

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011217\
 Data File : BF092217.D
 Acq On : 12 Jan 2017 19:42
 Operator : UM/SJ
 Sample : I1030-01
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMP-0011

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	116753	187074	3.67%	0.428%
2	4.721	245	248	261	rVB	1570334	2806836	55.11%	6.428%
3	5.190	287	289	292	rBV	2689025	3888131	76.33%	8.904%
4	6.264	380	383	390	rBV	4573542	5093551	100.00%	11.665%
5	6.367	390	392	395	rVB	4667375	4549418	89.32%	10.419%
6	6.596	409	412	414	rBV	833706	816077	16.02%	1.869%
7	6.756	423	426	428	rBV	2173451	3016801	59.23%	6.909%
8	7.167	459	462	464	rBV	3163970	3171505	62.27%	7.263%
9	7.876	522	524	527	rBV	1168871	1415098	27.78%	3.241%
10	8.962	616	619	621	rBV	4689724	4521299	88.77%	10.354%
11	9.362	652	654	656	rBV	374344	336682	6.61%	0.771%
12	9.625	675	677	680	rBV	1384040	1361799	26.74%	3.119%
13	10.082	715	717	718	rVB	63587	75363	1.48%	0.173%
14	10.413	744	746	749	rBV2	2045696	2809655	55.16%	6.434%
15	10.551	755	758	762	rBV	148377	192602	3.78%	0.441%
16	10.996	795	797	798	rBV2	103906	101446	1.99%	0.232%
17	11.099	804	806	809	rBV	1111868	1408938	27.66%	3.227%
18	11.659	853	855	859	rBV2	422775	395836	7.77%	0.907%
19	12.311	910	912	914	rBV	90099	80840	1.59%	0.185%
20	12.437	921	923	928	rBV	68643	91394	1.79%	0.209%
21	12.539	928	932	934	rVV	80471	111991	2.20%	0.256%
22	12.688	943	945	948	rVB	3124985	4043632	79.39%	9.260%
23	13.602	1022	1025	1034	rBV	254002	388217	7.62%	0.889%
24	13.728	1034	1036	1039	rBV	882209	974297	19.13%	2.231%
25	14.231	1076	1080	1087	rBV4	39599	113286	2.22%	0.259%
26	14.722	1121	1123	1128	rBV2	29812	82821	1.63%	0.190%
27	14.814	1128	1131	1132	rBV	44710	61779	1.21%	0.141%
28	15.088	1153	1155	1158	rBV	803621	964202	18.93%	2.208%
29	15.500	1188	1191	1193	rBV	47644	62419	1.23%	0.143%
30	15.557	1193	1196	1199	rBV2	32000	81101	1.59%	0.186%
31	16.334	1261	1264	1268	rBV	28532	64876	1.27%	0.149%
32	16.551	1280	1283	1284	rBV3	44585	96907	1.90%	0.222%
33	16.585	1284	1286	1292	rVB	88450	191384	3.76%	0.438%
34	16.814	1302	1306	1312	rBV6	45896	108721	2.13%	0.249%

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ALS Vial : 14 Sample Multiplier: 1

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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

