LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052523\
Data File : VN077899.D
Acq On : 25 May 2023 14:03
Operator : JC\MD
Sample : 02850-05
Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TRE-1729

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: VN077899.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.848	137	152	154	rBV4	54859	189632	8.15%	0.836%
2	4.453	414	425	434	rBV	20828	67725	2.91%	0.299%
3	5.271	554	564	574	rBV5	9965	34161	1.47%	0.151%
4	8.171	1047	1057	1061	rBV	310917	731266	31.42%	3.223%
5	8.230	1061	1067	1078	rVV	599428	1397493	60.04%	6.160%
6	8.324	1078	1083	1093	rVB3	19743	45926	1.97%	0.202%
7	8.447	1096	1104	1117	rBV	73998	166745	7.16%	0.735%
8	8.582	1117	1127	1140	rBV2	320013	729226	31.33%	3.214%
9	8.706	1140	1148	1157	rBV8	10340	29216	1.26%	0.129%
10	8.971	1184	1193	1199	rBV2	62886	121979	5.24%	0.538%
11	9.106	1207	1216	1233	rVB	810389	1676521	72.02%	7.390%
12	9.600	1288	1300	1305	rBV8	9424	30170	1.30%	0.133%
13	10.571	1456	1465	1471	rBV	1239677	2327707	100.00%	10.261%
14	10.635	1471	1476	1488	rVB	591625	1087952	46.74%	4.796%
15	11.871	1677	1686	1698	rBV	1127138	2007163	86.23%	8.848%
16	11.970	1698	1703	1709	rVV3	12902	24565	1.06%	0.108%
17	12.076	1713	1721	1732	rVV3	59328	123657	5.31%	0.545%
18	12.406	1767	1777	1785	rBV6	28413	69214	2.97%	0.305%
19	12.853	1847	1853	1864	rVB	918637	1627169	69.90%	7.173%
20	13.100	1890	1895	1899	rVV2	38643	69673	2.99%	0.307%
21	13.165	1899	1906	1914	rVV4	108178	236163	10.15%	1.041%
22	13.341	1927	1936	1942	rBV3	21263	59755	2.57%	0.263%
23	13.400	1943	1946	1952	rVB3	22973	34593	1.49%	0.152%
24	13.488	1956	1961	1966	rBV	84993	138059	5.93%	0.609%
25	13.676	1988	1993	1998	rBV5	44806	90598	3.89%	0.399%
26	13.729	1998	2002	2005	rVV4	30032	50083	2.15%	0.221%
27	13.800	2007	2014	2022	rVV	995548	1729303	74.29%	7.623%
28	13.864	2022	2025	2031	rVB2	35417	54511	2.34%	0.240%
29	13.982	2031	2045	2050	rBV3	86274	252779	10.86%	1.114%
30	14.029	2050	2053	2058	rVV2	63935	106053	4.56%	0.467%
31	14.112	2062	2067	2073	rBV	248533	382778	16.44%	1.687%
32	14.194	2078	2081	2085	rVV2	35252	52076	2.24%	0.230%
33	14.253	2087	2091	2093	rVV2	55153	88626	3.81%	0.391%
34	14.282	2093	2096	2100	rVV2	68136	96774	4.16%	0.427%
35	14.335	2100	2105	2110	rVB	90737	146292	6.28%	0.645%
36	14.447	2118	2124	2129	rBV3	96368	174810	7.51%	0.771%

LSC Area Percent Report

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Operator : JC\MD
Sample : 02850-05
Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TRE-1729

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

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

37	14.523	2129	2137	2141	rBV7	29966	69208	2.97%	0.305%
38	14.582	2141	2147	2151	rVV5	54870	114435	4.92%	0.504%
39	14.635	2151	2156	2158	rVV4	121230	194733	8.37%	0.858%
40	14.664	2159	2161	2164	rVV3	86504	110424	4.74%	0.487%
41	14.700	2164	2167	2170	rVV	93597	121194	5.21%	0.534%
42	14.741	2170	2174	2177	rVV3	104691	140647	6.04%	0.620%
43	14.776	2177	2180	2188	rVB7	89531	190951	8.20%	0.842%
44	14.882	2188	2198	2202	rBV5	103507	243314	10.45%	1.073%
45	14.964	2202	2212	2218	rBV6	295928	681464	29.28%	3.004%
46	15.053	2219	2227	2234	rBV7	208302	675913	29.04%	2.979%
47	15.106	2234	2236	2246	rVB6	104021	182249	7.83%	0.803%
48	15.217	2250	2255	2261	rVB2	115907	226519	9.73%	0.999%
49	15.282	2262	2266	2269	rBV6	35956	64132	2.76%	0.283%
50	15.329	2269	2274	2277	rBV4	97448	163958	7.04%	0.723%
51	15.441	2287	2293	2300	rBV6	105206	244115	10.49%	1.076%
52	15.606	2315	2321	2323	rBV4	83699	146620	6.30%	0.646%
53	15.706	2333	2338	2342	rBV2	111743	202258	8.69%	0.892%
54	15.753	2343	2346	2350	rVV5	80510	132012	5.67%	0.582%
55	15.841	2357	2361	2371	rVB5	209050	468793	20.14%	2.066%
56	15.953	2372	2380	2388	rBV5	120321	330511	14.20%	1.457%
57	16.029	2391	2393	2397	rVB4	26946	31944	1.37%	0.141%
58	16.123	2405	2409	2413	rBV5	62279	132126	5.68%	0.582%
59	16.176	2413	2418	2424	rVB2	283277	545204	23.42%	2.403%
60	16.353	2443	2448	2452	rBV5	43215	88310	3.79%	0.389%
61	16.511	2465	2475	2480	rBV4	170228	454968	19.55%	2.006%
62	16.717	2503	2510	2517	rVB2	220571	479415	20.60%	2.113%

