LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV062320\
Data File : VV017053.D
Acq On : 23 Jun 2020 14:11
Operator : SY/MD
Sample : L3067-01DL 40X
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : BFXF8DL

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_V\METHOD\SOMVTR061720WMA.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	1.315	62	70	81	rVB	79993	85044	3.55%	0.964%
2	1.579	143	152	165	rVB	62223	72221	3.02%	0.819%
3	2.126	311	322	336	rBV3	146660	235122	9.82%	2.666%
4	3.209	645	659	676	rVB	233152	481211	20.10%	5.456%
5	3.933	870	884	914	rBV3	72984	268412	11.21%	3.043%
6	4.380	1003	1023	1048	rBV	103733	281915	11.77%	3.196%
7	4.634	1080	1102	1127	rBV	964778	2394352	100.00%	27.145%
8	5.071	1220	1238	1266	rBV3	256209	629838	26.31%	7.141%
9	5.643	1402	1416	1440	rBV2	211380	434188	18.13%	4.923%
10	6.097	1545	1557	1575	rVB	140929	282413	11.79%	3.202%
11	6.341	1623	1633	1651	rVB2	25990	55037	2.30%	0.624%
12	7.010	1832	1841	1862	rVB	74125	134219	5.61%	1.522%
13	7.164	1874	1889	1905	rVB3	17818	38472	1.61%	0.436%
14	7.338	1932	1943	1960	rBV	306921	533764	22.29%	6.051%
15	7.643	2024	2038	2051	rBV2	45884	83079	3.47%	0.942%
16	8.113	2173	2184	2215	rBV	270787	529237	22.10%	6.000%
17	8.875	2406	2421	2447	rBV	326685	559316	23.36%	6.341%
18	9.756	2684	2695	2707	rBV2	40573	70375	2.94%	0.798%
19	10.238	2834	2845	2857	rBV	99769	155914	6.51%	1.768%
20	10.502	2915	2927	2942	rBV	240737	407329	17.01%	4.618%
21	11.270	3152	3166	3181	rBV	352794	545850	22.80%	6.188%
22	11.553	3245	3254	3268	rVB8	14855	26836	1.12%	0.304%
23	11.646	3268	3283	3305	rBV	319398	516311	21.56%	5.854%

