LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX092122\
Data File : VX031526.D
Acq On : 21 Sep 2022 15:53
Operator : JC/MD
Sample : N4614-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
H-3RB

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: VX031526.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	25	29	39	rBV2	14576	28222	3.73%	0.774%
2	1.618	77	87	88	rBV6	6525	15528	2.05%	0.426%
3	2.337	197	205	210	rBV	7200	13000	1.72%	0.357%
4	2.776	268	277	288	rVB2	8007	18023	2.39%	0.494%
5	2.983	298	311	323	rBV3	5593	18677	2.47%	0.512%
6	3.117	323	333	345	rVV	102817	237696	31.46%	6.521%
7	5.385	693	705	722	rBV2	91191	261176	34.56%	7.165%
8	5.556	722	733	745	rVV2	81667	232675	30.79%	6.383%
9	5.958	789	799	816	rVB2	98991	261468	34.60%	7.173%
10	6.251	837	847	858	rBV2	33528	100768	13.34%	2.764%
11	6.763	920	931	943	rBV	125140	301177	39.86%	8.262%
12	7.982	1125	1131	1140	rVB3	5510	10904	1.44%	0.299%
13	8.110	1144	1152	1161	rBV2	7615	16373	2.17%	0.449%
14	8.433	1198	1205	1211	rBV	14715	25872	3.42%	0.710%
15	8.507	1211	1217	1224	rVV	23505	39693	5.25%	1.089%
16	8.653	1231	1241	1249	rBV	477321	755633	100.00%	20.730%
17	8.842	1263	1272	1282	rBV	20810	36332	4.81%	0.997%
18	8.964	1286	1292	1300	rVB4	5727	10204	1.35%	0.280%
19	9.049	1300	1306	1311	rBV2	6105	9101	1.20%	0.250%
20	10.055	1460	1471	1477	rBV	278804	374599	49.57%	10.277%
21	10.147	1483	1486	1492	rVB2	8176	10767	1.42%	0.295%
22	11.079	1634	1639	1650	rBV	385309	494600	65.46%	13.569%
23	12.024	1789	1794	1802	rVB	274190	334475	44.26%	9.176%
24	12.244	1826	1830	1834	rBV2	8254	11010	1.46%	0.302%
25	13.780	2076	2082	2090	rVB2	4065	7760	1.03%	0.213%
26	14.603	2210	2217	2221	rBV	6055	9294	1.23%	0.255%
27	14.786	2240	2247	2251	rBV3	6059	10106	1.34%	0.277%

Sum of corrected areas: 3645133

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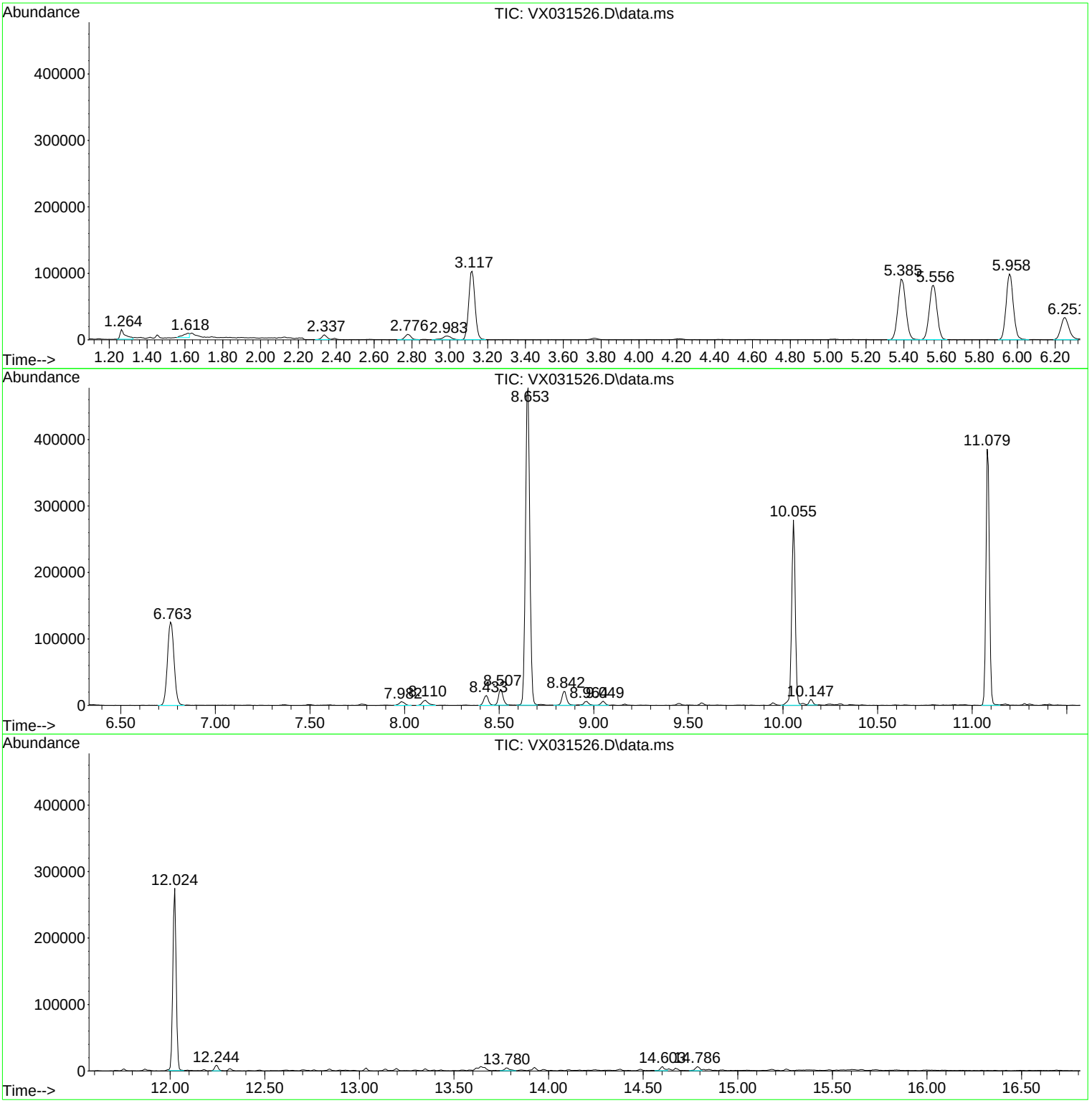
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091922W.M
Quant Title : SW846 8260

