

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050417\
 Data File : BF094887.D
 Acq On : 4 May 2017 22:15
 Operator : SJ/MA
 Sample : I2916-03
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-04-COMP(0-7.5)

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-BF050217.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	5.019	520	524	542	rBV	243411	470782	20.90%	2.272%
2	5.666	629	634	654	rBV	1334219	1971098	87.50%	9.513%
3	6.242	727	732	739	rVB2	16545	26243	1.16%	0.127%
4	7.260	900	905	921	rBV	1465503	2072773	92.01%	10.003%
5	7.384	921	926	936	rVB	1678838	2252787	100.00%	10.872%
6	7.719	979	983	993	rVB	396917	449272	19.94%	2.168%
7	7.960	1018	1024	1031	rBV	1308847	1778138	78.93%	8.581%
8	8.436	1101	1105	1111	rVB	21931	23973	1.06%	0.116%
9	8.619	1130	1136	1155	rBV	1057835	1344594	59.69%	6.489%
10	9.742	1322	1327	1344	rBV	472691	614628	27.28%	2.966%
11	11.513	1623	1628	1643	rBV	1704844	2037499	90.44%	9.833%
12	12.207	1741	1746	1753	rBV	141219	178005	7.90%	0.859%
13	12.571	1803	1808	1819	rBV2	519078	717829	31.86%	3.464%
14	13.865	2022	2028	2041	rBV	998906	1390038	61.70%	6.708%
15	14.189	2079	2083	2085	rBV	26735	32900	1.46%	0.159%
16	14.918	2203	2207	2211	rVB2	22437	25665	1.14%	0.124%
17	14.965	2211	2215	2227	rVB2	592860	792220	35.17%	3.823%
18	15.183	2248	2252	2263	rBV4	55256	108728	4.83%	0.525%
19	15.659	2323	2333	2345	rBV4	74525	192662	8.55%	0.930%
20	15.812	2354	2359	2367	rVB3	29658	42039	1.87%	0.203%
21	15.936	2375	2380	2392	rBV2	138324	179112	7.95%	0.864%
22	17.024	2561	2565	2568	rBV4	23899	28994	1.29%	0.140%
23	17.295	2605	2611	2620	rBV	1531183	1786798	79.31%	8.623%
24	18.542	2818	2823	2834	rBV	143802	296717	13.17%	1.432%
25	18.636	2834	2839	2847	rVV	577102	729985	32.40%	3.523%
26	18.700	2847	2850	2855	rVB2	22412	28107	1.25%	0.136%
27	19.342	2954	2959	2971	rBV3	99788	212120	9.42%	1.024%
28	19.771	3029	3032	3040	rVB	58675	62265	2.76%	0.300%
29	20.053	3076	3080	3083	rBV	68413	76269	3.39%	0.368%
30	20.089	3083	3086	3090	rVV4	28079	41621	1.85%	0.201%
31	20.294	3117	3121	3130	rBV	434061	550363	24.43%	2.656%
32	20.400	3136	3139	3143	rVB4	26403	28864	1.28%	0.139%
33	20.777	3199	3203	3207	rBV	46985	59345	2.63%	0.286%
34	22.106	3424	3429	3436	rVB8	25080	49159	2.18%	0.237%

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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-04-COMP(0-7.5)

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

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35	22.500	3491	3496	3503	rVB8	17611	34278	1.52%	0.165%
36	23.753	3702	3709	3716	rVB9	13828	34811	1.55%	0.168%