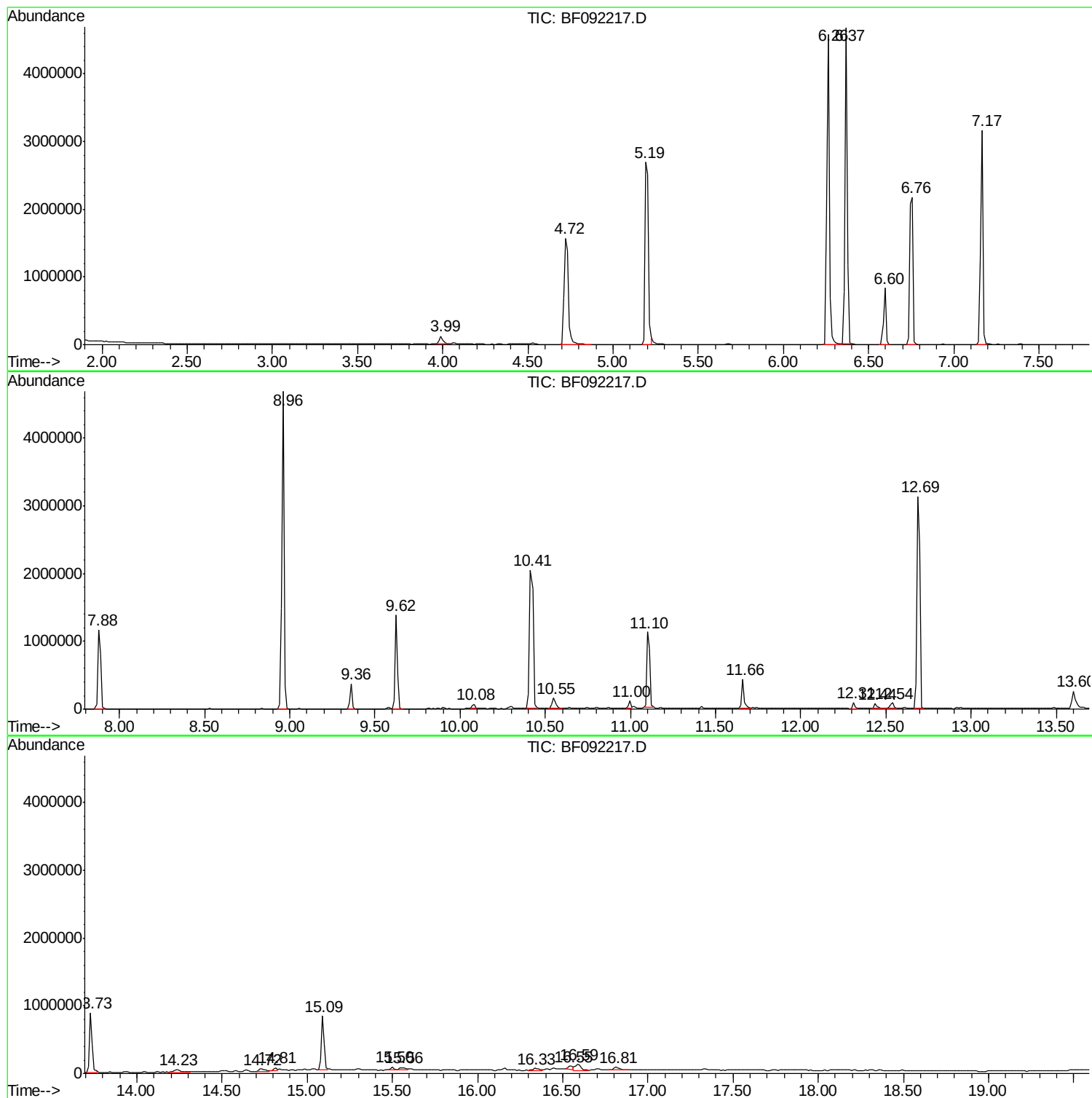
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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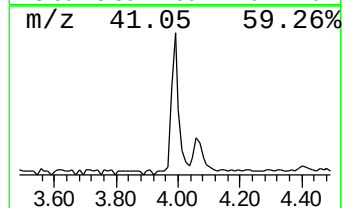
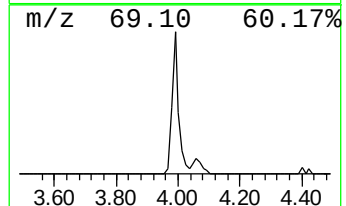
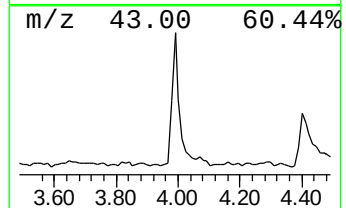
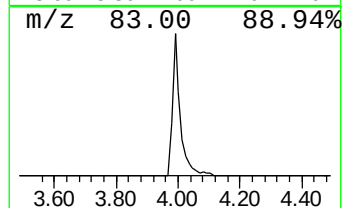
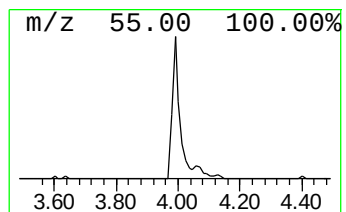
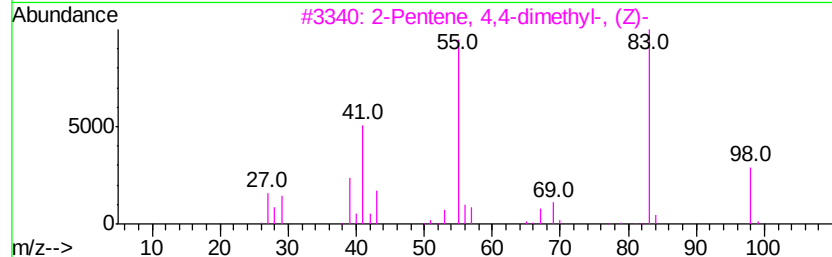
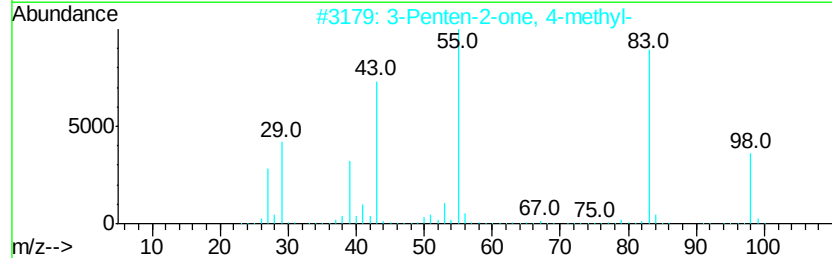
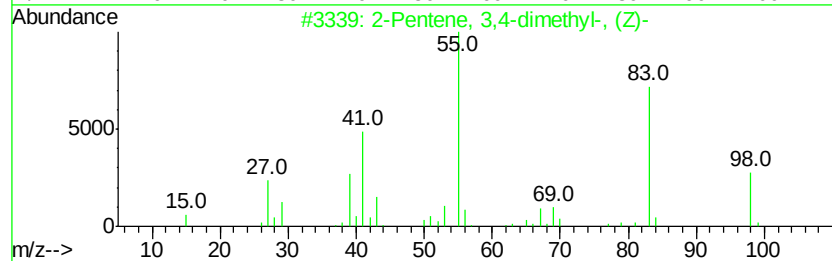
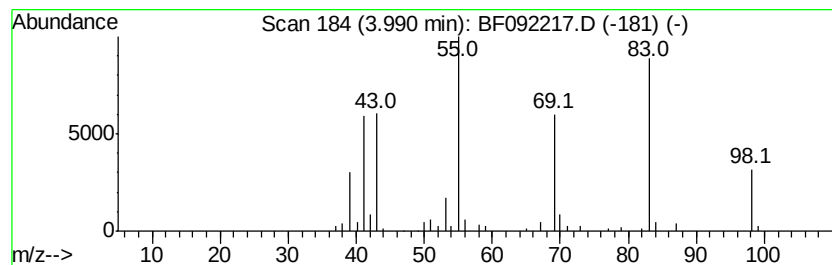
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentene, 3,4-dimethyl-, (Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.99	4.58 ng	187074	1,4-Dichlorobenzene-d4	6.60

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	90
2		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	87
3		2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	86
4		2-Pentene, 4,4-dimethyl-	98	C7H14	026232-98-4	86
5		3-Hexen-2-one	98	C6H10O	000763-93-9	72



