LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX091522\
Data File : VX031394.D
Acq On : 16 Sep 2022 08:08
Operator : JC/MD
Sample : N4537-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW2

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_X\Method\82X091422W.M
Title : SW846 8260

Signal : TIC: VX031394.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.282	24	32	42	rBV	58694	184476	22.56%	4.194%
2	1.550	73	76	83	rBV	15000	22689	2.77%	0.516%
3	1.953	139	142	149	rVB2	8579	12533	1.53%	0.285%
4	2.386	207	213	226	rBV	42455	96847	11.84%	2.202%
5	2.520	229	235	238	rBV2	6443	13053	1.60%	0.297%
6	2.575	238	244	258	rVB3	4960	21037	2.57%	0.478%
7	2.788	276	279	289	rVB5	3600	8414	1.03%	0.191%
8	2.946	296	305	320	rVB	16948	41130	5.03%	0.935%
9	4.574	562	572	582	rBV2	11513	37256	4.56%	0.847%
10	5.099	644	658	669	rVB4	5512	18002	2.20%	0.409%
11	5.385	695	705	719	rBV	97685	283882	34.72%	6.454%
12	5.556	722	733	748	rVB	97496	273571	33.46%	6.220%
13	5.958	789	799	810	rBV	111345	289070	35.35%	6.572%
14	6.037	810	812	820	rVB3	4271	8291	1.01%	0.188%
15	6.763	922	931	946	rBV	148243	354719	43.38%	8.065%
16	7.464	1042	1046	1054	rVB	4131	8234	1.01%	0.187%
17	8.415	1197	1202	1209	rBV3	5717	9854	1.21%	0.224%
18	8.653	1234	1241	1249	rBV	518889	817657	100.00%	18.589%
19	10.055	1465	1471	1483	rBV	323241	427771	52.32%	9.725%
20	11.079	1634	1639	1647	rBV	427000	544504	66.59%	12.379%
21	11.475	1701	1704	1711	rVB	6267	10002	1.22%	0.227%
22	11.805	1754	1758	1764	rBV	42455	55233	6.76%	1.256%
23	11.860	1764	1767	1776	rVB5	6319	10648	1.30%	0.242%
24	12.024	1787	1794	1801	rVB	334575	450375	55.08%	10.239%
25	12.244	1822	1830	1836	rBV	68294	91658	11.21%	2.084%
26	12.408	1851	1857	1864	rBV9	3403	9567	1.17%	0.218%
27	12.701	1900	1905	1912	rVB4	7921	15159	1.85%	0.345%
28	13.164	1967	1981	1991	rBV9	16165	58940	7.21%	1.340%
29	13.292	1997	2002	2007	rVB2	11427	17286	2.11%	0.393%
30	13.426	2019	2024	2029	rVB4	8176	13250	1.62%	0.301%
31	13.548	2040	2044	2047	rBV2	5596	8327	1.02%	0.189%
32	13.774	2078	2081	2088	rVB2	5414	9382	1.15%	0.213%
33	13.865	2088	2096	2101	rBV3	6265	13520	1.65%	0.307%
34	14.079	2125	2131	2133	rBV6	4473	8714	1.07%	0.198%
35	14.377	2175	2180	2188	rVB5	13651	21311	2.61%	0.485%
36	14.481	2193	2197	2203	rBV6	5665	9423	1.15%	0.214%

LSC Area Percent Report

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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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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091422W.M
Title : SW846 8260

37	14.603	2212	2217	2220	rBV3	6949	14775	1.81%	0.336%
38	14.780	2240	2246	2251	rBV	23404	36274	4.44%	0.825%
39	15.188	2308	2313	2320	rVB7	4352	8561	1.05%	0.195%
40	15.371	2336	2343	2344	rBV6	5731	10444	1.28%	0.237%
41	15.475	2355	2360	2364	rBV4	7092	11331	1.39%	0.258%
42	15.615	2377	2383	2386	rBV3	8382	13480	1.65%	0.306%
43	15.652	2386	2389	2394	rVB3	6212	9049	1.11%	0.206%
44	15.847	2417	2421	2428	rVB4	4584	9121	1.12%	0.207%
45	15.993	2439	2445	2454	rVB4	3437	9680	1.18%	0.220%

