

Data Path : Z:\HPCHEM1\BNA_F\Data\BF031817\
 Data File : BF093745.D
 Acq On : 18 Mar 2017 11:16
 Operator : SJ/MA
 Sample : I2263-04
 Misc :
 ALS Vial : 28 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-101D

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	2.344	34	40	44	rVV	907483	1507421	24.64%	3.012%
2	2.470	48	51	57	rBV	167955	269115	4.40%	0.538%
3	4.515	227	230	233	rBV	469168	532412	8.70%	1.064%
4	5.007	271	273	279	rVB	197234	295678	4.83%	0.591%
5	5.441	308	311	313	rBV	2591536	2541444	41.54%	5.078%
6	6.470	398	401	403	rBV	1771121	1801149	29.44%	3.599%
7	6.607	410	413	416	rBV	3380010	4116333	67.28%	8.224%
8	6.847	432	434	436	rBV	1349319	1212132	19.81%	2.422%
9	7.007	445	448	450	rVB	3798559	4061926	66.39%	8.116%
10	7.407	480	483	485	rBV	3183723	3278391	53.58%	6.550%
11	7.841	516	521	531	rBV	106695	239257	3.91%	0.478%
12	8.127	544	546	548	rVB	1661895	1527008	24.96%	3.051%
13	8.356	564	566	567	rBV	66559	75186	1.23%	0.150%
14	8.390	567	569	574	rVB	77345	120242	1.97%	0.240%
