

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102122\
 Data File : VX032291.D
 Acq On : 21 Oct 2022 16:12
 Operator : JC/MD
 Sample : N5185-11
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-10

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\82X101922W.M
 Title : SW846 8260

Signal : TIC: VX032291.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	23	29	43	rBV	503125	638368	2.93%	0.379%
2	1.368	43	46	52	rBV	2989078	3486935	15.99%	2.068%
3	1.746	103	108	128	rBV	15525511	21801792	100.00%	12.931%
4	1.953	137	142	155	rVB	3914059	5594006	25.66%	3.318%
5	2.069	156	161	167	rBV	298479	405457	1.86%	0.240%
6	2.215	180	185	195	rVB	676370	984543	4.52%	0.584%
7	2.343	198	206	225	rVB	277598	573448	2.63%	0.340%
8	2.782	270	278	281	rVV	876523	1919993	8.81%	1.139%
9	2.825	281	285	290	rVV	1657003	3628886	16.64%	2.152%
10	2.867	290	292	305	rVB2	792468	1585442	7.27%	0.940%
11	3.105	321	331	349	rVB2	1411638	3162287	14.50%	1.876%
12	3.318	357	366	377	rBV	151208	333426	1.53%	0.198%
13	3.447	377	387	399	rBV	401861	877709	4.03%	0.521%
14	3.733	427	434	443	rVB	355943	842686	3.87%	0.500%
15	3.837	443	451	458	rBV	207443	530616	2.43%	0.315%
16	4.105	482	495	503	rVB2	213845	600000	2.75%	0.356%
17	4.215	503	513	519	rVV	303838	883025	4.05%	0.524%
18	4.306	519	528	540	rVV	1979433	5606999	25.72%	3.326%
19	4.428	540	548	564	rVB4	79026	256849	1.18%	0.152%
20	5.196	666	674	688	rVB2	185514	585371	2.68%	0.347%
21	5.385	690	705	711	rBV	95963	297722	1.37%	0.177%
22	5.501	711	724	736	rVV6	526262	2698275	12.38%	1.600%
23	5.623	737	744	765	rVB	570035	1866056	8.56%	1.107%
24	5.830	765	778	790	rBV	527523	1551446	7.12%	0.920%
25	5.958	790	799	805	rVV	91894	243262	1.12%	0.144%
26	6.044	805	813	823	rVV	510226	1366149	6.27%	0.810%
27	6.159	823	832	839	rVV3	269472	938767	4.31%	0.557%
28	6.257	840	848	857	rVV2	627731	1957643	8.98%	1.161%
29	6.361	857	865	877	rVB2	186264	536803	2.46%	0.318%
30	6.611	892	906	918	rBV3	115335	306872	1.41%	0.182%
31	6.763	923	931	937	rVV	230528	594931	2.73%	0.353%
32	6.848	940	945	958	rVB4	142036	416474	1.91%	0.247%
33	7.379	1019	1032	1044	rBV4	468556	1310689	6.01%	0.777%
34	7.659	1073	1078	1089	rVB	162589	319962	1.47%	0.190%
35	7.885	1104	1115	1122	rBV4	72449	253801	1.16%	0.151%
36	7.988	1122	1132	1143	rVB	252391	584039	2.68%	0.346%

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37	8.110	1143	1152	1156	rBV	445919	967920	4.44%	0.574%
38	8.507	1212	1217	1224	rVB2	230715	404115	1.85%	0.240%
39	8.604	1224	1233	1236	rBV4	112918	272440	1.25%	0.162%
40	8.647	1236	1240	1247	rVB	463287	772130	3.54%	0.458%
41	8.720	1247	1252	1257	rBV	241313	380035	1.74%	0.225%
42	8.842	1264	1272	1278	rVB5	101225	266396	1.22%	0.158%
43	9.378	1355	1360	1365	rBV	222742	310530	1.42%	0.184%
44	9.458	1365	1373	1377	rBV	272809	434465	1.99%	0.258%
45	10.055	1466	1471	1476	rVB	454102	605020	2.78%	0.359%
46	10.201	1489	1495	1500	rBV	13672111	18312822	84.00%	10.861%
47	10.305	1506	1512	1518	rVB	9220546	12162667	55.79%	7.214%
48	10.640	1562	1567	1578	rVB	1978930	2586234	11.86%	1.534%
49	10.963	1614	1620	1626	rBV	1330596	1643997	7.54%	0.975%
50	11.085	1635	1640	1645	rBV	410718	553155	2.54%	0.328%
51	11.305	1671	1676	1681	rVB	3659493	4348640	19.95%	2.579%
52	11.384	1683	1689	1690	rBV	1258279	1730687	7.94%	1.026%
53	11.402	1690	1692	1696	rVV	1873005	1836187	8.42%	1.089%
54	11.451	1696	1700	1705	rVB	1368104	1628789	7.47%	0.966%
55	11.616	1721	1727	1736	rVB	3888205	4778591	21.92%	2.834%
56	11.756	1744	1750	1755	rBV	6384255	7663772	35.15%	4.545%
57	11.866	1762	1768	1770	rBV	200836	257771	1.18%	0.153%
58	11.890	1770	1772	1781	rVB	227077	269027	1.23%	0.160%
59	12.024	1789	1794	1799	rVB	570405	711932	3.27%	0.422%
60	12.091	1799	1805	1810	rBV	6214420	7305222	33.51%	4.333%
61	12.244	1825	1830	1837	rBV	6329347	7758227	35.59%	4.601%
62	12.317	1837	1842	1851	rVB3	671589	1337067	6.13%	0.793%
63	12.408	1852	1857	1861	rBV2	208510	270748	1.24%	0.161%
64	12.463	1861	1866	1872	rVB	660191	800336	3.67%	0.475%
65	12.530	1872	1877	1880	rBV	398358	546483	2.51%	0.324%
66	12.616	1885	1891	1894	rVV	2097549	2537922	11.64%	1.505%
67	12.646	1894	1896	1900	rVV	312381	329636	1.51%	0.196%
68	12.701	1900	1905	1913	rVB2	930766	1395314	6.40%	0.828%
69	12.847	1924	1929	1934	rVB	456840	555274	2.55%	0.329%
70	12.920	1934	1941	1945	rBV	1054571	1362190	6.25%	0.808%
71	12.963	1945	1948	1953	rVB	421128	480155	2.20%	0.285%
72	13.024	1953	1958	1964	rBV2	182712	283427	1.30%	0.168%
73	13.170	1978	1982	1986	rVB	937942	1054367	4.84%	0.625%
74	13.292	1998	2002	2007	rVB2	1935222	2556460	11.73%	1.516%
75	13.372	2012	2015	2020	rVV	193801	241955	1.11%	0.144%
76	13.426	2020	2024	2031	rVB	273009	356597	1.64%	0.211%

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77	13.579	2046	2049	2056	rVV3	310046	480853	2.21%	0.285%
78	13.670	2060	2064	2069	rVB3	173482	314573	1.44%	0.187%
79	13.774	2076	2081	2091	rBV	3090275	3955083	18.14%	2.346%
80	14.213	2149	2153	2160	rBV	138093	225043	1.03%	0.133%
81	14.640	2218	2223	2233	rVB	971373	1238737	5.68%	0.735%
82	14.780	2241	2246	2251	rBV	653386	781230	3.58%	0.463%

