

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091817\
 Data File : BF098623.D
 Acq On : 19 Sep 2017 1:44
 Operator : SJ/JU
 Sample : I5260-04
 Misc :
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 091317-SIDI-E-U-S

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-BF091117.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	4.804	458	462	474	rBV	196863	243066	4.92%	0.918%
2	5.240	533	536	551	rBV	1084121	1238256	25.07%	4.679%
3	6.287	711	714	728	rBV	919414	940572	19.04%	3.554%
4	6.404	730	734	746	rVB	2510038	2414085	48.88%	9.122%
5	6.634	769	773	782	rBV	1027132	854063	17.29%	3.227%
6	6.792	795	800	803	rBV	3177499	3012478	60.99%	11.383%
7	7.210	865	871	874	rBV	2484520	2369343	47.97%	8.953%
8	7.916	987	991	999	rBV	1246902	1095176	22.17%	4.138%
9	8.998	1169	1175	1178	rBV	5296756	4939250	100.00%	18.664%
10	9.392	1239	1242	1246	rBV	166591	127880	2.59%	0.483%
11	9.669	1285	1289	1299	rVB	1431811	1240169	25.11%	4.686%
12	10.457	1419	1423	1435	rVB	1570608	1409106	28.53%	5.325%
13	11.151	1537	1541	1544	rBV	1250383	1041373	21.08%	3.935%
14	12.733	1805	1810	1814	rBV	3472419	3401345	68.86%	12.853%
15	13.786	1985	1989	1999	rVB	852879	799424	16.19%	3.021%
16	15.180	2221	2226	2235	rBV	640620	756954	15.33%	2.860%
17	15.574	2288	2293	2299	rBV	54908	87259	1.77%	0.330%
18	16.021	2365	2369	2376	rVB	64225	105500	2.14%	0.399%
19	16.539	2452	2457	2467	rVB	45480	91853	1.86%	0.347%
20	17.157	2556	2562	2575	rVB3	45482	125560	2.54%	0.474%
21	17.886	2675	2686	2694	rBV7	30901	100989	2.04%	0.382%
22	18.739	2823	2831	2843	rBV9	19290	70575	1.43%	0.267%

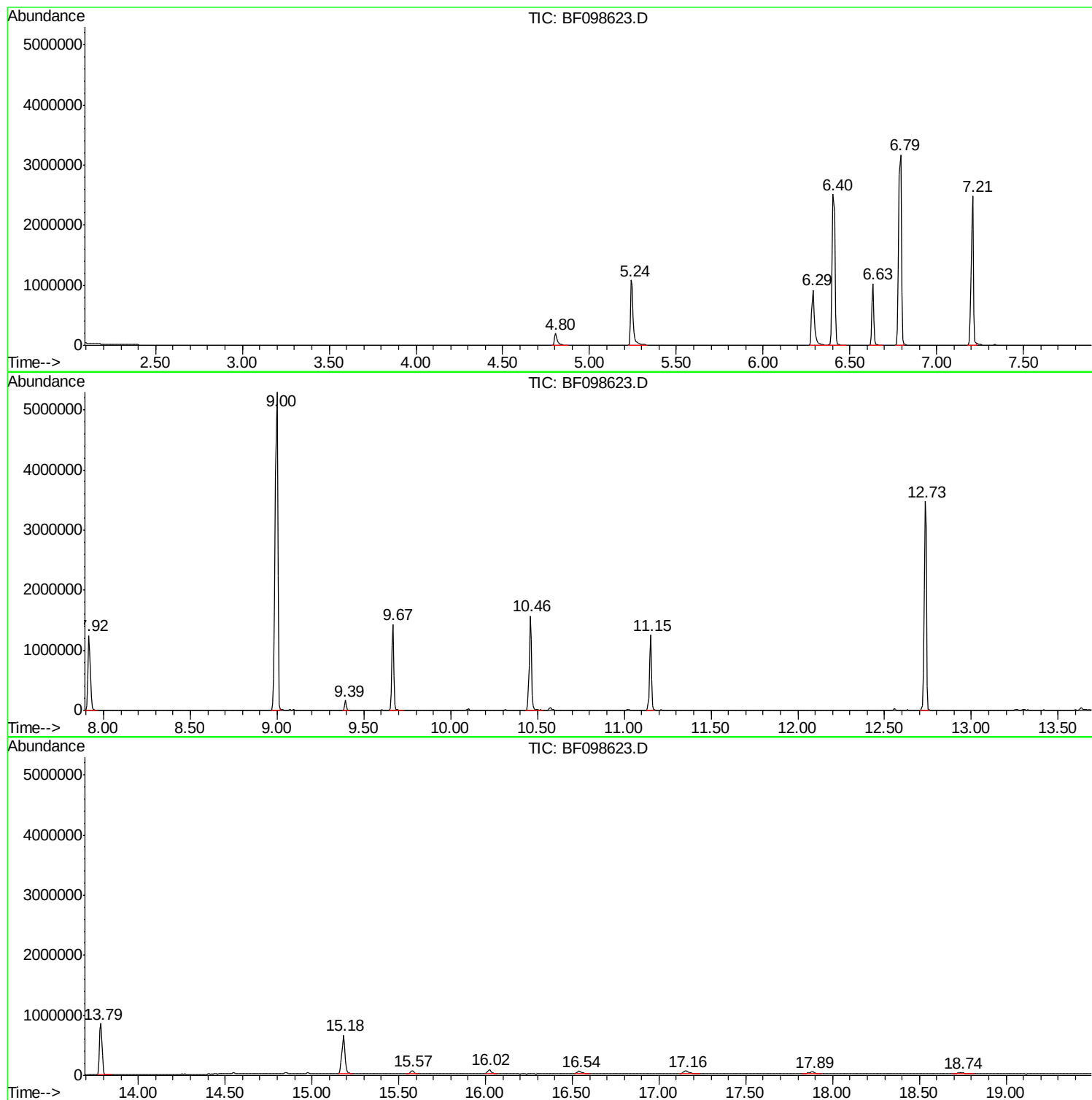
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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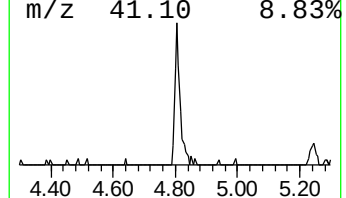
