

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011217\
 Data File : BF092218.D
 Acq On : 12 Jan 2017 20:11
 Operator : UM/SJ
 Sample : I1030-03
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMP-0012

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	3.990	181	184	188	rBV	78740	125464	2.40%	0.272%
2	4.721	245	248	263	rVB	1532484	2791702	53.47%	6.060%
3	5.190	287	289	292	rBV	4001075	5221550	100.00%	11.334%
4	6.264	380	383	390	rBV	3835432	4505205	86.28%	9.779%
5	6.367	390	392	395	rVB	4185977	3856261	73.85%	8.371%
6	6.596	410	412	414	rBV	1056510	1044189	20.00%	2.267%
7	6.744	423	425	428	rBV	2811623	3539031	67.78%	7.682%
8	7.167	459	462	464	rBV	2863065	2964144	56.77%	6.434%
9	7.876	522	524	527	rBV	1145567	1270107	24.32%	2.757%
10	8.962	616	619	621	rBV	4805942	4660089	89.25%	10.115%
11	9.362	651	654	656	rBV	371334	321683	6.16%	0.698%
12	9.625	675	677	680	rBV	1416406	1436476	27.51%	3.118%
13	10.082	715	717	718	rVB	83327	90139	1.73%	0.196%
14	10.425	744	747	749	rBV2	2066308	3004328	57.54%	6.521%
15	10.551	756	758	762	rBV	151568	184388	3.53%	0.400%
16	10.996	795	797	798	rBV2	125951	114838	2.20%	0.249%
17	11.111	804	807	809	rBV	1194374	1616792	30.96%	3.510%
18	11.659	853	855	859	rBV2	551005	532190	10.19%	1.155%
19	12.436	921	923	928	rBV	94588	116743	2.24%	0.253%
20	12.539	929	932	934	rVB2	45956	68084	1.30%	0.148%
21	12.688	943	945	948	rBV	3402972	4527837	86.71%	9.828%
22	13.602	1022	1025	1034	rBV	204599	307962	5.90%	0.668%
23	13.728	1034	1036	1039	rBV	887540	1018776	19.51%	2.211%
24	14.242	1076	1081	1087	rBV2	51313	141109	2.70%	0.306%
25	15.088	1152	1155	1158	rBV	999623	1187742	22.75%	2.578%
26	15.500	1188	1191	1193	rBV	119929	159638	3.06%	0.347%
27	15.557	1193	1196	1198	rBV2	29199	65095	1.25%	0.141%
28	15.922	1224	1228	1232	rBV2	33862	83365	1.60%	0.181%
29	16.403	1267	1270	1272	rBV	130371	255067	4.88%	0.554%
30	16.448	1272	1274	1280	rVV2	110649	226568	4.34%	0.492%
31	16.551	1280	1283	1284	rVV2	71188	140411	2.69%	0.305%
32	16.585	1284	1286	1291	rVB2	108206	225401	4.32%	0.489%
33	16.814	1302	1306	1311	rVB6	51872	128202	2.46%	0.278%
34	17.660	1375	1380	1385	rVB3	43684	138435	2.65%	0.300%

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ALS Vial : 15 Sample Multiplier: 1

Instrument :
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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

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

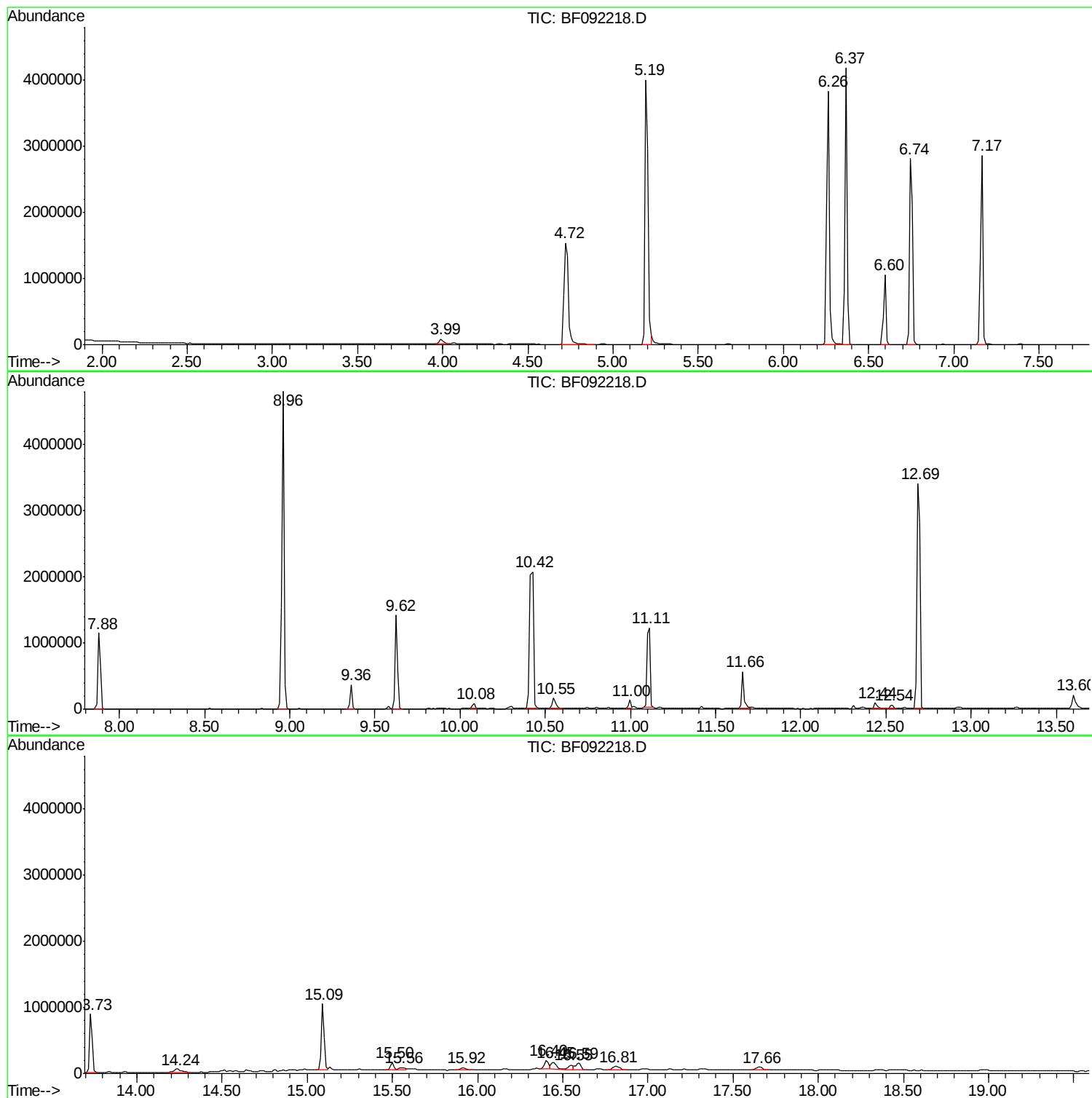
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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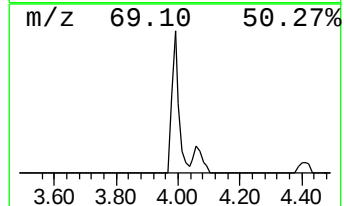
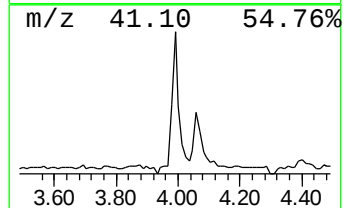
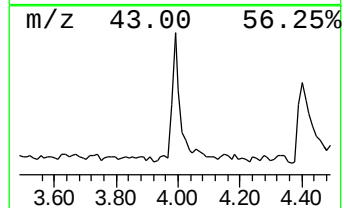
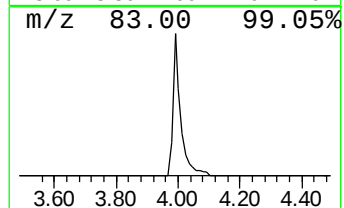
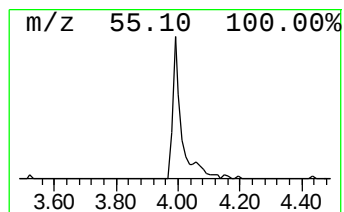
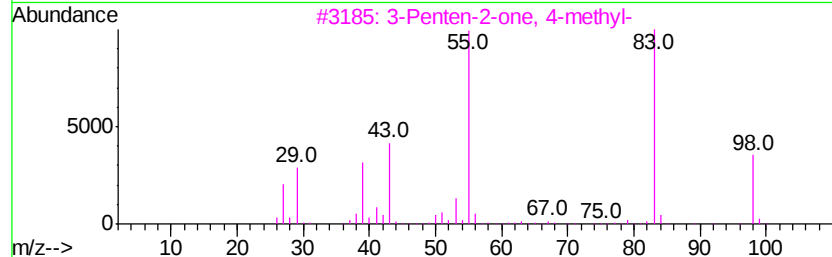
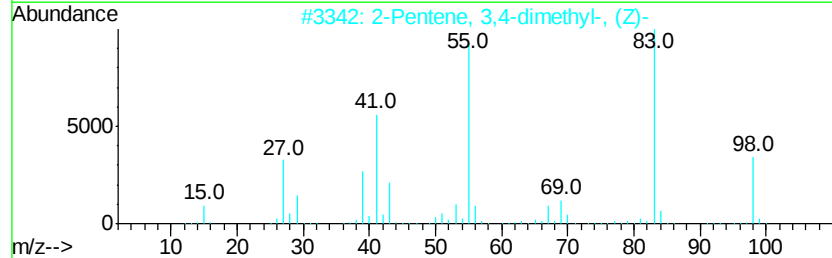
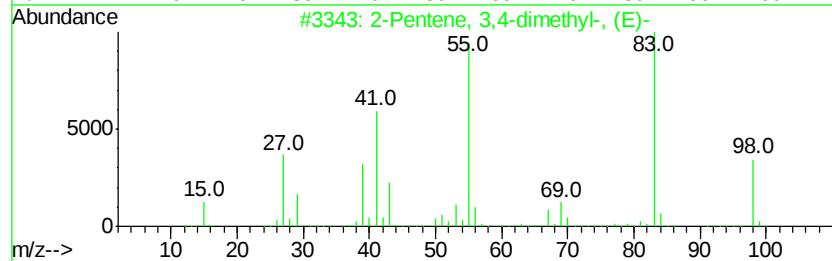
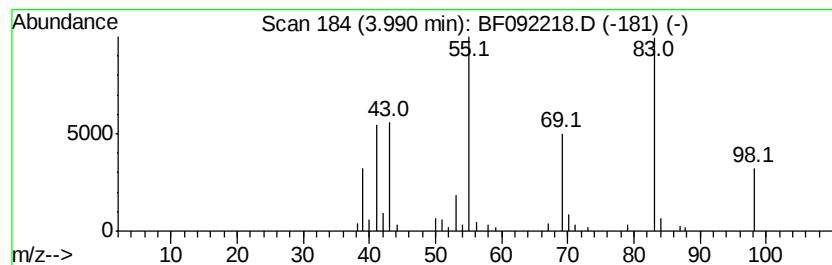
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentene, 3,4-dimethyl-, (E)- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.99	2.40 ng	125464	1,4-Dichlorobenzene-d4	6.60

