LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
Data File : VN074546.D
Acq On : 17 Sep 2022 06:34
Operator : JC\MD
Sample : N4549-18
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 52 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-62

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: VN074546.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.198	47	53	59	rBV	267626	494921	24.90%	3.398%
2	2.693	132	137	139	rBV2	62763	109347	5.50%	0.751%
3	7.228	901	908	919	rBV2	14928	37444	1.88%	0.257%
4	7.951	1021	1031	1036	rBV2	277751	645487	32.48%	4.431%
5	8.016	1036	1042	1051	rVB2	401124	912798	45.93%	6.266%
6	8.369	1093	1102	1112	rBV2	312764	717237	36.09%	4.924%
7	8.904	1178	1193	1205	rBV	683953	1387762	69.82%	9.527%
8	10.380	1436	1444	1453	rBV	1107051	1987490	100.00%	13.644%
9	10.580	1471	1478	1485	rVB7	12278	26321	1.32%	0.181%
10	11.686	1658	1666	1674	rBV	1050790	1842150	92.69%	12.646%
11	12.521	1802	1808	1814	rBV	62063	96574	4.86%	0.663%
12	12.674	1827	1834	1844	rBV	874313	1468981	73.91%	10.084%
13	12.862	1861	1866	1872	rVB	70716	107383	5.40%	0.737%
14	13.162	1910	1917	1925	rBV2	22156	39432	1.98%	0.271%
15	13.427	1956	1962	1970	rBV5	23146	56088	2.82%	0.385%
16	13.615	1986	1994	2007	rBV	1062882	1799095	90.52%	12.350%
17	13.715	2007	2011	2016	rVB3	17166	26621	1.34%	0.183%
18	13.780	2016	2022	2024	rBV2	62105	100872	5.08%	0.692%
19	13.815	2024	2028	2034	rVV	449341	742306	37.35%	5.096%
20	13.862	2034	2036	2041	rVV3	41892	54400	2.74%	0.373%
21	13.945	2044	2050	2056	rVB3	36658	59906	3.01%	0.411%
22	14.092	2069	2075	2081	rBV3	47992	84239	4.24%	0.578%
23	14.157	2081	2086	2092	rVV2	64657	106099	5.34%	0.728%
24	14.221	2092	2097	2099	rVV3	37397	50516	2.54%	0.347%
25	14.268	2100	2105	2111	rVV	215641	349311	17.58%	2.398%
26	14.345	2111	2118	2122	rVV8	12140	28777	1.45%	0.198%
27	14.409	2123	2129	2133	rVV2	18449	31470	1.58%	0.216%
28	14.480	2135	2141	2148	rVB	156297	250934	12.63%	1.723%
29	14.704	2169	2179	2183	rBV4	25865	44541	2.24%	0.306%
30	14.751	2183	2187	2194	rVB4	25456	48797	2.46%	0.335%
31	14.874	2200	2208	2213	rBV	183969	315543	15.88%	2.166%
32	14.939	2215	2219	2224	rVB7	17923	31769	1.60%	0.218%
33	15.021	2229	2233	2238	rVB6	17800	27275	1.37%	0.187%
34	15.139	2245	2253	2257	rBV3	38601	75280	3.79%	0.517%
35	15.227	2262	2268	2269	rBV2	14230	21805	1.10%	0.150%
36	15.439	2300	2304	2309	rVV5	13974	23754	1.20%	0.163%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
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ALS Vial : 52 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-62

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\82N091522W.M
Title : SW846 8260

37	15.498	2309	2314	2318	rVV3	37514	66850	3.36%	0.459%
38	15.580	2319	2328	2337	rVB4	42264	121477	6.11%	0.834%
39	15.815	2362	2368	2372	rBV8	10858	21950	1.10%	0.151%
40	16.039	2400	2406	2413	rBV6	11857	27874	1.40%	0.191%
41	16.121	2415	2420	2426	rVB6	12721	24059	1.21%	0.165%
42	16.262	2439	2444	2451	rBV7	9655	20533	1.03%	0.141%
43	16.745	2517	2526	2532	rBV5	31966	81642	4.11%	0.560%

