LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
Data File : VN074531.D
Acq On : 17 Sep 2022 00:30
Operator : JC\MD
Sample : N4549-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-48

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\82N091522W.M
Title : SW846 8260

Signal : TIC: VN074531.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.199	47	53	60	rBV	222527	439777	21.82%	2.325%
2	2.693	130	137	141	rBV2	71654	166533	8.26%	0.880%
3	3.763	311	319	329	rBV5	19303	49059	2.43%	0.259%
4	5.099	538	546	560	rVB2	17588	63863	3.17%	0.338%
5	5.275	560	576	592	rBV3	58770	223062	11.07%	1.179%
6	5.534	605	620	632	rBV2	100711	349859	17.36%	1.850%
7	6.410	759	769	780	rBV4	35884	114589	5.69%	0.606%
8	7.069	869	881	888	rBV4	23183	66774	3.31%	0.353%
9	7.240	898	910	917	rBV2	22549	66409	3.29%	0.351%
10	7.951	1021	1031	1036	rBV2	282930	667357	33.11%	3.528%
11	8.016	1036	1042	1054	rVB	456458	1032076	51.21%	5.456%
12	8.369	1092	1102	1113	rBV	313491	719666	35.71%	3.805%
13	8.516	1123	1127	1132	rVB6	12658	23653	1.17%	0.125%
14	8.639	1141	1148	1153	rVB8	10616	22326	1.11%	0.118%
15	8.904	1184	1193	1206	rBV	731937	1513710	75.10%	8.002%
16	9.351	1261	1269	1273	rBV6	12147	29639	1.47%	0.157%
17	9.910	1358	1364	1370	rBV5	15041	32177	1.60%	0.170%
18	10.139	1396	1403	1410	rBV5	27289	51363	2.55%	0.272%
19	10.263	1419	1424	1431	rVB6	16506	30243	1.50%	0.160%
20	10.381	1435	1444	1452	rBV	1121424	2015499	100.00%	10.655%
21	10.581	1472	1478	1485	rBV	185160	315427	15.65%	1.668%
22	10.657	1485	1491	1498	rVB	198668	337524	16.75%	1.784%
23	10.798	1510	1515	1521	rVB5	12969	21619	1.07%	0.114%
24	11.157	1572	1576	1581	rBV5	14082	26524	1.32%	0.140%
25	11.686	1658	1666	1678	rBV	1110061	1940246	96.27%	10.257%
26	11.792	1678	1684	1692	rVB10	12699	30669	1.52%	0.162%
27	11.898	1695	1702	1706	rBV5	17547	34430	1.71%	0.182%
28	12.027	1720	1724	1728	rBV4	16018	25485	1.26%	0.135%
29	12.522	1801	1808	1814	rVB	231449	376915	18.70%	1.993%
30	12.674	1826	1834	1844	rBV	912876	1516909	75.26%	8.019%
31	12.863	1860	1866	1876	rVB	190899	333433	16.54%	1.763%
32	13.163	1911	1917	1924	rVB2	34994	55420	2.75%	0.293%
33	13.439	1956	1964	1971	rVB5	39747	93370	4.63%	0.494%
34	13.616	1987	1994	2006	rVV	1091564	1788859	88.76%	9.457%
35	13.716	2006	2011	2016	rVB2	34262	53140	2.64%	0.281%
36	13.780	2016	2022	2023	rBV2	99809	129701	6.44%	0.686%

LSC Area Percent Report

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Sample : N4549-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MW-48

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\82N091522W.M
Title : SW846 8260

37	13.816	2023	2028	2035	rVB	855105	1399041	69.41%	7.396%
38	13.945	2044	2050	2057	rBV2	56174	90964	4.51%	0.481%
39	14.092	2069	2075	2080	rBV2	26047	44085	2.19%	0.233%
40	14.157	2080	2086	2092	rBV	136832	217472	10.79%	1.150%
41	14.221	2092	2097	2100	rBV3	43118	70348	3.49%	0.372%
42	14.268	2100	2105	2112	rVV	288800	481031	23.87%	2.543%
43	14.410	2124	2129	2134	rBV3	29216	50767	2.52%	0.268%
44	14.480	2134	2141	2148	rVB	267061	432427	21.46%	2.286%
45	14.704	2175	2179	2183	rVB3	25401	35530	1.76%	0.188%
46	14.757	2183	2188	2194	rBV4	38868	65086	3.23%	0.344%
47	14.868	2200	2207	2213	rBV2	173840	363276	18.02%	1.920%
48	14.939	2213	2219	2224	rVB7	27935	51538	2.56%	0.272%
49	15.133	2244	2252	2257	rBV5	48856	104255	5.17%	0.551%
50	15.239	2263	2270	2277	rVB10	30507	80648	4.00%	0.426%
51	15.498	2308	2314	2320	rBV	49923	84524	4.19%	0.447%
52	15.574	2320	2327	2339	rVB2	59251	139992	6.95%	0.740%
53	15.739	2346	2355	2361	rBV9	16344	38213	1.90%	0.202%
54	15.821	2363	2369	2373	rVB8	12079	27536	1.37%	0.146%
55	16.033	2400	2405	2414	rBV6	14344	39576	1.96%	0.209%
56	16.262	2439	2444	2450	rVB9	14607	31653	1.57%	0.167%
57	16.474	2474	2480	2485	rVB3	24374	51592	2.56%	0.273%
58	16.557	2485	2494	2501	rBV3	7667	20288	1.01%	0.107%
59	16.739	2516	2525	2533	rBV2	99227	238817	11.85%	1.263%

