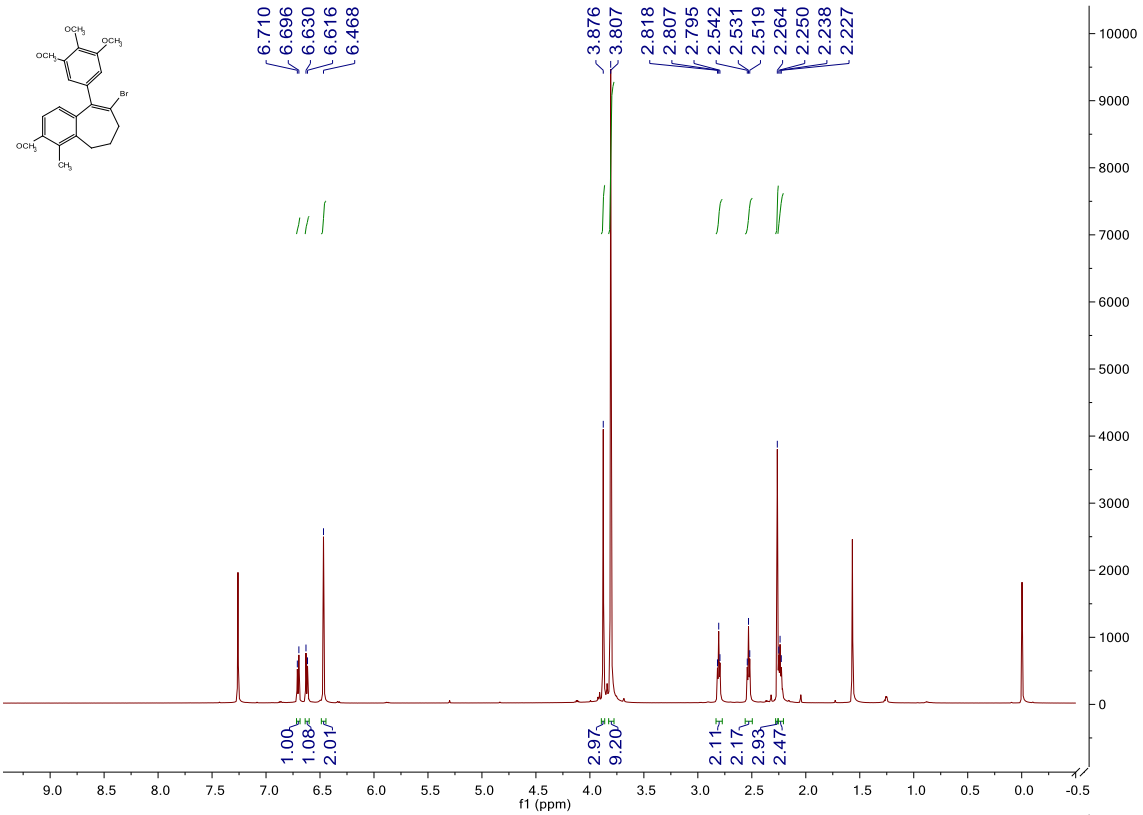
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.716	BB	0.1266	26.65558	3.21928	2.4140
2	17.538	BB	0.1302	1077.56128	128.05251	97.5860
Totals :				1104.21686	131.27178	

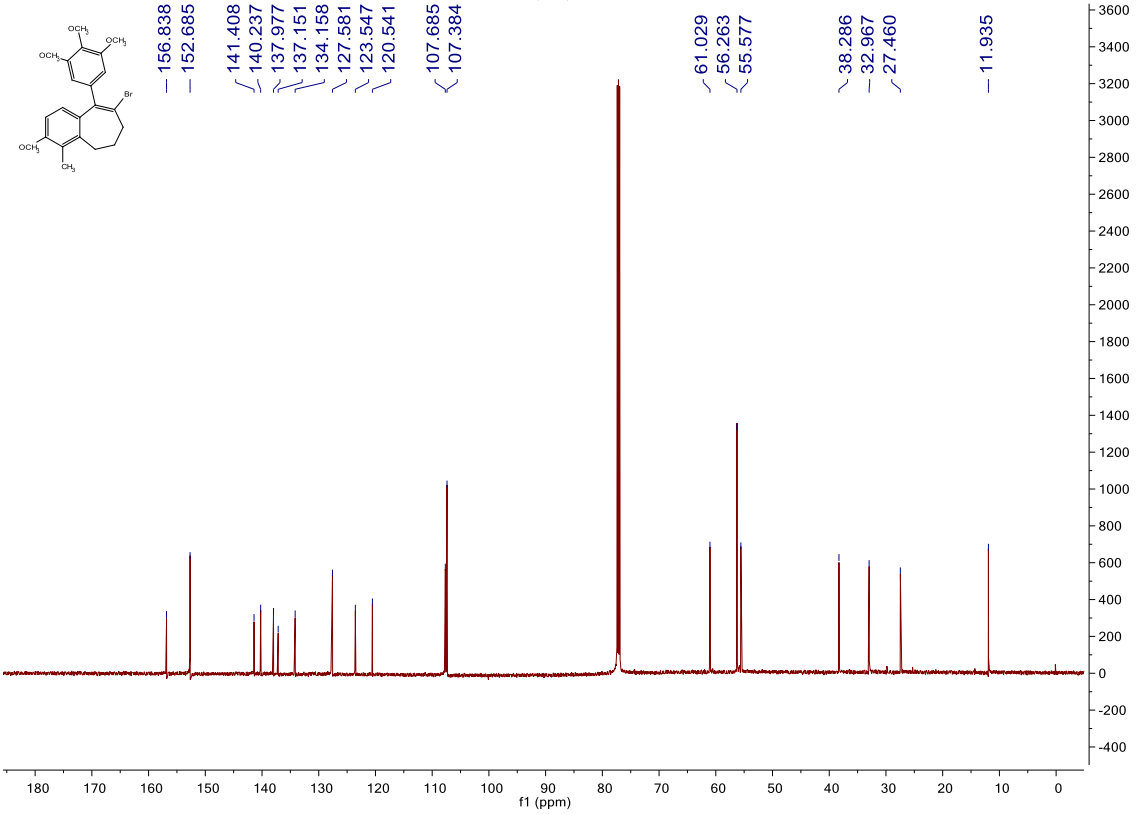
Signal 5: DAD1 H, Sig=320,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.716	BB	0.1324	16.67204	1.90032	9.5029
2	17.538	BB	0.1310	158.76990	18.70619	90.4971
Totals :				175.44194	20.60651	

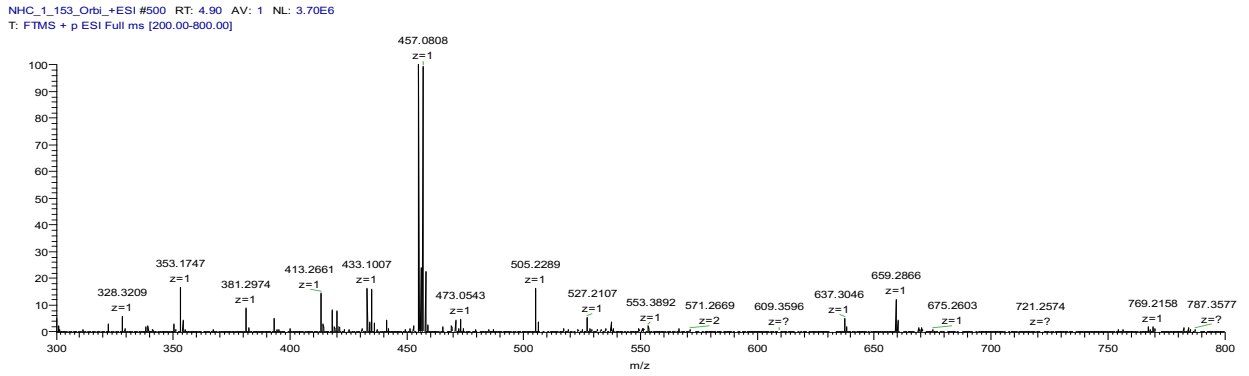
*** End of Report ***

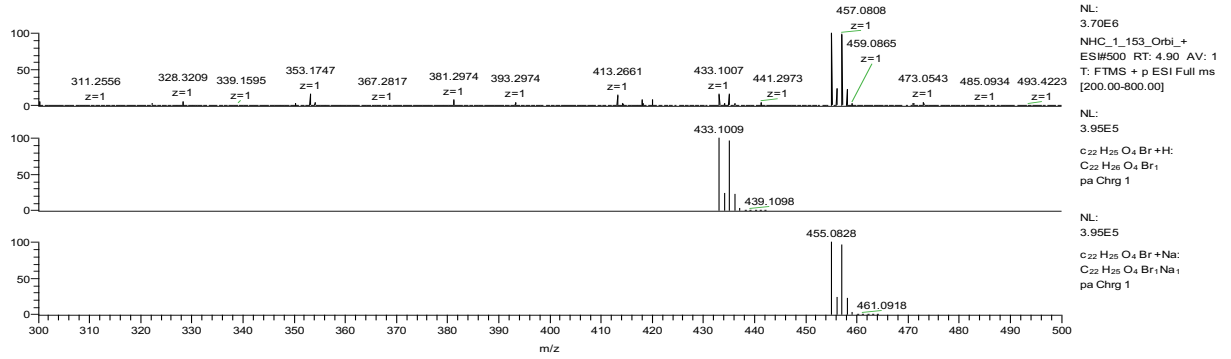
14. 8-Bromo-3-methoxy-4-methyl-9-(3,4,5-trimethoxyphenyl)-6,7-dihydro-5H-benzo[7]annulene





C:\Xcalibur\...\NHC_1_153_Orbi_+ESI 11/26/2014 5:19:04 PM NHC_1_153





Data File C:\CHEM32\1\DATA\HAICHAN NIU\KGP432PURE00002.D
Sample Name: KGP432PURE

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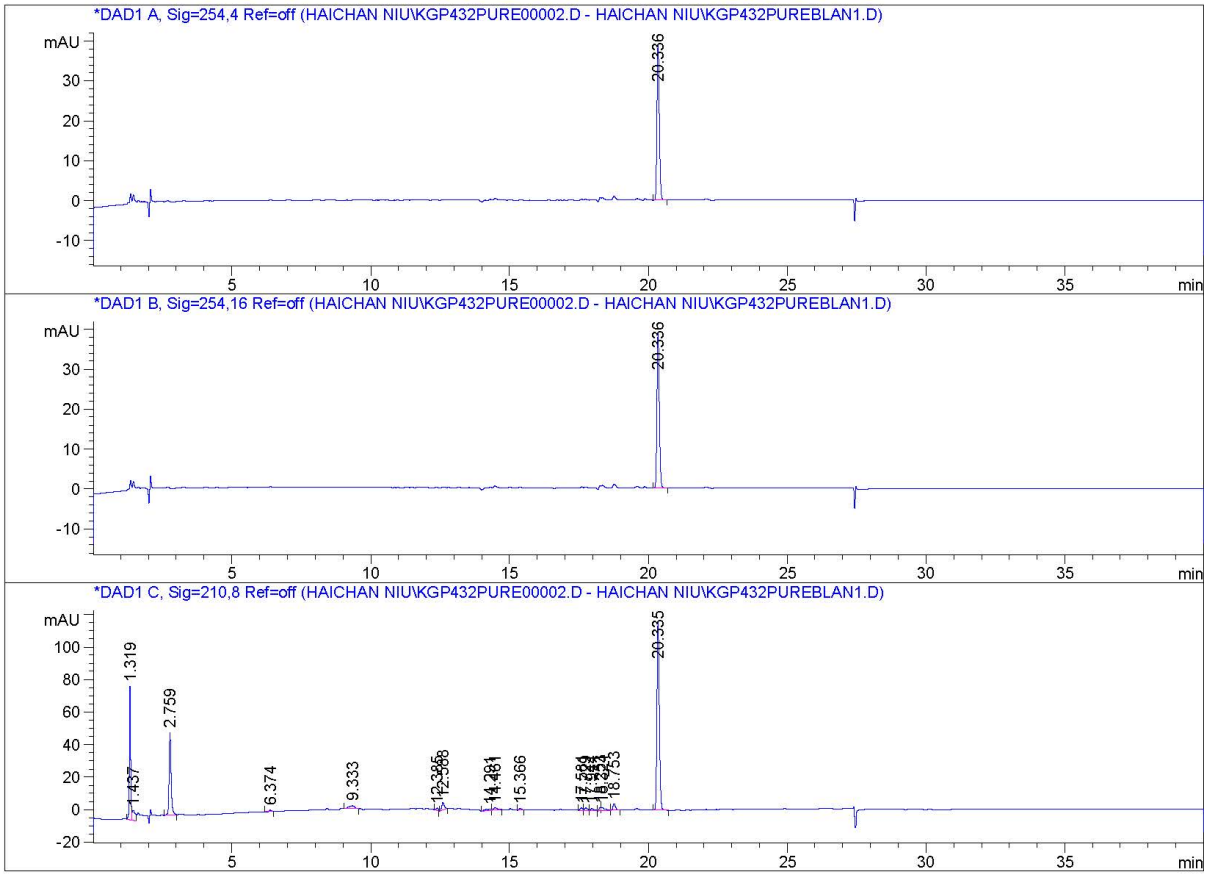
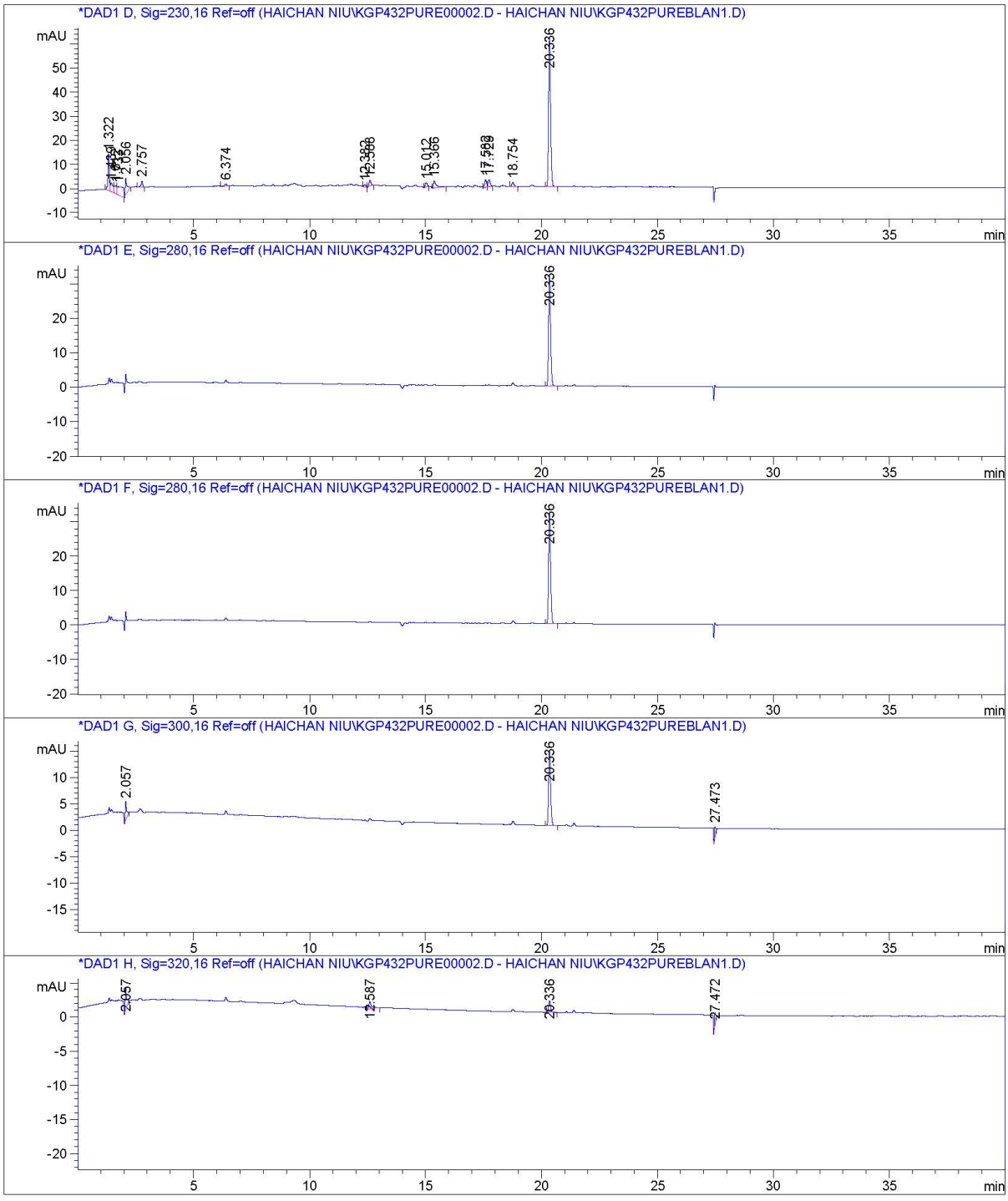
==========================================================================
Acq. Operator   : HAICHAN NIU
Acq. Instrument : Instrument 1                    Location :   -
Injection Date  : 12/17/2014 11:14:21 AM
Acq. Method     : C:\CHEM32\1\METHODS\MASTERMETHOD.M
Last changed    : 12/17/2014 11:09:46 AM by HAICHAN NIU
Analysis Method : C:\CHEM32\1\DATA\HAICHAN NIU\KGP432PURE00002.D\DA.M (MASTERMETHOD.M)
Last changed    : 12/17/2014 12:07:43 PM by HAICHAN NIU
Sample Info     : KGP432PURE
```



Data File C:\CHEM32\1\DATA\HAICHAN NIU\KGP432PURE00002.D
Sample Name: KGP432PURE



Data File C:\CHEM32\1\DATA\HAICHAN NIU\KGP432PURE00002.D
Sample Name: KGP432PURE

Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,4 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	20.336	BB	0.0911	232.63359	39.28381	100.0000
Totals :				232.63359	39.28381	

Signal 2: DAD1 B, Sig=254,16 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	20.336	BB	0.0911	231.28467	39.05958	100.0000
Totals :				231.28467	39.05958	

Signal 3: DAD1 C, Sig=210,8 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.319	BV	0.0489	260.75351	82.55019	17.7987
2	1.437	VV	0.1036	47.33643	6.16161	3.2311
3	2.759	BB	0.0768	255.48390	50.70833	17.4390
4	6.374	BB	0.0823	5.57547	1.01177	0.3806
5	9.333	BB	0.1893	24.71848	1.81080	1.6872
6	12.385	BB	0.0865	8.75978	1.58423	0.5979
7	12.588	BB	0.0978	31.46048	4.83926	2.1474
8	14.291	BV	0.2076	17.33635	1.07805	1.1834
9	14.461	VB	0.1360	15.93825	1.63093	1.0879
10	15.366	BB	0.0970	6.95629	1.11114	0.4748
11	17.581	BV	0.0945	10.15225	1.72910	0.6930
12	17.729	VV	0.1199	14.59630	1.77480	0.9963
13	17.944	VB	0.1494	15.66255	1.41234	1.0691

Data File C:\CHEM32\1\DATA\HAICHAN NIU\KGP432PURE00002.D
Sample Name: KGP432PURE

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
14	18.253	BV	0.0658	9.19920	2.15420	0.6279
15	18.324	VV	0.1435	22.91031	2.13003	1.5638
16	18.753	VB	0.1015	27.17989	3.98938	1.8553
17	20.335	BB	0.0912	690.99847	116.52905	47.1666
Totals :				1465.01791	282.20521	

Signal 4: DAD1 D, Sig=230,16 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.322	BV	0.0560	57.86644	15.32926	8.0494
2	1.439	VV	0.1102	29.74799	3.60819	4.1380
3	1.612	VV	0.0992	23.27344	3.18779	3.2374
4	1.733	VB	0.2284	63.24105	3.44190	8.7970
5	2.056	BB	0.0847	43.10315	7.11233	5.9958
6	2.757	BB	0.0821	13.99879	2.54623	1.9473
7	6.374	BB	0.0871	5.96154	1.03719	0.8293
8	12.382	VB	0.0990	6.91451	1.10573	0.9618
9	12.588	BB	0.0956	15.90767	2.52272	2.2128
10	15.012	BB	0.0996	12.44775	1.92126	1.7315
11	15.366	BB	0.1353	28.05904	2.94050	3.9031
12	17.582	BV	0.0904	18.50554	3.35373	2.5742
13	17.729	VB	0.0968	18.37617	2.94478	2.5562
14	18.754	BB	0.0956	11.36227	1.80087	1.5805
15	20.336	BB	0.0912	370.12521	62.44468	51.4856
Totals :				718.89054	115.29715	

Signal 5: DAD1 E, Sig=280,16 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	20.336	BB	0.0912	192.61380	32.48762	100.0000
Totals :				192.61380	32.48762	

Data File C:\CHEM32\1\DATA\HAICHAN NIU\KGP432PURE00002.D
Sample Name: KGP432PURE

Signal 6: DAD1 F, Sig=280,16 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	20.336	BB	0.0912	192.61380	32.48762	100.0000
Totals :				192.61380	32.48762	

Signal 7: DAD1 G, Sig=300,16 Ref=off
Signal has been modified after loading from rawdata file!

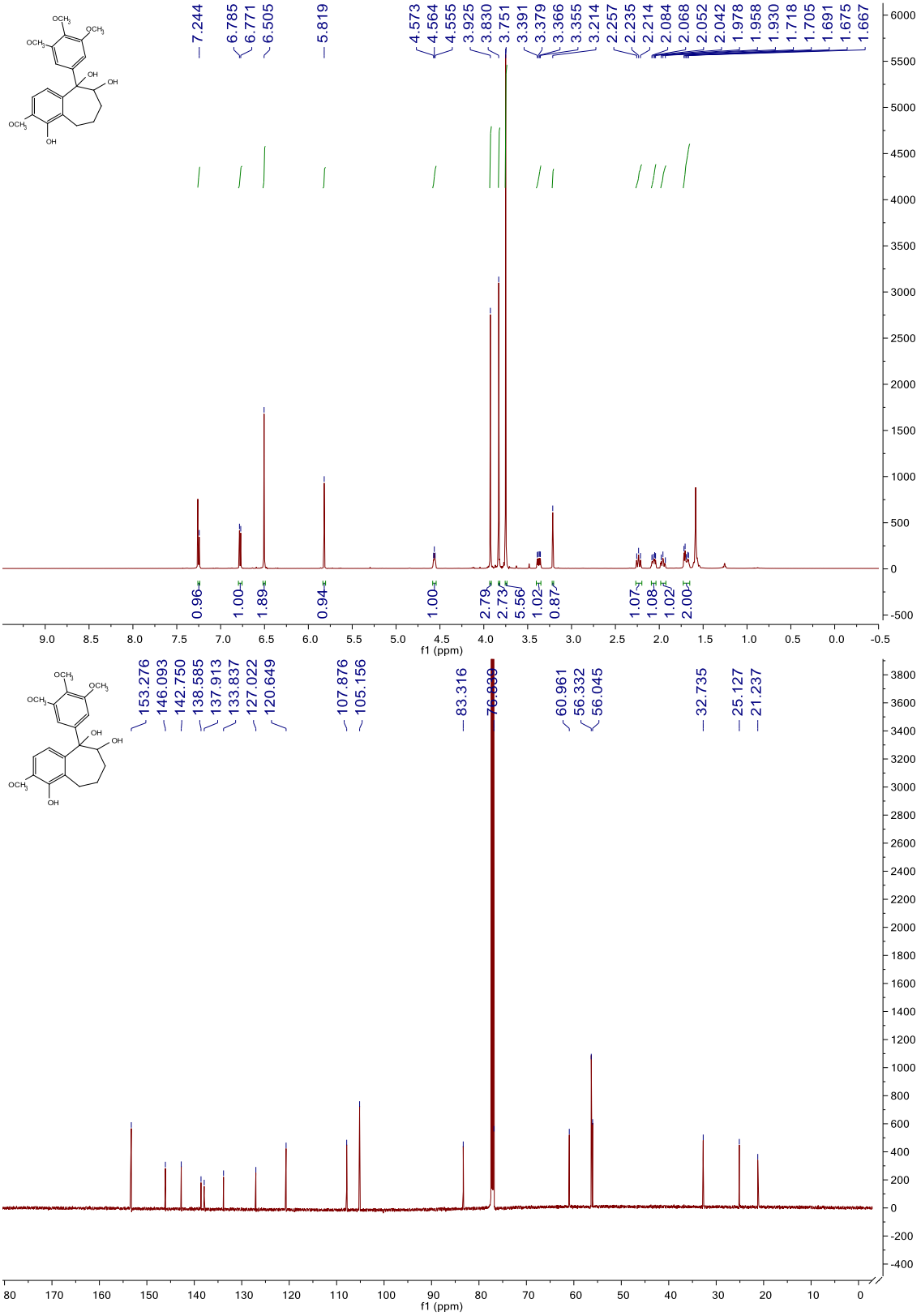
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.057	BB	0.0691	17.22527	3.64822	15.5859
2	20.336	BB	0.0912	85.20393	14.35921	77.0948
3	27.473	BB	0.0559	8.08915	2.15147	7.3193
Totals :				110.51835	20.15891	

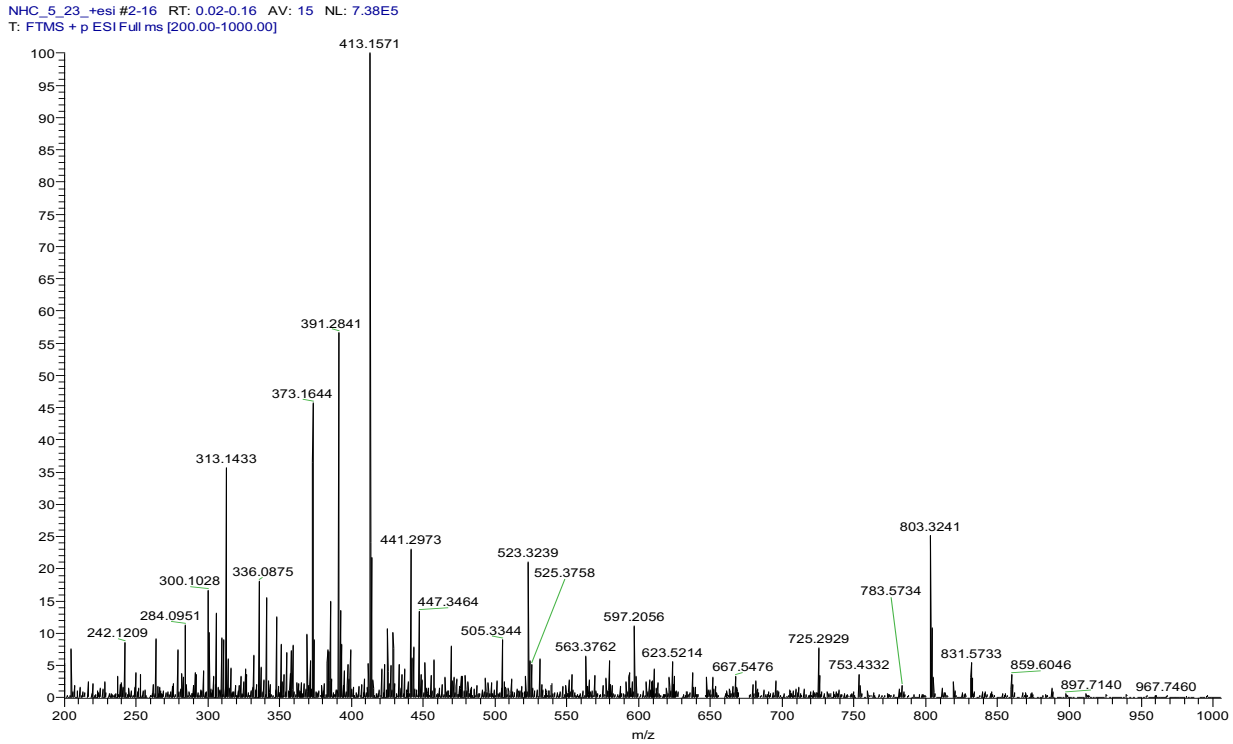
Signal 8: DAD1 H, Sig=320,16 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.057	BB	0.0679	15.75689	3.41272	35.8994
2	12.587	BB	0.1215	9.52415	1.11658	21.6992
3	20.336	BB	0.0922	10.25658	1.70470	23.3679
4	27.472	BB	0.0601	8.35416	2.11248	19.0335
Totals :				43.89178	8.34649	

*** End of Report ***

15. 2-methoxy-5-(3,4,5-trimethoxyphenyl)-6,7,8,9-tetrahydro-5H-benzo[7]annulene-1,5,6-triol



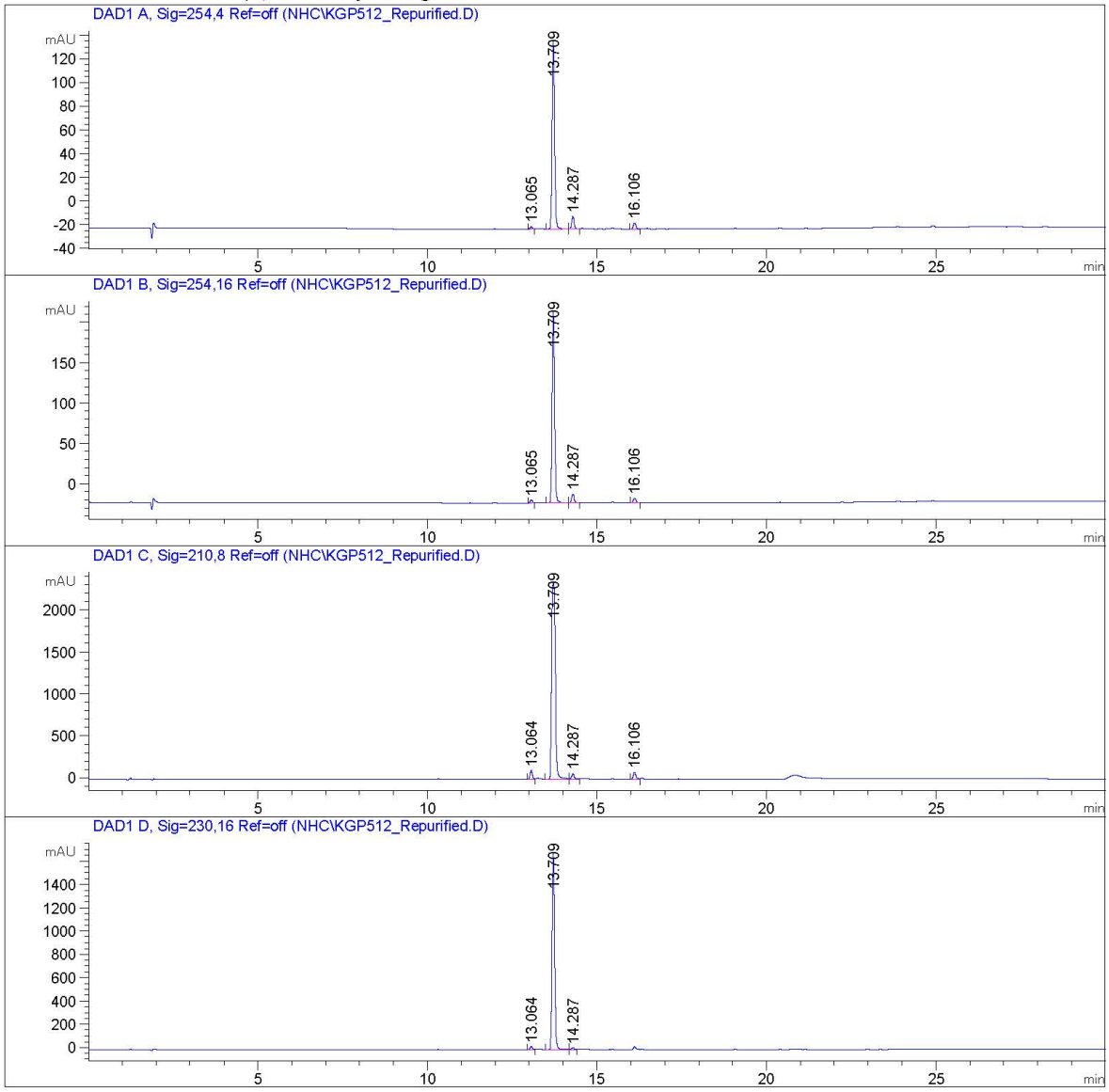

NHC_5_23_+esi #2-16 RT: 0.02-0.16 AV: 15 NL: 7.38E5
T: FTMS + p ESI Full ms [200.00-1000.00]
413.1571
391.2841
373.1644
313.1433
441.2973
523.3239
525.3758
803.3241
336.0875
300.1028
783.5734
447.3464
284.0951
597.2056
505.3344
242.1209
725.2929
563.3762
623.5214
831.5733
753.4332
667.5476
859.6046
897.7140
967.7460
m/z

Data File C:\Chem32\1\Data\NHC\KGP512_Repurified.D
Sample Name: KGP512_Repurified

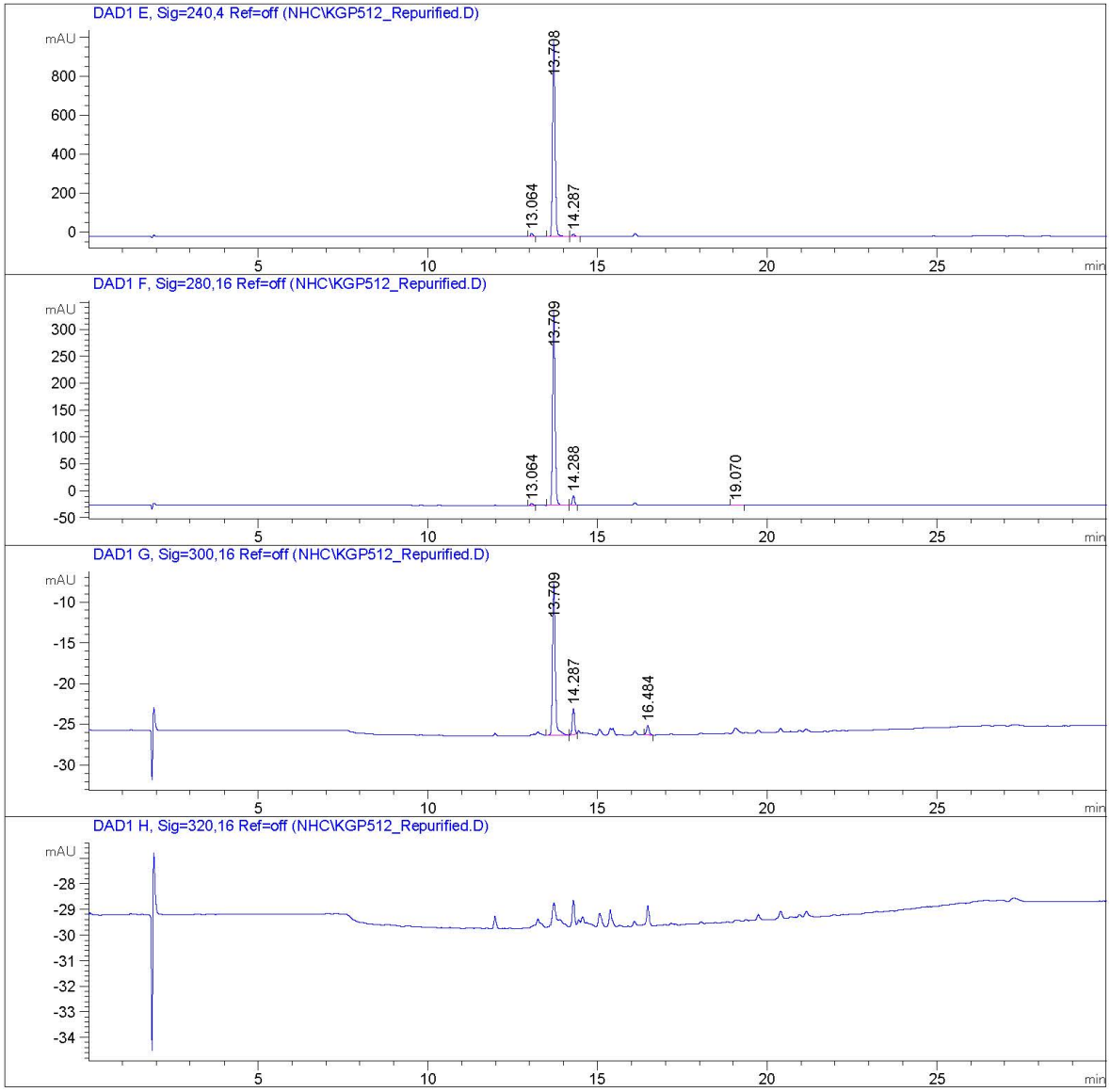
```
==========================================================================
Acq. Operator   : SYSTEM
Sample Operator : SYSTEM
Acq. Instrument : 1200 HPLC                    Location :   1
Injection Date  : 8/23/2017 9:28:27 AM
                                             Inj Volume : No inj
Acq. Method     : C:\CHEM32\1\METHODS\MASTERMETHOD2.M
Last changed    : 12/2/2015 12:37:42 PM by Eric Lin
Analysis Method : C:\CHEM32\1\METHODS\RT-ACNWASH 2.M
Last changed    : 7/9/2015 2:27:22 PM by Blake
Method Info     : General Column Wash Method

Sample Info     : sample

Additional Info : Peak(s) manually integrated
```



Data File C:\Chem32\1\Data\NHC\KGP512_Repurified.D
Sample Name: KGP512_Repurified



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Area Percent Report

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Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Data File C:\Chem32\1\Data\NHC\KGP512_Repurified.D
Sample Name: KGP512_Repurified

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.065	BB	0.0701	9.77358	2.18956	1.0897
2	13.709	BB	0.0768	803.74414	159.43422	89.6147
3	14.287	BV	0.0774	53.67685	10.53643	5.9848
4	16.106	BV	0.0852	29.69427	5.31389	3.3108
Totals :				896.88884	177.47410	

Signal 2: DAD1 B, Sig=254,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.065	BB	0.0707	14.80410	3.27786	1.1408
2	13.709	BB	0.0764	1192.41064	238.00854	91.8902
3	14.287	BV	0.0773	56.18486	11.06061	4.3297
4	16.106	BV	0.0854	34.24756	6.11318	2.6392
Totals :				1297.64717	258.46019	

Signal 3: DAD1 C, Sig=210,8 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.064	BV	0.0737	503.09753	105.46986	2.6442
2	13.709	BV	0.1216	1.76493e4	2351.60596	92.7631
3	14.287	VV	0.0888	395.12784	65.10931	2.0768
4	16.106	BV	0.0856	478.67270	85.10723	2.5159
Totals :				1.90262e4	2607.29237	

Signal 4: DAD1 D, Sig=230,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.064	BV	0.0745	136.84071	28.25139	1.5156
2	13.709	BV	0.0806	8801.68359	1694.72278	97.4875
3	14.287	VV	0.0841	89.99856	15.89352	0.9968
Totals :				9028.52287	1738.86769	

Data File C:\Chem32\1\Data\NHC\KGP512_Repurified.D
Sample Name: KGP512_Repurified

Signal 5: DAD1 E, Sig=240,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.064	BV	0.0753	74.07280	15.07936	1.4233
2	13.708	BV	0.0764	5061.45850	1011.85809	97.2548
3	14.287	VV	0.0864	68.79644	11.72970	1.3219
Totals :				5204.32774	1038.66716	

Signal 6: DAD1 F, Sig=280,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.064	BV	0.0791	17.30797	3.30291	0.9096
2	13.709	BB	0.0757	1789.19055	362.00397	94.0249
3	14.288	BV	0.0758	86.48084	17.46020	4.5447
4	19.070	BB	0.1397	9.91008	1.05404	0.5208
Totals :				1902.88944	383.82111	

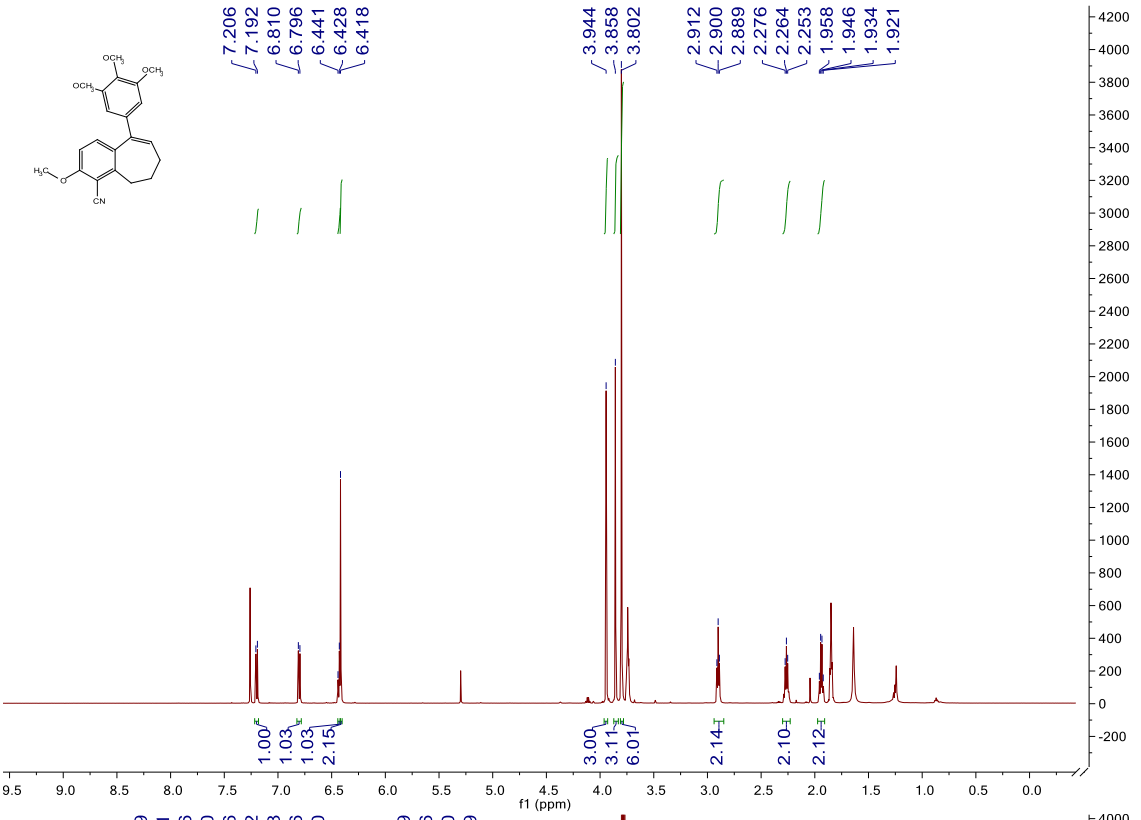
Signal 7: DAD1 G, Sig=300,16 Ref=off

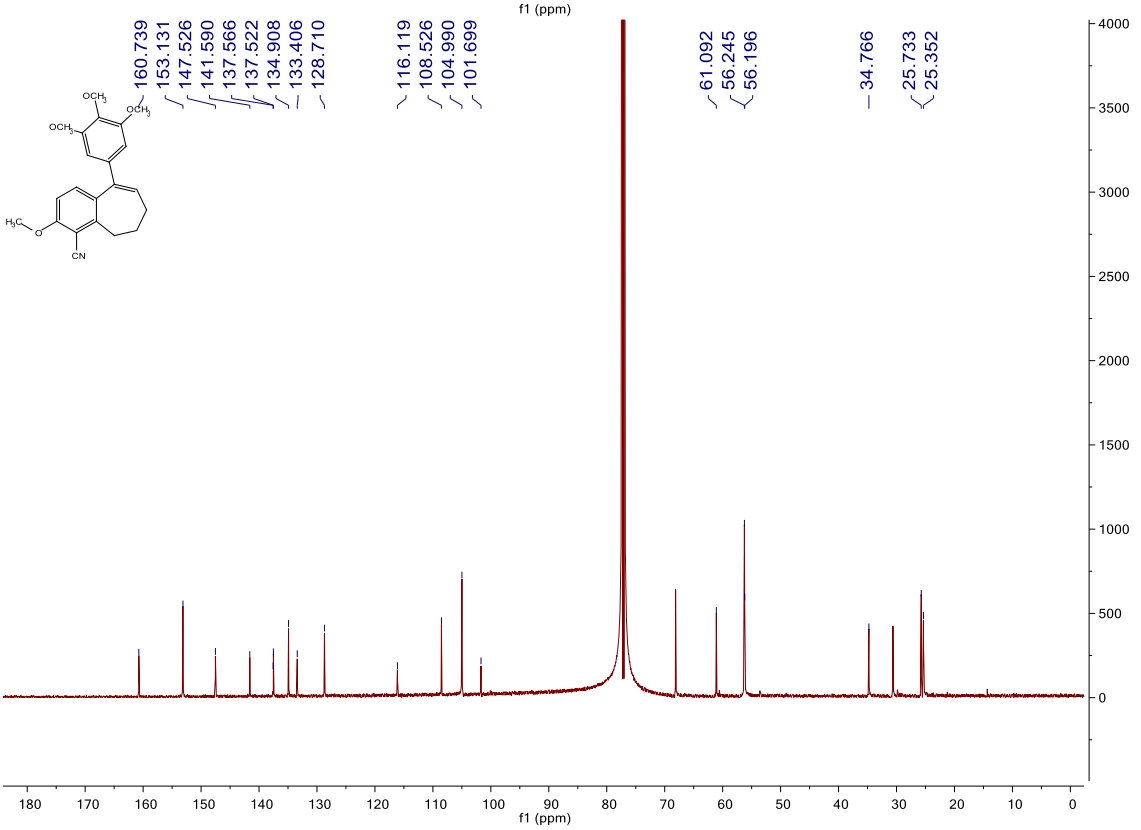
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.709	BB	0.0833	102.49873	18.90524	82.9384
2	14.287	BV	0.0750	15.30013	3.13398	12.3803
3	16.484	BB	0.0806	5.78537	1.11370	4.6813
Totals :				123.58423	23.15292	

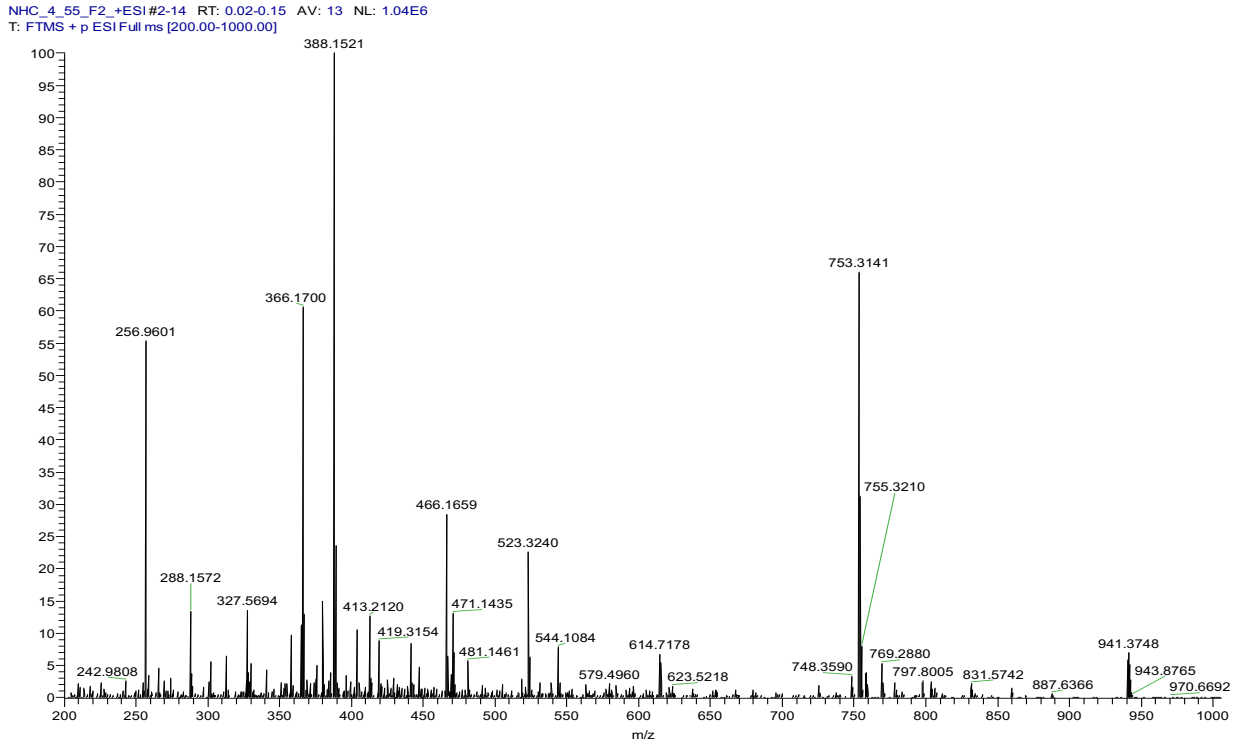
Signal 8: DAD1 H, Sig=320,16 Ref=off

*** End of Report ***

18. 3-methoxy-9-(3,4,5-trimethoxyphenyl)-6,7-dihydro-5H-benzo[7]annulene-4-carbonitrile





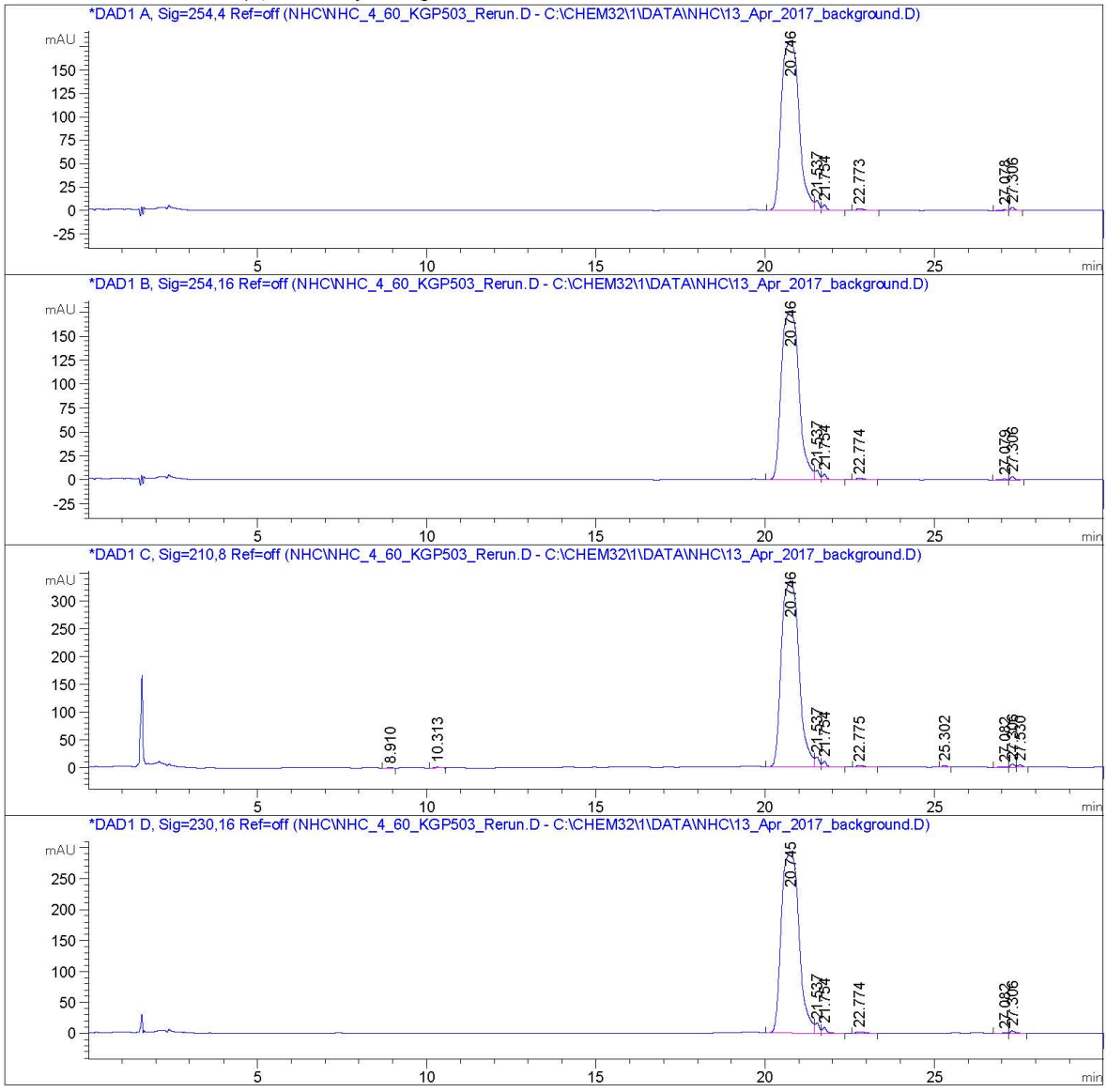

NHC_4_55_F2_+ESI #2-14 RT: 0.02-0.15 AV: 13 NL: 1.04E6
T: FTMS + p ESI Full ms [200.00-1000.00]
388.1521
753.3141
366.1700
256.9601
755.3210
466.1659
523.3240
288.1572
327.5694
413.2120
471.1435
419.3154
544.1084
481.1461
614.7178
769.2880
941.3748
748.3590
797.8005
831.5742
943.8765
579.4960
623.5218
887.6366
970.6692
242.9808
m/z

Data File C:\Chem32\1\Data\NHC\NHC_4_60_KGP503_Rerun.D
Sample Name: KGP503_NHC_4_60_Rerun

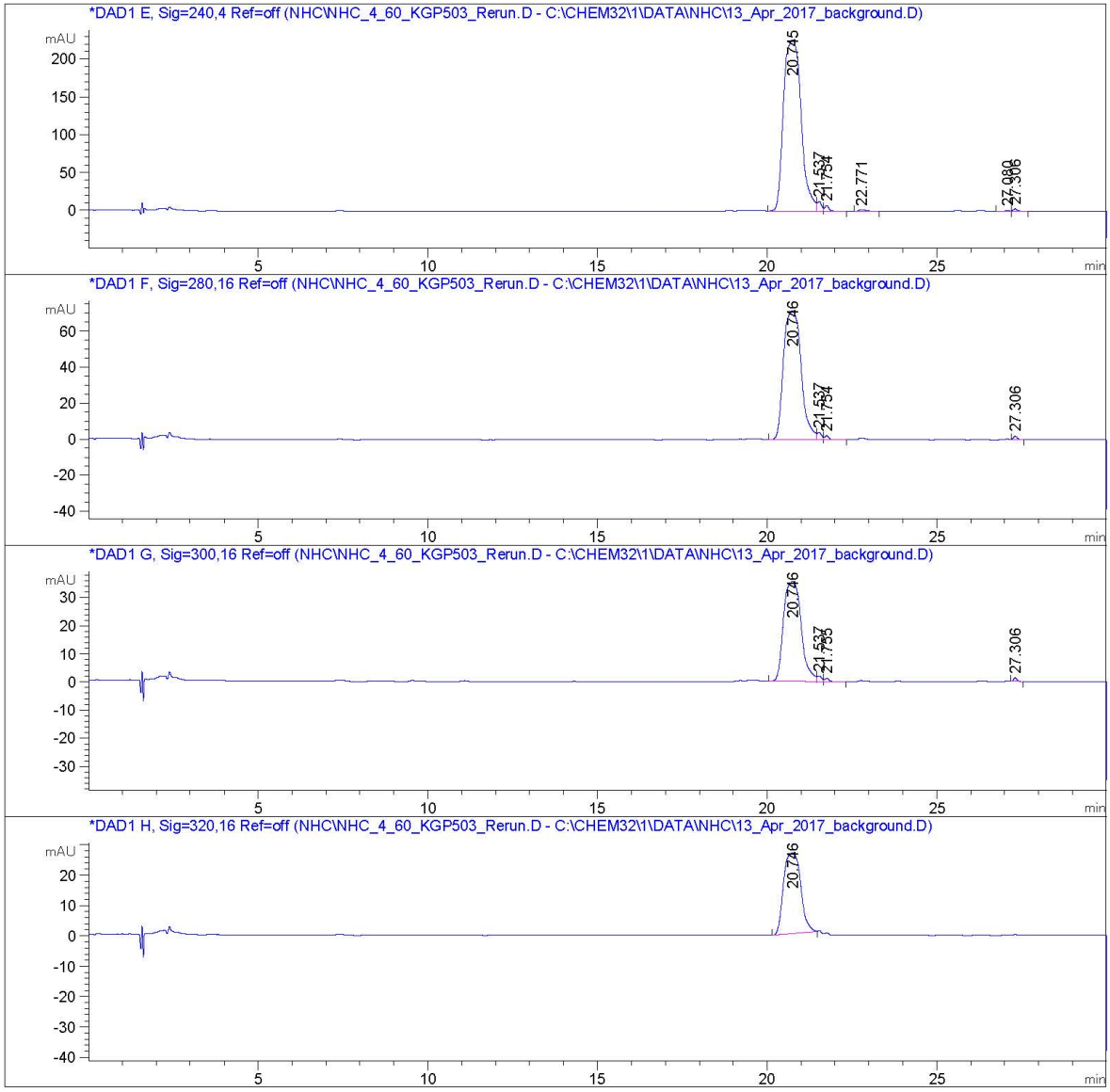
```
==========================================================================
Acq. Operator   : SYSTEM
Sample Operator : SYSTEM
Acq. Instrument : 1200 HPLC                    Location :   1
Injection Date  : 4/13/2017 6:13:07 PM
                                              Inj Volume : No inj
Acq. Method     : C:\Chem32\1\Methods\MASTERMETHOD2.M
Last changed    : 12/2/2015 12:37:42 PM by Eric Lin
Analysis Method : C:\CHEM32\1\METHODS\RT-ACNWASH 2.M
Last changed    : 7/9/2015 2:27:22 PM by Blake
Method Info     : General Column Wash Method

