

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062416\
 Data File : BF088353.D
 Acq On : 25 Jun 2016 1:40
 Operator : UM/SJ
 Sample : H3607-05
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TE-MW-2-23D

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-BF060716.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.712	10	11	27	rVB	1200775	2403659	89.65%	10.963%
2	4.707	271	273	286	rBV	36354	63116	2.35%	0.288%
3	5.176	312	314	326	rBV	699455	1057039	39.42%	4.821%
4	6.250	406	408	415	rBV	540560	665937	24.84%	3.037%
5	6.353	415	417	420	rBV	1568557	1752724	65.37%	7.994%
6	6.582	435	437	443	rBV	512023	543630	20.27%	2.479%
7	6.742	449	451	453	rBV	1766850	1906626	71.11%	8.696%
8	7.039	474	477	485	rBV	78688	164797	6.15%	0.752%
9	7.164	485	488	490	rBV	1255602	1537535	57.34%	7.012%
10	7.873	547	550	552	rBV	606428	702215	26.19%	3.203%
11	8.947	641	644	647	rBV	2057060	2681292	100.00%	12.229%
12	9.348	677	679	683	rVB	45982	43116	1.61%	0.197%
13	9.610	700	702	705	rBV	635420	744091	27.75%	3.394%
14	10.056	739	741	743	rVB2	38170	42755	1.59%	0.195%
15	10.410	769	772	774	rBV	974037	1301252	48.53%	5.935%
16	10.525	780	782	789	rVB2	34814	61372	2.29%	0.280%
17	11.096	829	832	834	rBV	440422	626472	23.36%	2.857%
18	11.839	895	897	906	rVB3	57482	110813	4.13%	0.505%
19	12.514	953	956	958	rBV	454061	565547	21.09%	2.579%
20	12.559	958	960	961	rBV	43907	38397	1.43%	0.175%
21	12.582	961	962	965	rVB	107157	96021	3.58%	0.438%
22	12.674	967	970	973	rBV	1797330	1911783	71.30%	8.719%
23	12.914	985	991	993	rBV	38410	42615	1.59%	0.194%
24	13.211	1015	1017	1019	rBV	439507	390436	14.56%	1.781%
25	13.256	1019	1021	1022	rBV	82641	84823	3.16%	0.387%
26	13.439	1035	1037	1038	rBV	32105	48539	1.81%	0.221%
27	13.474	1038	1040	1044	rVB	18255	30137	1.12%	0.137%
28	13.576	1047	1049	1055	rVB	117650	153731	5.73%	0.701%
29	13.714	1059	1061	1065	rBV2	562783	693992	25.88%	3.165%
30	13.897	1074	1077	1079	rBV	118296	120080	4.48%	0.548%
31	14.194	1101	1103	1106	rBV	88469	105879	3.95%	0.483%
32	14.491	1125	1129	1131	rBV	133088	146992	5.48%	0.670%
33	14.777	1152	1154	1157	rBV	113937	118447	4.42%	0.540%
34	15.074	1177	1180	1191	rBV	399069	598279	22.31%	2.729%

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062416\
Data File : BF088353.D
Acq On : 25 Jun 2016 1:40
Operator : UM/SJ
Sample : H3607-05
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TE-MW-2-23D

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-BF060716.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.451	1210	1213	1216	rBV	63059	93762	3.50%	0.428%
36	15.862	1246	1249	1252	rBV	46958	76833	2.87%	0.350%
37	16.342	1288	1291	1294	rBV	23594	48493	1.81%	0.221%
38	16.754	1323	1327	1332	rBV4	39356	110296	4.11%	0.503%
39	16.914	1338	1341	1346	rVB2	18549	42222	1.57%	0.193%

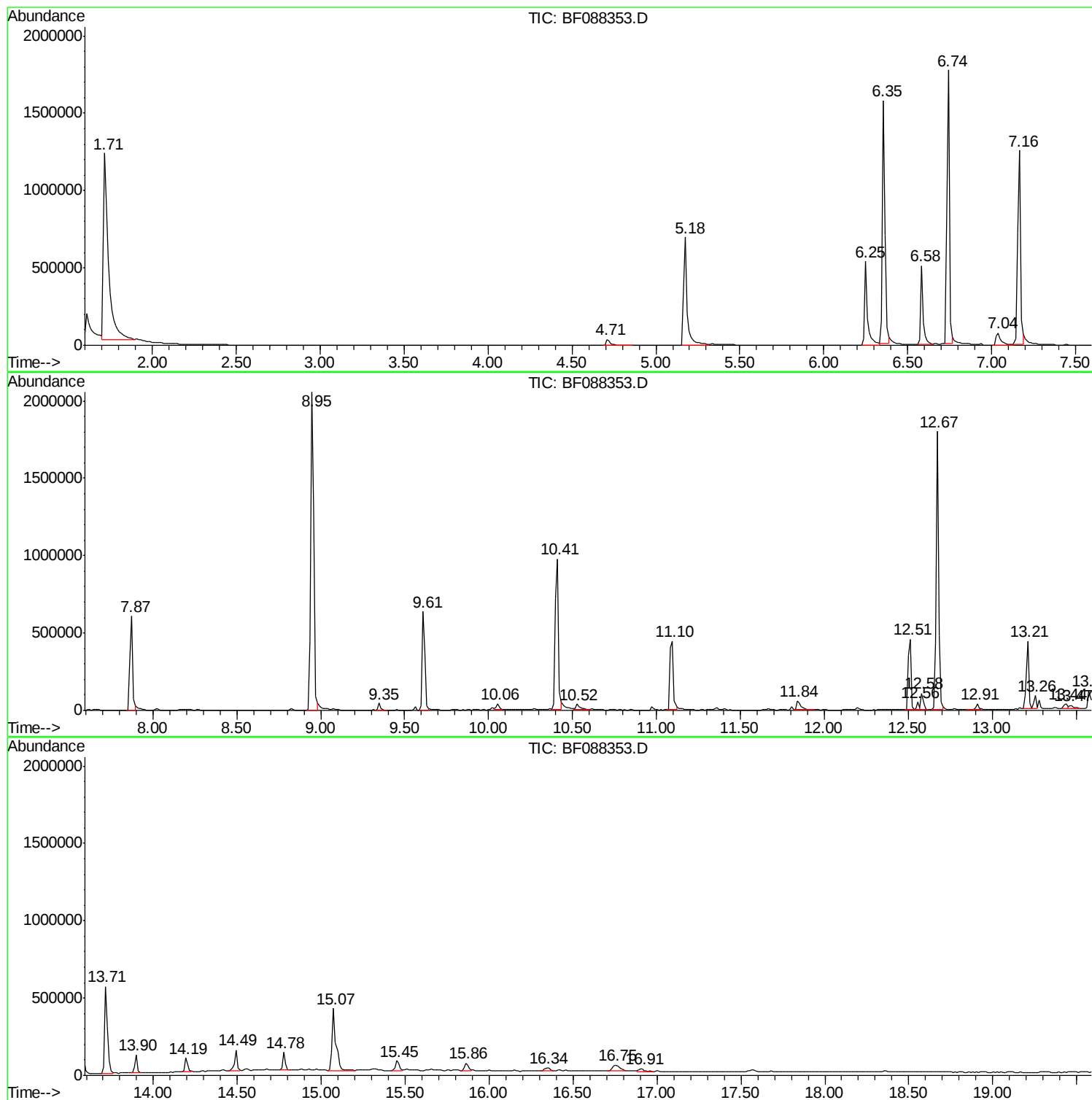
Sum of corrected areas: 21925745

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062416\
Data File : BF088353.D
Acq On : 25 Jun 2016 1:40
Operator : UM/SJ
Sample : H3607-05
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TE-MW-2-23D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062416\
Data File : BF088353.D
Acq On : 25 Jun 2016 1:40
Operator : UM/SJ
Sample : H3607-05
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TE-MW-2-23D

