

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020516\
 Data File : BF084857.D
 Acq On : 5 Feb 2016 14:04
 Operator : SJ/IZ
 Sample : H1329-05
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S4-B006(17-19)

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-BF020116.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	4.819	236	239	250	rVB	899331	1555341	29.62%	3.029%
2	5.253	274	277	280	rBV	3982888	5250663	100.00%	10.226%
3	6.316	367	370	373	rBV	4283941	4921458	93.73%	9.585%
4	6.430	377	380	383	rVV	4900682	4981745	94.88%	9.702%
5	6.659	398	400	402	rBV	1358414	1099859	20.95%	2.142%
6	6.819	411	414	416	rBV	4502809	4161362	79.25%	8.104%
7	7.230	447	450	453	rBV	2892201	3229476	61.51%	6.290%
8	7.950	510	513	515	rVB	1350245	1457855	27.77%	2.839%
9	9.025	604	607	610	rBV	4511798	5019039	95.59%	9.775%
10	9.425	640	642	644	rBV	832602	681529	12.98%	1.327%
11	9.642	653	661	663	rBV	92681	111259	2.12%	0.217%
12	9.699	663	666	668	rBV	1465004	1615583	30.77%	3.146%
13	10.145	701	705	706	rBV	113474	112741	2.15%	0.220%
14	10.362	721	724	727	rBV	38633	57914	1.10%	0.113%
15	10.488	732	735	737	rBV	3697689	4033682	76.82%	7.856%
16	10.614	744	746	753	rVB	126136	139910	2.66%	0.272%
17	11.174	792	795	797	rBV	1824858	1565248	29.81%	3.048%
18	11.722	841	843	850	rBV2	151306	196075	3.73%	0.382%
19	12.282	889	892	894	rVB	316195	323422	6.16%	0.630%
20	12.591	917	919	922	rBV	135161	182116	3.47%	0.355%
21	12.648	922	924	925	rBV	86994	72181	1.37%	0.141%
22	12.762	931	934	936	rBV	4518072	4273568	81.39%	8.323%
23	13.002	953	955	957	rVB	570392	521330	9.93%	1.015%
24	13.300	979	981	983	rBV	156800	144708	2.76%	0.282%
25	13.345	983	985	988	rVB	66872	82768	1.58%	0.161%
26	13.665	1011	1013	1022	rBV	1013907	1372089	26.13%	2.672%
27	13.802	1022	1025	1027	rBV	1304500	1251184	23.83%	2.437%
28	13.985	1039	1041	1045	rBV	56874	98654	1.88%	0.192%
29	14.305	1066	1069	1075	rBV	215482	443634	8.45%	0.864%
30	14.591	1089	1094	1098	rBV4	31197	96226	1.83%	0.187%
31	14.911	1117	1122	1125	rBV2	116297	282522	5.38%	0.550%
32	15.163	1142	1144	1147	rBV	573023	899129	17.12%	1.751%
33	15.585	1179	1181	1183	rBV	52618	77128	1.47%	0.150%
34	15.631	1183	1185	1196	rVB2	181780	499674	9.52%	0.973%

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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

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.M
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35	16.523	1260	1263	1267	rBV	24940	53092	1.01%	0.103%
36	16.626	1267	1272	1275	rBV4	34780	116104	2.21%	0.226%
37	16.934	1296	1299	1303	rBV5	29052	85718	1.63%	0.167%
38	17.117	1312	1315	1319	rVB2	25247	63125	1.20%	0.123%
39	17.826	1372	1377	1383	rBV2	24734	73645	1.40%	0.143%
40	18.671	1445	1451	1459	rVB5	34561	143791	2.74%	0.280%