Sum of corrected areas: 22685830

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Sample : 02850-05
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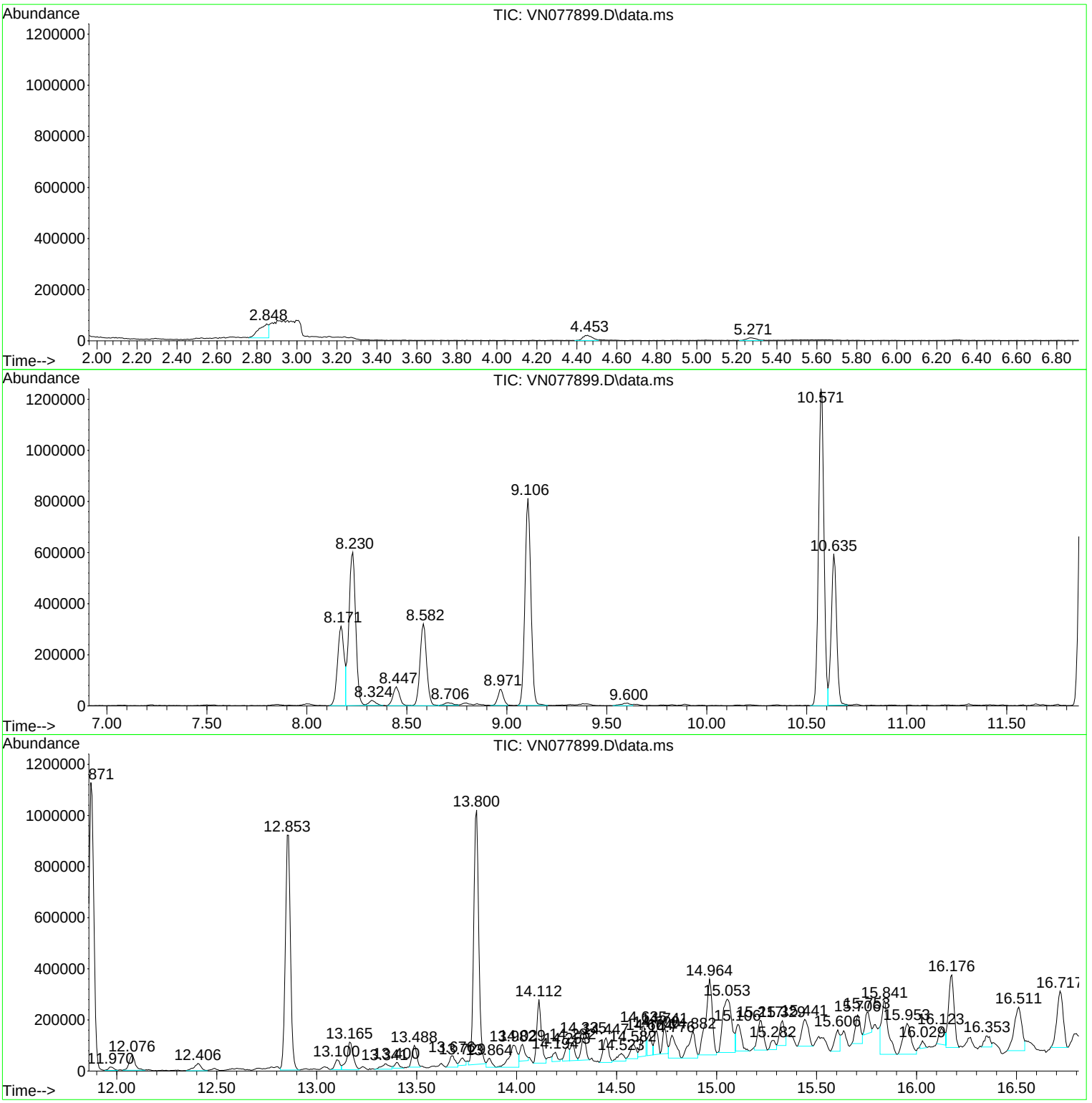
Instrument :
MSVOA_N
ClientSampleId :
TRE-1729

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052523\
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Acq On : 25 May 2023 14:03
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ClientSampleId :
TRE-1729

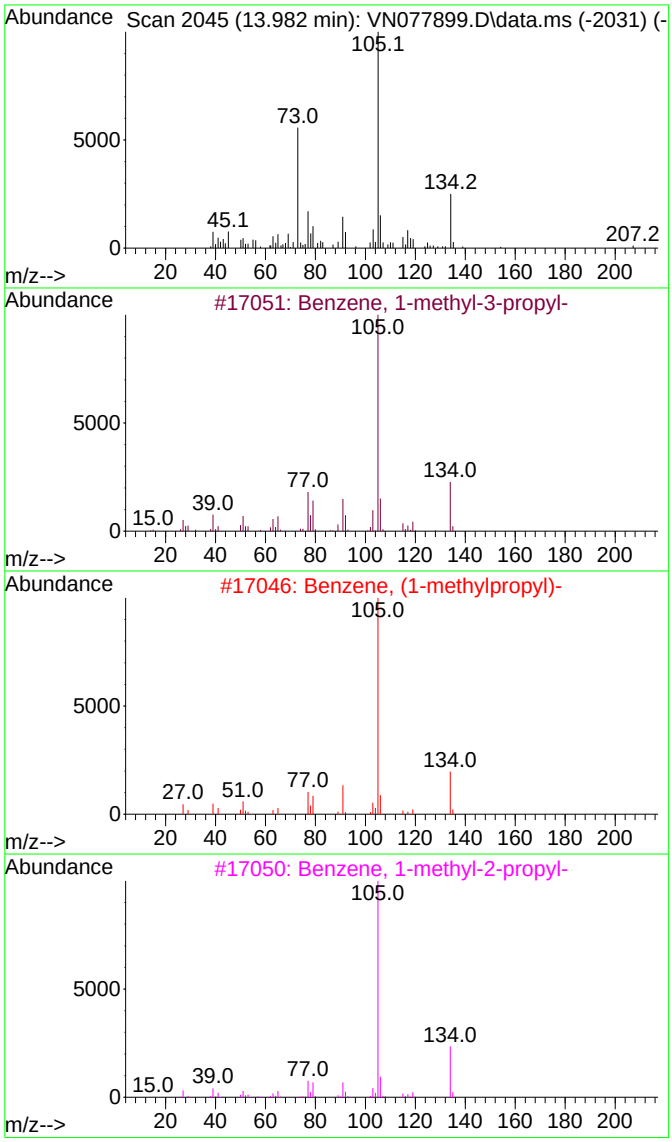
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

