

Structure Guided Design, Synthesis, and Biological Evaluation of Oxetane-Containing Indole Analogues

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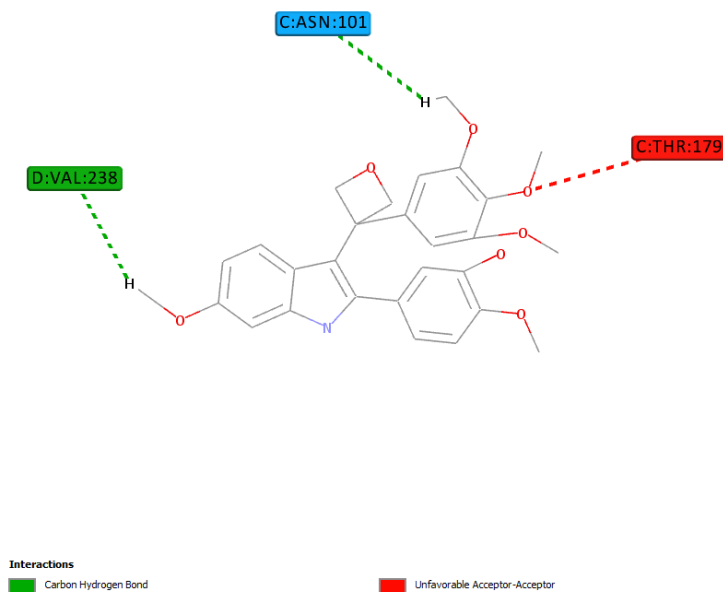
†Authors contributed equally

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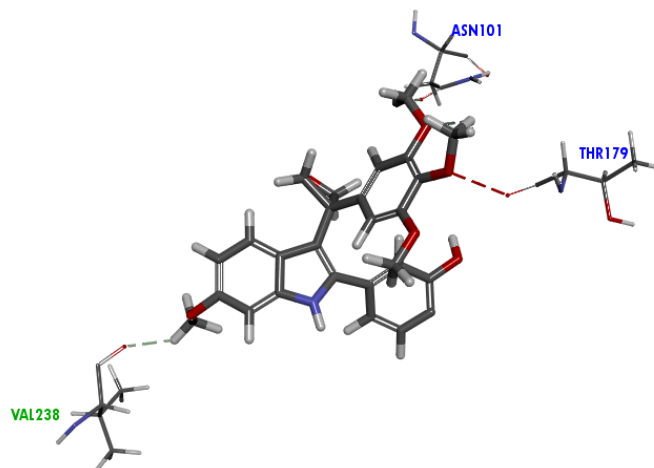
Molecular Docking SI	S3
¹H NMR, ¹³C NMR, HRMS of compound 3	S4–S6
¹H NMR, ¹³C NMR, HRMS, and HPLC for 5a	S7–S13
¹H NMR, ¹³C NMR, HRMS, and HPLC for 5b	S14–S21
¹H NMR, ¹³C NMR, HRMS, and HPLC for 5c	S22–S28
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¹H NMR, ¹³C NMR, HRMS, and HPLC for 5n	S95–S100
Table of Compound Purity by HPLC (wavelength 254 nm)	S101

2D and 3D Representations of Compound 5m Binding Interaction

Discovery Studio Client 4.5 (Accelrys), and X-ray structure of N-deacetyl-N-(2-mercaptoacetyl)-colchicine (DAMA-colchicine) co-crystallized with tubulin (1SA0) was used in docking procedure for Compound **5m**. 2D structure of **5m** in colchicine site of tubulin. Carbon-hydrogen bonding indicated in green dashed line, acceptor-acceptor clash indicated in red dashed line. Residues THR179 and ASN101 located on α -subunit, VAL238 located on β -subunit.

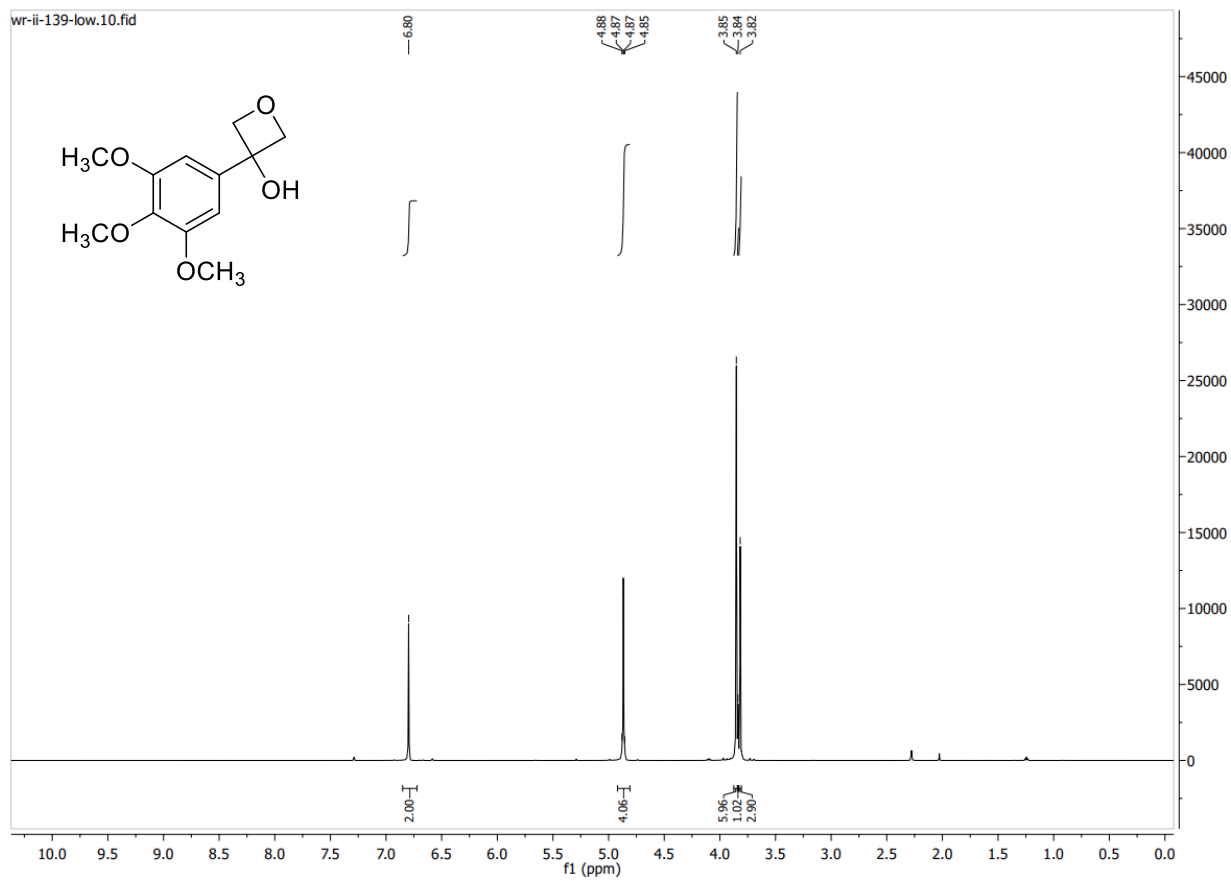


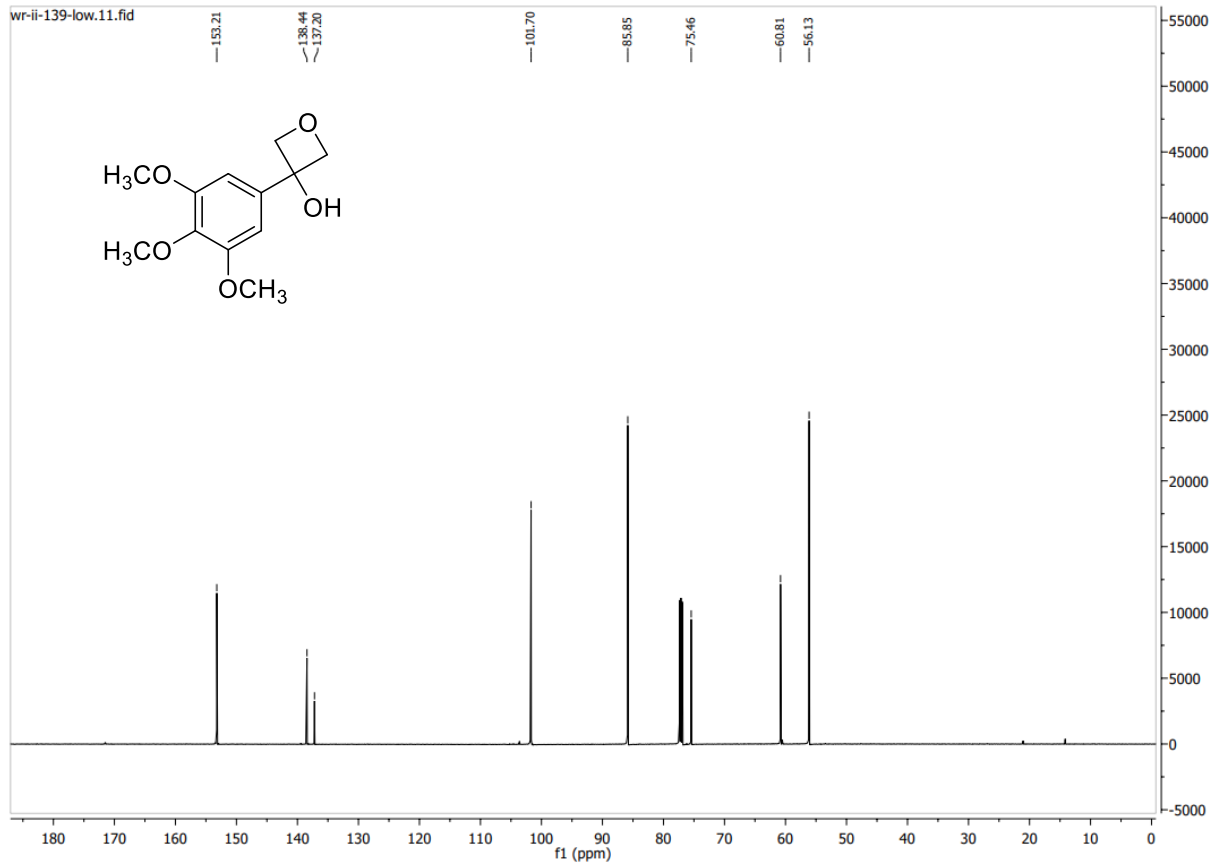
3D structure of compound **5m** within the colchicine site of tubulin indicated below. Residues on β -



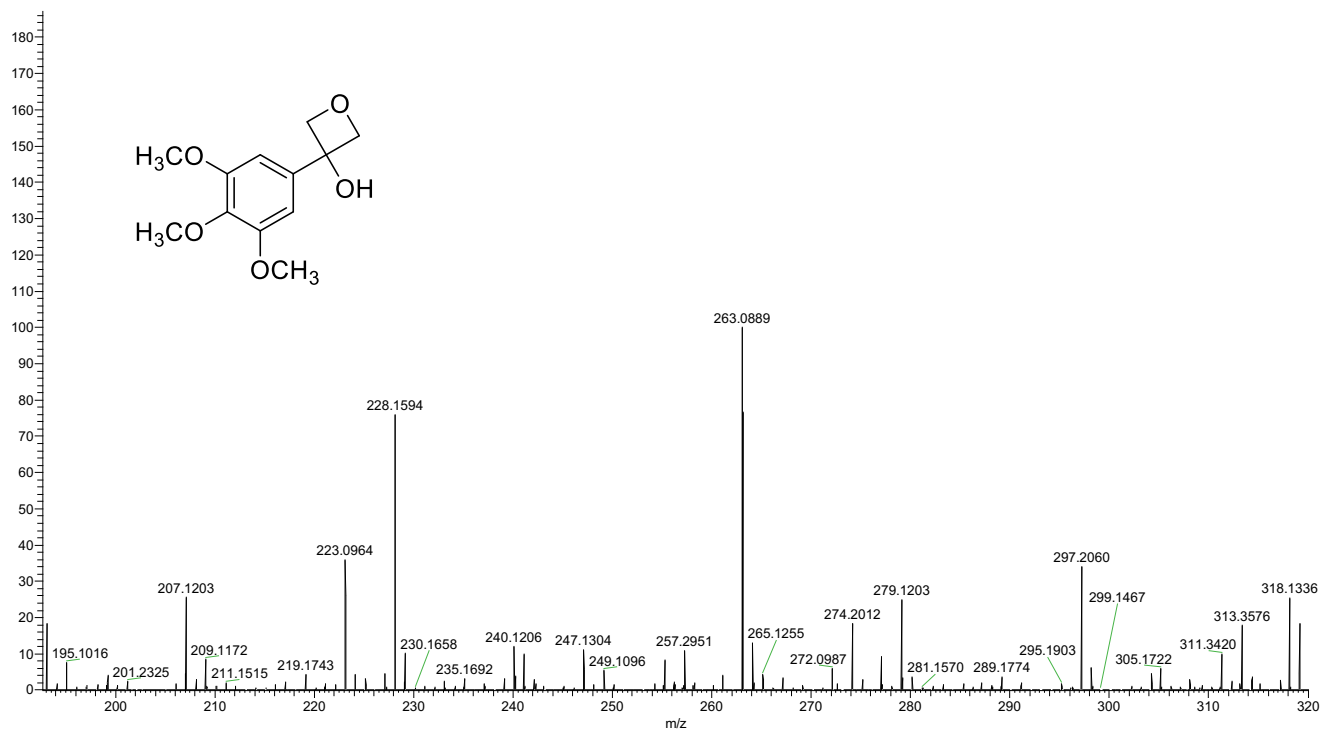
subunit indicated in green, α -subunit in blue. Interactions same as indicated above.

Compound 3

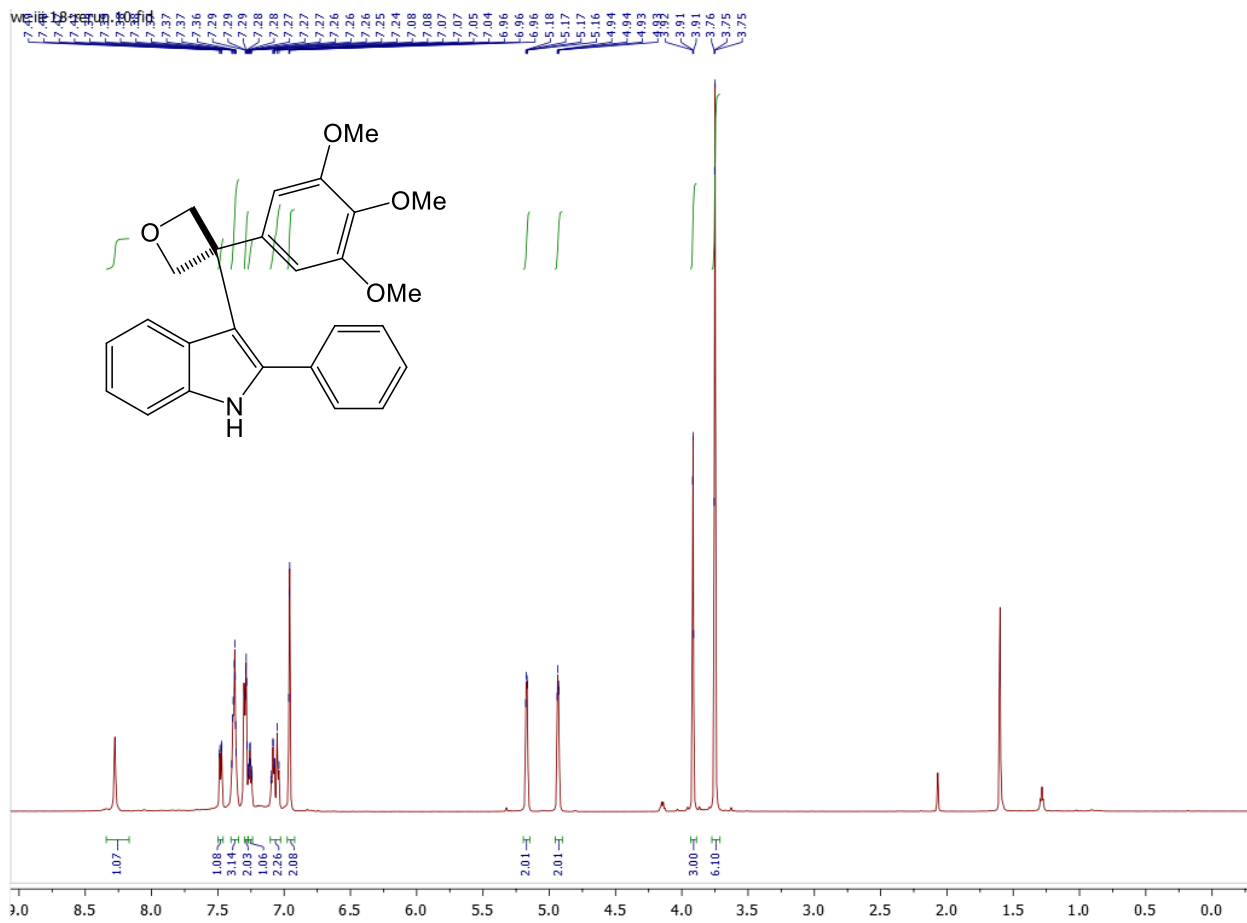




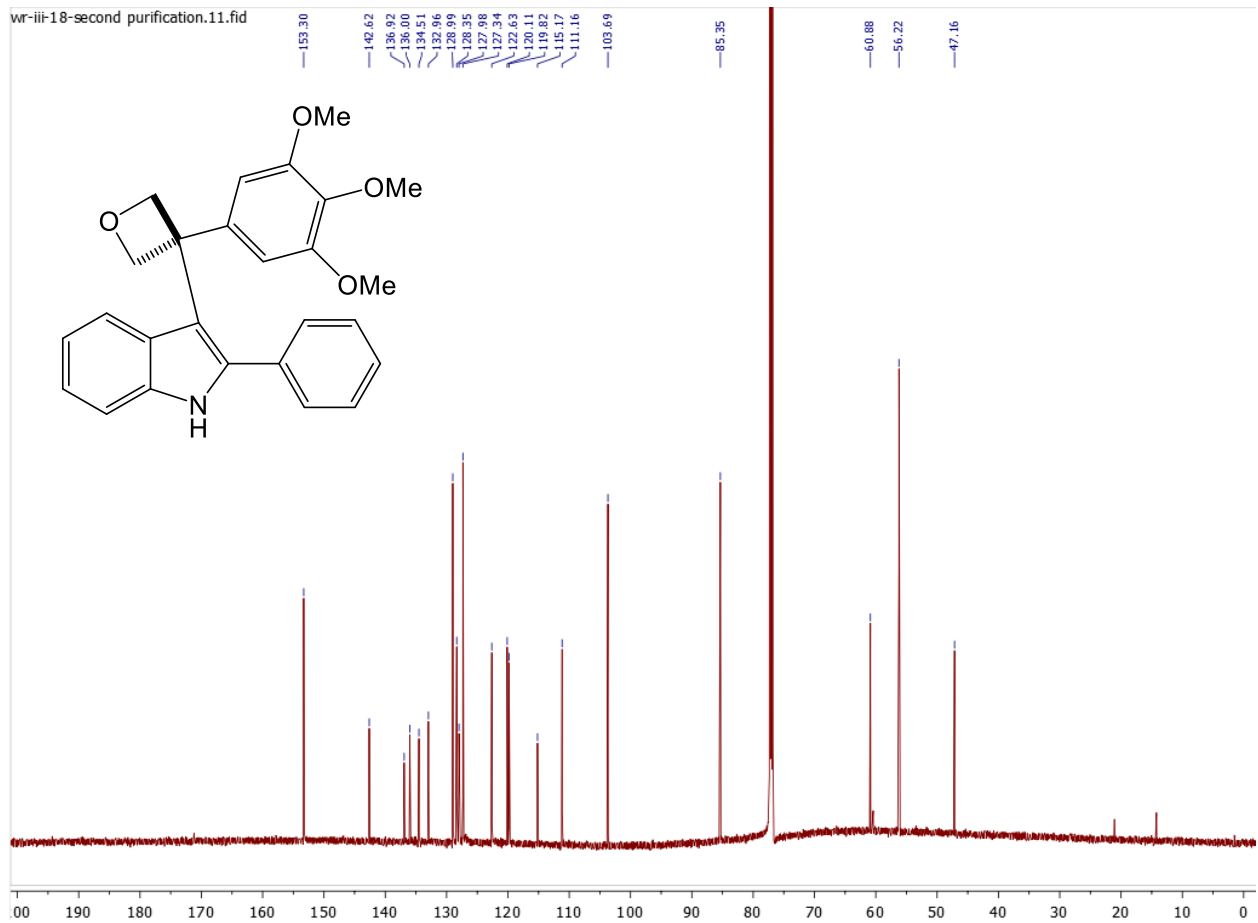
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T: FTMS + p ESI Full lock ms [50.0000-750.0000]



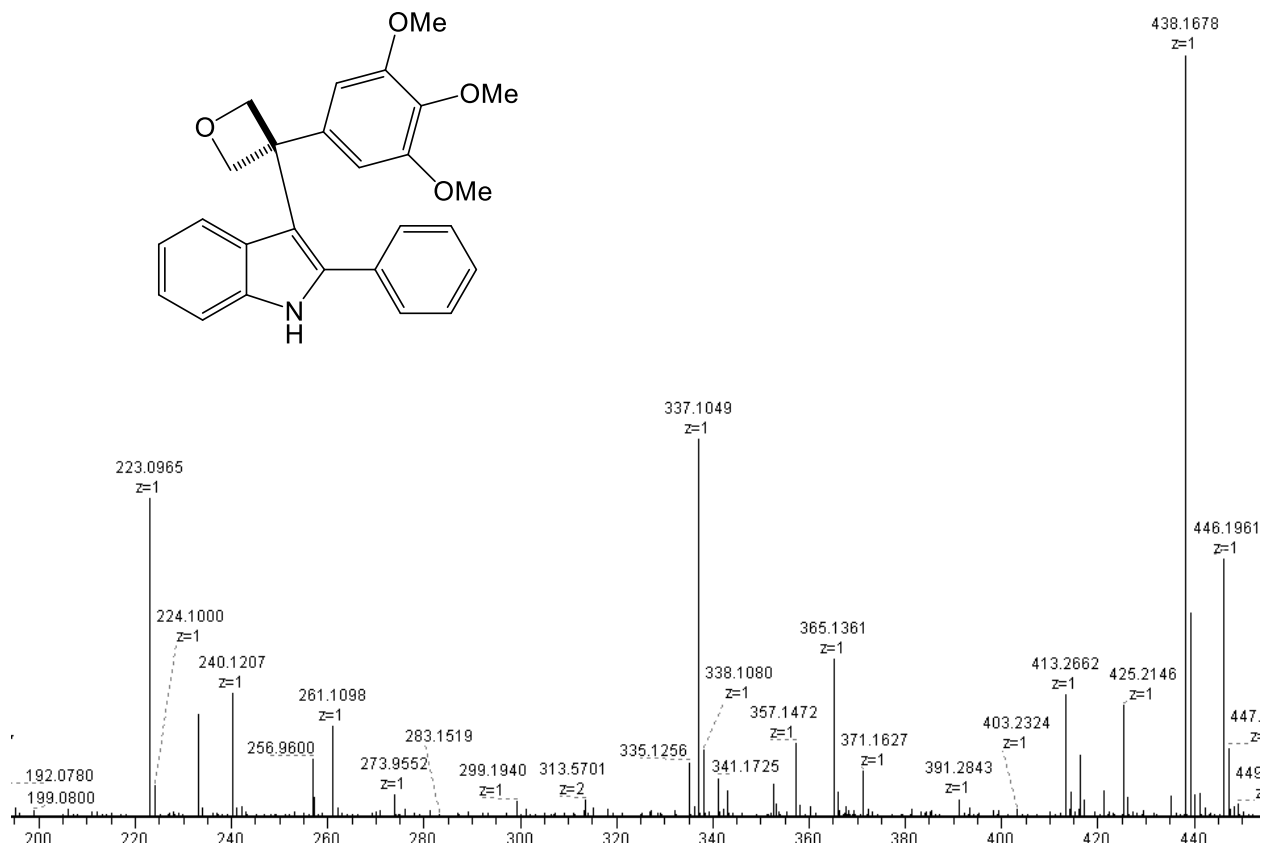
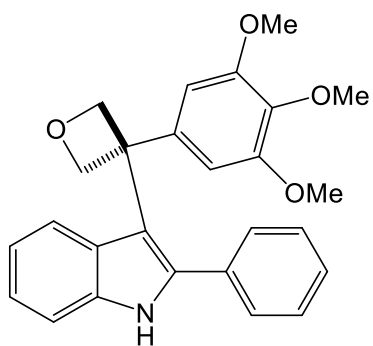
Compound 5a



wr-iii-18-second purification.11.fid

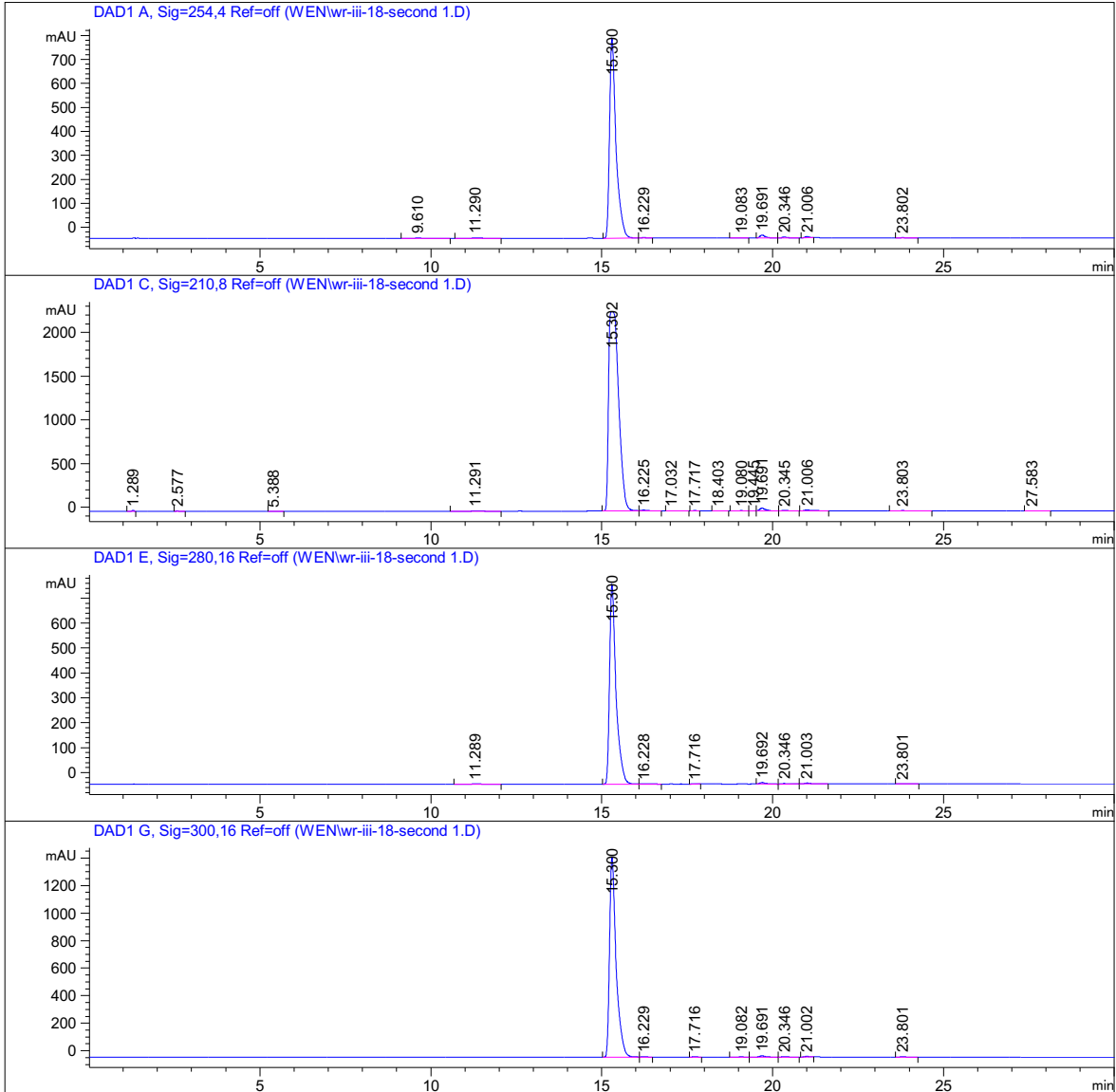


[105.00-1000.00]
V Stable=15min TmpDiff Lock(1/1, 0ppm)

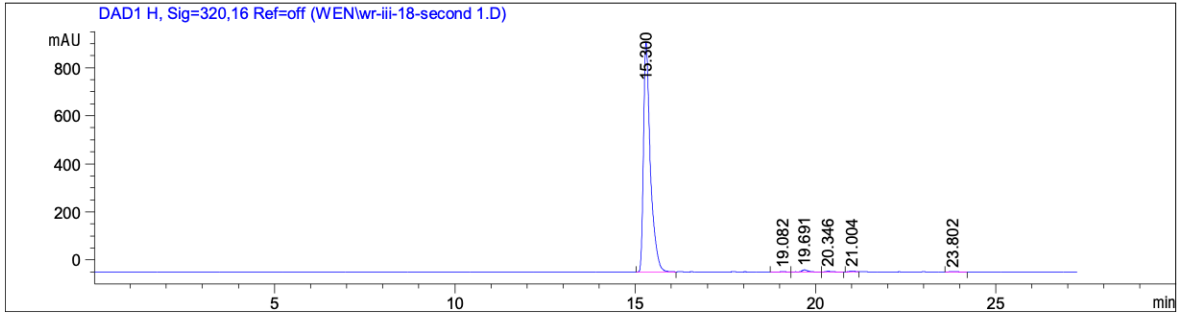


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Acq. Instrument : 1200 HPLC Location : 1
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Acq. Method : C:\Chem32\1\Methods\GRAD 2 30-90 ACN.M
Last changed : 4/2/2014 4:04:33 PM by ERICA P
Analysis Method : C:\Chem32\1\Methods\GRAD 2 50-90 ACN.M
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Data File C:\Chem32\1\Data\WEN\wr-iii-18-second 1.D
 Sample Name: wr-iii-18-second 1



=====
 Area Percent Report
 =====

Sorted By : Signal
 Multiplier : 1.0000
 Dilution : 1.0000
 Sample Amount : 1.00000 [ng/ul] (not used in calc.)
 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	9.610	BB	0.3935	50.88453	1.65124	0.4498
2	11.290	BB	0.3030	43.81142	1.85861	0.3873
3	15.300	BV	0.1931	1.09083e4	831.13947	96.4245
4	16.229	VB	0.1572	21.32360	2.05218	0.1885
5	19.083	BV	0.1971	15.88195	1.17960	0.1404
6	19.691	VB	0.1775	148.94395	12.45326	1.3166
7	20.346	BB	0.1776	51.86376	4.33408	0.4585
8	21.006	BB	0.1526	48.75811	4.96491	0.4310
9	23.802	BB	0.2009	23.02287	1.66884	0.2035

Totals : 1.13128e4 861.30219

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.289	BV	0.0627	47.49611	10.93599	0.0999
2	2.577	VB	0.0957	25.65813	3.95584	0.0540
3	5.388	BB	0.1421	16.62289	1.69929	0.0350
4	11.291	BB	0.2661	108.78239	5.37504	0.2289
5	15.302	BV	0.3167	4.63041e4	2282.54517	97.4413
6	16.225	VB	0.2117	149.55894	10.04549	0.3147
7	17.032	BB	0.1960	39.63947	2.89018	0.0834
8	17.717	BB	0.1274	26.63814	3.32658	0.0561
9	18.403	BB	0.1812	22.03388	1.87311	0.0464

Data File C:\Chem32\11\Data\WEN\wr-iii-18-second 1.D
 Sample Name: wr-iii-18-second 1

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
10	19.080	BB	0.1652	40.12218	3.68057	0.0844
11	19.445	BV	0.1084	11.72943	1.70139	0.0247
12	19.691	VB	0.1790	376.99915	31.18987	0.7933
13	20.345	BB	0.1738	75.69845	6.59981	0.1593
14	21.006	BB	0.2431	188.33199	10.92349	0.3963
15	23.803	BB	0.2811	66.29834	3.20865	0.1395
16	27.583	BB	0.2334	20.30258	1.23755	0.0427

Totals : 4.75200e4 2381.18801

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.289	BB	0.2404	42.65485	2.38809	0.3981
2	15.300	BV	0.1924	1.04607e4	800.96173	97.6407
3	16.228	VB	0.2064	28.73530	1.99055	0.2682
4	17.716	BB	0.1327	10.29597	1.21641	0.0961
5	19.692	BB	0.1735	66.74614	5.74819	0.6230
6	20.346	BV	0.1761	23.10314	1.98006	0.2156
7	21.003	VB	0.2364	63.97304	3.83996	0.5971
8	23.801	BB	0.1955	17.25001	1.29383	0.1610

Totals : 1.07134e4 819.41881

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.300	BV	0.1953	1.93009e4	1449.67871	98.6764
2	16.229	VB	0.1685	21.21124	1.89572	0.1084
3	17.716	BB	0.1372	17.33678	1.96051	0.0886
4	19.082	BB	0.1685	16.28374	1.43374	0.0833
5	19.691	BV	0.1768	106.77357	8.97469	0.5459
6	20.346	VB	0.1738	34.34324	2.95115	0.1756
7	21.002	BB	0.1570	39.90841	3.98044	0.2040
8	23.801	BB	0.1920	23.03045	1.76766	0.1177

