

Data Path : Z:\HPCHEM1\BNA_F\Data\BF031817\
 Data File : BF093746.D
 Acq On : 18 Mar 2017 11:44
 Operator : SJ/MA
 Sample : I2263-05
 Misc :
 ALS Vial : 29 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-102S

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-BF031817.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	271	274	277	rBV	296390	366138	4.07%	0.592%
2	5.442	308	311	313	rBV	2819601	2644774	29.40%	4.278%
3	6.470	398	401	403	rBV	1994430	1945844	21.63%	3.147%
4	6.607	410	413	416	rBV	3497576	4424660	49.19%	7.156%
5	6.847	432	434	436	rBV	1362344	1252044	13.92%	2.025%
6	7.007	445	448	450	rVB	3947943	4285278	47.64%	6.931%
7	7.407	480	483	485	rBV	3369465	3529883	39.24%	5.709%
8	7.830	515	520	527	rBV2	74913	191830	2.13%	0.310%
9	8.128	544	546	549	rBV	1801162	1626275	18.08%	2.630%
10	9.213	638	641	643	rVB	5404896	6418055	71.35%	10.380%
11	9.876	697	699	702	rBV	1415473	1780374	19.79%	2.879%
12	10.665	765	768	771	rBV	2878522	3262810	36.27%	5.277%
13	10.802	778	780	784	rVB	75361	97284	1.08%	0.157%
14	11.042	798	801	804	rBV	537427	855199	9.51%	1.383%
15	11.362	826	829	831	rVB	1865607	1849546	20.56%	2.991%
16	11.842	868	871	874	rBV	139387	405087	4.50%	0.655%
17	11.922	874	878	888	rVV	4080205	6697122	74.45%	10.832%
18	12.082	890	892	897	rVV3	35288	100769	1.12%	0.163%
19	12.196	899	902	904	rVV2	91069	146403	1.63%	0.237%
20	12.631	934	940	944	rBV	3046055	8995156	100.00%	14.548%
21	12.699	944	946	951	rVV	1046605	1630738	18.13%	2.637%
22	12.779	951	953	957	rVB	130526	188662	2.10%	0.305%
23	12.951	965	968	970	rVB	4715757	5278906	58.69%	8.538%
24	12.997	970	972	975	rVB	111738	141171	1.57%	0.228%
25	13.054	975	977	979	rBV2	81125	127994	1.42%	0.207%
26	13.191	986	989	992	rBV3	48098	95380	1.06%	0.154%
27	13.237	992	993	996	rVV	73530	91035	1.01%	0.147%
28	13.328	999	1001	1006	rVV4	49879	116161	1.29%	0.188%
29	13.865	1045	1048	1051	rBV	87106	139073	1.55%	0.225%
30	13.991	1056	1059	1061	rBV	1580221	1751976	19.48%	2.834%
31	15.397	1179	1182	1185	rBV	931461	1393885	15.50%	2.254%

