

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060123\
 Data File : VN078013.D
 Acq On : 01 Jun 2023 16:26
 Operator : JC\MD
 Sample : 02958-01
 Misc : 1.09g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 ORA-0588

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\82N051523W.M
 Title : SW846 8260

Signal : TIC: VN078013.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.224	1059	1066	1076	rVB3	2040514	4877151	9.00%	3.077%
2	8.330	1076	1084	1094	rVB2	594129	1419043	2.62%	0.895%
3	8.447	1094	1104	1112	rBV	2421467	5399159	9.97%	3.406%
4	8.582	1120	1127	1139	rVB2	322501	736369	1.36%	0.465%
5	8.712	1139	1149	1157	rBV4	333823	946173	1.75%	0.597%
6	8.971	1184	1193	1204	rBV	1843469	3645939	6.73%	2.300%
7	9.106	1207	1216	1226	rBV	803252	1645888	3.04%	1.038%
8	9.606	1283	1301	1318	rBV	519915	1389488	2.57%	0.877%
9	10.576	1457	1466	1470	rBV	1296822	2525140	4.66%	1.593%
10	10.641	1470	1477	1490	rVV2	28781516	54162179	100.00%	34.172%
11	11.876	1680	1687	1696	rBV	1044313	1933967	3.57%	1.220%
12	11.970	1696	1703	1713	rBV	929943	1699925	3.14%	1.073%
13	12.076	1713	1721	1732	rVV	2723878	5229000	9.65%	3.299%
14	12.406	1764	1777	1786	rBV	1270076	2737169	5.05%	1.727%
15	12.859	1848	1854	1863	rVB2	957205	1790868	3.31%	1.130%
16	13.041	1878	1885	1890	rBV	591283	1004193	1.85%	0.634%
17	13.106	1890	1896	1900	rBV	1628941	2865638	5.29%	1.808%
18	13.170	1903	1907	1914	rVB3	1250780	2731262	5.04%	1.723%
19	13.341	1928	1936	1943	rBV	696729	1393220	2.57%	0.879%
20	13.488	1955	1961	1968	rBV	2543569	4223185	7.80%	2.665%
21	13.682	1988	1994	1999	rBV3	438172	859437	1.59%	0.542%
22	13.800	2009	2014	2017	rBV2	1136827	2064282	3.81%	1.302%
23	13.959	2033	2041	2042	rBV5	317500	576103	1.06%	0.363%
24	13.994	2042	2047	2051	rBV2	845764	1581730	2.92%	0.998%
25	14.111	2063	2067	2074	rBV	1691299	2933621	5.42%	1.851%
26	14.253	2087	2091	2093	rVV	459837	731815	1.35%	0.462%
27	14.282	2093	2096	2100	rVV	543559	837735	1.55%	0.529%
28	14.335	2100	2105	2110	rVB	754458	1157512	2.14%	0.730%
29	14.453	2119	2125	2130	rVB2	761722	1314392	2.43%	0.829%
30	14.582	2142	2147	2151	rBV5	478975	867479	1.60%	0.547%
31	14.635	2151	2156	2159	rVV	869284	1397850	2.58%	0.882%
32	14.664	2159	2161	2164	rVV2	511172	659424	1.22%	0.416%
33	14.700	2164	2167	2171	rVB	629401	792121	1.46%	0.500%
34	14.741	2171	2174	2178	rVB	552235	658013	1.21%	0.415%
35	14.800	2178	2184	2189	rVB5	368178	884794	1.63%	0.558%
36	14.882	2189	2198	2203	rBV4	477264	1194267	2.20%	0.753%

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If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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37	14.964	2203	2212	2219	rBV5	1665936	3921372	7.24%	2.474%
38	15.058	2220	2228	2235	rBV4	1421484	4173810	7.71%	2.633%
39	15.217	2250	2255	2262	rVB	844565	1580021	2.92%	0.997%
40	15.323	2269	2273	2278	rBV2	538725	964837	1.78%	0.609%
41	15.470	2287	2298	2315	rVB2	6810037	13261559	24.48%	8.367%
42	15.606	2316	2321	2324	rBV4	305163	581119	1.07%	0.367%
43	15.705	2333	2338	2342	rBV	467984	879755	1.62%	0.555%
44	15.758	2342	2347	2350	rVV2	374742	623353	1.15%	0.393%
45	15.841	2357	2361	2372	rVB3	924311	1987080	3.67%	1.254%
46	15.953	2372	2380	2387	rBV3	662883	1672565	3.09%	1.055%
47	16.135	2404	2411	2412	rBV4	321816	607287	1.12%	0.383%
48	16.176	2413	2418	2427	rVB	1210765	2469513	4.56%	1.558%
49	16.352	2439	2448	2454	rBV5	362825	1004345	1.85%	0.634%
50	16.511	2464	2475	2481	rBV3	710493	2075821	3.83%	1.310%
51	16.717	2502	2510	2517	rBV3	762783	1828838	3.38%	1.154%