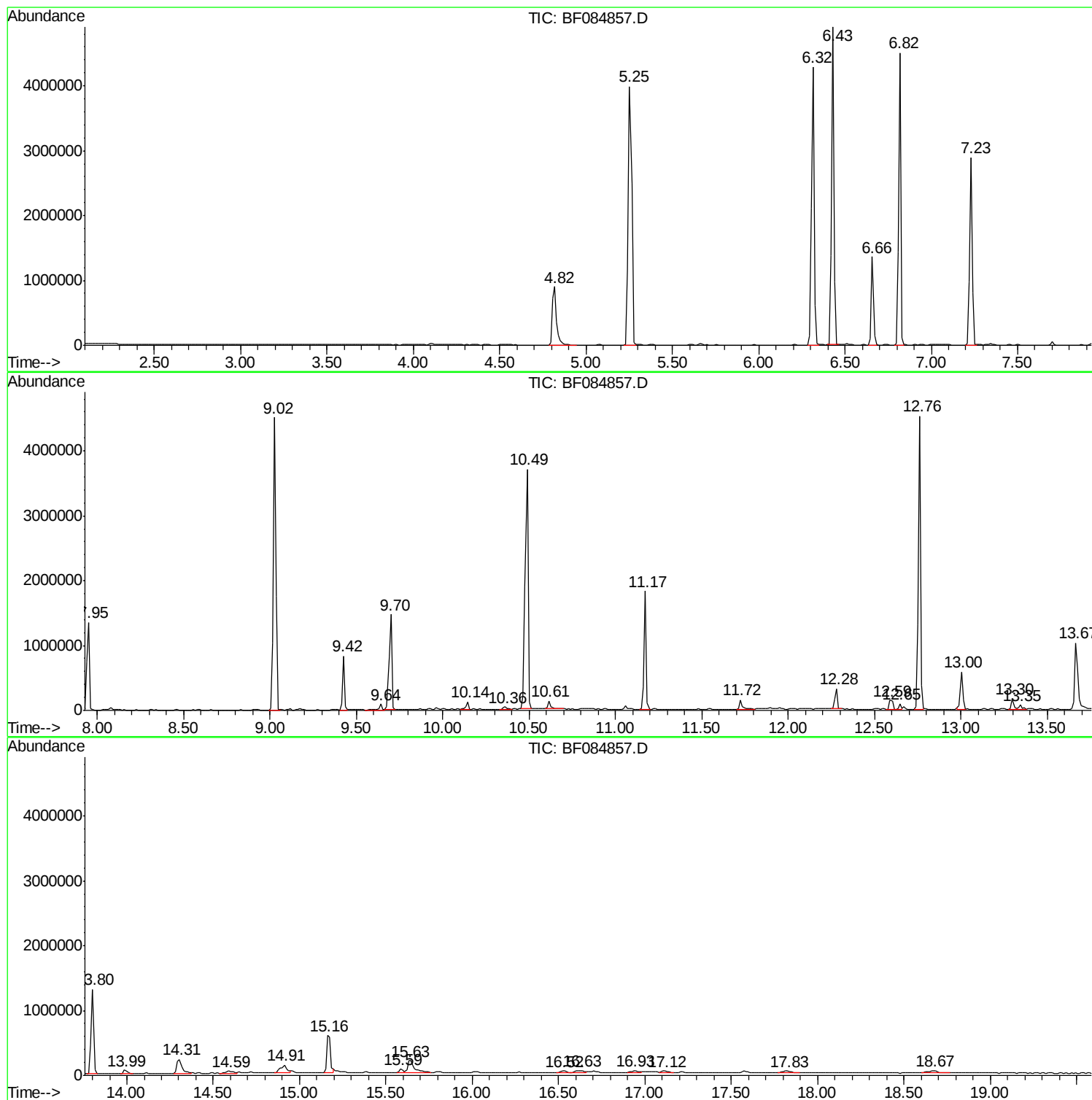
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ClientSampled :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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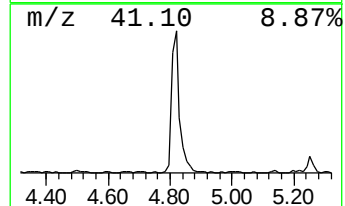
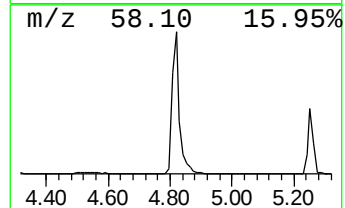
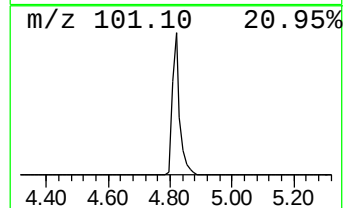
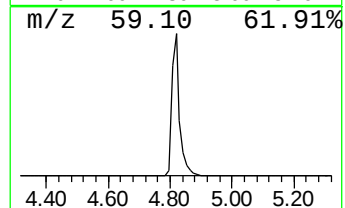
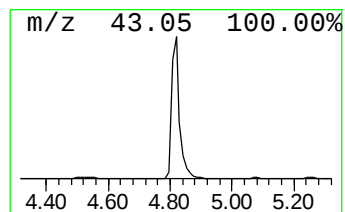
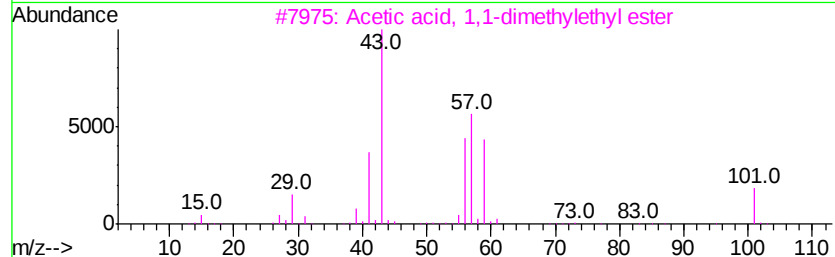
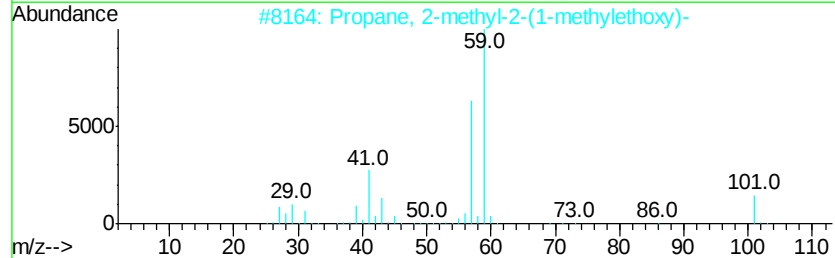
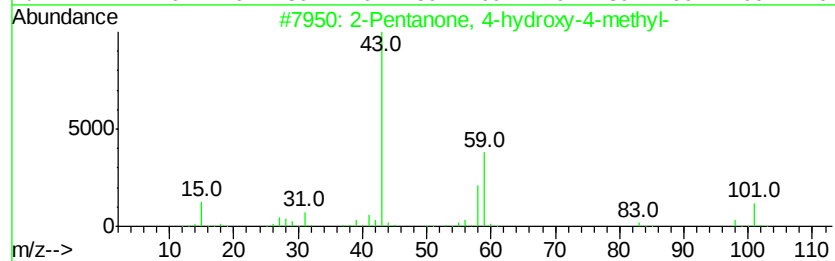
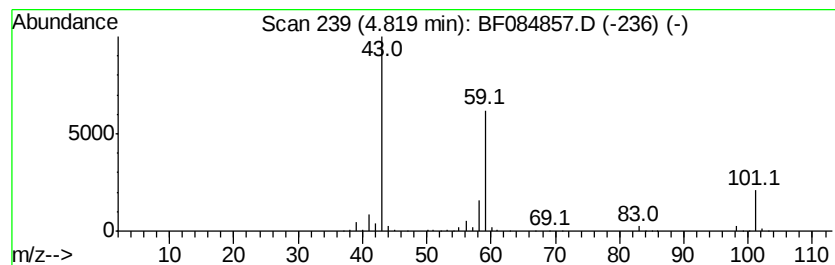
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.82	28.28 ng	1555340	1,4-Dichlorobenzene-d4	6.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Propane, 2-methyl-2-(1-methylethyl)-	116	C7H16O	017348-59-3	53
3		Acetic acid, 1,1-dimethylethyl ester	116	C6H12O2	000540-88-5	39
4		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
5		Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	23



