

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX053023\
 Data File : VX035906.D
 Acq On : 30 May 2023 15:14
 Operator : JC/MD
 Sample : 02902-01
 Misc : 1.15g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 FMC-0096

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\82X052623W.M
 Title : SW846 8260

Signal : TIC: VX035906.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.422	209	219	263	rBV	2422182	11613999	46.94%	8.609%
2	5.111	643	660	681	rVB2	99420	373943	1.51%	0.277%
3	5.391	695	706	711	rBV	95637	292063	1.18%	0.217%
4	5.489	711	722	735	rVV2	1186338	4297089	17.37%	3.185%
5	5.611	735	742	763	rVV4	610137	2317019	9.36%	1.718%
6	5.812	763	775	789	rVB	1490597	4335211	17.52%	3.214%
7	5.952	789	798	808	rBV	144583	397397	1.61%	0.295%
8	6.172	819	834	841	rBV3	153670	624144	2.52%	0.463%
9	6.245	841	846	854	rVV2	106328	284485	1.15%	0.211%
10	6.342	854	862	875	rVB2	101502	285052	1.15%	0.211%
11	6.598	890	904	917	rBV	927617	2228245	9.01%	1.652%
12	6.757	921	930	952	rVV	358125	905735	3.66%	0.671%
13	7.373	1018	1031	1042	rBV	357466	838080	3.39%	0.621%
14	8.647	1235	1240	1245	rVV	719490	1164275	4.71%	0.863%
15	8.720	1245	1252	1259	rVV	15178902	24744281	100.00%	18.343%
16	8.909	1277	1283	1289	rBV	275245	409084	1.65%	0.303%
17	9.903	1442	1446	1451	rVB	274193	377342	1.52%	0.280%
18	10.006	1456	1463	1467	rBV	261725	368799	1.49%	0.273%
19	10.055	1467	1471	1476	rVB	688709	940862	3.80%	0.697%
20	10.195	1488	1494	1499	rVB	1100825	1483463	6.00%	1.100%
21	10.299	1499	1511	1517	rBV	3938304	5705125	23.06%	4.229%
22	10.360	1517	1521	1527	rVB	900255	1097666	4.44%	0.814%
23	10.585	1551	1558	1562	rBV2	221700	341809	1.38%	0.253%
24	10.640	1562	1567	1575	rVV	1827062	2585014	10.45%	1.916%
25	10.780	1582	1590	1594	rBV2	697288	1079662	4.36%	0.800%
26	10.854	1594	1602	1606	rVV2	449469	852460	3.45%	0.632%
27	10.896	1606	1609	1614	rVB	293277	389980	1.58%	0.289%
28	10.963	1614	1620	1623	rBV2	340002	551610	2.23%	0.409%
29	11.085	1634	1640	1650	rVB3	1100072	2290902	9.26%	1.698%
30	11.189	1650	1657	1660	rBV	519359	835634	3.38%	0.619%
31	11.219	1660	1662	1670	rVB3	361199	412543	1.67%	0.306%
32	11.305	1670	1676	1679	rBV	724939	964316	3.90%	0.715%
33	11.378	1684	1688	1694	rVV	2394957	4414362	17.84%	3.272%
34	11.451	1694	1700	1702	rVV2	1328523	2536347	10.25%	1.880%
35	11.475	1702	1704	1709	rVB	2817001	3149165	12.73%	2.334%
36	11.579	1717	1721	1723	rBV2	178592	252781	1.02%	0.187%

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37	11.616	1723	1727	1734	rVB	1201140	1802465	7.28%	1.336%
38	11.713	1740	1743	1746	rBV	705273	835216	3.38%	0.619%
39	11.756	1746	1750	1759	rVB	4760022	6498654	26.26%	4.817%
40	11.890	1765	1772	1777	rVB3	521318	843730	3.41%	0.625%

41	11.945	1777	1781	1784	rBV3	911051	1352515	5.47%	1.003%
42	11.969	1784	1785	1789	rVB2	513120	491228	1.99%	0.364%
43	12.030	1789	1795	1799	rBV3	810975	1478543	5.98%	1.096%
44	12.091	1799	1805	1811	rVB	1705012	2636229	10.65%	1.954%
45	12.170	1812	1818	1823	rVB3	325079	591165	2.39%	0.438%

46	12.225	1823	1827	1829	rBV	1122647	1458875	5.90%	1.081%
47	12.268	1832	1834	1838	rVB	1029307	1152318	4.66%	0.854%
48	12.317	1838	1842	1849	rVB3	1525713	2764692	11.17%	2.049%
49	12.420	1849	1859	1863	rBV	1973885	2770052	11.19%	2.053%
50	12.463	1863	1866	1872	rVB	820684	1168562	4.72%	0.866%

51	12.536	1873	1878	1879	rBV	712170	899509	3.64%	0.667%
52	12.555	1879	1881	1885	rVB	681759	732282	2.96%	0.543%
53	12.615	1887	1891	1895	rVB	834638	936373	3.78%	0.694%
54	12.725	1899	1909	1913	rBV5	473359	1396928	5.65%	1.036%
55	12.847	1926	1929	1932	rVB2	255836	297305	1.20%	0.220%

56	12.890	1932	1936	1938	rBV2	279943	389597	1.57%	0.289%
57	12.920	1938	1941	1945	rVB	416513	514988	2.08%	0.382%
58	12.963	1945	1948	1951	rBV	786667	1078340	4.36%	0.799%
59	13.042	1956	1961	1964	rVV4	184787	319731	1.29%	0.237%
60	13.164	1974	1981	1985	rVB4	355036	666898	2.70%	0.494%

61	13.213	1985	1989	1992	rBV2	222023	258045	1.04%	0.191%
62	13.268	1992	1998	1999	rBV3	448574	731293	2.96%	0.542%
63	13.292	1999	2002	2007	rVB2	1049185	1445932	5.84%	1.072%
64	13.426	2019	2024	2032	rVB4	401968	838868	3.39%	0.622%
65	13.585	2046	2050	2055	rBV3	219614	395995	1.60%	0.294%

66	13.670	2060	2064	2071	rVB5	124561	256049	1.03%	0.190%
67	13.774	2077	2081	2084	rBV	401560	535046	2.16%	0.397%
68	13.810	2084	2087	2091	rVV	957249	1187574	4.80%	0.880%
69	13.853	2091	2094	2100	rVB	1151564	1500688	6.06%	1.112%
70	13.926	2100	2106	2111	rBV	1675652	2220114	8.97%	1.646%

71	13.981	2111	2115	2120	rVV2	266585	349164	1.41%	0.259%
72	14.438	2185	2190	2195	rBV	1727421	2132748	8.62%	1.581%
73	14.633	2216	2222	2226	rBV	553145	831946	3.36%	0.617%
74	14.780	2239	2246	2251	rBV2	279065	436332	1.76%	0.323%
75	15.091	2292	2297	2303	rBV	193330	292378	1.18%	0.217%

