

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011217\
 Data File : BF092213.D
 Acq On : 12 Jan 2017 17:49
 Operator : UM/SJ
 Sample : I1029-13
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMP-007

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-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	3.990	181	184	189	rBV	62626	111655	2.00%	0.240%
2	4.721	245	248	260	rVB	1551486	2658490	47.56%	5.714%
3	5.190	287	289	302	rBV	3834336	4864064	87.01%	10.455%
4	6.264	380	383	385	rBV	4896864	5590249	100.00%	12.016%
5	6.367	390	392	394	rBV	5100648	4666078	83.47%	10.030%
6	6.596	409	412	414	rBV	1073005	1117566	19.99%	2.402%
7	6.744	423	425	428	rBV	2942481	3667457	65.60%	7.883%
8	7.167	459	462	464	rBV	3186594	3388839	60.62%	7.284%
9	7.876	522	524	527	rBV	1329029	1548672	27.70%	3.329%
10	8.962	616	619	621	rBV	5129956	5113389	91.47%	10.991%
11	9.362	652	654	656	rBV	420761	358980	6.42%	0.772%
12	9.625	675	677	680	rVB	1721166	1833531	32.80%	3.941%
13	10.082	712	717	718	rBV	72852	83871	1.50%	0.180%
14	10.425	744	747	749	rBV2	1889039	2764842	49.46%	5.943%
15	10.551	756	758	762	rBV	125475	158077	2.83%	0.340%
16	10.996	795	797	798	rBV2	92945	83901	1.50%	0.180%
17	11.111	804	807	809	rBV	1045884	1385709	24.79%	2.979%
18	11.659	853	855	865	rBV2	373930	389007	6.96%	0.836%
19	12.436	921	923	930	rBV2	107486	156001	2.79%	0.335%
20	12.699	943	946	948	rBV	2855312	3836965	68.64%	8.248%
21	13.602	1022	1025	1034	rBV	203306	303990	5.44%	0.653%
22	13.728	1034	1036	1039	rBV	838873	1030222	18.43%	2.214%
23	14.231	1075	1080	1089	rBV	55036	144928	2.59%	0.312%
24	15.088	1153	1155	1158	rBV	668072	825617	14.77%	1.775%
25	16.448	1271	1274	1280	rVV4	74748	142989	2.56%	0.307%
26	16.551	1280	1283	1284	rVV	34166	66505	1.19%	0.143%
27	16.585	1284	1286	1292	rVB	74299	160683	2.87%	0.345%
28	16.814	1303	1306	1312	rVB7	27571	69811	1.25%	0.150%

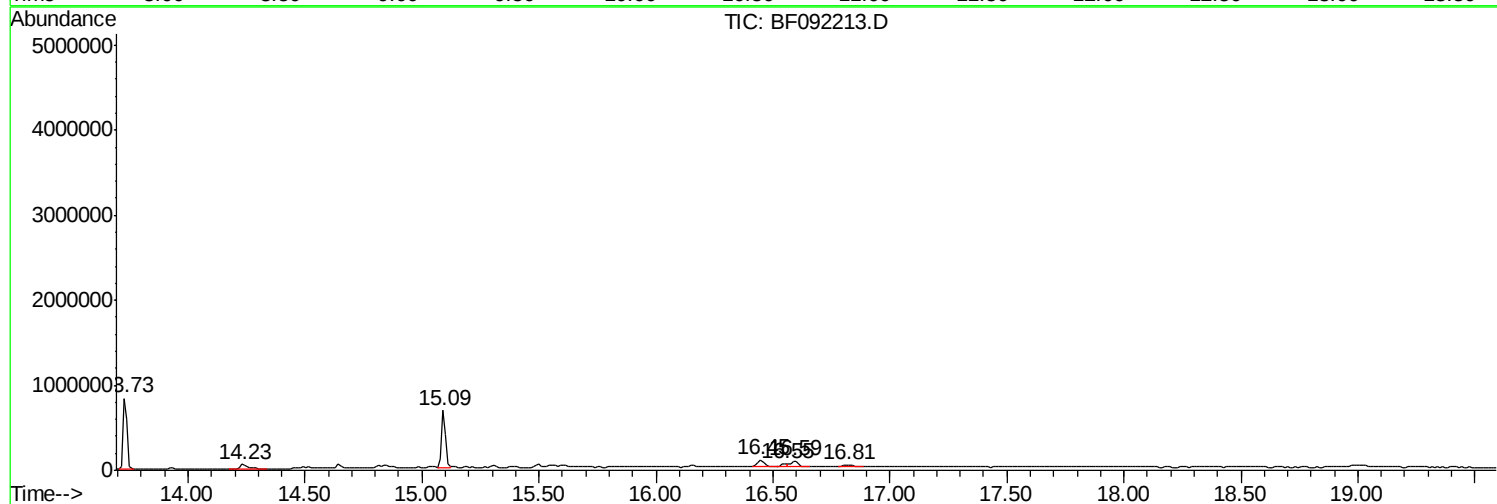
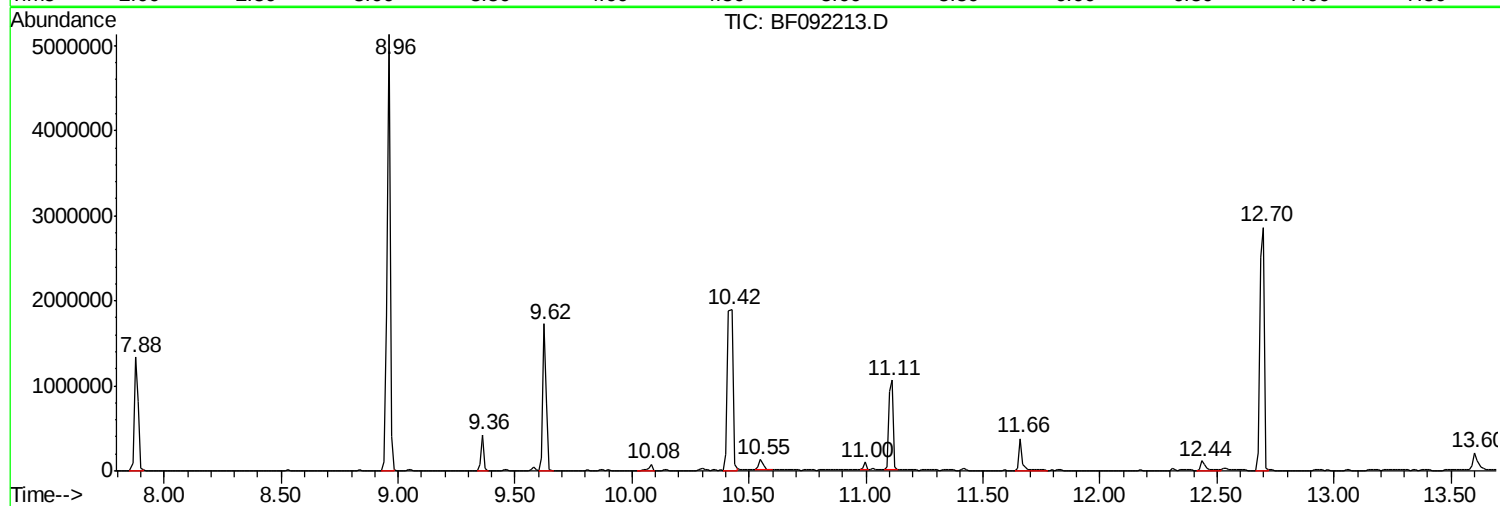
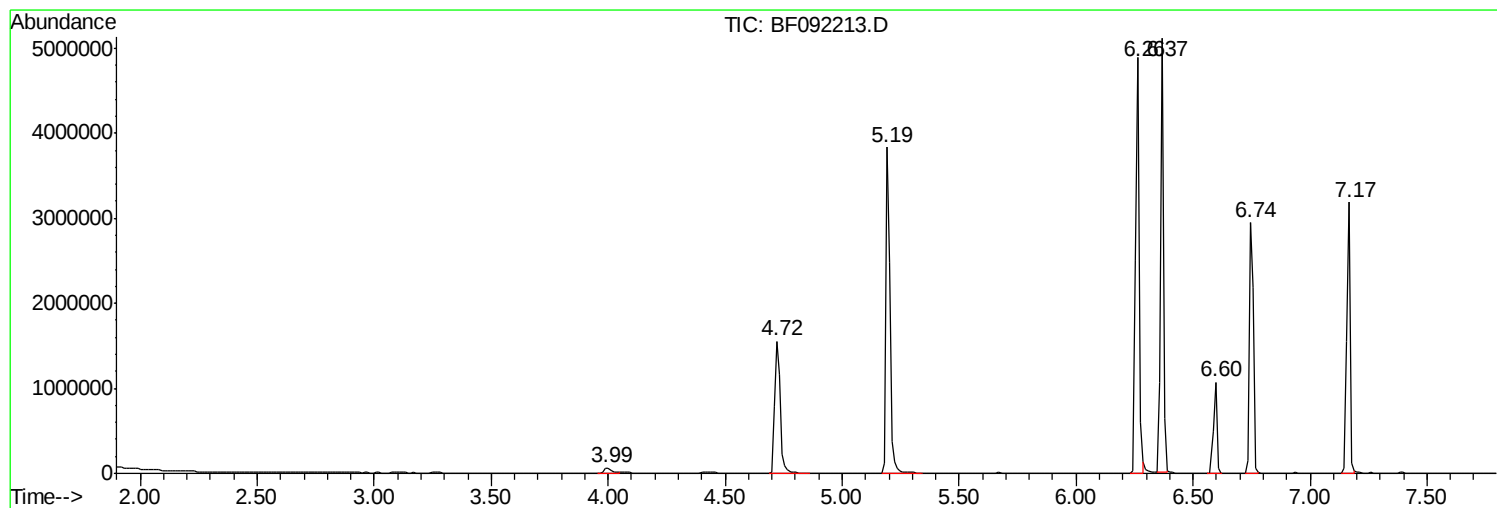
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BNA_F
ClientSampled :
COMP-007

