

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY100623\
 Data File : VY015869.D
 Acq On : 06 Oct 2023 17:57
 Operator : SY/MD
 Sample : 04767-09
 Misc : 5.17g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 Q-1(5-10)

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_Y\methods\82Y100523S.M
 Title : SW846 8260

Signal : TIC: VY015869.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.070	33	41	47	rBV	35192	49294	3.08%	0.349%
2	2.235	66	68	77	rVB3	10691	16891	1.05%	0.119%
3	2.387	88	93	101	rBV	23153	49775	3.11%	0.352%
4	2.887	169	175	188	rVB	28289	62341	3.89%	0.441%
5	3.241	225	233	241	rBV2	7283	17197	1.07%	0.122%
6	3.972	339	353	375	rBV	12285	50935	3.18%	0.360%
7	4.186	379	388	398	rVB	23291	62083	3.88%	0.439%
8	4.710	461	474	499	rVB4	32787	142585	8.90%	1.008%
9	5.228	544	559	571	rBV4	5056	18839	1.18%	0.133%
10	5.740	633	643	654	rBV4	7751	24646	1.54%	0.174%
11	6.789	807	815	832	rVB2	9295	30097	1.88%	0.213%
12	7.002	837	850	863	rBV2	6753	23749	1.48%	0.168%
13	7.716	955	967	972	rBV	187152	450104	28.10%	3.183%
14	7.783	972	978	988	rVV	408723	945275	59.02%	6.684%
15	7.868	988	992	1002	rVB3	12278	28163	1.76%	0.199%
16	8.142	1028	1037	1051	rBV2	295304	785759	49.06%	5.556%
17	8.411	1074	1081	1091	rVB3	15617	41269	2.58%	0.292%
18	8.545	1097	1103	1110	rBV4	10057	22983	1.43%	0.163%
19	8.685	1117	1126	1141	rBV	580836	1133158	70.75%	8.012%
20	9.179	1194	1207	1216	rBV	159684	339383	21.19%	2.400%
21	9.453	1242	1252	1259	rBV6	6936	17359	1.08%	0.123%
22	9.606	1269	1277	1283	rVB4	8617	17995	1.12%	0.127%
23	9.819	1306	1312	1324	rVB3	13786	34276	2.14%	0.242%
24	9.935	1324	1331	1345	rBV4	8161	25099	1.57%	0.177%
25	10.179	1363	1371	1377	rBV	908125	1595740	99.63%	11.283%
26	10.240	1377	1381	1388	rVB	176743	296023	18.48%	2.093%
27	10.343	1393	1398	1399	rBV	14412	19274	1.20%	0.136%
28	10.520	1410	1427	1432	rBV2	23877	54333	3.39%	0.384%
29	10.800	1468	1473	1477	rVB2	10899	16677	1.04%	0.118%
30	11.032	1507	1511	1515	rVV	22981	31538	1.97%	0.223%
31	11.087	1515	1520	1525	rVV	58054	94352	5.89%	0.667%
32	11.203	1533	1539	1545	rBV2	23711	37469	2.34%	0.265%
33	11.282	1545	1552	1559	rVB7	7012	17047	1.06%	0.121%
34	11.489	1577	1586	1595	rBV	752537	1247324	77.87%	8.819%
35	11.593	1595	1603	1611	rVB2	22889	44721	2.79%	0.316%
36	11.697	1611	1620	1626	rBV	110568	222510	13.89%	1.573%