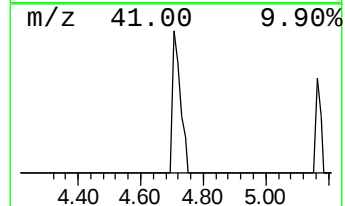
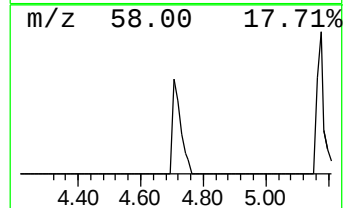
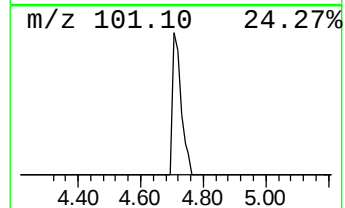
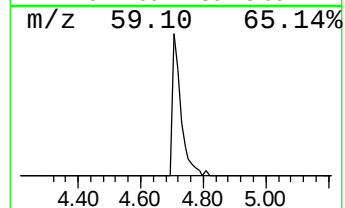
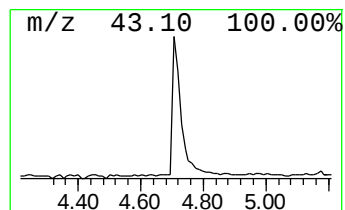
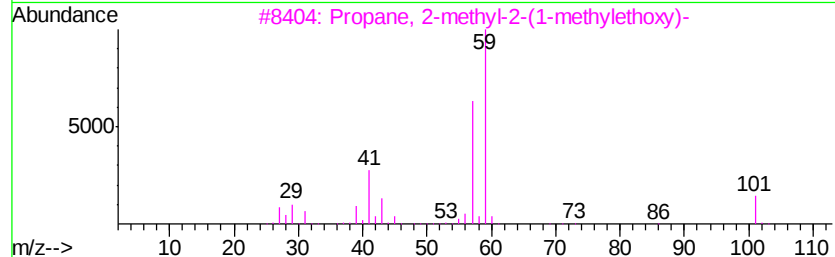
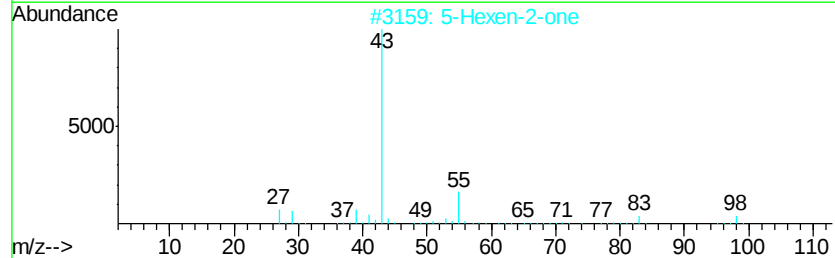
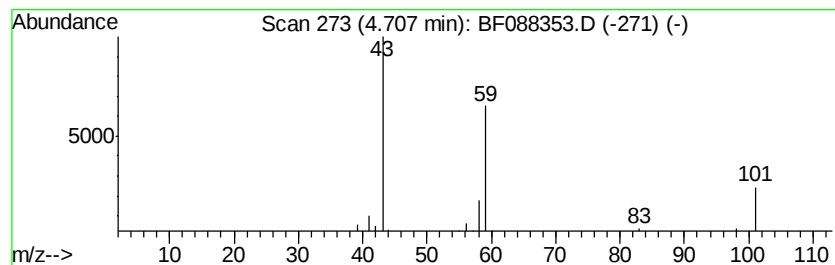
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.71	2.32 ng	63116	1,4-Dichlorobenzene-d4	6.58

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		5-Hexen-2-one	98	C6H10O	000109-49-9	9
3		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	9
4		3-Octanol	130	C8H18O	000589-98-0	9
5		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062416\
Data File : BF088353.D
Acq On : 25 Jun 2016 1:40
Operator : UM/SJ
Sample : H3607-05
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TE-MW-2-23D

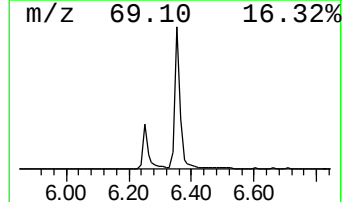
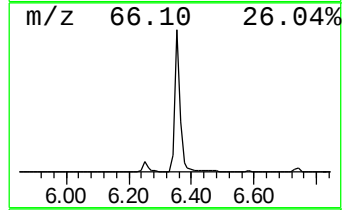
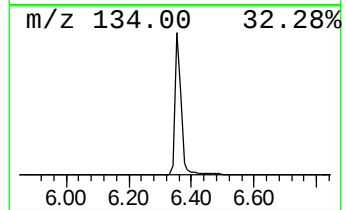
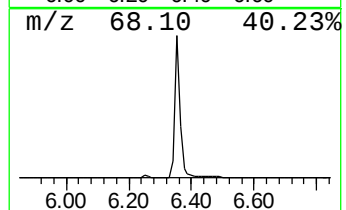
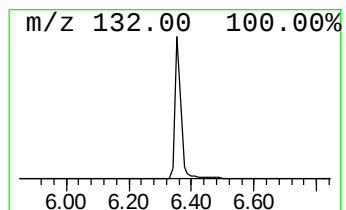
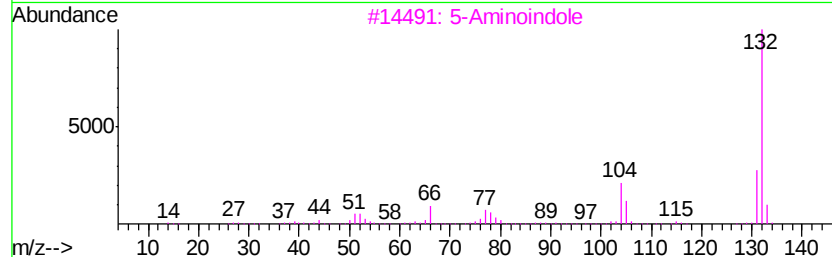
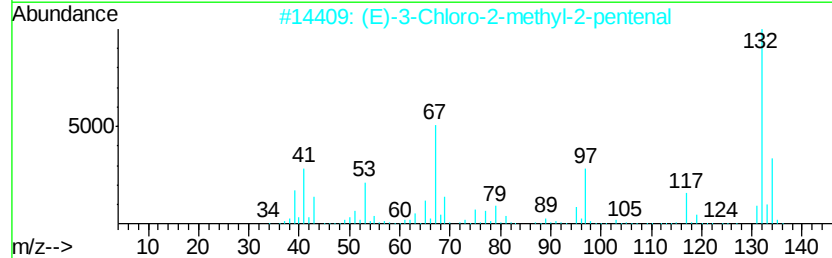
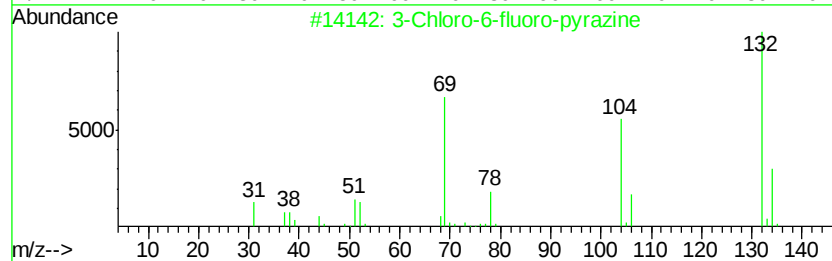
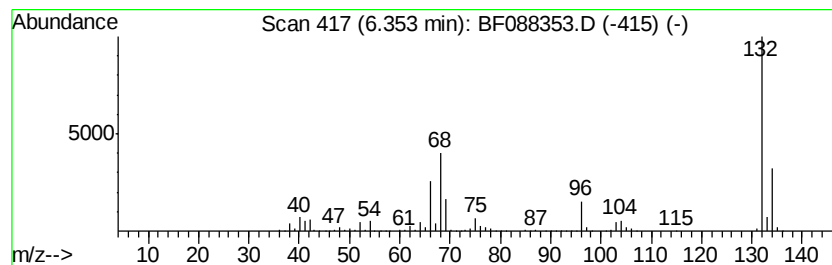
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.35 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.35	64.48 ng	1752720	1,4-Dichlorobenzene-d4	6.58

