

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011317\
 Data File : BF092278.D
 Acq On : 14 Jan 2017 11:58
 Operator : UM/SJ
 Sample : I1162-10
 Misc :
 ALS Vial : 37 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-48-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	4.701	252	255	272	rBV	1552191	2622479	47.23%	5.604%
2	5.170	294	296	313	rBV	4880718	5552755	100.00%	11.867%
3	6.244	387	390	397	rBV	4747704	5522983	99.46%	11.803%
4	6.347	397	399	402	rVV	5211676	4991885	89.90%	10.668%
5	6.576	416	419	421	rBV	1319929	1312457	23.64%	2.805%
6	6.724	430	432	435	rBV	3013709	4002816	72.09%	8.554%
7	7.147	466	469	471	rBV	3213626	3201707	57.66%	6.842%
8	7.856	529	531	534	rBV	1239731	1620681	29.19%	3.464%
9	8.942	623	626	629	rBV	4859130	4695418	84.56%	10.034%
10	9.342	659	661	664	rBV	637024	546799	9.85%	1.169%
11	9.605	682	684	687	rBV	1464207	1687573	30.39%	3.606%
12	10.062	720	724	725	rBV	117447	135742	2.44%	0.290%
13	10.279	740	743	744	rBV	57741	70318	1.27%	0.150%
14	10.393	751	753	756	rBV2	1817001	2636714	47.48%	5.635%
15	10.531	763	765	768	rVB	146996	181007	3.26%	0.387%
16	10.976	802	804	805	rBV	96427	84159	1.52%	0.180%
17	11.091	811	814	816	rBV	906138	1109223	19.98%	2.370%
18	11.639	860	862	866	rBV	65537	82124	1.48%	0.176%
19	12.508	937	938	941	rVB2	123308	115186	2.07%	0.246%
20	12.668	950	952	955	rBV	2437183	2788011	50.21%	5.958%
21	13.217	997	1000	1001	rBV	84353	86186	1.55%	0.184%
22	13.605	1030	1034	1041	rBV	71453	184523	3.32%	0.394%
23	13.708	1041	1043	1046	rBV	936876	1093585	19.69%	2.337%
24	14.245	1088	1090	1096	rVB3	25679	56910	1.02%	0.122%
25	14.359	1098	1100	1103	rBV	1109441	1019017	18.35%	2.178%
26	14.474	1108	1110	1114	rVV2	64468	96990	1.75%	0.207%
27	14.840	1139	1142	1149	rBV2	66418	186640	3.36%	0.399%
28	15.068	1159	1162	1164	rBV	768693	863988	15.56%	1.846%
29	15.571	1202	1206	1210	rVB7	25253	85607	1.54%	0.183%
30	15.823	1225	1228	1231	rBV3	19200	62000	1.12%	0.132%
31	15.880	1231	1233	1239	rVB2	39727	97552	1.76%	0.208%

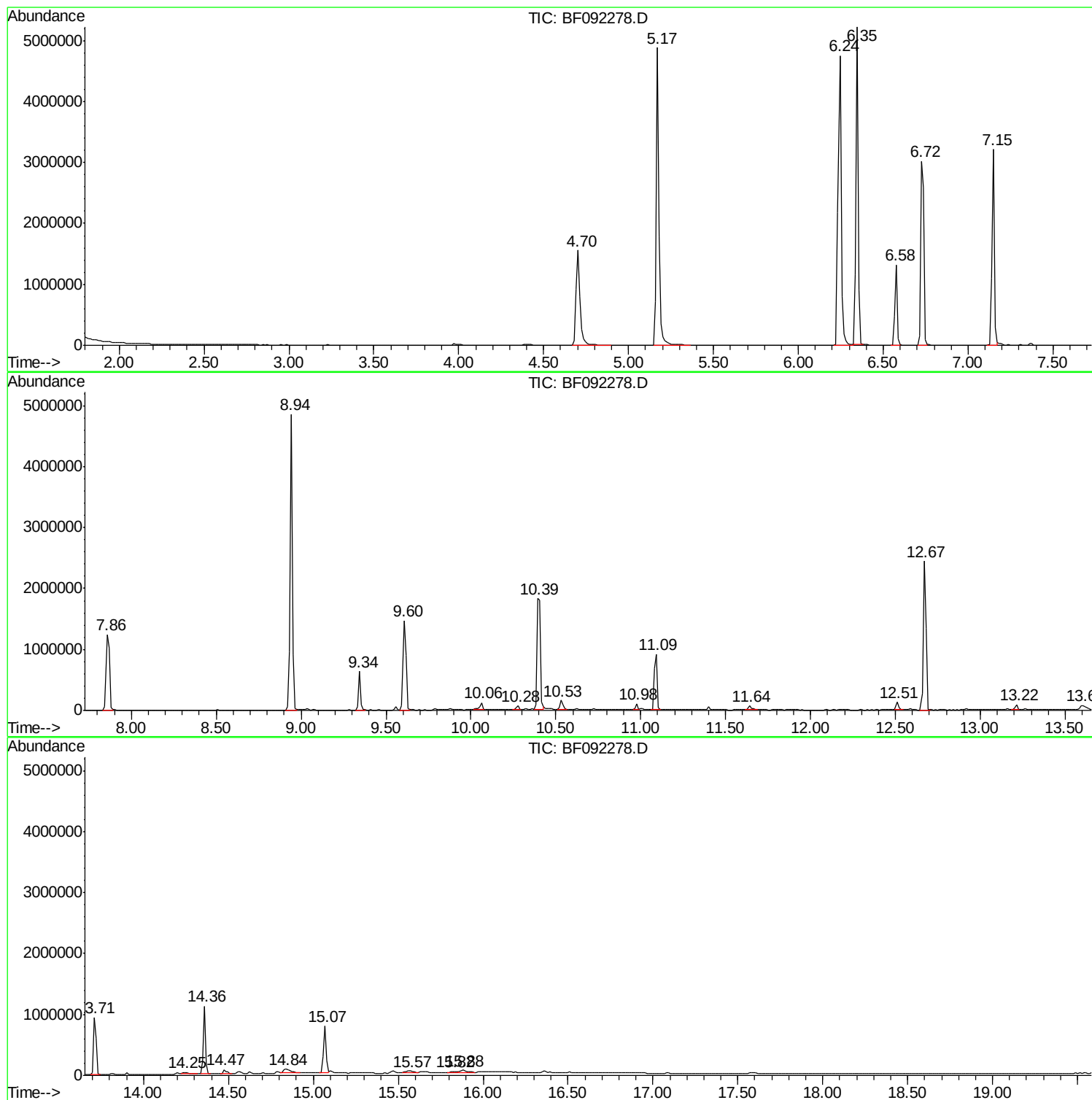
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ClientSampleId :
SB-48-COMP