Sum of corrected areas: 14567110

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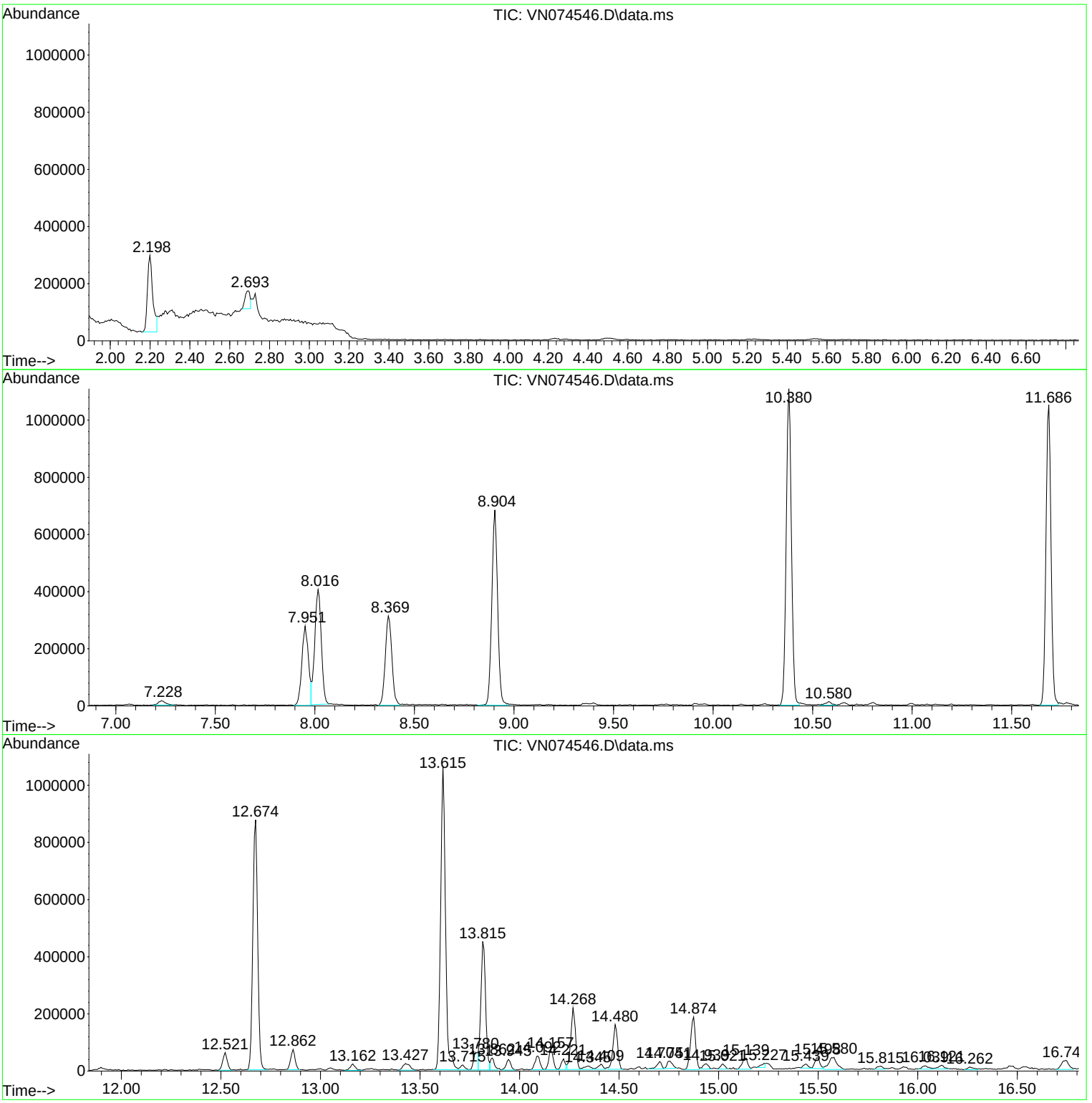
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

