

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042022\
 Data File : VX028210.D
 Acq On : 20 Apr 2022 20:04
 Operator : JC/MD
 Sample : N2459-07
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 31577

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\82X041922W.M
 Title : SW846 8260

Signal : TIC: VX028210.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.264	26	29	39	rVB	138581	142267	1.70%	0.377%
2	1.374	41	47	53	rBV	857540	898902	10.73%	2.383%
3	1.752	103	109	120	rVB	460734	634334	7.58%	1.682%
4	1.953	138	142	152	rVB2	208448	341260	4.08%	0.905%
5	2.062	152	160	173	rVV	4904809	8373707	100.00%	22.201%
6	2.166	173	177	181	rVV	49895	92072	1.10%	0.244%
7	2.215	181	185	195	rVB	120868	185397	2.21%	0.492%
8	2.867	288	292	304	rVB	57726	123139	1.47%	0.326%
9	4.306	519	528	542	rVB2	50934	146945	1.75%	0.390%
10	5.391	691	706	715	rBV	296201	862590	10.30%	2.287%
11	5.556	724	733	754	rVB	406988	1175922	14.04%	3.118%
12	5.958	789	799	805	rBV	287722	754061	9.01%	1.999%
13	6.043	805	813	826	rVB	611413	1621886	19.37%	4.300%
14	6.763	921	931	944	rBV	636028	1501072	17.93%	3.980%
15	8.653	1234	1241	1246	rBV	1489560	2356646	28.14%	6.248%
16	8.720	1246	1252	1265	rVB	3076898	4729305	56.48%	12.539%
17	10.055	1465	1471	1481	rBV	1416714	1859922	22.21%	4.931%
18	10.195	1489	1494	1505	rVB	313936	412609	4.93%	1.094%
19	10.305	1505	1512	1519	rBV	344496	484695	5.79%	1.285%
20	10.646	1562	1568	1581	rVB	490177	657245	7.85%	1.743%
21	11.085	1634	1640	1653	rVB	1295471	1694878	20.24%	4.494%
22	11.384	1683	1689	1690	rBV	138713	178475	2.13%	0.473%
23	11.451	1696	1700	1708	rVB	127170	164707	1.97%	0.437%
24	11.616	1721	1727	1735	rBV	142520	181941	2.17%	0.482%
25	12.024	1789	1794	1800	rVV	1519246	1876600	22.41%	4.975%
26	12.085	1800	1804	1810	rVB	234310	303759	3.63%	0.805%
27	12.244	1822	1830	1838	rBV4	357306	639316	7.63%	1.695%
28	12.317	1838	1842	1849	rVB2	149439	211828	2.53%	0.562%
29	12.463	1862	1866	1872	rVB	74956	90969	1.09%	0.241%
30	12.615	1885	1891	1894	rBV	129790	155217	1.85%	0.412%
31	12.719	1900	1908	1913	rBV3	144748	344525	4.11%	0.913%
32	12.920	1933	1941	1945	rVV	77148	113899	1.36%	0.302%
33	12.963	1945	1948	1954	rVB	136718	168866	2.02%	0.448%
34	13.170	1978	1982	1986	rVB2	123576	154919	1.85%	0.411%
35	13.292	1992	2002	2007	rBV2	443969	690509	8.25%	1.831%
36	13.426	2019	2024	2032	rVB	344440	474076	5.66%	1.257%

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37	13.585	2046	2050	2055	rVV3	85675	132534	1.58%	0.351%
38	13.664	2060	2063	2070	rVB2	102015	147958	1.77%	0.392%
39	13.774	2077	2081	2088	rVB	104968	161467	1.93%	0.428%
40	13.853	2088	2094	2100	rVB	148959	213406	2.55%	0.566%
41	13.926	2100	2106	2111	rBV2	157307	235747	2.82%	0.625%
42	14.079	2127	2131	2134	rBV	91616	109966	1.31%	0.292%
43	14.231	2149	2156	2163	rBV	335070	539152	6.44%	1.429%
44	14.371	2176	2179	2183	rVB	110645	136372	1.63%	0.362%
45	14.481	2192	2197	2207	rBV2	301590	414403	4.95%	1.099%
46	14.615	2215	2219	2221	rBV	153828	196615	2.35%	0.521%
47	14.676	2226	2229	2233	rVB2	92513	117505	1.40%	0.312%
48	14.902	2262	2266	2273	rBV2	64650	107741	1.29%	0.286%
49	15.182	2308	2312	2315	rBV2	115657	158551	1.89%	0.420%
50	15.487	2357	2362	2366	rBV2	90014	152746	1.82%	0.405%
51	15.615	2378	2383	2386	rBV3	59141	95610	1.14%	0.253%

