

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011915\
 Data File : BF076926.D
 Acq On : 19 Jan 2015 13:04
 Operator : IZ / TP
 Sample : G1101-04
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PO-002

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-BF011415.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	1.213	3	11	12	rVB	14159	45130	2.27%	0.422%
2	1.464	30	33	44	rBV	30586	69792	3.51%	0.652%
3	2.093	80	88	89	rBV2	7872	25019	1.26%	0.234%
4	2.150	89	93	95	rVV4	9554	34962	1.76%	0.327%
5	2.207	95	98	101	rVB3	13050	40387	2.03%	0.377%
6	2.801	141	150	151	rBV3	7039	28654	1.44%	0.268%
7	4.104	262	264	272	rBV	16142	34418	1.73%	0.321%
8	4.870	329	331	333	rVB	35949	48816	2.46%	0.456%
9	5.030	342	345	352	rVB2	110779	305072	15.35%	2.849%
10	5.602	386	395	397	rBV3	11674	46850	2.36%	0.438%
11	7.396	546	552	555	rBV2	538078	921044	46.33%	8.603%
12	7.465	555	558	566	rVB	228364	378654	19.05%	3.537%
13	7.979	599	603	606	rBV	114721	202116	10.17%	1.888%
14	8.299	627	631	634	rBV	286595	499478	25.12%	4.665%
15	9.133	701	704	712	rBV2	20446	43133	2.17%	0.403%
16	9.271	712	716	722	rVB	249215	408194	20.53%	3.813%
17	10.619	825	834	839	rBV3	18574	60328	3.03%	0.563%
18	10.722	839	843	849	rVB2	12243	28785	1.45%	0.269%
19	10.882	853	857	860	rBV	196199	289544	14.56%	2.704%
20	11.979	937	953	959	rBV	188648	1013459	50.98%	9.466%
21	12.162	966	969	975	rVB6	8121	23378	1.18%	0.218%
22	12.345	982	985	989	rBV	19186	33104	1.67%	0.309%
23	12.517	997	1000	1004	rBV	187623	312474	15.72%	2.919%
24	13.248	1046	1064	1066	rBV	339348	1988028	100.00%	18.568%
25	13.534	1085	1089	1092	rVB	563440	830194	41.76%	7.754%
26	14.597	1179	1182	1185	rVB	18863	27429	1.38%	0.256%
27	15.008	1215	1218	1224	rVB	212780	348912	17.55%	3.259%
28	15.465	1253	1258	1263	rVB	12075	23659	1.19%	0.221%
29	15.923	1293	1298	1303	rBV2	12818	25692	1.29%	0.240%
30	16.620	1356	1359	1361	rBV	46495	58209	2.93%	0.544%
31	16.677	1361	1364	1367	rVB	274599	327508	16.47%	3.059%
32	17.774	1457	1460	1463	rBV	310653	340111	17.11%	3.177%
33	18.711	1540	1542	1544	rBV2	23541	24551	1.23%	0.229%
34	18.757	1544	1546	1554	rVB2	47623	70394	3.54%	0.657%

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Integration Parameters: rteint.p
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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

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Peak separation: 5

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35	19.466	1606	1608	1611	rVB	126500	170159	8.56%	1.589%
36	20.003	1653	1655	1658	rVB	832253	850282	42.77%	7.942%
37	21.272	1761	1766	1769	rBV	301129	416910	20.97%	3.894%
38	22.472	1868	1871	1874	rVV	22923	29547	1.49%	0.276%
39	22.918	1907	1910	1913	rBV	228412	282157	14.19%	2.635%

