

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012215\
 Data File : BF077021.D
 Acq On : 22 Jan 2015 20:13
 Operator : TP/IZ
 Sample : G1136-12
 Misc : S
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-17-COMP

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	1.350	21	23	28	rBV	29234	48773	5.95%	0.963%
2	1.418	28	29	42	rVB	359170	819222	100.00%	16.176%
3	3.944	247	250	260	rVB	54062	115848	14.14%	2.288%
4	4.904	331	334	347	rBV	152738	345307	42.15%	6.818%
5	7.259	537	540	545	rBV	201736	352120	42.98%	6.953%
6	7.350	545	548	557	rVB	228444	401996	49.07%	7.938%
7	7.853	589	592	596	rVB	83087	131506	16.05%	2.597%
8	8.173	616	620	624	rBV	180073	292558	35.71%	5.777%
9	9.145	702	705	714	rVB	148297	228487	27.89%	4.512%
10	10.756	843	846	850	rBV	116304	179969	21.97%	3.554%
11	13.408	1075	1078	1082	rBV	279125	439296	53.62%	8.674%
12	14.482	1169	1172	1175	rBV	10927	16937	2.07%	0.334%
13	14.883	1204	1207	1211	rBV	132976	199616	24.37%	3.942%
14	16.574	1353	1355	1359	rVB	151601	231284	28.23%	4.567%
15	17.683	1450	1452	1455	rBV	143535	203559	24.85%	4.019%
16	19.374	1598	1600	1603	rBV2	37581	47852	5.84%	0.945%
17	19.820	1636	1639	1644	rVB2	20422	30424	3.71%	0.601%
18	19.923	1645	1648	1651	rVB	469444	472254	57.65%	9.325%
19	21.192	1755	1759	1761	rBV	183624	260739	31.83%	5.149%
20	21.329	1768	1771	1773	rBV	9883	10137	1.24%	0.200%
21	22.838	1900	1903	1906	rBV	155635	188806	23.05%	3.728%
22	23.421	1952	1954	1956	rBV2	5175	8935	1.09%	0.176%
23	23.466	1956	1958	1965	rVB5	6141	20006	2.44%	0.395%
24	24.621	2055	2059	2063	rVB4	3253	9774	1.19%	0.193%
25	26.484	2217	2222	2223	rBV3	3516	8916	1.09%	0.176%

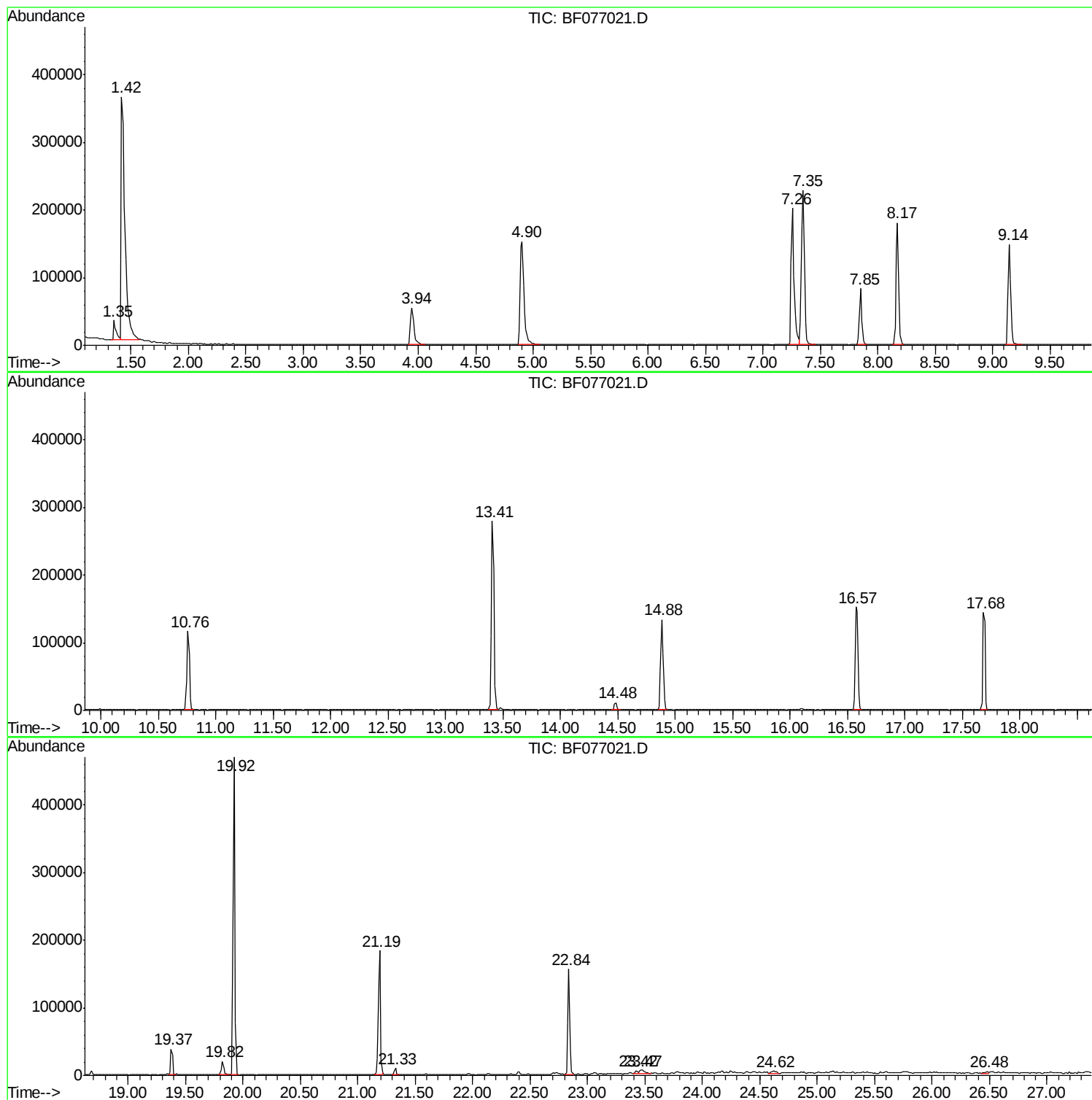
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF011415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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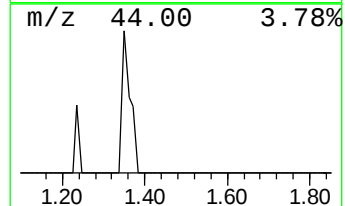