Sum of corrected areas: 18915964

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ClientSampleId :
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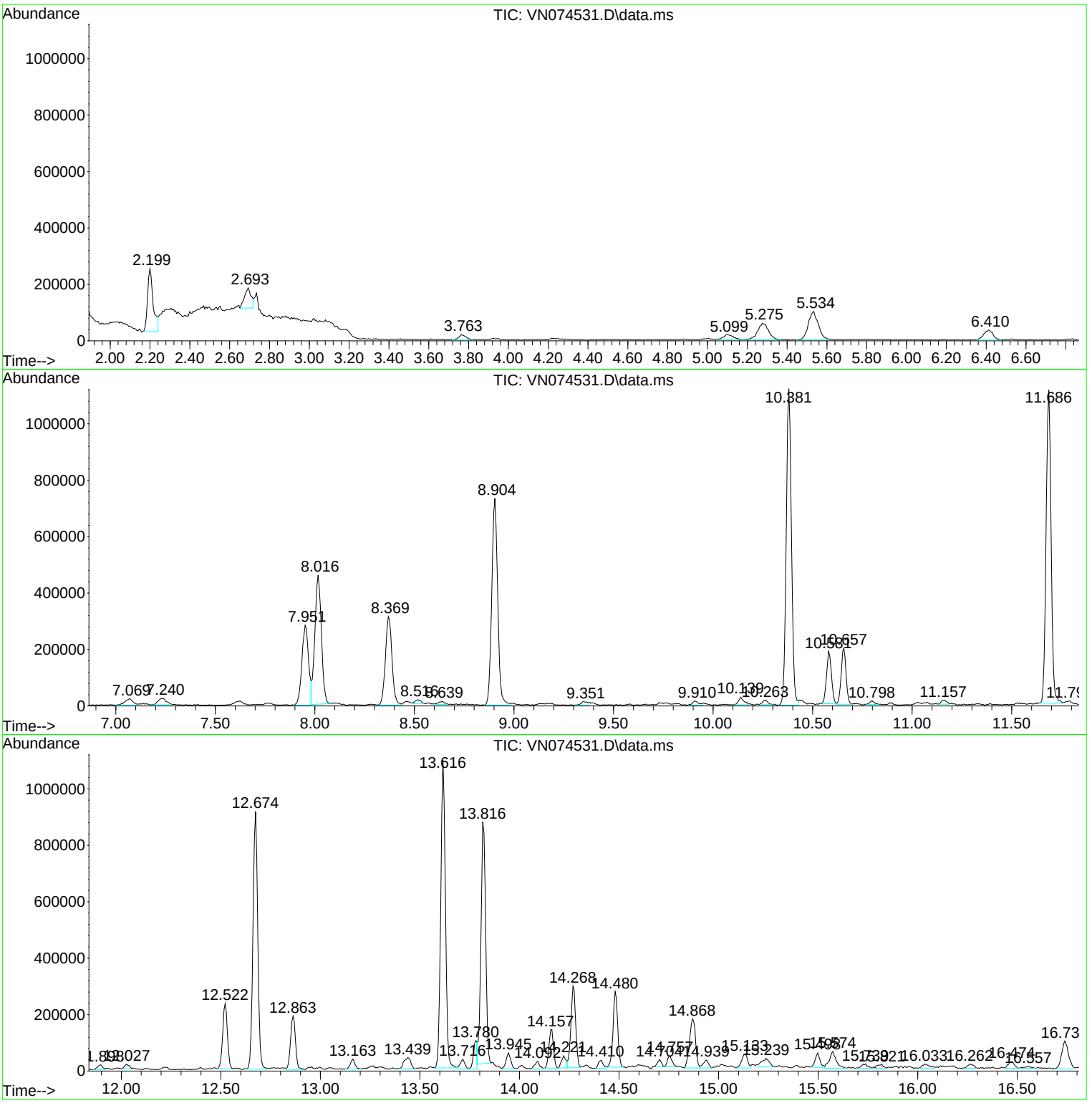
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

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



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Data File : VN074531.D
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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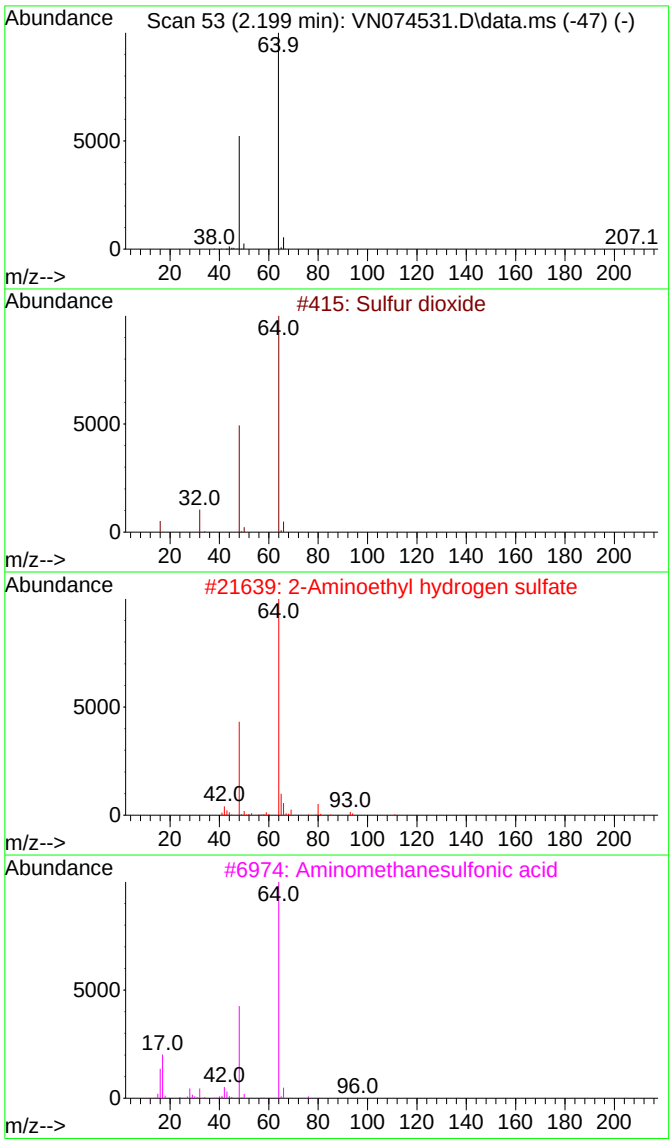
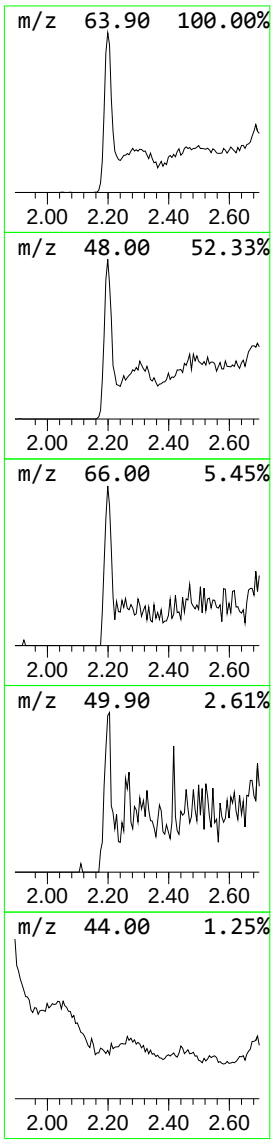
****
Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.199	21.31 ug/l	439777	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	90
2	2-Aminoethyl hydrogen sulfate	141	C2H7NO4S	000926-39-6	74
3	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4	Thiosulfuric acid (H2S2O3), S-(2...	320	C11H16N2O3S3	040284-00-2	9
5	2-Benzimidazolyl methane thiosul...	244	C8H8N2O3S2	1010256-39-2	9





