LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU102419\
Data File : VU035466.D
Acq On : 24 Oct 2019 18:09
Operator : JC/SP
Sample : K5488-12DL 4X
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : H0G54DL

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.1 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_U\METHOD\SOMUTR101719WMA.M
Title : TRACE VOA SOM01.0

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.372	5	10	16	rBV	10358	11156	1.26%	0.135%
2	1.507	46	52	60	rVB	31714	32414	3.65%	0.393%
3	1.613	75	85	94	rBV2	199437	230963	26.02%	2.797%
4	1.932	176	184	197	rVB	70956	94410	10.63%	1.143%
5	2.012	199	209	225	rVB	493897	667747	75.22%	8.086%
6	2.231	269	277	291	rVB4	11924	23796	2.68%	0.288%
7	2.594	379	390	410	rBV	107682	191190	21.54%	2.315%
8	3.076	524	540	556	rBV3	37864	98616	11.11%	1.194%
9	3.166	556	568	580	rVV	100562	202809	22.85%	2.456%
10	3.234	580	589	600	rVB2	16566	33363	3.76%	0.404%
11	3.427	625	649	676	rBV	254195	625580	70.47%	7.575%
12	4.375	931	944	956	rBV5	5083	10672	1.20%	0.129%
13	4.575	992	1006	1019	rBV2	13912	31767	3.58%	0.385%
14	4.655	1019	1031	1036	rVV2	15738	29715	3.35%	0.360%
15	4.713	1036	1049	1086	rVB2	156316	476097	53.63%	5.765%
16	5.115	1157	1174	1198	rBV	125187	295636	33.30%	3.580%
17	5.430	1259	1272	1285	rVB6	7824	17522	1.97%	0.212%
18	5.771	1358	1378	1408	rBV2	236501	664100	74.81%	8.042%
19	5.932	1418	1428	1440	rVB10	6036	13602	1.53%	0.165%
20	6.292	1525	1540	1562	rBV	274619	537132	60.51%	6.504%
21	6.735	1661	1678	1695	rBV	165787	330160	37.19%	3.998%
22	7.604	1934	1948	1967	rBV	66782	131749	14.84%	1.595%
23	7.935	2036	2051	2067	rBV	231508	412042	46.41%	4.989%
24	8.218	2128	2139	2154	rBV	43517	77486	8.73%	0.938%
25	8.684	2272	2284	2320	rBV	390615	887748	100.00%	10.750%
26	8.832	2321	2330	2355	rVB3	65455	138199	15.57%	1.673%
27	8.960	2360	2370	2383	rBV6	8419	19717	2.22%	0.239%
28	9.449	2509	2522	2534	rBV	386275	659655	74.31%	7.988%
29	9.861	2639	2650	2669	rBV2	81619	150654	16.97%	1.824%
30	10.314	2780	2791	2801	rBV6	6610	10715	1.21%	0.130%
31	10.394	2807	2816	2828	rVV6	7202	12105	1.36%	0.147%
32	10.787	2926	2938	2963	rVB	145964	261038	29.40%	3.161%
33	11.841	3250	3266	3284	rBV	262319	496939	55.98%	6.017%
34	12.221	3371	3384	3400	rBV	213164	381847	43.01%	4.624%

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If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR101719WMA.M
Title : TRACE VOA SOM01.0

