LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090322\
Data File : VN074332.D
Acq On : 03 Sep 2022 21:24
Operator : JC\MD
Sample : N4355-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-31

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\82N090222W.M
Title : SW846 8260

Signal : TIC: VN074332.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.275	50	66	78	rBV	539025	3157386	82.27%	12.200%
2	2.693	133	137	151	rVB2	263044	853613	22.24%	3.298%
3	5.287	567	578	592	rBV3	59410	207460	5.41%	0.802%
4	5.534	606	620	638	rBV	1092240	3837717	100.00%	14.829%
5	6.416	758	770	779	rBV3	27101	92286	2.40%	0.357%
6	7.069	871	881	889	rBV5	30141	86565	2.26%	0.334%
7	7.951	1021	1031	1037	rBV2	278962	685307	17.86%	2.648%
8	8.016	1037	1042	1053	rVB	466704	1013923	26.42%	3.918%
9	8.387	1092	1105	1116	rBV3	521957	1479833	38.56%	5.718%
10	8.904	1184	1193	1207	rBV2	672513	1400965	36.51%	5.413%
11	9.904	1358	1363	1369	rBV3	20648	39707	1.03%	0.153%
12	10.381	1435	1444	1451	rBV	1010681	1815683	47.31%	7.016%
13	10.445	1451	1455	1466	rVB	42509	89904	2.34%	0.347%
14	10.581	1466	1478	1485	rBV2	59437	115775	3.02%	0.447%
15	10.657	1485	1491	1499	rVV2	61661	109003	2.84%	0.421%
16	11.686	1658	1666	1676	rBV	971230	1755834	45.75%	6.785%
17	11.786	1676	1683	1692	rVV	280766	473620	12.34%	1.830%
18	11.898	1694	1702	1713	rVB	375522	681405	17.76%	2.633%
19	12.222	1750	1757	1764	rBV	168333	292642	7.63%	1.131%
20	12.516	1801	1807	1814	rBV	121270	199811	5.21%	0.772%
21	12.669	1826	1833	1842	rBV	834578	1377878	35.90%	5.324%
22	12.857	1857	1865	1872	rVV	134848	218002	5.68%	0.842%
23	12.957	1872	1882	1885	rVV	60886	109743	2.86%	0.424%
24	12.998	1885	1889	1895	rVB3	50821	80808	2.11%	0.312%
25	13.157	1908	1916	1924	rBV	239780	406502	10.59%	1.571%
26	13.310	1935	1942	1950	rVB	213743	343389	8.95%	1.327%
27	13.439	1956	1964	1969	rBV3	18492	38815	1.01%	0.150%
28	13.610	1986	1993	2007	rBV2	1008629	1997124	52.04%	7.717%
29	13.774	2015	2021	2022	rBV2	49758	60651	1.58%	0.234%
30	13.816	2022	2028	2034	rVB	541970	869254	22.65%	3.359%
31	13.998	2053	2059	2066	rVV3	37495	68599	1.79%	0.265%
32	14.157	2080	2086	2091	rBV	75380	110677	2.88%	0.428%
33	14.216	2091	2096	2099	rBV3	29857	47346	1.23%	0.183%
34	14.269	2099	2105	2110	rVB2	159270	272106	7.09%	1.051%
35	14.474	2132	2140	2144	rBV2	62568	107836	2.81%	0.417%
36	14.516	2144	2147	2152	rVB	37012	56182	1.46%	0.217%

LSC Area Percent Report

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Operator : JC\MD
Sample : N4355-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-31

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\82N090222W.M
Title : SW846 8260

37	14.751	2181	2187	2192	rVV	59226	97631	2.54%	0.377%
38	14.868	2198	2207	2213	rBV3	152868	352080	9.17%	1.360%
39	14.933	2213	2218	2223	rVB5	37964	65985	1.72%	0.255%
40	15.016	2226	2232	2242	rBV4	46313	84809	2.21%	0.328%
41	15.127	2244	2251	2256	rBV7	37846	79098	2.06%	0.306%
42	15.433	2297	2303	2310	rVB	140270	248272	6.47%	0.959%
43	15.539	2316	2321	2325	rBV6	21337	43402	1.13%	0.168%
44	15.892	2373	2381	2386	rBV8	17652	50761	1.32%	0.196%
45	16.104	2411	2417	2433	rVB8	19690	80082	2.09%	0.309%
46	16.262	2437	2444	2454	rBV8	18461	47273	1.23%	0.183%
47	16.739	2515	2525	2532	rBV3	69298	176517	4.60%	0.682%

