LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN013123\
Data File : VN076480.D
Acq On : 31 Jan 2023 12:11
Operator : JC\MD
Sample : 01345-01
Misc : 5.01g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
RBR200007

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\82N011623W.M
Title : SW846 8260

Signal : TIC: VN076480.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	1028	1040	1044	rBV	266721	641541	34.02%	3.569%
2	8.224	1044	1049	1061	rVB	524339	1157277	61.37%	6.439%
3	8.582	1100	1110	1120	rBV	274373	622674	33.02%	3.465%
4	8.759	1129	1140	1141	rBV4	8022	20446	1.08%	0.114%
5	9.100	1189	1198	1211	rBV	700867	1425788	75.61%	7.933%
6	10.565	1437	1447	1455	rBV	1030840	1885708	100.00%	10.492%
7	10.629	1455	1458	1465	rVB	28683	51642	2.74%	0.287%
8	11.865	1659	1668	1680	rBV	893251	1592667	84.46%	8.862%
9	11.965	1680	1685	1690	rBV	17896	28287	1.50%	0.157%
10	12.071	1696	1703	1708	rBV	48631	101065	5.36%	0.562%
11	12.400	1748	1759	1765	rBV4	36058	86171	4.57%	0.479%
12	12.623	1793	1797	1802	rVB3	13690	19899	1.06%	0.111%
13	12.853	1829	1836	1844	rVB	679267	1166771	61.87%	6.492%
14	12.947	1844	1852	1855	rBV9	8400	21360	1.13%	0.119%
15	13.035	1861	1867	1872	rVB5	21297	43385	2.30%	0.241%
16	13.100	1872	1878	1881	rBV3	40955	75296	3.99%	0.419%
17	13.135	1881	1884	1886	rVV3	29761	46386	2.46%	0.258%
18	13.170	1886	1890	1897	rVV3	66330	139195	7.38%	0.774%
19	13.223	1897	1899	1905	rVB6	15736	24948	1.32%	0.139%
20	13.335	1911	1918	1922	rVB3	13854	26102	1.38%	0.145%
21	13.423	1925	1933	1938	rVB9	16891	38811	2.06%	0.216%
22	13.482	1938	1943	1951	rBV	85495	146615	7.78%	0.816%
23	13.617	1962	1966	1970	rBV3	29778	43325	2.30%	0.241%
24	13.670	1971	1975	1981	rVV4	37218	74214	3.94%	0.413%
25	13.729	1981	1985	1989	rVB2	28407	40569	2.15%	0.226%
26	13.794	1989	1996	2005	rBV	878318	1511621	80.16%	8.411%
27	13.941	2013	2021	2025	rBV7	22538	68465	3.63%	0.381%
28	13.988	2025	2029	2032	rVV2	47965	76538	4.06%	0.426%
29	14.023	2032	2035	2040	rVB3	29390	54728	2.90%	0.305%
30	14.123	2046	2052	2058	rBV4	107044	213533	11.32%	1.188%
31	14.247	2066	2073	2075	rBV5	30806	59953	3.18%	0.334%
32	14.276	2076	2078	2082	rVV	36265	47131	2.50%	0.262%
33	14.329	2082	2087	2093	rVB2	67005	118384	6.28%	0.659%
34	14.441	2100	2106	2112	rBV2	182846	305624	16.21%	1.700%
35	14.517	2113	2119	2124	rBV4	79007	154236	8.18%	0.858%
36	14.576	2124	2129	2133	rVB4	57574	92199	4.89%	0.513%

LSC Area Percent Report

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ClientSampleId :
RBR200007

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
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Peak separation: 5

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Title : SW846 8260

37	14.629	2133	2138	2140	rBV2	112628	163915	8.69%	0.912%
38	14.664	2140	2144	2147	rVB2	79724	109986	5.83%	0.612%
39	14.741	2153	2157	2160	rBV2	49035	75940	4.03%	0.423%
40	14.794	2160	2166	2171	rVB5	90590	204387	10.84%	1.137%
41	14.847	2171	2175	2178	rBV5	64578	116031	6.15%	0.646%
42	14.941	2185	2191	2192	rBV3	57591	93926	4.98%	0.523%
43	14.970	2193	2196	2201	rVB2	69524	107710	5.71%	0.599%
44	15.035	2201	2207	2208	rBV3	147715	217571	11.54%	1.211%
45	15.112	2216	2220	2224	rBV4	140246	228731	12.13%	1.273%
46	15.217	2233	2238	2242	rBV	169044	303352	16.09%	1.688%
47	15.270	2243	2247	2252	rVV6	184349	355962	18.88%	1.981%
48	15.329	2252	2257	2263	rVB5	151592	356043	18.88%	1.981%
49	15.700	2315	2320	2326	rBV3	203054	455884	24.18%	2.537%
50	15.782	2331	2334	2343	rVB4	181976	374809	19.88%	2.085%
51	15.941	2354	2361	2363	rBV6	111003	272162	14.43%	1.514%
52	16.170	2395	2400	2406	rBV4	345209	649752	34.46%	3.615%
53	16.506	2453	2457	2464	rVB5	328312	696462	36.93%	3.875%
54	16.711	2486	2492	2499	rBV	419426	967689	51.32%	5.384%

