

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY100623\
 Data File : VY015864.D
 Acq On : 06 Oct 2023 15:59
 Operator : SY/MD
 Sample : 04767-01
 Misc : 4.95g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 D-1(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\82Y100523S.M
 Title : SW846 8260

Signal : TIC: VY015864.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.972	343	353	365	rBV	11857	46238	3.84%	0.493%
2	4.180	379	387	403	rVB2	7319	19996	1.66%	0.213%
3	4.704	461	473	486	rBV2	37138	116624	9.69%	1.244%
4	5.734	633	642	654	rBV5	3679	12081	1.00%	0.129%
5	6.984	837	847	866	rVB3	18807	54369	4.52%	0.580%
6	7.716	956	967	972	rBV	173800	414195	34.42%	4.420%
7	7.783	972	978	992	rVB	296880	655188	54.45%	6.991%
8	8.136	1026	1036	1049	rBV	194025	449758	37.38%	4.799%
9	8.685	1117	1126	1146	rBV	446522	885062	73.56%	9.444%
10	8.935	1160	1167	1177	rBV	64801	124167	10.32%	1.325%
11	10.179	1361	1371	1378	rBV	697107	1203210	100.00%	12.839%
12	10.240	1378	1381	1388	rVB	12267	21326	1.77%	0.228%
13	10.715	1452	1459	1469	rVB	199405	340774	28.32%	3.636%
14	11.489	1578	1586	1598	rBV	667041	1064800	88.50%	11.362%
15	11.697	1612	1620	1632	rVV2	6732	14151	1.18%	0.151%
16	12.483	1742	1749	1757	rBV	525585	814888	67.73%	8.696%
17	12.733	1785	1790	1794	rBV	7833	12747	1.06%	0.136%
18	12.806	1798	1802	1812	rVB4	12022	23043	1.92%	0.246%
19	13.117	1849	1853	1858	rBV2	10227	15512	1.29%	0.166%
20	13.422	1897	1903	1916	rVB	660960	1015514	84.40%	10.836%
21	13.623	1932	1936	1940	rBV	26948	42948	3.57%	0.458%
22	13.660	1940	1942	1950	rVB2	15909	23754	1.97%	0.253%
23	13.965	1987	1992	1999	rVB3	20650	33677	2.80%	0.359%
24	14.080	2005	2011	2016	rVB	31724	48772	4.05%	0.520%
25	14.562	2086	2090	2096	rBV2	16650	29628	2.46%	0.316%
26	14.684	2102	2110	2116	rBV3	57966	106935	8.89%	1.141%
27	14.940	2142	2152	2156	rBV2	12623	27159	2.26%	0.290%
28	15.050	2162	2170	2180	rVB4	17399	46521	3.87%	0.496%
29	15.233	2191	2200	2207	rBV	335087	559596	46.51%	5.971%
30	15.336	2212	2217	2223	rVV3	19161	39622	3.29%	0.423%
31	15.391	2223	2226	2232	rVB	11604	17577	1.46%	0.188%
32	15.525	2242	2248	2253	rBV	12651	21234	1.76%	0.227%
33	15.690	2264	2275	2285	rBV4	13617	40754	3.39%	0.435%
34	15.818	2291	2296	2301	rBV8	4946	12938	1.08%	0.138%
35	15.891	2303	2308	2313	rVB3	10122	20731	1.72%	0.221%
36	16.226	2353	2363	2367	rBV6	11590	34350	2.85%	0.367%

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D-1(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

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37	16.287	2367	2373	2387	rVB	234837	469071	38.98%	5.005%
38	16.488	2397	2406	2415	rVB	237402	492426	40.93%	5.255%