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



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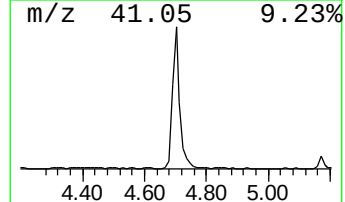
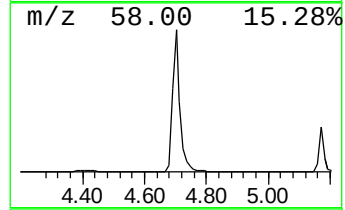
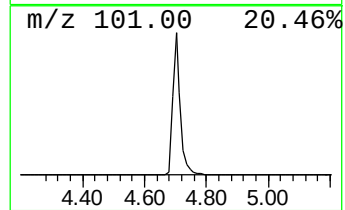
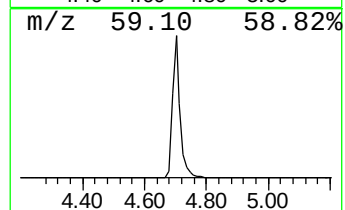
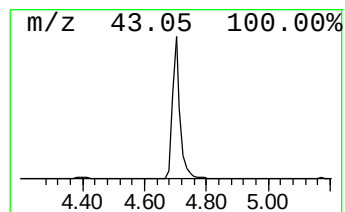
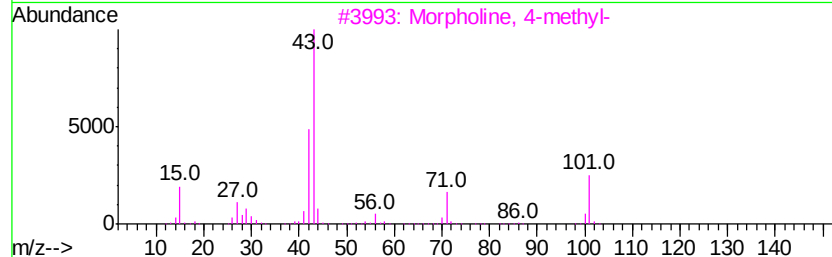
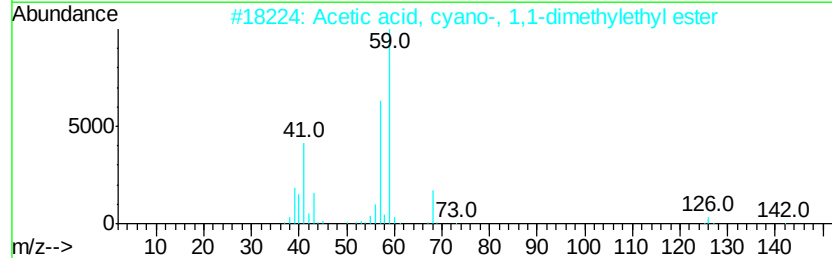
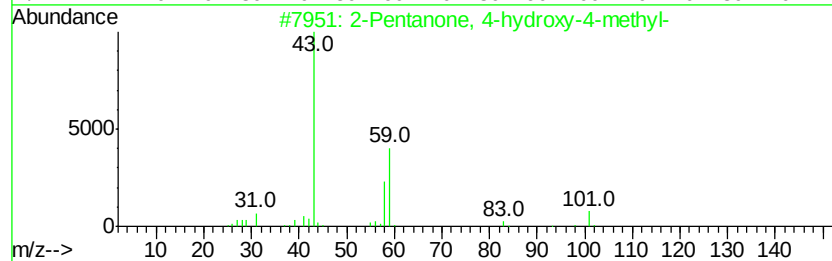
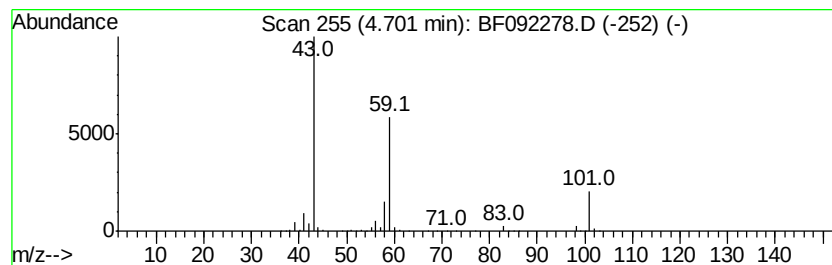
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.70	39.96 ng	2622480	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		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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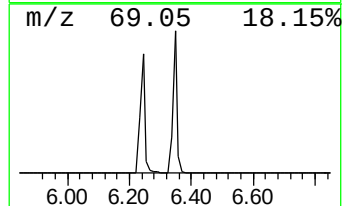
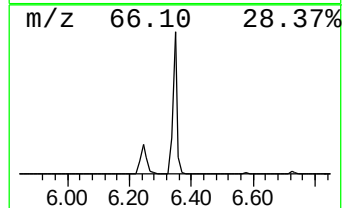
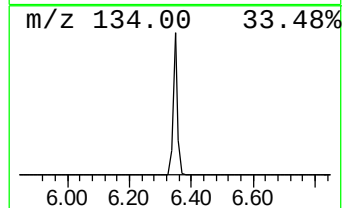
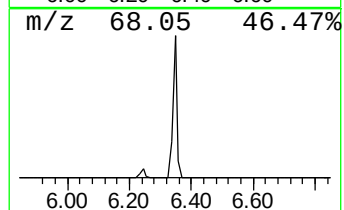
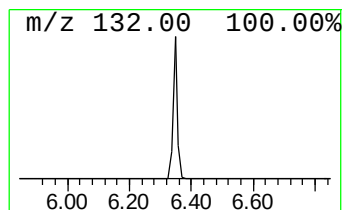
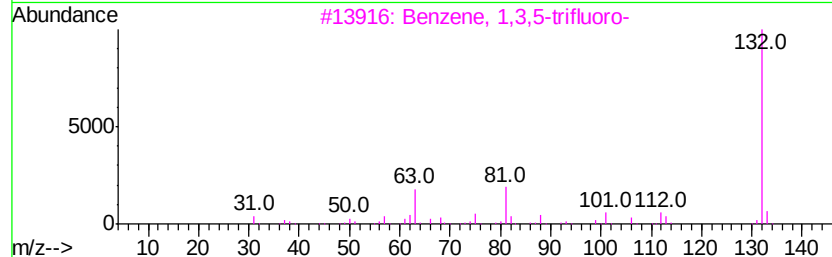
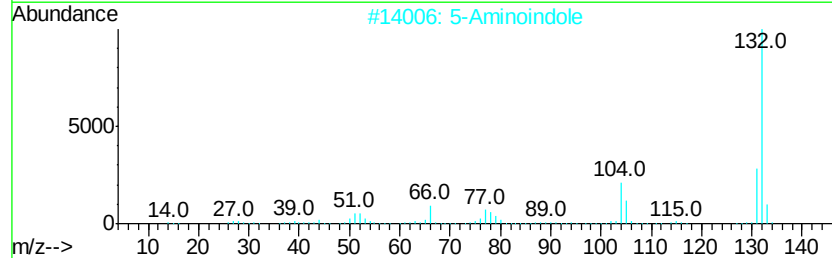
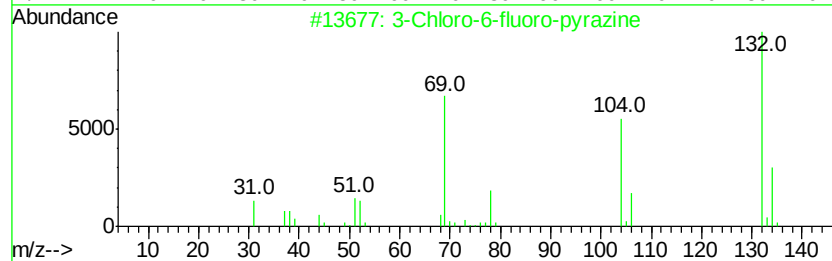
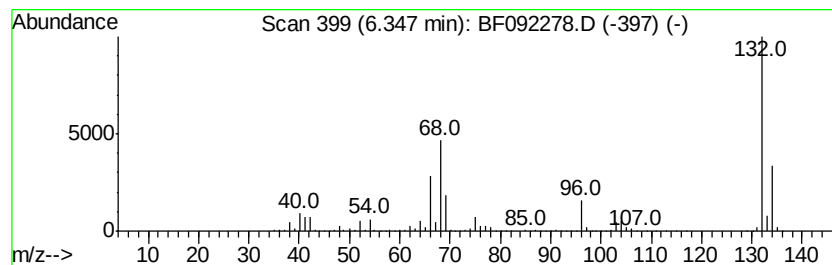
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Peak Number 2 unknown6.35 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.35	76.07 ng	4991890	1,4-Dichlorobenzene-d4	6.58

