

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010322\
 Data File : VX026224.D
 Acq On : 03 Jan 2022 16:47
 Operator : JC/MD
 Sample : M5335-02
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 20967

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\82X123021W.M
 Title : SW846 8260

Signal : TIC: VX026224.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.380	203	212	217	rBV	11005	18217	1.75%	0.213%
2	5.391	694	706	721	rBV2	120996	354049	34.08%	4.141%
3	5.556	721	733	752	rVB	203952	580194	55.85%	6.786%
4	5.958	788	799	816	rBV	142505	377864	36.37%	4.419%
5	6.763	920	931	948	rBV	329834	803934	77.39%	9.402%
6	8.580	1224	1229	1234	rBV2	8739	15308	1.47%	0.179%
7	8.653	1234	1241	1247	rVV	648811	1038858	100.00%	12.150%
8	8.720	1247	1252	1263	rVB	68645	108452	10.44%	1.268%
9	10.055	1465	1471	1488	rVB	667787	909037	87.50%	10.631%
10	11.079	1634	1639	1653	rBV	530823	685523	65.99%	8.017%
11	11.378	1683	1688	1690	rBV	8746	11574	1.11%	0.135%
12	11.451	1697	1700	1704	rVV	14088	15866	1.53%	0.186%
13	11.616	1723	1727	1732	rBV	11696	15554	1.50%	0.182%
14	11.750	1744	1749	1757	rVB	12920	17794	1.71%	0.208%
15	12.024	1788	1794	1801	rVV	663903	839608	80.82%	9.819%
16	12.085	1801	1804	1809	rVB	13664	17072	1.64%	0.200%
17	12.250	1828	1831	1832	rVV2	14442	16995	1.64%	0.199%
18	12.268	1832	1834	1838	rVB	15818	17273	1.66%	0.202%
19	12.317	1838	1842	1850	rVB2	40708	57359	5.52%	0.671%
20	12.463	1861	1866	1872	rVB	15046	18491	1.78%	0.216%
21	12.530	1872	1877	1879	rBV	10348	14051	1.35%	0.164%
22	12.555	1879	1881	1885	rVB	12592	13425	1.29%	0.157%
23	12.616	1885	1891	1894	rBV	32846	39314	3.78%	0.460%
24	12.701	1901	1905	1906	rBV	15445	17853	1.72%	0.209%
25	12.799	1917	1921	1924	rBV	10751	14281	1.37%	0.167%
26	12.847	1924	1929	1934	rVB2	17370	25409	2.45%	0.297%
27	12.921	1934	1941	1945	rBV	24962	37912	3.65%	0.443%
28	12.963	1945	1948	1954	rVB	38918	46230	4.45%	0.541%
29	13.030	1954	1959	1960	rBV2	15567	21444	2.06%	0.251%
30	13.140	1973	1977	1979	rBV2	13711	19086	1.84%	0.223%
31	13.164	1979	1981	1985	rVV2	16304	20380	1.96%	0.238%
32	13.213	1985	1989	1992	rVB4	10387	14606	1.41%	0.171%
33	13.256	1992	1996	1998	rBV3	15474	20701	1.99%	0.242%
34	13.292	1998	2002	2007	rVV2	61521	90376	8.70%	1.057%
35	13.341	2007	2010	2013	rVB3	9734	13068	1.26%	0.153%
36	13.427	2019	2024	2032	rVB3	36426	60005	5.78%	0.702%

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Integrator: RTE

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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	13.506	2032	2037	2040	rBV	16019	23561	2.27%	0.276%
38	13.548	2040	2044	2046	rVV	32306	45610	4.39%	0.533%
39	13.585	2046	2050	2055	rVV3	50559	98096	9.44%	1.147%
40	13.640	2056	2059	2061	rVV	28439	43884	4.22%	0.513%
41	13.664	2061	2063	2069	rVB3	38583	58631	5.64%	0.686%
42	13.798	2080	2085	2089	rVV3	11353	16007	1.54%	0.187%
43	13.853	2089	2094	2099	rVB2	48960	69347	6.68%	0.811%
44	13.926	2099	2106	2110	rBV2	64158	91350	8.79%	1.068%
45	13.975	2110	2114	2117	rVV	18557	22149	2.13%	0.259%
46	14.073	2126	2130	2135	rBV2	37448	51401	4.95%	0.601%
47	14.176	2139	2147	2150	rVV3	27285	48295	4.65%	0.565%
48	14.231	2150	2156	2159	rVV2	106747	201103	19.36%	2.352%
49	14.262	2159	2161	2164	rVV	31473	39187	3.77%	0.458%
50	14.323	2167	2171	2176	rVV	51339	65548	6.31%	0.767%
51	14.371	2176	2179	2184	rVB	63789	81698	7.86%	0.955%
52	14.420	2184	2187	2192	rVB2	18035	23685	2.28%	0.277%
53	14.481	2192	2197	2202	rBV2	105345	148609	14.31%	1.738%
54	14.591	2210	2215	2216	rBV3	7098	11307	1.09%	0.132%
55	14.615	2216	2219	2225	rVV3	62415	113220	10.90%	1.324%
56	14.670	2225	2228	2234	rVB	57068	81171	7.81%	0.949%
57	14.731	2234	2238	2241	rBV2	16924	23611	2.27%	0.276%
58	14.823	2248	2253	2255	rVV4	32012	51276	4.94%	0.600%
59	14.847	2255	2257	2262	rVB4	26481	30560	2.94%	0.357%
60	14.902	2262	2266	2272	rBV3	42677	73155	7.04%	0.856%
61	14.987	2276	2280	2286	rVB2	36751	53672	5.17%	0.628%
62	15.054	2286	2291	2294	rVB3	13985	20417	1.97%	0.239%
63	15.109	2296	2300	2302	rBV3	14410	18562	1.79%	0.217%
64	15.146	2302	2306	2309	rBV	33541	45364	4.37%	0.531%
65	15.182	2309	2312	2320	rVB	91346	152725	14.70%	1.786%
66	15.255	2320	2324	2326	rBV3	9637	14566	1.40%	0.170%
67	15.316	2330	2334	2336	rBV2	18023	25307	2.44%	0.296%
68	15.377	2341	2344	2352	rVB7	19929	47026	4.53%	0.550%
69	15.481	2357	2361	2364	rBV2	21247	30109	2.90%	0.352%
70	15.524	2364	2368	2373	rVB3	16740	24094	2.32%	0.282%
71	15.615	2378	2383	2386	rVV5	24314	45414	4.37%	0.531%
72	15.652	2386	2389	2397	rVB5	15609	31234	3.01%	0.365%
73	15.749	2398	2405	2408	rBV7	10764	23852	2.30%	0.279%
74	15.847	2417	2421	2425	rBV6	9456	15160	1.46%	0.177%
75	15.993	2439	2445	2457	rVB9	9185	29130	2.80%	0.341%
76	16.127	2457	2467	2469	rBV9	4696	14305	1.38%	0.167%