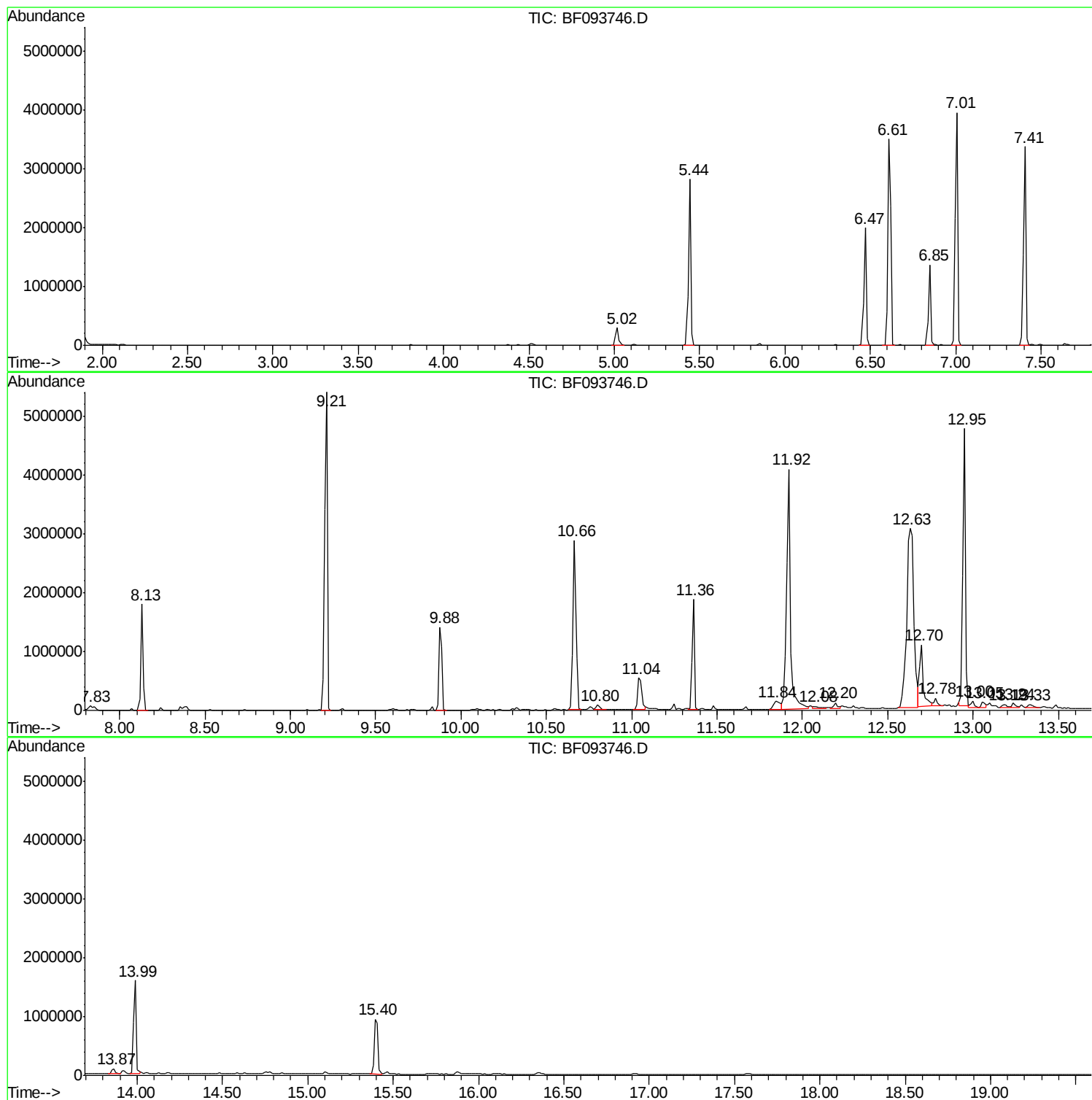
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Instrument :
BNA_F
ClientSampled :
MW-102S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031817.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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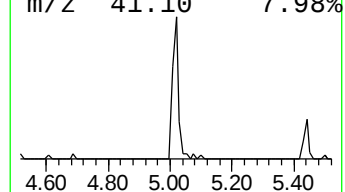
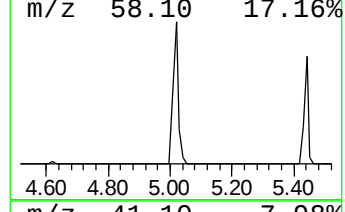
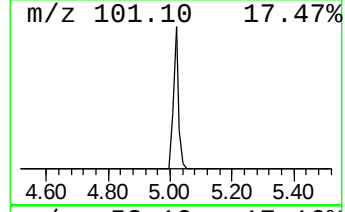
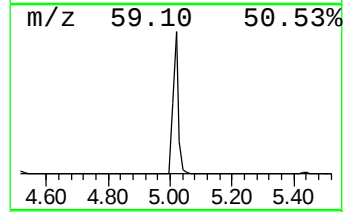
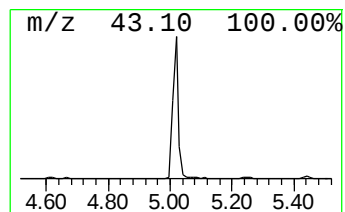
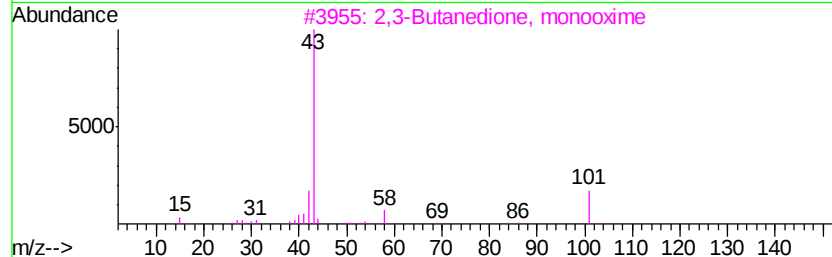
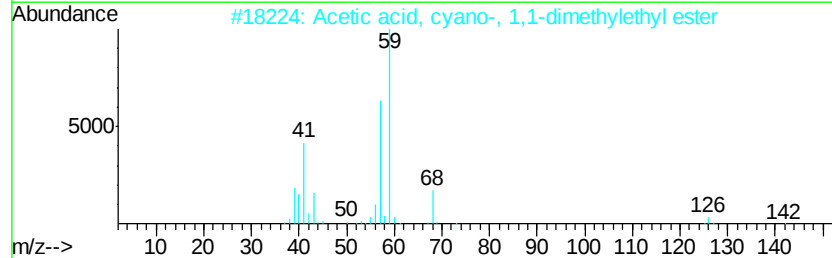
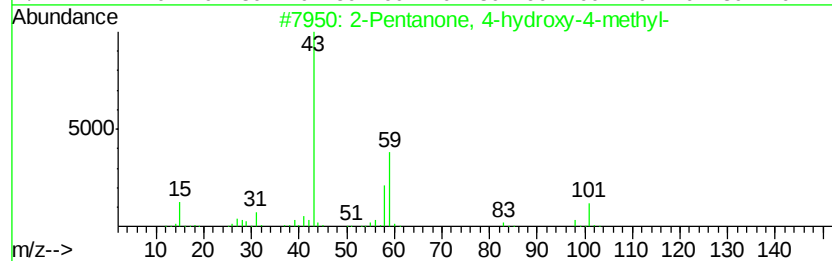
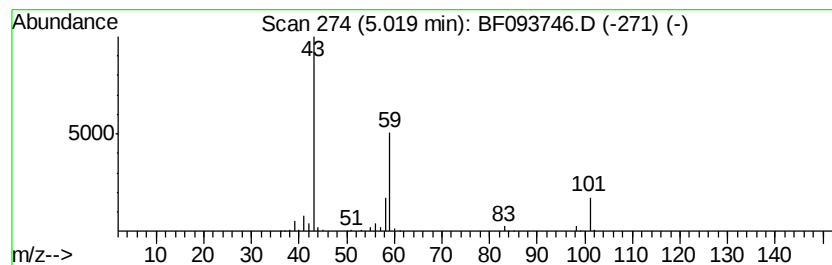
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031817.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	5.85 ng	366138	1,4-Dichlorobenzene-d4	6.85

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59	
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25	
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16	
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10	
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9	



