

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032823\
 Data File : VX034810.D
 Acq On : 28 Mar 2023 21:51
 Operator : JC/MD
 Sample : 02084-02
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 34 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-5B

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\82X031023W.M
 Title : SW846 8260

Signal : TIC: VX034810.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.368	43	46	52	rBV	3268926	3415269	6.71%	0.729%
2	1.752	103	109	125	rBV	13019757	17698451	34.78%	3.779%
3	1.959	138	143	156	rVV2	4735530	7638352	15.01%	1.631%
4	2.069	156	161	168	rVV	1233607	1713329	3.37%	0.366%
5	2.166	172	177	181	rVV	693275	1031562	2.03%	0.220%
6	2.215	181	185	198	rVB	2770738	4166826	8.19%	0.890%
7	2.343	198	206	218	rBV	614491	1225477	2.41%	0.262%
8	2.782	257	278	281	rBV2	1936768	4988605	9.80%	1.065%
9	2.825	281	285	289	rVV	3870409	7991389	15.71%	1.706%
10	2.867	289	292	312	rVB2	2485401	5502329	10.81%	1.175%
11	3.105	317	331	352	rVB	3541067	7967897	15.66%	1.701%
12	3.319	356	366	378	rBV	464738	1131353	2.22%	0.242%
13	3.447	378	387	400	rVB	1267625	2772056	5.45%	0.592%
14	3.581	400	409	416	rBV2	252356	654367	1.29%	0.140%
15	3.666	416	423	427	rBV	224776	522035	1.03%	0.111%
16	3.733	427	434	443	rVB	901757	2137414	4.20%	0.456%
17	3.837	443	451	457	rBV	726738	1847386	3.63%	0.394%
18	4.105	484	495	505	rVB	687207	1838650	3.61%	0.393%
19	4.306	518	528	540	rVV	4969995	14269371	28.04%	3.047%
20	4.428	540	548	561	rVB	362071	1088626	2.14%	0.232%
21	5.190	644	673	689	rVB	927876	3369928	6.62%	0.720%
22	5.385	690	705	710	rBV3	243051	807904	1.59%	0.172%
23	5.477	710	720	736	rVV4	1981480	7937551	15.60%	1.695%
24	5.617	738	743	766	rVB3	546087	2043151	4.02%	0.436%
25	5.830	766	778	791	rBV5	762300	2420221	4.76%	0.517%
26	6.160	818	832	843	rBV3	620483	2788502	5.48%	0.595%
27	6.257	843	848	856	rVV2	609734	1632288	3.21%	0.349%
28	6.361	856	865	875	rVB2	656760	1853041	3.64%	0.396%
29	6.611	893	906	914	rBV3	388024	998449	1.96%	0.213%
30	6.763	923	931	934	rBV	494082	1142096	2.24%	0.244%
31	6.848	935	945	954	rVB5	831610	3236652	6.36%	0.691%
32	7.172	989	998	1008	rBV2	749657	1720139	3.38%	0.367%
33	7.379	1019	1032	1044	rBV4	2313562	6048169	11.89%	1.291%
34	7.659	1070	1078	1089	rVB	450502	894847	1.76%	0.191%
35	7.854	1103	1110	1112	rBV2	277610	534036	1.05%	0.114%
36	7.879	1112	1114	1121	rVB	314842	518754	1.02%	0.111%

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37	8.141	1143	1157	1162	rBV	1509335	2924497	5.75%	0.624%
38	8.501	1209	1216	1226	rVB	970230	1766766	3.47%	0.377%
39	8.647	1235	1240	1246	rVB	1011417	1606190	3.16%	0.343%
40	8.720	1246	1252	1258	rBV	7588344	11523685	22.65%	2.460%
41	8.921	1278	1285	1290	rBV3	315496	560287	1.10%	0.120%
42	9.159	1319	1324	1335	rVB	684063	1113471	2.19%	0.238%
43	10.055	1466	1471	1475	rVB	971398	1275488	2.51%	0.272%
44	10.195	1489	1494	1500	rVB	19001859	25606756	50.33%	5.467%
45	10.305	1504	1512	1518	rVB	30800261	46131770	90.67%	9.850%
46	10.640	1562	1567	1578	rVB	11900135	15740969	30.94%	3.361%
47	10.964	1614	1620	1628	rBV	2372111	3013582	5.92%	0.643%
48	11.079	1635	1639	1644	rBV	875834	1072762	2.11%	0.229%
49	11.305	1668	1676	1683	rBV	8738406	10617677	20.87%	2.267%
50	11.384	1683	1689	1690	rVV	8713385	11958103	23.50%	2.553%
51	11.402	1690	1692	1696	rVV	10924762	11074303	21.77%	2.364%
52	11.451	1696	1700	1707	rVB	3916604	4630889	9.10%	0.989%
53	11.616	1721	1727	1736	rVB	10892372	14011647	27.54%	2.992%
54	11.756	1744	1750	1755	rBV	35448198	50880587	100.00%	10.863%
55	11.890	1770	1772	1778	rVB	482151	523371	1.03%	0.112%
56	11.969	1780	1785	1789	rBV	723503	916346	1.80%	0.196%
57	12.018	1789	1793	1799	rVB2	1304152	1941010	3.81%	0.414%
58	12.085	1799	1804	1810	rBV	10706486	13673484	26.87%	2.919%
59	12.244	1824	1830	1837	rBV2	10236120	14540305	28.58%	3.104%
60	12.311	1837	1841	1849	rVV3	3298007	5301060	10.42%	1.132%
61	12.408	1850	1857	1861	rVV2	720798	1000330	1.97%	0.214%
62	12.463	1861	1866	1872	rVB	1756699	2034740	4.00%	0.434%
63	12.530	1872	1877	1879	rBV	4795319	5893254	11.58%	1.258%
64	12.555	1879	1881	1886	rVB	4318617	4563045	8.97%	0.974%
65	12.616	1886	1891	1894	rBV	7241687	8954148	17.60%	1.912%
66	12.646	1894	1896	1900	rVB	2103009	2152344	4.23%	0.460%
67	12.701	1900	1905	1912	rBV2	5995317	8044453	15.81%	1.718%
68	12.847	1924	1929	1934	rVB	2135788	2582231	5.08%	0.551%
69	12.921	1934	1941	1944	rBV	4431572	5357554	10.53%	1.144%
70	12.963	1944	1948	1954	rVB	6388954	7383510	14.51%	1.576%
71	13.024	1954	1958	1964	rBV3	337450	810218	1.59%	0.173%
72	13.170	1978	1982	1987	rVB	5420609	6575078	12.92%	1.404%
73	13.292	1997	2002	2007	rVB2	9581243	12566042	24.70%	2.683%
74	13.420	2019	2023	2031	rVB	1302524	1640296	3.22%	0.350%
75	13.506	2031	2037	2040	rBV2	556735	754881	1.48%	0.161%
76	13.542	2040	2043	2046	rVV	1236480	1595293	3.14%	0.341%

