

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031622\
 Data File : VN071323.D
 Acq On : 16 Mar 2022 16:24
 Operator : JC\MD
 Sample : N1886-04
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 30970

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_N\methods\82N030722W.M
 Title : SW846 8260

Signal : TIC: VN071323.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.681	277	288	313	rBV	1237258	3305291	20.50%	3.129%
2	4.281	378	390	400	rBV	726678	2126810	13.19%	2.013%
3	4.563	425	438	458	rBV	321689	1094125	6.78%	1.036%
4	4.851	477	487	504	rVB	89868	289374	1.79%	0.274%
5	6.569	769	779	797	rBV2	177733	579493	3.59%	0.549%
6	7.063	850	863	875	rBV2	90342	285776	1.77%	0.271%
7	7.334	895	909	918	rBV2	77959	240261	1.49%	0.227%
8	8.022	1015	1026	1031	rBV	562355	1415176	8.78%	1.340%
9	8.081	1031	1036	1051	rVB	1145123	2541039	15.76%	2.406%
10	8.434	1084	1096	1107	rBV	665935	1562255	9.69%	1.479%
11	8.963	1175	1186	1208	rVB	1634656	3375077	20.93%	3.195%
12	9.151	1208	1218	1254	rBV	7220365	16126845	100.00%	15.267%
13	10.251	1395	1405	1410	rBV	85918	185956	1.15%	0.176%
14	10.328	1410	1418	1429	rBV	2914907	5193600	32.20%	4.917%
15	10.439	1429	1437	1444	rBV	2540302	4580538	28.40%	4.336%
16	10.939	1513	1522	1538	rBV	2815893	5246014	32.53%	4.966%
17	11.127	1549	1554	1559	rVV	319126	554729	3.44%	0.525%
18	11.457	1603	1610	1617	rBV	260089	464434	2.88%	0.440%
19	11.739	1647	1658	1668	rBV	2305273	4342913	26.93%	4.111%
20	11.945	1685	1693	1705	rVB	1619524	2757300	17.10%	2.610%
21	12.098	1713	1719	1726	rBV	199947	333875	2.07%	0.316%
22	12.174	1726	1732	1738	rVV	165000	281313	1.74%	0.266%
23	12.345	1756	1761	1770	rVB	122996	204781	1.27%	0.194%
24	12.727	1819	1826	1835	rBV	2007348	3509641	21.76%	3.323%
25	12.816	1835	1841	1848	rVV	715422	1357467	8.42%	1.285%
26	12.927	1855	1860	1866	rVB	316962	501532	3.11%	0.475%
27	13.057	1876	1882	1888	rVB	168778	279795	1.73%	0.265%
28	13.174	1894	1902	1911	rBV3	105420	216391	1.34%	0.205%
29	13.304	1918	1924	1935	rBV4	109185	373971	2.32%	0.354%
30	13.580	1965	1971	1980	rVB	3441242	5558395	34.47%	5.262%
31	13.668	1980	1986	1994	rBV	2056411	3772356	23.39%	3.571%
32	13.763	1994	2002	2009	rVV	3955742	6401378	39.69%	6.060%
33	13.833	2010	2014	2023	rVB6	151983	325264	2.02%	0.308%
34	14.133	2056	2065	2073	rBV3	242206	546119	3.39%	0.517%
35	14.268	2083	2088	2092	rBV4	88638	177640	1.10%	0.168%
36	14.345	2092	2101	2107	rBV	591690	1783395	11.06%	1.688%

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37	14.415	2107	2113	2121	rBV	4120382	6710312	41.61%	6.353%
38	14.521	2127	2131	2135	rBV	536436	788817	4.89%	0.747%
39	14.563	2135	2138	2139	rBV	185566	218866	1.36%	0.207%
40	14.586	2139	2142	2144	rBV2	190344	221517	1.37%	0.210%
41	14.621	2144	2148	2151	rBV	1575929	2277883	14.12%	2.156%
42	14.663	2151	2155	2161	rBV2	2048223	4388447	27.21%	4.155%
43	14.780	2170	2175	2182	rVB	1033363	1593146	9.88%	1.508%
44	14.963	2201	2206	2210	rBV2	643182	1255827	7.79%	1.189%
45	15.098	2219	2229	2231	rBV6	485544	1249781	7.75%	1.183%
46	15.133	2232	2235	2237	rVV3	360044	593829	3.68%	0.562%
47	15.162	2237	2240	2244	rVB	456081	768091	4.76%	0.727%
48	15.286	2255	2261	2265	rBV2	851394	1733264	10.75%	1.641%
49	15.439	2274	2287	2297	rVB5	498958	1939974	12.03%	1.837%

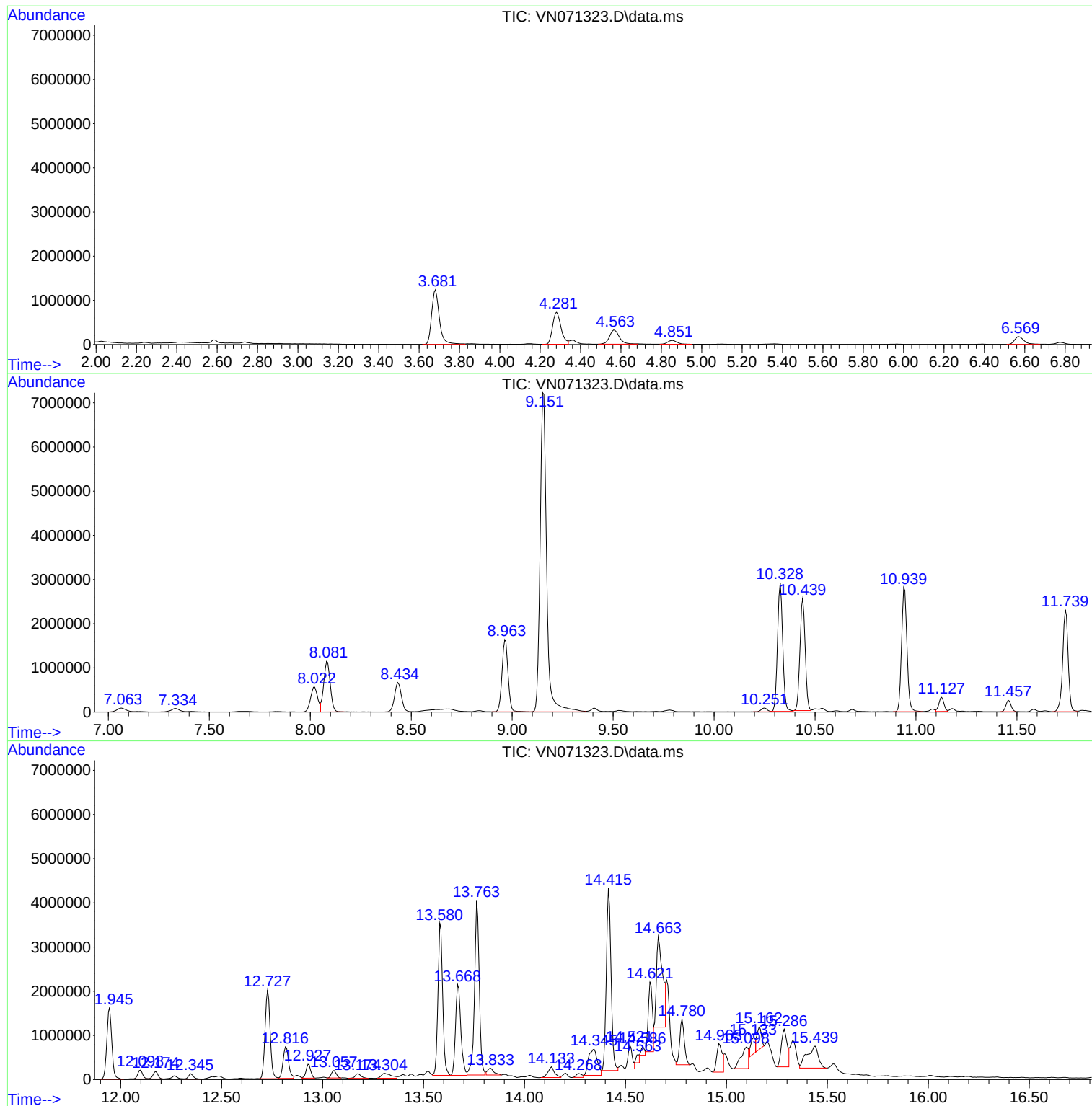
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030722W.M
Quant Title : SW846 8260

