

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101317\
 Data File : BF099461.D
 Acq On : 14 Oct 2017 1:21
 Operator : SJ/JU
 Sample : I5819-12
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 3915-PA4

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-BF092317.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	2.134	4	8	28	rVB	196884	343816	12.98%	1.960%
2	5.081	505	509	520	rBV	129127	167856	6.34%	0.957%
3	5.481	573	577	586	rBV	1368303	1279630	48.31%	7.295%
4	6.487	745	748	760	rBV	836861	742768	28.04%	4.234%
5	6.628	768	772	775	rBV	2462587	2153221	81.29%	12.274%
6	6.851	807	810	816	rBV	646343	536236	20.24%	3.057%
7	7.010	833	837	840	rBV	2425264	2125230	80.23%	12.115%
8	7.422	902	907	910	rBV	1708105	1594064	60.18%	9.087%
9	8.134	1025	1028	1034	rBV	809708	651909	24.61%	3.716%
10	8.416	1073	1076	1083	rBV	205867	184642	6.97%	1.053%
11	9.210	1206	1211	1214	rBV	3047286	2648826	100.00%	15.100%
12	9.886	1323	1326	1333	rVB	641761	602539	22.75%	3.435%
13	10.680	1457	1461	1470	rBV	1240082	1125923	42.51%	6.418%
14	10.798	1478	1481	1489	rVB	49067	56101	2.12%	0.320%
15	11.374	1576	1579	1583	rBV	522196	475911	17.97%	2.713%
16	12.116	1701	1705	1714	rBV	60717	100809	3.81%	0.575%
17	12.963	1844	1849	1852	rBV	1946889	1762066	66.52%	10.045%
18	14.021	2026	2029	2033	rBV	515804	447407	16.89%	2.550%
19	15.498	2276	2280	2290	rVB	405679	543323	20.51%	3.097%

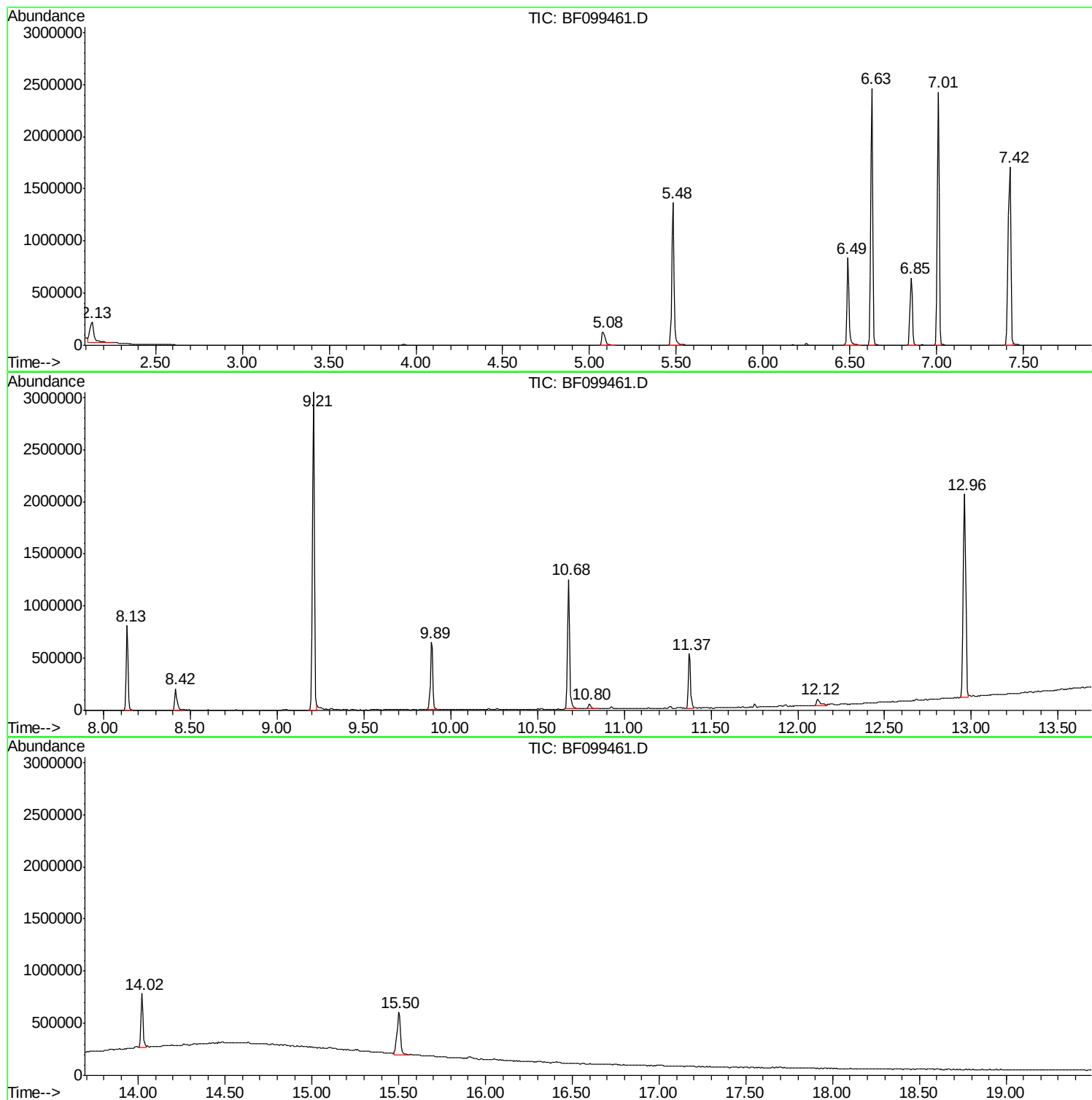
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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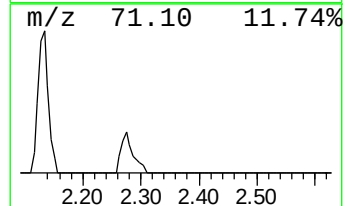
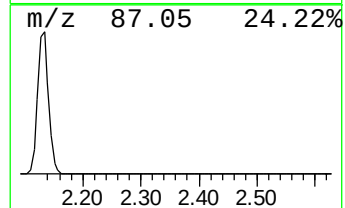
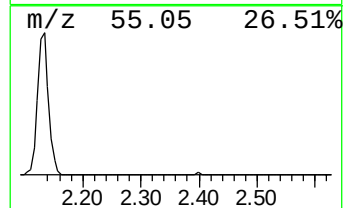
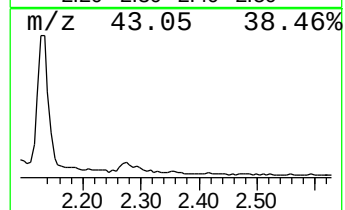