Sum of corrected areas: 17972866

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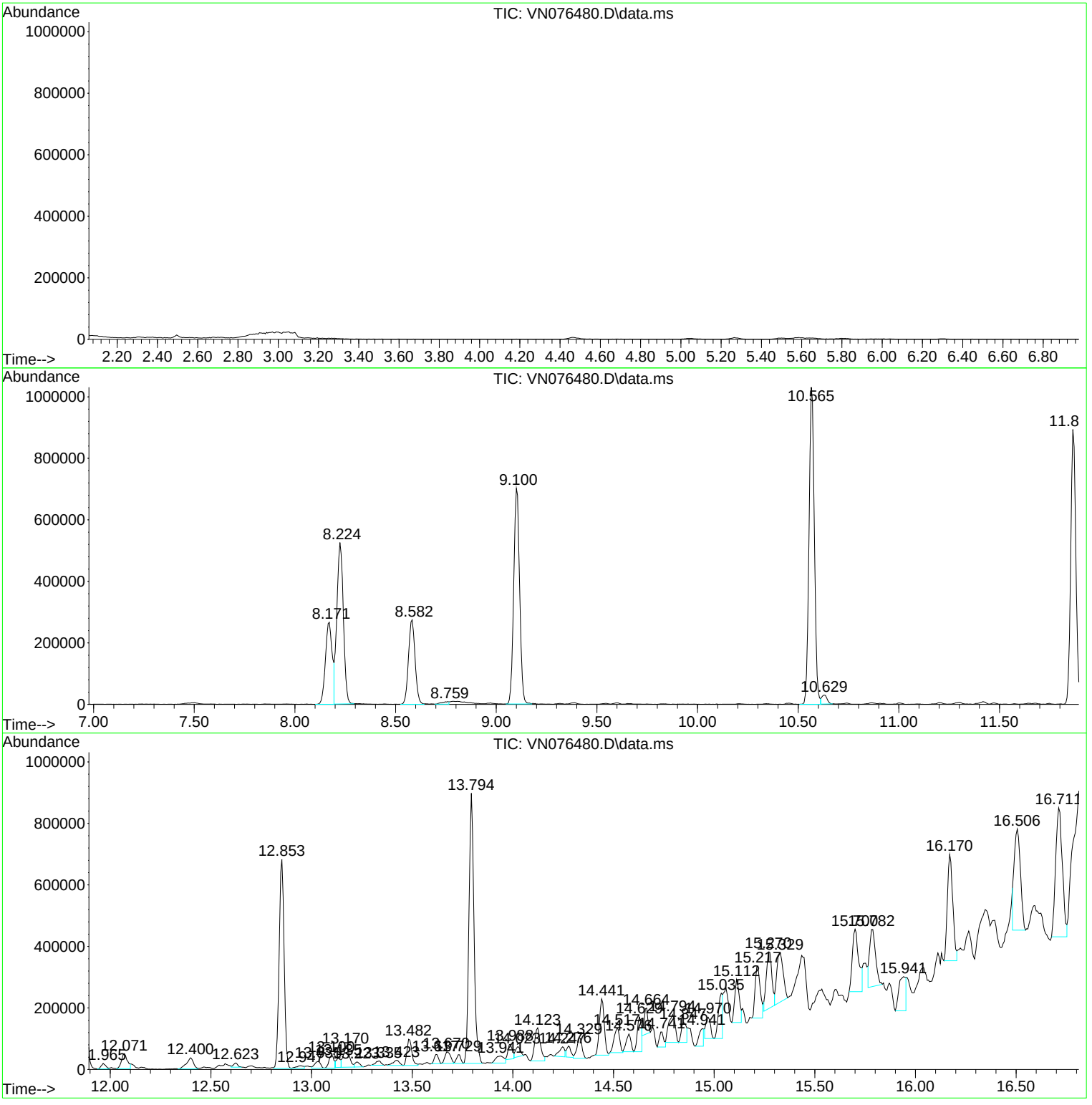
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
RBR200007

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011623W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN013123\
Data File : VN076480.D
Acq On : 31 Jan 2023 12:11
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RBR200007

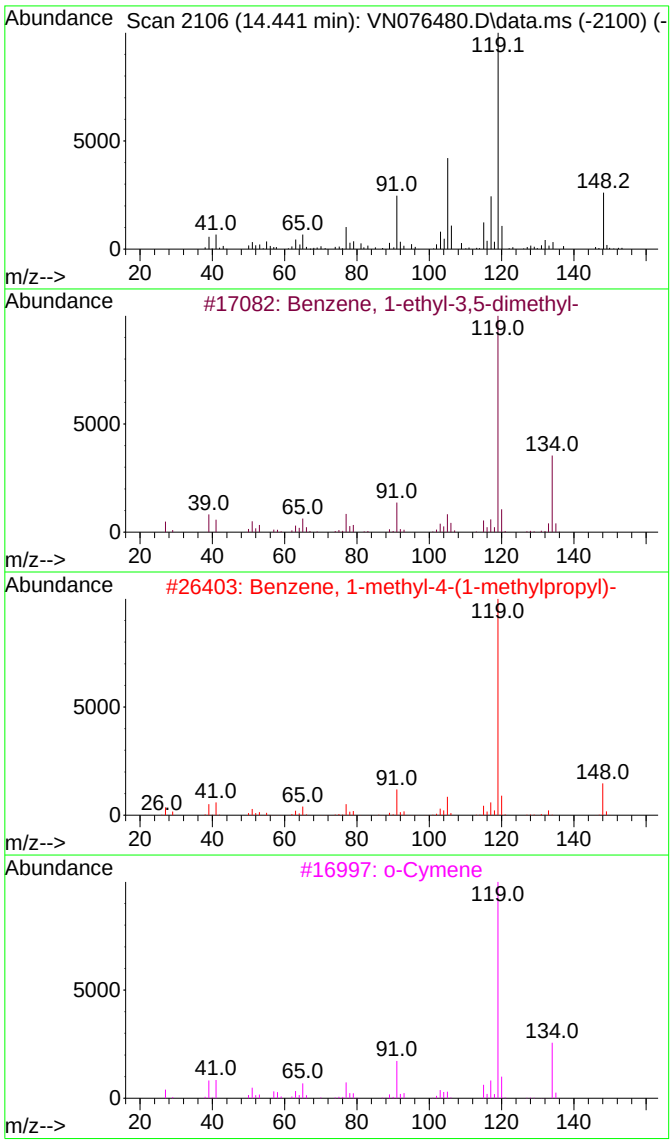
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011623W.M
Quant Title : SW846 8260

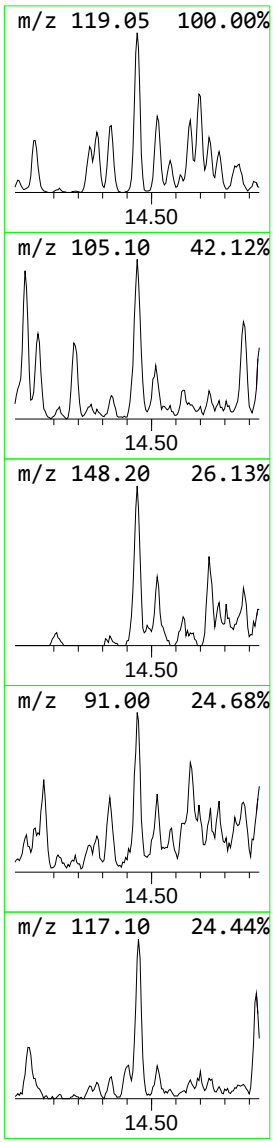
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Benzene, 1-ethyl-3,5-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.441	10.11 ug/l	305624	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	68
2	Benzene, 1-methyl-4-(1-methylpro...	148	C11H16	001595-16-0	64
3	o-Cymene	134	C10H14	000527-84-4	64
4	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	59
5	7-Methoxymethyl-2,7-dimethylcycl...	164	C11H16O	073992-48-0	59