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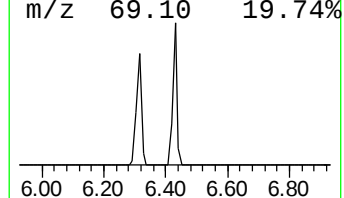
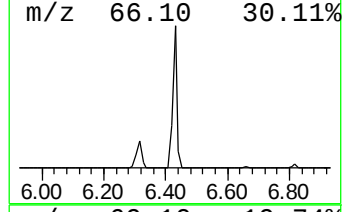
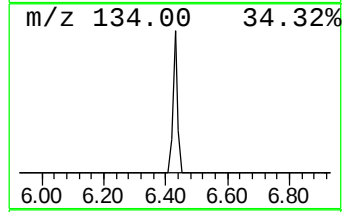
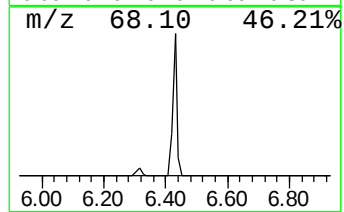
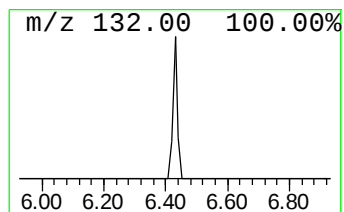
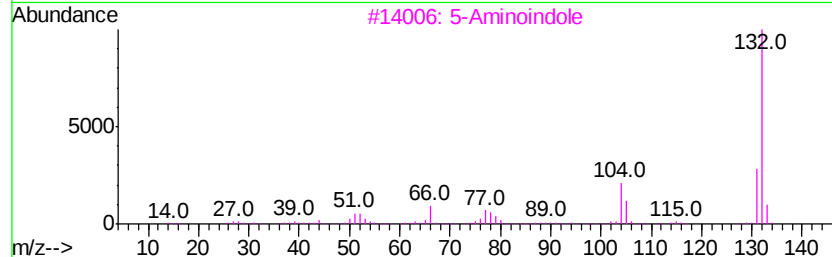
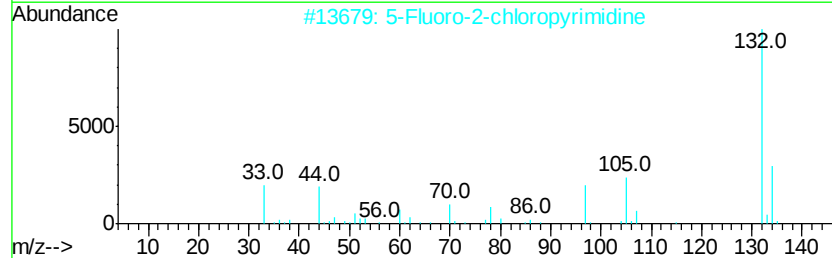
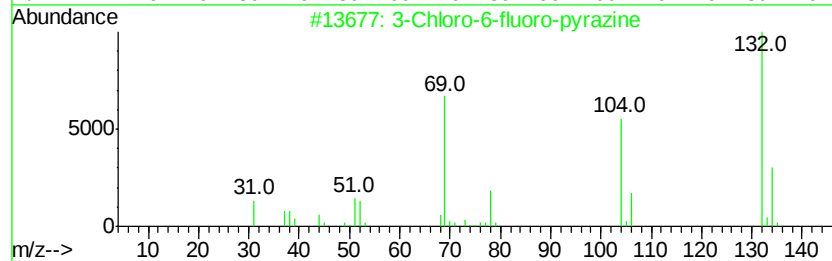
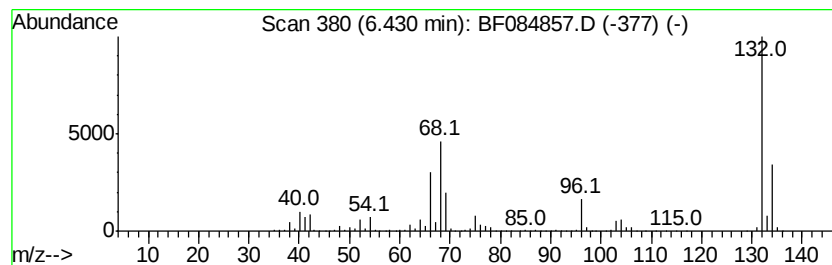
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown6.43 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.43	90.59 ng	4981750	1,4-Dichlorobenzene-d4	6.66

