

Data Path : Z:\HPCHEM1\BNA F\DATA\BF111315\
 Data File : BF082913.D
 Acq On : 13 Nov 2015 22:53
 Operator : UM/IZ
 Sample : G4370-02
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P001-TS002-01

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-BF110715.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	4.979	250	253	256	rVB	1613393	1903894	49.17%	4.505%
2	5.424	290	292	295	rBV	2718372	3580222	92.47%	8.472%
3	6.464	381	383	386	rBV	2934144	3765156	97.24%	8.910%
4	6.590	391	394	396	rBV	3178113	3871930	100.00%	9.162%
5	6.807	411	413	415	rBV	1952054	1567716	40.49%	3.710%
6	6.967	424	427	429	rBV	3163178	2968601	76.67%	7.025%
7	7.367	459	462	465	rBV	2245069	2249101	58.09%	5.322%
8	7.847	501	504	506	rBV2	64213	83618	2.16%	0.198%
9	8.099	523	526	528	rBV	2148134	2013067	51.99%	4.764%
10	8.453	554	557	559	rBV	54602	56500	1.46%	0.134%
11	9.059	608	610	612	rBV	30034	46173	1.19%	0.109%
12	9.173	618	620	623	rVB	3623389	3166710	81.79%	7.494%
13	9.573	653	655	657	rVV	1029791	942286	24.34%	2.230%
14	9.790	673	674	677	rVB	62247	61362	1.58%	0.145%
15	9.848	677	679	682	rBV2	1752562	2036268	52.59%	4.819%
16	10.030	689	695	696	rBV4	20382	42656	1.10%	0.101%
17	10.293	717	718	720	rVB	158628	117722	3.04%	0.279%
18	10.511	734	737	740	rBV	47784	101392	2.62%	0.240%
19	10.636	746	748	751	rBV2	1703111	2206504	56.99%	5.221%
20	10.762	758	759	764	rVB	135748	215426	5.56%	0.510%
21	10.865	766	768	770	rVV2	39082	60515	1.56%	0.143%
22	10.899	770	771	774	rVB2	33896	46300	1.20%	0.110%
23	10.968	774	777	779	rBV2	28011	56024	1.45%	0.133%
24	11.013	779	781	783	rVB3	34188	49662	1.28%	0.118%
25	11.048	783	784	786	rBV	37078	43124	1.11%	0.102%
26	11.093	786	788	790	rVB3	27911	39405	1.02%	0.093%
27	11.219	794	799	800	rBV	82725	116147	3.00%	0.275%
28	11.333	807	809	812	rVV	2156028	1870751	48.32%	4.427%
29	11.402	812	815	818	rVB3	49151	76885	1.99%	0.182%
30	11.642	833	836	839	rBV2	37726	64633	1.67%	0.153%
31	11.699	839	841	847	rBV7	15000	61916	1.60%	0.147%
32	11.802	848	850	852	rBV	45194	65329	1.69%	0.155%
33	11.882	854	857	861	rVV2	167890	284285	7.34%	0.673%
34	12.031	867	870	874	rBV5	23049	80898	2.09%	0.191%

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.168	880	882	884	rBV	42141	50866	1.31%	0.120%
36	12.225	884	887	888	rVV2	27810	44921	1.16%	0.106%
37	12.328	893	896	899	rBV	34757	74644	1.93%	0.177%
38	12.385	899	901	903	rVV	57807	103834	2.68%	0.246%
39	12.419	903	904	907	rVB2	39673	53942	1.39%	0.128%
40	12.579	913	918	923	rBV3	161329	605209	15.63%	1.432%
41	12.659	923	925	927	rVV	100731	120754	3.12%	0.286%
42	12.728	929	931	932	rVB	69858	73887	1.91%	0.175%
43	12.774	932	935	937	rBV2	82602	144623	3.74%	0.342%
44	12.922	946	948	950	rBV	2677069	2286616	59.06%	5.411%
45	13.082	960	962	965	rBV	68779	141129	3.64%	0.334%
46	13.219	972	974	977	rVB3	36079	49282	1.27%	0.117%
47	13.402	989	990	992	rVB	79724	65062	1.68%	0.154%
48	13.585	1004	1006	1007	rVB	58512	59969	1.55%	0.142%
49	13.837	1025	1028	1032	rBV2	152618	257012	6.64%	0.608%
50	13.905	1032	1034	1036	rVB2	51149	61076	1.58%	0.145%
51	13.974	1037	1040	1042	rBV	1549390	1482183	38.28%	3.507%
52	14.465	1081	1083	1090	rBV4	77471	157411	4.07%	0.372%
53	14.831	1113	1115	1117	rVB	92683	90203	2.33%	0.213%
54	15.391	1161	1164	1167	rBV	1028932	1457866	37.65%	3.450%
55	17.368	1335	1337	1342	rVB3	167300	321643	8.31%	0.761%
56	19.266	1499	1503	1509	rVB3	205665	644177	16.64%	1.524%