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	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062416\
Data File : BF088353.D
Acq On : 25 Jun 2016 1:40
Operator : UM/SJ
Sample : H3607-05
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TE-MW-2-23D

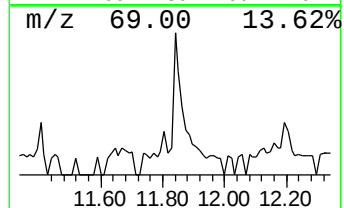
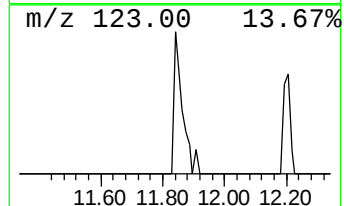
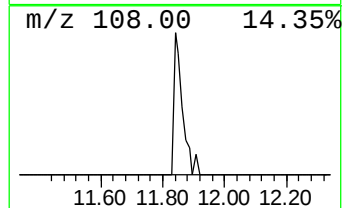
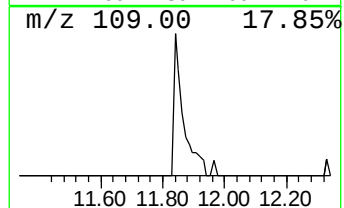
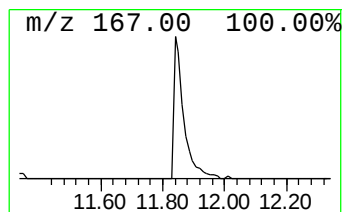
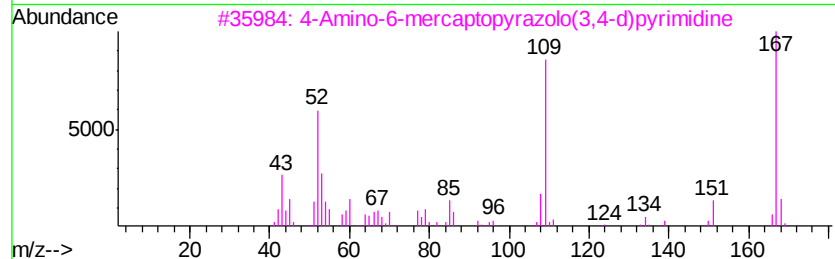
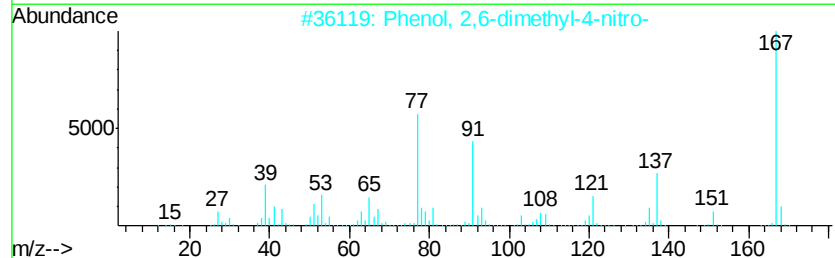
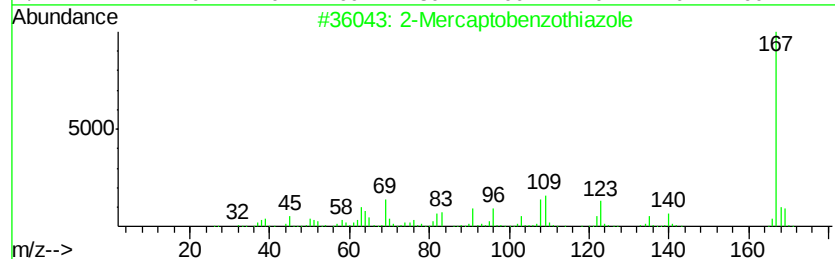
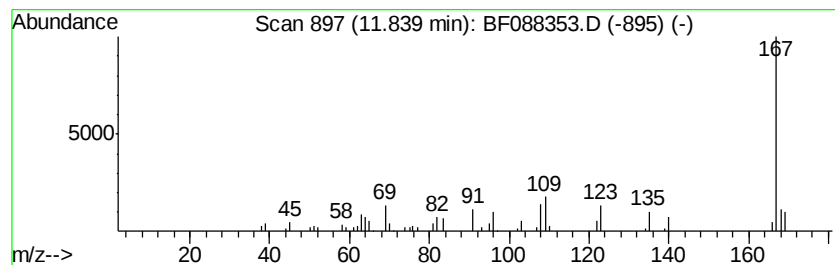
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 2-Mercaptobenzothiazole Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.84	3.54 ng	110813	Phenanthrene-d10	11.10

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Mercaptobenzothiazole	167	C7H5NS2	000149-30-4	97
2		Phenol, 2,6-dimethyl-4-nitro-	167	C8H9NO3	002423-71-4	53
3		4-Amino-6-mercaptopyrazolo(3,4-d...	167	C5H5N5S	023771-52-0	50
4		Thioguanine	167	C5H5N5S	000154-42-7	50
5		2-Methoxythiobenzamide	167	C8H9NOS	042590-97-6	50



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062416\
Data File : BF088353.D
Acq On : 25 Jun 2016 1:40
Operator : UM/SJ
Sample : H3607-05
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TE-MW-2-23D