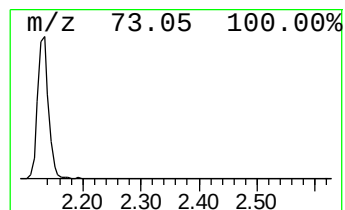
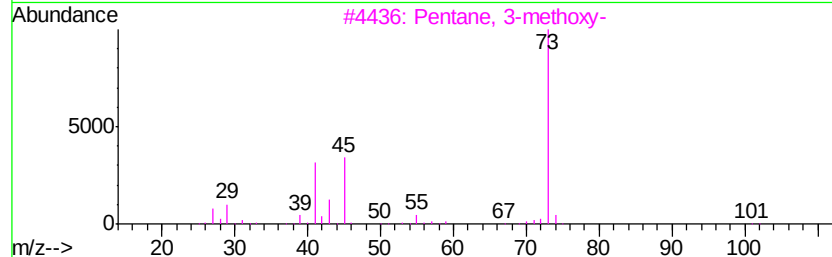
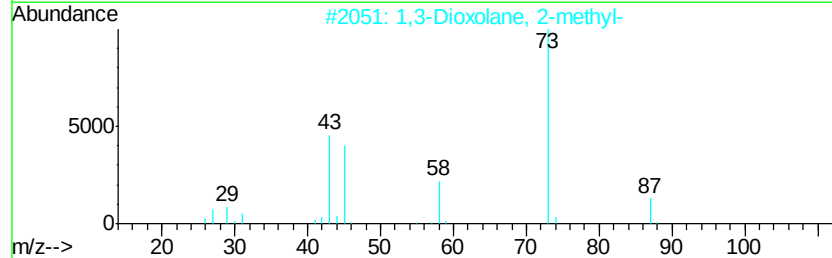
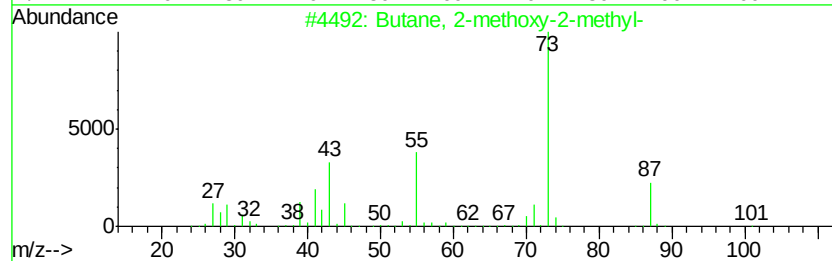
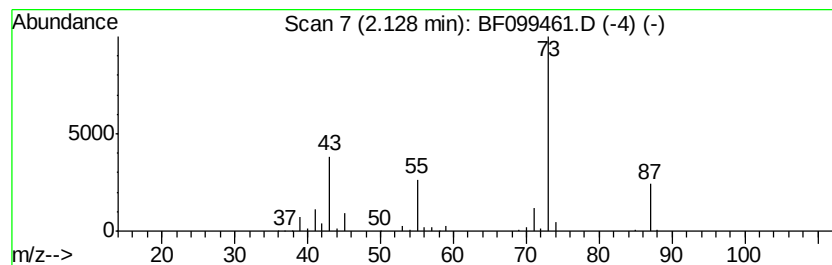
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.13	12.82 ng	343816	1,4-Dichlorobenzene-d4	6.85

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	64
2			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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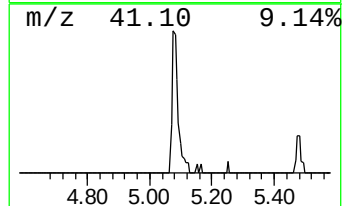
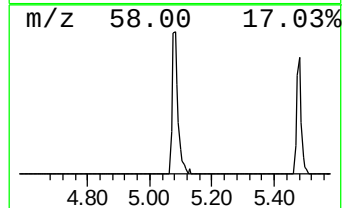
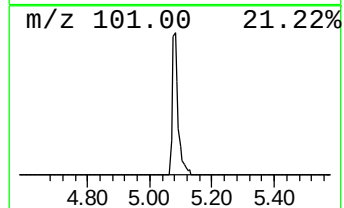
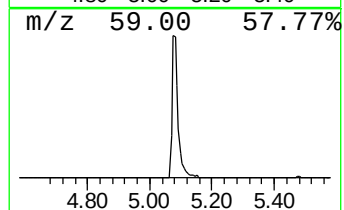
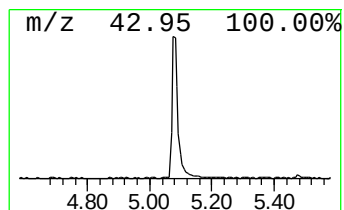
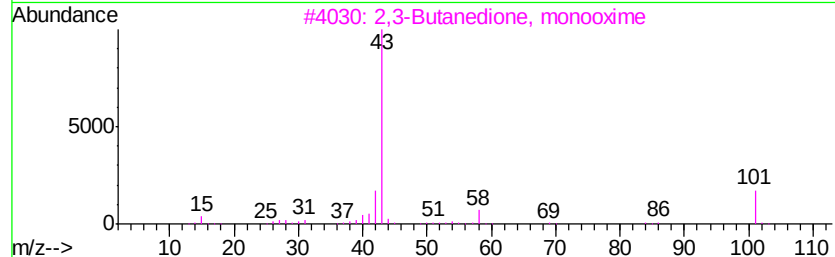
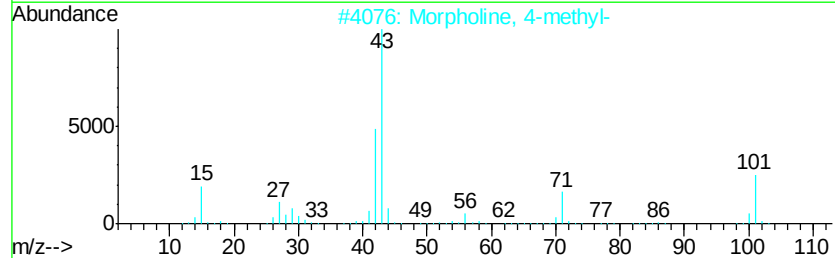
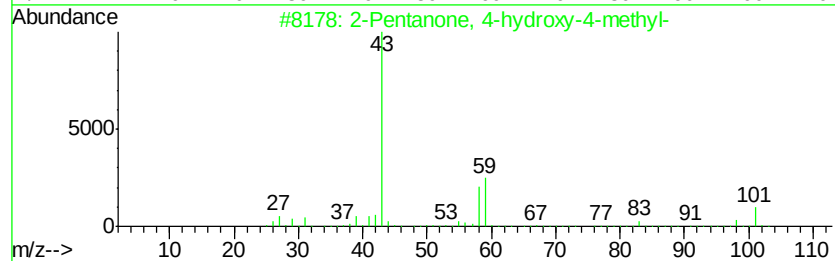
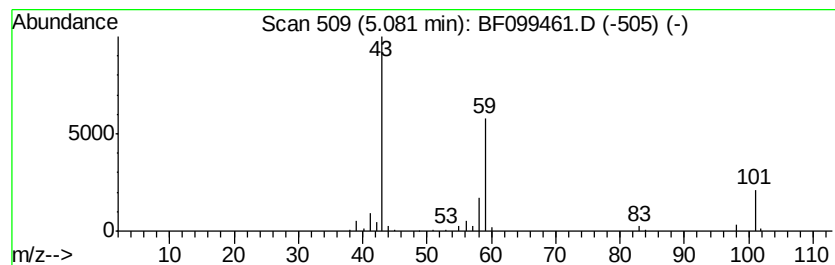
