

Data Path : Z:\HPCHEM1\BNA F\DATA\BF030917\
 Data File : BF093509.D
 Acq On : 10 Mar 2017 7:43
 Operator : SJ/MA
 Sample : I2132-01
 Misc :
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 W-21

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-BF030717.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	4.904	262	264	277	rBV	54665	142323	8.86%	0.830%
2	5.361	302	304	321	rBV	227758	461751	28.76%	2.692%
3	6.424	396	397	404	rBV3	179609	333504	20.77%	1.945%
4	6.527	404	406	417	rVB	797667	929710	57.91%	5.421%
5	6.676	417	419	423	rVB	13010	19154	1.19%	0.112%
6	6.744	423	425	428	rBV	955373	1113865	69.38%	6.495%
7	6.904	437	439	447	rBV	807100	795673	49.56%	4.639%
8	7.327	474	476	484	rBV	541704	668627	41.65%	3.899%
9	7.590	497	499	506	rVB	50069	65665	4.09%	0.383%
10	7.899	524	526	528	rBV	38401	29959	1.87%	0.175%
11	8.036	536	538	541	rBV	1737517	1527874	95.16%	8.908%
12	8.985	619	621	624	rBV2	18824	22810	1.42%	0.133%
13	9.042	624	626	630	rBV	1161713	1294580	80.63%	7.548%
14	9.110	630	632	634	rVB	1355826	1204254	75.01%	7.022%
15	9.510	665	667	670	rVB	76481	64267	4.00%	0.375%
16	9.785	689	691	693	rBV	1881592	1605506	100.00%	9.361%
17	10.013	709	711	717	rBV3	29662	56950	3.55%	0.332%
18	10.310	735	737	738	rBV	42880	47919	2.98%	0.279%
19	10.573	758	760	768	rVB2	500074	615372	38.33%	3.588%
20	10.710	768	772	774	rVB2	38485	58006	3.61%	0.338%
21	10.756	774	776	777	rBV	144512	130252	8.11%	0.759%
22	10.790	777	779	781	rVV2	142941	211604	13.18%	1.234%
23	10.825	781	782	785	rVV2	145704	187293	11.67%	1.092%
24	10.905	785	789	790	rVV2	49744	112623	7.01%	0.657%
25	10.939	790	792	793	rVV	97193	136274	8.49%	0.795%
26	10.973	793	795	797	rVV	164551	184166	11.47%	1.074%
27	11.008	797	798	801	rVB	53052	70718	4.40%	0.412%
28	11.133	807	809	810	rBV	21117	22004	1.37%	0.128%
29	11.156	810	811	814	rVB2	15247	24066	1.50%	0.140%
30	11.271	819	821	823	rBV	1635303	1462320	91.08%	8.526%
31	11.476	838	839	843	rBV4	8945	18940	1.18%	0.110%
32	11.556	843	846	849	rVB	23790	28056	1.75%	0.164%
33	12.539	929	932	934	rBV	112726	118988	7.41%	0.694%
34	12.608	937	938	949	rVV	199449	336060	20.93%	1.959%

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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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35	12.848	957	959	962	rBV	796324	707567	44.07%	4.126%
36	13.408	1007	1008	1010	rVB	21118	22428	1.40%	0.131%
37	13.911	1050	1052	1056	rBV	1015741	997062	62.10%	5.813%
38	14.185	1073	1076	1079	rBV5	6261	21793	1.36%	0.127%
39	14.962	1142	1144	1148	rBV4	16470	26907	1.68%	0.157%
40	15.317	1172	1175	1181	rBV	769963	1032637	64.32%	6.021%
41	15.579	1193	1198	1205	rVV5	25544	117002	7.29%	0.682%
42	15.694	1206	1208	1210	rVB2	22098	28672	1.79%	0.167%
43	16.140	1245	1247	1254	rVB2	21775	45903	2.86%	0.268%
44	16.665	1290	1293	1297	rBV6	16118	49733	3.10%	0.290%