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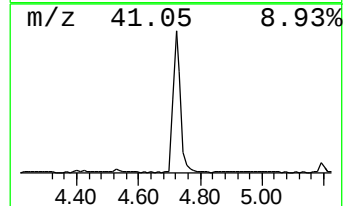
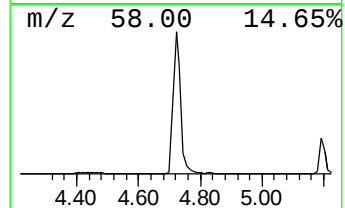
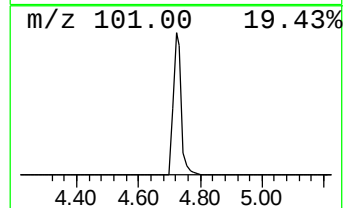
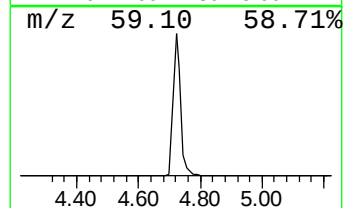
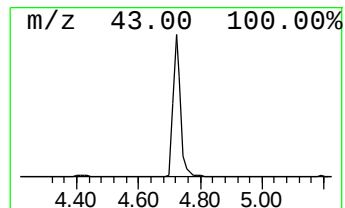
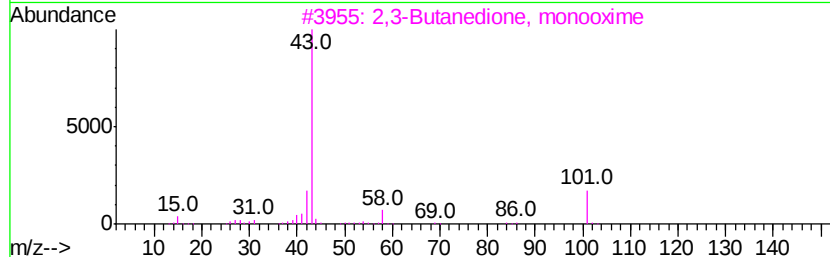
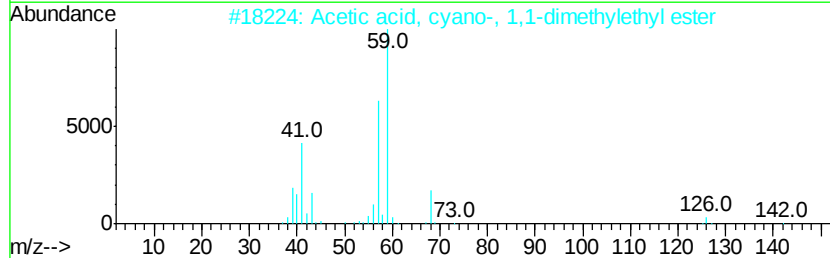
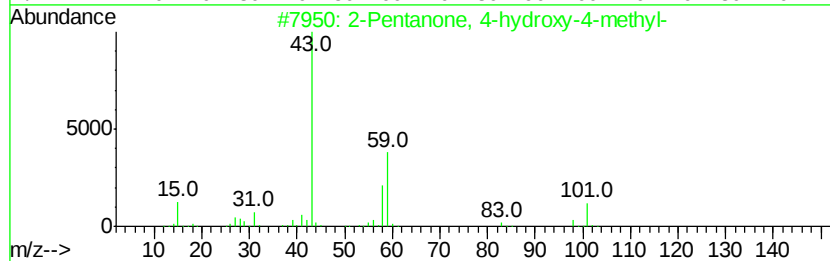
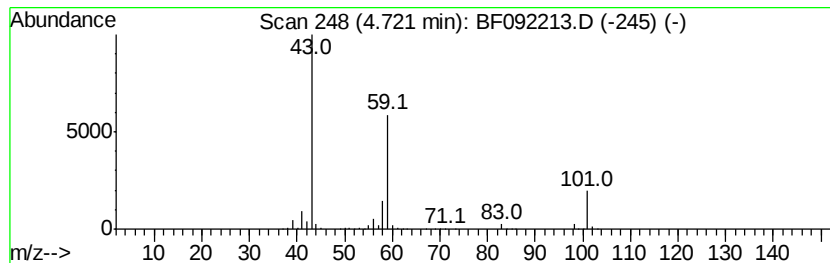
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.72	47.58 ng	2658490	1,4-Dichlorobenzene-d4	6.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		t-Butyl ethyl ether	102	C6H14O	1000118-18-4	9



