LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX092222\
Data File : VX031579.D
Acq On : 22 Sep 2022 18:41
Operator : JC/MD
Sample : N4614-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 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: VX031579.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.624	79	88	89	rBV5	4557	10697	1.75%	0.351%
2	2.337	200	205	210	rBV5	3838	8135	1.33%	0.267%
3	2.782	269	278	286	rBV	4244	9033	1.48%	0.296%
4	2.947	297	305	308	rBV	4862	11301	1.85%	0.371%
5	3.117	322	333	344	rVB	82505	187419	30.66%	6.152%
6	5.391	691	706	719	rBV	73183	207726	33.98%	6.818%
7	5.556	722	733	744	rBV	72896	198960	32.55%	6.531%
8	5.958	789	799	812	rBV	77723	206598	33.80%	6.781%
9	6.251	834	847	861	rBV2	37899	121288	19.84%	3.981%
10	6.763	921	931	945	rBV	111197	260571	42.63%	8.553%
11	8.104	1144	1151	1162	rBV6	4143	10014	1.64%	0.329%
12	8.434	1198	1205	1211	rBV	14649	26725	4.37%	0.877%
13	8.507	1211	1217	1227	rVB2	29634	52206	8.54%	1.714%
14	8.647	1233	1240	1261	rVB	390940	611250	100.00%	20.063%
15	8.842	1264	1272	1280	rBV2	28489	47324	7.74%	1.553%
16	8.958	1285	1291	1298	rVB3	5270	9705	1.59%	0.319%
17	9.049	1301	1306	1311	rBV2	6021	8840	1.45%	0.290%
18	9.574	1387	1392	1401	rVB4	5176	8152	1.33%	0.268%
19	10.055	1460	1471	1477	rBV	245593	331388	54.21%	10.877%
20	10.147	1482	1486	1492	rVB2	9985	15268	2.50%	0.501%
21	11.079	1634	1639	1645	rBV	309171	392680	64.24%	12.889%
22	12.024	1789	1794	1802	rBV	237656	293343	47.99%	9.629%
23	13.640	2052	2059	2061	rBV3	6033	9850	1.61%	0.323%
24	13.658	2061	2062	2071	rVB2	6907	8123	1.33%	0.267%

Sum of corrected areas: 3046596

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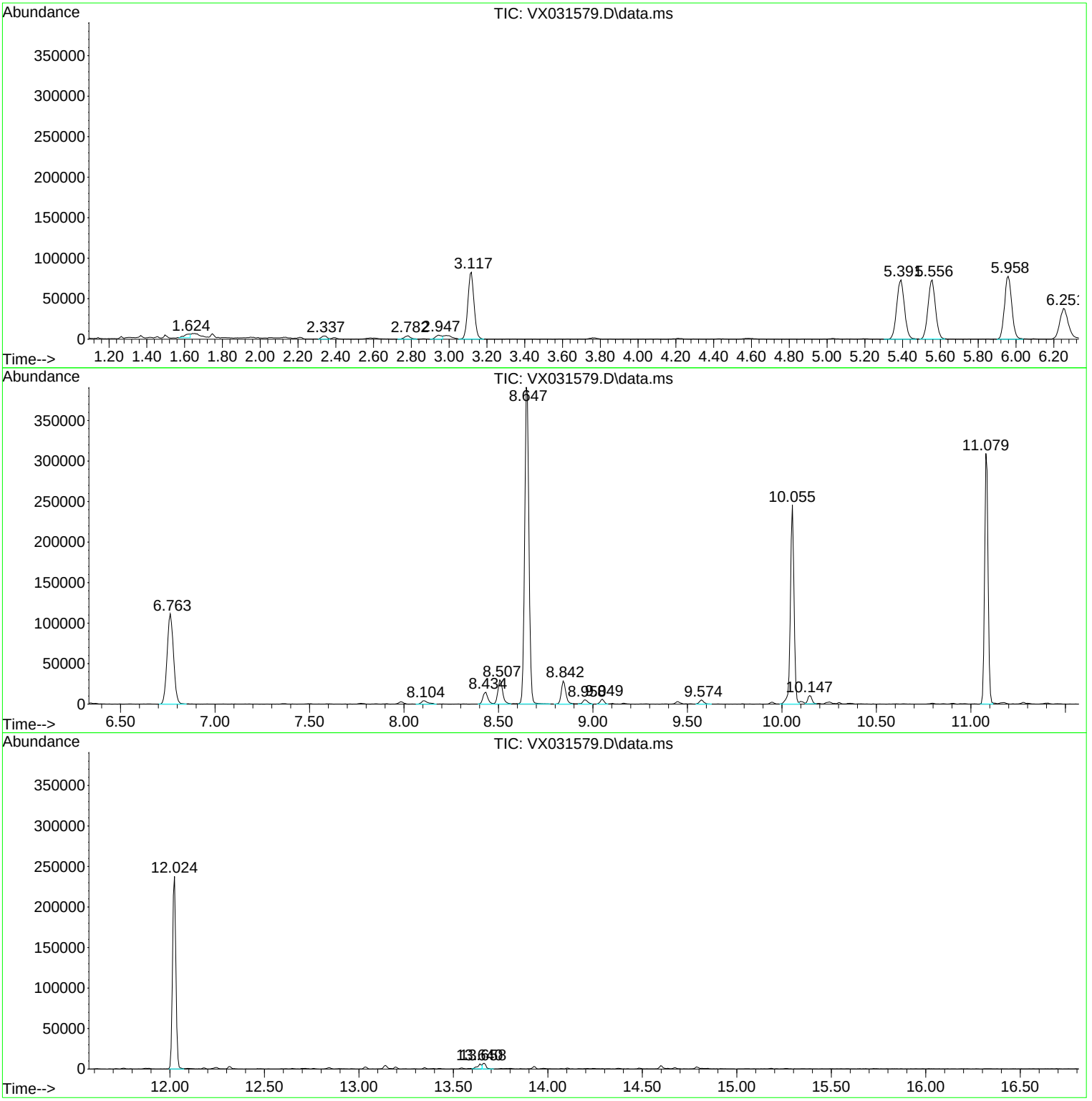
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091922W.M
Quant Title : SW846 8260

