

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050615\
 Data File : BF078958.D
 Acq On : 6 May 2015 14:11
 Operator : TP/IZ
 Sample : G2116-07
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-46D

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	1.507	25	28	30	rVB	5533664	7112029	100.00%	24.011%
2	1.644	37	40	49	rVB	1644405	308836	4.34%	1.043%
3	1.770	49	51	54	rVV	128955	216919	3.05%	0.732%
4	1.827	54	56	60	rVV	174233	253099	3.56%	0.855%
5	1.896	60	62	96	rVB	1352790	2357848	33.15%	7.960%
6	5.153	345	347	352	rVB	78677	91919	1.29%	0.310%
7	5.644	387	390	392	rBV	1515133	1519693	21.37%	5.131%
8	6.902	497	500	502	rBV	1285993	1638452	23.04%	5.532%
9	7.050	511	513	516	rBV	1146025	1606937	22.59%	5.425%
10	7.348	536	539	541	rBV	522372	455964	6.41%	1.539%
11	7.530	553	555	558	rBV	1182485	1187904	16.70%	4.011%
12	8.033	597	599	602	rBV	959154	915921	12.88%	3.092%
13	8.925	674	677	679	rBV	671285	642310	9.03%	2.169%
14	10.274	792	795	797	rBV	1396616	1757697	24.71%	5.934%
15	11.096	865	867	870	rBV2	633322	689433	9.69%	2.328%
16	11.439	895	897	907	rVB	51082	100678	1.42%	0.340%
17	11.999	944	946	949	rVB	114764	101171	1.42%	0.342%
18	12.079	950	953	956	rBV	1301836	1256148	17.66%	4.241%
19	12.948	1026	1029	1030	rBV	774912	740228	10.41%	2.499%
20	12.971	1030	1031	1033	rVB	86761	87717	1.23%	0.296%
21	14.148	1131	1134	1136	rBV	70416	83203	1.17%	0.281%
22	14.457	1159	1161	1163	rBV	169504	158211	2.22%	0.534%
23	14.548	1165	1169	1172	rVB	87919	160286	2.25%	0.541%
24	14.731	1183	1185	1188	rBV	131554	185687	2.61%	0.627%
25	14.800	1189	1191	1198	rVB	65270	106657	1.50%	0.360%
26	14.948	1201	1204	1206	rBV	1455250	1876819	26.39%	6.336%
27	15.108	1215	1218	1220	rBV	127936	149891	2.11%	0.506%
28	16.126	1304	1307	1311	rBV	241222	404979	5.69%	1.367%
29	16.251	1315	1318	1320	rVV	784718	1080426	15.19%	3.648%
30	16.286	1320	1321	1327	rVB2	103595	160892	2.26%	0.543%
31	16.548	1340	1344	1346	rBV3	38397	77570	1.09%	0.262%
32	16.766	1360	1363	1366	rBV2	33218	82381	1.16%	0.278%
33	17.371	1413	1416	1421	rBV4	27856	81416	1.14%	0.275%
34	17.589	1431	1435	1440	rBV	82607	243954	3.43%	0.824%

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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

35	17.909	1457	1463	1467	rBV2	106510	383952	5.40%	1.296%
36	17.977	1467	1469	1473	rVV	84523	141531	1.99%	0.478%
37	18.046	1473	1475	1478	rVV	653413	875464	12.31%	2.956%
38	18.194	1485	1488	1495	rVB2	57085	166413	2.34%	0.562%
39	19.543	1604	1606	1611	rVB2	31437	73346	1.03%	0.248%
40	19.989	1643	1645	1651	rVB	36412	85471	1.20%	0.289%