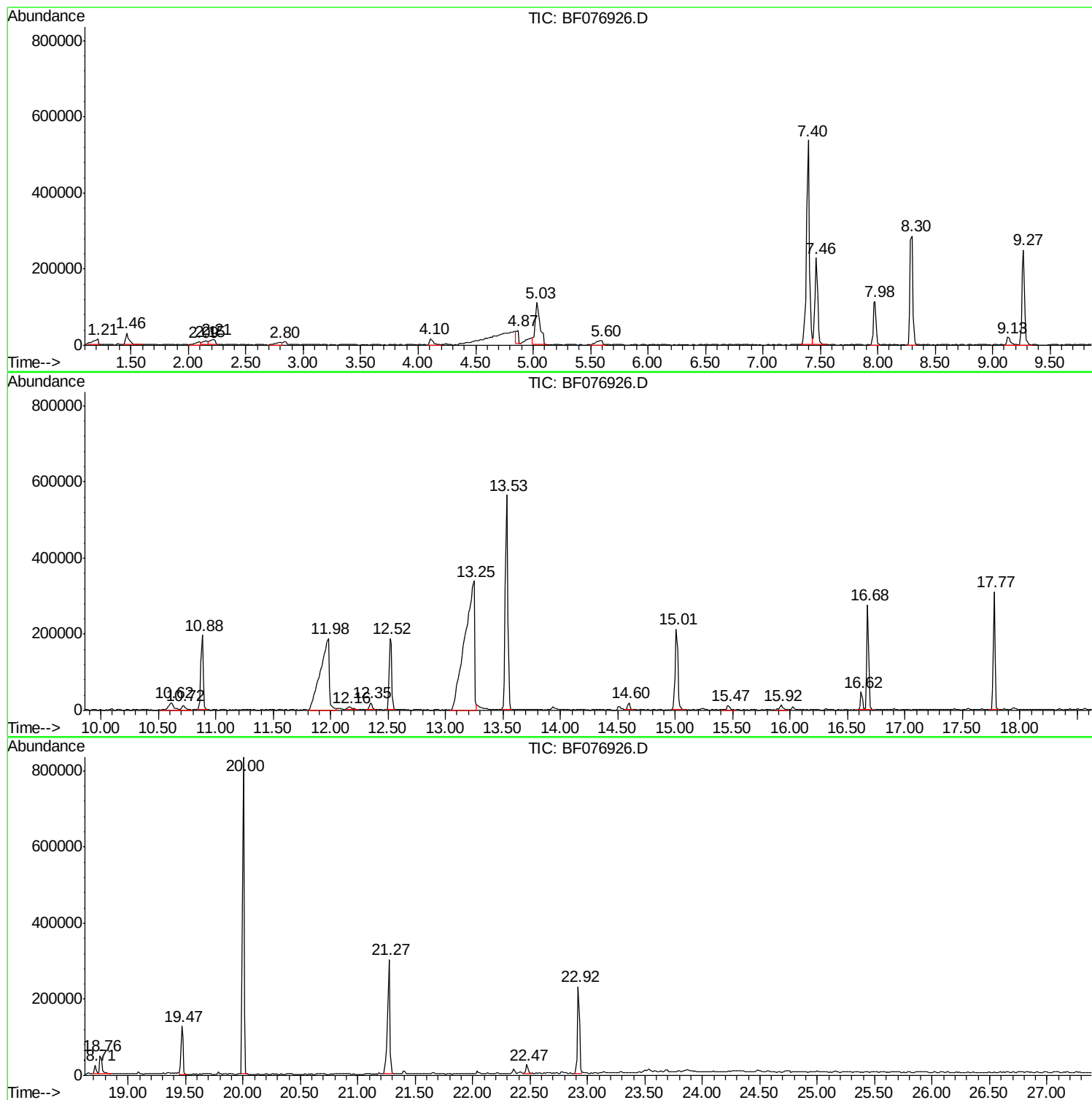
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF011415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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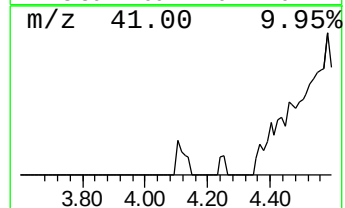
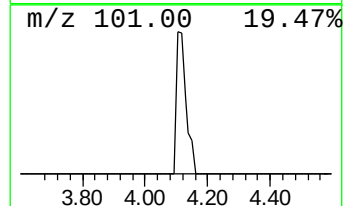
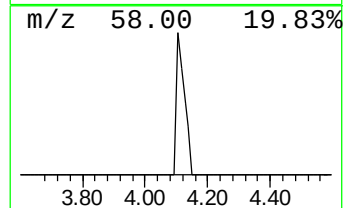
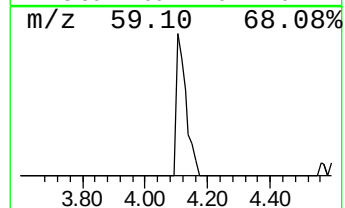
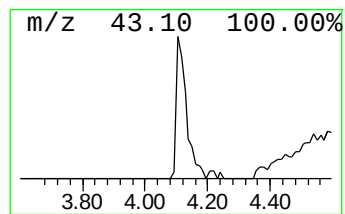
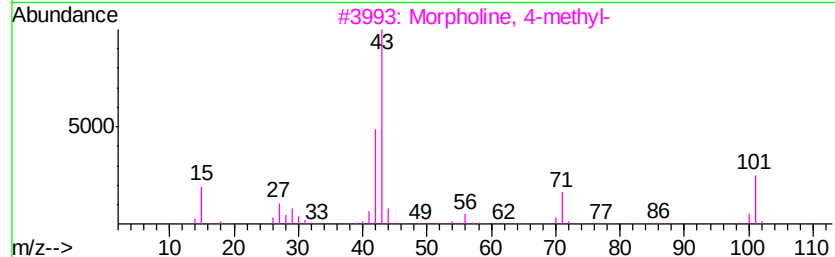
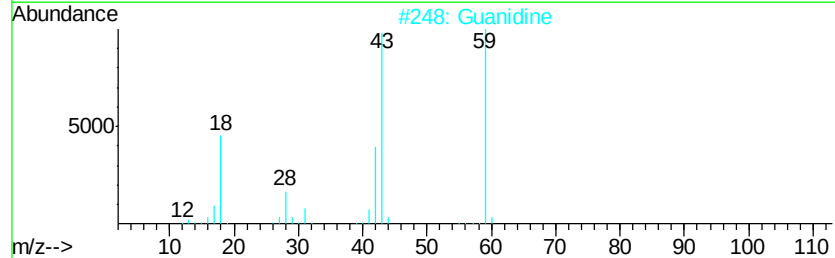
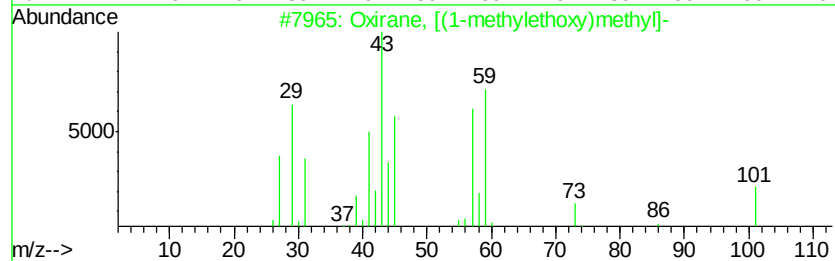
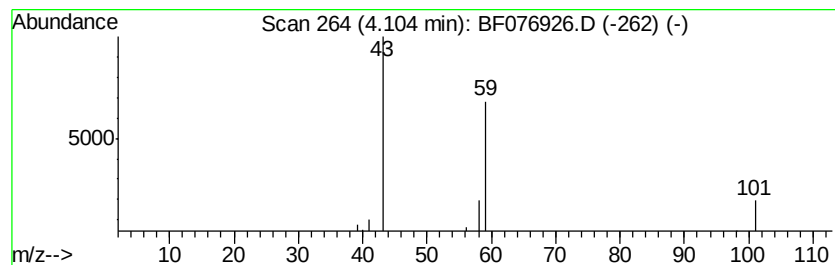
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Oxirane, [(1-methylethoxy)m... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.10	3.41 ng	34418	1,4-Dichlorobenzene-d4	7.98

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Oxirane, [(1-methylethoxy)methyl]-	116	C6H12O2	004016-14-2	64
2		Guanidine	59	CH5N3	000113-00-8	5
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	5
4		5-Hexen-2-one	98	C6H10O	000109-49-9	5
5		2-Propanone, 1-cyclopropyl-	98	C6H10O	004160-75-2	5



