

Data Path : Z:\HPCHEM1\BNA F\DATA\BF120215\
 Data File : BF083421.D
 Acq On : 2 Dec 2015 16:43
 Operator : UM/IZ
 Sample : G4584-07
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-P3WC-14(8-15.5)

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-BF113015.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	4.613	254	256	258	rBV	112008	161681	2.68%	0.303%
2	4.659	258	260	275	rVB	888672	1679327	27.84%	3.144%
3	4.933	281	284	292	rVB	168471	246858	4.09%	0.462%
4	5.139	299	302	304	rBV	4086790	5551302	92.03%	10.393%
5	6.213	393	396	399	rBV	4830853	5552426	92.05%	10.395%
6	6.316	403	405	407	rBV	5682852	5561646	92.21%	10.412%
7	6.533	422	424	427	rBV	757738	986998	16.36%	1.848%
8	6.693	436	438	443	rBV2	3927476	4300589	71.30%	8.051%
9	6.807	445	448	453	rVB	72099	126964	2.10%	0.238%
10	7.116	472	475	477	rBV	3396713	3889020	64.48%	7.281%
11	7.265	484	488	494	rVB	167531	246272	4.08%	0.461%
12	7.607	517	518	526	rVB2	39957	71759	1.19%	0.134%
13	7.825	535	537	541	rBV	1454044	1471951	24.40%	2.756%
14	8.910	629	632	634	rBV	5793102	6031771	100.00%	11.292%
15	9.310	665	667	669	rBV	1109064	980475	16.26%	1.836%
16	9.528	684	686	688	rBV	77549	91358	1.51%	0.171%
17	9.573	688	690	692	rVV	1577582	1470073	24.37%	2.752%
18	9.996	721	727	728	rBV	51347	73089	1.21%	0.137%
19	10.030	728	730	732	rVB	179647	161594	2.68%	0.303%
20	10.248	746	749	752	rBV	62994	109351	1.81%	0.205%
21	10.362	756	759	762	rVB	3368128	3519059	58.34%	6.588%
22	10.511	769	772	778	rVB	163719	285928	4.74%	0.535%
23	11.002	813	815	816	rBV	96661	108090	1.79%	0.202%
24	11.105	822	824	827	rBV	1136330	1422940	23.59%	2.664%
25	11.505	857	859	862	rBV	53470	66093	1.10%	0.124%
26	11.699	872	876	880	rBV2	28705	85402	1.42%	0.160%
27	11.814	883	886	891	rBV2	276096	405177	6.72%	0.759%
28	12.156	913	916	920	rVB	31145	61470	1.02%	0.115%
29	12.454	939	942	944	rBV	56265	85361	1.42%	0.160%
30	12.888	977	980	982	rBV	70075	123746	2.05%	0.232%
31	12.934	982	984	987	rVV2	52524	96287	1.60%	0.180%
32	13.014	990	991	996	rVB2	45451	71283	1.18%	0.133%
33	13.208	1004	1008	1010	rBV	3860914	5660707	93.85%	10.598%
34	14.637	1130	1133	1138	rBV2	187966	330266	5.48%	0.618%

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SB-P3WC-14(8-15.5)

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-BF113015.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.728	1138	1141	1144	rVV	938835	1250183	20.73%	2.341%
36	16.214	1268	1271	1274	rVB	107709	151000	2.50%	0.283%
37	16.785	1318	1321	1327	rBV	620813	926917	15.37%	1.735%

