

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120221\
 Data File : VX025458.D
 Acq On : 03 Dec 2021 03:40
 Operator : JC/MD
 Sample : M4918-02
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 46 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-38

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\82X111721W.M
 Title : SW846 8260

Signal : TIC: VX025458.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.245	22	26	28	rBV	224593	272064	2.02%	0.303%
2	1.270	28	30	41	rVV	94257	148182	1.10%	0.165%
3	1.373	41	47	52	rVB	294005	334518	2.48%	0.373%
4	1.745	103	108	122	rVB	378189	547490	4.06%	0.610%
5	1.959	138	143	155	rVB2	213042	452234	3.36%	0.504%
6	2.068	156	161	169	rVV	252689	352287	2.61%	0.393%
7	2.166	171	177	181	rVV	162471	251332	1.86%	0.280%
8	2.215	181	185	195	rVB	395621	571374	4.24%	0.637%
9	2.751	258	273	281	rBV	202221	477329	3.54%	0.532%
10	2.867	287	292	301	rVB	187869	380455	2.82%	0.424%
11	2.959	301	307	321	rVB	306108	649005	4.82%	0.724%
12	3.111	322	332	349	rVB3	157300	397899	2.95%	0.444%
13	3.733	428	434	445	rVB3	77206	216776	1.61%	0.242%
14	4.105	486	495	506	rBV	56437	147128	1.09%	0.164%
15	4.306	518	528	540	rVB	212916	613544	4.55%	0.684%
16	5.196	663	674	688	rVB	61165	188825	1.40%	0.211%
17	5.391	691	706	712	rBV	68288	204969	1.52%	0.229%
18	5.476	712	720	727	rVV2	99531	284930	2.11%	0.318%
19	5.556	727	733	743	rVB	84445	227654	1.69%	0.254%
20	5.964	790	800	803	rBV	63624	158415	1.18%	0.177%
21	6.049	803	814	827	rVV	5070656	13476813	100.00%	15.026%
22	6.208	827	840	856	rVV6	98256	504116	3.74%	0.562%
23	6.763	923	931	939	rBV	171021	430273	3.19%	0.480%
24	7.385	1021	1033	1044	rBV4	107175	285821	2.12%	0.319%
25	8.147	1153	1158	1163	rVB	104363	176124	1.31%	0.196%
26	8.506	1210	1217	1226	rVB	104377	176421	1.31%	0.197%
27	8.653	1235	1241	1246	rBV	360048	545351	4.05%	0.608%
28	8.720	1246	1252	1260	rVB	849070	1281707	9.51%	1.429%
29	9.457	1364	1373	1378	rBV2	154451	258807	1.92%	0.289%
30	9.945	1447	1453	1461	rBV	97063	143361	1.06%	0.160%
31	10.055	1461	1471	1476	rBV	362265	527800	3.92%	0.588%
32	10.201	1489	1495	1506	rVB	6957535	8930257	66.26%	9.957%
33	10.311	1506	1513	1518	rBV	9766372	12785927	94.87%	14.256%
34	10.646	1562	1568	1578	rVB	6219986	7837806	58.16%	8.739%
35	10.963	1613	1620	1626	rVB	482544	605035	4.49%	0.675%
36	11.085	1635	1640	1645	rBV	305962	381007	2.83%	0.425%

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37	11.305	1668	1676	1683	rBV	1127054	1380390	10.24%	1.539%
38	11.384	1683	1689	1691	rBV	1858484	2739889	20.33%	3.055%
39	11.457	1696	1701	1706	rVB	1233397	1553356	11.53%	1.732%
40	11.616	1721	1727	1735	rBV	1651566	2008583	14.90%	2.240%
41	11.756	1745	1750	1755	rVB	6423076	7546253	55.99%	8.414%
42	12.024	1789	1794	1798	rVV2	430762	550170	4.08%	0.613%
43	12.091	1798	1805	1810	rVB	2131157	2555431	18.96%	2.849%
44	12.243	1825	1830	1838	rBV	2422855	3315954	24.60%	3.697%
45	12.317	1838	1842	1850	rVB3	421895	661289	4.91%	0.737%
46	12.414	1852	1858	1862	rBV2	225652	297926	2.21%	0.332%
47	12.463	1862	1866	1872	rVB	172675	217836	1.62%	0.243%
48	12.536	1872	1878	1880	rBV	317628	446520	3.31%	0.498%
49	12.554	1880	1881	1886	rVV	234789	221046	1.64%	0.246%
50	12.615	1886	1891	1894	rVV	662919	788228	5.85%	0.879%
51	12.646	1894	1896	1900	rVB	150601	163573	1.21%	0.182%
52	12.701	1900	1905	1913	rBV2	466276	661054	4.91%	0.737%
53	12.847	1924	1929	1934	rVB2	164995	219358	1.63%	0.245%
54	12.926	1934	1942	1945	rBV	382876	489349	3.63%	0.546%
55	12.963	1945	1948	1954	rVB	461924	546902	4.06%	0.610%
56	13.170	1978	1982	1987	rVB	439074	501286	3.72%	0.559%
57	13.292	1997	2002	2007	rVB2	959443	1291917	9.59%	1.440%
58	13.426	2019	2024	2031	rVB	312398	391510	2.91%	0.437%
59	13.585	2047	2050	2056	rVB2	96748	148641	1.10%	0.166%
60	13.664	2061	2063	2070	rVB2	101267	152849	1.13%	0.170%
61	13.780	2074	2082	2091	rBV	2134602	2675155	19.85%	2.983%
62	14.225	2149	2155	2160	rBV3	99612	198397	1.47%	0.221%
63	14.639	2210	2223	2228	rBV	949766	1208199	8.97%	1.347%
64	14.780	2241	2246	2255	rBV	702451	909291	6.75%	1.014%
65	15.481	2354	2361	2366	rBV	125774	194065	1.44%	0.216%
66	15.615	2374	2383	2387	rBV	178653	290594	2.16%	0.324%
67	15.651	2387	2389	2396	rVB	108617	139445	1.03%	0.155%