Sum of corrected areas: 4398500

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ClientSampleId :
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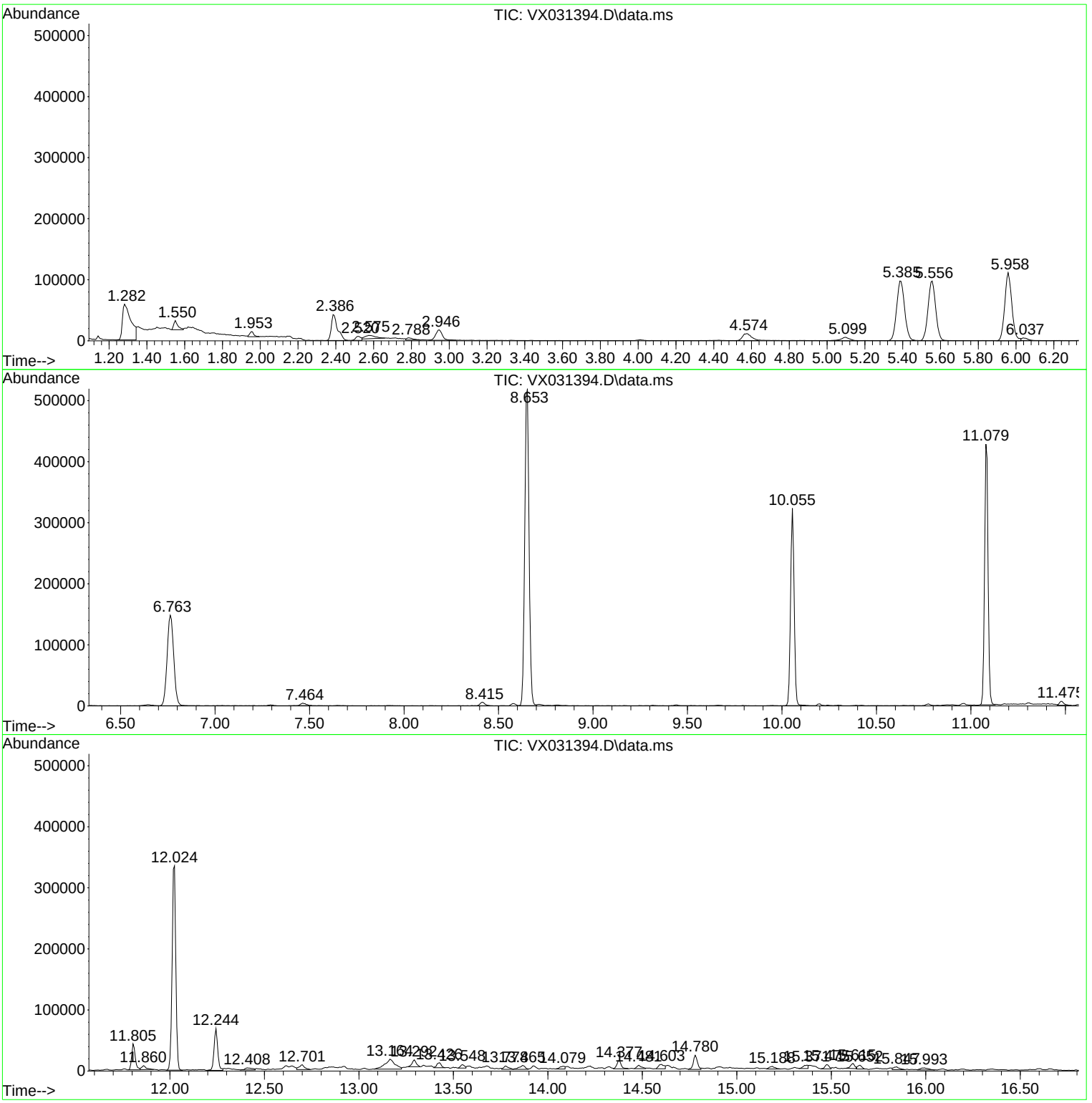
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091422W.M
Quant Title : SW846 8260

