

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121315\
 Data File : BF083769.D
 Acq On : 14 Dec 2015 10:13
 Operator : UM/IZ
 Sample : G4648-19
 Misc :
 ALS Vial : 59 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-08(0-0.16)

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-BF121315.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	2.235	11	13	22	rVB2	17701	34682	1.15%	0.132%
2	5.116	262	265	269	rBV	478198	614108	20.45%	2.344%
3	5.527	298	301	304	rVB	2360645	2540447	84.58%	9.697%
4	6.544	387	390	393	rBV	2067742	2789886	92.89%	10.649%
5	6.693	400	403	405	rBV	2247270	3003563	100.00%	11.464%
6	6.750	405	408	413	rVB2	42739	51992	1.73%	0.198%
7	6.922	420	423	425	rBV	832454	766746	25.53%	2.927%
8	7.082	434	437	439	rBV	1821578	2103236	70.02%	8.028%
9	7.482	469	472	474	rBV	1883714	1993870	66.38%	7.610%
10	7.562	477	479	482	rVB	25100	35616	1.19%	0.136%
11	8.202	533	535	537	rBV	1155113	1004607	33.45%	3.835%
12	9.276	626	629	632	rBV	2522462	2465177	82.08%	9.409%
13	9.402	638	640	642	rVB	91656	94075	3.13%	0.359%
14	9.665	661	663	666	rVB	331956	375481	12.50%	1.433%
15	9.893	682	683	686	rBV	55100	40171	1.34%	0.153%
16	9.950	686	688	691	rBV	752399	981169	32.67%	3.745%
17	10.396	723	727	728	rBV	80996	93788	3.12%	0.358%
18	10.613	743	746	749	rBV	30658	48994	1.63%	0.187%
19	10.739	754	757	760	rVV	1665217	1545776	51.46%	5.900%
20	10.865	766	768	772	rVB	96357	107282	3.57%	0.409%
21	11.311	804	807	809	rBV	50601	52566	1.75%	0.201%
22	11.436	816	818	820	rBV	940352	829268	27.61%	3.165%
23	11.962	863	864	866	rBV	53826	51999	1.73%	0.198%
24	12.145	876	880	883	rBV2	22911	39418	1.31%	0.150%
25	12.476	908	909	912	rBV2	47843	59966	2.00%	0.229%
26	12.842	940	941	945	rVB2	148652	155971	5.19%	0.595%
27	12.922	947	948	950	rVB	86252	60868	2.03%	0.232%
28	13.014	954	956	959	rBV	1622608	1514758	50.43%	5.782%
29	13.174	968	970	973	rBV2	18154	32130	1.07%	0.123%
30	13.254	975	977	980	rVB	26951	31981	1.06%	0.122%
31	13.505	996	999	1000	rVB2	25366	38499	1.28%	0.147%
32	13.551	1000	1003	1006	rBV	175772	177457	5.91%	0.677%
33	13.597	1006	1007	1010	rVV2	58611	88017	2.93%	0.336%
34	13.677	1012	1014	1015	rVV2	46888	49258	1.64%	0.188%

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121315\
Data File : BF083769.D
Acq On : 14 Dec 2015 10:13
Operator : UM/IZ
Sample : G4648-19
Misc :
ALS Vial : 59 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-08(0-0.16)

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-BF121315.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.722	1015	1018	1021	rVB2	22959	41736	1.39%	0.159%
36	13.917	1033	1035	1038	rBV2	126356	188808	6.29%	0.721%
37	13.985	1038	1041	1044	rBV	41469	50436	1.68%	0.193%
38	14.031	1044	1045	1046	rBV	26814	32659	1.09%	0.125%
39	14.065	1046	1048	1050	rVB	687349	692293	23.05%	2.642%
40	14.237	1061	1063	1065	rVB	82135	78602	2.62%	0.300%
41	14.545	1088	1090	1092	rBV	104270	101736	3.39%	0.388%
42	14.739	1104	1107	1108	rBV3	27094	40313	1.34%	0.154%
43	14.785	1108	1111	1114	rVV	80503	143693	4.78%	0.548%
44	14.842	1114	1116	1118	rVV	70161	91487	3.05%	0.349%
45	14.922	1121	1123	1125	rVB	37369	39993	1.33%	0.153%
46	15.174	1143	1145	1149	rBV	59435	81991	2.73%	0.313%
47	15.505	1171	1174	1177	rBV	436999	557701	18.57%	2.129%
48	15.551	1177	1178	1185	rVB	46025	66692	2.22%	0.255%
49	15.985	1213	1216	1218	rBV	30519	43722	1.46%	0.167%
50	16.477	1257	1259	1262	rBV2	19223	41025	1.37%	0.157%
51	17.745	1368	1370	1376	rVB5	11899	33392	1.11%	0.127%