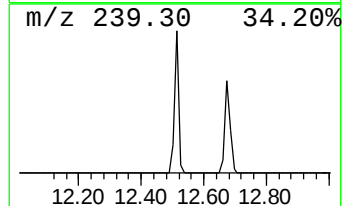
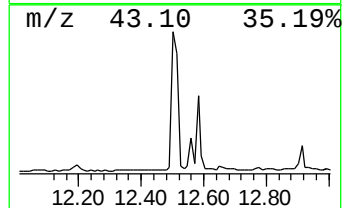
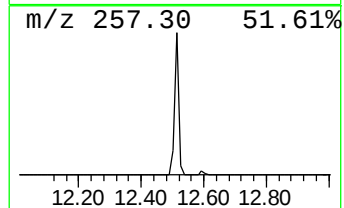
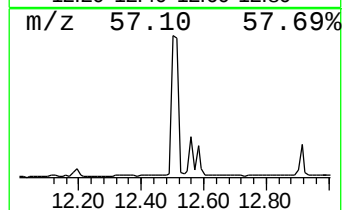
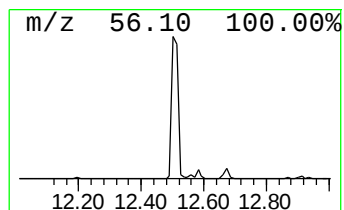
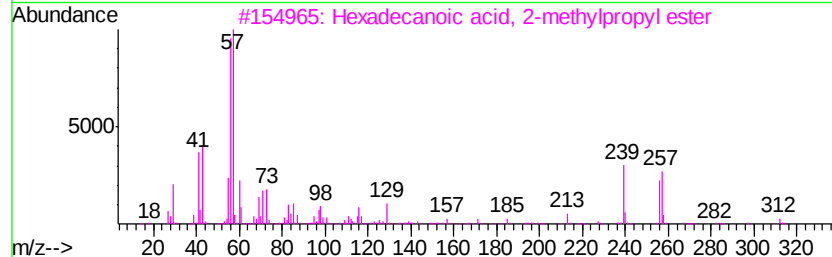
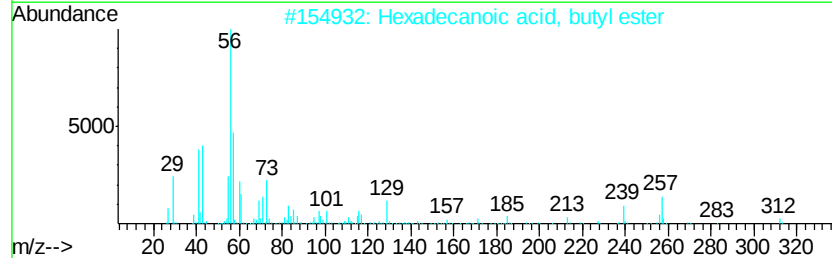
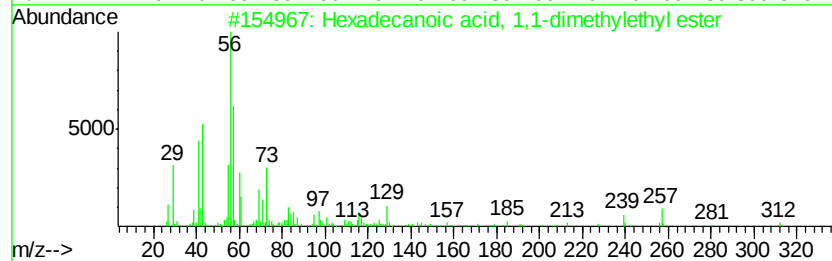
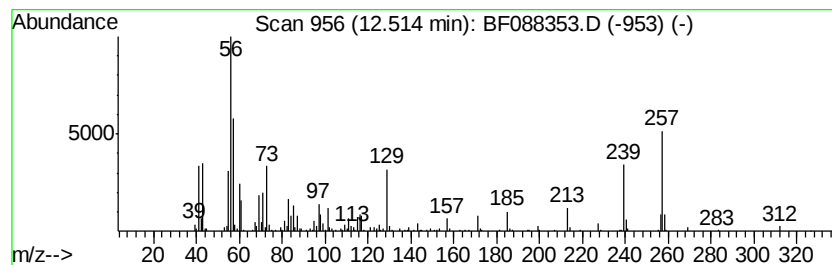
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Hexadecanoic acid, 1,1-dime... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.51	16.30 ng	565547	Chrysene-d12	13.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	95
2		Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	95
3		Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	93
4		Benz[c]acridine, 7,8-dimethyl-	257	C19H15N	003518-01-2	35
5		5-Carbamoyl-2,3,4,6-tetrahydro-1...	257	C13H11N3O3	1000241-45-9	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062416\
Data File : BF088353.D
Acq On : 25 Jun 2016 1:40
Operator : UM/SJ
Sample : H3607-05
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TE-MW-2-23D

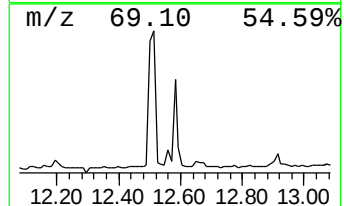
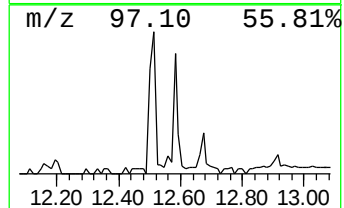
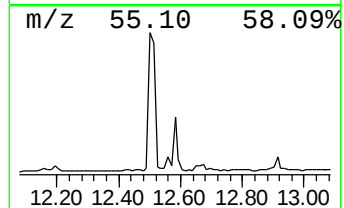
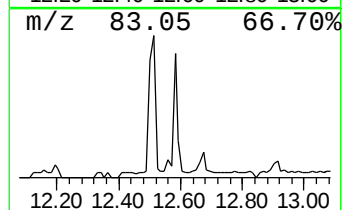
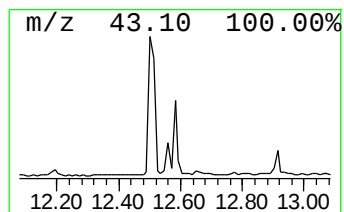
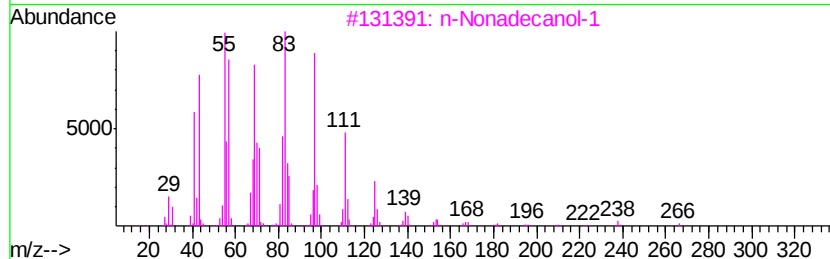
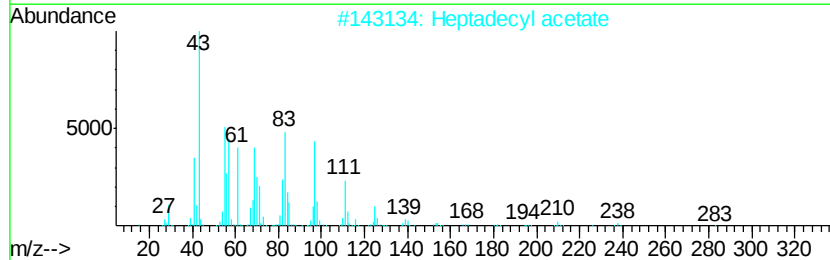
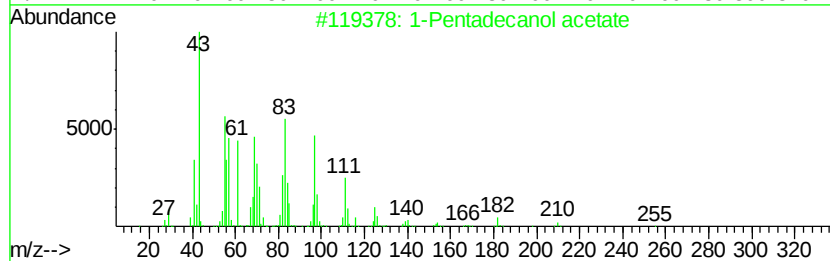
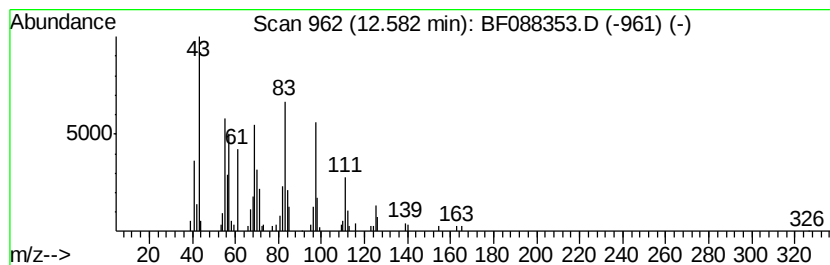
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 1-Pentadecanol acetate Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.58	2.77 ng	96021	Chrysene-d12	13.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Pentadecanol acetate	270	C17H34O2	000629-58-3	94
2		Heptadecyl acetate	298	C19H38O2	000822-20-8	94
3		n-Nonadecanol-1	284	C19H40O	001454-84-8	93
4		n-Heptadecanol-1	256	C17H36O	001454-85-9	93
5		n-Pentadecanol	228	C15H32O	000629-76-5	93



