LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090324\
Data File : VN083635.D
Acq On : 03 Sep 2024 19:33
Operator : JC\MD
Sample : P3811-02
Misc : 1.47g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DRUM-2

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\82N083024W.M
Title : SW846 8260

Signal : TIC: VN083635.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.289	52	57	63	rBV	53271	90808	8.45%	0.859%
2	2.806	138	145	146	rBV4	9526	18041	1.68%	0.171%
3	4.430	413	421	435	rVB2	17471	51008	4.74%	0.483%
4	5.024	514	522	534	rBV2	4439	14483	1.35%	0.137%
5	7.241	892	899	902	rBV3	4928	11677	1.09%	0.110%
6	8.165	1046	1056	1060	rBV2	125566	305865	28.45%	2.893%
7	8.218	1060	1065	1078	rVB	211854	466970	43.43%	4.417%
8	8.577	1114	1126	1132	rBV	128064	295923	27.52%	2.799%
9	8.683	1132	1144	1179	rVB3	131491	954367	88.76%	9.028%
10	9.094	1205	1214	1230	rVB	350451	731436	68.03%	6.919%
11	10.565	1454	1464	1472	rBV	487428	904045	84.08%	8.552%
12	11.865	1677	1685	1694	rBV	588213	1035233	96.28%	9.793%
13	12.065	1713	1719	1726	rBV	29826	51644	4.80%	0.489%
14	12.394	1766	1775	1782	rBV2	18370	34388	3.20%	0.325%
15	12.847	1840	1852	1862	rVB	436688	761266	70.80%	7.201%
16	13.100	1889	1895	1898	rBV5	13273	28251	2.63%	0.267%
17	13.170	1902	1907	1913	rVV5	25045	53395	4.97%	0.505%
18	13.482	1955	1960	1965	rBV2	38093	64156	5.97%	0.607%
19	13.618	1978	1983	1987	rBV6	7948	14900	1.39%	0.141%
20	13.676	1987	1993	1998	rBV7	17392	38044	3.54%	0.360%
21	13.788	2006	2012	2021	rVB	597190	1075215	100.00%	10.171%
22	13.935	2030	2037	2041	rBV8	9775	24625	2.29%	0.233%
23	13.982	2041	2045	2048	rBV4	24379	38821	3.61%	0.367%
24	14.023	2048	2052	2056	rVB2	19318	34267	3.19%	0.324%
25	14.117	2062	2068	2076	rBV6	54617	133333	12.40%	1.261%
26	14.241	2083	2089	2091	rBV5	16261	29214	2.72%	0.276%
27	14.329	2100	2104	2108	rVB2	37211	55564	5.17%	0.526%
28	14.435	2117	2122	2127	rBV2	60638	105166	9.78%	0.995%
29	14.512	2128	2135	2139	rBV6	39098	79922	7.43%	0.756%
30	14.570	2140	2145	2150	rBV7	37876	69752	6.49%	0.660%
31	14.623	2150	2154	2157	rBV4	74530	121649	11.31%	1.151%
32	14.659	2157	2160	2163	rVB2	49193	60278	5.61%	0.570%
33	14.729	2169	2172	2175	rBV5	32434	46081	4.29%	0.436%
34	14.770	2175	2179	2181	rBV2	38828	56932	5.29%	0.539%
35	14.847	2187	2192	2195	rBV6	35445	60710	5.65%	0.574%
36	14.959	2202	2211	2218	rBV10	69256	204799	19.05%	1.937%

LSC Area Percent Report

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ClientSampleId :
DRUM-2

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

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Peak separation: 5

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Title : SW846 8260

37	15.059	2218	2228	2232	rVV5	80394	274912	25.57%	2.600%
38	15.106	2232	2236	2241	rVB6	60293	114502	10.65%	1.083%
39	15.212	2249	2254	2259	rBV	117786	221758	20.62%	2.098%
40	15.264	2259	2263	2268	rVB5	81231	130796	12.16%	1.237%
41	15.317	2268	2272	2279	rBV6	77387	178004	16.56%	1.684%
42	15.594	2316	2319	2328	rVB6	52978	107141	9.96%	1.013%
43	15.700	2332	2337	2343	rBV4	128105	280302	26.07%	2.651%
44	15.953	2371	2380	2385	rBV9	72429	274742	25.55%	2.599%
45	16.170	2412	2417	2423	rBV7	173504	339729	31.60%	3.214%
46	16.706	2503	2508	2514	rBV2	247944	527394	49.05%	4.989%

