LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU060120\
Data File : VU038465.D
Acq On : 01 Jun 2020 13:01
Operator : JC/MD
Sample : L2789-03
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 2 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFX76

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\SOMUTR053120WMA.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	1.369	3	9	18	rBV	70092	68635	4.27%	0.601%
2	1.613	75	85	96	rBV	121869	138456	8.62%	1.213%
3	1.932	174	184	199	rVB	107942	141357	8.80%	1.238%
4	2.594	376	390	405	rBV	213263	353621	22.02%	3.097%
5	2.678	406	416	437	rVB2	9806	30886	1.92%	0.271%
6	3.221	572	585	600	rVB2	10615	24185	1.51%	0.212%
7	4.681	1017	1039	1074	rBV	208756	694774	43.27%	6.086%
8	4.848	1076	1091	1125	rVB	361734	862810	53.73%	7.558%
9	5.102	1153	1170	1201	rVB2	241290	538485	33.53%	4.717%
10	5.761	1352	1375	1409	rBV2	423205	1112512	69.28%	9.745%
11	6.282	1522	1537	1556	rBV	361873	705735	43.95%	6.182%
12	6.719	1658	1673	1694	rBV	261066	507403	31.60%	4.444%
13	7.070	1768	1782	1808	rBV	150360	271743	16.92%	2.380%
14	7.591	1931	1944	1966	rBV	136703	241485	15.04%	2.115%
15	7.922	2032	2047	2066	rBV	469278	850874	52.99%	7.453%
16	8.202	2120	2134	2151	rBV	89157	149773	9.33%	1.312%
17	8.655	2261	2275	2314	rBV	848919	1605785	100.00%	14.065%
18	9.436	2505	2518	2555	rVB	528289	902274	56.19%	7.903%
19	10.771	2919	2933	2951	rVB	224068	360844	22.47%	3.161%
20	11.822	3248	3260	3279	rVB	545585	867354	54.01%	7.597%
21	12.083	3328	3341	3362	rBV4	14544	33177	2.07%	0.291%
22	12.205	3366	3379	3394	rVB	526605	844021	52.56%	7.393%
23	17.388	4981	4991	5005	rVB2	60984	110333	6.87%	0.966%

