

Data Path : Z:\HPCHEM1\BNA F\DATA\BF073116\
 Data File : BF089492.D
 Acq On : 1 Aug 2016 3:32
 Operator : UM/SJ
 Sample : H4222-06
 Misc :
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-05-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-BF072716.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	1.655	5	6	41	rVB	983805	2381098	100.00%	17.166%
2	4.581	259	262	270	rBV	229525	459413	19.29%	3.312%
3	5.061	302	304	327	rBV	834042	1208808	50.77%	8.715%
4	6.159	398	400	407	rBV	1026102	1228476	51.59%	8.856%
5	6.262	407	409	427	rVB	1240843	1288967	54.13%	9.292%
6	6.490	427	429	440	rBV3	194212	230870	9.70%	1.664%
7	6.650	440	443	445	rBV	982658	971214	40.79%	7.002%
8	7.073	477	480	490	rBV	411979	699596	29.38%	5.044%
9	7.782	540	542	544	rBV	240283	247124	10.38%	1.782%
10	8.856	634	636	639	rBV	1048920	1052793	44.21%	7.590%
11	9.256	669	671	674	rBV	167091	165363	6.94%	1.192%
12	9.519	692	694	697	rBV	271503	251751	10.57%	1.815%
13	10.308	761	763	773	rVV	618485	605808	25.44%	4.367%
14	10.445	773	775	781	rVV	25731	31032	1.30%	0.224%
15	10.993	821	823	828	rBV	261272	268684	11.28%	1.937%
16	11.553	870	872	875	rBV	99048	105388	4.43%	0.760%
17	12.194	926	928	930	rBV	86991	80704	3.39%	0.582%
18	12.331	938	940	945	rBV2	75044	110527	4.64%	0.797%
19	12.422	945	948	950	rBV	92330	92751	3.90%	0.669%
20	12.582	959	962	964	rBV	931322	1112413	46.72%	8.020%
21	13.485	1039	1041	1049	rBV2	71292	108405	4.55%	0.782%
22	13.611	1049	1052	1060	rBV2	317933	419892	17.63%	3.027%
23	14.114	1095	1096	1100	rVB2	21823	33223	1.40%	0.240%
24	14.468	1125	1127	1129	rBV	80088	77319	3.25%	0.557%
25	14.525	1130	1132	1135	rBV	28813	33896	1.42%	0.244%
26	14.605	1136	1139	1143	rBV	37193	69963	2.94%	0.504%
27	14.708	1145	1148	1151	rBV2	34027	76252	3.20%	0.550%
28	14.902	1163	1165	1167	rBV	16806	25324	1.06%	0.183%
29	14.948	1167	1169	1172	rBV	162548	229577	9.64%	1.655%
30	15.337	1201	1203	1205	rBV	25238	34363	1.44%	0.248%
31	15.634	1227	1229	1233	rVV	44278	83556	3.51%	0.602%
32	15.702	1233	1235	1243	rVB3	15123	42393	1.78%	0.306%
33	16.548	1305	1309	1315	rBV4	15157	44206	1.86%	0.319%

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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-BF072716.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

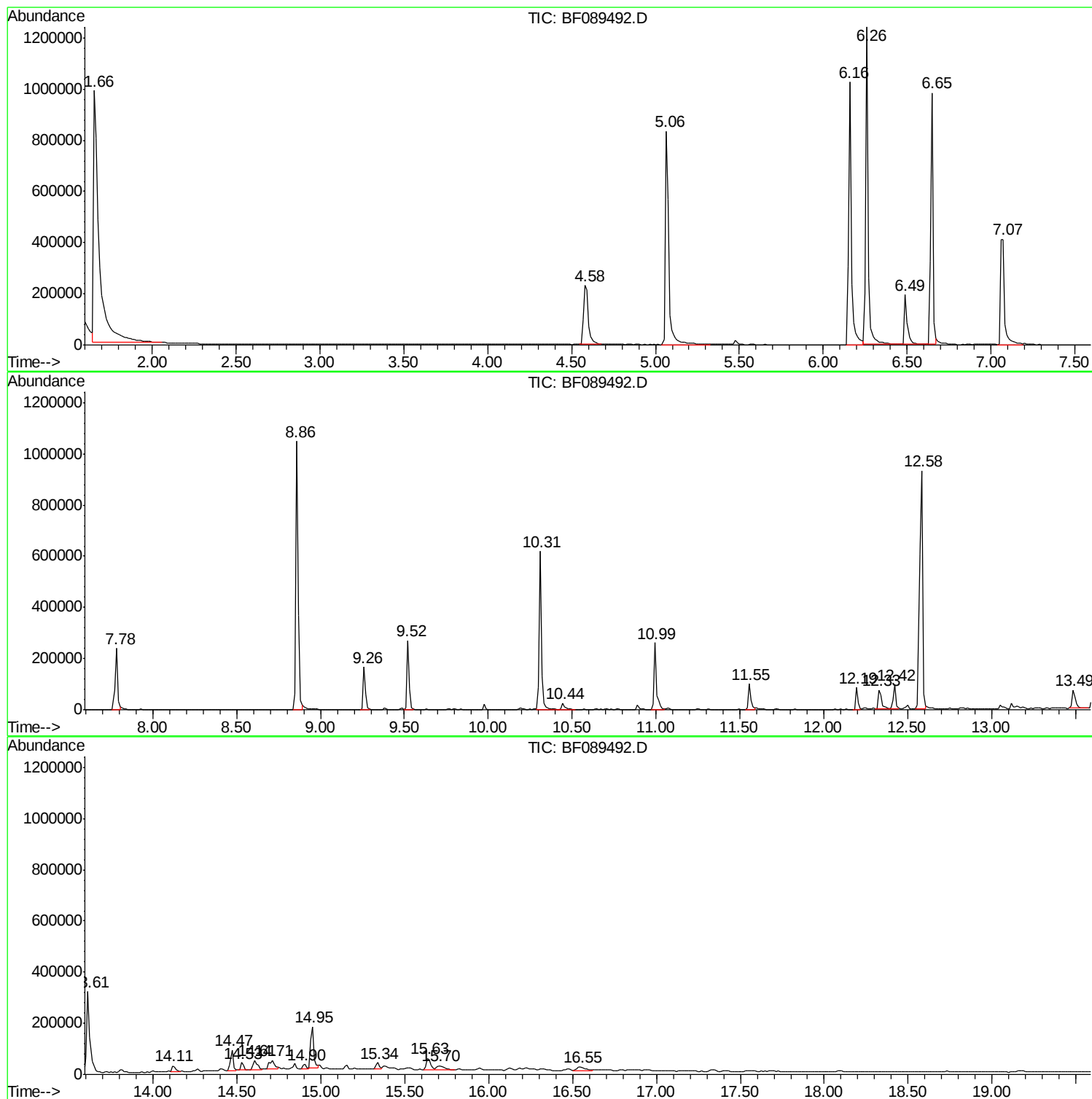
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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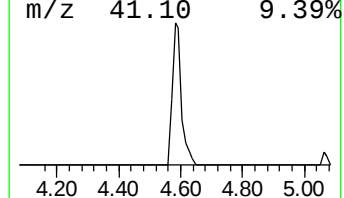
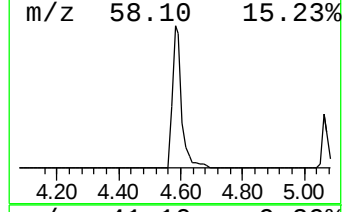
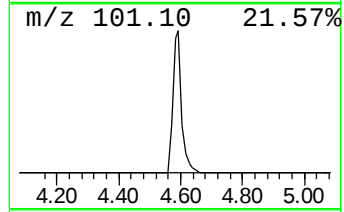
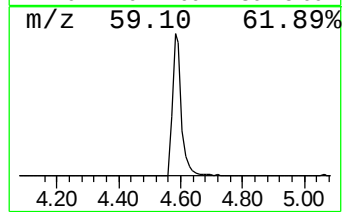
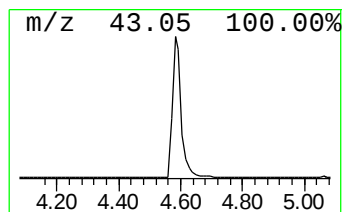
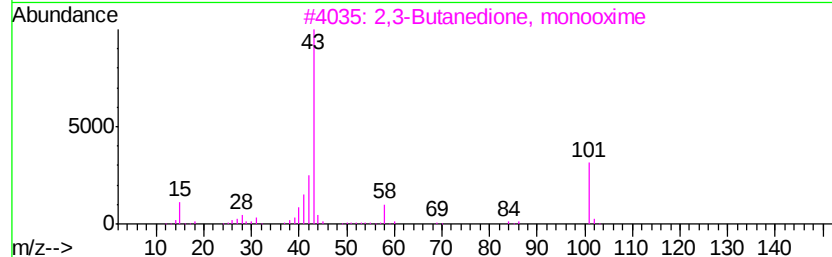
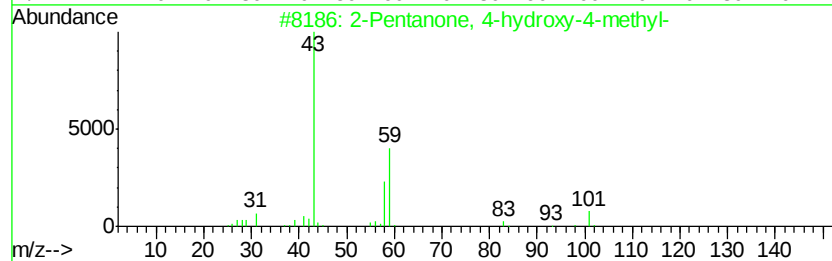
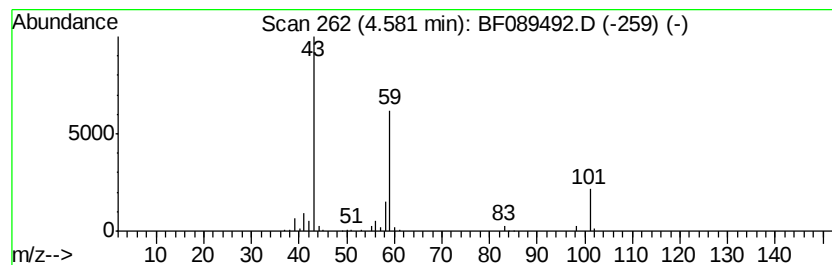
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.58	39.80 ng	459413	1,4-Dichlorobenzene-d4	6.49