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



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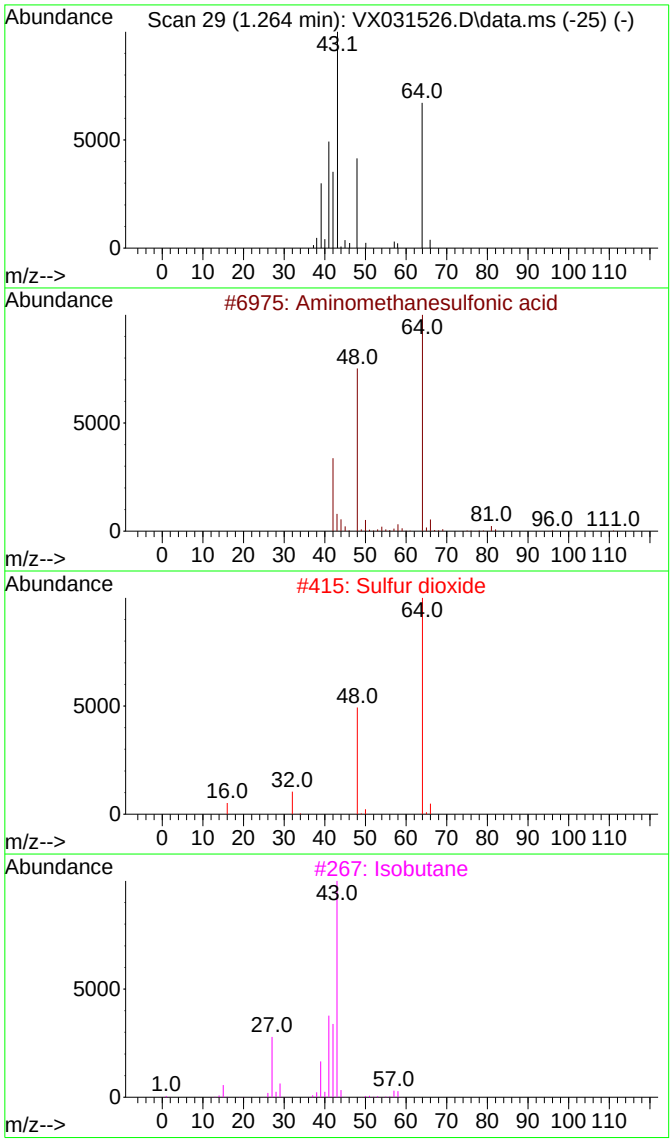
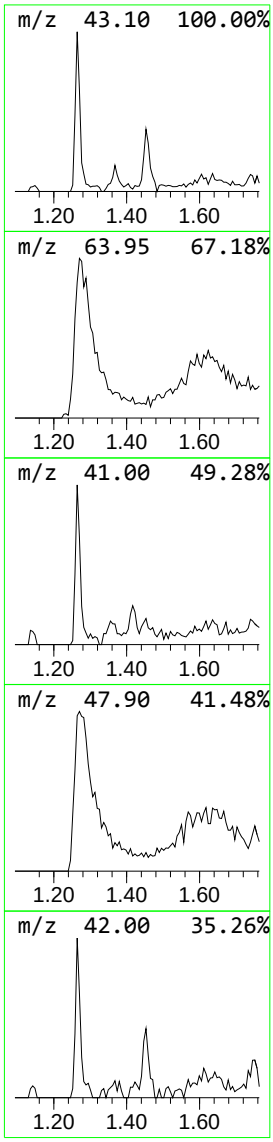
****
Peak Number 1 Aminomethanesulfonic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.264	6.06 ug/l	28222	Pentafluorobenzene	5.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
2	Sulfur dioxide	64	O2S	007446-09-5	45
3	Isobutane	58	C4H10	000075-28-5	9
4	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5	Ethene, 1,2-difluoro-	64	C2H2F2	001691-13-0	5