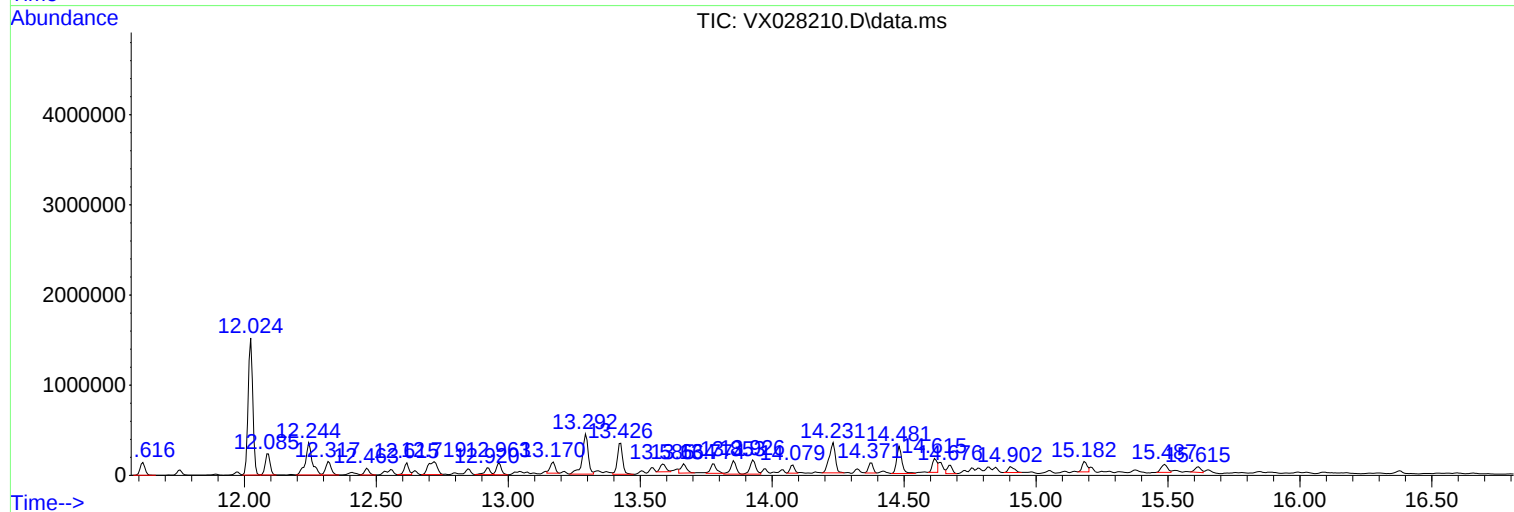
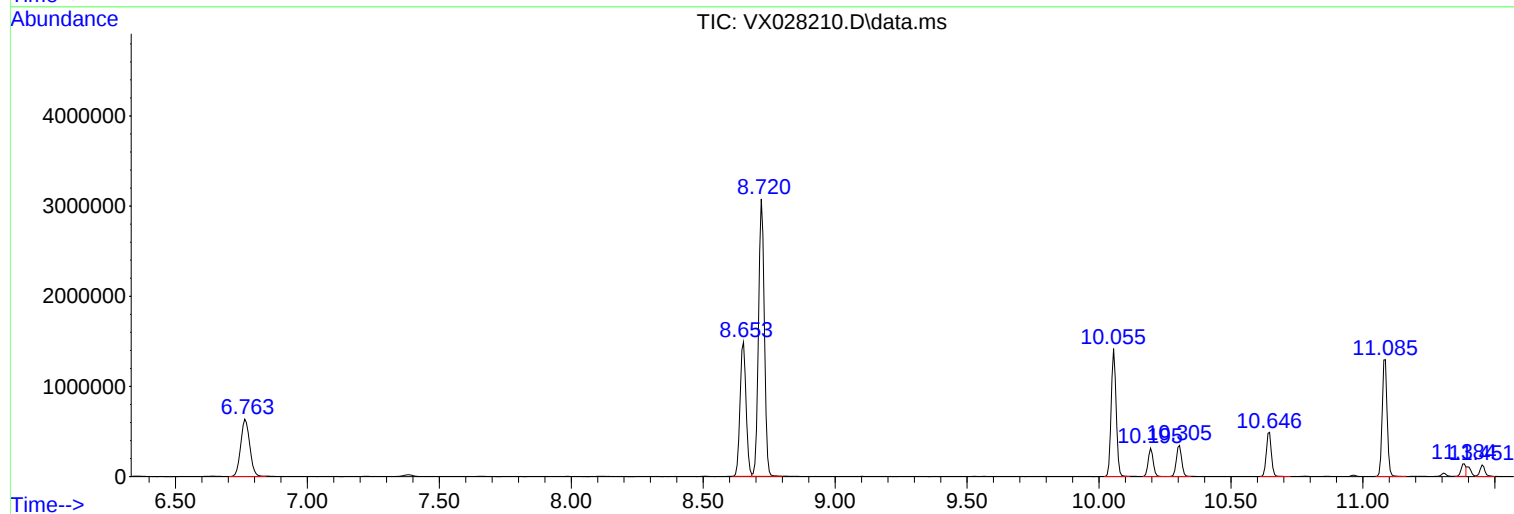
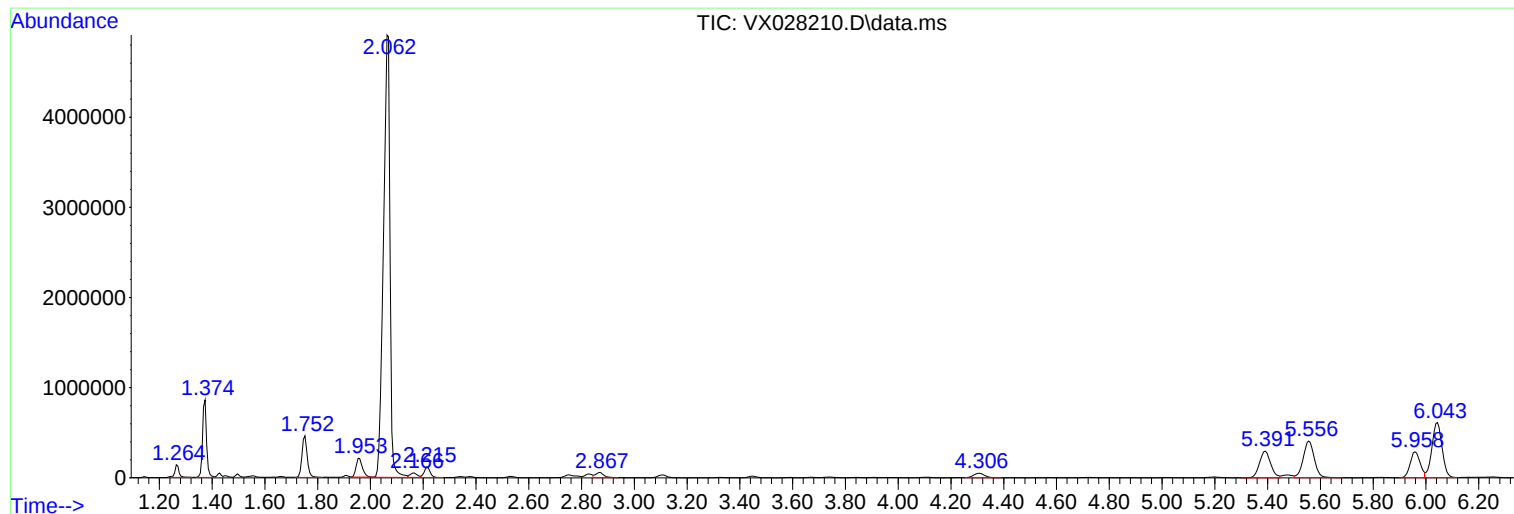
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

