

Data Path : Z:\HPCHEM1\BNA F\DATA\BF022717\
 Data File : BF093214.D
 Acq On : 27 Feb 2017 19:45
 Operator : SJ/MA
 Sample : I1997-06
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 E2-BB6-WSW

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-BF013017.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	3.116	88	90	101	rBV	61285	215033	4.05%	0.457%
2	3.699	138	141	145	rBV	371405	607274	11.45%	1.292%
3	4.990	251	254	264	rBV	1409717	2176854	41.04%	4.630%
4	5.424	289	292	295	rBV	4243589	4506278	84.95%	9.585%
5	6.476	380	384	386	rBV	3920037	5304430	100.00%	11.283%
6	6.590	391	394	396	rBV	4437309	4346753	81.95%	9.246%
7	6.819	412	414	416	rBV	854770	901707	17.00%	1.918%
8	6.967	425	427	430	rBV	2662059	3482824	65.66%	7.408%
9	7.390	461	464	466	rBV	3085566	3398234	64.06%	7.228%
10	7.493	469	473	479	rVB	49585	65357	1.23%	0.139%
11	8.099	524	526	529	rBV	1307750	1207966	22.77%	2.569%
12	9.185	617	621	623	rBV	4020701	4990700	94.09%	10.616%
13	9.573	653	655	658	rBV	1199461	1391911	26.24%	2.961%
14	9.791	671	674	677	rBV	41951	67765	1.28%	0.144%
15	9.859	677	680	682	rVB	1335308	1390571	26.22%	2.958%
16	10.282	713	717	719	rBV2	64345	95768	1.81%	0.204%
17	10.648	746	749	752	rBV	2298664	2768195	52.19%	5.888%
18	10.762	757	759	762	rBV	91346	120471	2.27%	0.256%
19	11.208	796	798	799	rBV	112690	102661	1.94%	0.218%
20	11.345	807	810	812	rBV	1501746	1438762	27.12%	3.060%
21	11.631	833	835	839	rBV	72629	70458	1.33%	0.150%
22	12.042	867	871	876	rVB2	38823	60528	1.14%	0.129%
23	12.934	946	949	951	rBV	4190901	4287711	80.83%	9.121%
24	13.825	1024	1027	1032	rBV2	197657	321140	6.05%	0.683%
25	13.985	1038	1041	1043	rBV	1320407	1355972	25.56%	2.884%
26	14.454	1078	1082	1094	rBV5	52880	315589	5.95%	0.671%
27	15.060	1132	1135	1137	rBV	40077	56157	1.06%	0.119%
28	15.414	1163	1166	1169	rBV	845258	1199022	22.60%	2.550%
29	15.825	1199	1202	1204	rBV	73534	120504	2.27%	0.256%
30	16.294	1240	1243	1246	rVB	89079	151134	2.85%	0.321%
31	16.843	1288	1291	1296	rVB	87470	178204	3.36%	0.379%
32	17.494	1344	1348	1352	rVB	65417	175006	3.30%	0.372%
33	18.260	1411	1415	1421	rVB	50040	140784	2.65%	0.299%