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3	Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5	Aminoindole	132	C8H8N2	005192-03-0	12
3		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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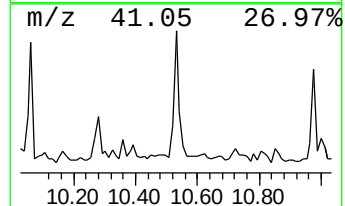
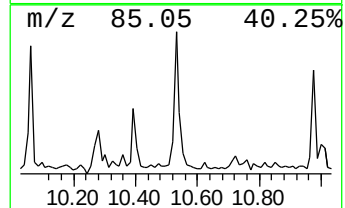
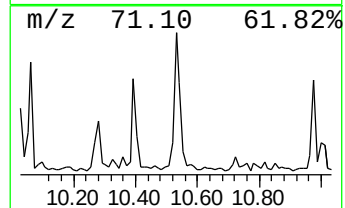
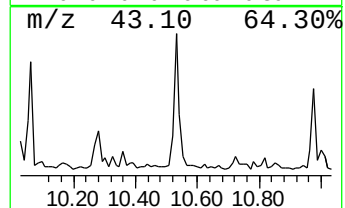
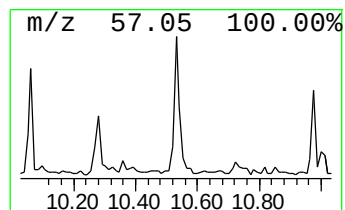
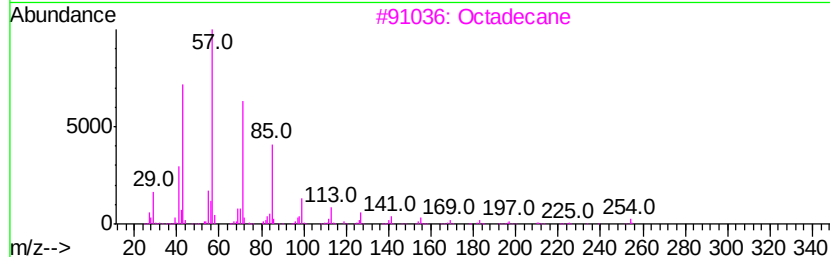
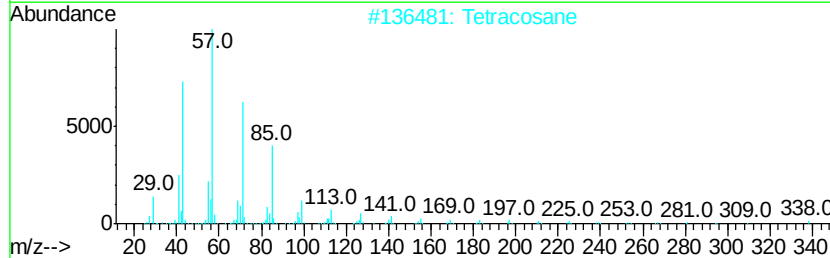
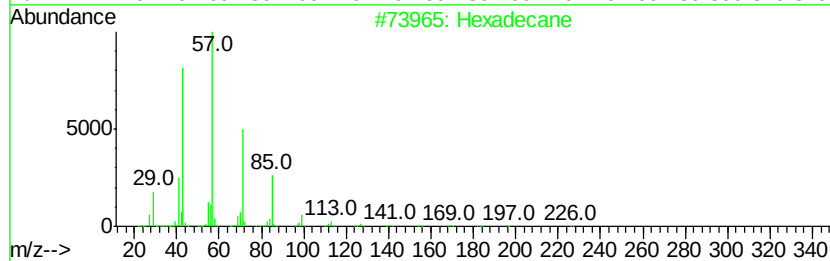
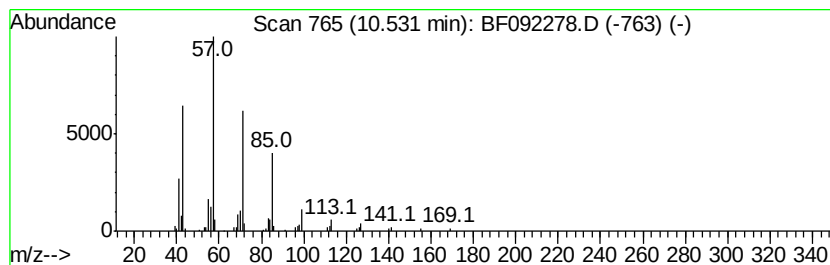
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Peak Number 4 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.53	3.26 ng	181007	Phenanthrene-d10		11.09
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Tetracosane	338	C24H50	000646-31-1	90
3	Octadecane	254	C18H38	000593-45-3	86
4	Heptacosane	380	C27H56	000593-49-7	78
5	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	78