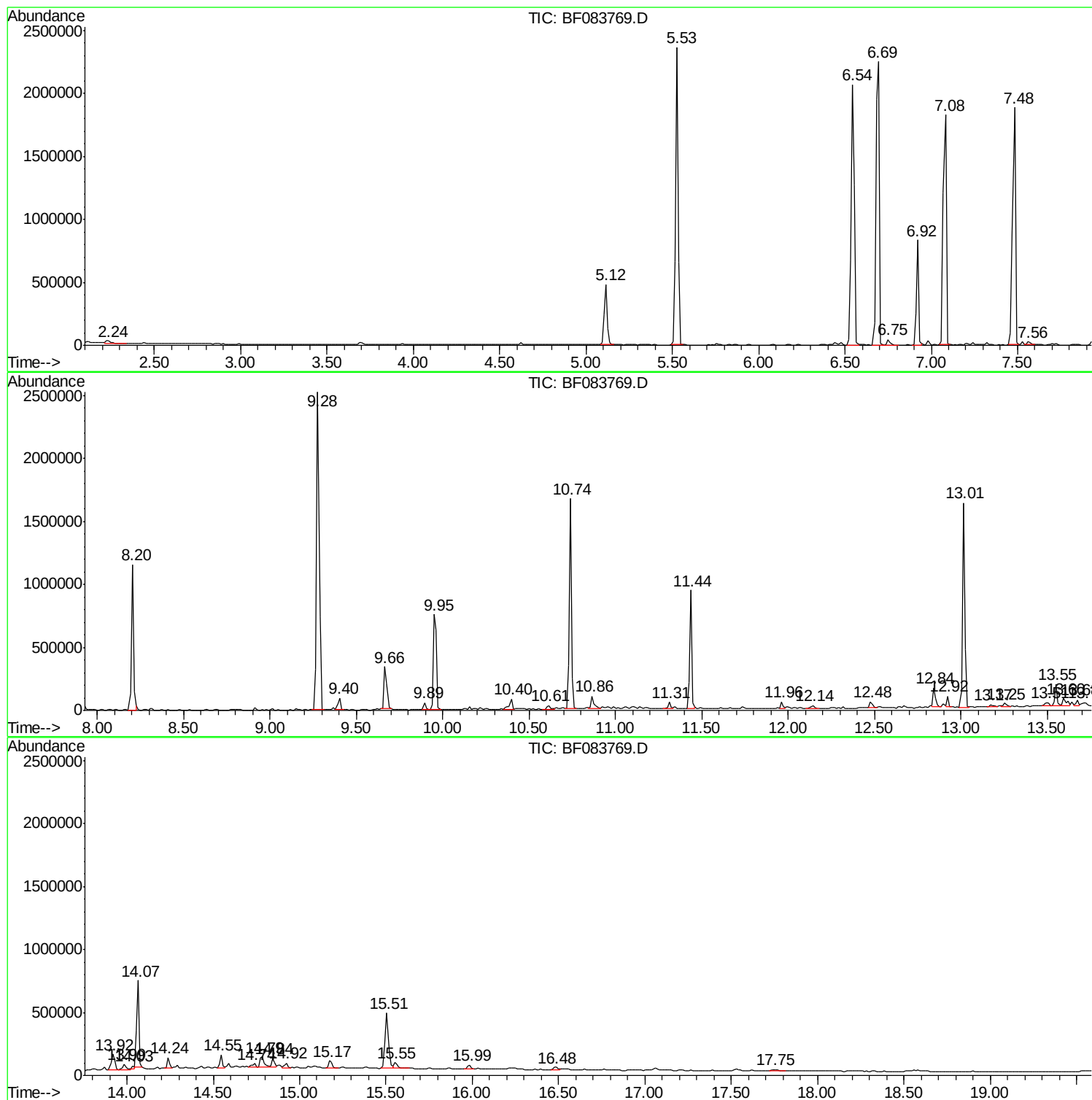
Sum of corrected areas: 26199101

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121315\
Data File : BF083769.D
Acq On : 14 Dec 2015 10:13
Operator : UM/IZ
Sample : G4648-19
Misc :
ALS Vial : 59 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-08(0-0.16)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
Data File : BF083769.D
Acq On : 14 Dec 2015 10:13
Operator : UM/IZ
Sample : G4648-19
Misc :
ALS Vial : 59 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-08(0-0.16)

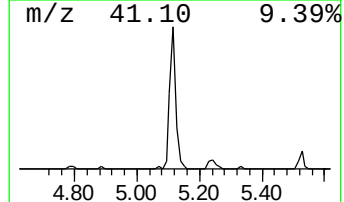
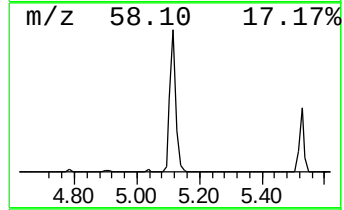
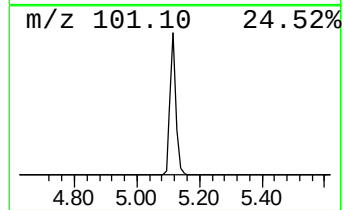
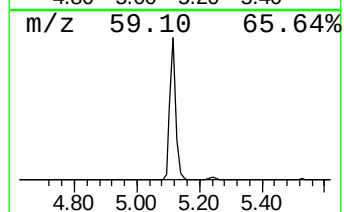
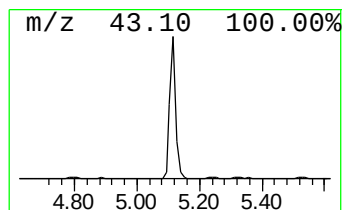
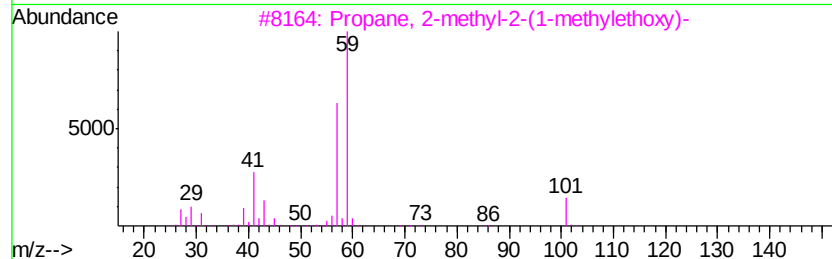
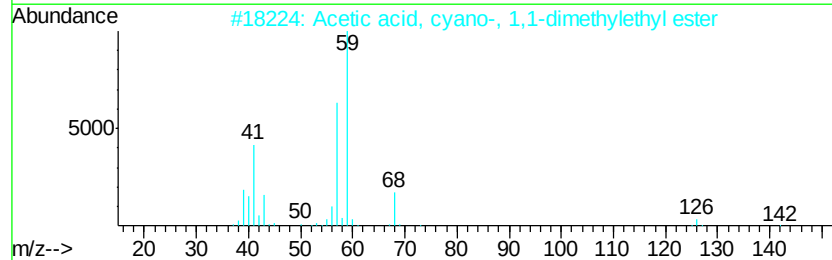
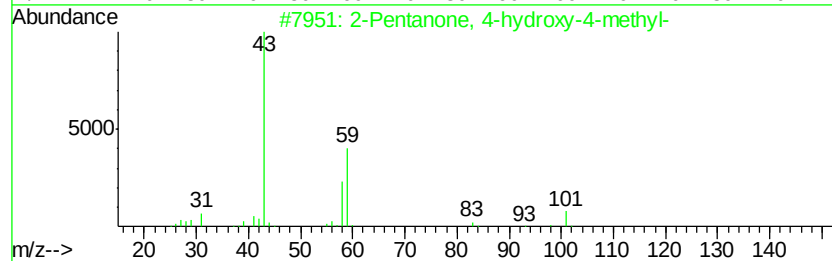
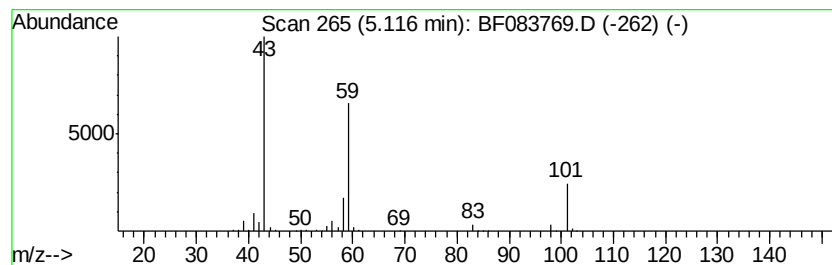
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.12	16.02 ng	614108	1,4-Dichlorobenzene-d4	6.92