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



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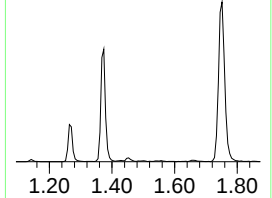
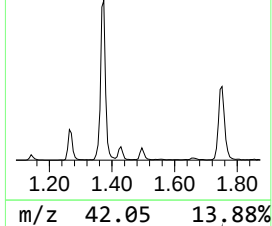
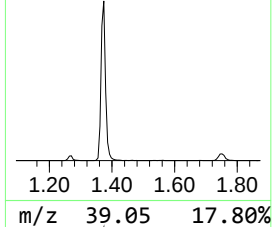
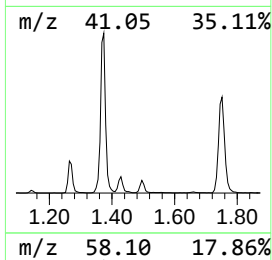
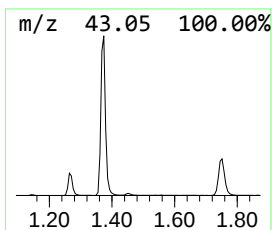
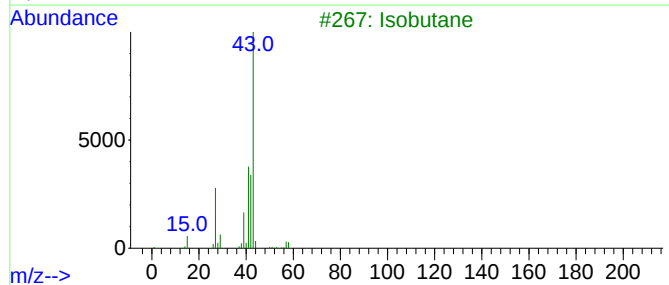
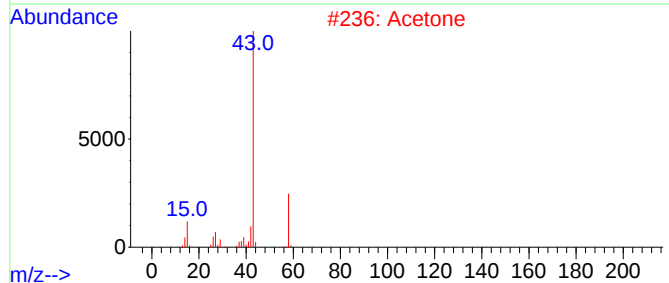
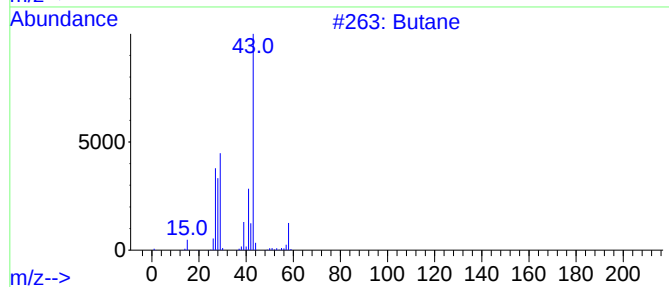
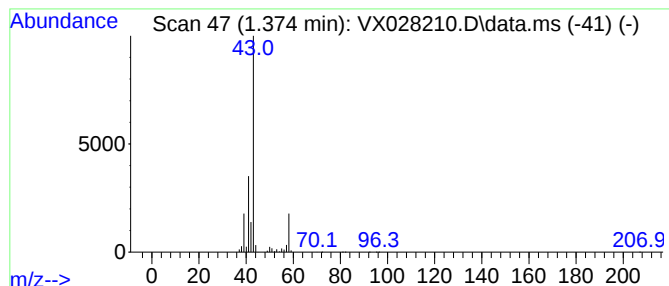
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.374	38.22 ug/l	898902	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane	58	C4H10	000106-97-8	72
2			Acetone	58	C3H6O	000067-64-1	9
3			Isobutane	58	C4H10	000075-28-5	9
4			Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9
5			Propane, 1-nitro-	89	C3H7NO2	000108-03-2	9



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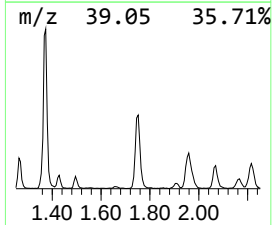
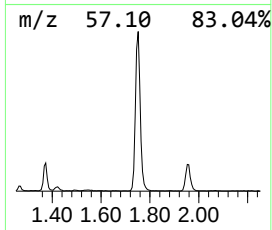
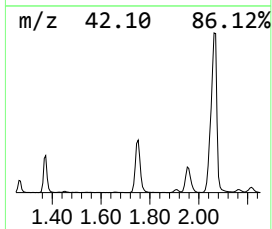
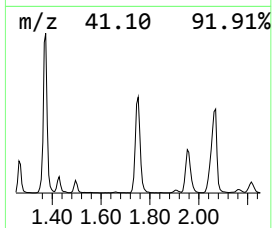
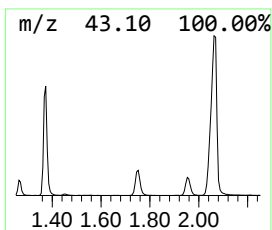
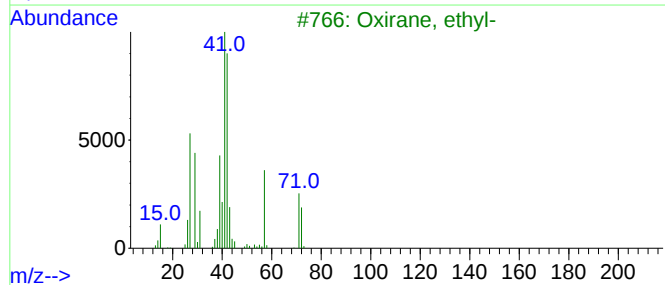
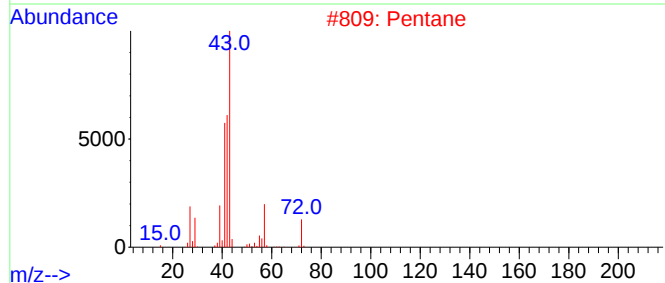
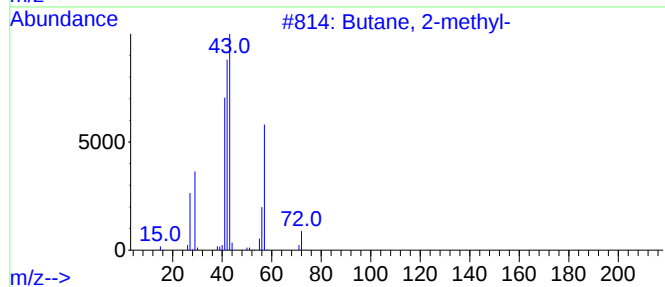
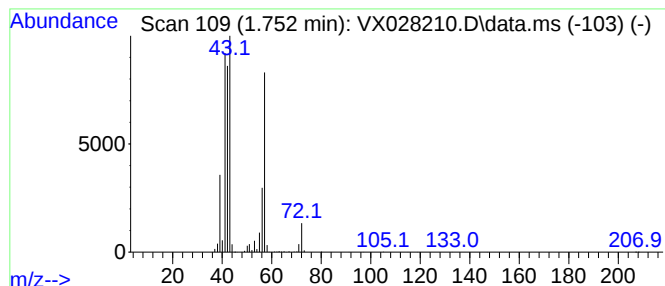
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

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

Peak Number 2 Butane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.752	26.97 ug/l	634334	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	86
2			Pentane	72	C5H12	000109-66-0	58
3			Oxirane, ethyl-	72	C4H8O	000106-88-7	47
4			Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	27
5			1-Propene, 2-methyl-	56	C4H8	000115-11-7	10



