LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN111422\
Data File : VN075269.D
Acq On : 14 Nov 2022 16:51
Operator : JC\MD
Sample : N5582-04
Misc : 5.08g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
31979

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\82N102622W.M
Title : SW846 8260

Signal : TIC: VN075269.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.171	1029	1040	1044	rBV	323660	807264	32.14%	4.456%
2	8.224	1044	1049	1059	rVB	601890	1300762	51.79%	7.180%
3	8.577	1099	1109	1121	rBV	358819	808336	32.18%	4.462%
4	9.100	1188	1198	1208	rBV	881711	1783179	71.00%	9.843%
5	10.565	1438	1447	1464	rBV	1387612	2511541	100.00%	13.863%
6	11.865	1660	1668	1682	rBV	1204131	2109118	83.98%	11.642%
7	12.071	1696	1703	1713	rBV4	16227	30802	1.23%	0.170%
8	12.847	1829	1835	1845	rVB	904557	1538986	61.28%	8.495%
9	13.100	1871	1878	1882	rBV	16410	32576	1.30%	0.180%
10	13.159	1882	1888	1896	rVV3	76771	151432	6.03%	0.836%
11	13.394	1924	1928	1934	rVB2	25452	41784	1.66%	0.231%
12	13.482	1934	1943	1947	rBV	32121	59487	2.37%	0.328%
13	13.671	1970	1975	1980	rBV5	23932	51644	2.06%	0.285%
14	13.712	1980	1982	1986	rVV4	25509	38359	1.53%	0.212%
15	13.794	1986	1996	2003	rVV	1192958	2058732	81.97%	11.364%
16	13.853	2003	2006	2012	rVB	31917	48176	1.92%	0.266%
17	13.941	2014	2021	2024	rBV6	11673	26511	1.06%	0.146%
18	13.982	2024	2028	2031	rBV2	24536	35612	1.42%	0.197%
19	14.023	2031	2035	2043	rVB4	23123	44410	1.77%	0.245%
20	14.106	2043	2049	2055	rBV	193726	323160	12.87%	1.784%
21	14.265	2070	2076	2082	rBV6	30297	67155	2.67%	0.371%
22	14.323	2082	2086	2090	rBV3	36645	54523	2.17%	0.301%
23	14.365	2090	2093	2100	rVB6	26393	46588	1.85%	0.257%
24	14.435	2100	2105	2110	rBV3	49444	91700	3.65%	0.506%
25	14.500	2111	2116	2122	rBV7	17932	36687	1.46%	0.203%
26	14.582	2124	2130	2133	rBV4	54186	101900	4.06%	0.562%
27	14.623	2133	2137	2141	rVV4	93481	141289	5.63%	0.780%
28	14.659	2141	2143	2146	rVV2	48082	55066	2.19%	0.304%
29	14.688	2146	2148	2152	rVB	32450	40098	1.60%	0.221%
30	14.735	2152	2156	2159	rBV3	71201	96556	3.84%	0.533%
31	14.788	2159	2165	2171	rVB5	32854	77852	3.10%	0.430%
32	14.847	2171	2175	2176	rBV4	30389	40554	1.61%	0.224%
33	14.959	2184	2194	2200	rBV4	284745	531783	21.17%	2.935%
34	15.053	2201	2210	2213	rBV5	110341	325632	12.97%	1.797%
35	15.212	2233	2237	2243	rVB3	60526	128805	5.13%	0.711%
36	15.270	2243	2247	2250	rBV6	24358	40624	1.62%	0.224%

LSC Area Percent Report

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Operator : JC\MD
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Misc : 5.08g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
31979

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\82N102622W.M
Title : SW846 8260

37	15.317	2250	2255	2259	rBV4	72740	123646	4.92%	0.682%
38	15.441	2269	2276	2282	rBV5	63208	170383	6.78%	0.940%
39	15.506	2284	2287	2296	rVB6	57363	143217	5.70%	0.791%
40	15.594	2297	2302	2307	rBV5	71577	158568	6.31%	0.875%
41	15.700	2316	2320	2324	rBV3	37597	62181	2.48%	0.343%
42	15.747	2324	2328	2332	rBV4	43679	74293	2.96%	0.410%
43	15.829	2338	2342	2353	rVB3	210274	437779	17.43%	2.416%
44	15.947	2353	2362	2369	rBV4	99747	277612	11.05%	1.532%
45	16.165	2394	2399	2408	rVB2	171434	354563	14.12%	1.957%
46	16.500	2448	2456	2462	rBV3	100472	275148	10.96%	1.519%
47	16.712	2485	2492	2499	rBV	135313	289554	11.53%	1.598%
48	16.782	2499	2504	2505	rBV3	49374	71347	2.84%	0.394%