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



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

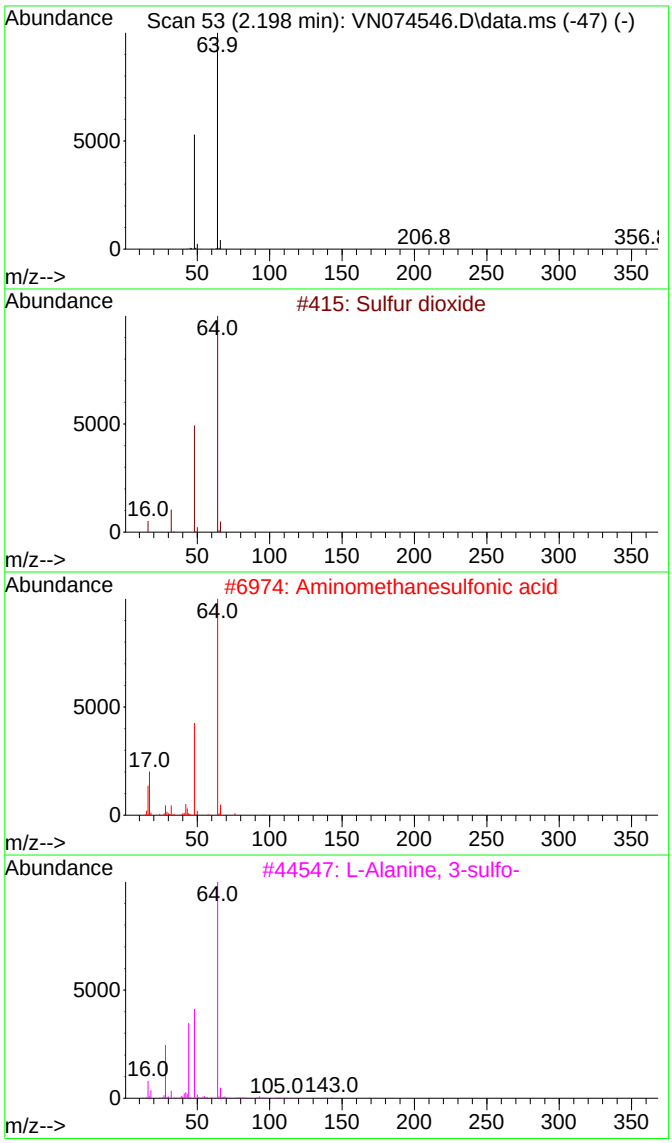
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

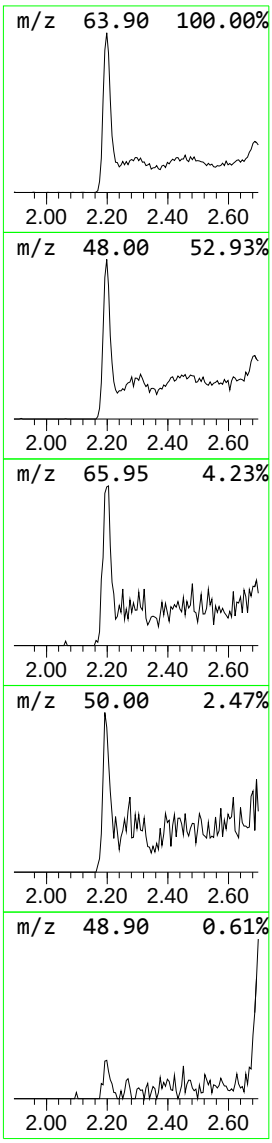
****

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.198	27.11 ug/l	494921	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	90
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5	Ethyl Chloride	64	C2H5Cl	000075-00-3	3





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ALS Vial : 52 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-62

