LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062222\
Data File : VX029704.D
Acq On : 22 Jun 2022 17:10
Operator : JC/MD
Sample : N3293-19
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
30986

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\82X061822W.M
Title : SW846 8260

Signal : TIC: VX029704.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.276	26	31	44	rBV2	33971	128206	4.07%	0.896%
2	1.453	56	60	65	rBV	29645	32138	1.02%	0.225%
3	2.379	205	212	218	rBV	202260	336422	10.67%	2.351%
4	2.544	230	239	253	rBV2	81931	219701	6.97%	1.535%
5	2.702	259	265	276	rBV	291391	504849	16.02%	3.527%
6	2.964	299	308	324	rVB2	33658	95742	3.04%	0.669%
7	4.562	562	570	588	rBV2	43715	129533	4.11%	0.905%
8	5.019	635	645	656	rBV4	9987	33945	1.08%	0.237%
9	5.281	671	688	697	rBV	130543	374851	11.89%	2.619%
10	5.391	697	706	722	rVV	150955	451122	14.31%	3.152%
11	5.555	722	733	751	rVB	277059	778020	24.69%	5.436%
12	5.958	787	799	808	rBV	157830	418398	13.28%	2.923%
13	6.043	808	813	821	rVB2	20265	52409	1.66%	0.366%
14	6.763	921	931	946	rBV	408325	992323	31.49%	6.933%
15	7.458	1040	1045	1057	rVB	16235	34593	1.10%	0.242%
16	7.695	1078	1084	1095	rVB6	26428	66811	2.12%	0.467%
17	7.951	1122	1126	1137	rVB2	18139	32761	1.04%	0.229%
18	8.220	1160	1170	1178	rBV	36820	61382	1.95%	0.429%
19	8.415	1194	1202	1208	rBV2	16187	32354	1.03%	0.226%
20	8.652	1234	1241	1248	rBV	843140	1303845	41.37%	9.110%
21	8.720	1248	1252	1256	rVV	32533	50987	1.62%	0.356%
22	8.768	1256	1260	1272	rVB	80022	132258	4.20%	0.924%
23	9.457	1364	1373	1375	rBV4	37951	73650	2.34%	0.515%
24	9.488	1375	1378	1384	rVB	120833	175960	5.58%	1.229%
25	10.055	1461	1471	1475	rBV	809625	1134354	35.99%	7.926%
26	10.097	1475	1478	1483	rVV	172289	233212	7.40%	1.629%
27	10.152	1483	1487	1492	rVV	61542	80290	2.55%	0.561%
28	10.305	1508	1512	1520	rVB	27946	45474	1.44%	0.318%
29	10.408	1523	1529	1532	rBV	28587	46306	1.47%	0.324%
30	10.506	1541	1545	1551	rBV2	34407	46337	1.47%	0.324%
31	10.646	1563	1568	1571	rBV	24019	35764	1.13%	0.250%
32	10.756	1581	1586	1599	rBV	143988	233984	7.42%	1.635%
33	10.859	1599	1603	1608	rVV3	31052	52639	1.67%	0.368%
34	10.908	1608	1611	1619	rVB3	26924	40329	1.28%	0.282%
35	11.085	1634	1640	1645	rBV	625684	841312	26.69%	5.878%
36	11.134	1645	1648	1654	rVB2	34422	49317	1.56%	0.345%

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Integration Parameters: RTEINT.P
Integrator: RTE
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Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Title : SW846 8260

37	11.280	1663	1672	1676	rBV3	31286	52248	1.66%	0.365%
38	11.353	1680	1684	1689	rVB	55769	76978	2.44%	0.538%
39	11.573	1712	1720	1723	rBV	72017	102652	3.26%	0.717%
40	11.603	1723	1725	1729	rVV	65304	98144	3.11%	0.686%
41	11.634	1729	1730	1738	rVV5	31291	59210	1.88%	0.414%
42	11.756	1746	1750	1755	rBV	27114	36928	1.17%	0.258%
43	11.871	1765	1769	1776	rVB	90232	123546	3.92%	0.863%
44	12.024	1789	1794	1801	rVB	865696	1049757	33.31%	7.335%
45	12.219	1821	1826	1836	rBV	2521671	3151688	100.00%	22.021%
46	12.304	1837	1840	1845	rVB2	61890	88716	2.81%	0.620%
47	12.804	1912	1922	1928	rBV2	43131	74900	2.38%	0.523%
48	12.957	1942	1947	1953	rVB6	25154	46036	1.46%	0.322%

