

Data Path : Z:\HPCHEM1\BNA F\DATA\BF110515\
 Data File : BF082710.D
 Acq On : 4 Nov 2015 19:42
 Operator : UM/IZ
 Sample : G4241-04
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-16(4)

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-BF103015.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	2.201	8	10	19	rVB	100828	180550	2.49%	0.259%
2	5.059	256	260	269	rVB	2055819	3094027	42.74%	4.432%
3	5.481	293	297	299	rBV	4398843	6550069	90.48%	9.382%
4	6.499	382	386	388	rVB	5305967	5879341	81.22%	8.421%
5	6.636	395	398	400	rBV	6389336	6788410	93.77%	9.723%
6	6.864	415	418	420	rBV	1524511	1341214	18.53%	1.921%
7	7.024	429	432	434	rVB	4720621	4911966	67.85%	7.036%
8	7.425	464	467	469	rVB	3603310	3901598	53.90%	5.589%
9	8.145	528	530	533	rBV	1528942	1587066	21.92%	2.273%
10	9.105	612	614	616	rBV	137311	117120	1.62%	0.168%
11	9.230	622	625	627	rBV	6823764	6810820	94.08%	9.756%
12	9.345	633	635	637	rVB	74090	103433	1.43%	0.148%
13	9.619	656	659	661	rBV	1411873	1204313	16.64%	1.725%
14	9.905	681	684	686	rBV	2245113	2092839	28.91%	2.998%
15	10.316	706	720	722	rBV2	217423	864446	11.94%	1.238%
16	10.419	728	729	734	rVB3	41917	74333	1.03%	0.106%
17	10.693	749	753	755	rBV	5217186	5532738	76.43%	7.925%
18	10.819	762	764	768	rVB	143764	168810	2.33%	0.242%
19	10.911	769	772	773	rBV2	64530	73621	1.02%	0.105%
20	11.265	801	803	805	rBV	130815	115500	1.60%	0.165%
21	11.379	811	813	816	rVB2	1794060	2025145	27.97%	2.901%
22	11.562	826	829	831	rBV2	39244	81246	1.12%	0.116%
23	11.619	832	834	836	rVV	722832	642009	8.87%	0.920%
24	11.688	838	840	843	rVB	57067	85920	1.19%	0.123%
25	11.928	858	861	863	rBV	1047612	1029096	14.22%	1.474%
26	12.179	881	883	886	rBV	84609	133665	1.85%	0.191%
27	12.442	894	906	908	rBV3	308562	1030489	14.23%	1.476%
28	12.488	908	910	912	rVV	73637	112699	1.56%	0.161%
29	12.705	927	929	936	rVB	256614	338935	4.68%	0.485%
30	12.865	941	943	947	rVV3	72552	135815	1.88%	0.195%
31	12.979	950	953	955	rVB	6617209	7239167	100.00%	10.369%
32	13.219	972	974	976	rVB2	82232	85402	1.18%	0.122%
33	13.459	993	995	998	rVB2	47867	79695	1.10%	0.114%
34	13.871	1029	1031	1041	rVB	1138314	1300357	17.96%	1.863%

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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-BF103015.M
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35	14.019	1041	1044	1046	rBV	2344872	2117482	29.25%	3.033%
36	14.511	1085	1087	1090	rBV	112206	144867	2.00%	0.208%
37	14.820	1111	1114	1117	rBV2	39351	80858	1.12%	0.116%
38	15.460	1166	1170	1172	rBV	976365	1443932	19.95%	2.068%
39	15.974	1213	1215	1220	rBV	129791	235106	3.25%	0.337%
40	17.071	1308	1311	1317	rBV7	24028	80447	1.11%	0.115%

