

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112522\
 Data File : VX033074.D
 Acq On : 25 Nov 2022 17:37
 Operator : JC/MD
 Sample : N5742-10
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 DUP111822

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\82X112222W.M
 Title : SW846 8260

Signal : TIC: VX033074.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.374	41	47	53	rBV	711750	771290	2.03%	0.332%
2	1.752	104	109	126	rVB	3622779	4648594	12.21%	2.003%
3	1.959	138	143	156	rVB2	2000236	3013010	7.91%	1.298%
4	2.069	156	161	168	rVV	374855	542160	1.42%	0.234%
5	2.215	181	185	196	rVB	771217	1185888	3.11%	0.511%
6	2.782	258	278	281	rBV3	376558	1164766	3.06%	0.502%
7	2.831	281	286	289	rVV	1073741	2203662	5.79%	0.949%
8	2.867	289	292	308	rVB2	830185	1926511	5.06%	0.830%
9	3.105	321	331	349	rVB	833986	1883376	4.95%	0.811%
10	3.447	378	387	400	rBV	561278	1247753	3.28%	0.538%
11	3.672	416	424	428	rBV	161503	382567	1.00%	0.165%
12	3.733	428	434	443	rVB	396546	936423	2.46%	0.403%
13	3.837	443	451	457	rBV	246884	622894	1.64%	0.268%
14	4.105	485	495	505	rVB	282164	732690	1.92%	0.316%
15	4.312	518	529	540	rVB	2221264	6319873	16.60%	2.722%
16	5.196	664	674	689	rVB	308269	965823	2.54%	0.416%
17	5.477	710	720	730	rBV	1272108	4024525	10.57%	1.734%
18	5.623	739	744	765	rVB3	162747	598743	1.57%	0.258%
19	5.830	766	778	791	rBV5	189471	614944	1.62%	0.265%
20	6.044	804	813	823	rVB	881524	2251825	5.91%	0.970%
21	6.166	823	833	836	rBV	183108	501567	1.32%	0.216%
22	6.257	843	848	857	rVB2	234923	633634	1.66%	0.273%
23	6.361	857	865	876	rVB2	211413	599833	1.58%	0.258%
24	6.763	924	931	936	rBV	227521	580488	1.52%	0.250%
25	6.848	940	945	954	rVB4	237003	679546	1.78%	0.293%
26	7.178	990	999	1007	rBV2	196984	457486	1.20%	0.197%
27	7.385	1017	1033	1045	rBV3	1072319	2720607	7.15%	1.172%
28	8.147	1152	1158	1163	rVB	460514	782152	2.05%	0.337%
29	8.507	1210	1217	1226	rVB	422364	733270	1.93%	0.316%
30	8.647	1235	1240	1246	rVB	368232	620495	1.63%	0.267%
31	8.720	1246	1252	1258	rBV	1511354	2275892	5.98%	0.980%
32	8.958	1287	1291	1300	rVB	312572	533066	1.40%	0.230%
33	9.049	1300	1306	1311	rBV	287090	453829	1.19%	0.196%
34	10.055	1461	1471	1476	rBV	487049	700626	1.84%	0.302%
35	10.201	1489	1495	1500	rVB	13811899	18680381	49.06%	8.047%
36	10.311	1506	1513	1518	rBV	23964916	38072916	100.00%	16.401%

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37	10.646	1562	1568	1578	rVB	8227537	10363652	27.22%	4.464%
38	10.963	1613	1620	1627	rBV	1257319	1561003	4.10%	0.672%
39	11.079	1635	1639	1644	rVB	323907	412246	1.08%	0.178%
40	11.305	1668	1676	1682	rVB	3318574	3957332	10.39%	1.705%
41	11.384	1683	1689	1696	rVV	8708075	17075687	44.85%	7.356%
42	11.457	1696	1701	1707	rVB	4430013	5622248	14.77%	2.422%
43	11.616	1721	1727	1737	rBV	5853175	7161071	18.81%	3.085%
44	11.762	1745	1751	1755	rVB	20352103	26420133	69.39%	11.381%
45	12.024	1789	1794	1798	rVV2	594428	820372	2.15%	0.353%
46	12.091	1798	1805	1810	rVB	6722363	8093590	21.26%	3.487%
47	12.244	1824	1830	1838	rBV2	6156176	8532749	22.41%	3.676%
48	12.317	1838	1842	1852	rVB3	1429203	2103682	5.53%	0.906%
49	12.408	1852	1857	1862	rBV2	384490	538687	1.41%	0.232%
50	12.463	1862	1866	1872	rVB	516400	594614	1.56%	0.256%
51	12.530	1872	1877	1879	rBV	1143072	1389037	3.65%	0.598%
52	12.555	1879	1881	1886	rVB	990460	1082840	2.84%	0.466%
53	12.616	1886	1891	1894	rBV	1971121	2313644	6.08%	0.997%
54	12.646	1894	1896	1900	rVB	573446	579754	1.52%	0.250%
55	12.701	1900	1905	1913	rBV2	1666721	2231427	5.86%	0.961%
56	12.847	1924	1929	1934	rVB	579506	703342	1.85%	0.303%
57	12.920	1934	1941	1945	rBV	1159701	1449717	3.81%	0.625%
58	12.963	1945	1948	1954	rVB	1770377	1974245	5.19%	0.850%
59	13.170	1978	1982	1987	rVB	1483372	1685530	4.43%	0.726%
60	13.292	1997	2002	2007	rVB2	3114315	3995262	10.49%	1.721%
61	13.426	2019	2024	2032	rVB	813069	1078932	2.83%	0.465%
62	13.585	2046	2050	2056	rVB3	278235	437184	1.15%	0.188%
63	13.664	2061	2063	2069	rVB2	327327	430913	1.13%	0.186%
64	13.780	2074	2082	2090	rBV	5856343	7500672	19.70%	3.231%
65	14.225	2149	2155	2164	rVB3	251816	529720	1.39%	0.228%
66	14.640	2218	2223	2233	rVB	2693762	3345887	8.79%	1.441%
67	14.780	2241	2246	2255	rBV	1725939	2185471	5.74%	0.941%
68	15.475	2354	2360	2365	rBV	241429	383230	1.01%	0.165%
69	15.615	2373	2383	2386	rBV	334826	519354	1.36%	0.224%