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		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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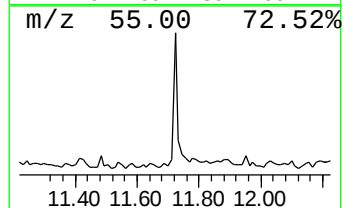
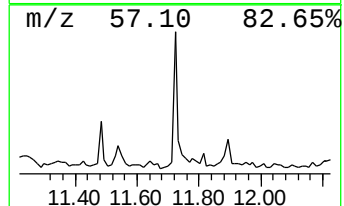
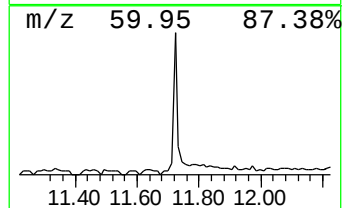
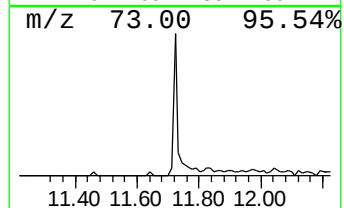
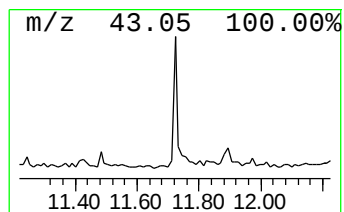
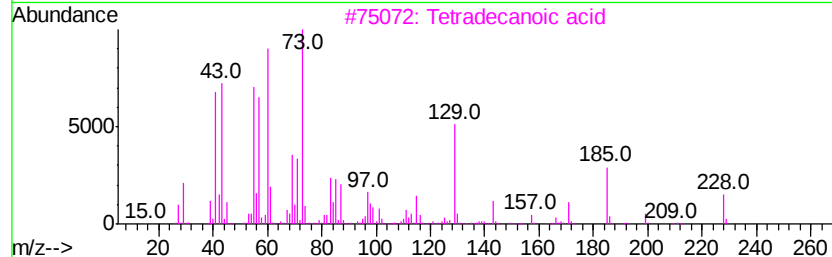
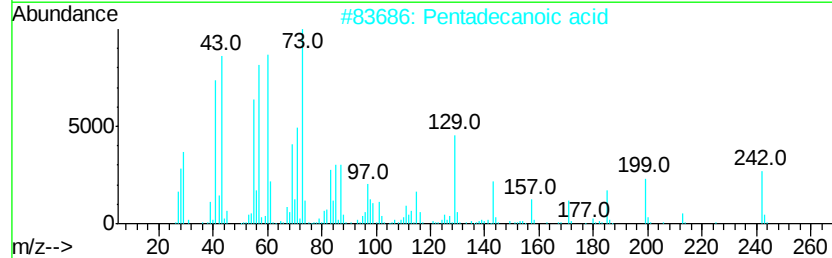
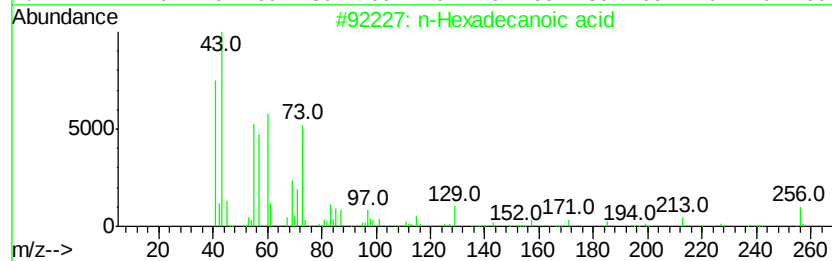
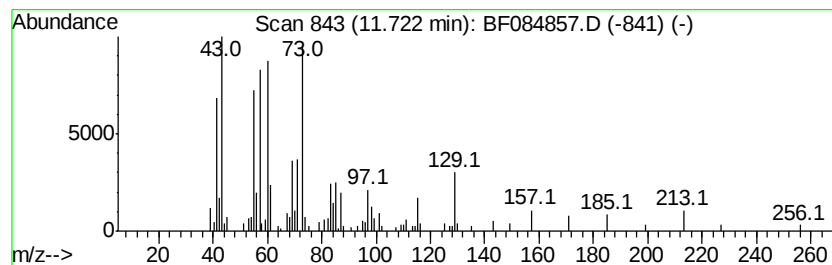
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.72	2.51 ng	196075	Phenanthrene-d10	11.17

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	86
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4		Tridecanoic acid	214	C13H26O2	000638-53-9	72
5		Dodecanoic acid	200	C12H24O2	000143-07-7	64



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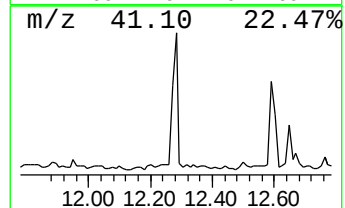
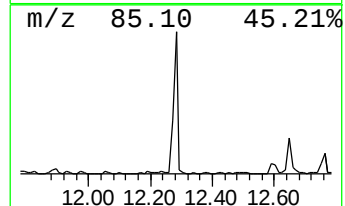
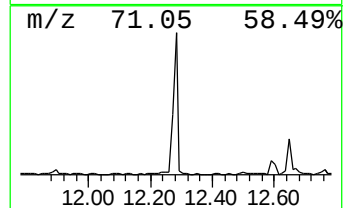
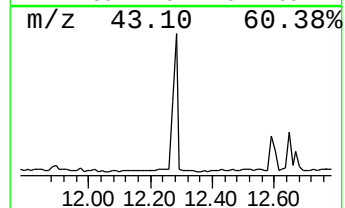
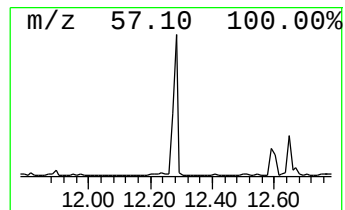
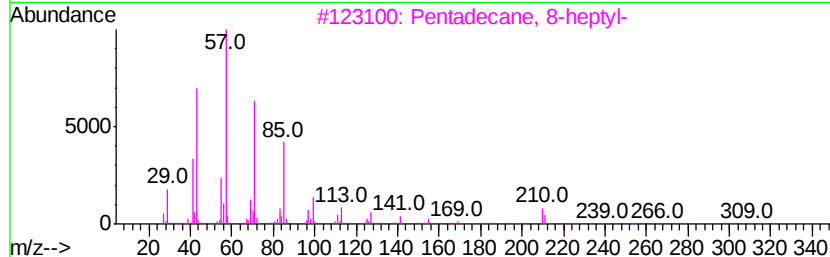
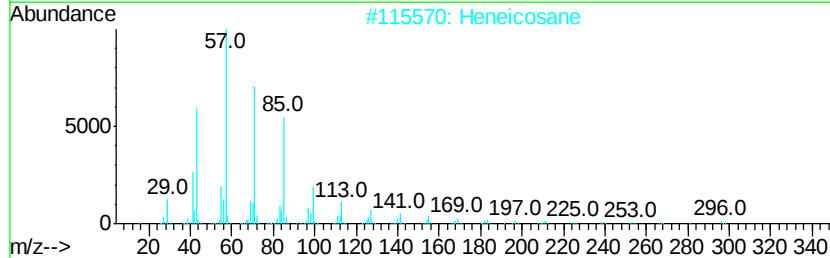
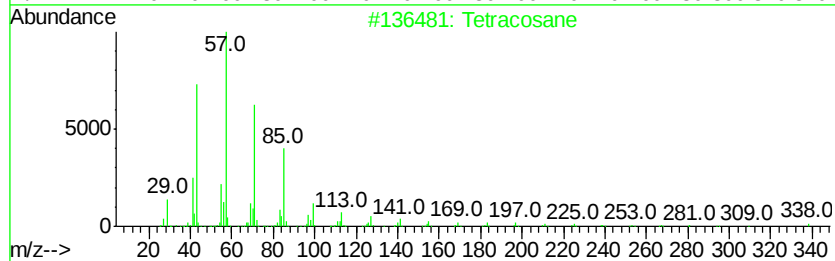
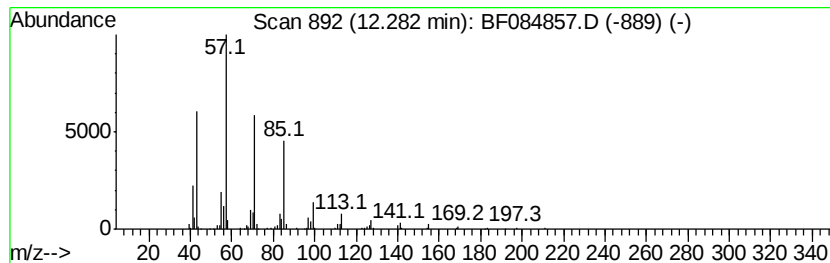
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 Tetracosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.28	4.13 ng	323422	Phenanthrene-d10	11.17