15	9.213	637	641	643	rBV	5314428	6118201	100.00%	12.224%
16	9.876	697	699	702	rVB	1370958	1675248	27.38%	3.347%
17	10.665	765	768	771	rBV	2842841	3156536	51.59%	6.307%
18	10.802	778	780	784	rVB	50407	65164	1.07%	0.130%
19	11.042	799	801	804	rBV	104314	133123	2.18%	0.266%
20	11.248	817	819	820	rBV2	67746	62289	1.02%	0.124%
21	11.362	826	829	831	rVB	1684774	1721850	28.14%	3.440%
22	11.830	867	870	874	rBV	70764	123552	2.02%	0.247%
23	11.899	874	876	887	rVV	557214	724901	11.85%	1.448%
24	12.619	934	939	944	rBV	2493184	4734379	77.38%	9.459%
25	12.688	944	945	952	rVV	707663	988404	16.16%	1.975%
26	12.951	965	968	970	rBV	4796751	5155595	84.27%	10.301%
27	13.865	1045	1048	1056	rBV	50264	79627	1.30%	0.159%
28	13.991	1056	1059	1061	rBV	1485597	1662534	27.17%	3.322%
29	15.099	1154	1156	1159	rBV	62807	76763	1.25%	0.153%
30	15.397	1179	1182	1185	rBV	924350	1305391	21.34%	2.608%
31	15.465	1185	1188	1195	rVB	105272	158233	2.59%	0.316%
32	15.877	1221	1224	1228	rBV	93240	153010	2.50%	0.306%