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



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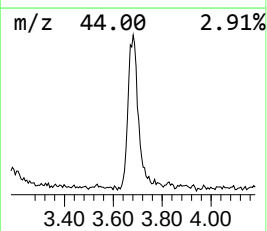
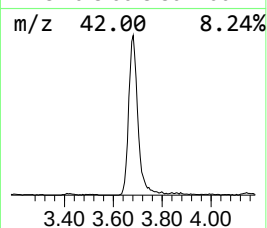
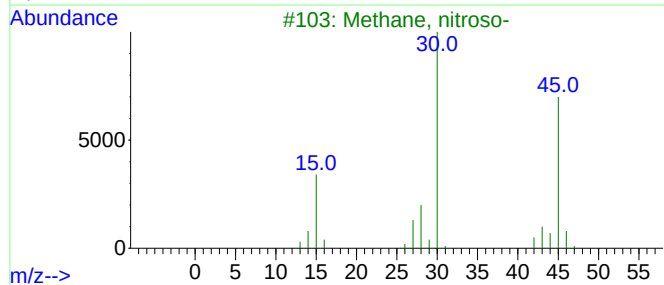
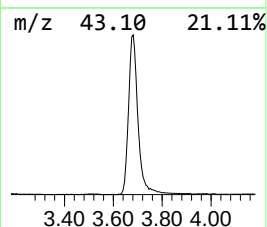
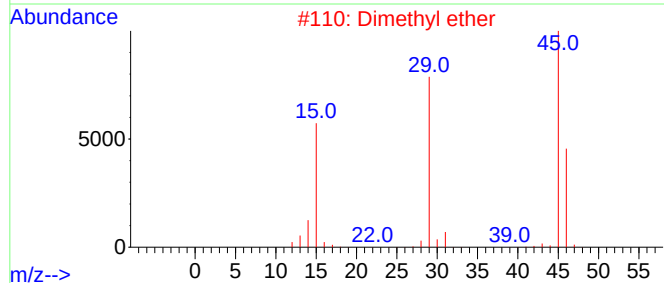
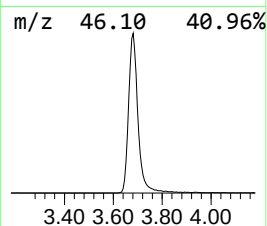
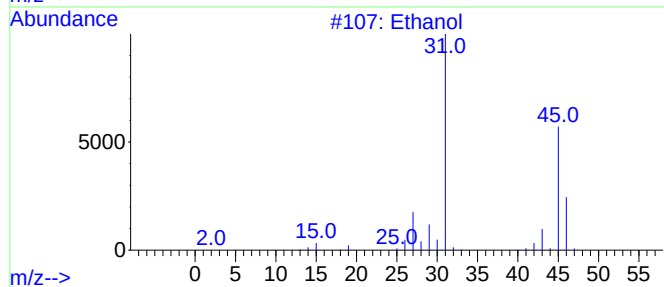
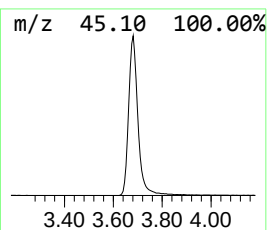
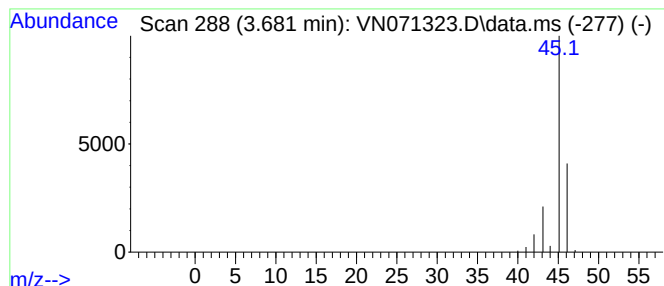
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030722W.M
Quant Title : SW846 8260

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

Peak Number 1 Ethanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.681	65.04 ug/l	3305290	Pentafluorobenzene	8.081

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol			46	C2H6O	000064-17-5	74
2	Dimethyl ether			46	C2H6O	000115-10-6	9
3	Methane, nitroso-			45	CH3NO	000865-40-7	4
4	Formic acid			46	CH2O2	000064-18-6	4
5	Oxalic acid			90	C2H2O4	000144-62-7	4



