

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX083023\
 Data File : VX037382.D
 Acq On : 30 Aug 2023 12:26
 Operator : JC/MD
 Sample : 04110-14
 Misc : 4.28g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 TP-21(3-4)

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081723W.M
 Title : SW846 8260

Signal : TIC: VX037382.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.623	84	88	97	rBV	56238	67865	10.15%	1.188%
2	1.709	99	102	107	rVB3	5880	7633	1.14%	0.134%
3	1.879	127	130	143	rVB8	4412	13551	2.03%	0.237%
4	2.733	262	270	273	rBV2	5115	10378	1.55%	0.182%
5	2.782	273	278	291	rVB4	8280	21787	3.26%	0.381%
6	2.946	299	305	314	rBV2	4006	9557	1.43%	0.167%
7	3.062	317	324	335	rVB3	4520	9928	1.49%	0.174%
8	4.275	513	523	533	rBV2	7333	20302	3.04%	0.355%
9	5.391	693	706	722	rBV2	70005	234764	35.12%	4.109%
10	5.543	722	731	750	rVB	140624	409287	61.22%	7.164%
11	5.806	767	774	785	rVB6	2711	8220	1.23%	0.144%
12	5.958	789	799	807	rVV	78343	208829	31.24%	3.655%
13	6.025	807	810	821	rVV3	9479	23611	3.53%	0.413%
14	6.141	821	829	838	rVV5	3235	9809	1.47%	0.172%
15	6.238	838	845	853	rVV5	2970	8100	1.21%	0.142%
16	6.342	853	862	873	rVB4	6032	16528	2.47%	0.289%
17	6.757	921	930	944	rBV	200860	478280	71.54%	8.371%