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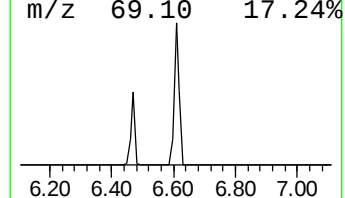
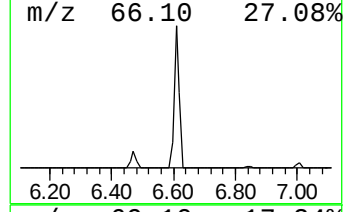
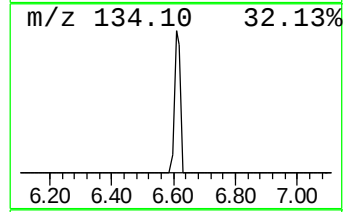
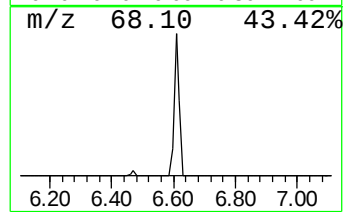
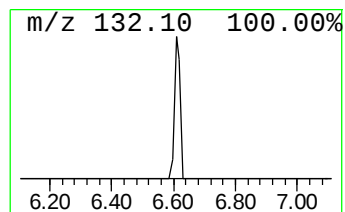
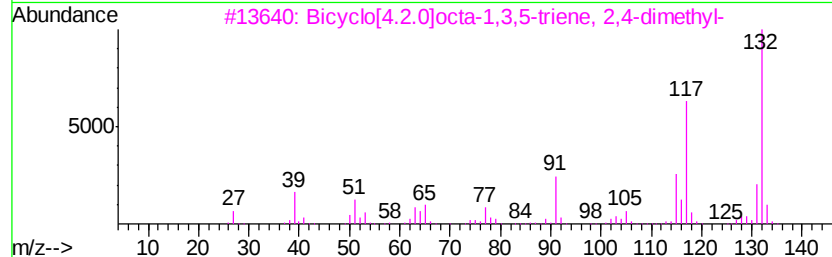
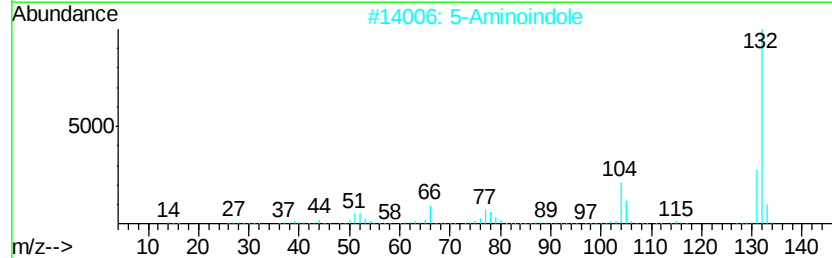
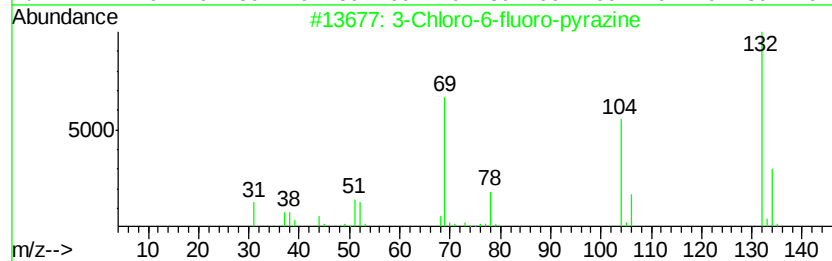
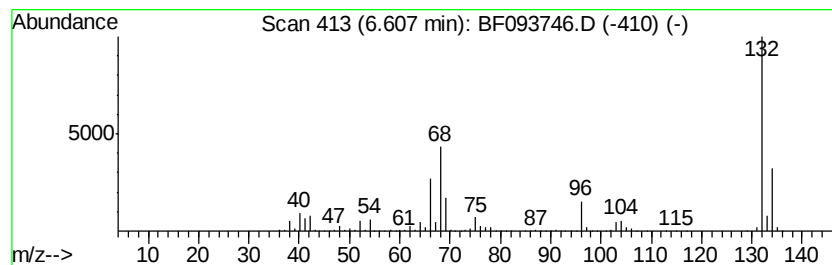
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Peak Number 2 unknown6.61 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	70.68 ng	4424660	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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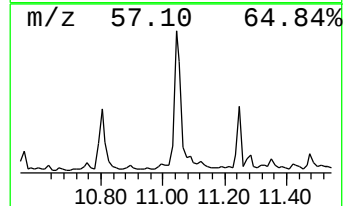
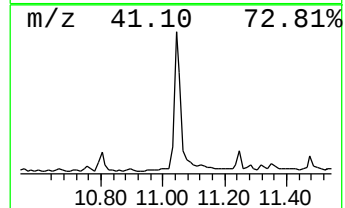
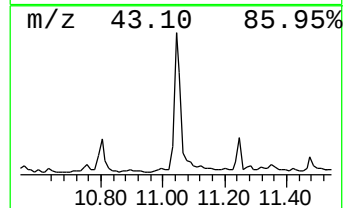
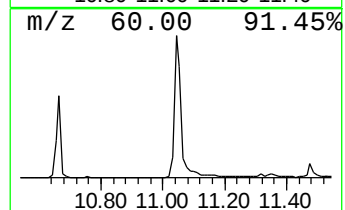
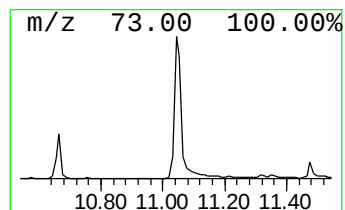
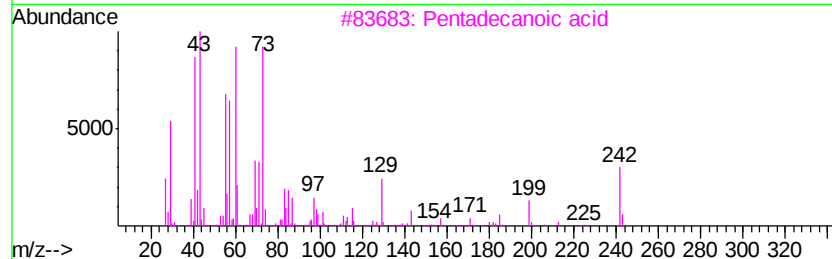
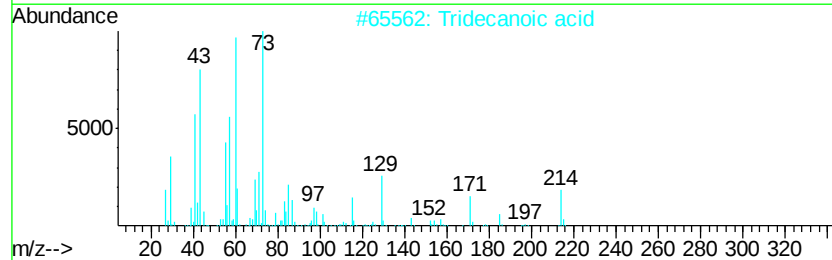
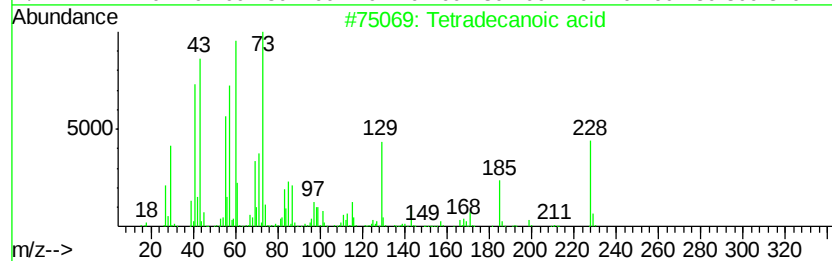
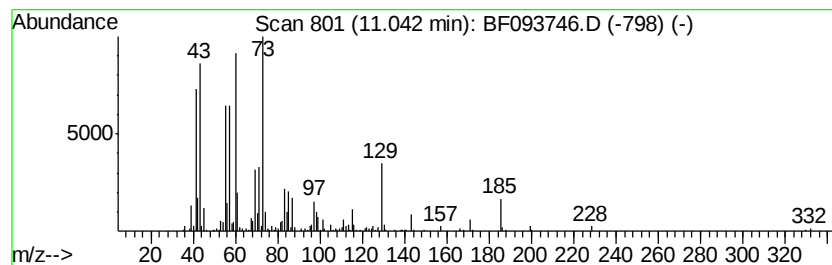
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Tetradecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.04	9.25 ng	855199	Phenanthrene-d10	11.36