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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

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Title : SW846 8260

77	16.176	2471	2475	2481	rVB5	10733	20443	1.97%	0.239%
78	16.261	2481	2489	2493	rBV3	11059	23622	2.27%	0.276%
79	16.542	2528	2535	2540	rVB9	5425	15840	1.52%	0.185%

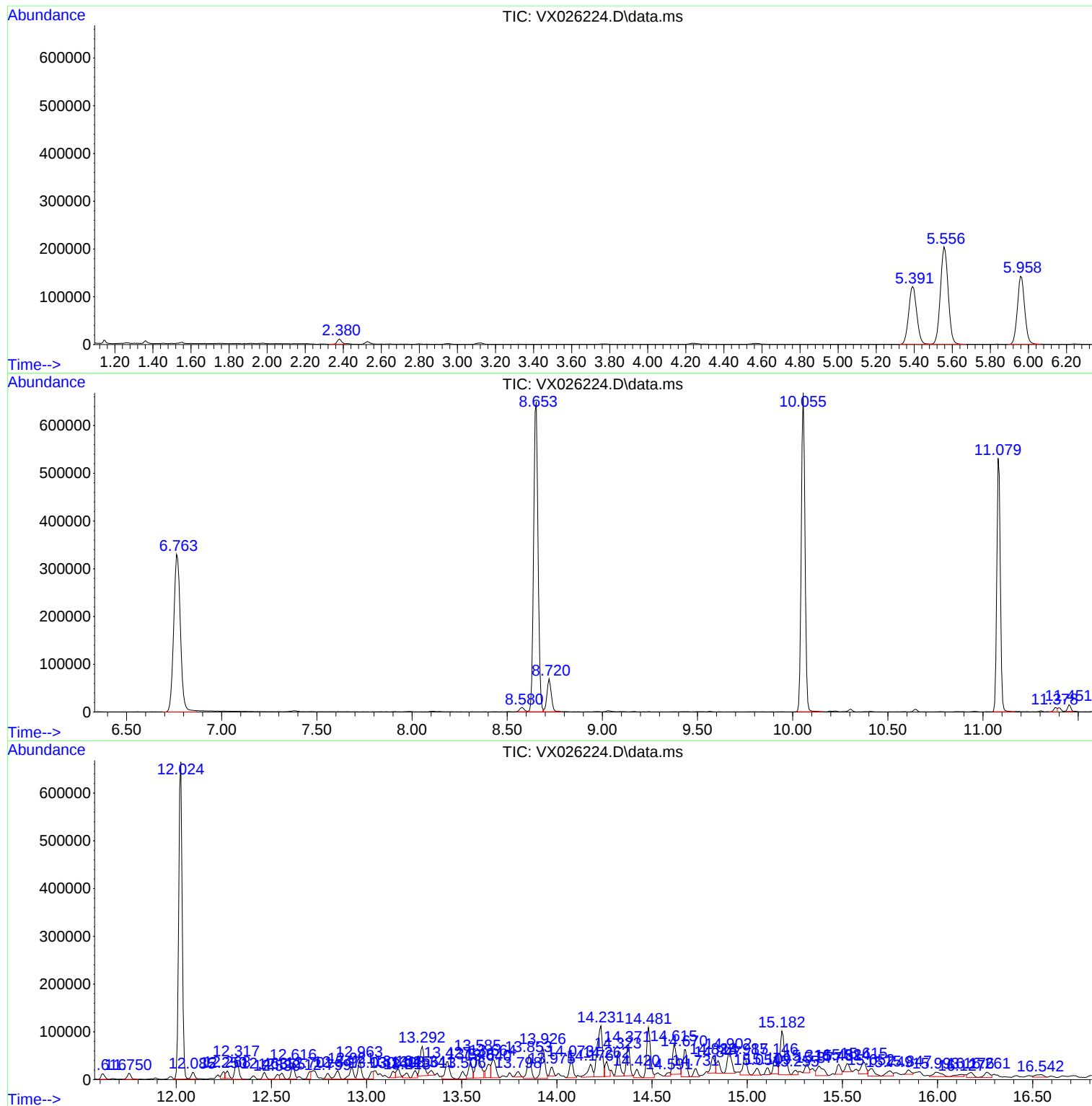
Sum of corrected areas: 8550466

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X123021W.M
Quant Title : SW846 8260