76	15.731	2397	2402	2413	rVB5	134192	317839	1.28%	0.236%
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Title : SW846 8260

77	16.133	2460	2468	2478	rVB	1012969	2103612	8.50%	1.559%
78	16.688	2552	2559	2572	rVB	114745	250247	1.01%	0.186%

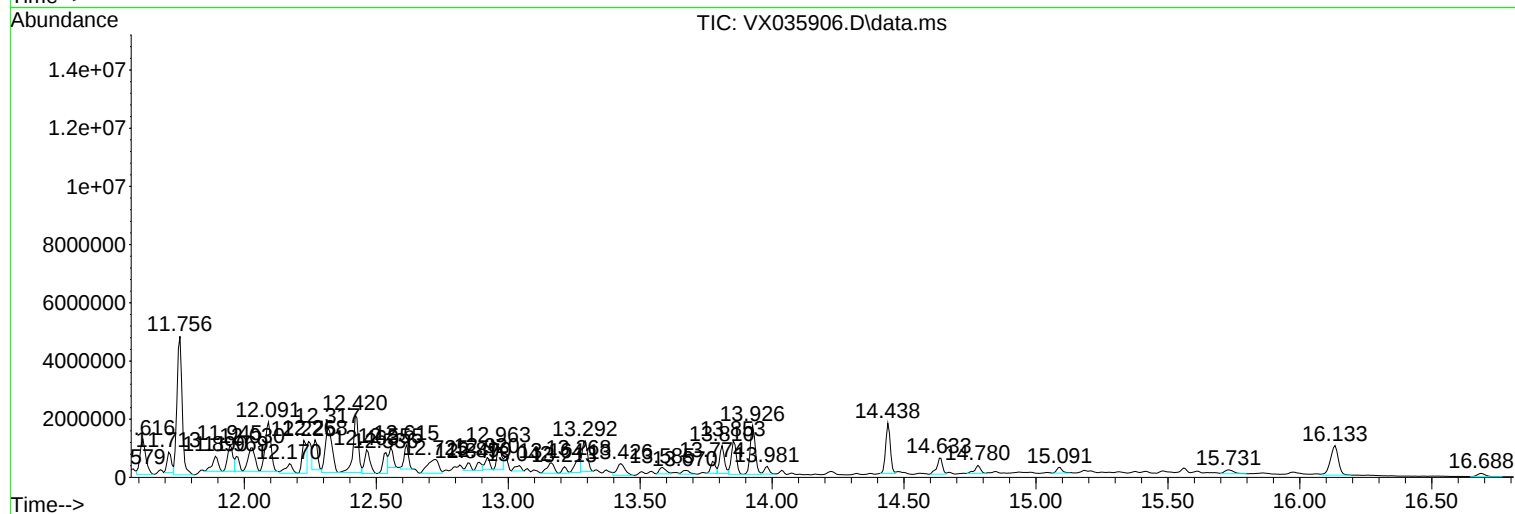
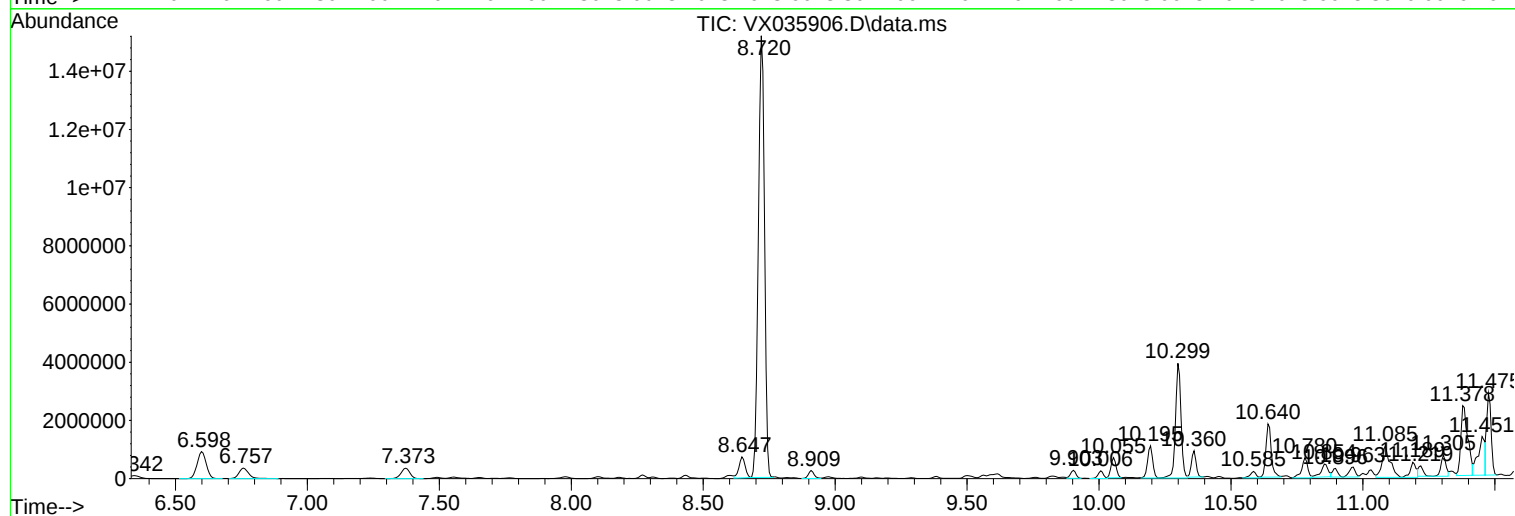
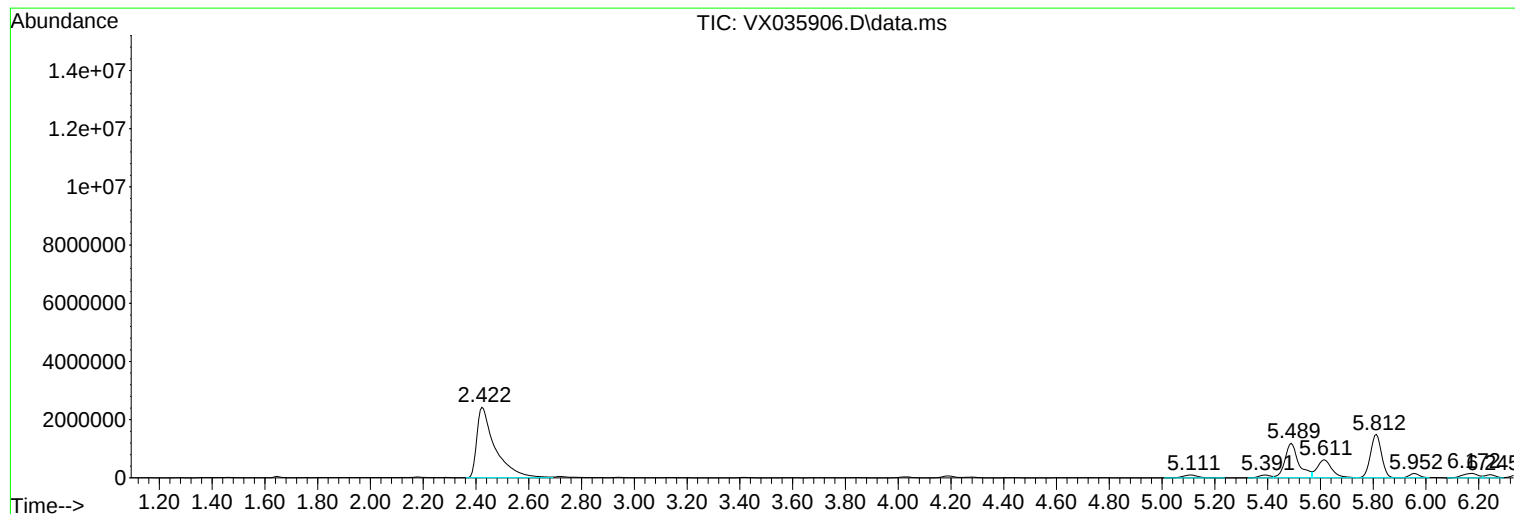
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X052623W.M
Quant Title : SW846 8260