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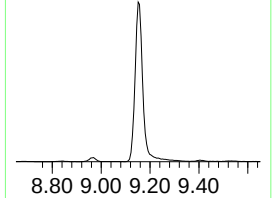
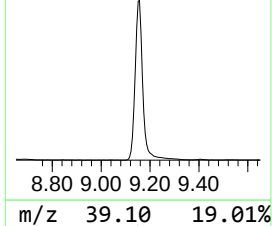
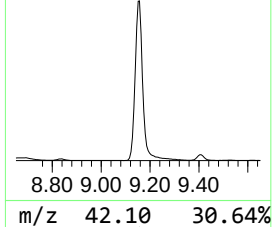
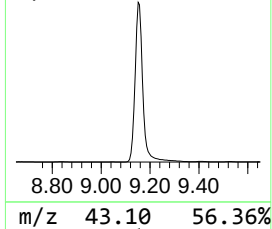
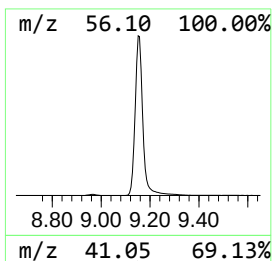
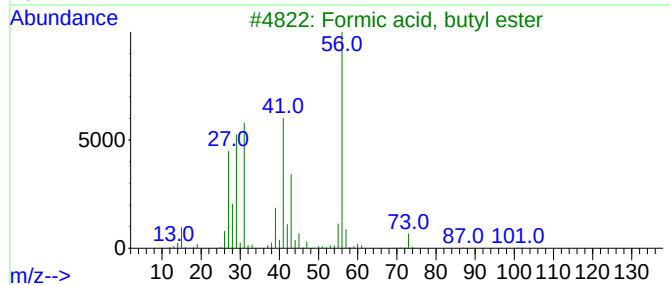
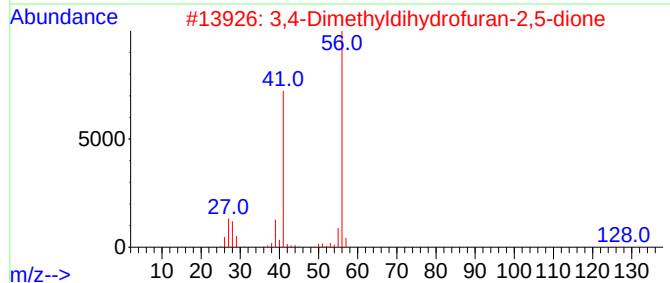
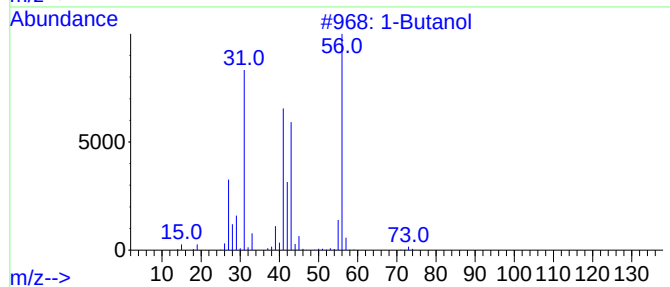
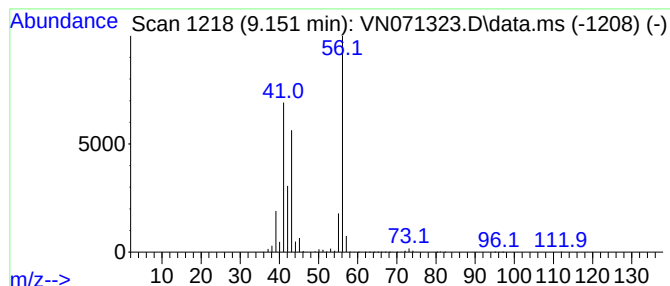
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030722W.M
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 1-Butanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.151	238.91 ug/l	16126800	1,4-Difluorobenzene	8.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol			74	C4H10O	000071-36-3	91
2	3,4-Dimethyldihydrofuran-2,5-dione			128	C6H8O3	007475-92-5	9
3	Formic acid, butyl ester			102	C5H10O2	000592-84-7	9
4	Oxetane, 3,3-dimethyl-			86	C5H10O	006921-35-3	9
5	2-Methanesulfonylethanamine			123	C3H9NO2S	049773-20-8	9



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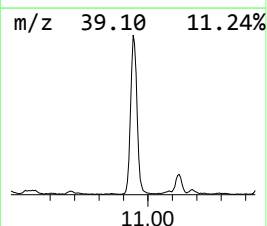
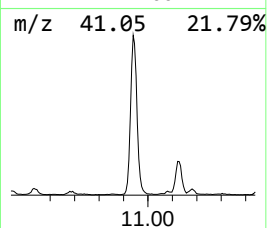
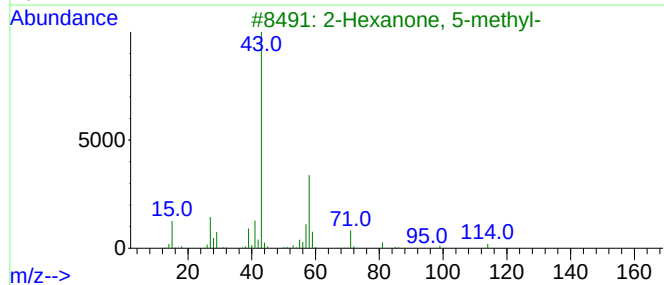
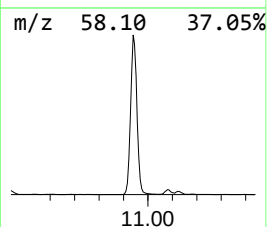
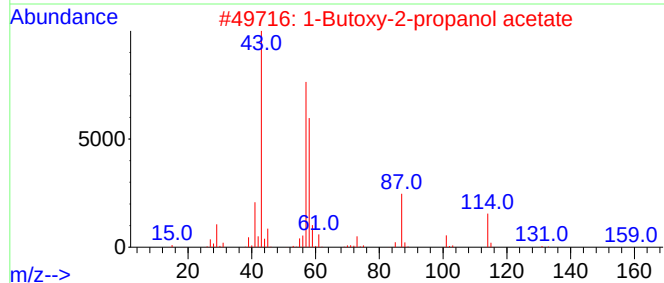
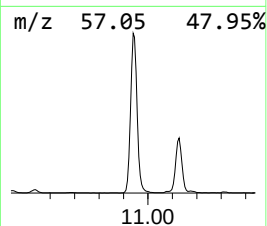
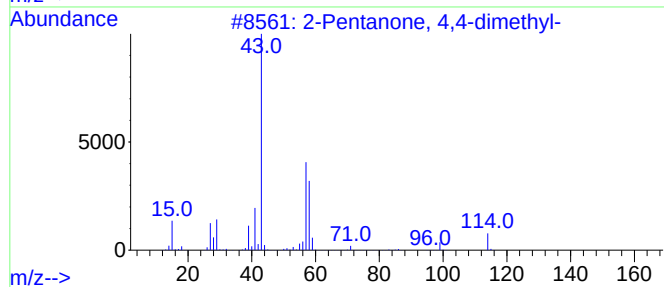
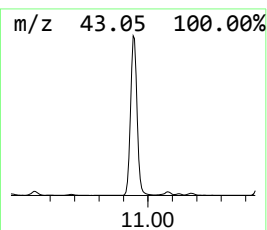
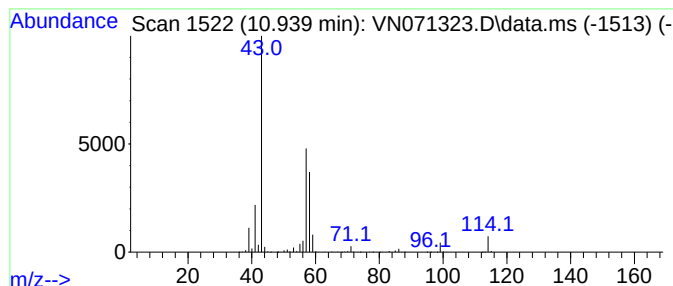
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4,4-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.939	60.40 ug/l	5246010	Chlorobenzene-d5	11.739