Sum of corrected areas: 14312381

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MSVOA_X
ClientSampleId :
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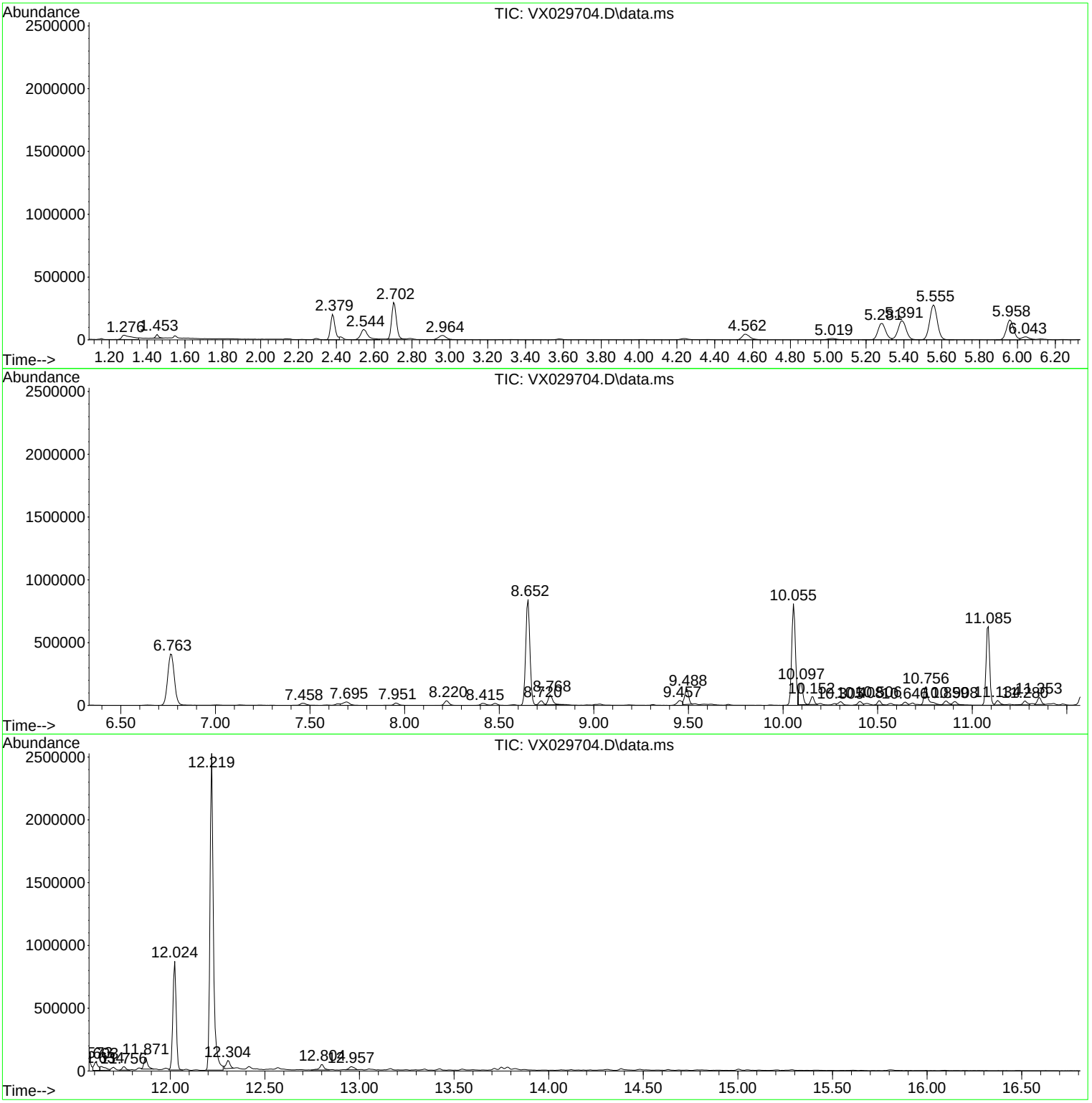
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