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



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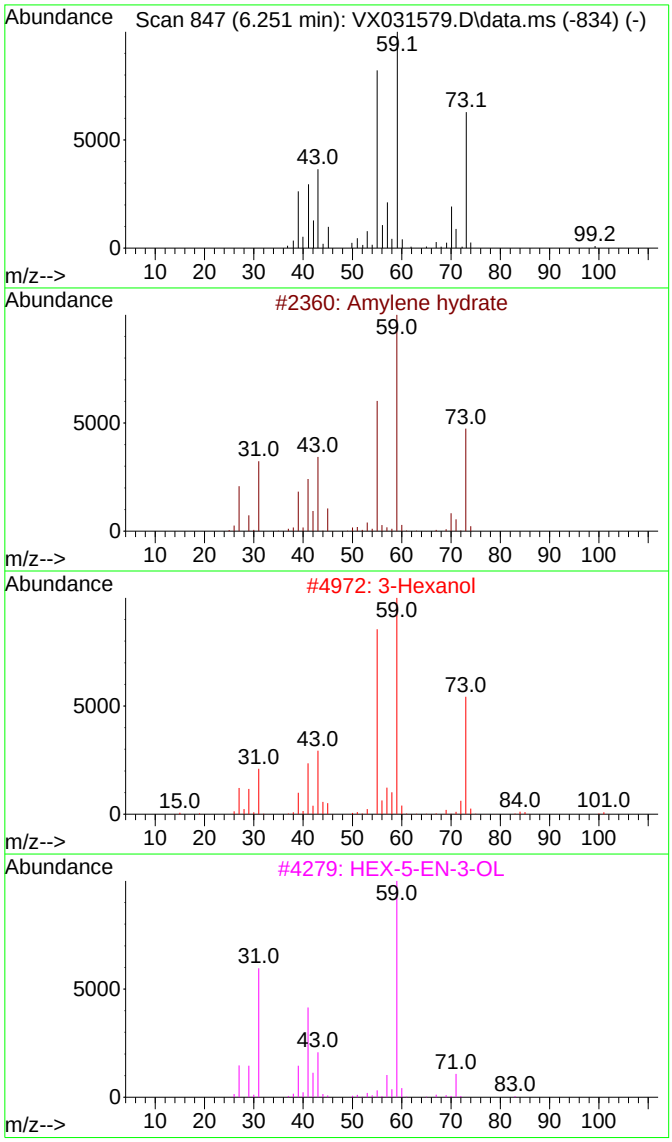
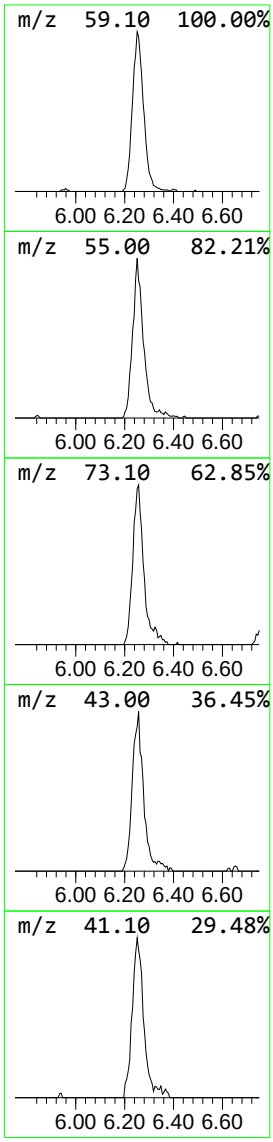
****
Peak Number 1 Amylene hydrate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.251	23.27 ug/l	121288	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Amylene hydrate	88	C5H12O	000075-85-4	72
2	3-Hexanol	102	C6H14O	000623-37-0	50
3	HEX-5-EN-3-OL	100	C6H12O	000688-99-3	38
4	Acetaldoxime	59	C2H5NO	000107-29-9	37
5	3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	36





