LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021517\
Data File : BF092956.D
Acq On : 15 Feb 2017 17:41
Operator : SJ/MA
Sample : I1826-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP1-2-COMP14

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:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.681	50	52	59	rVB	287863	402422	8.21%	1.010%
2	4.407	200	203	207	rBV	64635	102741	2.10%	0.258%
3	4.613	218	221	225	rBV	55017	70936	1.45%	0.178%
4	5.059	257	260	270	rBV	1269776	1991156	40.63%	4.999%
5	5.482	294	297	299	rBV	3748755	3836219	78.28%	9.631%
6	6.510	384	387	390	rBV	3123902	3210557	65.51%	8.060%
7	6.647	396	399	401	rBV	3522515	4342928	88.62%	10.903%
8	6.693	401	403	410	rVB	102592	102090	2.08%	0.256%
9	6.876	416	419	421	rBV	755882	868054	17.71%	2.179%
10	7.025	430	432	435	rBV	2737660	3031247	61.85%	7.610%
11	7.436	465	468	471	rVB	2371524	2534776	51.72%	6.363%
12	7.893	506	508	510	rBV	66848	66883	1.36%	0.168%
13	8.156	528	531	535	rBV2	1339326	1502521	30.66%	3.772%
14	9.231	622	625	627	rBV	4453625	4515652	92.15%	11.336%
15	9.825	669	677	682	rBV	119765	261386	5.33%	0.656%
16	9.905	682	684	686	rBV	1576937	1367351	27.90%	3.433%
17	10.694	750	753	756	rBV	2417155	2713251	55.37%	6.811%
18	11.391	811	814	816	rBV	1493663	1464560	29.89%	3.677%