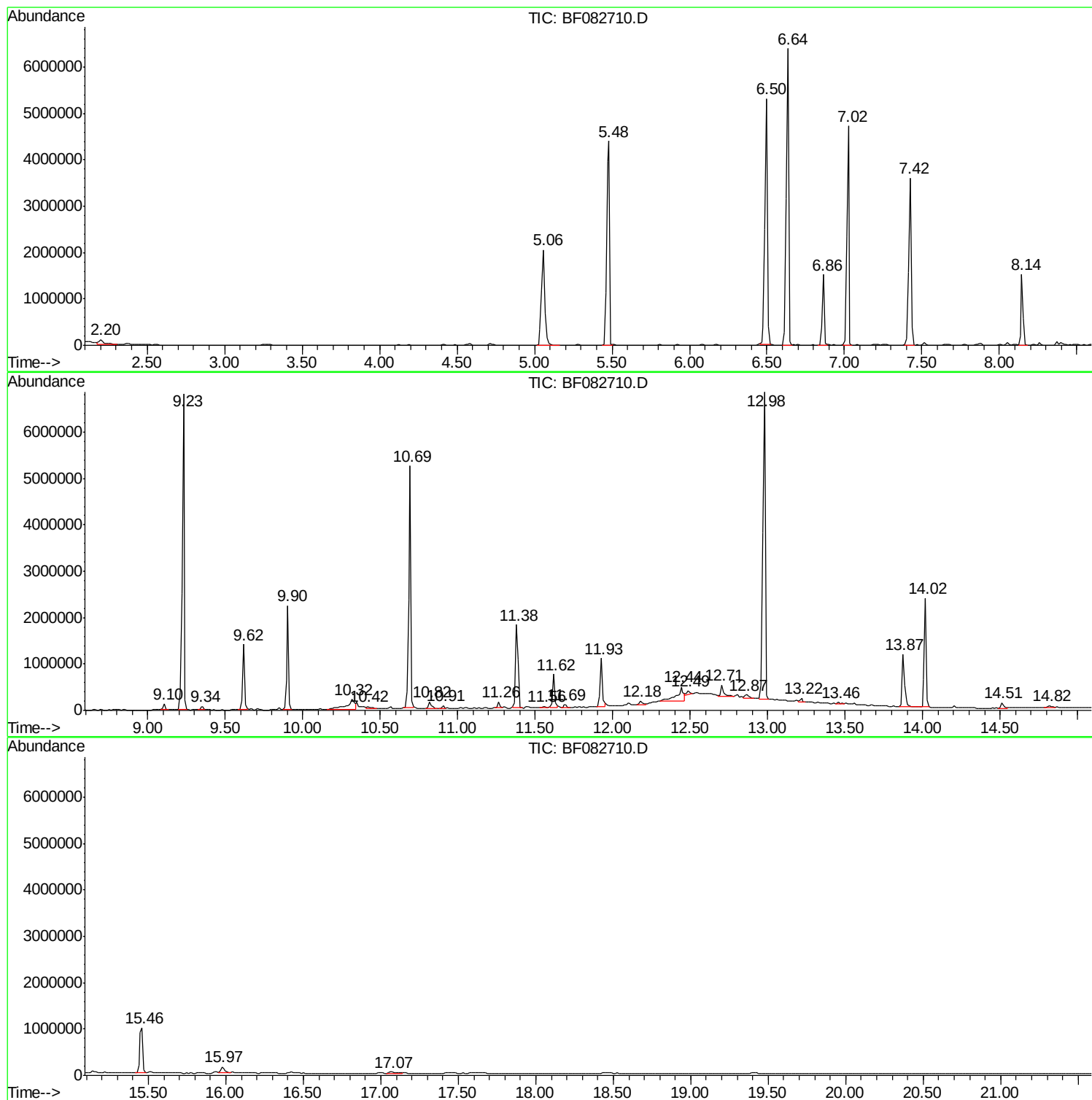
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF103015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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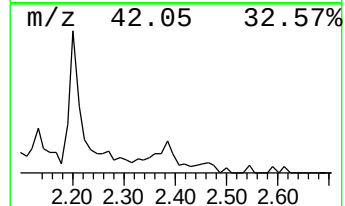
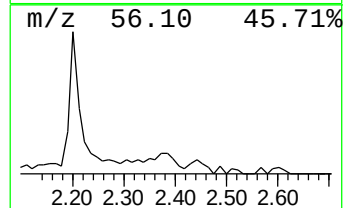
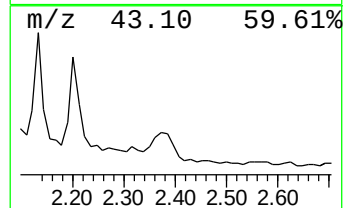
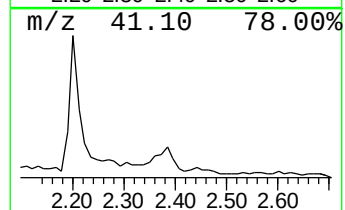
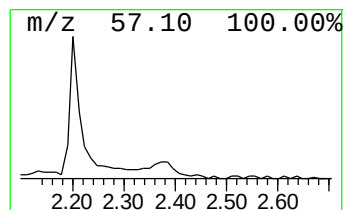
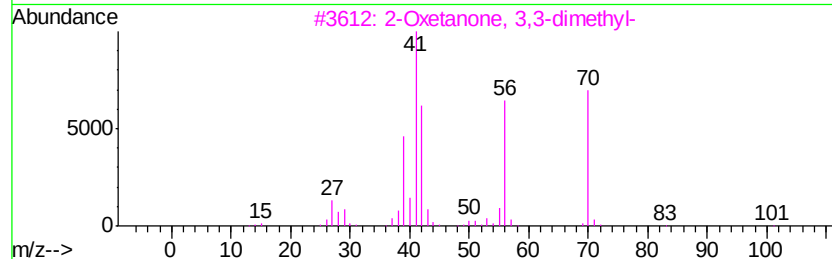
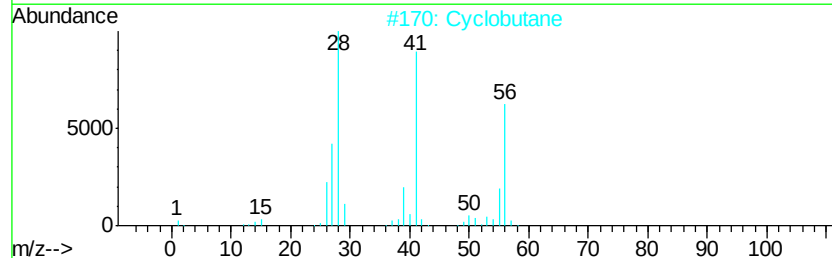
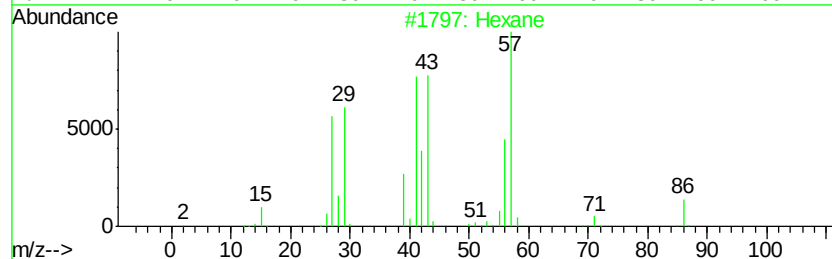
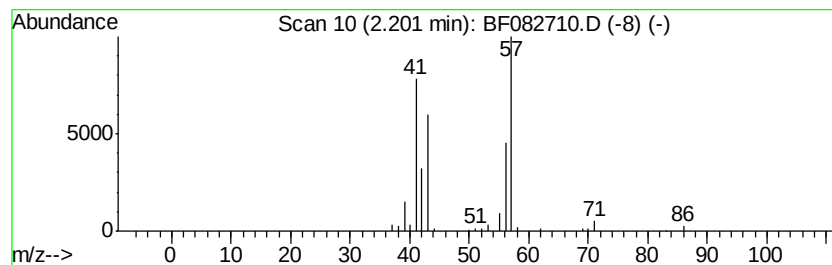
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF103015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Hexane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.20	2.69 ng	180550	1,4-Dichlorobenzene-d4	6.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane			86	C6H14	000110-54-3	78
2	Cyclobutane			56	C4H8	000287-23-0	38
3	2-Oxetanone, 3,3-dimethyl-			100	C5H8O2	001955-45-9	36
4	1-Pentene, 4-methyl-			84	C6H12	000691-37-2	33
5	Pentane, 2,2,3,4-tetramethyl-			128	C9H20	001186-53-4	25