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Integrator: RTE

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Filtering: 5

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37	12.026	1663	1674	1682	rBV2	89112	179508	11.21%	1.269%
38	12.203	1698	1703	1706	rBV3	20668	34063	2.13%	0.241%
39	12.233	1706	1708	1714	rVB4	16800	27112	1.69%	0.192%
40	12.331	1719	1724	1729	rVB2	31297	47121	2.94%	0.333%
41	12.477	1742	1748	1756	rBV	565880	905066	56.51%	6.399%
42	12.642	1770	1775	1783	rVB3	13815	31513	1.97%	0.223%
43	12.733	1783	1790	1793	rBV	25754	42808	2.67%	0.303%
44	12.806	1797	1802	1810	rVB2	53689	90717	5.66%	0.641%
45	12.971	1821	1829	1836	rBV	23071	40697	2.54%	0.288%
46	13.038	1836	1840	1848	rVB8	10102	18243	1.14%	0.129%
47	13.117	1848	1853	1858	rBV	72243	114615	7.16%	0.810%
48	13.166	1858	1861	1866	rVB2	22147	31380	1.96%	0.222%
49	13.343	1881	1890	1892	rBV5	15747	36226	2.26%	0.256%
50	13.422	1897	1903	1913	rVB	653599	1075497	67.15%	7.604%
51	13.526	1916	1920	1929	rVB5	11877	20079	1.25%	0.142%
52	13.623	1929	1936	1940	rBV	28972	49244	3.07%	0.348%
53	13.660	1940	1942	1950	rVB4	16261	25601	1.60%	0.181%
54	13.751	1951	1957	1960	rBV4	16905	28799	1.80%	0.204%
55	13.806	1960	1966	1973	rVV2	29705	58472	3.65%	0.413%
56	13.879	1974	1978	1981	rVV2	11162	19698	1.23%	0.139%
57	13.916	1981	1984	1988	rVV	12057	18263	1.14%	0.129%
58	13.965	1988	1992	1997	rVB3	21797	35947	2.24%	0.254%
59	14.074	2005	2010	2015	rBV2	19859	37536	2.34%	0.265%
60	14.208	2027	2032	2037	rBV3	11827	17372	1.08%	0.123%
61	14.294	2043	2046	2049	rVV2	11720	18086	1.13%	0.128%
62	14.330	2049	2052	2056	rVB	15292	20950	1.31%	0.148%
63	14.574	2086	2092	2095	rBV5	10146	19852	1.24%	0.140%
64	14.672	2103	2108	2115	rBV3	30616	68447	4.27%	0.484%
65	14.751	2115	2121	2125	rVB7	9276	18049	1.13%	0.128%
66	14.830	2129	2134	2138	rBV4	14793	24999	1.56%	0.177%
67	14.940	2148	2152	2155	rBV4	12691	18194	1.14%	0.129%
68	15.050	2165	2170	2176	rVB4	10174	19886	1.24%	0.141%
69	15.233	2190	2200	2208	rBV	986517	1601718	100.00%	11.325%
70	15.336	2211	2217	2222	rBV2	24351	46875	2.93%	0.331%
71	15.525	2242	2248	2253	rBV4	8656	16272	1.02%	0.115%
72	15.684	2265	2274	2277	rBV8	10890	24229	1.51%	0.171%
73	16.031	2323	2331	2336	rBV5	9552	23476	1.47%	0.166%
74	16.220	2356	2362	2366	rBV5	11149	23923	1.49%	0.169%
75	16.287	2366	2373	2389	rVB	275456	567249	35.42%	4.011%
76	16.488	2398	2406	2414	rVB	279389	578959	36.15%	4.094%

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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

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y100523S.M
Title : SW846 8260