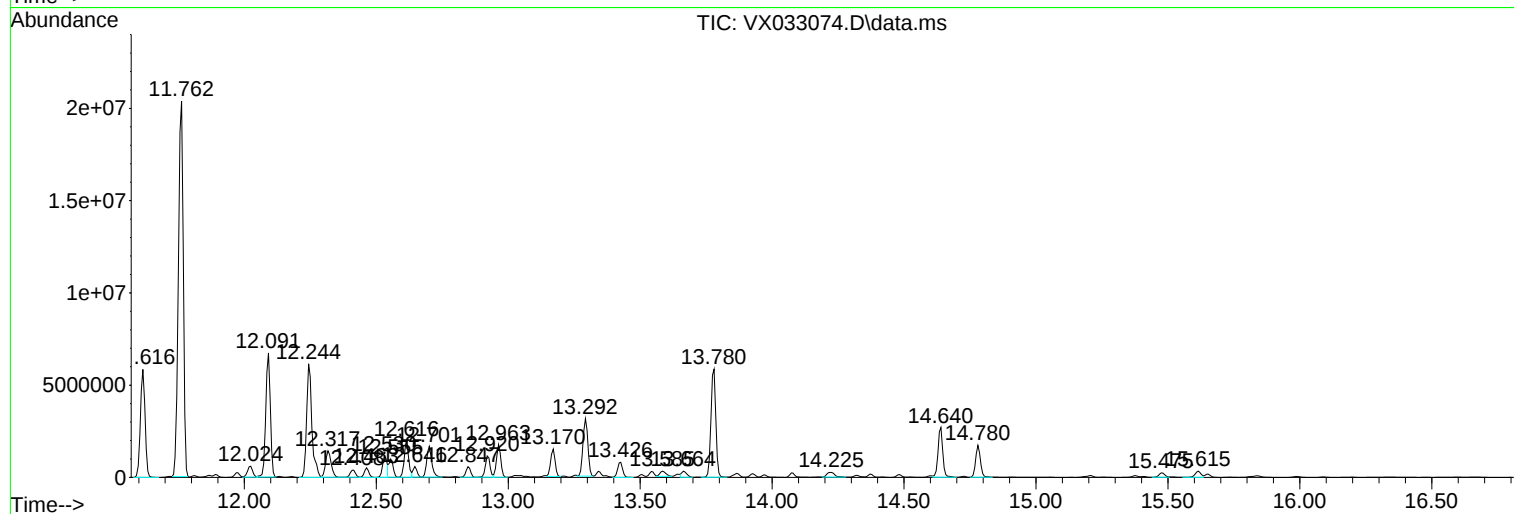
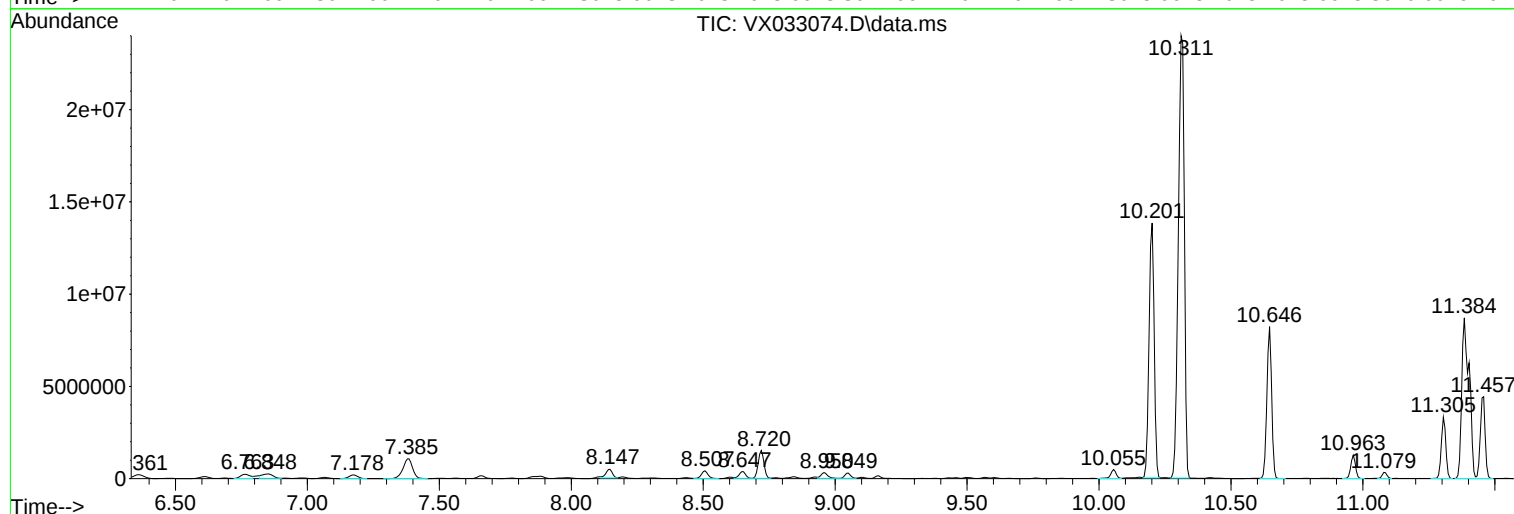
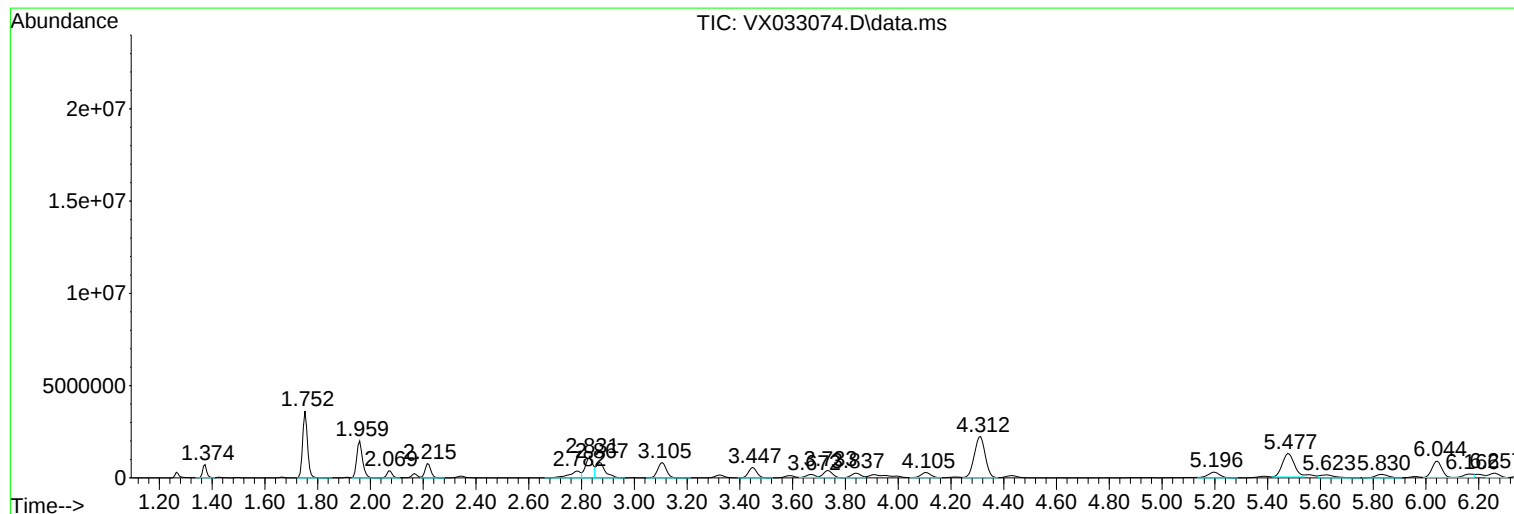
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Instrument :
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ClientSampleId :
DUP111822