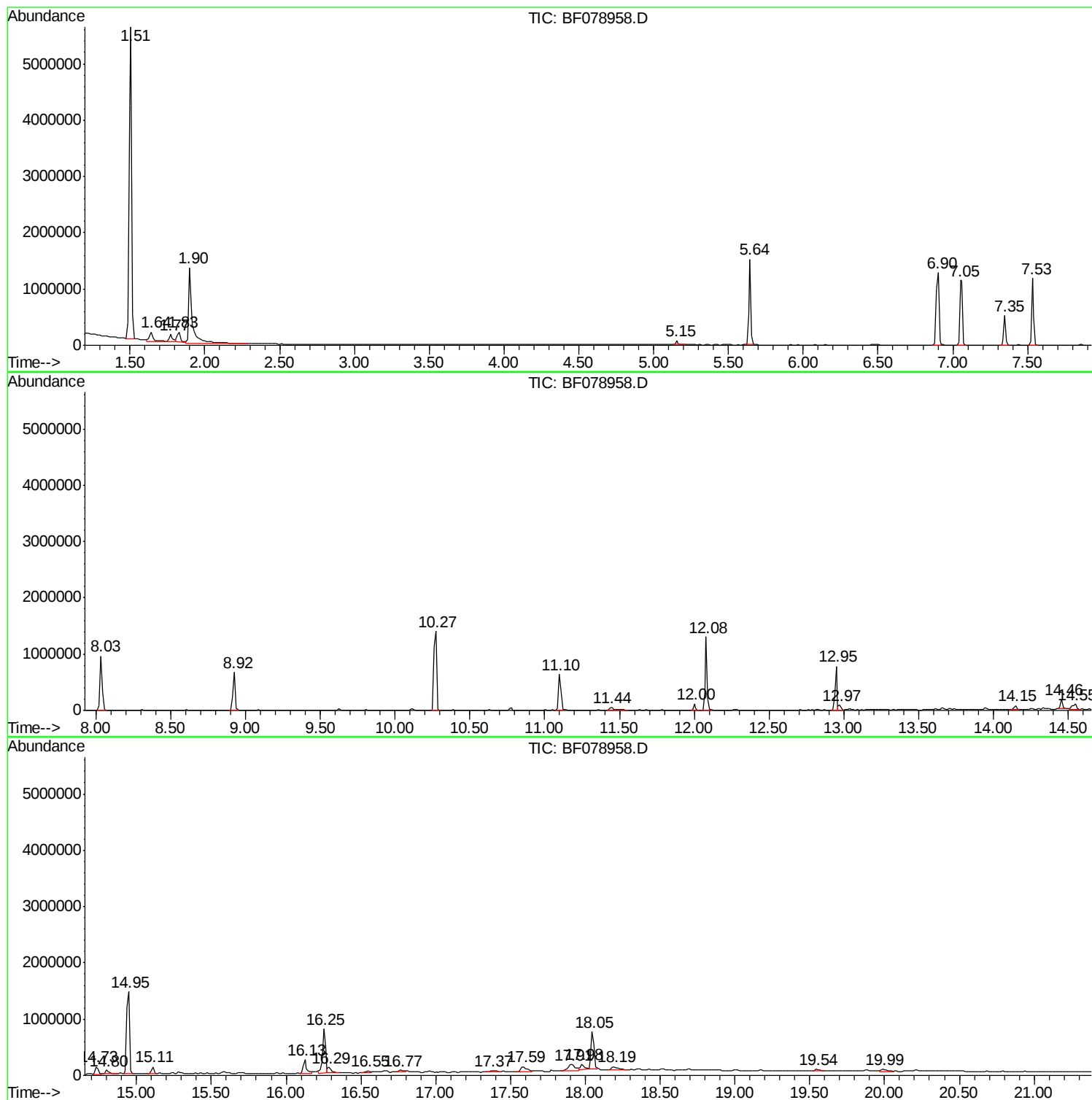
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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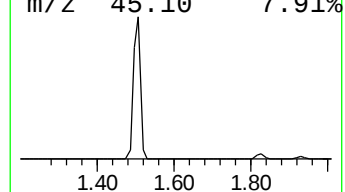
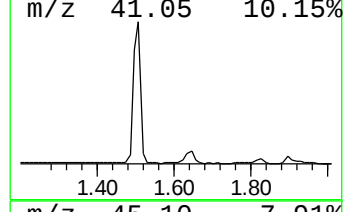
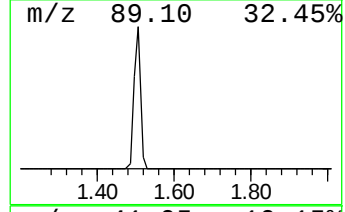
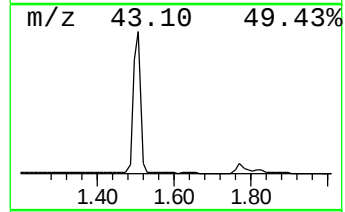
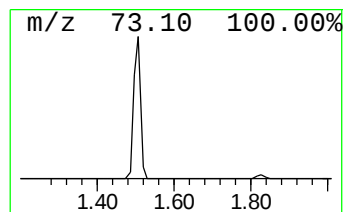
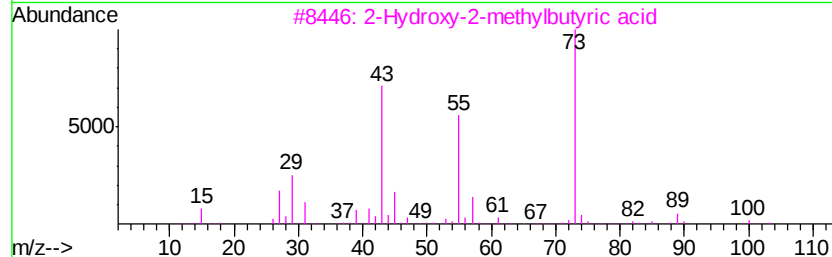
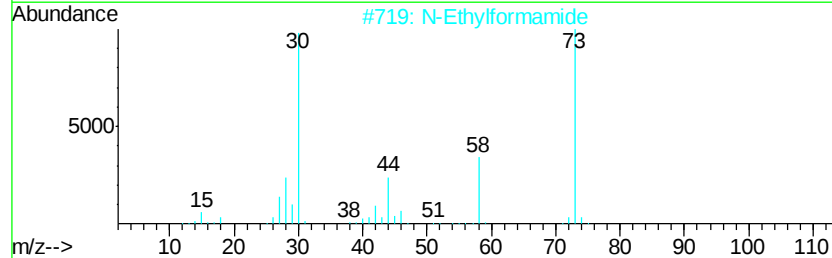
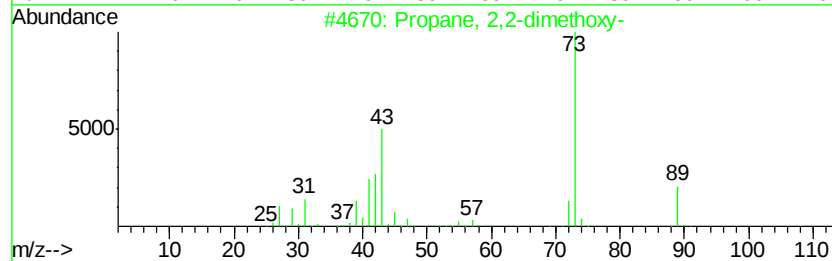
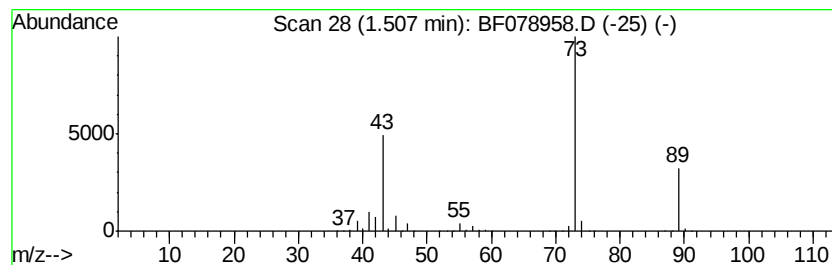
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.51	311.96 ng	7112030	1,4-Dichlorobenzene-d4	7.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	56
2		N-Ethylformamide	73	C3H7NO	000627-45-2	9
3		2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9
4		1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9