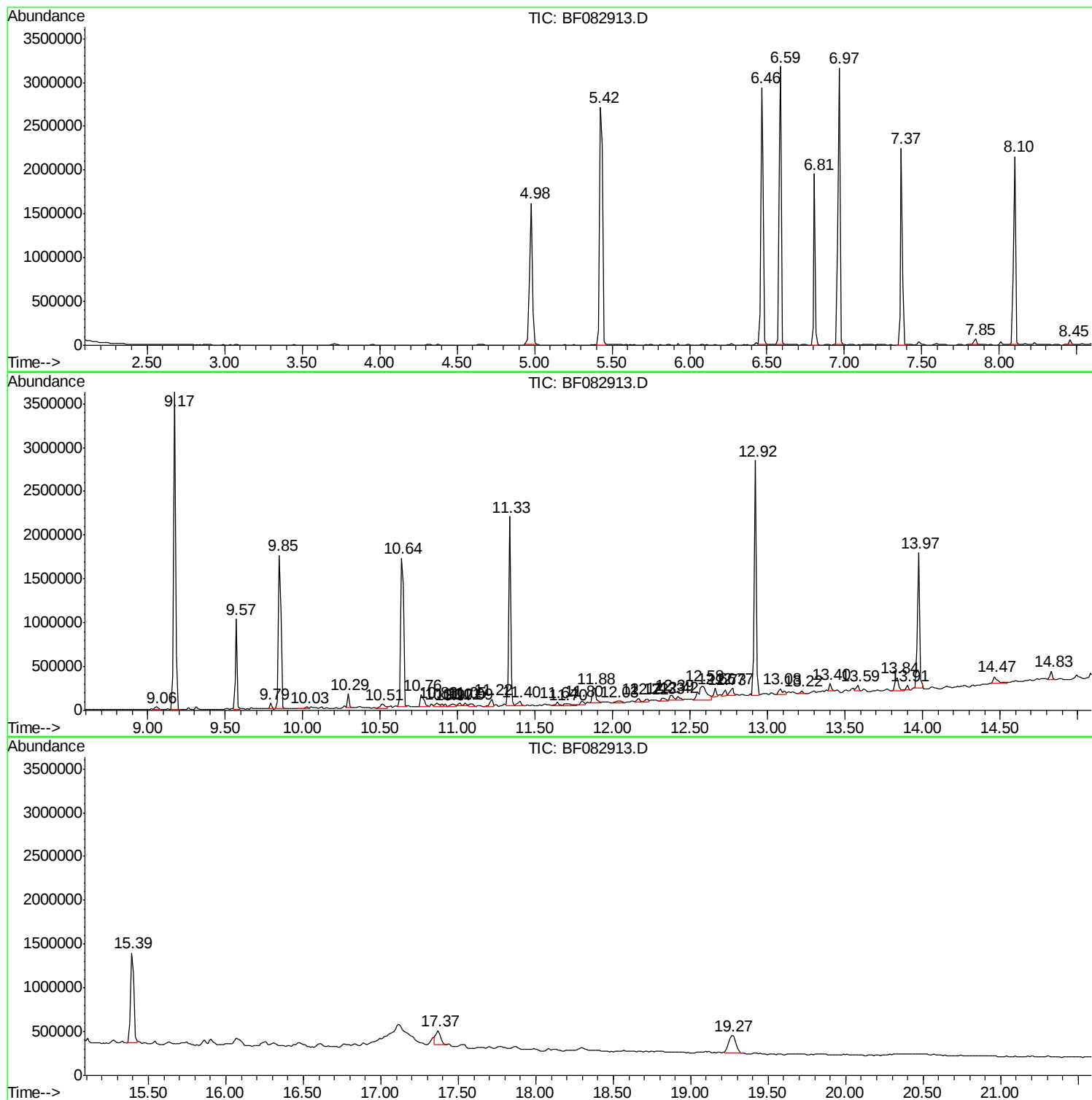
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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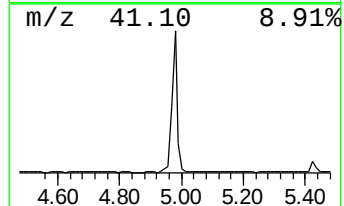
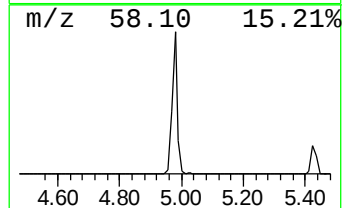
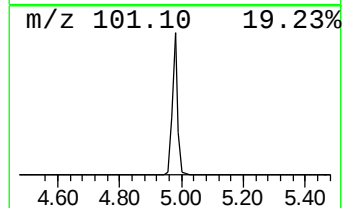
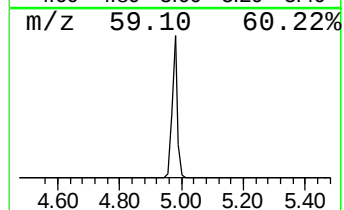
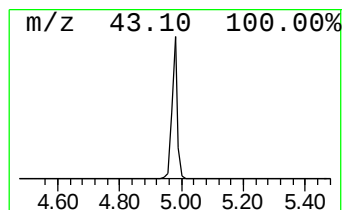
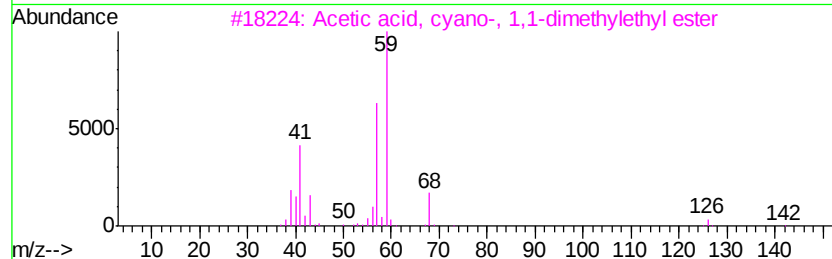
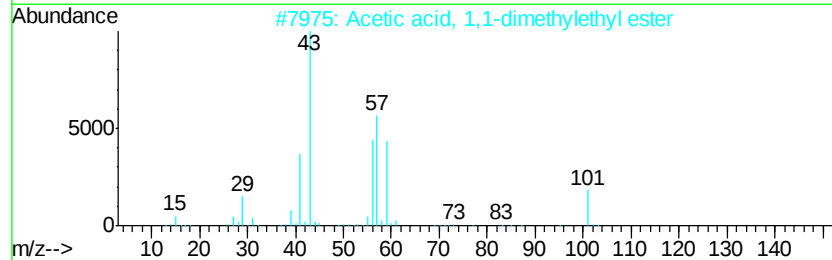
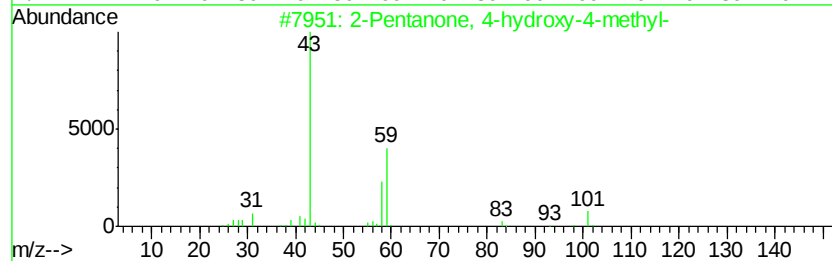
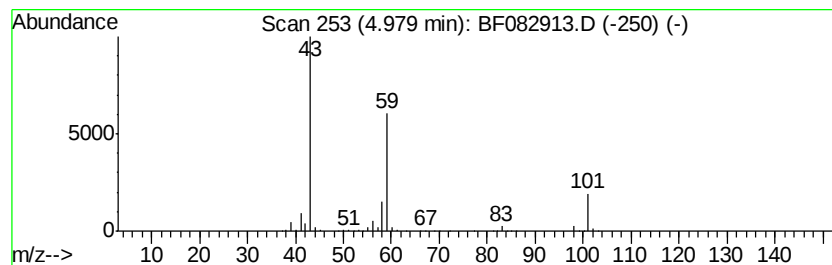
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF110715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.98	24.29 ng	1903890	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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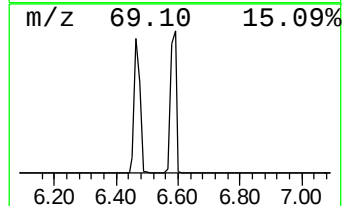
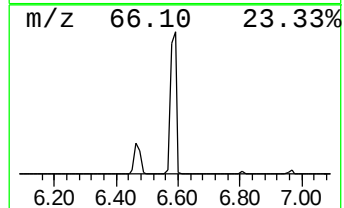
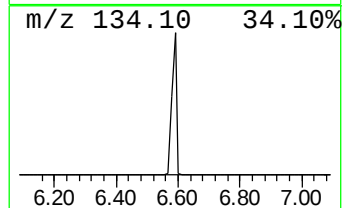
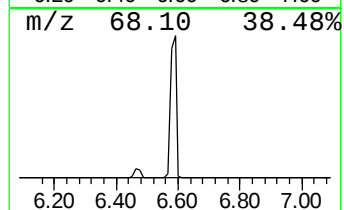
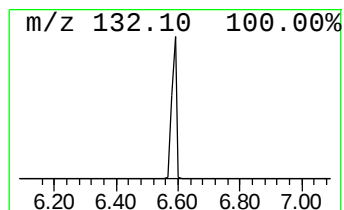
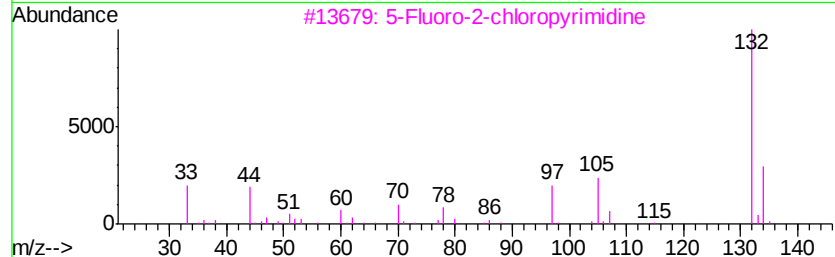
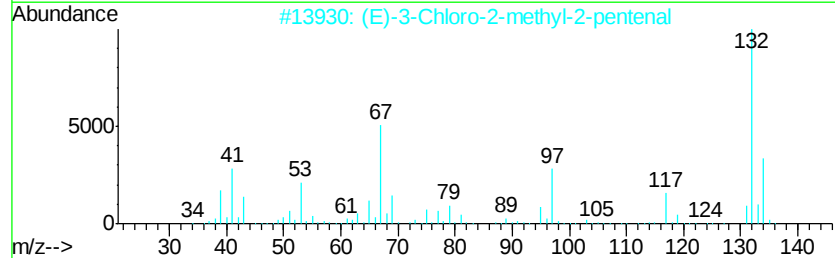
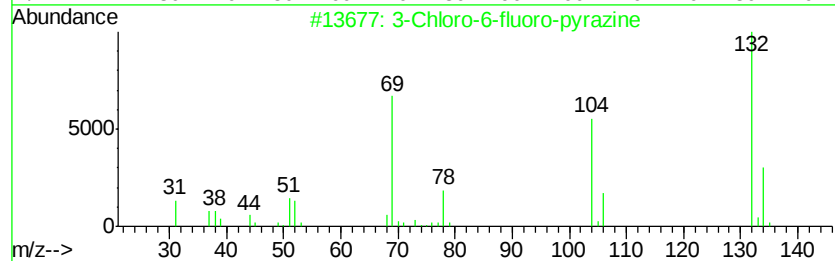
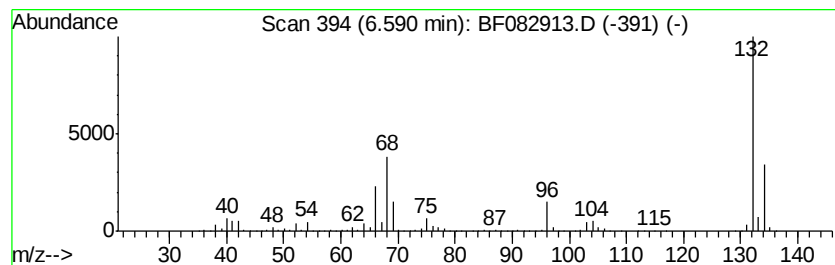
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.59 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.59	49.40 ng	3871930	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9