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4,4-dimethyl-	114	C7H14O	000590-50-1	91		
2	1-Butoxy-2-propanol acetate	174	C9H18O3	085409-76-3	72		
3	2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	64		
4	2-Heptanone	114	C7H14O	000110-43-0	53		
5	Butanal, 2-methyl-	86	C5H10O	000096-17-3	23		



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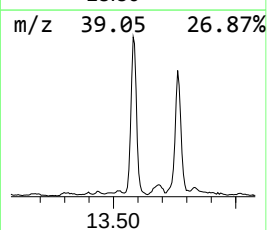
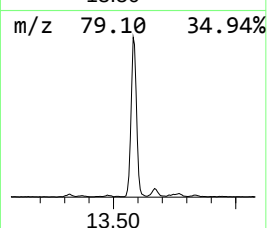
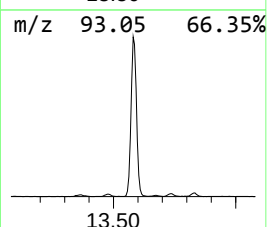
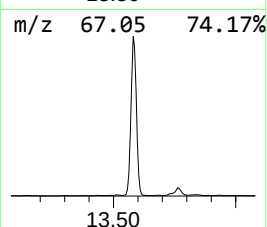
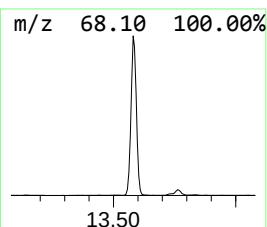
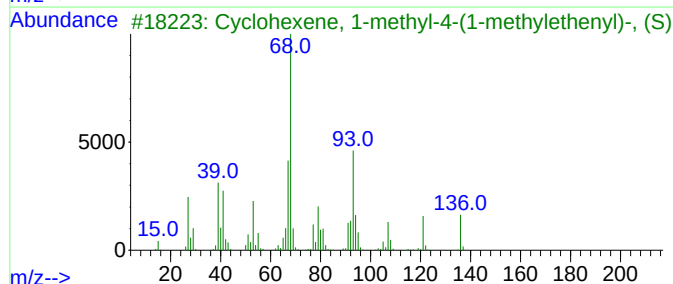
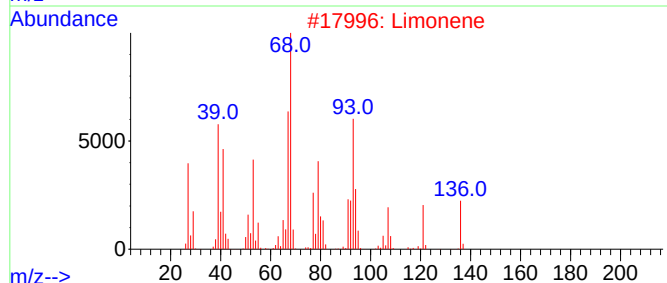
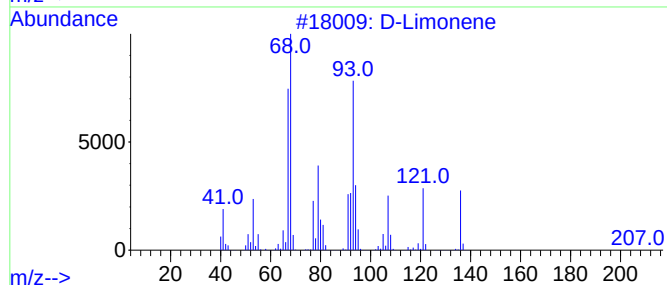
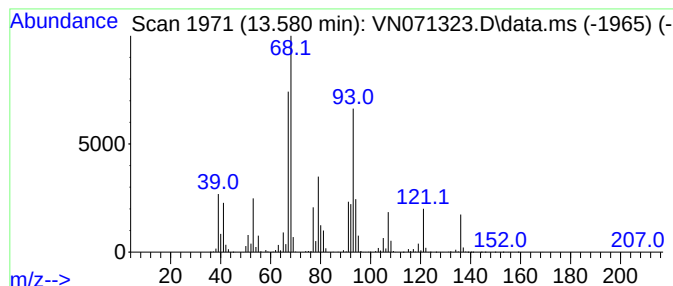
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Quant Title : SW846 8260

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

Peak Number 4 D-Limonene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.580	73.67 ug/l	5558400	1,4-Dichlorobenzene-d4	13.669

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			D-Limonene	136	C10H16	005989-27-5	97
2			Limonene	136	C10H16	000138-86-3	87
3			Cyclohexene, 1-methyl-4-(1-methy...	136	C10H16	005989-54-8	74
4			Cyclohexanol, 1-methyl-4-(1-meth...	196	C12H20O2	010198-23-9	72
5			Cyclohexene, 1-methyl-5-(1-methy...	136	C10H16	013898-73-2	55



