

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031924\
 Data File : VN081483.D
 Acq On : 19 Mar 2024 20:08
 Operator : JC\MD
 Sample : P1772-01
 Misc : 1.09g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 1151

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\82N031824W.M
 Title : SW846 8260

Signal : TIC: VN081483.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.495	80	92	99	rBV3	51596	174054	1.53%	0.228%
2	6.677	792	803	817	rBV5	34298	134219	1.18%	0.176%
3	8.165	1045	1056	1060	rBV	345099	842368	7.41%	1.103%
4	8.218	1060	1065	1074	rVV	772726	1746245	15.37%	2.287%
5	8.324	1076	1083	1091	rVB2	45686	114810	1.01%	0.150%
6	8.441	1094	1103	1111	rBV	229386	519455	4.57%	0.680%
7	8.577	1117	1126	1135	rBV	368684	828985	7.30%	1.086%
8	8.694	1140	1146	1155	rVV5	39703	115708	1.02%	0.152%
9	8.965	1182	1192	1201	rBV	433649	877450	7.72%	1.149%
10	9.100	1207	1215	1225	rBV	940634	1930837	16.99%	2.528%
11	9.594	1288	1299	1304	rBV5	80643	215163	1.89%	0.282%
12	10.565	1456	1464	1471	rBV	1387274	2615552	23.02%	3.425%
13	10.629	1471	1475	1488	rVV	121496	252485	2.22%	0.331%
14	10.741	1489	1494	1503	rVB2	65181	120438	1.06%	0.158%
15	11.641	1642	1647	1651	rBV4	90485	176539	1.55%	0.231%
16	11.747	1660	1665	1670	rVB	98475	166437	1.46%	0.218%
17	11.865	1678	1685	1695	rVB	1166249	2157394	18.99%	2.825%
18	11.965	1697	1702	1706	rBV2	138239	243083	2.14%	0.318%
19	12.071	1712	1720	1725	rBV	896430	1611559	14.18%	2.110%
20	12.400	1766	1776	1782	rBV2	326649	873615	7.69%	1.144%
21	12.482	1785	1790	1796	rVB2	173913	293156	2.58%	0.384%
22	12.606	1803	1811	1812	rBV4	106191	235976	2.08%	0.309%
23	12.770	1836	1839	1842	rBV3	111361	171365	1.51%	0.224%
24	12.853	1847	1853	1862	rVB2	1021486	2001563	17.62%	2.621%
25	13.035	1878	1884	1889	rBV	197203	355411	3.13%	0.465%
26	13.100	1889	1895	1898	rVV	624311	1090145	9.59%	1.428%
27	13.159	1899	1905	1913	rVV2	1666724	3671635	32.31%	4.808%
28	13.229	1913	1917	1922	rVB2	202701	326664	2.87%	0.428%
29	13.341	1927	1936	1941	rBV2	341782	1057778	9.31%	1.385%
30	13.394	1941	1945	1954	rVB2	668598	1239238	10.91%	1.623%
31	13.482	1955	1960	1965	rBV	1096068	1730378	15.23%	2.266%
32	13.523	1965	1967	1972	rVB2	139423	201494	1.77%	0.264%
33	13.576	1972	1976	1979	rBV2	263505	356229	3.14%	0.466%
34	13.617	1980	1983	1985	rBV3	122883	149799	1.32%	0.196%
35	13.676	1989	1993	1997	rVV5	576955	1176310	10.35%	1.540%
36	13.717	1997	2000	2003	rVV3	647484	914980	8.05%	1.198%

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37	13.753	2003	2006	2008	rVV	410942	532876	4.69%	0.698%
38	13.788	2008	2012	2017	rVV2	1694064	3165185	27.86%	4.145%
39	13.853	2021	2023	2031	rVB2	871729	1375978	12.11%	1.802%
40	13.941	2032	2038	2041	rBV5	296042	611219	5.38%	0.800%
41	13.988	2042	2046	2056	rBV4	578579	1763117	15.52%	2.309%
42	14.106	2061	2066	2072	rBV	7170531	11362751	100.00%	14.880%
43	14.217	2082	2085	2088	rVB3	292811	332808	2.93%	0.436%
44	14.264	2088	2093	2098	rBV5	742802	1509788	13.29%	1.977%
45	14.370	2108	2111	2117	rVB4	990884	1551725	13.66%	2.032%
46	14.441	2118	2123	2127	rBV4	526737	1023850	9.01%	1.341%
47	14.506	2130	2134	2139	rBV4	466779	772015	6.79%	1.011%
48	14.582	2142	2147	2150	rBV3	1156846	2225296	19.58%	2.914%
49	14.629	2151	2155	2158	rVV3	2308116	3526541	31.04%	4.618%
50	14.664	2158	2161	2164	rVB	784544	933623	8.22%	1.223%
51	14.735	2169	2173	2176	rBV2	993187	1422147	12.52%	1.862%
52	14.770	2176	2179	2180	rBV	348703	370010	3.26%	0.485%
53	14.959	2206	2211	2217	rBV	4245671	6019022	52.97%	7.882%
54	15.041	2219	2225	2230	rBV4	1690256	3878154	34.13%	5.079%
55	16.476	2462	2469	2481	rVB	1482755	3298570	29.03%	4.320%