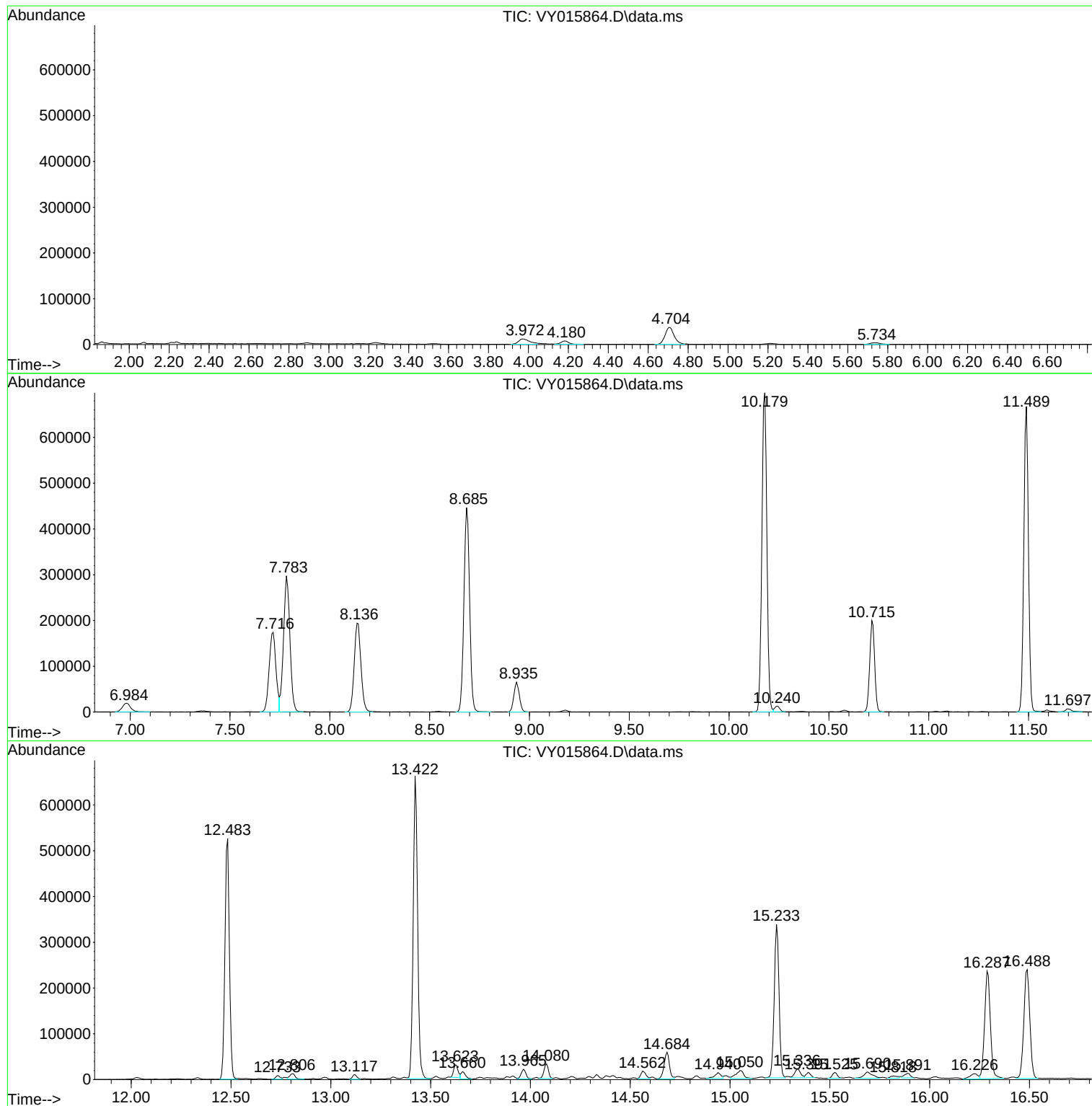
Sum of corrected areas: 9371336

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



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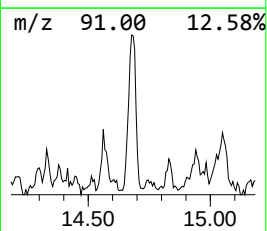
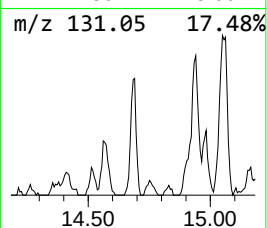
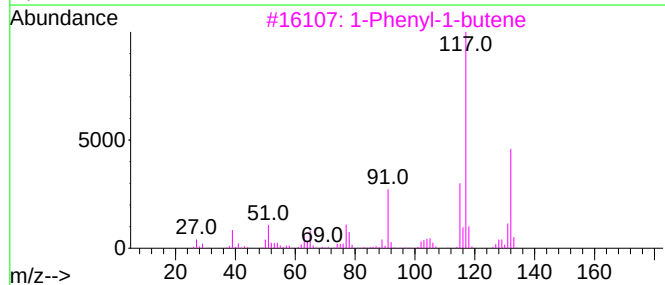
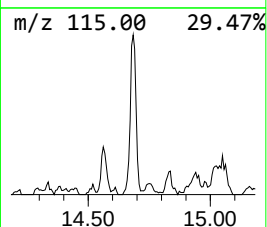
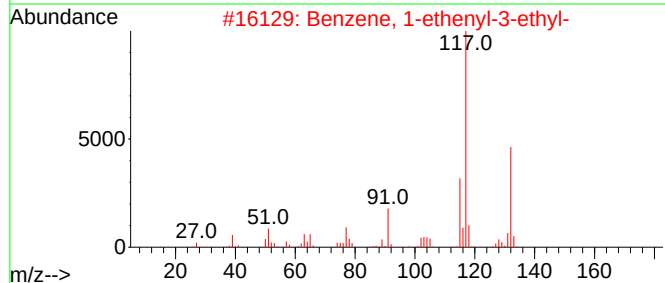
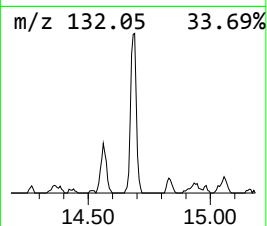
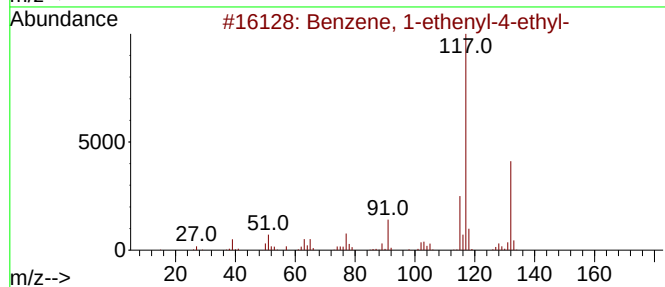
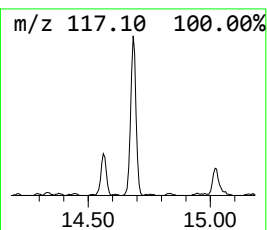
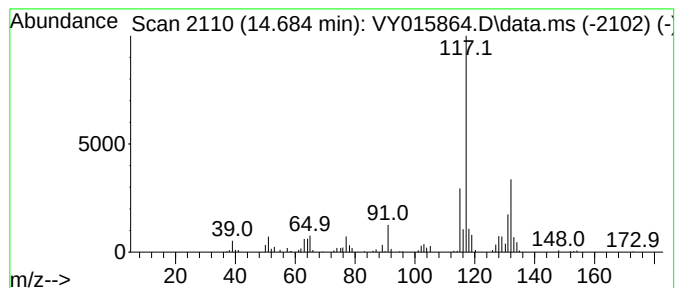
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y100523S.M
Quant Title : SW846 8260

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

Peak Number 2 Benzene, 1-ethenyl-4-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.684	5.27 ug/l	106935	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
2			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	90
3			1-Phenyl-1-butene	132	C10H12	000824-90-8	90
4			1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	87
5			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	87



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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
D-1(0-5)