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

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



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Sample : N5742-10
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DUP111822

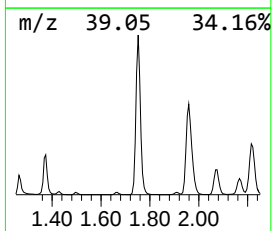
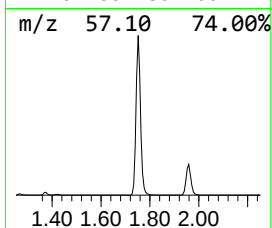
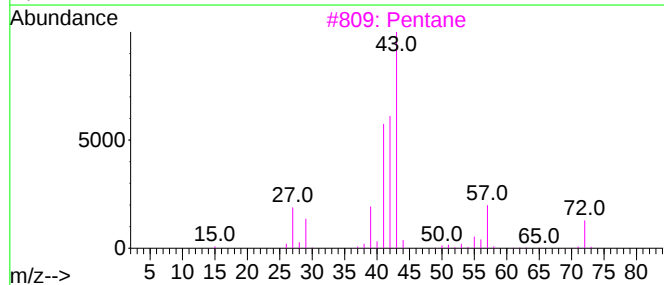
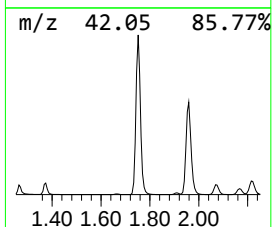
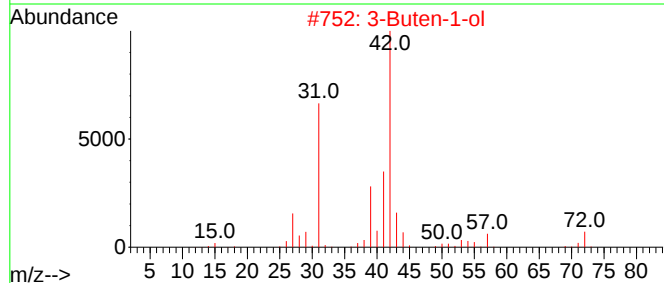
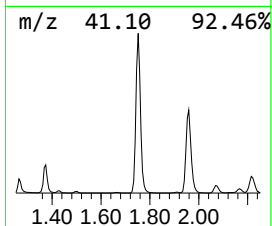
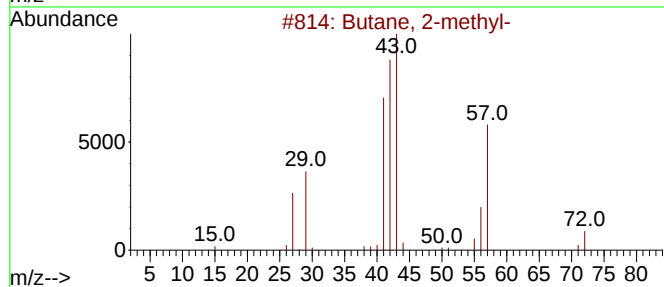
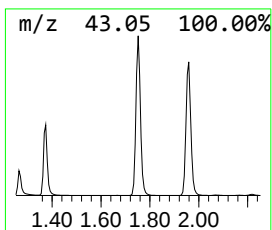
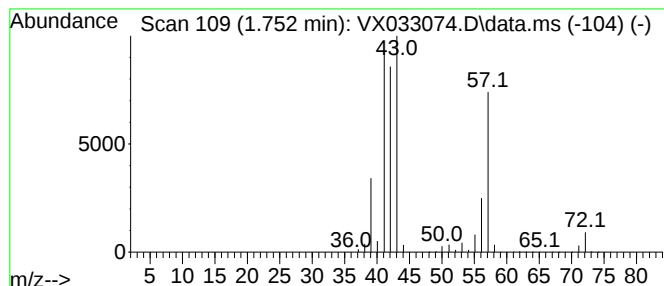
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.752	388.20 ug/l	4648590	Pentafluorobenzene	5.556

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	43
3			Pentane	72	C5H12	000109-66-0	28
4			Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	10
5			Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	10



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MSVOA_X
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DUP111822

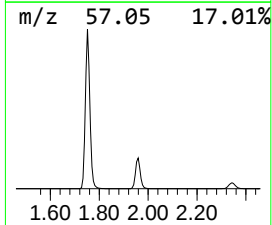
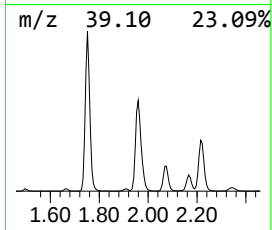
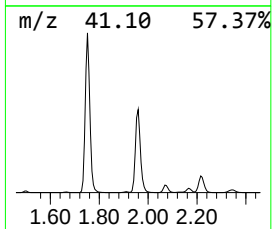
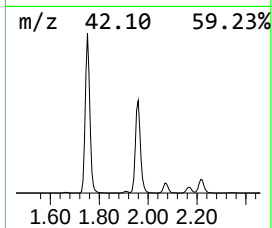
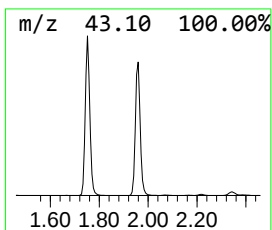
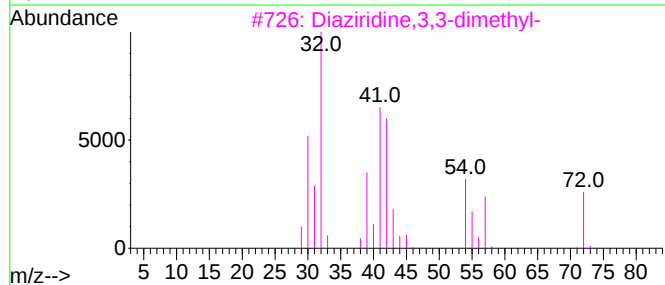
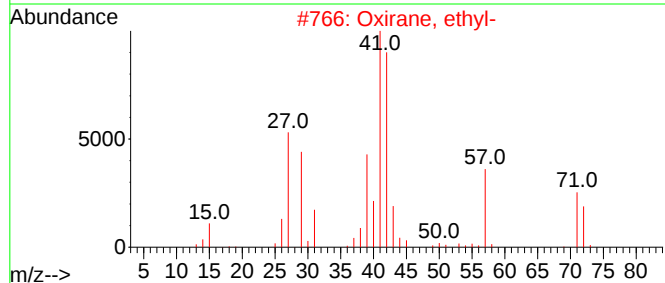
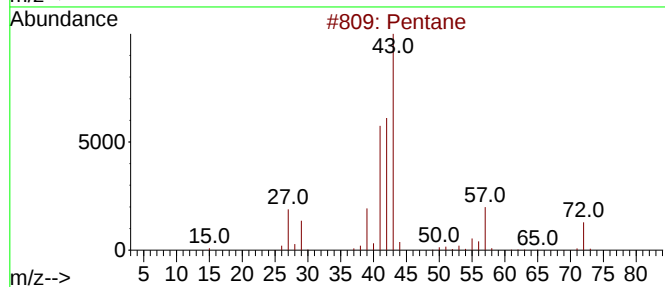
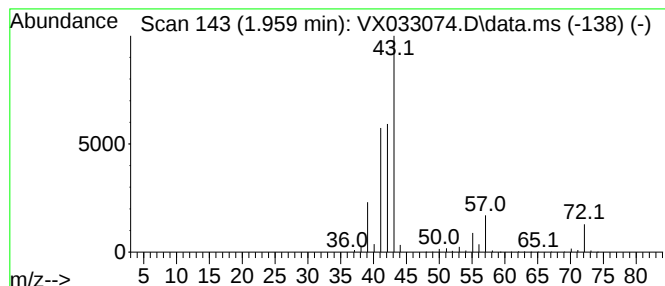
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