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Data File : VN074531.D
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ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-48

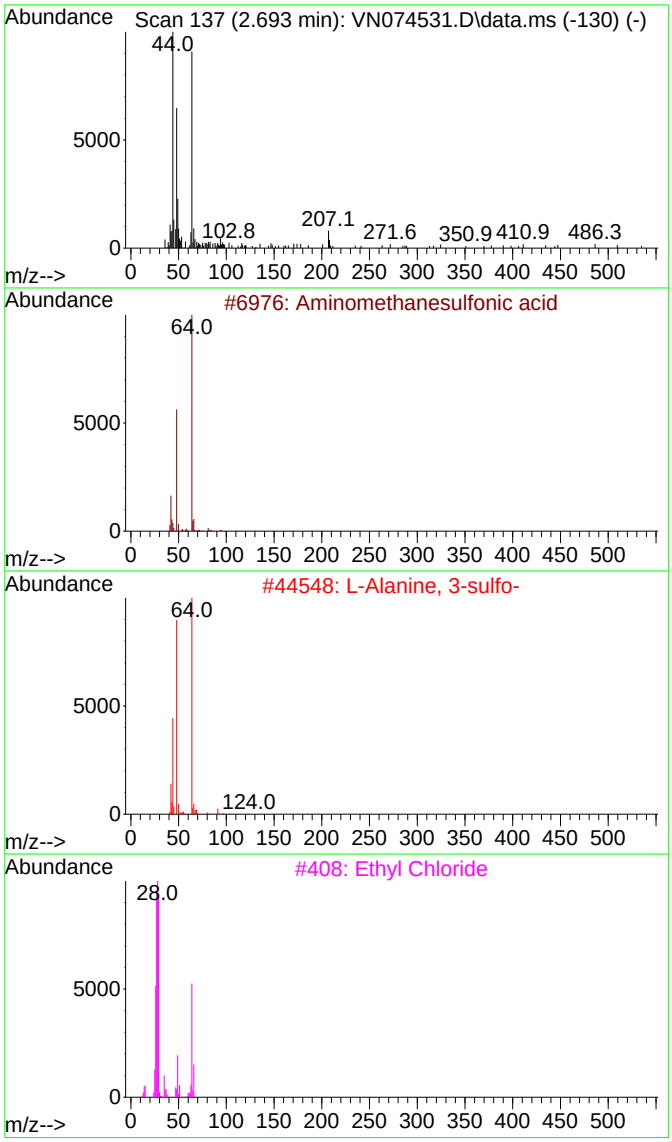
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

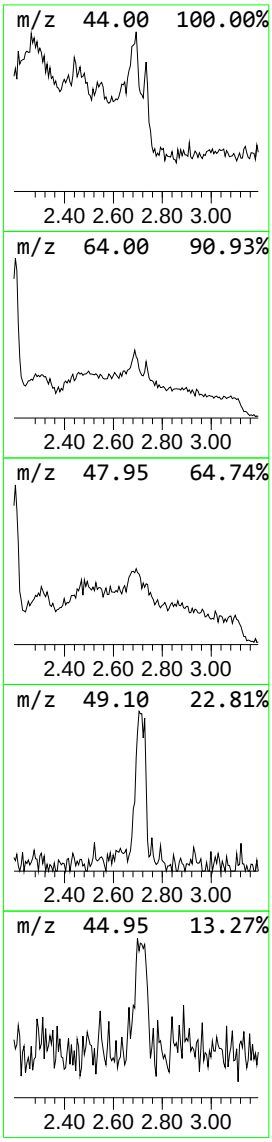
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Aminomethanesulfonic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.693	8.07 ug/l	166533	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	50
2	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	45
3	Ethyl Chloride	64	C2H5Cl	000075-00-3	45
4	Dihydropyrimidine-2-methyl thios...	208	C5H8N2O3S2	1000256-28-8	40
5	Sulfur dioxide	64	O2S	007446-09-5	40





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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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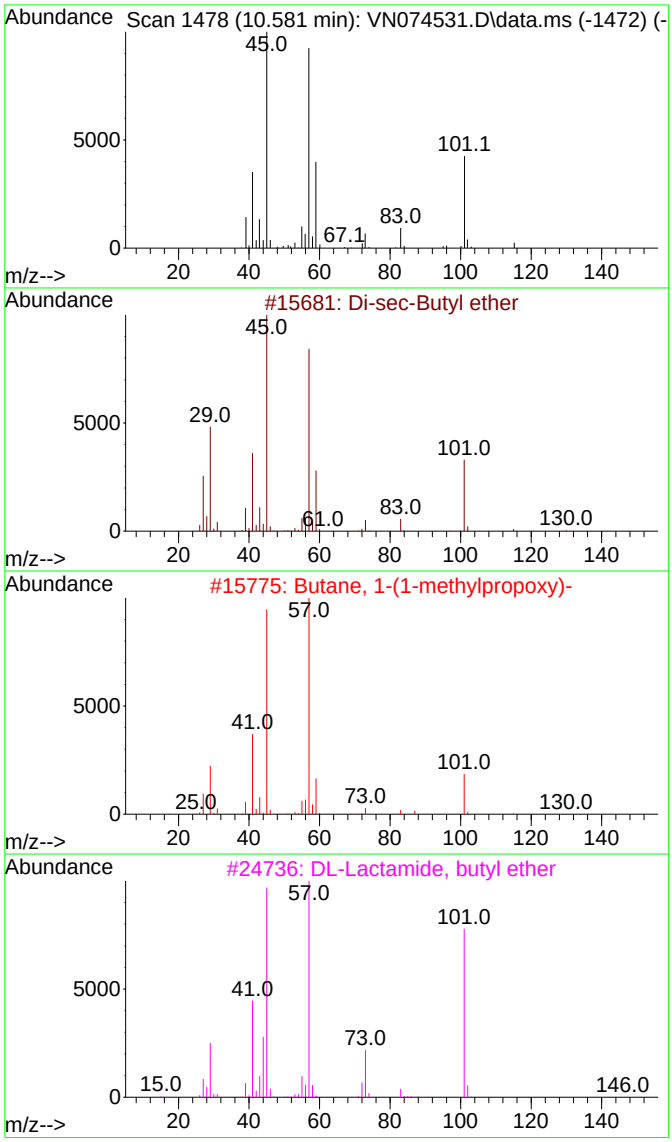
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