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



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Data File : VX031394.D
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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091422W.M
Quant Title : SW846 8260

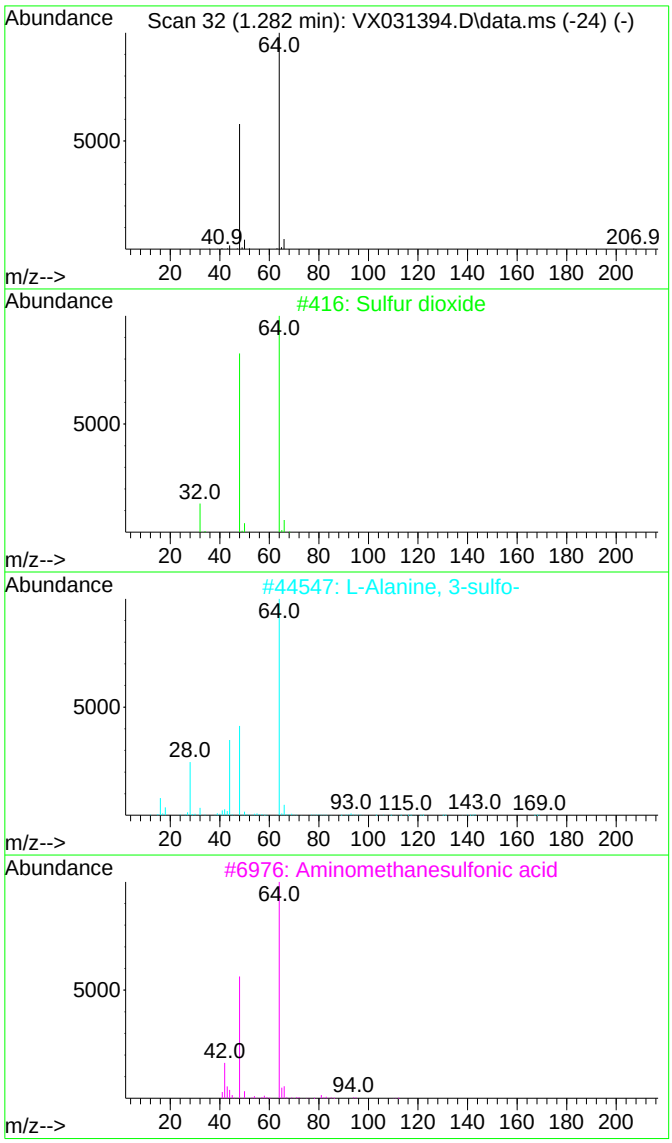
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

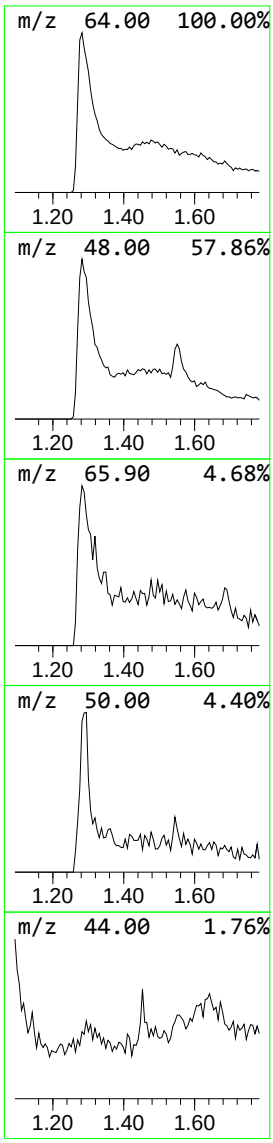
****

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.282	33.72 ug/l	184476	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	83
2	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
3	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	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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Instrument :
MSVOA_X
ClientSampleId :
MW2