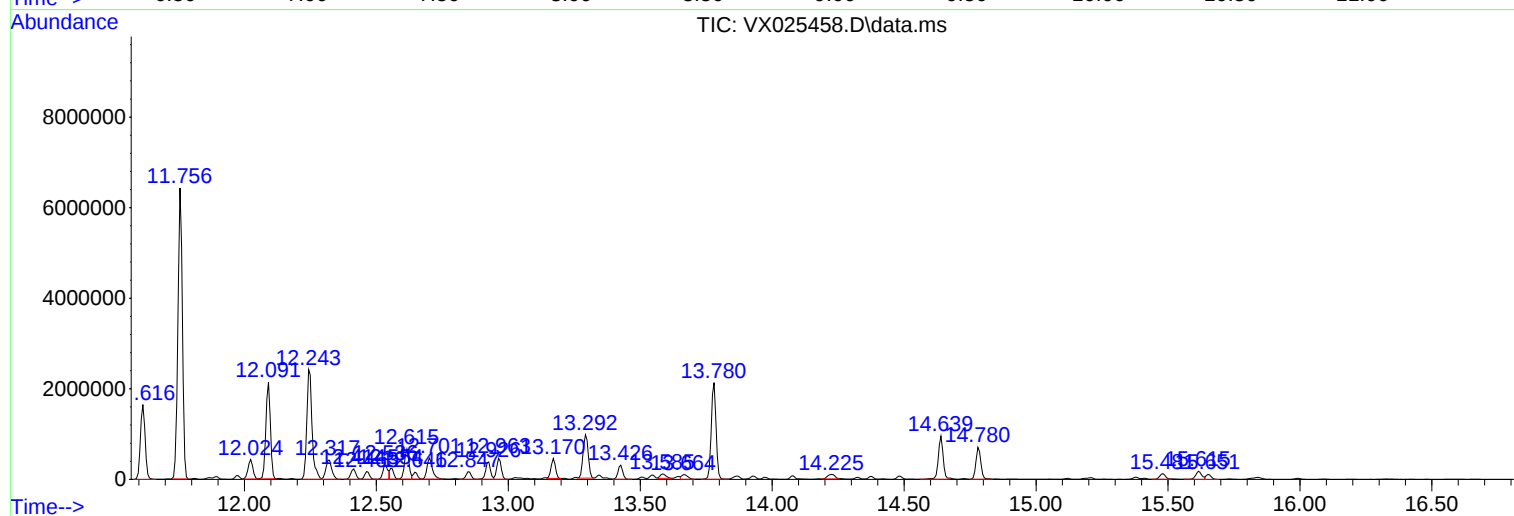
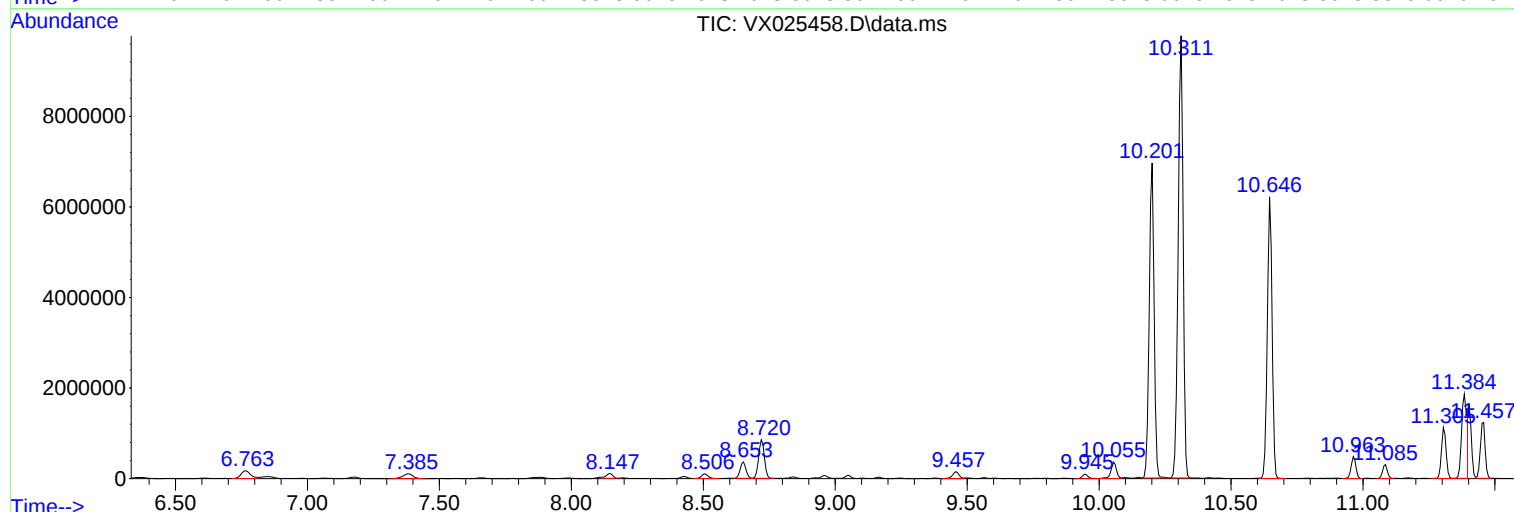
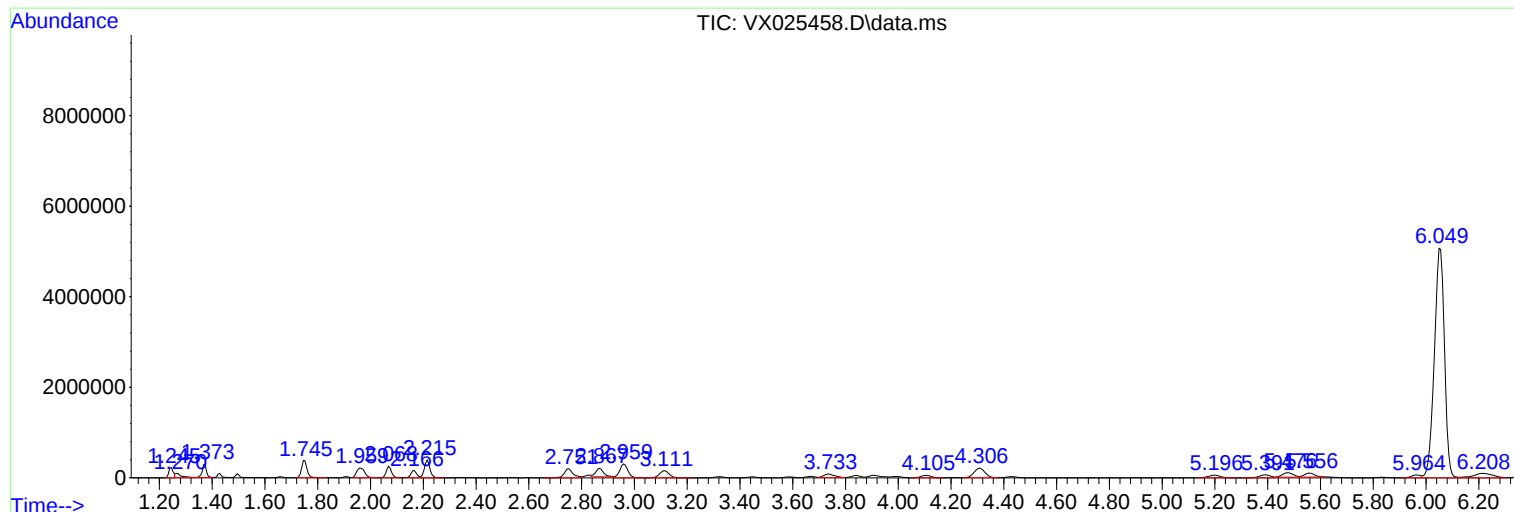
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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