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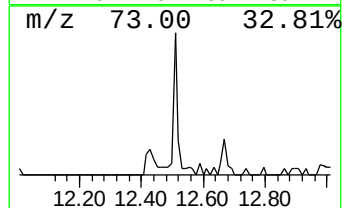
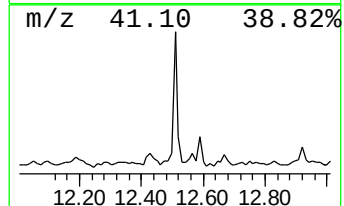
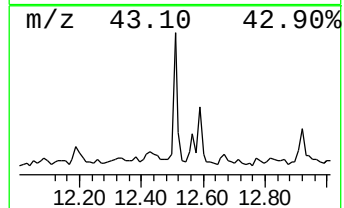
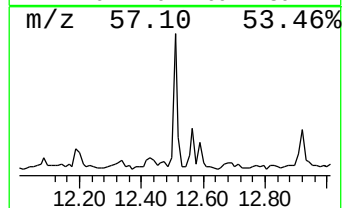
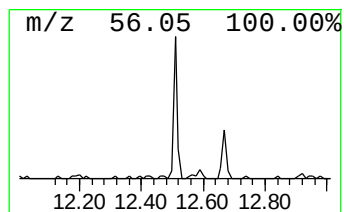
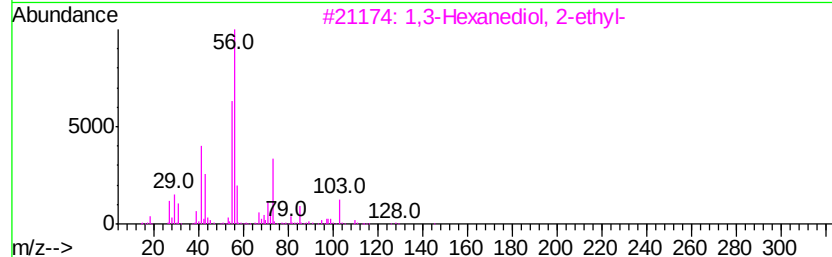
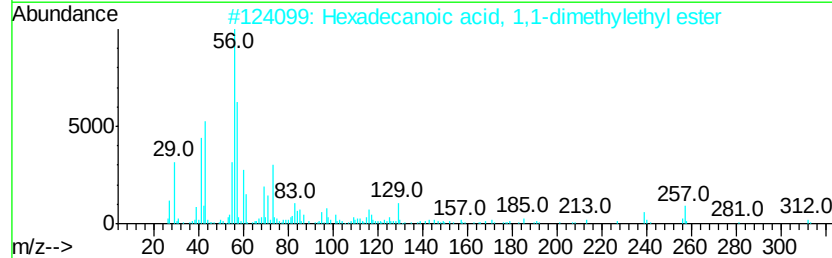
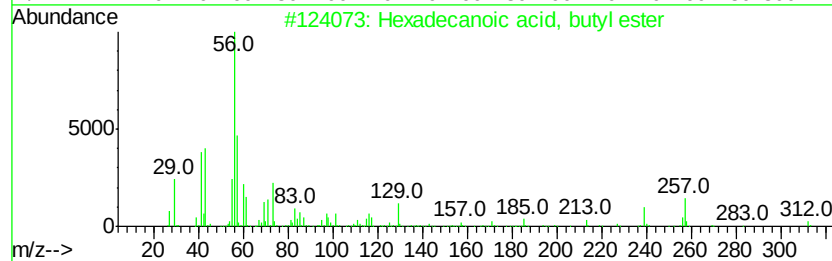
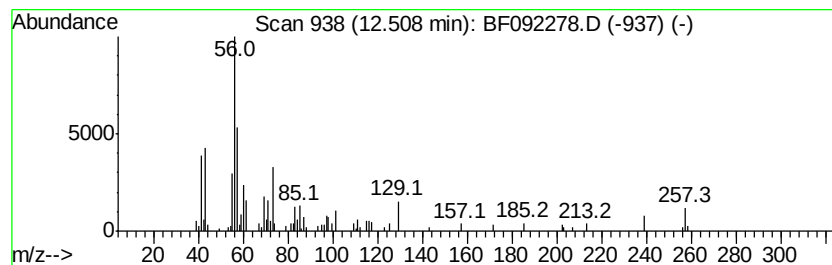
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.51	2.11 ng	115186	Chrysene-d12	13.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	43
3		1,3-Hexanediol, 2-ethyl-	146	C8H18O2	000094-96-2	38
4		Decane, 2,2,3-trimethyl-	184	C13H28	062338-09-4	38
5		1-Heptene, 2-methyl-	112	C8H16	015870-10-7	38