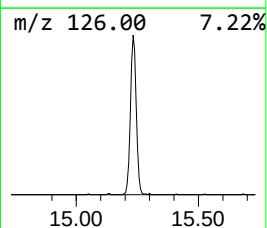
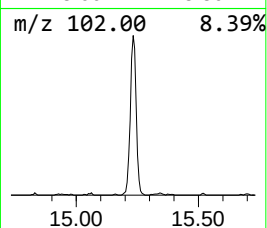
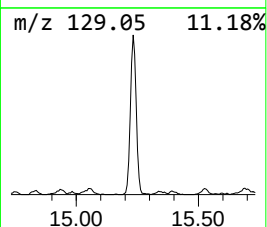
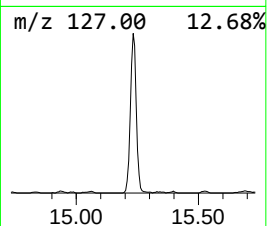
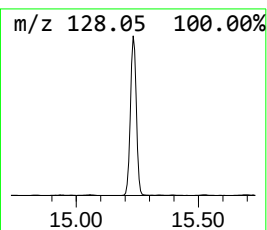
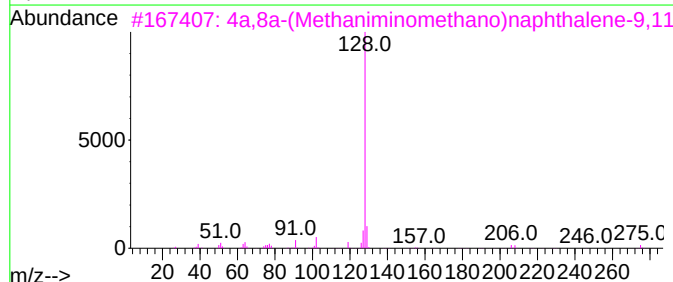
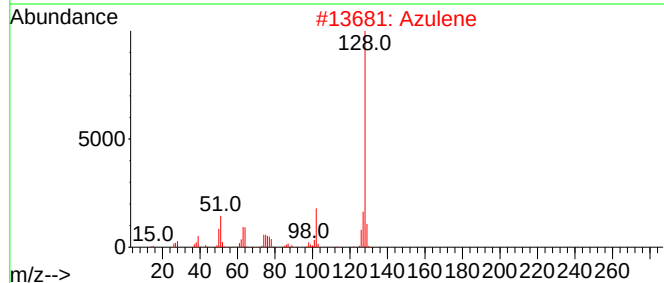
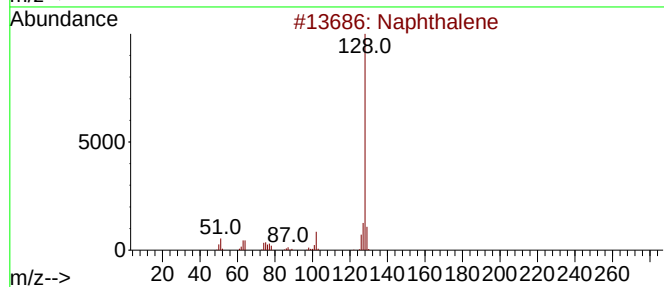
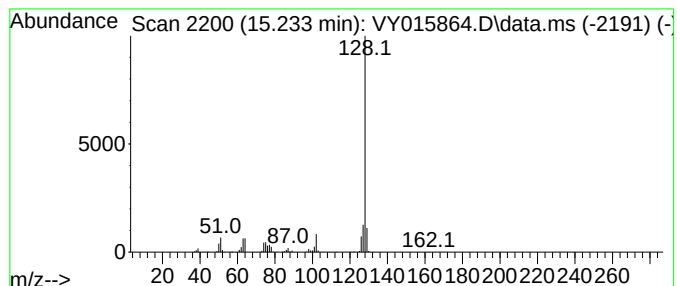
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y100523S.M
Quant Title : SW846 8260

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

Peak Number 3 Azulene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.233	27.55 ug/l	559596	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			4a,8a-(Methaniminomethano)naphth...	275	C18H13NO2	069915-10-2	64
4			1,3-Dicyanobenzene	128	C8H4N2	000626-17-5	64
5			[4.2.2]Propella-2,4,7,9-tetraene	128	C10H8	088090-34-0	50