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Operator : JC\MD
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Misc : 5.01g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
RBR200007

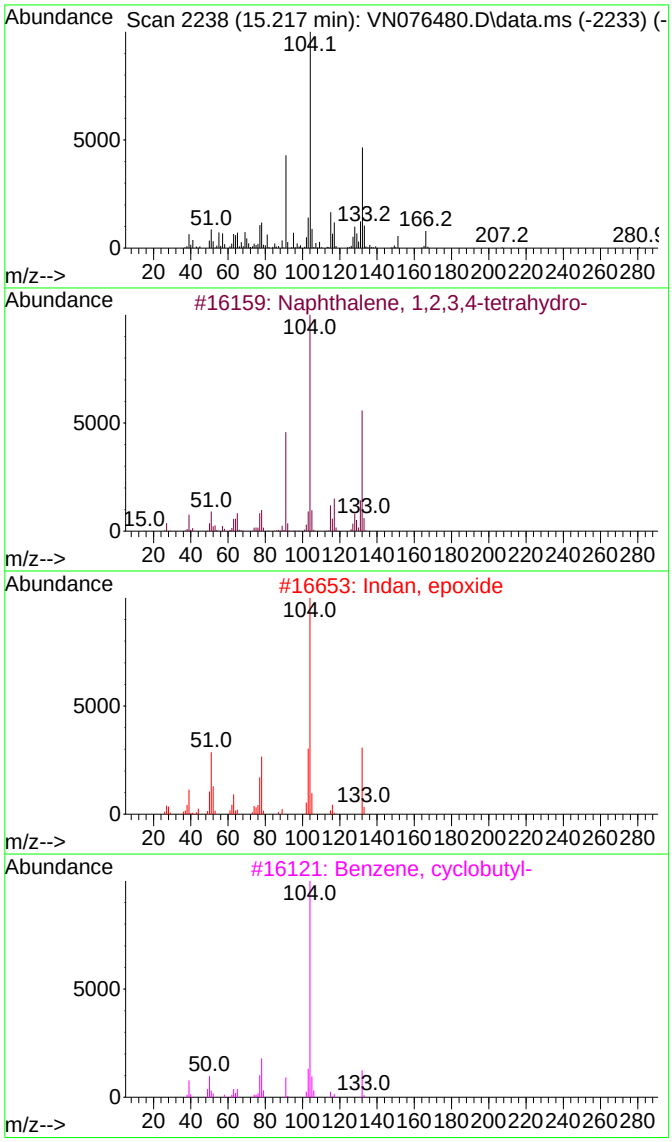
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011623W.M
Quant Title : SW846 8260

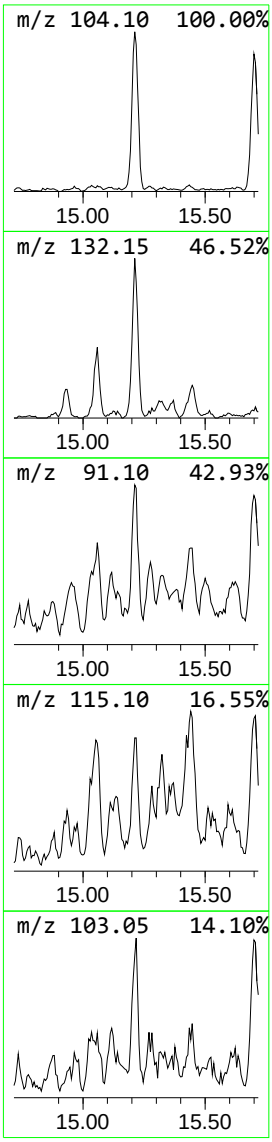
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.217	10.03 ug/l	303352	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-	132	C10H12	000119-64-2	95
2	Indan, epoxide	132	C9H8O	000768-22-9	64
3	Benzene, cyclobutyl-	132	C10H12	004392-30-7	53
4	2H-Inden-2-one, 1,3-dihydro-	132	C9H8O	000615-13-4	50
5	2-Methylbenzyl cyanide	131	C9H9N	022364-68-7	46





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN013123\
Data File : VN076480.D
Acq On : 31 Jan 2023 12:11
Operator : JC\MD
Sample : 01345-01
Misc : 5.01g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
RBR200007

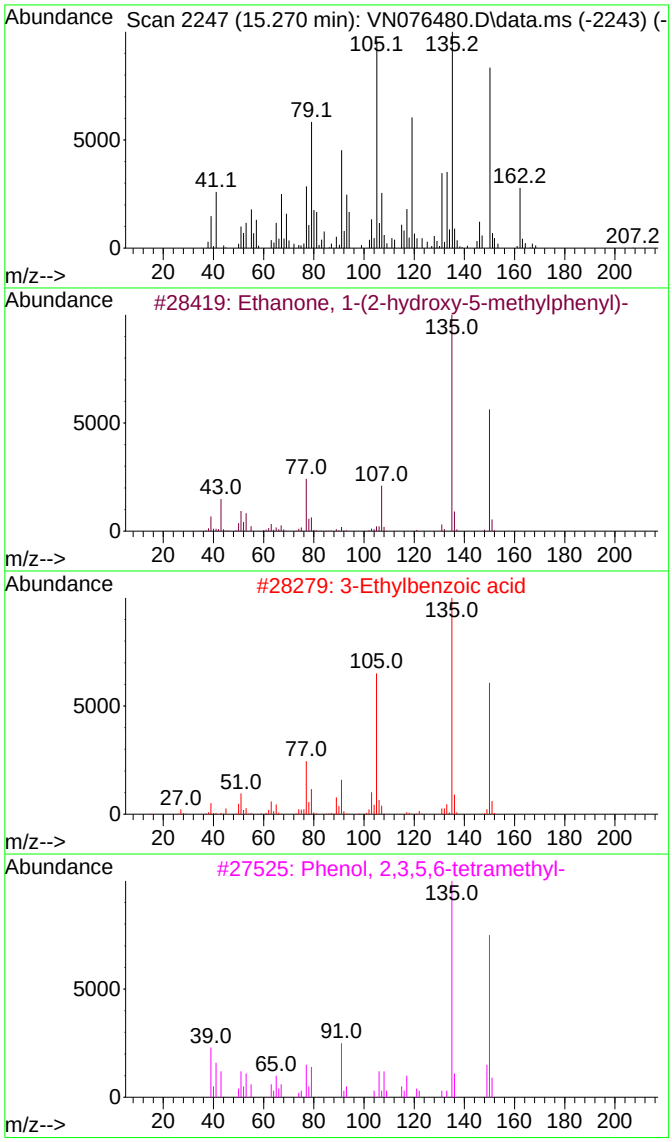
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011623W.M
Quant Title : SW846 8260