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



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Data File : VX029704.D
Acq On : 22 Jun 2022 17:10
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ALS Vial : 21 Sample Multiplier: 1

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MSVOA_X
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

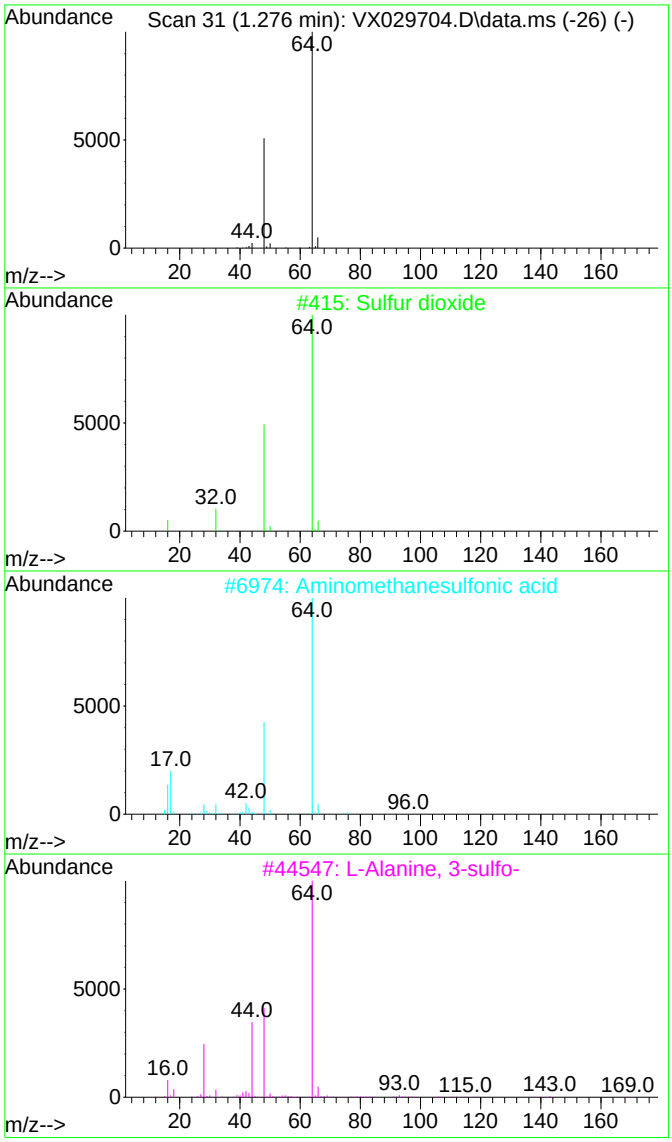
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

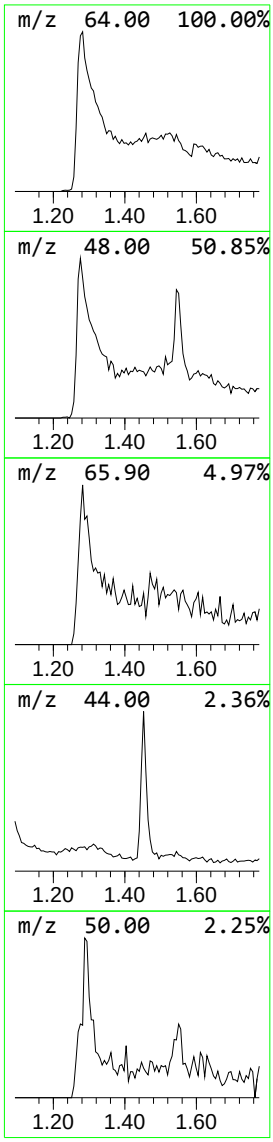
****

Peak Number 1 Sulfur dioxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.276	8.24 ug/l	128206	Pentafluorobenzene	5.555