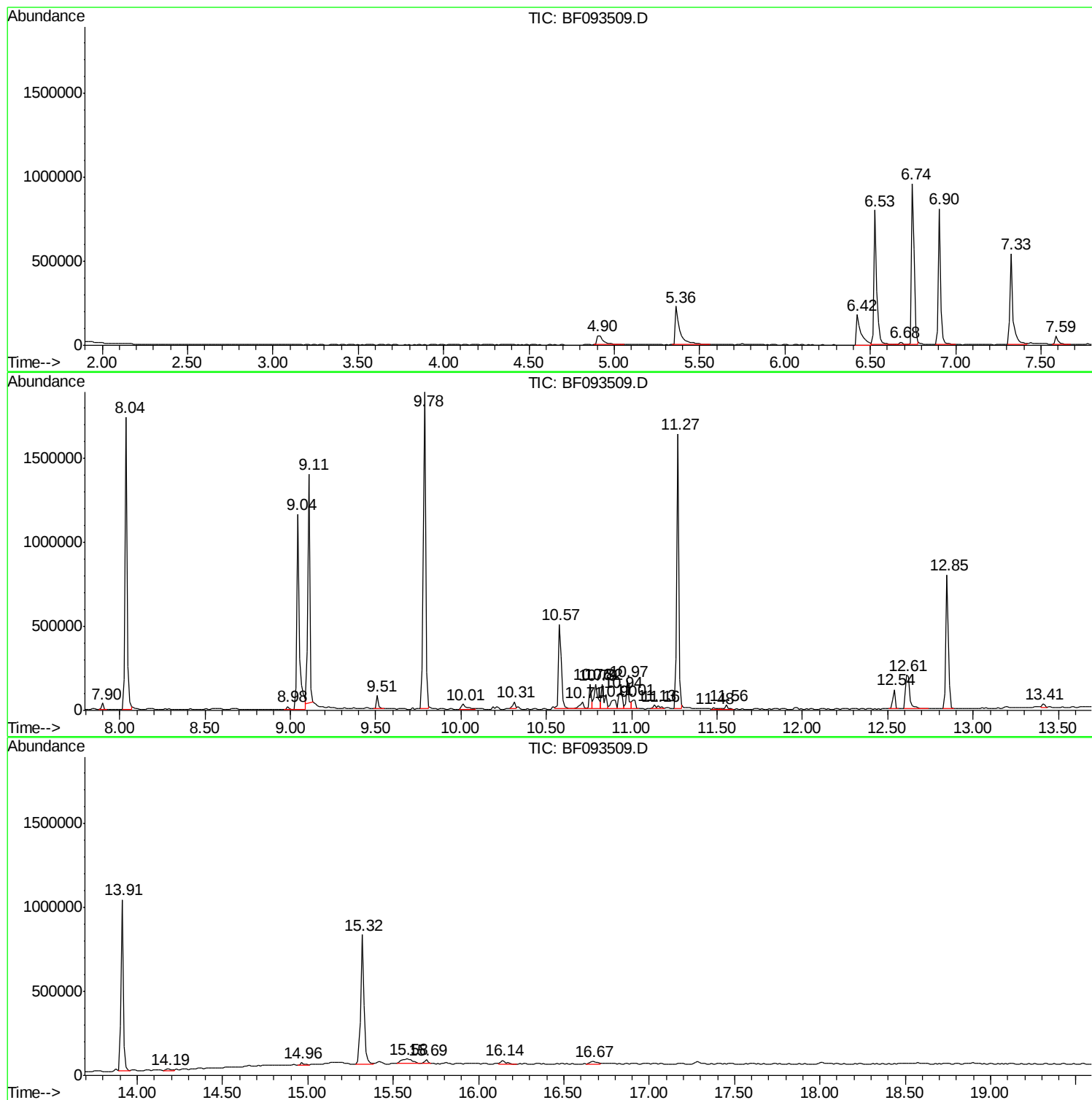
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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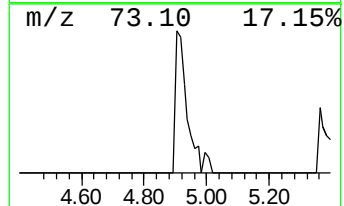
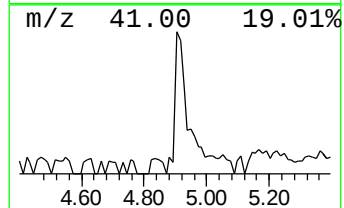
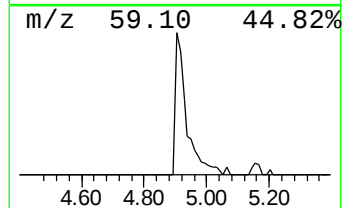
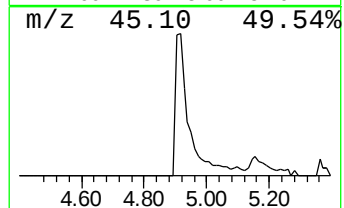
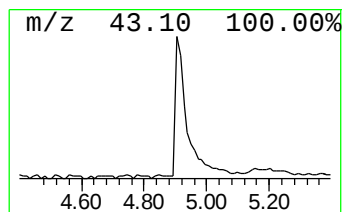
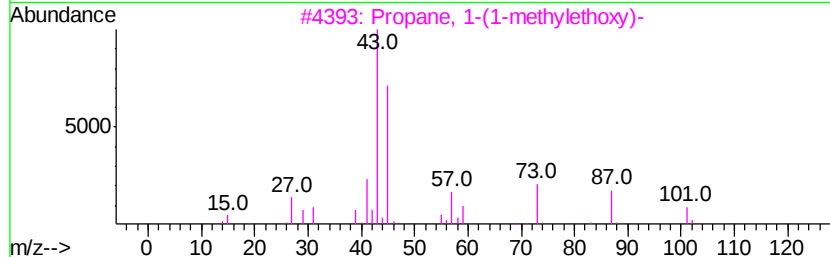
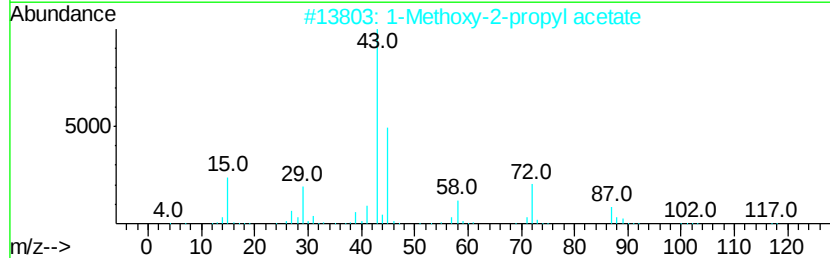
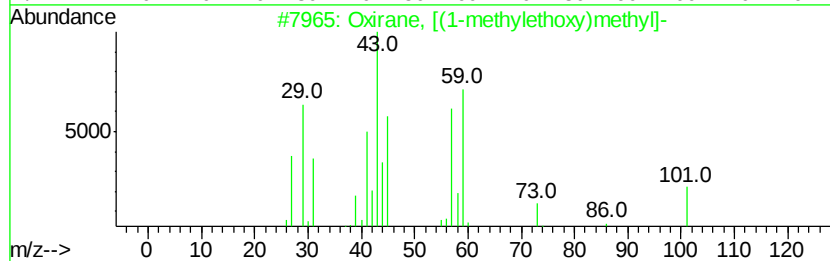
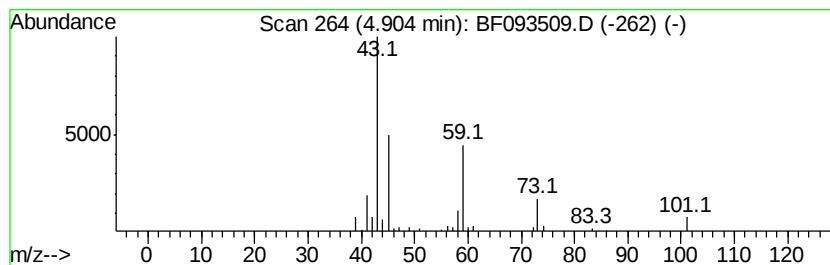
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown4.90 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	2.56 ng	142323	1,4-Dichlorobenzene-d4	6.74

