

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112222\
 Data File : VN075377.D
 Acq On : 22 Nov 2022 18:55
 Operator : JC\MD
 Sample : N5675-01
 Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 AUD-1673

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\82N112122W.M
 Title : SW846 8260

Signal : TIC: VN075377.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.295	35	41	53	rVB2	13652	41203	2.01%	0.430%
2	2.507	70	77	79	rBV3	11959	22616	1.10%	0.236%
3	8.165	1031	1039	1042	rBV	64292	138589	6.75%	1.447%
4	8.224	1042	1049	1058	rVV2	240150	567471	27.64%	5.926%
5	8.318	1058	1065	1074	rVB3	14781	36005	1.75%	0.376%
6	8.441	1078	1086	1094	rBV2	60160	138690	6.76%	1.448%
7	8.583	1101	1110	1120	rVB	51048	116760	5.69%	1.219%
8	8.706	1121	1131	1138	rBV4	20875	69086	3.37%	0.721%
9	8.965	1169	1175	1188	rVB2	36665	75507	3.68%	0.788%
10	9.100	1188	1198	1206	rBV	273180	568262	27.68%	5.934%
11	10.565	1440	1447	1452	rBV	155664	288874	14.07%	3.017%
12	10.630	1452	1458	1473	rVV	1120517	2052881	100.00%	21.437%
13	11.647	1622	1631	1634	rBV3	11845	25634	1.25%	0.268%
14	11.747	1642	1648	1654	rVB2	12930	21323	1.04%	0.223%
15	11.865	1661	1668	1677	rBV	359699	647259	31.53%	6.759%
16	11.965	1680	1685	1689	rBV2	14691	23655	1.15%	0.247%
17	12.071	1696	1703	1708	rBV2	86646	150261	7.32%	1.569%
18	12.400	1746	1759	1766	rBV4	25629	75420	3.67%	0.788%
19	12.482	1766	1773	1778	rVB2	24890	41201	2.01%	0.430%
20	12.600	1778	1793	1805	rBV8	26282	110159	5.37%	1.150%
21	12.700	1805	1810	1813	rBV5	10708	20895	1.02%	0.218%
22	12.853	1830	1836	1846	rVB	225406	415114	20.22%	4.335%
23	13.024	1859	1865	1871	rVB5	24389	49750	2.42%	0.520%
24	13.100	1871	1878	1881	rBV2	44320	81079	3.95%	0.847%
25	13.159	1881	1888	1896	rVV3	162222	327400	15.95%	3.419%
26	13.224	1896	1899	1904	rVB4	18728	28421	1.38%	0.297%
27	13.353	1906	1921	1925	rBV4	33591	116210	5.66%	1.214%
28	13.394	1925	1928	1938	rVB	34721	61477	2.99%	0.642%
29	13.482	1938	1943	1948	rBV	64884	107579	5.24%	1.123%
30	13.535	1948	1952	1958	rVB	75806	109727	5.35%	1.146%
31	13.706	1969	1981	1990	rBV10	56427	184386	8.98%	1.925%
32	13.794	1990	1996	2005	rVV2	376649	676959	32.98%	7.069%
33	13.871	2005	2009	2016	rVB4	43338	89565	4.36%	0.935%
34	13.947	2017	2022	2024	rBV4	18553	28493	1.39%	0.298%
35	13.988	2024	2029	2031	rBV2	44319	64523	3.14%	0.674%
36	14.023	2032	2035	2044	rVB4	59675	128670	6.27%	1.344%

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37	14.106	2044	2049	2055	rBV2	101246	175060	8.53%	1.828%
38	14.188	2060	2063	2068	rVV	33445	53702	2.62%	0.561%
39	14.247	2068	2073	2075	rVV2	51445	84256	4.10%	0.880%
40	14.276	2075	2078	2082	rVV	56989	86093	4.19%	0.899%
41	14.329	2082	2087	2100	rVB	114141	214392	10.44%	2.239%
42	14.435	2100	2105	2113	rBV3	41567	85708	4.18%	0.895%
43	14.576	2123	2129	2134	rBV4	36375	73611	3.59%	0.769%
44	14.629	2134	2138	2140	rVV3	46137	65535	3.19%	0.684%
45	14.659	2140	2143	2146	rVV2	53685	82556	4.02%	0.862%
46	14.694	2146	2149	2153	rVV	47798	66395	3.23%	0.693%
47	14.735	2153	2156	2160	rVB4	34013	42624	2.08%	0.445%
48	14.794	2160	2166	2170	rVB8	15235	34769	1.69%	0.363%
49	14.847	2170	2175	2177	rBV3	15697	26109	1.27%	0.273%
50	14.935	2185	2190	2191	rBV4	36321	52624	2.56%	0.550%
51	14.959	2192	2194	2201	rVB2	46565	61271	2.98%	0.640%
52	15.041	2201	2208	2215	rBV6	46533	142974	6.96%	1.493%
53	15.270	2243	2247	2252	rBV6	16236	31042	1.51%	0.324%
54	15.318	2252	2255	2263	rVB8	20283	38206	1.86%	0.399%
55	15.594	2297	2302	2306	rBV6	23603	45162	2.20%	0.472%
56	15.747	2323	2328	2333	rBV5	22070	37552	1.83%	0.392%
57	15.835	2339	2343	2348	rVB7	16028	21029	1.02%	0.220%
58	15.947	2354	2362	2363	rBV7	17867	39370	1.92%	0.411%
59	16.017	2369	2374	2385	rVB9	14267	34187	1.67%	0.357%
60	16.112	2385	2390	2394	rBV8	16601	33430	1.63%	0.349%
61	16.165	2396	2399	2407	rVB10	19798	38037	1.85%	0.397%
62	16.482	2447	2453	2461	rBV4	42650	99222	4.83%	1.036%
63	16.712	2486	2492	2498	rBV5	28213	69024	3.36%	0.721%
64	16.782	2499	2504	2505	rBV4	27493	41322	2.01%	0.431%