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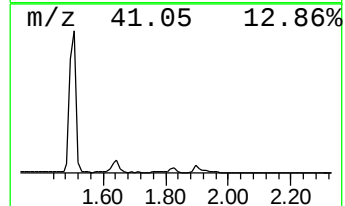
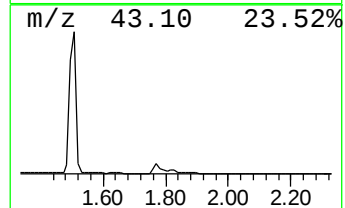
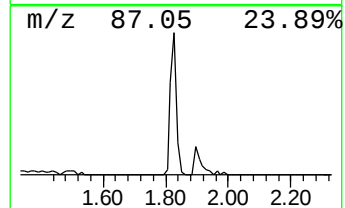
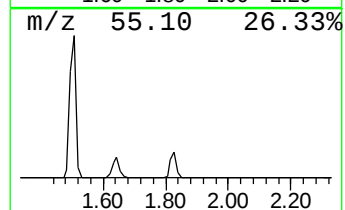
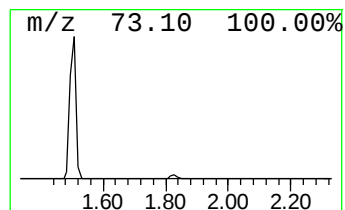
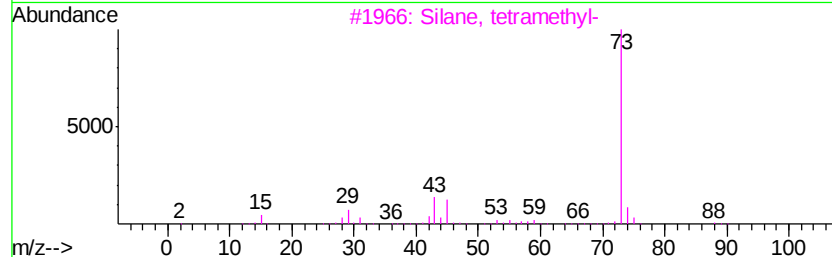
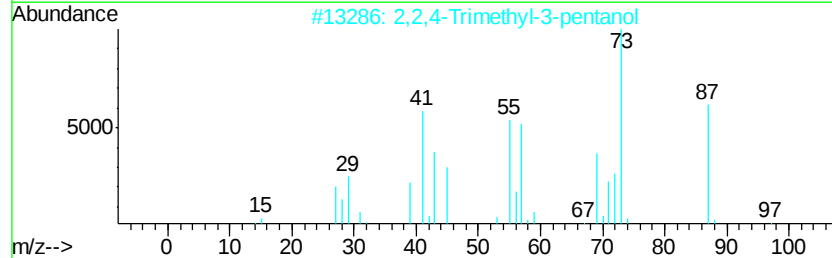
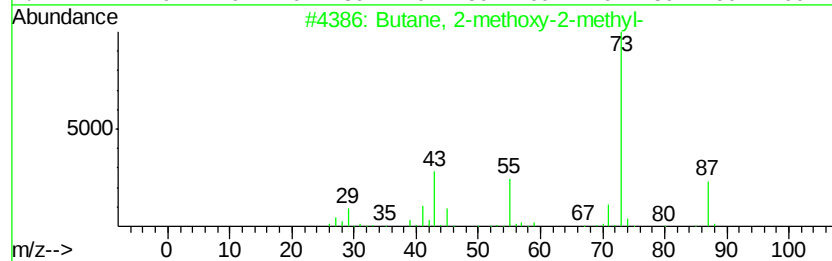
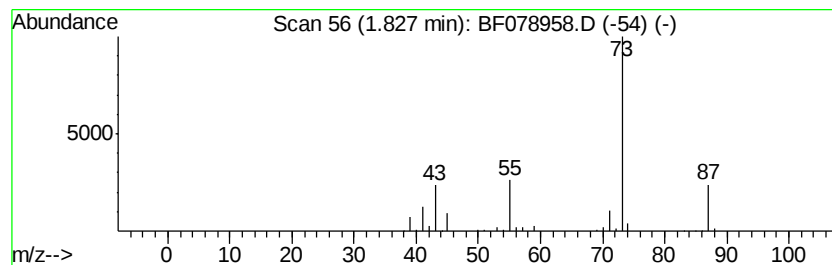
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.83	11.10 ng	253099	1,4-Dichlorobenzene-d4	7.35

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	90
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		Silane, tetramethyl-	88	C4H12Si	000075-76-3	23
4		N-Ethylformamide	73	C3H7NO	000627-45-2	9
5		Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	9



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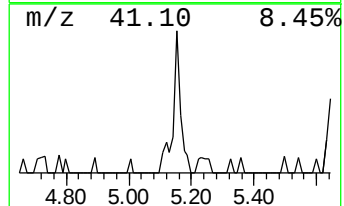
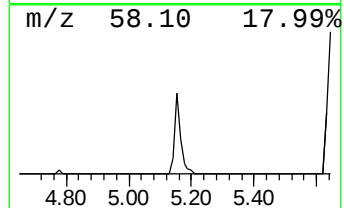
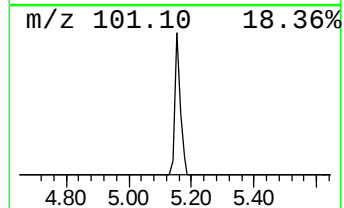
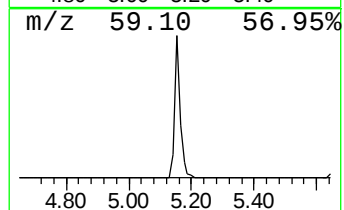
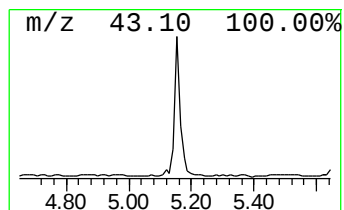
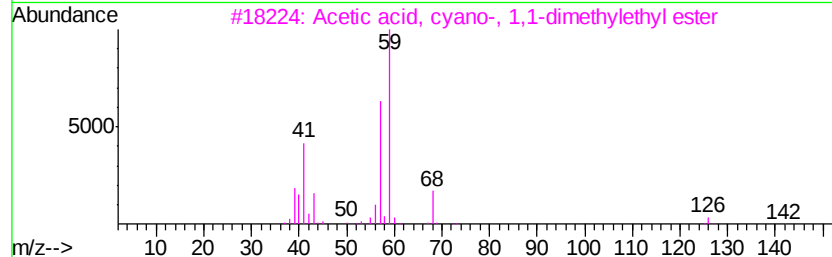
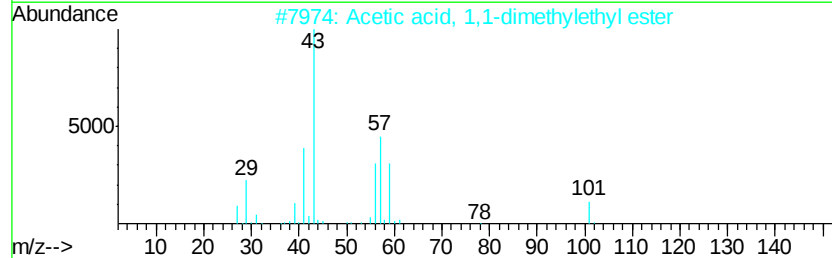
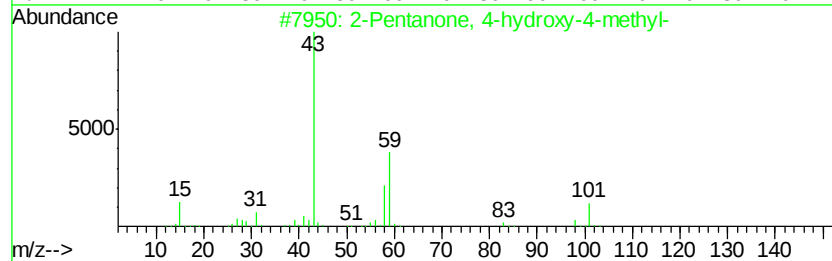
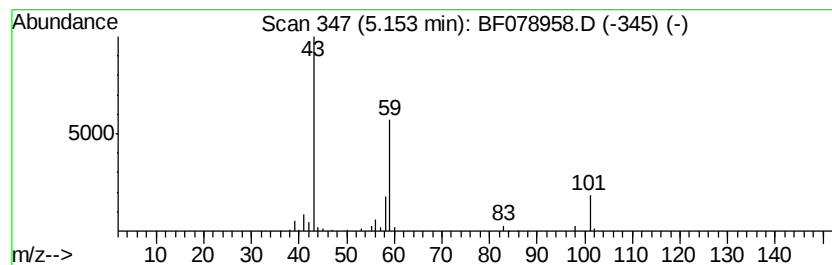
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	4.03 ng	91919	1,4-Dichlorobenzene-d4	7.35

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5			5-Hexen-2-one	98	C6H10O	000109-49-9	9