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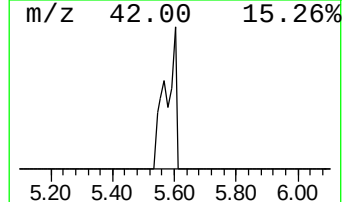
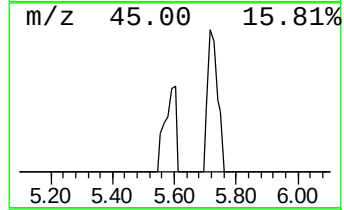
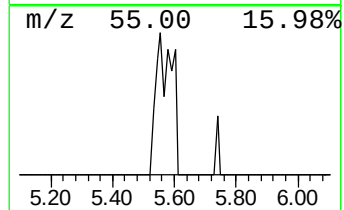
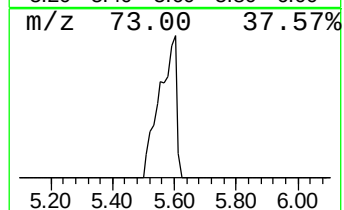
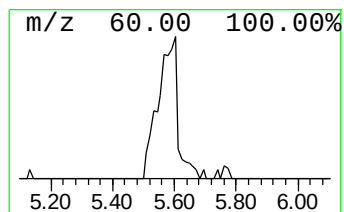
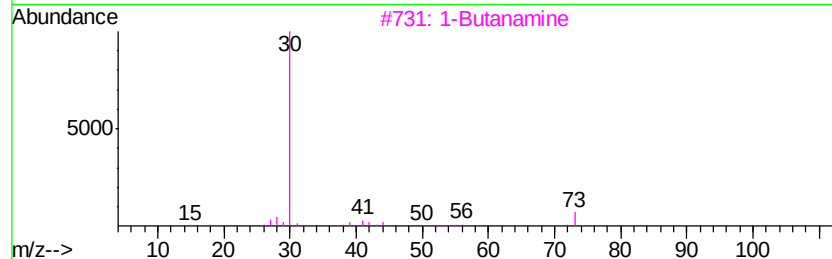
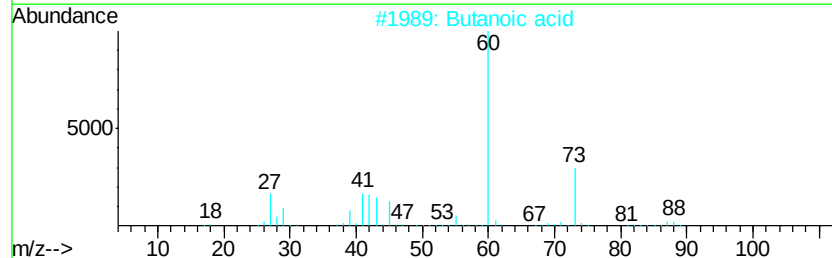
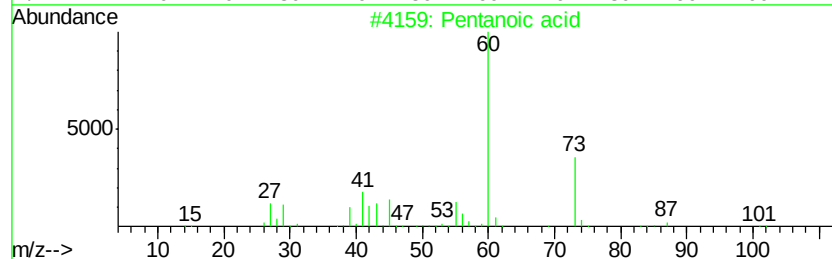
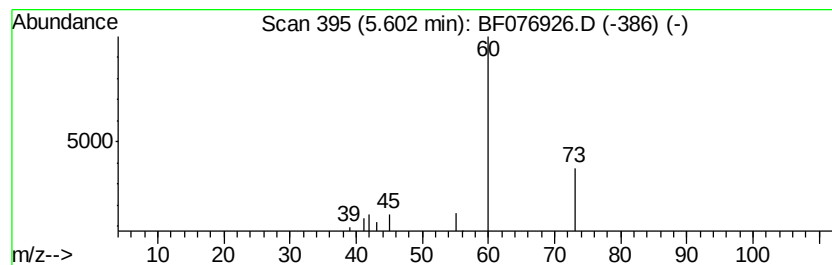
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Pentanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.60	4.64 ng	46850	1,4-Dichlorobenzene-d4	7.98

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentanoic acid	102	C5H10O2	000109-52-4	74
2		Butanoic acid	88	C4H8O2	000107-92-6	64
3		1-Butanamine	73	C4H11N	000109-73-9	7
4		Isobutylamine	73	C4H11N	000078-81-9	5
5		Formic acid hydrazide	60	CH4N2O	000624-84-0	4



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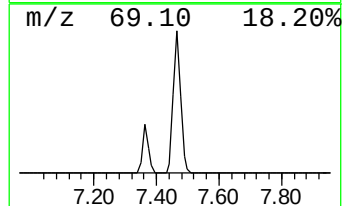
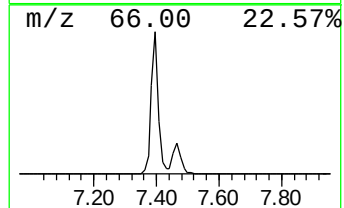
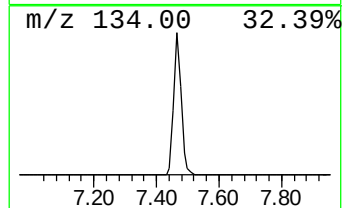
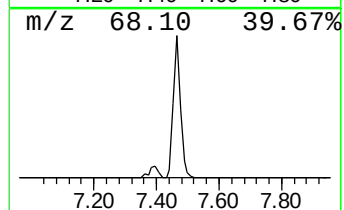
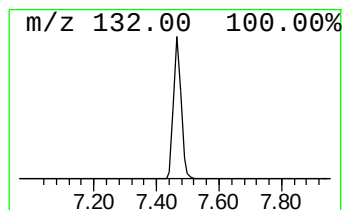
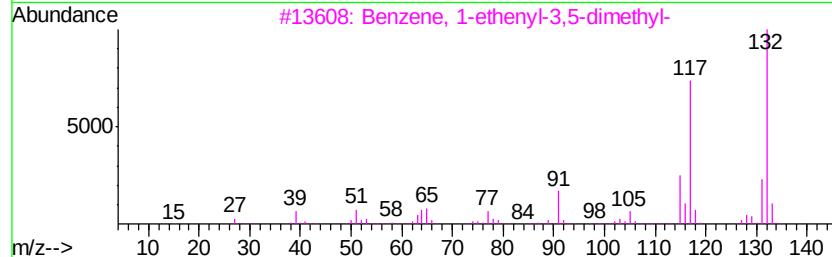
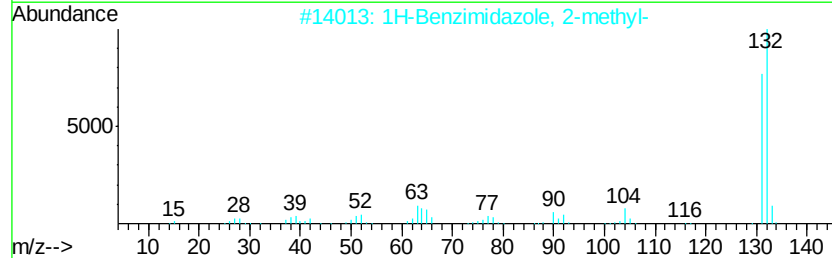
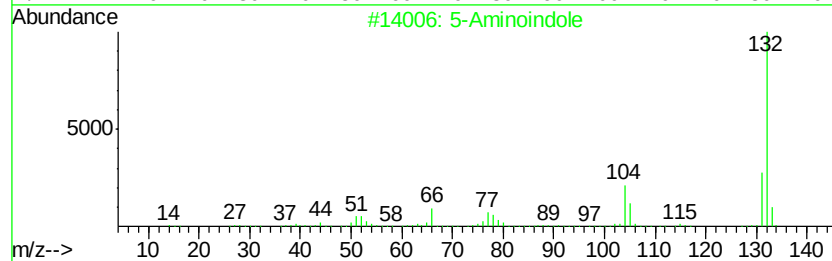
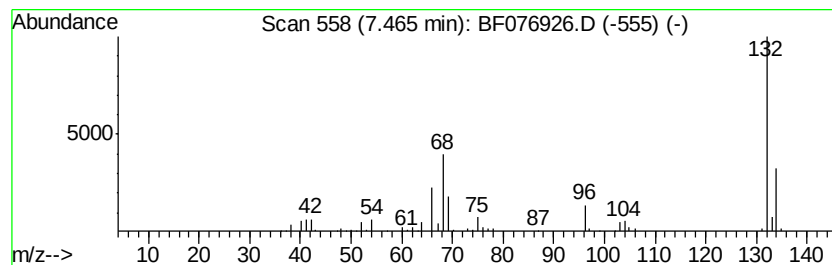
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 unknown7.46 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.46	37.47 ng	378654	1,4-Dichlorobenzene-d4	7.98