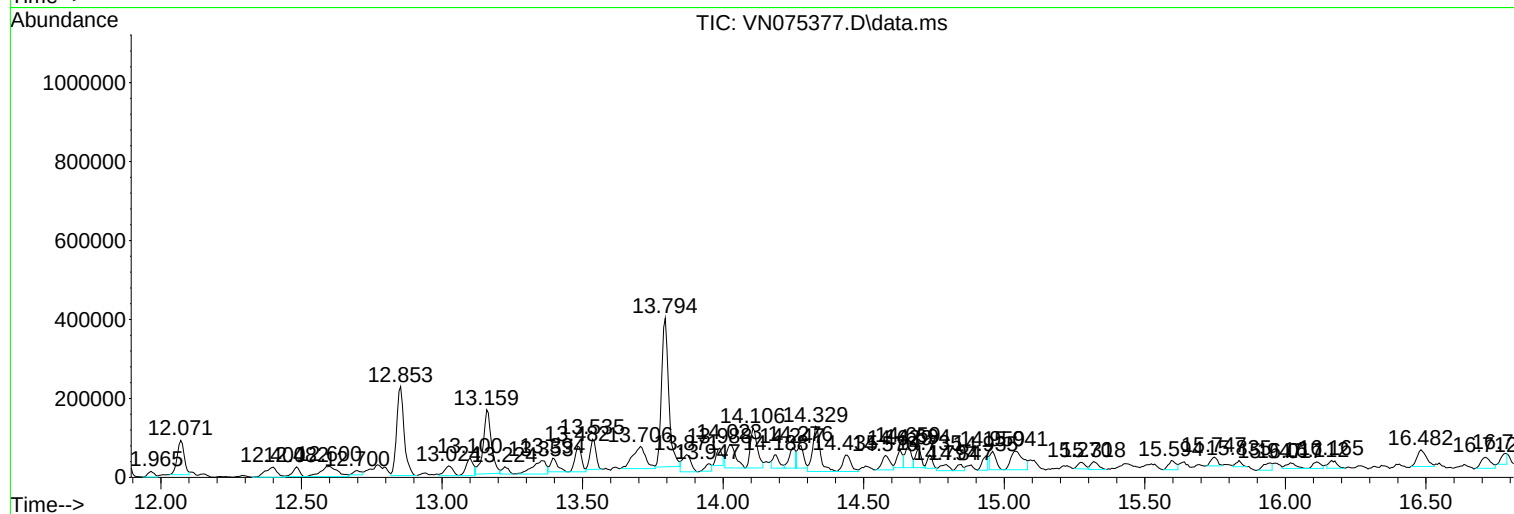
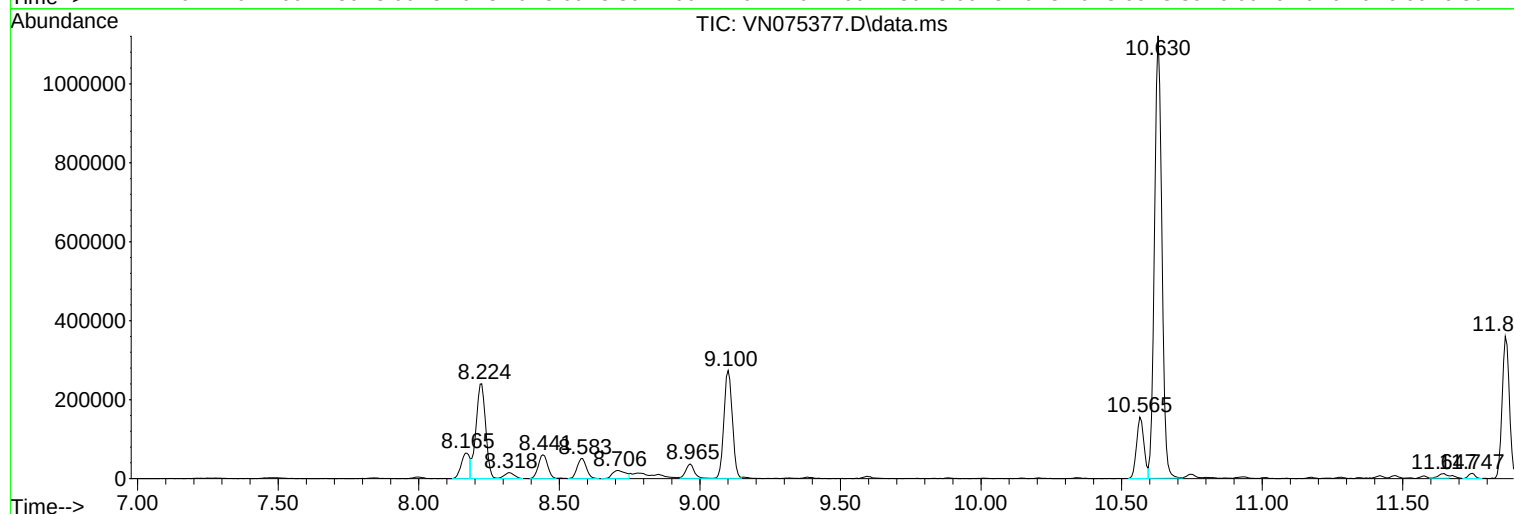
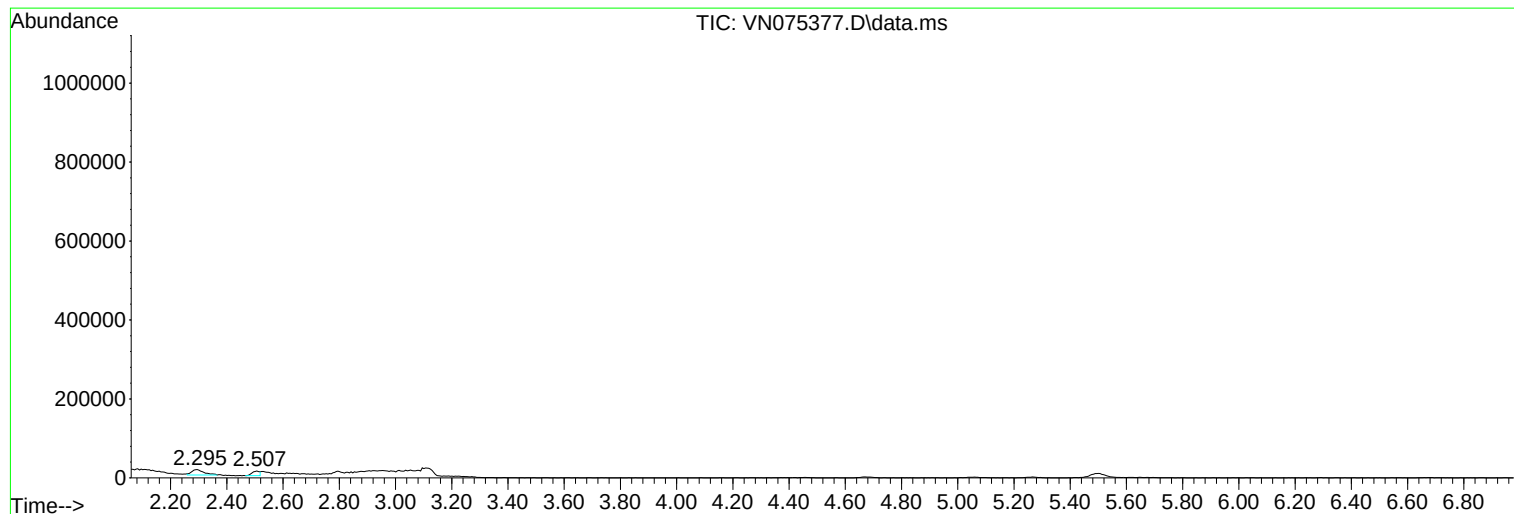
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112122W.M
Quant Title : SW846 8260