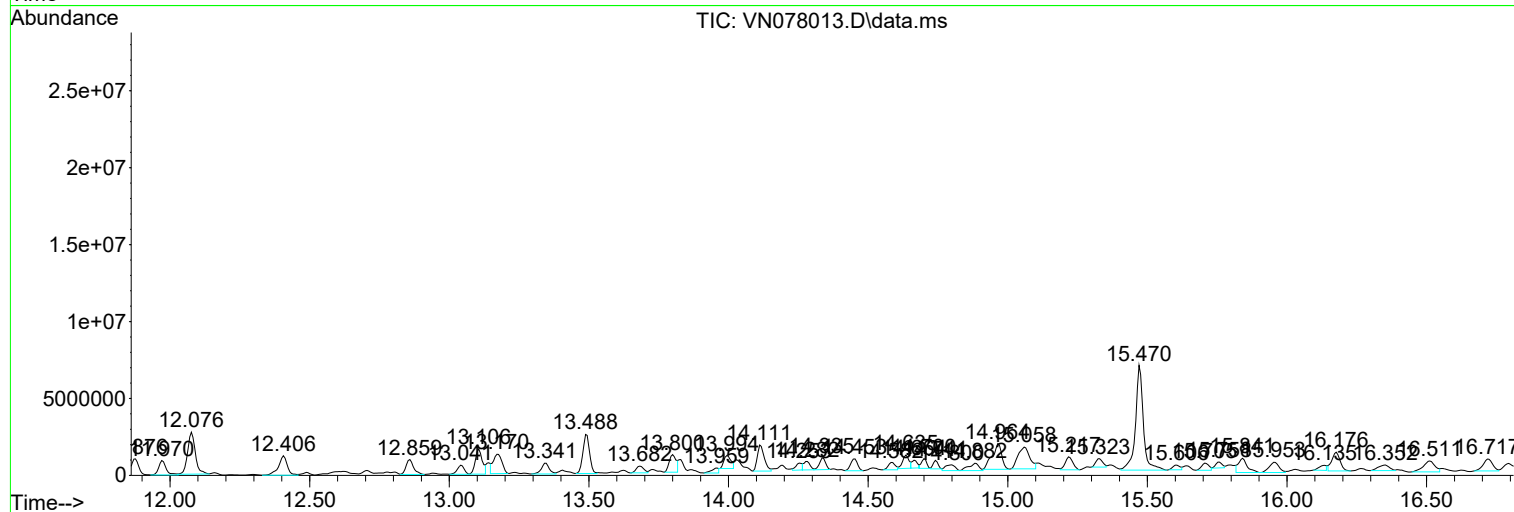
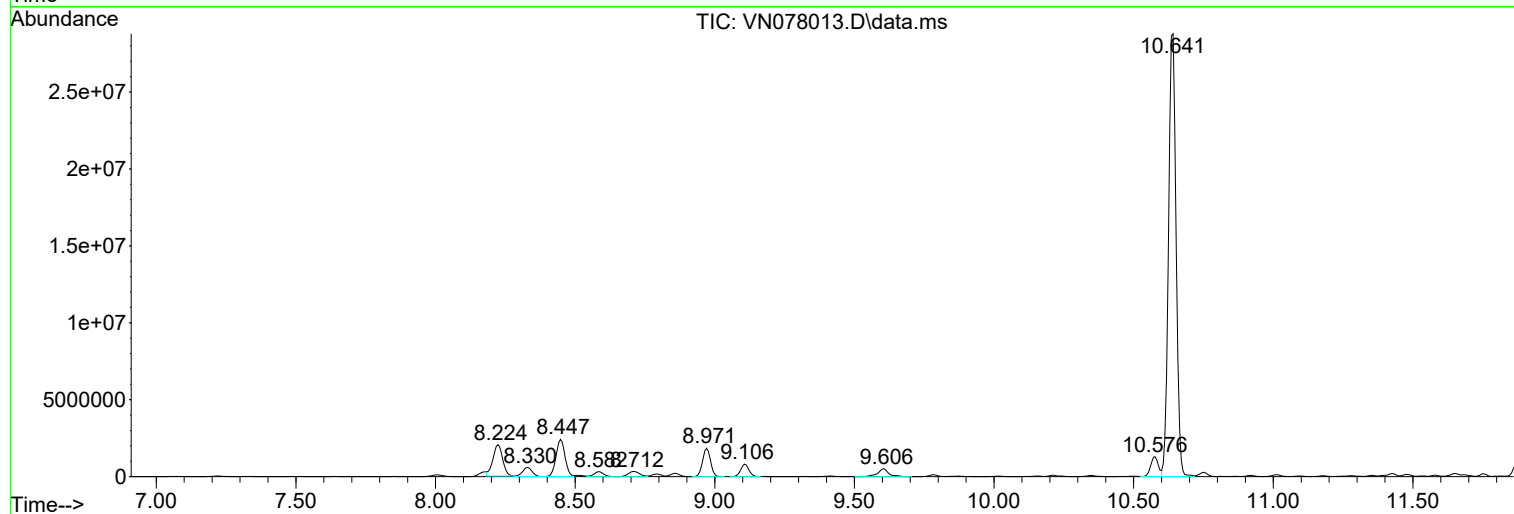
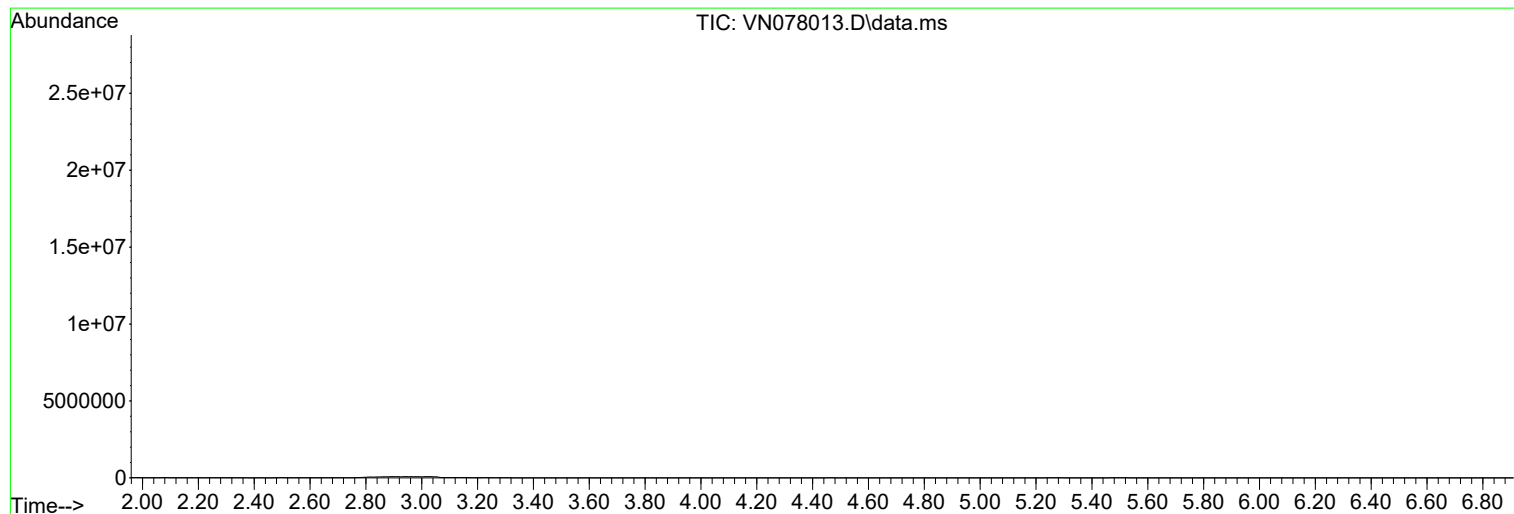
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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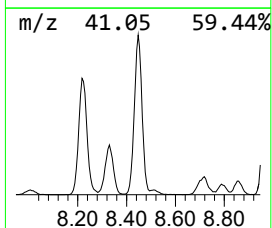
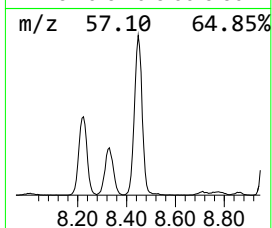
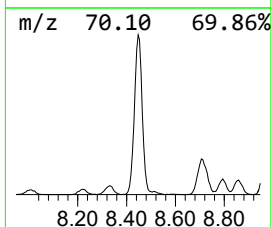
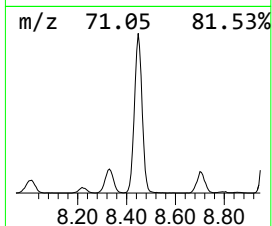
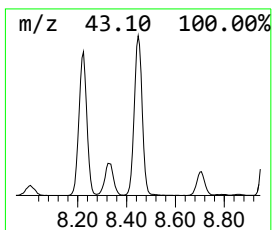
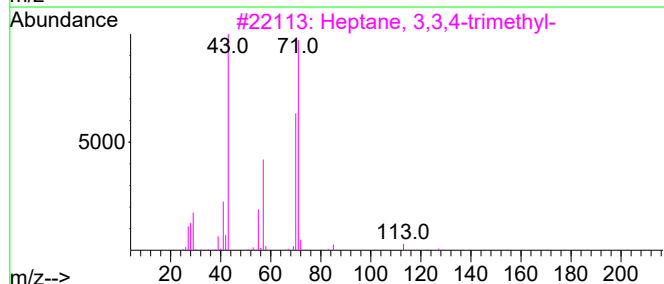
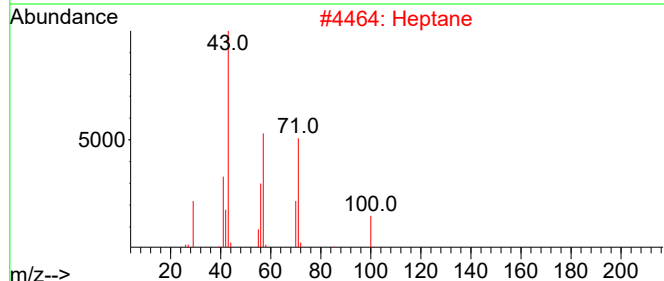
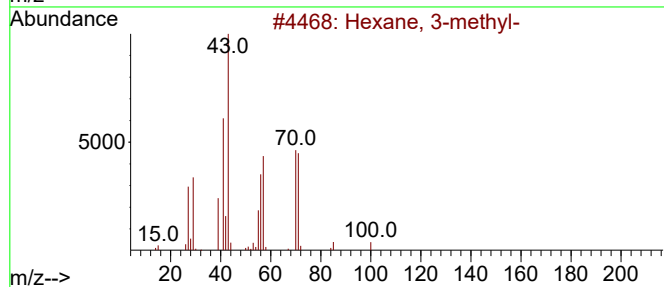
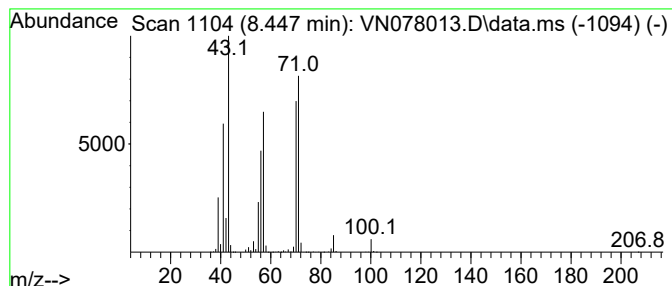
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