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetradecanoic acid	228	C14H28O2	000544-63-8	96
2		Tridecanoic acid	214	C13H26O2	000638-53-9	90
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	86
4		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	78
5		Undecanoic acid	186	C11H22O2	000112-37-8	72



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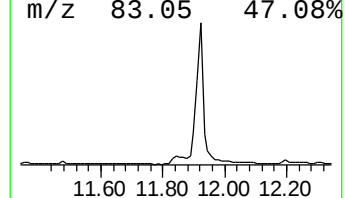
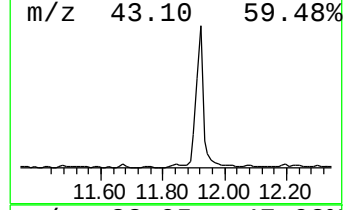
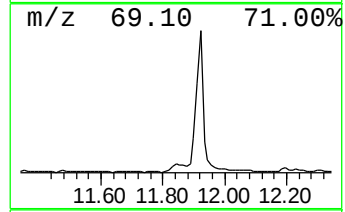
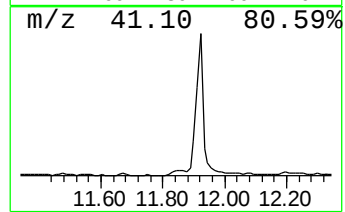
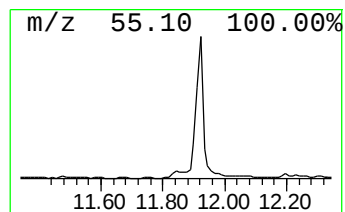
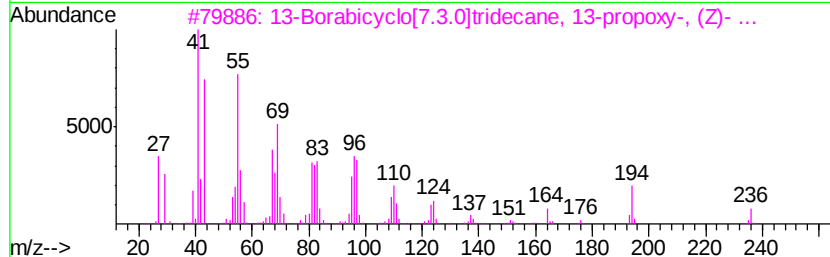
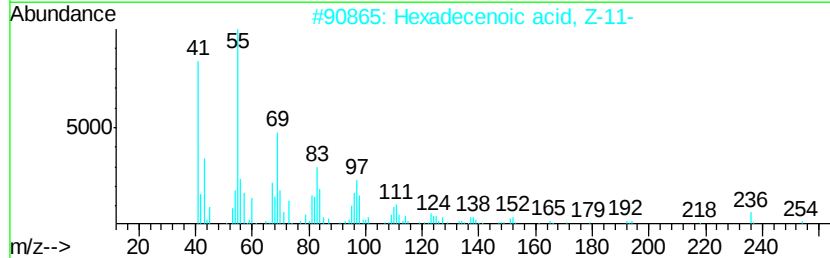
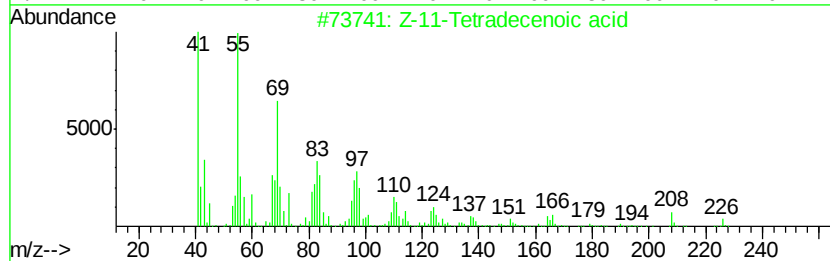
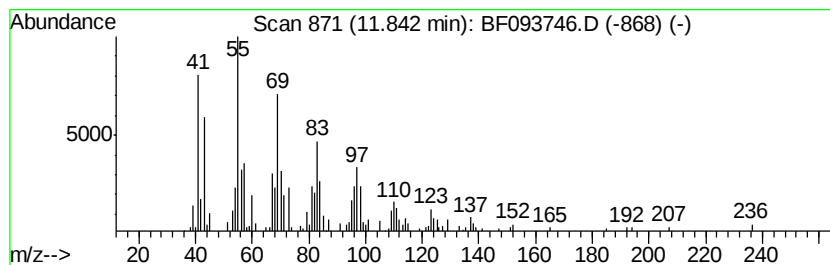
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Peak Number 5 Z-11-Tetradecenoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.84	4.38 ng	405087	Phenanthrene-d10	11.36

