

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY100423\
 Data File : VY015835.D
 Acq On : 04 Oct 2023 18:12
 Operator : SY/MD
 Sample : 04693-04
 Misc : 6.17g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 S-3(0-5)

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\82Y091923S.M
 Title : SW846 8260

Signal : TIC: VY015835.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.863	3	7	20	rVB2	16139	24650	2.46%	0.294%
2	2.211	59	64	66	rBV	7374	11751	1.17%	0.140%
3	2.235	66	68	73	rVB2	9661	12615	1.26%	0.150%
4	2.894	167	176	185	rVB3	5688	14033	1.40%	0.167%
5	3.241	224	233	244	rVB4	4214	12406	1.24%	0.148%
6	3.948	338	349	368	rBV	62536	181968	18.14%	2.169%
7	4.186	377	388	404	rBV2	11055	37318	3.72%	0.445%
8	4.704	461	473	493	rBV	41462	135601	13.52%	1.617%
9	5.735	632	642	653	rBV2	14637	44961	4.48%	0.536%
10	6.984	835	847	861	rBV	27379	76767	7.65%	0.915%
11	7.710	957	966	972	rBV2	139757	335970	33.49%	4.005%
12	7.783	972	978	989	rVB	257090	581874	58.00%	6.937%
13	8.136	1027	1036	1049	rBV2	156421	369307	36.81%	4.403%
14	8.685	1118	1126	1139	rBV	383760	747907	74.55%	8.916%
15	9.179	1195	1207	1213	rBV4	9351	22101	2.20%	0.263%
16	10.179	1362	1371	1377	rBV	590505	1003226	100.00%	11.960%
17	10.240	1377	1381	1389	rVB	33157	56930	5.67%	0.679%
18	11.490	1578	1586	1597	rBV	522091	839174	83.65%	10.004%
19	11.587	1597	1602	1610	rBV	5849	11637	1.16%	0.139%
20	11.697	1615	1620	1628	rVB	16828	33004	3.29%	0.393%
21	12.032	1662	1675	1682	rBV4	13593	30752	3.07%	0.367%
22	12.331	1714	1724	1732	rBV	146434	247449	24.67%	2.950%
23	12.477	1742	1748	1760	rVV	395240	639076	63.70%	7.619%
24	12.581	1761	1765	1770	rVB3	6535	10684	1.06%	0.127%
25	12.806	1798	1802	1808	rVB	14916	24117	2.40%	0.288%
26	12.892	1810	1816	1822	rBV2	22643	46509	4.64%	0.554%
27	13.117	1849	1853	1858	rVV	19175	27489	2.74%	0.328%
28	13.166	1858	1861	1867	rVB3	6844	10940	1.09%	0.130%
29	13.367	1887	1894	1898	rBV	70854	107096	10.68%	1.277%
30	13.422	1898	1903	1912	rVB	488106	753182	75.08%	8.979%
31	13.526	1915	1920	1925	rBV2	10789	17897	1.78%	0.213%
32	13.623	1932	1936	1939	rBV3	8161	14061	1.40%	0.168%
33	13.660	1939	1942	1950	rVB4	11501	18502	1.84%	0.221%
34	13.806	1960	1966	1974	rVB3	11519	21714	2.16%	0.259%
35	13.910	1974	1983	1987	rBV4	7407	18042	1.80%	0.215%
36	13.965	1987	1992	1997	rBV2	17882	27619	2.75%	0.329%

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37	14.294	2042	2046	2049	rBV	9545	14233	1.42%	0.170%
38	14.331	2049	2052	2057	rVB	24498	32713	3.26%	0.390%
39	14.410	2063	2065	2075	rVB6	5160	13259	1.32%	0.158%
40	14.568	2086	2091	2095	rBV6	4956	10470	1.04%	0.125%
41	14.672	2102	2108	2114	rBV3	29866	63416	6.32%	0.756%
42	14.745	2114	2120	2128	rVB6	16690	36241	3.61%	0.432%
43	14.830	2128	2134	2138	rBV2	26487	42656	4.25%	0.509%
44	14.940	2147	2152	2156	rBV6	8025	14705	1.47%	0.175%
45	15.050	2164	2170	2177	rBV3	9624	17894	1.78%	0.213%
46	15.233	2193	2200	2206	rBV	232170	378468	37.73%	4.512%
47	15.330	2212	2216	2221	rBV3	7411	15143	1.51%	0.181%
48	15.391	2221	2226	2237	rVB10	9167	28517	2.84%	0.340%
49	15.519	2242	2247	2252	rBV5	4807	10432	1.04%	0.124%
50	15.708	2265	2278	2284	rBV5	11513	41464	4.13%	0.494%
51	15.824	2291	2297	2302	rBV4	11797	27746	2.77%	0.331%
52	16.031	2322	2331	2335	rBV10	5585	13621	1.36%	0.162%
53	16.220	2355	2362	2366	rBV2	12504	28232	2.81%	0.337%
54	16.287	2366	2373	2387	rVB	224280	448404	44.70%	5.346%
55	16.483	2397	2405	2414	rBV	284697	582256	58.04%	6.941%