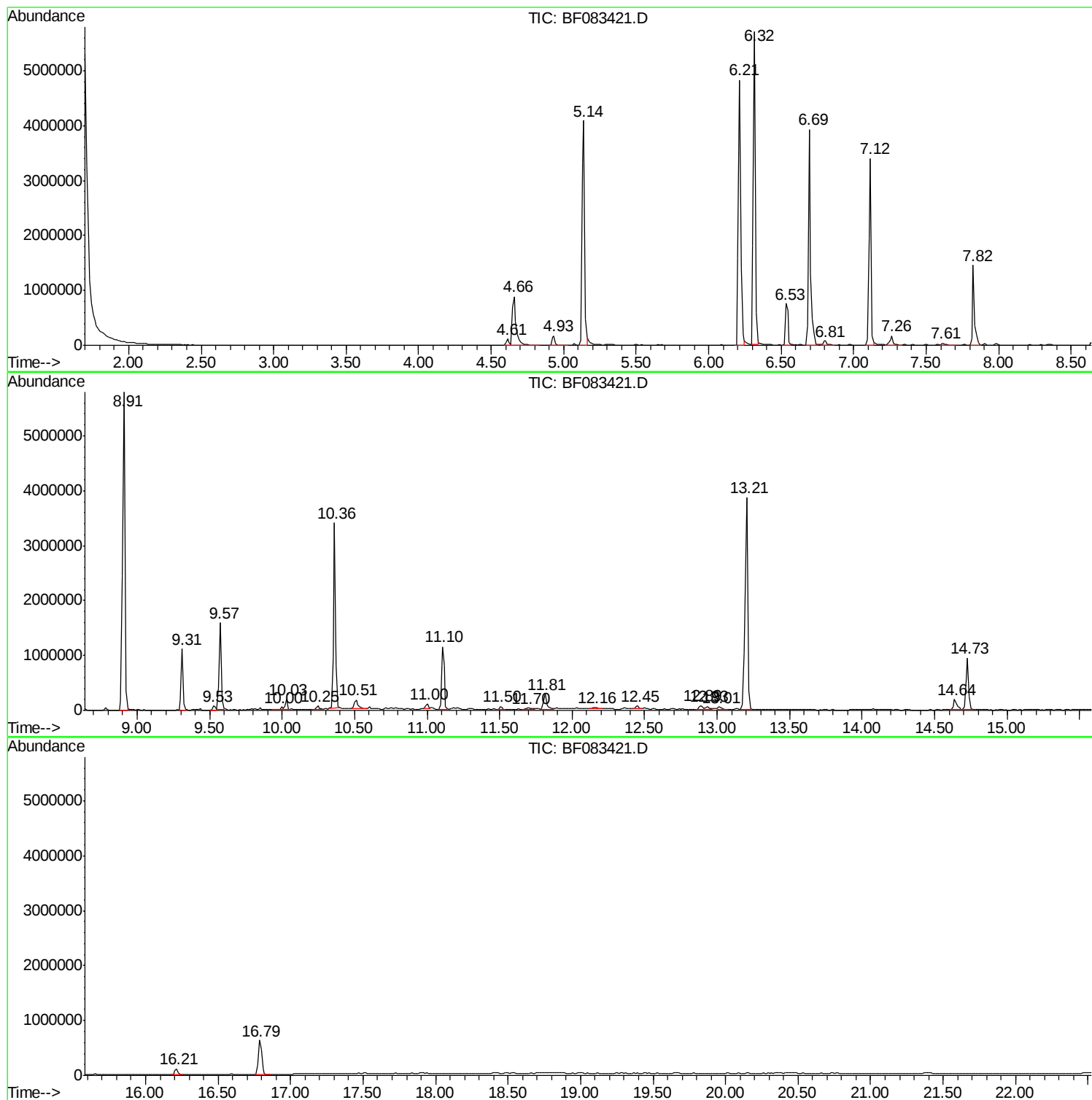
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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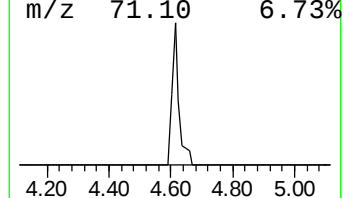
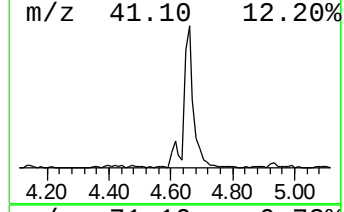
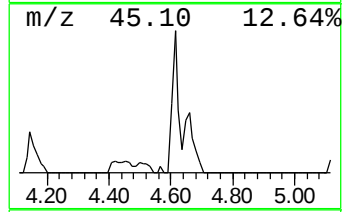
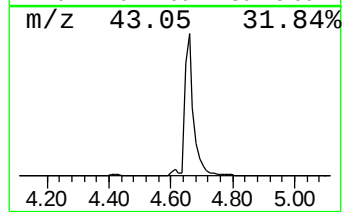
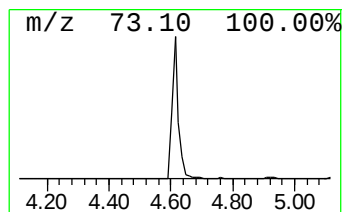
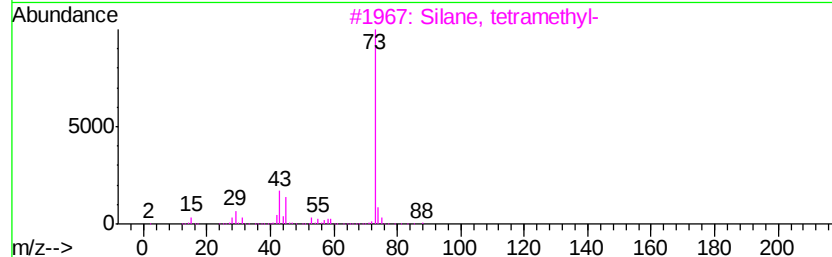
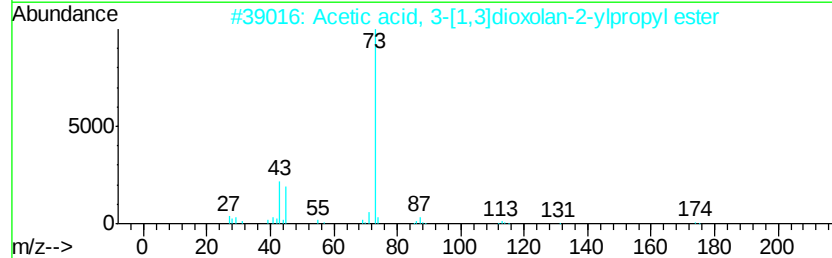
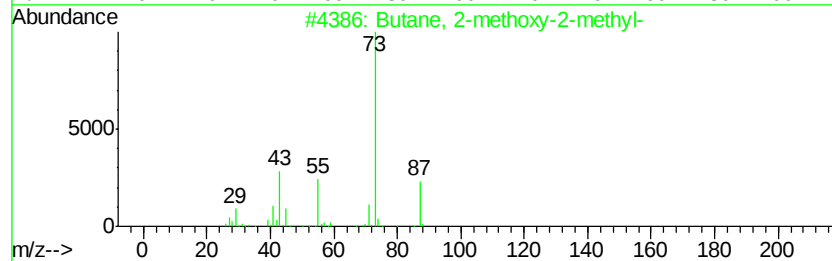
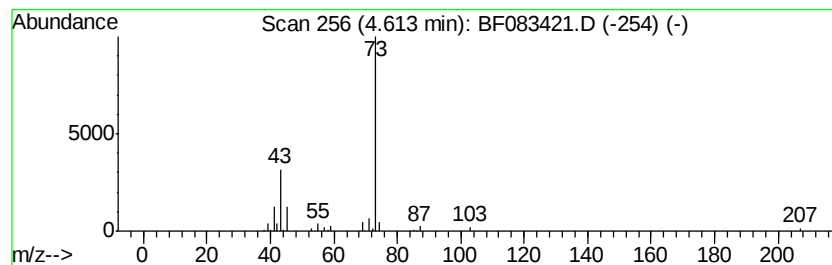
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown4.61 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.61	3.28 ng	161681	1,4-Dichlorobenzene-d4	6.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	42
2		Acetic acid, 3-[1,3]dioxolan-2-ylpropyl ester	174	C8H14O4	1000186-02-3	28
3		Silane, tetramethyl-	88	C4H12Si	000075-76-3	28
4		Methane, isothiocyanato-	73	C2H3NS	000556-61-6	9
5		2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9