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

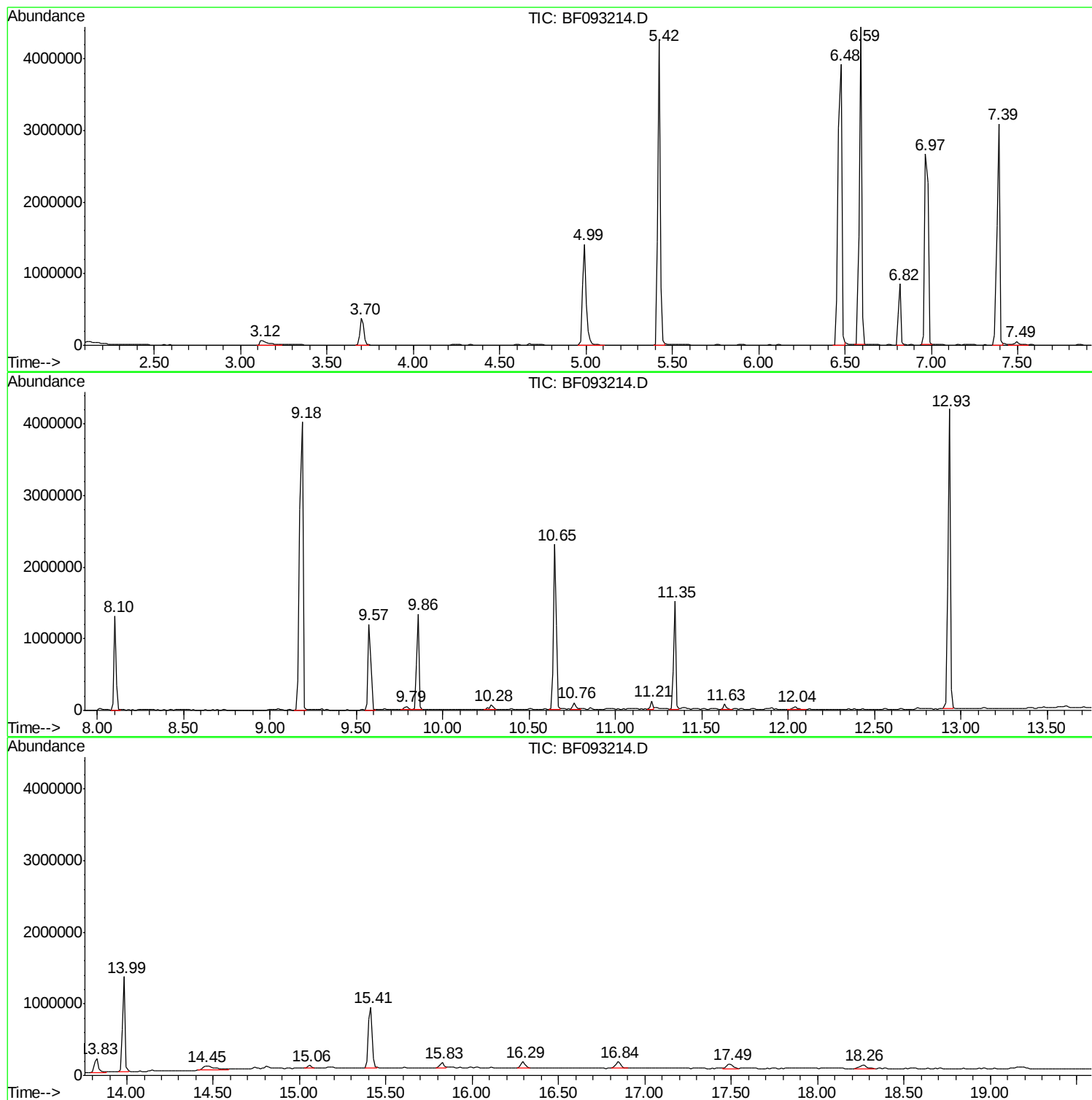
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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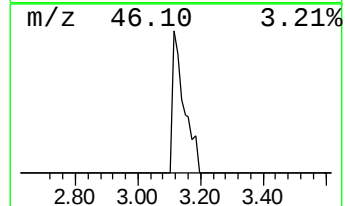
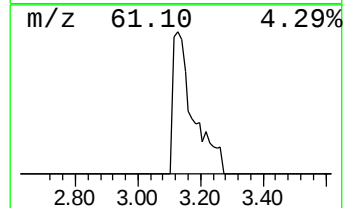
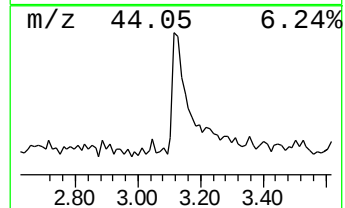
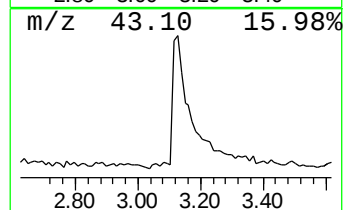
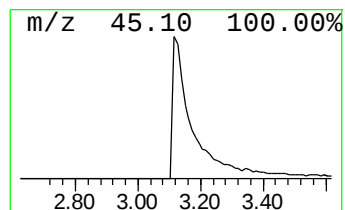
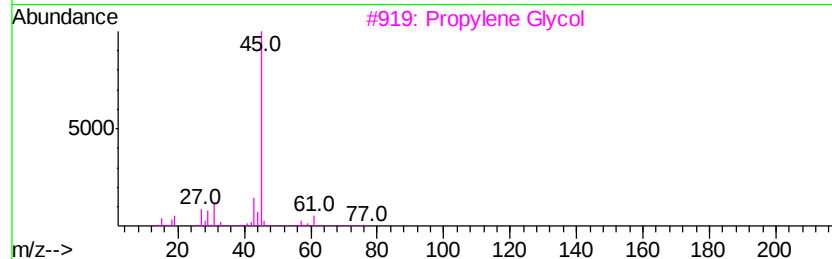
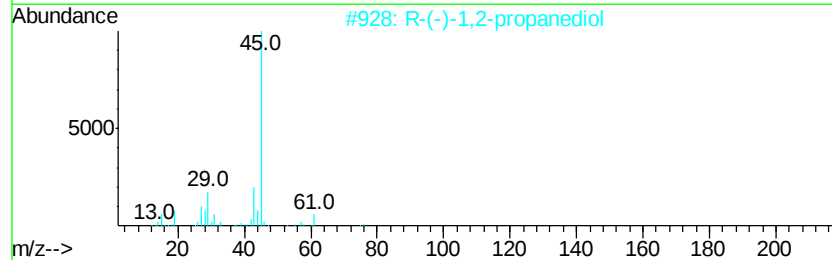
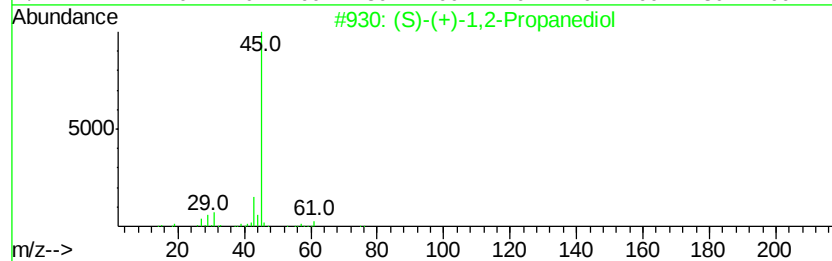
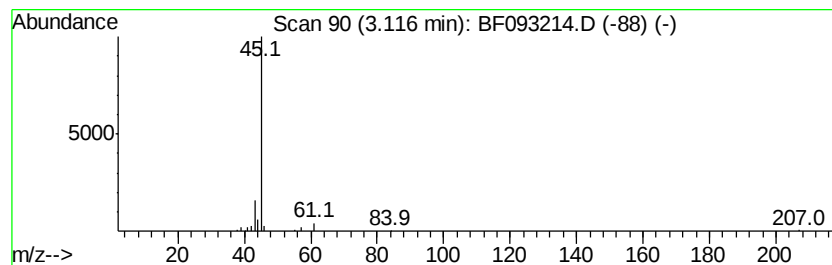
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 (S)-(+)-1,2-Propanediol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.12	4.77 ng	215033	1,4-Dichlorobenzene-d4	6.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	43
3	Propylene Glycol	76	C3H8O2	000057-55-6	9
4	Propane, 2-ethoxy-	88	C5H12O	000625-54-7	9
5	2-Pentanol	88	C5H12O	006032-29-7	9