Sum of corrected areas: 18116974

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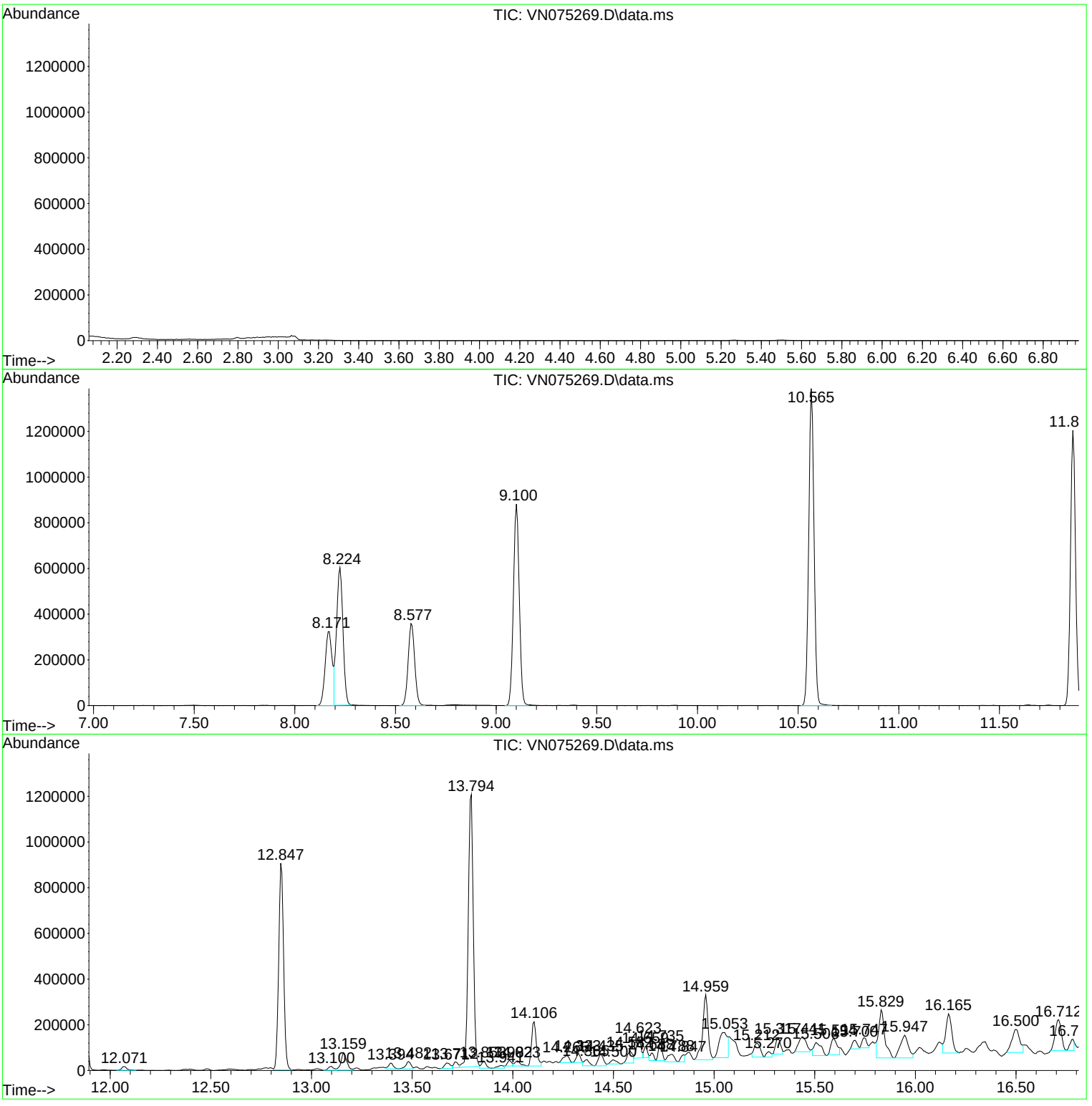
MSVOA_N
ClientSampleId :
31979

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102622W.M
Quant Title : SW846 8260

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



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Quant Title : SW846 8260

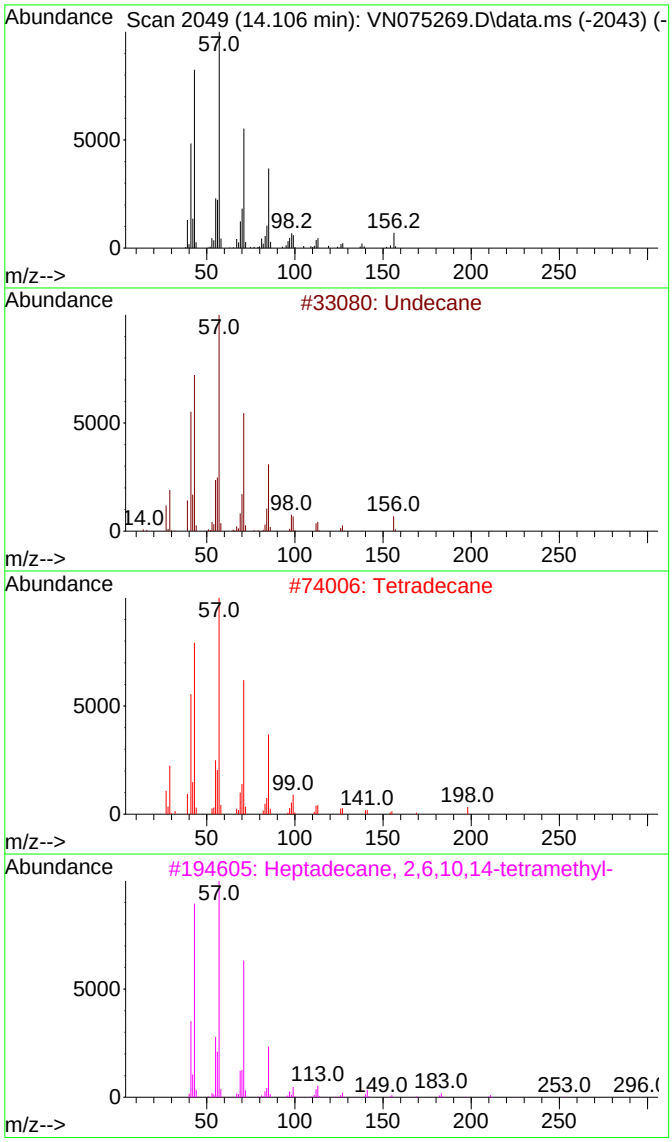
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