Totals : 1.95598e4 1472.64262

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

Data File C:\Chem32\1\Data\WEN\wr-iii-18-second 1.D

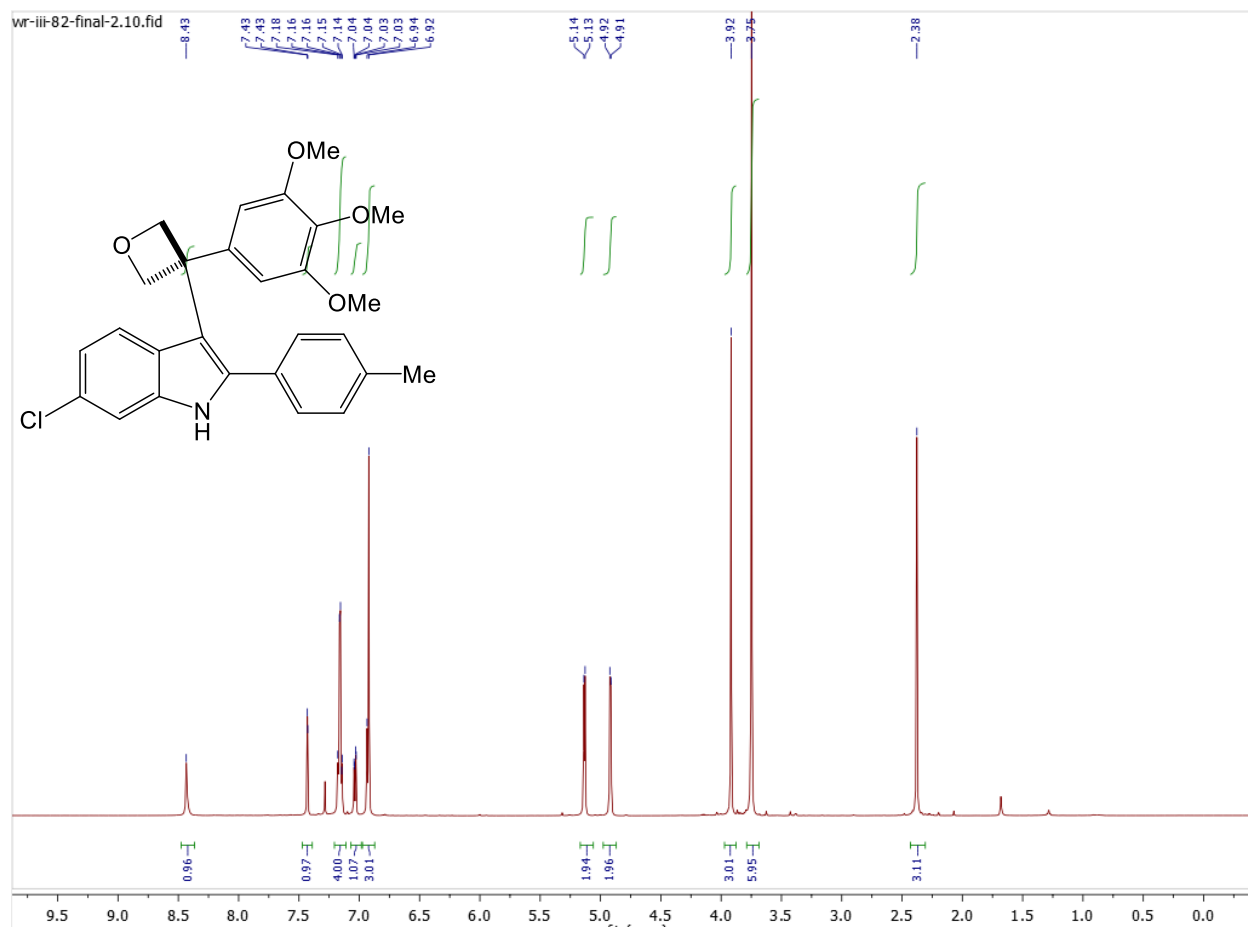
Sample Name: wr-iii-18-second 1

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.300	BB	0.1934	1.25478e4	954.53064	98.3924
2	19.082	BB	0.1754	12.47272	1.05871	0.0978
3	19.691	BB	0.1782	106.48537	8.86263	0.8350
4	20.346	BB	0.1740	33.53300	2.87756	0.2629
5	21.004	BB	0.1547	32.84745	3.34219	0.2576
6	23.802	BB	0.1934	19.67611	1.49605	0.1543

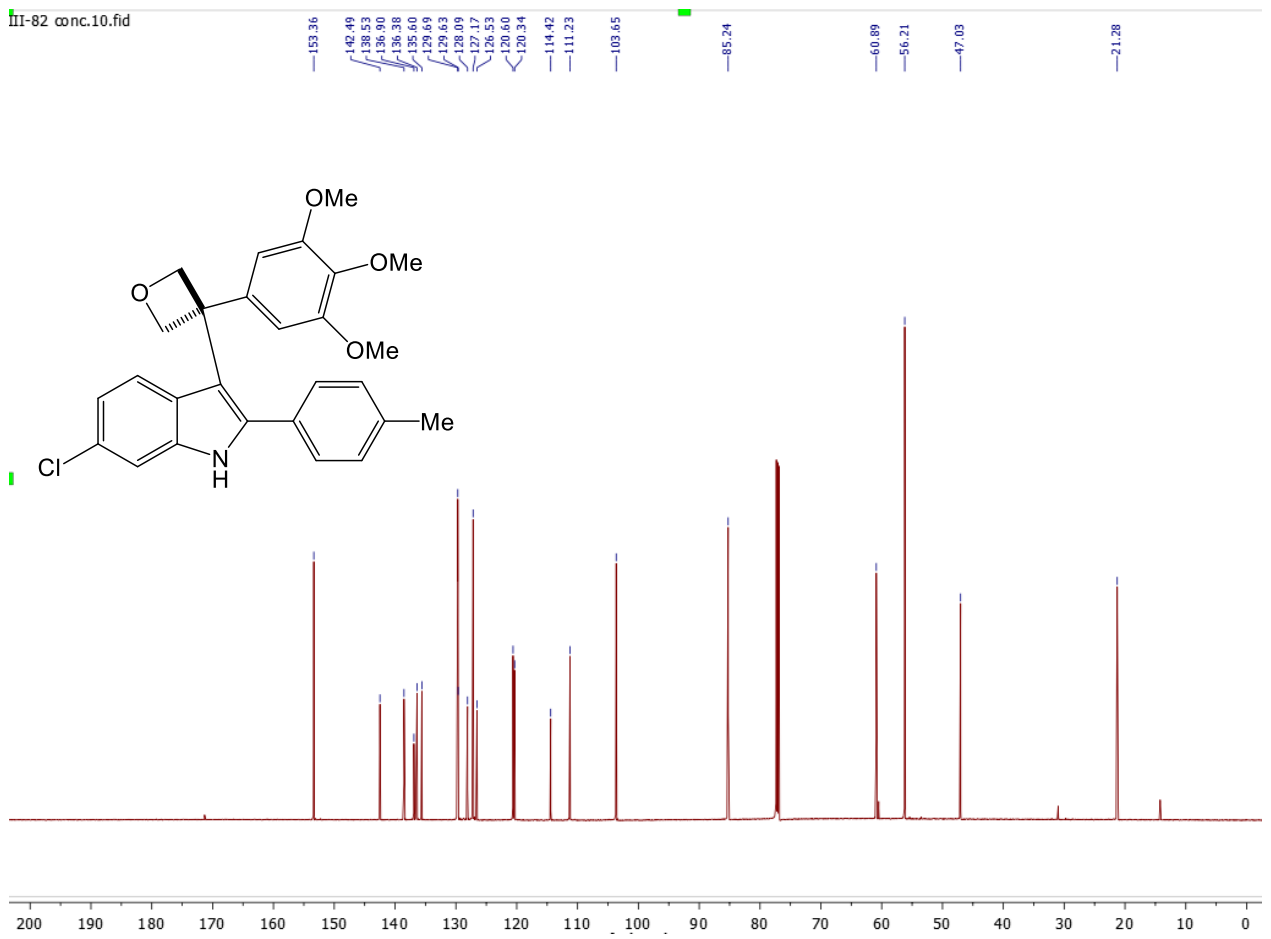
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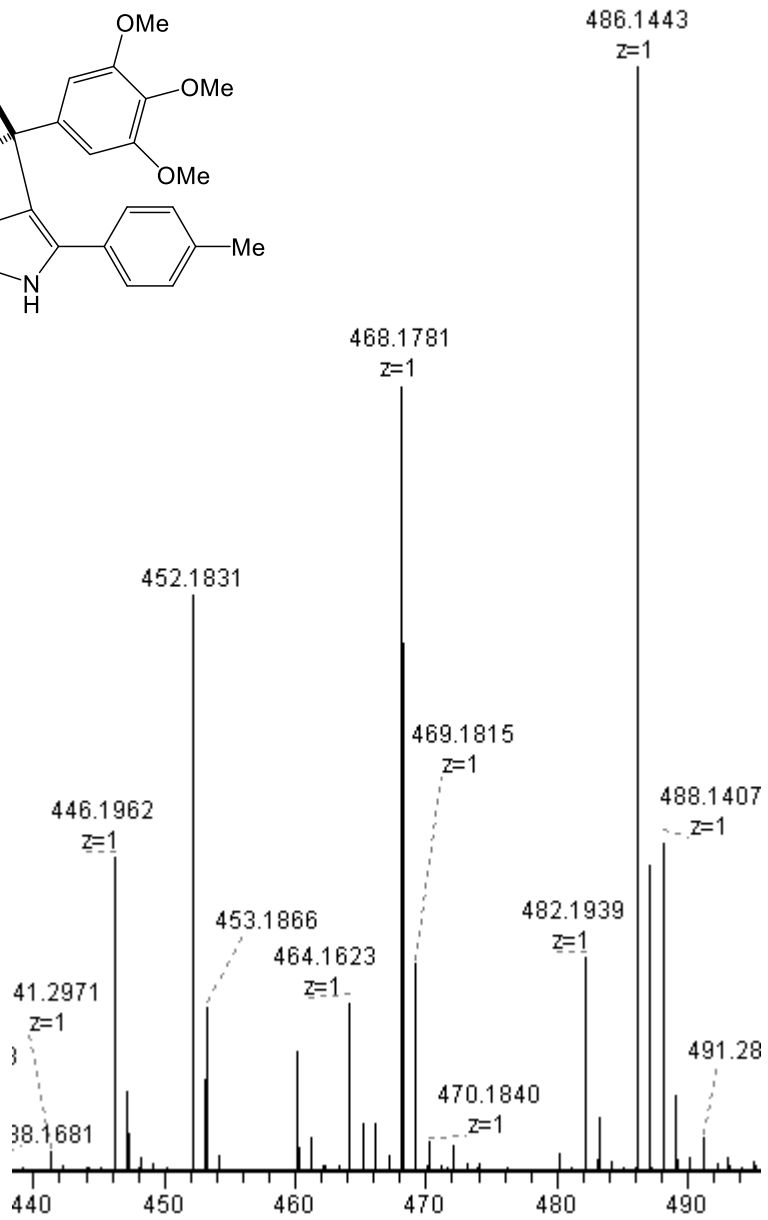
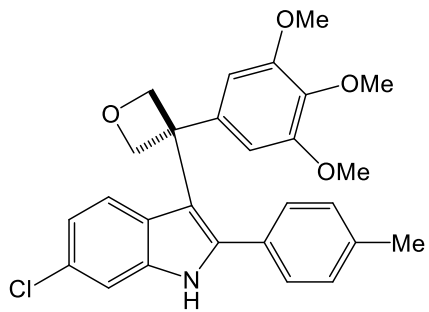
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Compound 5b



III-82 conc.10.fid

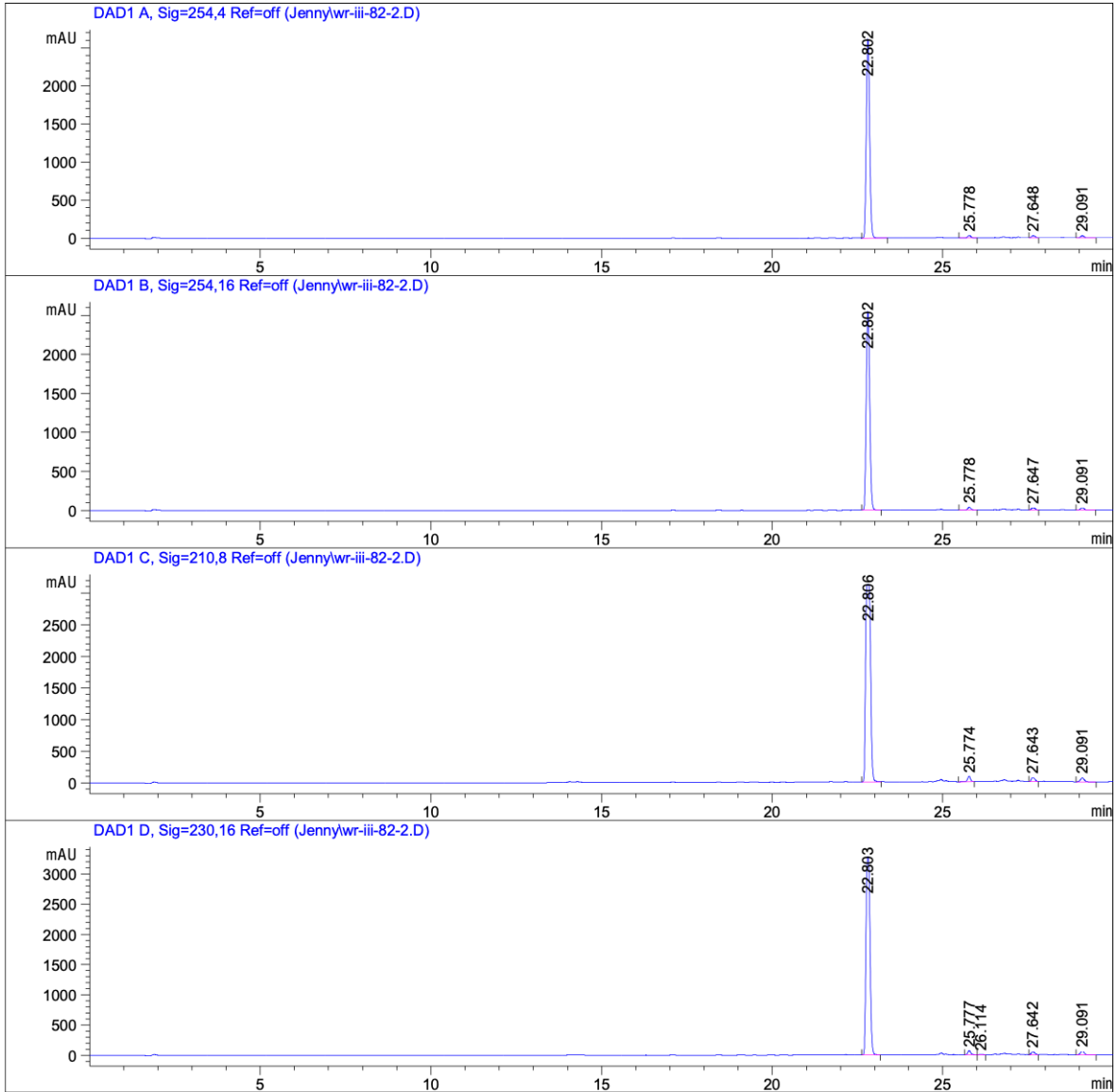




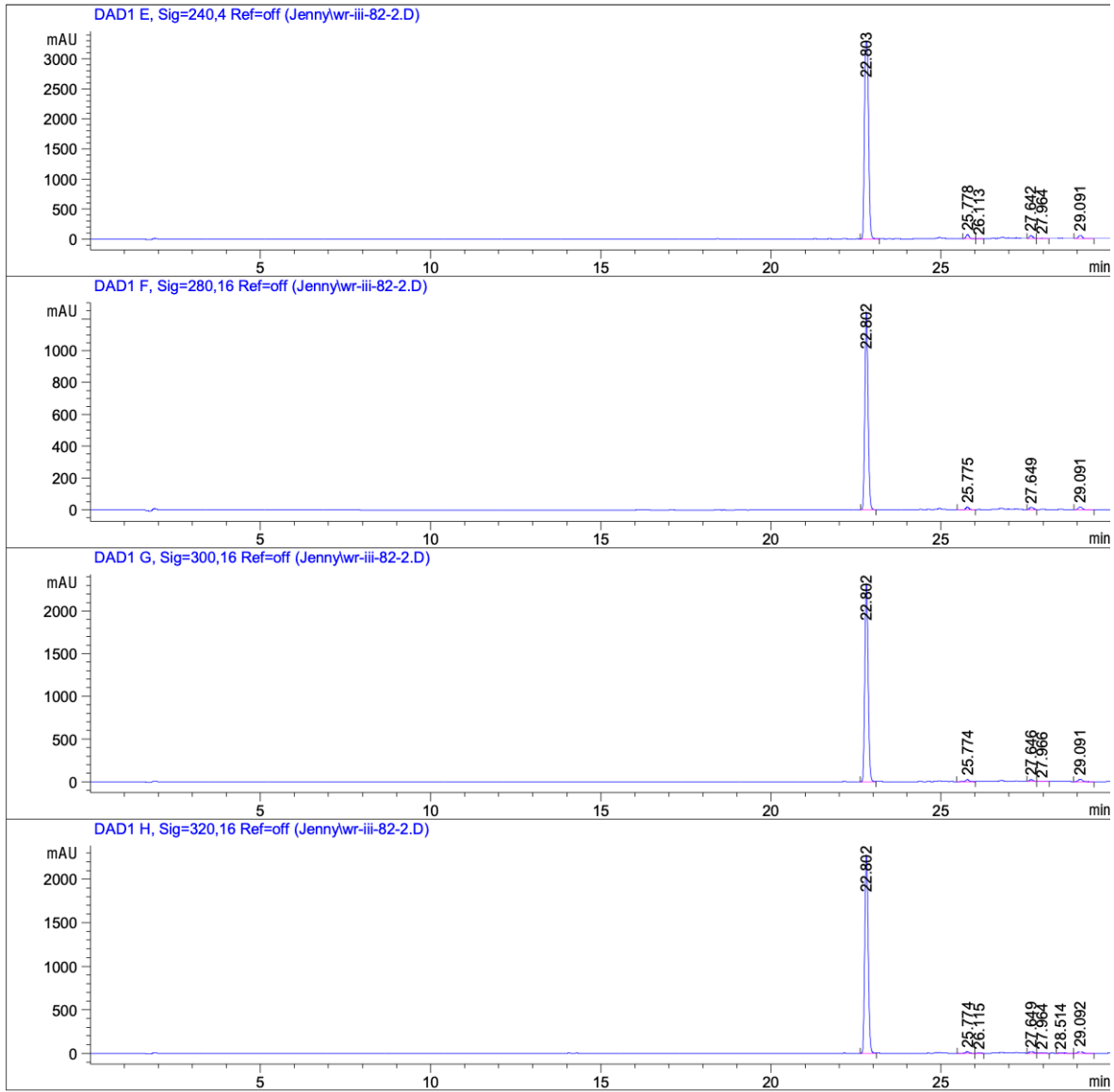
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Sample Name: wr-iii-82-2

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Sample Operator : SYSTEM
Acq. Instrument : 1200 HPLC Location : 1
Injection Date : 3/6/2023 10:43:59 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



Data File C:\Chem32\1\Data\Jenny\wr-iii-82-2.D
Sample Name: wr-iii-82-2



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Area Percent Report
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Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Sample Amount: : 1.00000 [ng/ul] (not used in calc.)
Use Multiplier & Dilution Factor with ISTDs

Data File C:\Chem32\1\Data\Jenny\wr-iii-82-2.D
Sample Name: wr-iii-82-2

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	22.802	BB	0.1059	1.74398e4	2611.20264	96.3533
2	25.778	BV	0.1006	222.11363	33.83608	1.2272
3	27.648	BV	0.1239	217.25757	28.84854	1.2003
4	29.091	BB	0.1156	220.68309	29.40542	1.2193

Totals : 1.80999e4 2703.29268

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	22.802	BV	0.1116	1.78087e4	2546.18042	96.1686
2	25.778	BV	0.1002	241.12387	36.91934	1.3021
3	27.647	BV	0.1228	229.19749	30.81300	1.2377
4	29.091	BB	0.1154	239.18097	31.91086	1.2916

Totals : 1.85182e4 2645.82362

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	22.806	BV	0.1606	3.07292e4	3128.47729	95.5157
2	25.774	BV	0.0916	523.00793	87.62906	1.6257
3	27.643	BB	0.1166	455.57166	65.96323	1.4161
4	29.091	BB	0.1155	464.11362	61.87204	1.4426

Totals : 3.21719e4 3343.94163

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	22.803	BV	0.1291	2.62145e4	3283.87793	95.3522
2	25.777	VV	0.0941	426.34061	68.97872	1.5508
3	26.114	VB	0.1089	33.17459	4.45482	0.1207
4	27.642	BB	0.1132	336.02618	49.52521	1.2223
5	29.091	BB	0.1150	482.23447	64.63055	1.7541

Totals : 2.74923e4 3471.46724

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	22.803	BV	0.1295	2.64089e4	3295.79419	95.0437
2	25.778	VV	0.0959	460.40836	72.64408	1.6570
3	26.113	VB	0.1052	32.45143	4.44567	0.1168
4	27.642	BV	0.1123	361.85648	52.56580	1.3023
5	27.964	VB	0.1360	47.60092	4.86992	0.1713
6	29.091	VB	0.1150	474.85211	63.64465	1.7090

Totals : 2.77860e4 3493.96431

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	22.802	BV	0.0973	7791.44824	1239.91174	95.6818
2	25.775	BV	0.0950	102.90936	16.45016	1.2638
3	27.649	BV	0.1250	109.79018	14.38403	1.3483
4	29.091	BB	0.1160	138.93817	18.41994	1.7062

Totals : 8143.08596 1289.16588

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	22.802	BV	0.1022	1.51269e4	2316.49438	96.4544
2	25.774	BV	0.0930	145.56303	23.90901	0.9282
3	27.646	BV	0.1224	168.88388	22.81687	1.0769
4	27.966	VV	0.1415	21.33482	2.04874	0.1360
5	29.091	BB	0.1155	220.27505	29.36234	1.4046

Totals : 1.56830e4 2394.63135

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	22.802	BV	0.1066	1.53179e4	2274.95142	96.7437
2	25.774	BB	0.0952	111.76621	17.80715	0.7059
3	26.115	BB	0.0960	14.98379	2.29961	0.0946
4	27.649	BV	0.1243	158.13374	20.88873	0.9987
5	27.964	VV	0.1515	20.69553	1.83599	0.1307
6	28.514	BB	0.1464	23.99650	2.32529	0.1516

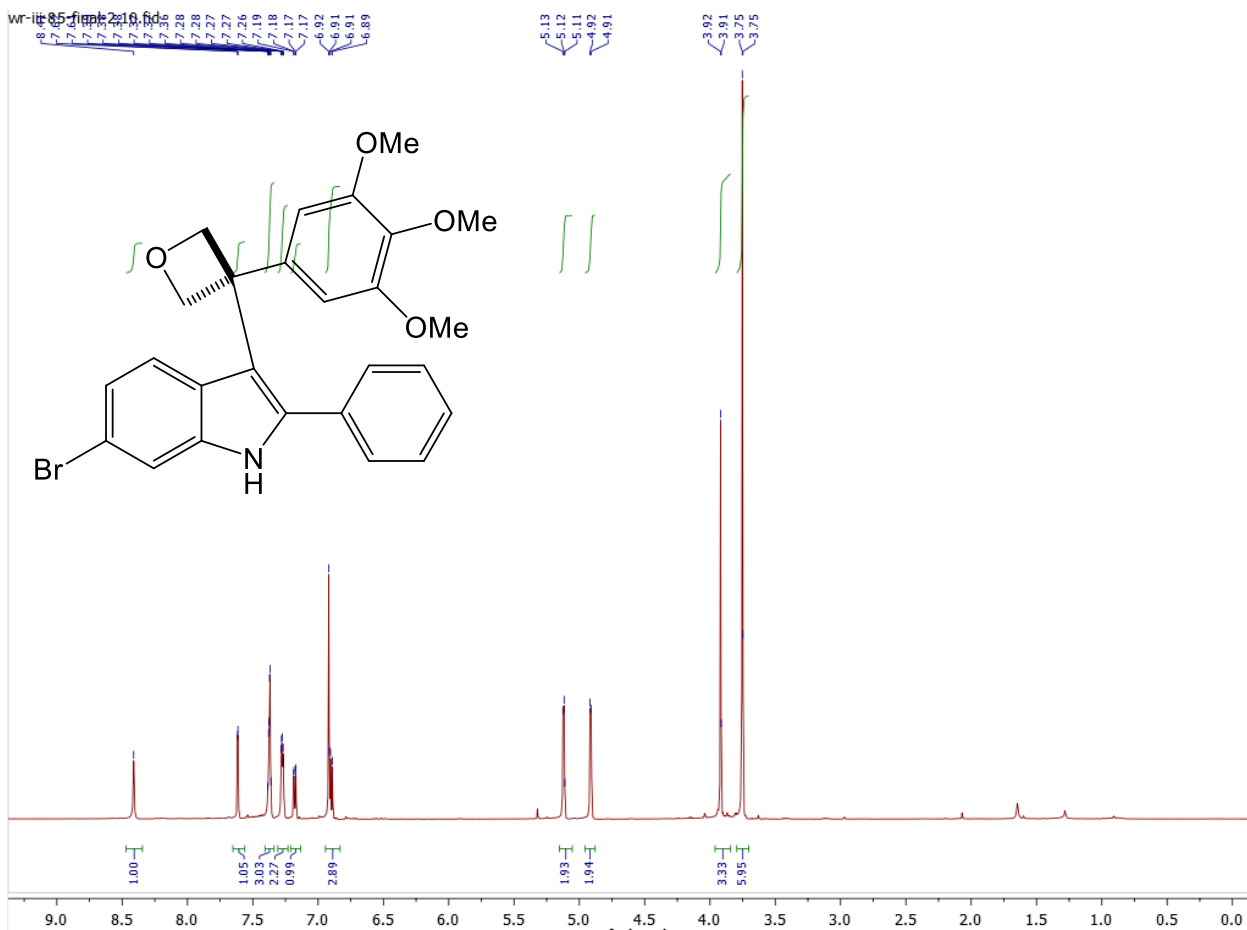
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Sample Name: wr-iii-82-2

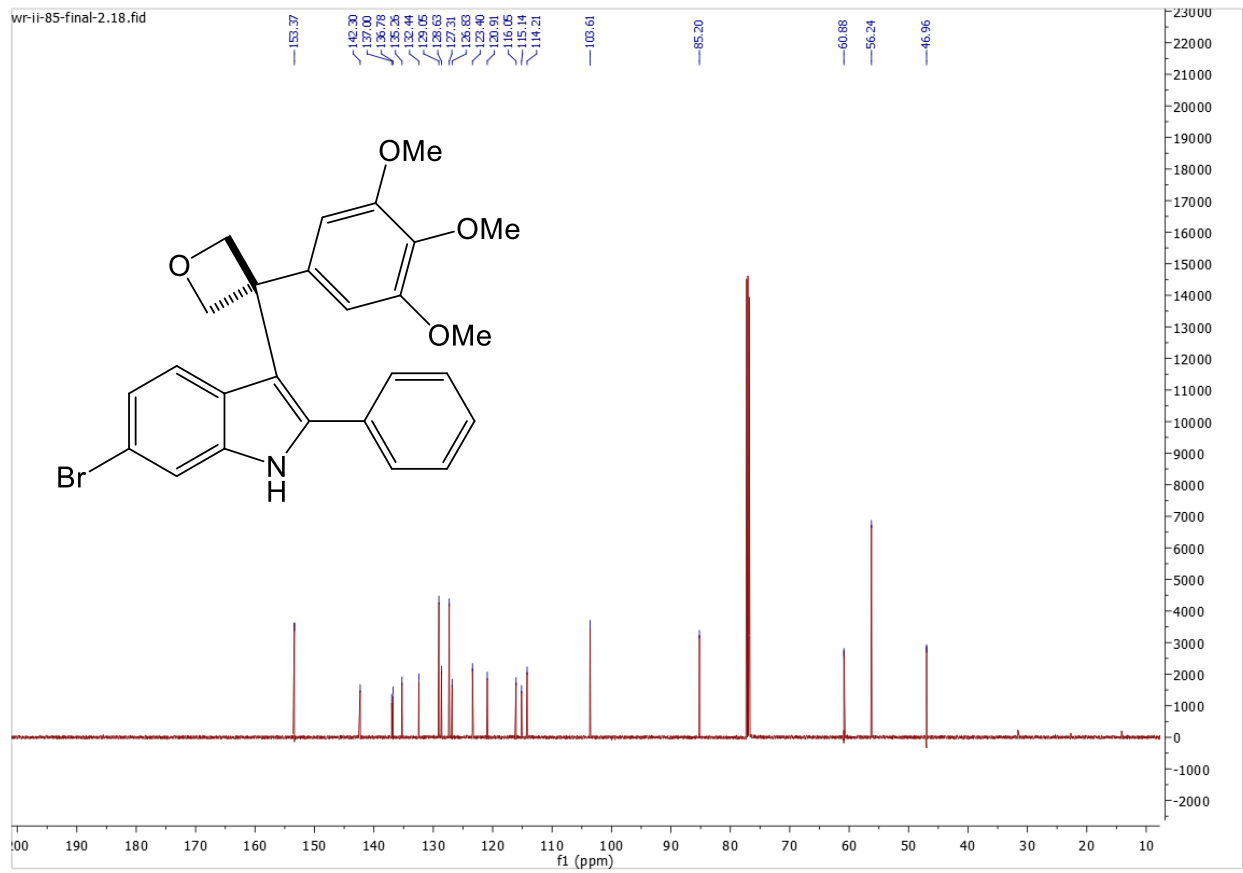
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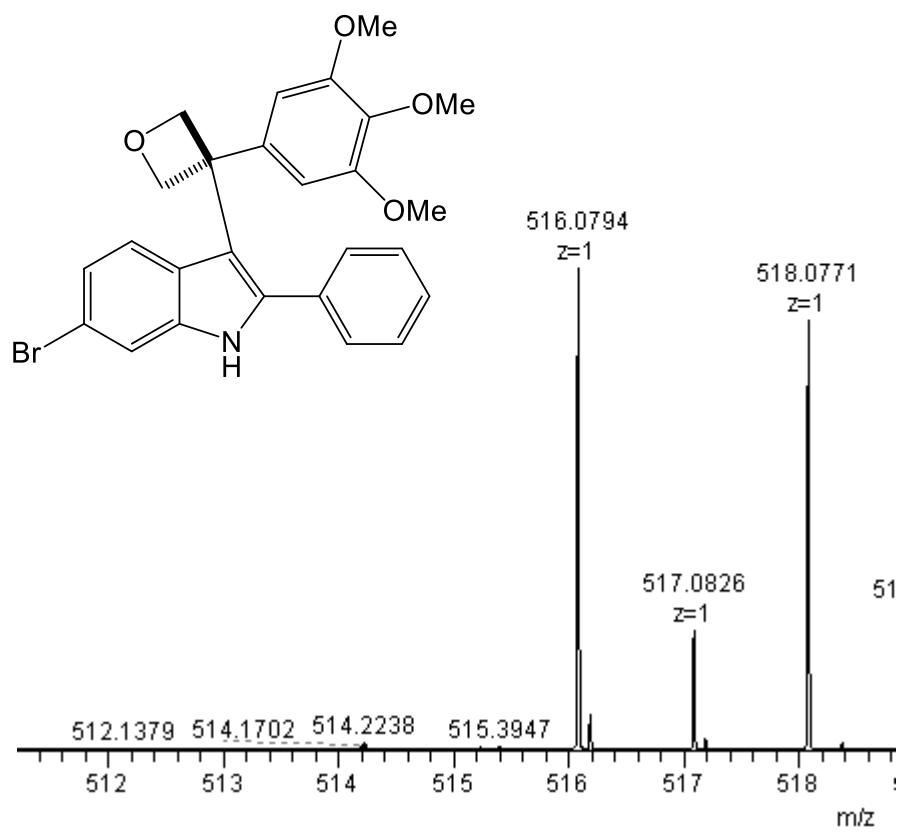
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*** End of Report ***

