

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050515\
 Data File : BF078949.D
 Acq On : 5 May 2015 19:23
 Operator : TP/IZ
 Sample : G2044-18
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-49D

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-BF043015.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	1.518	26	29	32	rVB	5837184	6619940	100.00%	21.131%
2	1.655	38	41	44	rVB	144461	262823	3.97%	0.839%
3	1.770	50	51	55	rBV	109055	149562	2.26%	0.477%
4	1.838	55	57	60	rVB	233568	292053	4.41%	0.932%
5	1.907	60	63	84	rVB	459476	979330	14.79%	3.126%
6	5.164	346	348	356	rVB	211505	263327	3.98%	0.841%
7	5.656	388	391	393	rBV	2325937	2348220	35.47%	7.496%
8	6.913	498	501	503	rBV	1645353	2349975	35.50%	7.501%
9	7.062	512	514	517	rBV	1920854	2437374	36.82%	7.780%
10	7.359	537	540	542	rBV	481164	443930	6.71%	1.417%
11	7.542	554	556	559	rVB	1851769	1694804	25.60%	5.410%
12	8.045	598	600	603	rBV	1565699	1375416	20.78%	4.390%
13	8.936	675	678	680	rBV	500397	600399	9.07%	1.916%
14	10.273	793	795	798	rBV	1854023	2262652	34.18%	7.222%
15	10.776	837	839	842	rBV	78978	90133	1.36%	0.288%
16	11.108	866	868	871	rVB	713986	662975	10.01%	2.116%
17	11.451	896	898	908	rVB	43668	69767	1.05%	0.223%
18	12.091	951	954	956	rBV	1660742	1783236	26.94%	5.692%
19	12.948	1027	1029	1031	rBV	522429	705487	10.66%	2.252%
20	14.559	1164	1170	1172	rVB	86702	133339	2.01%	0.426%
21	14.742	1183	1186	1187	rBV	65533	78413	1.18%	0.250%
22	14.811	1190	1192	1196	rBV	685303	767789	11.60%	2.451%
23	14.948	1202	1204	1207	rBV	2187677	2452790	37.05%	7.829%
24	15.588	1257	1260	1262	rBV	61022	122067	1.84%	0.390%
25	16.125	1304	1307	1311	rBV	95484	199637	3.02%	0.637%
26	16.251	1315	1318	1320	rVV	802071	833416	12.59%	2.660%
27	16.537	1338	1343	1349	rVB3	55466	138199	2.09%	0.441%
28	16.948	1377	1379	1386	rVB2	37659	67604	1.02%	0.216%
29	17.554	1430	1432	1438	rVB	30932	77608	1.17%	0.248%
30	17.828	1452	1456	1459	rBV2	37335	120062	1.81%	0.383%
31	17.886	1459	1461	1465	rVB2	39344	76876	1.16%	0.245%
32	18.023	1470	1473	1477	rVB	615392	868722	13.12%	2.773%

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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-BF043015.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