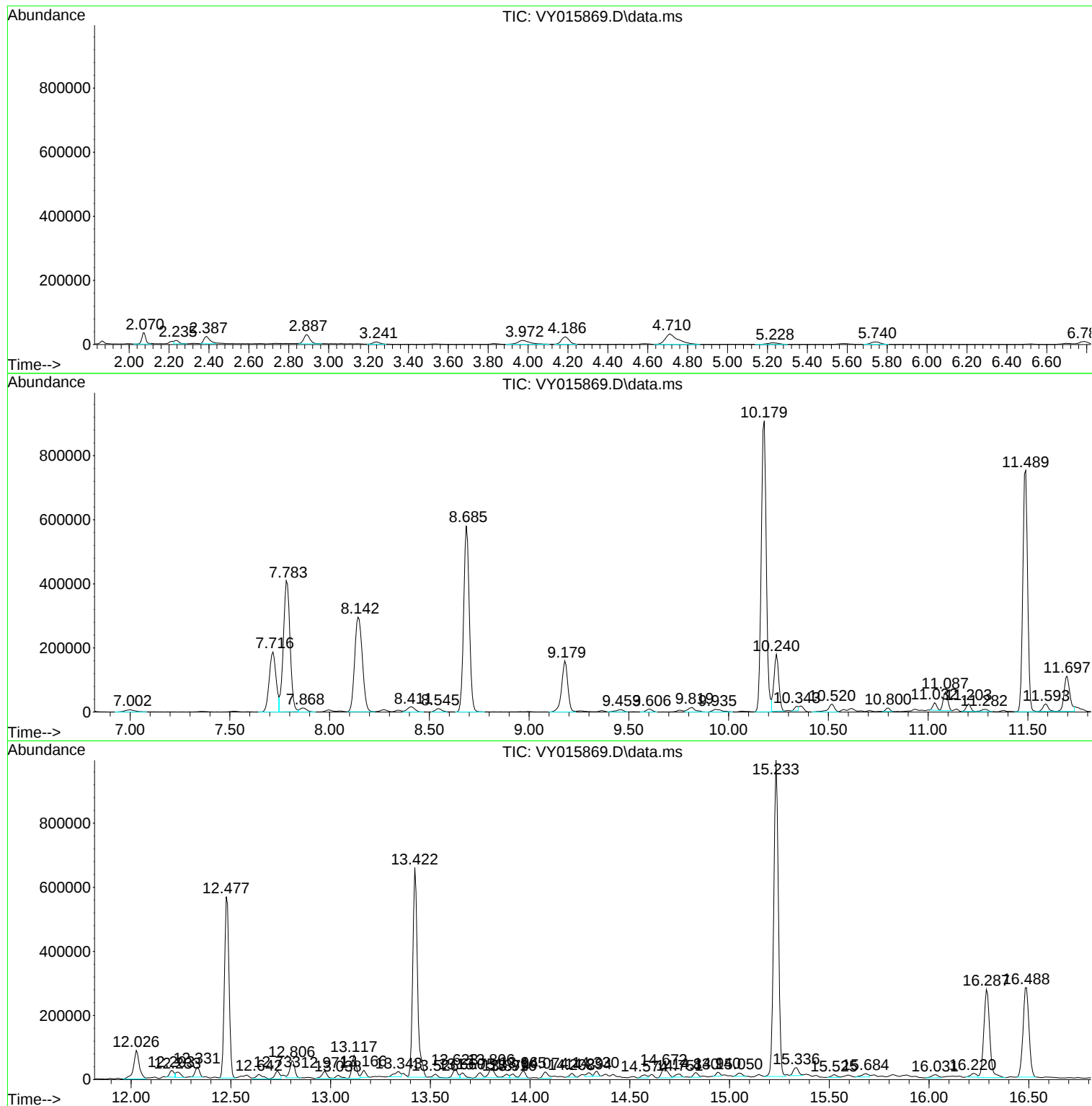
Sum of corrected areas: 14143004

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Data File : VY015869.D
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Misc : 5.17g/5.0mL/MSVOA_Y/SOIL
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Instrument :
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y100523S.M
Quant Title : SW846 8260

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



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ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
Q-1(5-10)

