

Data Path : Z:\HPCHEM1\BNA_F\Data\BF031817\
 Data File : BF093750.D
 Acq On : 18 Mar 2017 13:33
 Operator : SJ/MA
 Sample : I2263-09
 Misc :
 ALS Vial : 33 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-102D

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	152056	220646	3.72%	0.534%
2	5.441	308	311	313	rBV	2675690	2635089	44.37%	6.378%
3	6.470	398	401	403	rBV	2021012	1949297	32.83%	4.718%
4	6.607	410	413	416	rBV	3272948	4043114	68.08%	9.787%
5	6.847	431	434	436	rBV	1338506	1190581	20.05%	2.882%
6	7.007	445	448	450	rVB	3584221	3758627	63.29%	9.098%
7	7.407	480	483	485	rBV	3051132	3148913	53.03%	7.622%
8	8.127	544	546	549	rVB	1587674	1504683	25.34%	3.642%
9	9.213	637	641	643	rBV	4934306	5938367	100.00%	14.374%
10	9.830	693	695	697	rVB	143277	176464	2.97%	0.427%
11	9.876	697	699	702	rBV	1284372	1690707	28.47%	4.092%
12	10.322	734	738	740	rVB2	32483	60252	1.01%	0.146%
13	10.665	765	768	771	rBV	2813462	3149052	53.03%	7.622%