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	23
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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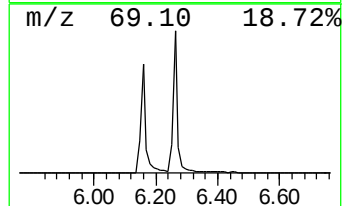
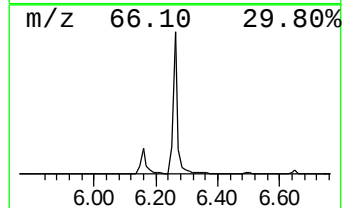
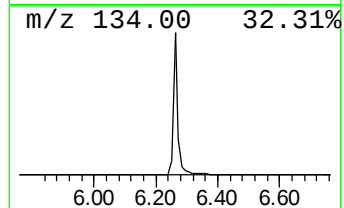
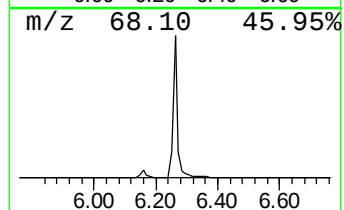
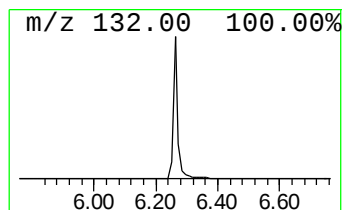
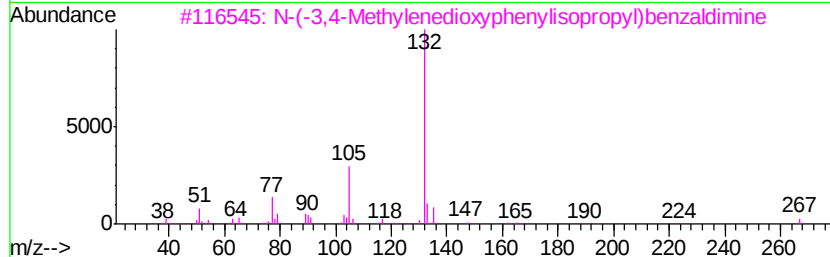
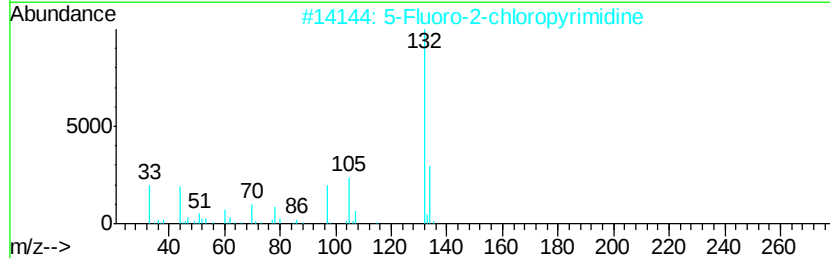
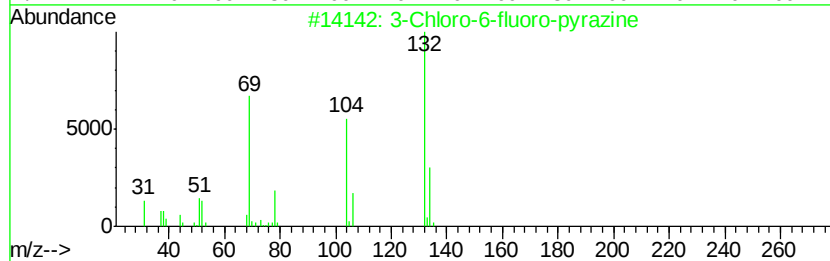
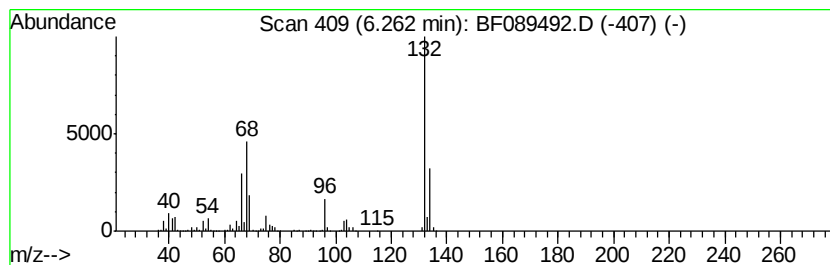
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TIC Library : C:\Database\NIST11.L
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Peak Number 3 unknown6.26 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.26	111.66 ng	1288970	1,4-Dichlorobenzene-d4	6.49