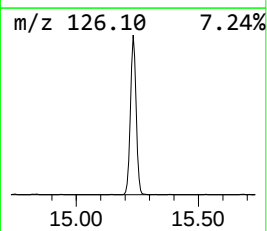
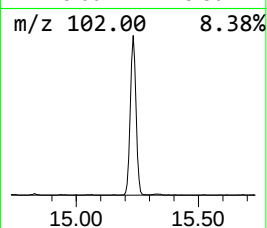
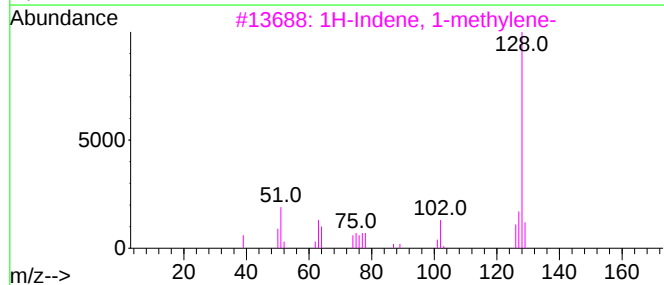
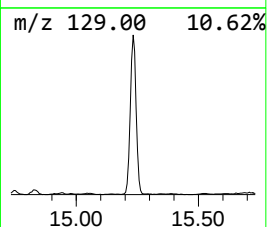
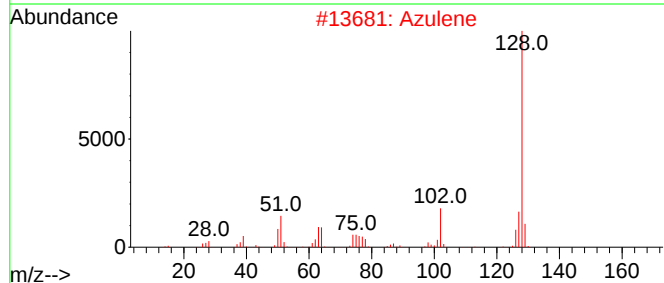
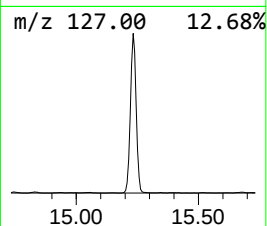
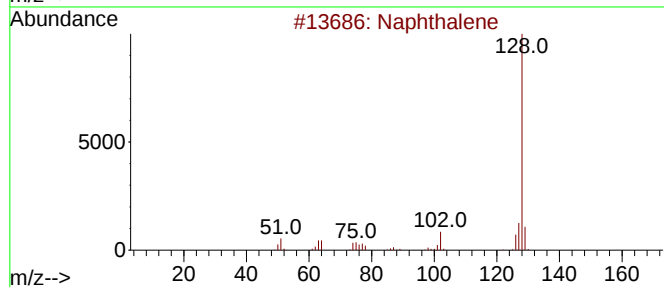
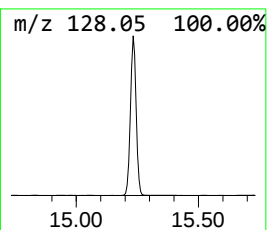
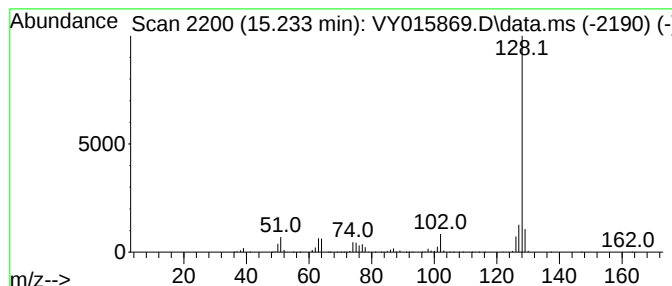
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y100523S.M
Quant Title : SW846 8260

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.
15.233	74.46 ug/l	1601720	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	95
2			Azulene	128	C10H8	000275-51-4	91
3			1H-Indene, 1-methylene-	128	C10H8	002471-84-3	87
4			4a,8a-(Methaniminomethano)naphth...	275	C18H13NO2	069915-10-2	64
5			1,3-Dicyanobenzene	128	C8H4N2	000626-17-5	64



