

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111715\
 Data File : BF082992.D
 Acq On : 18 Nov 2015 3:53
 Operator : UM/IZ
 Sample : G4407-11
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-17

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-BF110715.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	2.178	5	8	26	rVB2	116653	321299	4.84%	0.681%
2	4.373	196	200	202	rVV	1141495	1570708	23.66%	3.327%
3	4.899	242	246	249	rBV	786151	1127007	16.97%	2.387%
4	5.356	283	286	288	rBV	2857668	2670713	40.22%	5.657%
5	6.396	375	377	380	rBV	1868589	1570420	23.65%	3.326%
6	6.522	385	388	390	rBV	4015553	4026769	60.65%	8.529%
7	6.750	406	408	411	rBV	1406888	1155709	17.41%	2.448%
8	6.876	417	419	420	rBV	151281	149092	2.25%	0.316%
9	6.910	420	422	424	rVB	4538074	3930347	59.20%	8.325%
10	7.322	455	458	460	rBV	3640999	3906845	58.84%	8.275%
11	7.950	511	513	515	rBV	82656	98259	1.48%	0.208%
12	8.042	518	521	522	rVV	1477754	1544042	23.26%	3.271%
13	8.087	522	525	528	rVB2	30081	69117	1.04%	0.146%
14	8.510	560	562	564	rBV	73951	74008	1.11%	0.157%
15	8.705	577	579	581	rVB	111839	91507	1.38%	0.194%
16	8.807	586	588	593	rVB3	193369	246156	3.71%	0.521%
17	8.887	593	595	597	rBV	131350	169019	2.55%	0.358%
18	9.025	603	607	610	rBV2	75196	115395	1.74%	0.244%
19	9.116	612	615	618	rVV	4627999	6045718	91.06%	12.806%
20	9.253	625	627	628	rBV	89324	81240	1.22%	0.172%
21	9.276	628	629	632	rVV2	68395	103046	1.55%	0.218%
22	9.322	632	633	635	rVB	109519	110792	1.67%	0.235%
23	9.516	645	650	651	rBV	99122	123059	1.85%	0.261%
24	9.630	657	660	664	rBV3	26164	78166	1.18%	0.166%
25	9.790	672	674	677	rVB	1987539	1763413	26.56%	3.735%
26	9.928	684	686	688	rVB	65025	70789	1.07%	0.150%
27	10.213	709	711	715	rVB2	43693	73286	1.10%	0.155%
28	10.579	740	743	746	rBV	3555417	3850930	58.00%	8.157%
29	10.682	750	752	753	rVV	137202	151058	2.28%	0.320%
