

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012017\
 Data File : BF092367.D
 Acq On : 20 Jan 2017 12:30
 Operator : UM/SJ
 Sample : I1260-01
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MH-0-12FT-COMP

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-BF122116.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	4.633	246	249	264	rBV	1052087	1878167	29.21%	3.755%
2	5.101	288	290	293	rBV	2802325	3845268	59.81%	7.687%
3	6.187	383	385	392	rBV	3408226	3919116	60.96%	7.835%
4	6.290	392	394	397	rVB	3809420	3658057	56.90%	7.313%
5	6.519	412	414	417	rBV	955388	878149	13.66%	1.756%
6	6.679	425	428	430	rBV	3043272	3353032	52.15%	6.703%
7	7.102	462	465	467	rBV	2559121	3623450	56.36%	7.244%
8	7.810	524	527	529	rBV	1780135	1793634	27.90%	3.586%
9	8.896	618	622	624	rBV	4765577	6429399	100.00%	12.854%
10	9.296	655	657	659	rBV	596523	595373	9.26%	1.190%
11	9.513	674	676	677	rBV	79801	76027	1.18%	0.152%
12	9.559	677	680	682	rBV	1860157	1972155	30.67%	3.943%
13	10.005	717	719	721	rVB	132778	138066	2.15%	0.276%
14	10.222	735	738	742	rBV	47606	82215	1.28%	0.164%
15	10.348	746	749	751	rBV	3413810	3550633	55.22%	7.098%
16	10.473	758	760	765	rVB	160560	268158	4.17%	0.536%
17	10.919	797	799	801	rBV	110923	153216	2.38%	0.306%
18	11.033	807	809	812	rBV	2092784	1907613	29.67%	3.814%
19	11.353	834	837	839	rBV	87927	104514	1.63%	0.209%
20	11.594	855	858	862	rBV2	163281	210082	3.27%	0.420%
21	12.462	932	934	937	rBV2	53862	76880	1.20%	0.154%
22	12.622	945	948	950	rBV	5118422	5278316	82.10%	10.552%
23	13.114	988	991	996	rBV	1724188	1756311	27.32%	3.511%
24	13.194	996	998	1004	rVB2	58957	112180	1.74%	0.224%
25	13.582	1026	1032	1036	rBV3	66169	280900	4.37%	0.562%
26	13.662	1036	1039	1044	rVB	1552220	1632804	25.40%	3.264%
27	14.451	1103	1108	1111	rBV2	74011	215823	3.36%	0.431%
28	14.508	1111	1113	1119	rVB	116974	180311	2.80%	0.360%
29	15.011	1155	1157	1159	rBV	969078	1182967	18.40%	2.365%
30	15.400	1188	1191	1195	rVB	73710	116466	1.81%	0.233%
31	15.560	1203	1205	1211	rVB6	30008	71204	1.11%	0.142%
32	15.800	1223	1226	1233	rVV	78472	156183	2.43%	0.312%
33	16.268	1264	1267	1273	rVB2	63346	130941	2.04%	0.262%
34	16.817	1308	1315	1325	rBV	53987	227969	3.55%	0.456%

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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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	17.468	1367	1372	1378	rVB3	28045	96997	1.51%	0.194%
36	18.234	1435	1439	1446	rVB2	20924	67727	1.05%	0.135%