Sum of corrected areas: 11416522

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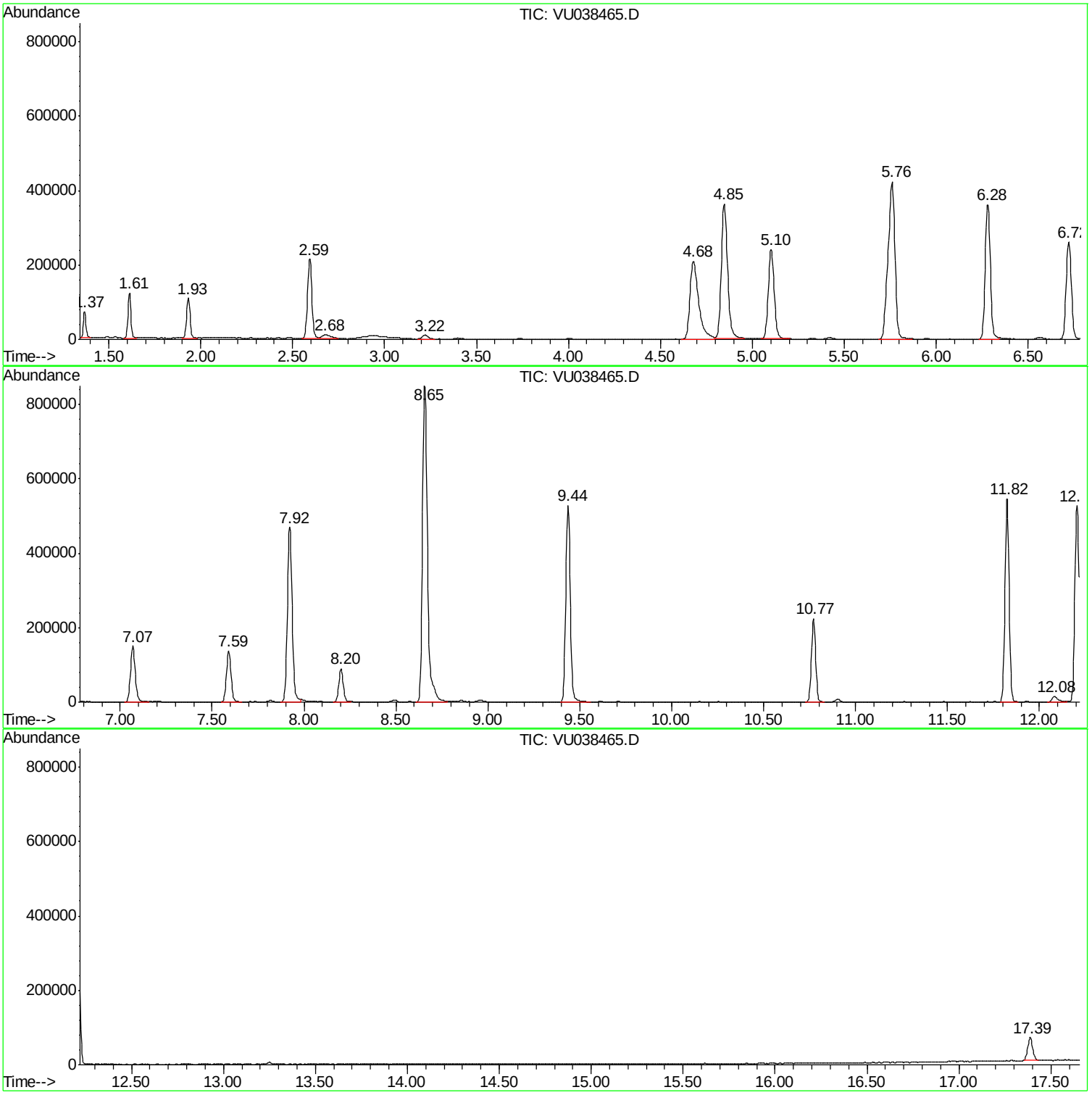
ALS Vial : 2 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFX76

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR053120WMA.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 U\DATA\VU060120\
Data File : VU038465.D
Acq On : 01 Jun 2020 13:01
Operator : JC/MD
Sample : L2789-03
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 2 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFX76

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR053120WMA.M
Quant Title : TRACE VOA SOM01.0