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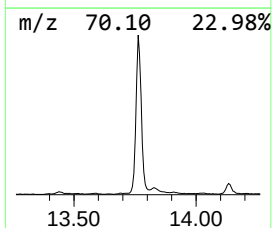
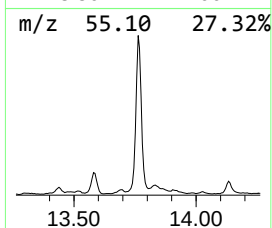
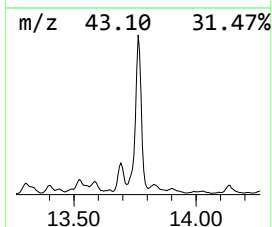
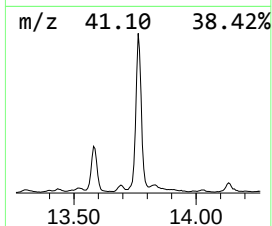
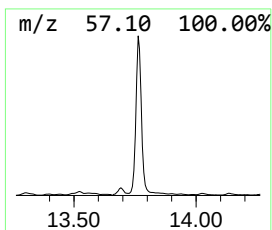
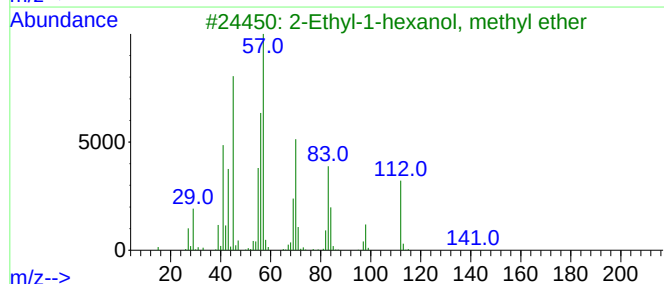
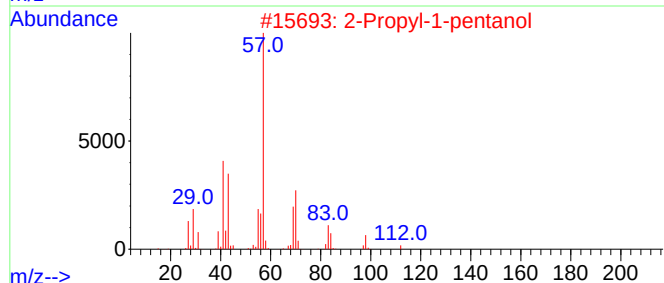
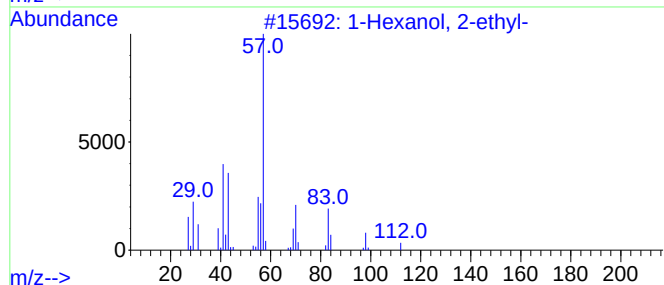
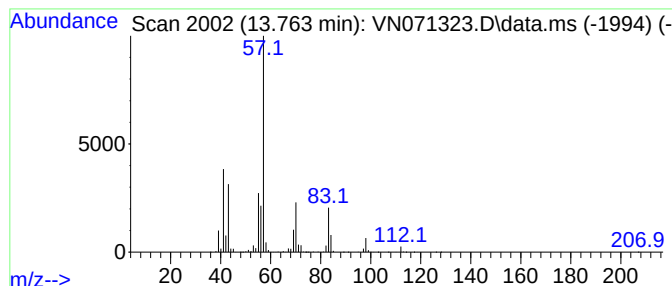
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Quant Title : SW846 8260

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

Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.763	84.85 ug/l	6401380	1,4-Dichlorobenzene-d4	13.669

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53
3			2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	47
4			1-Decene, 2,4-dimethyl-	168	C12H24	055170-80-4	47
5			Pentadecafluorooctanoic acid, 2-...	526	C16H17F15O2	1000406-80-9	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031622\
Data File : VN071323.D
Acq On : 16 Mar 2022 16:24
Operator : JC\MD
Sample : N1886-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
30970

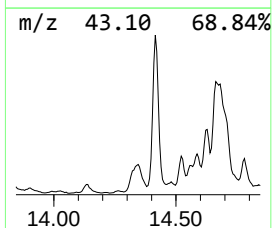
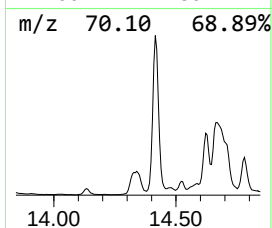
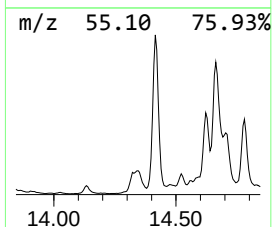
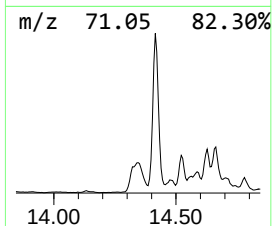
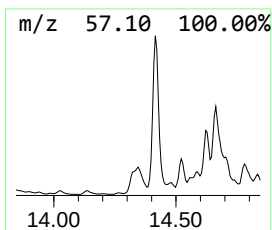
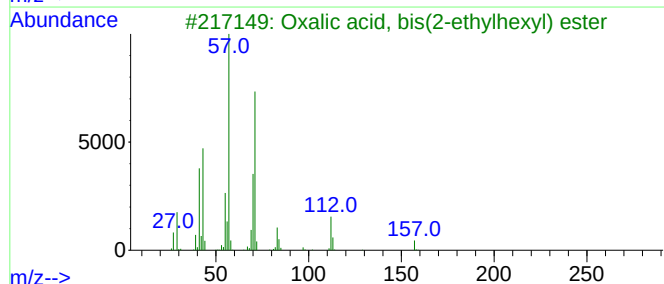
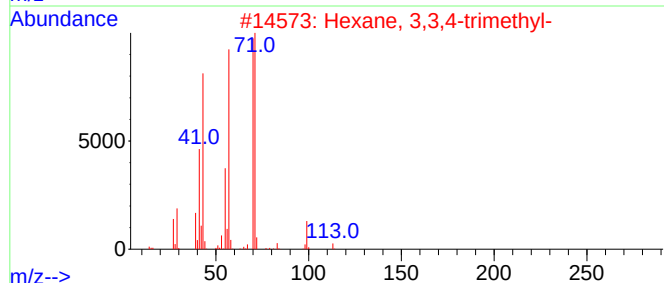
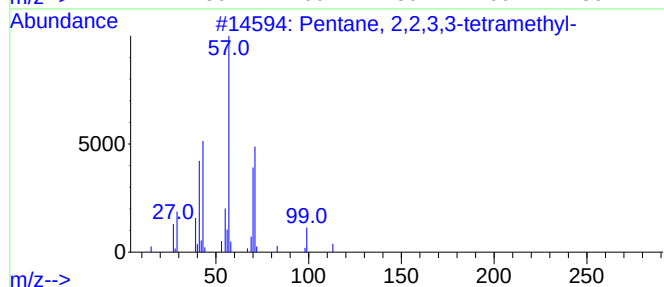
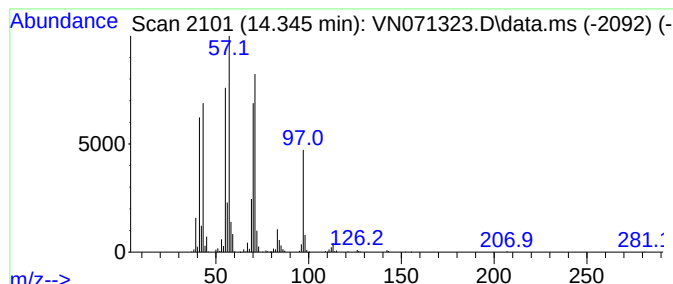
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Quant Title : SW846 8260