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Z-11-Tetradecenoic acid	226	C14H26O2	1000130-83-3	87
2		Hexadecenoic acid, Z-11-	254	C16H30O2	002416-20-8	83
3		13-Borabicyclo[7.3.0]tridecane, ...	236	C15H29B0	1000156-41-7	81
4		Myristoleic acid	226	C14H26O2	000544-64-9	74
5		Z-7-Tetradecenoic acid	226	C14H26O2	1000130-98-4	68



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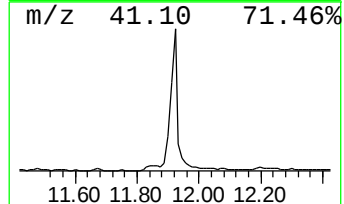
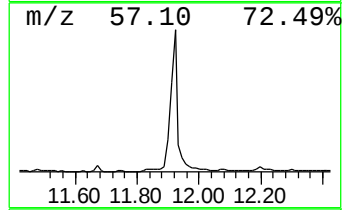
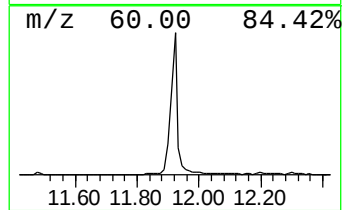
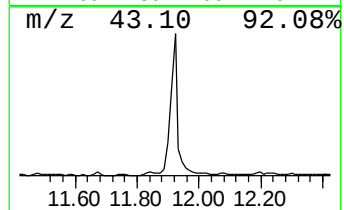
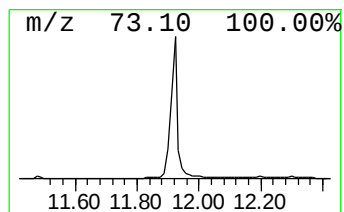
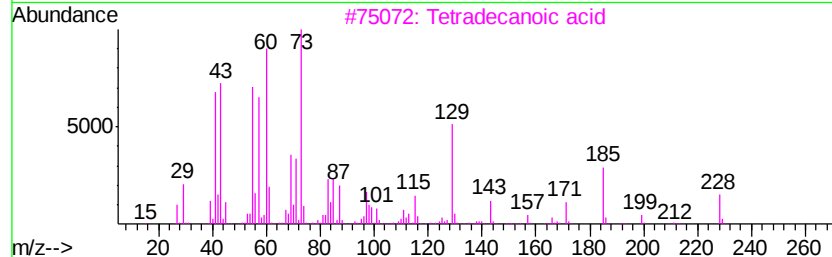
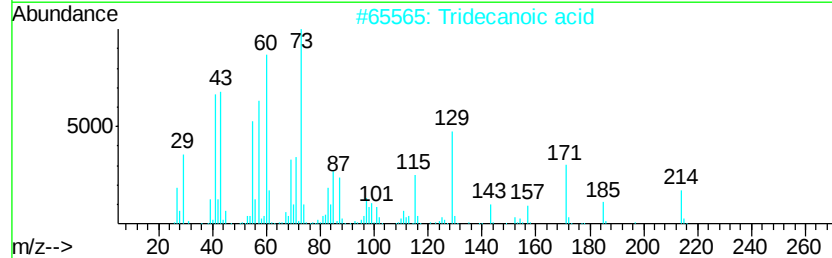
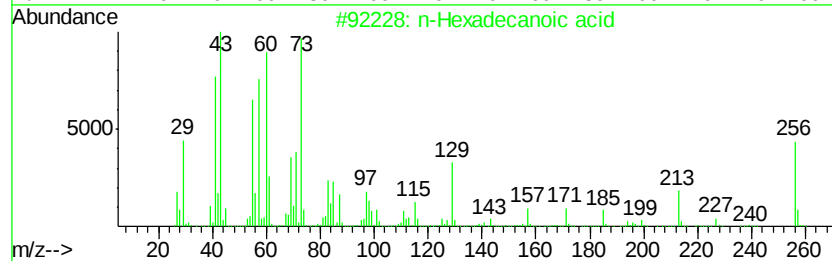
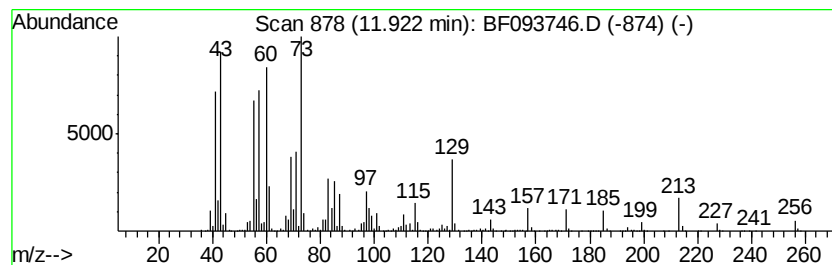
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Peak Number 6 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.		
11.92	72.42 ng	6697120	Phenanthrene-d10	11.36		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tridecanoic acid	214	C13H26O2	000638-53-9	95
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4		Dodecane	170	C12H26	000112-40-3	11
5		Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	11