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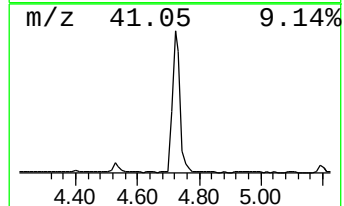
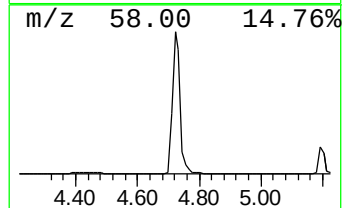
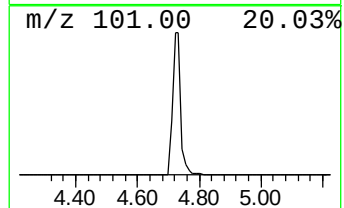
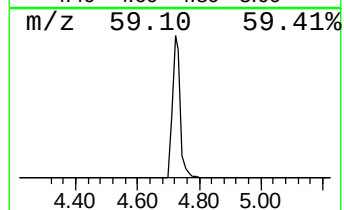
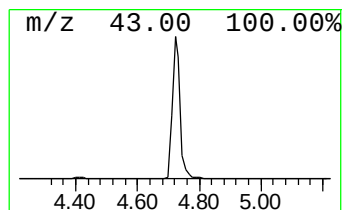
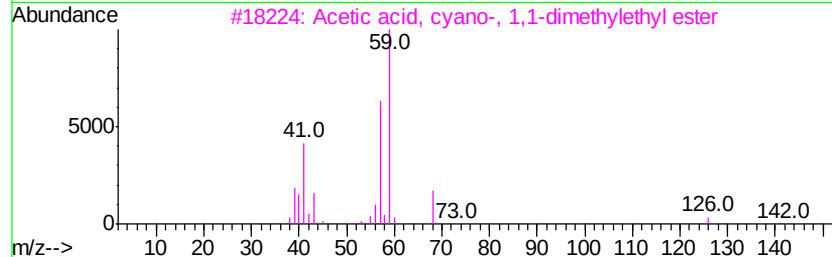
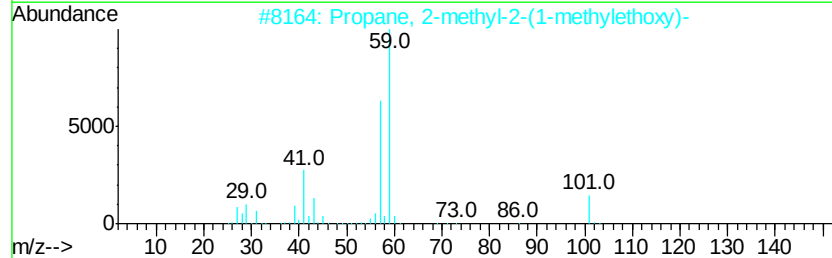
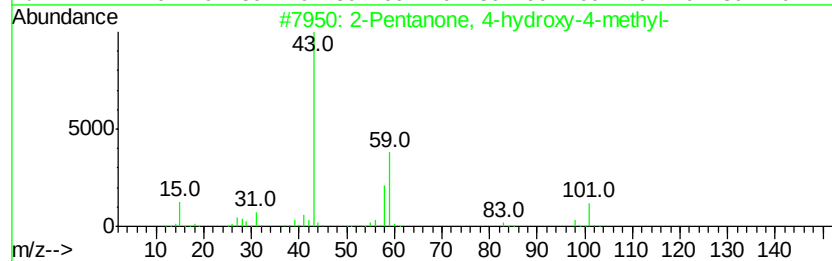
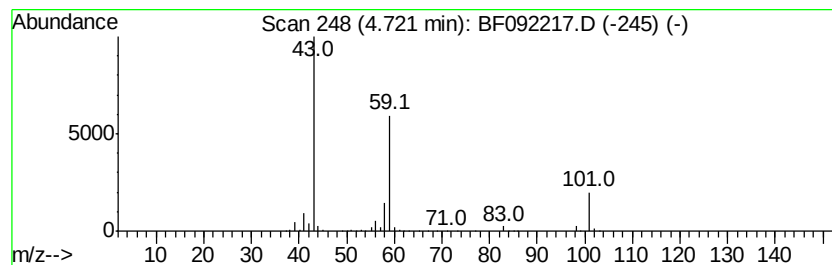
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.72	68.79 ng	2806840	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		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
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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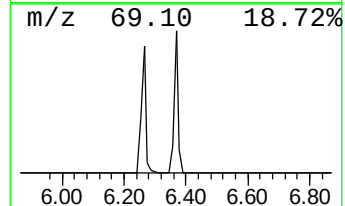
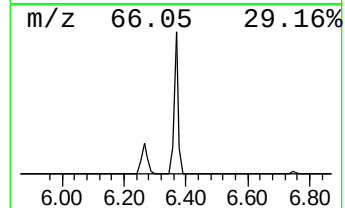
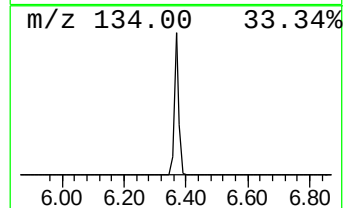
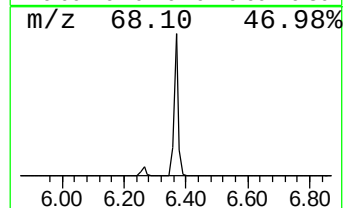
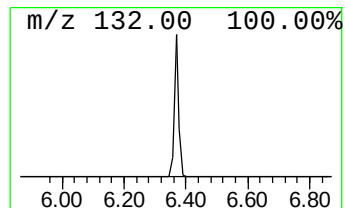
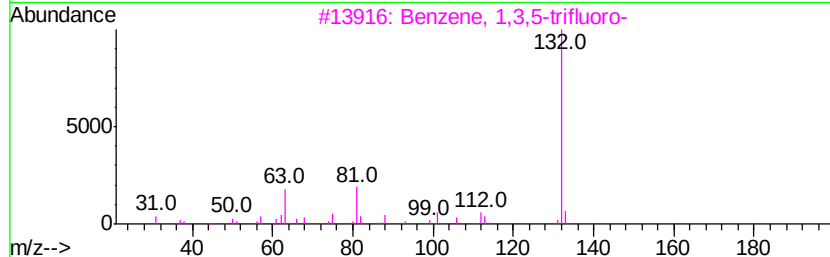
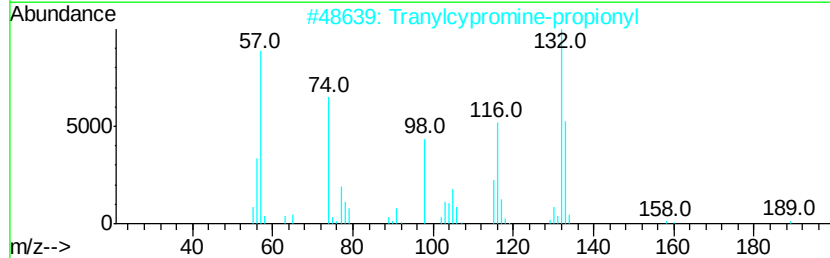
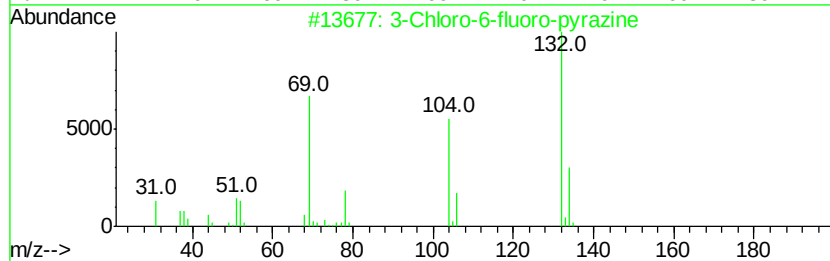
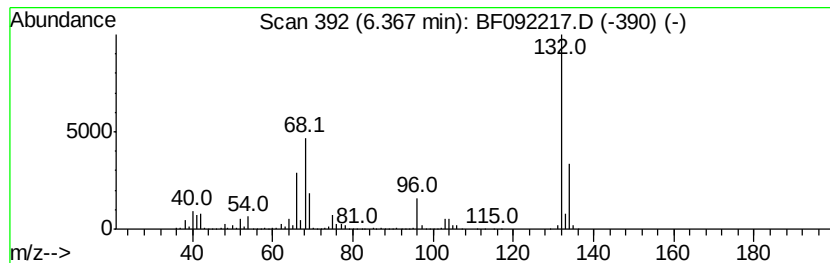
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.37 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.37	111.50 ng	4549420	1,4-Dichlorobenzene-d4	6.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
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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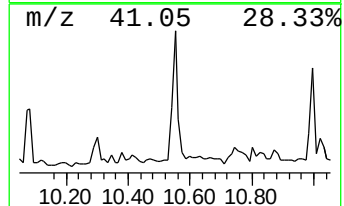
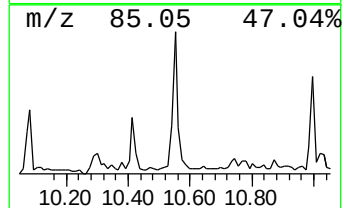
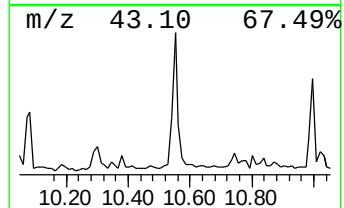
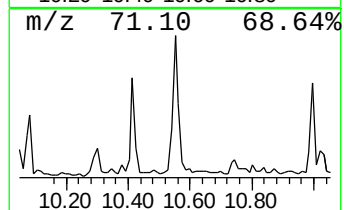
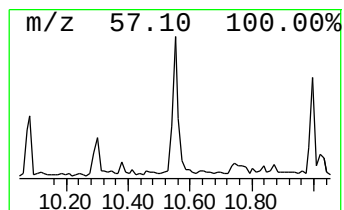
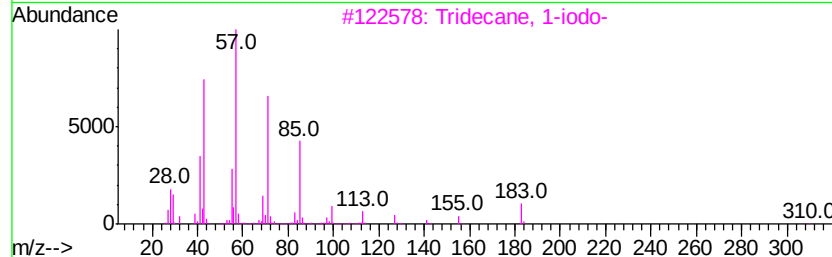
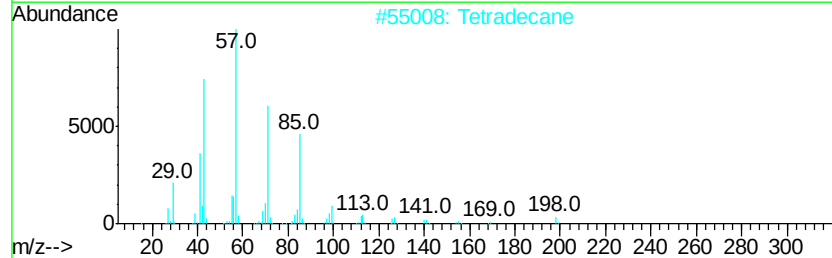
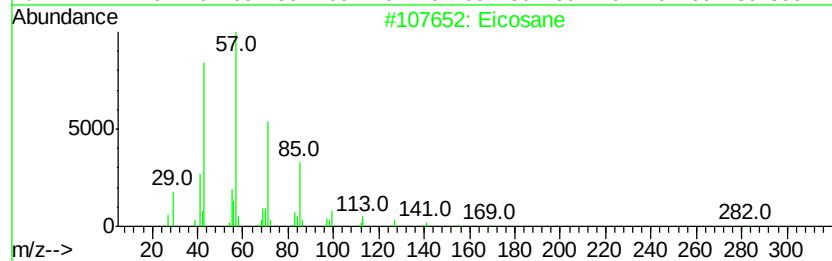
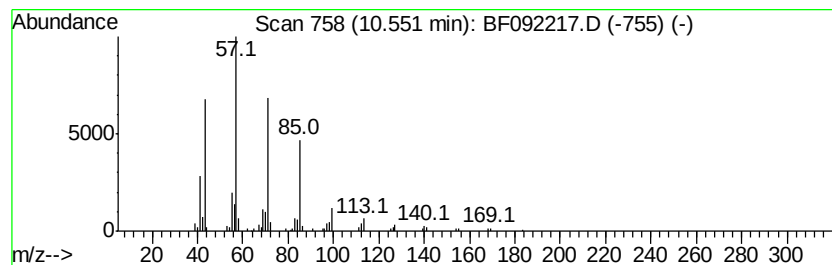
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.55	2.73 ng	192602	Phenanthrene-d10	11.10