Sample Info     : sample

Additional Info : Peak(s) manually integrated
```



Data File C:\Chem32\1\Data\NHC\NHC_4_60_KGP503_Rerun.D
Sample Name: KGP503_NHC_4_60_Rerun



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Area Percent Report

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Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Data File C:\Chem32\1\Data\NHC\NHC_4_60_KGP503_Rerun.D
Sample Name: KGP503_NHC_4_60_Rerun

Signal 1: DAD1 A, Sig=254,4 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	20.746	BV	0.5806	6496.62305	181.07161	96.8448
2	21.537	VV	0.1249	87.63673	10.13339	1.3064
3	21.754	VB	0.1259	48.88611	5.70871	0.7287
4	22.773	BB	0.2493	28.75137	1.68332	0.4286
5	27.078	BV	0.1778	15.20079	1.19977	0.2266
6	27.306	VB	0.1239	31.18135	3.71487	0.4648
Totals :				6708.27940	203.51166	

Signal 2: DAD1 B, Sig=254,16 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	20.746	BV	0.5806	6318.01221	176.10487	96.8661
2	21.537	VV	0.1249	85.17250	9.85030	1.3058
3	21.754	VB	0.1260	47.56451	5.54766	0.7292
4	22.774	BB	0.2526	26.80340	1.57420	0.4109
5	27.079	BV	0.1803	14.68895	1.15591	0.2252
6	27.306	VB	0.1249	30.17599	3.56095	0.4627
Totals :				6522.41755	197.79389	

Signal 3: DAD1 C, Sig=210,8 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.910	BB	0.2193	19.95940	1.13417	0.1596
2	10.313	BB	0.0907	11.23343	1.80299	0.0899
3	20.746	BV	0.5806	1.20101e4	334.73129	96.0626
4	21.537	VV	0.1248	161.23265	18.66839	1.2896
5	21.754	VB	0.1269	91.25467	10.55160	0.7299
6	22.775	BB	0.2788	55.21412	3.14467	0.4416
7	25.302	BB	0.1264	28.33697	3.50110	0.2267
8	27.082	BV	0.1789	24.07454	1.91226	0.1926
9	27.306	VV	0.1174	52.81111	6.74406	0.4224
10	27.530	VB	0.1599	48.15096	4.53419	0.3851
Totals :				1.25023e4	386.72474	

Data File C:\Chem32\1\Data\NHC\NHC_4_60_KGP503_Rerun.D
Sample Name: KGP503_NHC_4_60_Rerun

Signal 4: DAD1 D, Sig=230,16 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	20.745	BV	0.5804	1.05244e4	293.48941	97.0376
2	21.537	VV	0.1248	140.95088	16.32036	1.2996
3	21.754	VB	0.1272	79.96591	9.21827	0.7373
4	22.774	BB	0.2516	36.94115	2.15940	0.3406
5	27.082	BV	0.1828	19.33566	1.49573	0.1783
6	27.306	VB	0.1401	44.10019	4.50837	0.4066
Totals :				1.08457e4	327.19153	

Signal 5: DAD1 E, Sig=240,4 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	20.745	BV	0.5805	8119.95264	226.37668	97.1078
2	21.537	VV	0.1249	108.94429	12.60018	1.3029
3	21.754	VB	0.1275	61.87254	7.10915	0.7399
4	22.771	BB	0.2471	25.56801	1.49789	0.3058
5	27.080	BV	0.1745	14.83483	1.19784	0.1774
6	27.306	VB	0.1345	30.61814	3.29323	0.3662
Totals :				8361.79044	252.07496	

Signal 6: DAD1 F, Sig=280,16 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	20.746	BV	0.5806	2565.01343	71.48746	97.3831
2	21.537	VV	0.1244	34.30706	3.98565	1.3025
3	21.754	VB	0.1269	19.40143	2.24244	0.7366
4	27.306	BB	0.1114	15.21854	2.07902	0.5778
Totals :				2633.94046	79.79456	

Signal 7: DAD1 G, Sig=300,16 Ref=off
Signal has been modified after loading from rawdata file!

Data File C:\Chem32\1\Data\NHC\NHC_4_60_KGP503_Rerun.D
Sample Name: KGP503_NHC_4_60_Rerun

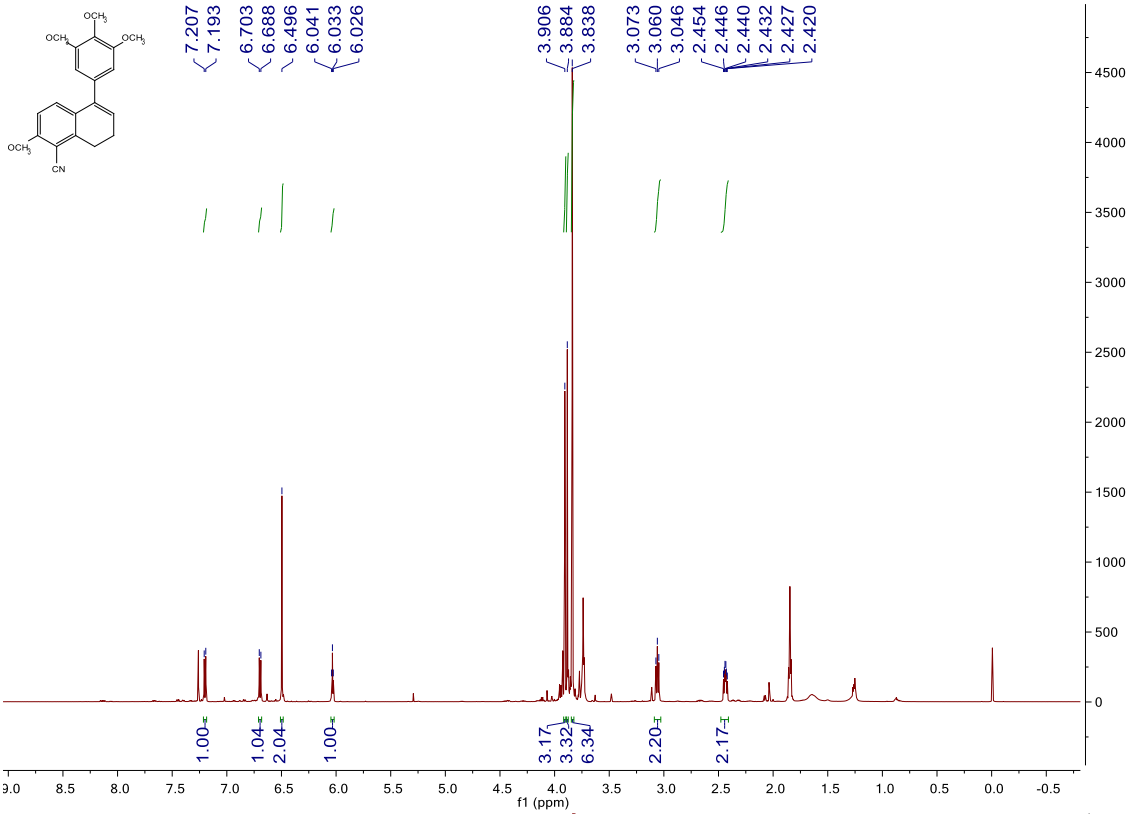
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	20.746	BV	0.5805	1271.03320	35.42966	97.2825
2	21.537	VV	0.1247	17.07931	1.97868	1.3072
3	21.755	VB	0.1249	9.63400	1.11392	0.7374
4	27.306	BB	0.1101	8.79221	1.21982	0.6729
Totals :				1306.53873	39.74207	

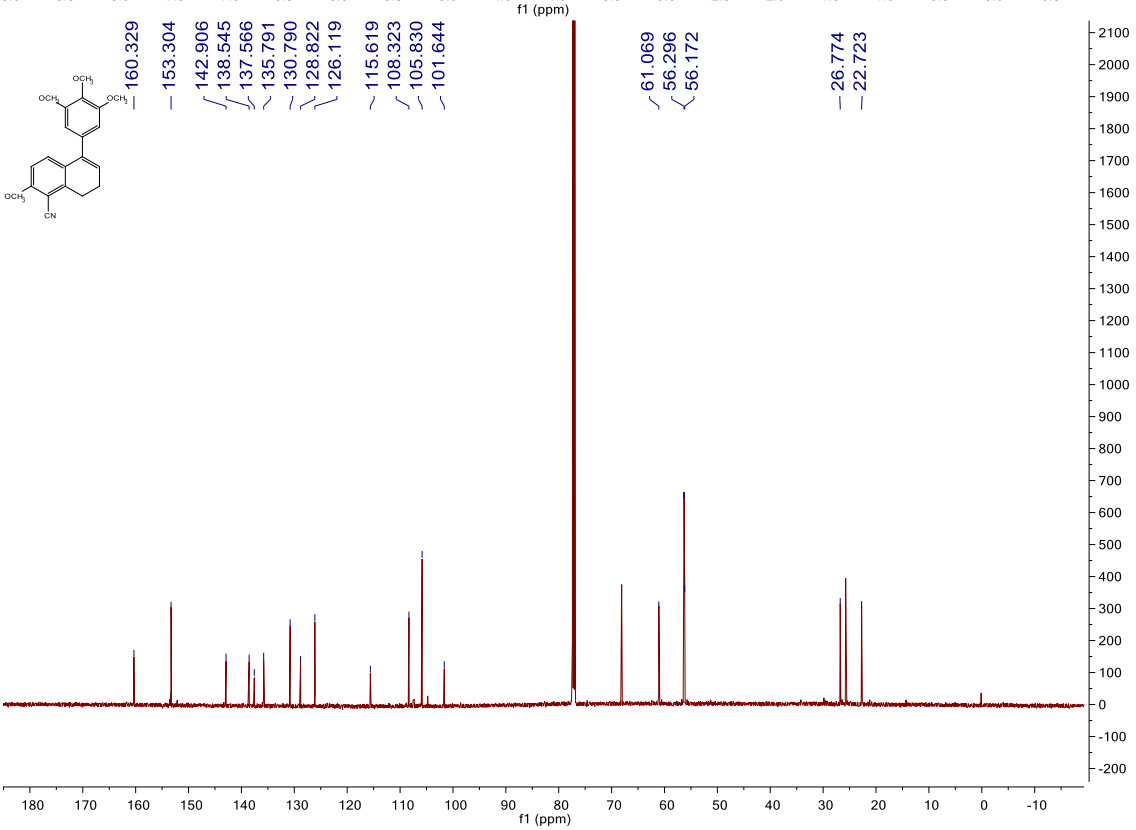
Signal 8: DAD1 H, Sig=320,16 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	20.746	BB	0.5668	923.98254	26.62748	100.0000
Totals :				923.98254	26.62748	

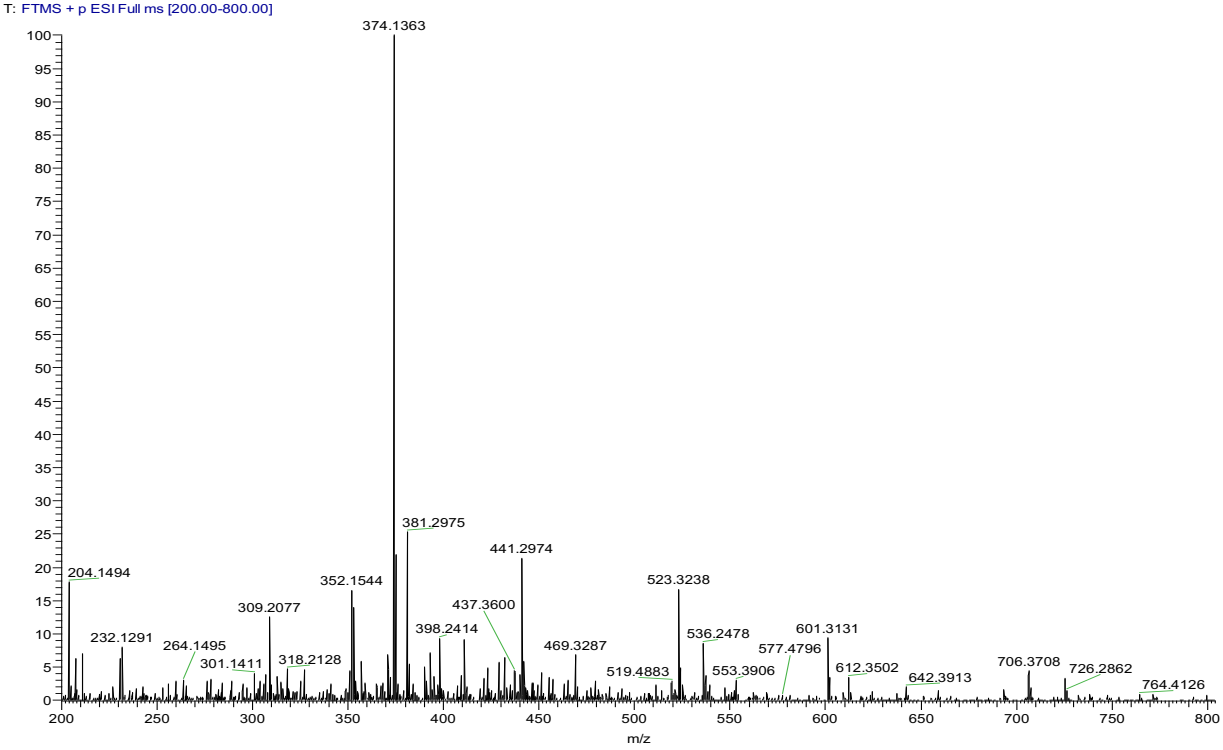
*** End of Report ***

19. 2-methoxy-5-(3,4,5-trimethoxyphenyl)-7,8-dihydronaphthalene-1-carbonitrile





NHC_3_79_nitrile group_Orbi+ESI #1-43 RT: 0.01-0.37 AV: 43 NL: 1.95E6
T: FTMS + p ESI Full ms [200.00-800.00]



Data File C:\Chem32\1\Data\NHC\KGP483-Repurified-20160628.D
Sample Name: KGP483-Repurified-20160628

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======================================================================
Acq. Operator   : SYSTEM
Sample Operator : SYSTEM
Acq. Instrument : 1200 HPLC                    Location :     -
Injection Date  : 6/28/2016 11:50:12 AM
                                             Inj Volume : No inj
Acq. Method     : C:\CHEM32\1\METHODS\MASTERMETHOD2.M
Last changed    : 12/2/2015 12:37:42 PM by Eric Lin
Analysis Method : C:\CHEM32\1\METHODS\RT-ACNWASH 2.M
Last changed    : 7/9/2015 2:27:22 PM by Blake
Method Info     : General Column Wash Method

Additional Info : Peak(s) manually integrated
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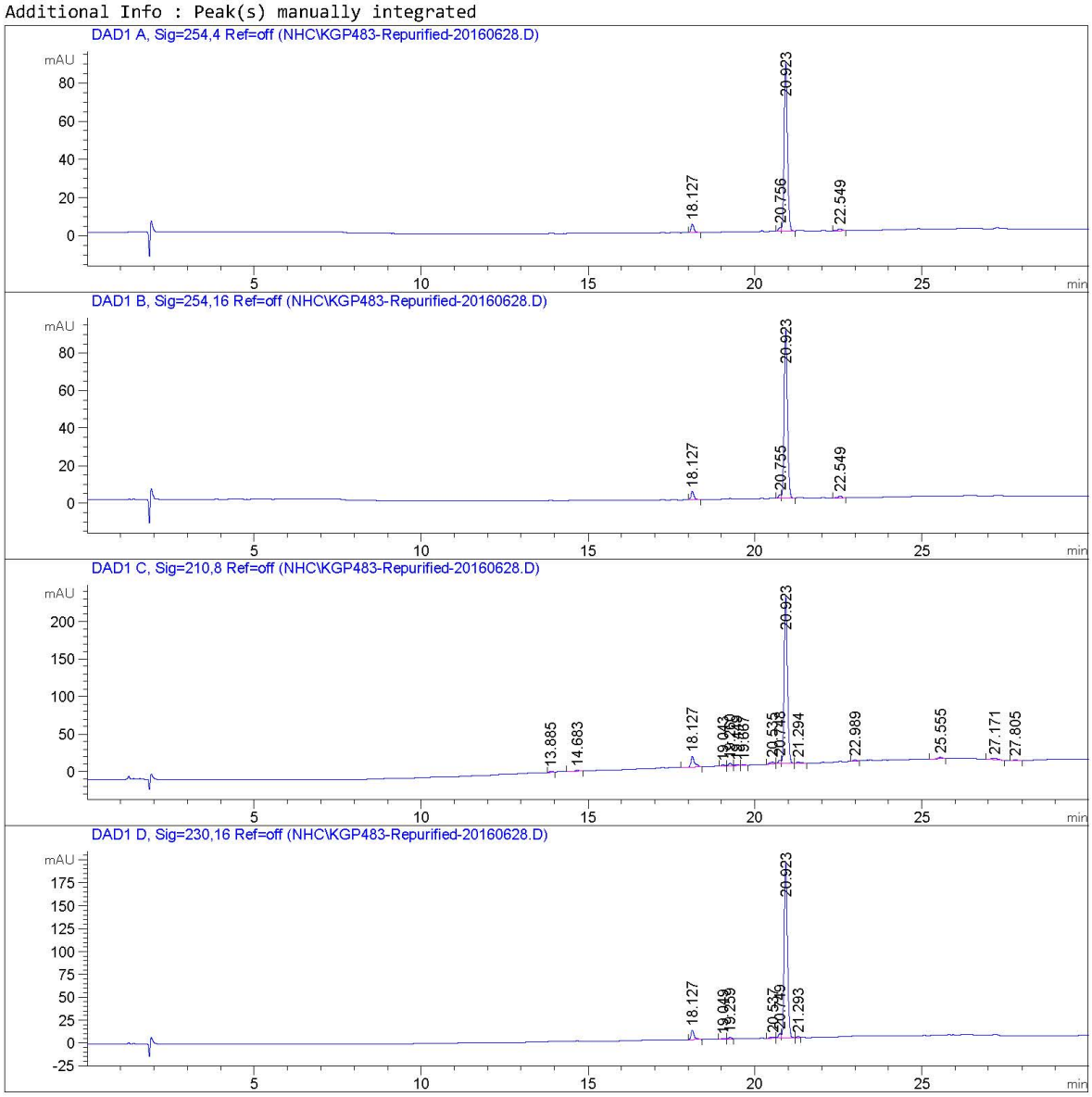
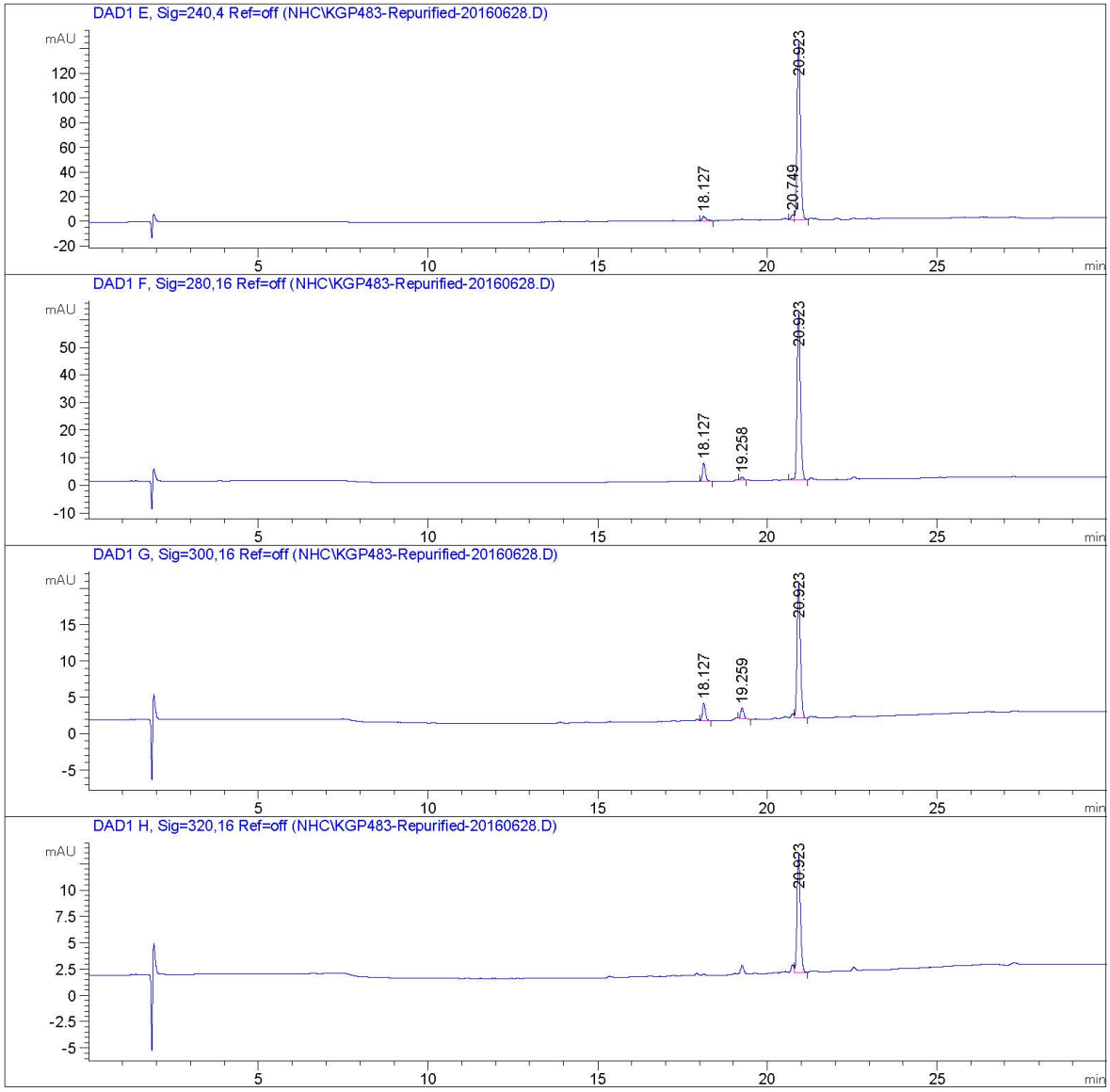


Data File C:\Chem32\1\Data\NHC\KGP483-Repurified-20160628.D
Sample Name: KGP483-Repurified-20160628



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Area Percent Report

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Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Data File C:\Chem32\1\Data\NHC\KGP483-Repurified-20160628.D
Sample Name: KGP483-Repurified-20160628

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.127	BB	0.0969	27.52547	4.40697	4.3551
2	20.756	BV	0.0855	10.64724	1.95639	1.6846
3	20.923	VB	0.1028	586.03583	89.03397	92.7231
4	22.549	BB	0.1083	7.81904	1.10814	1.2371
Totals :				632.02759	96.50547	

Signal 2: DAD1 B, Sig=254,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.127	BB	0.0974	27.72689	4.40723	4.3001
2	20.755	BV	0.0852	10.39476	1.91779	1.6121
3	20.923	VV	0.1029	598.92731	90.91395	92.8865
4	22.549	BB	0.1084	7.74590	1.09634	1.2013
Totals :				644.79486	98.33531	

Signal 3: DAD1 C, Sig=210,8 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.885	BB	0.0883	6.42959	1.13223	0.3603
2	14.683	BB	0.1255	9.13448	1.04989	0.5119
3	18.127	BB	0.1134	111.79525	14.58452	6.2650
4	19.043	BV	0.1023	12.28498	1.83074	0.6884
5	19.260	VV	0.1059	25.93017	3.69388	1.4531
6	19.449	VV	0.1173	10.99650	1.40448	0.6162
7	19.667	VB	0.1030	7.81470	1.15372	0.4379
8	20.535	BB	0.1283	24.38312	2.62631	1.3664
9	20.748	BV	0.0844	22.24938	4.16101	1.2468
10	20.923	VV	0.1024	1471.93042	224.68059	82.4866
11	21.294	VB	0.1225	16.36377	1.89992	0.9170
12	22.989	BB	0.0973	11.10314	1.76728	0.6222
13	25.555	BB	0.1172	15.61706	2.09044	0.8752
14	27.171	BB	0.2373	26.69373	1.71804	1.4959
15	27.805	BB	0.1501	11.72167	1.21965	0.6569
Totals :				1784.44796	265.01271	

Data File C:\Chem32\1\Data\NHC\KGP483-Repurified-20160628.D
Sample Name: KGP483-Repurified-20160628

Signal 4: DAD1 D, Sig=230,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.127	BB	0.1033	71.34565	10.49653	5.0712
2	19.049	BV	0.1174	9.14095	1.16693	0.6497
3	19.259	VV	0.1052	15.23248	2.18955	1.0827
4	20.537	BB	0.1186	9.69208	1.14647	0.6889
5	20.749	BV	0.0854	25.20602	4.63971	1.7916
6	20.923	VB	0.1026	1268.52246	193.30789	90.1650
7	21.293	BV	0.0905	7.75009	1.32033	0.5509
Totals :				1406.88974	214.26741	

Signal 5: DAD1 E, Sig=240,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.127	BB	0.1068	25.16262	3.54622	2.5109
2	20.749	BV	0.0865	20.52419	3.70993	2.0481
3	20.923	VB	0.1026	956.43463	145.60522	95.4410
Totals :				1002.12143	152.86138	

Signal 6: DAD1 F, Sig=280,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.127	BB	0.0966	40.78636	6.55303	9.0081
2	19.258	BB	0.0897	6.65932	1.18173	1.4708
3	20.923	BV	0.1032	405.33044	61.26882	89.5212
Totals :				452.77612	69.00358	

Signal 7: DAD1 G, Sig=300,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.127	BB	0.0949	14.47020	2.38239	9.8791
2	19.259	BB	0.0963	9.02615	1.45748	6.1623
3	20.923	VB	0.1026	122.97638	18.74084	83.9586
Totals :				146.47272	22.58071	

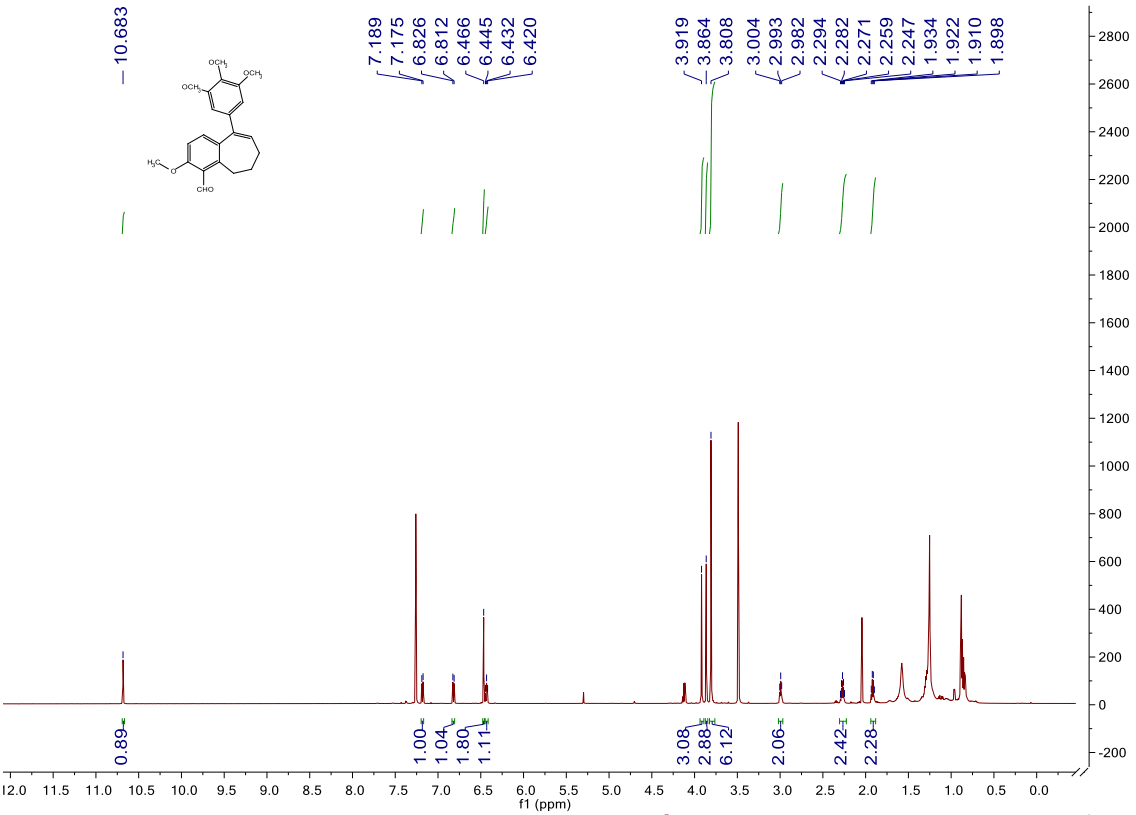
Data File C:\Chem32\1\Data\NHC\KGP483-Repurified-20160628.D
Sample Name: KGP483-Repurified-20160628

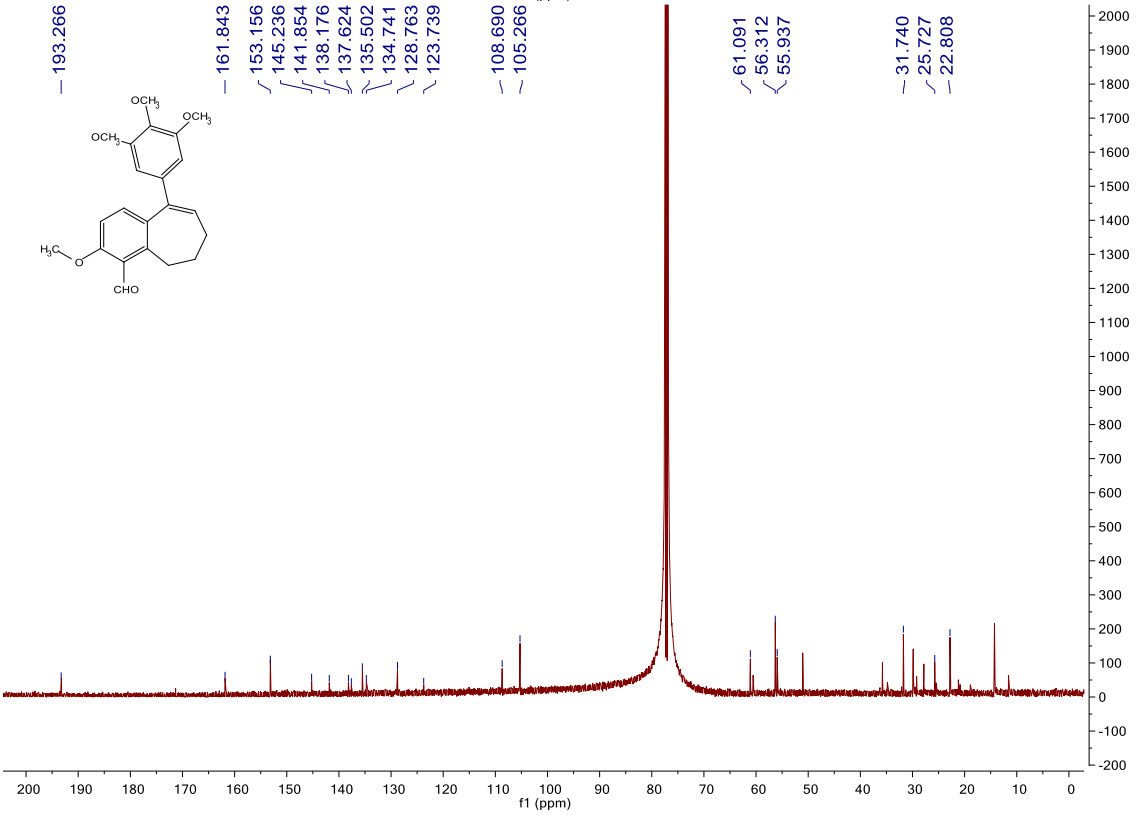
Signal 8: DAD1 H, Sig=320,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	20.923	VB	0.1028	74.78910	11.35700	100.0000
Totals :				74.78910	11.35700	

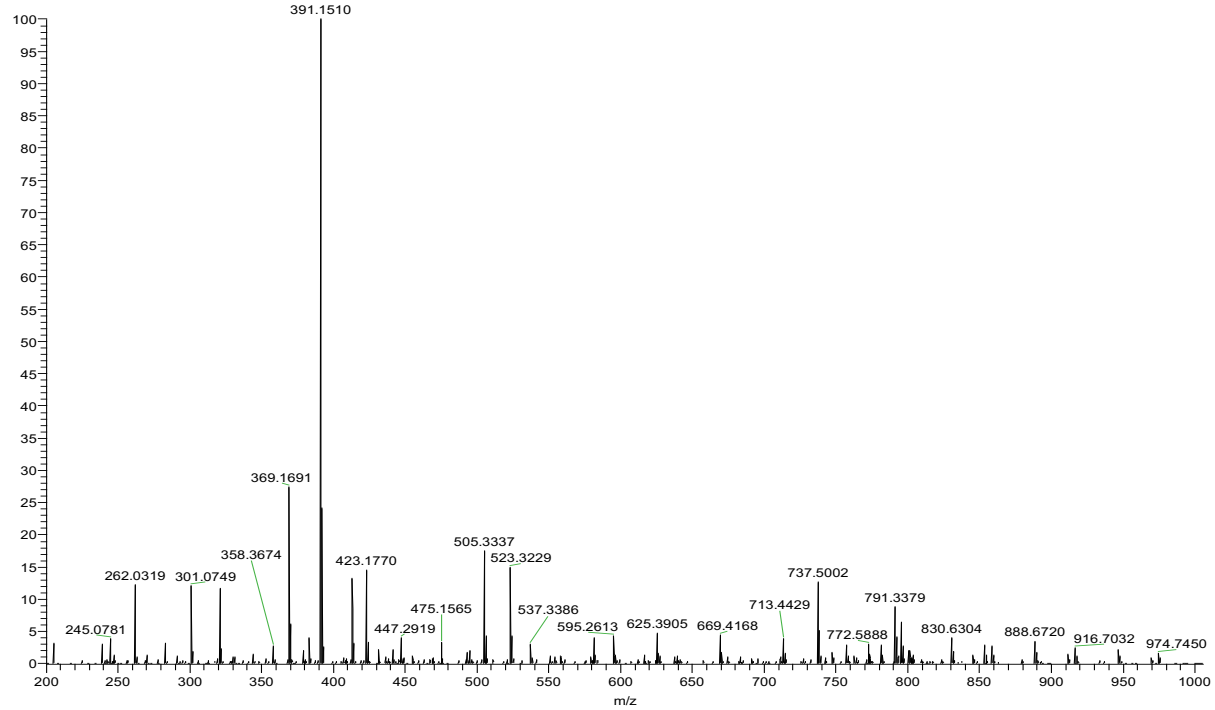
*** End of Report ***

20. 3-methoxy-9-(3,4,5-trimethoxyphenyl)-6,7-dihydro-5H-benzo[7]annulene-4-carbaldehyde





NHC_4_89_aldehyde_Cali #2-17 RT: 0.01-0.15 AV: 16 NL: 8.06E6
T: FTMS + p ESI Full ms [200.00-1000.00]



Data File C:\Chem32\1\Data\NHC\NHC_4_123_sample.D
Sample Name: NHC_4_123_sample

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Acq. Operator   : SYSTEM
Sample Operator : SYSTEM
Acq. Instrument : 1200 HPLC                    Location :     -
Injection Date  : 6/13/2017 9:38:03 AM
                                             Inj Volume : No inj
Acq. Method     : C:\Chem32\1\Methods\MASTERMETHOD2.M
Last changed    : 12/2/2015 12:37:42 PM by Eric Lin
Analysis Method : C:\CHEM32\1\METHODS\RT-ACNWASH 2.M
Last changed    : 7/9/2015 2:27:22 PM by Blake
Method Info     : General Column Wash Method

Sample Info     : run

Additional Info : Peak(s) manually integrated
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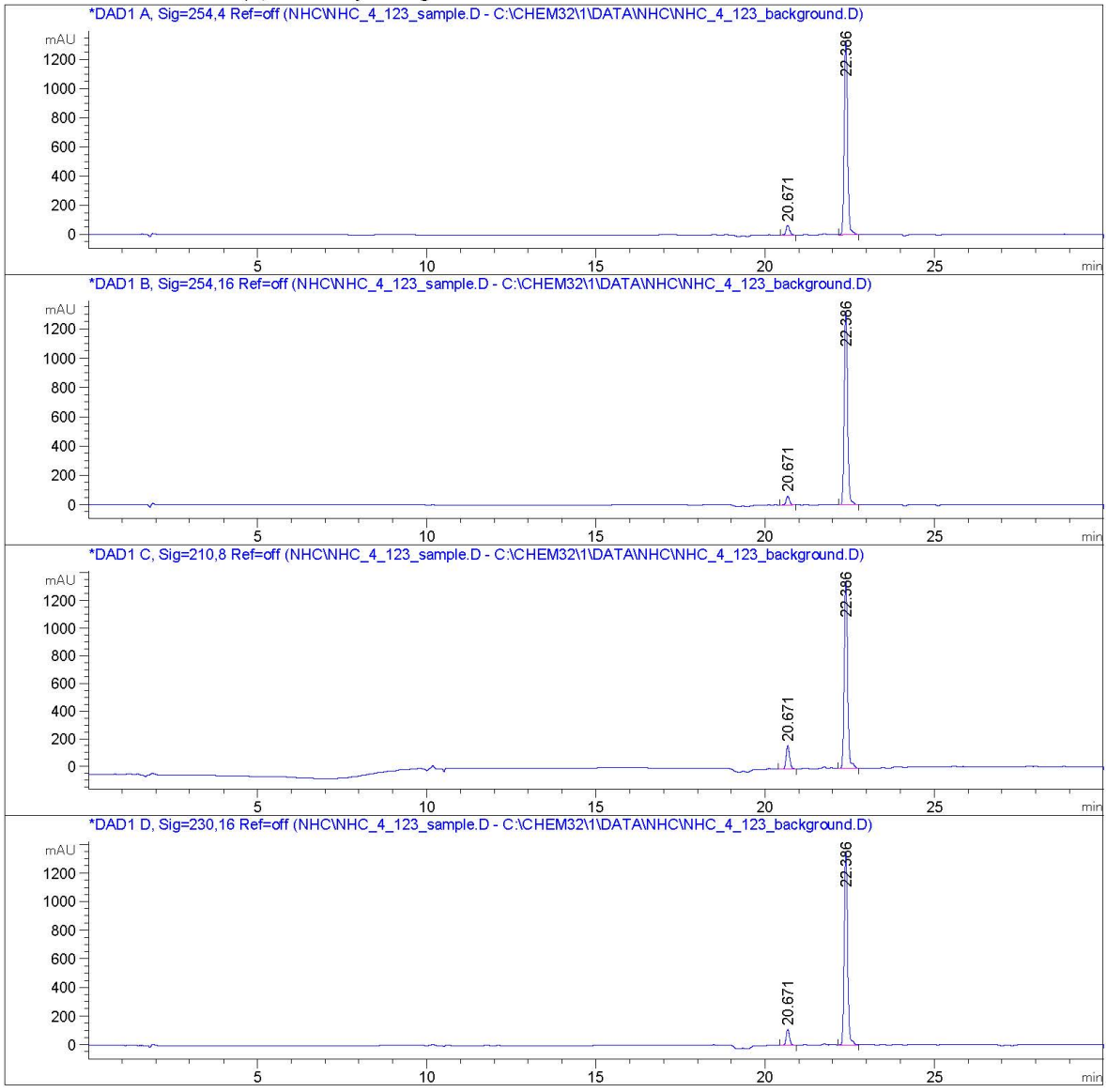
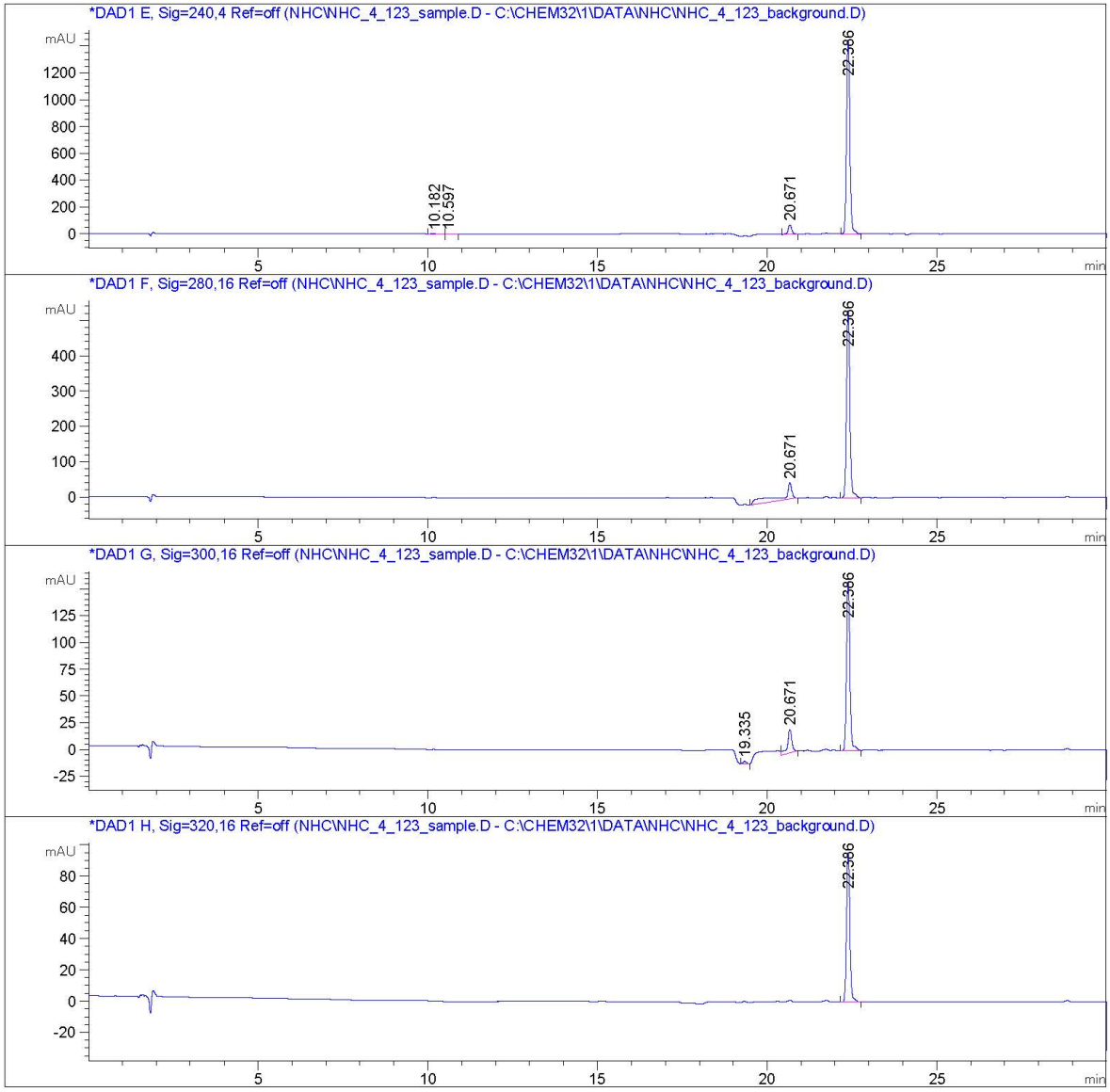


Data File C:\Chem32\1\Data\NHC\NHC_4_123_sample.D
Sample Name: NHC_4_123_sample



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Area Percent Report

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Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Data File C:\Chem32\1\Data\NHC\NHC_4_123_sample.D
Sample Name: NHC_4_123_sample

Signal 1: DAD1 A, Sig=254,4 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	20.671	BB	0.1050	433.03525	63.92846	4.4639
2	22.386	VV	0.1071	9267.71973	1333.79065	95.5361
Totals :				9700.75497	1397.71911	

Signal 2: DAD1 B, Sig=254,16 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	20.671	BB	0.1051	416.58456	61.43745	4.3303
2	22.386	VV	0.1070	9203.54297	1325.31763	95.6697
Totals :				9620.12753	1386.75507	

Signal 3: DAD1 C, Sig=210,8 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	20.671	BV	0.1057	1161.26270	170.09296	10.8772
2	22.386	VB	0.1079	9514.88281	1356.19568	89.1228
Totals :				1.06761e4	1526.28864	

Signal 4: DAD1 D, Sig=230,16 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	20.671	BB	0.1049	739.92719	109.43777	7.2504
2	22.386	VV	0.1075	9465.35449	1355.30701	92.7496
Totals :				1.02053e4	1464.74478	

Data File C:\Chem32\1\Data\NHC\NHC_4_123_sample.D
Sample Name: NHC_4_123_sample

Signal 5: DAD1 E, Sig=240,4 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.182	BB	0.1720	38.17877	2.89298	0.3557
2	10.597	BB	0.1553	15.93288	1.46076	0.1484
3	20.671	VB	0.1146	533.87170	70.33253	4.9741
4	22.386	VV	0.1075	1.01450e4	1451.47473	94.5217
Totals :				1.07330e4	1526.16101	

Signal 6: DAD1 F, Sig=280,16 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	20.671	BB	0.2770	989.67731	45.99776	21.2272
2	22.386	BB	0.1070	3672.63428	529.19031	78.7728
Totals :				4662.31158	575.18806	

Signal 7: DAD1 G, Sig=300,16 Ref=off
Signal has been modified after loading from rawdata file!

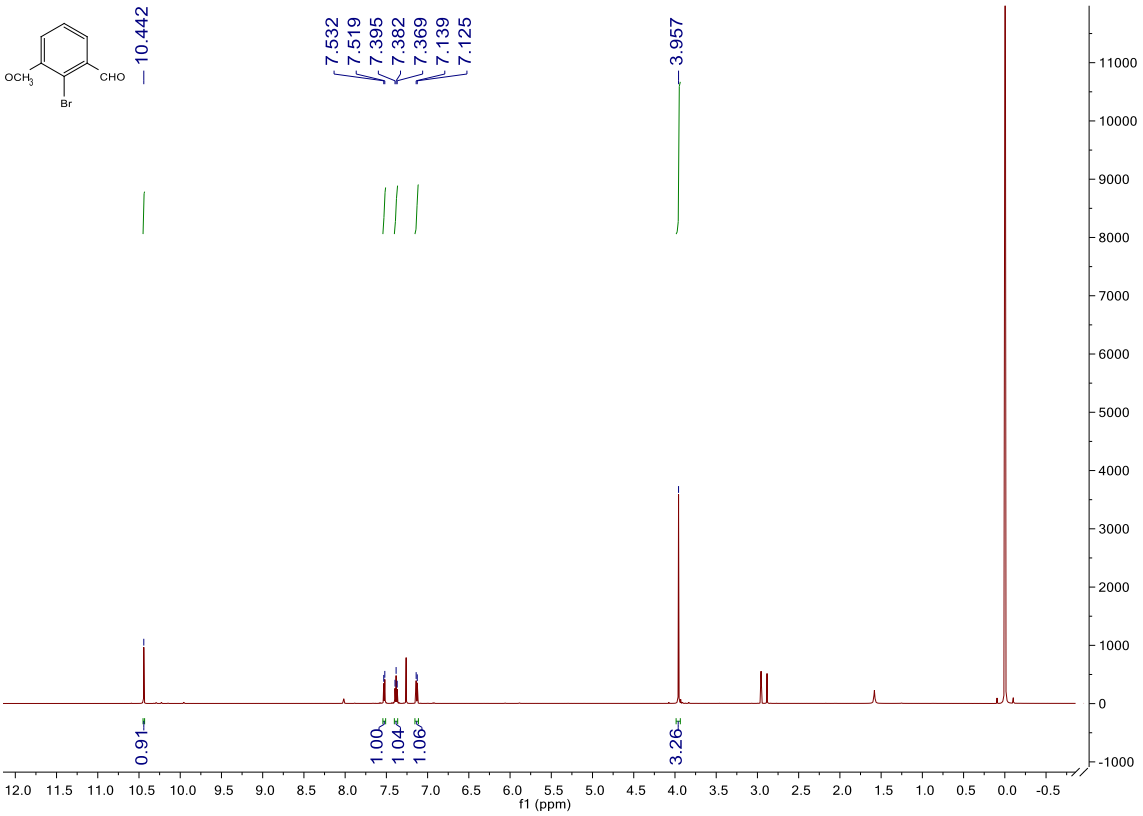
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.335	BB	0.1093	15.72323	2.25735	1.2006
2	20.671	VB	0.1297	194.43983	21.88058	14.8473
3	22.386	BB	0.1073	1099.43250	157.75989	83.9521
Totals :				1309.59556	181.89782	

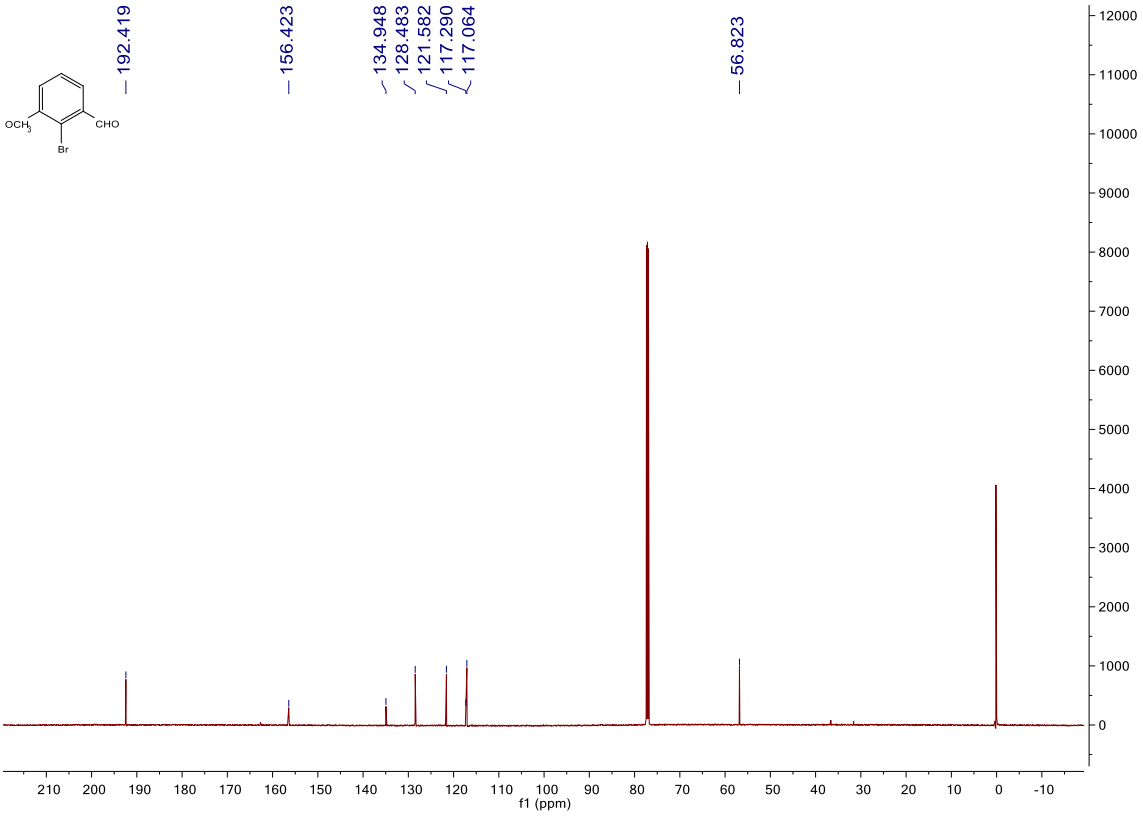
Signal 8: DAD1 H, Sig=320,16 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	22.386	BB	0.1064	658.00146	95.42596	100.0000
Totals :				658.00146	95.42596	

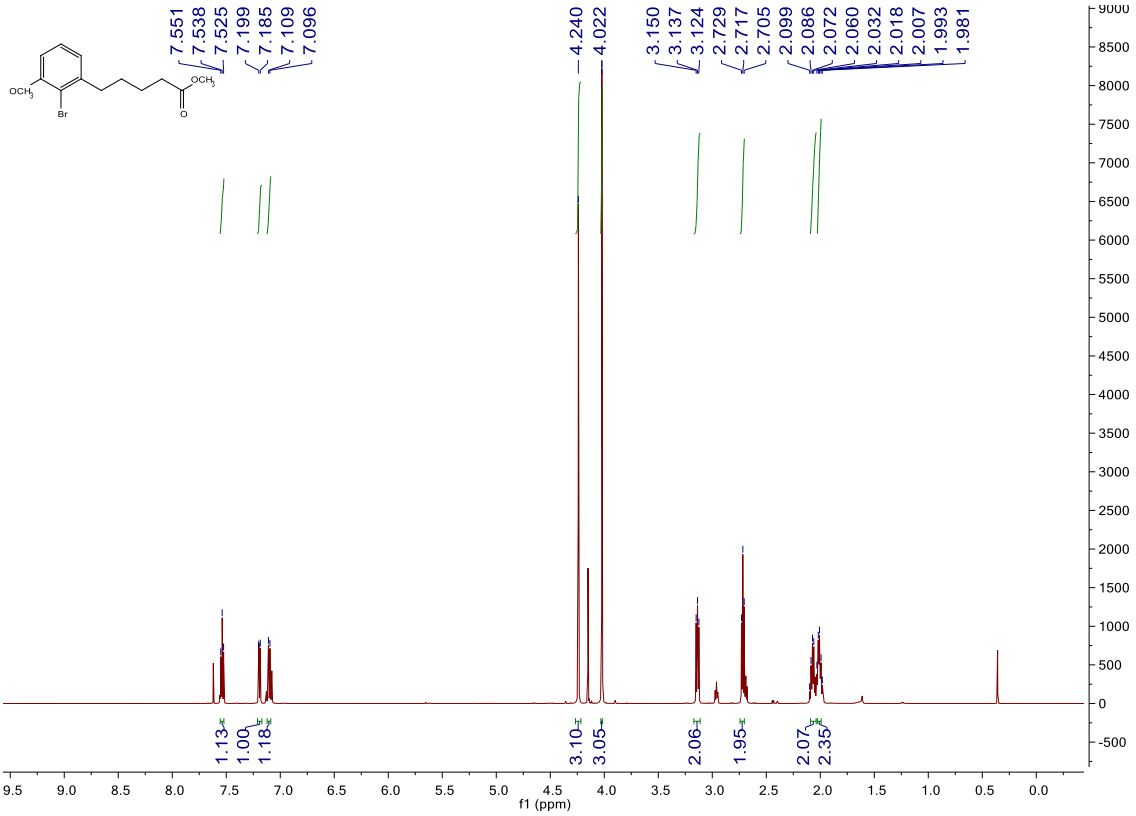
*** End of Report ***

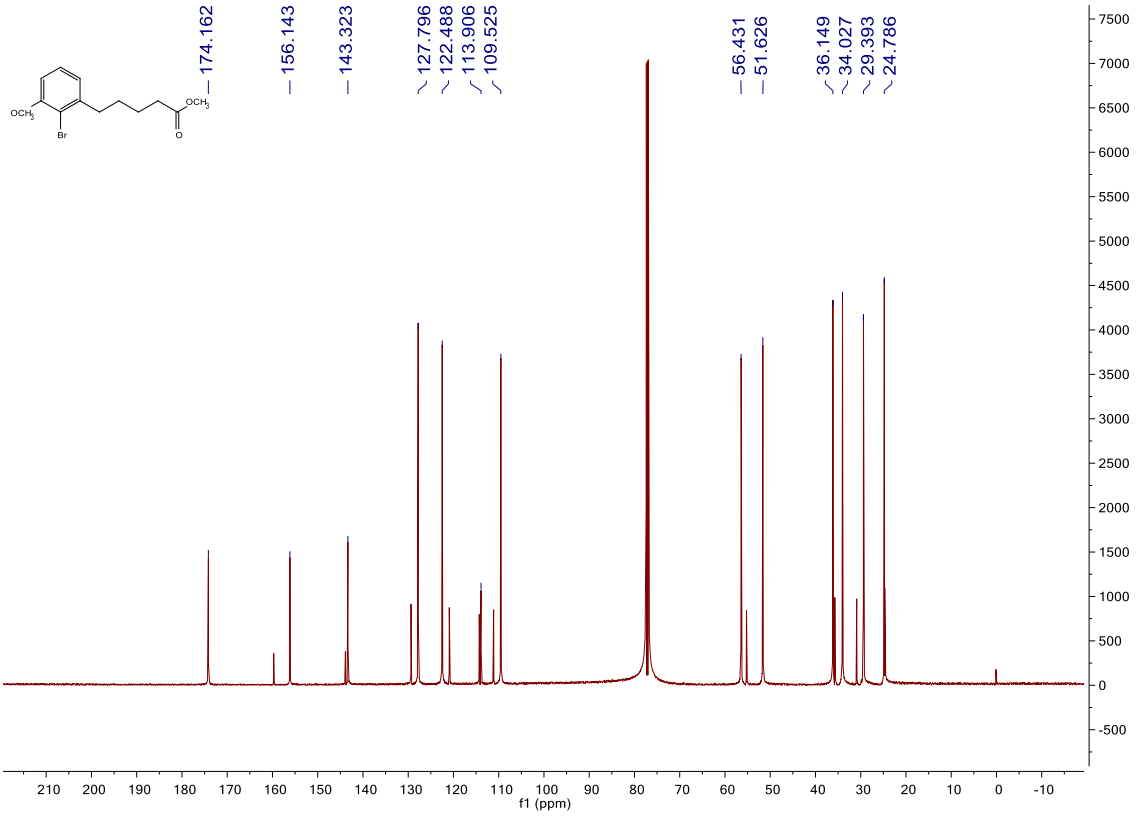
22. 2-bromo-3-methoxybenzaldehyde



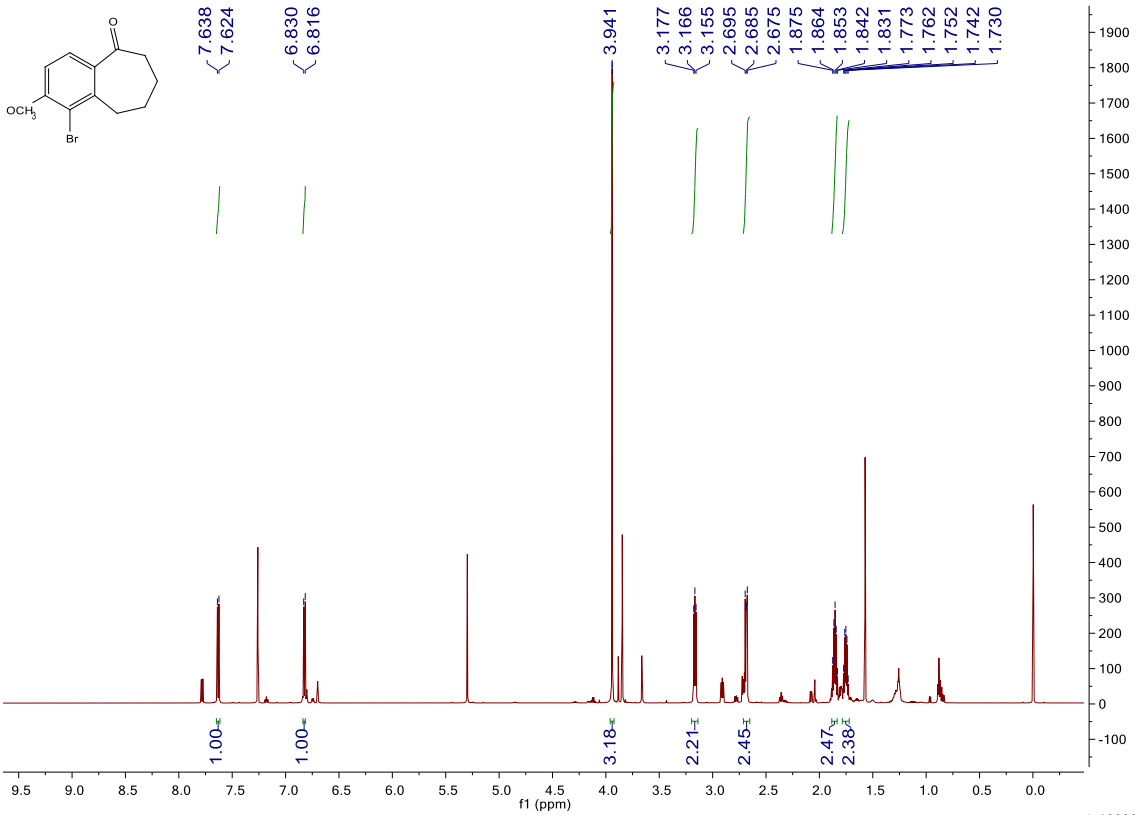


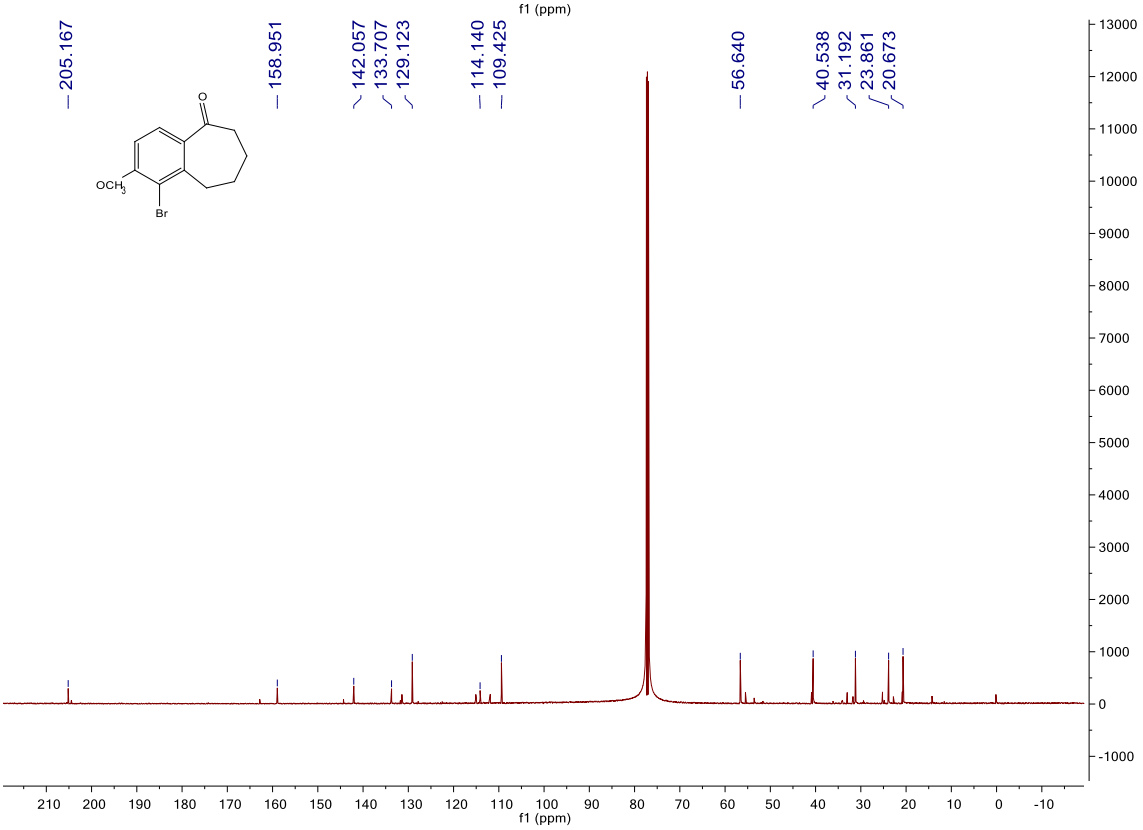
24. methyl 5-(2-bromo-3-methoxyphenyl)pentanoate



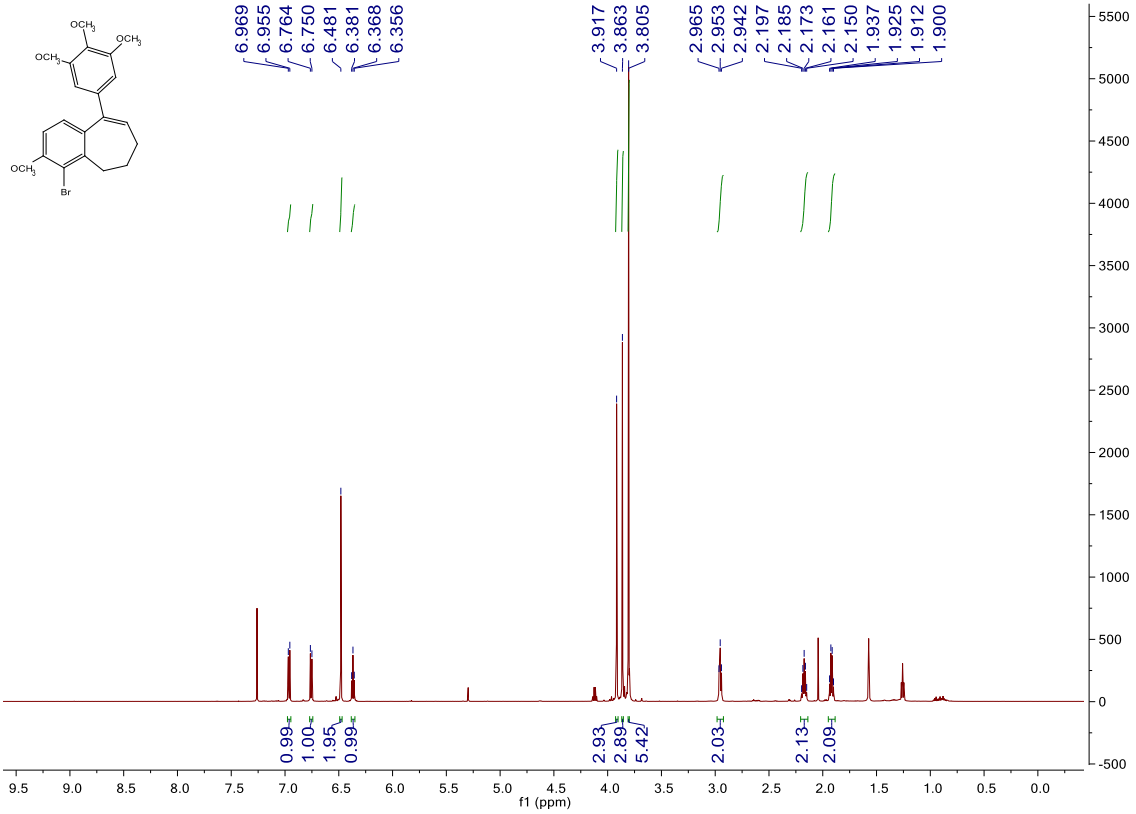


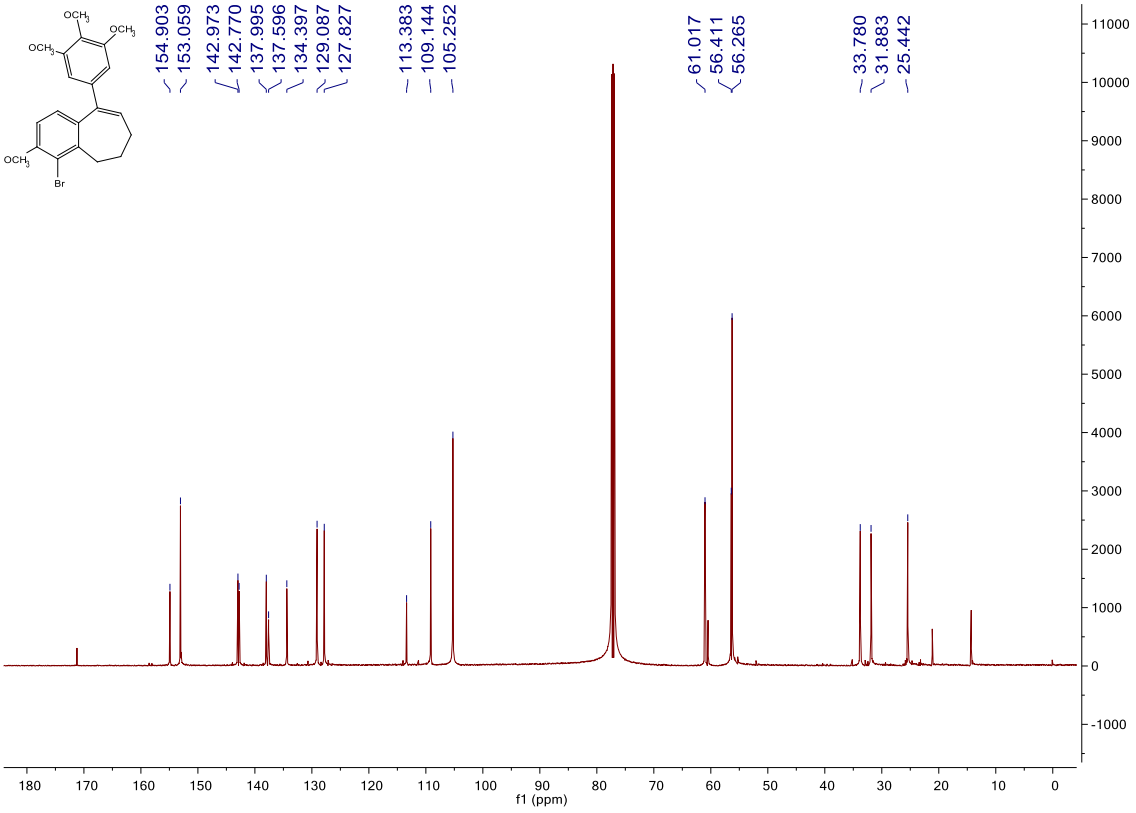
25. 1-bromo-2-methoxy-6,7,8,9-tetrahydro-5H-benzo[7]annulen-5-one



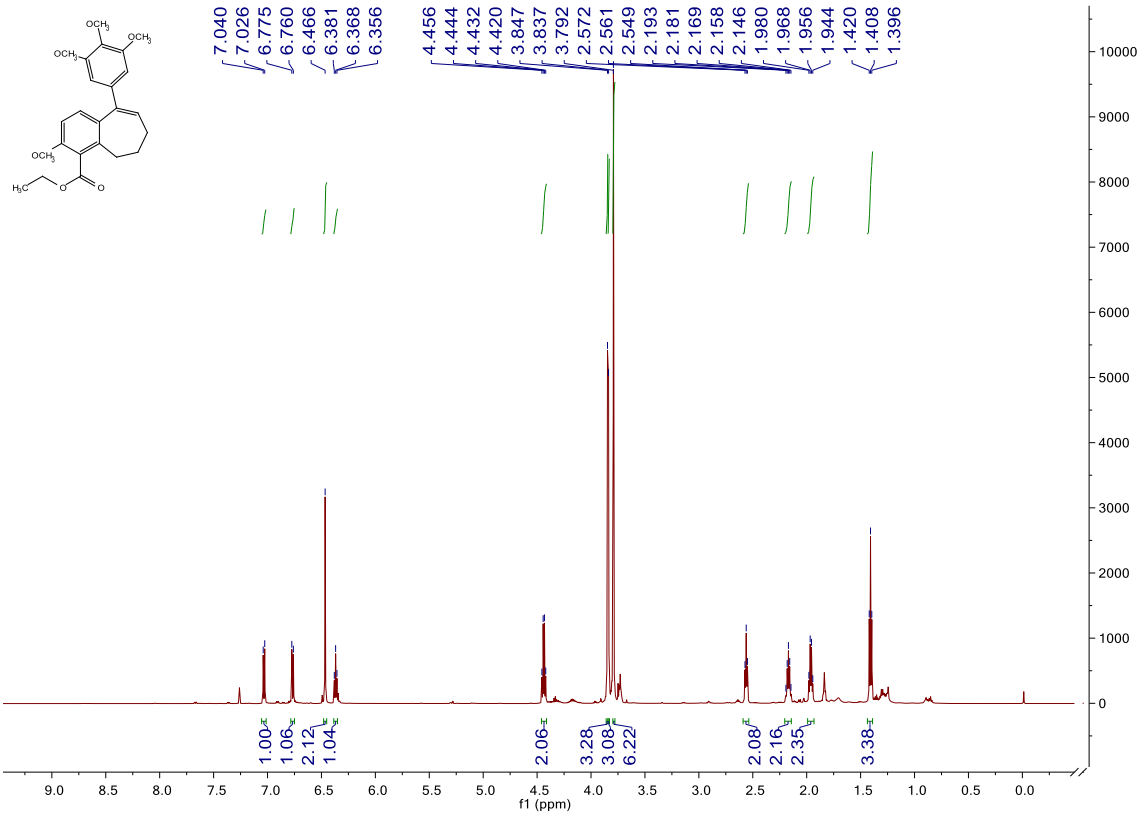


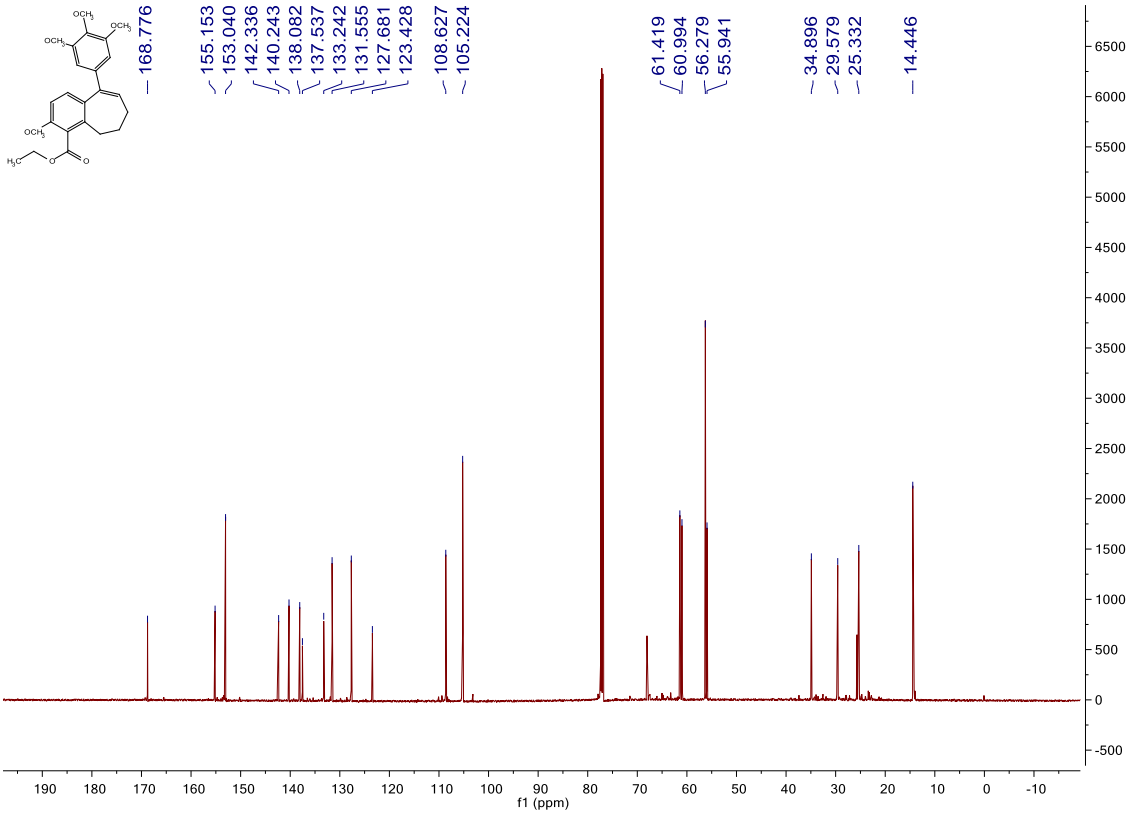
26. 4-bromo-3-methoxy-9-(3,4,5-trimethoxyphenyl)-6,7-dihydro-5H-benzo[7]annulene



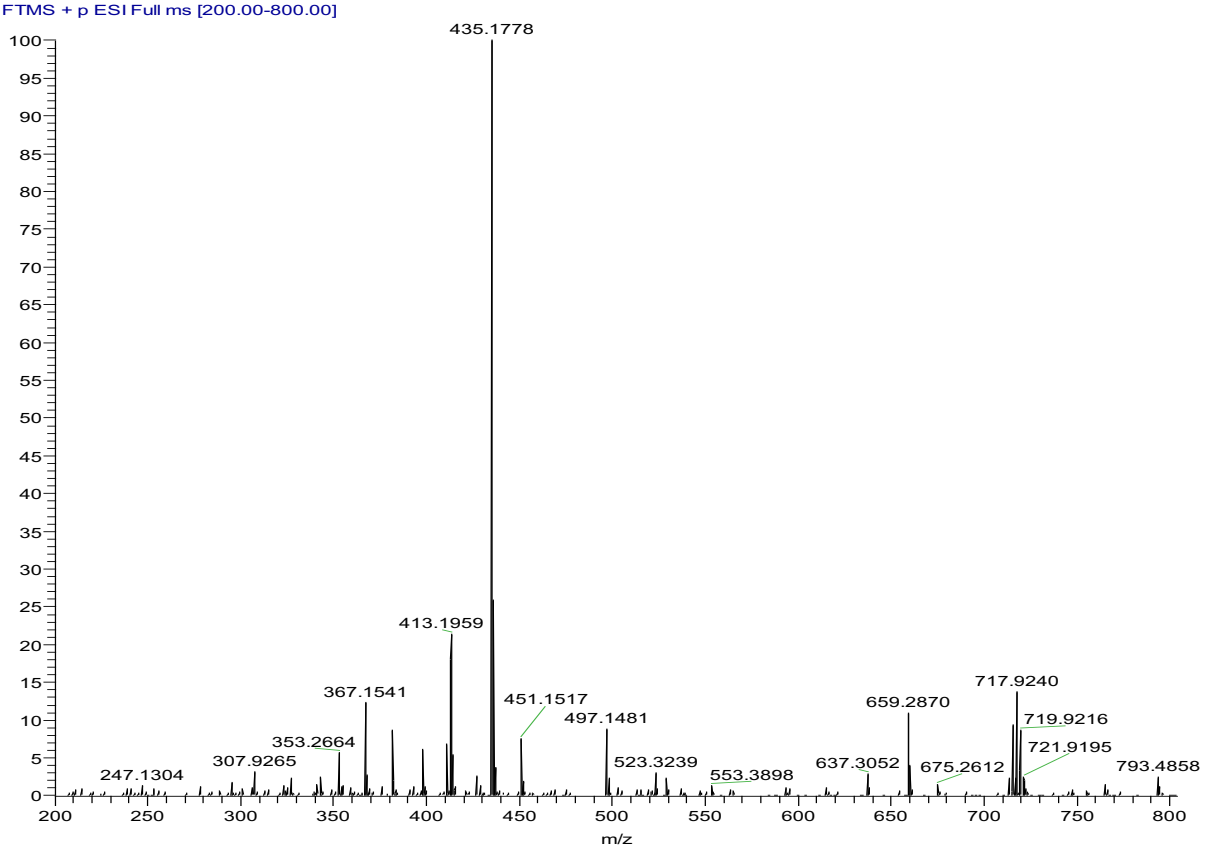


27. ethyl 3-methoxy-9-(3,4,5-trimethoxyphenyl)-6,7-dihydro-5H-benzo[7]annulene-4-carboxylate





NHC_3_86_F2_Orbi+ESI #2-42 RT: 0.01-0.37 AV: 41 NL: 4.59E6
T: FTMS + p ESI Full ms [200.00-800.00]



Data File C:\Chem32\1\Data\NHC\KGP485_Concentrated.D
Sample Name: KGP485_Concentrated

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======================================================================
Acq. Operator   : SYSTEM
Sample Operator : SYSTEM
Acq. Instrument : 1200 HPLC                    Location :   1
Injection Date  : 2/28/2018 1:25:24 PM
                                             Inj Volume : No inj
Acq. Method     : C:\CHEM32\1\METHODS\MASTERMETHOD2.M
Last changed    : 12/2/2015 12:37:42 PM by Eric Lin
Analysis Method : C:\CHEM32\1\METHODS\RT-ACNWASH 2.M
Last changed    : 7/9/2015 2:27:22 PM by Blake
Method Info     : General Column Wash Method

Sample Info     : 20180228

Additional Info : Peak(s) manually integrated
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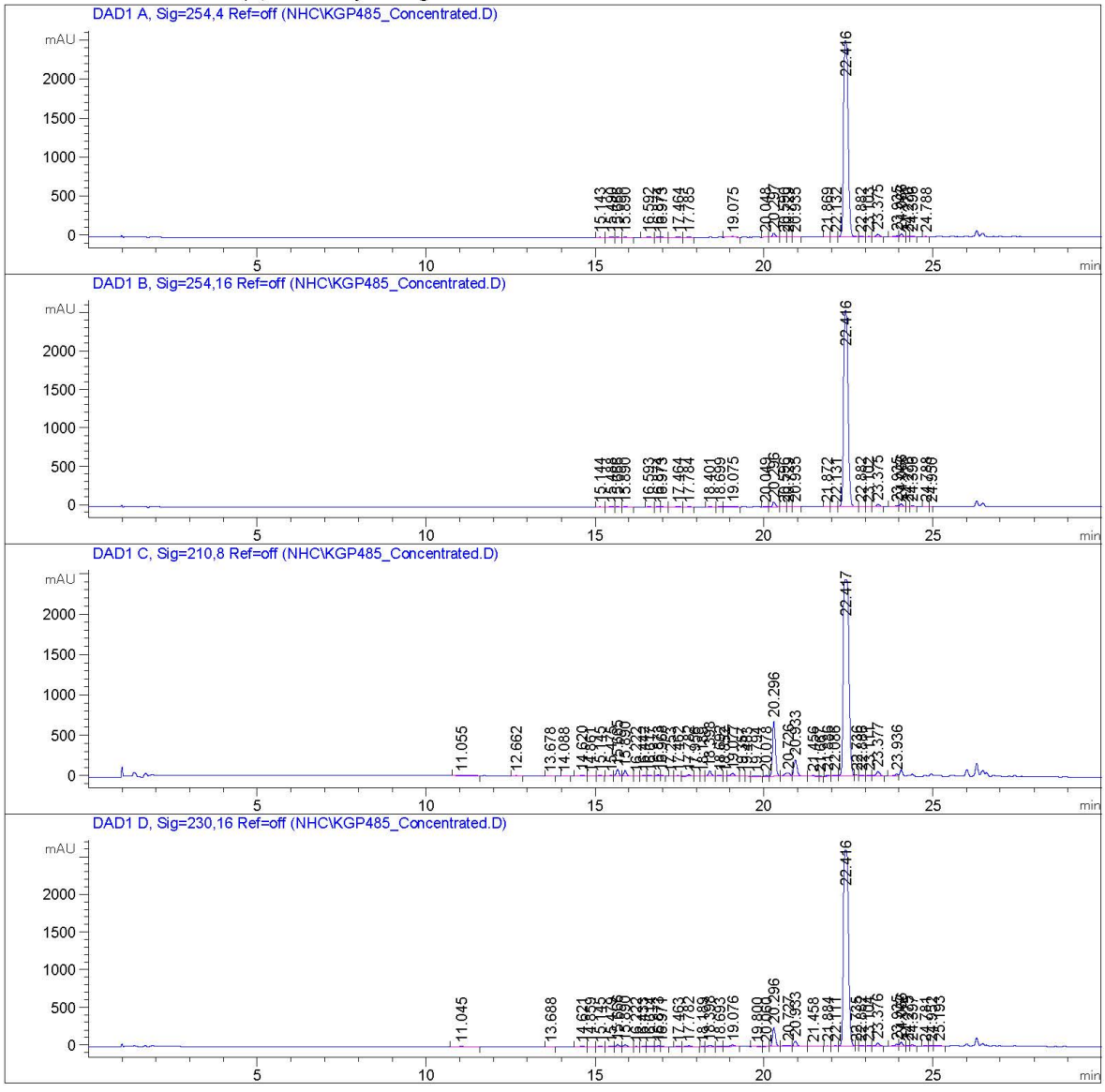
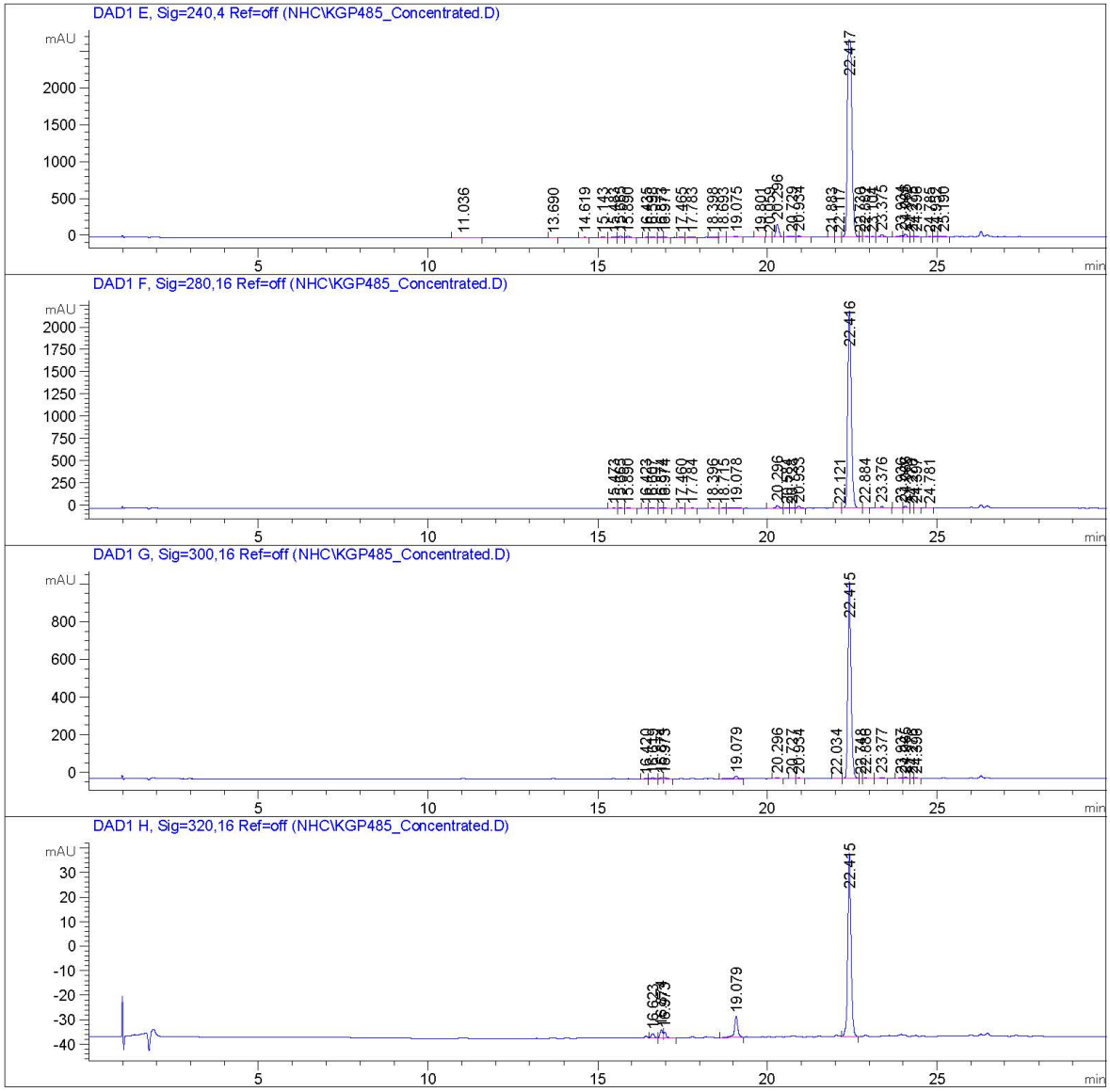


Data File C:\Chem32\1\Data\NHC\KGP485_Concentrated.D
Sample Name: KGP485_Concentrated



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Area Percent Report

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Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Data File C:\Chem32\1\Data\NHC\KGP485_Concentrated.D
Sample Name: KGP485_Concentrated

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.143	BB	0.0934	8.33023	1.40075	0.0331
2	15.490	BV	0.1346	19.58883	2.31746	0.0779
3	15.666	VV	0.0866	13.02673	2.35240	0.0518
4	15.890	VB	0.0998	14.21835	2.13269	0.0565
5	16.592	BV	0.1322	14.25762	1.62774	0.0567
6	16.874	VV	0.0833	11.05103	1.97438	0.0439
7	16.973	VB	0.0832	7.92460	1.41708	0.0315
8	17.464	BB	0.1036	24.72286	3.53347	0.0983
9	17.785	BB	0.0990	12.09403	1.88184	0.0481
10	19.075	BB	0.1148	54.89812	7.05413	0.2182
11	20.048	BV	0.0942	6.91471	1.14876	0.0275
12	20.297	VB	0.0954	317.10803	51.84093	1.2603
13	20.590	BV	0.1084	31.91162	4.40917	0.1268
14	20.729	VV	0.1084	32.33943	4.46839	0.1285
15	20.935	VB	0.1010	31.78071	4.81521	0.1263
16	21.869	BB	0.0924	8.85594	1.55649	0.0352
17	22.132	BV	0.1201	17.63049	2.23430	0.0701
18	22.416	VV	0.1498	2.37362e4	2522.00586	94.3347
19	22.882	VV	0.1106	66.47027	8.95987	0.2642
20	23.103	VV	0.1140	31.11934	4.12341	0.1237
21	23.375	VV	0.1083	238.31810	33.79056	0.9471
22	23.935	BV	0.1021	107.65102	14.93505	0.4278
23	24.066	VB	0.0900	222.35457	38.15697	0.8837
24	24.276	BV	0.0744	37.09813	7.67267	0.1474
25	24.396	VB	0.0917	78.43112	13.13635	0.3117
26	24.788	BB	0.0955	17.38949	3.00463	0.0691
Totals :				2.51616e4	2741.95056	

Signal 2: DAD1 B, Sig=254,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.144	BB	0.0915	9.29218	1.56085	0.0371
2	15.488	BV	0.1338	18.43984	2.19968	0.0736
3	15.666	VB	0.0863	18.93161	3.43537	0.0755
4	15.890	BB	0.0953	19.25417	3.06369	0.0768
5	16.593	VV	0.1209	14.35085	1.84228	0.0572