30	10.716	753	755	758	rVB3	36741	86462	1.30%	0.183%
31	11.151	790	793	795	rVB3	70009	97200	1.46%	0.206%
32	11.265	801	803	806	rVB	1304226	1756893	26.46%	3.721%
33	12.705	926	929	931	rBV	71376	97260	1.46%	0.206%
34	12.865	940	943	945	rBV	6168436	6639494	100.00%	14.064%

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.905	1031	1034	1036	rBV	1514470	1829910	27.56%	3.876%
36	14.762	1106	1109	1111	rVB	85275	113501	1.71%	0.240%
37	15.300	1153	1156	1158	rBV	971888	1301958	19.61%	2.758%

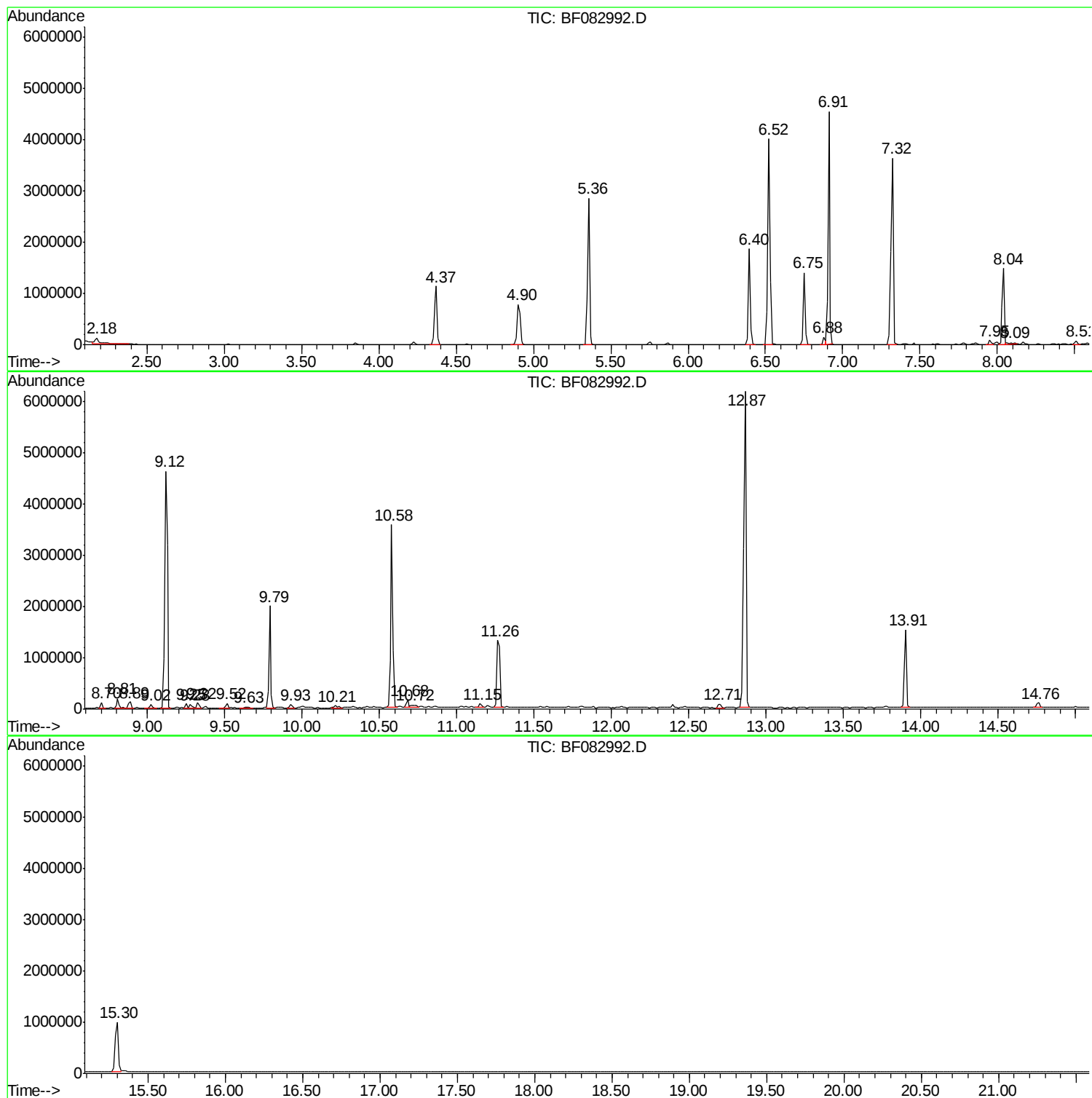
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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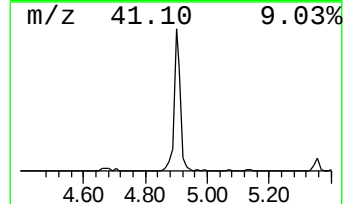
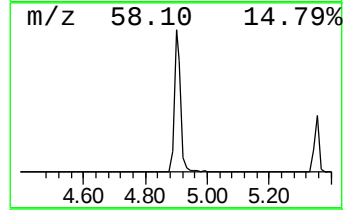
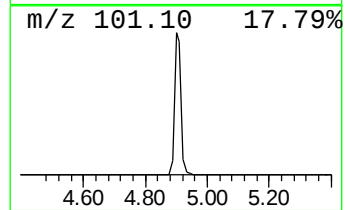
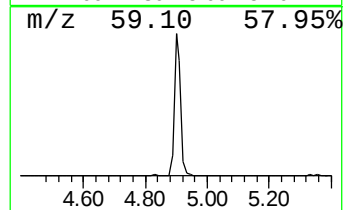
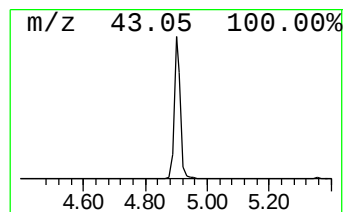
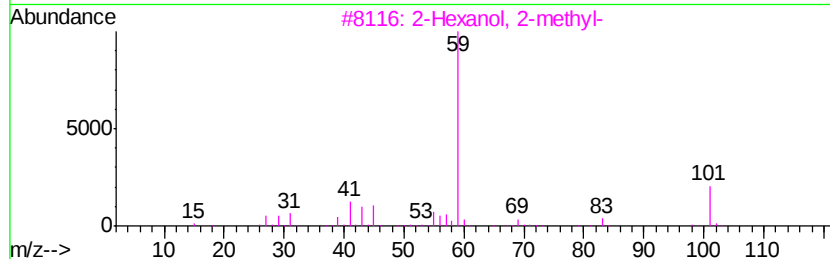
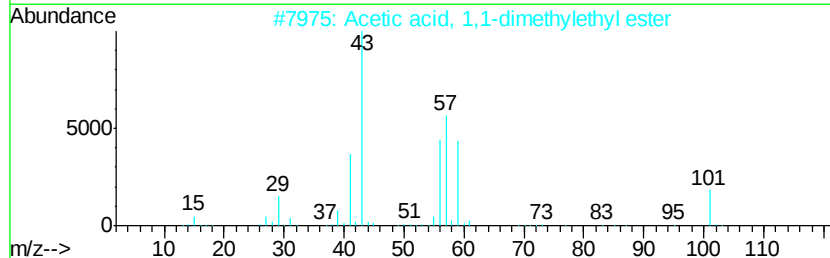
