

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021017\
 Data File : BF092897.D
 Acq On : 10 Feb 2017 21:45
 Operator : SJ/MA
 Sample : I1769-02
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 9717

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 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	2.750	56	58	65	rVB	182301	295440	5.27%	0.650%
2	4.441	203	206	211	rVB	59812	82180	1.47%	0.181%
3	5.093	260	263	268	rBV	1385546	2287945	40.84%	5.037%
4	5.207	268	273	279	rVB	41640	136833	2.44%	0.301%
5	5.516	297	300	302	rBV	3736582	4568745	81.55%	10.058%
6	6.544	386	390	392	rBV	3035829	4416132	78.82%	9.722%
7	6.670	398	401	403	rBV	4369561	4737674	84.56%	10.430%
8	6.899	418	421	423	rBV	865548	979855	17.49%	2.157%
9	7.047	432	434	437	rBV	2598935	3408748	60.84%	7.504%
10	7.459	467	470	472	rBV	2317926	2979841	53.19%	6.560%
11	8.179	530	533	539	rVB	1412715	1367637	24.41%	3.011%
12	8.442	553	556	562	rBV	111954	159705	2.85%	0.352%
13	9.265	624	628	630	rBV	3620336	5602638	100.00%	12.334%
14	9.859	672	680	684	rBV	75993	163690	2.92%	0.360%
15	9.939	684	687	689	rVV	1347974	1612934	28.79%	3.551%
16	10.728	752	756	759	rBV	2713288	3178548	56.73%	6.997%
17	11.425	814	817	819	rBV	1275527	1623459	28.98%	3.574%
18	12.751	932	933	936	rBV	66909	94394	1.68%	0.208%
19	13.014	953	956	958	rBV	4489160	5292251	94.46%	11.651%
20	14.054	1045	1047	1050	rBV	1362317	1339808	23.91%	2.950%
21	15.505	1171	1174	1182	rBV	849189	1095757	19.56%	2.412%

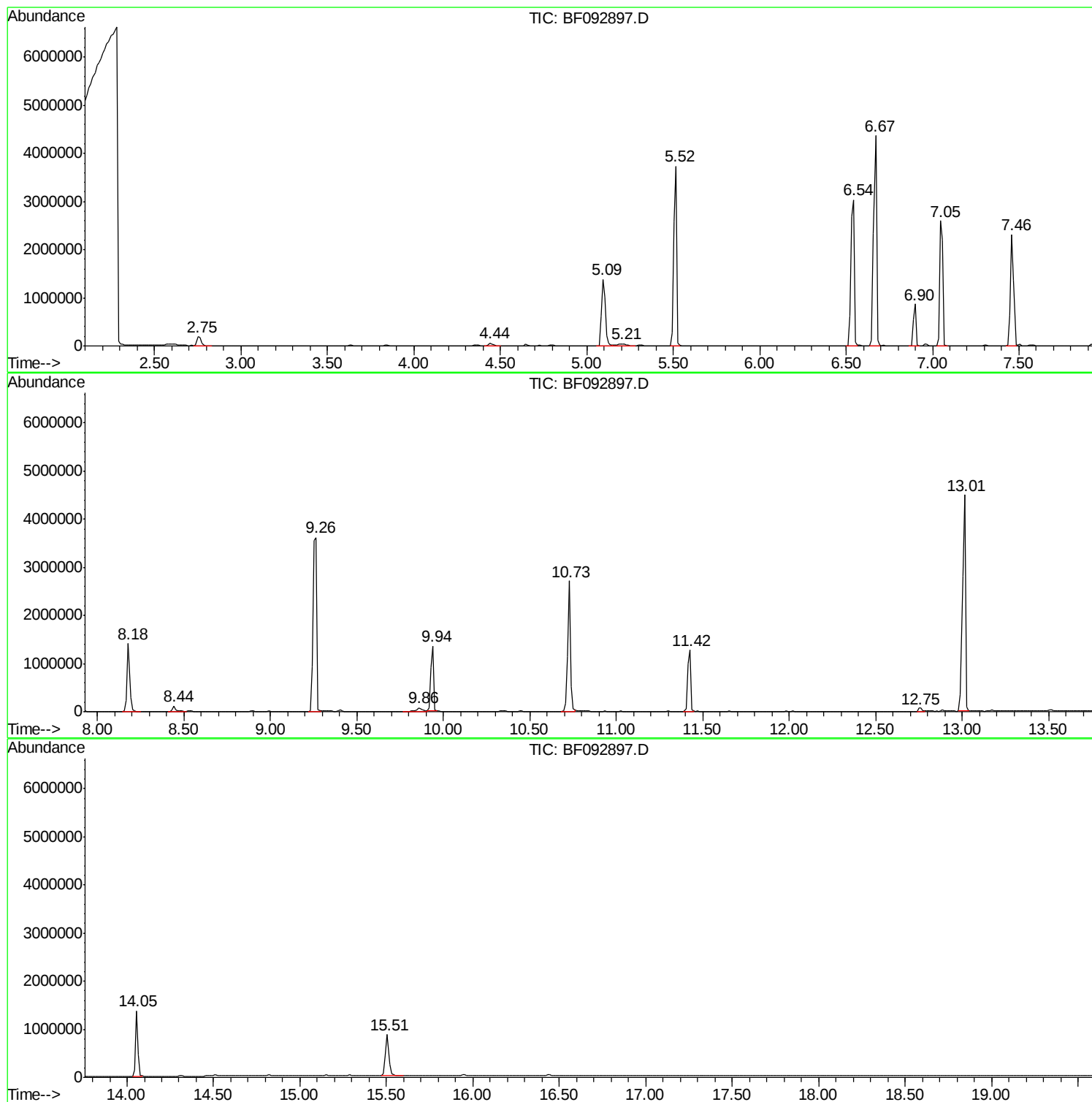
Sum of corrected areas: 45424214

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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



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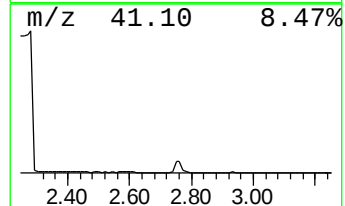
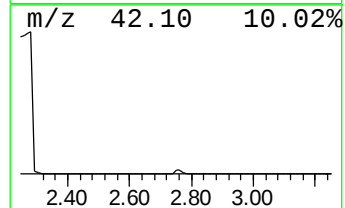
