

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112322\
 Data File : VN075409.D
 Acq On : 23 Nov 2022 20:22
 Operator : JC\MD
 Sample : N5692-03
 Misc : 1.32g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 HS-SPILL-DRUM-11-16

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: VN075409.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.500	71	76	78	rBV4	5489	8433	1.32%	0.145%
2	2.800	122	127	131	rBV3	5919	10704	1.67%	0.184%
3	3.071	170	173	182	rVB6	20766	50153	7.85%	0.861%
4	5.053	496	510	517	rBV3	2738	10631	1.66%	0.183%
5	5.500	578	586	598	rVB3	3582	11898	1.86%	0.204%
6	8.171	1030	1040	1043	rBV	63916	139868	21.88%	2.401%
7	8.224	1043	1049	1058	rVB	197186	439396	68.74%	7.543%
8	8.577	1100	1109	1120	rVB	46918	104136	16.29%	1.788%
9	8.694	1122	1129	1130	rBV2	17105	29430	4.60%	0.505%
10	9.100	1189	1198	1208	rBV	267453	556829	87.11%	9.559%
11	10.570	1439	1448	1455	rBV	140167	262492	41.07%	4.506%
12	11.282	1564	1569	1578	rBV5	2914	6845	1.07%	0.118%
13	11.865	1661	1668	1681	rVB	353791	639211	100.00%	10.974%
14	12.853	1829	1836	1846	rVB	203882	352658	55.17%	6.054%
15	13.117	1871	1881	1885	rBV5	16567	32206	5.04%	0.553%
16	13.164	1885	1889	1892	rVV3	19272	33374	5.22%	0.573%
17	13.206	1892	1896	1903	rVB	40255	68732	10.75%	1.180%
18	13.359	1916	1922	1927	rBV3	9269	16305	2.55%	0.280%
19	13.482	1937	1943	1948	rBV2	14342	20748	3.25%	0.356%
20	13.664	1970	1974	1980	rBV6	7935	14791	2.31%	0.254%
21	13.794	1989	1996	2004	rVV	366146	613727	96.01%	10.536%
22	13.864	2004	2008	2014	rVB5	9038	18634	2.92%	0.320%
23	13.988	2024	2029	2032	rBV2	8606	12281	1.92%	0.211%
24	14.023	2032	2035	2040	rVB5	7119	11033	1.73%	0.189%
25	14.106	2044	2049	2056	rBV	33494	50670	7.93%	0.870%
26	14.253	2067	2074	2076	rBV4	6195	11849	1.85%	0.203%
27	14.329	2083	2087	2092	rVB3	9966	16192	2.53%	0.278%
28	14.441	2101	2106	2112	rBV5	10557	20646	3.23%	0.354%
29	14.564	2122	2127	2129	rBV4	11577	19204	3.00%	0.330%
30	14.582	2129	2130	2134	rVV4	11853	12270	1.92%	0.211%
31	14.629	2134	2138	2141	rVV5	18696	27998	4.38%	0.481%
32	14.658	2141	2143	2147	rVV3	12847	17062	2.67%	0.293%
33	14.694	2147	2149	2153	rVB2	10914	11146	1.74%	0.191%
34	14.735	2153	2156	2160	rVB3	16959	20993	3.28%	0.360%
35	14.782	2160	2164	2165	rBV3	5708	6735	1.05%	0.116%
36	14.876	2172	2180	2184	rBV9	12689	27652	4.33%	0.475%

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37	14.958	2190	2194	2202	rVB2	93702	145253	22.72%	2.494%
38	15.047	2202	2209	2213	rBV6	36477	93181	14.58%	1.600%
39	15.217	2233	2238	2244	rVB7	18204	38375	6.00%	0.659%
40	15.276	2244	2248	2251	rBV5	9313	17811	2.79%	0.306%
41	15.317	2251	2255	2260	rBV5	25140	46505	7.28%	0.798%
42	15.447	2269	2277	2284	rBV8	28570	89672	14.03%	1.539%
43	15.511	2284	2288	2297	rVB7	29601	72746	11.38%	1.249%
44	15.600	2297	2303	2307	rBV2	48917	105565	16.51%	1.812%
45	15.700	2314	2320	2324	rBV6	19174	46303	7.24%	0.795%
46	15.753	2324	2329	2333	rVV4	39001	69232	10.83%	1.189%
47	15.835	2338	2343	2354	rVB2	191571	389842	60.99%	6.693%
48	15.947	2354	2362	2369	rBV7	62383	198199	31.01%	3.403%
49	16.123	2388	2392	2395	rBV6	19493	36914	5.77%	0.634%
50	16.170	2395	2400	2407	rVB4	89540	163120	25.52%	2.800%
51	16.329	2421	2427	2428	rBV4	42708	72979	11.42%	1.253%
52	16.500	2450	2456	2461	rBV4	57060	129482	20.26%	2.223%
53	16.711	2485	2492	2499	rBV2	142924	354194	55.41%	6.081%
54	16.782	2500	2504	2505	rBV4	33595	48668	7.61%	0.836%