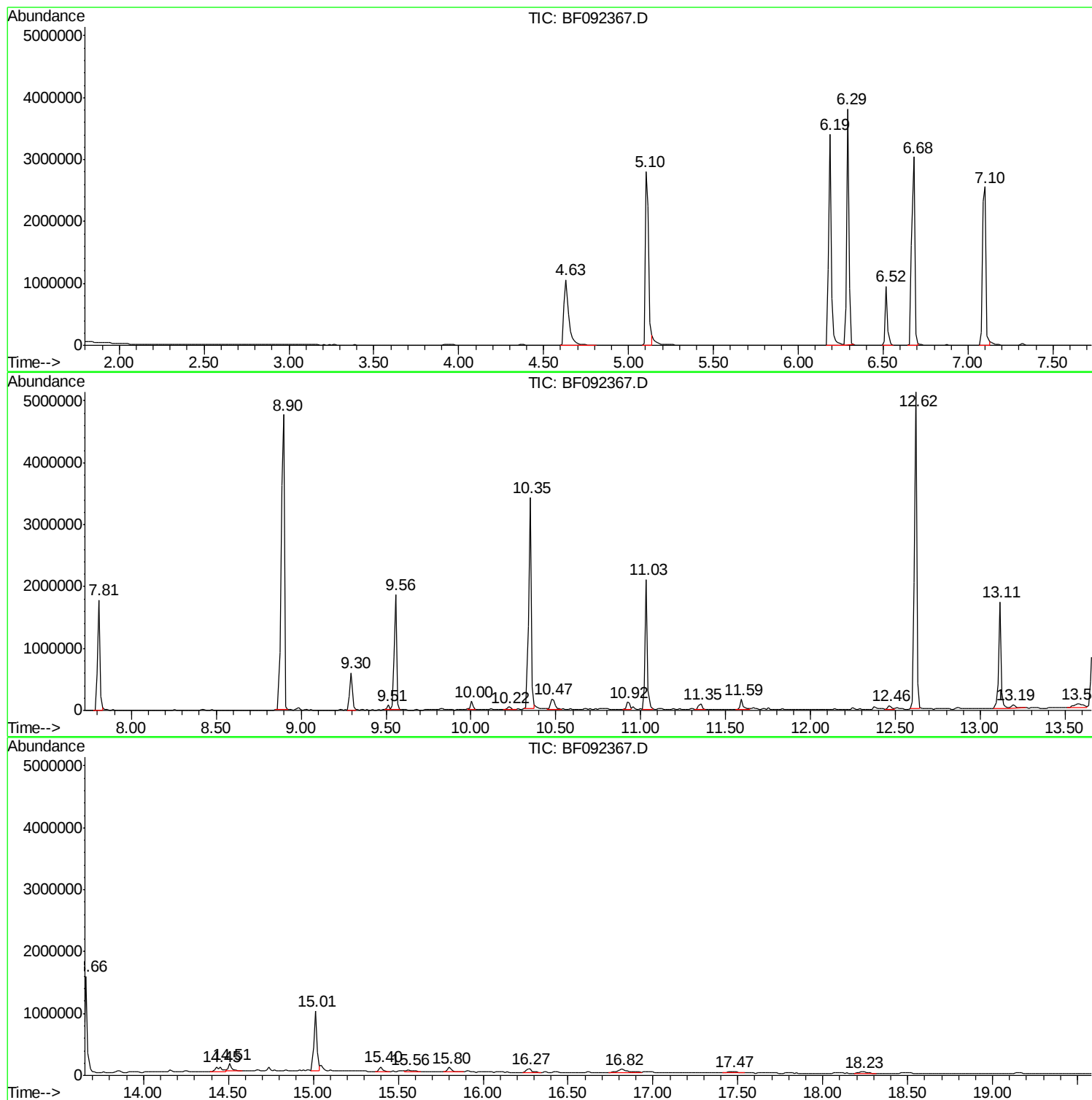
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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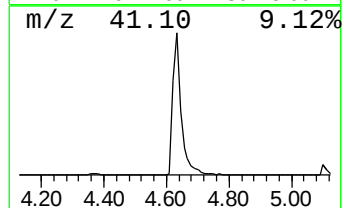
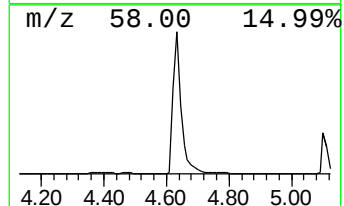
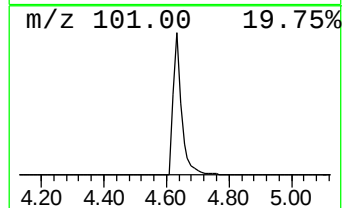
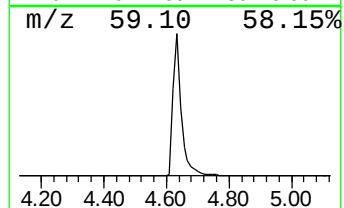
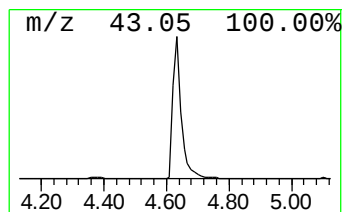
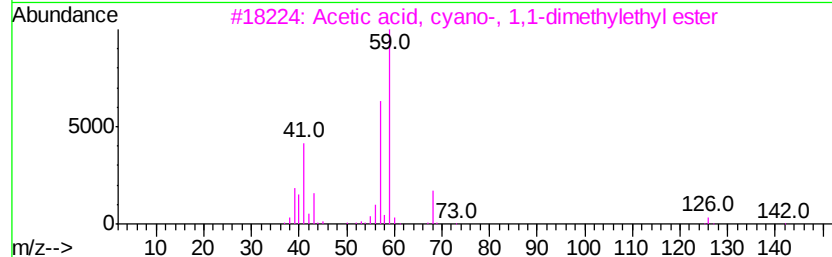
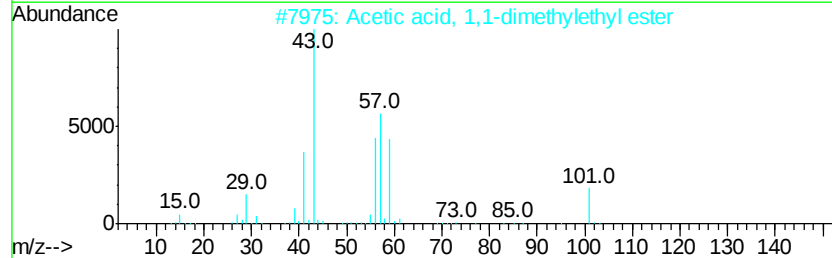
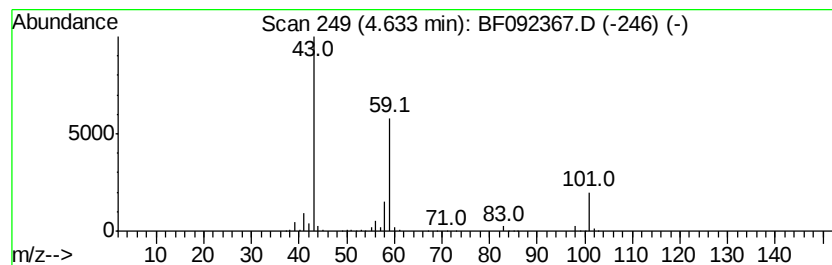
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.63	42.78 ng	1878170	1,4-Dichlorobenzene-d4	6.52

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
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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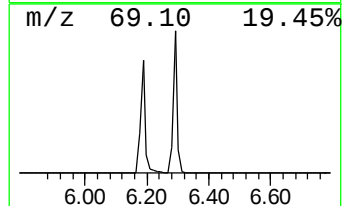
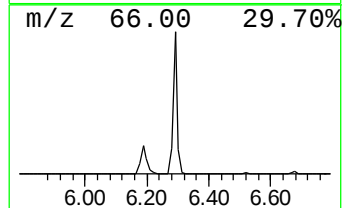
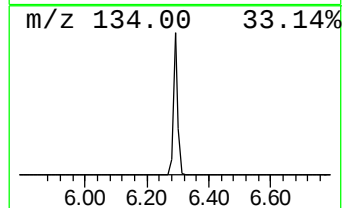
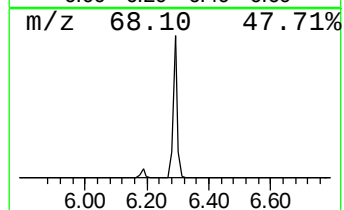
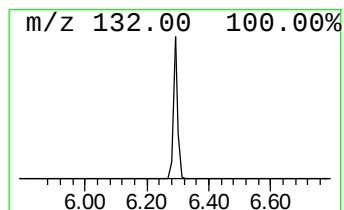
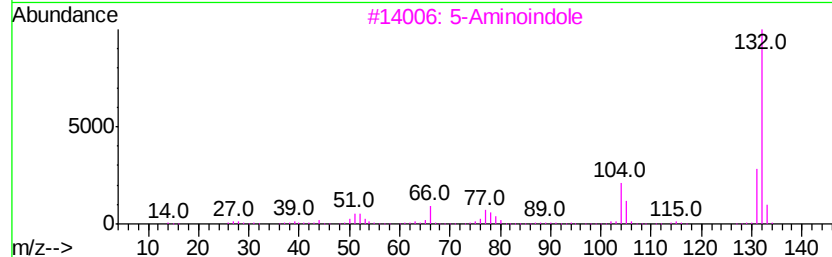
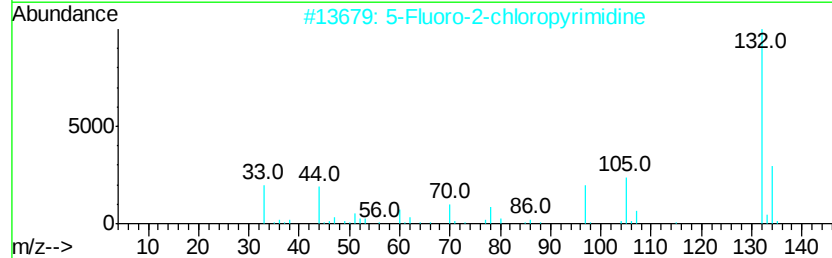
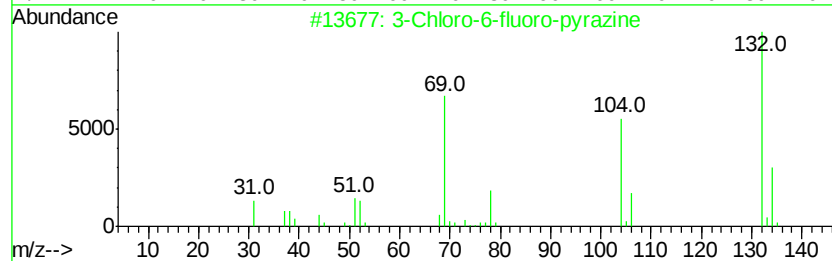
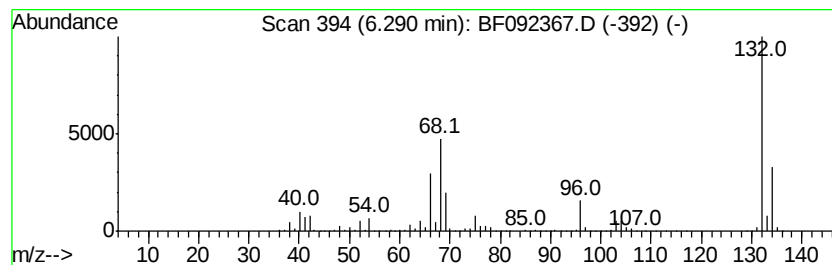
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.29 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.29	83.31 ng	3658060	1,4-Dichlorobenzene-d4	6.52