6	16.874	VV	0.0850	13.25696	2.30894	0.0529
7	16.973	VB	0.0825	9.07843	1.64111	0.0362
8	17.464	BB	0.1044	24.08924	3.40893	0.0961
9	17.784	BB	0.0996	13.88108	2.14120	0.0554
10	18.401	VV	0.1121	7.61204	1.00774	0.0304
11	18.699	VV	0.1006	7.69934	1.17225	0.0307
12	19.075	VB	0.1212	63.89308	7.67159	0.2549
13	20.049	BV	0.0976	7.32312	1.19334	0.0292
14	20.296	VB	0.0952	388.06714	63.54612	1.5479
15	20.596	BV	0.1111	32.03711	4.39342	0.1278

Data File C:\Chem32\1\Data\NHC\KGP485_Concentrated.D
Sample Name: KGP485_Concentrated

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
16	20.729	VV	0.1076	38.02944	5.18166	0.1517
17	20.935	VB	0.1000	37.83025	5.80485	0.1509
18	21.872	BB	0.0948	9.74633	1.70142	0.0389
19	22.131	BV	0.1203	17.17916	2.17097	0.0685
20	22.416	VV	0.1475	2.35526e4	2555.71948	93.9472
21	22.882	VV	0.1101	64.40833	8.72951	0.2569
22	23.102	VV	0.1139	29.15085	3.86712	0.1163
23	23.375	VV	0.1086	223.20885	31.51183	0.8903
24	23.935	BV	0.1025	106.19034	14.65690	0.4236
25	24.066	VB	0.0900	211.35193	36.27748	0.8430
26	24.276	BV	0.0747	36.76686	7.55985	0.1467
27	24.396	VB	0.0916	74.12943	12.42585	0.2957
28	24.788	BB	0.0922	16.13047	2.84184	0.0643
29	24.950	BV	0.0666	6.11324	1.40885	0.0244
Totals :				2.50700e4	2790.44412	

Signal 3: DAD1 C, Sig=210,8 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.055	BB	0.1966	36.57398	2.87157	0.0976
2	12.662	BB	0.1116	12.97379	1.68982	0.0346
3	13.678	BV	0.1316	16.00774	1.87440	0.0427
4	14.088	BB	0.1459	10.34158	1.20807	0.0276
5	14.620	BV	0.0955	74.50301	11.82868	0.1989
6	14.861	VB	0.1026	18.75695	2.78270	0.0501
7	15.145	BB	0.0912	52.52161	9.12137	0.1402
8	15.475	BV	0.1205	35.56589	4.69095	0.0950
9	15.665	VV	0.0875	490.90030	87.41347	1.3106
10	15.890	VB	0.0884	391.59515	68.81618	1.0455
11	16.222	BB	0.0792	21.70162	4.42820	0.0579
12	16.442	BV	0.1021	43.47946	6.84939	0.1161
13	16.617	VV	0.1246	67.78275	7.86437	0.1810
14	16.873	VV	0.0959	106.51293	16.36972	0.2844
15	16.968	VB	0.0688	47.62775	10.52875	0.1272
16	17.253	BB	0.0607	5.19991	1.35574	0.0139
17	17.462	BB	0.0851	34.02348	6.28659	0.0908
18	17.782	BV	0.1142	143.01854	18.50416	0.3818
19	17.956	VB	0.0971	8.89701	1.31285	0.0238
20	18.189	BV	0.0859	11.31681	2.00217	0.0302
21	18.398	VB	0.0962	422.01907	68.17153	1.1267
22	18.692	BV	0.1024	104.86539	15.59619	0.2800
23	18.852	VV	0.0790	27.79159	5.14861	0.0742
24	19.077	VB	0.1125	280.21582	36.10938	0.7481
25	19.357	BV	0.0811	9.11958	1.80034	0.0243
26	19.483	VB	0.1048	7.72842	1.23935	0.0206
27	19.794	BB	0.1226	46.20218	5.58166	0.1234
28	20.078	BV	0.1179	47.84826	6.65499	0.1277
29	20.296	VB	0.0952	4129.25684	676.39777	11.0243
30	20.726	BV	0.1503	425.86432	38.72407	1.1370

Data File C:\Chem32\1\Data\NHC\KGP485_Concentrated.D
Sample Name: KGP485_Concentrated

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
31	20.933	VB	0.0991	1299.64380	201.85574	3.4698
32	21.456	BV	0.1294	67.31625	7.17869	0.1797
33	21.667	VB	0.0747	8.72522	1.79655	0.0233
34	21.886	BB	0.0904	83.43248	14.66684	0.2227
35	22.086	BV	0.1109	74.13023	9.95198	0.1979
36	22.417	VV	0.1868	2.79993e4	2422.46143	74.7524
37	22.736	VB	0.0761	45.81138	9.53544	0.1223
38	22.886	BB	0.0906	55.70490	10.06568	0.1487
39	23.111	BV	0.0911	74.66079	12.98298	0.1993
40	23.377	VB	0.1123	443.88904	58.61972	1.1851
41	23.936	BV	0.0981	173.23309	25.24012	0.4625
Totals :				3.74561e4	3897.57820	

Signal 4: DAD1 D, Sig=230,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.045	BB	0.2194	29.27055	2.06513	0.0933
2	13.688	BB	0.1232	11.77030	1.53882	0.0375
3	14.621	BV	0.0931	35.99555	5.90601	0.1147
4	14.859	VB	0.0975	8.33657	1.32295	0.0266
5	15.145	BB	0.0930	36.36981	6.14930	0.1159
6	15.479	BV	0.1275	28.64103	3.57461	0.0913
7	15.666	VV	0.0874	158.09705	28.22238	0.5039
8	15.890	VB	0.0896	132.87042	22.94082	0.4235
9	16.222	BB	0.0779	7.39274	1.54263	0.0236
10	16.433	BV	0.0943	18.97336	3.14760	0.0605
11	16.614	VV	0.1223	41.46205	5.13063	0.1322
12	16.873	VV	0.0893	55.88730	9.14154	0.1781
13	16.971	VB	0.0788	32.72037	6.27800	0.1043
14	17.463	VB	0.0931	28.95014	4.89059	0.0923
15	17.782	BB	0.1146	66.25149	8.53588	0.2112
16	18.189	BV	0.0861	6.57483	1.16062	0.0210
17	18.398	VB	0.0969	102.63708	16.42999	0.3272
18	18.693	BV	0.1008	41.62845	6.32242	0.1327
19	19.076	VB	0.1200	181.93646	22.11270	0.5799
20	19.800	BB	0.1352	16.81750	1.97700	0.0536
21	20.060	BV	0.1147	23.13130	3.26328	0.0737
22	20.296	VB	0.0952	1519.28369	248.78177	4.8427
23	20.727	BV	0.1617	180.74738	15.09073	0.5761
24	20.933	VB	0.0982	441.48798	69.43363	1.4072
25	21.458	BB	0.1728	33.95776	2.59314	0.1082
26	21.884	BB	0.0884	24.60236	4.45423	0.0784
27	22.111	BB	0.1204	20.61290	2.91938	0.0657
28	22.416	BV	0.1660	2.68171e4	2606.61255	85.4789
29	22.735	VB	0.0662	16.28876	3.78488	0.0519
30	22.882	BB	0.0880	46.95659	8.55824	0.1497
31	23.104	BV	0.0925	25.99397	4.56100	0.0829
32	23.376	VB	0.1088	289.25766	40.76824	0.9220
33	23.935	BV	0.1000	157.03195	22.33052	0.5005

Data File C:\Chem32\1\Data\NHC\KGP485_Concentrated.D
Sample Name: KGP485_Concentrated

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
34	24.066	VB	0.0898	316.73645	54.52169	1.0096
35	24.275	BV	0.0780	61.73699	12.41080	0.1968
36	24.397	VB	0.0912	106.41171	17.94668	0.3392
37	24.781	BV	0.0971	45.17023	7.41248	0.1440
38	24.952	VV	0.0852	51.01236	9.12754	0.1626
39	25.193	VB	0.1575	152.65260	14.66224	0.4866
Totals :				3.13727e4	3307.62267	

Signal 5: DAD1 E, Sig=240,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.036	BB	0.2282	22.70355	1.52069	0.0810
2	13.690	BB	0.1199	9.10374	1.20780	0.0325
3	14.619	BB	0.0942	10.79468	1.74490	0.0385
4	15.143	BB	0.0903	26.74286	4.56801	0.0954
5	15.483	BV	0.1275	18.80848	2.34639	0.0671
6	15.665	VB	0.0863	85.24845	15.45822	0.3042
7	15.890	BB	0.0890	72.26150	12.58268	0.2578
8	16.435	BV	0.0934	7.35842	1.23639	0.0263
9	16.598	VV	0.1275	23.67183	2.83132	0.0845
10	16.873	VV	0.0905	30.06336	4.83900	0.1073
11	16.971	VB	0.0763	16.86926	3.26388	0.0602
12	17.465	BB	0.0854	18.74666	3.44851	0.0669
13	17.783	BB	0.1021	35.21133	5.26137	0.1256
14	18.398	VB	0.0973	39.57500	6.29728	0.1412
15	18.693	BV	0.0987	25.74167	4.02147	0.0918
16	19.075	VB	0.1222	115.23772	13.68551	0.4112
17	19.801	BB	0.1311	8.76465	1.05334	0.0313
18	20.059	BV	0.1109	13.13572	1.89430	0.0469
19	20.296	VB	0.0952	1072.81409	175.84843	3.8279
20	20.729	BV	0.1573	136.37468	11.75892	0.4866
21	20.934	VB	0.1012	115.88248	17.98977	0.4135
22	21.883	BB	0.0920	19.25364	3.40578	0.0687
23	22.117	BV	0.1262	19.28736	2.49549	0.0688
24	22.417	VV	0.1517	2.51929e4	2680.38184	89.8914
25	22.730	VB	0.0616	9.99581	2.55773	0.0357
26	22.882	BB	0.0885	39.25538	7.10551	0.1401
27	23.104	BV	0.0895	17.64683	3.14221	0.0630
28	23.375	VB	0.1067	196.51772	28.41080	0.7012
29	23.934	BV	0.1043	136.12515	18.39413	0.4857
30	24.066	VB	0.0899	219.46948	37.71962	0.7831
31	24.275	BV	0.0790	49.67536	9.82261	0.1772
32	24.396	VB	0.0907	72.79107	12.36407	0.2597
33	24.785	BB	0.0884	17.38600	3.25111	0.0620
34	24.952	BV	0.0782	30.21395	5.85291	0.1078
35	25.190	VB	0.1578	100.28733	9.60244	0.3578
Totals :				2.80259e4	3117.36442	

Data File C:\Chem32\1\Data\NHC\KGP485_Concentrated.D
Sample Name: KGP485_Concentrated

Signal 6: DAD1 F, Sig=280,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.473	BV	0.1265	11.01561	1.41958	0.0632
2	15.665	VB	0.0851	13.77363	2.54522	0.0791
3	15.890	BB	0.0946	18.42481	2.96128	0.1058
4	16.423	BV	0.0821	6.27473	1.21838	0.0360
5	16.607	VB	0.1146	26.63526	3.76305	0.1529
6	16.874	BV	0.0779	25.99045	5.06250	0.1492
7	16.974	VB	0.0824	21.19812	3.83990	0.1217
8	17.460	BB	0.0882	11.98845	2.11153	0.0688
9	17.784	BB	0.1032	9.76219	1.43794	0.0561
10	18.396	VB	0.1104	11.03026	1.48952	0.0633
11	18.715	BV	0.1082	7.61201	1.08086	0.0437
12	19.078	VB	0.1172	87.54132	10.73143	0.5026
13	20.296	BB	0.0961	179.89883	29.11555	1.0329
14	20.584	BV	0.0955	14.32021	2.27442	0.0822
15	20.728	VV	0.1070	23.98289	3.37284	0.1377
16	20.933	VB	0.0983	124.59994	19.55870	0.7154
17	22.121	BV	0.1405	10.69543	1.09004	0.0614
18	22.416	VV	0.1184	1.64326e4	2218.00977	94.3514
19	22.884	VV	0.1074	29.37505	4.20932	0.1687
20	23.376	BB	0.1085	116.49738	16.48240	0.6689
21	23.936	BV	0.0995	48.21041	6.90030	0.2768
22	24.066	VB	0.0897	114.10828	19.66980	0.6552
23	24.276	BV	0.0737	17.08398	3.57947	0.0981
24	24.397	VB	0.0916	40.58337	6.80235	0.2330
25	24.781	BB	0.0938	13.17234	2.26540	0.0756
Totals :				1.74163e4	2370.99155	

Signal 7: DAD1 G, Sig=300,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.420	BV	0.0851	8.01321	1.48085	0.1082
2	16.619	VV	0.1049	25.07796	3.61711	0.3387
3	16.874	VV	0.0792	30.45059	5.80377	0.4113
4	16.973	VB	0.0824	23.86242	4.32461	0.3223
5	19.079	BB	0.1116	92.54210	12.05236	1.2500
6	20.296	BB	0.0976	37.01918	5.87041	0.5000
7	20.727	VV	0.1007	13.54648	1.95953	0.1830
8	20.934	VB	0.1087	23.00213	3.16829	0.3107
9	22.034	BV	0.1484	10.83307	1.00026	0.1463
10	22.415	VV	0.1040	6989.56543	1046.03650	94.4082
11	22.748	VV	0.0838	6.04228	1.07059	0.0816
12	22.886	VB	0.1253	16.57144	1.94612	0.2238
13	23.377	BB	0.1097	37.73441	5.13532	0.5097
14	23.937	BV	0.0976	22.62986	3.31826	0.3057
15	24.065	VB	0.0896	43.96283	7.58438	0.5938
16	24.276	BV	0.0786	9.02400	1.79778	0.1219

Data File C:\Chem32\1\Data\NHC\KGP485_Concentrated.D
Sample Name: KGP485_Concentrated

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
17	24.396	VB	0.0897	13.67874	2.35766	0.1848
Totals :				7403.55613	1108.52379	

Signal 8: DAD1 H, Sig=320,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.623	VV	0.0985	12.29826	1.87665	2.0106
2	16.874	VV	0.0792	17.02584	3.24417	2.7835
3	16.973	VB	0.0842	13.60806	2.39984	2.2247
4	19.079	BB	0.1051	60.78568	8.53374	9.9377
5	22.415	BB	0.1032	507.95117	74.83036	83.0435
Totals :				611.66900	90.88476	

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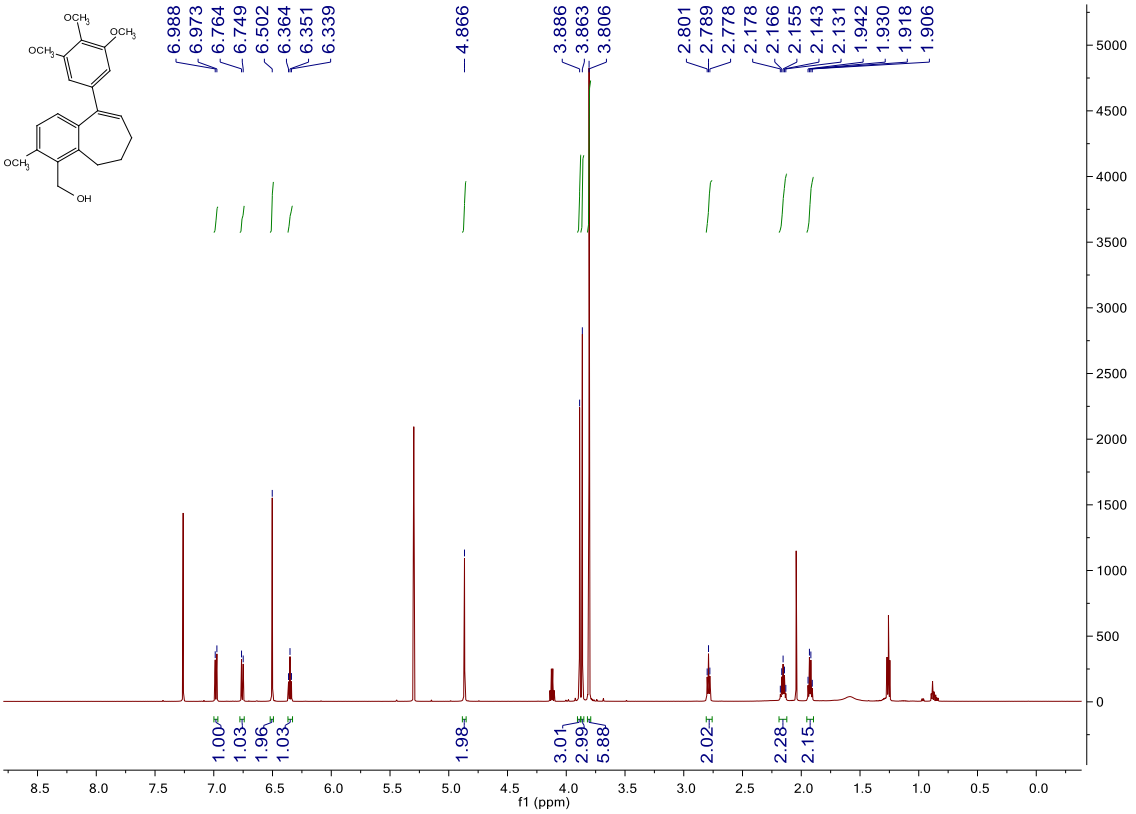
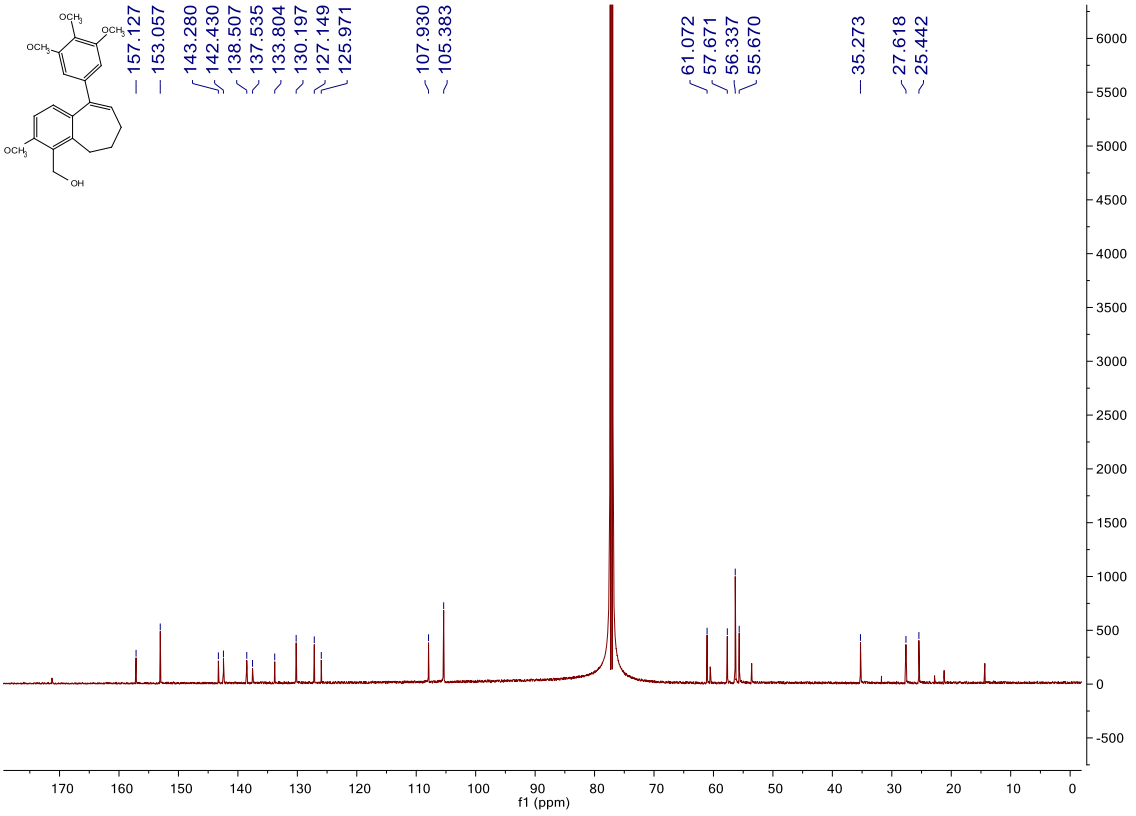
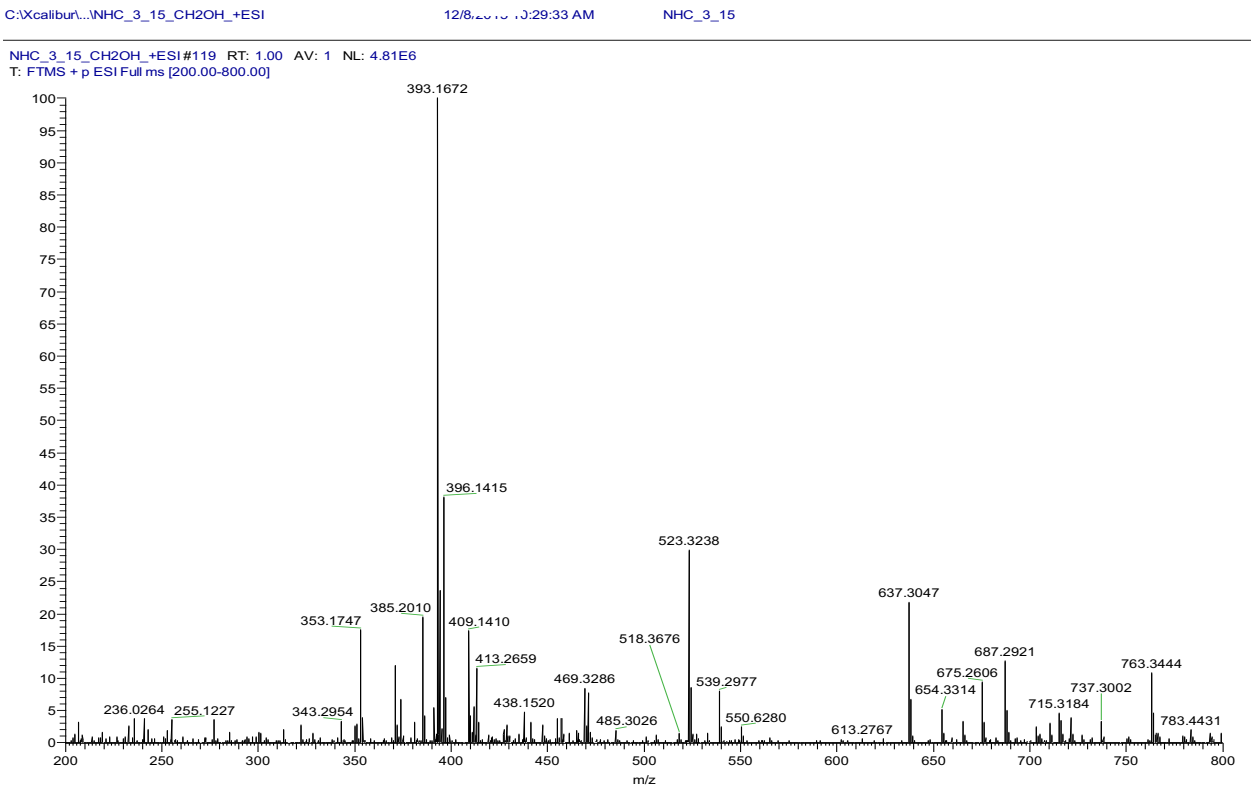
*** End of Report ***

28. (3-methoxy-9-(3,4,5-trimethoxyphenyl)-6,7-dihydro-5H-benzo[7]annulen-4-yl)methanol






C:\Xcalibur\...\NHC_3_15_CH2OH_+ESI
12/8/2015 10:29:33 AM
NHC_3_15
NHC_3_15_CH2OH_+ESI #119 RT: 1.00 AV: 1 NL: 4.81E6
T: FTMS + p ESI Full ms [200.00-800.00]
393.1672
396.1415
523.3238
637.3047
385.2010
353.1747
409.1410
518.3676
687.2921
763.3444
413.2659
675.2606
469.3286
539.2977
654.3314
737.3002
438.1520
715.3184
236.0264
255.1227
343.2954
485.3026
550.6280
613.2767
783.4431
m/z

Data File C:\Chem32\1\Data\NHC\KGP479-Remake-20160628.D
Sample Name: KGP483-Remake-20160628

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==========================================================================
Acq. Operator   : SYSTEM
Sample Operator : SYSTEM
Acq. Instrument : 1200 HPLC                    Location :     -
Injection Date  : 6/28/2016 12:35:47 PM
                                             Inj Volume : No inj
Acq. Method     : C:\CHEM32\1\METHODS\MASTERMETHOD2.M
Last changed    : 12/2/2015 12:37:42 PM by Eric Lin
Analysis Method : C:\CHEM32\1\METHODS\RT-ACNWASH 2.M
Last changed    : 7/9/2015 2:27:22 PM by Blake
Method Info     : General Column Wash Method
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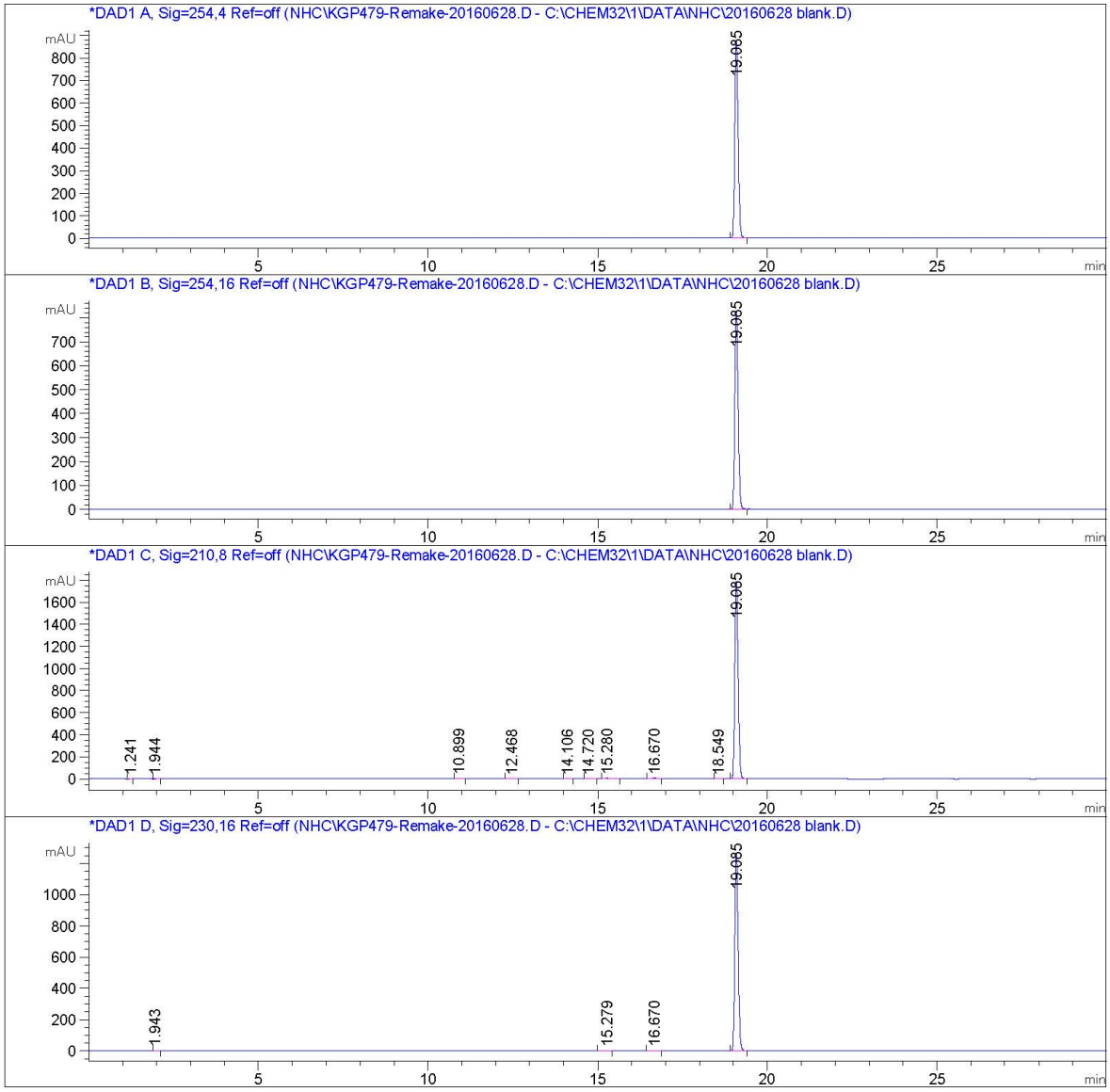
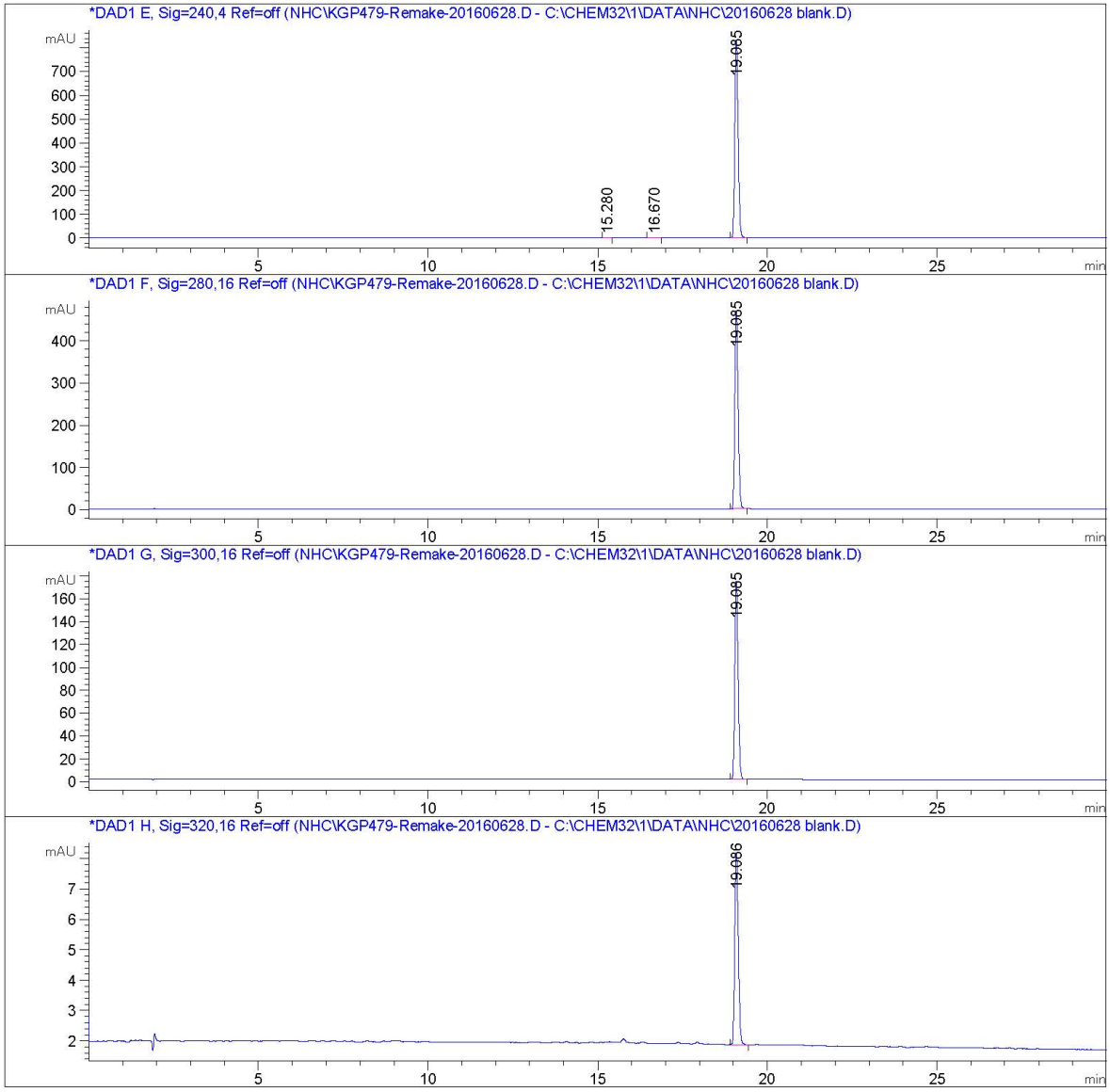


Data File C:\Chem32\1\Data\NHC\KGP479-Remake-20160628.D
Sample Name: KGP483-Remake-20160628



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Area Percent Report

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Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

Data File C:\Chem32\1\Data\NHC\KGP479-Remake-20160628.D
Sample Name: KGP483-Remake-20160628

Signal 1: DAD1 A, Sig=254,4 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.085	BB	0.1008	5794.88574	880.20862	100.0000
Totals :				5794.88574	880.20862	

Signal 2: DAD1 B, Sig=254,16 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.085	BB	0.1008	5458.21191	829.09521	100.0000
Totals :				5458.21191	829.09521	

Signal 3: DAD1 C, Sig=210,8 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.241	BB	0.0576	15.66318	4.19107	0.1304
2	1.944	BB	0.0763	6.04444	1.13141	0.0503
3	10.899	BB	0.0800	19.40668	3.77627	0.1616
4	12.468	BB	0.0904	10.92510	1.86384	0.0910
5	14.106	BB	0.0904	12.37679	2.11183	0.1030
6	14.720	BB	0.1209	8.41541	1.01281	0.0701
7	15.280	BV	0.0971	28.64273	4.56986	0.2385
8	16.670	BB	0.0997	36.99091	5.70152	0.3080
9	18.549	BV	0.1031	7.54006	1.05901	0.0628
10	19.085	BB	0.1015	1.18652e4	1786.20667	98.7844
Totals :				1.20112e4	1811.62430	

Signal 4: DAD1 D, Sig=230,16 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.943	BB	0.0761	5.69901	1.07124	0.0677
2	15.279	BB	0.0997	10.85100	1.67169	0.1289
3	16.670	BB	0.1036	12.63866	1.85169	0.1502
4	19.085	BB	0.1011	8386.12500	1269.11670	99.6531

Data File C:\Chem32\1\Data\NHC\KGP479-Remake-20160628.D
Sample Name: KGP483-Remake-20160628

Totals : 8415.31368 1273.71131

Signal 5: DAD1 E, Sig=240,4 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.280	BB	0.0923	5.85575	1.00086	0.1064
2	16.670	BB	0.1017	9.01613	1.35412	0.1638
3	19.085	BB	0.1008	5489.83496	833.59961	99.7298

Totals : 5504.70684 835.95460

Signal 6: DAD1 F, Sig=280,16 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.085	BB	0.1008	3100.32178	470.76486	100.0000

Totals : 3100.32178 470.76486

Signal 7: DAD1 G, Sig=300,16 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.085	BB	0.1011	1146.14038	173.54346	100.0000

Totals : 1146.14038 173.54346

Signal 8: DAD1 H, Sig=320,16 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.086	BB	0.1110	45.00113	6.32842	100.0000

Totals : 45.00113 6.32842

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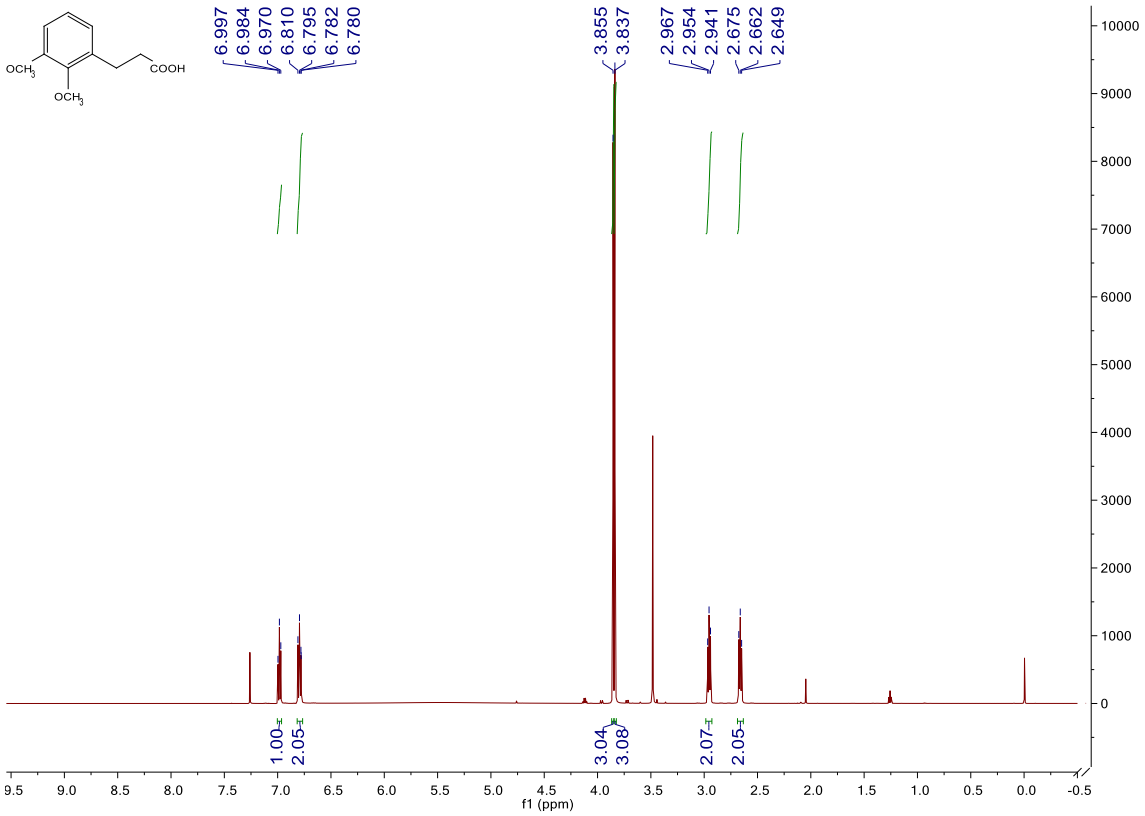
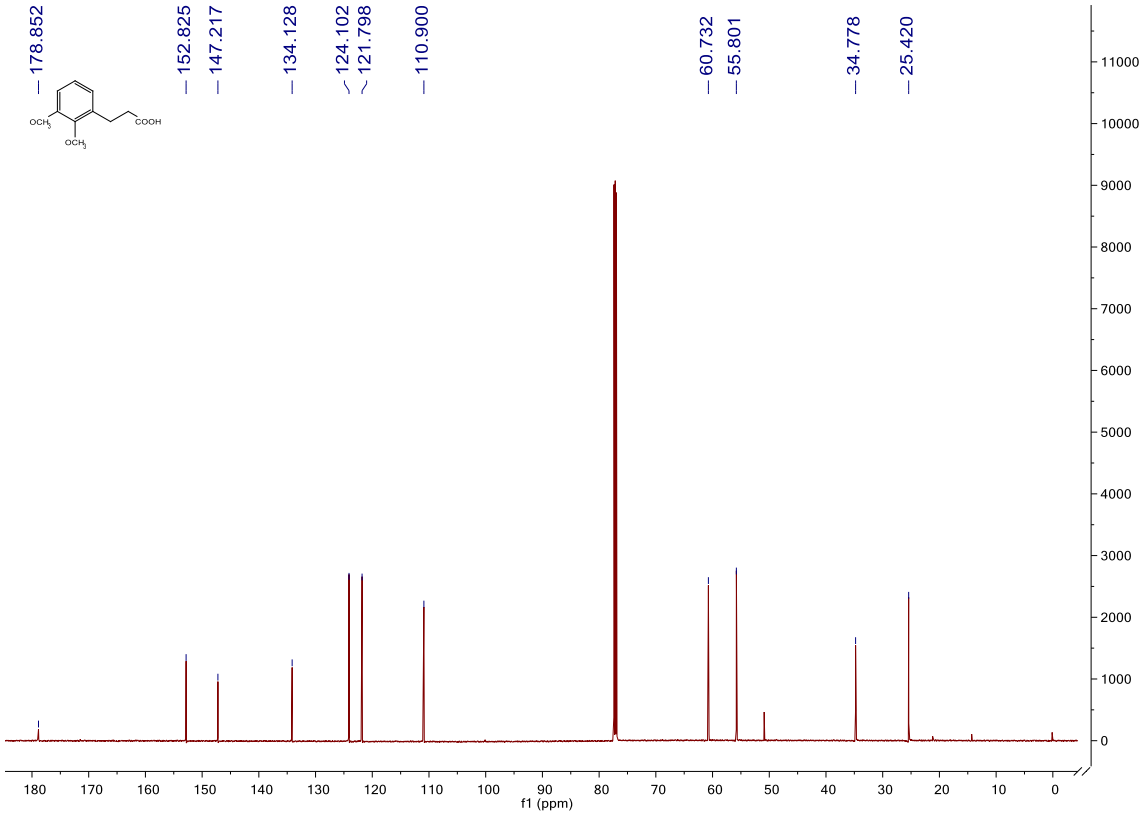
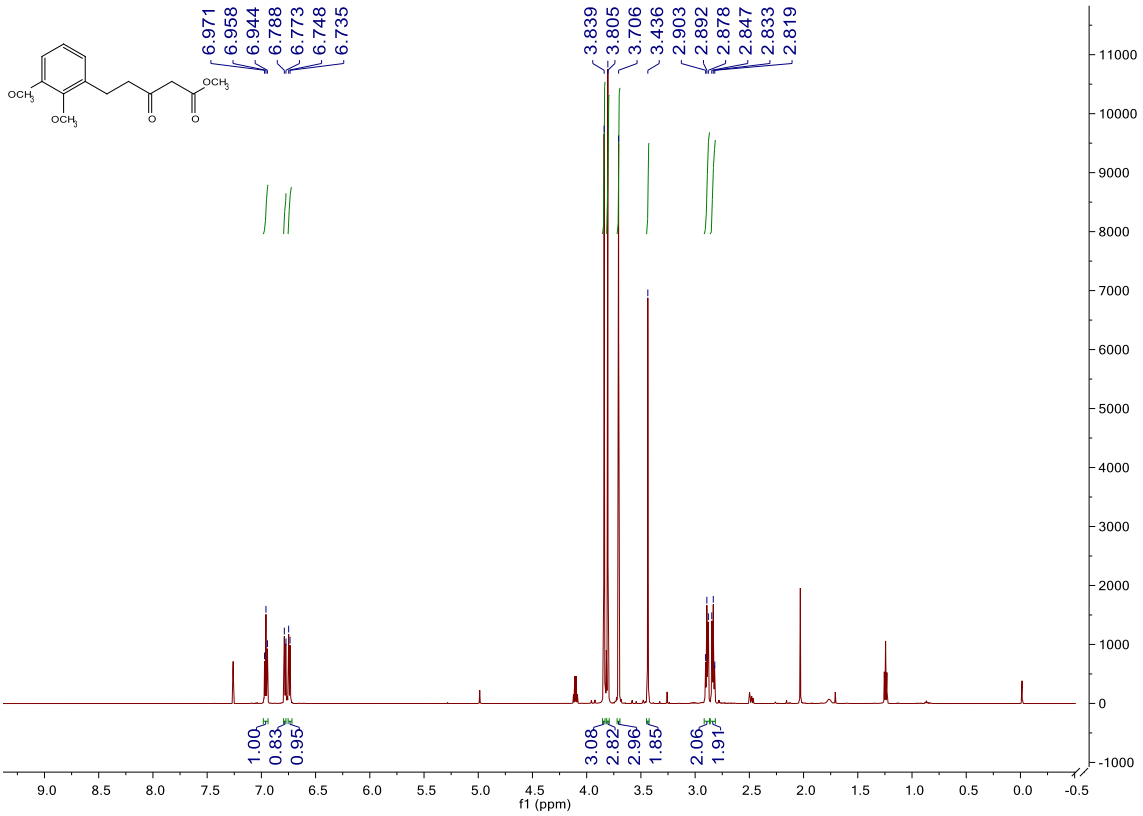
*** End of Report ***

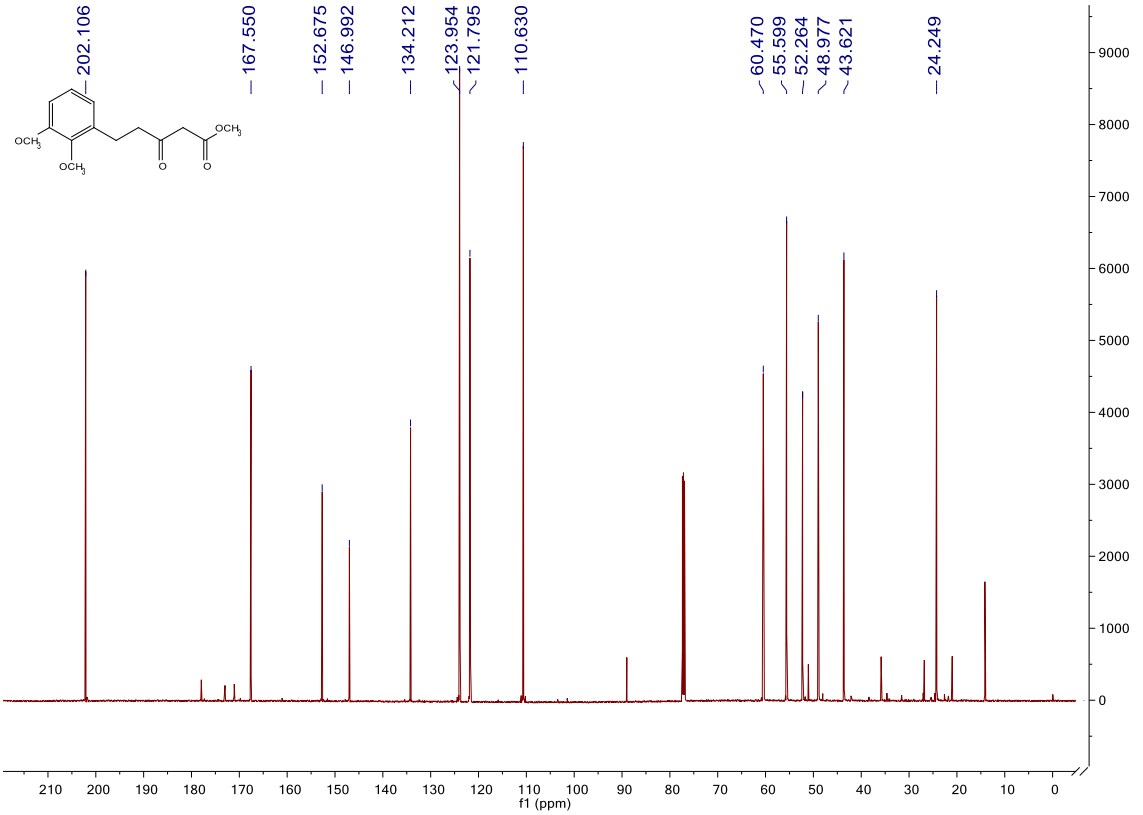
30. 3-(2,3-Dimethoxyphenyl)propanoic acid



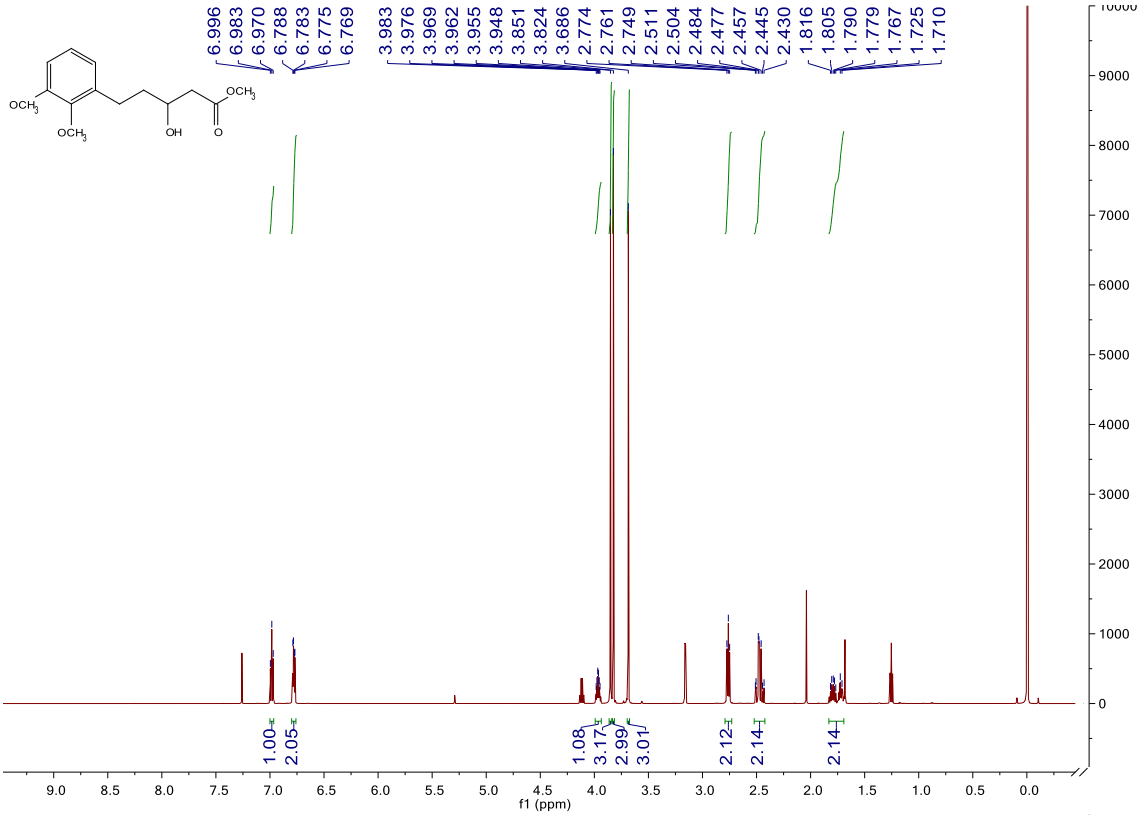


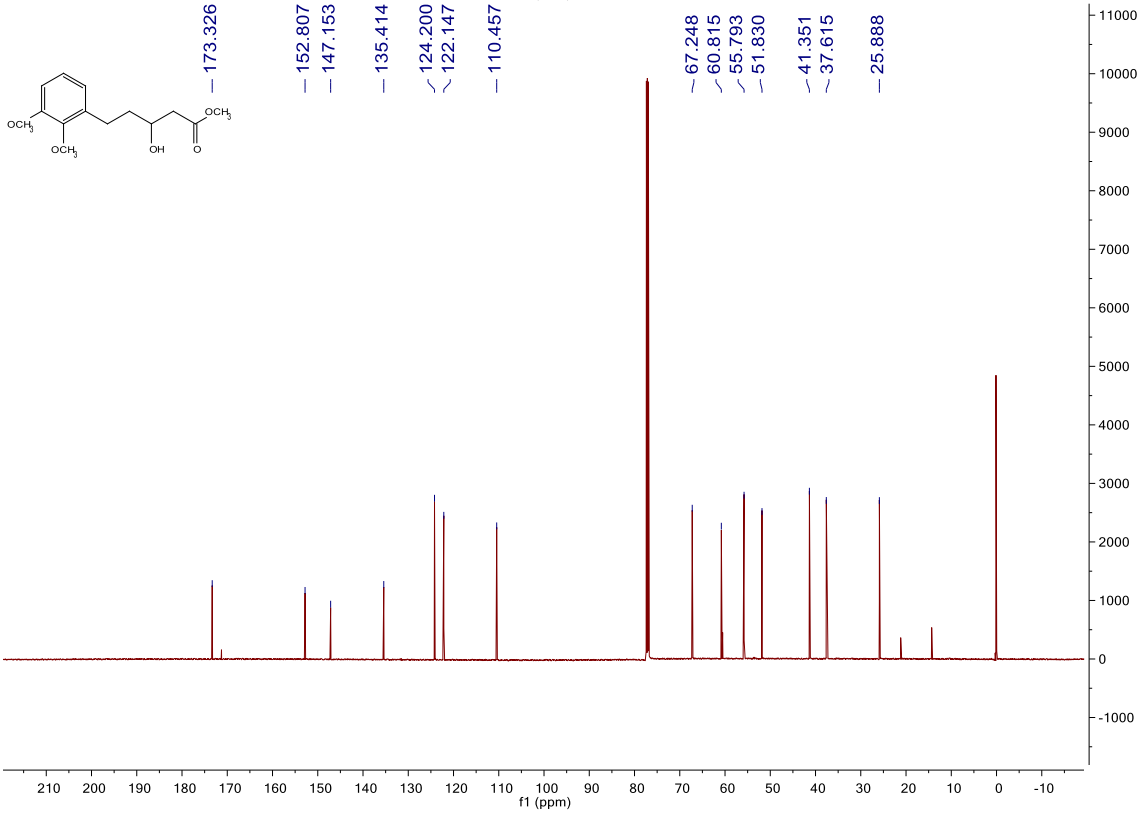
31. Methyl 5-(2,3-dimethoxyphenyl)-3-oxopentanoate



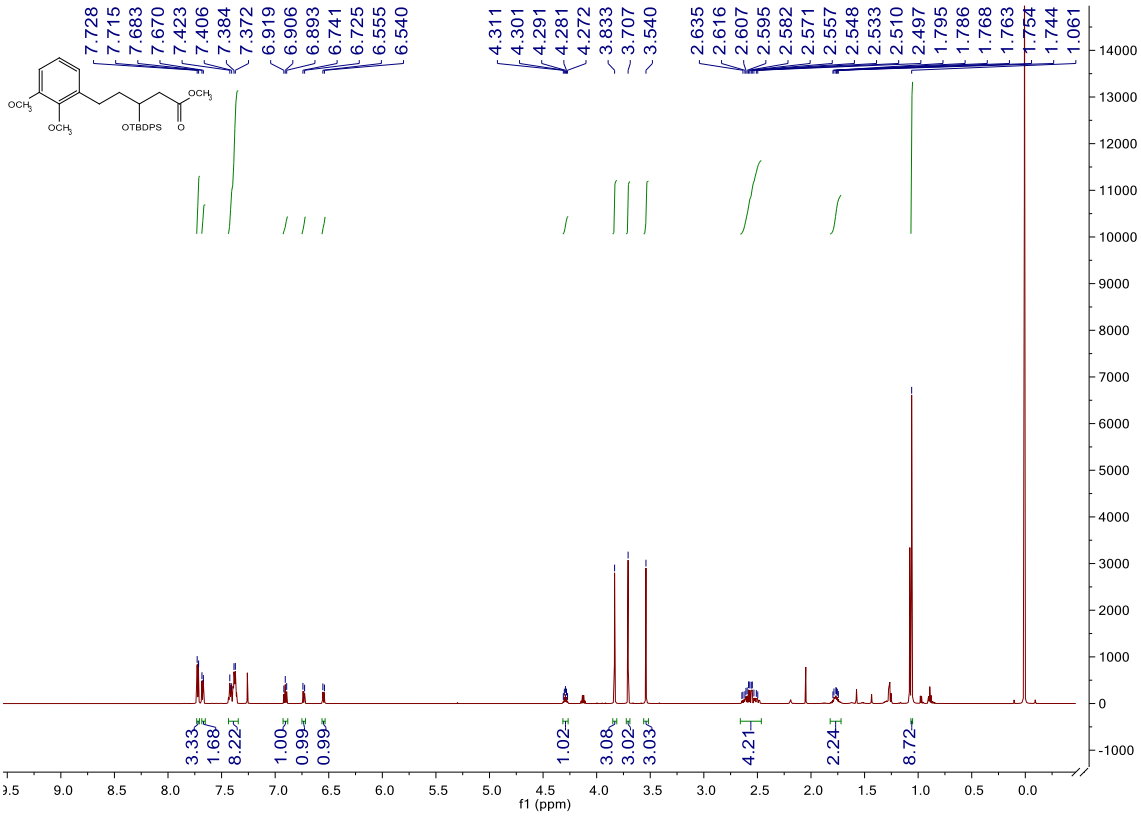


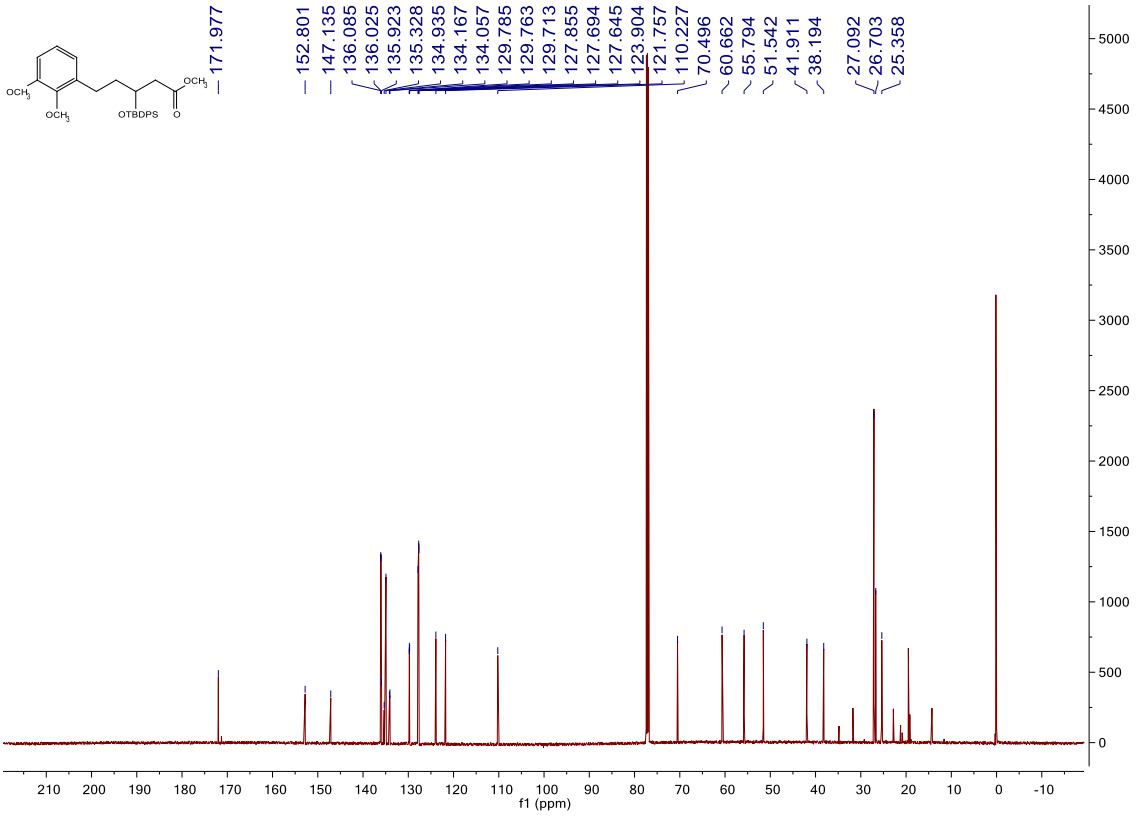
32. Methyl 5-(2,3-dimethoxyphenyl)-3-hydroxypentanoate



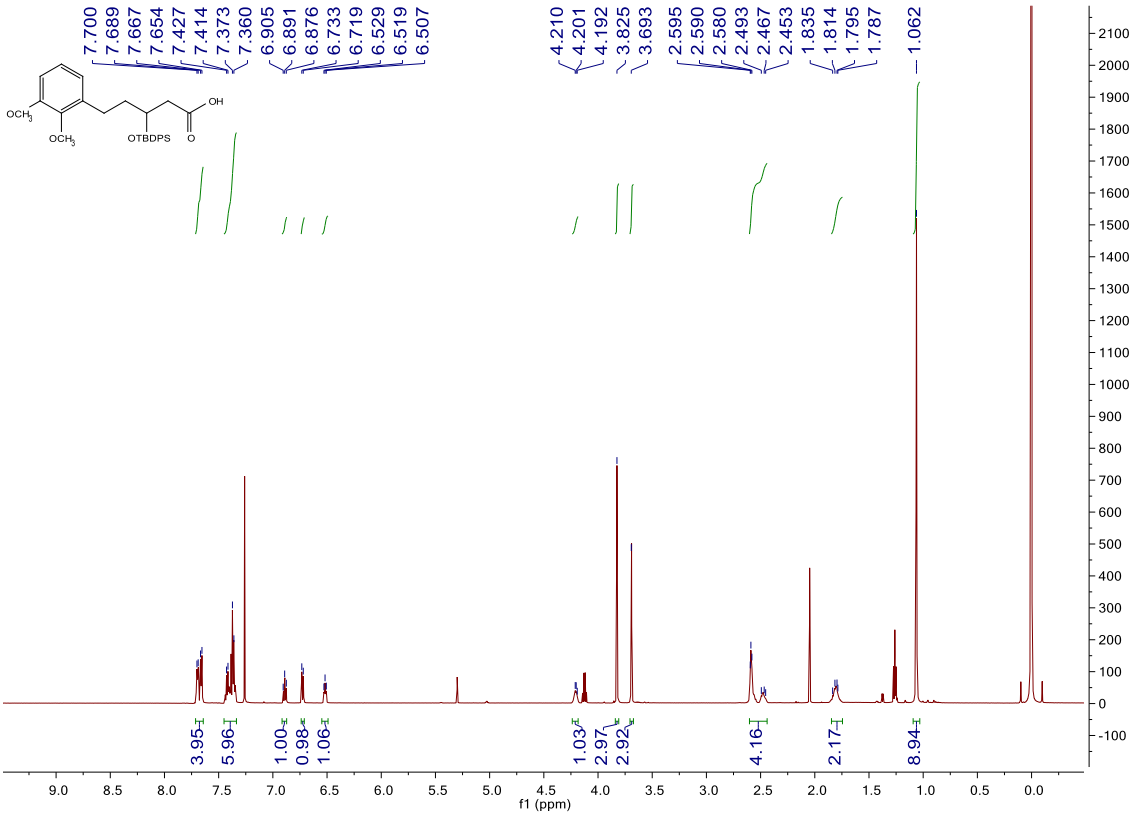


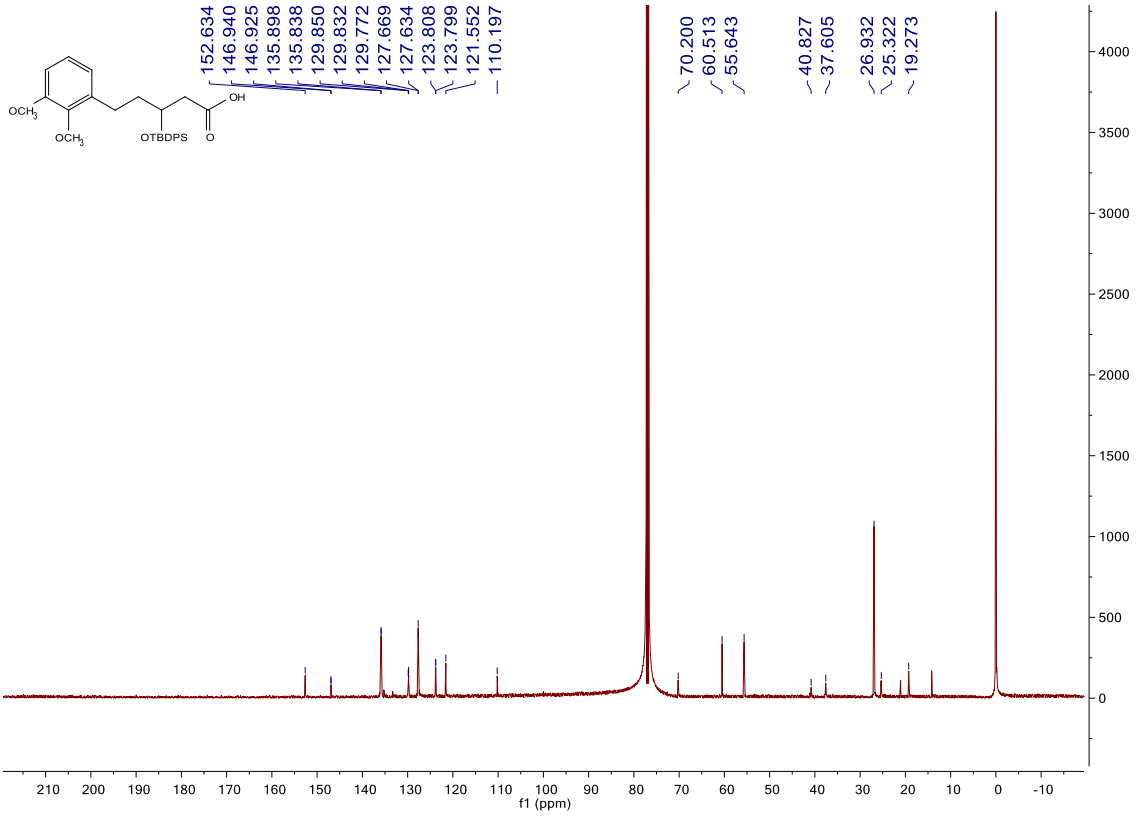
33. Methyl 3-((tert-butyldiphenylsilyl)oxy)-5-(2,3-dimethoxyphenyl)pentanoate



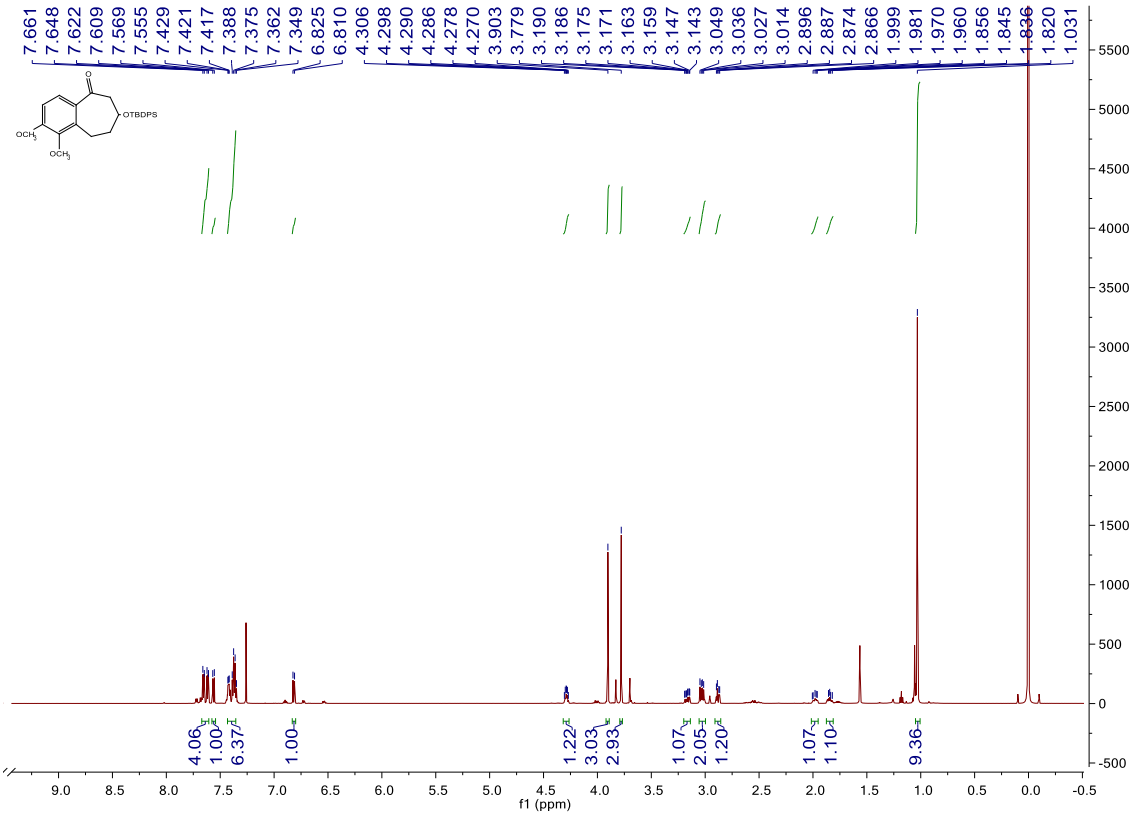


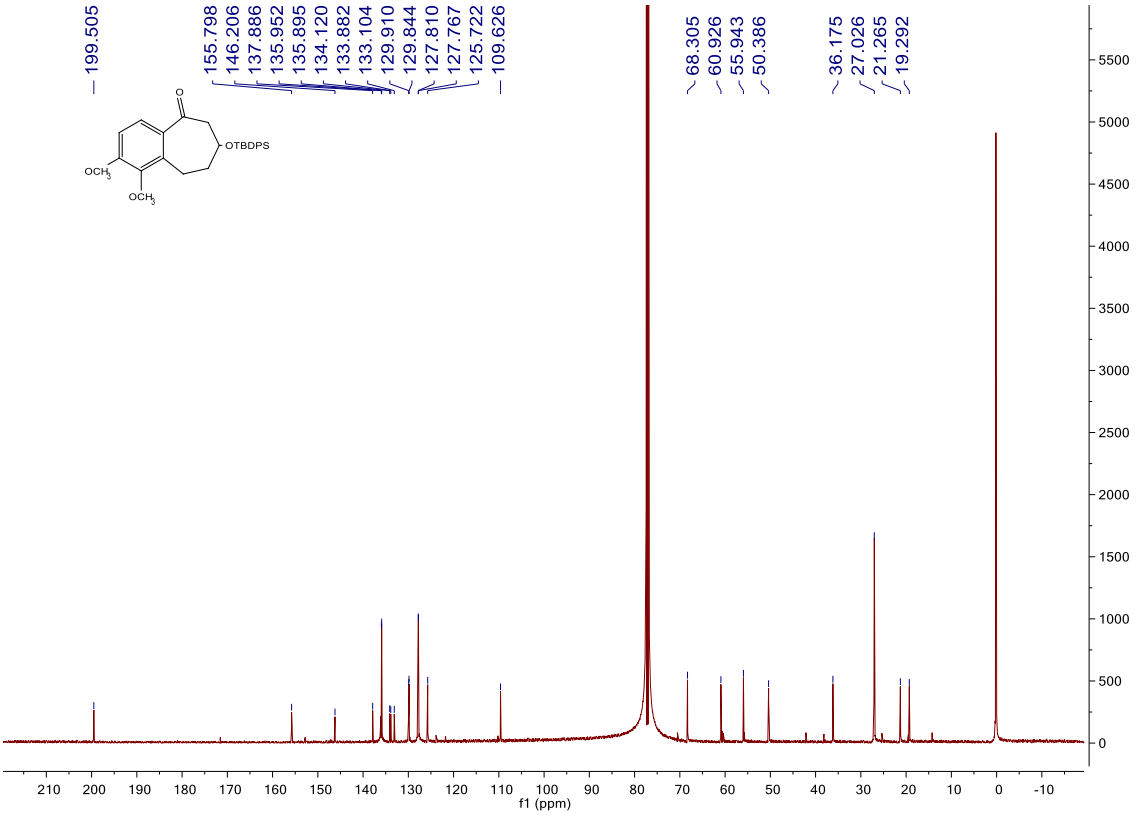
34. 3-((tert-butyldiphenylsilyl)oxy)-5-(2,3-dimethoxyphenyl)pentanoic acid



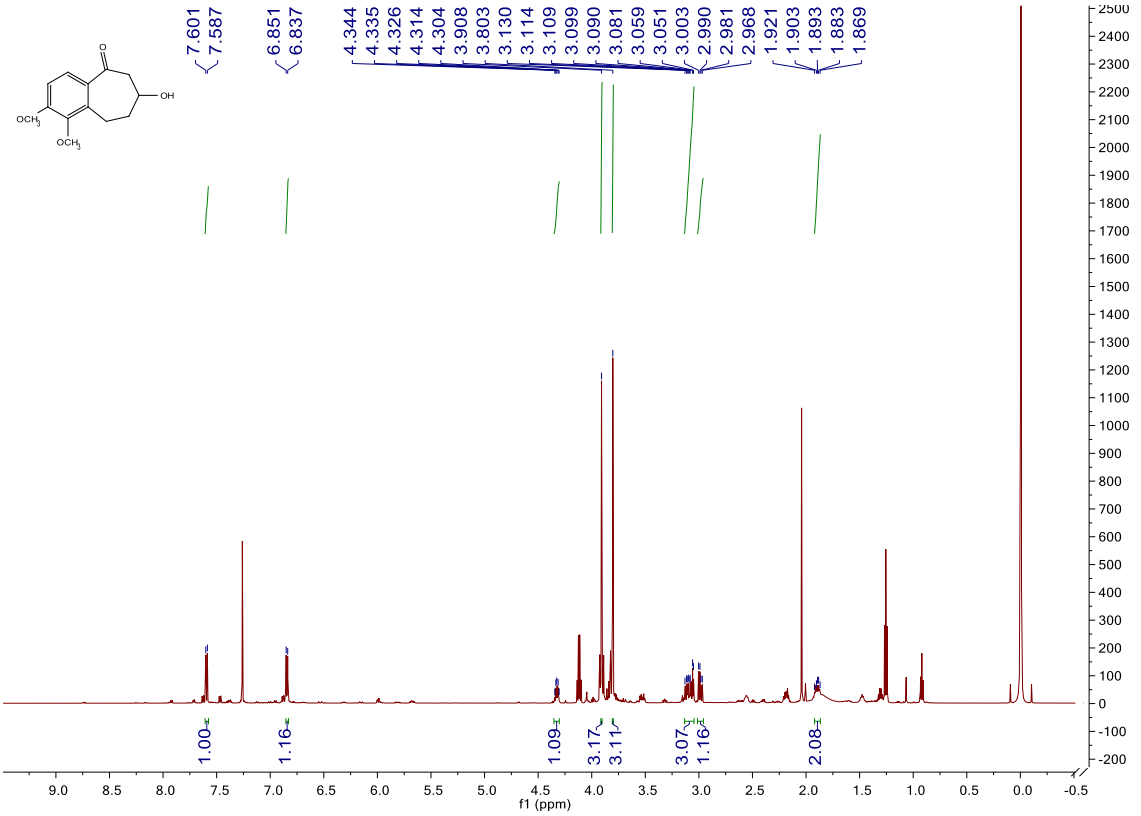


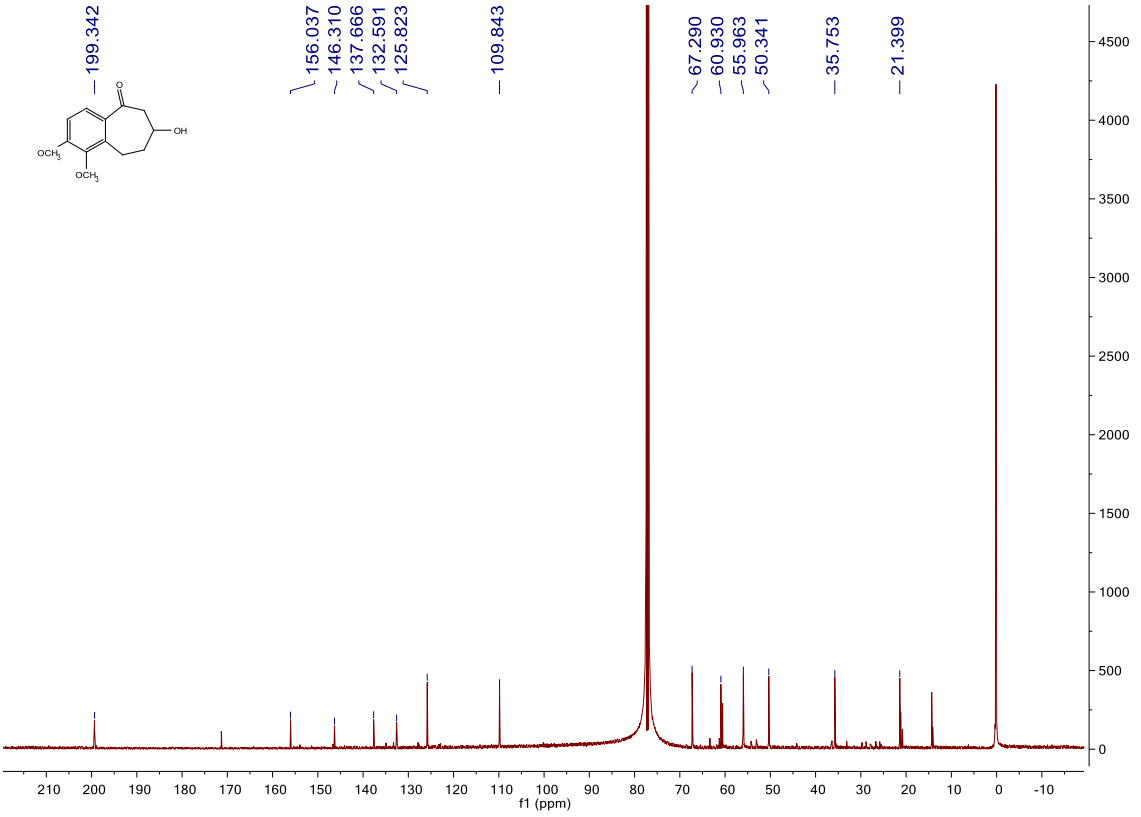
35. 7-((tert-butyldiphenylsilyl)oxy)-1,2-dimethoxy-6,7,8,9-tetrahydro-5H-benzo[7]annulen-5-one



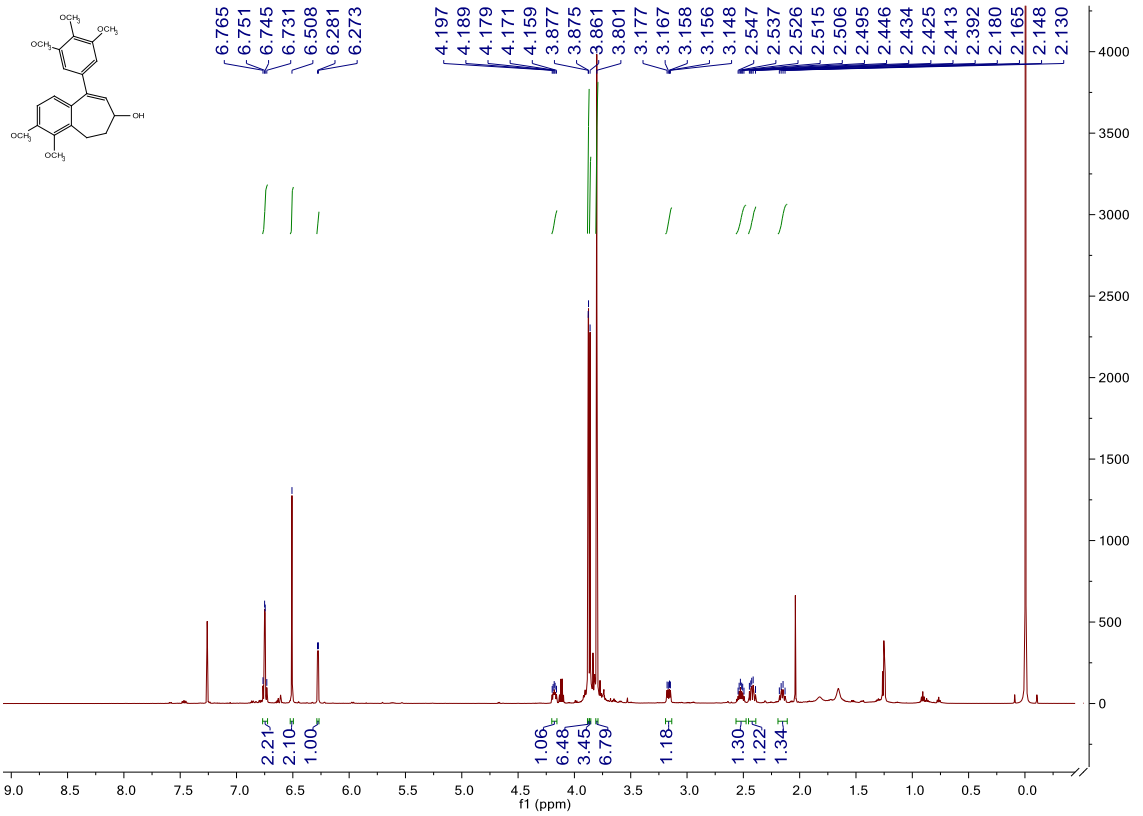


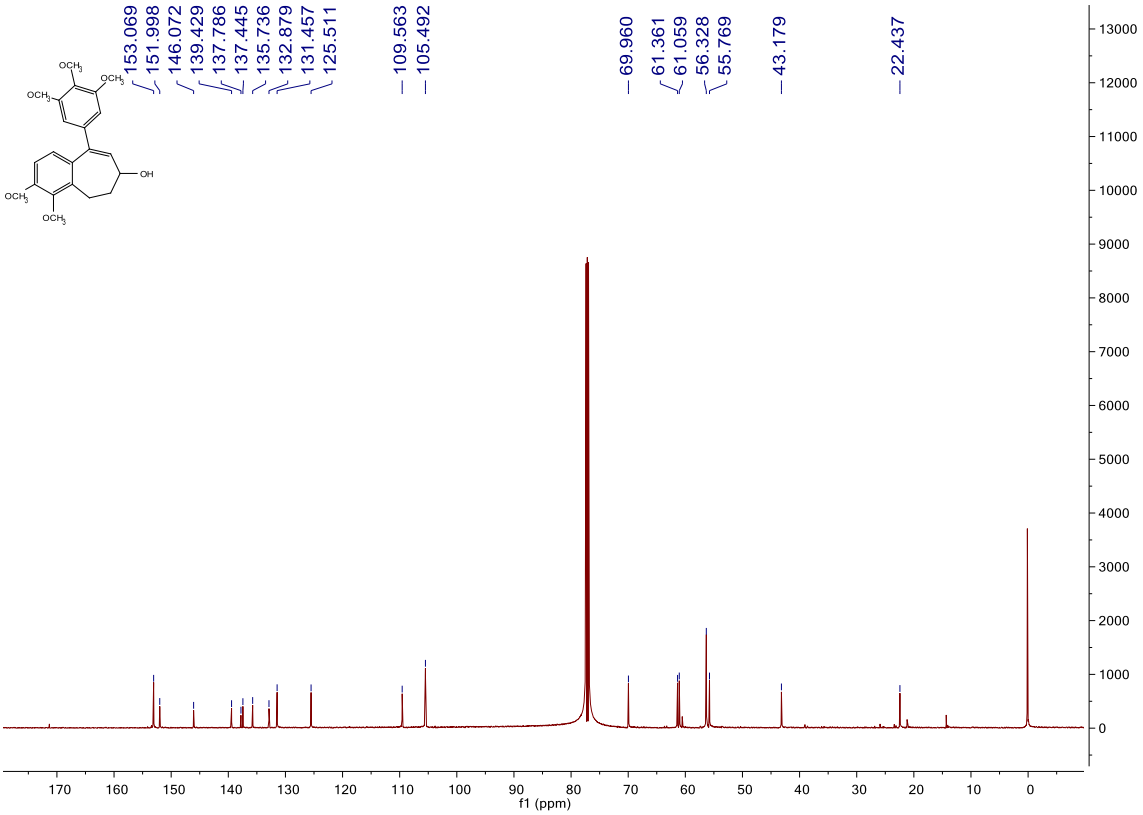
36. 7-hydroxy-1,2-dimethoxy-6,7,8,9-tetrahydro-5H-benzo[7]annulen-5-one





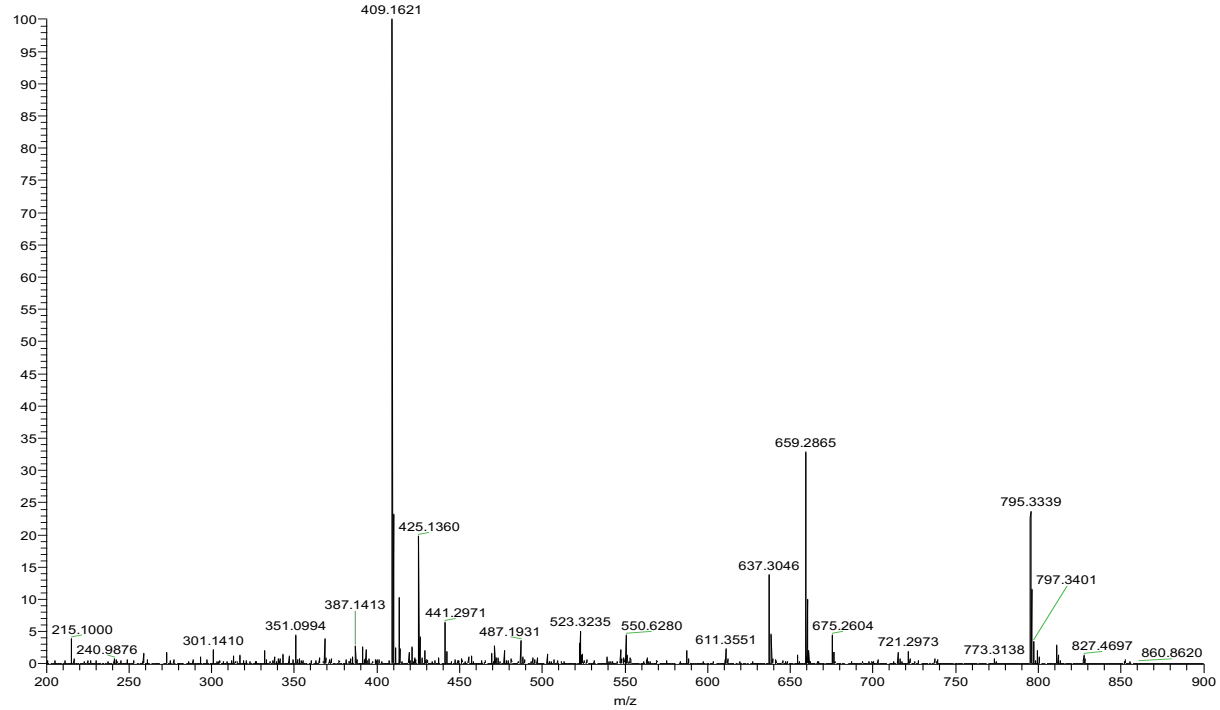
37. 3,4-dimethoxy-9-(3,4,5-trimethoxyphenyl)-6,7-dihydro-5H-benzo[7]annulen-7-ol





C:\Xcalibur\...\NHC_3_05_KGP471 11/1[illegible] 3:12:31 PM

NHC_3_05_KGP471 #200 RT: 1.69 AV: 1 NL: 8.53E6
T: FTMS + p ESI Full ms [200.00-900.00]



Data File C:\Chem32\1\Data\NHC\KGP471_Concentrated.D
Sample Name: KGP471_Concentrated