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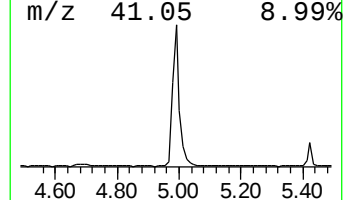
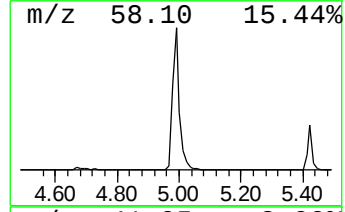
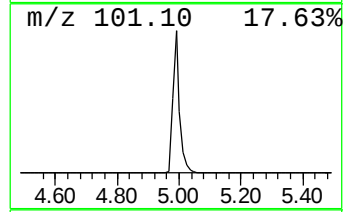
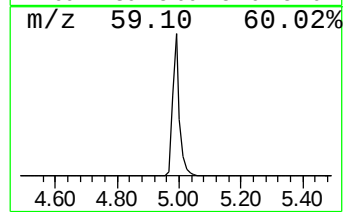
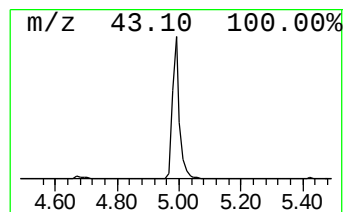
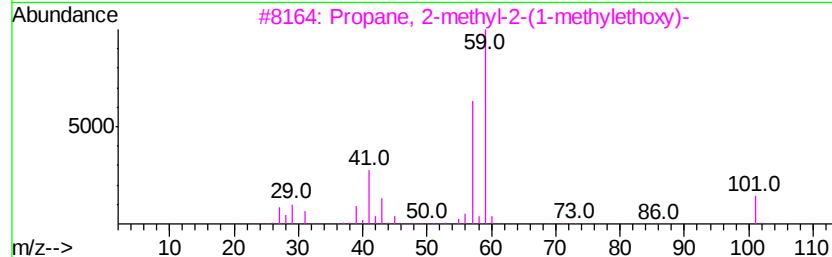
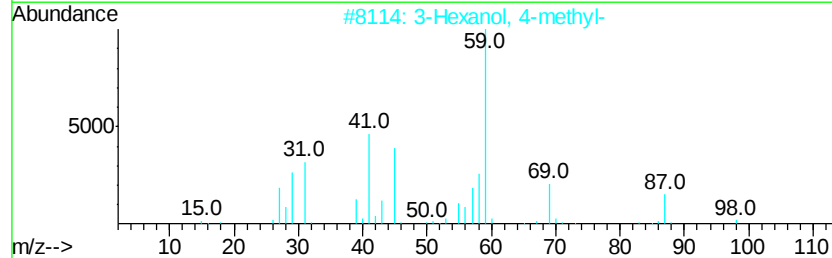
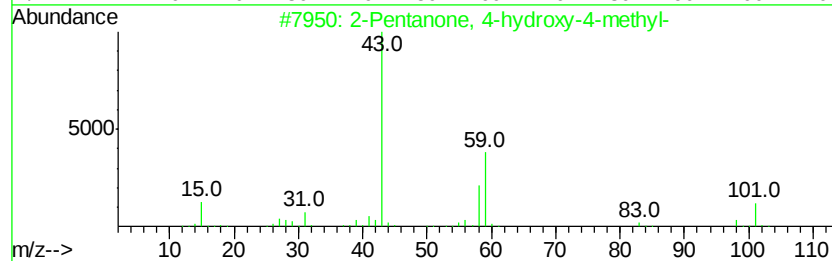
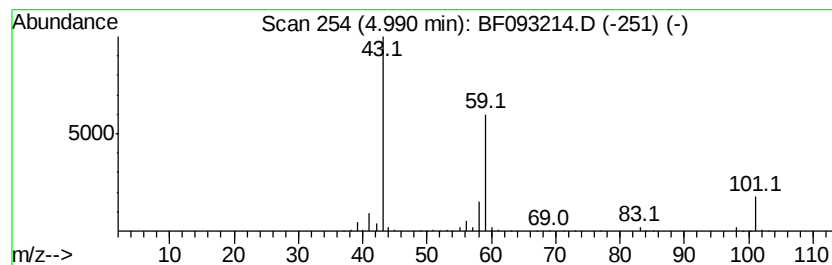
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.99	48.28 ng	2176850	1,4-Dichlorobenzene-d4	6.82

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



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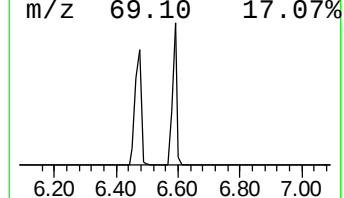
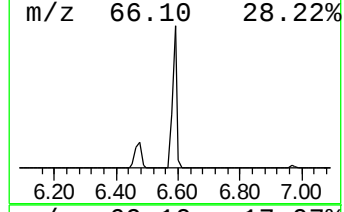
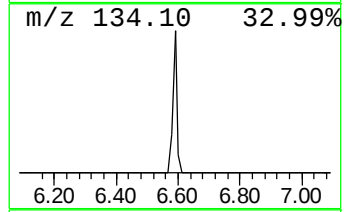
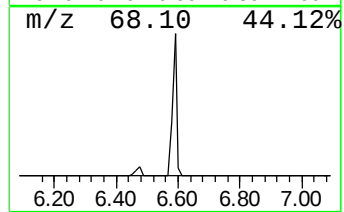
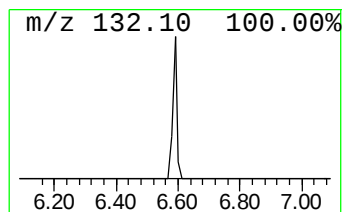
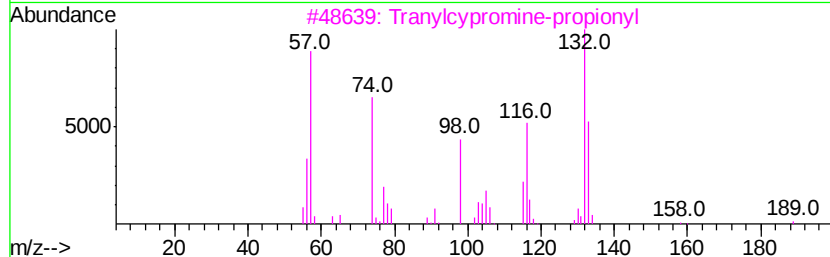
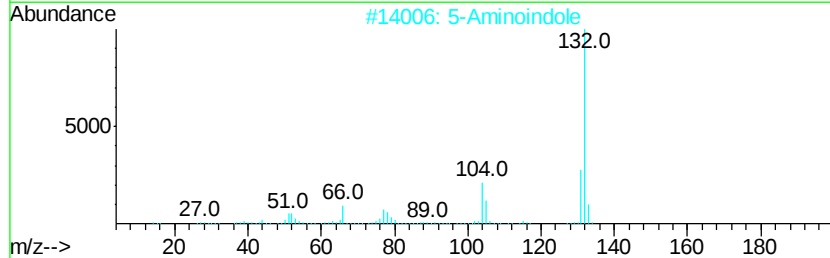
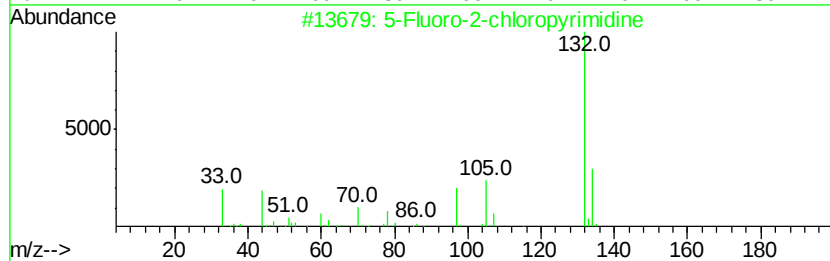
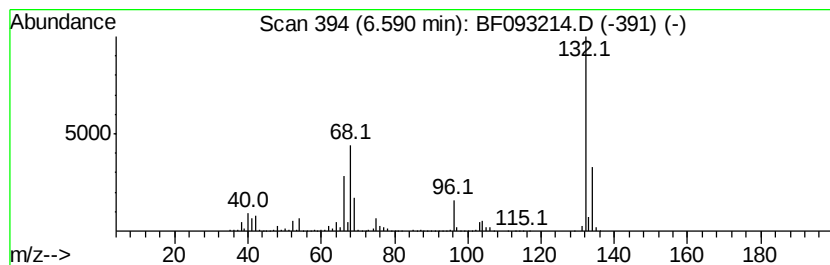
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown6.59 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.59	96.41 ng	4346750	1,4-Dichlorobenzene-d4	6.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
4		2H-Cyclopentadipyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9



