LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061923\
Data File : VN078275.D
Acq On : 19 Jun 2023 13:23
Operator : JC\MD
Sample : 03241-01
Misc : 1.13g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
30852

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\82N060623W.M
Title : SW846 8260

Signal : TIC: VN078275.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	1046	1057	1061	rBV	273281	640018	3.16%	0.586%
2	8.230	1061	1067	1080	rVB	467197	1073276	5.31%	0.983%
3	8.583	1116	1127	1138	rBV	293103	700139	3.46%	0.641%
4	9.106	1206	1216	1227	rBV	668165	1413699	6.99%	1.295%
5	10.571	1457	1465	1473	rBV	1065495	1952878	9.66%	1.789%
6	11.871	1677	1686	1697	rBV	942546	1706361	8.44%	1.563%
7	12.406	1766	1777	1784	rBV	464096	832945	4.12%	0.763%
8	12.706	1819	1828	1837	rBV2	960292	1844276	9.12%	1.690%
9	12.853	1846	1853	1861	rVB	764043	1317200	6.51%	1.207%
10	12.965	1861	1872	1878	rBV	134028	269871	1.33%	0.247%
11	13.041	1878	1885	1890	rBV	2159783	3500228	17.31%	3.207%
12	13.100	1890	1895	1899	rBV	7844101	13334542	65.93%	12.217%
13	13.135	1899	1901	1905	rVV	3655697	4835403	23.91%	4.430%
14	13.176	1905	1908	1915	rVB	4193657	6423470	31.76%	5.885%
15	13.265	1916	1923	1929	rBV	5168905	7868410	38.91%	7.209%
16	13.341	1929	1936	1943	rVB	3472448	5505465	27.22%	5.044%
17	13.488	1953	1961	1972	rBV	11431887	20223796	100.00%	18.528%
18	13.612	1974	1982	1988	rBV3	1310009	2369884	11.72%	2.171%
19	13.712	1988	1999	2001	rBV	1543312	3434374	16.98%	3.146%
20	13.823	2008	2018	2023	rBV2	4370928	8858647	43.80%	8.116%
21	13.959	2033	2041	2042	rBV3	475263	749409	3.71%	0.687%
22	13.994	2042	2047	2050	rVV2	1396636	2925088	14.46%	2.680%
23	14.023	2050	2052	2062	rVV2	1245794	2181429	10.79%	1.999%
24	14.112	2062	2067	2074	rVV2	757134	1439564	7.12%	1.319%
25	14.188	2076	2080	2083	rVV	263525	422759	2.09%	0.387%
26	14.241	2083	2089	2093	rVV3	1007480	1951215	9.65%	1.788%
27	14.276	2093	2095	2100	rVV	478317	733514	3.63%	0.672%
28	14.335	2100	2105	2110	rVB	725839	1115126	5.51%	1.022%
29	14.582	2141	2147	2151	rBV4	194105	405145	2.00%	0.371%
30	14.629	2151	2155	2159	rBV2	487696	793597	3.92%	0.727%
31	14.665	2159	2161	2164	rVB2	214883	225864	1.12%	0.207%
32	14.800	2177	2184	2188	rVV2	320236	575705	2.85%	0.527%
33	14.847	2188	2192	2198	rVB7	145565	267684	1.32%	0.245%
34	14.965	2205	2212	2216	rBV	354096	659752	3.26%	0.604%
35	15.047	2221	2226	2228	rBV4	215419	377227	1.87%	0.346%
36	15.082	2228	2232	2235	rBV	311844	514703	2.55%	0.472%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061923\
Data File : VN078275.D
Acq On : 19 Jun 2023 13:23
Operator : JC\MD
Sample : 03241-01
Misc : 1.13g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
30852

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\82N060623W.M
Title : SW846 8260

37	15.182	2244	2249	2253	rBV7	131626	278325	1.38%	0.255%
38	15.229	2253	2257	2261	rVV5	272948	499628	2.47%	0.458%
39	15.270	2261	2264	2268	rVB3	279217	394952	1.95%	0.362%
40	15.323	2269	2273	2280	rVB7	165347	385981	1.91%	0.354%
41	15.429	2284	2291	2295	rBV7	209892	522367	2.58%	0.479%
42	15.517	2301	2306	2308	rBV4	286119	493484	2.44%	0.452%
43	15.600	2315	2320	2327	rVB3	540929	1142519	5.65%	1.047%
44	15.694	2328	2336	2345	rBV8	292144	1060626	5.24%	0.972%
45	15.929	2371	2376	2379	rBV5	115774	242825	1.20%	0.222%
46	16.176	2413	2418	2425	rBV7	118926	246225	1.22%	0.226%
47	16.512	2470	2475	2486	rVB2	163737	441917	2.19%	0.405%