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



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Instrument :
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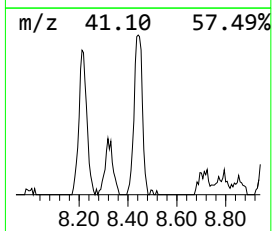
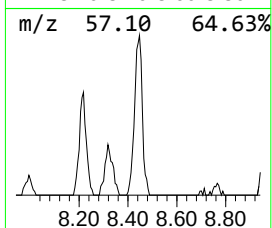
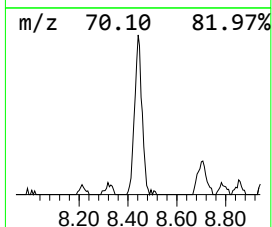
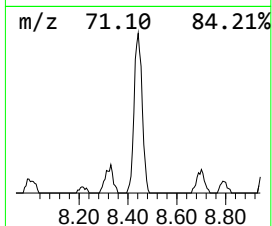
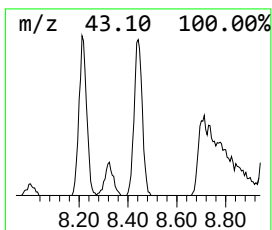
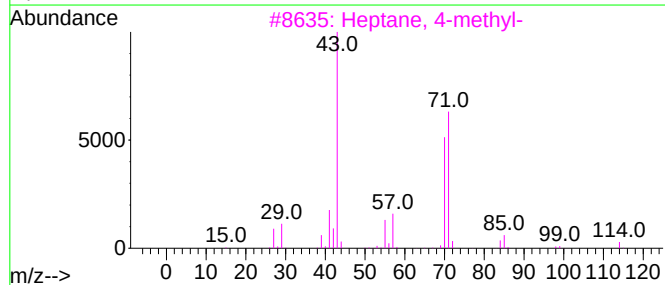
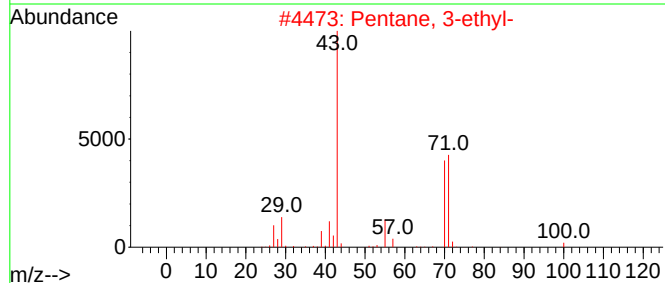
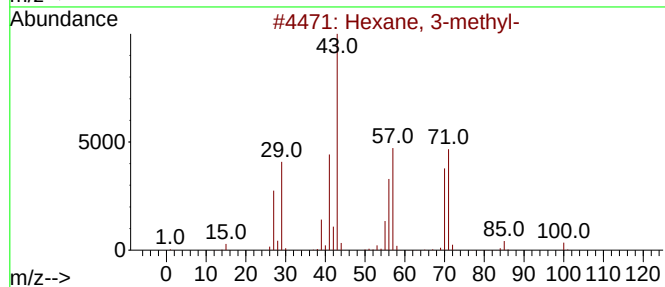
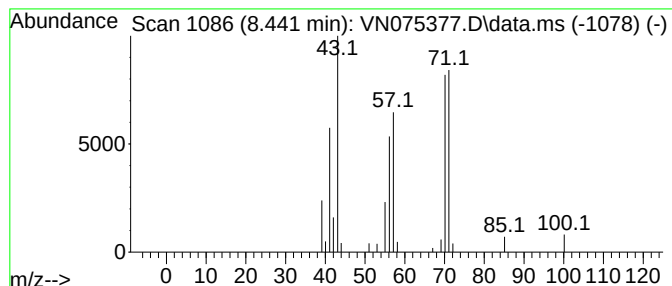
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.441	12.22 ug/l	138690	Pentafluorobenzene	8.224

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexane, 3-methyl-	100	C7H16	000589-34-4	91
2		Pentane, 3-ethyl-	100	C7H16	000617-78-7	64
3		Heptane, 4-methyl-	114	C8H18	000589-53-7	64
4		Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	64
5		Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	59



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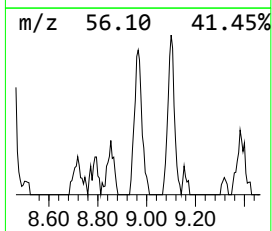
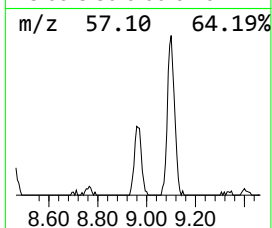
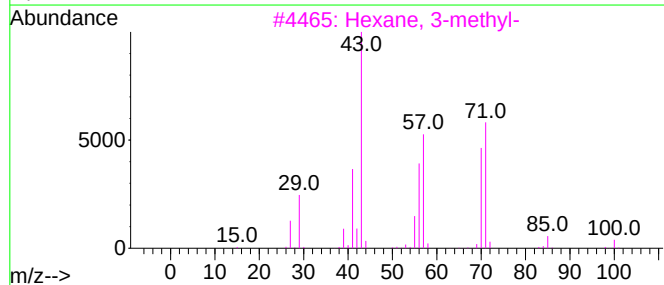
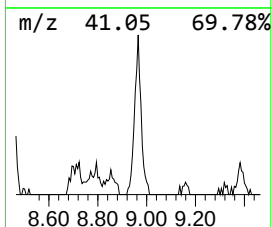
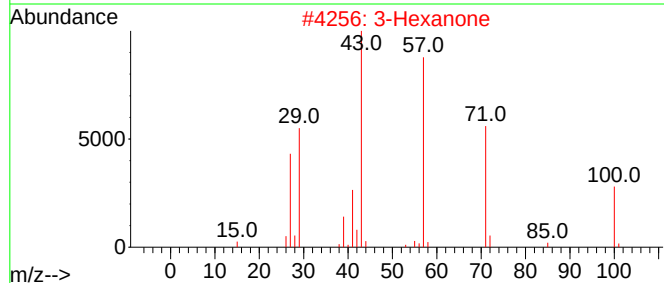
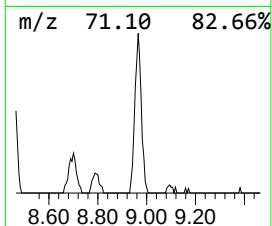
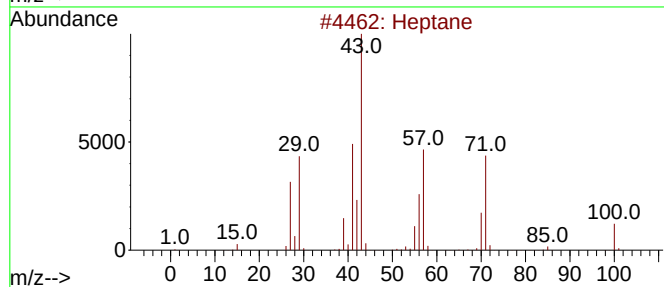
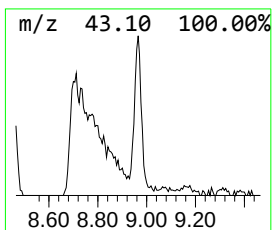
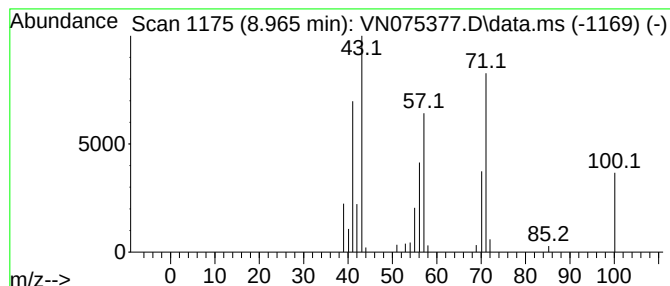
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112122W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Heptane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.965	6.64 ug/l	75507	1,4-Difluorobenzene	9.100