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	91
2	Tetradecane		198	C14H30	000629-59-4	91
3	Tridecane, 1-iodo-		310	C13H27I	035599-77-0	87
4	Pentadecane		212	C15H32	000629-62-9	86
5	Dodecane, 1-iodo-		296	C12H25I	004292-19-7	80



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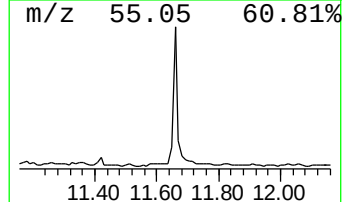
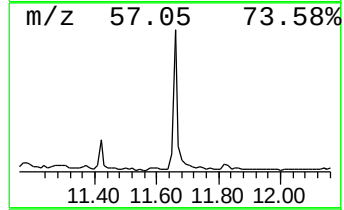
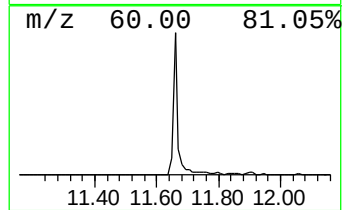
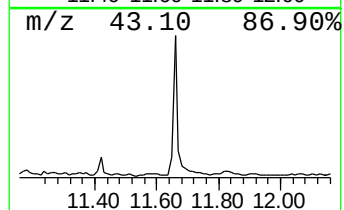
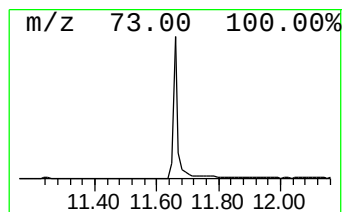
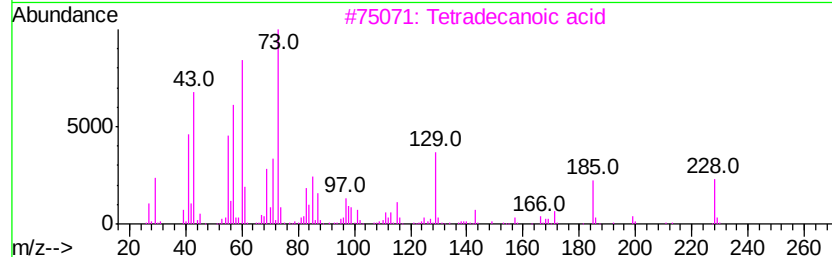
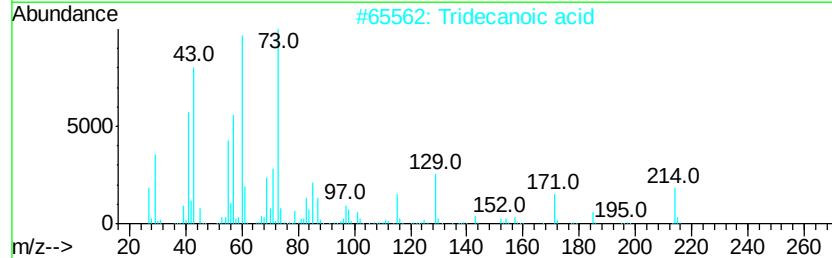
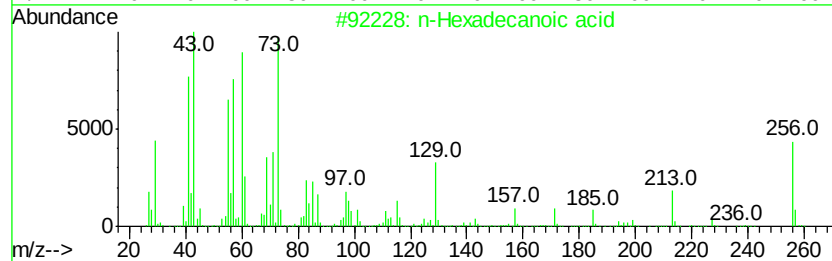
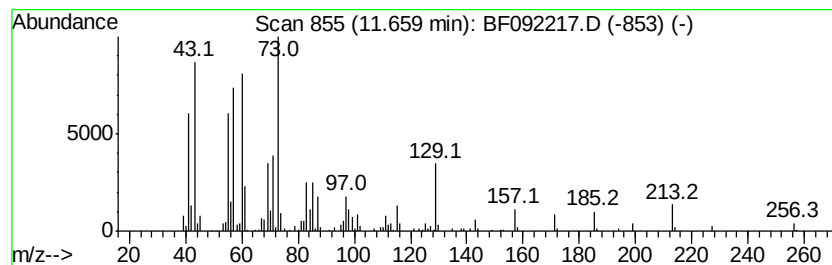
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.66	5.62 ng	395836	Phenanthrene-d10	11.10