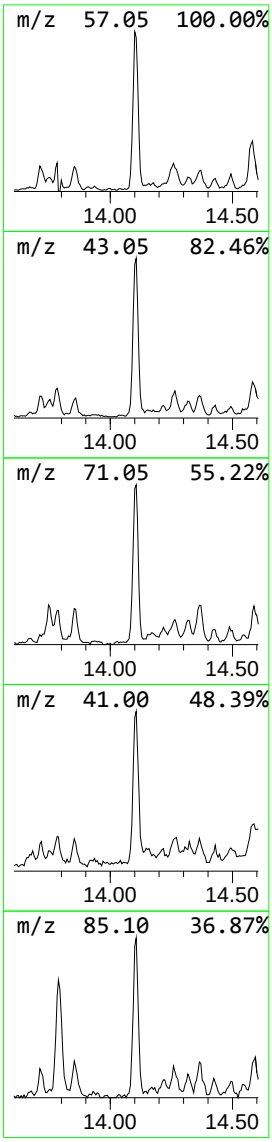
****

Peak Number 1 Undecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.106	7.85 ug/l	323160	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane	156	C11H24	001120-21-4	96
2	Tetradecane	198	C14H30	000629-59-4	86
3	Heptadecane, 2,6,10,14-tetramethyl-	296	C21H44	018344-37-1	80
4	Hexadecane	226	C16H34	000544-76-3	72
5	Octacosane	394	C28H58	000630-02-4	59





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Operator : JC\MD
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Misc : 5.08g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
31979

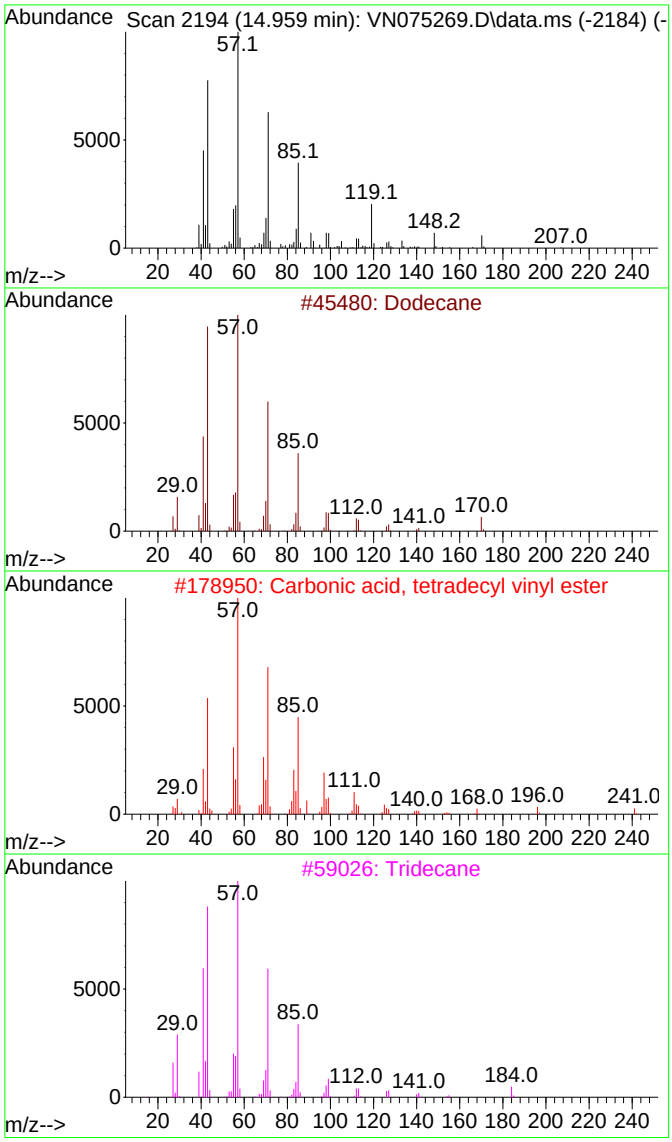
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102622W.M
Quant Title : SW846 8260