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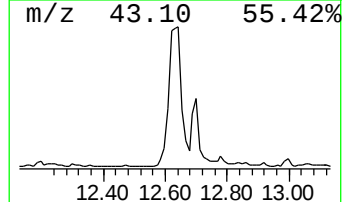
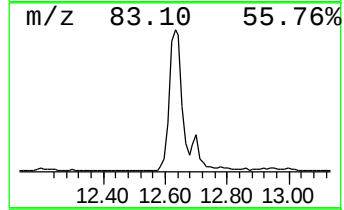
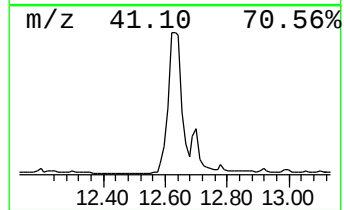
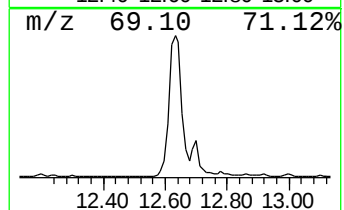
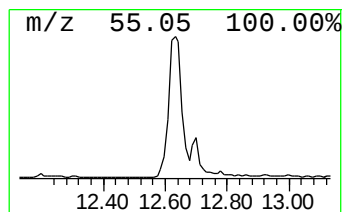
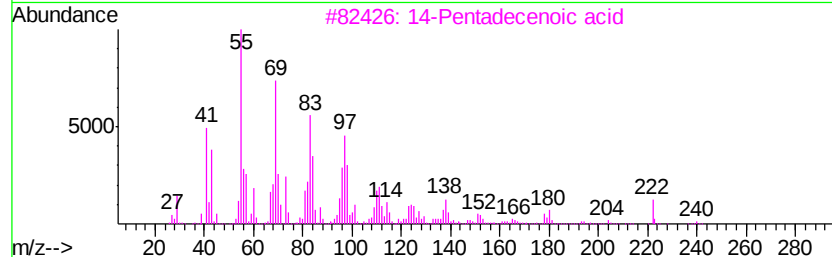
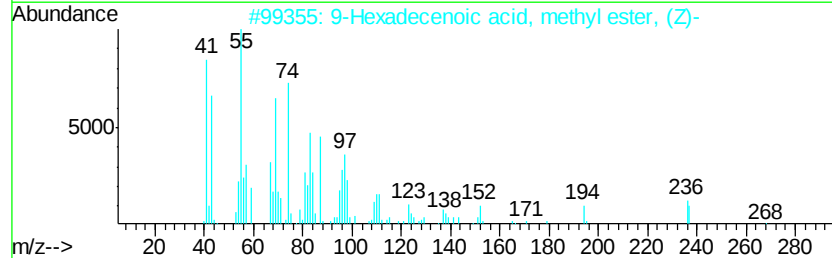
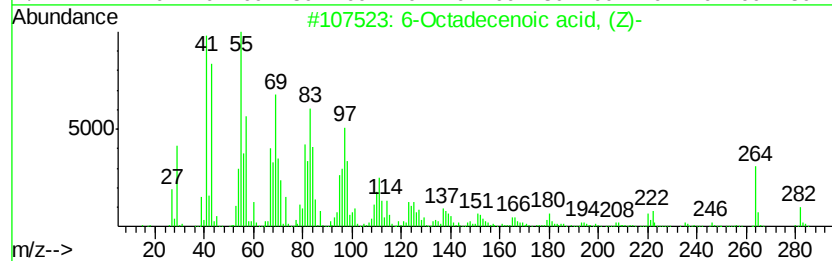
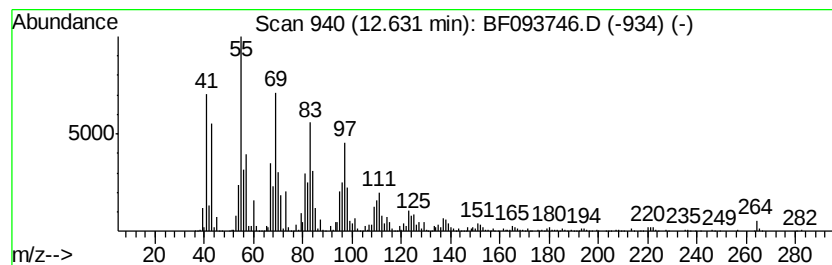
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 6-Octadecenoic acid, (Z)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.63	97.27 ng	8995160	Phenanthrene-d10	11.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	6-Octadecenoic acid, (Z)-	282	C18H34O2	000593-39-5	95
2		9-Hexadecenoic acid, methyl este...	268	C17H32O2	001120-25-8	83
3		14-Pentadecenoic acid	240	C15H28O2	017351-34-7	83
4		9-Hexadecenoic acid	254	C16H30O2	002091-29-4	81
5		Oleic Acid	282	C18H34O2	000112-80-1	55