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062416\
Data File : BF088353.D
Acq On : 25 Jun 2016 1:40
Operator : UM/SJ
Sample : H3607-05
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TE-MW-2-23D

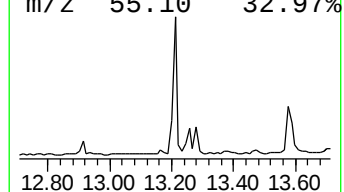
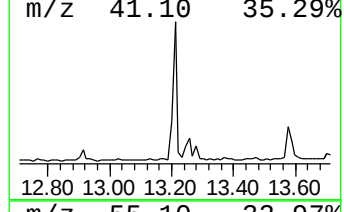
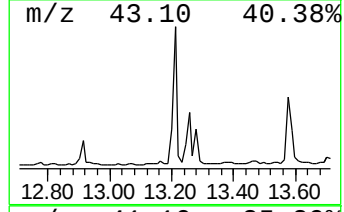
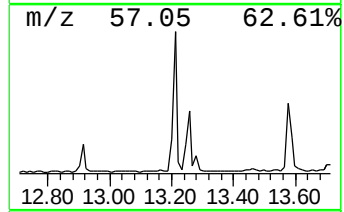
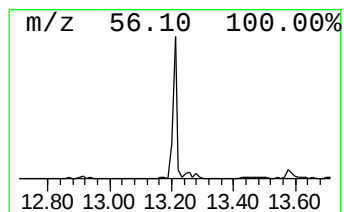
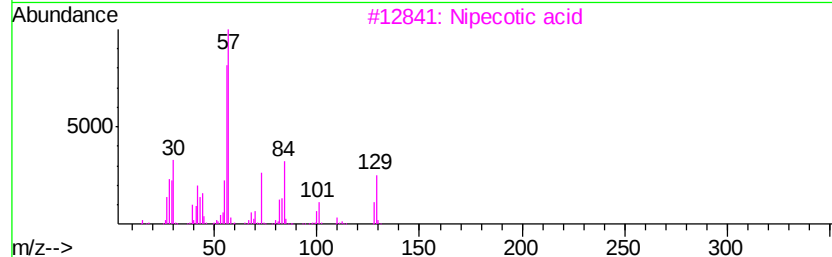
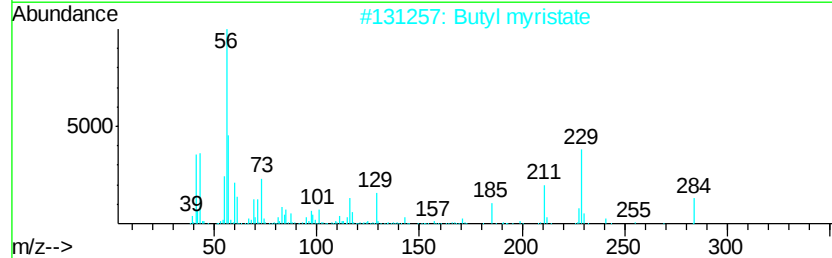
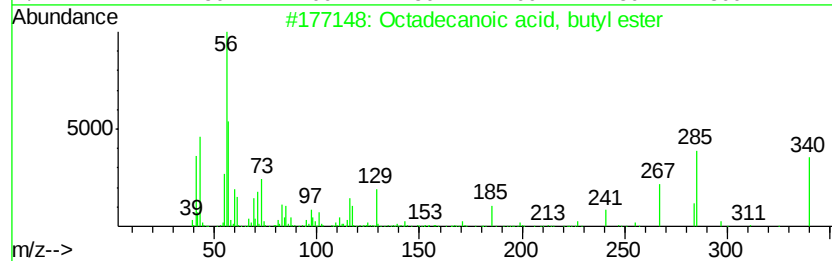
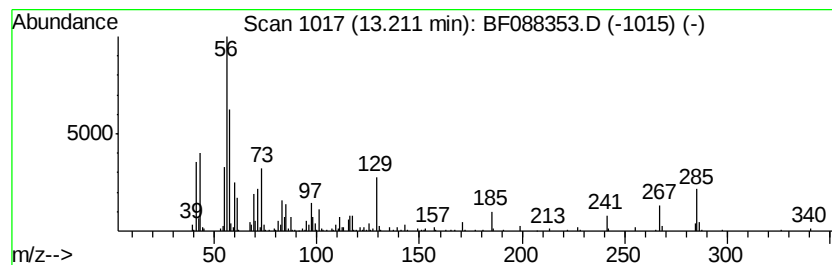
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Octadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.21	11.25 ng	390436	Chrysene-d12	13.71

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	72
2		Butyl myristate	284	C18H36O2	000110-36-1	64
3		Nipecotic acid	129	C6H11NO2	000498-95-3	50
4		Butyl 15-methylhexadecanoate	326	C21H42O2	1000336-52-4	42
5		Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062416\
Data File : BF088353.D
Acq On : 25 Jun 2016 1:40
Operator : UM/SJ
Sample : H3607-05
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TE-MW-2-23D