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, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	23
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
Data File : BF083769.D
Acq On : 14 Dec 2015 10:13
Operator : UM/IZ
Sample : G4648-19
Misc :
ALS Vial : 59 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-08(0-0.16)

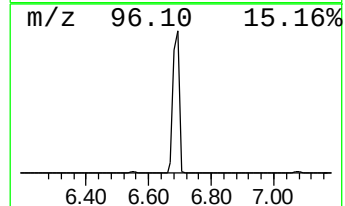
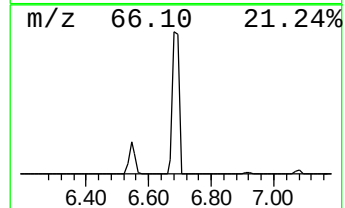
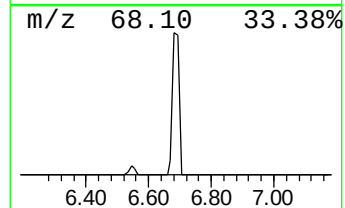
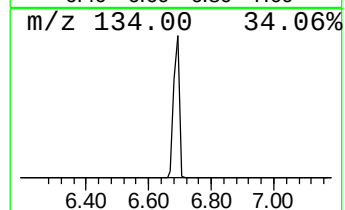
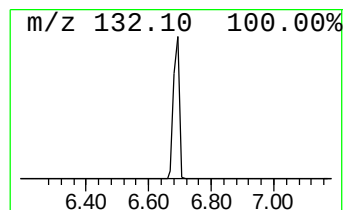
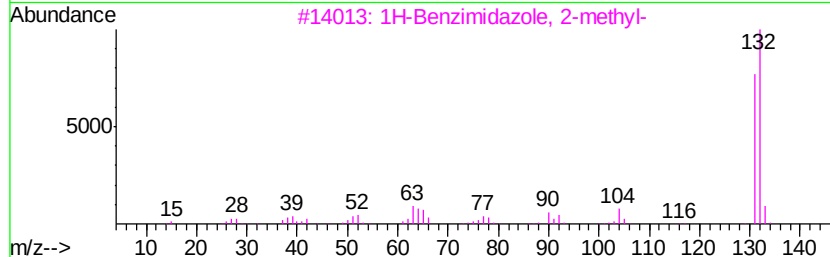
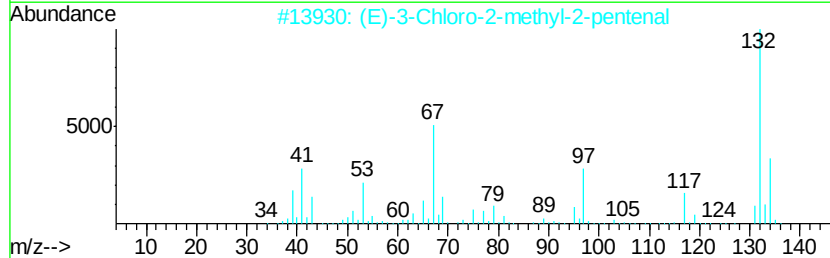
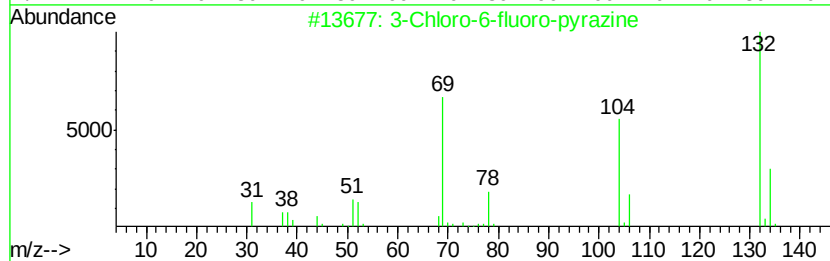
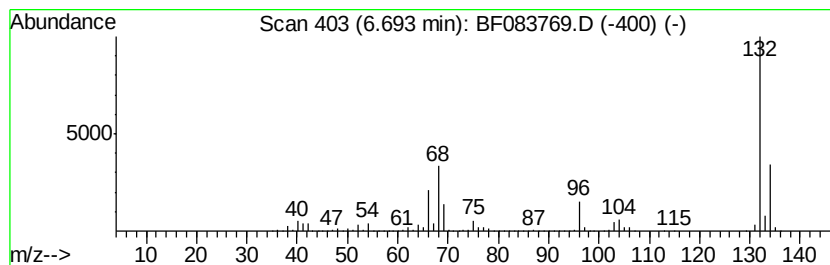
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	78.35 ng	3003560	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	12
4		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
Data File : BF083769.D
Acq On : 14 Dec 2015 10:13
Operator : UM/IZ
Sample : G4648-19
Misc :
ALS Vial : 59 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-08(0-0.16)