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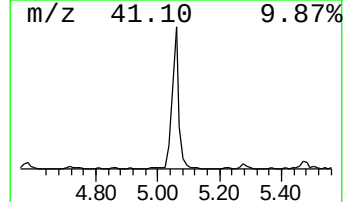
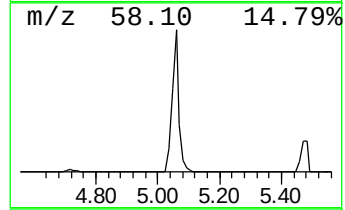
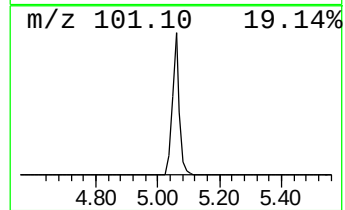
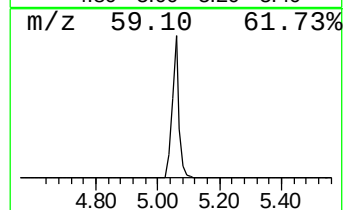
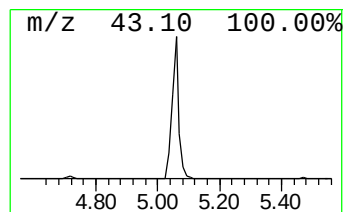
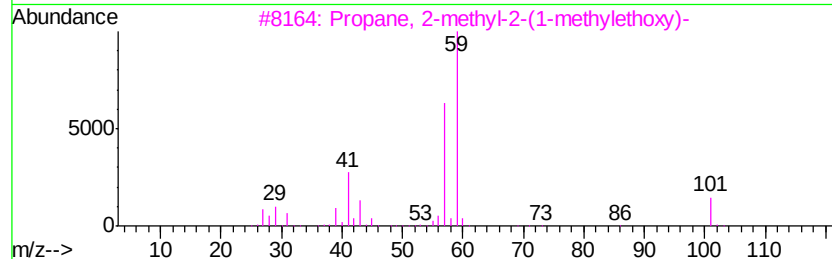
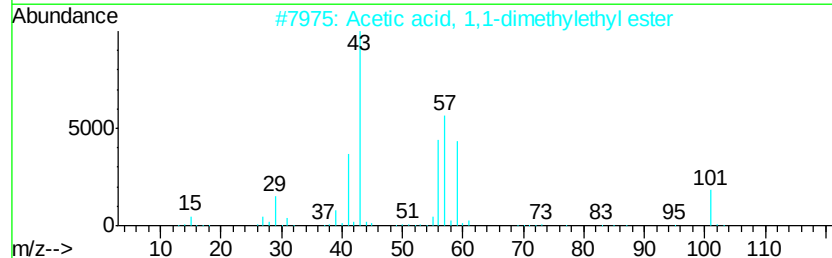
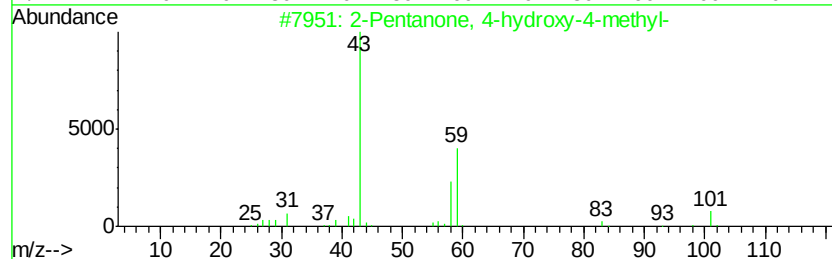
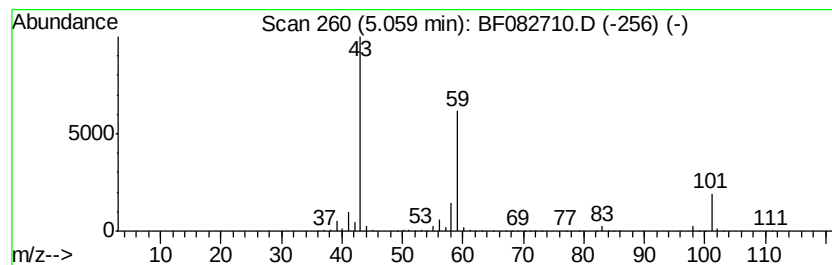
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF103015.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	46.14 ng	3094030	1,4-Dichlorobenzene-d4	6.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
4			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



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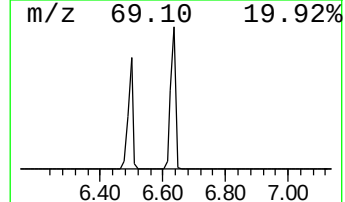
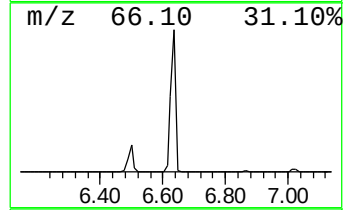
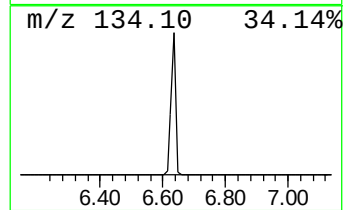
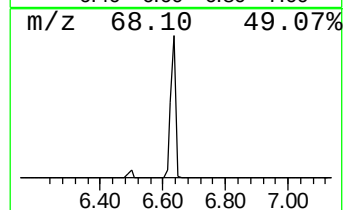
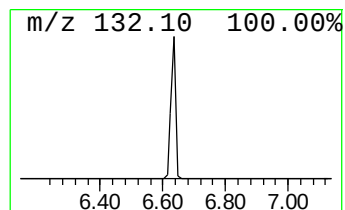
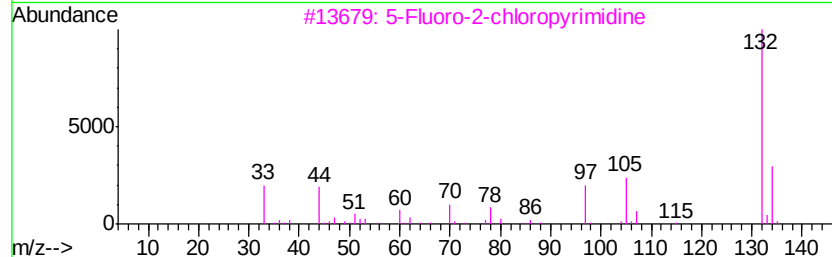
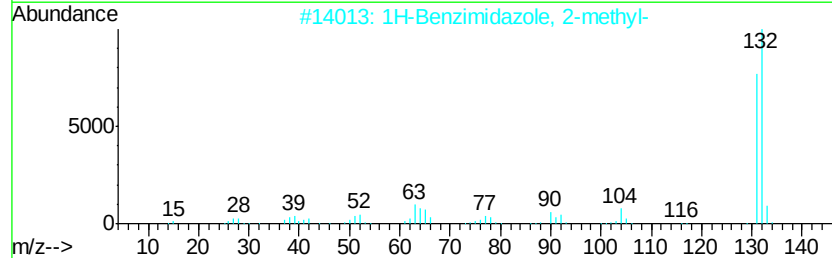
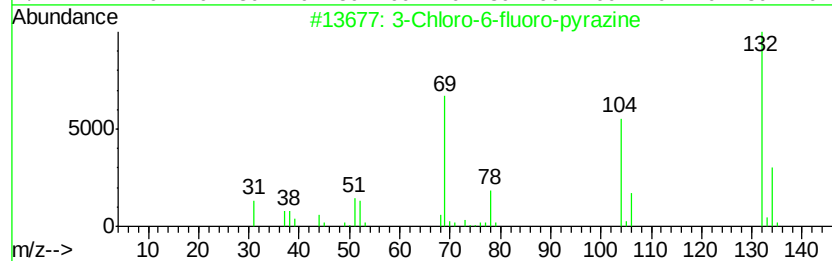
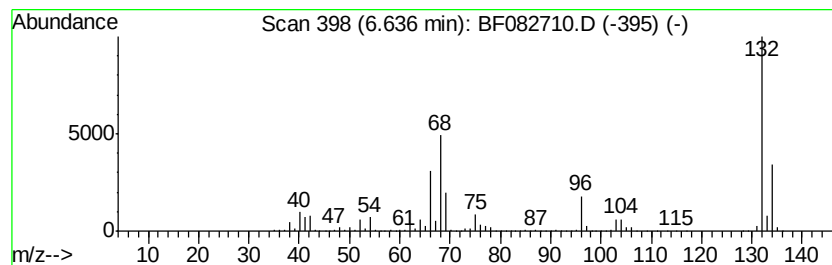
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.64 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.64	101.23 ng	6788410	1,4-Dichlorobenzene-d4	6.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine			132	C4H2ClFN2	1000146-10-7	27
2	1H-Benzimidazole, 2-methyl-			132	C8H8N2	000615-15-6	22
3	5-Fluoro-2-chloropyrimidine			132	C4H2ClFN2	062802-42-0	12
4	Tranylcypromine-propionyl			189	C12H15NO	1000123-86-3	10
5	(5-METHYL-2-PYRIDYL)ACETONITRILE			132	C8H8N2	1000241-93-9	10