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane	100	C7H16	000142-82-5	90
2			3-Hexanone	100	C6H12O	000589-38-8	47
3			Hexane, 3-methyl-	100	C7H16	000589-34-4	45
4			Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	42
5			Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	38



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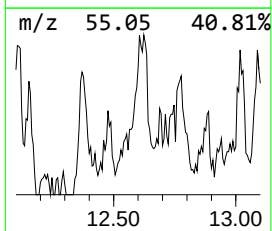
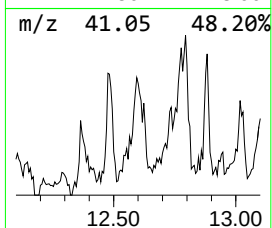
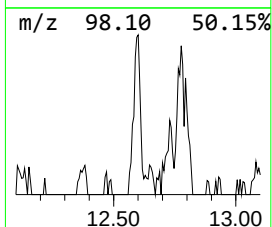
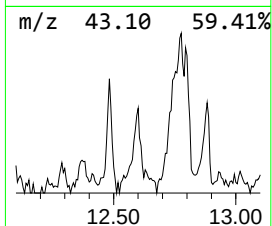
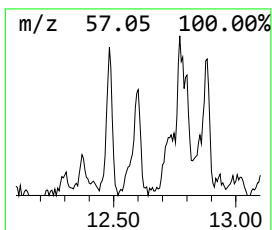
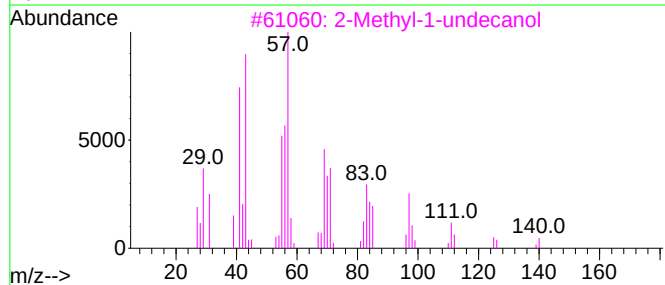
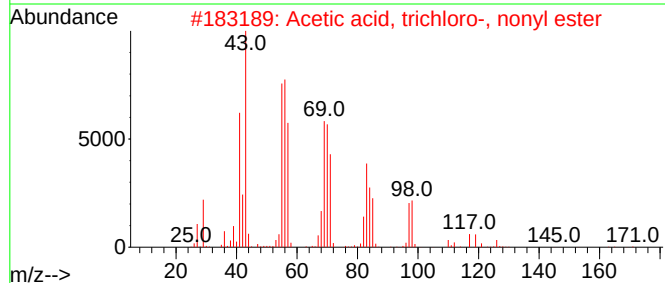
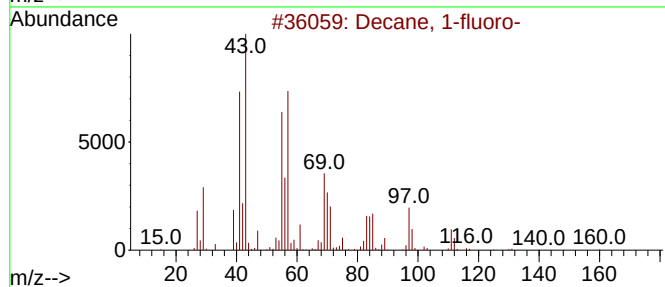
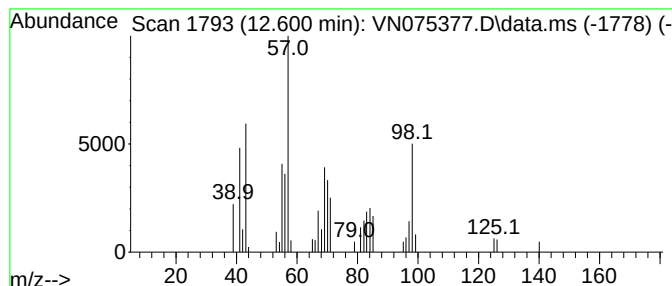
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Peak Number 3 unknown12.600 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.600	8.51 ug/l	110159	Chlorobenzene-d5	11.865

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 1-fluoro-	160	C10H21F	000334-56-5	47
2			Acetic acid, trichloro-, nonyl e...	288	C11H19Cl3O2	065611-32-7	43
3			2-Methyl-1-undecanol	186	C12H26O	010522-26-6	43
4			1-Fluorononane	146	C9H19F	000463-18-3	43
5			Dichloroacetic acid, nonyl ester	254	C11H20Cl2O2	083004-99-3	43



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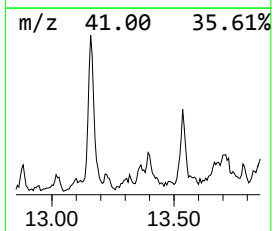
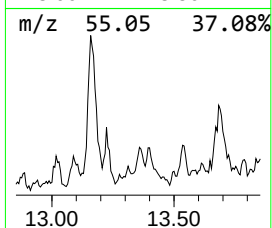
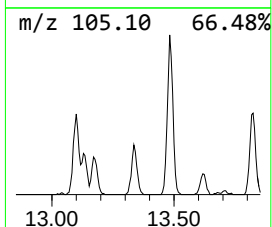
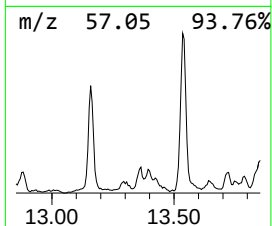
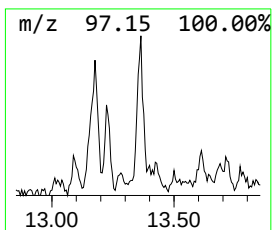
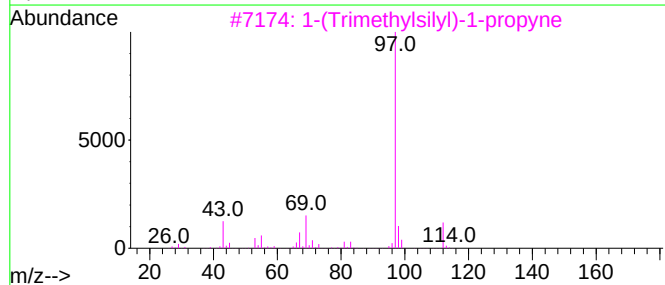
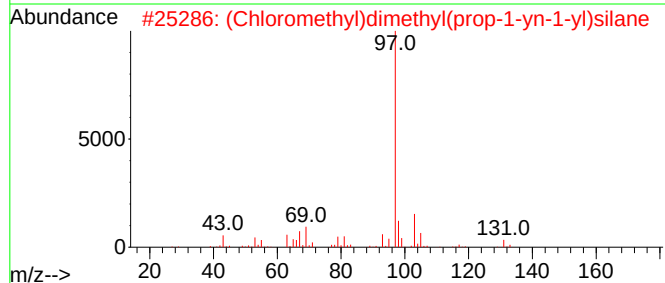
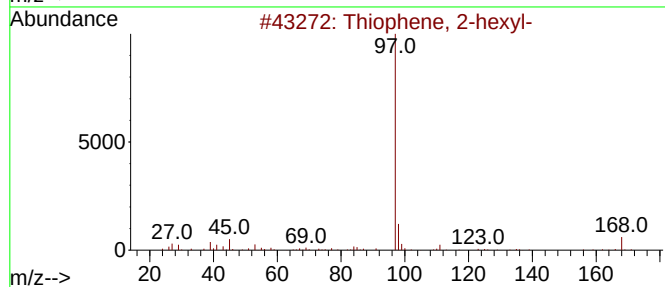
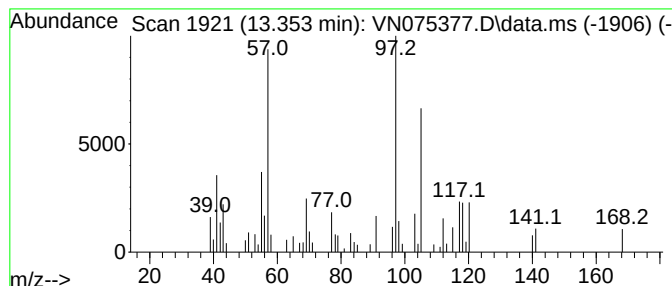
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112122W.M
Quant Title : SW846 8260