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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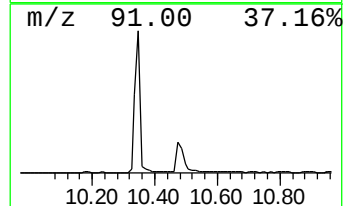
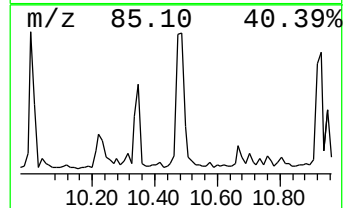
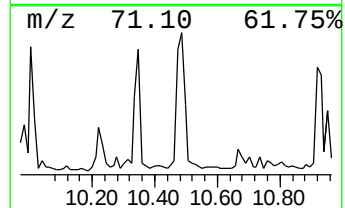
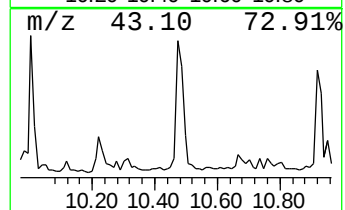
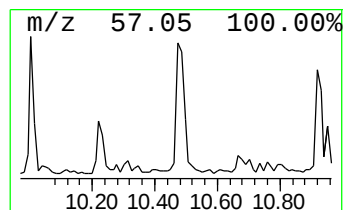
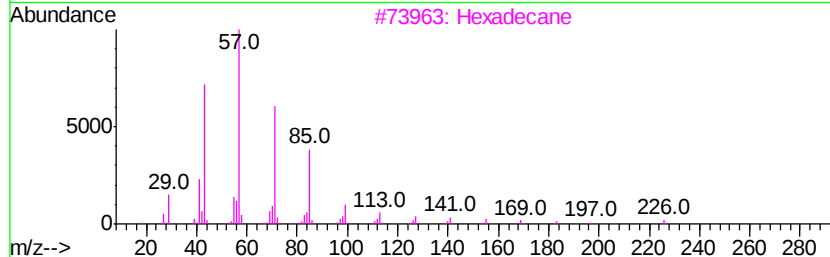
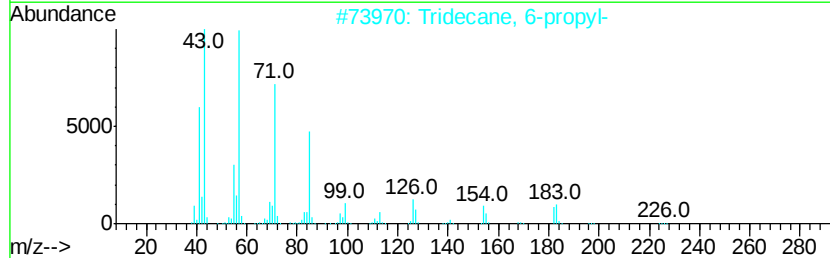
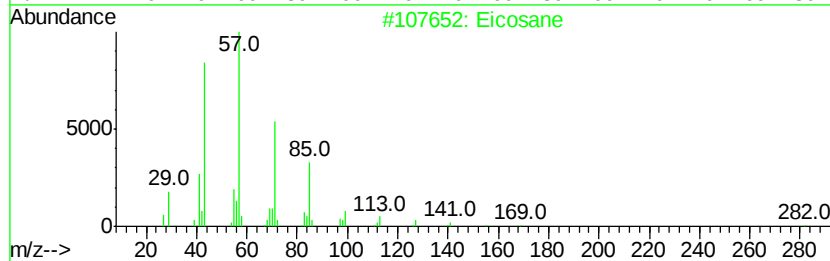
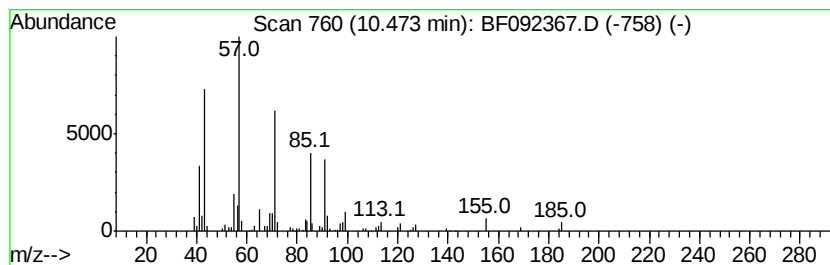
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.47	2.81 ng	268158	Phenanthrene-d10	11.03

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	87
2	Tridecane, 6-propyl-		226	C16H34	055045-10-8	86
3	Hexadecane		226	C16H34	000544-76-3	86
4	Octacosane		394	C28H58	000630-02-4	86
5	Pentadecane		212	C15H32	000629-62-9	86