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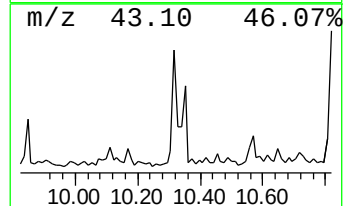
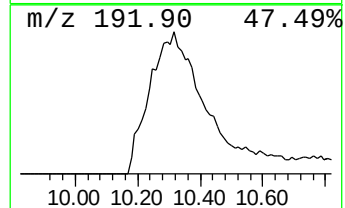
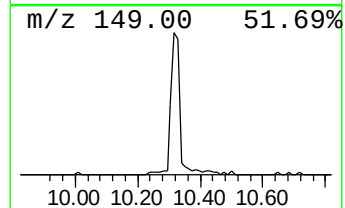
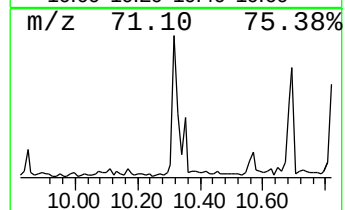
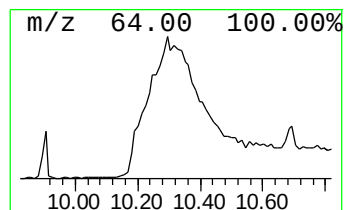
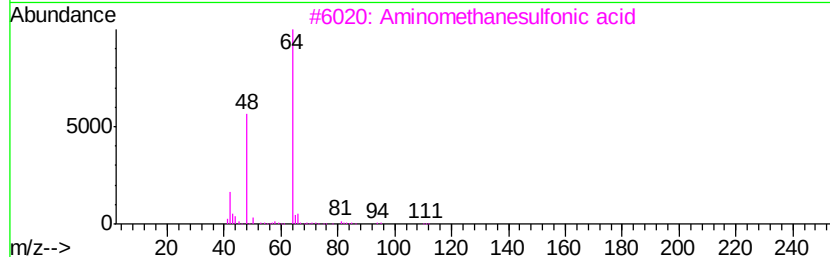
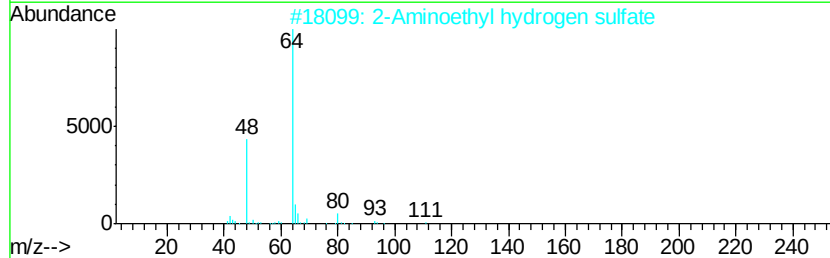
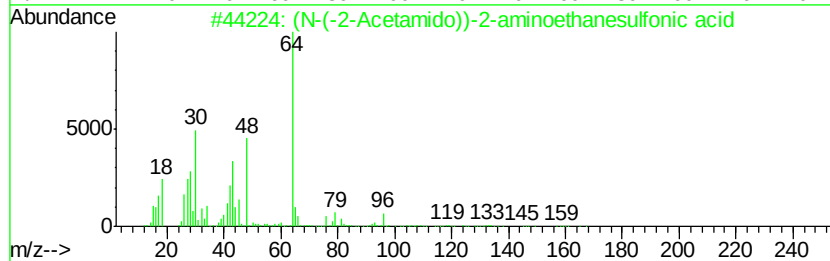
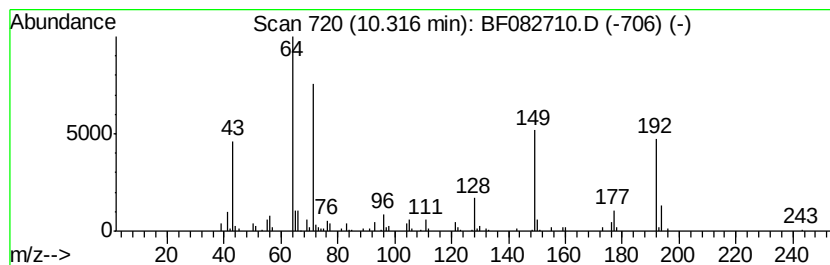
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown10.32 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.32	8.26 ng	864446	Acenaphthene-d10	9.90	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(N-(-2-Acetamido))-2-aminoethane...	182	C4H10N2O4S	007365-82-4	28
2	2-Aminoethyl hydrogen sulfate	141	C2H7N04S	000926-39-6	28
3	Aminomethanesulfonic acid	111	CH5N03S	013881-91-9	28
4	4-Methoxypyrrolo[2,3-d]pyrimidine	149	C7H7N3O	004786-76-9	10
5	Sulfur dioxide	64	O2S	007446-09-5	7