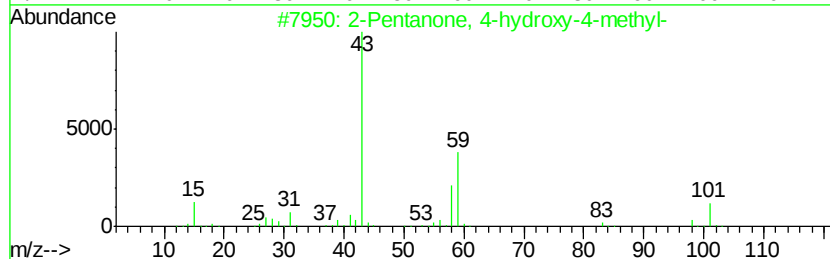
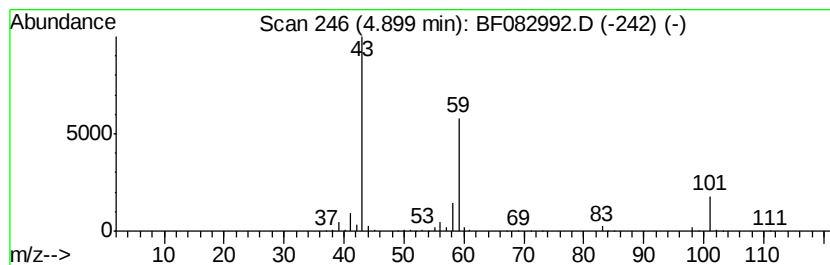
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	19.50 ng	1127010	1,4-Dichlorobenzene-d4	6.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4		3-Hexanol	102	C6H14O	000623-37-0	33
5		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33



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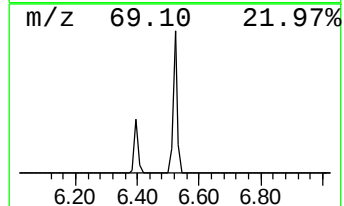
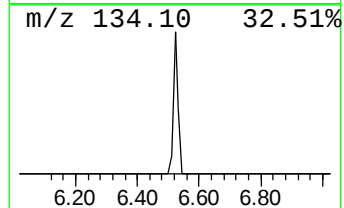
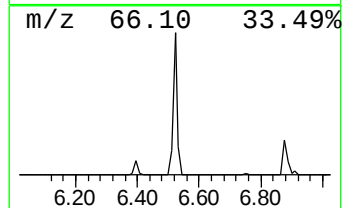
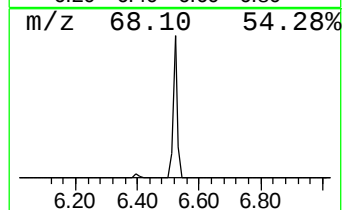
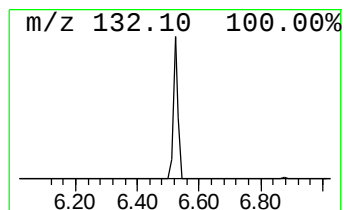
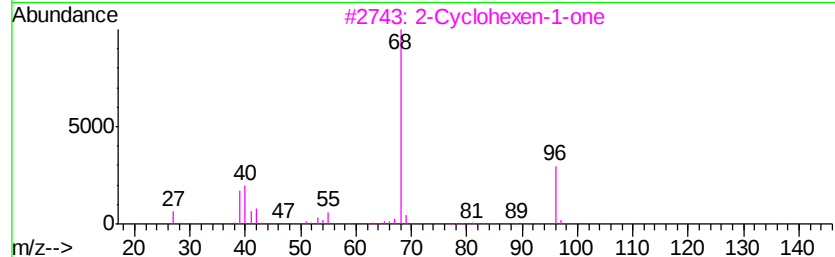
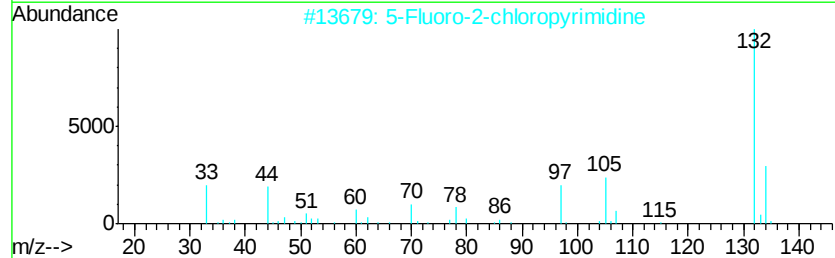
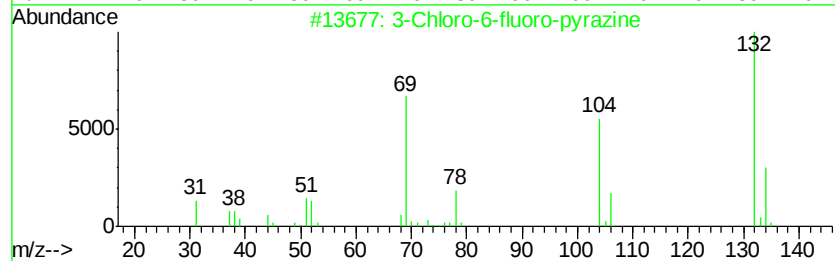
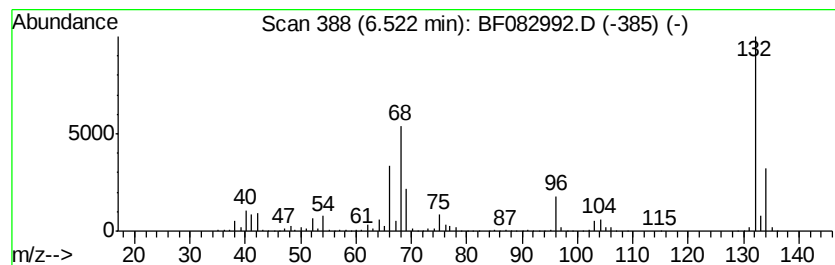
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown6.52 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.52	69.68 ng	4026770	1,4-Dichlorobenzene-d4	6.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10