19	12.979	950	953	955	rBV	4432066	4900580	100.00%	12.303%
20	14.020	1042	1044	1047	rBV	1369769	1326746	27.07%	3.331%
21	15.460	1167	1170	1180	rVB	899039	1221748	24.93%	3.067%

Sum of corrected areas: 39833804

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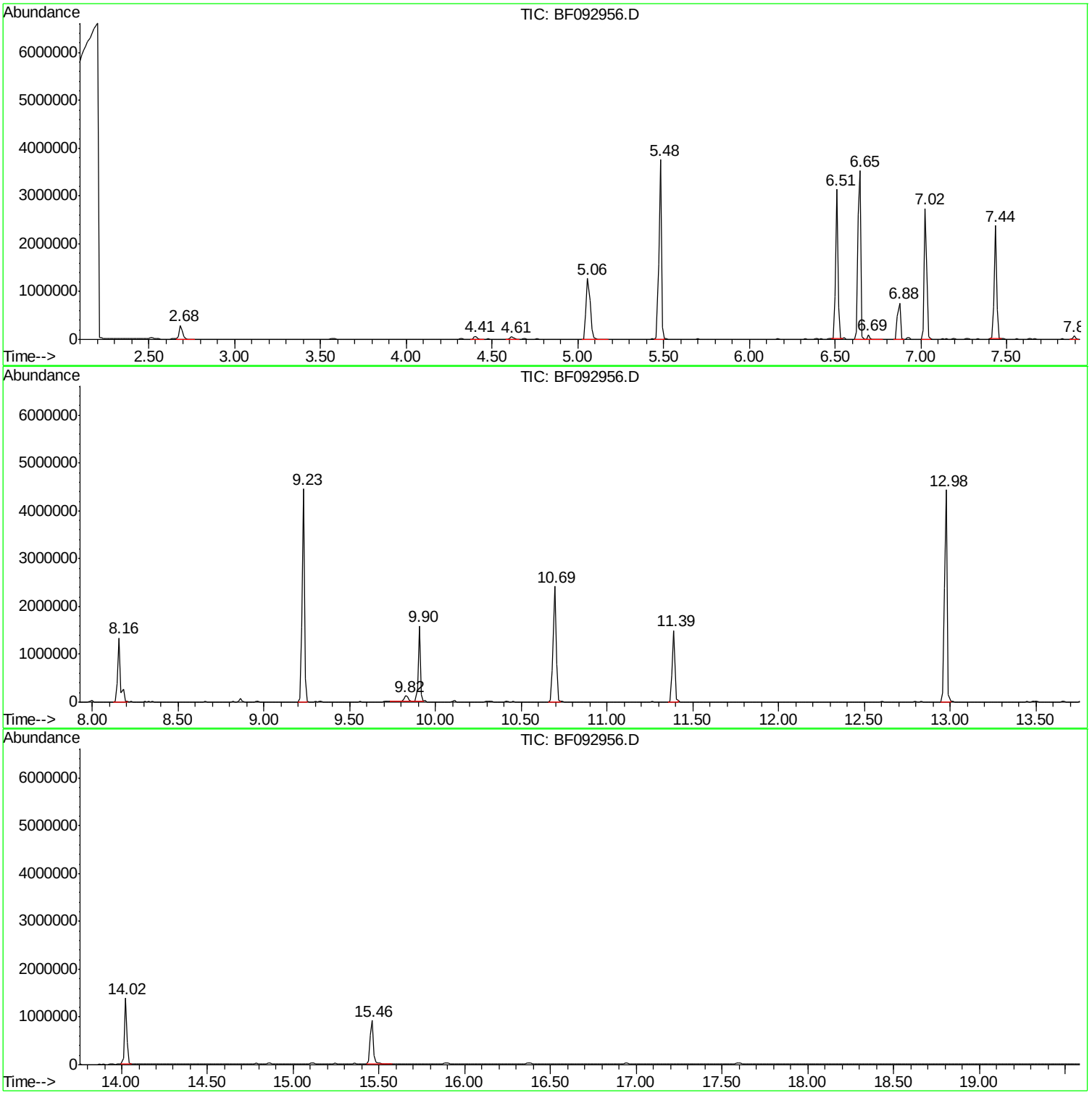
BNA_F
ClientSampleId :
TP1-2-COMP14

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

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Data File : BF092956.D
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Operator : SJ/MA
Sample : I1826-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP1-2-COMP14