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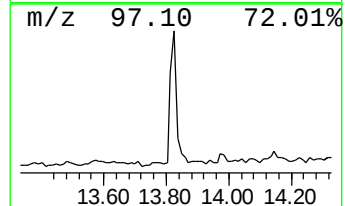
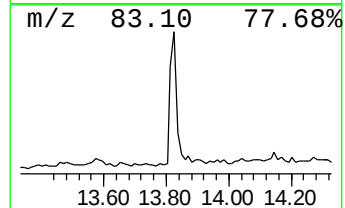
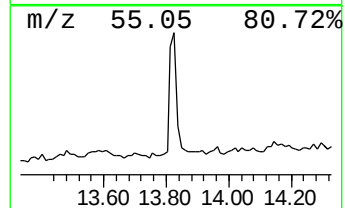
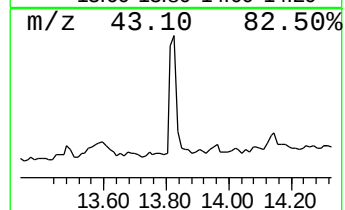
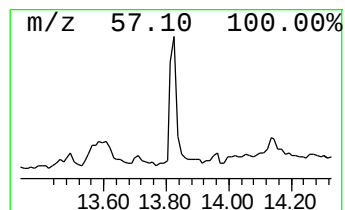
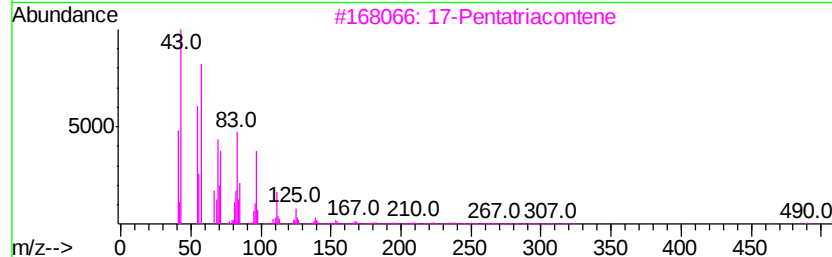
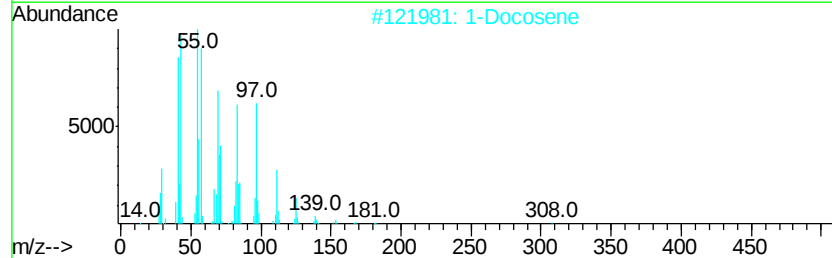
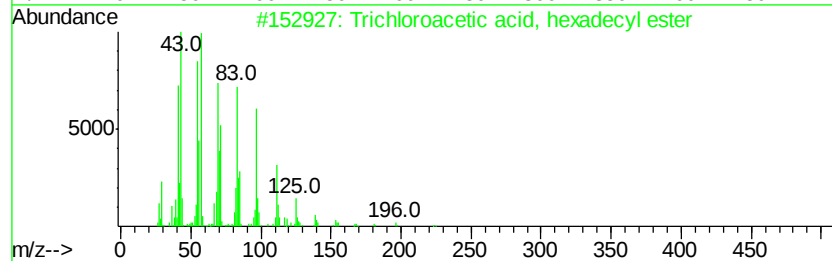
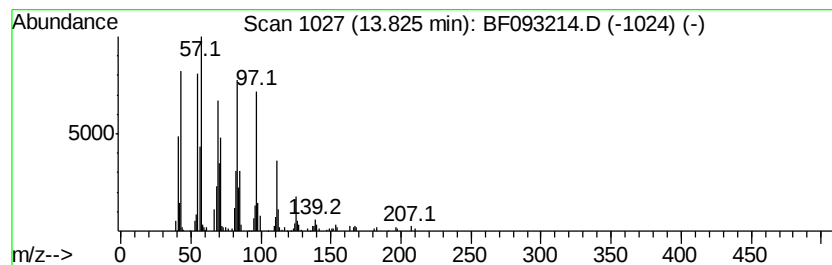
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 Trichloroacetic acid, hexad... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	4.74 ng	321140	Chrysene-d12	13.99

