

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012517\
 Data File : BF092491.D
 Acq On : 25 Jan 2017 21:57
 Operator : SJ/MA
 Sample : I1398-06
 Misc :
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-7-012017

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-BF012417.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	5.138	265	267	270	rBV	501127	557598	11.24%	1.593%
2	5.550	300	303	306	rBV	1994534	1949285	39.31%	5.570%
3	6.579	390	393	395	rBV	1520612	1481569	29.88%	4.234%
4	6.727	403	406	408	rBV	3496260	3294095	66.43%	9.413%
5	6.967	424	427	429	rBV	994353	1000399	20.17%	2.859%
6	7.127	438	441	443	rVB	2643956	3192828	64.39%	9.124%
7	7.527	473	476	479	rBV	2245489	2615857	52.75%	7.475%
8	8.259	537	540	542	rBV	1402358	1328877	26.80%	3.797%
9	9.345	631	635	637	rBV	4507856	4764841	96.09%	13.616%
10	10.019	691	694	697	rBV	1569138	1447097	29.18%	4.135%
11	10.453	728	732	734	rVB	48991	54402	1.10%	0.155%
12	10.808	760	763	766	rBV2	2194431	2777365	56.01%	7.937%
13	10.933	772	774	777	rVB	47386	73501	1.48%	0.210%
14	11.505	822	824	827	rBV	1495564	1452873	29.30%	4.152%
15	12.042	868	871	873	rBV	105617	142756	2.88%	0.408%
16	12.831	937	940	946	rBV2	36511	71872	1.45%	0.205%
17	13.105	960	964	966	rBV	3808217	4958934	100.00%	14.171%
18	13.996	1040	1042	1050	rBV	113783	172106	3.47%	0.492%
19	14.145	1052	1055	1058	rBV	1554546	1460643	29.45%	4.174%
20	15.277	1152	1154	1160	rVB	37219	58197	1.17%	0.166%
21	15.620	1181	1184	1187	rBV	917478	1221711	24.64%	3.491%
22	15.665	1187	1188	1194	rVB	77184	105473	2.13%	0.301%
23	16.111	1224	1227	1231	rBV	82582	140223	2.83%	0.401%
24	16.637	1269	1273	1281	rVB	95485	196517	3.96%	0.562%
25	17.243	1322	1326	1333	rBV	76298	184635	3.72%	0.528%
26	17.963	1384	1389	1397	rBV	64907	184052	3.71%	0.526%
27	18.820	1459	1464	1469	rBV	35037	106644	2.15%	0.305%

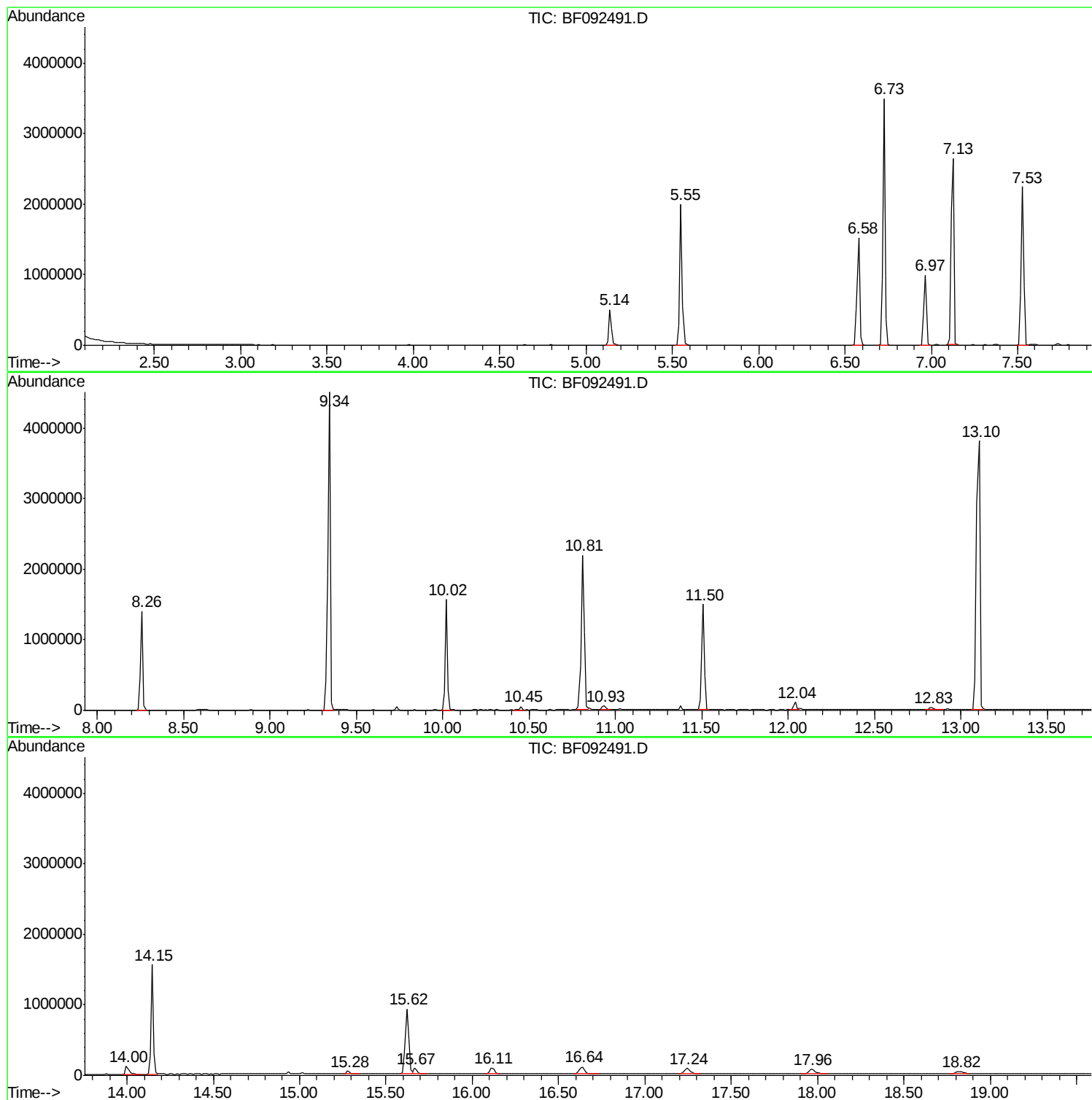