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

Peak Number 4 unknown13.353 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.353	8.58 ug/l	116210	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thiophene, 2-hexyl-	168	C10H16S	018794-77-9	43
2			(Chloromethyl)dimethyl(prop-1-yn...	146	C6H11ClSi	1000390-26-6	38
3			1-(Trimethylsilyl)-1-propyne	112	C6H12Si	006224-91-5	38
4			4-Hepten-3-one, 2,6-dimethyl-	140	C9H16O	056259-14-4	38
5			Cyclohexane, 1,1-dimethyl-	112	C8H16	000590-66-9	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112222\
Data File : VN075377.D
Acq On : 22 Nov 2022 18:55
Operator : JC\MD
Sample : N5675-01
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
AUD-1673

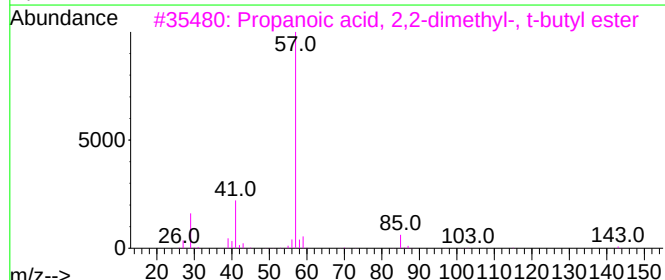
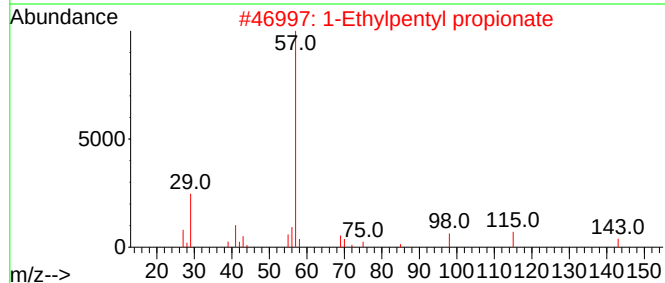
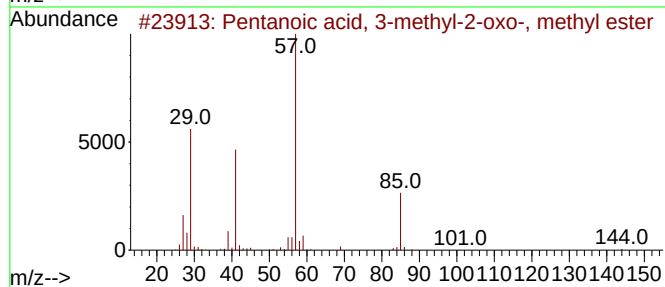
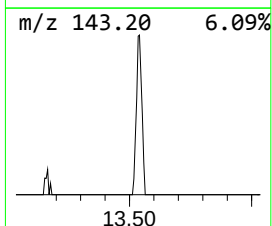
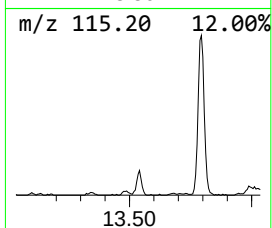
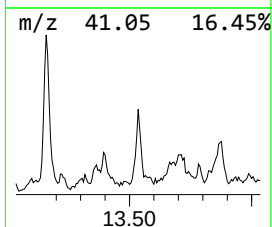
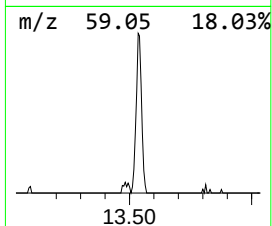
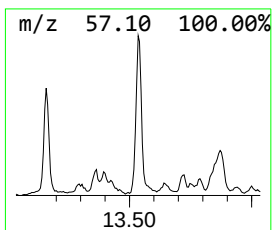
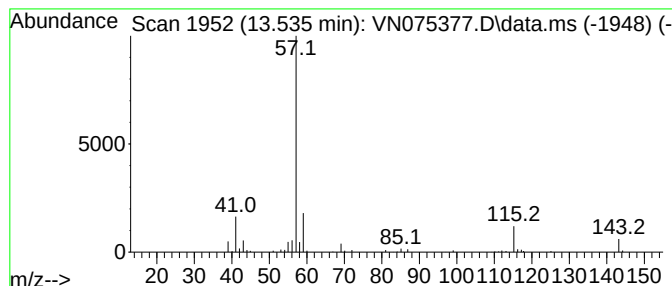
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Quant Title : SW846 8260

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

Peak Number 5 unknown13.535 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.535	8.10 ug/l	109727	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentanoic acid, 3-methyl-2-oxo-,...	144	C7H12O3	003682-42-6	32
2			1-Ethylpentyl propionate	172	C10H20O2	1000430-89-7	32
3			Propanoic acid, 2,2-dimethyl-, t...	158	C9H18O2	016474-43-4	23
4			Propane, 1-(1,1-dimethylethoxy)-...	130	C8H18O	033021-02-2	23
5			Thiolane-3,4-dicarbonitrile, 2,5...	386	C16H20F6N2S	1000260-74-6	17



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112222\
Data File : VN075377.D
Acq On : 22 Nov 2022 18:55
Operator : JC\MD
Sample : N5675-01
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
AUD-1673