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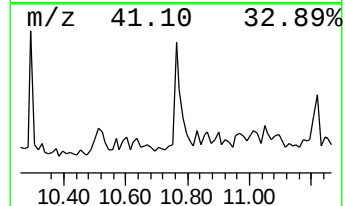
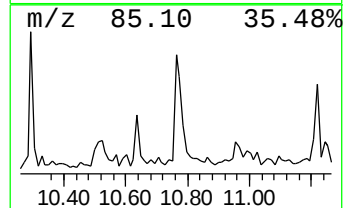
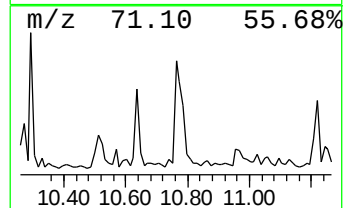
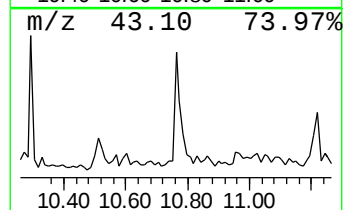
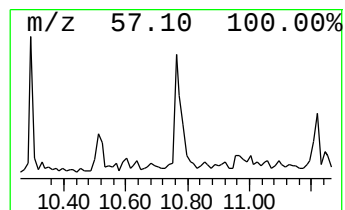
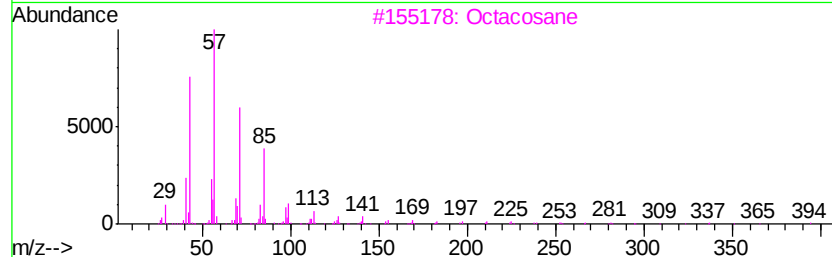
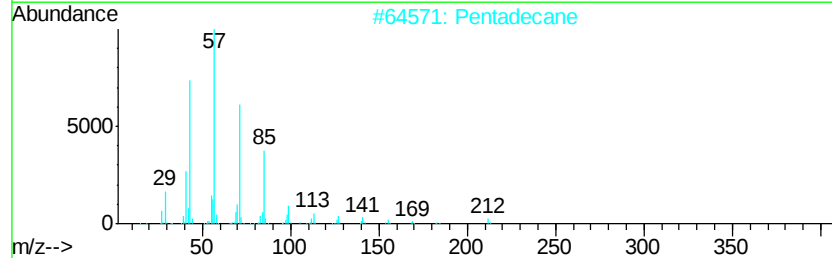
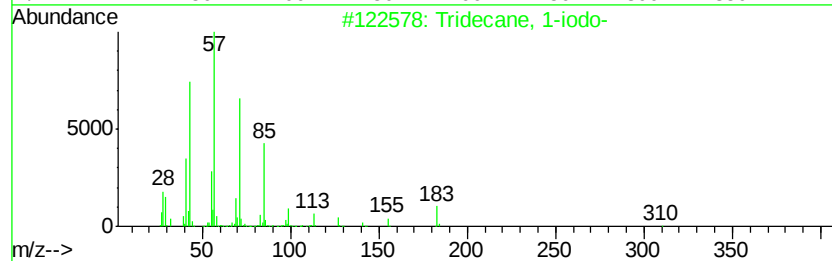
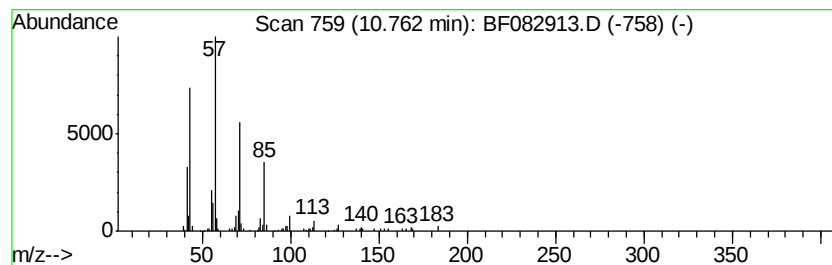
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Tridecane, 1-iodo- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.76	2.30 ng	215426	Phenanthrene-d10	11.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	90
2		Pentadecane	212	C15H32	000629-62-9	90
3		Octacosane	394	C28H58	000630-02-4	83
4		Decane, 2,3,7-trimethyl-	184	C13H28	062238-13-5	72
5		Hexadecane	226	C16H34	000544-76-3	72