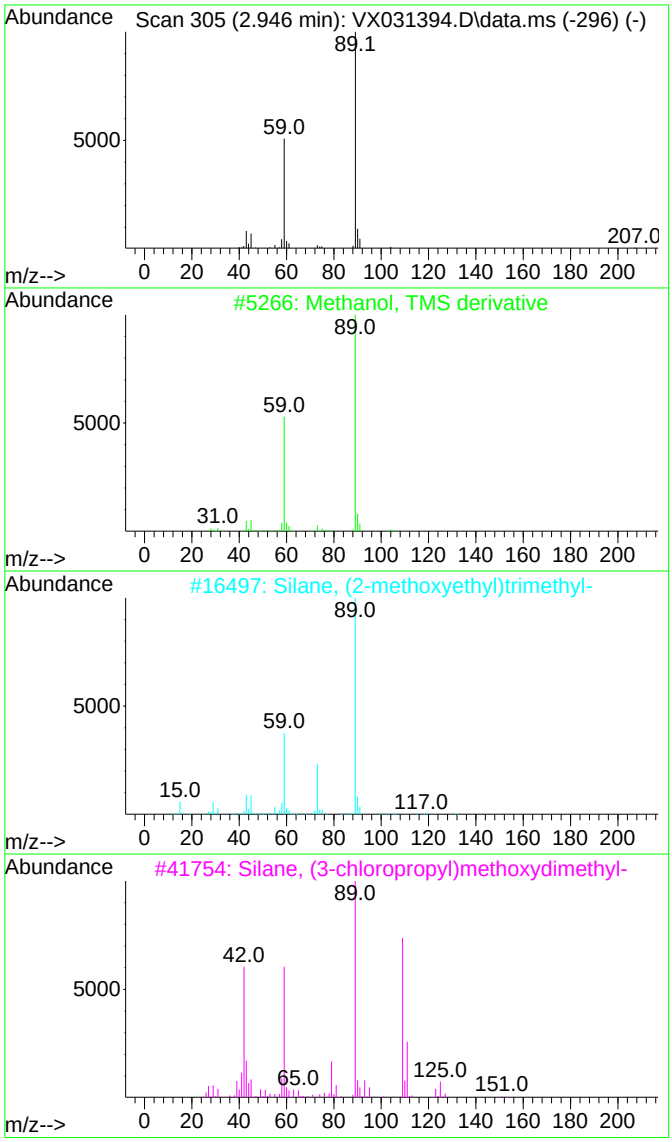
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091422W.M
Quant Title : SW846 8260

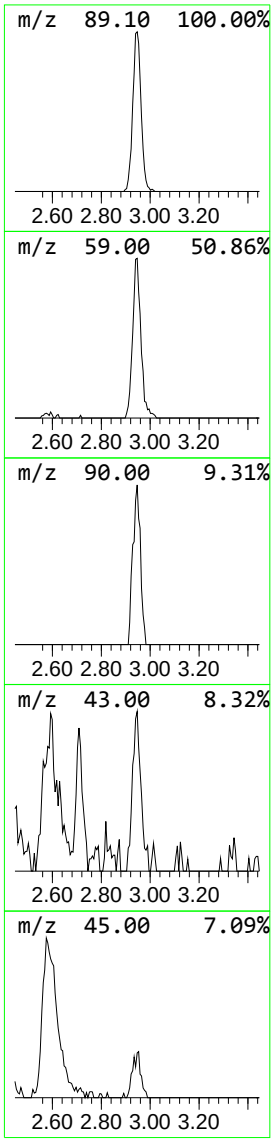
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Methanol, TMS derivative Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.946	7.52 ug/l	41130	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methanol, TMS derivative	104	C4H12OSi	001825-61-2	91
2	Silane, (2-methoxyethyl)trimethyl-	132	C6H16OSi	018173-63-2	83
3	Silane, (3-chloropropyl)methoxyd...	166	C6H15ClOSi	018171-14-7	83
4	Ethyl(dimethyl)methoxysilane	118	C5H14OSi	052686-75-6	74
5	Dimethyl(chloromethyl)methoxysilane	138	C4H11ClOSi	018143-33-4	64





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Data File : VX031394.D
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Operator : JC/MD
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ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW2