Data Path : Z:\HPCHEM1\BNA_F\Data\BF031817\
Data File : BF093746.D
Acq On : 18 Mar 2017 11:44
Operator : SJ/MA
Sample : I2263-05
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-102S

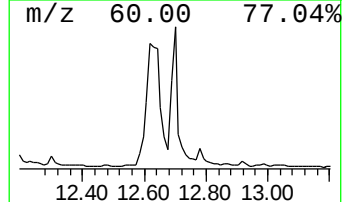
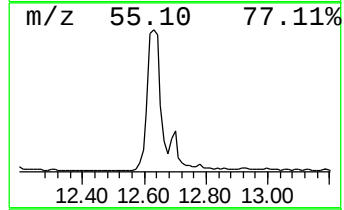
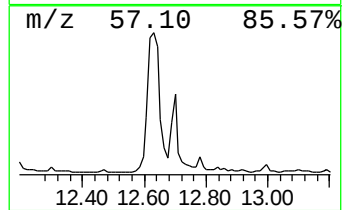
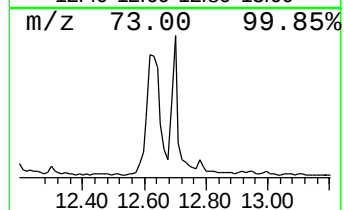
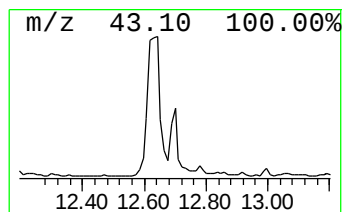
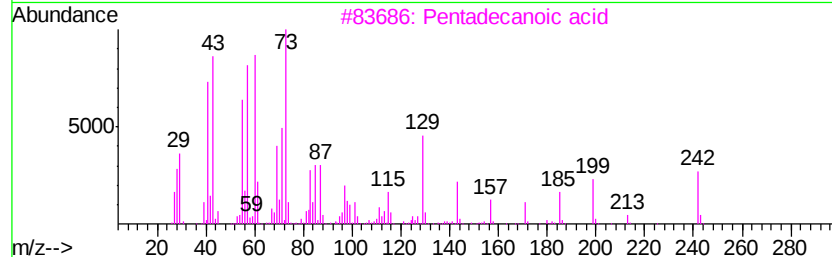
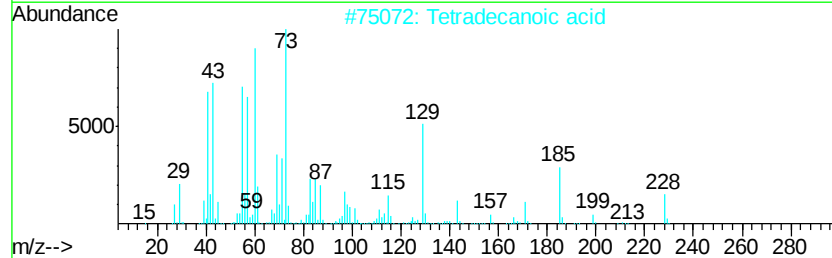
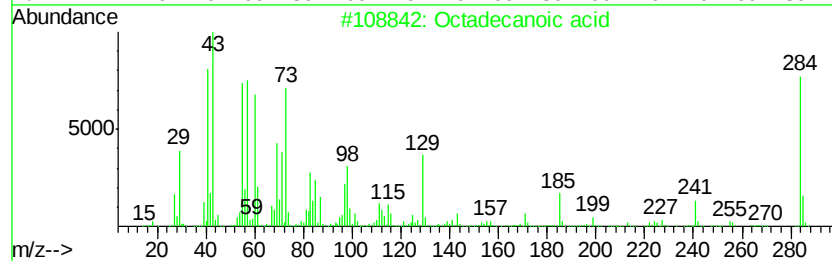
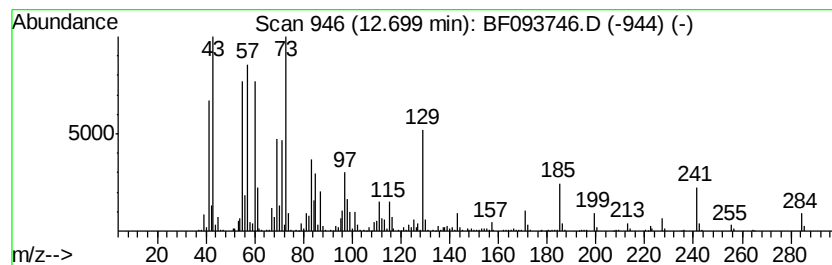
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.70	18.62 ng	1630740	Chrysene-d12	13.99

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	95
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	81
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4		n-Decanoic acid	172	C10H20O2	000334-48-5	70
5		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	42



Data Path : Z:\HPCHEM1\BNA_F\Data\BF031817\
Data File : BF093746.D
Acq On : 18 Mar 2017 11:44
Operator : SJ/MA
Sample : I2263-05
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-102S