```
======================================================================
Acq. Operator   : SYSTEM
Sample Operator : SYSTEM
Acq. Instrument : 1200 HPLC                    Location :   1
Injection Date  : 2/28/2018 3:57:48 PM
                                             Inj Volume : No inj
Acq. Method     : C:\CHEM32\1\METHODS\MASTERMETHOD2.M
Last changed    : 12/2/2015 12:37:42 PM by Eric Lin
Analysis Method : C:\CHEM32\1\METHODS\RT-ACNWASH 2.M
Last changed    : 7/9/2015 2:27:22 PM by Blake
Method Info     : General Column Wash Method

Sample Info     : 20180228

Additional Info : Peak(s) manually integrated
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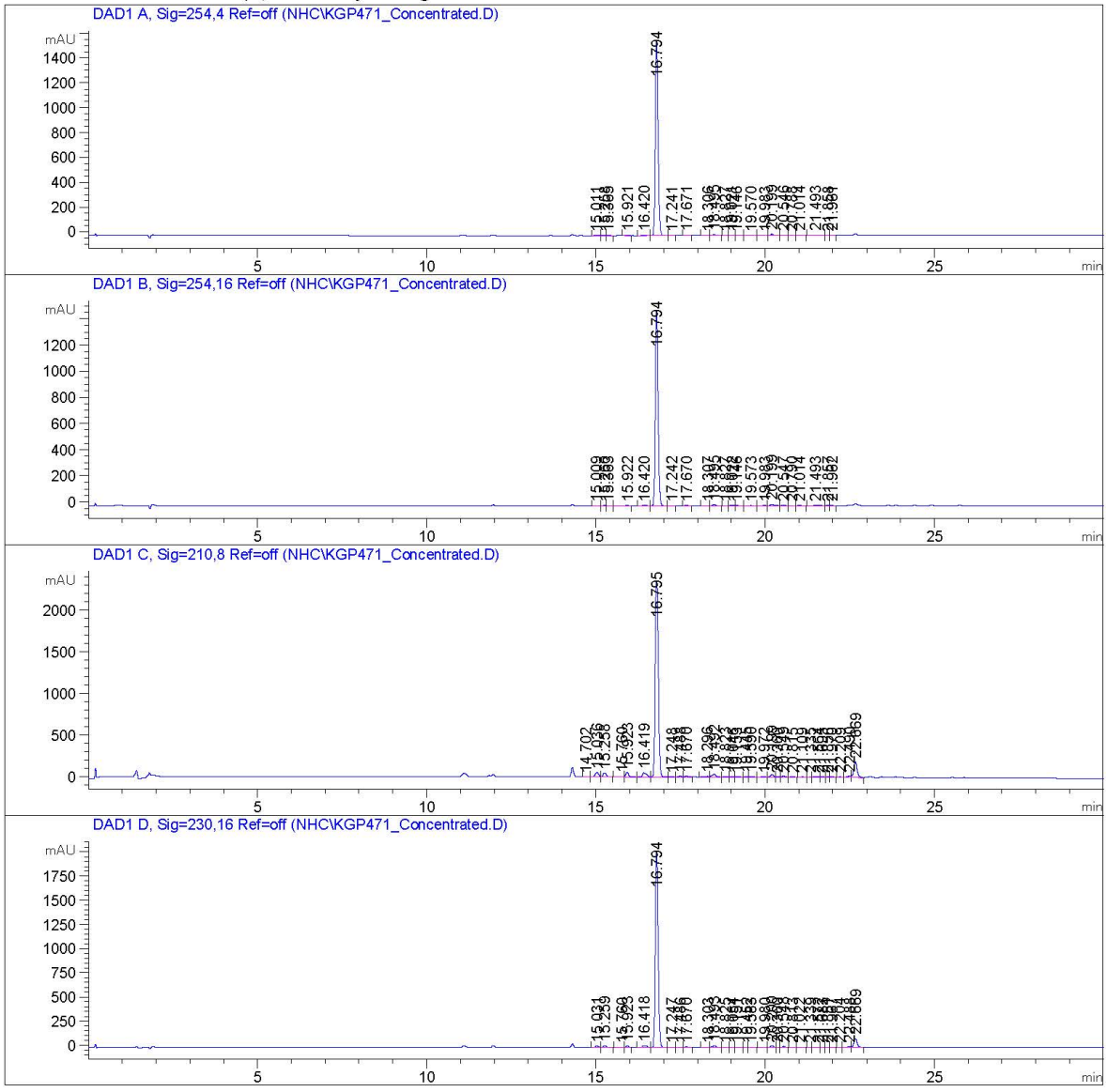
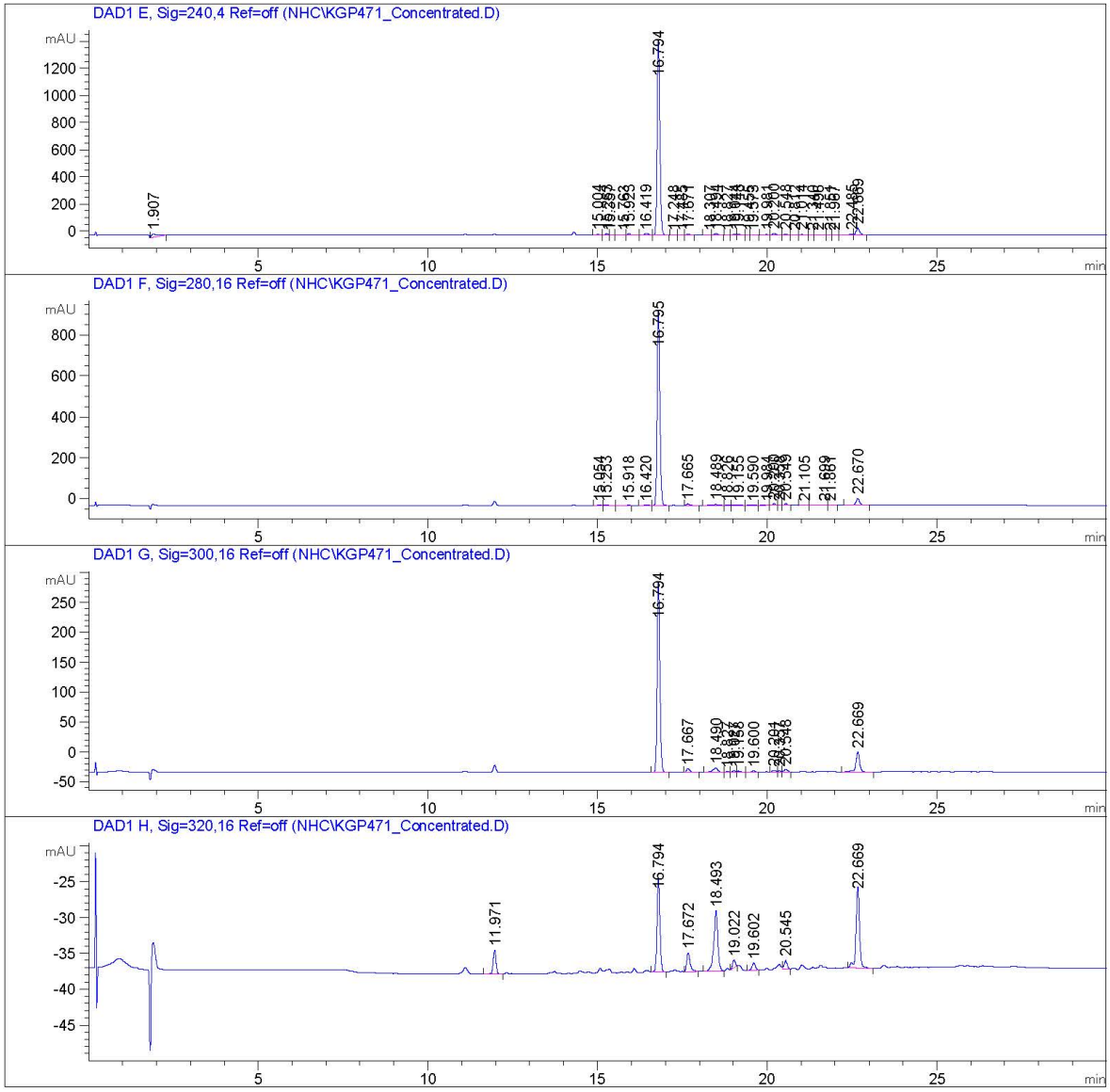


Data File C:\Chem32\1\Data\NHC\KGP471_Concentrated.D
Sample Name: KGP471_Concentrated



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Area Percent Report

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Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Data File C:\Chem32\1\Data\NHC\KGP471_Concentrated.D
Sample Name: KGP471_Concentrated

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.011	BV	0.1228	16.78301	2.15665	0.1759
2	15.258	VV	0.0939	19.06440	3.01132	0.1999
3	15.365	VB	0.0889	18.88440	3.19873	0.1980
4	15.921	BB	0.0820	19.30542	3.63033	0.2024
5	16.420	BV	0.1259	35.84679	3.87537	0.3758
6	16.794	VV	0.0892	9045.49707	1571.56372	94.8299
7	17.241	VB	0.1066	9.07631	1.31312	0.0952
8	17.671	BB	0.0944	23.82453	3.94665	0.2498
9	18.306	BV	0.1229	8.85831	1.11226	0.0929
10	18.495	VB	0.1106	57.96413	7.80660	0.6077
11	18.827	BB	0.0851	8.71520	1.61229	0.0914
12	19.021	BV	0.1045	31.15117	4.63042	0.3266
13	19.146	VB	0.0895	13.83794	2.32390	0.1451
14	19.570	BB	0.1808	20.15080	1.74433	0.2113
15	19.983	BV	0.1038	16.59275	2.42658	0.1740
16	20.199	VV	0.1155	82.05315	10.23953	0.8602
17	20.546	VB	0.1115	26.82783	3.57529	0.2813
18	20.788	BV	0.1174	7.54420	1.08062	0.0791
19	21.014	VB	0.1096	21.30884	2.97477	0.2234
20	21.493	BB	0.1949	32.57446	2.19746	0.3415
21	21.858	BV	0.0866	9.82635	1.77480	0.1030
22	21.961	VB	0.0962	12.97055	2.03957	0.1360
Totals :				9538.65762	1638.23433	

Signal 2: DAD1 B, Sig=254,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.009	BV	0.1187	19.69266	2.59083	0.2165
2	15.260	VV	0.0960	22.51476	3.54811	0.2475
3	15.363	VB	0.0843	17.73131	3.11892	0.1949
4	15.922	BB	0.1068	33.91423	4.55857	0.3729
5	16.420	BV	0.1261	40.41064	4.35957	0.4443
6	16.794	VV	0.0890	8576.89941	1493.45435	94.2937
7	17.242	VB	0.1033	9.02361	1.32713	0.0992
8	17.670	BB	0.0946	26.00756	4.29688	0.2859
9	18.307	BV	0.1263	10.75583	1.33136	0.1182
10	18.495	VB	0.1118	57.88004	7.68681	0.6363
11	18.827	BB	0.0849	8.41770	1.56167	0.0925
12	19.022	BV	0.1052	30.40357	4.47882	0.3343
13	19.146	VB	0.0911	14.91885	2.44737	0.1640
14	19.573	BB	0.1808	21.14986	1.83007	0.2325
15	19.983	BV	0.1054	17.28123	2.47573	0.1900
16	20.199	VV	0.1161	79.53284	9.85869	0.8744
17	20.547	VB	0.1101	27.89582	3.77982	0.3067
18	20.790	BV	0.1195	7.68341	1.07381	0.0845
19	21.014	VB	0.1103	20.02006	2.77150	0.2201

Data File C:\Chem32\1\Data\NHC\KGP471_Concentrated.D
Sample Name: KGP471_Concentrated

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
20	21.493	BB	0.2000	31.95560	2.09449	0.3513
21	21.857	BV	0.0864	9.35524	1.69430	0.1029
22	21.962	VB	0.0963	12.49788	1.96129	0.1374
Totals :				9095.94211	1562.30010	

Signal 3: DAD1 C, Sig=210,8 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.702	VB	0.1445	20.89368	2.33278	0.1015
2	15.036	BV	0.1198	380.04733	51.67448	1.8457
3	15.258	VB	0.1079	353.74332	49.17688	1.7180
4	15.760	BV	0.1364	101.28828	10.15446	0.4919
5	15.923	VB	0.0902	350.39801	58.23767	1.7017
6	16.419	BV	0.1264	459.97971	50.44131	2.2339
7	16.795	VB	0.1086	1.59109e4	2360.23047	77.2715
8	17.248	BB	0.1050	20.54396	3.19528	0.0998
9	17.488	BV	0.0982	94.50442	14.84969	0.4590
10	17.670	VB	0.1092	115.13950	15.41124	0.5592
11	18.296	BV	0.1542	125.05814	11.74608	0.6073
12	18.492	VB	0.1226	289.30923	34.22702	1.4050
13	18.823	BB	0.0913	43.79387	7.59260	0.2127
14	19.046	BV	0.0992	31.37870	5.00320	0.1524
15	19.153	VB	0.1094	46.74327	5.96928	0.2270
16	19.445	BV	0.0908	52.65433	8.92726	0.2557
17	19.590	VB	0.1255	72.24635	8.82945	0.3509
18	19.972	BB	0.1197	49.28241	6.13389	0.2393
19	20.199	BV	0.0973	211.37521	32.75731	1.0265
20	20.360	VV	0.0844	31.71260	5.74937	0.1540
21	20.549	VB	0.0977	107.52854	17.02164	0.5222
22	20.815	BB	0.1320	50.41508	6.39358	0.2448
23	21.109	BB	0.1056	34.80313	5.09877	0.1690
24	21.335	BV	0.0851	19.84887	3.55851	0.0964
25	21.564	VV	0.1601	51.62708	4.23828	0.2507
26	21.695	VB	0.0920	30.91896	5.15103	0.1502
27	21.856	BV	0.0713	13.69423	2.99670	0.0665
28	21.970	VB	0.0986	45.20246	7.06660	0.2195
29	22.209	BB	0.0942	24.45537	4.18358	0.1188
30	22.490	BV	0.1015	116.57590	17.55134	0.5662
31	22.669	VB	0.1075	1334.84619	186.52919	6.4827
Totals :				2.05909e4	3002.42895	

Data File C:\Chem32\1\Data\NHC\KGP471_Concentrated.D
Sample Name: KGP471_Concentrated

Signal 4: DAD1 D, Sig=230,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.031	BV	0.1231	123.01094	16.11219	0.8704
2	15.259	VB	0.1177	137.69258	17.14124	0.9743
3	15.760	BV	0.1358	32.35648	3.26066	0.2289
4	15.923	VB	0.0837	103.20261	18.89578	0.7302
5	16.418	BV	0.1237	180.76074	19.94655	1.2790
6	16.794	VB	0.0935	1.20898e4	2030.49292	85.5450
7	17.247	BB	0.1021	15.79870	2.48903	0.1118
8	17.486	BV	0.0989	28.58271	4.57275	0.2022
9	17.670	VB	0.1019	63.44791	9.49903	0.4489
10	18.303	BV	0.1372	39.76471	4.32592	0.2814
11	18.493	VB	0.1188	138.13828	16.99601	0.9774
12	18.825	BB	0.0888	20.79643	3.74540	0.1472
13	19.054	BV	0.0984	27.34455	4.40886	0.1935
14	19.151	VB	0.1102	39.40737	5.09501	0.2788
15	19.452	BV	0.0836	17.59227	3.22742	0.1245
16	19.583	VB	0.1305	40.85652	4.74193	0.2891
17	19.980	BB	0.1026	27.63213	4.10041	0.1955
18	20.200	BV	0.0988	112.75363	17.13424	0.7978
19	20.360	VV	0.0832	16.33440	2.92357	0.1156
20	20.548	VB	0.0997	65.66751	10.12673	0.4647
21	20.813	BB	0.1243	15.12977	2.04473	0.1071
22	21.022	BB	0.1382	20.19997	1.99454	0.1429
23	21.339	BV	0.0833	8.66180	1.59627	0.0613
24	21.572	VV	0.1579	26.18093	2.15257	0.1853
25	21.683	VB	0.0943	12.75117	2.05733	0.0902
26	21.851	BV	0.0821	11.75560	2.20898	0.0832
27	21.967	VB	0.0965	20.46784	3.29585	0.1448
28	22.204	BB	0.0991	6.07440	1.02629	0.0430
29	22.488	BV	0.1078	55.69608	7.75810	0.3941
30	22.669	VB	0.1073	634.81122	88.90147	4.4918
Totals :				1.41326e4	2312.27178	

Signal 5: DAD1 E, Sig=240,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.907	BB	0.1950	328.73831	25.07483	3.3271
2	15.004	BV	0.1061	51.31367	7.29355	0.5193
3	15.263	VV	0.0976	62.24531	9.60111	0.6300
4	15.357	VB	0.0682	21.71208	4.85475	0.2197
5	15.763	BV	0.1371	25.40589	2.53059	0.2571
6	15.923	VB	0.0928	72.77342	11.65710	0.7365
7	16.419	BV	0.1258	103.88537	11.24391	1.0514
8	16.794	VB	0.0888	8252.48730	1440.60889	83.5229
9	17.248	BB	0.0968	11.21957	1.84825	0.1136
10	17.485	BV	0.1008	14.97330	2.33399	0.1515
11	17.671	VB	0.0992	42.64151	6.61279	0.4316

Data File C:\Chem32\1\Data\NHC\KGP471_Concentrated.D
Sample Name: KGP471_Concentrated

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
12	18.307	BV	0.1365	25.33621	2.82830	0.2564
13	18.494	VB	0.1159	82.44463	10.46401	0.8344
14	18.827	BB	0.0853	11.33137	2.08773	0.1147
15	19.044	BV	0.1069	27.64451	4.08846	0.2798
16	19.148	VB	0.0993	27.50285	3.94891	0.2784
17	19.455	BV	0.0805	11.40575	2.19782	0.1154
18	19.573	VB	0.1374	28.12904	3.11255	0.2847
19	19.981	BV	0.1117	30.73274	4.08729	0.3110
20	20.200	VV	0.1193	92.54539	11.10138	0.9366
21	20.548	VB	0.1086	42.49094	5.85888	0.4300
22	20.812	BV	0.1303	10.64117	1.37527	0.1077
23	21.014	VB	0.1086	23.62852	3.33868	0.2391
24	21.340	BV	0.0902	7.94307	1.35793	0.0804
25	21.496	VV	0.2137	44.34917	2.67170	0.4489
26	21.851	VV	0.0976	15.62197	2.34779	0.1581
27	21.967	VB	0.1020	17.11787	2.55977	0.1732
28	22.485	BV	0.1276	48.70327	5.48500	0.4929
29	22.669	VB	0.1084	345.54871	47.74048	3.4973
Totals :				9880.51291	1640.31171	

Signal 6: DAD1 F, Sig=280,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.054	BV	0.1090	21.55566	2.89076	0.3510
2	15.253	VB	0.1328	25.26513	2.70890	0.4114
3	15.918	BV	0.1589	18.24239	1.53263	0.2971
4	16.420	BV	0.1314	22.02534	2.26597	0.3587
5	16.795	VV	0.0888	5463.79248	954.54541	88.9759
6	17.665	VB	0.1030	49.65844	7.32952	0.8087
7	18.489	BB	0.1571	61.46814	5.30905	1.0010
8	18.826	BV	0.0900	10.56657	1.81397	0.1721
9	19.155	VB	0.2009	27.99067	1.95659	0.4558
10	19.590	BB	0.1397	15.81760	1.68285	0.2576
11	19.984	BB	0.1088	8.06416	1.10894	0.1313
12	20.200	BV	0.0984	48.82339	7.45521	0.7951
13	20.358	VV	0.0862	9.29252	1.63643	0.1513
14	20.549	VB	0.0976	47.25852	7.49552	0.7696
15	21.105	BB	0.1234	8.84723	1.01785	0.1441
16	21.699	BV	0.2320	28.07697	1.55971	0.4572
17	21.861	VB	0.1606	18.40672	1.54969	0.2997
18	22.670	BB	0.1149	255.60170	32.81970	4.1624
Totals :				6140.75362	1036.67870	

Data File C:\Chem32\1\Data\NHC\KGP471_Concentrated.D
Sample Name: KGP471_Concentrated

Signal 7: DAD1 G, Sig=300,16 Ref=off

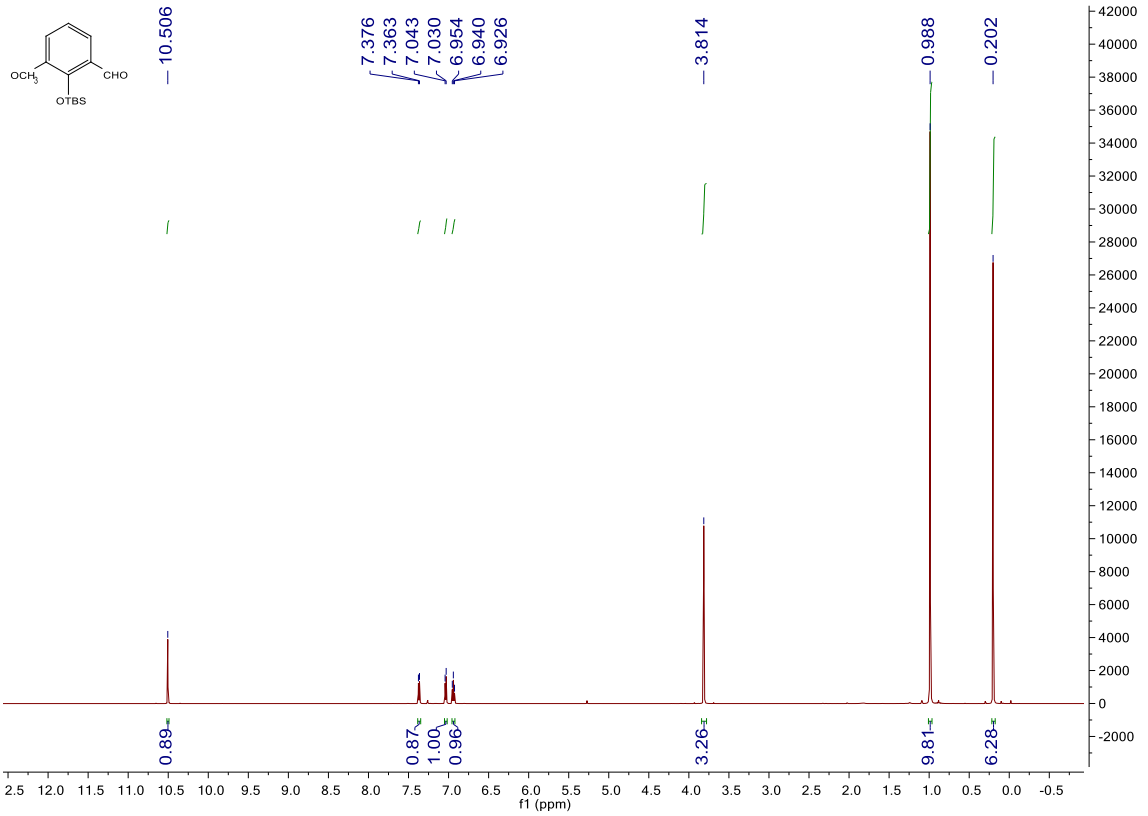
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.794	BB	0.0889	1830.76514	319.25458	79.8437
2	17.667	BB	0.1006	38.43918	5.70514	1.6764
3	18.490	BB	0.1338	70.64924	7.37258	3.0812
4	18.827	BV	0.0881	6.82989	1.20498	0.2979
5	19.027	VV	0.1107	12.07432	1.66306	0.5266
6	19.158	VB	0.1229	11.56161	1.48363	0.5042
7	19.600	BB	0.1145	13.01811	1.71548	0.5677
8	20.201	BV	0.1000	17.34897	2.59544	0.7566
9	20.357	VV	0.0996	9.24838	1.38995	0.4033
10	20.548	VB	0.0983	31.45959	4.94228	1.3720
11	22.669	BB	0.1117	251.54092	33.47738	10.9703
Totals :				2292.93535	380.80451	