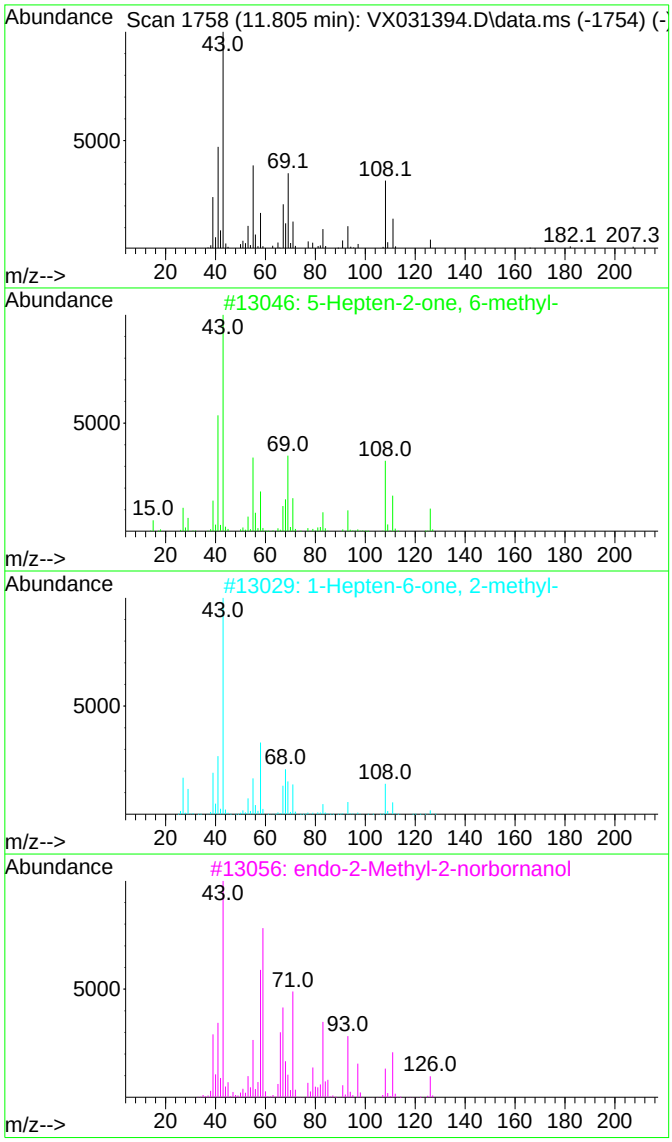
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091422W.M
Quant Title : SW846 8260

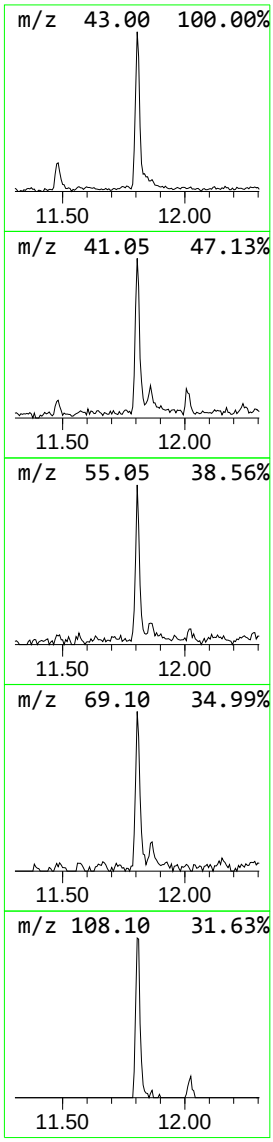
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 5-Hepten-2-one, 6-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.805	6.13 ug/l	55233	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Hepten-2-one, 6-methyl-	126	C8H14O	000110-93-0	74
2	1-Hepten-6-one, 2-methyl-	126	C8H14O	010408-15-8	52
3	endo-2-Methyl-2-norbornanol	126	C8H14O	003212-16-6	25
4	2-Oxabicyclo[2.2.2]octan-6-ol, 1...	170	C10H18O2	018679-48-6	16
5	2-(Diacetoxymethyl)-5-nitrofuran	243	C9H9NO7	000092-55-7	10





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Instrument :
MSVOA_X
ClientSampleId :
MW2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091422W.M
Quant Title : SW846 8260