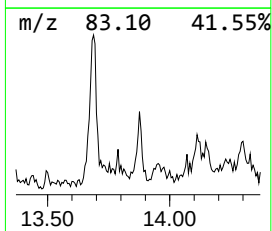
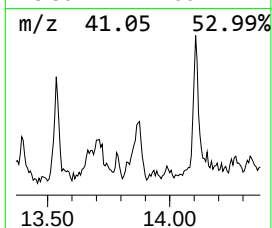
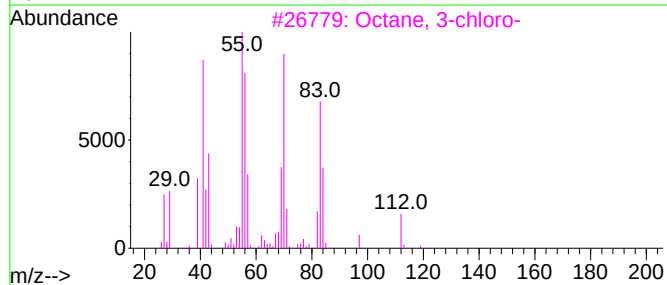
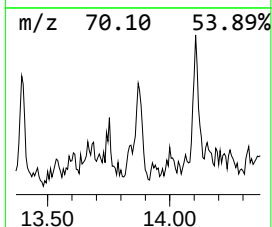
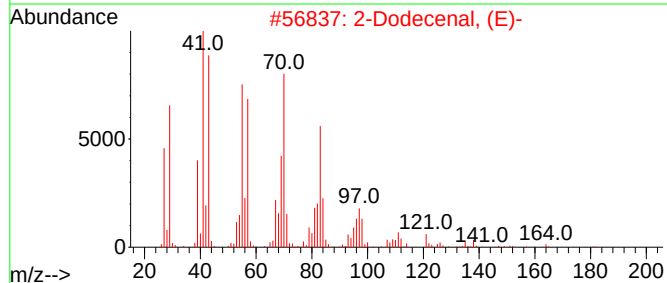
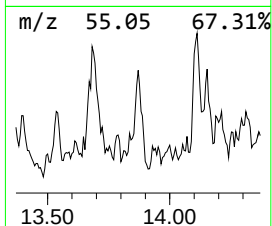
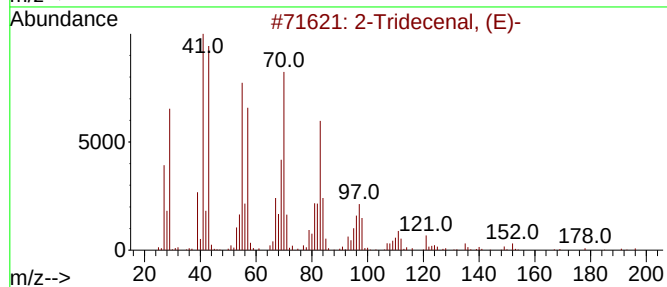
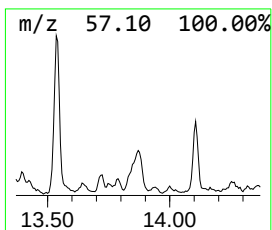
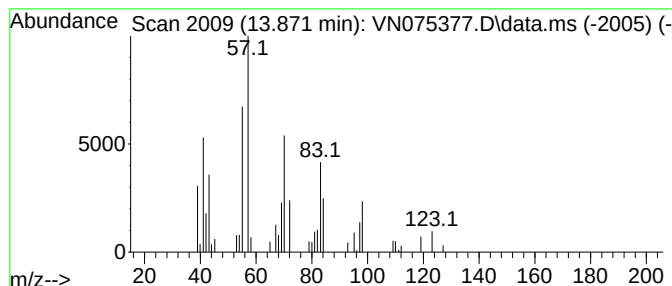
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Quant Title : SW846 8260

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

Peak Number 6 unknown13.871 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.871	6.62 ug/l	89565	1,4-Dichlorobenzene-d4	13.794

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Tridecenal, (E)-		196	C13H24O	007069-41-2	43
2	2-Dodecenal, (E)-		182	C12H22O	020407-84-5	43
3	Octane, 3-chloro-		148	C8H17Cl	001117-79-9	38
4	1-Pentene, 2,3-dimethyl-		98	C7H14	003404-72-6	38
5	Heptyl isobutyl carbonate		216	C12H24O3	959068-08-7	27



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112222\
Data File : VN075377.D
Acq On : 22 Nov 2022 18:55
Operator : JC\MD
Sample : N5675-01
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
AUD-1673

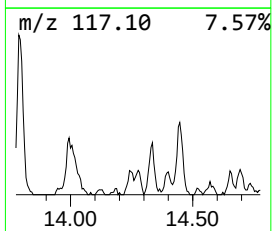
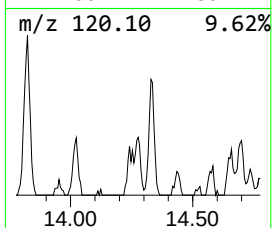
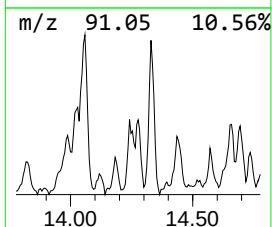
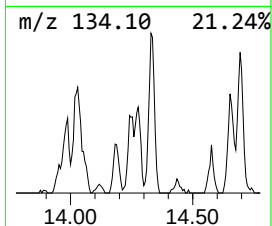
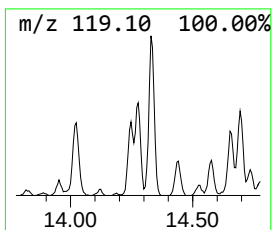
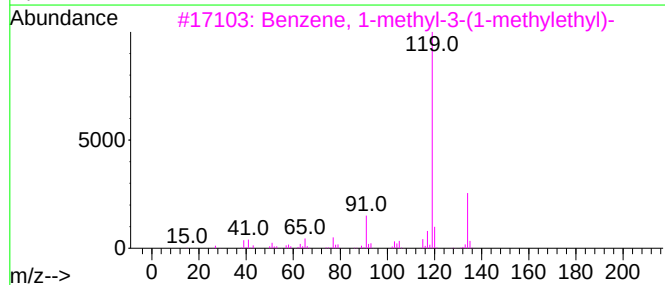
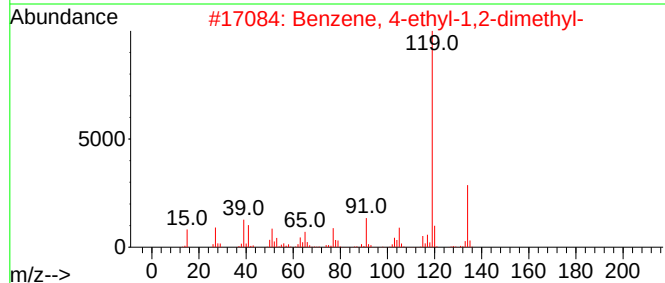
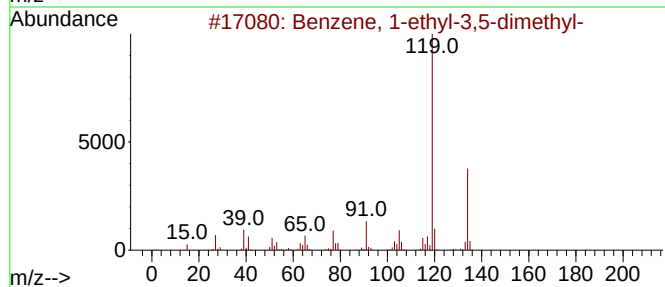
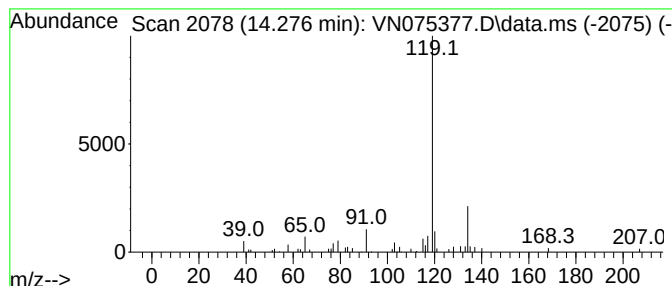
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1-ethyl-3,5-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.276	6.36 ug/l	86093	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	90
2			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	87
3			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	87
4			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	87
5			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112222\
Data File : VN075377.D
Acq On : 22 Nov 2022 18:55
Operator : JC\MD
Sample : N5675-01
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 23 Sample Multiplier: 1