Sum of corrected areas: 10571508

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ClientSampleId :
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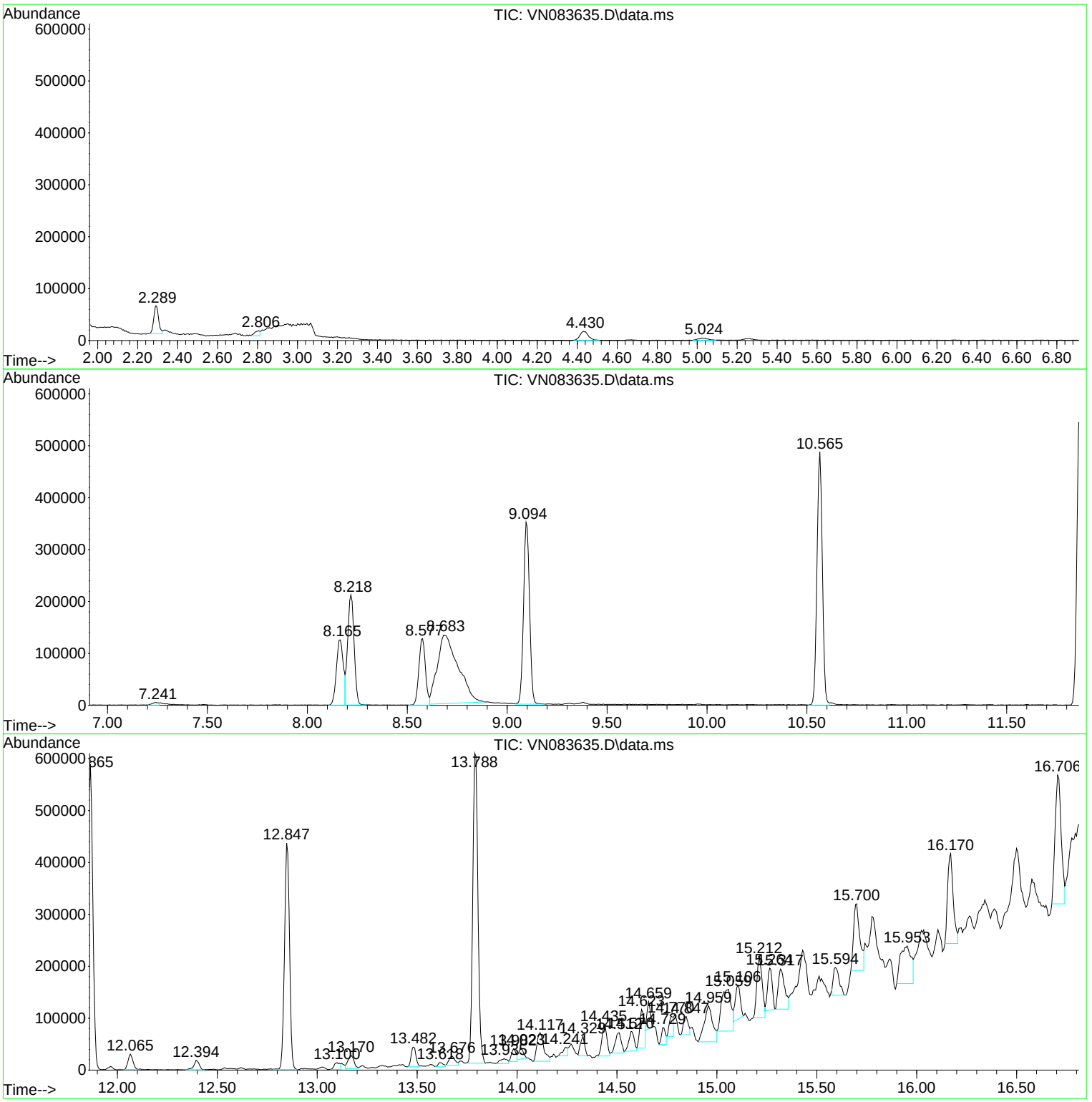
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083024W.M
Quant Title : SW846 8260

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



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Data File : VN083635.D
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Operator : JC\MD
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083024W.M
Quant Title : SW846 8260

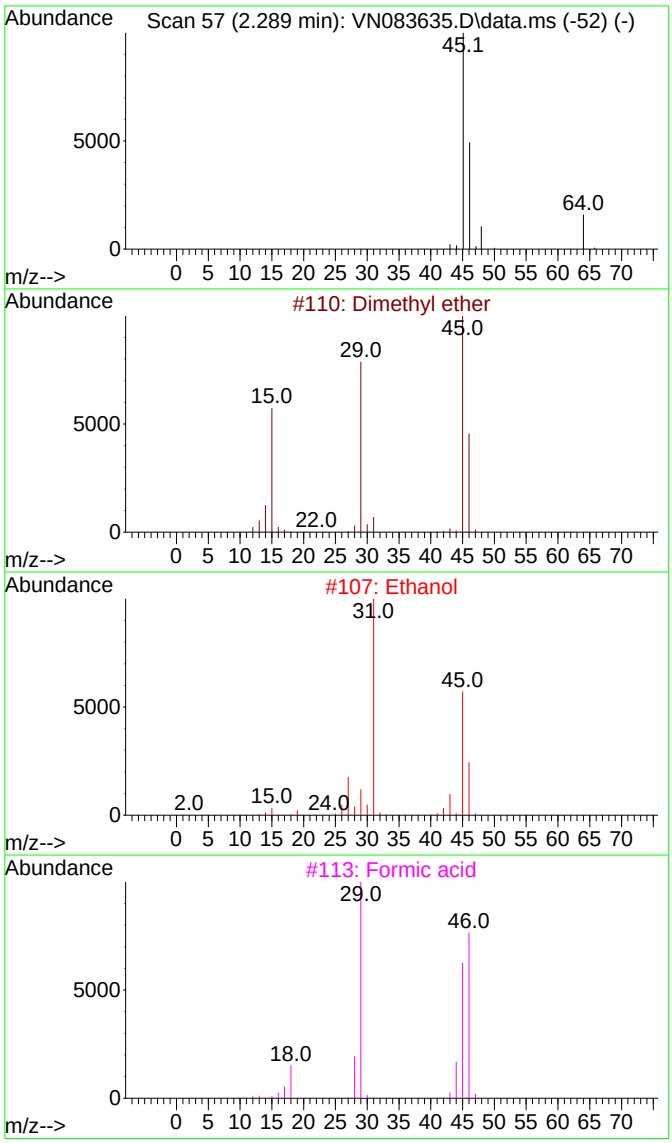
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

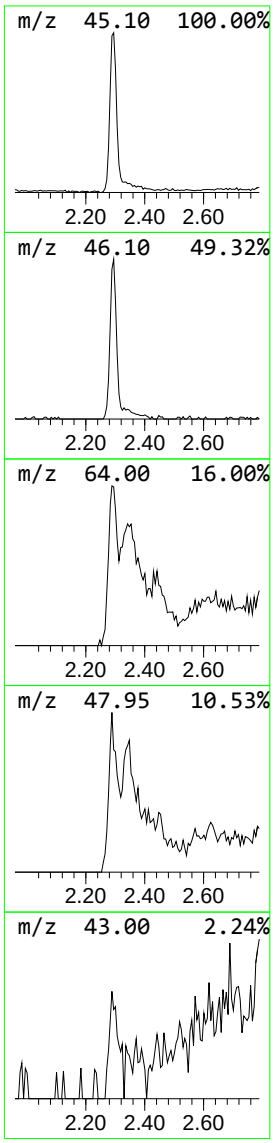
****

Peak Number 1 Dimethyl ether Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.289	9.72 ug/l	90808	Pentafluorobenzene	8.218

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dimethyl ether	46	C2H6O	000115-10-6	56
2	Ethanol	46	C2H6O	000064-17-5	9
3	Formic acid	46	CH2O2	000064-18-6	5
4	Oxalic acid	90	C2H2O4	000144-62-7	4
5	Methane, nitroso-	45	CH3NO	000865-40-7	3





