

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120216\
 Data File : BF091407.D
 Acq On : 2 Dec 2016 23:33
 Operator : UM/SJ
 Sample : H5760-02
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 GRID-MM4-5

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-BF112916.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	5.053	238	242	249	rVB	1597748	2370393	42.88%	4.384%
2	5.464	275	278	281	rVB	4555426	5068561	91.69%	9.373%
3	6.493	364	368	371	rBV	4345667	5528184	100.00%	10.223%
4	6.630	377	380	382	rBV	5372105	5426906	98.17%	10.036%
5	6.859	398	400	402	rBV	1678191	1381851	25.00%	2.555%
6	7.019	411	414	416	rVB	4656350	4212876	76.21%	7.791%
7	7.430	446	450	452	rBV	2555278	3788107	68.52%	7.005%
8	8.139	510	512	515	rBV	1284516	1761096	31.86%	3.257%
9	9.225	604	607	609	rBV	5956999	5499863	99.49%	10.171%
10	9.613	639	641	643	rBV	360831	295149	5.34%	0.546%
11	9.899	663	666	668	rBV	2398294	1996757	36.12%	3.693%
12	10.333	703	704	706	rVB	82993	76662	1.39%	0.142%
13	10.688	732	735	737	rBV	3564042	3589341	64.93%	6.638%