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

Peak Number 6 Pentane, 2,2,3,3-tetramethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.345	23.64 ug/l	1783400	1,4-Dichlorobenzene-d4	13.669

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,2,3,3-tetramethyl-	128	C9H20	007154-79-2	50
2			Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	47
3			Oxalic acid, bis(2-ethylhexyl) e...	314	C18H34O4	1000309-39-0	47
4			3-Bromooctane	192	C8H17Br	000999-64-4	43
5			4-Methyl-3-heptanol, heptafluoro...	326	C12H17F7O2	1000365-51-5	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031622\
Data File : VN071323.D
Acq On : 16 Mar 2022 16:24
Operator : JC\MD
Sample : N1886-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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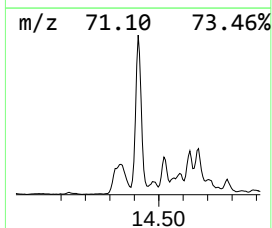
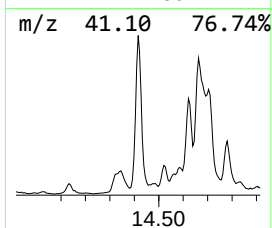
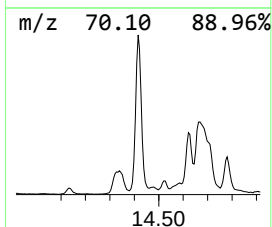
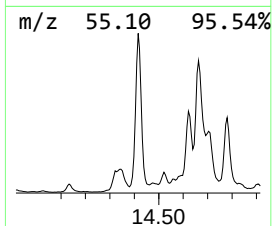
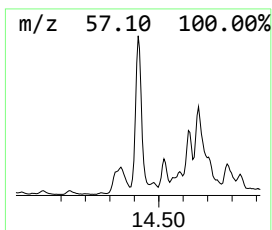
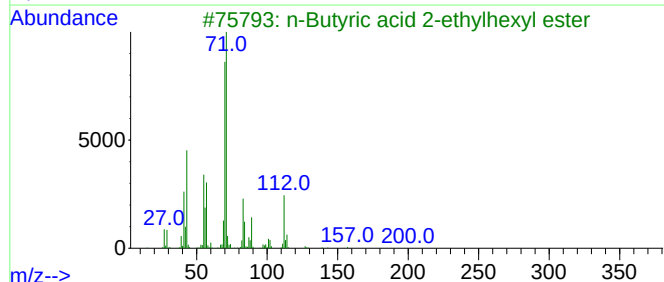
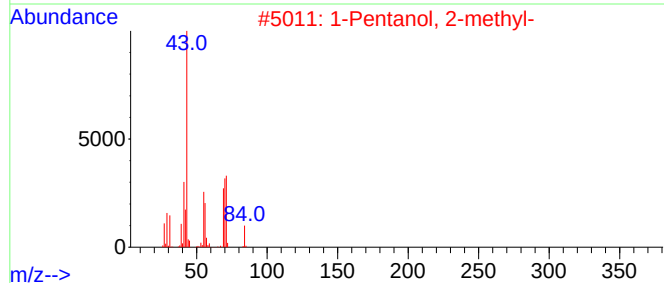
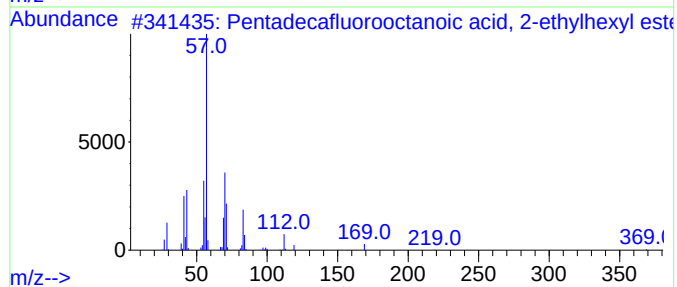
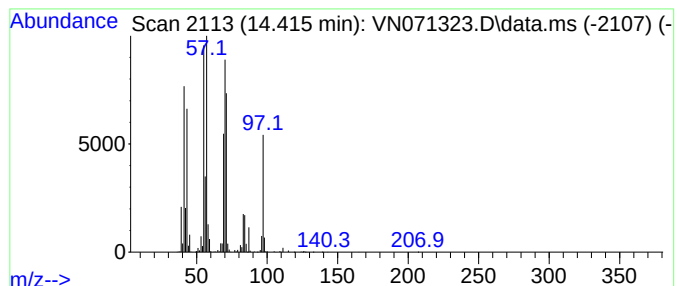
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Quant Title : SW846 8260

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

Peak Number 7 Pentadecafluorooctanoic aci... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.416	88.94 ug/l	6710310	1,4-Dichlorobenzene-d4	13.669