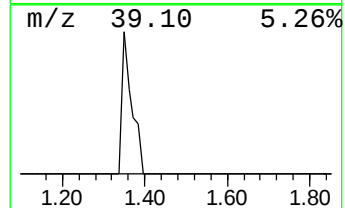
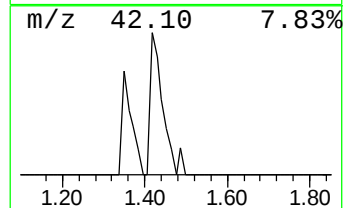
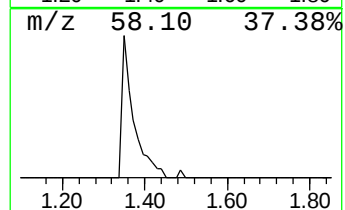
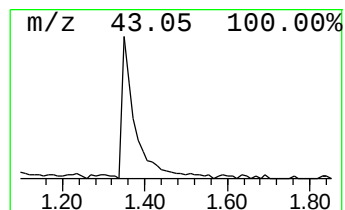
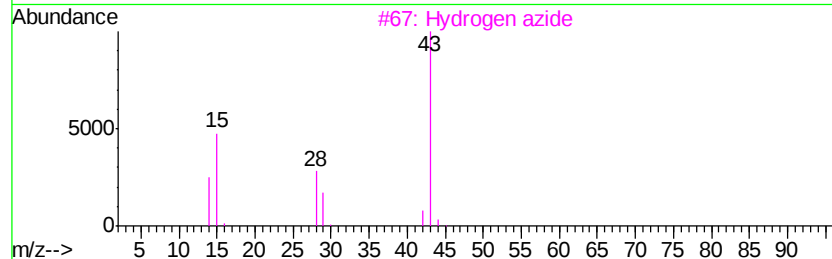
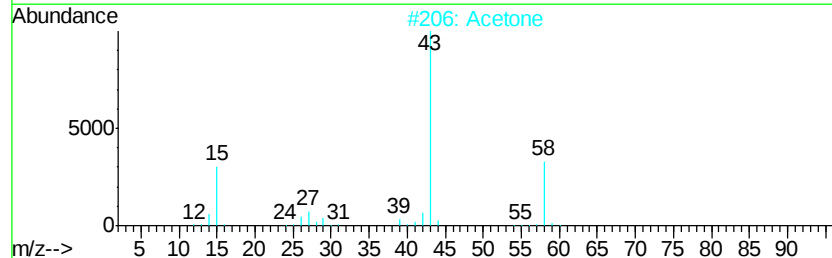
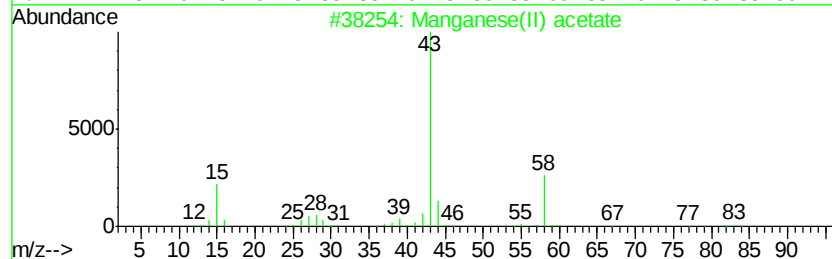
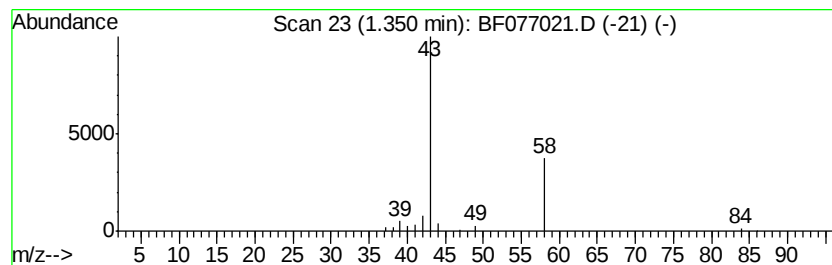
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown1.35 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.35	7.42 ng	48773	1,4-Dichlorobenzene-d4	7.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Manganese(II) acetate	173	C4H6MnO4	006156-78-1	39
2		Acetone	58	C3H6O	000067-64-1	9
3		Hydrogen azide	43	HN3	007782-79-8	4
4		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	4
5		Butanedial	86	C4H6O2	000638-37-9	4



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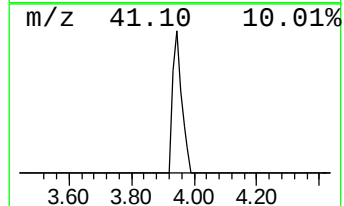
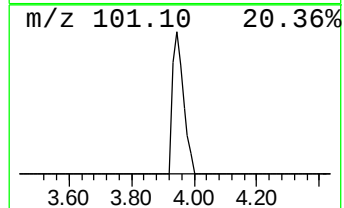
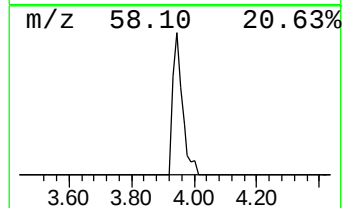