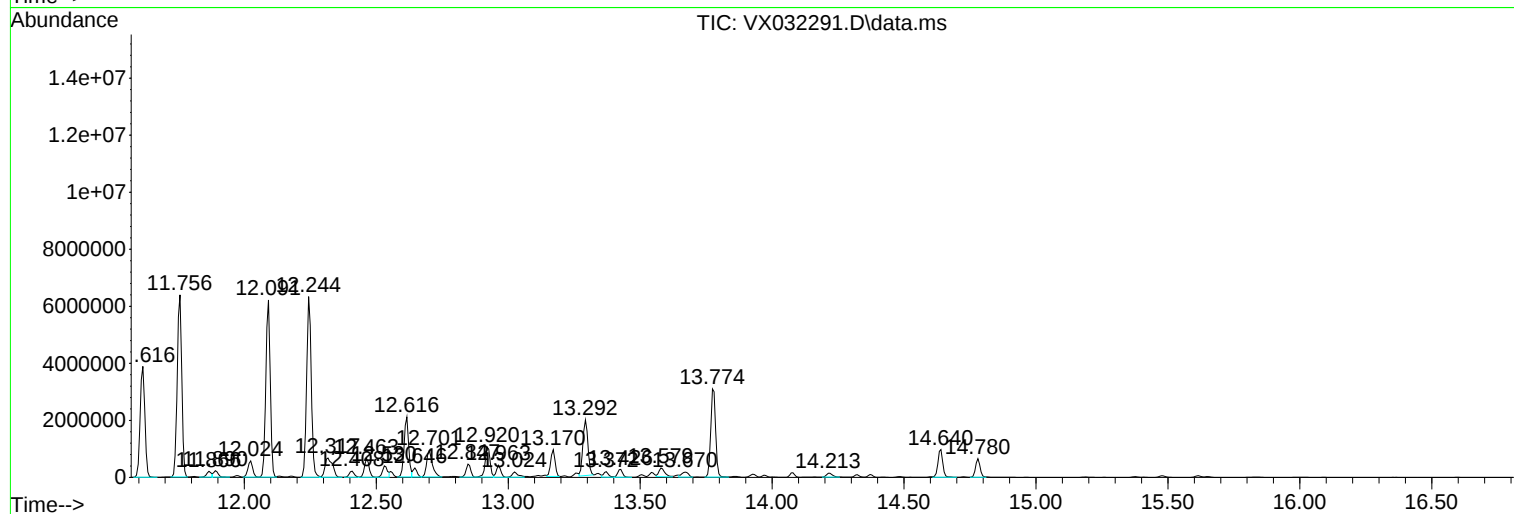
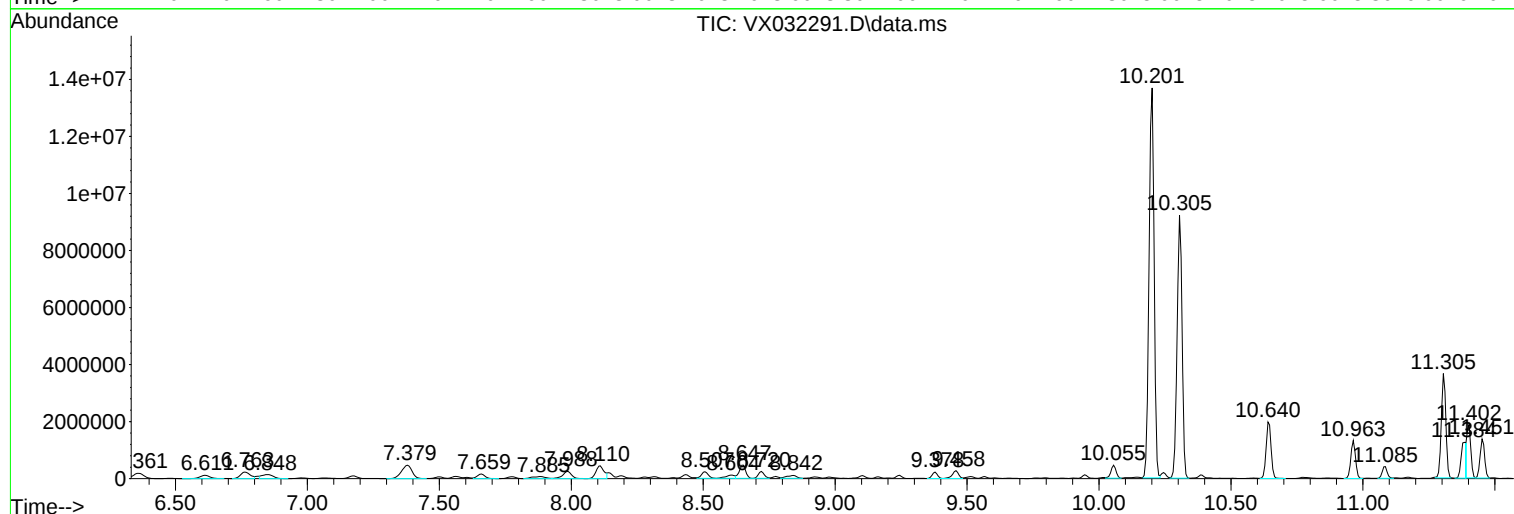
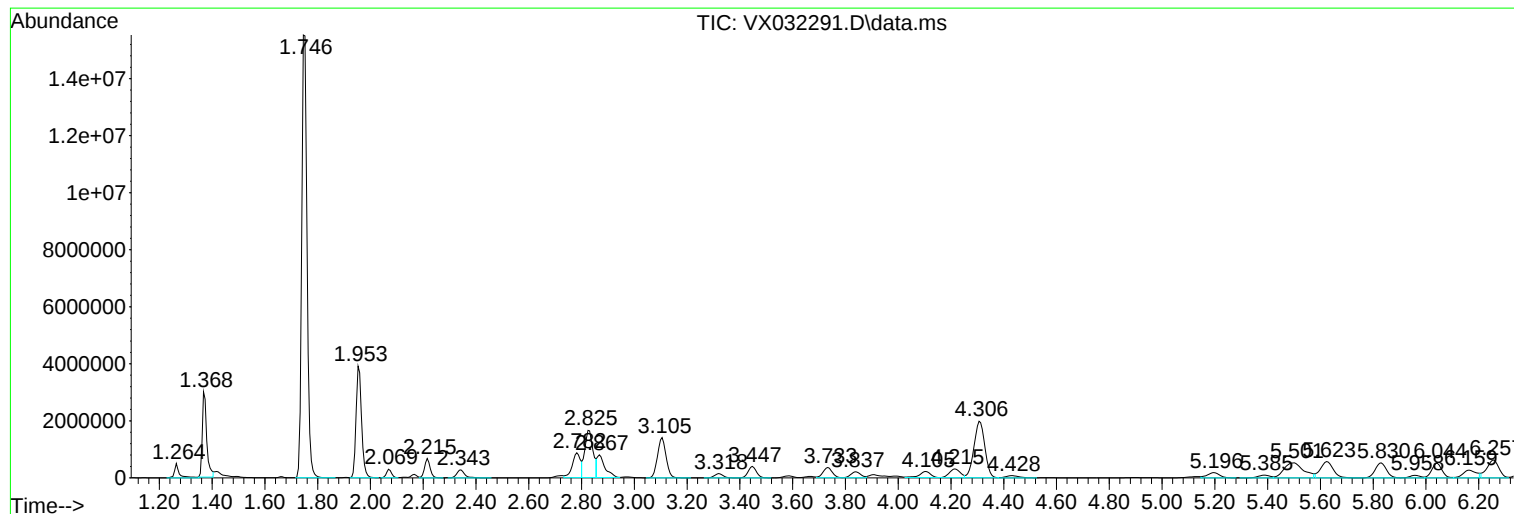
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.M
Quant Title : SW846 8260