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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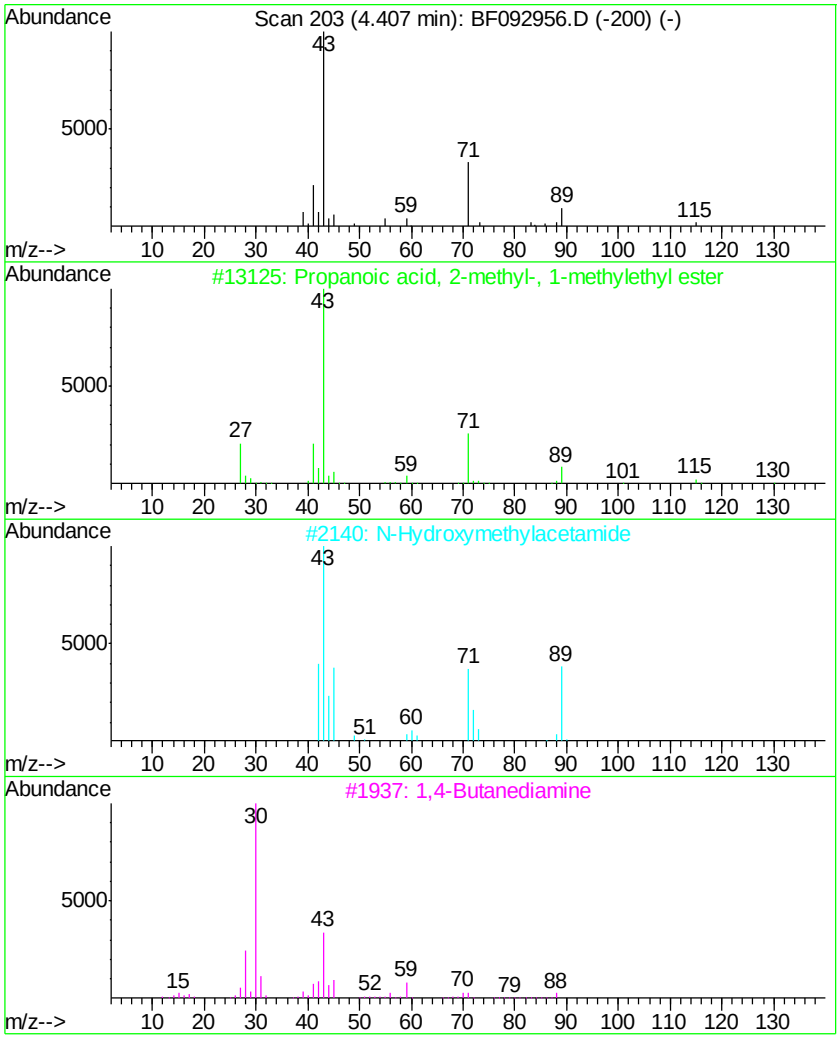
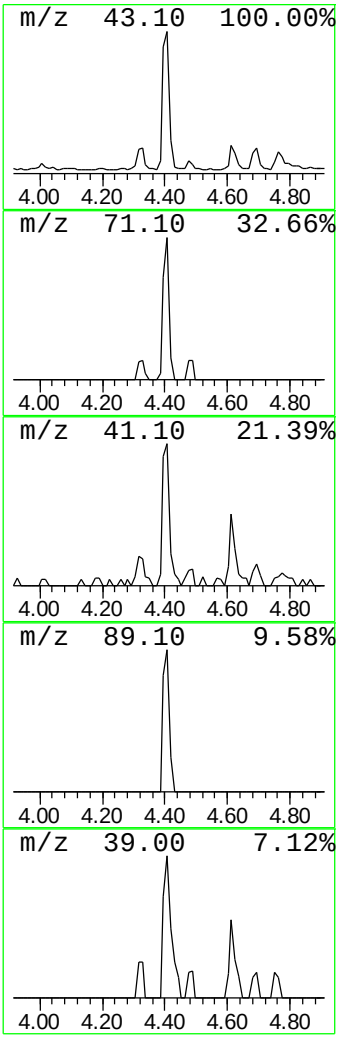
Peak Number 2 Propanoic acid, 2-methyl-, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.41	2.37 ng	102741	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72
2	N-Hydroxymethylacetamide	89	C3H7NO2	000625-51-4	9
3	1,4-Butanediamine	88	C4H12N2	000110-60-1	9
4	2-Oxo-n-valeric acid	116	C5H8O3	001821-02-9	9
5	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	9





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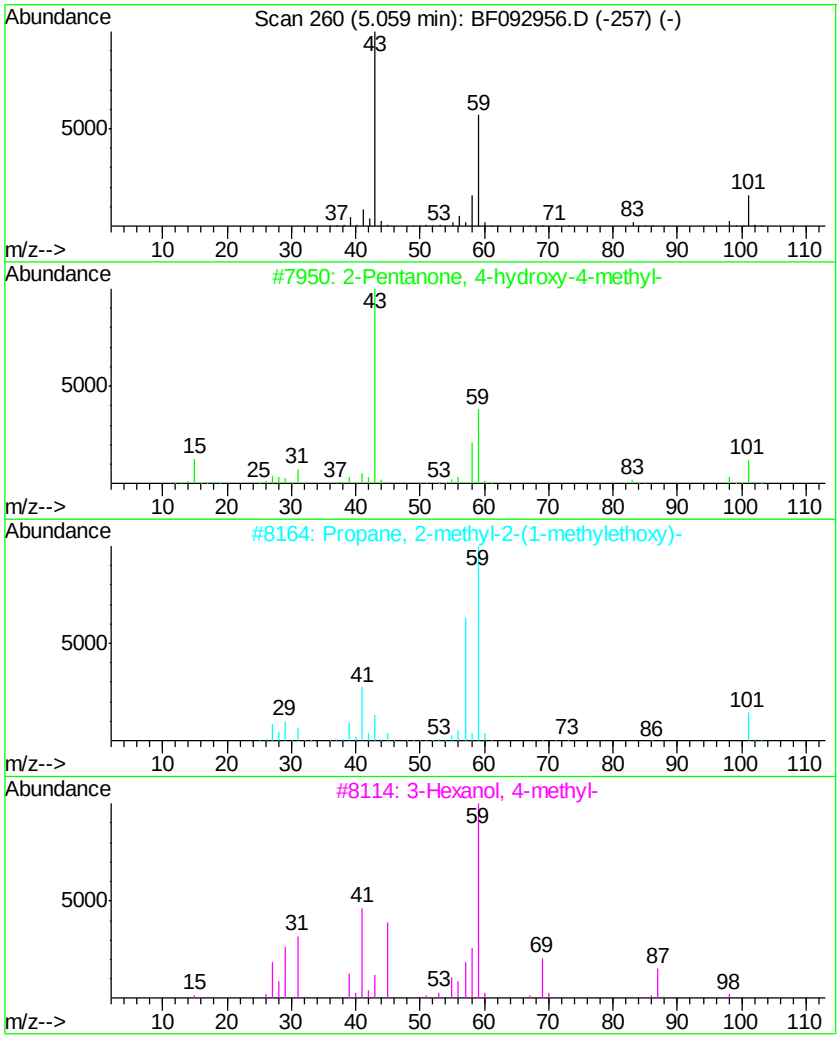
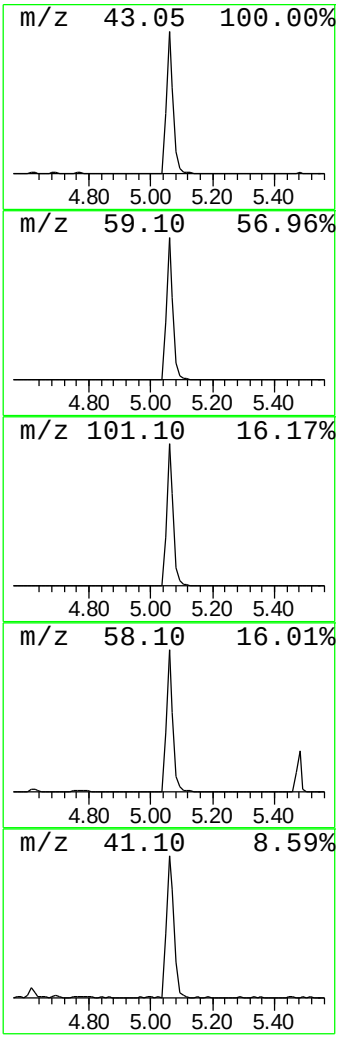