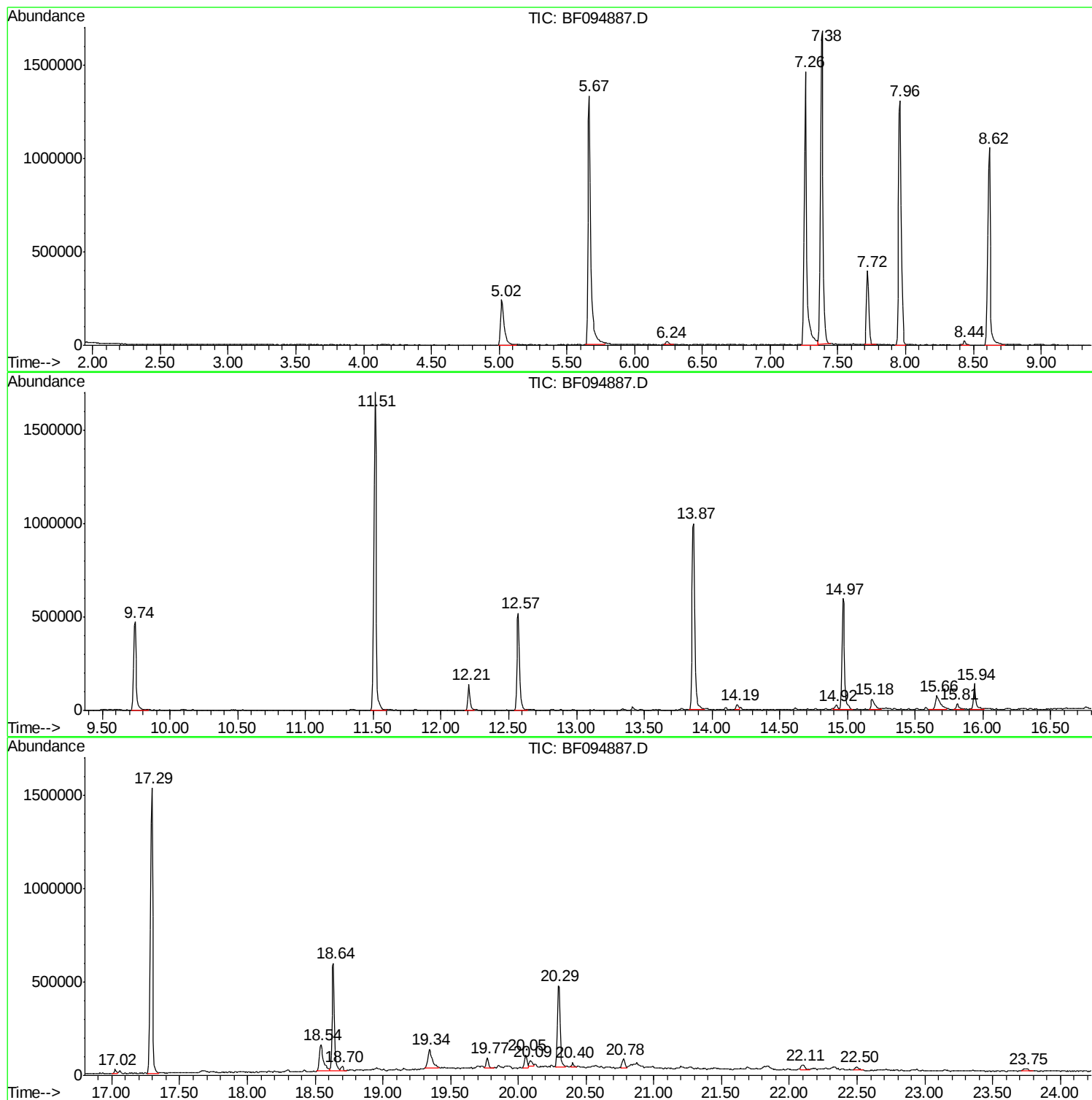
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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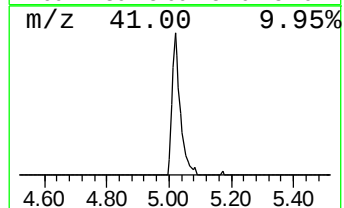
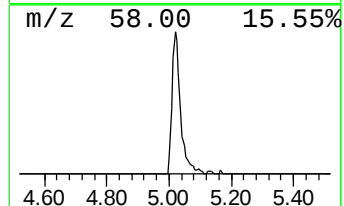
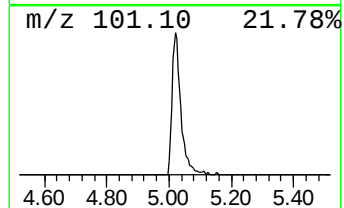
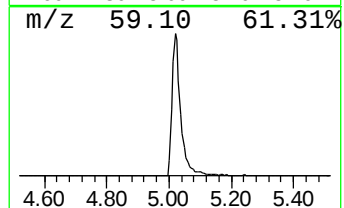
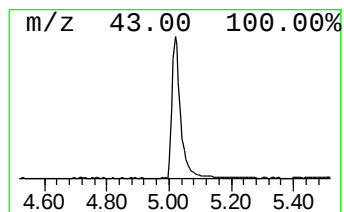
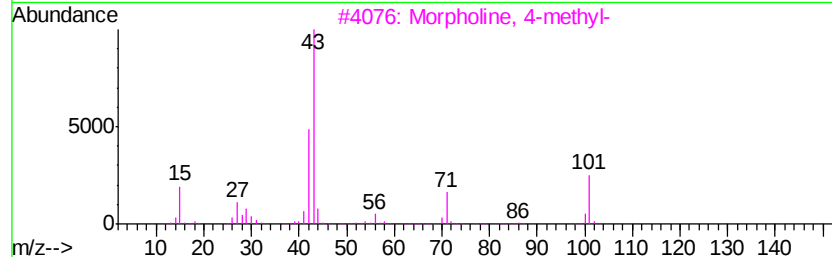
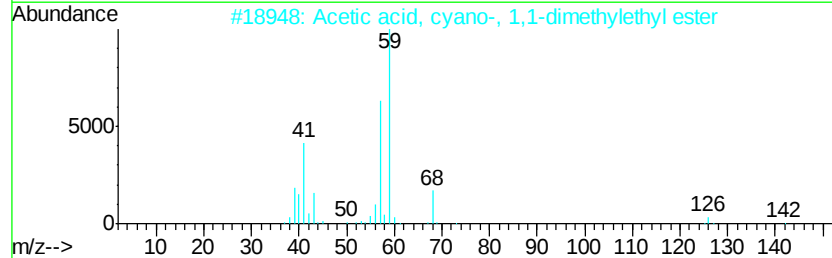
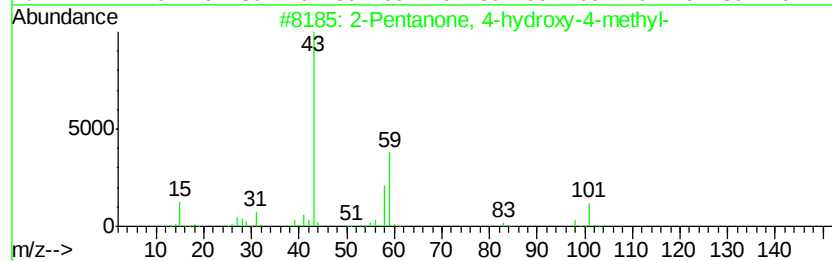
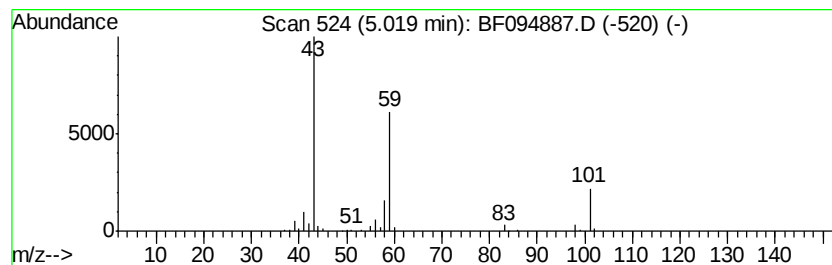
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	20.96 ng	470782	1,4-Dichlorobenzene-d4	7.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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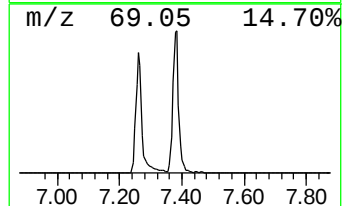
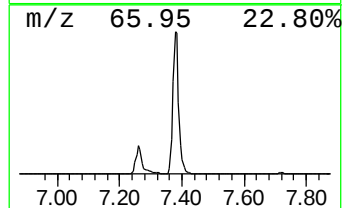
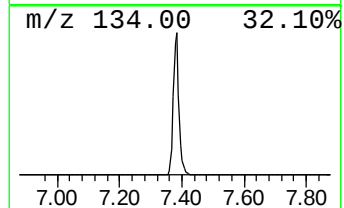
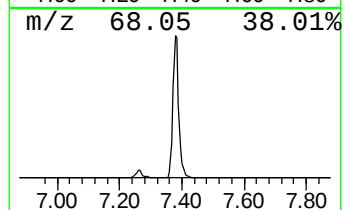
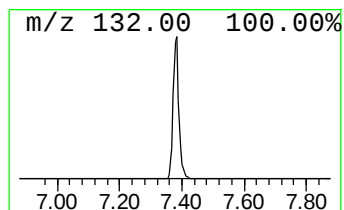
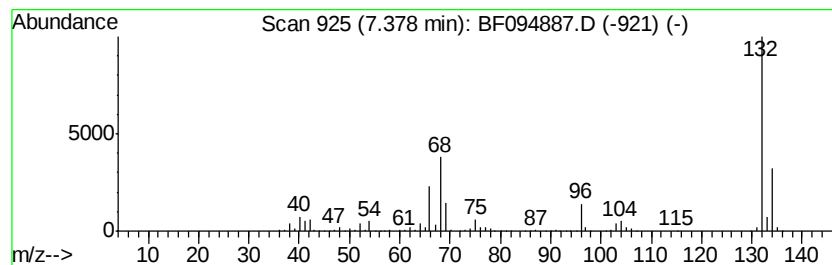
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown7.38 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.38	100.29 ng	2252790	1,4-Dichlorobenzene-d4	7.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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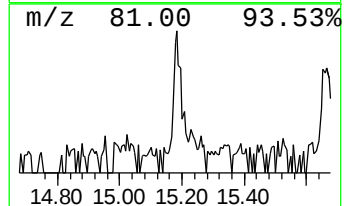
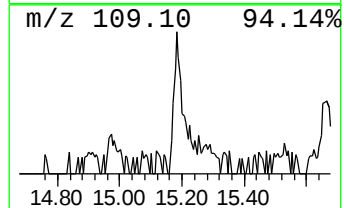
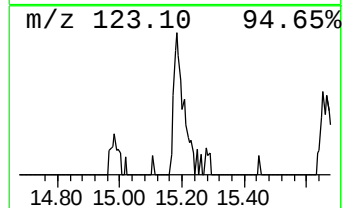
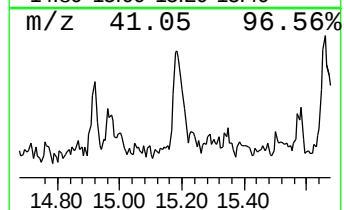
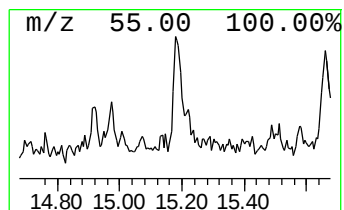
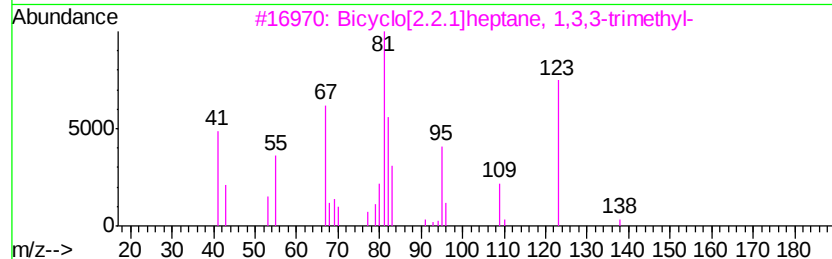
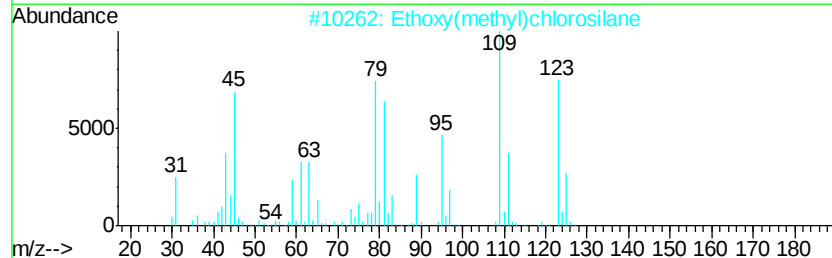
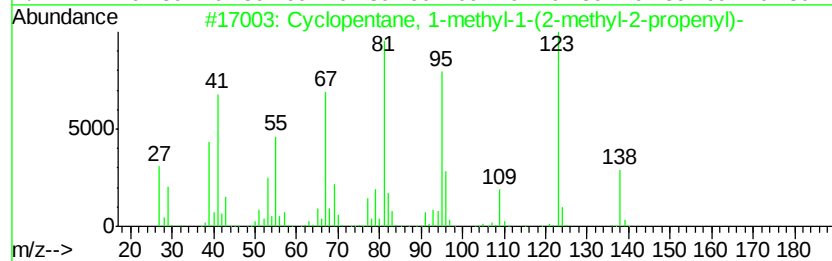
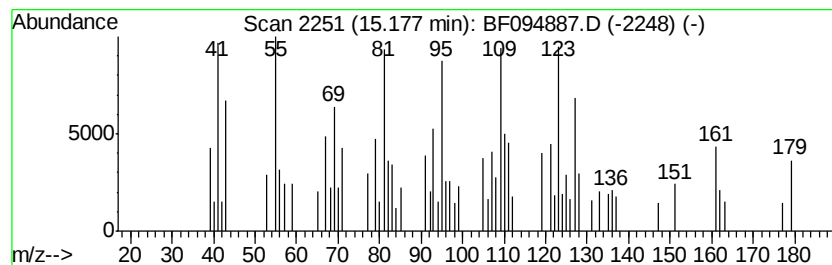
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown15.18 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.18	2.74 ng	108728	Phenanthrene-d10	14.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentane, 1-methyl-1-(2-meth...	138	C10H18	074764-47-9	35
2		Ethoxy(methyl)chlorosilane	124	C3H9ClOSi	018191-33-8	27
3		Bicyclo[2.2.1]heptane, 1,3,3-tri...	138	C10H18	006248-88-0	27
4		6-Methyl-3,5-heptadiene-2-one	124	C8H12O	001604-28-0	22
5		[2-(1-butenyl)-2,2-dimethylcyclo...	163	C11H17N	1000111-15-4	22