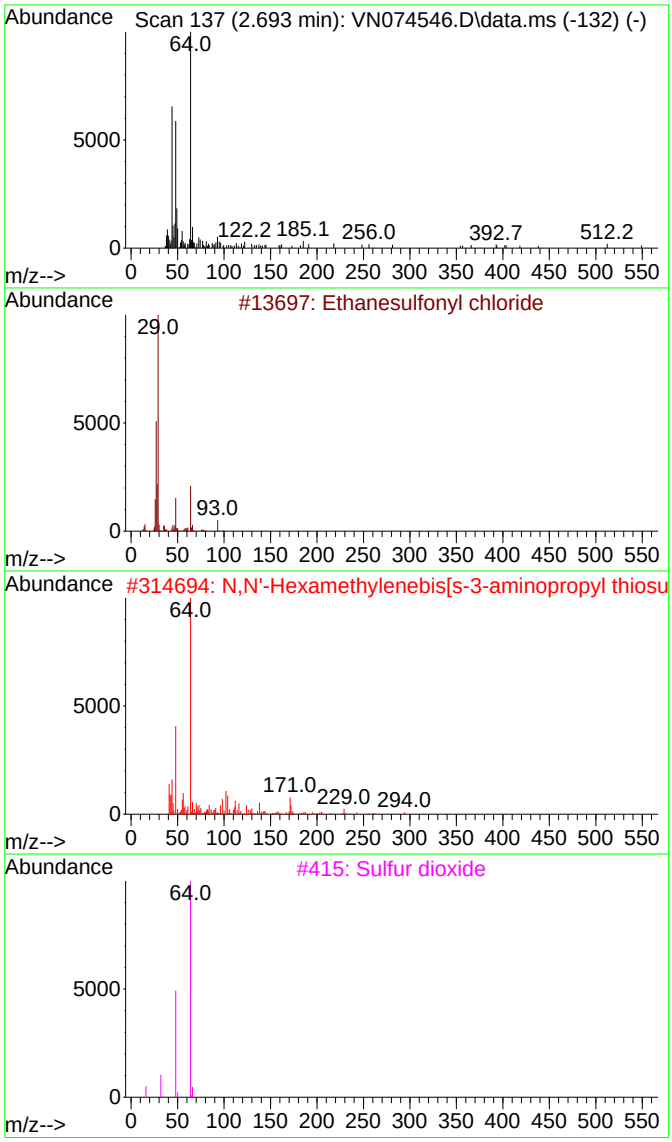
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

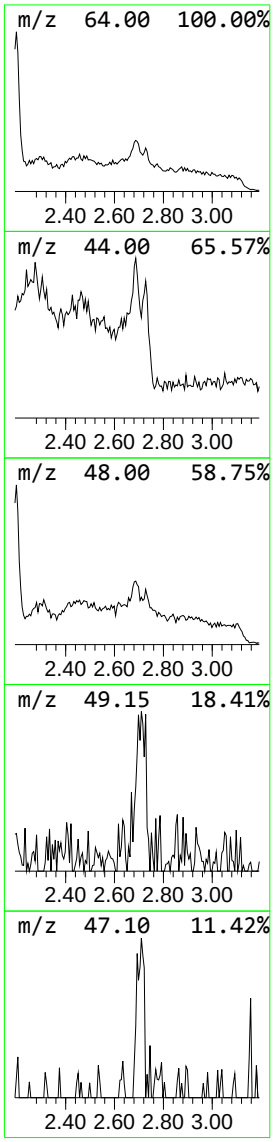
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Ethanesulfonyl chloride Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.693	5.99 ug/l	109347	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanesulfonyl chloride	128	C2H5ClO2S	000594-44-5	72
2	N,N'-Hexamethylenebis[s-3-aminop...	424	C12H28N2O6S4	035871-55-7	56
3	Sulfur dioxide	64	O2S	007446-09-5	50
4	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	50
5	1,3-Dioxane, 5,5-difluoro-	124	C4H6F2O2	036301-44-7	45





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ALS Vial : 52 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-62