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.08	6.26 ng	167856	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9
5		Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	9



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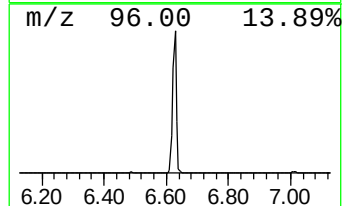
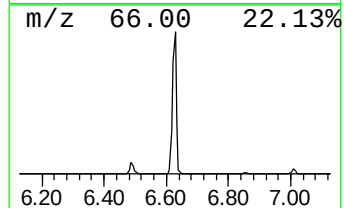
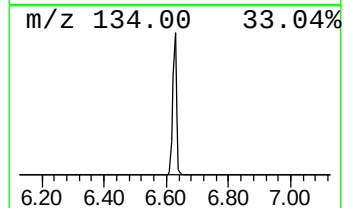
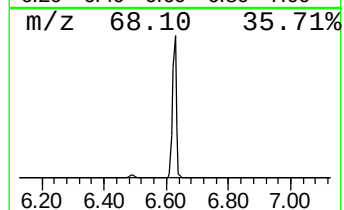
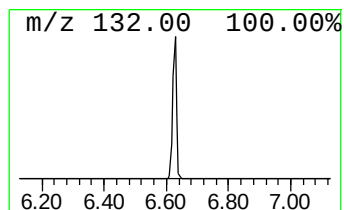
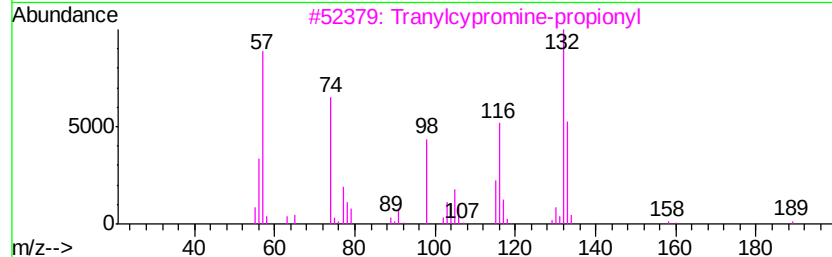
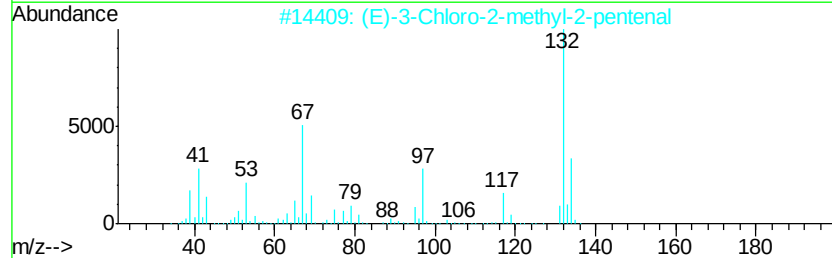
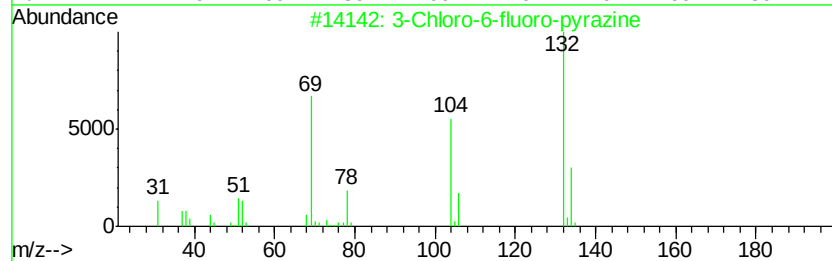
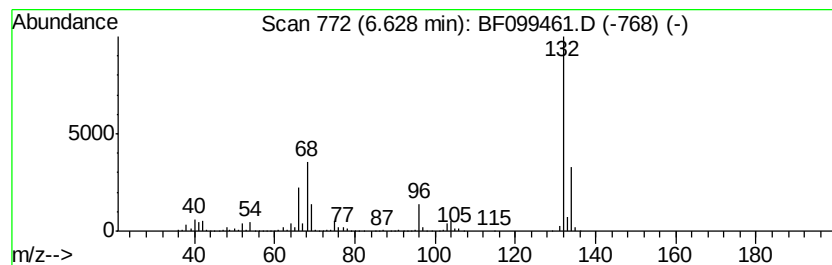
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Peak Number 3 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	80.31 ng	2153220	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		Xenon	132	Xe	007440-63-3	9