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

Peak Number 1 Hexane, 3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.447	55.35 ug/l	5399160	Pentafluorobenzene	8.229

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 3-methyl-	100	C7H16	000589-34-4	96
2			Heptane	100	C7H16	000142-82-5	80
3			Heptane, 3,3,4-trimethyl-	142	C10H22	020278-87-9	59
4			Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	59
5			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	59



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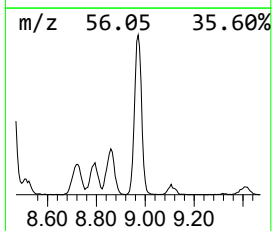
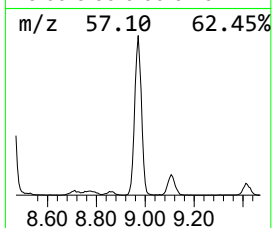
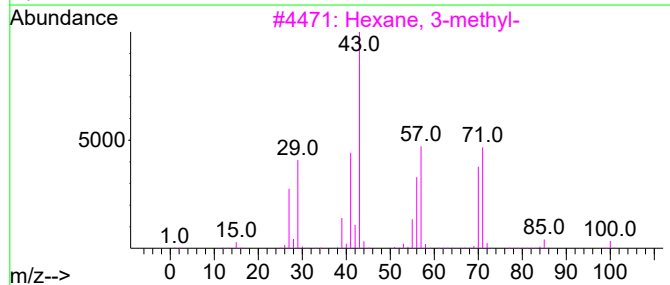
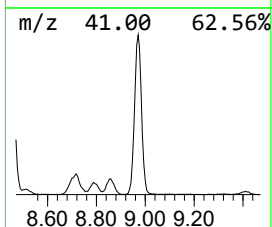
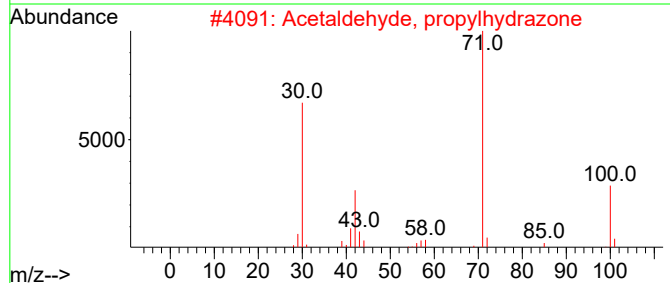
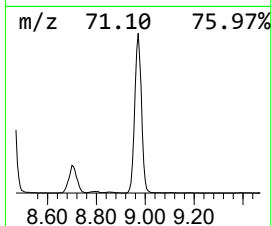
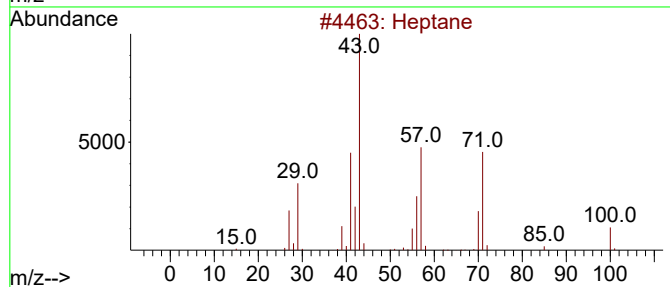
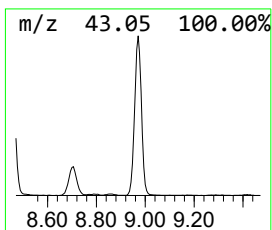
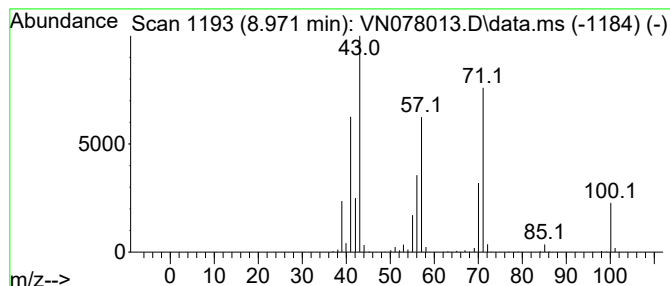
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

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

Peak Number 2 Heptane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.971	110.76 ug/l	3645940	1,4-Difluorobenzene	9.106

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane	100	C7H16	000142-82-5	86
2			Acetaldehyde, propylhydrazone	100	C5H12N2	007422-88-0	53
3			Hexane, 3-methyl-	100	C7H16	000589-34-4	50
4			Pentane, 2-methyl-	86	C6H14	000107-83-5	50
5			Oxirane, butyl-	100	C6H12O	001436-34-6	47