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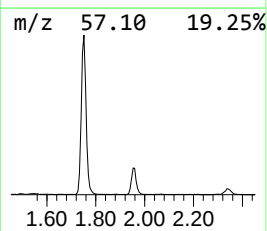
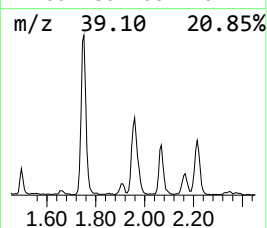
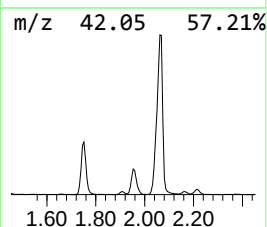
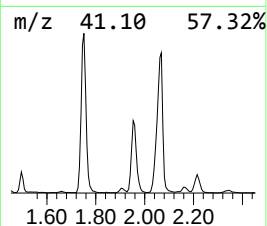
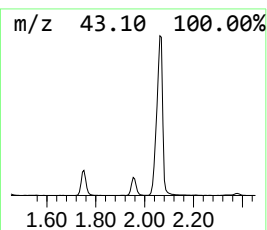
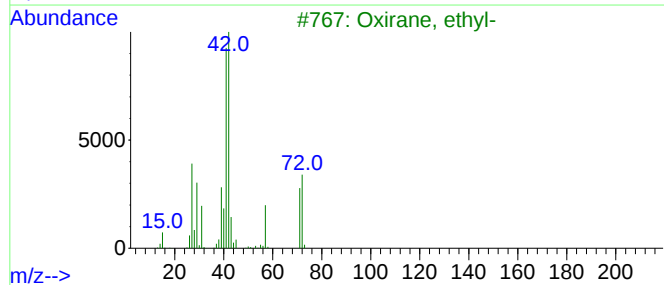
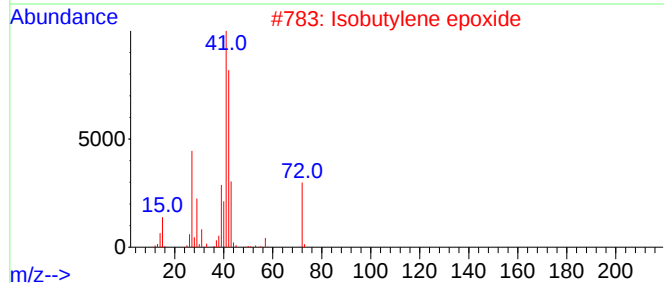
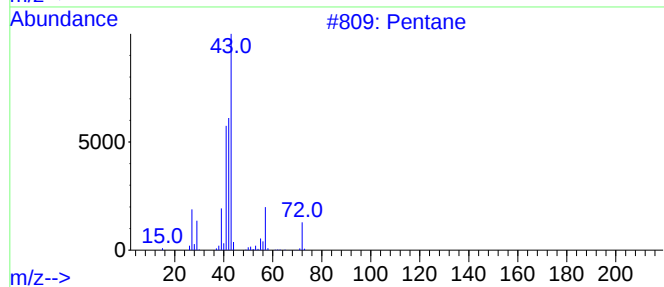
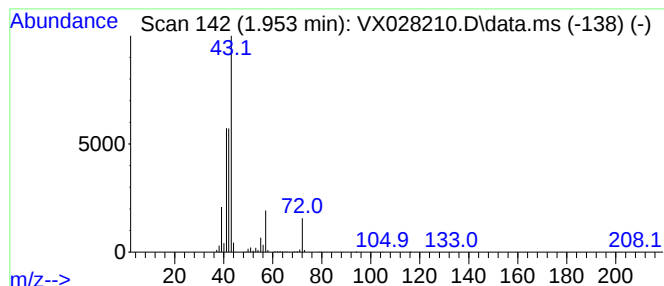
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Pentane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.953	14.51 ug/l	341260	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane	72	C5H12	000109-66-0	91
2			Isobutylene epoxide	72	C4H8O	000558-30-5	47
3			Oxirane, ethyl-	72	C4H8O	000106-88-7	40
4			Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	38
5			Tetrahydrofuran	72	C4H8O	000109-99-9	38



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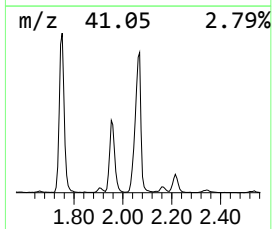
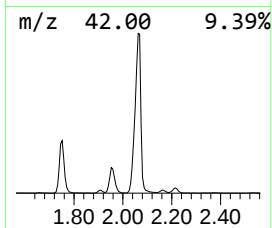
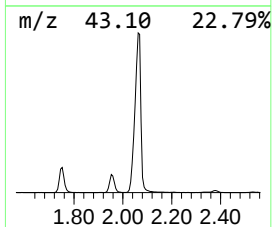
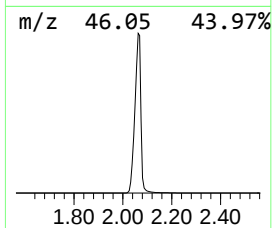
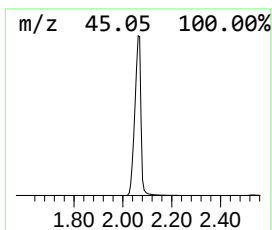
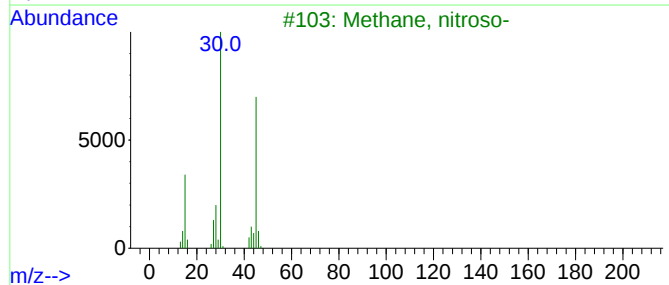
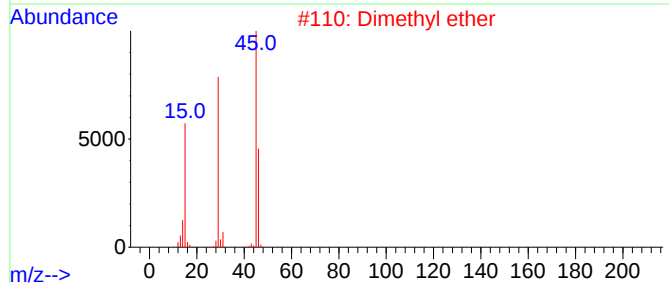
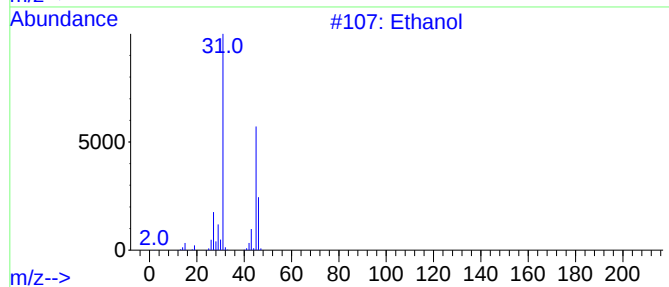
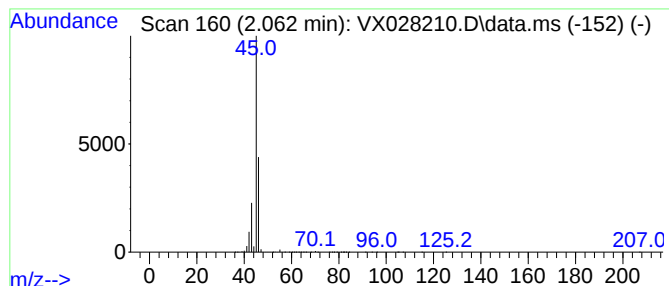
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Quant Title : SW846 8260