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
2			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	83
3			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	80
4			3-Hexen-2-one	98	C6H10O	000763-93-9	80
5			2-Pentene, 3,4-dimethyl-	98	C7H14	024910-63-2	80



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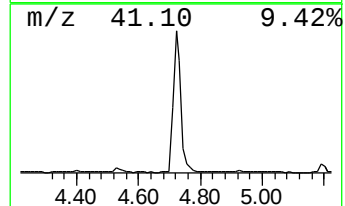
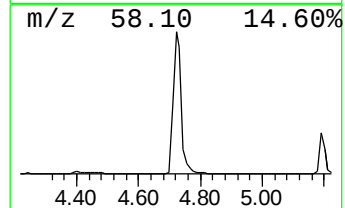
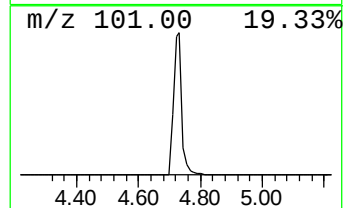
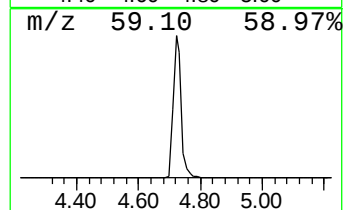
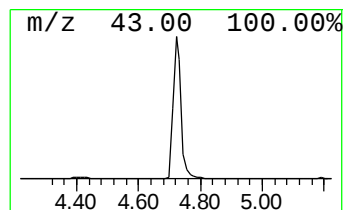
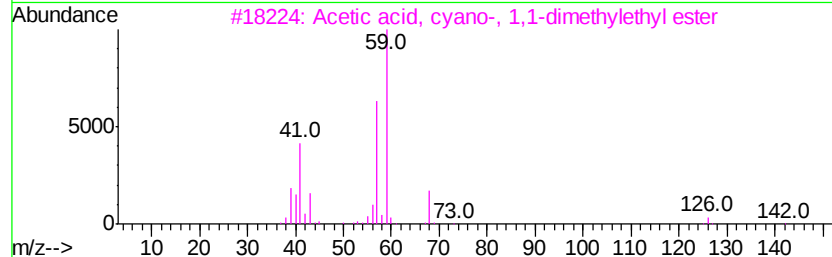
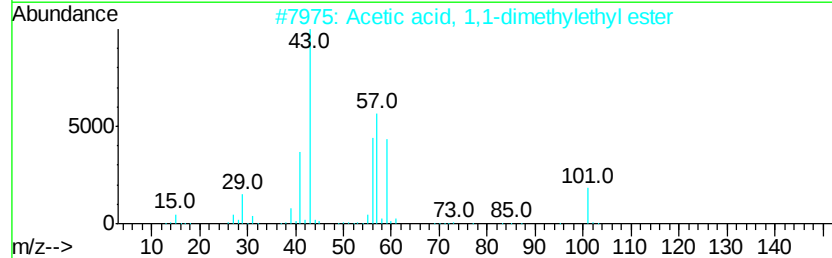
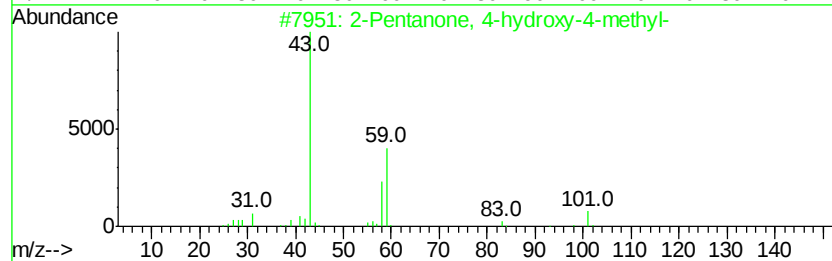
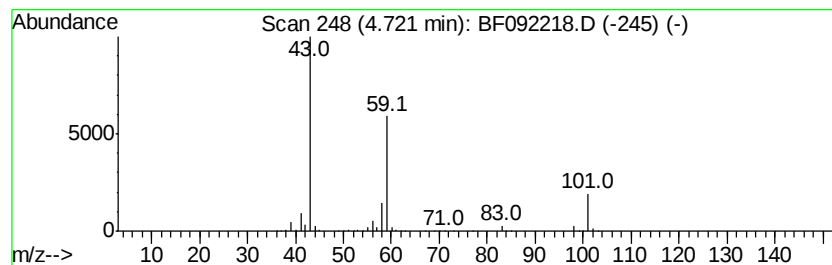
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.72	53.47 ng	2791700	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	56
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		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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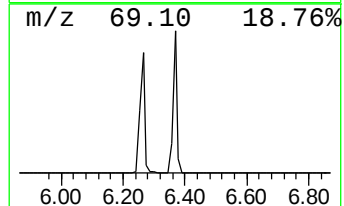
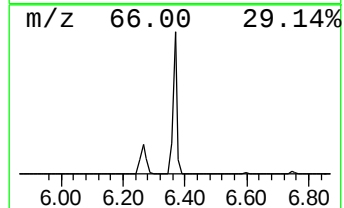
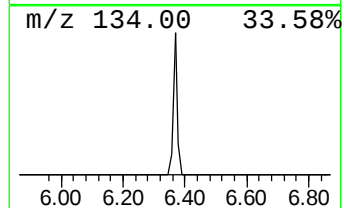
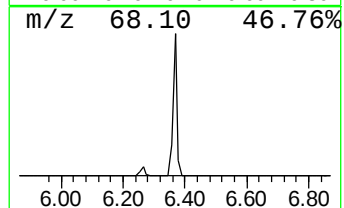
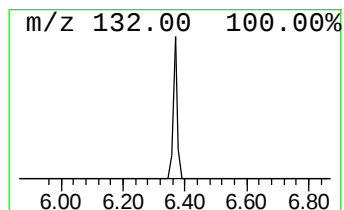
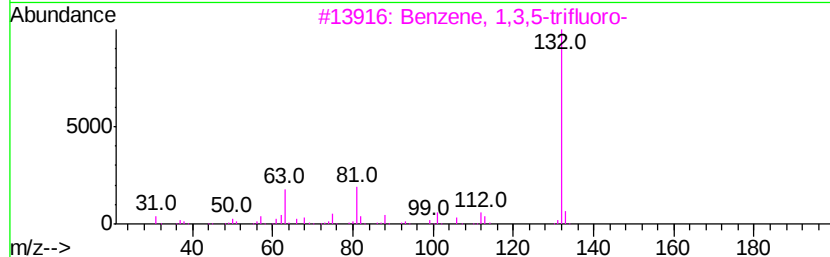