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2			1-Docosene	308	C22H44	001599-67-3	94
3			17-Pentatriacontene	491	C35H70	006971-40-0	91
4			11-Tricosene	322	C23H46	052078-56-5	90
5			2-Bromopropionic acid, pentadec...	362	C18H35BrO2	1000292-44-2	90



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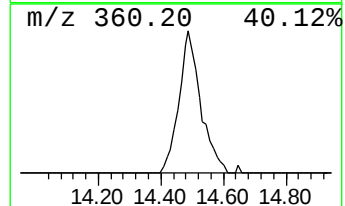
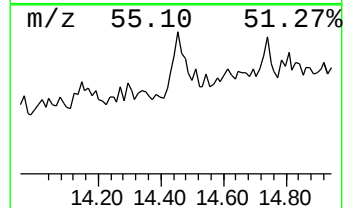
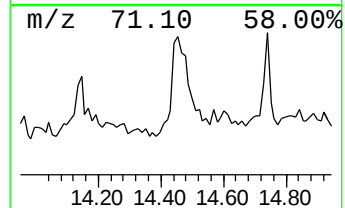
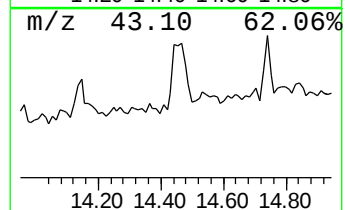
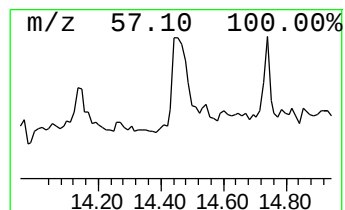
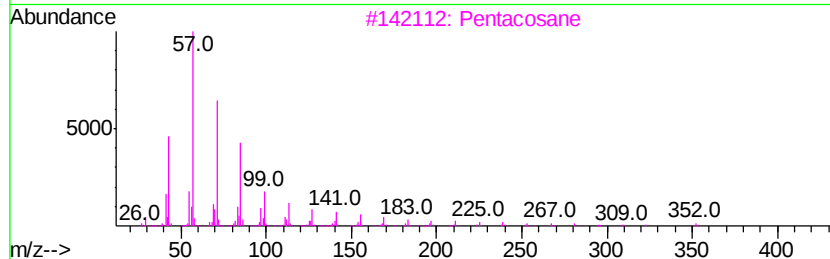
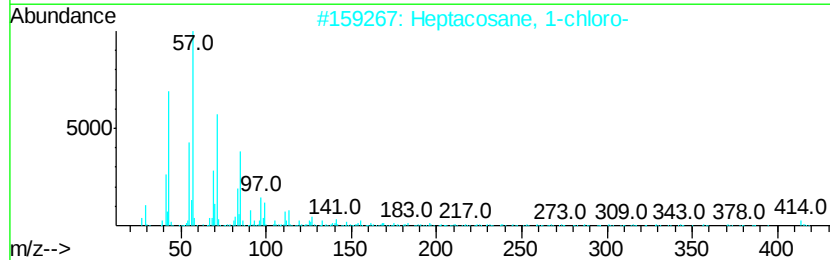
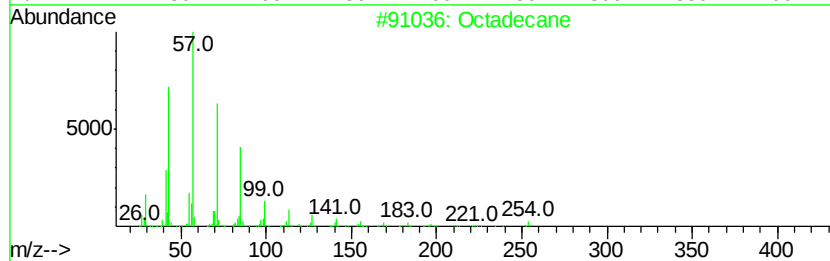
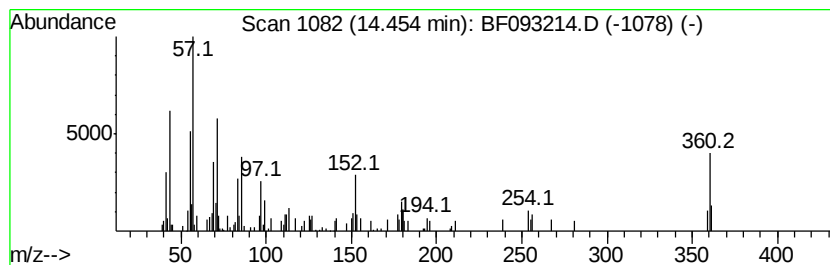
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Peak Number 7 unknown14.45 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.45	4.65 ng	315589	Chrysene-d12	13.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecane	254	C18H38	000593-45-3	49
2		Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	30
3		Pentacosane	352	C25H52	000629-99-2	30
4		Docosane	310	C22H46	000629-97-0	30
5		Tetratriacontane	479	C34H70	014167-59-0	30