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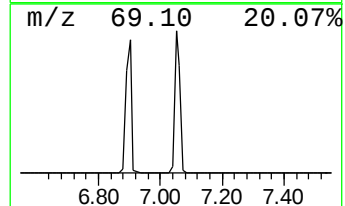
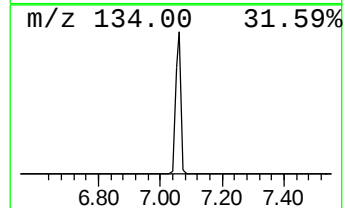
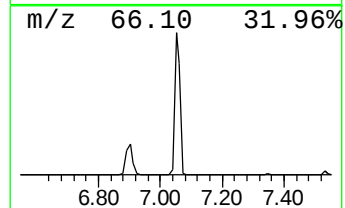
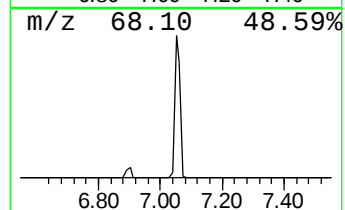
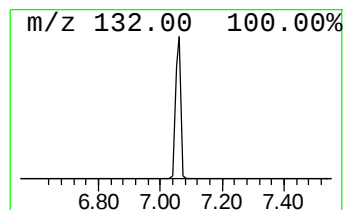
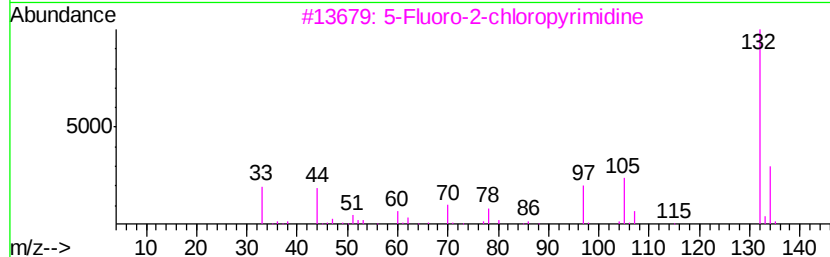
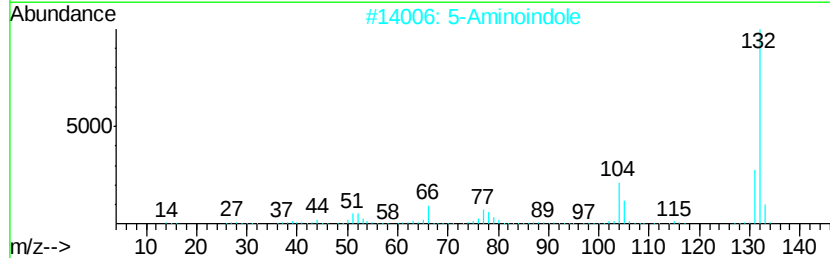
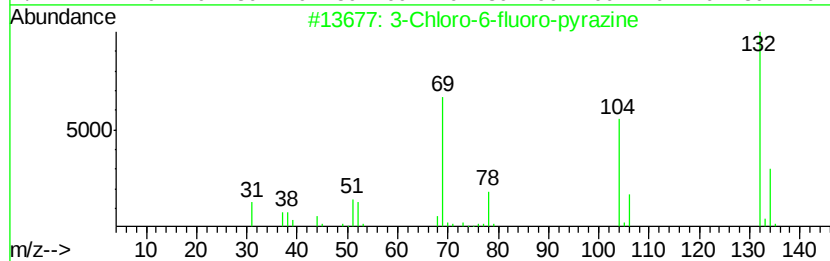
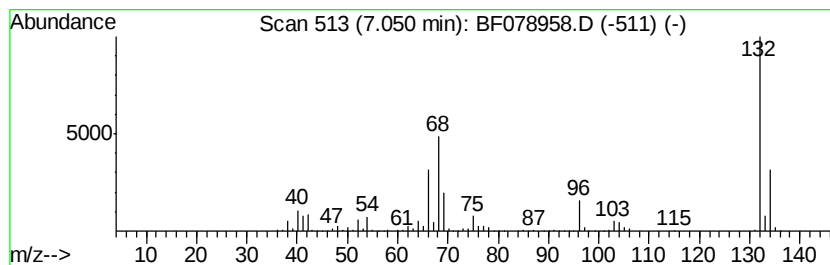
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 7 unknown7.05 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.05	70.49 ng	1606940	1,4-Dichlorobenzene-d4	7.35

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	22
3	5	Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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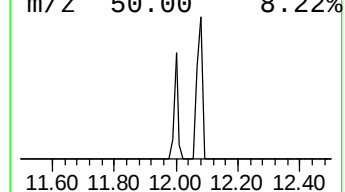
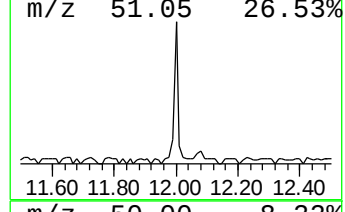
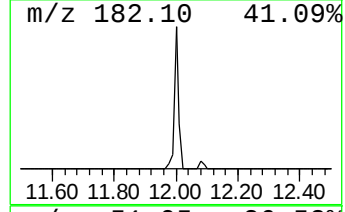
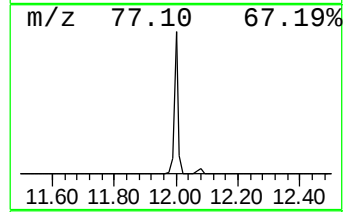
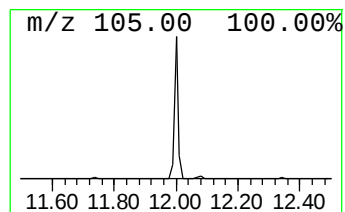
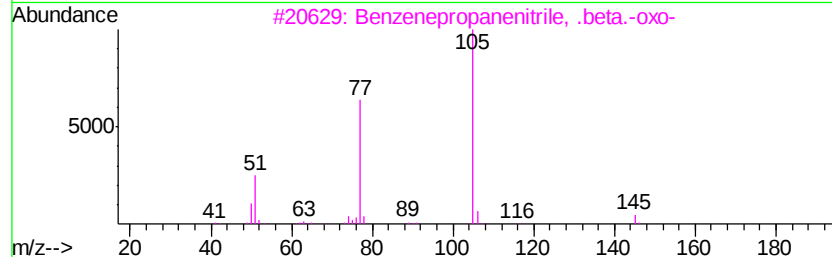
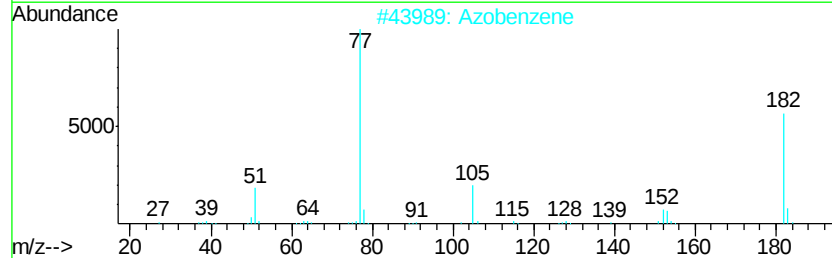
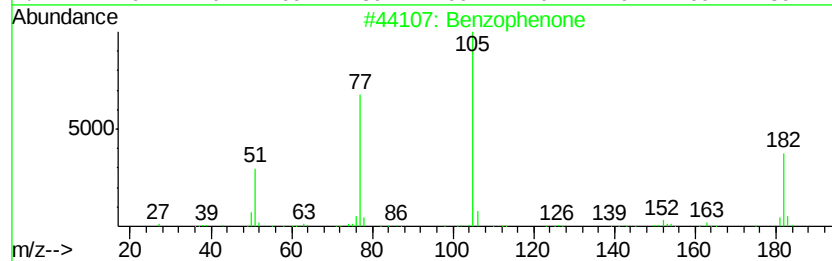
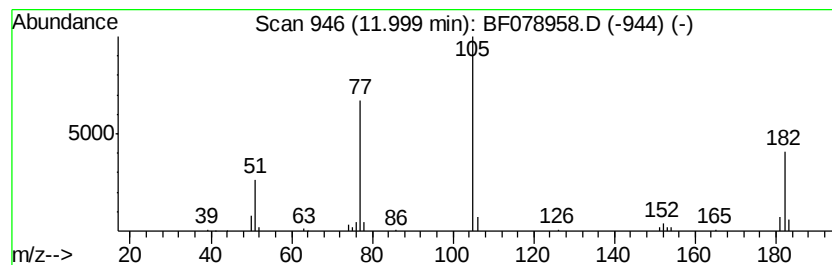
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Benzophenone Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD		R.T.
12.00	2.93 ng	101171	Acenaphthene-d10		11.10
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Azobenzene	182	C12H10N2	000103-33-3	59
3	Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	47
4	Benzoylformic acid	150	C8H6O3	000611-73-4	47
5	Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	47