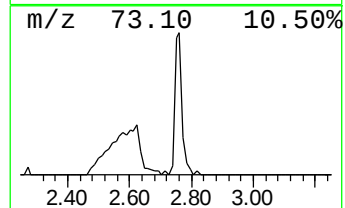
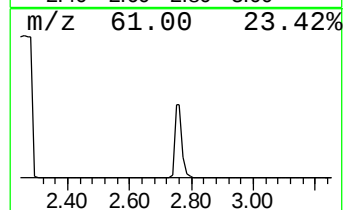
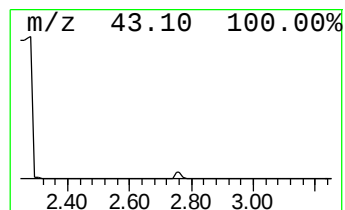
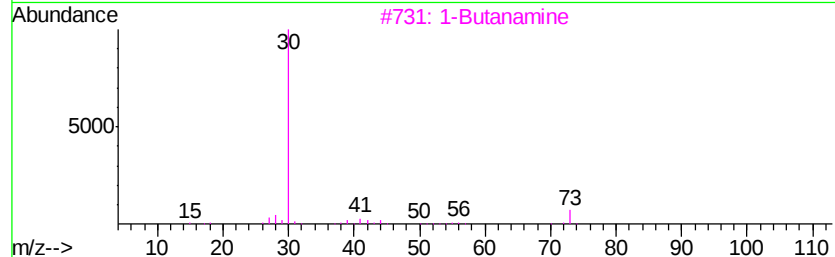
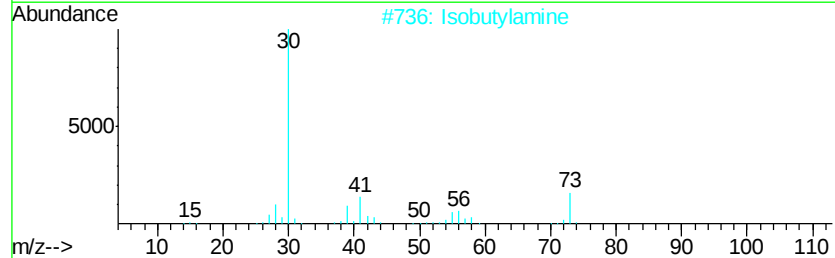
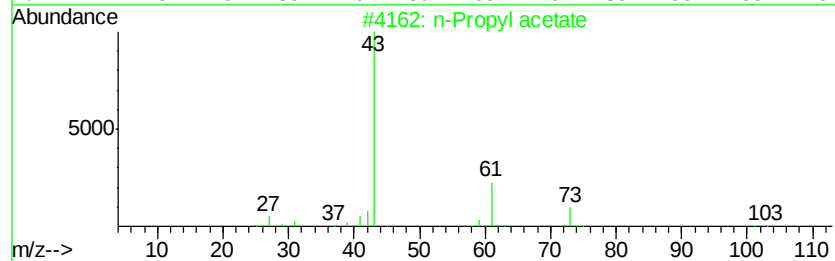
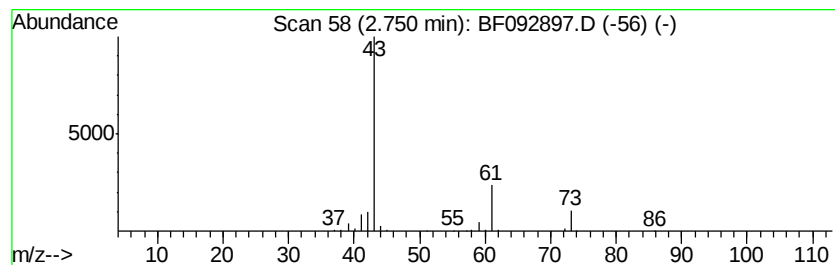
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 n-Propyl acetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.75	6.03 ng	295440	1,4-Dichlorobenzene-d4	6.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Propyl acetate	102	C5H10O2	000109-60-4	83
2		Isobutylamine	73	C4H11N	000078-81-9	7
3		1-Butanamine	73	C4H11N	000109-73-9	7
4		Hydrogen azide	43	HN3	007782-79-8	4
5		1,4-Butanediol, diacetate	174	C8H14O4	000628-67-1	4



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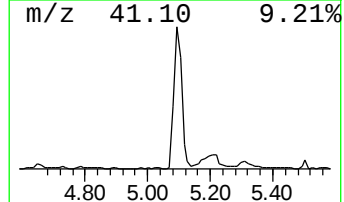
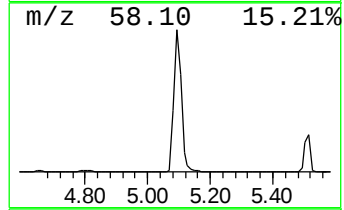
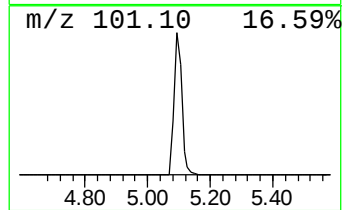