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

Peak Number 2 Pentane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.959	251.61 ug/l	3013010	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			Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	38
4			Butanal, 2,2-dimethyl-	100	C6H12O	002094-75-9	12
5			2-Propanone, hydrazone	72	C3H8N2	005281-20-9	10



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ClientSampleId :
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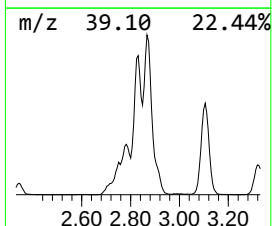
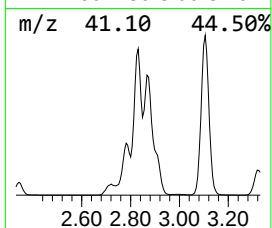
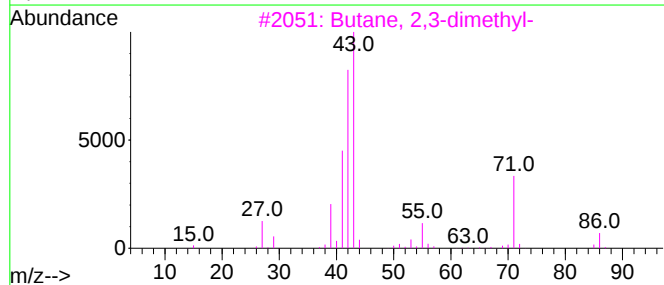
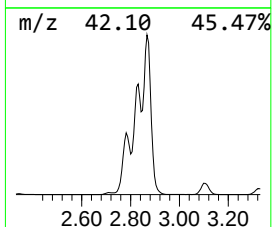
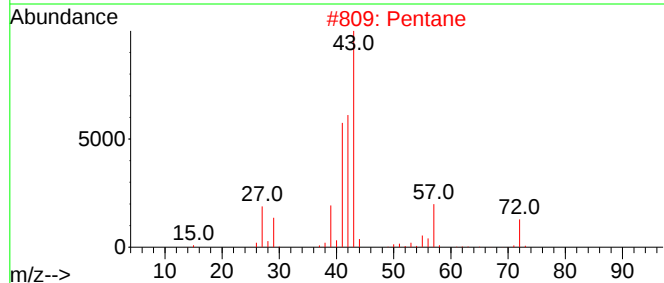
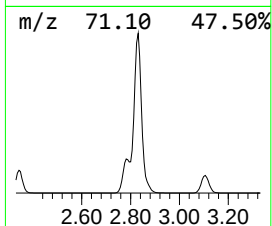
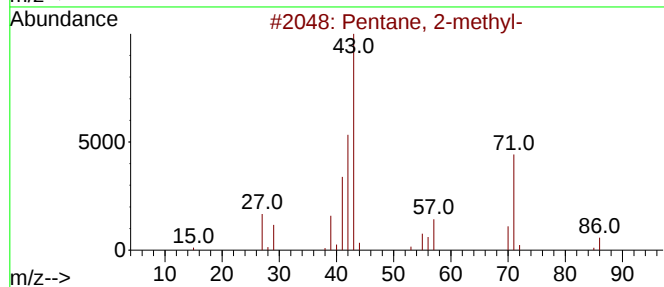
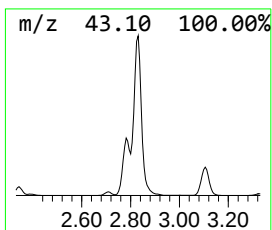
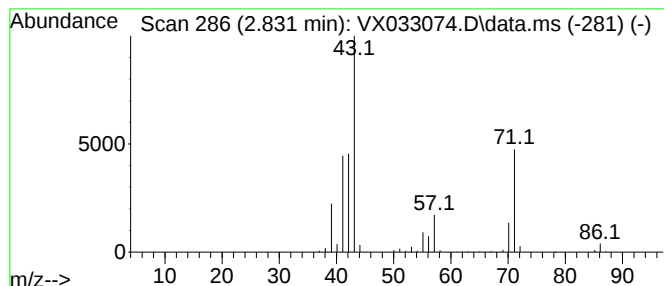
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Quant Title : SW846 8260

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

Peak Number 3 Pentane, 2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.831	184.02 ug/l	2203660	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2-methyl-	86	C6H14	000107-83-5	91
2			Pentane	72	C5H12	000109-66-0	49
3			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	38
4			Pentane, 3,3-dimethyl-	100	C7H16	000562-49-2	37
5			1-Butanol, 2,3-dimethyl-	102	C6H14O	019550-30-2	36