Sum of corrected areas: 8258341

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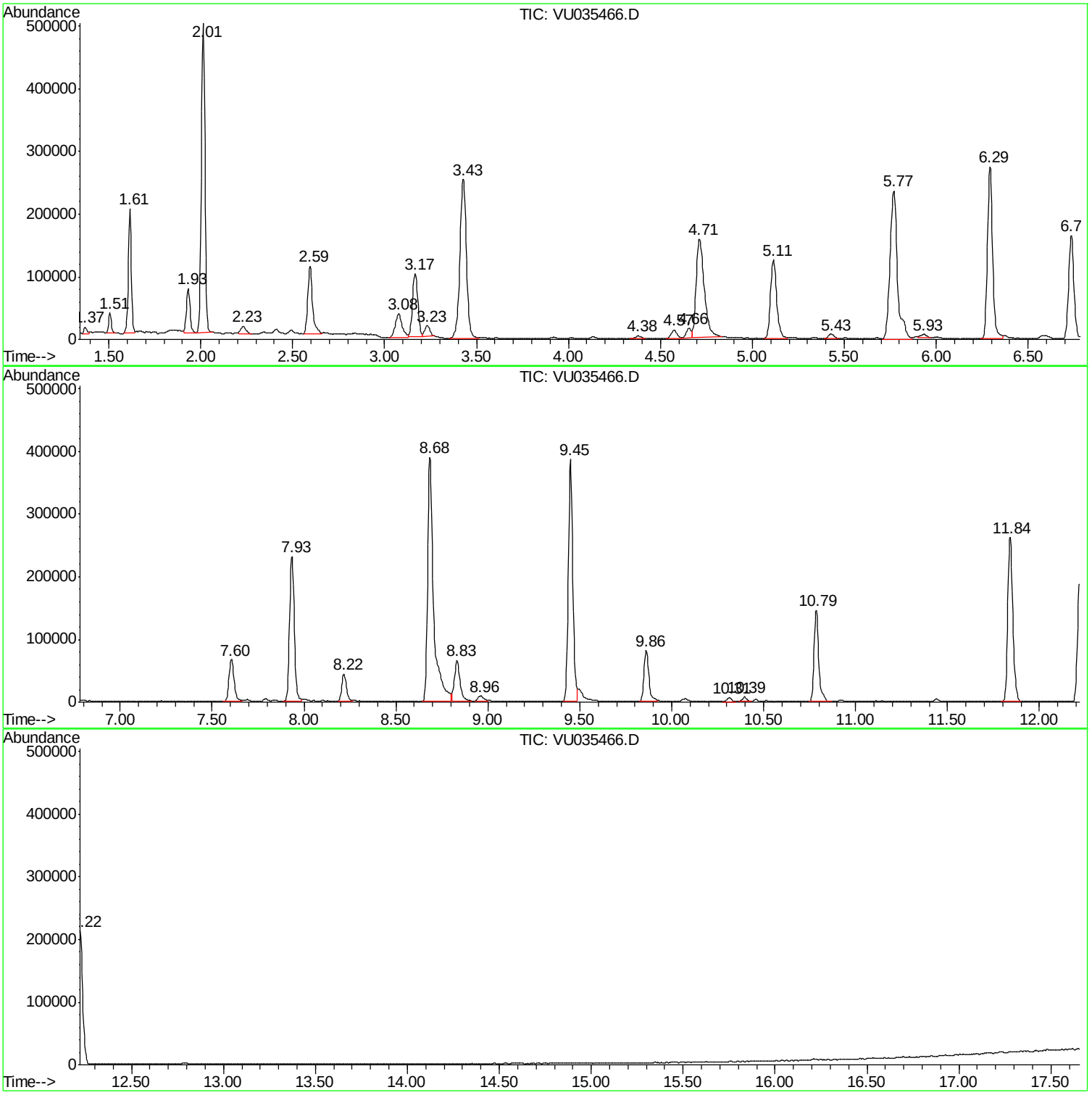
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR101719WMA.M
Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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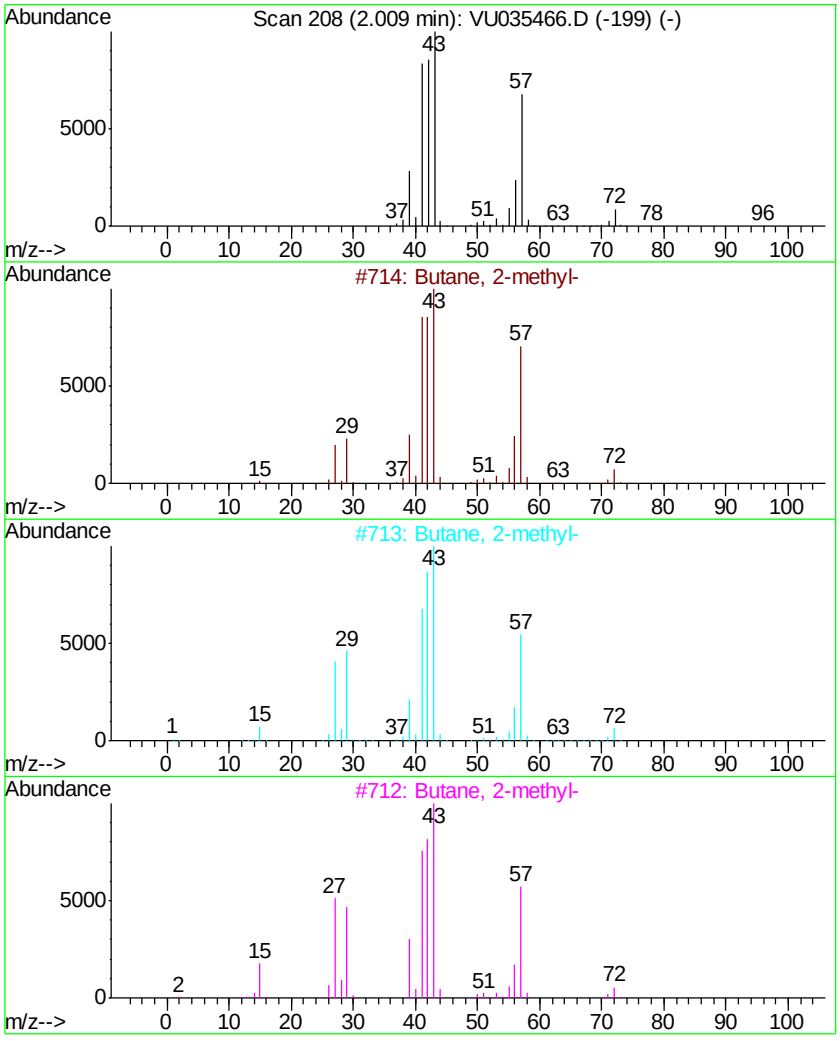