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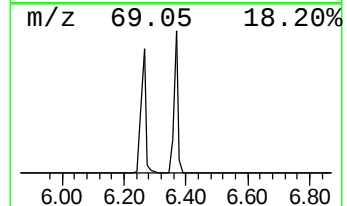
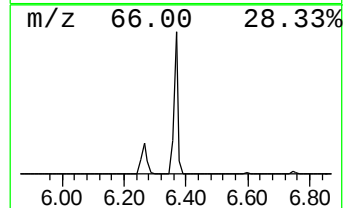
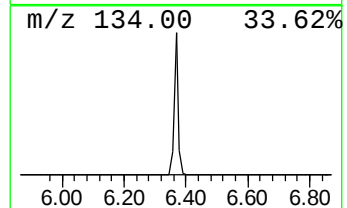
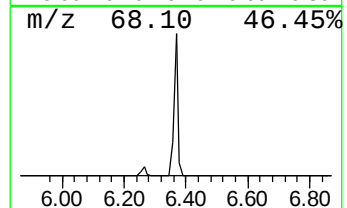
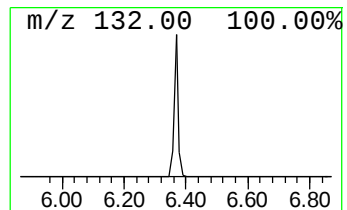
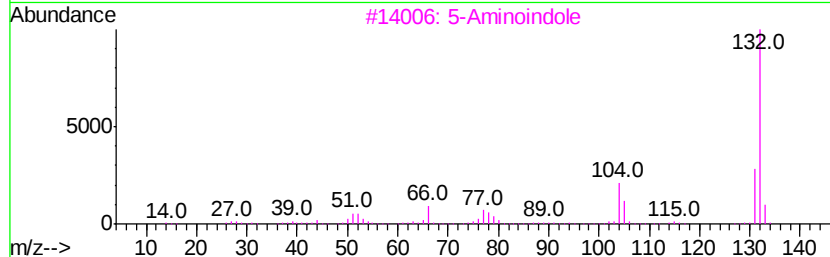
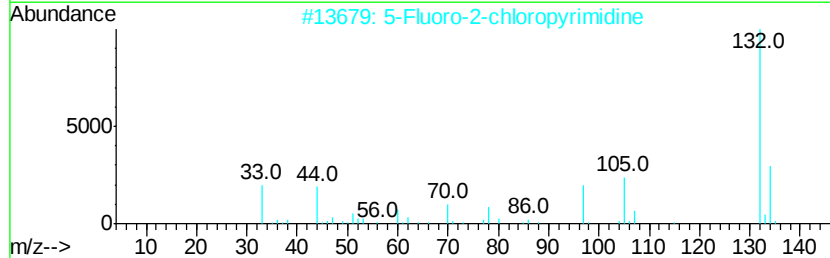
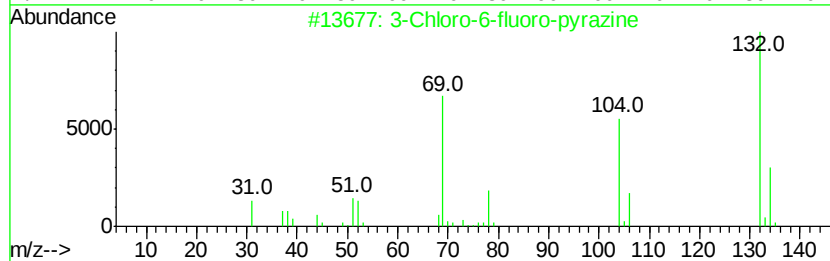
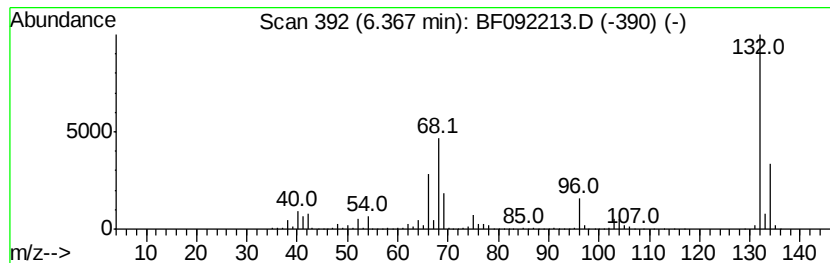
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Peak Number 2 unknown6.37 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.37	83.50 ng	4666080	1,4-Dichlorobenzene-d4	6.60