18	7.372	1022	1031	1041	rBV	56817	127601	19.09%	2.233%
19	7.769	1088	1096	1103	rBV2	3795	7902	1.18%	0.138%
20	7.951	1118	1126	1135	rBV4	4092	8228	1.23%	0.144%
21	8.268	1173	1178	1183	rBV3	4072	6991	1.05%	0.122%
22	8.598	1225	1232	1234	rBV2	10667	17705	2.65%	0.310%
23	8.646	1234	1240	1245	rVV	411046	668549	100.00%	11.702%
24	8.714	1245	1251	1257	rVV2	85283	236633	35.40%	4.142%
25	8.768	1257	1260	1264	rVB4	5271	7373	1.10%	0.129%
26	8.848	1269	1273	1278	rVV5	4076	6753	1.01%	0.118%
27	8.909	1278	1283	1288	rVV2	7459	11039	1.65%	0.193%
28	8.976	1288	1294	1300	rVB2	10588	17559	2.63%	0.307%
29	9.274	1338	1343	1348	rBV3	5202	8057	1.21%	0.141%
30	9.384	1355	1361	1370	rBV	5770	8710	1.30%	0.152%
31	9.512	1375	1382	1385	rVV5	3399	6951	1.04%	0.122%
32	9.561	1385	1390	1394	rVV2	11952	17509	2.62%	0.306%
33	9.616	1394	1399	1403	rVV	7939	12690	1.90%	0.222%
34	9.817	1426	1432	1442	rBV4	6566	12541	1.88%	0.220%
35	10.006	1457	1463	1466	rBV3	4214	6731	1.01%	0.118%
36	10.055	1466	1471	1479	rVV	385209	521777	78.05%	9.133%

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37	10.195	1487	1494	1501	rVV	14080	19091	2.86%	0.334%
38	10.299	1501	1511	1517	rVV	71984	110682	16.56%	1.937%
39	10.360	1517	1521	1529	rVB4	12829	19409	2.90%	0.340%
40	10.585	1550	1558	1563	rBV5	4052	8058	1.21%	0.141%