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Aminoindole	132	C8H8N2	005192-03-0	12
2		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
3		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
4		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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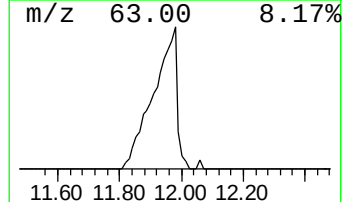
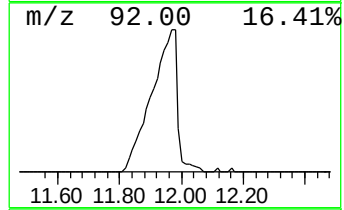
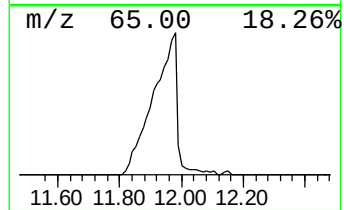
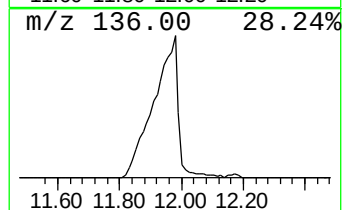
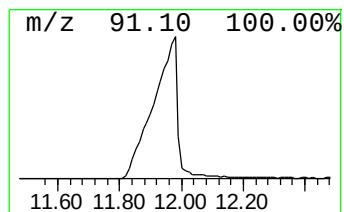
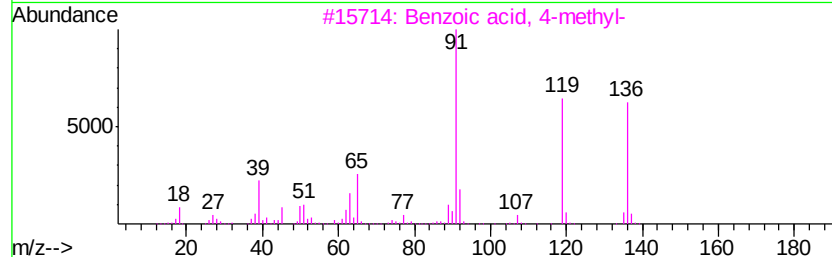
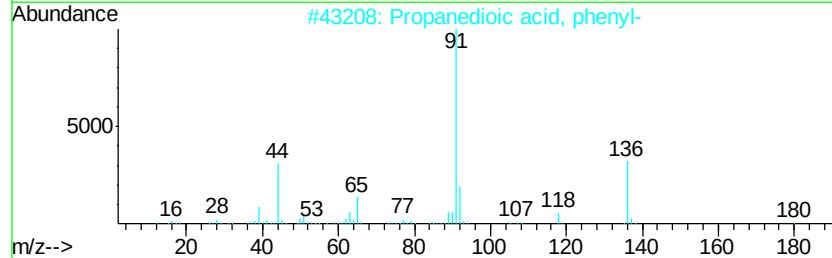
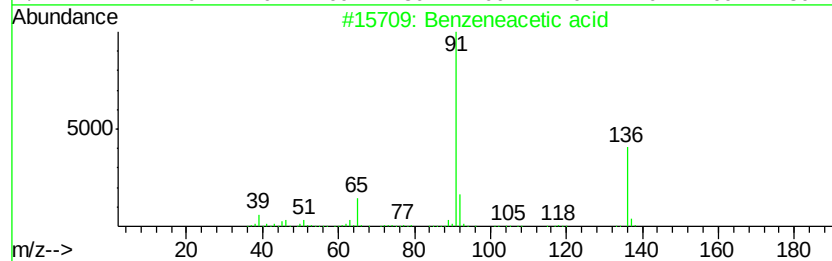
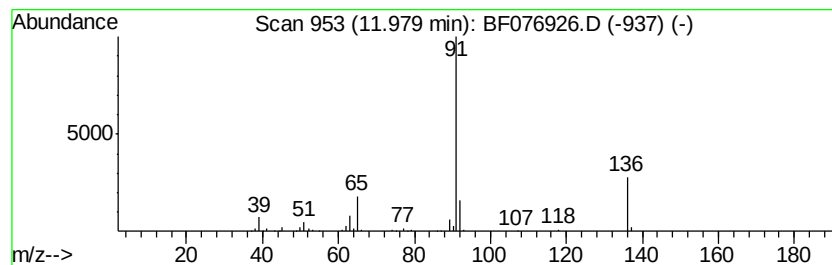
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Benzeneacetic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.98	70.00 ng	1013460	Napthalene-d8	10.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzeneacetic acid	136	C8H8O2	000103-82-2	86
2		Propanedioic acid, phenyl-	180	C9H8O4	002613-89-0	78
3		Benzoic acid, 4-methyl-	136	C8H8O2	000099-94-5	72
4		p-Methylbenzeneboronic acid	136	C7H9BO2	005720-05-8	59
5		Benzyl 2-chloroethyl sulfone	218	C9H11ClO2S	066998-67-2	50