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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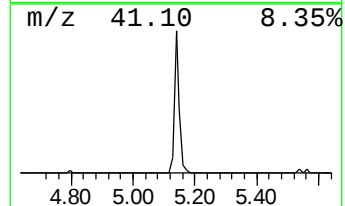
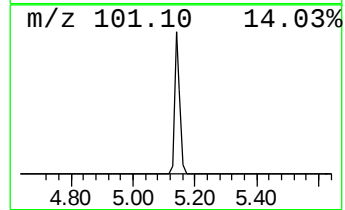
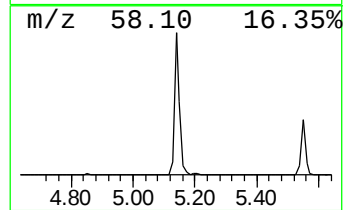
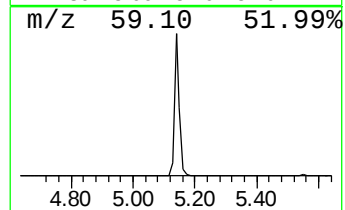
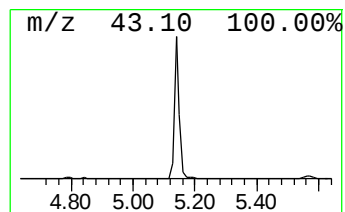
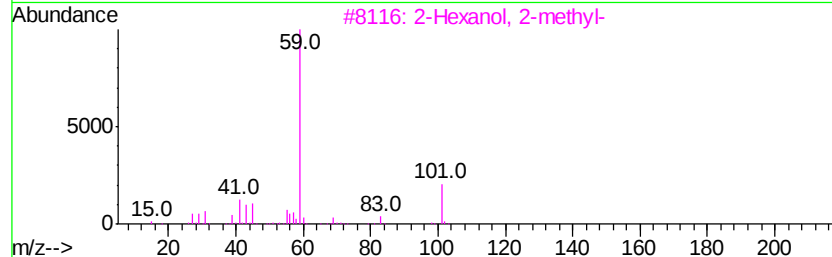
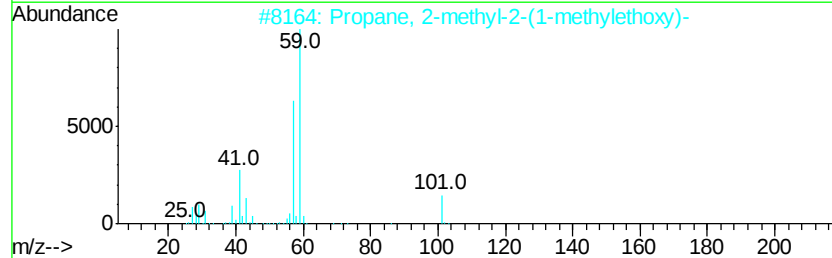
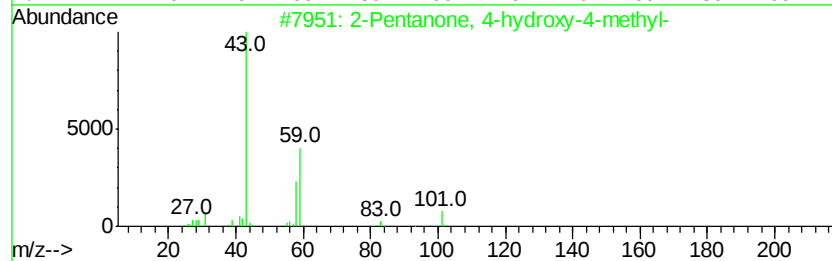
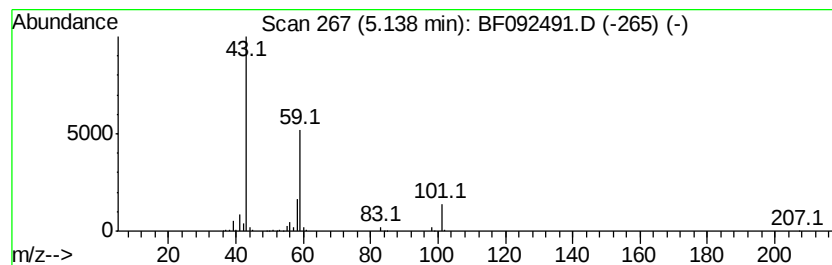
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	11.15 ng	557598	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Propane, 2-methyl-2-(1-methylethoxy)-	116	C7H16O	017348-59-3	36
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5		Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	25



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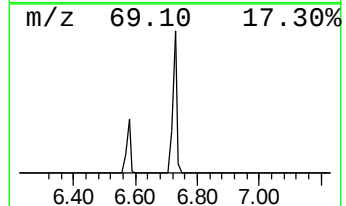
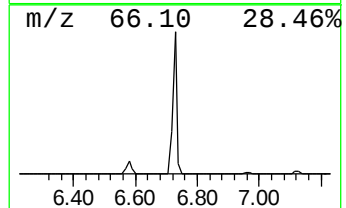
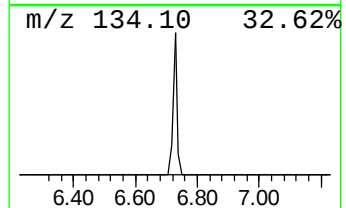