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxirane, [(1-methylethoxy)methyl]-	116	C6H12O2	004016-14-2	39
2			1-Methoxy-2-propyl acetate	132	C6H12O3	000108-65-6	32
3			Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	28
4			Oxirane, 2,3-dimethyl-	72	C4H8O	003266-23-7	25
5			2-Ethoxyethyl acetate	132	C6H12O3	000111-15-9	25



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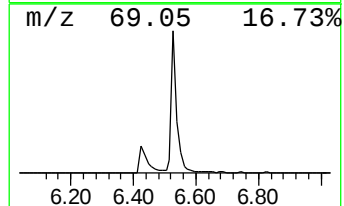
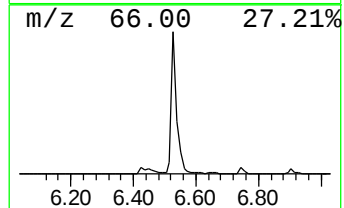
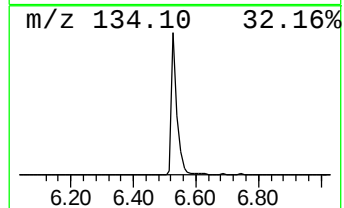
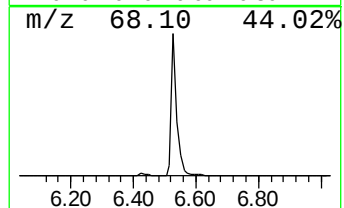
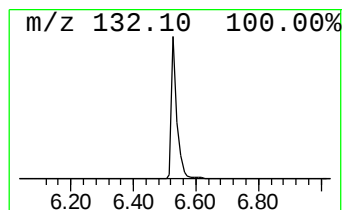
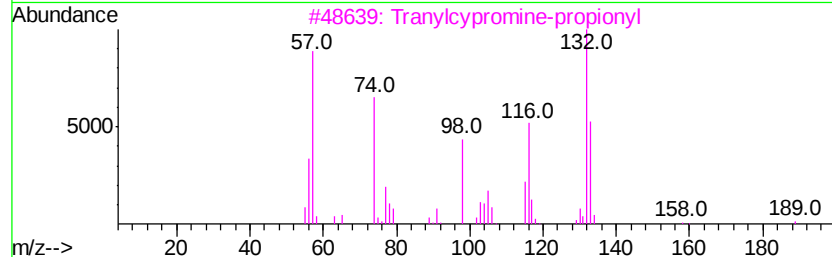
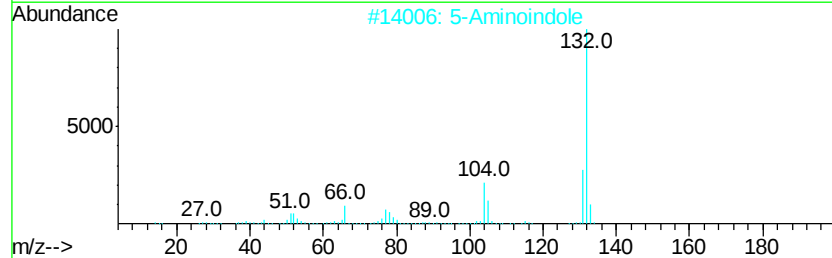
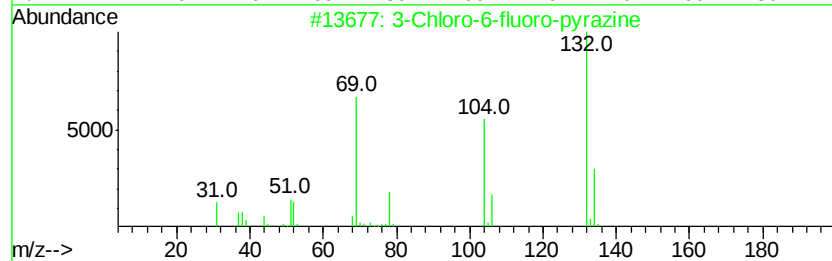
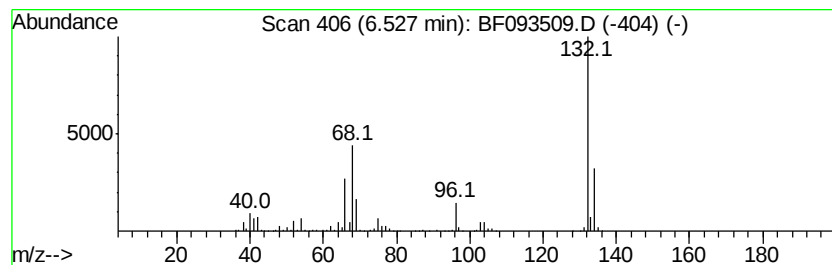
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Peak Number 2 unknown6.53 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.53	16.69 ng	929710	1,4-Dichlorobenzene-d4	6.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27	
2	5-Aminoindole	132	C8H8N2	005192-03-0	12	
3	Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10	
4	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9	
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9	