Sum of corrected areas: 25879261

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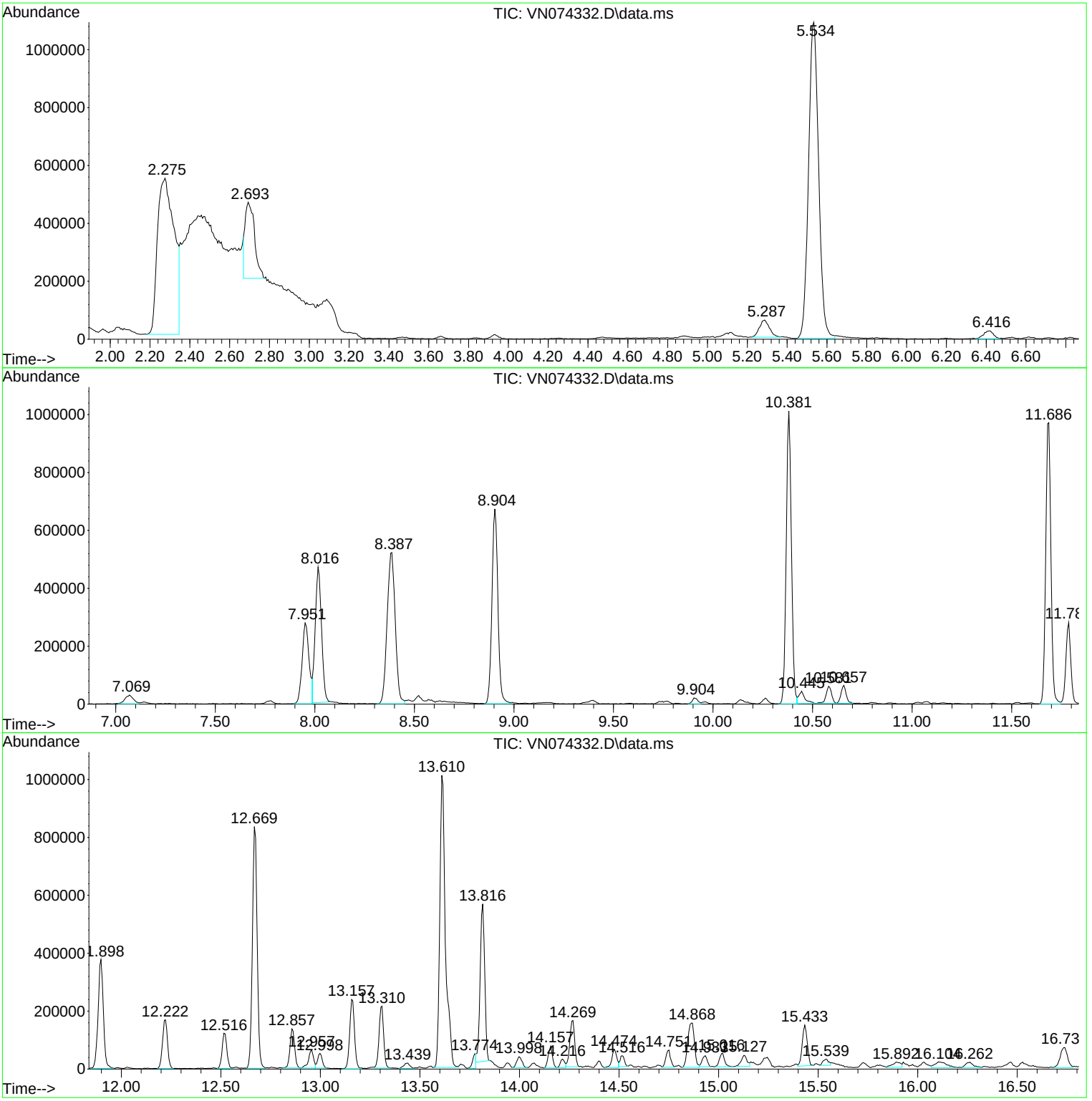
Instrument :
MSVOA_N
ClientSampleId :
MW-31