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050615\
Data File : BF078958.D
Acq On : 6 May 2015 14:11
Operator : TP/IZ
Sample : G2116-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-46D

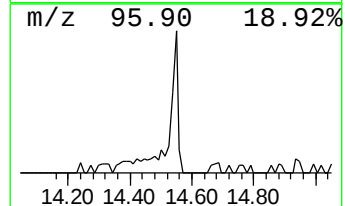
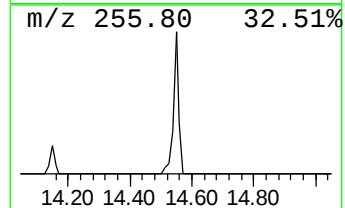
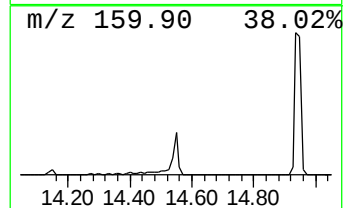
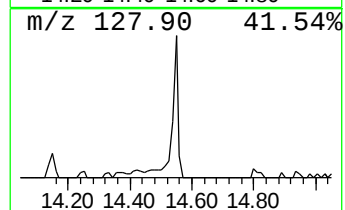
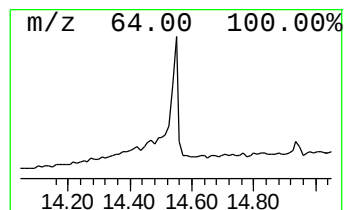
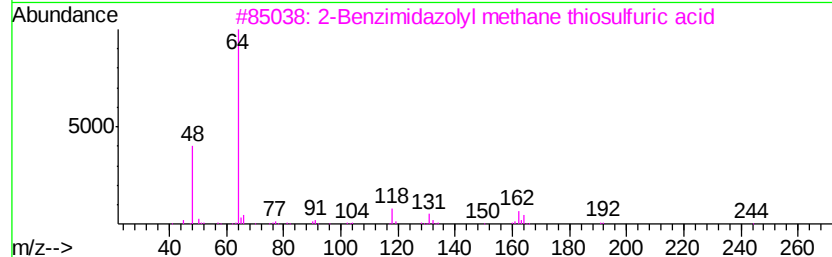
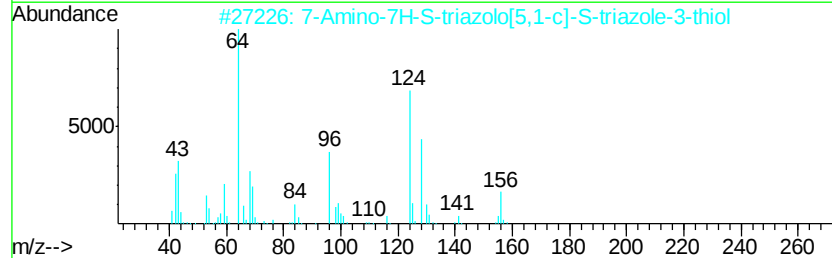
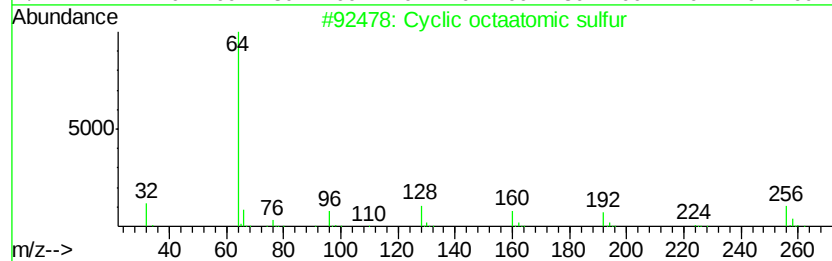
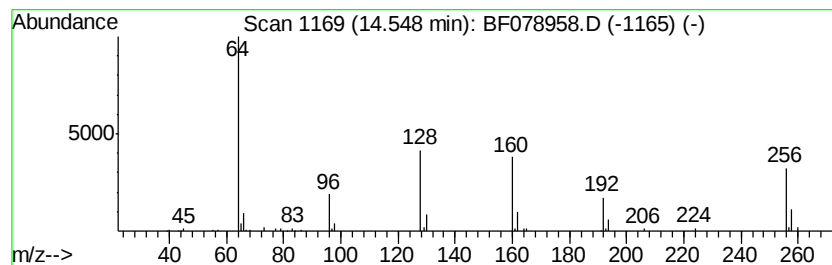
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Cyclic octaatomic sulfur Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.55	4.33 ng	160286	Phenanthrene-d10	12.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclic octaatomic sulfur	256	S8	010544-50-0	94
2		7-Amino-7H-S-triazolo[5,1-c]-S-t...	156	C3H4N6S	013728-28-4	39
3		2-Benzimidazolyl methane thiosul...	244	C8H8N2O3S2	1000256-39-2	38
4		Methanethiol, N-(p-methoxyphenet...	304	C11H16N2O4S2	040283-94-1	9
5		Dihydropyrimidine-2-methyl thios...	208	C5H8N2O3S2	1000256-28-8	9