14	10.813	744	746	750	rVB	103701	149368	2.70%	0.276%
15	11.259	781	785	786	rBV	105786	101239	1.83%	0.187%
16	11.385	793	796	798	rBV	1564203	1797252	32.51%	3.324%
17	11.454	799	802	804	rBV	85320	80488	1.46%	0.149%
18	11.911	840	842	844	rBV2	431379	485414	8.78%	0.898%
19	11.991	847	849	854	rVB2	47084	78259	1.42%	0.145%
20	12.585	899	901	903	rBV	404164	374812	6.78%	0.693%
21	12.699	908	911	917	rBV	197313	266897	4.83%	0.494%
22	12.814	917	921	924	rBV	404222	439295	7.95%	0.812%
23	12.974	932	935	937	rVB	3344493	4406465	79.71%	8.149%
24	13.145	946	950	952	rBV	84844	99851	1.81%	0.185%
25	13.214	954	956	957	rBV	87034	90242	1.63%	0.167%
26	13.648	992	994	996	rBV	43418	62112	1.12%	0.115%
27	13.762	1001	1004	1005	rBV2	66853	91405	1.65%	0.169%
28	13.865	1011	1013	1016	rBV2	286658	304624	5.51%	0.563%
29	14.014	1023	1026	1027	rBV2	1586573	1720367	31.12%	3.182%
30	14.780	1091	1093	1095	rBV	185666	281073	5.08%	0.520%
31	15.031	1112	1115	1120	rVB	215733	437544	7.91%	0.809%
32	15.328	1138	1141	1143	rVB	102998	155659	2.82%	0.288%