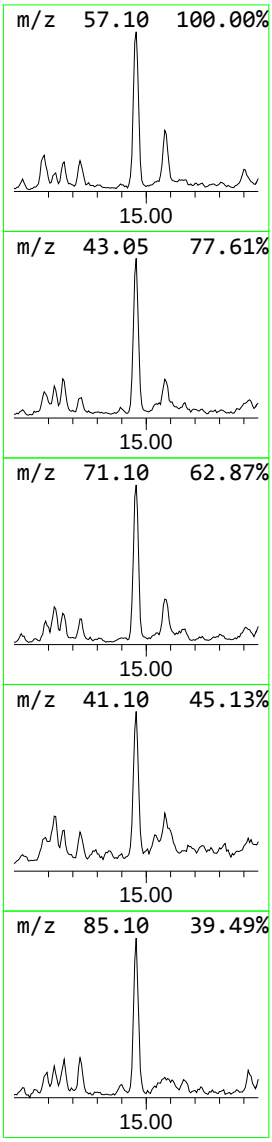
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Dodecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.959	12.92 ug/l	531783	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane	170	C12H26	000112-40-3	96
2	Carbonic acid, tetradecyl vinyl ...	284	C17H32O3	1000382-54-5	64
3	Tridecane	184	C13H28	000629-50-5	64
4	Nonane	128	C9H20	000111-84-2	60
5	Tetradecane	198	C14H30	000629-59-4	58





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Operator : JC\MD
Sample : N5582-04
Misc : 5.08g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
31979

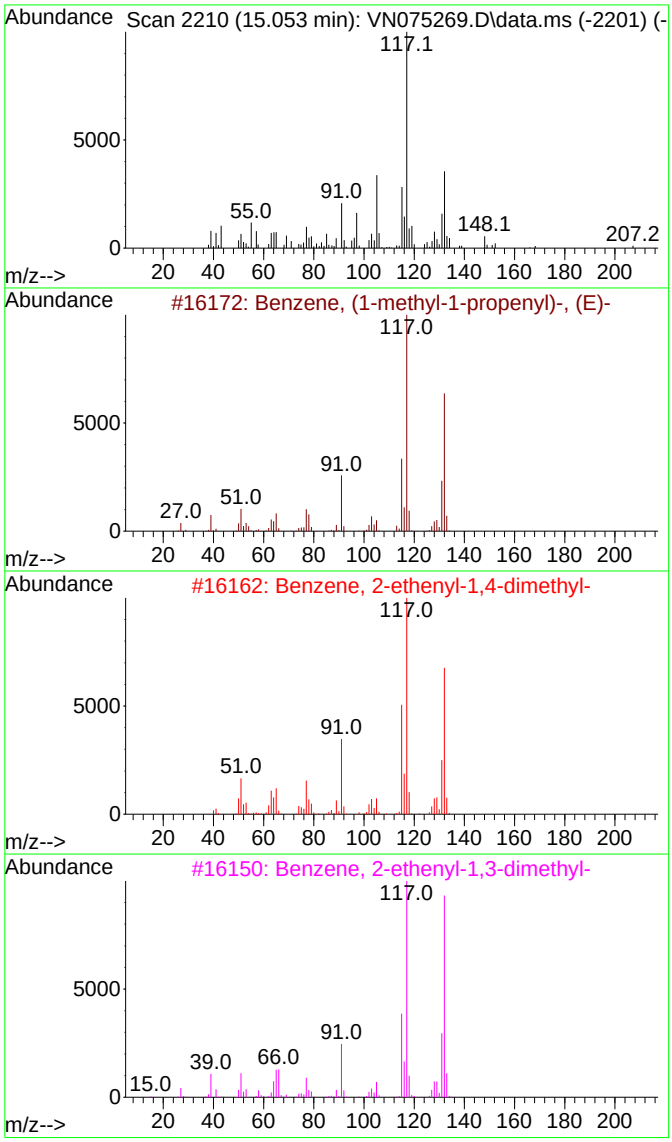
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102622W.M
Quant Title : SW846 8260

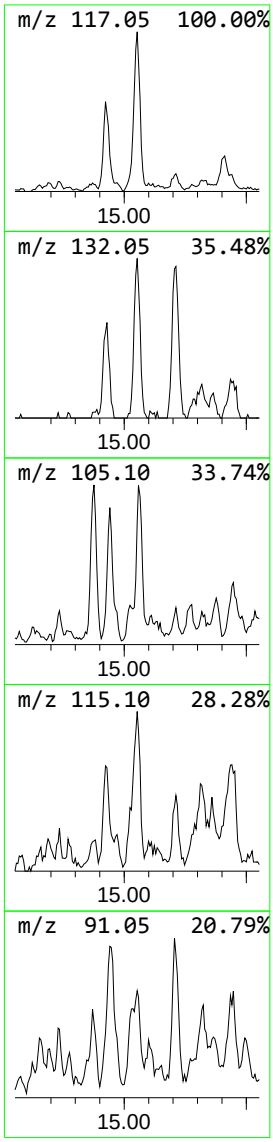
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Benzene, (1-methyl-1-propen... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.053	7.91 ug/l	325632	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	95
2	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	95
3	Benzene, 2-ethenyl-1,3-dimethyl-	132	C10H12	002039-90-9	93
4	1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	91
5	1-Phenyl-1-butene	132	C10H12	000824-90-8	89