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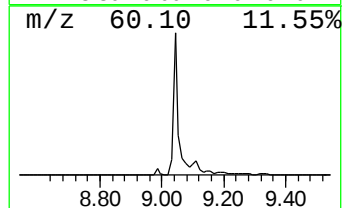
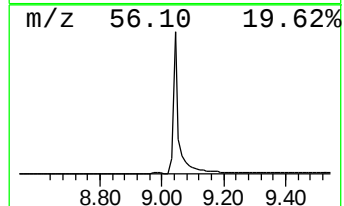
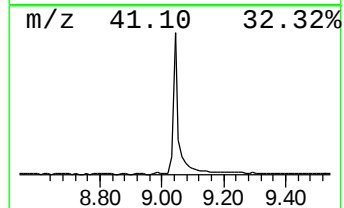
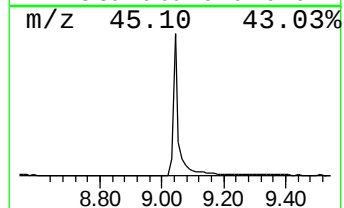
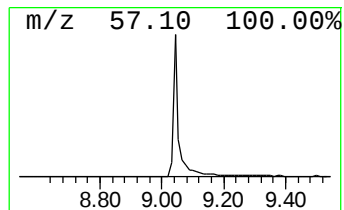
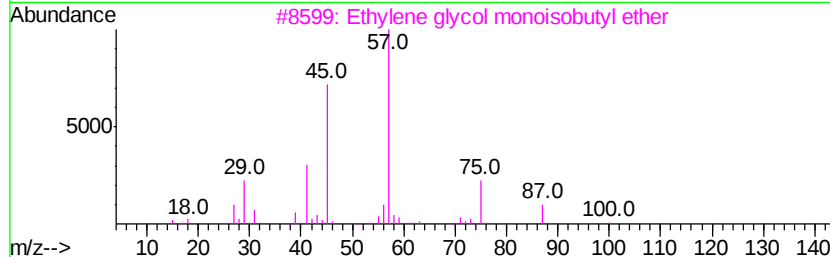
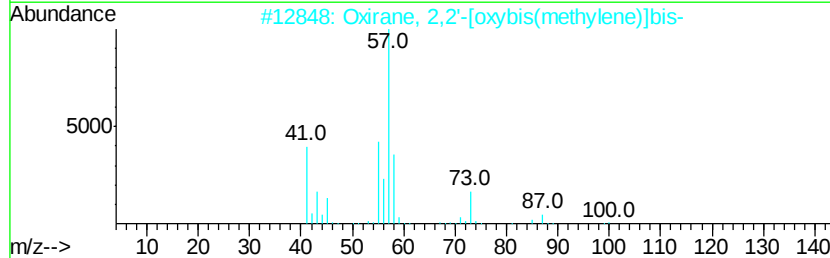
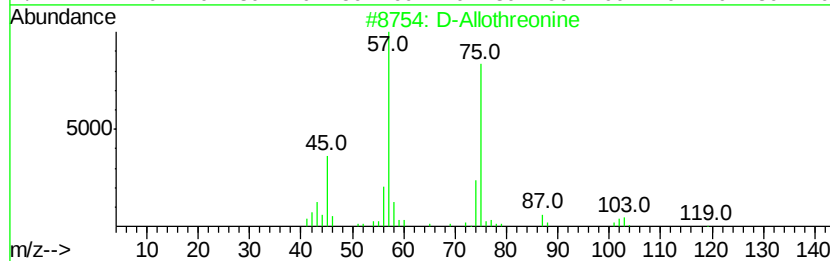
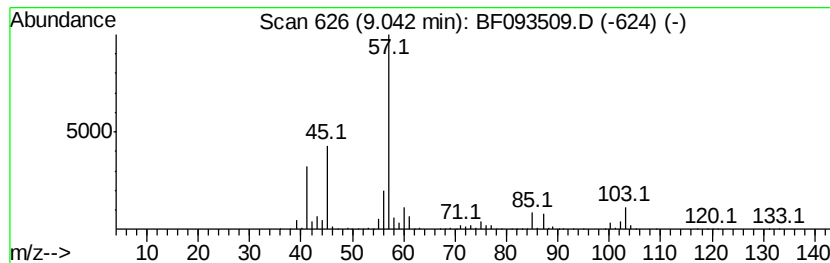
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown9.04 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.04	16.13 ng	1294580	Acenaphthene-d10	9.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	D-Allothreonine	119	C4H9NO3	024830-94-2	39
2		Oxirane, 2,2'-[oxybis(methylene)]...	130	C6H10O3	002238-07-5	38
3		Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	37
4		Carbonic acid, bis(1-methylpropyl)...	174	C9H18O3	000623-63-2	37
5		Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	37