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

Peak Number 4 Ethanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.062	356.05 ug/l	8373710	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol			46	C2H6O	000064-17-5	78
2	Dimethyl ether			46	C2H6O	000115-10-6	9
3	Methane, nitroso-			45	CH3NO	000865-40-7	4
4	Formic acid			46	CH2O2	000064-18-6	4
5	Oxalic acid			90	C2H2O4	000144-62-7	4



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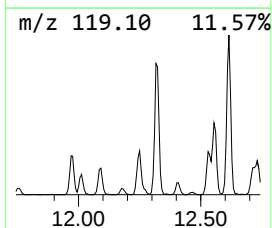
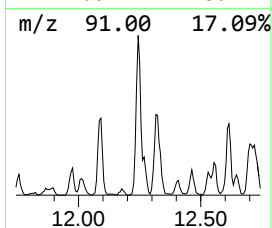
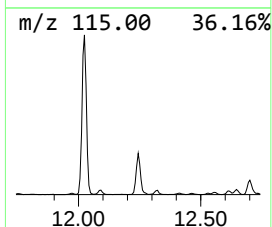
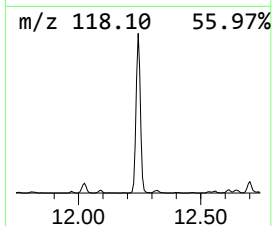
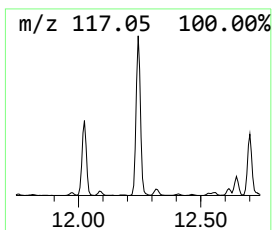
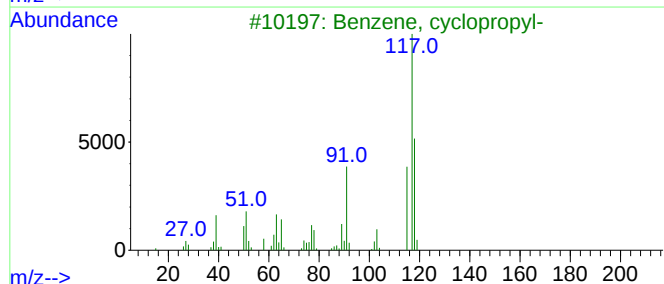
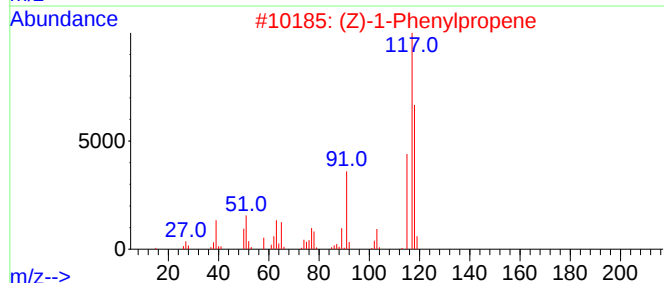
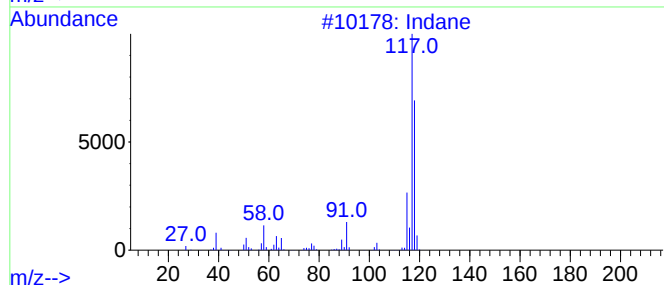
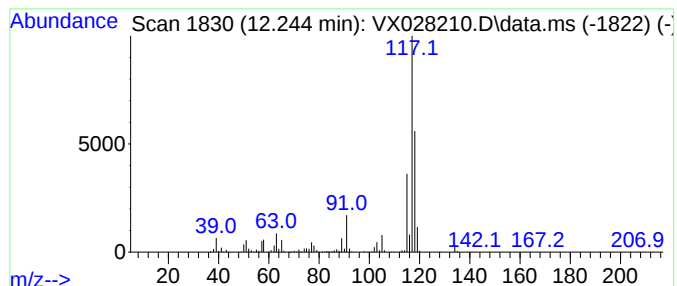
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Quant Title : SW846 8260

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

Peak Number 5 Indane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	17.03 ug/l	639316	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	87
2			(Z)-1-Phenylpropene	118	C9H10	000766-90-5	81
3			Benzene, cyclopropyl-	118	C9H10	000873-49-4	81
4			Benzene, 2-propenyl-	118	C9H10	000300-57-2	74
5			Deltacyclene	118	C9H10	007785-10-6	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042022\
Data File : VX028210.D
Acq On : 20 Apr 2022 20:04
Operator : JC/MD
Sample : N2459-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31577