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Operator : JC\MD
Sample : N5582-04
Misc : 5.08g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
31979

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102622W.M
Quant Title : SW846 8260

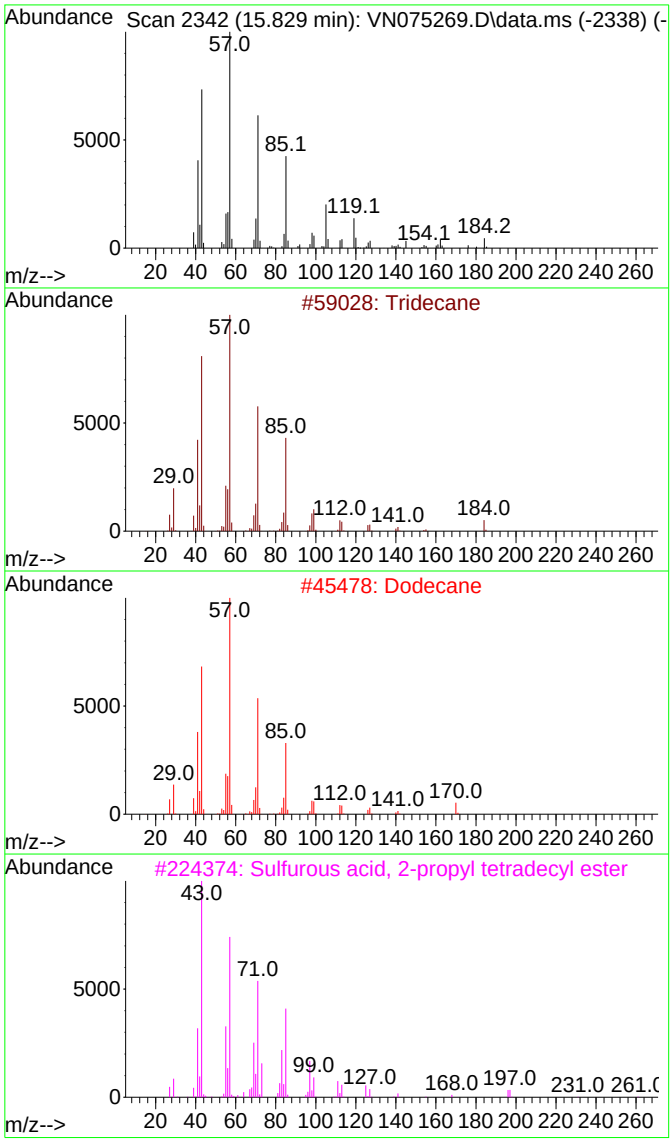
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

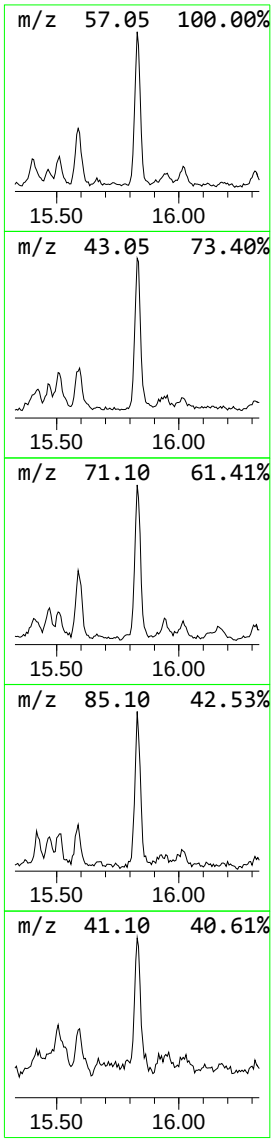
****

Peak Number 4 Tridecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.829	10.63 ug/l	437779	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	76
2	Dodecane	170	C12H26	000112-40-3	58
3	Sulfurous acid, 2-propyl tetrade...	320	C17H36O3S	1010309-12-5	47
4	Oxalic acid, 6-ethyloct-3-yl pro...	272	C15H28O4	1000309-34-0	43
5	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	38