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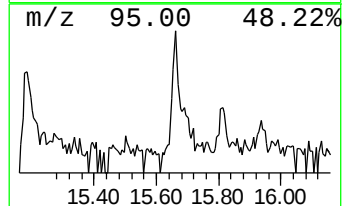
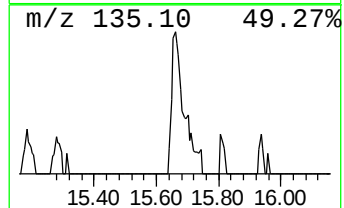
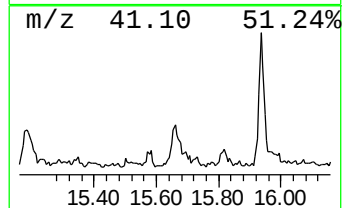
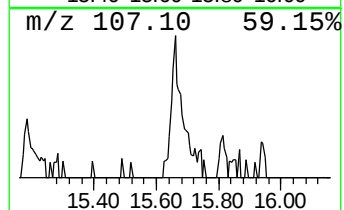
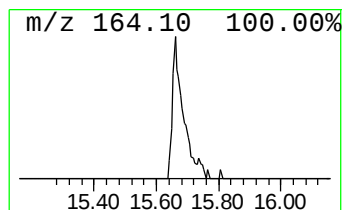
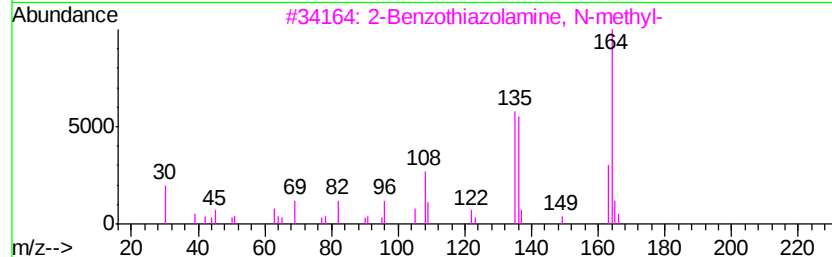
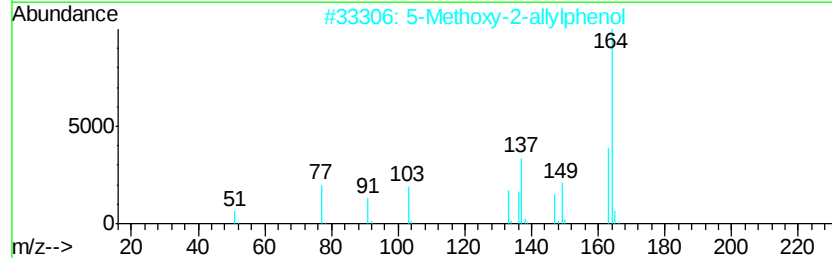
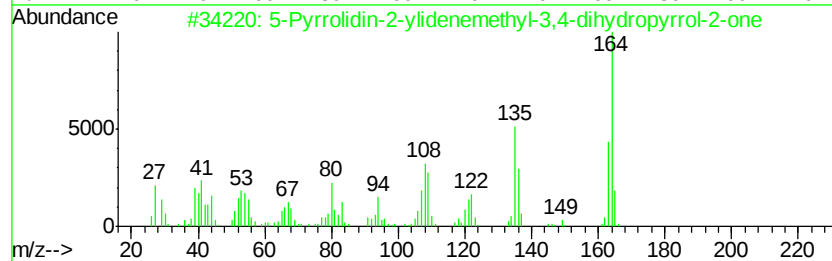
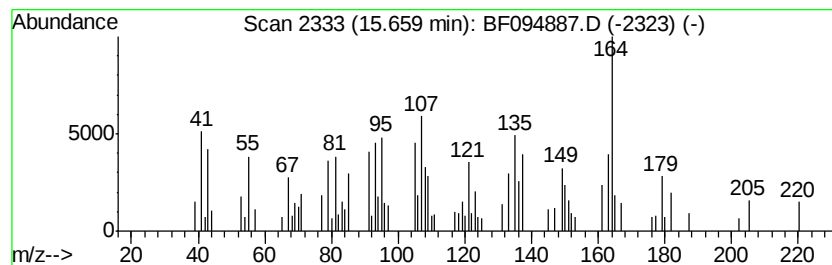
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown15.66 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.66	4.86 ng	192662	Phenanthrene-d10	14.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Pyrrolidin-2-ylidenemethyl-3,4...	164	C9H12N2O	1000192-09-5	46
2		5-Methoxy-2-allylphenol	164	C10H12O2	1000306-52-6	38
3		2-Benzothiazolamine, N-methyl-	164	C8H8N2S	016954-69-1	30
4		1-Benzothiepin, 2,3,4,5-tetrahydro-	164	C10H12S	004370-78-9	25
5		2-Benzothiazolamine, 4-methyl-	164	C8H8N2S	001477-42-5	25