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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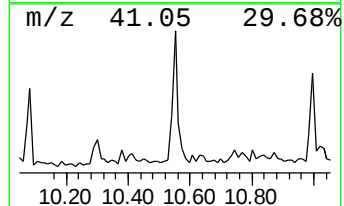
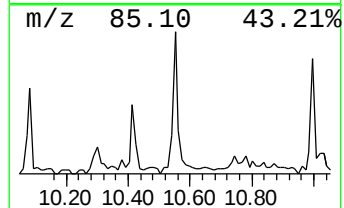
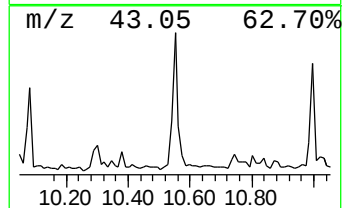
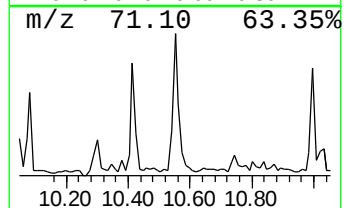
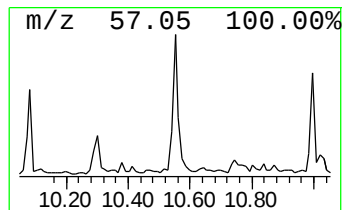
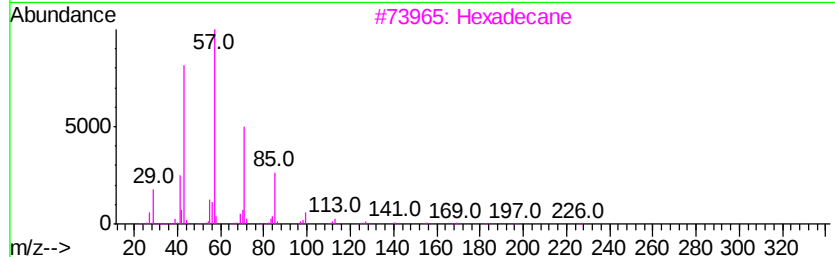
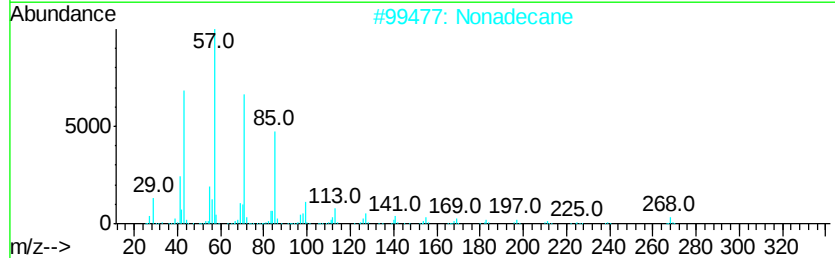
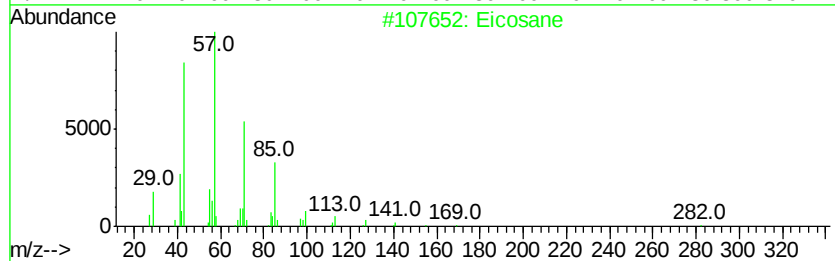
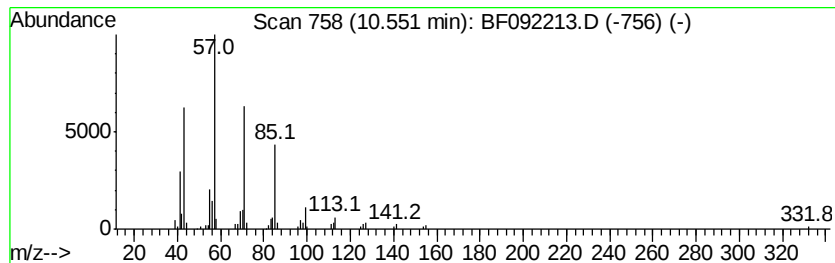
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Peak Number 4 Eicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.55	2.28 ng	158077	Phenanthrene-d10	11.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	91
2		Nonadecane	268	C19H40	000629-92-5	90
3		Hexadecane	226	C16H34	000544-76-3	90
4		Heneicosane	296	C21H44	000629-94-7	90
5		Dodecane, 2-methyl-	184	C13H28	001560-97-0	86



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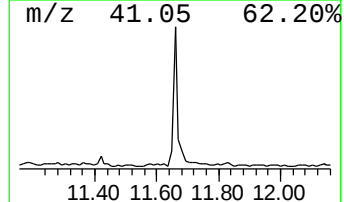
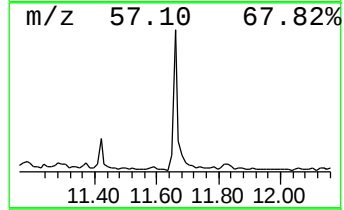
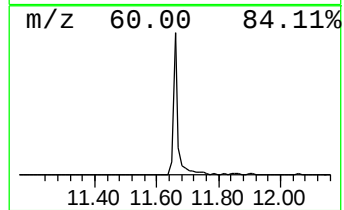
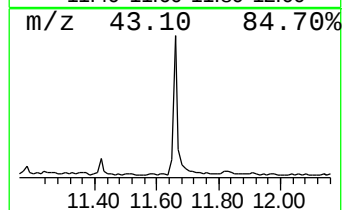
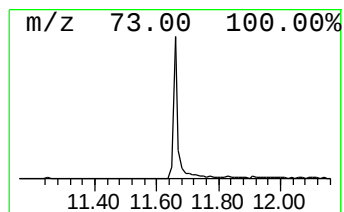
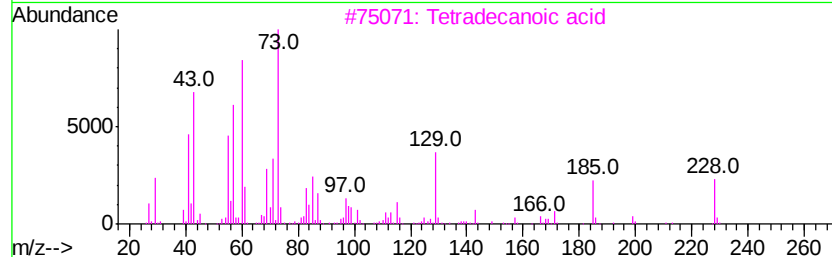
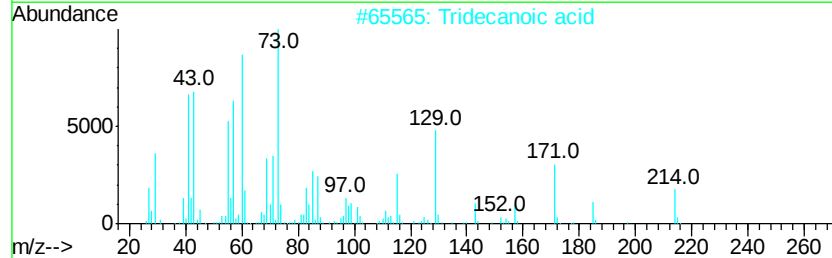
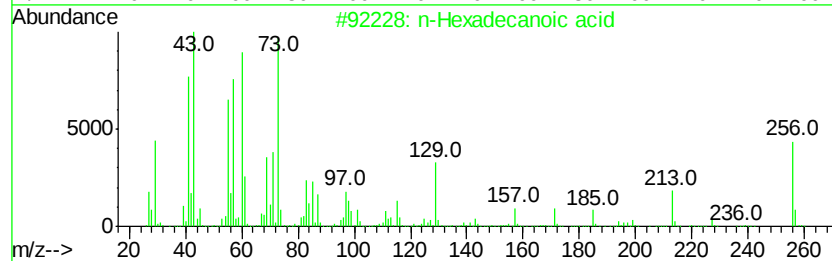
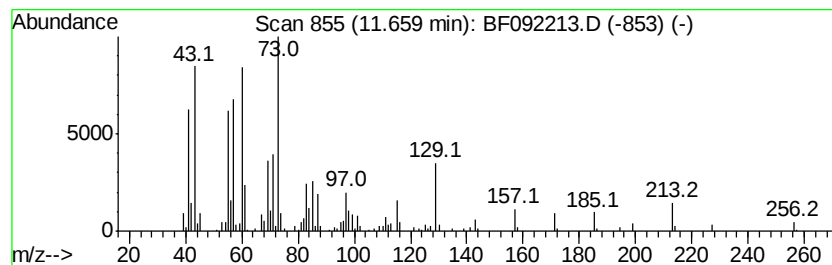
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.66	5.61 ng	389007	Phenanthrene-d10	11.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	91
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	52
5		N-Acetylisoaxazolidine	115	C5H9NO2	115615-36-6	18