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090222W.M
Quant Title : SW846 8260

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



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Data File : VN074332.D
Acq On : 03 Sep 2022 21:24
Operator : JC\MD
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ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-31

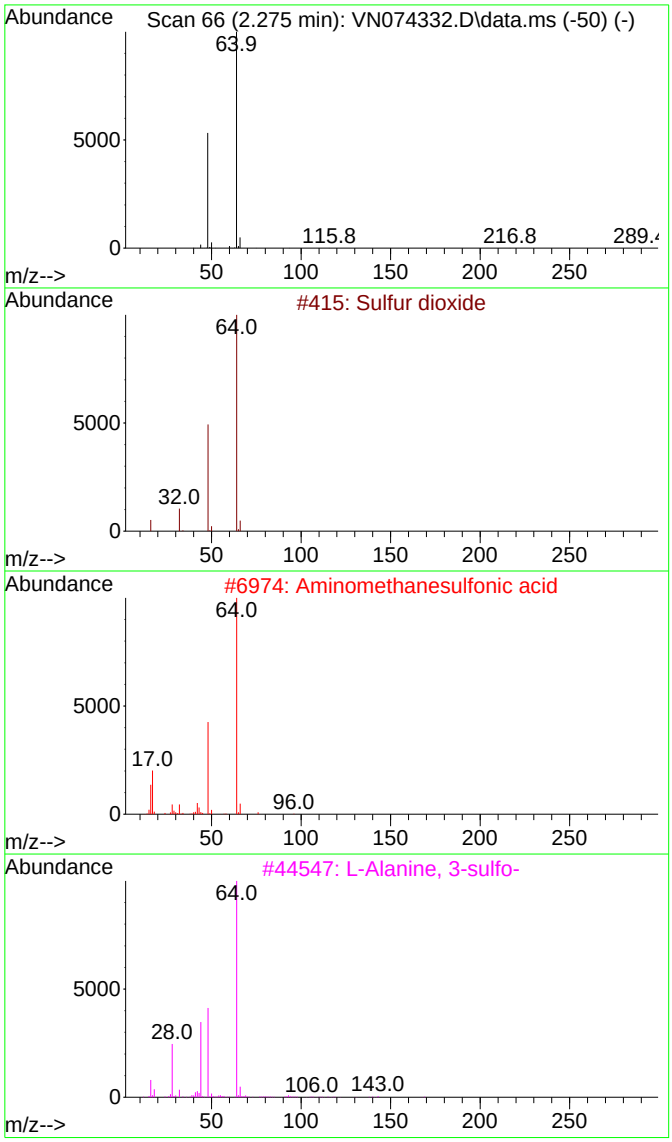
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090222W.M
Quant Title : SW846 8260

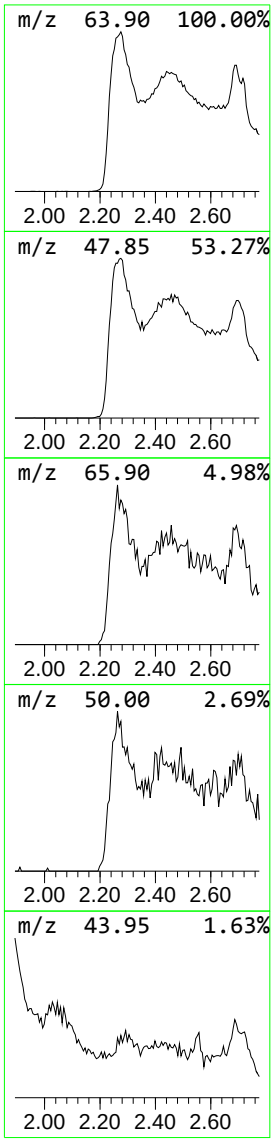
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.275	155.70 ug/l	3157390	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	83
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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Operator : JC\MD
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ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-31