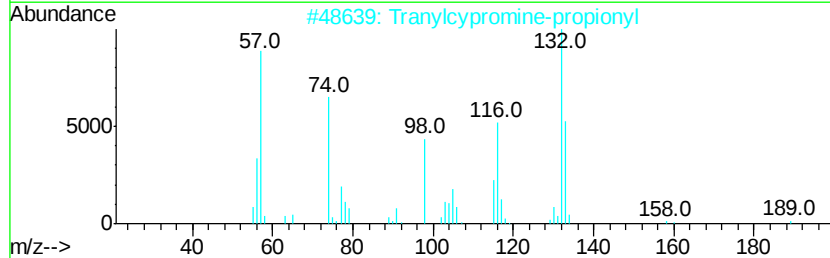
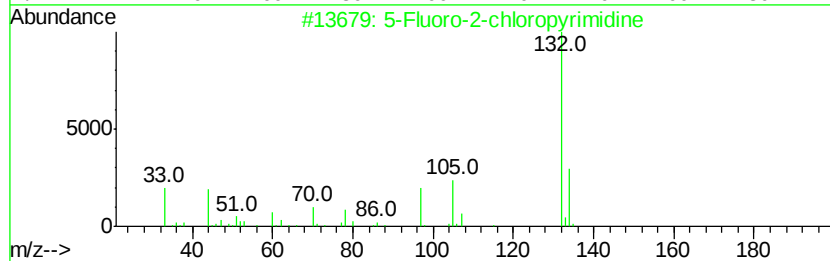
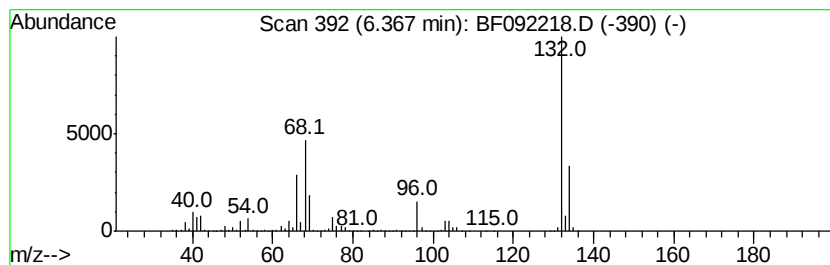
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.37 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.37	73.86 ng	3856260	1,4-Dichlorobenzene-d4	6.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
4		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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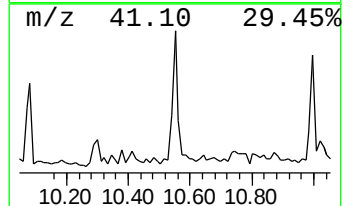
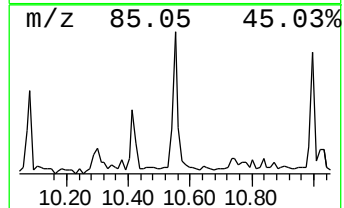
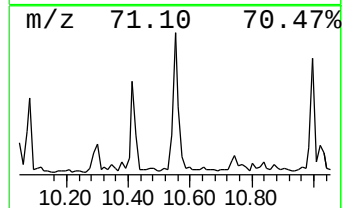
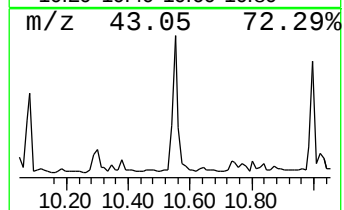
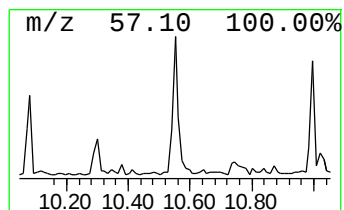
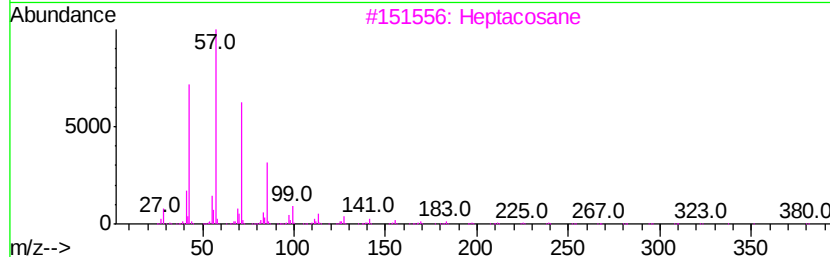
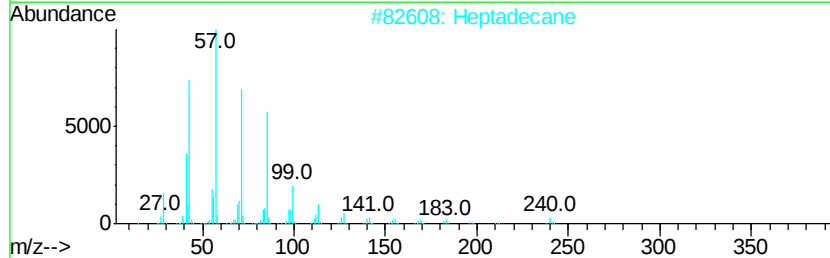
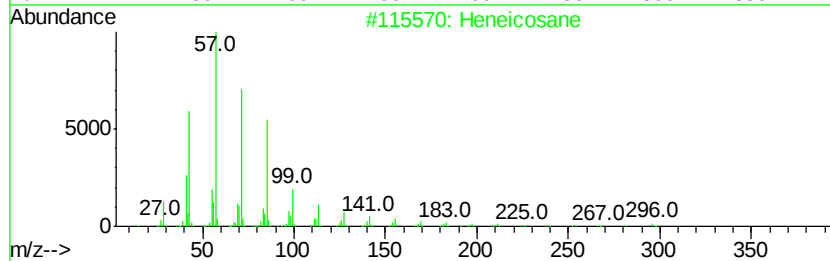
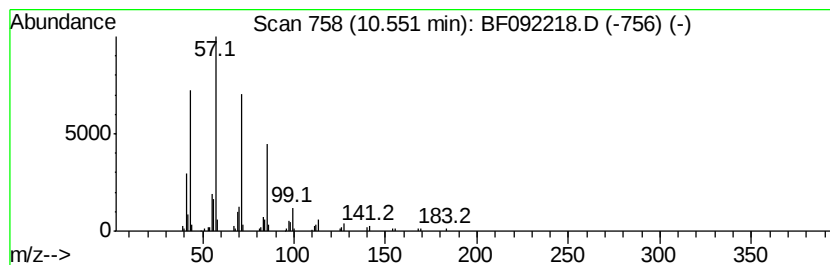
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Heneicosane Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.55	2.28 ng	184388	Phenanthrene-d10	11.11

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Heptadecane		240	C17H36	000629-78-7	91
3	Heptacosane		380	C27H56	000593-49-7	91
4	Hexadecane		226	C16H34	000544-76-3	90
5	Tridecane, 1-iodo-		310	C13H27I	035599-77-0	90