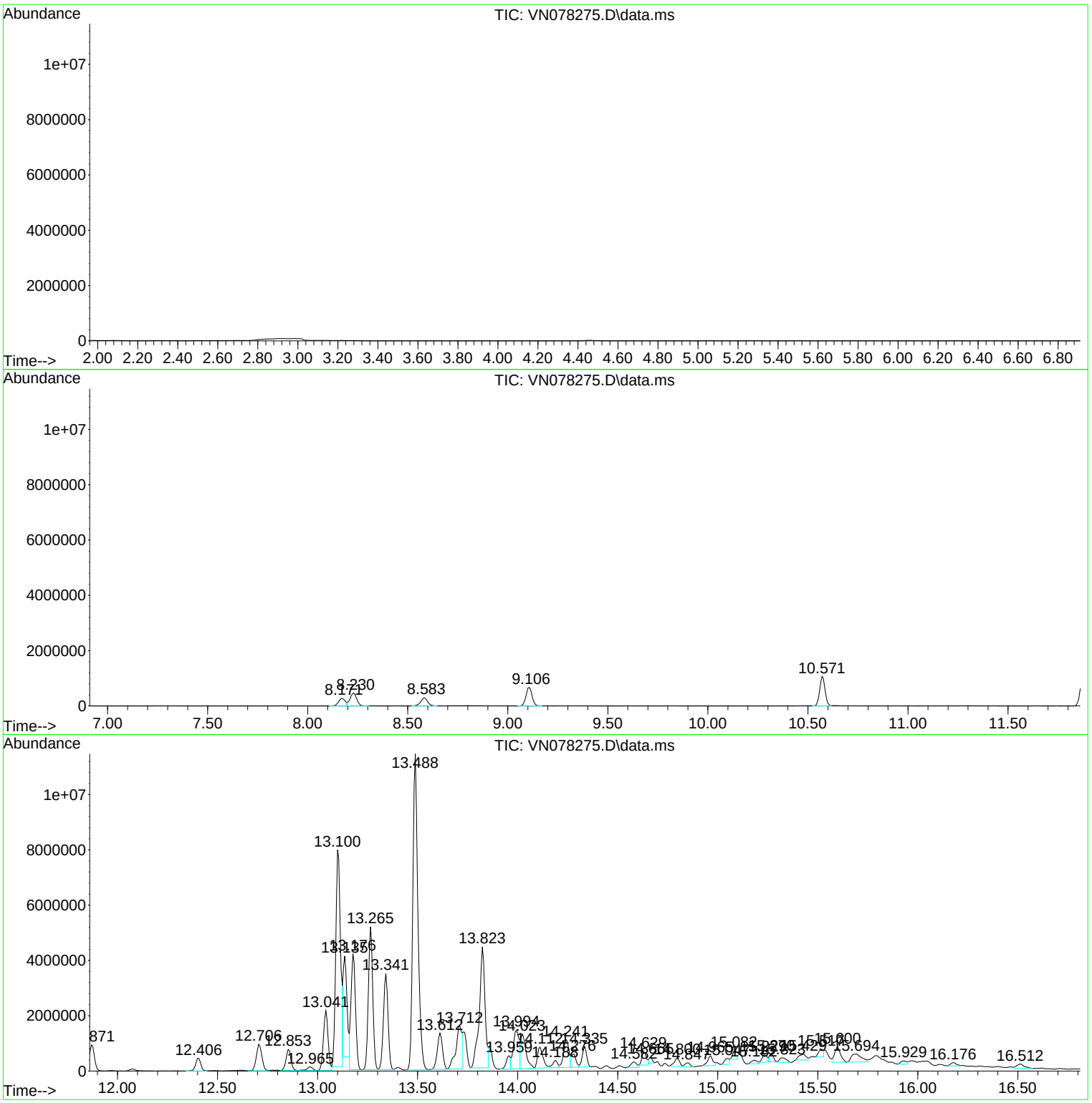
Sum of corrected areas: 109151512

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061923\
Data File : VN078275.D
Acq On : 19 Jun 2023 13:23
Operator : JC\MD
Sample : 03241-01
Misc : 1.13g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
30852

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060623W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061923\
Data File : VN078275.D
Acq On : 19 Jun 2023 13:23
Operator : JC\MD
Sample : 03241-01
Misc : 1.13g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
30852

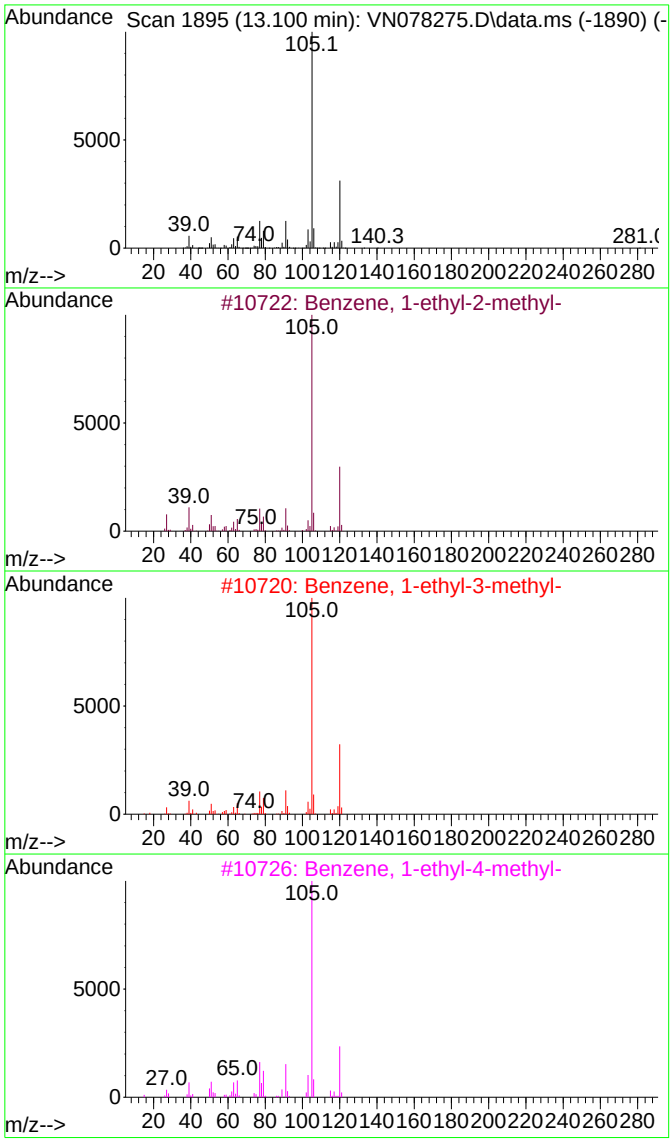
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060623W.M
Quant Title : SW846 8260

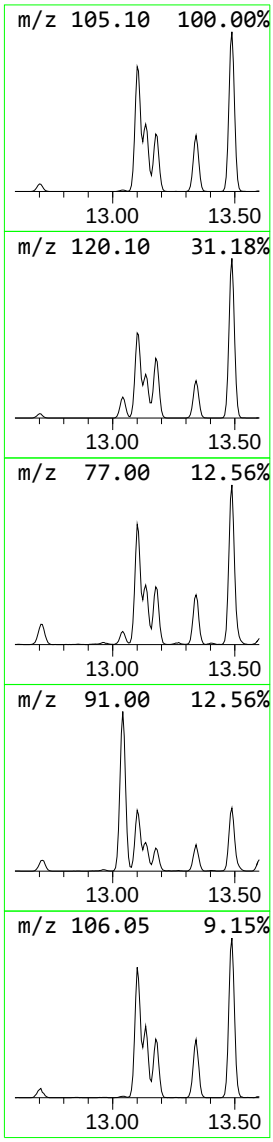
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Benzene, 1-ethyl-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.100	75.26 ug/l	13334500	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	94
3	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4	Mesitylene	120	C9H12	000108-67-8	91
5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061923\
Data File : VN078275.D
Acq On : 19 Jun 2023 13:23
Operator : JC\MD
Sample : 03241-01
Misc : 1.13g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
30852