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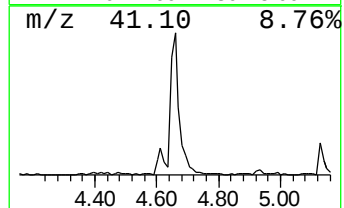
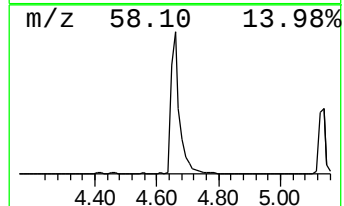
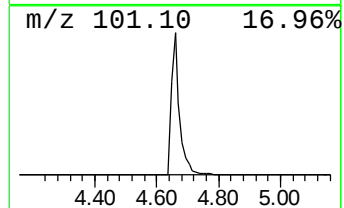
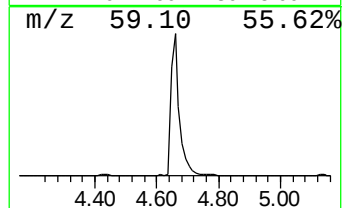
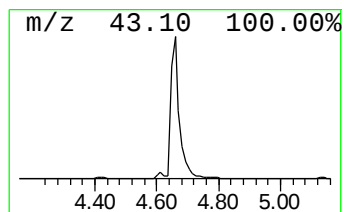
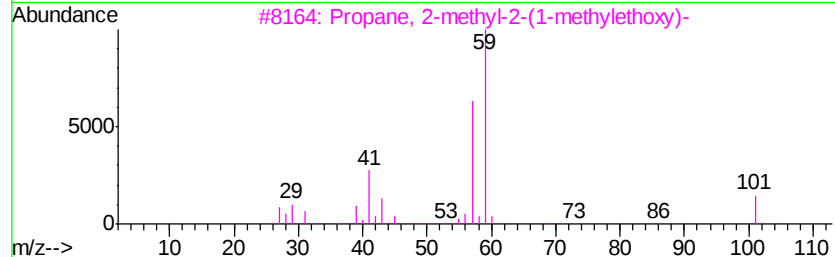
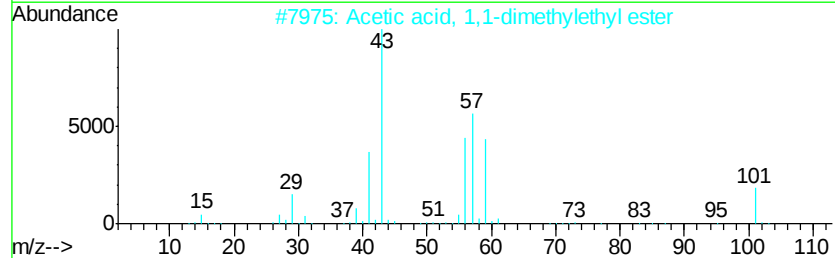
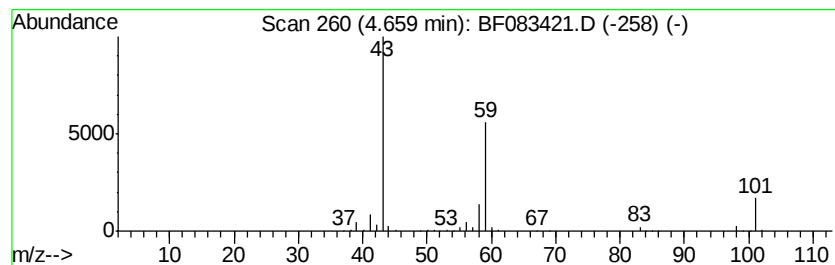
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.66	34.03 ng	1679330	1,4-Dichlorobenzene-d4	6.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
4		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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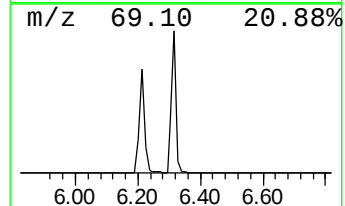
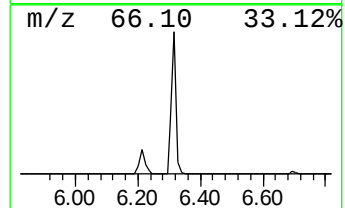
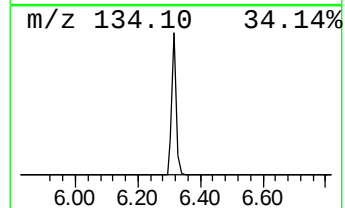
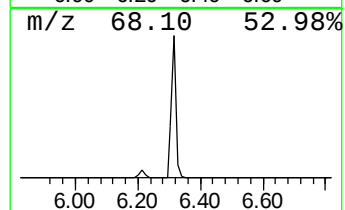
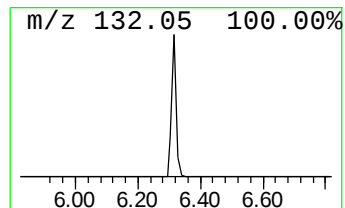
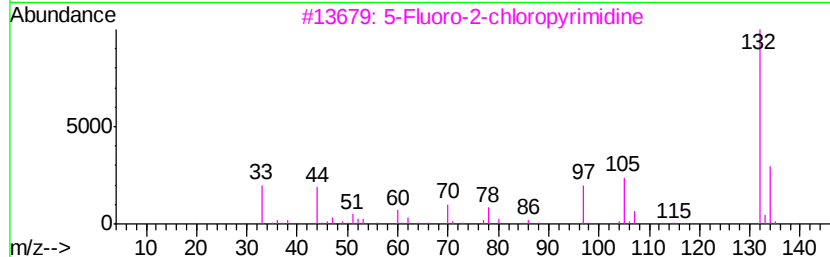
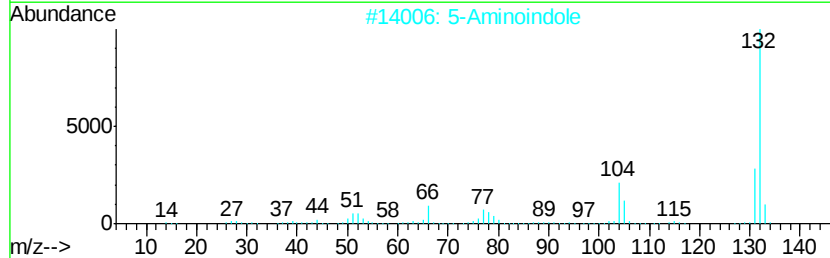
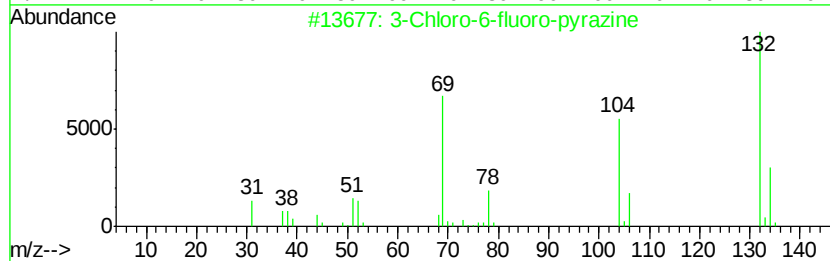
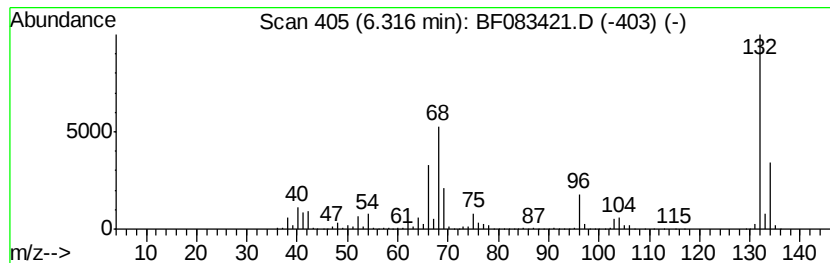
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown6.32 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.32	112.70 ng	5561650	1,4-Dichlorobenzene-d4	6.54

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	22
3	5	Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4	1H	Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	12
5	2	Cyclohexen-1-one	96	C6H8O	000930-68-7	10