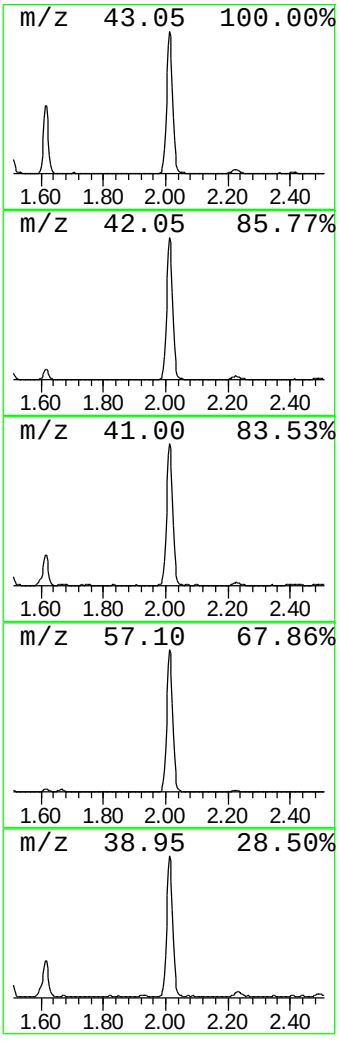
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.01	6.22 ug/L	667747	1,4-Difluorobenzene	6.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	94
2	Butane, 2-methyl-	72	C5H12	000078-78-4	91
3	Butane, 2-methyl-	72	C5H12	000078-78-4	86
4	Pentane	72	C5H12	000109-66-0	42
5	3-Buten-1-ol	72	C4H8O	000627-27-0	28