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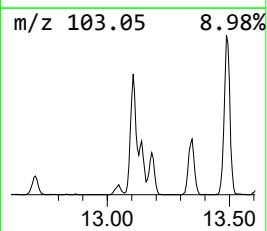
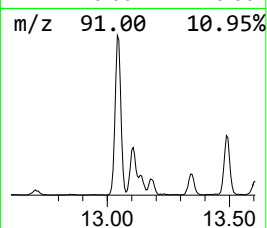
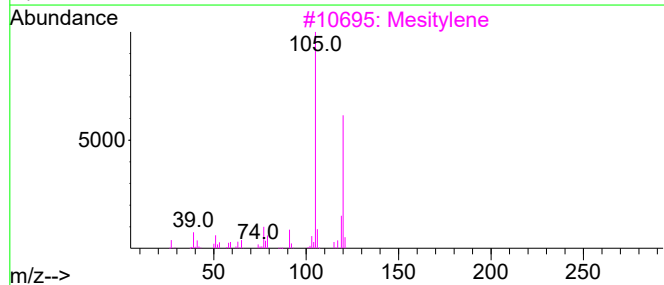
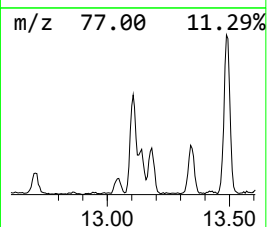
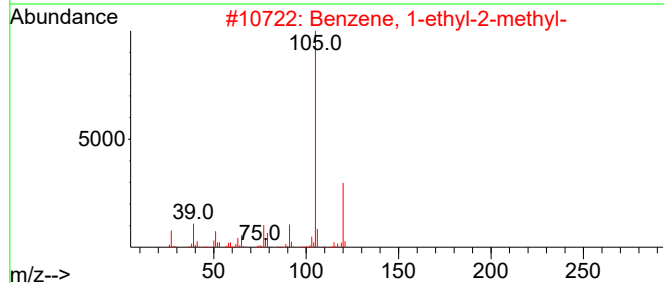
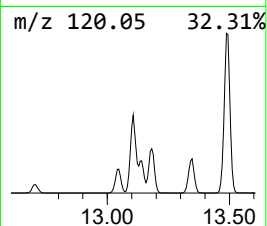
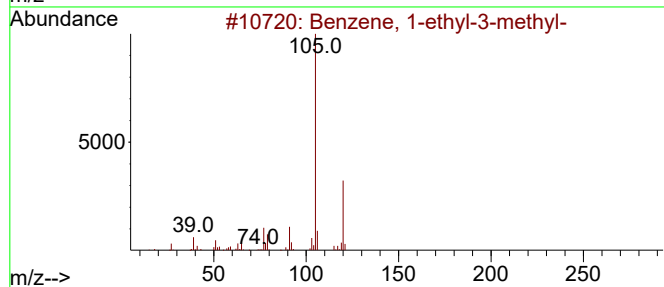
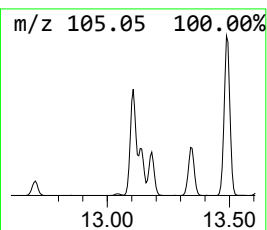
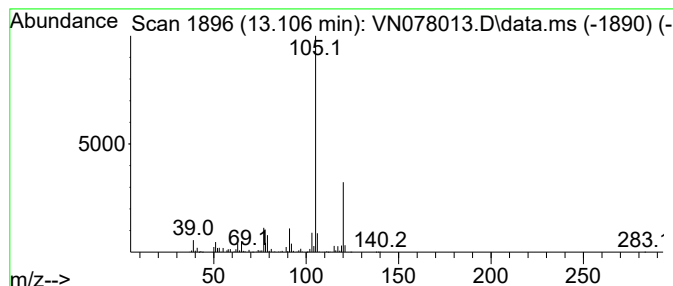
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzene, 1-ethyl-3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.106	69.41 ug/l	2865640	1,4-Dichlorobenzene-d4	13.800

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
2			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
3			Mesitylene	120	C9H12	000108-67-8	91
4			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91



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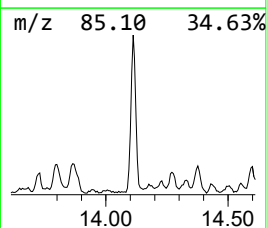
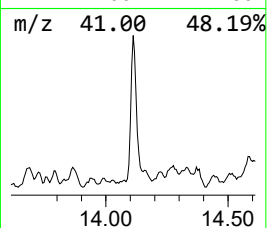
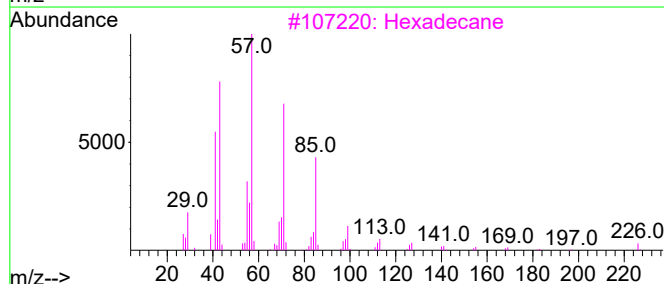
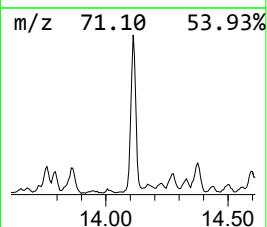
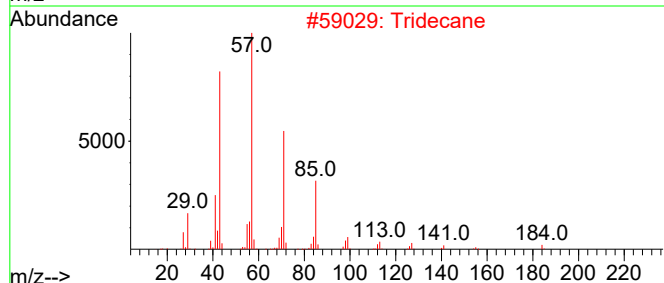
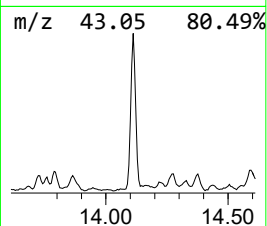
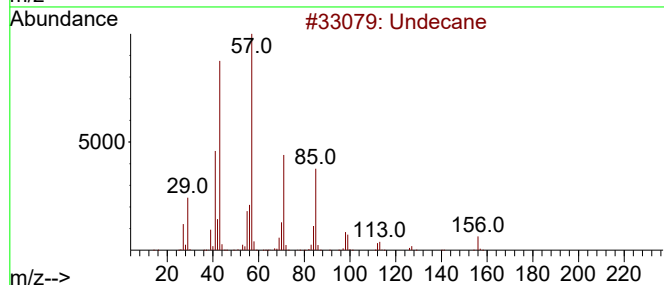
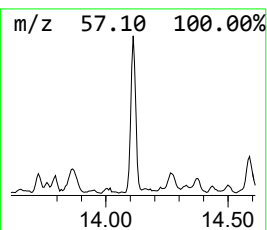
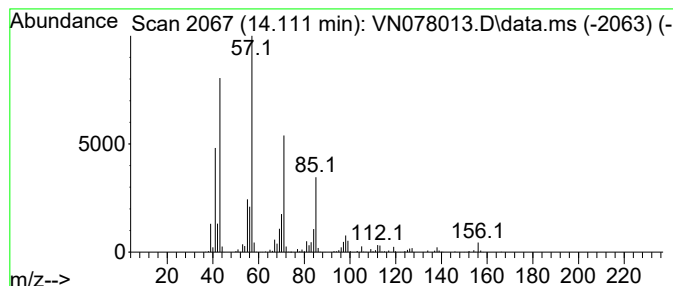
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