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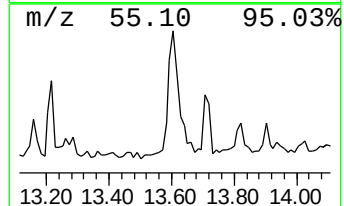
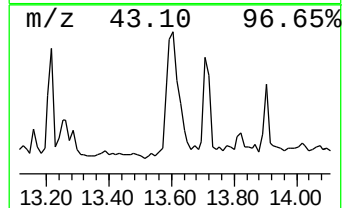
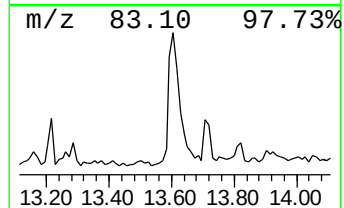
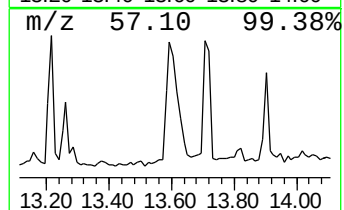
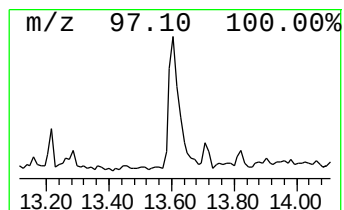
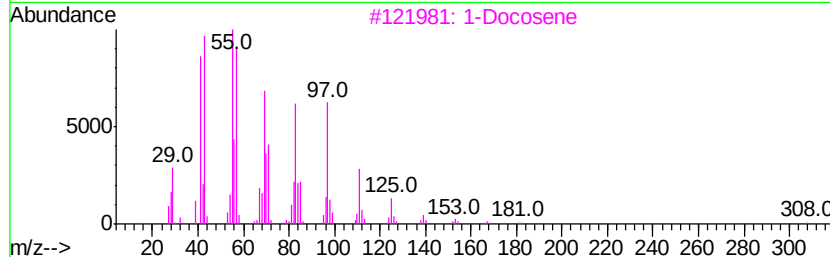
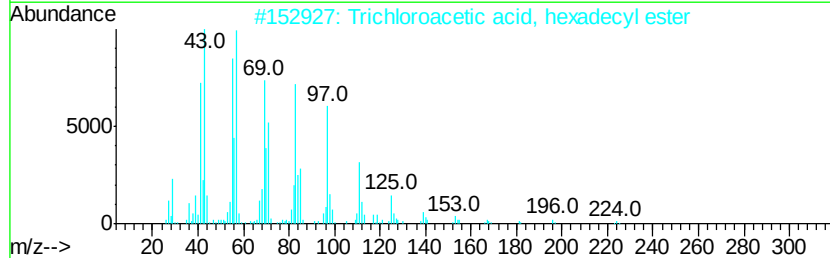
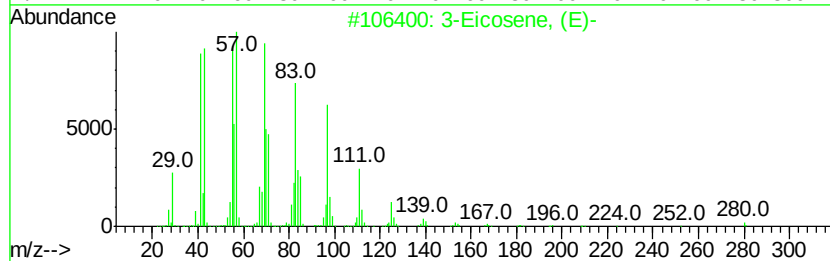
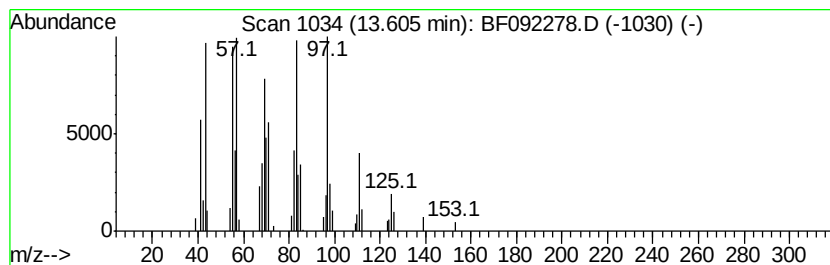
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Peak Number 6 3-Eicosene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.61	3.37 ng	184523	Chrysene-d12	13.71	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	81
3	1-Docosene	308	C22H44	001599-67-3	81
4	1-Heptadecanol	256	C17H36O	001454-85-9	81
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	81