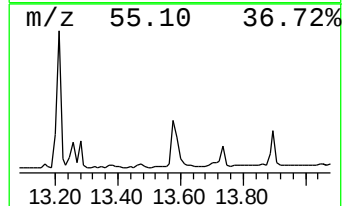
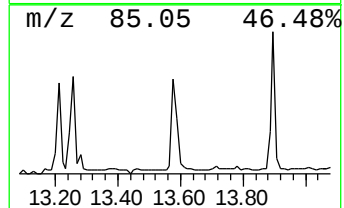
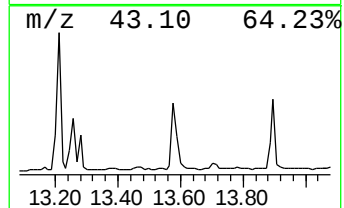
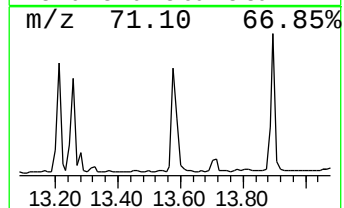
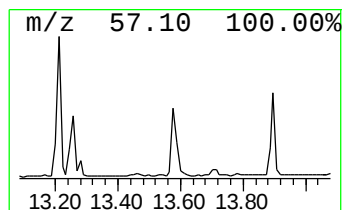
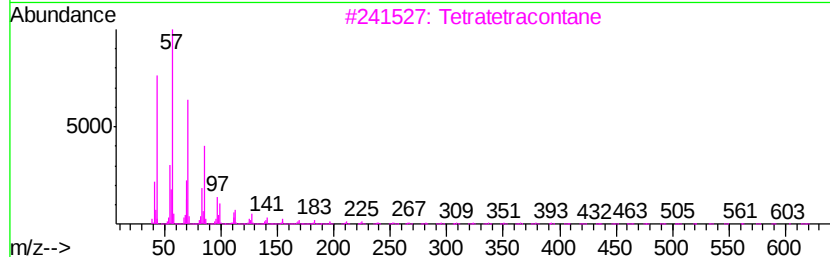
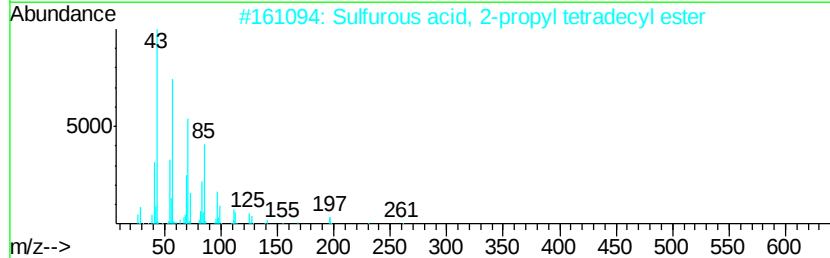
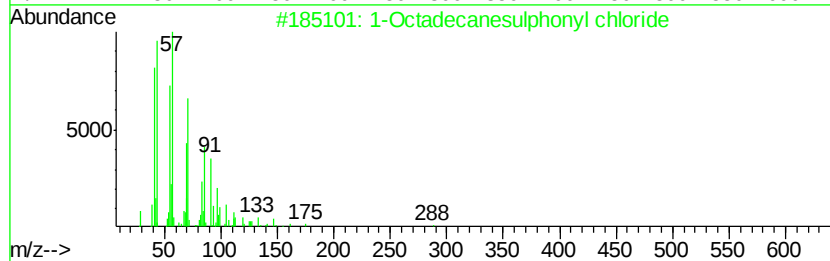
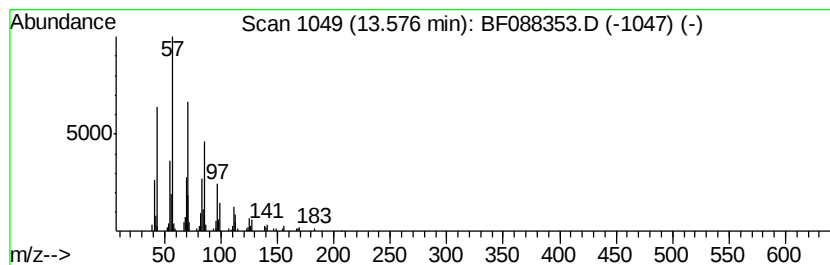
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 1-Octadecanesulphonyl chloride Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.58	4.43 ng	153731	Chrysene-d12	13.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	91
2			Sulfurous acid, 2-propyl tetradec...	320	C17H36O3S	1000309-12-5	91
3			Tetratetracontane	619	C44H90	007098-22-8	90
4			Sulfurous acid, pentadecyl 2-pro...	334	C18H38O3S	1000309-12-6	90
5			Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	83



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062416\
Data File : BF088353.D
Acq On : 25 Jun 2016 1:40
Operator : UM/SJ
Sample : H3607-05
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TE-MW-2-23D

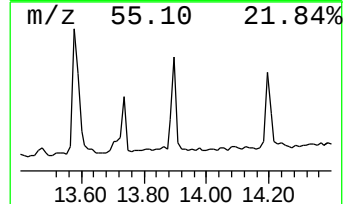
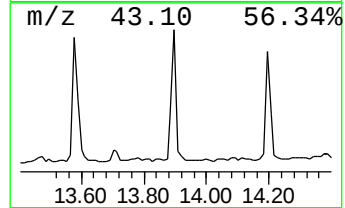
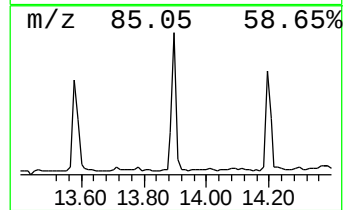
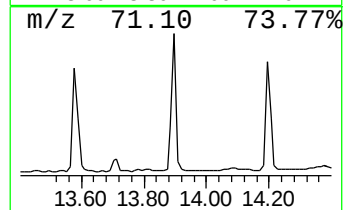
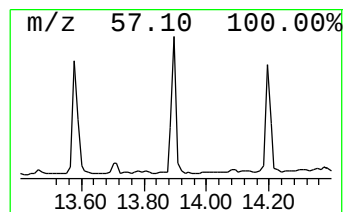
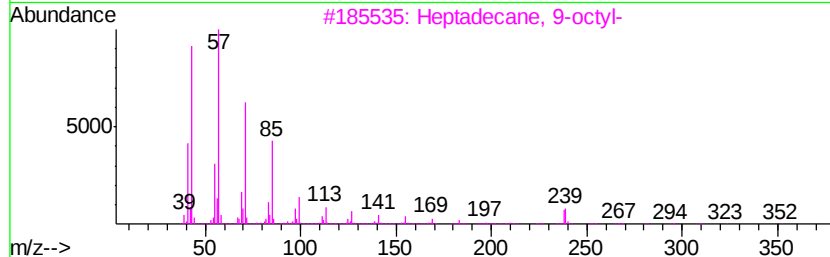
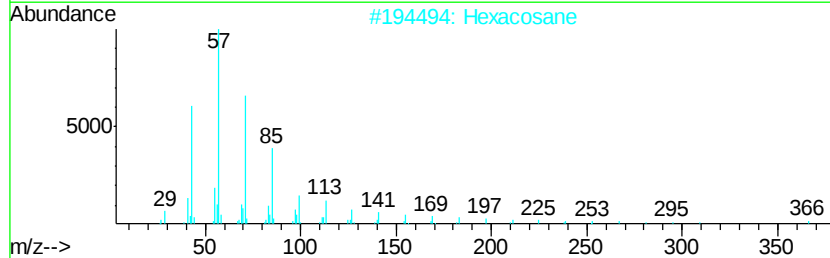
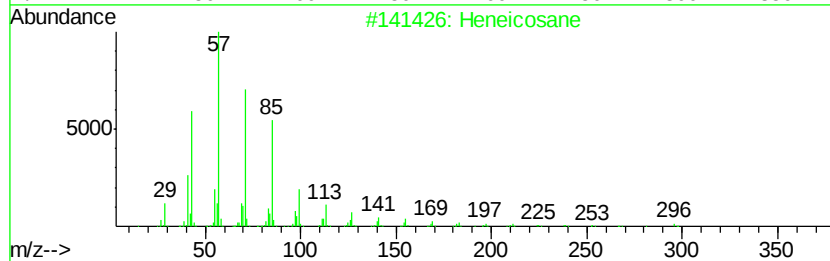
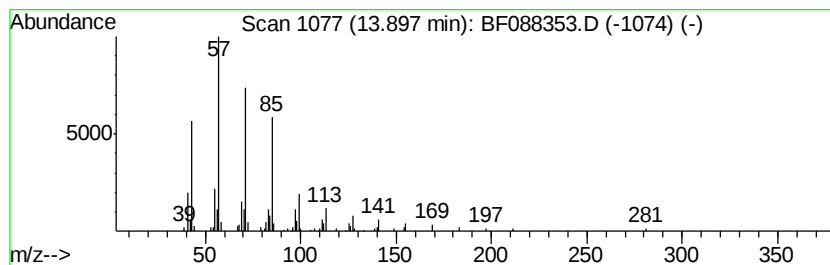
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Heneicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.90	3.46 ng	120080	Chrysene-d12	13.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	91
2		Hexacosane	366	C26H54	000630-01-3	91
3		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4		Octacosane	394	C28H58	000630-02-4	90
5		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062416\
Data File : BF088353.D
Acq On : 25 Jun 2016 1:40
Operator : UM/SJ
Sample : H3607-05
Misc :
ALS Vial : 23 Sample Multiplier: 1