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Data File : VN083635.D
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Operator : JC\MD
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Misc : 1.47g/10mL/100uL/5.00mL/MSVOA_N/MEOH
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Instrument :
MSVOA_N
ClientSampleId :
DRUM-2

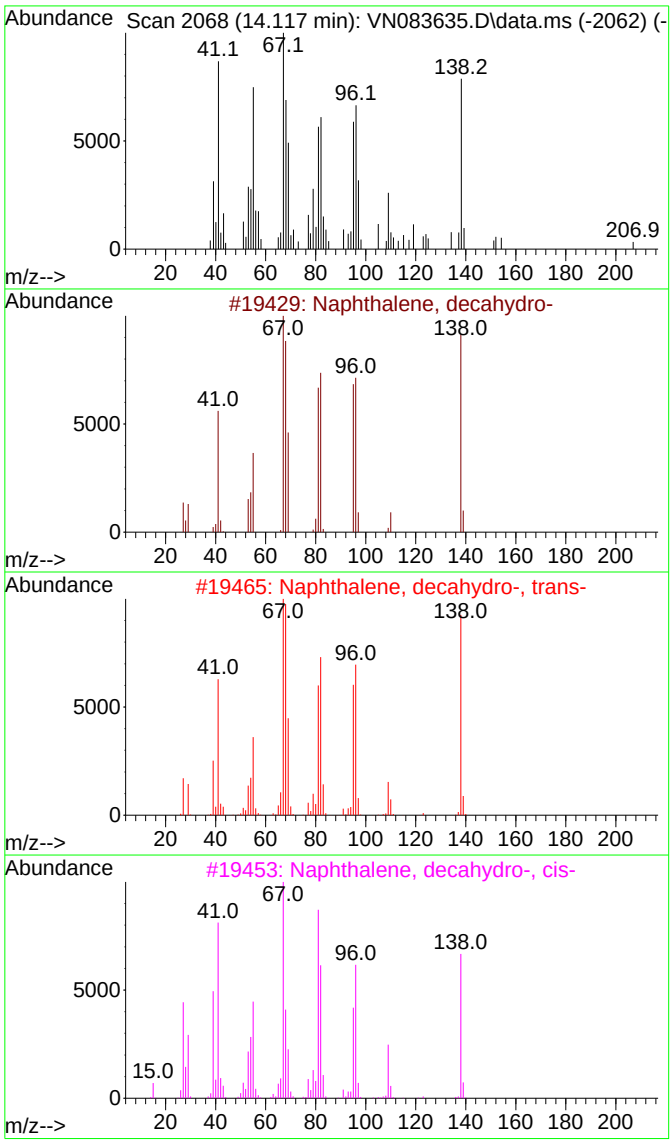
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083024W.M
Quant Title : SW846 8260

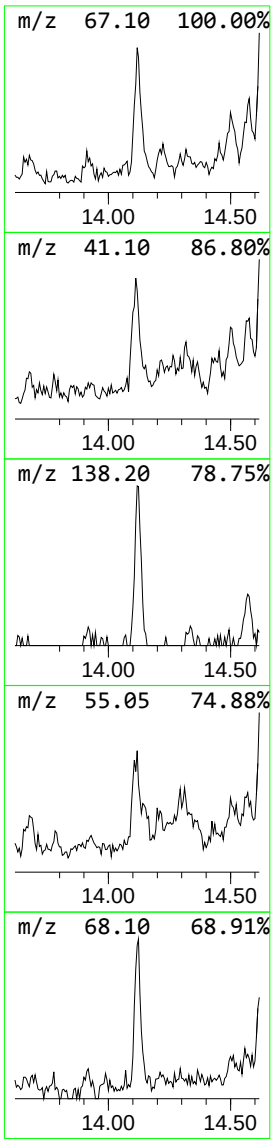
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Naphthalene, decahydro- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.118	6.20 ug/l	133333	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, decahydro-	138	C10H18	000091-17-8	95
2	Naphthalene, decahydro-, trans-	138	C10H18	000493-02-7	95
3	Naphthalene, decahydro-, cis-	138	C10H18	000493-01-6	90
4	9-Borabicyclo[3.3.1]nonane, 9-hy...	138	C8H15BO	063366-65-4	90
5	Cyclodecene	138	C10H18	003618-12-0	83





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Data File : VN083635.D
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Misc : 1.47g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083024W.M
Quant Title : SW846 8260

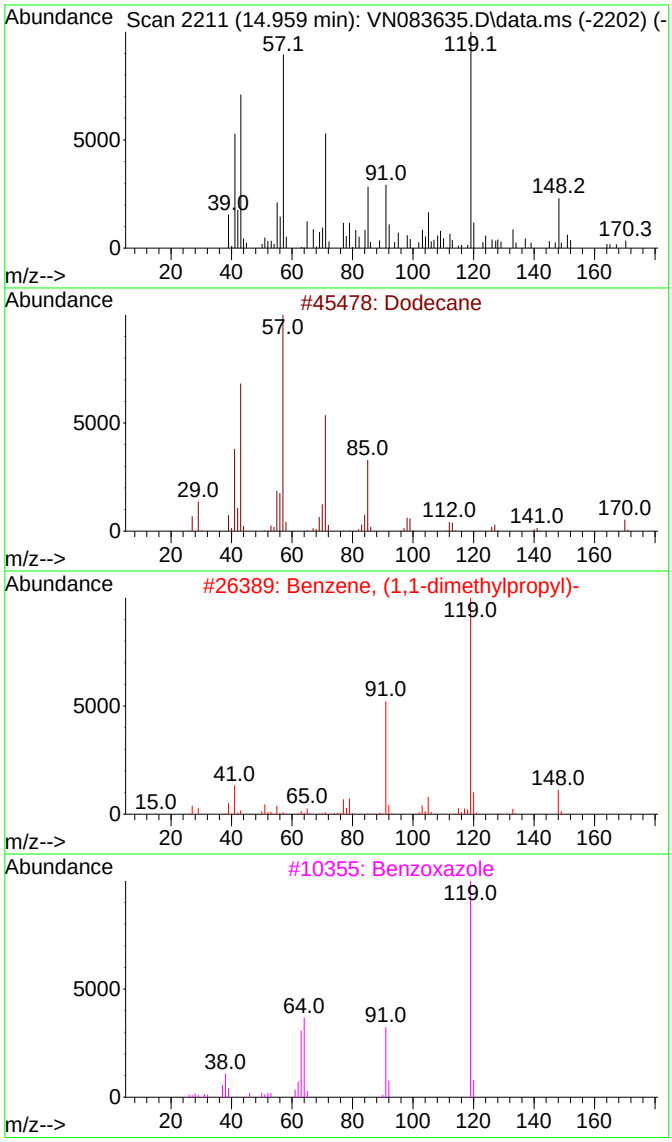
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