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



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Instrument :
MSVOA_X
ClientSampleId :
MW-10

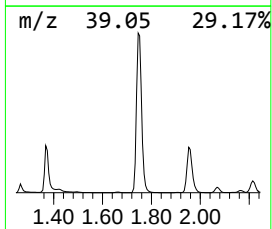
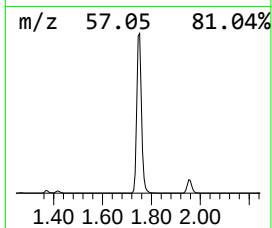
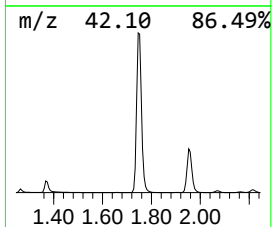
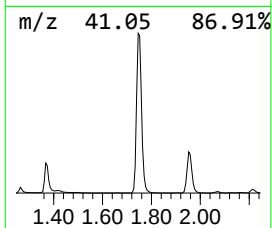
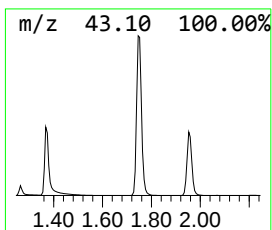
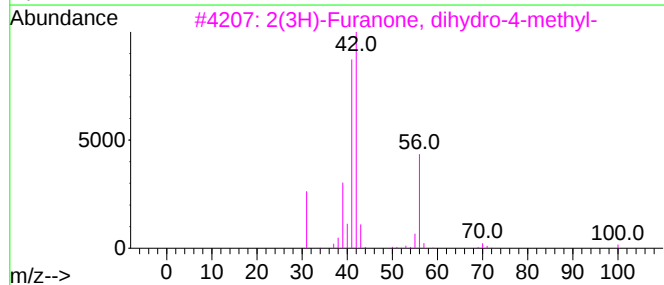
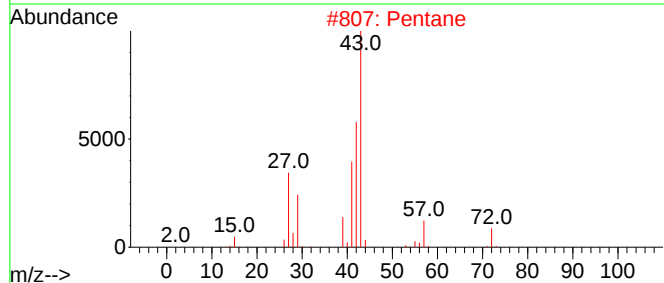
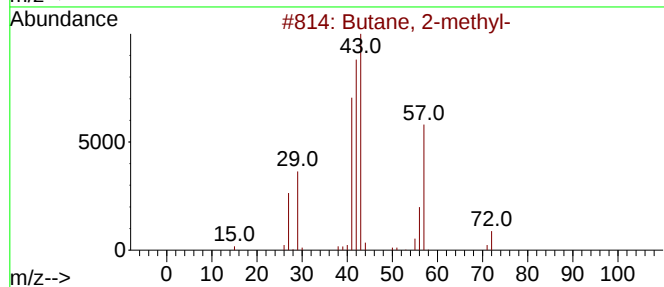
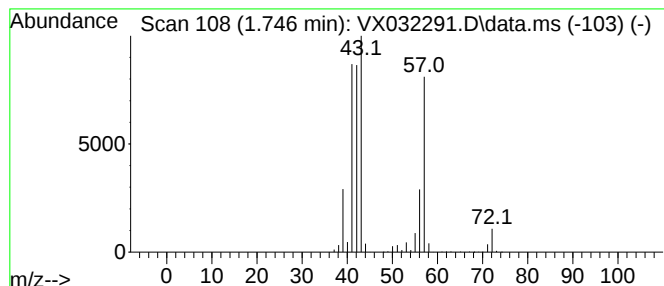
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.746	404.00 ug/l	21801800	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	91
2			Pentane	72	C5H12	000109-66-0	42
3			2(3H)-Furanone, dihydro-4-methyl-	100	C5H8O2	001679-49-8	36
4			3-Buten-1-ol	72	C4H8O	000627-27-0	28
5			Oxalic acid, butyl propyl ester	188	C9H16O4	1000309-25-6	17



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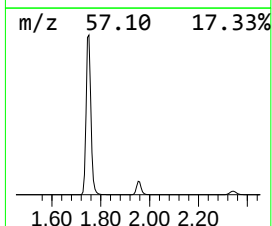
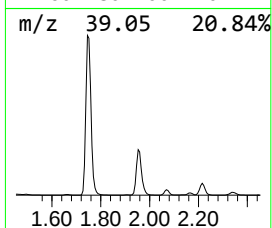
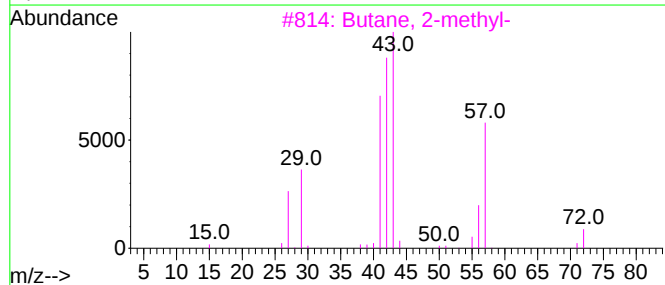
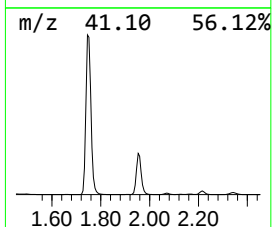
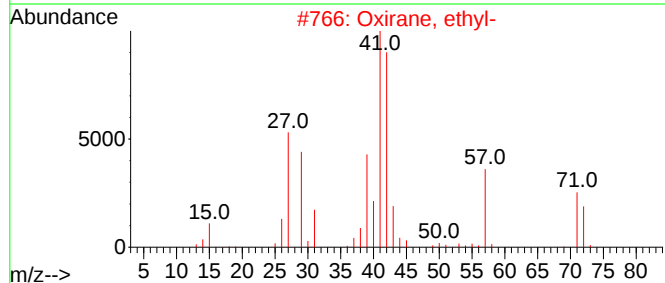
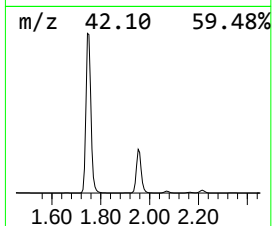
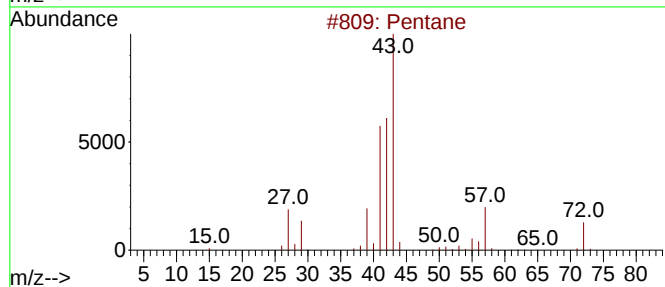
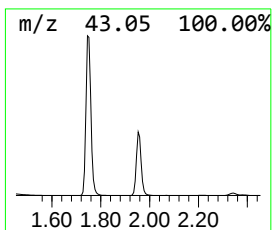
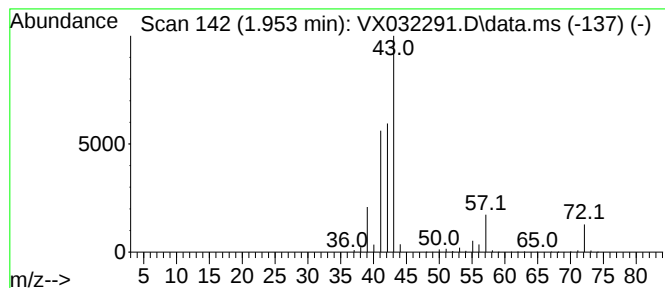
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Pentane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.953	103.66 ug/l	5594010	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane	72	C5H12	000109-66-0	91
2			Oxirane, ethyl-	72	C4H8O	000106-88-7	50
3			Butane, 2-methyl-	72	C5H12	000078-78-4	50
4			Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	38
5			Butanenitrile, 2-hydroxy-3-methyl-	99	C5H9NO	010021-64-4	9