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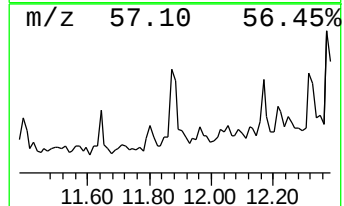
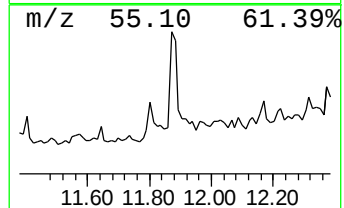
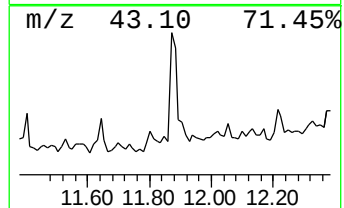
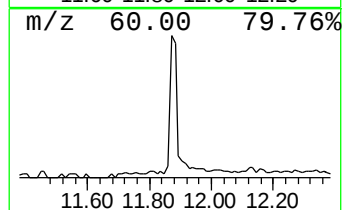
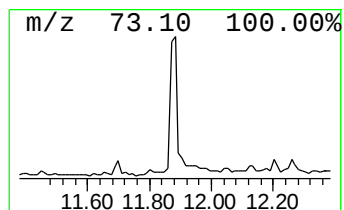
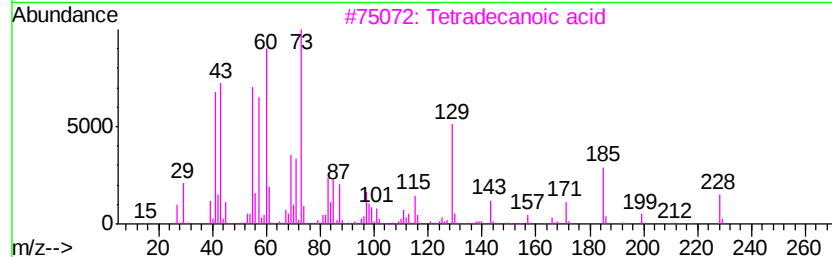
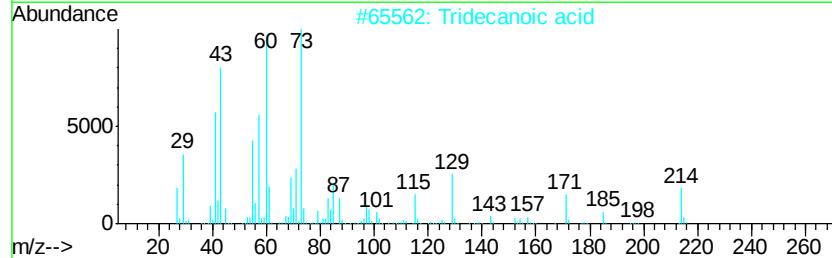
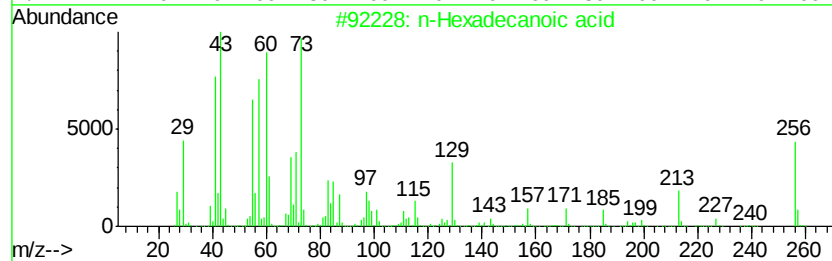
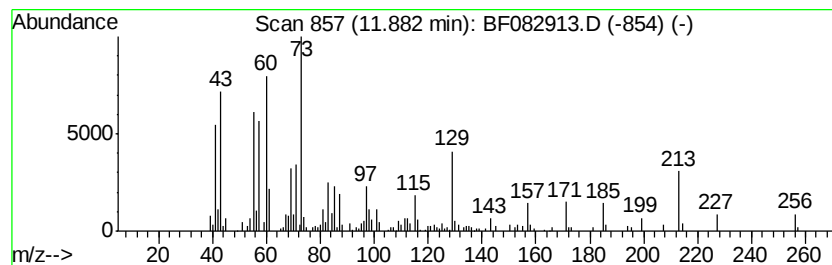
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.88	3.04 ng	284285	Phenanthrene-d10	11.33