33	16.357	1262	1266	1274	rVB	88261	177413	2.90%	0.354%
34	16.917	1311	1315	1326	rBV	46477	117445	1.92%	0.235%

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ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_F
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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

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35	17.580	1369	1373	1380	rbV	27889	83976	1.37%	0.168%
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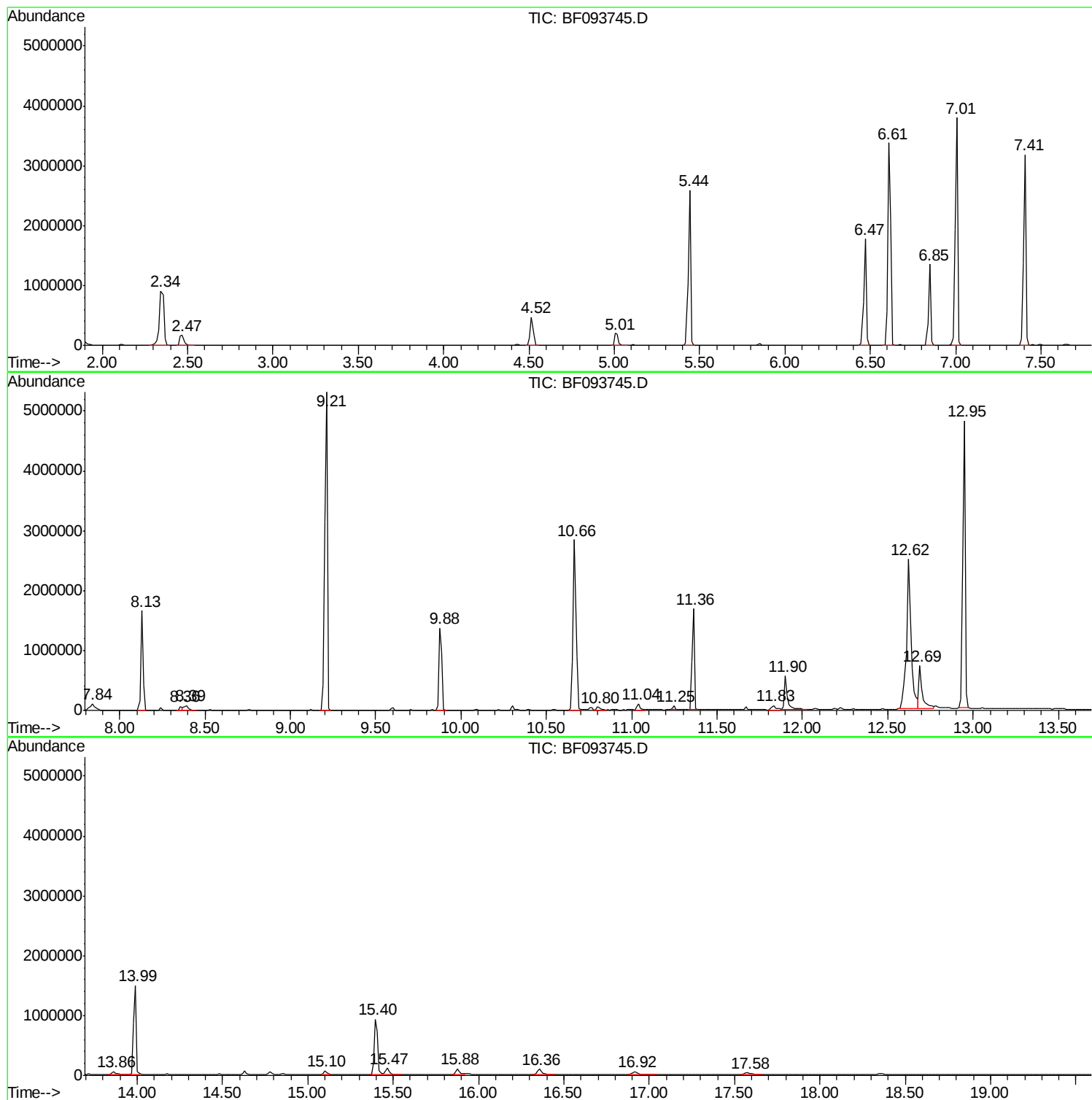
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031817.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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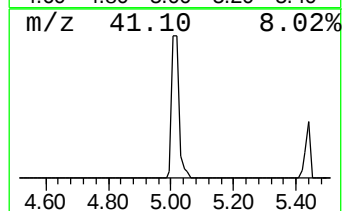
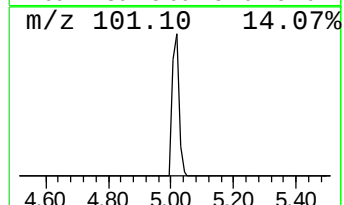
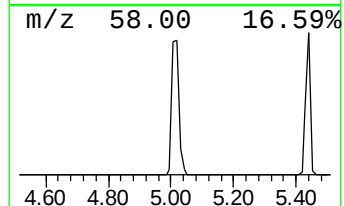
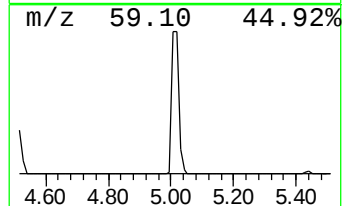
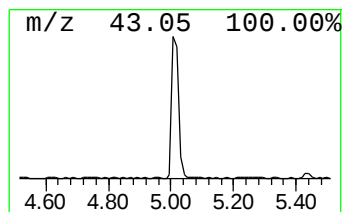
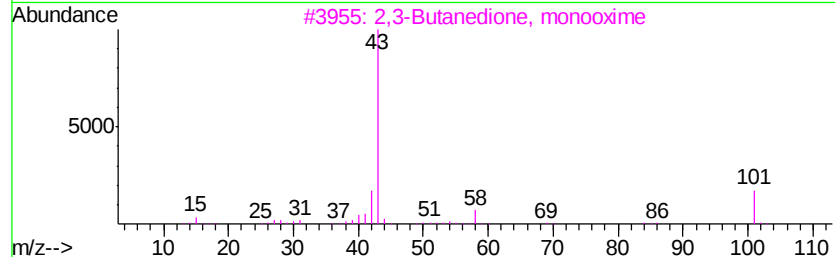
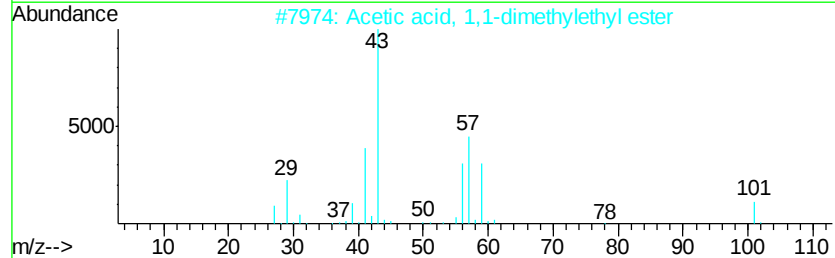
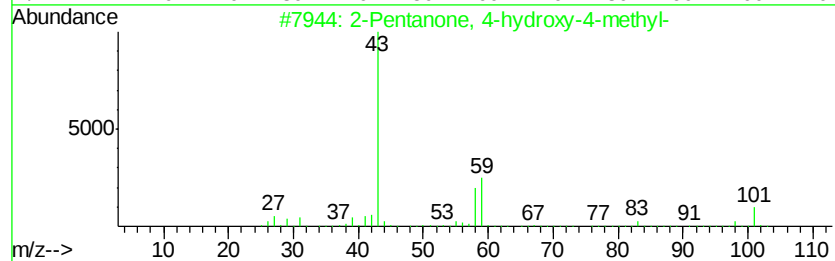