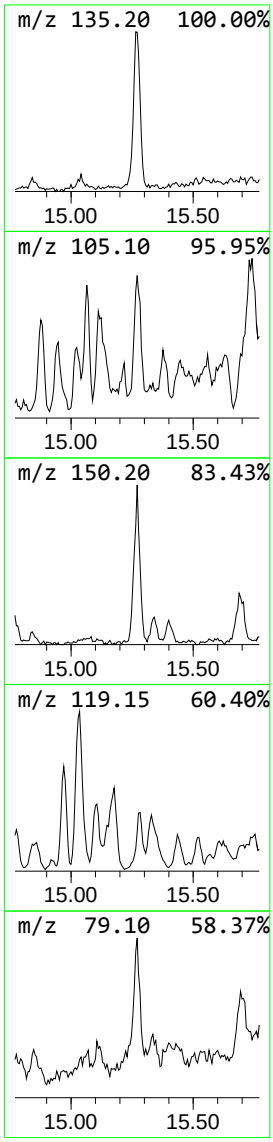
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Ethanone, 1-(2-hydroxy-5-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.270	11.77 ug/l	355962	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanone, 1-(2-hydroxy-5-methylp...	150	C9H10O2	001450-72-2	55
2	3-Ethylbenzoic acid	150	C9H10O2	000619-20-5	50
3	Phenol, 2,3,5,6-tetramethyl-	150	C10H14O	000527-35-5	50
4	3,9-Epoxy-p-mentha-1,8(10)-diene	150	C10H14O	1000111-14-8	49
5	2,3,5-Trimethylanizole	150	C10H14O	1000342-42-3	46





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN013123\
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ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
RBR200007

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011623W.M
Quant Title : SW846 8260

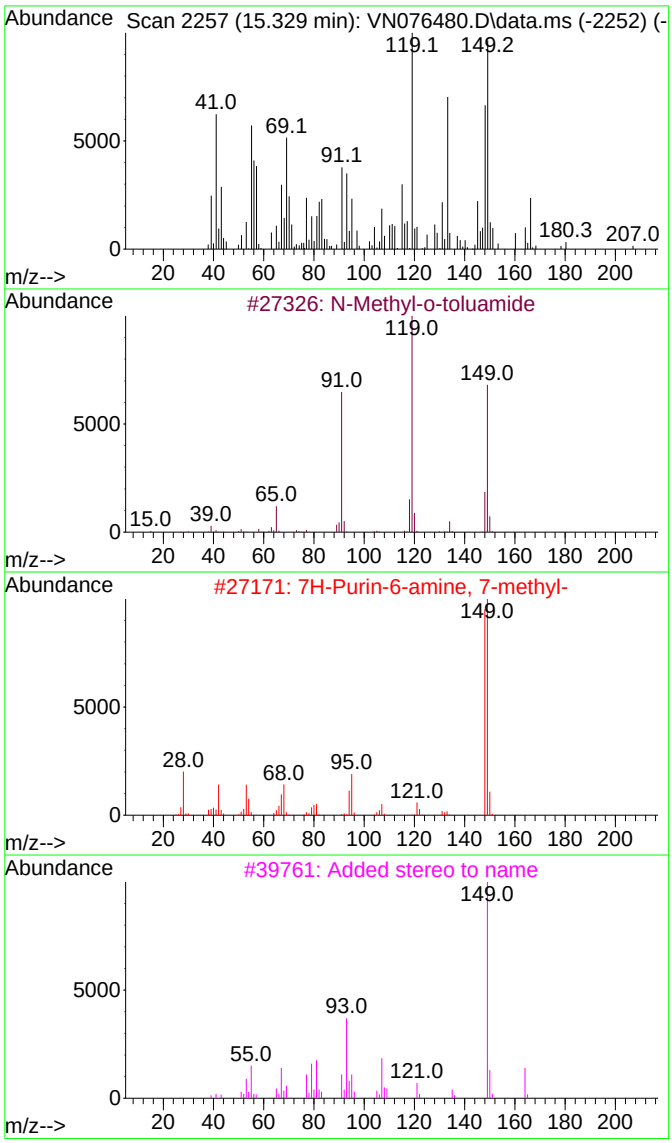
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

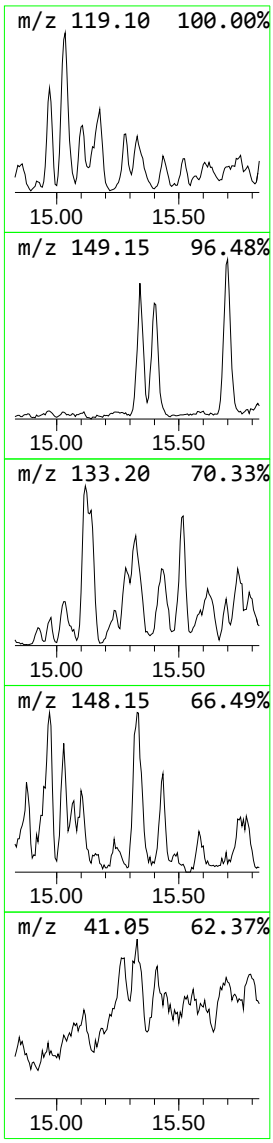
****

Peak Number 4 unknown15.329 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.329	11.78 ug/l	356043	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N-Methyl-o-toluamide	149	C9H11NO	002170-09-4	35
2	7H-Purin-6-amine, 7-methyl-	149	C6H7N5	000935-69-3	30
3	Added stereo to name	164	C12H20	024145-89-9	25
4	Added stereo to name	164	C12H20	024145-88-8	25
5	2-(1-Methyl-2-propenyl)phenol	148	C10H12O	1000432-85-2	25