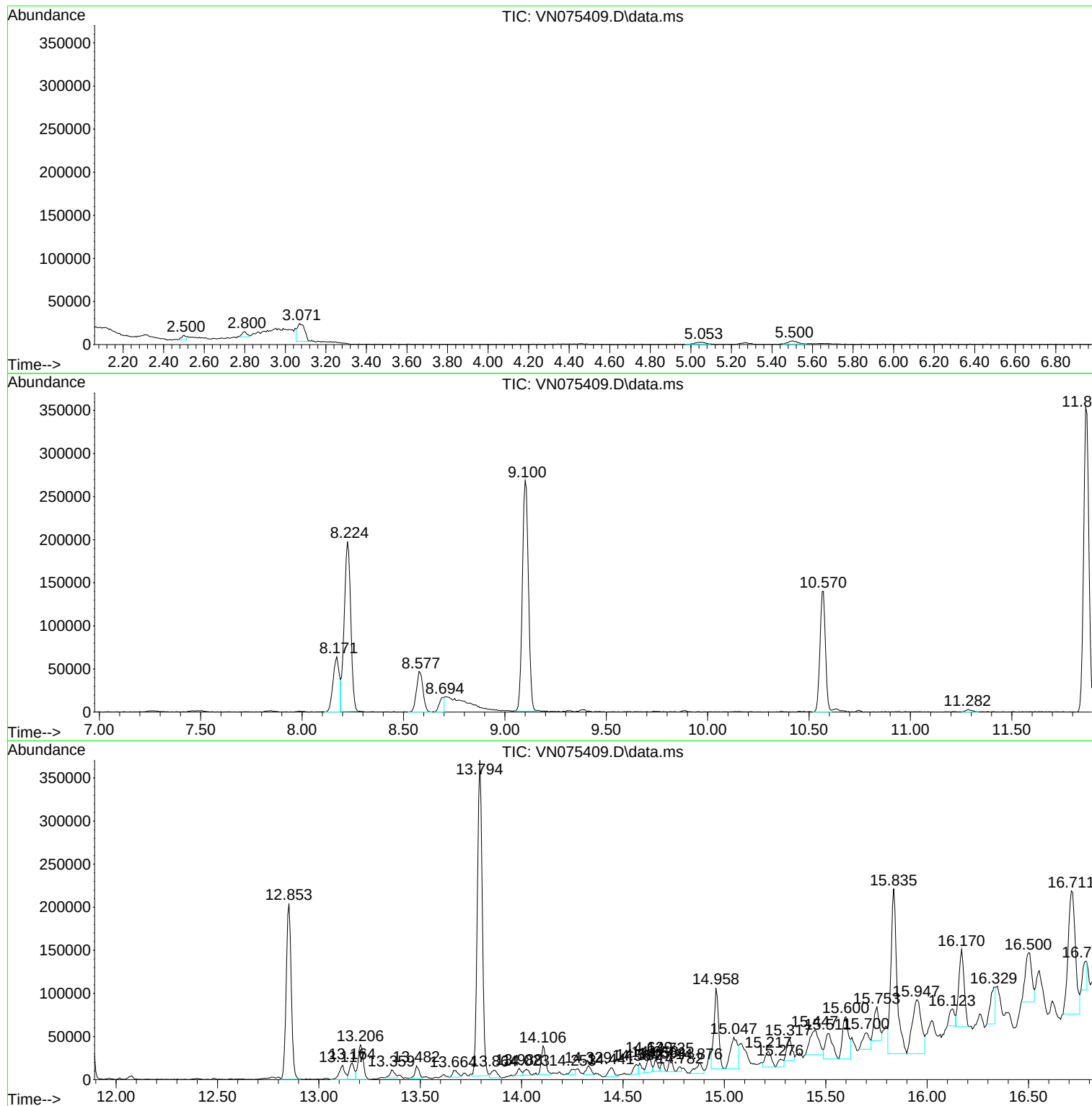
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112122W.M
Quant Title : SW846 8260

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



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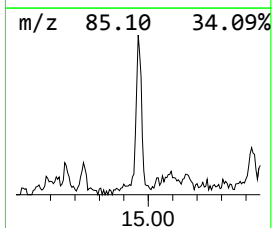
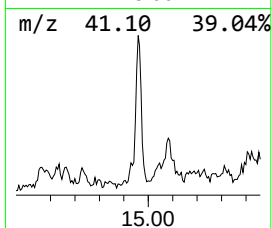
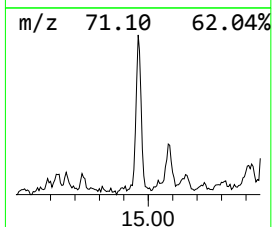
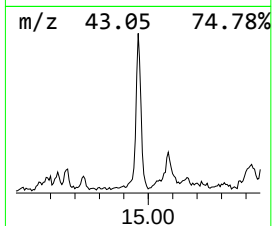
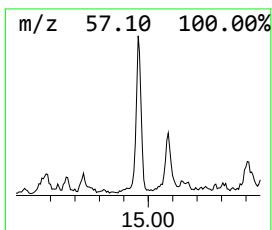
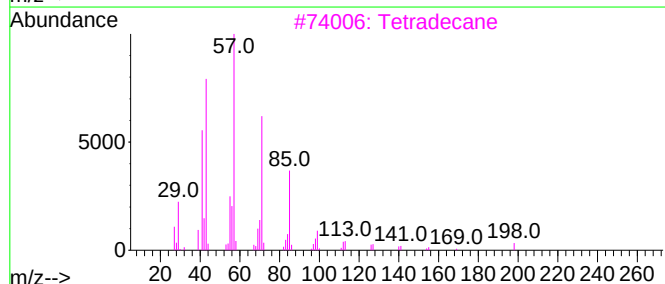
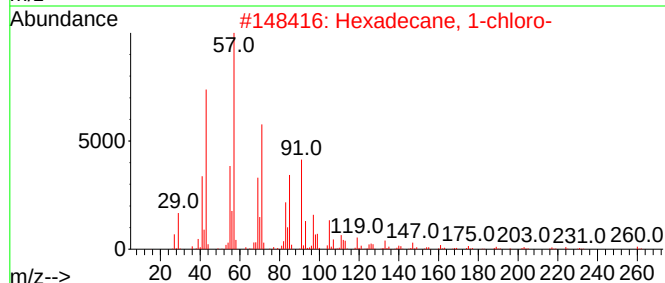
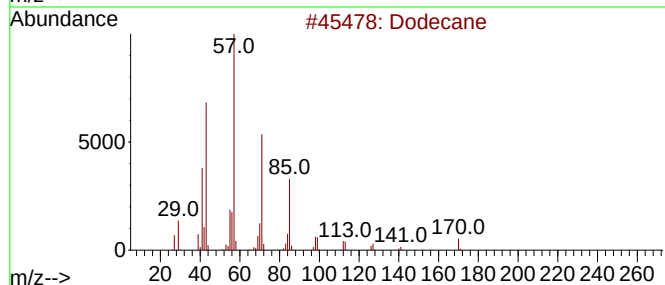
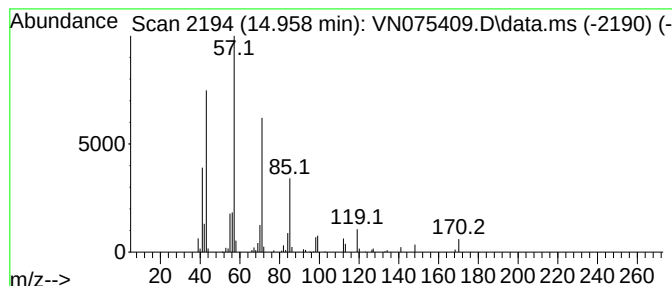
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112122W.M
Quant Title : SW846 8260