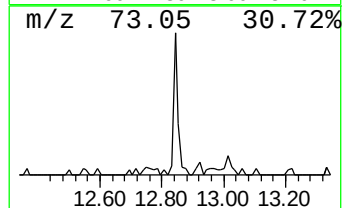
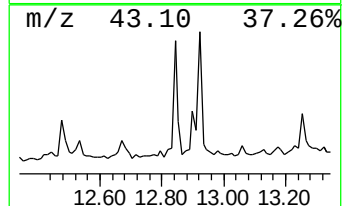
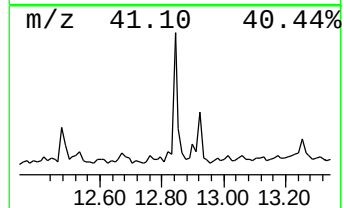
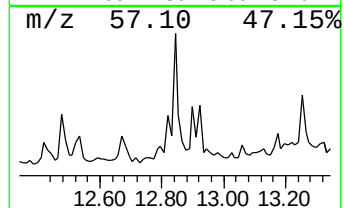
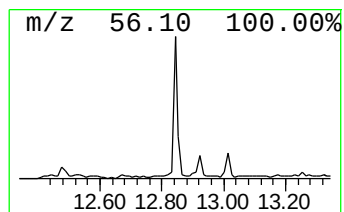
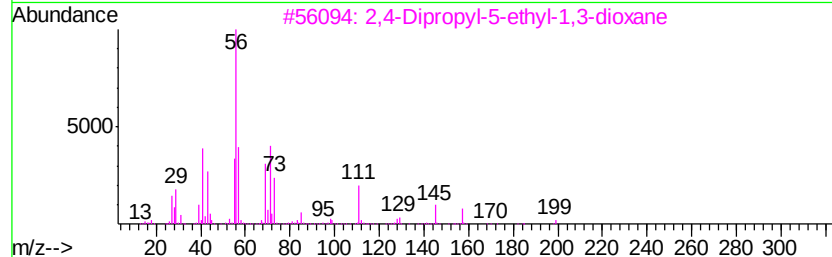
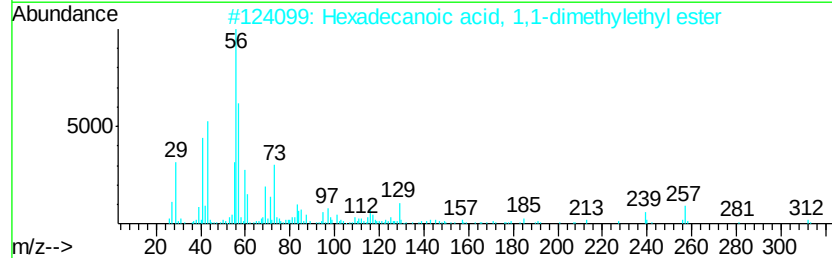
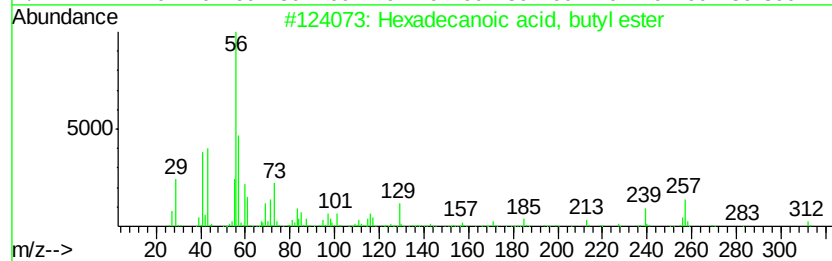
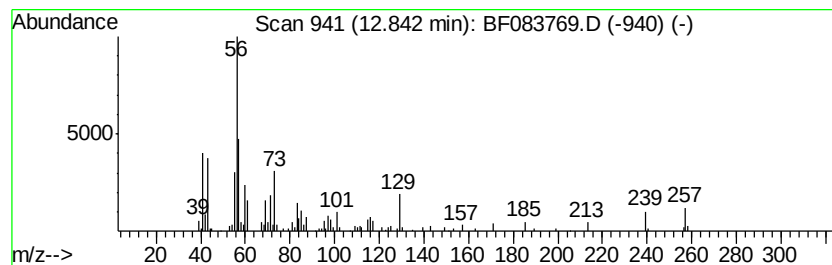
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Hexadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.84	4.51 ng	155971	Chrysene-d12	14.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	91
3		2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	38
4		Cyclopropane, 1-(1-methylethyl)-...	210	C15H30	041977-39-3	35
5		Cyclohexanol, 2-amino-, trans-	115	C6H13NO	006982-39-4	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121315\
Data File : BF083769.D
Acq On : 14 Dec 2015 10:13
Operator : UM/IZ
Sample : G4648-19
Misc :
ALS Vial : 59 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-08(0-0.16)

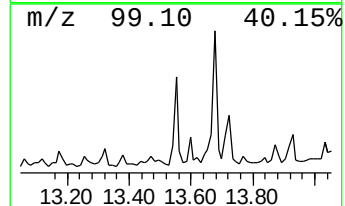
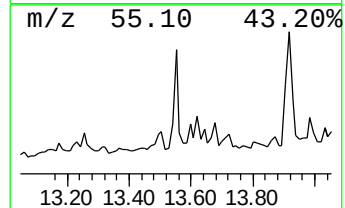
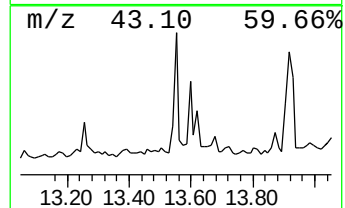
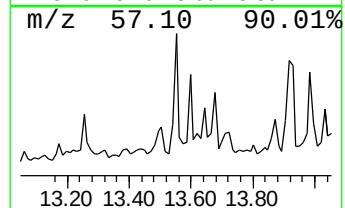
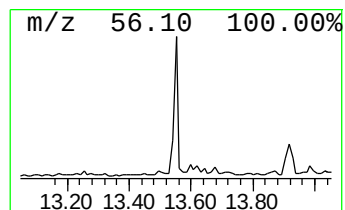
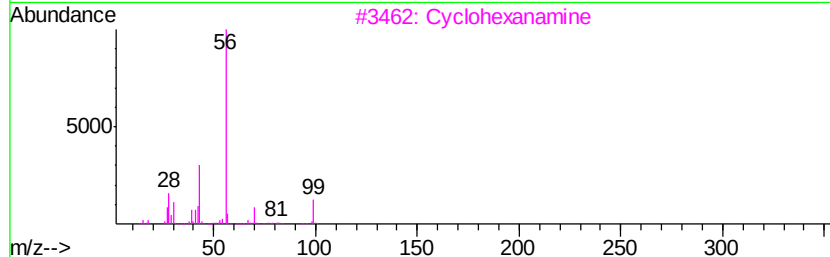
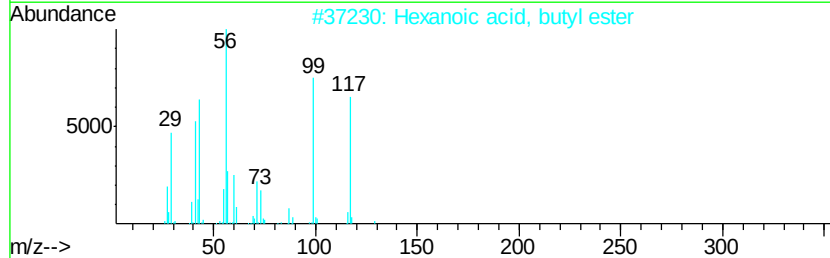
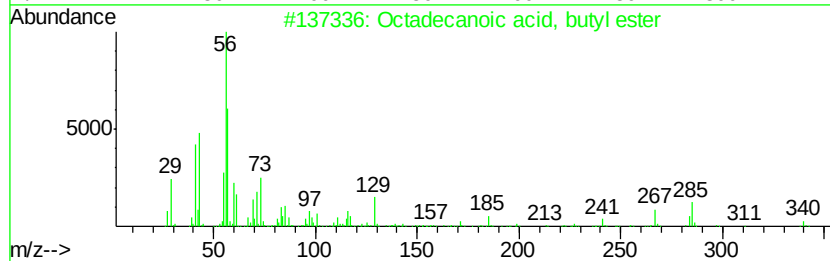
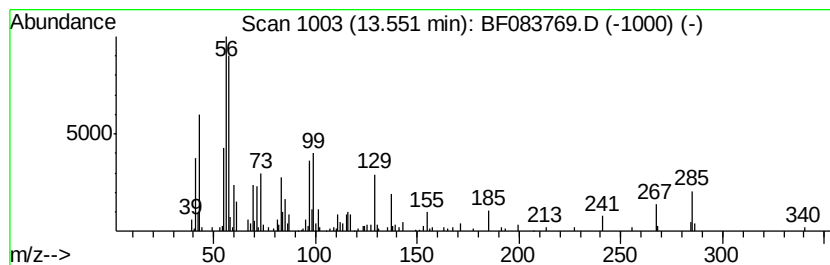
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown13.55 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.55	5.13 ng	177457	Chrysene-d12	14.07