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



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ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FMC-0096

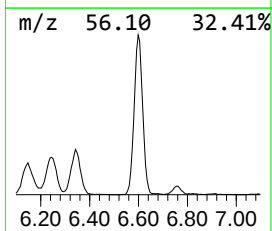
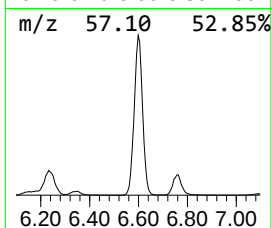
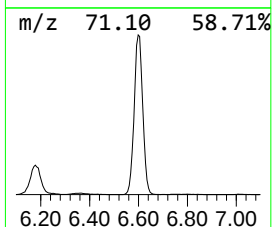
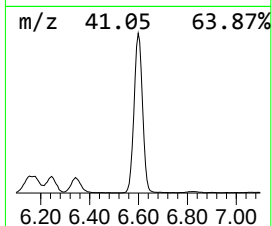
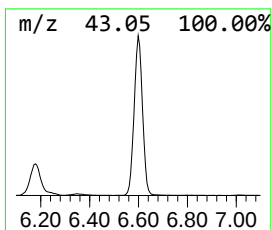
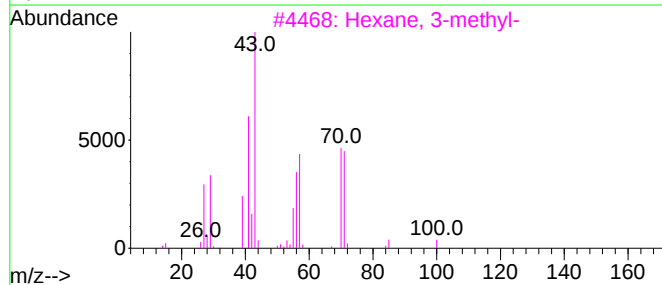
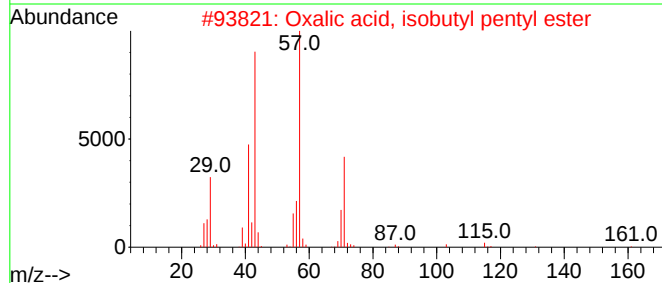
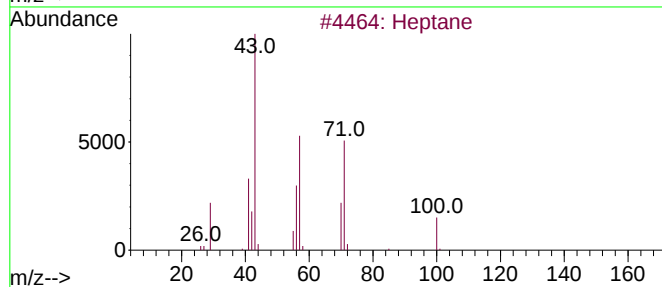
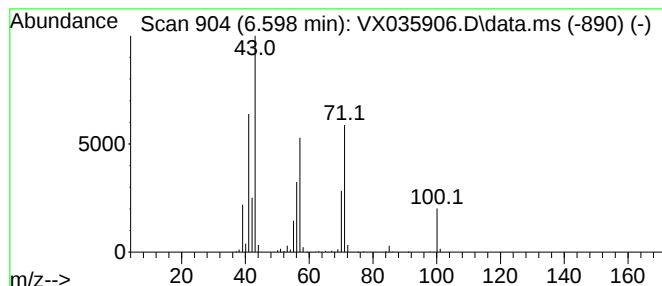
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X052623W.M
Quant Title : SW846 8260

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

Peak Number 1 Heptane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.598	123.01 ug/l	2228250	1,4-Difluorobenzene	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane	100	C7H16	000142-82-5	91
2			Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	42
3			Hexane, 3-methyl-	100	C7H16	000589-34-4	40
4			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	38
5			Acetaldehyde, propylhydrazone	100	C5H12N2	007422-88-0	38