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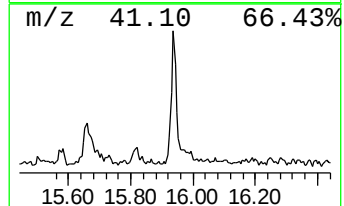
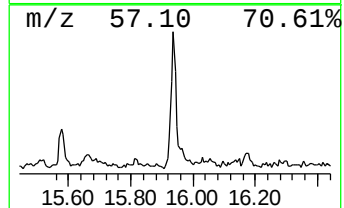
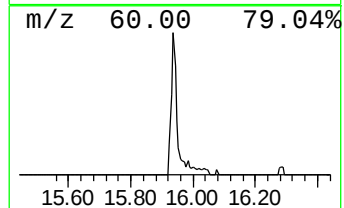
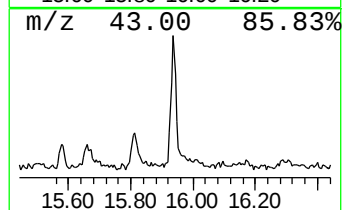
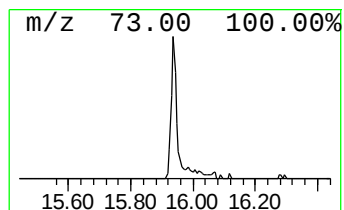
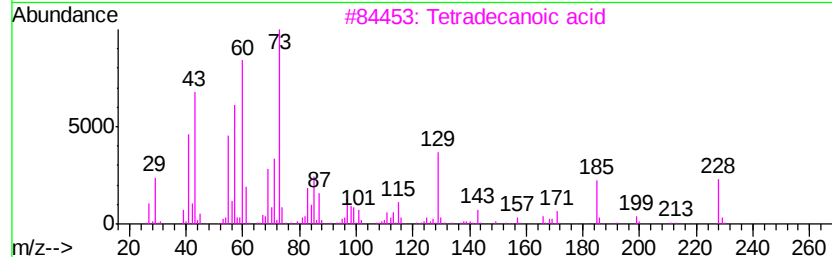
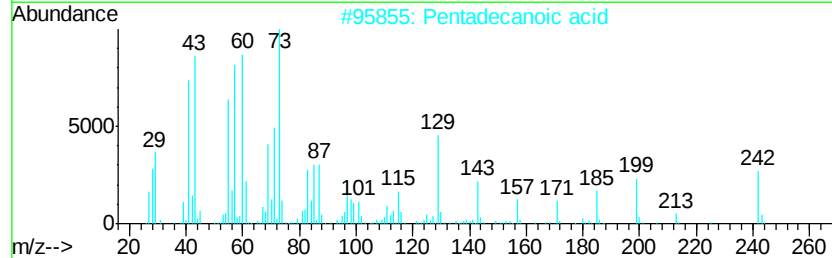
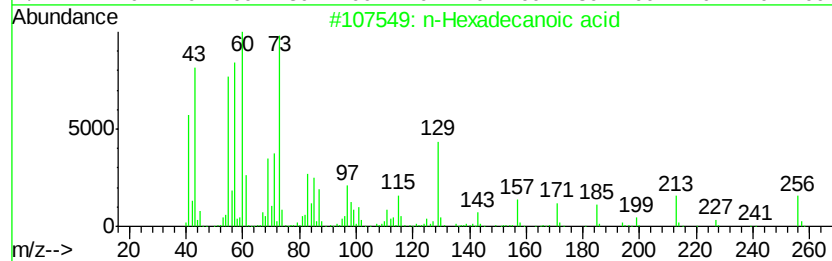
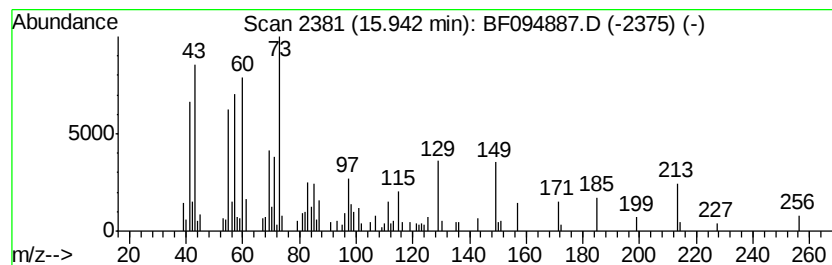
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Peak Number 6 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.94	4.52 ng	179112	Phenanthrene-d10	14.97