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tridecanoic acid	214	C13H26O2	000638-53-9	93
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4		Dodecanoic acid	200	C12H24O2	000143-07-7	64
5		Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	49



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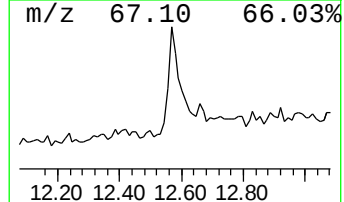
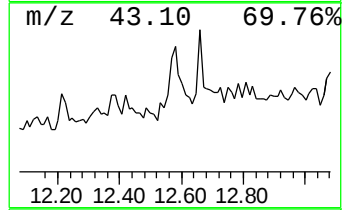
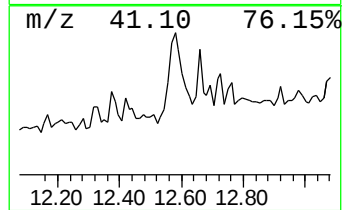
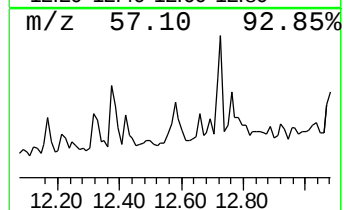
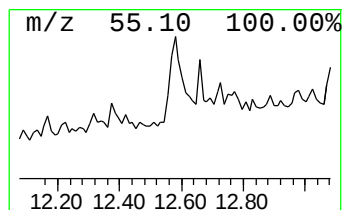
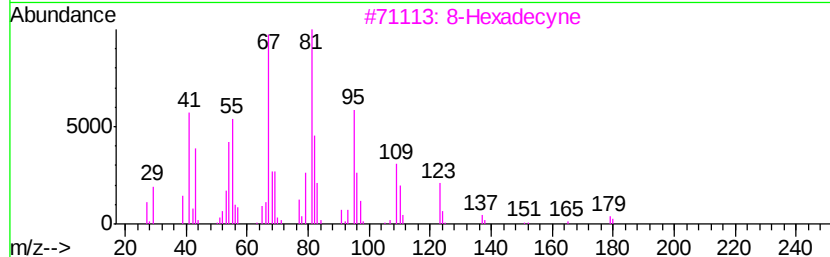
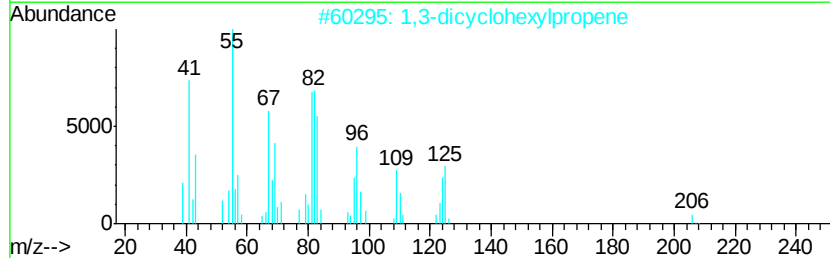
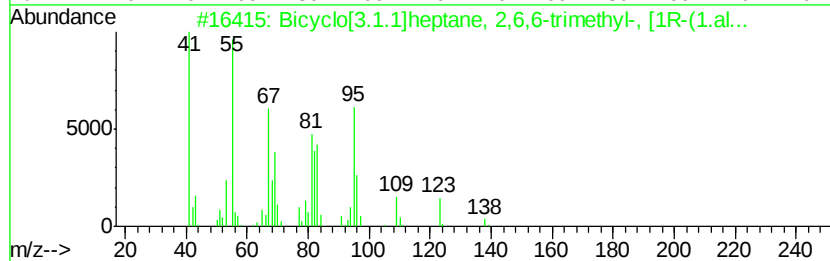
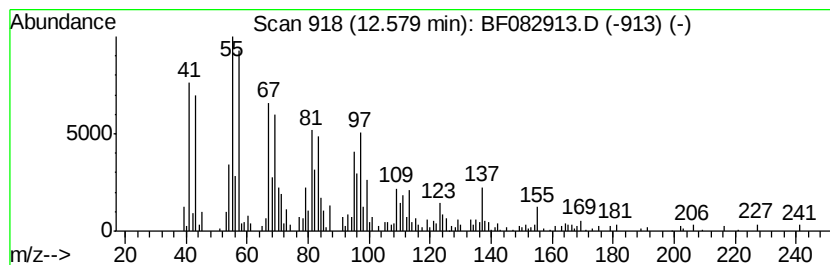
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown12.58 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.58	6.47 ng	605209	Phenanthrene-d10	11.33

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Bicyclo[3.1.1]heptane, 2,6,6-tri...	138	C10H18	004863-59-6	41
2		1,3-dicyclohexylpropene	206	C15H26	1000214-96-8	38
3		8-Hexadecyne	222	C16H30	019781-86-3	38
4		2,8-Nonadienoic acid, methyl ester	168	C10H16O2	078709-46-3	38
5		3,4-Octadiene, 7-methyl-	124	C9H16	037050-05-8	30



Data Path : Z:\HPCHEM1\BNA F\DATA\BF111315\
Data File : BF082913.D
Acq On : 13 Nov 2015 22:53
Operator : UM/IZ
Sample : G4370-02
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P001-TS002-01