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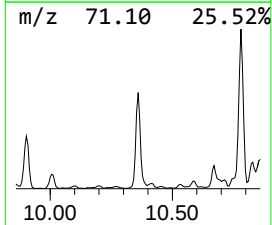
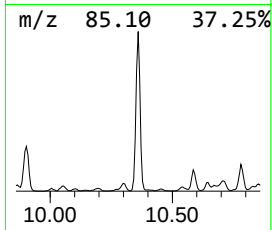
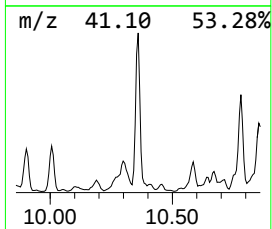
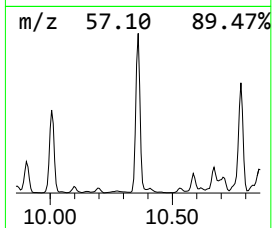
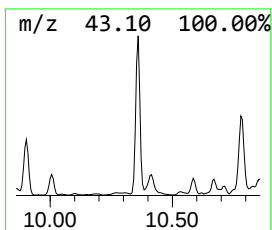
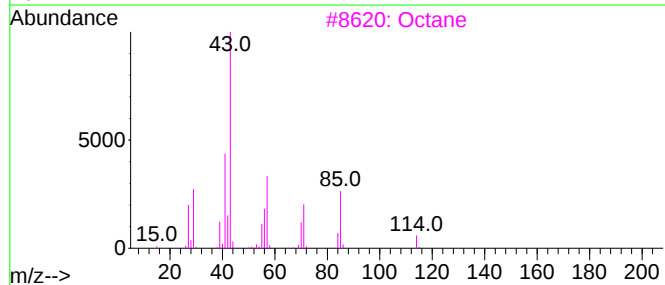
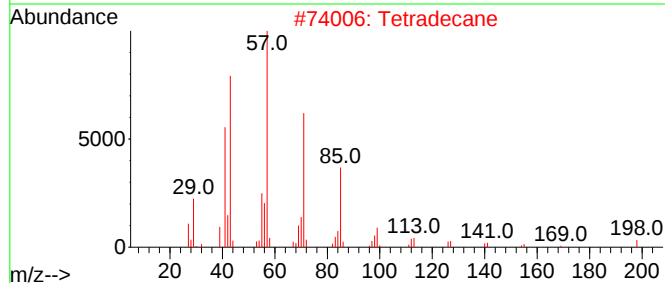
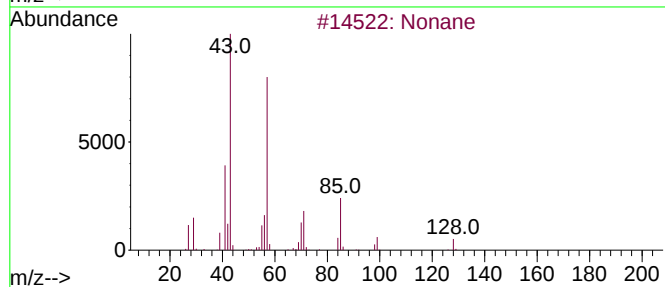
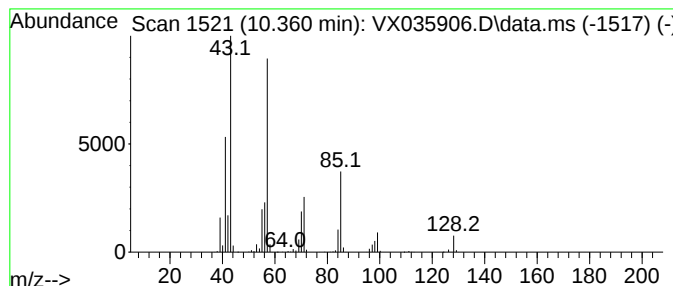
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Nonane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.360	58.33 ug/l	1097670	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonane	128	C9H20	000111-84-2	91
2			Tetradecane	198	C14H30	000629-59-4	59
3			Octane	114	C8H18	000111-65-9	53
4			Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	53
5			Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	50



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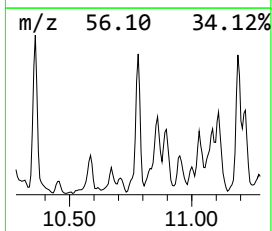
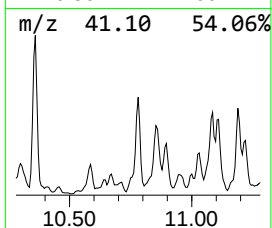
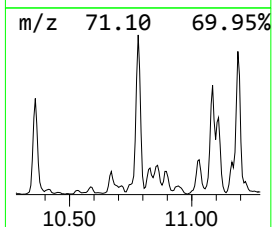
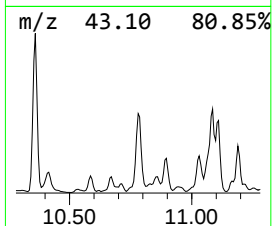
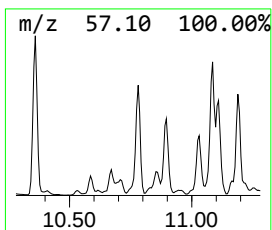
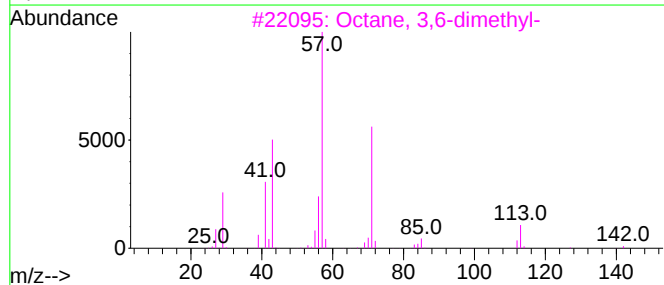
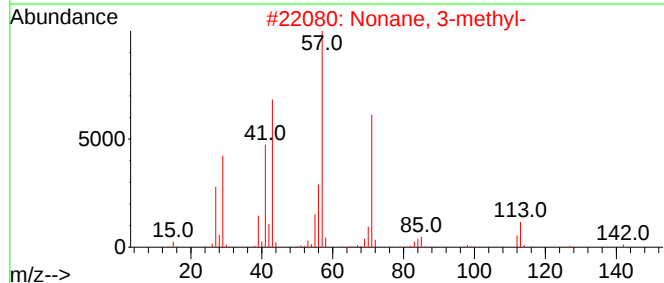
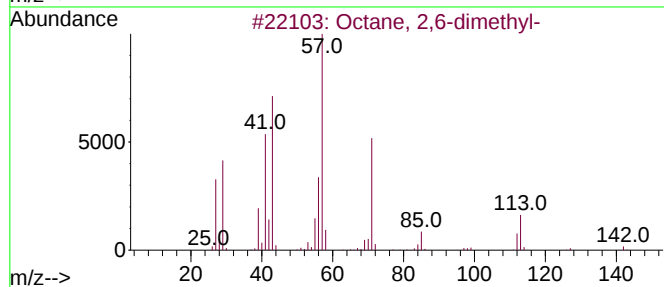
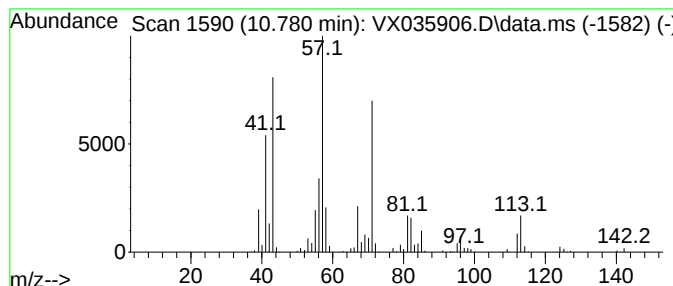
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X052623W.M
Quant Title : SW846 8260