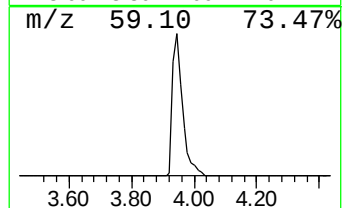
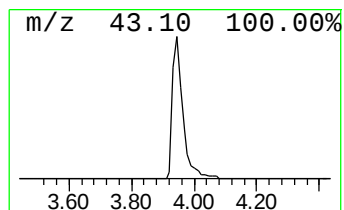
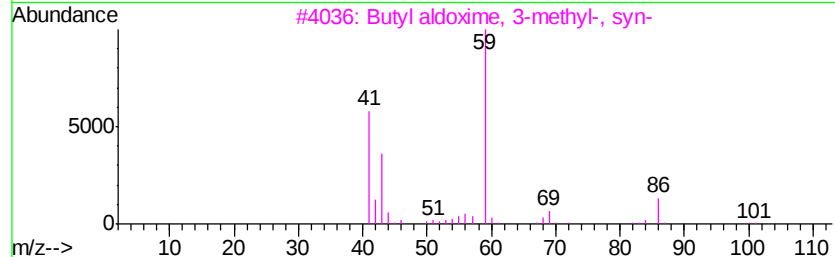
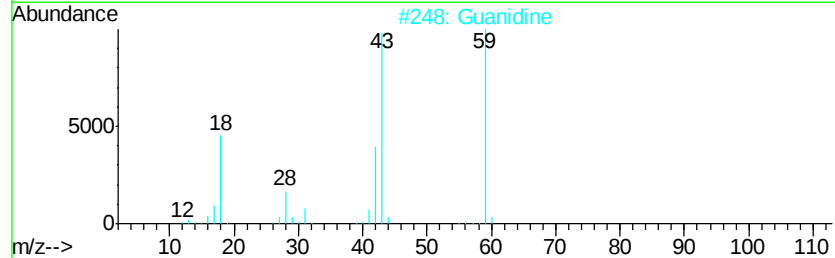
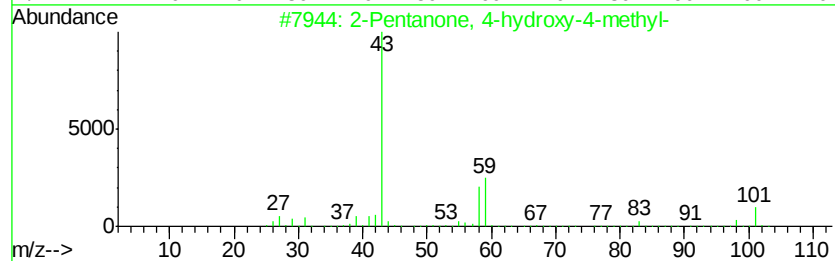
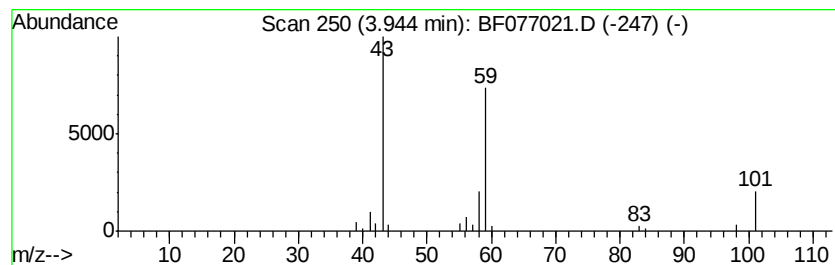
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.94	17.62 ng	115848	1,4-Dichlorobenzene-d4	7.85

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Guanidine	59	CH5N3	000113-00-8	50
3			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	38
4			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5			1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	25



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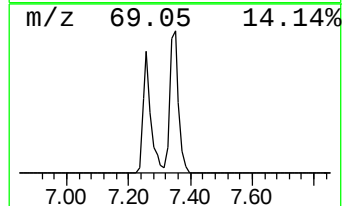
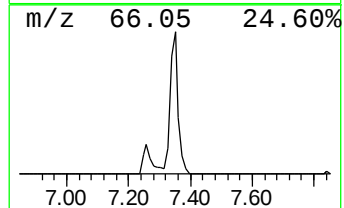
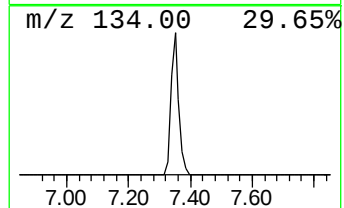
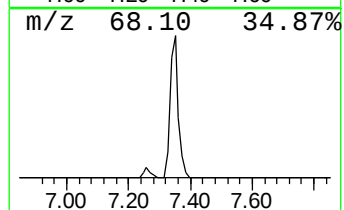
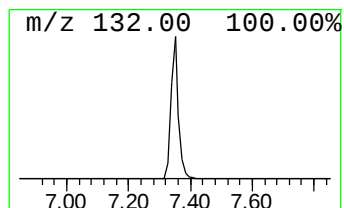
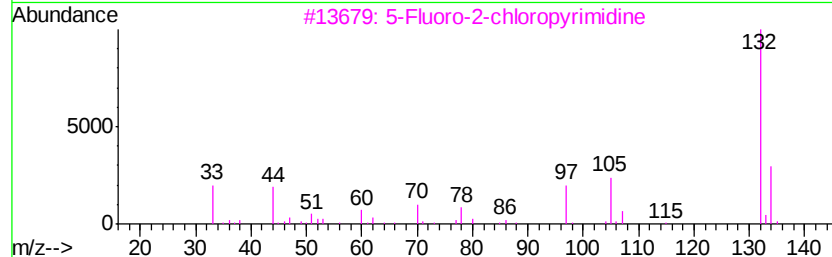