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ClientSampleId :
E2-BB6-WSW

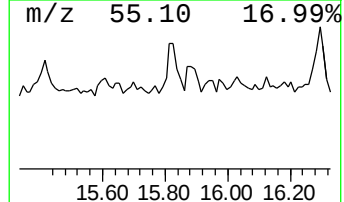
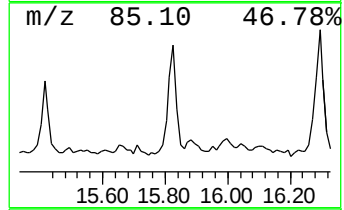
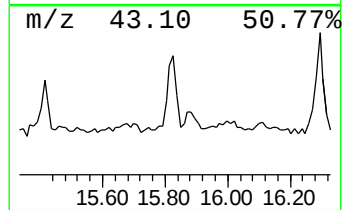
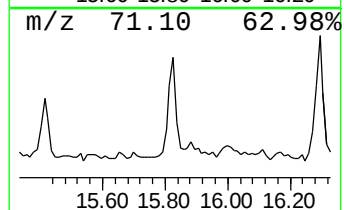
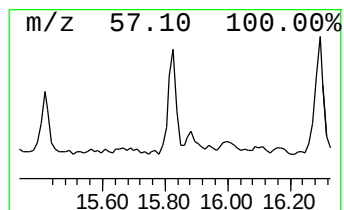
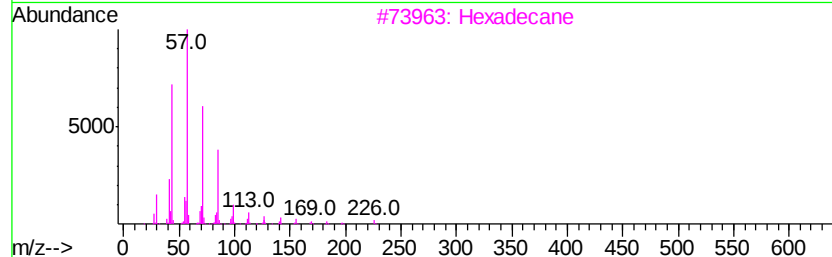
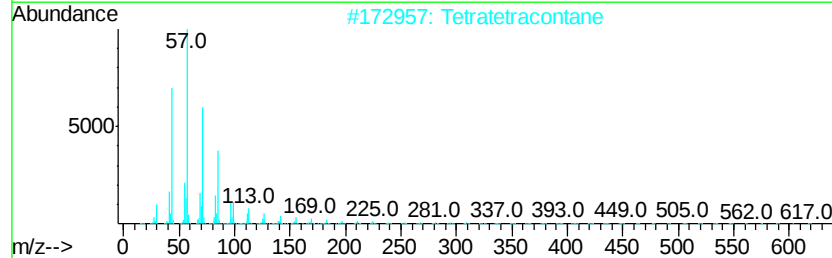
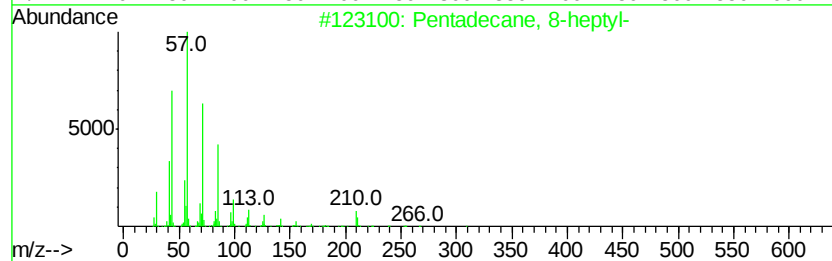
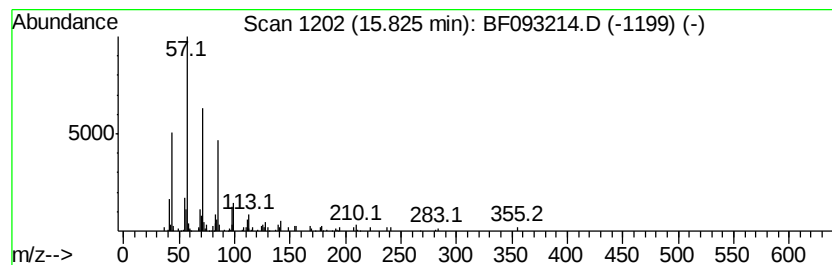
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Pentadecane, 8-heptyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.83	2.01 ng	120504	Perylene-d12	15.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	87
2		Tetratetracontane	619	C44H90	007098-22-8	86
3		Hexadecane	226	C16H34	000544-76-3	80
4		Heptacosane	380	C27H56	000593-49-7	80
5		Octacosane	394	C28H58	000630-02-4	80



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022717\
Data File : BF093214.D
Acq On : 27 Feb 2017 19:45
Operator : SJ/MA
Sample : I1997-06
Misc :
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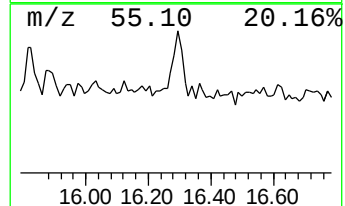
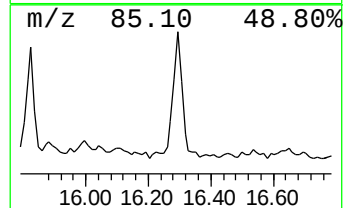
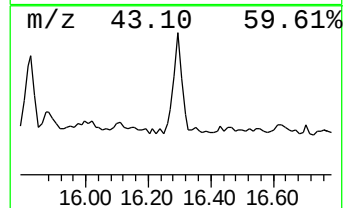
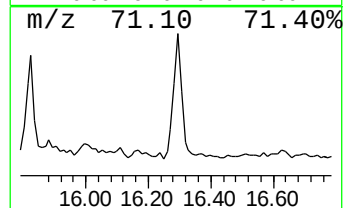
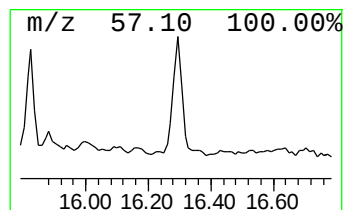
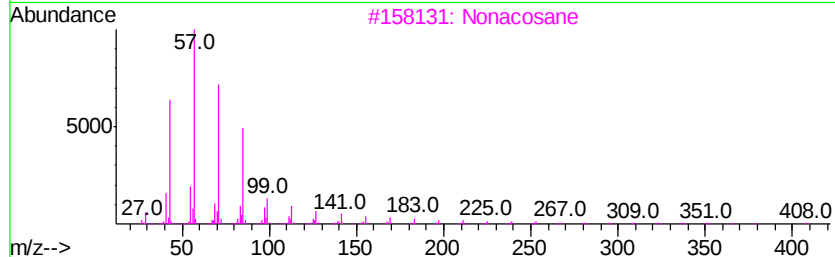
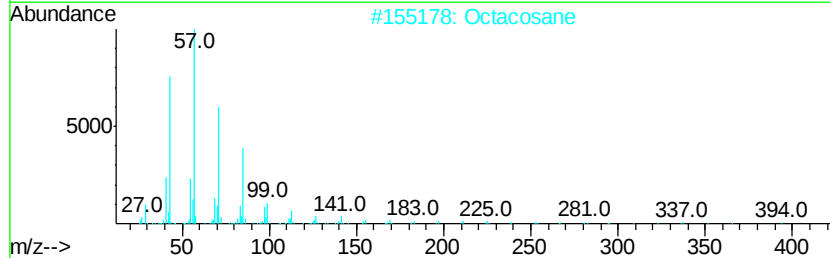
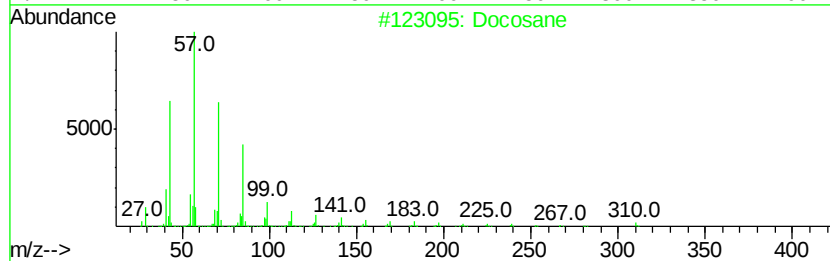
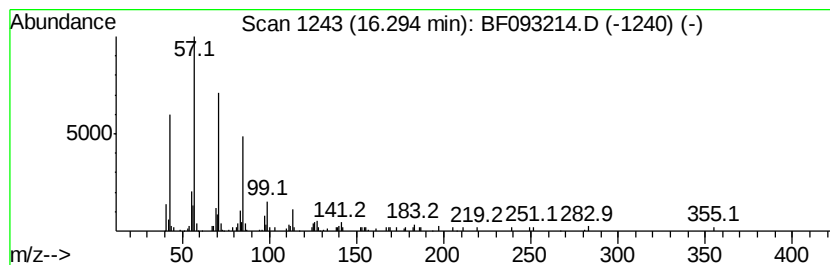
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Docosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.29	2.52 ng	151134	Perylene-d12	15.41
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Docosane		310 C22H46	000629-97-0 87
2	Octacosane		394 C28H58	000630-02-4 87
3	Nonacosane		408 C29H60	000630-03-5 86
4	Pentadecane, 8-heptyl-		310 C22H46	071005-15-7 83
5	Heneicosane		296 C21H44	000629-94-7 83