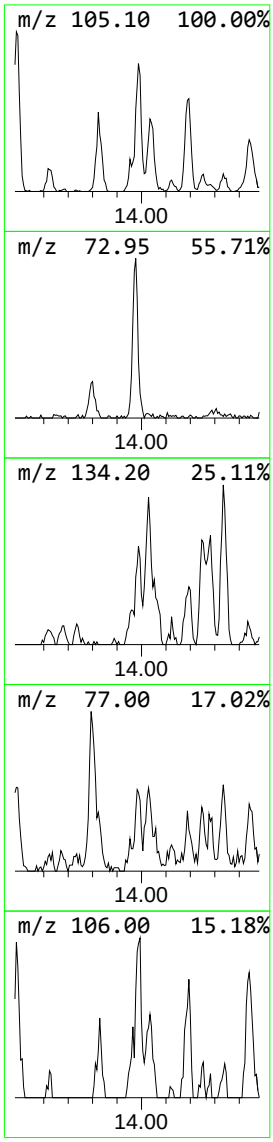
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Benzene, 1-methyl-3-propyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.982	7.31 ug/l	252779	1,4-Dichlorobenzene-d4	13.800

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-methyl-3-propyl-	134	C10H14	001074-43-7	90
2	Benzene, (1-methylpropyl)-	134	C10H14	000135-98-8	76
3	Benzene, 1-methyl-2-propyl-	134	C10H14	001074-17-5	64
4	Benzene, 1-methyl-4-propyl-	134	C10H14	001074-55-1	62
5	2-Tolyloxirane	134	C9H10O	002783-26-8	52





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052523\
Data File : VN077899.D
Acq On : 25 May 2023 14:03
Operator : JC\MD
Sample : 02850-05
Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TRE-1729

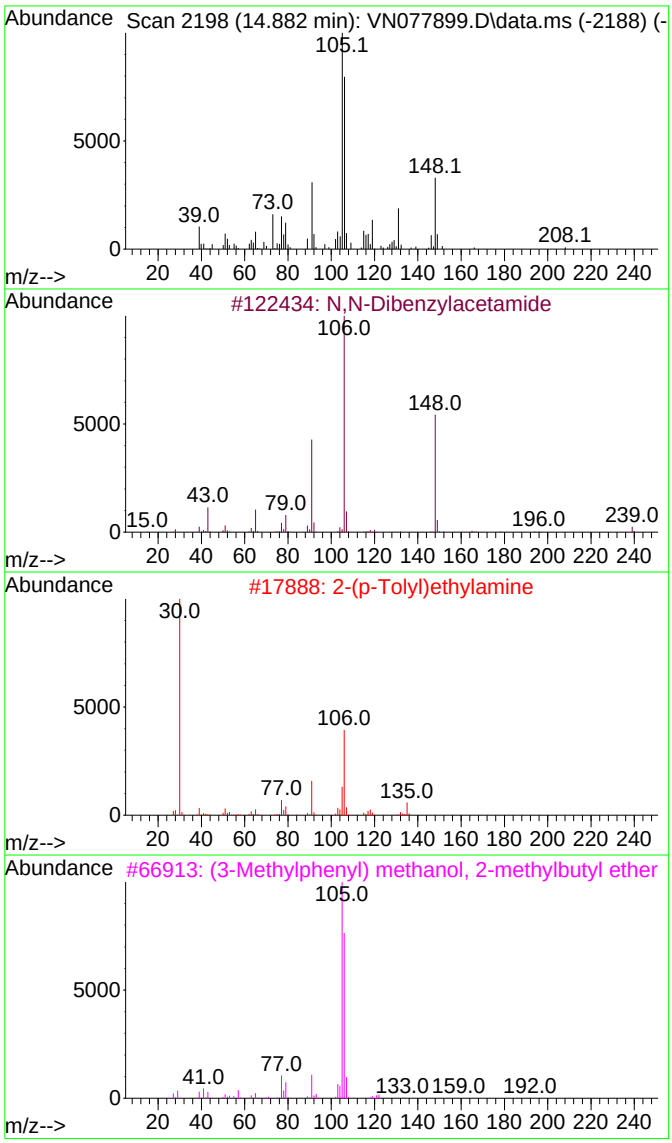
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

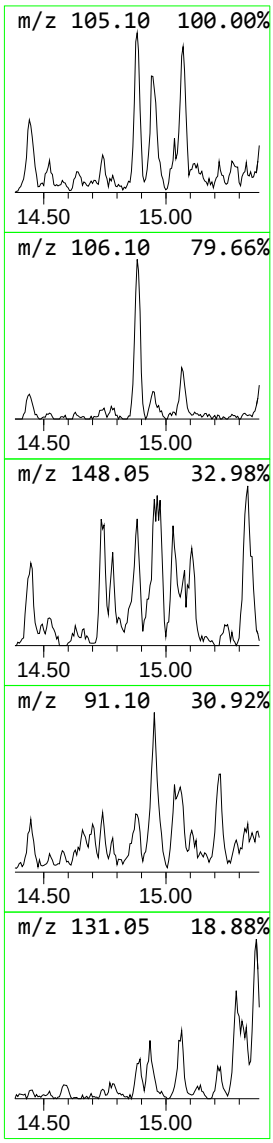
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 unknown14.882 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.882	7.04 ug/l	243314	1,4-Dichlorobenzene-d4	13.800

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N,N-Dibenzylacetamide	239	C16H17NO	010479-30-8	47
2	2-(p-Tolyl)ethylamine	135	C9H13N	003261-62-9	47
3	(3-Methylphenyl) methanol, 2-met...	192	C13H20O	1000374-43-9	43
4	(1H)Pyrrole-3-carbonitrile, 2-me...	106	C6H6N2	026187-27-9	43
5	Tricyclo[4.2.2.0(1,5)]dec-7-ene	134	C10H14	1000190-45-2	43





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052523\
Data File : VN077899.D
Acq On : 25 May 2023 14:03
Operator : JC\MD
Sample : 02850-05
Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TRE-1729