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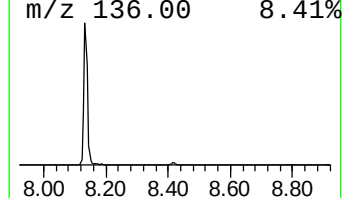
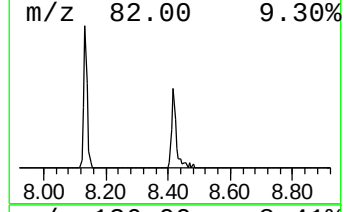
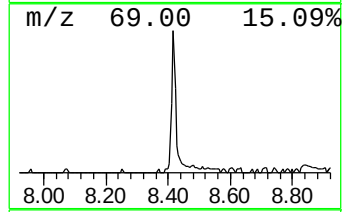
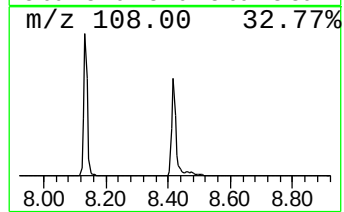
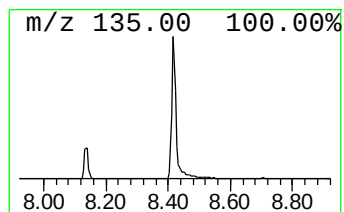
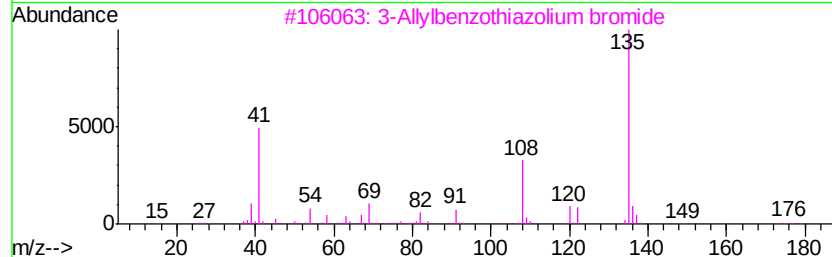
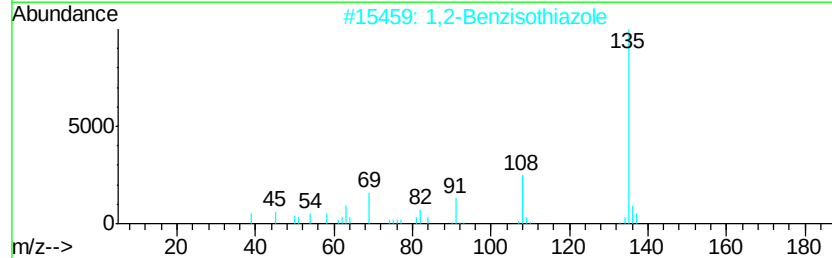
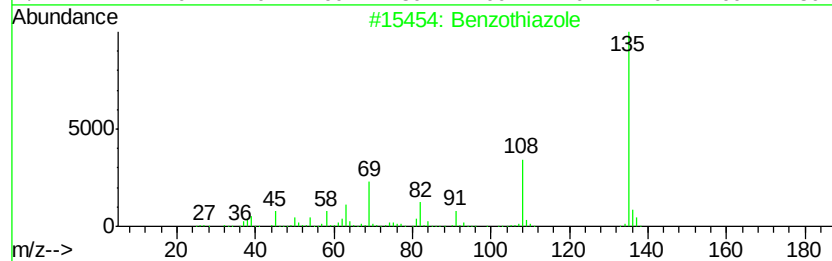
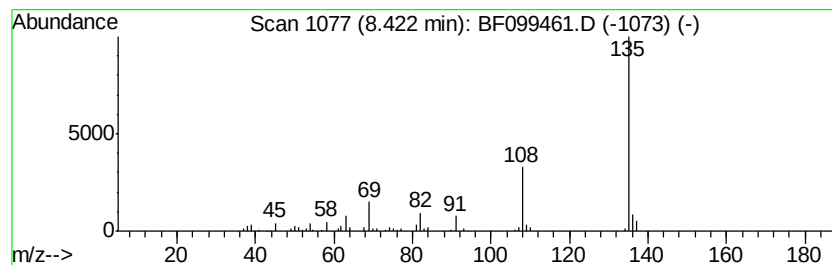
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Benzothiazole Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.42	5.66 ng	184642	Naphthalene-d8	8.13

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzothiazole	135	C7H5NS	000095-16-9	95
2		1,2-Benzisothiazole	135	C7H5NS	000272-16-2	90
3		3-Allylbenzothiazolium bromide	255	C10H10BrNS	016407-55-9	83
4		1H-Indole, 5-fluoro-	135	C8H6FN	000399-52-0	64