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77	13.585	2046	2050	2055	rVV3	1174149	2170547	4.27%	0.463%
78	13.640	2055	2059	2060	rVV2	628962	799200	1.57%	0.171%
79	13.664	2060	2063	2069	rVB2	1187118	1691969	3.33%	0.361%
80	13.774	2074	2081	2090	rVB	3616748	4595000	9.03%	0.981%
81	13.865	2090	2096	2100	rBV2	354715	525587	1.03%	0.112%
82	13.926	2100	2106	2110	rVV2	450803	644389	1.27%	0.138%
83	14.073	2126	2130	2137	rBV	832556	995207	1.96%	0.212%
84	14.213	2149	2153	2159	rBV	624789	1042767	2.05%	0.223%
85	14.371	2176	2179	2184	rVB	441421	517444	1.02%	0.110%
86	14.634	2219	2222	2233	rVB	715127	980719	1.93%	0.209%
87	14.780	2241	2246	2257	rVB	1999435	2541684	5.00%	0.543%

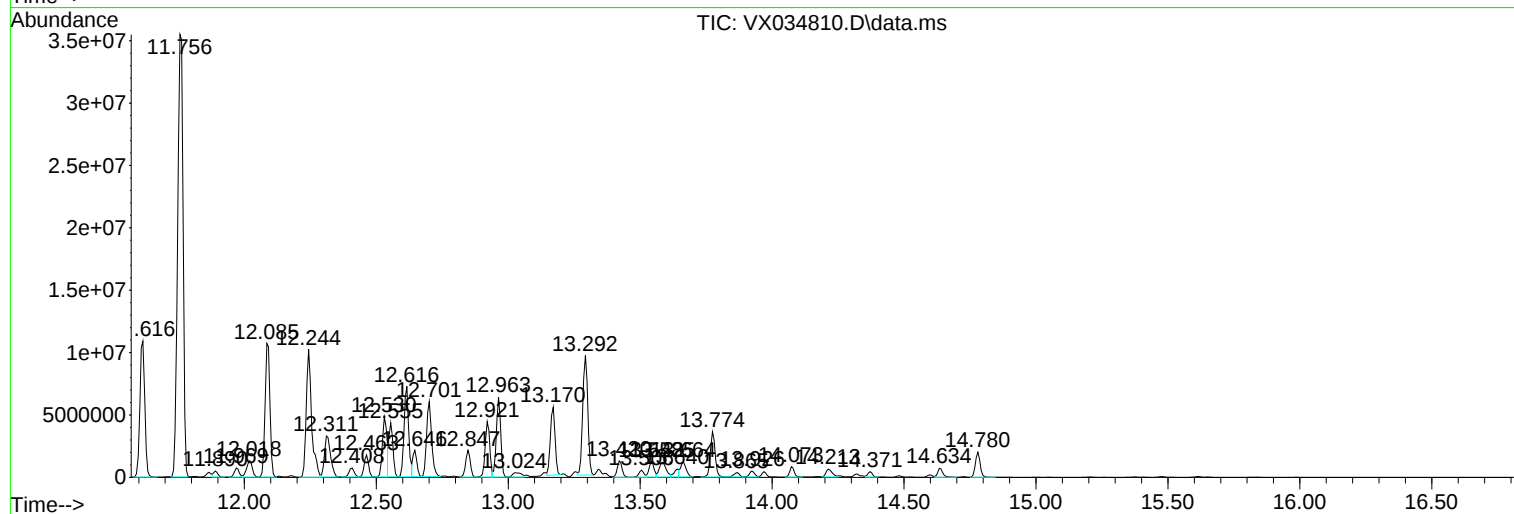
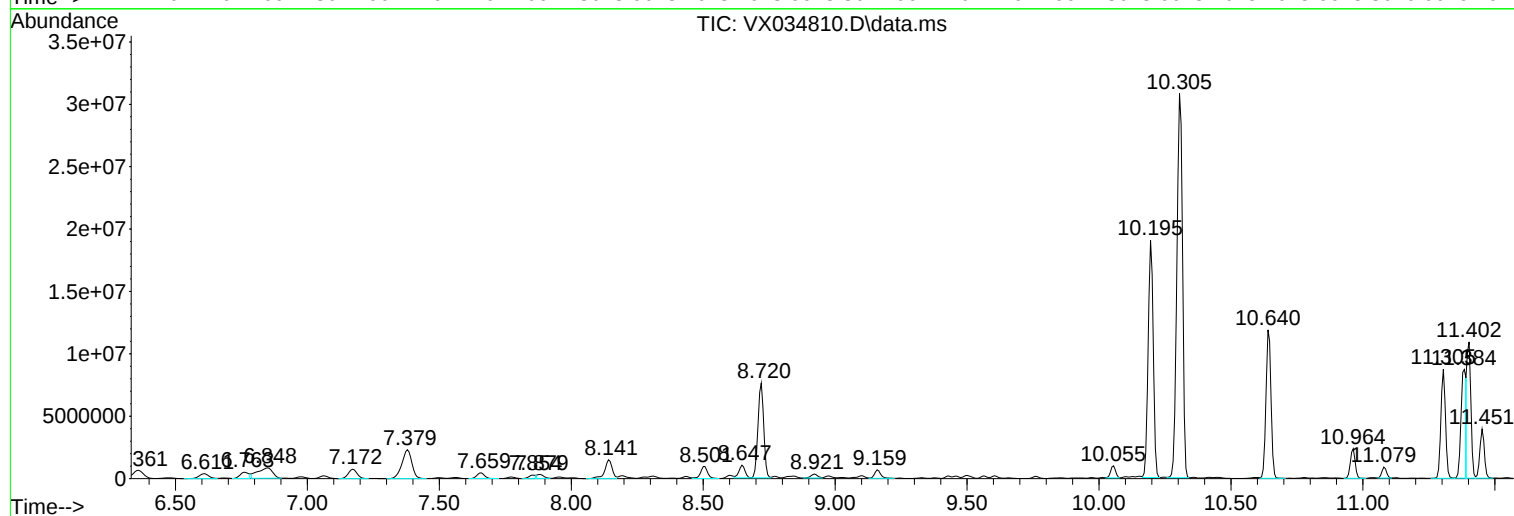
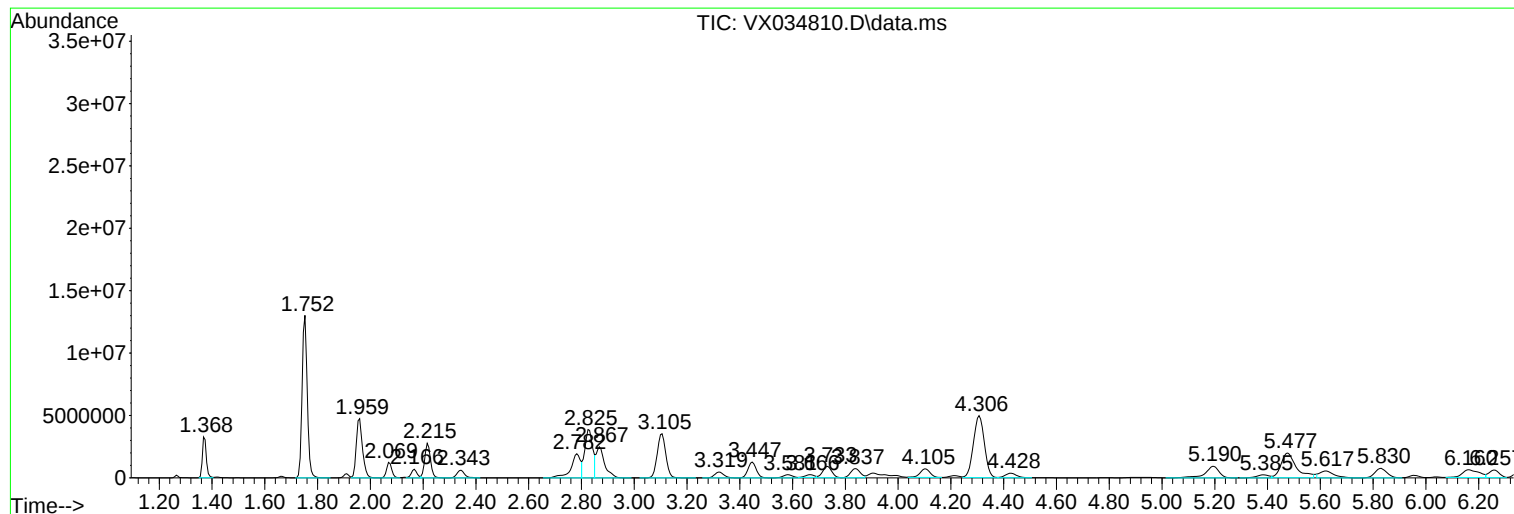
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MSVOA_X
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