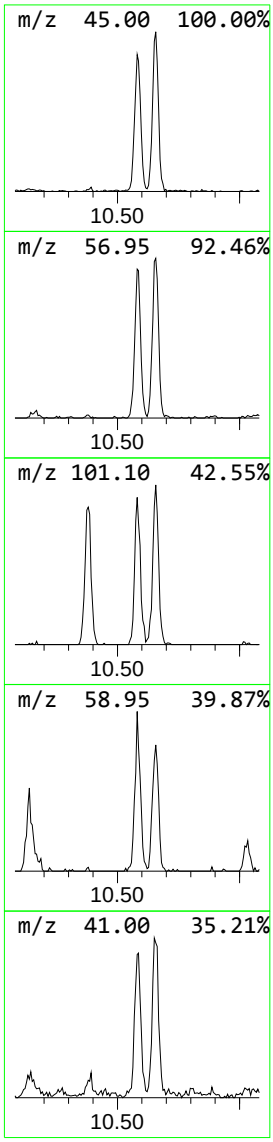
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Di-sec-Butyl ether Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.581	8.13 ug/l	315427	Chlorobenzene-d5	11.686

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Di-sec-Butyl ether	130	C8H18O	006863-58-7	90
2	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	47
3	DL-Lactamide, butyl ether	145	C7H15NO2	1000452-56-5	42
4	1-Octene, 3-(methoxymethoxy)-	172	C10H20O2	088738-34-5	38
5	2-Hydroxy-3-pentanone	102	C5H10O2	005704-20-1	36





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ALS Vial : 37 Sample Multiplier: 1

Instrument :
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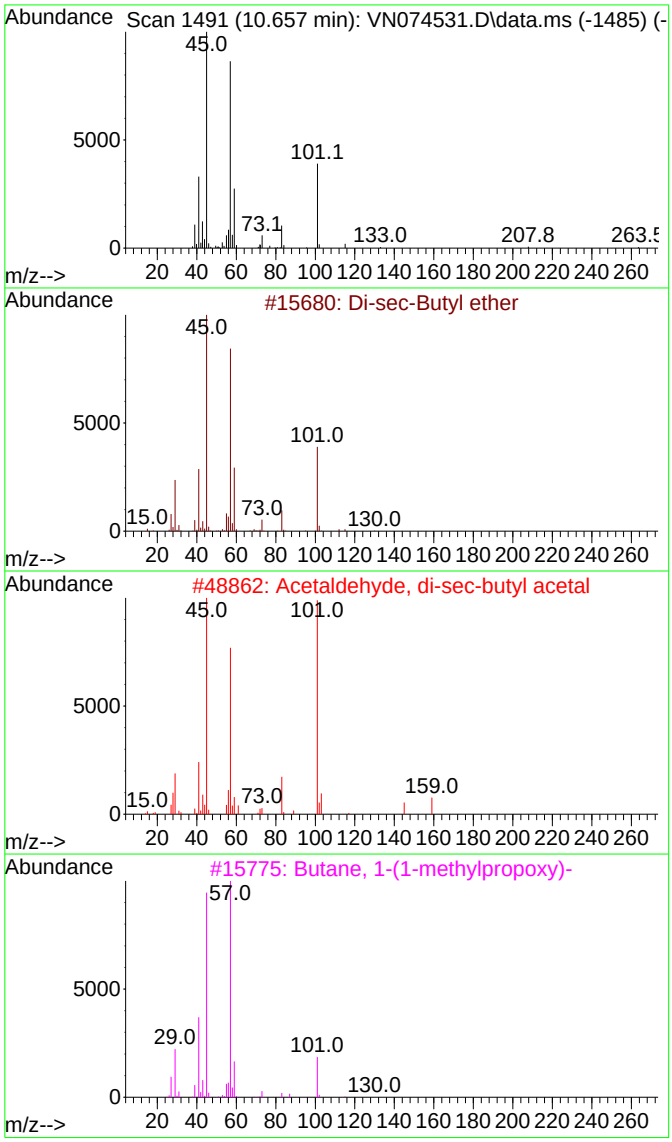
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

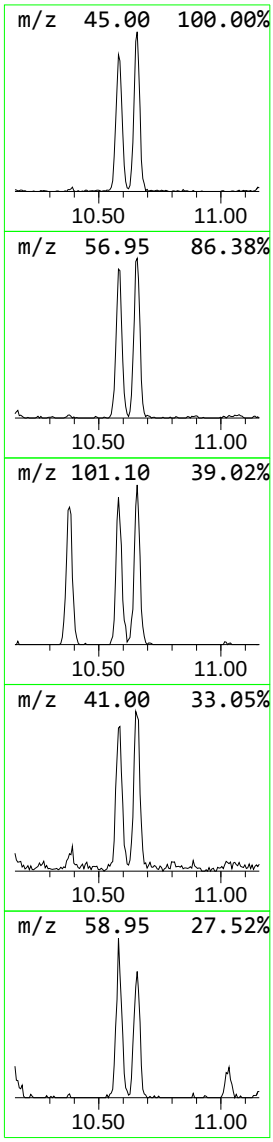
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Acetaldehyde, di-sec-butyl ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.657	8.70 ug/l	337524	Chlorobenzene-d5	11.686