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

Peak Number 1 Dodecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.958	11.83 ug/l	145253	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	91
2			Hexadecane, 1-chloro-	260	C16H33Cl	004860-03-1	72
3			Tetradecane	198	C14H30	000629-59-4	72
4			Tetradecane, 1-chloro-	232	C14H29Cl	002425-54-9	72
5			Hexadecane	226	C16H34	000544-76-3	64



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ALS Vial : 26 Sample Multiplier: 1

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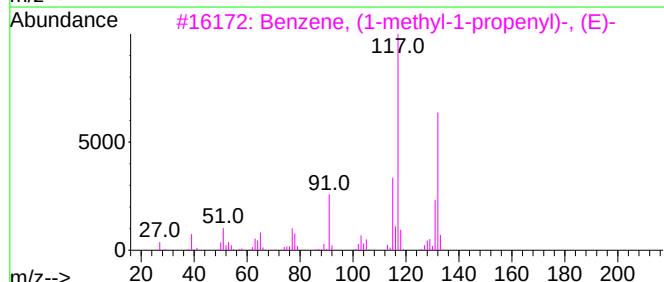
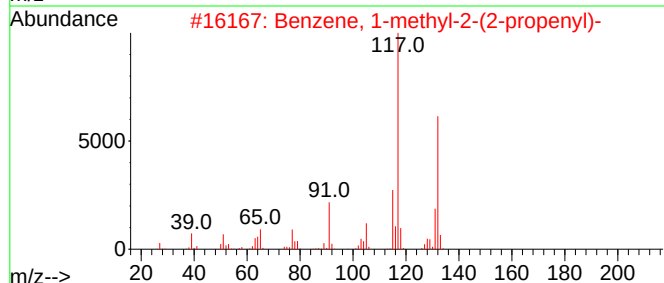
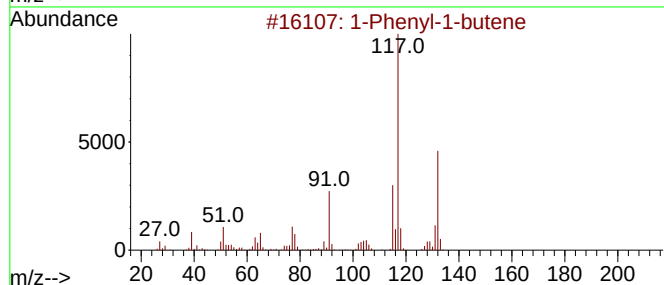
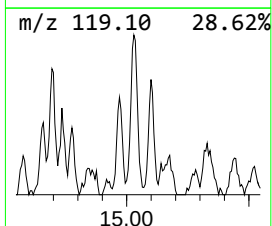
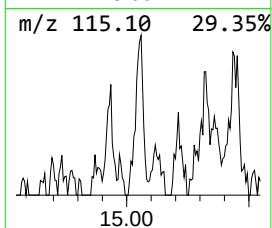
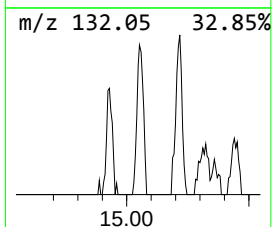
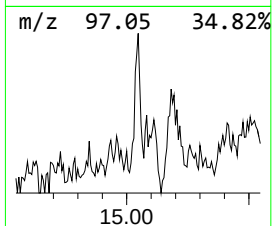
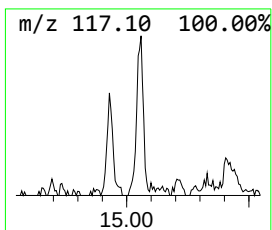
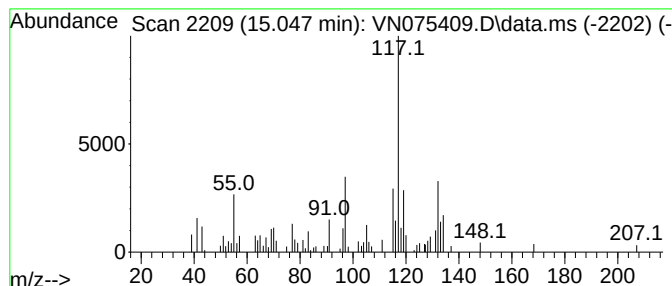
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112122W.M
Quant Title : SW846 8260

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

Peak Number 2 1-Phenyl-1-butene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.047	7.59 ug/l	93181	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenyl-1-butene	132	C10H12	000824-90-8	70
2			Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	62
3			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	62
4			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000767-99-7	62
5			Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	60



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Misc : 1.32g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 26 Sample Multiplier: 1