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



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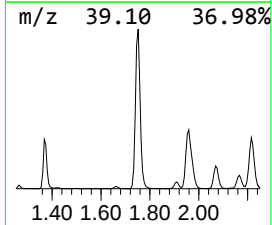
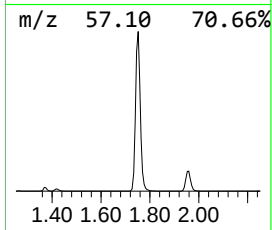
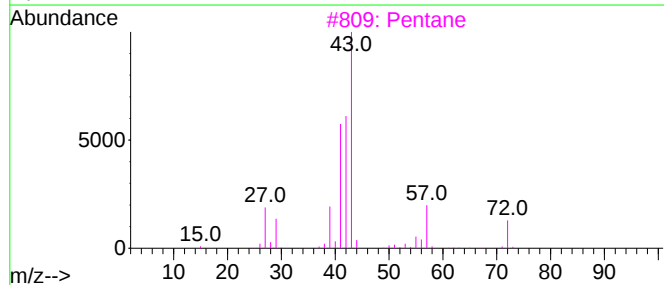
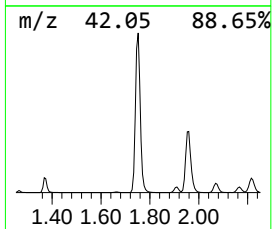
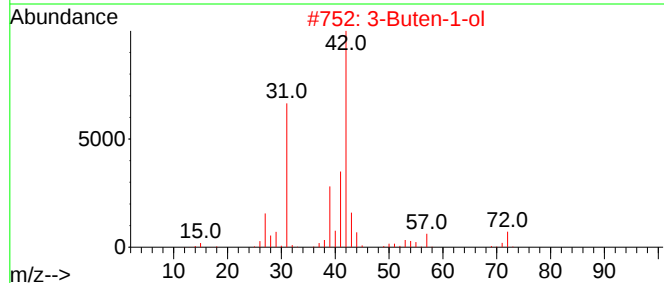
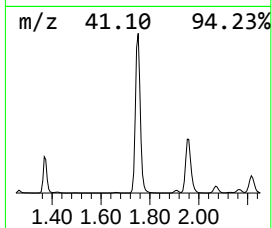
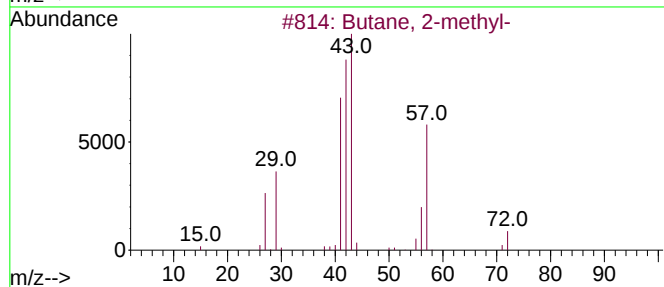
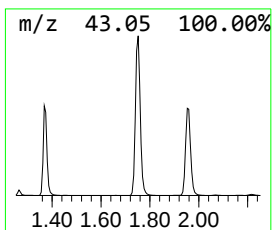
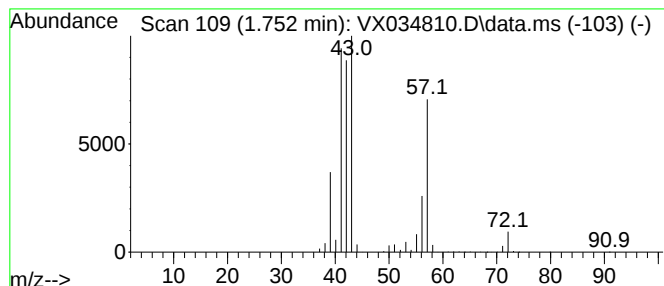
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.752	433.12 ug/l	17698500	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	86
2			3-Buten-1-ol	72	C4H8O	000627-27-0	47
3			Pentane	72	C5H12	000109-66-0	33
4			Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	16
5			1-Propene, 2-methyl-	56	C4H8	000115-11-7	10