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Instrument :
MSVOA_X
ClientSampleId :
MW-38

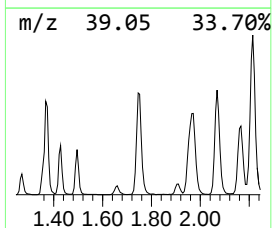
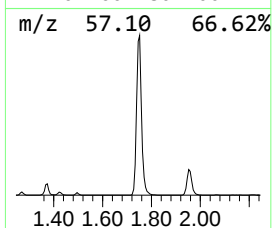
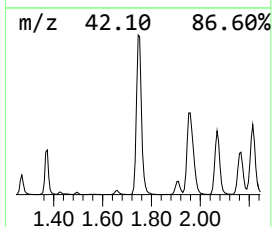
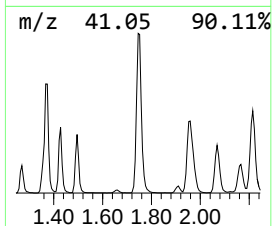
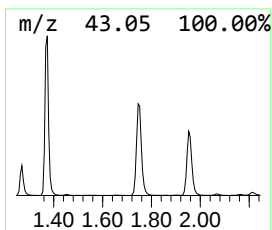
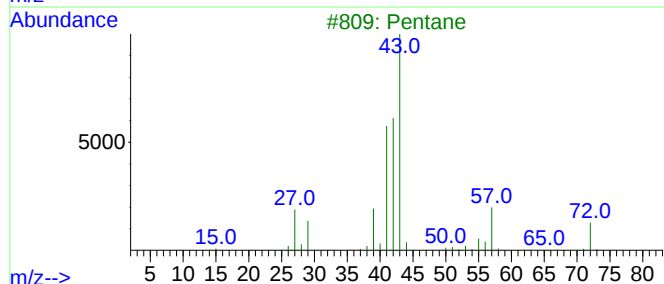
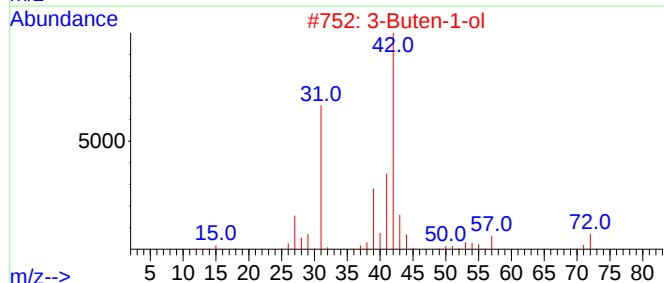
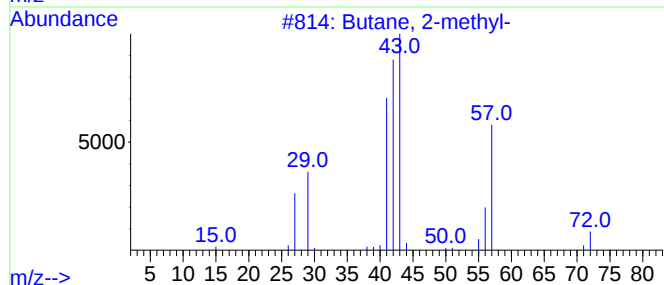
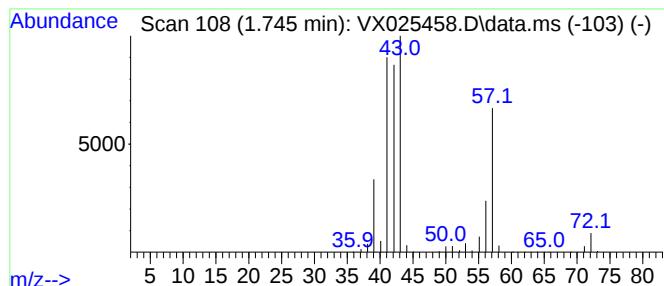
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.745	120.25 ug/l	547490	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	90
2			3-Buten-1-ol	72	C4H8O	000627-27-0	47
3			Pentane	72	C5H12	000109-66-0	36
4			1-Butene	56	C4H8	000106-98-9	10
5			1-Propene, 2-methyl-	56	C4H8	000115-11-7	10