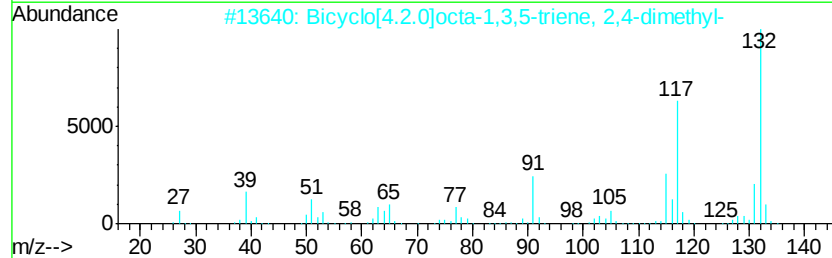
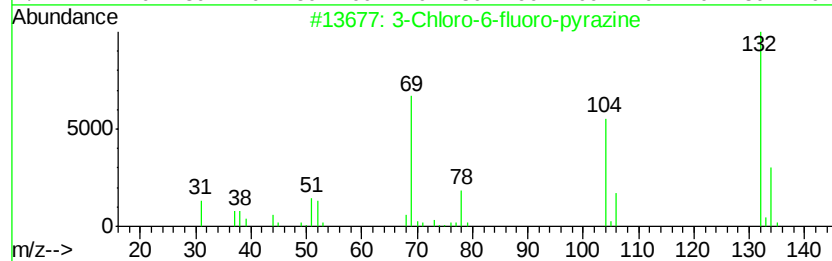
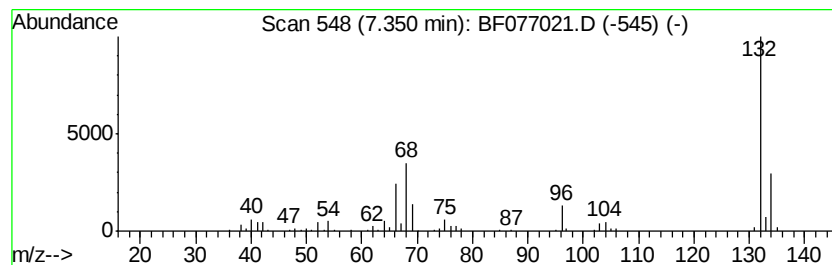
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown7.35 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.35	61.14 ng	401996	1,4-Dichlorobenzene-d4	7.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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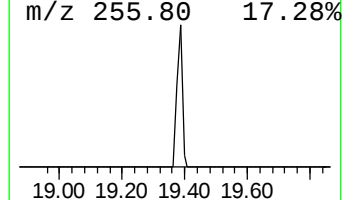
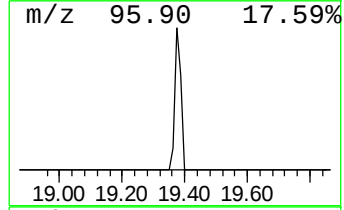
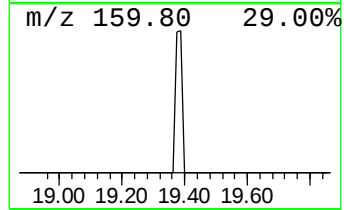
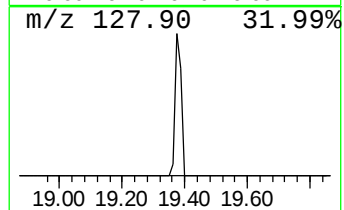
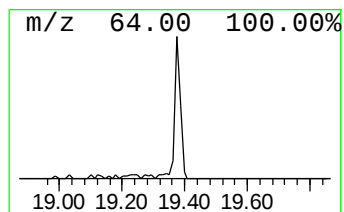
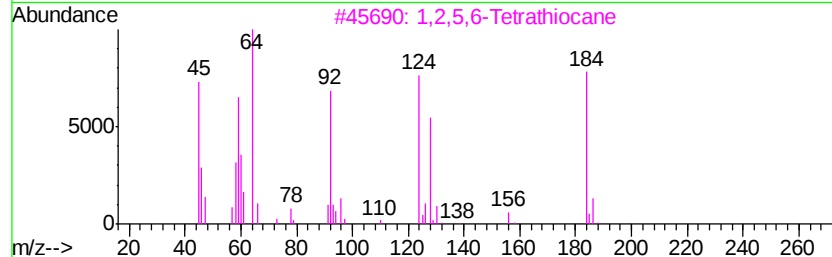
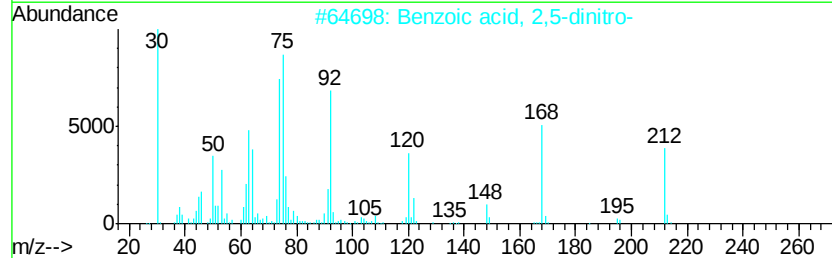
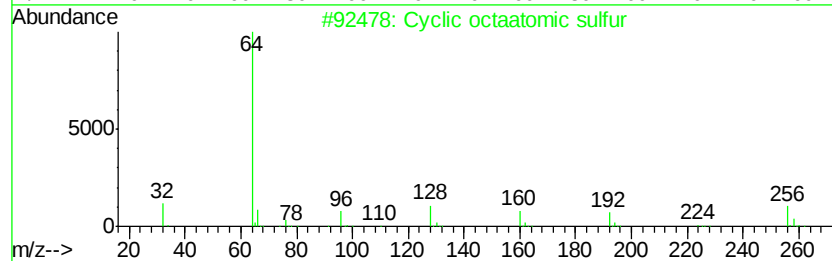
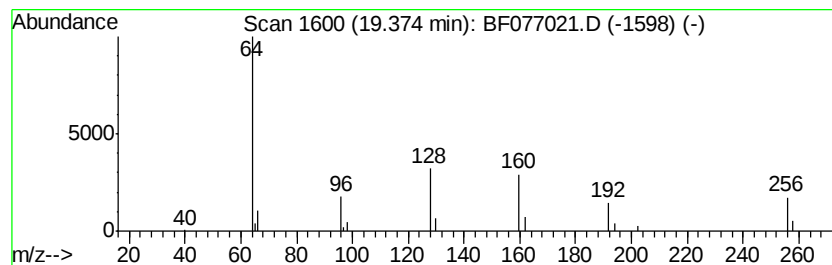
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Cyclic octaatomic sulfur Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.37	4.70 ng	47852	Phenanthrene-d10	17.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclic octaatomic sulfur	256	S8	010544-50-0	90