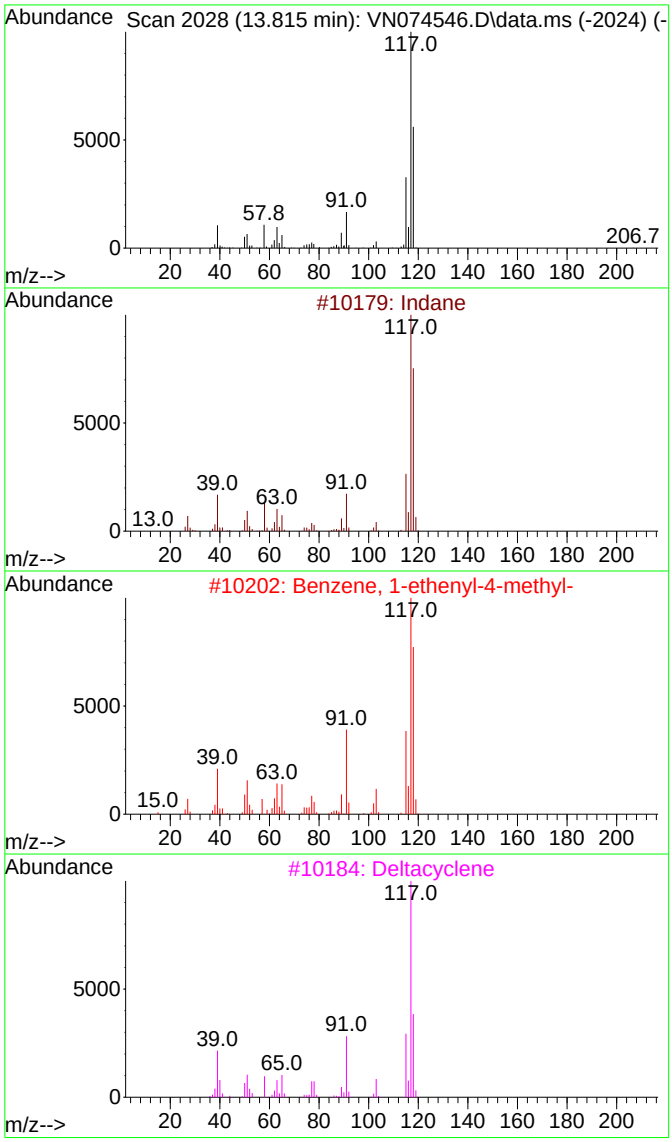
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

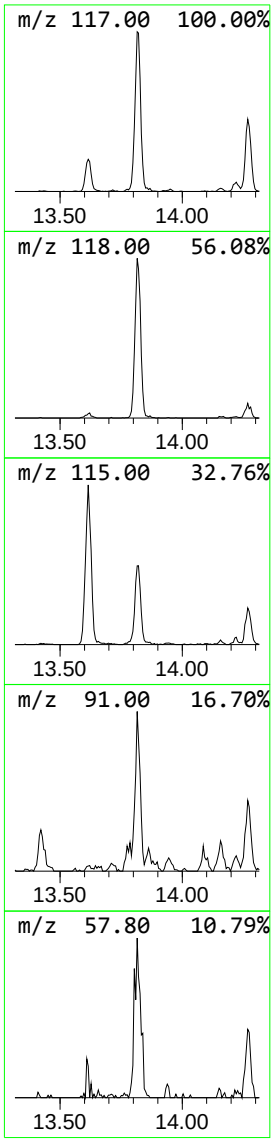
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Indane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.815	20.63 ug/l	742306	1,4-Dichlorobenzene-d4	13.615

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	94
2	Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	74
3	Deltacyclene	118	C9H10	007785-10-6	72
4	(Z)-1-Phenylpropene	118	C9H10	000766-90-5	64
5	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	64





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Instrument :
MSVOA_N
ClientSampleId :
MW-62

