

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY052424\
 Data File : VY018367.D
 Acq On : 24 May 2024 15:56
 Operator : SY/MD
 Sample : P2330-22
 Misc : 4.92g/5.0mL/MSVOA_Y/SOIL/A
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 H-3(5.0-6.0)

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\82Y052224S.M
 Title : SW846 8260

Signal : TIC: VY018367.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.857	3	6	13	rVB3	16234	22974	3.45%	0.586%
2	2.211	59	64	74	rVB3	12265	28355	4.26%	0.724%
3	4.180	379	387	395	rBV	7286	21122	3.17%	0.539%
4	4.692	462	471	483	rBV2	17665	58895	8.85%	1.503%
5	5.735	634	642	653	rVB3	9047	28792	4.32%	0.735%
6	7.704	954	965	971	rBV2	92118	217804	32.71%	5.559%
7	7.777	971	977	990	rVB	153881	345307	51.86%	8.813%
8	8.130	1026	1035	1046	rBV	85598	186151	27.96%	4.751%
9	8.679	1116	1125	1136	rBV	248214	505626	75.94%	12.904%
10	10.173	1363	1370	1378	rBV	391694	665784	100.00%	16.992%
11	11.490	1577	1586	1596	rBV	314964	538090	80.82%	13.733%
12	11.703	1614	1621	1624	rBV4	3364	8433	1.27%	0.215%
13	12.008	1662	1671	1673	rBV7	5431	12779	1.92%	0.326%
14	12.197	1699	1702	1705	rVV5	4013	6908	1.04%	0.176%
15	12.233	1705	1708	1715	rVB6	4030	8972	1.35%	0.229%
16	12.477	1741	1748	1756	rBV	197562	312389	46.92%	7.973%
17	12.648	1772	1776	1783	rVB9	5195	10753	1.62%	0.274%
18	12.733	1784	1790	1792	rBV7	3868	7098	1.07%	0.181%
19	12.806	1798	1802	1808	rVB6	8448	14075	2.11%	0.359%
20	13.117	1847	1853	1858	rBV	8330	12477	1.87%	0.318%
21	13.422	1897	1903	1916	rVB	193127	304798	45.78%	7.779%
22	13.623	1932	1936	1941	rBV2	21472	35134	5.28%	0.897%
23	13.739	1951	1955	1964	rBV8	4397	8327	1.25%	0.213%
24	13.965	1988	1992	1997	rVB2	8249	14090	2.12%	0.360%
25	14.081	2005	2011	2016	rVB3	10126	16418	2.47%	0.419%
26	14.331	2049	2052	2057	rVB2	5497	7781	1.17%	0.199%
27	14.562	2086	2090	2096	rBV4	8993	14408	2.16%	0.368%
28	14.684	2102	2110	2115	rBV3	20798	41621	6.25%	1.062%
29	14.940	2148	2152	2157	rBV5	4440	7860	1.18%	0.201%
30	15.050	2167	2170	2175	rVB6	4701	8519	1.28%	0.217%
31	15.233	2194	2200	2206	rVB	91552	155029	23.29%	3.957%
32	15.330	2211	2216	2223	rBV5	8220	16326	2.45%	0.417%
33	15.422	2228	2231	2239	rVB7	3542	6859	1.03%	0.175%
34	15.526	2239	2248	2254	rBV5	5179	10318	1.55%	0.263%
35	16.227	2356	2363	2367	rBV5	3858	7362	1.11%	0.188%
36	16.288	2367	2373	2384	rVB	74544	151479	22.75%	3.866%

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Instrument :
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ClientSampleId :
H-3(5.0-6.0)

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\82Y052224S.M
Title : SW846 8260