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

Peak Number 4 Undecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.111	71.06 ug/l	2933620	1,4-Dichlorobenzene-d4	13.800

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane	156	C11H24	001120-21-4	94
2	Tridecane	184	C13H28	000629-50-5	80
3	Hexadecane	226	C16H34	000544-76-3	64
4	Nonane	128	C9H20	000111-84-2	59
5	Tetradecane	198	C14H30	000629-59-4	59



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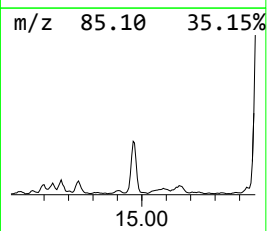
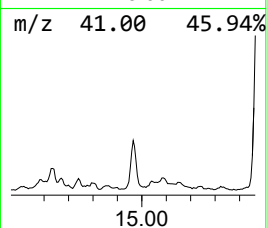
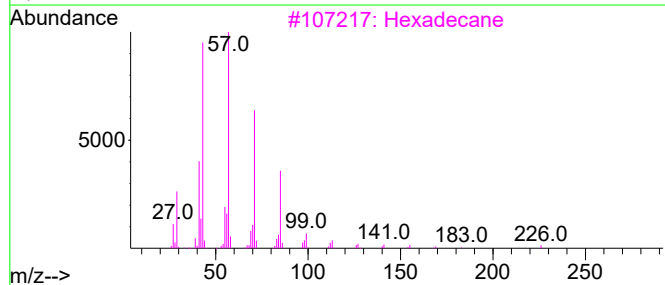
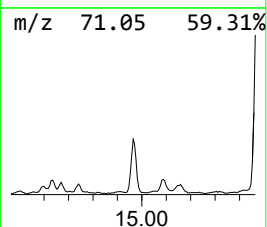
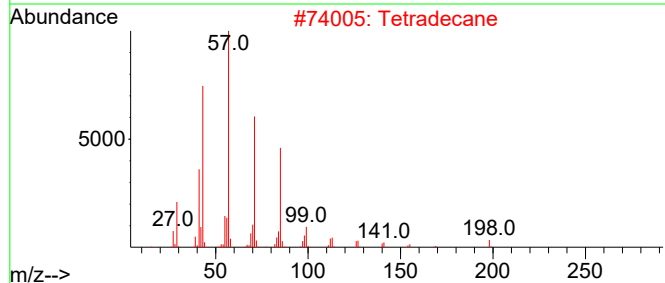
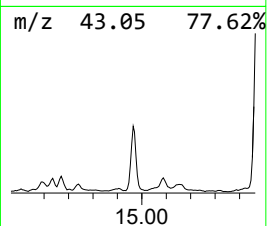
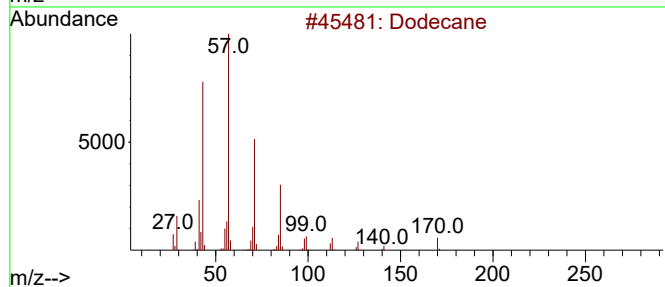
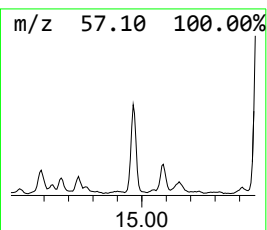
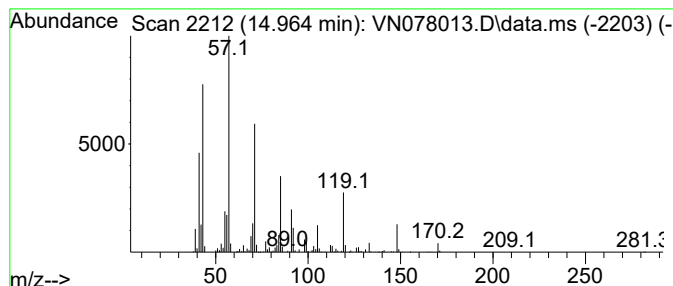
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Quant Title : SW846 8260

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

Peak Number 5 Dodecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.964	94.98 ug/l	3921370	1,4-Dichlorobenzene-d4	13.800

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	55
2			Tetradecane	198	C14H30	000629-59-4	46
3			Hexadecane	226	C16H34	000544-76-3	46
4			Decane, 6-ethyl-2-methyl-	184	C13H28	062108-21-8	43
5			Tridecane	184	C13H28	000629-50-5	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060123\
Data File : VN078013.D
Acq On : 01 Jun 2023 16:26
Operator : JC\MD
Sample : 02958-01
Misc : 1.09g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
ORA-0588