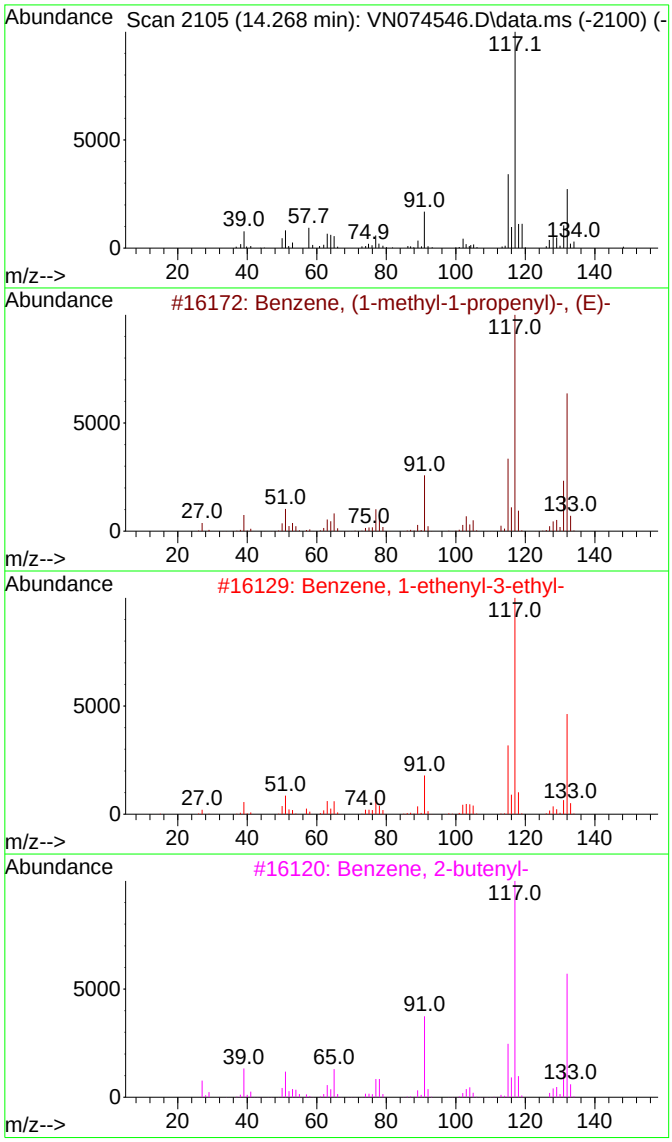
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

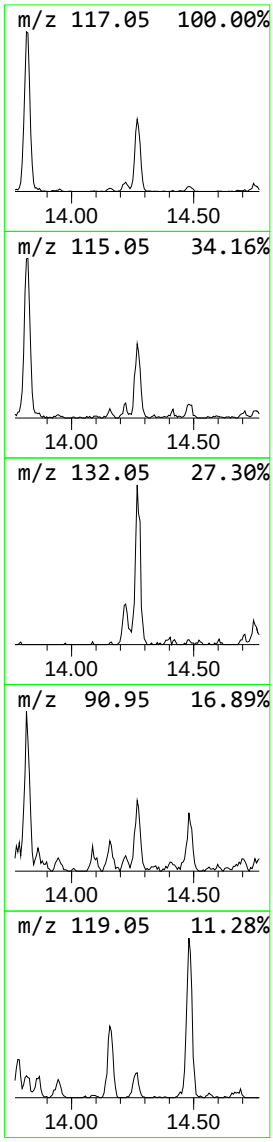
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Benzene, (1-methyl-1-propen... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.268	9.71 ug/l	349311	1,4-Dichlorobenzene-d4	13.615

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	90
2	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	83
3	Benzene, 2-butenyl-	132	C10H12	001560-06-1	80
4	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000767-99-7	80
5	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	80





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ALS Vial : 52 Sample Multiplier: 1