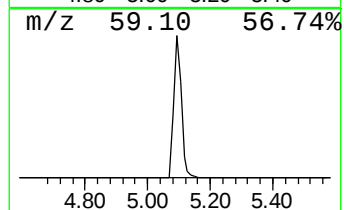
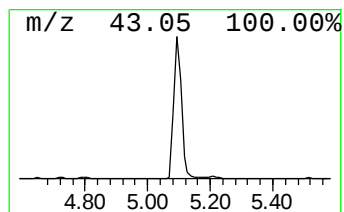
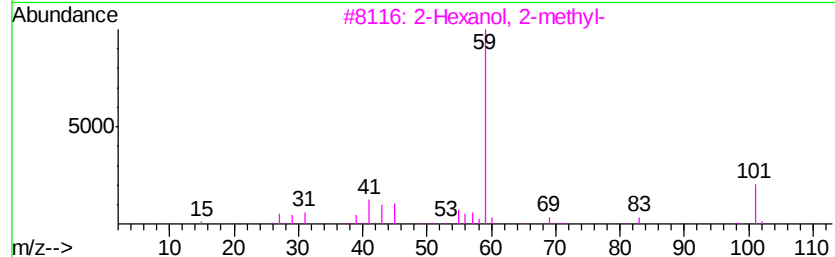
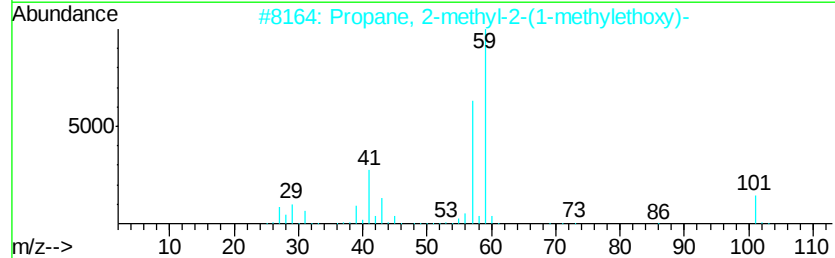
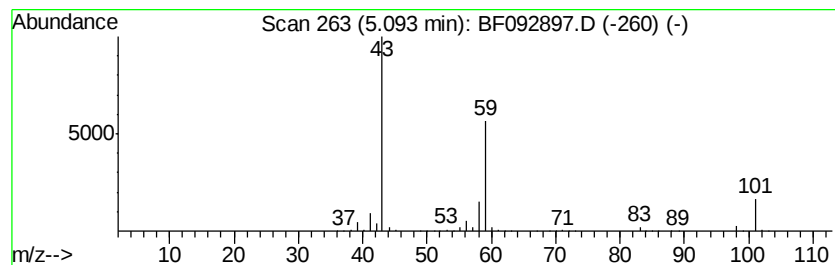
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	46.70 ng	2287950	1,4-Dichlorobenzene-d4	6.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32



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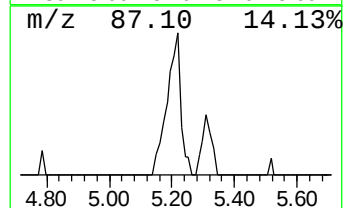
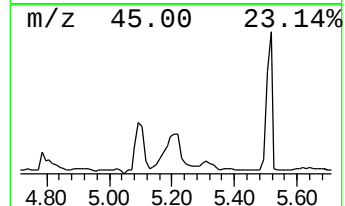
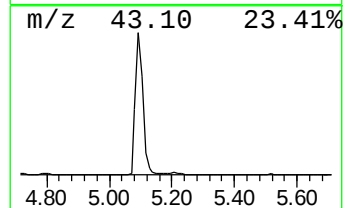
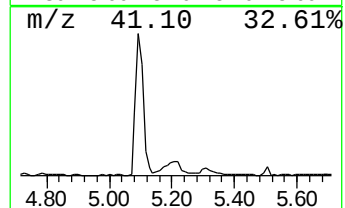
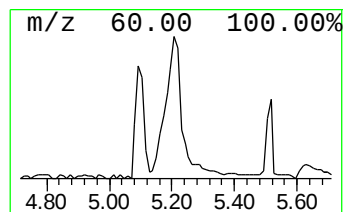
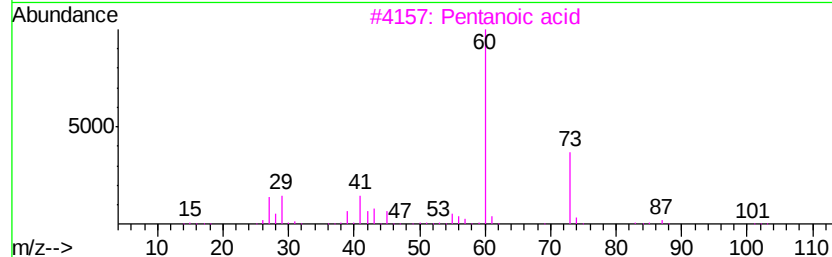
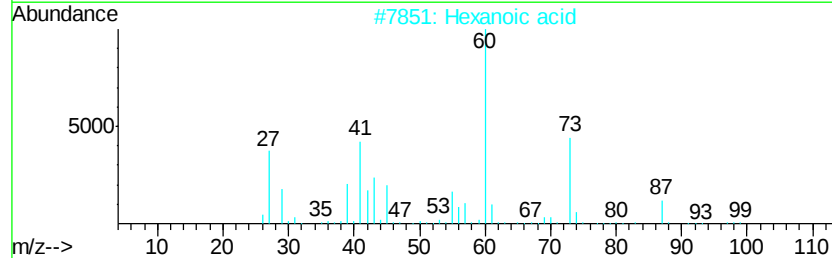
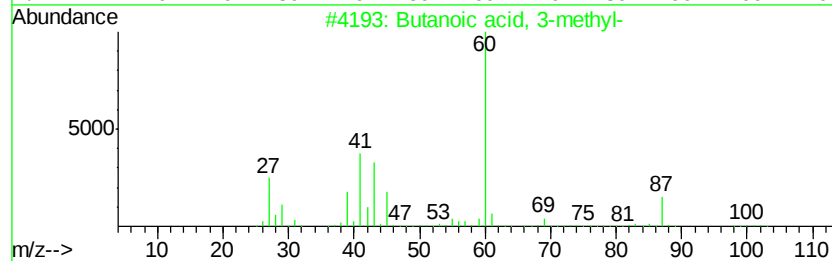
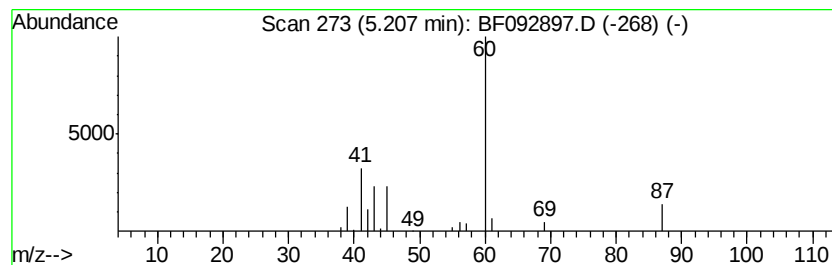