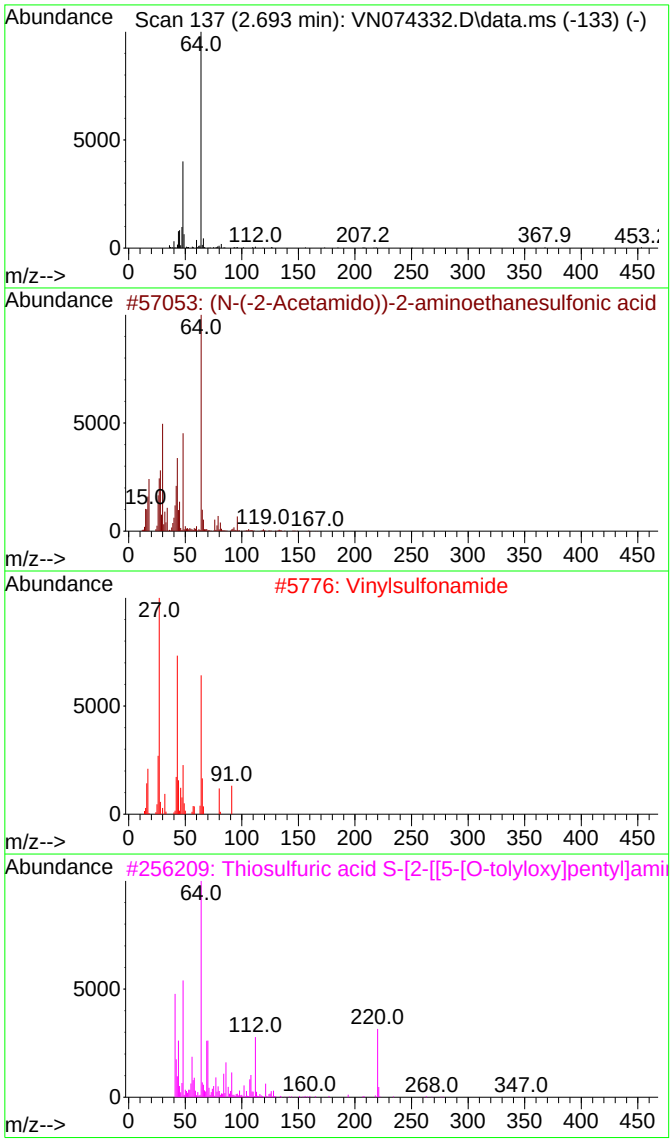
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090222W.M
Quant Title : SW846 8260

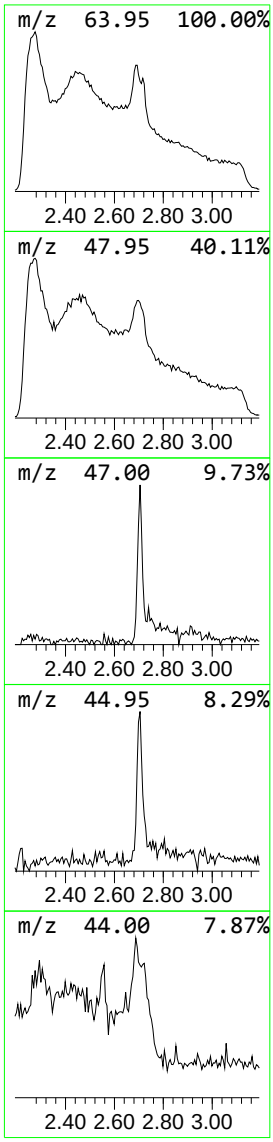
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 (N-(-2-Acetamido))-2-aminoe... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.693	42.09 ug/l	853613	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(N-(-2-Acetamido))-2-aminoethane...	182	C4H10N2O4S	007365-82-4	78
2	Vinylsulfonamide	107	C2H5NO2S	002386-58-5	64
3	Thiosulfuric acid S-[2-[[5-[O-to...	347	C15H25NO4S2	038920-47-7	64
4	Sulfur dioxide	64	O2S	007446-09-5	64
5	6-Amino-2,3-diphenyl-8-[p-sulfam...	482	C26H22N6O2S	021271-90-9	64