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



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Data File : VX026224.D
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Instrument :
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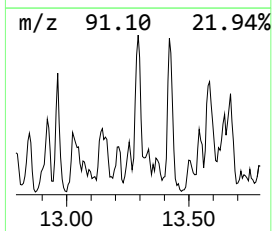
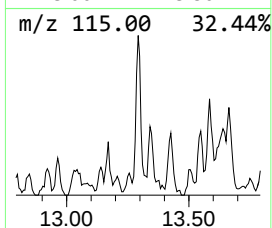
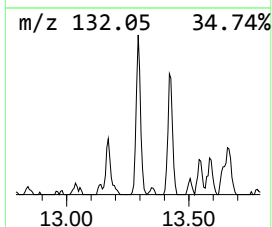
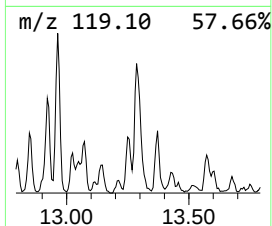
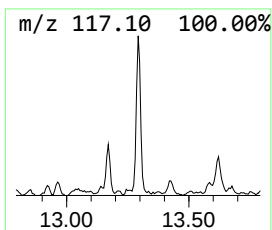
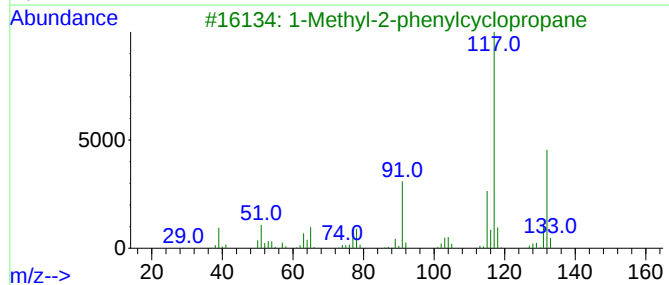
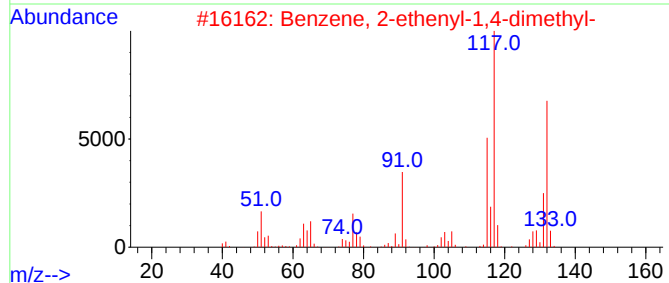
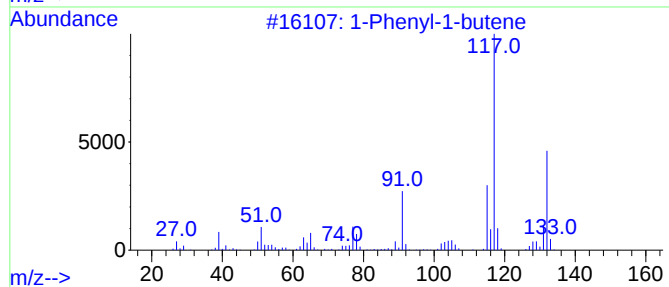
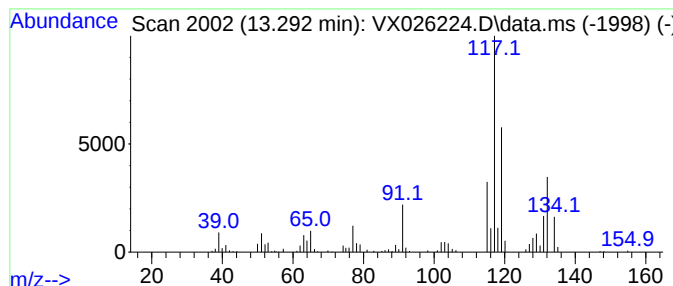
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X123021W.M
Quant Title : SW846 8260

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

Peak Number 1 1-Phenyl-1-butene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	5.38 ug/l	90376	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenyl-1-butene	132	C10H12	000824-90-8	93
2			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	87
3			1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	70
4			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	70
5			Benzene, 2-butenyl-	132	C10H12	001560-06-1	70