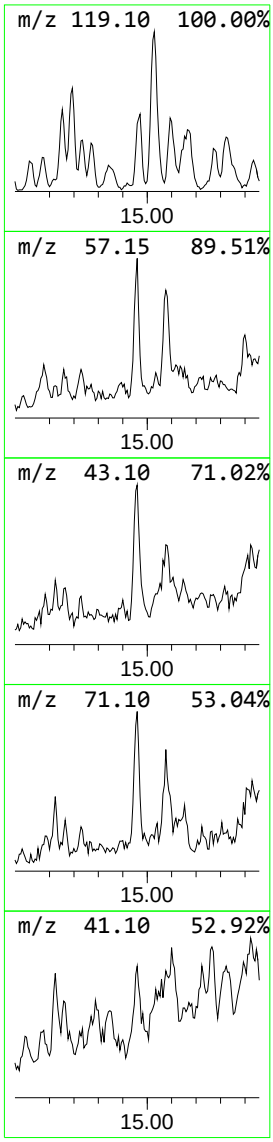
****

Peak Number 3 unknown14.959 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.959	9.52 ug/l	204799	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane	170	C12H26	000112-40-3	42
2	Benzene, (1,1-dimethylpropyl)-	148	C11H16	002049-95-8	38
3	Benzoxazole	119	C7H5NO	000273-53-0	35
4	o-Cymene	134	C10H14	000527-84-4	30
5	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	30





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Operator : JC\MD
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Misc : 1.47g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DRUM-2

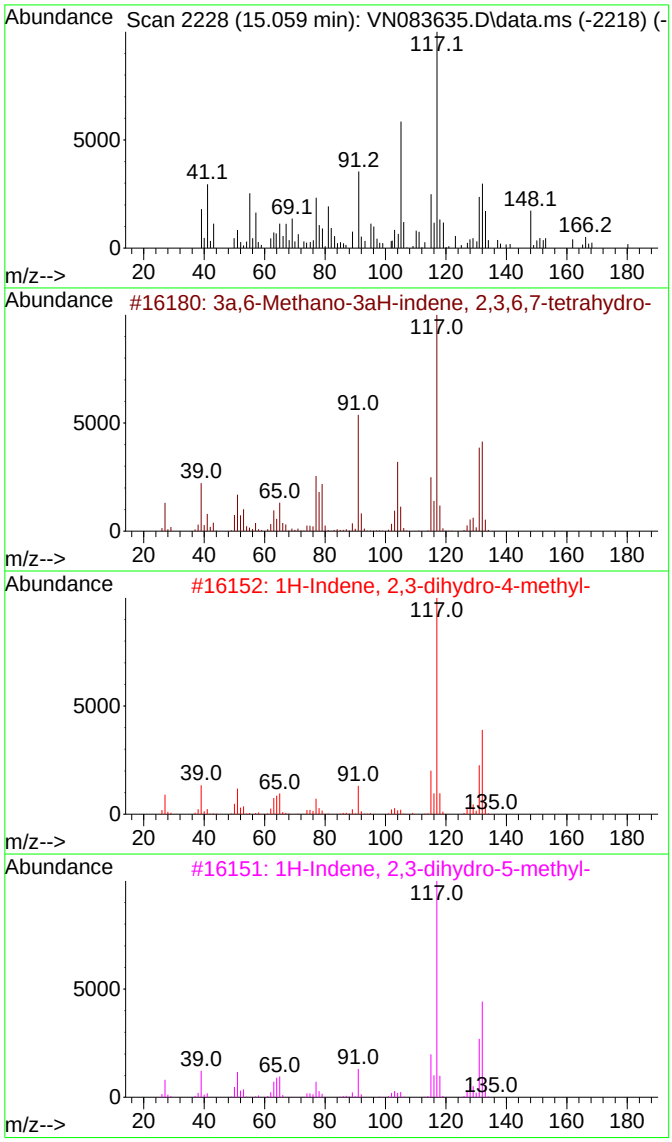
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083024W.M
Quant Title : SW846 8260

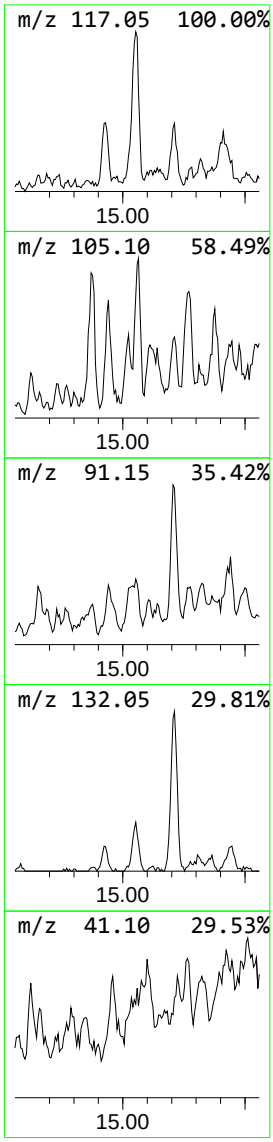
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 3a,6-Methano-3aH-indene, 2,... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.059	12.78 ug/l	274912	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3a,6-Methano-3aH-indene, 2,3,6,7...	132	C10H12	098640-29-0	81
2	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	76
3	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	76
4	Benzene, 2-butenyl-	132	C10H12	001560-06-1	70
5	1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	70