33	15.385	1143	1146	1148	rBV	103280	147132	2.66%	0.272%
34	15.442	1148	1151	1154	rBV	811854	1154655	20.89%	2.135%

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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-BF112916.M
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35	15.957	1195	1196	1203	rVB4	46992	107357	1.94%	0.199%
36	16.140	1210	1212	1218	rVB2	49298	91230	1.65%	0.169%
37	16.837	1270	1273	1276	rBV2	45165	88997	1.61%	0.165%
38	17.248	1307	1309	1313	rVB	33863	66452	1.20%	0.123%

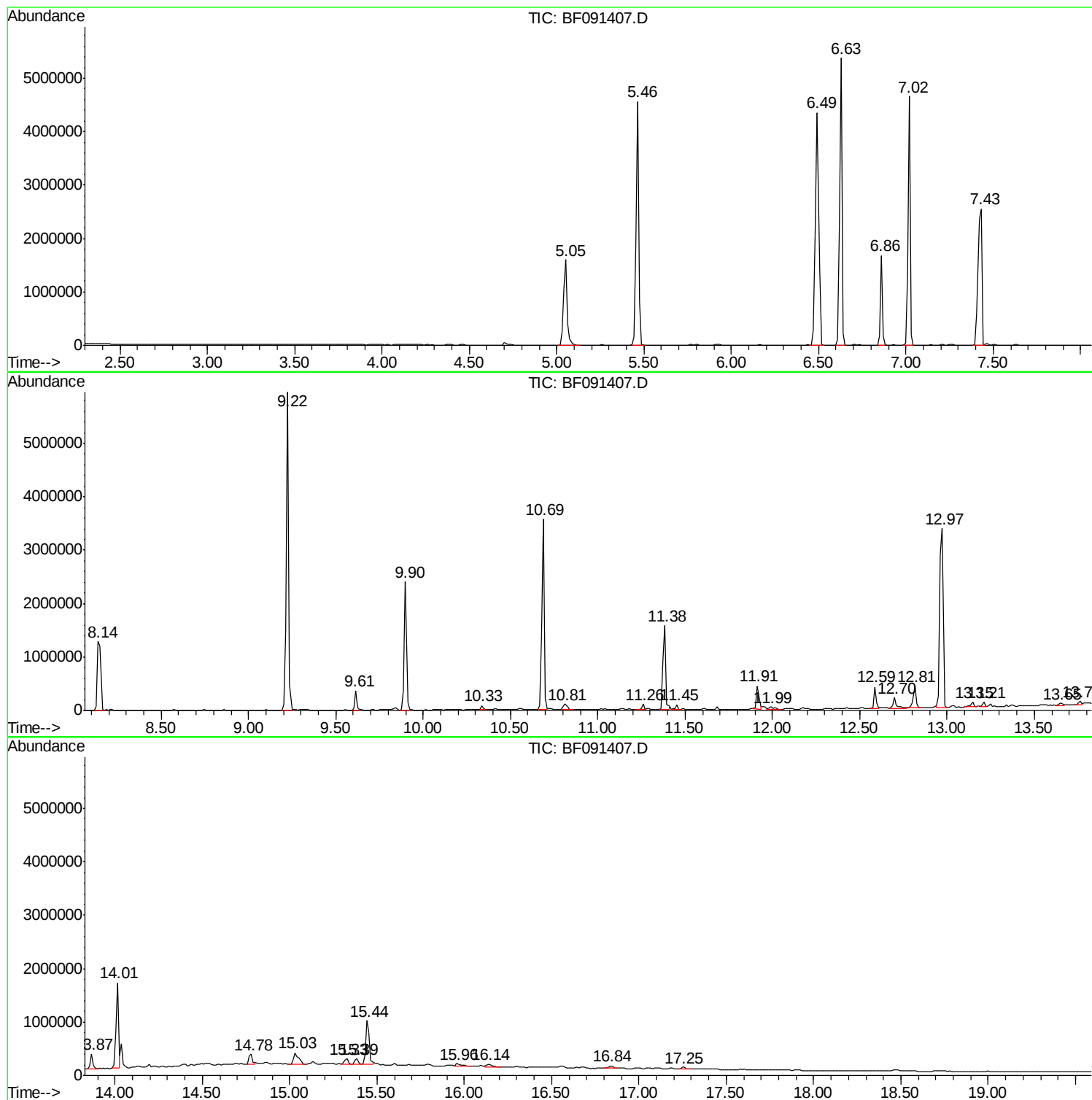
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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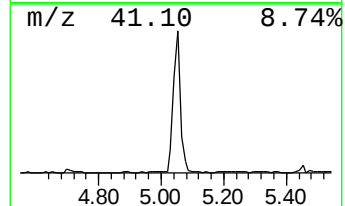
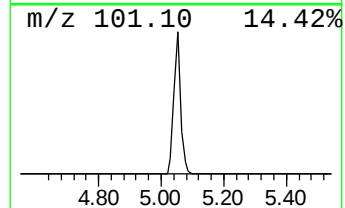
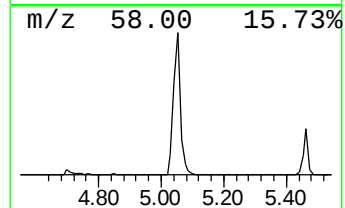
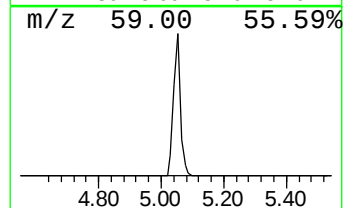
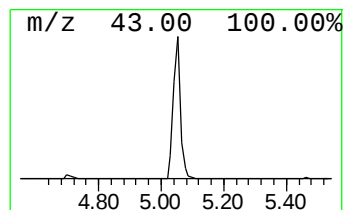
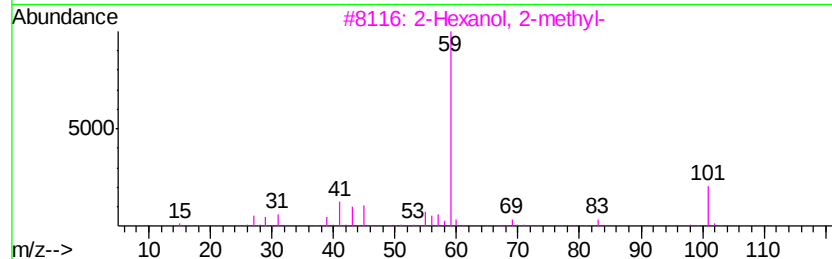
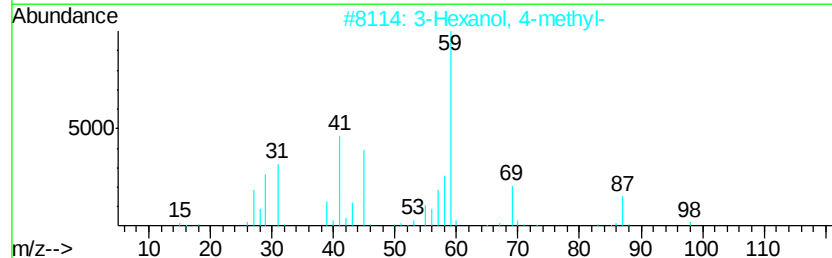
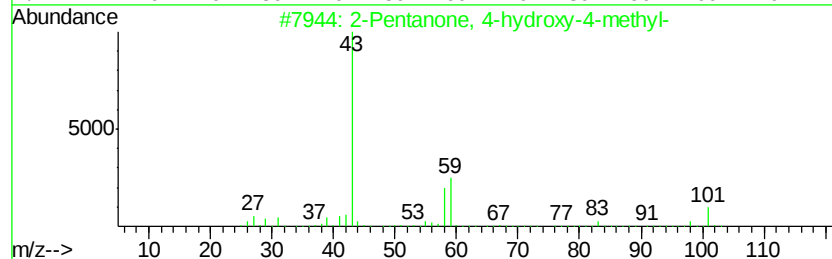