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Acq On : 6 May 2015 14:11
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Sample : G2116-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-46D

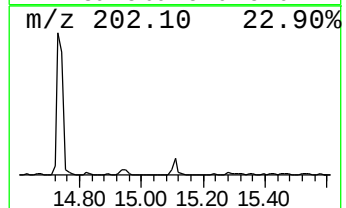
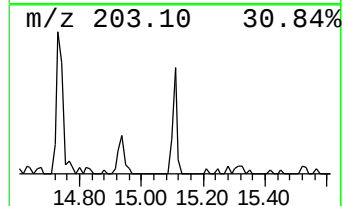
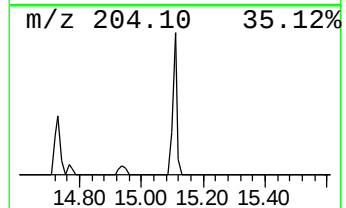
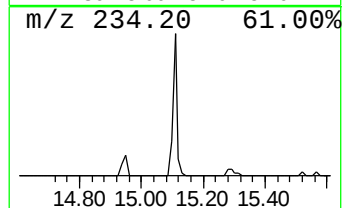
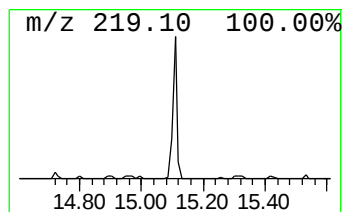
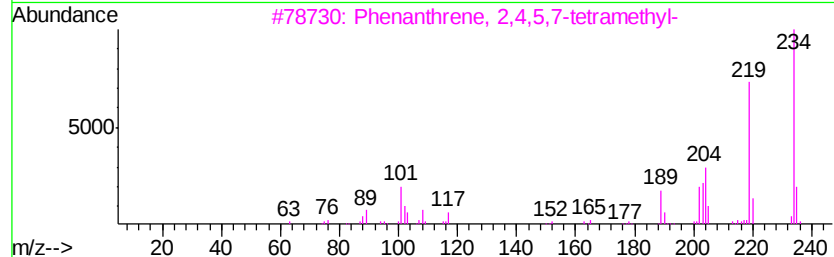
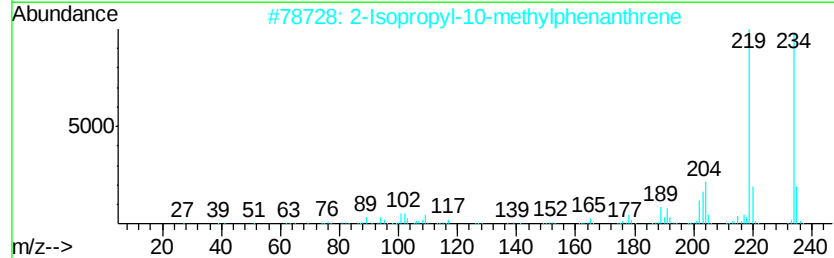
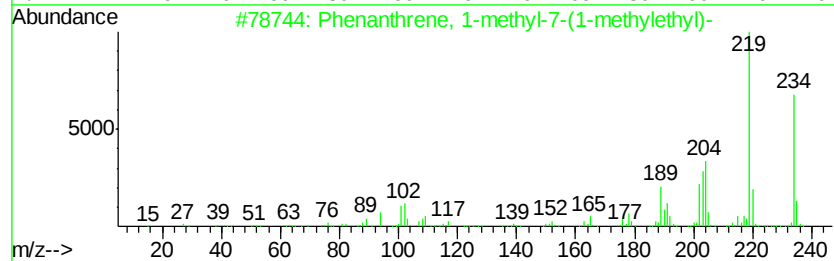
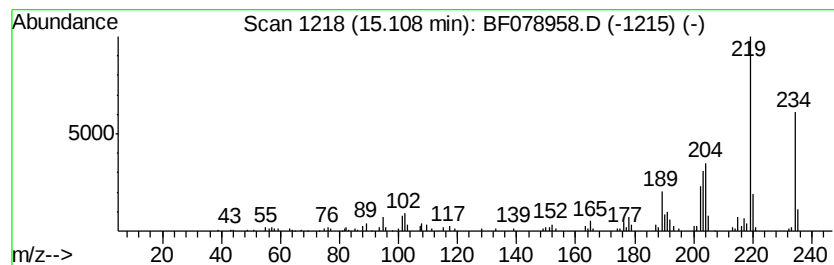
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Phenanthrene, 1-methyl-7-(1... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.11	2.77 ng	149891	Chrysene-d12	16.25

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenanthrene, 1-methyl-7-(1-meth...	234	C18H18	000483-65-8	99
2			2-Isopropyl-10-methylphenanthrene	234	C18H18	066552-97-4	94
3			Phenanthrene, 2,4,5,7-tetramethyl-	234	C18H18	007396-38-5	62
4			1-(10-Methylanthracen-9-yl)ethanone	234	C17H14O	036778-18-4	58
5			Phenanthrene, 3,4,5,6-tetramethyl-	234	C18H18	007343-06-8	53



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050615\
Data File : BF078958.D
Acq On : 6 May 2015 14:11
Operator : TP/IZ
Sample : G2116-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