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Operator : JC\MD
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ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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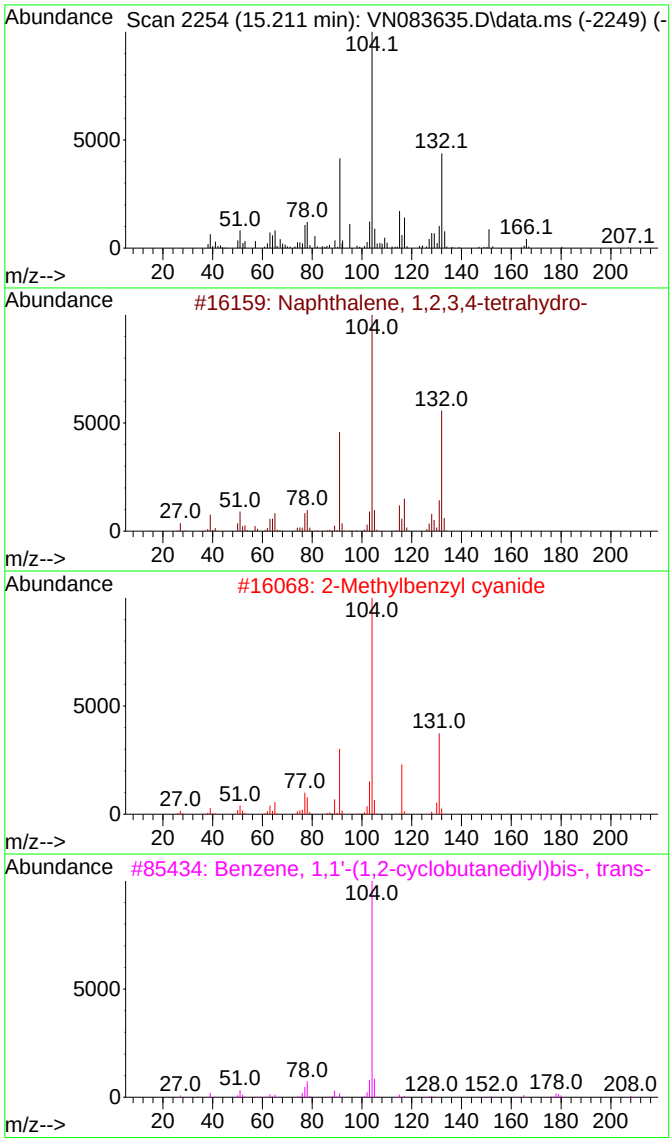
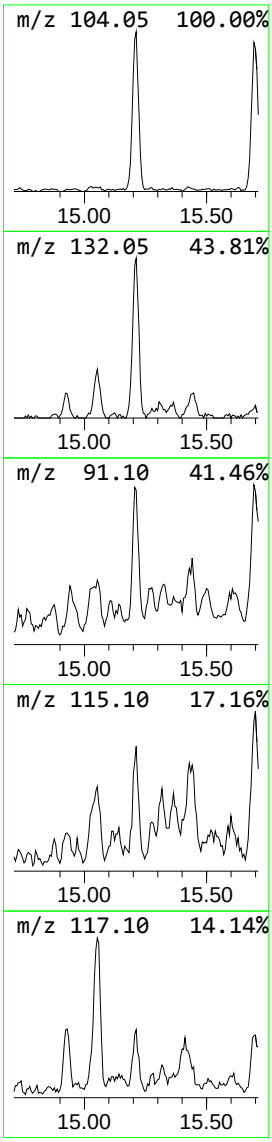
****
Peak Number 5 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.211	10.31 ug/l	221758	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-	132	C10H12	000119-64-2	96
2	2-Methylbenzyl cyanide	131	C9H9N	022364-68-7	43
3	Benzene, 1,1'-(1,2-cyclobutanedi...	208	C16H16	020071-09-4	38
4	4H-Pyran-4-one 2,3-dihydro-2-phe...	174	C11H10O2	1010163-21-2	38
5	2-Bromopropionic acid, 2-phenyle...	256	C11H13BrO2	043216-34-8	38





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TIC Library : C:\Database\NIST20.L
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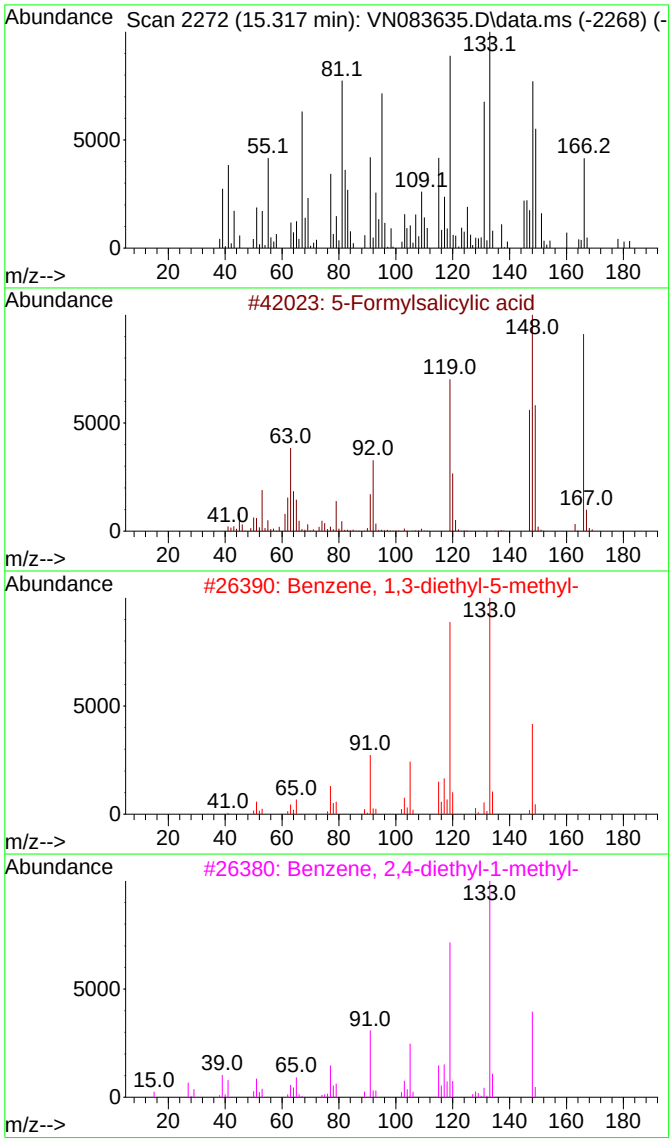
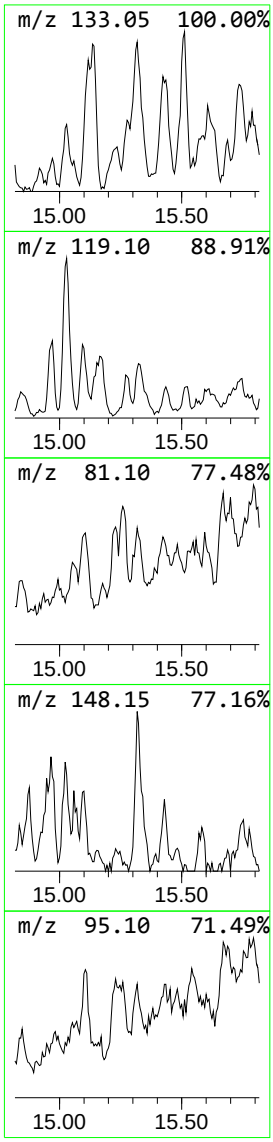
****