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Instrument :
MSVOA_N
ClientSampleId :
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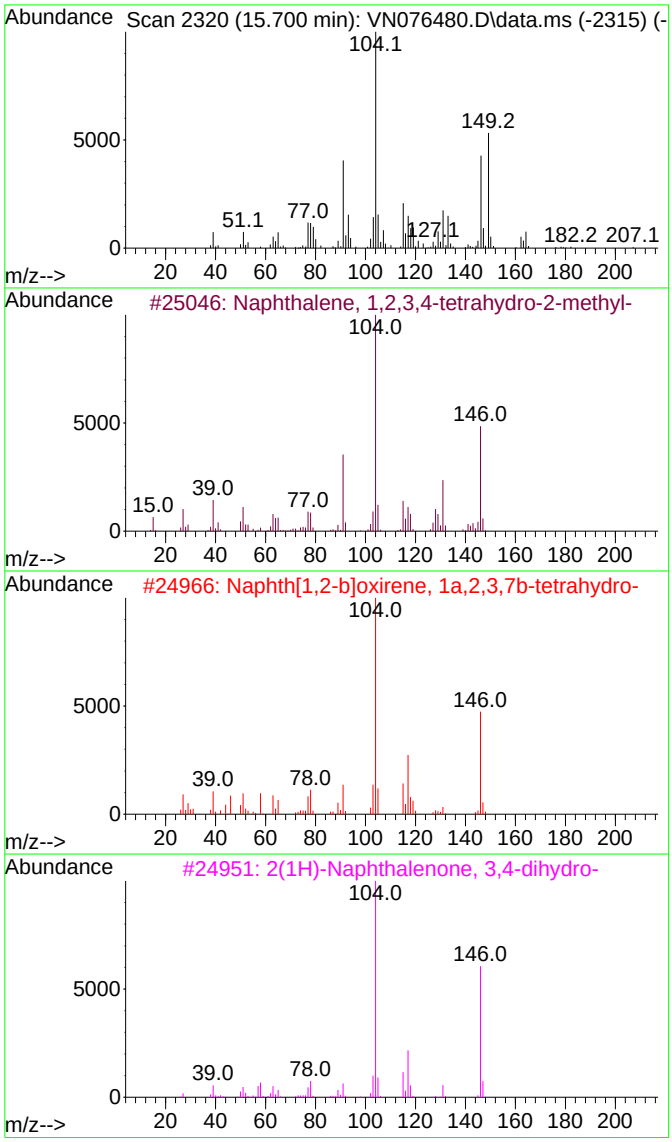
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011623W.M
Quant Title : SW846 8260

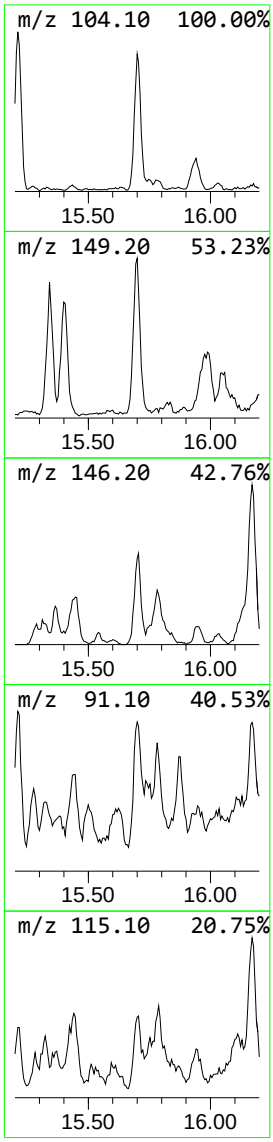
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.700	15.08 ug/l	455884	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	003877-19-8	86
2	Naphth[1,2-b]oxirene, 1a,2,3,7b-...	146	C10H10O	002461-34-9	58
3	2(1H)-Naphthalenone, 3,4-dihydro-	146	C10H10O	000530-93-8	52
4	Cyclopropane, 1-cyclopropylethyn...	164	C11H16O	1010274-98-5	38
5	Benzenepropanoic acid, methyl ester	164	C10H12O2	000103-25-3	38





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Quant Title : SW846 8260

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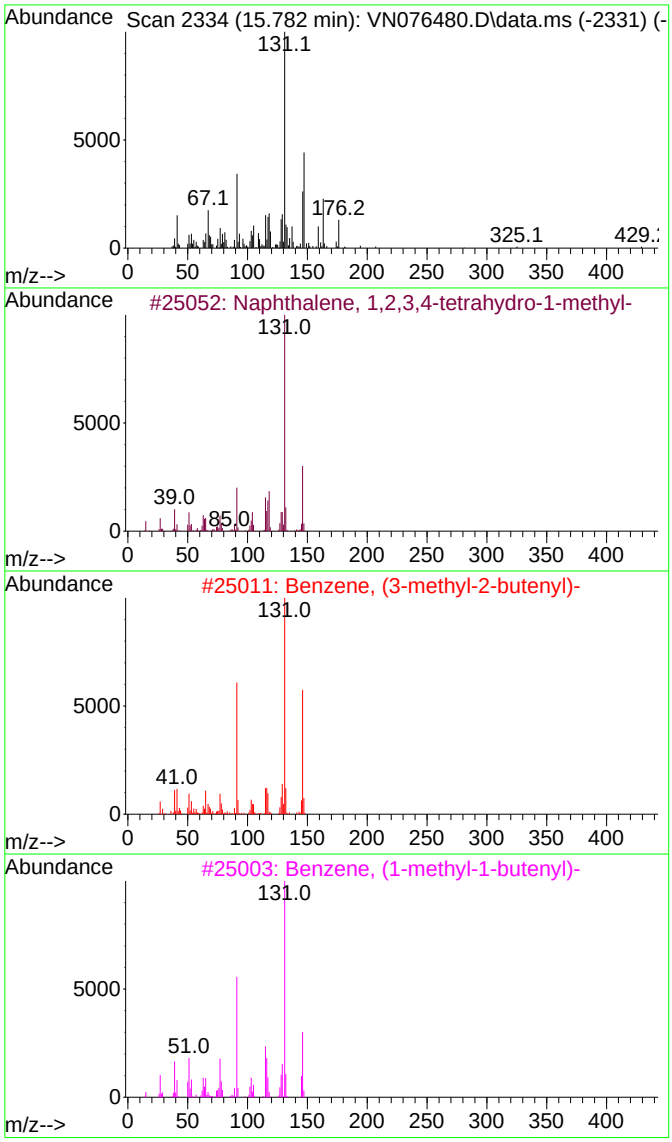
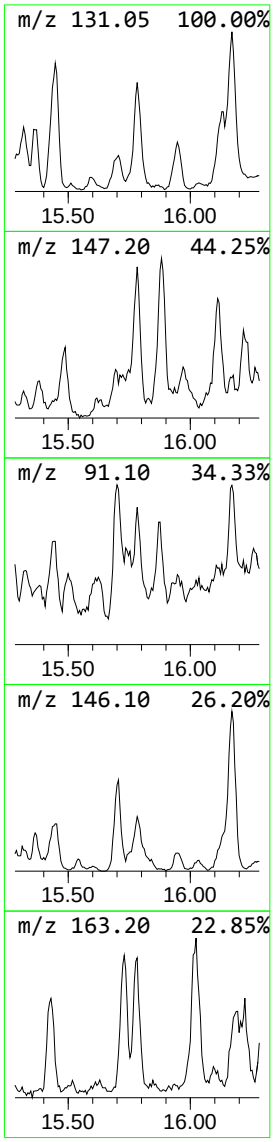
****
Peak Number 6 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.782	12.40 ug/l	374809	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001559-81-5	55
2	Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	55
3	Benzene, (1-methyl-1-butenyl)-	146	C11H14	053172-84-2	55
4	Benzene, 1-methyl-2-(1-methyl-2-...	146	C11H14	097664-19-2	49
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	146	C11H14	027087-54-3	49