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	49
2		Hexanoic acid, butyl ester	172	C10H20O2	000626-82-4	47
3		Cyclohexanamine	99	C6H13N	000108-91-8	35
4		Cyclohexane, 1-(1,1-dimethylethy...	154	C11H22	075736-66-2	27
5		5-Methyl-2-hexyl methylphosphono...	196	C8H18FO2P	199850-62-9	25



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
Data File : BF083769.D
Acq On : 14 Dec 2015 10:13
Operator : UM/IZ
Sample : G4648-19
Misc :
ALS Vial : 59 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-08(0-0.16)

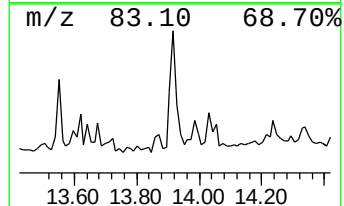
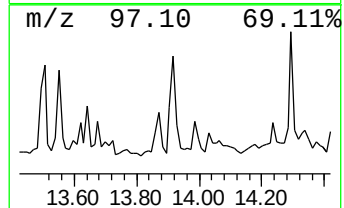
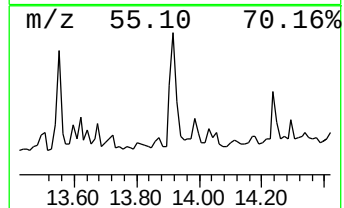
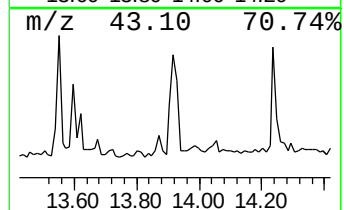
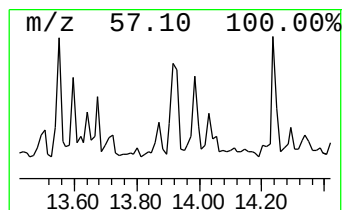
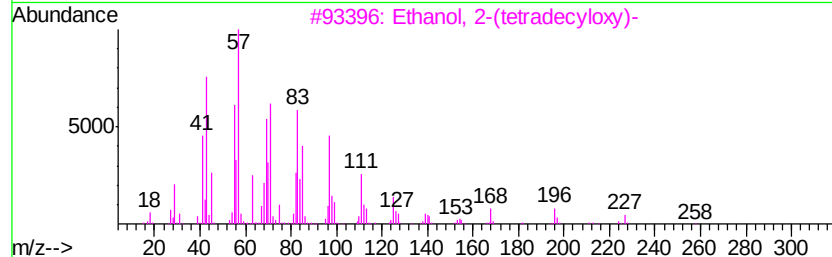
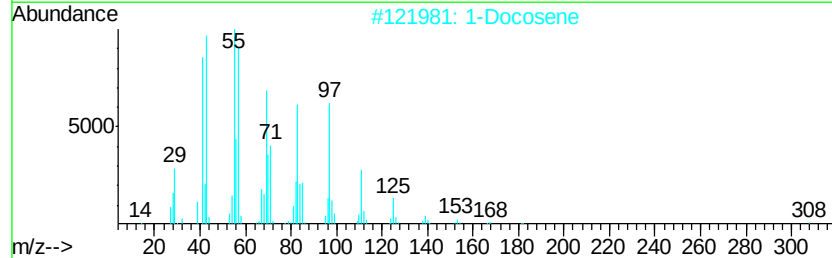
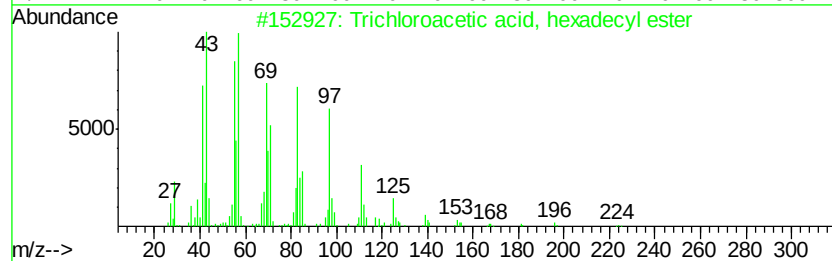
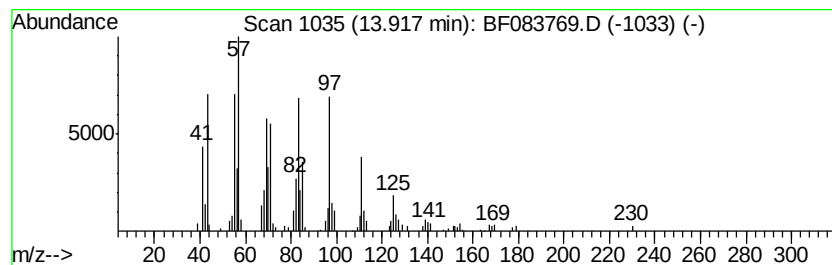
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Trichloroacetic acid, hexad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.92	5.45 ng	188808	Chrysene-d12	14.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
2		1-Docosene	308	C22H44	001599-67-3	91
3		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
4		17-Pentatriacontene	491	C35H70	006971-40-0	90
5		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	83



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121315\
Data File : BF083769.D
Acq On : 14 Dec 2015 10:13
Operator : UM/IZ
Sample : G4648-19
Misc :
ALS Vial : 59 Sample Multiplier: 1