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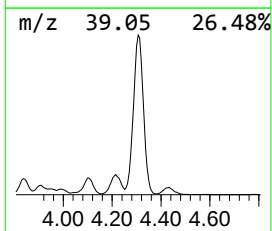
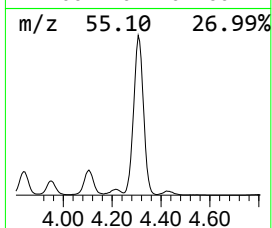
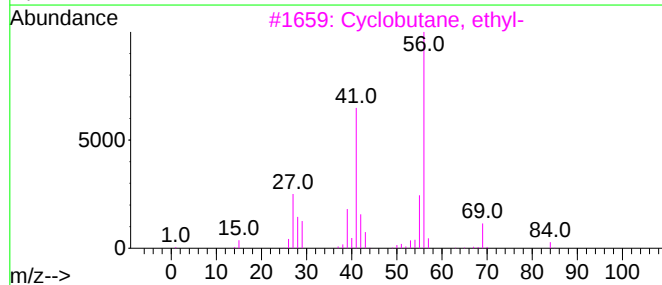
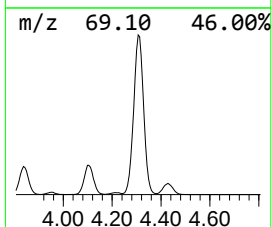
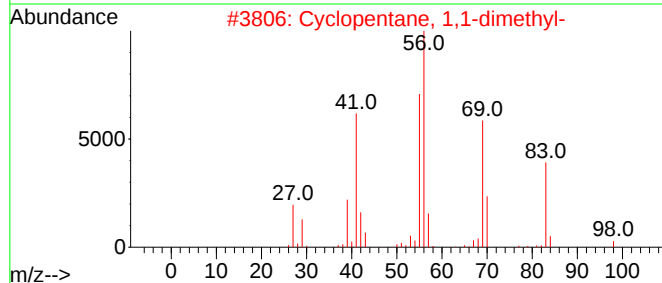
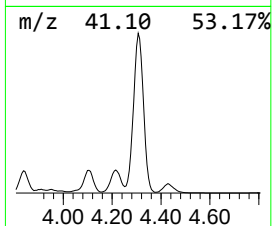
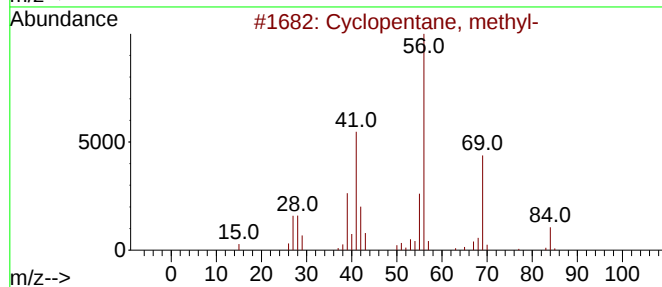
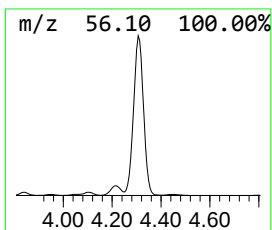
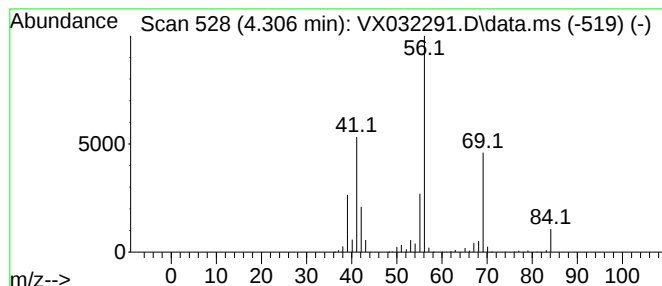
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.M
Quant Title : SW846 8260

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

Peak Number 3 Cyclopentane, methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	103.90 ug/l	5607000	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2			Cyclopentane, 1,1-dimethyl-	98	C7H14	001638-26-2	72
3			Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
4			1-Pentene, 2-methyl-	84	C6H12	000763-29-1	56
5			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	56