37	16.489	2398	2406	2414	rVB	47465	99104	14.89%	2.529%
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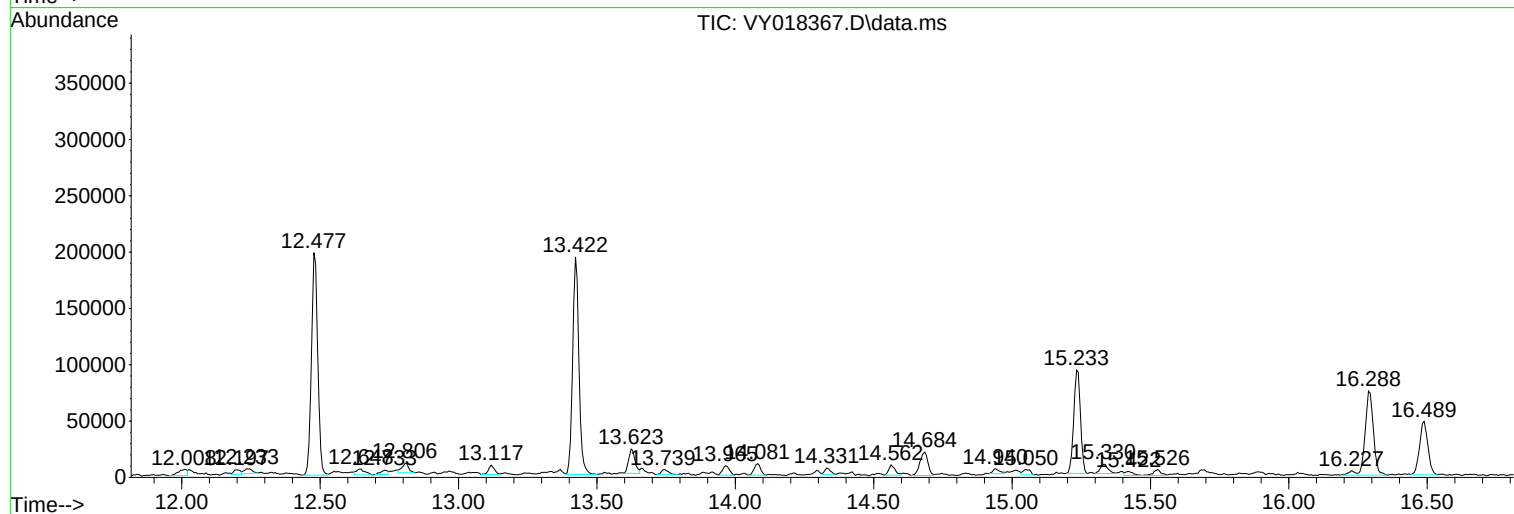