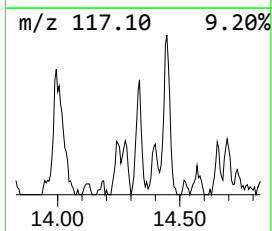
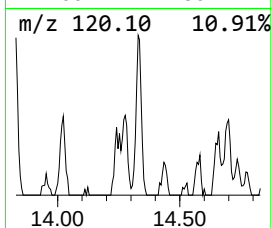
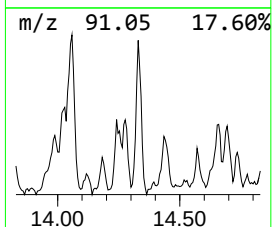
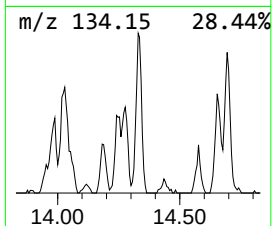
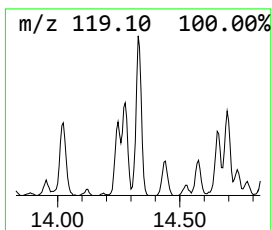
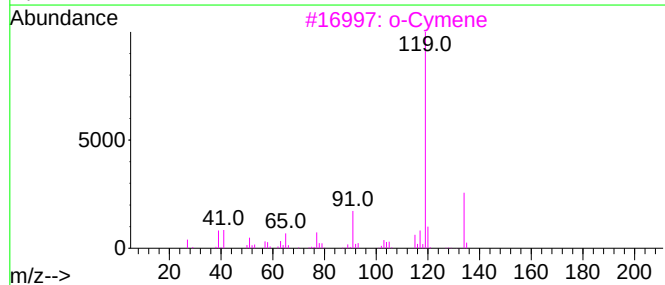
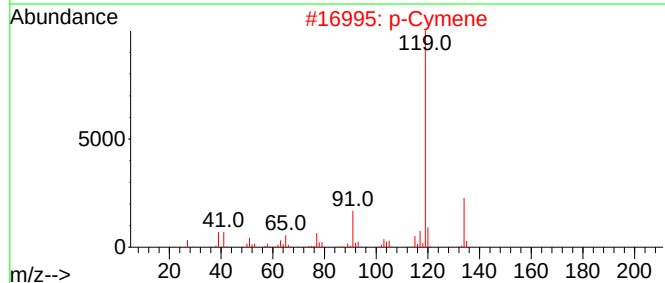
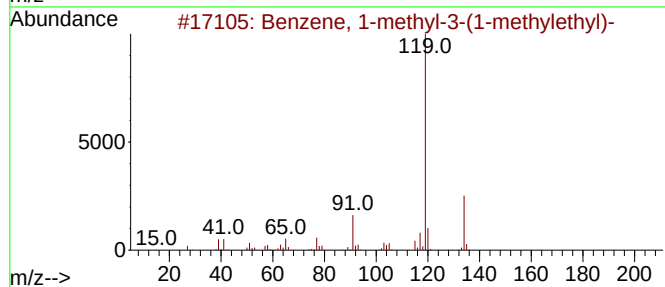
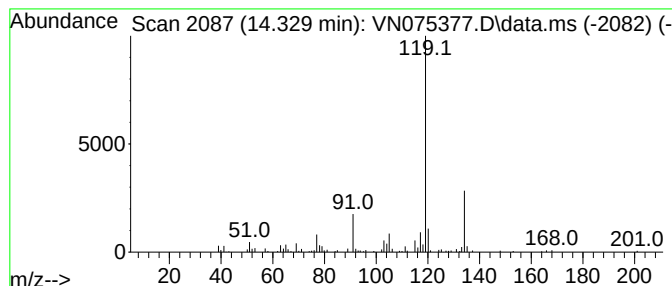
Instrument :
MSVOA_N
ClientSampleId :
AUD-1673

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112122W.M
Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1-methyl-3-(1-meth... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.329	15.83 ug/l	214392	1,4-Dichlorobenzene-d4		13.794	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Benzene, 1-methyl-3-(1-methyleth...		134	C10H14	000535-77-3	95
2	p-Cymene		134	C10H14	000099-87-6	95
3	o-Cymene		134	C10H14	000527-84-4	95
4	Benzene, 2-ethyl-1,4-dimethyl-		134	C10H14	001758-88-9	94
5	Benzene, 2-ethyl-1,3-dimethyl-		134	C10H14	002870-04-4	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112222\
Data File : VN075377.D
Acq On : 22 Nov 2022 18:55
Operator : JC\MD
Sample : N5675-01
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
AUD-1673

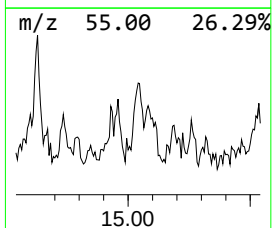
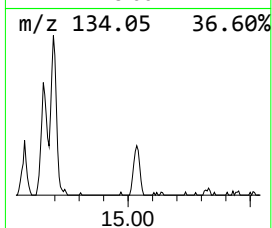
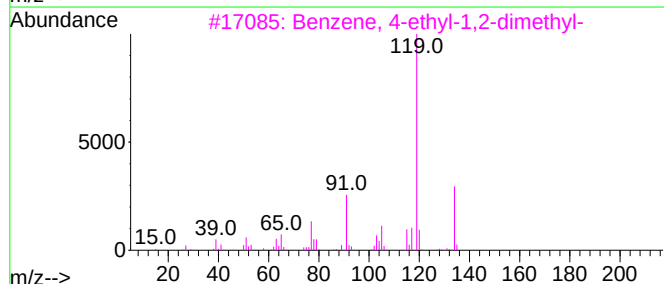
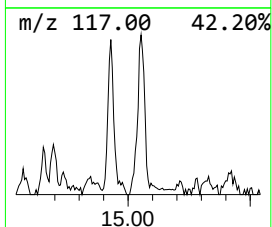
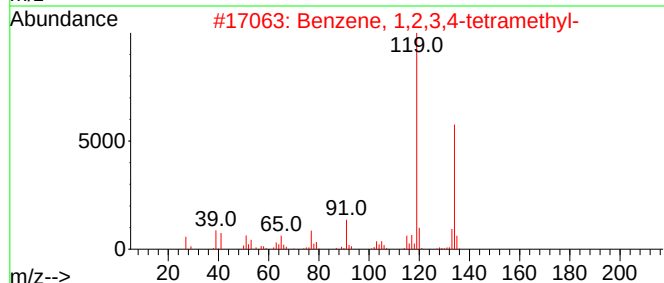
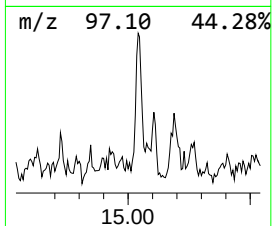
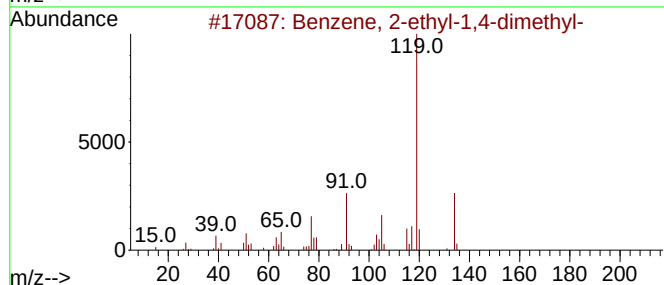
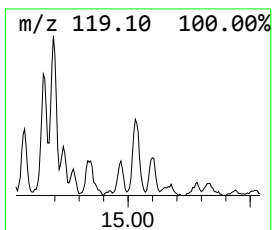
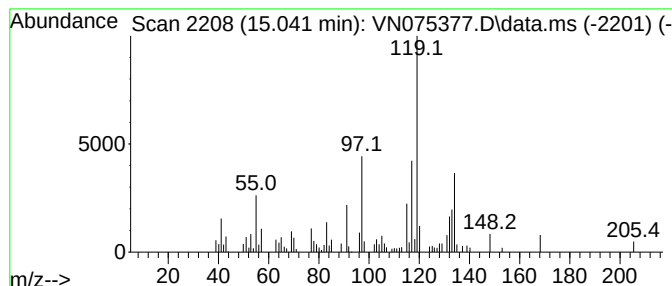
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, 2-ethyl-1,4-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.041	10.56 ug/l	142974	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	50
2			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	50
3			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	50
4			o-Cymene	134	C10H14	000527-84-4	50
5			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112222\
Data File : VN075377.D
Acq On : 22 Nov 2022 18:55
Operator : JC\MD
Sample : N5675-01
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
AUD-1673