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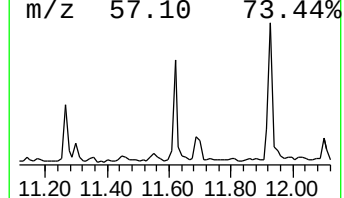
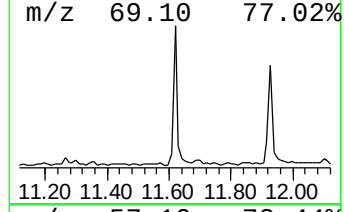
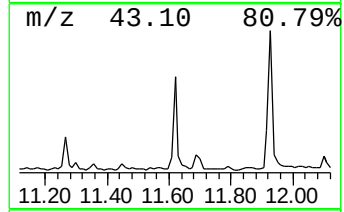
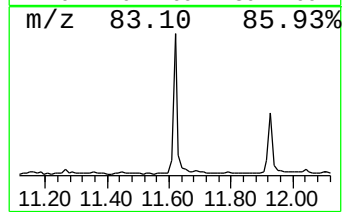
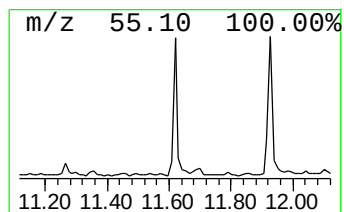
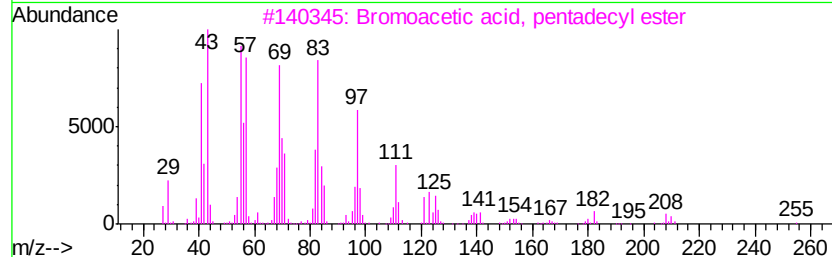
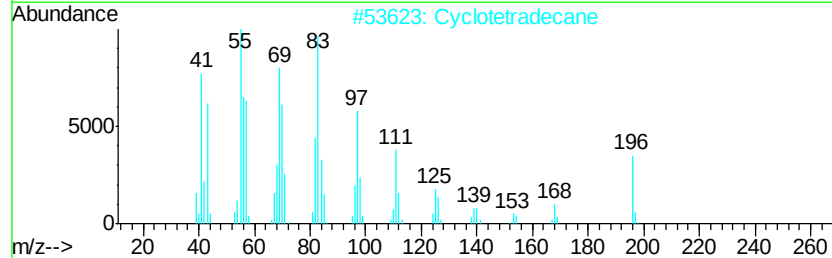
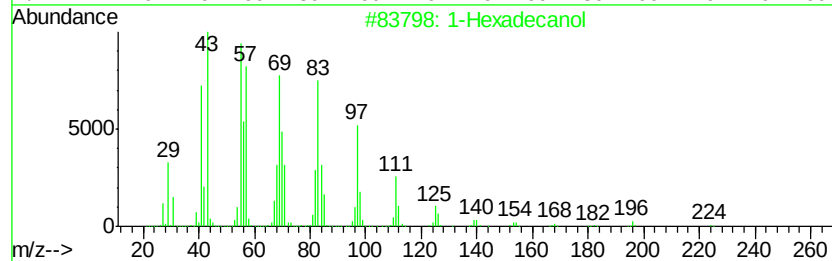
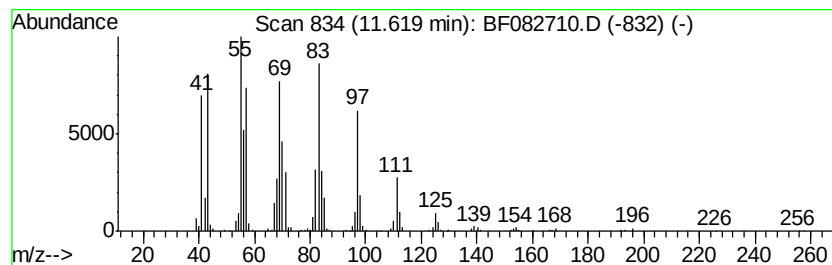
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 1-Hexadecanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.62	6.34 ng	642009	Phenanthrene-d10		11.38
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecanol	242	C16H34O	036653-82-4	94
2	Cyclotetradecane	196	C14H28	000295-17-0	94
3	Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	91
4	1-Pentadecanol	228	C15H32O	000629-76-5	91
5	1-Pentadecene	210	C15H30	013360-61-7	91



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Sample : G4241-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-16(4)

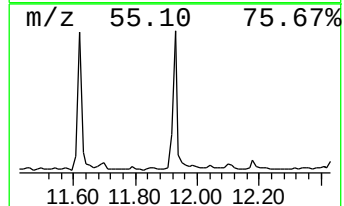
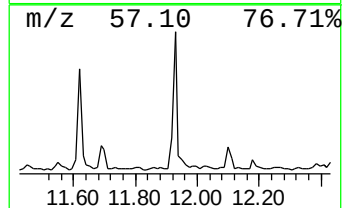
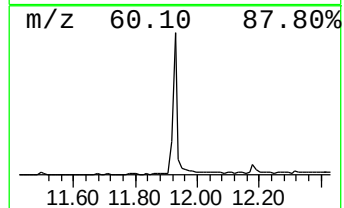
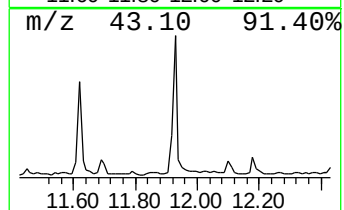
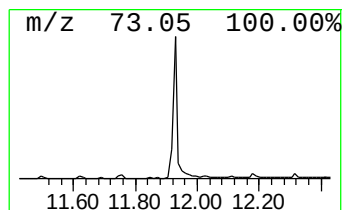
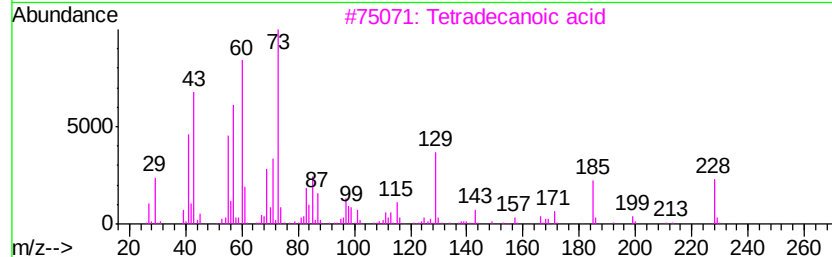
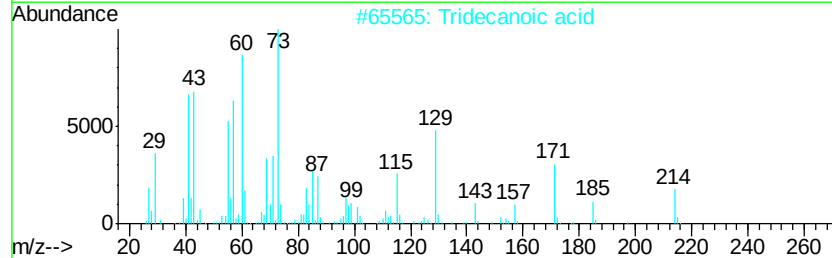
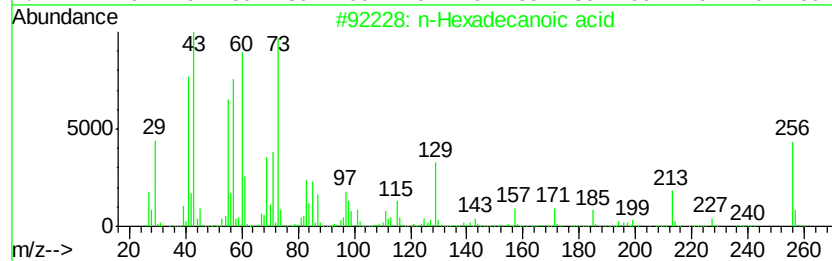
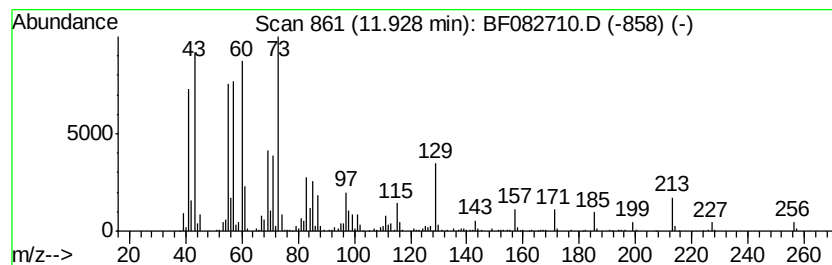
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.93	10.16 ng	1029100	Phenanthrene-d10	11.38