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

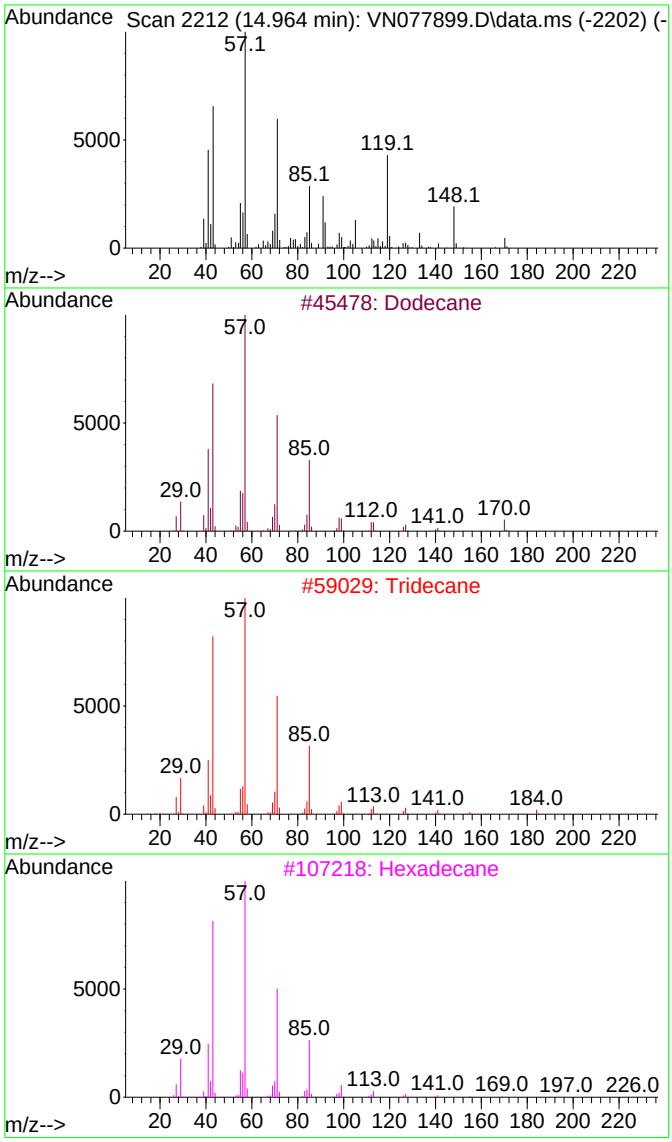
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

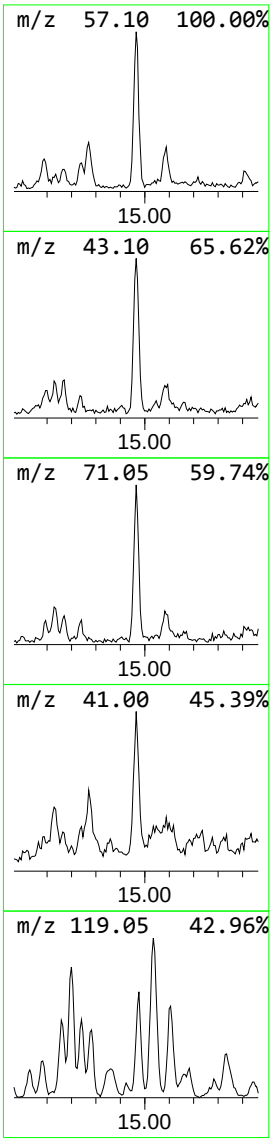
****

Peak Number 3 Dodecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.964	19.70 ug/l	681464	1,4-Dichlorobenzene-d4	13.800

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane	170	C12H26	000112-40-3	90
2	Tridecane	184	C13H28	000629-50-5	43
3	Hexadecane	226	C16H34	000544-76-3	43
4	Heptacosane	380	C27H56	000593-49-7	38
5	Heptadecane, 7-methyl-	254	C18H38	020959-33-5	27





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052523\
Data File : VN077899.D
Acq On : 25 May 2023 14:03
Operator : JC\MD
Sample : 02850-05
Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TRE-1729

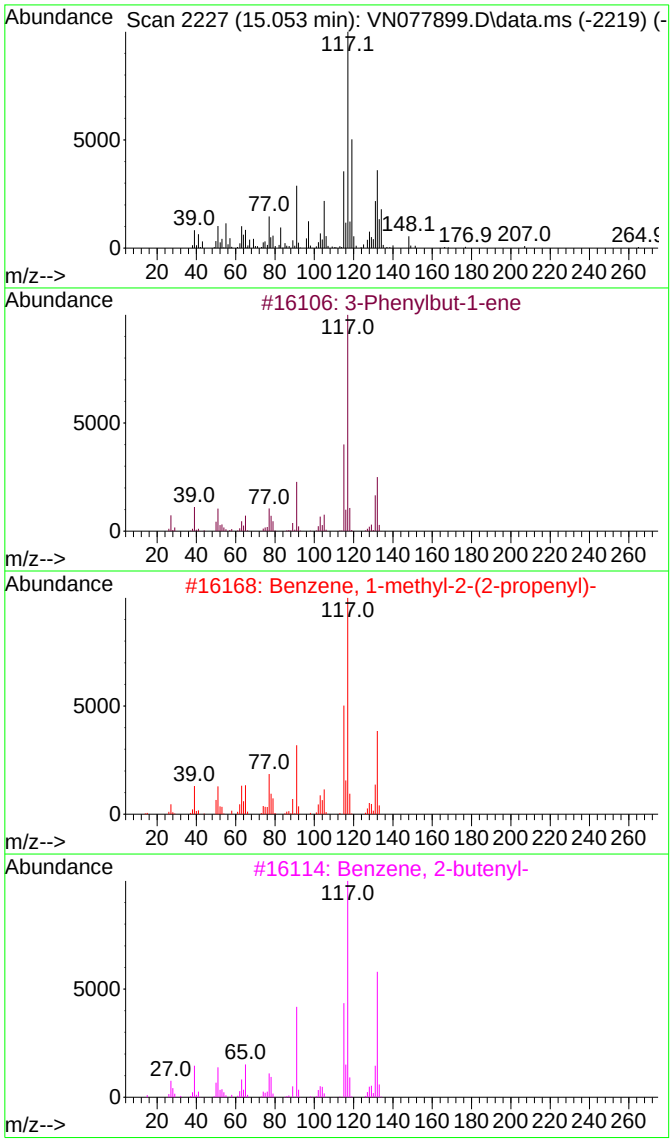
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

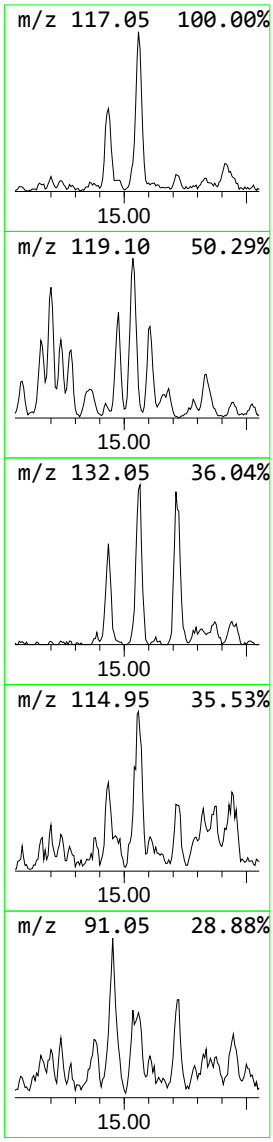
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 3-Phenylbut-1-ene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.053	19.54 ug/l	675913	1,4-Dichlorobenzene-d4	13.800