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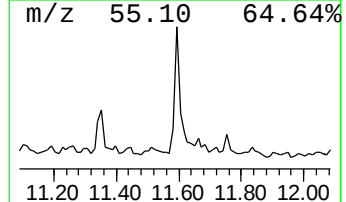
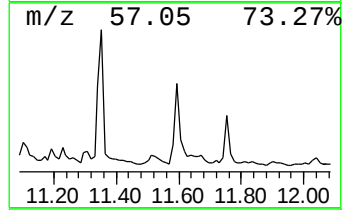
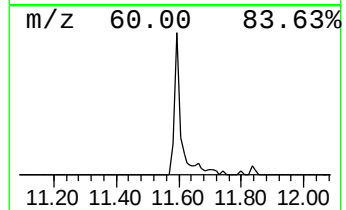
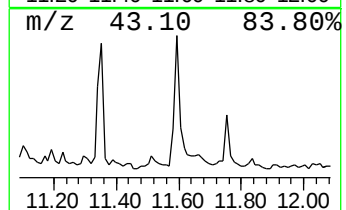
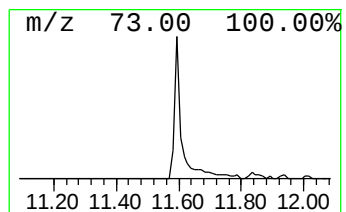
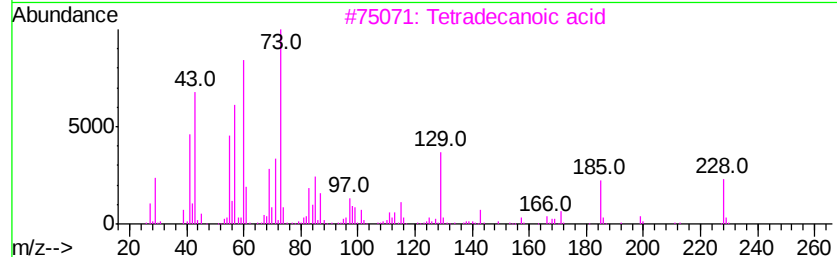
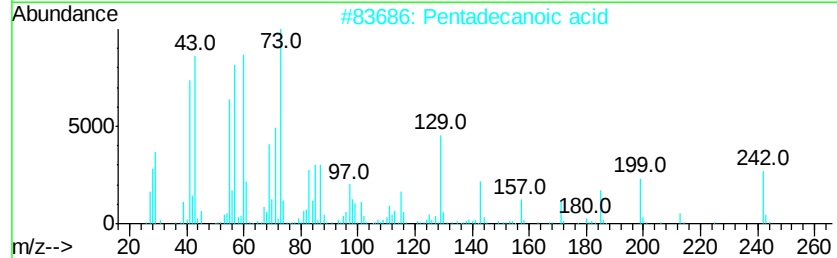
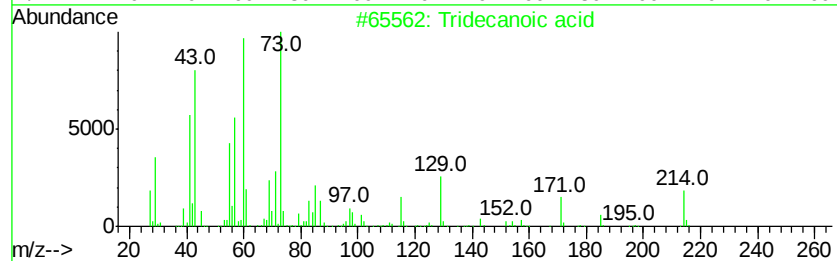
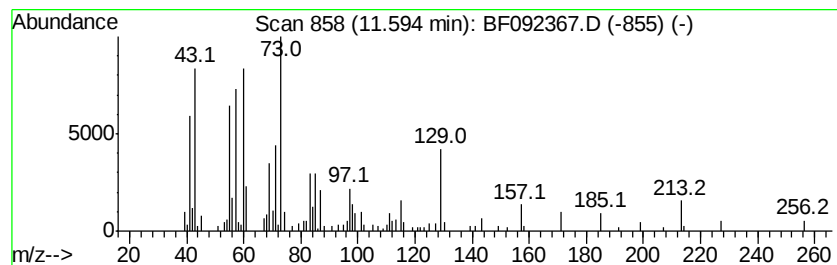
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Tridecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.59	2.20 ng	210082	Phenanthrene-d10	11.03

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tridecanoic acid	214	C13H26O2	000638-53-9	87
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	86
4		2H-Pyran-2-one, tetrahydro-4-hyd...	130	C6H10O3	000503-48-0	11
5		Ethanol, 2-(dodecyloxy)-	230	C14H30O2	004536-30-5	11



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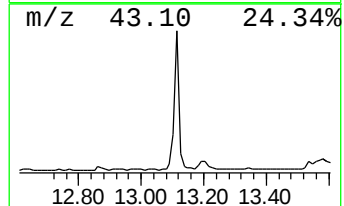
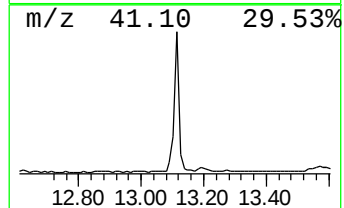
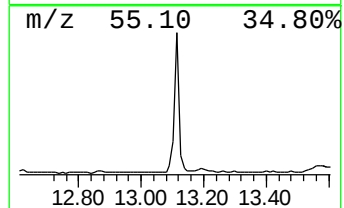
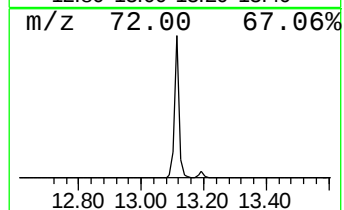
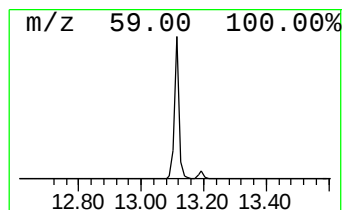
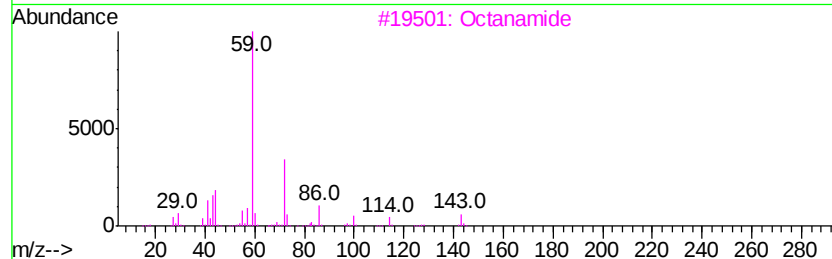
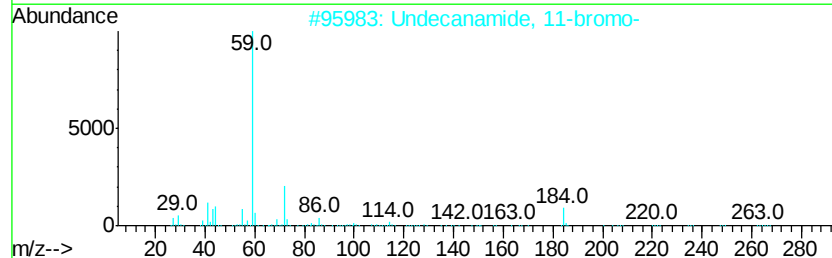
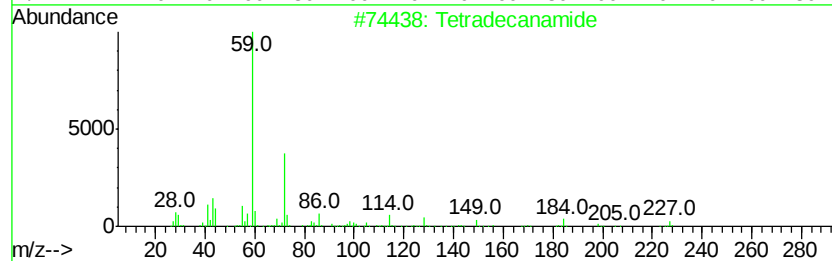
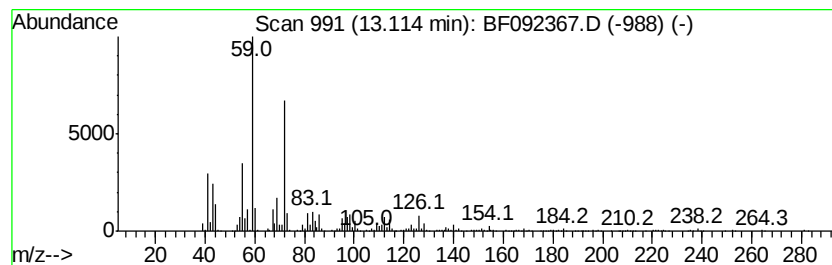
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Tetradecanamide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.11	21.51 ng	1756310	Chrysene-d12	13.66

