LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX092122\
Data File : VX031525.D
Acq On : 21 Sep 2022 15:29
Operator : JC/MD
Sample : N4614-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
H-3RA

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\82X091922W.M
Title : SW846 8260

Signal : TIC: VX031525.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.264	23	29	43	rBV3	11321	35703	4.30%	0.820%
2	1.453	57	60	65	rBV	9877	12593	1.52%	0.289%
3	1.611	76	86	99	rVB	8935	28631	3.45%	0.658%
4	1.752	104	109	114	rVB4	6457	9825	1.18%	0.226%
5	2.337	200	205	210	rBV2	4693	9193	1.11%	0.211%
6	2.569	235	243	256	rVB2	4122	12249	1.48%	0.281%
7	2.776	271	277	289	rVB2	5677	12750	1.54%	0.293%
8	2.953	297	306	308	rBV	10730	23851	2.88%	0.548%
9	3.117	323	333	345	rBV	117223	269501	32.49%	6.189%
10	5.391	694	706	718	rBV	99679	286059	34.48%	6.569%
11	5.556	722	733	752	rVB	98771	277607	33.47%	6.375%
12	5.958	789	799	818	rBV	108418	287149	34.62%	6.594%
13	6.245	834	846	857	rBV2	53687	157851	19.03%	3.625%
14	6.763	921	931	942	rBV	150404	351478	42.37%	8.072%
15	8.110	1145	1152	1163	rVB4	5434	13047	1.57%	0.300%
16	8.427	1198	1204	1211	rBV	20078	36527	4.40%	0.839%
17	8.507	1211	1217	1226	rVV2	39821	69000	8.32%	1.585%
18	8.653	1231	1241	1249	rBV	522273	829525	100.00%	19.050%
19	8.842	1264	1272	1282	rBV	38208	62519	7.54%	1.436%
20	8.958	1287	1291	1299	rVV2	7699	13179	1.59%	0.303%
21	9.049	1301	1306	1312	rVB2	7705	11356	1.37%	0.261%
22	9.567	1387	1391	1401	rVB3	6941	11567	1.39%	0.266%
23	10.055	1460	1471	1477	rBV	319742	440249	53.07%	10.110%
24	10.146	1482	1486	1491	rVB	14226	18974	2.29%	0.436%
25	11.079	1634	1639	1649	rBV	426025	545070	65.71%	12.518%
26	12.024	1789	1794	1801	rVB	312431	385187	46.43%	8.846%
27	12.244	1826	1830	1836	rBV2	7425	9940	1.20%	0.228%
28	12.317	1838	1842	1848	rVB4	5432	8422	1.02%	0.193%
29	12.616	1884	1891	1894	rBV2	5569	8829	1.06%	0.203%
30	13.134	1964	1976	1980	rBV6	5226	17198	2.07%	0.395%
31	13.640	2052	2059	2061	rBV2	8250	15503	1.87%	0.356%
32	13.664	2061	2063	2069	rVV	11384	12888	1.55%	0.296%
33	13.780	2072	2082	2091	rVB	10207	18244	2.20%	0.419%
34	14.603	2212	2217	2220	rBV	6974	10832	1.31%	0.249%
35	14.780	2240	2246	2255	rBV2	12493	23305	2.81%	0.535%
36	15.481	2355	2361	2365	rBV3	5023	8396	1.01%	0.193%

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H-3RA

Integration Parameters: RTEINT.P
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Sampling : 1 Min Area: 3 % of largest Peak
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Stop Thrs : 0 Peak Location: TOP