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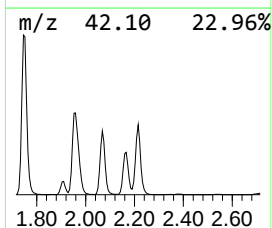
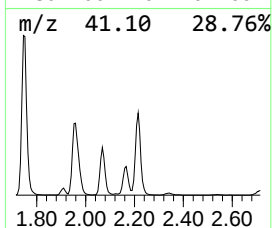
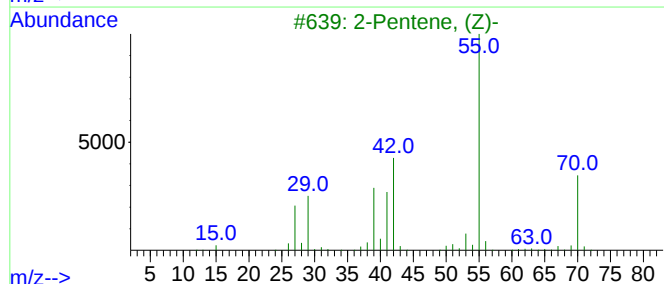
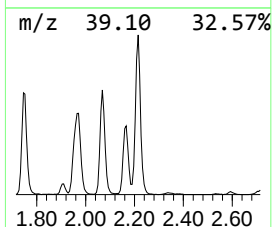
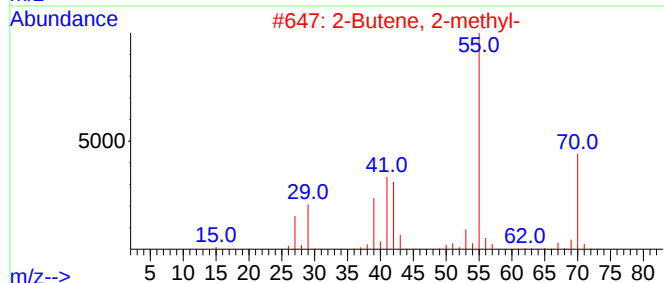
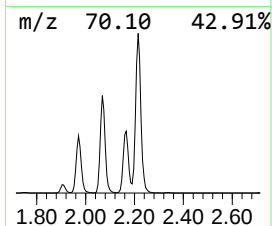
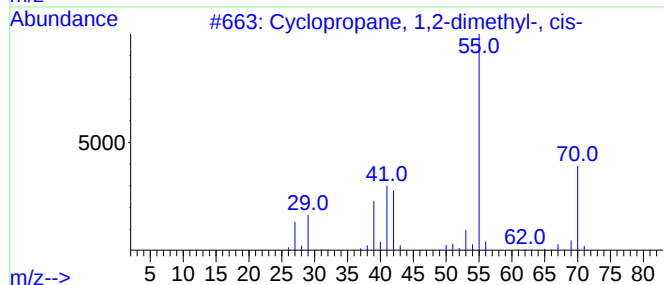
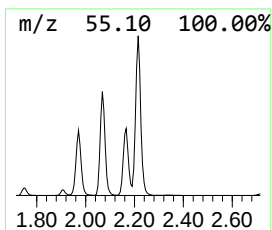
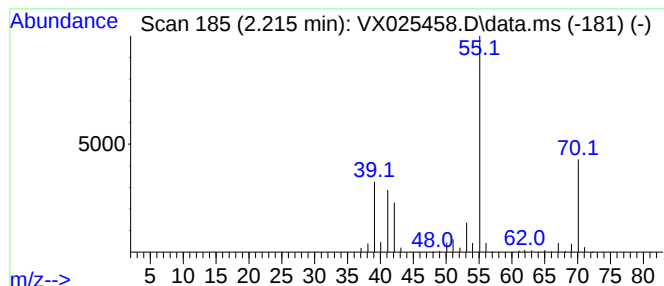
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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

Peak Number 2 Cyclopropane, 1,2-dimethyl-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.215	125.49 ug/l	571374	Pentafluorobenzene	5.556

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	90
2		2-Butene, 2-methyl-	70	C5H10	000513-35-9	86
3		2-Pentene, (Z)-	70	C5H10	000627-20-3	81
4		Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	80
5		1-Butene, 3-methyl-	70	C5H10	000563-45-1	78



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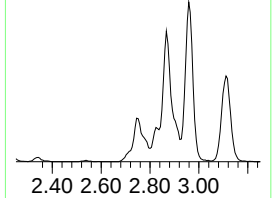
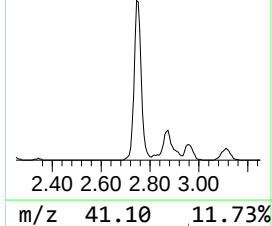
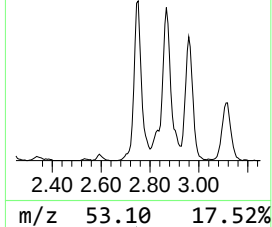
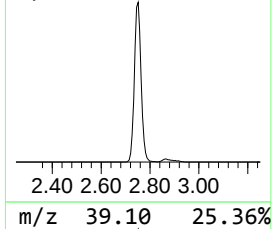
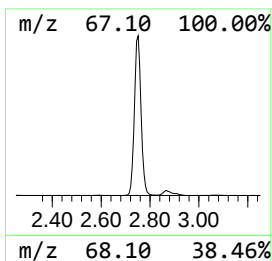
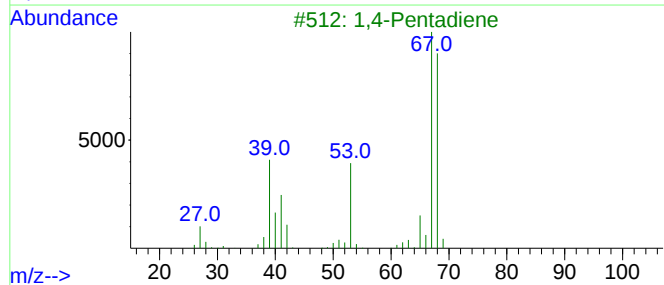
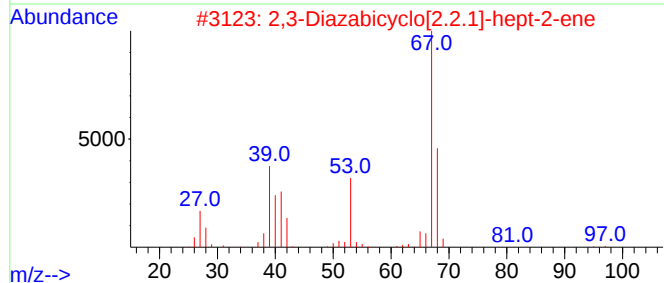
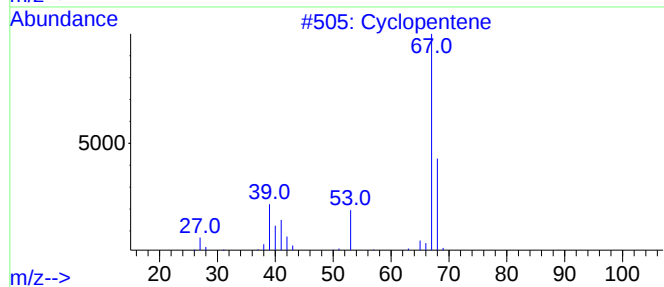
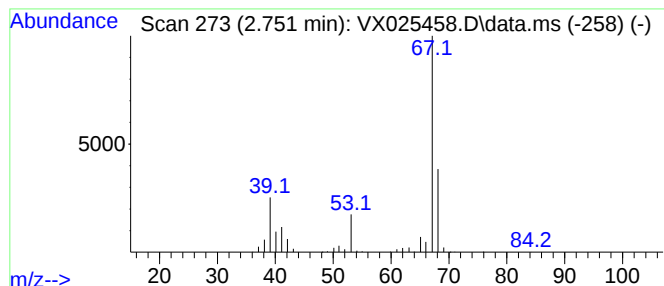
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Cyclopentene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.751	104.84 ug/l	477329	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentene	68	C5H8	000142-29-0	91
2			2,3-Diazabicyclo[2.2.1]-hept-2-ene	96	C5H8N2	002721-32-6	78
3			1,4-Pentadiene	68	C5H8	000591-93-5	62
4			1,3-Pentadiene, (Z)-	68	C5H8	001574-41-0	53
5			1-Butyne, 3-methyl-	68	C5H8	000598-23-2	53