14	10.768	774	777	778	rVV	480535	411781	6.93%	0.997%
15	10.802	778	780	784	rVB	70066	91006	1.53%	0.220%
16	11.248	816	819	820	rBV2	69718	63117	1.06%	0.153%
17	11.362	826	829	831	rVB	1691133	1726953	29.08%	4.180%
18	11.899	873	876	885	rBV	199874	260604	4.39%	0.631%
19	12.608	935	938	942	rBV3	24130	63086	1.06%	0.153%
20	12.688	942	945	951	rVV	365620	456877	7.69%	1.106%
21	12.951	965	968	970	rBV	4604655	5100062	85.88%	12.345%
22	13.431	1003	1010	1013	rBV3	20998	66684	1.12%	0.161%
23	13.865	1045	1048	1056	rVB	44249	92444	1.56%	0.224%
24	13.991	1056	1059	1061	rBV	1556691	1690509	28.47%	4.092%
25	14.848	1132	1134	1137	rBV	151732	153097	2.58%	0.371%
26	15.340	1174	1177	1180	rBV	47762	64497	1.09%	0.156%
27	15.397	1180	1182	1185	rVV	854001	1257180	21.17%	3.043%
28	15.465	1185	1188	1191	rVB	58183	82698	1.39%	0.200%
29	15.877	1221	1224	1229	rBV	51380	85148	1.43%	0.206%
30	16.357	1261	1266	1275	rVB	51344	119347	2.01%	0.289%