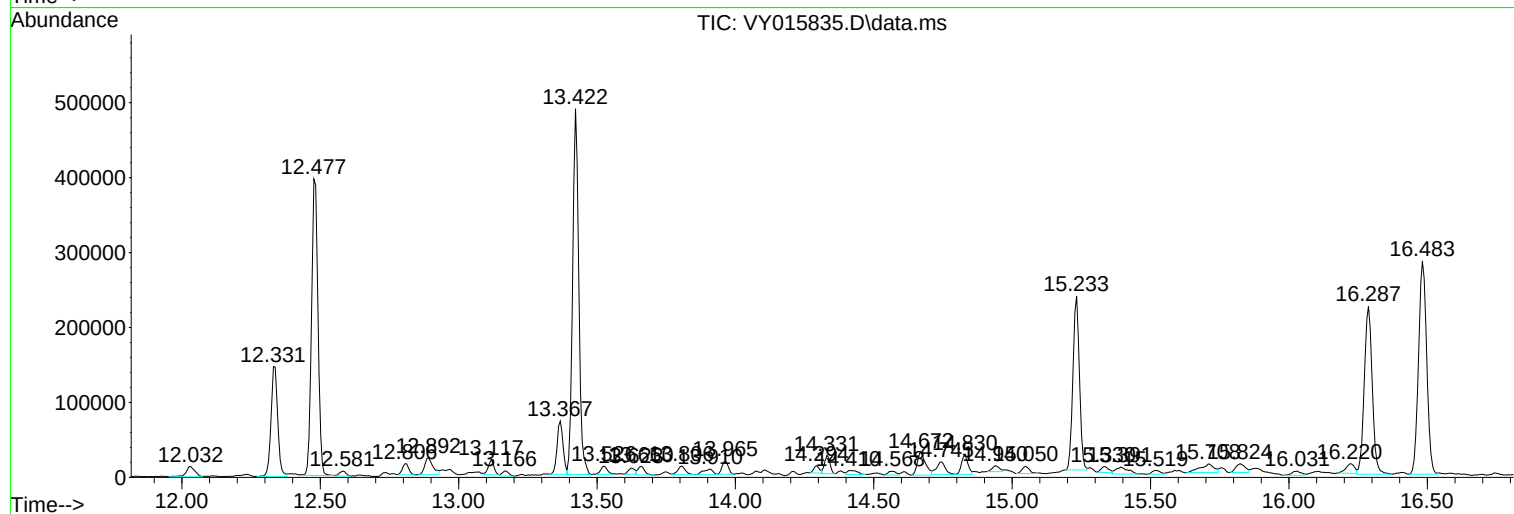
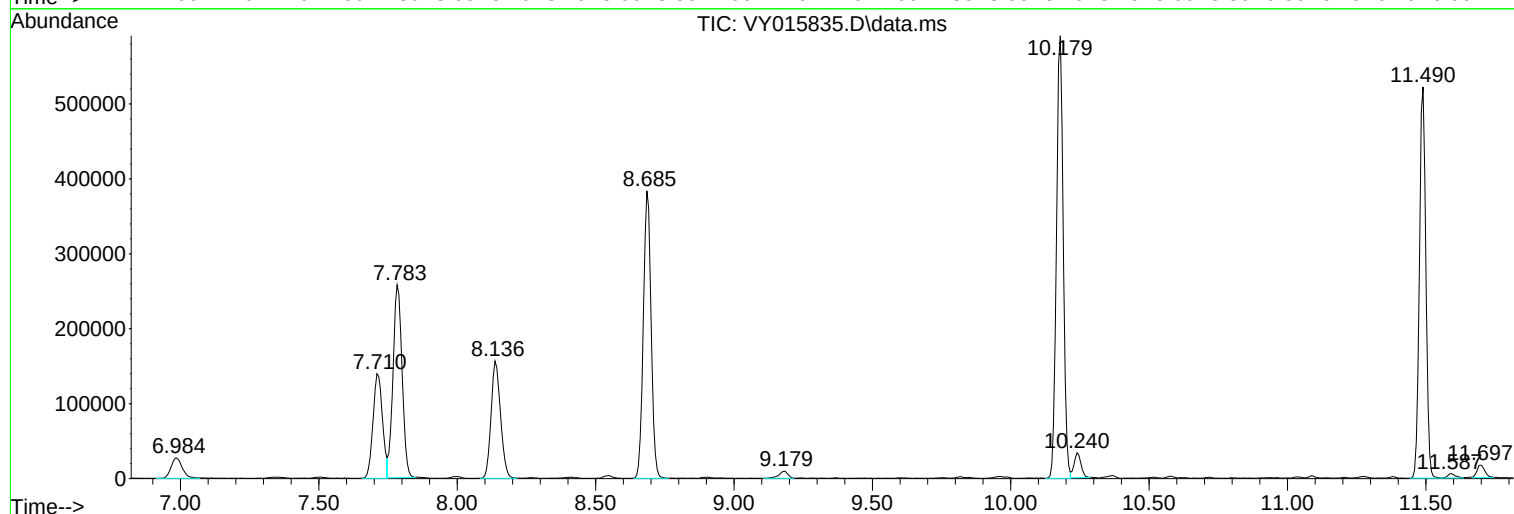
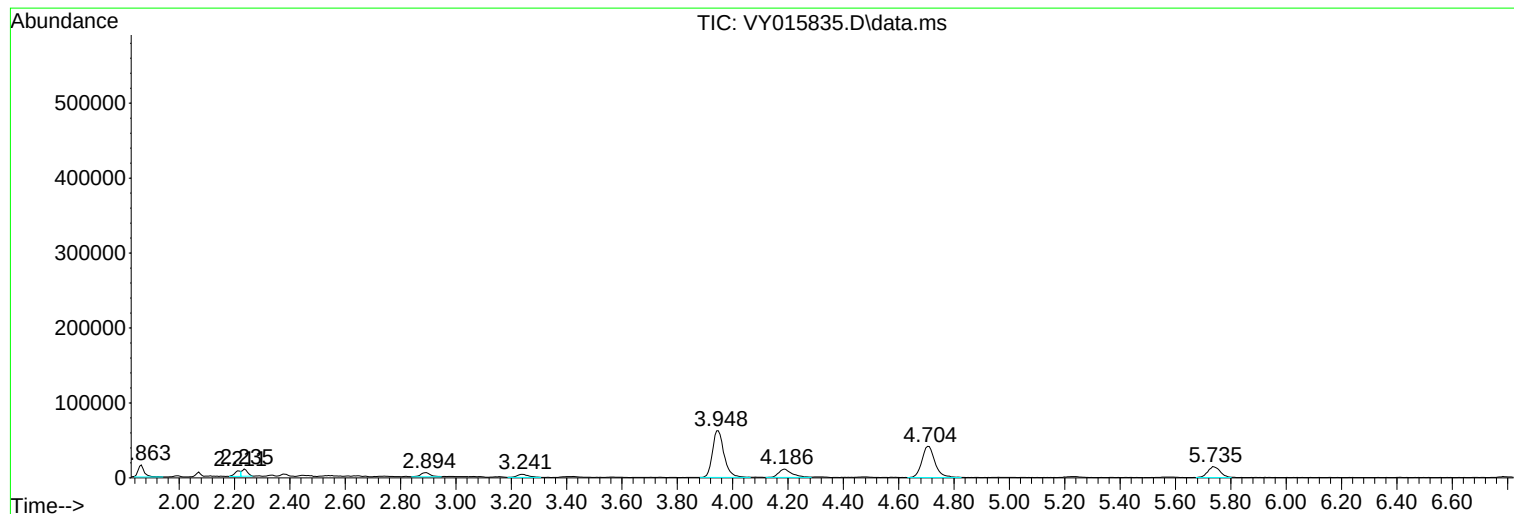
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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