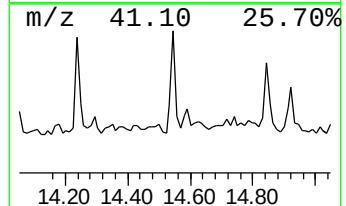
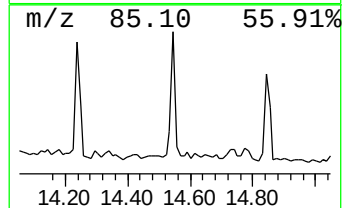
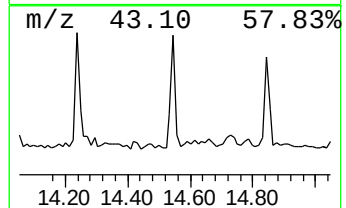
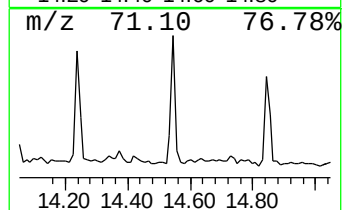
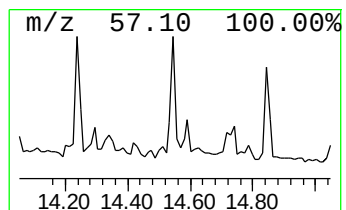
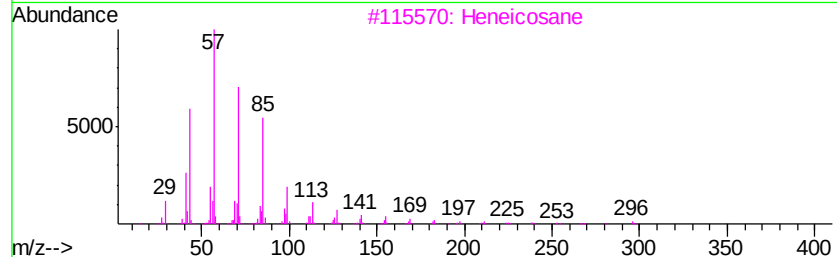
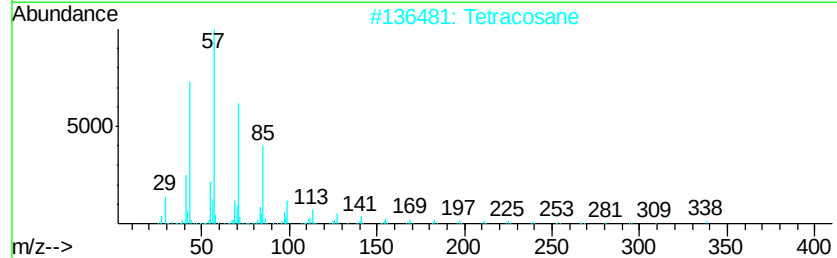
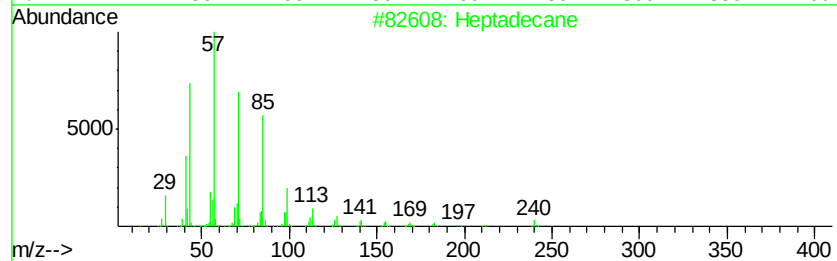
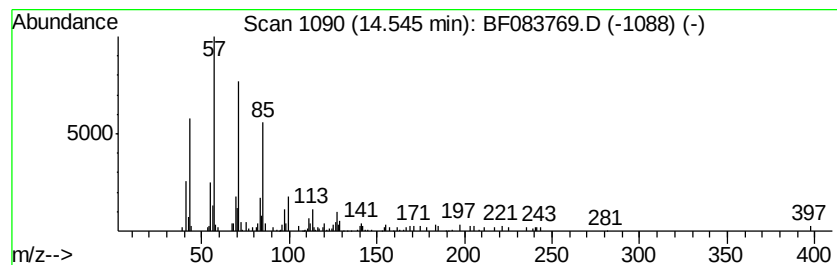
Instrument :
BNA_F
ClientSampleId :
SB-08(0-0.16)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.55	2.94 ng	101736	Chrysene-d12		14.07
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	94
2	Tetracosane	338	C24H50	000646-31-1	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Nonacosane	408	C29H60	000630-03-5	90
5	Heptadecane, 8-methyl-	254	C18H38	013287-23-5	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121315\
Data File : BF083769.D
Acq On : 14 Dec 2015 10:13
Operator : UM/IZ
Sample : G4648-19
Misc :
ALS Vial : 59 Sample Multiplier: 1