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetradecanamide	227	C14H29NO	000638-58-4	72
2		Undecanamide, 11-bromo-	263	C11H22BrNO	005875-26-3	59
3		Octanamide	143	C8H17NO	000629-01-6	56
4		Hexadecanamide	255	C16H33NO	000629-54-9	56
5		Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	50



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ALS Vial : 3 Sample Multiplier: 1

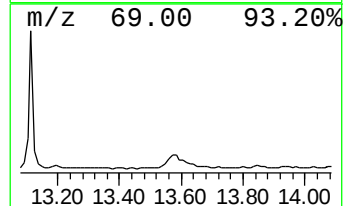
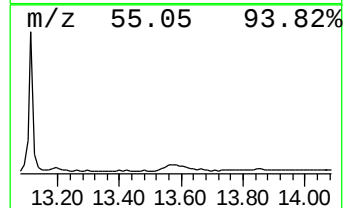
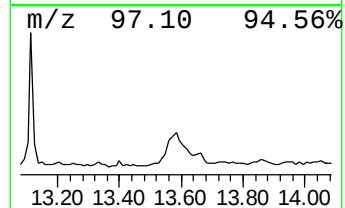
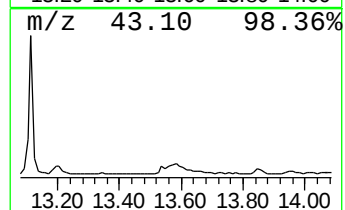
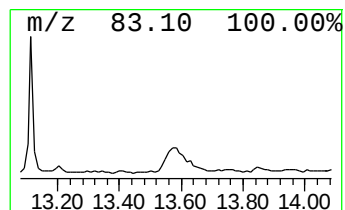
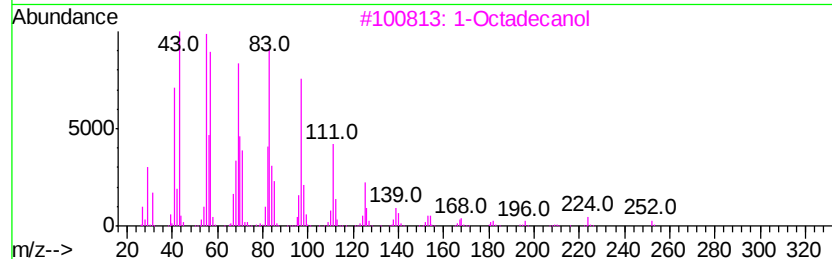
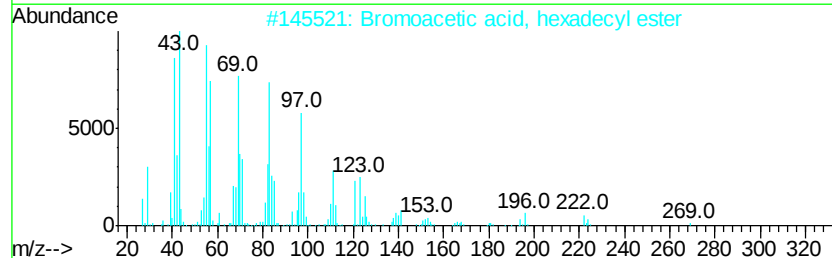
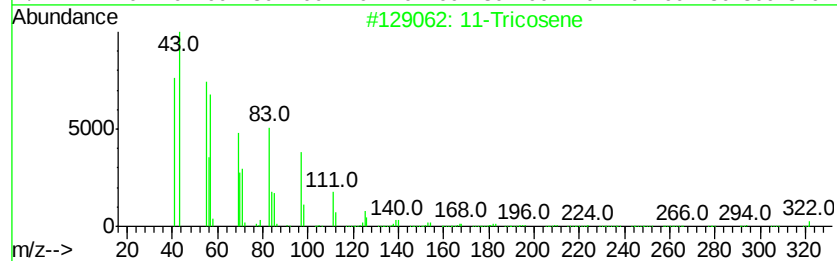
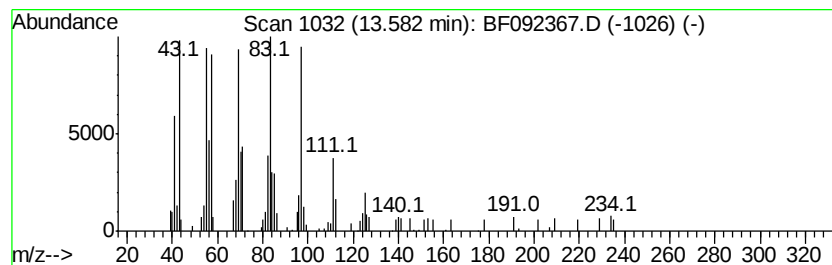
Instrument :
BNA_F
ClientSampleId :
MH-0-12FT-COMP