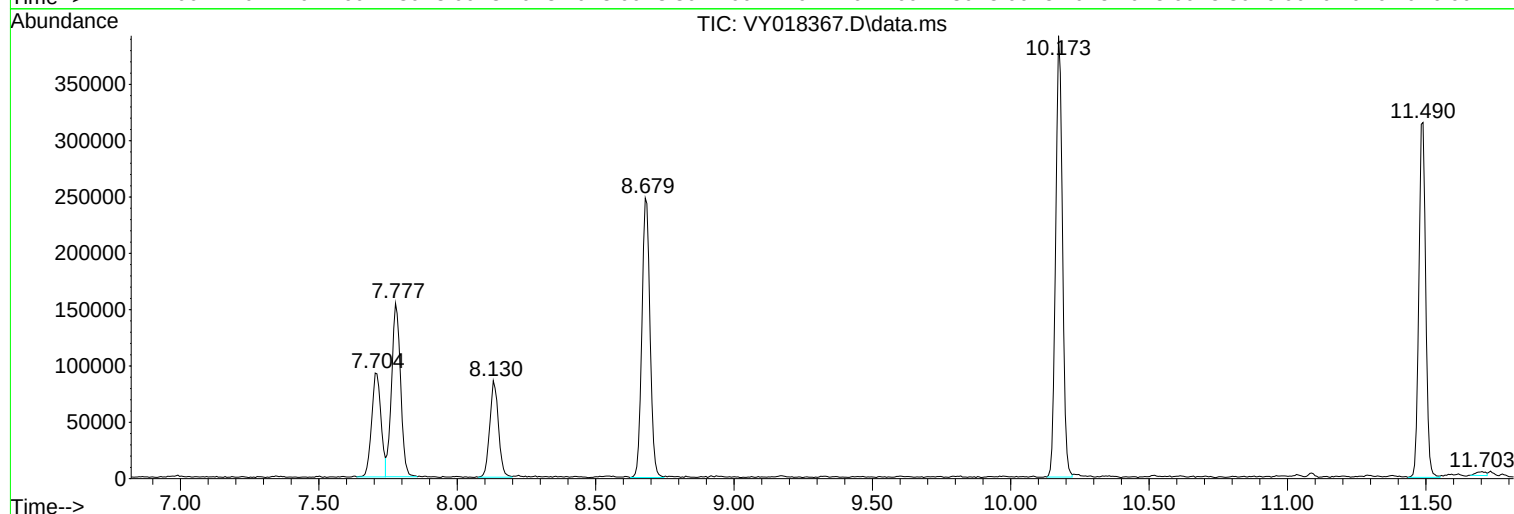
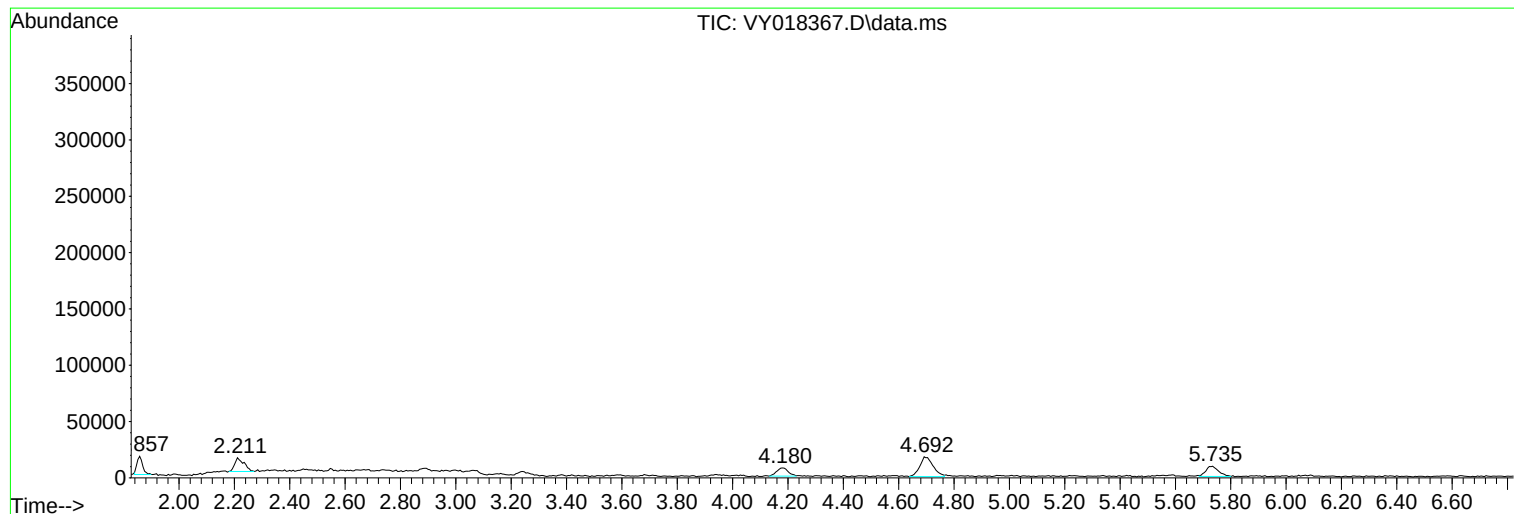
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y052224S.M
Quant Title : SW846 8260