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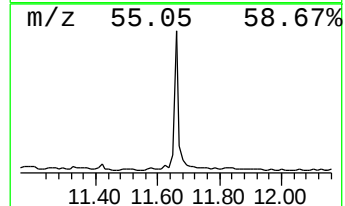
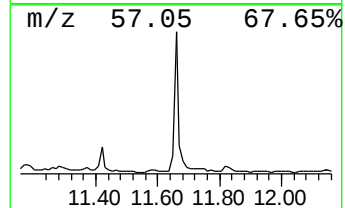
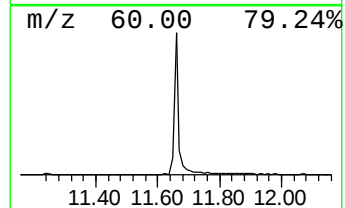
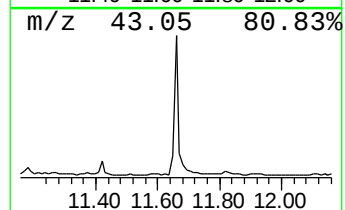
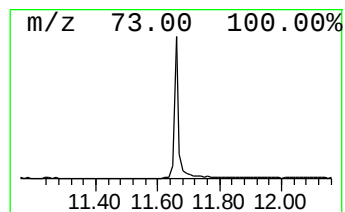
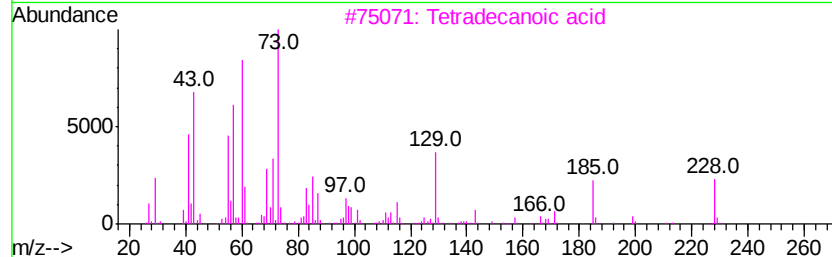
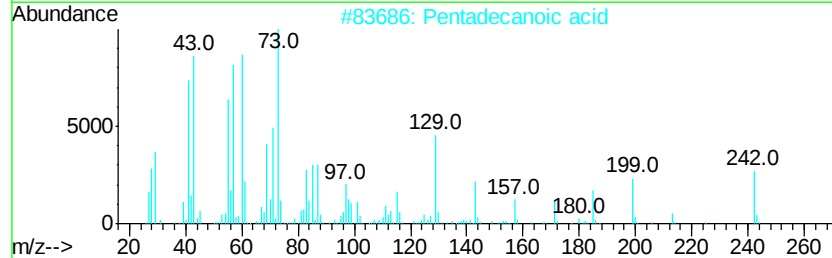
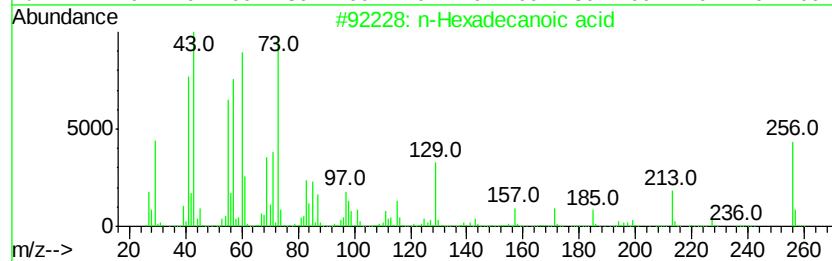
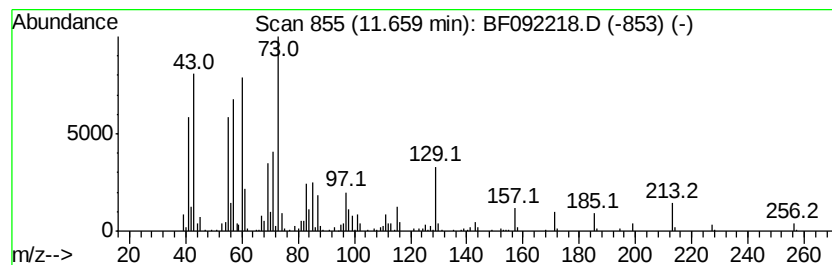
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.66	6.58 ng	532190	Phenanthrene-d10	11.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4		Tridecanoic acid	214	C13H26O2	000638-53-9	72
5		Estra-1,3,5(10)-trien-17.beta.-ol	256	C18H24O	002529-64-8	30



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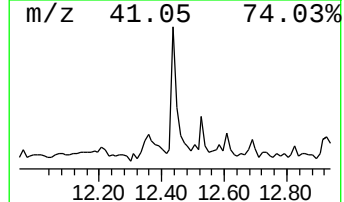
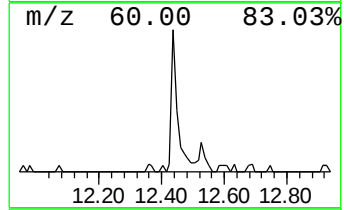
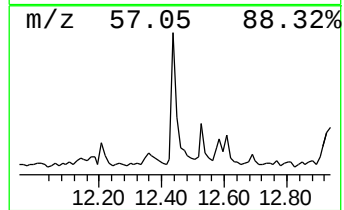
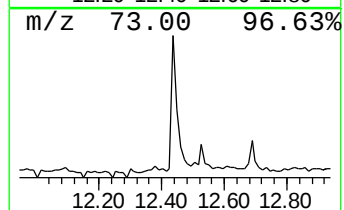
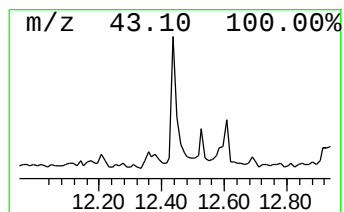
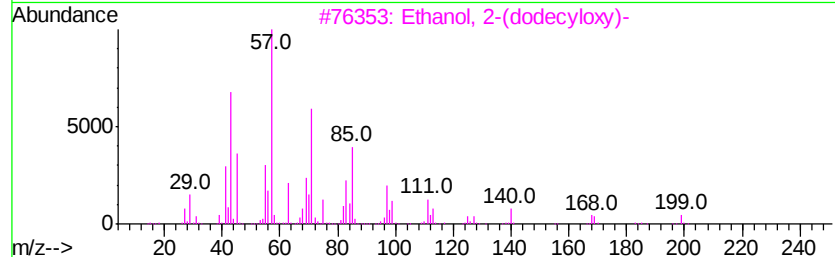
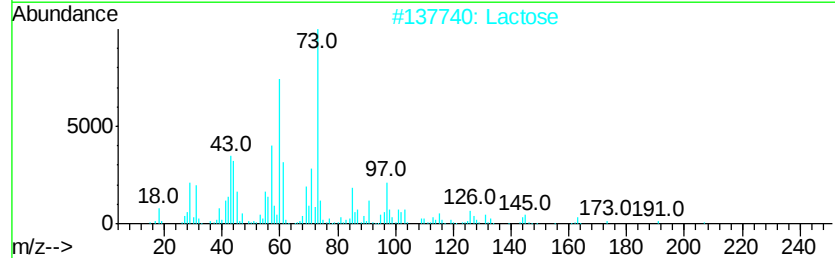
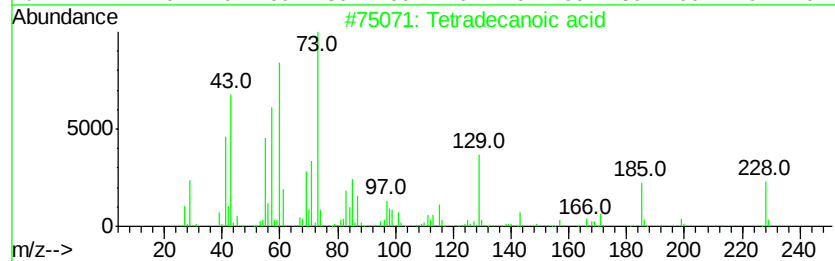
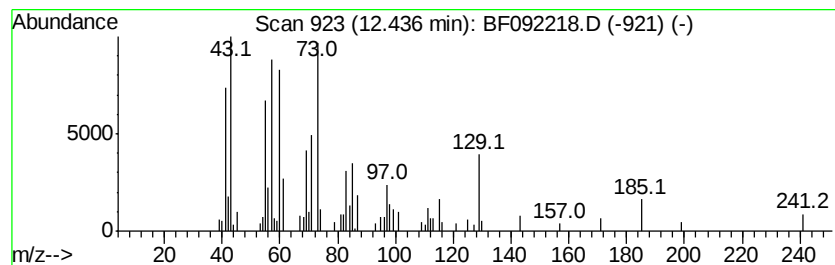
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tetradecanoic acid Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.44	2.29 ng	116743	Chrysene-d12	13.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetradecanoic acid	228	C14H28O2	000544-63-8	59
2		Lactose	342	C12H22O11	000063-42-3	50
3		Ethanol, 2-(dodecyloxy)-	230	C14H30O2	004536-30-5	18
4		Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	14
5		1-Octanol, 2-butyl-	186	C12H26O	003913-02-8	14



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011217\
Data File : BF092218.D
Acq On : 12 Jan 2017 20:11
Operator : UM/SJ
Sample : I1030-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