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

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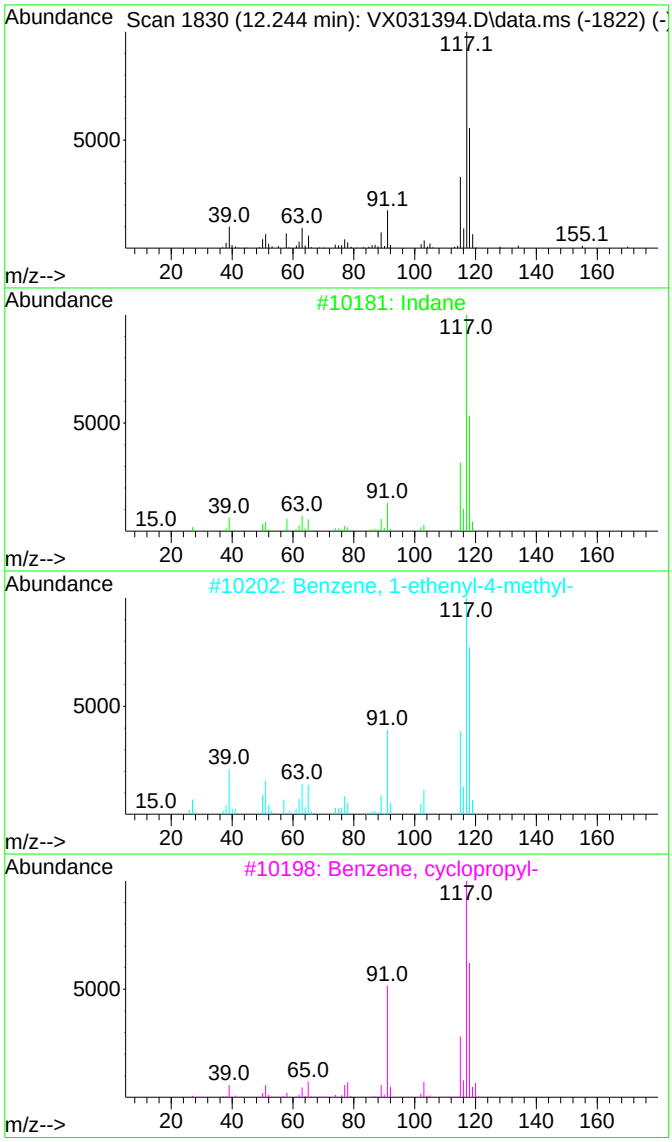
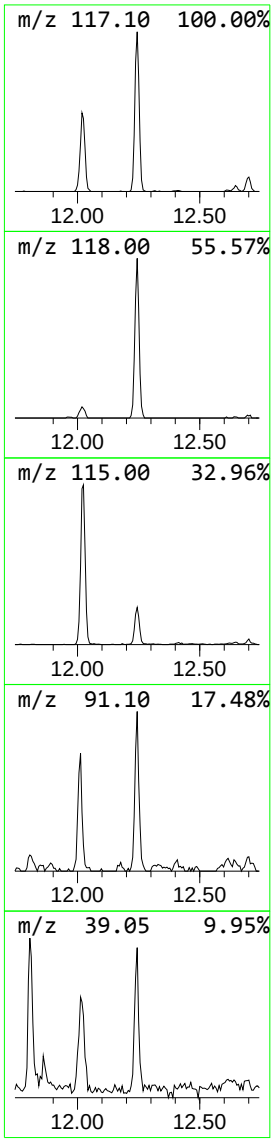
Peak Number 4 Indane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	10.18 ug/l	91658	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	93
2	Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	83
3	Benzene, cyclopropyl-	118	C9H10	000873-49-4	74
4	1,4:5,8-Dimethanobiphenylene, 1,...	184	C14H16	001624-13-1	72
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	118	C9H10	055337-80-9	72





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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW2