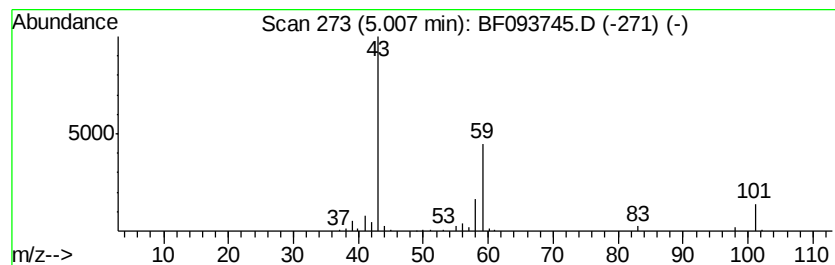
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.01	4.88 ng	295678	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	50	
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28	
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10	
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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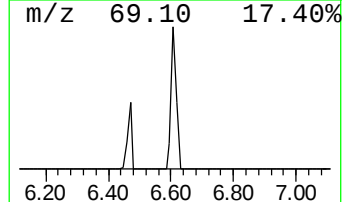
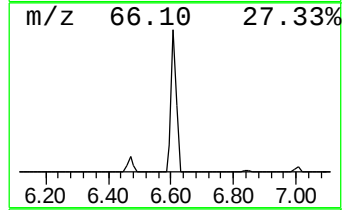
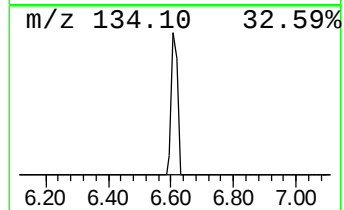
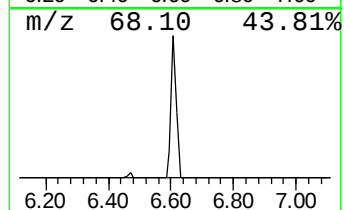
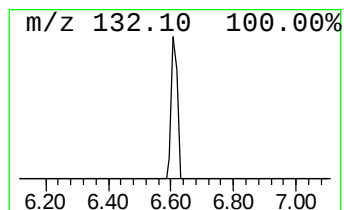
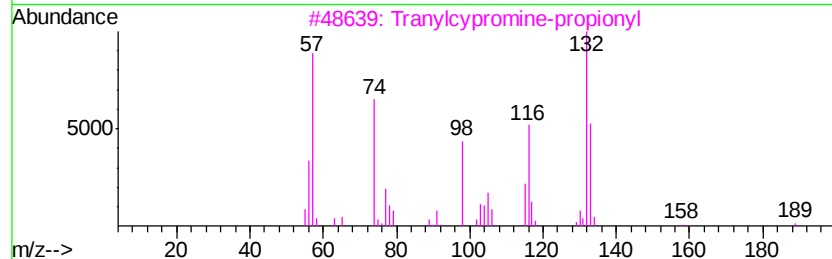
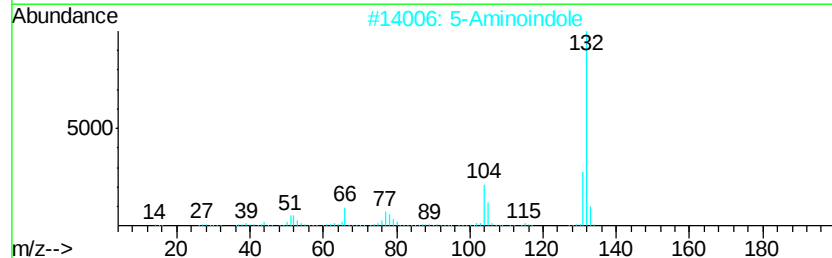
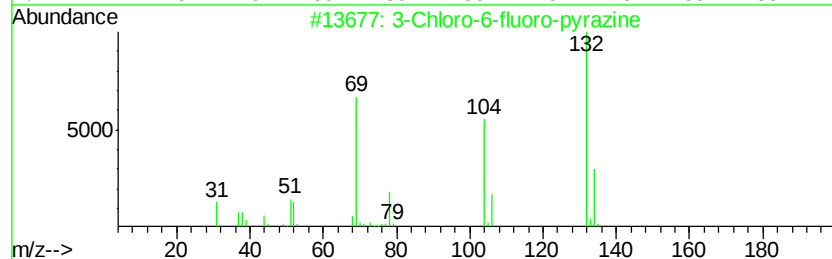
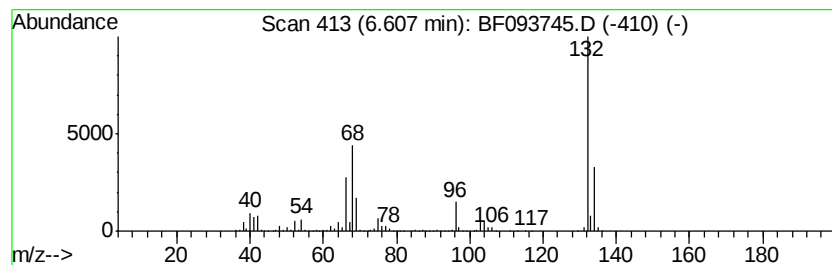
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 4 unknown6.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	67.92 ng	4116330	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		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