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	87
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	62
5		N-Acetylisoaxazolidine	115	C5H9NO2	115615-36-6	25



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COMP-0011

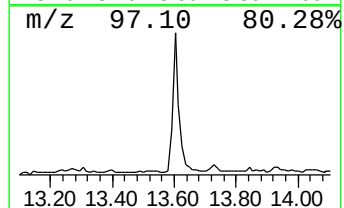
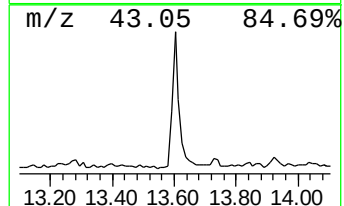
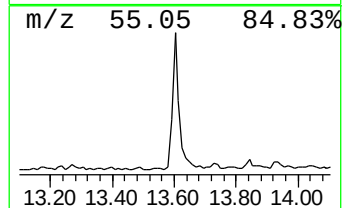
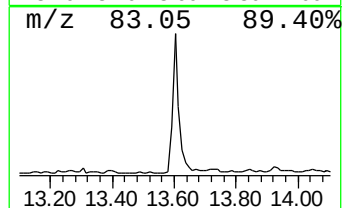
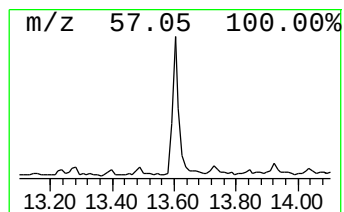
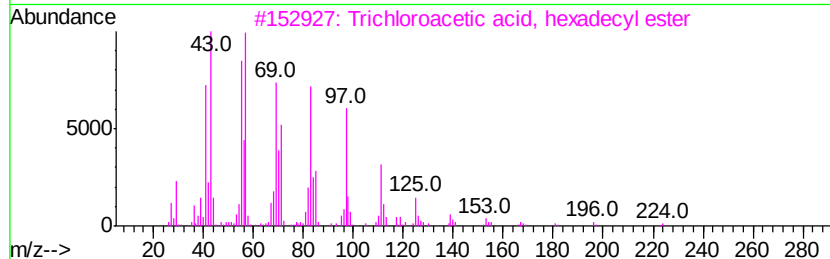
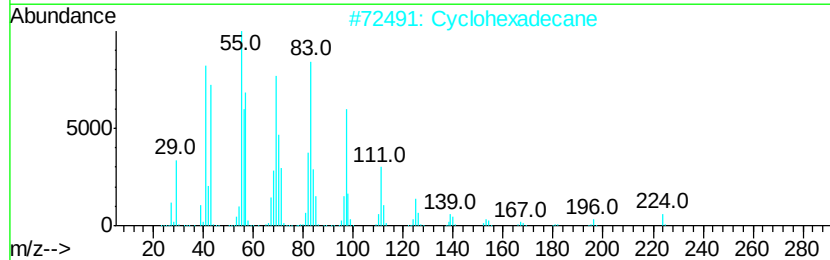
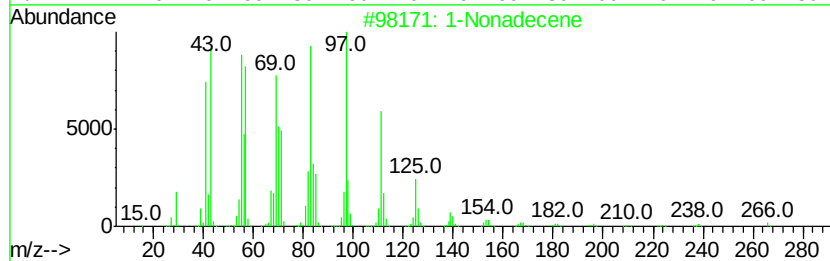
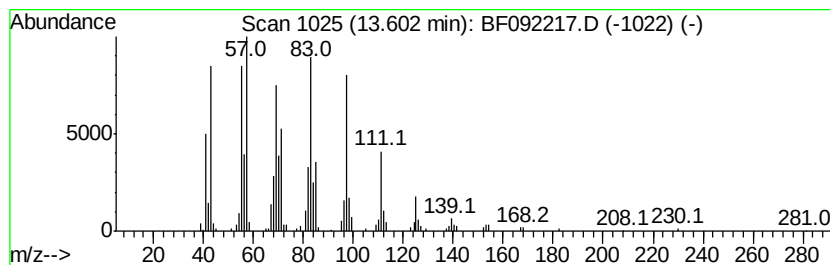
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Nonadecene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.60	7.97 ng	388217	Chrysene-d12	13.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Nonadecene	266	C19H38	018435-45-5	91
2		Cyclohexadecane	224	C16H32	000295-65-8	87
3		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	87
4		17-Pentatriacontene	491	C35H70	006971-40-0	80
5		Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	74



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011217\
Data File : BF092217.D
Acq On : 12 Jan 2017 19:42
Operator : UM/SJ
Sample : I1030-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-0011