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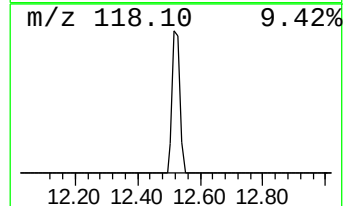
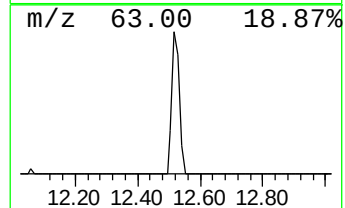
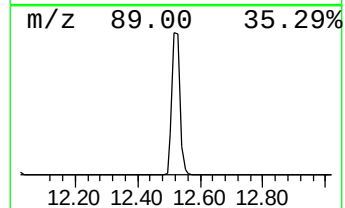
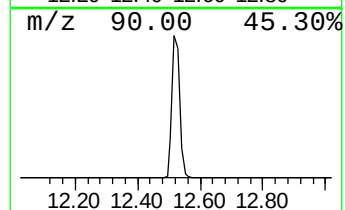
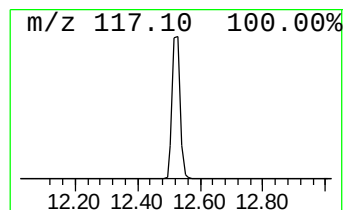
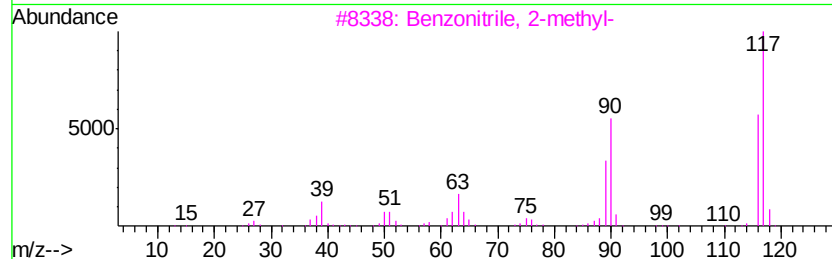
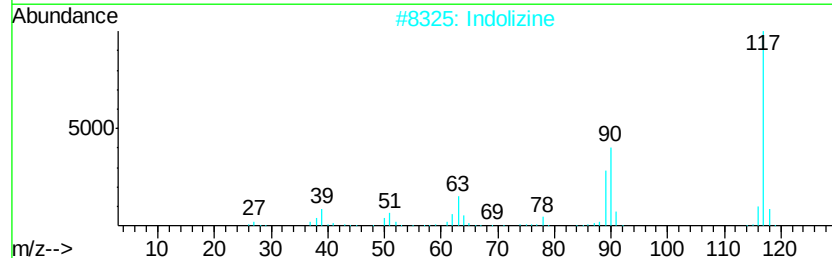
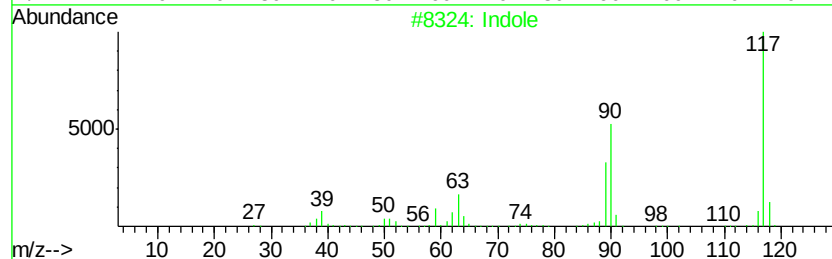
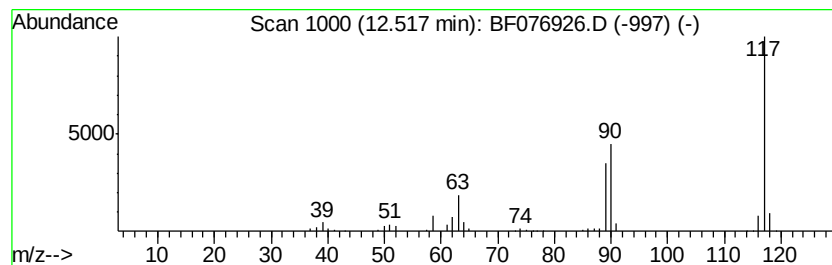
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Peak Number 15 Indole Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.52	21.58 ng	312474	Naphthalene-d8	10.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Indole	117	C8H7N	000120-72-9	95
2		Indolizine	117	C8H7N	000274-40-8	91
3		Benzonitrile, 2-methyl-	117	C8H7N	000529-19-1	91
4		Benzyl nitrile	117	C8H7N	000140-29-4	91
5		Benzene, 1-isocyano-4-methyl-	117	C8H7N	007175-47-5	90