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3			N-(-3,4-Methylenedioxyphenylisopropyl)benzaldimine	267	C17H17NO2	1000378-96-6	10
4			Tranvlcypropine-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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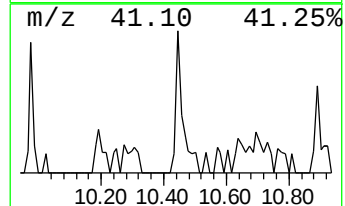
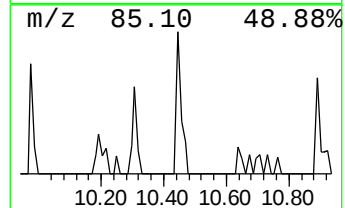
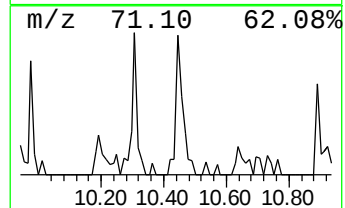
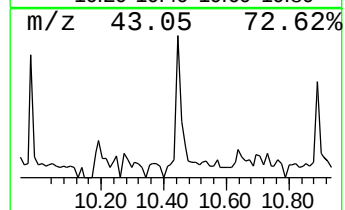
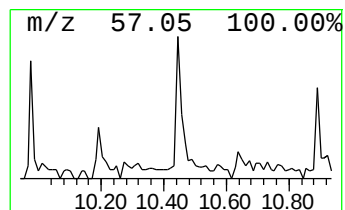
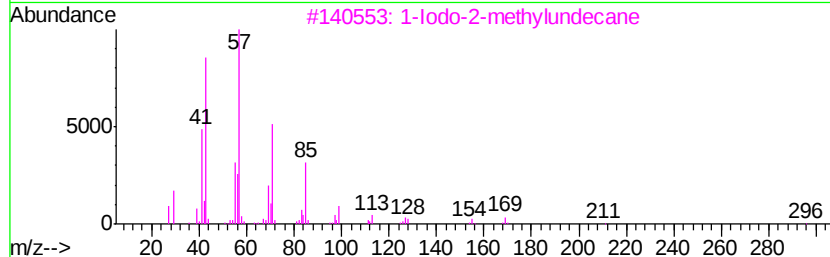
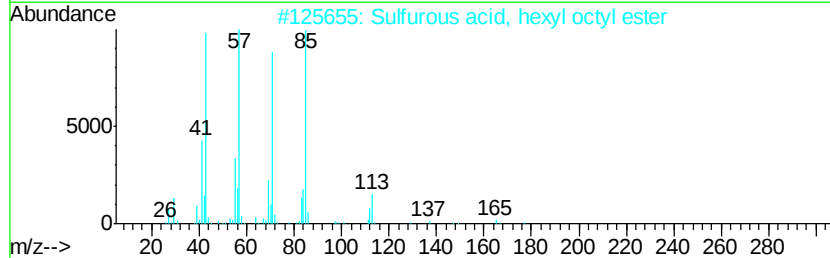
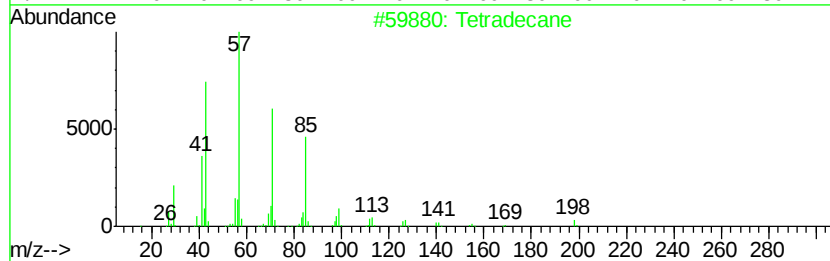
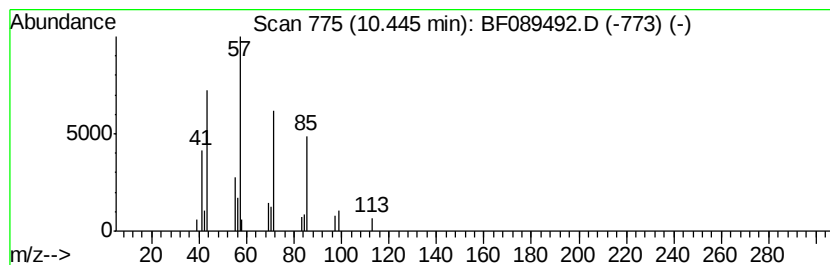
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Tetradecane Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.44	2.31 ng	31032	Phenanthrene-d10	10.99	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	78
2	Sulfurous acid, hexyl octyl ester	278	C14H30O3S	1000309-13-0	72
3	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	64
4	Tridecane	184	C13H28	000629-50-5	64
5	Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	59



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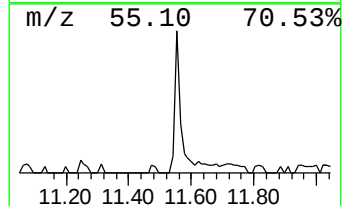
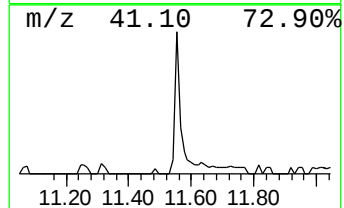
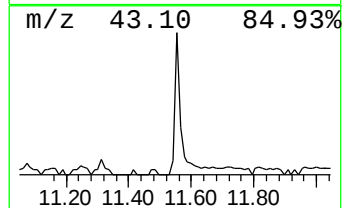
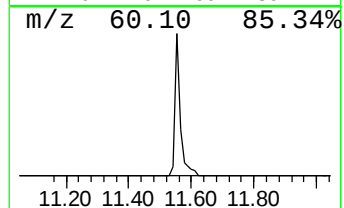
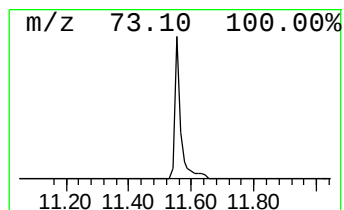
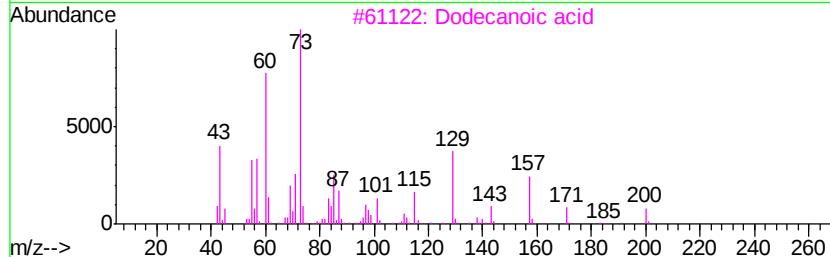
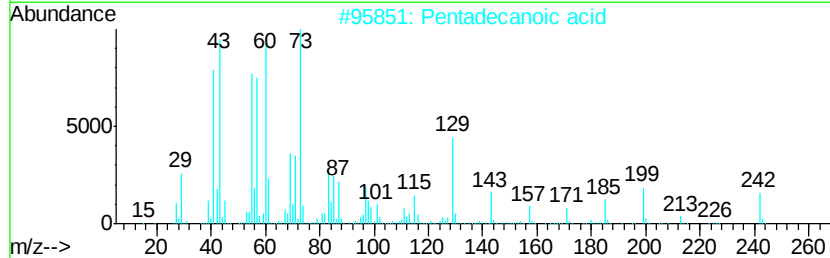
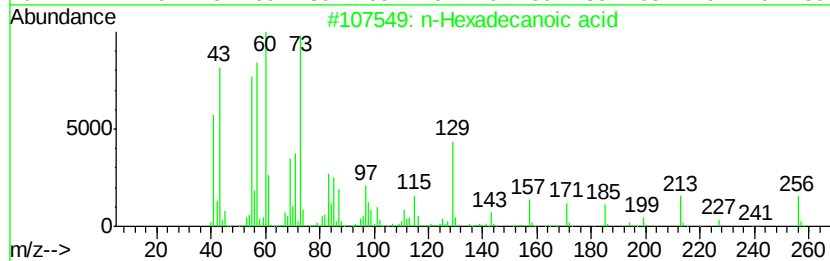
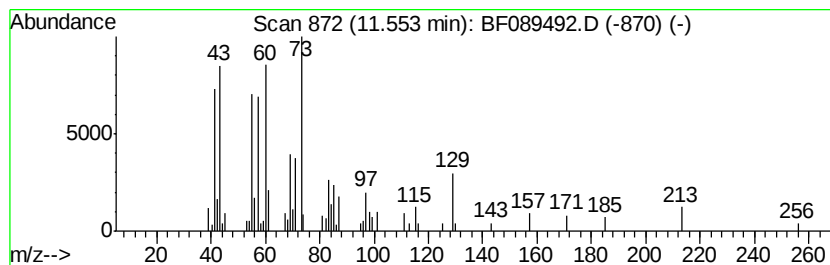
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.55	7.84 ng	105388	Phenanthrene-d10	10.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Dodecanoic acid	200	C12H24O2	000143-07-7	72
4	Undecanoic acid	186	C11H22O2	000112-37-8	72
5	Tridecanoic acid	214	C13H26O2	000638-53-9	64