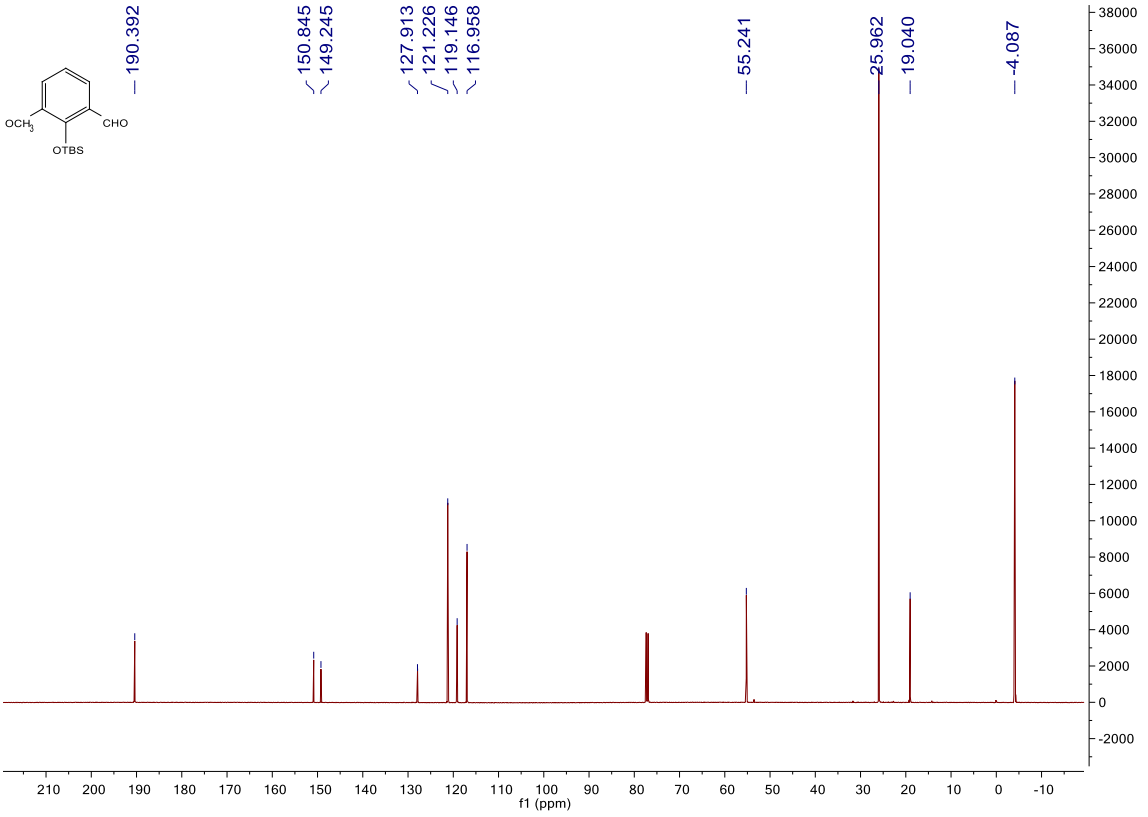
Signal 8: DAD1 H, Sig=320,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.971	BB	0.0906	19.63272	3.34000	6.8334
2	16.794	BB	0.0954	78.59277	12.83918	27.3551
3	17.672	BB	0.1042	18.18523	2.64584	6.3296
4	18.493	BB	0.1162	66.79688	8.44772	23.2494
5	19.022	BB	0.0961	6.15215	1.05459	2.1413
6	19.602	BB	0.1039	7.03116	1.02682	2.4473
7	20.545	VB	0.0977	7.51448	1.19022	2.6155
8	22.669	BB	0.1096	83.40063	11.36270	29.0285
Totals :				287.30603	41.90707	

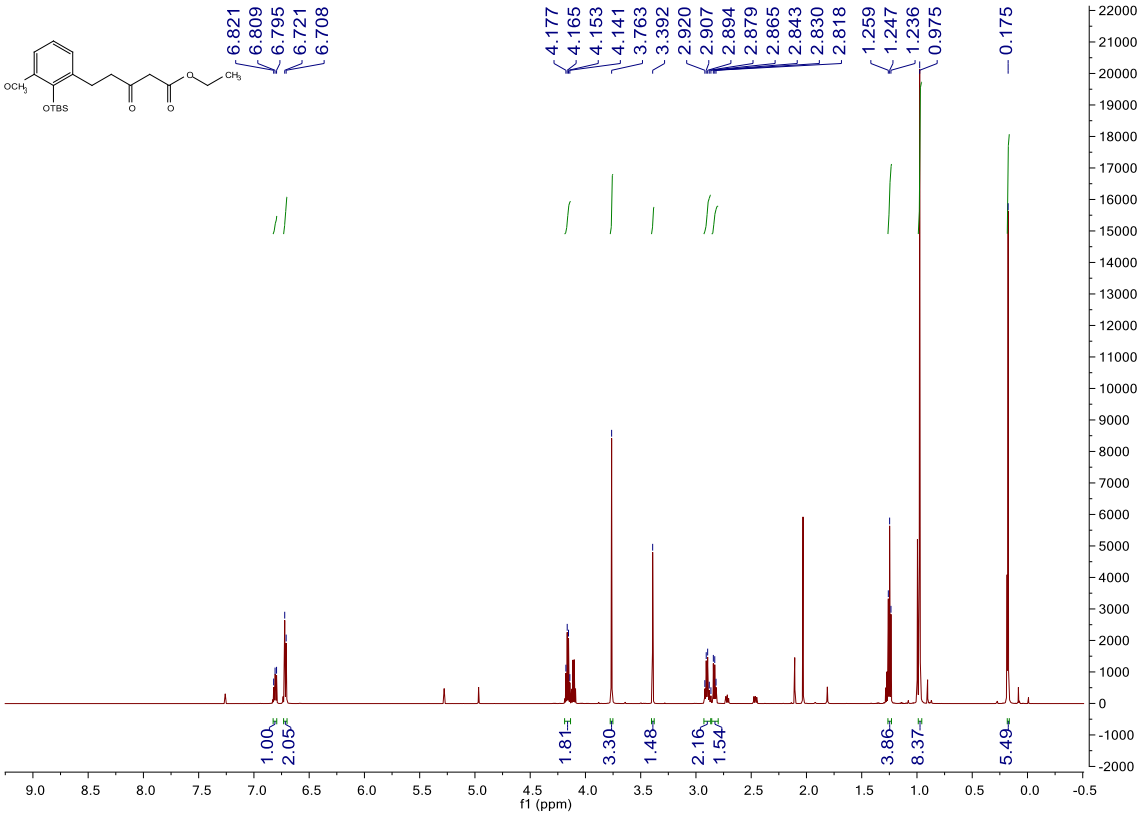
*** End of Report ***

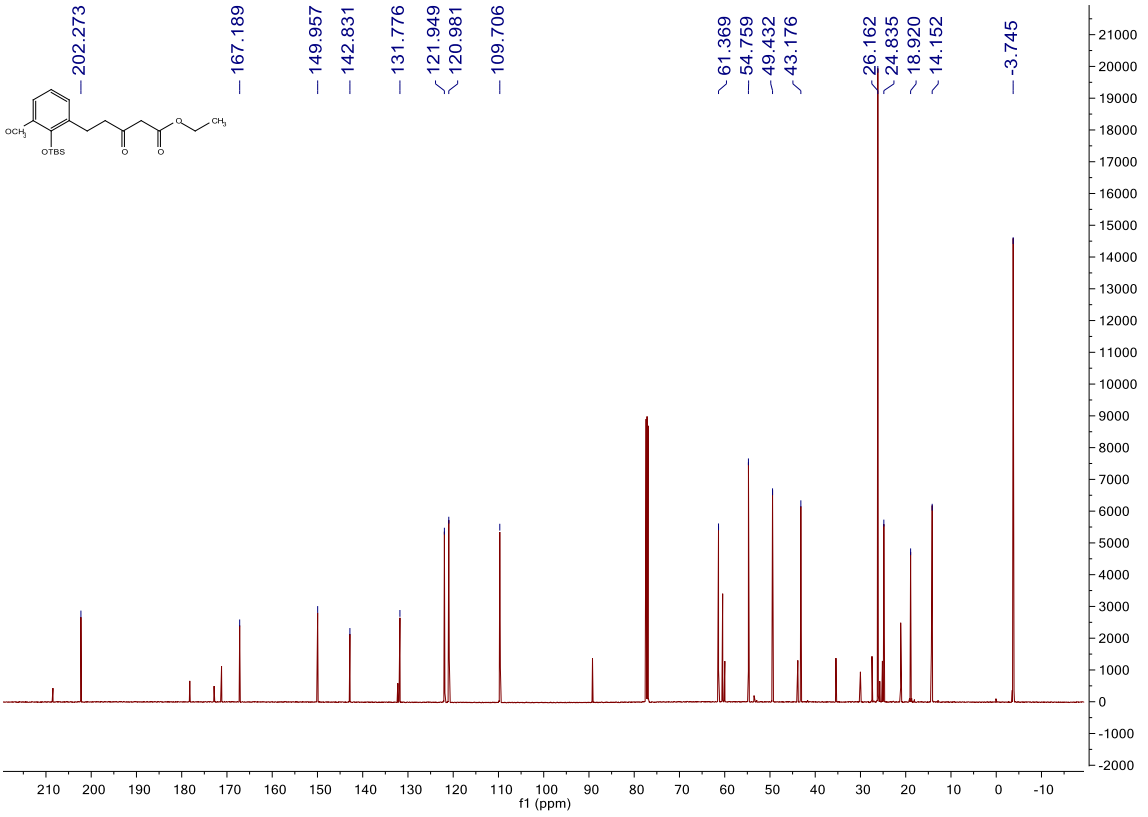
39. 2-((tert-butyldimethylsilyl)oxy)-3-methoxybenzaldehyde



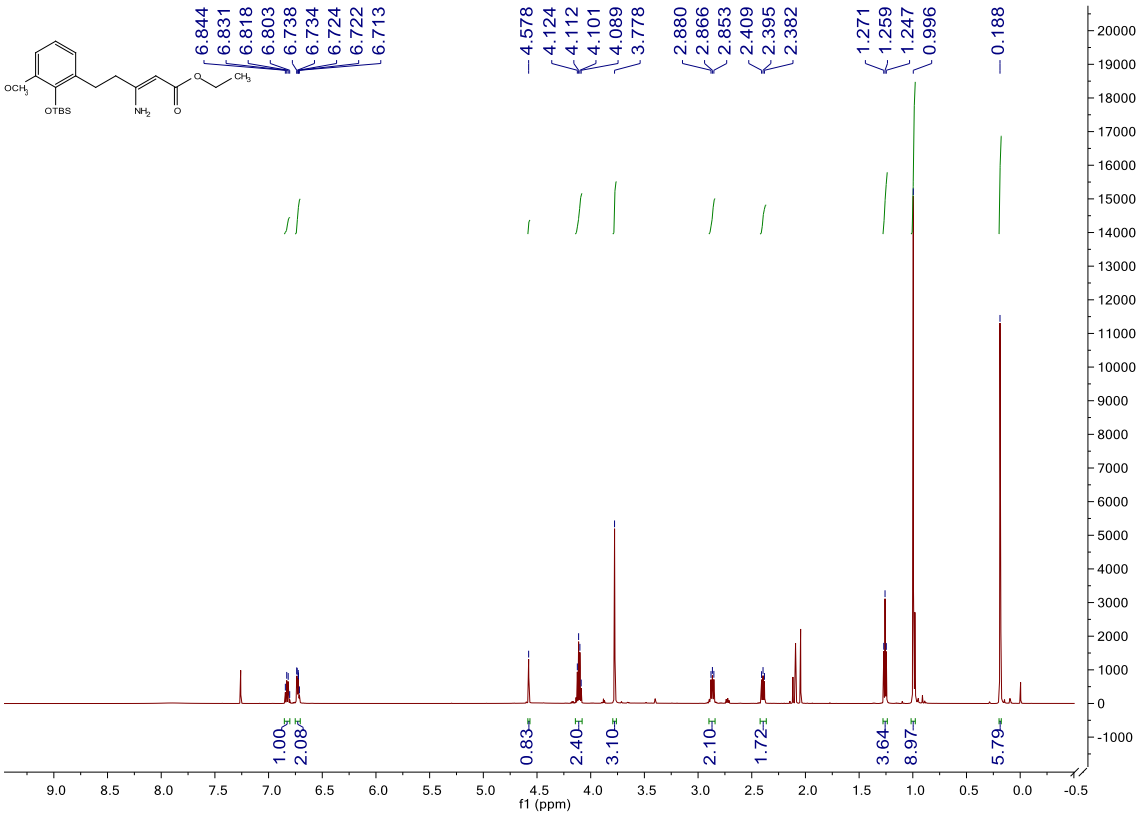


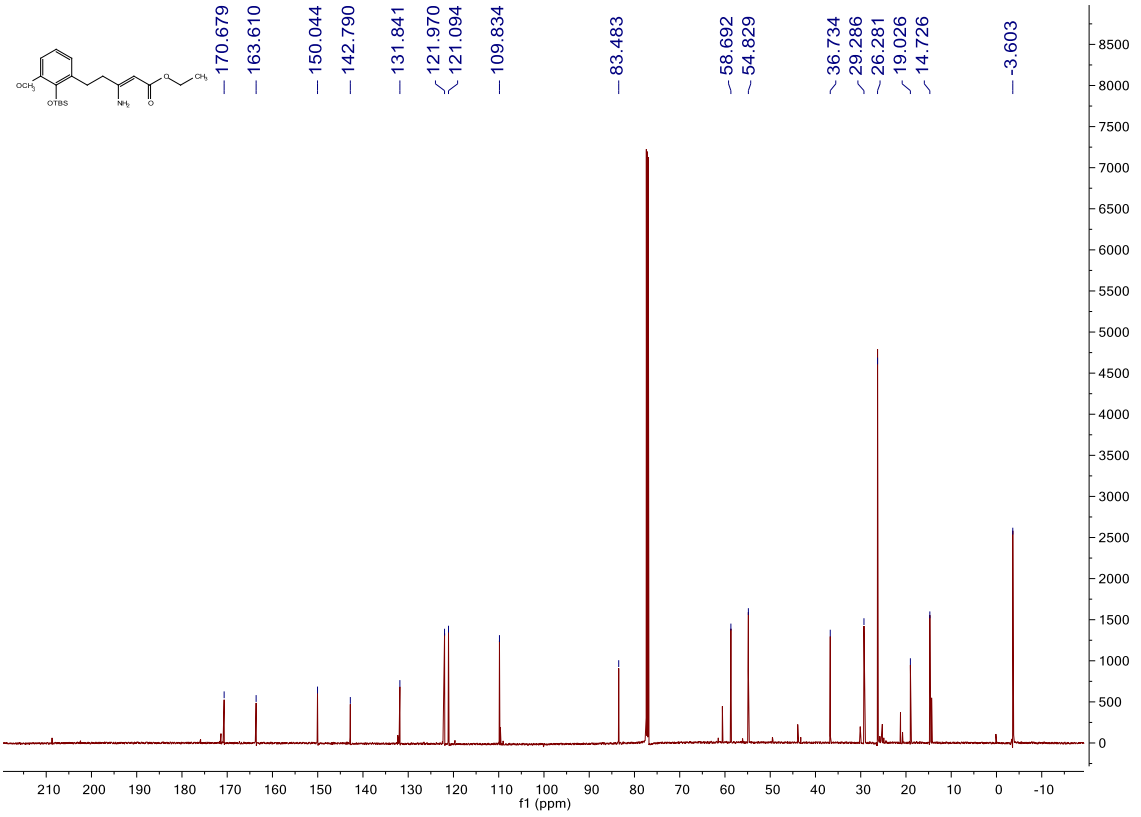
41. ethyl 5-(2-((tert-butyldimethylsilyl)oxy)-3-methoxyphenyl)-3-oxopentanoate



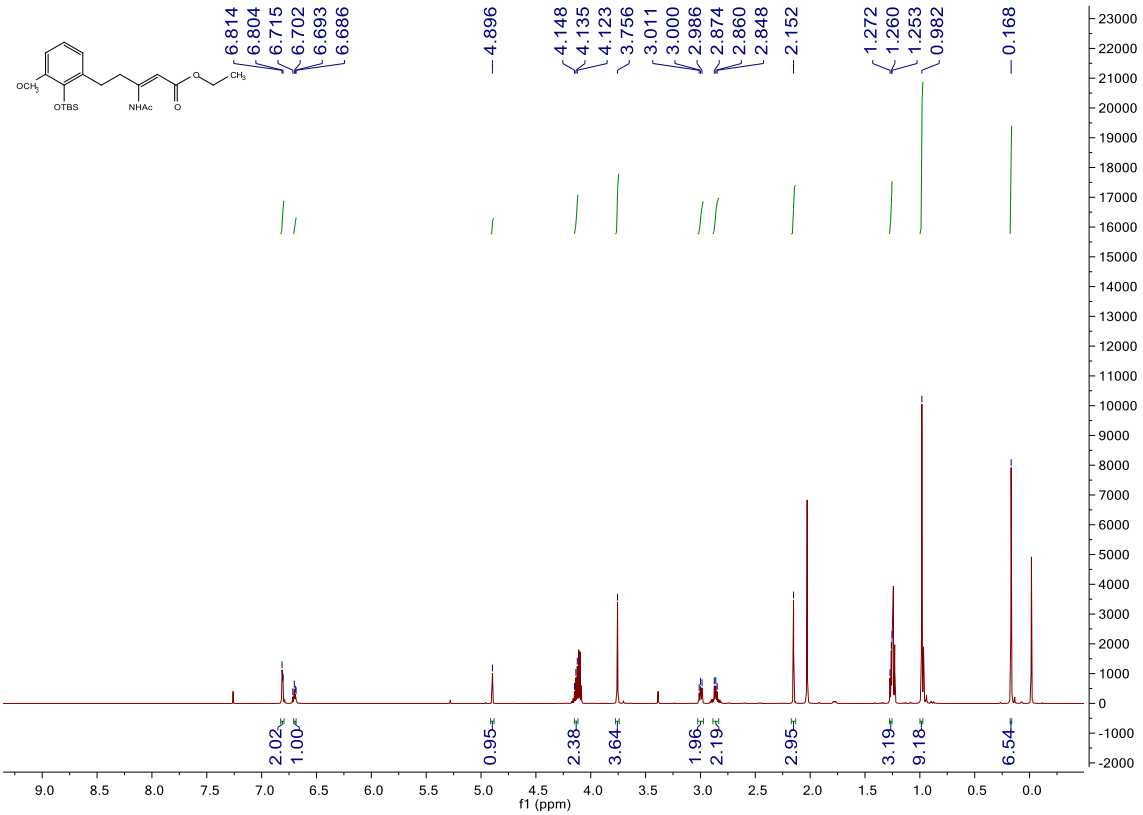


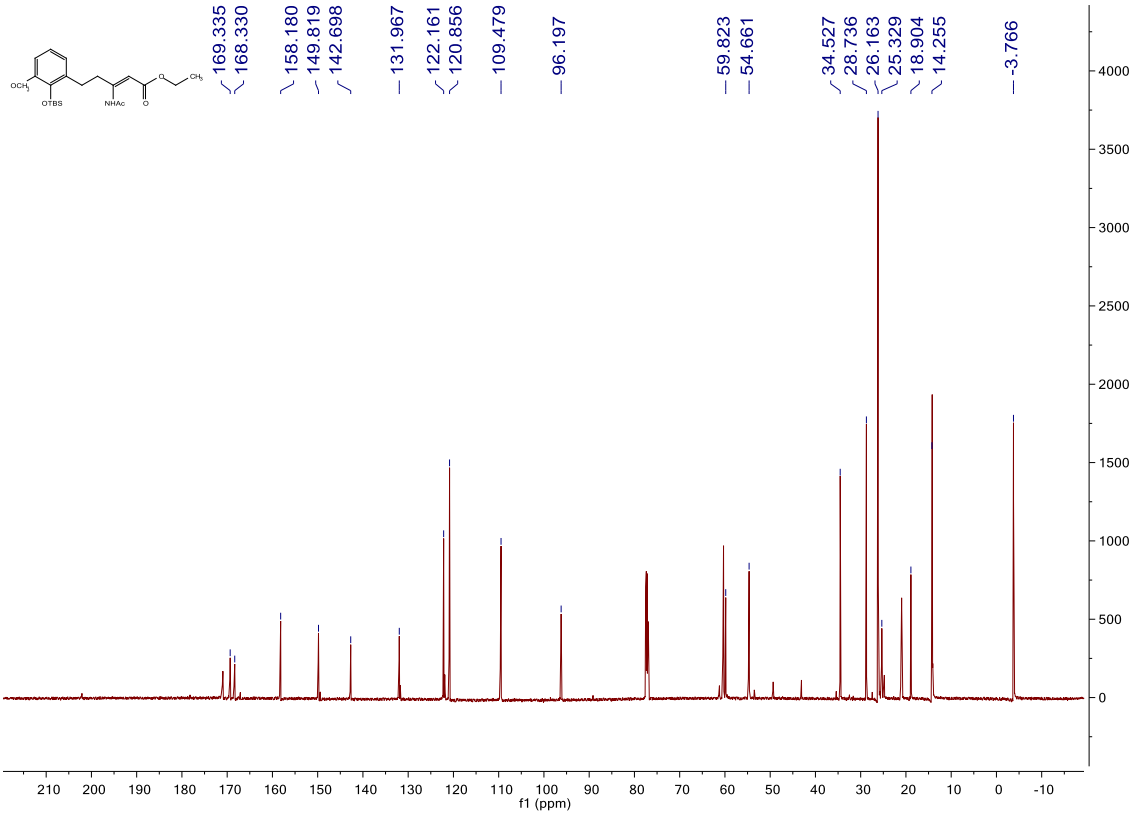
42. ethyl (Z)-3-amino-5-(2-((tert-butyldimethylsilyl)oxy)-3-methoxyphenyl)pent-2-enoate



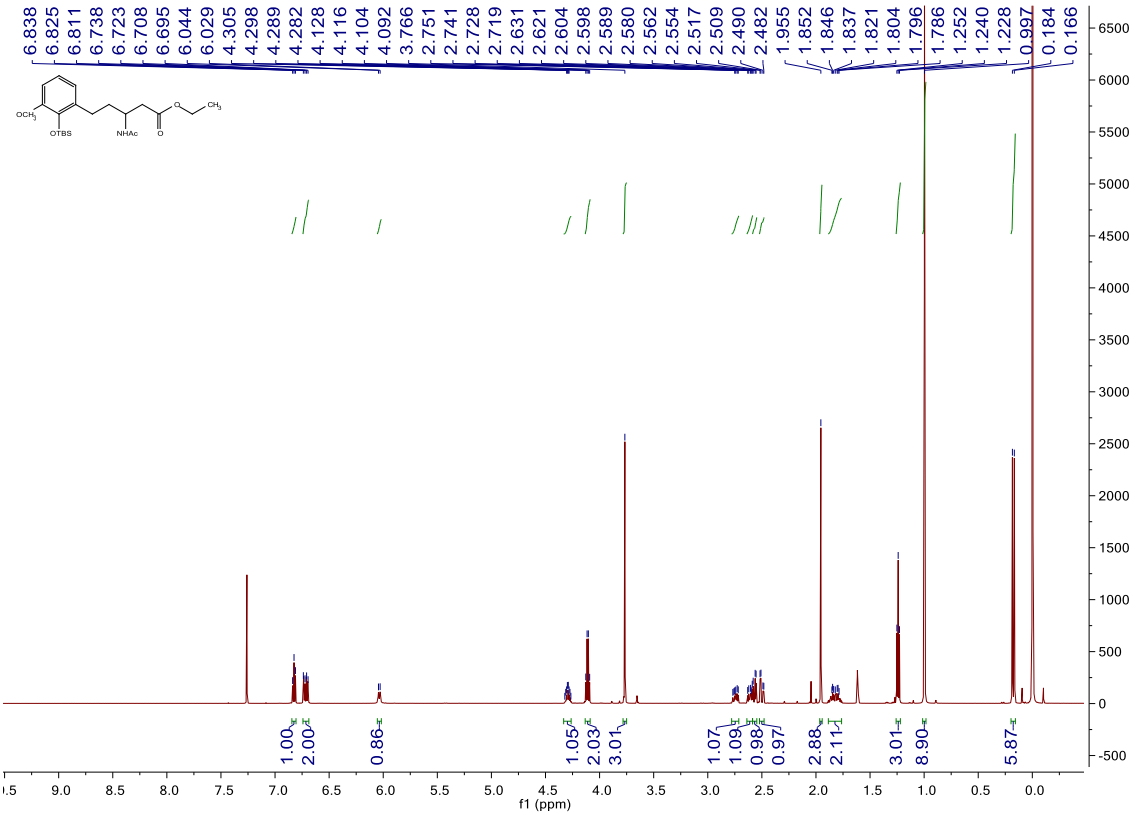


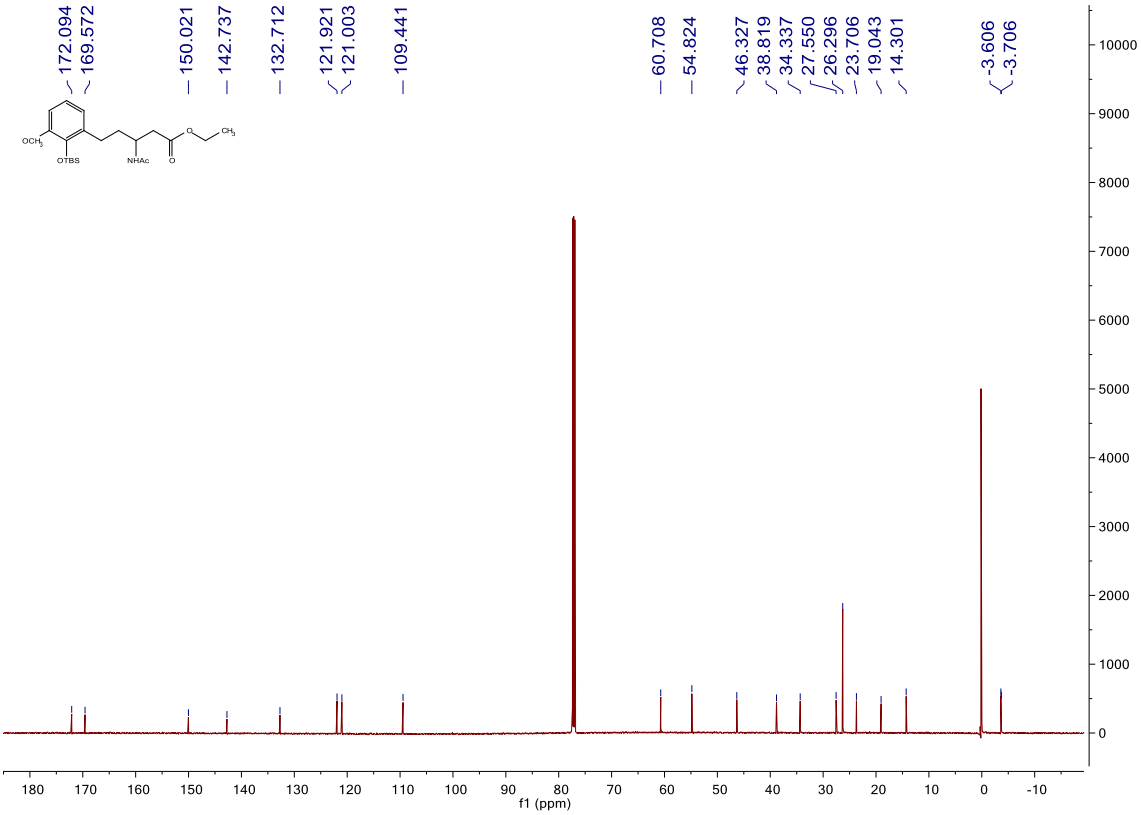
43. ethyl (Z)-3-acetamido-5-(2-((tert-butyldimethylsilyl)oxy)-3-methoxyphenyl)pent-2-enoate



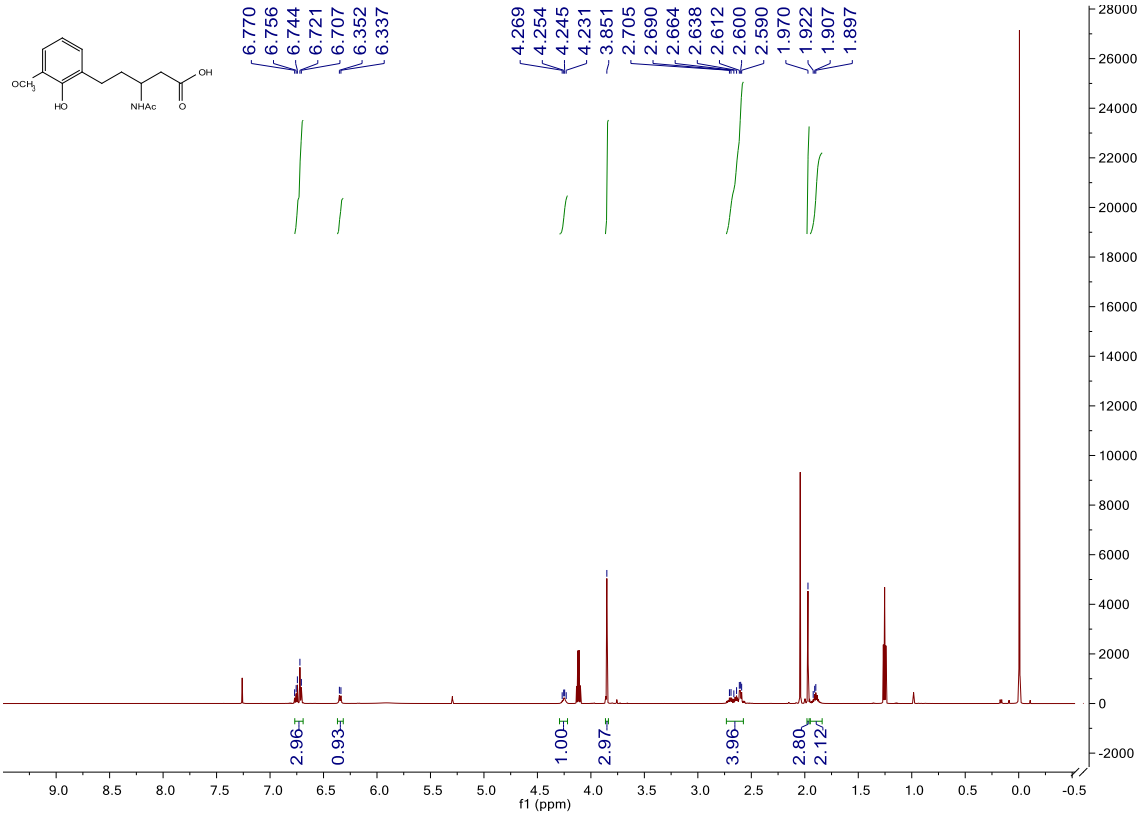


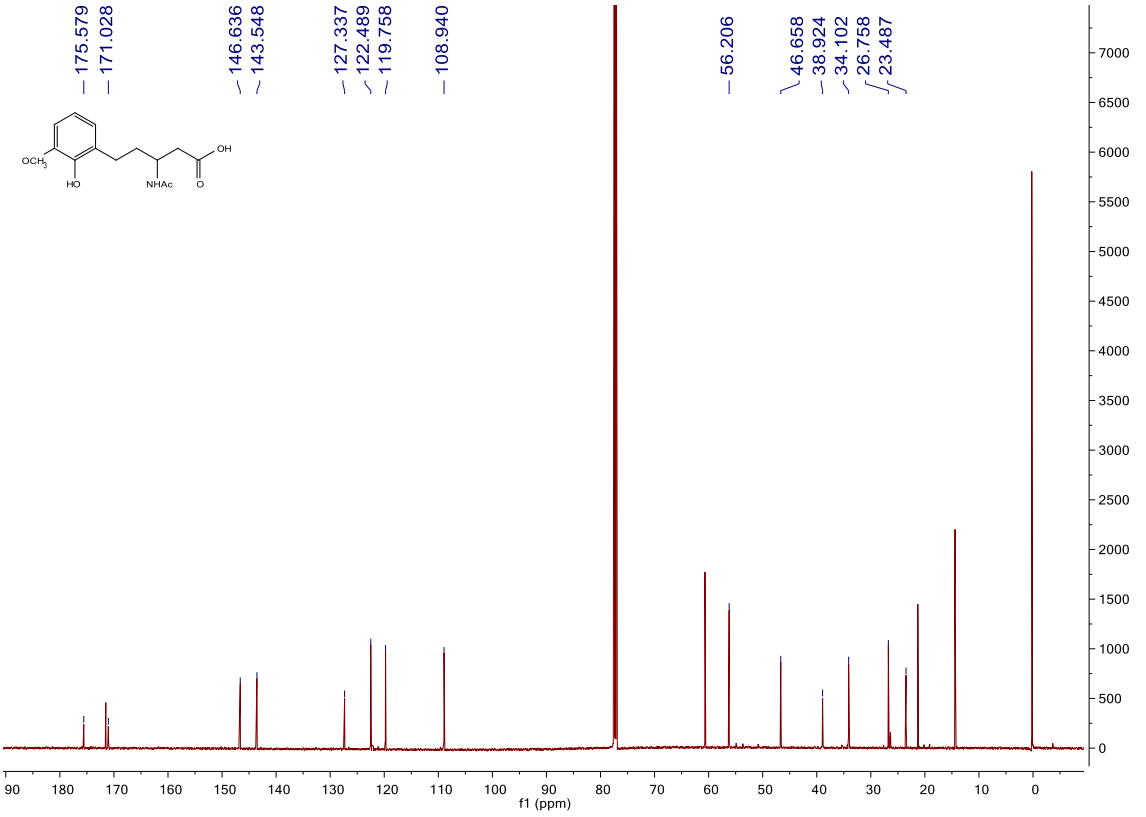
44. ethyl 3-acetamido-5-(2-((tert-butyldimethylsilyl)oxy)-3-methoxyphenyl)pentanoate



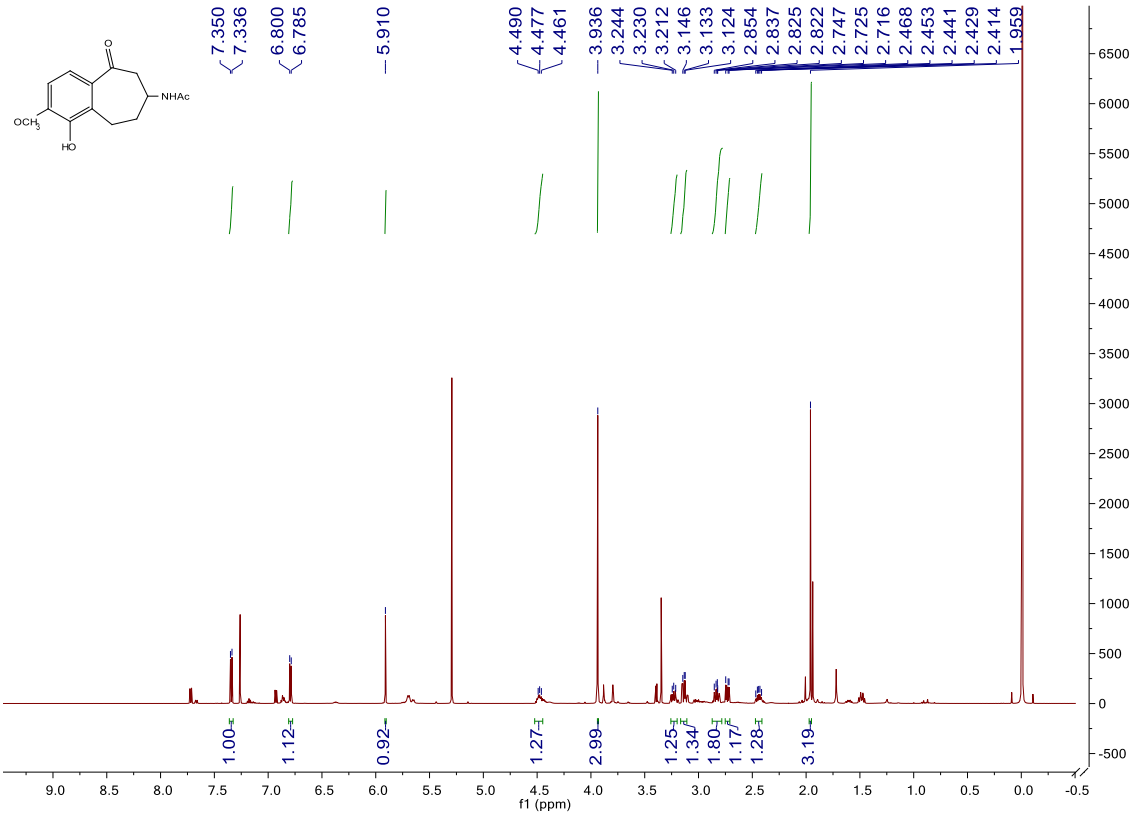


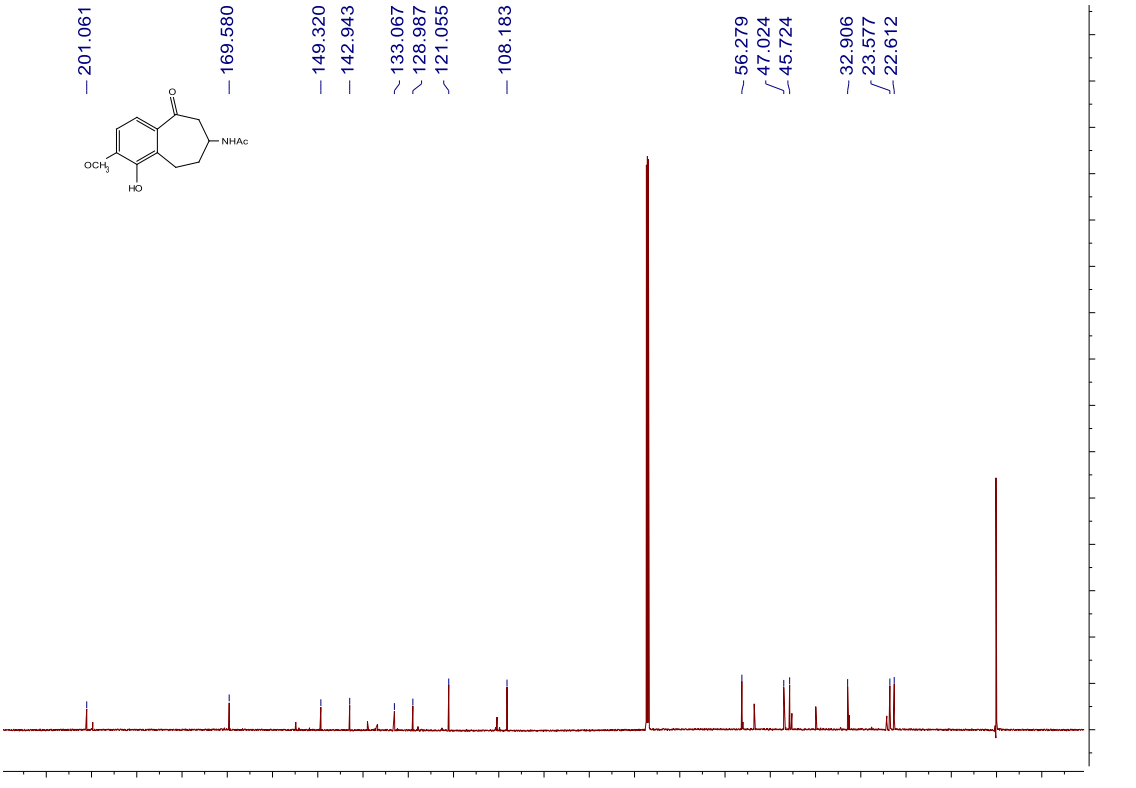
45. 3-acetamido-5-(2-hydroxy-3-methoxyphenyl)pentanoic acid



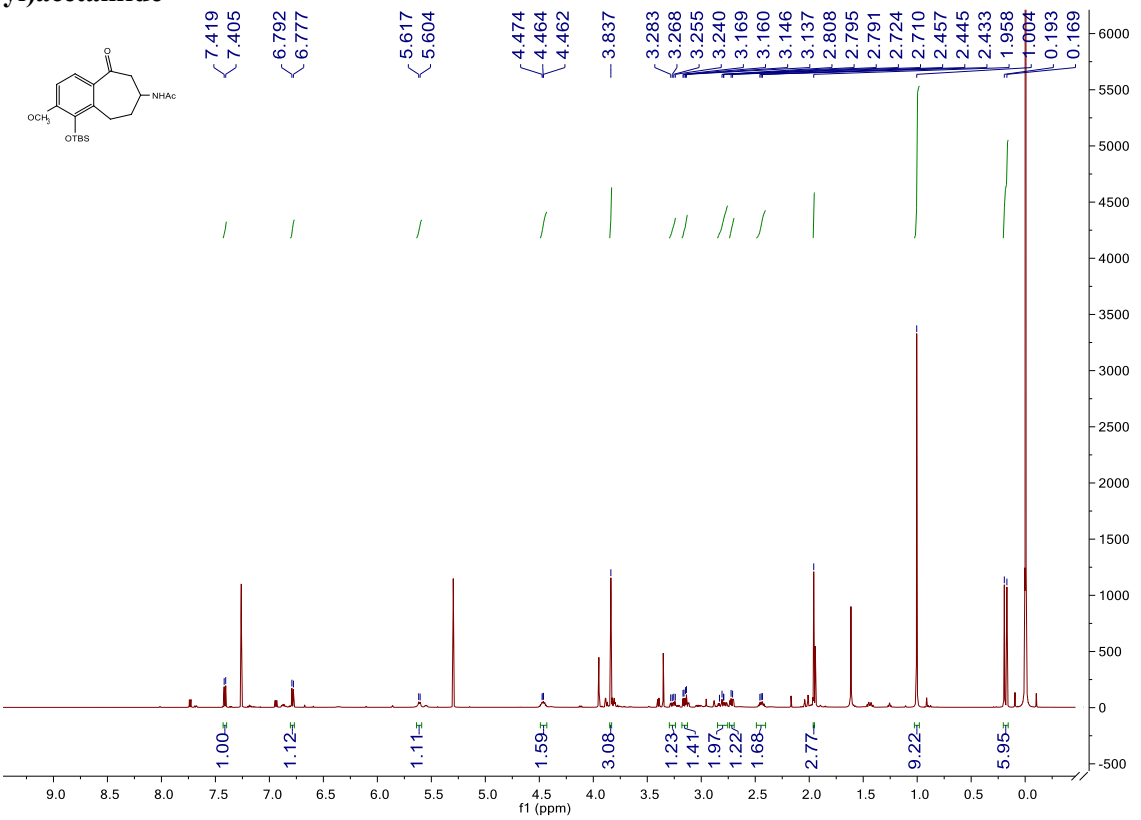


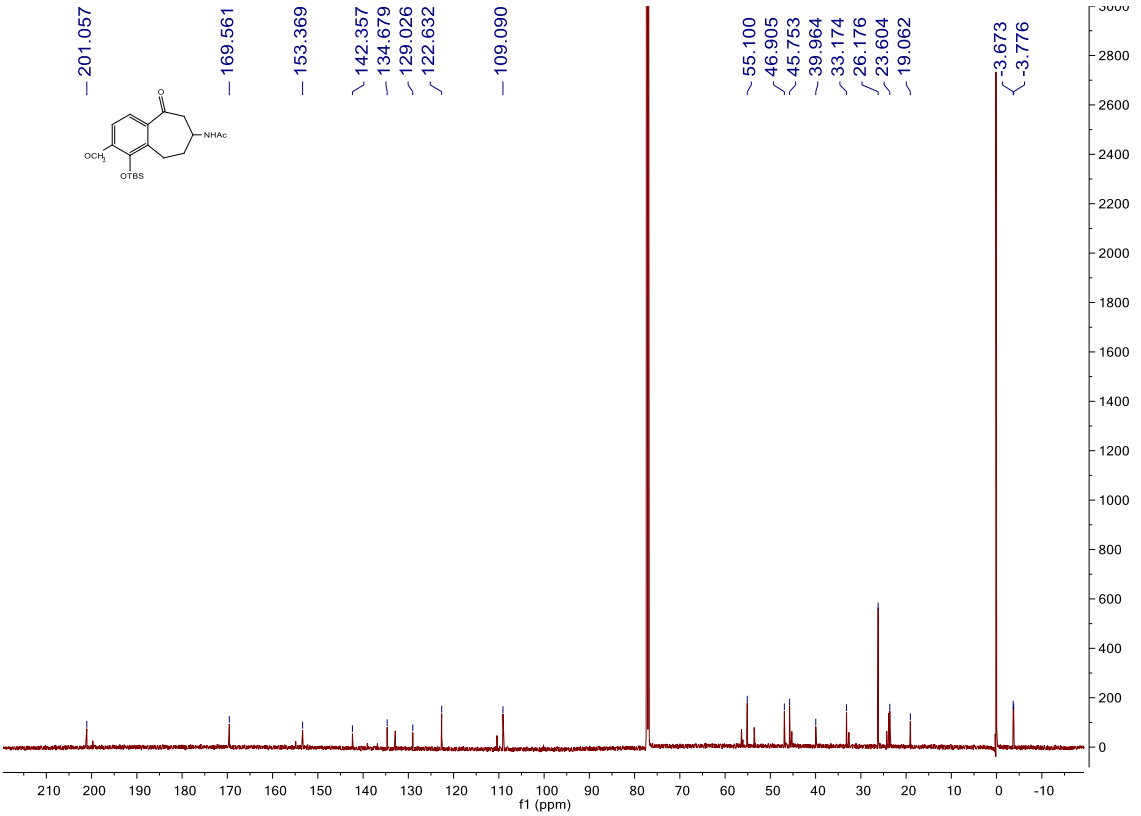
46. N-(1-hydroxy-2-methoxy-5-oxo-6,7,8,9-tetrahydro-5H-benzo[7]annulen-7-yl)acetamide



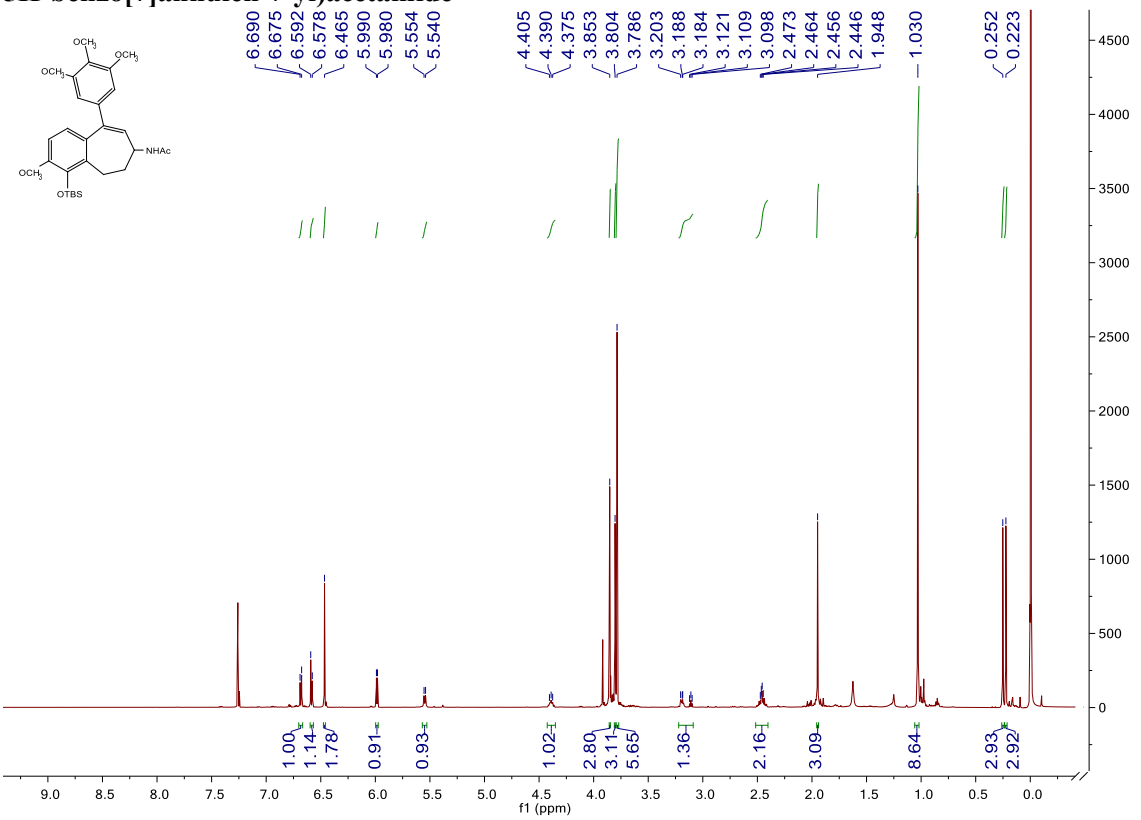


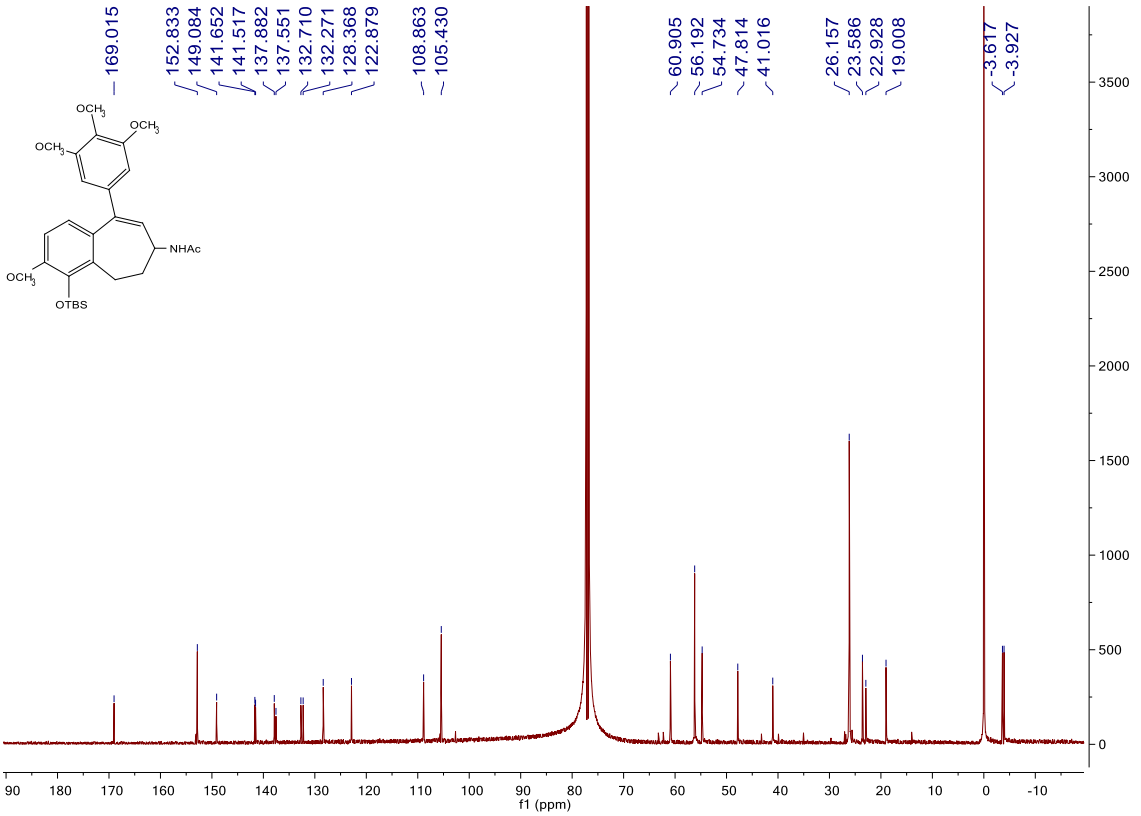
47. N-(1-((tert-butyldimethylsilyl)oxy)-2-methoxy-5-oxo-6,7,8,9-tetrahydro-5H-benzo[7]annulen-7-yl)acetamide



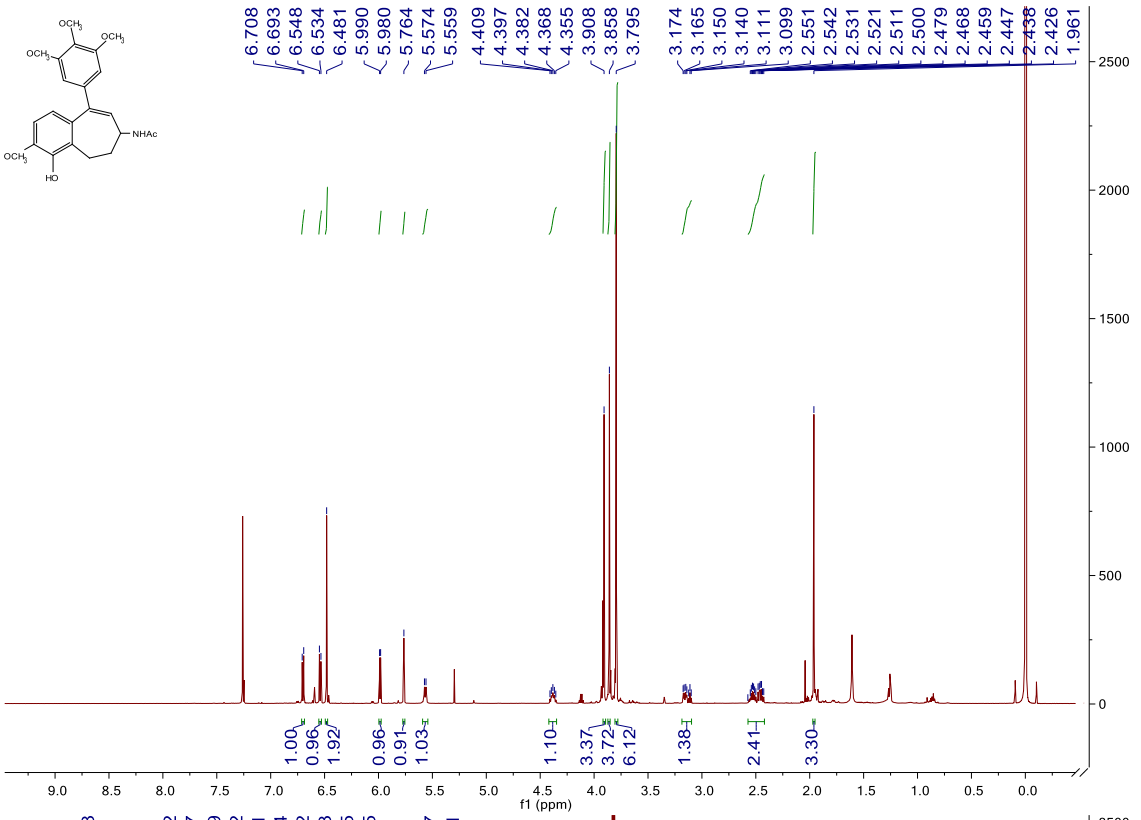


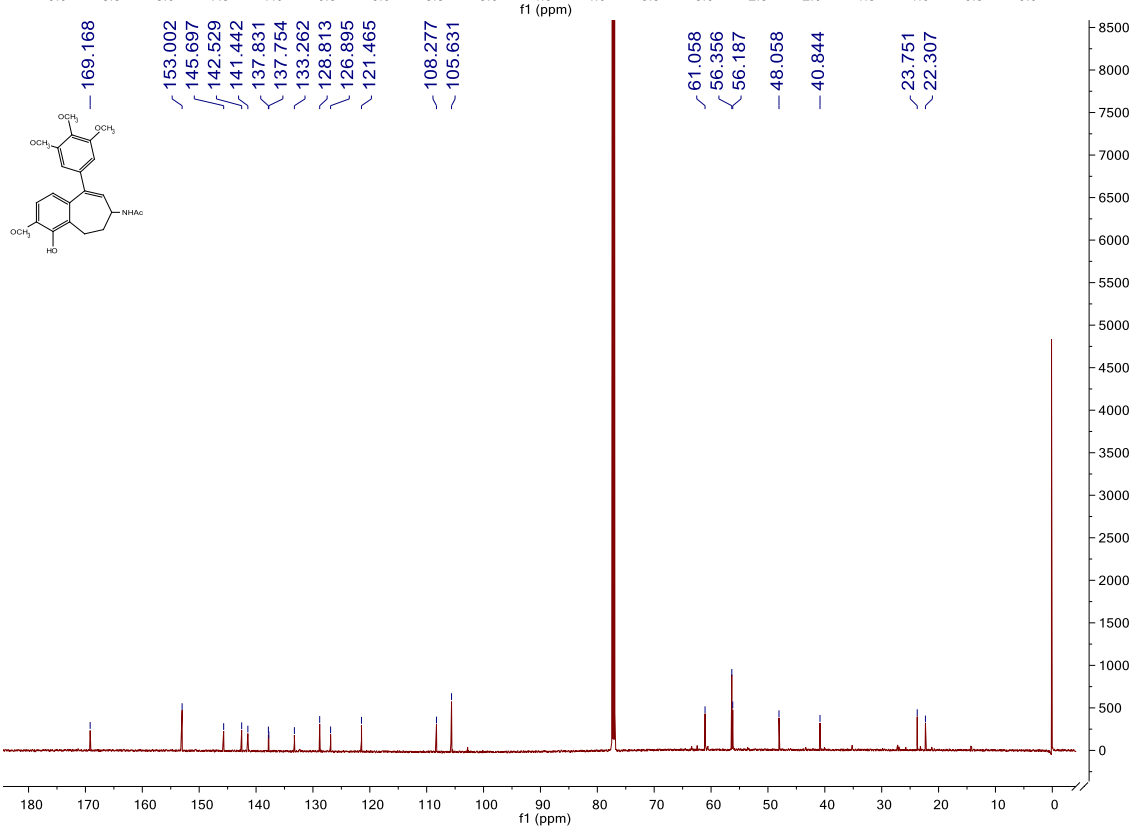
48. N-(1-((tert-butyldimethylsilyl)oxy)-2-methoxy-5-(3,4,5-trimethoxyphenyl)-6,7,8,9-tetrahydro-5H-benzo[7]annulen-7-yl)acetamide





49. N-(1-hydroxy-2-methoxy-5-(3,4,5-trimethoxyphenyl)-6,7,8,9-tetrahydro-5H-benzo[7]annulen-7-yl)acetamide





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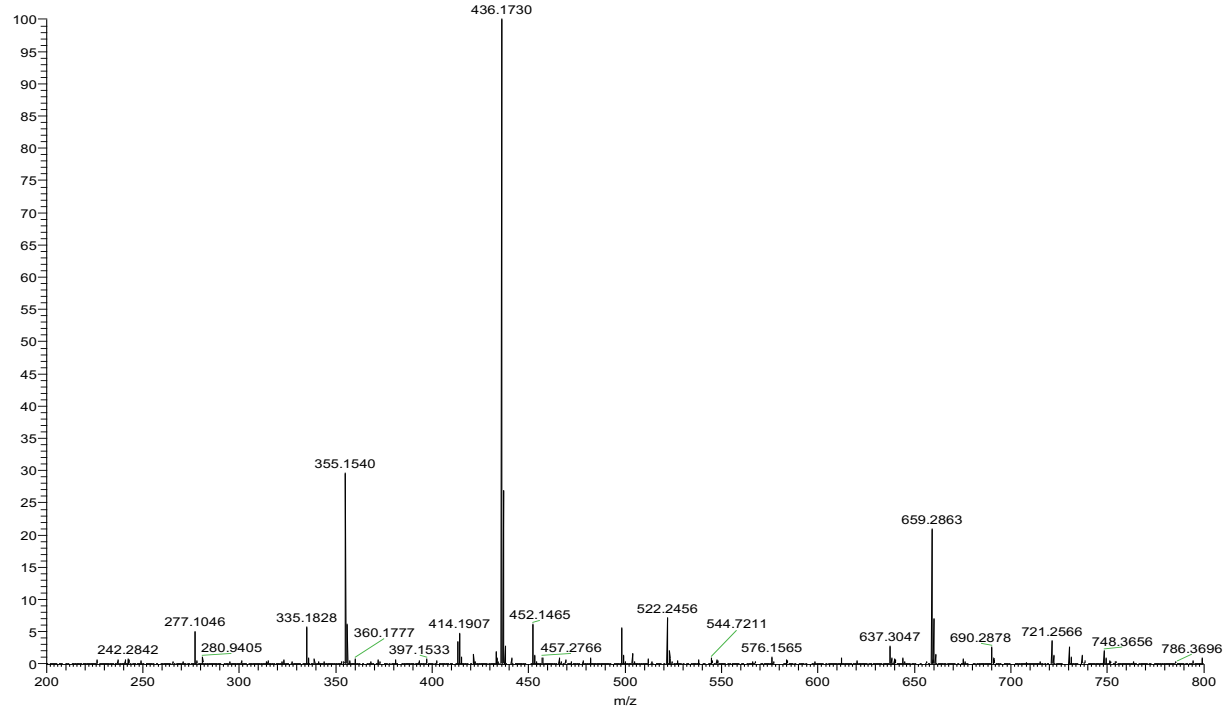

Data File C:\CHEM32\1\DATA\HAICHAN NIU\KGP472SAMPLE001.D
Sample Name: KGP472sample

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Acq. Instrument : Instrument 1 Location : -
Injection Date : 11/19/2015 11:51:41 AM
Acq. Method : C:\CHEM32\1\METHODS\MASTERMETHOD.M
Last changed : 11/19/2015 11:44:37 AM by Haichan Niu
Analysis Method : C:\CHEM32\1\DATA\HAICHAN NIU\KGP472SAMPLE001.D\DA.M (MASTERMETHOD.M)
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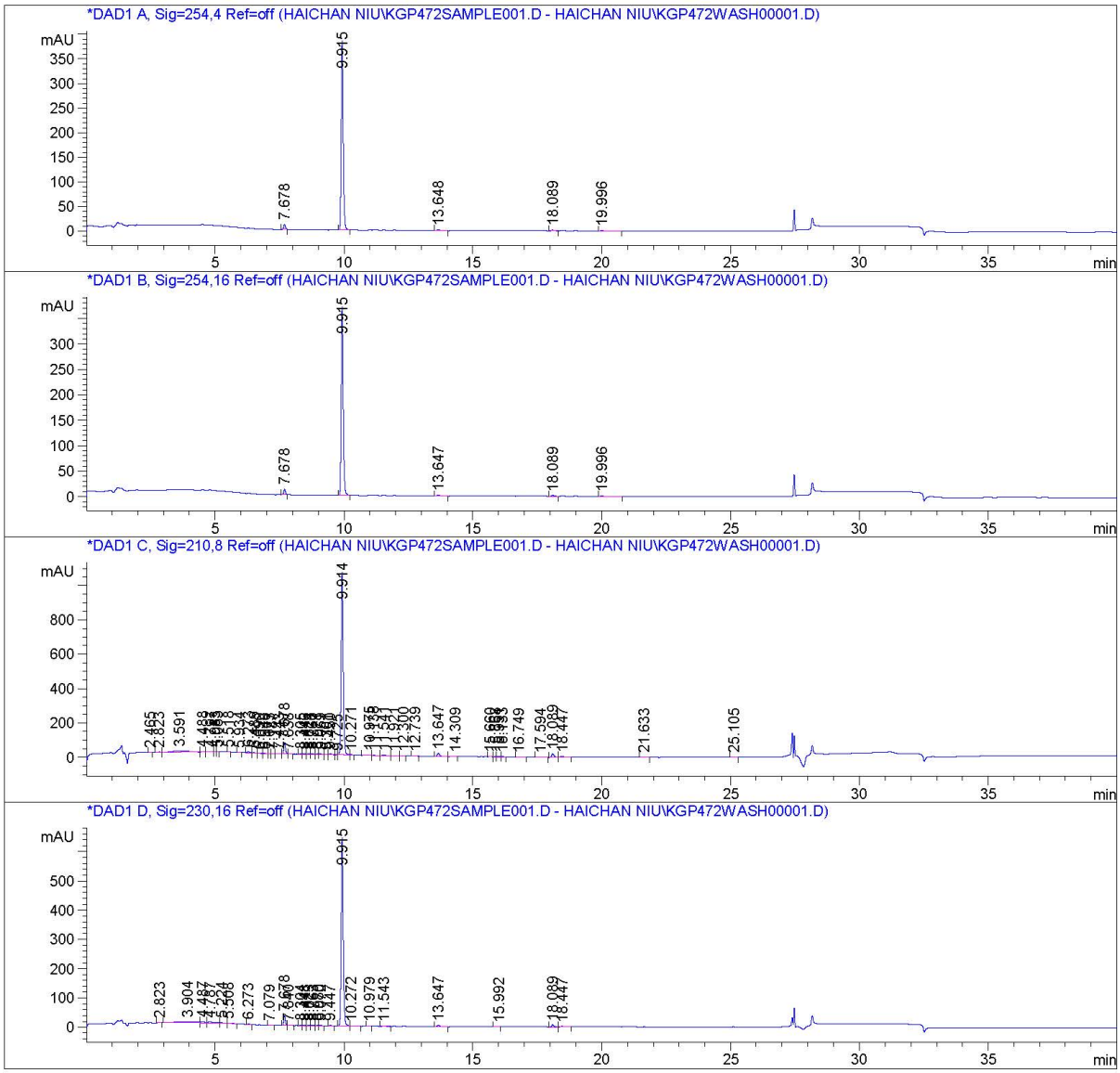