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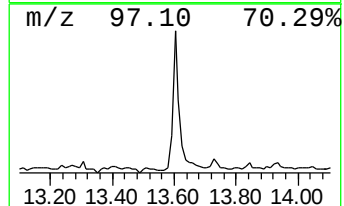
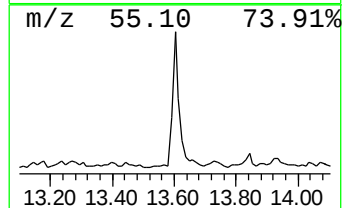
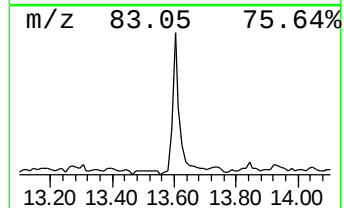
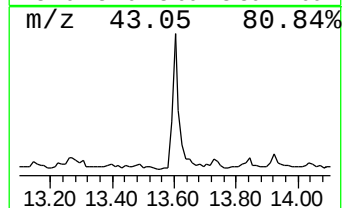
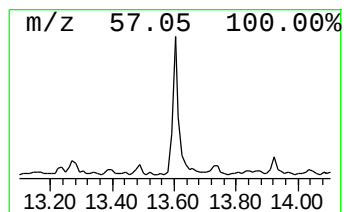
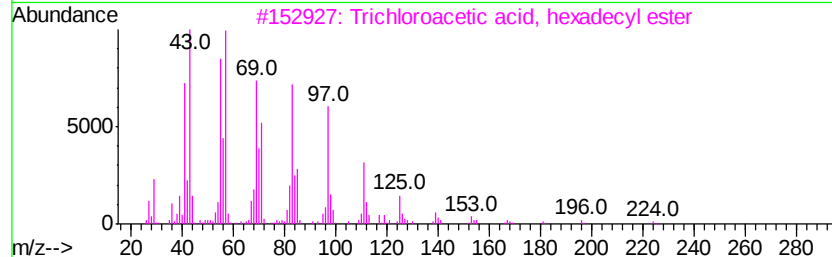
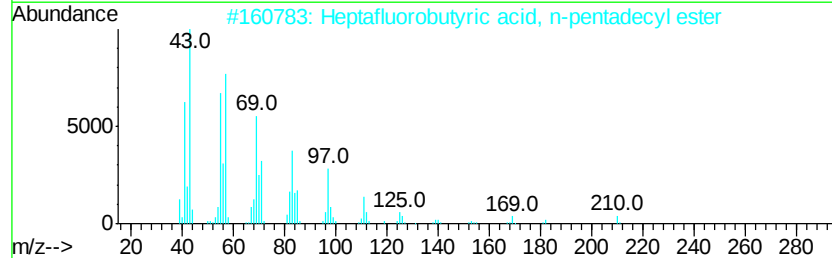
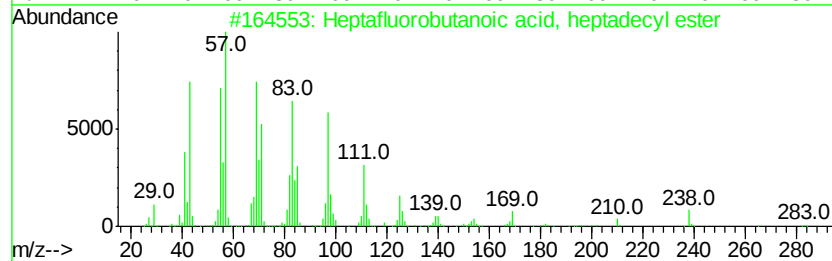
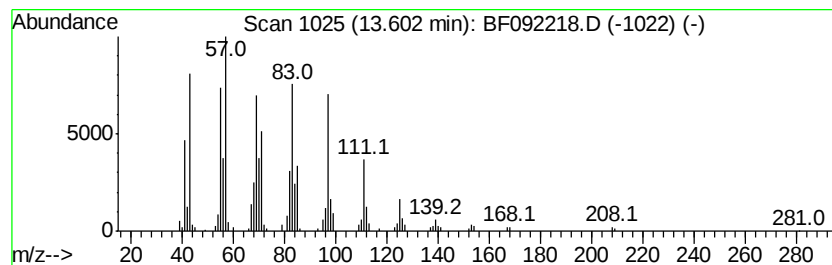
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptafluorobutanoic acid, h... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.60	6.05 ng	307962	Chrysene-d12	13.73

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	94
2		Heptafluorobutyric acid, n-penta...	424	C19H31F7O2	1000216-79-3	91
3		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	91
5		Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011217\
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ClientSampleId :
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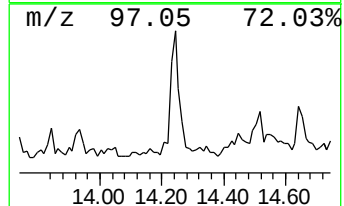
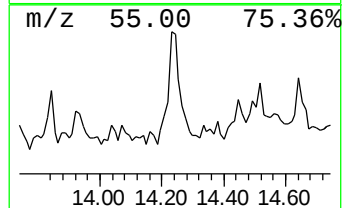
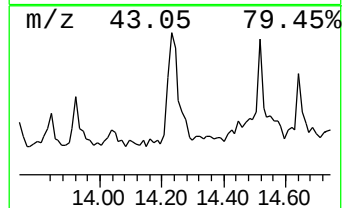
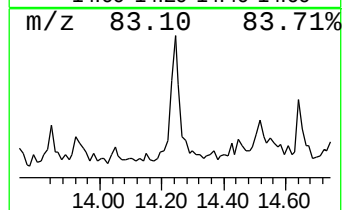
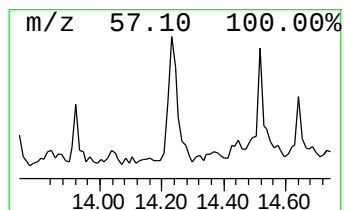
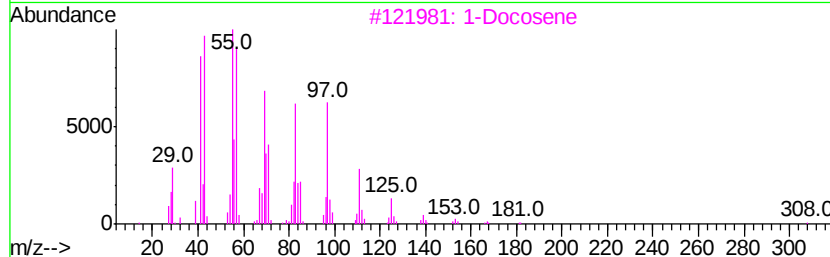
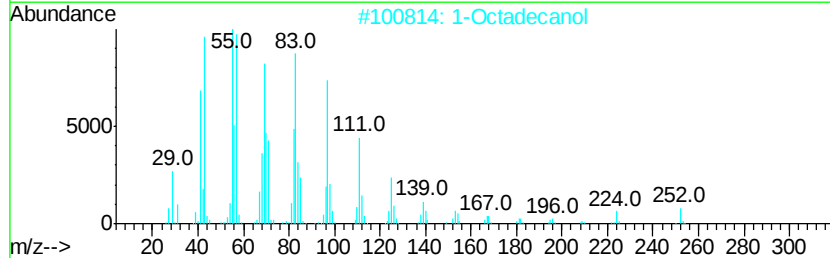
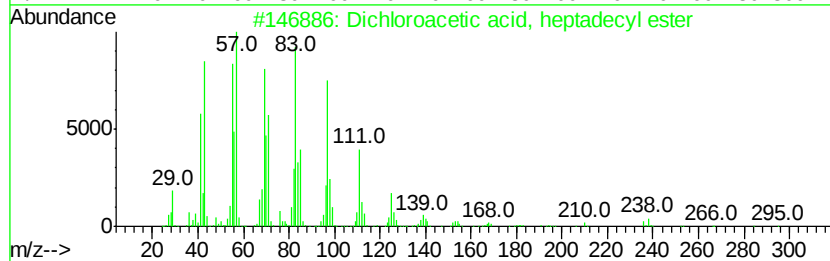
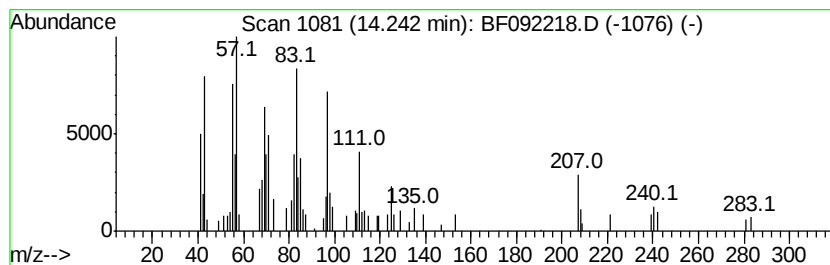
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Dichloroacetic acid, heptad... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.24	2.77 ng	141109	Chrysene-d12	13.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	93
2		1-Octadecanol	270	C18H38O	000112-92-5	93
3		1-Docosene	308	C22H44	001599-67-3	87
4		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	81
5		1-Nonadecanol	284	C19H40O	001454-84-8	76