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Phenylbut-1-ene	132	C10H12	000934-10-1	70
2	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	64
3	Benzene, 2-butenyl-	132	C10H12	001560-06-1	60
4	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	60
5	1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	60





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052523\
Data File : VN077899.D
Acq On : 25 May 2023 14:03
Operator : JC\MD
Sample : 02850-05
Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TRE-1729

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

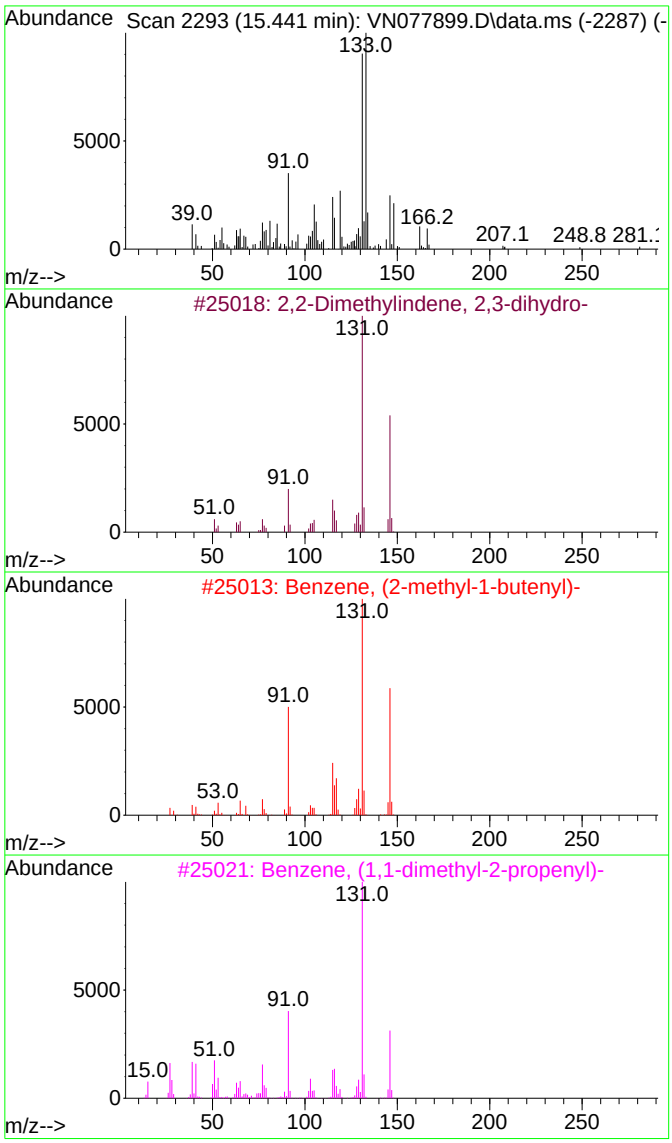
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

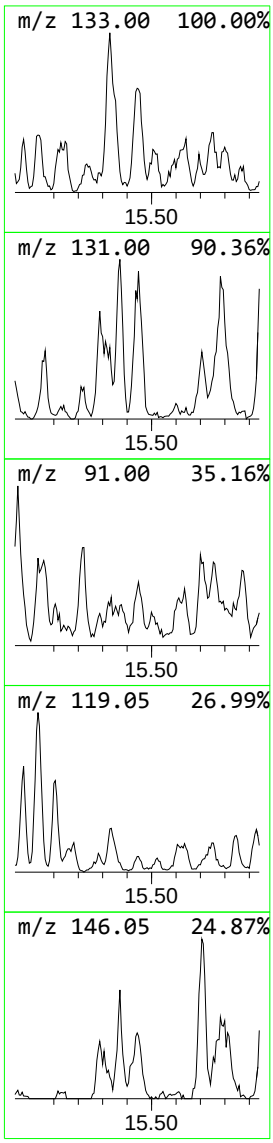
****

Peak Number 5 unknown15.441 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.441	7.06 ug/l	244115	1,4-Dichlorobenzene-d4	13.800

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2-Dimethylindene, 2,3-dihydro-	146	C11H14	020836-11-7	46
2	Benzene, (2-methyl-1-butenyl)-	146	C11H14	056253-64-6	46
3	Benzene, (1,1-dimethyl-2-propenyl)-	146	C11H14	018321-36-3	46
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	146	C11H14	027087-54-3	46
5	2-Butene, 3-chloro-1-phenyl-, (Z)-	166	C10H11Cl	016608-68-7	42





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Instrument :
MSVOA_N
ClientSampleId :
TRE-1729

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

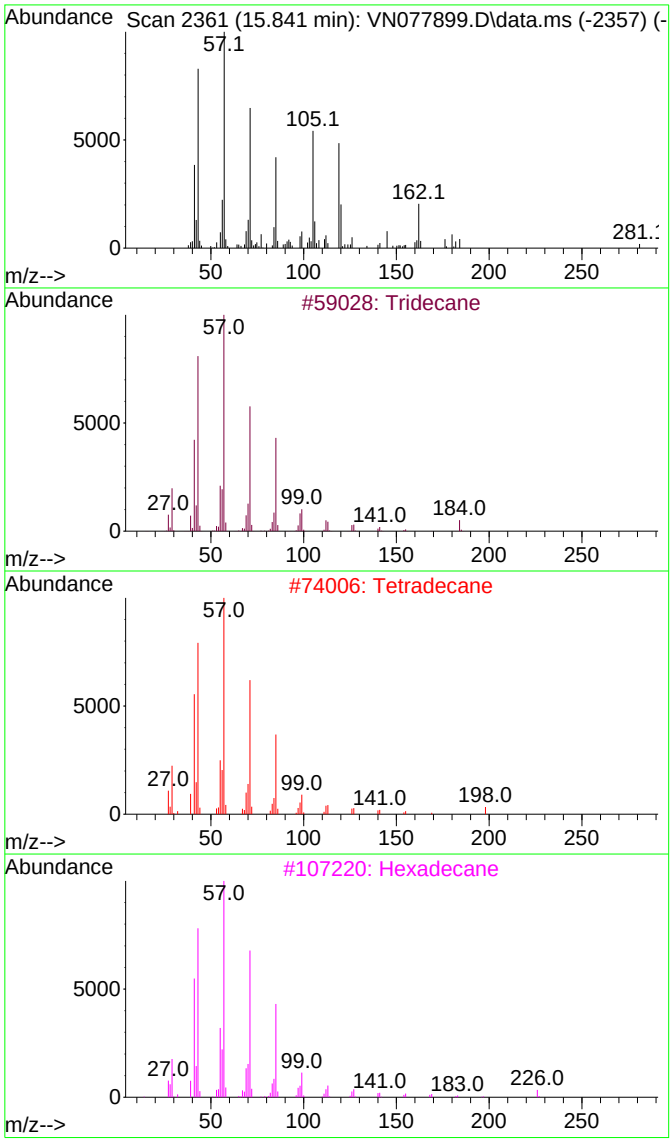
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