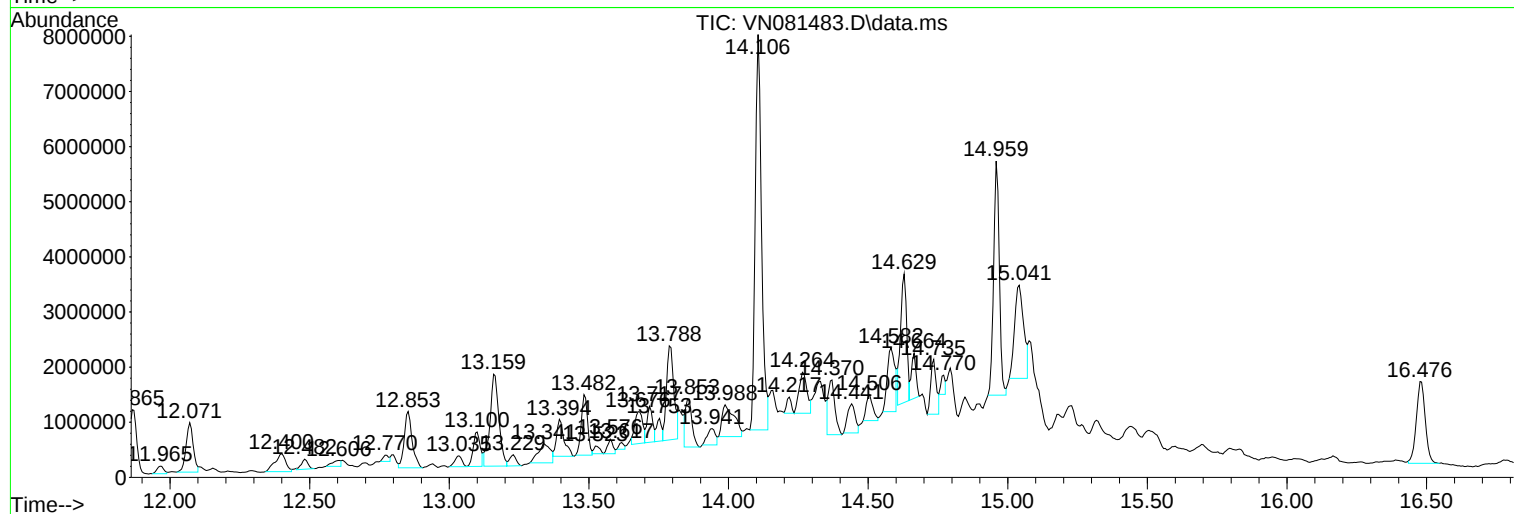
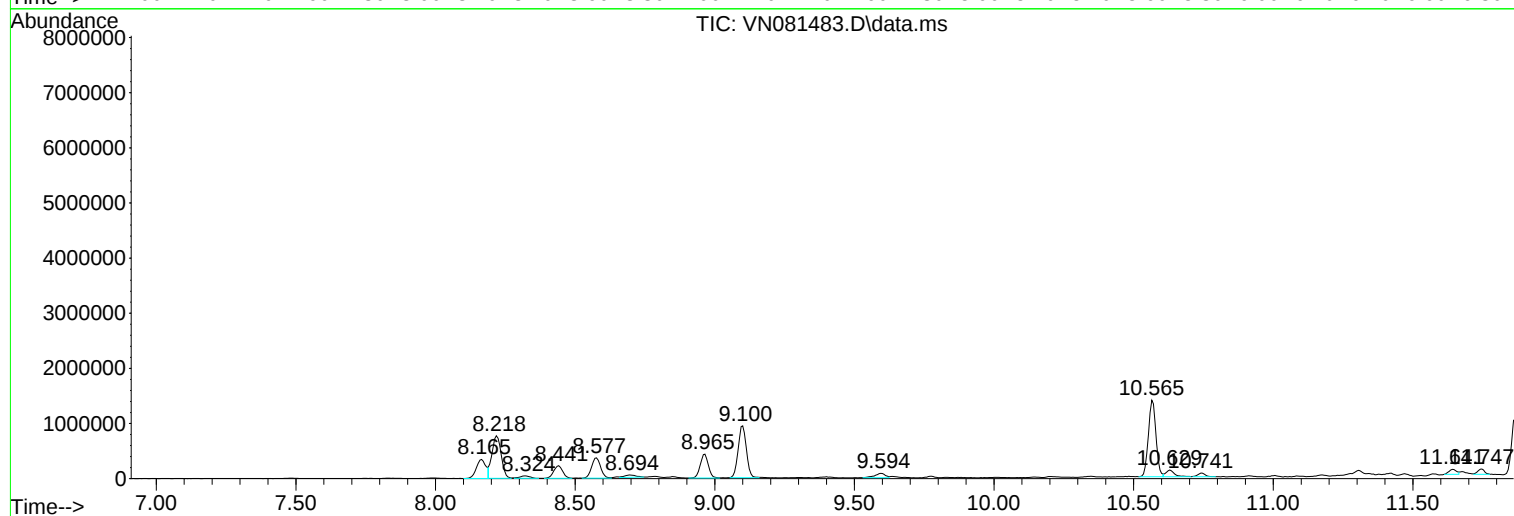
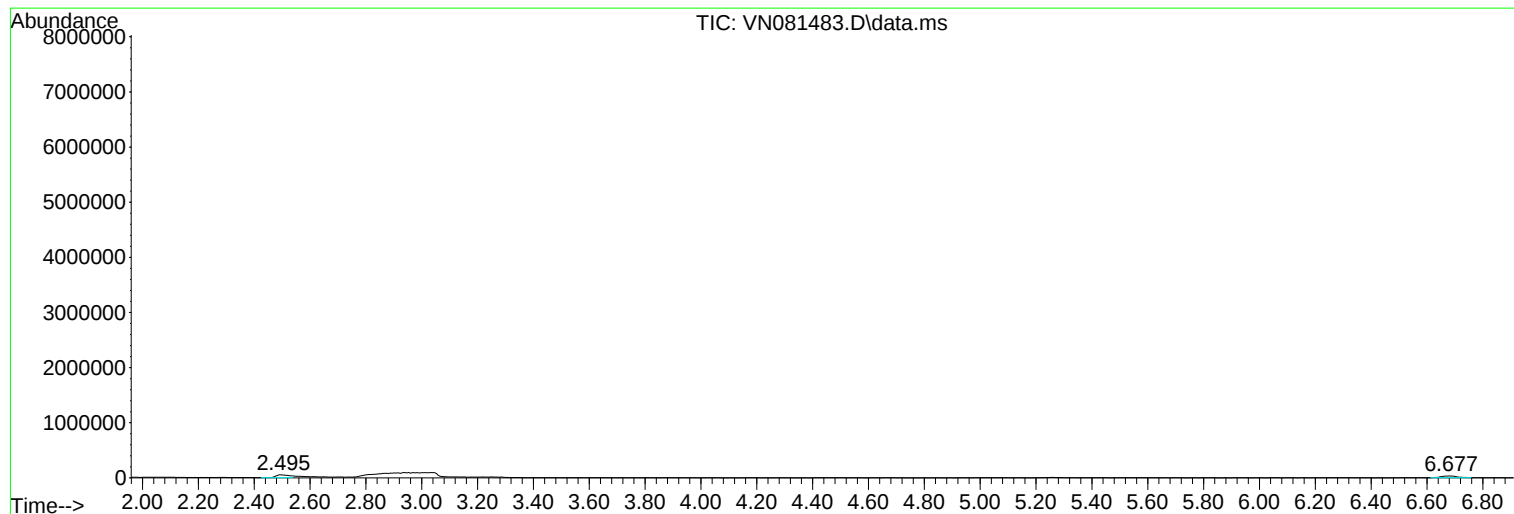
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Quant Title : SW846 8260