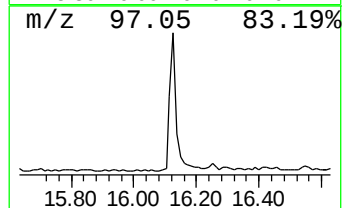
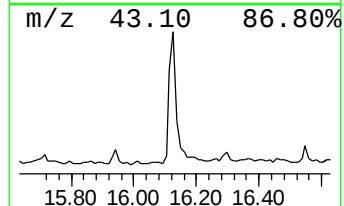
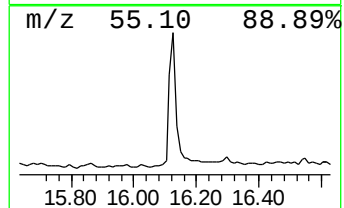
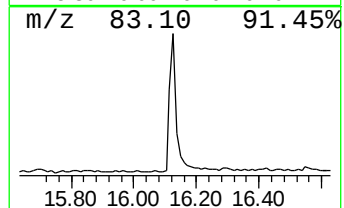
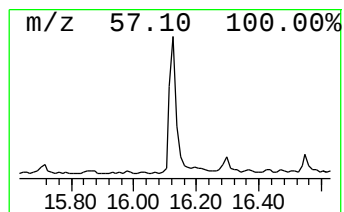
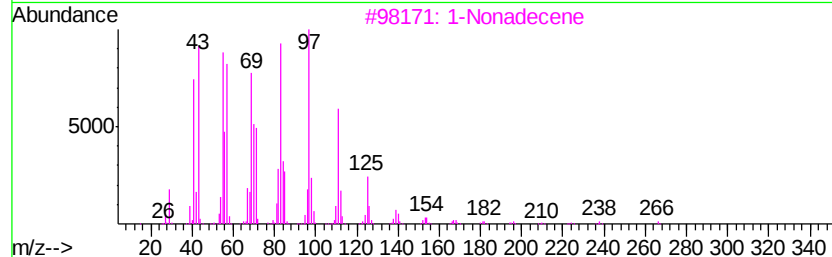
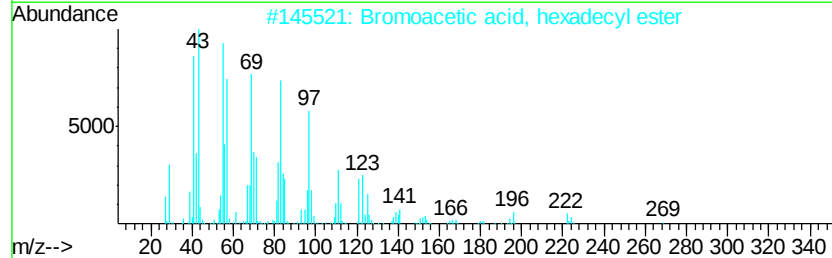
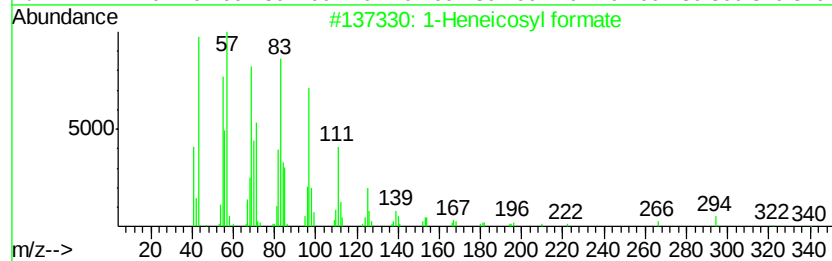
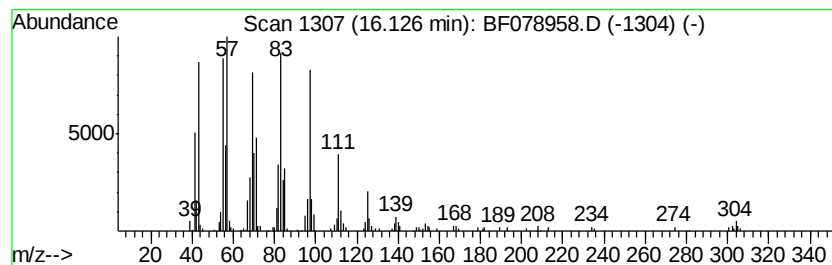
Instrument :
BNA_F
ClientSampleId :
SB-46D

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 14 1-Heneicosyl formate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.		
16.13	7.50 ng	404979	Chrysene-d12	16.25		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heneicosyl formate	340	C22H44O2	077899-03-7	95
2		Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	94
3		1-Nonadecene	266	C19H38	018435-45-5	91
4		Trifluoroacetic acid, n-octadecyl ...	366	C20H37F3O2	079392-43-1	91
5		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91



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Data File : BF078958.D
Acq On : 6 May 2015 14:11
Operator : TP/IZ
Sample : G2116-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-46D

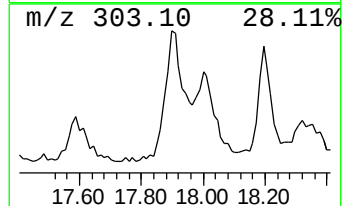
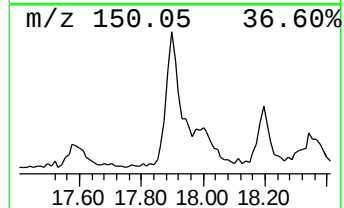
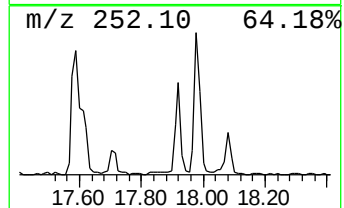
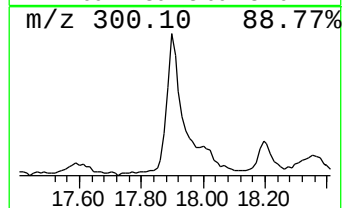
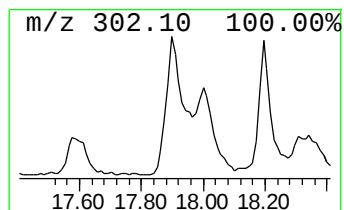
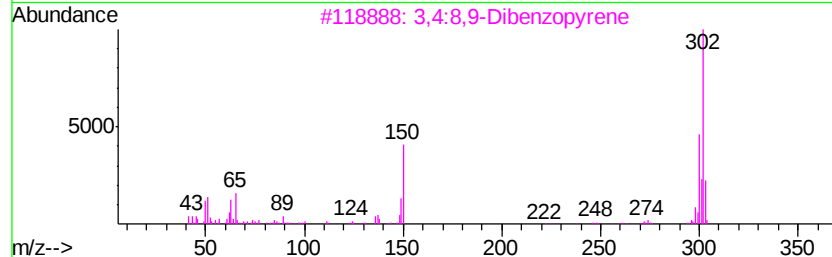
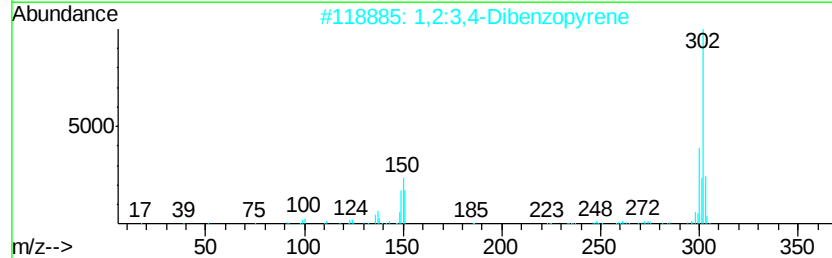
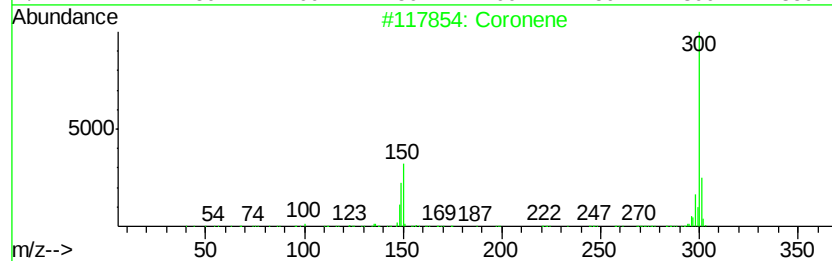
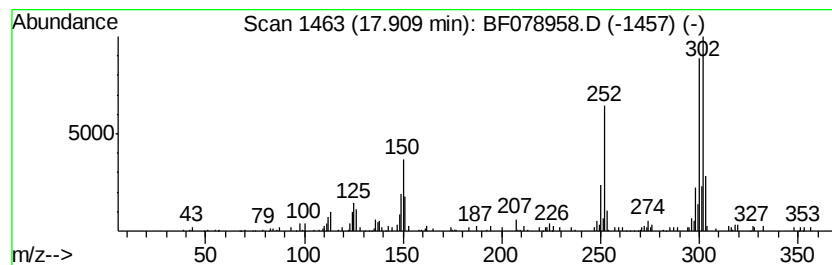
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Coronene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.91	8.77 ng	383952	Perylene-d12	18.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Coronene	300	C24H12	000191-07-1	89
2		1,2:3,4-Dibenzopyrene	302	C24H14	000191-30-0	64
3		3,4:8,9-Dibenzopyrene	302	C24H14	000189-64-0	46
4		Indeno[1,2,3-f]naphthacene	302	C24H14	000203-11-2	46
5		4'-Bromo-flavone	300	C15H9BrO2	020525-20-6	38