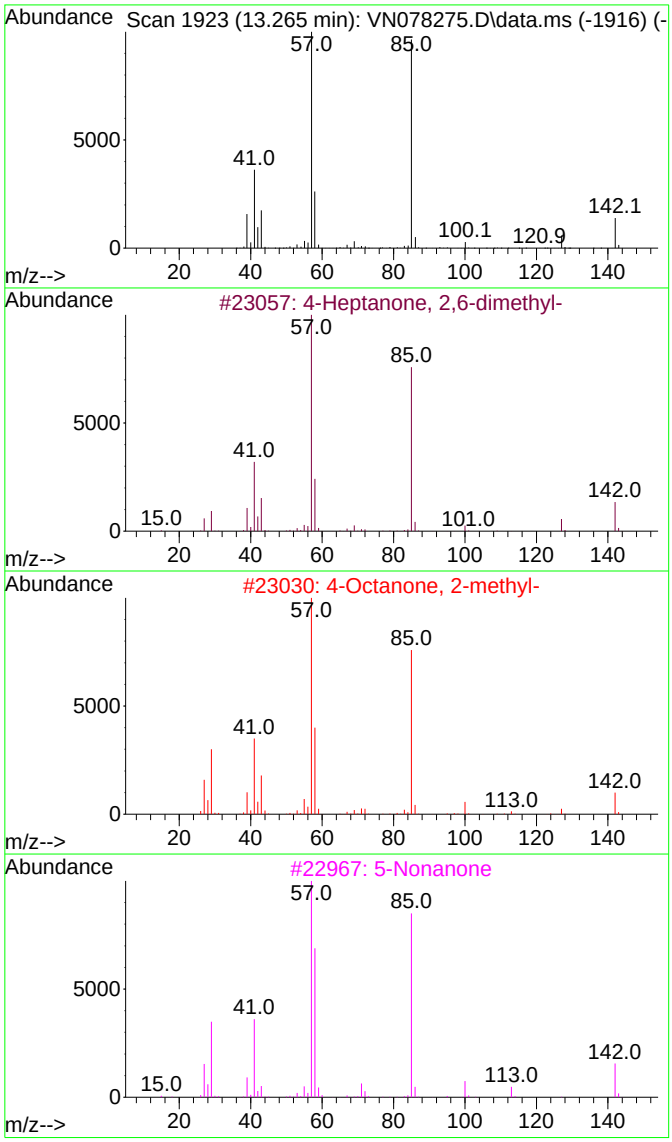
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060623W.M
Quant Title : SW846 8260

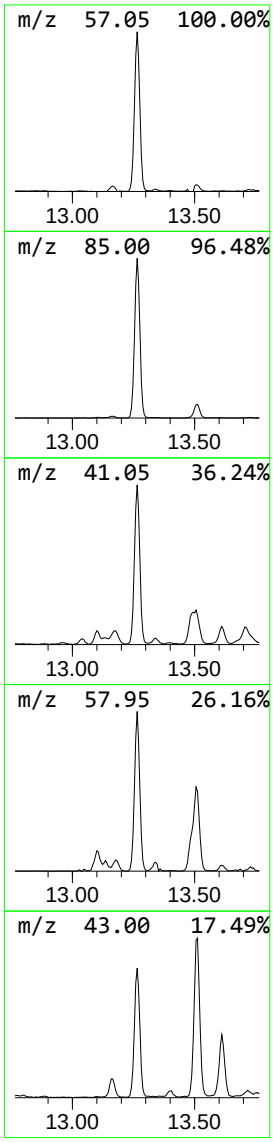
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 4-Heptanone, 2,6-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.265	44.41 ug/l	7868410	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanone, 2,6-dimethyl-	142	C9H18O	000108-83-8	94
2	4-Octanone, 2-methyl-	142	C9H18O	007492-38-8	64
3	5-Nonanone	142	C9H18O	000502-56-7	59
4	3-Buten-2-ol, 2,3-dimethyl-	100	C6H12O	010473-13-9	53
5	2,4-Heptanedione, 6-methyl-	142	C8H14O2	003002-23-1	45





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061923\
Data File : VN078275.D
Acq On : 19 Jun 2023 13:23
Operator : JC\MD
Sample : 03241-01
Misc : 1.13g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
30852

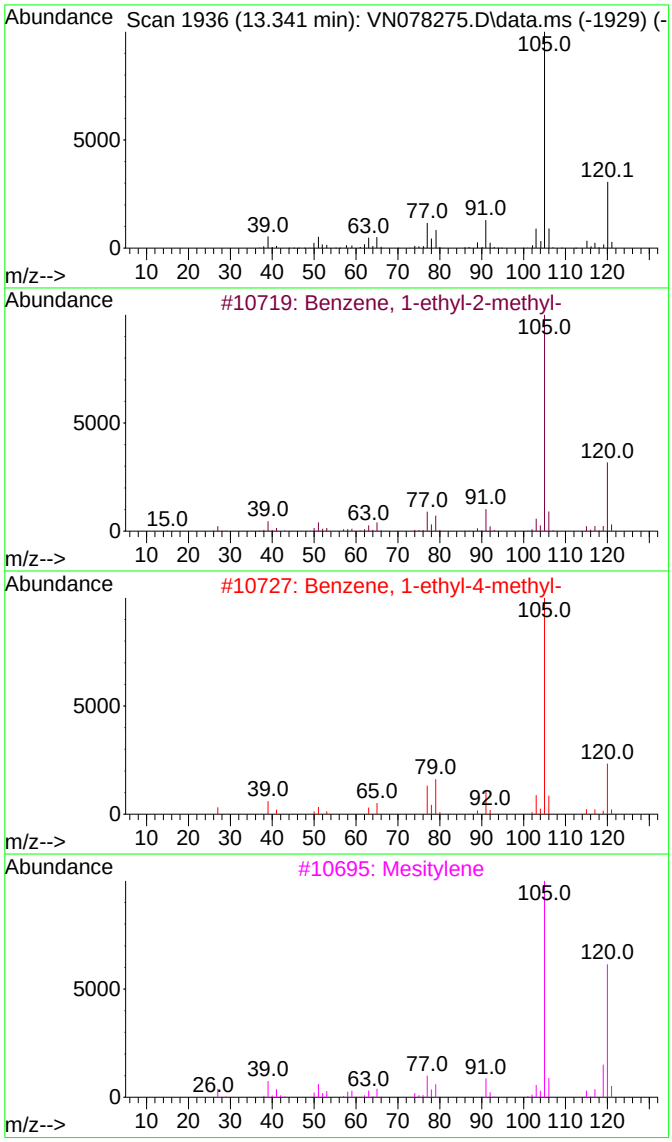
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060623W.M
Quant Title : SW846 8260