Sum of corrected areas: 8820455

LSC Report - Integrated Chromatogram

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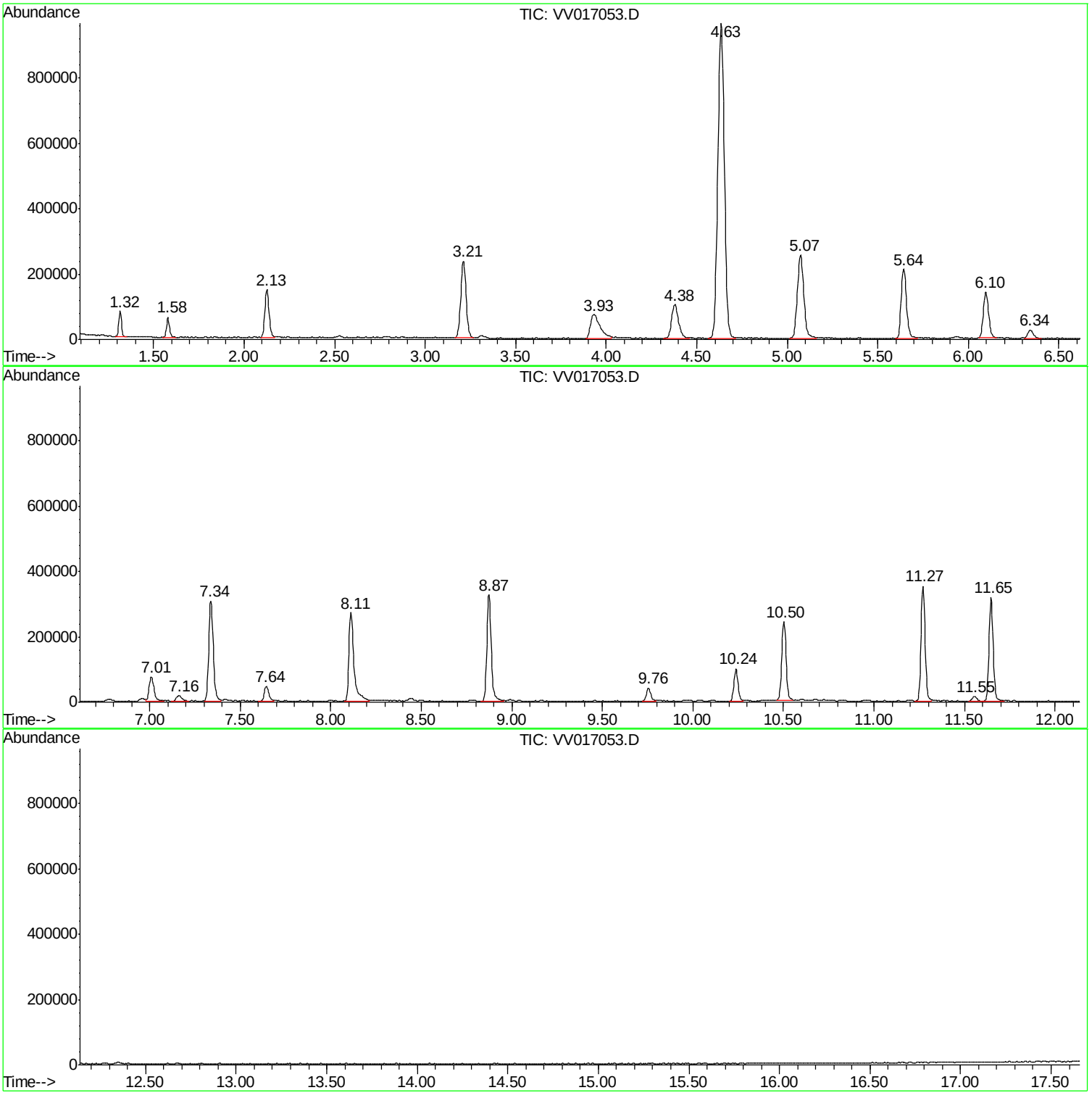
Instrument : MSVOA_V
ClientSampleId : BFXF8DL

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

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



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV062320\
Data File : VV017053.D
Acq On : 23 Jun 2020 14:11
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ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : BFXF8DL

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

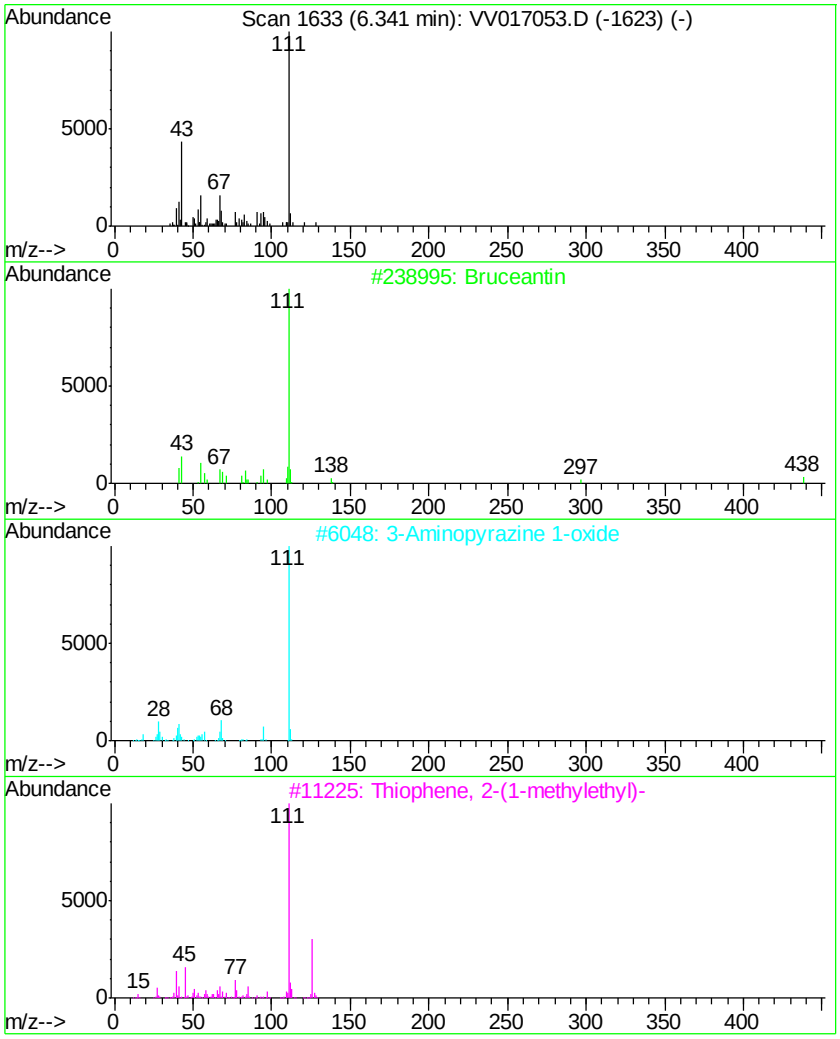
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