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Di-sec-Butyl ether	130	C8H18O	006863-58-7	90
2	Acetaldehyde, di-sec-butyl acetal	174	C10H22O2	005314-41-0	72
3	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	56
4	Formic acid, 1-methylpropyl ester	102	C5H10O2	000589-40-2	47
5	Butane, 1,1'-[ethylidenebis(oxy)...	174	C10H22O2	000871-22-7	45





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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
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TIC Library : C:\Database\NIST20.L
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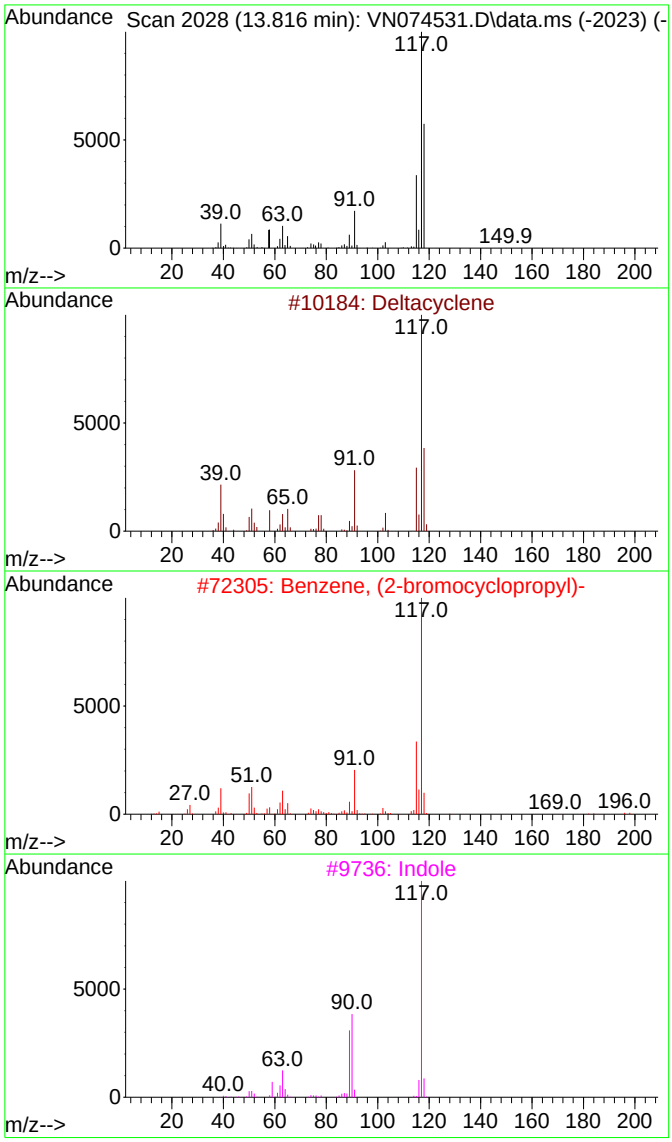
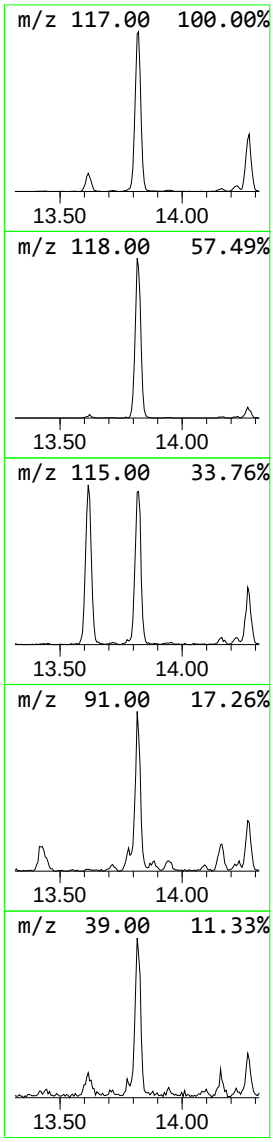
****
Peak Number 5 Benzene, (2-bromocyclopropyl)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.816	39.10 ug/l	1399040	1,4-Dichlorobenzene-d4	13.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Deltacyclene	118	C9H10	007785-10-6	59
2	Benzene, (2-bromocyclopropyl)-	196	C9H9Br	036617-02-4	50
3	Indole	117	C8H7N	000120-72-9	50
4	4-Ethynylaniline	117	C8H7N	014235-81-5	47
5	Indolizine	117	C8H7N	000274-40-8	47





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Instrument :
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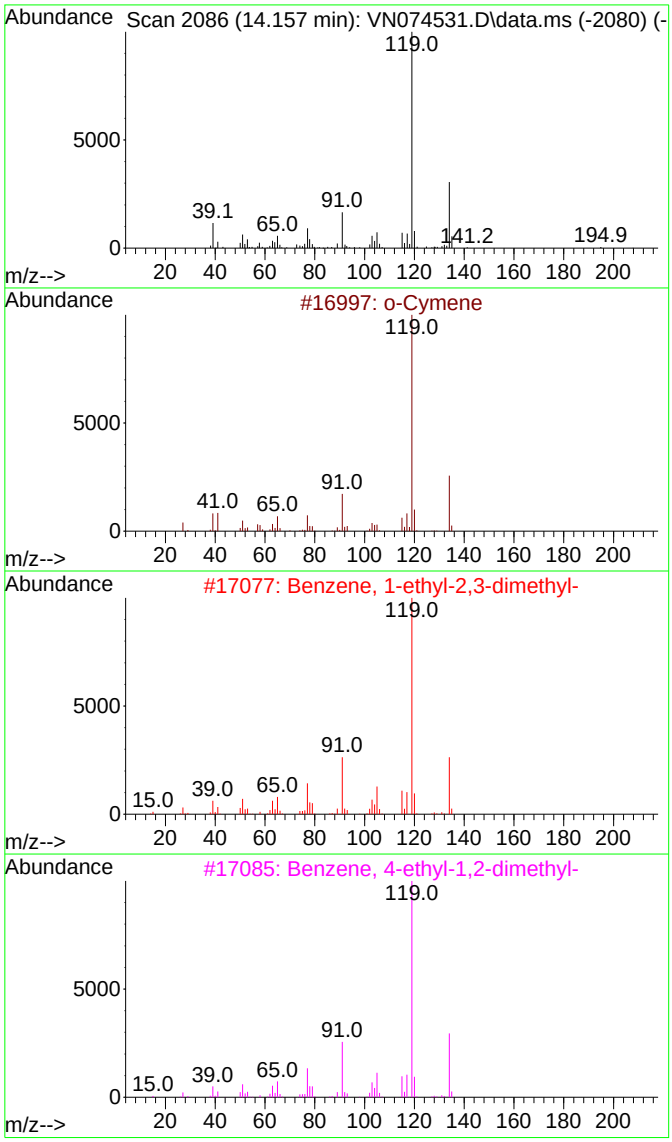
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