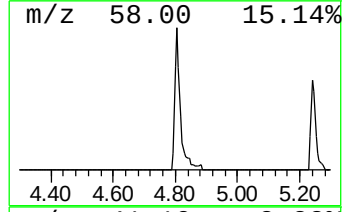
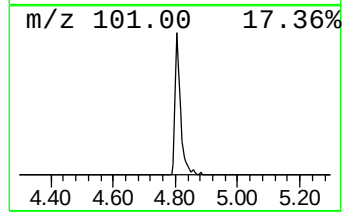
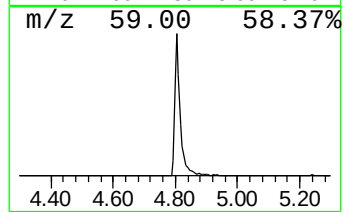
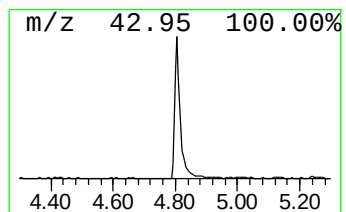
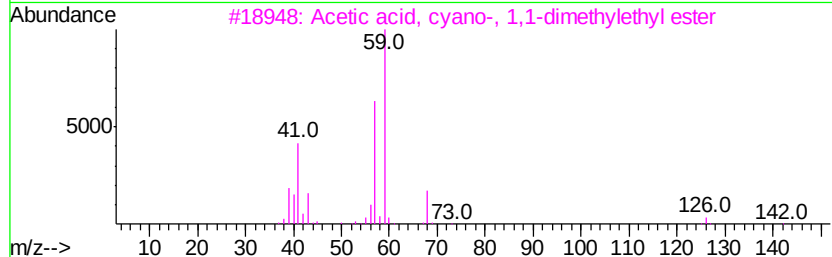
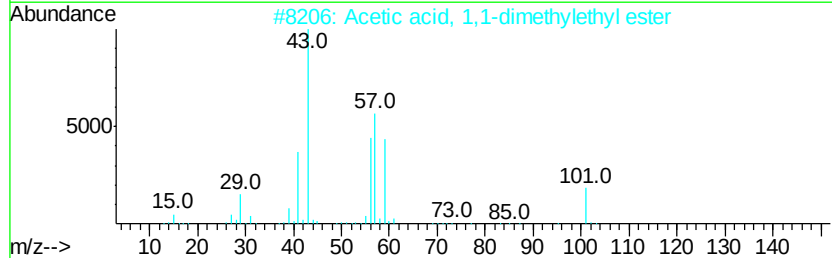
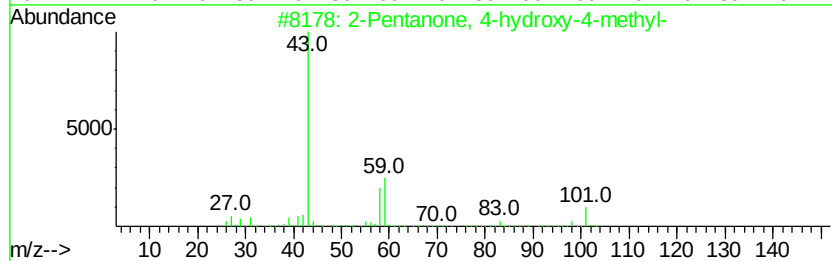
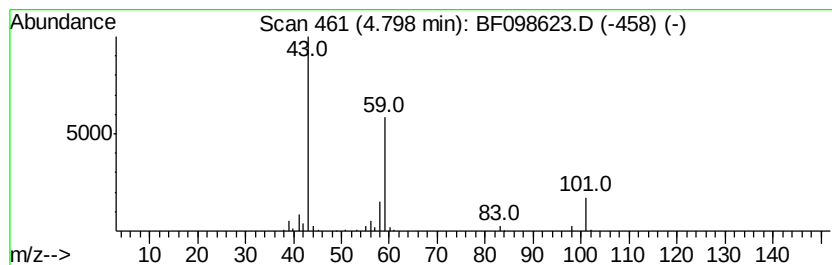
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.80	5.69 ng	243066	1,4-Dichlorobenzene-d4	6.63

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, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	37
4			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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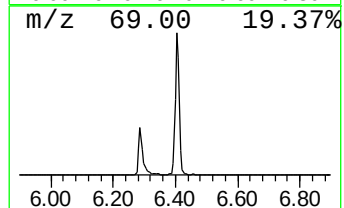
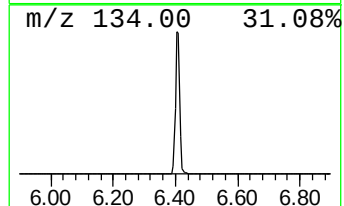
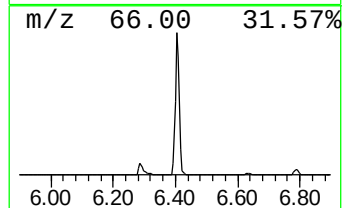
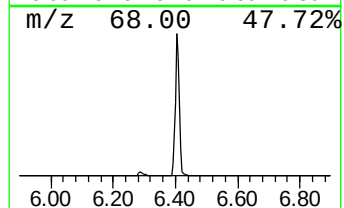