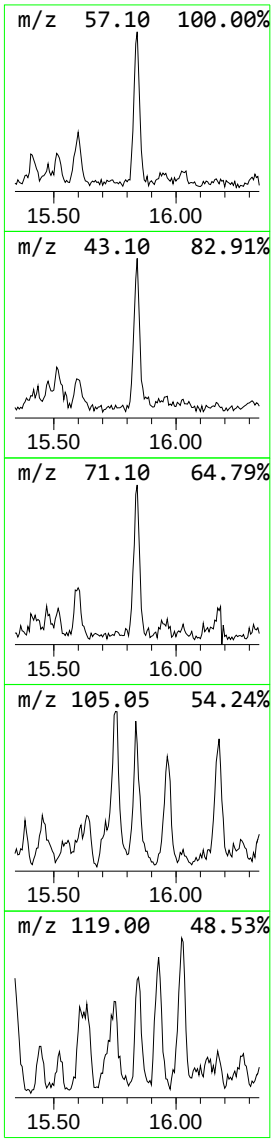
****

Peak Number 6 Tridecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.841	13.55 ug/l	468793	1,4-Dichlorobenzene-d4	13.800

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	78
2	Tetradecane	198	C14H30	000629-59-4	46
3	Hexadecane	226	C16H34	000544-76-3	43
4	Dodecane	170	C12H26	000112-40-3	43
5	3,5-Dimethyldodecane	198	C14H30	107770-99-0	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052523\
Data File : VN077899.D
Acq On : 25 May 2023 14:03
Operator : JC\MD
Sample : 02850-05
Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TRE-1729

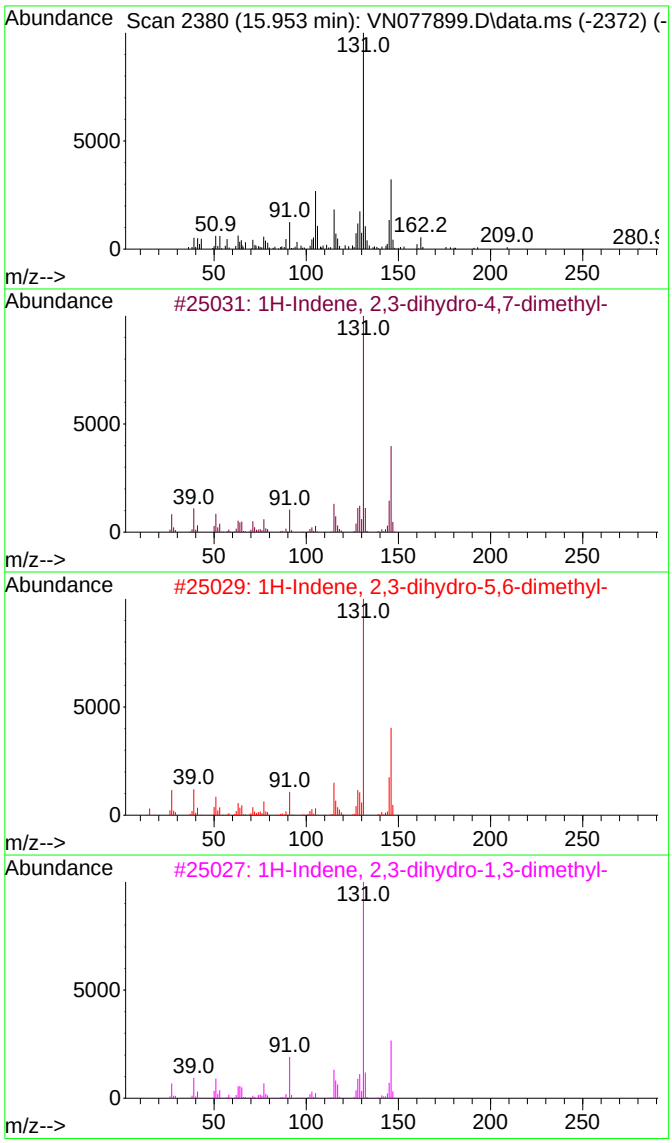
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

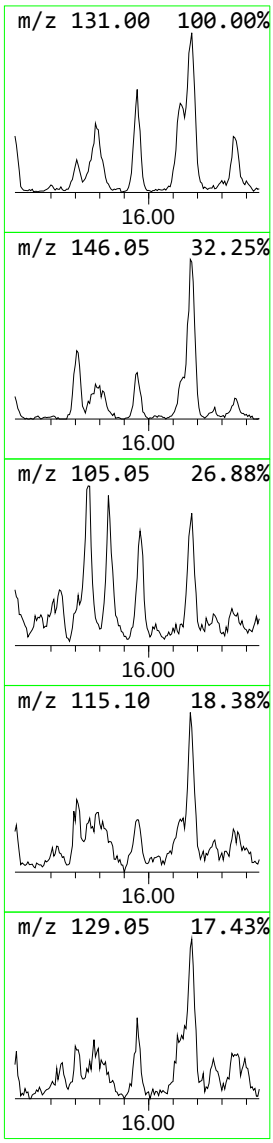
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.953	9.56 ug/l	330511	1,4-Dichlorobenzene-d4	13.800

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	93
2	1H-Indene, 2,3-dihydro-5,6-dimet...	146	C11H14	001075-22-5	93
3	1H-Indene, 2,3-dihydro-1,3-dimet...	146	C11H14	004175-53-5	81
4	Benzene, 1-methyl-3-(1-methyl-2-...	146	C11H14	052161-57-6	81
5	1H-Indene, 2,3-dihydro-1,6-dimet...	146	C11H14	017059-48-2	74





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052523\
Data File : VN077899.D
Acq On : 25 May 2023 14:03
Operator : JC\MD
Sample : 02850-05
Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TRE-1729