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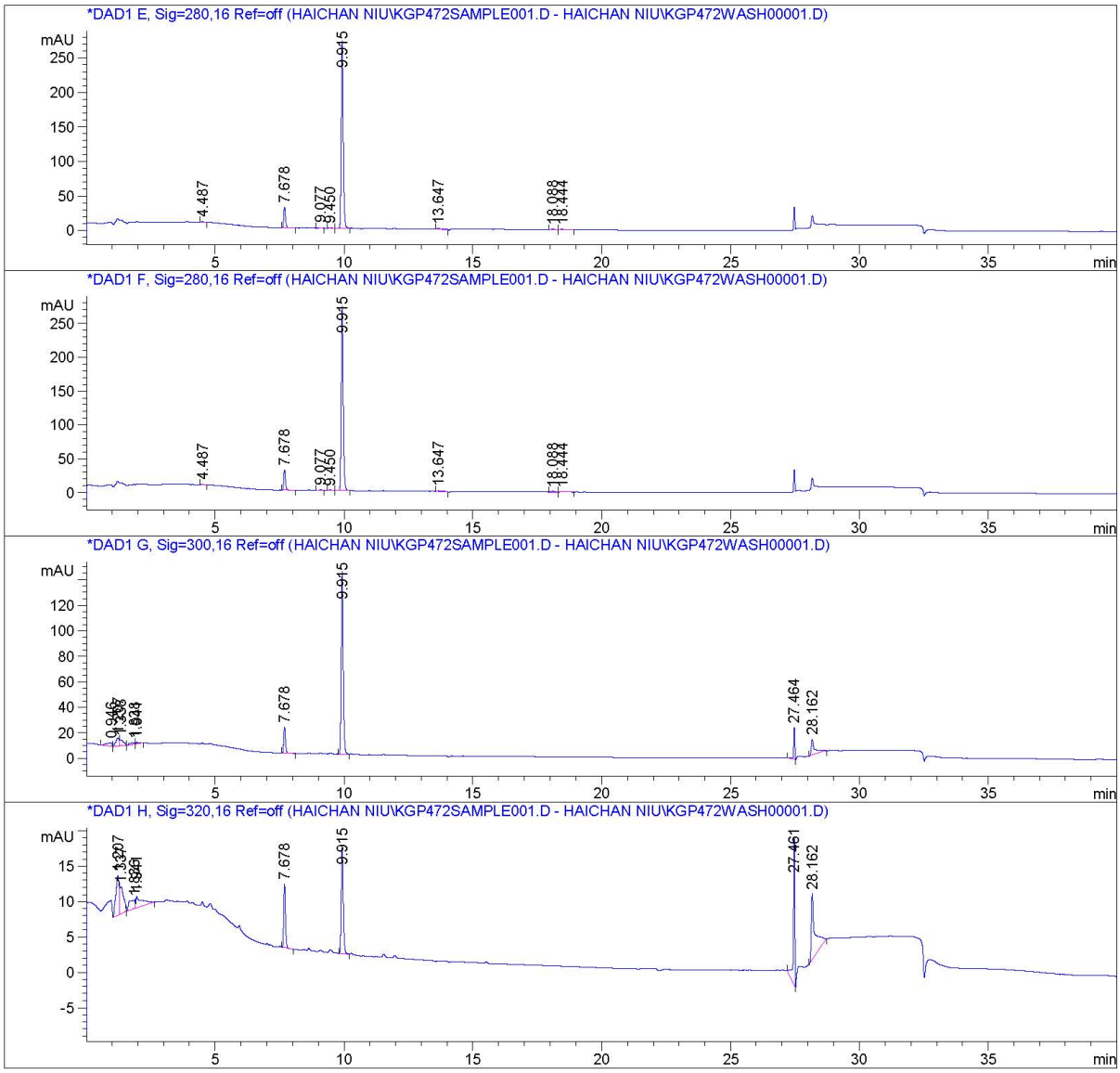

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Area Percent Report

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Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Data File C:\CHEM32\1\DATA\HAICHAN NIU\KGP472SAMPLE001.D
Sample Name: KGP472sample

Signal 1: DAD1 A, Sig=254,4 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.678	BB	0.0711	46.21363	10.15255	2.1300
2	9.915	VV	0.0830	2073.97314	384.31497	95.5878
3	13.648	BB	0.1682	23.80234	1.92531	1.0970
4	18.089	BB	0.1011	11.36394	1.63549	0.5238
5	19.996	BB	0.1441	14.35070	1.37145	0.6614
Totals :				2169.70375	399.39977	

Signal 2: DAD1 B, Sig=254,16 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.678	BB	0.0710	49.87946	10.97051	2.3697
2	9.915	VV	0.0830	2002.73462	370.84903	95.1466
3	13.647	BB	0.1675	26.67926	2.16874	1.2675
4	18.089	BB	0.1004	12.34215	1.79001	0.5864
5	19.996	BB	0.1451	13.25722	1.25599	0.6298
Totals :				2104.89270	387.03428	

Signal 3: DAD1 C, Sig=210,8 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.465	VB	0.0730	9.21492	1.95298	0.1193
2	2.823	BV	0.0740	13.67571	2.84675	0.1771
3	3.591	VB	0.5699	371.93463	8.54350	4.8161
4	4.488	BB	0.0692	12.43935	2.72876	0.1611
5	4.797	BV	0.1443	29.23532	3.09089	0.3786
6	4.983	VV	0.0886	6.62762	1.09460	0.0858
7	5.083	VB	0.0706	5.55790	1.18729	0.0720
8	5.518	BB	0.0604	6.27346	1.64733	0.0812
9	5.934	VB	0.0903	6.31640	1.11128	0.0818
10	6.273	VV	0.0864	45.44395	7.32318	0.5884
11	6.489	VB	0.0758	18.87074	3.80848	0.2444
12	6.690	BB	0.0757	6.63320	1.25443	0.0859
13	6.940	BV	0.0848	8.05059	1.36426	0.1042
14	7.073	VV	0.0751	5.32454	1.01643	0.0689

Data File C:\CHEM32\1\DATA\HAICHAN NIU\KGP472SAMPLE001.D
Sample Name: KGP472sample

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
15	7.187	VB	0.0757	6.04263	1.14239	0.0782
16	7.443	BV	0.1166	21.37668	2.53029	0.2768
17	7.678	VV	0.0736	298.55148	62.63482	3.8659
18	7.838	VB	0.0840	9.48736	1.53790	0.1228
19	8.305	BV	0.0768	20.84925	4.13497	0.2700
20	8.446	VB	0.0781	13.63189	2.64709	0.1765
21	8.624	BV	0.0747	21.20205	4.36395	0.2745
22	8.760	VB	0.0847	15.64381	2.73620	0.2026
23	8.971	BV	0.0940	12.98660	2.22650	0.1682
24	9.069	VB	0.0870	17.10794	2.89372	0.2215
25	9.301	BV	0.0710	9.81547	2.24416	0.1271
26	9.450	VB	0.1128	42.31837	6.26343	0.5480
27	9.725	BV	0.0625	7.17496	1.80194	0.0929
28	9.914	VV	0.0857	5990.85889	1064.61560	77.5740
29	10.271	VB	0.0838	9.81505	1.79614	0.1271
30	10.975	BV	0.1434	41.16666	4.02217	0.5331
31	11.138	VB	0.1752	28.90885	2.11892	0.3743
32	11.541	BV	0.1442	58.38725	5.48608	0.7560
33	11.921	VB	0.1604	15.28566	1.45678	0.1979
34	12.300	BV	0.1220	9.04627	1.19947	0.1171
35	12.739	BB	0.0983	14.84690	2.27004	0.1922
36	13.647	BB	0.1092	142.22536	19.47558	1.8416
37	14.309	BB	0.1597	12.45613	1.04055	0.1613
38	15.660	BB	0.0920	13.71918	2.42600	0.1776
39	15.868	BV	0.0750	8.28239	1.69400	0.1072
40	15.991	VV	0.0912	24.20039	3.96467	0.3134
41	16.133	VB	0.0860	8.22338	1.45466	0.1065
42	16.749	BB	0.1041	7.04374	1.02647	0.0912
43	17.594	BB	0.3381	57.08141	2.10664	0.7391
44	18.089	BV	0.1082	159.52197	21.58679	2.0656
45	18.447	VB	0.1480	62.66870	5.80069	0.8115
46	21.633	BB	0.1406	9.47685	1.05676	0.1227
47	25.105	BB	0.1075	7.76048	1.13821	0.1005
Totals :				7722.76234	1281.86374	

Signal 4: DAD1 D, Sig=230,16 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.823	BB	0.0705	8.73210	1.93966	0.1941
2	3.904	BV	0.6768	248.98193	4.43586	5.5347
3	4.487	VV	0.1522	61.88265	5.30089	1.3756
4	4.787	VV	0.3186	111.43323	4.59977	2.4771
5	5.224	VV	0.1754	39.09641	2.82544	0.8691
6	5.508	VB	0.1585	23.49368	1.92330	0.5222

Data File C:\CHEM32\1\DATA\HAICHAN NIU\KGP472SAMPLE001.D
Sample Name: KGP472sample

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
7	6.273	BV	0.0749	16.03098	3.06964	0.3564
8	7.079	VB	0.1190	11.69650	1.29917	0.2600
9	7.678	VV	0.0734	162.24304	34.16079	3.6065
10	7.840	VB	0.0797	11.34244	2.01415	0.2521
11	8.304	BV	0.0761	7.69742	1.54601	0.1711
12	8.448	VB	0.0728	11.99849	2.55425	0.2667
13	8.623	BV	0.0733	7.45083	1.57185	0.1656
14	8.763	VB	0.0939	6.07437	1.04311	0.1350
15	8.980	BV	0.0860	5.26994	1.02468	0.1171
16	9.070	VB	0.0904	9.96891	1.60540	0.2216
17	9.447	BB	0.1139	13.49196	2.01943	0.2999
18	9.915	VV	0.0840	3529.10742	643.14319	78.4491
19	10.272	VB	0.1578	21.52843	1.82222	0.4786
20	10.979	BB	0.0865	8.80346	1.59313	0.1957
21	11.543	BB	0.1176	22.38876	2.73258	0.4977
22	13.647	BB	0.1523	61.38229	5.58113	1.3645
23	15.992	BV	0.1239	8.95901	1.00621	0.1992
24	18.089	BV	0.1070	61.69706	8.46725	1.3715
25	18.447	VB	0.1340	27.84542	2.90000	0.6190
Totals :				4498.59674	740.17910	

Signal 5: DAD1 E, Sig=280,16 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.487	BB	0.0762	5.84106	1.13265	0.3481
2	7.678	BB	0.0727	141.08772	30.06461	8.4077
3	9.077	BB	0.0935	6.99596	1.11009	0.4169
4	9.450	BB	0.1138	7.17926	1.02409	0.4278
5	9.915	BV	0.0830	1472.46619	272.47473	87.7469
6	13.647	BB	0.2469	26.35899	1.37962	1.5708
7	18.088	BB	0.1113	9.28397	1.18590	0.5532
8	18.444	BB	0.1216	8.87055	1.03903	0.5286
Totals :				1678.08371	309.41074	

Signal 6: DAD1 F, Sig=280,16 Ref=off
Signal has been modified after loading from rawdata file!

Data File C:\CHEM32\1\DATA\HAICHAN NIU\KGP472SAMPLE001.D
Sample Name: KGP472sample

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.487	BB	0.0762	5.83992	1.13265	0.3480
2	7.678	BB	0.0728	141.09488	30.06471	8.4080
3	9.077	BB	0.0935	6.99577	1.11009	0.4169
4	9.450	BB	0.1138	7.17983	1.02459	0.4279
5	9.915	BV	0.0830	1472.46594	272.47427	87.7463
6	13.647	BB	0.2468	26.36662	1.38079	1.5712
7	18.088	BB	0.1113	9.28435	1.18593	0.5533
8	18.444	BB	0.1216	8.86765	1.03896	0.5284
Totals :				1678.09496	309.41201	

Signal 7: DAD1 G, Sig=300,16 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	0.946	BB	0.1929	41.73813	2.75312	3.3407
2	1.207	BV	0.1318	62.59555	6.77686	5.0101
3	1.338	VB	0.1402	46.74639	4.77595	3.7415
4	1.838	BV	0.2338	21.82882	1.16929	1.7472
5	1.941	VB	0.1033	11.75556	1.53634	0.9409
6	7.678	BB	0.0724	95.35380	20.46690	7.6320
7	9.915	BV	0.0828	769.89136	143.04012	61.6211
8	27.464	BB	0.0480	76.92471	24.95676	6.1570
9	28.162	BB	0.1328	122.56091	12.45418	9.8096
Totals :				1249.39522	217.92952	

Signal 8: DAD1 H, Sig=320,16 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.207	BV	0.1307	52.14275	5.59459	12.0450
2	1.337	VB	0.1374	37.02372	3.81054	8.5525
3	1.836	BV	0.2130	20.42301	1.20949	4.7177
4	1.941	VB	0.2092	28.18526	1.68497	6.5108
5	7.678	BB	0.0718	41.36581	8.97630	9.5555
6	9.915	BB	0.0830	82.23476	15.23933	18.9963
7	27.461	BB	0.0559	74.66927	20.81409	17.2487
8	28.162	BB	0.1387	96.85426	9.36135	22.3734
Totals :				432.89884	66.69066	

Data File C:\CHEM32\1\DATA\HAICHAN NIU\KGP472SAMPLE001.D
Sample Name: KGP472sample

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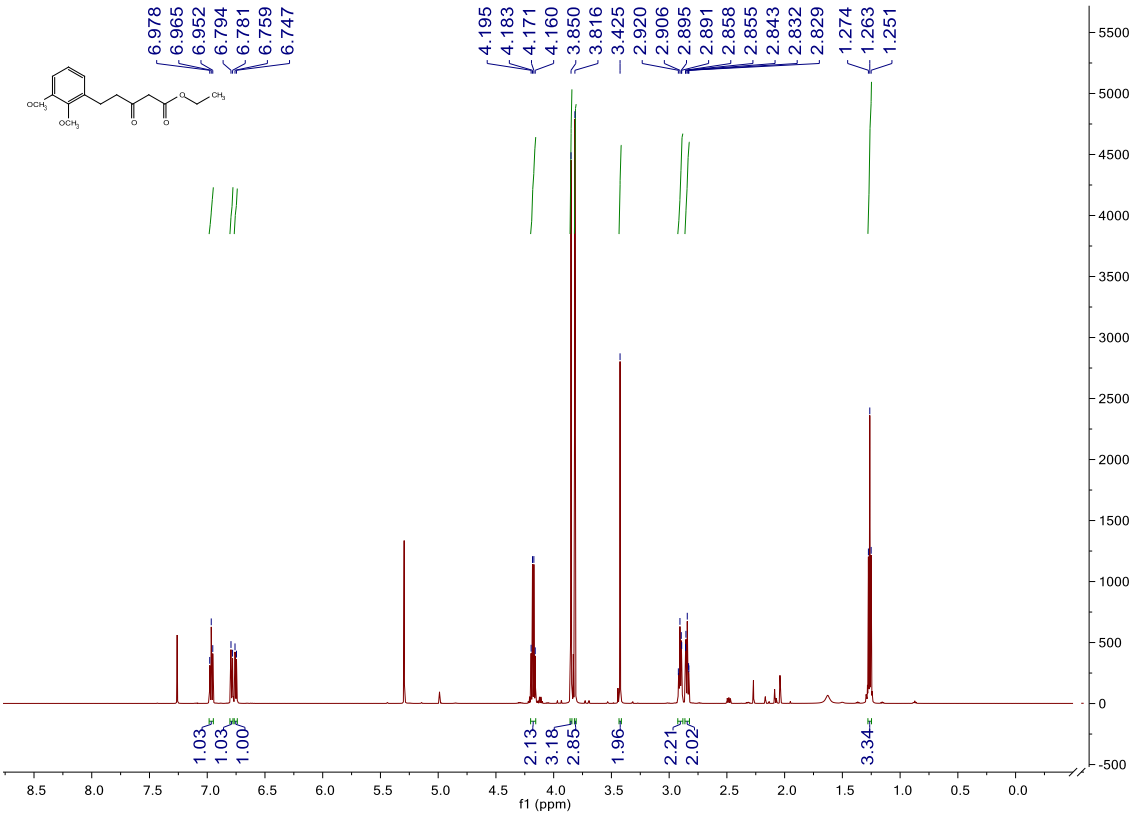
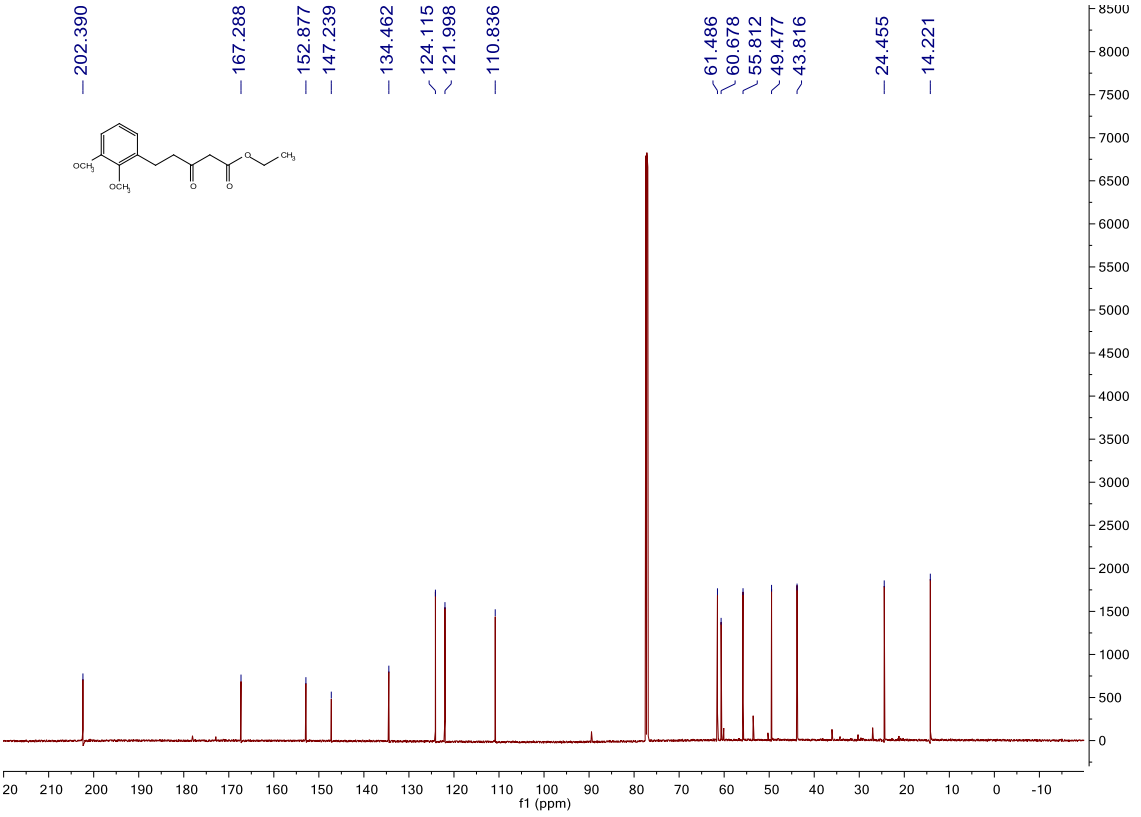
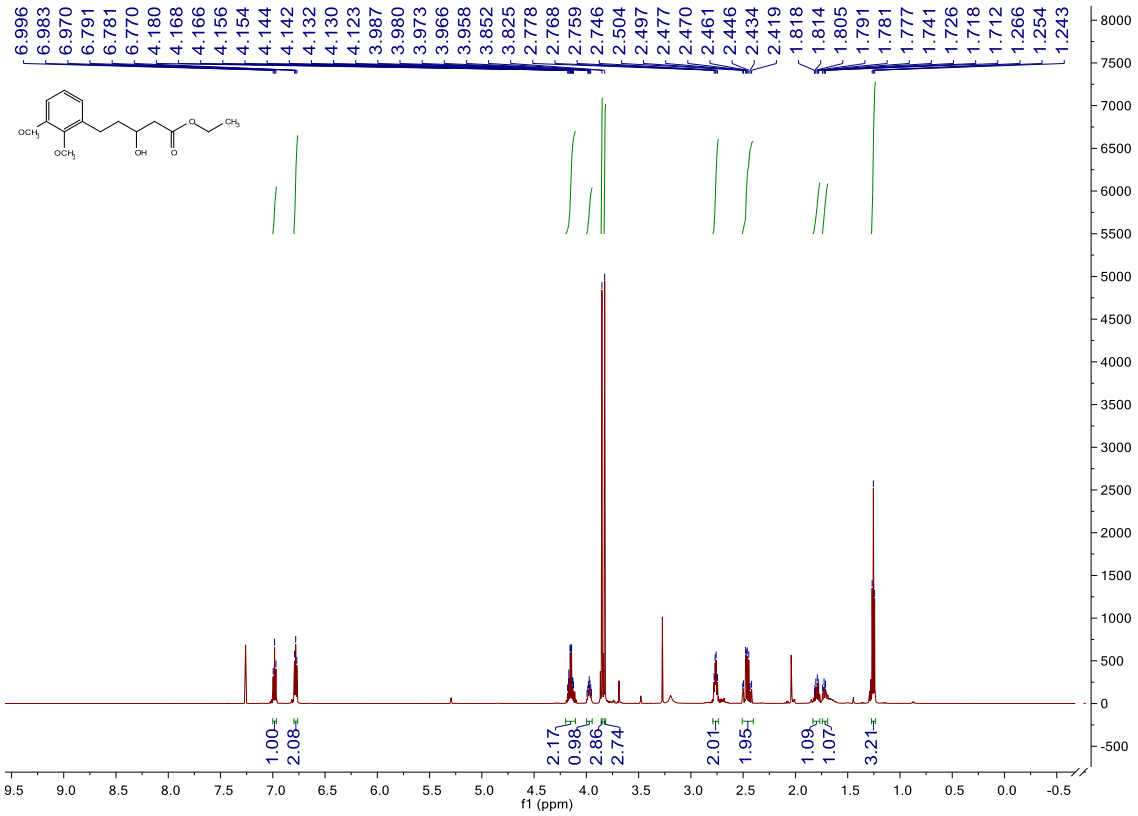
*** End of Report ***

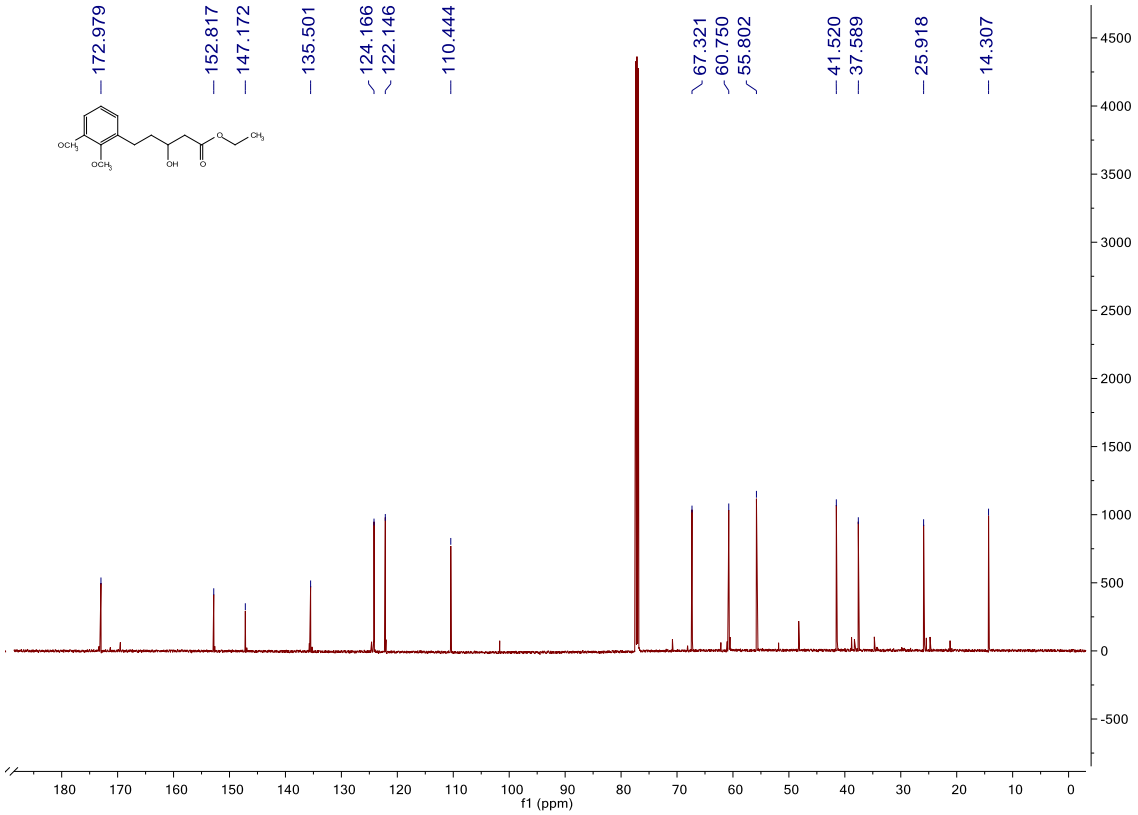
52. ethyl 5-(2,3-dimethoxyphenyl)-3-oxopentanoate



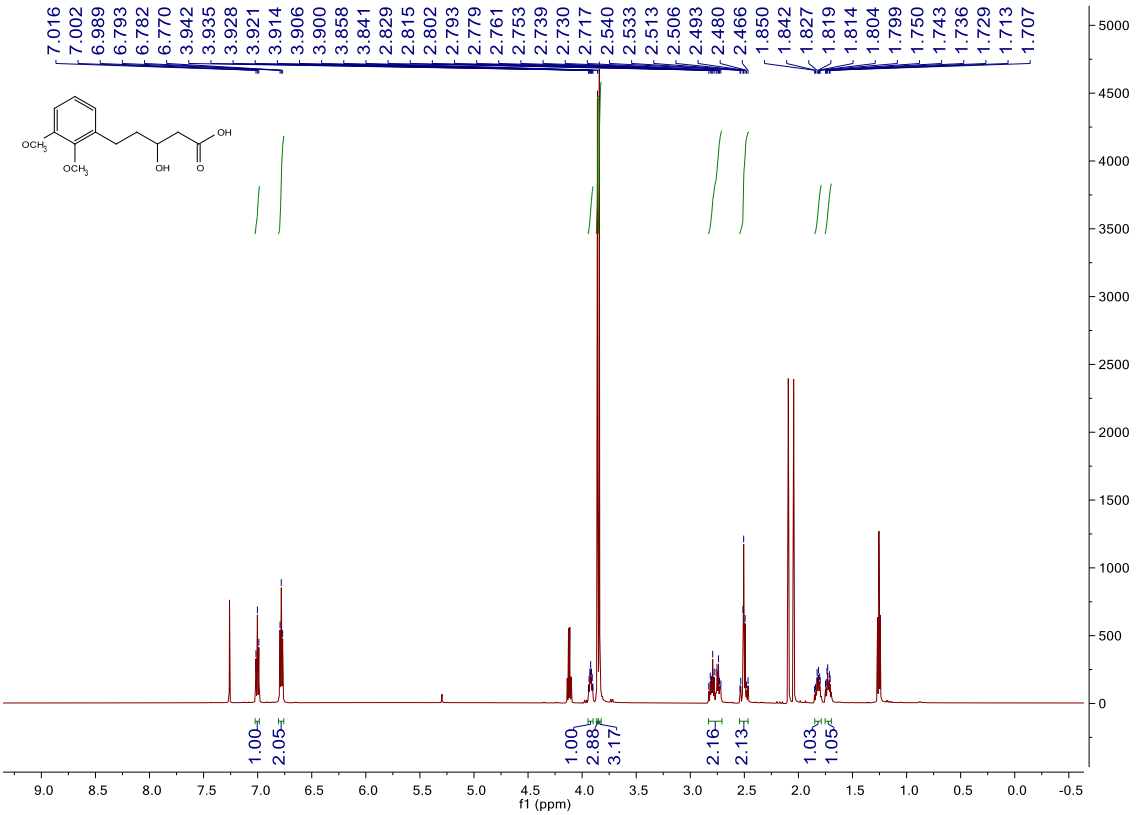


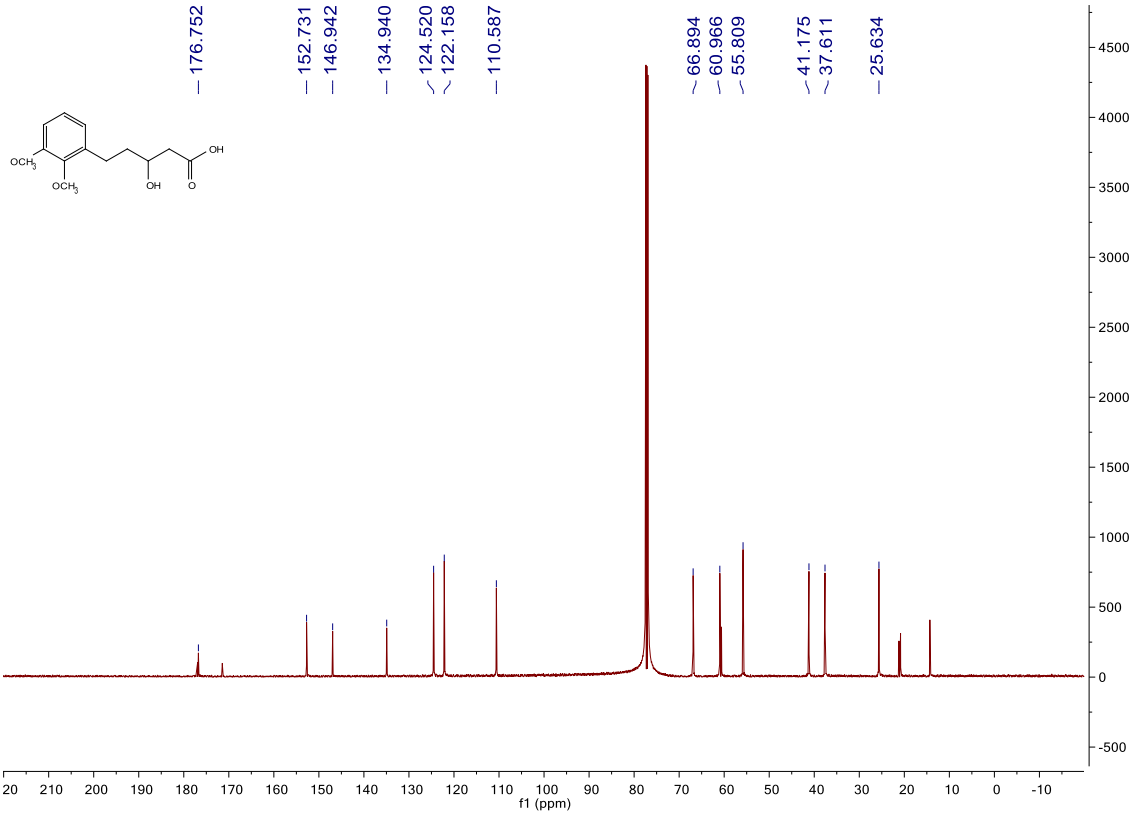
53. ethyl 5-(2,3-dimethoxyphenyl)-3-hydroxypentanoate



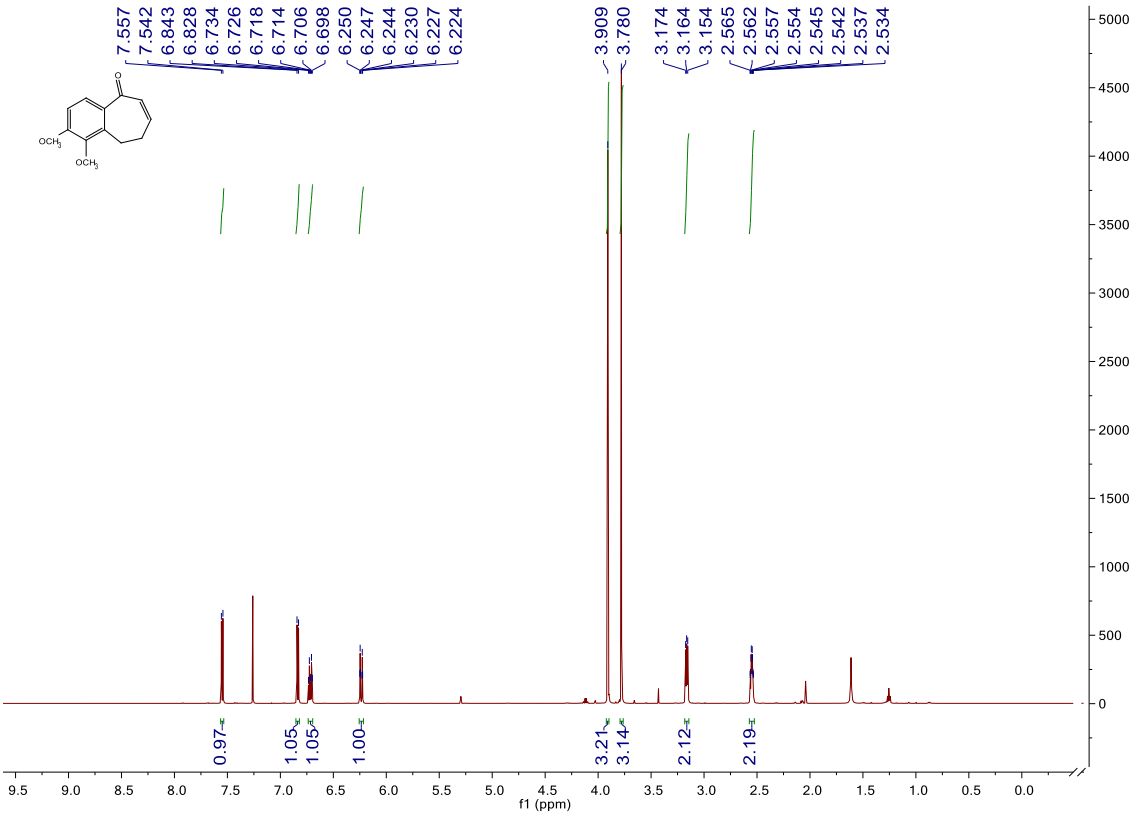


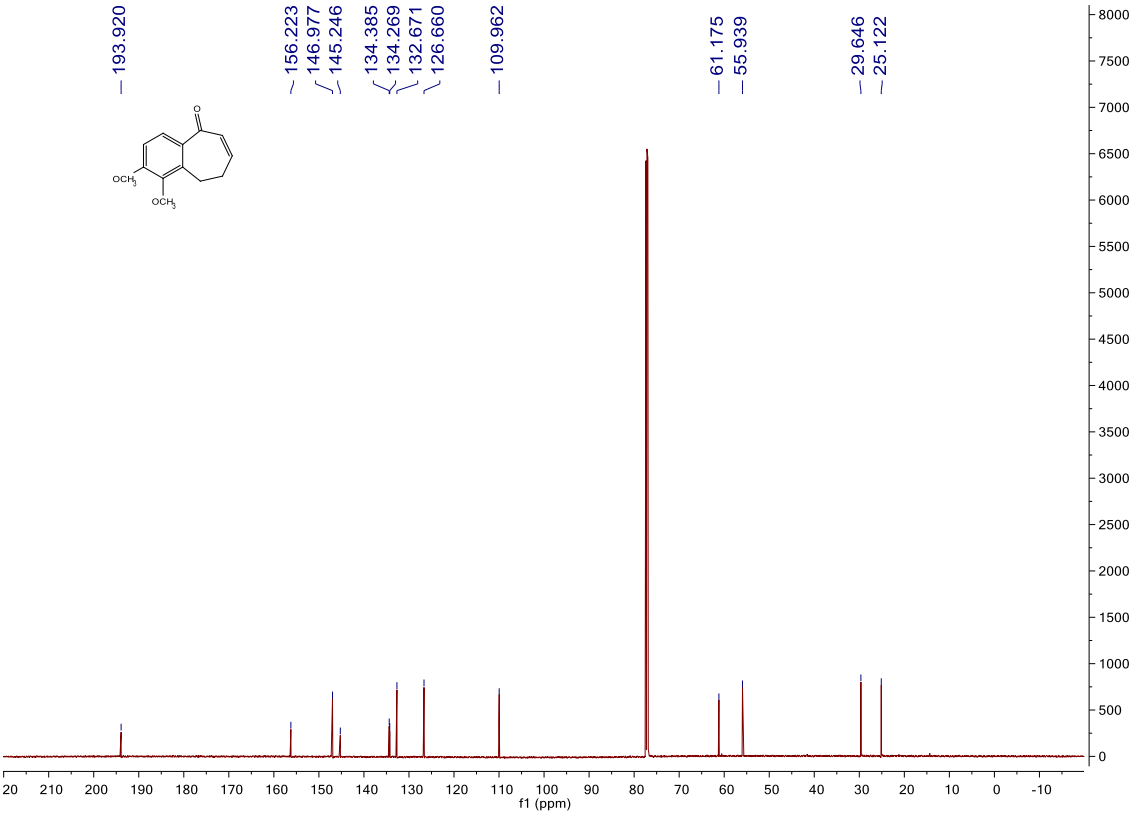
54. 5-(2,3-dimethoxyphenyl)-3-hydroxypentanoic acid



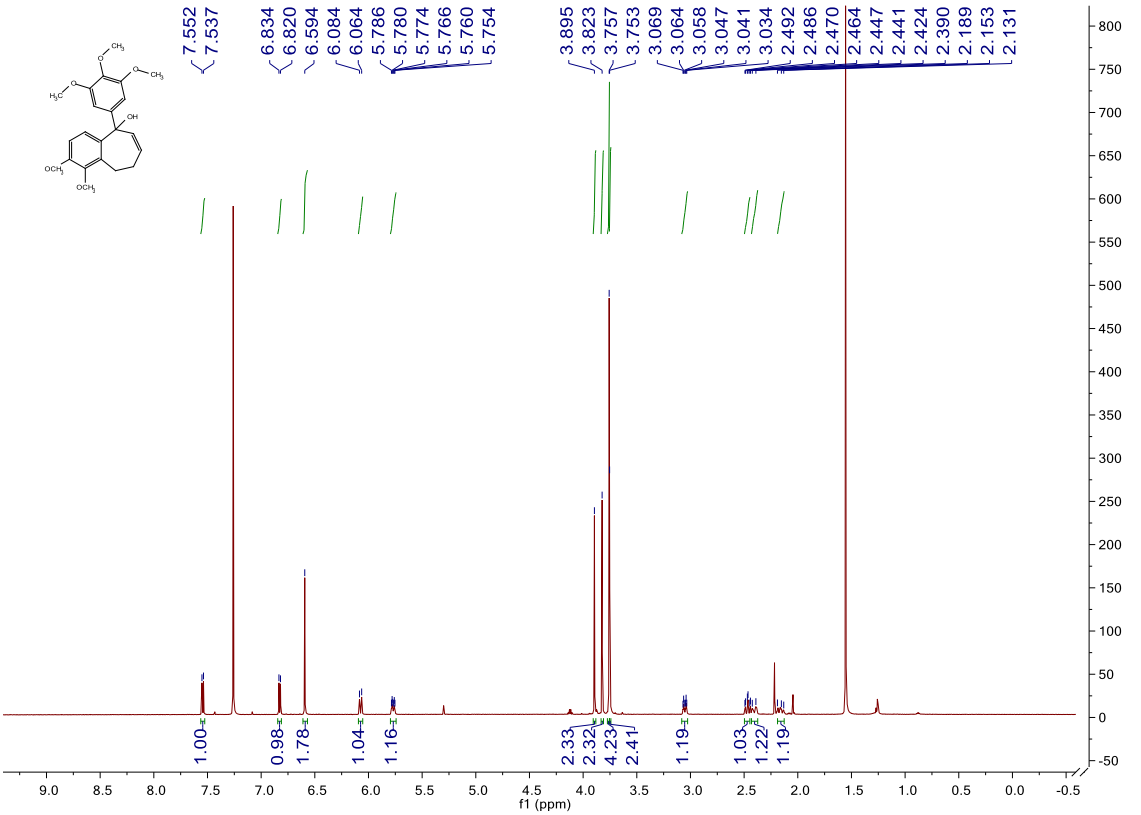


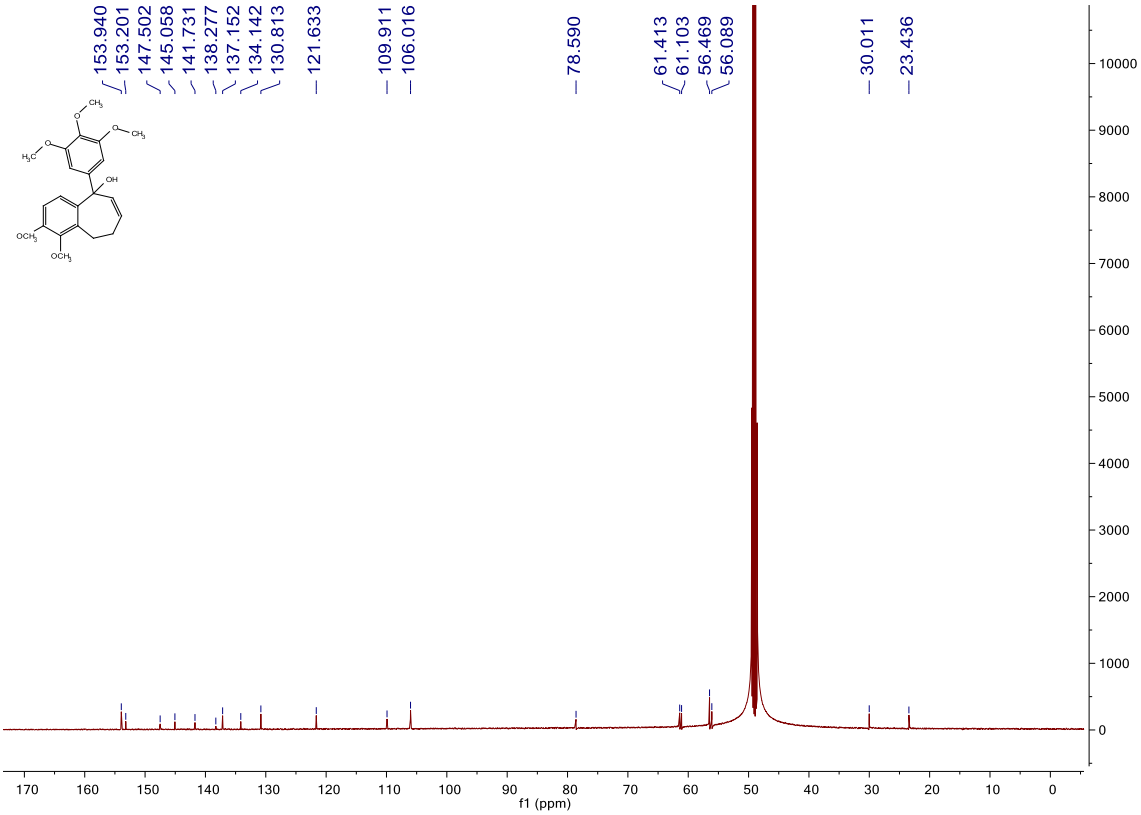
55. 1,2-dimethoxy-8,9-dihydro-5H-benzo[7]annulen-5-one

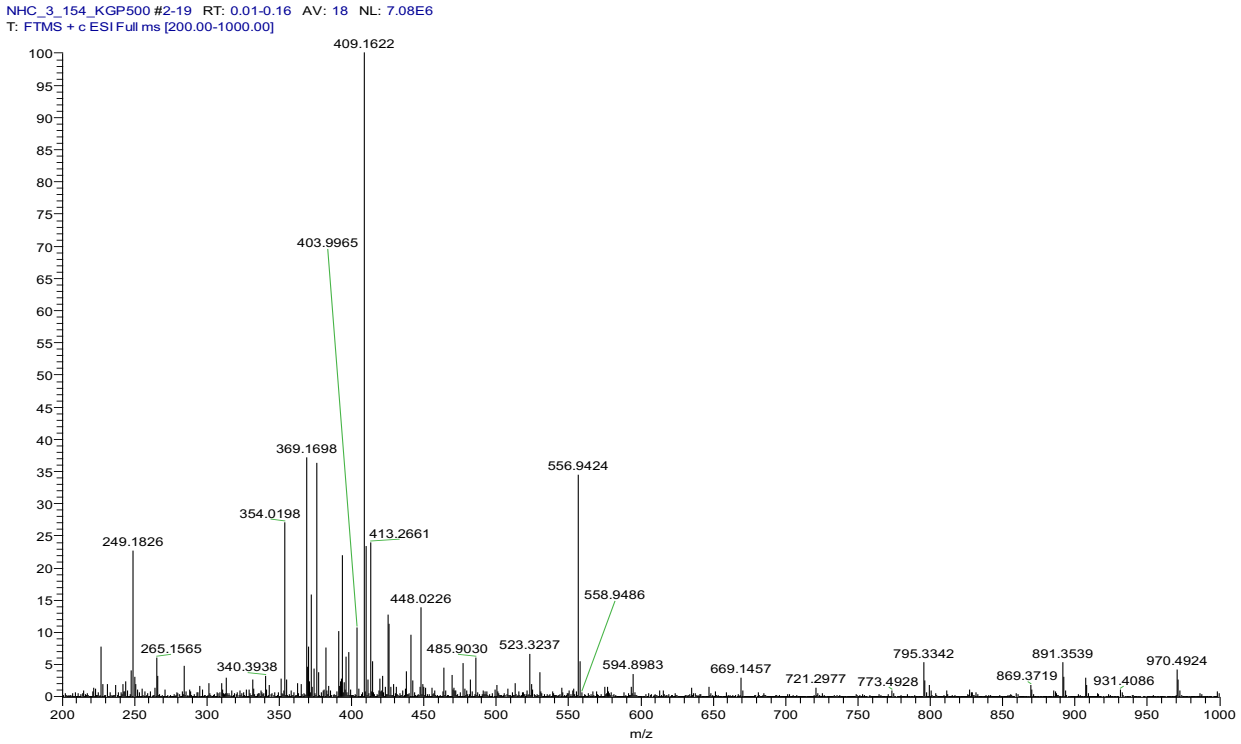




56. 1,2-dimethoxy-5-(3,4,5-trimethoxyphenyl)-8,9-dihydro-5H-benzo[7]annulen-5-ol






NHC_3_154_KGP500 #2-19 RT: 0.01-0.16 AV: 18 NL: 7.08E6
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931.4086
970.4924
m/z

Data File C:\Chem32\1\Data\NHC\NHC_3_154_KGP500 20170203.D
Sample Name: NHC_3_154_KGP500_20170203

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======================================================================
Acq. Operator   : SYSTEM
Sample Operator : SYSTEM
Acq. Instrument : 1200 HPLC                    Location :   1
Injection Date  : 2/3/2017 8:34:01 AM
                                             Inj Volume : No inj
Acq. Method     : C:\Chem32\1\Methods\MASTERMETHOD2.M
Last changed    : 12/2/2015 12:37:42 PM by Eric Lin
Analysis Method : C:\CHEM32\1\METHODS\RT-ACNWASH 2.M
Last changed    : 2/3/2017 9:24:08 AM by SYSTEM
                  (modified after loading)
Method Info     : General Column Wash Method

Sample Info     : KGP500

Additional Info : Peak(s) manually integrated
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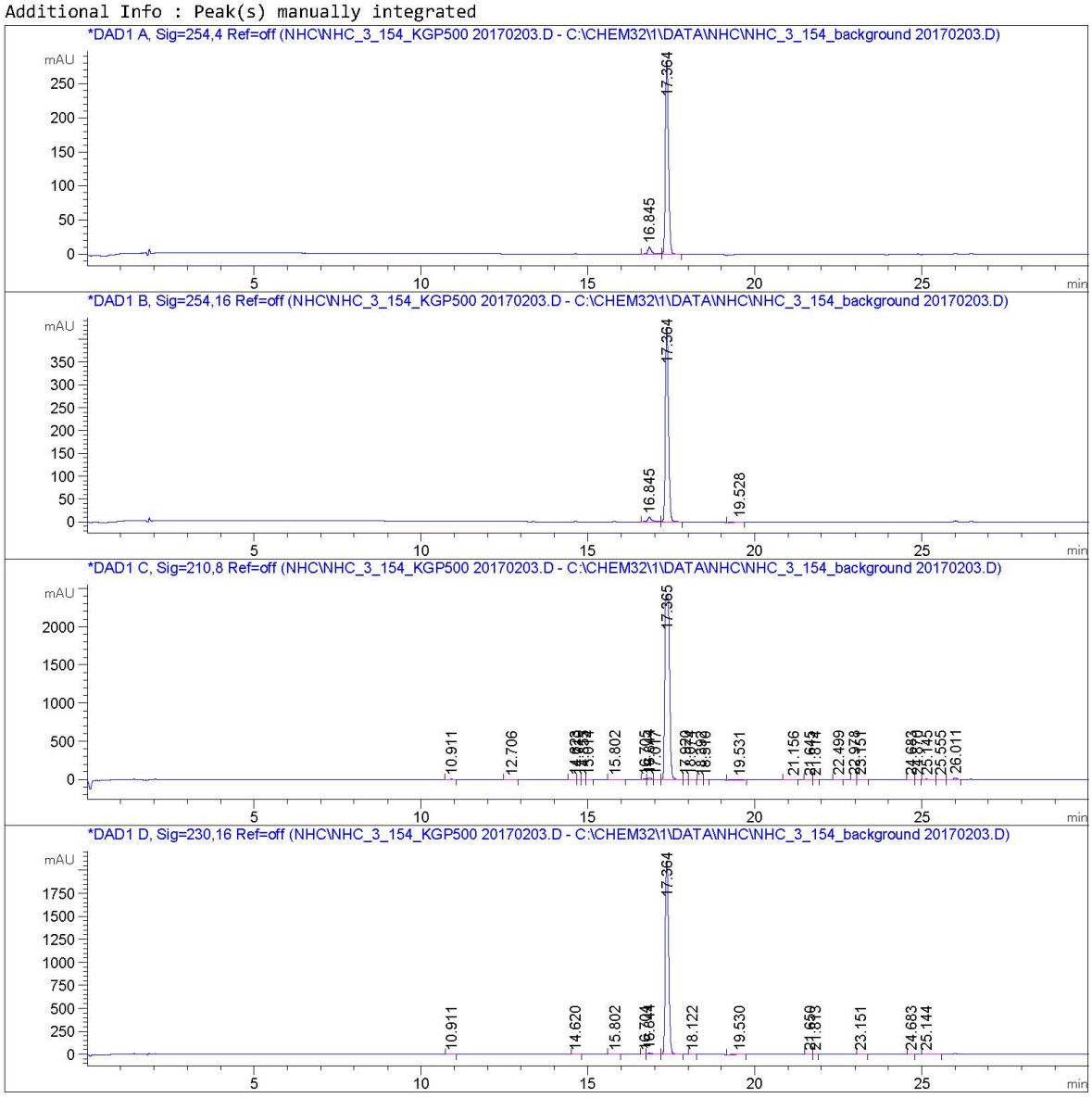
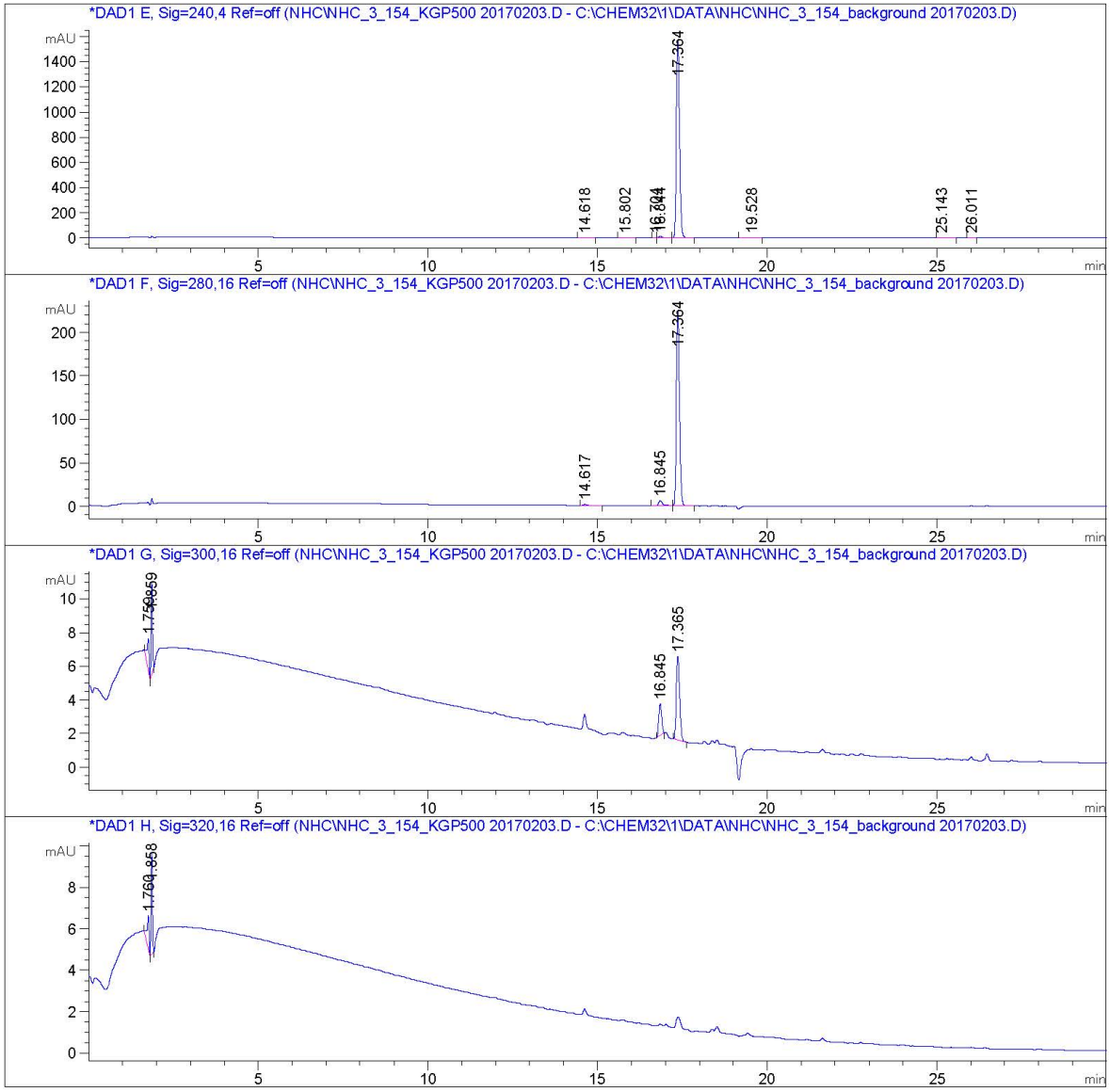


Data File C:\Chem32\1\Data\NHC\NHC_3_154_KGP500 20170203.D
Sample Name: NHC_3_154_KGP500_20170203



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Area Percent Report

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Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

Data File C:\Chem32\1\Data\NHC\NHC_3_154_KGP500 20170203.D
Sample Name: NHC_3_154_KGP500_20170203

Signal 1: DAD1 A, Sig=254,4 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.845	BV	0.1217	85.85909	10.47208	4.4690
2	17.364	VB	0.1016	1835.37573	283.17236	95.5310
Totals :				1921.23482	293.64444	

Signal 2: DAD1 B, Sig=254,16 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.845	BV	0.1226	81.98203	9.89646	2.8747
2	17.364	VB	0.1015	2747.77808	424.72995	96.3504
3	19.528	BB	0.2779	22.10064	1.01566	0.7750
Totals :				2851.86075	435.64207	

Signal 3: DAD1 C, Sig=210,8 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.911	BB	0.1149	57.66664	7.56772	0.2360
2	12.706	BB	0.1147	8.27689	1.08912	0.0339
3	14.623	BV	0.0910	13.19409	2.16835	0.0540
4	14.710	VV	0.0904	13.25748	2.13539	0.0543
5	14.855	VV	0.0994	10.74688	1.62052	0.0440
6	15.014	VB	0.1058	16.50654	2.35352	0.0675
7	15.802	BB	0.1072	37.58694	5.26771	0.1538
8	16.705	BV	0.0855	49.76601	9.14854	0.2037
9	16.844	VV	0.1047	146.81279	21.76399	0.6008
10	17.017	VB	0.0986	21.63904	3.29418	0.0886
11	17.365	BV	0.1597	2.36245e4	2423.54004	96.6755
12	17.920	VV	0.1140	31.22889	4.05004	0.1278
13	18.074	VB	0.1307	29.21334	3.52332	0.1195
14	18.392	BV	0.0984	9.68995	1.51892	0.0397
15	18.510	VB	0.0864	5.96369	1.08057	0.0244
16	19.531	BB	0.2901	50.02998	2.21045	0.2047
17	21.156	BB	0.1203	11.18060	1.47691	0.0458
18	21.645	BV	0.1201	9.27212	1.22721	0.0379
19	21.814	VB	0.0914	5.95397	1.03069	0.0244
20	22.499	BB	0.1159	10.01805	1.33036	0.0410
21	22.978	VV	0.0924	6.67292	1.10559	0.0273
22	23.151	VB	0.1100	31.31748	4.35191	0.1282
23	24.683	VV	0.1119	37.72108	5.24394	0.1544

Data File C:\Chem32\1\Data\NHC\NHC_3_154_KGP500 20170203.D
Sample Name: NHC_3_154_KGP500_20170203

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
24	24.870	VB	0.1046	9.98686	1.48269	0.0409
25	25.145	BV	0.1252	48.47191	5.70342	0.1984
26	25.555	VV	0.1134	20.82845	2.84694	0.0852
27	26.011	VB	0.1010	119.40503	18.57635	0.4886
Totals :				2.44369e4	2536.70837	

Signal 4: DAD1 D, Sig=230,16 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.911	BB	0.1121	13.09853	1.73546	0.0878
2	14.620	BB	0.1186	13.36771	1.61384	0.0896
3	15.802	BB	0.1057	12.76321	1.86743	0.0856
4	16.704	BV	0.0805	16.05019	3.09411	0.1076
5	16.844	VV	0.1198	117.29995	14.59164	0.7863
6	17.364	VB	0.1113	1.46344e4	2100.98071	98.1036
7	18.122	VB	0.1431	8.70244	1.02423	0.0583
8	19.530	BB	0.3048	51.65467	2.16144	0.3463
9	21.650	BV	0.1101	8.40199	1.16571	0.0563
10	21.813	VB	0.0888	6.30786	1.13566	0.0423
11	23.151	VB	0.1063	8.41046	1.22168	0.0564
12	24.683	BV	0.1116	10.55525	1.47300	0.0708
13	25.144	BB	0.1348	16.27417	1.74585	0.1091
Totals :				1.49173e4	2133.81077	

Signal 5: DAD1 E, Sig=240,4 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.618	BB	0.1181	8.61762	1.06867	0.0825
2	15.802	BB	0.1116	8.87661	1.18186	0.0850
3	16.704	BV	0.0800	10.13652	1.97227	0.0971
4	16.844	VV	0.1203	76.82481	9.50258	0.7358
5	17.364	VB	0.1022	1.02631e4	1572.32544	98.3015
6	19.528	BB	0.3100	40.08093	1.64677	0.3839
7	25.143	BB	0.1399	10.35311	1.04220	0.0992
8	26.011	BB	0.0972	22.43824	3.67601	0.2149
Totals :				1.04404e4	1592.41580	

Data File C:\Chem32\1\Data\NHC\NHC_3_154_KGP500 20170203.D
Sample Name: NHC_3_154_KGP500_20170203

Signal 6: DAD1 F, Sig=280,16 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.617	BB	0.1221	12.44602	1.47997	0.8296
2	16.845	BV	0.1243	52.75229	6.26000	3.5163
3	17.364	VB	0.1006	1435.04431	224.35574	95.6541
Totals :				1500.24263	232.09571	

Signal 7: DAD1 G, Sig=300,16 Ref=off
Signal has been modified after loading from rawdata file!