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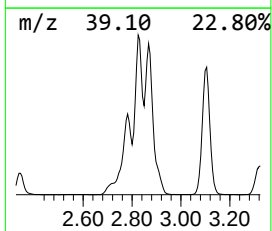
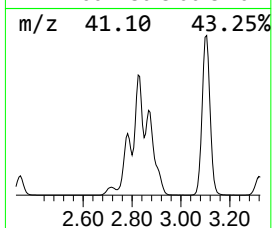
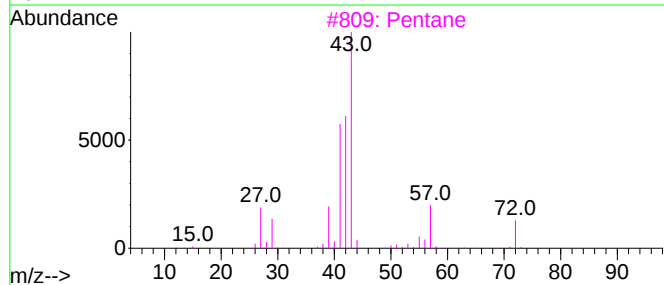
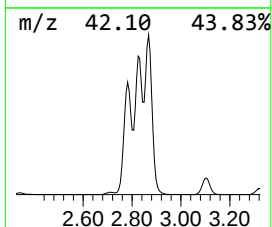
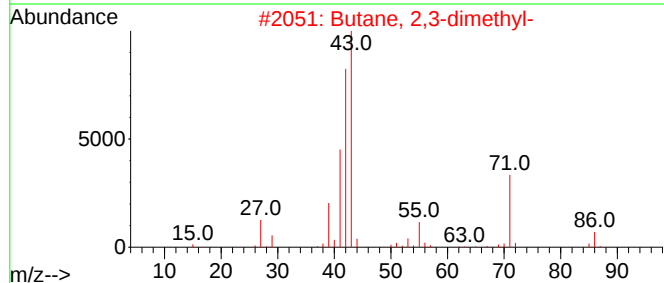
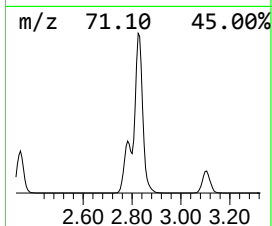
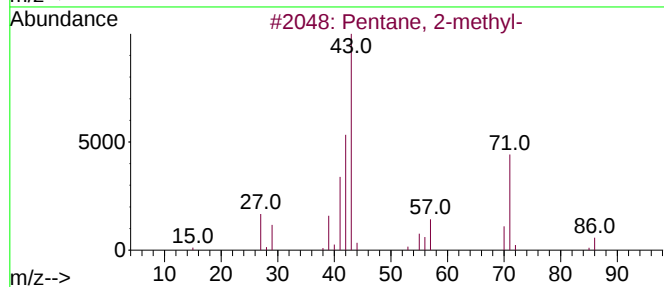
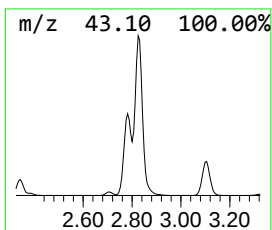
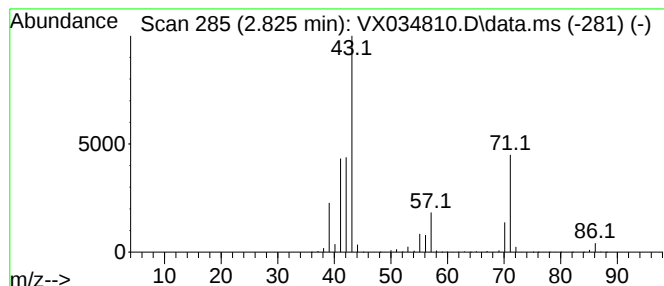
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

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

Peak Number 2 Pentane, 2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.825	195.57 ug/l	7991390	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2-methyl-	86	C6H14	000107-83-5	91
2			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	43
3			Pentane	72	C5H12	000109-66-0	38
4			Pentane, 3,3-dimethyl-	100	C7H16	000562-49-2	38
5			Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	28



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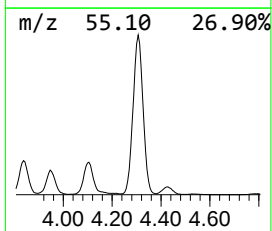
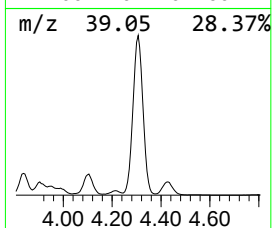
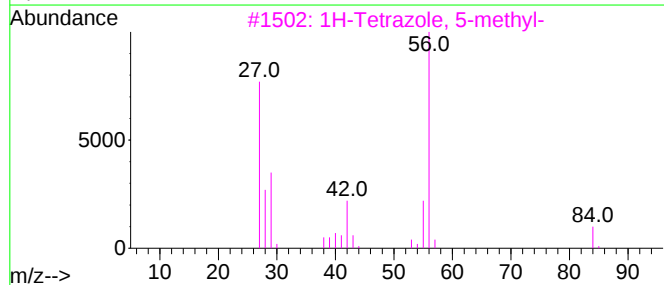
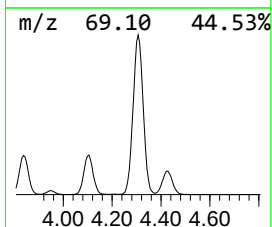
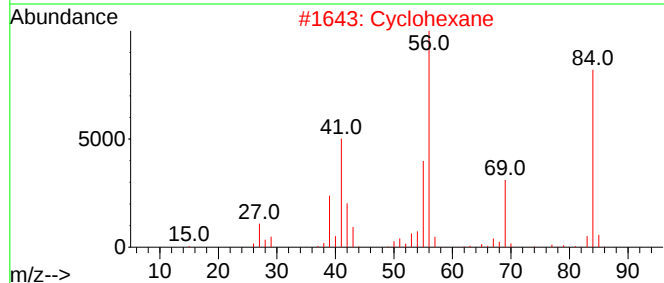
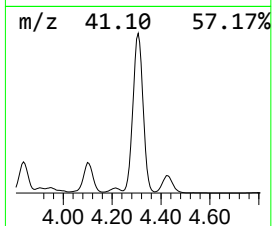
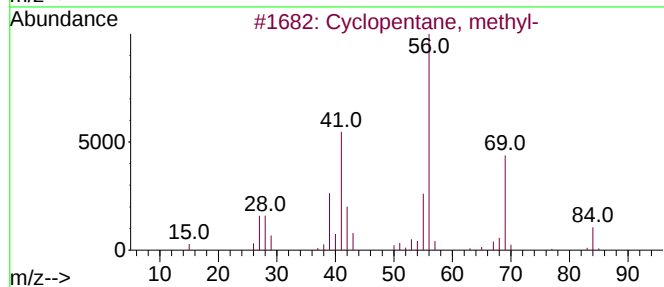
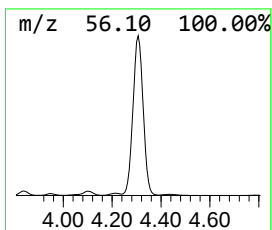
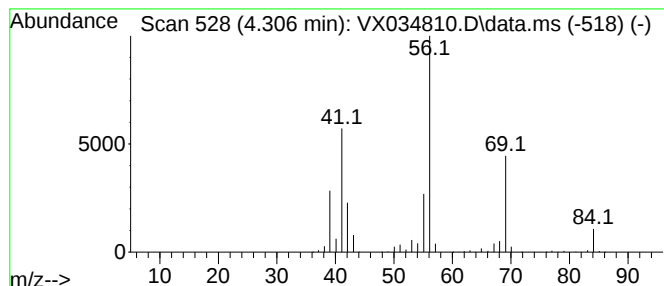
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