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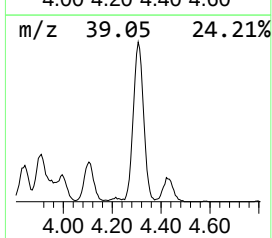
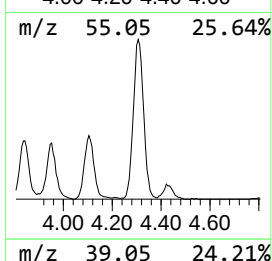
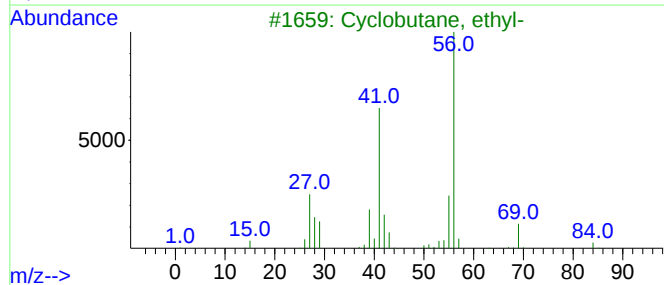
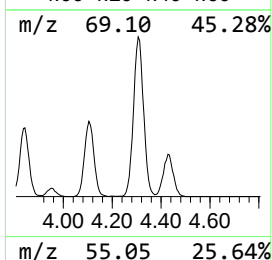
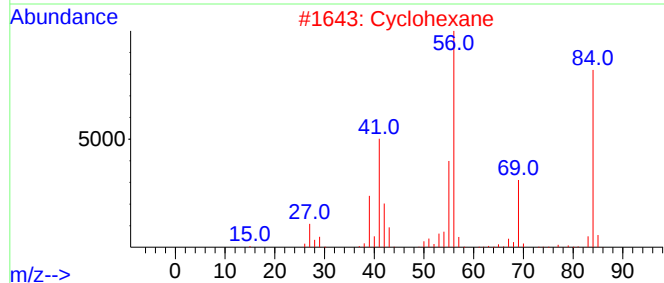
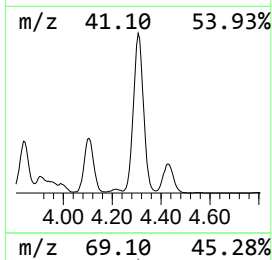
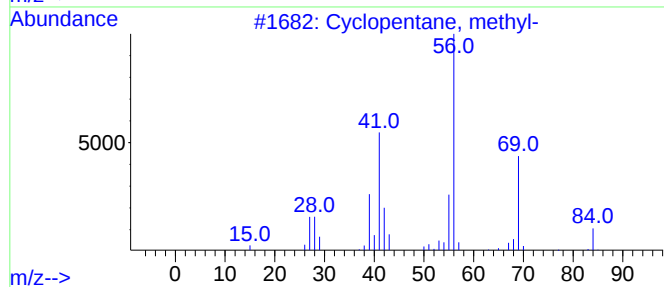
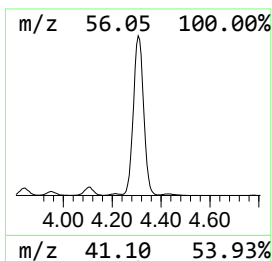
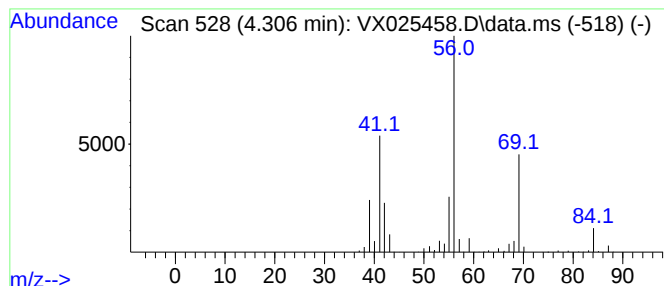
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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

Peak Number 4 Cyclopentane, methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	134.75 ug/l	613544	Pentafluorobenzene	5.556

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2		Cyclohexane	84	C6H12	000110-82-7	72
3		Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
4		1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	64
5		Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120221\
Data File : VX025458.D
Acq On : 03 Dec 2021 03:40
Operator : JC/MD
Sample : M4918-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-38

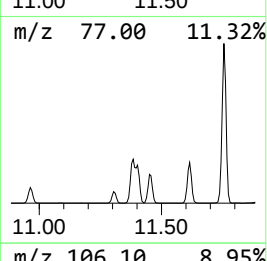
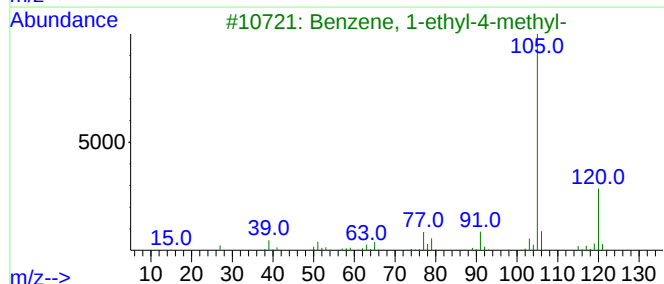
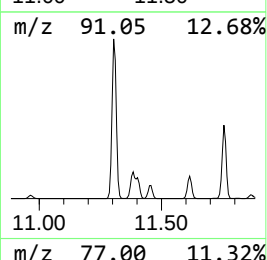
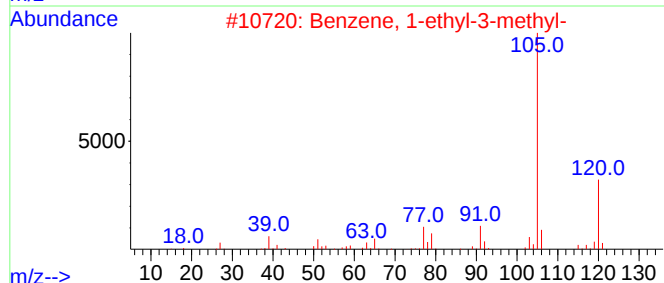
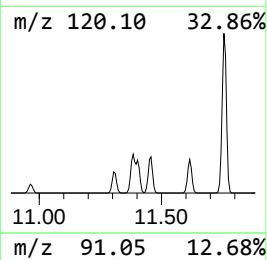
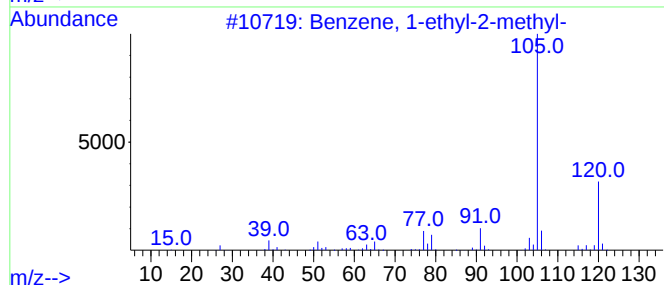
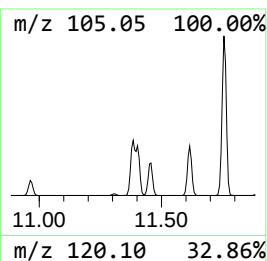
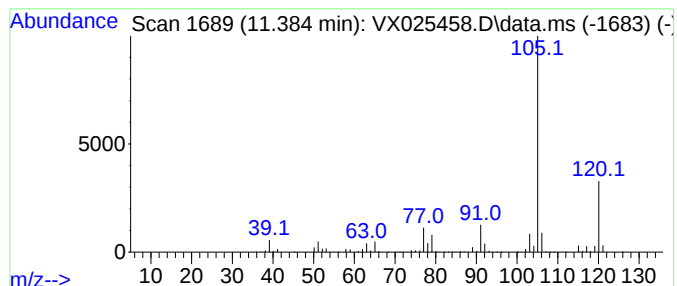
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Quant Title : SW846 8260