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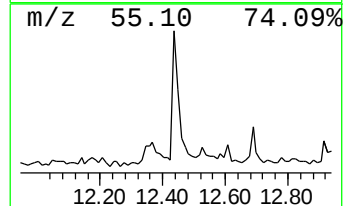
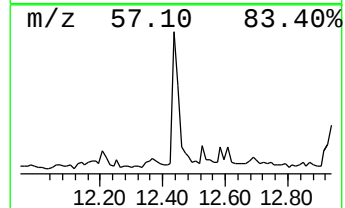
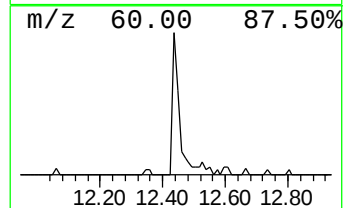
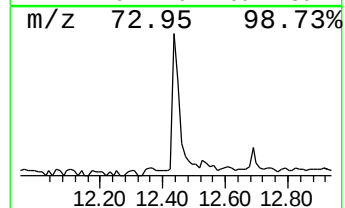
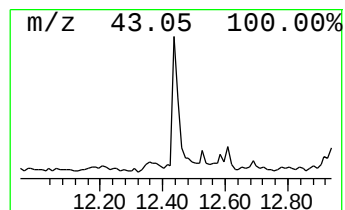
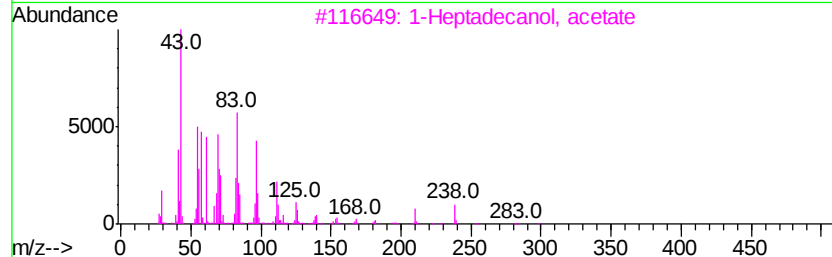
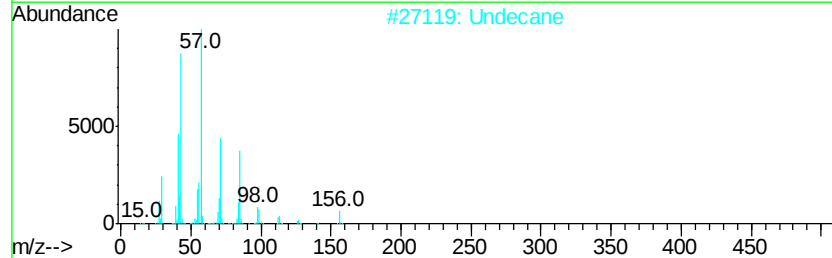
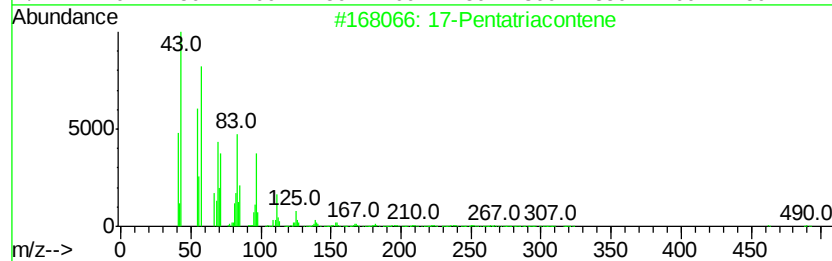
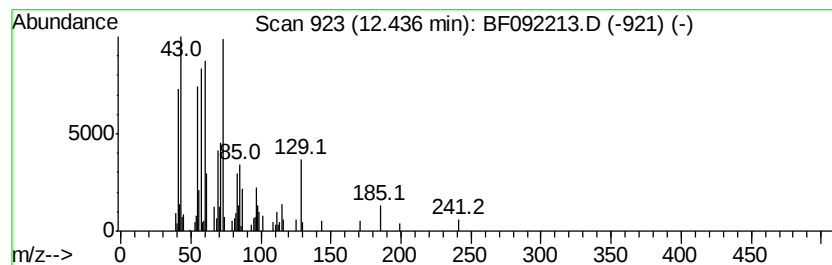
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Peak Number 6 unknown12.44 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.44	3.03 ng	156001	Chrysene-d12	13.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	17-Pentatriacontene	491	C35H70	006971-40-0	11
2		Undecane	156	C11H24	001120-21-4	11
3		1-Heptadecanol, acetate	298	C19H38O2	000822-20-8	10
4		1-Iodoundecane	282	C11H23I	004282-44-4	10
5		Methoxyacetic acid, 2-tetradecyl...	286	C17H34O3	1000282-04-8	10