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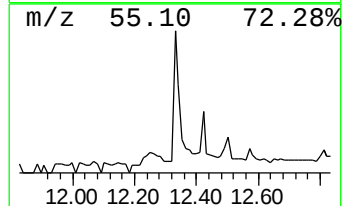
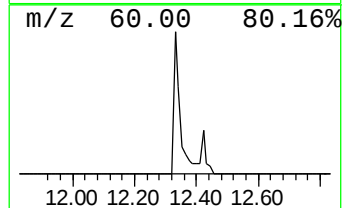
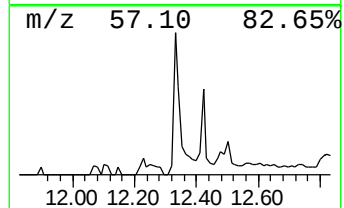
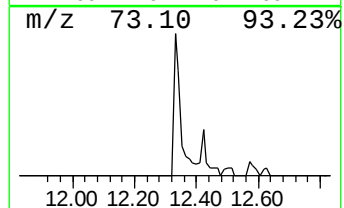
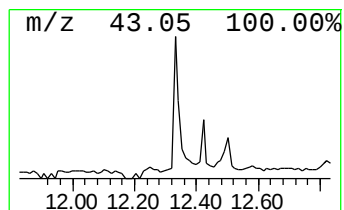
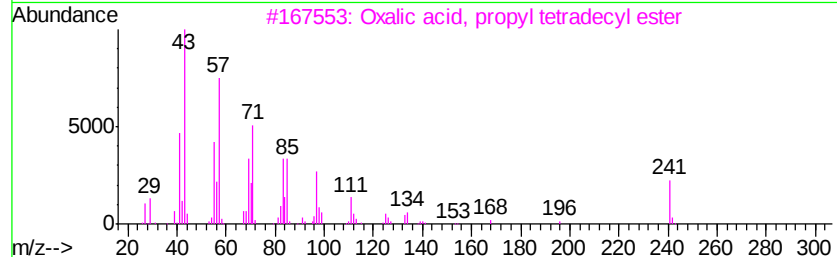
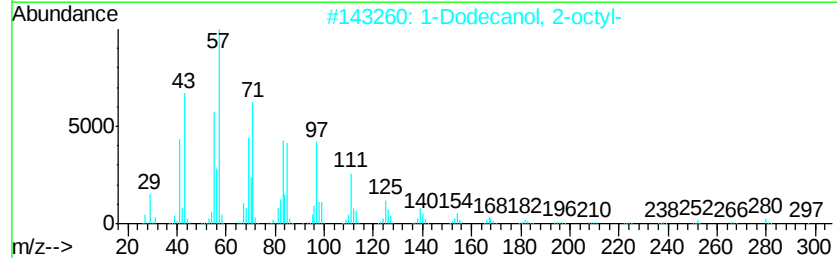
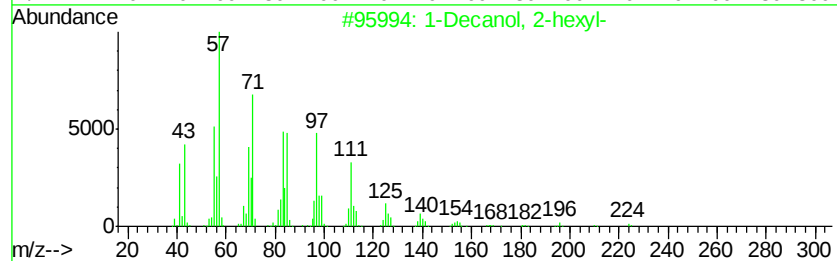
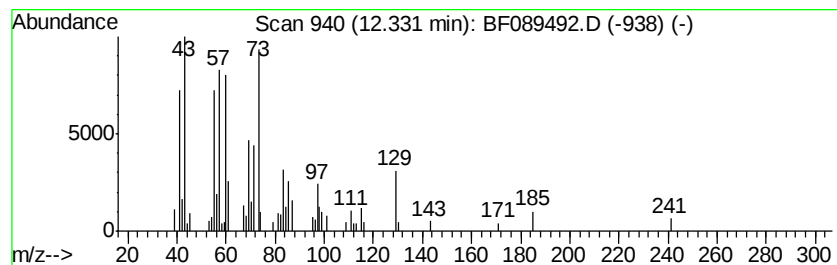
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Peak Number 7 unknown12.33 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.33	5.26 ng	110527	Chrysene-d12	13.61	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	30
2	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	30
3	Oxalic acid, propyl tetradecyl e...	328	C19H36O4	1000309-26-7	30
4	Oxalic acid, cyclobutyl octadecv...	396	C24H44O4	1000309-70-8	30
5	1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	30



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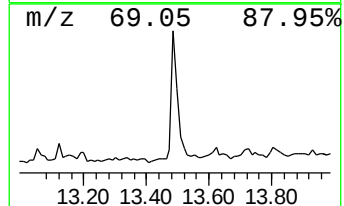
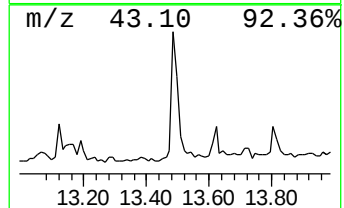
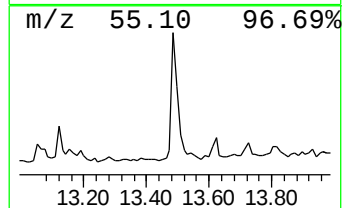
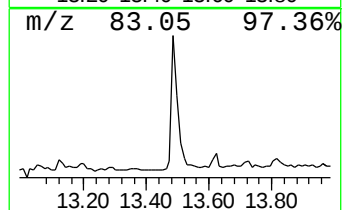
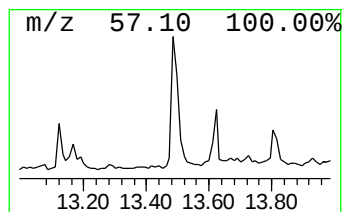
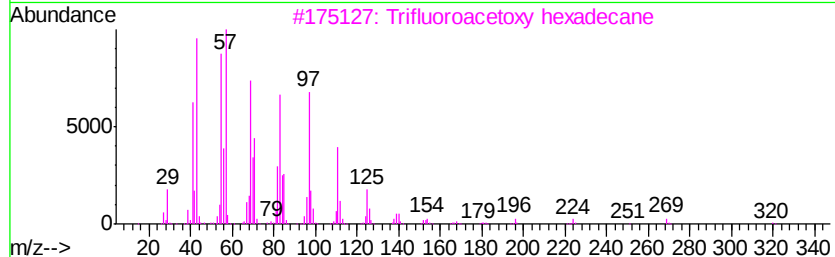
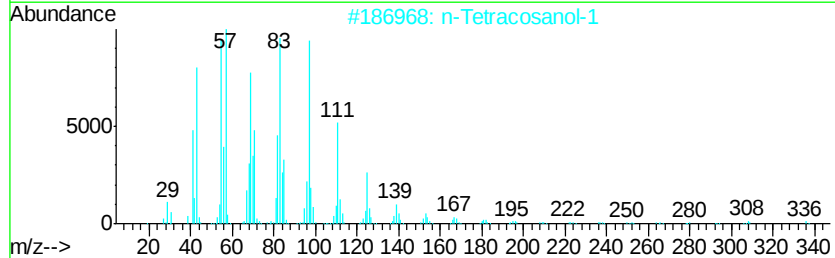
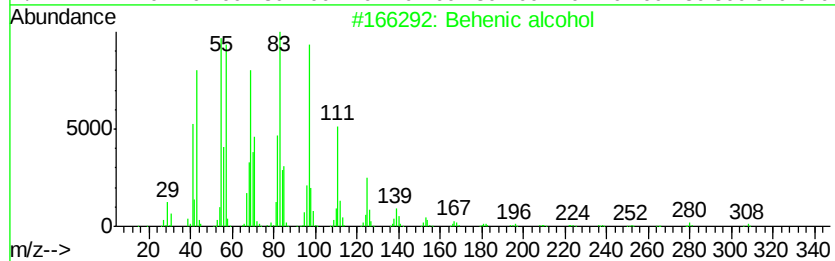
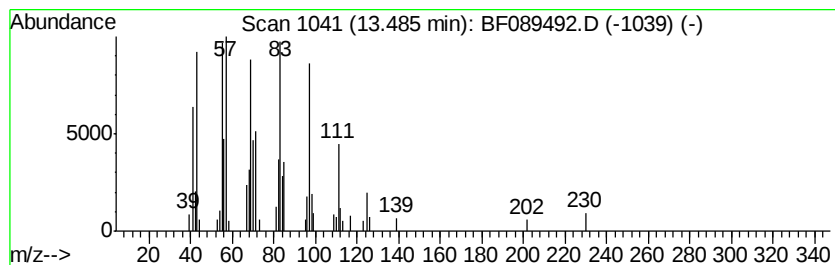
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Behenic alcohol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.49	5.16 ng	108405	Chrysene-d12	13.61
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Behenic alcohol	326 C22H46O	000661-19-8 94
2		n-Tetracosanol-1	354 C24H50O	000506-51-4 94
3		Trifluoroacetoxv hexadecane	338 C18H33F3O2	006222-03-3 93
4		1-Heneicosanol	312 C21H44O	015594-90-8 91
5		Pentafluoropropionic acid, penta...	374 C18H31F5O2	959092-08-1 91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF073116\
Data File : BF089492.D
Acq On : 1 Aug 2016 3:32
Operator : UM/SJ
Sample : H4222-06
Misc :
ALS Vial : 27 Sample Multiplier: 1