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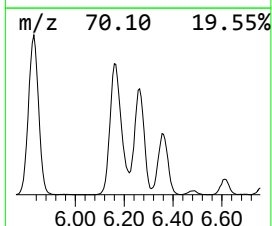
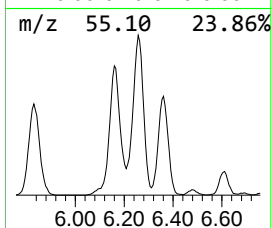
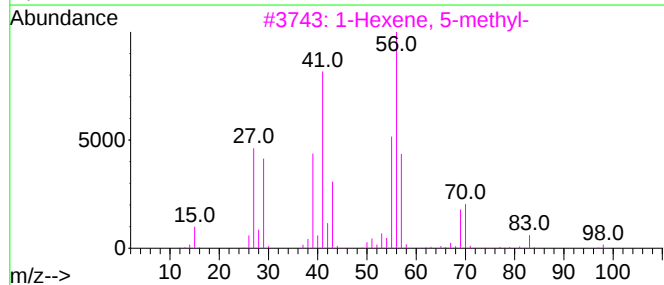
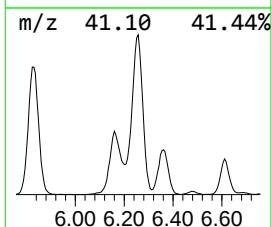
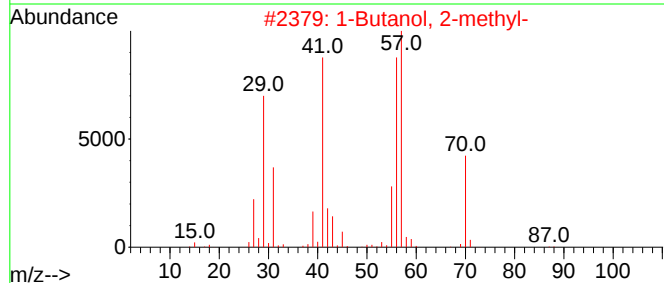
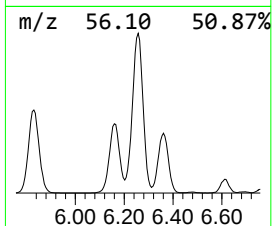
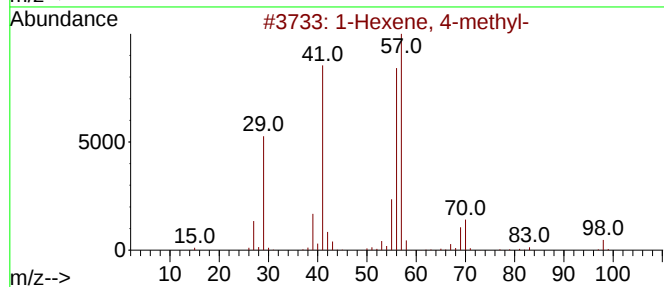
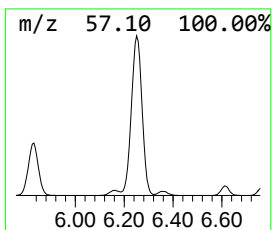
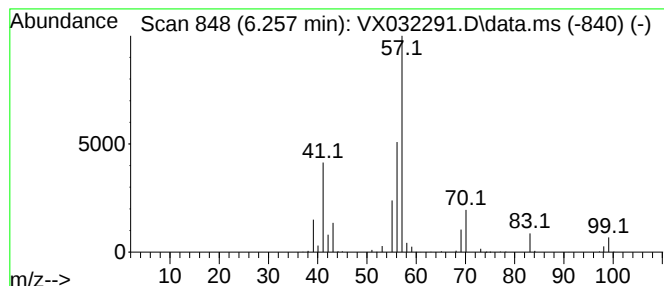
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Quant Title : SW846 8260

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

Peak Number 4 1-Hexene, 4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.257	164.53 ug/l	1957640	1,4-Difluorobenzene	6.763

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Hexene, 4-methyl-	98	C7H14	003769-23-1	50
2		1-Butanol, 2-methyl-	88	C5H12O	000137-32-6	50
3		1-Hexene, 5-methyl-	98	C7H14	003524-73-0	38
4		Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	38
5		2,2,7,7-Tetramethyloctane	170	C12H26	001071-31-4	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102122\
Data File : VX032291.D
Acq On : 21 Oct 2022 16:12
Operator : JC/MD
Sample : N5185-11
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-10

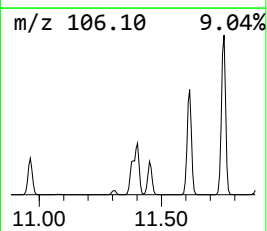
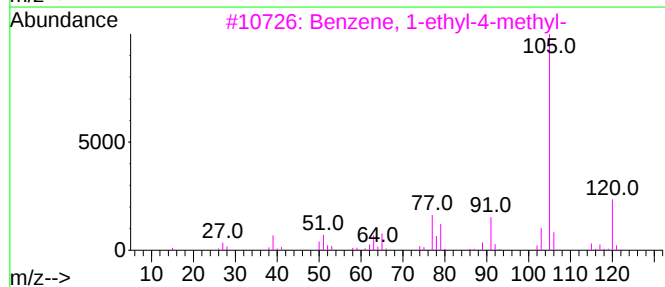
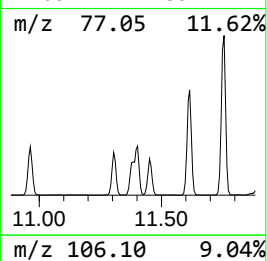
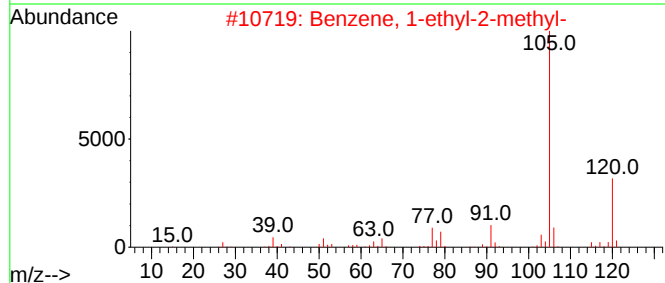
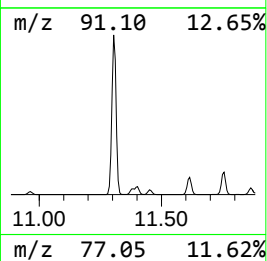
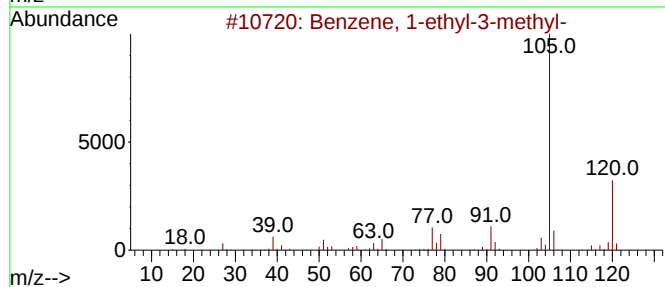
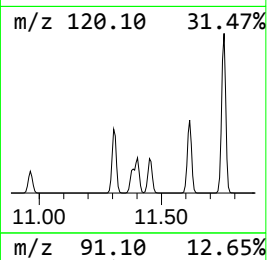
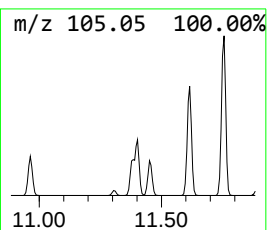
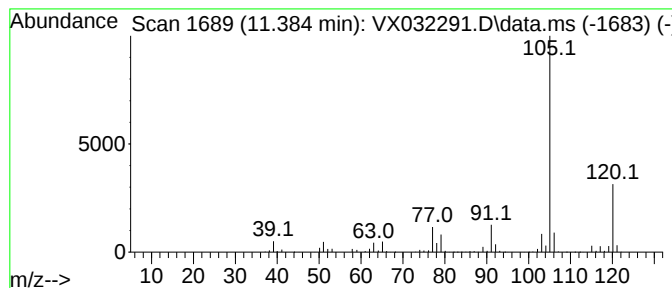
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Quant Title : SW846 8260

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

Peak Number 5 Benzene, 1-ethyl-3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.384	121.55 ug/l	1730690	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
2			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	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	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102122\
Data File : VX032291.D
Acq On : 21 Oct 2022 16:12
Operator : JC/MD
Sample : N5185-11
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-10