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Instrument :
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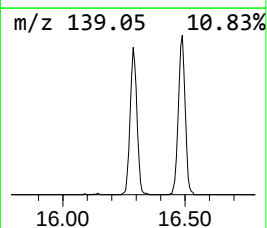
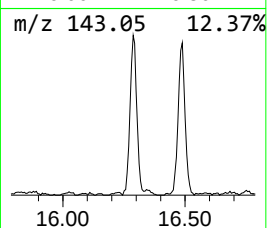
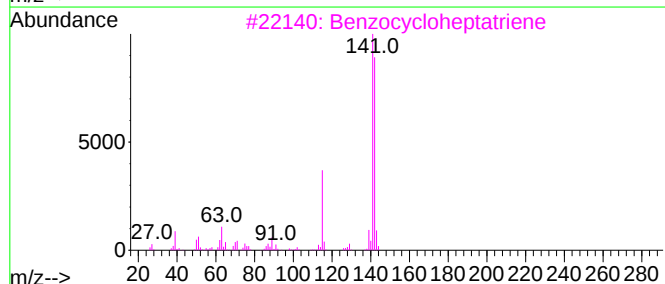
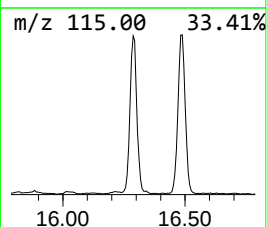
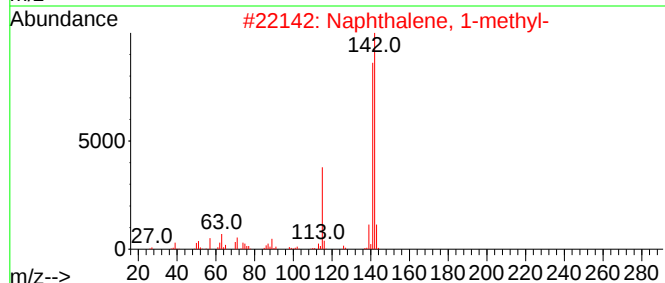
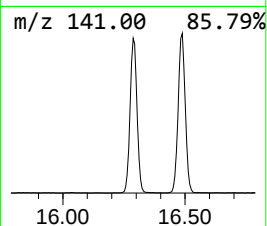
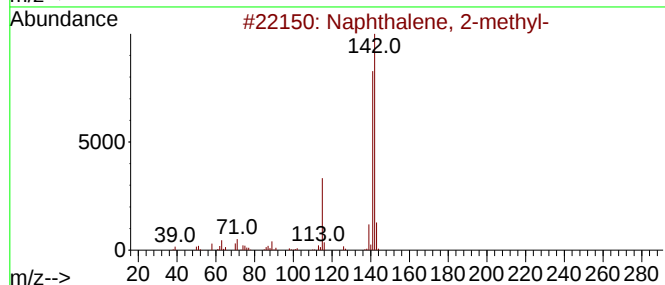
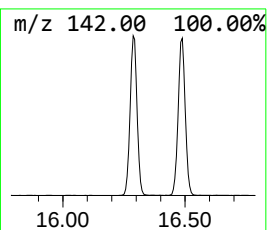
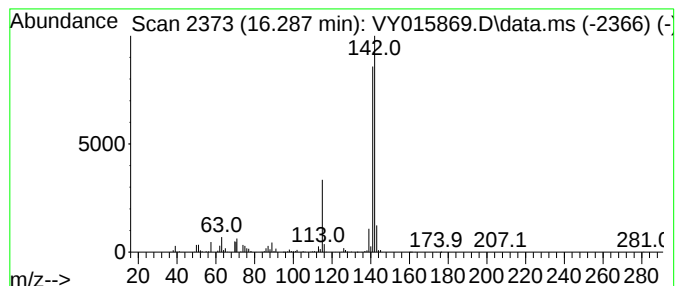
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y100523S.M
Quant Title : SW846 8260

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

Peak Number 3 Benzocycloheptatriene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.287	26.37 ug/l	567249	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3			Benzocycloheptatriene	142	C11H10	000264-09-5	91
4			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	90
5			1H-Indole-4-carbonitrile	142	C9H6N2	016136-52-0	46