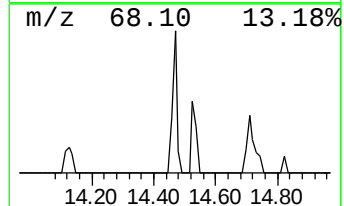
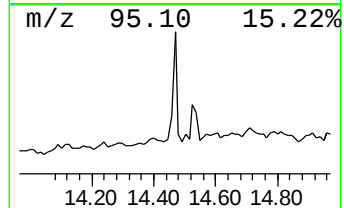
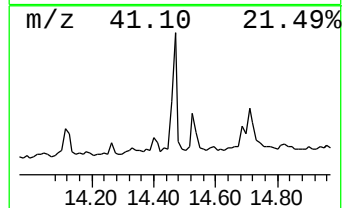
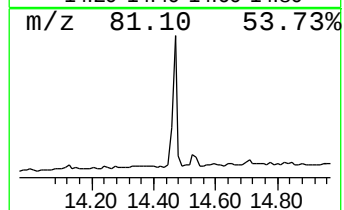
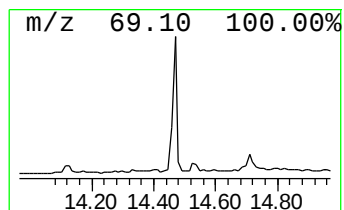
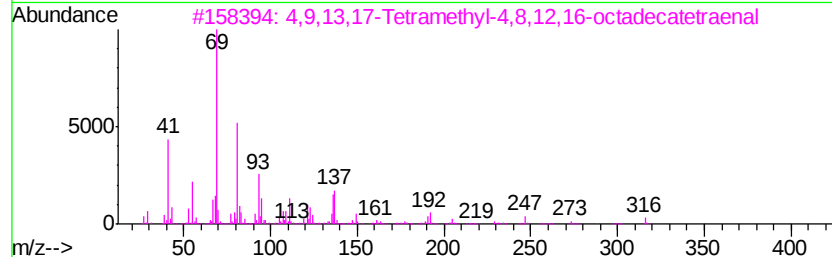
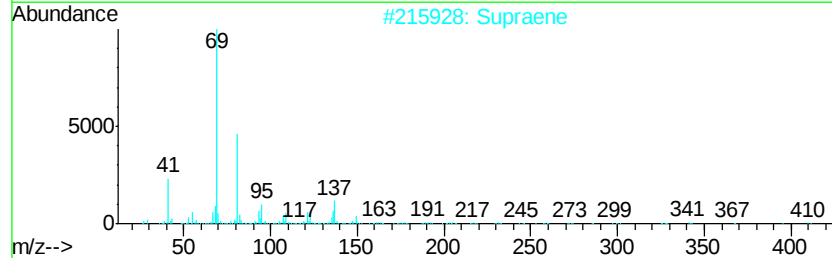
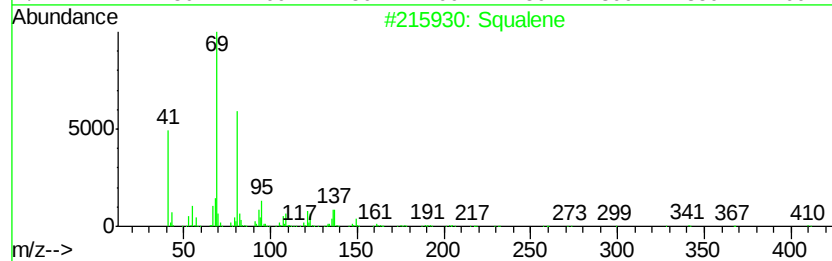
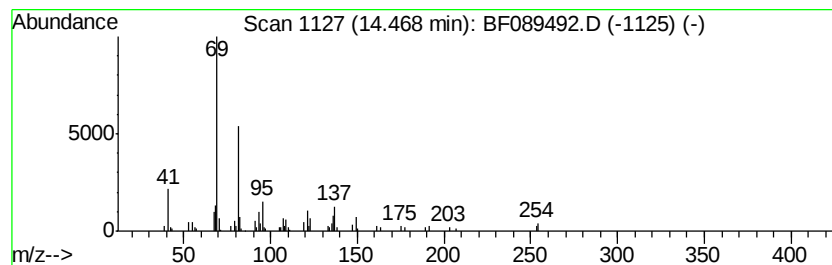
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.47	6.74 ng	77319	Perylene-d12		14.95
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	91
3	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	78
4	trans-Farnesol	222	C15H26O	000106-28-5	59
5	2,6-Octadiene, 2,6-dimethyl-	138	C10H18	002792-39-4	50



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF073116\
Data File : BF089492.D
Acq On : 1 Aug 2016 3:32
Operator : UM/SJ
Sample : H4222-06
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-05-COMP

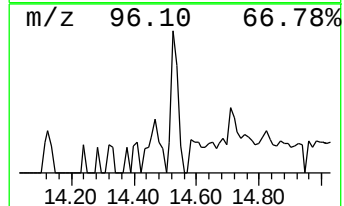
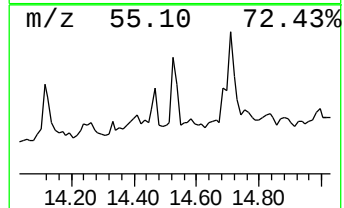
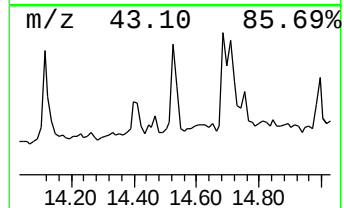
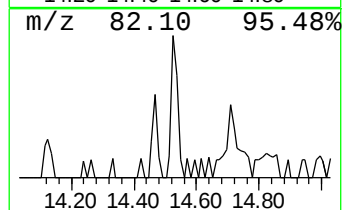
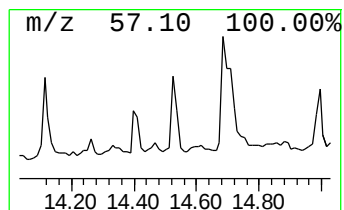
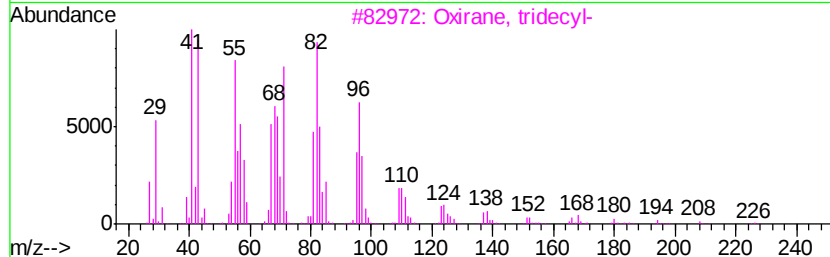
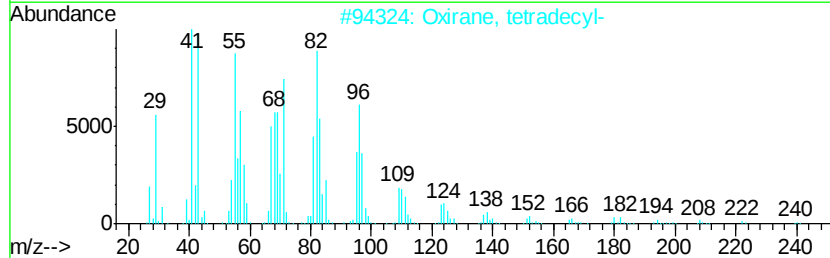
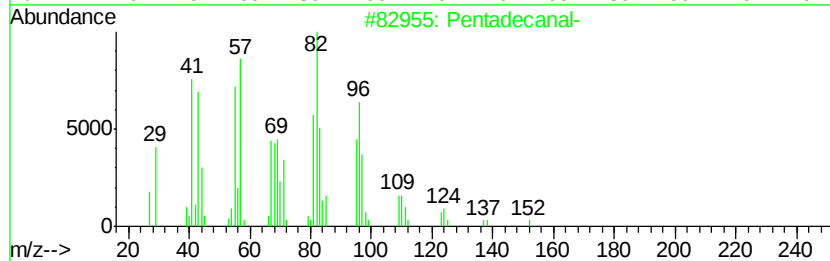
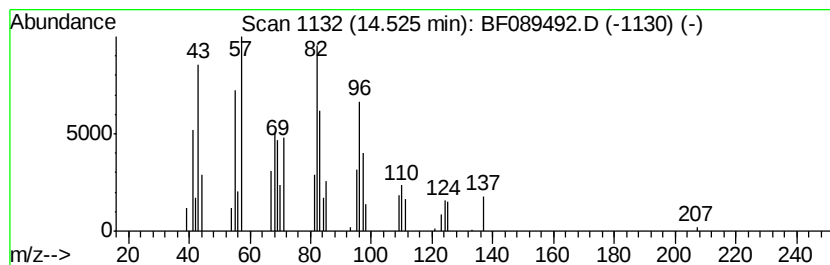
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Pentadecanal- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.53	2.95 ng	33896	Perylene-d12	14.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecanal-	226	C15H30O	002765-11-9	80
2		Oxirane, tetradecyl-	240	C16H32O	007320-37-8	72
3		Oxirane, tridecyl-	226	C15H30O	018633-25-5	72
4		1,19-Eicosadiene	278	C20H38	014811-95-1	64
5		1-Dodecen-1-ol, acetate	226	C14H26O2	056438-08-5	47