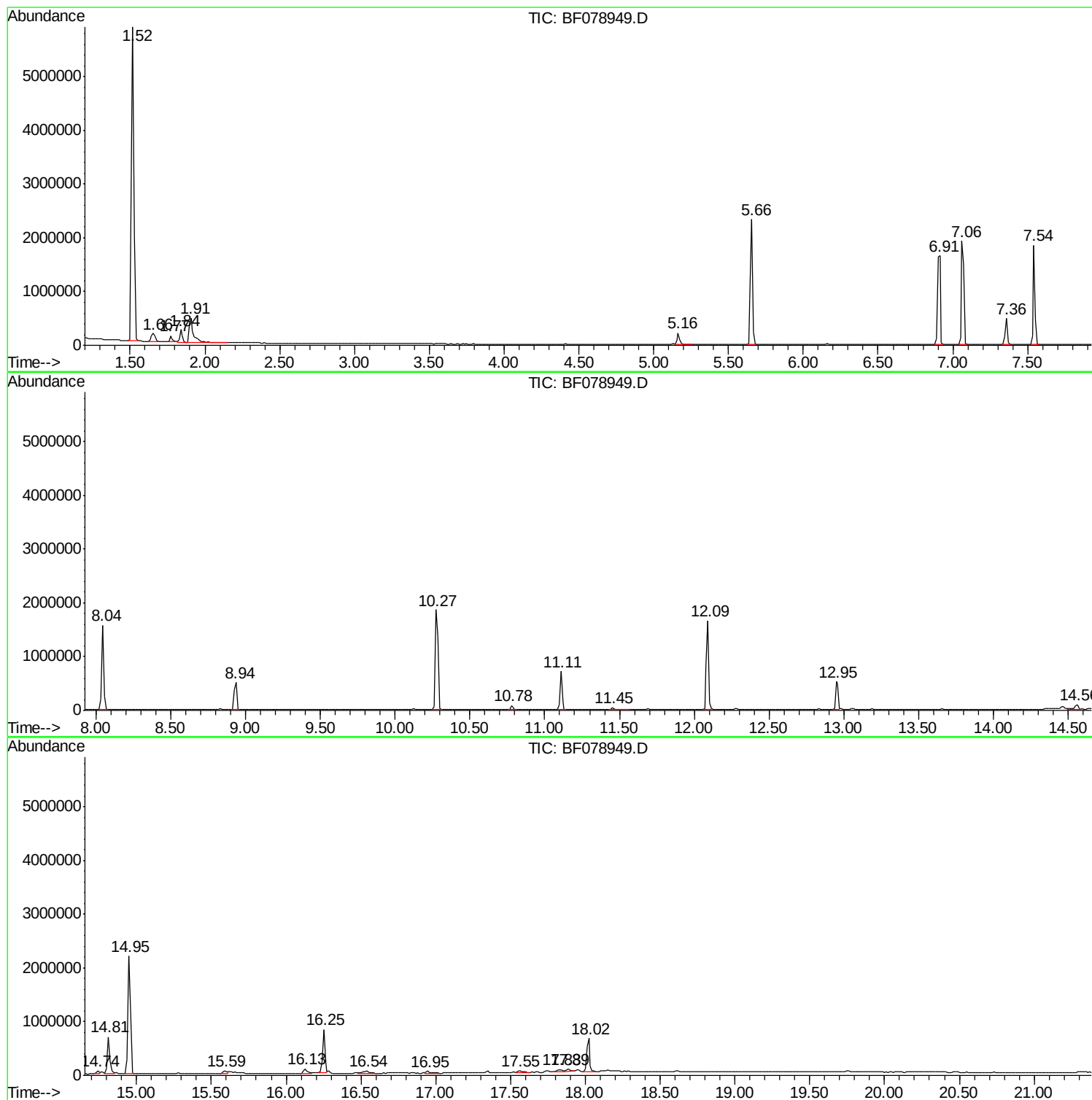
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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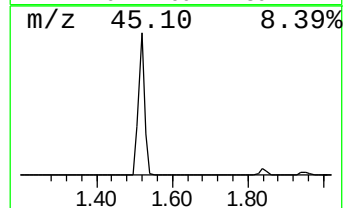
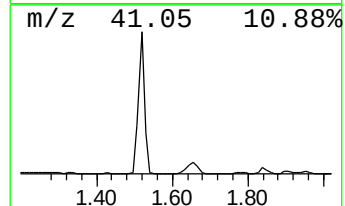
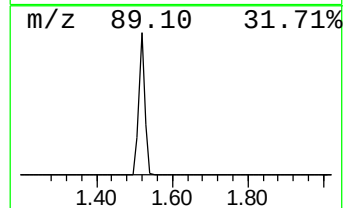
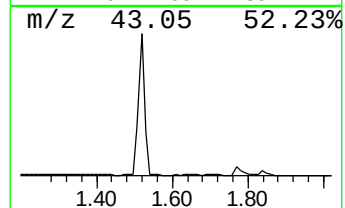
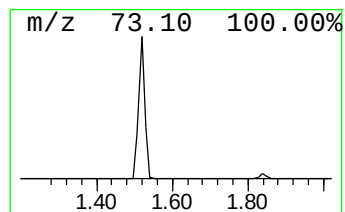
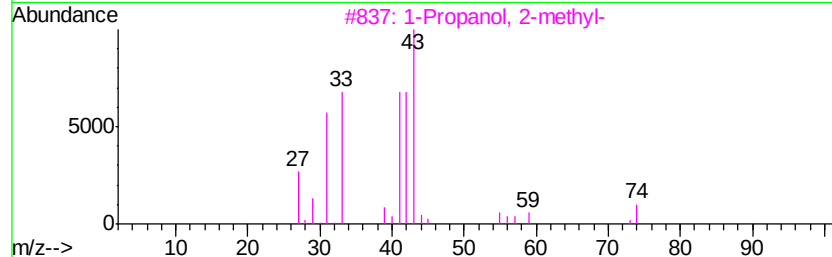
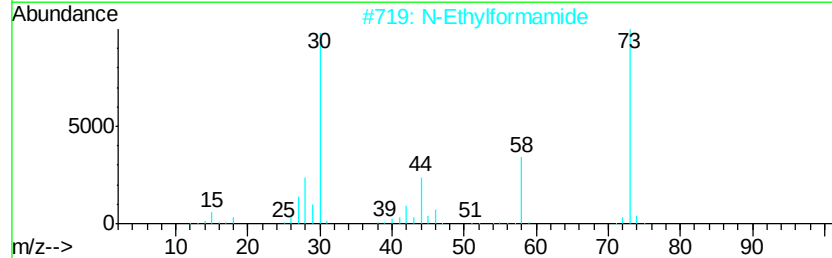
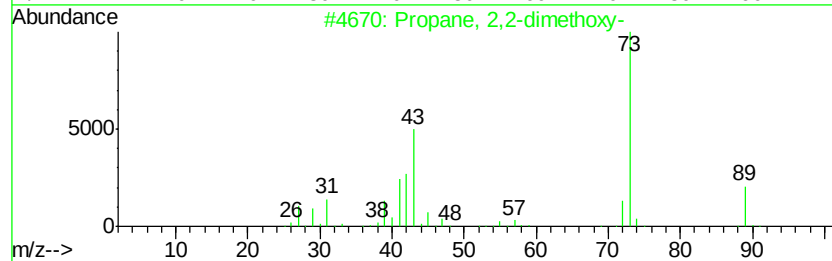
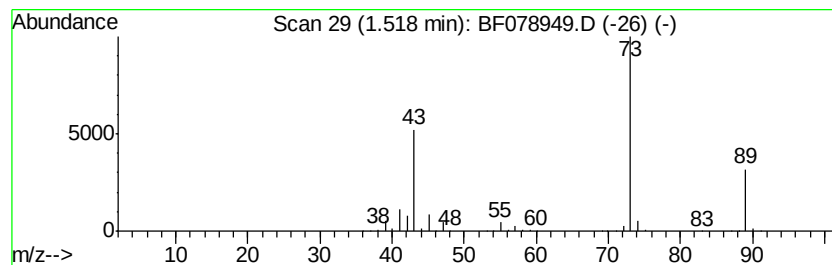
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown1.52 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.52	298.24 ng	6619940	1,4-Dichlorobenzene-d4	7.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	38
2		N-Ethylformamide	73	C3H7NO	000627-45-2	9
3		1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
4		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
5		1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9



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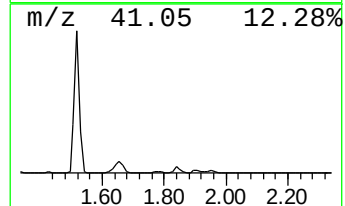
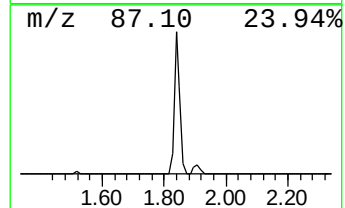
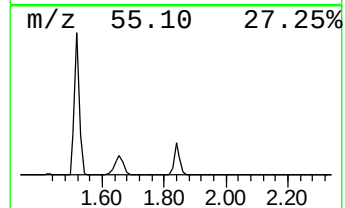
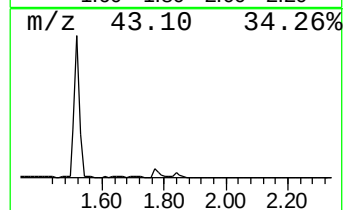
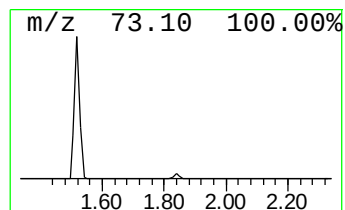
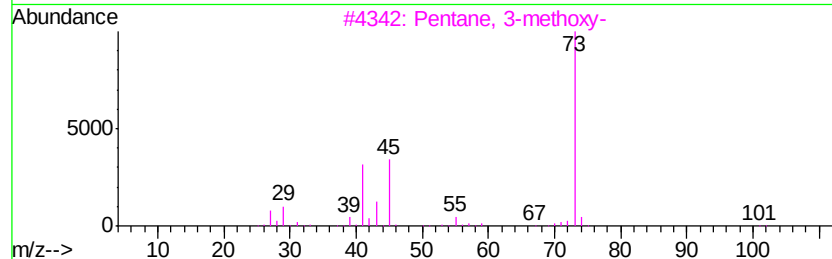
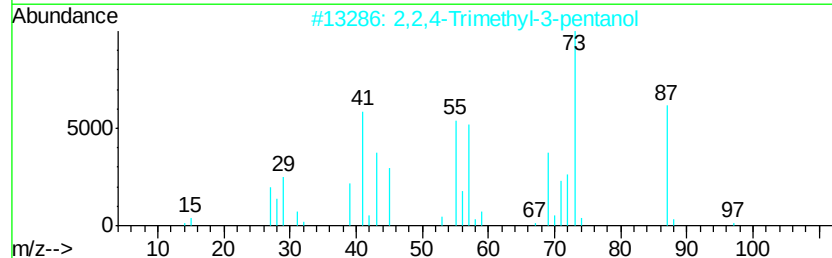
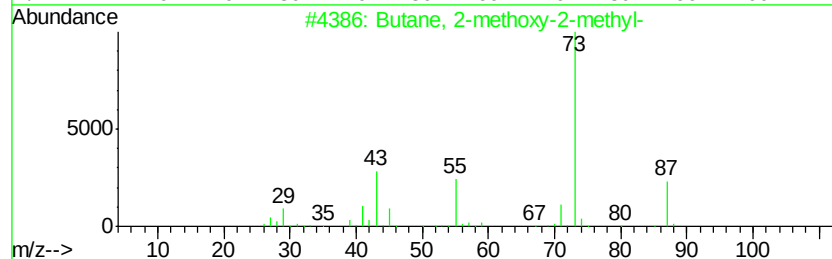
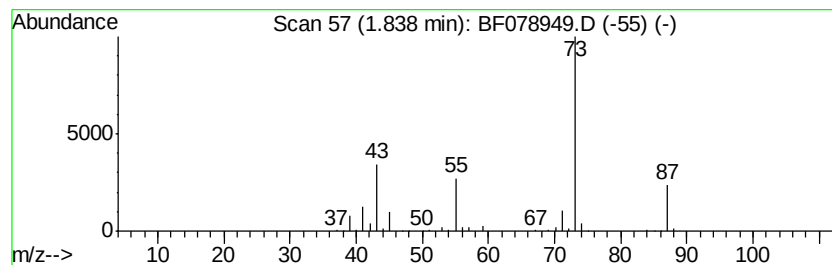
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.84	13.16 ng	292053	1,4-Dichlorobenzene-d4	7.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4		Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
5		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	10