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



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Instrument :
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ClientSampleId :
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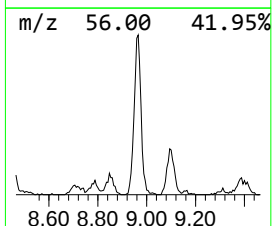
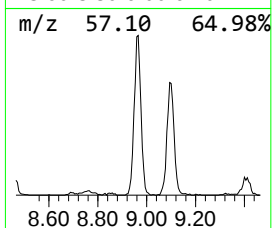
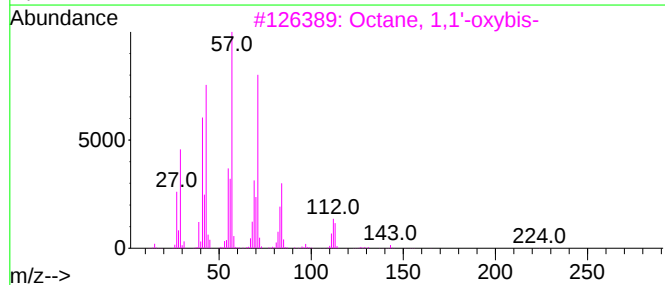
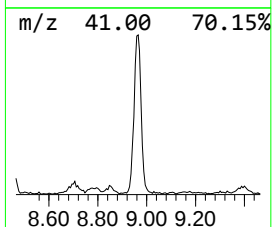
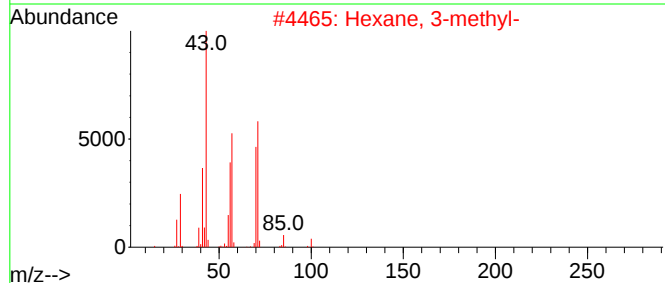
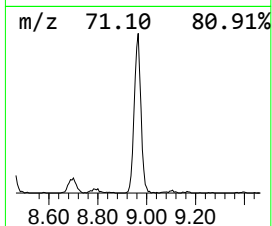
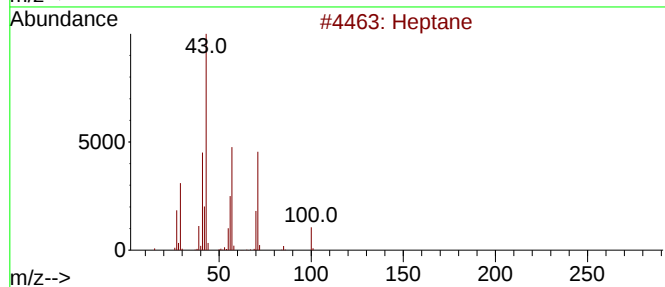
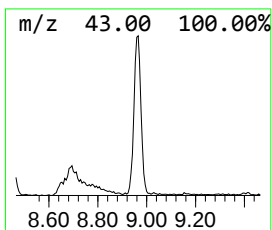
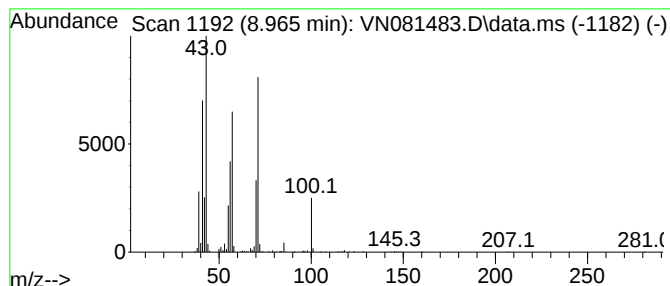
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.M
Quant Title : SW846 8260

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

Peak Number 1 Heptane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.965	22.72 ug/l	877450	1,4-Difluorobenzene	9.100

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane	100	C7H16	000142-82-5	91
2			Hexane, 3-methyl-	100	C7H16	000589-34-4	50
3			Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	50
4			3-Hexanone	100	C6H12O	000589-38-8	49
5			Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	47



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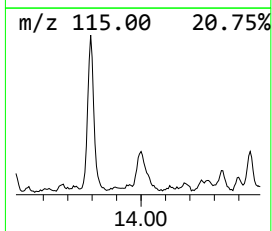
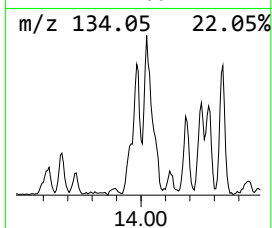
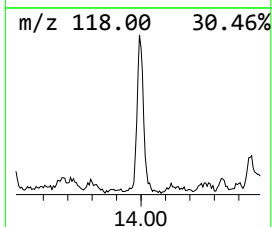
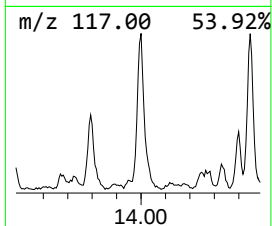
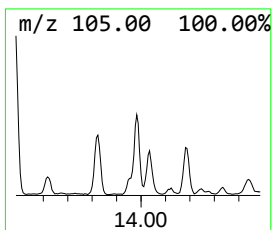
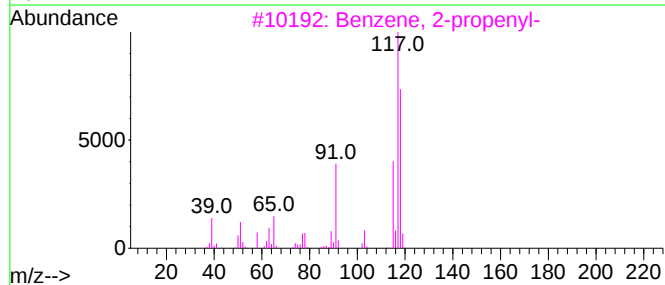
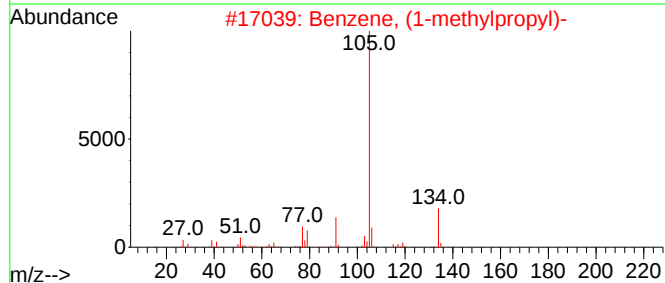
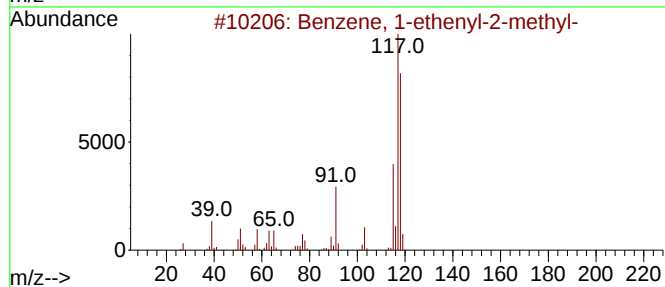
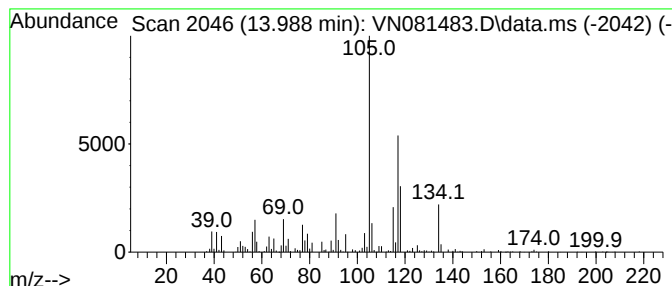
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown13.988 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.988	27.85 ug/l	1763120	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	46
2			Benzene, (1-methylpropyl)-	134	C10H14	000135-98-8	42
3			Benzene, 2-propenyl-	118	C9H10	000300-57-2	41
4			Benzene, cyclopropyl-	118	C9H10	000873-49-4	38
5			Benzene, 1-methyl-3-propyl-	134	C10H14	001074-43-7	38