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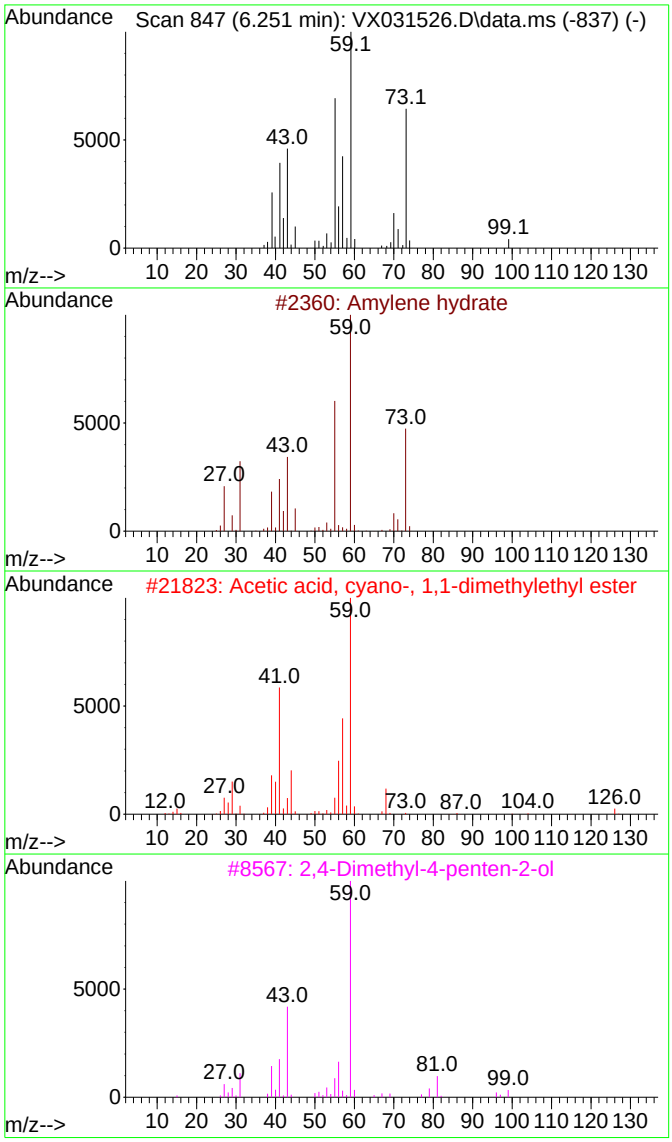
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091922W.M
Quant Title : SW846 8260

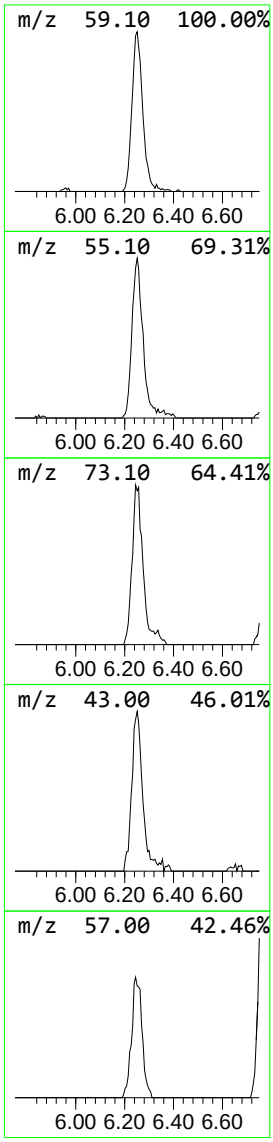
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Amylene hydrate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.251	16.73 ug/l	100768	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Amylene hydrate	88	C5H12O	000075-85-4	59
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	53
3	2,4-Dimethyl-4-penten-2-ol	114	C7H14O	019781-53-4	50
4	HEX-5-EN-3-OL	100	C6H12O	000688-99-3	40
5	Acetaldoxime	59	C2H5NO	000107-29-9	37