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Title : SW846 8260

37	15.615	2377	2383	2386	rBV4	6478	10214	1.23%	0.235%

Sum of corrected areas: 4354411

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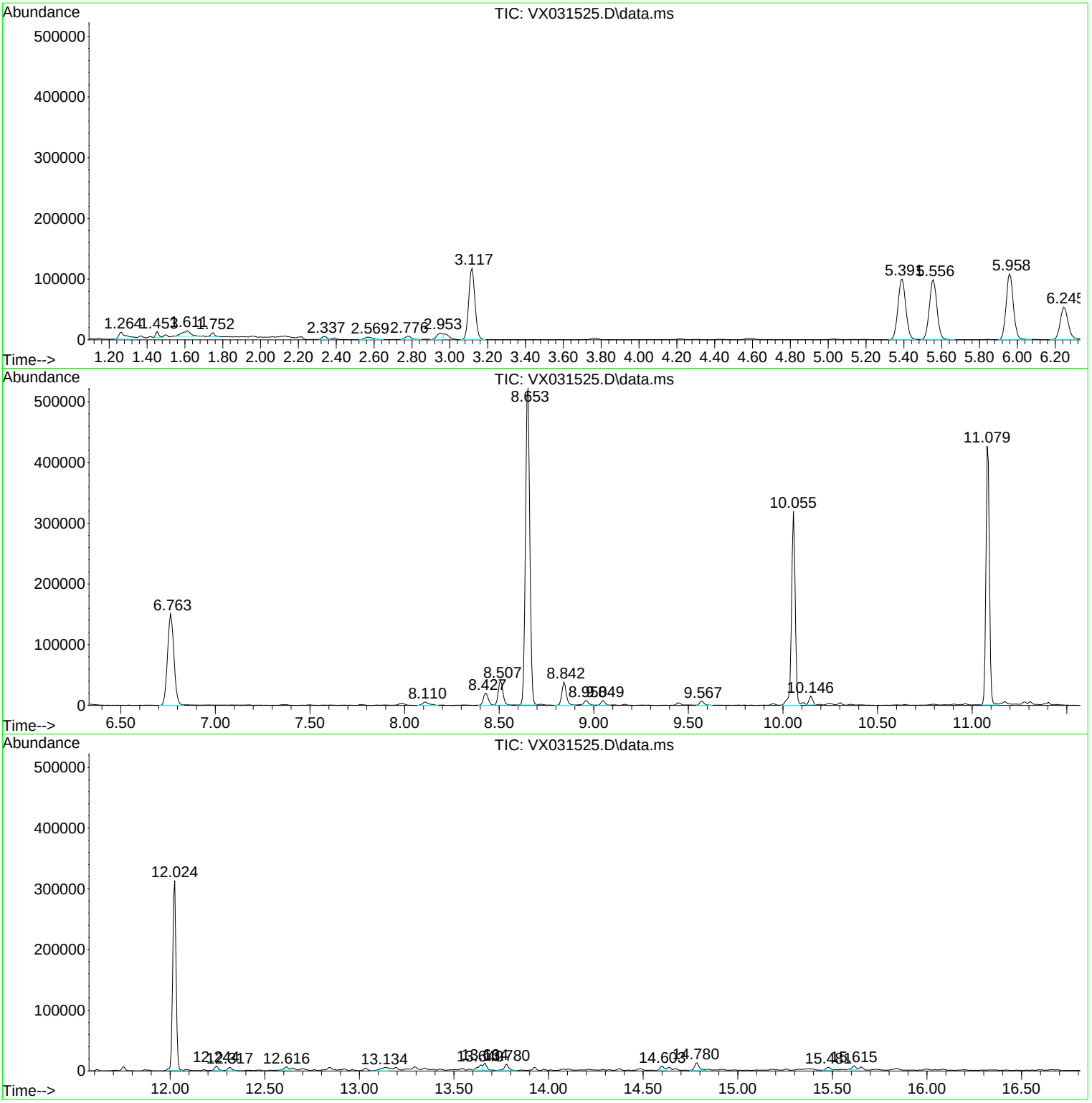
ClientSampleId :
H-3RA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091922W.M
Quant Title : SW846 8260