Compound 5c





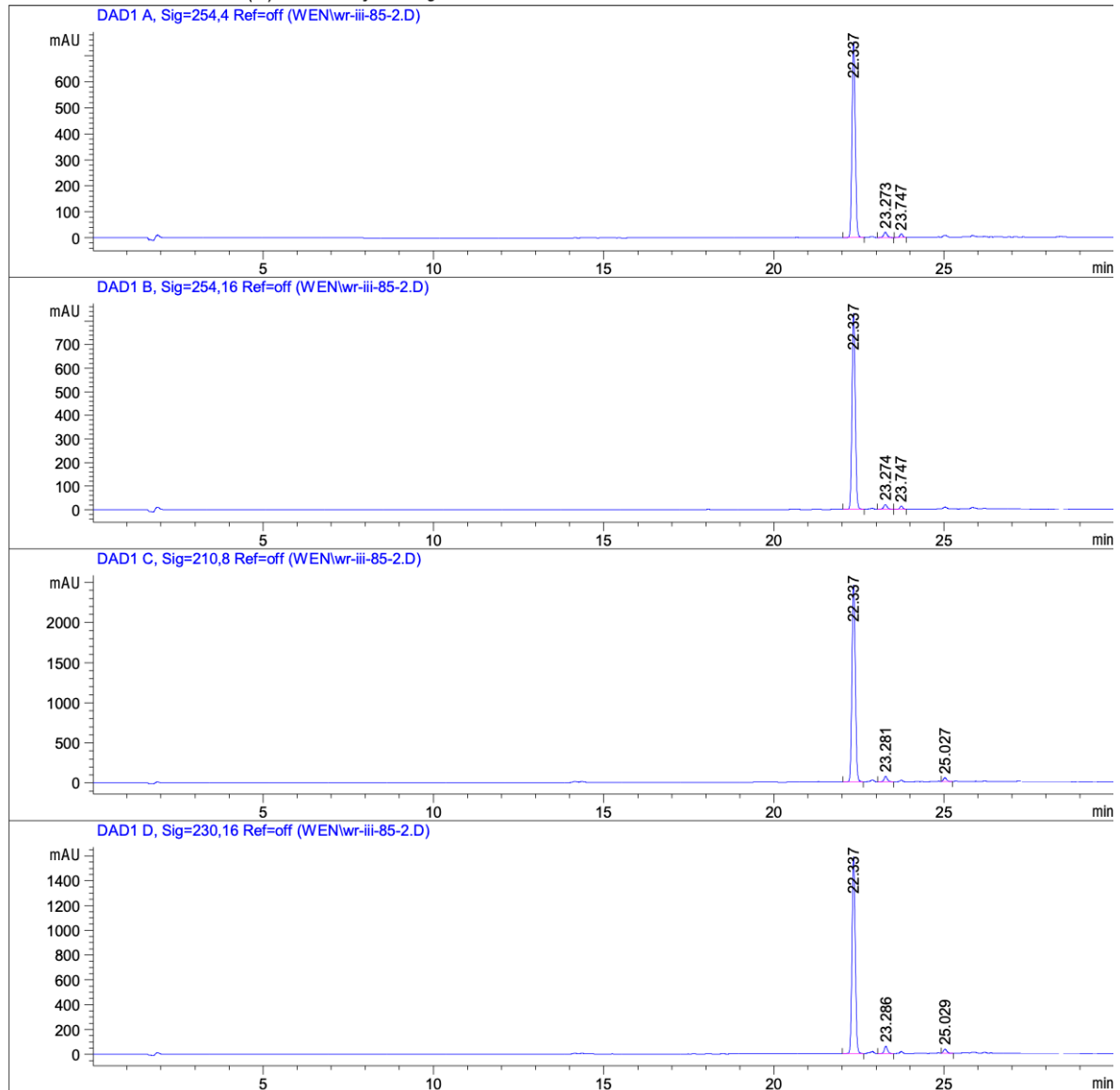


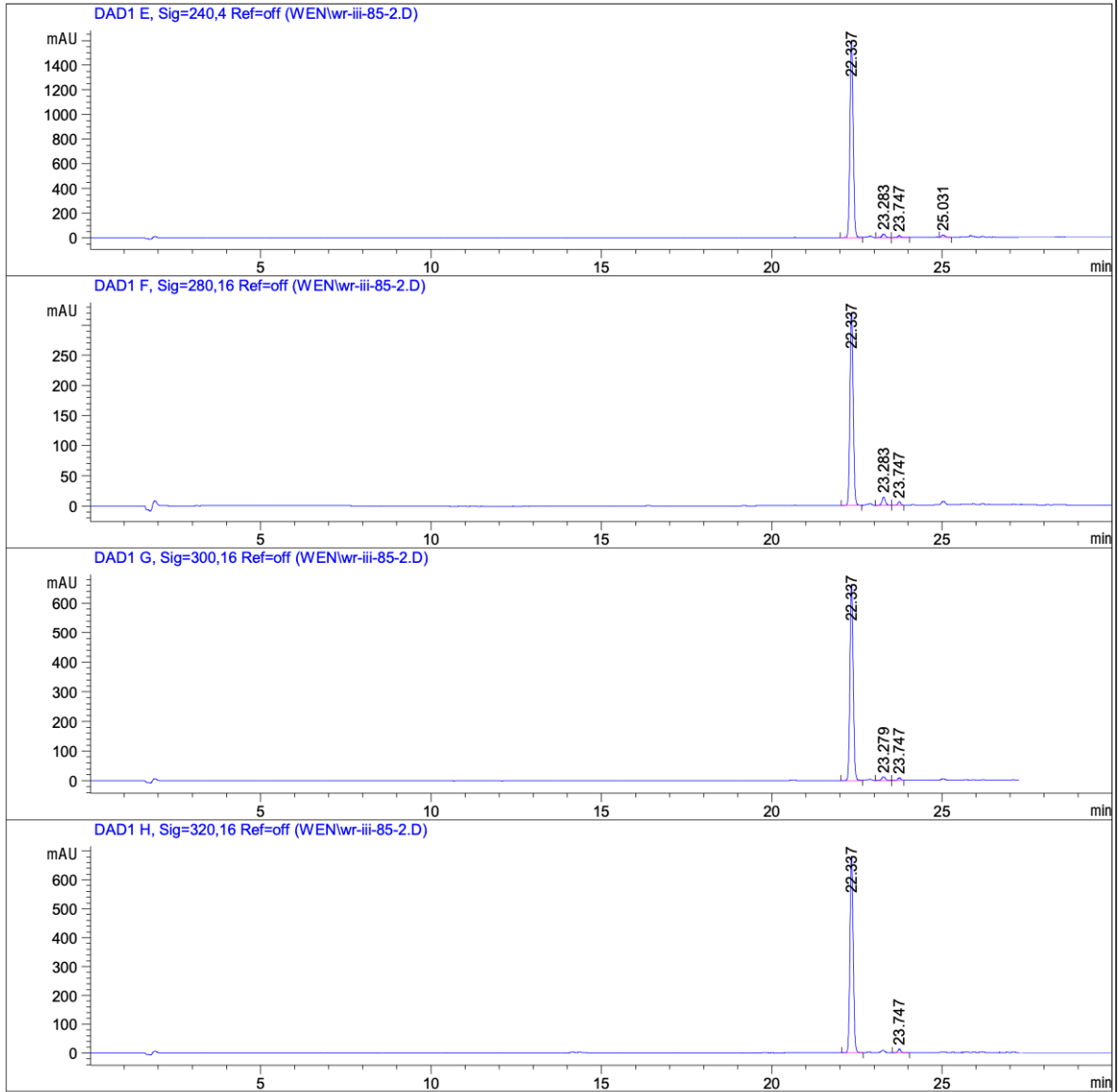
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Sample Operator : SYSTEM
Acq. Instrument : 1200 HPLC Location : 1
Injection Date : 3/6/2023 1:44:33 PM Inj Volume : No inj

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

Additional Info : Peak(s) manually integrated





=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Sample Amount : 1.00000 [ng/ul] (not used in calc.)
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	22.337	BB	0.0996	4875.91992	752.84637	95.3813
2	23.273	BB	0.1130	152.40520	20.43799	2.9813
3	23.747	BB	0.0909	83.70277	14.16718	1.6374

Totals : 5112.02789 787.45155

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	22.337	BV	0.0997	5400.87549	832.27887	95.8953
2	23.274	BB	0.1129	150.52261	20.21642	2.6726
3	23.747	BB	0.0912	80.65516	13.59647	1.4321

Totals : 5632.05326 866.09176

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	22.337	BV	0.1045	1.65231e4	2454.30737	95.3167
2	23.281	BB	0.1080	492.30078	68.34073	2.8399
3	25.027	VB	0.1078	319.54886	46.69796	1.8434

Totals : 1.73350e4 2569.34606

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	22.337	BV	0.1016	1.02993e4	1588.89661	94.1846
2	23.286	BB	0.1020	399.33817	59.73422	3.6519
3	25.029	VV	0.1116	236.58698	33.01656	2.1635

Totals : 1.09352e4 1681.64739

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	22.337	BV	0.1017	1.03912e4	1600.69543	95.9015
2	23.283	BB	0.1060	206.19827	29.32318	1.9030
3	23.747	BB	0.0960	98.42836	15.51506	0.9084
4	25.031	VV	0.1187	139.45804	18.33497	1.2871

Totals : 1.08353e4 1663.86864

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	22.337	BB	0.0993	2072.29517	320.92938	93.9197
2	23.283	BB	0.1070	97.21315	13.65925	4.4059
3	23.747	BV	0.0933	36.94506	6.04259	1.6744

Totals : 2206.45338 340.63122

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	22.337	BV	0.0994	4285.17529	663.46387	96.6767
2	23.279	VB	0.1123	92.88168	12.56342	2.0955
3	23.747	BV	0.0926	54.42215	8.99362	1.2278

Totals : 4432.47912 685.02091

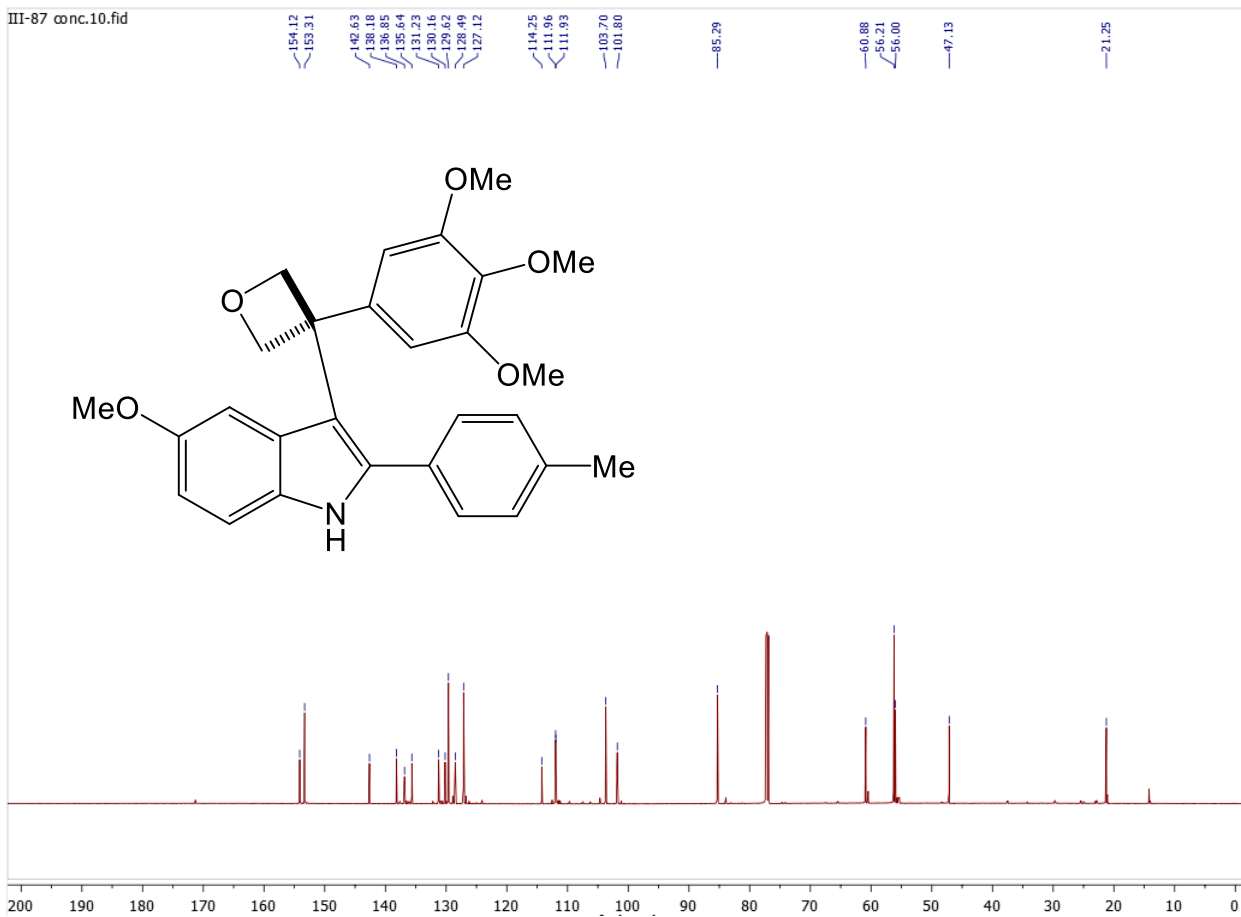
Signal 8: DAD1 H, Sig=320,16 Ref=off

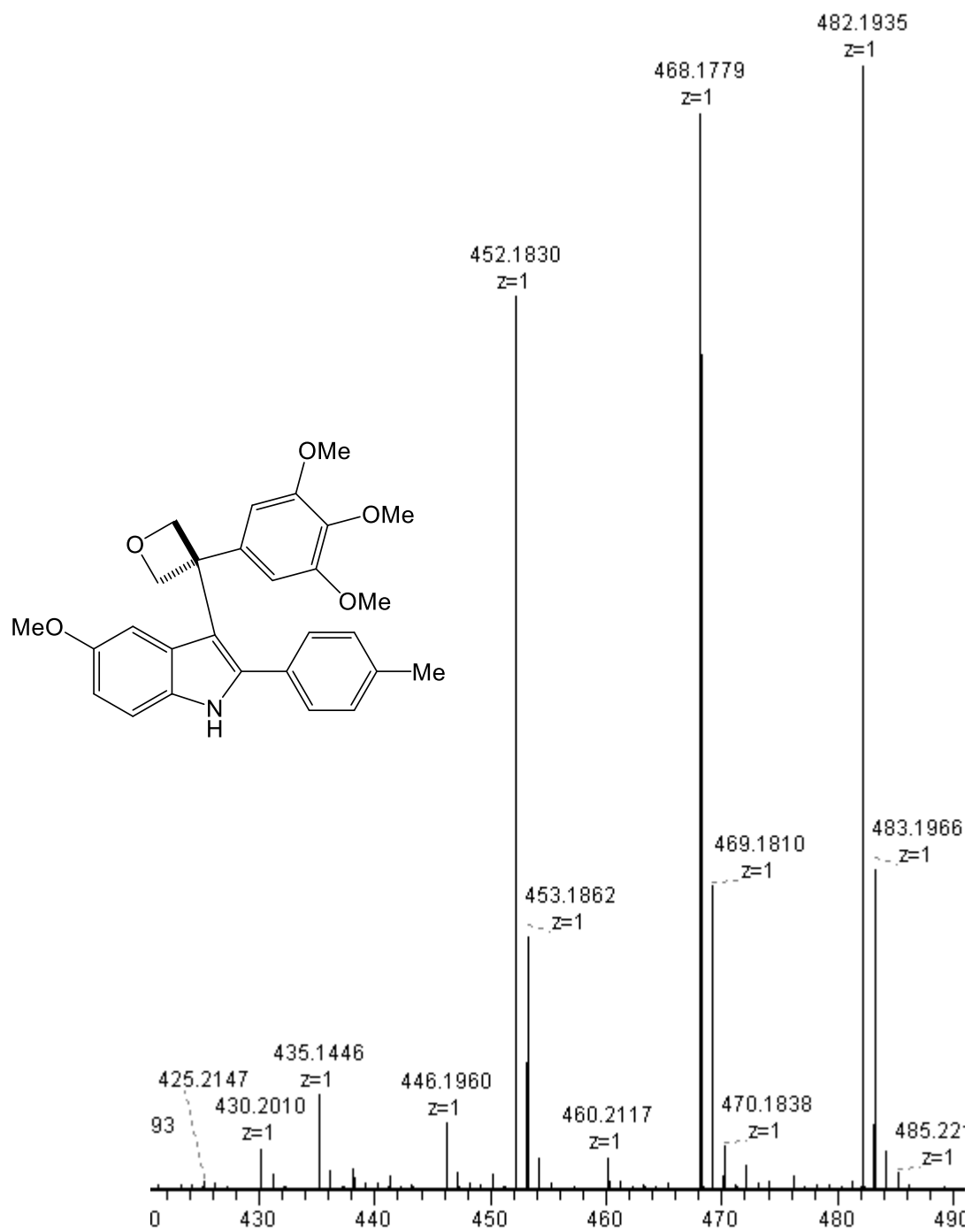
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	22.337	BB	0.0992	4397.05615	681.85901	98.3067
2	23.747	BB	0.0954	75.73710	12.37473	1.6933

Totals : 4472.79325 694.23374

=====
*** End of Report ***

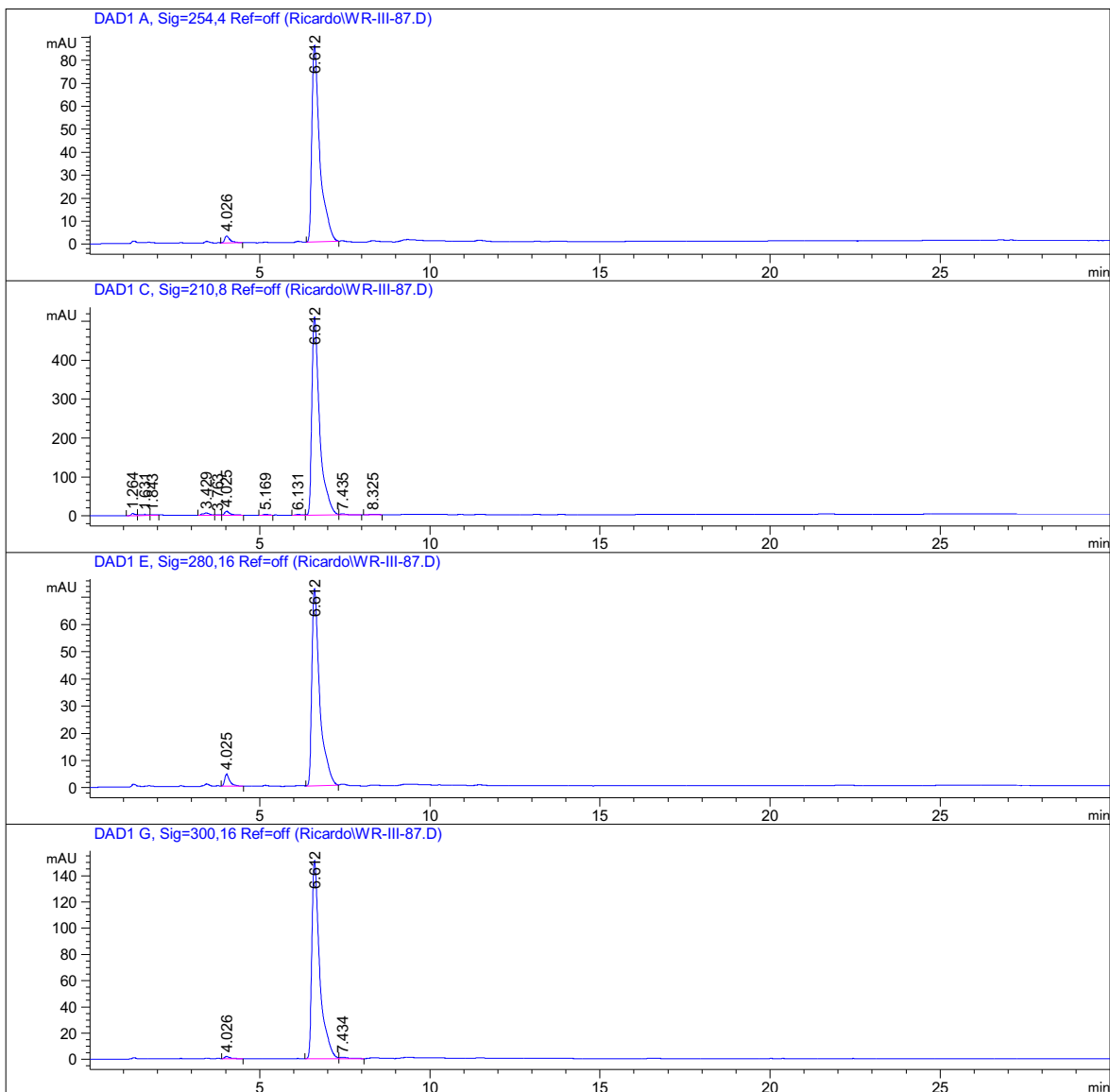
III-87 conc.10.fid



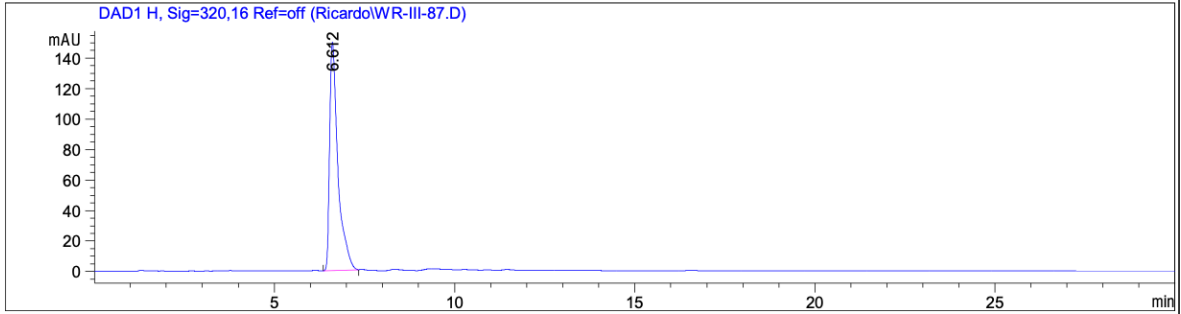


Data File C:\Chem32\1\Data\Ricardo\WR-III-87.D
Sample Name: WR-III-87

=====
Acq. Operator : SYSTEM
Sample Operator : SYSTEM
Acq. Instrument : 1200 HPLC Location : 1
Injection Date : 7/31/2020 2:13:12 PM Inj Volume : No inj
Method : C:\Chem32\1\Methods\GRAD 2 50-90 ACN.M
Last changed : 4/30/2014 1:53:57 AM by ERICAP
Sample Info : 50-90 ACN:WATER



Data File C:\Chem32\1\Data\Ricardo\WR-III-87.D
 Sample Name: WR-III-87



=====
 Area Percent Report
 =====

Sorted By : Signal
 Multiplier : 1.0000
 Dilution : 1.0000
 Sample Amount : 1.00000 [ng/ul] (not used in calc.)
 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	4.026	BB	0.1617	32.49809	2.96934	2.2947
2	6.612	BB	0.2367	1383.73792	85.57095	97.7053

Totals : 1416.23600 88.54029

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.264	BV	0.1150	46.49942	5.83297	0.5480
2	1.631	VV	0.2115	38.71789	2.28751	0.4563
3	1.843	VV	0.1425	18.79692	1.78976	0.2215
4	3.429	BV	0.2192	90.58074	6.03350	1.0675
5	3.763	VV	0.1266	12.87899	1.49301	0.1518
6	4.025	VB	0.1706	119.14664	10.17709	1.4041
7	5.169	BB	0.1560	23.23737	2.33717	0.2738
8	6.131	BV	0.1952	23.11951	1.78397	0.2725
9	6.612	VV	0.2324	8053.87842	509.51855	94.9124
10	7.435	VB	0.2111	39.75042	2.70999	0.4684
11	8.325	BB	0.2260	18.98729	1.35048	0.2238

Totals : 8485.59361 545.31401

Data File C:\Chem32\1\Data\Ricardo\WR-III-87.D
Sample Name: WR-III-87

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.025	BB	0.1574	46.51346	4.39775	3.8769
2	6.612	BB	0.2319	1153.25342	72.37313	96.1231

Totals : 1199.76688 76.77088

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.026	BB	0.1592	17.16919	1.60029	0.7054
2	6.612	BV	0.2314	2400.26563	151.02991	98.6166
3	7.434	VB	0.2196	16.50172	1.07221	0.6780

Totals : 2433.93654 153.70241

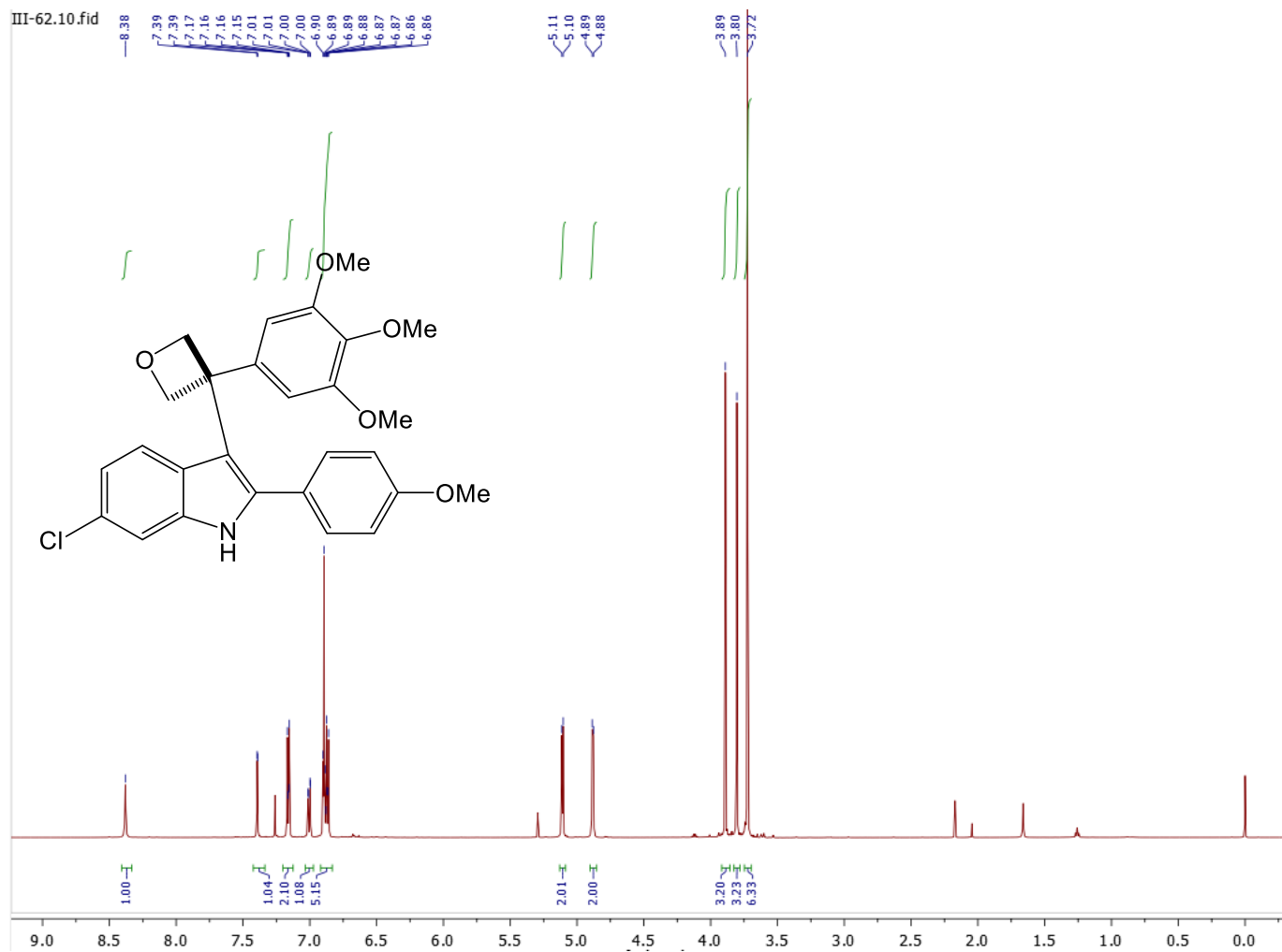
Signal 5: DAD1 H, Sig=320,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.612	BB	0.2317	2382.69189	149.70708	100.0000

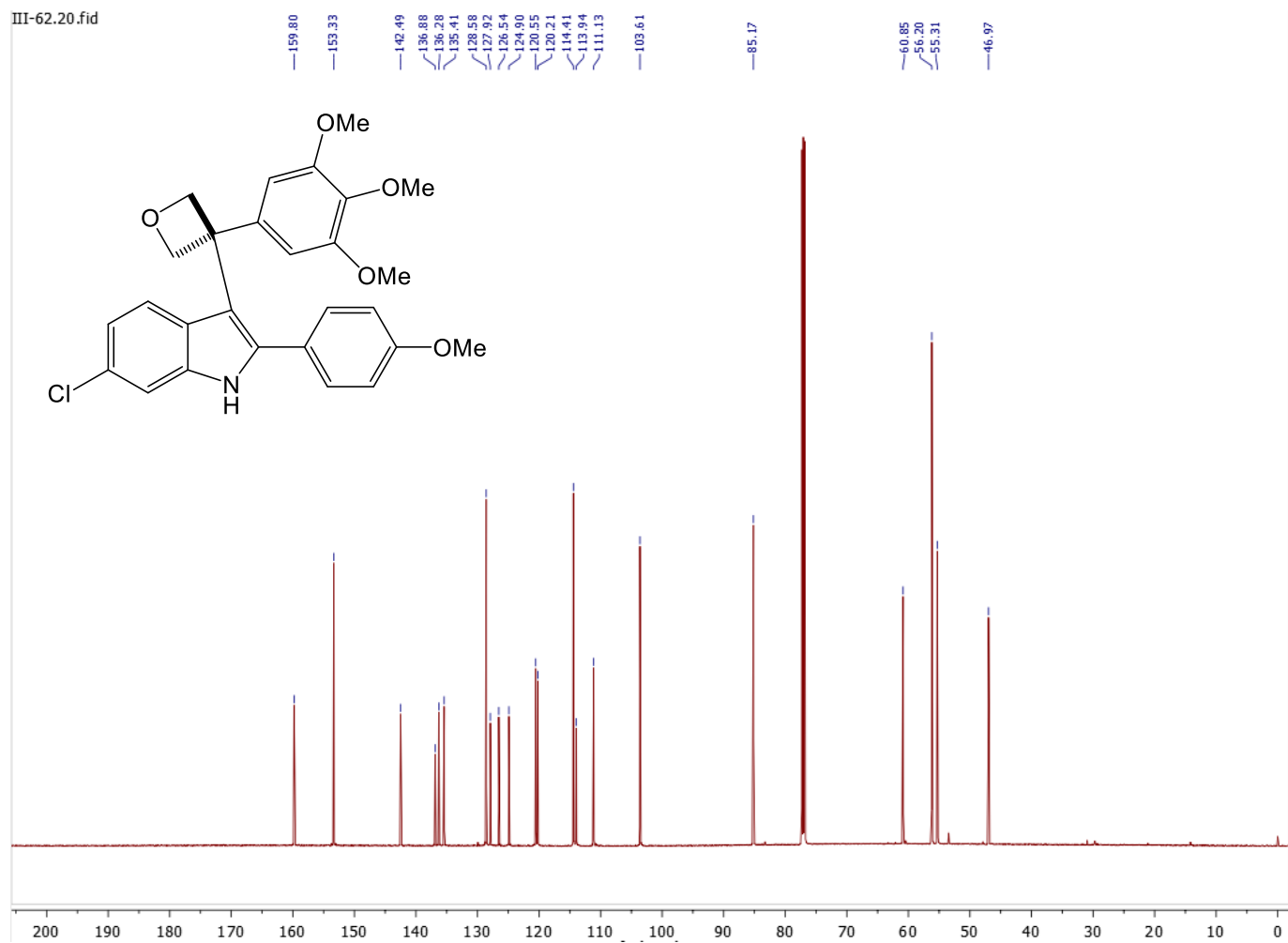
Totals : 2382.69189 149.70708

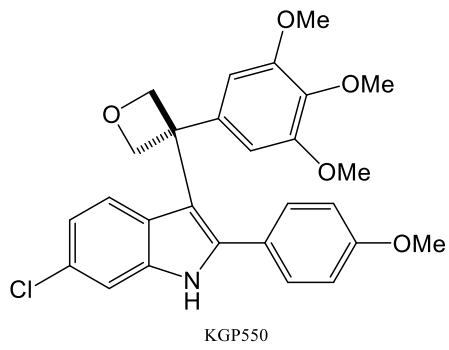
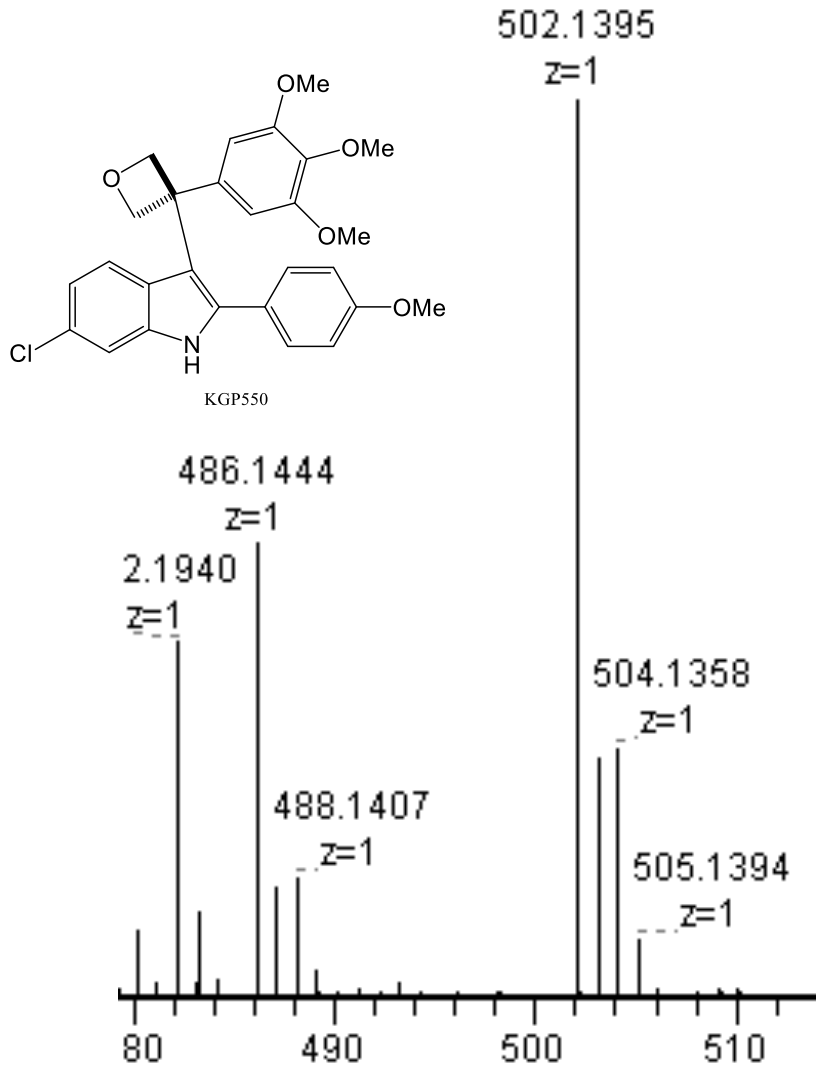
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*** End of Report ***