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	5
5	Ethyl Chloride	64	C2H5Cl	000075-00-3	4





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Instrument :
MSVOA_X
ClientSampleId :
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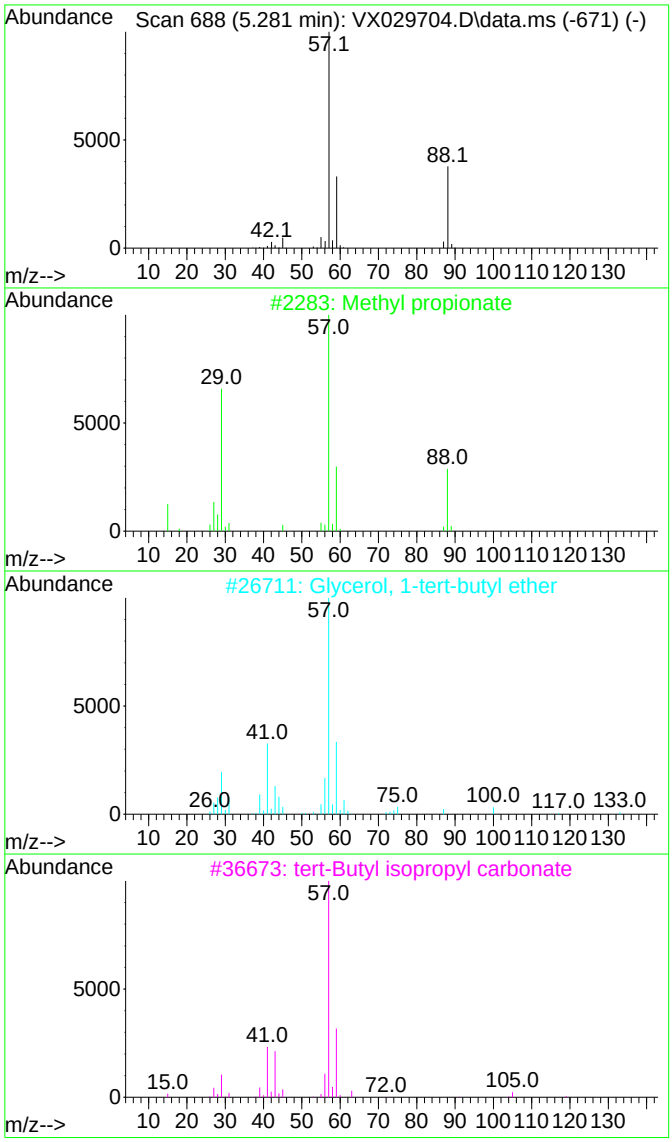
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

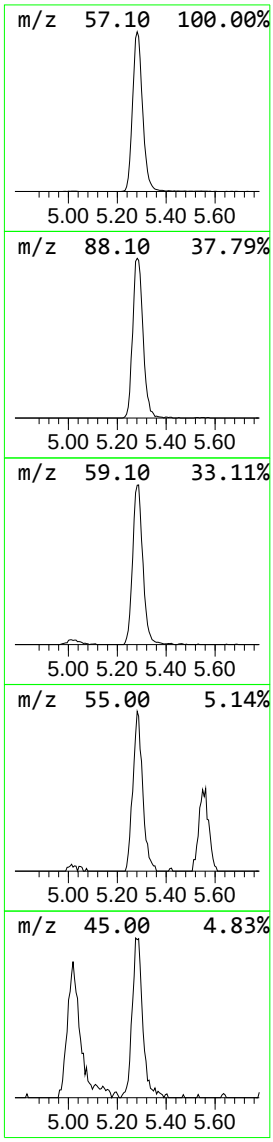
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Methyl propionate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.281	24.09 ug/l	374851	Pentafluorobenzene	5.555

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl propionate	88	C4H8O2	000554-12-1	90
2	Glycerol, 1-tert-butyl ether	148	C7H16O3	1010381-75-8	33
3	tert-Butyl isopropyl carbonate	160	C8H16O3	030221-21-7	9
4	Hydrazinecarboxylic acid, 1,1-di...	132	C5H12N2O2	000870-46-2	9
5	Urea, N,N'-dimethyl-	88	C3H8N2O	000096-31-1	5