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022717\
Data File : BF093214.D
Acq On : 27 Feb 2017 19:45
Operator : SJ/MA
Sample : I1997-06
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
E2-BB6-WSW

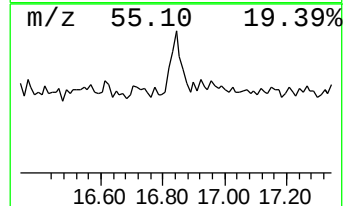
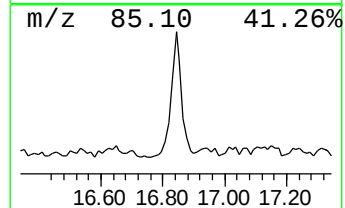
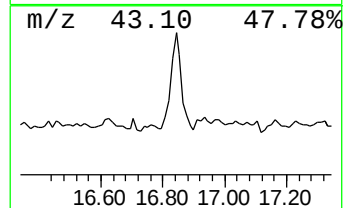
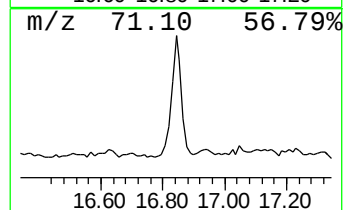
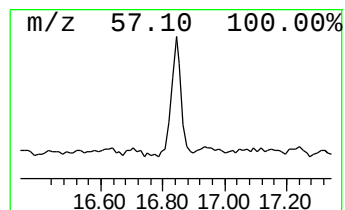
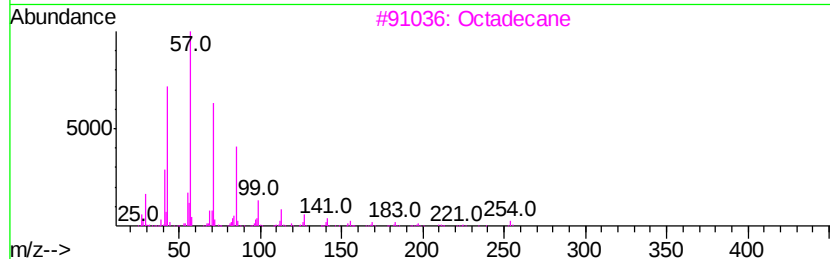
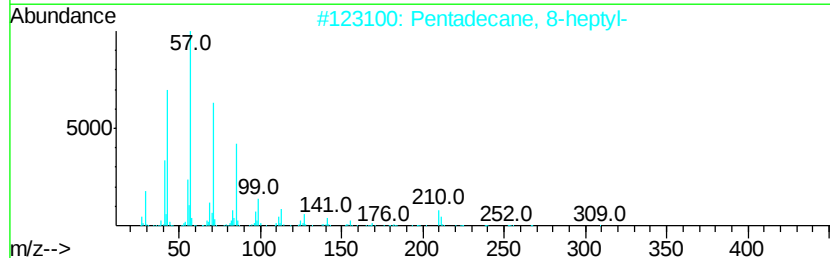
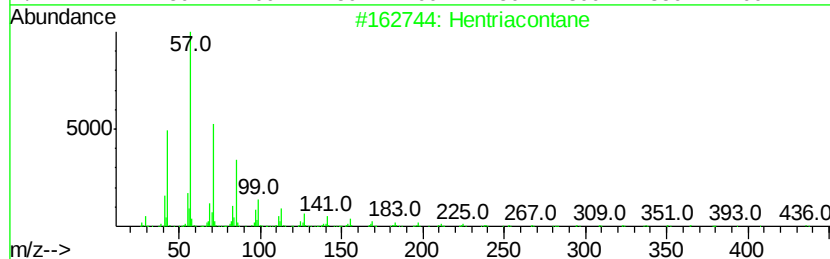
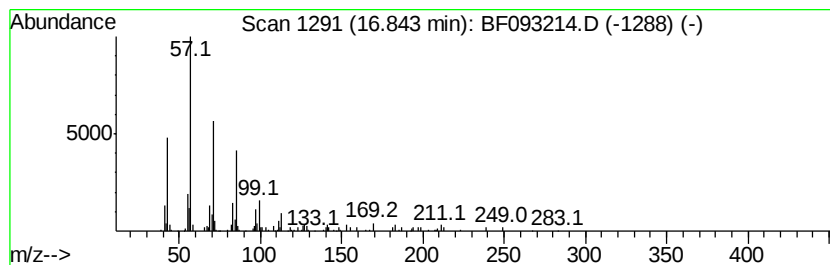
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hentriacontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.84	2.97 ng	178204	Perylene-d12	15.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hentriacontane	437	C31H64	000630-04-6	90
2		Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	86
3		Octadecane	254	C18H38	000593-45-3	80
4		Eicosane	282	C20H42	000112-95-8	80
5		Octadecane, 1-iodo-	380	C18H37I	000629-93-6	80