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

Peak Number 3 Cyclopentane, methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	349.20 ug/l	14269400	Pentafluorobenzene	5.550

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	80
3		1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
4		1-Pentene, 2-methyl-	84	C6H12	000763-29-1	64
5		Cyclobutane, ethyl-	84	C6H12	004806-61-5	64



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ClientSampleId :
MW-5B

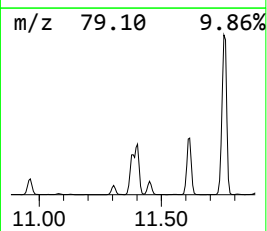
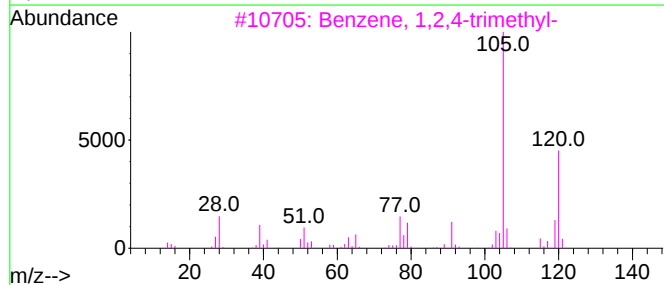
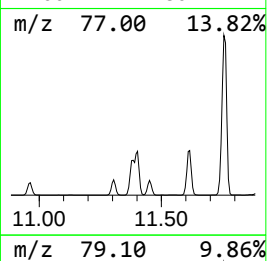
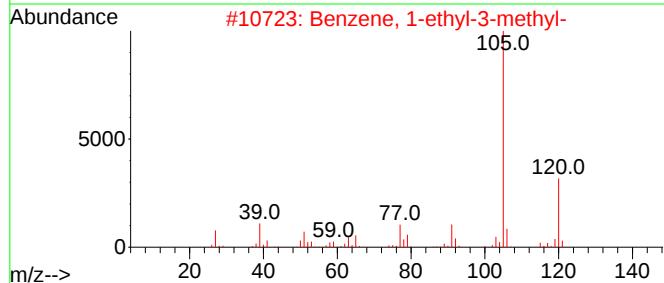
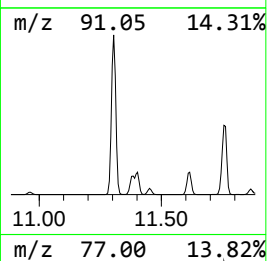
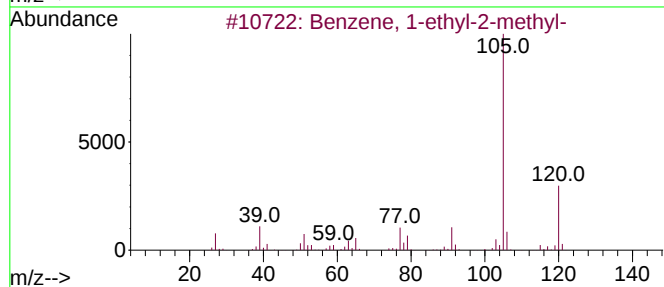
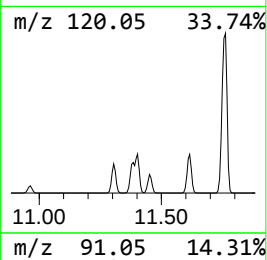
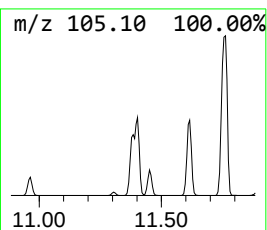
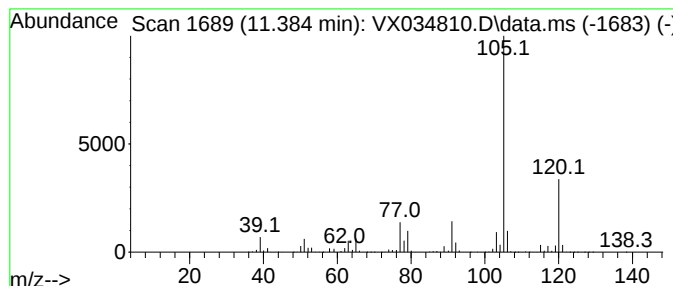
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Quant Title : SW846 8260

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

Peak Number 4 Benzene, 1-ethyl-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.384	308.04 ug/l	11958100	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	94
3			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4			Mesitylene	120	C9H12	000108-67-8	91
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032823\
Data File : VX034810.D
Acq On : 28 Mar 2023 21:51
Operator : JC/MD
Sample : 02084-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 34 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-5B