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF073116\
Data File : BF089492.D
Acq On : 1 Aug 2016 3:32
Operator : UM/SJ
Sample : H4222-06
Misc :
ALS Vial : 27 Sample Multiplier: 1

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ClientSampleId :
SB-05-COMP

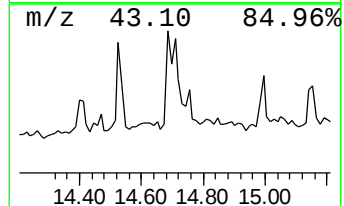
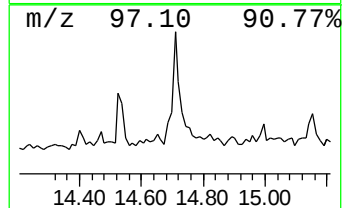
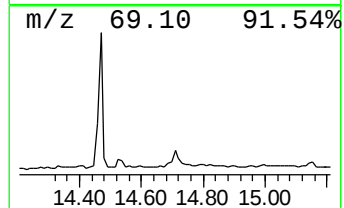
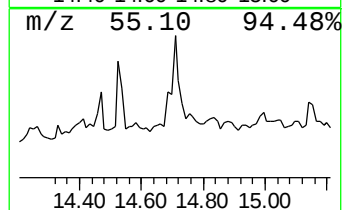
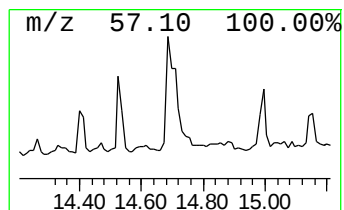
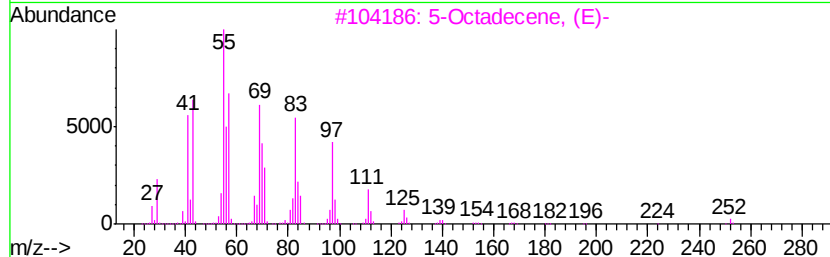
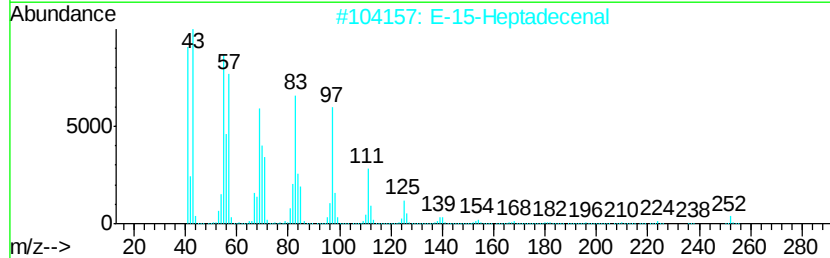
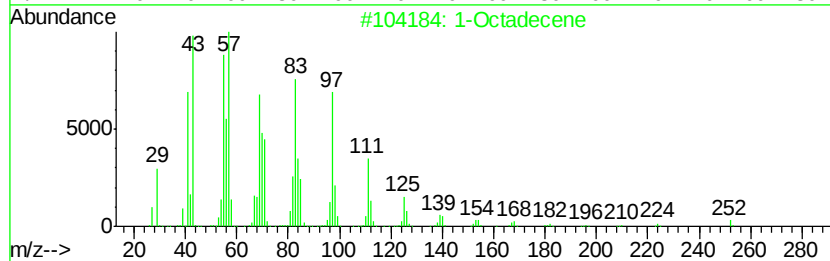
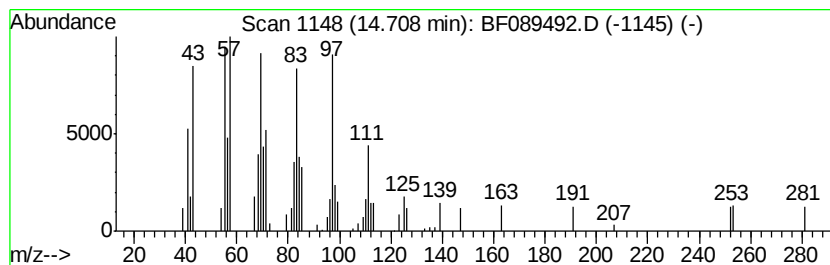
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 1-Octadecene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.71	6.64 ng	76252	Perylene-d12	14.95

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octadecene	252	C18H36	000112-88-9	99
2			E-15-Heptadecenal	252	C17H32O	1000130-97-9	98
3			5-Octadecene, (E)-	252	C18H36	007206-21-5	96
4			Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	95
5			Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	95



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF073116\
Data File : BF089492.D
Acq On : 1 Aug 2016 3:32
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Misc :
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ClientSampleId :
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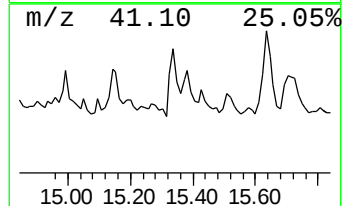
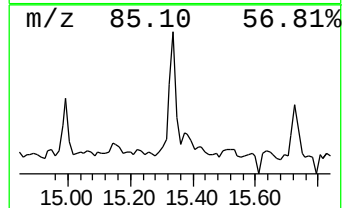
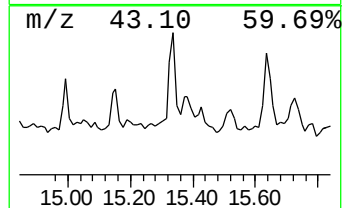
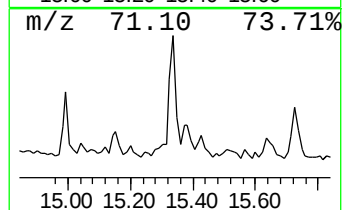
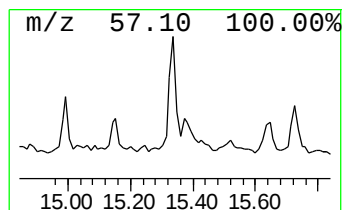
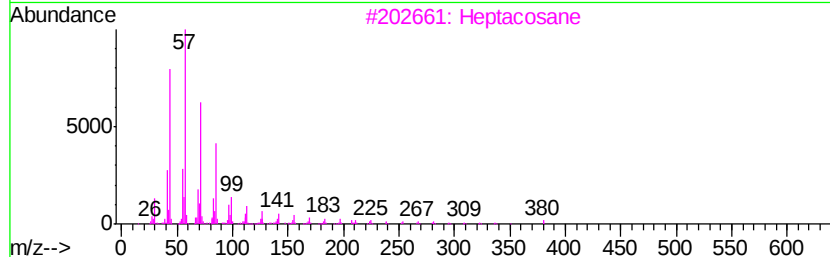
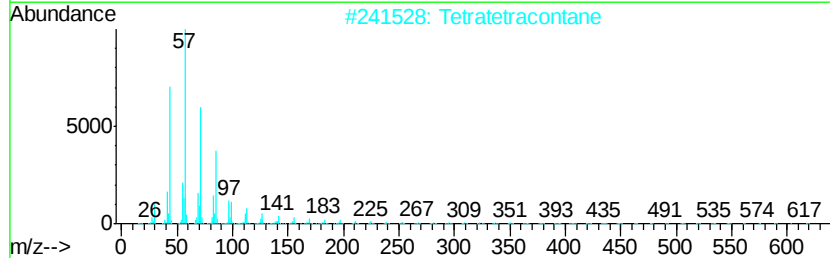
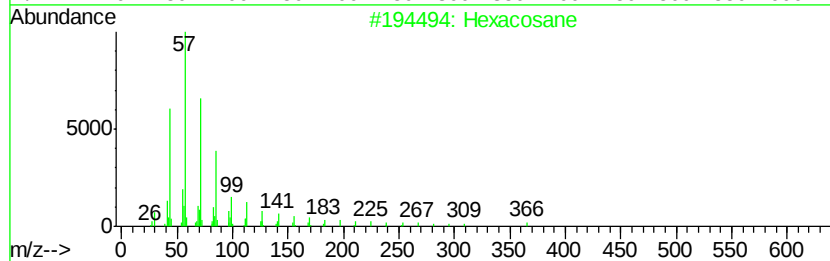
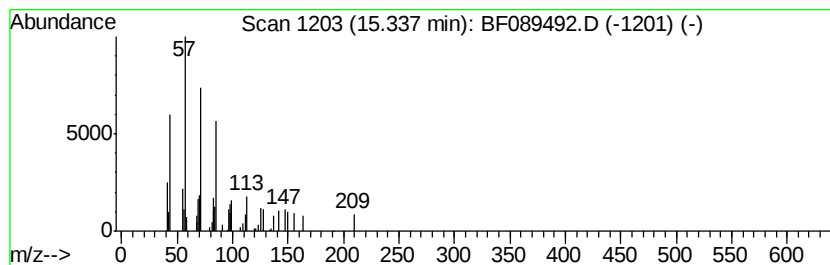
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Hexacosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.34	2.99 ng	34363	Perylene-d12	14.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	80
2		Tetratetracontane	619	C44H90	007098-22-8	80
3		Heptacosane	380	C27H56	000593-49-7	80
4		Octacosane	394	C28H58	000630-02-4	72
5		triacontane	422	C30H62	000638-68-6	72