Peak Number 6 unknown15.317 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.317	8.28 ug/l	178004	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Formylsalicylic acid	166	C8H6O4	000616-76-2	41
2	Benzene, 1,3-diethyl-5-methyl-	148	C11H16	002050-24-0	35
3	Benzene, 2,4-diethyl-1-methyl-	148	C11H16	001758-85-6	27
4	1H-Indene, 1-ethyloctahydro-7a-m...	166	C12H22	056324-71-1	20
5	3(2H)-Benzofuranone, 5-methyl-	148	C9H8O2	054120-66-0	15





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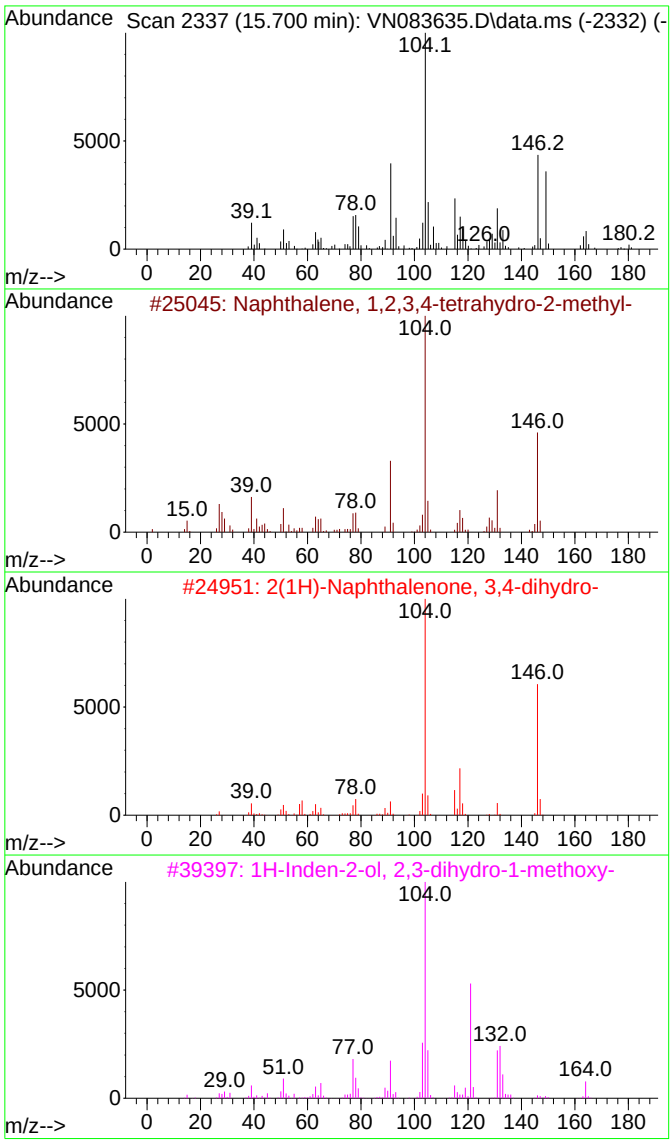
Quant Title : SW846 8260

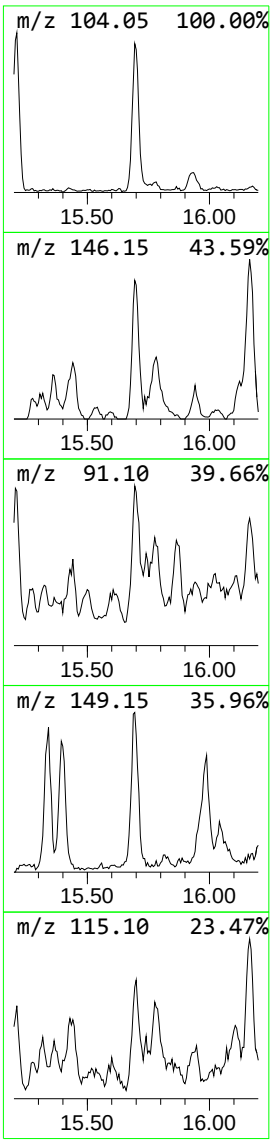
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.700	13.03 ug/l	280302	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	003877-19-8	86
2	2(1H)-Naphthalenone, 3,4-dihydro-	146	C10H10O	000530-93-8	58
3	1H-Inden-2-ol, 2,3-dihydro-1-met...	164	C10H12O2	071720-52-0	46
4	Phthalic acid, decyl 2-phenyleth...	410	C26H34O4	1000309-77-9	38
5	Benzenemethanol, 2-methyl-, acetate	164	C10H12O2	017373-93-2	38