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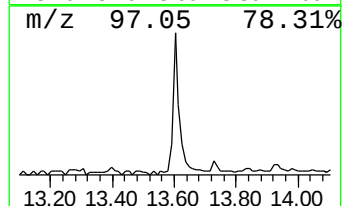
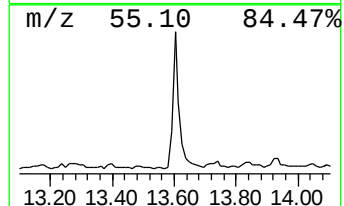
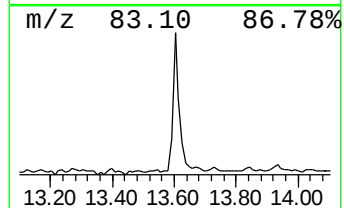
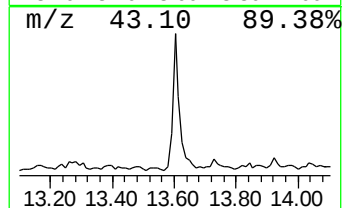
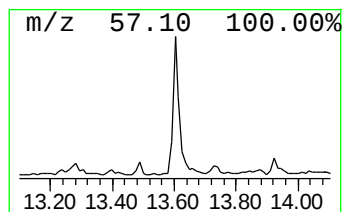
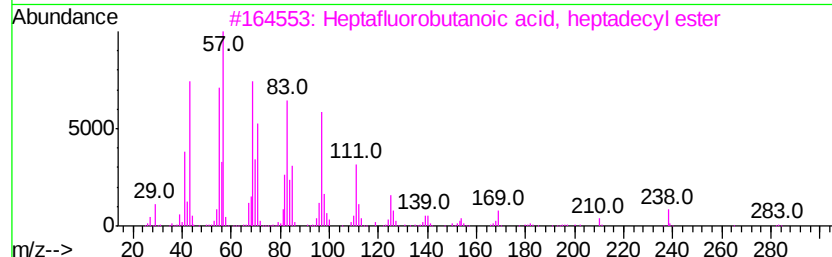
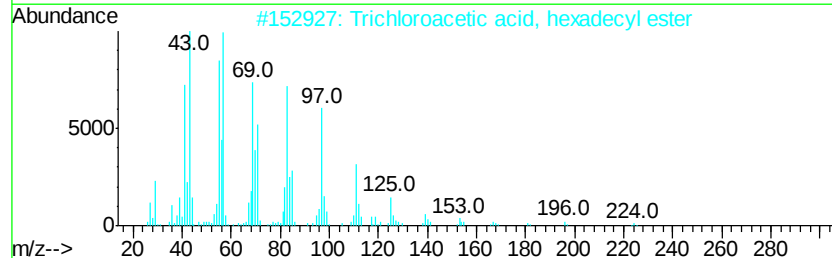
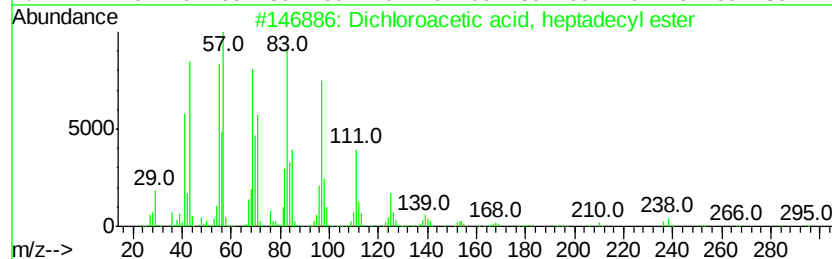
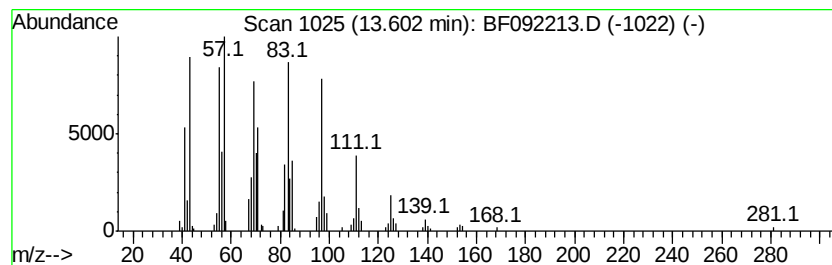
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Dichloroacetic acid, heptad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.60	5.90 ng	303990	Chrysene-d12	13.73

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
2			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3			Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	94
4			3-Eicosene, (E)-	280	C20H40	074685-33-9	91
5			Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011217\
Data File : BF092213.D
Acq On : 12 Jan 2017 17:49
Operator : UM/SJ
Sample : I1029-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-007

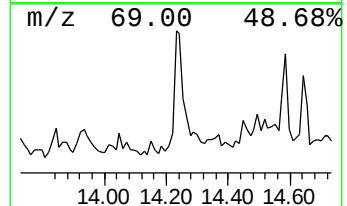
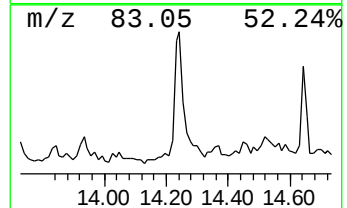
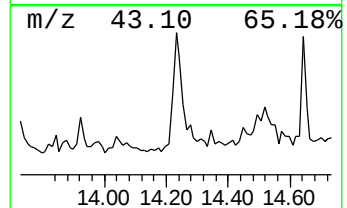
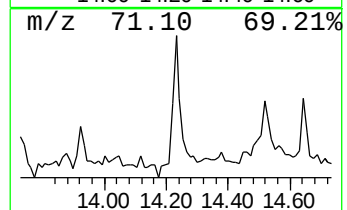
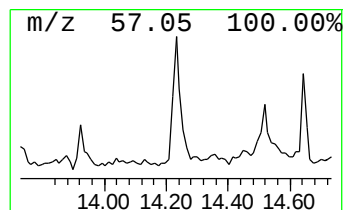
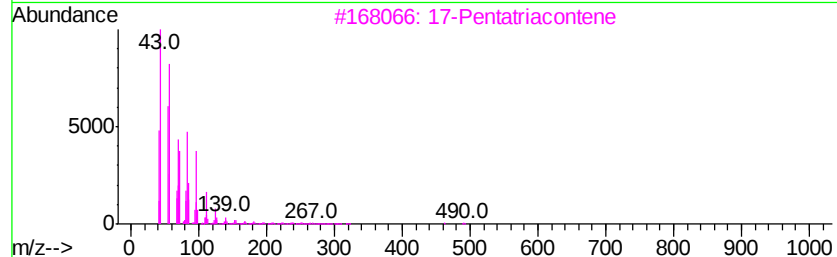
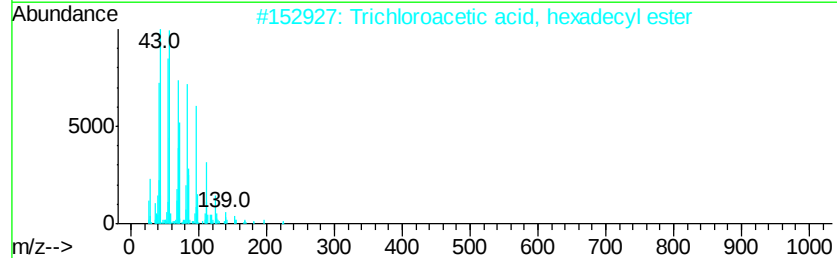
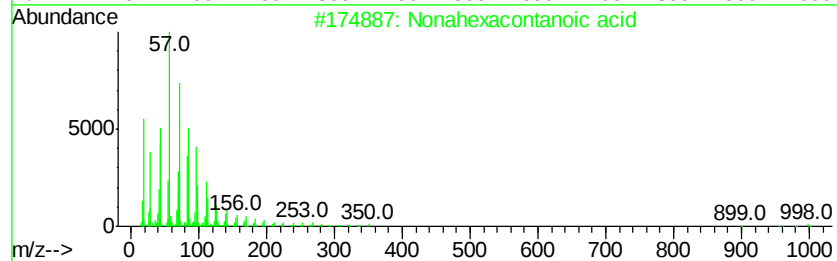
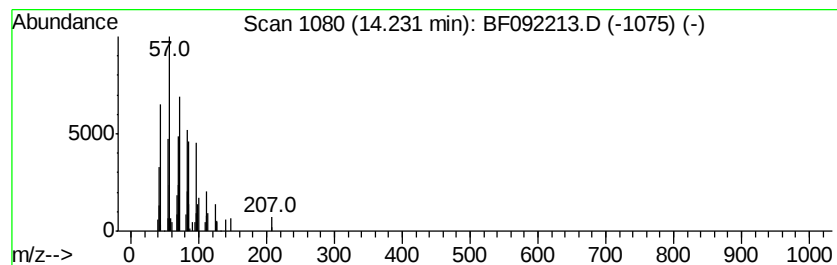
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Nonaheptacontanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.23	2.81 ng	144928	Chrysene-d12	13.73