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



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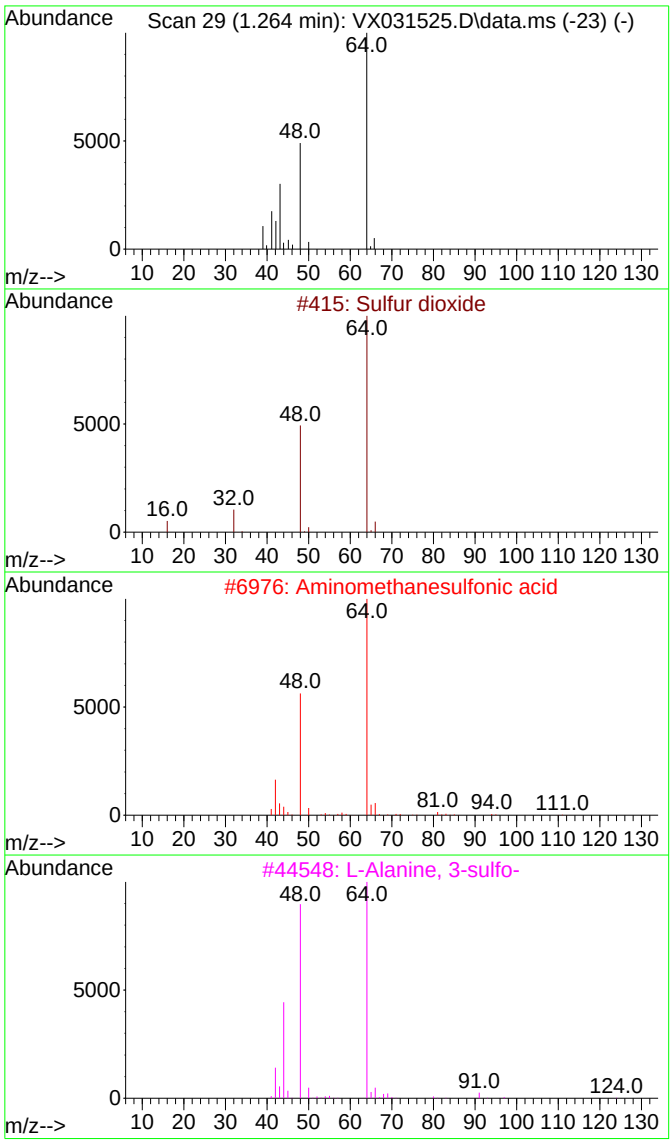
Quant Title : SW846 8260

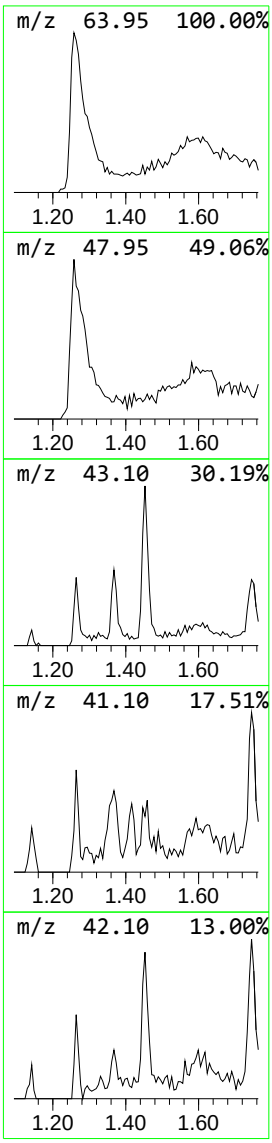
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Sulfur dioxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.264	6.43 ug/l	35703	Pentafluorobenzene	5.556

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	83
3	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	7
5	Ethyl Chloride	64	C2H5Cl	000075-00-3	3





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Instrument :
MSVOA_X
ClientSampleId :
H-3RA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091922W.M
Quant Title : SW846 8260