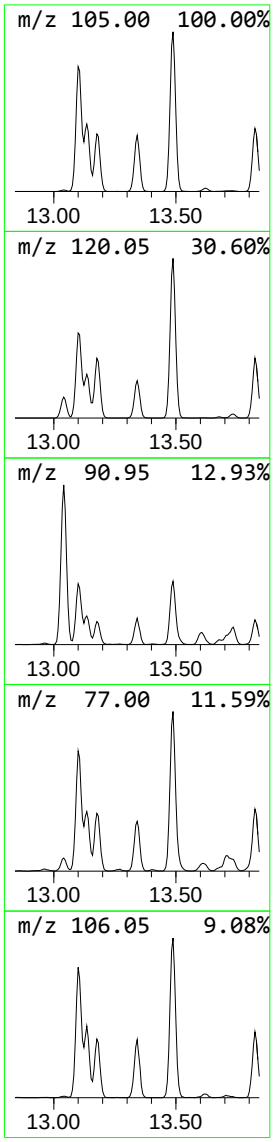
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Benzene, 1-ethyl-4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.341	31.07 ug/l	5505470	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	94
3	Mesitylene	120	C9H12	000108-67-8	90
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90
5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	90





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061923\
Data File : VN078275.D
Acq On : 19 Jun 2023 13:23
Operator : JC\MD
Sample : 03241-01
Misc : 1.13g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
30852

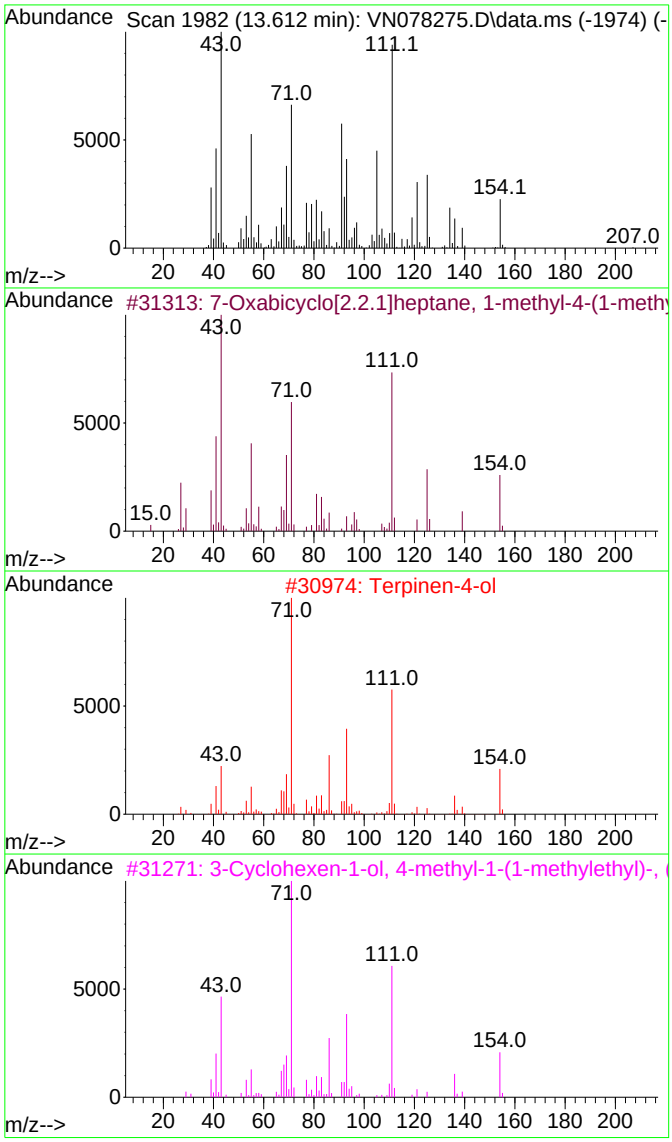
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060623W.M
Quant Title : SW846 8260

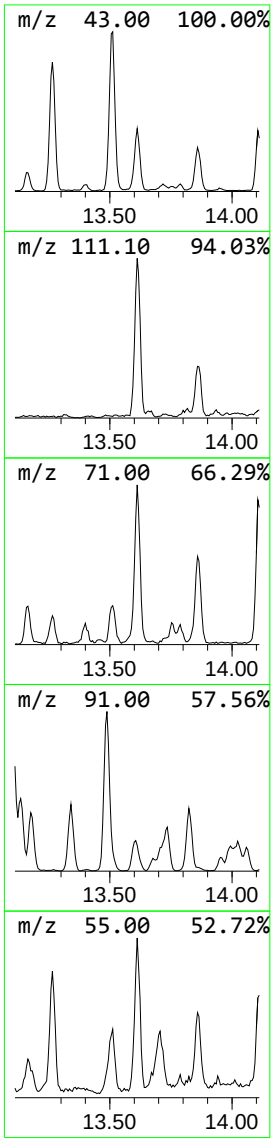
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 7-Oxabicyclo[2.2.1]heptane,... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.612	13.38 ug/l	2369880	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Oxabicyclo[2.2.1]heptane, 1-me...	154	C10H18O	000470-67-7	91
2	Terpinen-4-ol	154	C10H18O	000562-74-3	76
3	3-Cyclohexen-1-ol, 4-methyl-1-(1...	154	C10H18O	020126-76-5	76
4	4-Hepten-3-one, 2,5,6-trimethyl-	154	C10H18O	016466-21-0	35
5	1,2-Propanedione, 1-(2-thienyl)-	154	C7H6O2S	013678-69-8	27





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061923\
Data File : VN078275.D
Acq On : 19 Jun 2023 13:23
Operator : JC\MD
Sample : 03241-01
Misc : 1.13g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
30852