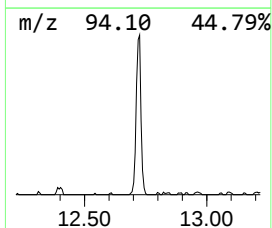
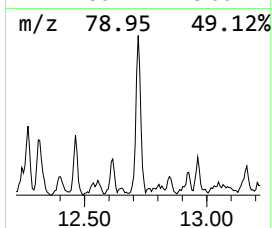
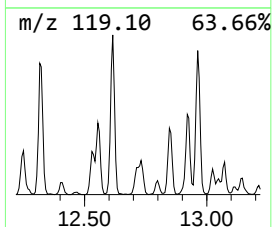
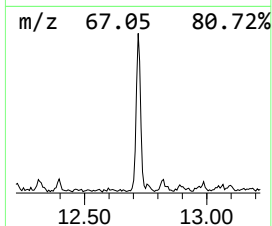
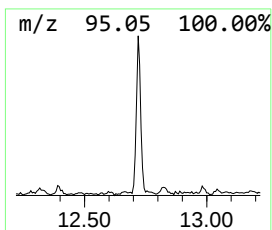
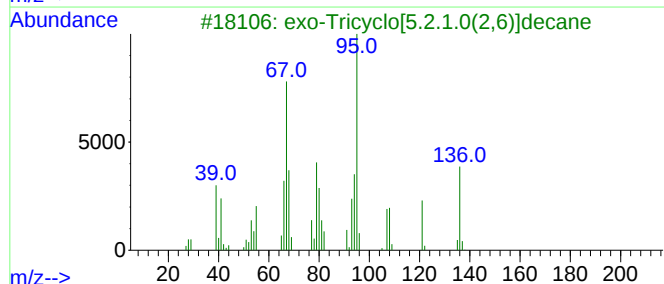
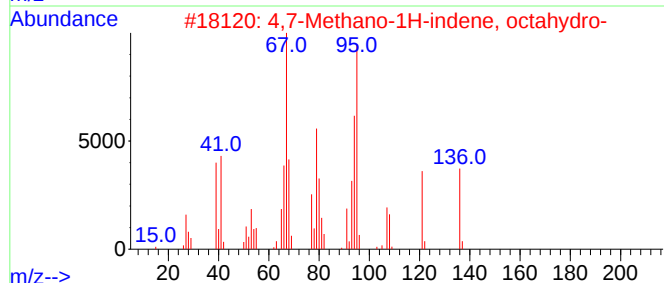
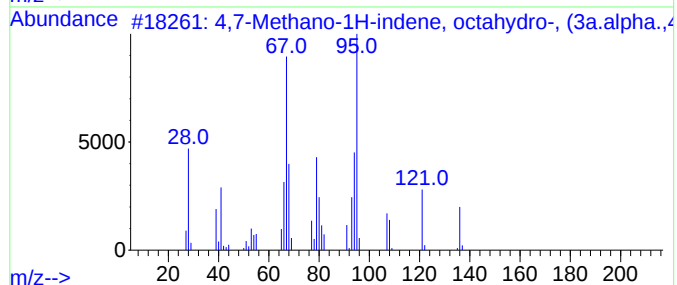
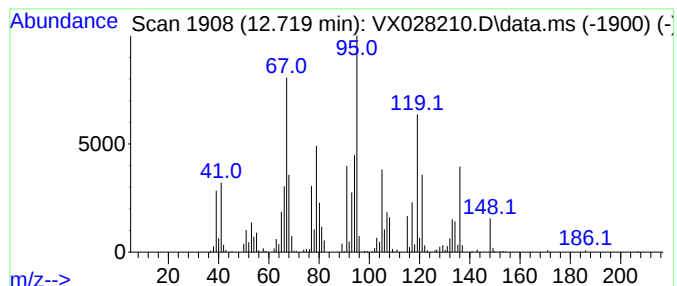
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Quant Title : SW846 8260

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

Peak Number 6 4,7-Methano-1H-indene, octa... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.719	9.18 ug/l	344525	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4,7-Methano-1H-indene, octahydro...	136	C10H16	002825-83-4	98
2			4,7-Methano-1H-indene, octahydro-	136	C10H16	006004-38-2	96
3			exo-Tricyclo[5.2.1.0(2,6)]decane	136	C10H16	002825-82-3	95
4			3-Cyclopentylcyclopentene	136	C10H16	002690-17-7	76
5			1-Cyclopentylcyclopentene	136	C10H16	004884-21-3	52



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042022\
Data File : VX028210.D
Acq On : 20 Apr 2022 20:04
Operator : JC/MD
Sample : N2459-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31577

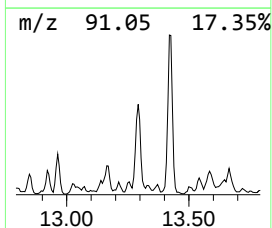
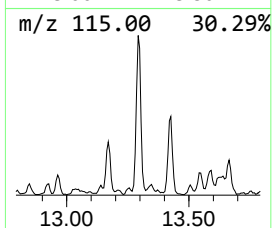
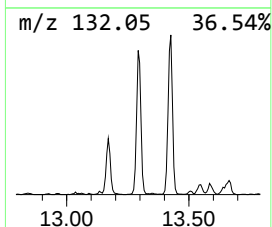
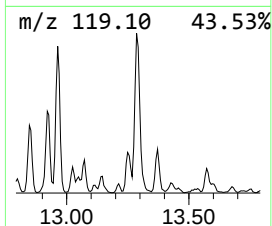
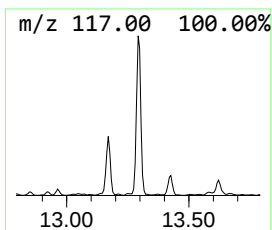
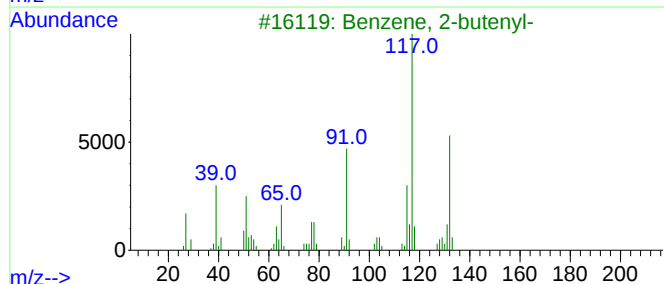
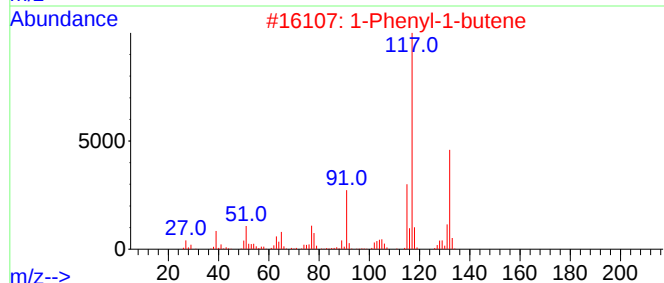
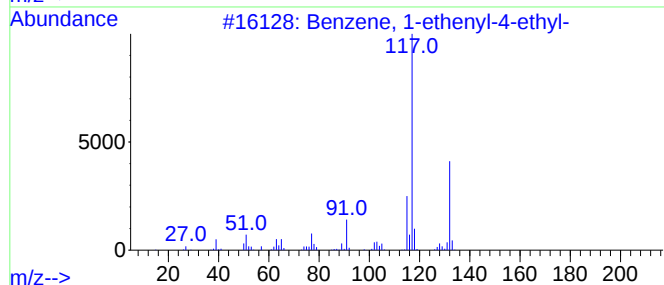
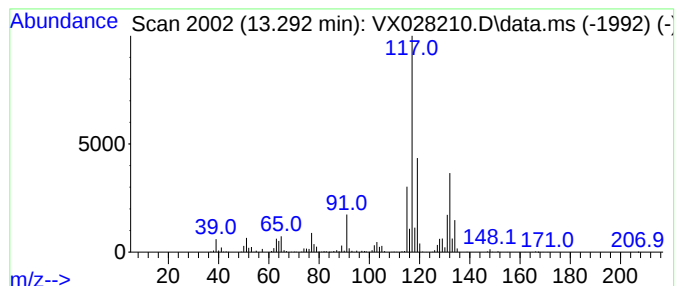
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1-ethenyl-4-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	18.40 ug/l	690509	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	93
2			1-Phenyl-1-butene	132	C10H12	000824-90-8	76
3			Benzene, 2-butenyl-	132	C10H12	001560-06-1	76
4			Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	76
5			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	76