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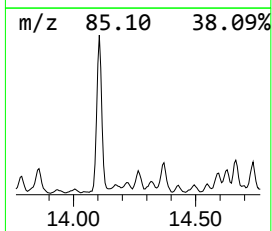
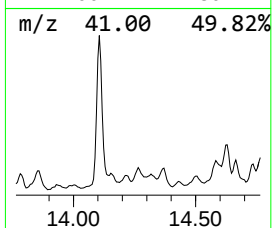
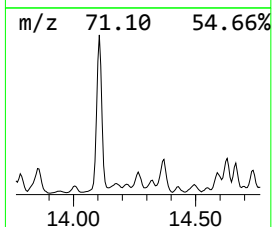
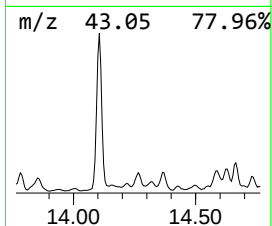
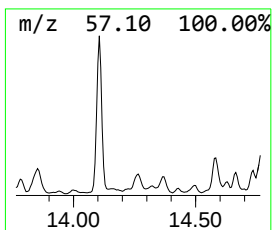
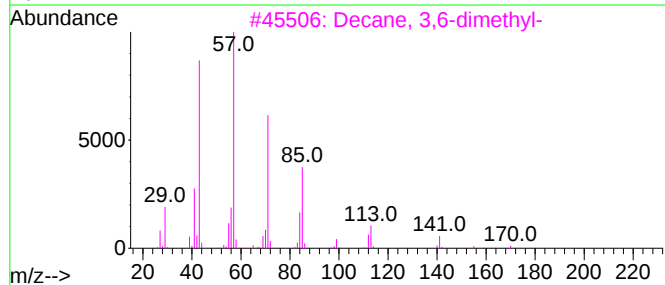
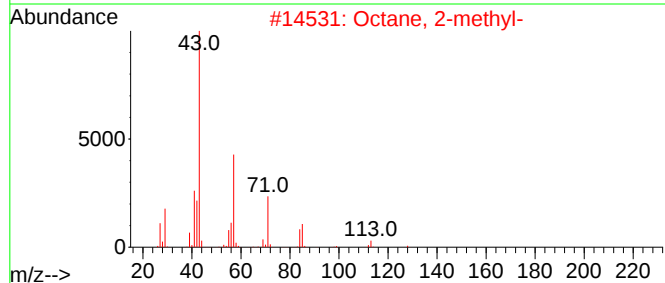
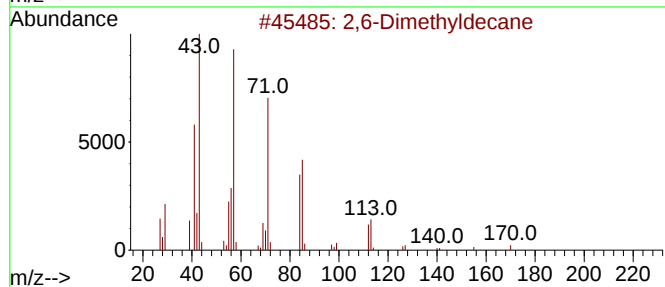
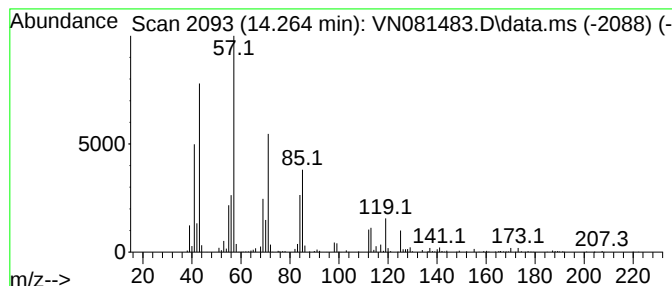
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2,6-Dimethyldecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.265	23.85 ug/l	1509790	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,6-Dimethyldecane	170	C12H26	013150-81-7	96
2			Octane, 2-methyl-	128	C9H20	003221-61-2	81
3			Decane, 3,6-dimethyl-	170	C12H26	017312-53-7	76
4			Octane, 2,3,3-trimethyl-	156	C11H24	062016-30-2	64
5			Heptadecane	240	C17H36	000629-78-7	53



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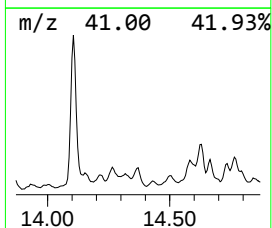
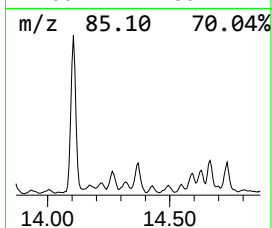
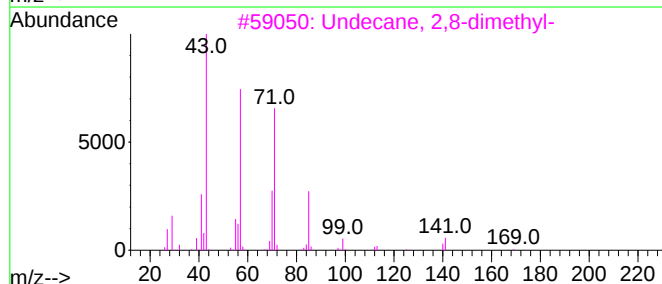
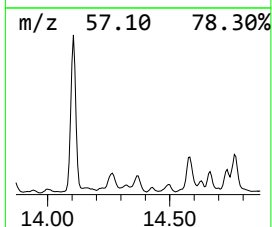
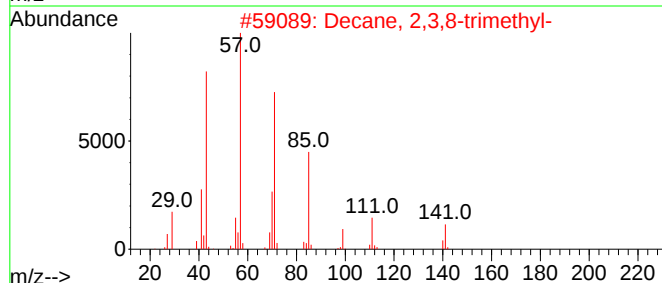
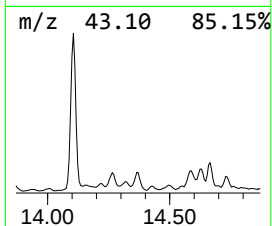
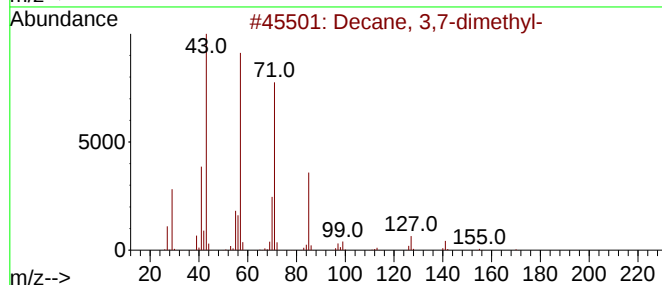
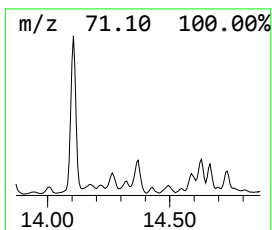
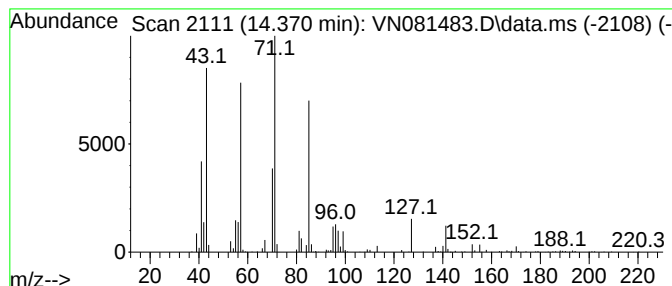
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Quant Title : SW846 8260