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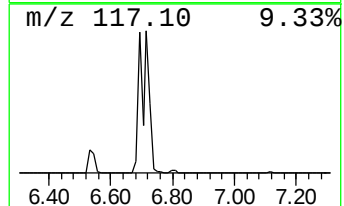
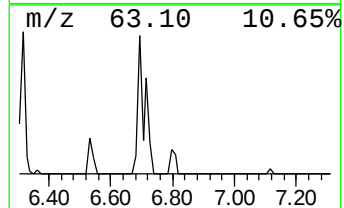
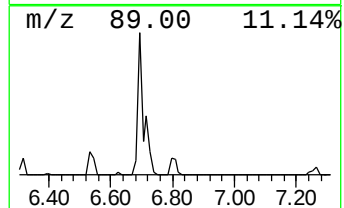
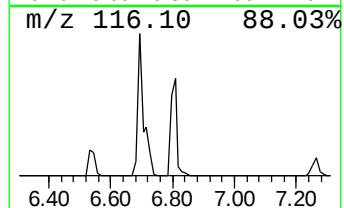
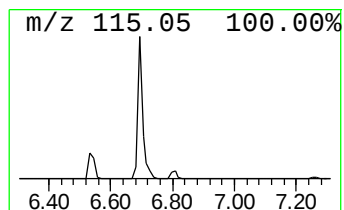
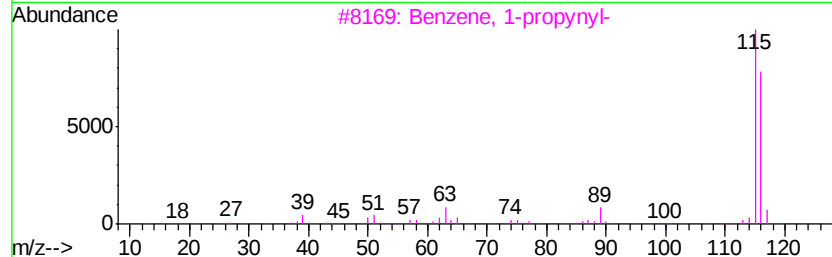
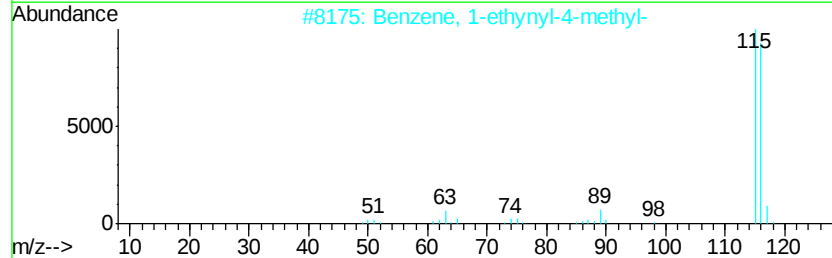
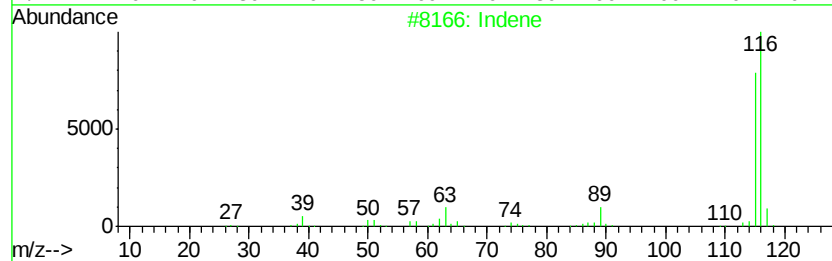
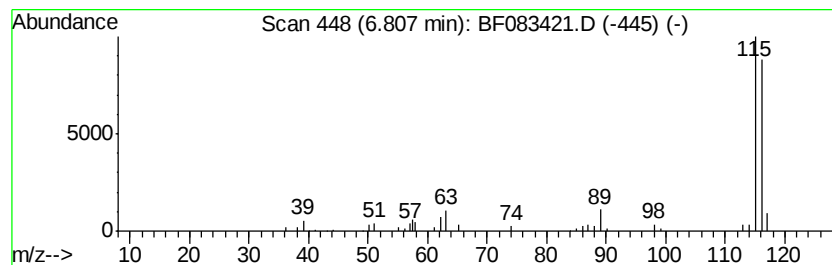
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 Indene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.81	2.57 ng	126964	1,4-Dichlorobenzene-d4	6.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Indene	116	C9H8	000095-13-6	94
2		Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	90
3		Benzene, 1-propynyl-	116	C9H8	000673-32-5	90
4		Benzene, 1-ethynyl-2-methyl-	116	C9H8	000766-47-2	90
5		Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	80