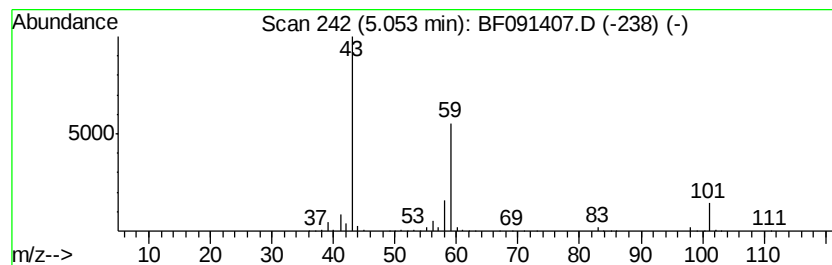
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	34.31 ng	2370390	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	59	
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33	
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33	
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25	
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	17	



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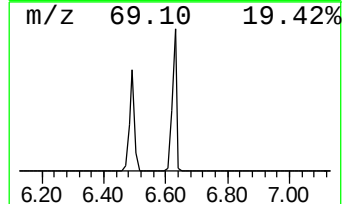
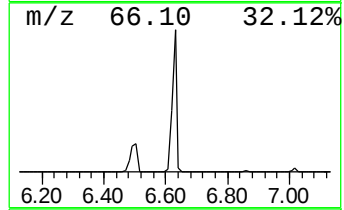
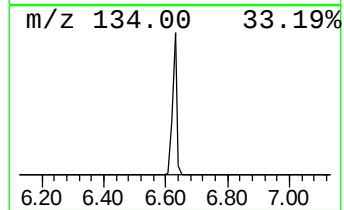
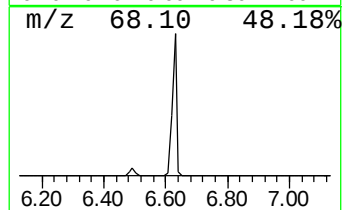
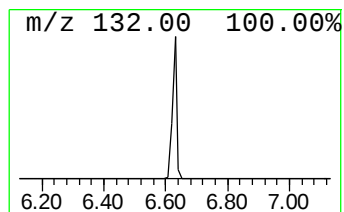
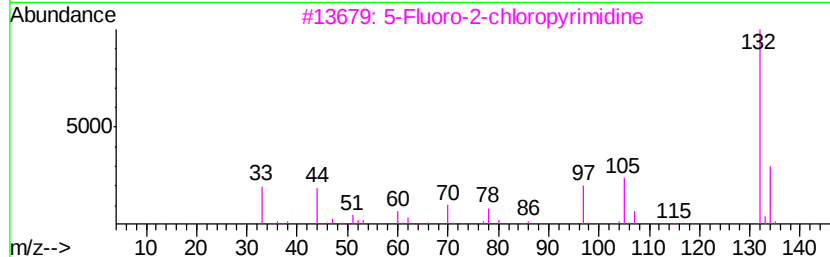
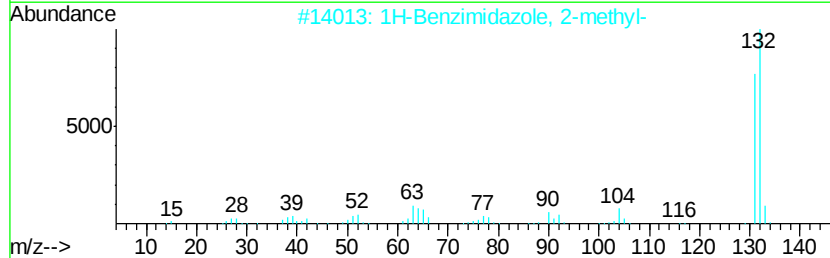
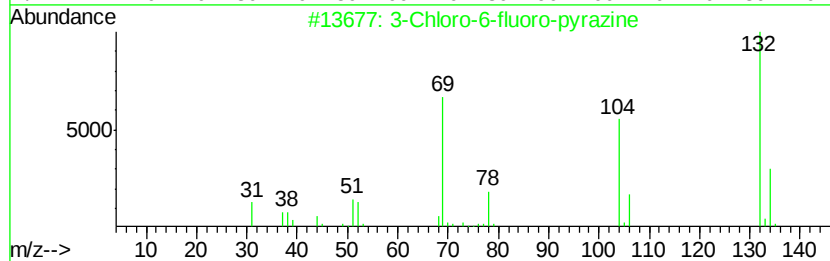
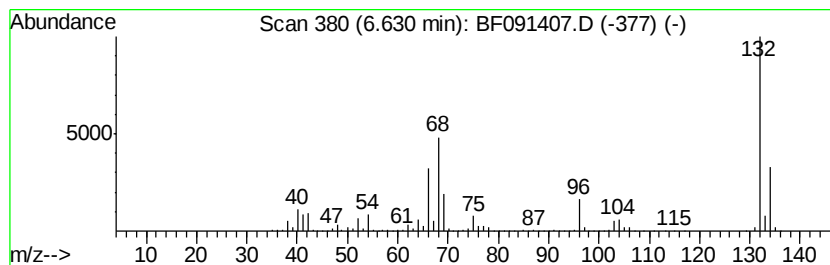
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	78.55 ng	5426910	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	16
4	(5-METHYL-2-PYRIDYL)ACETONITRILE			132	C8H8N2	1000241-93-9	10