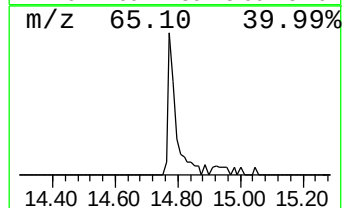
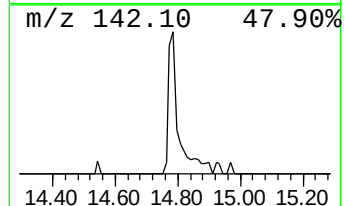
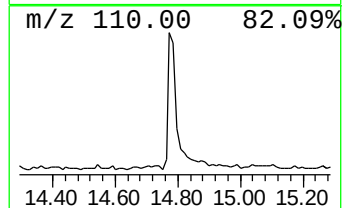
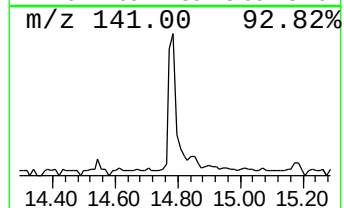
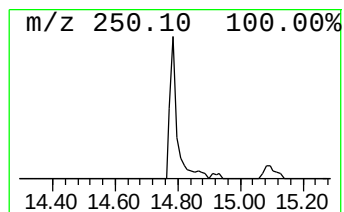
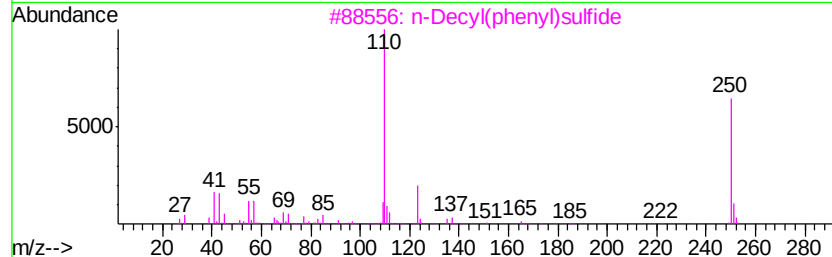
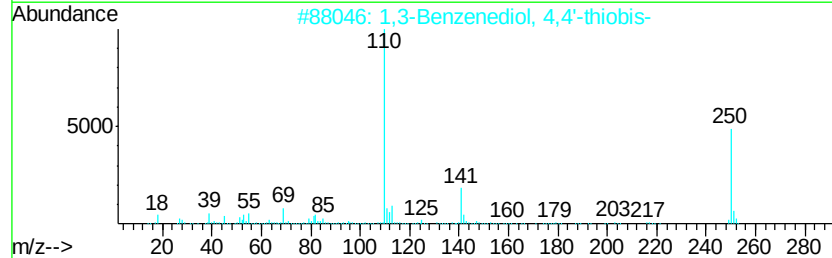
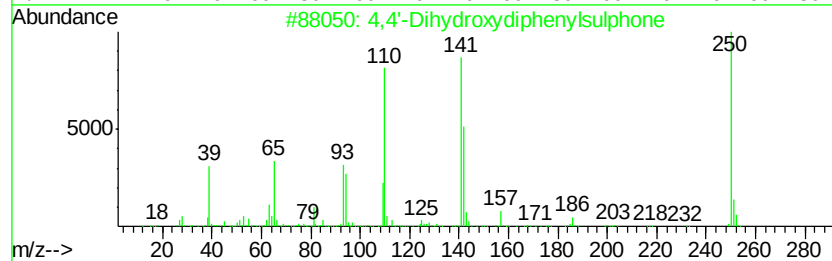
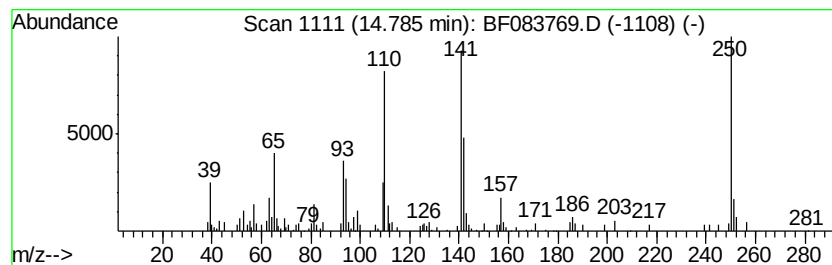
Instrument :
BNA_F
ClientSampleId :
SB-08(0-0.16)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 4,4'-Dihydroxydiphenylsulphone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.79	4.15 ng	143693	Chrysene-d12	14.07	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,4'-Dihydroxydiphenylsulphone	250	C12H10O4S	000080-09-1	99
2	1,3-Benzenediol, 4,4'-thiobis-	250	C12H10O4S	000097-29-0	43
3	n-Decyl(phenyl)sulfide	250	C16H26S	013910-18-4	30
4	[2,2'-Bifuran]-5,5'-dicarboxylic...	250	C12H10O6	005905-02-2	10
5	[(4-Hydroxyphenoxy)formamido]sul...	279	C7H6F5N3S	090597-98-1	10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121315\
Data File : BF083769.D
Acq On : 14 Dec 2015 10:13
Operator : UM/IZ
Sample : G4648-19
Misc :
ALS Vial : 59 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-08(0-0.16)

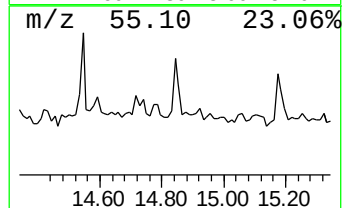
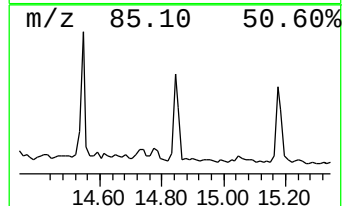
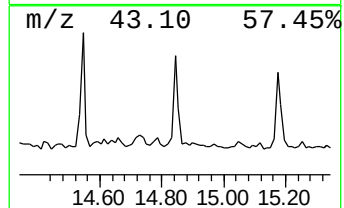
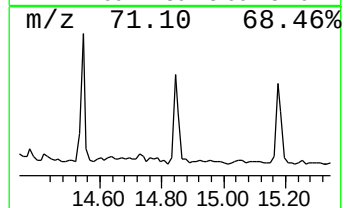
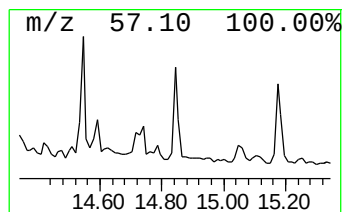
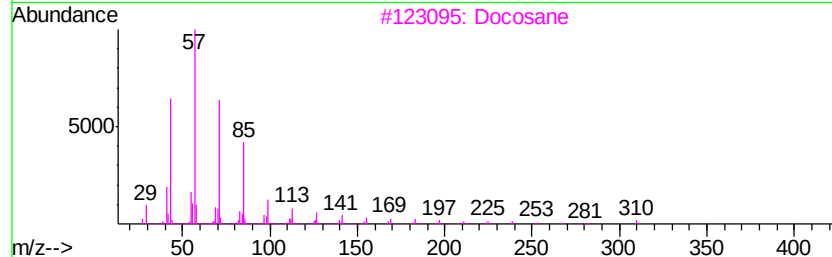
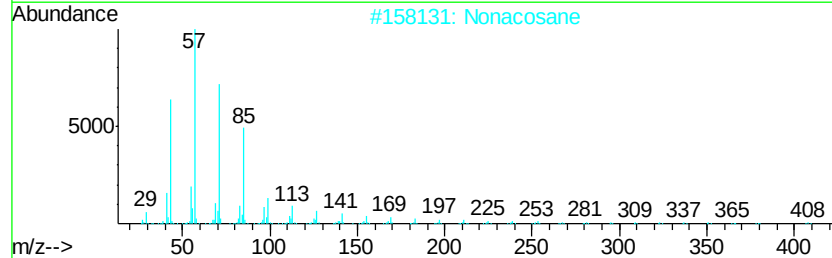
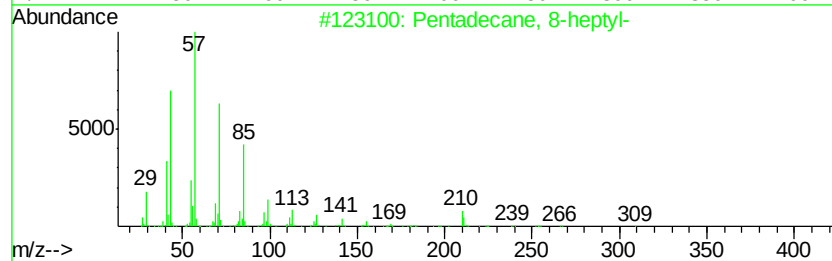
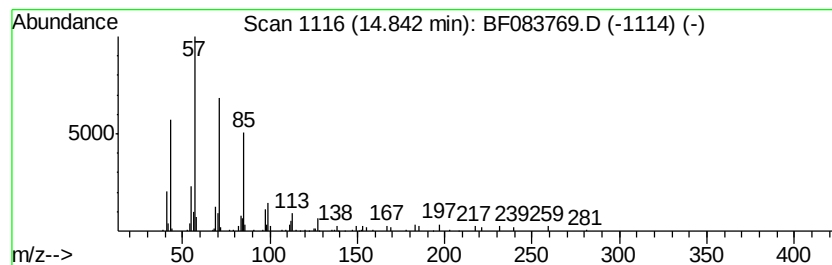
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Pentadecane, 8-heptyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.84	3.28 ng	91487	Perylene-d12	15.51