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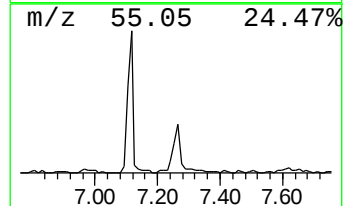
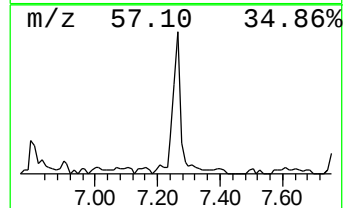
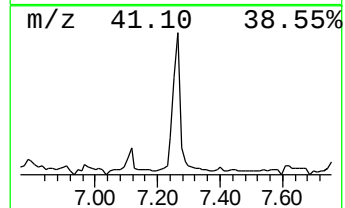
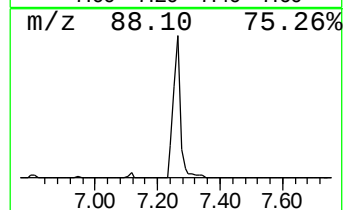
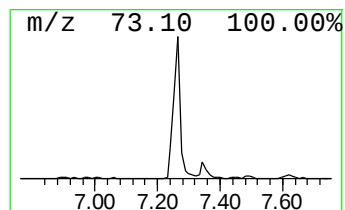
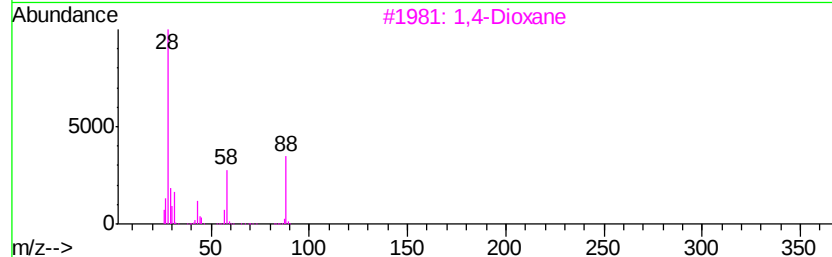
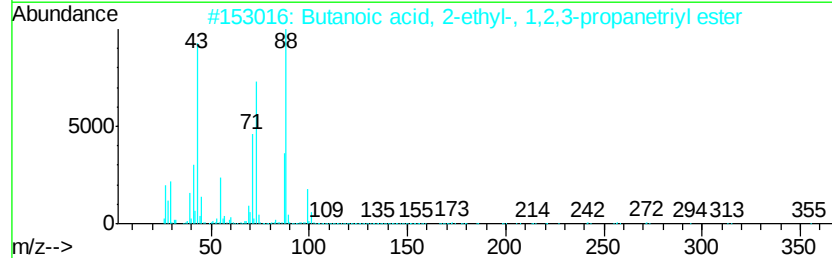
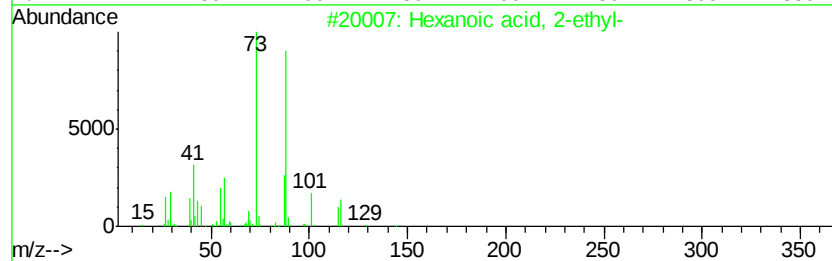
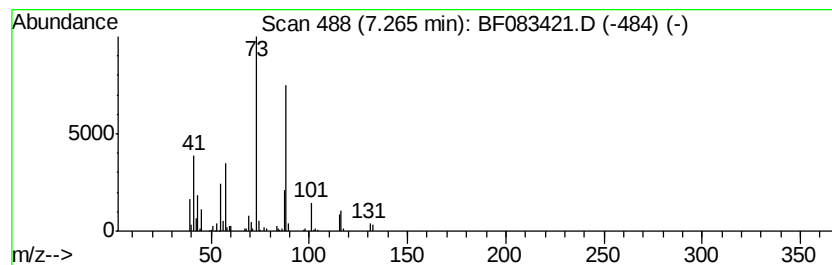
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Peak Number 7 Hexanoic acid, 2-ethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.26	3.35 ng	246272	Naphthalene-d8	7.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	86
2		Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	53
3		1,4-Dioxane	88	C4H8O2	000123-91-1	47
4		Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	45
5		Isoasparagine	132	C4H8N2O3	1000130-17-5	45



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Operator : UM/IZ
Sample : G4584-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

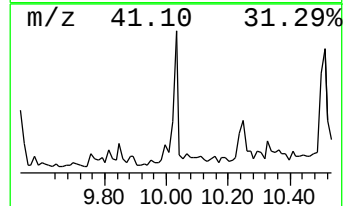
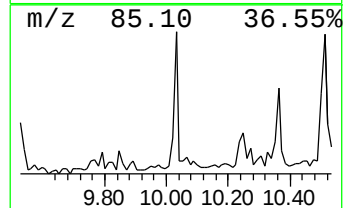
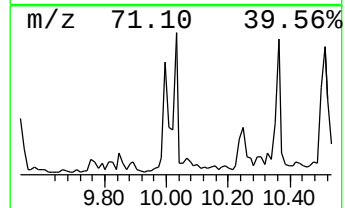
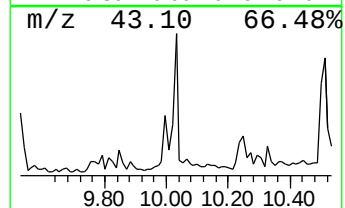
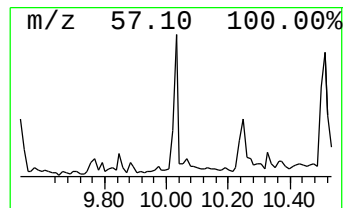
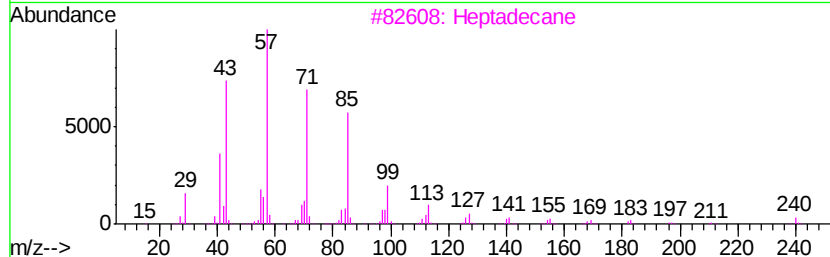
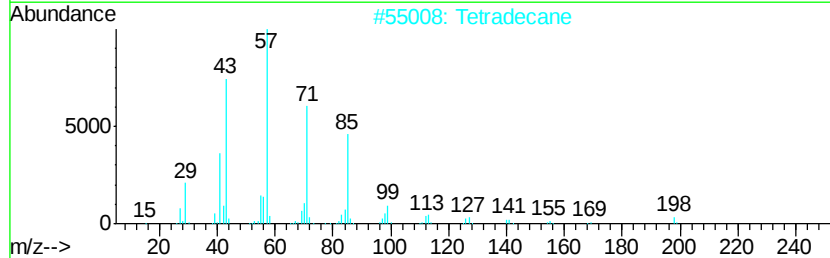
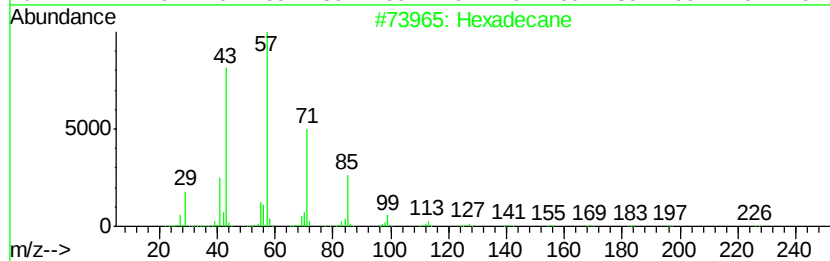
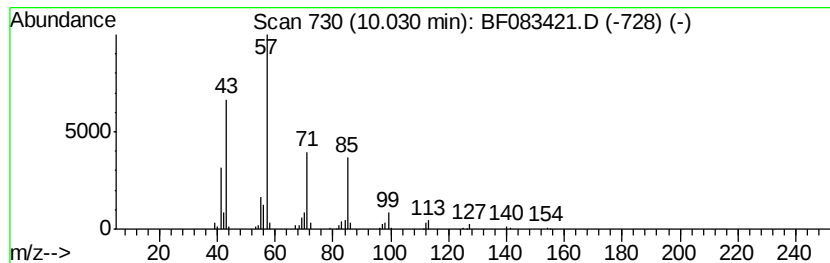
Instrument :
BNA_F
ClientSampleId :
SB-P3WC-14(8-15.5)