Library Search Compound Report

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Instrument : MSVOA_U
ClientSampleId : H0G54DL

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR101719WMA.M
Quant Title : TRACE VOA SOM01.0

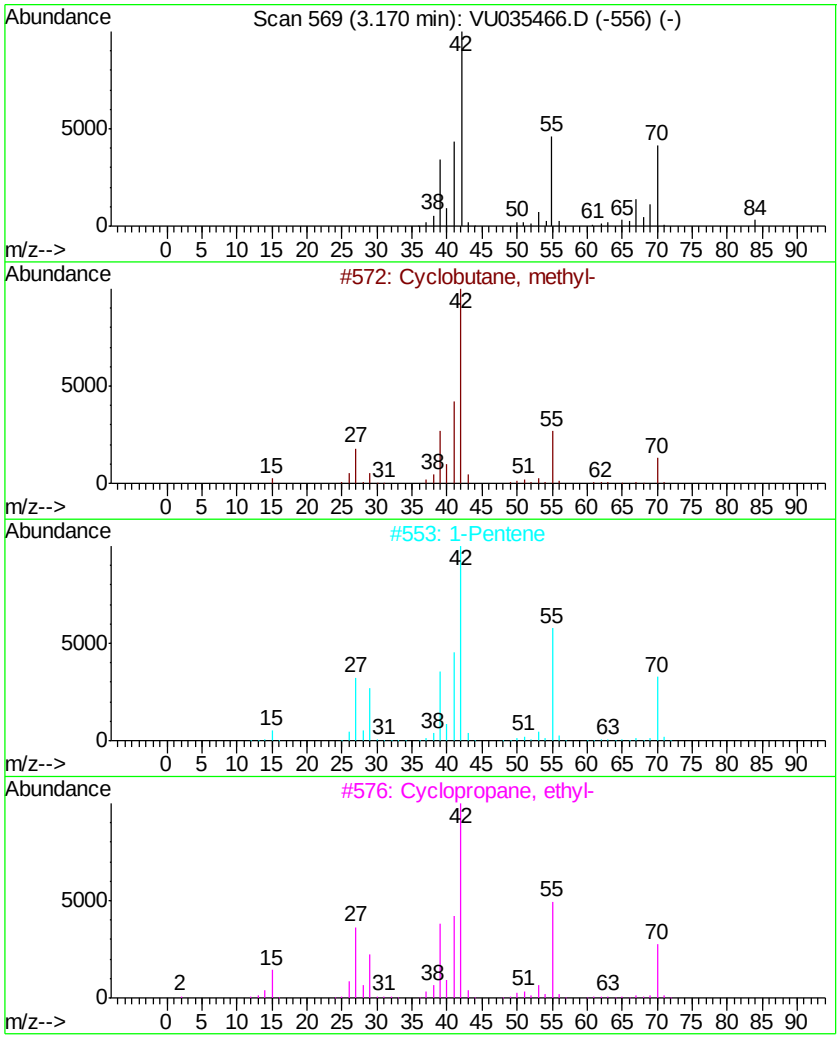
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

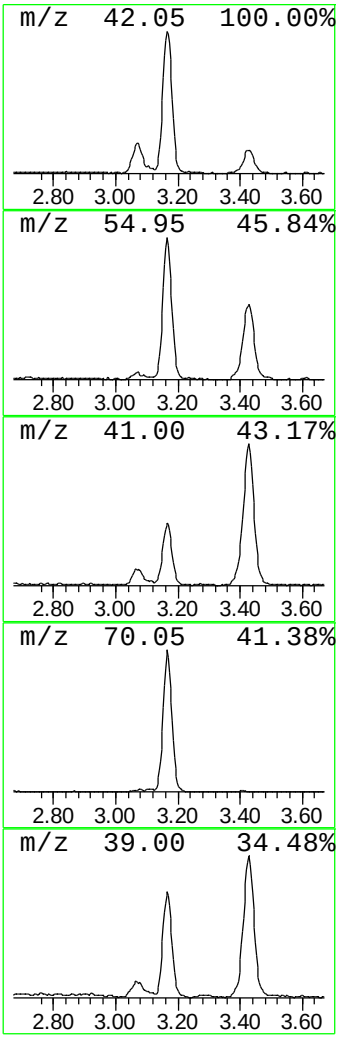
****

Peak Number 2 (DEL) Alkane: Cyclic3.17 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.17	1.89 ug/L	202809	1,4-Difluorobenzene	6.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclobutane, methyl-	70	C5H10	000598-61-8	72
2	1-Pentene	70	C5H10	000109-67-1	59
3	Cyclopropane, ethyl-	70	C5H10	001191-96-4	50
4	Cyclopropane, ethyl-	70	C5H10	001191-96-4	50
5	Cyclopentane	70	C5H10	000287-92-3	50





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ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : H0G54DL

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR101719WMA.M
Quant Title : TRACE VOA SOM01.0