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ClientSampleId :
RBR200007

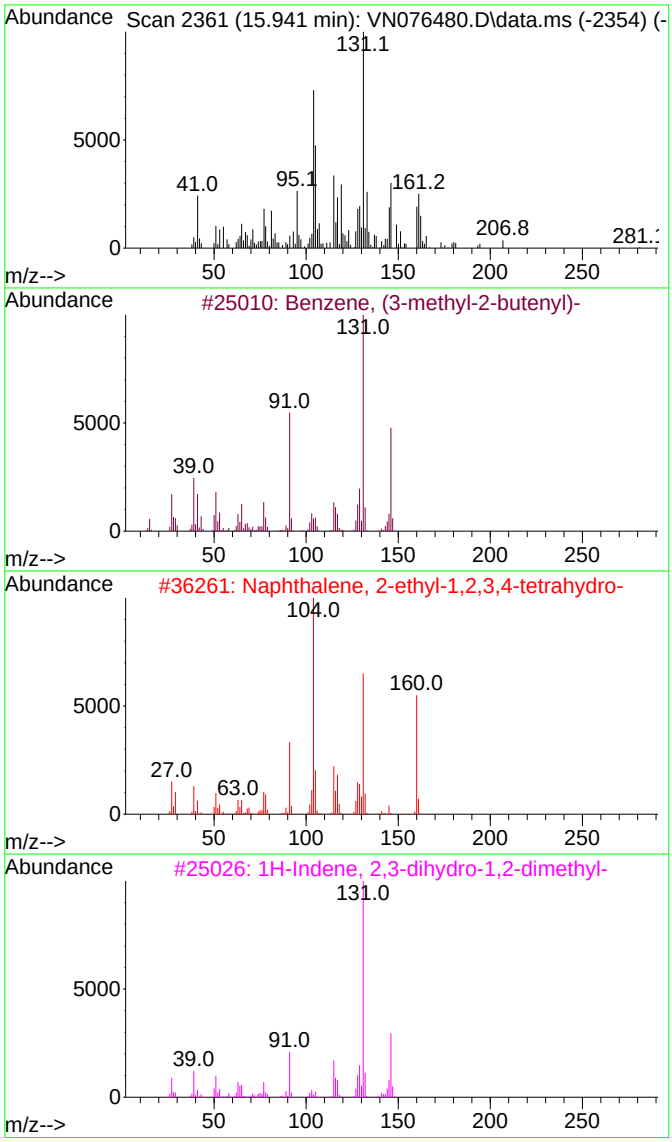
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011623W.M
Quant Title : SW846 8260

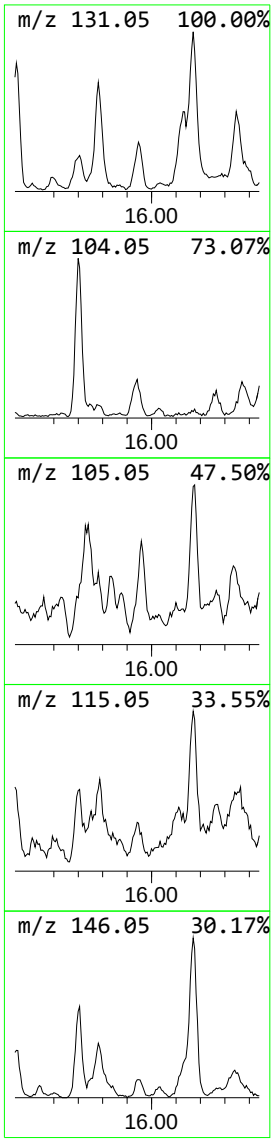
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, (3-methyl-2-butenyl)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.941	9.00 ug/l	272162	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	55
2	Naphthalene, 2-ethyl-1,2,3,4-tet...	160	C12H16	032367-54-7	50
3	1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	46
4	Naphthalene, 6-ethyl-1,2,3,4-tet...	160	C12H16	022531-20-0	43
5	2-Propenal, 3-(4-methylphenyl)-	146	C10H10O	001504-75-2	41





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN013123\
Data File : VN076480.D
Acq On : 31 Jan 2023 12:11
Operator : JC\MD
Sample : 01345-01
Misc : 5.01g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
RBR200007