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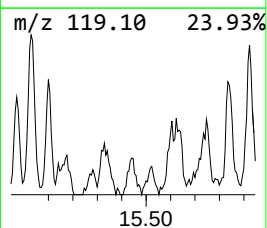
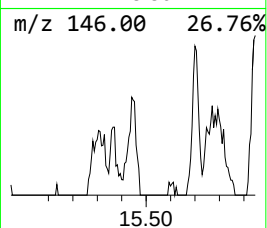
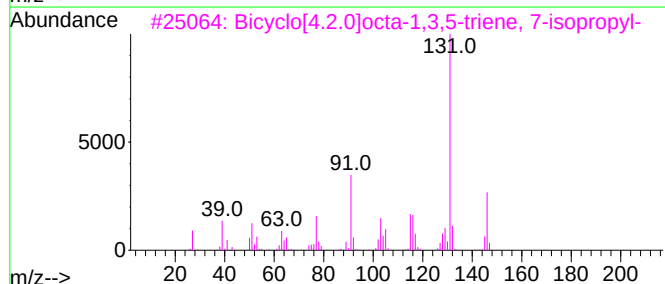
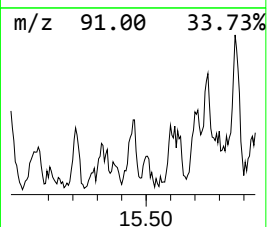
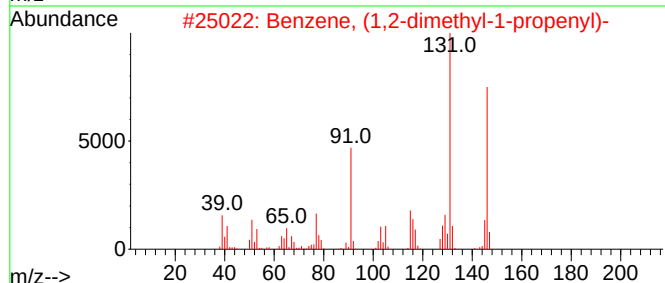
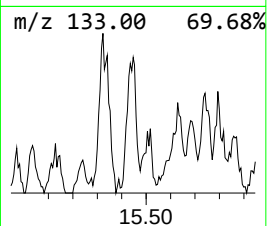
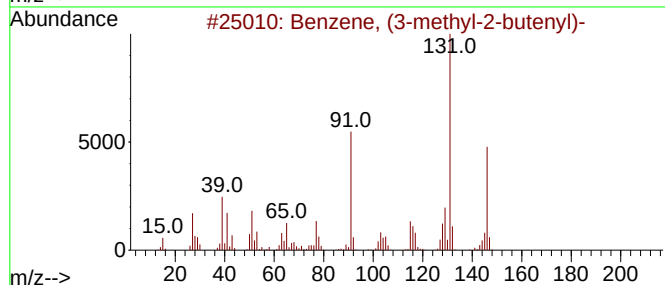
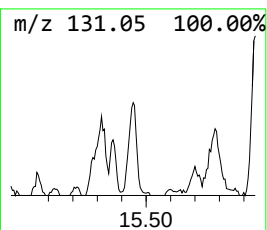
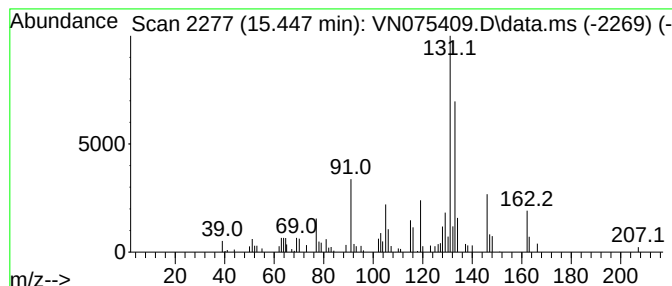
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112122W.M
Quant Title : SW846 8260

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

Peak Number 3 Benzene, (3-methyl-2-butenyl)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.447	7.31 ug/l	89672	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	60
2			Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	60
3			Bicyclo[4.2.0]octa-1,3,5-triene,...	146	C11H14	027087-54-3	49
4			2-Propenal, 3-(2-methoxyphenyl)-	162	C10H10O2	001504-74-1	49
5			1H-Indene, 2,3-dihydro-1,6-dimet...	146	C11H14	017059-48-2	49



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Instrument :
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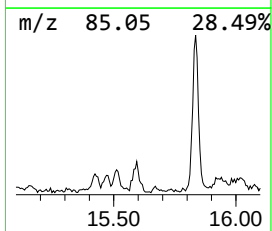
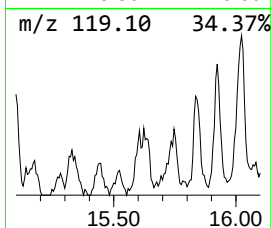
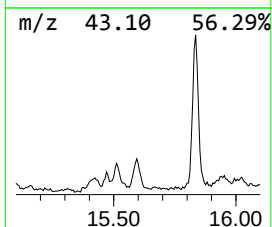
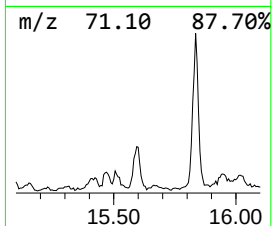
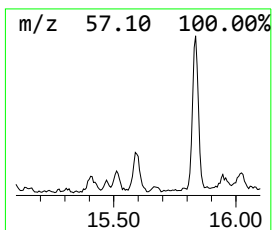
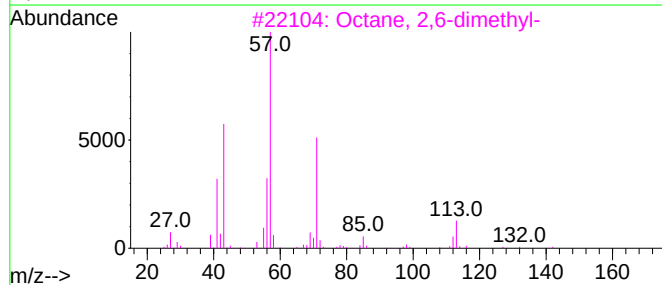
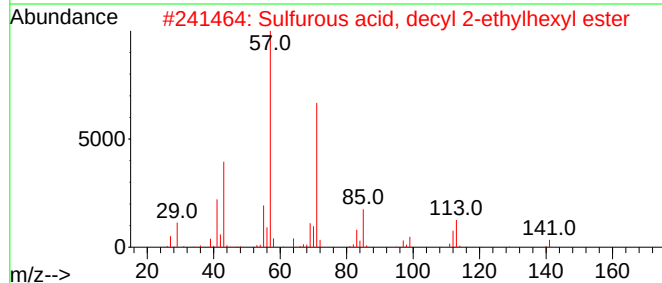
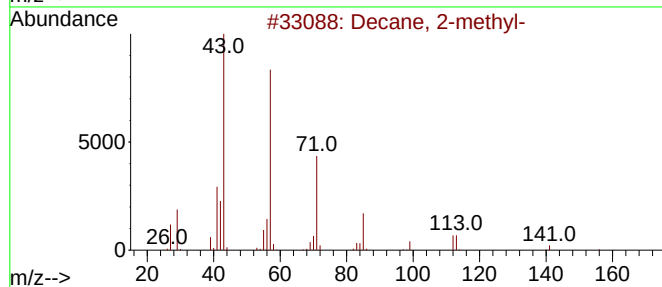
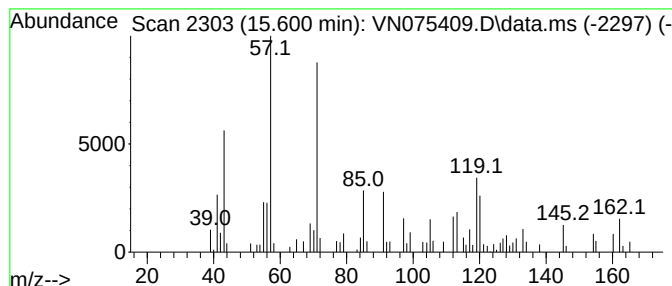
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Quant Title : SW846 8260