2	Benzoic acid, 2,5-dinitro-	212	C7H4N2O6	000610-28-6	59
3	1,2,5,6-Tetrathiocane	184	C4H8S4	001940-01-8	39
4	Acetonitrile, 2-(5-chloro-3-oxo-...	248	C8H9ClN2OS2	1000269-94-4	9
5	2,3-Diazabicyclo[3.2.0]hept-2-en...	176	C7H7F3N2	1000258-92-2	9



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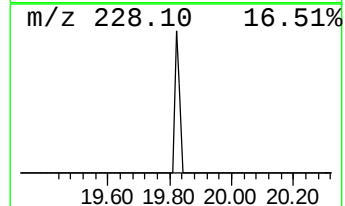
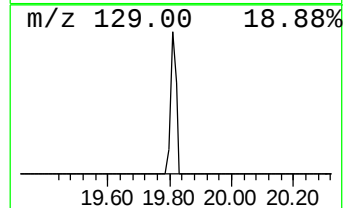
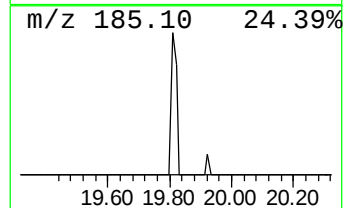
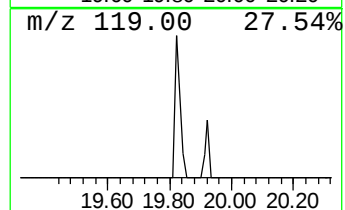
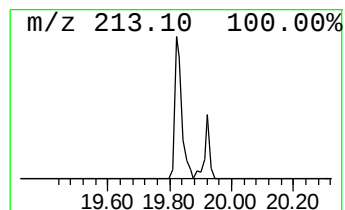
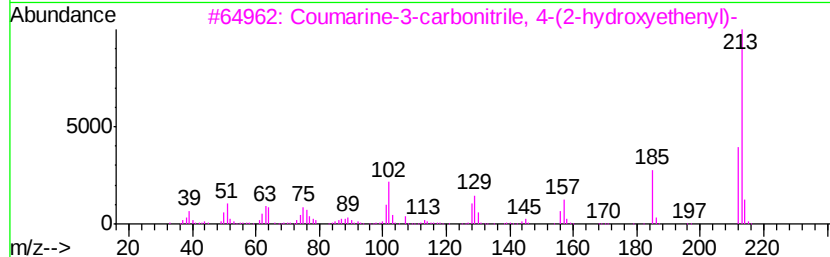
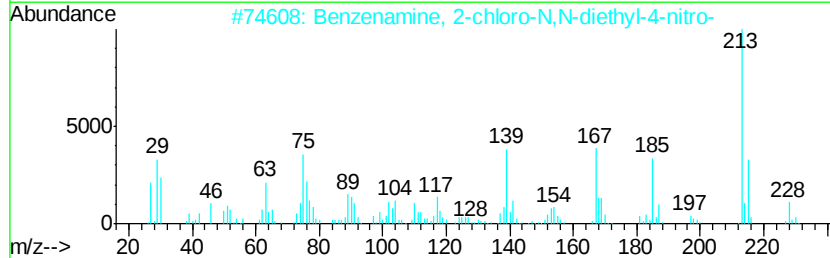
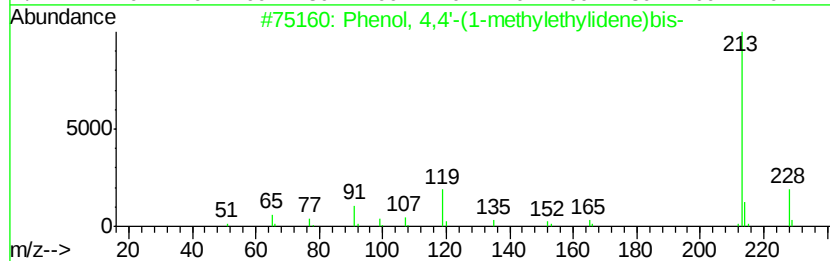
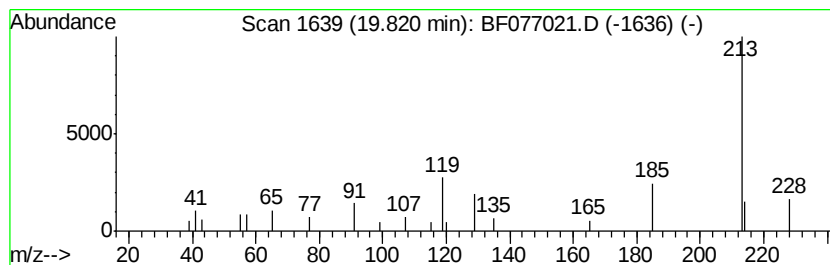
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Phenol, 4,4'-(1-methylethyl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.82	2.33 ng	30424	Chrysene-d12	21.19