4		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
5		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9



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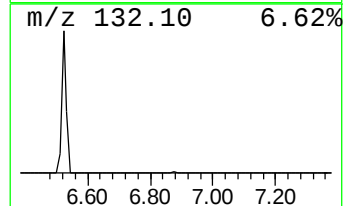
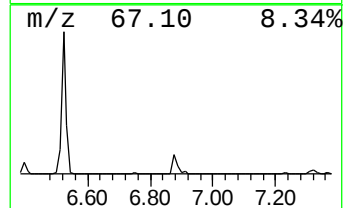
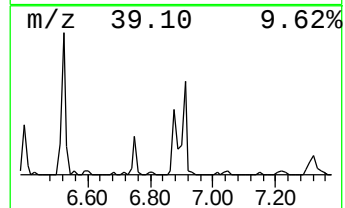
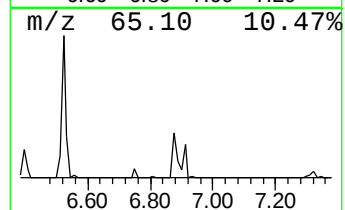
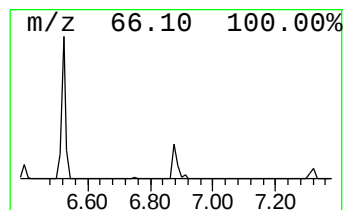
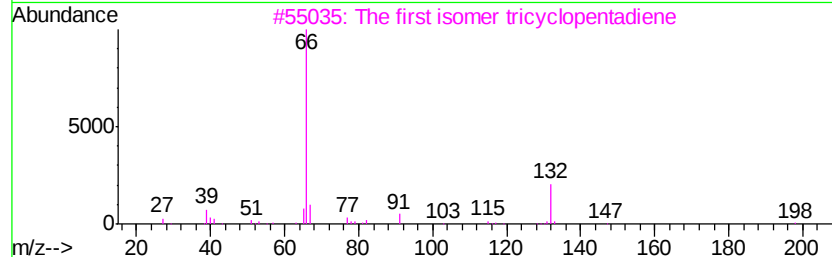
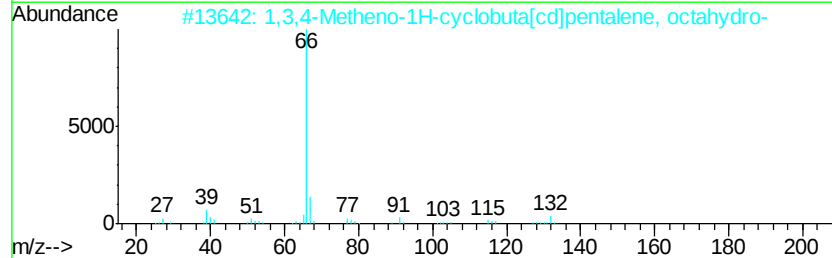
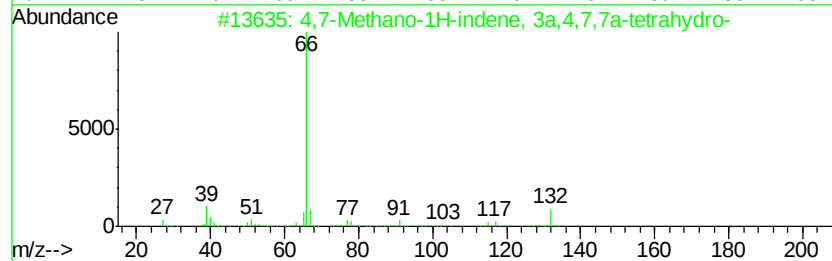
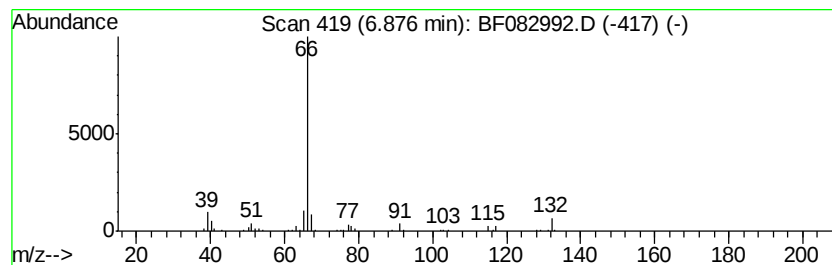
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Peak Number 5 4,7-Methano-1H-indene, 3a,4... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.88	2.58 ng	149092	1,4-Dichlorobenzene-d4	6.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4,7-Methano-1H-indene, 3a,4,7,7a...	132	C10H12	000077-73-6	91