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Instrument :
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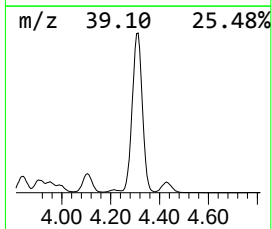
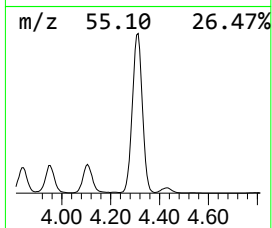
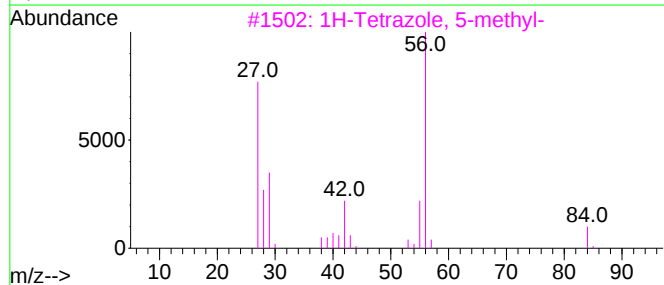
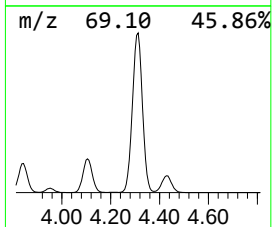
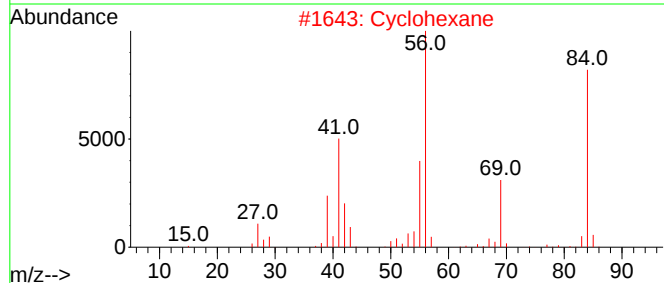
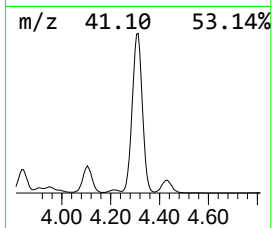
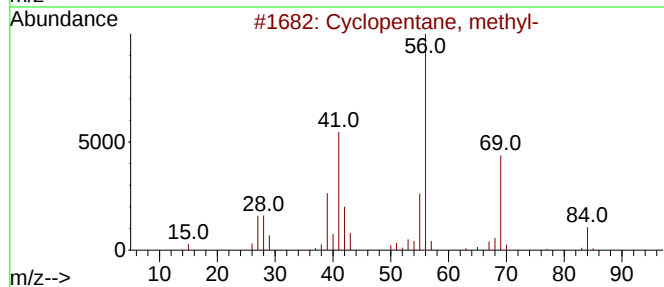
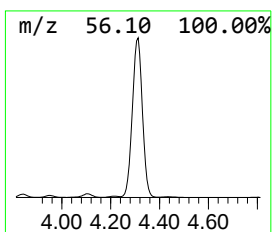
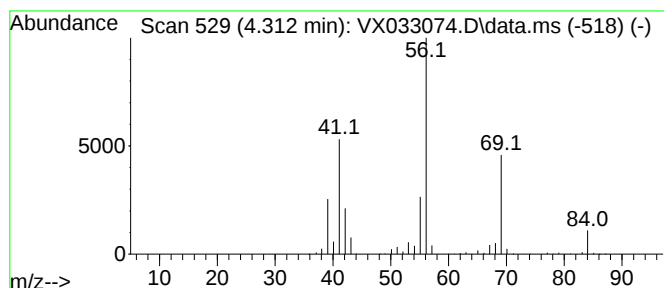
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

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

Peak Number 4 Cyclopentane, methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.312	527.76 ug/l	6319870	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	80
3			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
4			Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
5			Cyclopentane, 1,1-dimethyl-	98	C7H14	001638-26-2	56



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112522\
Data File : VX033074.D
Acq On : 25 Nov 2022 17:37
Operator : JC/MD
Sample : N5742-10
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DUP111822

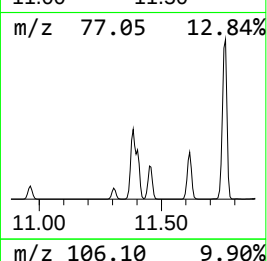
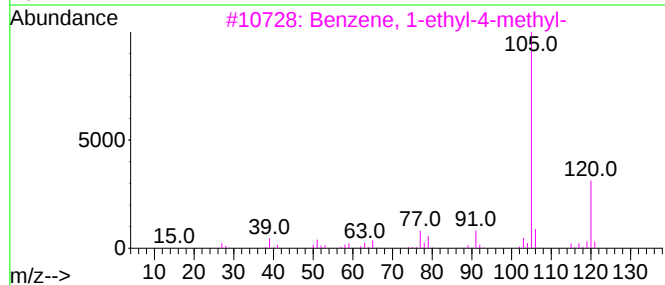
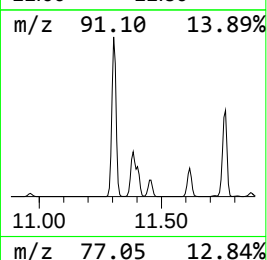
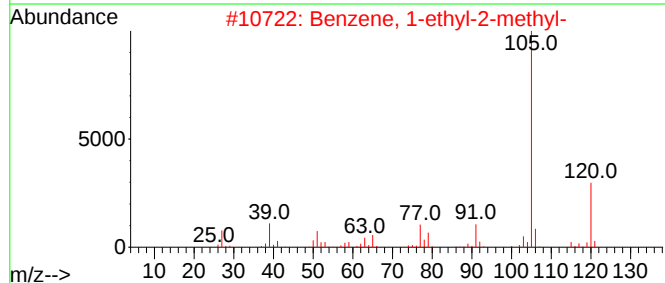
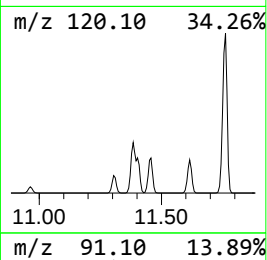
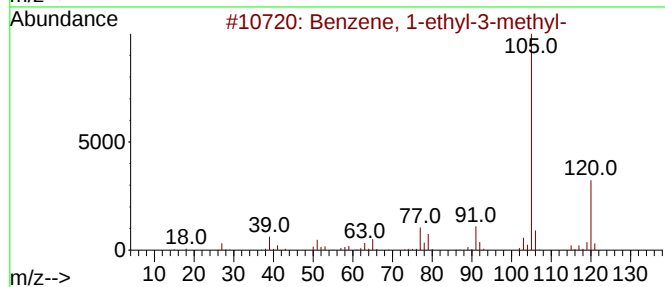
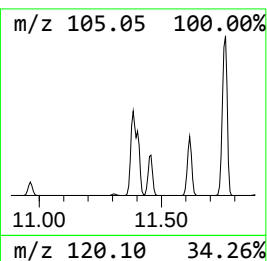
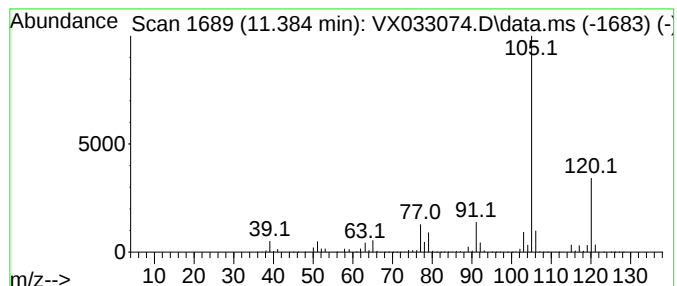
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.384	1040.73 ug/l	17075700	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	97
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, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112522\
Data File : VX033074.D
Acq On : 25 Nov 2022 17:37
Operator : JC/MD
Sample : N5742-10
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DUP111822