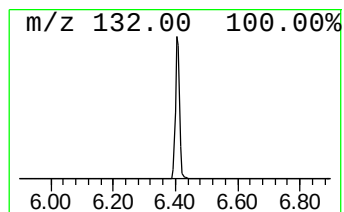
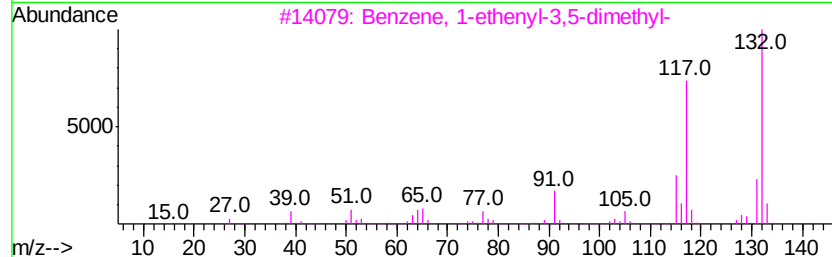
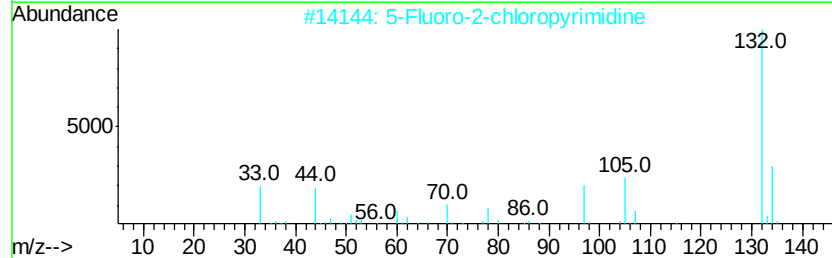
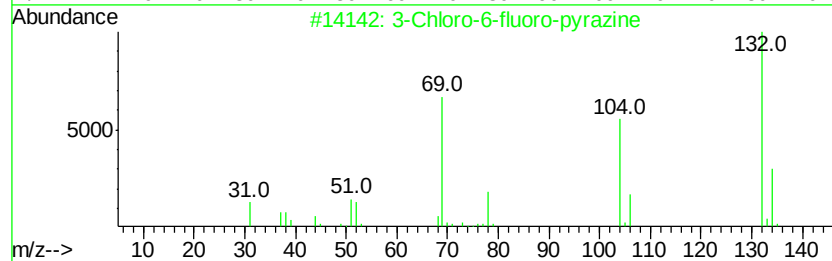
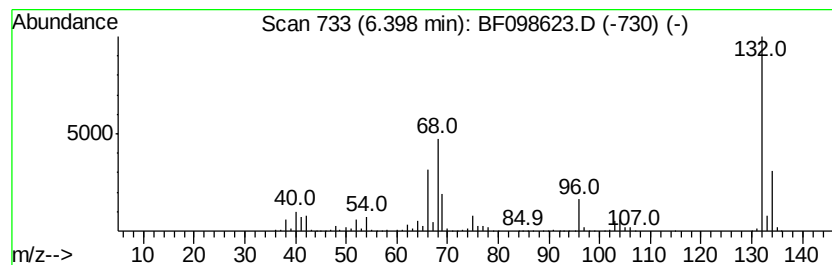
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.40 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.40	56.53 ng	2414090	1,4-Dichlorobenzene-d4	6.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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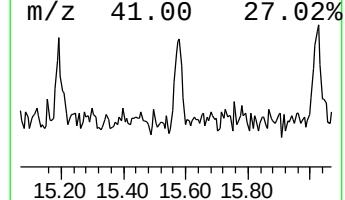
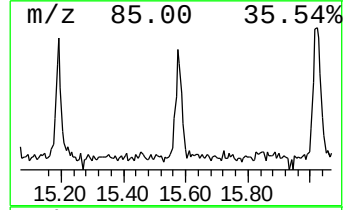
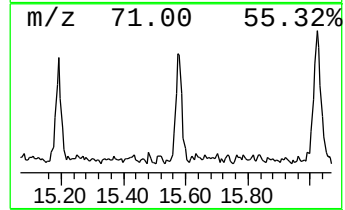
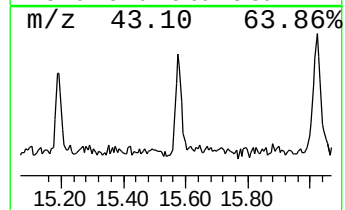
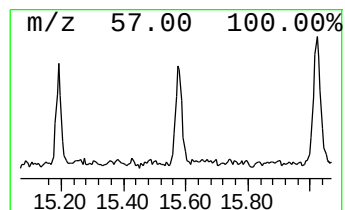
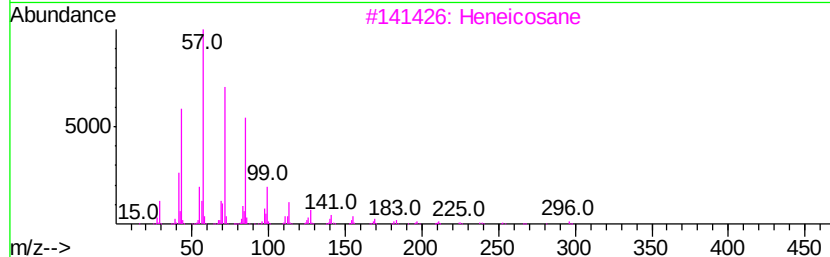
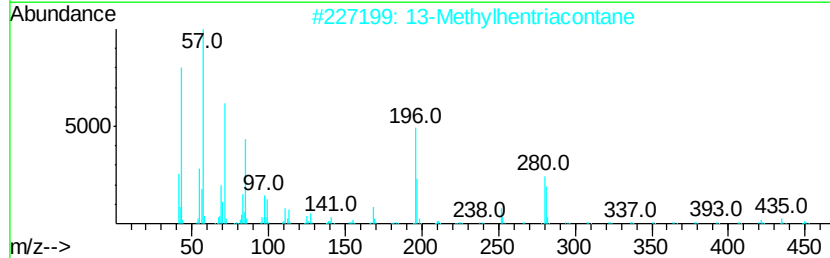
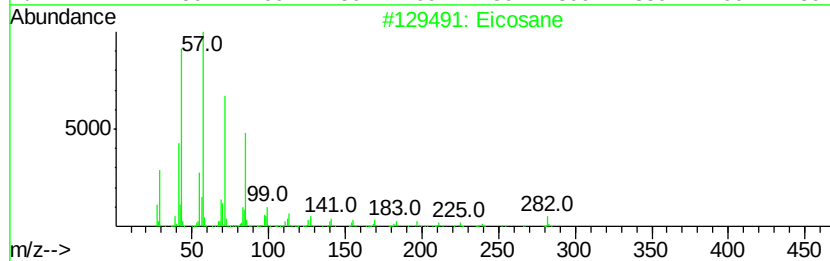
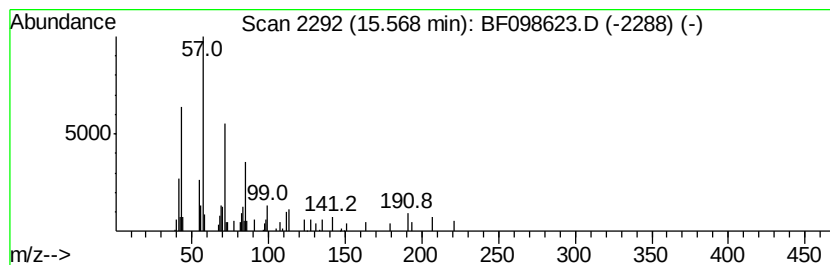