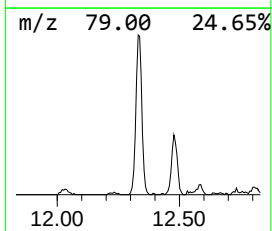
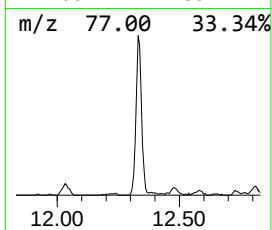
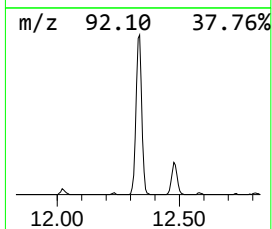
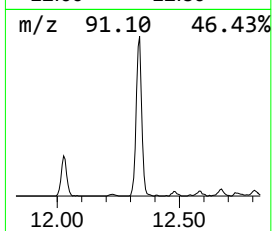
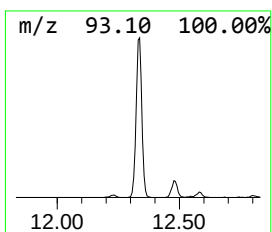
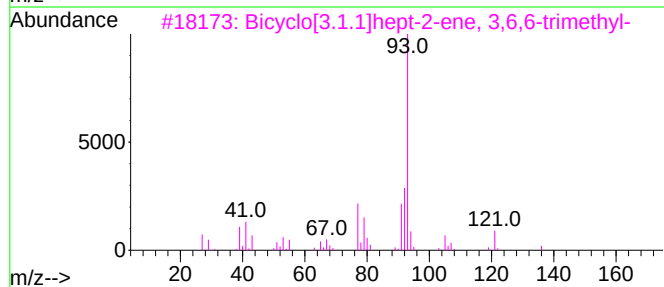