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 11-Tricosene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.58	3.44 ng	280900	Chrysene-d12	13.66	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11-Tricosene	322	C23H46	052078-56-5	90
2	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	90
3	1-Octadecanol	270	C18H38O	000112-92-5	90
4	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	87
5	Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012017\
Data File : BF092367.D
Acq On : 20 Jan 2017 12:30
Operator : UM/SJ
Sample : I1260-01
Misc :
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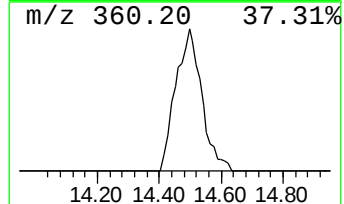
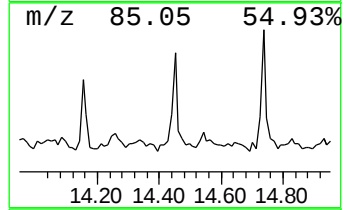
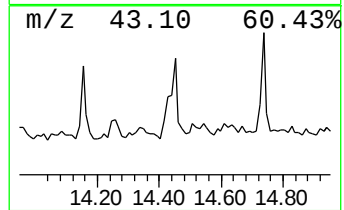
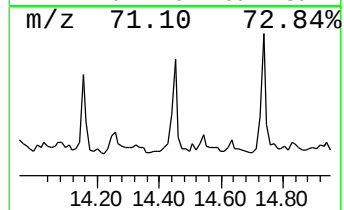
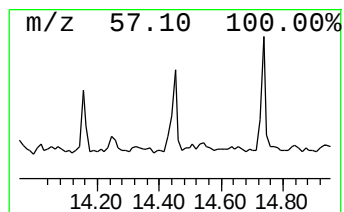
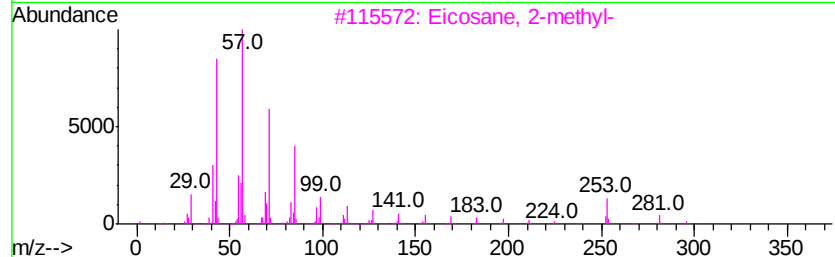
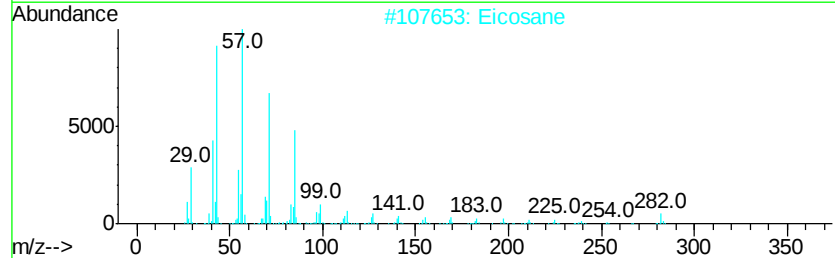
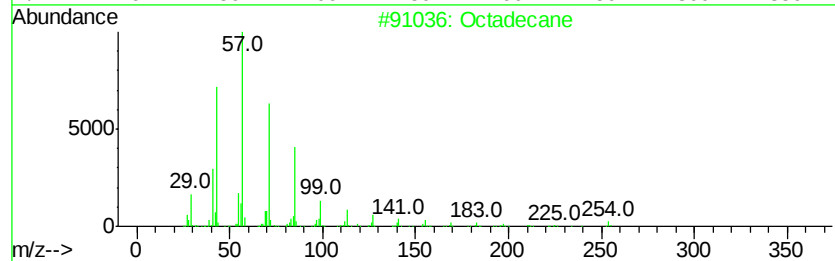
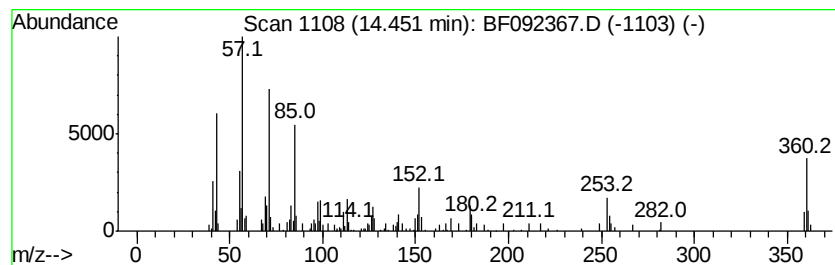
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.45	3.65 ng	215823	Perylene-d12	15.01	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	64
2	Eicosane	282	C20H42	000112-95-8	64
3	Eicosane, 2-methyl-	296	C21H44	001560-84-5	49
4	Triacontane	422	C30H62	000638-68-6	43
5	Octacosane	394	C28H58	000630-02-4	41



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012017\
Data File : BF092367.D
Acq On : 20 Jan 2017 12:30
Operator : UM/SJ
Sample : I1260-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-0-12FT-COMP