Data Path : Z:\HPCHEM1\BNA F\DATA\BF073116\
Data File : BF089492.D
Acq On : 1 Aug 2016 3:32
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Sample : H4222-06
Misc :
ALS Vial : 27 Sample Multiplier: 1

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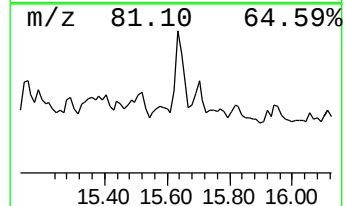
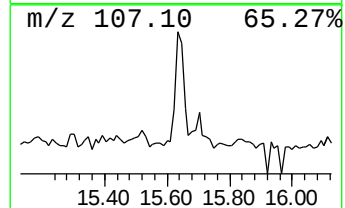
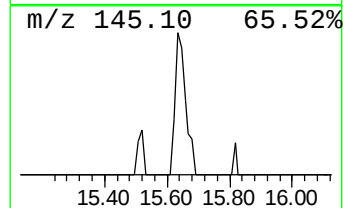
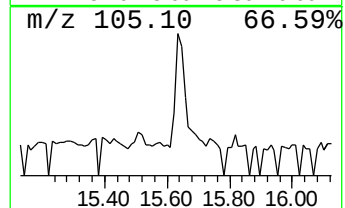
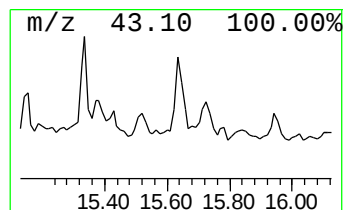
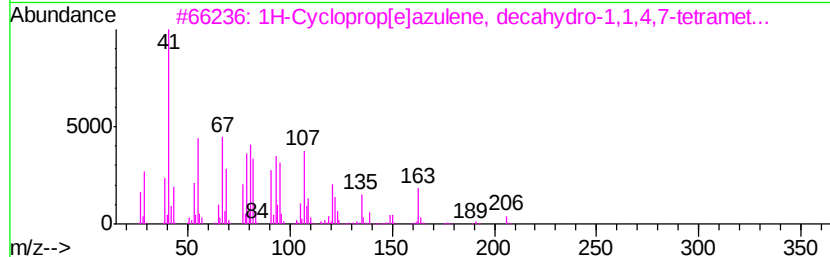
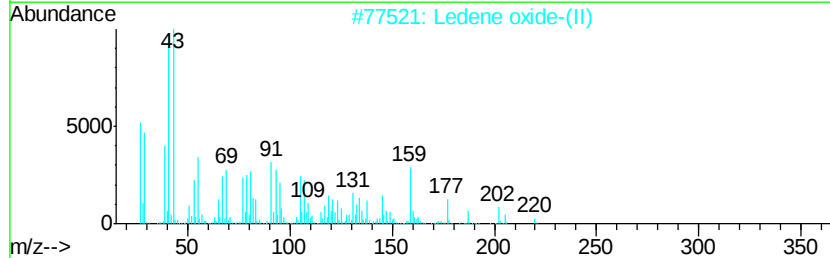
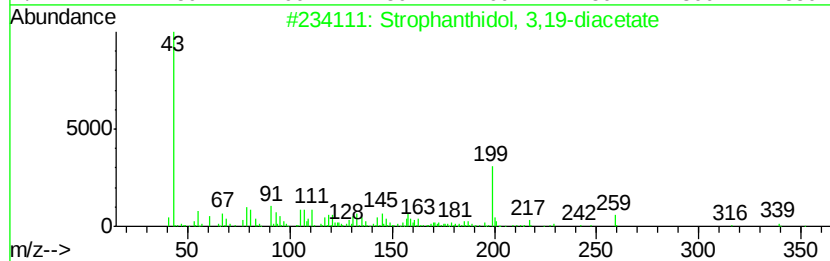
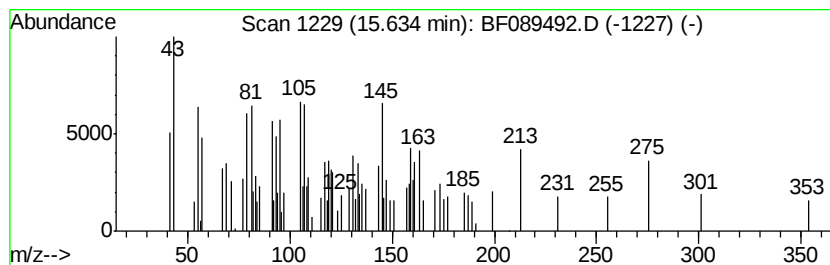
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown15.63 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.63	7.28 ng	83556	Perylene-d12	14.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Strophanthidol, 3,19-diacetate	490	C27H38O8	083349-11-5	38
2		Ledene oxide-(II)	220	C15H24O	1000159-36-7	16
3		1H-Cycloprop[elazulene, decahydr...	206	C15H26	028580-43-0	12
4		Andrographolide	350	C20H30O5	005508-58-7	12
5		2H-Pyran, 2-(7-heptadecynyloxy)t...	336	C22H40O2	056599-50-9	11



Data Path : Z:\HPCHEM1\BNA F\DATA\BF073116\
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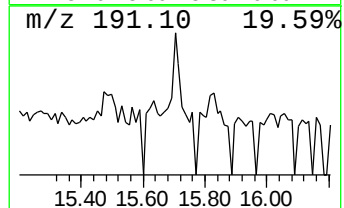
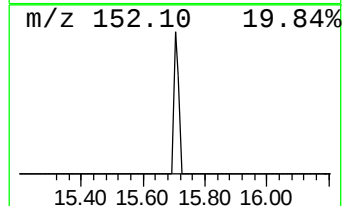
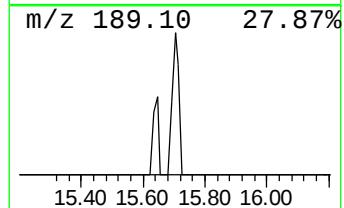
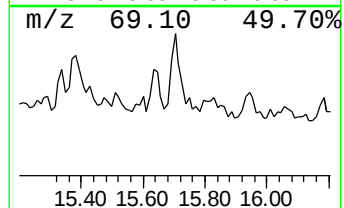
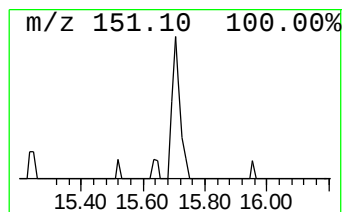
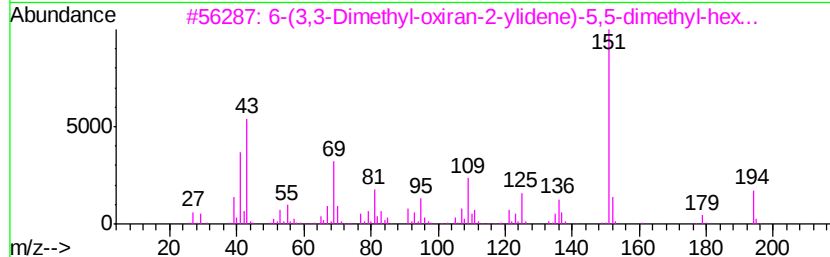
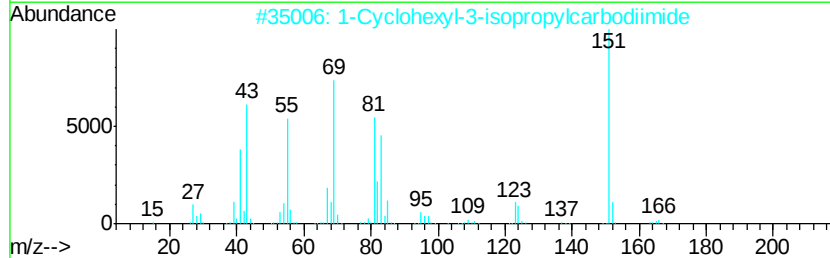
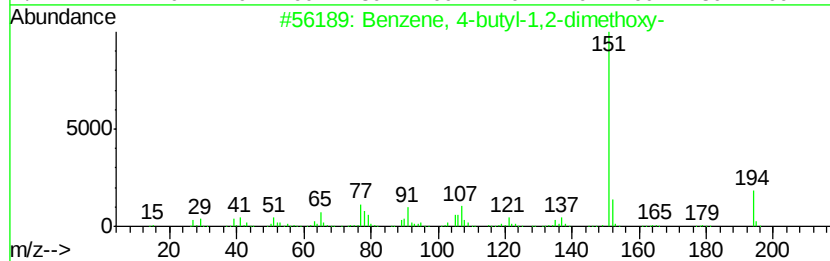
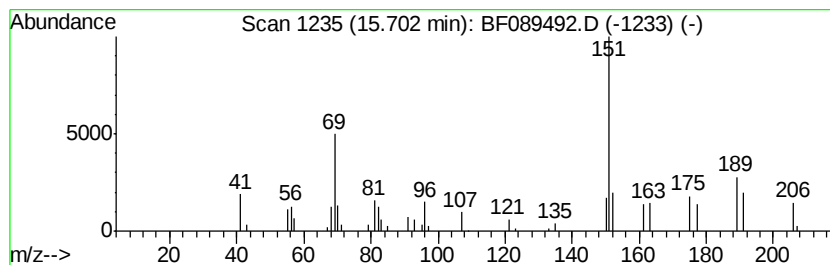
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown15.70 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.70	3.69 ng	42393	Perylene-d12	14.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 4-butyl-1,2-dimethoxy-	194	C12H18O2	059056-76-7	38
2		1-Cyclohexyl-3-isopropylcarbodiimide...	166	C10H18N2	003496-83-1	17
3		6-(3,3-Dimethyl-oxiran-2-ylidene)...	194	C12H18O2	1000187-66-2	17
4		2-Methyl-7-oxo-4,7-dihydro-triaz...	151	C5H5N5O	057351-75-4	16
5		Ethanethioamide, N-phenyl-	151	C8H9NS	000637-53-6	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF073116\
Data File : BF089492.D
Acq On : 1 Aug 2016 3:32
Operator : UM/SJ
Sample : H4222-06
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-05-COMP