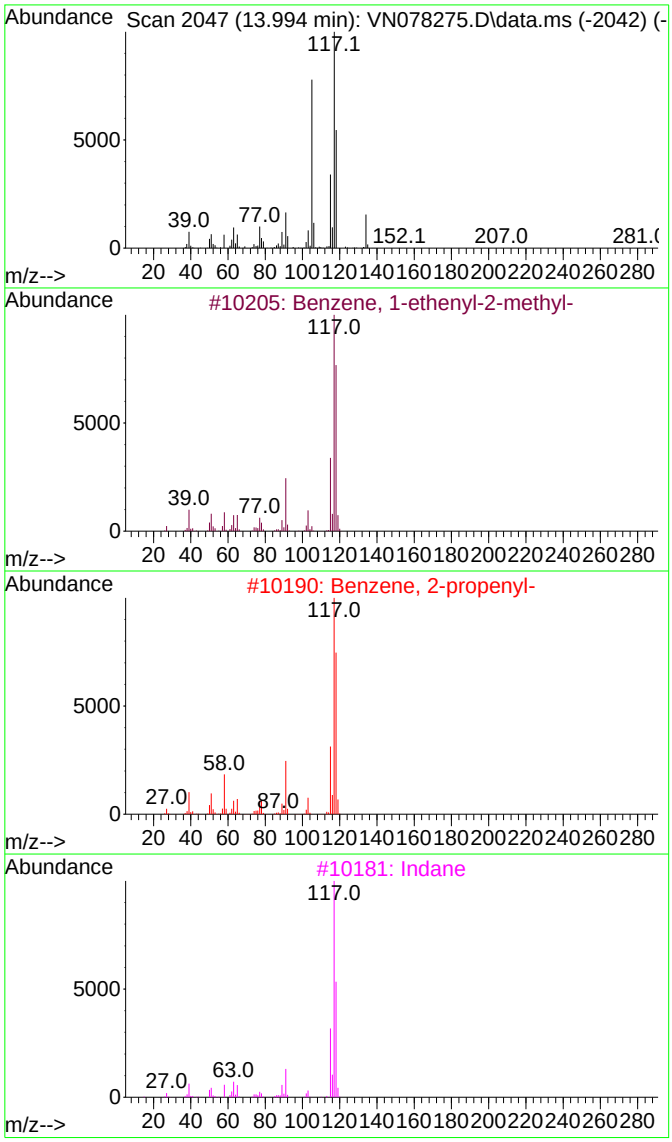
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060623W.M
Quant Title : SW846 8260

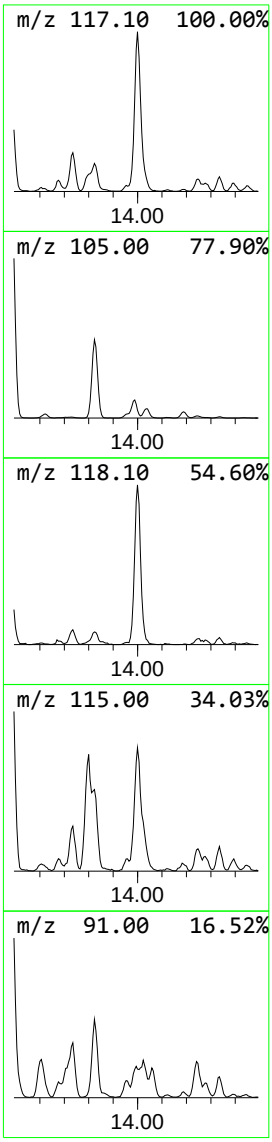
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzene, 1-ethenyl-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.994	16.51 ug/l	2925090	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	70
2	Benzene, 2-propenyl-	118	C9H10	000300-57-2	70
3	Indane	118	C9H10	000496-11-7	70
4	Benzene, cyclopropyl-	118	C9H10	000873-49-4	64
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	118	C9H10	055337-80-9	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061923\
Data File : VN078275.D
Acq On : 19 Jun 2023 13:23
Operator : JC\MD
Sample : 03241-01
Misc : 1.13g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
30852

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060623W.M
Quant Title : SW846 8260

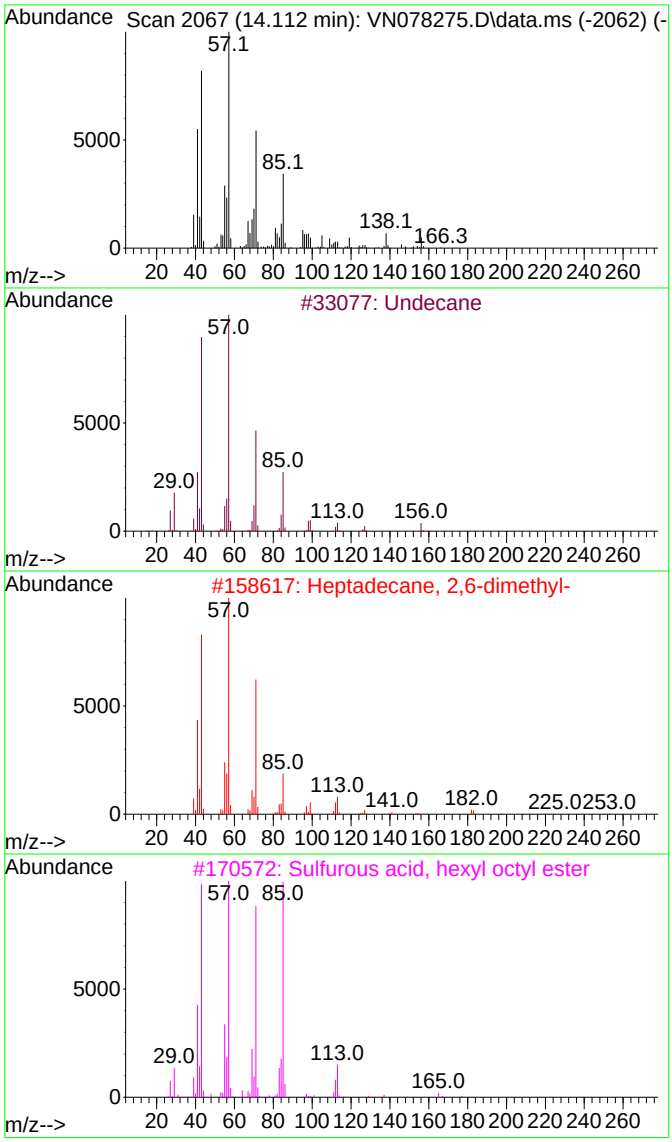
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