5	Benzene, 1,3,5-trifluoro-			132	C6H3F3	000372-38-3	9



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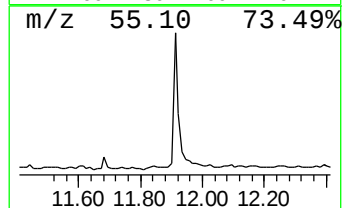
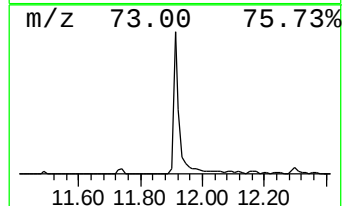
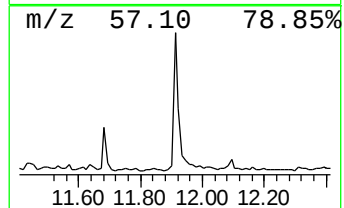
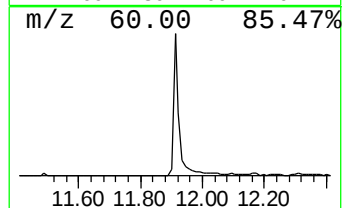
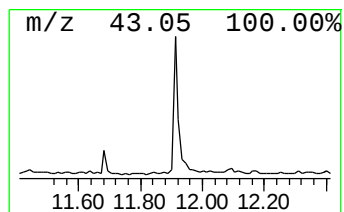
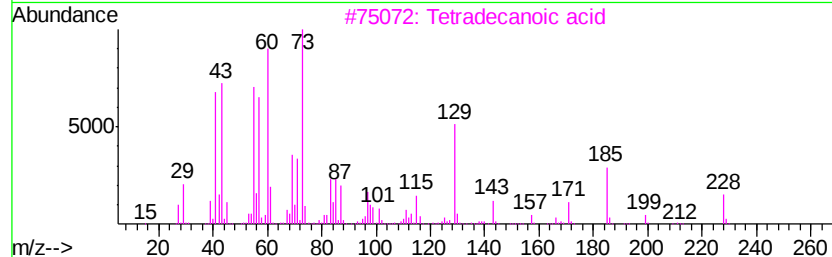
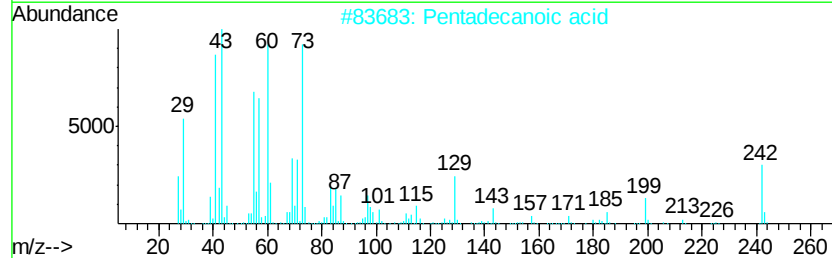
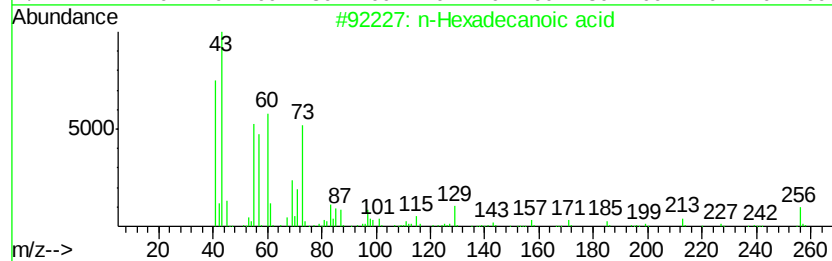
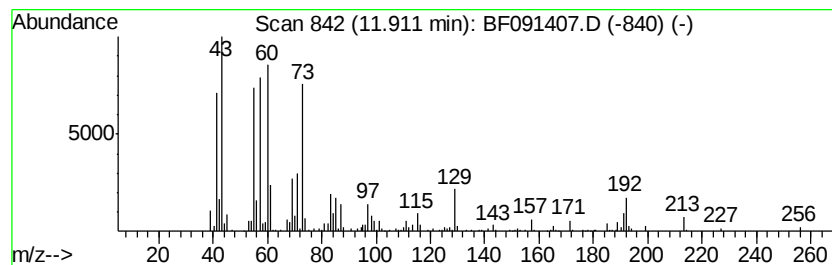
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.91	5.40 ng	485414	Phenanthrene-d10	11.38

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4		Tridecanoic acid	214	C13H26O2	000638-53-9	72
5		Undecanoic acid	186	C11H22O2	000112-37-8	72



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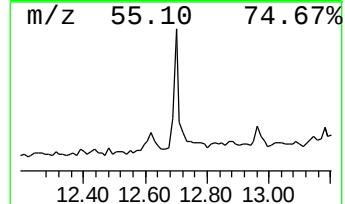
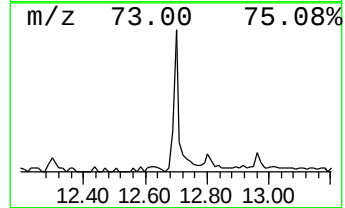
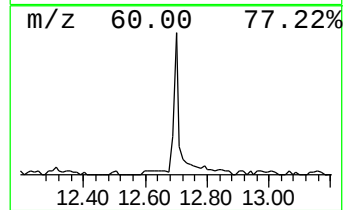
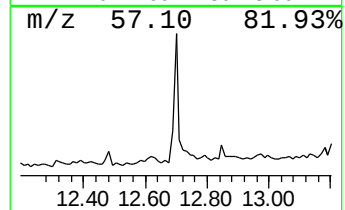
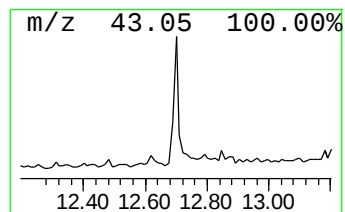
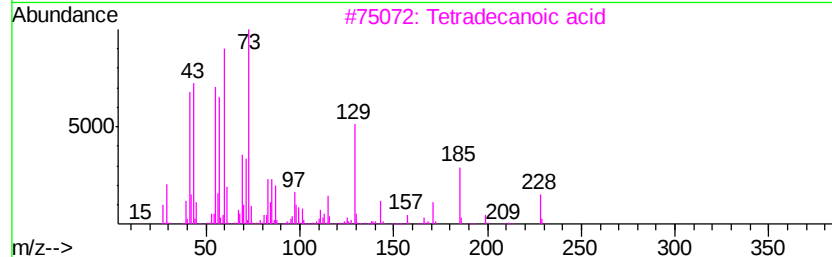