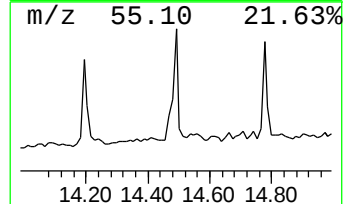
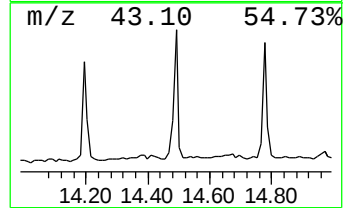
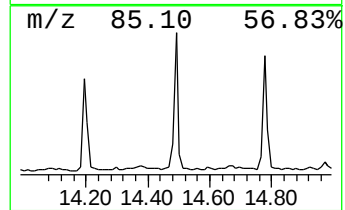
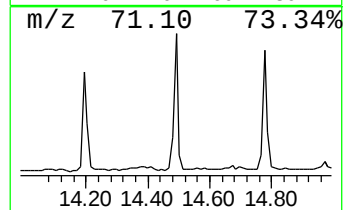
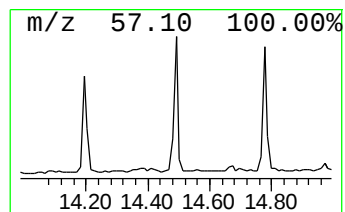
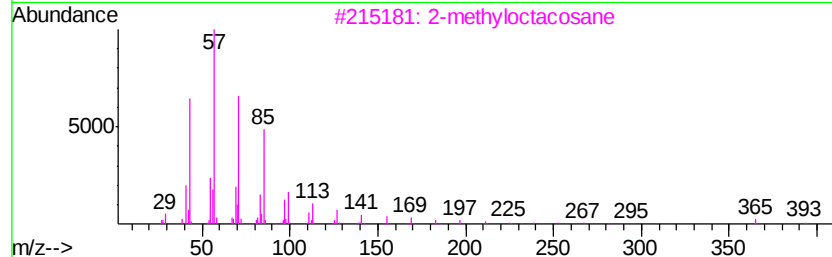
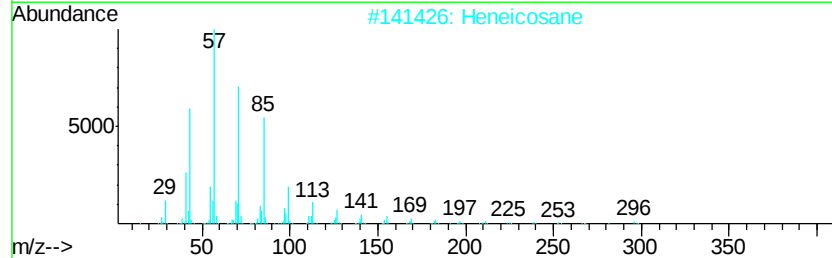
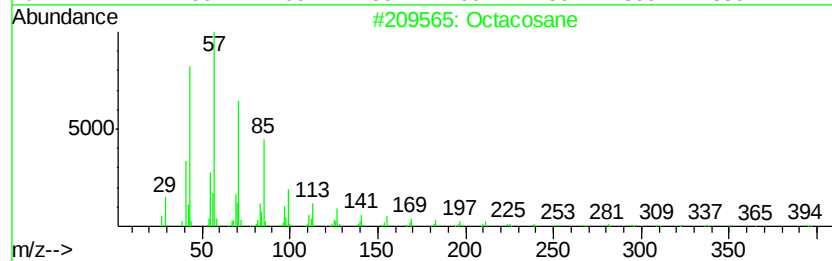
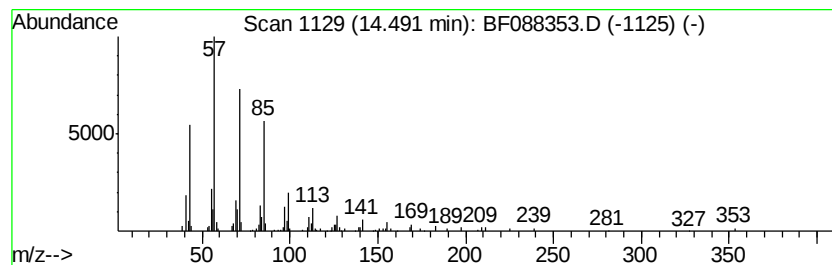
Instrument :
BNA_F
ClientSampleId :
TE-MW-2-23D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Octacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.49	4.91 ng	146992	Perylene-d12	15.07	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Octadecane	254	C18H38	000593-45-3	91
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062416\
Data File : BF088353.D
Acq On : 25 Jun 2016 1:40
Operator : UM/SJ
Sample : H3607-05
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TE-MW-2-23D

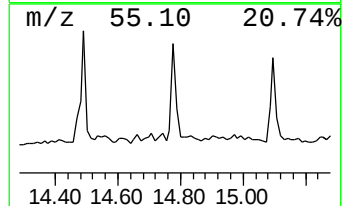
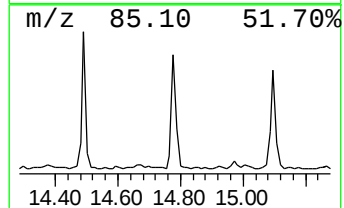
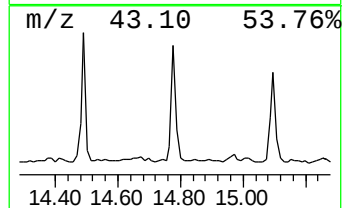
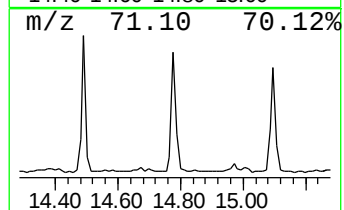
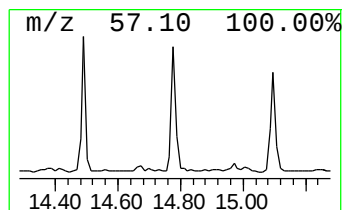
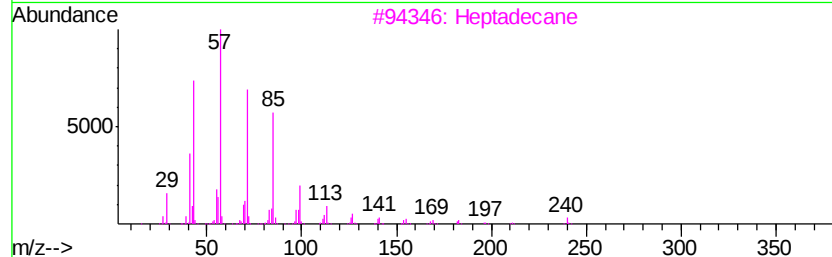
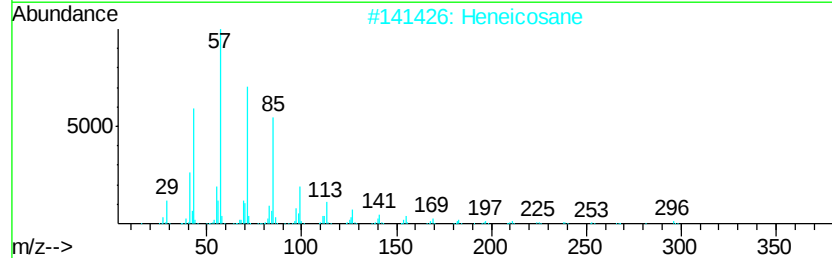
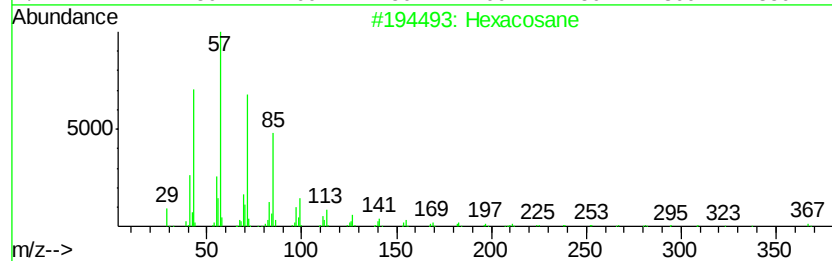
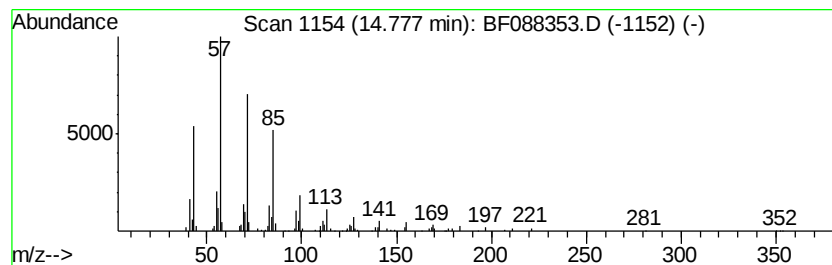
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 Hexacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.78	3.96 ng	118447	Perylene-d12	15.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Heptadecane	240	C17H36	000629-78-7	91
4		Tetracosane	338	C24H50	000646-31-1	91
5		Octacosane	394	C28H58	000630-02-4	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062416\
Data File : BF088353.D
Acq On : 25 Jun 2016 1:40
Operator : UM/SJ
Sample : H3607-05
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TE-MW-2-23D