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

Peak Number 5 Benzene, 1-ethyl-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.384	249.00 ug/l	2739890	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4			Mesitylene	120	C9H12	000108-67-8	91
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120221\
Data File : VX025458.D
Acq On : 03 Dec 2021 03:40
Operator : JC/MD
Sample : M4918-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-38

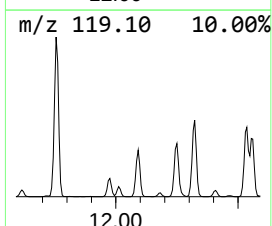
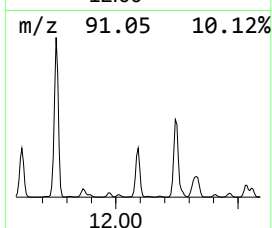
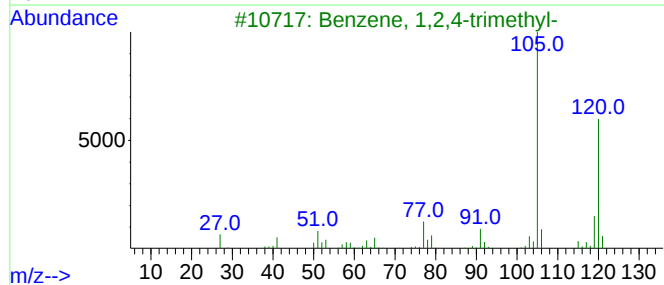
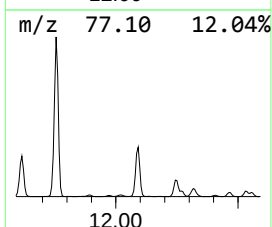
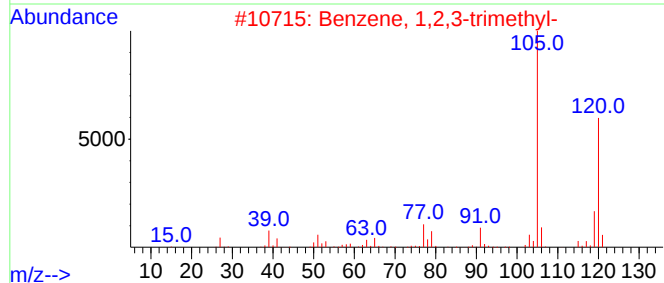
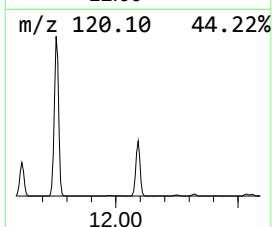
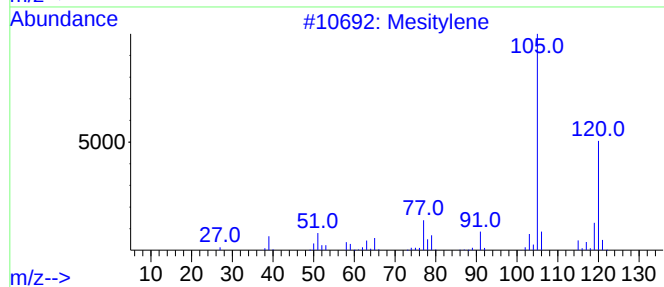
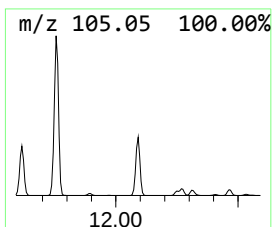
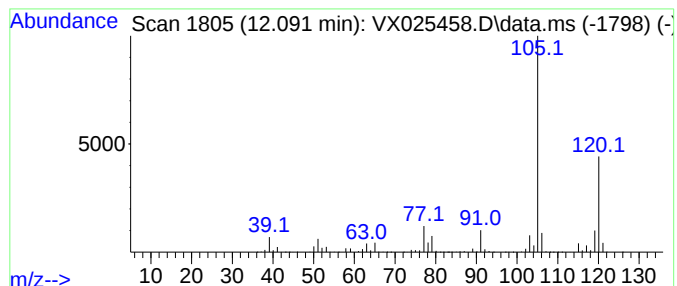
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.091	232.24 ug/l	2555430	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Mesitylene	120	C9H12	000108-67-8	97
2			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
3			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120221\
Data File : VX025458.D
Acq On : 03 Dec 2021 03:40
Operator : JC/MD
Sample : M4918-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-38