31	16.917	1311	1315	1318	rBV	28245	61772	1.04%	0.150%

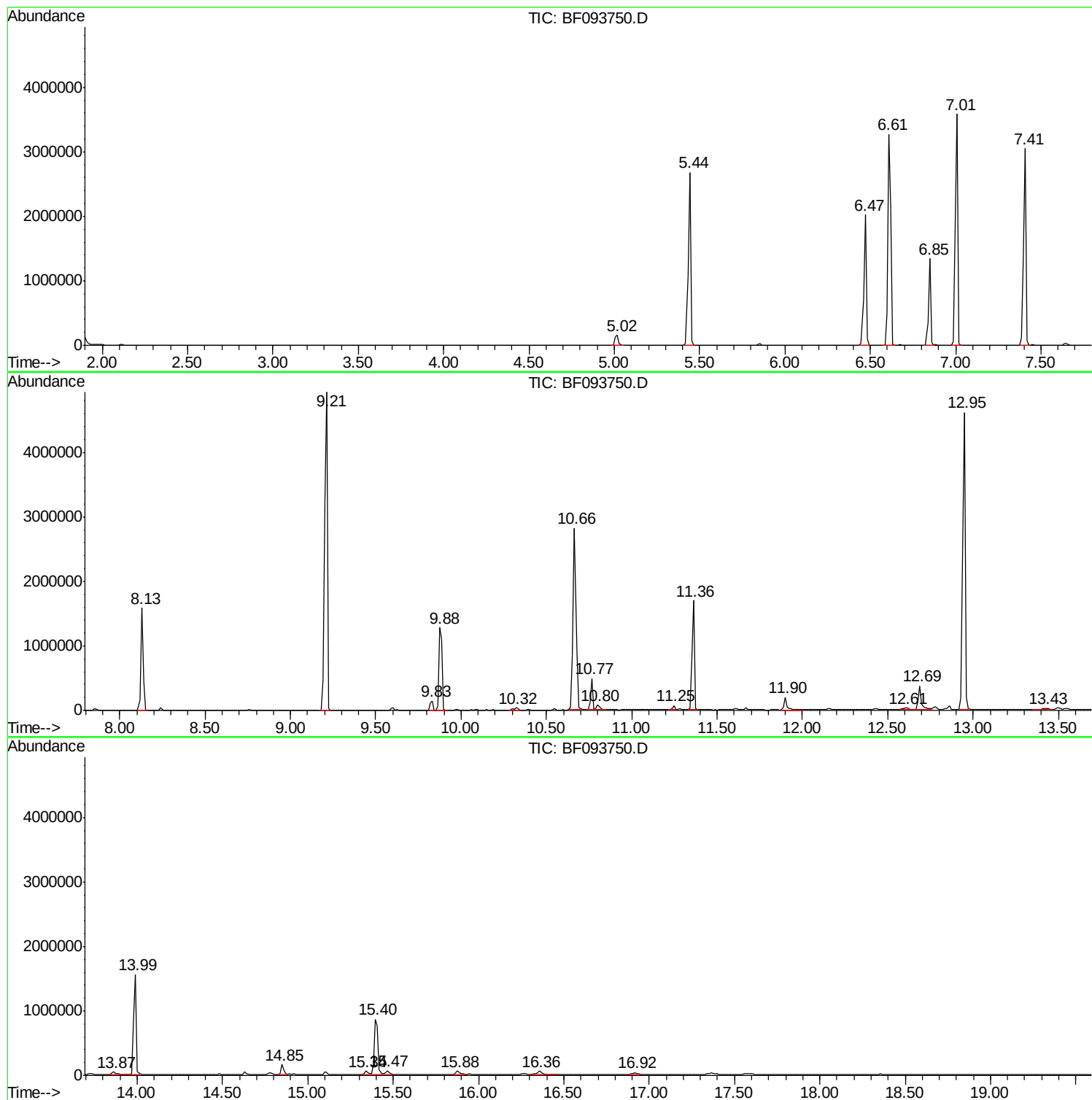
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Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-102D

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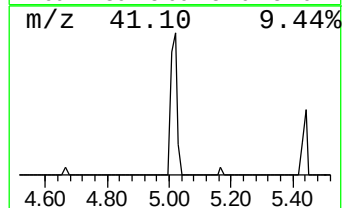
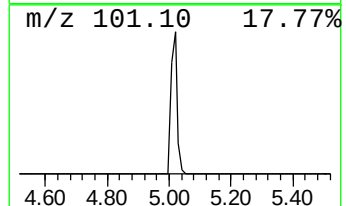
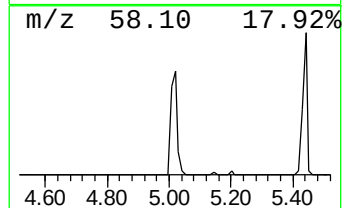
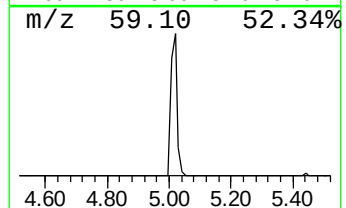
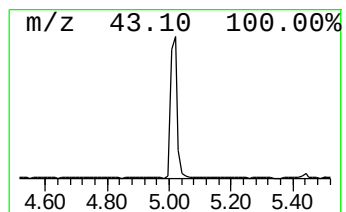
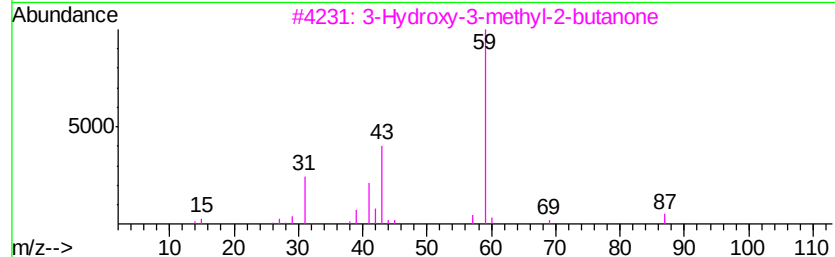
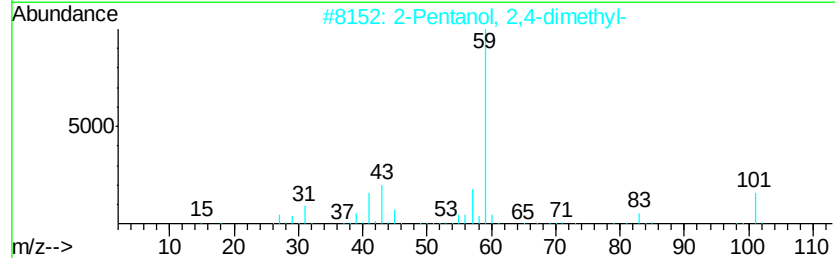
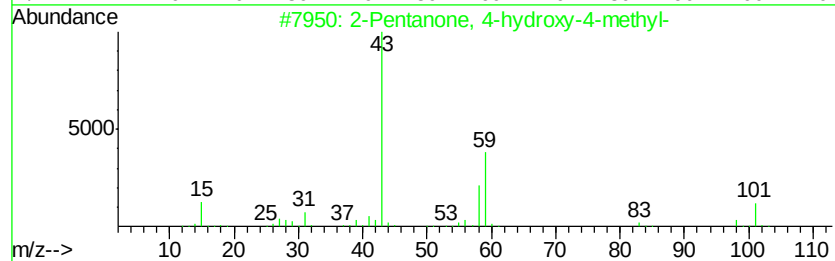
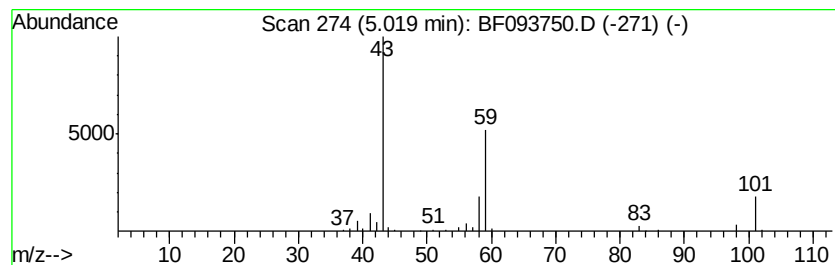
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.02	3.71 ng	220646	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	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	28
3	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	23
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9