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

Peak Number 3 Octane, 2,6-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.781	57.38 ug/l	1079660	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	92
2			Nonane, 3-methyl-	142	C10H22	005911-04-6	70
3			Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	53
4			Sulfurous acid, butyl 2-ethylhex...	250	C12H26O3S	1000309-18-8	47
5			Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	43



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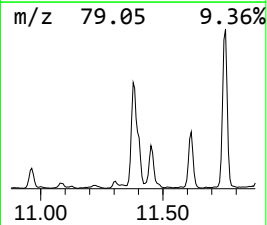
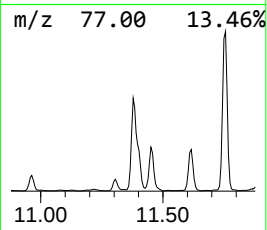
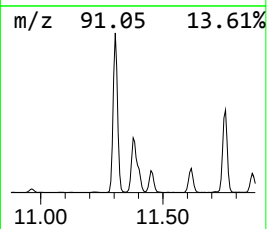
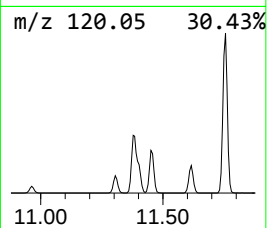
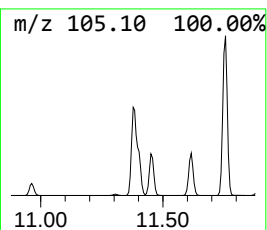
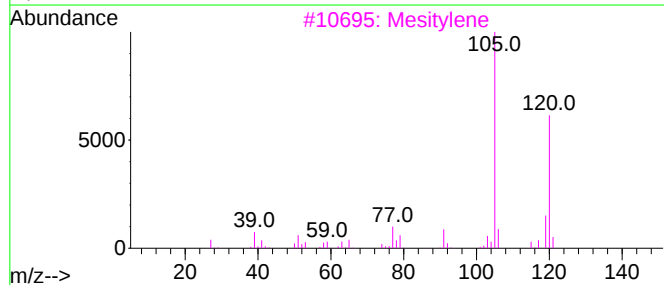
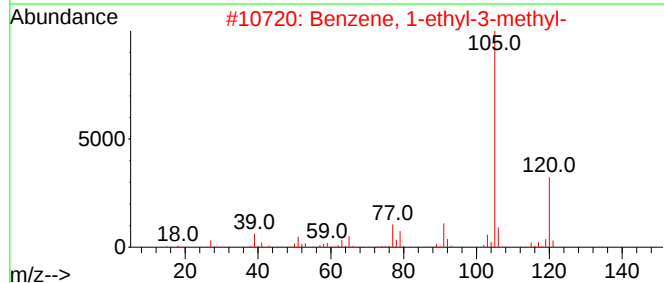
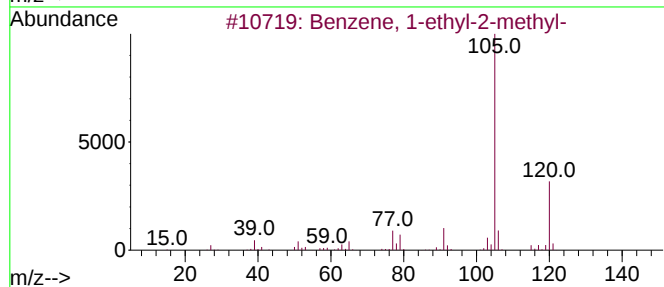
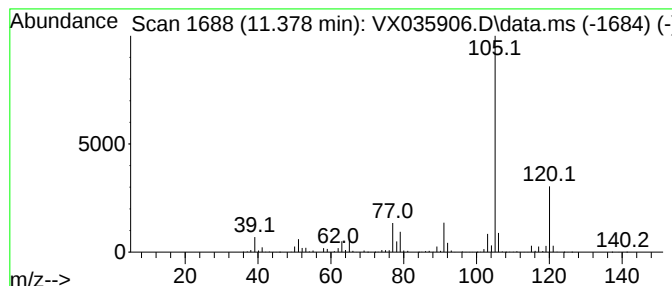
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	149.28 ug/l	4414360	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			Mesitylene	120	C9H12	000108-67-8	91
4			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX053023\
Data File : VX035906.D
Acq On : 30 May 2023 15:14
Operator : JC/MD
Sample : 02902-01
Misc : 1.15g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FMC-0096

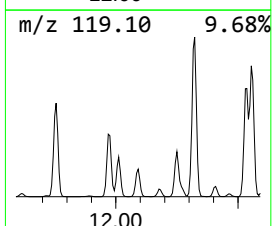
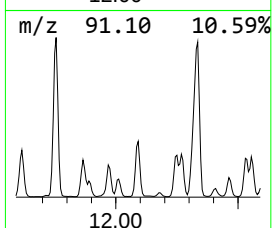
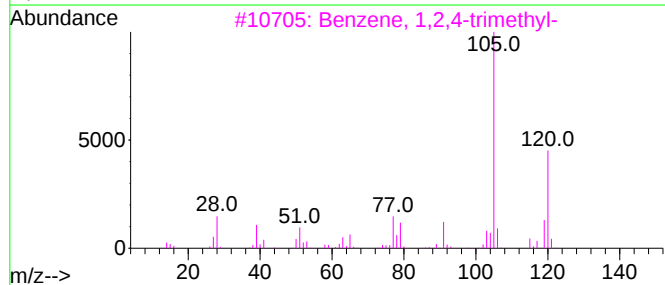
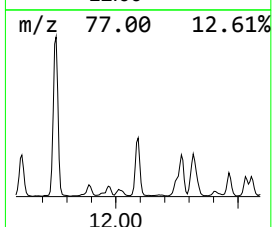
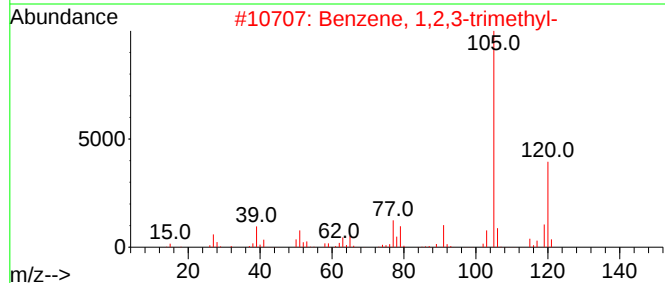
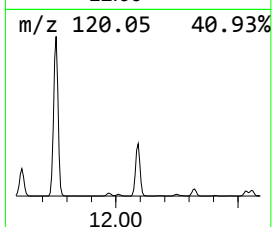
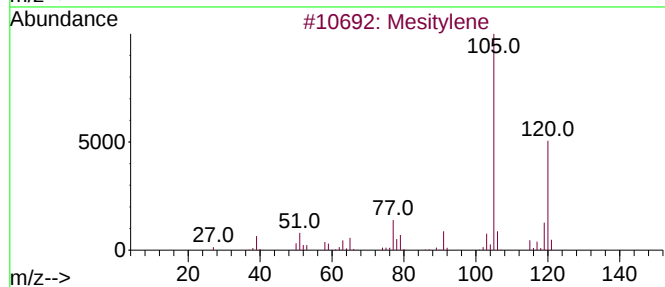
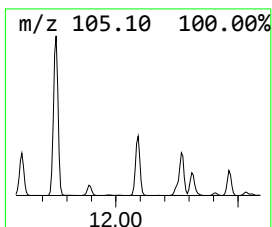
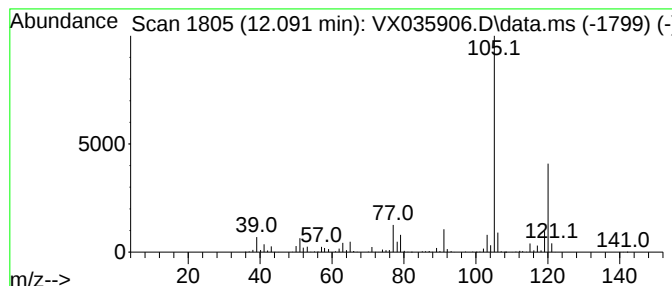
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, 1,2,3-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.091	89.15 ug/l	2636230	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	90
5			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX053023\
Data File : VX035906.D
Acq On : 30 May 2023 15:14
Operator : JC/MD
Sample : 02902-01
Misc : 1.15g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FMC-0096