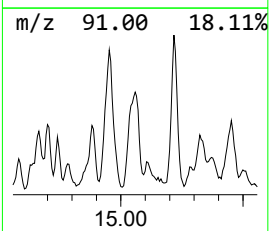
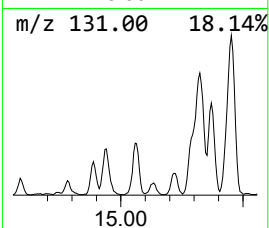
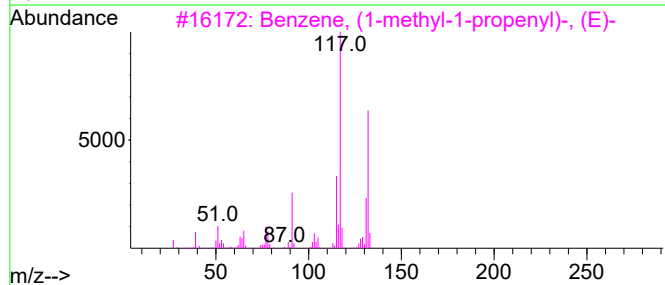
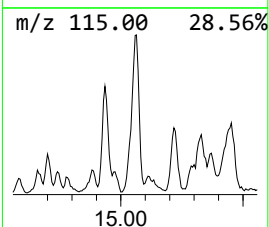
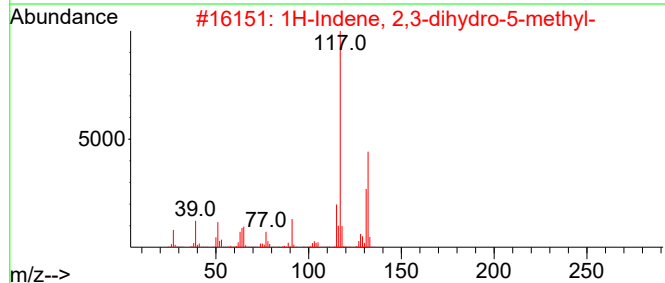
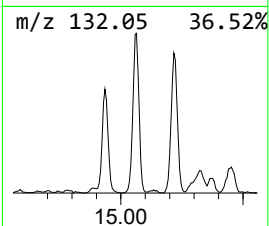
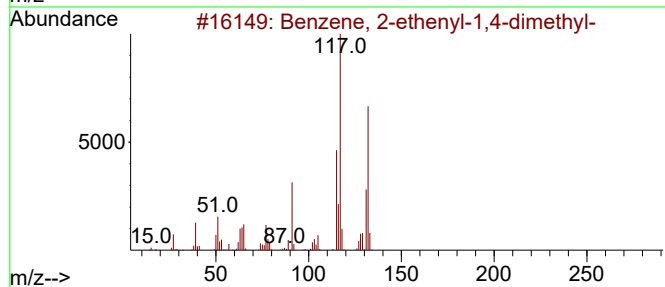
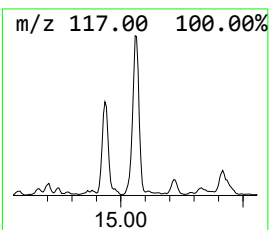
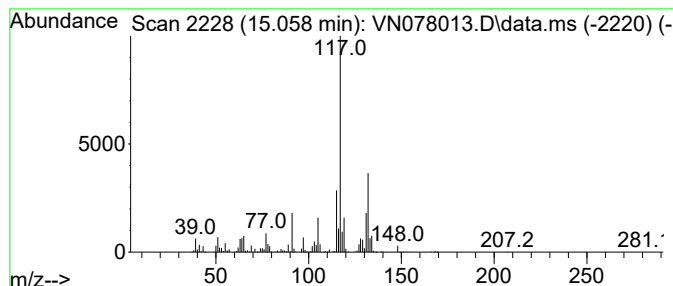
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.059	101.10 ug/l	4173810	1,4-Dichlorobenzene-d4	13.800

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	96
2			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	91
3			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	90
4			Benzene, 2-butenyl-	132	C10H12	001560-06-1	90
5			3-Phenylbut-1-ene	132	C10H12	000934-10-1	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060123\
Data File : VN078013.D
Acq On : 01 Jun 2023 16:26
Operator : JC\MD
Sample : 02958-01
Misc : 1.09g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
ORA-0588

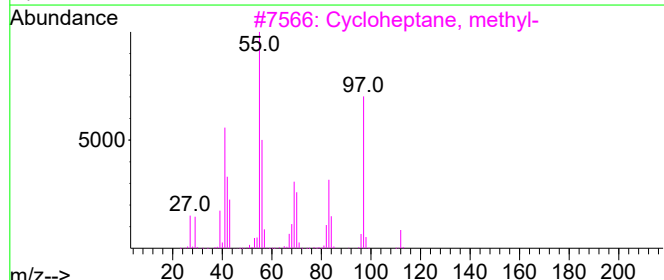
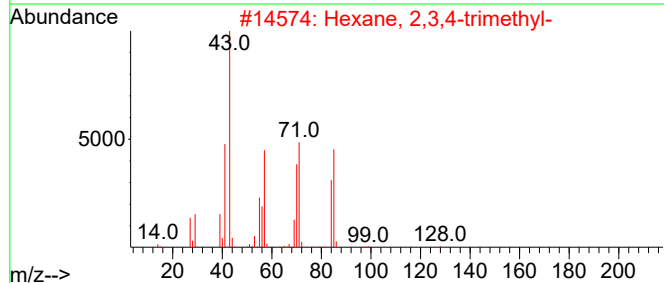
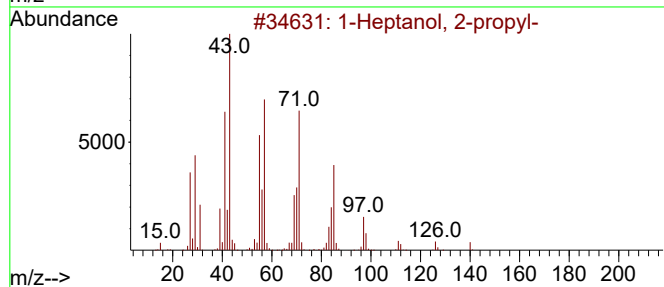
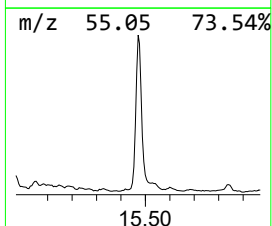
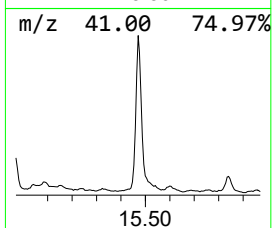
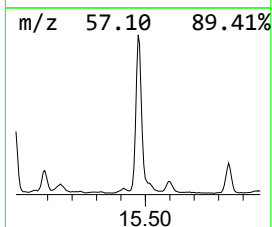
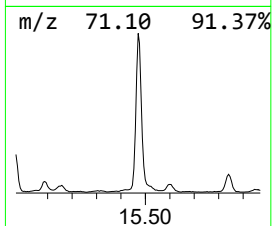
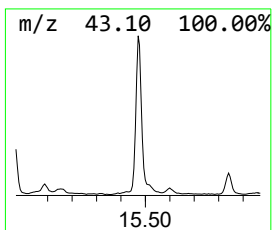
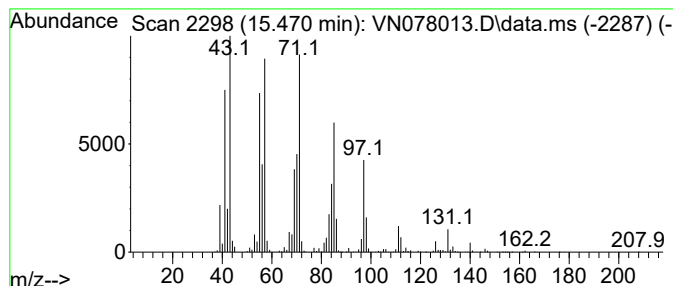
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Quant Title : SW846 8260

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

Peak Number 7 1-Heptanol, 2-propyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.470	321.21 ug/l	13261600	1,4-Dichlorobenzene-d4	13.800

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heptanol, 2-propyl-	158	C10H22O	010042-59-8	80
2			Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	46
3			Cycloheptane, methyl-	112	C8H16	004126-78-7	35
4			1-Decene	140	C10H20	000872-05-9	30
5			Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	27



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060123\
Data File : VN078013.D
Acq On : 01 Jun 2023 16:26
Operator : JC\MD
Sample : 02958-01
Misc : 1.09g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
ORA-0588