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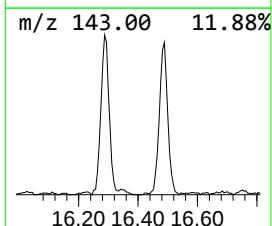
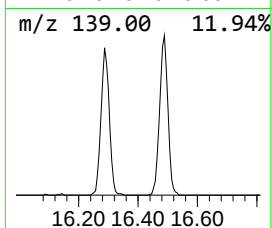
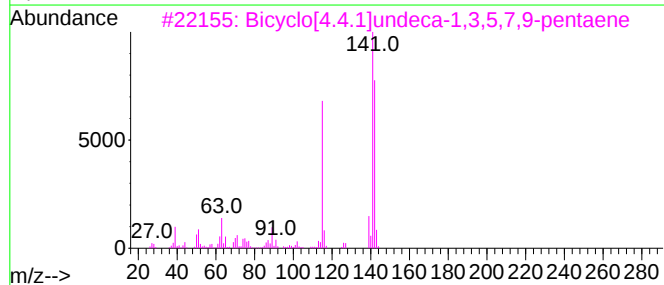
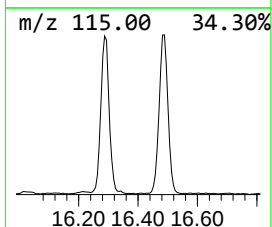
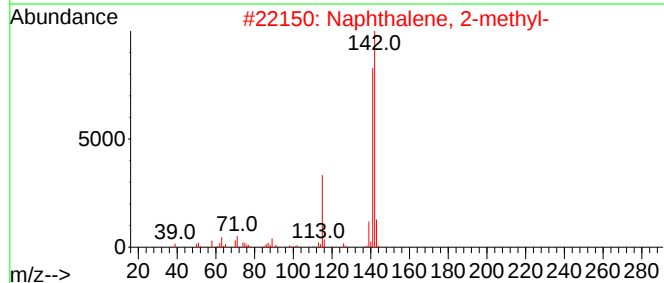
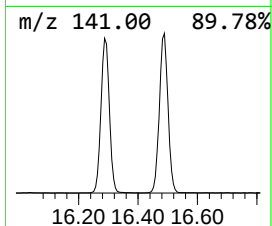
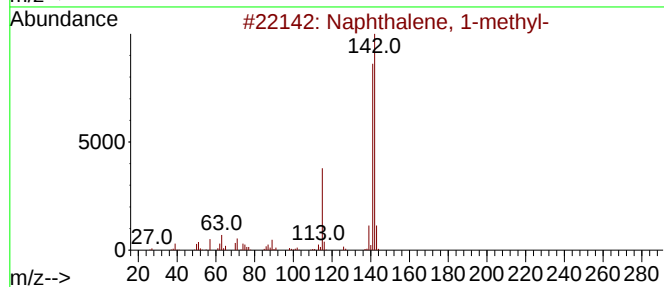
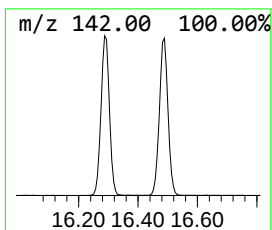
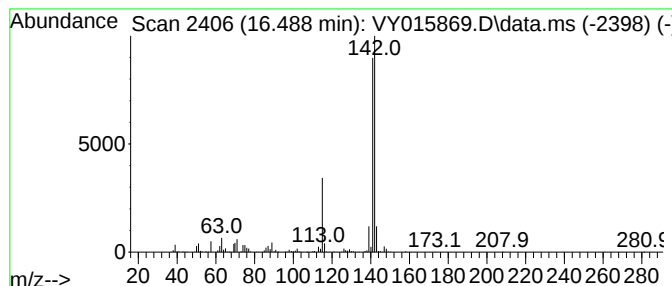
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Quant Title : SW846 8260

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

Peak Number 4 Bicyclo[4.4.1]undeca-1,3,5,... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.488	26.92 ug/l	578959	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
3			Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	91
4			Benzocycloheptatriene	142	C11H10	000264-09-5	91
5			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91



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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	15.233	74.5	ug/l	1601720	4	13.422	1075500	50.0
Benzocyclohepta...	16.287	26.4	ug/l	567249	4	13.422	1075500	50.0
Bicyclo[4.4.1]u...	16.488	26.9	ug/l	578959	4	13.422	1075500	50.0