Compound 5e

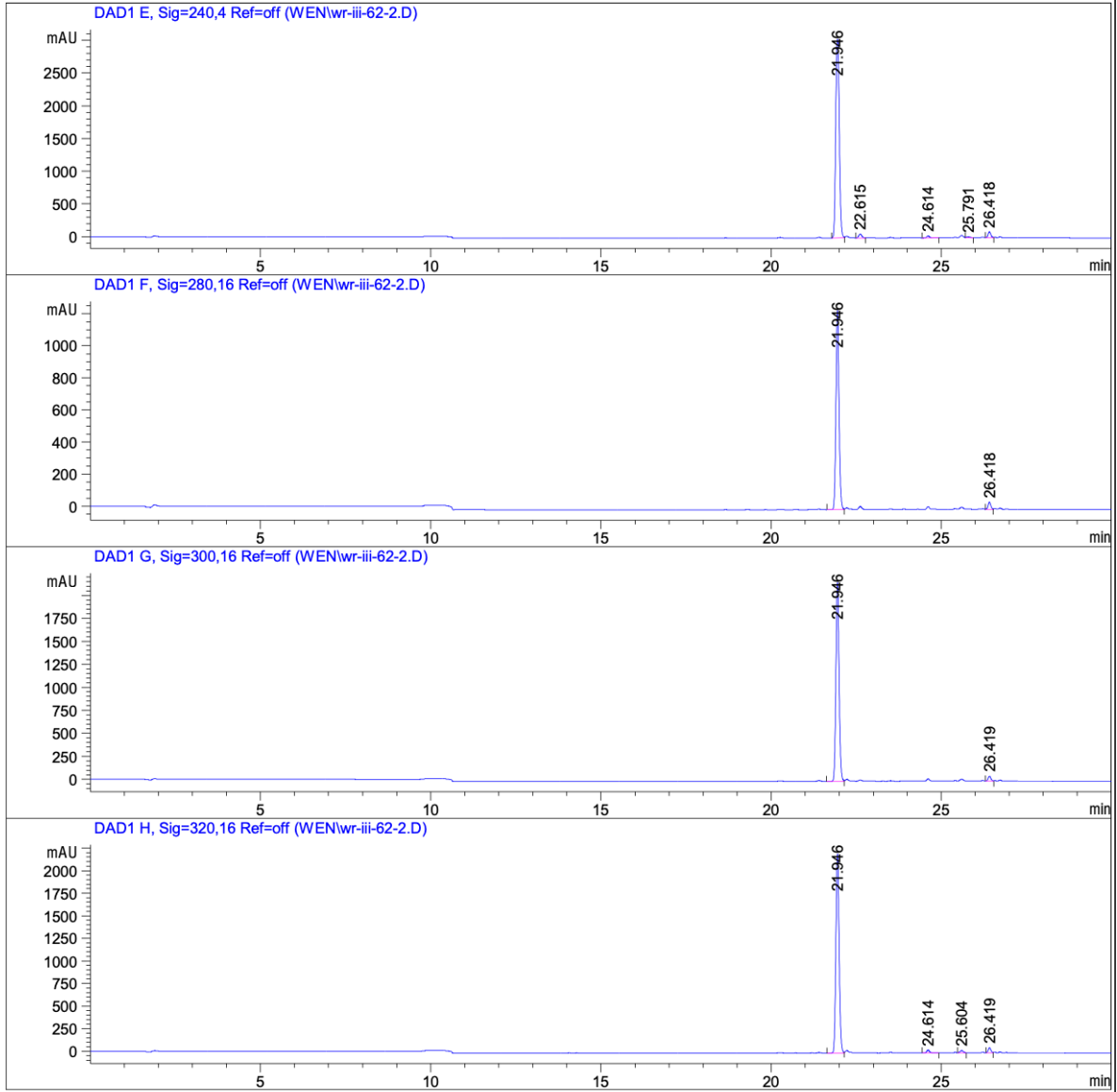


III-62.20.fid





Data File C:\Chem32\1\Data\WEN\wr-iii-62-2.D
Sample Name: wr-iii-62-2



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Area Percent Report
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Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Sample Amount : 1.00000 [ng/ul] (not used in calc.)
Use Multiplier & Dilution Factor with ISTDs

Sample Name: wr-iii-62-2

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	21.946	BV	0.1138	1.95699e4	2723.57715	95.3497
2	24.614	BV	0.0929	240.41814	39.56171	1.1714
3	25.604	VV	0.1003	235.66830	36.03448	1.1482
4	26.418	BV	0.0840	478.34830	87.21782	2.3306

Totals : 2.05244e4 2886.39116

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	21.946	BV	0.1136	1.90123e4	2653.70630	97.5943
2	26.418	BV	0.0841	468.65009	85.34182	2.4057

Totals : 1.94810e4 2739.04812

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	21.945	BV	0.1619	2.79597e4	2813.27002	92.3256
2	22.222	VB	0.1130	439.50073	56.33816	1.4513
3	22.615	BV	0.0976	568.56976	90.11728	1.8775
4	22.836	VV	0.0994	48.75050	7.35133	0.1610
5	24.614	BB	0.1006	342.69827	50.85356	1.1316
6	26.416	BV	0.0832	879.20251	162.38976	2.9032
7	26.581	VV	0.0817	45.38559	8.31196	0.1499

Totals : 3.02838e4 3188.63206

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	21.946	BV	0.1229	2.28210e4	2994.35864	94.9970
2	22.615	BV	0.0977	389.15082	61.61694	1.6199
3	24.614	BB	0.0997	219.72202	32.97391	0.9146
4	25.410	BV	0.0837	45.79996	8.65896	0.1907
5	26.417	BV	0.0841	519.87256	94.68971	2.1641
6	26.581	VV	0.0789	27.31297	5.23220	0.1137

Totals : 2.40229e4 3197.53037

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	21.946	BV	0.1212	2.26830e4	3033.90234	95.0158
2	22.615	BV	0.0975	383.66473	60.86258	1.6071
3	24.614	BB	0.0996	216.13211	32.48325	0.9053
4	25.791	VB	0.0922	92.76106	14.99069	0.3886
5	26.418	BV	0.0849	497.31873	89.36918	2.0832

Totals : 2.38729e4 3231.60804

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	21.946	BV	0.0986	7922.77832	1238.73938	97.0708
2	26.418	BV	0.0832	239.07545	44.10551	2.9292

Totals : 8161.85378 1282.84489

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	21.946	BV	0.1030	1.42424e4	2156.98999	97.9902
2	26.419	BV	0.0838	292.11990	53.43065	2.0098

Totals : 1.45345e4 2210.42064

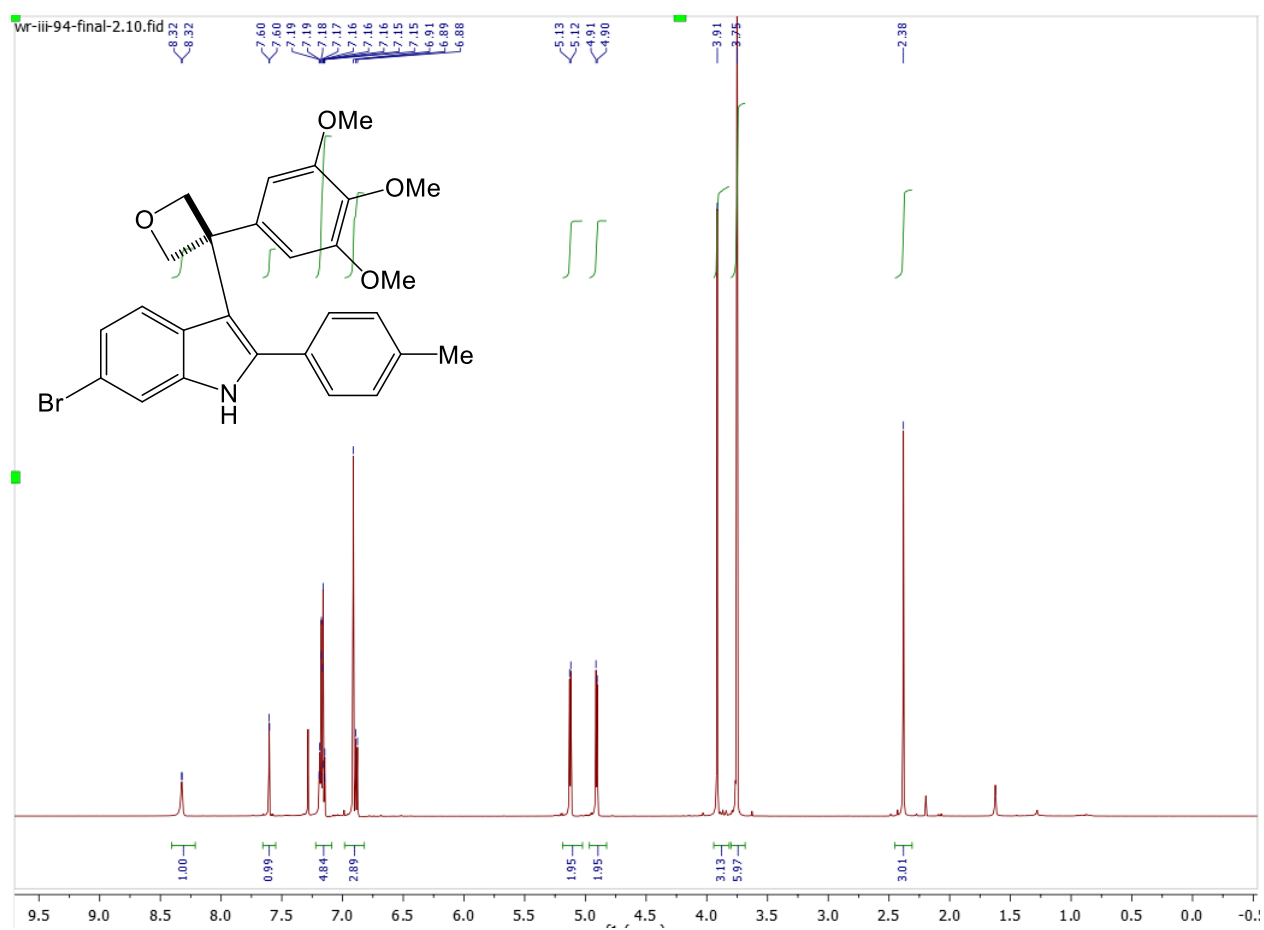
Signal 8: DAD1 H, Sig=320,16 Ref=off

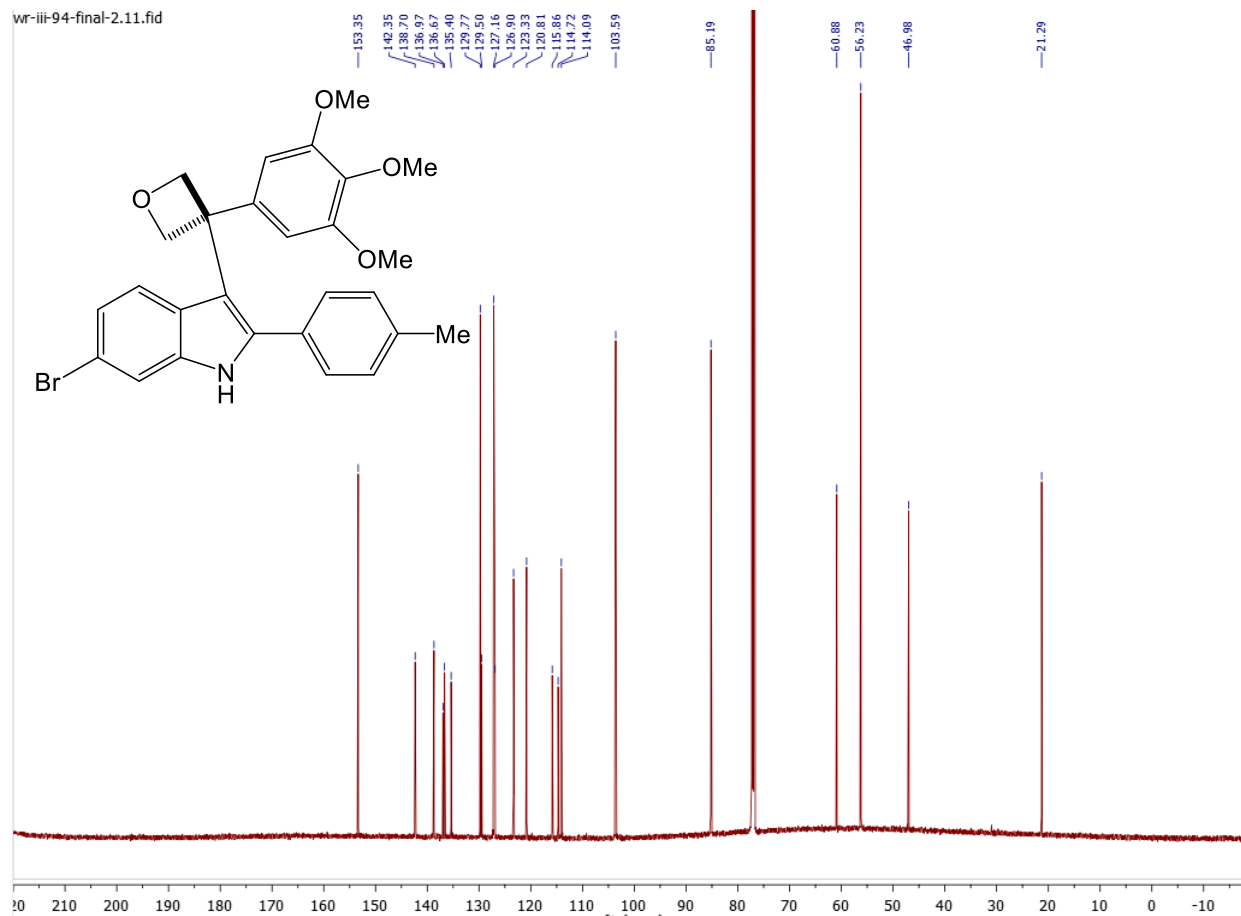
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	21.946	BV	0.1074	1.49590e4	2199.20264	95.5721
2	24.614	BV	0.0967	208.00969	32.48122	1.3290
3	25.604	VV	0.1024	176.03522	26.19173	1.1247
4	26.419	BV	0.0856	309.01193	56.70751	1.9743

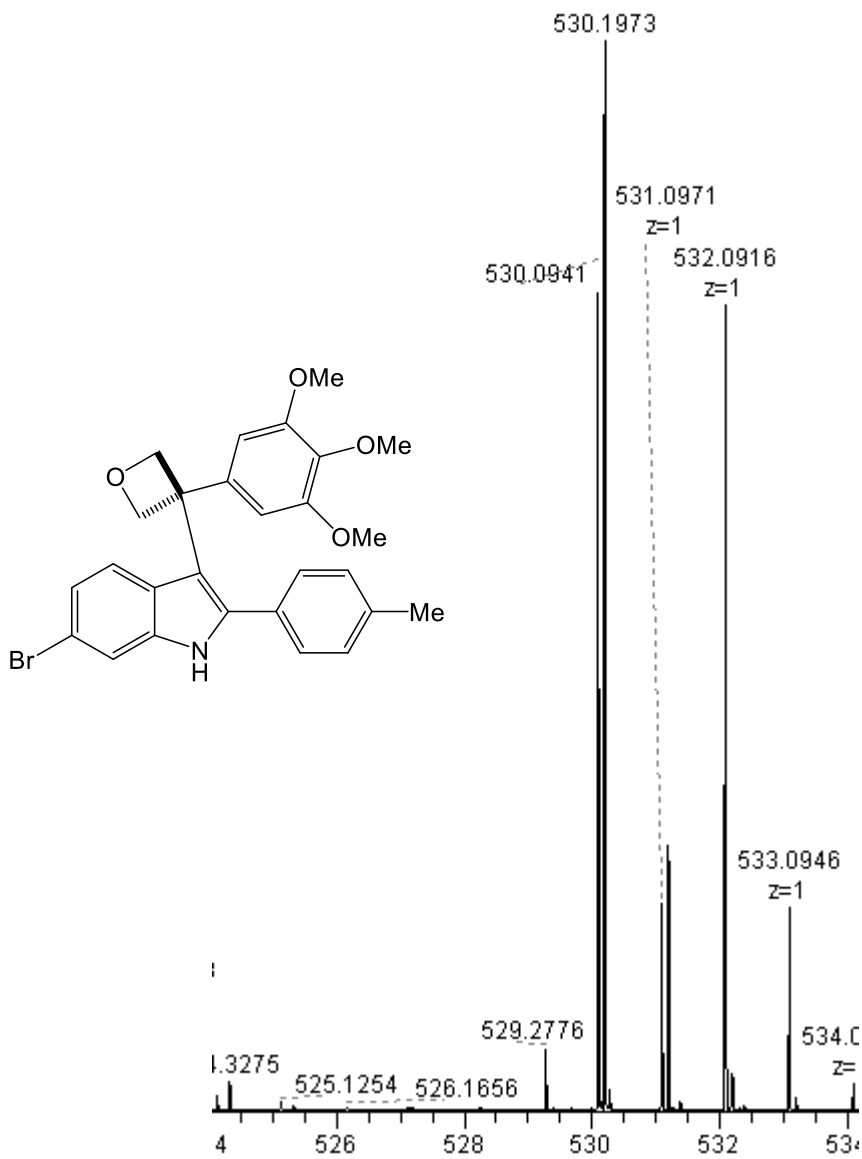
Totals : 1.56520e4 2314.58310

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*** End of Report ***

Compound 5f







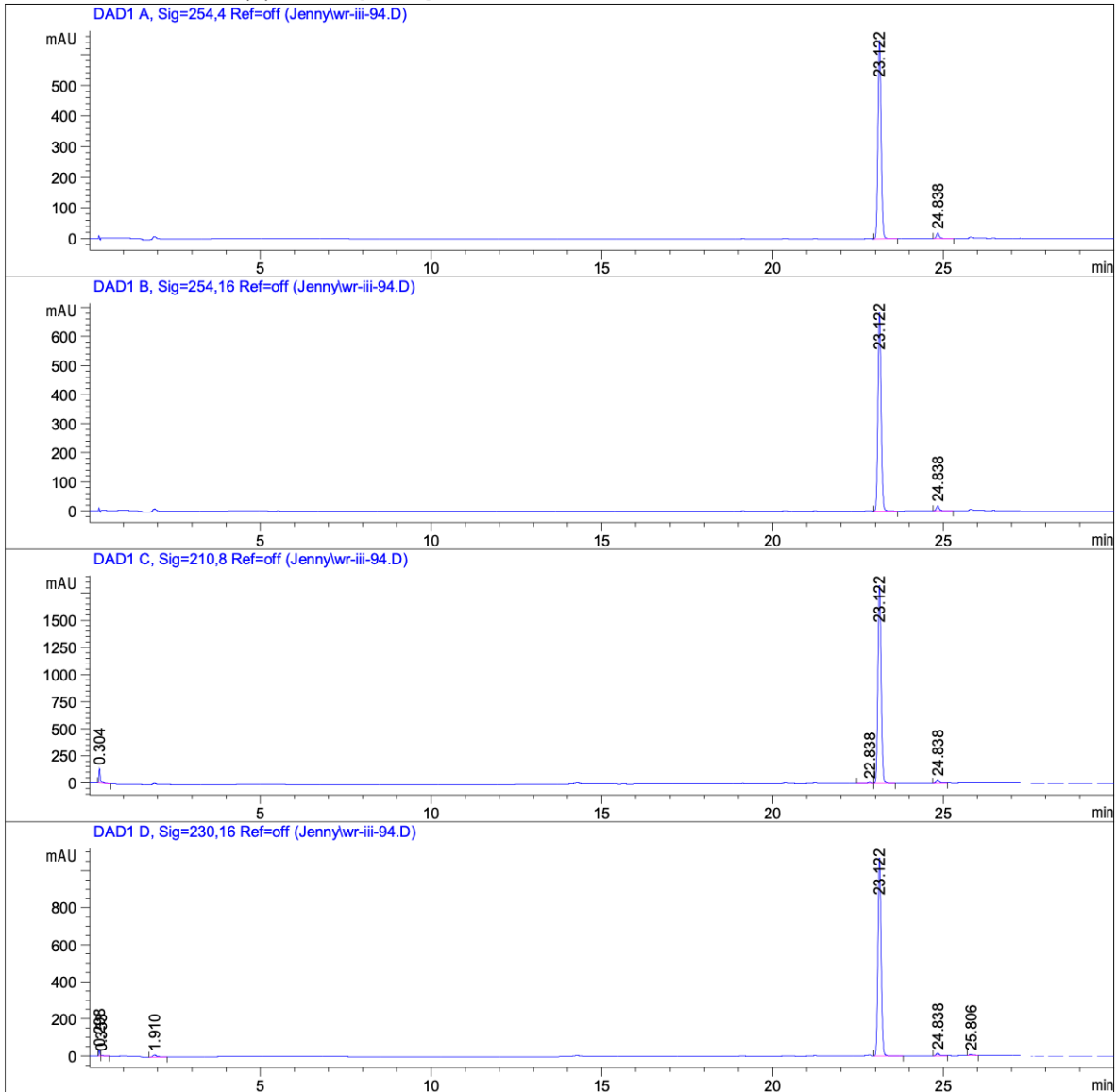
Data File C:\Chem32\1\Data\Jenny\wr-iii-94.D
Sample Name: wr-iii-94

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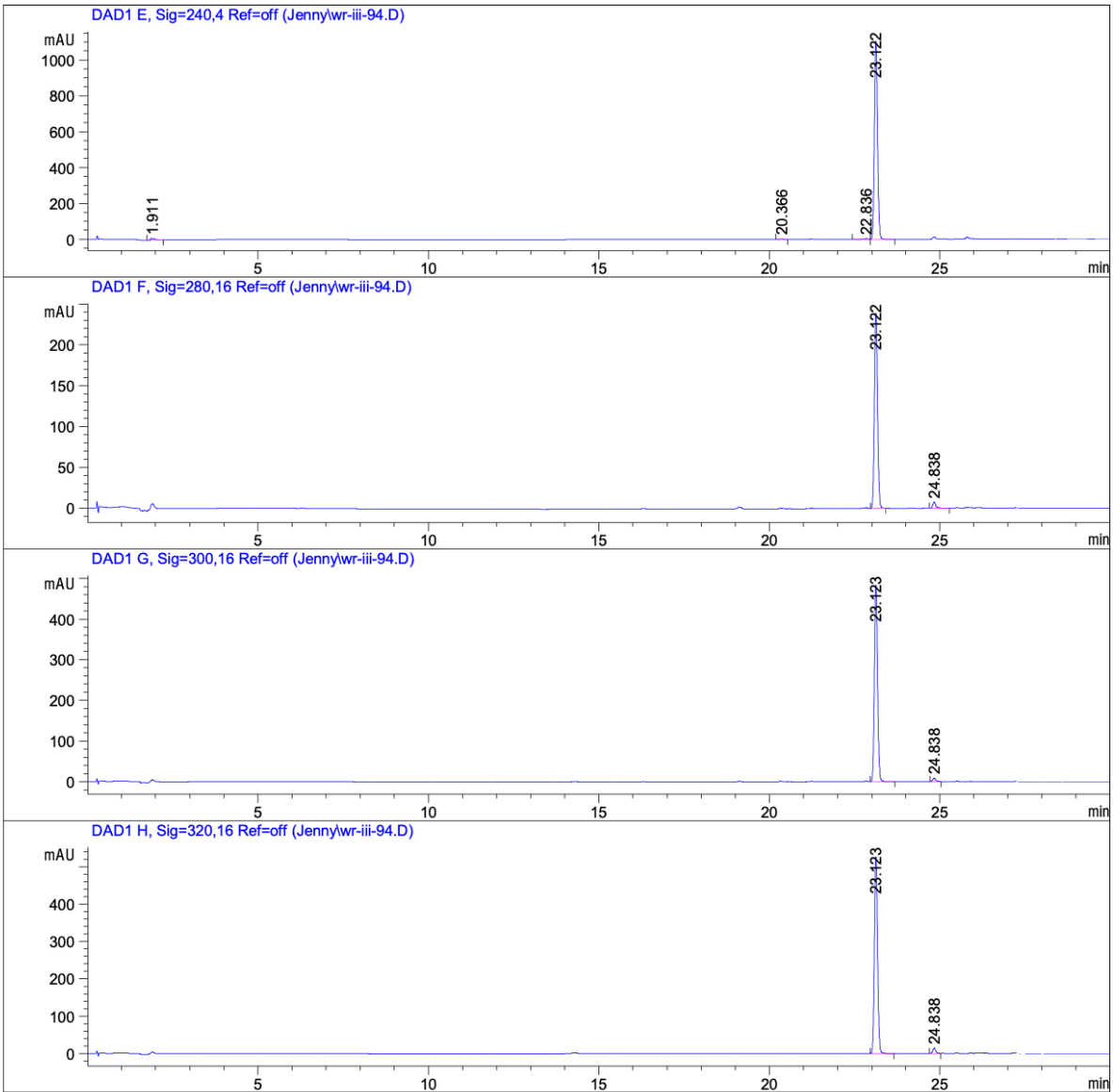
Acq. Operator : SYSTEM
Sample Operator : SYSTEM
Acq. Instrument : 1200 HPLC Location : 1
Injection Date : 3/6/2023 10:03:25 AM Inj Volume : No inj

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



Data File C:\Chem32\1\Data\Jenny\wr-iii-94.D
Sample Name: wr-iii-94



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Area Percent Report
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Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Sample Amount: : 1.00000 [ng/ul] (not used in calc.)
Use Multiplier & Dilution Factor with ISTDs

Data File C:\Chem32\1\Data\Jenny\wr-iii-94.D
Sample Name: wr-iii-94

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	23.122	VB	0.0982	4125.98682	648.82428	97.2443
2	24.838	BB	0.0970	116.92339	18.19571	2.7557

Totals : 4242.91021 667.01999

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	23.122	VB	0.0982	4349.37842	684.22589	97.4473
2	24.838	BB	0.0973	113.93318	17.65711	2.5527

Totals : 4463.31160 701.88300

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	0.304	BB	0.0475	402.72342	132.38976	3.2112
2	22.838	BV	0.1092	68.90028	9.21509	0.5494
3	23.122	VB	0.0995	1.18459e4	1829.84180	94.4569
4	24.838	BV	0.0977	223.53879	34.43666	1.7825

Totals : 1.25411e4 2005.88331

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	0.298	BV	0.0410	75.36086	30.35119	1.0520
2	0.353	VB	0.0904	13.37091	2.28021	0.1866
3	1.910	BB	0.1407	103.51208	11.11344	1.4449
4	23.122	VB	0.0981	6814.51074	1072.81458	95.1230
5	24.838	BV	0.1033	107.00661	15.36334	1.4937
6	25.806	BB	0.1063	50.12897	6.77747	0.6997

Totals : 7163.89017 1138.70023

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.911	BB	0.1368	92.79232	10.33375	1.2916
2	20.366	BB	0.1573	22.33437	2.34197	0.3109
3	22.836	BV	0.1278	41.62230	4.59004	0.5793
4	23.122	VB	0.0980	7027.65430	1107.47095	97.8182

Totals : 7184.40328 1124.73671

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	23.122	BB	0.0978	1515.68567	239.59666	96.7121
2	24.838	BB	0.1013	51.52903	7.57881	3.2879

Totals : 1567.21469 247.17548

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	23.123	VB	0.0980	3073.97559	484.62503	98.3636
2	24.838	BB	0.0920	51.13946	8.52290	1.6364

Totals : 3125.11505 493.14793

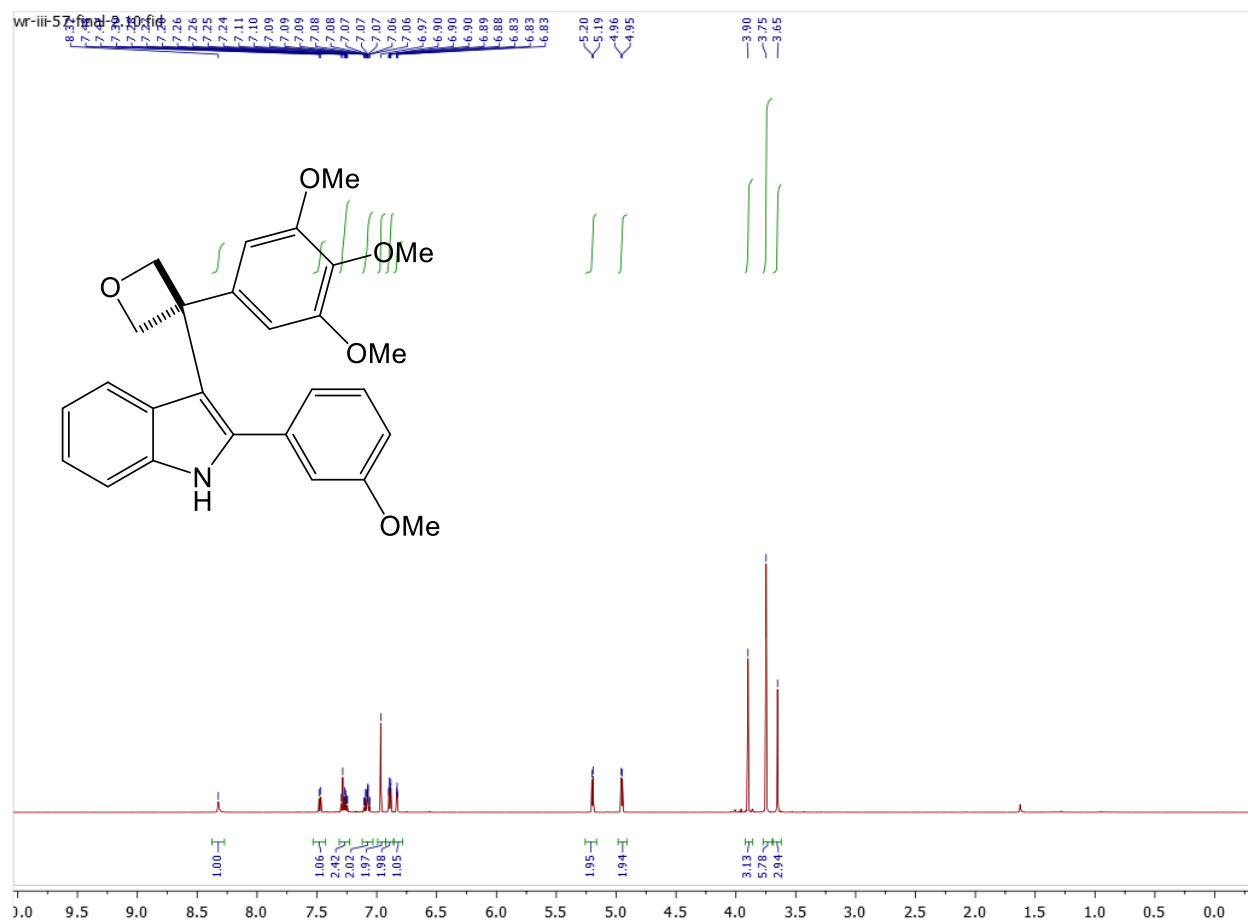
Signal 8: DAD1 H, Sig=320,16 Ref=off

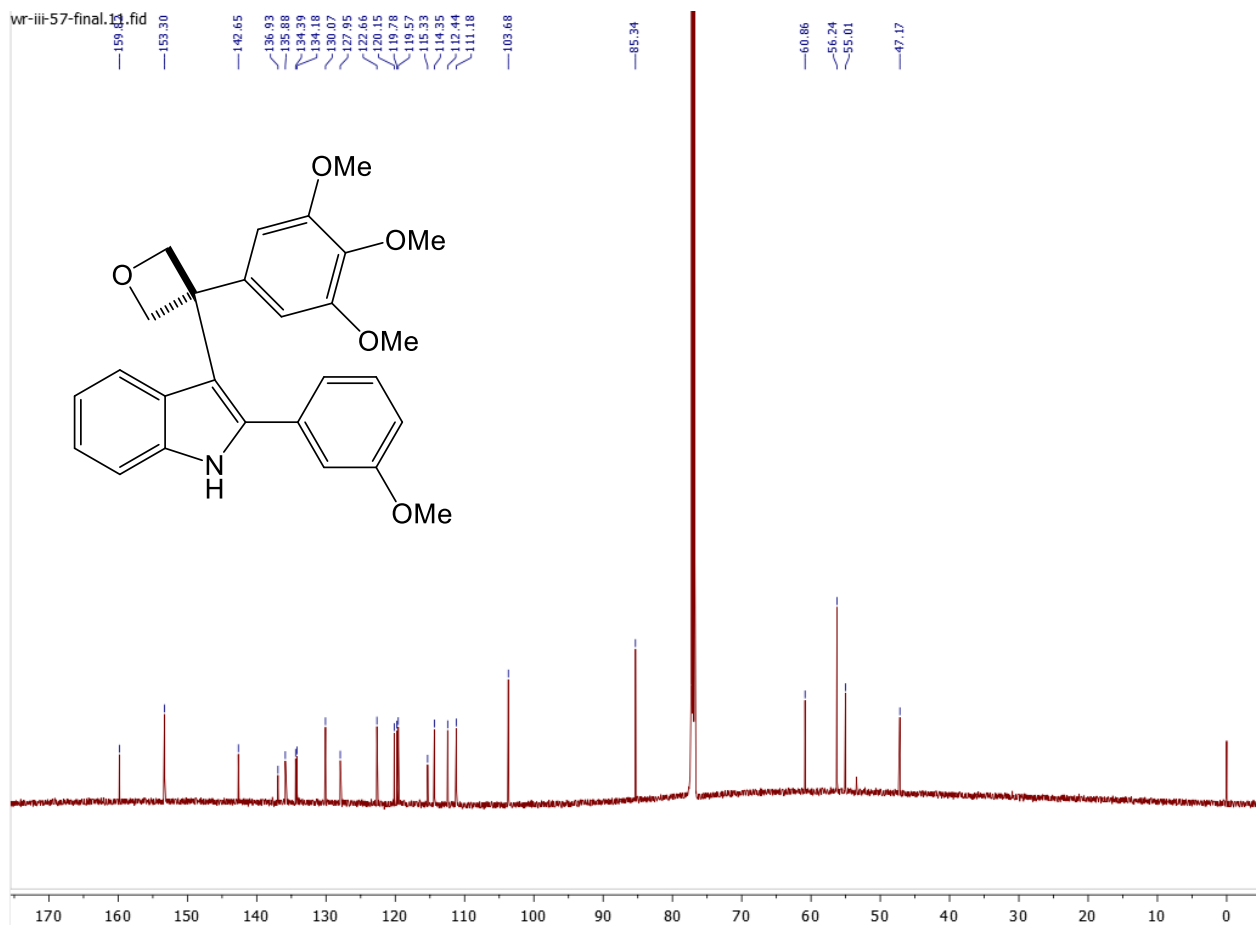
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	23.123	BB	0.0980	3347.94092	527.78351	97.5633
2	24.838	BB	0.0909	83.61826	14.15893	2.4367