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Quant Title : SW846 8260

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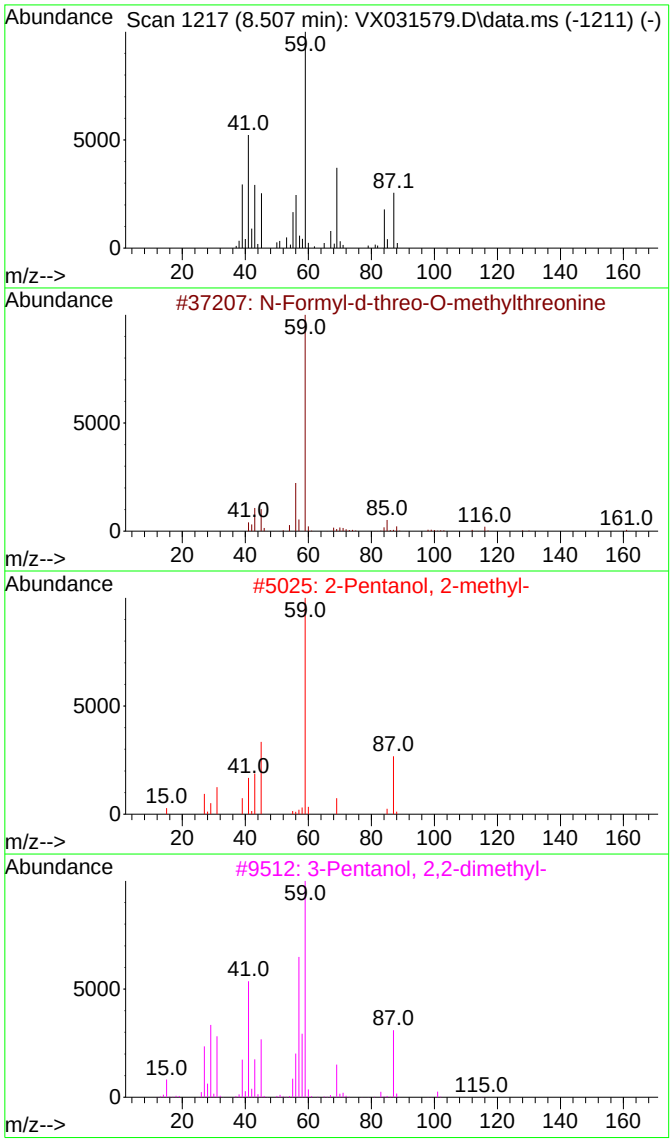
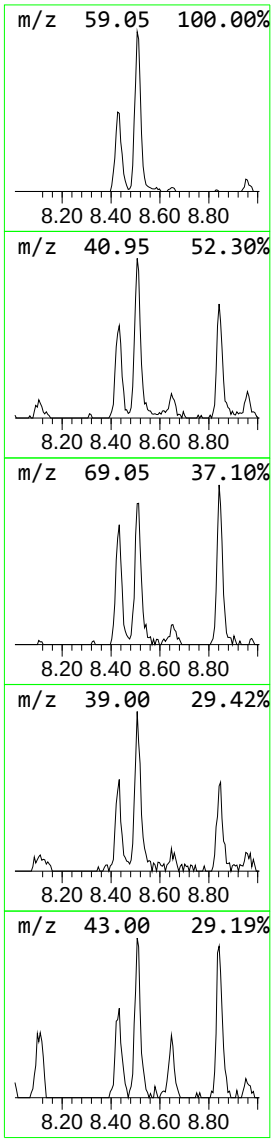
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 N-Formyl-d-threo-O-methylth... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.507	7.88 ug/l	52206	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N-Formyl-d-threo-O-methylthreonine	161	C6H11NO4	1000214-69-5	53
2	2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	50
3	3-Pentanol, 2,2-dimethyl-	116	C7H16O	003970-62-5	40
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	28
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	25