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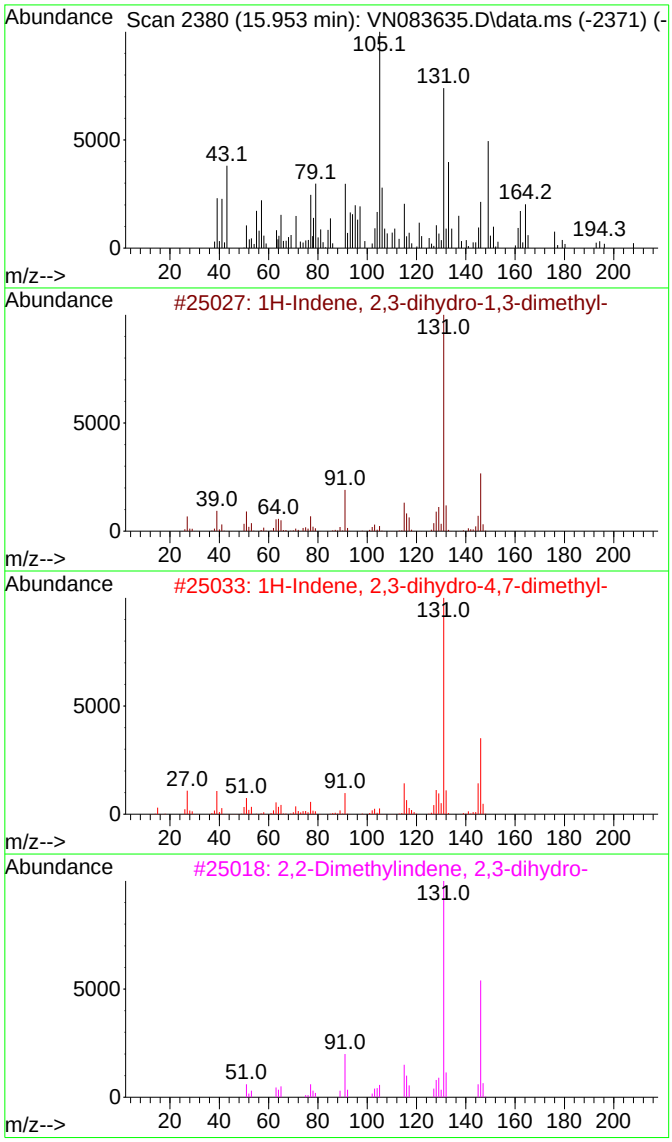
TIC Integration Parameters: LSCINT.P

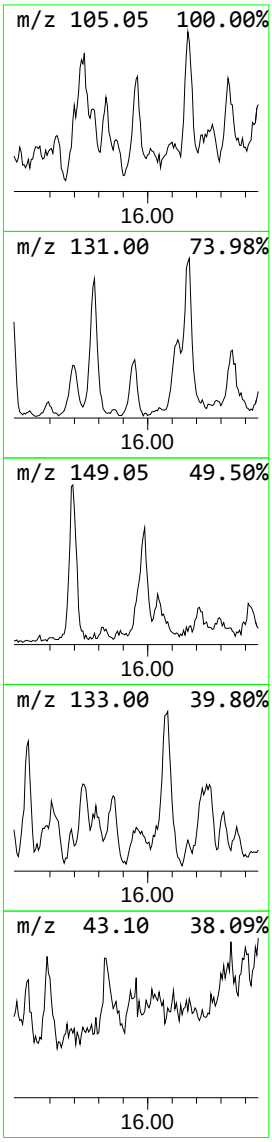
****

Peak Number 8 unknown15.953 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.953	12.78 ug/l	274742	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-1,3-dimet...	146	C11H14	004175-53-5	38
2	1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	38
3	2,2-Dimethylindene, 2,3-dihydro-	146	C11H14	020836-11-7	30
4	1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	30
5	1H-Indene, 2,3-dihydro-1,6-dimet...	146	C11H14	017059-48-2	25





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Data File : VN083635.D
Acq On : 03 Sep 2024 19:33
Operator : JC\MD
Sample : P3811-02
Misc : 1.47g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DRUM-2

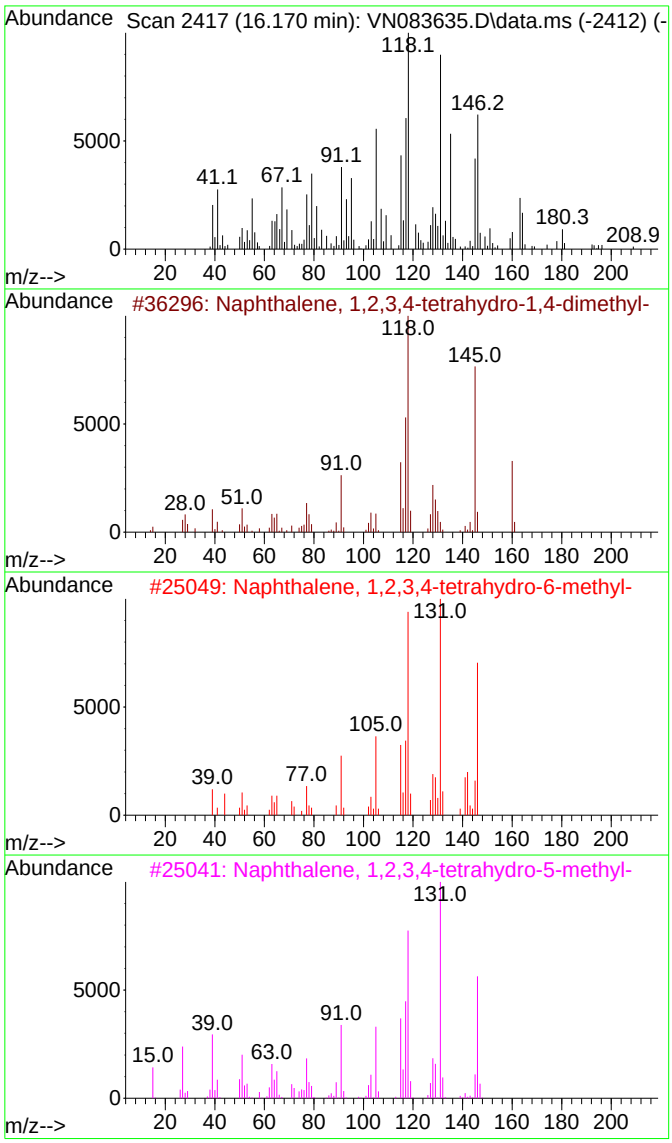
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083024W.M
Quant Title : SW846 8260