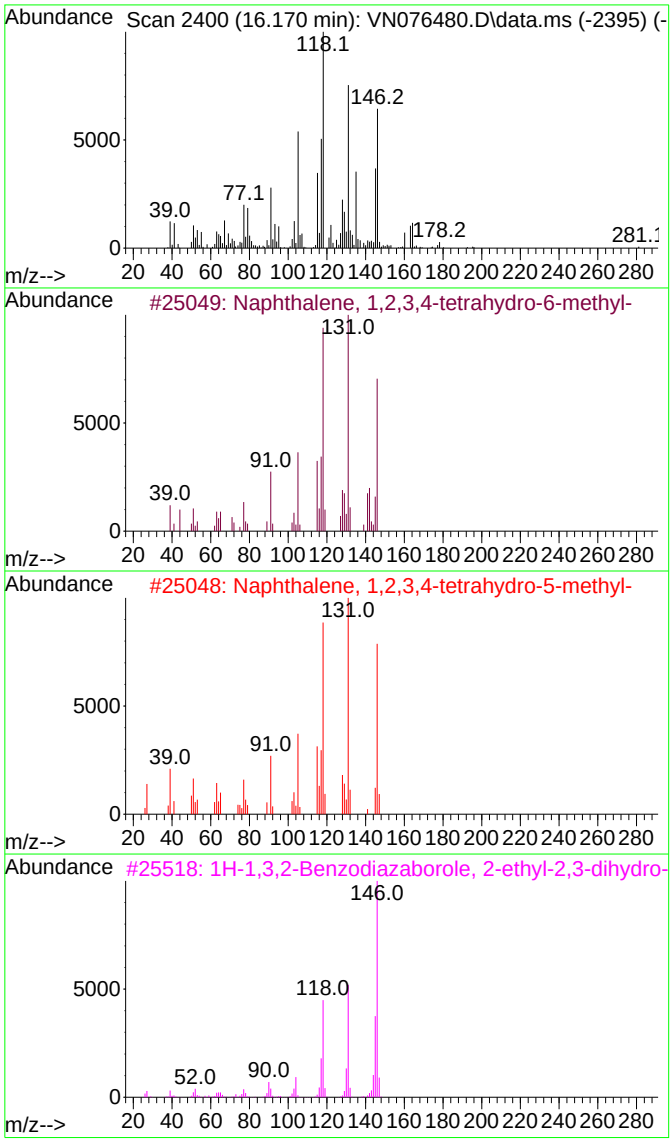
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011623W.M
Quant Title : SW846 8260

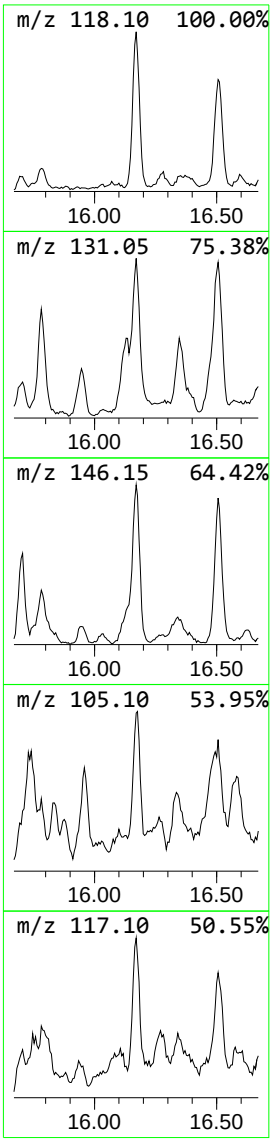
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.170	21.49 ug/l	649752	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	90
2	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	76
3	1H-1,3,2-Benzodiazaborole, 2-eth...	146	C8H11BN2	074663-81-3	58
4	2-Propyn-1-ol, 3-(4-methylphenyl)-	146	C10H10O	016017-24-6	45
5	Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	41





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN013123\
Data File : VN076480.D
Acq On : 31 Jan 2023 12:11
Operator : JC\MD
Sample : 01345-01
Misc : 5.01g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
RBR200007

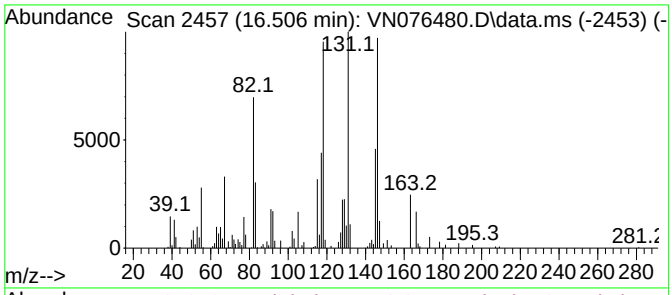
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011623W.M
Quant Title : SW846 8260

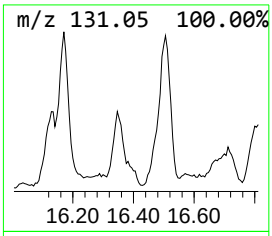
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

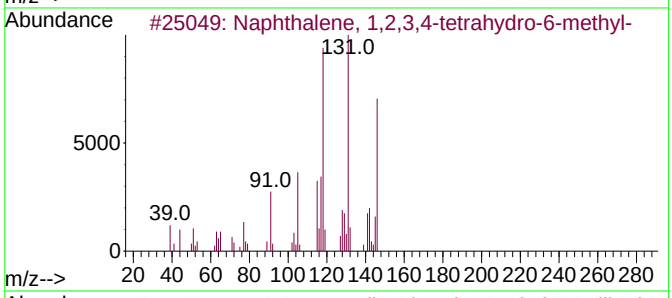
****
Peak Number 9 1H-1,3,2-Benzodiazaborole, ... Concentration Rank 2

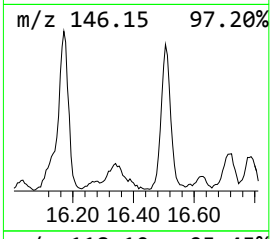
R.T.	EstConc	Area	Relative to ISTD	R.T.
16.506	23.04 ug/l	696462	1,4-Dichlorobenzene-d4	13.794

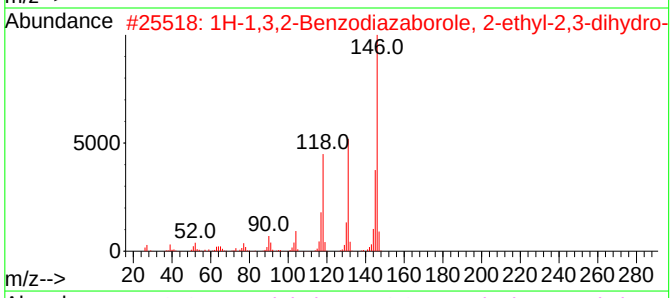
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	89
2	1H-1,3,2-Benzodiazaborole, 2-eth...	146	C8H11BN2	074663-81-3	76
3	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	70
4	2,3,4,5,6,7-Hexahydro-1H-cyclope...	146	C11H14	1010189-31-0	52
5	Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	50