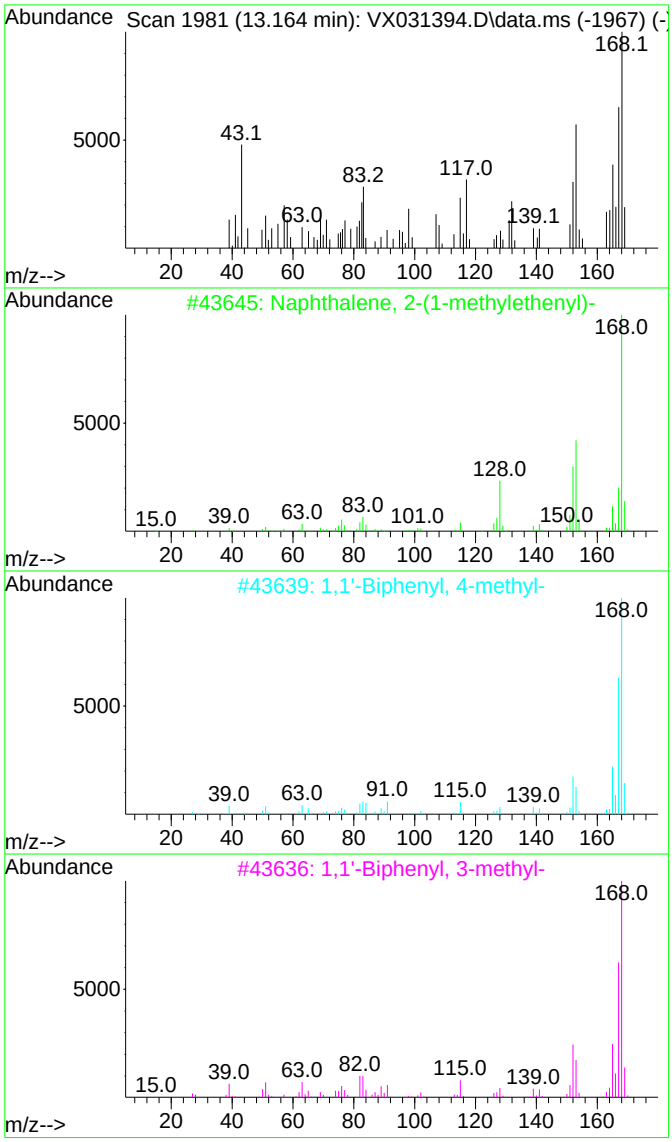
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091422W.M
Quant Title : SW846 8260

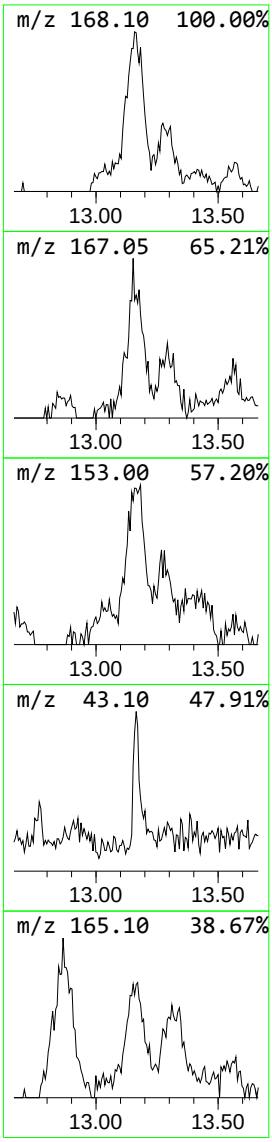
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Naphthalene, 2-(1-methyleth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.164	6.54 ug/l	58940	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-(1-methylethenyl)-	168	C13H12	003710-23-4	60
2	1,1'-Biphenyl, 4-methyl-	168	C13H12	000644-08-6	55
3	1,1'-Biphenyl, 3-methyl-	168	C13H12	000643-93-6	53
4	1-Isopropenylnaphthalene	168	C13H12	001855-47-6	50
5	1,1'-Biphenyl, 2-methyl-	168	C13H12	000643-58-3	46





Tentatively Identified Compound (LSC) summary

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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	1.282	33.7	ug/l	184476	1	5.550	273571	50.0
Methanol, TMS d...	2.946	7.5	ug/l	41130	1	5.550	273571	50.0
5-Hepten-2-one,...	11.805	6.1	ug/l	55233	4	12.024	450375	50.0
Indane	12.244	10.2	ug/l	91658	4	12.024	450375	50.0
Naphthalene, 2-...	13.164	6.5	ug/l	58940	4	12.024	450375	50.0