Totals : 3431.55917 541.94244

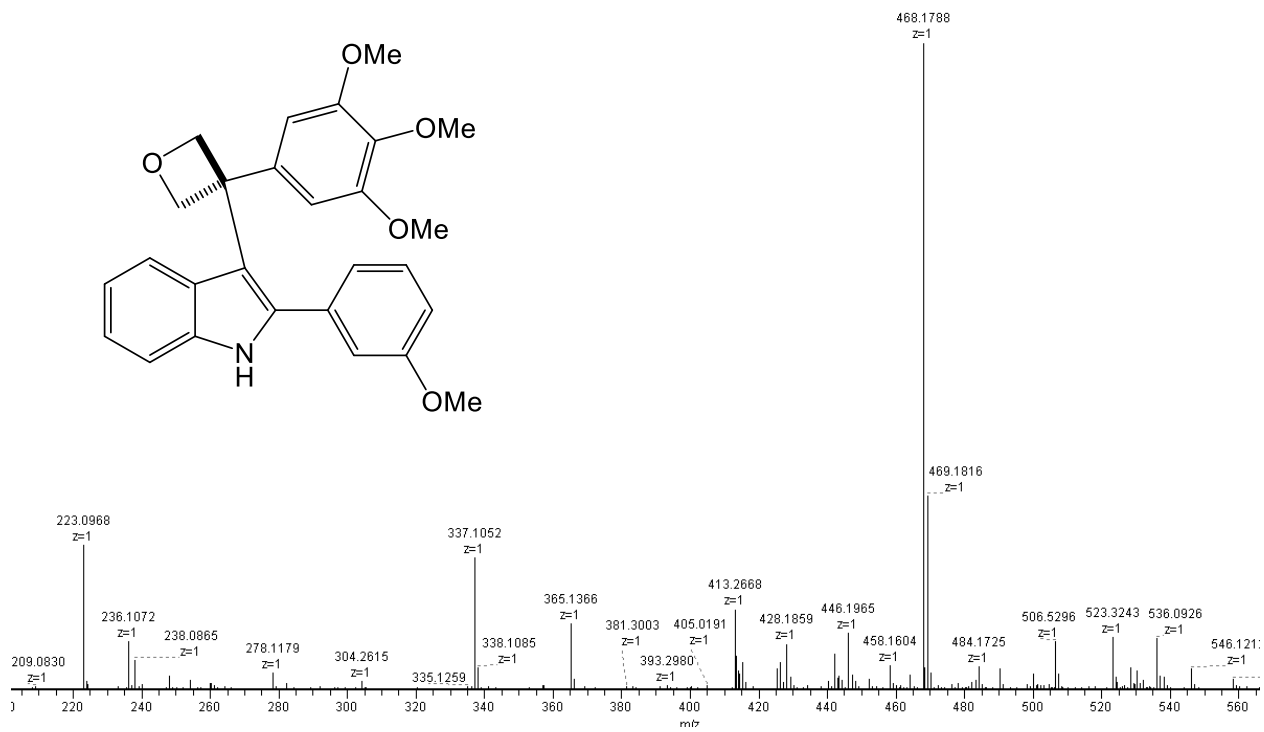
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*** End of Report ***

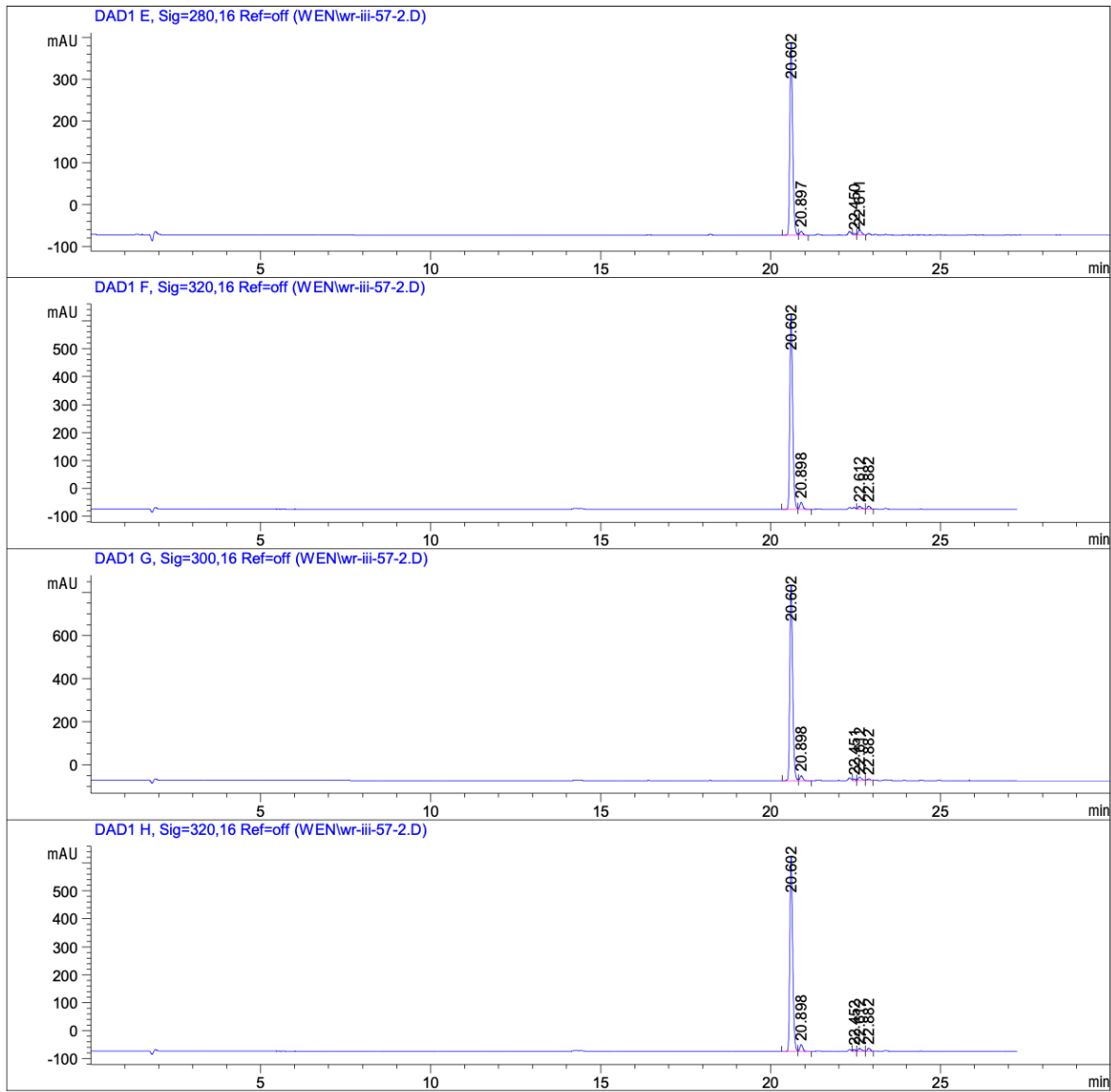
Compound 5g





T: 59.084 ST: 0.79 uS: 1 CS: 1 AMW: 467.17 NL: 1.39E7
+ p ESI Full ms [200.00-600.00]
I=3d RF=2300V TmpDiff Lock(In)391.3, 1f1, +2ppm)





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Area Percent Report
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Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Sample Amount: : 1.00000 [ng/ul] (not used in calc.)
Use Multiplier & Dilution Factor with ISTDs

Data File C:\Chem32\1\Data\WEN\wr-iii-57-2.D
Sample Name: wr-iii-57-2

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	20.602	BV	0.0908	3384.96973	574.10345	95.7475
2	20.898	VB	0.0893	74.94018	12.60932	2.1198
3	22.451	VV	0.0787	29.80915	5.72974	0.8432
4	22.882	BV	0.0861	45.58938	8.30036	1.2895

Totals : 3535.30844 600.74287

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	20.602	BV	0.0908	3713.72681	629.62360	92.3811
2	20.897	VB	0.0903	76.63709	12.71002	1.9064
3	21.391	BB	0.1113	20.75458	2.77405	0.5163
4	22.320	BV	0.0836	58.92662	10.80842	1.4658
5	22.611	VB	0.1014	103.29552	15.16912	2.5695
6	22.882	BV	0.0861	46.66776	8.48902	1.1609

Totals : 4020.00837 679.57422

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	20.602	BV	0.1109	1.59760e4	2302.89453	95.6203
2	20.897	VV	0.0936	216.18344	34.27876	1.2939
3	22.321	BV	0.0826	105.30437	19.61131	0.6303
4	22.614	VB	0.1019	220.87402	31.48221	1.3220
5	22.882	BV	0.0864	189.39507	34.33472	1.1336

Totals : 1.67077e4 2422.60153

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	20.602	BV	0.0932	1.15400e4	1890.37732	94.9799
2	20.897	VB	0.0915	182.24625	29.75588	1.5000
3	22.321	BV	0.0822	74.02666	13.88464	0.6093
4	22.452	VV	0.0800	63.90585	12.03197	0.5260
5	22.613	VB	0.1006	162.21931	23.48679	1.3351
6	22.882	BV	0.0863	109.05629	19.78951	0.8976

Sample Name: wr-iii-57-2

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
7	23.076	VB	0.0831	18.47762	3.41738	0.1521

Totals : 1.21499e4 1992.74349

Signal 5: DAD1 E, Sig=280,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	20.602	BV	0.0905	2707.83374	461.14719	94.4635
2	20.897	VB	0.0894	56.78530	9.55181	1.9810
3	22.450	VV	0.0781	19.28189	3.74140	0.6727
4	22.611	VB	0.1000	82.63763	12.36380	2.8828

Totals : 2866.53856 486.80420

Signal 6: DAD1 F, Sig=320,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	20.602	BV	0.0906	4121.34521	700.93152	93.5993
2	20.898	VB	0.0881	147.19968	25.22091	3.3430
3	22.612	VB	0.1011	71.32451	10.26158	1.6198
4	22.882	BV	0.0867	63.31134	11.41986	1.4379

Totals : 4403.18074 747.83387

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	20.602	BV	0.0907	5344.69971	907.99390	94.2988
2	20.898	VB	0.0892	133.21346	22.46591	2.3503
3	22.451	VV	0.0796	34.93911	6.61825	0.6164
4	22.612	VB	0.0994	109.13794	16.45338	1.9256
5	22.882	BV	0.0863	45.84373	8.31994	0.8088

Totals : 5667.83394 961.85137

Data File C:\Chem32\1\Data\WEN\wr-iii-57-2.D
Sample Name: wr-iii-57-2

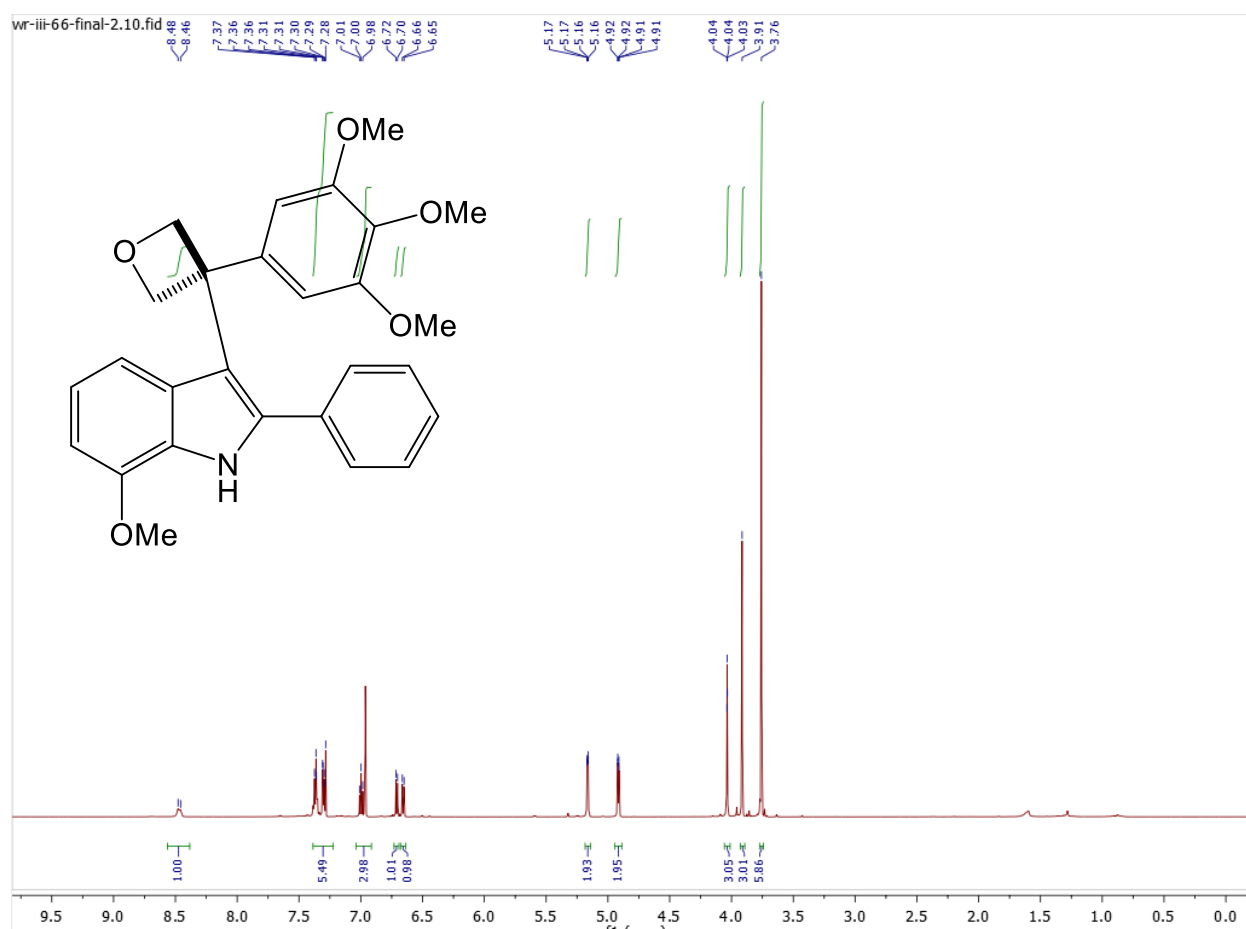
Signal 8: DAD1 H, Sig=320,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	20.602	BV	0.0906	4121.34521	700.93152	92.8695
2	20.898	VB	0.0881	147.19968	25.22091	3.3170
3	22.452	VV	0.0826	34.60011	6.45276	0.7797
4	22.612	VB	0.1011	71.32451	10.26158	1.6072
5	22.882	BV	0.0867	63.31134	11.41986	1.4266

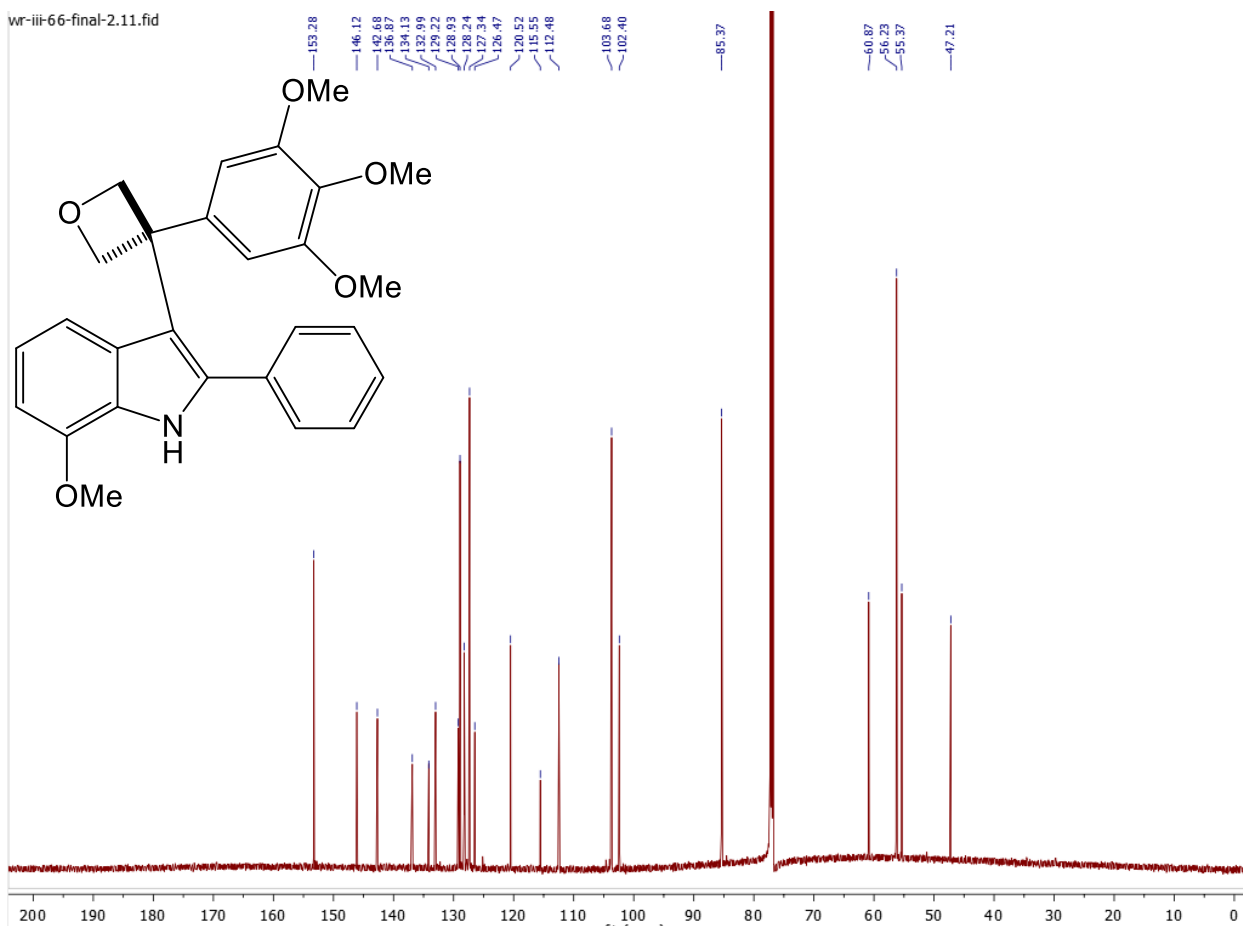
Totals : 4437.78086 754.28663

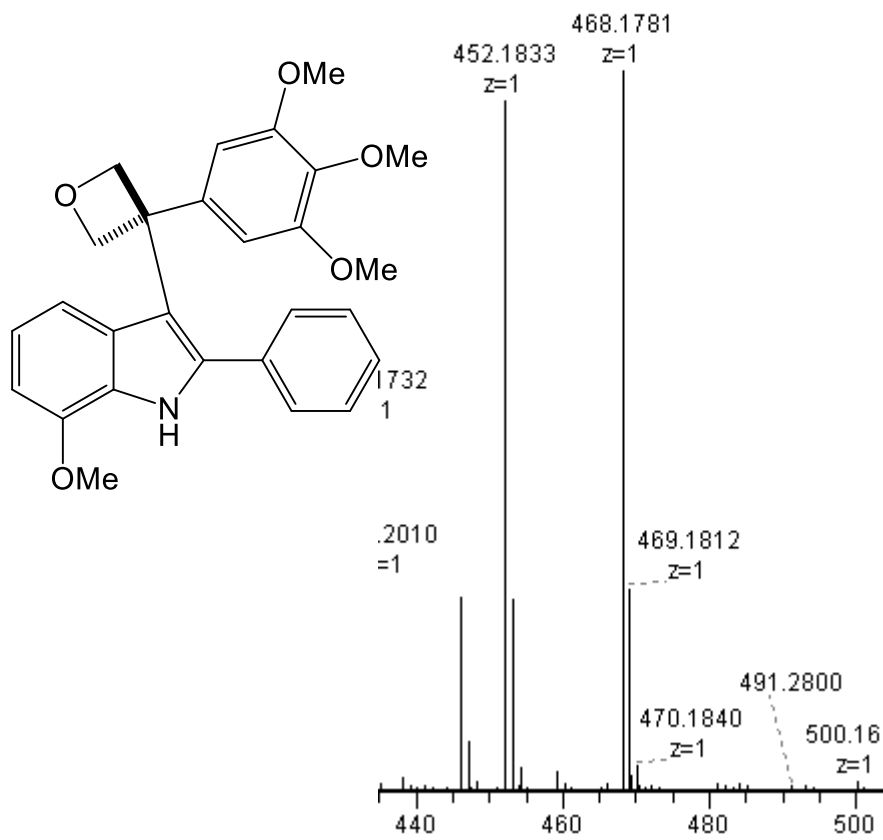
=====
*** End of Report ***

Compound 5h



wr-iii-66-final-2.11.fid



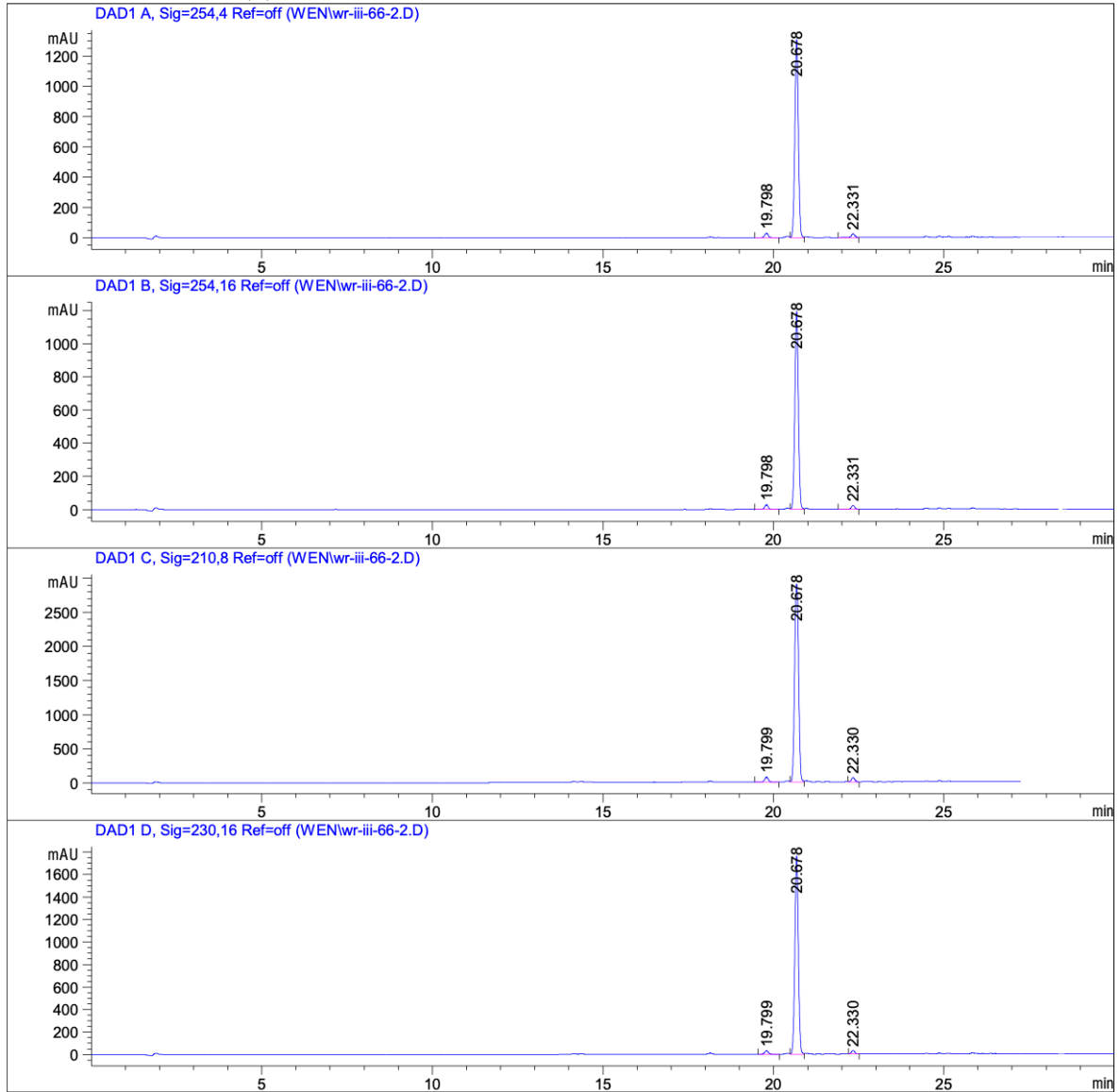


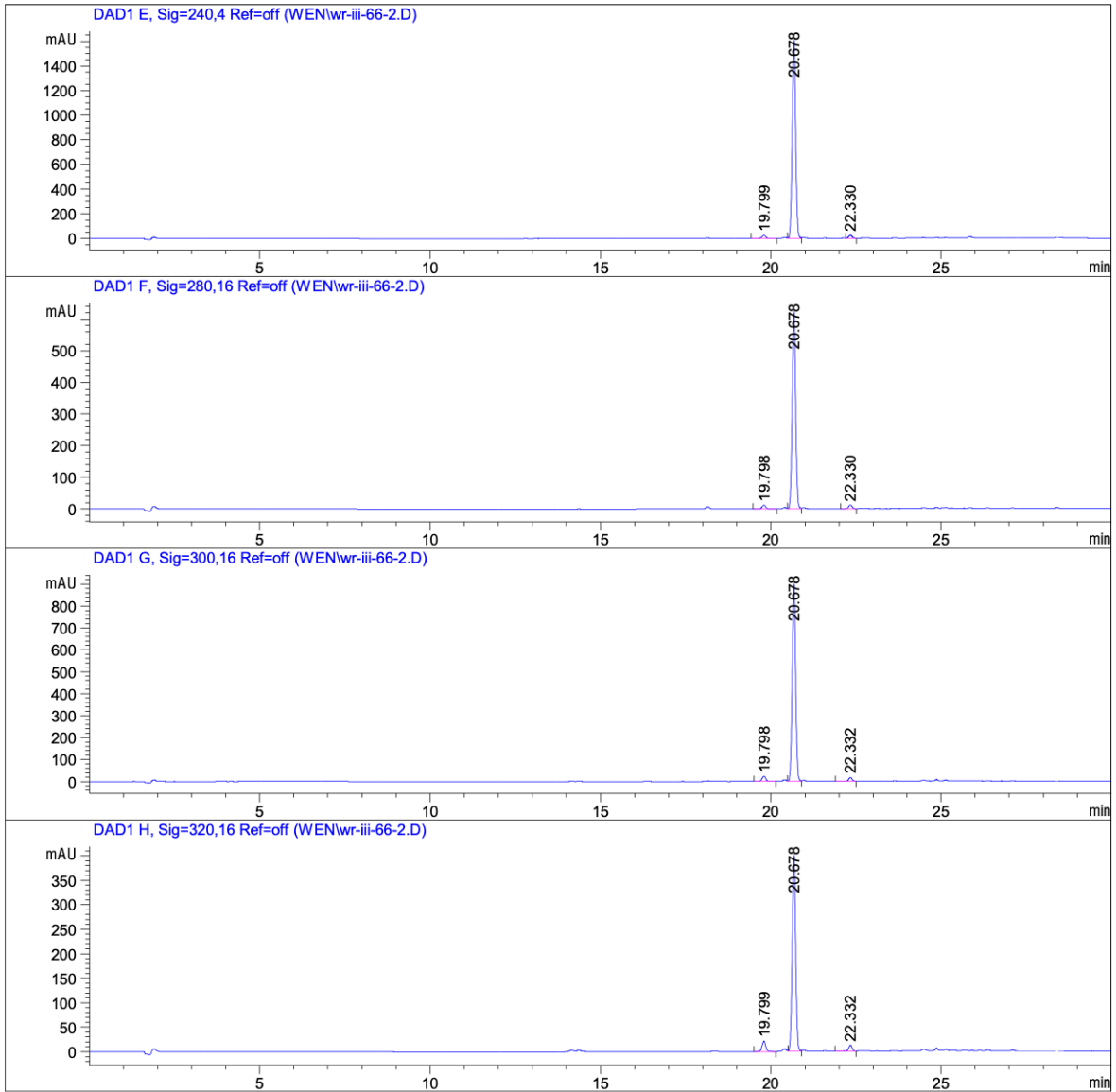
Data File C:\Chem32\1\Data\WEN\wr-iii-66-2.D
Sample Name: wr-iii-66-2

=====

Acq. Operator	: SYSTEM		
Sample Operator	: SYSTEM		
Acq. Instrument	: 1200 HPLC	Location	: 1
Injection Date	: 3/6/2023 1:03:39 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		

Additional Info : Peak(s) manually integrated





=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Sample Amount : 1.00000 [ng/ul] (not used in calc.)
Use Multiplier & Dilution Factor with ISTDs

Sample Name: wr-iii-66-2

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.798	BB	0.1097	215.90776	29.38068	2.2578
2	20.678	VV	0.1076	9165.81250	1309.95911	95.8476
3	22.331	BV	0.1104	181.17979	25.04303	1.8946

Totals : 9562.90005 1364.38282

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.798	BB	0.1099	207.12729	28.14017	2.3687
2	20.678	VV	0.1077	8361.29102	1194.12231	95.6214
3	22.331	BV	0.1109	175.74190	24.14511	2.0098

Totals : 8744.16020 1246.40760

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.799	VB	0.1124	558.50012	73.69063	2.3253
2	20.678	VV	0.1266	2.30417e4	2904.21143	95.9336
3	22.330	VB	0.1033	418.17468	63.08693	1.7411

Totals : 2.40183e4 3040.98898

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.799	BB	0.1100	227.12460	30.81322	1.7822
2	20.678	VV	0.1075	1.23009e4	1760.76233	96.5234
3	22.330	VB	0.1050	215.92987	31.88265	1.6944

Totals : 1.27440e4 1823.45820

Data File C:\Chem32\1\Data\WEN\wr-iii-66-2.D
Sample Name: wr-iii-66-2

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.799	BB	0.1114	192.46979	25.69604	1.6666
2	20.678	VV	0.1073	1.11849e4	1605.06494	96.8526
3	22.330	VB	0.1054	171.00220	25.12363	1.4807

Totals : 1.15484e4 1655.88461

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.798	BB	0.1113	89.84528	12.00837	1.9956
2	20.678	VV	0.1072	4326.65234	621.65009	96.1036
3	22.330	BV	0.1080	85.57549	12.17355	1.9008

Totals : 4502.07310 645.83201

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.798	BB	0.1099	181.20651	24.60402	2.7572
2	20.678	VV	0.1072	6264.99658	899.87030	95.3267
3	22.332	BV	0.1077	125.92751	17.54367	1.9161