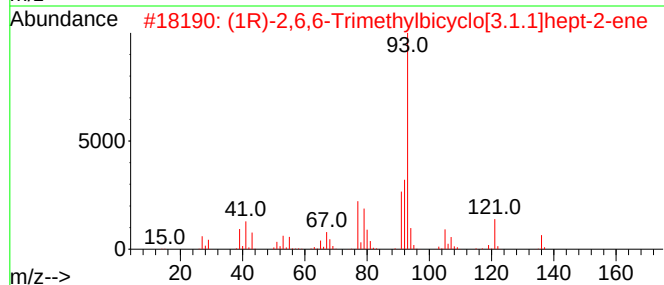
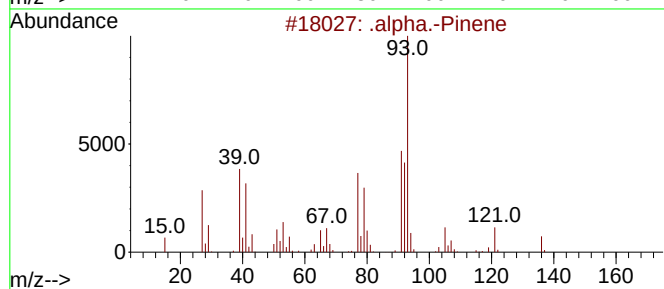
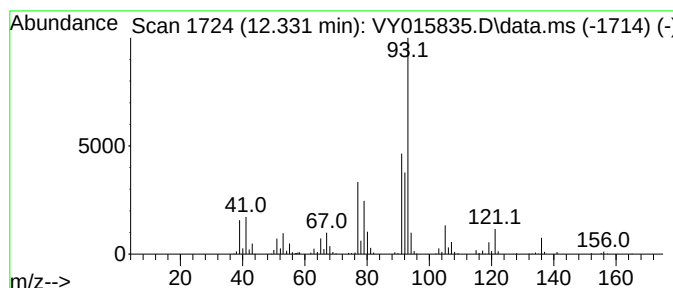
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y091923S.M
Quant Title : SW846 8260