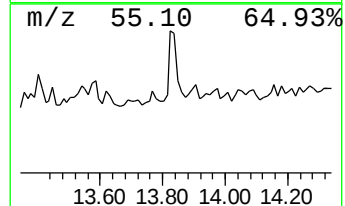
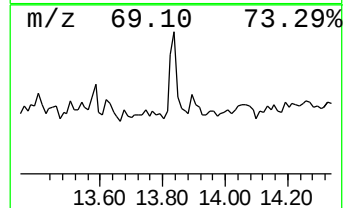
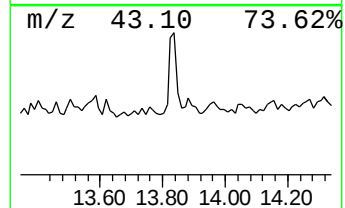
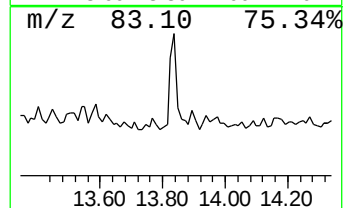
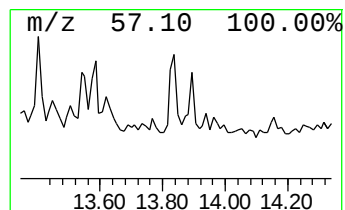
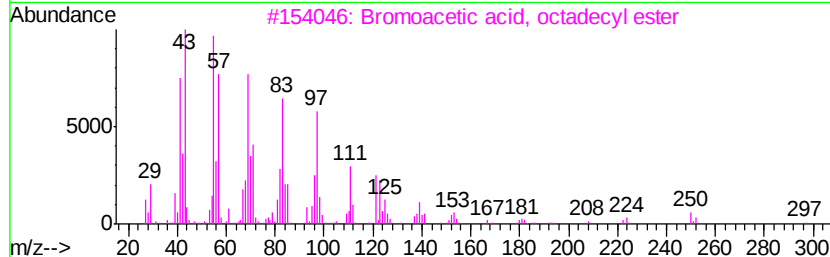
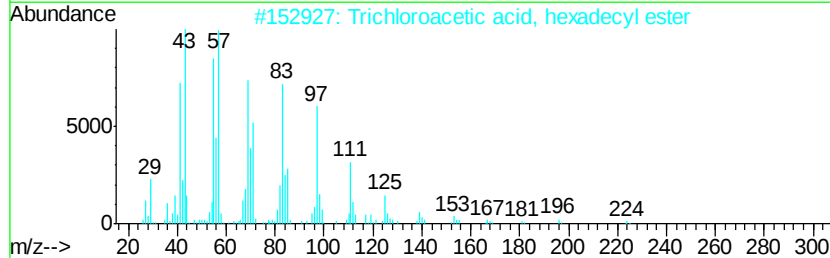
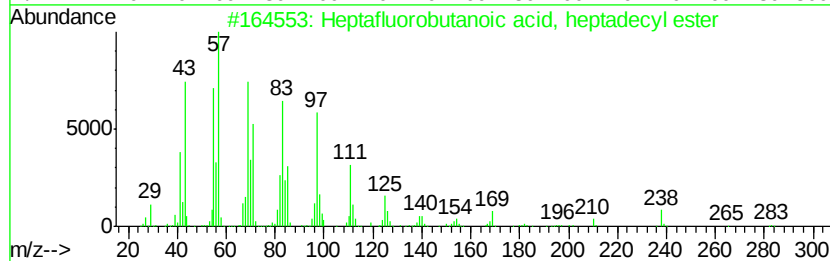
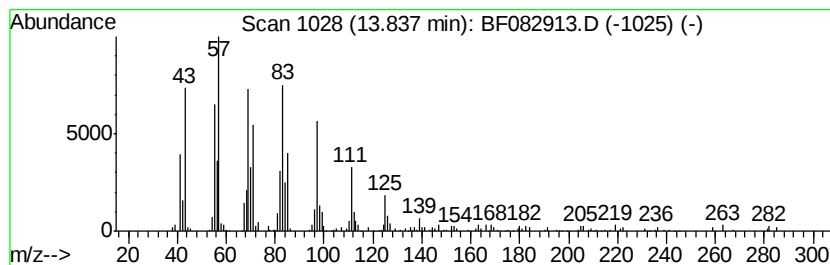
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptafluorobutanoic acid, h... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.84	3.47 ng	257012	Chrysene-d12	13.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	91
2		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90
3		Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	87
4		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	87
5		Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	81



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111315\
Data File : BF082913.D
Acq On : 13 Nov 2015 22:53
Operator : UM/IZ
Sample : G4370-02
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P001-TS002-01

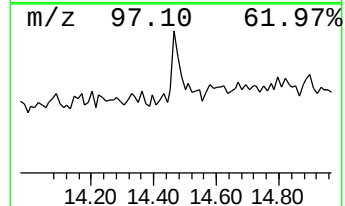
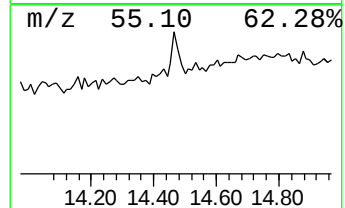
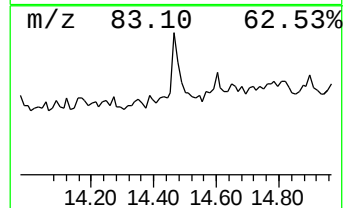
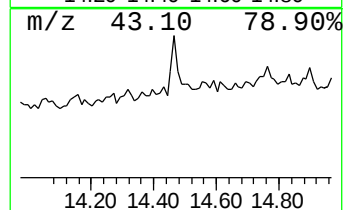
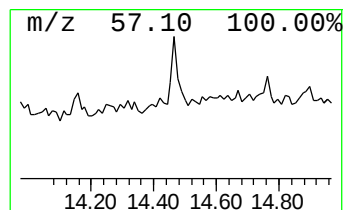
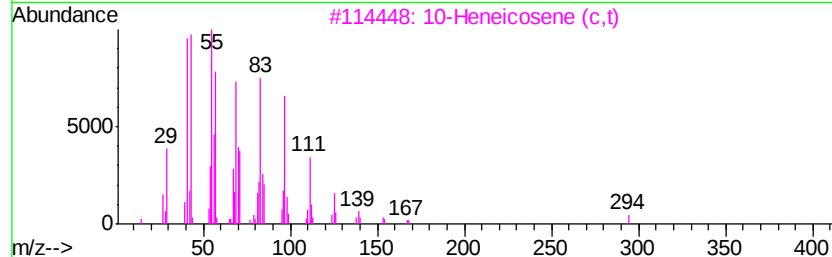
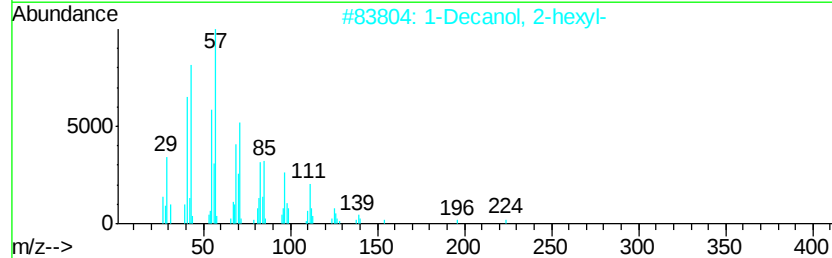
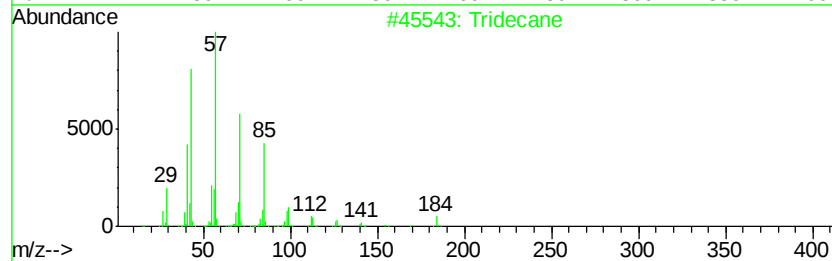
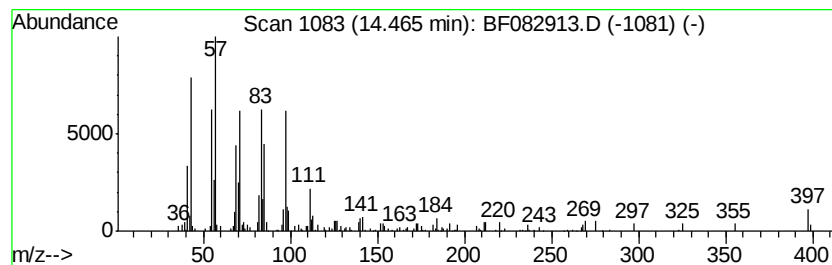
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tridecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.47	2.12 ng	157411	Chrysene-d12	13.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tridecane	184	C13H28	000629-50-5	55
2		1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	52
3		10-Heneicosene (c,t)	294	C21H42	095008-11-0	45
4		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	43
5		Pentadecane	212	C15H32	000629-62-9	42