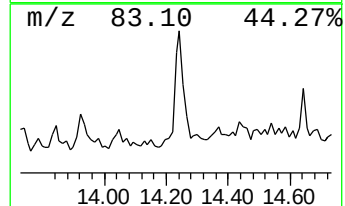
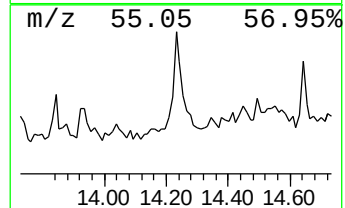
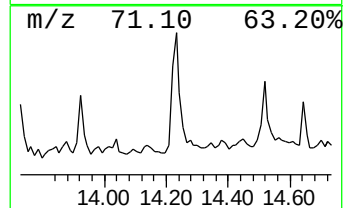
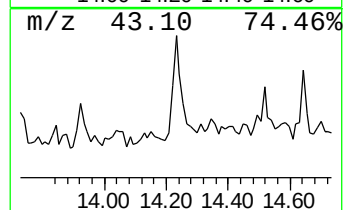
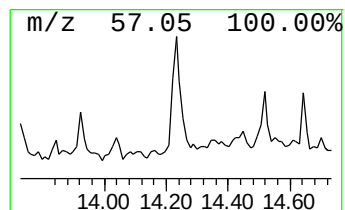
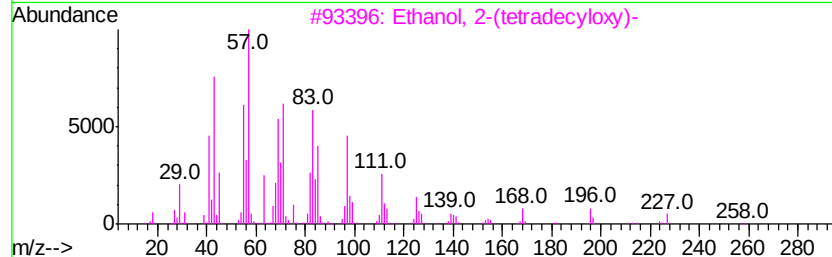
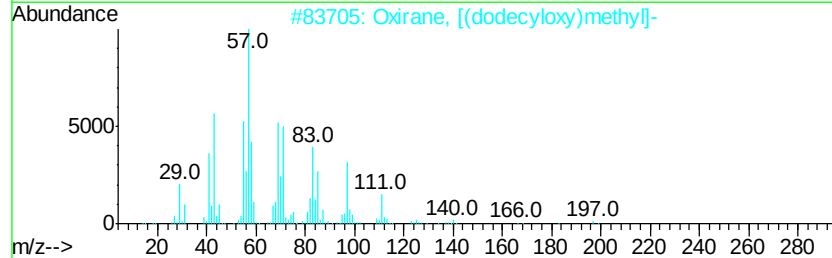
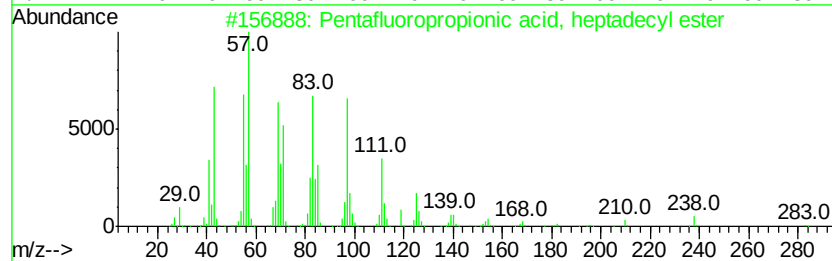
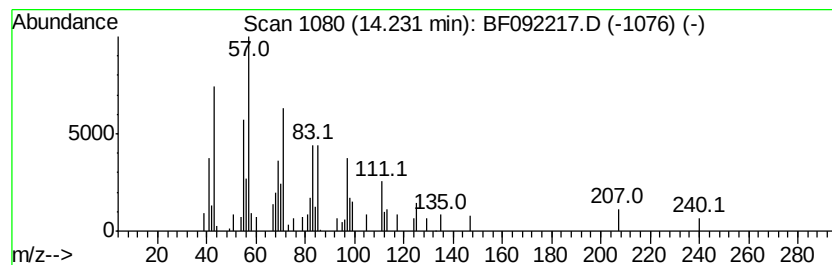
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Pentafluoropropionic acid, ... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.23	2.33 ng	113286	Chrysene-d12	13.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	50
2		Oxirane, [(dodecyloxy)methyl]-	242	C15H30O2	002461-18-9	50
3		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	49
4		Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	47
5		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	46



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011217\
Data File : BF092217.D
Acq On : 12 Jan 2017 19:42
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Sample : I1030-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