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

Peak Number 4 unknown15.600 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.600	8.60 ug/l	105565	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 2-methyl-	156	C11H24	006975-98-0	47
2			Sulfurous acid, decyl 2-ethylhex...	334	C18H38O3S	1000309-19-3	46
3			Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	46
4			Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	43
5			Sulfurous acid, 2-ethylhexyl non...	320	C17H36O3S	1010309-19-2	43



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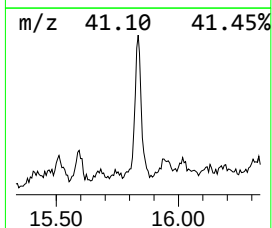
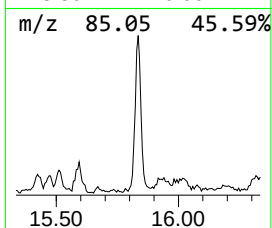
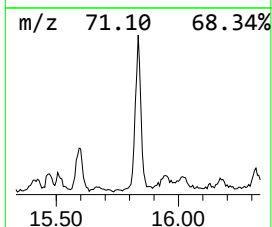
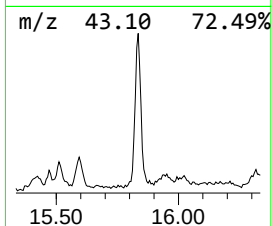
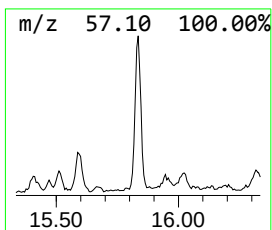
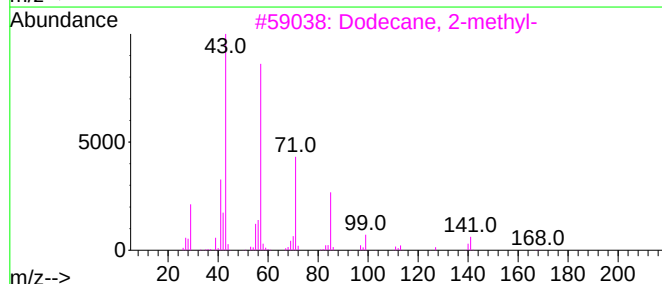
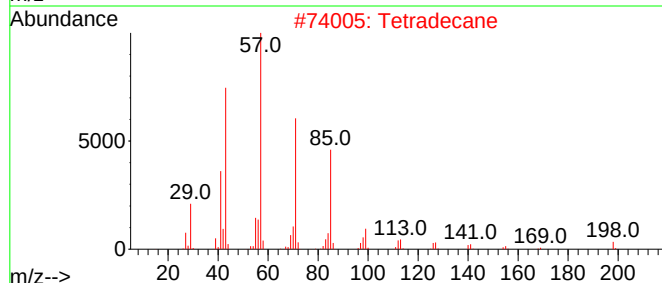
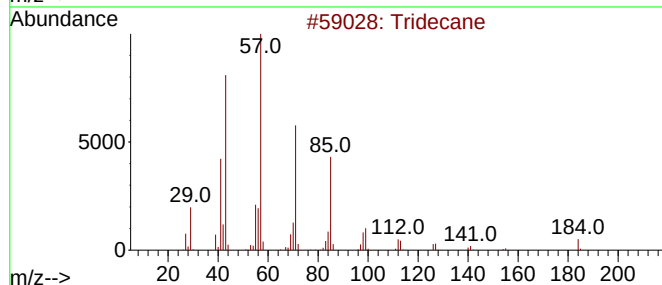
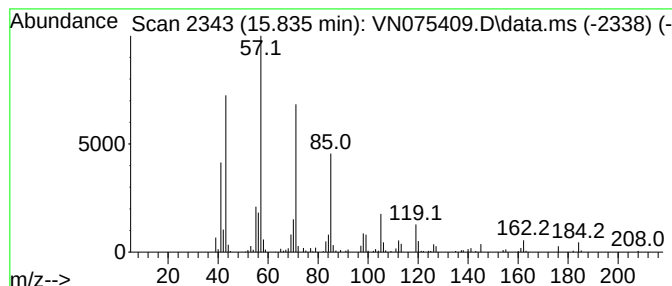
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Quant Title : SW846 8260

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

Peak Number 5 Tridecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.835	31.76 ug/l	389842	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	97
2			Tetradecane	198	C14H30	000629-59-4	68
3			Dodecane, 2-methyl-	184	C13H28	001560-97-0	59
4			Carbonic acid, tetradecyl vinyl ...	284	C17H32O3	1000382-54-5	59
5			Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112322\
Data File : VN075409.D
Acq On : 23 Nov 2022 20:22
Operator : JC\MD
Sample : N5692-03
Misc : 1.32g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
HS-SPILL-DRUM-11-16