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2		Tridecanoic acid	214	C13H26O2	000638-53-9	95
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	94
4		Estra-1,3,5(10)-trien-17.β.-ol	256	C18H24O	002529-64-8	25
5		Dodecane	170	C12H26	000112-40-3	11



Data Path : Z:\HPCHEM1\BNA F\DATA\BF110515\
Data File : BF082710.D
Acq On : 4 Nov 2015 19:42
Operator : UM/IZ
Sample : G4241-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

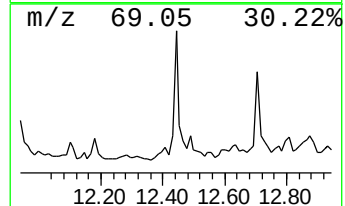
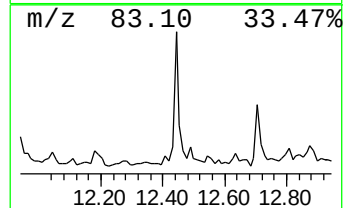
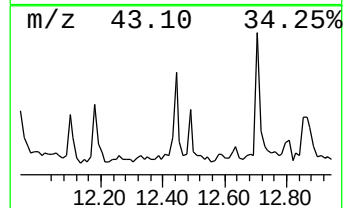
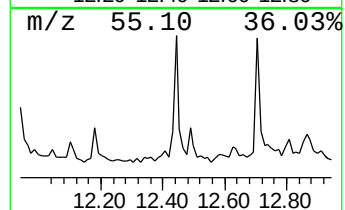
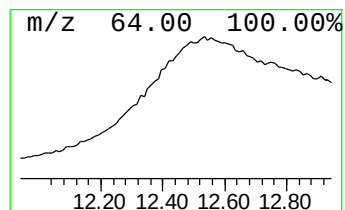
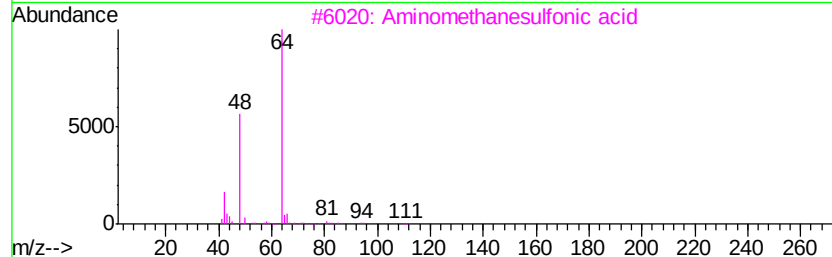
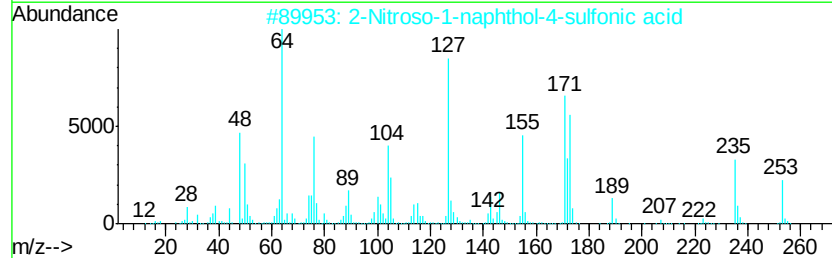
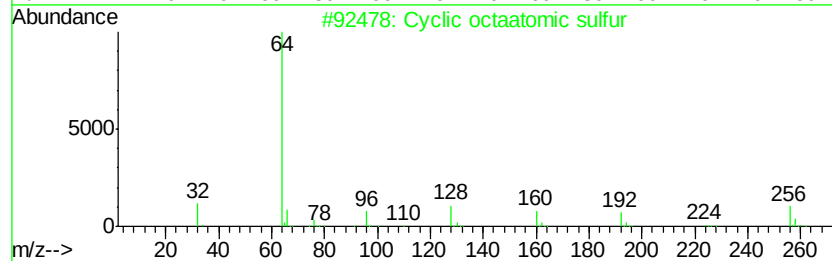
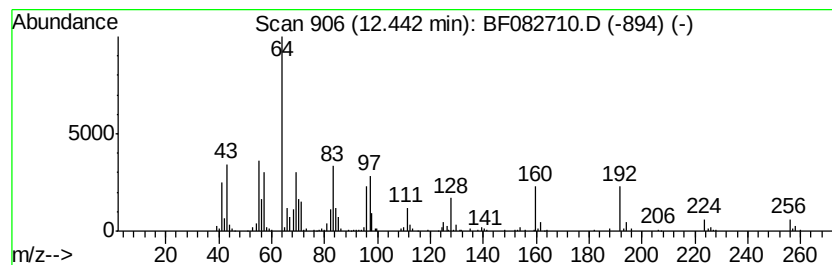
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown12.44 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.44	10.18 ng	1030490	Phenanthrene-d10	11.38
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Cyclic octaatomic sulfur	256 S8	010544-50-0 35
2		2-Nitroso-1-naphthol-4-sulfonic ...	253 C10H7NO5S	003682-32-4 9
3		Aminomethanesulfonic acid	111 CH5NO3S	013881-91-9 9
4		Thiosulfuric acid (H2S2O3), S-(2...	320 C11H16N2O3S3	040284-00-2 9
5		Piperazine-1,4-diium, 1,4-di(2-c...	338 C12H26Cl4N2	1000273-25-4 9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF110515\
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Sample : G4241-04
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ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-16(4)