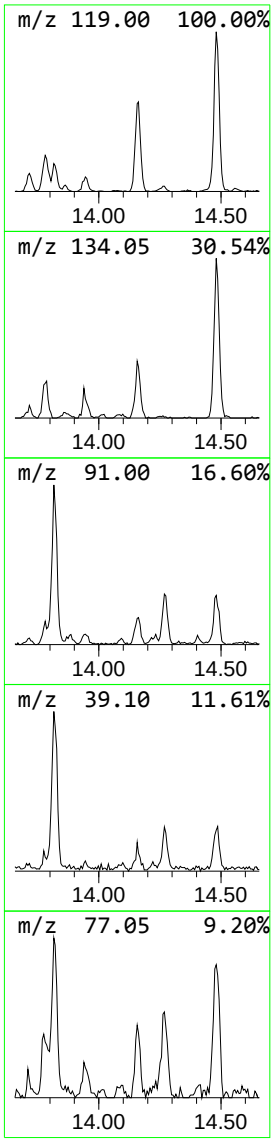
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 o-Cymene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.157	6.08 ug/l	217472	1,4-Dichlorobenzene-d4	13.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	o-Cymene	134	C10H14	000527-84-4	95
2	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	94
3	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	94
4	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	94
5	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	91





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Instrument :
MSVOA_N
ClientSampleId :
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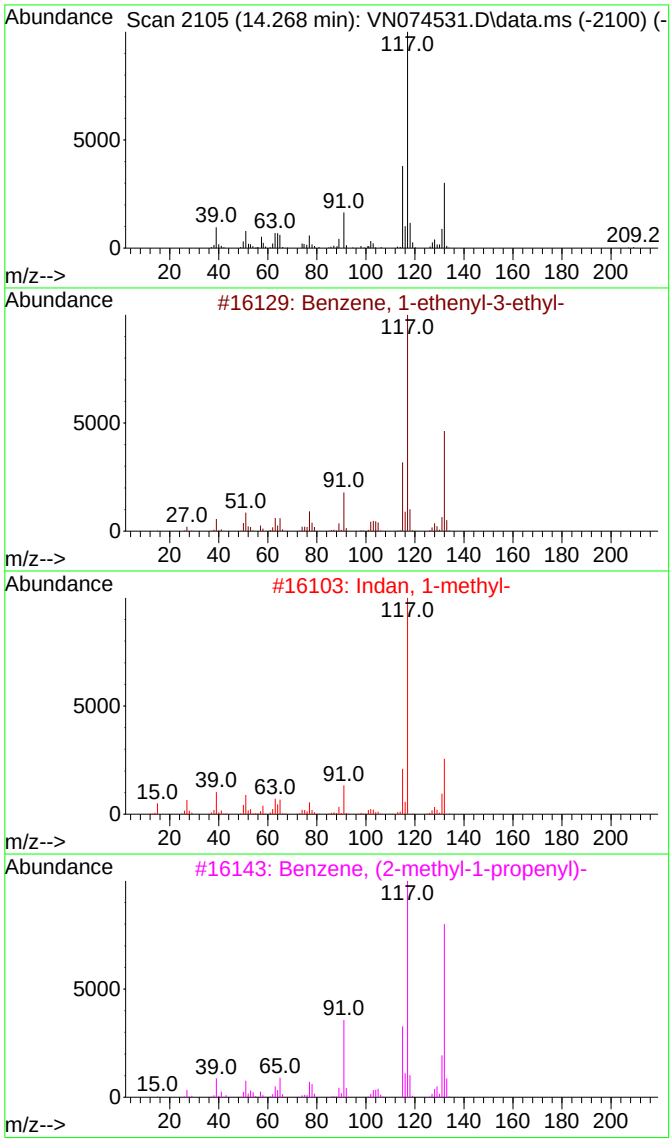
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

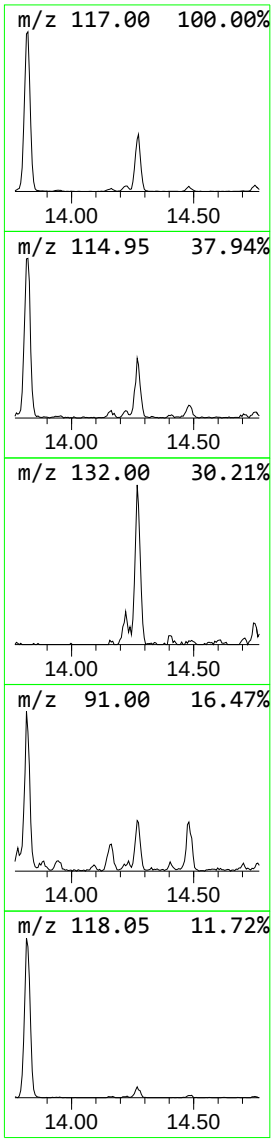
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, 1-ethenyl-3-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.269	13.45 ug/l	481031	1,4-Dichlorobenzene-d4	13.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	91
2	Indan, 1-methyl-	132	C10H12	000767-58-8	91
3	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	86
4	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	86
5	1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	83