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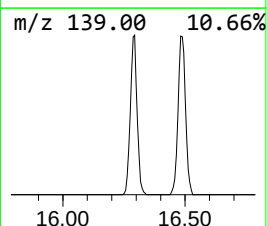
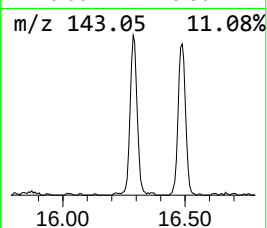
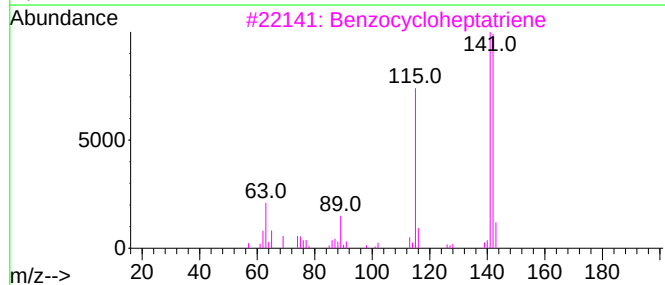
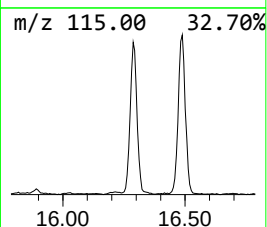
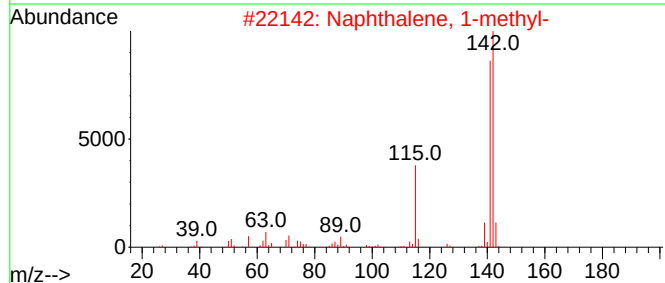
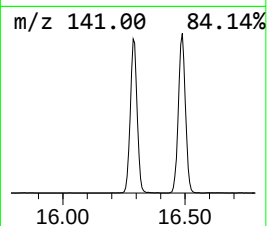
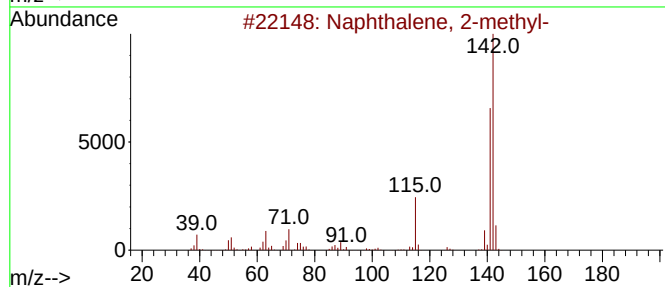
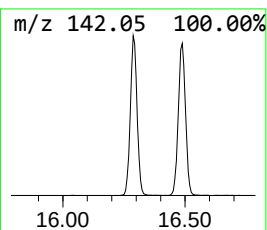
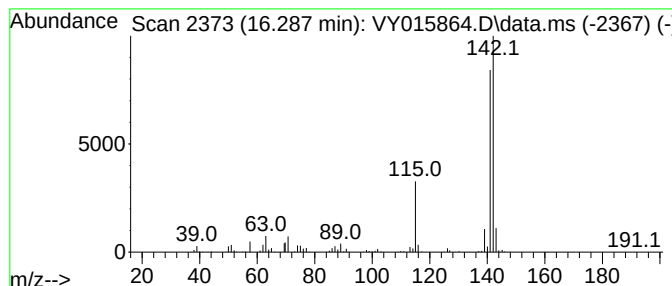
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Quant Title : SW846 8260

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

Peak Number 4 Benzocycloheptatriene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.287	23.10 ug/l	469071	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	91
5			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	59



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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
D-1(0-5)