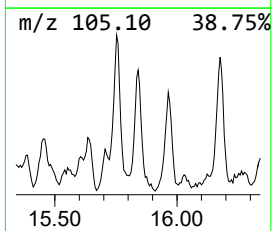
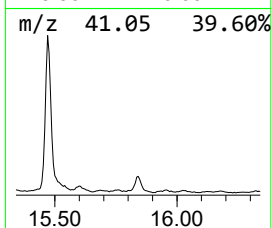
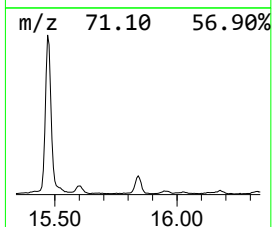
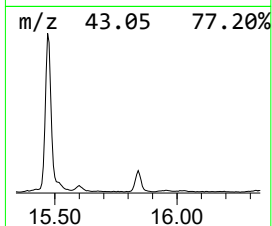
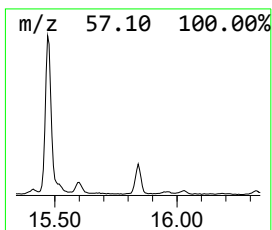
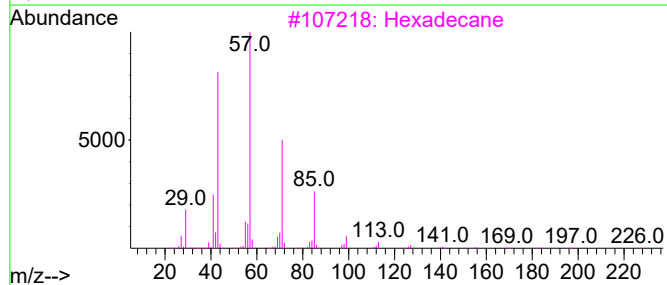
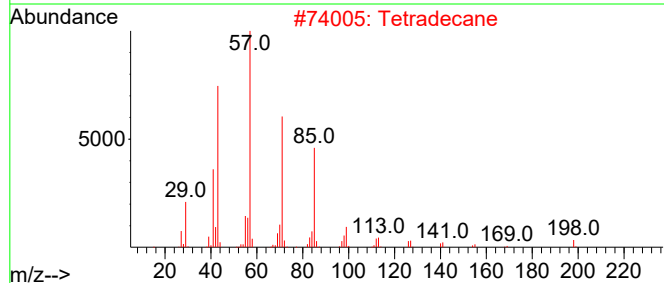
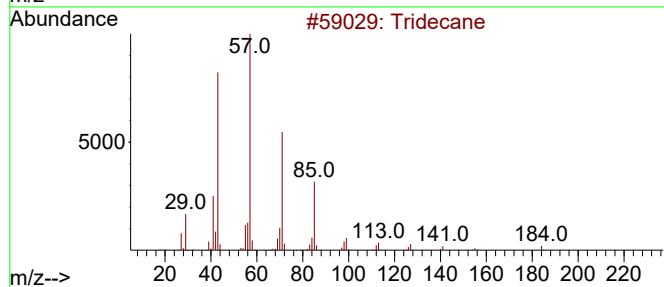
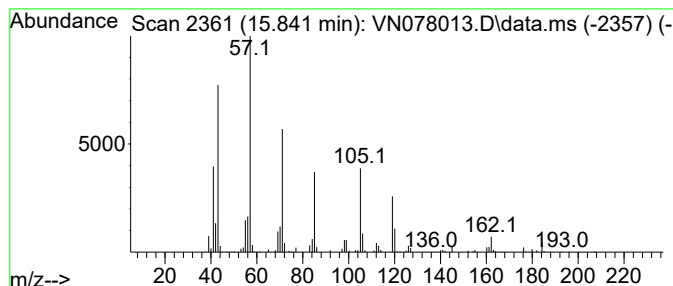
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Quant Title : SW846 8260

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

Peak Number 8 Tridecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.841	48.13 ug/l	1987080	1,4-Dichlorobenzene-d4	13.800

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	83
2			Tetradecane	198	C14H30	000629-59-4	52
3			Hexadecane	226	C16H34	000544-76-3	49
4			Decane, 6-ethyl-2-methyl-	184	C13H28	062108-21-8	47
5			Nonane, 5-(2-methylpropyl)-	184	C13H28	062185-53-9	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060123\
Data File : VN078013.D
Acq On : 01 Jun 2023 16:26
Operator : JC\MD
Sample : 02958-01
Misc : 1.09g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
ORA-0588

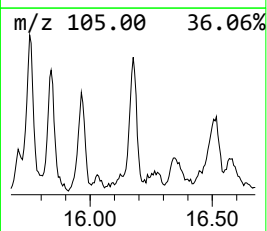
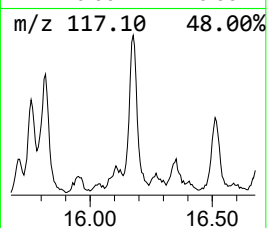
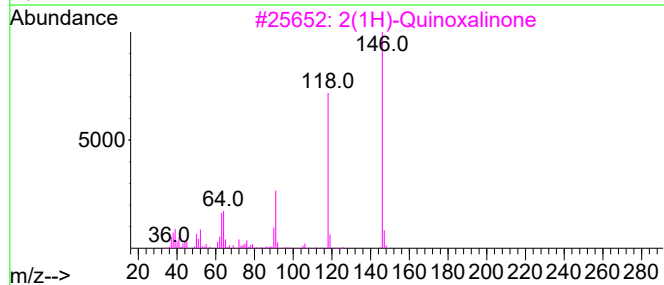
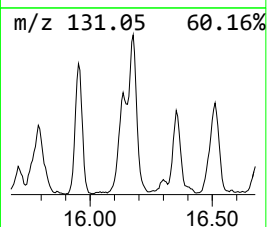
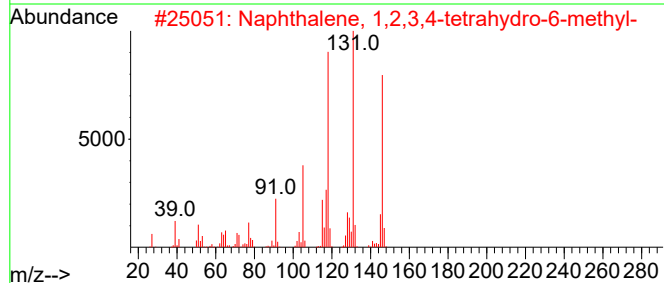
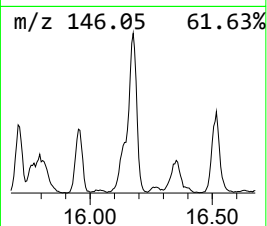
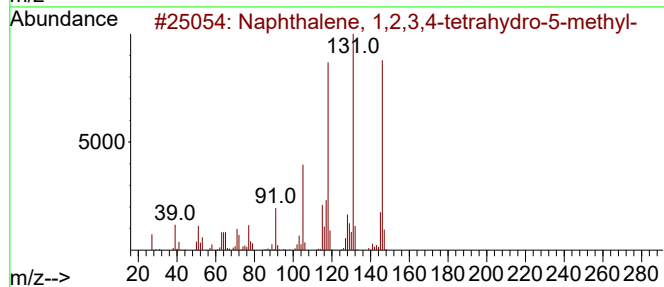
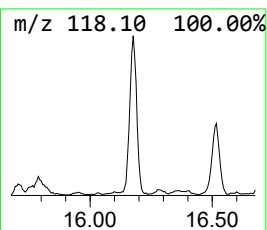
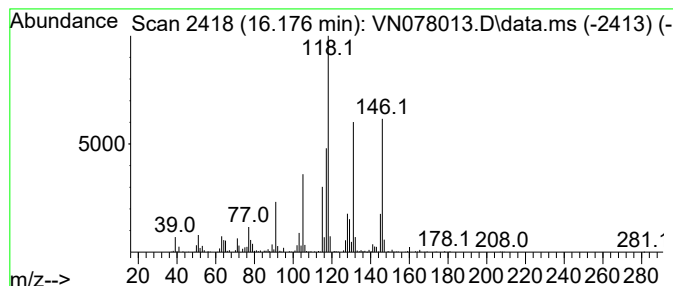
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Quant Title : SW846 8260