Totals : 6572.13060 942.01800

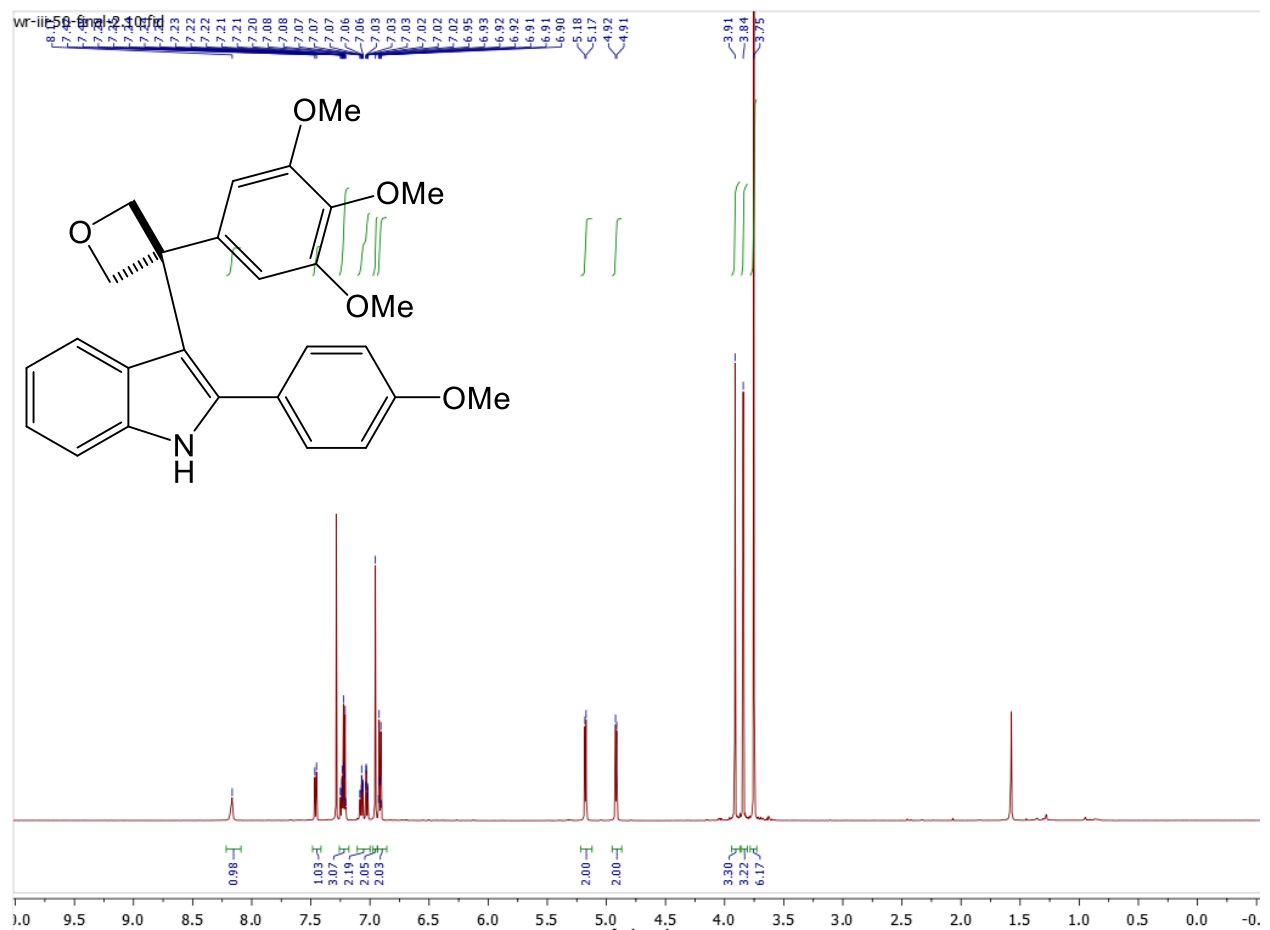
Signal 8: DAD1 H, Sig=320,16 Ref=off

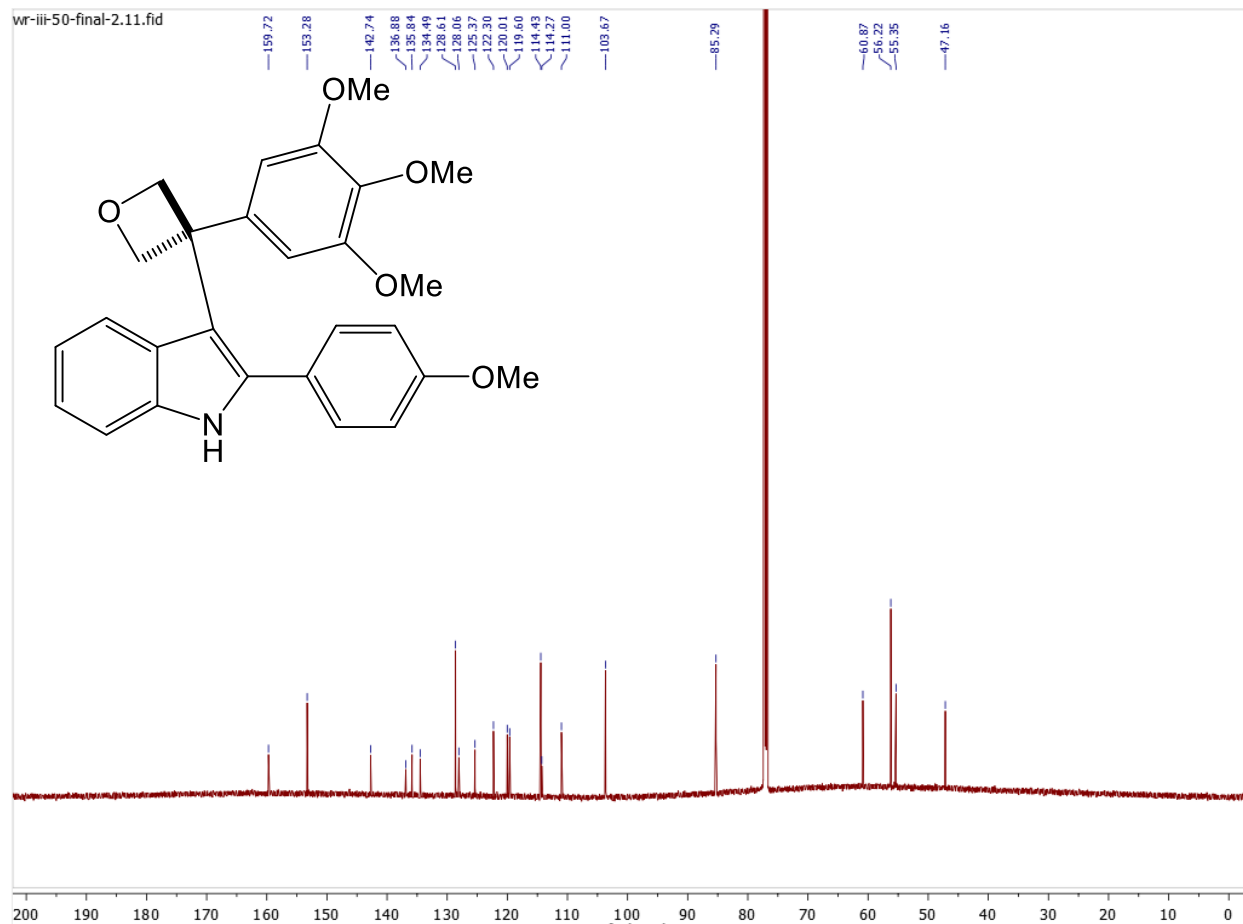
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.799	BB	0.1097	157.65778	21.45697	5.1899
2	20.678	VV	0.1073	2786.78467	399.75082	91.7375
3	22.332	BV	0.1102	93.34043	12.63743	3.0726

Totals : 3037.78288 433.84522

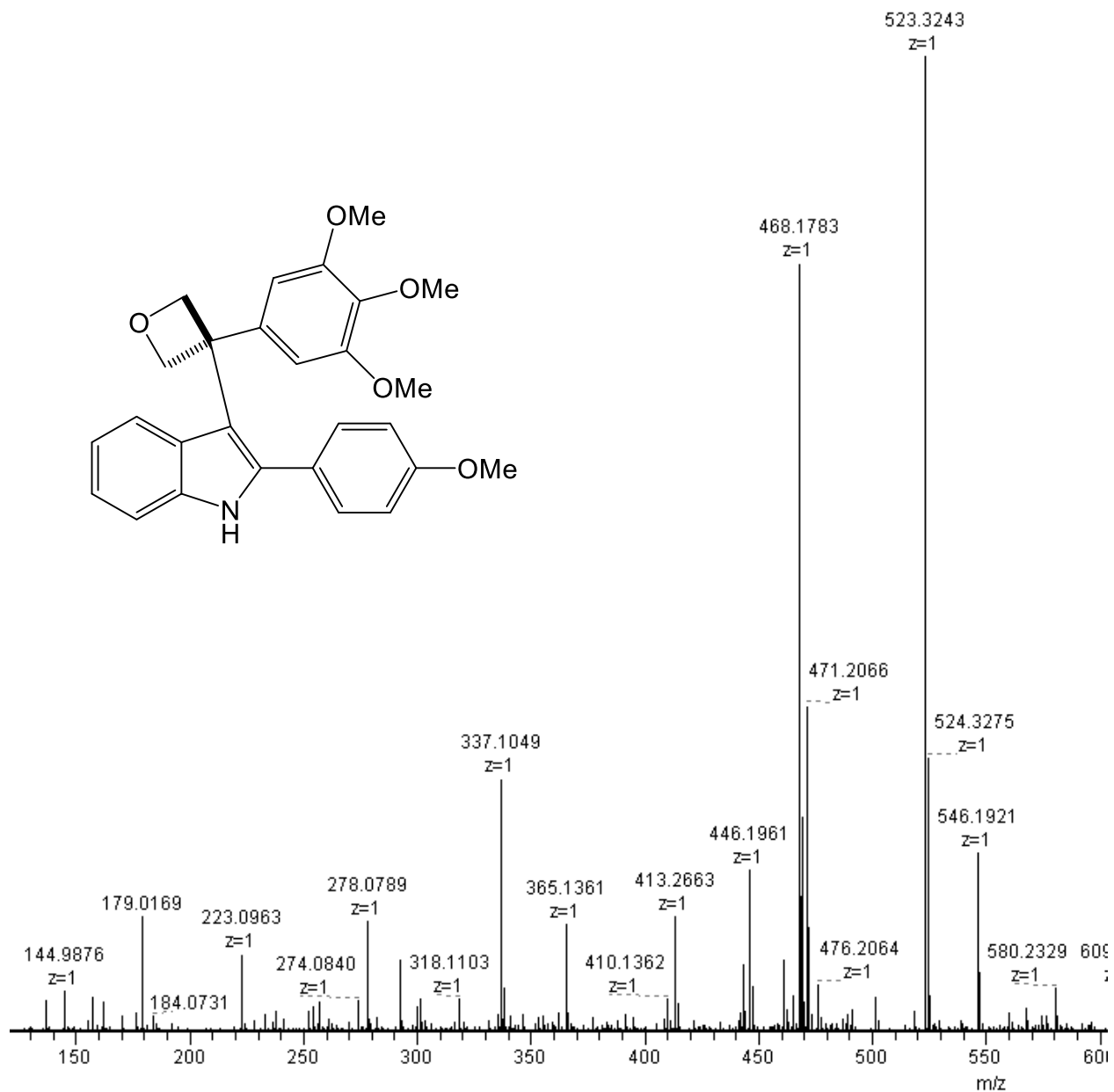
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*** End of Report ***

Compound 5i

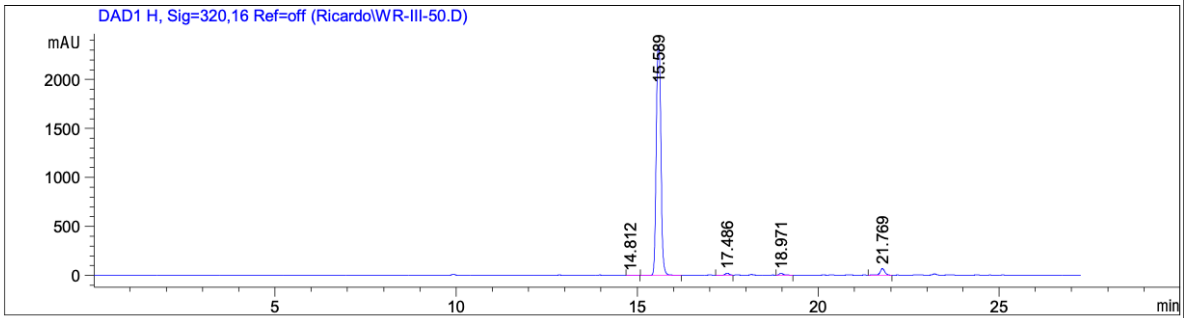




d RF=1240V Stable=4min TmpDiff Lock(1/1, +1ppm)



Data File C:\Chem32\1\Data\Ricardo\WR-III-50.D
 Sample Name: wr-iii-50



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 Area Percent Report
 =====

Sorted By : Signal
 Multiplier : 1.0000
 Dilution : 1.0000
 Sample Amount : 1.00000 [ng/ul] (not used in calc.)
 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	15.588	BV	0.1412	2.69445e4	3045.55371	99.8622
2	16.323	VV	0.1431	11.69677	1.20699	0.0434
3	17.007	VB	0.1287	25.48516	2.95151	0.0945

Totals : 2.69816e4 3049.71221

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.811	BB	0.1826	67.21581	5.00893	0.1499
2	15.576	BV	0.2234	4.18274e4	3061.66992	93.2925
3	17.485	VV	0.1179	380.36926	49.33554	0.8484
4	20.368	VB	0.1208	409.29581	52.59023	0.9129
5	20.855	BB	0.1739	650.81262	58.47007	1.4516
6	21.271	BV	0.1204	346.76022	44.74298	0.7734
7	21.786	VB	0.1685	717.54639	58.73730	1.6004
8	23.208	BB	0.1214	435.27579	55.55922	0.9708

Totals : 4.48347e4 3386.11420

Data File C:\Chem32\1\Data\Ricardo\WR-III-50.D
Sample Name: wr-iii-50

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.589	BB	0.1245	1.96185e4	2474.63892	98.7383
2	21.771	VV	0.1518	250.69673	24.02147	1.2617

Totals : 1.98692e4 2498.66038

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.588	BV	0.1553	2.77497e4	2857.06152	97.6041
2	18.971	VV	0.1275	185.84741	21.35965	0.6537
3	21.770	VV	0.1474	495.32086	49.22616	1.7422

Totals : 2.84309e4 2927.64733

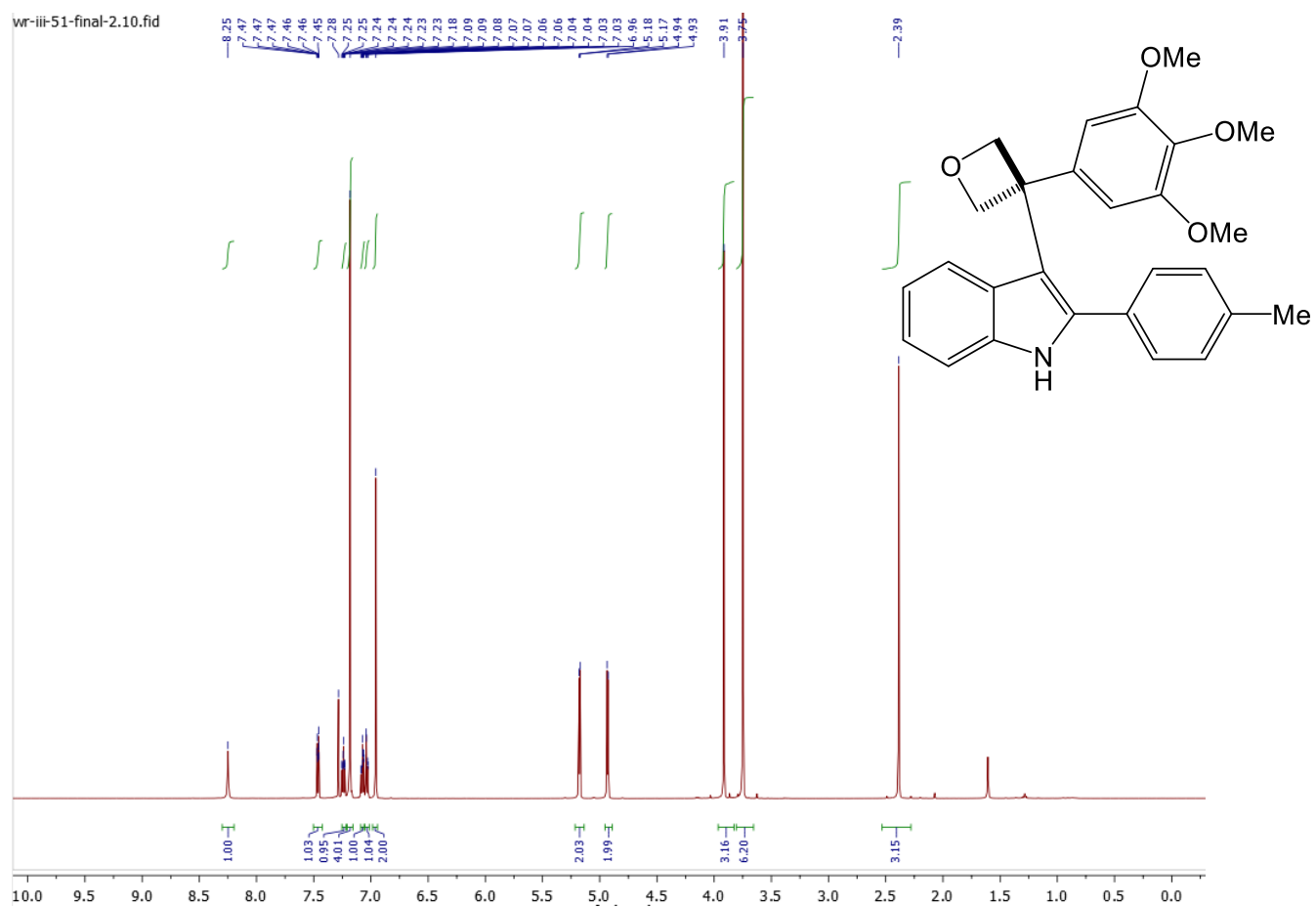
Signal 5: DAD1 H, Sig=320,16 Ref=off

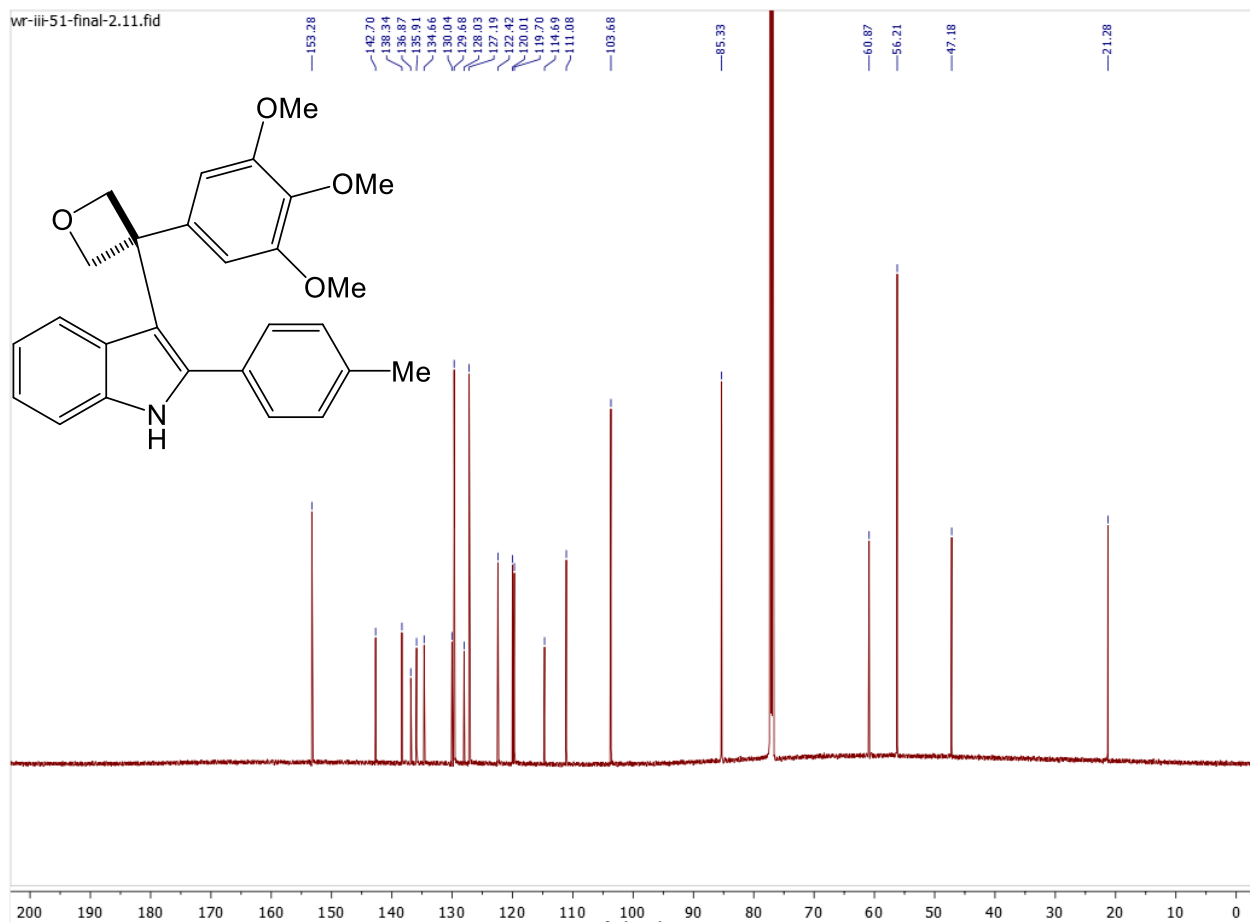
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.812	VB	0.1156	17.77576	2.31534	0.0811
2	15.589	BB	0.1417	2.09100e4	2351.58032	95.4370
3	17.486	BV	0.1195	172.93491	22.04464	0.7893
4	18.971	VV	0.1267	182.44273	21.14190	0.8327
5	21.769	VV	0.1363	626.57568	68.79659	2.8598

Totals : 2.19097e4 2465.87879

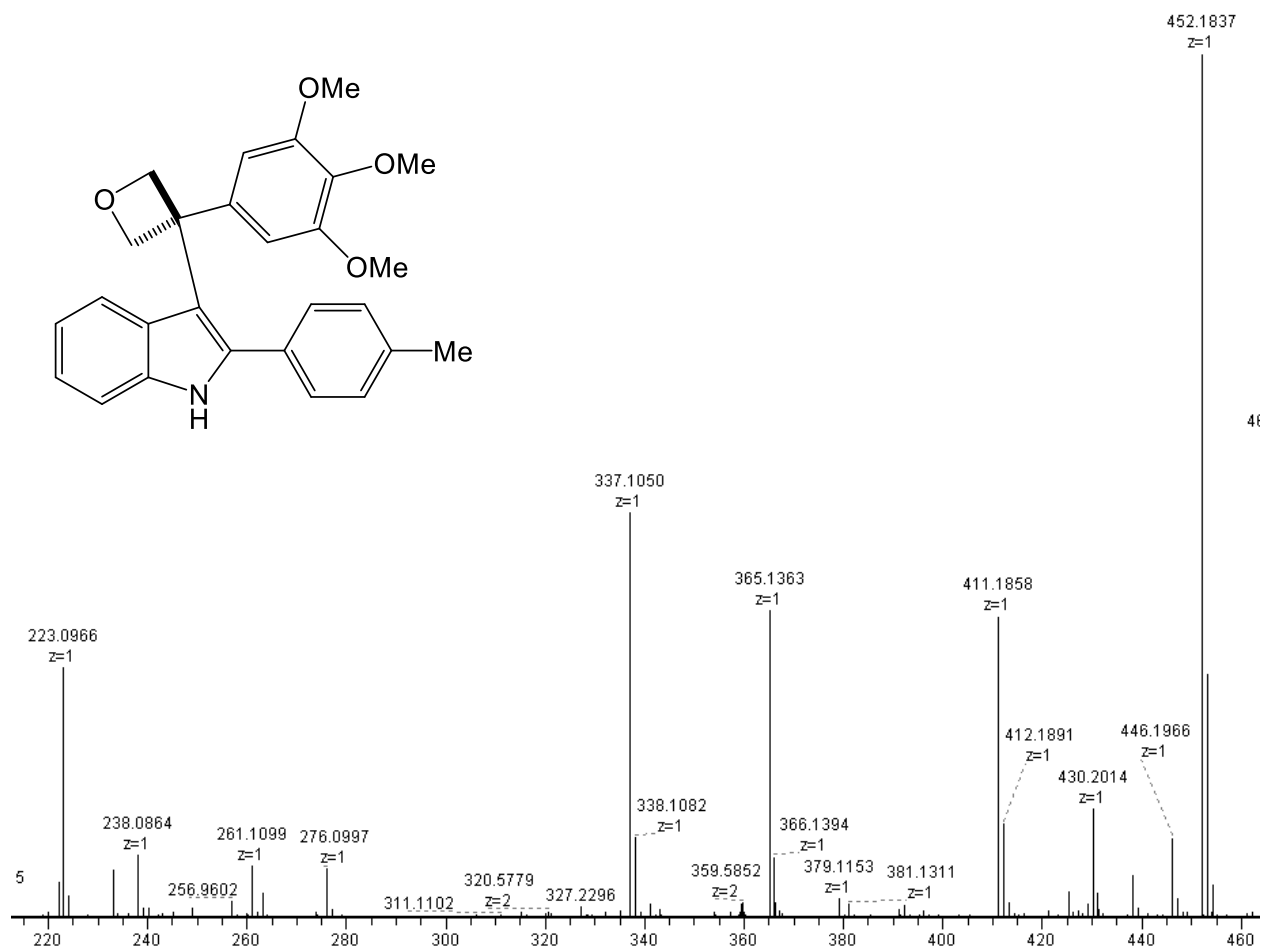
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*** End of Report ***

Compound 5j





10.00]
min TmpDiff Lock(inj391.3, 1/1, 0ppm)



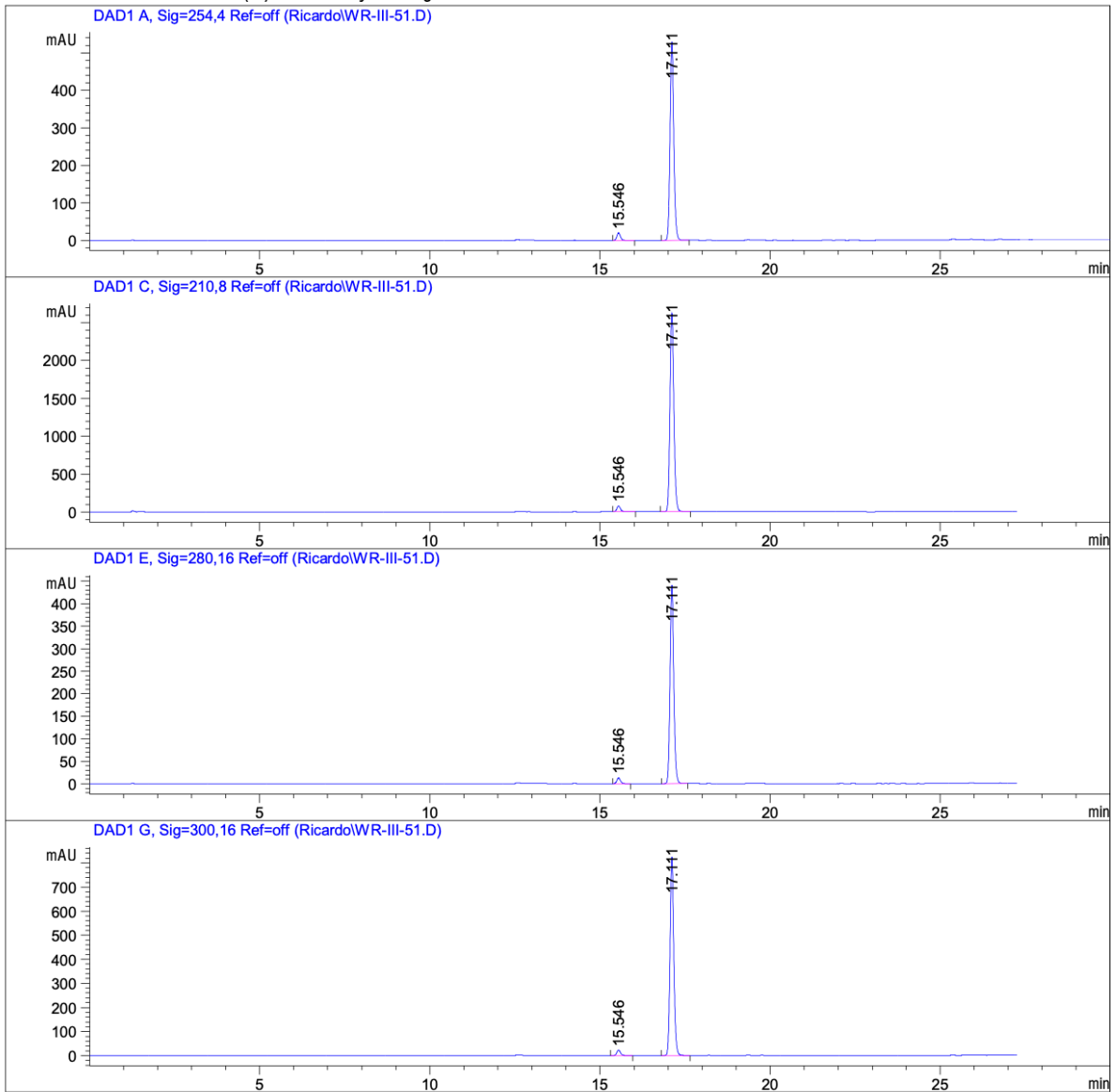
Data File C:\Chem32\1\Data\Ricardo\WR-III-51.D
Sample Name: wr-iii-51

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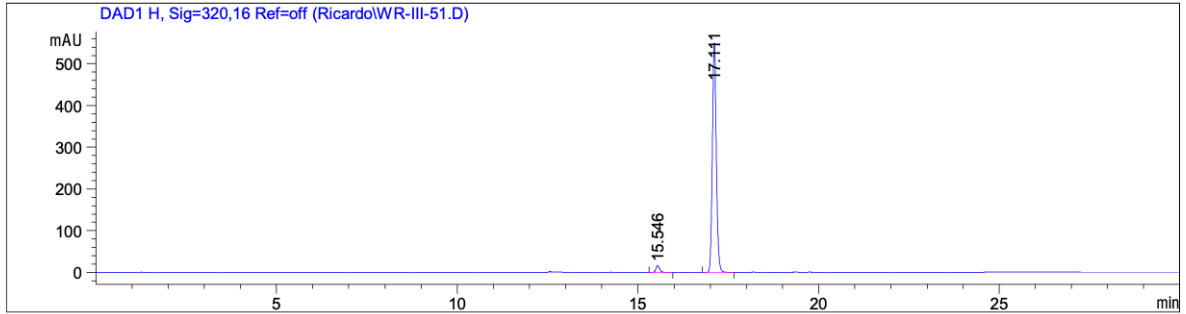
Acq. Operator	: SYSTEM		
Sample Operator	: SYSTEM		
Acq. Instrument	: 1200 HPLC	Location	: 1
Injection Date	: 3/30/2021 2:41:01 PM	Inj Volume	: No inj
Acq. Method	: C:\Chem32\1\Methods\GRAD 2 30-90 ACN.M		
Last changed	: 4/2/2014 4:04:33 PM by ERICA P		
Analysis Method	: C:\Chem32\1\Methods\RT-ACNWASH 2.M		
Last changed	: 7/9/2015 2:27:22 PM by Blake		
Method Info	: General Column Wash Method		

Sample Info : 30-90 ACN wr-iii-51

Additional Info : Peak(s) manually integrated



Data File C:\Chem32\1\Data\Ricardo\WR-III-51.D
 Sample Name: wr-iii-51



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 Area Percent Report
 =====

Sorted By : Signal
 Multiplier : 1.0000
 Dilution : 1.0000
 Sample Amount : 1.00000 [ng/ul] (not used in calc.)
 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	15.546	BB	0.1158	155.17206	20.62951	3.6327
2	17.111	BB	0.1187	4116.32666	529.73645	96.3673

Totals : 4271.49872 550.36596

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.546	VV	0.1186	608.21960	78.34319	2.7868
2	17.111	BB	0.1264	2.12170e4	2622.46924	97.2132

Totals : 2.18252e4 2700.81242

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.546	BB	0.1156	99.22981	13.22059	2.8255
2	17.111	BB	0.1182	3412.71826	441.37155	97.1745

Totals : 3511.94807 454.59215

Data File C:\Chem32\1\Data\Ricardo\WR-III-51.D
Sample Name: wr-iii-51

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.546	BB	0.1160	178.06367	23.61539	2.7060
2	17.111	BB	0.1184	6402.19385	826.61566	97.2940