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane		338	C24H50	000646-31-1	91
2	Heneicosane		296	C21H44	000629-94-7	90
3	Pentadecane, 8-heptyl-		310	C22H46	071005-15-7	90
4	Pentacosane		352	C25H52	000629-99-2	90
5	Hexadecane		226	C16H34	000544-76-3	90



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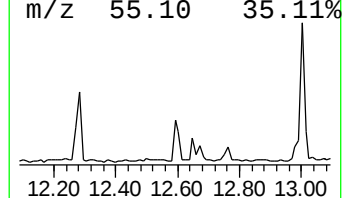
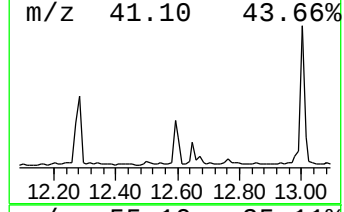
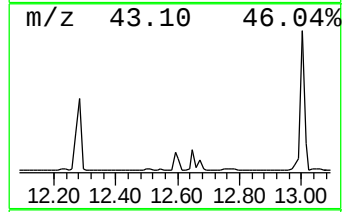
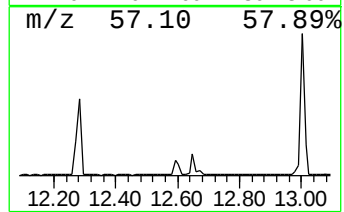
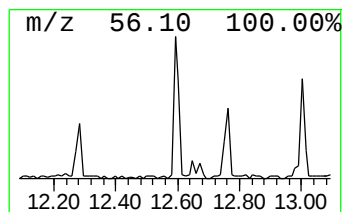
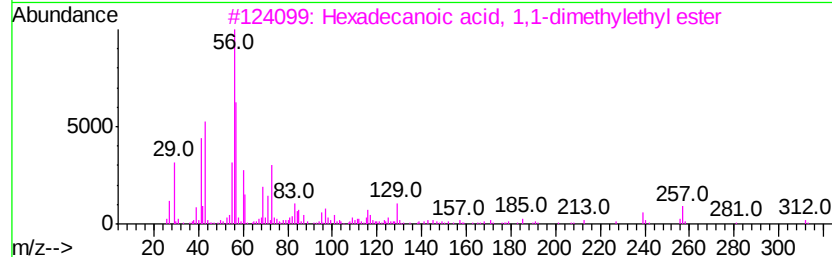
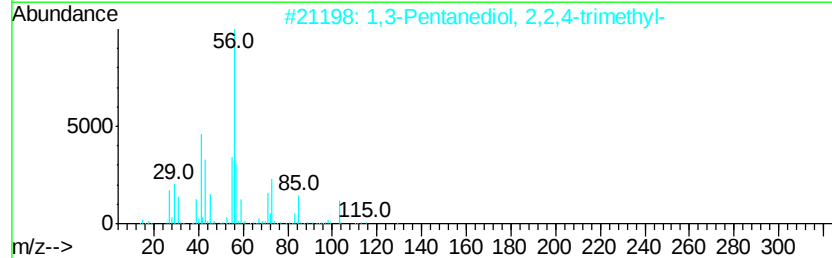
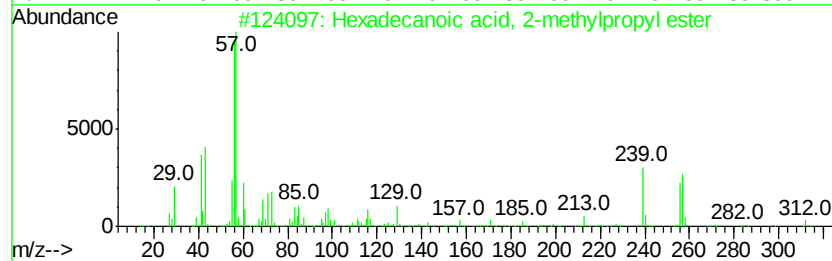
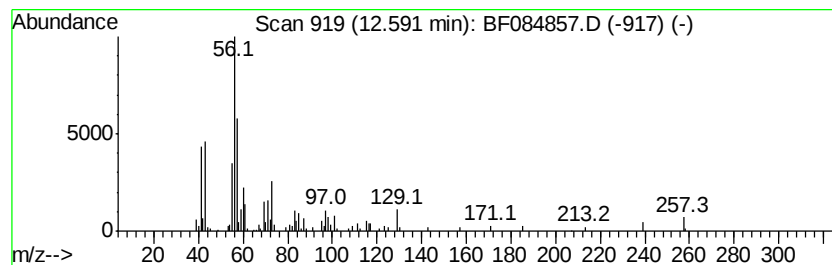
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Hexadecanoic acid, 2-methyl... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.59	2.91 ng	182116	Chrysene-d12	13.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, 2-methylpropyl...	312	C20H40O2	000110-34-9	59
2		1,3-Pentenediol, 2,2,4-trimethyl-	146	C8H18O2	000144-19-4	50
3		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	49
4		2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	40
5		Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	38