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042022\
Data File : VX028210.D
Acq On : 20 Apr 2022 20:04
Operator : JC/MD
Sample : N2459-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31577

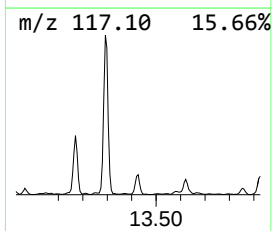
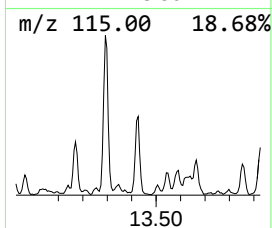
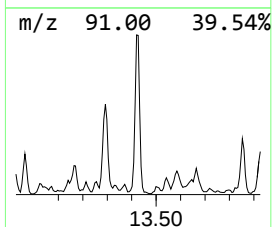
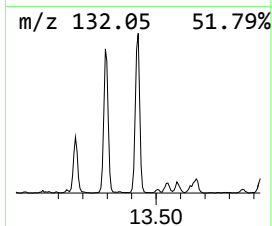
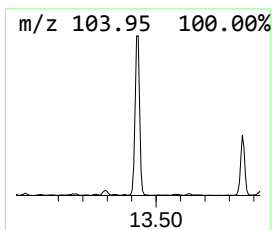
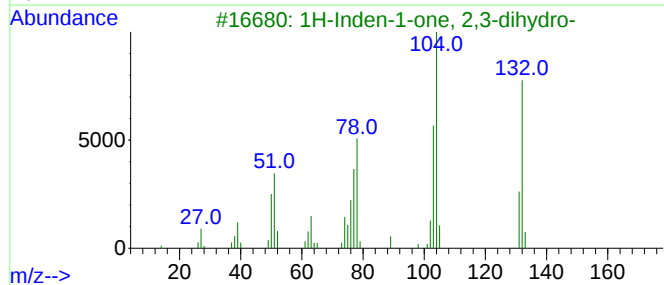
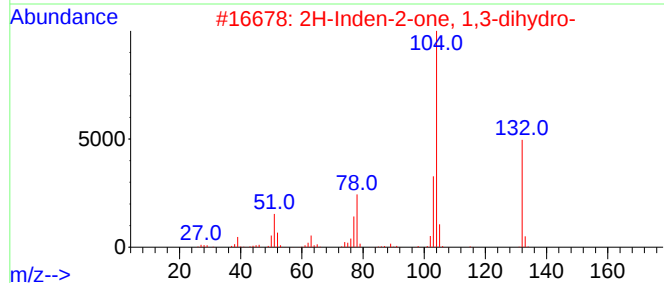
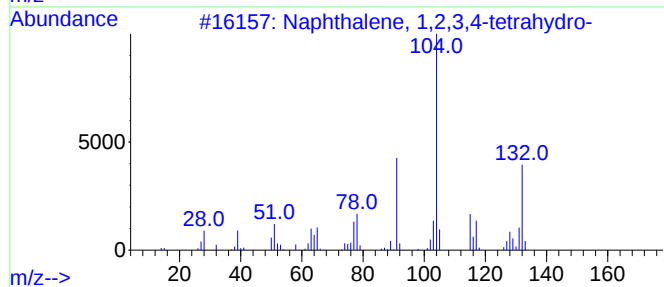
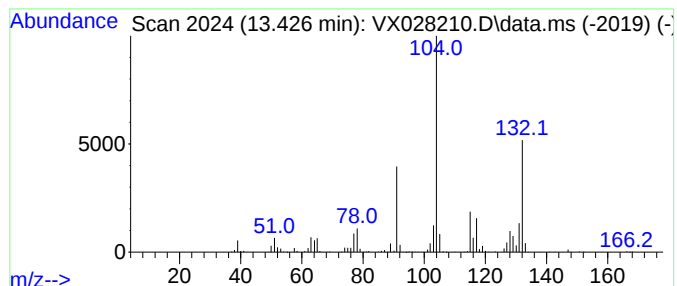
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Quant Title : SW846 8260

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

Peak Number 8 Naphthalene, 1,2,3,4-tetrahydro... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.426	12.63 ug/l	474076	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-	132	C10H12	000119-64-2	96
2			2H-Inden-2-one, 1,3-dihydro-	132	C9H8O	000615-13-4	53
3			1H-Inden-1-one, 2,3-dihydro-	132	C9H8O	000083-33-0	38
4			Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	38
5			Isoquinoline, 1,2,3,4-tetrahydro-	133	C9H11N	000091-21-4	27



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042022\
Data File : VX028210.D
Acq On : 20 Apr 2022 20:04
Operator : JC/MD
Sample : N2459-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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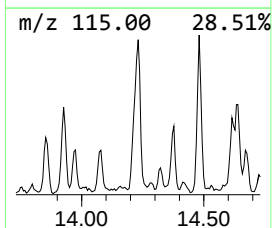
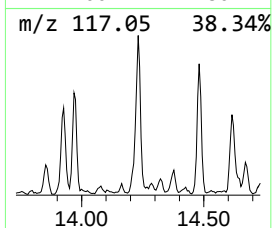
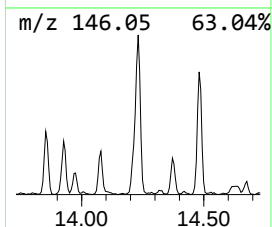
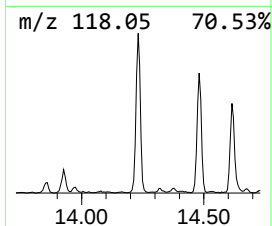
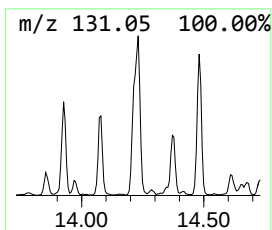
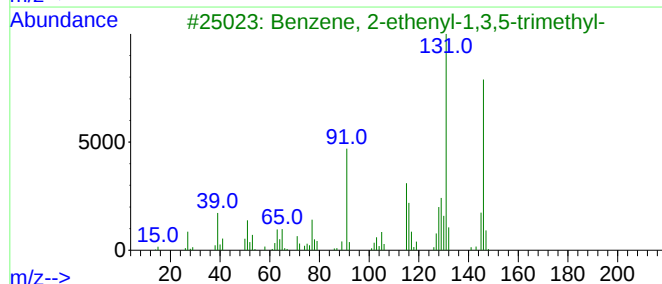
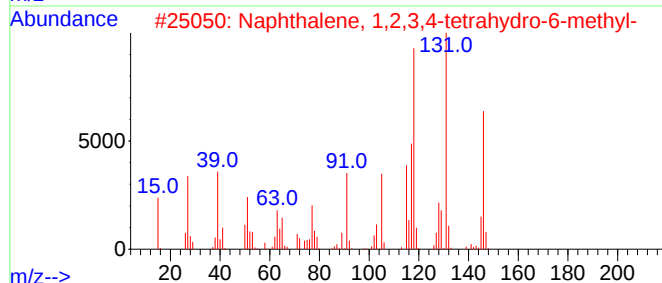
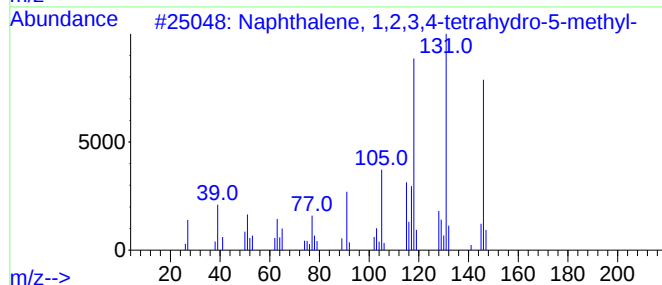
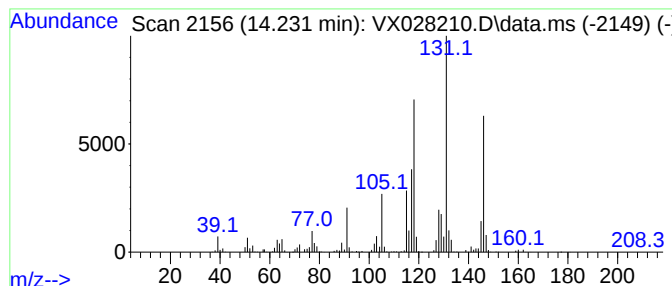
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