41	10.640	1563	1567	1577	rVB	51355	71935	10.76%	1.259%
42	10.756	1581	1586	1587	rBV2	5116	6944	1.04%	0.122%
43	10.780	1587	1590	1594	rVB2	12958	16378	2.45%	0.287%
44	10.853	1594	1602	1606	rBV2	10287	16217	2.43%	0.284%
45	10.896	1606	1609	1614	rVB2	7191	10027	1.50%	0.176%
46	10.963	1614	1620	1624	rBV	10917	14335	2.14%	0.251%
47	11.085	1634	1640	1651	rVB	298235	395319	59.13%	6.919%
48	11.305	1671	1676	1680	rBV	10867	15131	2.26%	0.265%
49	11.384	1683	1689	1695	rVV2	19727	35544	5.32%	0.622%
50	11.451	1695	1700	1702	rVV2	16780	25030	3.74%	0.438%
51	11.475	1702	1704	1710	rVB	19231	22538	3.37%	0.394%
52	11.615	1722	1727	1734	rBV	15047	20527	3.07%	0.359%
53	11.713	1740	1743	1746	rBV	14654	17604	2.63%	0.308%
54	11.756	1746	1750	1759	rVB	54858	75003	11.22%	1.313%
55	11.890	1769	1772	1777	rVB	9310	11727	1.75%	0.205%
56	11.939	1777	1780	1783	rBV4	5054	7427	1.11%	0.130%
57	11.975	1783	1786	1789	rVB2	9707	11585	1.73%	0.203%
58	12.024	1789	1794	1801	rBV	395355	490286	73.34%	8.581%
59	12.091	1801	1805	1813	rVB	23452	36297	5.43%	0.635%
60	12.176	1813	1819	1826	rVB7	3629	6846	1.02%	0.120%
61	12.243	1826	1830	1832	rBV2	5891	7637	1.14%	0.134%
62	12.329	1838	1844	1851	rVB5	13465	28936	4.33%	0.506%
63	12.426	1851	1860	1864	rBV	21320	31481	4.71%	0.551%