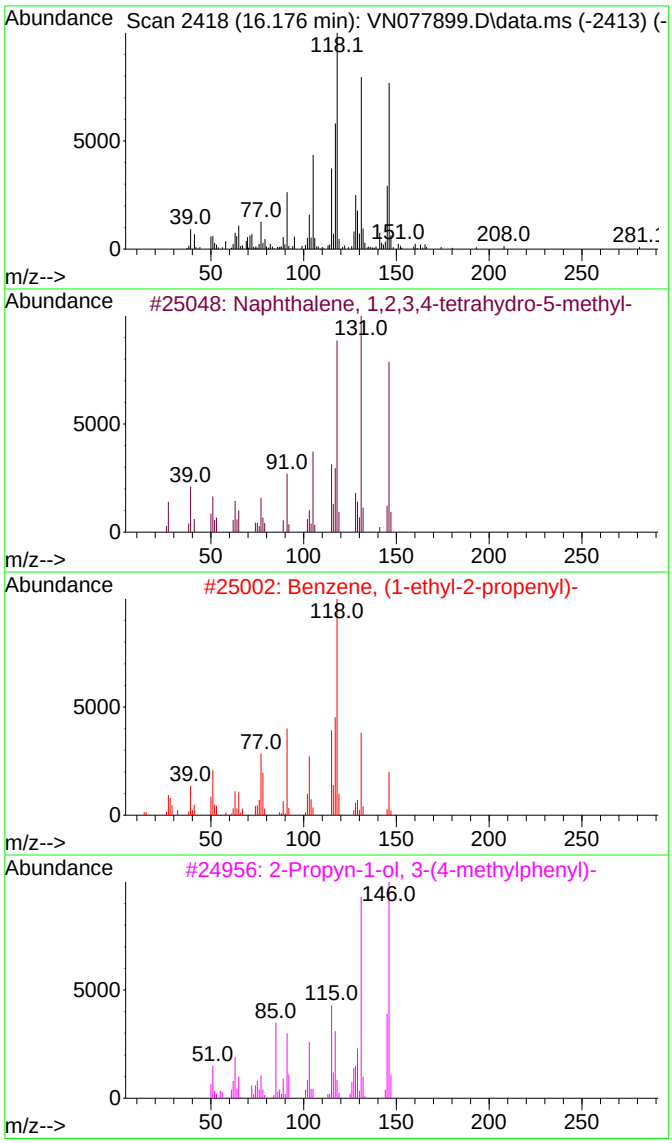
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

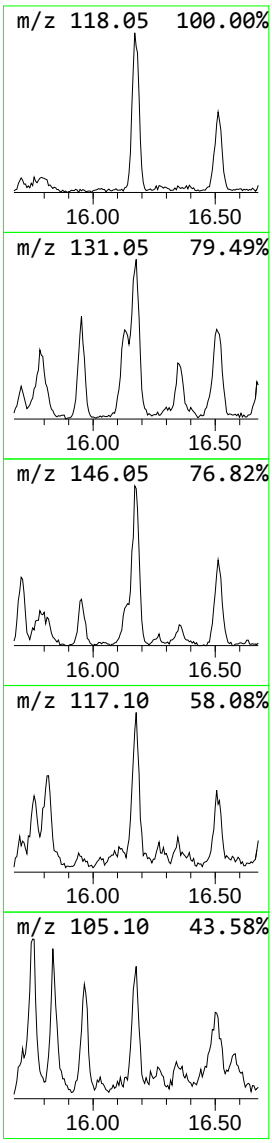
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.176	15.76 ug/l	545204	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	87
2	Benzene, (1-ethyl-2-propenyl)-	146	C11H14	019947-22-9	86
3	2-Propyn-1-ol, 3-(4-methylphenyl)-	146	C10H10O	016017-24-6	83
4	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	83
5	Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	60





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052523\
Data File : VN077899.D
Acq On : 25 May 2023 14:03
Operator : JC\MD
Sample : 02850-05
Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TRE-1729

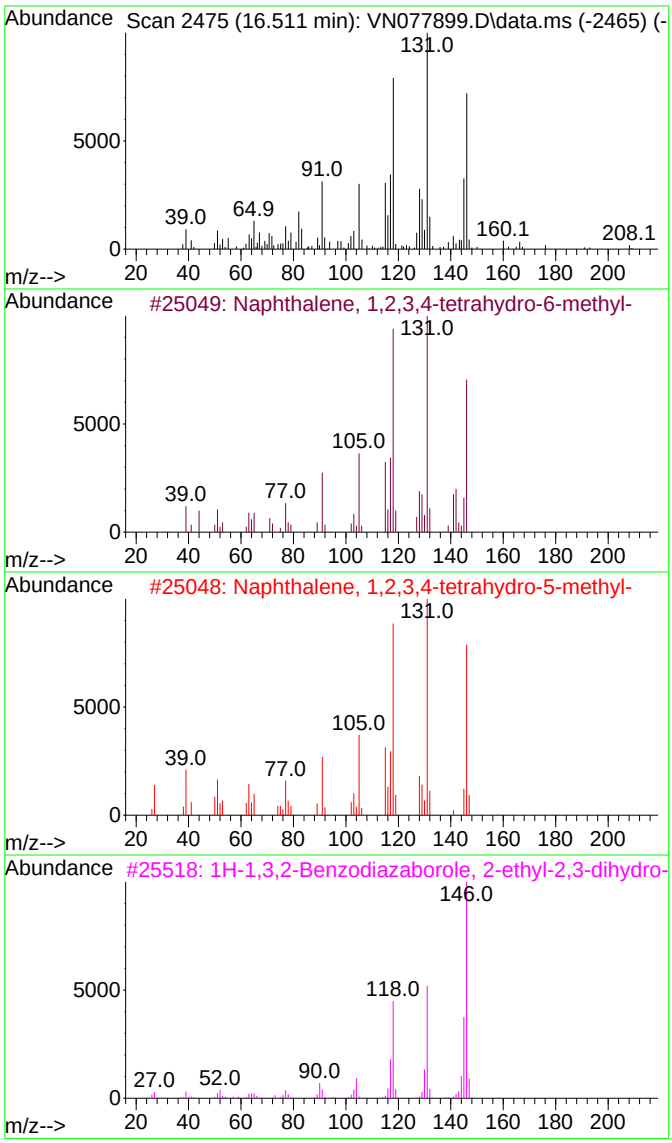
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