2		1,3,4-Metheno-1H-cyclobuta[cd]pe...	132	C10H12	006707-88-6	90
3		The first isomer tricyclopentadiene	198	C15H18	1000222-21-0	83
4		Bicyclo[2.2.1]hept-5-en-2-ol	110	C7H10O	013080-90-5	83
5		5-Ethyl bicyclo[2.2.1]-2-heptene	122	C9H14	015403-89-1	74



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ClientSampled :
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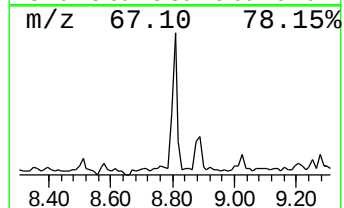
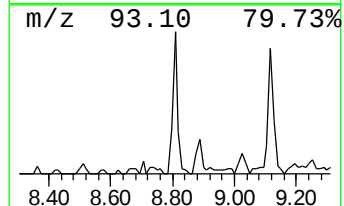
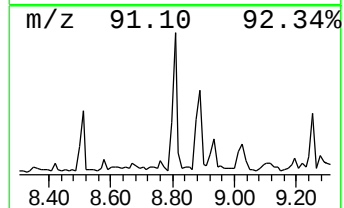
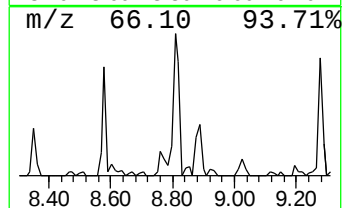
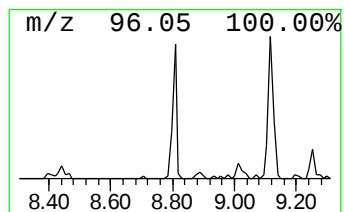
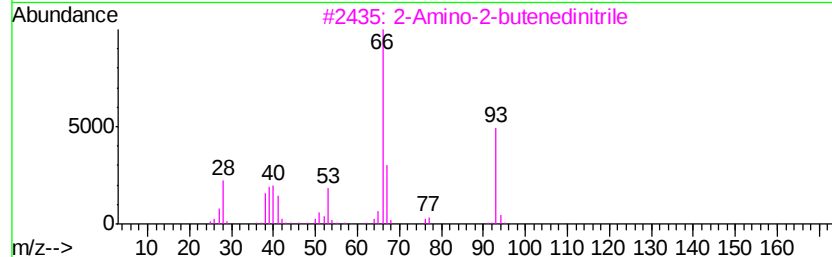
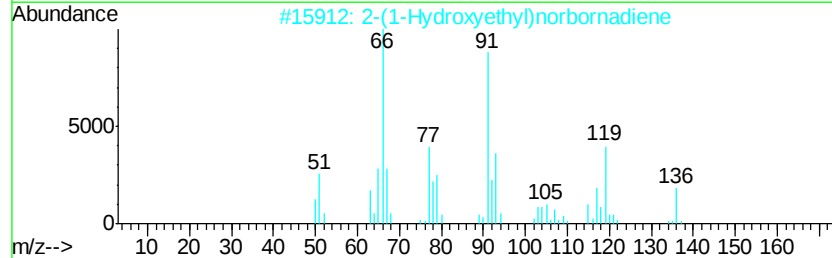
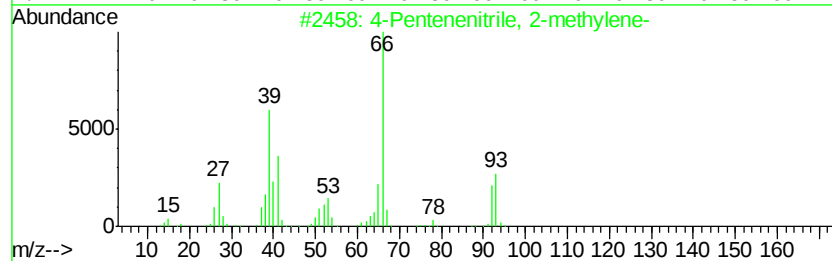
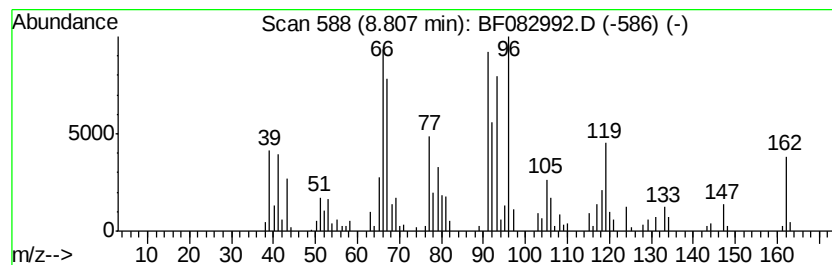
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 7 unknown8.81 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.81	3.19 ng	246156	Naphthalene-d8	8.04