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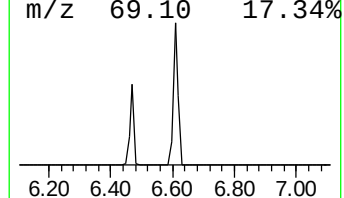
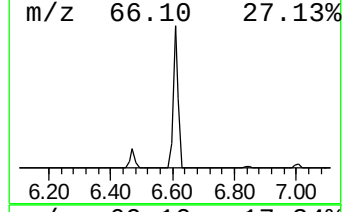
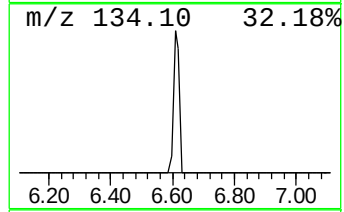
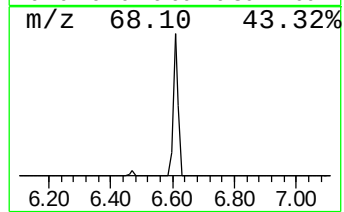
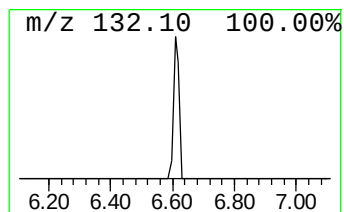
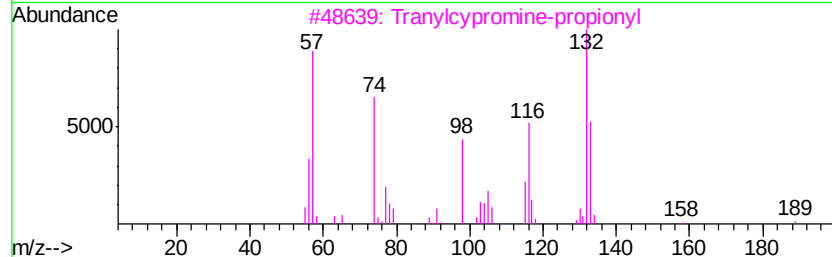
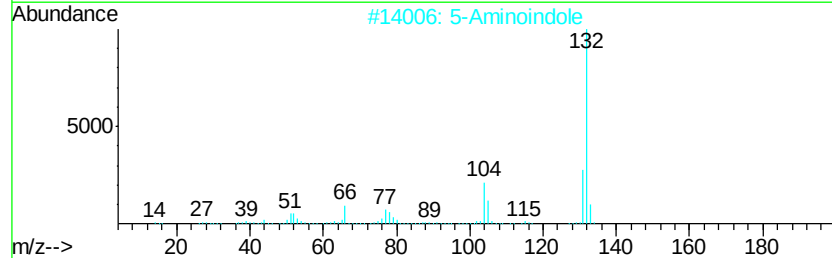
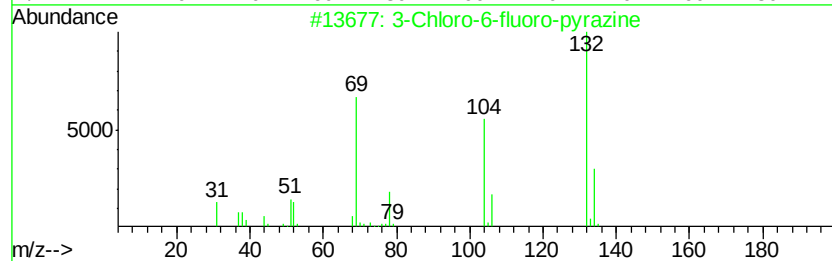
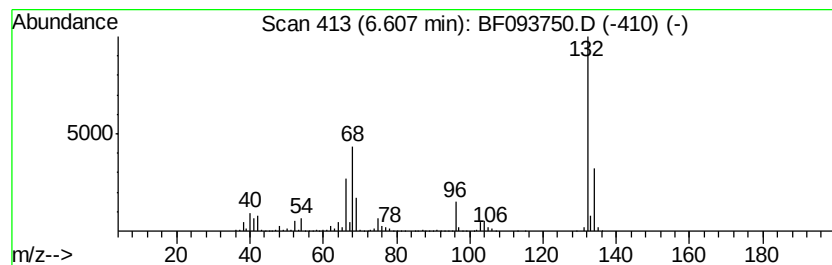
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Peak Number 2 unknown6.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	67.92 ng	4043110	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		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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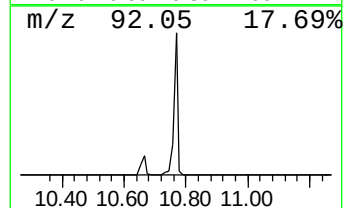
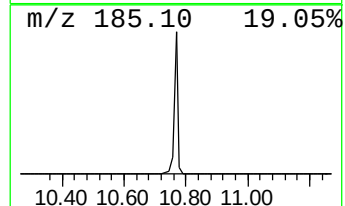
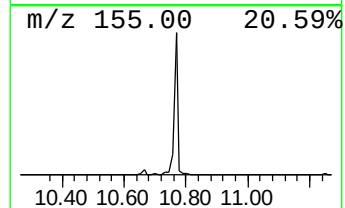
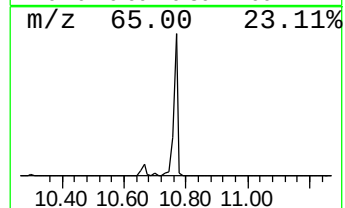
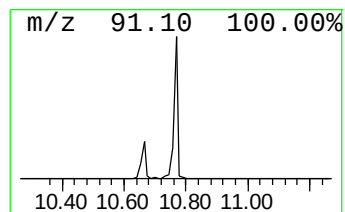
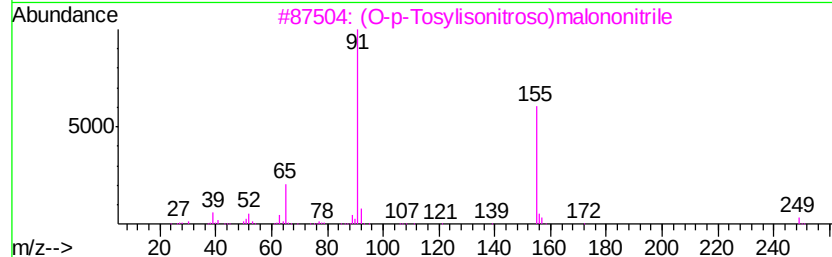