Data Path : Z:\HPCHEM1\BNA F\DATA\BF020516\
Data File : BF084857.D
Acq On : 5 Feb 2016 14:04
Operator : SJ/IZ
Sample : H1329-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
S4-B006(17-19)

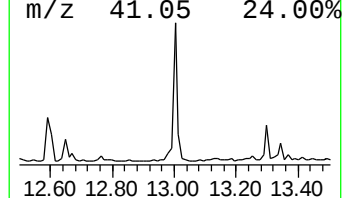
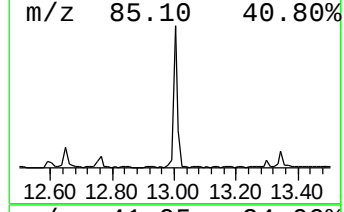
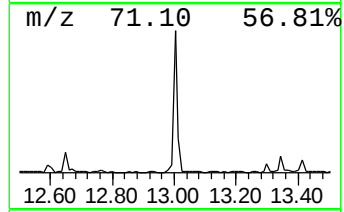
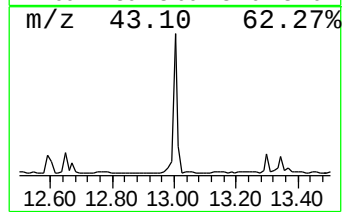
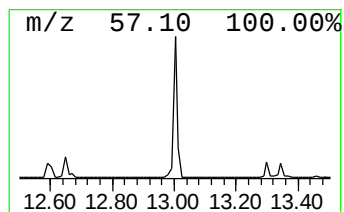
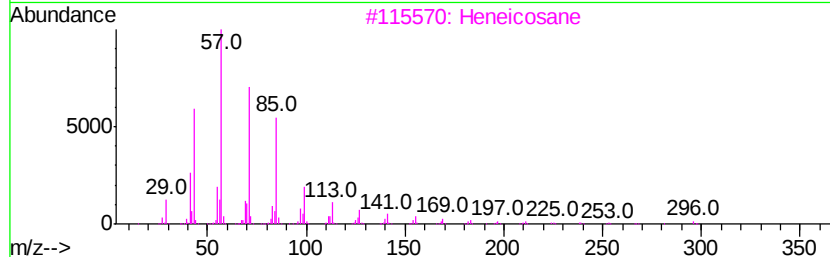
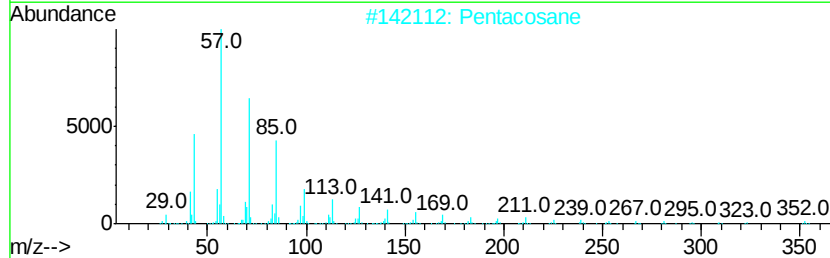
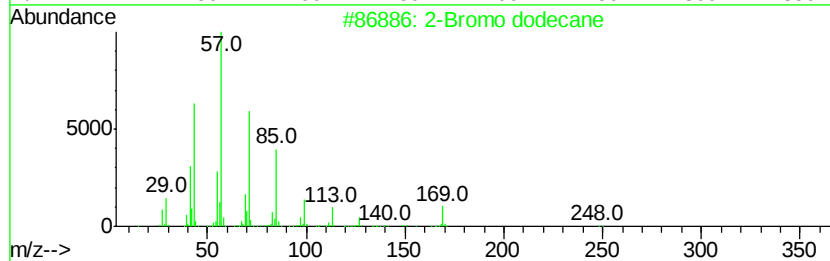
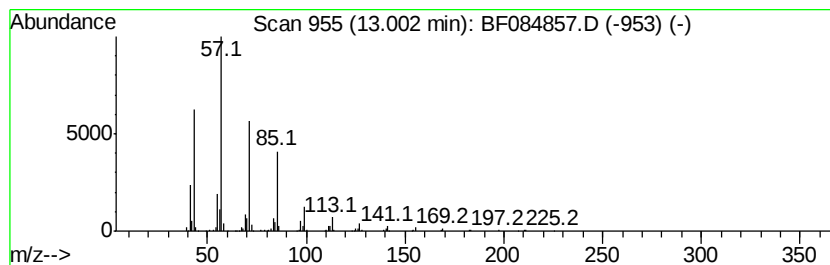
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 2-Bromo dodecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.00	8.33 ng	521330	Chrysene-d12	13.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Bromo dodecane	248	C12H25Br	013187-99-0	90
2		Pentacosane	352	C25H52	000629-99-2	90
3		Heneicosane	296	C21H44	000629-94-7	90
4		Tetracosane	338	C24H50	000646-31-1	90
5		Octadecane	254	C18H38	000593-45-3	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020516\
Data File : BF084857.D
Acq On : 5 Feb 2016 14:04
Operator : SJ/IZ
Sample : H1329-05
Misc :
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Instrument :
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ClientSampleId :
S4-B006(17-19)