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF113015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.03	2.20 ng	161594	Acenaphthene-d10	9.57
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexadecane	226 C16H34	000544-76-3	90
2	Tetradecane	198 C14H30	000629-59-4	83
3	Heptadecane	240 C17H36	000629-78-7	78
4	Pentadecane	212 C15H32	000629-62-9	78
5	Silane, trichlorooctadecyl-	386 C18H37Cl3Si	000112-04-9	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120215\
Data File : BF083421.D
Acq On : 2 Dec 2015 16:43
Operator : UM/IZ
Sample : G4584-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-P3WC-14(8-15.5)

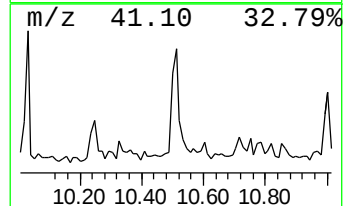
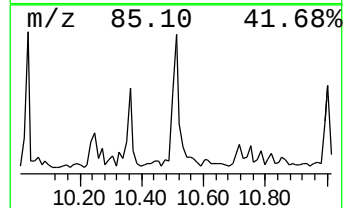
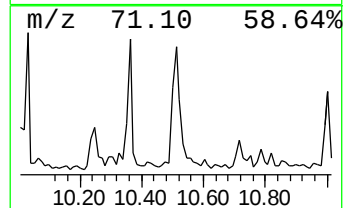
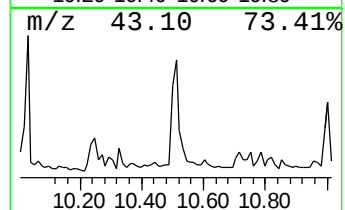
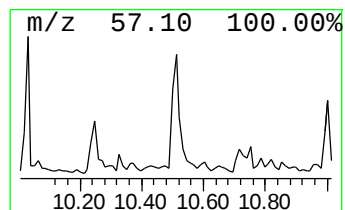
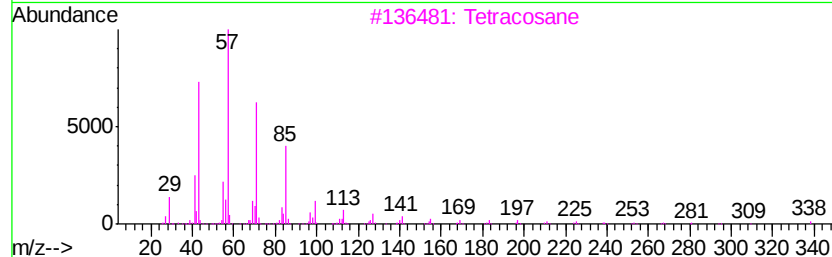
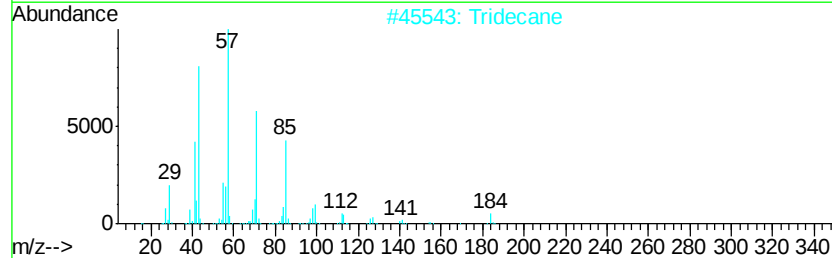
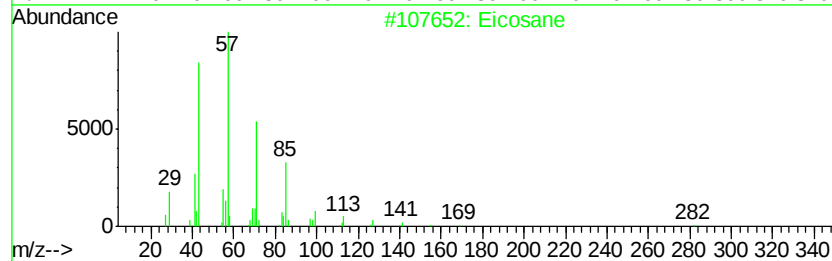
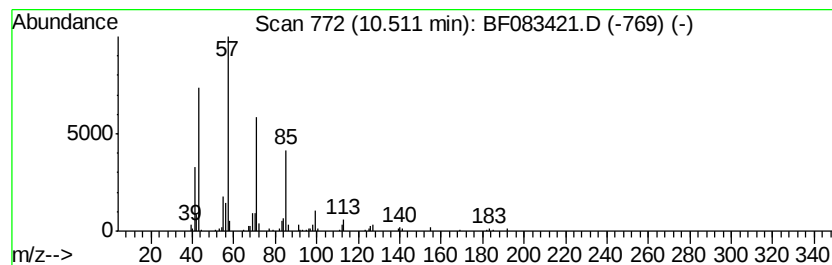
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.51	4.02 ng	285928	Phenanthrene-d10	11.10

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	91
2	Tridecane		184	C13H28	000629-50-5	86
3	Tetracosane		338	C24H50	000646-31-1	86
4	Dodecane, 1-iodo-		296	C12H25I	004292-19-7	86
5	Tetradecane		198	C14H30	000629-59-4	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120215\
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Acq On : 2 Dec 2015 16:43
Operator : UM/IZ
Sample : G4584-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