64	12.463	1864	1866	1873	rVB2	5550	7670	1.15%	0.134%
65	12.536	1873	1878	1880	rBV	10686	15819	2.37%	0.277%
66	12.713	1899	1907	1913	rBV7	6180	15233	2.28%	0.267%
67	12.920	1938	1941	1945	rVV2	6591	8782	1.31%	0.154%
68	12.969	1945	1949	1955	rVB3	8661	15238	2.28%	0.267%
69	13.036	1955	1960	1964	rBV5	3865	7047	1.05%	0.123%
70	13.268	1992	1998	2000	rBV	17884	25120	3.76%	0.440%
71	13.383	2013	2017	2020	rBV3	4851	6687	1.00%	0.117%
72	13.426	2020	2024	2031	rVB7	4436	9920	1.48%	0.174%
73	13.585	2045	2050	2054	rBV4	12159	19933	2.98%	0.349%
74	13.774	2076	2081	2088	rVB	155139	207651	31.06%	3.634%
75	13.841	2088	2092	2095	rBV2	6023	7298	1.09%	0.128%
76	14.036	2120	2124	2127	rBV2	10956	12310	1.84%	0.215%

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77	14.633	2216	2222	2227	rBV	114694	157570	23.57%	2.758%
78	14.780	2239	2246	2253	rVB	100932	133852	20.02%	2.343%
79	15.206	2313	2316	2322	rVB3	9356	12645	1.89%	0.221%
80	15.377	2338	2344	2347	rBV2	13515	20371	3.05%	0.357%
81	15.407	2347	2349	2353	rVV	6378	7788	1.16%	0.136%
82	15.475	2353	2360	2370	rVV	23322	42139	6.30%	0.738%
83	15.615	2376	2383	2386	rBV	38190	60748	9.09%	1.063%
84	15.651	2386	2389	2396	rVB	25857	38554	5.77%	0.675%
85	15.834	2409	2419	2431	rBV	15175	40328	6.03%	0.706%