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	87
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4		Tridecanoic acid	214	C13H26O2	000638-53-9	81
5		Ethanol, 2-(hexadecyloxy)-	286	C18H38O2	002136-71-2	18



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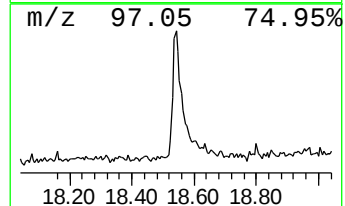
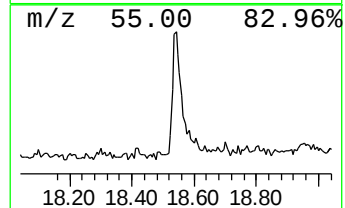
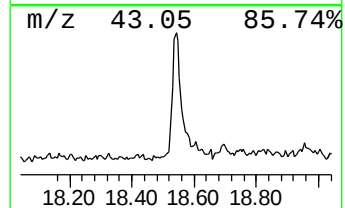
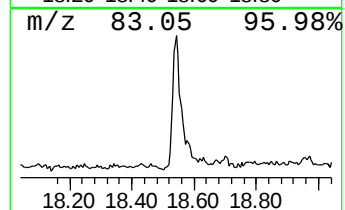
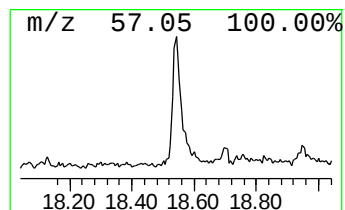
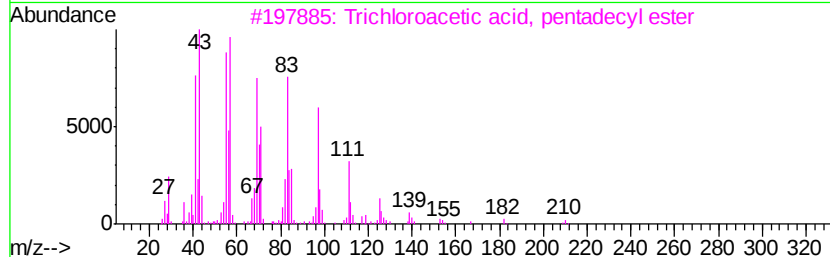
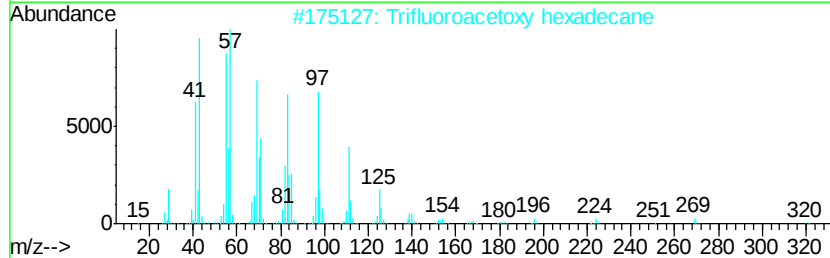
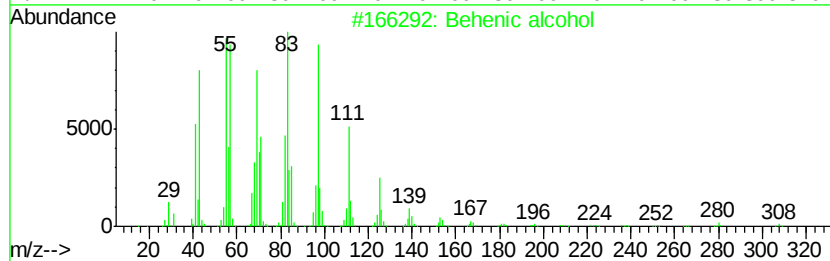
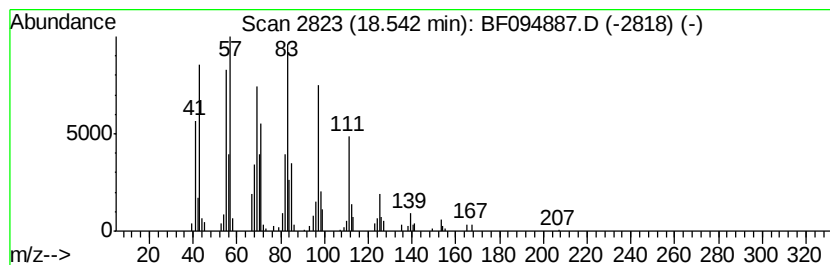
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Behenic alcohol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.54	8.13 ng	296717	Chrysene-d12	18.64

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Behenic alcohol	326	C22H46O	000661-19-8	95
2		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
3		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
4		3-Eicosene, (E)-	280	C20H40	074685-33-9	91
5		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050417\
Data File : BF094887.D
Acq On : 4 May 2017 22:15
Operator : SJ/MA
Sample : I2916-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-04-COMP(0-7.5)