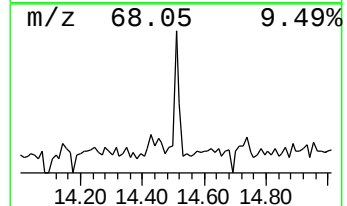
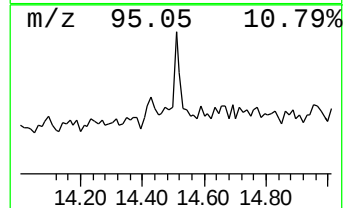
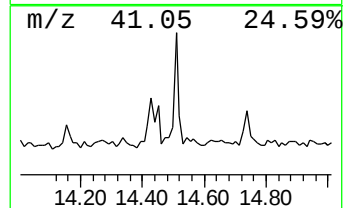
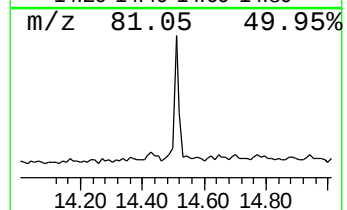
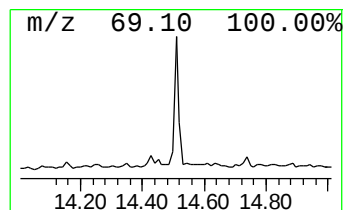
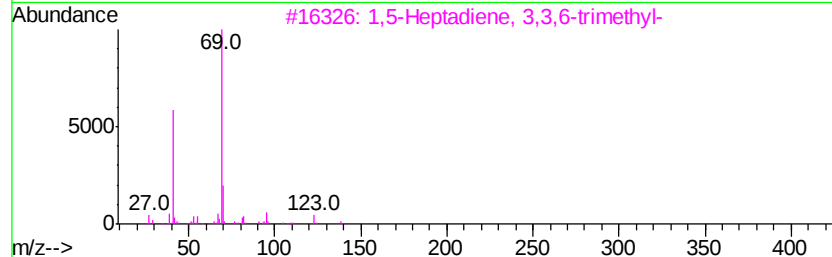
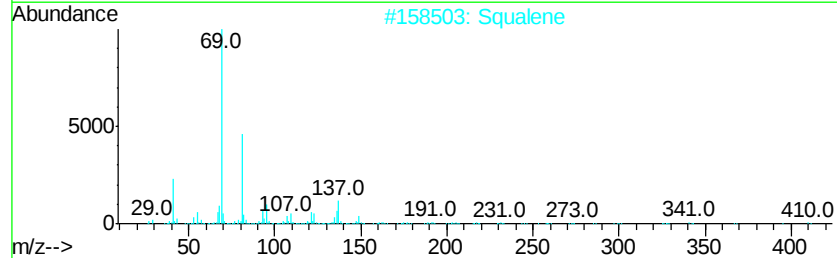
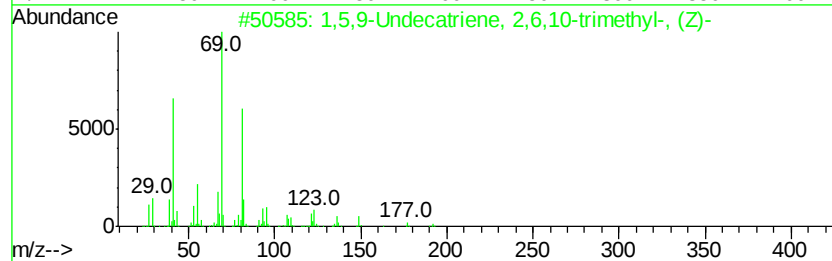
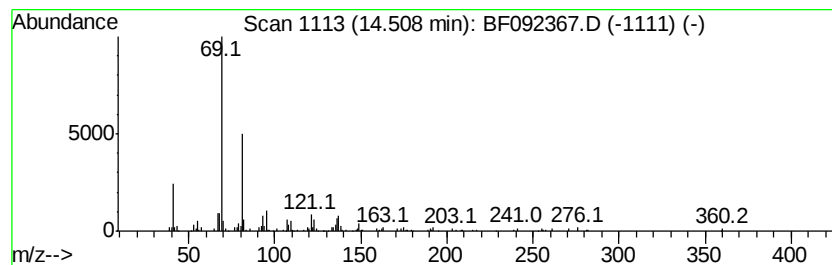
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1,5,9-Undecatriene, 2,6,10-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.51	3.05 ng	180311	Perylene-d12	15.01

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	90
2			Squalene	410	C30H50	007683-64-9	83
3			1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	64
4			1,6-Octadiene, 3,5-dimethyl-, tr...	138	C10H18	074630-87-8	64
5			4-Methyl-1,5-Heptadiene	110	C8H14	000998-94-7	59



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012017\
Data File : BF092367.D
Acq On : 20 Jan 2017 12:30
Operator : UM/SJ
Sample : I1260-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MH-0-12FT-COMP

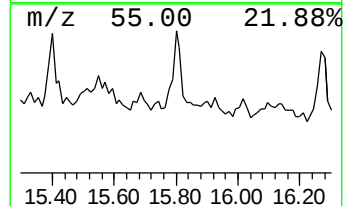
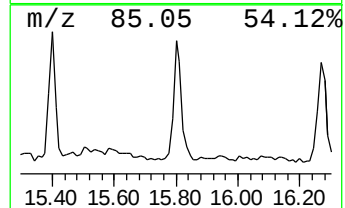
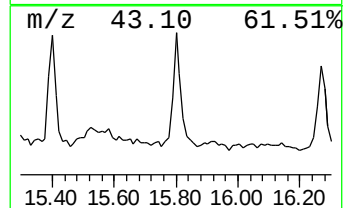
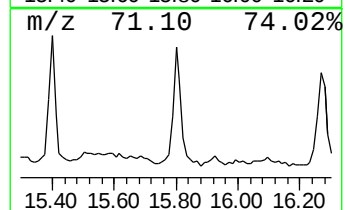
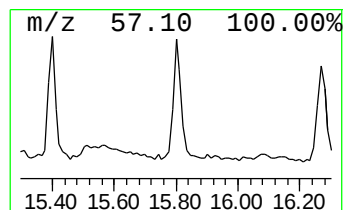
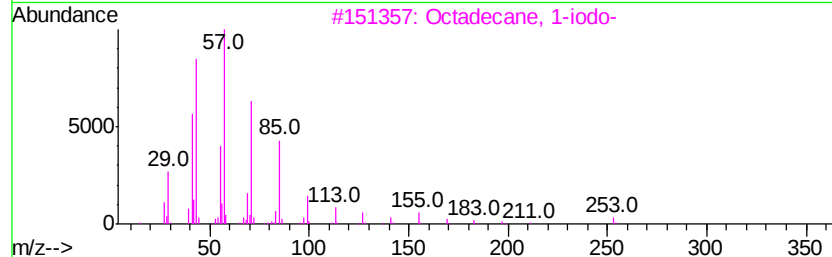
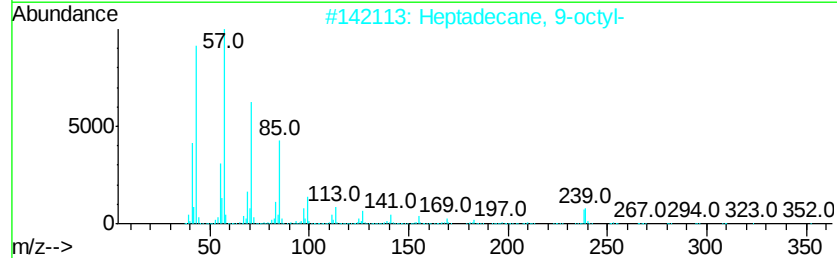
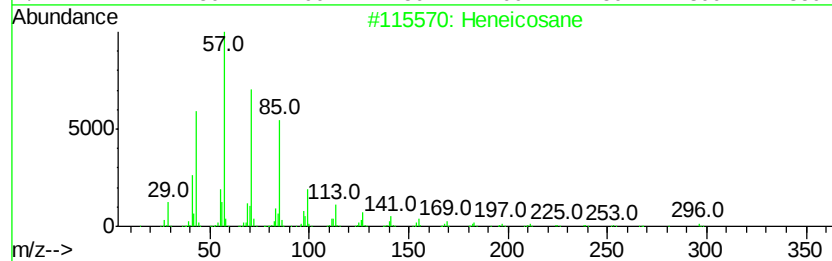
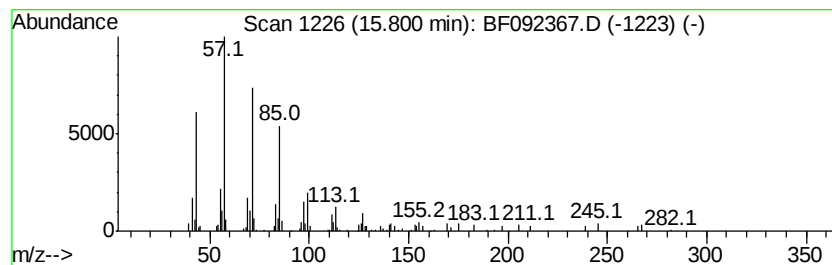
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heneicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.80	2.64 ng	156183	Perylene-d12	15.01