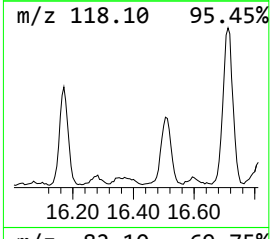


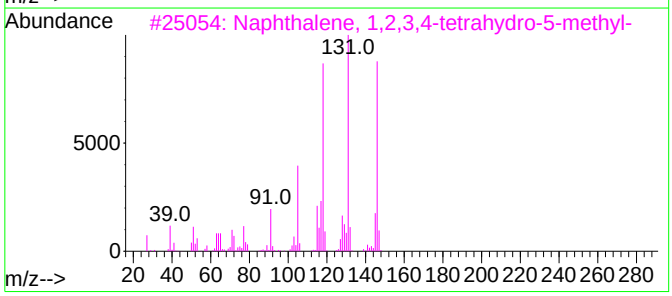


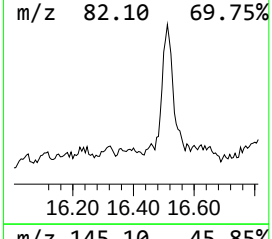


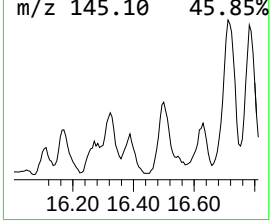












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Data File : VN076480.D
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ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
RBR200007

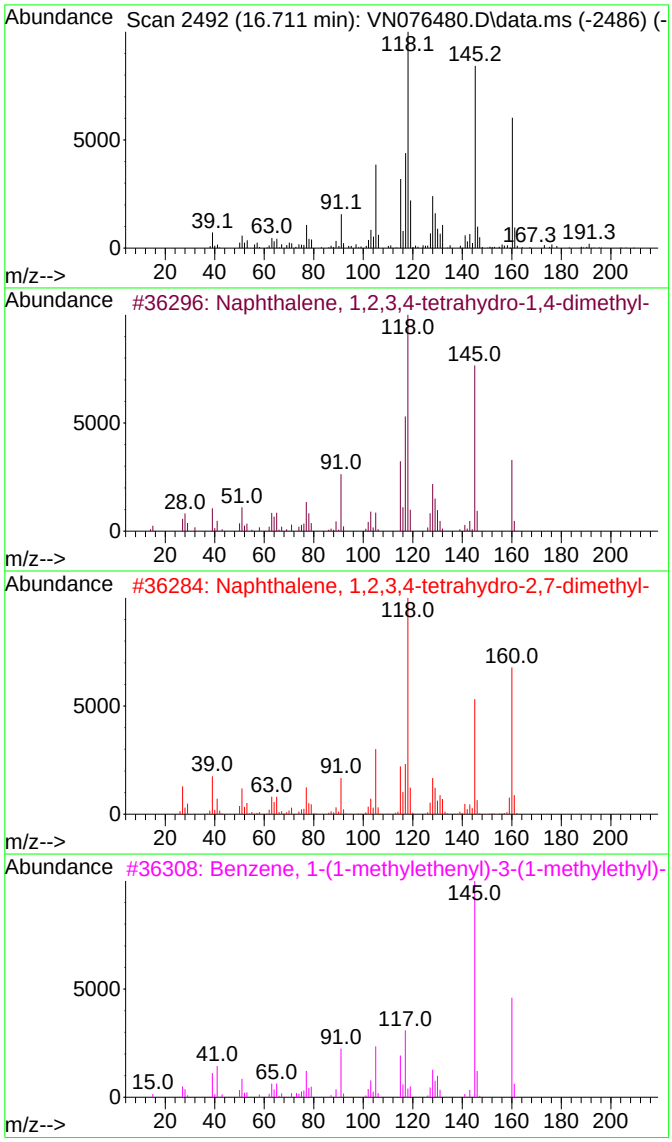
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011623W.M
Quant Title : SW846 8260

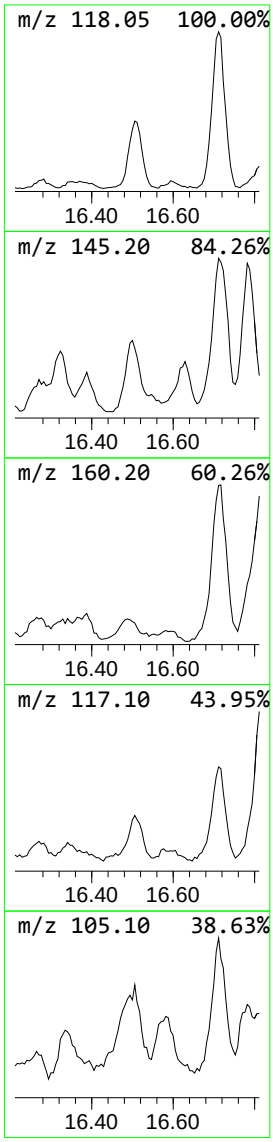
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.711	32.01 ug/l	967689	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	94
2	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	013065-07-1	87
3	Benzene, 1-(1-methylethenyl)-3-(...	160	C12H16	001129-29-9	64
4	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	020027-77-4	60
5	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	025419-33-4	58





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN013123\
Data File : VN076480.D
Acq On : 31 Jan 2023 12:11
Operator : JC\MD
Sample : 01345-01
Misc : 5.01g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
RBR200007

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011623W.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-ethy...	14.441	10.1	ug/l	305624	4	13.794	1511620	50.0
Naphthalene, 1,...	15.217	10.0	ug/l	303352	4	13.794	1511620	50.0
Ethanone, 1-(2-...	15.270	11.8	ug/l	355962	4	13.794	1511620	50.0
unknown15.329	15.329	11.8	ug/l	356043	4	13.794	1511620	50.0
Naphthalene, 1,...	15.700	15.1	ug/l	455884	4	13.794	1511620	50.0
Naphthalene, 1,...	15.782	12.4	ug/l	374809	4	13.794	1511620	50.0
Benzene, (3-met...	15.941	9.0	ug/l	272162	4	13.794	1511620	50.0
Naphthalene, 1,...	16.170	21.5	ug/l	649752	4	13.794	1511620	50.0
1H-1,3,2-Benzod...	16.506	23.0	ug/l	696462	4	13.794	1511620	50.0
Naphthalene, 1,...	16.711	32.0	ug/l	967689	4	13.794	1511620	50.0