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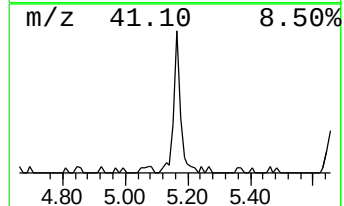
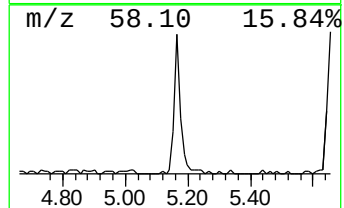
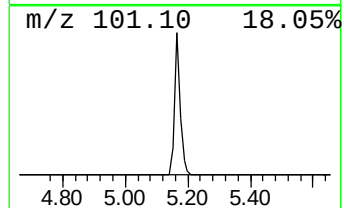
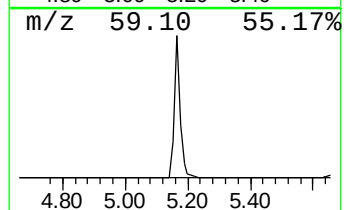
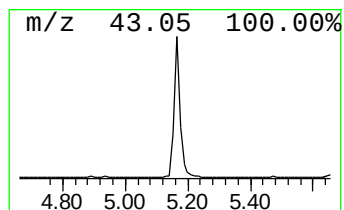
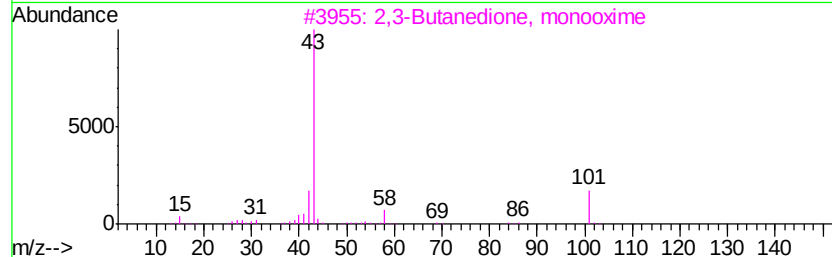
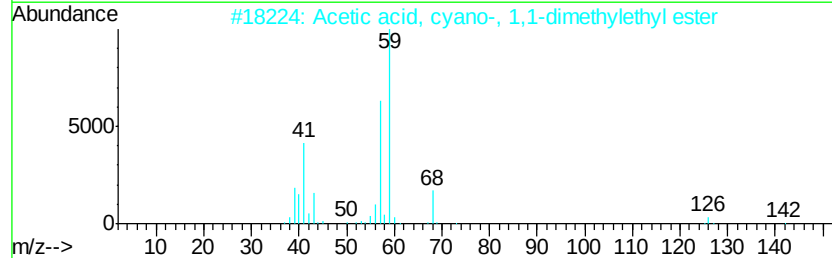
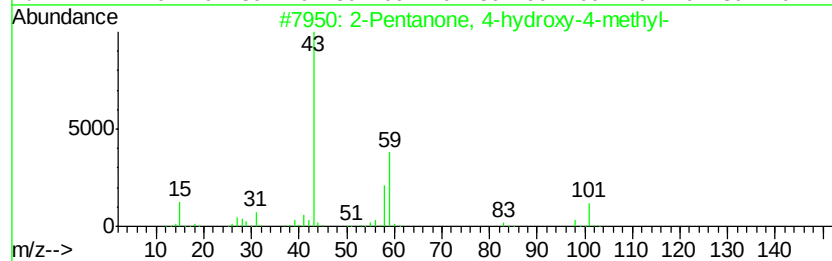
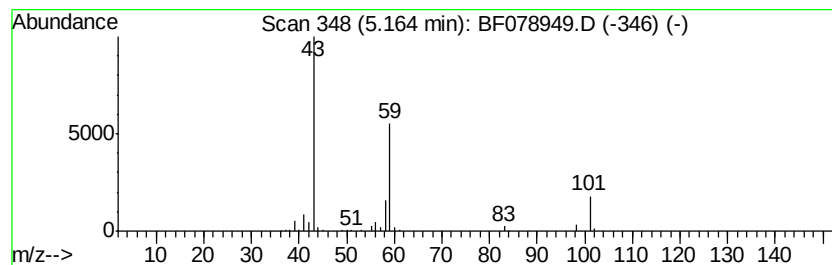
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.16	11.86 ng	263327	1,4-Dichlorobenzene-d4	7.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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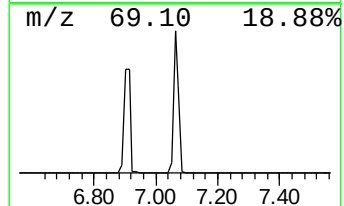
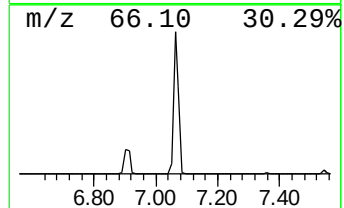
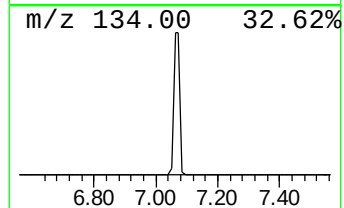
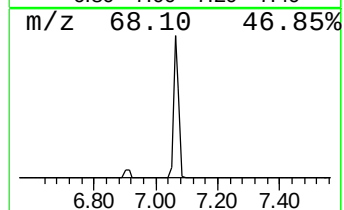
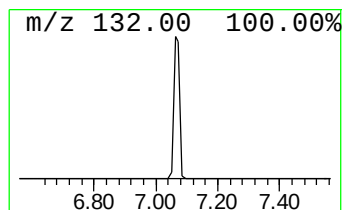
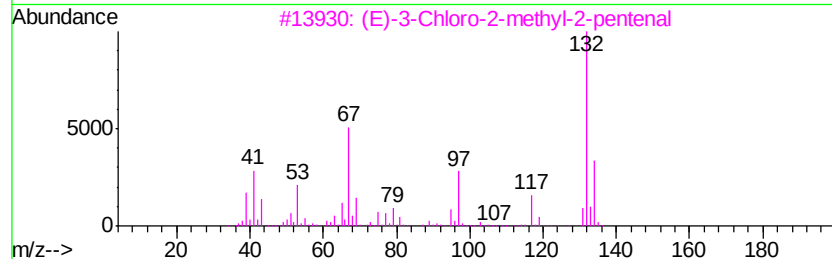
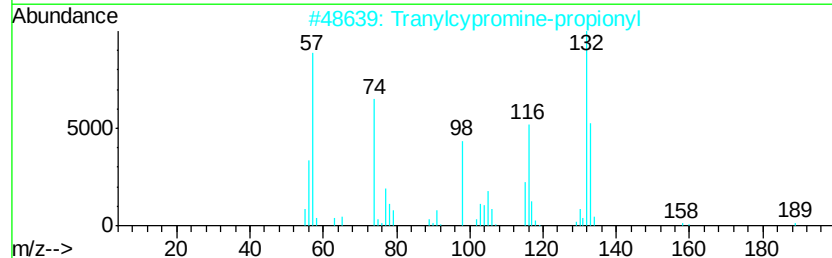
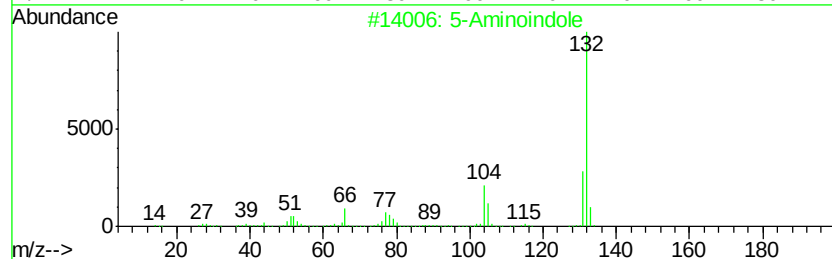
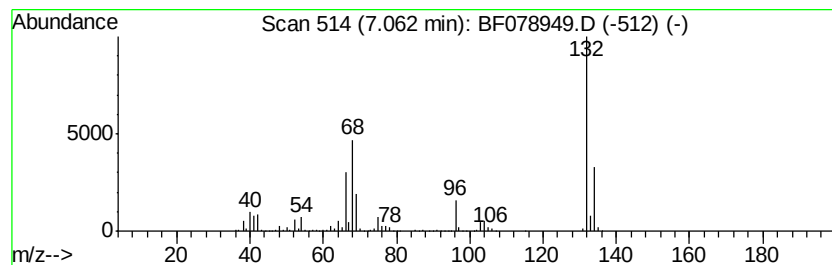
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown7.06 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.06	109.81 ng	2437370	1,4-Dichlorobenzene-d4	7.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Aminoindole	132	C8H8N2	005192-03-0	12
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9