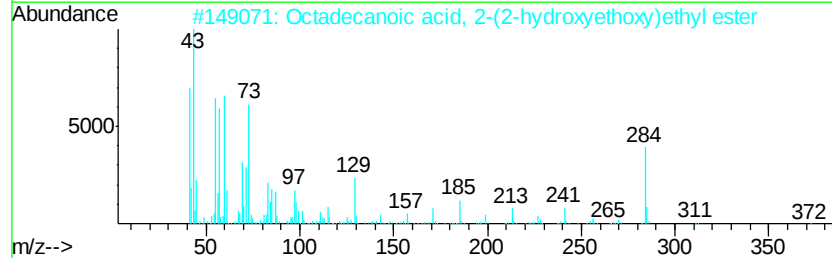
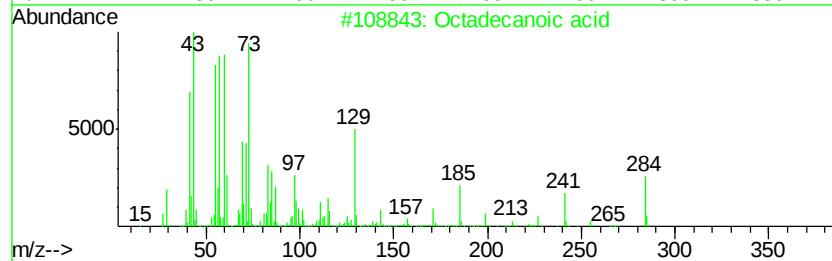
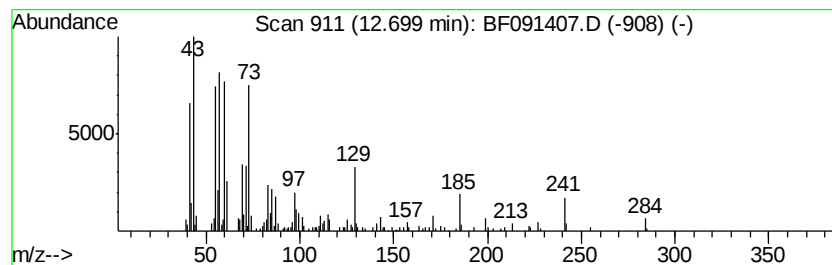
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.70	2.97 ng	266897	Phenanthrene-d10	11.38

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	91
2			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	80
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	64
5			Tridecanoic acid	214	C13H26O2	000638-53-9	64



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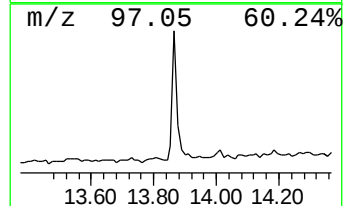
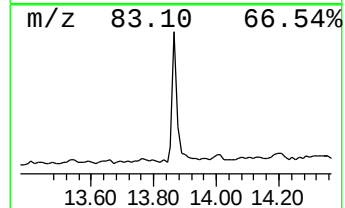
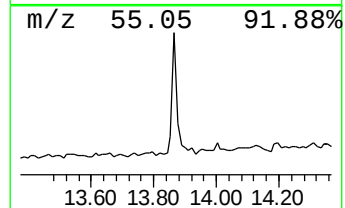
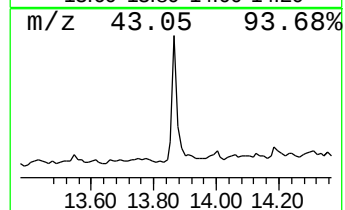
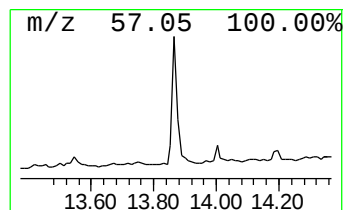
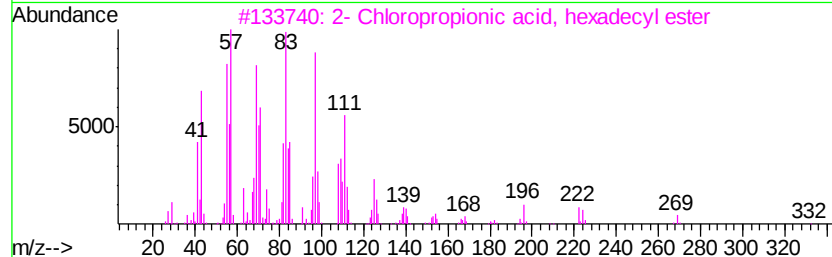
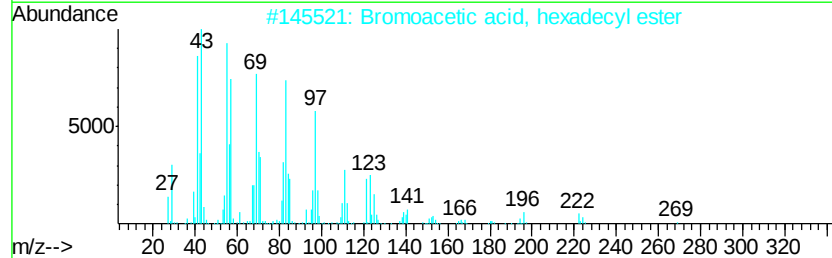
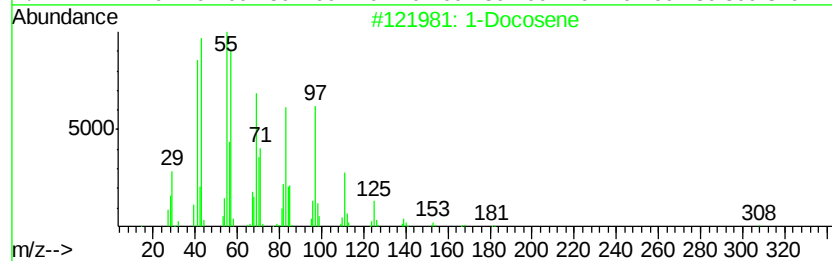
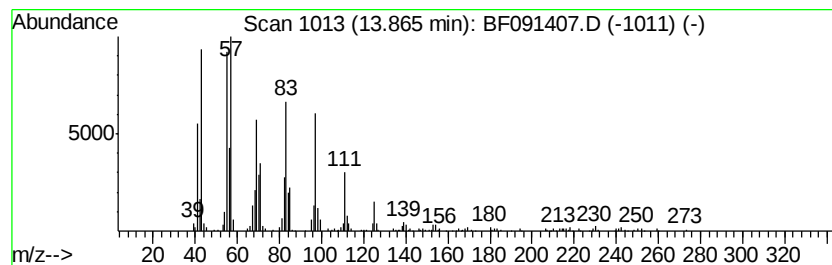
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ClientSampleId :
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Peak Number 6 1-Docosene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	3.54 ng	304624	Chrysene-d12	14.01