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

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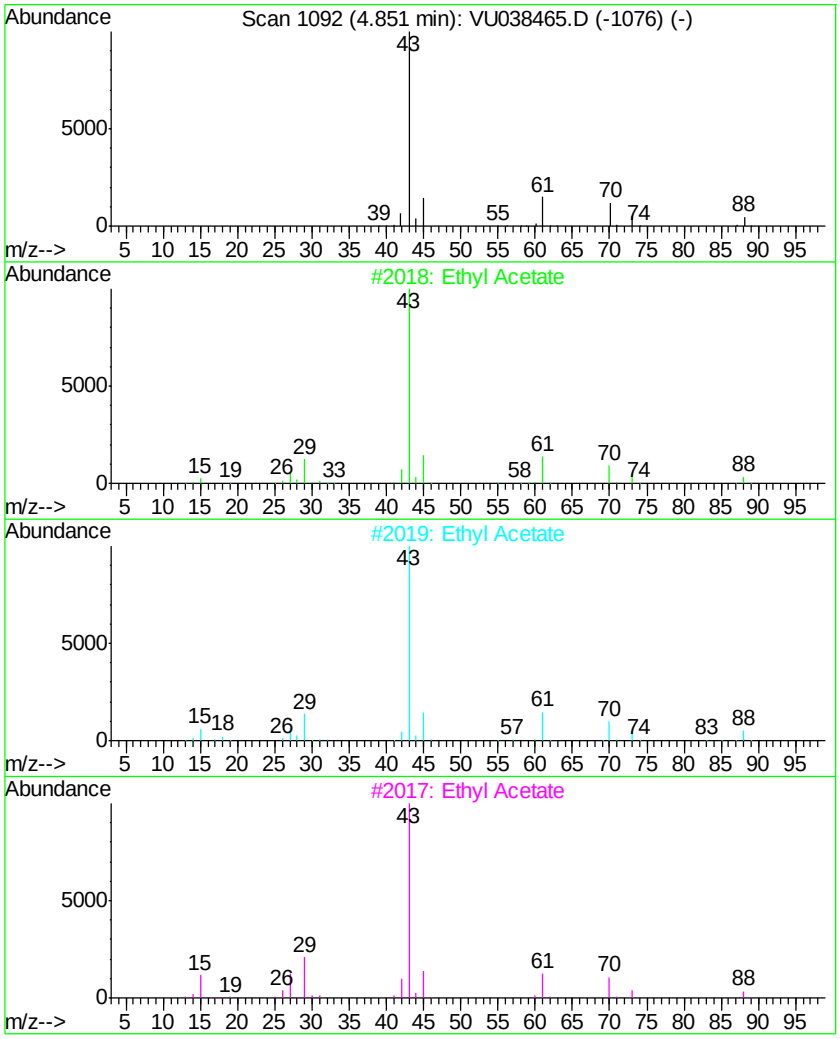
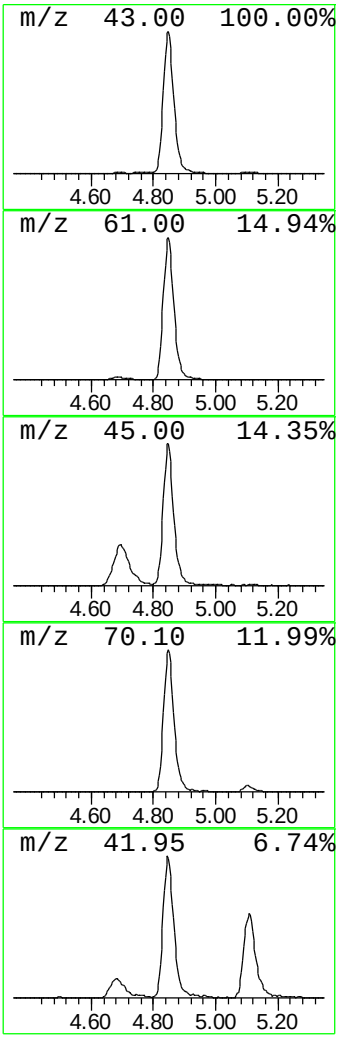
Peak Number 1 Ethyl Acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.85	6.11 ug/L	862810	1,4-Difluorobenzene	6.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethyl Acetate	88	C4H8O2	000141-78-6	90
2	Ethyl Acetate	88	C4H8O2	000141-78-6	90
3	Ethyl Acetate	88	C4H8O2	000141-78-6	90
4	Ethyl Acetate	88	C4H8O2	000141-78-6	86
5	CH3C(O)CH2CH2OH	88	C4H8O2	000590-90-9	40





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ALS Vial : 2 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFX76

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR053120WMA.M
Quant Title : TRACE VOA SOM01.0