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Instrument :
MSVOA_X
ClientSampleId :
30986

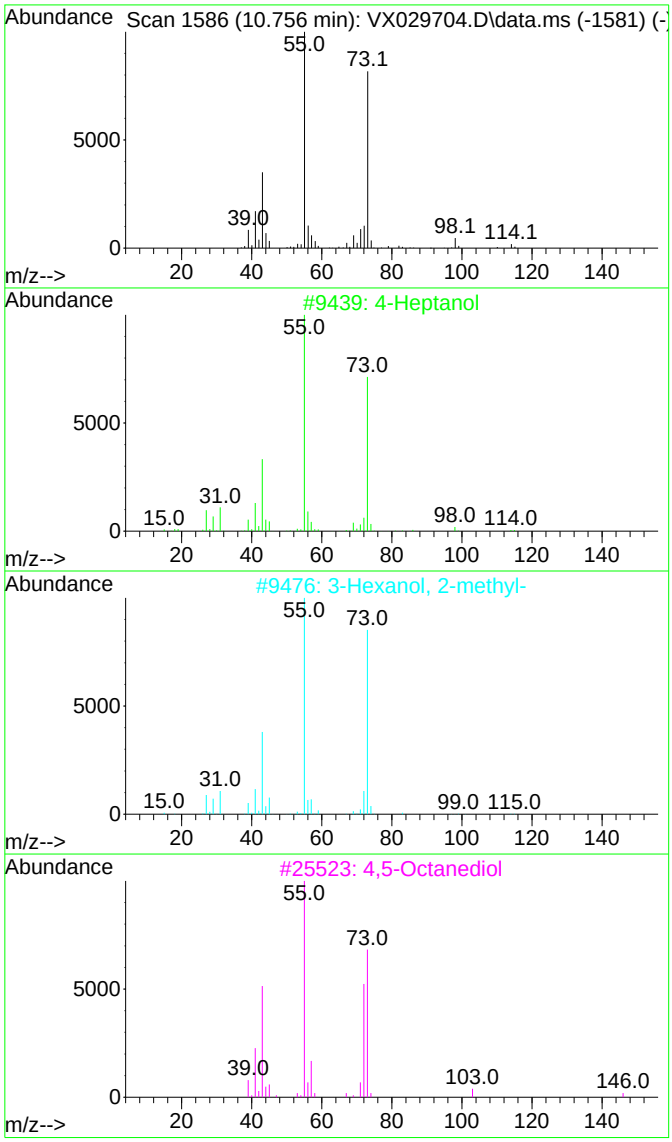
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

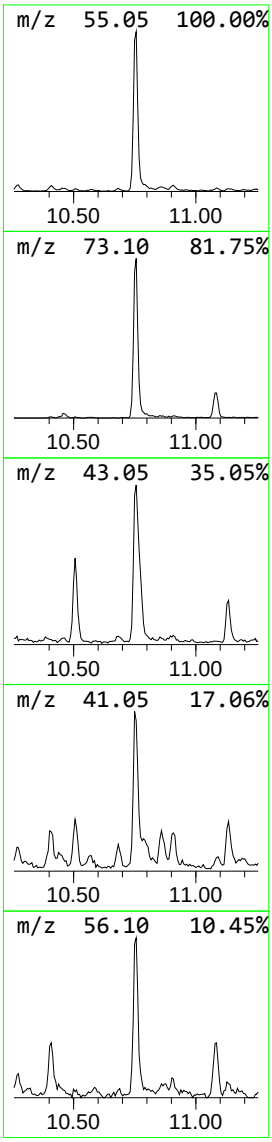
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 4-Heptanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.756	10.31 ug/l	233984	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanol	116	C7H16O	000589-55-9	72
2	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	50
3	4,5-Octanediol	146	C8H18O2	022607-10-9	42
4	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	38
5	5-Hydroxy-4-octanone	144	C8H16O2	000496-77-5	33