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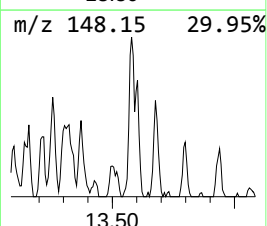
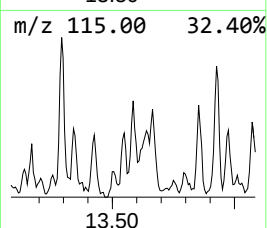
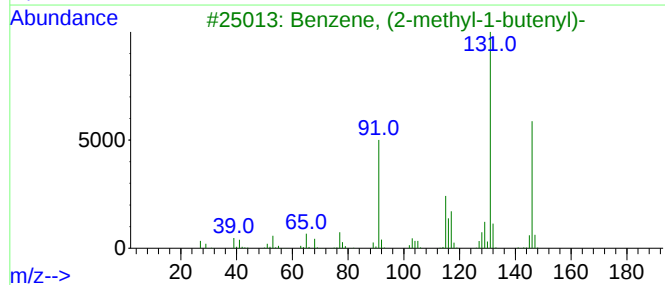
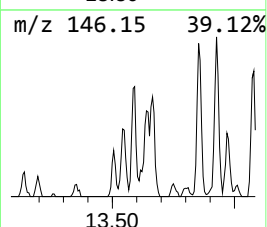
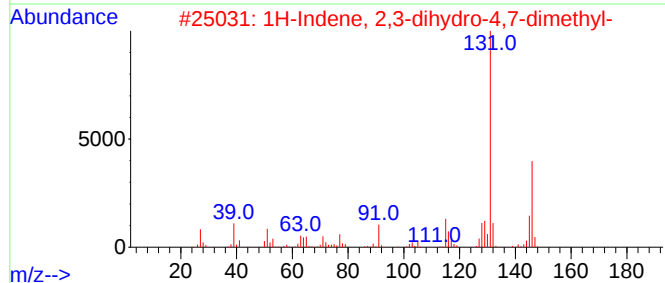
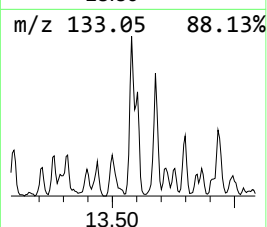
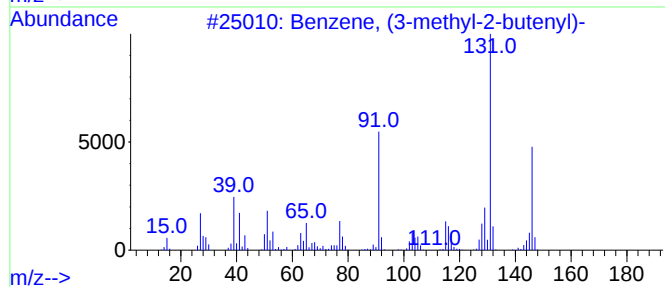
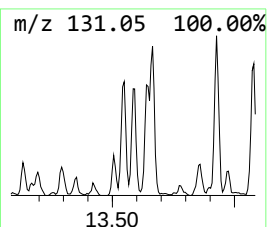
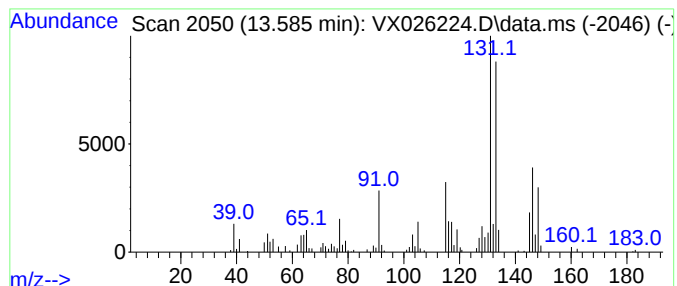
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X123021W.M
Quant Title : SW846 8260

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

Peak Number 2 Benzene, (3-methyl-2-butenyl)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.585	5.84 ug/l	98096	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	55
2			1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	55
3			Benzene, (2-methyl-1-butenyl)-	146	C11H14	056253-64-6	50
4			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001559-81-5	50
5			Benzene, (1-methyl-1-butenyl)-	146	C11H14	053172-84-2	50