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Peak Number 3 Butanoic acid, 3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.21	2.79 ng	136833	1,4-Dichlorobenzene-d4	6.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	74
2		Hexanoic acid	116	C6H12O2	000142-62-1	39
3		Pentanoic acid	102	C5H10O2	000109-52-4	9
4		Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	5
5		1-Pentanamine	87	C5H13N	000110-58-7	5



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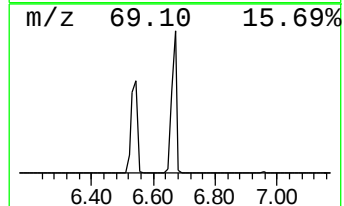
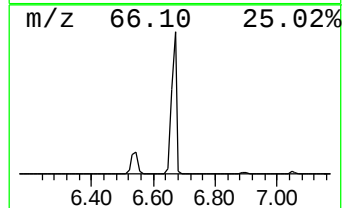
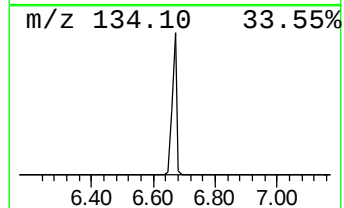
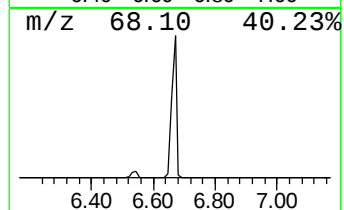
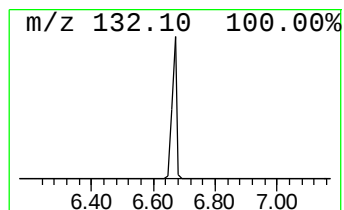
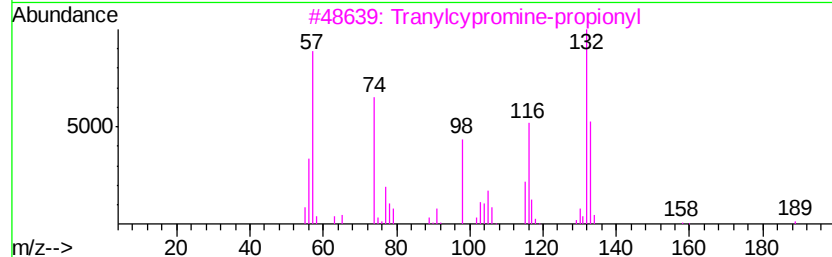
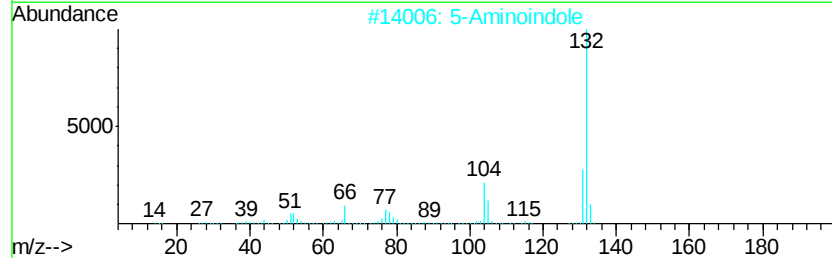
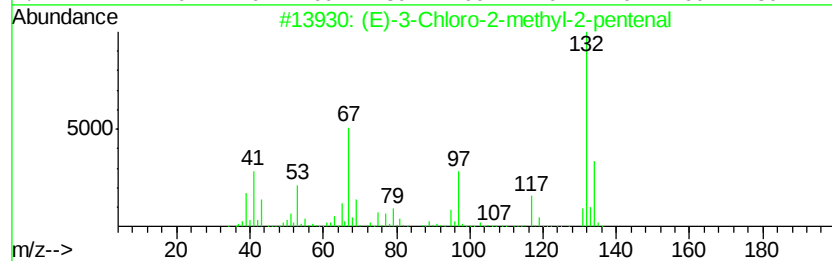
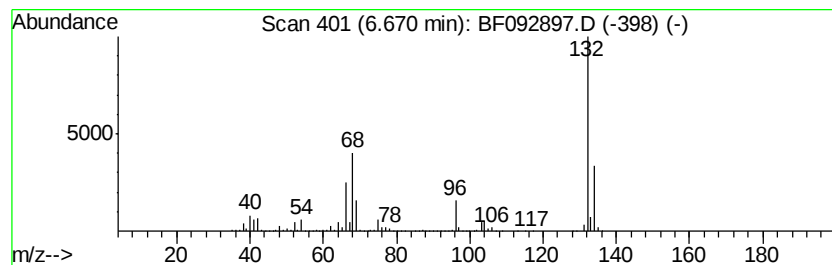
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 4 unknown6.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	96.70 ng	4737670	1,4-Dichlorobenzene-d4	6.90