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Pentenitrile, 2-methylene-	93	C6H7N	028769-50-8	43
2			2-(1-Hydroxyethyl)norbornadiene	136	C9H12O	1000139-55-9	43
3			2-Amino-2-butenedinitrile	93	C4H3N3	1000196-60-0	43
4			Nortricyclyl formate	138	C8H10O2	021892-95-5	38
5			Pyridine, 3-methyl-	93	C6H7N	000108-99-6	37



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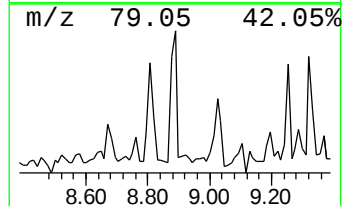
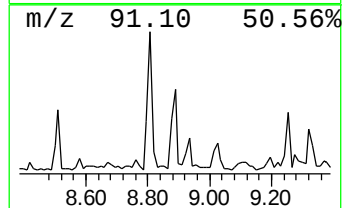
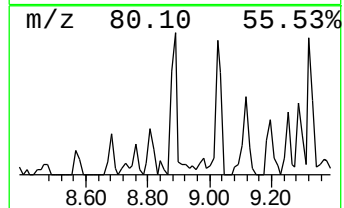
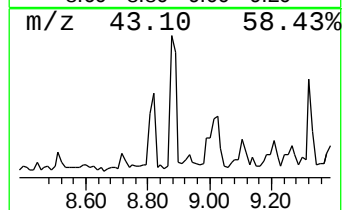
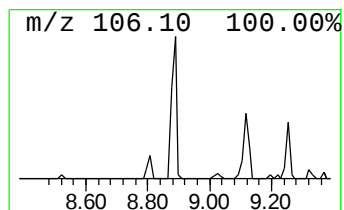
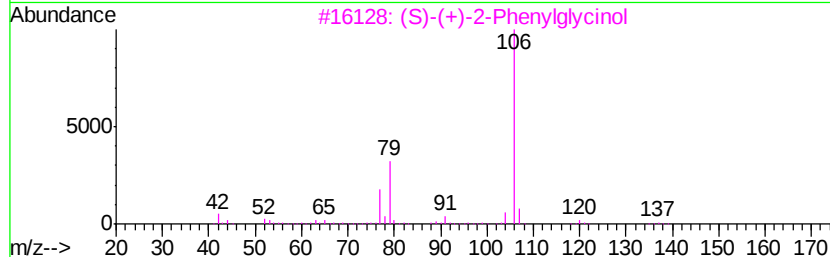
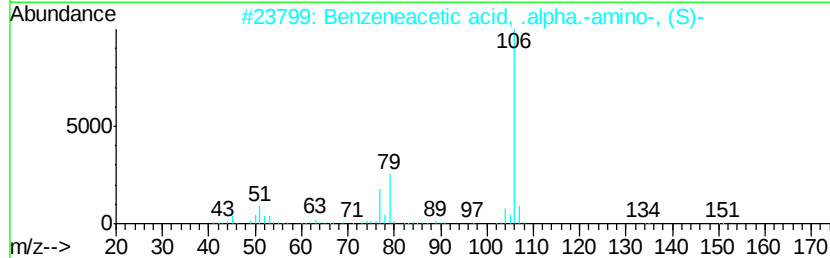
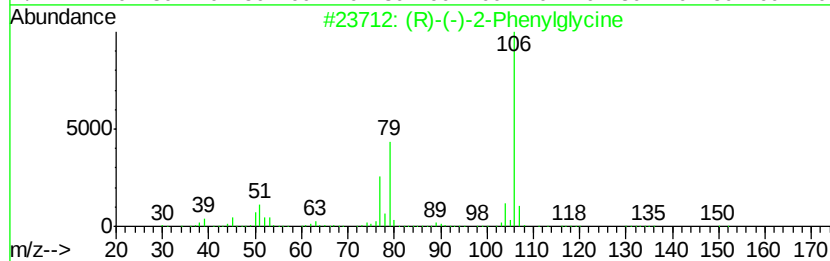
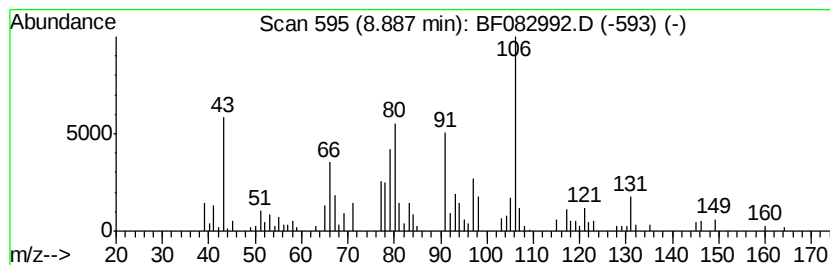
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Peak Number 8 unknown8.89 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.89	2.19 ng	169019	Napthalene-d8	8.04

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(R)-(-)-2-Phenylglycine		151	C8H9NO2		000875-74-1	27
2	Benzeneacetic acid, .alpha.-amin...		151	C8H9NO2		002935-35-5	27
3	(S)-(+)-2-Phenylglycinol		137	C8H11NO		020989-17-7	27
4	Benzenemethanamine, .alpha.-meth...		121	C8H11N		002627-86-3	27
5	Benzenemethanamine, .alpha.-meth...		121	C8H11N		000618-36-0	27



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Data File : BF082992.D
Acq On : 18 Nov 2015 3:53
Operator : UM/IZ
Sample : G4407-11
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-17

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.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
2-Pentanone, 4-hy...	4.90	19.5	ng	1127010	1	6.75	1155710	20.0
unknown6.52	6.52	69.7	ng	4026770	1	6.75	1155710	20.0
4,7-Methano-1H-in...	6.88	2.6	ng	149092	1	6.75	1155710	20.0
unknown8.81	8.81	3.2	ng	246156	2	8.04	1544040	20.0
unknown8.89	8.89	2.2	ng	169019	2	8.04	1544040	20.0