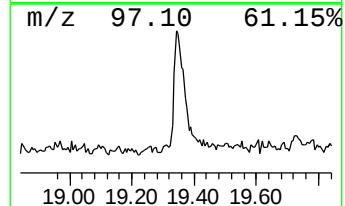
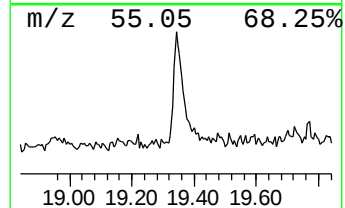
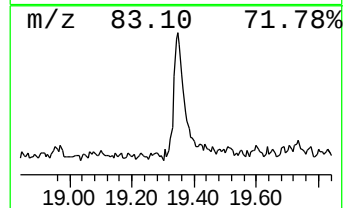
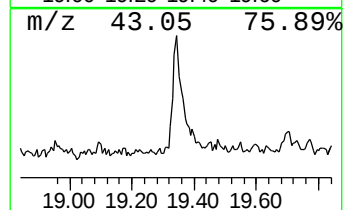
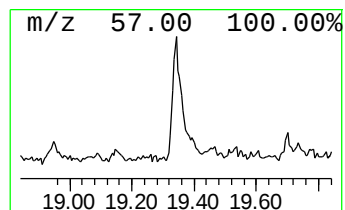
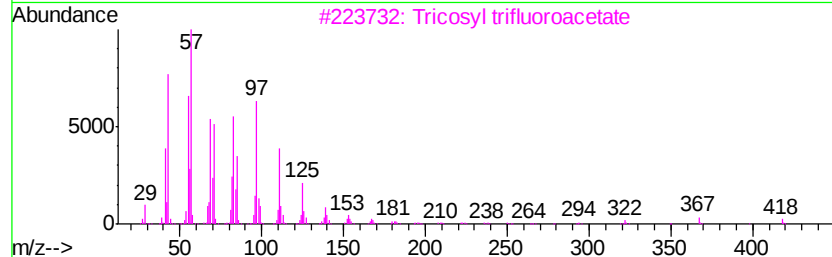
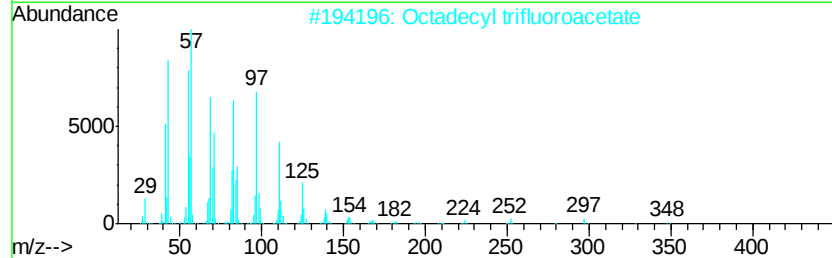
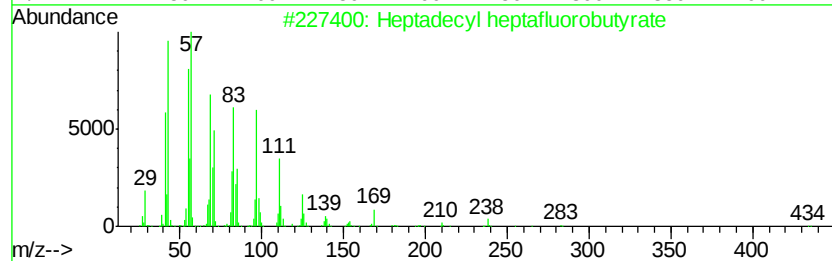
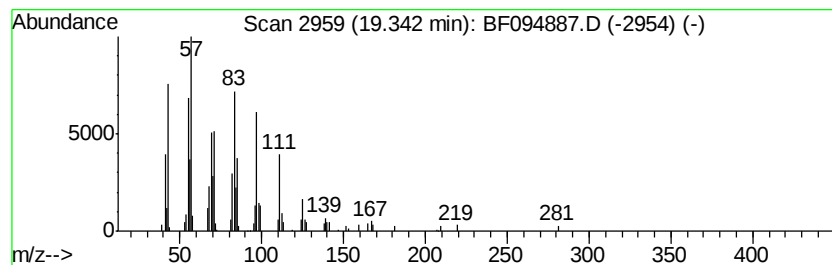
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Heptadecyl heptafluorobutyrate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.34	5.81 ng	212120	Chrysene-d12	18.64

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	95
2		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	94
3		Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	94
4		Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	94
5		Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050417\
Data File : BF094887.D
Acq On : 4 May 2017 22:15
Operator : SJ/MA
Sample : I2916-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-04-COMP(0-7.5)