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ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-31

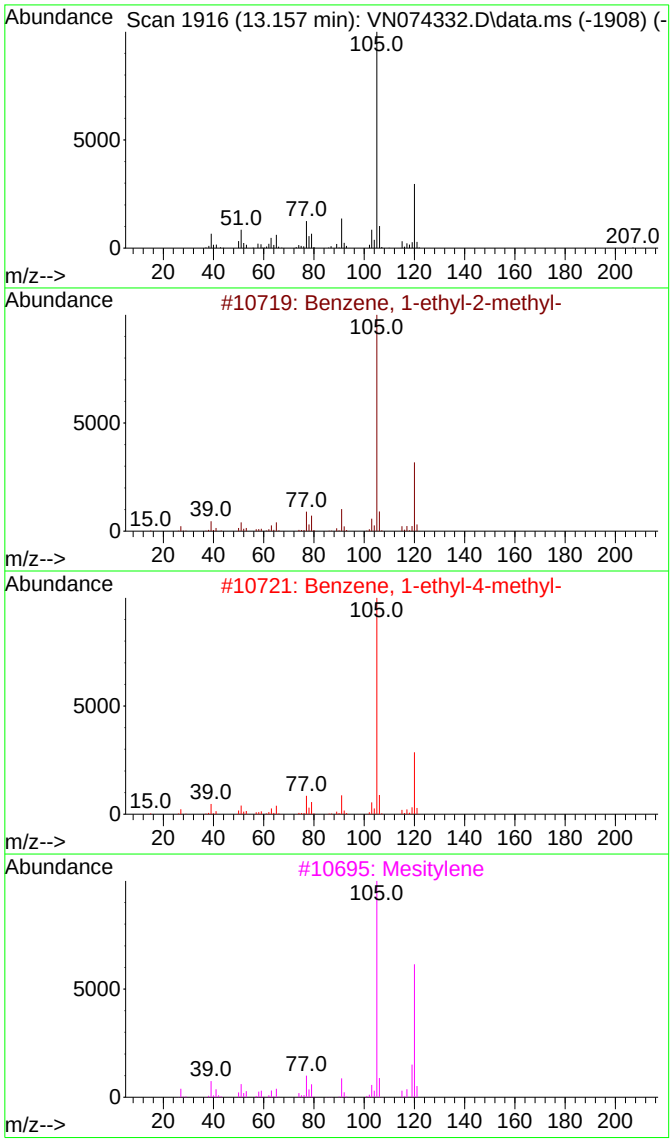
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090222W.M
Quant Title : SW846 8260

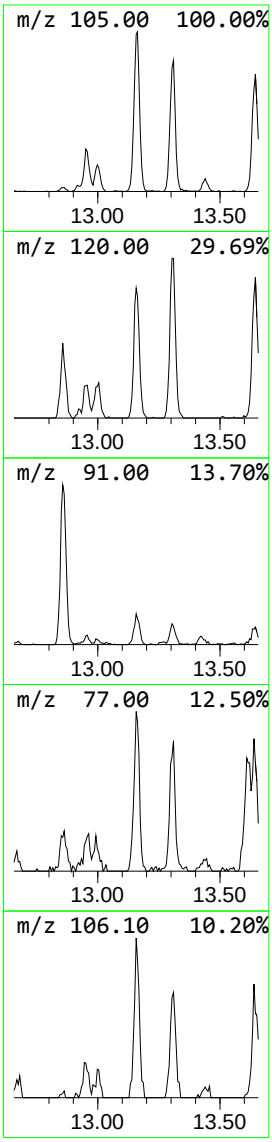
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Benzene, 1-ethyl-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.157	10.18 ug/l	406502	1,4-Dichlorobenzene-d4	13.610

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-4-methyl-	120	C9H12	000622-96-8	94
3	Mesitylene	120	C9H12	000108-67-8	91
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91





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ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-31