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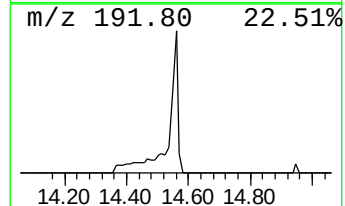
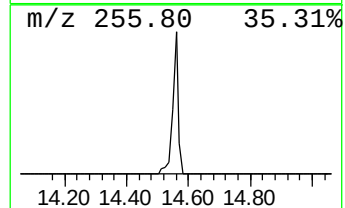
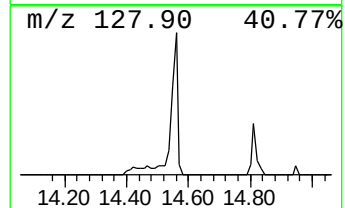
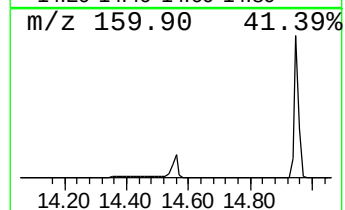
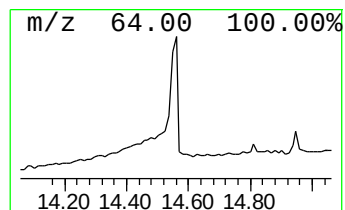
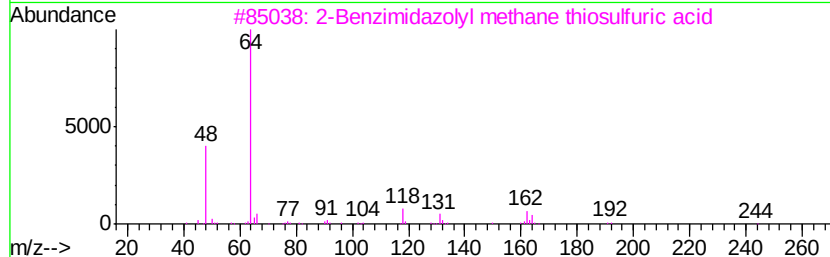
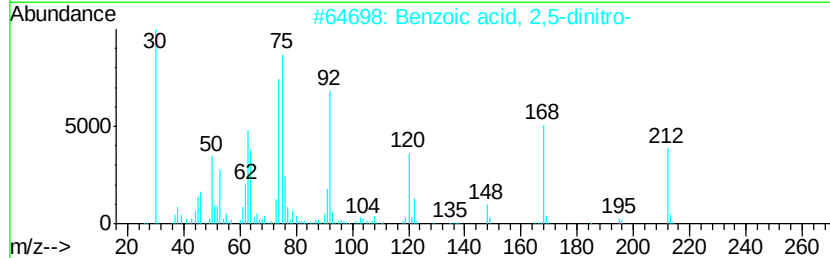
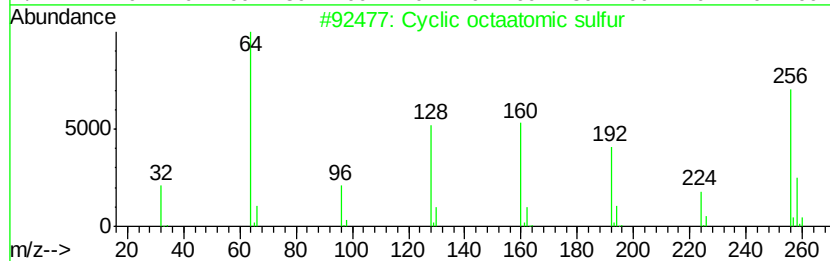
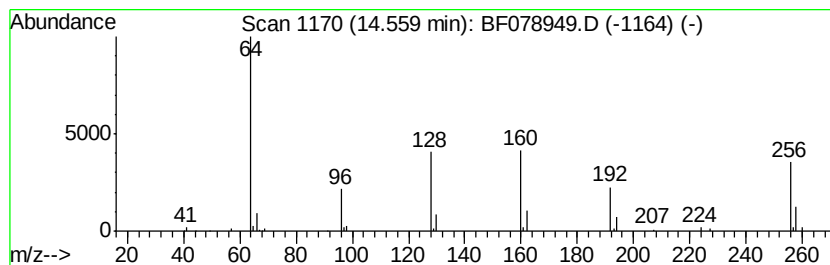
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 10 Cyclic octaatomic sulfur Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.56	3.78 ng	133339	Phenanthrene-d10	12.96