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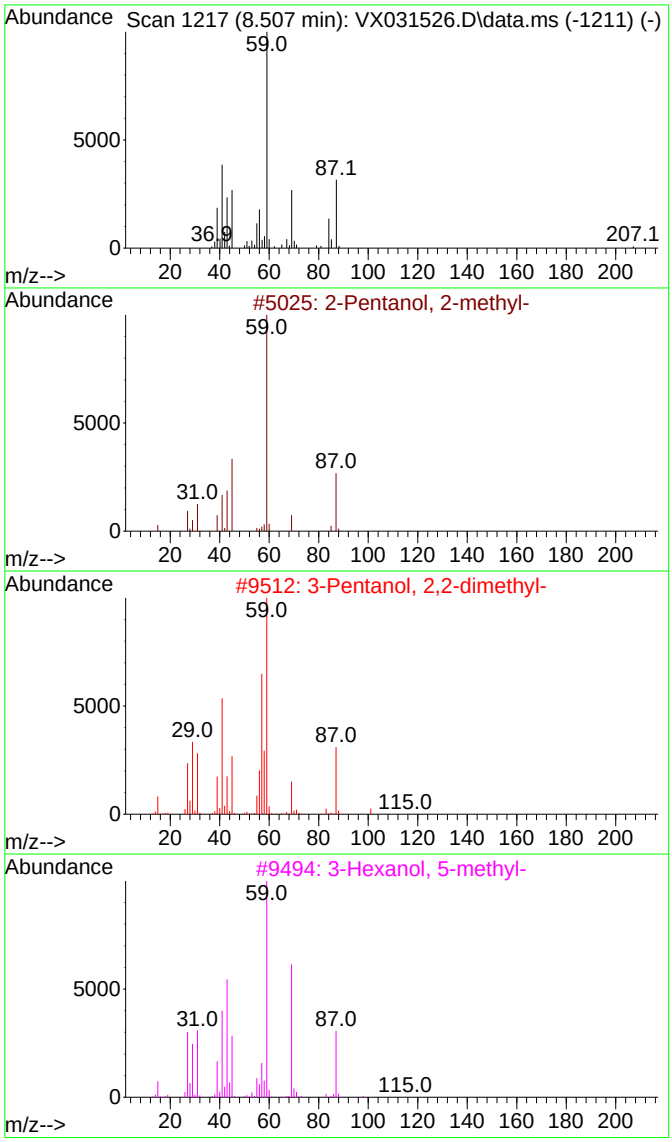
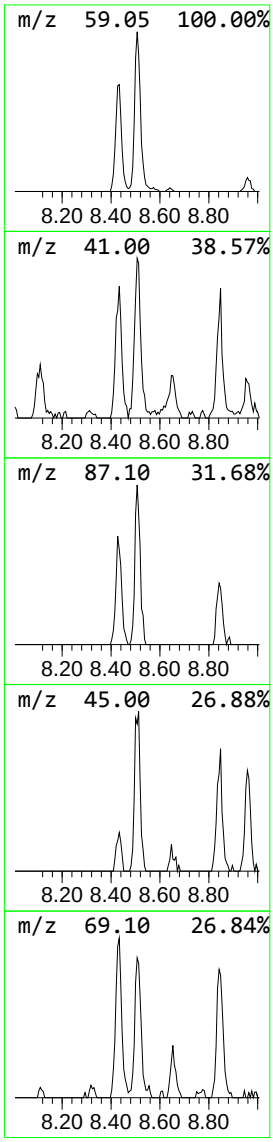
****
Peak Number 3 2-Pentanol, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.507	5.30 ug/l	39693	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	72
2	3-Pentanol, 2,2-dimethyl-	116	C7H16O	003970-62-5	50
3	3-Hexanol, 5-methyl-	116	C7H16O	000623-55-2	50
4	2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	45
5	Pentane, 2-methoxy-	102	C6H14O	006795-88-6	42





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
Aminomethanesul...	1.264	6.1	ug/l	28222	1	5.562	232675	50.0
Amylene hydrate	6.251	16.7	ug/l	100768	2	6.763	301177	50.0
2-Pentanol, 2-m...	8.507	5.3	ug/l	39693	3	10.055	374599	50.0