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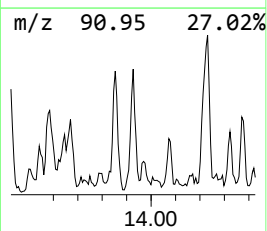
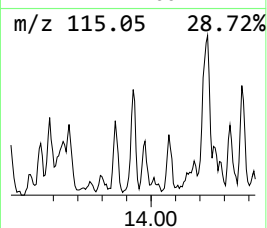
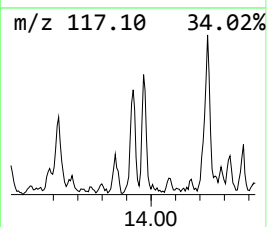
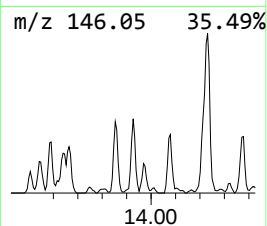
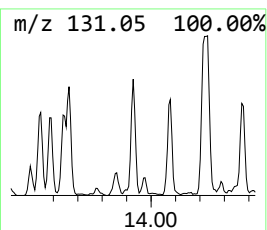
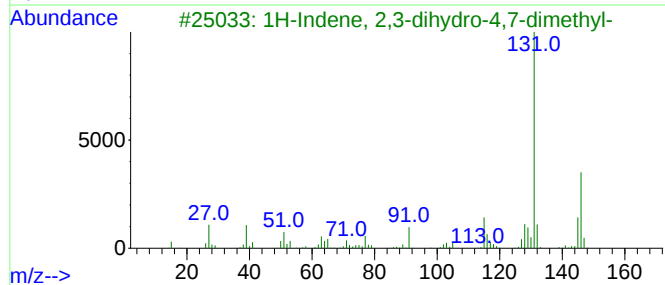
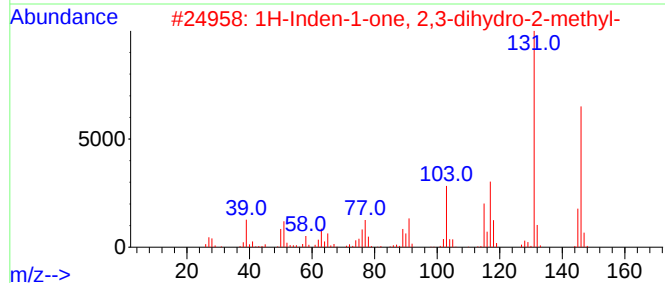
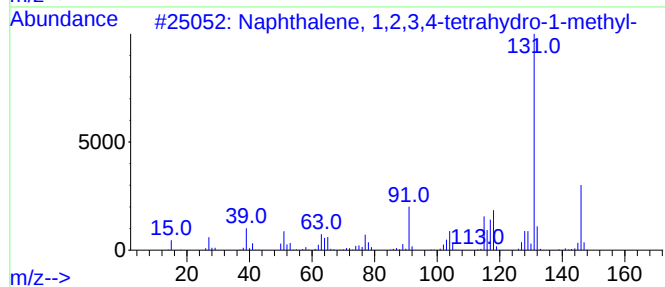
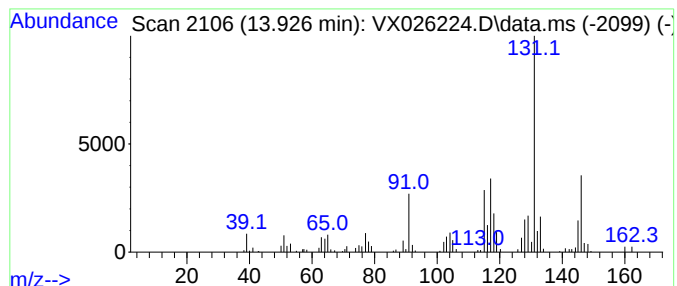
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X123021W.M
Quant Title : SW846 8260

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

Peak Number 3 Naphthalene, 1,2,3,4-tetrahydro-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.926	5.44 ug/l	91350	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001559-81-5	93
2			1H-Inden-1-one, 2,3-dihydro-2-methyl-	146	C10H10O	017496-14-9	89
3			1H-Indene, 2,3-dihydro-4,7-dimethyl-	146	C11H14	006682-71-9	76
4			Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	70
5			Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	70



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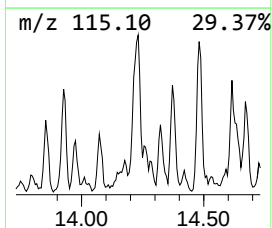
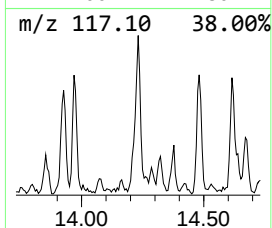
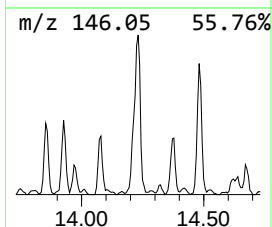
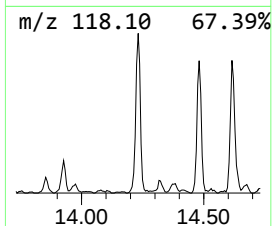
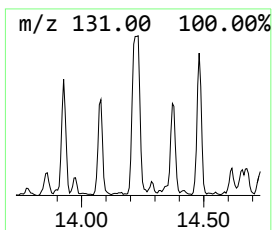
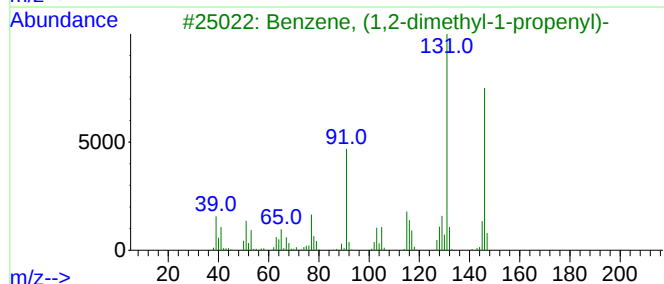
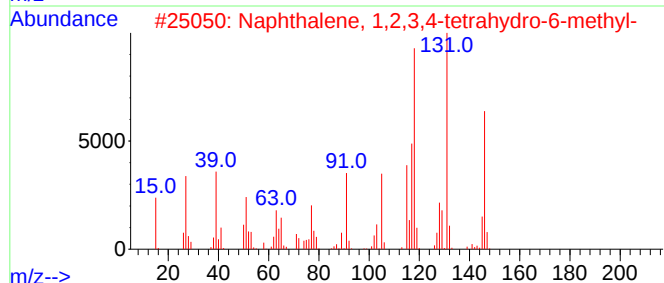
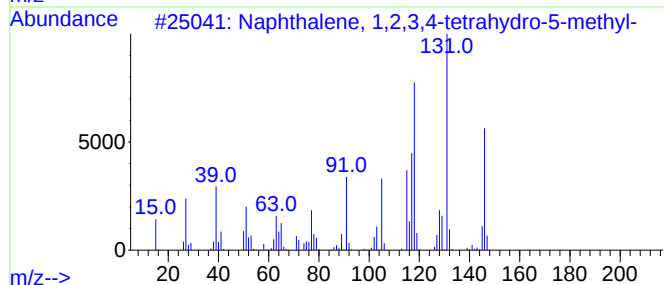
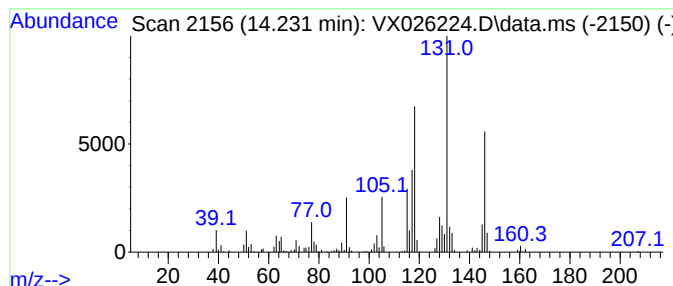
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Quant Title : SW846 8260