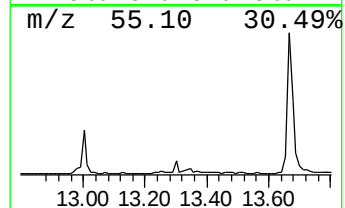
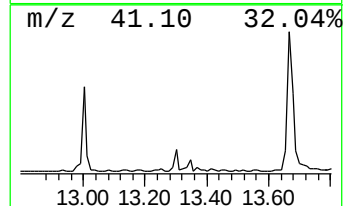
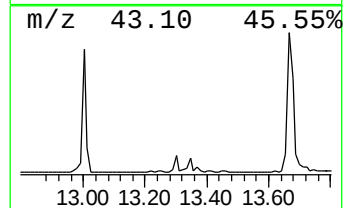
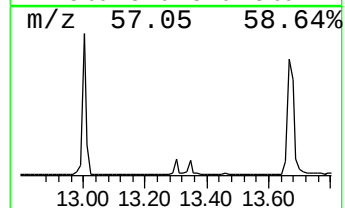
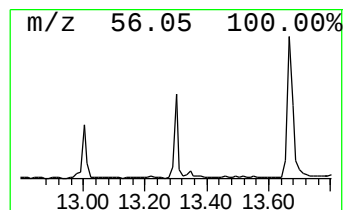
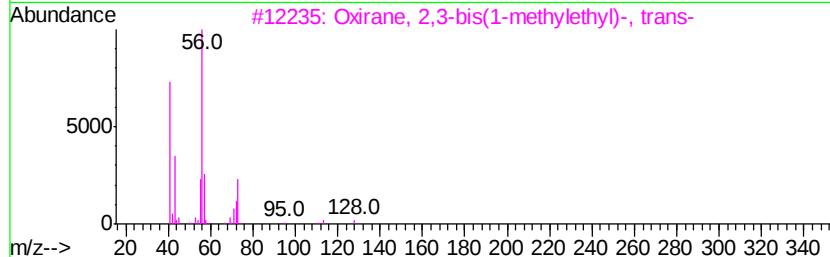
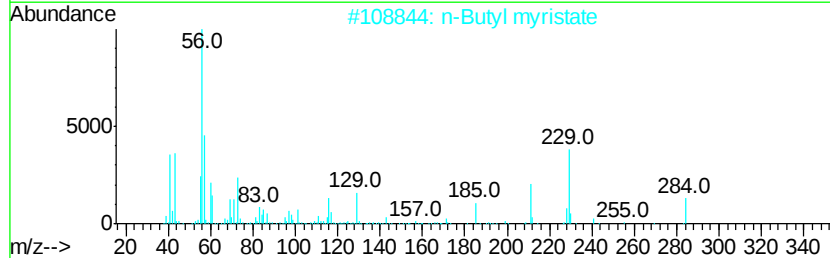
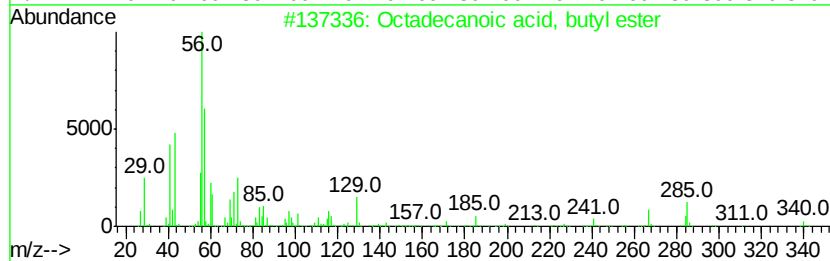
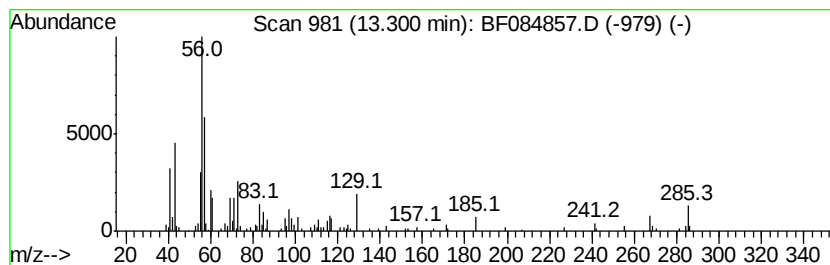
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid, butyl ester Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.30	2.31 ng	144708	Chrysene-d12	13.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	91
2		n-Butyl myristate	284	C18H36O2	000110-36-1	64
3		Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	43
4		Decane, 2,2,3-trimethyl-	184	C13H28	062338-09-4	38
5		Urea, N,N'-di-2-propenyl-	140	C7H12N2O	001801-72-5	38



Data Path : Z:\HPCHEM1\BNA F\DATA\BF020516\
 Data File : BF084857.D
 Acq On : 5 Feb 2016 14:04
 Operator : SJ/IZ
 Sample : H1329-05
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