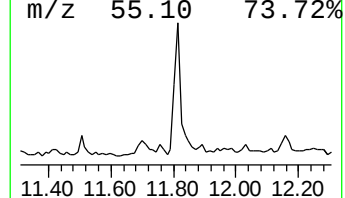
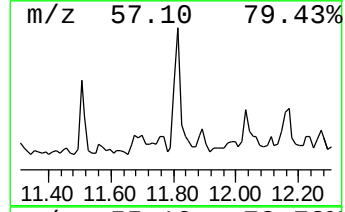
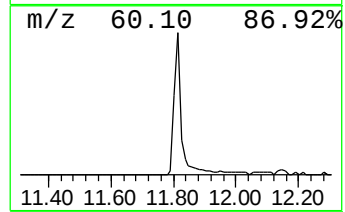
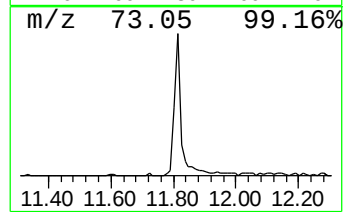
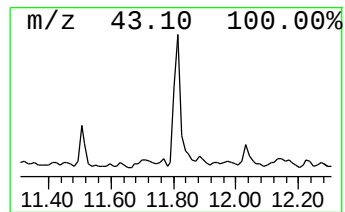
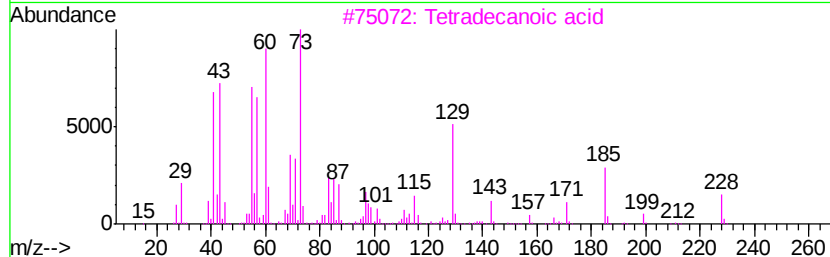
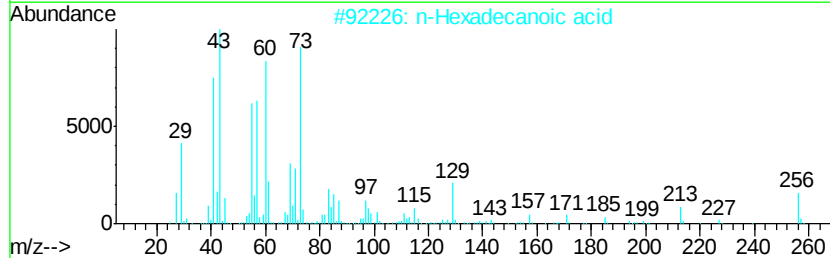
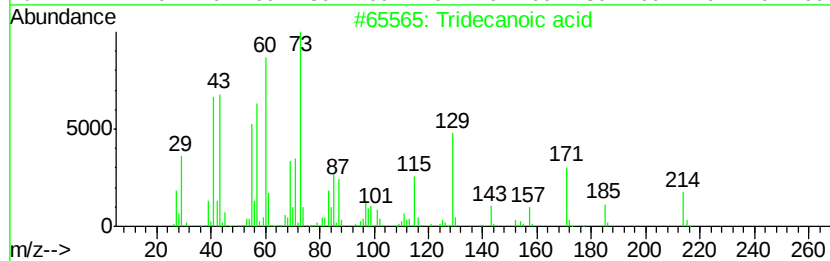
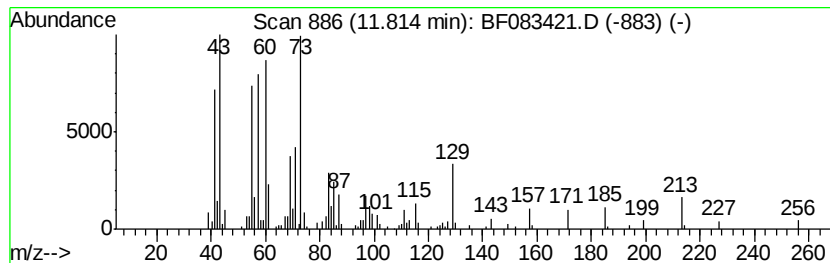
Instrument :
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ClientSampleId :
SB-P3WC-14(8-15.5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Tridecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.81	5.69 ng	405177	Phenanthrene-d10	11.10	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	95
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
5	Ethanol, 2-(dodecyloxy)-	230	C14H30O2	004536-30-5	11



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120215\
Data File : BF083421.D
Acq On : 2 Dec 2015 16:43
Operator : UM/IZ
Sample : G4584-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-P3WC-14(8-15.5)

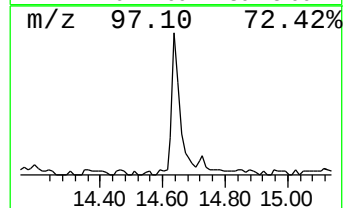
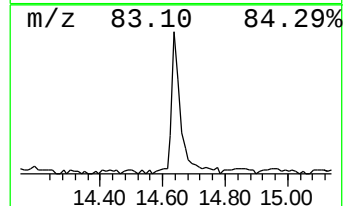
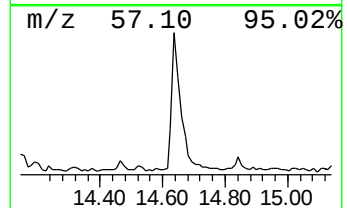
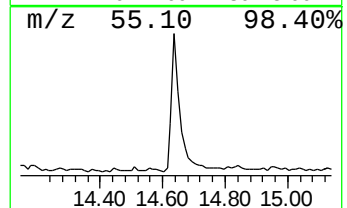
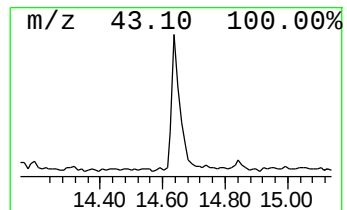
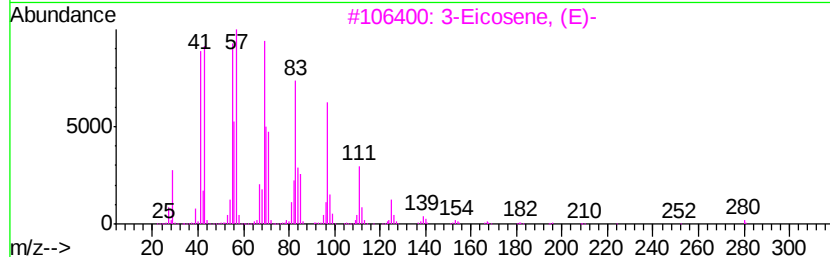
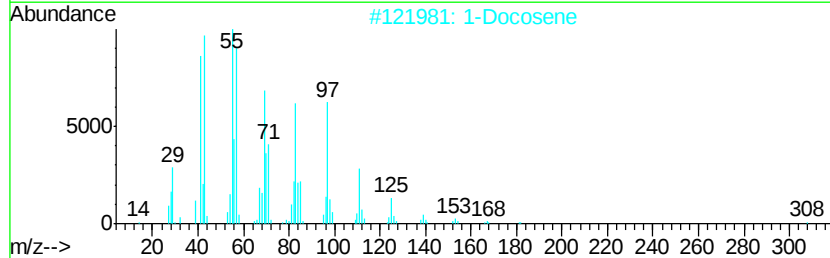
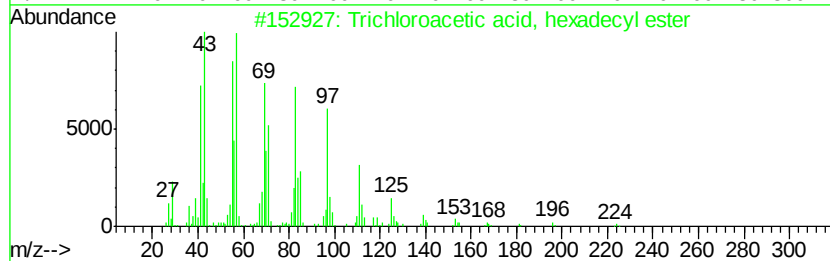
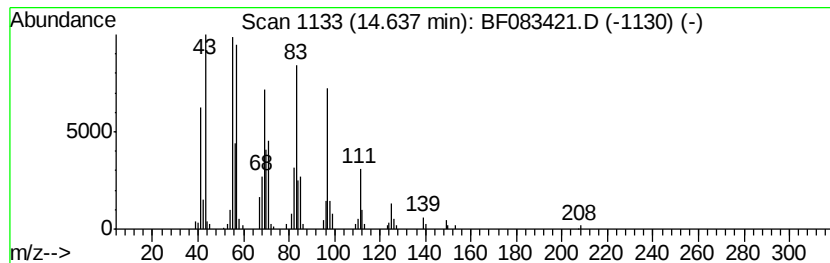
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Trichloroacetic acid, hexad... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	5.28 ng	330266	Chrysene-d12	14.73