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011217\
Data File : BF092218.D
Acq On : 12 Jan 2017 20:11
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Sample : I1030-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

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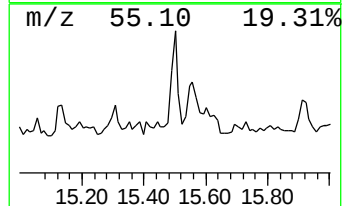
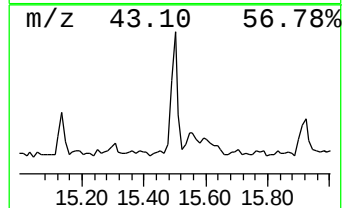
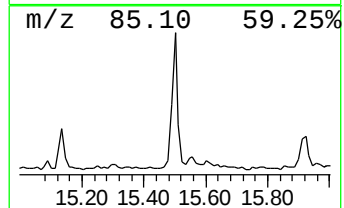
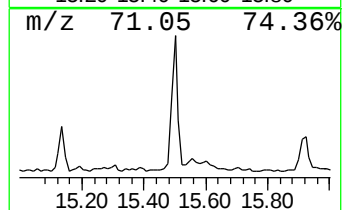
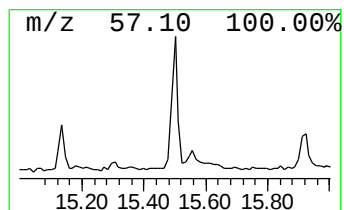
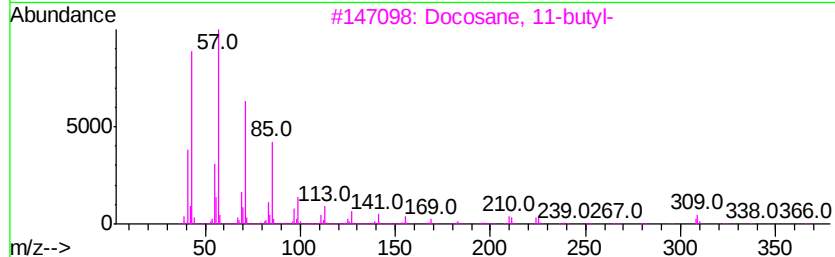
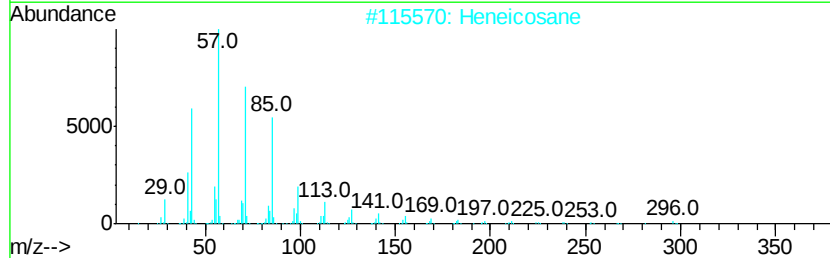
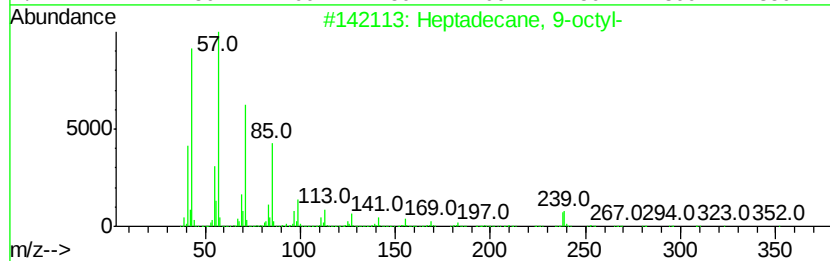
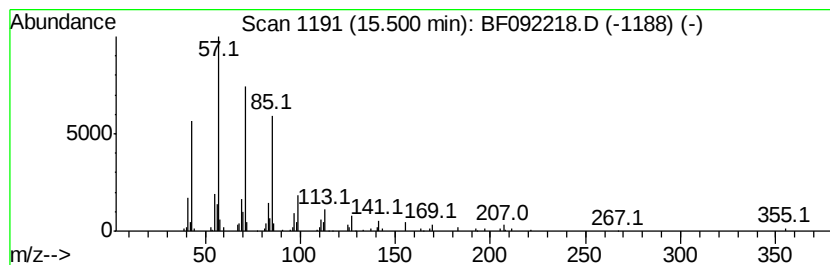
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.50	2.69 ng	159638	Perylene-d12	15.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Docosane, 11-butyl-	366	C26H54	013475-76-8	91
4		Eicosane	282	C20H42	000112-95-8	91
5		Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	91



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011217\
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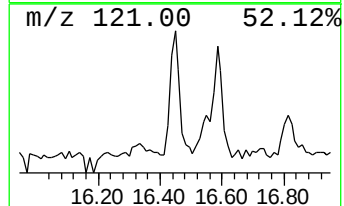
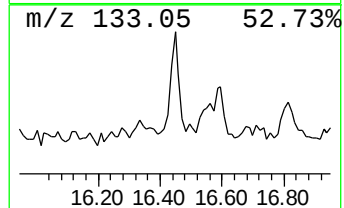
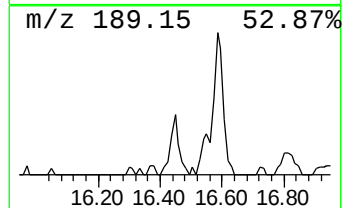
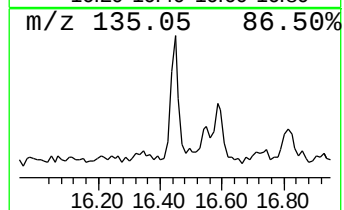
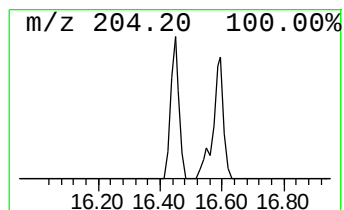
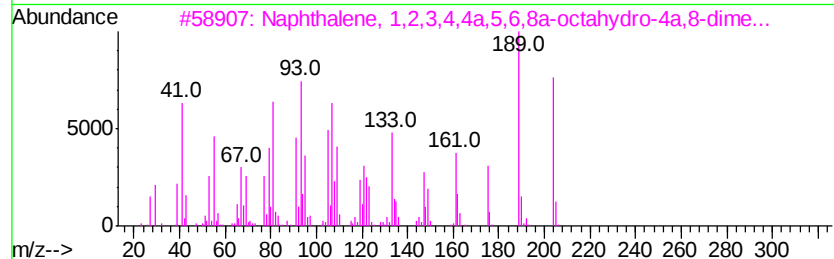
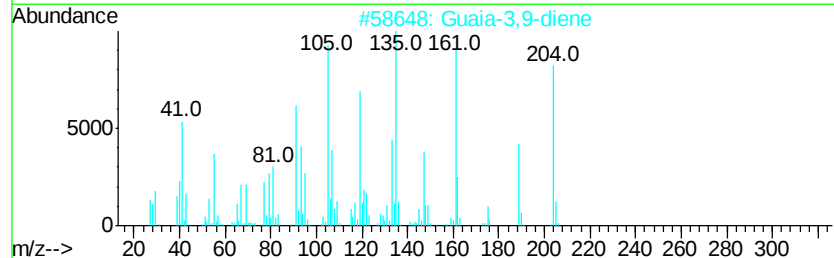
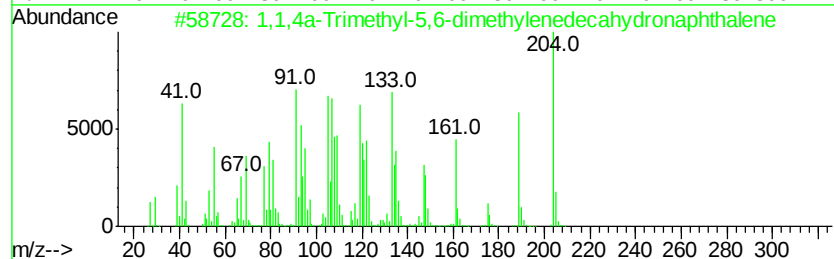
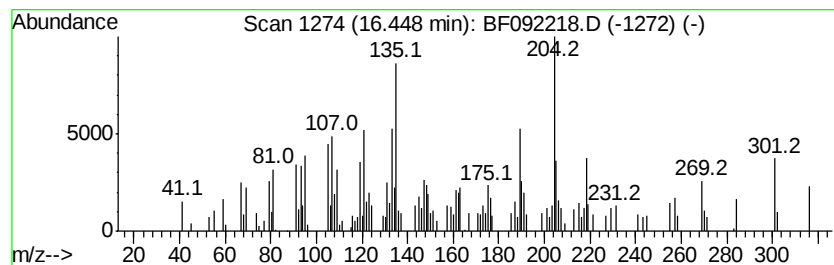
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 1,1,4a-Trimethyl-5,6-dimeth... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.45	3.82 ng	226568	Perylene-d12	15.09