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

Peak Number 4 Decane, 3,7-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.370	24.51 ug/l	1551730	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 3,7-dimethyl-	170	C12H26	017312-54-8	81
2			Decane, 2,3,8-trimethyl-	184	C13H28	062238-14-6	59
3			Undecane, 2,8-dimethyl-	184	C13H28	017301-25-6	59
4			Nonane, 5-methyl-5-propyl-	184	C13H28	017312-75-3	50
5			Sulfurous acid, hexyl 2-pentyl e...	236	C11H24O3S	1000309-15-6	47



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1151

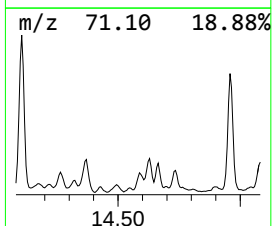
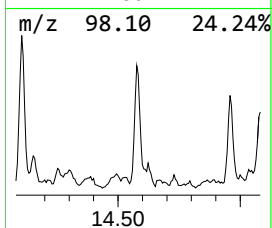
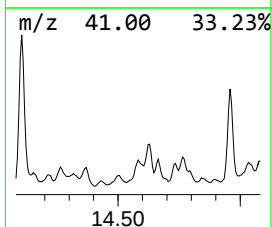
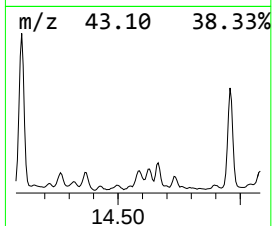
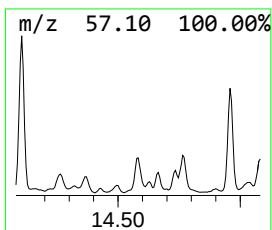
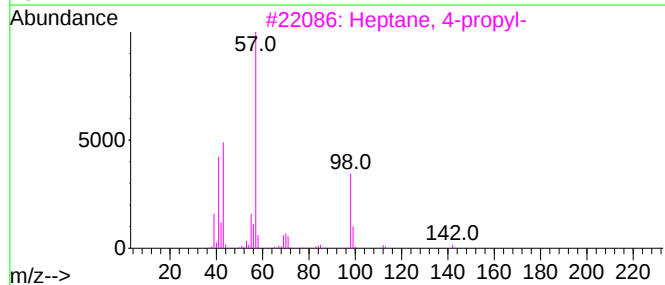
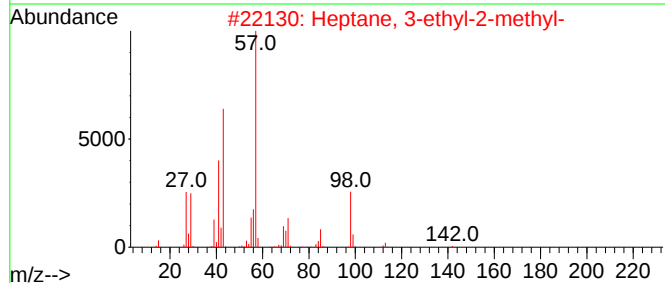
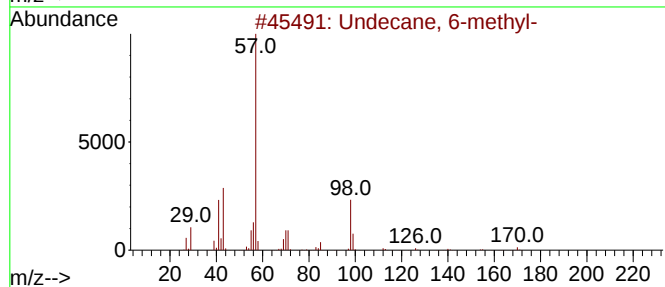
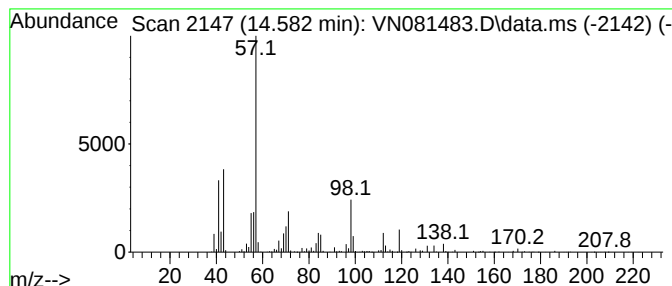
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Quant Title : SW846 8260

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

Peak Number 5 Undecane, 6-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.582	35.15 ug/l	2225300	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane, 6-methyl-	170	C12H26	017302-33-9	60
2			Heptane, 3-ethyl-2-methyl-	142	C10H22	014676-29-0	47
3			Heptane, 4-propyl-	142	C10H22	003178-29-8	43
4			Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	43
5			Carbonic acid, heptyl vinyl ester	186	C10H18O3	1010383-25-4	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031924\
Data File : VN081483.D
Acq On : 19 Mar 2024 20:08
Operator : JC\MD
Sample : P1772-01
Misc : 1.09g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1151