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	45.88 ng	1991160	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23





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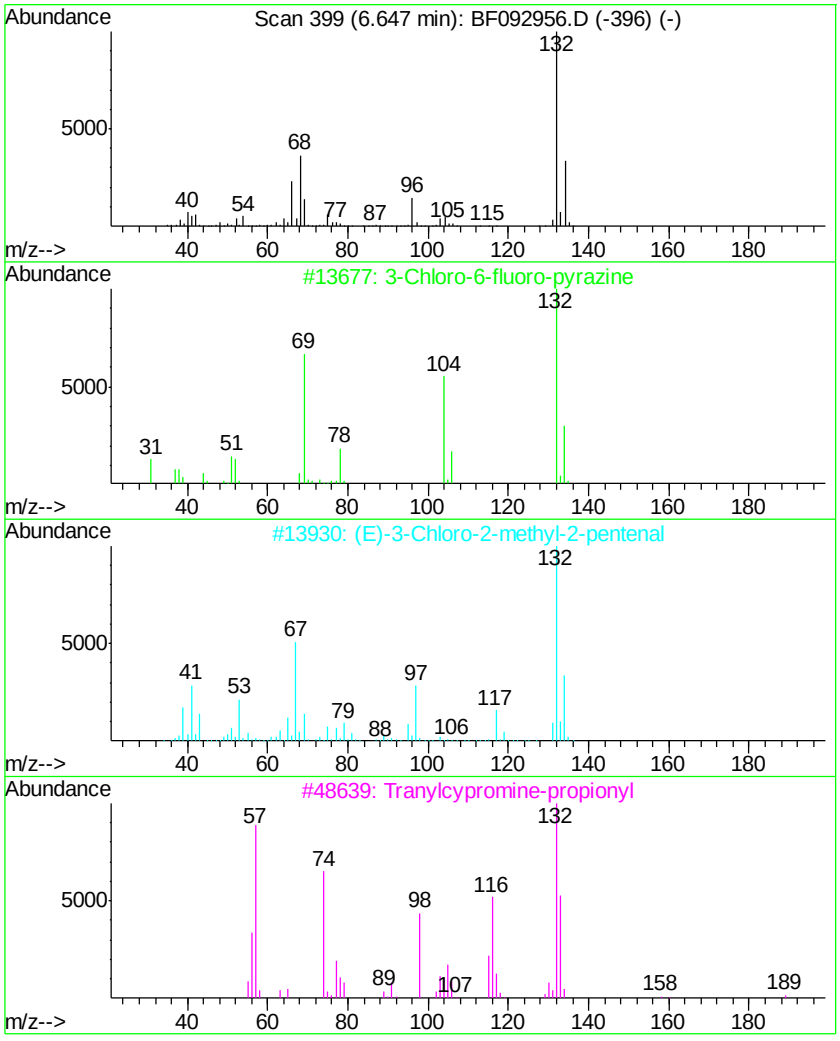
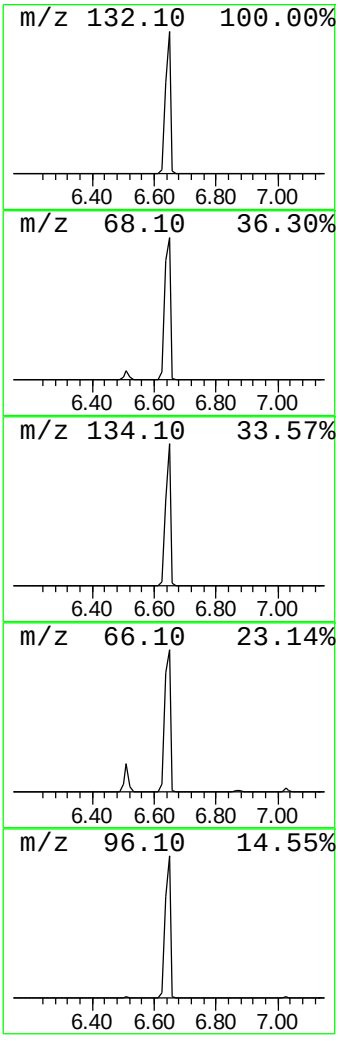
Peak Number 4 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	100.06 ng	4342930	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
4	5-Aminoindole	132	C8H8N2	005192-03-0	16
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
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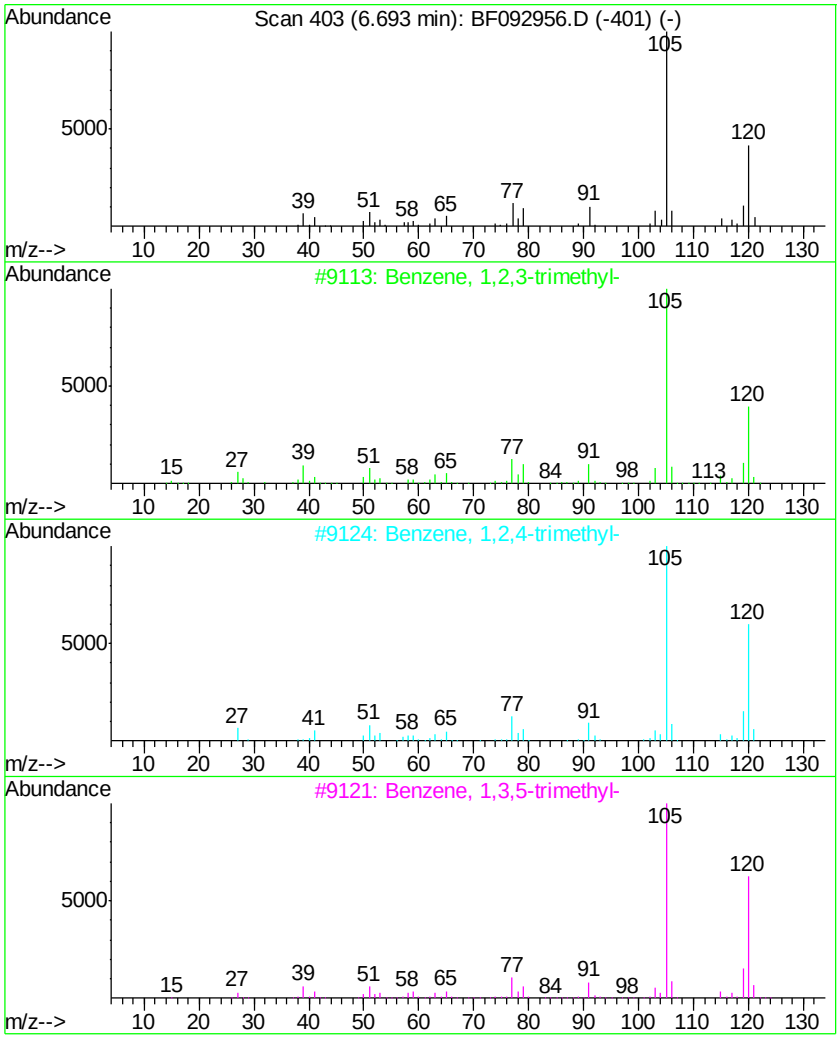
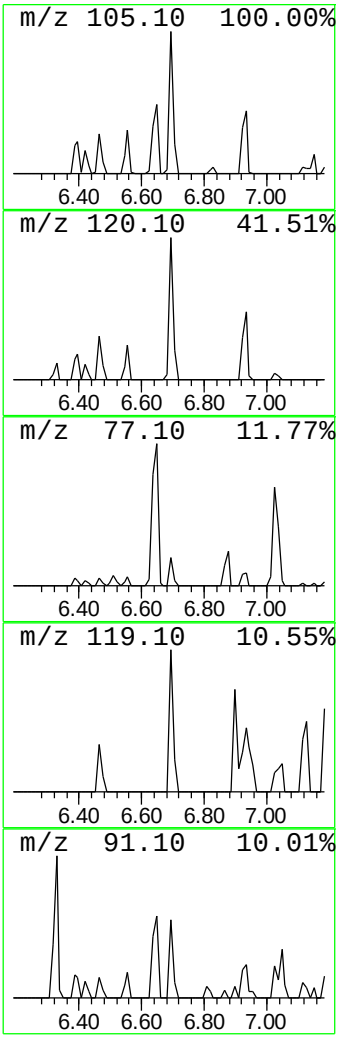