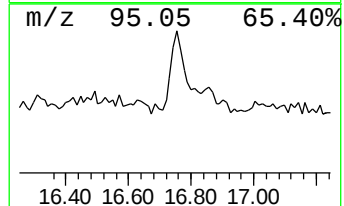
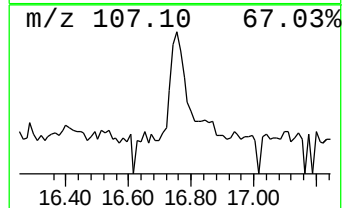
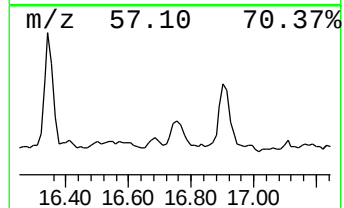
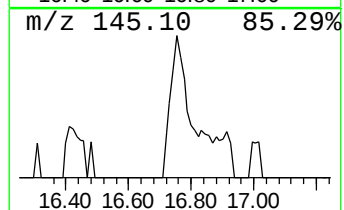
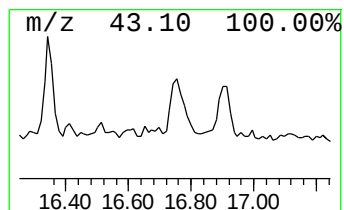
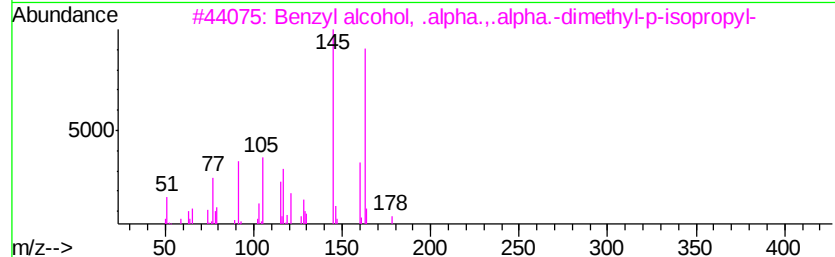
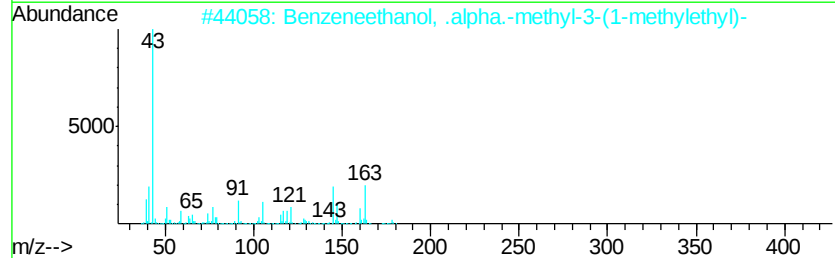
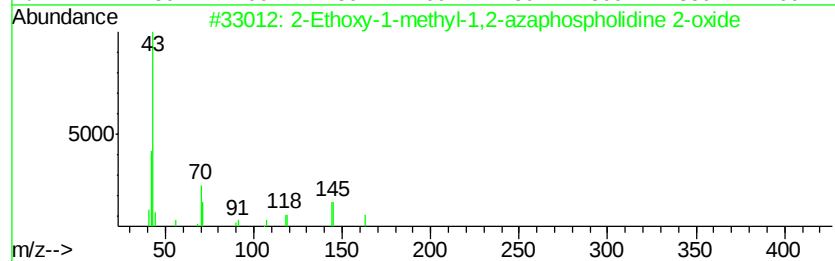
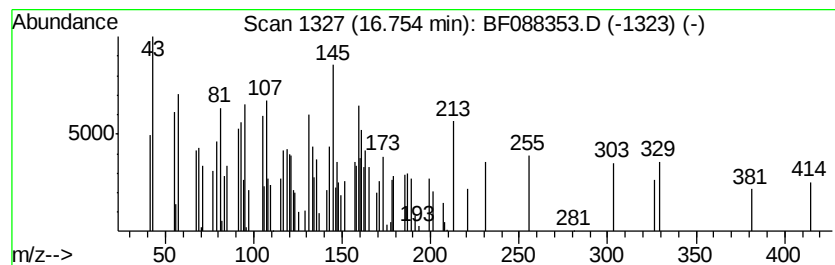
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 17 unknown16.75 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.75	3.69 ng	110296	Perylene-d12	15.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Ethoxy-1-methyl-1,2-azaphospho...	163	C6H14N02P	054008-32-1	22
2		Benzeneethanol, .alpha.-methyl-3...	178	C12H18O	054518-11-5	12
3		Benzyl alcohol, .alpha.,.alpha.-...	178	C12H18O	003445-42-9	12
4		N-(3-Chloro-4-fluorophenyl)aceta...	187	C8H7ClFNO	000877-90-7	11
5		Cyclopentane-3'-spirotricyclo[3....	188	C14H20	078578-93-5	10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062416\
 Data File : BF088353.D
 Acq On : 25 Jun 2016 1:40
 Operator : UM/SJ
 Sample : H3607-05
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TE-MW-2-23D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.71	2.3	ng	63116	1	6.58	543630	20.0
unknown6.35	6.35	64.5	ng	1752720	1	6.58	543630	20.0
2-Mercaptobenzoth...	11.84	3.5	ng	110813	4	11.10	626472	20.0
Hexadecanoic acid...	12.51	16.3	ng	565547	5	13.71	693992	20.0
1-Pentadecanol ac...	12.58	2.8	ng	96021	5	13.71	693992	20.0
Octadecanoic acid...	13.21	11.3	ng	390436	5	13.71	693992	20.0
1-Octadecanesulph...	13.58	4.4	ng	153731	5	13.71	693992	20.0
Heneicosane	13.90	3.5	ng	120080	5	13.71	693992	20.0
Octacosane	14.49	4.9	ng	146992	6	15.07	598279	20.0
Hexacosane	14.78	4.0	ng	118447	6	15.07	598279	20.0
unknown16.75	16.75	3.7	ng	110296	6	15.07	598279	20.0