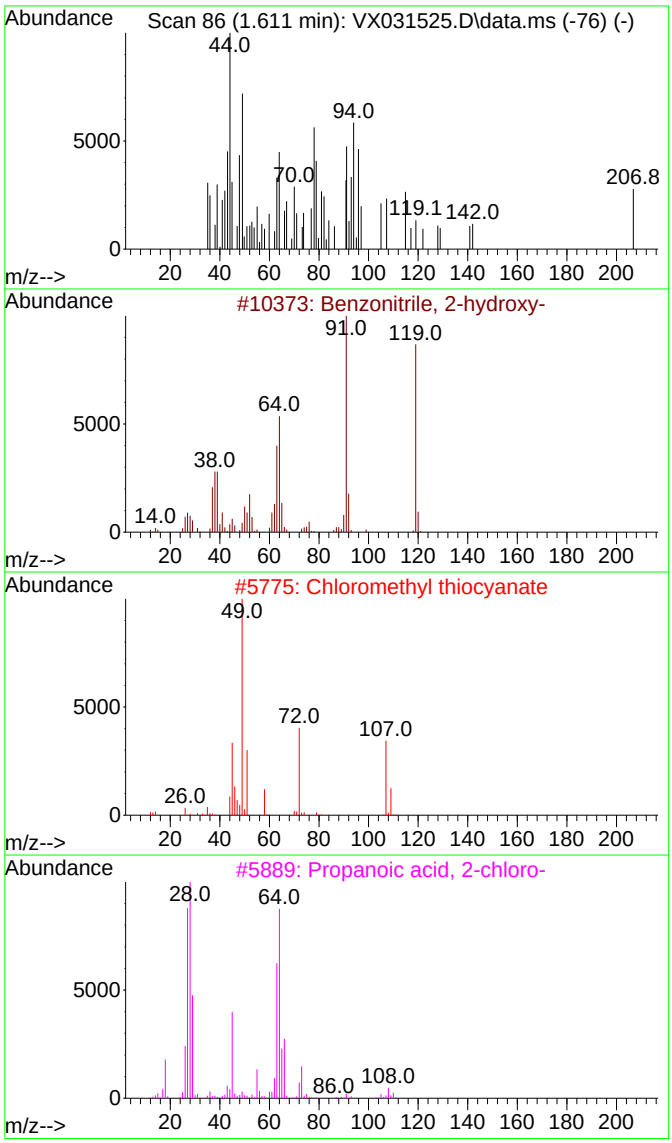
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

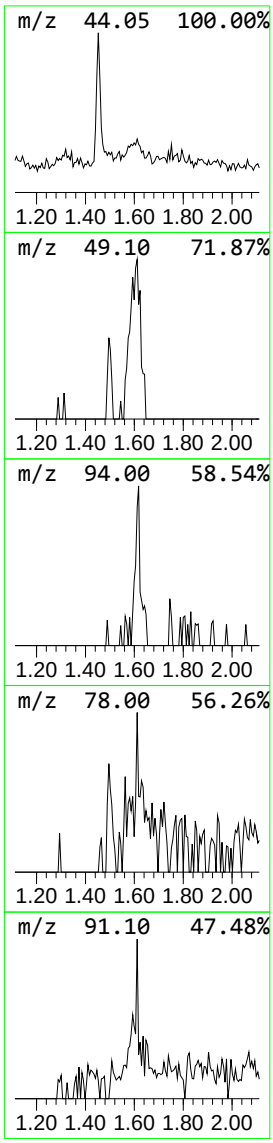
****

Peak Number 2 unknown1.611 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.611	5.16 ug/l	28631	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzonitrile, 2-hydroxy-	119	C7H5NO	000611-20-1	15
2	Chloromethyl thiocyanate	107	C2H2ClNS	003268-79-9	14
3	Propanoic acid, 2-chloro-	108	C3H5ClO2	000598-78-7	10
4	Benzene, azido-	119	C6H5N3	000622-37-7	10
5	Acetic acid, bromochloro-	172	C2H2BrClO2	005589-96-8	10





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Instrument :
MSVOA_X
ClientSampleId :
H-3RA