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2			5-Aminoindole	132	C8H8N2	005192-03-0	12
3			Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4			Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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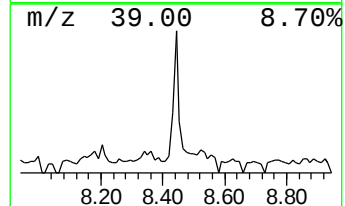
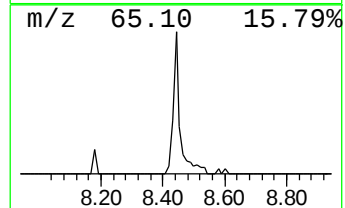
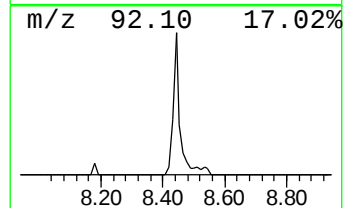
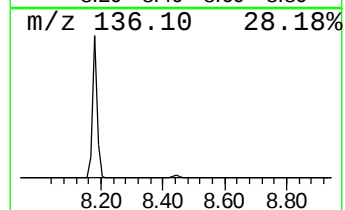
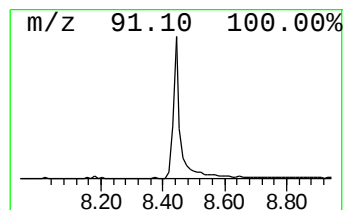
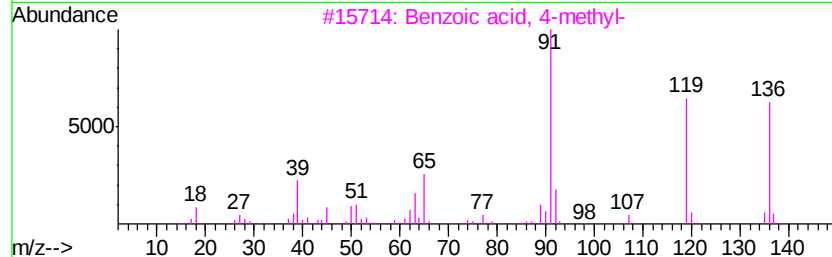
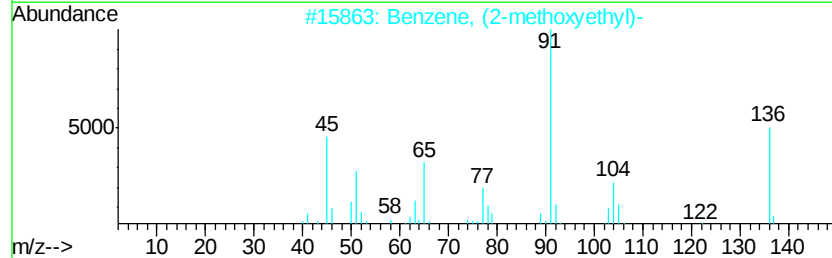
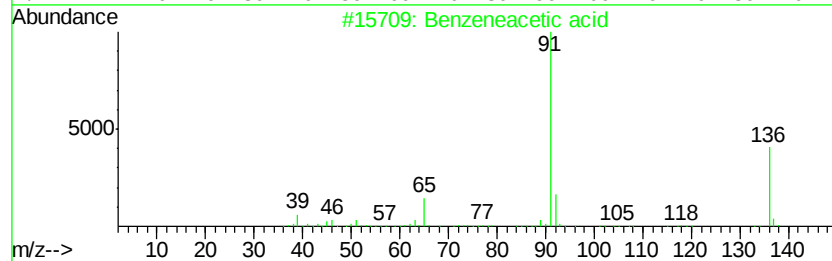
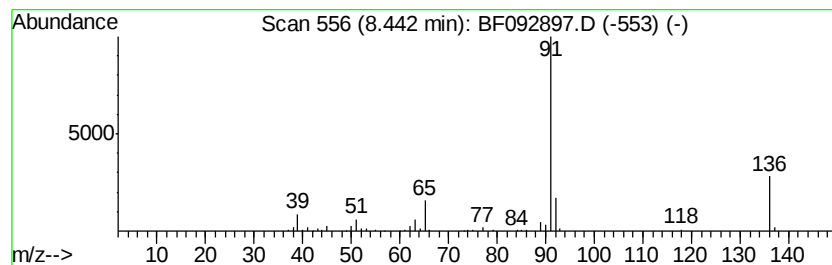
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Benzeneacetic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.44	2.34 ng	159705	Napthalene-d8	8.18

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzeneacetic acid	136	C8H8O2	000103-82-2	91