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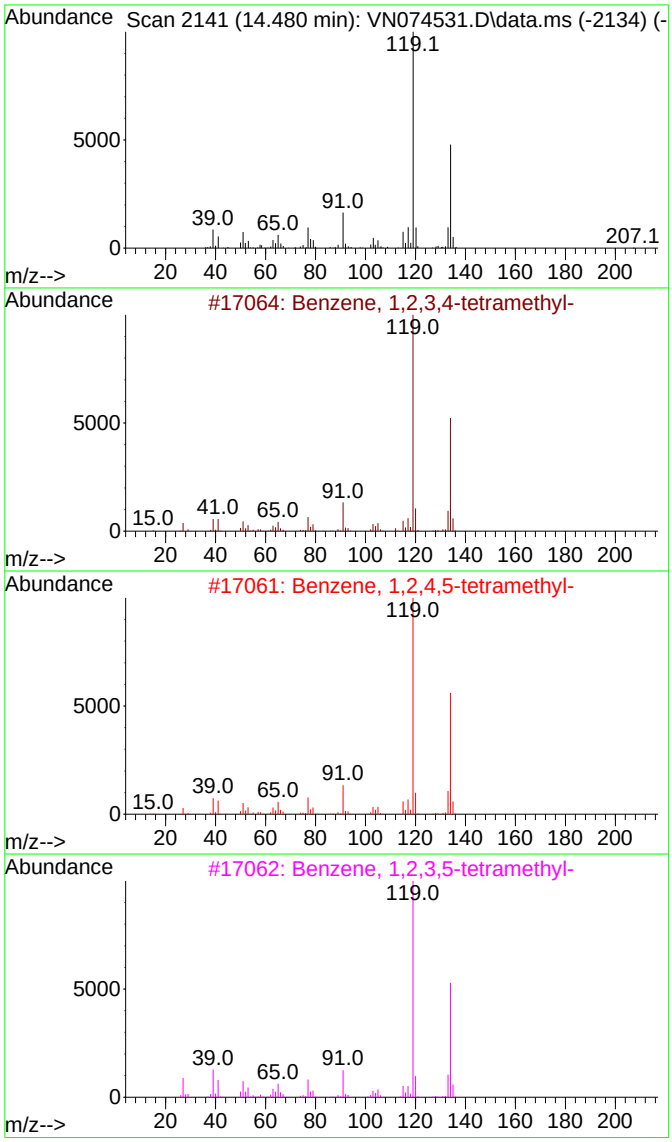
Quant Title : SW846 8260

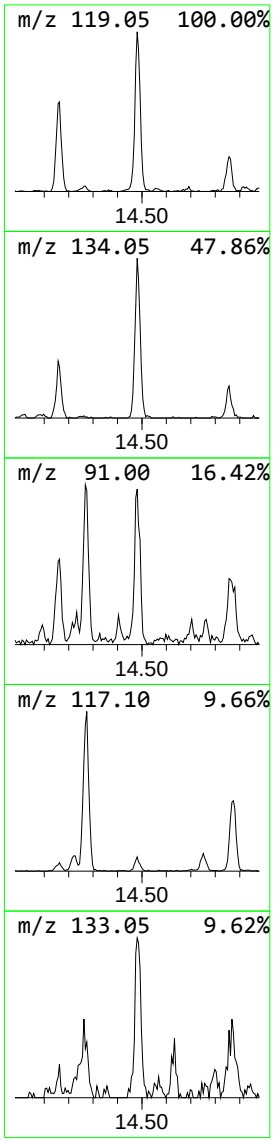
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.480	12.09 ug/l	432427	1,4-Dichlorobenzene-d4	13.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
2	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	95
3	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	94
4	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	93
5	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
Data File : VN074531.D
Acq On : 17 Sep 2022 00:30
Operator : JC\MD
Sample : N4549-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-48

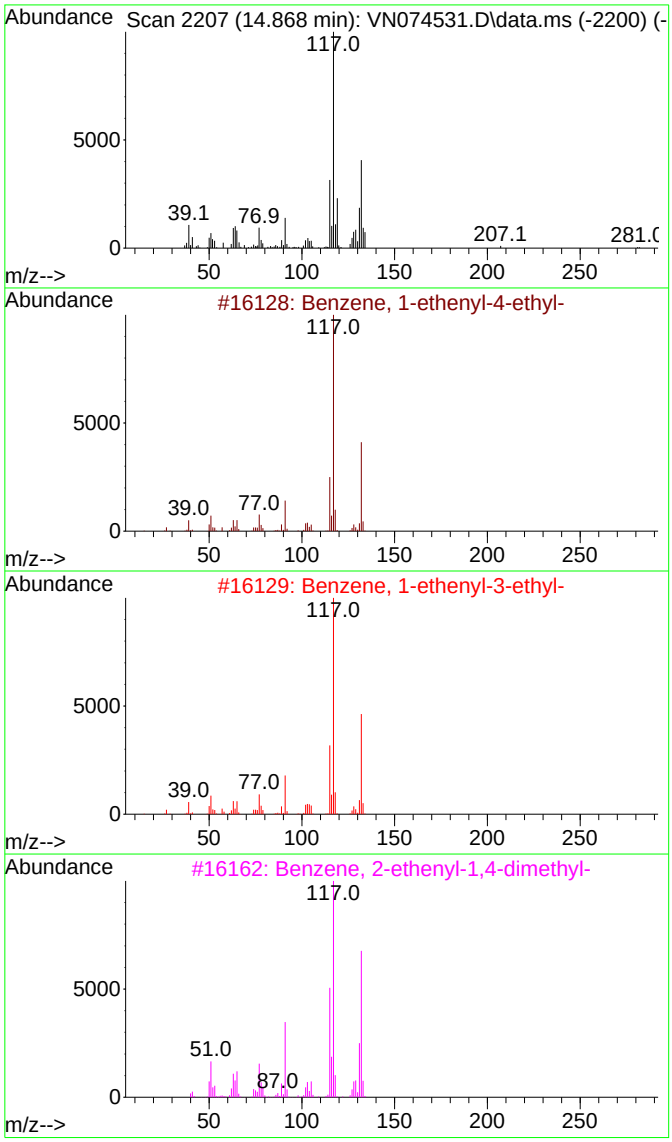
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