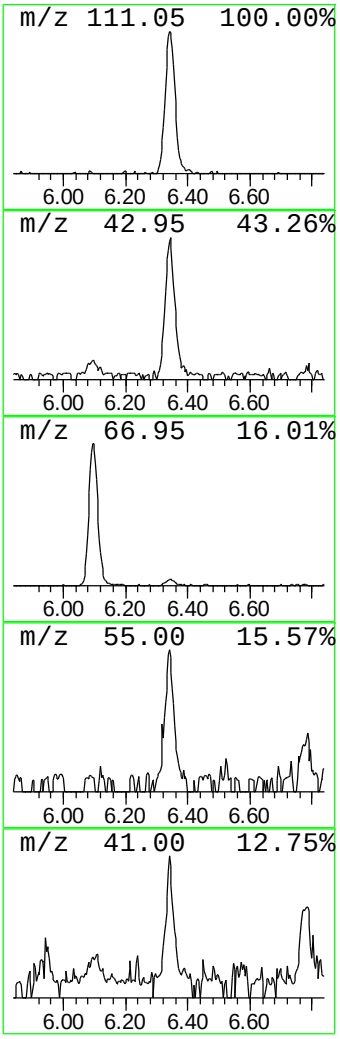
****

Peak Number 1 Bruceantin Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.34	0.63 ug/L	55037	1,4-Difluorobenzene	5.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bruceantin	548	C28H36O11	041451-75-6	64
2	3-Aminopyrazine 1-oxide	111	C4H5N3O	006863-77-0	59
3	Thiophene, 2-(1-methylethyl)-	126	C7H10S	004095-22-1	59
4	2(1H)-Pyrimidinone, 4-amino-	111	C4H5N3O	000071-30-7	59
5	2(1H)-Pyridinone, 3-hydroxy-	111	C5H5NO2	016867-04-2	53





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Instrument : MSVOA_V
ClientSampleId : BFXF8DL