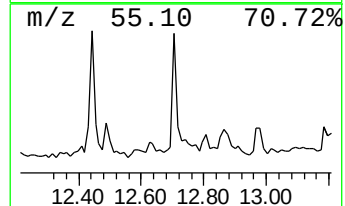
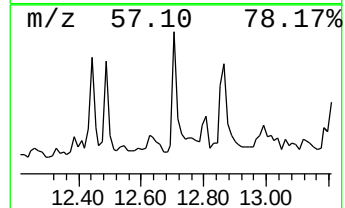
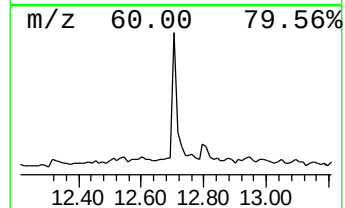
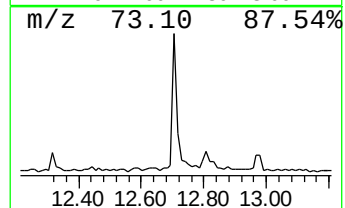
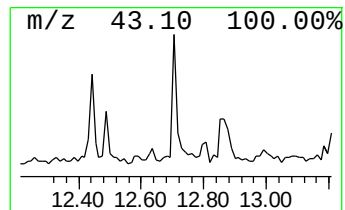
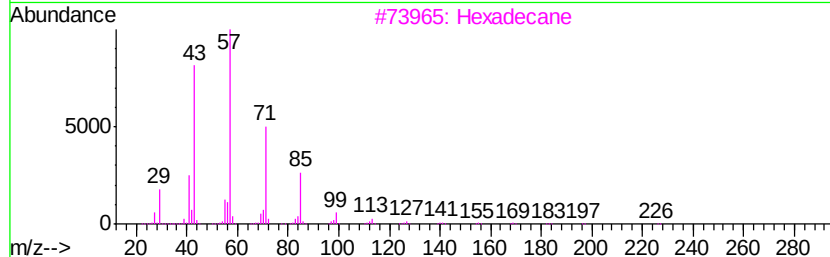
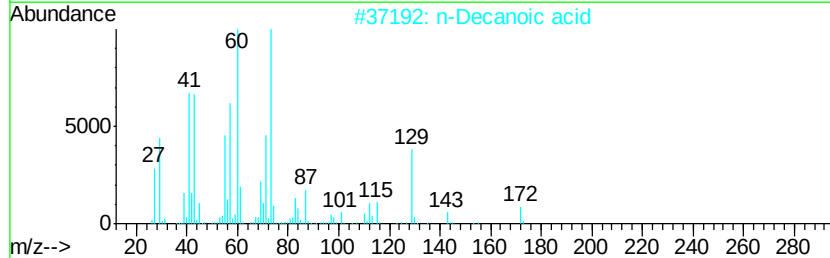
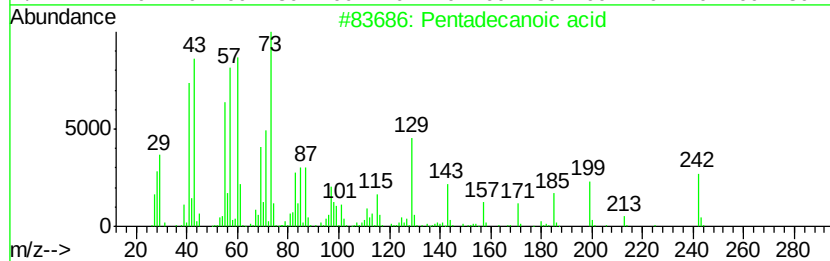
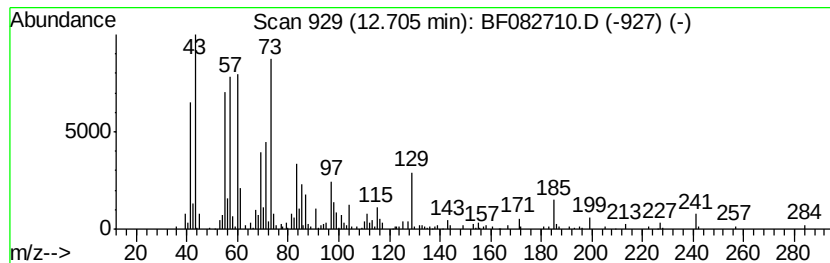
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Pentadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.71	3.20 ng	338935	Chrysene-d12	14.02

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentadecanoic acid	242	C15H30O2	001002-84-2	93
2		n-Decanoic acid	172	C10H20O2	000334-48-5	64
3		Hexadecane	226	C16H34	000544-76-3	25
4		Nonanoic acid	158	C9H18O2	000112-05-0	11
5		Undecane	156	C11H24	001120-21-4	11



Data Path : Z:\HPCHEM1\BNA F\DATA\BF110515\
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Sample : G4241-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-16(4)

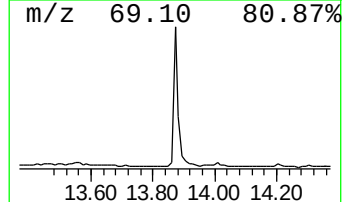
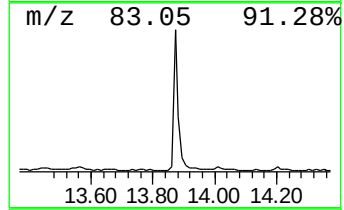
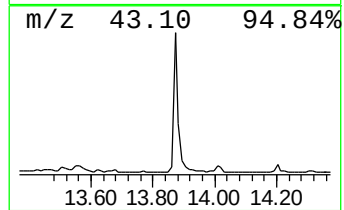
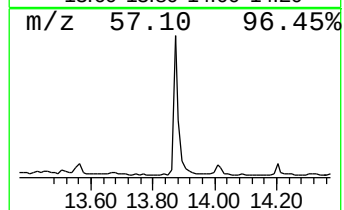
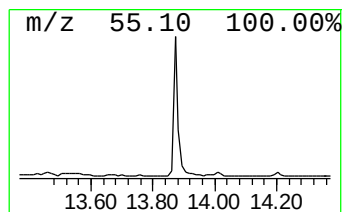
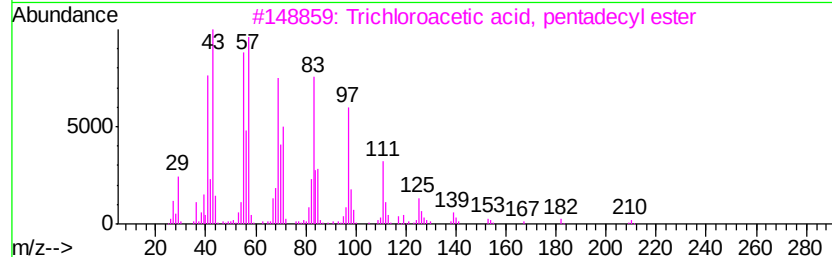
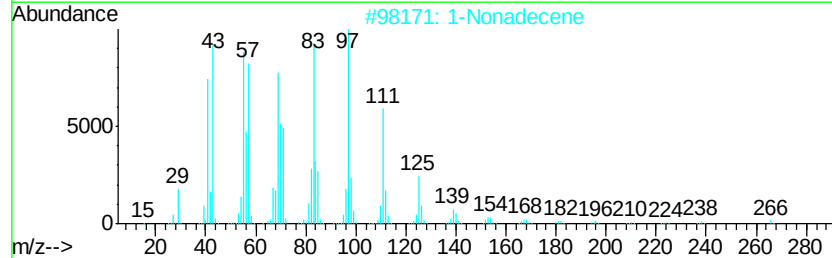
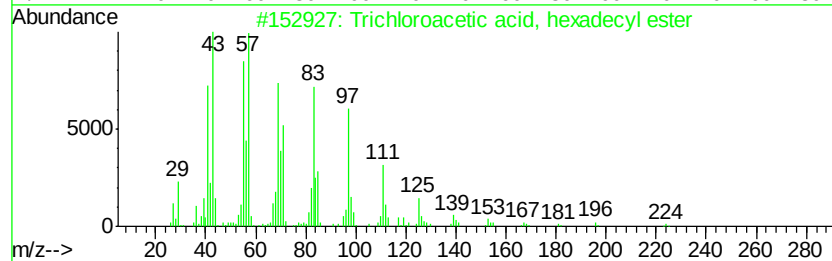
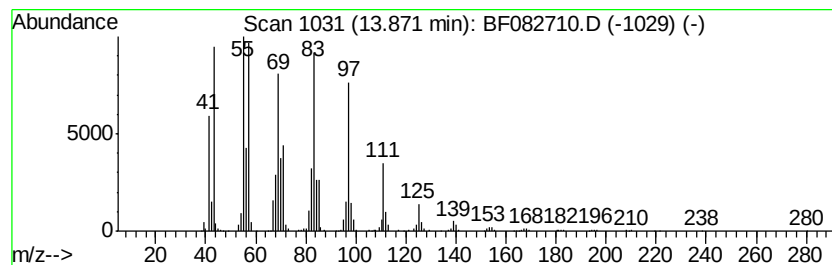
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Trichloroacetic acid, hexad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	12.28 ng	1300360	Chrysene-d12	14.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2		1-Nonadecene	266	C19H38	018435-45-5	91
3		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
4		Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
5		Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	90