Peak Number 5 Benzene, 1,2,3-trimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	2.35 ng	102090	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
2	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
3	Benzene, 1,3,5-trimethyl-	120	C9H12	000108-67-8	91
4	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	90
5	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90





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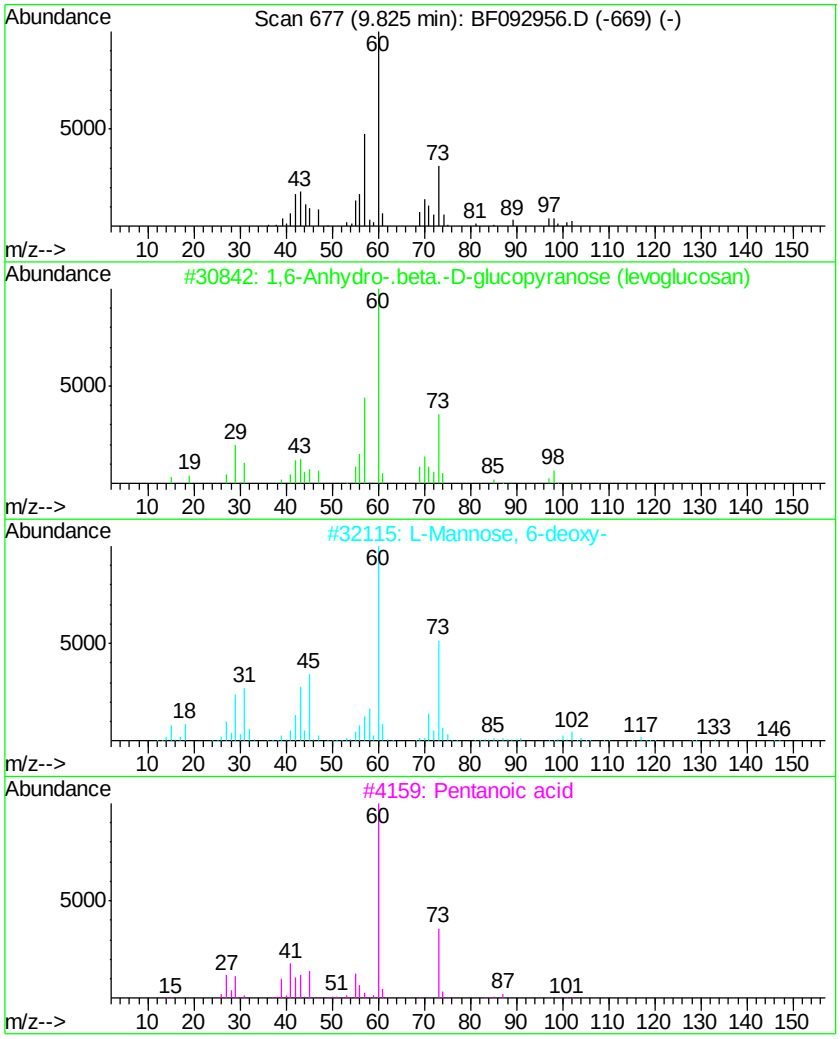
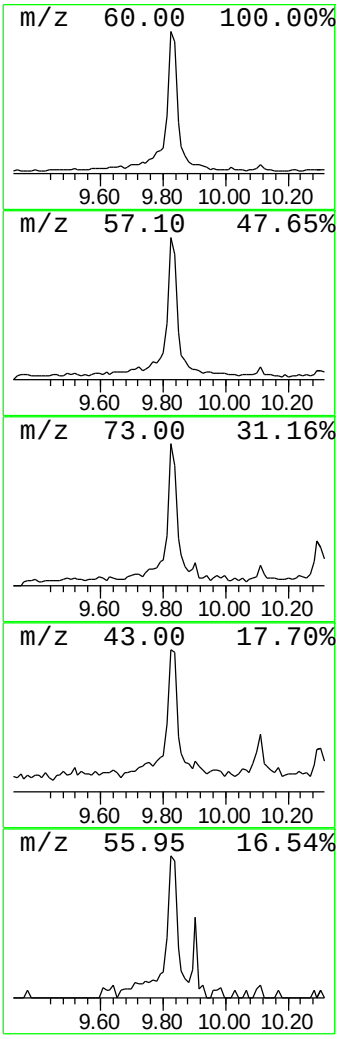
Peak Number 7 1,6-Anhydro-.beta.-D-glucop... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.82	3.82 ng	261386	Acenaphthene-d10	9.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,6-Anhydro-.beta.-D-glucopyrano...	162	C6H10O5	000498-07-7	64
2	L-Mannose, 6-deoxy-	164	C6H12O5	003615-41-6	56
3	Pentanoic acid	102	C5H10O2	000109-52-4	53
4	.beta.-D-Ribopyranoside, methyl	164	C6H12O5	017289-61-1	45
5	Heptanoic acid	130	C7H14O2	000111-14-8	45





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Propanoic acid, 2...	4.41	2.4	ng	102741	1	6.88	868054	20.0
2-Pentanone, 4-hy...	5.06	45.9	ng	1991160	1	6.88	868054	20.0
unknown6.65	6.65	100.1	ng	4342930	1	6.88	868054	20.0
Benzene, 1,2,3-tr...	6.69	2.4	ng	102090	1	6.88	868054	20.0
1,6-Anhydro-.beta...	9.82	3.8	ng	261386	3	9.90	1367350	20.0