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Peak Number 4 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.57	2.31 ng	87259	Perylene-d12	15.18

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	90
2	13-Methylhentriacontane		451	C32H66	1000131-19-4	86
3	Heneicosane		296	C21H44	000629-94-7	83
4	Octacosane		394	C28H58	000630-02-4	83
5	Nonadecane, 2-methyl-		282	C20H42	001560-86-7	80



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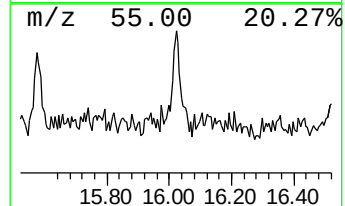
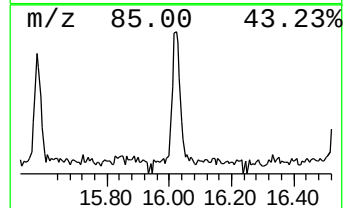
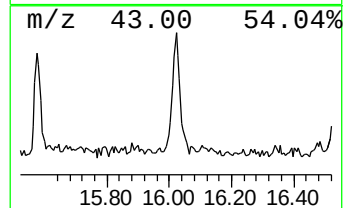
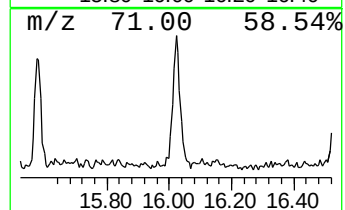
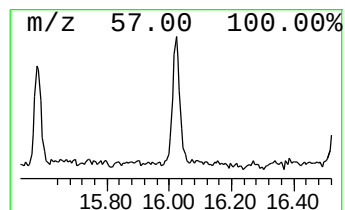
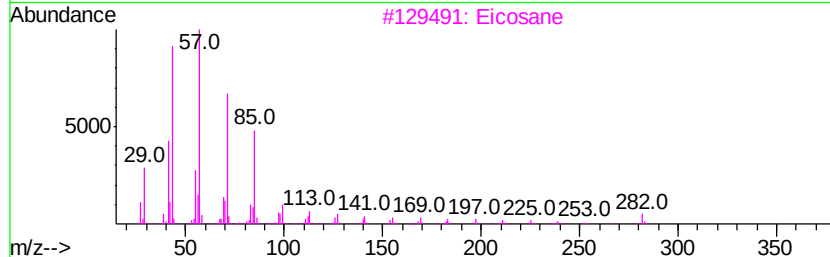
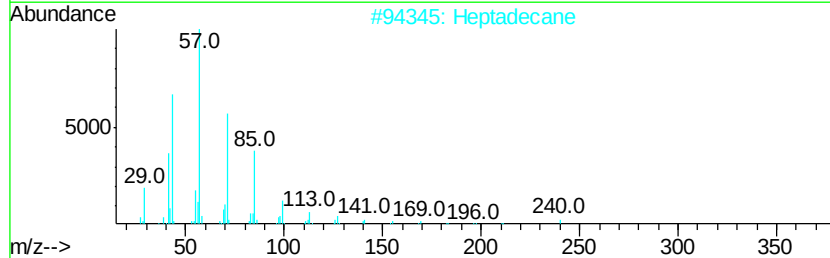
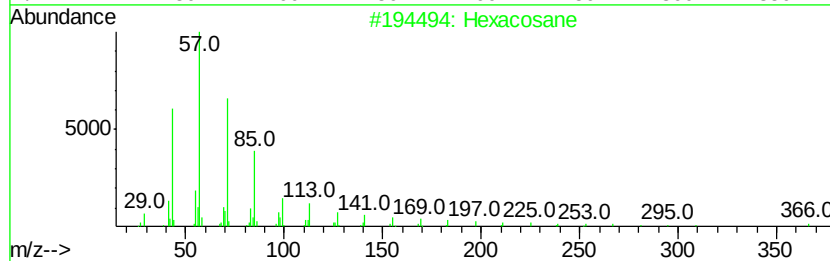
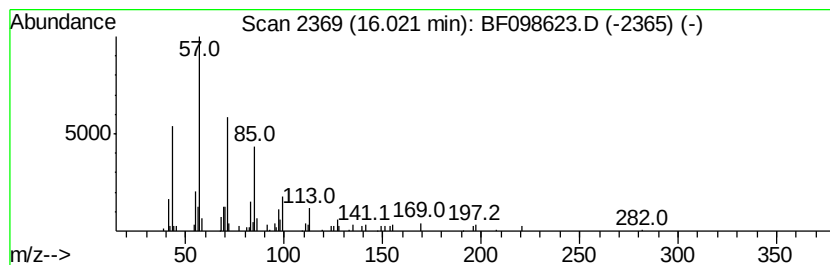
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.02	2.79 ng	105500	Perylene-d12	15.18