Totals : 6580.25752 850.23105

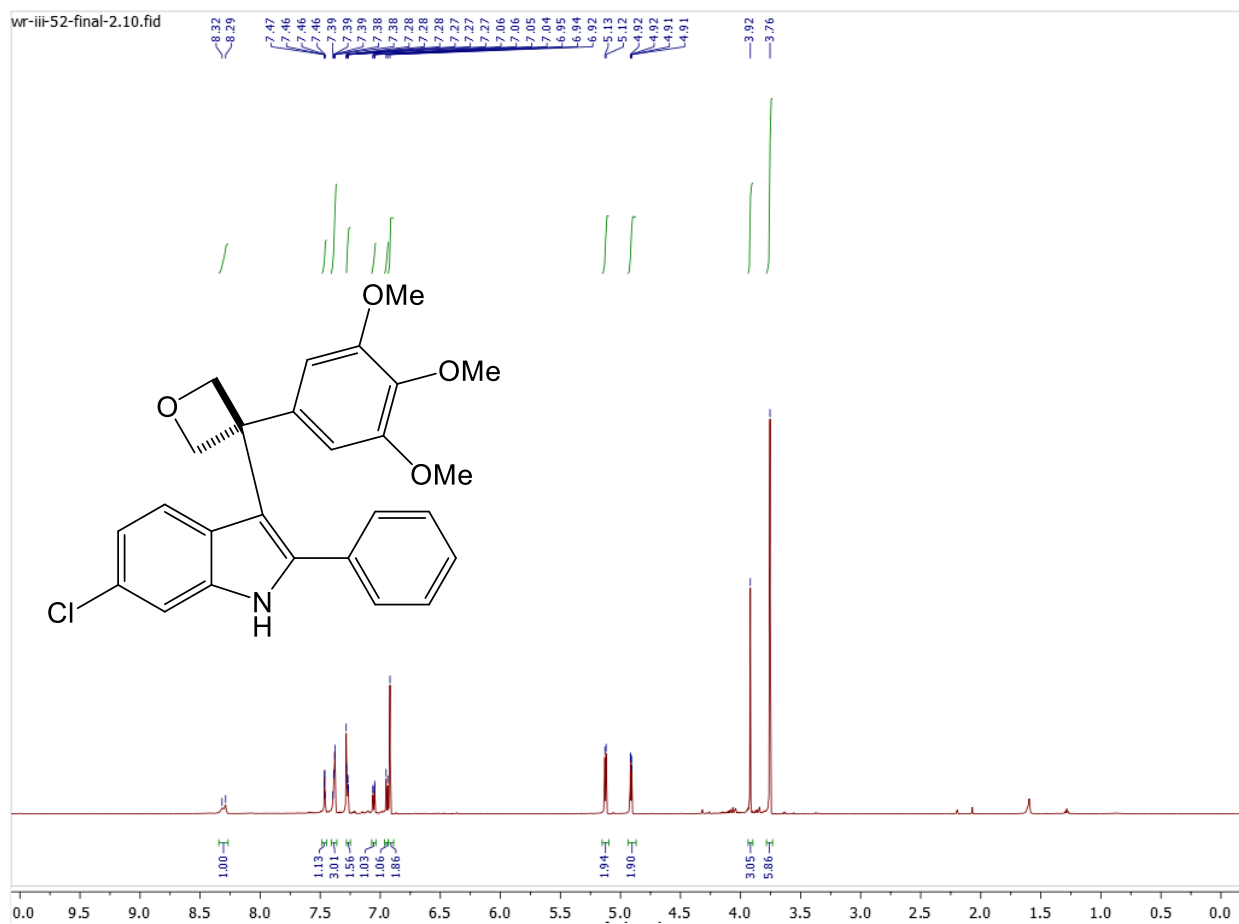
Signal 5: DAD1 H, Sig=320,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.546	BB	0.1165	122.06917	16.09184	2.7765
2	17.111	BB	0.1184	4274.45313	551.40344	97.2235

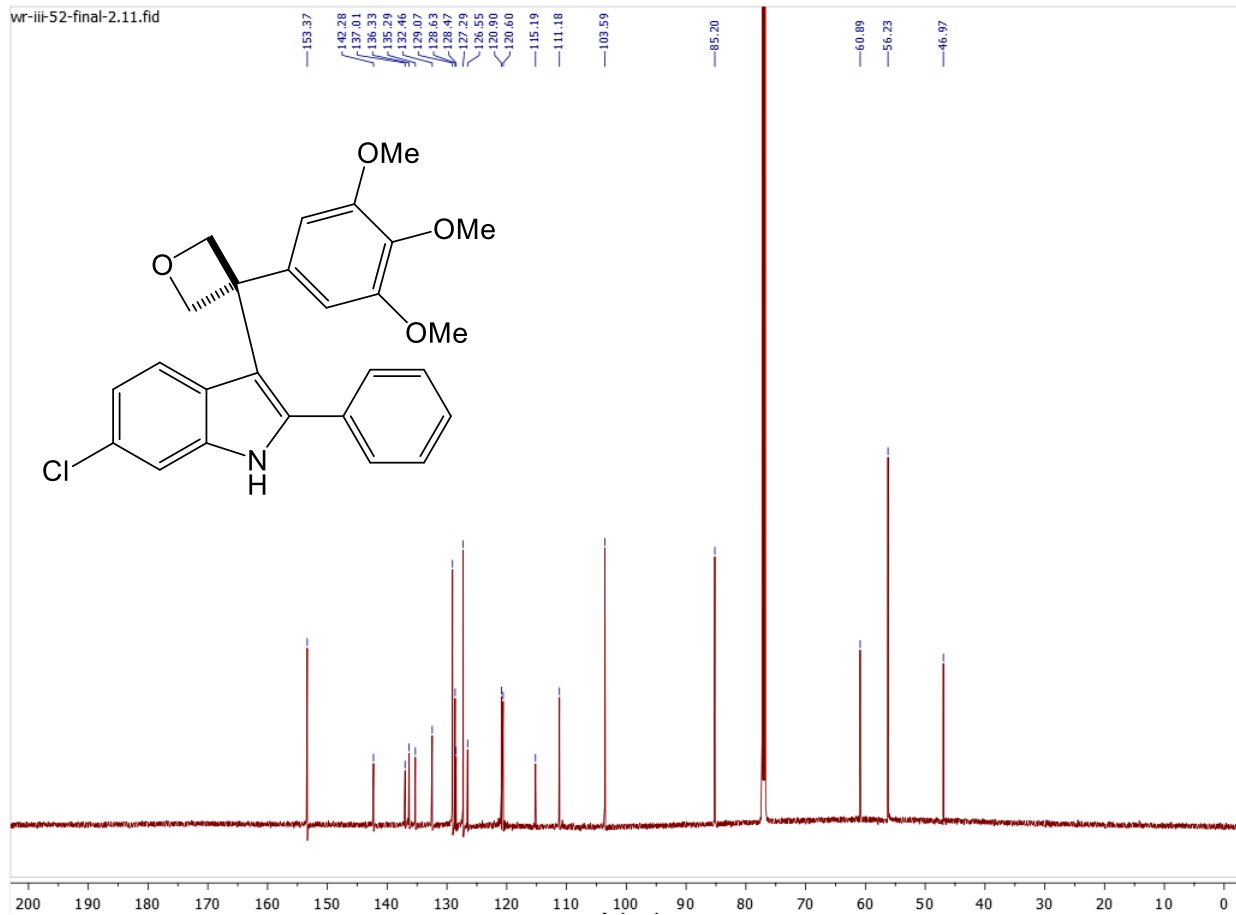
Totals : 4396.52229 567.49529

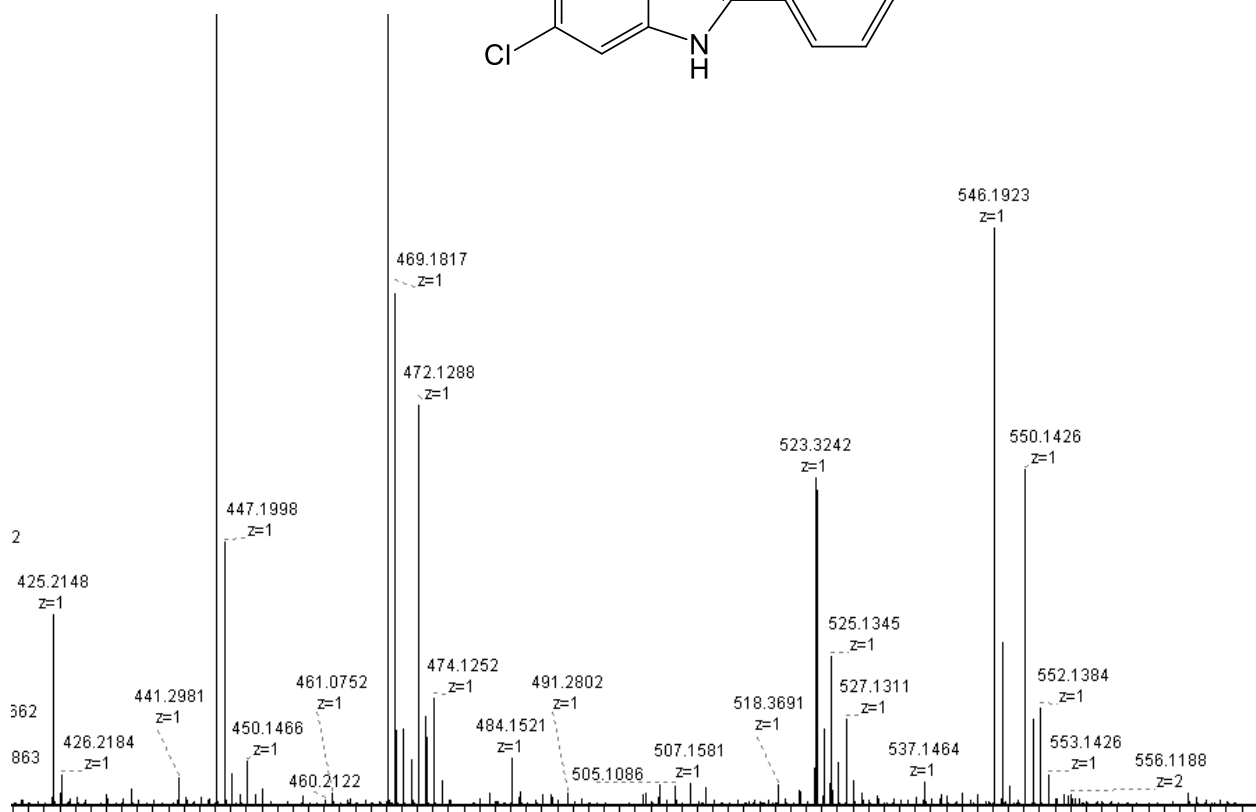
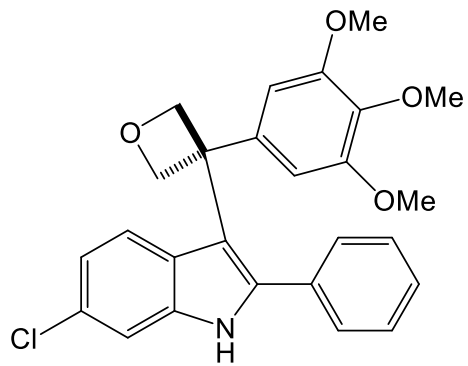
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*** End of Report ***

Compound 5k

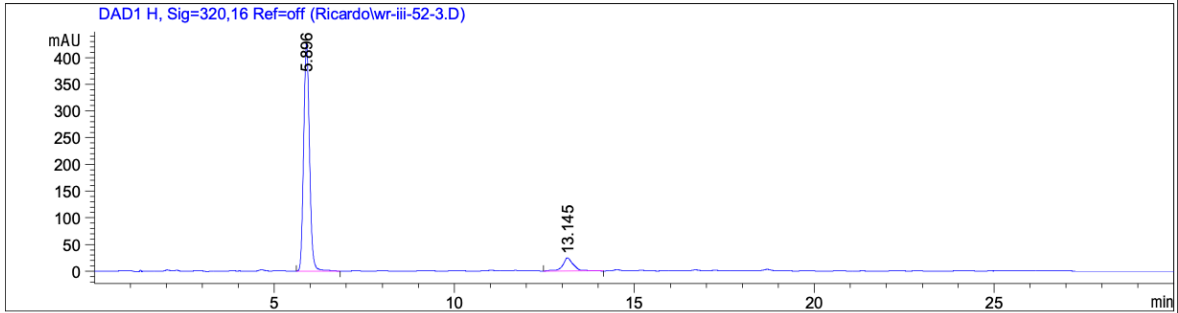


wr-iii-52-final-2.11.fid





Data File C:\Chem32\1\Data\Ricardo\wr-iii-52-3.D
 Sample Name: wr-iii-52-3



=====
 Area Percent Report
 =====

Sorted By : Signal
 Multiplier : 1.0000
 Dilution : 1.0000
 Sample Amount: : 1.00000 [ng/ul] (not used in calc.)
 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	5.896	BB	0.1798	4894.52197	426.67896	86.7160
2	13.149	VB	0.2784	749.79047	37.97300	13.2840

Totals : 5644.31244 464.65196

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.895	BV	0.1802	2.01088e4	1748.11218	92.7887
2	12.718	BV	0.2128	367.41565	26.00728	1.6954
3	13.142	VV	0.2755	1066.93445	54.71981	4.9232
4	13.676	VB	0.2697	128.44844	6.35697	0.5927

Totals : 2.16716e4 1835.19624

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.896	BB	0.1802	2419.03955	210.26505	83.0804
2	13.291	VB	0.3154	492.64685	21.17661	16.9196

Data File C:\Chem32\1\Data\Ricardo\wr-iii-52-3.D

Sample Name: wr-iii-52-3

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
Totals :				2911.68640	231.44165	

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

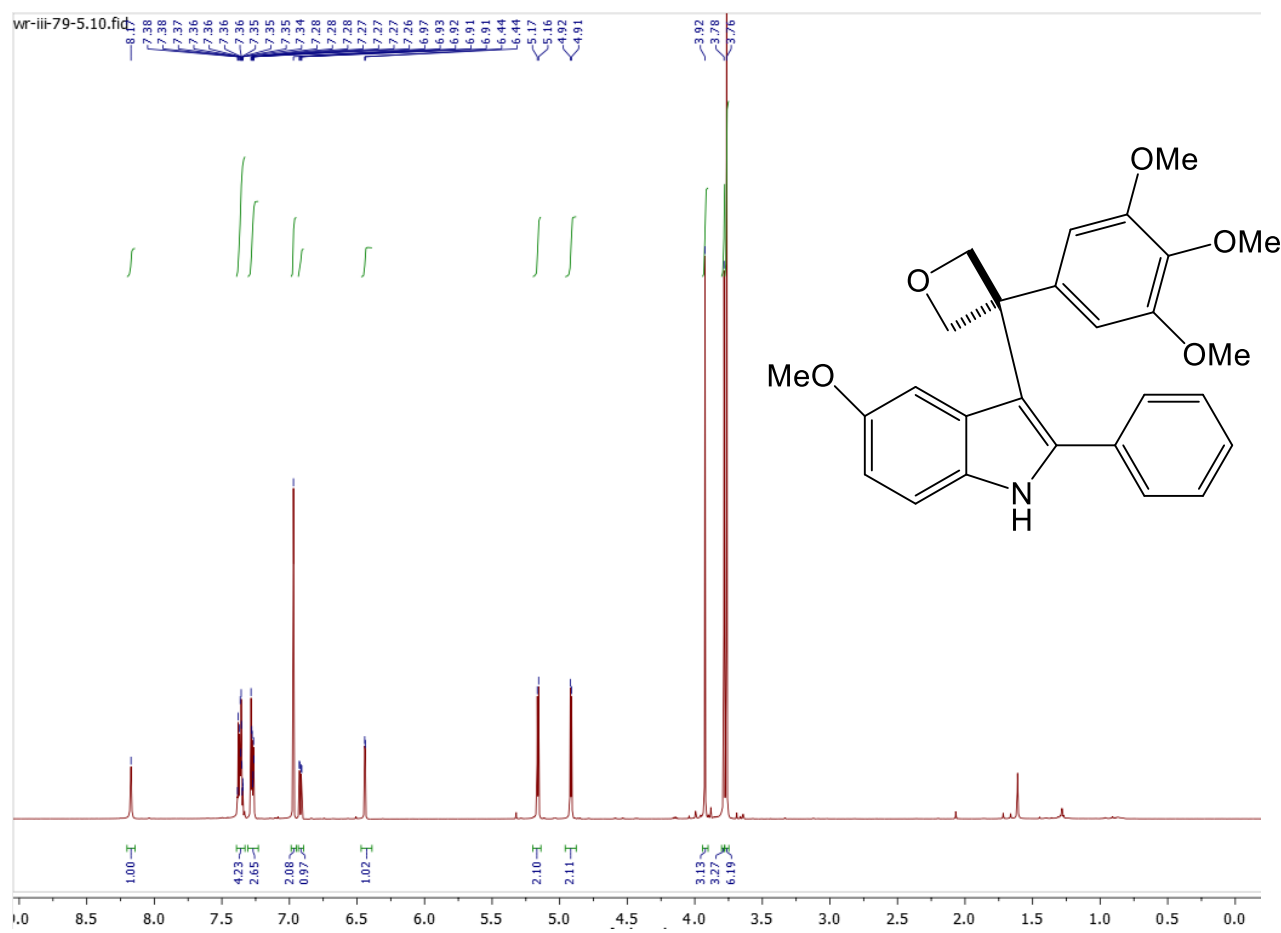
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.896	BB	0.1786	4907.32666	431.75131	89.8675
2	6.971	BB	0.1929	16.49167	1.40543	0.3020
3	12.728	BV	0.1817	28.02455	2.37365	0.5132
4	13.163	VB	0.3067	508.77982	22.76542	9.3172
Totals :				5460.62270	458.29581	

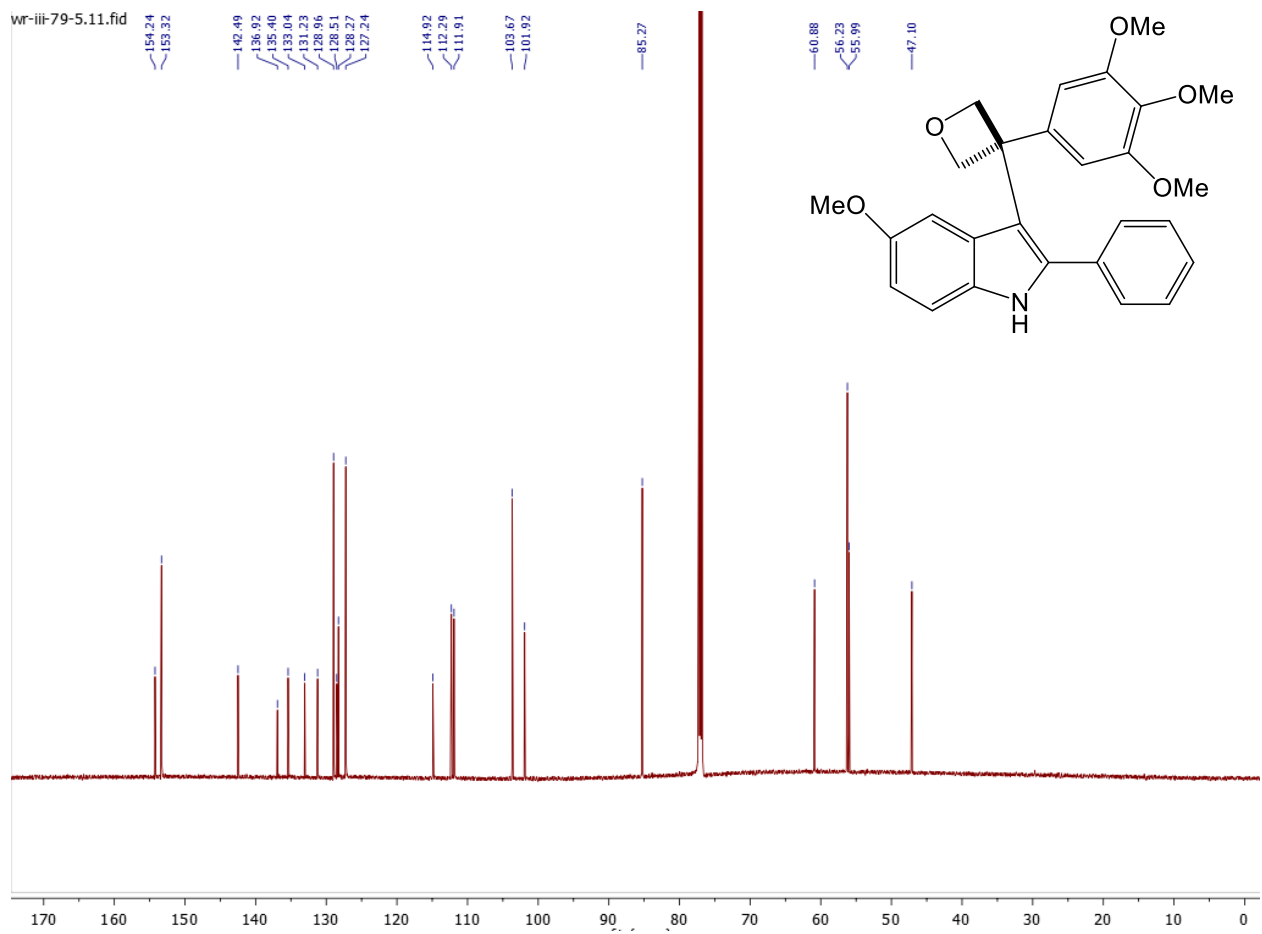
Signal 5: DAD1 H, Sig=320,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.896	BB	0.1785	4850.44922	427.23105	90.5085
2	13.145	BB	0.2884	508.65955	24.89326	9.4915
Totals :				5359.10876	452.12431	

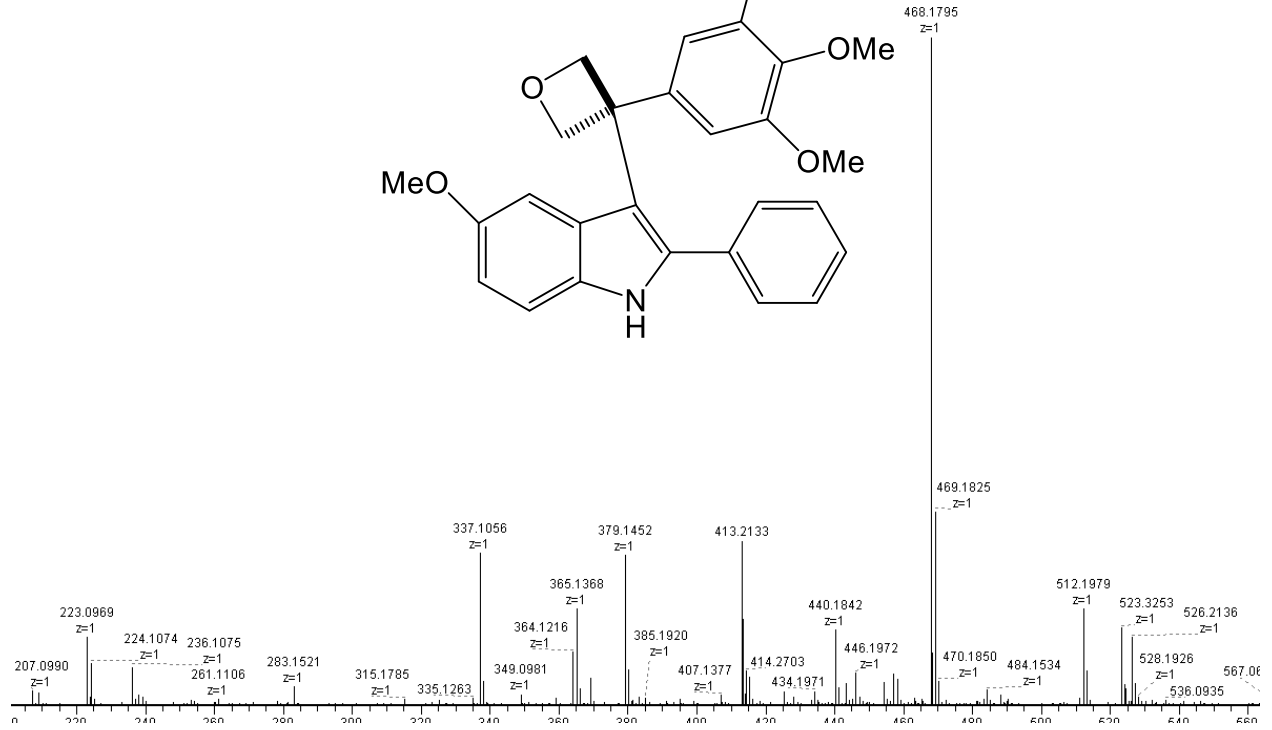
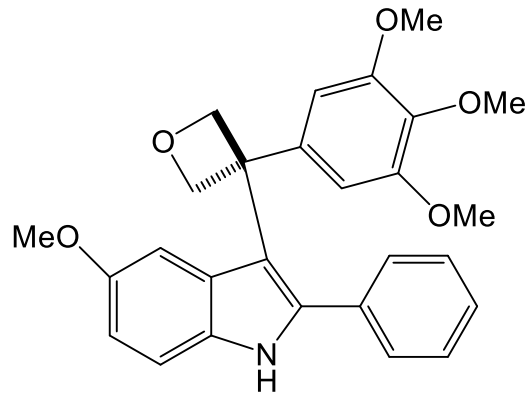
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*** End of Report ***

Compound 51

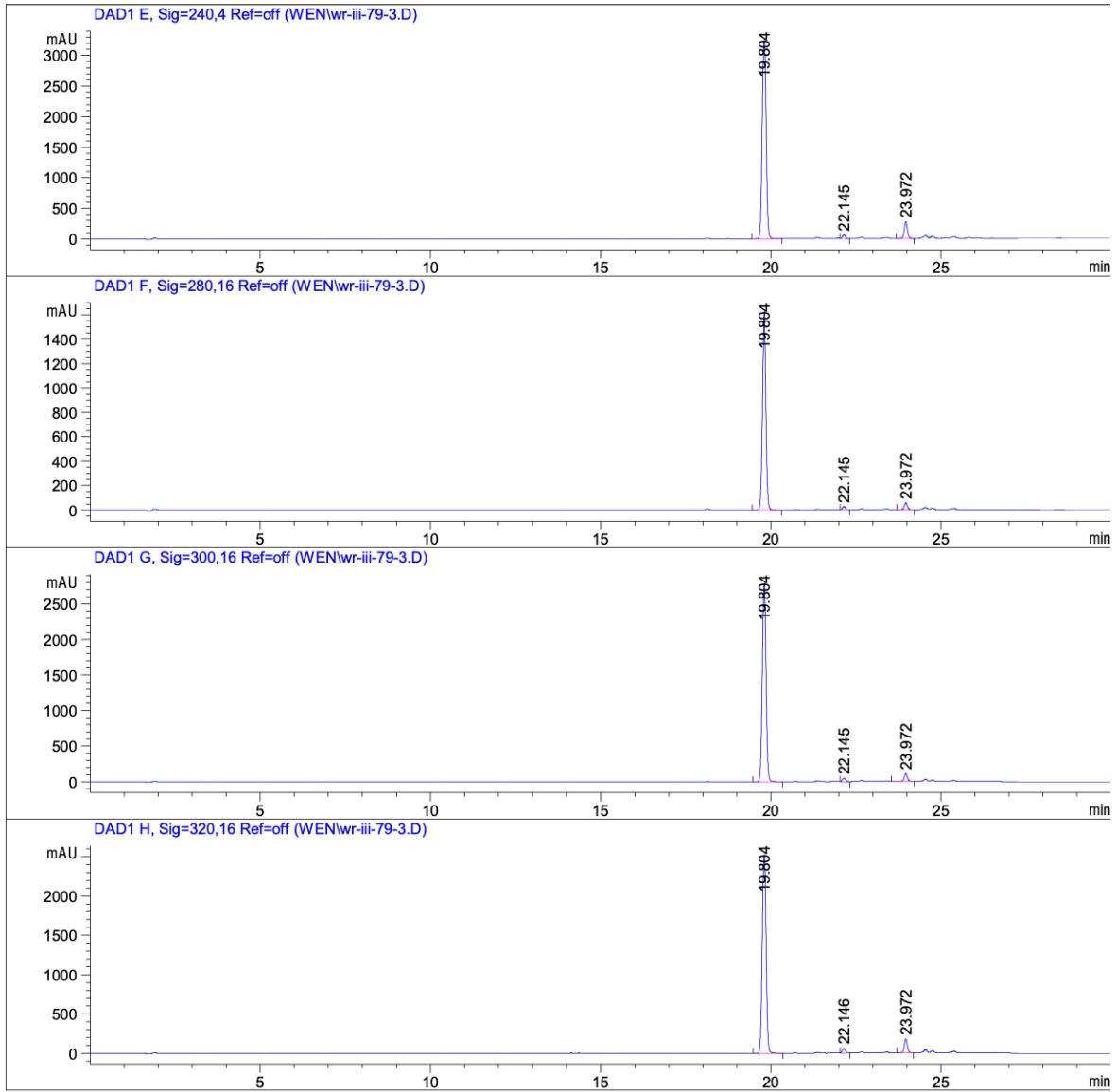




IT: 9.976 ST: 0.65 uS: 1 CS: 1 AMW: 467.17 NL: 4.08E7
+ p ESI Full ms [200.00-600.00]
il=3d RF=2300V TmpDiff Lock(1/1, +7ppm)



Data File C:\Chem32\1\Data\WEN\wr-iii-79-3.D
Sample Name: wr-iii-79-3



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Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Sample Amount: : 1.00000 [ng/ul] (not used in calc.)
Use Multiplier & Dilution Factor with ISTDs

Data File C:\Chem32\1\Data\WEN\wr-iii-79-3.D
Sample Name: wr-iii-79-3

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.804	BB	0.1070	1.19571e4	1721.52454	91.4717
2	22.145	VB	0.0945	256.08728	42.38355	1.9591
3	23.972	BB	0.0984	604.16827	94.75039	4.6219
4	24.549	BV	0.1110	254.55943	34.14898	1.9474

Totals : 1.30719e4 1892.80745

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.804	BB	0.1081	1.31459e4	1867.05139	94.9395
2	23.972	VB	0.0989	700.70874	109.17844	5.0605

Totals : 1.38466e4 1976.22983

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.807	VV	0.1839	3.70037e4	3272.19019	85.3839
2	22.145	VB	0.0941	521.38971	86.75980	1.2031
3	23.972	BB	0.0973	4413.84863	702.31647	10.1847
4	24.548	VV	0.1136	727.65814	94.72643	1.6790
5	25.385	VB	0.1249	671.43762	80.85714	1.5493

Totals : 4.33380e4 4236.85002

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.804	VV	0.1505	3.11274e4	3345.63794	93.2722
2	23.972	BV	0.0978	2245.23389	354.75153	6.7278

Totals : 3.33727e4 3700.38947

Data File C:\Chem32\1\Data\WEN\wr-iii-79-3.D
Sample Name: wr-iii-79-3

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.804	BV	0.1316	2.65419e4	3240.31958	92.6386
2	22.145	VB	0.0944	370.58215	61.39384	1.2934
3	23.972	BB	0.0977	1738.52783	275.15390	6.0679

Totals : 2.86510e4 3576.86732

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.804	BB	0.1070	1.12664e4	1623.22388	95.5305
2	22.145	VB	0.0945	167.03540	27.64040	1.4163
3	23.972	BB	0.0998	360.07422	55.39006	3.0531

Totals : 1.17935e4 1706.25433

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.804	BV	0.1219	2.14595e4	2785.30298	95.3193
2	22.145	VB	0.0948	312.22397	51.46977	1.3868
3	23.972	VB	0.1019	741.56122	111.10456	3.2939

Totals : 2.25133e4 2947.87731

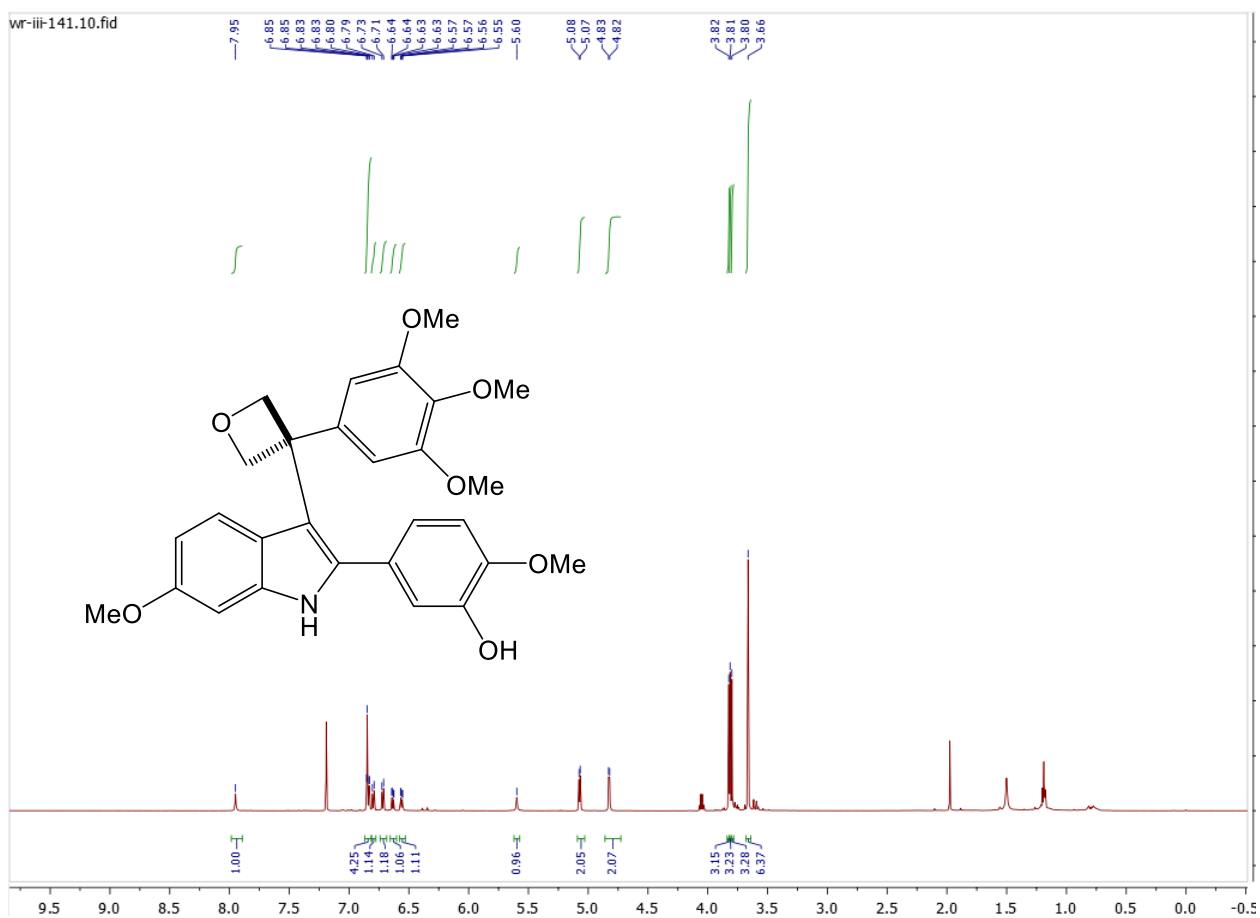
Signal 8: DAD1 H, Sig=320,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.804	BV	0.1271	2.01174e4	2520.65381	92.9423
2	22.146	VB	0.0947	366.05951	60.38461	1.6912
3	23.972	VB	0.0990	1161.58008	180.74988	5.3665