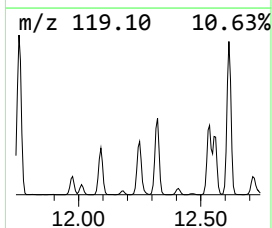
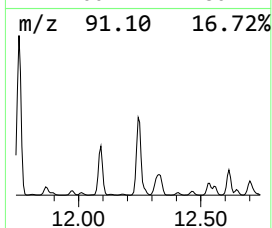
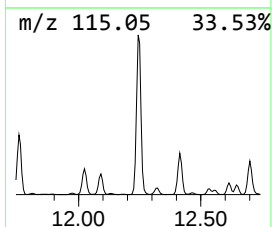
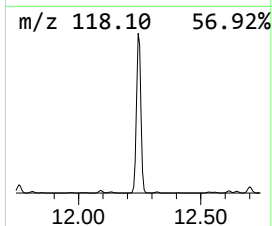
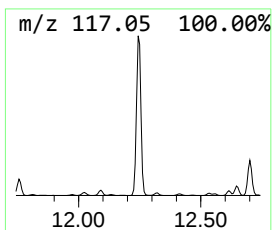
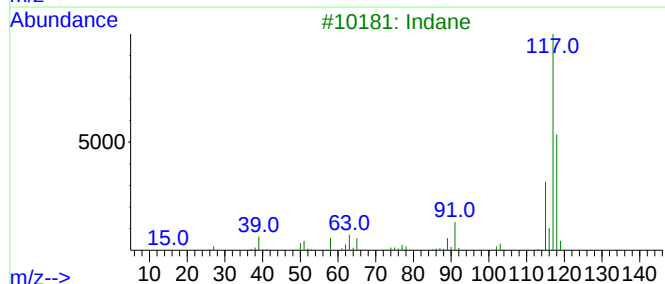
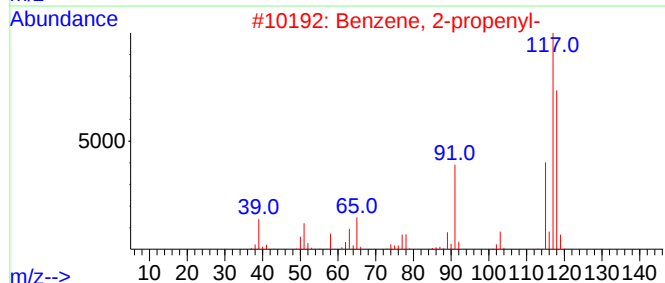
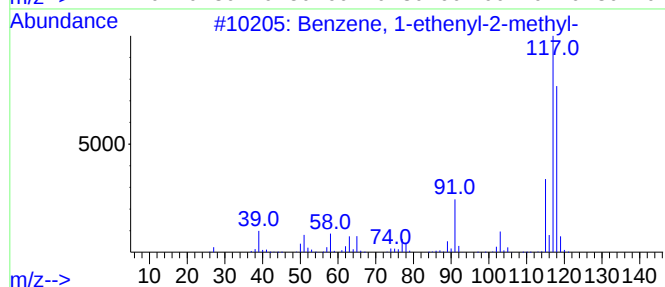
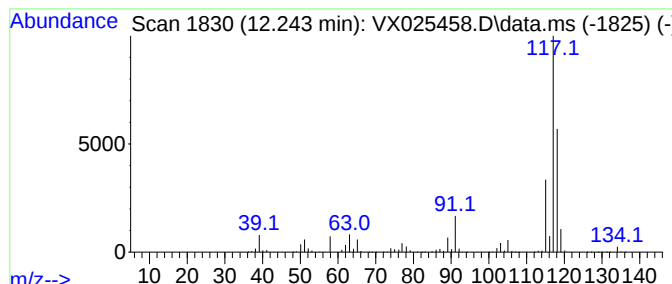
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1-ethenyl-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.243	301.36 ug/l	3315950	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	90
2			Benzene, 2-propenyl-	118	C9H10	000300-57-2	83
3			Indane	118	C9H10	000496-11-7	81
4			Benzene, cyclopropyl-	118	C9H10	000873-49-4	74
5			Benzene, 1-propenyl-	118	C9H10	000637-50-3	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120221\
Data File : VX025458.D
Acq On : 03 Dec 2021 03:40
Operator : JC/MD
Sample : M4918-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-38

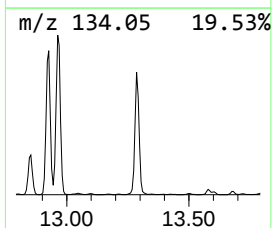
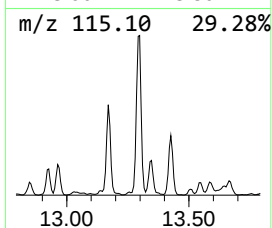
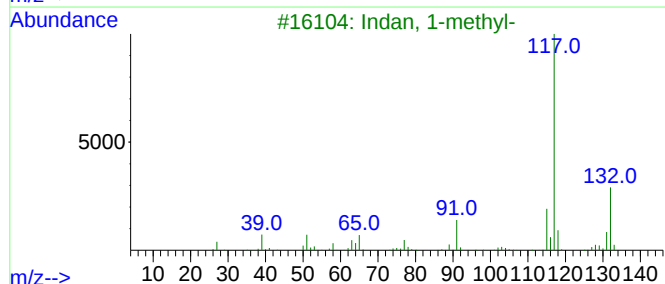
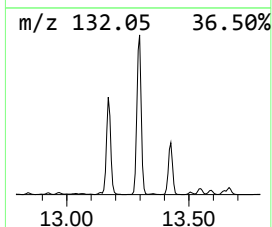
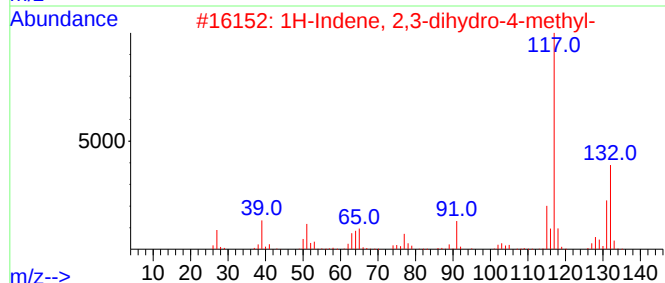
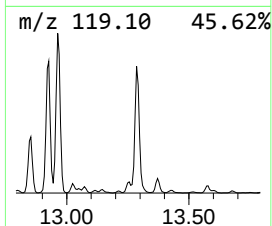
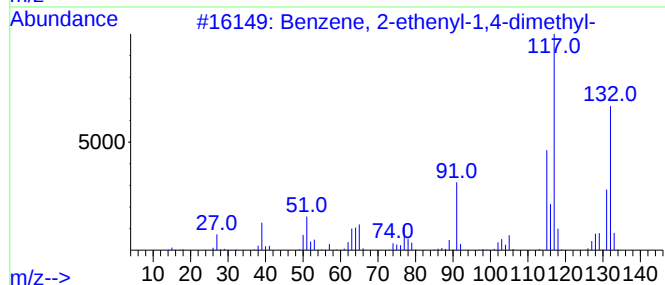
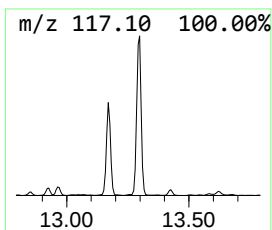
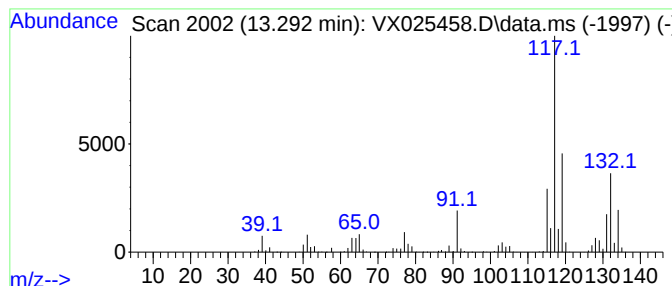
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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