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

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

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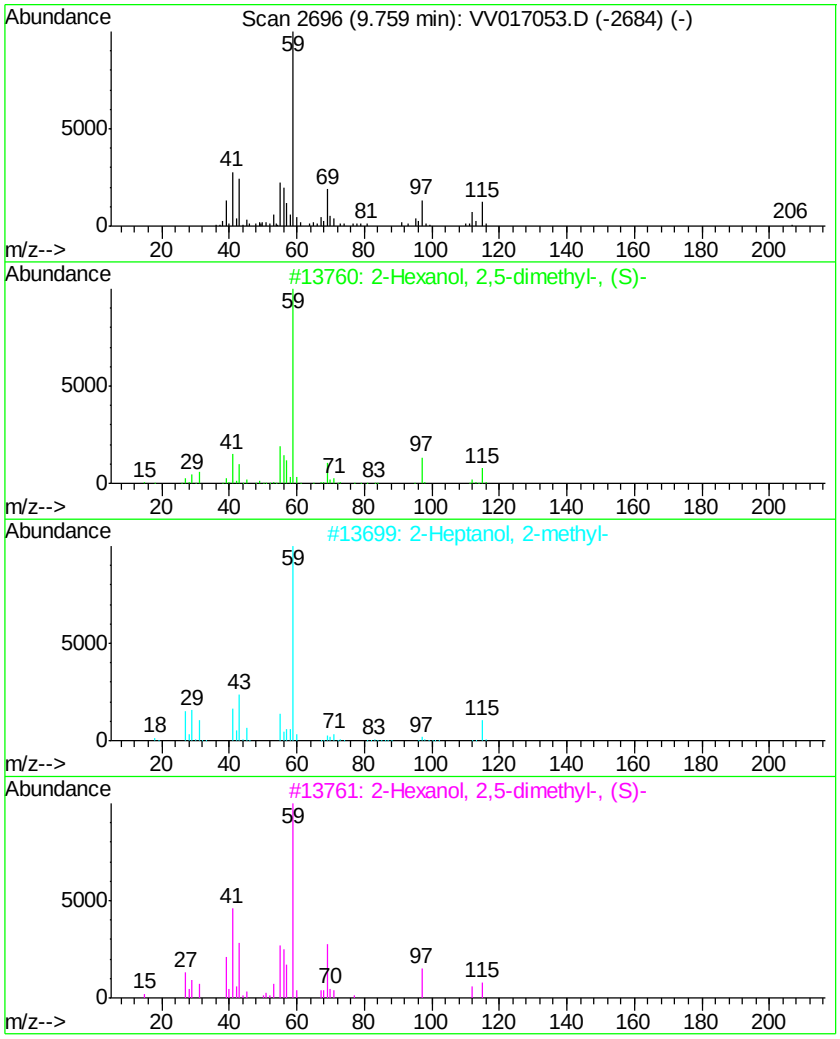
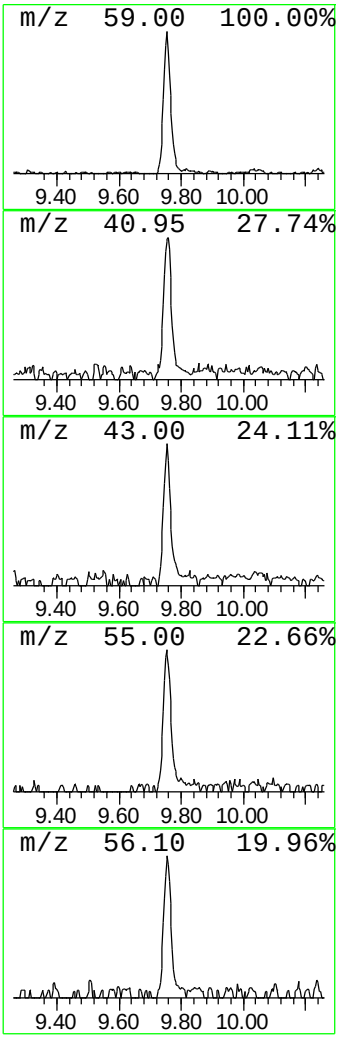
Peak Number 3 2-Hexanol, 2,5-dimethyl-, (S)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.76	0.63 ug/L	70375	Chlorobenzene-d5	8.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	78
2	2-Heptanol, 2-methyl-	130	C8H18O	000625-25-2	53
3	2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	50
4	2-Octanol, 2,6-dimethyl-	158	C10H22O	018479-57-7	45
5	2,4-Dimethyl-4-penten-2-ol	114	C7H14O	019781-53-4	40





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Instrument : MSVOA_V
ClientSampleId : BFXF8DL