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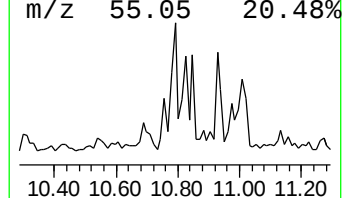
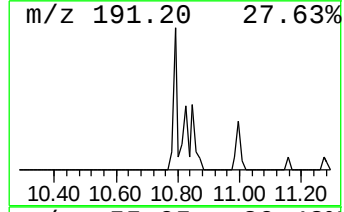
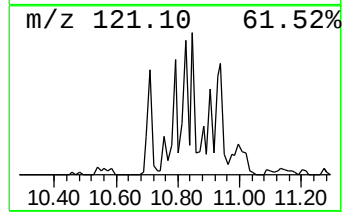
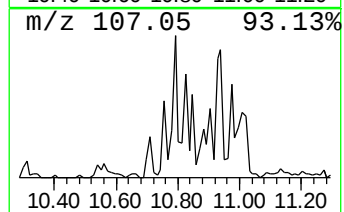
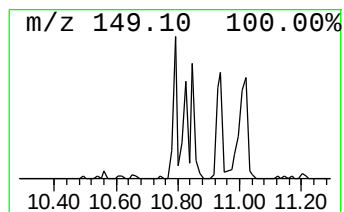
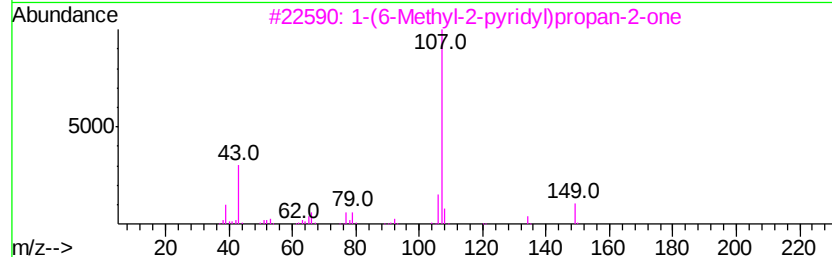
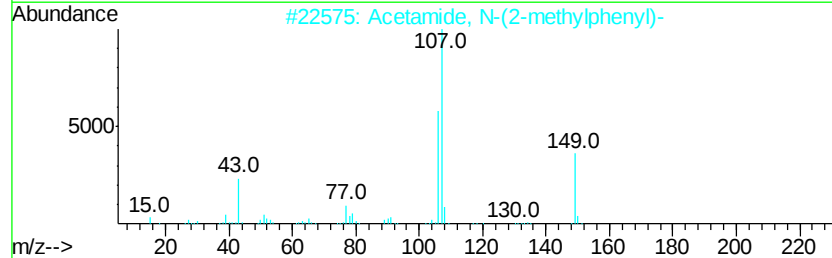
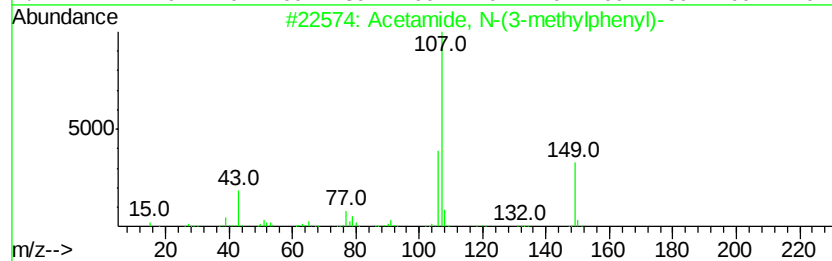
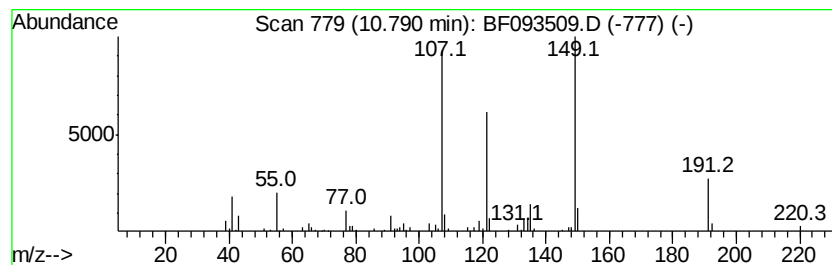
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Acetamide, N-(3-methylphenyl)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.79	2.89 ng	211604	Phenanthrene-d10	11.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Acetamide, N-(3-methylphenyl)-	149	C9H11NO	000537-92-8	64
2		Acetamide, N-(2-methylphenyl)-	149	C9H11NO	000120-66-1	59
3		1-(6-Methyl-2-pyridyl)propan-2-one	149	C9H11NO	065702-08-1	59
4		Pyridine-3-carbonitrile, 1,2-dih...	191	C9H9N3O2	220098-92-0	43
5		Butanamide, N-(2-methylphenyl)-3...	191	C11H13NO2	000093-68-5	43