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	78
2			Guaia-3,9-diene	204	C15H24	000489-83-8	64
3			Naphthalene, 1,2,3,4,4a,5,6,8a-o...	204	C15H24	000473-13-2	50
4			Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	004630-07-3	46
5			1,3a-Ethano-3aH-indene, 1,2,3,6,...	204	C15H24	004545-68-0	43



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011217\
Data File : BF092218.D
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Misc :
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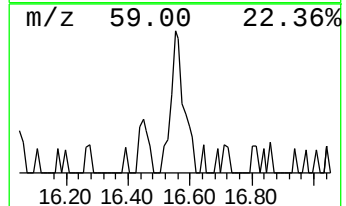
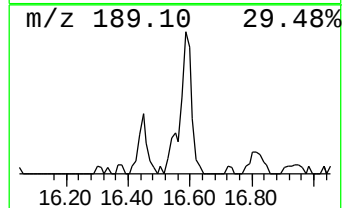
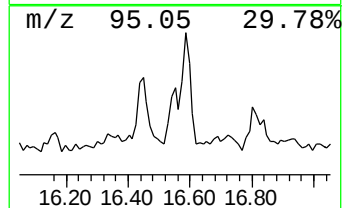
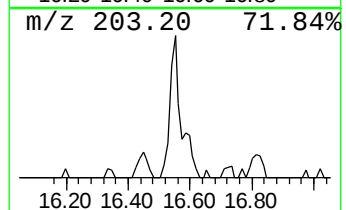
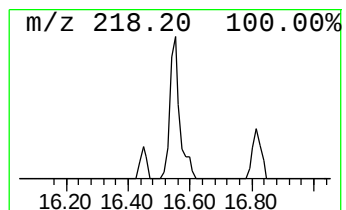
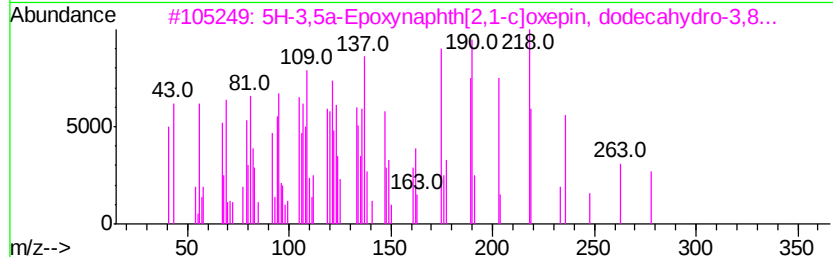
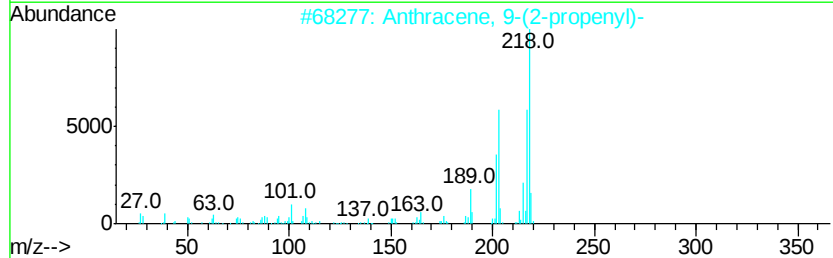
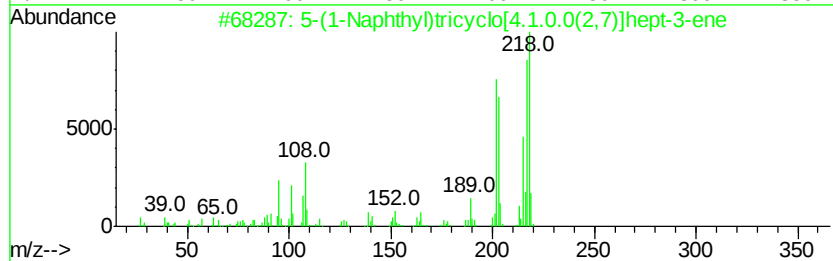
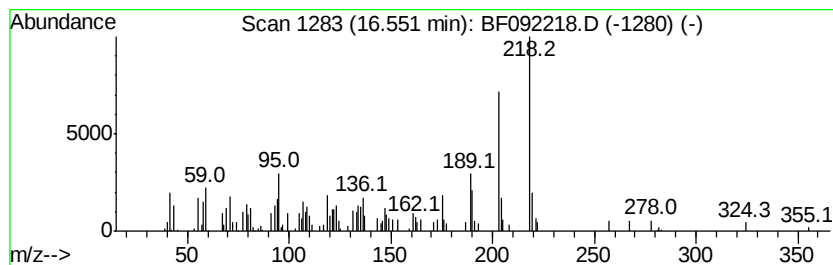
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 5-(1-Naphthyl)tricyclo[4.1.... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.55	2.36 ng	140411	Perylene-d12	15.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-(1-Naphthyl)tricyclo[4.1.0.0(2...]	218	C17H14	107729-05-5	64
2		Anthracene, 9-(2-propenyl)-	218	C17H14	023707-65-5	58
3		5H-3,5a-Epoxy-naphth[2,1-c]oxepin...	278	C18H30O2	001153-35-1	56
4		9-Phenyl-5H-benzocycloheptene	218	C17H14	138089-71-1	53
5		8-Amino-6,7-dimethoxy-4-methylqu...	218	C12H14N2O2	1000213-07-2	49



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011217\
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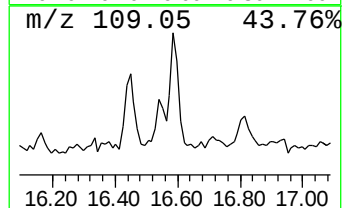
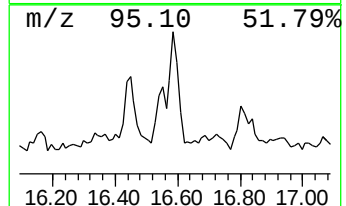
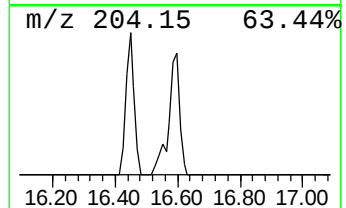
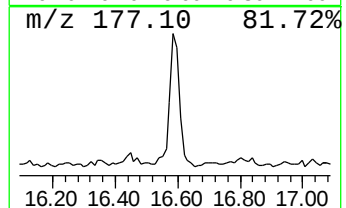
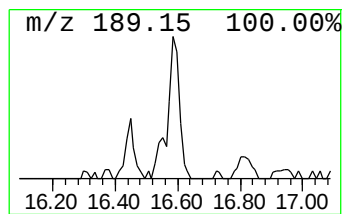
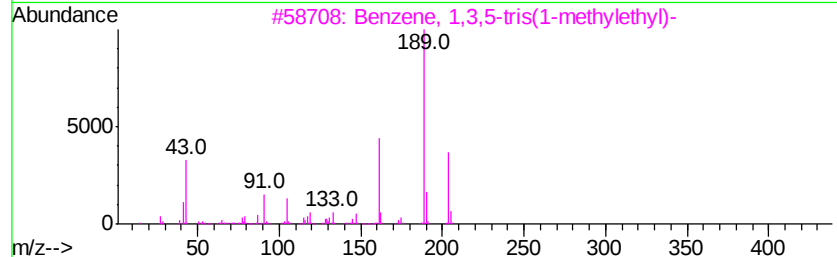
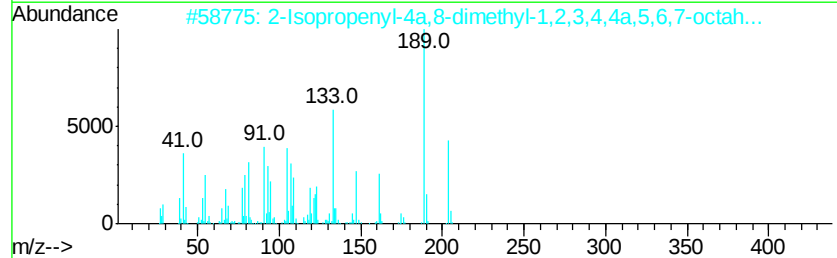
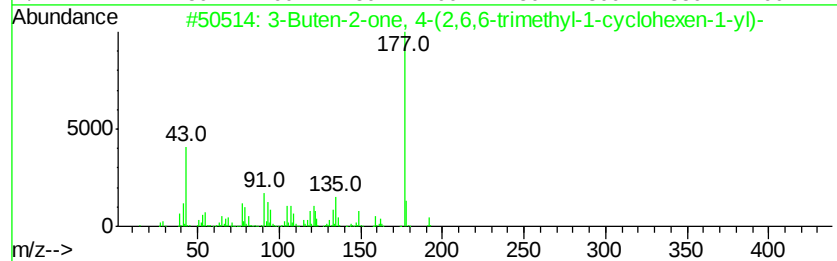
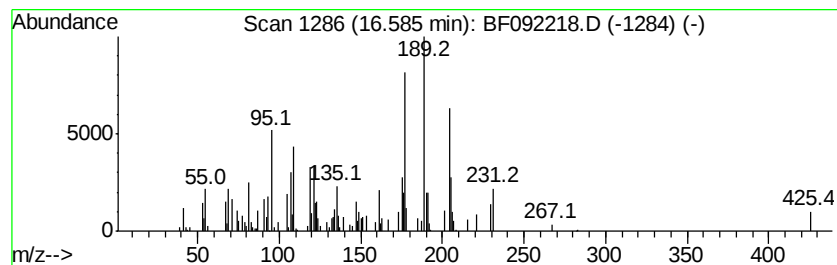
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown16.59 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.59	3.80 ng	225401	Perylene-d12	15.09	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Buten-2-one, 4-(2,6,6-trimethyl-2-phenyl-1,3-dioxane-5-carbonyl)-	192	C13H20O	014901-07-6	44
2	2-Isopropenyl-4a,8-dimethyl-1,2,3,4,8a,8b-hexahydro-2H-chromene	204	C15H24	1000192-43-5	41
3	Benzene, 1,3,5-tris(1-methylethyl)-	204	C15H24	000717-74-8	30
4	p-Trifluoromethoxybenzamide	205	C8H6F3NO2	000456-71-3	27
5	3,4-Dihydrocoumarin, 4,4,7,8-tetrahydro-2H-chromene	204	C13H16O2	040614-36-6	25