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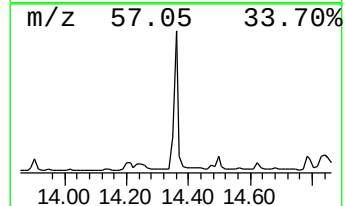
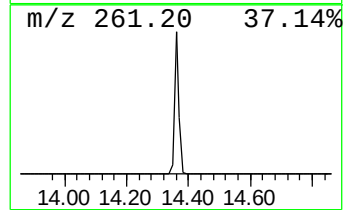
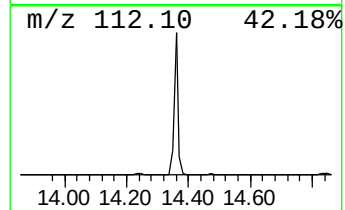
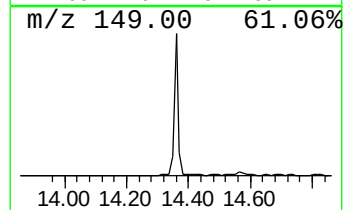
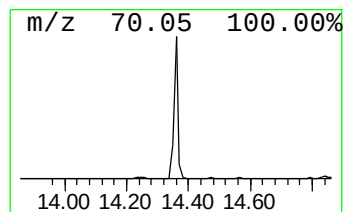
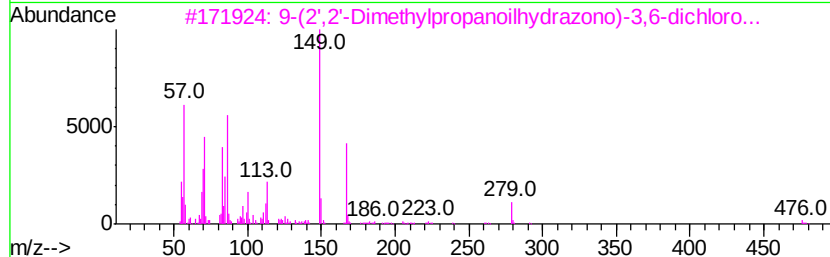
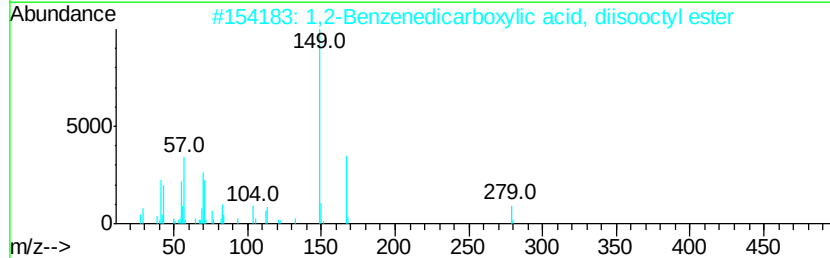
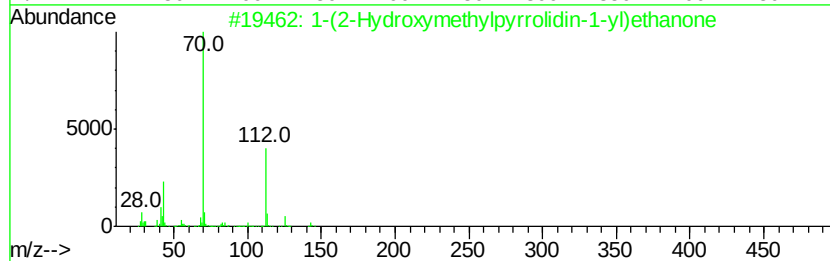
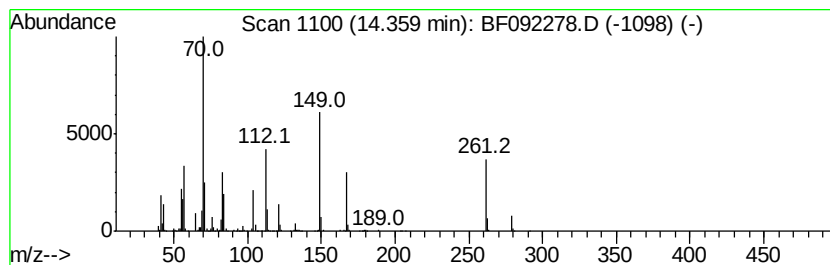
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown14.36 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.36	18.64 ng	1019020	Chrysene-d12	13.71

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-(2-Hydroxymethylpyrrolidin-1-yl)ethanone	143	C7H13NO2	1000192-83-2	23
2		1,2-Benzenedicarboxylic acid, diisooctyl ester	390	C24H38O4	027554-26-3	22
3		9-(2',2'-Dimethylpropanoimidohydrazono)-3,6-dichloro-3,4-dihydro-2H-pyridine	576	C30H42Cl2N4O3	1000111-04-6	22
4		Cyclohexaneamine, N-but-2-enylidene	167	C10H17NO	068048-01-1	16
5		Bromoacetic acid, 2-ethylhexyl ester	250	C10H19BrO2	068144-73-0	16



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011317\
Data File : BF092278.D
Acq On : 14 Jan 2017 11:58
Operator : UM/SJ
Sample : I1162-10
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-48-COMP

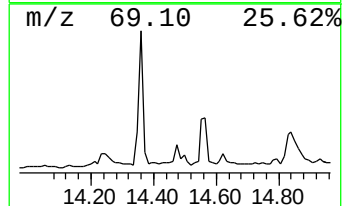
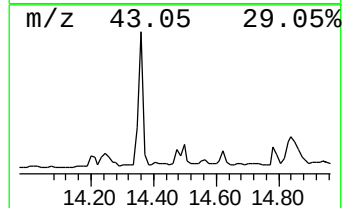
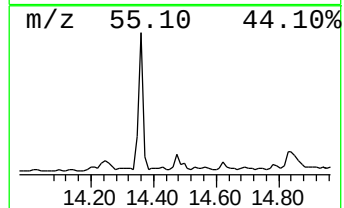
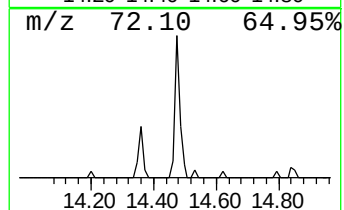
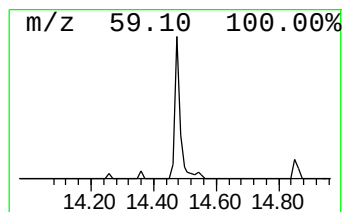
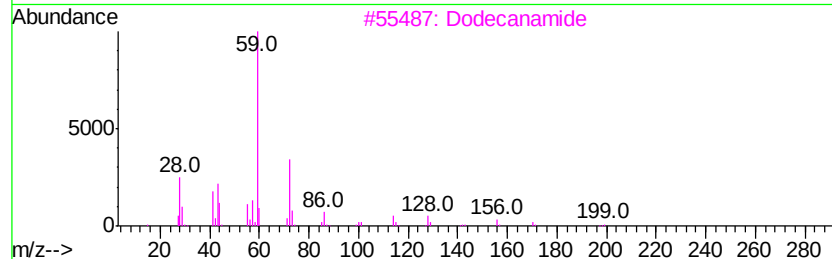
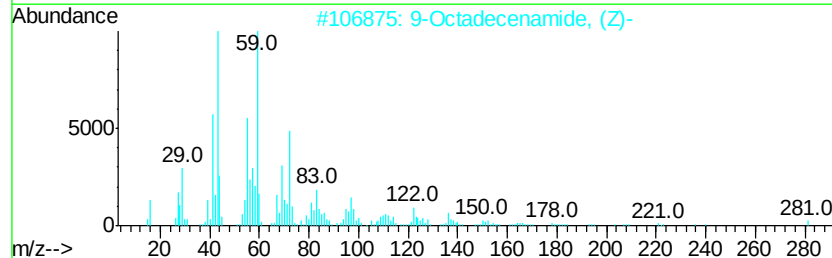
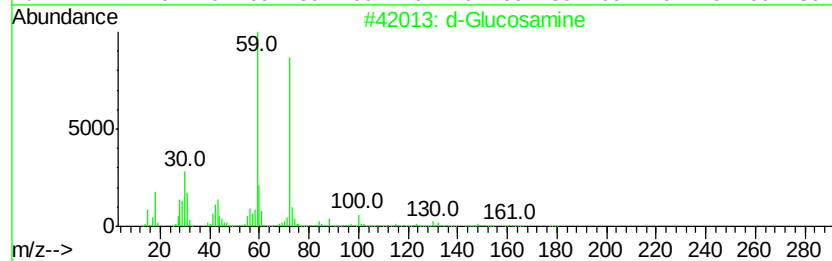
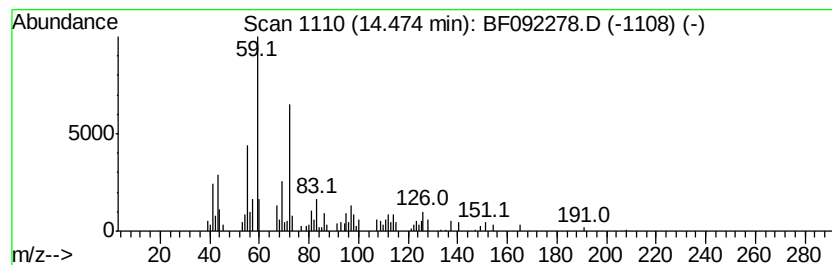
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 d-Glucosamine Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.47	2.25 ng	96990	Perylene-d12	15.07