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



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Instrument :
MSVOA_Y
ClientSampleId :
H-3(5.0-6.0)

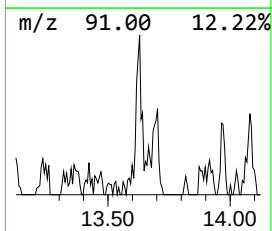
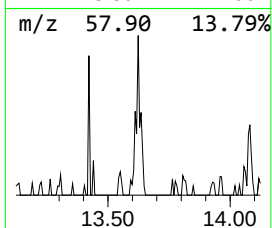
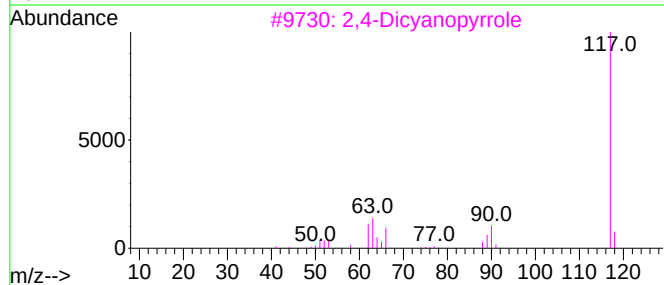
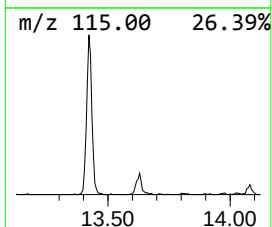
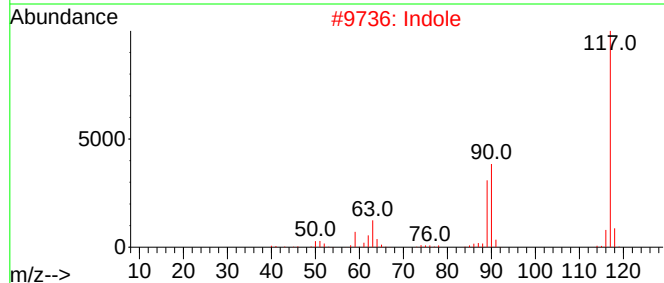
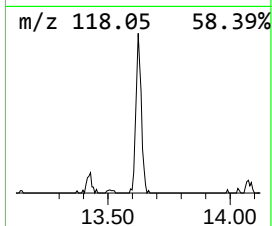
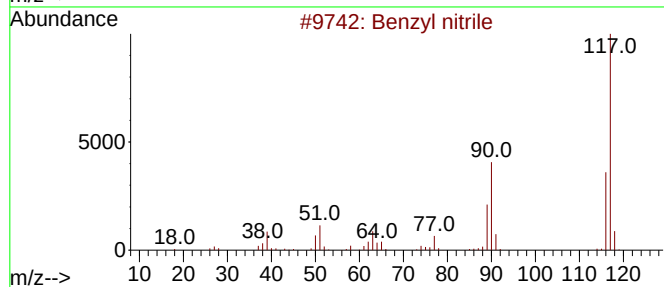
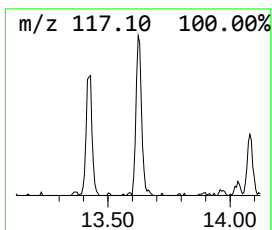
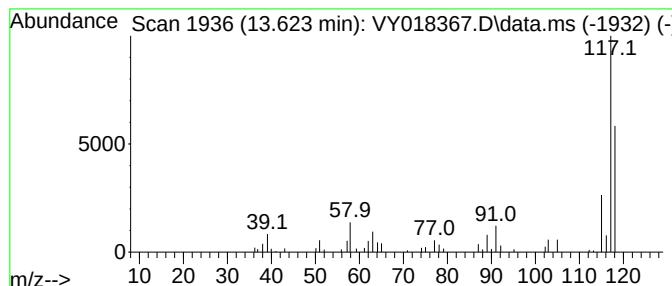
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y052224S.M
Quant Title : SW846 8260

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

Peak Number 1 unknown13.623 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.623	5.76 ug/l	35134	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzyl nitrile	117	C8H7N	000140-29-4	49
2			Indole	117	C8H7N	000120-72-9	47
3			2,4-Dicyanopyrrole	117	C6H3N3	074023-87-3	43
4			4-Ethynylaniline	117	C8H7N	014235-81-5	43
5			Benzene, 1,1'-(1,5-hexadiene-1,6...	234	C18H18	004439-45-6	42



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ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
H-3(5.0-6.0)