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	91
2		Heptadecane	240	C17H36	000629-78-7	90
3		Eicosane	282	C20H42	000112-95-8	90
4		Octacosane	394	C28H58	000630-02-4	90
5		Pentacosane	352	C25H52	000629-99-2	86



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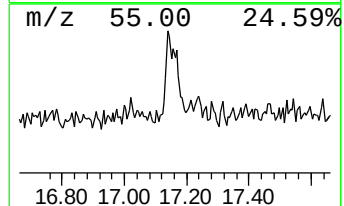
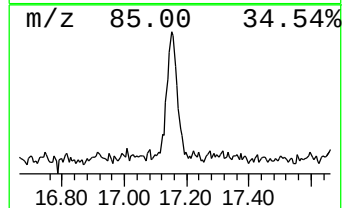
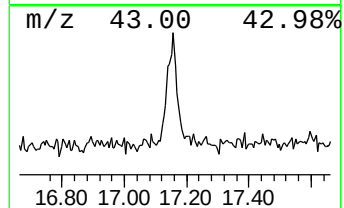
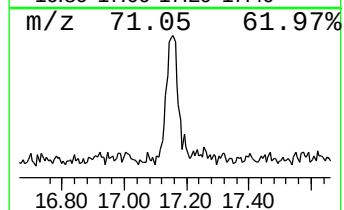
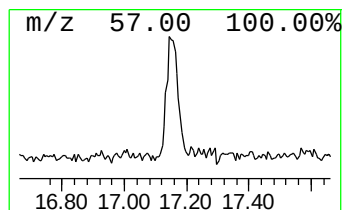
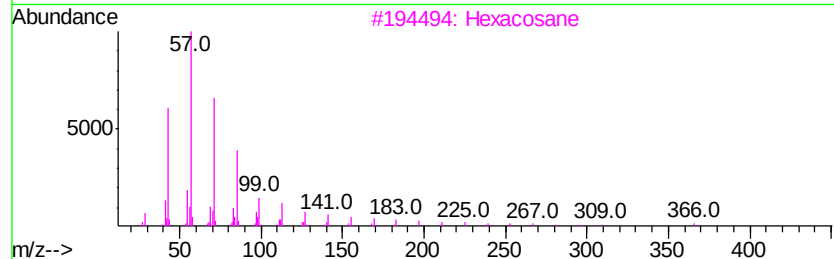
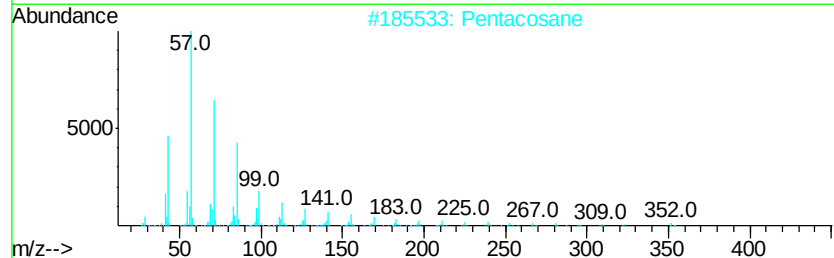
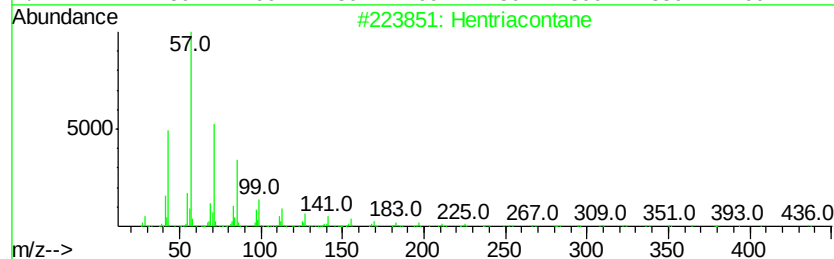
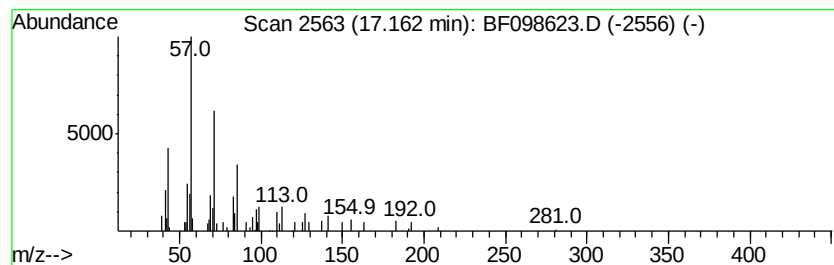
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Hentriacontane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.16	3.32 ng	125560	Perylene-d12	15.18

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hentriacontane	437	C31H64	000630-04-6	90