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ClientSampleId :
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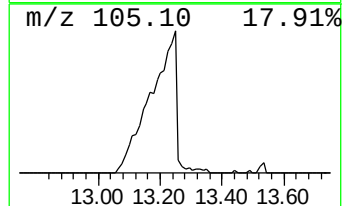
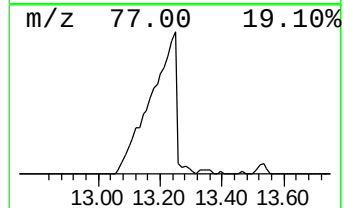
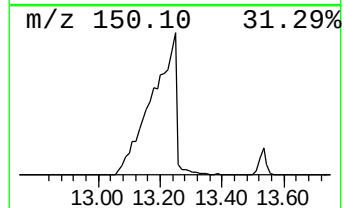
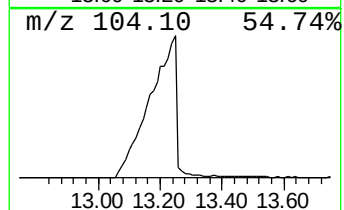
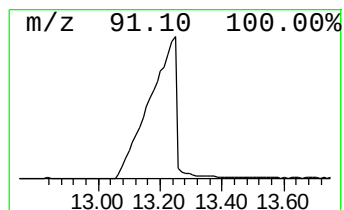
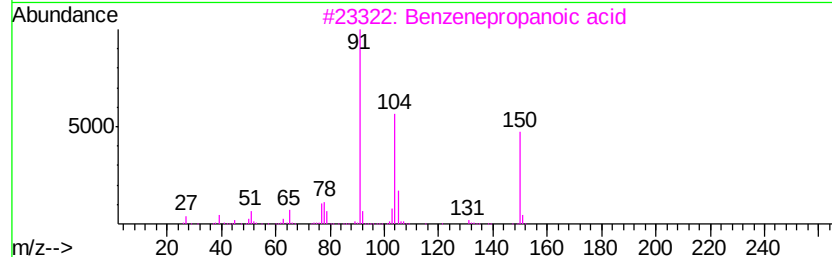
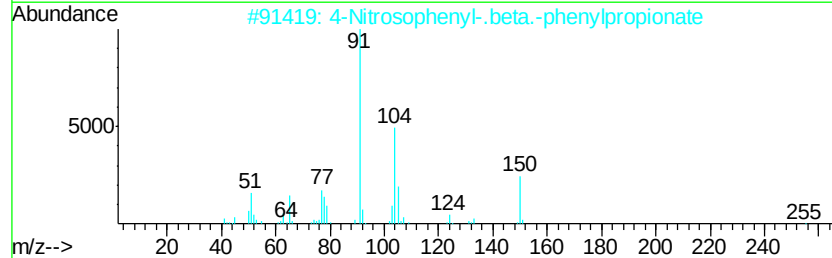
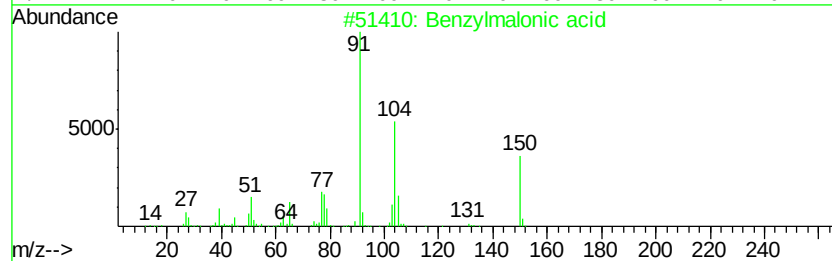
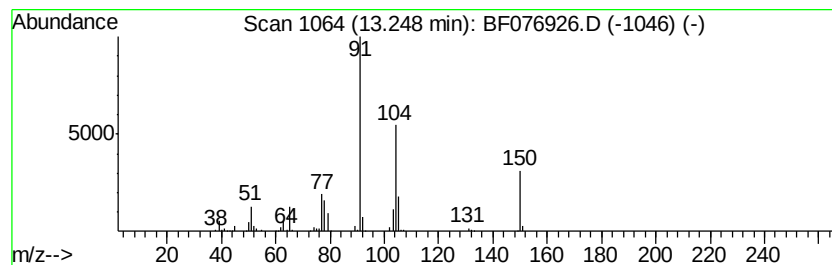
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 Benzylmalonic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.25	113.96 ng	1988030	Acenaphthene-d10	15.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzylmalonic acid	194	C10H10O4	000616-75-1	91
2		4-Nitrosophenyl-.beta.-phenylpro...	255	C15H13NO3	1000129-40-0	90
3		Benzenepropanoic acid	150	C9H10O2	000501-52-0	87
4		Acetic acid, trifluoro-, 2-pheny...	218	C10H9F3O2	055419-66-4	59
5		Formic acid, 2-phenylethyl ester	150	C9H10O2	000104-62-1	53



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011915\
Data File : BF076926.D
Acq On : 19 Jan 2015 13:04
Operator : IZ / TP
Sample : G1101-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

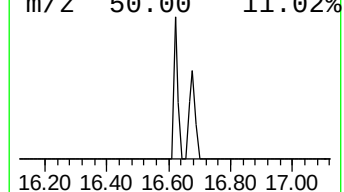
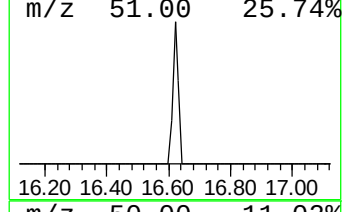
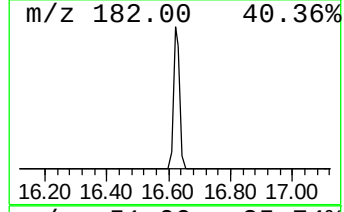
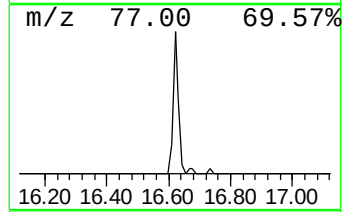
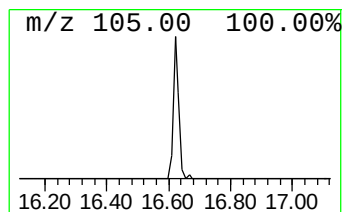
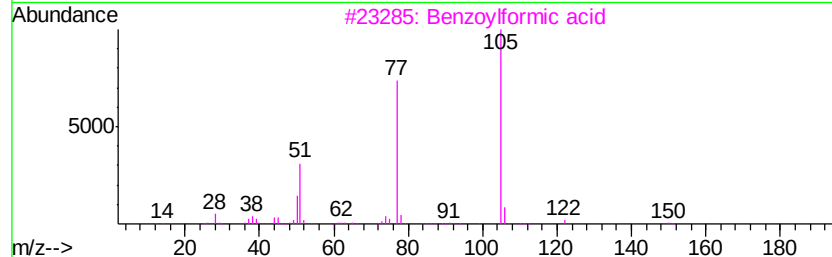
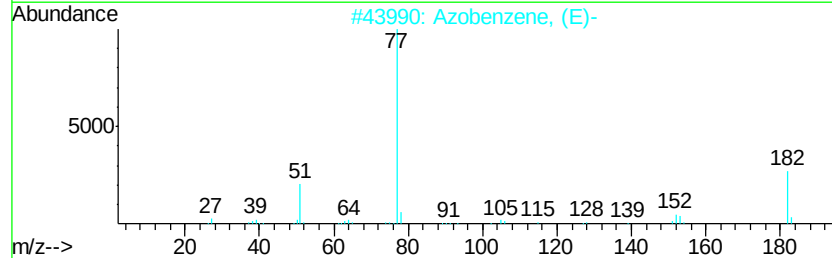
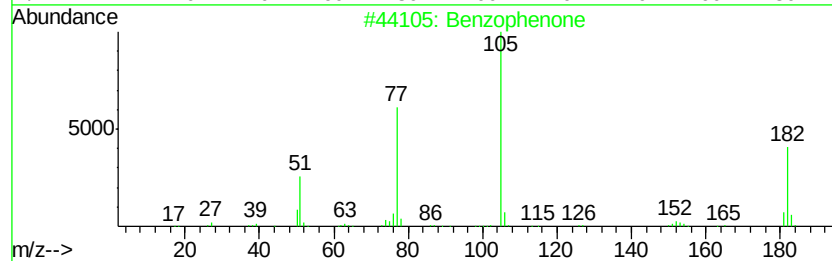
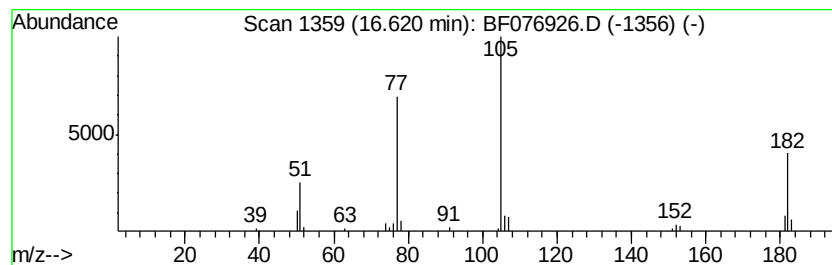
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 Benzophenone Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD		R.T.	
16.62	3.42 ng	58209	Phenanthrene-d10		17.77	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzophenone	182	C13H10O	000119-61-9	94
2		Azobenzene, (E)-	182	C12H10N2	017082-12-1	59
3		Benzoylformic acid	150	C8H6O3	000611-73-4	43
4		1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	43
5		1,2,4-Triazine-3,5(2H,4H)-dione, ...	249	C10H7N3O3S	024168-34-1	43