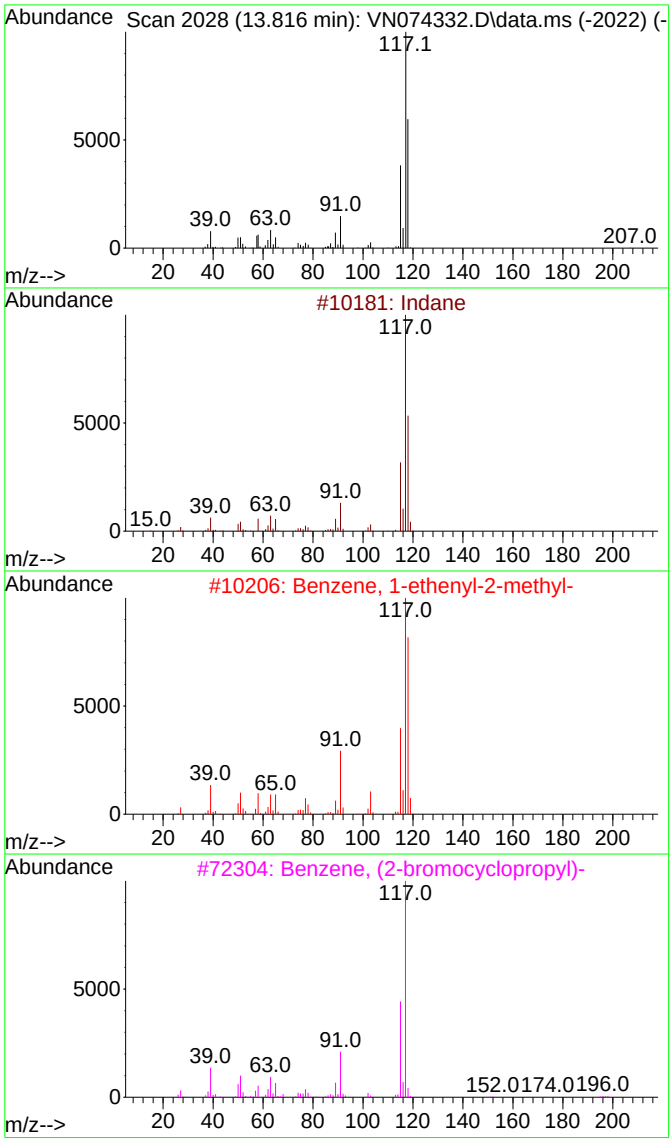
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090222W.M
Quant Title : SW846 8260

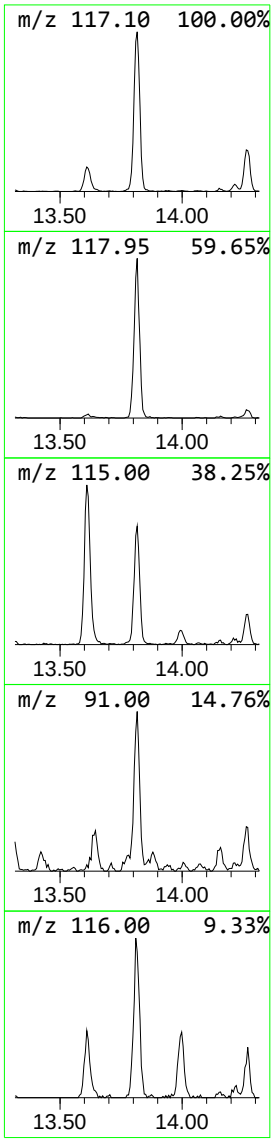
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Indane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.816	21.76 ug/l	869254	1,4-Dichlorobenzene-d4	13.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	94
2	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	76
3	Benzene, (2-bromocyclopropyl)-	196	C9H9Br	036617-02-4	64
4	Benzene, cyclopropyl-	118	C9H10	000873-49-4	58
5	(Z)-1-Phenylpropene	118	C9H10	000766-90-5	53