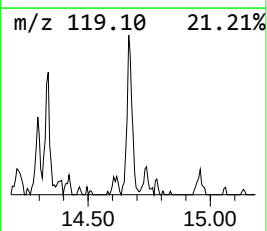
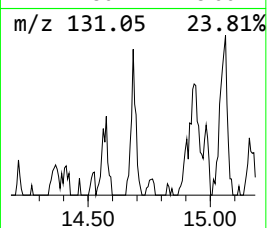
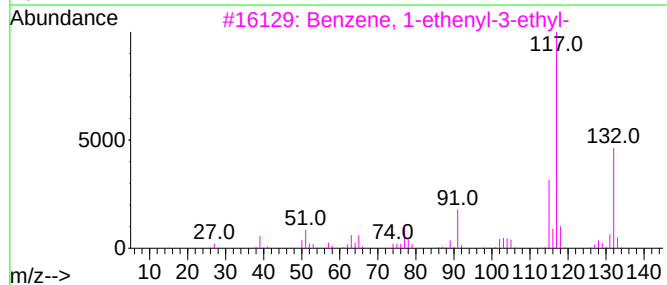
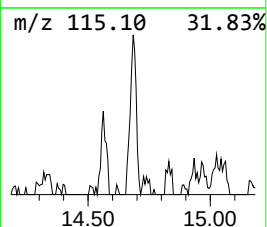
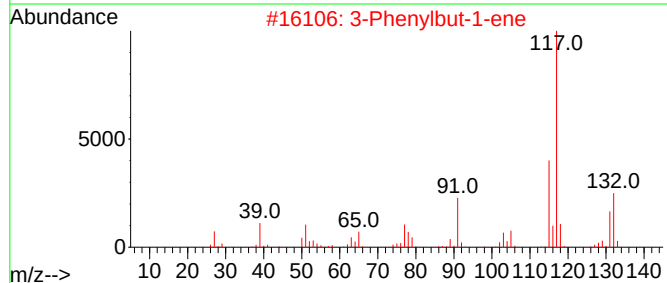
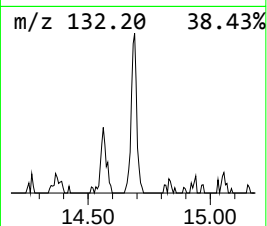
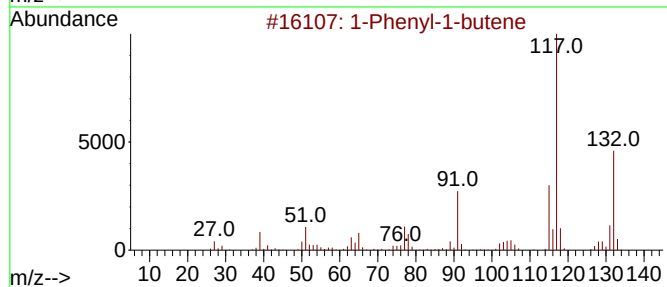
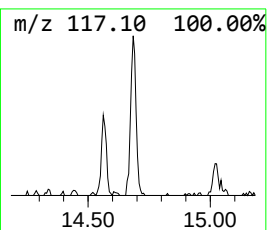
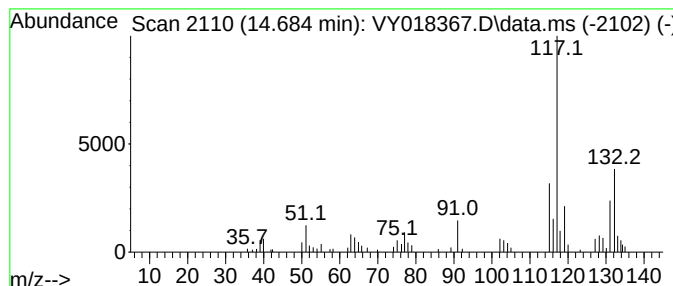
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 1-Phenyl-1-butene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.684	6.83 ug/l	41621	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenyl-1-butene	132	C10H12	000824-90-8	90
2			3-Phenylbut-1-ene	132	C10H12	000934-10-1	87
3			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	81
4			1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	81
5			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	81



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Instrument :
MSVOA_Y
ClientSampleId :
H-3(5.0-6.0)