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ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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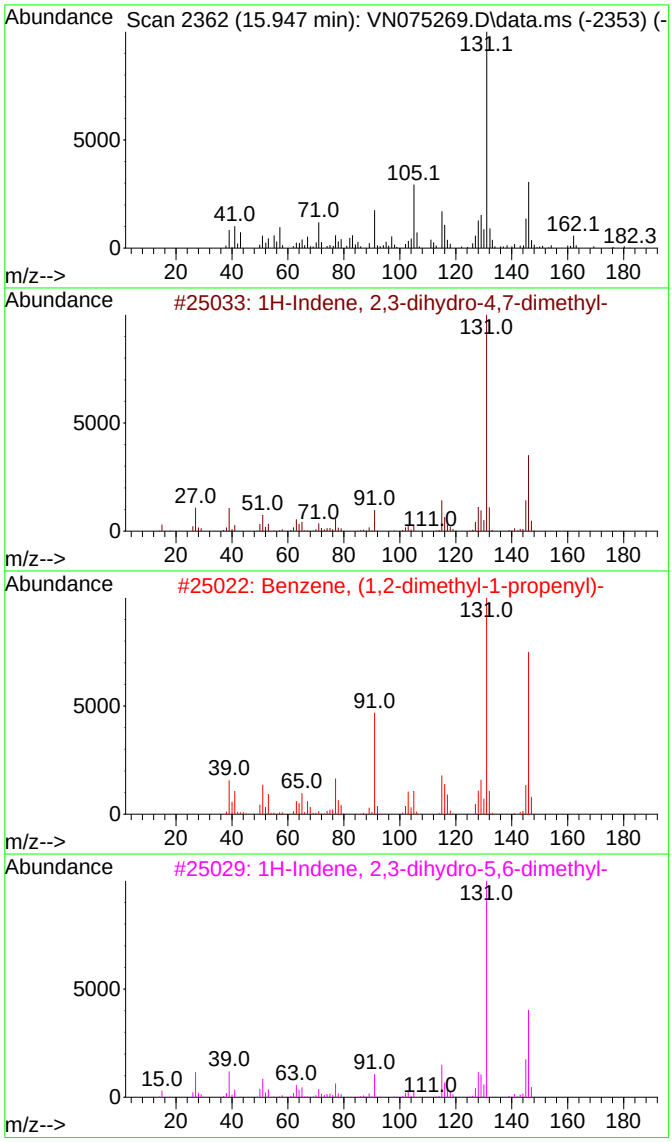
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102622W.M
Quant Title : SW846 8260

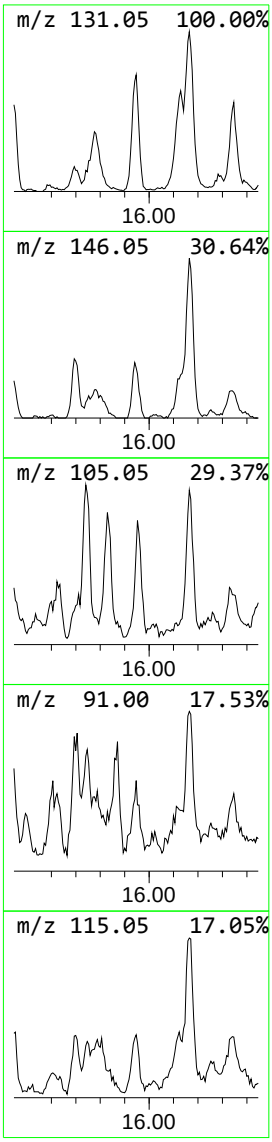
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1H-Indene, 2,3-dihydro-4,7-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.947	6.74 ug/l	277612	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	91
2	Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	87
3	1H-Indene, 2,3-dihydro-5,6-dimet...	146	C11H14	001075-22-5	76
4	1H-Indene, 2,3-dihydro-4,6-dimet...	146	C11H14	001685-82-1	76
5	1H-Indene, 2,3-dihydro-1,6-dimet...	146	C11H14	017059-48-2	74





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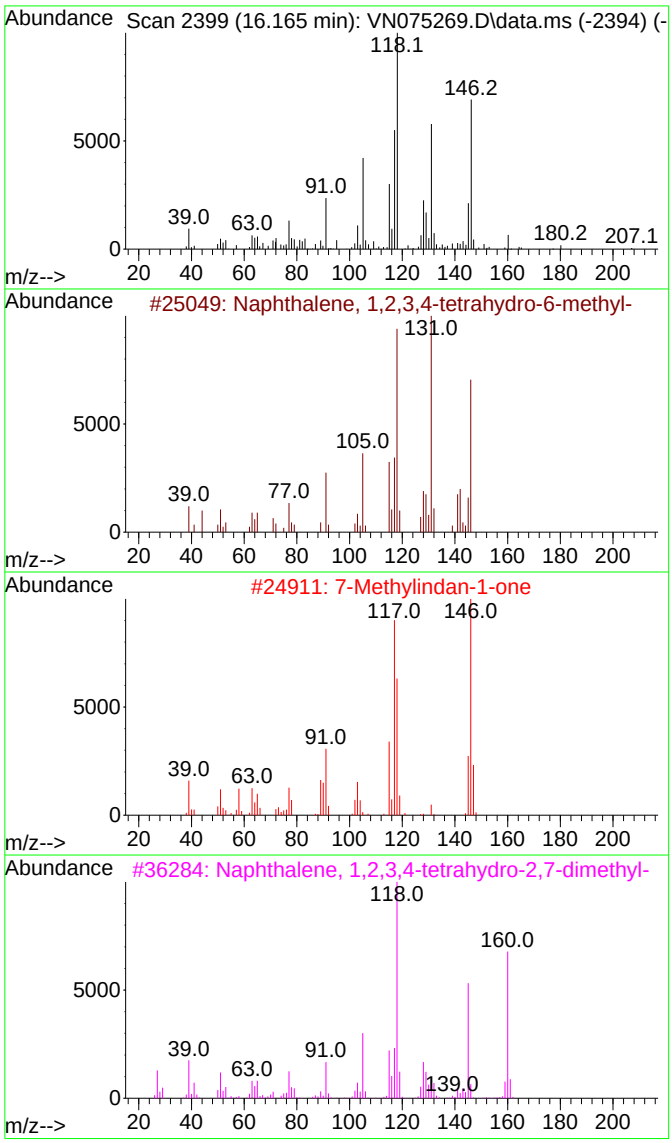
Quant Title : SW846 8260