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

Peak Number 4 Naphthalene, 1,2,3,4-tetrahydro-... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.231	11.98 ug/l	201103	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	96
2			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	95
3			Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	95
4			1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	86
5			2,2-Dimethylindene, 2,3-dihydro-	146	C11H14	020836-11-7	70



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010322\
Data File : VX026224.D
Acq On : 03 Jan 2022 16:47
Operator : JC/MD
Sample : M5335-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
20967

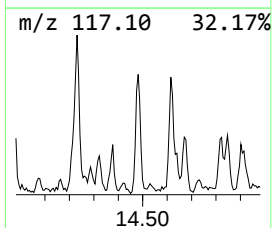
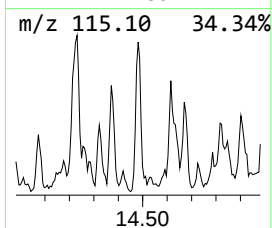
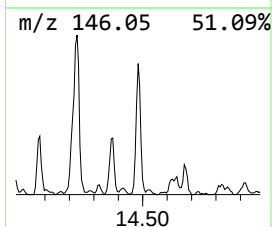
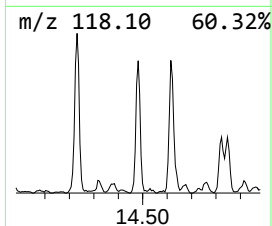
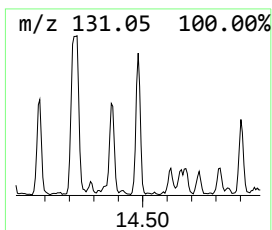
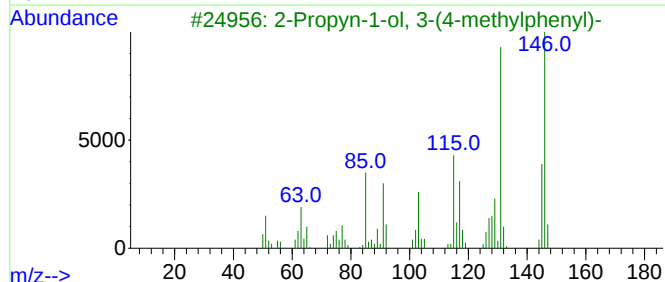
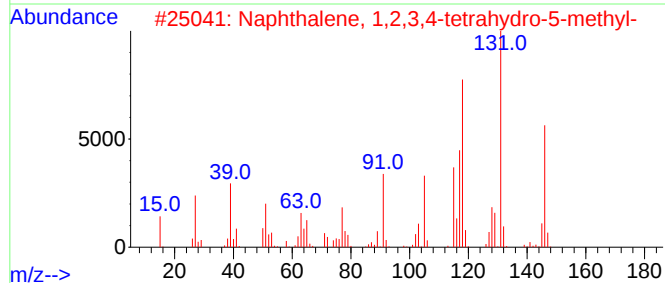
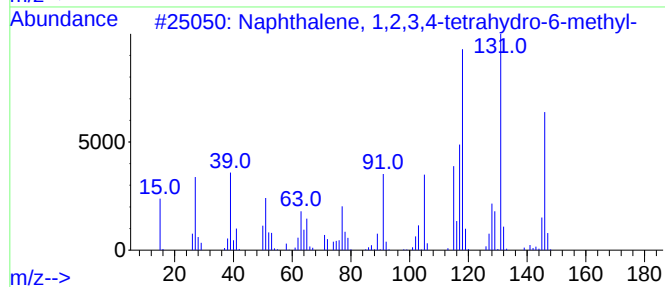
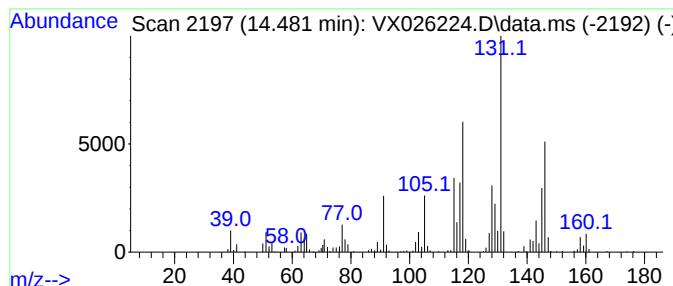
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Quant Title : SW846 8260