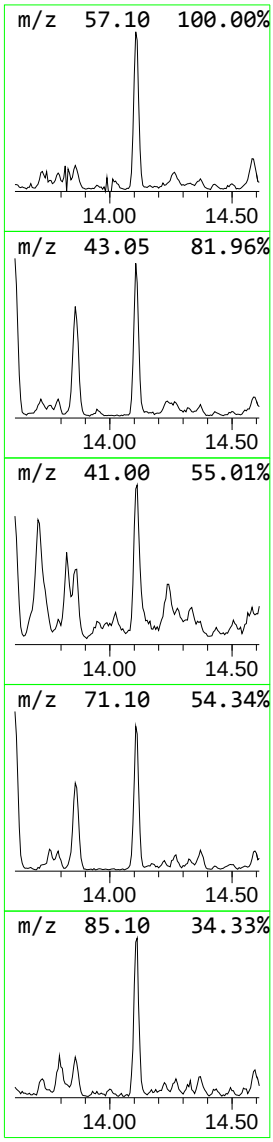
****

Peak Number 6 Undecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.112	8.13 ug/l	1439560	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane	156	C11H24	001120-21-4	74
2	Heptadecane, 2,6-dimethyl-	268	C19H40	054105-67-8	59
3	Sulfurous acid, hexyl octyl ester	278	C14H30O3S	1000309-13-0	59
4	Ether, hexyl pentyl	172	C11H24O	032357-83-8	52
5	Decane, 2,3,7-trimethyl-	184	C13H28	062238-13-5	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061923\
Data File : VN078275.D
Acq On : 19 Jun 2023 13:23
Operator : JC\MD
Sample : 03241-01
Misc : 1.13g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
30852

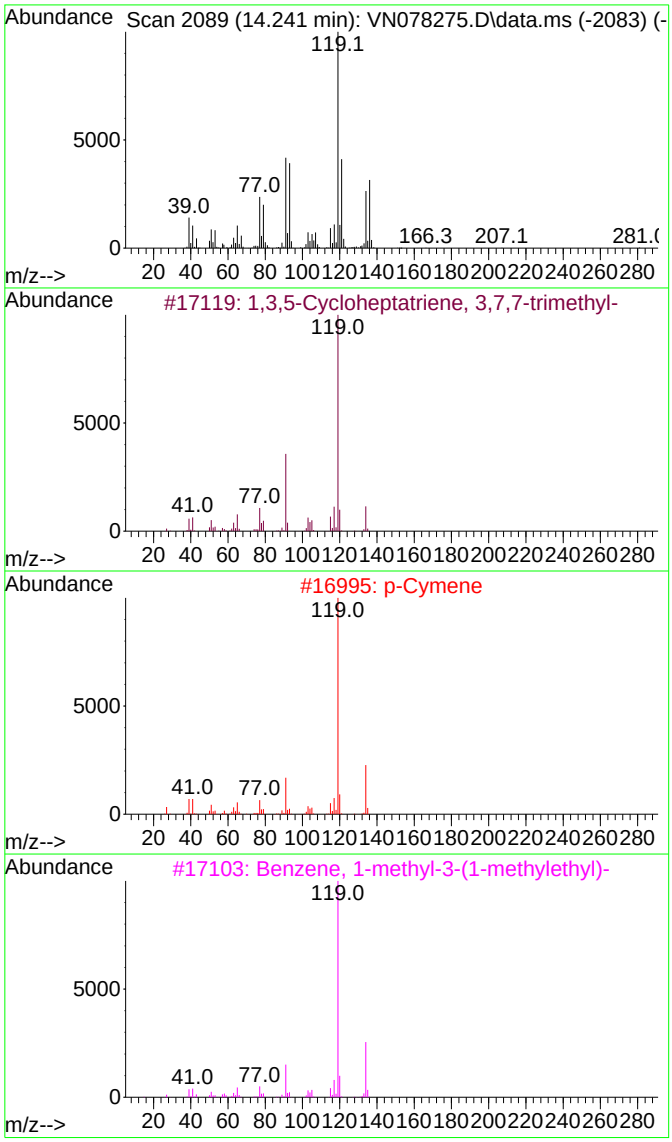
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060623W.M
Quant Title : SW846 8260

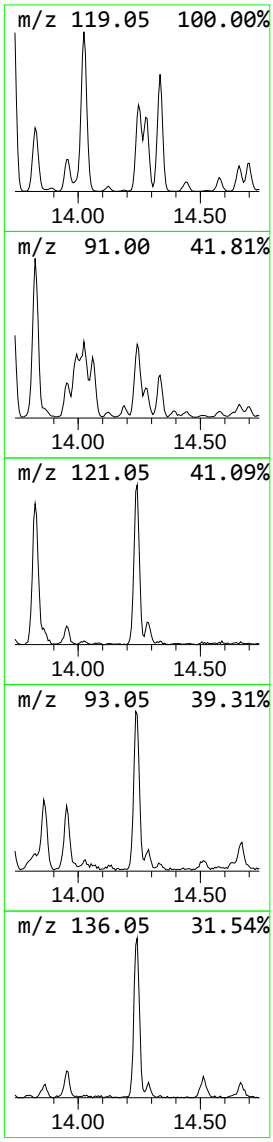
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 1,3,5-Cycloheptatriene, 3,7... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.241	11.01 ug/l	1951220	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,5-Cycloheptatriene, 3,7,7-tr...	134	C10H14	003479-89-8	91
2	p-Cymene	134	C10H14	000099-87-6	78
3	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	78
4	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	64
5	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061923\
Data File : VN078275.D
Acq On : 19 Jun 2023 13:23
Operator : JC\MD
Sample : 03241-01
Misc : 1.13g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
30852

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060623W.M
Quant Title : SW846 8260