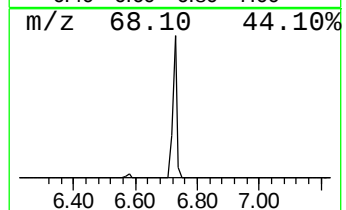
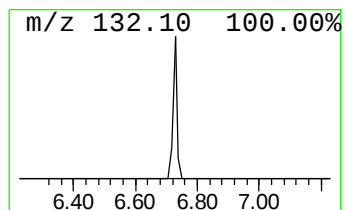
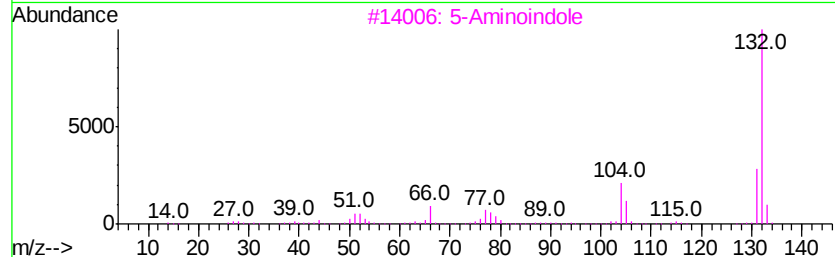
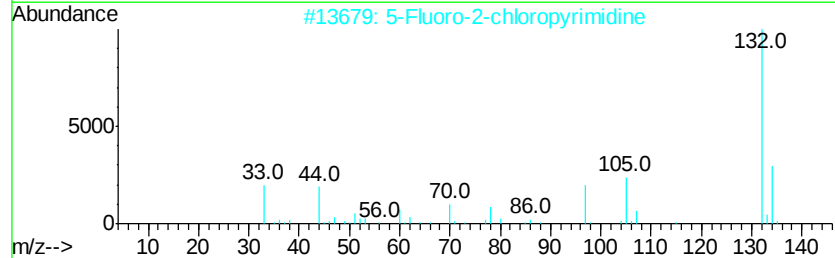
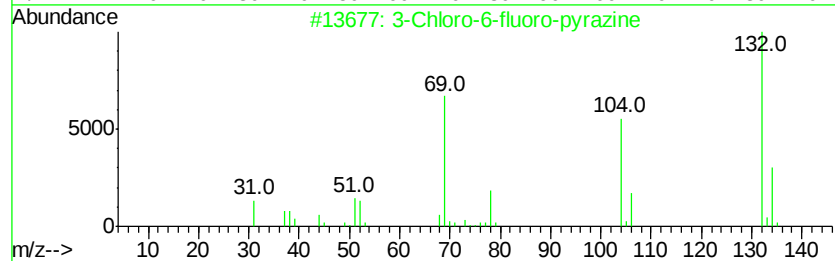
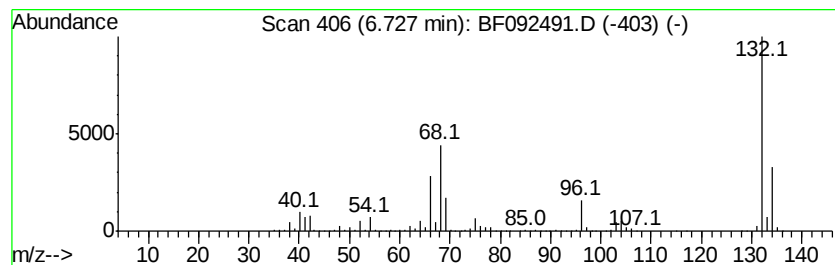
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown6.73 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	65.86 ng	3294100	1,4-Dichlorobenzene-d4	6.97

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3			5-Aminoindole	132	C8H8N2	005192-03-0	12
4			Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5			2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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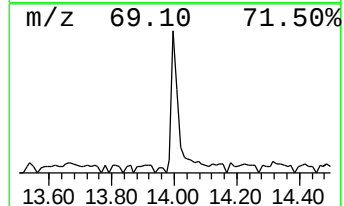
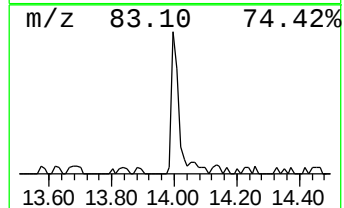
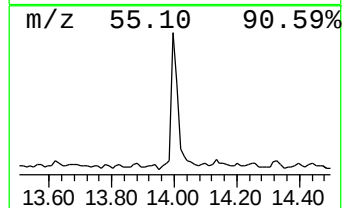
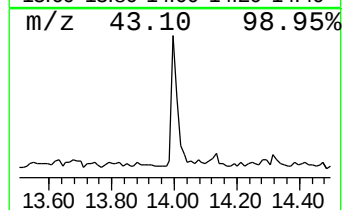
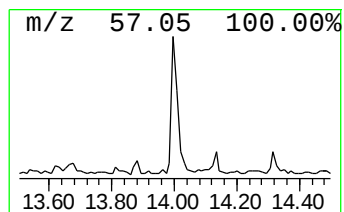
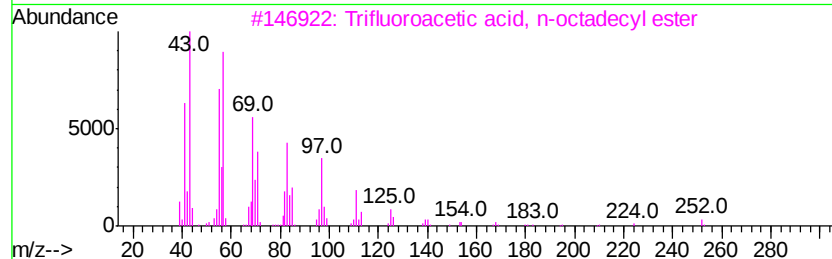
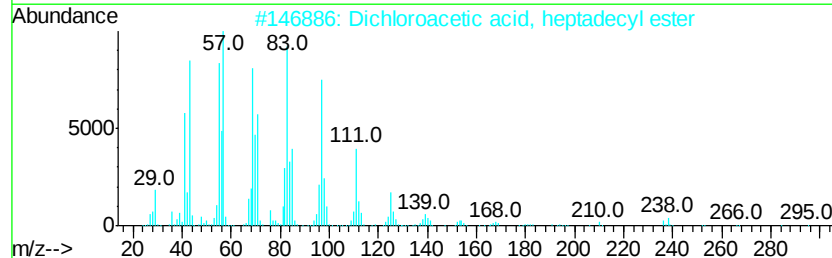