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

Peak Number 5 Naphthalene, 1,2,3,4-tetrahydro-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.481	8.85 ug/l	148609	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	94
2			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	90
3			2-Propyn-1-ol, 3-(4-methylphenyl)-	146	C10H10O	016017-24-6	68
4			Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	64
5			Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010322\
Data File : VX026224.D
Acq On : 03 Jan 2022 16:47
Operator : JC/MD
Sample : M5335-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
20967

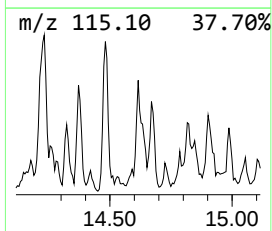
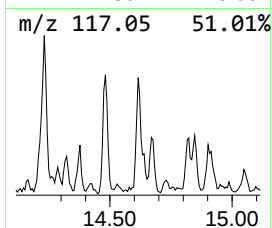
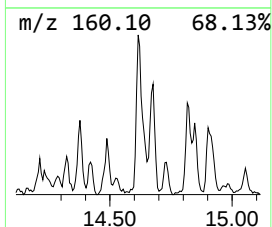
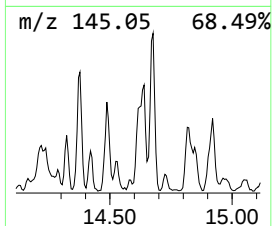
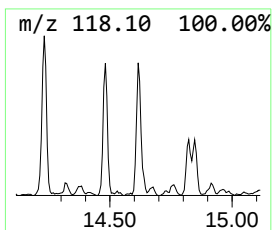
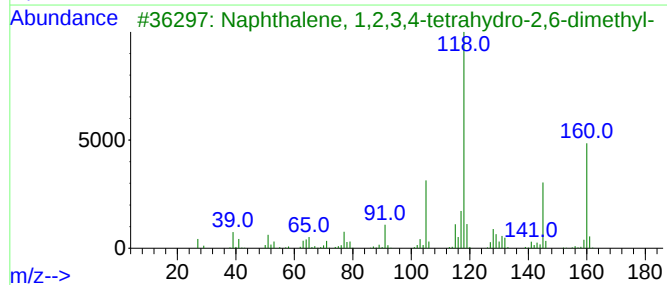
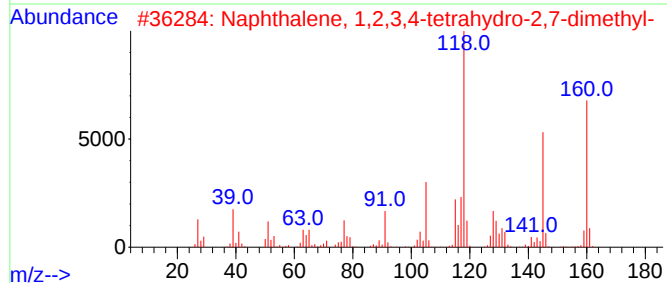
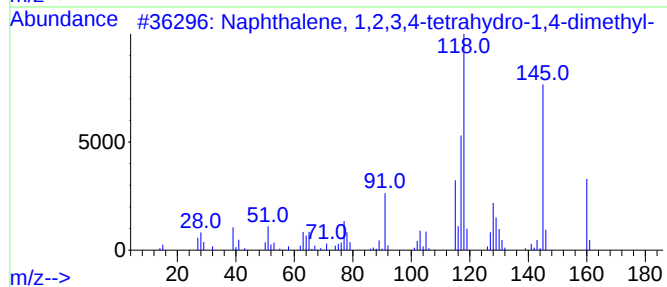
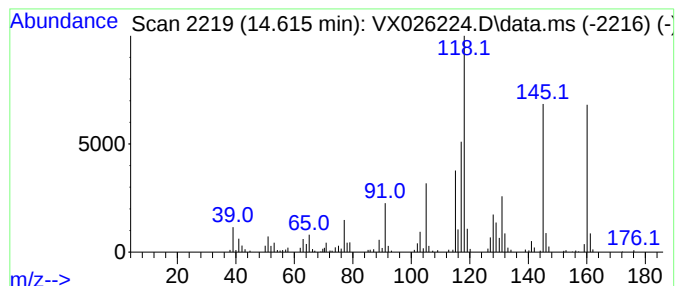
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Quant Title : SW846 8260

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

Peak Number 6 Naphthalene, 1,2,3,4-tetrahydro-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.615	6.74 ug/l	113220	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	95
2			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	013065-07-1	91
3			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	007524-63-2	70
4			Benzene, (3-methyl-1-methylenebu...	160	C12H16	038212-14-5	58
5			1(2H)-Naphthalenone, 3,4-dihydro...	160	C11H12O	001590-08-5	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010322\
Data File : VX026224.D
Acq On : 03 Jan 2022 16:47
Operator : JC/MD
Sample : M5335-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
20967