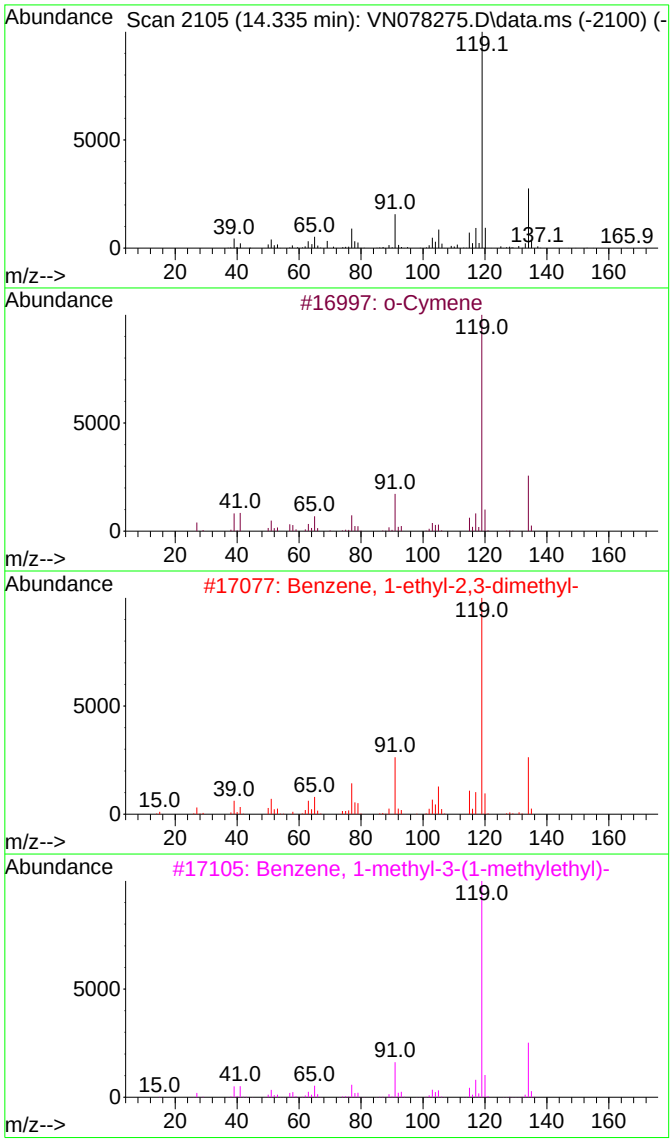
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

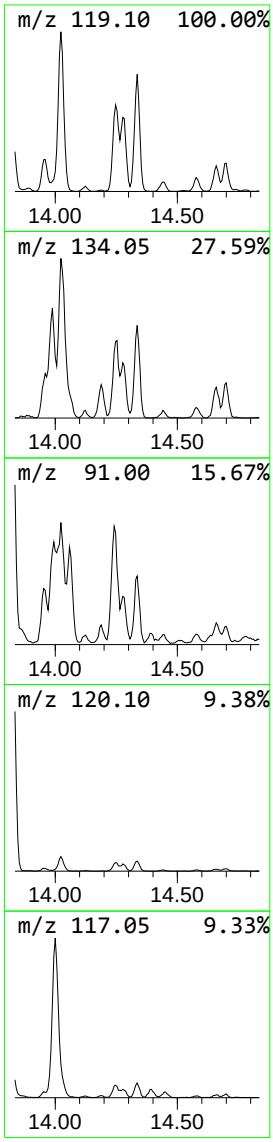
****

Peak Number 8 o-Cymene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.335	6.29 ug/l	1115130	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	o-Cymene	134	C10H14	000527-84-4	97
2	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	96
3	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	95
4	p-Cymene	134	C10H14	000099-87-6	95
5	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061923\
Data File : VN078275.D
Acq On : 19 Jun 2023 13:23
Operator : JC\MD
Sample : 03241-01
Misc : 1.13g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
30852

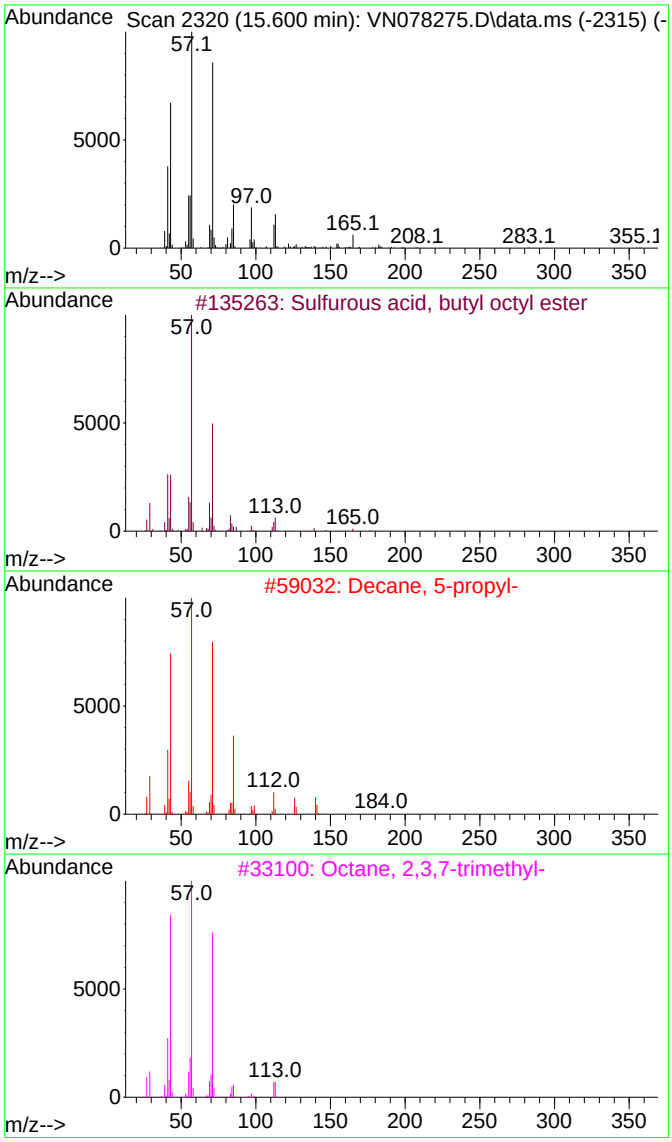
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060623W.M
Quant Title : SW846 8260