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclic octaatomic sulfur	256	S8	010544-50-0	94
2			Benzoic acid, 2,5-dinitro-	212	C7H4N2O6	000610-28-6	50
3			2-Benzimidazolyl methane thiosul...	244	C8H8N2O3S2	1000256-39-2	9
4			Methanethiol, N-(p-methoxyphenet...	304	C11H16N2O4S2	040283-94-1	9
5			1,2,5,6-Tetrathiocane	184	C4H8S4	001940-01-8	9



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SB-49D

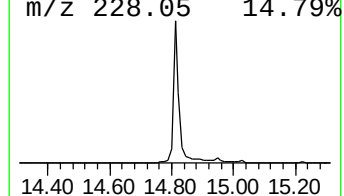
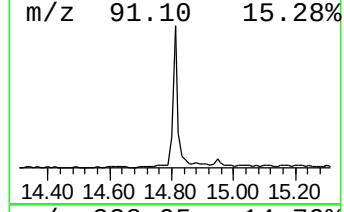
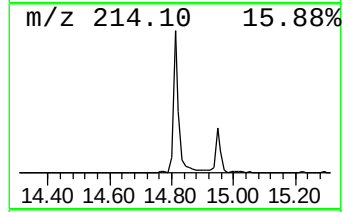
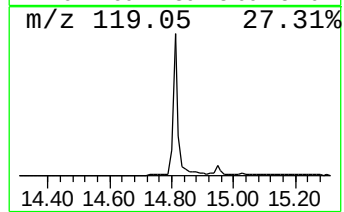
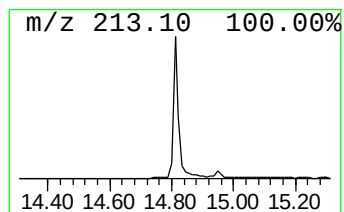
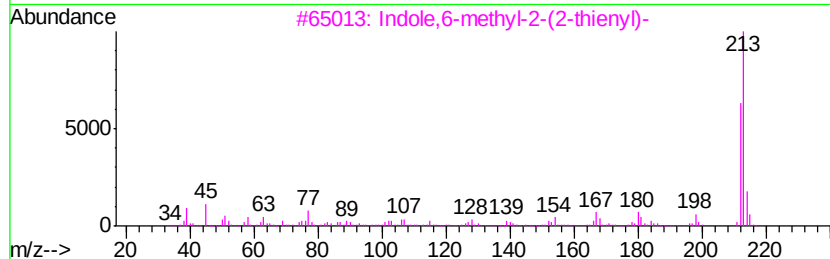
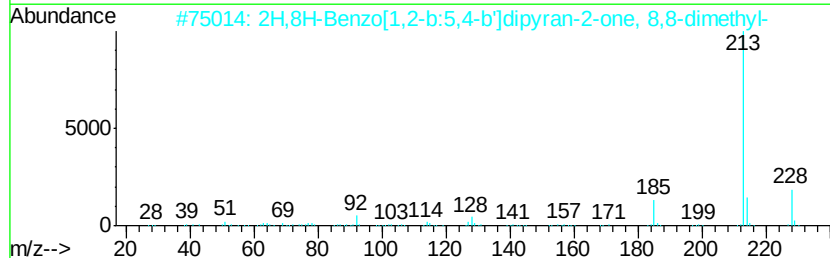
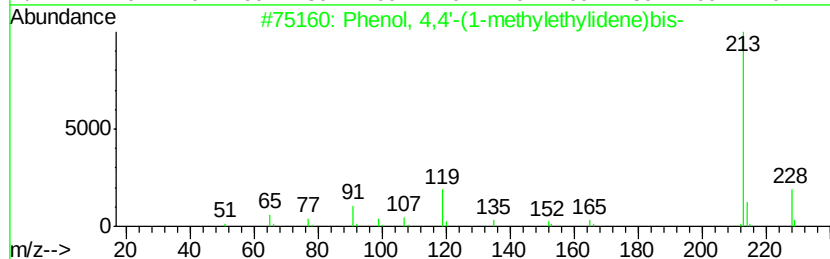
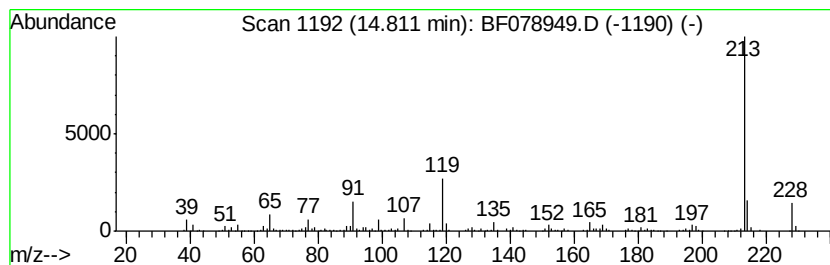
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Phenol, 4,4'-(1-methylethyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.81	18.43 ng	767789	Chrysene-d12	16.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	96
2		2H,8H-Benzo[1,2-b:5,4-b']dipyrans...	228	C14H12O3	000553-19-5	53
3		Indole,6-methyl-2-(2-thienyl)-	213	C13H11NS	296245-70-0	50
4		Carbanilic acid, p-phenyl-	213	C13H11NO2	004474-53-7	49
5		2H,8H-Benzo[1,2-b:3,4-b']dipyrans...	228	C14H12O3	000523-59-1	42



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050515\
Data File : BF078949.D
Acq On : 5 May 2015 19:23
Operator : TP/IZ
Sample : G2044-18
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-49D