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

Peak Number 1 .alpha.-Pinene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.331	14.74 ug/l	247449	Chlorobenzene-d5	11.490

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	.		.alpha.-Pinene	136	C10H16	000080-56-8	95
2	(1R)-2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene, 3,6,6-trimethyl-			136	C10H16	007785-70-8	94
3	Bicyclo[3.1.1]hept-2-ene, 3,6,6-trimethyl-			136	C10H16	004889-83-2	91
4	.gamma.-Terpinene			136	C10H16	000099-85-4	90
5	(+)-3-Carene			136	C10H16	000498-15-7	90



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Instrument :
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ClientSampleId :
S-3(0-5)

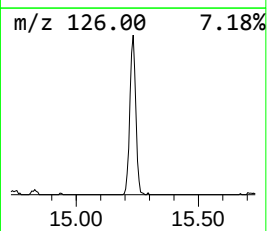
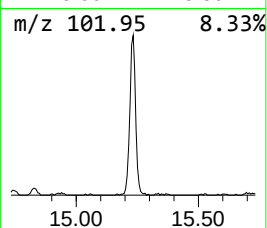
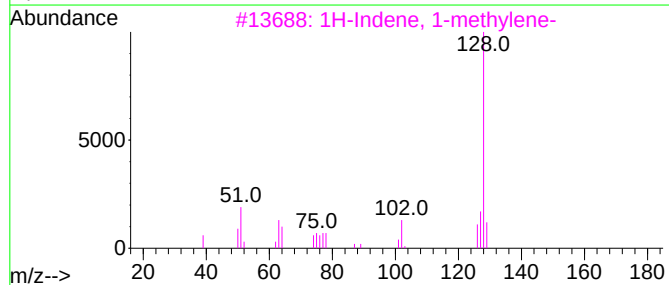
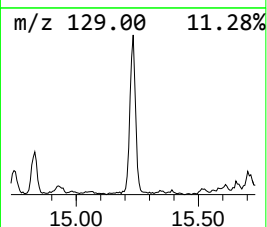
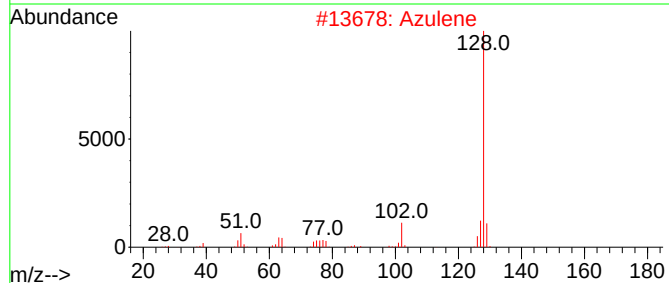
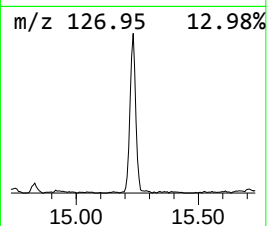
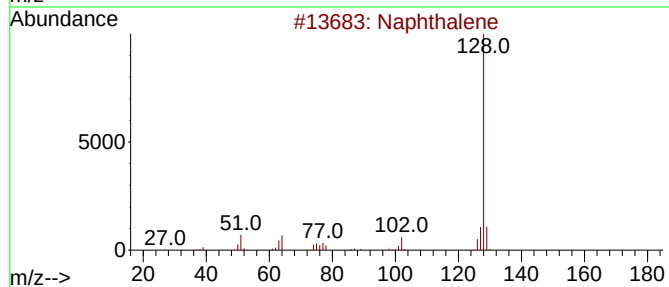
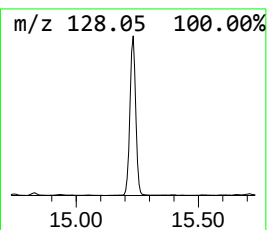
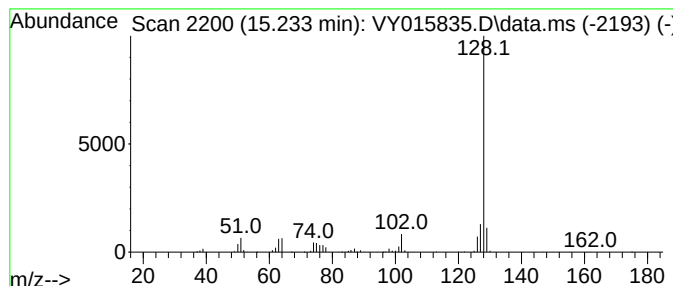
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y091923S.M
Quant Title : SW846 8260

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

Peak Number 2 Azulene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.233	25.12 ug/l	378468	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	94
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	59