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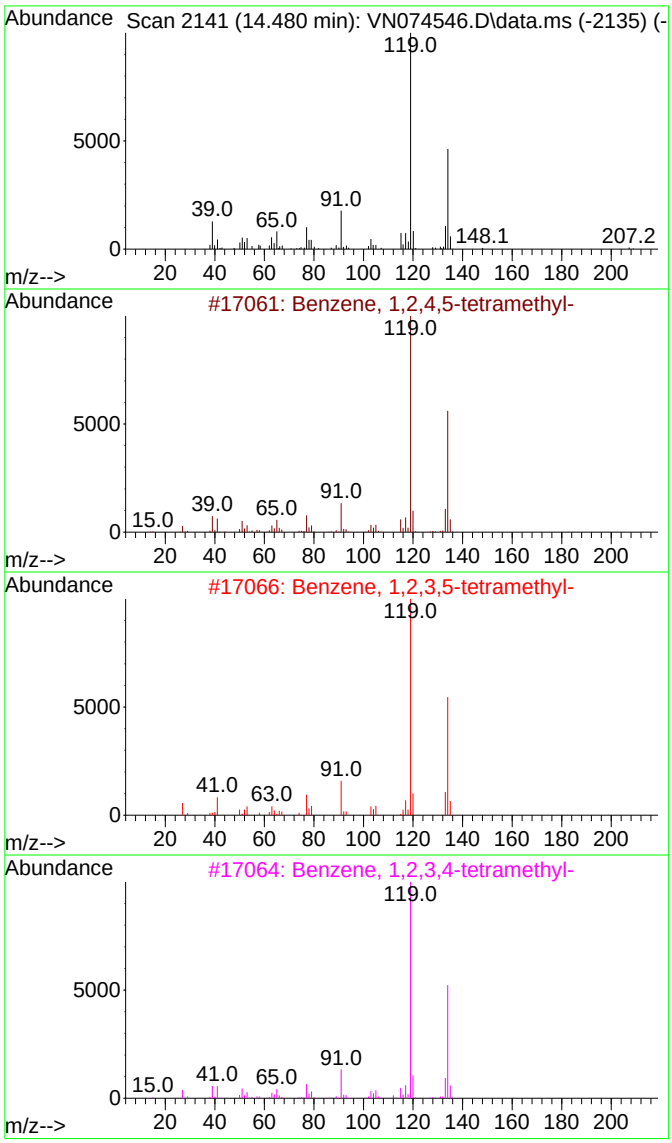
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

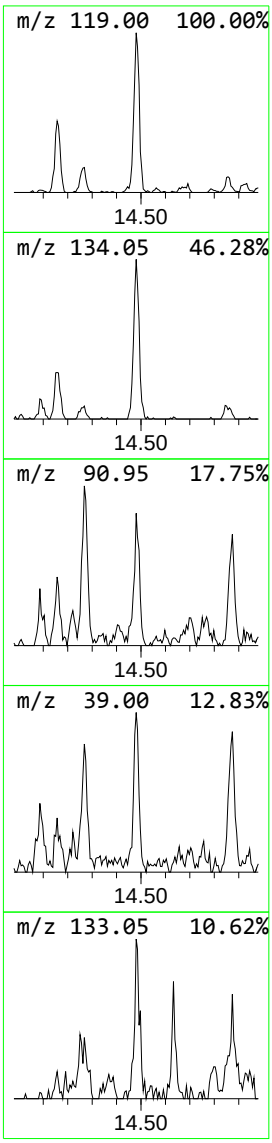
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.480	6.97 ug/l	250934	1,4-Dichlorobenzene-d4	13.615

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	94
2	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	91
3	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	91
4	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	91
5	1,3-Cyclopentadiene, 1,2,3,4-tet...	134	C10H14	076089-59-3	91