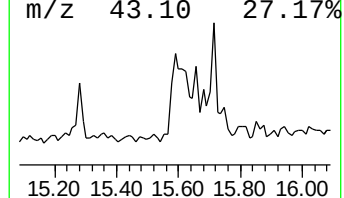
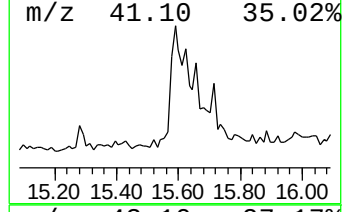
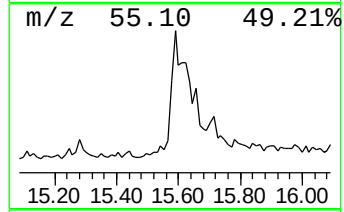
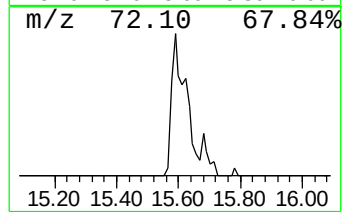
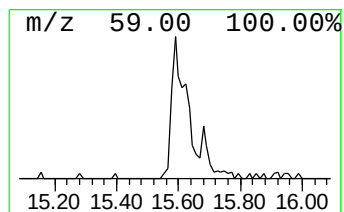
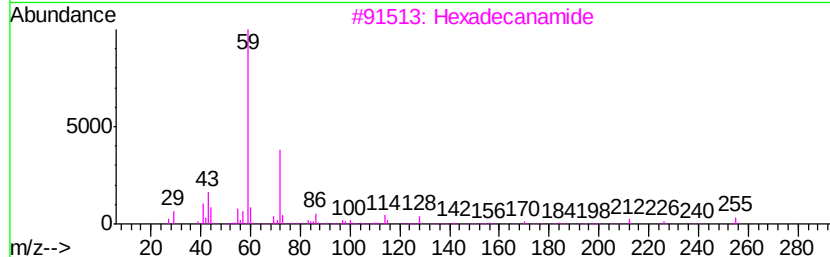
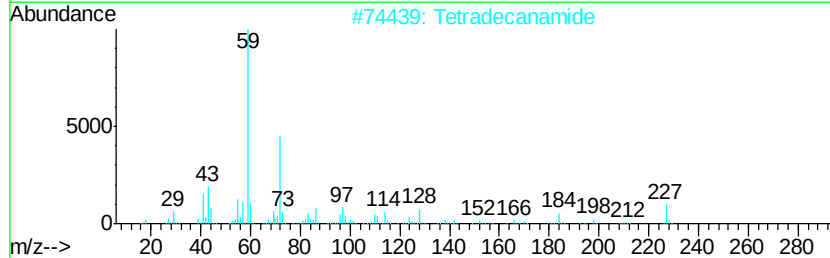
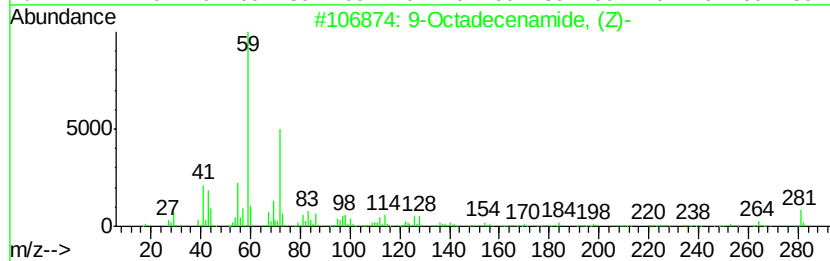
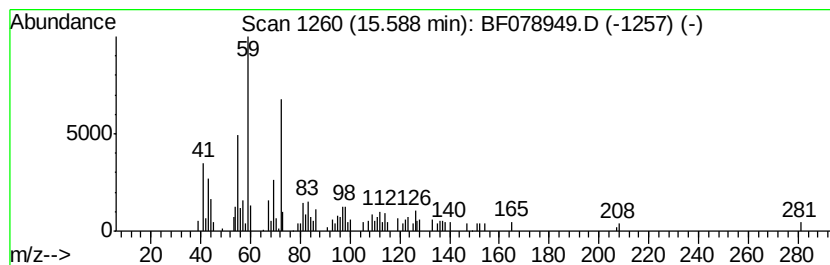
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 9-Octadecenamide, (Z)- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.59	2.93 ng	122067	Chrysene-d12	16.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	87
2		Tetradecanamide	227	C14H29NO	000638-58-4	53
3		Hexadecanamide	255	C16H33NO	000629-54-9	53
4		Octanamide	143	C8H17NO	000629-01-6	47
5		Dodecanamide	199	C12H25NO	001120-16-7	47



Data Path : Z:\HPCHEM1\BNA F\DATA\BF050515\
Data File : BF078949.D
Acq On : 5 May 2015 19:23
Operator : TP/IZ
Sample : G2044-18
Misc :
ALS Vial : 21 Sample Multiplier: 1