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Nonaheptacontanoic acid	999	C69H138O2	040710-32-5	72
2		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	64
3		17-Pentatriacontene	491	C35H70	006971-40-0	64
4		Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	64
5		Ethanol, 2-(dodecyloxy)-	230	C14H30O2	004536-30-5	53



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011217\
Data File : BF092213.D
Acq On : 12 Jan 2017 17:49
Operator : UM/SJ
Sample : I1029-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-007

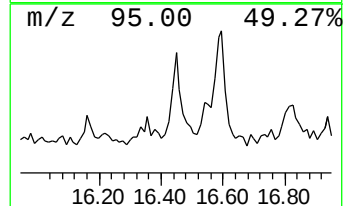
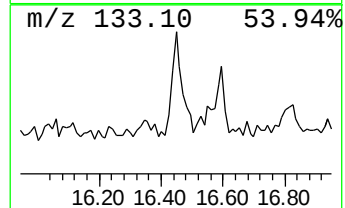
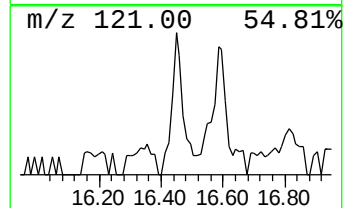
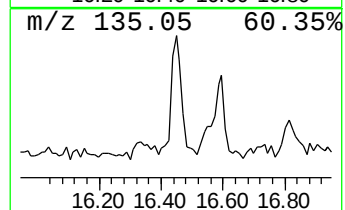
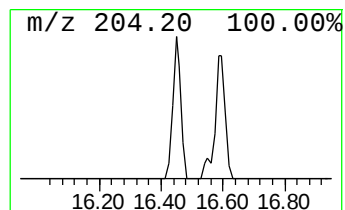
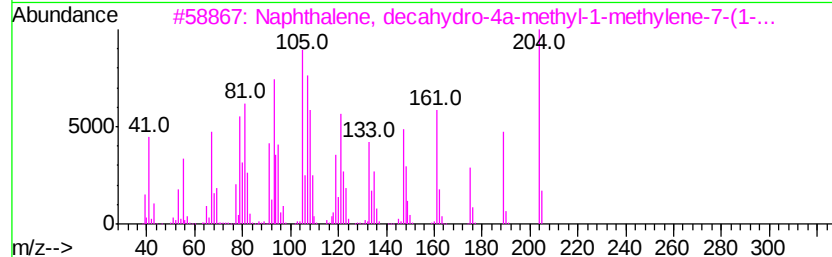
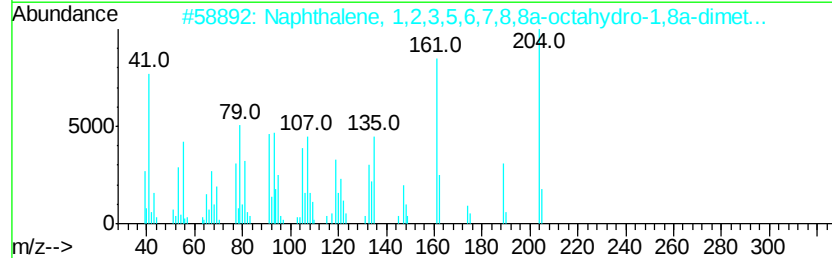
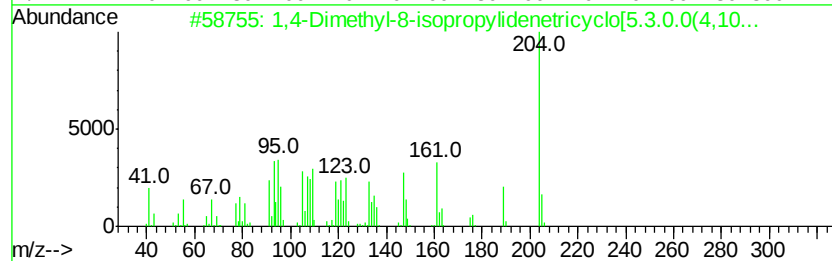
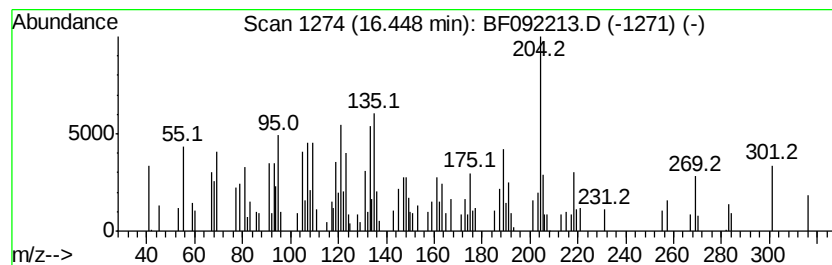
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1,4-Dimethyl-8-isopropylide... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.45	3.46 ng	142989	Perylene-d12	15.09