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Docosene	308 C22H44	001599-67-3	95
2	Bromoacetic acid, hexadecyl ester	362 C18H35BrO2	005454-48-8	91
3	2- Chloropropionic acid, hexadec...	332 C19H37ClO2	086711-81-1	91
4	Bromoacetic acid, pentadecyl ester	348 C17H33BrO2	131143-01-6	91
5	Trichloroacetic acid, hexadecyl ...	386 C18H33Cl3O2	074339-54-1	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120216\
Data File : BF091407.D
Acq On : 2 Dec 2016 23:33
Operator : UM/SJ
Sample : H5760-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GRID-MM4-5

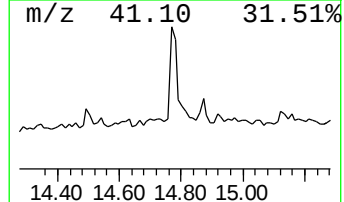
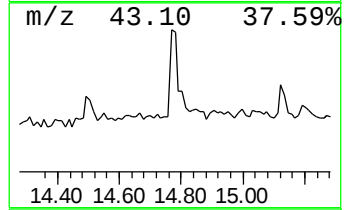
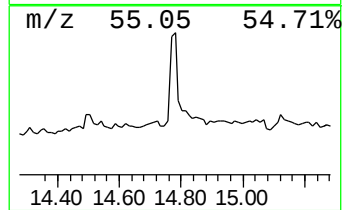
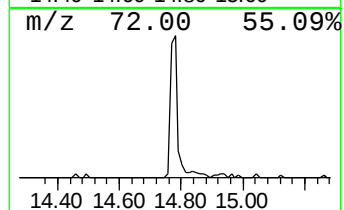
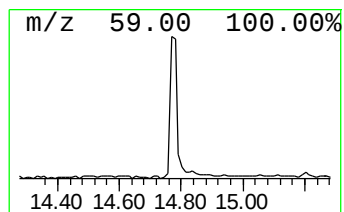
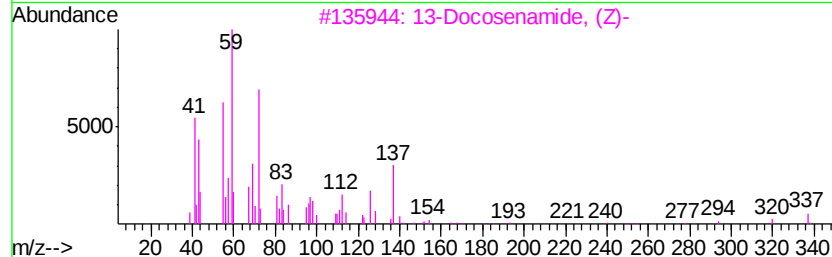
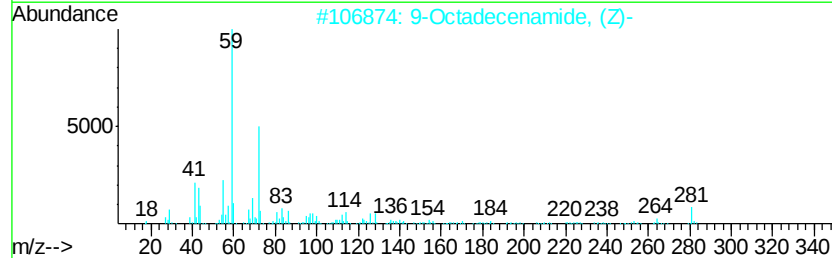
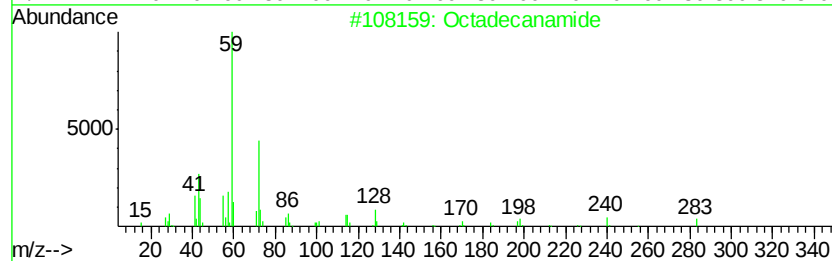
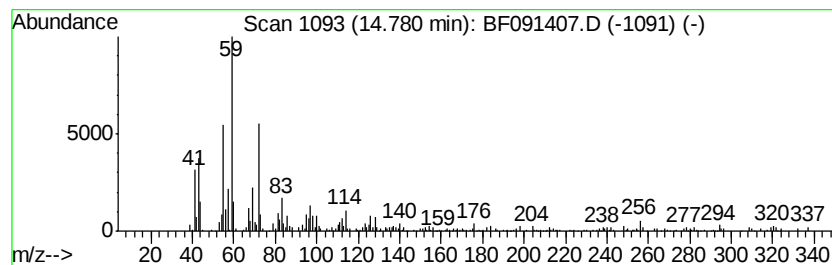
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanamide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.78	4.87 ng	281073	Perylene-d12	15.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanamide	283	C18H37NO	000124-26-5	91
2		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	90
3		13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	87
4		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	81
5		Tetradecanamide	227	C14H29NO	000638-58-4	78



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Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GRID-MM4-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.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
2-Pentanone, 4-hy...	5.05	34.3	ng	2370390	1	6.86	1381850	20.0
unknown6.63	6.63	78.5	ng	5426910	1	6.86	1381850	20.0
n-Hexadecanoic acid	11.91	5.4	ng	485414	4	11.38	1797250	20.0
Octadecanoic acid	12.70	3.0	ng	266897	4	11.38	1797250	20.0
1-Docosene	13.87	3.5	ng	304624	5	14.01	1720370	20.0
Octadecanamide	14.78	4.9	ng	281073	6	15.44	1154660	20.0