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		d-Glucosamine	179	C6H13NO5	000090-77-7	53
2		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	50
3		Dodecanamide	199	C12H25NO	001120-16-7	47
4		Tetradecanamide	227	C14H29NO	000638-58-4	45
5		Triisopropylsilane	158	C9H22Si	006485-79-6	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011317\
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Acq On : 14 Jan 2017 11:58
Operator : UM/SJ
Sample : I1162-10
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-48-COMP

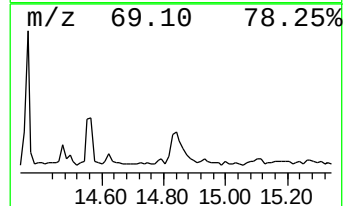
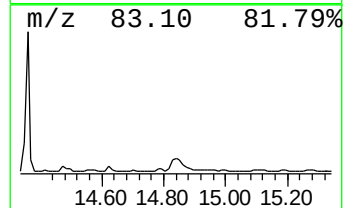
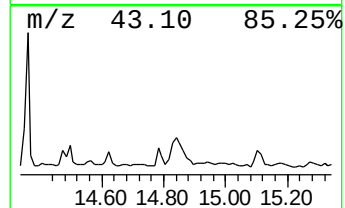
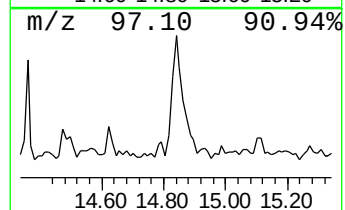
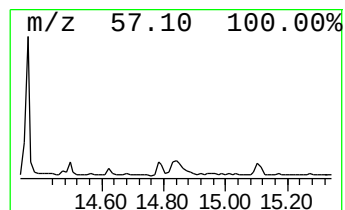
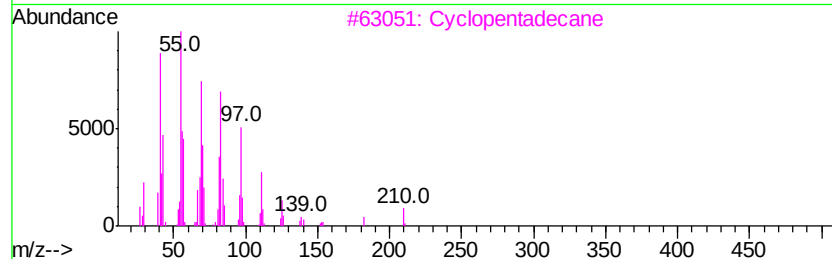
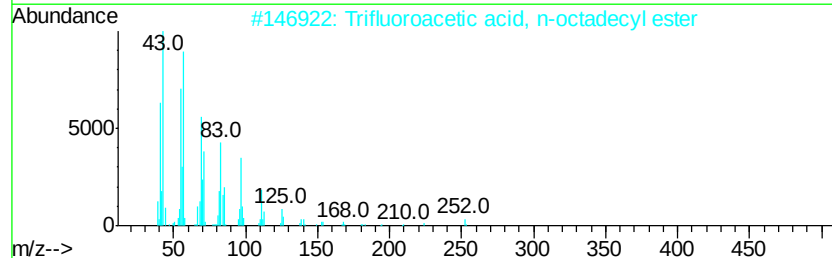
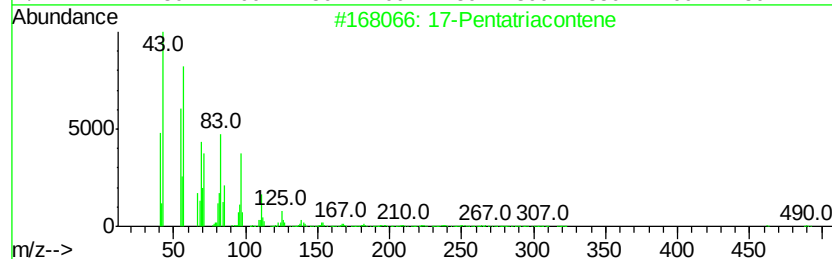
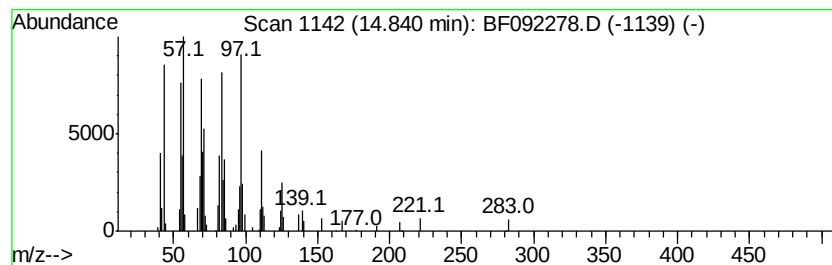
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 17-Pentatriacontene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.84	4.32 ng	186640	Perylene-d12	15.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	17-Pentatriacontene	491	C35H70	006971-40-0	91
2		Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	91
3		Cyclopentadecane	210	C15H30	000295-48-7	91
4		1-Nonadecene	266	C19H38	018435-45-5	90
5		2-Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	87