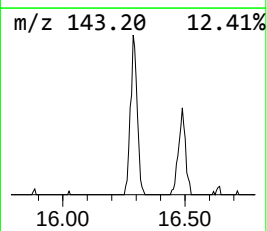
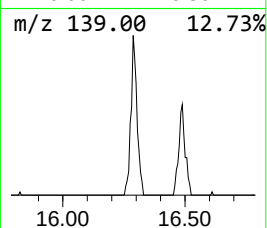
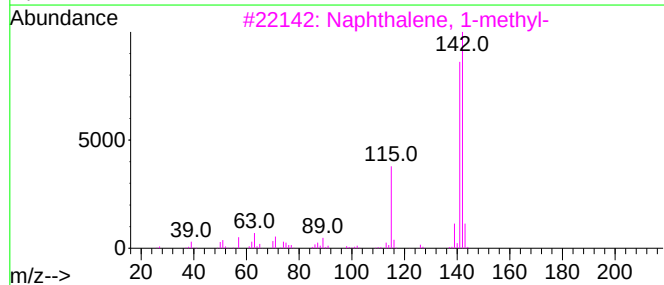
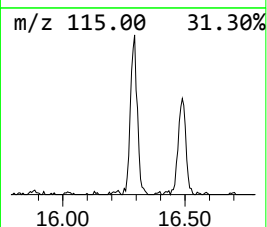
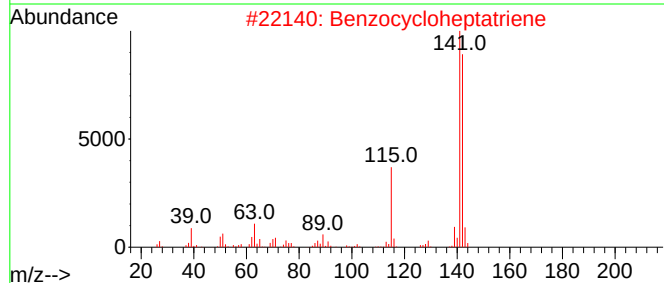
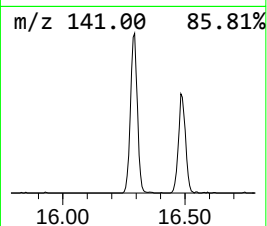
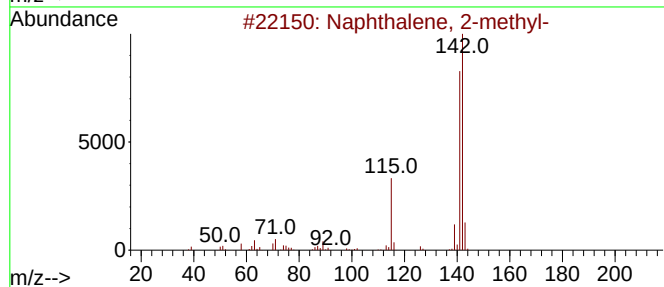
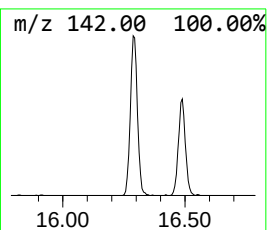
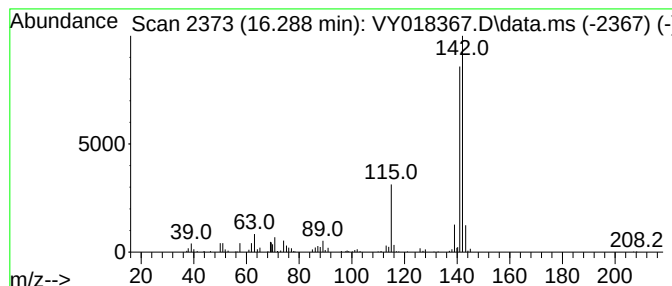
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y052224S.M
Quant Title : SW846 8260

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

Peak Number 3 Naphthalene, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.288	24.85 ug/l	151479	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			Benzocycloheptatriene	142	C11H10	000264-09-5	95
3			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	95
4			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	87
5			Naphthalene, 1-[(2-propenyloxy)m...	198	C14H14O	074685-39-5	64



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ClientSampleId :
H-3(5.0-6.0)