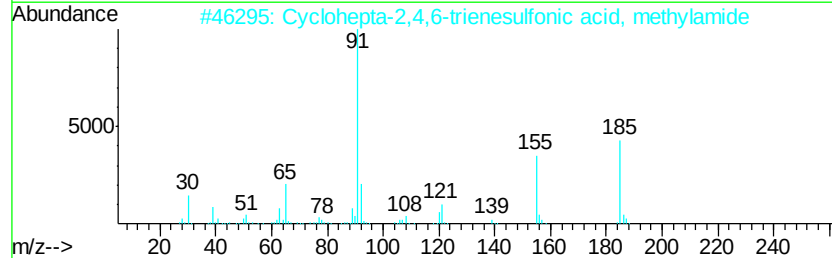
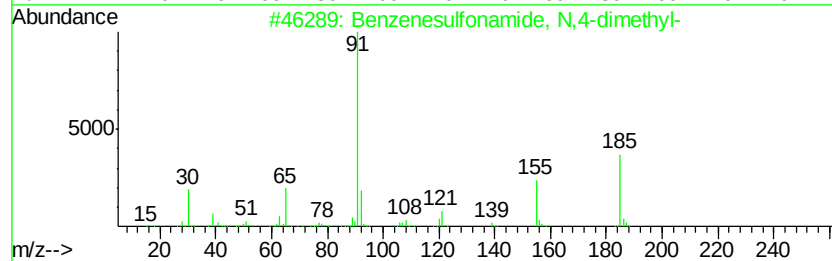
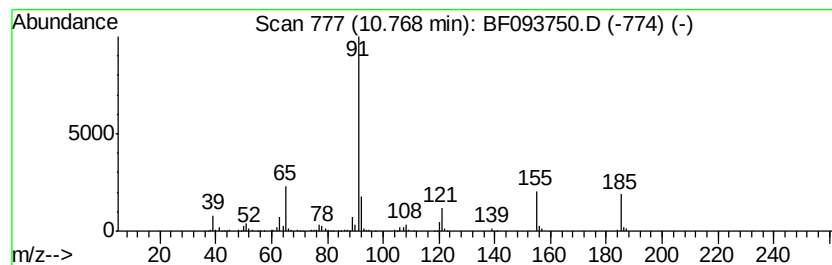
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Peak Number 4 Benzenesulfonamide, N,4-dim... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.77	4.77 ng	411781	Phenanthrene-d10	11.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzenesulfonamide, N,4-dimethyl-	185	C8H11NO2S	000640-61-9	93
2		Cyclohepta-2,4,6-trienesulfonic ...	185	C8H11NO2S	1000187-28-7	62
3		(O-p-Tosylisonitroso)malononitrile	249	C10H7N3O3S	020893-01-0	47
4		4-Toluenesulfonylmethylisocyanide	195	C9H9NO2S	036635-61-7	47
5		Toluene-4-sulfonic acid, 2-benzy...	366	C18H22O6S	118653-93-3	43



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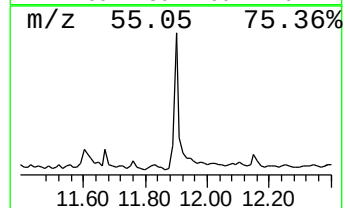
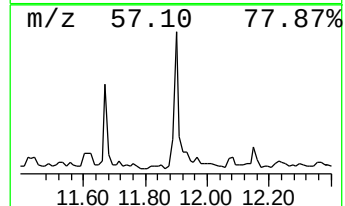
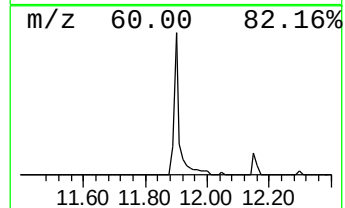
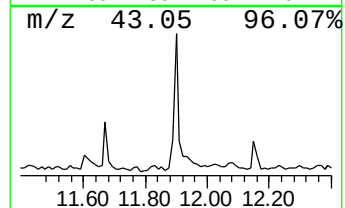
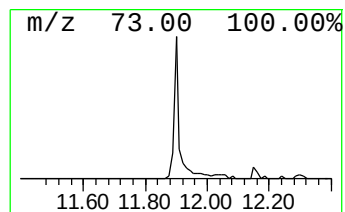