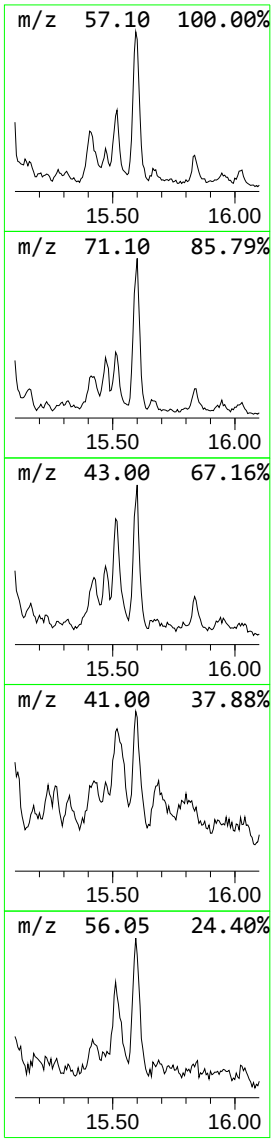
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Sulfurous acid, butyl octyl... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.600	6.45 ug/l	1142520	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, butyl octyl ester	250	C12H26O3S	1000309-17-5	64
2	Decane, 5-propyl-	184	C13H28	017312-62-8	64
3	Octane, 2,3,7-trimethyl-	156	C11H24	062016-34-6	59
4	Heptane, 3-[(ethenyloxy)methyl]-	156	C10H20O	000103-44-6	59
5	Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061923\
Data File : VN078275.D
Acq On : 19 Jun 2023 13:23
Operator : JC\MD
Sample : 03241-01
Misc : 1.13g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
30852

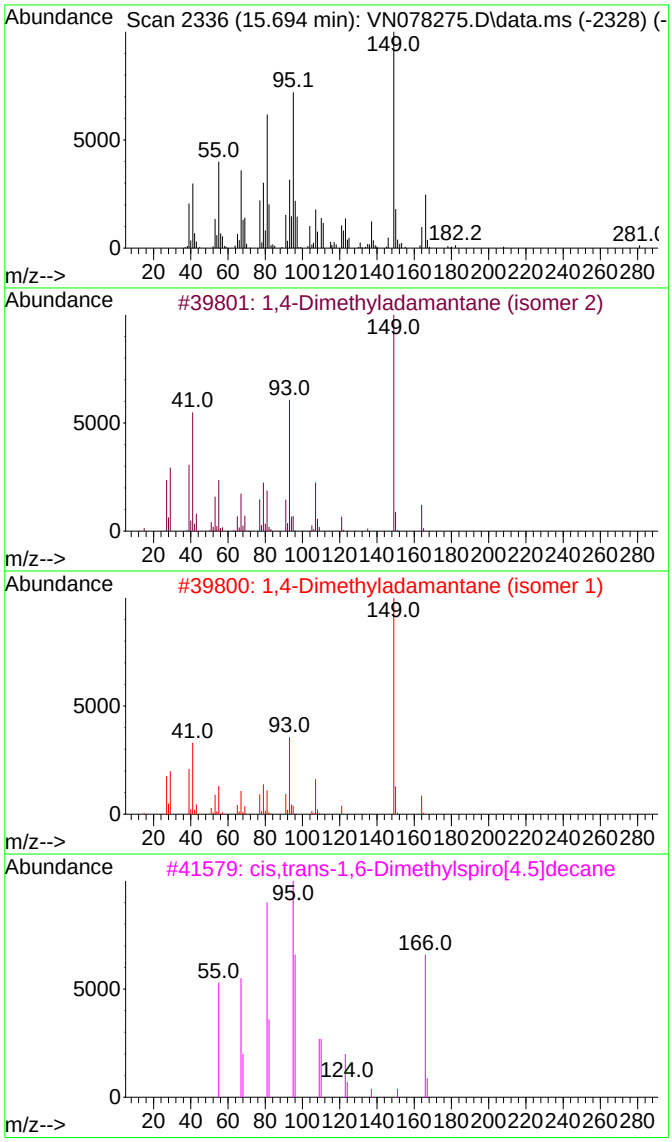
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060623W.M
Quant Title : SW846 8260

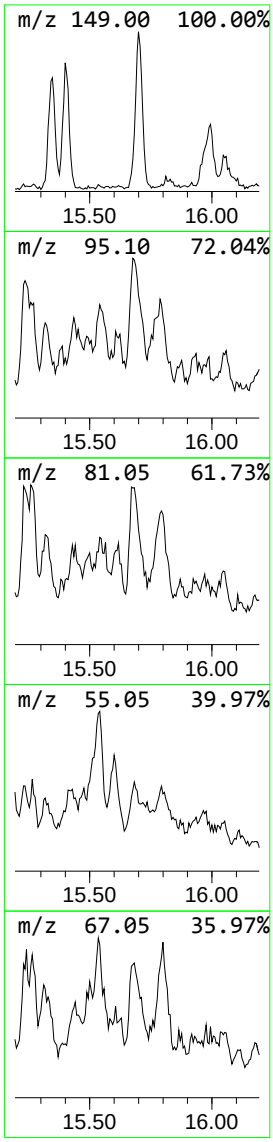
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 unknown15.694 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.694	5.99 ug/l	1060630	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Dimethyladamantane (isomer 2)	164	C12H20	1000460-67-1	43
2	1,4-Dimethyladamantane (isomer 1)	164	C12H20	1000460-67-0	38
3	cis,trans-1,6-Dimethylspiro[4.5]...	166	C12H22	1000111-72-3	35
4	5-Methylthieno[3,2-b]pyridine	149	C8H7NS	001759-29-1	35
5	2-(3-Methylbuta-1,3-dienyl)cyclo...	164	C11H16O	1000191-75-5	35





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061923\
Data File : VN078275.D
Acq On : 19 Jun 2023 13:23
Operator : JC\MD
Sample : 03241-01
Misc : 1.13g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
30852

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060623W.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...	13.100	75.3	ug/l	13334500	4	13.794	8858650	50.0
4-Heptanone, 2,...	13.265	44.4	ug/l	7868410	4	13.794	8858650	50.0
Benzene, 1-ethy...	13.341	31.1	ug/l	5505470	4	13.794	8858650	50.0
7-Oxabicyclo[2....	13.612	13.4	ug/l	2369880	4	13.794	8858650	50.0
Benzene, 1-ethe...	13.994	16.5	ug/l	2925090	4	13.794	8858650	50.0
Undecane	14.112	8.1	ug/l	1439560	4	13.794	8858650	50.0
1,3,5-Cyclohept...	14.241	11.0	ug/l	1951220	4	13.794	8858650	50.0
o-Cymene	14.335	6.3	ug/l	1115130	4	13.794	8858650	50.0
Sulfurous acid,...	15.600	6.5	ug/l	1142520	4	13.794	8858650	50.0
unknown15.694	15.694	6.0	ug/l	1060630	4	13.794	8858650	50.0