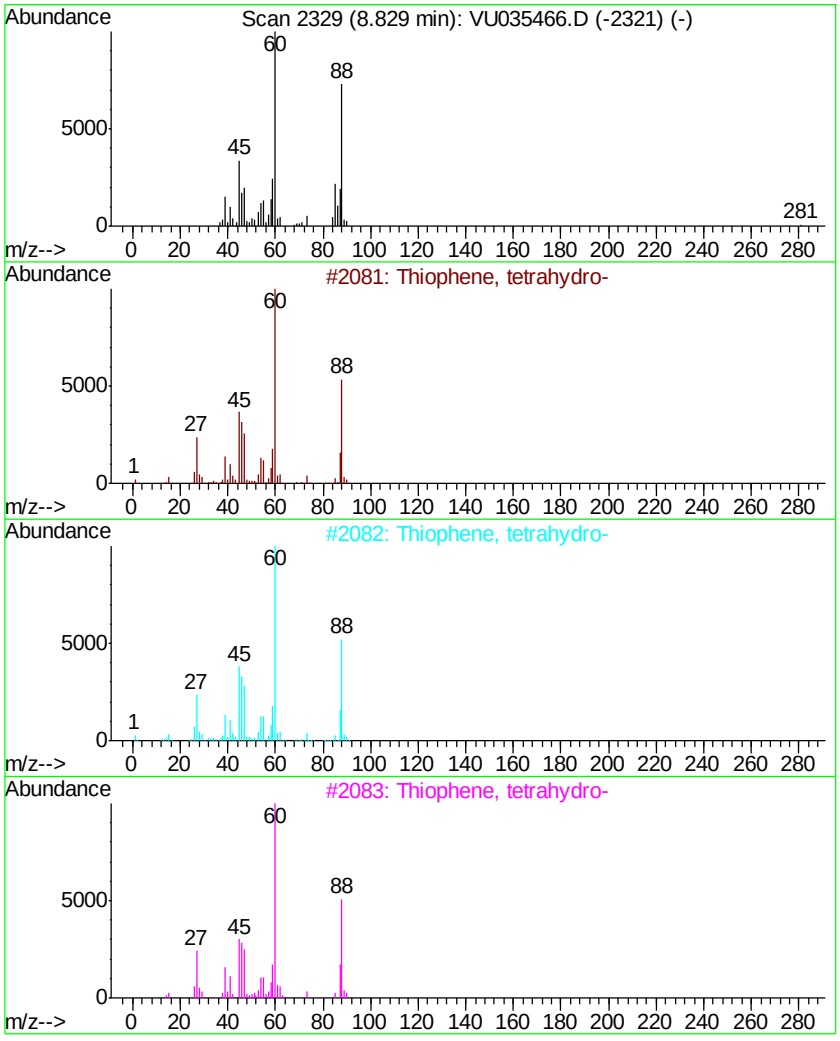
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

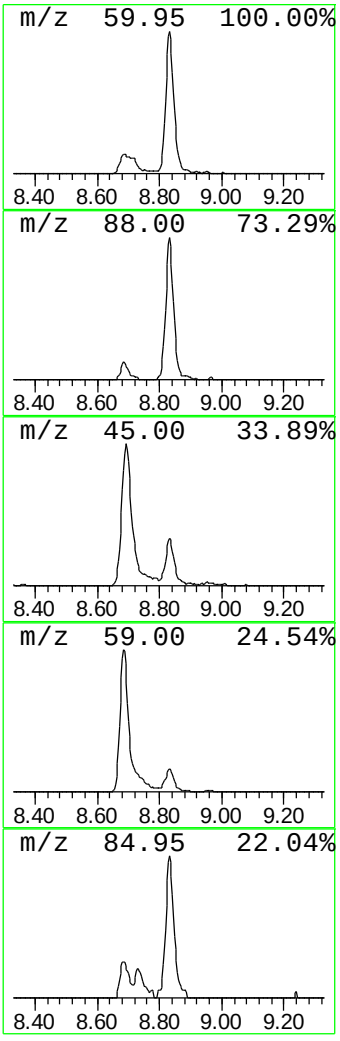
****

Peak Number 4 Thiophene, tetrahydro- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.83	1.05 ug/L	138199	Chlorobenzene-d5	9.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiophene, tetrahydro-	88	C4H8S	000110-01-0	87
2	Thiophene, tetrahydro-	88	C4H8S	000110-01-0	87
3	Thiophene, tetrahydro-	88	C4H8S	000110-01-0	68
4	Thietane, 2-methyl-	88	C4H8S	017837-41-1	64
5	Ethylvinyl sulfide	88	C4H8S	000627-50-9	47





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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR101719WMA.M
Quant Title : TRACE VOA SOM01.0