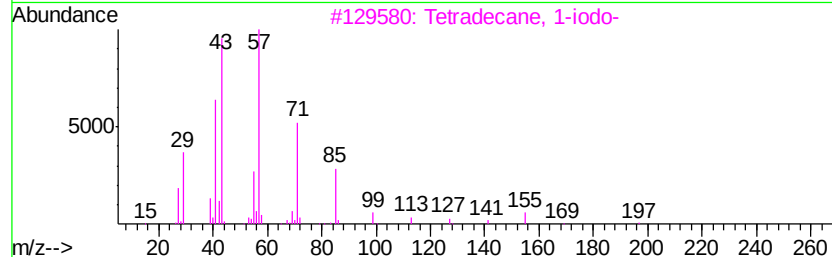
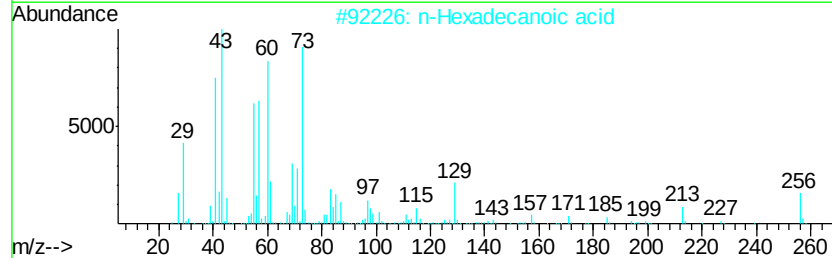
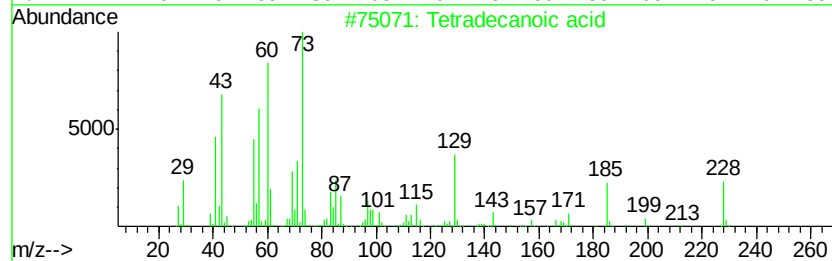
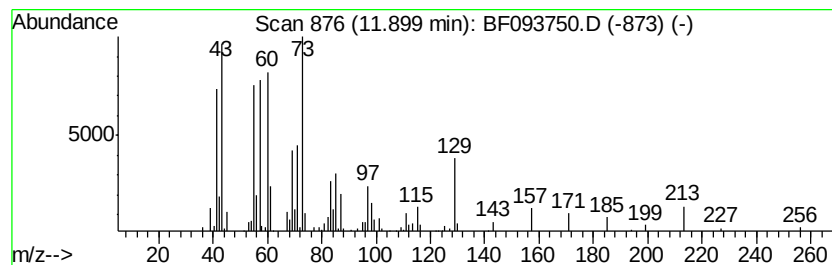
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 Tetradecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.90	3.02 ng	260604	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	49
3	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	11
4	Tridecane	184	C13H28	000629-50-5	11
5	Dodecane	170	C12H26	000112-40-3	11



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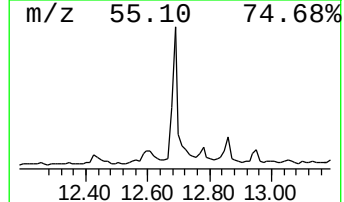
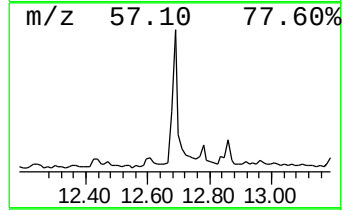
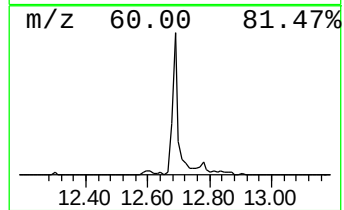
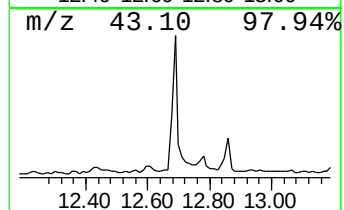
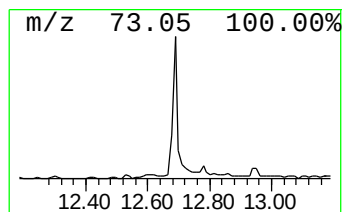
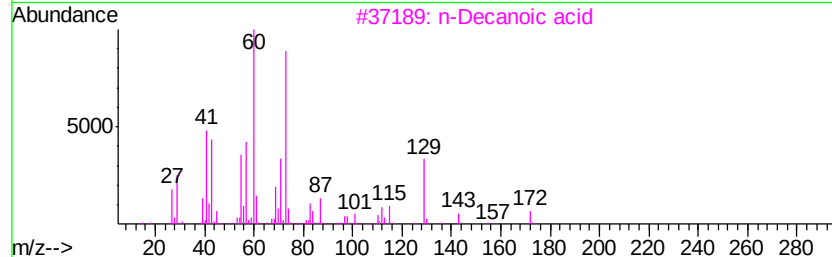
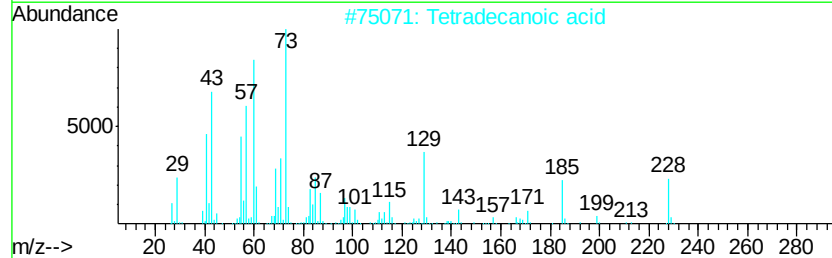
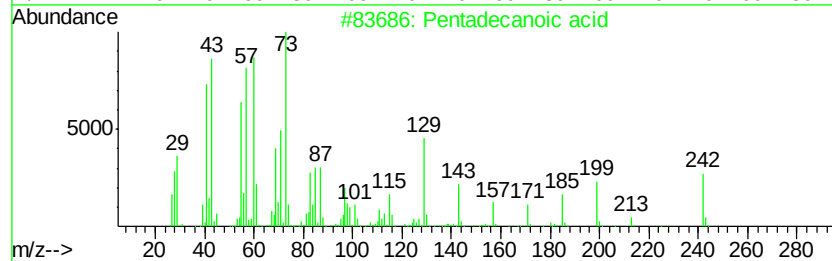
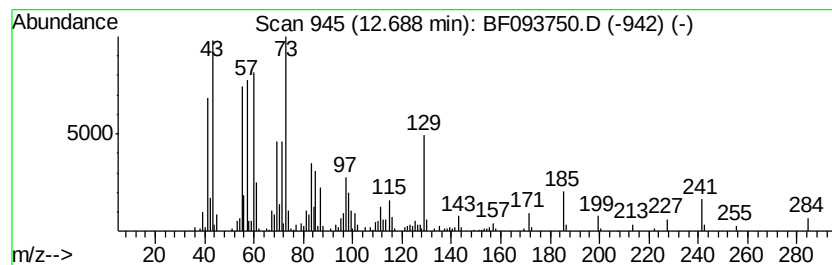