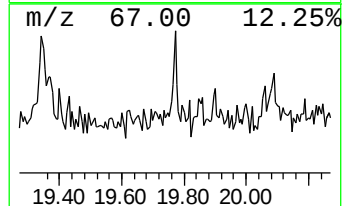
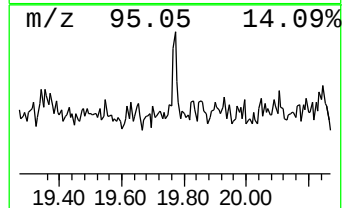
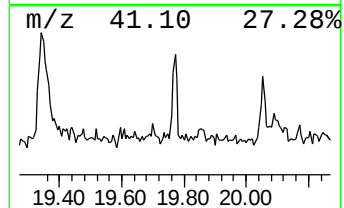
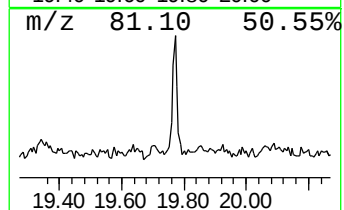
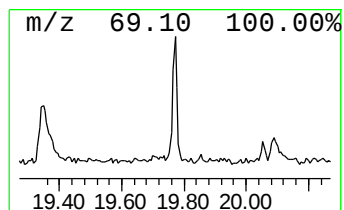
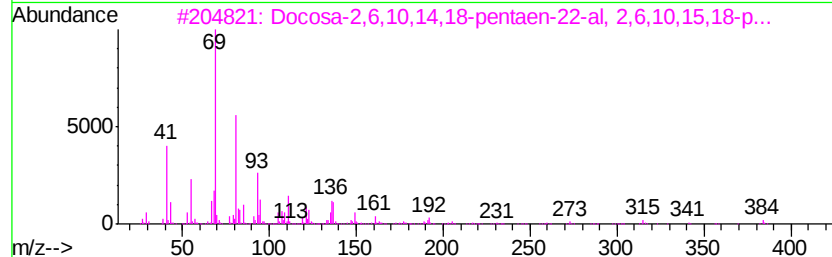
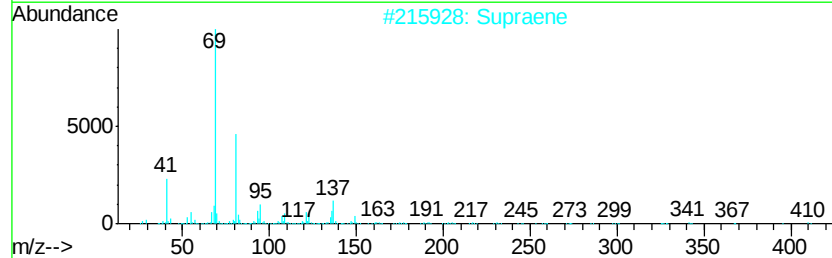
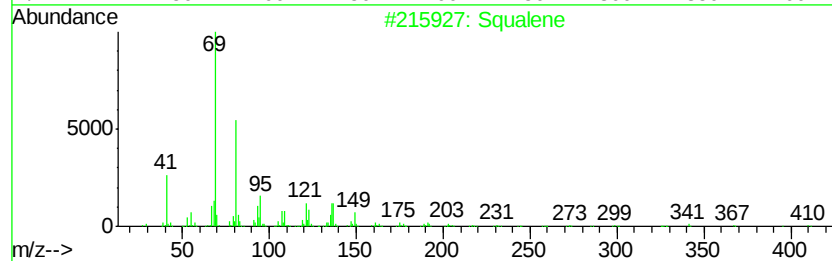
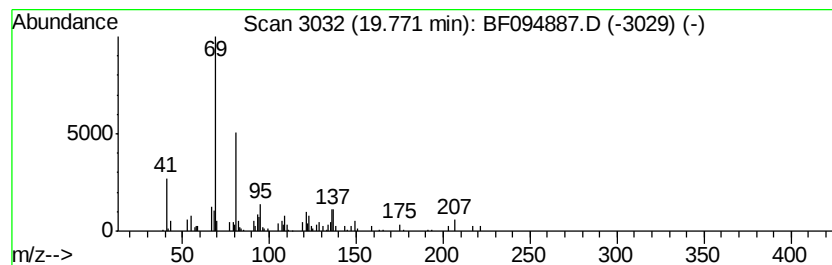
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Squalene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.77	2.26 ng	62265	Perylene-d12	20.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	87
2		Supraene	410	C30H50	007683-64-9	86
3		Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	78
4		3,7,11-Tridecatrienitrile, 4,8...	231	C16H25N	006006-01-5	64
5		Hexadeca-2,6,10,14-tetraen-1-ol,...	290	C20H34O	007614-21-3	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050417\
Data File : BF094887.D
Acq On : 4 May 2017 22:15
Operator : SJ/MA
Sample : I2916-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-04-COMP(0-7.5)