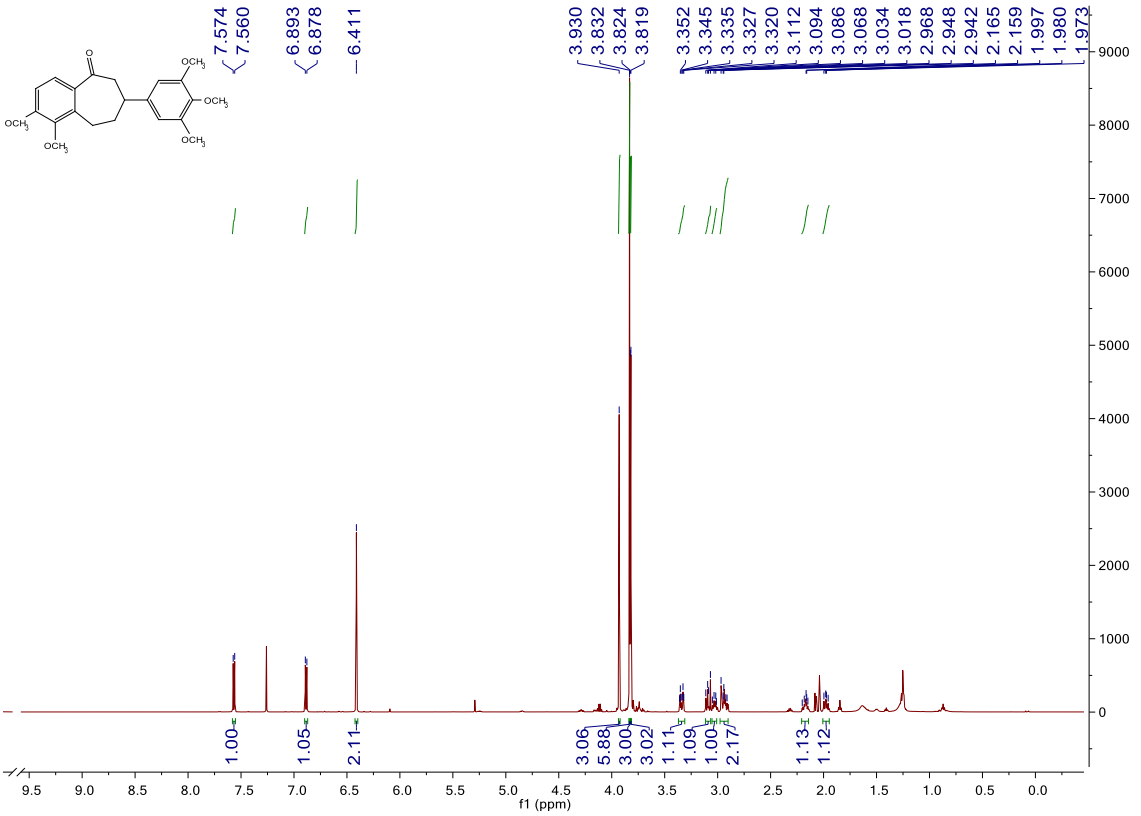
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.759	BB	0.0609	7.55375	1.87956	10.9323
2	1.859	BB	0.0462	16.25813	5.54189	23.5298
3	16.845	BB	0.0948	11.18299	1.89581	16.1848
4	17.365	BB	0.1082	34.10091	4.96056	49.3531
Totals :				69.09579	14.27782	

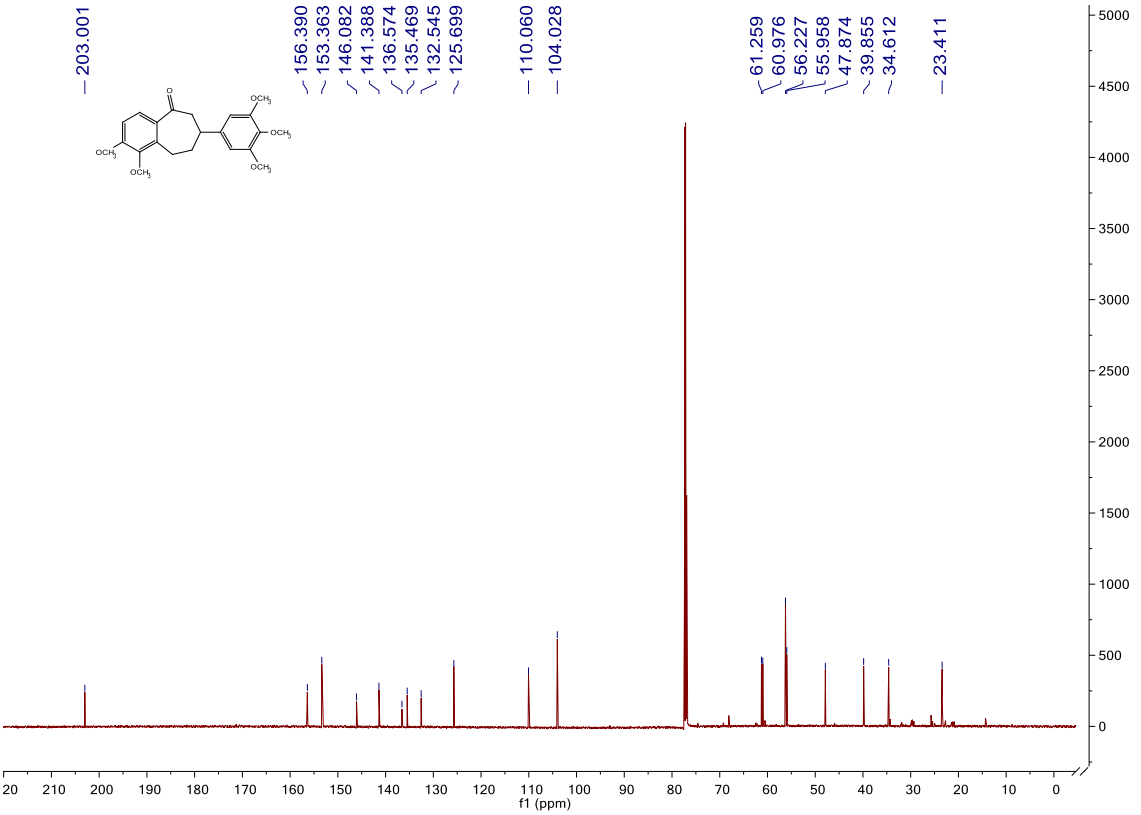
Signal 8: DAD1 H, Sig=320,16 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.760	BB	0.0613	6.44649	1.58956	31.1500
2	1.858	BB	0.0457	14.24850	4.92747	68.8500
Totals :				20.69498	6.51703	

*** End of Report ***

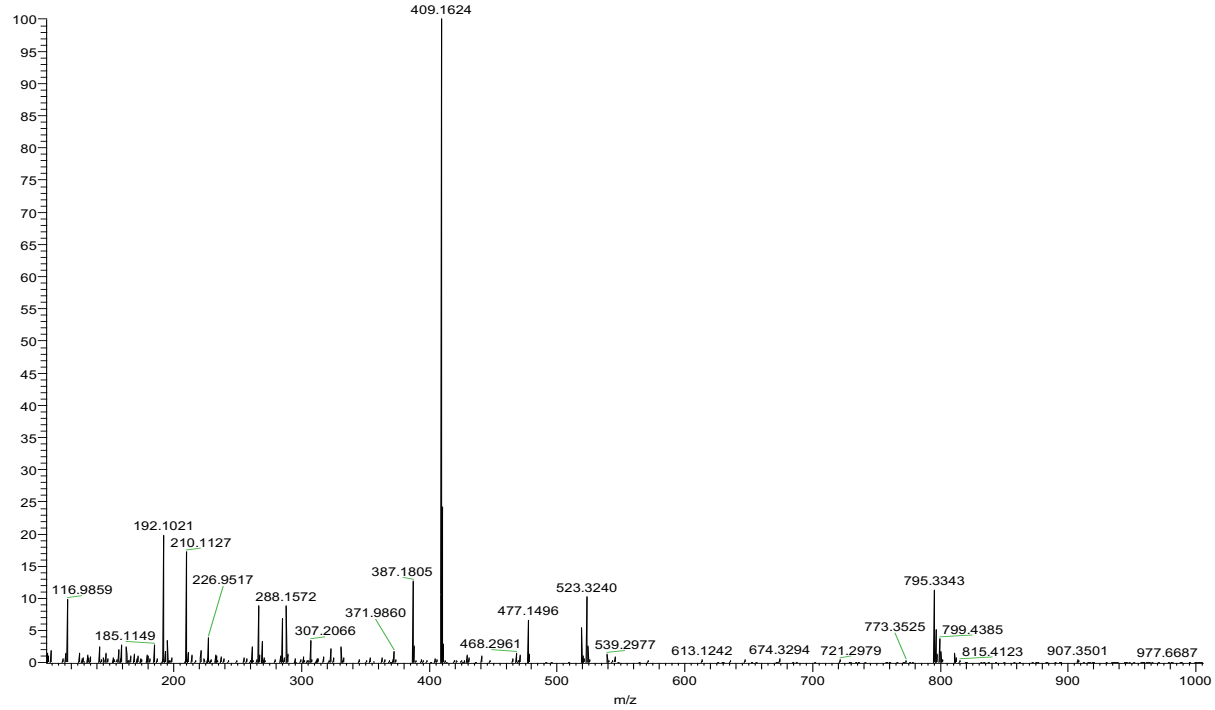
57. 1,2-dimethoxy-7-(3,4,5-trimethoxyphenyl)-6,7,8,9-tetrahydro-5H-benzo[7]annulen-5-one





C:\Xcalibur\...\NHC_4_17_Repurified_esi 2/16/2017 1:15:58 AM
NHC_4_17

NHC_4_17_Repurified_esi #2-19 RT: 0.01-0.15 AV: 18 NL: 2.39E7
T: FTMS + p ESI Full ms [100.00-1000.00]



Data File C:\Chem32\1\Data\NHC\NHC_4_17_KGP501_sample.D
Sample Name: NHC_4_17_KGP501_sample

```
=====================================================================
Acq. Operator   : SYSTEM
Sample Operator : SYSTEM
Acq. Instrument : 1200 HPLC                    Location :   1
Injection Date  : 3/3/2017 11:44:28 AM
                                             Inj Volume : No inj
Acq. Method     : C:\Chem32\1\Methods\MASTERMETHOD2.M
Last changed    : 12/2/2015 12:37:42 PM by Eric Lin
Analysis Method : C:\CHEM32\1\METHODS\RT-ACNWASH 2.M
Last changed    : 7/9/2015 2:27:22 PM by Blake
Method Info     : General Column Wash Method

Sample Info     : background 20170303

Additional Info : Peak(s) manually integrated
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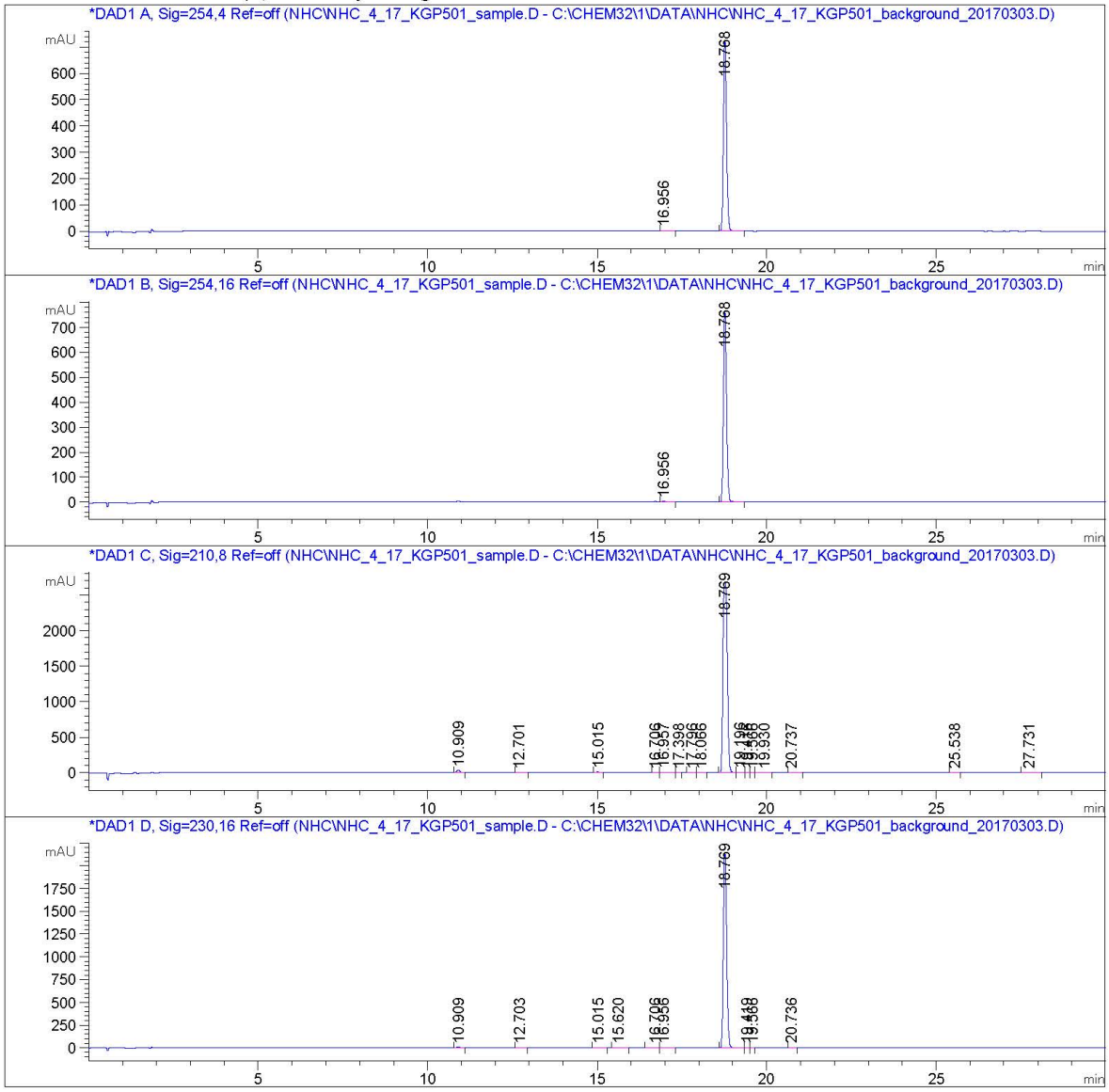
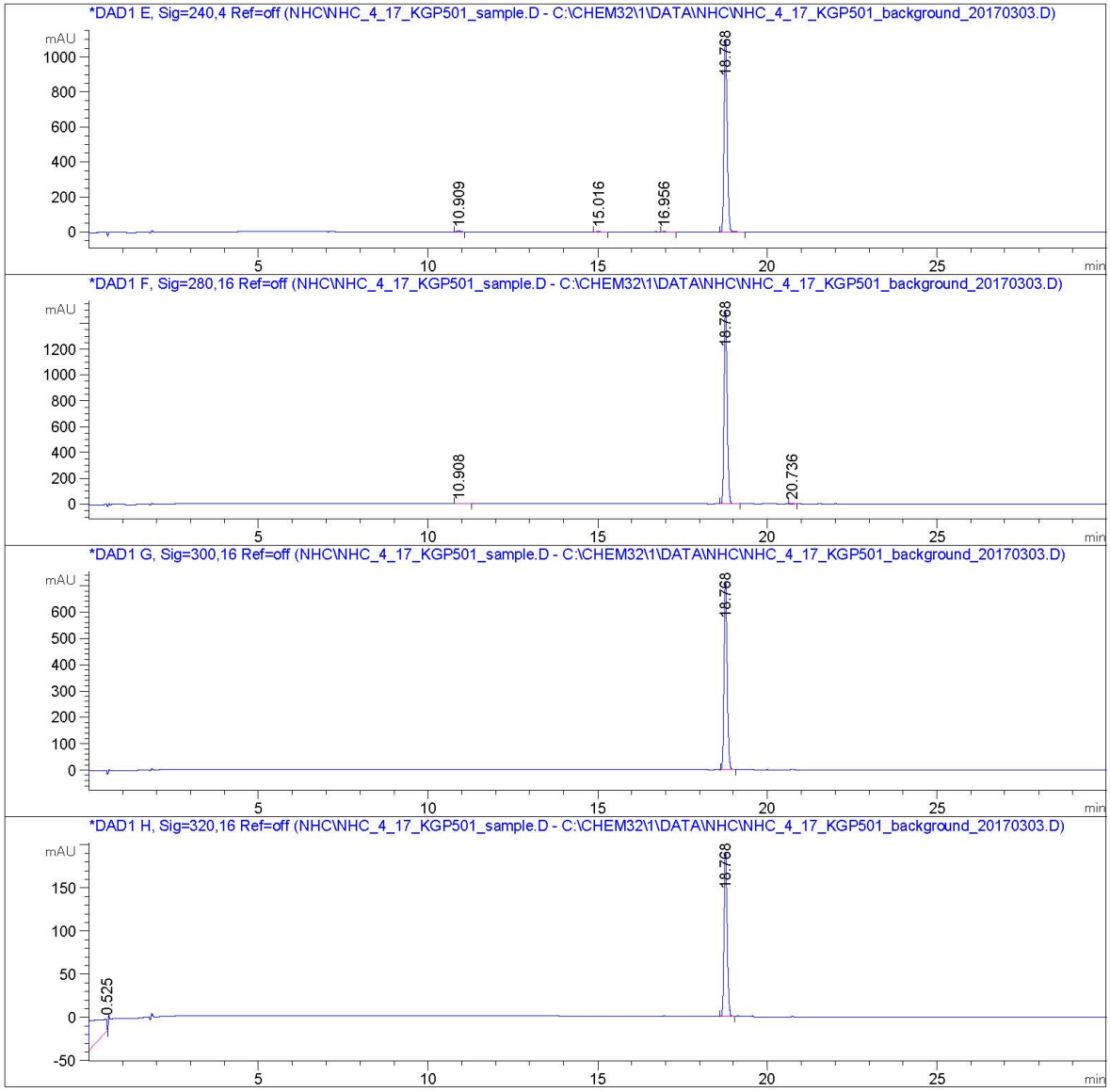


Data File C:\Chem32\1\Data\NHC\NHC_4_17_KGP501_sample.D
Sample Name: NHC_4_17_KGP501_sample



==========

Area Percent Report

==========

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

Data File C:\Chem32\1\Data\NHC\NHC_4_17_KGP501_sample.D
Sample Name: NHC_4_17_KGP501_sample

Signal 1: DAD1 A, Sig=254,4 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.956	VB	0.0960	9.14904	1.44154	0.2041
2	18.768	BB	0.0941	4472.67627	724.20117	99.7959
Totals :				4481.82531	725.64271	

Signal 2: DAD1 B, Sig=254,16 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.956	VB	0.0983	9.36114	1.43222	0.1979
2	18.768	BB	0.0941	4720.95898	763.91931	99.8021
Totals :				4730.32013	765.35153	

Signal 3: DAD1 C, Sig=210,8 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.909	VB	0.1029	227.68459	34.52555	0.9489
2	12.701	BB	0.0925	27.14396	4.49487	0.1131
3	15.015	BB	0.0878	68.21432	12.09876	0.2843
4	16.706	VV	0.1112	19.18409	2.51008	0.0800
5	16.957	VB	0.1237	52.35861	6.00665	0.2182
6	17.398	BB	0.0850	6.04696	1.15729	0.0252
7	17.796	BV	0.1082	15.01916	2.08054	0.0626
8	18.066	VB	0.1194	17.44163	2.13384	0.0727
9	18.769	BV	0.1417	2.33801e4	2683.31982	97.4383
10	19.196	VV	0.1604	66.49103	5.76986	0.2771
11	19.416	VV	0.1160	18.65642	2.36491	0.0778
12	19.566	VB	0.0814	12.95463	2.46306	0.0540
13	19.930	BB	0.2324	18.20497	1.12759	0.0759
14	20.737	BB	0.1145	16.43744	2.07270	0.0685
15	25.538	BB	0.0985	18.41706	2.88574	0.0768
16	27.731	BB	0.1576	30.42202	3.01753	0.1268
Totals :				2.39948e4	2768.02880	

Data File C:\Chem32\1\Data\NHC\NHC_4_17_KGP501_sample.D
Sample Name: NHC_4_17_KGP501_sample

Signal 4: DAD1 D, Sig=230,16 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.909	BB	0.1027	52.31738	7.95528	0.3643
2	12.703	BB	0.0951	6.79331	1.08438	0.0473
3	15.015	BB	0.0953	17.88387	2.84835	0.1245
4	15.620	BB	0.1899	13.54218	1.04021	0.0943
5	16.706	BV	0.1322	11.10396	1.17575	0.0773
6	16.956	VB	0.1122	24.10922	3.11717	0.1679
7	18.769	BV	0.1053	1.42072e4	2144.07983	98.9335
8	19.419	VV	0.1184	11.53812	1.39695	0.0803
9	19.566	VB	0.0775	7.21468	1.41562	0.0502
10	20.736	BB	0.0934	8.64906	1.45322	0.0602
Totals :				1.43603e4	2165.56676	

Signal 5: DAD1 E, Sig=240,4 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.909	BB	0.1030	23.75278	3.59800	0.3441
2	15.016	BB	0.0986	9.20544	1.40269	0.1333
3	16.956	VB	0.1113	11.48606	1.50115	0.1664
4	18.768	BB	0.0989	6859.28076	1097.56555	99.3562
Totals :				6903.72504	1104.06739	

Signal 6: DAD1 F, Sig=280,16 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.908	BB	0.1062	8.45509	1.22953	0.0908
2	18.768	BB	0.0985	9296.77246	1496.94958	99.8133
3	20.736	BB	0.0934	8.93848	1.50160	0.0960
Totals :				9314.16603	1499.68071	

Signal 7: DAD1 G, Sig=300,16 Ref=off
Signal has been modified after loading from rawdata file!

Data File C:\Chem32\1\Data\NHC\NHC_4_17_KGP501_sample.D
Sample Name: NHC_4_17_KGP501_sample

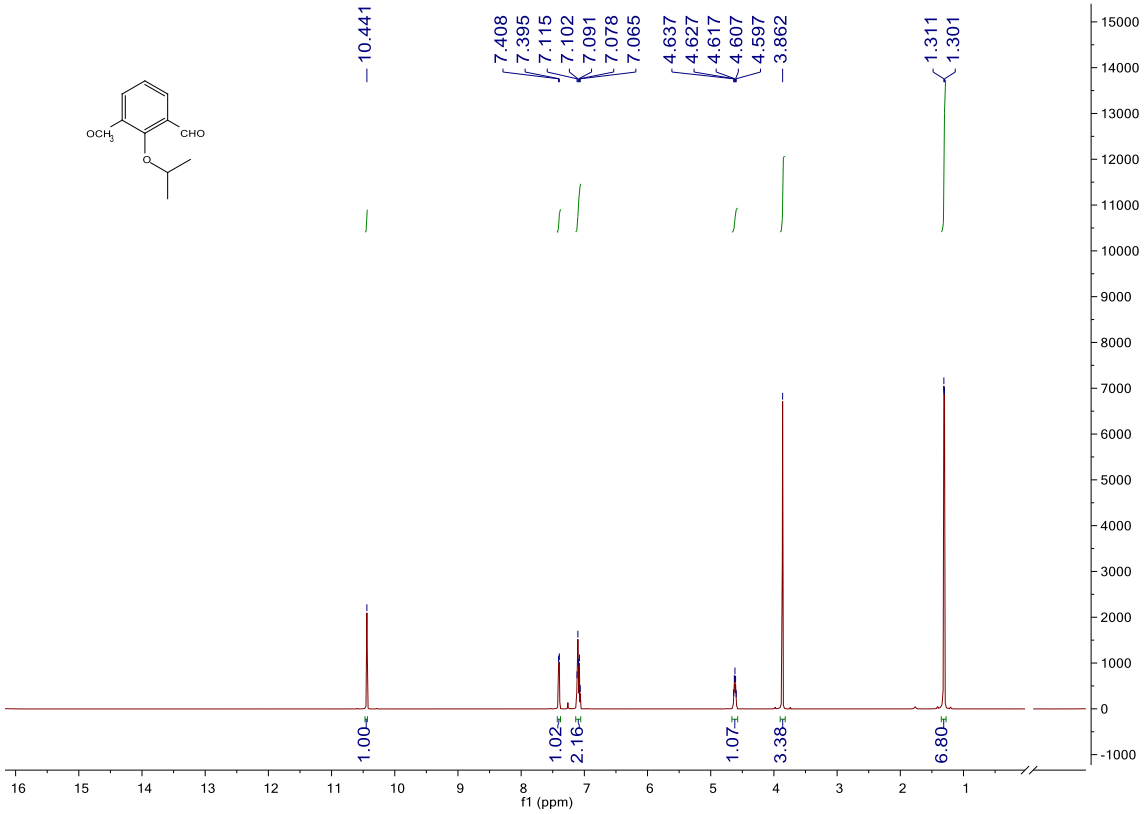
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.768	BB	0.0940	4402.45361	713.63989	100.0000
Totals :				4402.45361	713.63989	

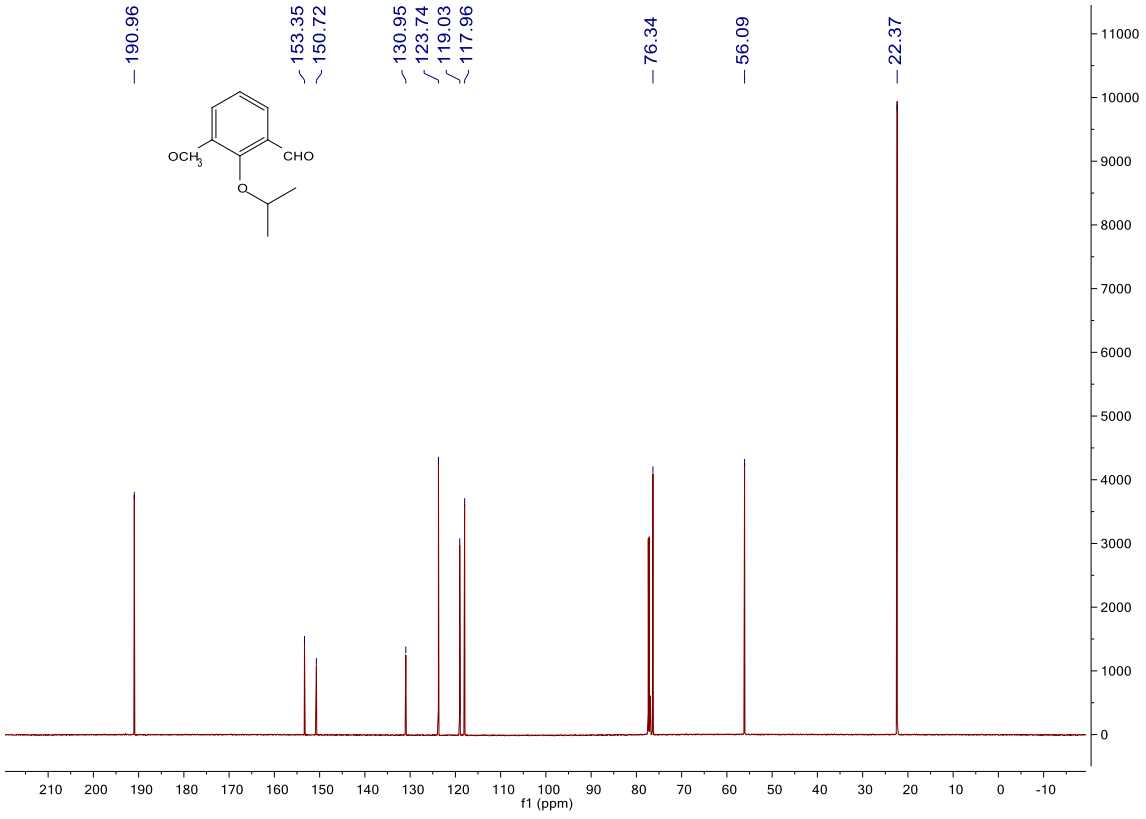
Signal 8: DAD1 H, Sig=320,16 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	0.525	BB	0.6315	786.67737	14.86395	40.1537
2	18.768	BV	0.0939	1172.48682	190.23064	59.8463
Totals :				1959.16418	205.09458	

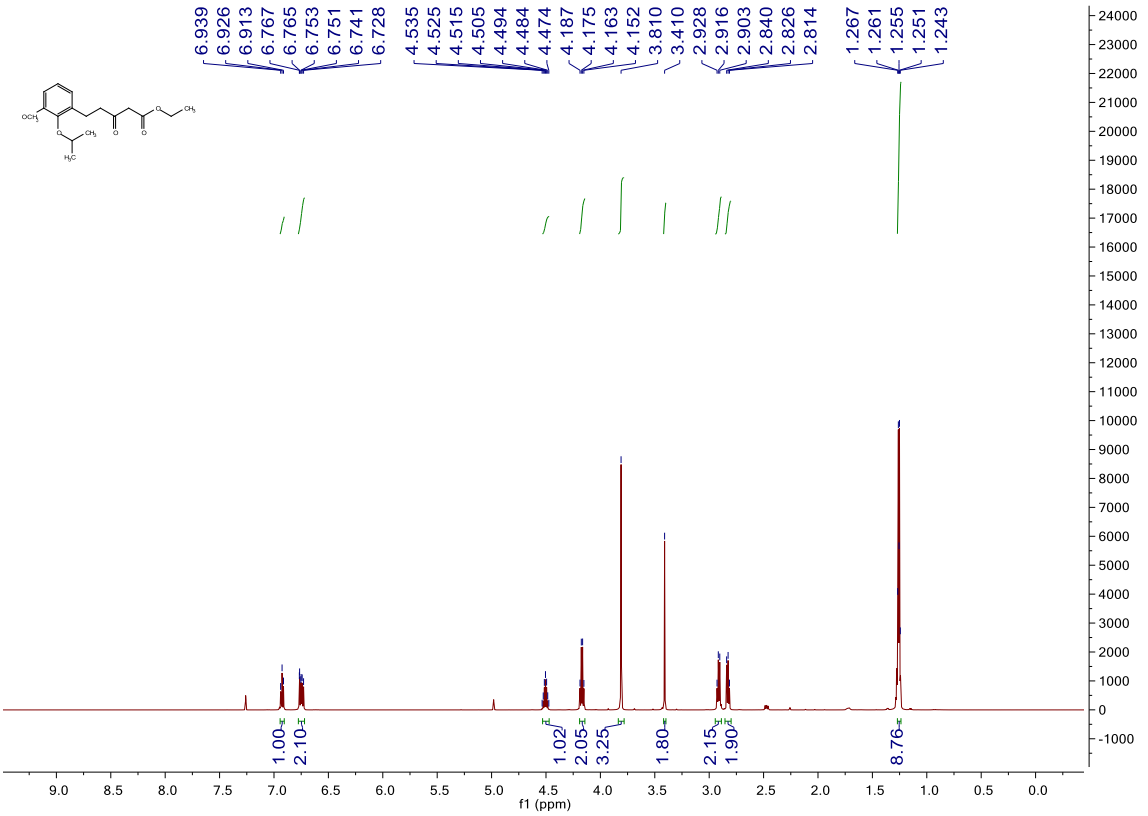
*** End of Report ***

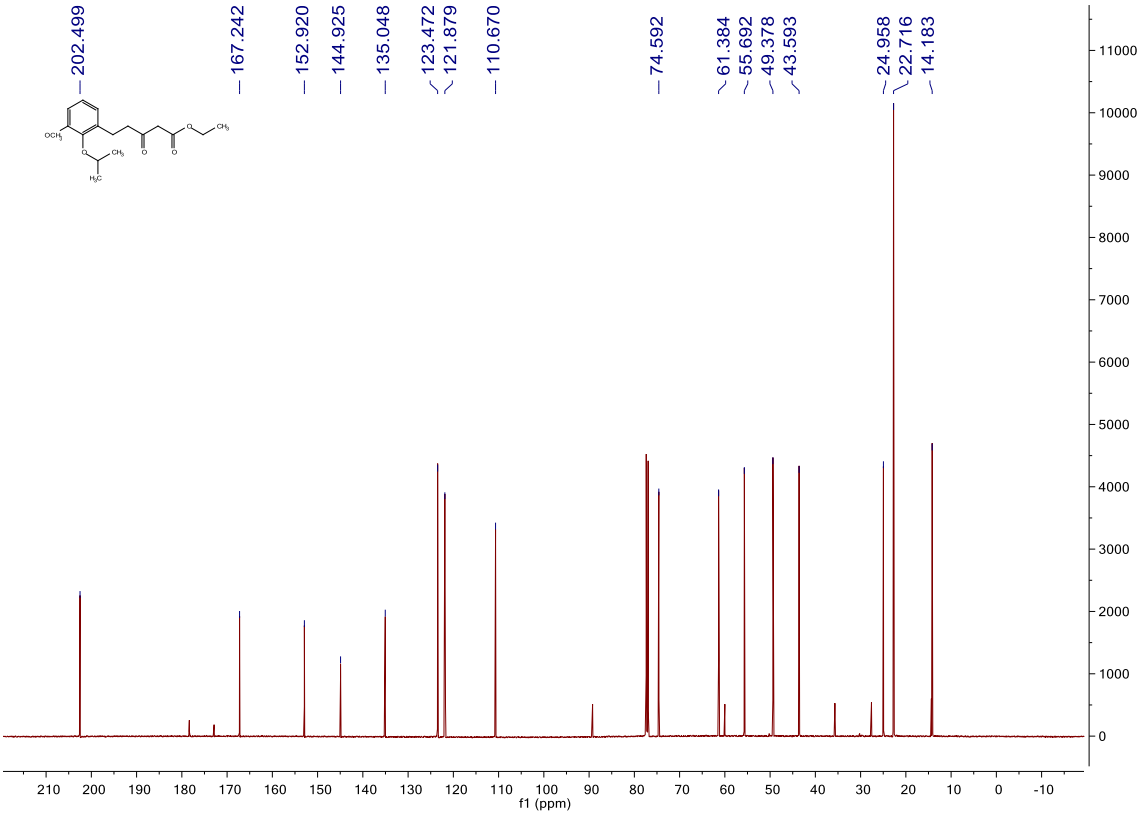
58. 2-isopropoxy-3-methoxybenzaldehyde



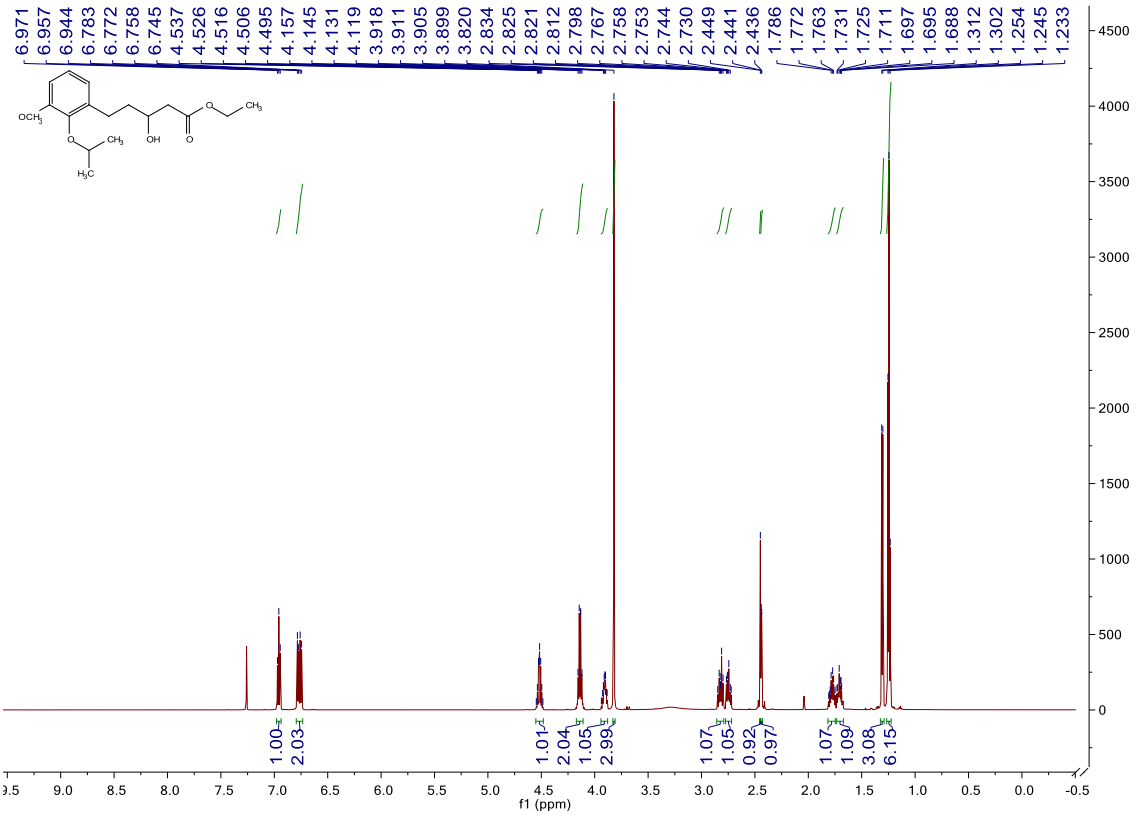


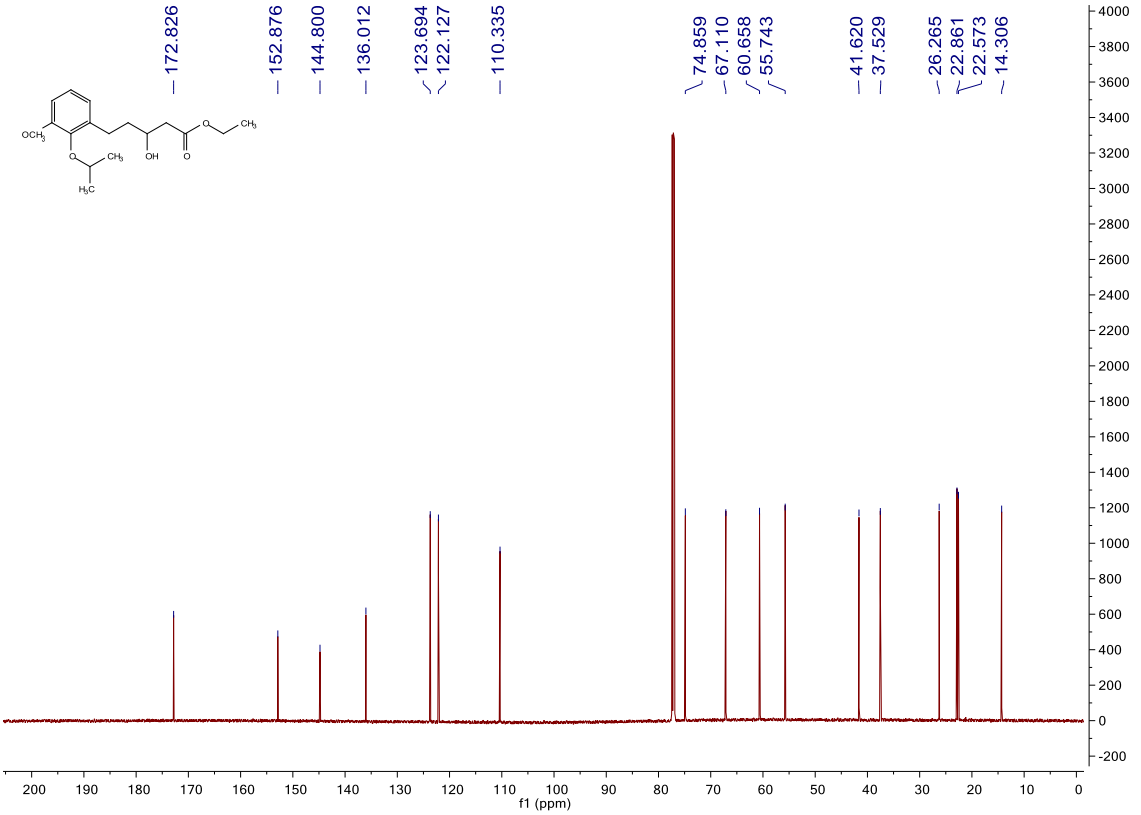
60. ethyl 5-(2-isopropoxy-3-methoxyphenyl)-3-oxopentanoate



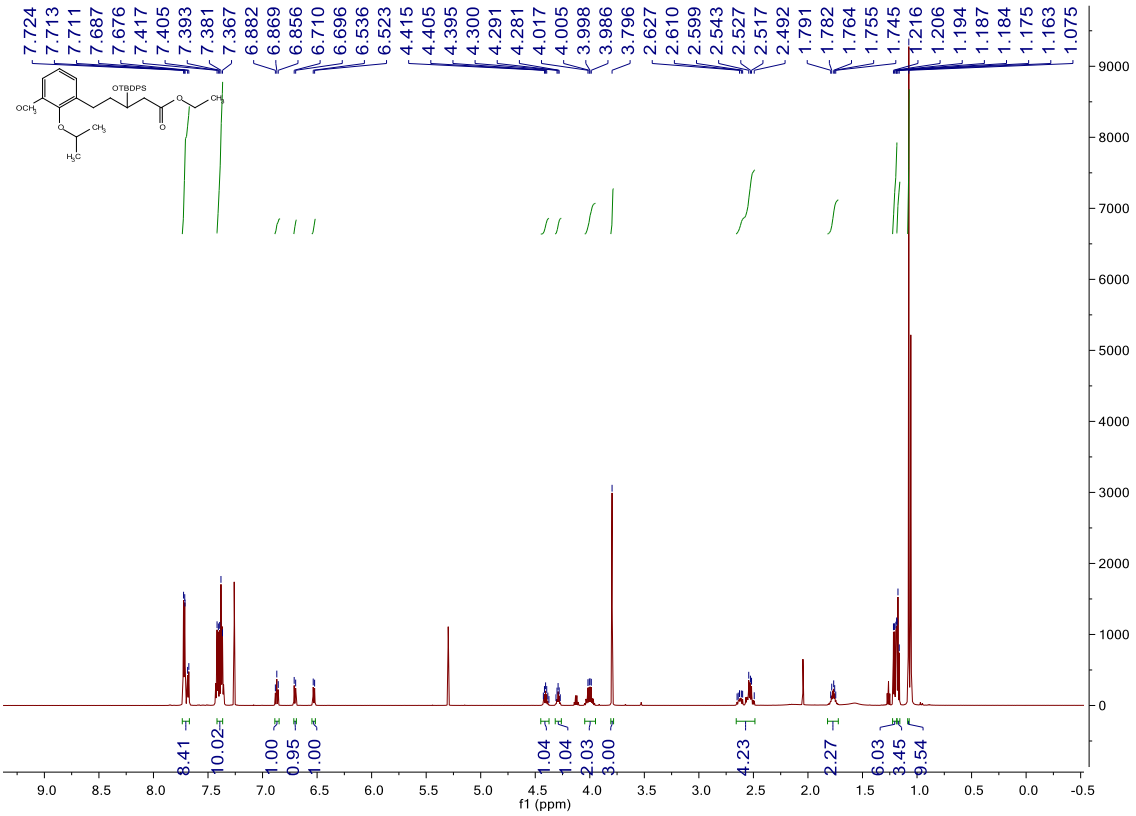


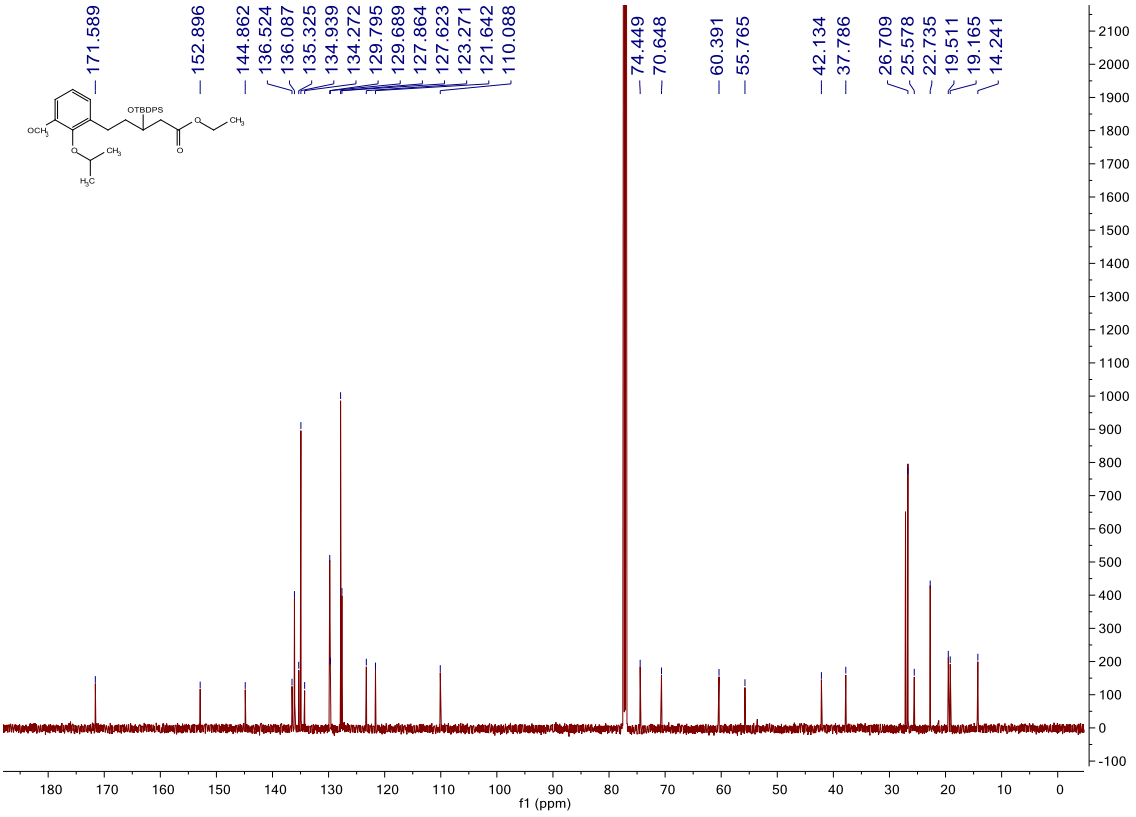
61. ethyl 3-hydroxy-5-(2-isopropoxy-3-methoxyphenyl)pentanoate



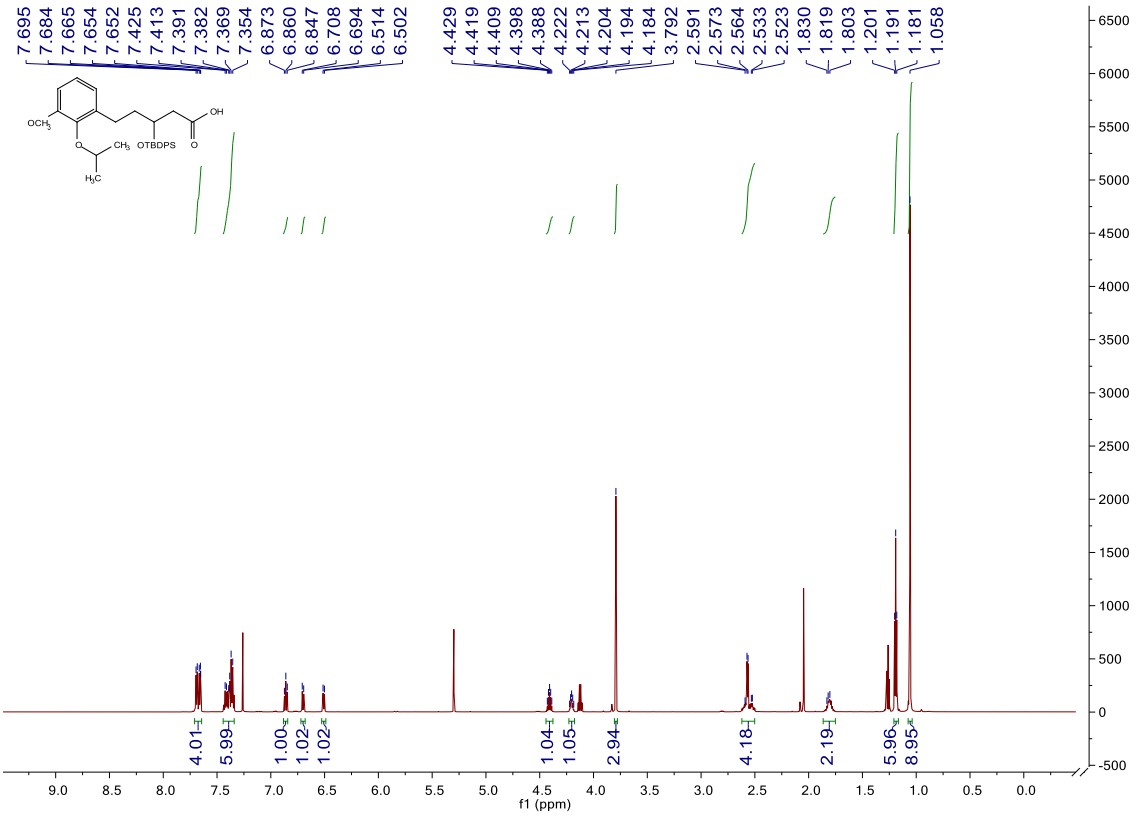


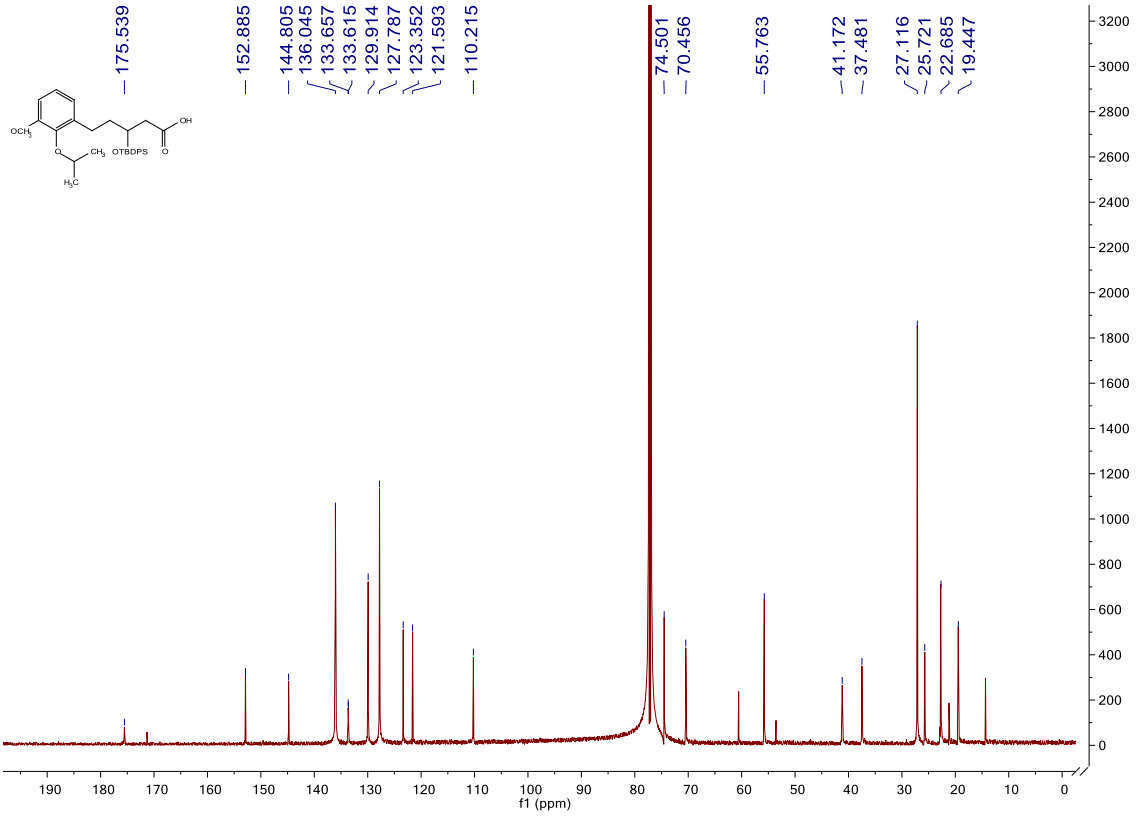
62. ethyl 3-((tert-butyldiphenylsilyl)oxy)-5-(2-isopropoxy-3-methoxyphenyl)pentanoate



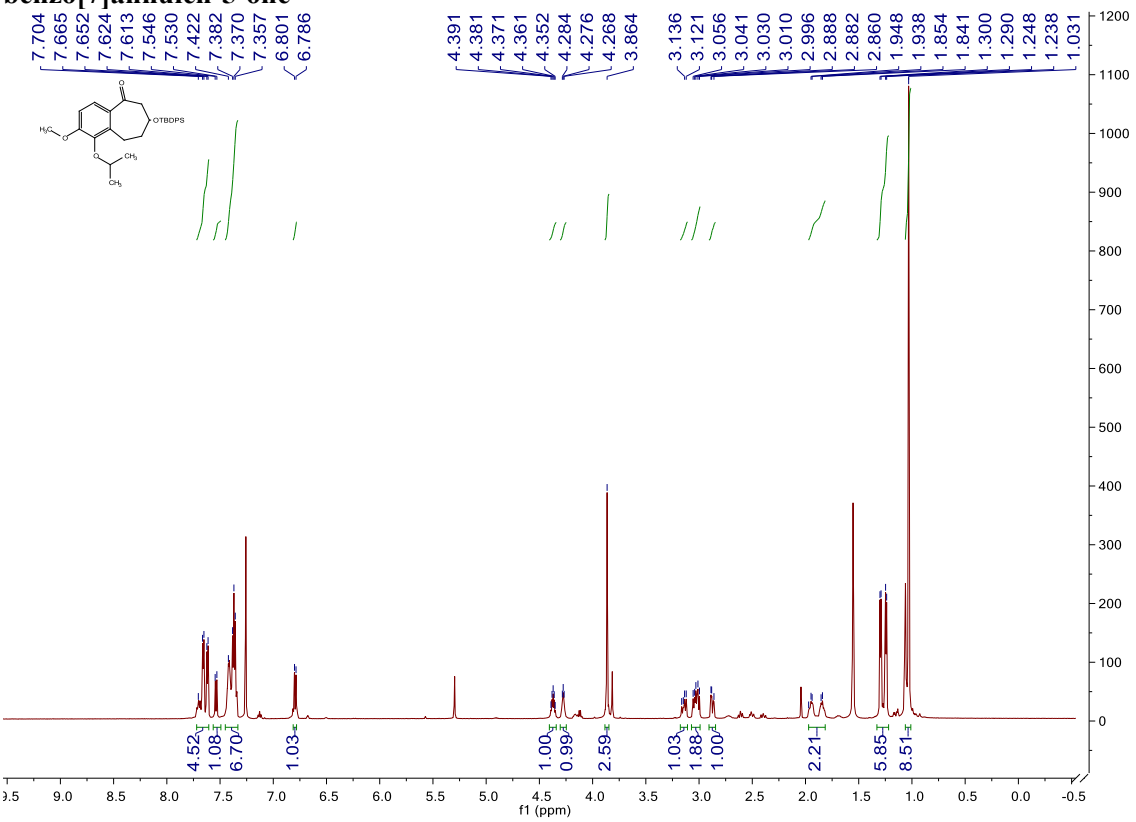


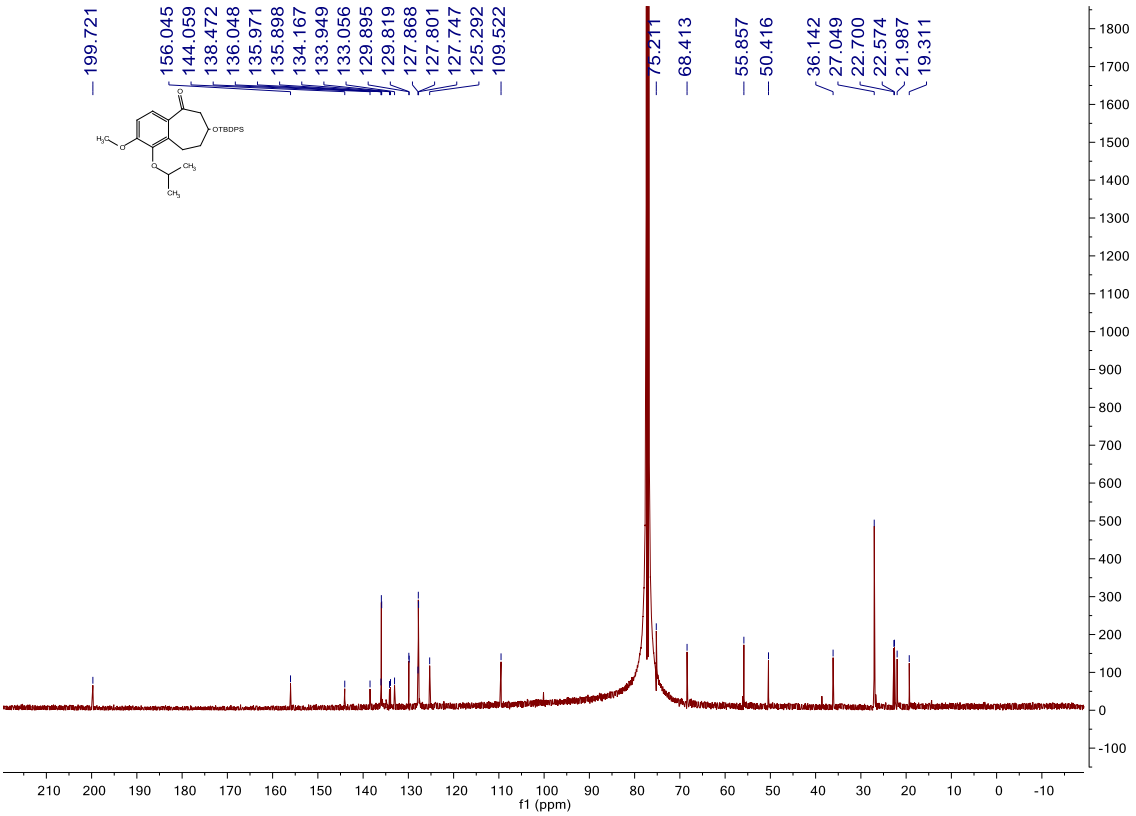
63. 3-((tert-butyldiphenylsilyl)oxy)-5-(2-isopropoxy-3-methoxyphenyl)pentanoic acid



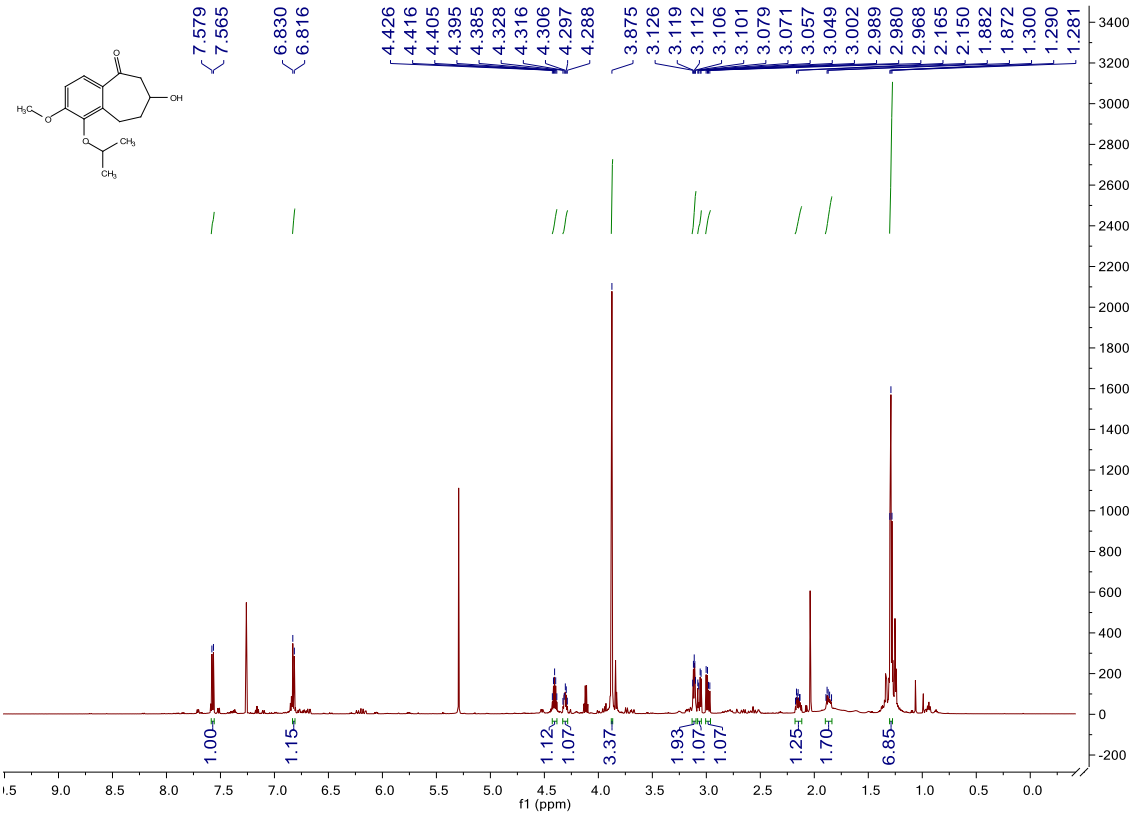


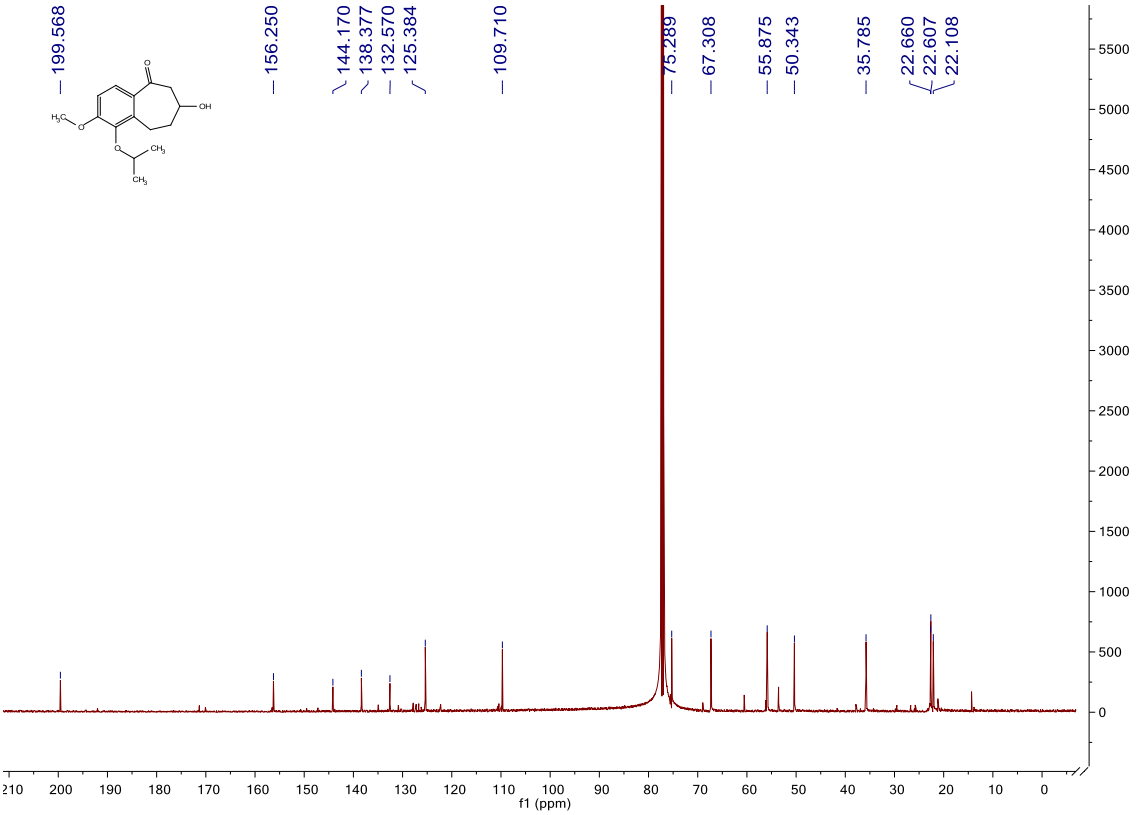
64. 7-((tert-butyldiphenylsilyl)oxy)-1-isopropoxy-2-methoxy-6,7,8,9-tetrahydro-5H-benzo[7]annulen-5-one



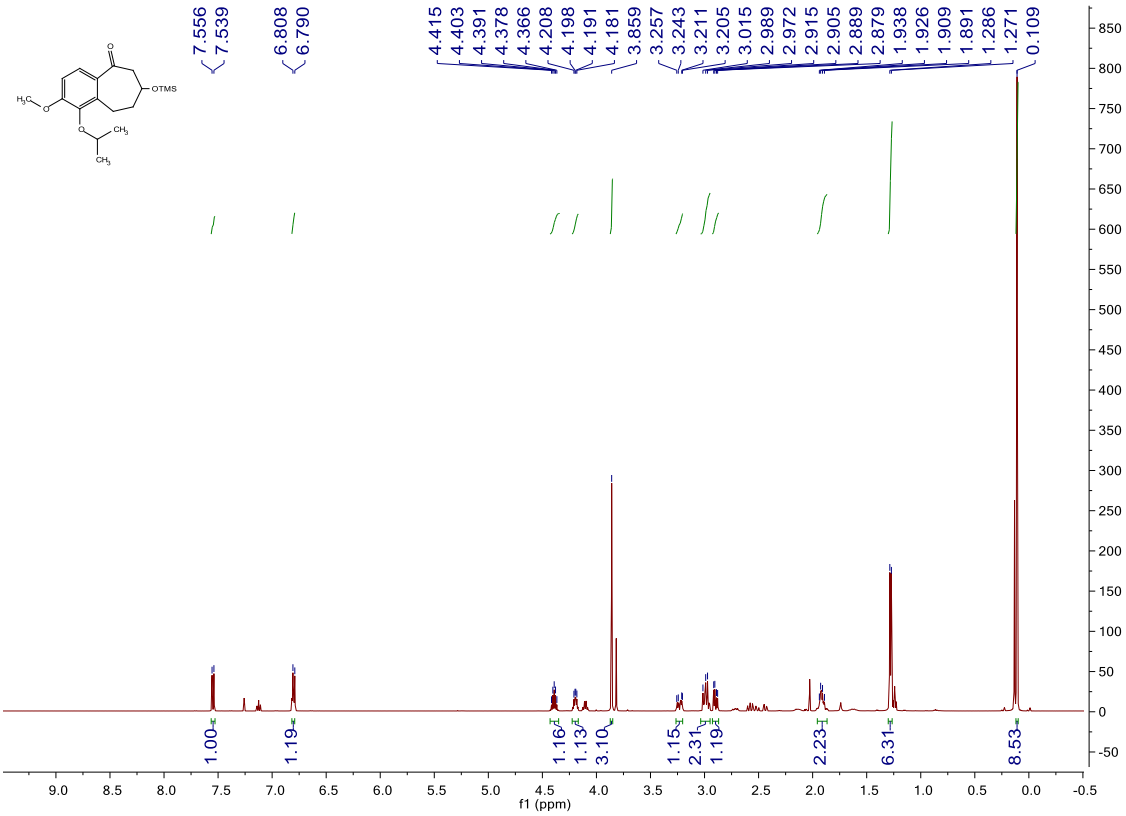


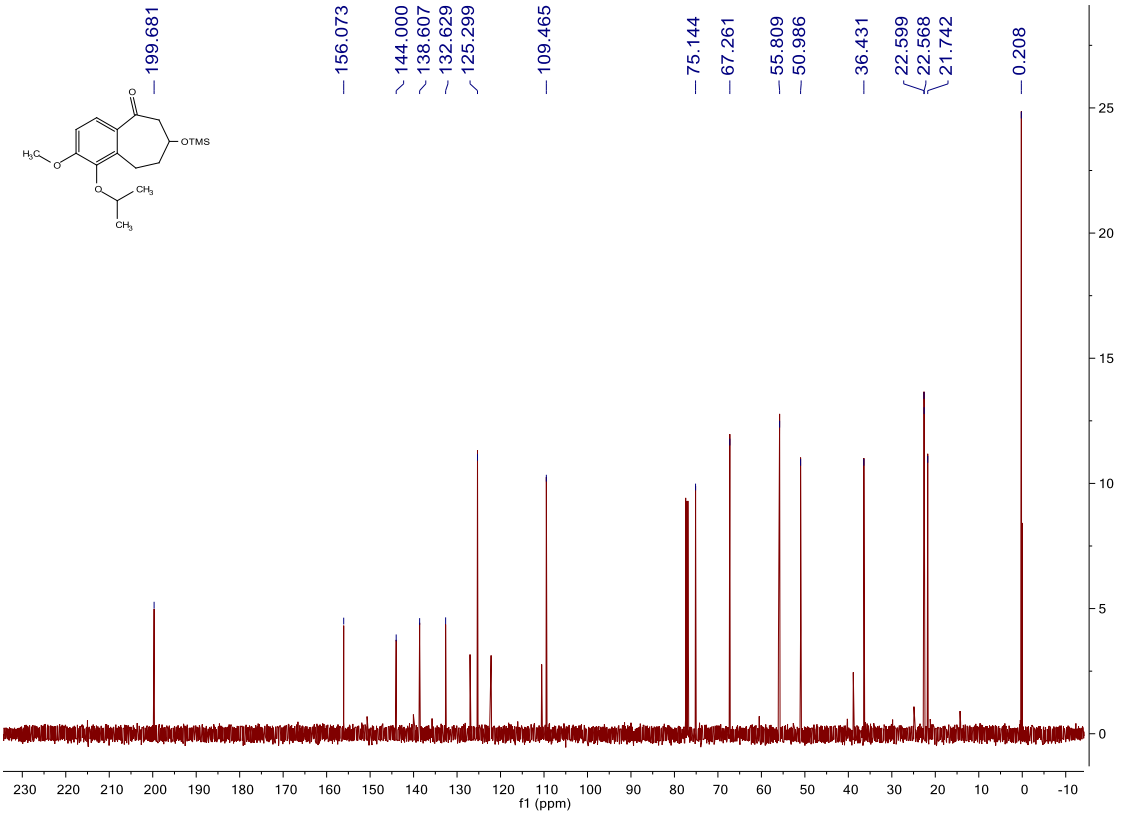
65. 7-hydroxy-1-isopropoxy-2-methoxy-6,7,8,9-tetrahydro-5H-benzo[7]annulen-5-one



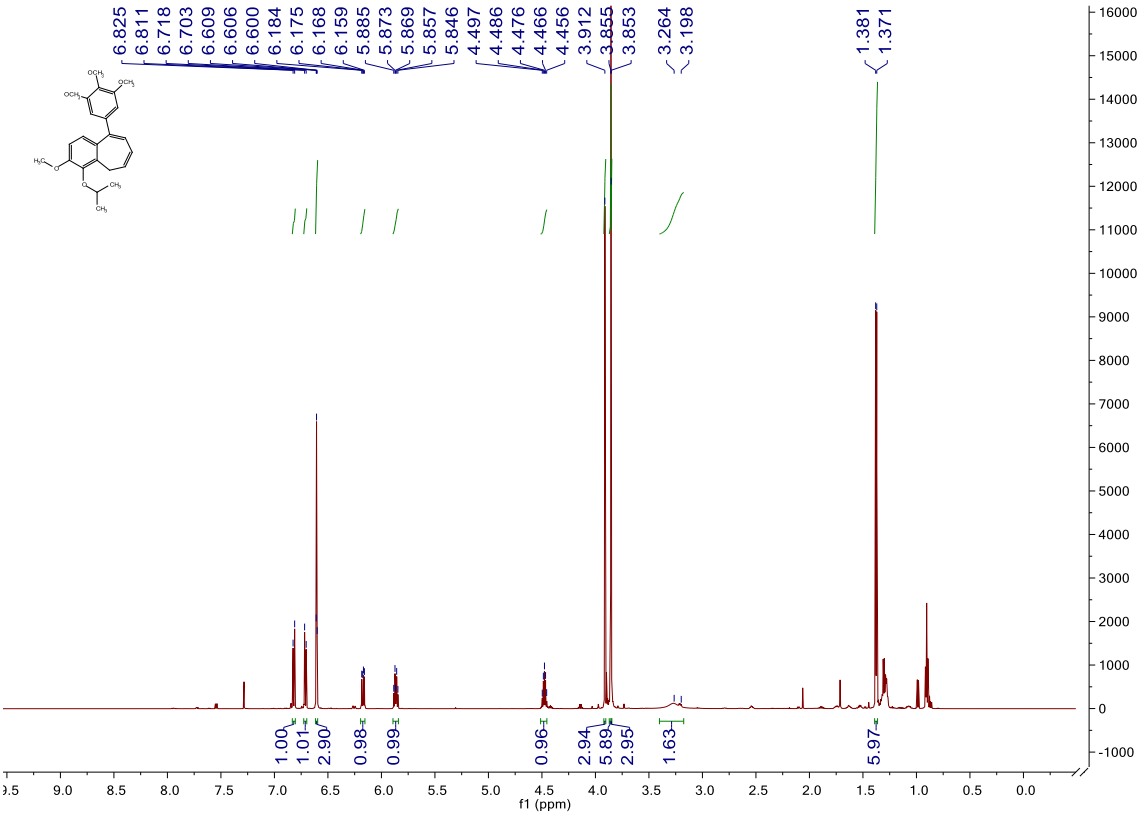


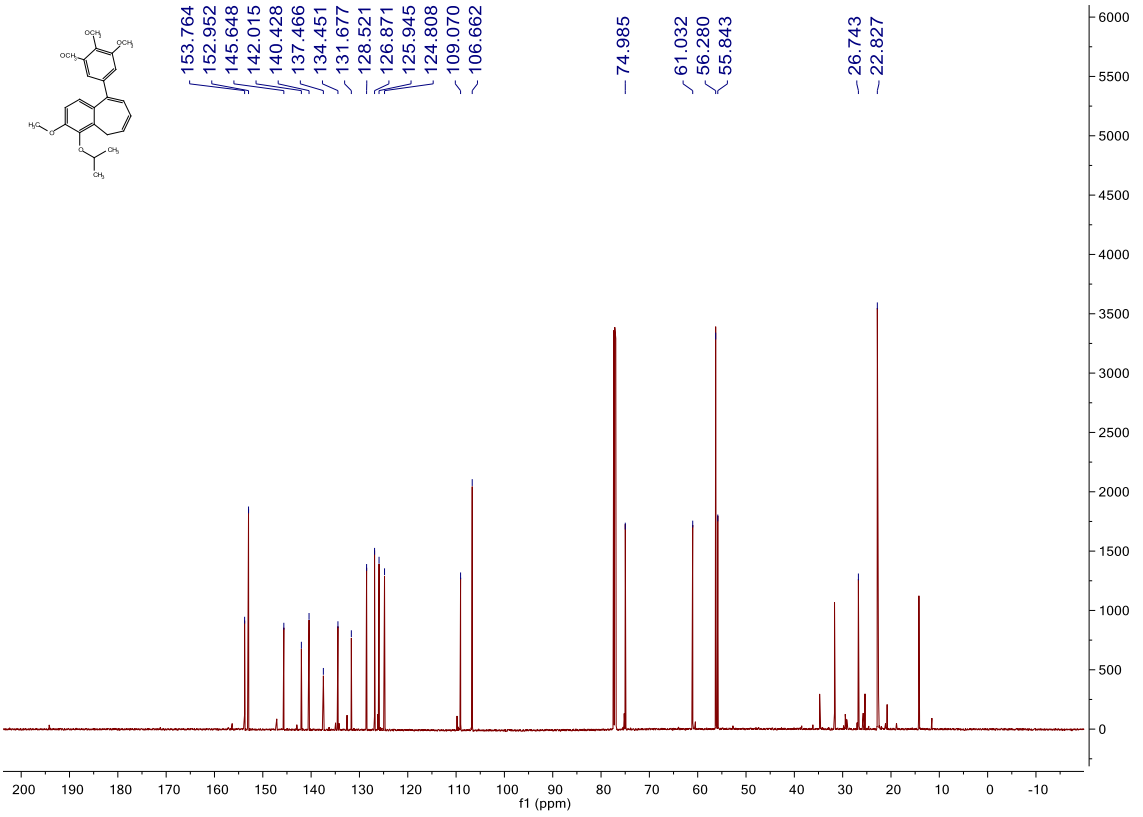
66. 1-isopropoxy-2-methoxy-7-((trimethylsilyl)oxy)-6,7,8,9-tetrahydro-5H-benzo[7]annulen-5-one



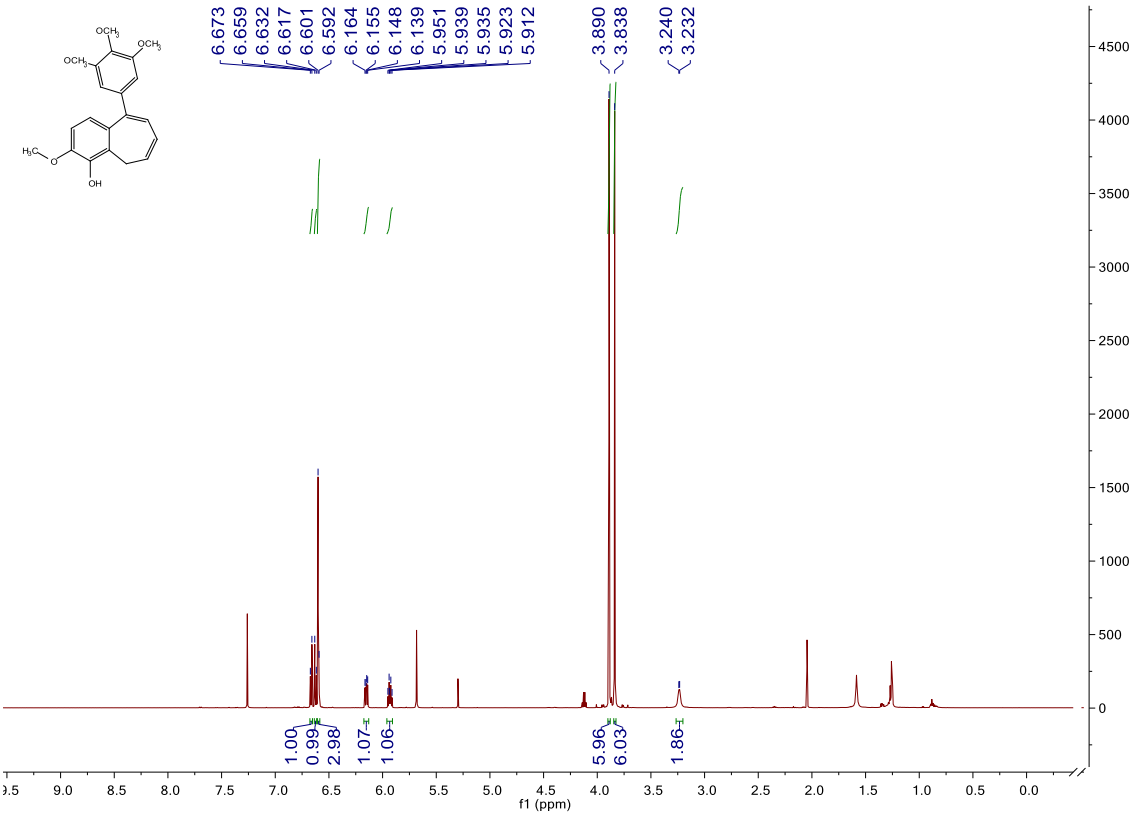


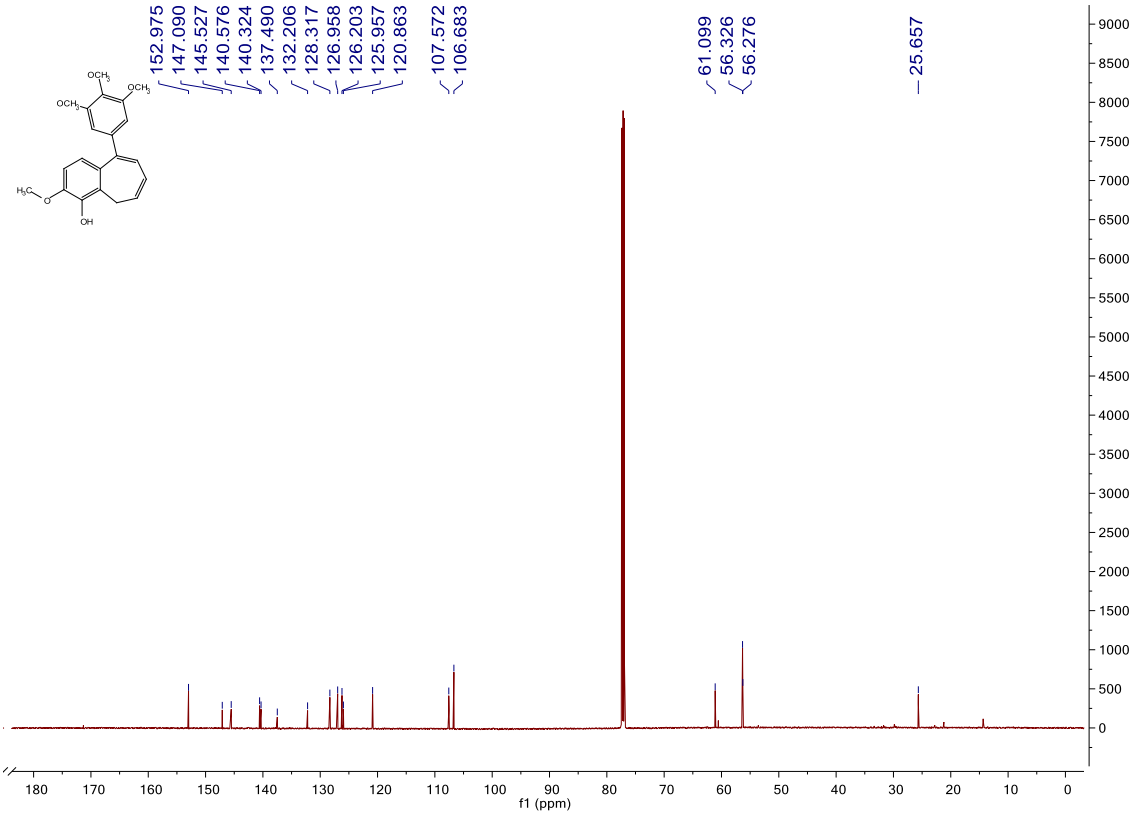
67. 4-isopropoxy-3-methoxy-9-(3,4,5-trimethoxyphenyl)-5H-benzo[7]annulene

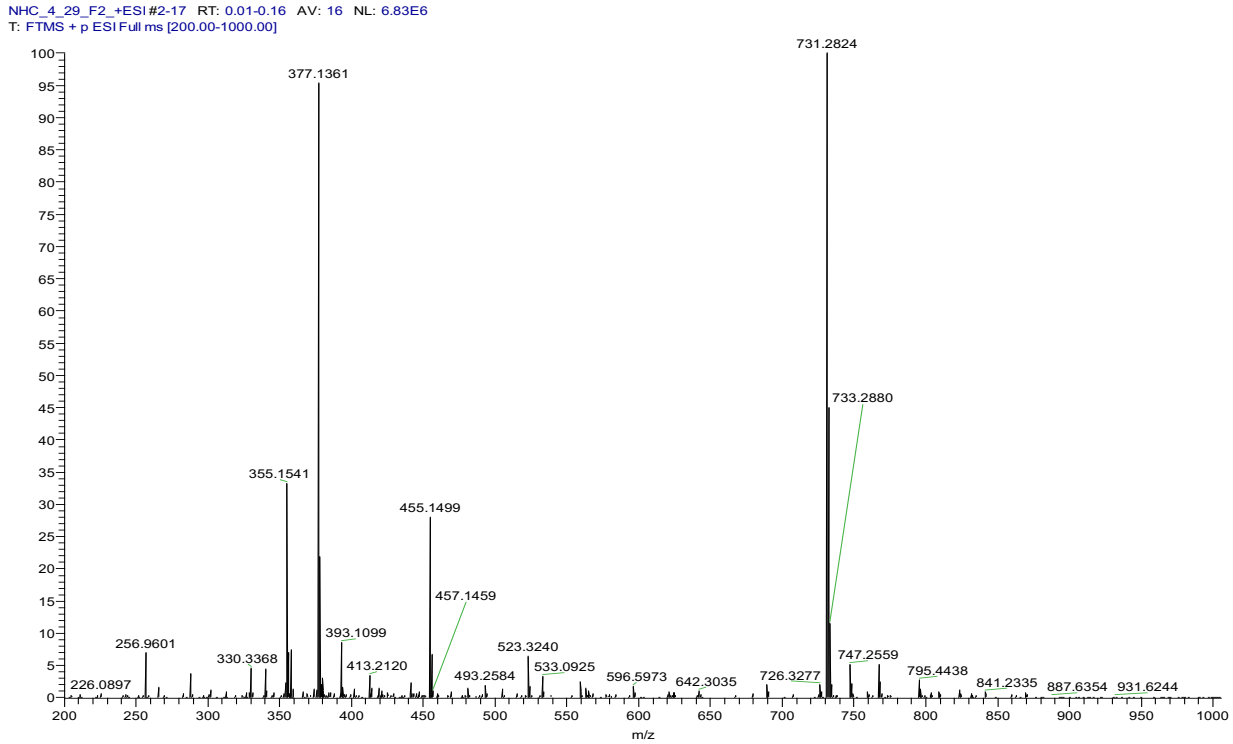




68. 3-methoxy-9-(3,4,5-trimethoxyphenyl)-5H-benzo[7]annulen-4-ol






NHC_4_29_F2_+ESI #2-17 RT: 0.01-0.16 AV: 16 NL: 6.83E6
T: FTMS + p ESI Full ms [200.00-1000.00]
731.2824
377.1361
733.2880
355.1541
455.1499
457.1459
393.1099
256.9601
523.3240
330.3368
413.2120
747.2559
533.0925
493.2584
795.4438
596.5973
642.3035
726.3277
841.2335
887.6354
931.6244
226.0897
m/z

Data File C:\Chem32\1\Data\NHC\NHC_4_29_F2.D
Sample Name: run