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011217\
Data File : BF092218.D
Acq On : 12 Jan 2017 20:11
Operator : UM/SJ
Sample : I1030-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-0012

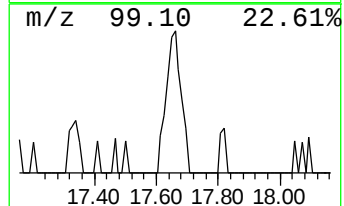
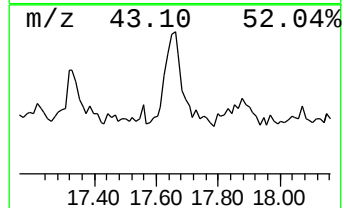
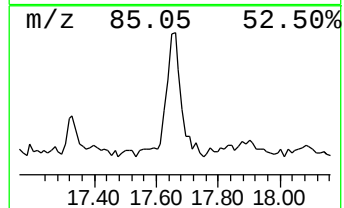
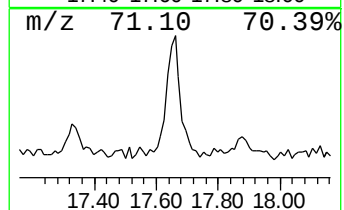
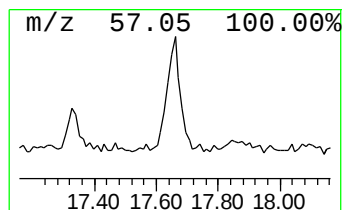
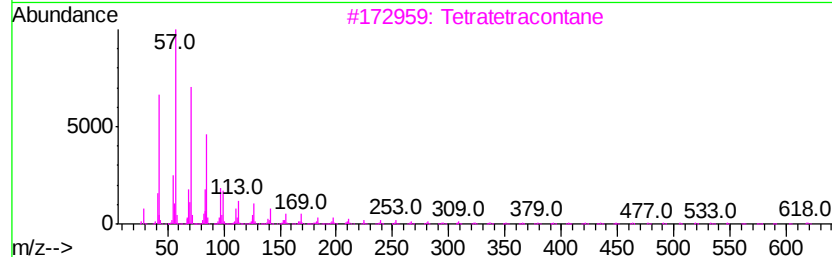
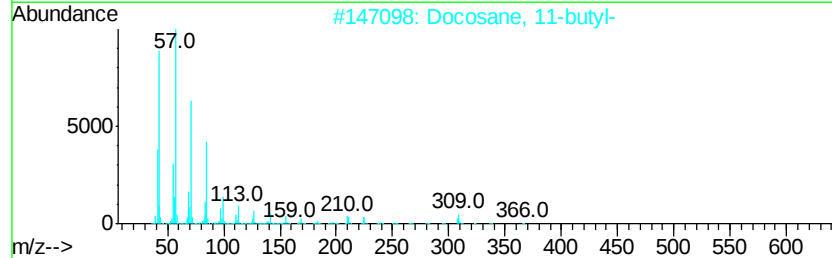
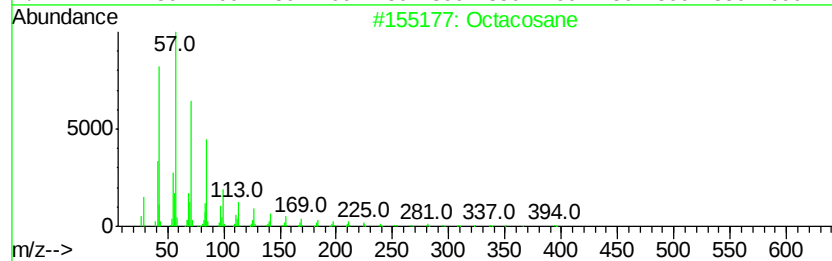
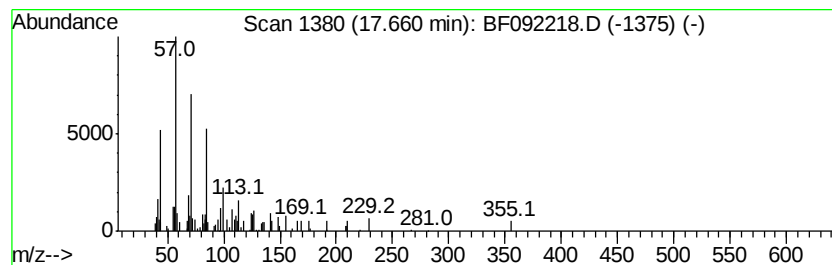
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 Octacosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.66	2.33 ng	138435	Perylene-d12	15.09

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	83
2			Docosane, 11-butyl-	366	C26H54	013475-76-8	83
3			Tetratetracontane	619	C44H90	007098-22-8	80
4			Tetracosane	338	C24H50	000646-31-1	80
5			Docosane	310	C22H46	000629-97-0	74



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011217\
 Data File : BF092218.D
 Acq On : 12 Jan 2017 20:11
 Operator : UM/SJ
 Sample : I1030-03
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMP-0012

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-Pentene, 3,4-di...	3.99	2.4	ng	125464	1	6.60	1044190	20.0
2-Pentanone, 4-hy...	4.72	53.5	ng	2791700	1	6.60	1044190	20.0
unknown6.37	6.37	73.9	ng	3856260	1	6.60	1044190	20.0
Heneicosane	10.55	2.3	ng	184388	4	11.11	1616790	20.0
n-Hexadecanoic acid	11.66	6.6	ng	532190	4	11.11	1616790	20.0
Tetradecanoic acid	12.44	2.3	ng	116743	5	13.73	1018780	20.0
Heptafluorobutano...	13.60	6.0	ng	307962	5	13.73	1018780	20.0
Dichloroacetic ac...	14.24	2.8	ng	141109	5	13.73	1018780	20.0
Heptadecane, 9-oc...	15.50	2.7	ng	159638	6	15.09	1187740	20.0
1,1,4a-Trimethyl-...	16.45	3.8	ng	226568	6	15.09	1187740	20.0
5-(1-Naphthyl)tri...	16.55	2.4	ng	140411	6	15.09	1187740	20.0
unknown16.59	16.59	3.8	ng	225401	6	15.09	1187740	20.0
2(1H)Naphthalenon...	16.81	2.2	ng	128202	6	15.09	1187740	20.0
Octacosane	17.66	2.3	ng	138435	6	15.09	1187740	20.0