5		Thiocyanic acid, phenyl ester	135	C7H5NS	005285-87-0	64



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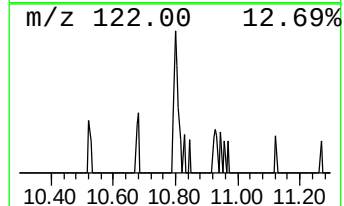
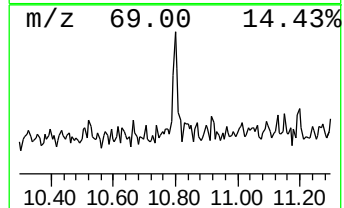
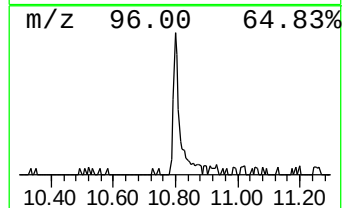
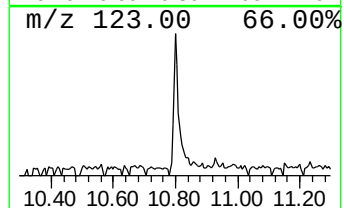
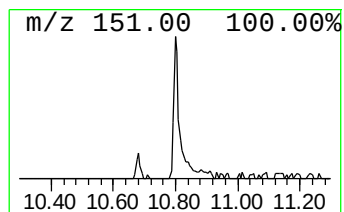
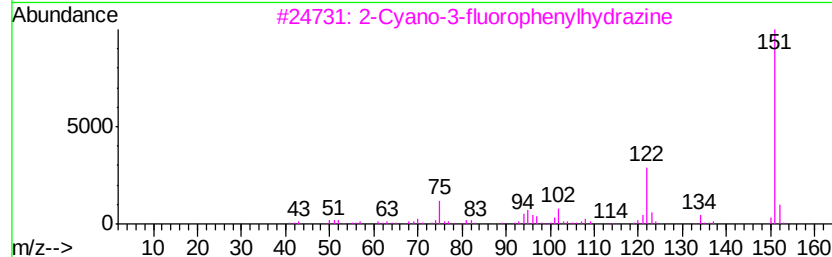
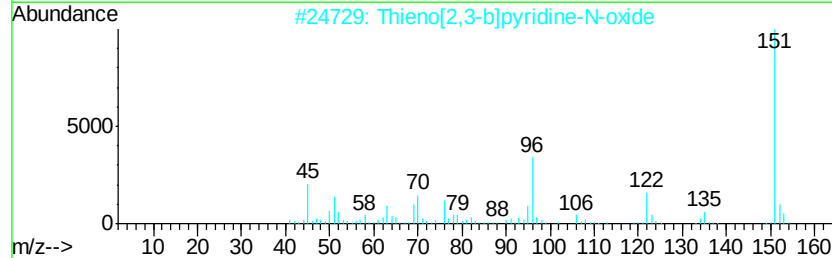
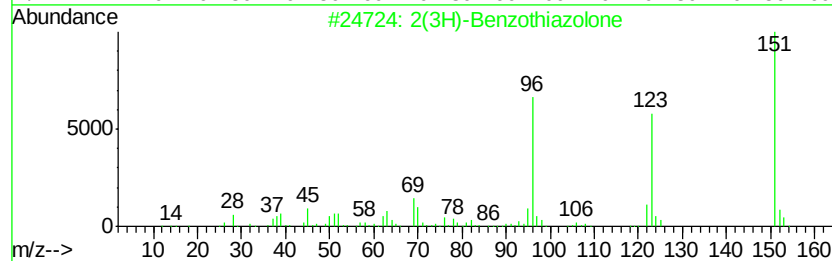
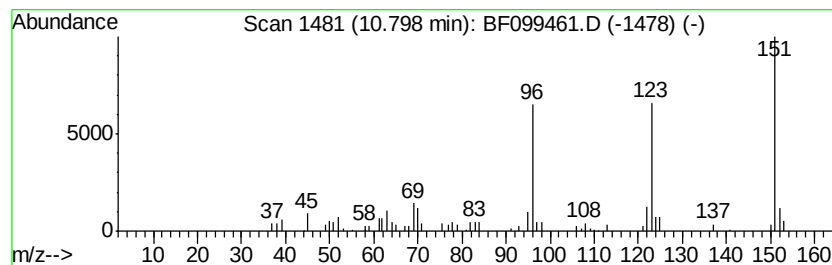
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Peak Number 6 2(3H)-Benzothiazolone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.		
10.80	2.36 ng	56101	Phenanthrene-d10	11.37		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(3H)-Benzothiazolone	151	C7H5NOS	000934-34-9	94	
2	Thieno[2,3-b]pyridine-N-oxide	151	C7H5NOS	025557-50-0	52	