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Instrument :
MSVOA_N
ClientSampleId :
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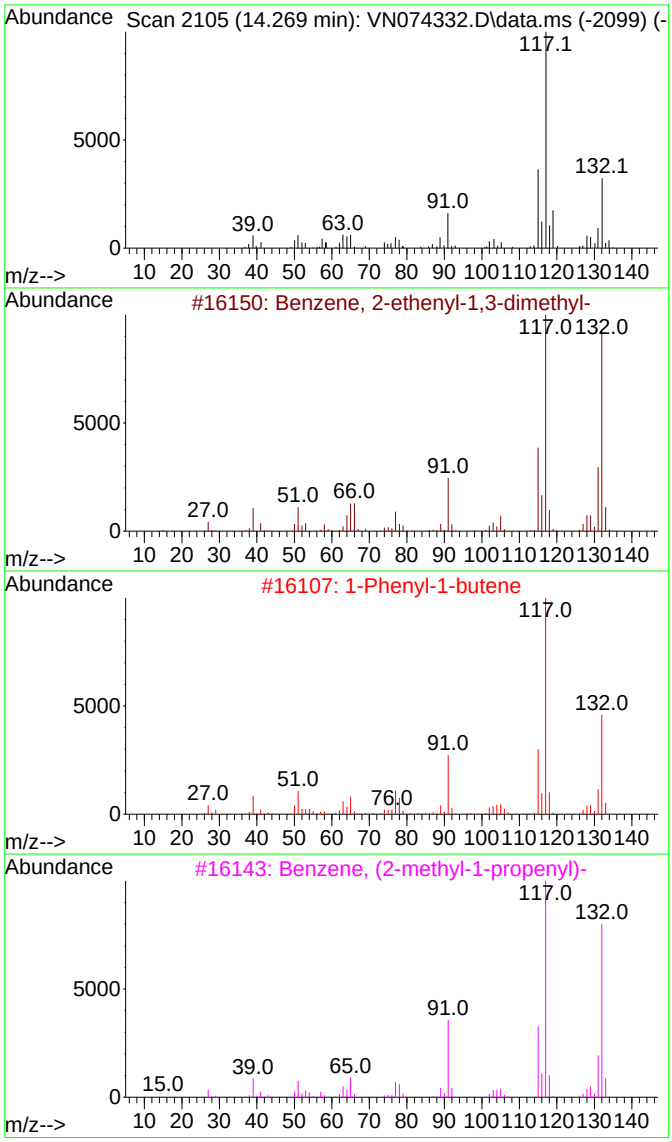
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090222W.M
Quant Title : SW846 8260

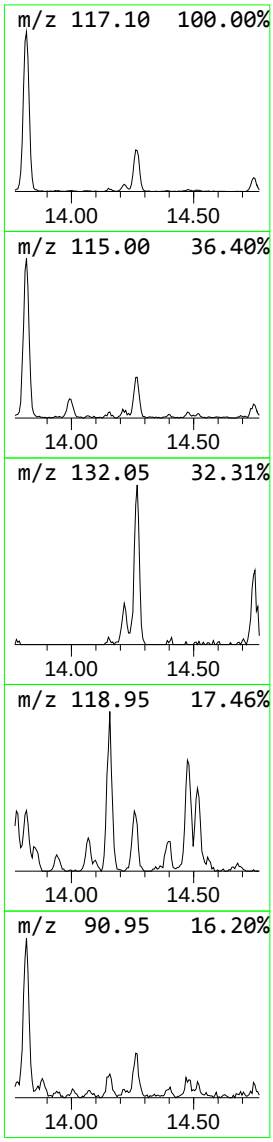
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzene, 2-ethenyl-1,3-dime... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.269	6.81 ug/l	272106	1,4-Dichlorobenzene-d4	13.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethenyl-1,3-dimethyl-	132	C10H12	002039-90-9	87
2	1-Phenyl-1-butene	132	C10H12	000824-90-8	87
3	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	86
4	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	83
5	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	83