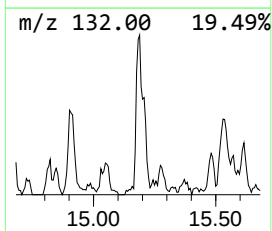
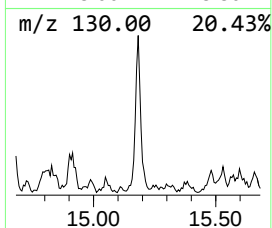
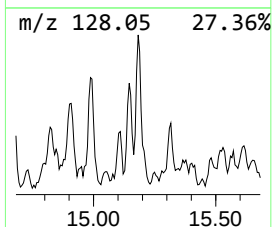
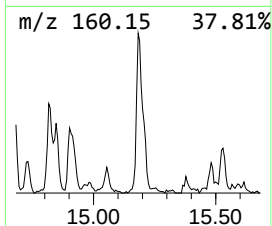
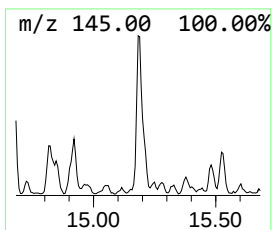
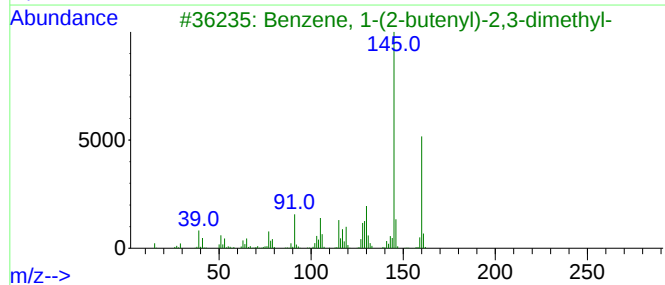
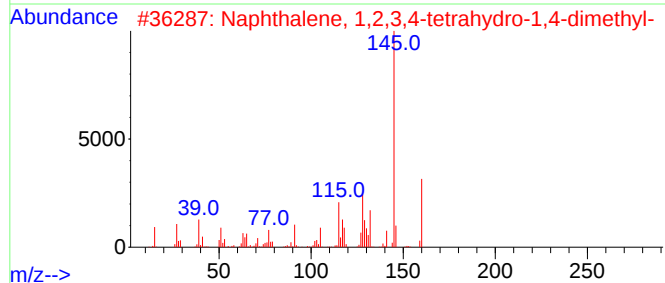
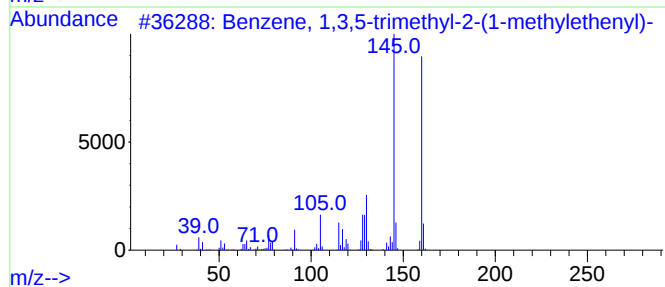
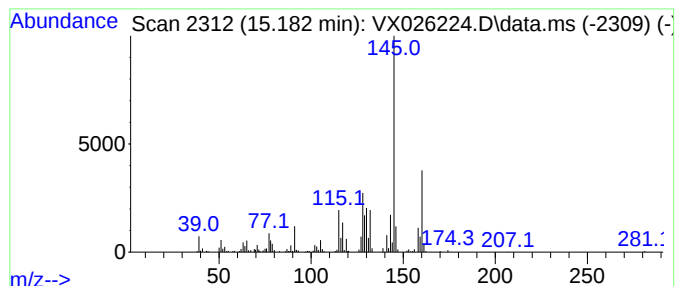
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X123021W.M
Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1,3,5-trimethyl-2-... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.182	9.10 ug/l	152725	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,3,5-trimethyl-2-(1-me...	160	C12H16	014679-13-1	93
2			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	93
3			Benzene, 1-(2-butenyl)-2,3-dimet...	160	C12H16	054340-85-1	76
4			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	021564-91-0	74
5			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	021693-54-9	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010322\
Data File : VX026224.D
Acq On : 03 Jan 2022 16:47
Operator : JC/MD
Sample : M5335-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
20967

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X123021W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Phenyl-1-butene	13.292	5.4	ug/l	90376	4	12.024	839608	50.0
Benzene, (3-met...	13.585	5.8	ug/l	98096	4	12.024	839608	50.0
Naphthalene, 1,...	13.926	5.4	ug/l	91350	4	12.024	839608	50.0
Naphthalene, 1,...	14.231	12.0	ug/l	201103	4	12.024	839608	50.0
Naphthalene, 1,...	14.481	8.8	ug/l	148609	4	12.024	839608	50.0
Naphthalene, 1,...	14.615	6.7	ug/l	113220	4	12.024	839608	50.0
Benzene, 1,3,5-...	15.182	9.1	ug/l	152725	4	12.024	839608	50.0