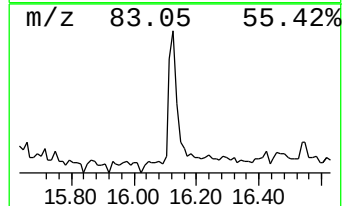
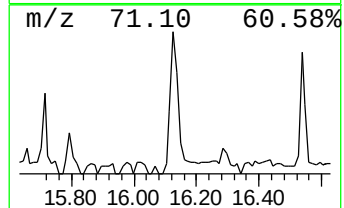
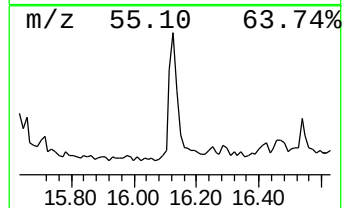
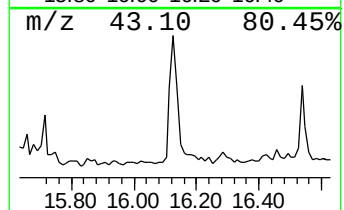
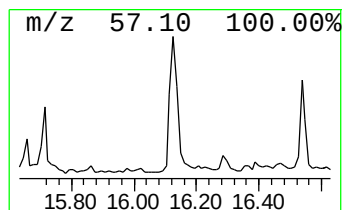
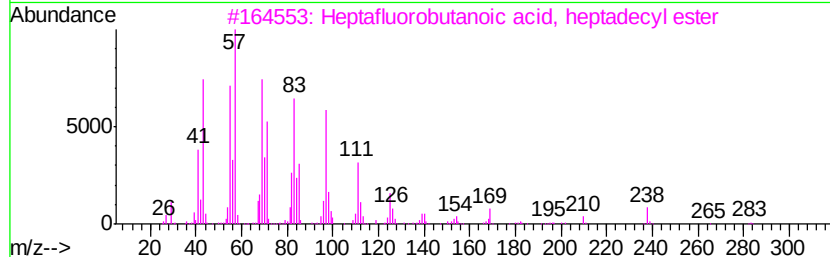
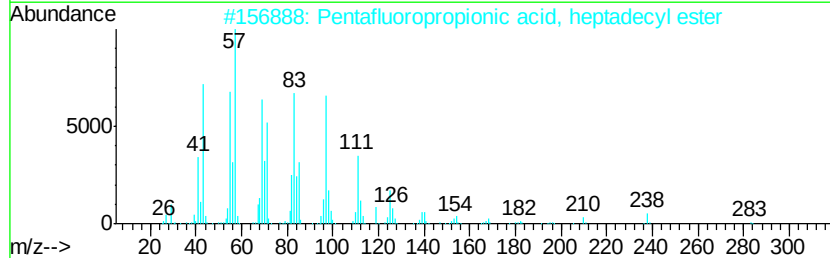
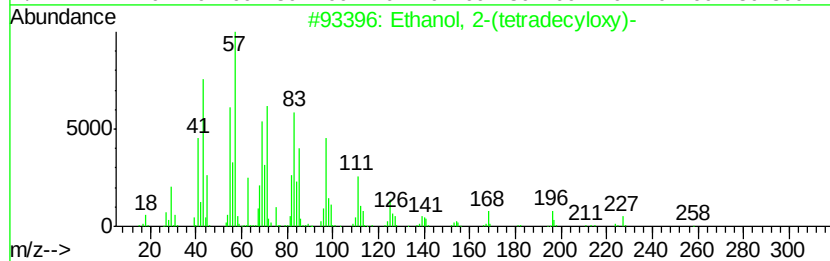
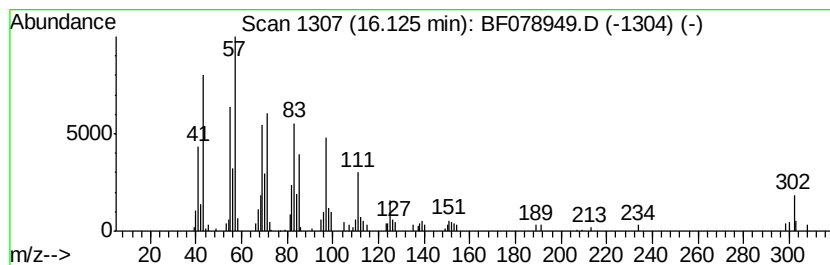
Instrument :
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ClientSampleId :
SB-49D

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF043015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Ethanol, 2-(tetradecyloxy)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.13	4.79 ng	199637	Chrysene-d12	16.25
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Ethanol, 2-(tetradecyloxy)-	258 C16H34O2	002136-70-1 87
2		Pentafluoropropionic acid, hepta...	402 C20H35F5O2	1000283-04-2 81
3		Heptafluorobutanoic acid, heptad...	452 C21H35F7O2	1000282-97-3 81
4		2-Ethyl-1-dodecanol	214 C14H30O	019780-33-7 74
5		Cyclopentane, (4-octyldodecyl)-	350 C25H50	005638-09-5 74



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050515\
Data File : BF078949.D
Acq On : 5 May 2015 19:23
Operator : TP/IZ
Sample : G2044-18
Misc :
ALS Vial : 21 Sample Multiplier: 1

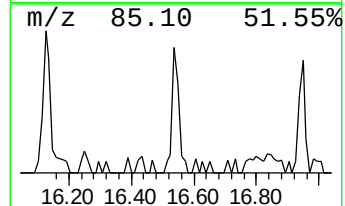
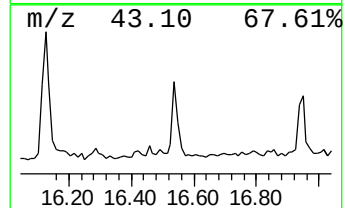
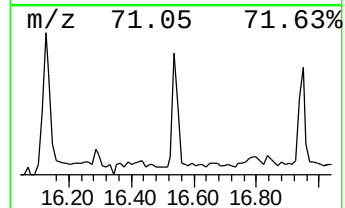
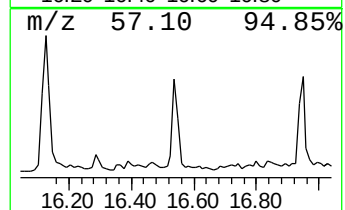
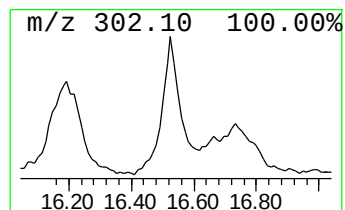
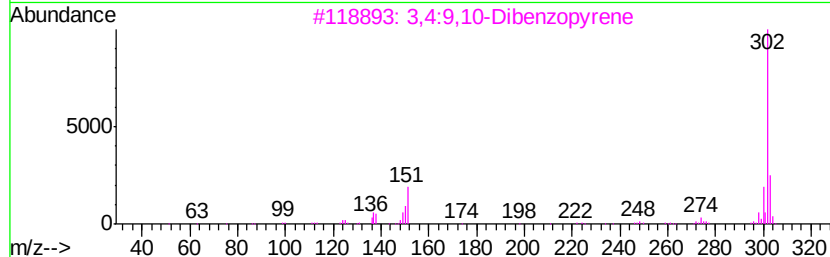
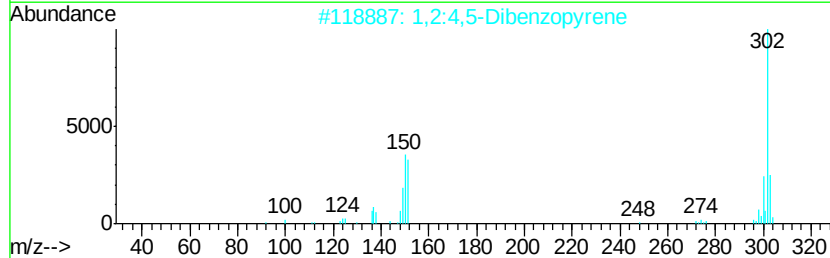
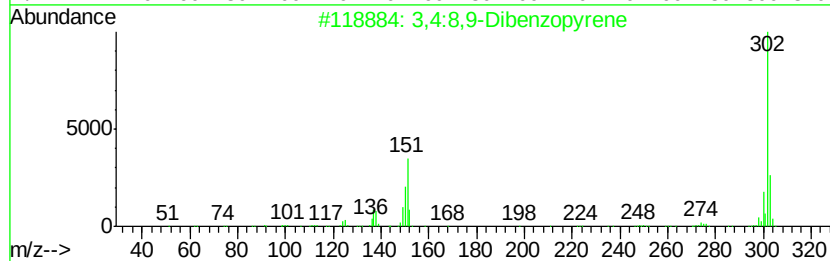
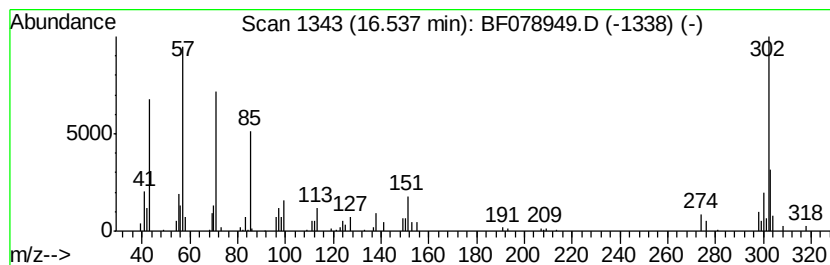
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 3,4:8,9-Dibenzopyrene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.54	3.32 ng	138199	Chrysene-d12	16.25	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,4:8,9-Dibenzopyrene	302	C24H14	000189-64-0	72
2	1,2:4,5-Dibenzopyrene	302	C24H14	000192-65-4	64
3	3,4:9,10-Dibenzopyrene	302	C24H14	000189-55-9	64
4	Nonadecane, 1-chloro-	302	C19H39Cl	062016-76-6	59
5	Dibenz(a,e)aceanthrylene	302	C24H14	005385-75-1	50