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022717\
Data File : BF093214.D
Acq On : 27 Feb 2017 19:45
Operator : SJ/MA
Sample : I1997-06
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
E2-BB6-WSW

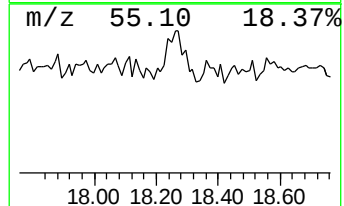
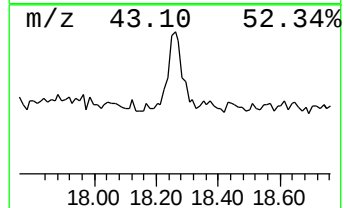
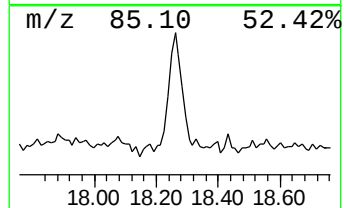
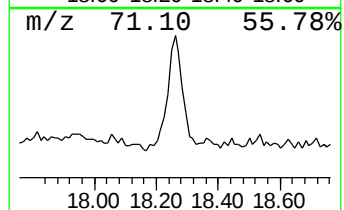
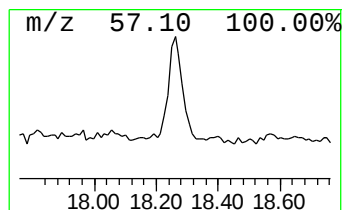
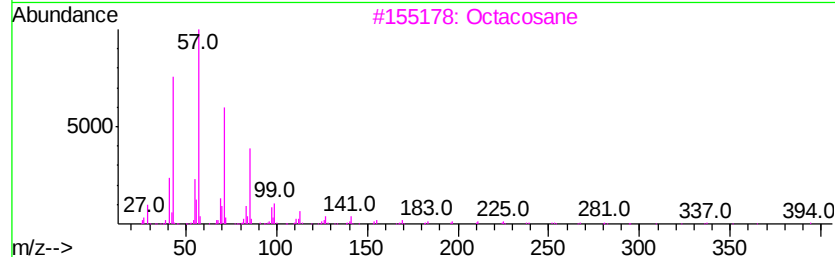
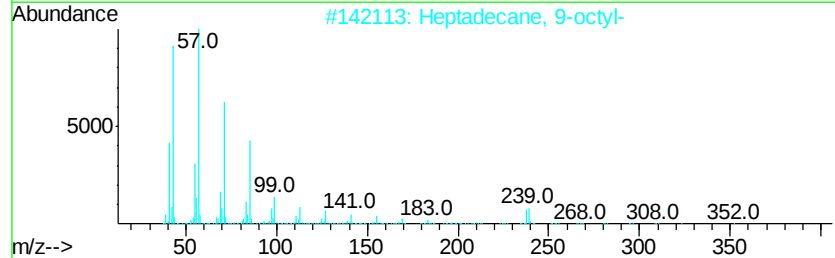
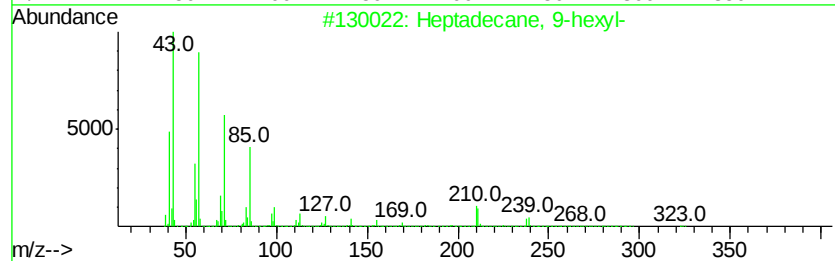
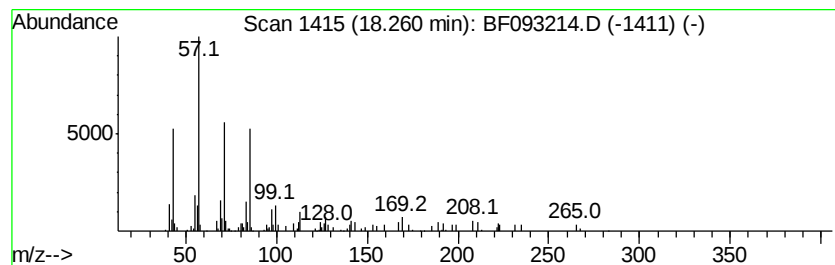
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Heptadecane, 9-hexyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.26	2.35 ng	140784	Perylene-d12	15.41

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane, 9-hexyl-	324	C23H48	055124-79-3	72
2			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	72
3			Octacosane	394	C28H58	000630-02-4	64
4			Hexacosane	366	C26H54	000630-01-3	64
5			Octadecane, 1-iodo-	380	C18H37I	000629-93-6	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022717\
Data File : BF093214.D
Acq On : 27 Feb 2017 19:45
Operator : SJ/MA
Sample : I1997-06
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
E2-BB6-WSW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.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
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2-Pentanone, 4-hy...	4.99	48.3	ng	2176850	1	6.82	901707	20.0
unknown6.59	6.59	96.4	ng	4346750	1	6.82	901707	20.0
Trichloroacetic a...	13.83	4.7	ng	321140	5	13.99	1355970	20.0
unknown14.45	14.45	4.7	ng	315589	5	13.99	1355970	20.0
Pentadecane, 8-he...	15.83	2.0	ng	120504	6	15.41	1199020	20.0
Docosane	16.29	2.5	ng	151134	6	15.41	1199020	20.0
Hentriacontane	16.84	3.0	ng	178204	6	15.41	1199020	20.0
Heptadecane, 9-he...	18.26	2.4	ng	140784	6	15.41	1199020	20.0