2		Pentacosane	352	C25H52	000629-99-2	86
3		Hexacosane	366	C26H54	000630-01-3	86
4		Octacosane	394	C28H58	000630-02-4	86
5		2-methyloctacosane	408	C29H60	1000376-72-8	86



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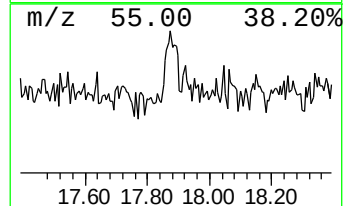
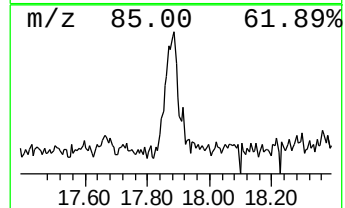
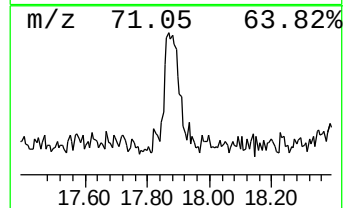
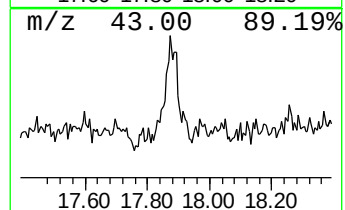
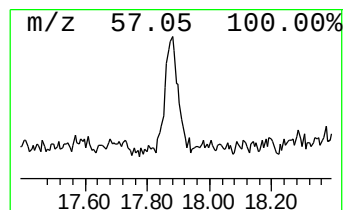
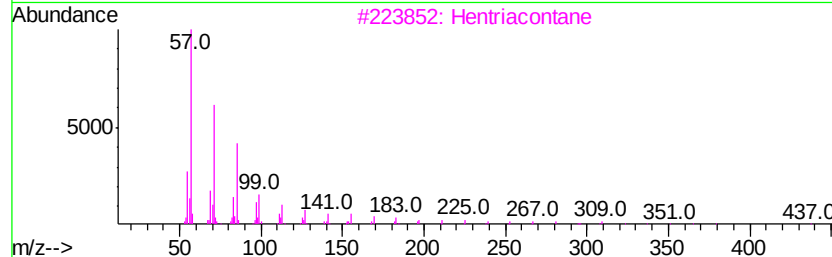
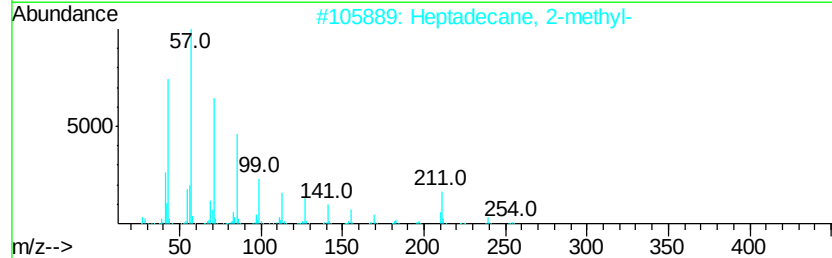
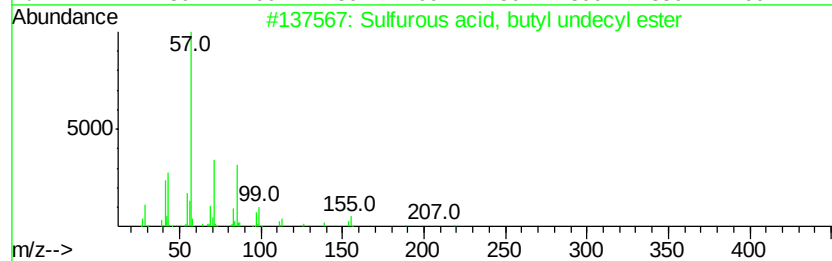
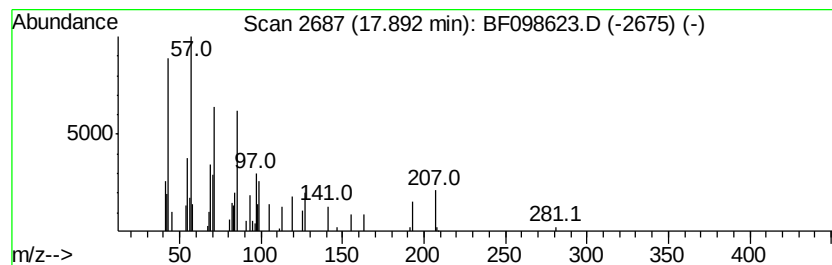
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown17.89 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.89	2.67 ng	100989	Perylene-d12	15.18

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfurous acid, butyl undecyl ester	292	C15H32O3S	1000309-17-8	47
2		Heptadecane, 2-methyl-	254	C18H38	001560-89-0	43
3		Hentriacontane	437	C31H64	000630-04-6	43
4		Octacosane	394	C28H58	000630-02-4	43
5		Tetratetracontane	619	C44H90	007098-22-8	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091817\
Data File : BF098623.D
Acq On : 19 Sep 2017 1:44
Operator : SJ/JU
Sample : I5260-04
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
091317-SIDI-E-U-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.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
2-Pentanone, 4-hy...	4.80	5.7	ng	243066	1	6.63	854063	20.0
unknown6.40	6.40	56.5	ng	2414090	1	6.63	854063	20.0
Eicosane	15.57	2.3	ng	87259	6	15.18	756954	20.0
Hexacosane	16.02	2.8	ng	105500	6	15.18	756954	20.0
Hentriacontane	17.16	3.3	ng	125560	6	15.18	756954	20.0
unknown17.89	17.89	2.7	ng	100989	6	15.18	756954	20.0