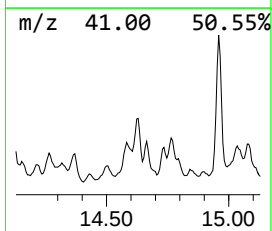
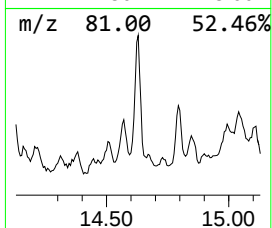
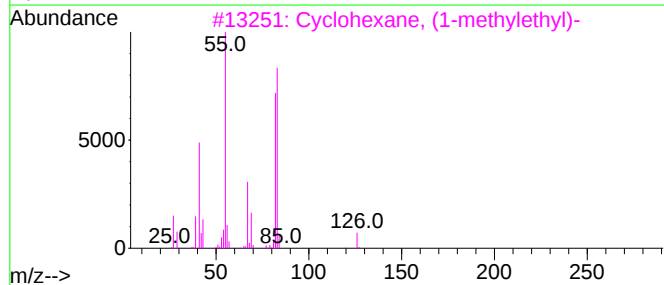
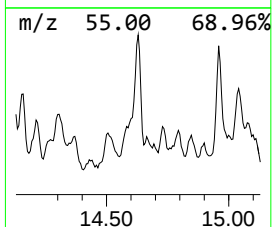
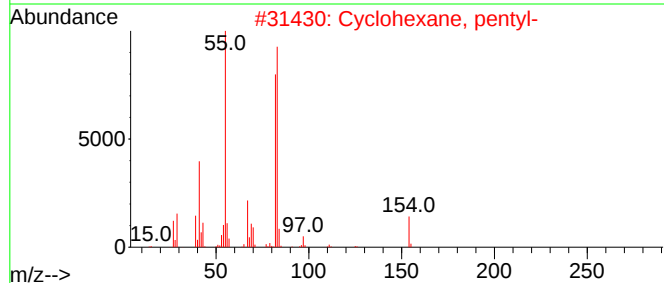
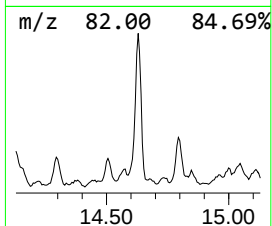
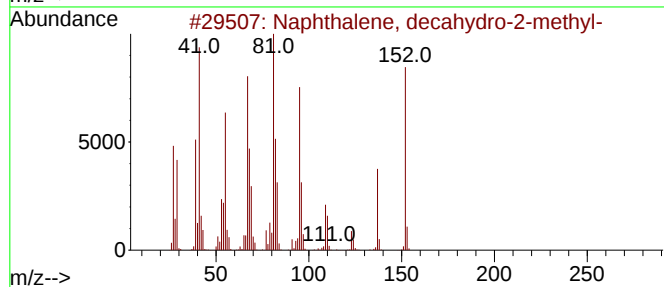
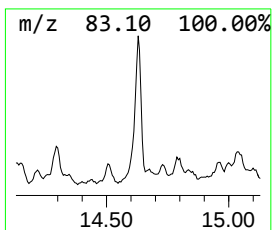
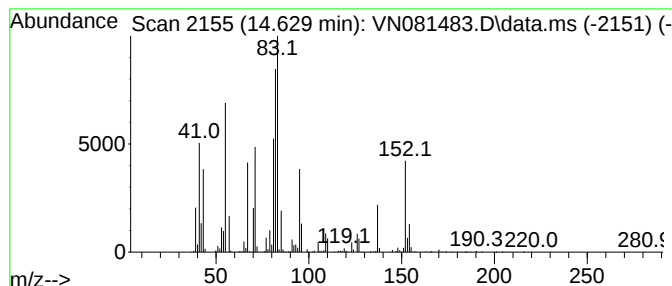
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Quant Title : SW846 8260

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

Peak Number 6 Naphthalene, decahydro-2-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.629	55.71 ug/l	3526540	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	86
2			Cyclohexane, pentyl-	154	C11H22	004292-92-6	38
3			Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	38
4			Cyclohexane, 2-propenyl-	124	C9H16	002114-42-3	37
5			(E)-2,6-Dimethylocta-3,7-diene-2...	170	C10H18O2	051276-34-7	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031924\
Data File : VN081483.D
Acq On : 19 Mar 2024 20:08
Operator : JC\MD
Sample : P1772-01
Misc : 1.09g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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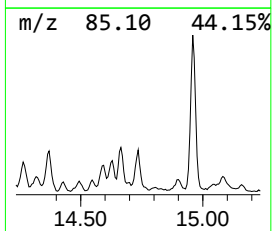
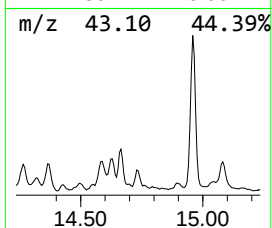
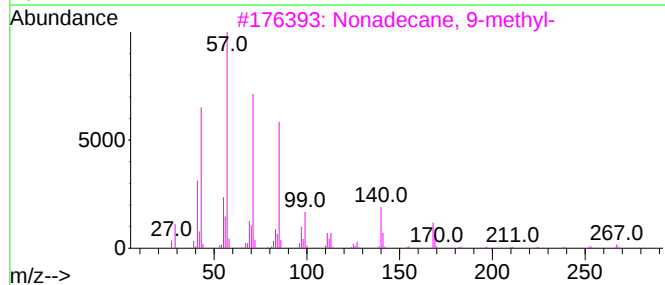
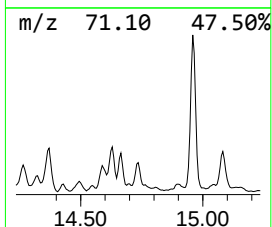
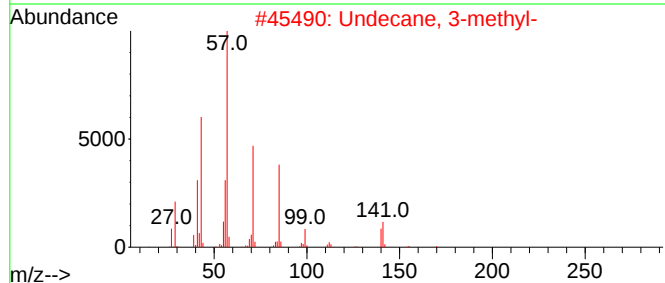
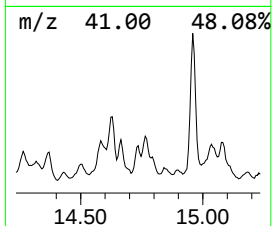
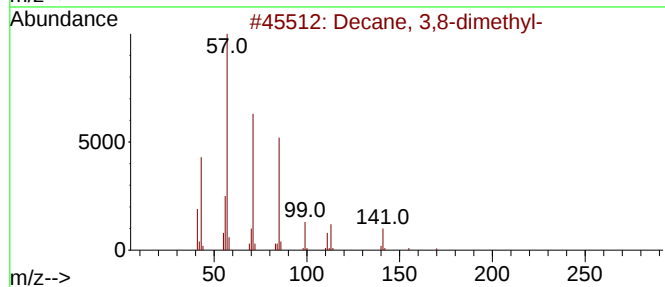
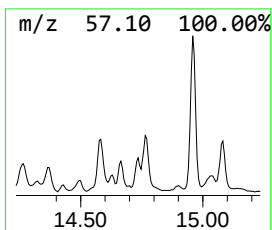
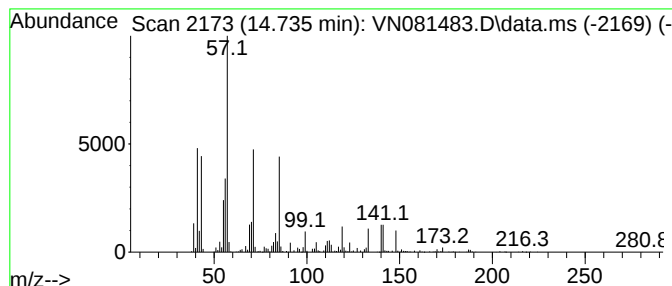
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Quant Title : SW846 8260