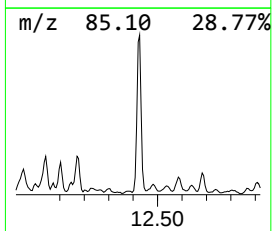
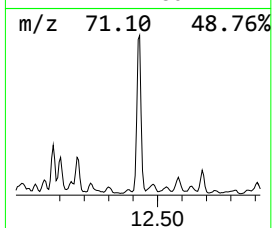
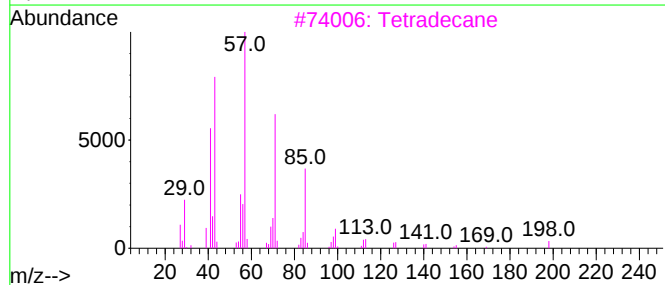
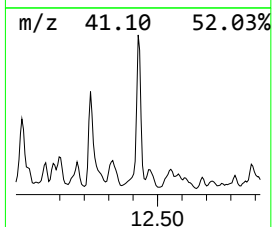
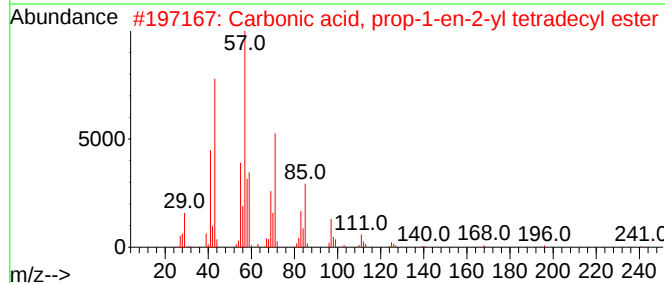
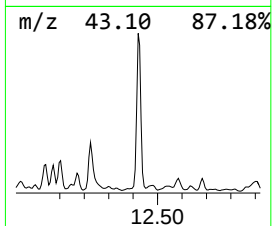
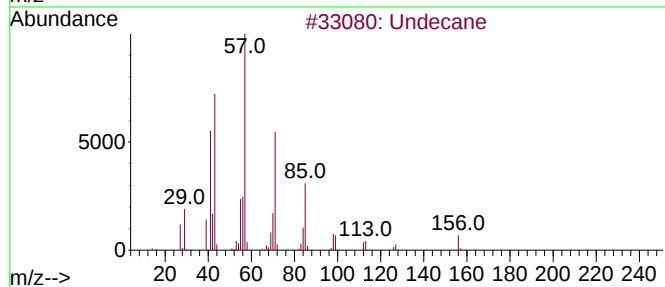
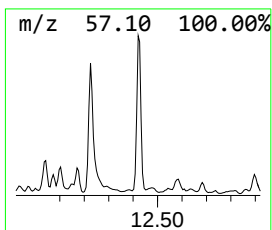
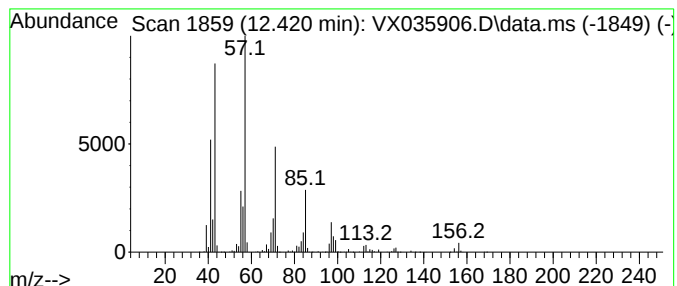
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Quant Title : SW846 8260

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

Peak Number 7 Undecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.420	93.68 ug/l	2770050	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane			156	C11H24	001120-21-4	94
2	Carbonic acid, prop-1-en-2-yl te...			298	C18H34O3	1000382-90-9	80
3	Tetradecane			198	C14H30	000629-59-4	72
4	Hexadecane			226	C16H34	000544-76-3	64
5	Tridecane			184	C13H28	000629-50-5	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX053023\
Data File : VX035906.D
Acq On : 30 May 2023 15:14
Operator : JC/MD
Sample : 02902-01
Misc : 1.15g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FMC-0096