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ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
S-3(0-5)

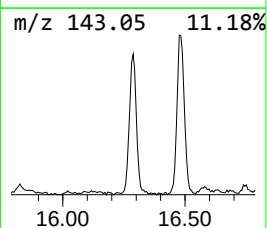
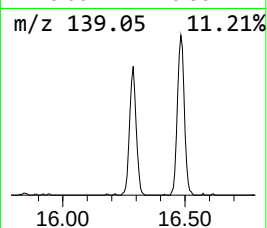
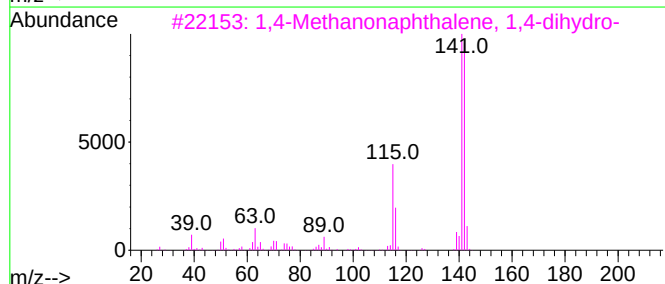
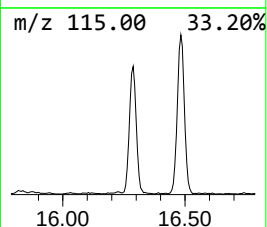
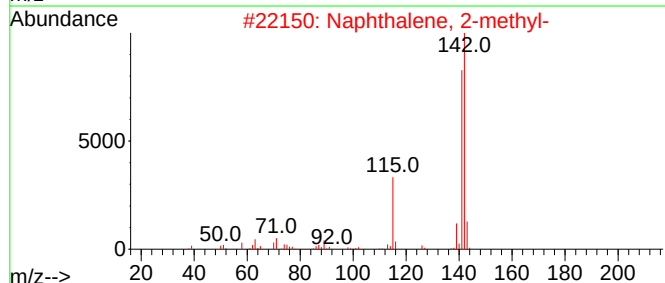
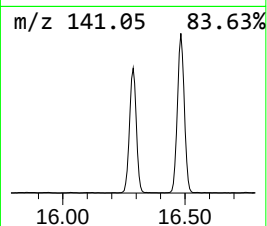
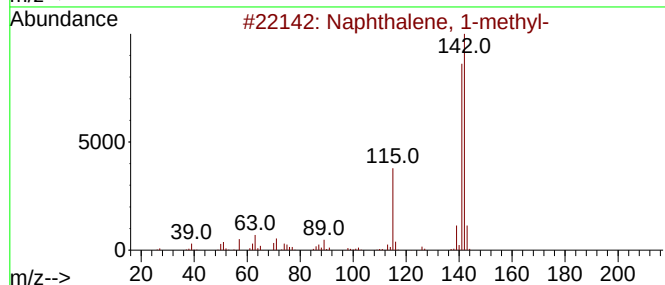
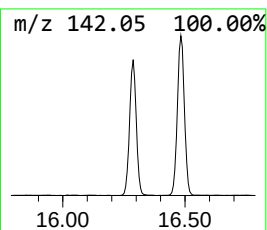
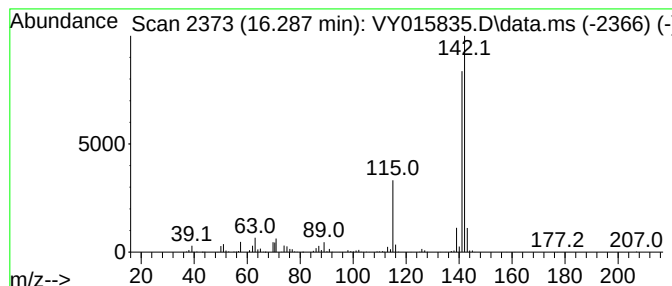
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1,4-Methanonaphthalene, 1,4... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.288	29.77 ug/l	448404	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			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	90
4			Benzocycloheptatriene	142	C11H10	000264-09-5	90
5			Naphthalene, 1-[(2-propenyloxy)m...	198	C14H14O	074685-39-5	78