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

Peak Number 7 Decane, 3,8-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.735	22.47 ug/l	1422150	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	74
2			Undecane, 3-methyl-	170	C12H26	001002-43-3	64
3			Nonadecane, 9-methyl-	282	C20H42	013287-24-6	53
4			Decane, 1-iodo-	268	C10H21I	002050-77-3	50
5			Undecane, 5-ethyl-	184	C13H28	017453-94-0	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031924\
Data File : VN081483.D
Acq On : 19 Mar 2024 20:08
Operator : JC\MD
Sample : P1772-01
Misc : 1.09g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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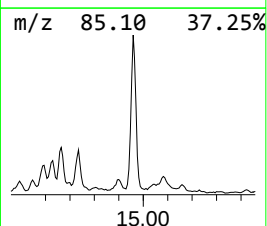
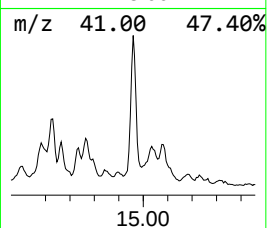
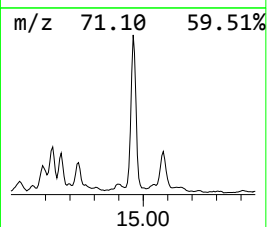
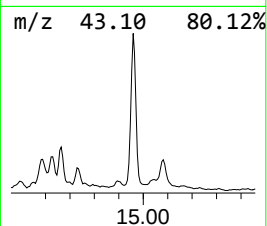
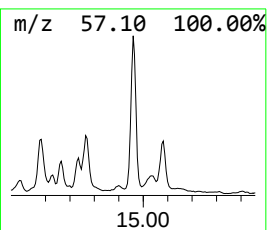
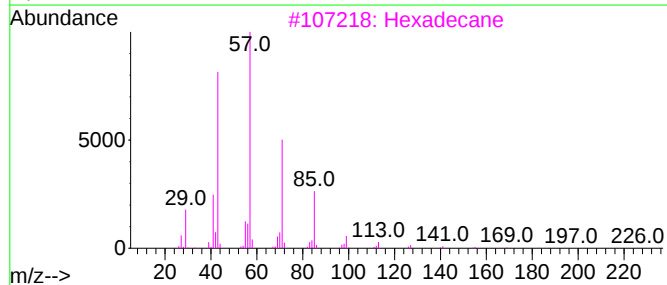
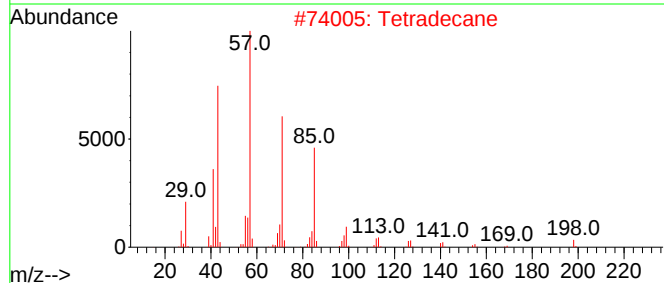
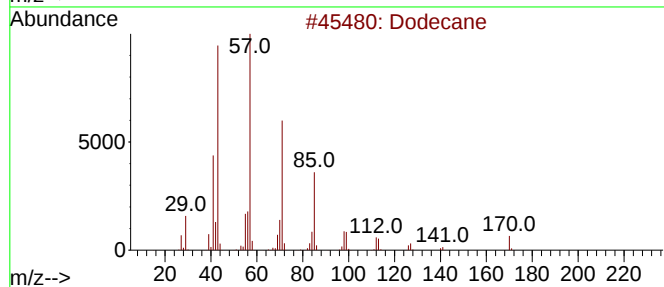
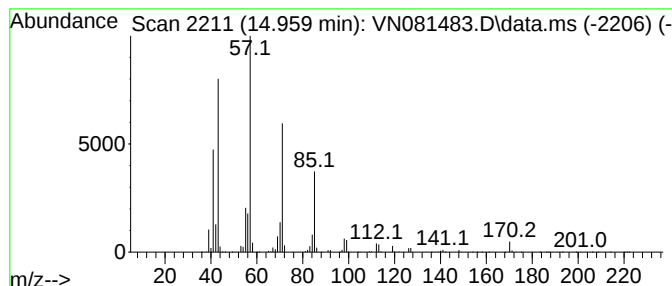
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Quant Title : SW846 8260

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

Peak Number 8 Dodecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.959	95.08 ug/l	6019020	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	97
2			Tetradecane	198	C14H30	000629-59-4	90
3			Hexadecane	226	C16H34	000544-76-3	86
4			Carbonic acid, prop-1-en-2-yl te...	298	C18H34O3	1000382-90-9	86
5			Undecane	156	C11H24	001120-21-4	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031924\
Data File : VN081483.D
Acq On : 19 Mar 2024 20:08
Operator : JC\MD
Sample : P1772-01
Misc : 1.09g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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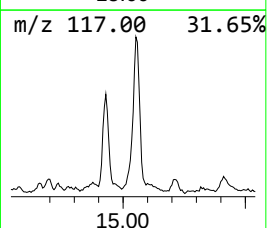
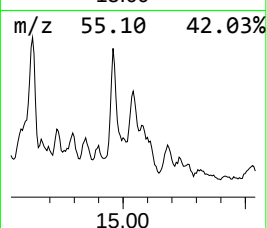
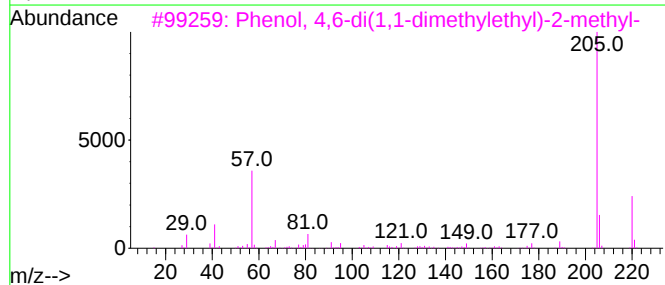
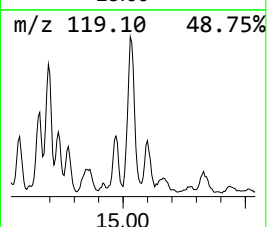
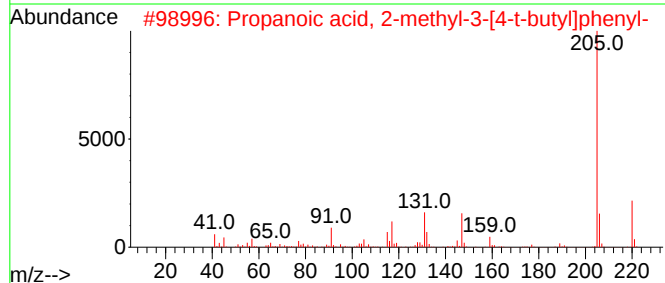
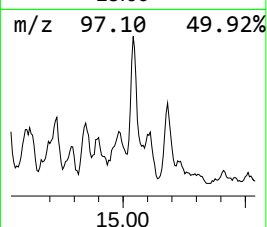
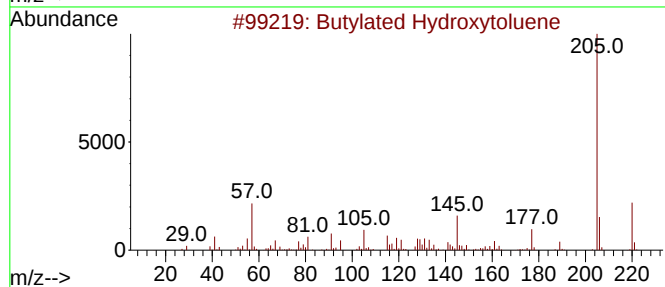
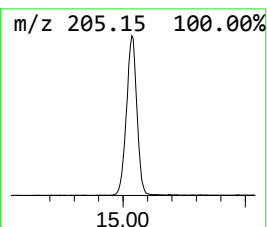
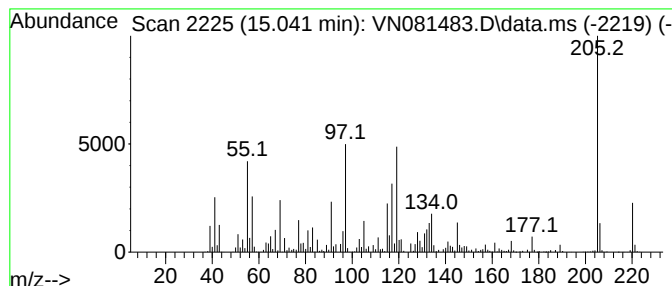
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Quant Title : SW846 8260