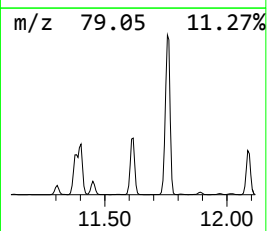
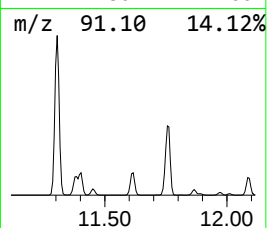
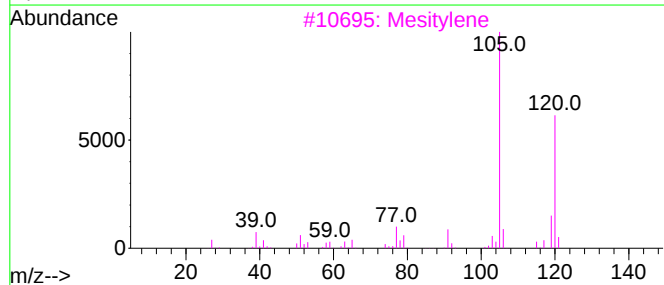
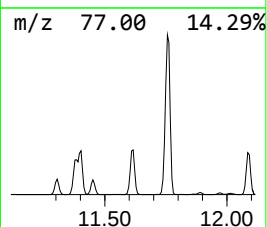
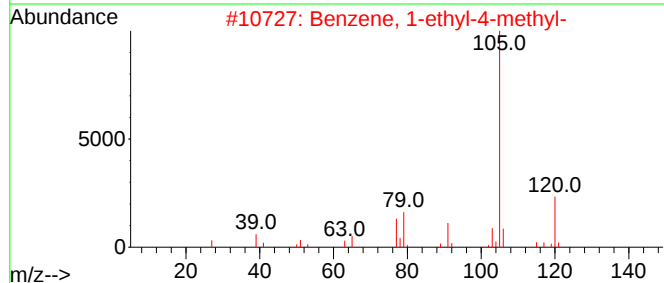
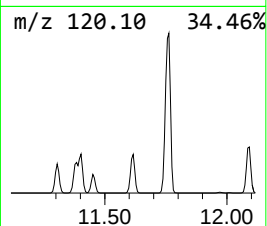
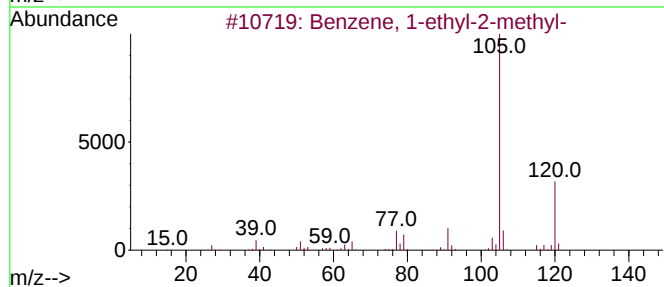
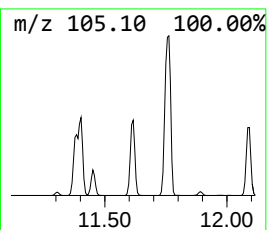
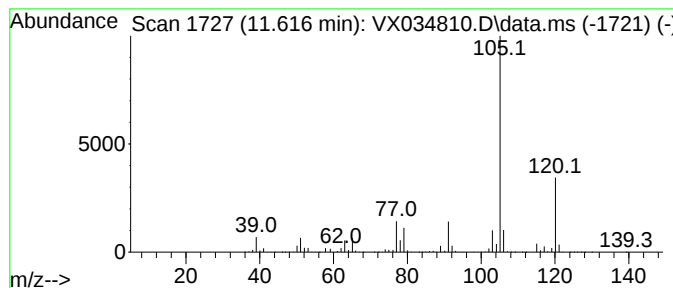
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Quant Title : SW846 8260

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

Peak Number 5 Benzene, 1-ethyl-4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	360.94 ug/l	14011600	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	94
2			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
3			Mesitylene	120	C9H12	000108-67-8	91
4			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032823\
Data File : VX034810.D
Acq On : 28 Mar 2023 21:51
Operator : JC/MD
Sample : 02084-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 34 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-5B

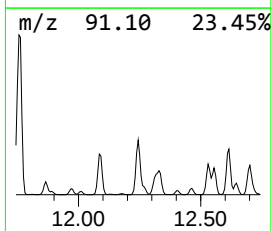
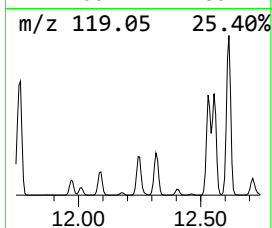
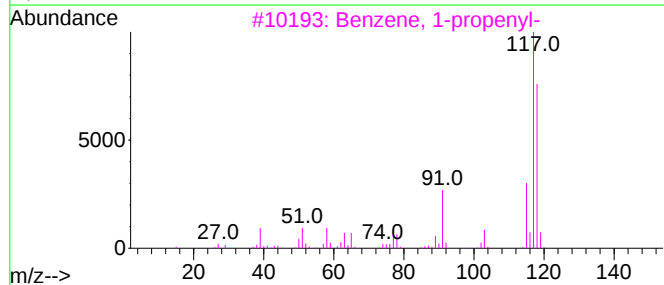
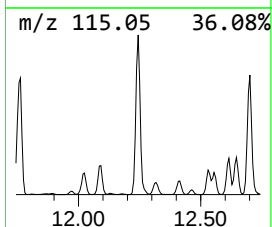
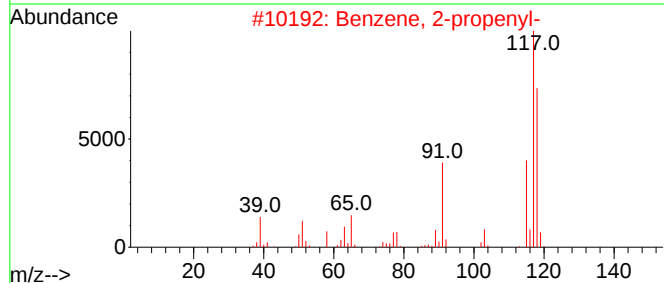
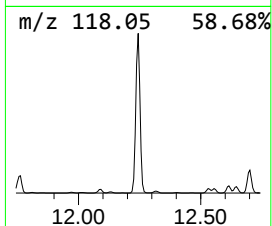
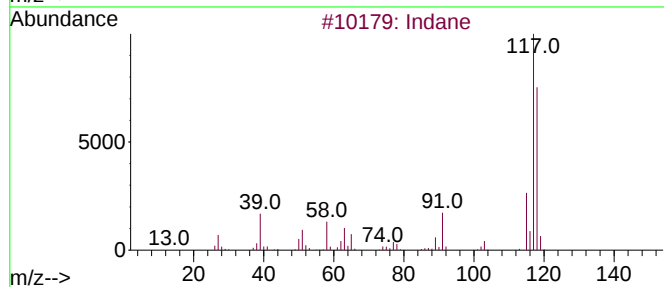
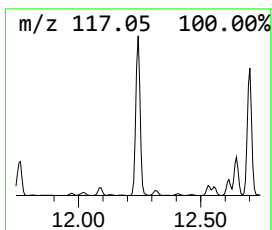
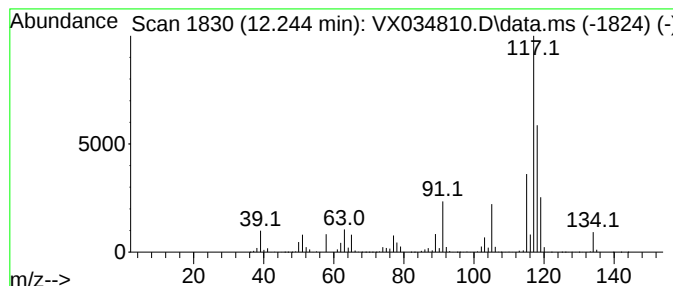
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Quant Title : SW846 8260

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

Peak Number 7 Indane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	374.56 ug/l	14540300	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	70
2			Benzene, 2-propenyl-	118	C9H10	000300-57-2	70
3			Benzene, 1-propenyl-	118	C9H10	000637-50-3	64
4			Benzene, cyclopropyl-	118	C9H10	000873-49-4	64
5			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032823\
Data File : VX034810.D
Acq On : 28 Mar 2023 21:51
Operator : JC/MD
Sample : 02084-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 34 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-5B