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Instrument :
MSVOA_X
ClientSampleId :
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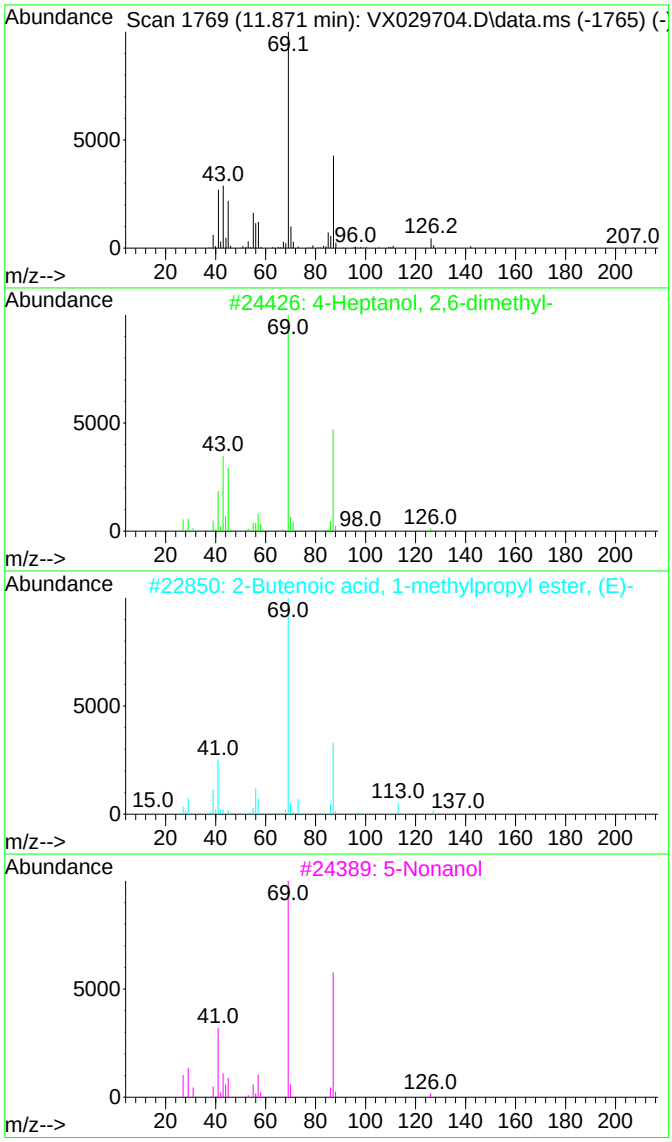
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

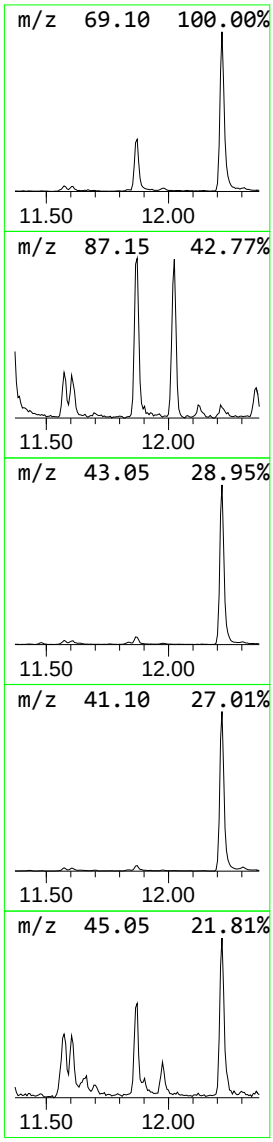
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 4-Heptanol, 2,6-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.871	5.88 ug/l	123546	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanol, 2,6-dimethyl-	144	C9H20O	000108-82-7	78
2	2-Butenoic acid, 1-methylpropyl ...	142	C8H14O2	010371-45-6	64
3	5-Nonanol	144	C9H20O	000623-93-8	64
4	1,2-Hexanediol	118	C6H14O2	006920-22-5	64
5	4-Octanol, 2-methyl-	144	C9H20O	040575-41-5	64





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MSVOA_X
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