Peak Number 9 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	117.41 ug/l	1291920	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	95
2			1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	91
3			Indan, 1-methyl-	132	C10H12	000767-58-8	70
4			Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	70
5			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	70



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120221\
Data File : VX025458.D
Acq On : 03 Dec 2021 03:40
Operator : JC/MD
Sample : M4918-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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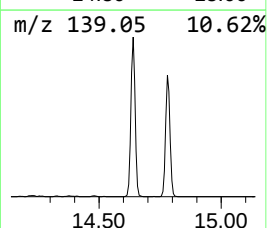
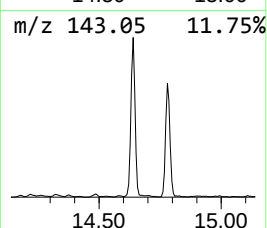
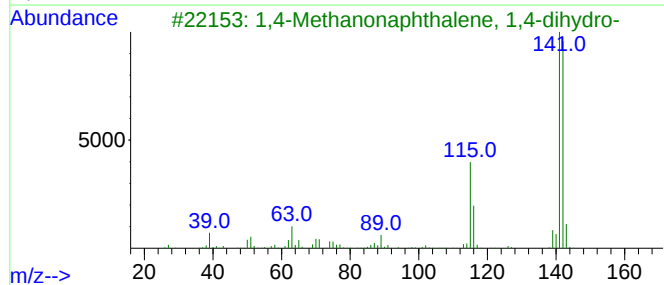
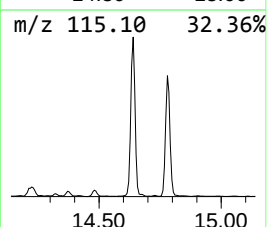
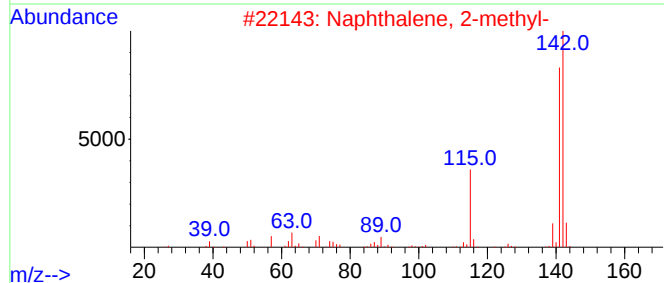
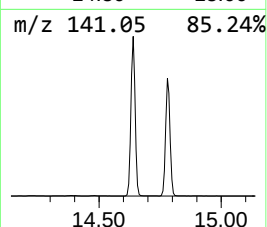
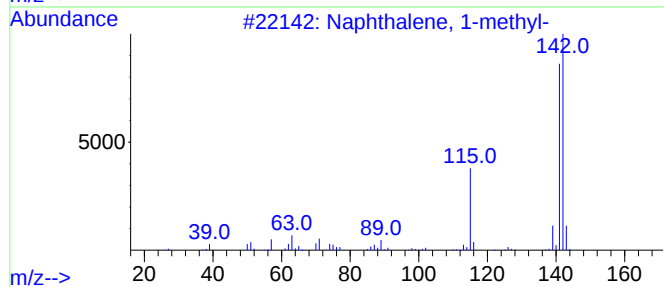
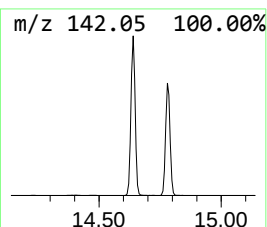
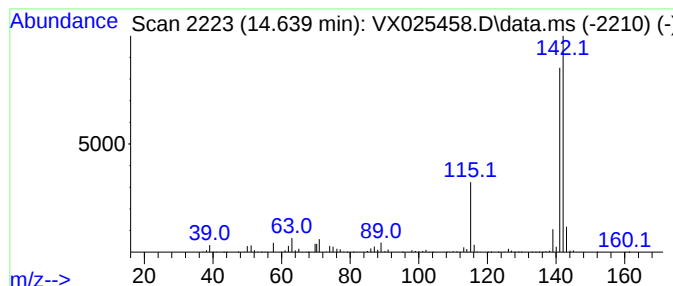
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Quant Title : SW846 8260

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

Peak Number 10 Naphthalene, 1-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.639	109.80 ug/l	1208200	1,4-Dichlorobenzene-d4	12.024

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	91
4			Benzocycloheptatriene	142	C11H10	000264-09-5	91
5			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120221\
Data File : VX025458.D
Acq On : 03 Dec 2021 03:40
Operator : JC/MD
Sample : M4918-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-38

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.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
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Cyclopropane, 1...	2.215	125.5	ug/l	571374	1	5.556	227654	50.0
Cyclopentene	2.751	104.8	ug/l	477329	1	5.556	227654	50.0
Cyclopentane, m...	4.306	134.8	ug/l	613544	1	5.556	227654	50.0
Benzene, 1-ethy...	11.384	249.0	ug/l	2739890	4	12.024	550170	50.0
Benzene, 1,2,3-...	12.091	232.2	ug/l	2555430	4	12.024	550170	50.0
Benzene, 1-ethe...	12.243	301.4	ug/l	3315950	4	12.024	550170	50.0
Benzene, 2-ethe...	13.292	117.4	ug/l	1291920	4	12.024	550170	50.0
Naphthalene, 1-...	14.639	109.8	ug/l	1208200	4	12.024	550170	50.0