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

Peak Number 9 Naphthalene, 1,2,3,4-tetra... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.231	14.37 ug/l	539152	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	97
2			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	96
3			Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	86
4			1H-Inden-1-one, 2,3-dihydro-2-me...	146	C10H10O	017496-14-9	68
5			Benzene, (1-methyl-1-butenyl)-	146	C11H14	053172-84-2	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042022\
Data File : VX028210.D
Acq On : 20 Apr 2022 20:04
Operator : JC/MD
Sample : N2459-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31577

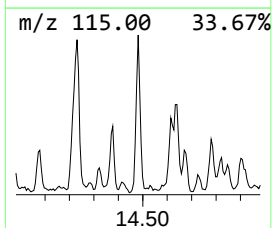
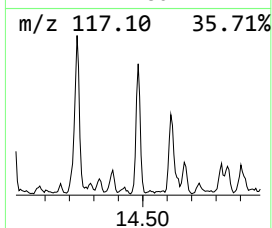
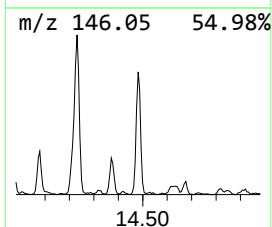
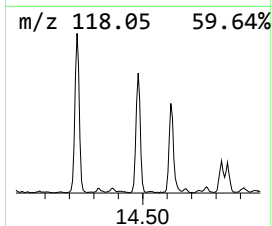
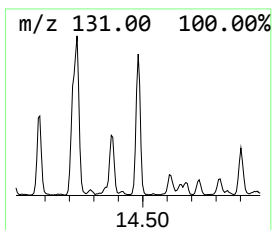
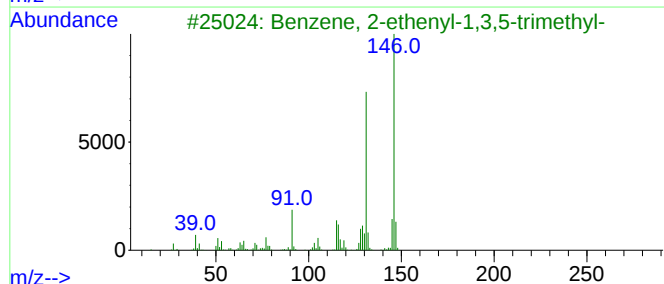
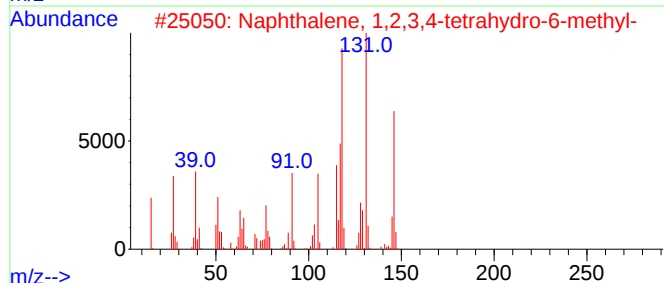
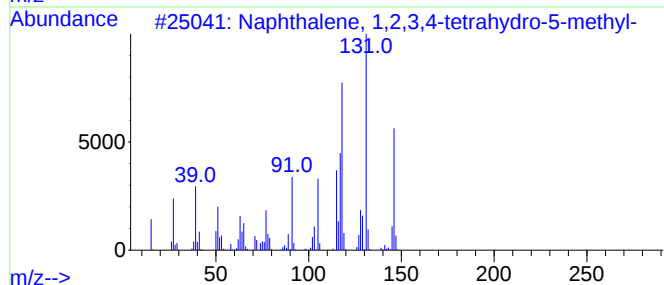
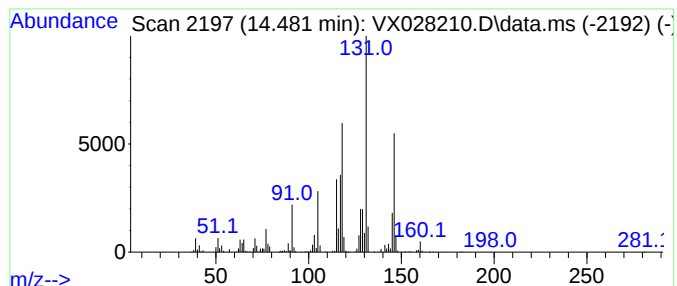
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

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

Peak Number 10 Naphthalene, 1,2,3,4-tetrahydro-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.481	11.04 ug/l	414403	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	94
2			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	94
3			Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	68
4			1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	64
5			Benzene, (1-methyl-1-butenyl)-	146	C11H14	053172-84-2	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042022\
Data File : VX028210.D
Acq On : 20 Apr 2022 20:04
Operator : JC/MD
Sample : N2459-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31577

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.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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Butane, 2-methyl-	1.752	27.0	ug/l	634334	1	5.556	1175920	50.0
Pentane	1.953	14.5	ug/l	341260	1	5.556	1175920	50.0
Ethanol	2.062	356.1	ug/l	8373710	1	5.556	1175920	50.0
Indane	12.244	17.0	ug/l	639316	4	12.024	1876600	50.0
4,7-Methano-1H-...	12.719	9.2	ug/l	344525	4	12.024	1876600	50.0
Benzene, 1-ethe...	13.292	18.4	ug/l	690509	4	12.024	1876600	50.0
Naphthalene, 1,...	13.426	12.6	ug/l	474076	4	12.024	1876600	50.0
Naphthalene, 1,...	14.231	14.4	ug/l	539152	4	12.024	1876600	50.0
Naphthalene, 1,...	14.481	11.0	ug/l	414403	4	12.024	1876600	50.0