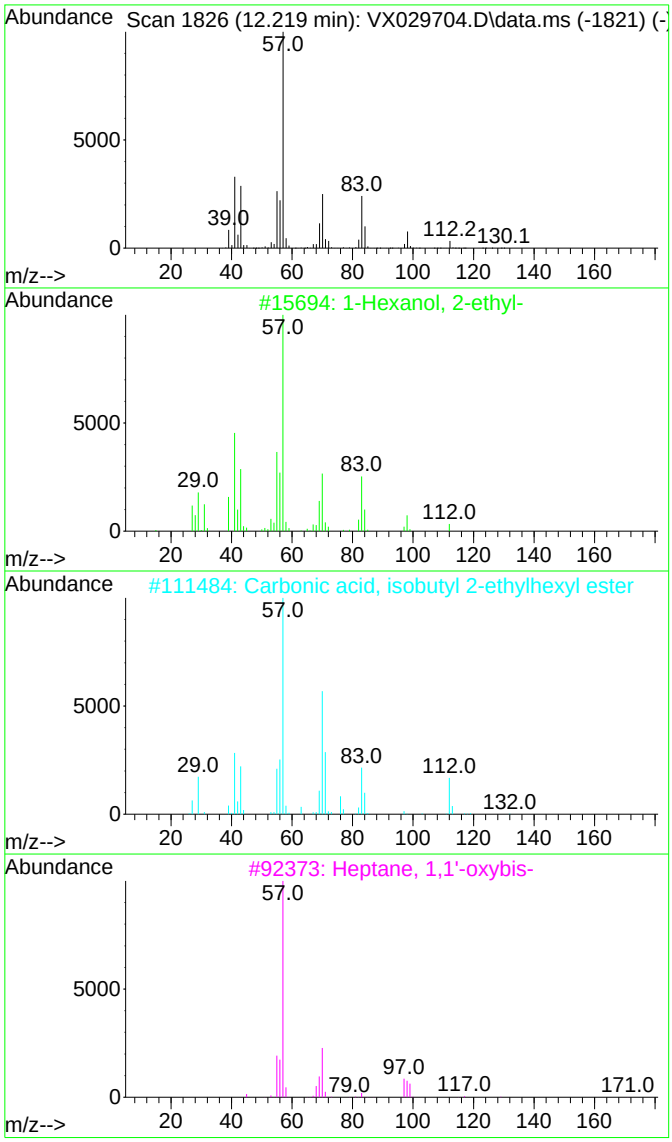
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

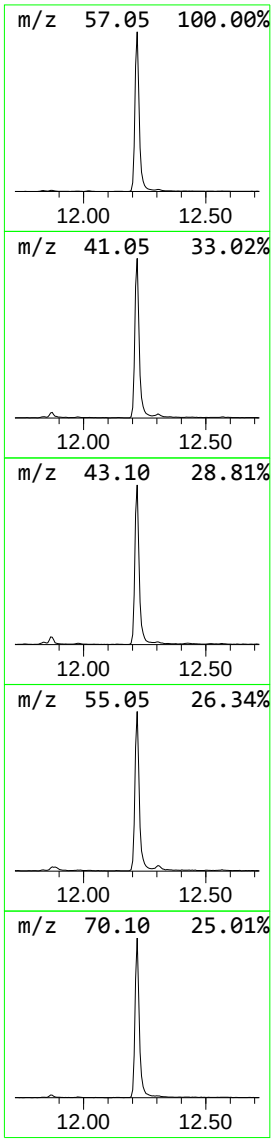
****

Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	150.12 ug/l	3151690	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2	Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000383-13-3	59
3	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
4	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
5	Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	47





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	1.276	8.2	ug/l	128206	1	5.555	778020	50.0
Methyl propionate	5.281	24.1	ug/l	374851	1	5.555	778020	50.0
4-Heptanol	10.756	10.3	ug/l	233984	3	10.055	1134350	50.0
4-Heptanol, 2,6...	11.871	5.9	ug/l	123546	4	12.024	1049760	50.0
1-Hexanol, 2-et...	12.219	150.1	ug/l	3151690	4	12.024	1049760	50.0