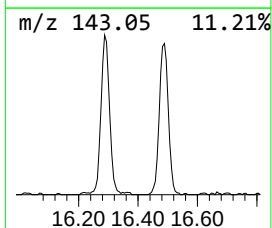
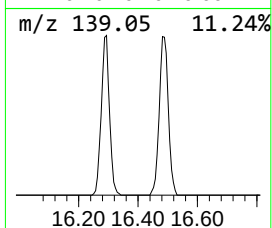
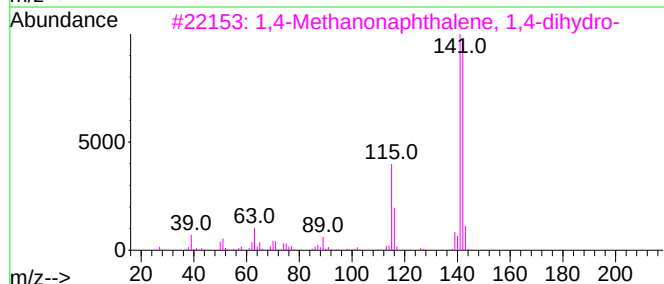
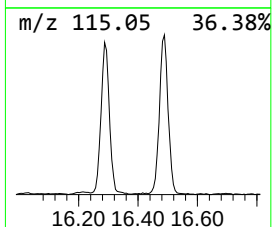
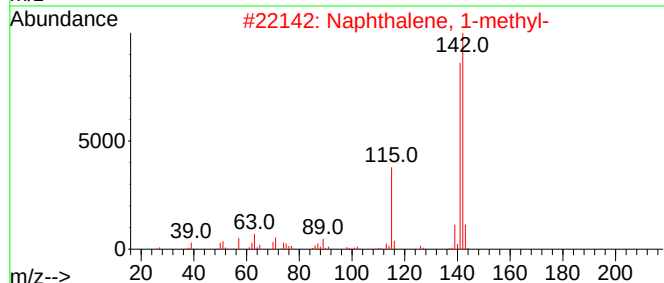
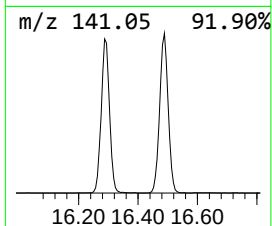
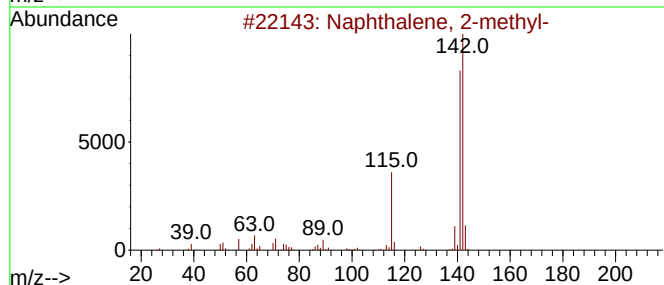
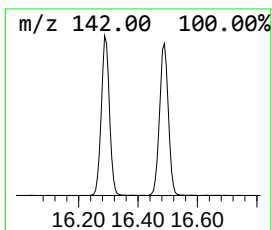
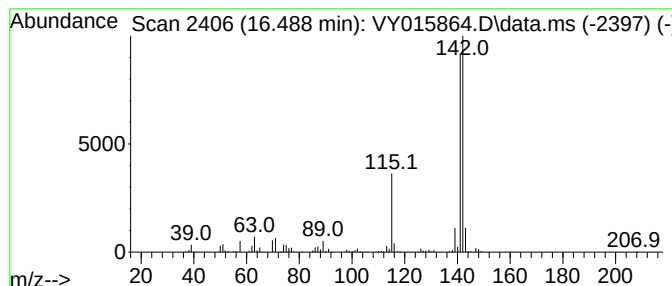
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1,4-Methanonaphthalene, 1,4... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.488	24.25 ug/l	492426	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			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
4			Benzocycloheptatriene	142	C11H10	000264-09-5	91
5			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	64



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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
Benzene, 1-ethe...	14.684	5.3	ug/l	106935	4	13.422	1015510	50.0
Azulene	15.233	27.6	ug/l	559596	4	13.422	1015510	50.0
Benzocyclohepta...	16.287	23.1	ug/l	469071	4	13.422	1015510	50.0
1,4-Methanonaph...	16.488	24.3	ug/l	492426	4	13.422	1015510	50.0