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	87
2	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	87
3	Octadecane, 1-iodo-		380	C18H37I	000629-93-6	87
4	Tridecane, 3-methyl-		198	C14H30	006418-41-3	86
5	triacontane		422	C30H62	000638-68-6	86



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012017\
Data File : BF092367.D
Acq On : 20 Jan 2017 12:30
Operator : UM/SJ
Sample : I1260-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MH-0-12FT-COMP

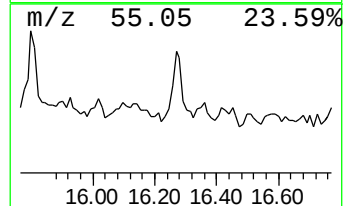
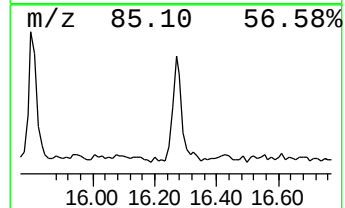
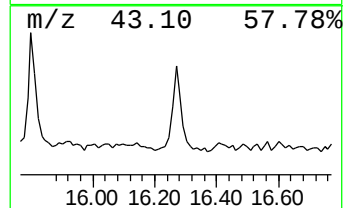
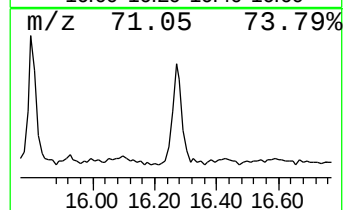
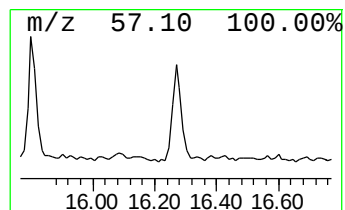
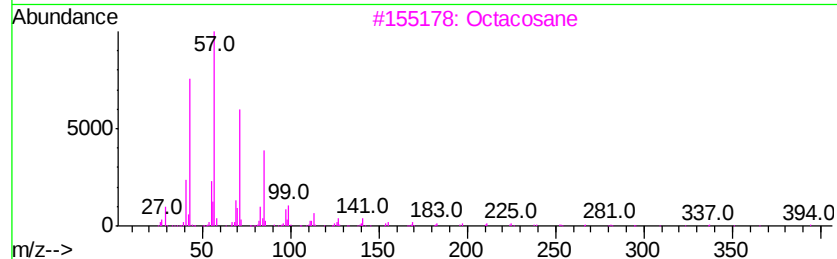
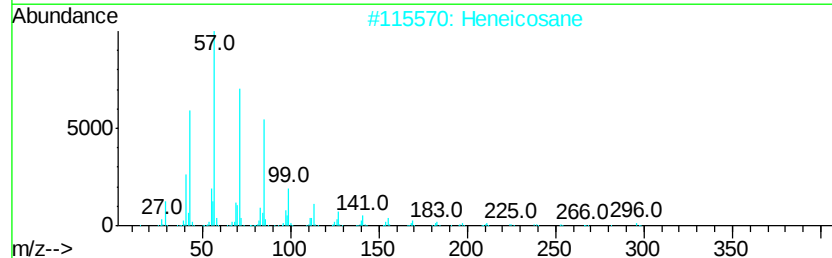
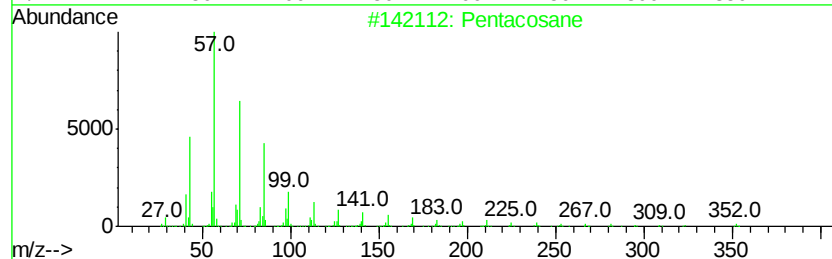
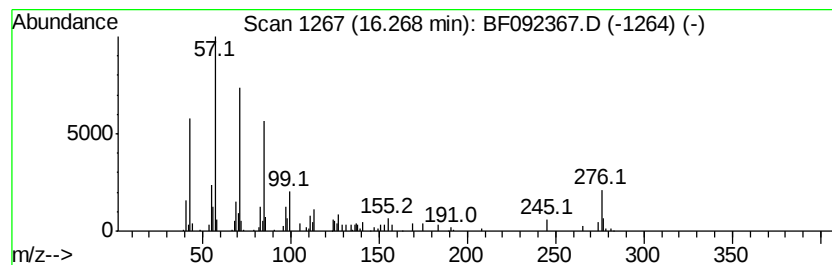
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Pentacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.27	2.21 ng	130941	Perylene-d12	15.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentacosane	352	C25H52	000629-99-2	81
2		Heneicosane	296	C21H44	000629-94-7	81
3		Octacosane	394	C28H58	000630-02-4	74
4		Triacontane	422	C30H62	000638-68-6	72
5		Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012017\
Data File : BF092367.D
Acq On : 20 Jan 2017 12:30
Operator : UM/SJ
Sample : I1260-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-0-12FT-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.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...	4.63	42.8	ng	1878170	1	6.52	878149	20.0
unknown6.29	6.29	83.3	ng	3658060	1	6.52	878149	20.0
Eicosane	10.47	2.8	ng	268158	4	11.03	1907610	20.0
Tridecanoic acid	11.59	2.2	ng	210082	4	11.03	1907610	20.0
Tetradecanamide	13.11	21.5	ng	1756310	5	13.66	1632800	20.0
11-Tricosene	13.58	3.4	ng	280900	5	13.66	1632800	20.0
Octadecane	14.45	3.6	ng	215823	6	15.01	1182970	20.0
1,5,9-Undecatrien...	14.51	3.0	ng	180311	6	15.01	1182970	20.0
Heneicosane	15.80	2.6	ng	156183	6	15.01	1182970	20.0
Pentacosane	16.27	2.2	ng	130941	6	15.01	1182970	20.0