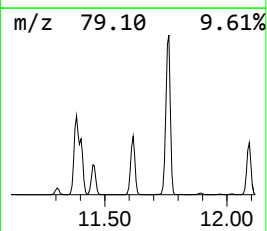
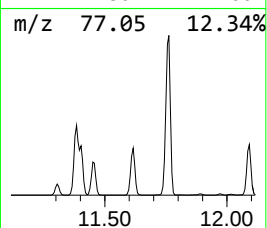
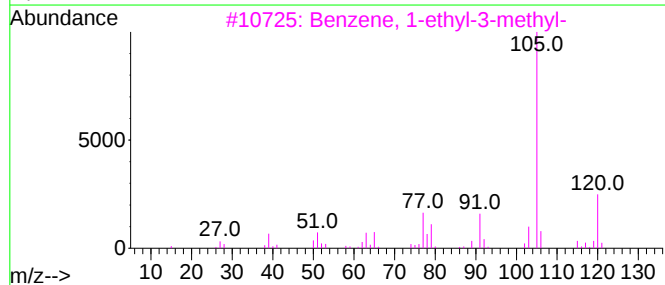
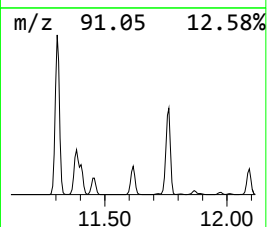
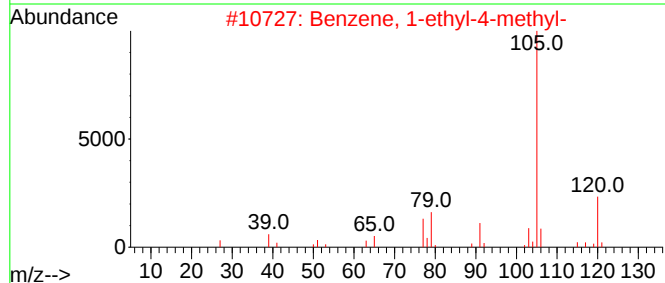
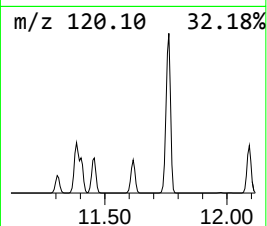
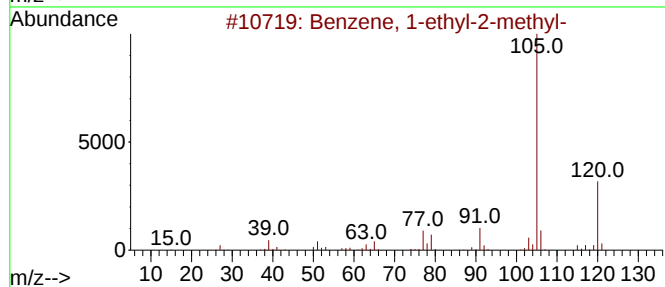
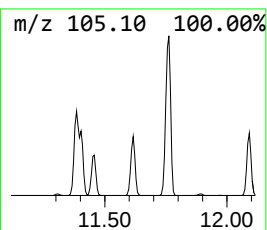
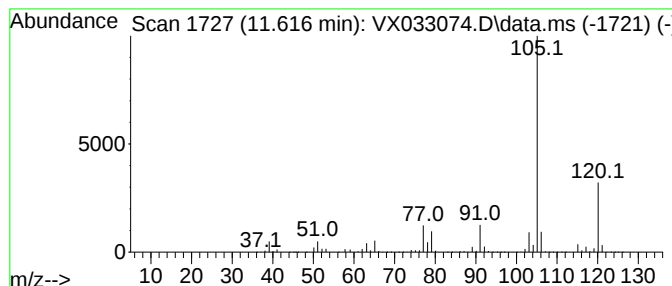
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, 1-ethyl-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	436.45 ug/l	7161070	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			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\VX112522\
Data File : VX033074.D
Acq On : 25 Nov 2022 17:37
Operator : JC/MD
Sample : N5742-10
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DUP111822

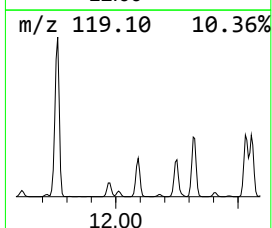
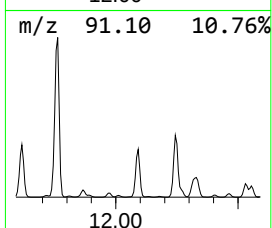
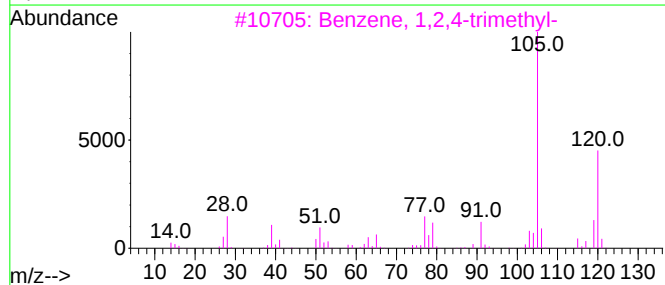
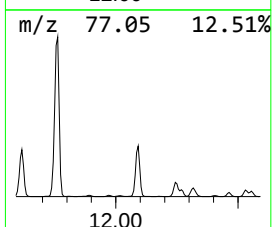
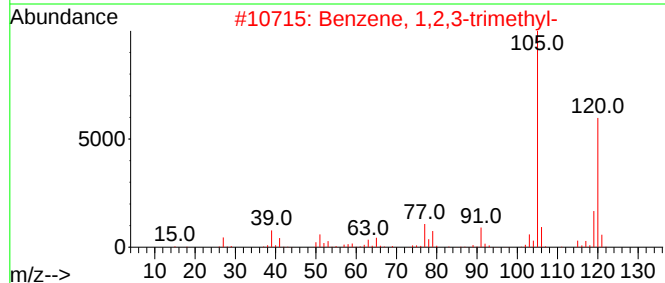
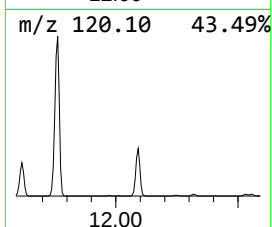
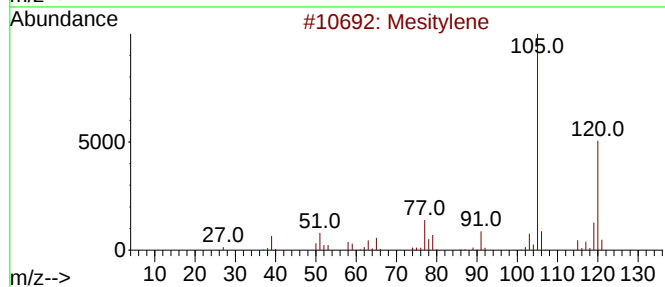
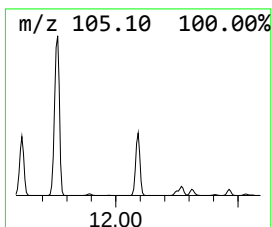
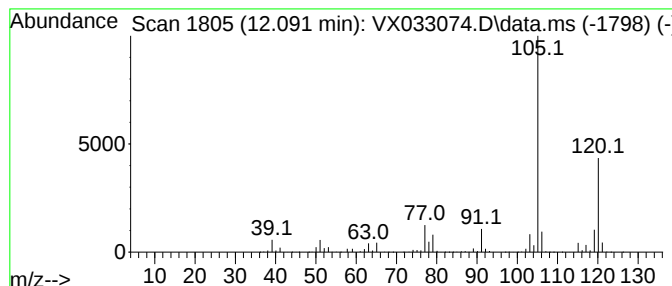
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1,2,3-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.091	493.29 ug/l	8093590	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	94
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\VX112522\
Data File : VX033074.D
Acq On : 25 Nov 2022 17:37
Operator : JC/MD
Sample : N5742-10
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DUP111822