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

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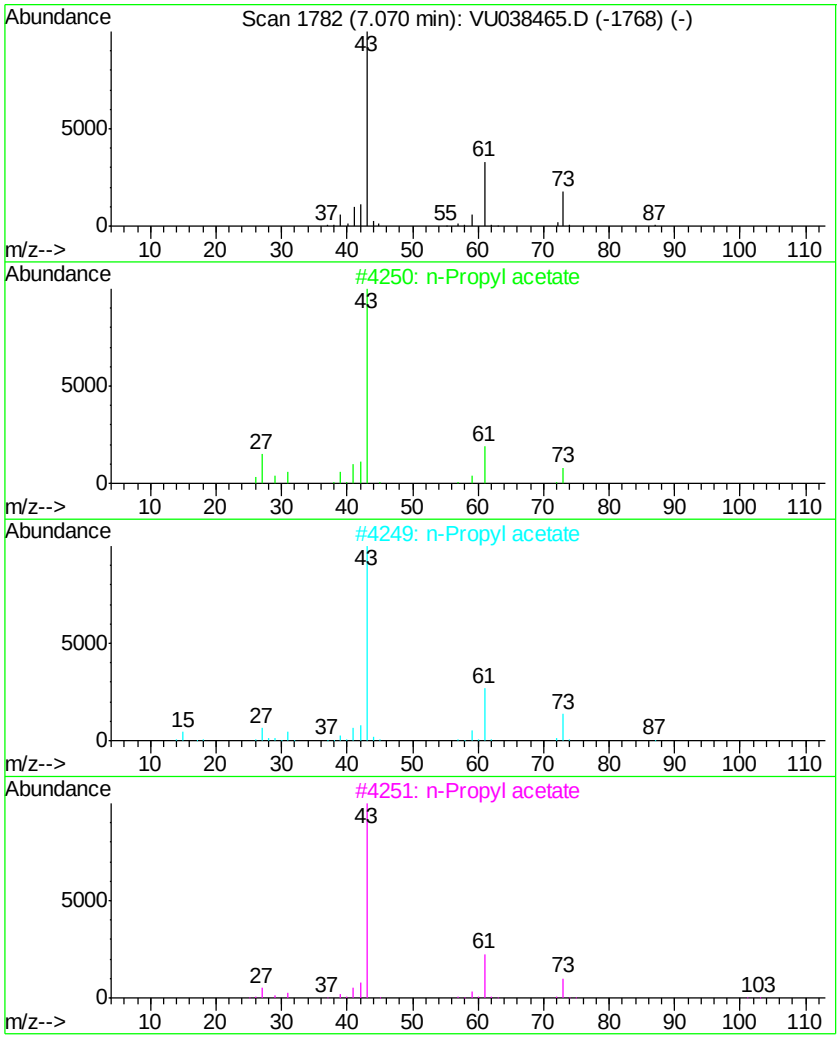
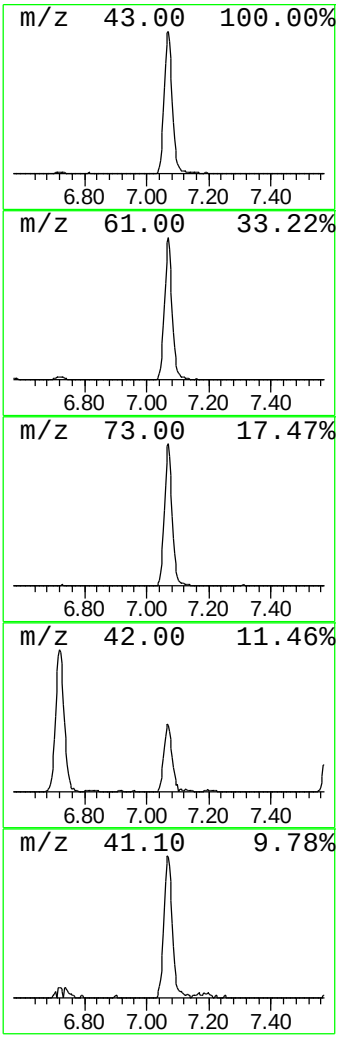
Peak Number 2 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.07	1.93 ug/L	271743	1,4-Difluorobenzene	6.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate	102	C5H10O2	000109-60-4	78
2	n-Propyl acetate	102	C5H10O2	000109-60-4	78
3	n-Propyl acetate	102	C5H10O2	000109-60-4	40
4	Propanal, 2,3-dihydroxy-, (S)-	90	C3H6O3	000497-09-6	36
5	Isobutylamine	73	C4H11N	000078-81-9	9





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ALS Vial : 2 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFX76

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR053120WMA.M
Quant Title : TRACE VOA SOM01.0