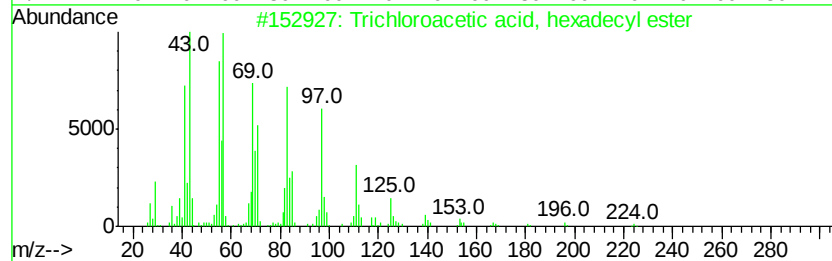
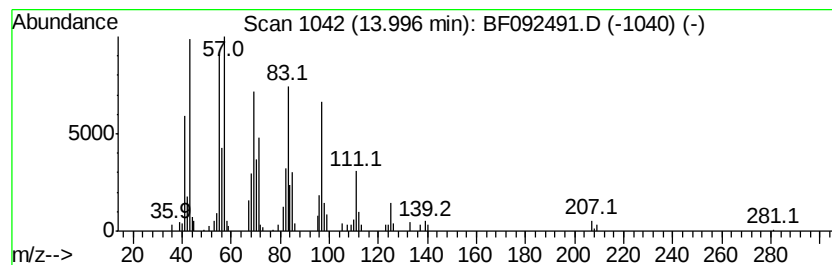
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Peak Number 4 Trichloroacetic acid, hexad... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.00	2.36 ng	172106	Chrysene-d12	14.15

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	95
2		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91
3		Trifluoroacetic acid, n-octadecyl ...	366	C20H37F3O2	079392-43-1	91
4		Heptafluorobutyric acid, n-octadecyl ...	466	C22H37F7O2	000400-57-7	91
5		1-Docosene	308	C22H44	001599-67-3	91



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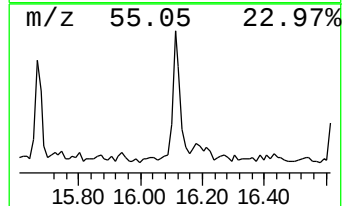
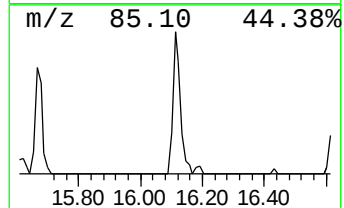
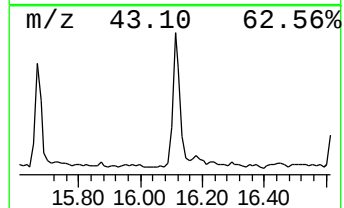
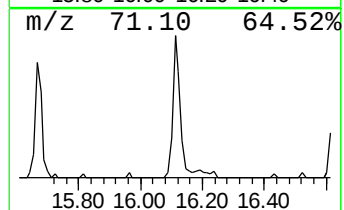
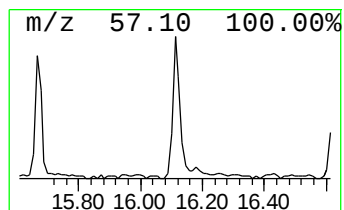
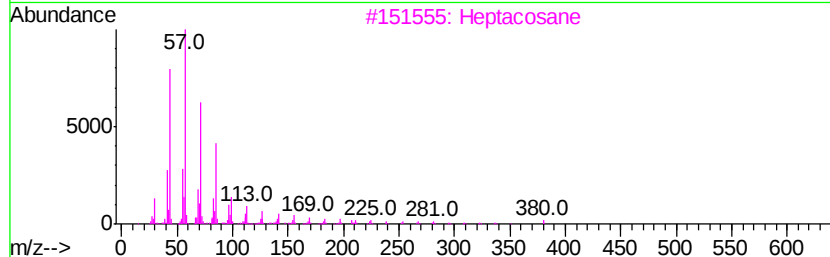
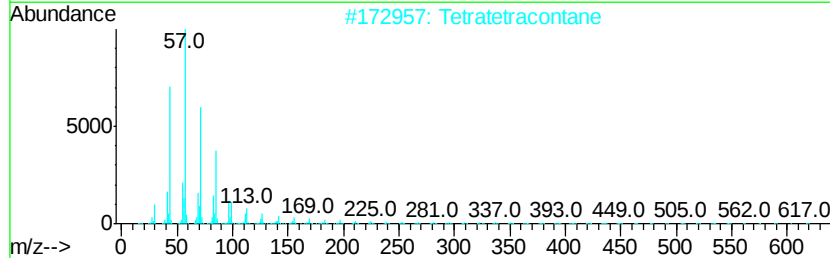