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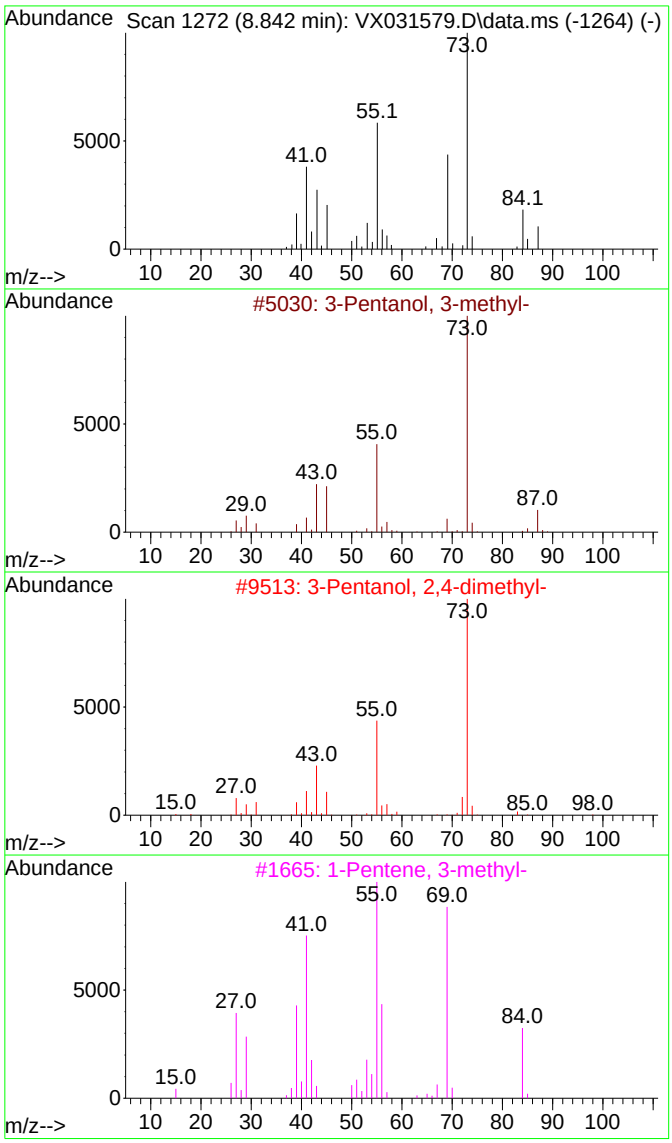
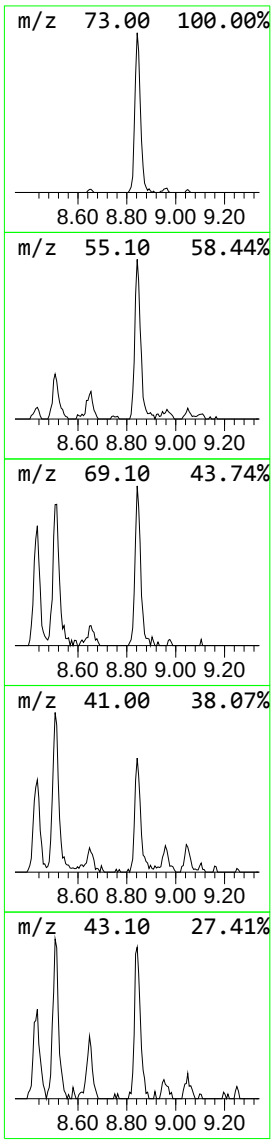
****
Peak Number 3 3-Pentanol, 3-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.842	7.14 ug/l	47324	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	53
2	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	32
3	1-Pentene, 3-methyl-	84	C6H12	000760-20-3	25
4	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	23
5	3-Hexene, (Z)-	84	C6H12	007642-09-3	22





Tentatively Identified Compound (LSC) summary

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					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Amylene hydrate	6.251	23.3	ug/l	121288	2	6.763	260571	50.0
N-Formyl-d-thre...	8.507	7.9	ug/l	52206	3	10.055	331388	50.0
3-Pentanol, 3-m...	8.842	7.1	ug/l	47324	3	10.055	331388	50.0