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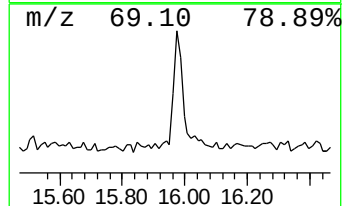
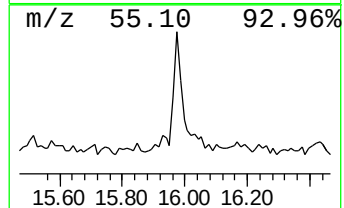
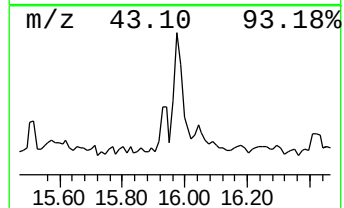
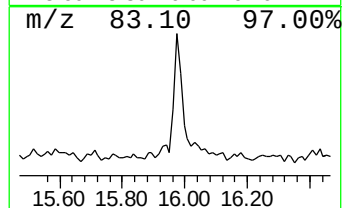
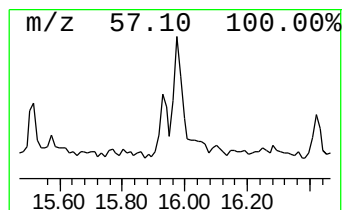
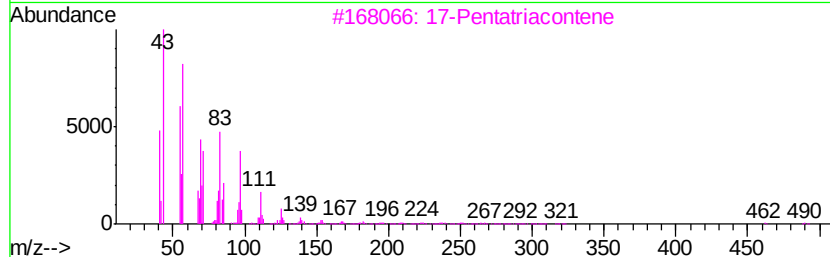
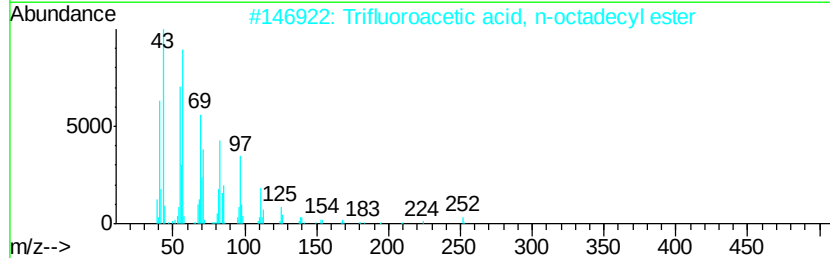
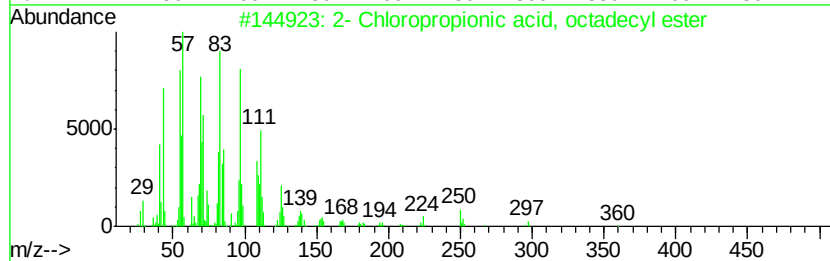
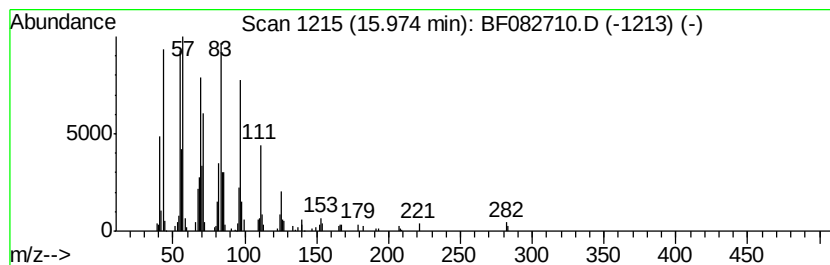
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 2- Chloropropionic acid, oc... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.97	3.26 ng	235106	Perylene-d12	15.46

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91
2		Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	90
3		17-Pentatriacontene	491	C35H70	006971-40-0	86
4		1-Tetracosanol	354	C24H50O	000506-51-4	74
5		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	62



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110515\
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TIC Library : C:\DATABASE\NIST02.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hexane	2.20	2.7	ng	180550	1	6.86	1341210	20.0
2-Pentanone, 4-hy...	5.06	46.1	ng	3094030	1	6.86	1341210	20.0
unknown6.64	6.64	101.2	ng	6788410	1	6.86	1341210	20.0
unknown10.32	10.32	8.3	ng	864446	3	9.90	2092840	20.0
1-Hexadecanol	11.62	6.3	ng	642009	4	11.38	2025150	20.0
n-Hexadecanoic acid	11.93	10.2	ng	1029100	4	11.38	2025150	20.0
unknown12.44	12.44	10.2	ng	1030490	4	11.38	2025150	20.0
Pentadecanoic acid	12.71	3.2	ng	338935	5	14.02	2117480	20.0
Trichloroacetic a...	13.87	12.3	ng	1300360	5	14.02	2117480	20.0
2- Chloropropioni...	15.97	3.3	ng	235106	6	15.46	1443930	20.0