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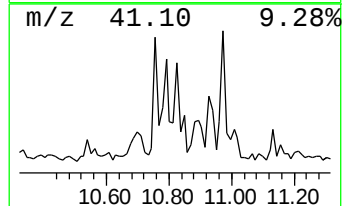
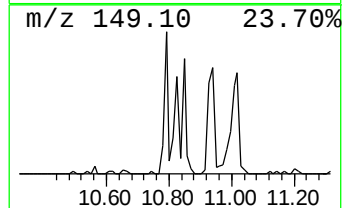
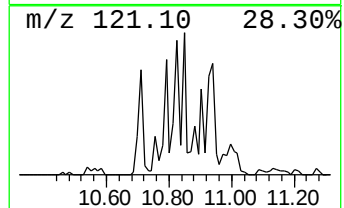
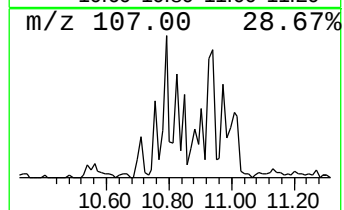
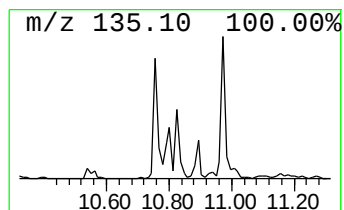
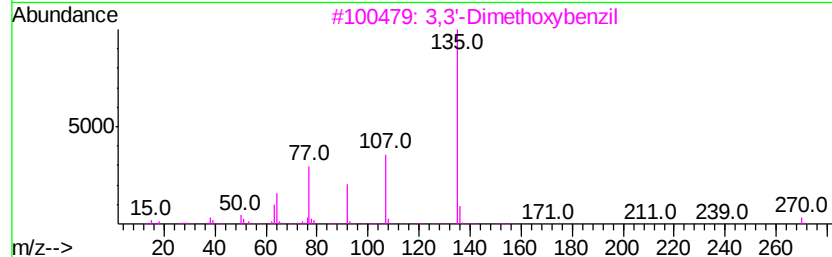
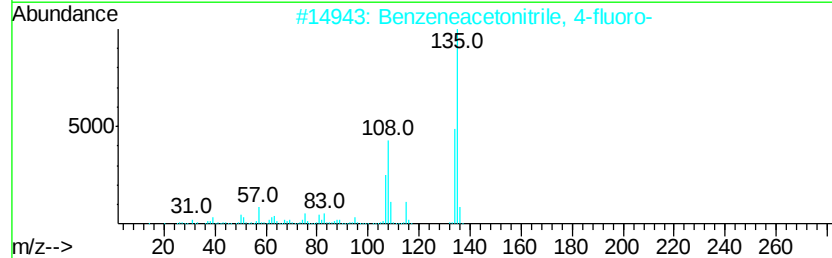
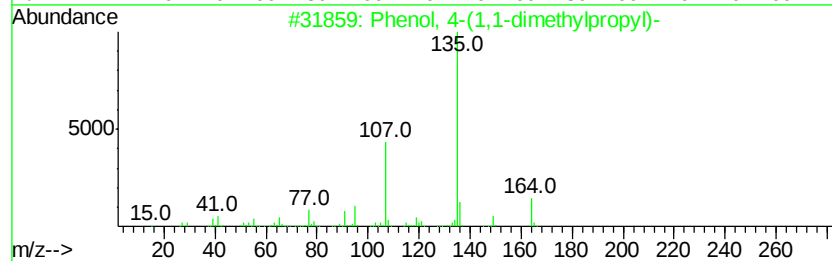
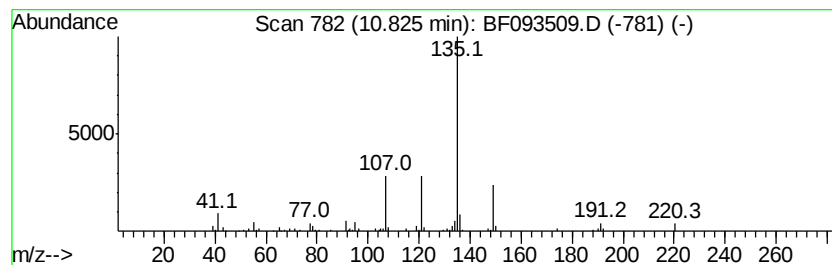
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Phenol, 4-(1,1-dimethylprop... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.82	2.56 ng	187293	Phenanthrene-d10	11.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	59
2	Benzeneacetonitrile, 4-fluoro-	135	C8H6FN	000459-22-3	53
3	3,3'-Dimethoxybenzil	270	C16H14O4	040101-17-5	53
4	Pentanoic acid, 5-hydroxy-, p-t-...	250	C15H22O3	166273-37-6	50
5	1-Adamantanecarboxylic acid chloride	198	C11H15ClO	002094-72-6	47



Data Path : Z:\HPCHEM1\BNA F\DATA\BF030917\
Data File : BF093509.D
Acq On : 10 Mar 2017 7:43
Operator : SJ/MA
Sample : I2132-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
W-21