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011915\
Data File : BF076926.D
Acq On : 19 Jan 2015 13:04
Operator : IZ / TP
Sample : G1101-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PO-002

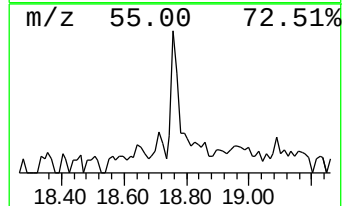
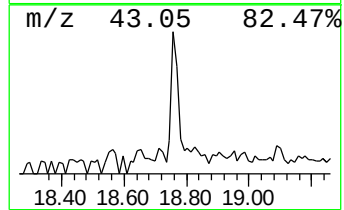
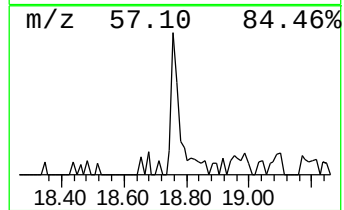
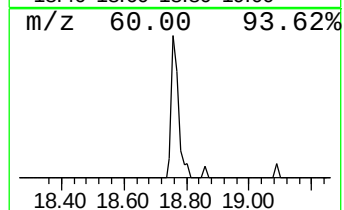
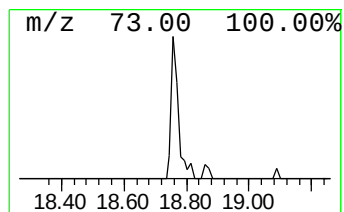
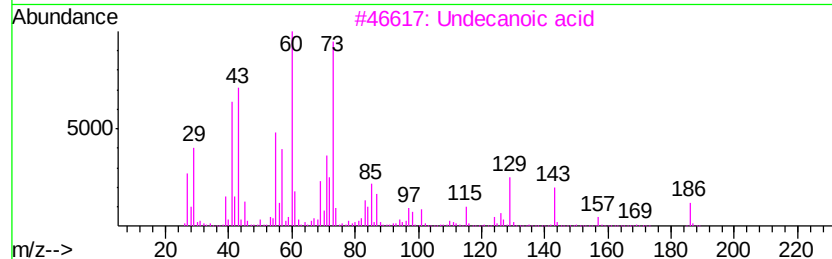
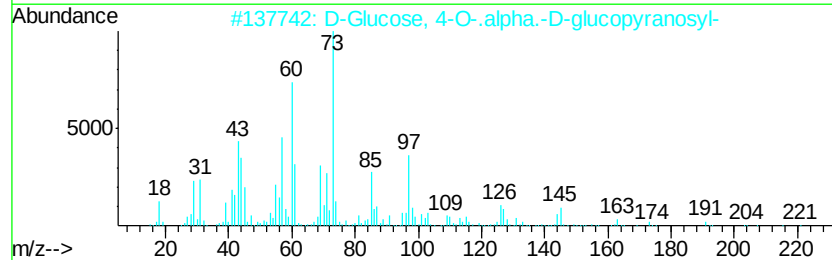
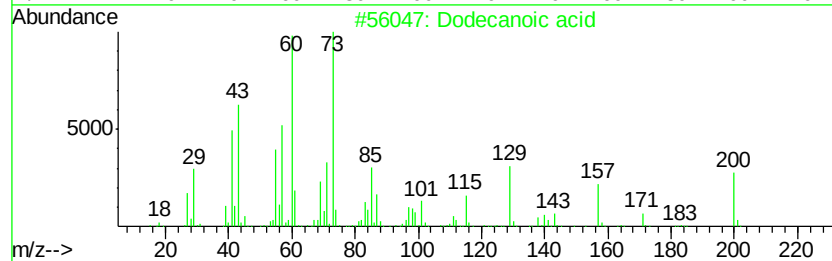
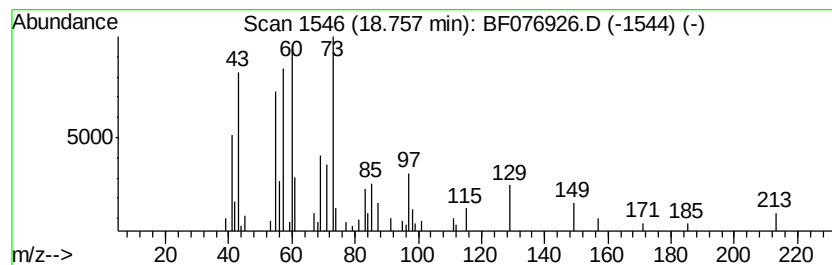
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 Dodecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.76	4.14 ng	70394	Phenanthrene-d10	17.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecanoic acid	200	C12H24O2	000143-07-7	59
2		D-Glucose, 4-O-.alpha.-D-glucopy...	342	C12H22O11	000069-79-4	53
3		Undecanoic acid	186	C11H22O2	000112-37-8	53
4		n-Decanoic acid	172	C10H20O2	000334-48-5	47
5		n-Capric acid isopropyl ester	214	C13H26O2	002311-59-3	47