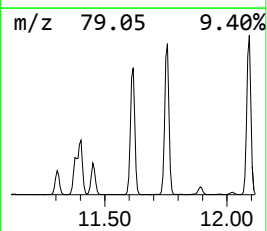
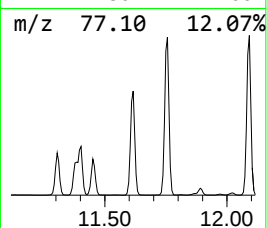
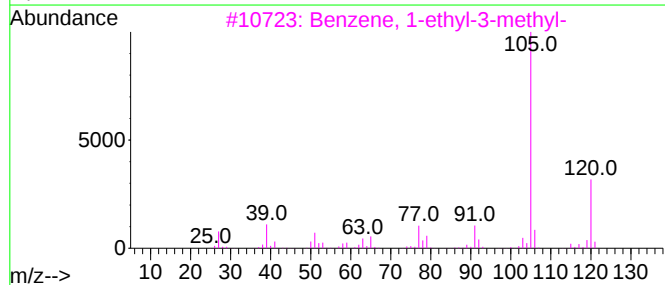
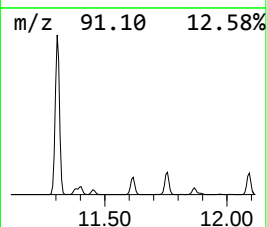
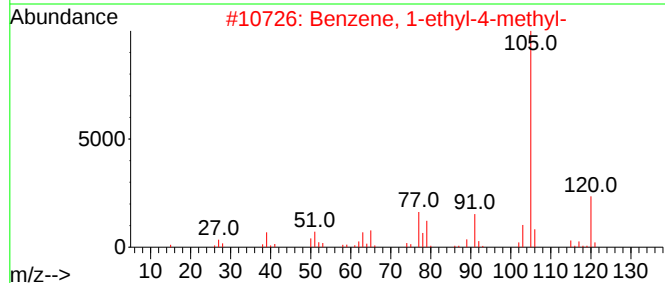
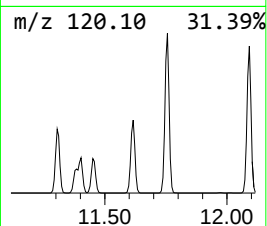
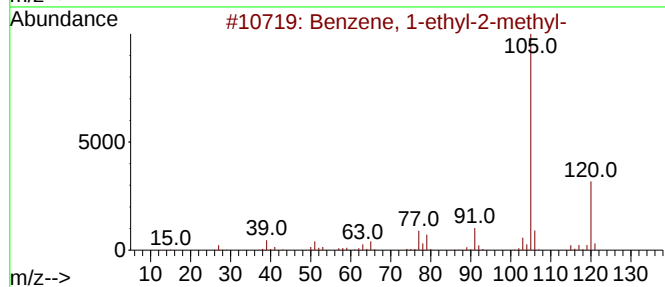
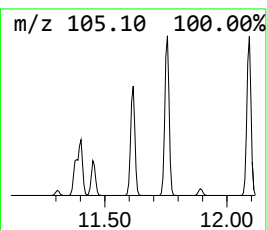
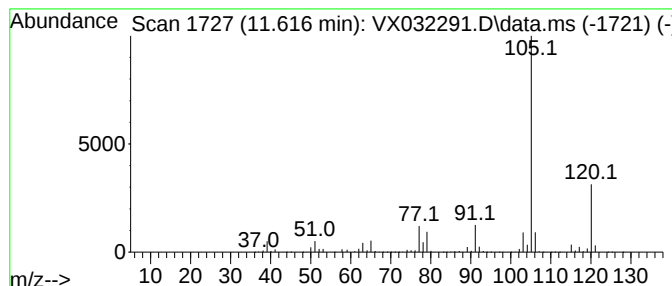
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, 1-ethyl-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	335.61 ug/l	4778590	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	94
3			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4			Mesitylene	120	C9H12	000108-67-8	91
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102122\
Data File : VX032291.D
Acq On : 21 Oct 2022 16:12
Operator : JC/MD
Sample : N5185-11
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-10

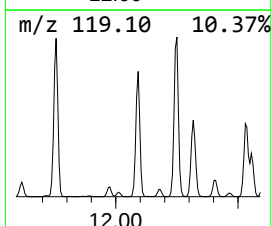
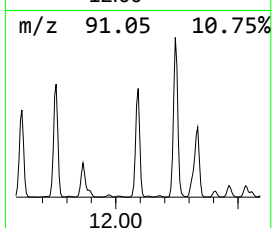
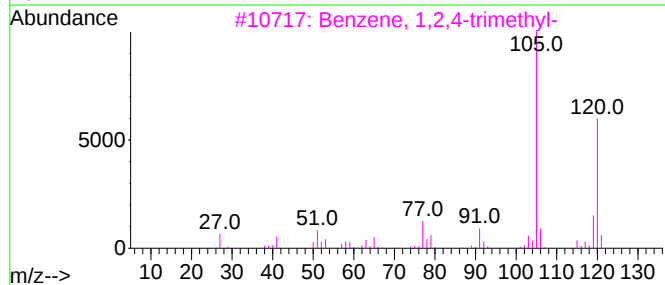
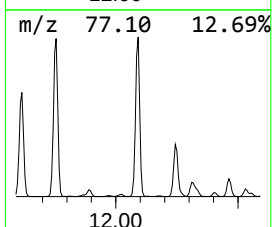
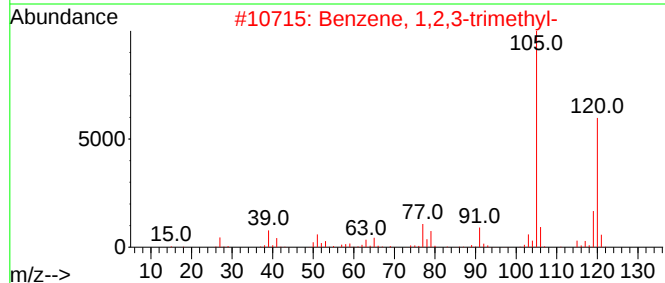
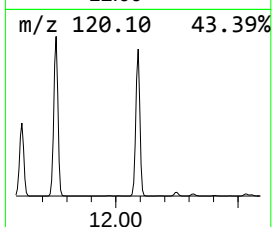
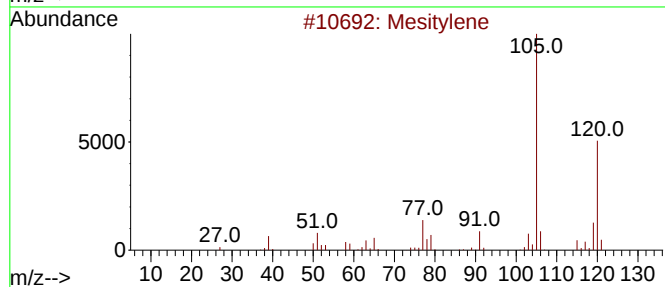
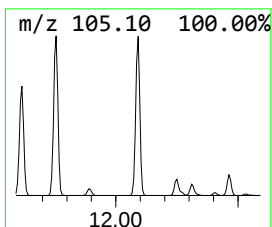
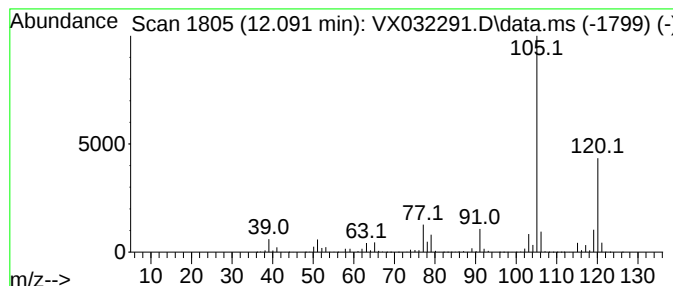
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.091	513.06 ug/l	7305220	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-2-methyl-	120	C9H12	000611-14-3	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102122\
Data File : VX032291.D
Acq On : 21 Oct 2022 16:12
Operator : JC/MD
Sample : N5185-11
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-10