Data Path : Z:\HPCHEM1\BNA F\DATA\BF111315\
Data File : BF082913.D
Acq On : 13 Nov 2015 22:53
Operator : UM/IZ
Sample : G4370-02
Misc :
ALS Vial : 23 Sample Multiplier: 1

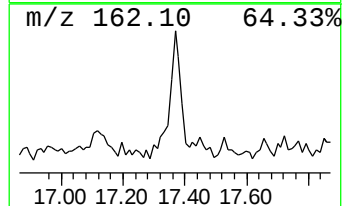
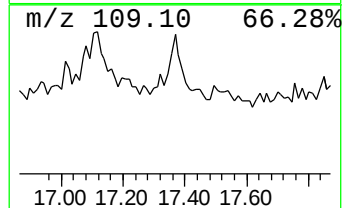
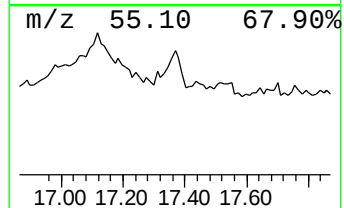
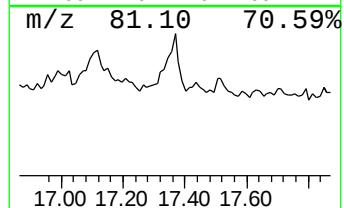
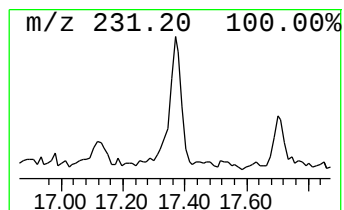
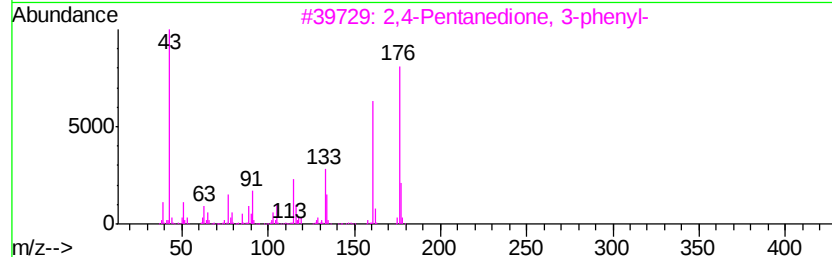
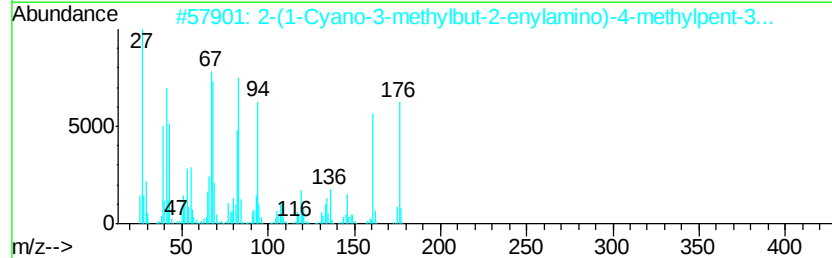
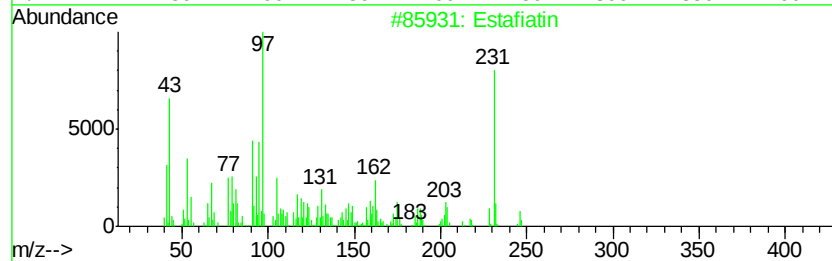
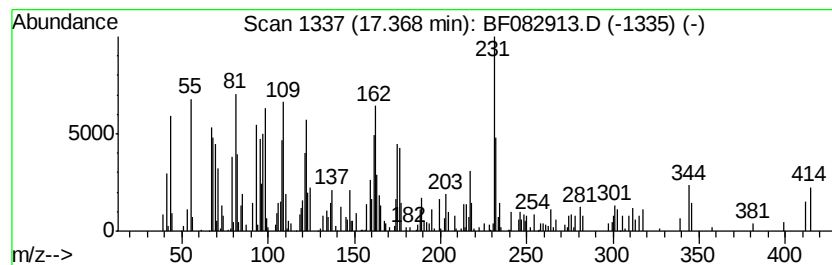
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF110715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown17.37 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.37	4.41 ng	321643	Perylene-d12	15.39
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Estafiatin	246	C15H18O3	010180-89-9 25
2	2-(1-Cyano-3-methylbut-2-enylami...	203	C12H17N3	1000191-53-7 11
3	2,4-Pentanedione, 3-phenyl-	176	C11H12O2	005910-25-8 11
4	1H-Indol-2(3H)-one, 3-aminomethyl-	162	C9H10N2O	1000262-27-9 11
5	4-Acetamido-6-methoxy-8-aminoqui...	231	C12H13N3O2	063456-99-5 11