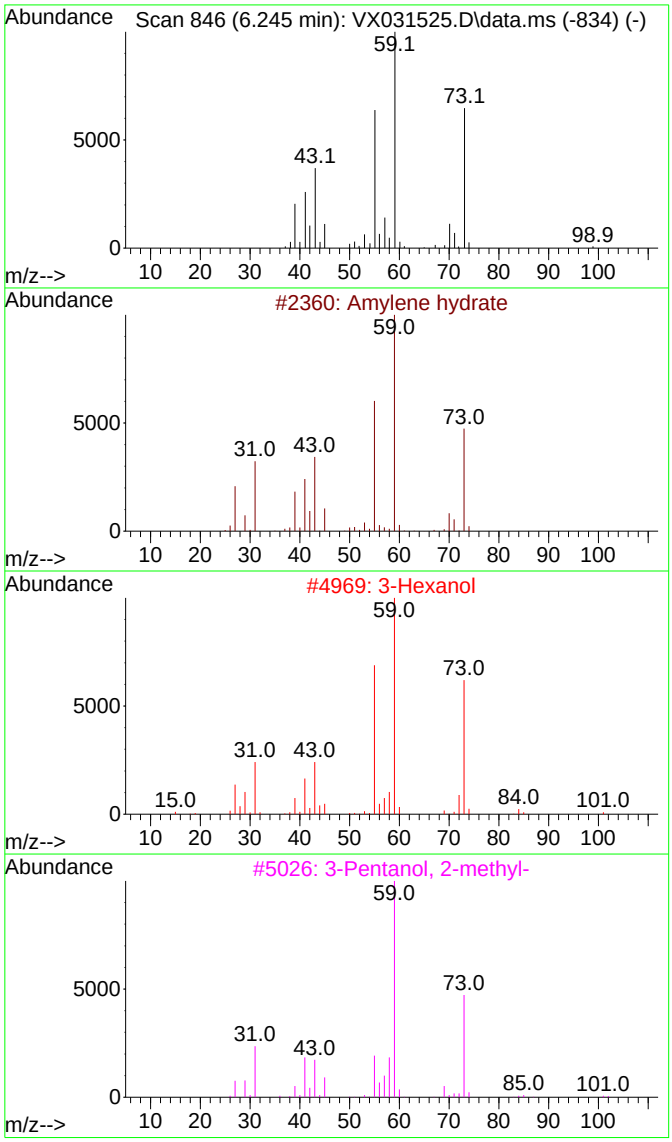
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091922W.M
Quant Title : SW846 8260

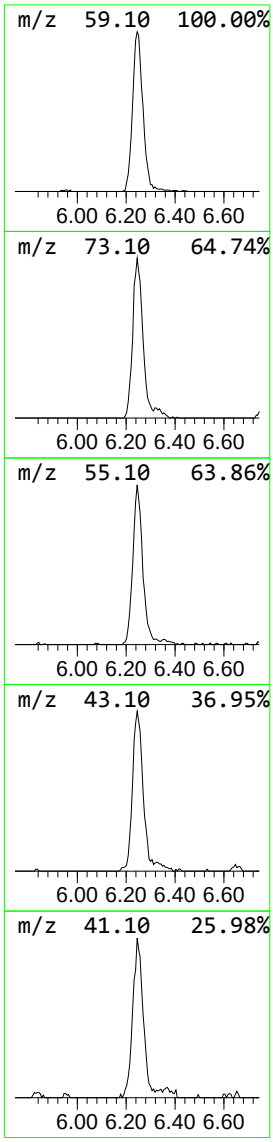
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Amylene hydrate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.245	22.46 ug/l	157851	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Amylene hydrate	88	C5H12O	000075-85-4	78
2	3-Hexanol	102	C6H14O	000623-37-0	59
3	3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	36
4	Carbonic acid, 3-pentyl propyl e...	174	C9H18O3	1000325-64-0	36
5	Propanenitrile, 3-ethoxy-	99	C5H9NO	002141-62-0	33





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ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
H-3RA