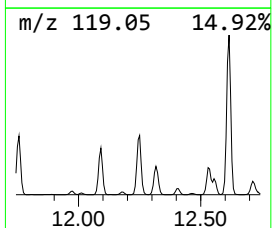
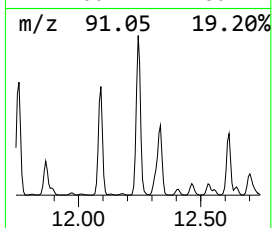
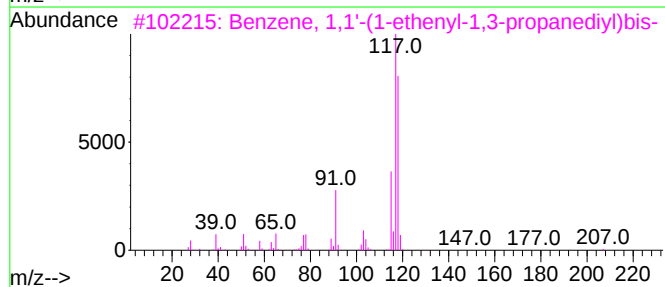
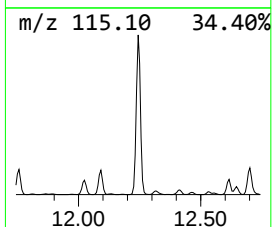
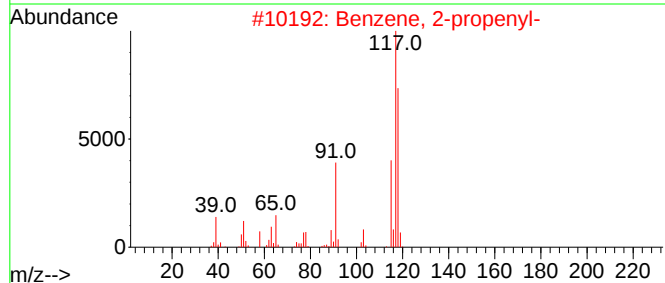
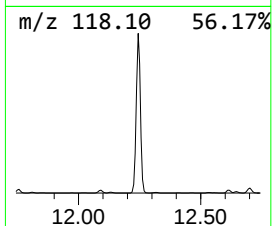
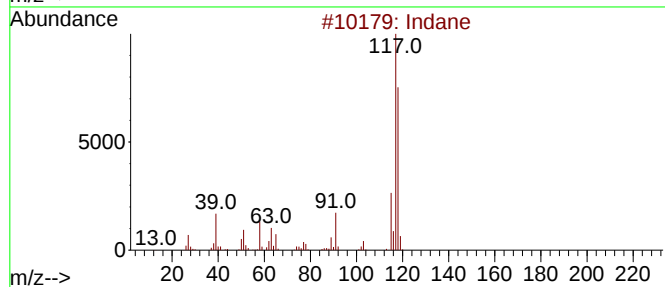
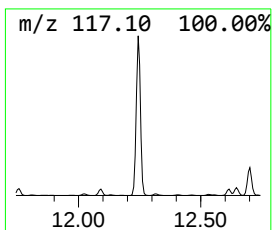
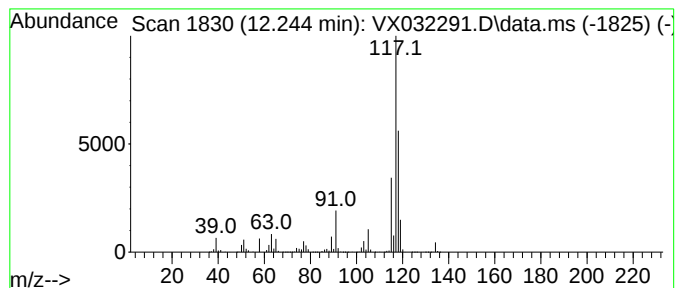
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Quant Title : SW846 8260

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

Peak Number 8 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	544.87 ug/l	7758230	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	76
2			Benzene, 2-propenyl-	118	C9H10	000300-57-2	76
3			Benzene, 1,1'-(1-ethenyl-1,3-pro...	222	C17H18	061141-97-7	72
4			Benzene, cyclopropyl-	118	C9H10	000873-49-4	70
5			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102122\
Data File : VX032291.D
Acq On : 21 Oct 2022 16:12
Operator : JC/MD
Sample : N5185-11
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-10