2		Benzene, (2-methoxyethyl)-	136	C9H12O	003558-60-9	72
3		Benzoic acid, 4-methyl-	136	C8H8O2	000099-94-5	59
4		Propanedioic acid, phenyl-	180	C9H8O4	002613-89-0	59
5		2-Benzyloxy-4-bromobutane-1,3-diol	274	C11H15BrO3	1000191-12-1	53



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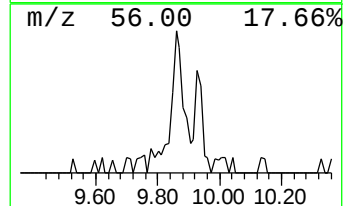
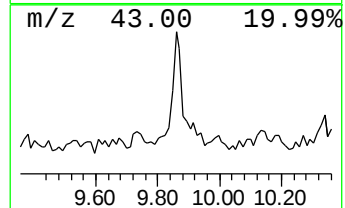
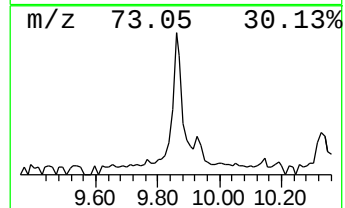
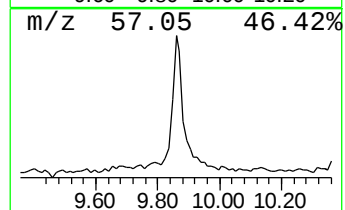
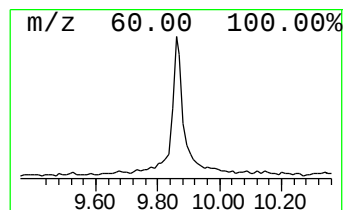
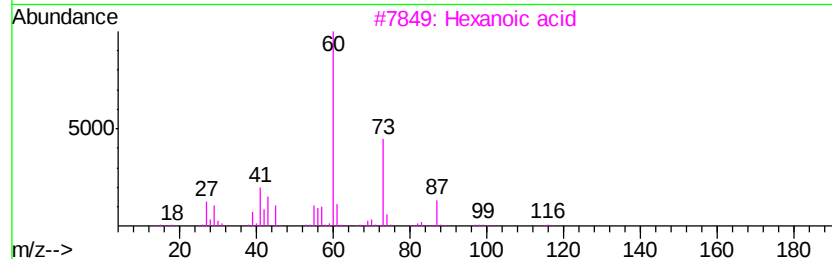
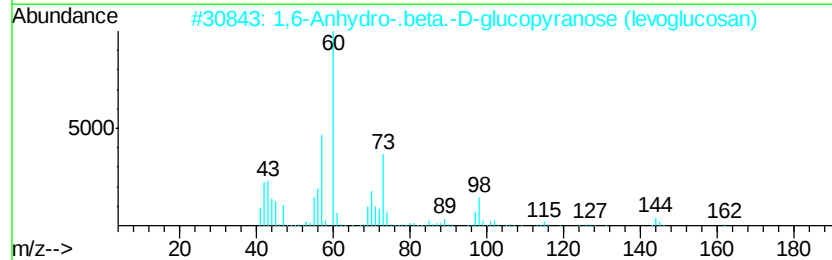
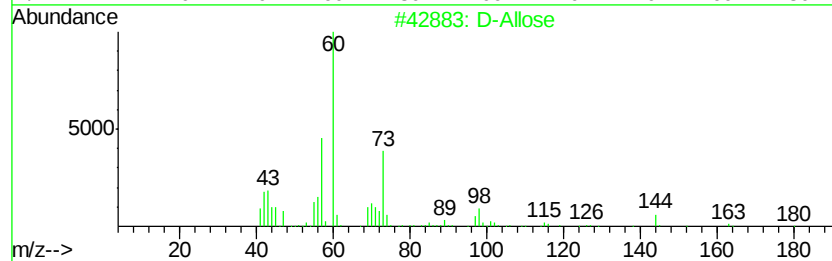
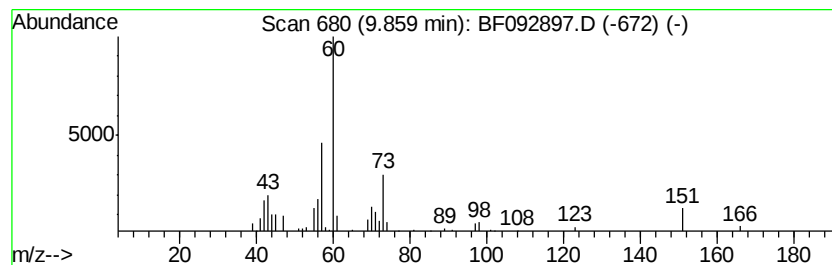
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TIC Integration Parameters: LSCINT.P

Peak Number 7 D-Allose Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.86	2.03 ng	163690	Acenaphthene-d10	9.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	D-Allose	180	C6H12O6	002595-97-3	80
2		1,6-Anhydro-.beta.-D-glucopyrano...	162	C6H10O5	000498-07-7	72
3		Hexanoic acid	116	C6H12O2	000142-62-1	53
4		Heptanoic acid	130	C7H14O2	000111-14-8	53
5		Pentanoic acid	102	C5H10O2	000109-52-4	53



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021017\
Data File : BF092897.D
Acq On : 10 Feb 2017 21:45
Operator : SJ/MA
Sample : I1769-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
9717

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Propyl acetate	2.75	6.0	ng	295440	1	6.90	979855	20.0
2-Pentanone, 4-hy...	5.09	46.7	ng	2287950	1	6.90	979855	20.0
Butanoic acid, 3-...	5.21	2.8	ng	136833	1	6.90	979855	20.0
unknown6.67	6.67	96.7	ng	4737670	1	6.90	979855	20.0
Benzeneacetic acid	8.44	2.3	ng	159705	2	8.18	1367640	20.0
D-Allose	9.86	2.0	ng	163690	3	9.94	1612930	20.0