3	2-Cyano-3-fluorophenylhydrazine	151	C7H6FN3	1000131-91-9	43	
4	4-Methoxyformanilide	151	C8H9NO2	005470-34-8	43	
5	4-Mercaptoimidazo[4,5-c]pyridine	151	C6H5N3S	034550-51-1	38	



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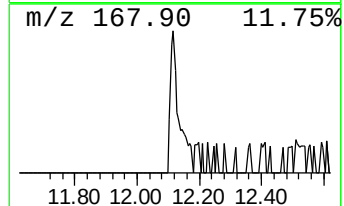
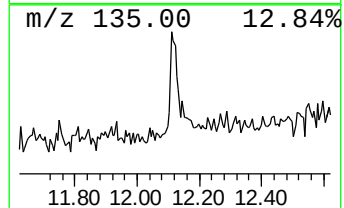
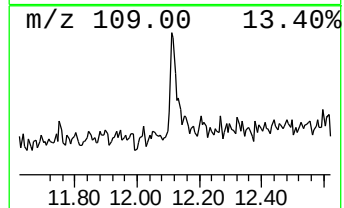
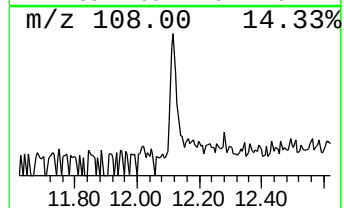
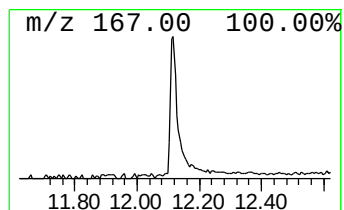
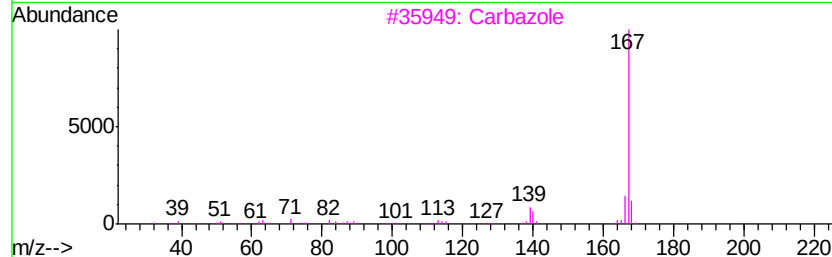
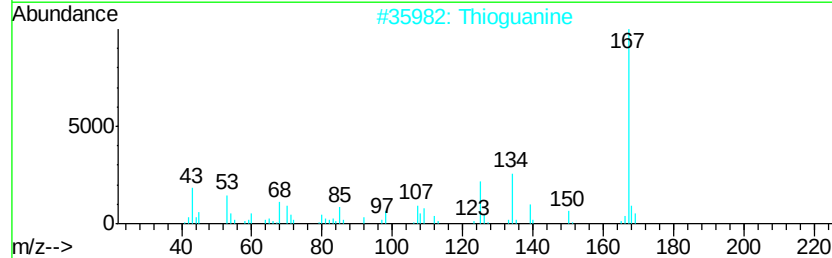
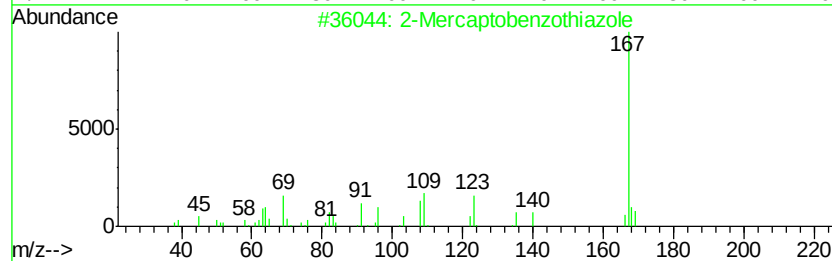
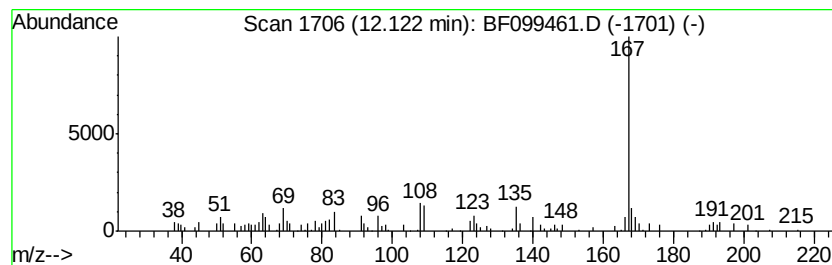
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 2-Mercaptobenzothiazole Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.12	4.24 ng	100809	Phenanthrene-d10	11.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Mercaptobenzothiazole	167	C7H5NS2	000149-30-4	97
2		Thioguanine	167	C5H5N5S	000154-42-7	53
3		Carbazole	167	C12H9N	000086-74-8	50
4		Benzaldehyde, 2-hydroxy-5-nitro-	167	C7H5NO4	000097-51-8	50
5		Benzene, 1,1',1''-(1-ethanyl-2-y...	258	C20H18	001520-42-9	47



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101317\
Data File : BF099461.D
Acq On : 14 Oct 2017 1:21
Operator : SJ/JU
Sample : I5819-12
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
3915-PA4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.13	12.8	ng	343816	1	6.85	536236	20.0
2-Pentanone, 4-hy...	5.08	6.3	ng	167856	1	6.85	536236	20.0
unknown6.63	6.63	80.3	ng	2153220	1	6.85	536236	20.0
Benzothiazole	8.42	5.7	ng	184642	2	8.13	651909	20.0
2(3H)-Benzothiazo...	10.80	2.4	ng	56101	4	11.37	475911	20.0
2-Mercaptobenzoth...	12.12	4.2	ng	100809	4	11.37	475911	20.0