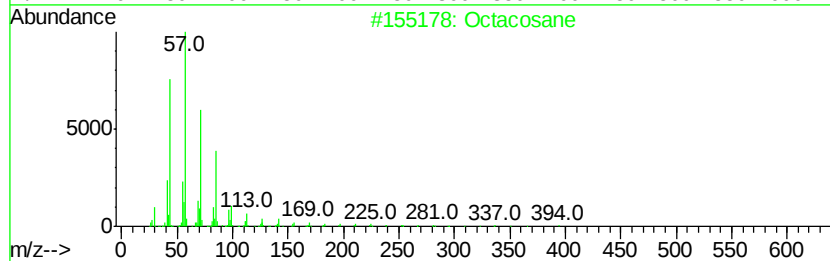
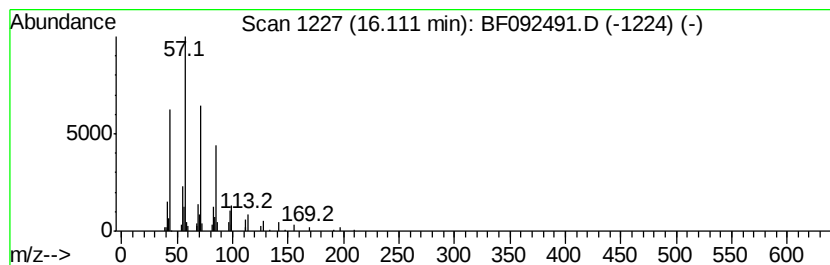
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.11	2.30 ng	140223	Perylene-d12	15.62

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane		394	C28H58	000630-02-4	91
2	Tetratetracontane		619	C44H90	007098-22-8	91
3	Heptacosane		380	C27H56	000593-49-7	91
4	Tetracosane		338	C24H50	000646-31-1	91
5	Nonacosane		408	C29H60	000630-03-5	90



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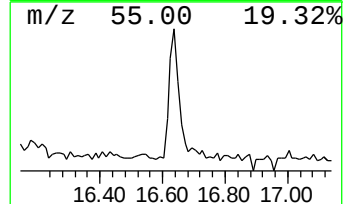
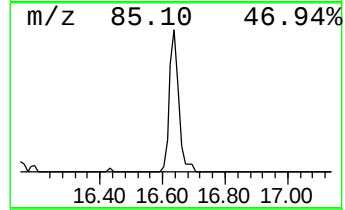
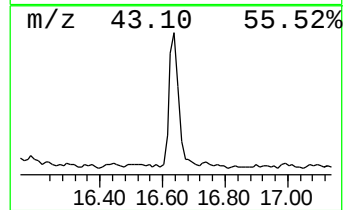
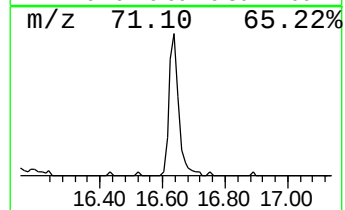
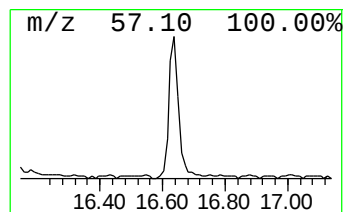
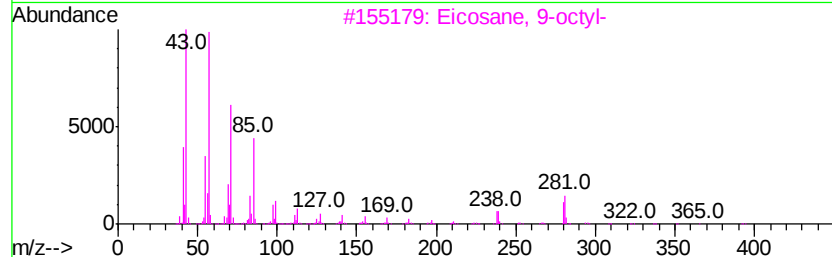
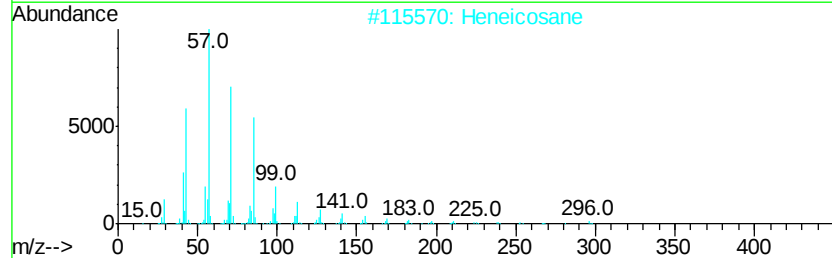
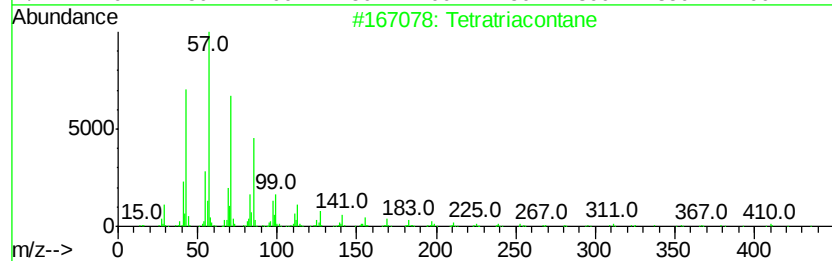
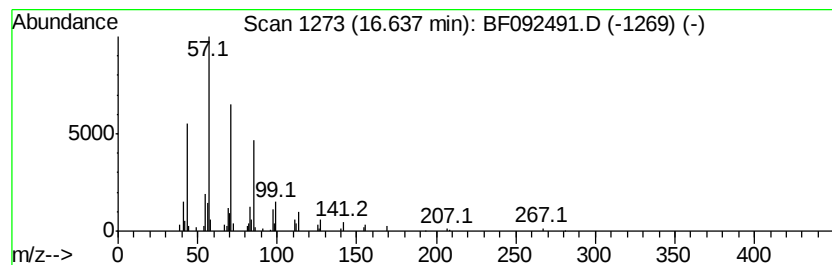
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 Tetratriacontane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.64	3.22 ng	196517	Perylene-d12	15.62