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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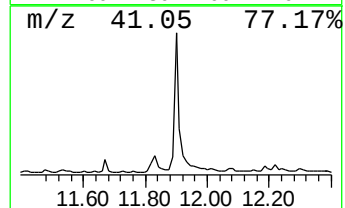
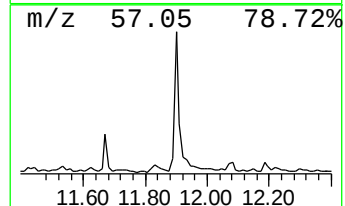
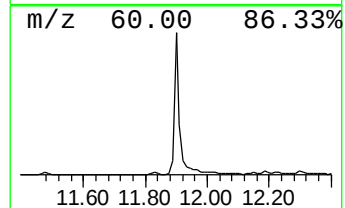
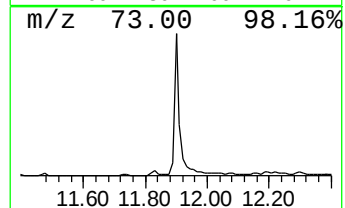
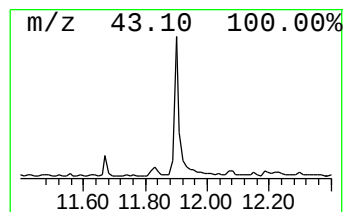
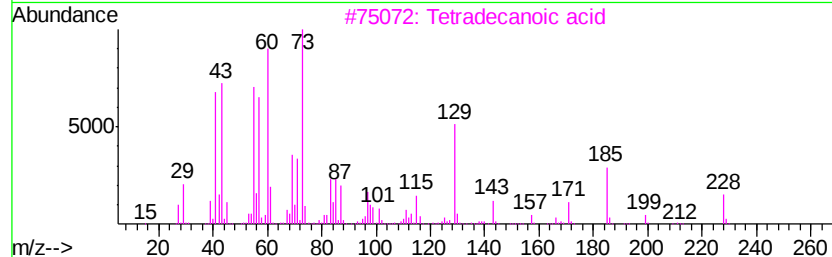
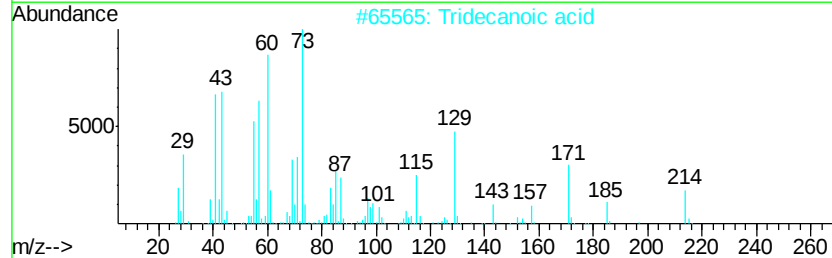
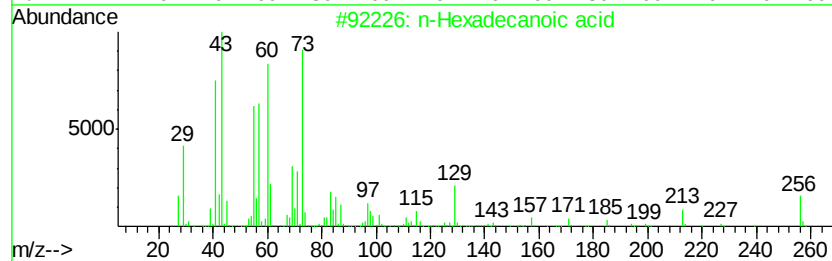
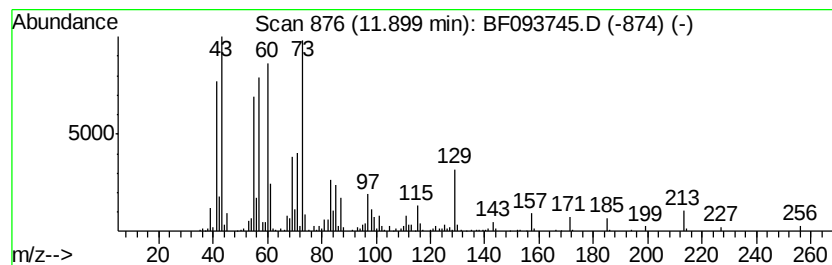
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.90	8.42 ng	724901	Phenanthrene-d10	11.36	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
2	Tridecanoic acid	214	C13H26O2	000638-53-9	76
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	Amyl Nitrite	117	C5H11NO2	000110-46-3	38
5	Undecane	156	C11H24	001120-21-4	11



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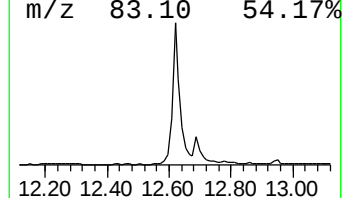
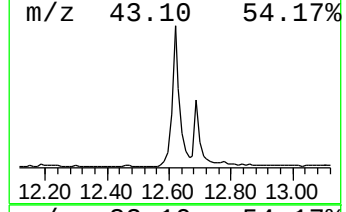
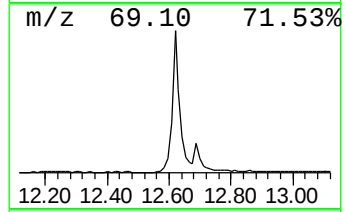