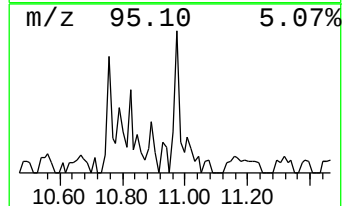
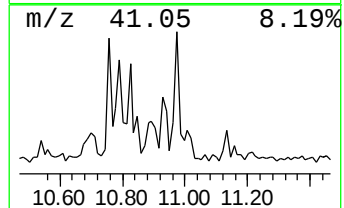
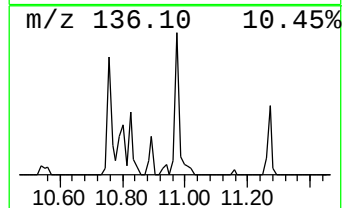
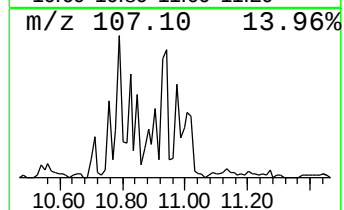
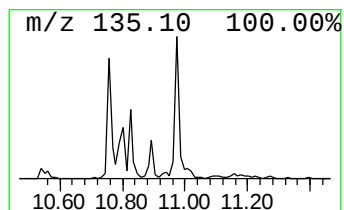
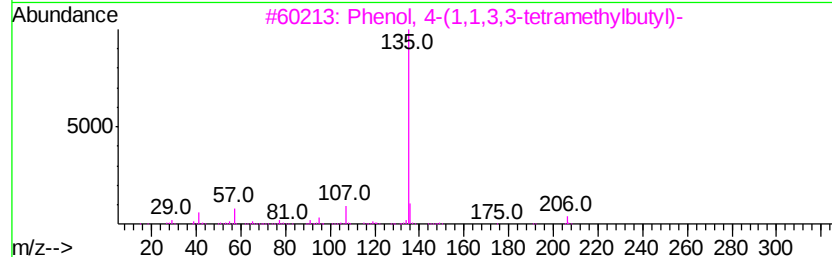
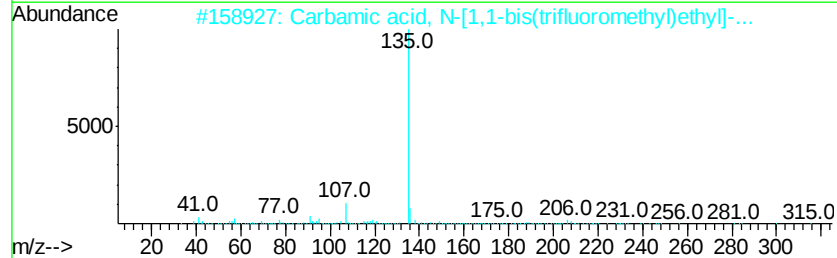
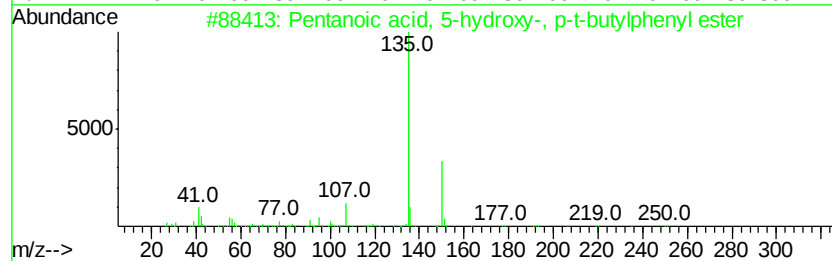
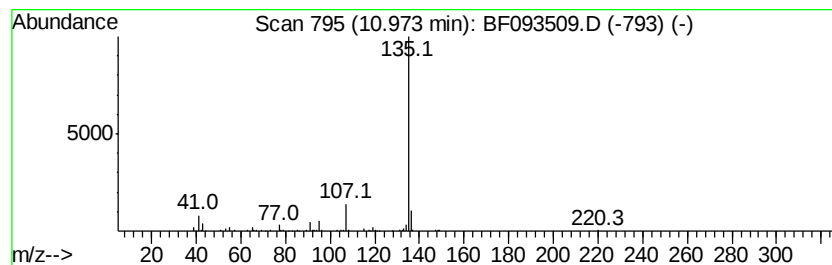
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Pentanoic acid, 5-hydroxy-,... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.97	2.52 ng	184166	Phenanthrene-d10	11.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentanoic acid, 5-hydroxy-, p-t-...	250	C15H22O3	166273-37-6	78
2		Carbamic acid, N-[1,1-bis(triflu...	413	C19H25F6N02	296242-69-8	78
3		Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	78
4		o-Methoxybenzoic acid, 2-chlorop...	262	C14H11ClO3	085965-92-0	59
5		((1,2-Diethylethylene)bis(p-phen...	354	C22H26O4	004547-76-6	56



Data Path : Z:\HPCHEM1\BNA F\DATA\BF030917\
Data File : BF093509.D
Acq On : 10 Mar 2017 7:43
Operator : SJ/MA
Sample : I2132-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
W-21