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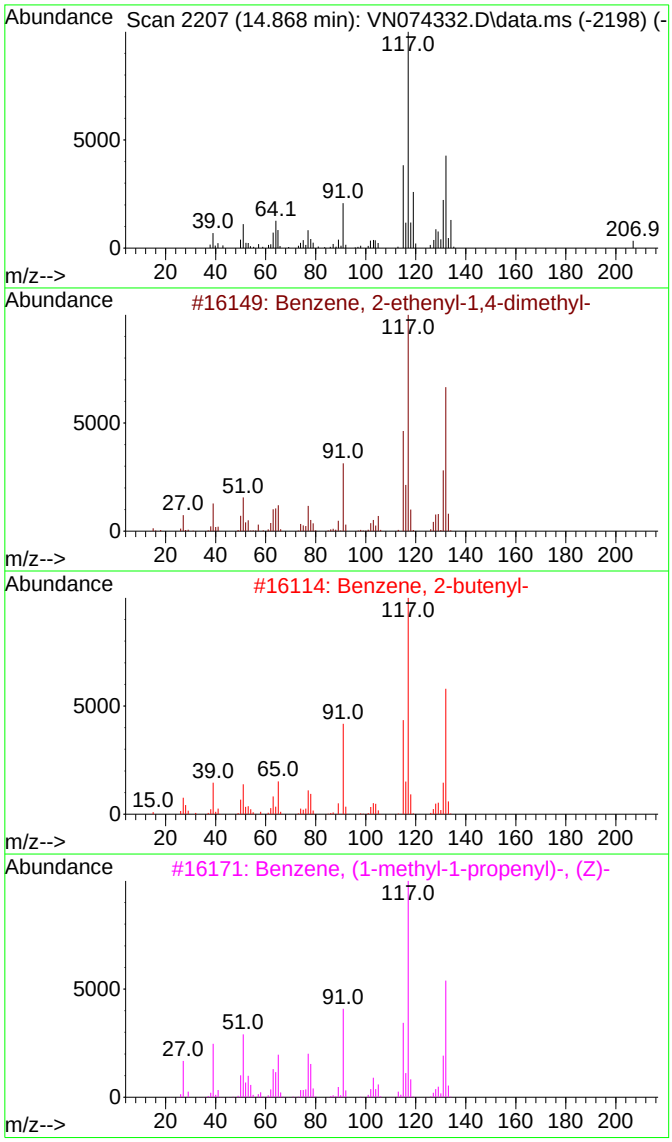
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090222W.M
Quant Title : SW846 8260

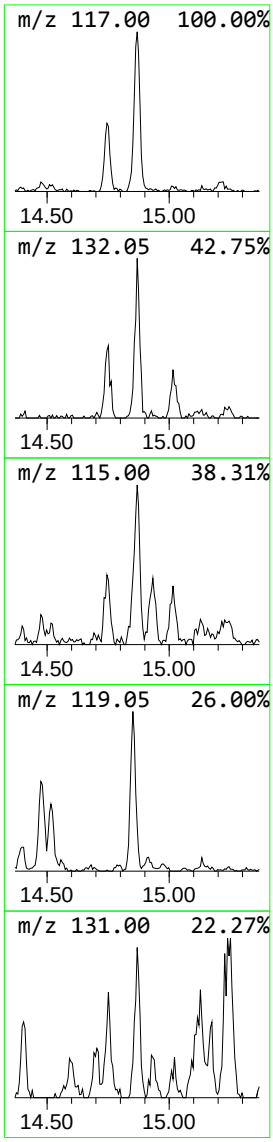
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.868	8.81 ug/l	352080	1,4-Dichlorobenzene-d4	13.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	90
2	Benzene, 2-butenyl-	132	C10H12	001560-06-1	89
3	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000767-99-7	87
4	3-Phenylbut-1-ene	132	C10H12	000934-10-1	81
5	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	76





Tentatively Identified Compound (LSC) summary

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090222W.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	2.275	155.7	ug/l	3157390	1	8.016	1013920	50.0
(N-(-2-Acetamid...	2.693	42.1	ug/l	853613	1	8.016	1013920	50.0
Benzene, 1-ethy...	13.157	10.2	ug/l	406502	4	13.610	1997120	50.0
Indane	13.816	21.8	ug/l	869254	4	13.610	1997120	50.0
Benzene, 2-ethe...	14.269	6.8	ug/l	272106	4	13.610	1997120	50.0
Benzene, 2-ethe...	14.868	8.8	ug/l	352080	4	13.610	1997120	50.0