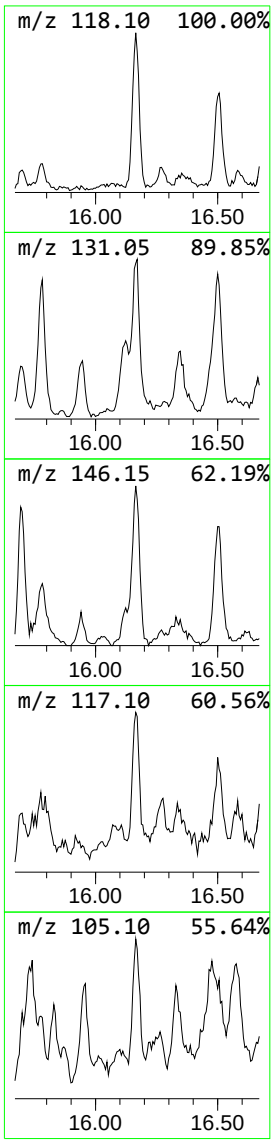
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.170	15.80 ug/l	339729	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	87
2	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	86
3	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	70
4	Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	46
5	1H-1,3,2-Benzodiazaborole, 2-eth...	146	C8H11BN2	074663-81-3	46





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090324\
Data File : VN083635.D
Acq On : 03 Sep 2024 19:33
Operator : JC\MD
Sample : P3811-02
Misc : 1.47g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DRUM-2

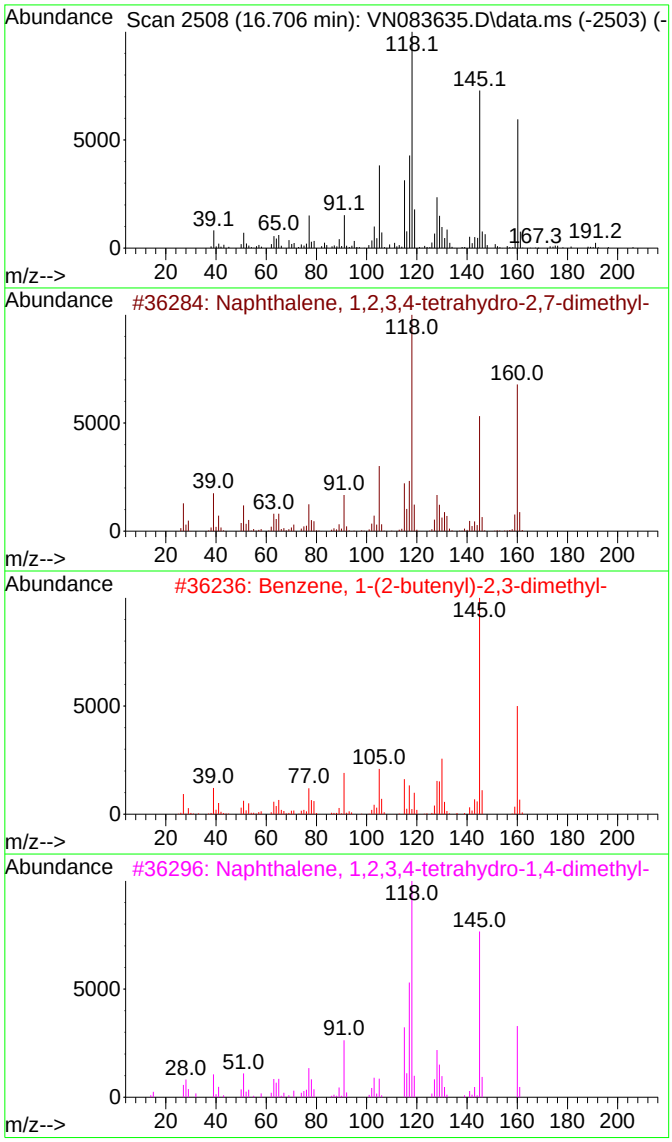
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083024W.M
Quant Title : SW846 8260

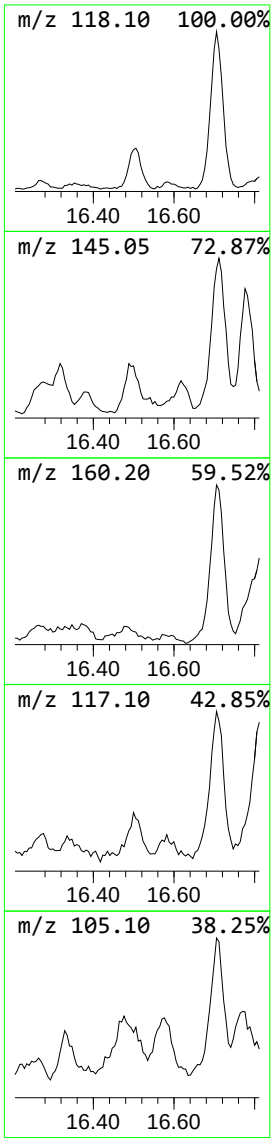
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.706	24.52 ug/l	527394	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	013065-07-1	91
2	Benzene, 1-(2-butenyl)-2,3-dimet...	160	C12H16	054340-85-1	64
3	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	64
4	Benzene, 1,3,5-trimethyl-2-(1-me...	160	C12H16	014679-13-1	62
5	Benzene, 1-(1-methylethenyl)-3-(...	160	C12H16	001129-29-9	60





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090324\
Data File : VN083635.D
Acq On : 03 Sep 2024 19:33
Operator : JC\MD
Sample : P3811-02
Misc : 1.47g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DRUM-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083024W.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
Dimethyl ether	2.289	9.7	ug/l	90808	1	8.218	466970	50.0
Naphthalene, de...	14.118	6.2	ug/l	133333	4	13.788	1075220	50.0
unknown14.959	14.959	9.5	ug/l	204799	4	13.788	1075220	50.0
3a,6-Methano-3a...	15.059	12.8	ug/l	274912	4	13.788	1075220	50.0
Naphthalene, 1,...	15.211	10.3	ug/l	221758	4	13.788	1075220	50.0
unknown15.317	15.317	8.3	ug/l	178004	4	13.788	1075220	50.0
Naphthalene, 1,...	15.700	13.0	ug/l	280302	4	13.788	1075220	50.0
unknown15.953	15.953	12.8	ug/l	274742	4	13.788	1075220	50.0
Naphthalene, 1,...	16.170	15.8	ug/l	339729	4	13.788	1075220	50.0
Naphthalene, 1,...	16.706	24.5	ug/l	527394	4	13.788	1075220	50.0