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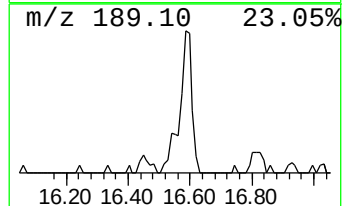
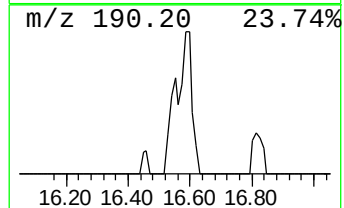
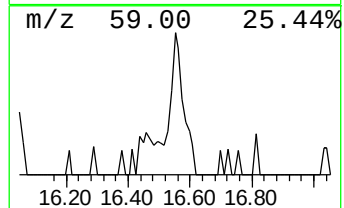
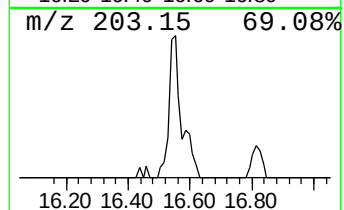
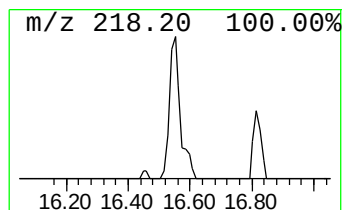
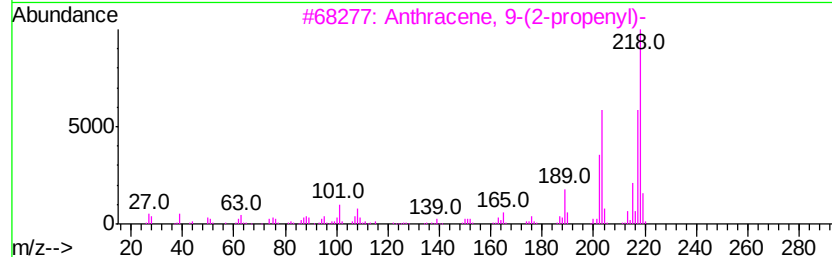
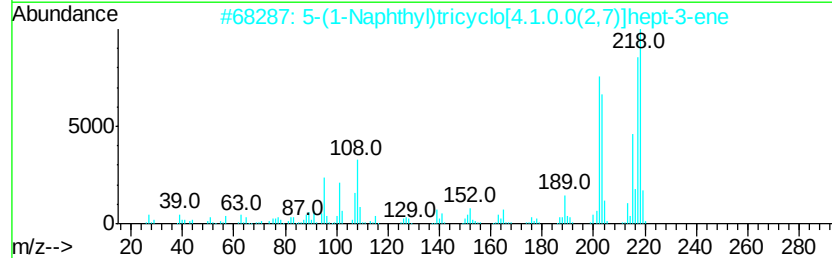
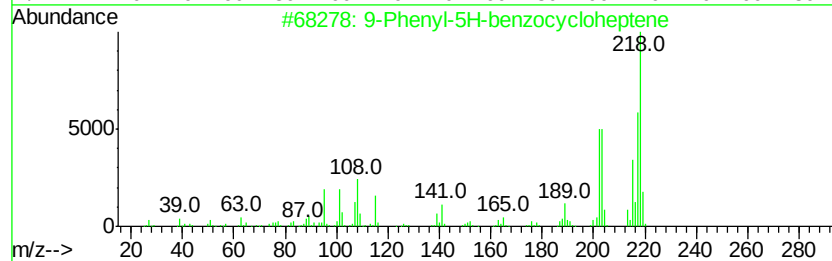
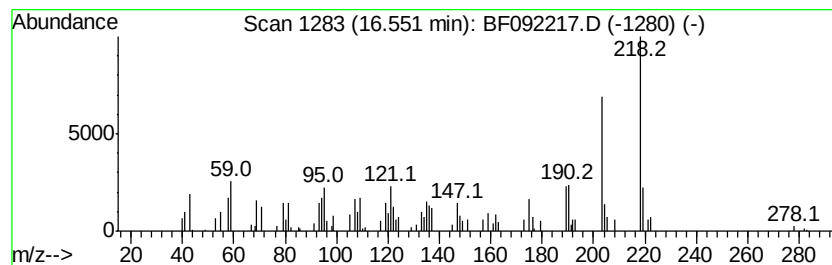
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 9-Phenyl-5H-benzocycloheptene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.55	2.01 ng	96907	Perylene-d12	15.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Phenyl-5H-benzocycloheptene	218	C17H14	138089-71-1	64
2		5-(1-Naphthyl)tricyclo[4.1.0.0(2...]	218	C17H14	107729-05-5	64
3		Anthracene, 9-(2-propenyl)-	218	C17H14	023707-65-5	62
4		2H-Cyclopropa[fa]naphthalen-2-one...	218	C15H22O	006831-17-0	60
5		6,7,8,9-Tetrahydrodibenzo[b,d]fu...	260	C15H16O4	1000196-34-3	53



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011217\
Data File : BF092217.D
Acq On : 12 Jan 2017 19:42
Operator : UM/SJ
Sample : I1030-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

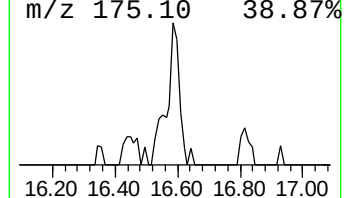
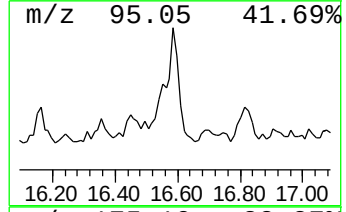
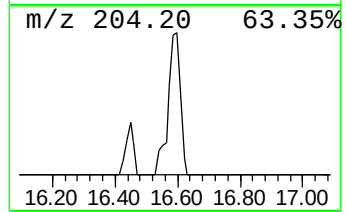
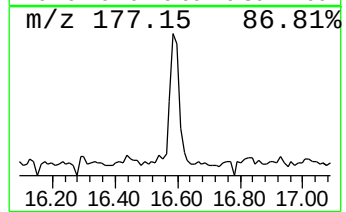
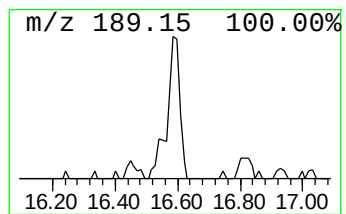
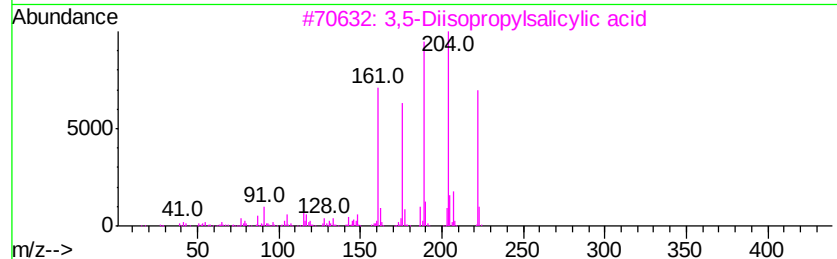
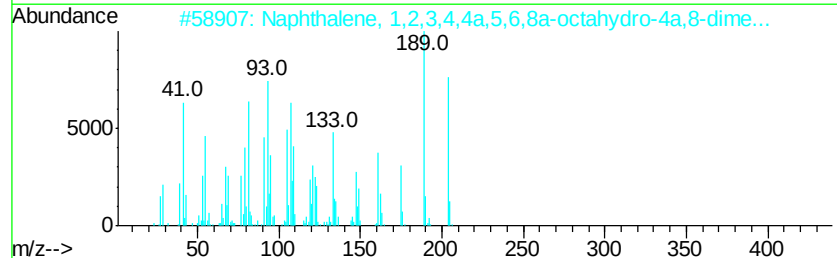
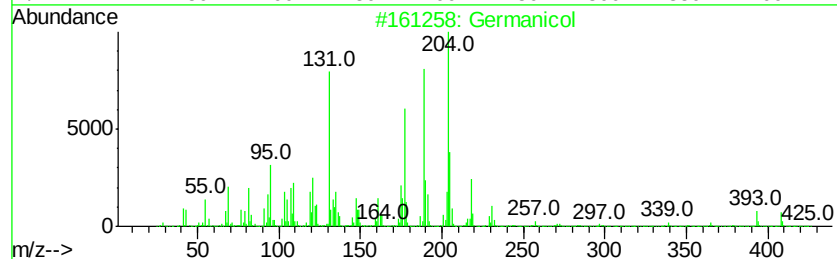
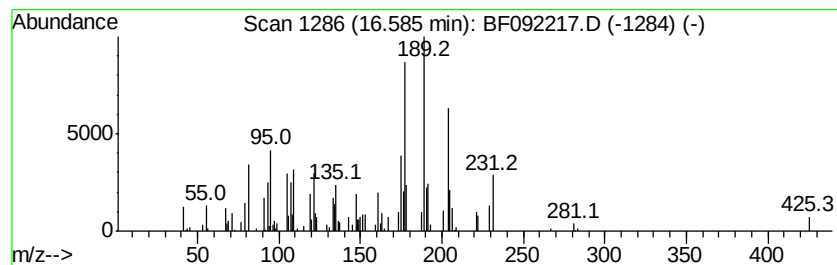
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Germanicol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.59	3.97 ng	191384	Perylene-d12	15.09
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Germanicol		426 C30H500	000465-02-1 68
2	Naphthalene, 1,2,3,4,4a,5,6,8a-o...		204 C15H24	000473-13-2 35
3	3,5-Diisopropylsalicylic acid		222 C13H18O3	002215-21-6 27
4	3,4-Dihydrocoumarin, 4,4-dimethy...		204 C13H16O2	029423-74-3 22
5	2,3-Dimethoxy-5-aminocinnamitrile		204 C11H12N2O2	1000214-46-5 22