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, 2-...	526	C16H17F15O2	1000406-80-9	59
2			1-Pentanol, 2-methyl-	102	C6H14O	000105-30-6	53
3			n-Butyric acid 2-ethylhexyl ester	200	C12H24O2	025415-84-3	50
4			1-Dodecanol, 3,7,11-trimethyl-	228	C15H32O	006750-34-1	50
5			1-Butanol, 2-ethyl-	102	C6H14O	000097-95-0	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031622\
Data File : VN071323.D
Acq On : 16 Mar 2022 16:24
Operator : JC\MD
Sample : N1886-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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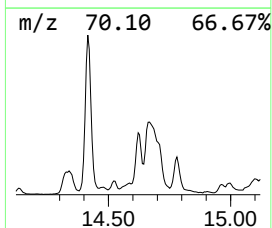
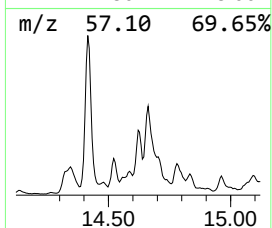
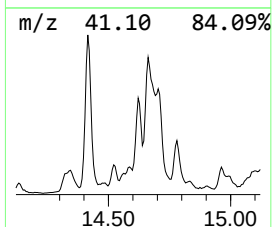
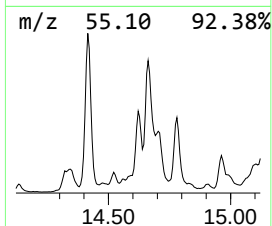
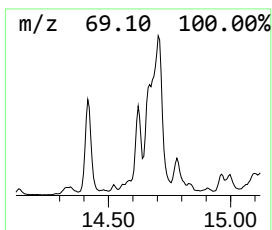
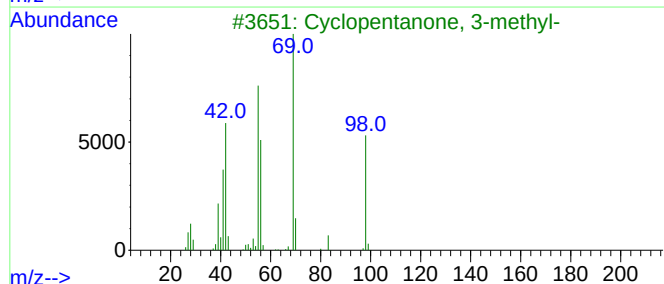
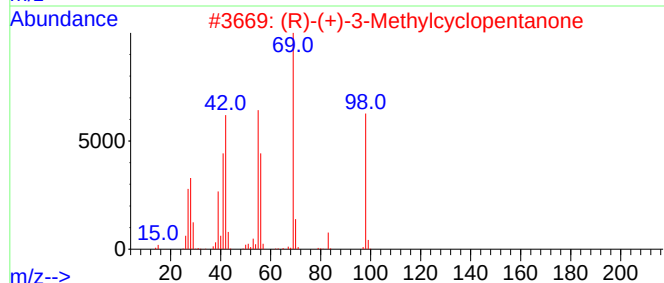
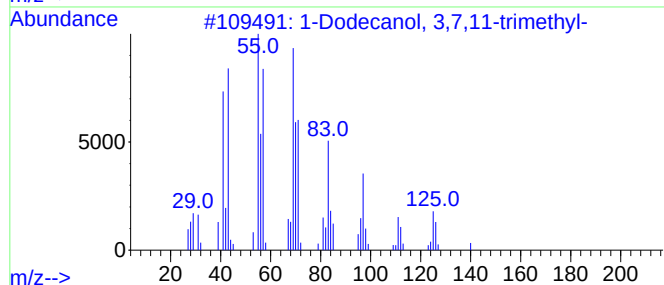
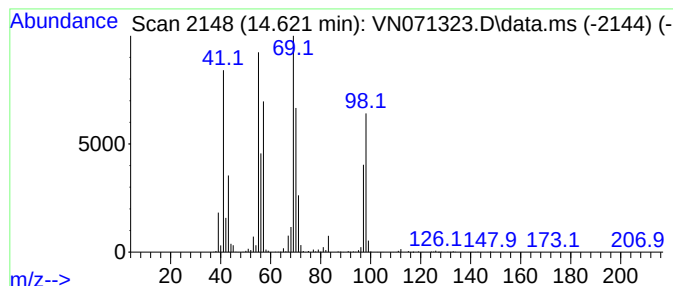
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Quant Title : SW846 8260

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

Peak Number 8 1-Dodecanol, 3,7,11-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.621	30.19 ug/l	2277880	1,4-Dichlorobenzene-d4	13.669

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Dodecanol, 3,7,11-trimethyl-	228	C15H32O	006750-34-1	59
2		(R)-(+)-3-Methylcyclopentanone	98	C6H10O	006672-30-6	52
3		Cyclopentanone, 3-methyl-	98	C6H10O	001757-42-2	52
4		1-Hexene, 3-methyl-	98	C7H14	003404-61-3	50
5		3-Heptene, 2-methyl-, (E)-	112	C8H16	000692-96-6	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031622\
Data File : VN071323.D
Acq On : 16 Mar 2022 16:24
Operator : JC\MD
Sample : N1886-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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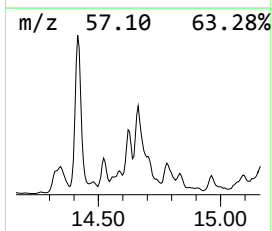
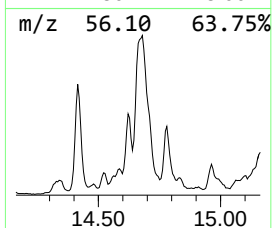
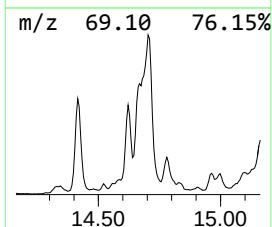
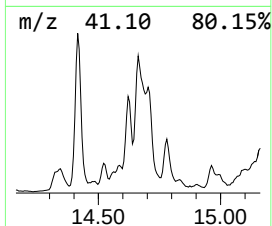
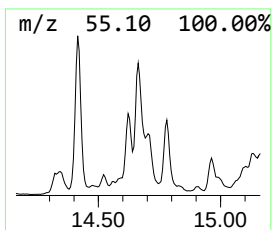
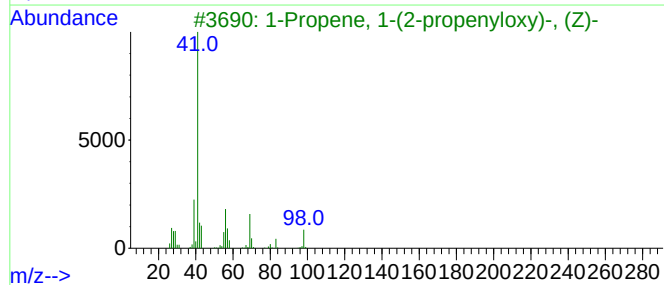
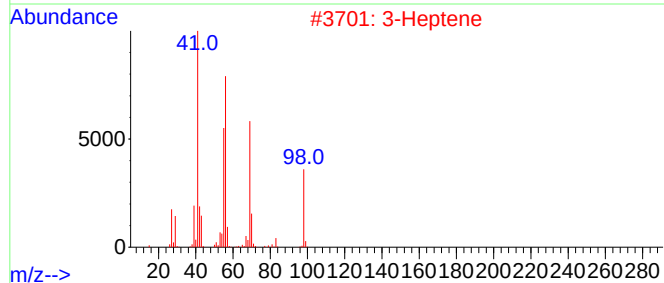
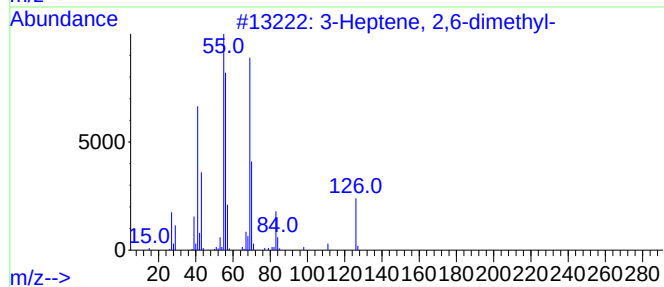
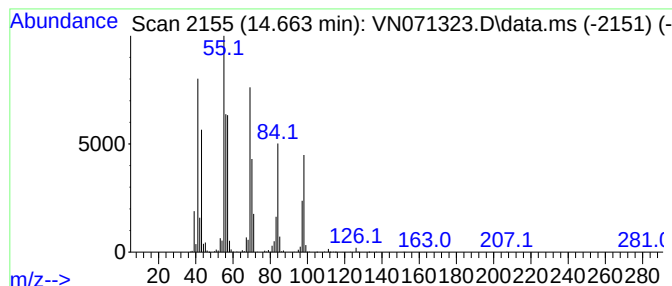
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Quant Title : SW846 8260