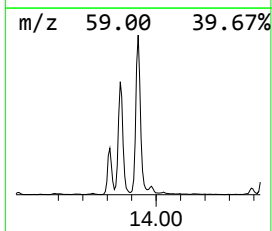
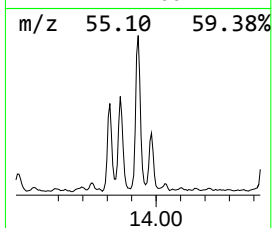
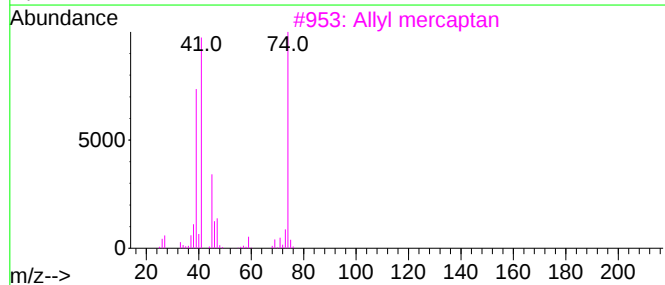
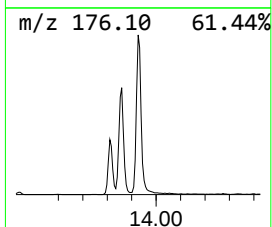
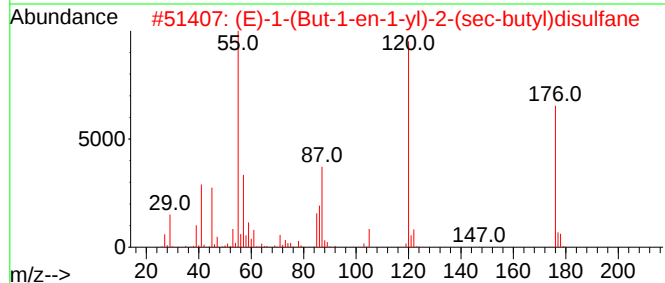
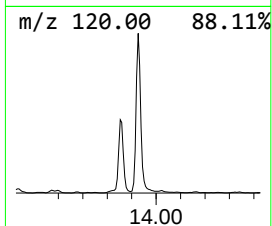
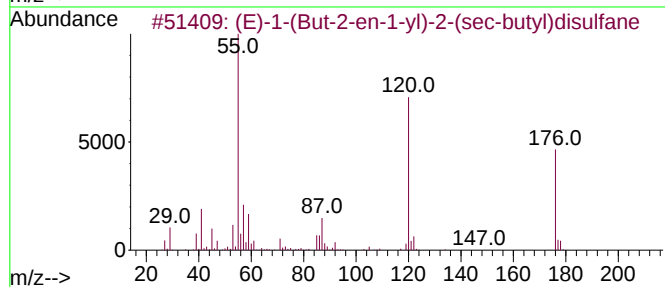
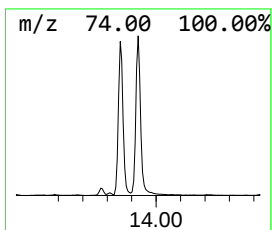
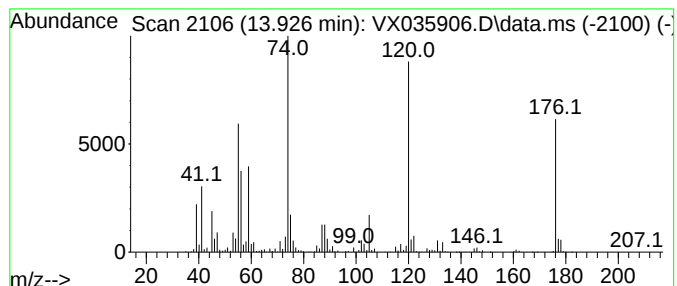
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Quant Title : SW846 8260

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

Peak Number 8 unknown13.926 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.926	75.08 ug/l	2220110	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-1-(But-2-en-1-yl)-2-(sec-but...	176	C8H16S2	110690-24-9	41		
2	(E)-1-(But-1-en-1-yl)-2-(sec-but...	176	C8H16S2	110690-22-7	38		
3	Allyl mercaptan	74	C3H6S	000870-23-5	30		
4	(Z)-1-(But-1-en-1-yl)-2-(sec-but...	176	C8H16S2	110690-21-6	30		
5	1,3-Dithiane	120	C4H8S2	000505-23-7	27		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX053023\
Data File : VX035906.D
Acq On : 30 May 2023 15:14
Operator : JC/MD
Sample : 02902-01
Misc : 1.15g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FMC-0096

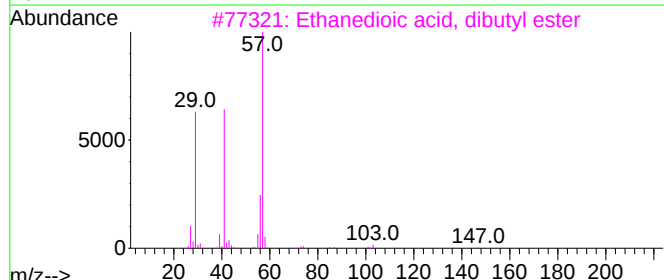
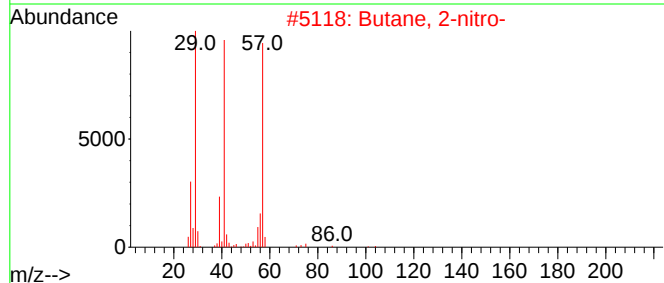
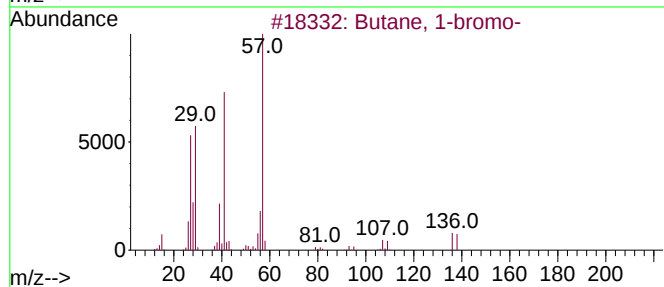
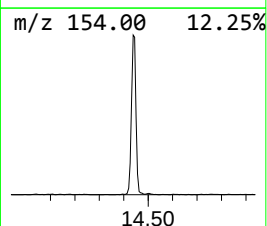
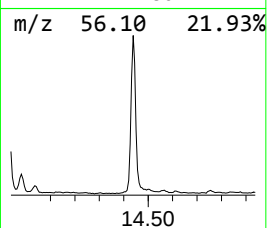
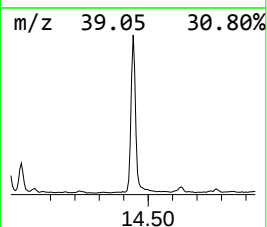
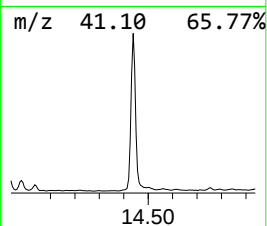
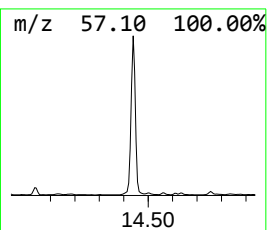
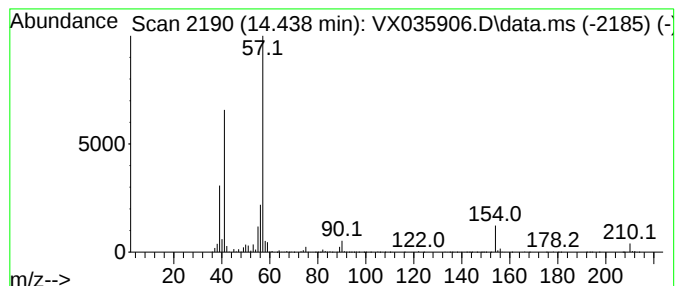
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 unknown14.438 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.438	72.12 ug/l	2132750	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 1-bromo-	136	C4H9Br	000109-65-9	32
2			Butane, 2-nitro-	103	C4H9NO2	000600-24-8	32
3			Ethanedioic acid, dibutyl ester	202	C10H18O4	002050-60-4	23
4			Hydrazinecarboxylic acid, 1,1-di...	132	C5H12N2O2	000870-46-2	23
5			Disulfide, (1-methylethyl) (1,1-...	164	C7H16S2	043022-60-2	16