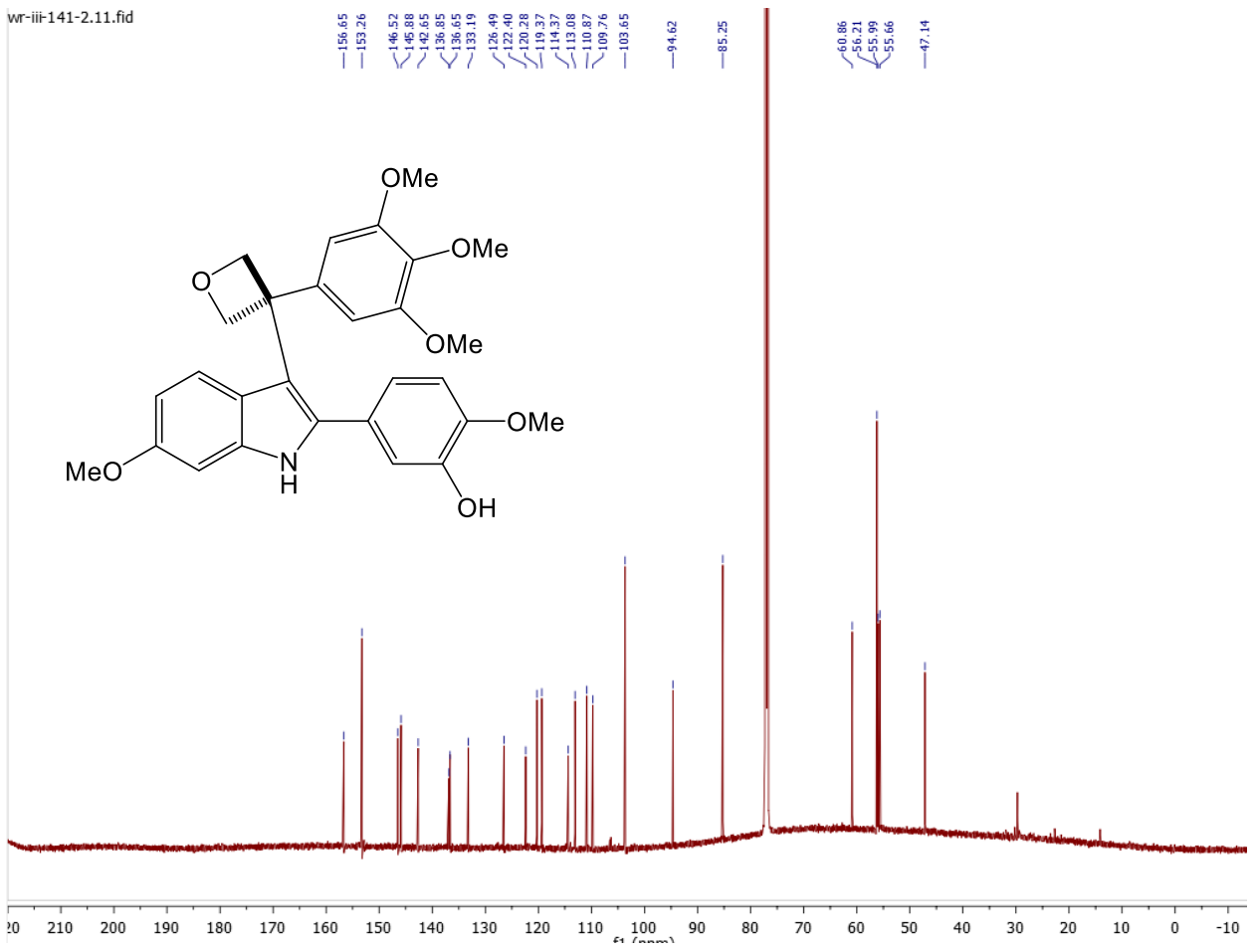
Totals : 2.16451e4 2761.78830

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*** End of Report ***

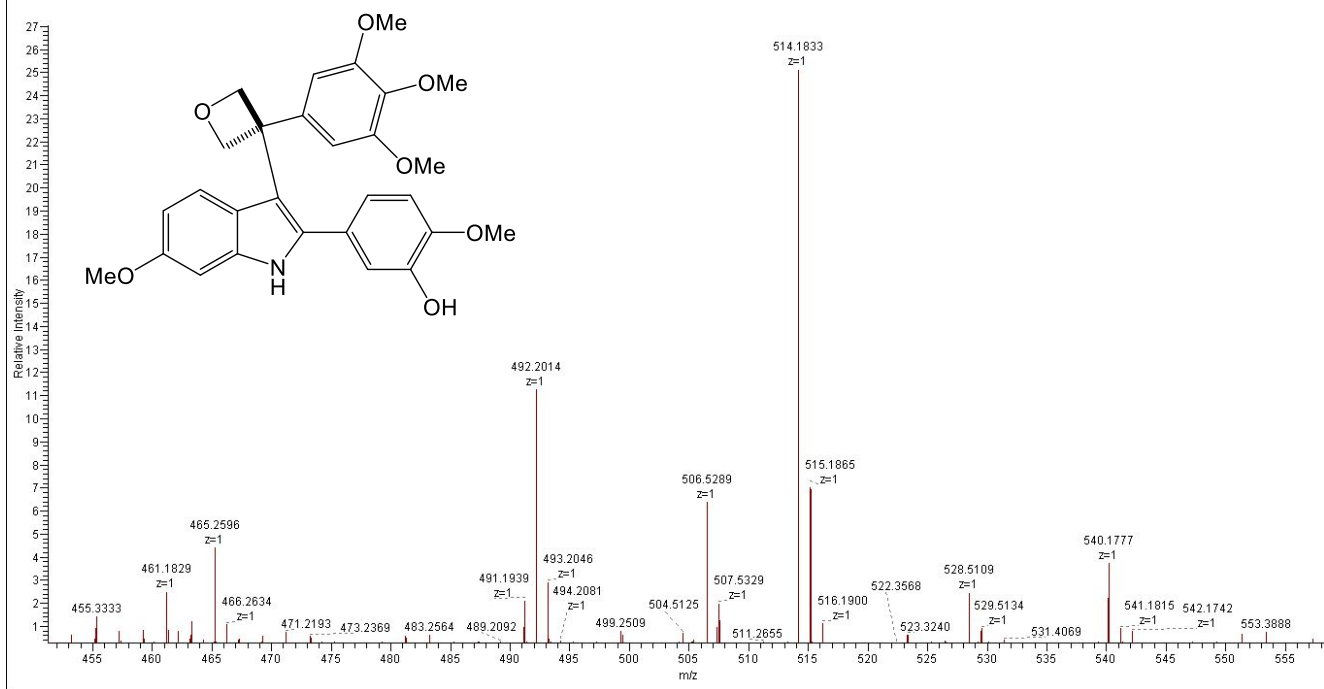
Compound 5m



wr-iii-141-2.11.fid



#1800 AV: 3 IT: 400.000 ST: 1.04 uS: 1 NL: 1.12E6
F: FTMS + p ESI Full ms [50.00-750.00]
Info: Ufill=0.01 RF=600V



Data File C:\Chem32\1\Data\Ricardo\WR-III-137.D
Sample Name: WR-III-137

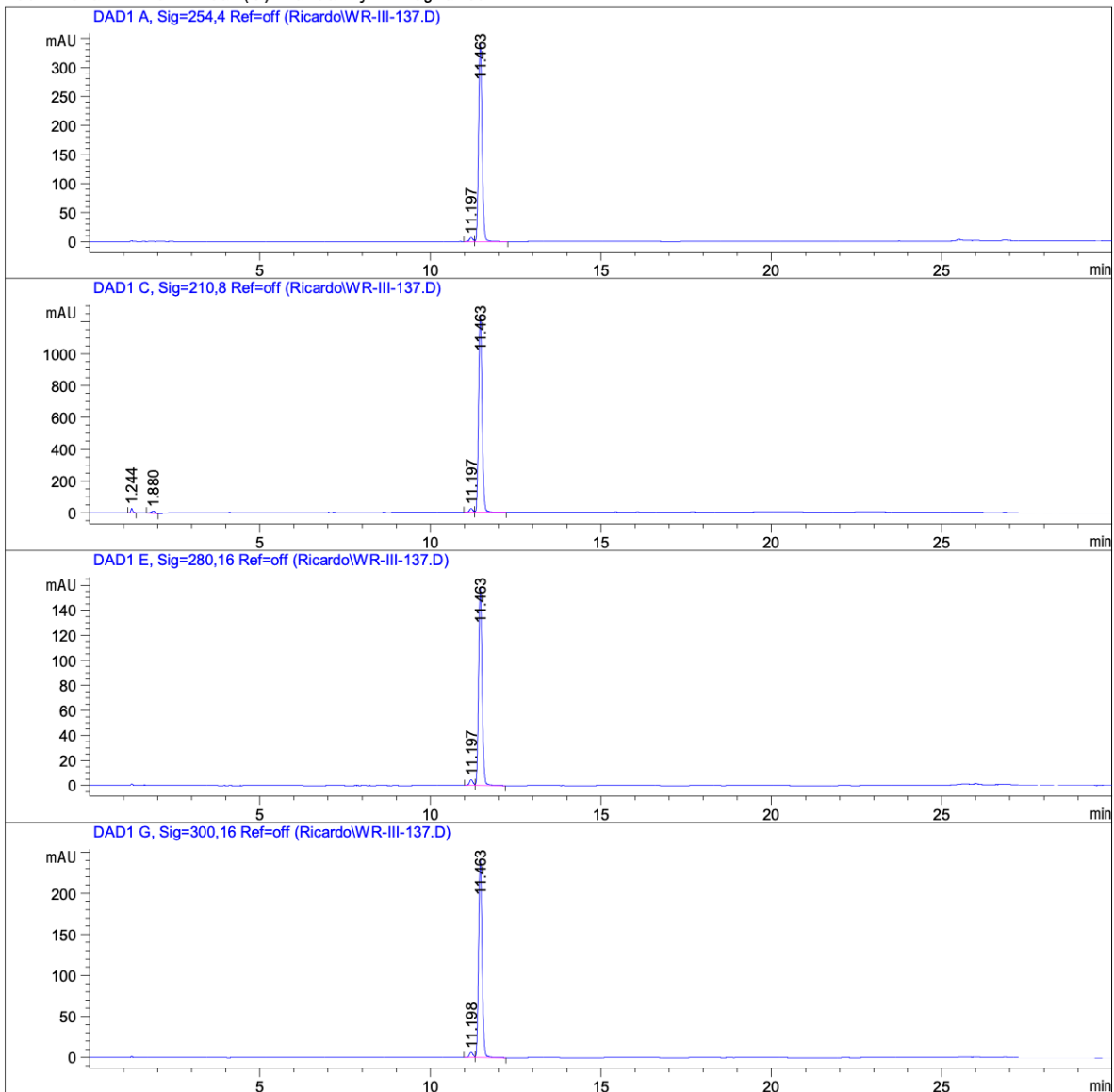
=====

Acq. Operator : SYSTEM
Sample Operator : SYSTEM
Acq. Instrument : 1200 HPLC Location : 1
Injection Date : 3/29/2021 2:11:46 PM Inj Volume : No inj

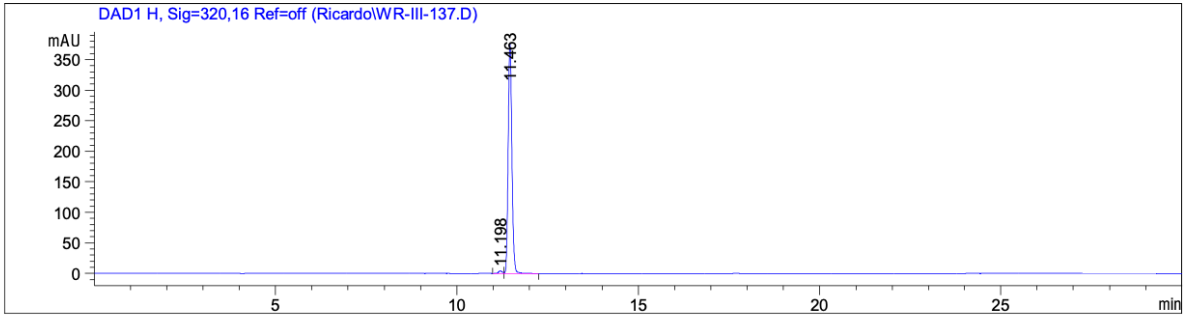
Acq. Method : C:\Chem32\1\Methods\GRAD 2 30-90 ACN.M
Last changed : 4/2/2014 4:04:33 PM by ERICA P
Analysis Method : C:\Chem32\1\Methods\RT-ACNWASH 2.M
Last changed : 7/9/2015 2:27:22 PM by Blake
Method Info : General Column Wash Method

Sample Info : WR-III-137 OXi8006 oxetane 30-90 ACN

Additional Info : Peak(s) manually integrated



Data File C:\Chem32\1\Data\Ricardo\WR-III-137.D
 Sample Name: WR-III-137



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 Area Percent Report
 =====

Sorted By : Signal
 Multiplier : 1.0000
 Dilution : 1.0000
 Sample Amount : 1.00000 [ng/ul] (not used in calc.)
 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	11.197	BV	0.1088	49.06672	6.90990	2.0152
2	11.463	VB	0.1073	2385.76221	342.48453	97.9848

Totals : 2434.82893 349.39443

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.244	BV	0.0587	104.28168	27.23908	1.1478
2	1.880	VB	0.1357	137.16713	14.85493	1.5097
3	11.197	BV	0.1062	163.59390	23.78542	1.8006
4	11.463	VB	0.1074	8680.57520	1243.79224	95.5419

Totals : 9085.61790 1309.67167

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.197	BV	0.1088	32.96772	4.64467	2.8806
2	11.463	VB	0.1076	1111.49072	158.95779	97.1194

Data File C:\Chem32\1\Data\Ricardo\WR-III-137.D
Sample Name: WR-III-137

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
----- ----- ----- ----- ----- ----- -----						
Totals :				1144.45844	163.60246	

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

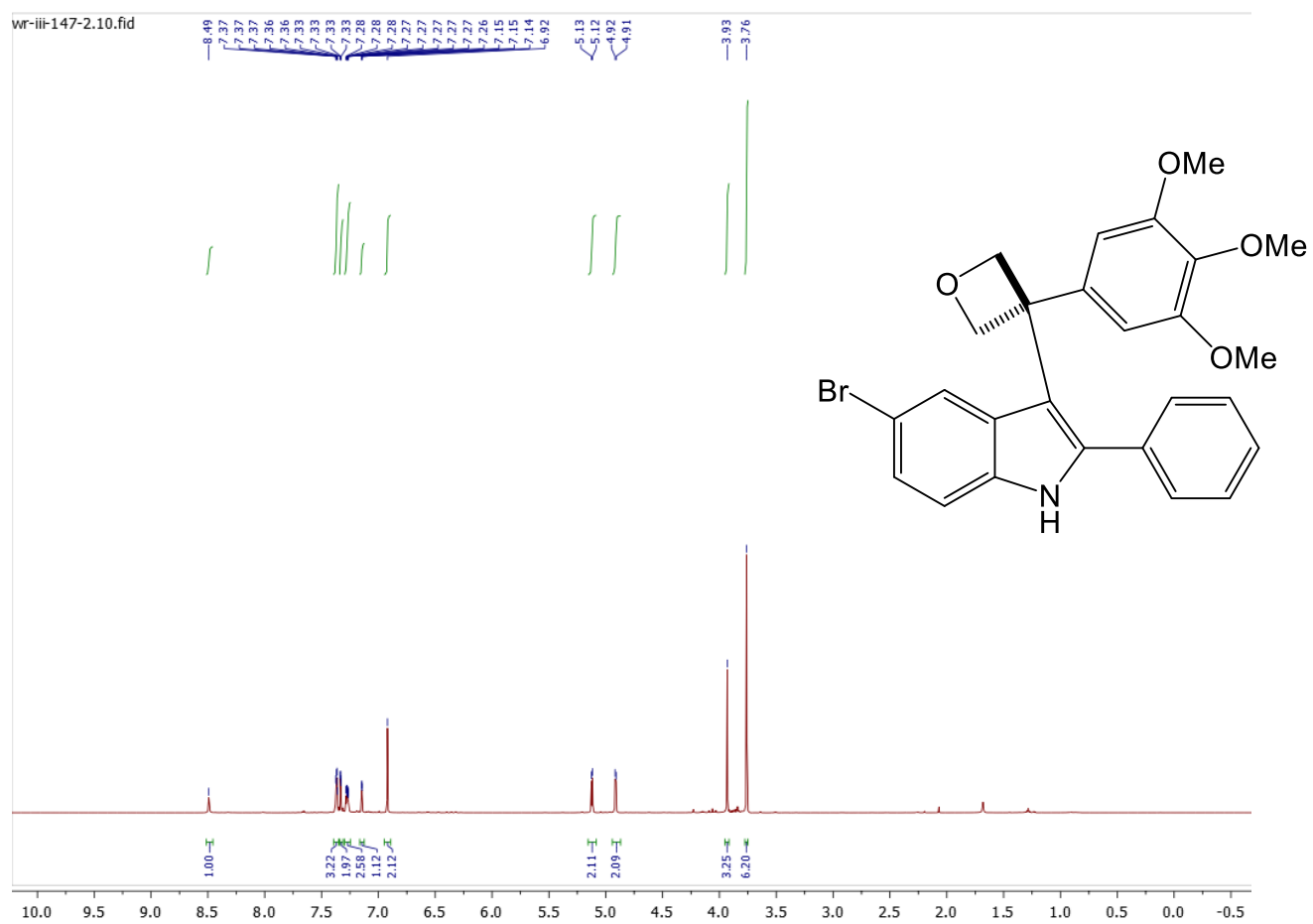
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
----- ----- ----- ----- ----- ----- -----						
1	11.198	BV	0.1081	46.57622	6.61492	2.6848
2	11.463	VB	0.1073	1688.24109	242.20956	97.3152
----- ----- ----- ----- ----- ----- -----						
Totals :				1734.81731	248.82448	

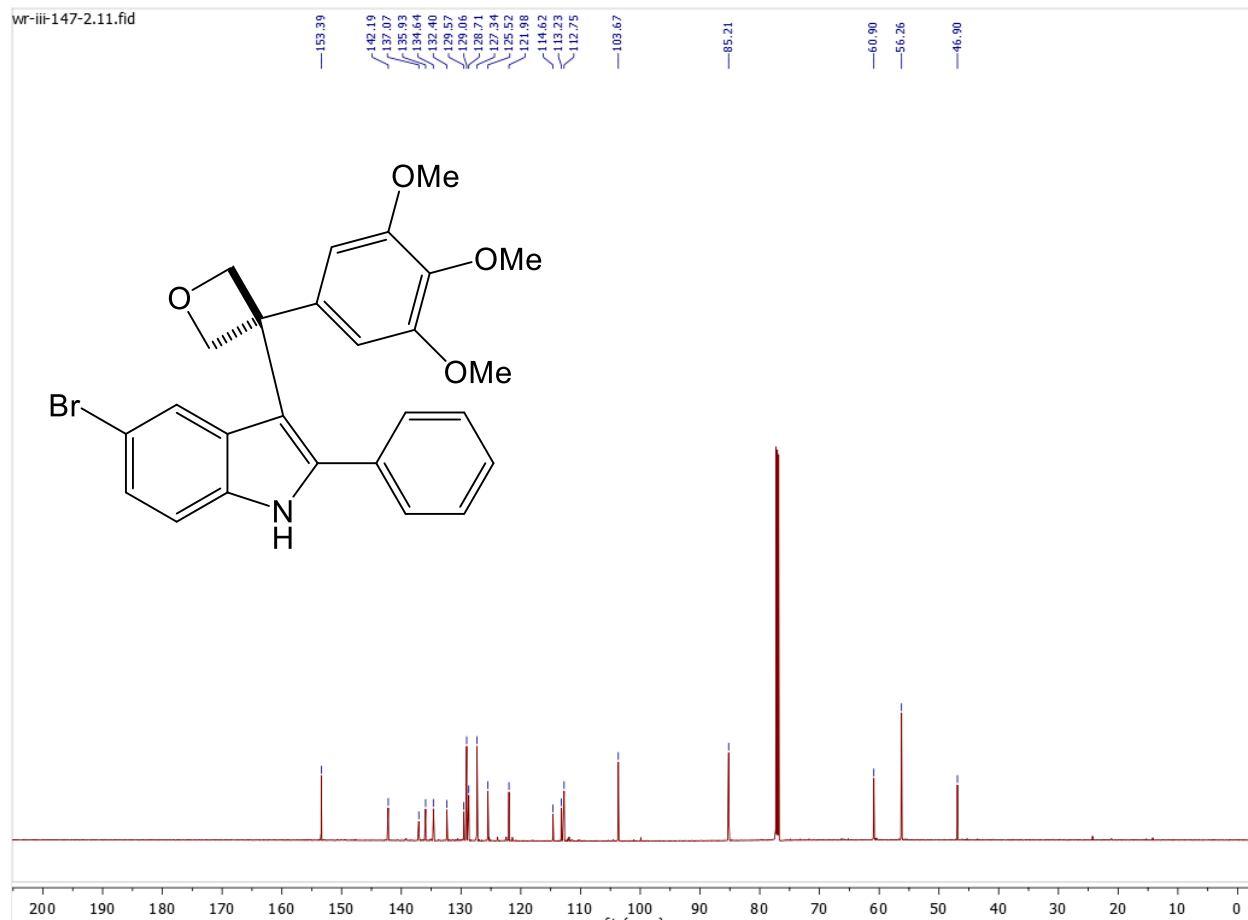
Signal 5: DAD1 H, Sig=320,16 Ref=off

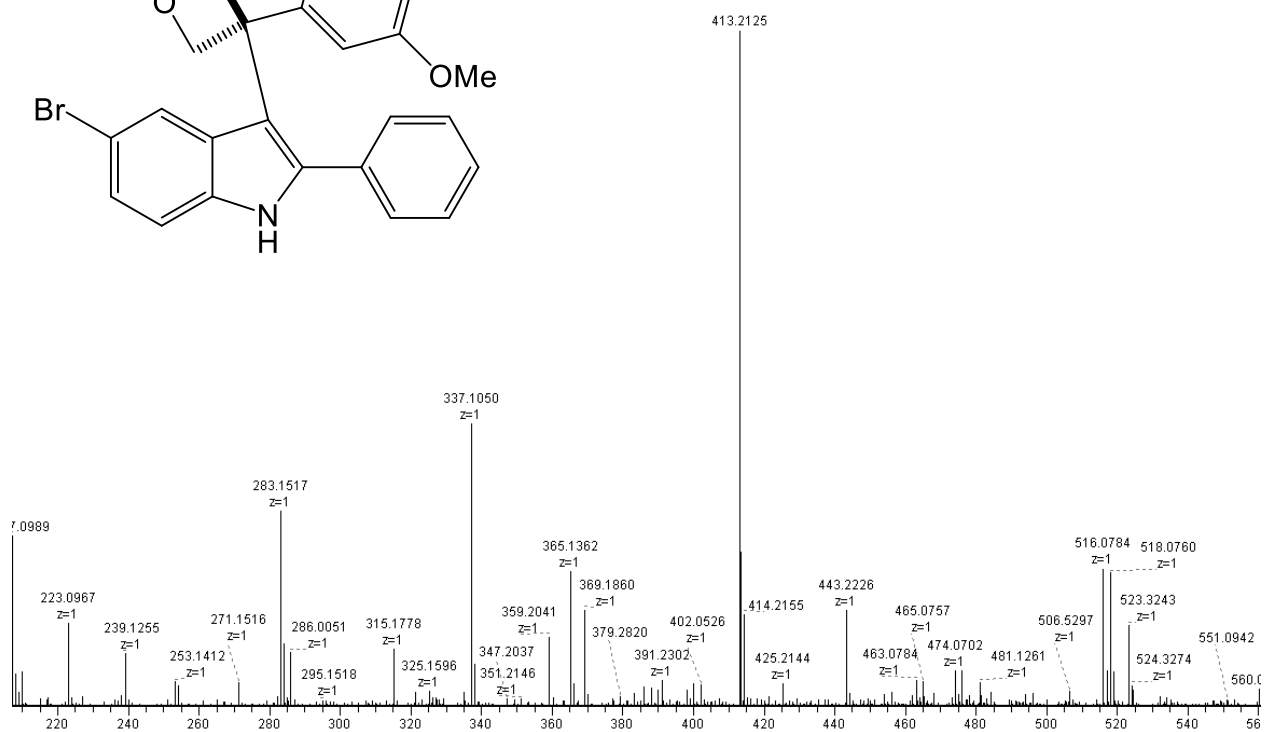
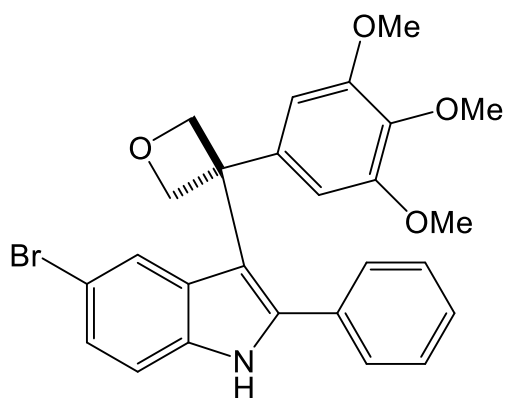
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
----- ----- ----- ----- ----- ----- -----						
1	11.198	BV	0.1103	30.92123	4.27715	1.1633
2	11.463	VB	0.1072	2627.15112	377.55621	98.8367
----- ----- ----- ----- ----- ----- -----						
Totals :				2658.07236	381.83337	

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*** End of Report ***

Compound 5n







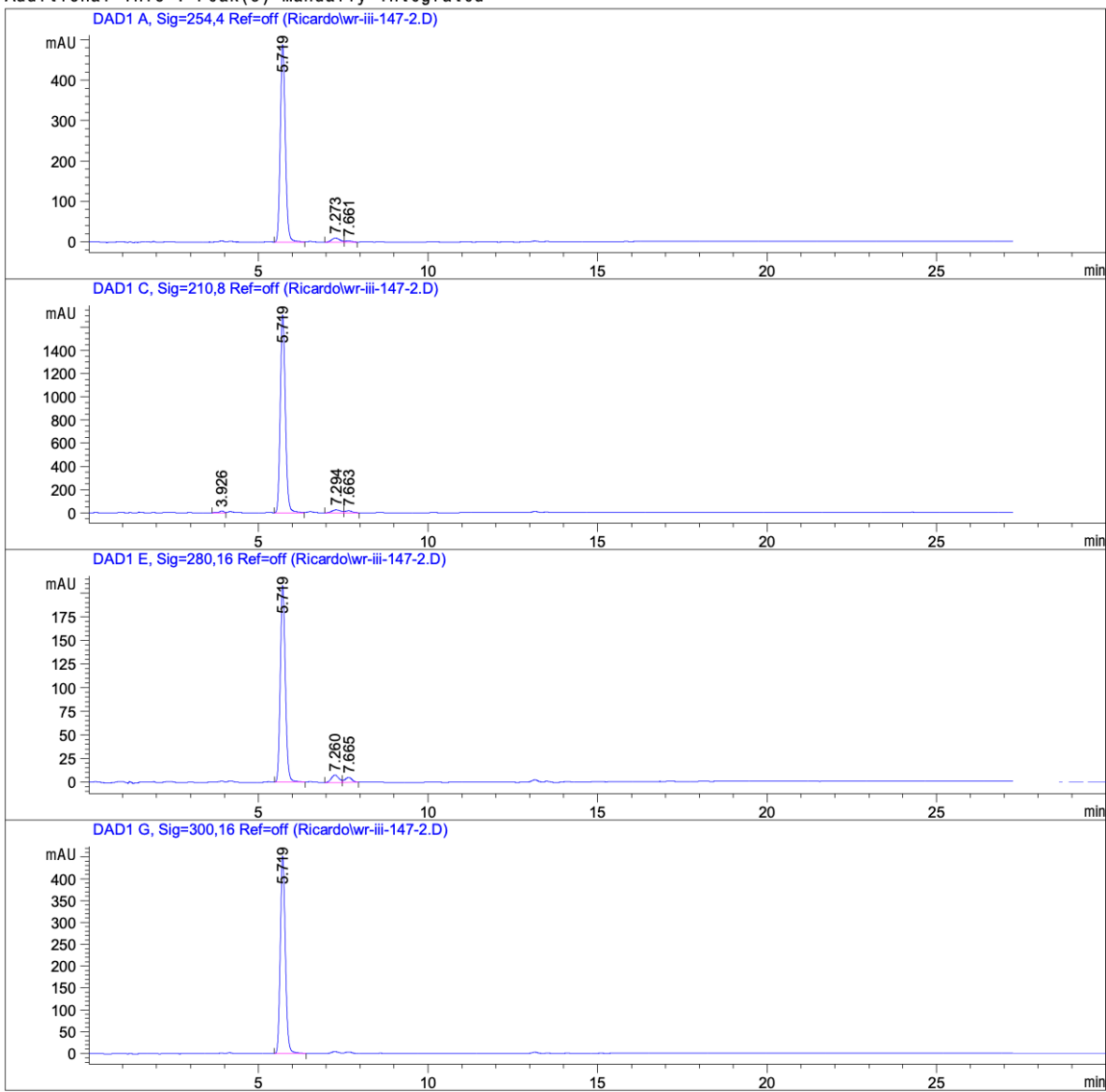
Data File C:\Chem32\1\Data\Ricardo\wr-iii-147-2.D
Sample Name: wr-iii-147-2

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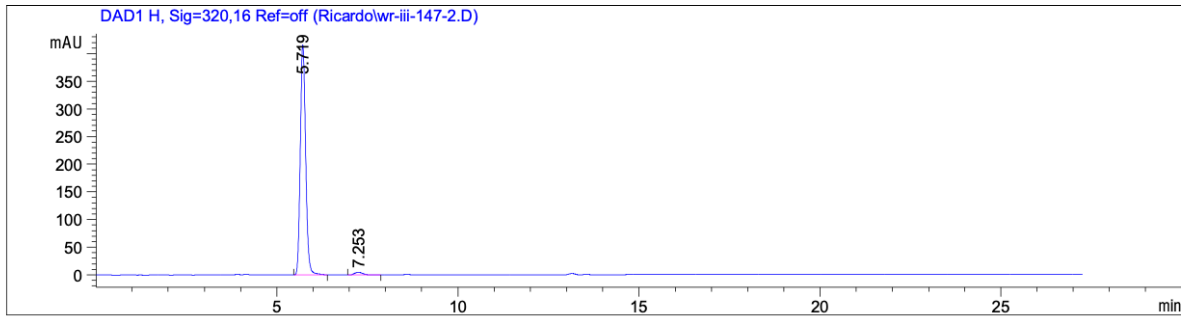
Acq. Operator	: SYSTEM		
Sample Operator	: SYSTEM		
Acq. Instrument	: 1200 HPLC	Location	: 1
Injection Date	: 4/8/2021 1:38:05 PM	Inj Volume	: No inj
Acq. Method	: C:\Chem32\1\Methods\GRAD 2 30-90 ACN.M		
Last changed	: 4/2/2014 4:04:33 PM by ERICA P		
Analysis Method	: C:\Chem32\1\Methods\RT-ACNWASH 2.M		
Last changed	: 7/9/2015 2:27:22 PM by Blake		
Method Info	: General Column Wash Method		

Sample Info : wr-iii-147-2 ACN 30:90

Additional Info : Peak(s) manually integrated



Data File C:\Chem32\1\Data\Ricardo\wr-iii-147-2.D
 Sample Name: wr-iii-147-2



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 Area Percent Report
 =====

Sorted By : Signal
 Multiplier : 1.0000
 Dilution : 1.0000
 Sample Amount : 1.00000 [ng/ul] (not used in calc.)
 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	5.719	VV	0.1646	5127.97217	488.12402	96.0488
2	7.273	BV	0.2630	171.96848	10.29084	3.2210
3	7.661	VB	0.1974	38.98065	3.00408	0.7301

Totals : 5338.92130 501.41894

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.926	BV	0.1294	129.58307	15.20400	0.6893
2	5.719	VV	0.1650	1.79987e4	1706.83838	95.7435
3	7.294	BV	0.2723	435.54669	25.37051	2.3169
4	7.663	VB	0.2104	235.03928	17.09587	1.2503

Totals : 1.87988e4 1764.50875

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

Data File C:\Chem32\1\Data\Ricardo\wr-iii-147-2.D
Sample Name: wr-iii-147-2

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.719	BB	0.1636	2171.55933	208.29308	91.8229
2	7.260	BV	0.2386	120.45528	7.87022	5.0934
3	7.665	VB	0.2175	72.92902	5.20343	3.0838

Totals : 2364.94363 221.36673

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.719	BB	0.1637	4710.84229	451.76431	100.0000

Totals : 4710.84229 451.76431

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.719	BB	0.1637	4334.10303	415.48242	98.1501
2	7.253	BB	0.2462	81.68601	5.11836	1.8499

Totals : 4415.78904 420.60078

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*** End of Report ***

Table of Compound Purity by HPLC (wavelength 254 nm)

Compound	HPLC Purity
5a	96.4%
5b	96.3%
5c	95.4%
5d	97.7%
5e	95.3%
5f	97.2%
5g	95.7%
5h	95.8%
5i	99.8%
5j	96.4%
5k	86.8%
5l	91.5%
5m	97.9%
5n	96.1%