Data Path : Z:\HPCHEM1\BNA F\DATA\BF050615\
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Misc :
ALS Vial : 8 Sample Multiplier: 1

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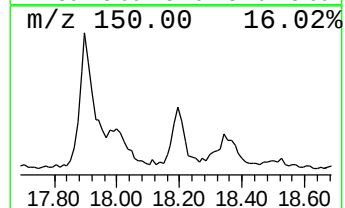
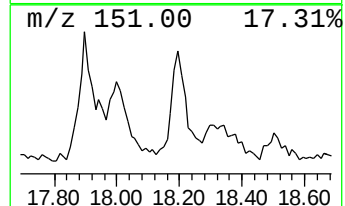
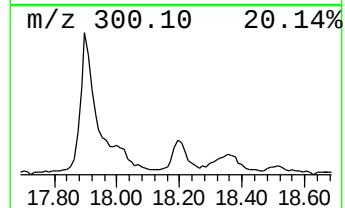
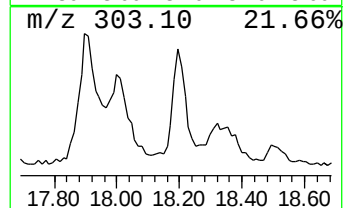
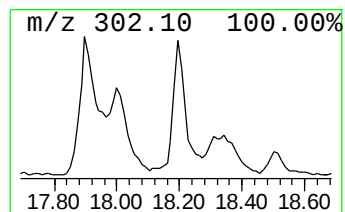
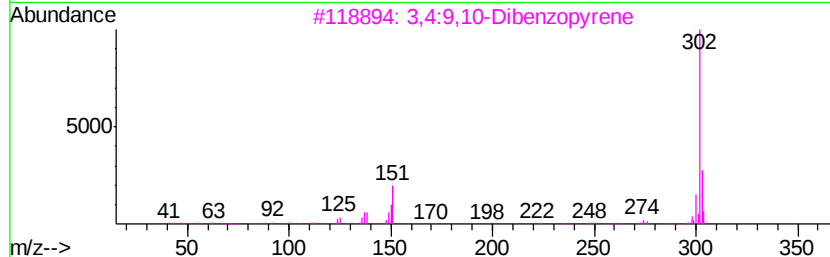
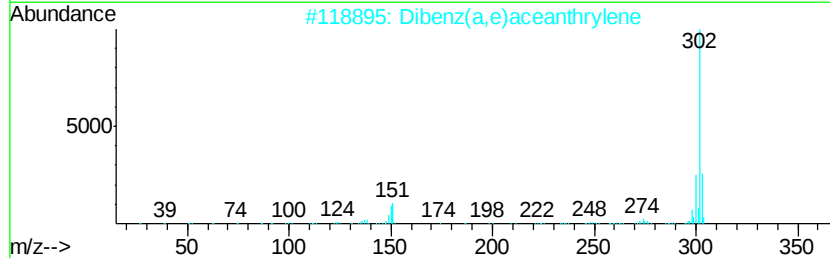
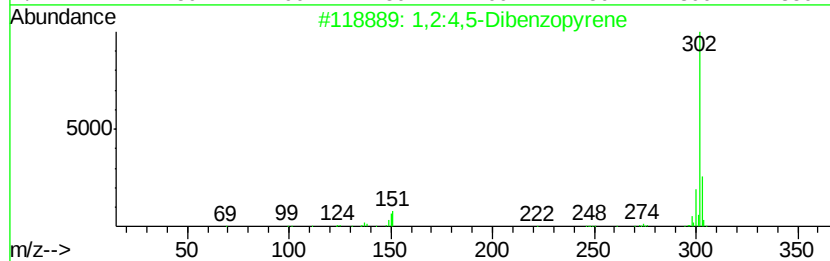
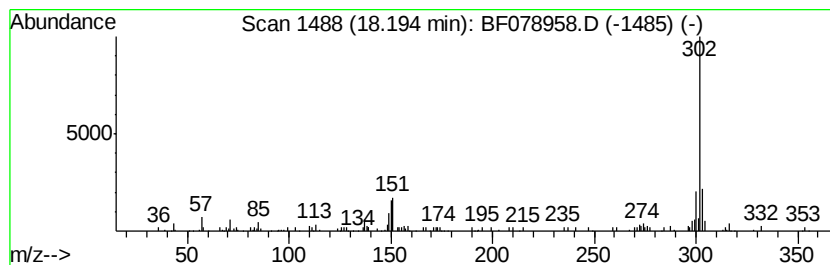
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 1,2:4,5-Dibenzopyrene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.19	3.80 ng	166413	Perylene-d12	18.05

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2:4,5-Dibenzopyrene	302	C24H14	000192-65-4	96
2			Dibenz(a,e)aceanthrylene	302	C24H14	005385-75-1	95
3			3,4:9,10-Dibenzopyrene	302	C24H14	000189-55-9	91
4			3,4:8,9-Dibenzopyrene	302	C24H14	000189-64-0	90
5			Indeno[1,2,3-fg]naphthacene	302	C24H14	000203-11-2	89



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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
Propane, 2,2-dime...	1.51	312.0	ng	7112030	1	7.35	455964	20.0
Butane, 2-methoxy...	1.83	11.1	ng	253099	1	7.35	455964	20.0
2-Pentanone, 4-hy...	5.15	4.0	ng	91919	1	7.35	455964	20.0
unknown7.05	7.05	70.5	ng	1606940	1	7.35	455964	20.0
Benzophenone	12.00	2.9	ng	101171	3	11.10	689433	20.0
unknown14.15	14.15	2.3	ng	83203	4	12.95	740228	20.0
Cyclic octaatomic...	14.55	4.3	ng	160286	4	12.95	740228	20.0
Phenanthrene, 1-m...	15.11	2.8	ng	149891	5	16.25	1080430	20.0
1-Heneicosyl formate	16.13	7.5	ng	404979	5	16.25	1080430	20.0
Coronene	17.91	8.8	ng	383952	6	18.05	875464	20.0
1,2:4,5-Dibenzopy...	18.19	3.8	ng	166413	6	18.05	875464	20.0