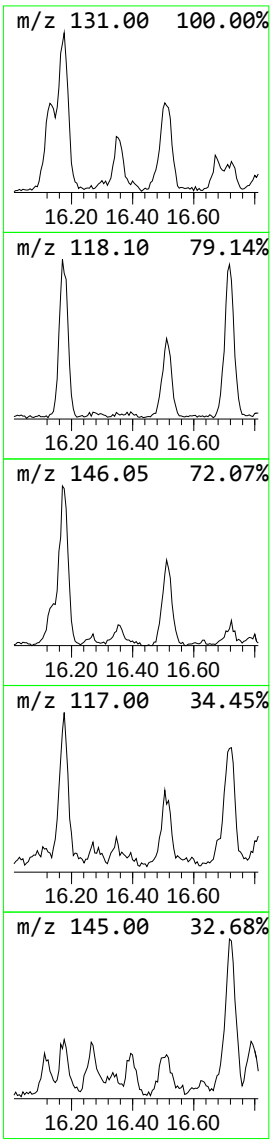
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.511	13.15 ug/l	454968	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	93
2	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	90
3	1H-1,3,2-Benzodiazaborole, 2-eth...	146	C8H11BN2	074663-81-3	81
4	Benzene, (1-methyl-1-butenyl)-	146	C11H14	053172-84-2	64
5	2-Propyn-1-ol, 3-(4-methylphenyl)-	146	C10H10O	016017-24-6	52





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052523\
Data File : VN077899.D
Acq On : 25 May 2023 14:03
Operator : JC\MD
Sample : 02850-05
Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TRE-1729

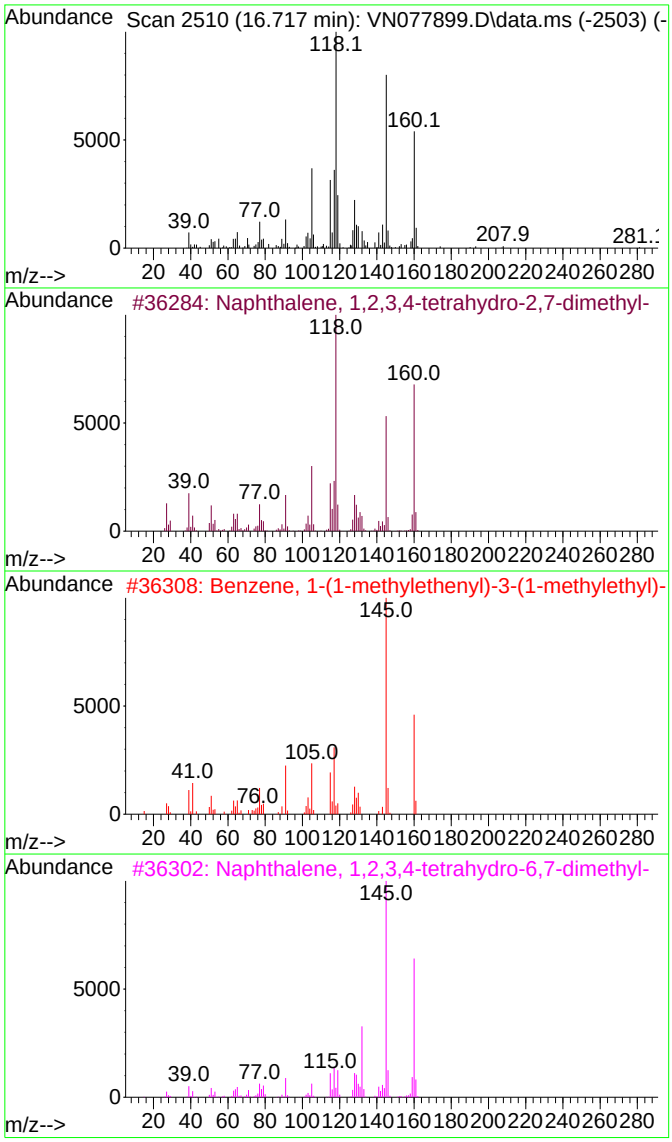
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

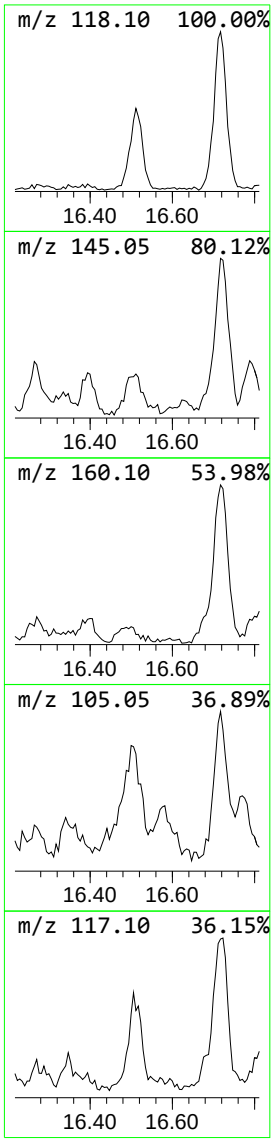
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.717	13.86 ug/l	479415	1,4-Dichlorobenzene-d4	13.800

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	013065-07-1	68
2	Benzene, 1-(1-methylethenyl)-3-(...	160	C12H16	001129-29-9	60
3	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	001076-61-5	58
4	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	020027-77-4	58
5	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	007524-63-2	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052523\
Data File : VN077899.D
Acq On : 25 May 2023 14:03
Operator : JC\MD
Sample : 02850-05
Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TRE-1729

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Benzene, 1-meth...	13.982	7.3	ug/l	252779	4	13.800	1729300	50.0
unknown14.882	14.882	7.0	ug/l	243314	4	13.800	1729300	50.0
Dodecane	14.964	19.7	ug/l	681464	4	13.800	1729300	50.0
3-Phenylbut-1-ene	15.053	19.5	ug/l	675913	4	13.800	1729300	50.0
unknown15.441	15.441	7.1	ug/l	244115	4	13.800	1729300	50.0
Tridecane	15.841	13.6	ug/l	468793	4	13.800	1729300	50.0
1H-Indene, 2,3-...	15.953	9.6	ug/l	330511	4	13.800	1729300	50.0
Naphthalene, 1,...	16.176	15.8	ug/l	545204	4	13.800	1729300	50.0
Naphthalene, 1,...	16.511	13.2	ug/l	454968	4	13.800	1729300	50.0
Naphthalene, 1,...	16.717	13.9	ug/l	479415	4	13.800	1729300	50.0