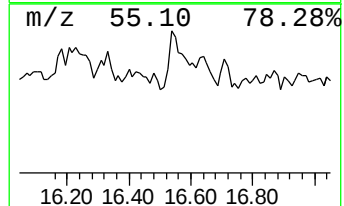
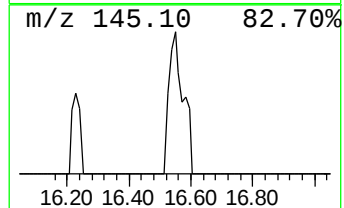
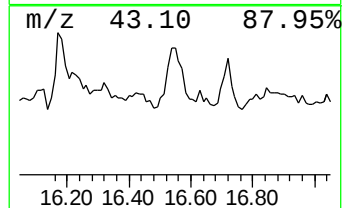
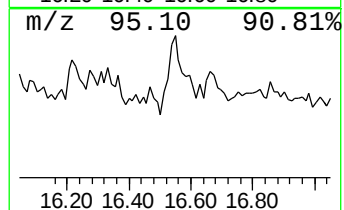
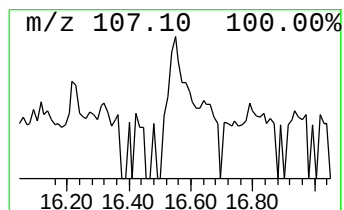
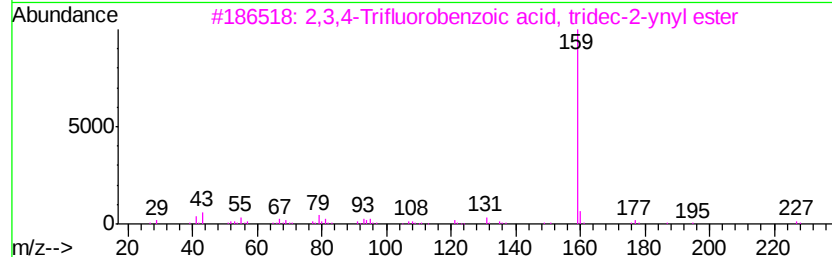
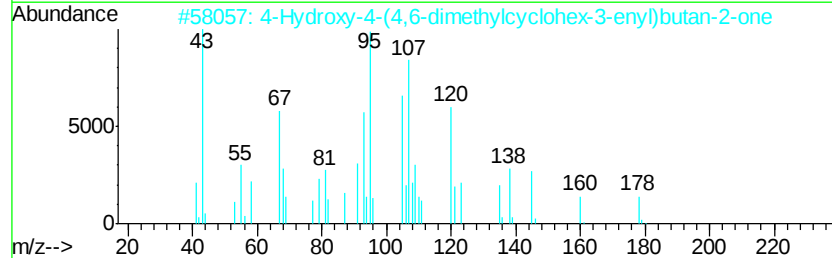
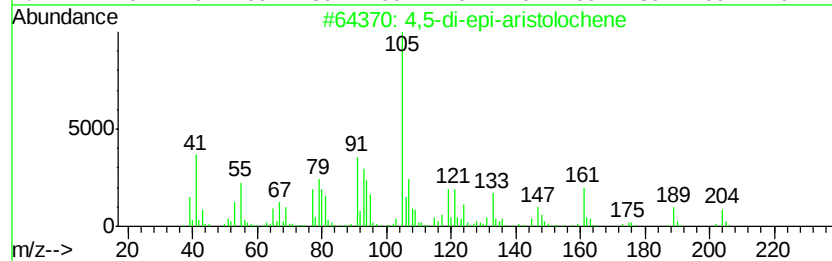
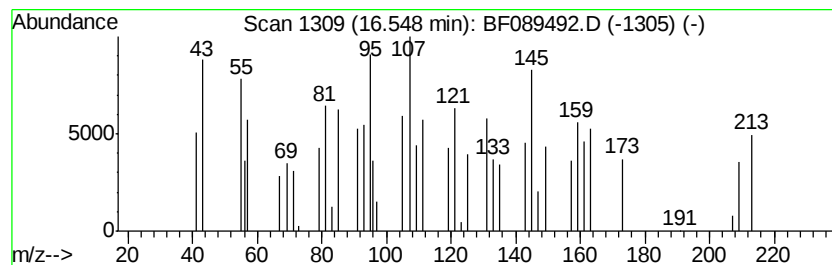
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 unknown16.55 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.55	3.85 ng	44206	Perylene-d12	14.95

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4,5-di-epi-aristolochene	204	C15H24	1000374-17-1	10
2			4-Hydroxy-4-(4,6-dimethylcyclohe...	196	C12H20O2	002316-79-2	10
3			2,3,4-Trifluorobenzoic acid, tri...	354	C20H25F3O2	1000292-56-0	9
4			Benzyl 2-bromoacetate	228	C9H9BrO2	005437-45-6	9
5			Pent-4-enoic acid, 2-(2-hydroxy-...	244	C12H24N2O3	1000302-98-5	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF073116\
 Data File : BF089492.D
 Acq On : 1 Aug 2016 3:32
 Operator : UM/SJ
 Sample : H4222-06
 Misc :
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-05-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.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...	4.58	39.8	ng	459413	1	6.49	230870	20.0
unknown6.26	6.26	111.7	ng	1288970	1	6.49	230870	20.0
Tetradecane	10.44	2.3	ng	31032	4	10.99	268684	20.0
n-Hexadecanoic acid	11.55	7.8	ng	105388	4	10.99	268684	20.0
unknown12.33	12.33	5.3	ng	110527	5	13.61	419892	20.0
Behenic alcohol	13.49	5.2	ng	108405	5	13.61	419892	20.0
Squalene	14.47	6.7	ng	77319	6	14.95	229577	20.0
Pentadecanal-	14.53	3.0	ng	33896	6	14.95	229577	20.0
1-Octadecene	14.71	6.6	ng	76252	6	14.95	229577	20.0
Hexacosane	15.34	3.0	ng	34363	6	14.95	229577	20.0
unknown15.63	15.63	7.3	ng	83556	6	14.95	229577	20.0
unknown15.70	15.70	3.7	ng	42393	6	14.95	229577	20.0
unknown16.55	16.55	3.9	ng	44206	6	14.95	229577	20.0