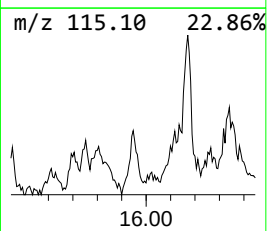
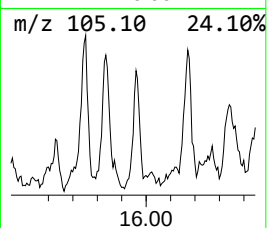
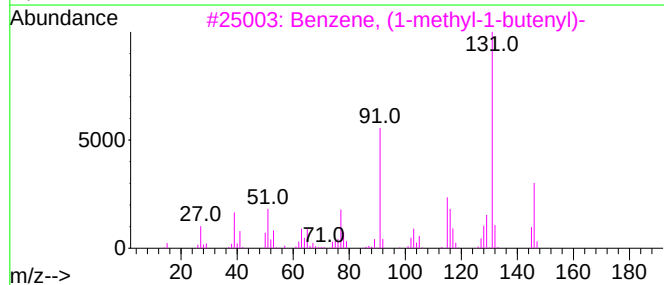
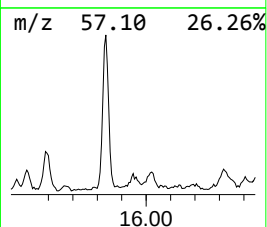
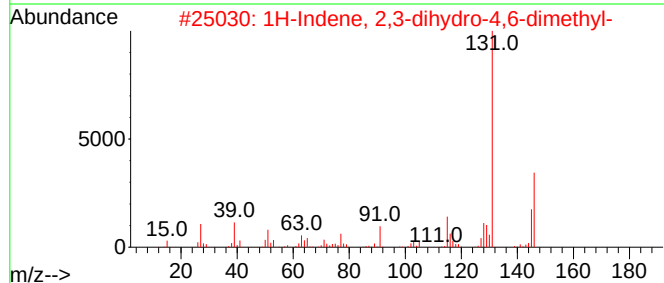
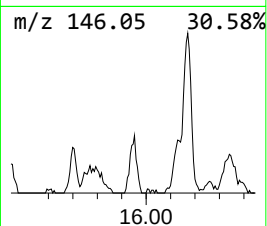
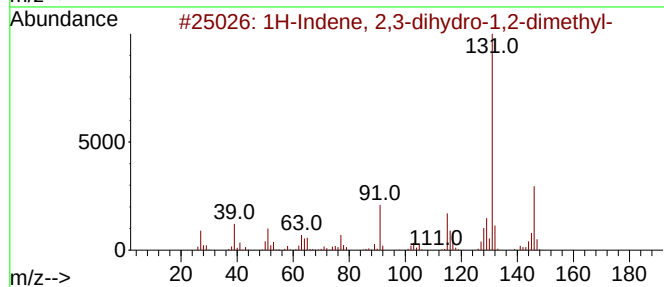
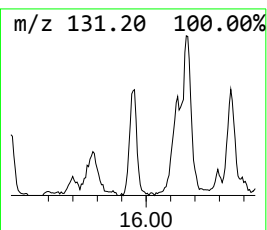
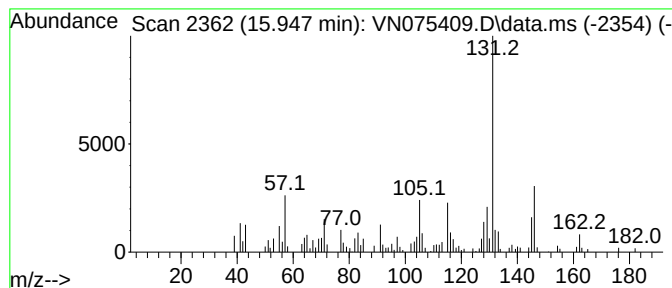
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Quant Title : SW846 8260

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

Peak Number 6 1H-Indene, 2,3-dihydro-1,2-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.947	16.15 ug/l	198199	1,4-Dichlorobenzene-d4	13.794

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	81
2		1H-Indene, 2,3-dihydro-4,6-dimet...	146	C11H14	001685-82-1	76
3		Benzene, (1-methyl-1-butenyl)-	146	C11H14	053172-84-2	74
4		1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	70
5		1H-Indene, 2,3-dihydro-1,6-dimet...	146	C11H14	017059-48-2	70



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112322\
Data File : VN075409.D
Acq On : 23 Nov 2022 20:22
Operator : JC\MD
Sample : N5692-03
Misc : 1.32g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
HS-SPILL-DRUM-11-16