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

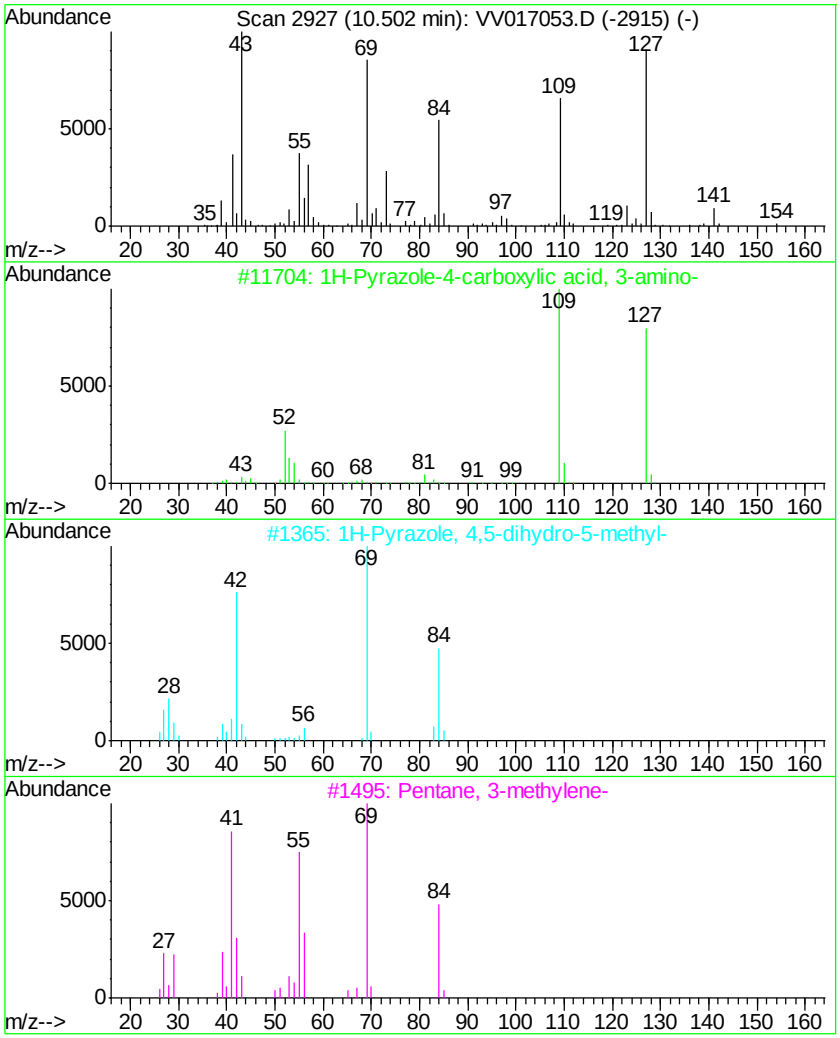
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

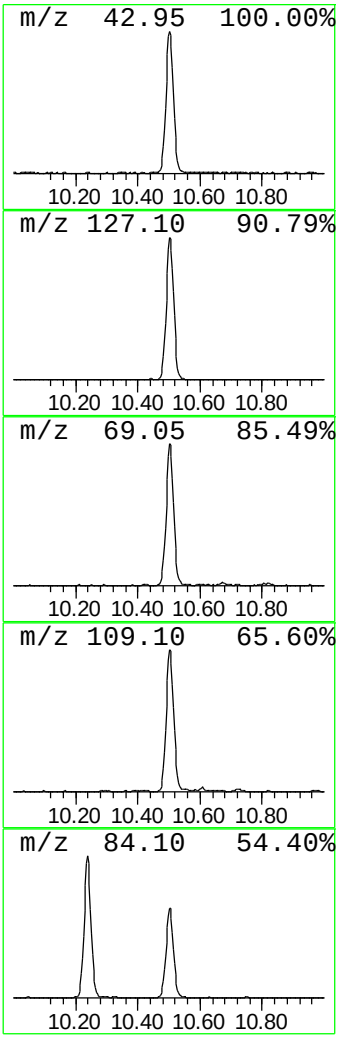
****

Peak Number 4 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.50	3.73 ug/L	407329	1,4-Dichlorobenzene-d4	11.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Pyrazole-4-carboxylic acid, 3...	127	C4H5N3O2	041680-34-6	35
2	1H-Pyrazole, 4,5-dihydro-5-methyl-	84	C4H8N2	001568-20-3	27
3	Pentane, 3-methylene-	84	C6H12	000760-21-4	27
4	Furan, 2,3-dihydro-3-methyl-	84	C5H8O	001708-27-6	27
5	4-Piperidinone, 1,3-dimethyl-	127	C7H13NO	004629-80-5	22





Tentatively Identified Compound (LSC) summary

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Quant Title : TRACE VOA SOM01.0

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Bruceantin	6.34	0.6	ug/L	55037	1	5.64	434188	5.0
2-Hexanol, 2,5-di...	9.76	0.6	ug/L	70375	2	8.87	559316	5.0
unknown-01	10.50	3.7	ug/L	407329	3	11.27	545850	5.0