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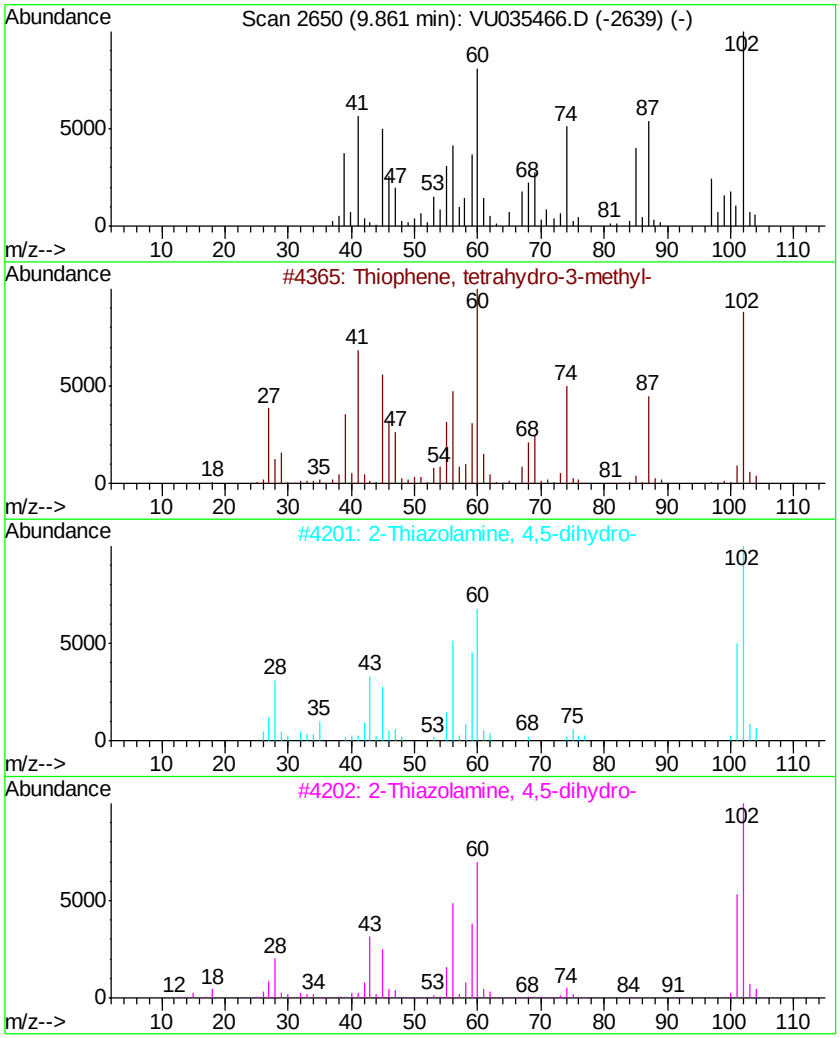
TIC Integration Parameters: LSCINT.P

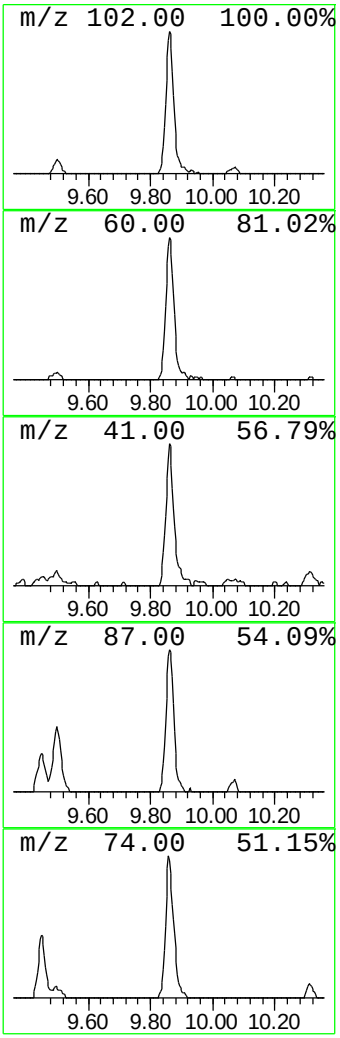
****

Peak Number 5 Thiophene, tetrahydro-3-met... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.86	1.14 ug/L	150654	Chlorobenzene-d5	9.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiophene, tetrahydro-3-methyl-	102	C5H10S	004740-00-5	93
2	2-Thiazolamine, 4,5-dihydro-	102	C3H6N2S	001779-81-3	49
3	2-Thiazolamine, 4,5-dihydro-	102	C3H6N2S	001779-81-3	46
4	2-Thiazolamine, 4,5-dihydro-	102	C3H6N2S	001779-81-3	46
5	2H-Thiopyran, tetrahydro-	102	C5H10S	001613-51-0	32





Tentatively Identified Compound (LSC) summary

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Quant Title : TRACE VOA SOM01.0

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
(DEL) Alkane: Str...	2.01	6.2	ug/L	667747	1	6.29	537132	5.0
(DEL) Alkane: Cyc...	3.17	1.9	ug/L	202809	1	6.29	537132	5.0
Thiophene, tetrah...	8.83	1.1	ug/L	138199	2	9.45	659655	5.0
Thiophene, tetrah...	9.86	1.1	ug/L	150654	2	9.45	659655	5.0