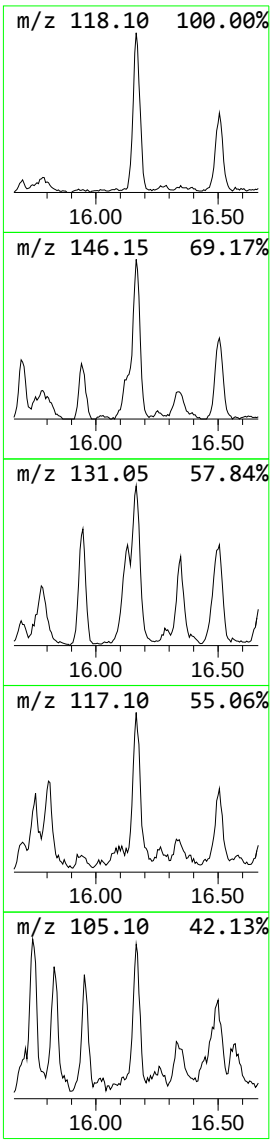
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.165	8.61 ug/l	354563	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	93
2	7-Methylindan-1-one	146	C10H10O	039627-61-7	49
3	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	013065-07-1	49
4	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	38
5	2-Trifluoromethylbenzoic acid, 3...	308	C17H15F3O2	1000282-29-3	38





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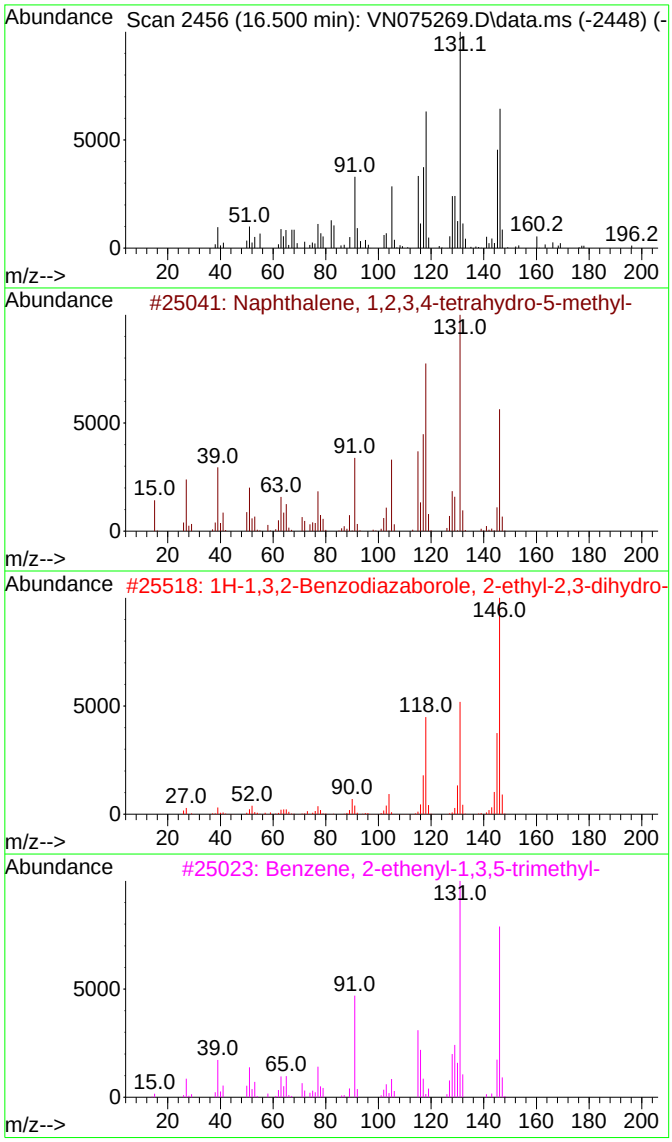
Quant Title : SW846 8260

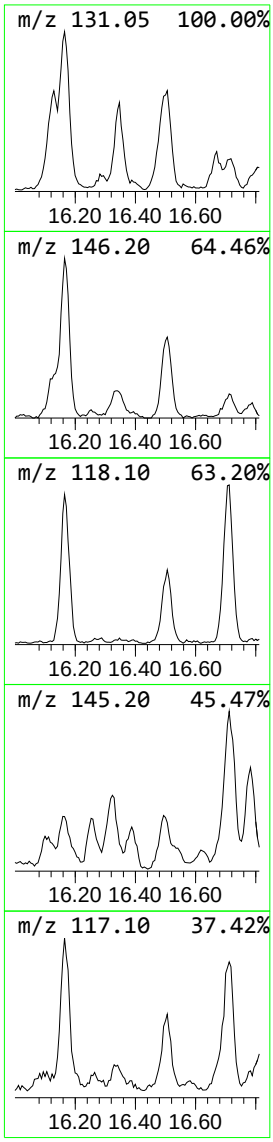
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.500	6.68 ug/l	275148	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	93
2	1H-1,3,2-Benzodiazaborole, 2-eth...	146	C8H11BN2	074663-81-3	64
3	Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	60
4	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	58
5	1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	53