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011915\
Data File : BF076926.D
Acq On : 19 Jan 2015 13:04
Operator : IZ / TP
Sample : G1101-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PO-002

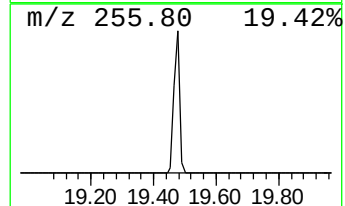
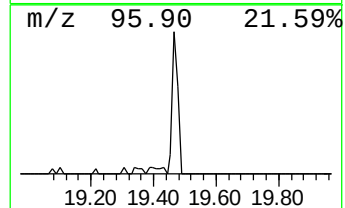
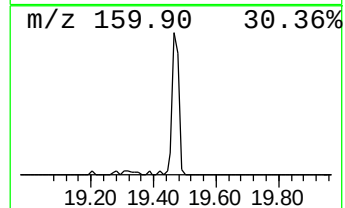
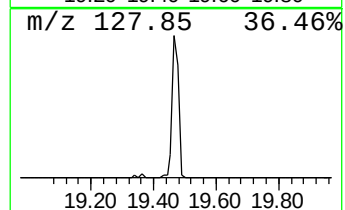
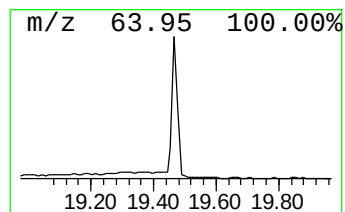
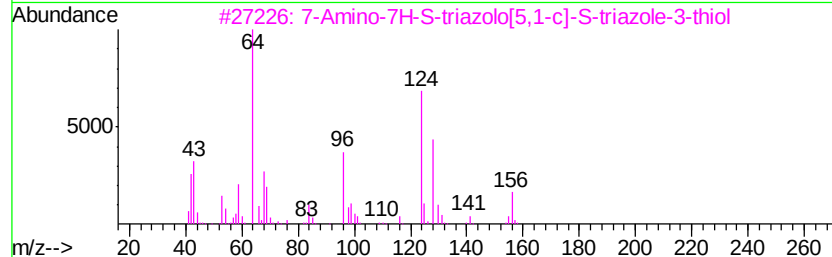
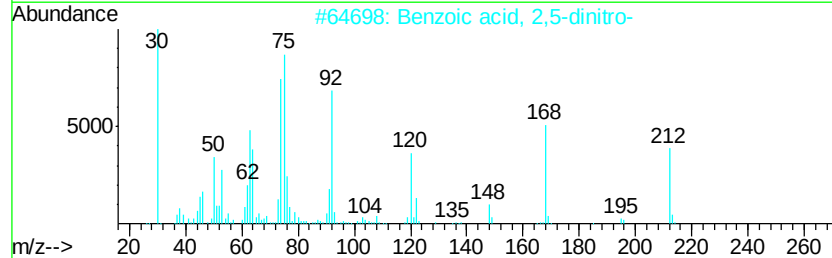
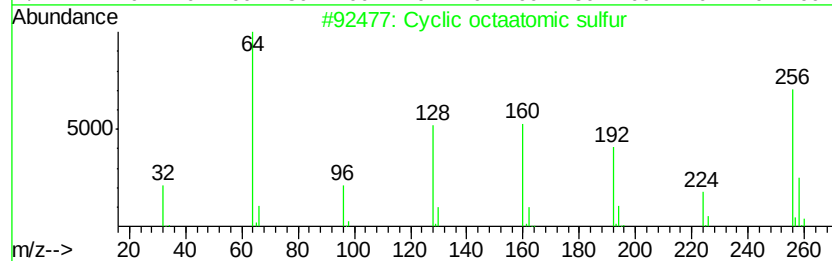
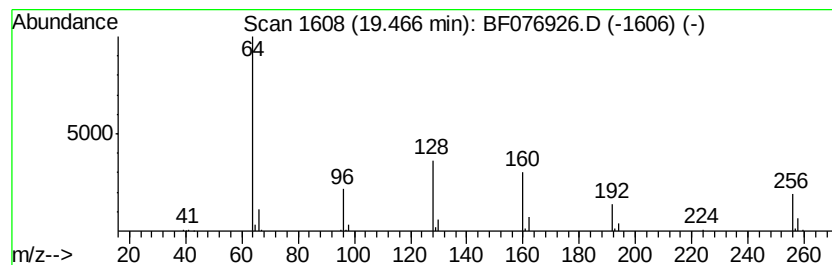
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 Cyclic octaatomic sulfur Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.47	10.01 ng	170159	Phenanthrene-d10	17.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclic octaatomic sulfur	256	S8	010544-50-0	94
2		Benzoic acid, 2,5-dinitro-	212	C7H4N2O6	000610-28-6	53
3		7-Amino-7H-S-triazolo[5,1-c]-S-t...	156	C3H4N6S	013728-28-4	9
4		1,2,5,6-Tetrathiocane	184	C4H8S4	001940-01-8	9
5		Acetonitrile, 2-(5-chloro-3-oxo-...	248	C8H9ClN2OS2	1000269-94-4	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011915\
Data File : BF076926.D
Acq On : 19 Jan 2015 13:04
Operator : IZ / TP
Sample : G1101-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.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
Oxirane, [(1-meth...	4.10	3.4	ng	34418	1	7.98	202116	20.0
Pentanoic acid	5.60	4.6	ng	46850	1	7.98	202116	20.0
unknown7.46	7.46	37.5	ng	378654	1	7.98	202116	20.0
Benzeneacetic acid	11.98	70.0	ng	1013460	2	10.88	289544	20.0
Indole	12.52	21.6	ng	312474	2	10.88	289544	20.0
Benzylmalonic acid	13.25	114.0	ng	1988030	3	15.01	348912	20.0
Benzophenone	16.62	3.4	ng	58209	4	17.77	340111	20.0
Dodecanoic acid	18.76	4.1	ng	70394	4	17.77	340111	20.0
Cyclic octaatomic...	19.47	10.0	ng	170159	4	17.77	340111	20.0