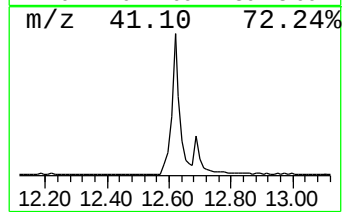
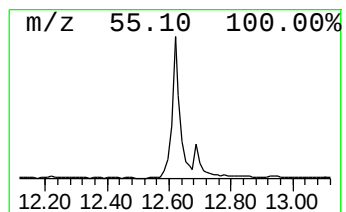
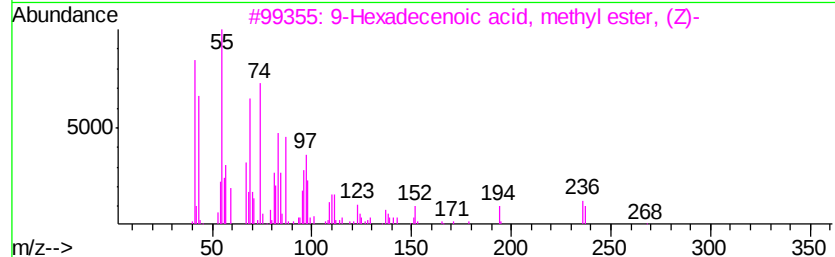
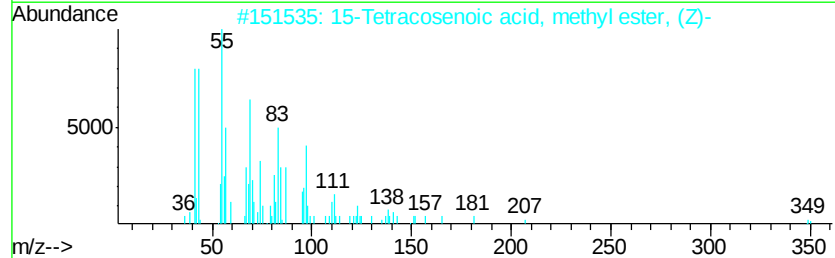
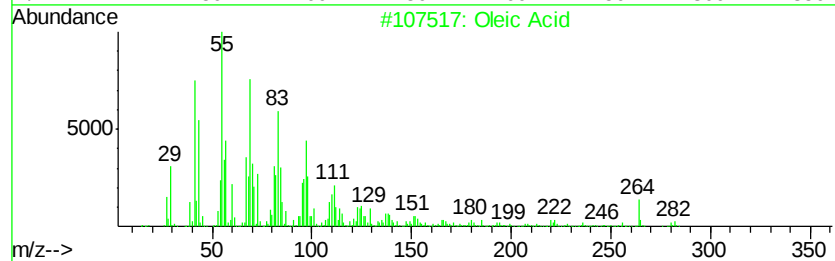
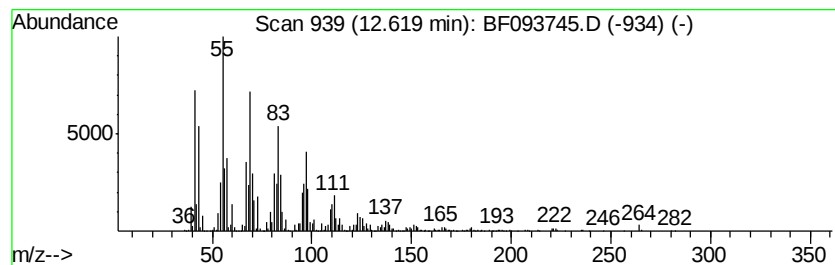
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Oleic Acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.62	54.99 ng	4734380	Phenanthrene-d10	11.36

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oleic Acid		282	C18H34O2	000112-80-1	93
2	15-Tetracosenoic acid, methyl es...		380	C25H48O2	002733-88-2	91
3	9-Hexadecenoic acid, methyl este...		268	C17H32O2	001120-25-8	91
4	6-Octadecenoic acid, (Z)-		282	C18H34O2	000593-39-5	90
5	Hexadecenoic acid, Z-11-		254	C16H30O2	002416-20-8	86



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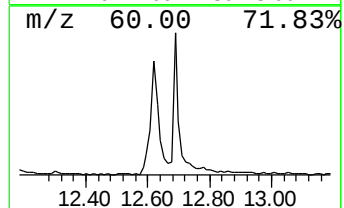
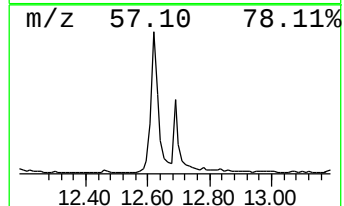
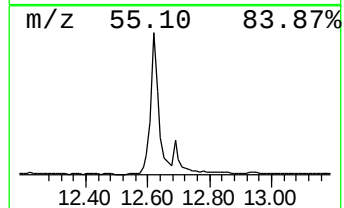
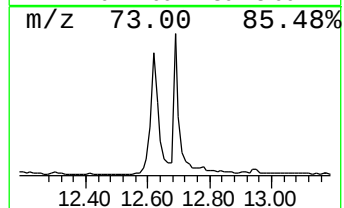
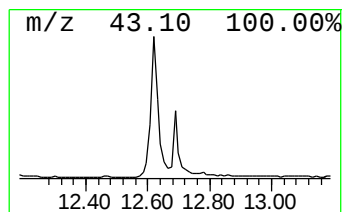