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111315\
Data File : BF082913.D
Acq On : 13 Nov 2015 22:53
Operator : UM/IZ
Sample : G4370-02
Misc :
ALS Vial : 23 Sample Multiplier: 1

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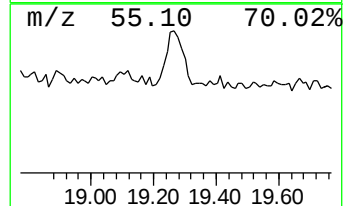
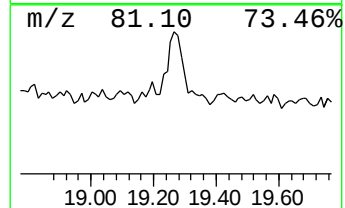
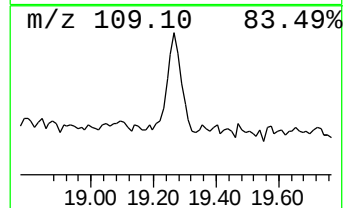
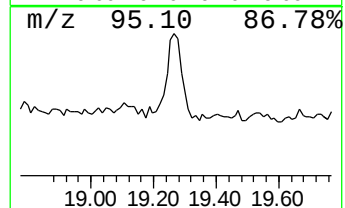
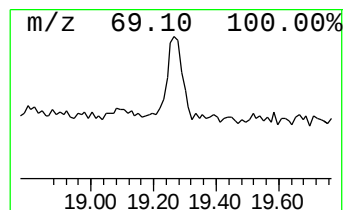
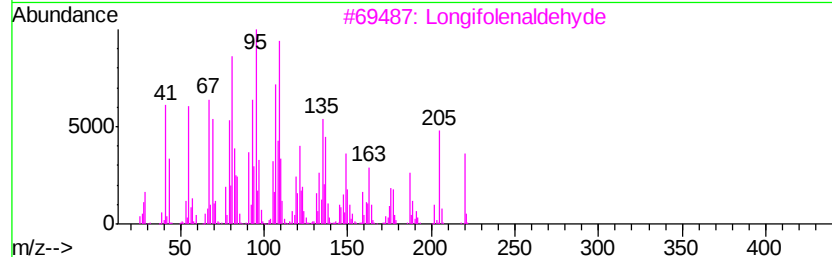
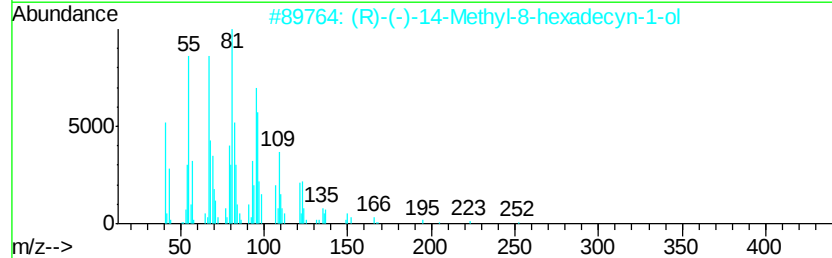
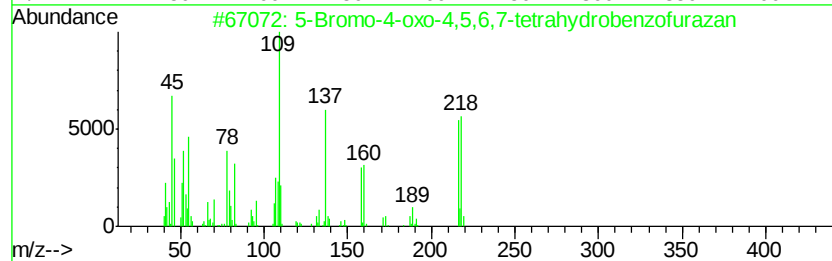
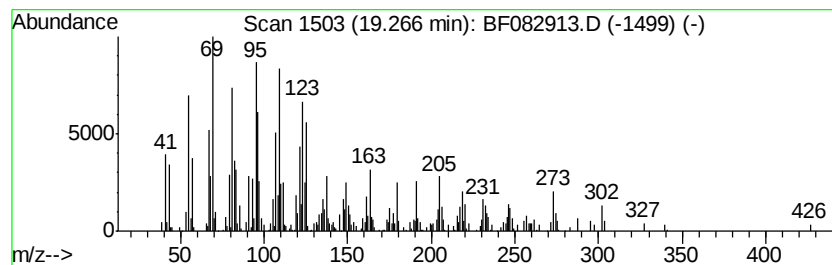
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 5-Bromo-4-oxo-4,5,6,7-tetra... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.27	8.84 ng	644177	Perylene-d12	15.39

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Bromo-4-oxo-4,5,6,7-tetrahydro...	216	C6H5BrN2O2	300574-36-1	59
2			(R)-(-)-14-Methyl-8-hexadecyn-1-ol	252	C17H32O	064566-18-3	49
3			Longifolenaldehyde	220	C15H24O	019890-84-7	49
4			2,2,6-Trimethyl-1-(2-methyl-cycl...	218	C15H22O	1000188-72-8	30
5			1-Hexadecyne	222	C16H30	000629-74-3	30



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111315\
Data File : BF082913.D
Acq On : 13 Nov 2015 22:53
Operator : UM/IZ
Sample : G4370-02
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.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...	4.98	24.3	ng	1903890	1	6.81	1567720	20.0
unknown6.59	6.59	49.4	ng	3871930	1	6.81	1567720	20.0
Tridecane, 1-iodo-	10.76	2.3	ng	215426	4	11.33	1870750	20.0
n-Hexadecanoic acid	11.88	3.0	ng	284285	4	11.33	1870750	20.0
unknown12.58	12.58	6.5	ng	605209	4	11.33	1870750	20.0
Heptafluorobutano...	13.84	3.5	ng	257012	5	13.97	1482180	20.0
Tridecane	14.47	2.1	ng	157411	5	13.97	1482180	20.0
unknown17.37	17.37	4.4	ng	321643	6	15.39	1457870	20.0
5-Bromo-4-oxo-4,5...	19.27	8.8	ng	644177	6	15.39	1457870	20.0