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Misc :
ALS Vial : 37 Sample Multiplier: 1

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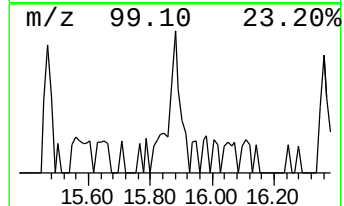
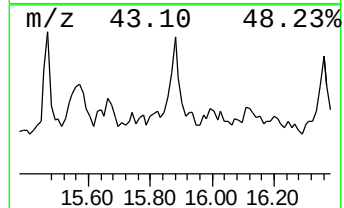
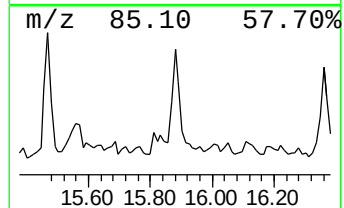
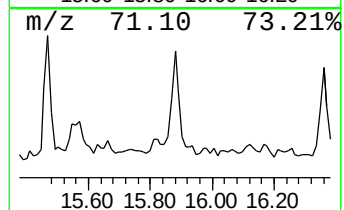
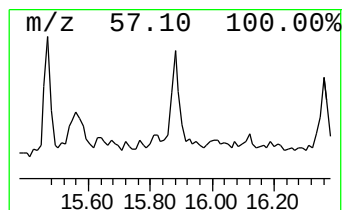
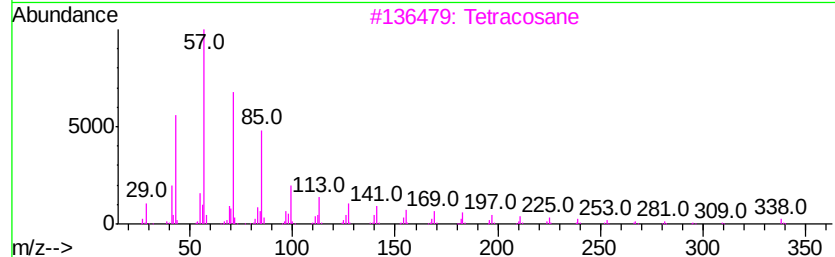
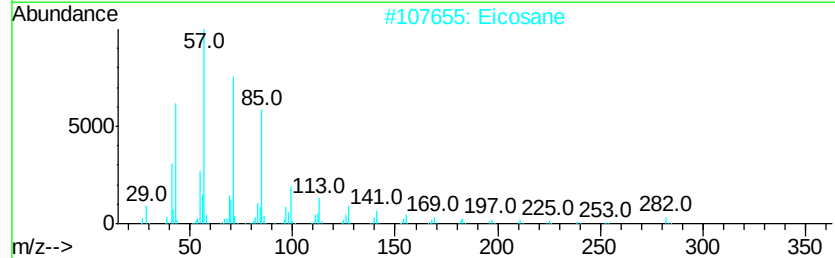
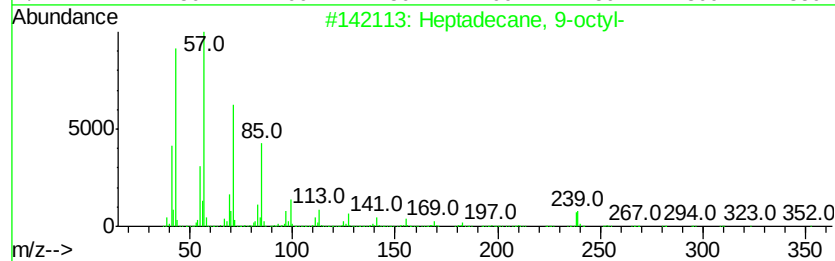
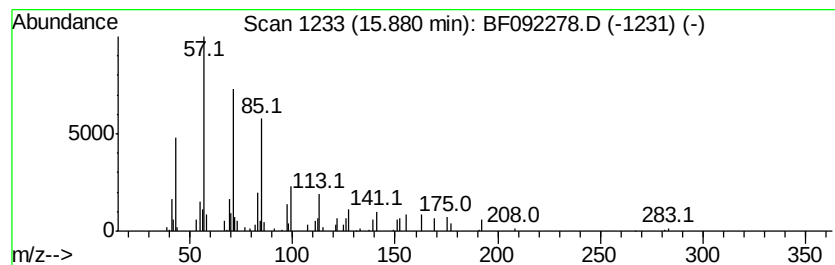
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heptadecane, 9-octyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.88	2.26 ng	97552	Perylene-d12	15.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86
2		Eicosane	282	C20H42	000112-95-8	80
3		Tetracosane	338	C24H50	000646-31-1	80
4		Hexacosane	366	C26H54	000630-01-3	80
5		Pentacosane	352	C25H52	000629-99-2	80



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ALS Vial : 37 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.70	40.0	ng	2622480	1	6.58	1312460	20.0
unknown6.35	6.35	76.1	ng	4991890	1	6.58	1312460	20.0
Hexadecane	10.53	3.3	ng	181007	4	11.09	1109220	20.0
Hexadecanoic acid...	12.51	2.1	ng	115186	5	13.71	1093590	20.0
3-Eicosene, (E)-	13.61	3.4	ng	184523	5	13.71	1093590	20.0
unknown14.36	14.36	18.6	ng	1019020	5	13.71	1093590	20.0
d-Glucosamine	14.47	2.3	ng	96990	6	15.07	863988	20.0
17-Pentatriacontene	14.84	4.3	ng	186640	6	15.07	863988	20.0
Heptadecane, 9-oc...	15.88	2.3	ng	97552	6	15.07	863988	20.0