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2			1-Docosene	308	C22H44	001599-67-3	94
3			3-Eicosene, (E)-	280	C20H40	074685-33-9	91
4			1-Nonadecene	266	C19H38	018435-45-5	91
5			9-Eicosene, (E)-	280	C20H40	074685-29-3	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120215\
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Acq On : 2 Dec 2015 16:43
Operator : UM/IZ
Sample : G4584-07
Misc :
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Instrument :
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ClientSampleId :
SB-P3WC-14(8-15.5)

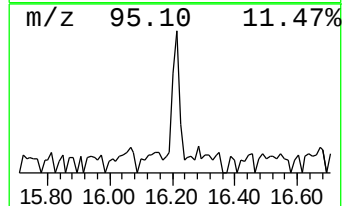
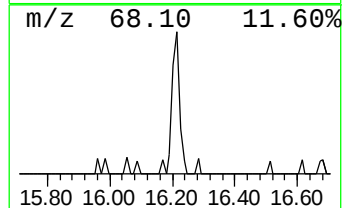
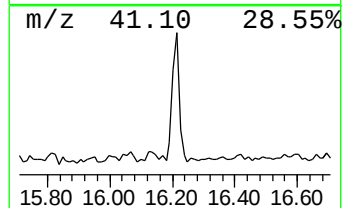
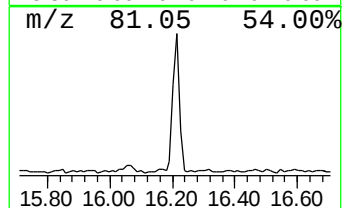
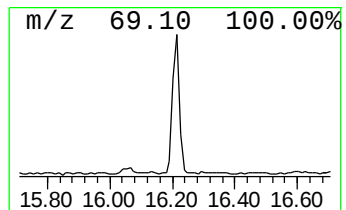
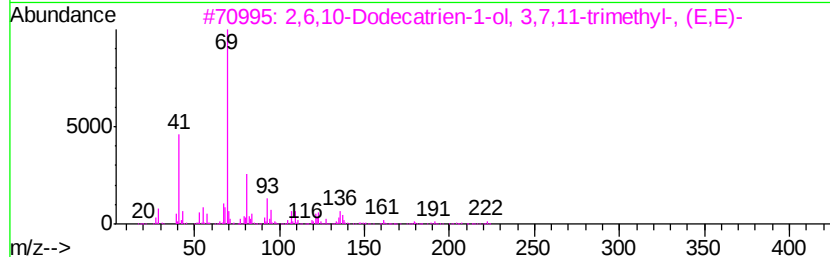
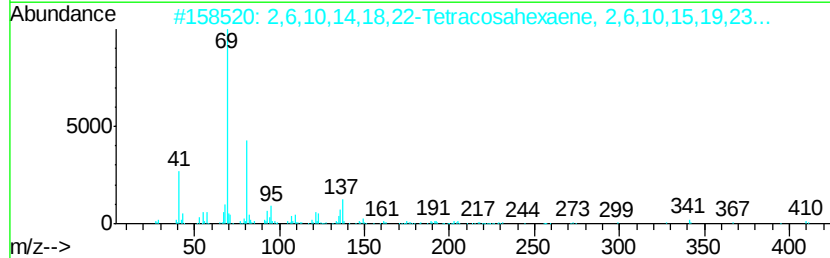
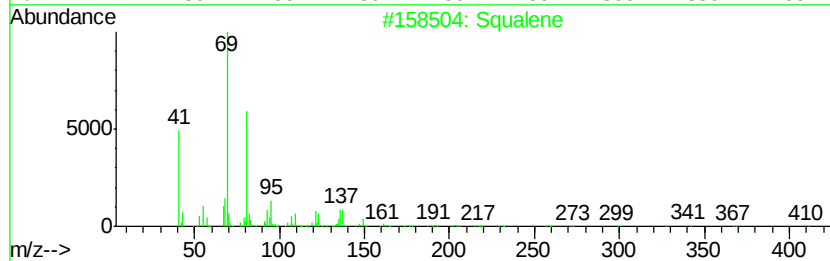
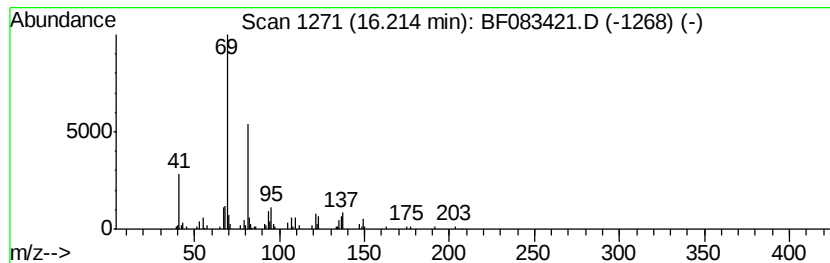
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Squalene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.21	3.26 ng	151000	Perylene-d12	16.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	007683-64-9	91
2		2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	90
3		2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	000106-28-5	78
4		4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72
5		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120215\
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Sample : G4584-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-P3WC-14(8-15.5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113015.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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2-Pentanone, 4-hy...	4.66	34.0	ng	1679330	1	6.54	986998	20.0
unknown6.32	6.32	112.7	ng	5561650	1	6.54	986998	20.0
Indene	6.81	2.6	ng	126964	1	6.54	986998	20.0
Hexanoic acid, 2-...	7.26	3.4	ng	246272	2	7.82	1471950	20.0
Hexadecane	10.03	2.2	ng	161594	3	9.57	1470070	20.0
Eicosane	10.51	4.0	ng	285928	4	11.10	1422940	20.0
Tridecanoic acid	11.81	5.7	ng	405177	4	11.10	1422940	20.0
Trichloroacetic a...	14.64	5.3	ng	330266	5	14.73	1250180	20.0
Squalene	16.21	3.3	ng	151000	6	16.79	926917	20.0