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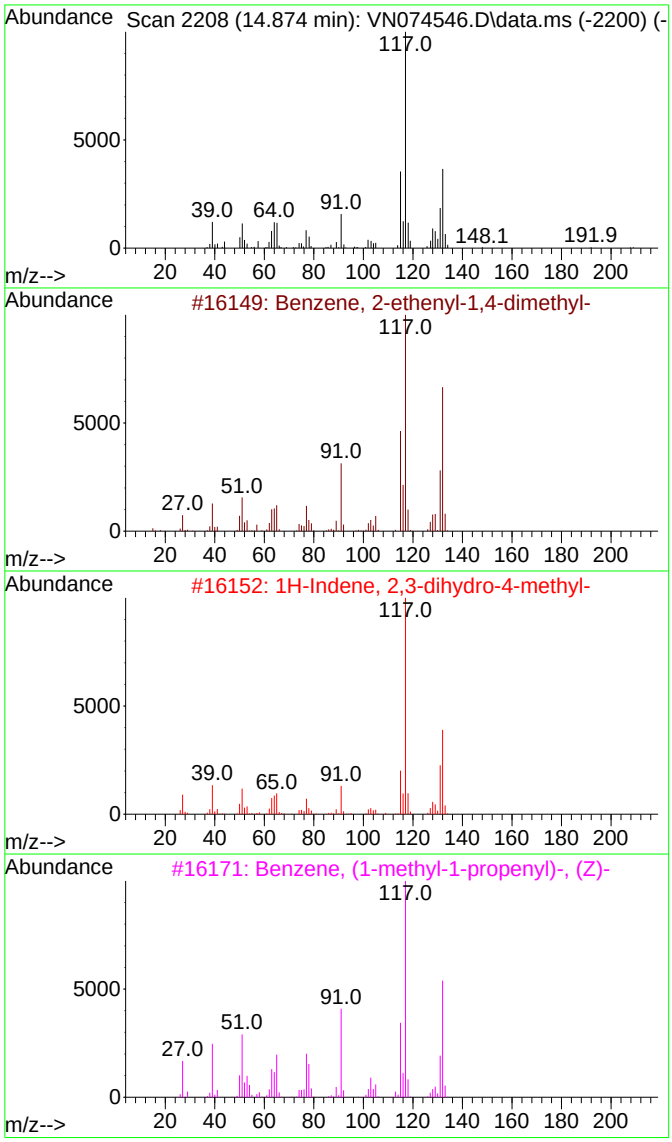
Quant Title : SW846 8260

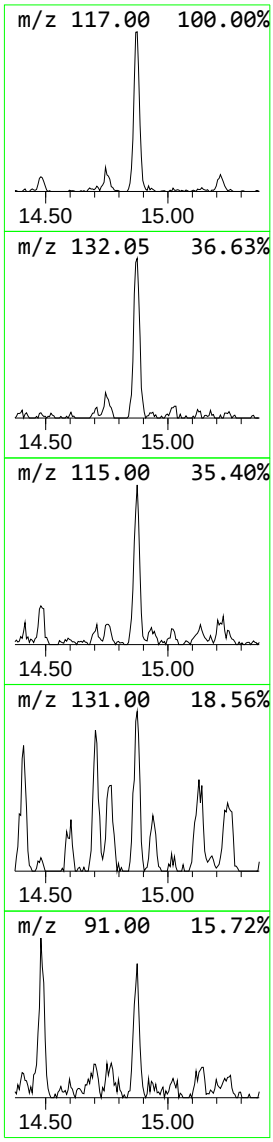
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.874	8.77 ug/l	315543	1,4-Dichlorobenzene-d4	13.615

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	96
2	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	93
3	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000767-99-7	90
4	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	90
5	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	87





Tentatively Identified Compound (LSC) summary

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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	2.198	27.1	ug/l	494921	1	8.016	912798	50.0
Ethanesulfonyl ...	2.693	6.0	ug/l	109347	1	8.016	912798	50.0
Indane	13.815	20.6	ug/l	742306	4	13.615	1799100	50.0
Benzene, (1-met...	14.268	9.7	ug/l	349311	4	13.615	1799100	50.0
Benzene, 1,2,4,...	14.480	7.0	ug/l	250934	4	13.615	1799100	50.0
Benzene, 2-ethe...	14.874	8.8	ug/l	315543	4	13.615	1799100	50.0