86	15.987	2439	2444	2453	rVB2	5240	9546	1.43%	0.167%
87	16.328	2493	2500	2512	rVB5	11869	29371	4.39%	0.514%

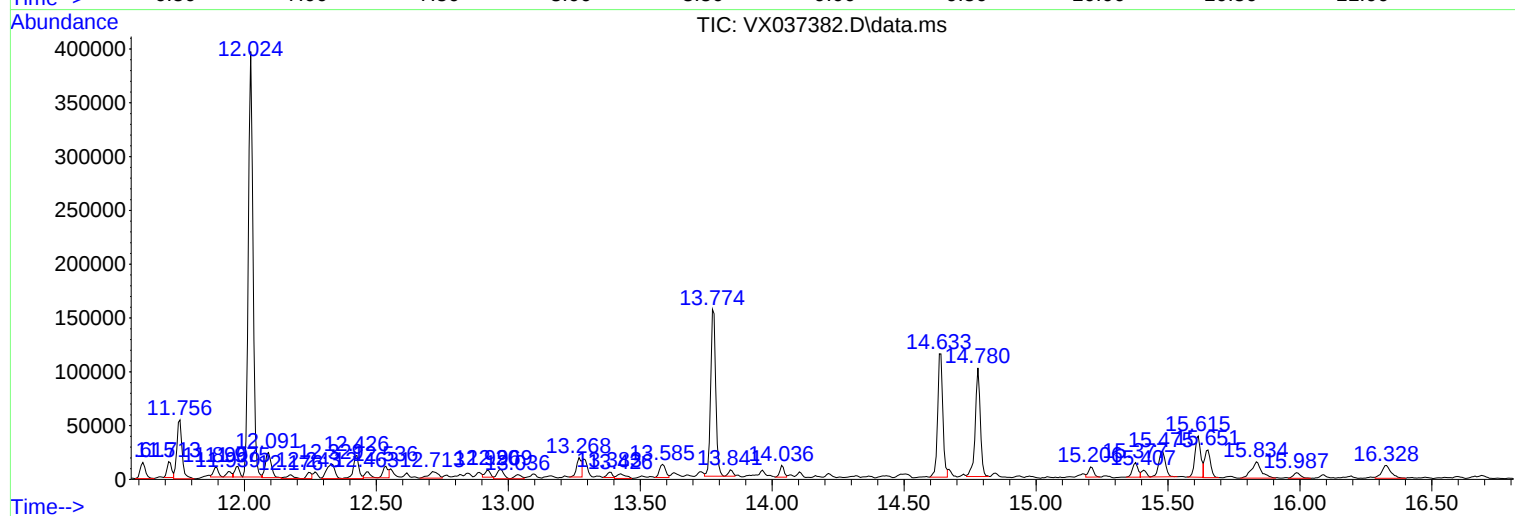
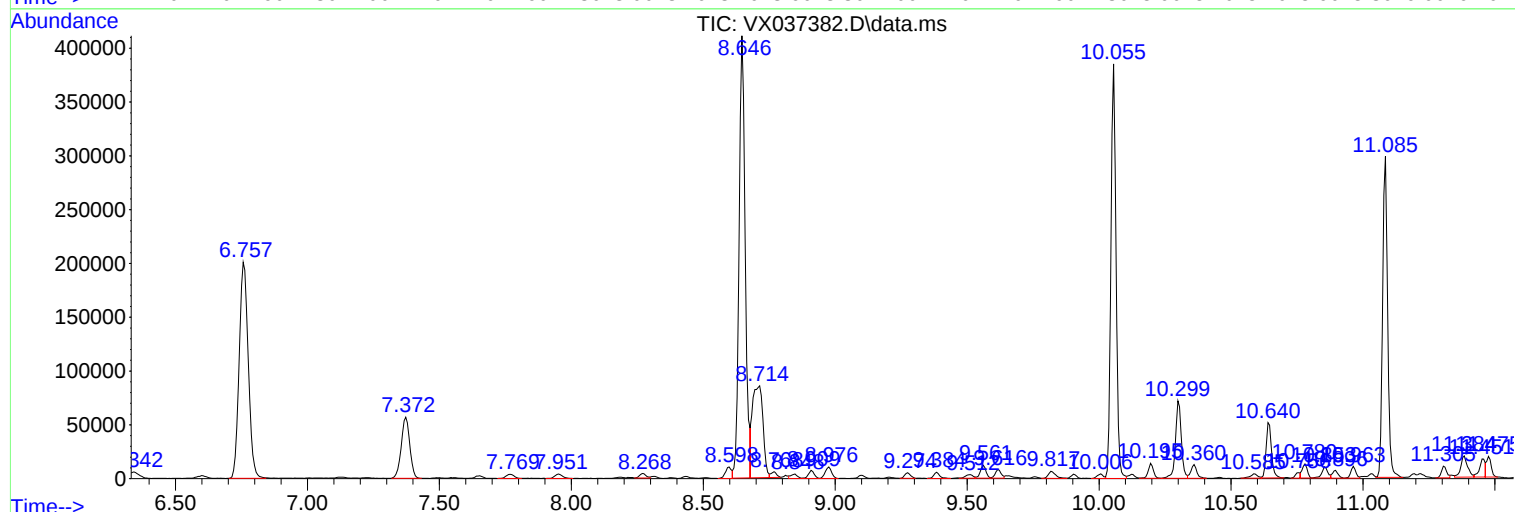
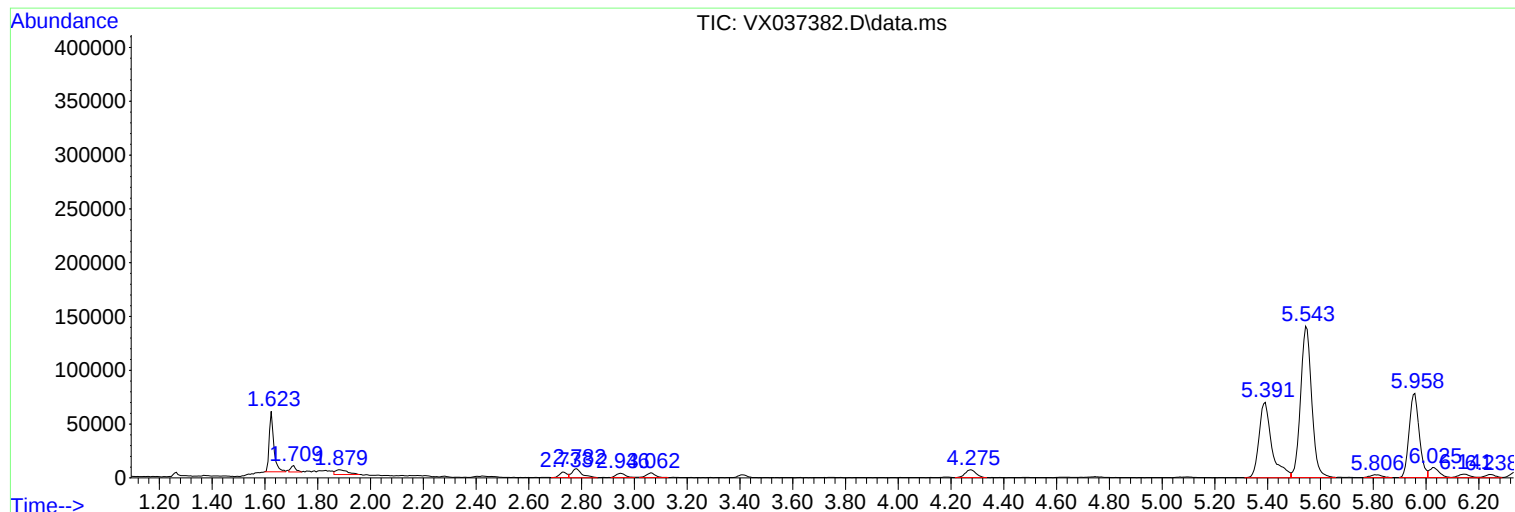
Sum of corrected areas: 5713342

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TP-21(3-4)

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081723W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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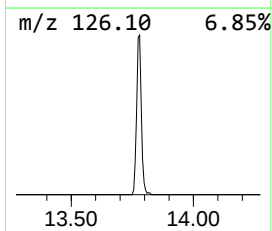
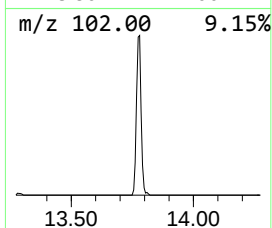
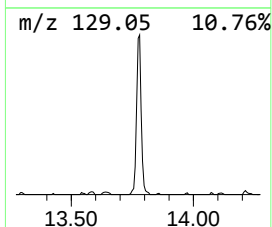
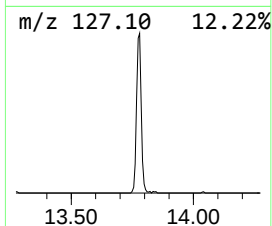
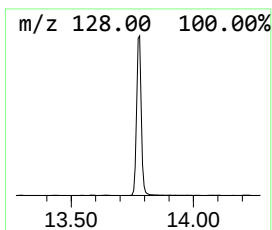
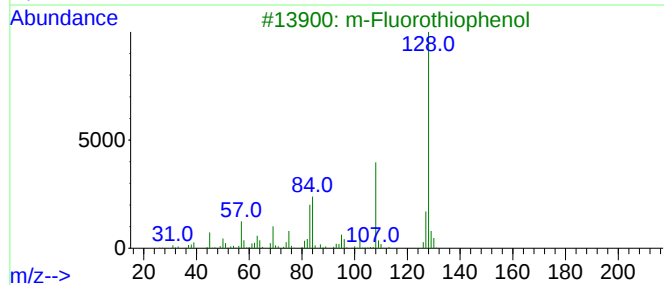
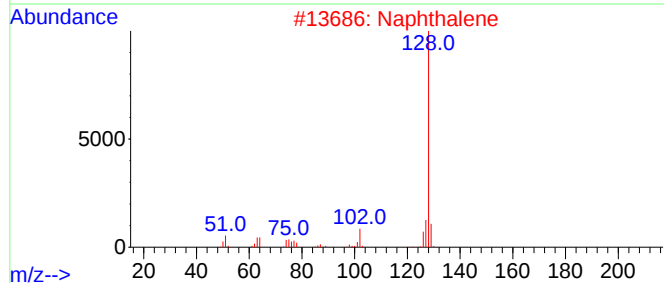
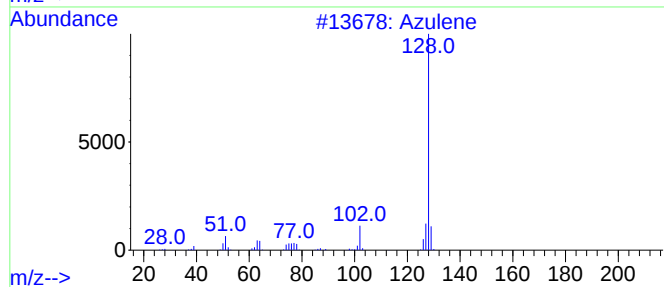
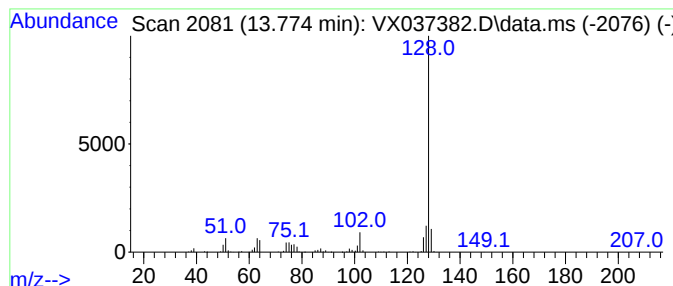
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081723W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Azulene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.774	21.18 ug/l	207651	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Azulene	128	C10H8	000275-51-4	95
2			Naphthalene	128	C10H8	000091-20-3	95
3			m-Fluorothiophenol	128	C6H5FS	002557-77-9	50