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phenol, 4,4'-(1-methylethylidene)bis-	228	C15H16O2	000080-05-7	81
2		Benzenamine, 2-chloro-N,N-diethyl-	228	C10H13ClN2O2	000086-49-7	58
3		Coumarine-3-carbonitrile, 4-(2-hydroxyethyl)-	213	C12H7N3O3	1000270-09-9	53
4		Pyrrolo[3,4-c]coumarine, 3,4-dihydro-	213	C12H7N3O3	040547-98-6	53
5		2H,8H-Benzo[1,2-b:3,4-b']dipyran-	228	C14H12O3	000523-59-1	53



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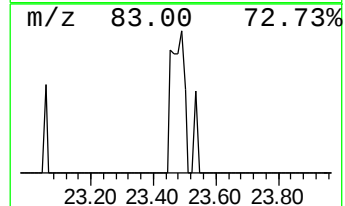
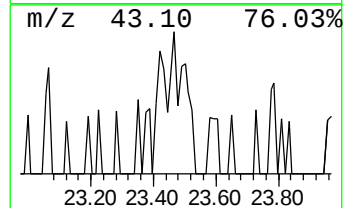
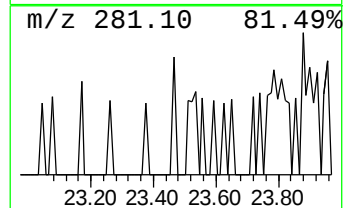
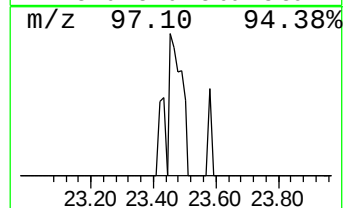
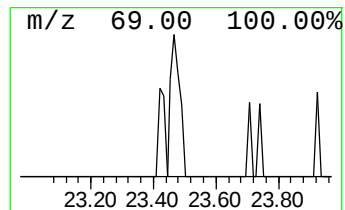
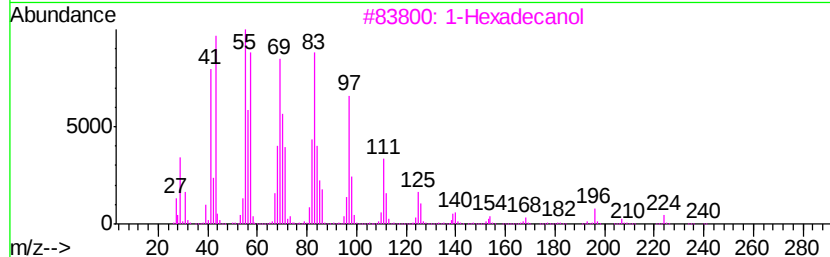
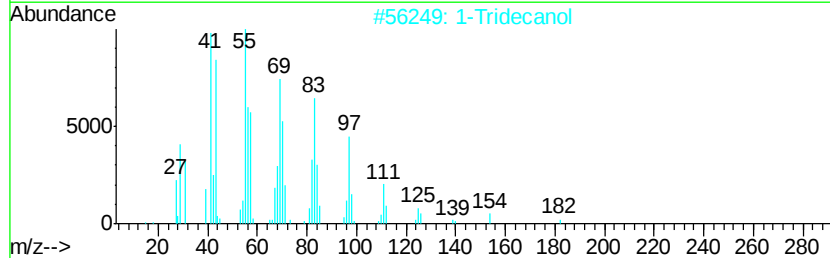
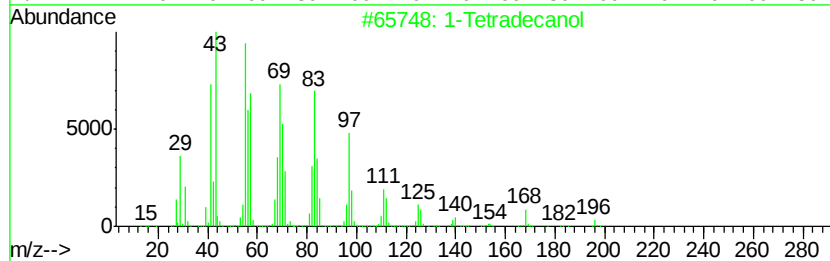
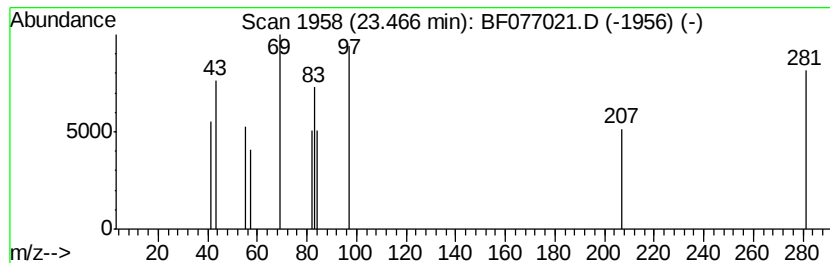
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown23.47 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.47	2.12 ng	20006	Perylene-d12	22.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Tetradecanol	214	C14H30O	000112-72-1	38
2		1-Tridecanol	200	C13H28O	000112-70-9	38
3		1-Hexadecanol	242	C16H34O	036653-82-4	28
4		1-Octadecanol	270	C18H38O	000112-92-5	28
5		Acetic acid, chloro-, hexadecyl ...	318	C18H35ClO2	052132-58-8	28



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012215\
Data File : BF077021.D
Acq On : 22 Jan 2015 20:13
Operator : TP/IZ
Sample : G1136-12
Misc : S
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-17-COMP

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
unknown1.35	1.35	7.4	ng	48773	1	7.85	131506	20.0
2-Pentanone, 4-hy...	3.94	17.6	ng	115848	1	7.85	131506	20.0
unknown7.35	7.35	61.1	ng	401996	1	7.85	131506	20.0
Cyclic octaatomic...	19.37	4.7	ng	47852	4	17.68	203559	20.0
Phenol, 4,4'-(1-m...	19.82	2.3	ng	30424	5	21.19	260739	20.0
unknown23.47	23.47	2.1	ng	20006	6	22.84	188806	20.0