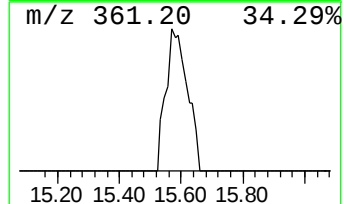
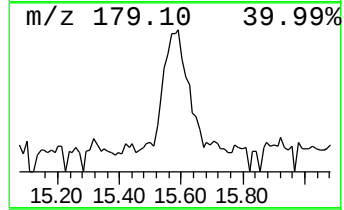
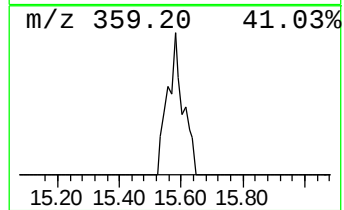
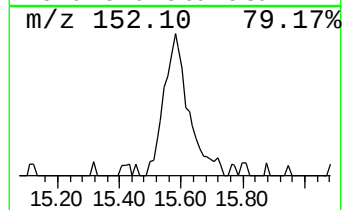
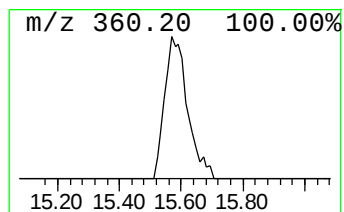
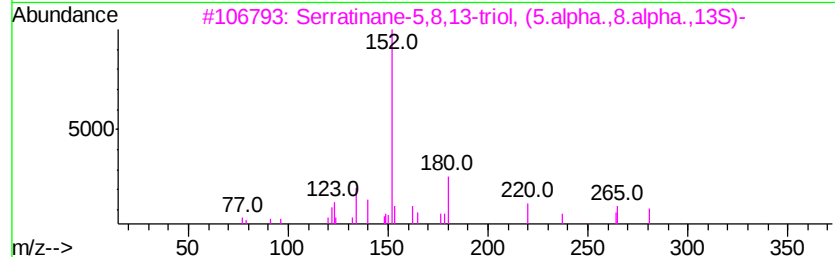
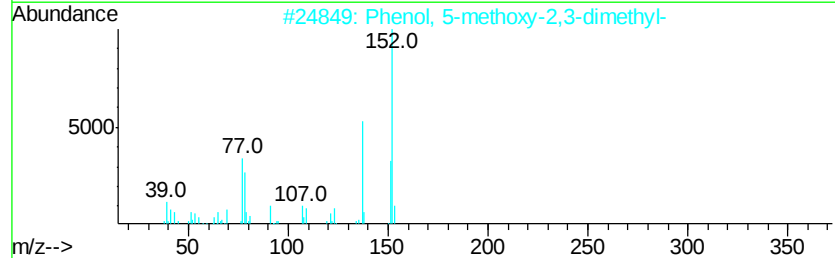
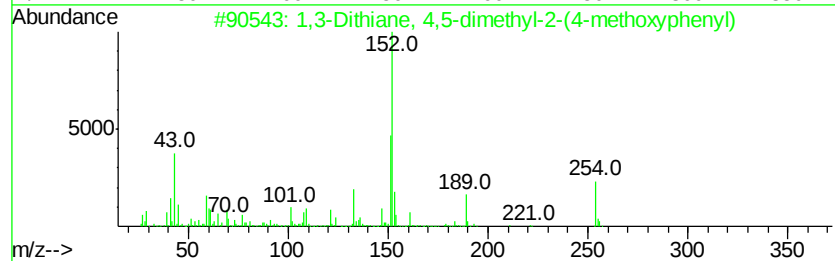
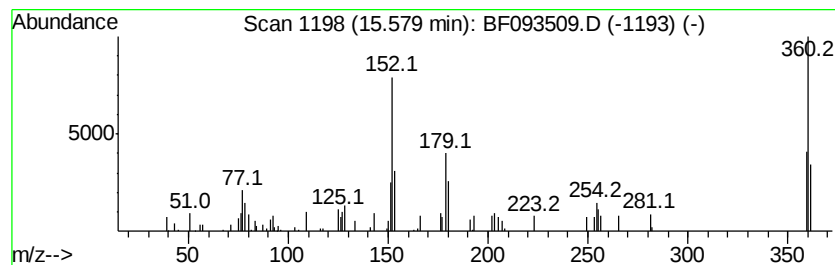
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown15.58 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.58	2.27 ng	117002	Perylene-d12	15.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Dithiane, 4,5-dimethyl-2-(4-...	254	C13H18OS2	1000197-88-6	22
2		Phenol, 5-methoxy-2,3-dimethyl-	152	C9H12O2	034883-01-7	18
3		Serratinane-5,8,13-triol, (5.alpha...	281	C16H27NO3	005532-22-9	14
4		2,4-Dinitro-11-phenyl-5H-dibenzo...	360	C19H12N4O4	071354-26-2	10
5		Acenaphthylene	152	C12H8	000208-96-8	9



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Sample : I2132-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
W-21

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.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
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unknown6.53	6.53	16.7	ng	929710	1	6.74	1113870	20.0
unknown9.04	9.04	16.1	ng	1294580	3	9.78	1605510	20.0
Acetamide, N-(3-m...	10.79	2.9	ng	211604	4	11.27	1462320	20.0
Phenol, 4-(1,1-di...	10.82	2.6	ng	187293	4	11.27	1462320	20.0
Pentanoic acid, 5...	10.97	2.5	ng	184166	4	11.27	1462320	20.0
unknown15.58	15.58	2.3	ng	117002	6	15.32	1032640	20.0