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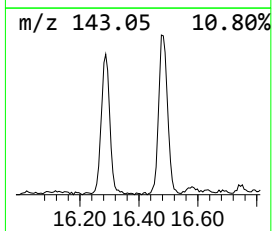
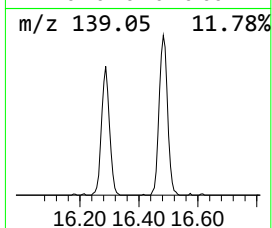
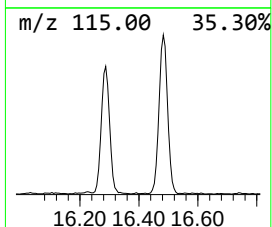
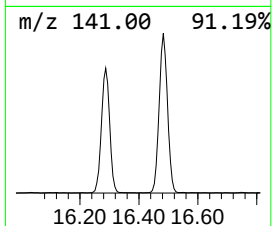
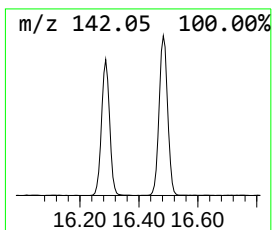
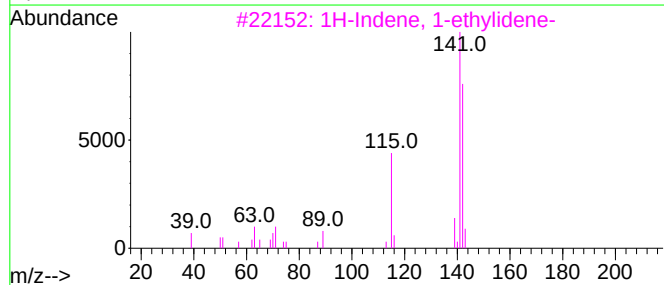
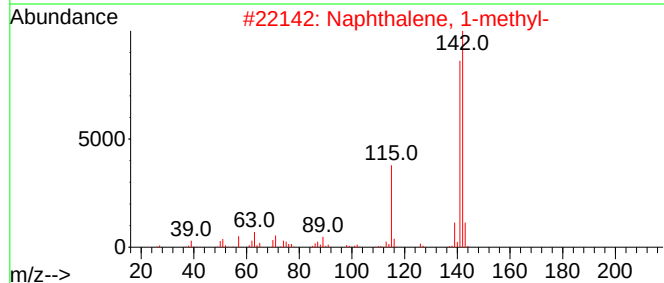
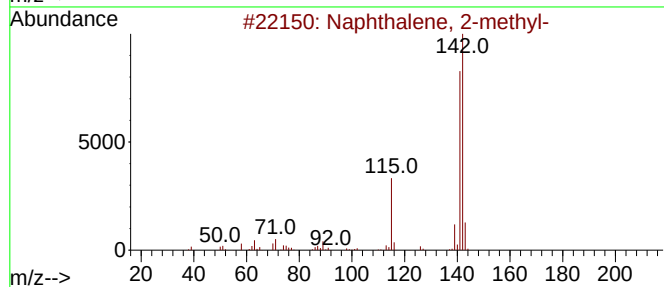
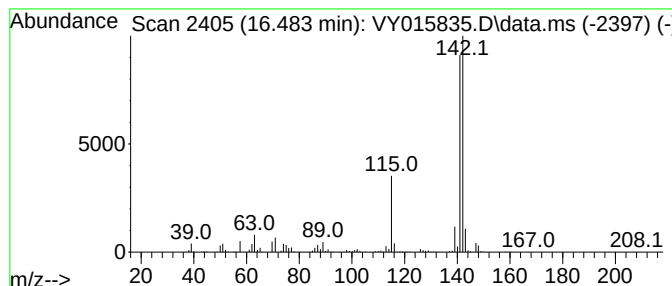
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y091923S.M
Quant Title : SW846 8260

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

Peak Number 4 1H-Indene, 1-ethylidene- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.483	38.65 ug/l	582256	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			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	94
4			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
5			Benzocycloheptatriene	142	C11H10	000264-09-5	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
.alpha.-Pinene	12.331	14.7	ug/l	247449	3	11.490	839174	50.0
Azulene	15.233	25.1	ug/l	378468	4	13.422	753182	50.0
1,4-Methanonaph...	16.288	29.8	ug/l	448404	4	13.422	753182	50.0
1H-Indene, 1-et...	16.483	38.6	ug/l	582256	4	13.422	753182	50.0