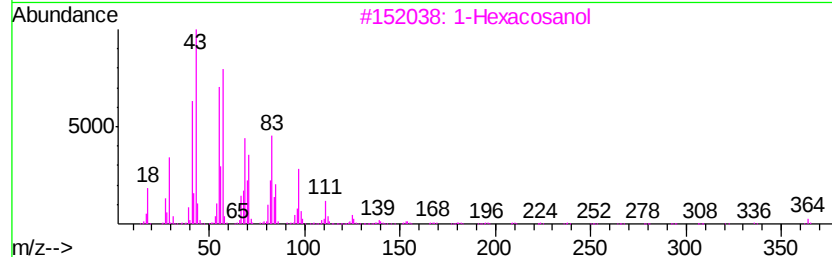
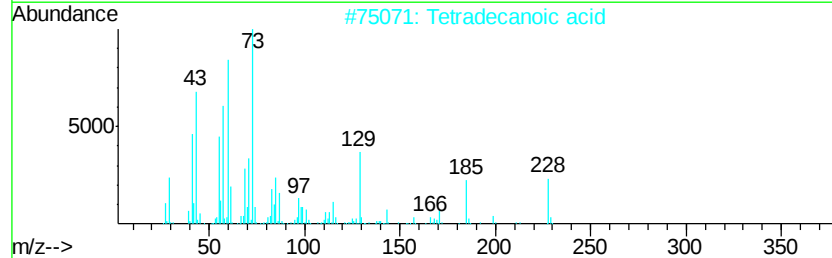
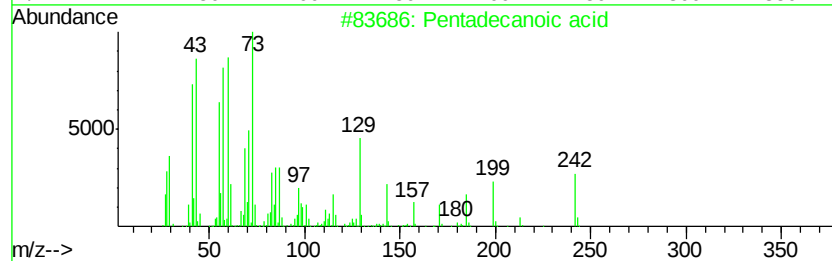
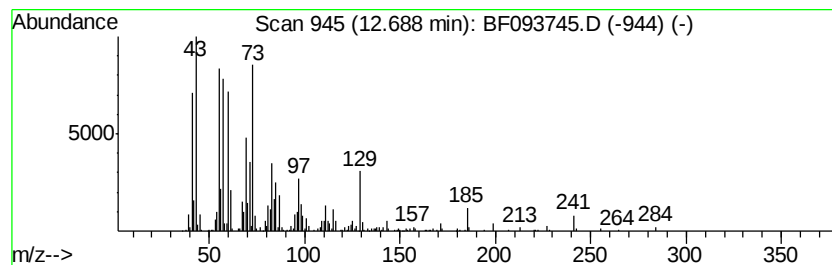
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Peak Number 8 Pentadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.69	11.89 ng	988404	Chrysene-d12	13.99

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentadecanoic acid	242	C15H30O2	001002-84-2	64
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	53
3		1-Hexacosanol	382	C26H54O	000506-52-5	30
4		Acetic acid, octadecyl ester	312	C20H40O2	000822-23-1	22
5		17-Pentatriacontene	491	C35H70	006971-40-0	20



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ClientSampleId :
MW-101D

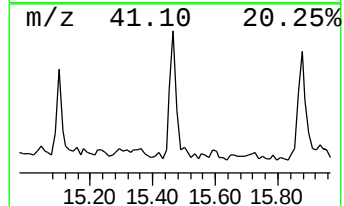
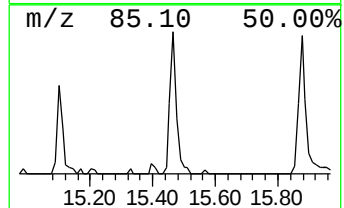
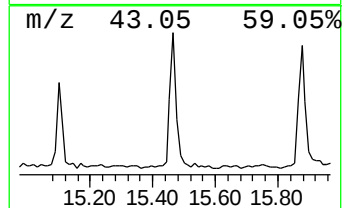
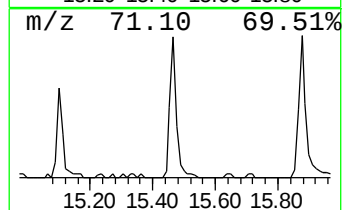
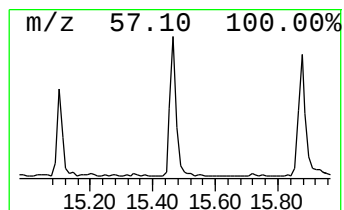
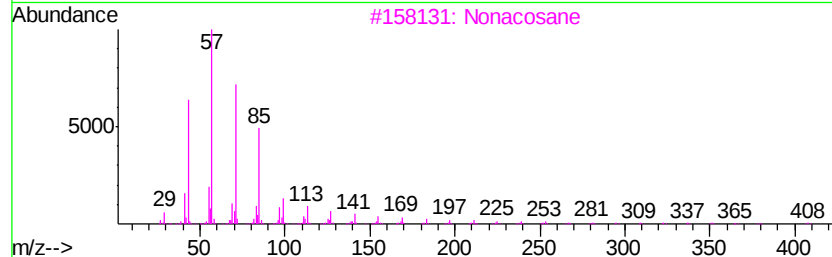
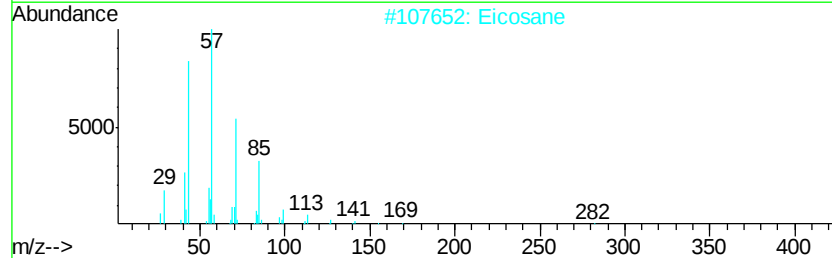