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011217\
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Sample : I1030-01
Misc :
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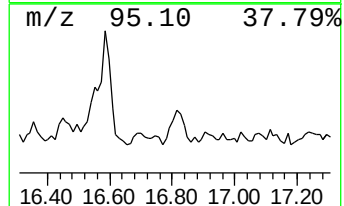
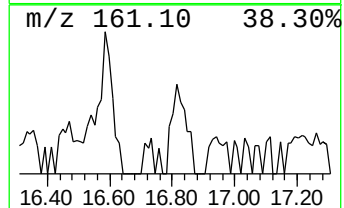
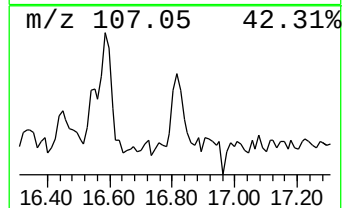
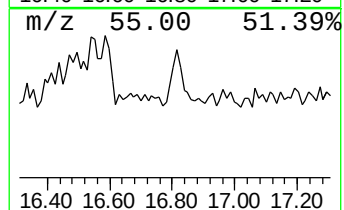
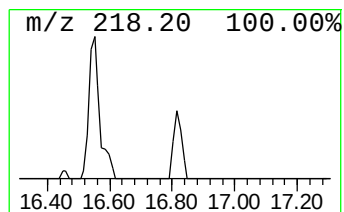
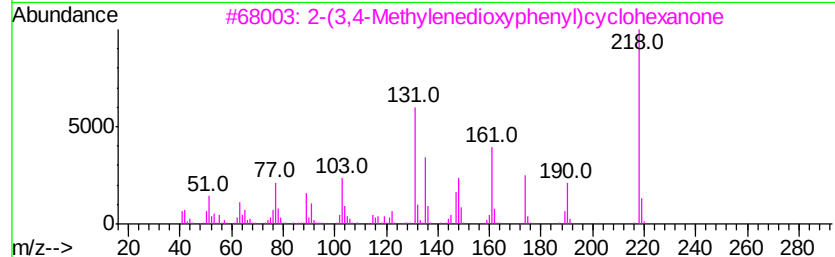
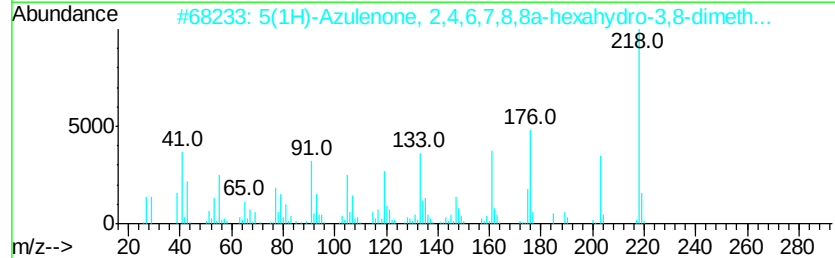
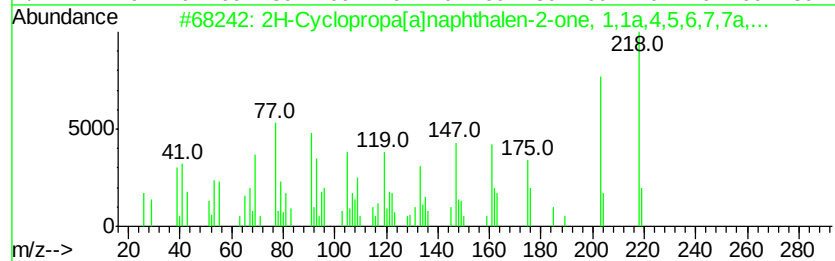
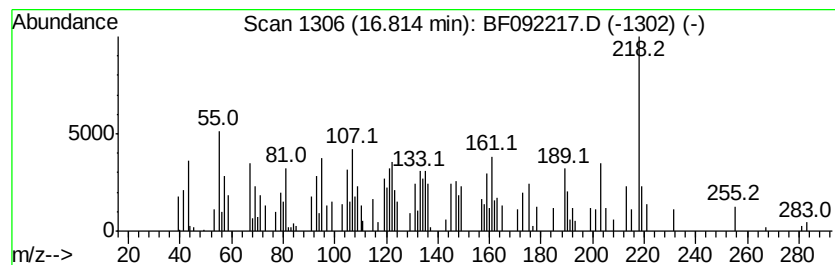
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 2H-Cyclopropa[a]naphthalen-... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.		
16.81	2.26 ng	108721	Perylene-d12	15.09		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2H-Cyclopropa[alnaphthalen-2-one...	218	C15H22O	006831-17-0	50
2		5(1H)-Azulenone, 2,4,6,7,8,8a-he...	218	C15H22O	006754-66-1	49
3		2-(3,4-Methylenedioxyphenyl)cycl...	218	C13H14O3	042866-86-4	43
4		8-Amino-2,6-dimethoxyepidine	218	C12H14N2O2	074509-65-2	43
5		Pyrrolo[2,3-b]indole, 1,2,3,3a,8...	218	C13H18N2O	046479-70-3	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011217\
Data File : BF092217.D
Acq On : 12 Jan 2017 19:42
Operator : UM/SJ
Sample : I1030-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
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-Pentene, 3,4-di...	3.99	4.6	ng	187074	1	6.60	816077	20.0
2-Pentanone, 4-hy...	4.72	68.8	ng	2806840	1	6.60	816077	20.0
unknown6.37	6.37	111.5	ng	4549420	1	6.60	816077	20.0
Eicosane	10.55	2.7	ng	192602	4	11.10	1408940	20.0
n-Hexadecanoic acid	11.66	5.6	ng	395836	4	11.10	1408940	20.0
1-Nonadecene	13.60	8.0	ng	388217	5	13.73	974297	20.0
Pentafluoropropio...	14.23	2.3	ng	113286	5	13.73	974297	20.0
9-Phenyl-5H-benzo...	16.55	2.0	ng	96907	6	15.09	964202	20.0
Germanicol	16.59	4.0	ng	191384	6	15.09	964202	20.0
2H-Cyclopropa[a]n...	16.81	2.3	ng	108721	6	15.09	964202	20.0