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	86	
2	Nonacosane	408	C29H60	000630-03-5	86	
3	Docosane	310	C22H46	000629-97-0	78	
4	Tetratriacontane	479	C34H70	014167-59-0	78	
5	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	78	



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121315\
Data File : BF083769.D
Acq On : 14 Dec 2015 10:13
Operator : UM/IZ
Sample : G4648-19
Misc :
ALS Vial : 59 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-08(0-0.16)

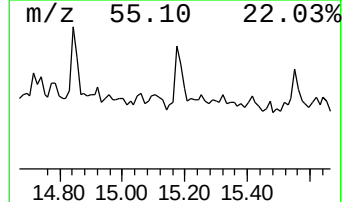
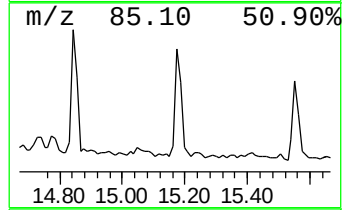
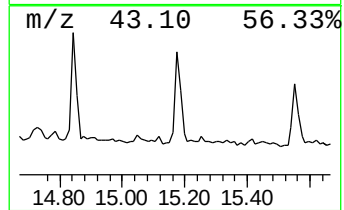
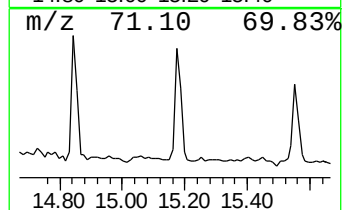
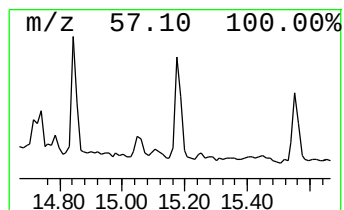
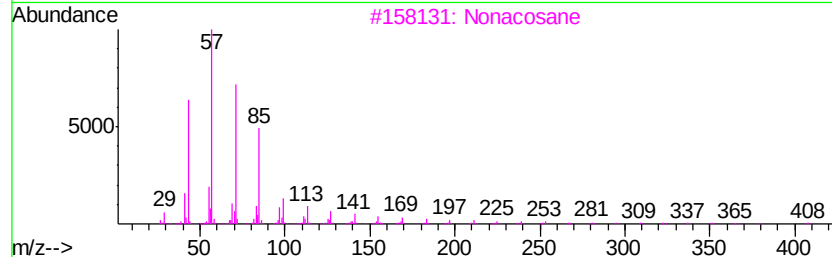
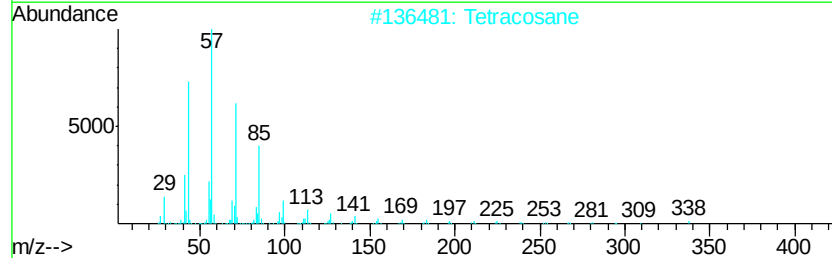
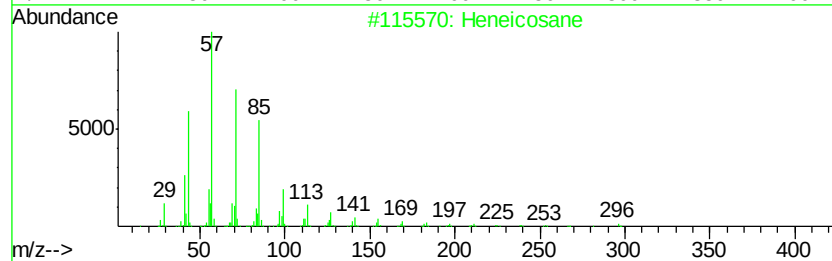
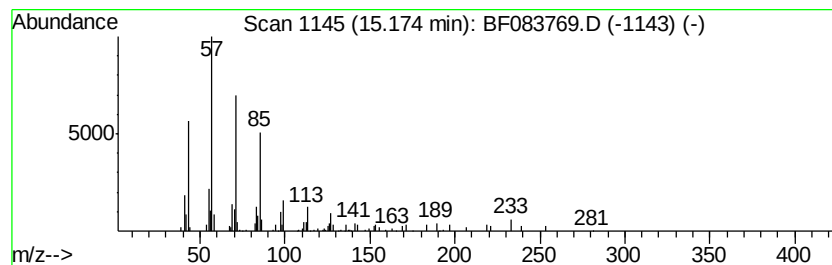
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.17	2.94 ng	81991	Perylene-d12	15.51

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	87
2		Tetracosane	338	C24H50	000646-31-1	86
3		Nonacosane	408	C29H60	000630-03-5	86
4		Hexadecane	226	C16H34	000544-76-3	86
5		Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121315\
Data File : BF083769.D
Acq On : 14 Dec 2015 10:13
Operator : UM/IZ
Sample : G4648-19
Misc :
ALS Vial : 59 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-08(0-0.16)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.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...	5.12	16.0	ng	614108	1	6.92	766746	20.0
unknown6.69	6.69	78.3	ng	3003560	1	6.92	766746	20.0
Hexadecanoic acid...	12.84	4.5	ng	155971	5	14.07	692293	20.0
unknown13.55	13.55	5.1	ng	177457	5	14.07	692293	20.0
Trichloroacetic a...	13.92	5.5	ng	188808	5	14.07	692293	20.0
Heptadecane	14.55	2.9	ng	101736	5	14.07	692293	20.0
4,4'-Dihydroxydip...	14.79	4.2	ng	143693	5	14.07	692293	20.0
Pentadecane, 8-he...	14.84	3.3	ng	91487	6	15.51	557701	20.0
Heneicosane	15.17	2.9	ng	81991	6	15.51	557701	20.0