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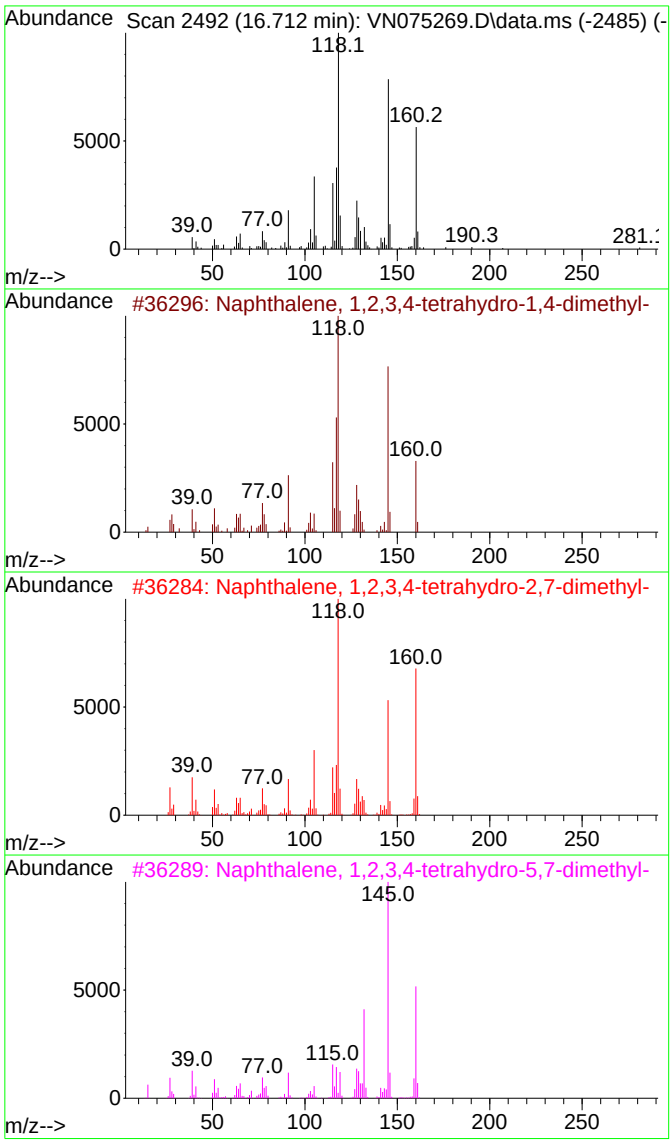
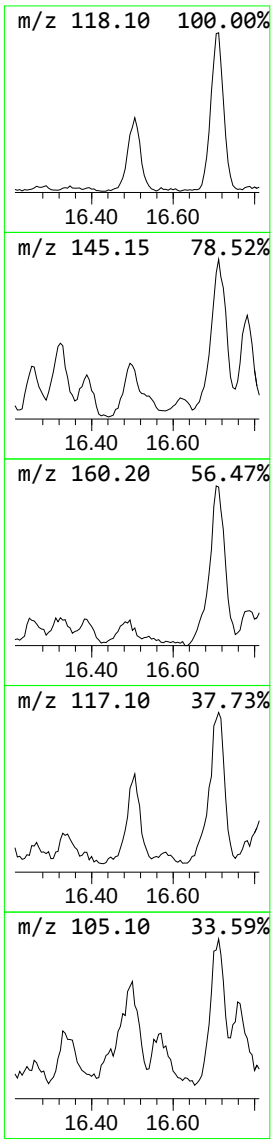
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.712	7.03 ug/l	289554	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	93
2	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	013065-07-1	91
3	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	021693-54-9	60
4	Benzene, 1-(1-methylethenyl)-2-(...	160	C12H16	005557-93-7	58
5	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	007524-63-2	58





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN111422\
Data File : VN075269.D
Acq On : 14 Nov 2022 16:51
Operator : JC\MD
Sample : N5582-04
Misc : 5.08g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
31979

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102622W.M
Quant Title : SW846 8260

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Undecane	14.106	7.8	ug/l	323160	4	13.794	2058730	50.0
Dodecane	14.959	12.9	ug/l	531783	4	13.794	2058730	50.0
Benzene, (1-met...	15.053	7.9	ug/l	325632	4	13.794	2058730	50.0
Tridecane	15.829	10.6	ug/l	437779	4	13.794	2058730	50.0
1H-Indene, 2,3-...	15.947	6.7	ug/l	277612	4	13.794	2058730	50.0
Naphthalene, 1,...	16.165	8.6	ug/l	354563	4	13.794	2058730	50.0
Naphthalene, 1,...	16.500	6.7	ug/l	275148	4	13.794	2058730	50.0
Naphthalene, 1,...	16.712	7.0	ug/l	289554	4	13.794	2058730	50.0