4			[4.2.2]Propella-2,4,7,9-tetraene	128	C10H8	088090-34-0	50
5			1H-Indene, 1-methylene-	128	C10H8	002471-84-3	50



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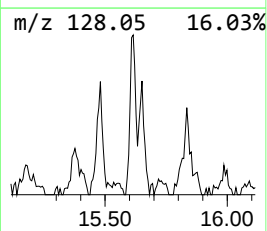
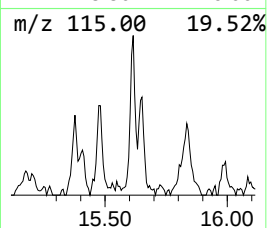
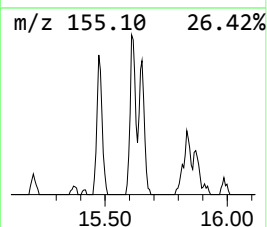
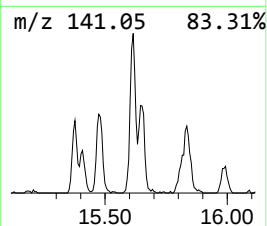
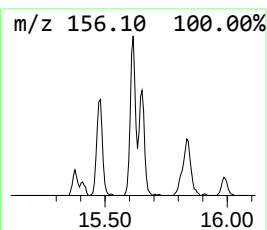
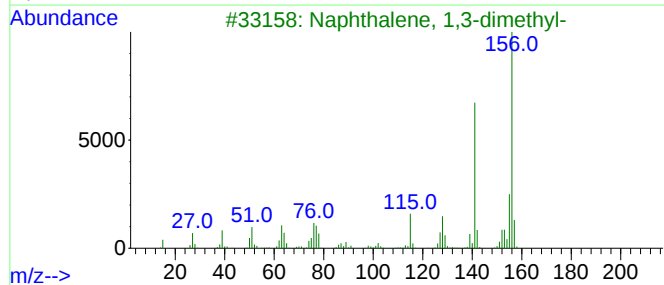
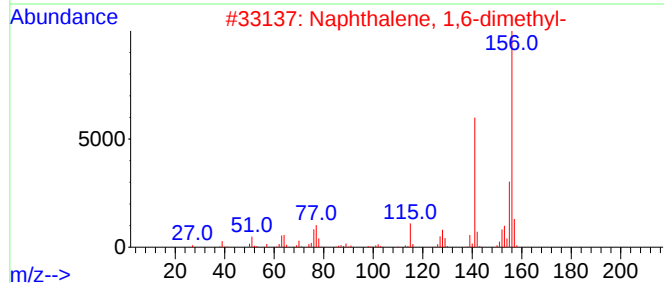
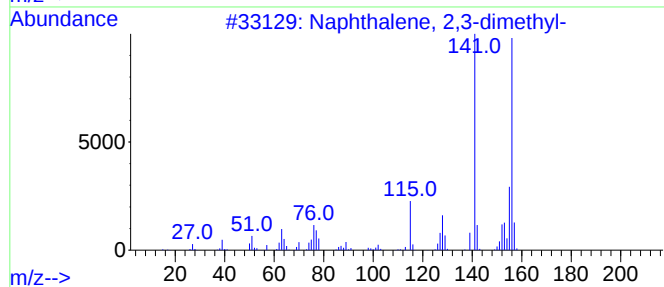
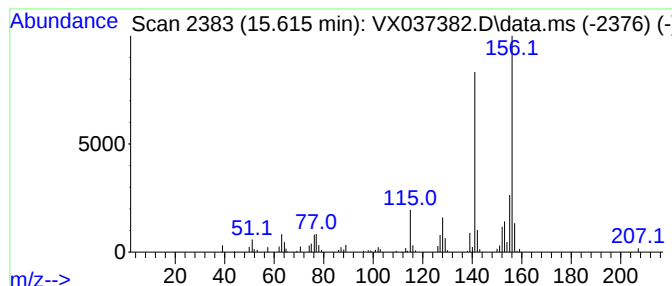
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081723W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Naphthalene, 2,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.615	6.20 ug/l	60748	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	98
2			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97
3			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	97
4			Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	97
5			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	96



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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Azulene	13.774	21.2	ug/l	207651	4	12.024	490286	50.0
Naphthalene, 2,...	15.615	6.2	ug/l	60748	4	12.024	490286	50.0