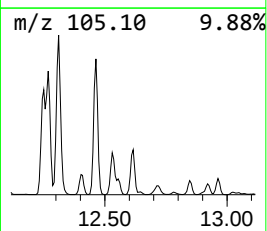
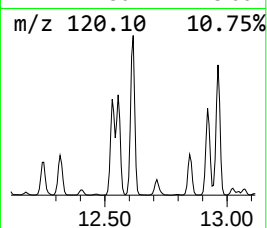
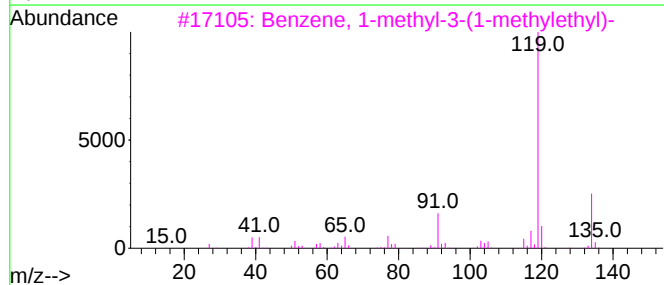
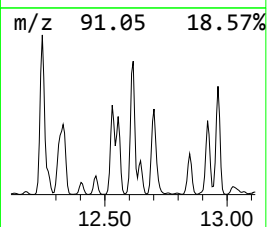
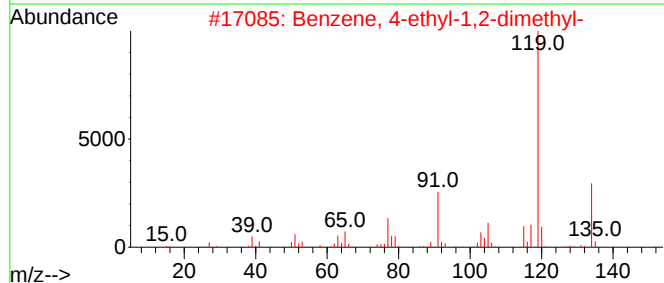
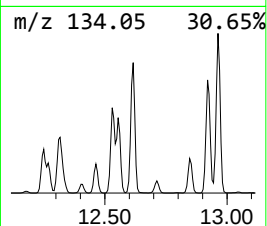
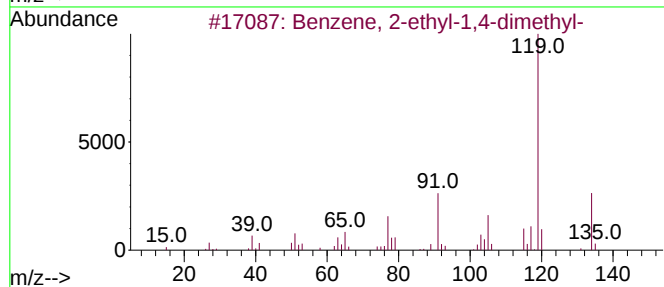
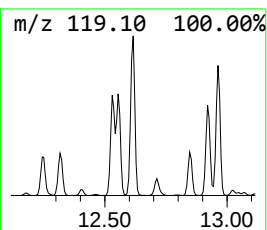
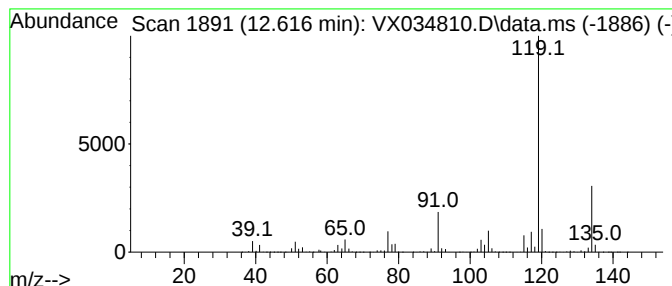
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 2-ethyl-1,4-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.616	230.66 ug/l	8954150	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	96
2			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
3			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	95
4			p-Cymene	134	C10H14	000099-87-6	95
5			o-Cymene	134	C10H14	000527-84-4	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032823\
Data File : VX034810.D
Acq On : 28 Mar 2023 21:51
Operator : JC/MD
Sample : 02084-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 34 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-5B

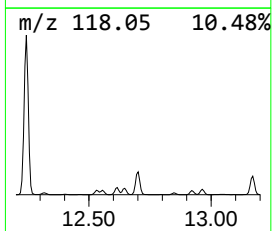
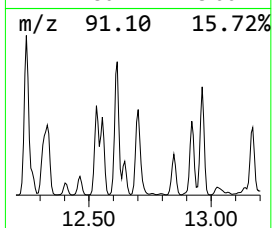
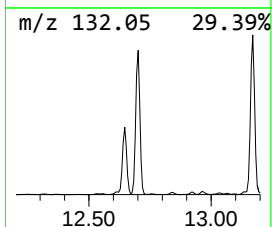
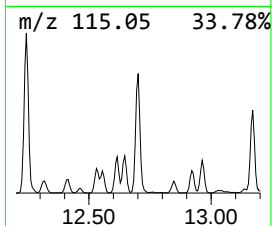
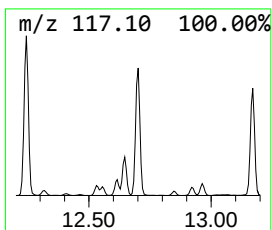
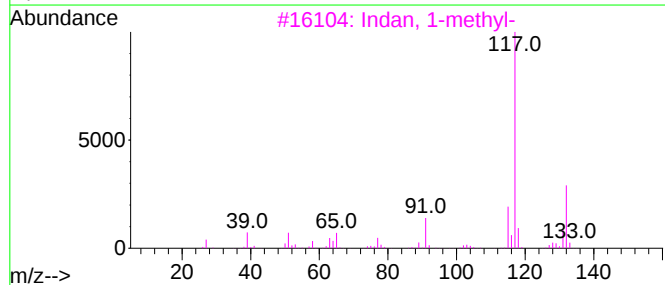
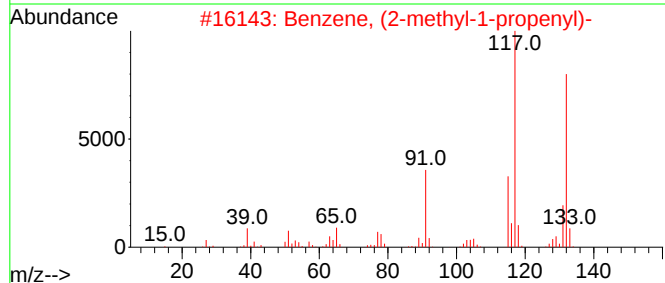
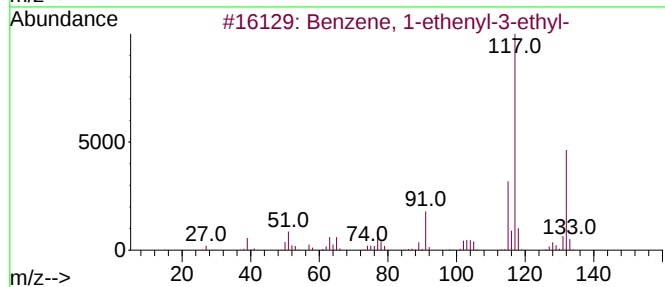
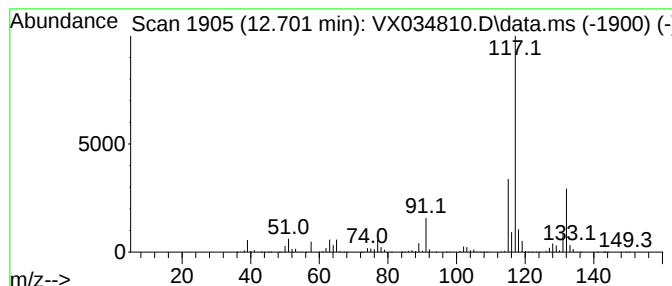
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, 1-ethenyl-3-ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.701	207.22 ug/l	8044450	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	91
2			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	90
3			Indan, 1-methyl-	132	C10H12	000767-58-8	87
4			1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	87
5			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032823\
Data File : VX034810.D
Acq On : 28 Mar 2023 21:51
Operator : JC/MD
Sample : 02084-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 34 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-5B