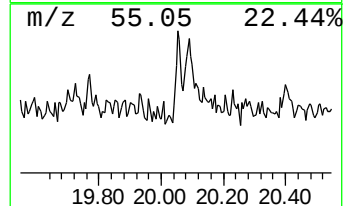
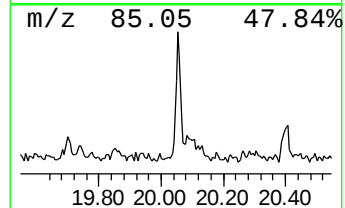
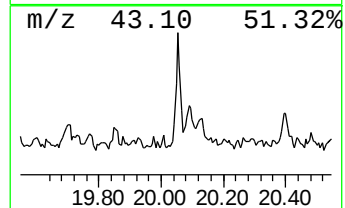
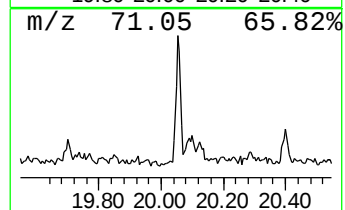
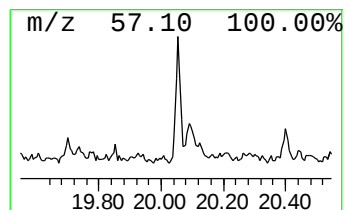
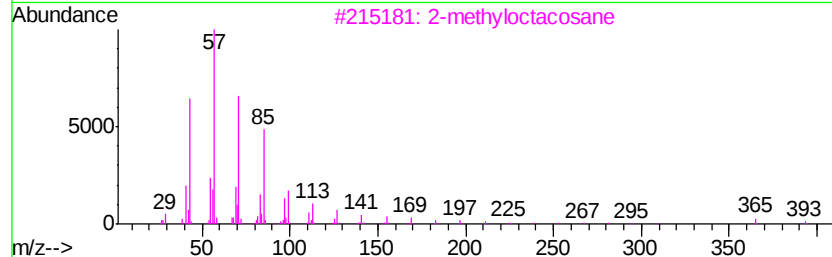
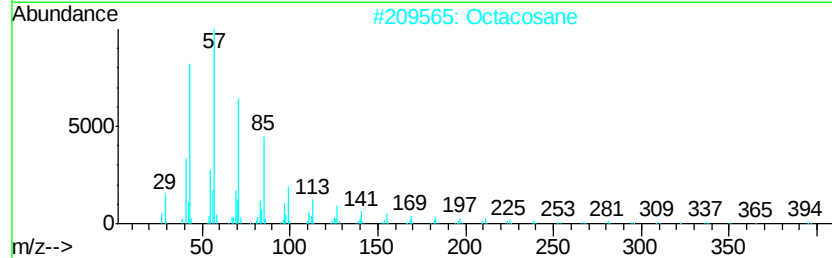
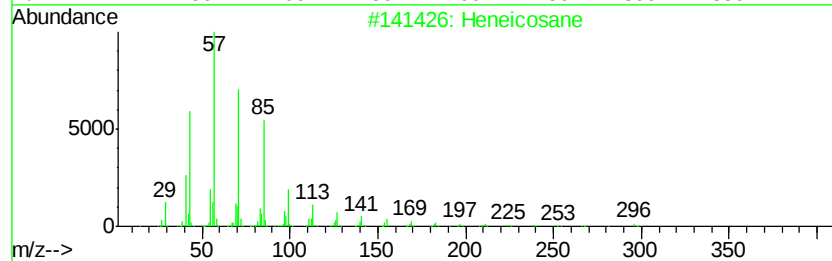
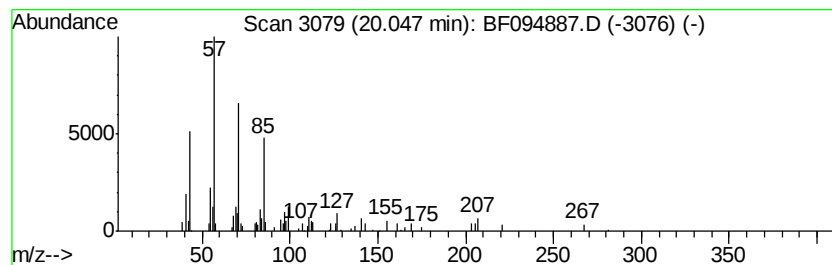
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.05	2.77 ng	76269	Perylene-d12	20.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	91
2		Octacosane	394	C28H58	000630-02-4	91
3		2-methyloctacosane	408	C29H60	1000376-72-8	91
4		Heptadecane	240	C17H36	000629-78-7	91
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050417\
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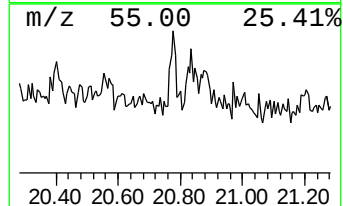
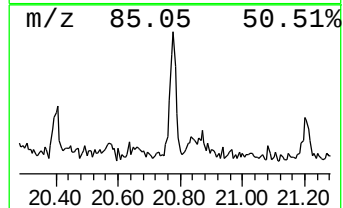
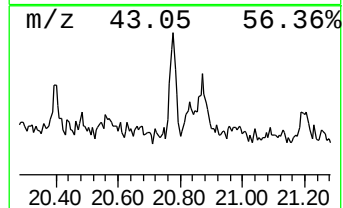
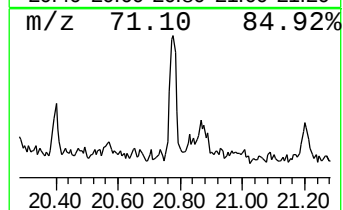
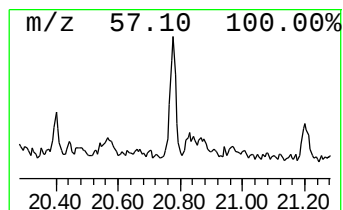
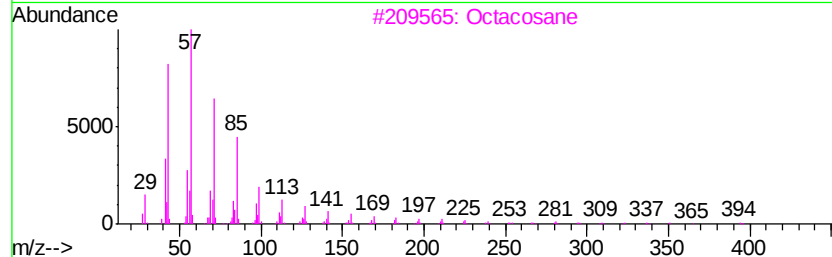
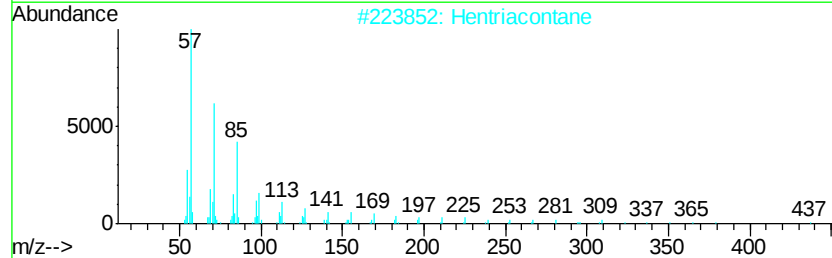
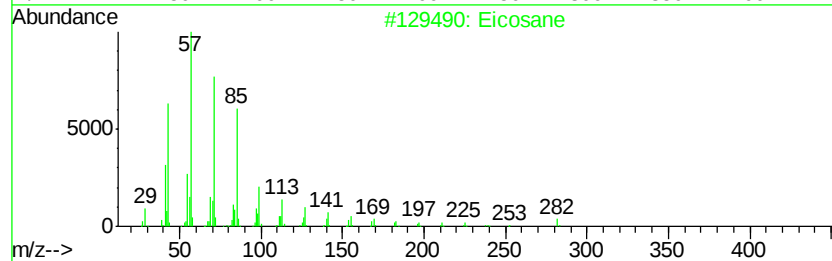
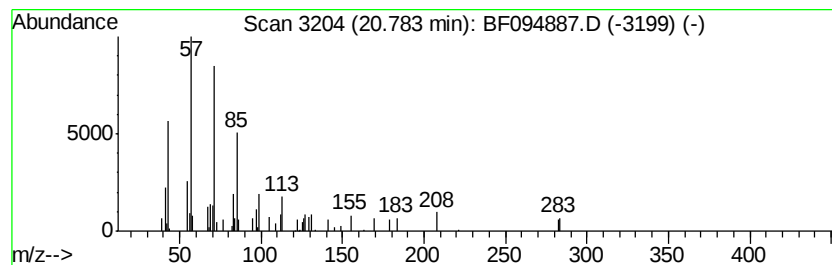
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Eicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.78	2.16 ng	59345	Perylene-d12	20.29
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Eicosane		282 C20H42	000112-95-8 93
2	Hentriacontane		437 C31H64	000630-04-6 87
3	Octacosane		394 C28H58	000630-02-4 83
4	Octadecane		254 C18H38	000593-45-3 83
5	Hexacosane		366 C26H54	000630-01-3 83



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050417\
Data File : BF094887.D
Acq On : 4 May 2017 22:15
Operator : SJ/MA
Sample : I2916-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-04-COMP(0-7.5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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unknown7.38	7.38	100.3	ng	2252790	1	7.72	449272	20.0
unknown15.18	15.18	2.7	ng	108728	4	14.97	792220	20.0
unknown15.66	15.66	4.9	ng	192662	4	14.97	792220	20.0
n-Hexadecanoic acid	15.94	4.5	ng	179112	4	14.97	792220	20.0
Behenic alcohol	18.54	8.1	ng	296717	5	18.64	729985	20.0
Heptadecyl heptaf...	19.34	5.8	ng	212120	5	18.64	729985	20.0
Squalene	19.77	2.3	ng	62265	6	20.29	550363	20.0
Heneicosane	20.05	2.8	ng	76269	6	20.29	550363	20.0
Eicosane	20.78	2.2	ng	59345	6	20.29	550363	20.0