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX053023\
Data File : VX035906.D
Acq On : 30 May 2023 15:14
Operator : JC/MD
Sample : 02902-01
Misc : 1.15g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FMC-0096

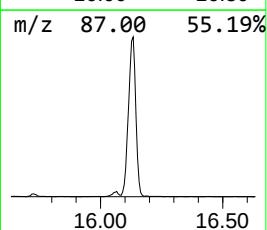
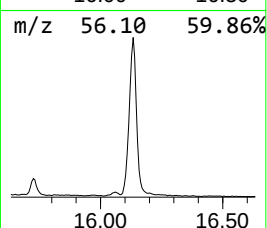
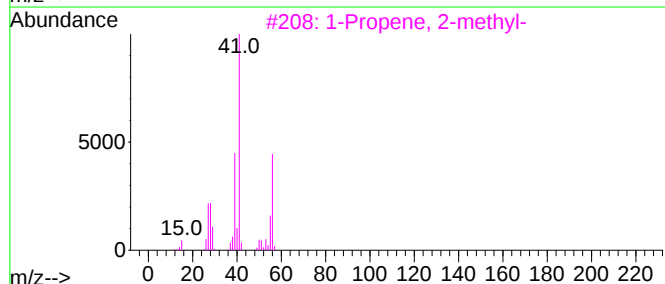
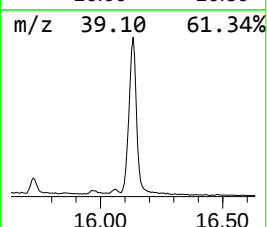
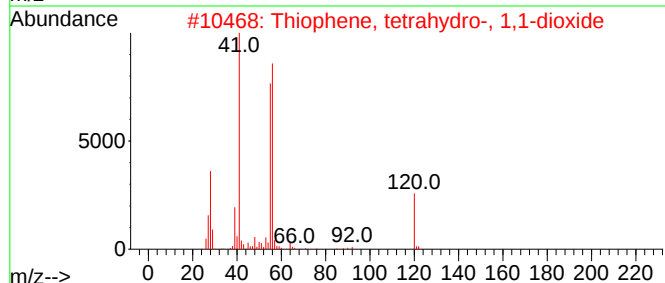
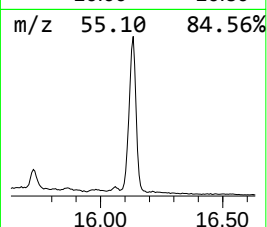
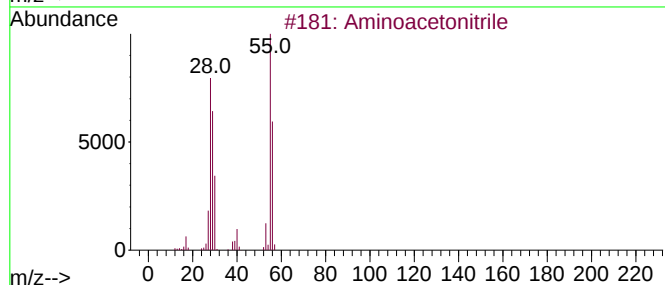
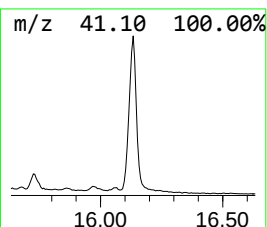
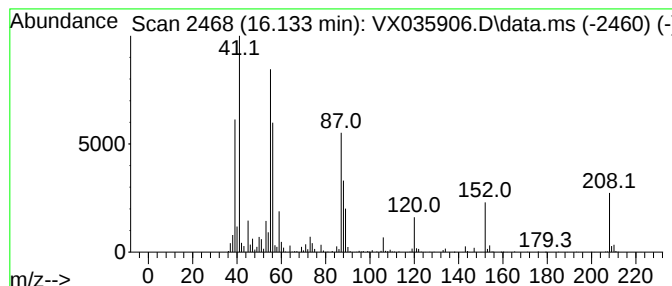
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Quant Title : SW846 8260

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

Peak Number 10 unknown16.133 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.133	71.14 ug/l	2103610	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Aminoacetonitrile	56	C2H4N2	000540-61-4	14
2		Thiophene, tetrahydro-, 1,1-dioxide	120	C4H8O2S	000126-33-0	14
3		1-Propene, 2-methyl-	56	C4H8	000115-11-7	11
4		2-Butene, (E)-	56	C4H8	000624-64-6	10
5		2-Butene	56	C4H8	000107-01-7	10



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX053023\
Data File : VX035906.D
Acq On : 30 May 2023 15:14
Operator : JC/MD
Sample : 02902-01
Misc : 1.15g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FMC-0096

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X052623W.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
Heptane	6.598	123.0	ug/l	2228250	2	6.757	905735	50.0
Nonane	10.360	58.3	ug/l	1097670	3	10.055	940862	50.0
Octane, 2,6-dim...	10.781	57.4	ug/l	1079660	3	10.055	940862	50.0
Benzene, 1-ethy...	11.378	149.3	ug/l	4414360	4	12.024	1478540	50.0
Benzene, 1,2,3-...	12.091	89.2	ug/l	2636230	4	12.024	1478540	50.0
Undecane	12.420	93.7	ug/l	2770050	4	12.024	1478540	50.0
unknown13.926	13.926	75.1	ug/l	2220110	4	12.024	1478540	50.0
unknown14.438	14.438	72.1	ug/l	2132750	4	12.024	1478540	50.0
unknown16.133	16.133	71.1	ug/l	2103610	4	12.024	1478540	50.0