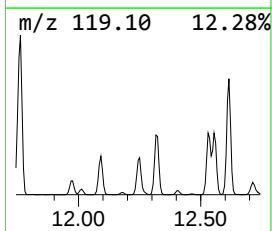
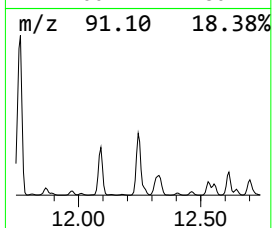
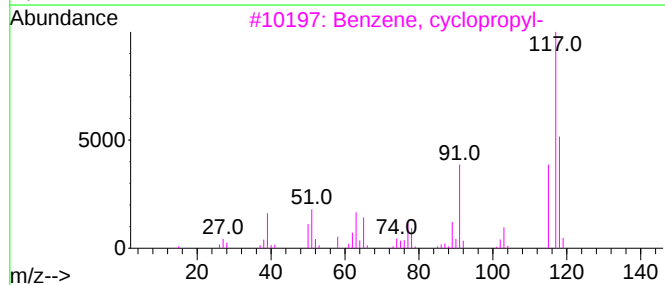
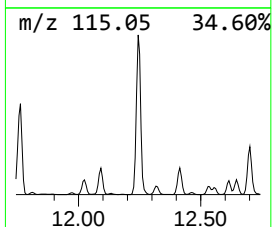
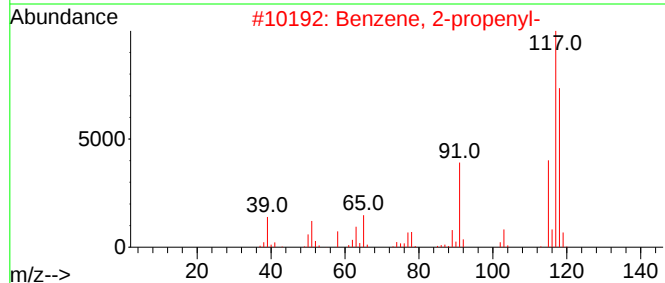
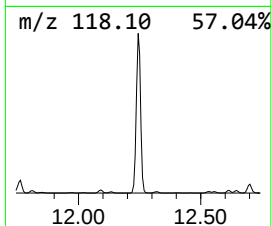
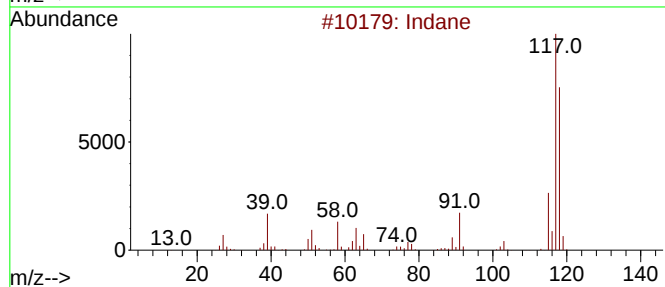
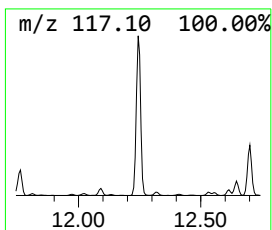
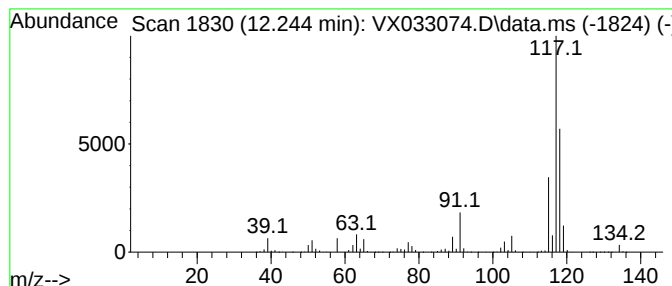
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Quant Title : SW846 8260

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

Peak Number 8 Indane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	520.05 ug/l	8532750	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	81
2			Benzene, 2-propenyl-	118	C9H10	000300-57-2	81
3			Benzene, cyclopropyl-	118	C9H10	000873-49-4	81
4			Delatcyclene	118	C9H10	007785-10-6	64
5			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	60



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112522\
Data File : VX033074.D
Acq On : 25 Nov 2022 17:37
Operator : JC/MD
Sample : N5742-10
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DUP111822

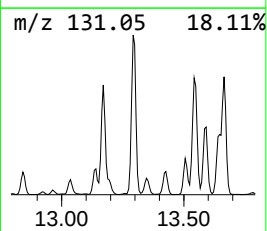
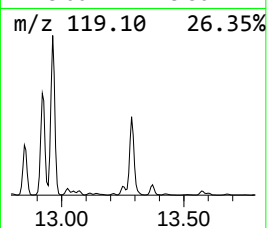
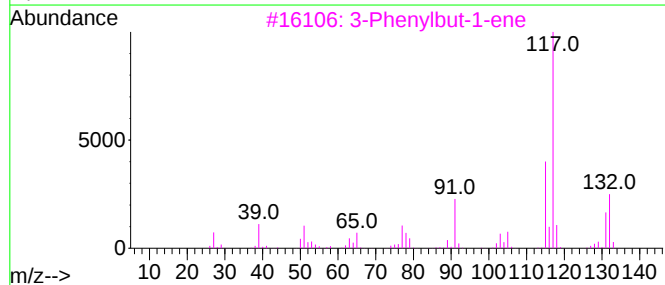
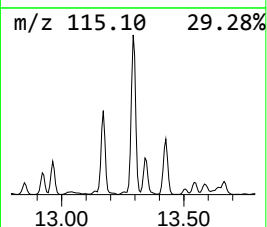
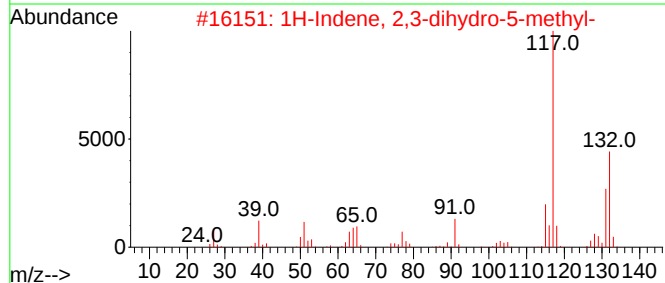
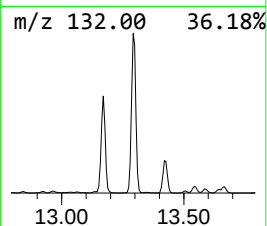
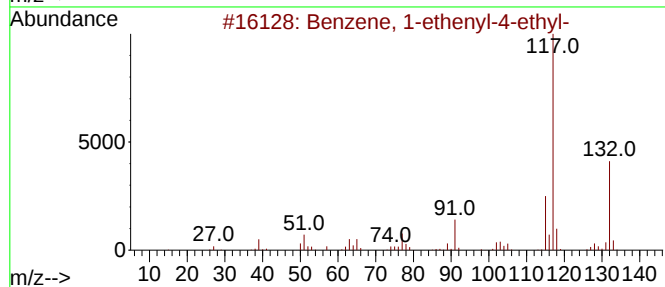
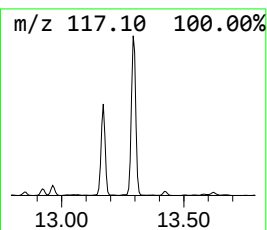
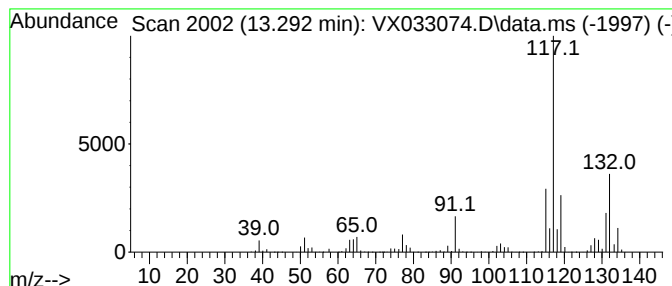
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, 1-ethenyl-4-ethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	243.50 ug/l	3995260	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	94
2			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	89
3			3-Phenylbut-1-ene	132	C10H12	000934-10-1	87
4			Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	83
5			Benzene, 2-butenyl-	132	C10H12	001560-06-1	81