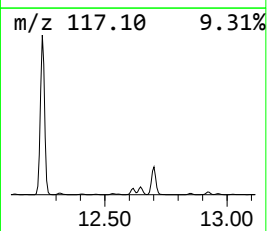
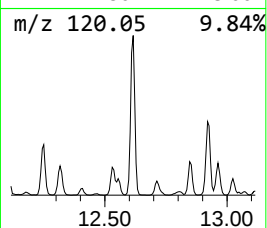
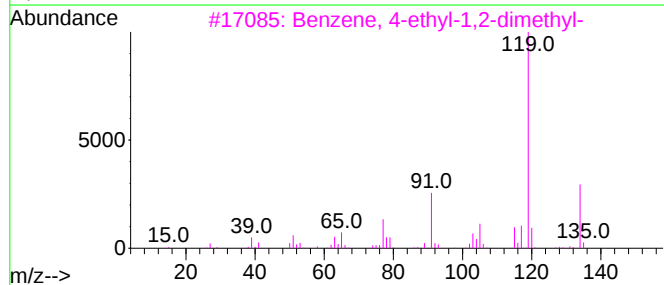
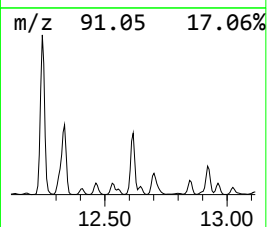
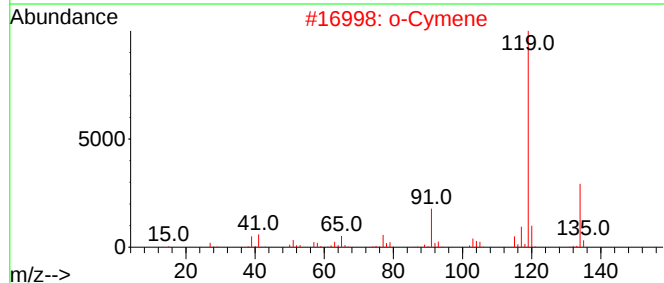
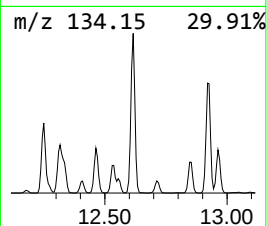
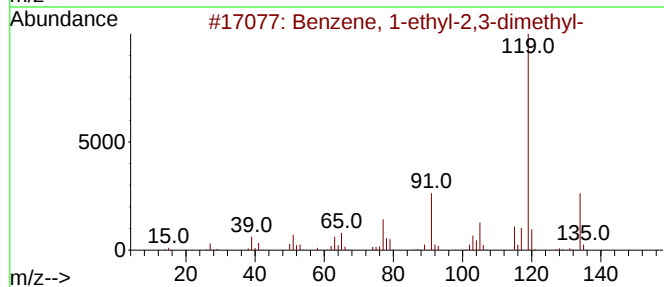
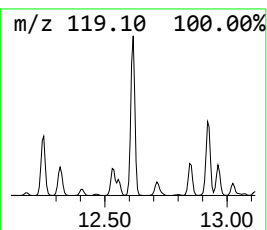
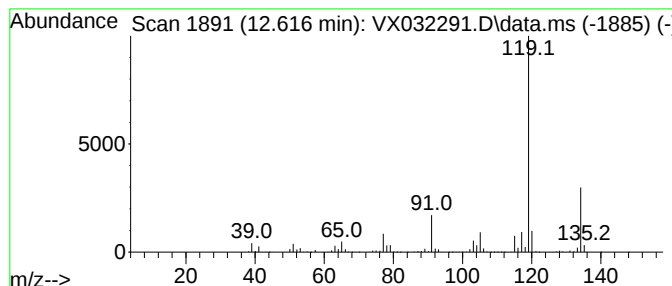
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, 1-ethyl-2,3-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.616	178.24 ug/l	2537920	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95
2			o-Cymene	134	C10H14	000527-84-4	95
3			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95
4			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	94
5			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102122\
Data File : VX032291.D
Acq On : 21 Oct 2022 16:12
Operator : JC/MD
Sample : N5185-11
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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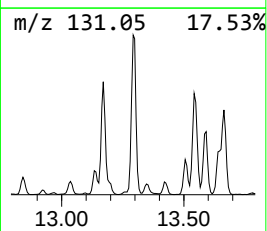
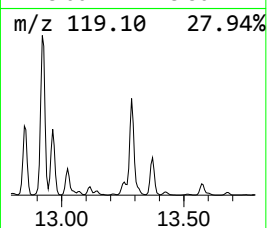
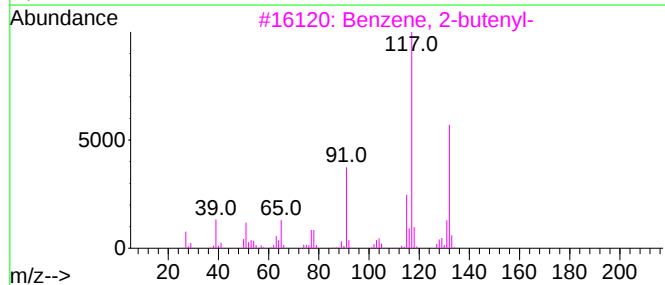
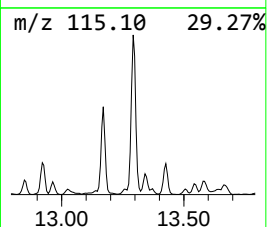
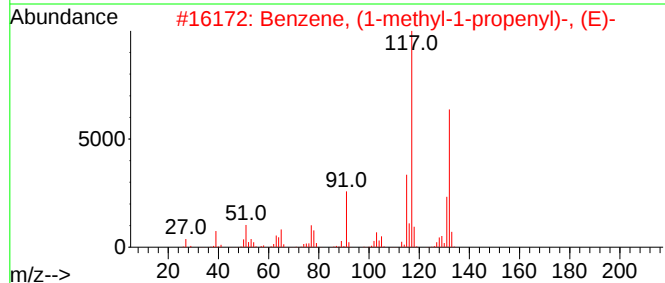
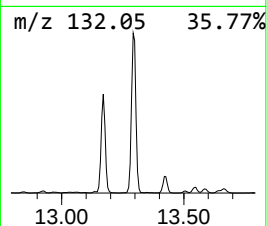
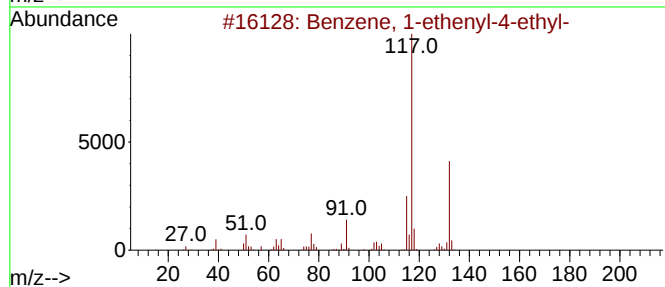
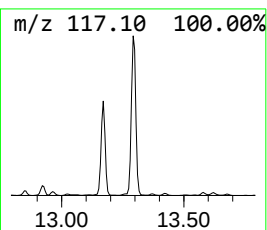
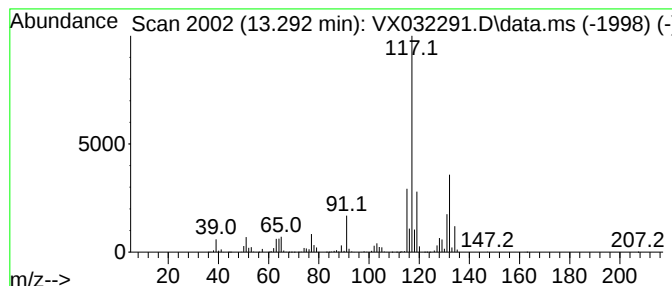
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.M
Quant Title : SW846 8260

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

Peak Number 10 Benzene, 1-ethenyl-4-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	179.54 ug/l	2556460	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	89
2			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	81
3			Benzene, 2-butenyl-	132	C10H12	001560-06-1	81
4			3-Phenylbut-1-ene	132	C10H12	000934-10-1	81
5			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102122\
Data File : VX032291.D
Acq On : 21 Oct 2022 16:12
Operator : JC/MD
Sample : N5185-11
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-10

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.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
Butane, 2-methyl-	1.746	404.0	ug/l	21801800	1	5.556	2698280	50.0
Pentane	1.953	103.7	ug/l	5594010	1	5.556	2698280	50.0
Cyclopentane, m...	4.306	103.9	ug/l	5607000	1	5.556	2698280	50.0
1-Hexene, 4-met...	6.257	164.5	ug/l	1957640	2	6.763	594931	50.0
Benzene, 1-ethy...	11.384	121.6	ug/l	1730690	4	12.024	711932	50.0
Benzene, 1-ethy...	11.616	335.6	ug/l	4778590	4	12.024	711932	50.0
Benzene, 1,2,3-...	12.091	513.1	ug/l	7305220	4	12.024	711932	50.0
Indane	12.244	544.9	ug/l	7758230	4	12.024	711932	50.0
Benzene, 1-ethy...	12.616	178.2	ug/l	2537920	4	12.024	711932	50.0
Benzene, 1-ethe...	13.292	179.5	ug/l	2556460	4	12.024	711932	50.0