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

Peak Number 9 3-Heptene, 2,6-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.663	58.17 ug/l	4388450	1,4-Dichlorobenzene-d4	13.669

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Heptene, 2,6-dimethyl-	126	C9H18	002738-18-3	53
2			3-Heptene	98	C7H14	000592-78-9	47
3			1-Propene, 1-(2-propenyloxy)-, (Z)-	98	C6H10O	061142-12-9	47
4			(R)-(+)-3-Methylcyclopentanone	98	C6H10O	006672-30-6	47
5			3-Heptene, (E)-	98	C7H14	014686-14-7	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031622\
Data File : VN071323.D
Acq On : 16 Mar 2022 16:24
Operator : JC\MD
Sample : N1886-04
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ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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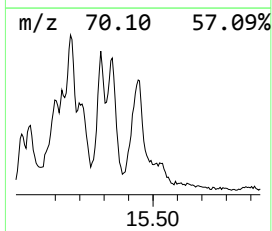
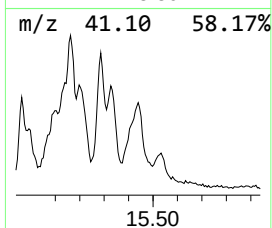
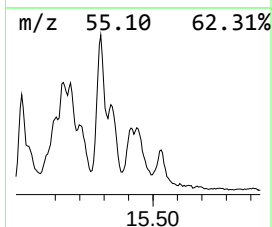
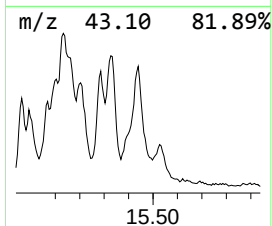
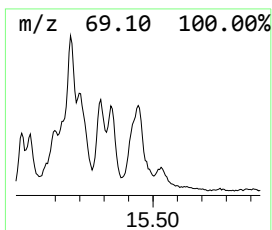
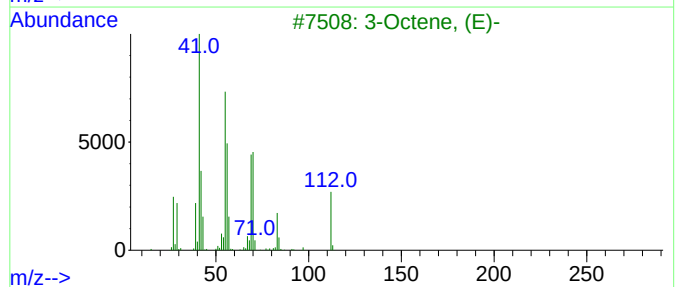
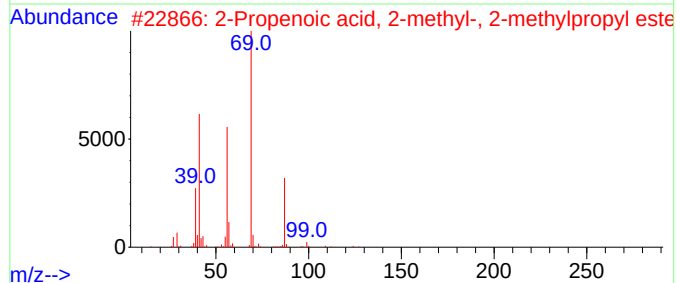
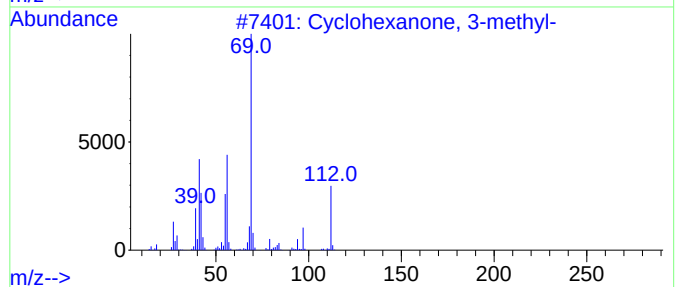
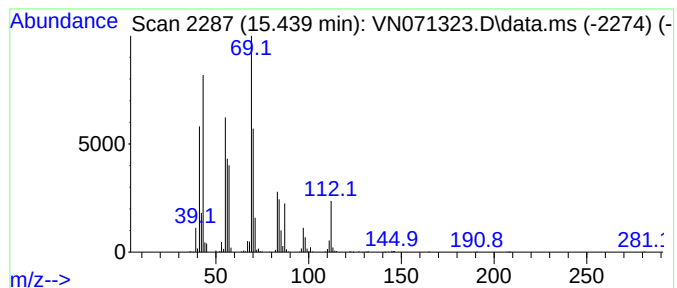
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Quant Title : SW846 8260

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

Peak Number 10 unknown15.439 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.439	25.71 ug/l	1939970	1,4-Dichlorobenzene-d4	13.669

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclohexanone, 3-methyl-	112	C7H12O	000591-24-2	49
2		2-Propenoic acid, 2-methyl-, 2-m...	142	C8H14O2	000097-86-9	43
3		3-Octene, (E)-	112	C8H16	014919-01-8	43
4		3-Octene, (Z)-	112	C8H16	014850-22-7	38
5		4-Octene, (Z)-	112	C8H16	007642-15-1	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031622\
Data File : VN071323.D
Acq On : 16 Mar 2022 16:24
Operator : JC\MD
Sample : N1886-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030722W.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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1-Butanol	9.151	238.9	ug/l	16126800	2	8.963	3375080	50.0
2-Pentanone, 4,...	10.939	60.4	ug/l	5246010	3	11.739	4342910	50.0
D-Limonene	13.580	73.7	ug/l	5558400	4	13.669	3772360	50.0
1-Hexanol, 2-et...	13.763	84.8	ug/l	6401380	4	13.669	3772360	50.0
Pentane, 2,2,3,...	14.345	23.6	ug/l	1783400	4	13.669	3772360	50.0
Pentadecafluoro...	14.416	88.9	ug/l	6710310	4	13.669	3772360	50.0
1-Dodecanol, 3,...	14.621	30.2	ug/l	2277880	4	13.669	3772360	50.0
3-Heptene, 2,6-...	14.663	58.2	ug/l	4388450	4	13.669	3772360	50.0
unknown15.439	15.439	25.7	ug/l	1939970	4	13.669	3772360	50.0