```
======================================================================
Acq. Operator   : SYSTEM
Sample Operator : SYSTEM
Acq. Instrument : 1200 HPLC                    Location :   1
Injection Date  : 4/13/2017 3:42:39 PM
                                             Inj Volume : No inj
Acq. Method     : C:\Chem32\1\Methods\MASTERMETHOD2.M
Last changed    : 12/2/2015 12:37:42 PM by Eric Lin
Analysis Method : C:\CHEM32\1\METHODS\RT-ACNWASH 2.M
Last changed    : 7/9/2015 2:27:22 PM by Blake
Method Info     : General Column Wash Method

Sample Info     : sample run

Additional Info : Peak(s) manually integrated
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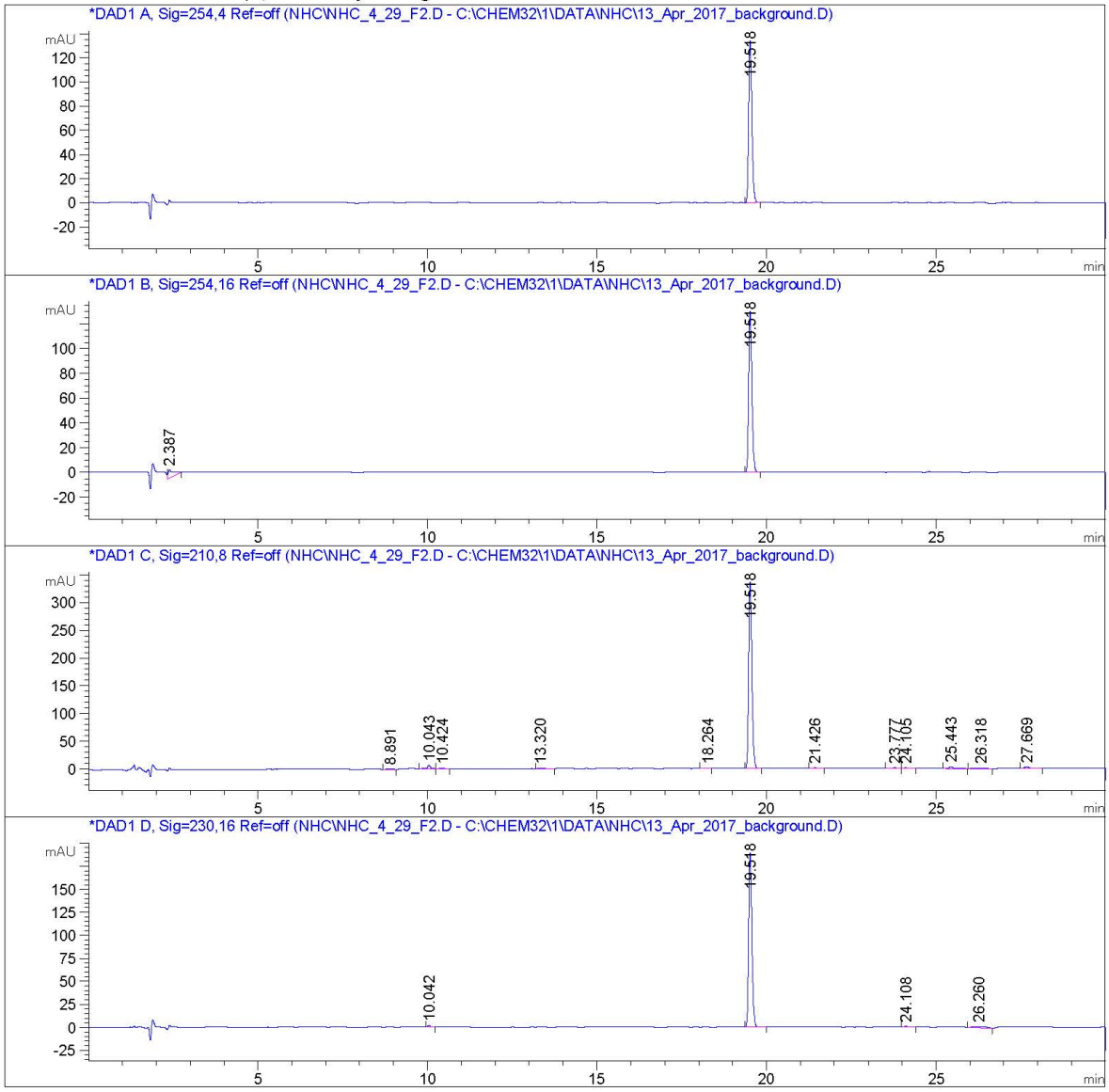
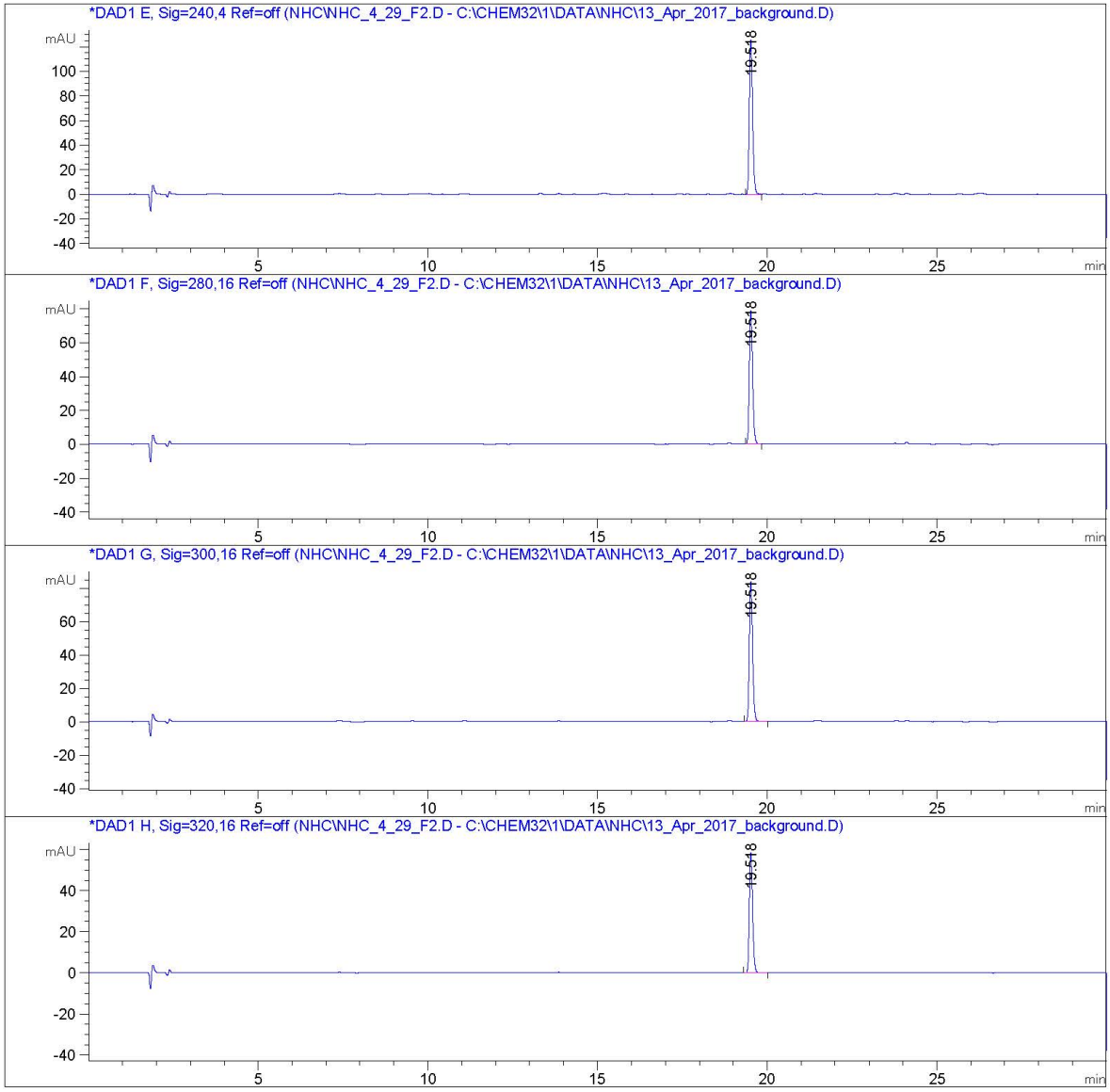


Data File C:\Chem32\1\Data\NHC\NHC_4_29_F2.D
Sample Name: run



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Area Percent Report

==========

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Data File C:\Chem32\1\Data\NHC\NHC_4_29_F2.D
Sample Name: run

Signal 1: DAD1 A, Sig=254,4 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.518	BB	0.1037	893.67578	134.17885	100.0000
Totals :				893.67578	134.17885	

Signal 2: DAD1 B, Sig=254,16 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.387	VB	0.1446	76.20650	6.91596	8.0878
2	19.518	BB	0.1037	866.02875	130.02982	91.9122
Totals :				942.23525	136.94578	

Signal 3: DAD1 C, Sig=210,8 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.891	BB	0.2174	21.26654	1.31029	0.8596
2	10.043	BB	0.0923	40.79895	6.40773	1.6491
3	10.424	BB	0.0892	8.80127	1.48347	0.3557
4	13.320	BB	0.0991	10.09099	1.52677	0.4079
5	18.264	BB	0.1176	8.73953	1.16396	0.3532
6	19.518	BB	0.1038	2244.24927	336.59158	90.7107
7	21.426	BB	0.1681	17.70563	1.45380	0.7156
8	23.777	BV	0.1809	16.40671	1.43975	0.6631
9	24.105	VB	0.1170	11.36482	1.49017	0.4594
10	25.443	BB	0.1471	32.64170	3.19694	1.3193
11	26.318	BB	0.3383	31.05574	1.41386	1.2552
12	27.669	BB	0.1670	30.95303	2.93546	1.2511
Totals :				2474.07416	360.41377	

Signal 4: DAD1 D, Sig=230,16 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.042	BB	0.0735	8.04291	1.69065	0.6140
2	19.518	BB	0.1039	1265.59241	189.50731	96.6177

Data File C:\Chem32\1\Data\NHC\NHC_4_29_F2.D
Sample Name: run

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
3	24.108	BB	0.1117	7.96165	1.11024	0.6078
4	26.260	BB	0.2896	28.30067	1.27207	2.1605
Totals :				1309.89764	193.58027	

Signal 5: DAD1 E, Sig=240,4 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.518	BB	0.1037	836.45416	125.52441	100.0000
Totals :				836.45416	125.52441	

Signal 6: DAD1 F, Sig=280,16 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.518	BB	0.1038	524.59283	78.70221	100.0000
Totals :				524.59283	78.70221	

Signal 7: DAD1 G, Sig=300,16 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.518	BB	0.1039	558.95642	83.67628	100.0000
Totals :				558.95642	83.67628	

Signal 8: DAD1 H, Sig=320,16 Ref=off
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.518	BB	0.1040	390.38800	58.39185	100.0000
Totals :				390.38800	58.39185	

Data File C:\Chem32\1\Data\NHC\NHC_4_29_F2.D
Sample Name: run

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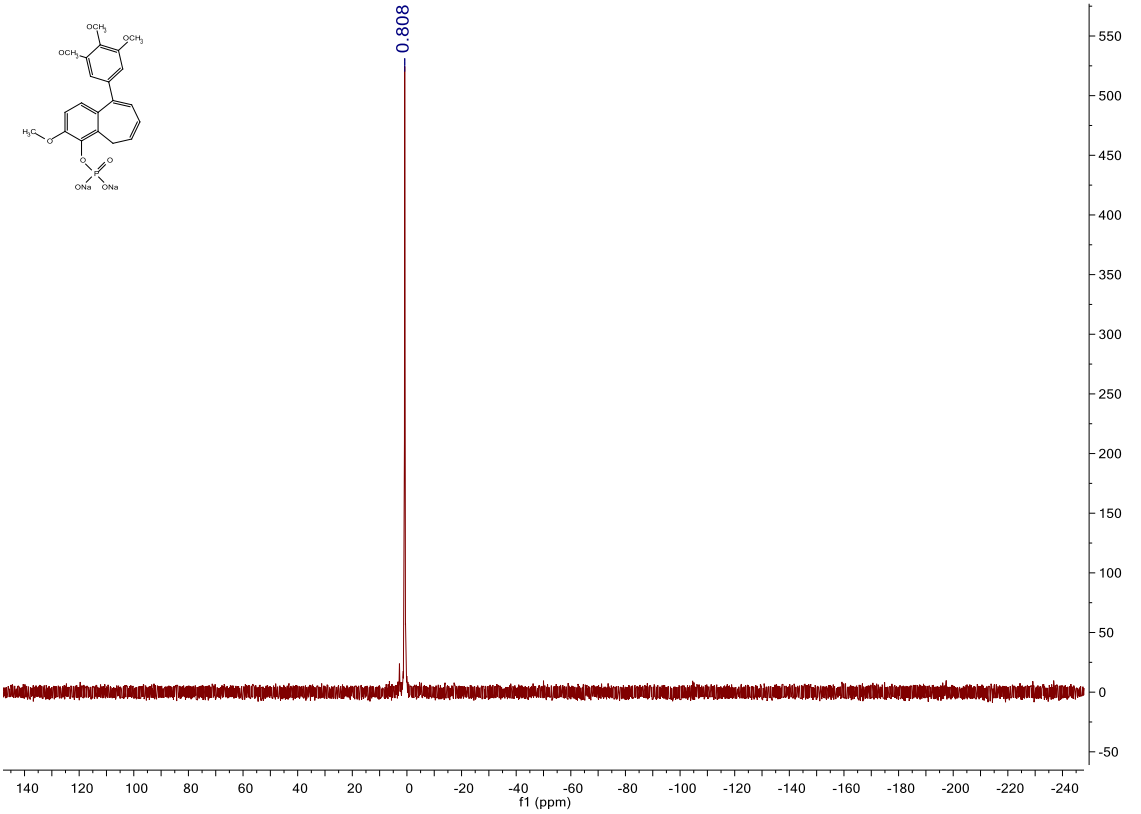
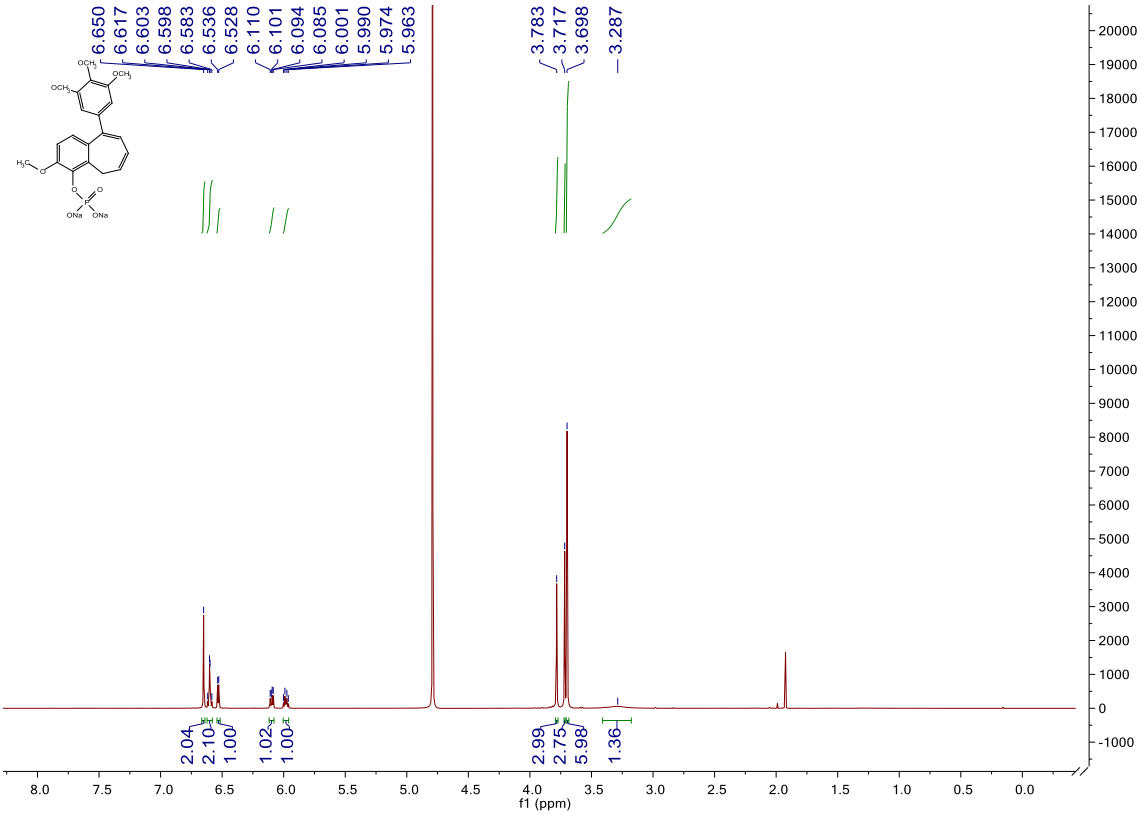
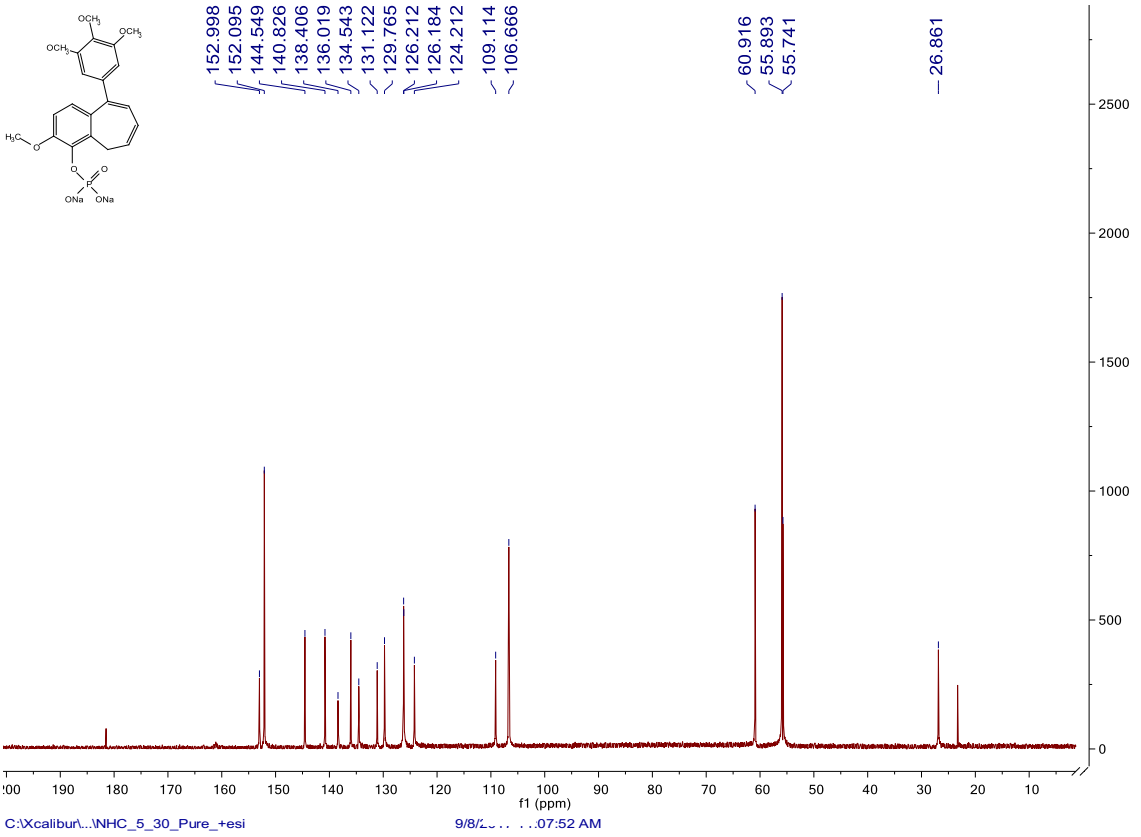
*** End of Report ***

69. Sodium 3-methoxy-9-(3,4,5-trimethoxyphenyl)-5H-benzo[7]annulen-4-yl phosphate



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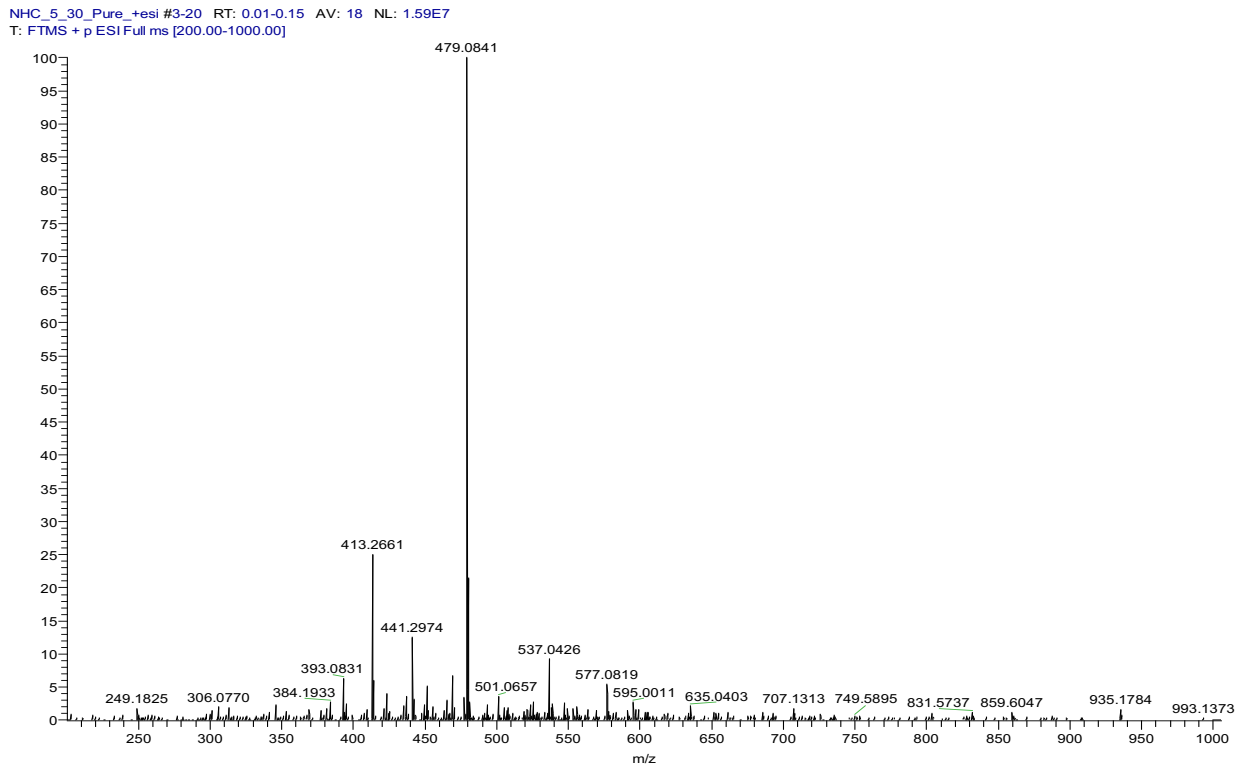
26.861
f1 (ppm)
C:\Xcalibur\...\NHC_5_30_Pure_+esi


NHC_5_30_Pure_+esi #3-20 RT: 0.01-0.15 AV: 18 NL: 1.59E7
T: FTMS + p ESI Full ms [200.00-1000.00]
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413.2661
441.2974
537.0426
577.0819
393.0831
501.0657
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635.0403
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249.1825
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384.1933
m/z

Data File C:\Chem32\1\Data\NHC\KGP513 salt_TFA.D
Sample Name: KGP513 salt_TFA

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    Sample Operator : SYSTEM
    Acq. Instrument : 1200 HPLC                    Location :   1
    Injection Date  : 2/23/2018 9:53:56 AM
                                                   Inj Volume : No inj
    Acq. Method     : C:\CHEM32\1\METHODS\MASTERMETHOD2.M
    Last changed    : 12/2/2015 12:37:42 PM by Eric Lin
    Analysis Method : C:\Users\CHEMISTRY\Desktop\CHRISTINE\VANIHINGEDPHEN1.D\ACQ.M
    Last changed    : 6/18/2014 3:18:53 PM by Christine
    Additional Info : Peak(s) manually integrated
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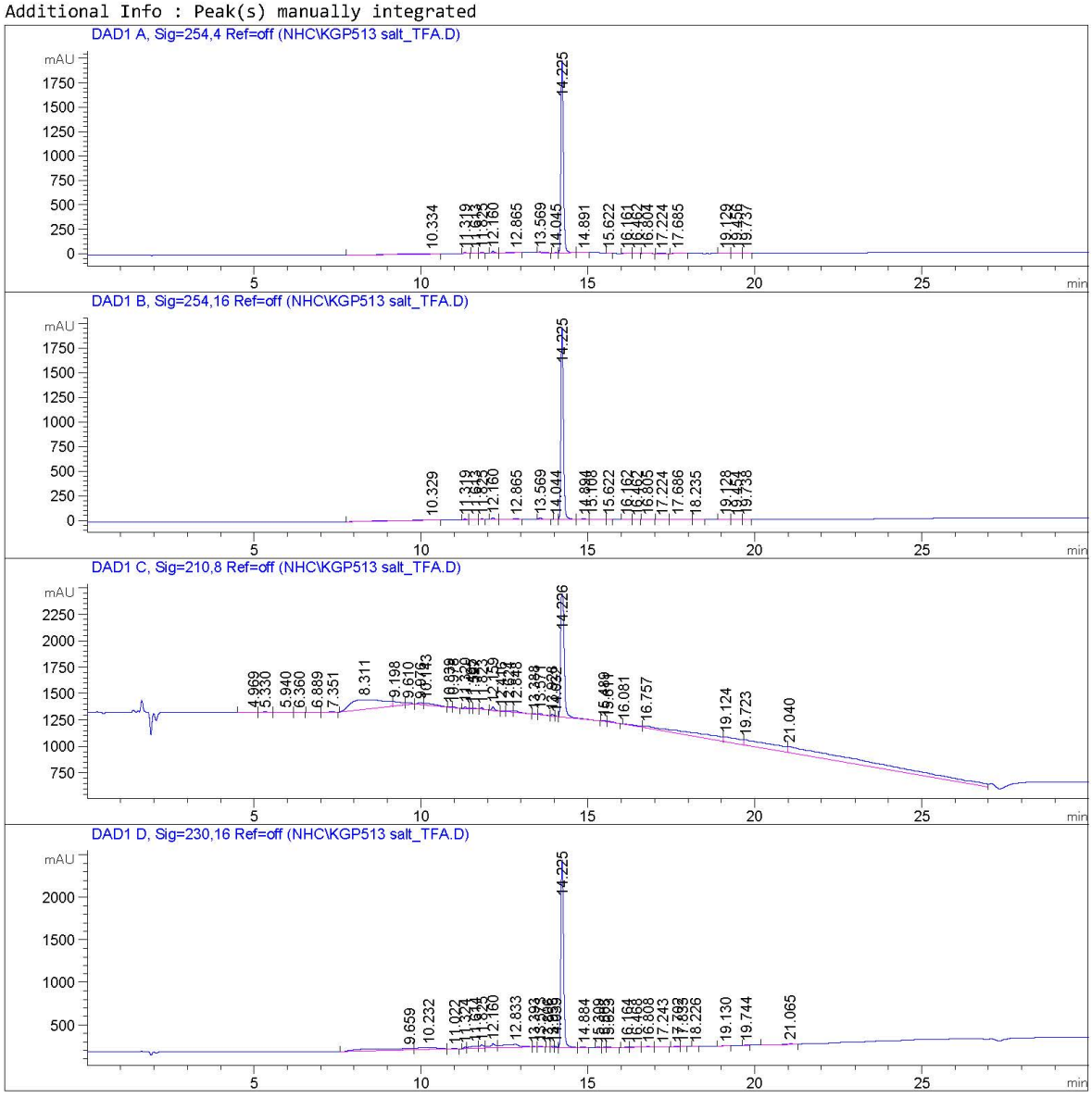
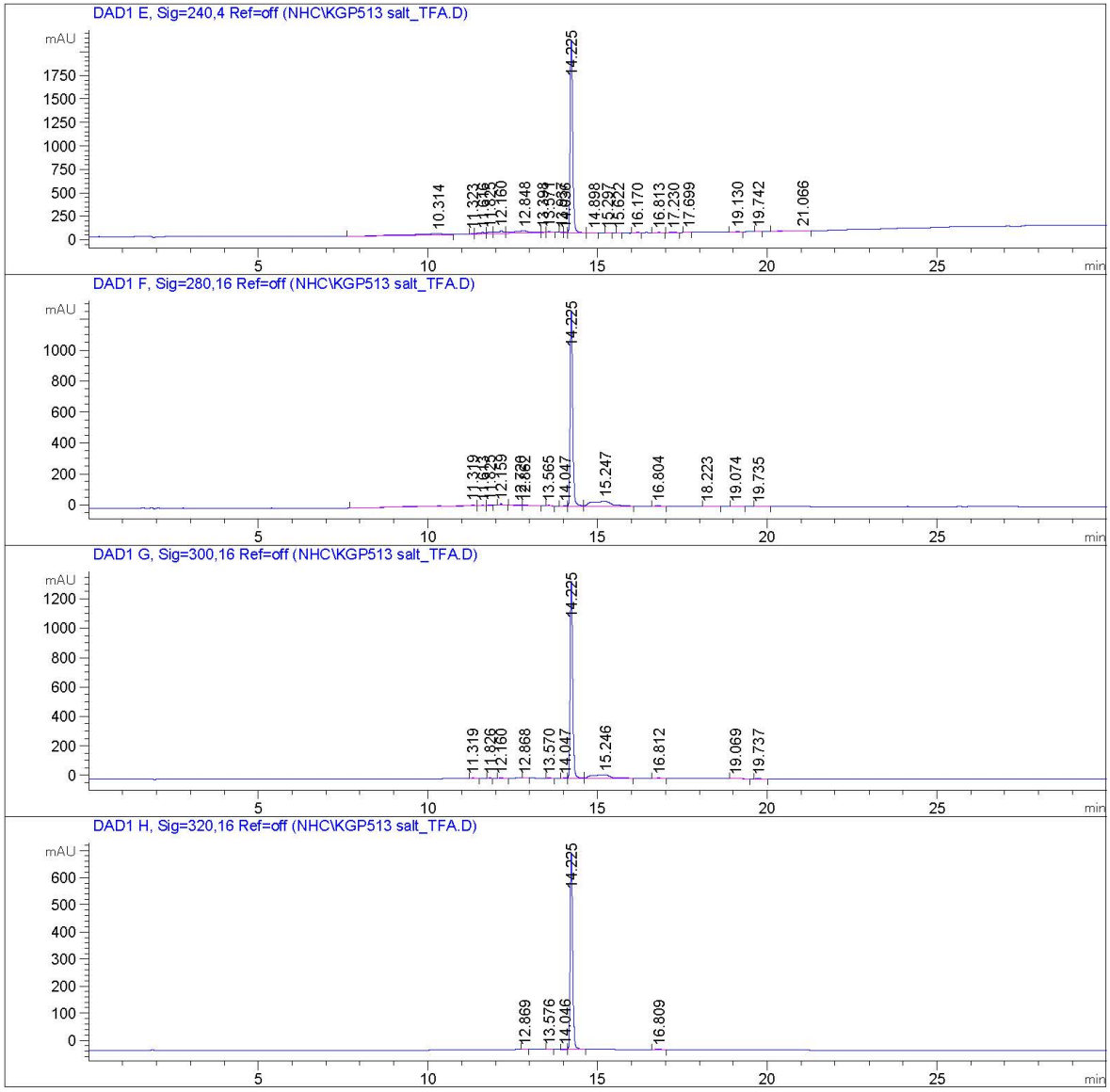


Data File C:\Chem32\1\Data\NHC\KGP513 salt_TFA.D
Sample Name: KGP513 salt_TFA



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Area Percent Report

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Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Data File C:\Chem32\1\Data\NHC\KGP513 salt_TFA.D
Sample Name: KGP513 salt_TFA

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.334	BV	1.0671	364.58389	4.11725	3.3269
2	11.319	BB	0.0710	45.74504	10.06239	0.4174
3	11.613	BV	0.0796	10.14485	1.92030	0.0926
4	11.825	VB	0.0692	41.18274	9.38475	0.3758
5	12.160	BV	0.0758	94.26627	19.02197	0.8602
6	12.865	VV	0.1586	66.90304	5.63251	0.6105
7	13.569	VB	0.0946	60.37288	9.44519	0.5509
8	14.045	BB	0.0768	13.17087	2.70600	0.1202
9	14.225	BV	0.0774	1.00198e4	1966.54004	91.4329
10	14.891	VB	0.1949	25.99766	1.77432	0.2372
11	15.622	BB	0.0753	12.42037	2.62129	0.1133
12	16.161	BB	0.1732	29.77633	2.91421	0.2717
13	16.462	BB	0.1034	8.09889	1.16108	0.0739
14	16.804	BB	0.1871	51.66618	4.59805	0.4715
15	17.224	BB	0.1824	19.26022	1.45491	0.1758
16	17.685	BB	0.2140	48.35583	3.09947	0.4413
17	19.129	BV	0.1471	19.89521	2.01628	0.1815
18	19.456	VV	0.1964	13.96277	1.14422	0.1274
19	19.737	VB	0.0987	13.02931	2.03628	0.1189
Totals :				1.09586e4	2051.65050	

Signal 2: DAD1 B, Sig=254,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.329	BB	1.0409	230.34048	2.66882	2.1198
2	11.319	BV	0.0739	47.52680	9.91320	0.4374
3	11.613	VV	0.1381	28.18924	2.73812	0.2594
4	11.825	VB	0.0718	42.28798	9.17143	0.3892
5	12.160	BV	0.0761	89.54153	17.98655	0.8240
6	12.865	VV	0.1690	74.79410	5.85496	0.6883
7	13.569	VV	0.0973	60.90246	9.19650	0.5605
8	14.044	VB	0.0770	14.26166	2.92002	0.1312
9	14.225	BB	0.0772	9885.65137	1947.65454	90.9765
10	14.894	BV	0.2143	63.55091	3.85523	0.5849
11	15.108	VB	0.2670	72.90054	3.61946	0.6709
12	15.622	BB	0.0747	11.40344	2.43370	0.1049
13	16.162	BB	0.1706	28.02155	2.75561	0.2579
14	16.462	BB	0.1050	8.63266	1.21278	0.0794
15	16.805	BB	0.1602	49.97883	4.47887	0.4599
16	17.224	BB	0.1812	19.59429	1.45408	0.1803
17	17.686	BV	0.2772	77.43287	3.65467	0.7126
18	18.235	VB	0.1801	14.42759	1.10688	0.1328
19	19.128	BV	0.1661	20.96198	2.07127	0.1929
20	19.454	VV	0.1706	13.06426	1.06877	0.1202
21	19.738	VB	0.0986	12.68909	1.98541	0.1168

Data File C:\Chem32\1\Data\NHC\KGP513 salt_TFA.D
Sample Name: KGP513 salt_TFA

Totals : 1.08662e4 2037.80087

Signal 3: DAD1 C, Sig=210,8 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.969	BV	0.2793	59.38541	2.77892	0.1432
2	5.330	VB	0.2216	73.94147	5.40461	0.1783
3	5.940	BV	0.2946	77.44138	3.81852	0.1868
4	6.360	VB	0.1848	22.55084	2.07509	0.0544
5	6.889	BV	0.2459	25.50157	1.30544	0.0615
6	7.351	VB	0.2053	36.07074	2.11196	0.0870
7	8.311	BV	0.8612	6154.67822	90.52409	14.8431
8	9.198	VV	0.2354	728.63788	40.99575	1.7572
9	9.610	VB	0.1724	253.50475	22.68634	0.6114
10	9.976	BV	0.1725	154.76651	13.42912	0.3732
11	10.143	VB	0.3489	449.89648	17.21574	1.0850
12	10.839	BV	0.1358	15.42967	1.58139	0.0372
13	10.978	VB	0.1482	50.63254	5.45940	0.1221
14	11.320	BV	0.0880	117.40595	19.57756	0.2831
15	11.495	VV	0.0768	36.16812	6.72010	0.0872
16	11.597	VB	0.0959	55.25023	8.27662	0.1332
17	11.823	BB	0.0796	88.95613	16.85888	0.2145
18	12.159	BV	0.0827	197.35747	35.61134	0.4760
19	12.416	VV	0.1276	39.75274	4.31197	0.0959
20	12.624	VV	0.1494	115.20856	10.38821	0.2778
21	12.848	VB	0.1537	188.60291	16.97095	0.4548
22	13.388	BV	0.0882	20.61618	3.52447	0.0497
23	13.571	VV	0.1081	110.04835	14.90671	0.2654
24	13.928	VV	0.0845	86.32745	15.60852	0.2082
25	14.032	VB	0.0662	31.06448	7.51463	0.0749
26	14.226	BB	0.1227	8867.73535	1166.39758	21.3861
27	15.489	BV	0.1075	44.92231	5.85696	0.1083
28	15.611	VB	0.1514	93.04314	8.26133	0.2244
29	16.081	BV	1.1458	184.40137	1.94552	0.4447
30	16.757	VV	2.4707	3879.17554	18.72643	9.3553
31	19.124	VV	0.4358	1657.07690	47.40188	3.9963
32	19.723	VV	0.9256	3799.64600	49.16460	9.1635
33	21.040	VV	2.8908	1.37497e4	55.95520	33.1599

Totals : 4.14649e4 1723.36583

Signal 4: DAD1 D, Sig=230,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.659	BV	1.5060	2057.79663	16.39898	11.2808
2	10.232	VB	0.4943	703.14252	17.29416	3.8546
3	11.022	BB	0.1598	13.03095	1.26887	0.0714
4	11.324	BV	0.0732	83.00867	16.91838	0.4551
5	11.614	VV	0.2130	393.77121	23.55556	2.1586

Data File C:\Chem32\1\Data\NHC\KGP513 salt_TFA.D
Sample Name: KGP513 salt_TFA

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
6	11.825	VV	0.1270	313.02353	33.51480	1.7160
7	12.160	VV	0.1766	651.90656	47.94473	3.5737
8	12.833	VB	0.4290	1204.33240	34.86694	6.6021
9	13.393	BV	0.0739	11.92508	2.58247	0.0654
10	13.573	VB	0.0887	56.84451	9.94573	0.3116
11	13.806	BV	0.0805	7.49349	1.44436	0.0411
12	13.936	VV	0.0877	46.04342	7.93402	0.2524
13	14.039	VB	0.0736	34.71891	7.28065	0.1903
14	14.225	BV	0.0867	1.22107e4	2201.18823	66.9388
15	14.884	VB	0.1742	18.08795	1.38621	0.0992
16	15.309	VV	0.1084	17.79687	2.40447	0.0976
17	15.503	VV	0.0942	18.77873	2.87648	0.1029
18	15.623	VB	0.1184	47.98247	5.69091	0.2630
19	16.164	BV	0.1546	31.26108	3.12757	0.1714
20	16.468	VB	0.2036	38.26526	2.40524	0.2098
21	16.808	BB	0.1507	65.37402	6.21731	0.3584
22	17.243	BB	0.2068	27.19472	1.69829	0.1491
23	17.702	BV	0.1366	28.63807	3.13377	0.1570
24	17.833	VB	0.1331	18.45650	2.01017	0.1012
25	18.226	BB	0.1032	6.52072	1.01138	0.0357
26	19.130	BB	0.1707	34.35279	3.26504	0.1883
27	19.744	BB	0.0907	15.74038	2.67236	0.0863
28	21.065	BB	0.2250	85.39493	4.90846	0.4681
Totals :				1.82416e4	2464.94556	

Signal 5: DAD1 E, Sig=240,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.314	BV	1.2834	1184.28394	11.05896	8.5940
2	11.323	BV	0.0734	55.45825	11.27322	0.4024
3	11.616	VV	0.2074	233.17108	14.36506	1.6921
4	11.825	VV	0.1262	198.36234	21.38090	1.4395
5	12.160	VV	0.1700	396.89346	30.46765	2.8801
6	12.848	VV	0.4686	853.10999	22.38571	6.1908
7	13.398	VV	0.1161	42.44704	5.26197	0.3080
8	13.571	VB	0.1033	68.13227	9.77712	0.4944
9	13.937	VV	0.0896	36.33102	6.08865	0.2636
10	14.036	VB	0.0705	23.63801	5.25450	0.1715
11	14.225	BB	0.0774	1.04506e4	2054.12817	75.8368
12	14.898	BB	0.1661	16.06753	1.30054	0.1166
13	15.297	BB	0.0937	6.60305	1.10592	0.0479
14	15.622	BV	0.0716	7.47353	1.68928	0.0542
15	16.170	BB	0.1577	22.95993	2.44143	0.1666
16	16.813	BB	0.1367	28.20684	2.97366	0.2047
17	17.230	BB	0.1888	30.37091	2.12414	0.2204
18	17.699	BB	0.1197	10.61716	1.35069	0.0770
19	19.130	BB	0.1738	26.68450	2.51552	0.1936
20	19.742	BB	0.0926	11.41683	1.88684	0.0828
21	21.066	BB	0.2772	77.54187	3.54540	0.5627

Data File C:\Chem32\1\Data\NHC\KGP513 salt_TFA.D
Sample Name: KGP513 salt_TFA

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
Totals :				1.37803e4	2212.37535	

Signal 6: DAD1 F, Sig=280,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.319	BV	0.8534	452.68979	6.32186	5.4969
2	11.613	VV	0.1253	16.51236	1.79485	0.2005
3	11.825	VV	0.0742	29.01138	6.02226	0.3523
4	12.159	BB	0.0751	53.81640	11.00502	0.6535
5	12.720	BV	0.1866	33.75927	2.33593	0.4099
6	12.862	VV	0.1300	34.69127	3.68000	0.4212
7	13.565	BB	0.0883	19.86325	3.49492	0.2412
8	14.047	BV	0.0785	14.99003	2.99162	0.1820
9	14.225	VV	0.0762	6291.78174	1261.78394	76.4000
10	15.247	VB	0.5383	1210.39124	28.56665	14.6976
11	16.804	BB	0.1623	40.61341	3.52855	0.4932
12	18.223	BB	0.1576	12.82129	1.23054	0.1557
13	19.074	BB	0.1487	17.04829	1.79632	0.2070
14	19.735	BB	0.0967	7.32975	1.14508	0.0890
Totals :				8235.31946	1335.69753	

Signal 7: DAD1 G, Sig=300,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.319	BB	0.0757	10.59825	2.14446	0.1368
2	11.826	BV	0.0683	9.12248	2.11537	0.1178
3	12.160	BB	0.0759	17.84779	3.59445	0.2304
4	12.868	BB	0.0739	10.27431	2.22548	0.1326
5	13.570	BV	0.0966	13.73831	2.14906	0.1773
6	14.047	BV	0.0889	24.15033	4.34292	0.3117
7	14.225	VV	0.0765	6716.51221	1339.15881	86.6968
8	15.246	VB	0.5408	902.18079	21.10354	11.6454
9	16.812	BB	0.1441	23.94751	2.32604	0.3091
10	19.069	BB	0.1415	11.56425	1.25546	0.1493
11	19.737	BB	0.0945	7.19147	1.15778	0.0928
Totals :				7747.12771	1381.57337	

Data File C:\Chem32\1\Data\NHC\KGP513 salt_TFA.D
Sample Name: KGP513 salt_TFA

Signal 8: DAD1 H, Sig=320,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.869	BB	0.0749	6.74006	1.43153	0.1842
2	13.576	BB	0.0840	10.08056	1.83758	0.2755
3	14.046	BV	0.0844	8.78677	1.69668	0.2402
4	14.225	VB	0.0760	3611.94531	726.27673	98.7219
5	16.809	BB	0.1528	21.15385	1.94576	0.5782
Totals :				3658.70655	733.18828	

*** End of Report ***

Inhibition of tubulin polymerization, percent inhibition of colchicine binding, and cytotoxicity of the benzosuberene and dihydronaphthalene analogues.

Compound	Inhibition of tubulin polymerization IC_{50} (μM) ± SD	% Inhibition of colchicine binding ± SD	GI_{50} (μM) SRB assay[a] ± SD		
			SK-OV-3	NCI-H460	DU-145
CA4	1.0[b]	84 ± 3 (1 μM), 98 ± 0.007 (5 μM)	0.00455	0.00223[c]	0.00327[c]
CA4P	>40[b]	ND	0.00119	0.00194[c]	0.00323[c]
KGP18	0.85 ± 0.02[d]	73 ± 5 (1 μM), 95 ± 0.5 (5 μM)	0.0000543[e]	0.0000418[e]	0.0000249[e]
KGP03	0.5[f]	90 ± 2 (1 μM), 98 ± 0.3 (5 μM)	0.0029[f]	0.0032[f]	0.00040[f]
Doxorubicin	ND	ND	0.0789±0.0551	0.123±0.066	0.134±0.0842
Paclitaxel	NR	NR	0.00134±0.000408	0.00176±0.000399	0.00147±0.000442
3	>20	ND	0.394±0.0134	0.173±0.167	0.0330±0.0146
6	1.2 ± 0.1	72 ± 2 (5 μM)	0.0314±0.0105	0.0476±0.0148	0.141±0.094
8	>20	ND	6.52±0.71	1.90±0.42	5.66±0.35
11	>20	ND	3.22±0.57	0.855±0.114	3.76±0.41
13	0.39 ± 0.06	88 ± 1 (5 μM)	0.0221±0.0011	0.0353±0.0095	0.0362±0.0111
14	4.9 ± 0.1	35 ± 5 (1 μM)	0.312±0.116	0.449±0.046	0.423±0.110
15	>20	0 (5 μM)	3.03±1.25	3.86±1.15	4.04±1.74
18	1.1 ± 0.1	62 ± 0.7 (5 μM)	0.0648±0.0088	0.434±0.122	0.860±0.267
19	0.37 ± 0.08	73 ± 0.6 (5 μM)	0.0384±0.0102	0.0605±0.0027	0.0252±0.00223
20	3.2 ± 0.08	61 ± 3 (5 μM)	0.0572±0.0110	0.0847±0.0087	0.0402±0.0155
27	1.0 ± 0.07	47 ± 1 (5 μM)	0.299±0.025	0.353±0.024	0.631±0.134
28	0.63 ± 0.03	76 ± 2 (5 μM)	0.0403±0.0028	0.0628±0.0013	ND
37	3.8 ± 0.5	28 ± 4 (5 μM)	0.263±0.019	0.432±0.169	0.439±0.220
49	>20	0.4 ± 0.6 (5 μM)	ND	0.334±0.004	1.20[g]
56	>20	0 (5 μM)	27.2±4.4	70.5±33.6	26.0±5.4
57	>20	0 (5 μM)	5.77±0.82	2.00±0.55	4.45±0.63
68	0.48 ± 0.08	68 ± 1 (0.5 μM), 95 ± 0.8 (5 μM)	0.00690±0.00215	0.0581±0.0206	0.0976±0.0352
69	16 ± 0.7	45 ± 2 (5 μM)	0.0153±0.0008	0.0291±0.0068	0.0239±0.0079

[a] Average of n ≥ 3 independent determinations (unless otherwise noted)
[b] Data from ref. 24[24] and ref.74[74]
[c] For additional data, see ref. 24[24]
[d] For additional data, see ref. 37[37]
[e] For additional data, see ref. 8[8]
[f] For additional data, see ref. 36[36] and ref. 75[75]

[g] Average of n = 2 independent determinations (of duplicates)
ND = Not Determined
NR = Not Relevant (paclitaxel enhances microtubule assembly)