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetratriacontane	479	C34H70	014167-59-0	91
2			Heneicosane	296	C21H44	000629-94-7	91
3			Eicosane, 9-octyl-	394	C28H58	013475-77-9	91
4			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	91
5			Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	91



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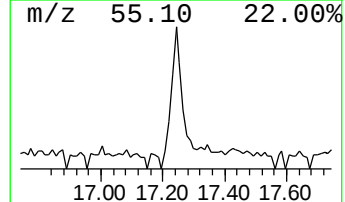
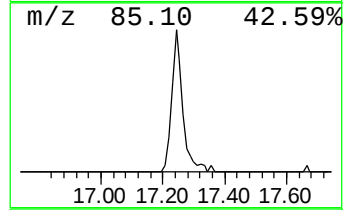
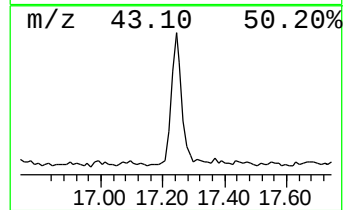
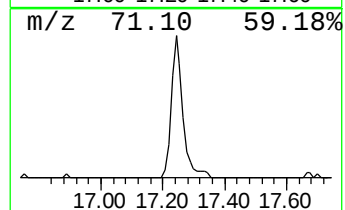
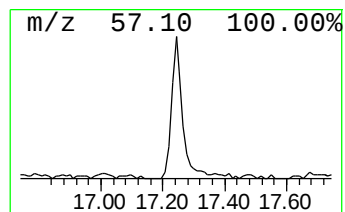
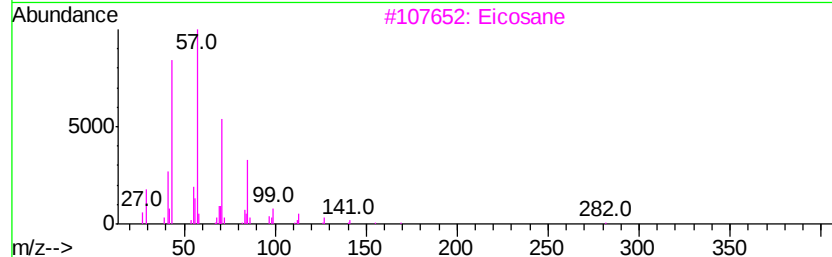
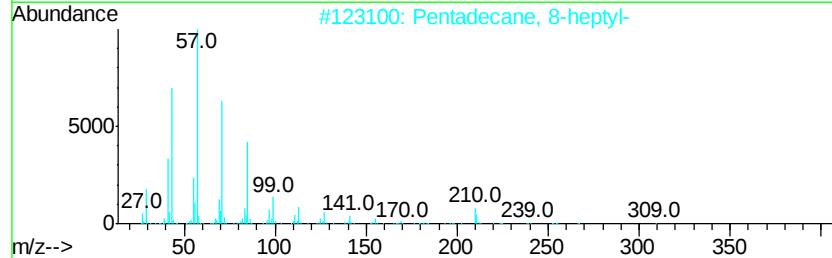
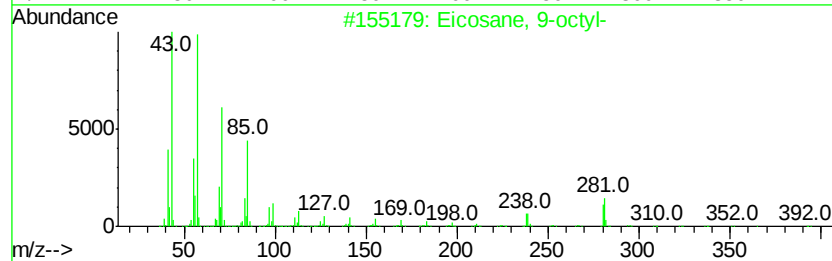
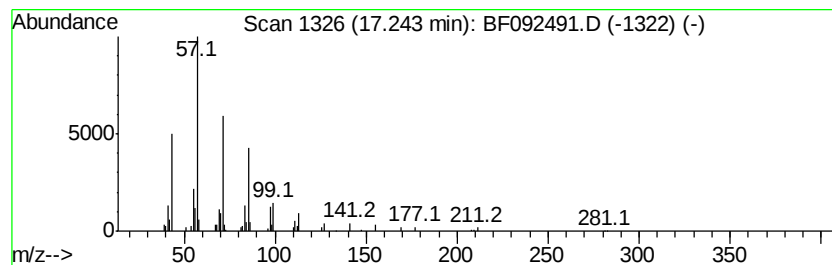
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Eicosane, 9-octyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.24	3.02 ng	184635	Perylene-d12	15.62

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane, 9-octyl-	394	C28H58	013475-77-9	90
2		Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	87
3		Eicosane	282	C20H42	000112-95-8	87
4		Octacosane	394	C28H58	000630-02-4	87
5		Heptacosane	380	C27H56	000593-49-7	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012517\
Data File : BF092491.D
Acq On : 25 Jan 2017 21:57
Operator : SJ/MA
Sample : I1398-06
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-7-012017

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.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...	5.14	11.2	ng	557598	1	6.97	1000400	20.0
unknown6.73	6.73	65.9	ng	3294100	1	6.97	1000400	20.0
Trichloroacetic a...	14.00	2.4	ng	172106	5	14.15	1460640	20.0
Octacosane	16.11	2.3	ng	140223	6	15.62	1221710	20.0
Tetratriacontane	16.64	3.2	ng	196517	6	15.62	1221710	20.0
Eicosane, 9-octyl-	17.24	3.0	ng	184635	6	15.62	1221710	20.0