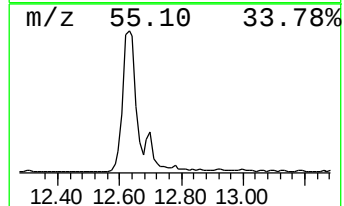
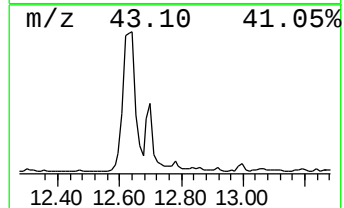
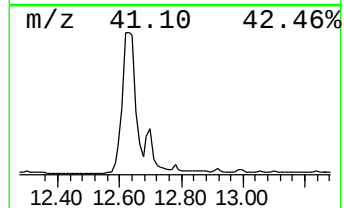
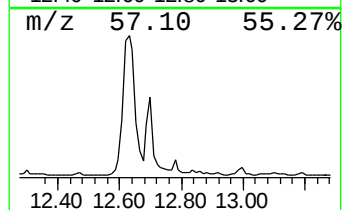
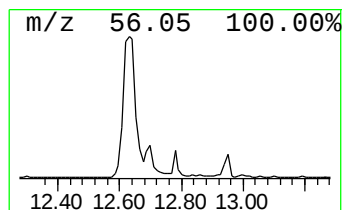
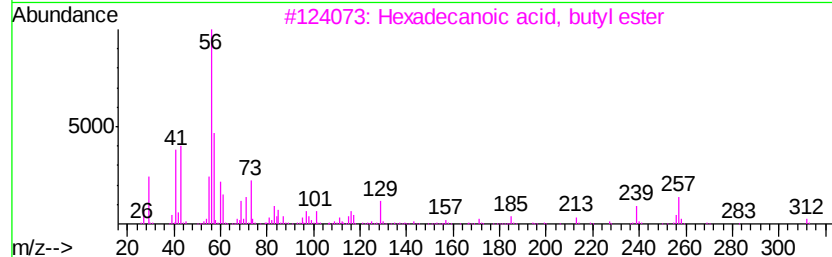
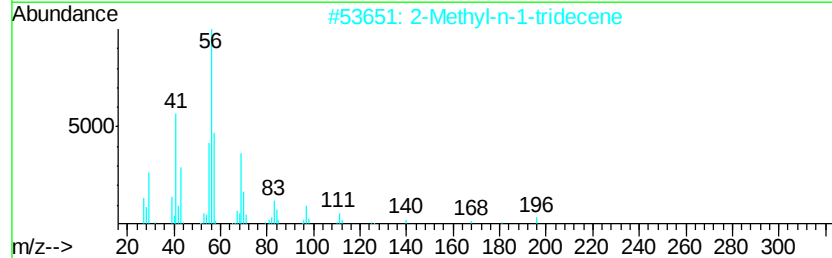
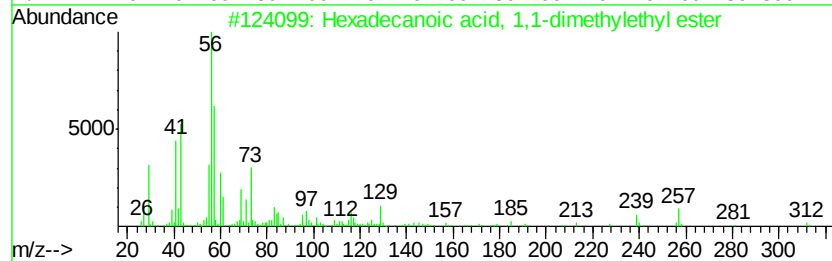
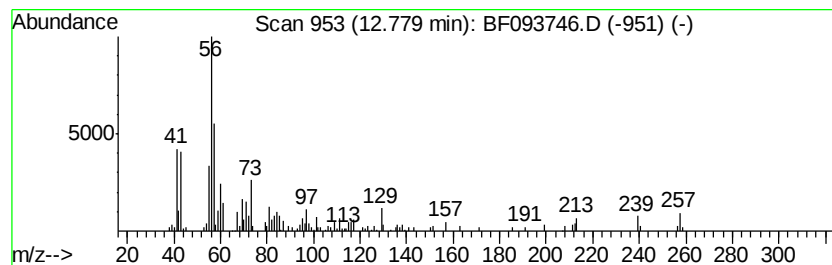
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexadecanoic acid, 1,1-dime... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.78	2.15 ng	188662	Chrysene-d12	13.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	58
2		2-Methyl-n-1-tridecene	196	C14H28	018094-01-4	43
3		Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	43
4		3-Undecene, 2-methyl-, (E)-	168	C12H24	074630-51-6	37
5		Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	37



Data Path : Z:\HPCHEM1\BNA_F\Data\BF031817\
Data File : BF093746.D
Acq On : 18 Mar 2017 11:44
Operator : SJ/MA
Sample : I2263-05
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-102S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.02	5.8	ng	366138	1	6.85	1252040	20.0
unknown6.61	6.61	70.7	ng	4424660	1	6.85	1252040	20.0
Tetradecanoic acid	11.04	9.3	ng	855199	4	11.36	1849550	20.0
Z-11-Tetradeceno...	11.84	4.4	ng	405087	4	11.36	1849550	20.0
n-Hexadecanoic acid	11.92	72.4	ng	6697120	4	11.36	1849550	20.0
6-Octadecenoic ac...	12.63	97.3	ng	8995160	4	11.36	1849550	20.0
Octadecanoic acid	12.70	18.6	ng	1630740	5	13.99	1751980	20.0
Hexadecanoic acid...	12.78	2.1	ng	188662	5	13.99	1751980	20.0