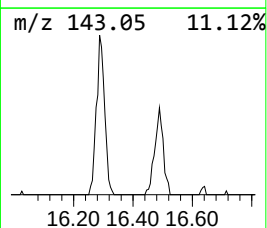
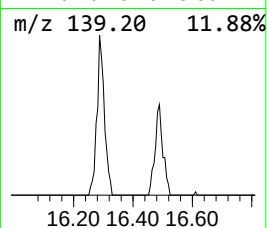
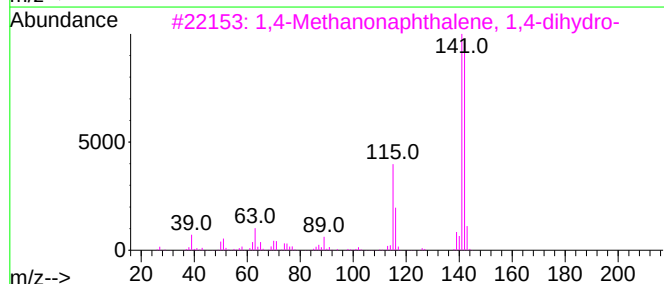
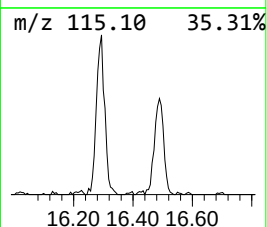
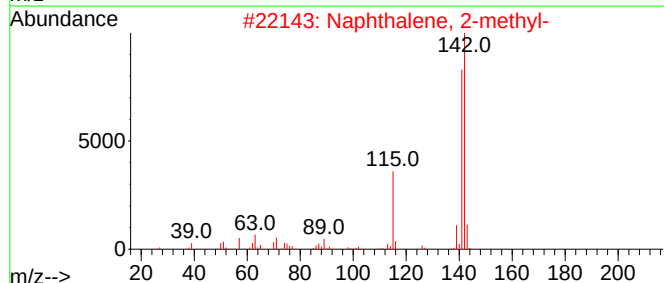
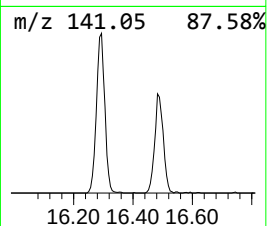
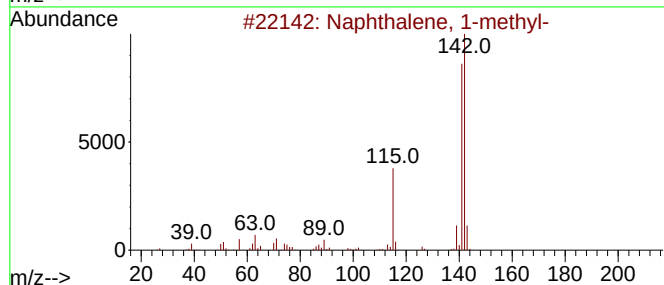
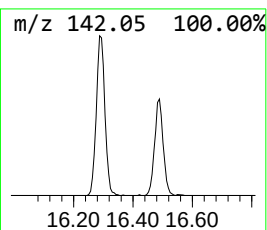
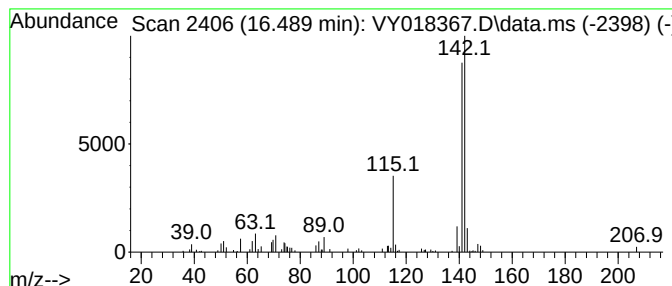
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Naphthalene, 1-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.489	16.26 ug/l	99104	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	95
2			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	95
3			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
4			Benzocycloheptatriene	142	C11H10	000264-09-5	90
5			3,4-Difluorobenzaldehyde	142	C7H4F2O	034036-07-2	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
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1-Phenyl-1-butene	14.684	6.8	ug/l	41621	4	13.422	304798	50.0
Naphthalene, 2-...	16.288	24.9	ug/l	151479	4	13.422	304798	50.0
Naphthalene, 1-...	16.489	16.3	ug/l	99104	4	13.422	304798	50.0