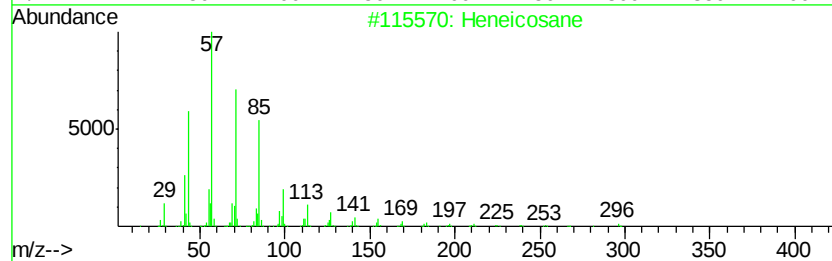
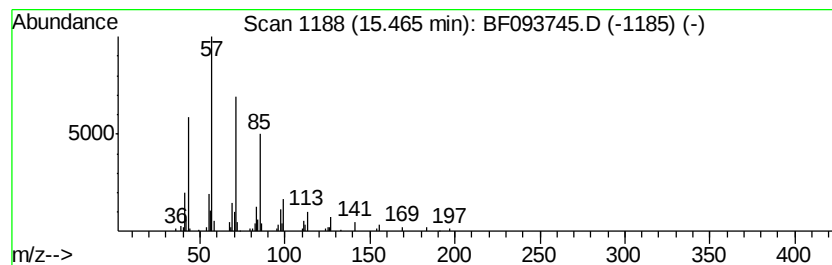
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heneicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.47	2.42 ng	158233	Perylene-d12	15.40

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Eicosane		282	C20H42	000112-95-8	91
3	Nonacosane		408	C29H60	000630-03-5	91
4	Heptadecane		240	C17H36	000629-78-7	90
5	Triacontane		422	C30H62	000638-68-6	90



Data Path : Z:\HPCHEM1\BNA_F\Data\BF031817\
Data File : BF093745.D
Acq On : 18 Mar 2017 11:16
Operator : SJ/MA
Sample : I2263-04
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-101D

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...	5.01	4.9	ng	295678	1	6.85	1212130	20.0
unknown6.61	6.61	67.9	ng	4116330	1	6.85	1212130	20.0
n-Hexadecanoic acid	11.90	8.4	ng	724901	4	11.36	1721850	20.0
Oleic Acid	12.62	55.0	ng	4734380	4	11.36	1721850	20.0
Pentadecanoic acid	12.69	11.9	ng	988404	5	13.99	1662530	20.0
Heneicosane	15.47	2.4	ng	158233	6	15.40	1305390	20.0