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Peak Number 6 Pentadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.69	5.41 ng	456877	Chrysene-d12		13.99	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
3		n-Decanoic acid	172	C10H20O2	000334-48-5	70
4		Undecanoic acid	186	C11H22O2	000112-37-8	43
5		Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	38



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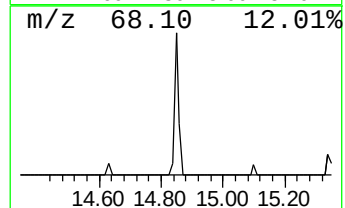
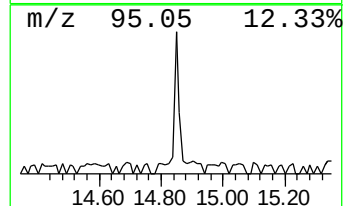
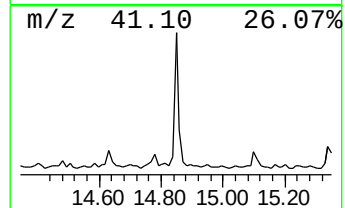
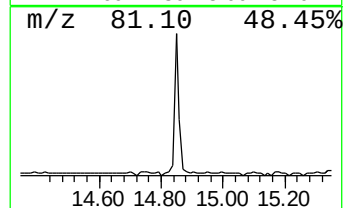
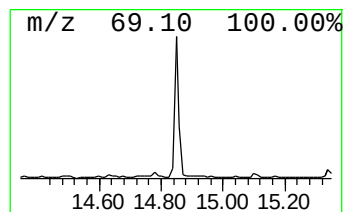
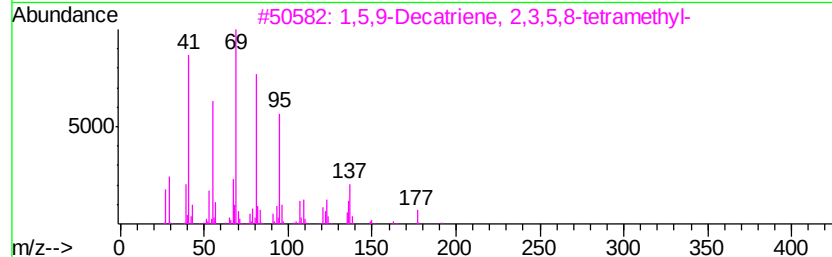
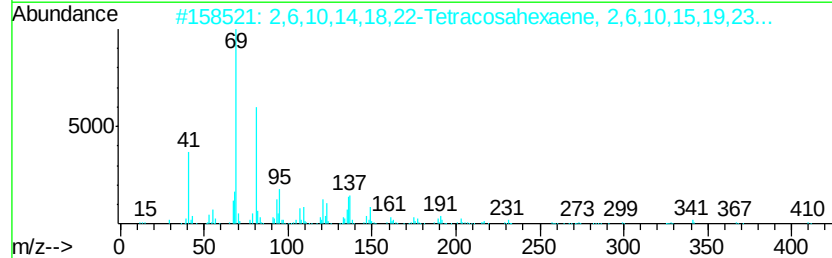
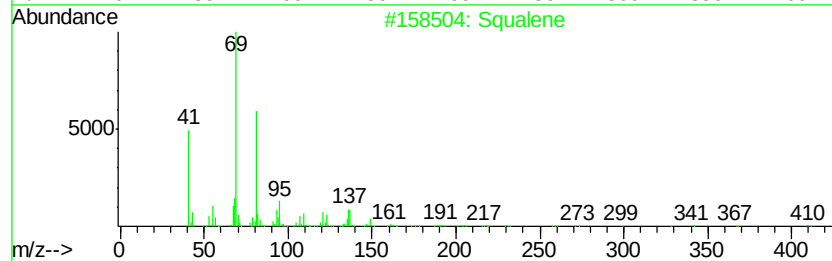
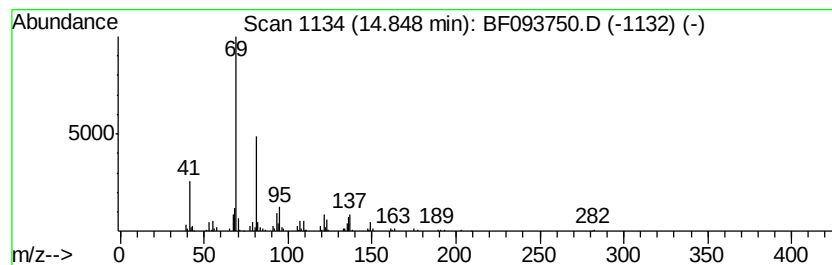
Instrument :
BNA_F
ClientSampleId :
MW-102D

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 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.85	2.44 ng	153097	Perylene-d12	15.41
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Squalene	410 C30H50	007683-64-9	91
2	2,6,10,14,18,22-Tetracosahexaene...	410 C30H50	000111-02-4	90
3	1,5,9-Decatriene, 2,3,5,8-tetram...	192 C14H24	230646-72-7	72
4	2,6,10-Dodecatrien-1-ol, 3,7,11-...	264 C17H28O2	004128-17-0	72
5	7,11-Dimethyldodeca-2,6,10-trien...	208 C14H24O	125529-10-4	72



Data Path : Z:\HPCHEM1\BNA_F\Data\BF031817\
Data File : BF093750.D
Acq On : 18 Mar 2017 13:33
Operator : SJ/MA
Sample : I2263-09
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-102D

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	3.7	ng	220646	1	6.85	1190580	20.0
unknown6.61	6.61	67.9	ng	4043110	1	6.85	1190580	20.0
Benzenesulfonamid...	10.77	4.8	ng	411781	4	11.36	1726950	20.0
Tetradecanoic acid	11.90	3.0	ng	260604	4	11.36	1726950	20.0
Pentadecanoic acid	12.69	5.4	ng	456877	5	13.99	1690510	20.0
Squalene	14.85	2.4	ng	153097	6	15.41	1257180	20.0