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

Peak Number 9 Naphthalene, 1,2,3,4-tetrahydro-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.176	59.82 ug/l	2469510	1,4-Dichlorobenzene-d4	13.800

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	81
2			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	70
3			2(1H)-Quinoxalinone	146	C8H6N2O	001196-57-2	46
4			1(2H)-Naphthalenone, 3,4-dihydro-	146	C10H10O	000529-34-0	46
5			Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060123\
Data File : VN078013.D
Acq On : 01 Jun 2023 16:26
Operator : JC\MD
Sample : 02958-01
Misc : 1.09g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
ORA-0588

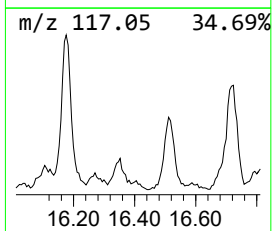
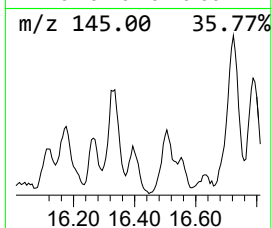
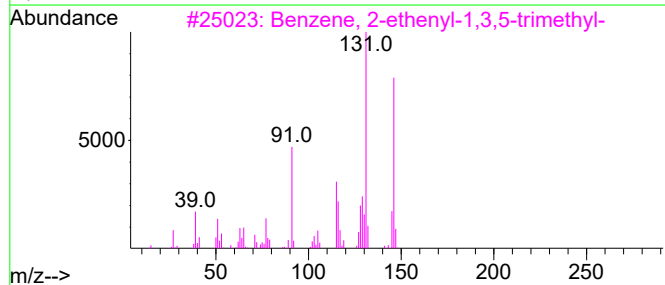
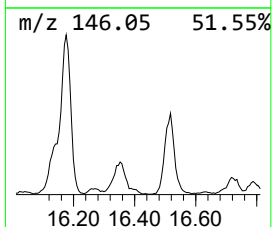
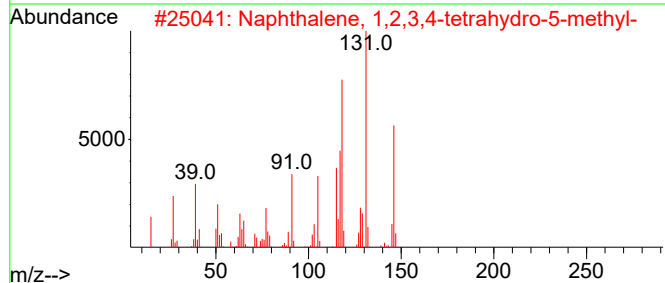
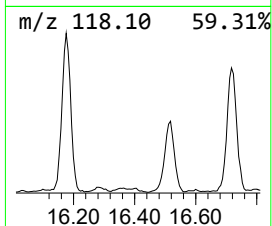
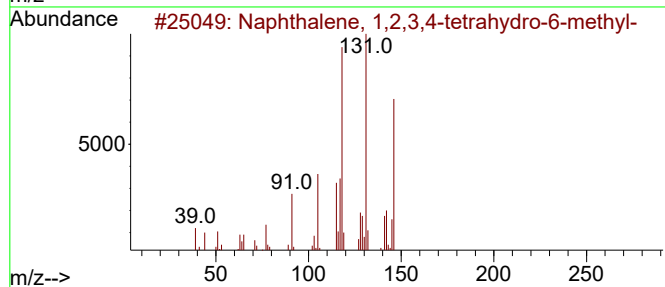
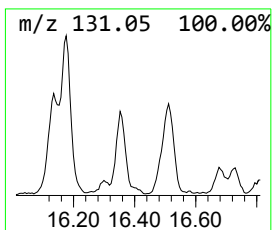
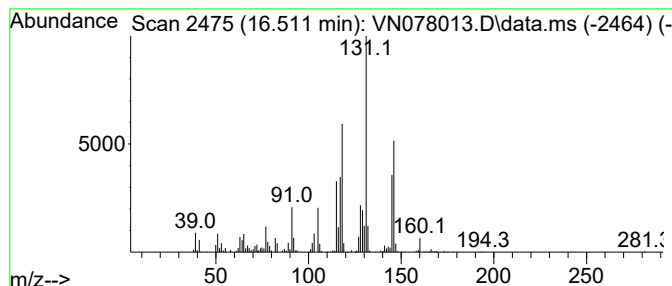
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

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

Peak Number 10 Naphthalene, 1,2,3,4-tetrahydro-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.511	50.28 ug/l	2075820	1,4-Dichlorobenzene-d4	13.800

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	91
2			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	87
3			Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	70
4			1H-Benzimidazole, 5,6-dimethyl-	146	C9H10N2	000582-60-5	64
5			2-Propenal, 3-(4-methylphenyl)-	146	C10H10O	001504-75-2	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060123\
Data File : VN078013.D
Acq On : 01 Jun 2023 16:26
Operator : JC\MD
Sample : 02958-01
Misc : 1.09g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
ORA-0588

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.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	8.971	110.8	ug/l	3645940	2	9.106	1645890	50.0
Benzene, 1-ethy...	13.106	69.4	ug/l	2865640	4	13.800	2064280	50.0
Undecane	14.111	71.1	ug/l	2933620	4	13.800	2064280	50.0
Dodecane	14.964	95.0	ug/l	3921370	4	13.800	2064280	50.0
Benzene, 2-ethe...	15.059	101.1	ug/l	4173810	4	13.800	2064280	50.0
1-Heptanol, 2-p...	15.470	321.2	ug/l	13261600	4	13.800	2064280	50.0
Tridecane	15.841	48.1	ug/l	1987080	4	13.800	2064280	50.0
Naphthalene, 1,...	16.176	59.8	ug/l	2469510	4	13.800	2064280	50.0
Naphthalene, 1,...	16.511	50.3	ug/l	2075820	4	13.800	2064280	50.0