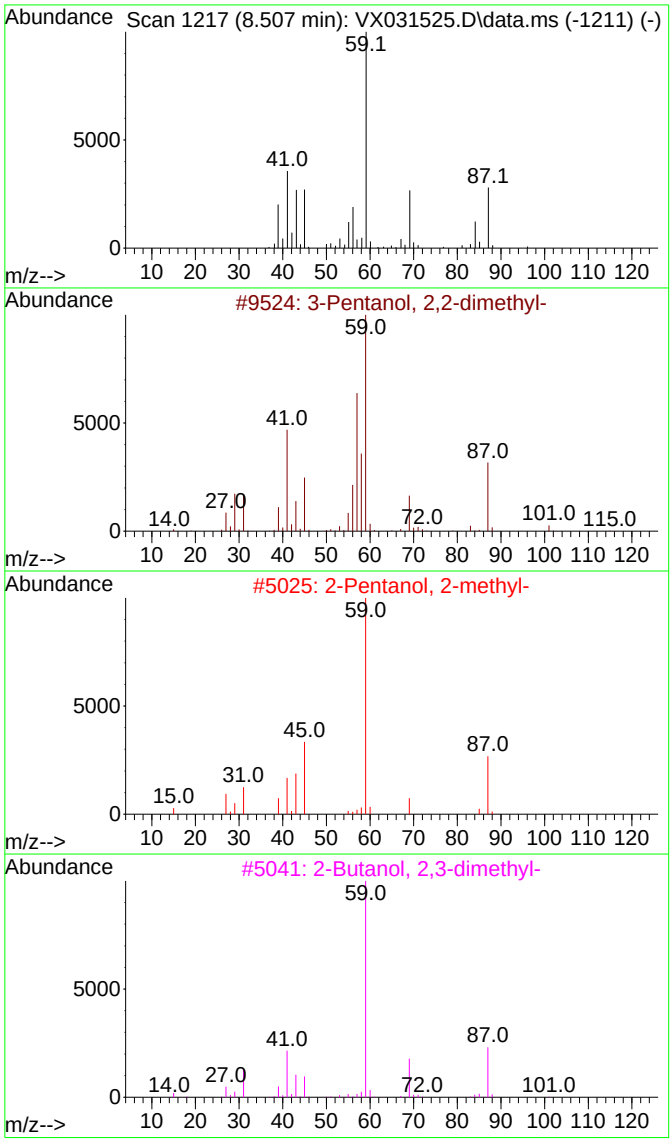
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091922W.M
Quant Title : SW846 8260

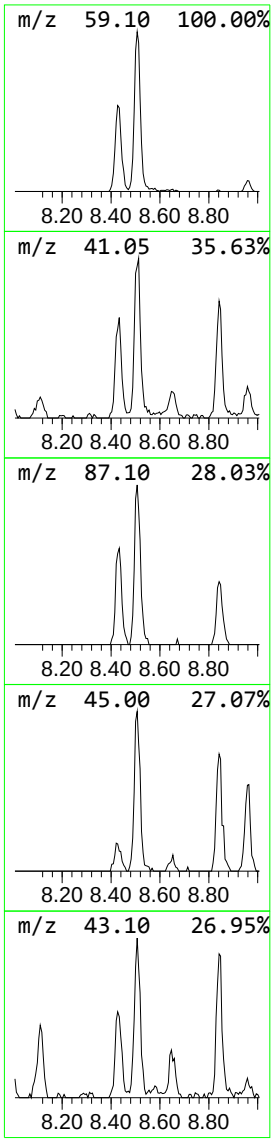
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 3-Pentanol, 2,2-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.507	7.84 ug/l	69000	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanol, 2,2-dimethyl-	116	C7H16O	003970-62-5	78
2	2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	72
3	2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	50
4	3-Hexanol, 5-methyl-	116	C7H16O	000623-55-2	38
5	4-Pentene-2-ol, 2-methyl	100	C6H12O	000624-97-5	37





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Instrument :
MSVOA_X
ClientSampleId :
H-3RA