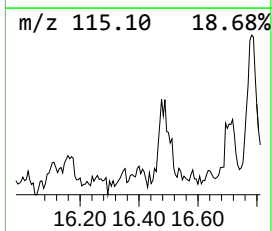
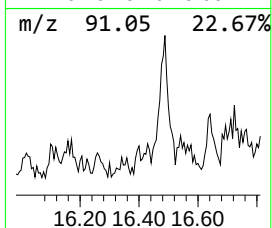
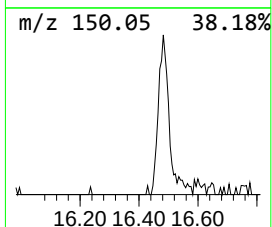
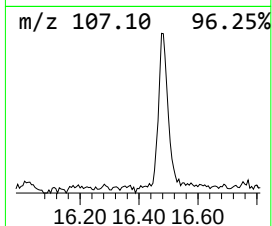
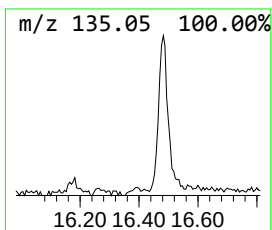
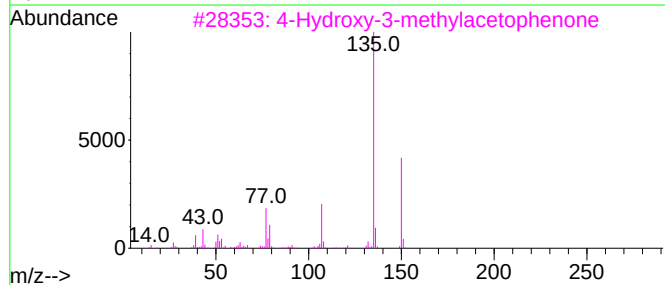
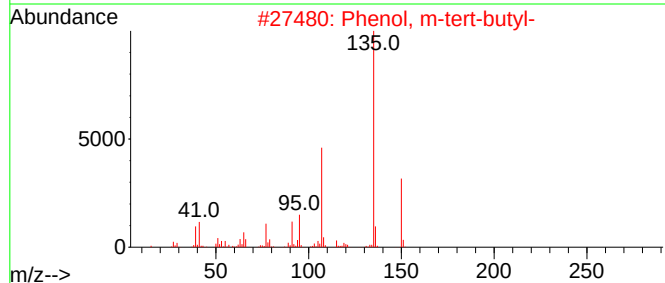
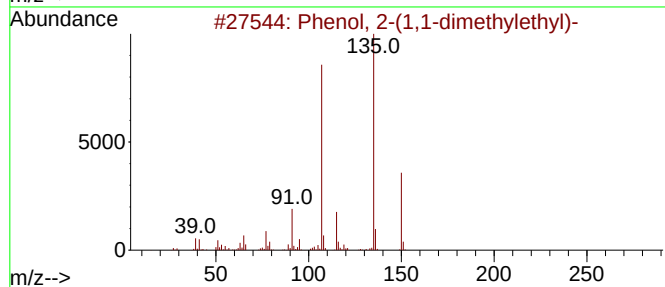
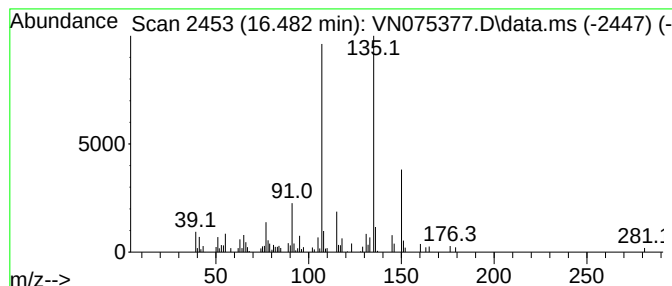
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Quant Title : SW846 8260

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

Peak Number 10 Phenol, 2-(1,1-dimethylethyl)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.482	7.33 ug/l	99222	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2-(1,1-dimethylethyl)-	150	C10H14O	000088-18-6	90
2			Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	64
3			4-Hydroxy-3-methylacetophenone	150	C9H10O2	000876-02-8	60
4			4-Hydroxy-2-methylacetophenone	150	C9H10O2	000875-59-2	58
5			2,5-Diethylphenol	150	C10H14O	000876-20-0	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112222\
Data File : VN075377.D
Acq On : 22 Nov 2022 18:55
Operator : JC\MD
Sample : N5675-01
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
AUD-1673

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112122W.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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Heptane	8.965	6.6	ug/l	75507	2	9.100	568262	50.0
unknown12.600	12.600	8.5	ug/l	110159	3	11.865	647259	50.0
unknown13.353	13.353	8.6	ug/l	116210	4	13.794	676959	50.0
unknown13.535	13.535	8.1	ug/l	109727	4	13.794	676959	50.0
unknown13.871	13.871	6.6	ug/l	89565	4	13.794	676959	50.0
Benzene, 1-ethy...	14.276	6.4	ug/l	86093	4	13.794	676959	50.0
Benzene, 1-meth...	14.329	15.8	ug/l	214392	4	13.794	676959	50.0
Benzene, 2-ethy...	15.041	10.6	ug/l	142974	4	13.794	676959	50.0
Phenol, 2-(1,1-...	16.482	7.3	ug/l	99222	4	13.794	676959	50.0