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112522\
Data File : VX033074.D
Acq On : 25 Nov 2022 17:37
Operator : JC/MD
Sample : N5742-10
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DUP111822

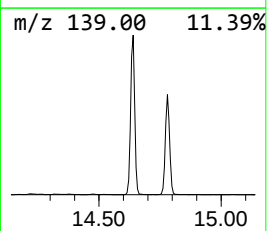
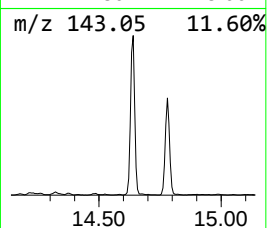
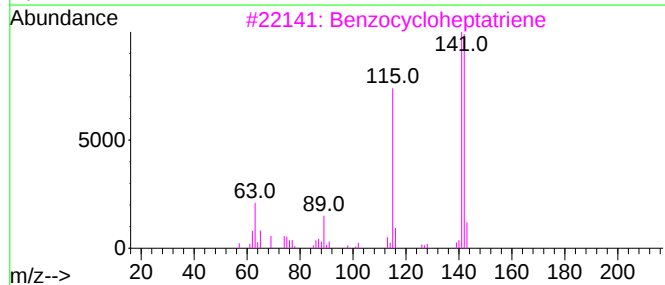
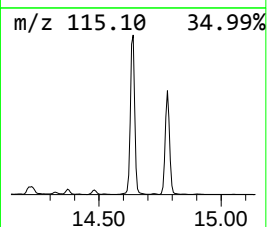
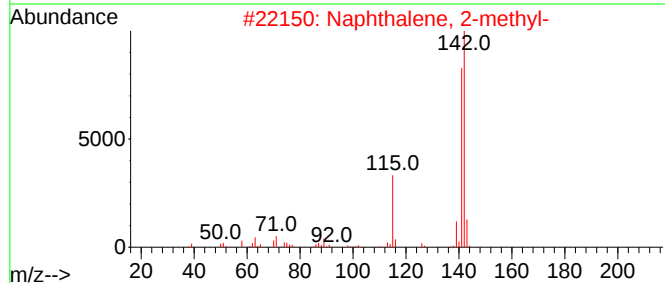
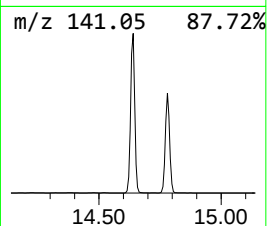
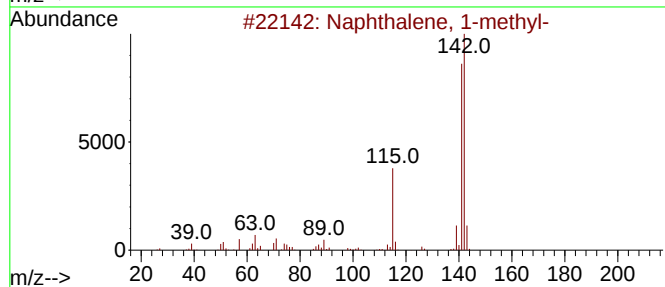
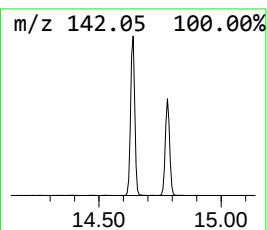
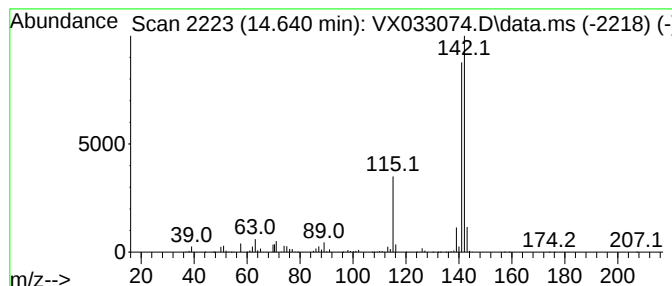
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Quant Title : SW846 8260

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

Peak Number 10 Benzocycloheptatriene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.640	203.93 ug/l	3345890	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			Benzocycloheptatriene	142	C11H10	000264-09-5	91
4			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
5			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112522\
Data File : VX033074.D
Acq On : 25 Nov 2022 17:37
Operator : JC/MD
Sample : N5742-10
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DUP111822

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.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	1.959	251.6	ug/l	3013010	1	5.556	598743	50.0
Pentane, 2-methyl-	2.831	184.0	ug/l	2203660	1	5.556	598743	50.0
Cyclopentane, m...	4.312	527.8	ug/l	6319870	1	5.556	598743	50.0
Benzene, 1-ethy...	11.384	1040.7	ug/l	17075700	4	12.024	820372	50.0
Benzene, 1-ethy...	11.616	436.4	ug/l	7161070	4	12.024	820372	50.0
Benzene, 1,2,3-...	12.091	493.3	ug/l	8093590	4	12.024	820372	50.0
Indane	12.244	520.0	ug/l	8532750	4	12.024	820372	50.0
Benzene, 1-ethe...	13.292	243.5	ug/l	3995260	4	12.024	820372	50.0
Benzocyclohepta...	14.640	203.9	ug/l	3345890	4	12.024	820372	50.0