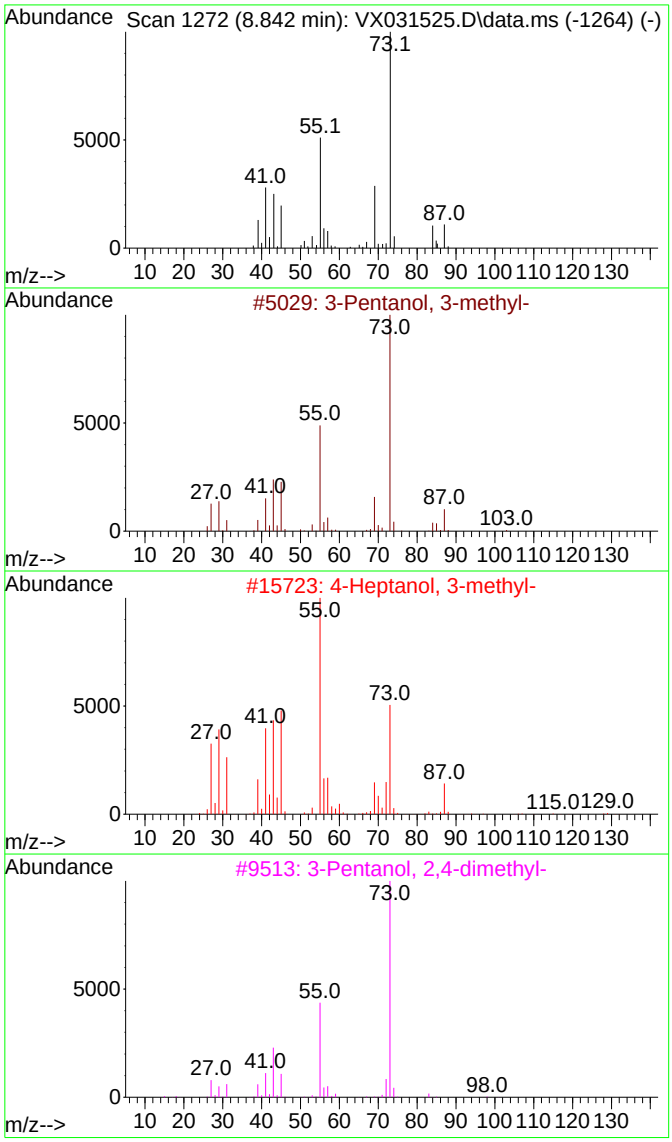
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091922W.M
Quant Title : SW846 8260

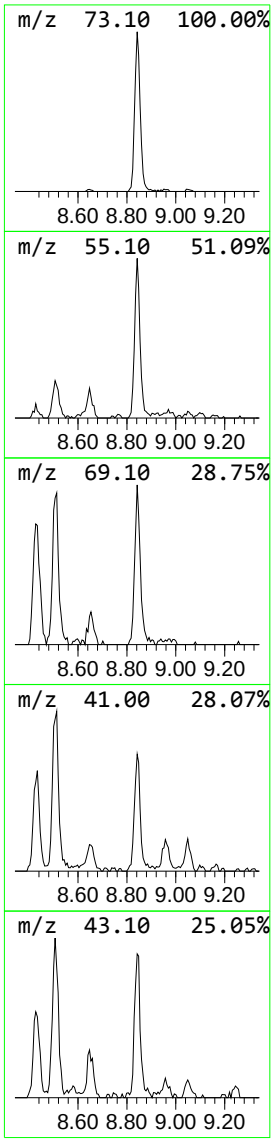
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 3-Pentanol, 3-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.842	7.10 ug/l	62519	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	83
2	4-Heptanol, 3-methyl-	130	C8H18O	001838-73-9	38
3	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	32
5	Methane, isothiocyanato-	73	C2H3NS	000556-61-6	25





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	1.264	6.4	ug/l	35703	1	5.556	277607	50.0
unknown1.611	1.611	5.2	ug/l	28631	1	5.556	277607	50.0
Amylene hydrate	6.245	22.5	ug/l	157851	2	6.763	351478	50.0
3-Pentanol, 2,2...	8.507	7.8	ug/l	69000	3	10.055	440249	50.0
3-Pentanol, 3-m...	8.842	7.1	ug/l	62519	3	10.055	440249	50.0