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Dimethyl-8-isopropylidenetri...	204	C15H24	1000140-07-7	64
2			Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	004630-07-3	52
3			Naphthalene, decahydro-4a-methyl...	204	C15H24	017066-67-0	43
4			1H-Cyclopropylazulene, 1a,2,3,4...	204	C15H24	000489-40-7	38
5			3-Isopropenyl-trans-8a-methyl-6-...	222	C14H22O2	013567-75-4	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011217\
Data File : BF092213.D
Acq On : 12 Jan 2017 17:49
Operator : UM/SJ
Sample : I1029-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-007

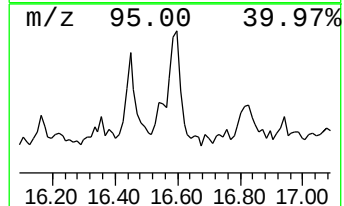
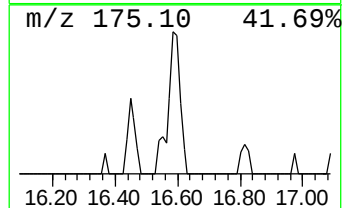
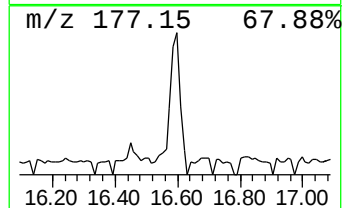
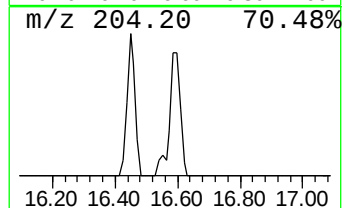
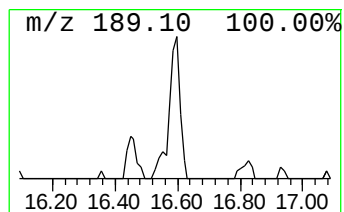
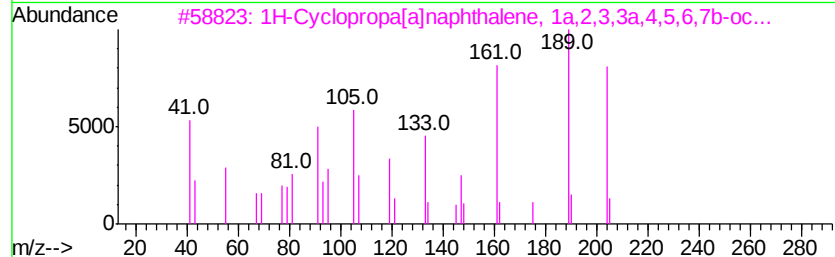
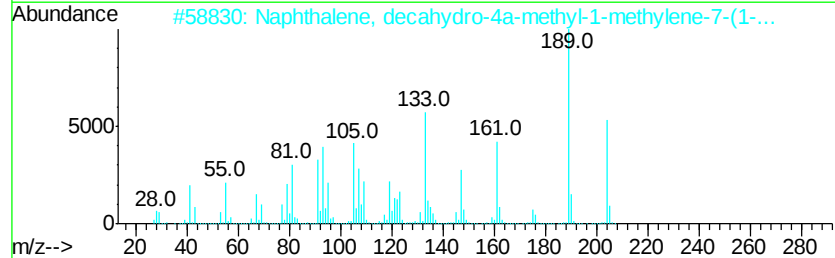
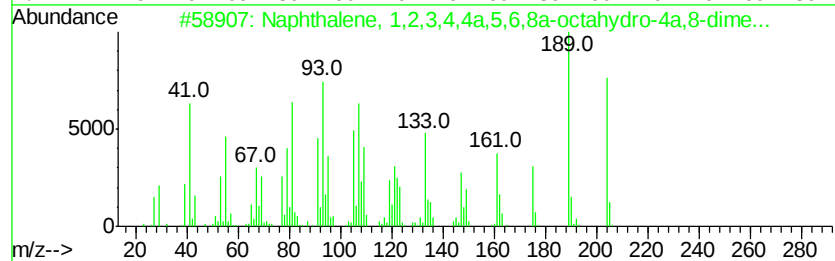
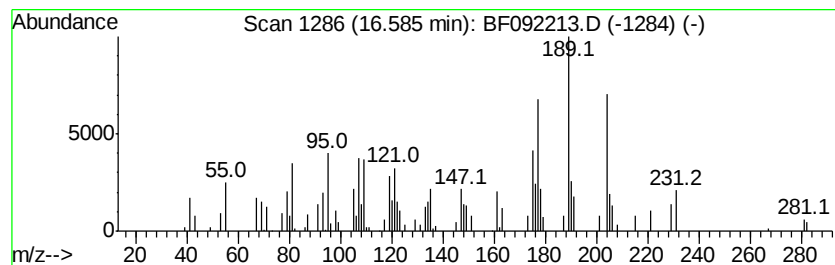
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Naphthalene, 1,2,3,4,4a,5,6... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.59	3.89 ng	160683	Perylene-d12	15.09

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4,4a,5,6,8a-o...	204	C15H24	000473-13-2	50
2			Naphthalene, decahydro-4a-methyl...	204	C15H24	000515-17-3	46
3			1H-Cyclopropafalnaphthalene, 1a,...	204	C15H24	1000147-32-8	43
4			1H-Cyclopropafalnaphthalene, 1a,...	204	C15H24	000489-29-2	38
5			2-Isopropenyl-4a,8-dimethyl-1,2,...	204	C15H24	1000193-57-0	30



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011217\
Data File : BF092213.D
Acq On : 12 Jan 2017 17:49
Operator : UM/SJ
Sample : I1029-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-007

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...	4.72	47.6	ng	2658490	1	6.60	1117570	20.0
unknown6.37	6.37	83.5	ng	4666080	1	6.60	1117570	20.0
Eicosane	10.55	2.3	ng	158077	4	11.11	1385710	20.0
n-Hexadecanoic acid	11.66	5.6	ng	389007	4	11.11	1385710	20.0
unknown12.44	12.44	3.0	ng	156001	5	13.73	1030220	20.0
Dichloroacetic ac...	13.60	5.9	ng	303990	5	13.73	1030220	20.0
Nonahexacontanoic...	14.23	2.8	ng	144928	5	13.73	1030220	20.0
1,4-Dimethyl-8-is...	16.45	3.5	ng	142989	6	15.09	825617	20.0
Naphthalene, 1,2,...	16.59	3.9	ng	160683	6	15.09	825617	20.0