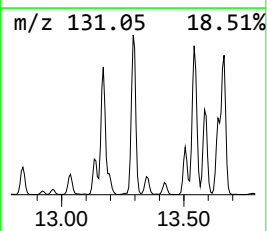
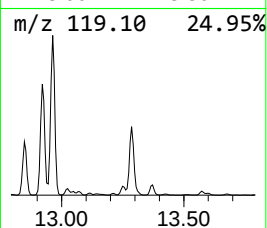
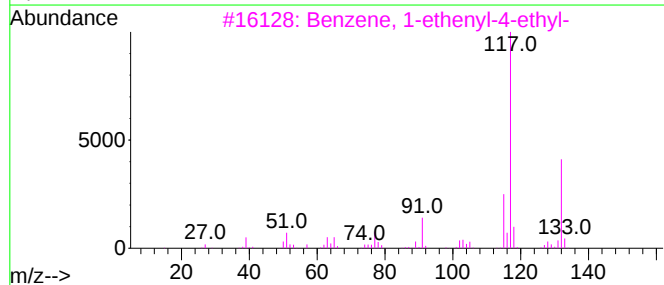
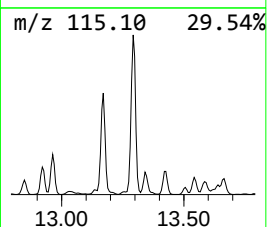
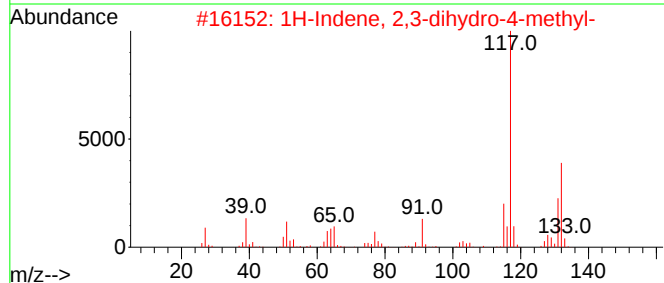
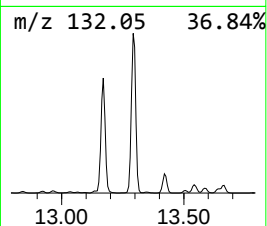
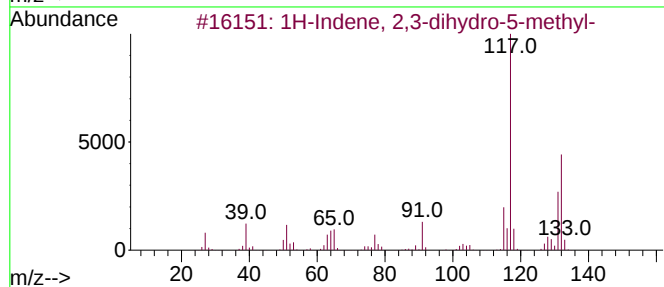
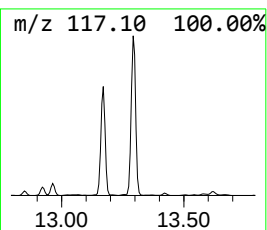
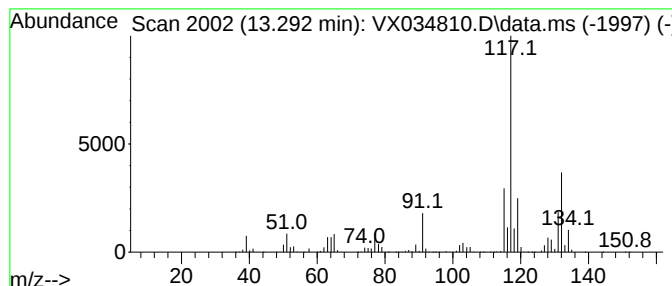
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Quant Title : SW846 8260

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

Peak Number 10 1H-Indene, 2,3-dihydro-5-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	323.70 ug/l	12566000	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	95	
2	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	93	
3	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	89	
4	Benzene, 2-ethenyl-1,3-dimethyl-	132	C10H12	002039-90-9	81	
5	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	81	



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032823\
Data File : VX034810.D
Acq On : 28 Mar 2023 21:51
Operator : JC/MD
Sample : 02084-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 34 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-5B

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.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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Pentane, 2-methyl-	2.825	195.6	ug/l	7991390	1	5.550	2043150	50.0
Cyclopentane, m...	4.306	349.2	ug/l	14269400	1	5.550	2043150	50.0
Benzene, 1-ethy...	11.384	308.0	ug/l	11958100	4	12.024	1941010	50.0
Benzene, 1-ethy...	11.616	360.9	ug/l	14011600	4	12.024	1941010	50.0
Indane	12.244	374.6	ug/l	14540300	4	12.024	1941010	50.0
Benzene, 2-ethy...	12.616	230.7	ug/l	8954150	4	12.024	1941010	50.0
Benzene, 1-ethe...	12.701	207.2	ug/l	8044450	4	12.024	1941010	50.0
1H-Indene, 2,3-...	13.292	323.7	ug/l	12566000	4	12.024	1941010	50.0