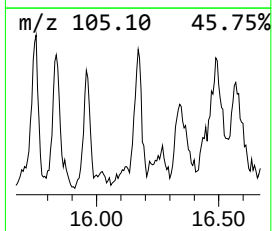
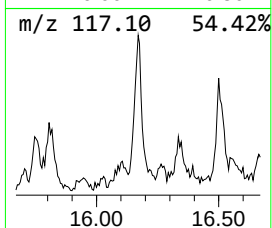
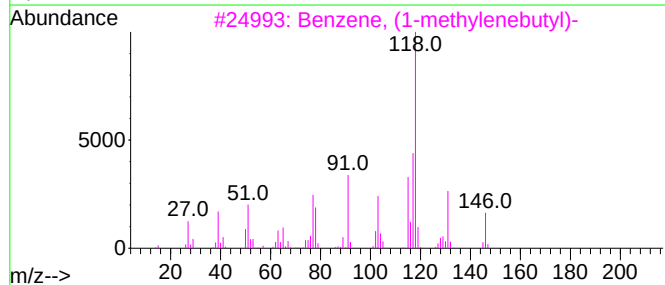
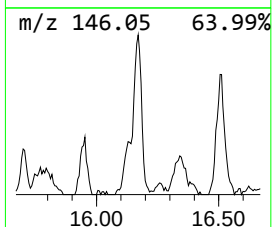
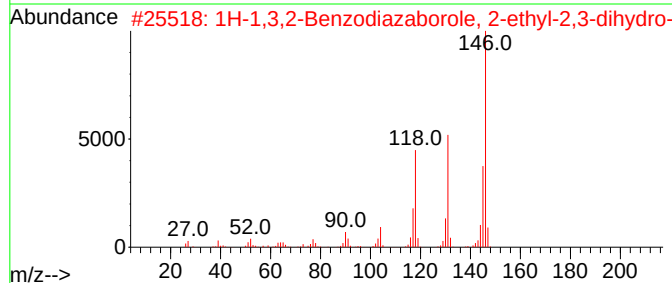
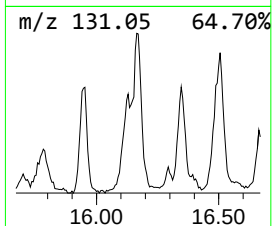
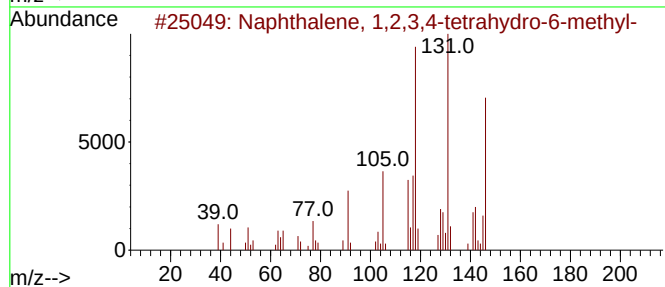
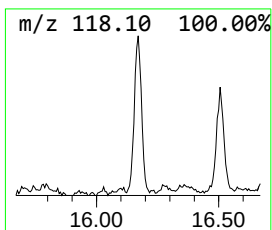
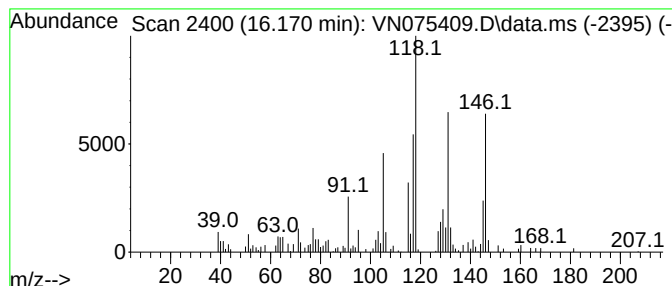
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.170	13.29 ug/l	163120	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	81
2			1H-1,3,2-Benzodiazaborole, 2-eth...	146	C8H11BN2	074663-81-3	68
3			Benzene, (1-methylenebutyl)-	146	C11H14	005676-32-4	64
4			2-Propyn-1-ol, 3-(4-methylphenyl)-	146	C10H10O	016017-24-6	60
5			Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	49



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112322\
Data File : VN075409.D
Acq On : 23 Nov 2022 20:22
Operator : JC\MD
Sample : N5692-03
Misc : 1.32g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
HS-SPILL-DRUM-11-16

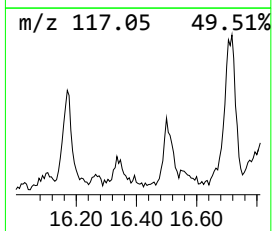
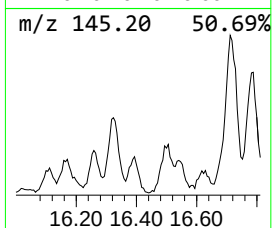
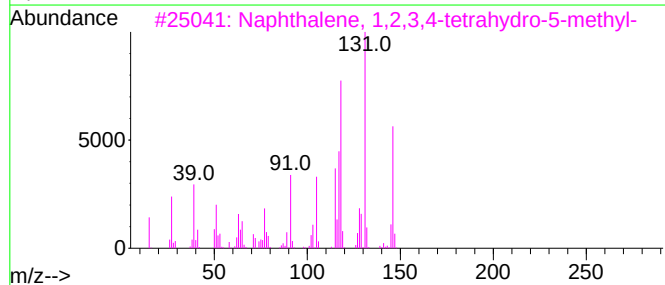
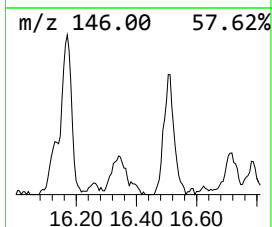
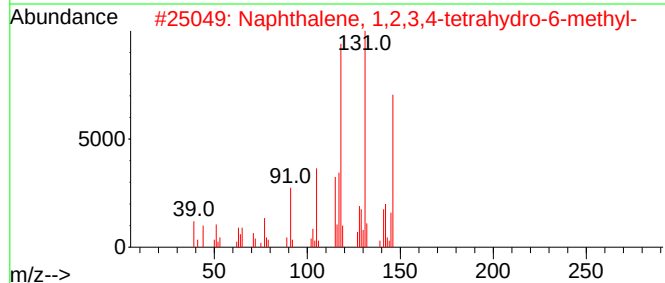
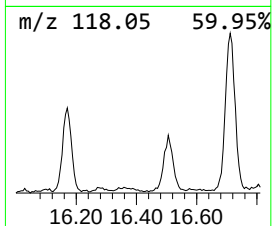
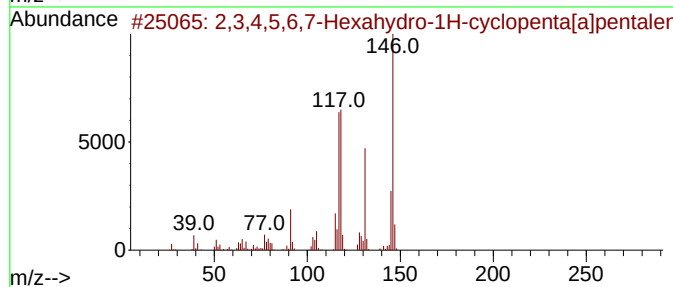
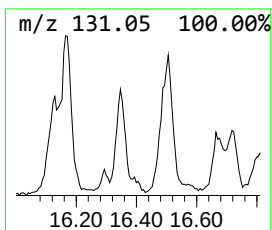
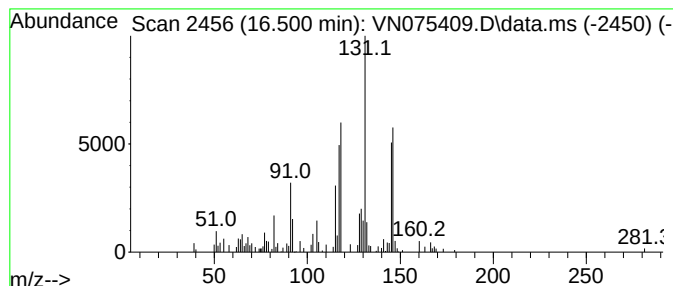
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Quant Title : SW846 8260