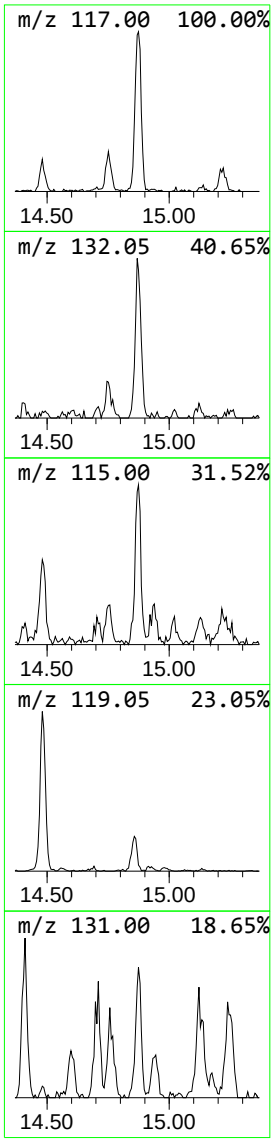
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 1-ethenyl-4-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.868	10.15 ug/l	363276	1,4-Dichlorobenzene-d4	13.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
2	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	93
3	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	92
4	1-Phenyl-1-butene	132	C10H12	000824-90-8	83
5	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000767-99-7	80





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
Data File : VN074531.D
Acq On : 17 Sep 2022 00:30
Operator : JC\MD
Sample : N4549-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-48

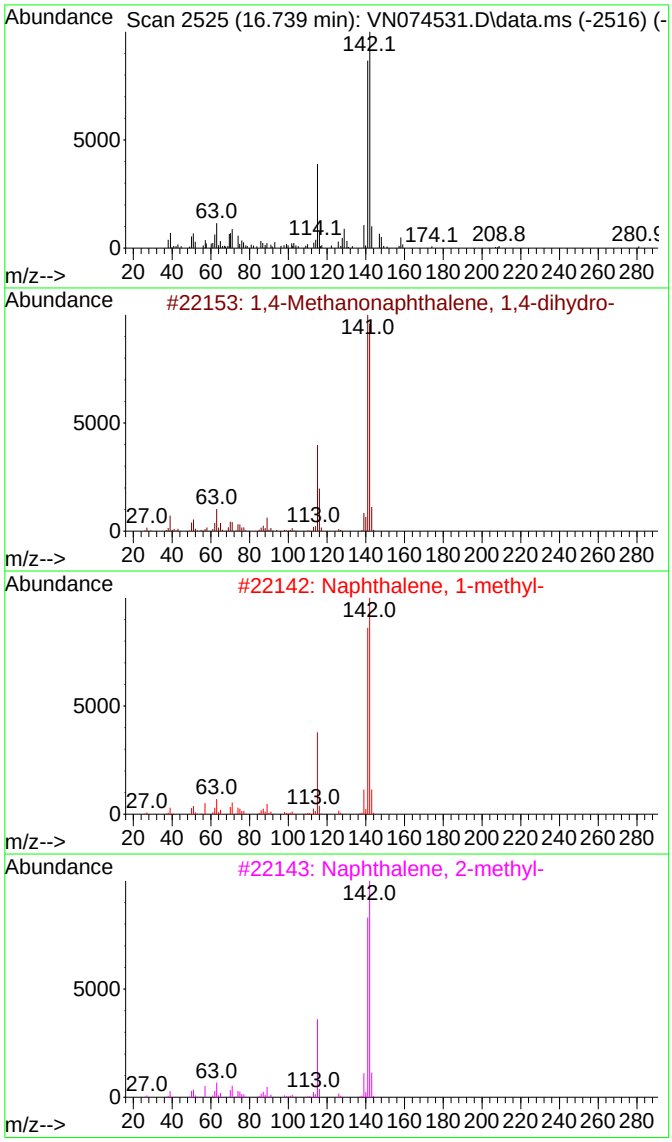
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

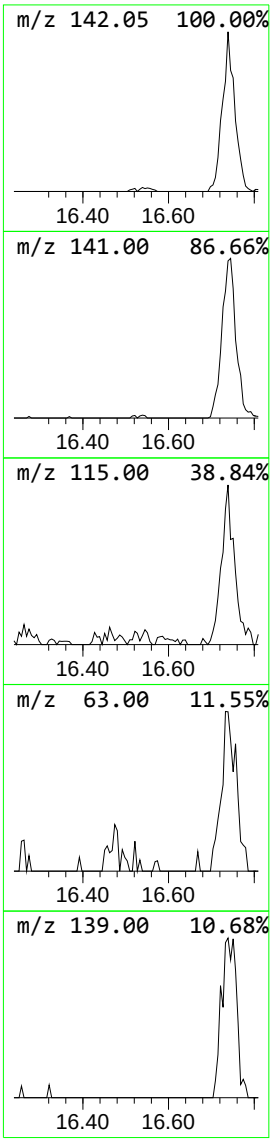
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 1,4-Methanonaphthalene, 1,4... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.739	6.68 ug/l	238817	1,4-Dichlorobenzene-d4	13.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	90
2	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	90
3	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	90
4	Benzocycloheptatriene	142	C11H10	000264-09-5	87
5	Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	59





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
Data File : VN074531.D
Acq On : 17 Sep 2022 00:30
Operator : JC\MD
Sample : N4549-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-48

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.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
Sulfur dioxide	2.199	21.3	ug/l	439777	1	8.016	1032080	50.0
Aminomethanesul...	2.693	8.1	ug/l	166533	1	8.016	1032080	50.0
Di-sec-Butyl ether	10.581	8.1	ug/l	315427	3	11.686	1940250	50.0
Acetaldehyde, d...	10.657	8.7	ug/l	337524	3	11.686	1940250	50.0
Benzene, (2-bro...	13.816	39.1	ug/l	1399040	4	13.616	1788860	50.0
o-Cymene	14.157	6.1	ug/l	217472	4	13.616	1788860	50.0
Benzene, 1-ethe...	14.269	13.4	ug/l	481031	4	13.616	1788860	50.0
Benzene, 1,2,3,...	14.480	12.1	ug/l	432427	4	13.616	1788860	50.0
Benzene, 1-ethe...	14.868	10.2	ug/l	363276	4	13.616	1788860	50.0
1,4-Methanonaph...	16.739	6.7	ug/l	238817	4	13.616	1788860	50.0