Data Path : Z:\HPCHEM1\BNA F\DATA\BF050515\
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Sample : G2044-18
Misc :
ALS Vial : 21 Sample Multiplier: 1

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ClientSampleId :
SB-49D

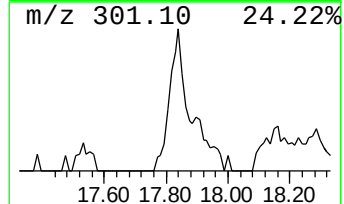
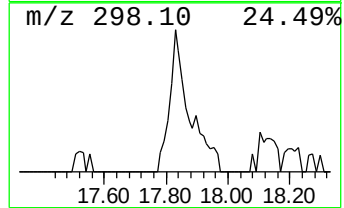
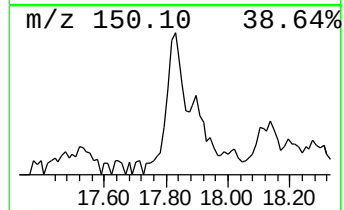
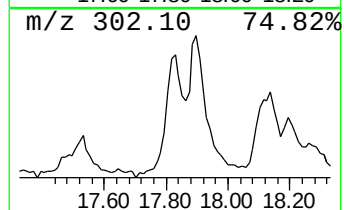
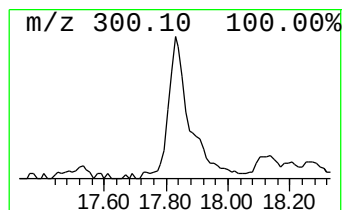
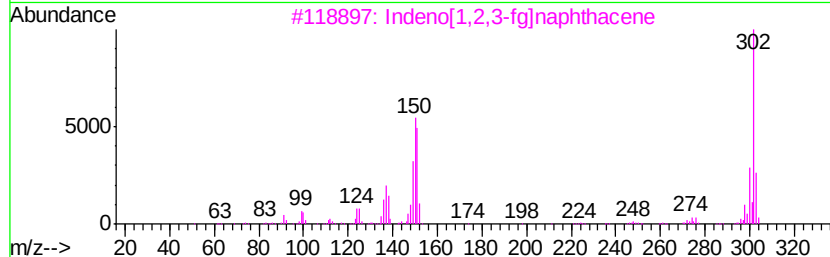
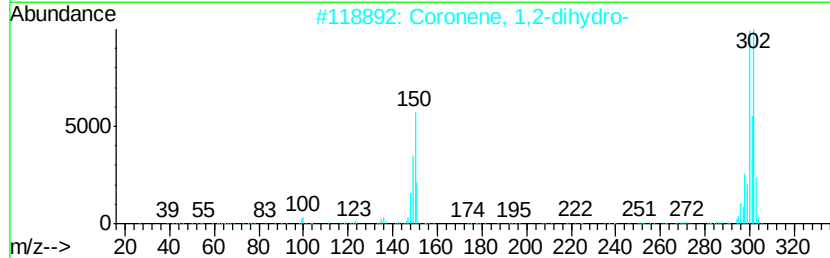
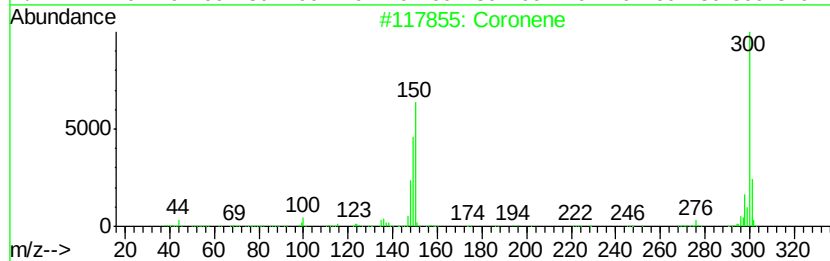
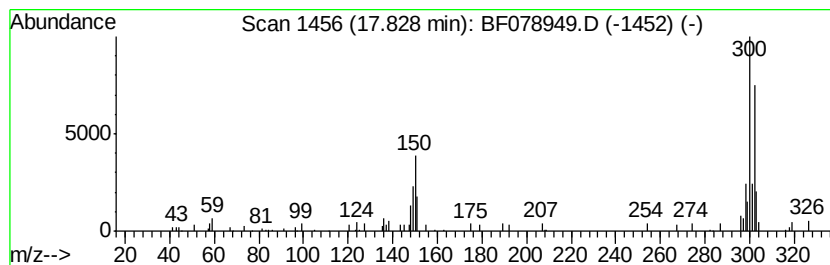
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Coronene Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.83	2.76 ng	120062	Perylene-d12	18.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Coronene	300	C24H12	000191-07-1	55
2		Coronene, 1,2-dihydro-	302	C24H14	107716-56-3	49
3		Indeno[1,2,3-fg]naphthacene	302	C24H14	000203-11-2	43
4		1,2:3,4-Dibenzopyrene	302	C24H14	000191-30-0	43
5		4'-Bromo-flavone	300	C15H9BrO2	020525-20-6	40



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050515\
Data File : BF078949.D
Acq On : 5 May 2015 19:23
Operator : TP/IZ
Sample : G2044-18
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.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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Butane, 2-methoxy...	1.84	13.2	ng	292053	1	7.36	443930	20.0
2-Pentanone, 4-hy...	5.16	11.9	ng	263327	1	7.36	443930	20.0
unknown7.06	7.06	109.8	ng	2437370	1	7.36	443930	20.0
Cyclic octaatomic...	14.56	3.8	ng	133339	4	12.96	705487	20.0
Phenol, 4,4'-(1-m...	14.81	18.4	ng	767789	5	16.25	833416	20.0
9-Octadecenamide,...	15.59	2.9	ng	122067	5	16.25	833416	20.0
Ethanol, 2-(tetra...	16.13	4.8	ng	199637	5	16.25	833416	20.0
3,4:8,9-Dibenzopy...	16.54	3.3	ng	138199	5	16.25	833416	20.0
Coronene	17.83	2.8	ng	120062	6	18.02	868722	20.0