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

Peak Number 9 2,3,4,5,6,7-Hexahydro-1H-cy... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.500	10.55 ug/l	129482	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3,4,5,6,7-Hexahydro-1H-cyclope...	146	C11H14	1010189-31-0	87		
2	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	81		
3	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	72		
4	Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	64		
5	1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	49		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112322\
Data File : VN075409.D
Acq On : 23 Nov 2022 20:22
Operator : JC\MD
Sample : N5692-03
Misc : 1.32g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
HS-SPILL-DRUM-11-16

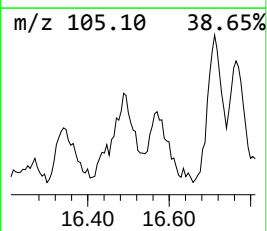
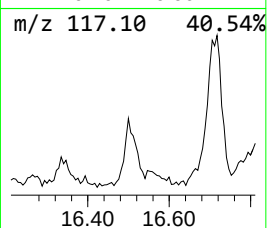
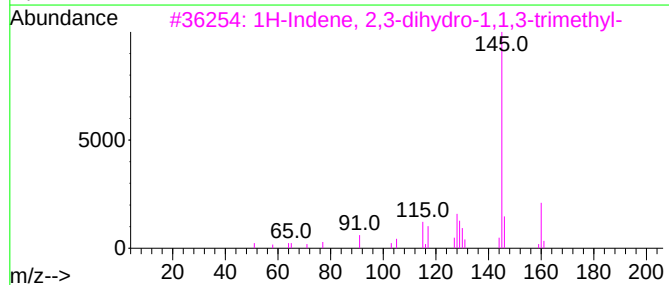
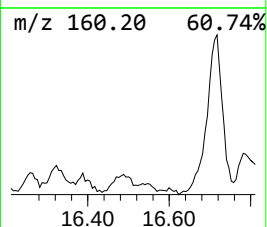
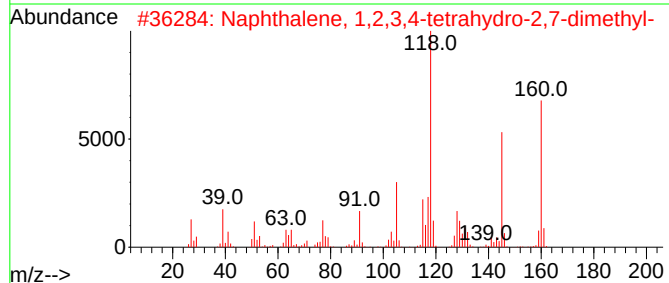
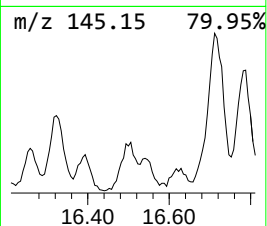
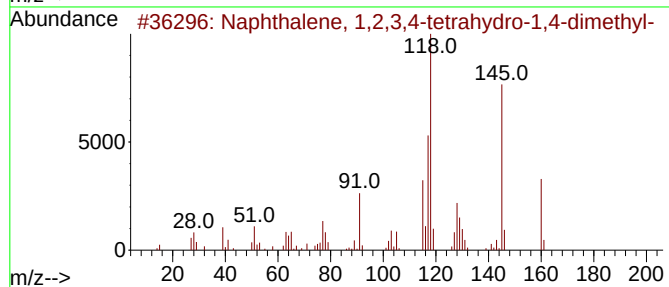
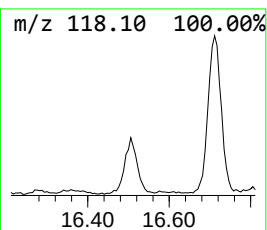
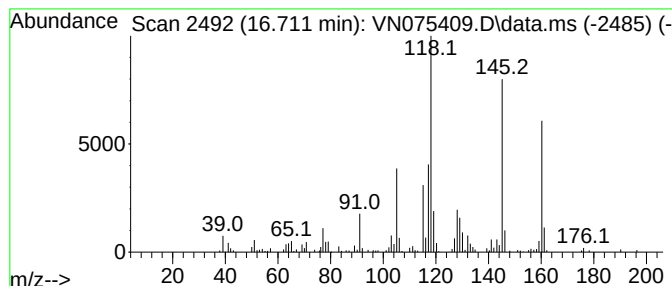
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112122W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.711	28.86 ug/l	354194	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	91
2			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	013065-07-1	90
3			1H-Indene, 2,3-dihydro-1,1,3-tri...	160	C12H16	002613-76-5	83
4			Benzene, 1-(2-butenyl)-2,3-dimet...	160	C12H16	054340-85-1	78
5			Benzene, 1-(1-methylethenyl)-3-(...	160	C12H16	001129-29-9	70



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112322\
Data File : VN075409.D
Acq On : 23 Nov 2022 20:22
Operator : JC\MD
Sample : N5692-03
Misc : 1.32g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
HS-SPILL-DRUM-11-16

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
Dodecane	14.958	11.8	ug/l	145253	4	13.794	613727	50.0
1-Phenyl-1-butene	15.047	7.6	ug/l	93181	4	13.794	613727	50.0
Benzene, (3-met...	15.447	7.3	ug/l	89672	4	13.794	613727	50.0
unknown15.600	15.600	8.6	ug/l	105565	4	13.794	613727	50.0
Tridecane	15.835	31.8	ug/l	389842	4	13.794	613727	50.0
1H-Indene, 2,3-...	15.947	16.1	ug/l	198199	4	13.794	613727	50.0
Naphthalene, 1,...	16.170	13.3	ug/l	163120	4	13.794	613727	50.0
Benzene, 1-(1-m...	16.329	6.0	ug/l	72979	4	13.794	613727	50.0
2,3,4,5,6,7-Hex...	16.500	10.6	ug/l	129482	4	13.794	613727	50.0
Naphthalene, 1,...	16.711	28.9	ug/l	354194	4	13.794	613727	50.0