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

Peak Number 9 Butylated Hydroxytoluene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.041	61.26 ug/l	3878150	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	95
2			Propanoic acid, 2-methyl-3-[4-t...	220	C14H20O2	1000131-87-0	46
3			Phenol, 4,6-di(1,1-dimethylethyl...	220	C15H24O	000616-55-7	42
4			Phenol, 2,4,6-tris(1-methylethyl)-	220	C15H24O	002934-07-8	41
5			Ethyl 4-oxo-2-phenylpentanoate	220	C13H16O3	1000427-11-2	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031924\
Data File : VN081483.D
Acq On : 19 Mar 2024 20:08
Operator : JC\MD
Sample : P1772-01
Misc : 1.09g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1151

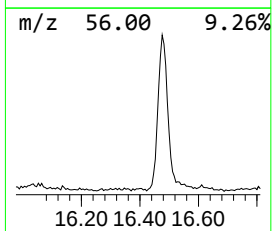
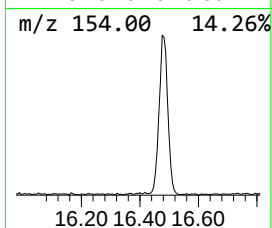
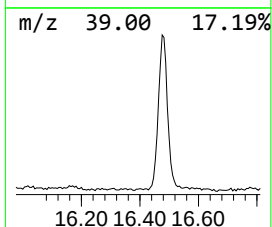
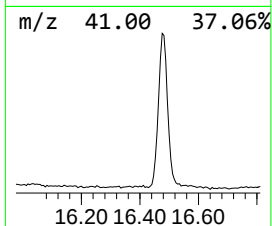
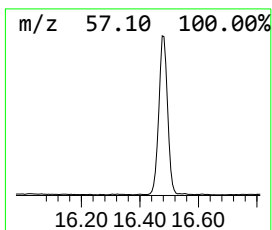
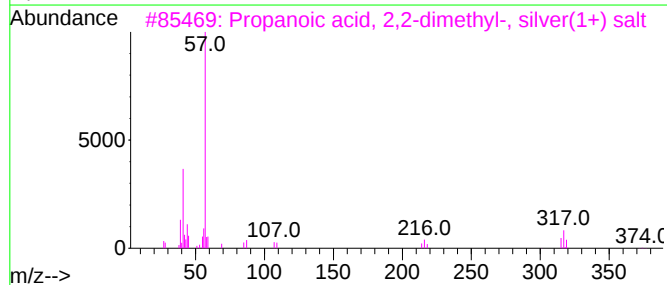
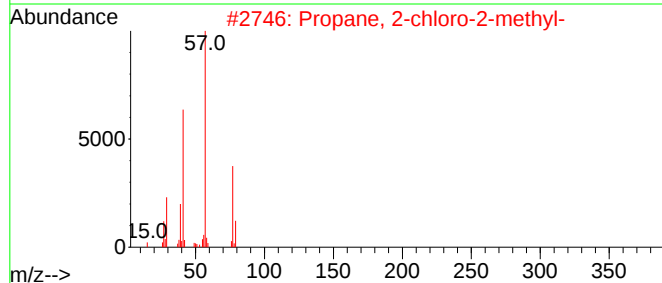
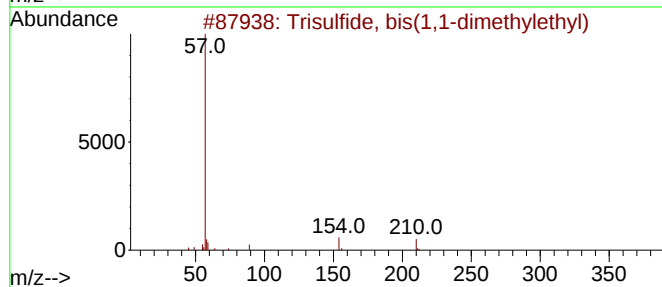
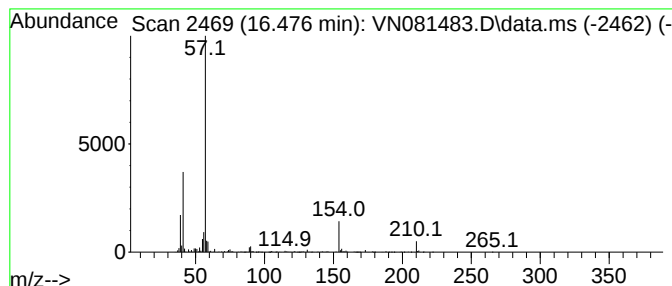
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Quant Title : SW846 8260

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

Peak Number 10 Trisulfide, bis(1,1-dimethy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.476	52.11 ug/l	3298570	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trisulfide, bis(1,1-dimethylethyl)	210	C8H18S3	004253-90-1	58
2			Propane, 2-chloro-2-methyl-	92	C4H9Cl	000507-20-0	43
3			Propanoic acid, 2,2-dimethyl-, s...	208	C5H9AgO2	007324-58-5	43
4			Di-tert-butyl disulfide	178	C8H18S2	000110-06-5	35
5			Butane, 2-bromo-	136	C4H9Br	000078-76-2	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031924\
Data File : VN081483.D
Acq On : 19 Mar 2024 20:08
Operator : JC\MD
Sample : P1772-01
Misc : 1.09g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.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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unknown13.988	13.988	27.9	ug/l	1763120	4	13.794	3165190	50.0
2,6-Dimethyldecane	14.265	23.9	ug/l	1509790	4	13.794	3165190	50.0
Decane, 3,7-dim...	14.370	24.5	ug/l	1551730	4	13.794	3165190	50.0
Undecane, 6-met...	14.582	35.1	ug/l	2225300	4	13.794	3165190	50.0
Naphthalene, de...	14.629	55.7	ug/l	3526540	4	13.794	3165190	50.0
Decane, 3,8-dim...	14.735	22.5	ug/l	1422150	4	13.794	3165190	50.0
Dodecane	14.959	95.1	ug/l	6019020	4	13.794	3165190	50.0
Butylated Hydro...	15.041	61.3	ug/l	3878150	4	13.794	3165190	50.0
Trisulfide, bis...	16.476	52.1	ug/l	3298570	4	13.794	3165190	50.0