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

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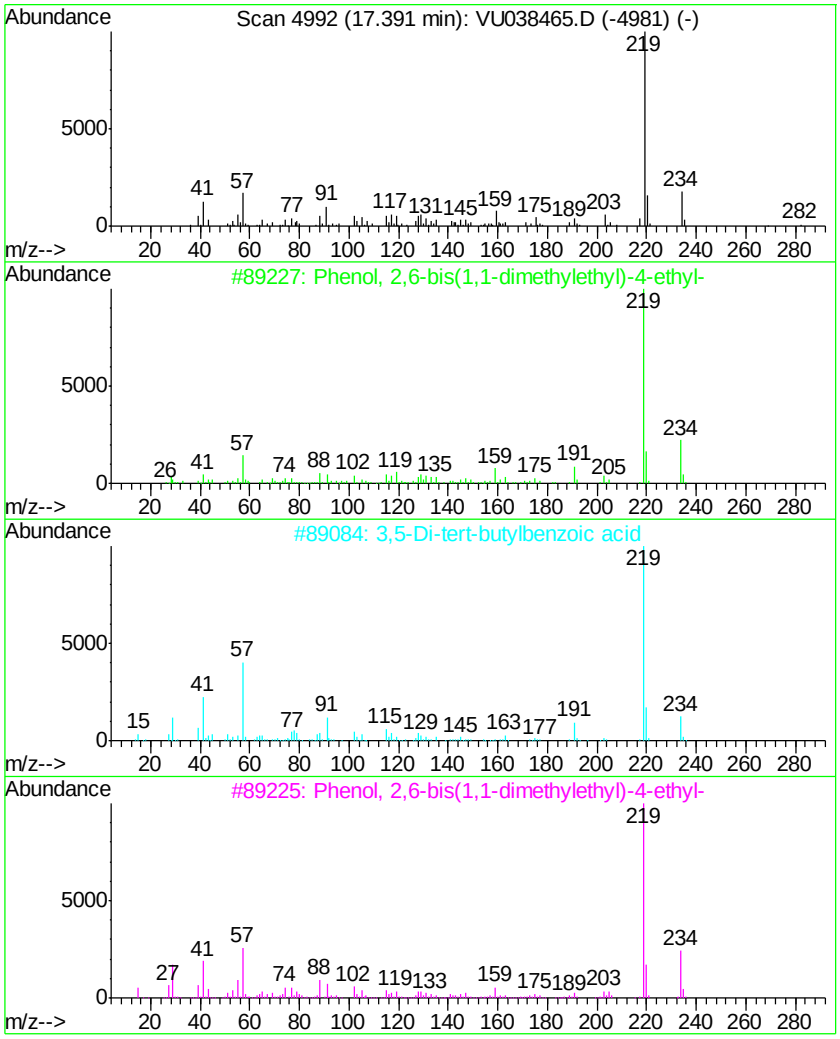
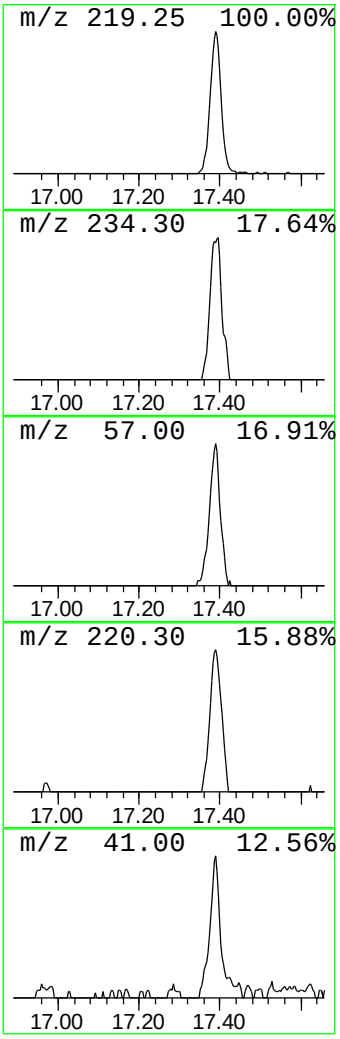
Peak Number 4 Phenol, 2,6-bis(1,1-dimethy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.39	0.64 ug/L	110333	1,4-Dichlorobenzene-d4	11.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,6-bis(1,1-dimethylethy...	234	C16H26O	004130-42-1	93
2	3,5-Di-tert-butylbenzoic acid	234	C15H22O2	016225-26-6	91
3	Phenol, 2,6-bis(1,1-dimethylethy...	234	C16H26O	004130-42-1	91
4	3,5-Di-tert-butylbenzoic acid	234	C15H22O2	016225-26-6	80
5	6-(1'-Hydroxyethyl)-7-methoxy-2,...	234	C14H18O3	1000360-28-8	80





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
Ethyl Acetate	4.85	6.1	ug/L	862810	1	6.28	705735	5.0
n-Propyl acetate	7.07	1.9	ug/L	271743	1	6.28	705735	5.0
Phenol, 2,6-bis(1...	17.39	0.6	ug/L	110333	3	11.83	867354	5.0