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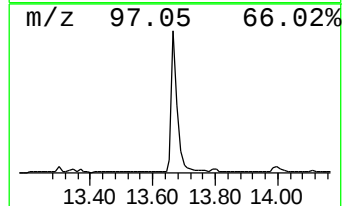
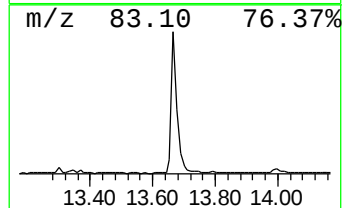
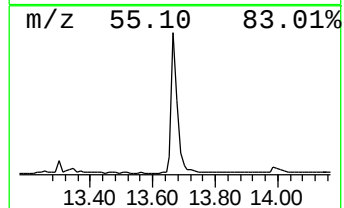
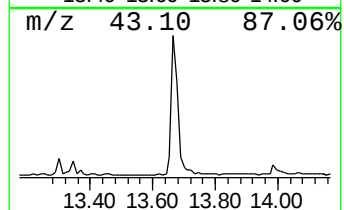
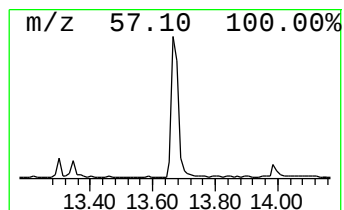
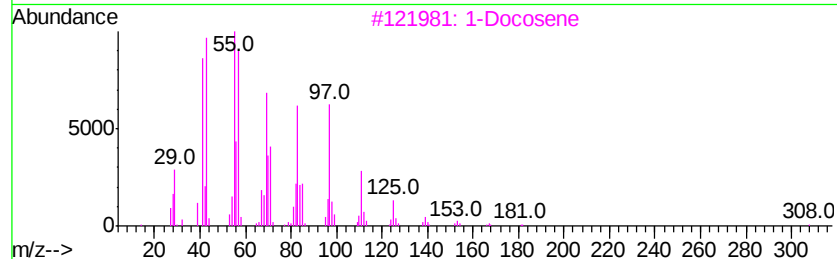
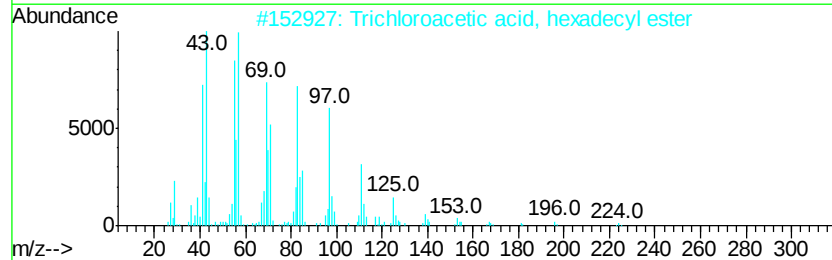
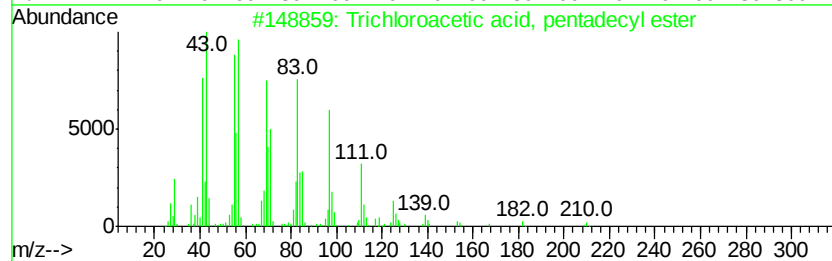
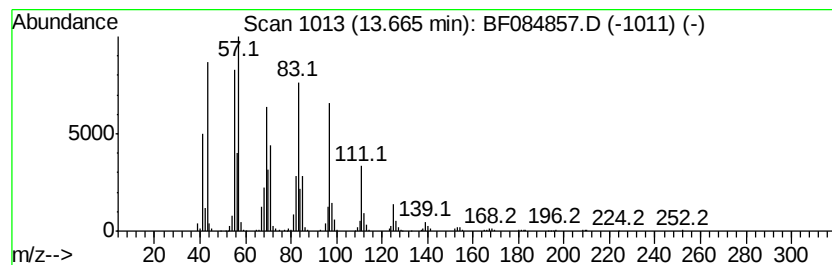
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 9 Trichloroacetic acid, penta... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.67	21.93 ng	1372090	Chrysene-d12	13.80

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
2		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3		1-Docosene	308	C22H44	001599-67-3	91
4		Trifluoroacetic acid, n-octadecyl...	366	C20H37F3O2	079392-43-1	91
5		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020516\
Data File : BF084857.D
Acq On : 5 Feb 2016 14:04
Operator : SJ/IZ
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Misc :
ALS Vial : 5 Sample Multiplier: 1

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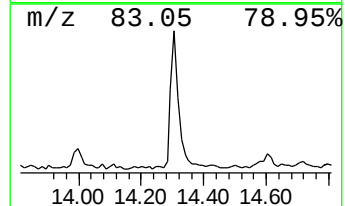
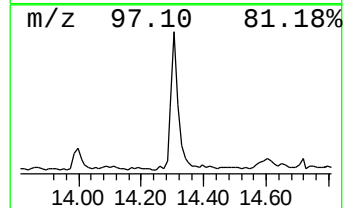
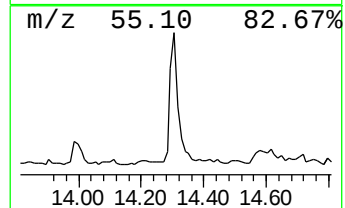
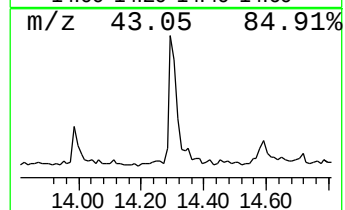
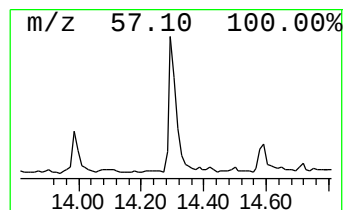
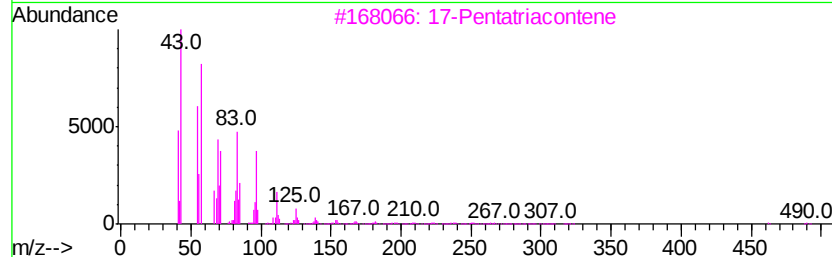
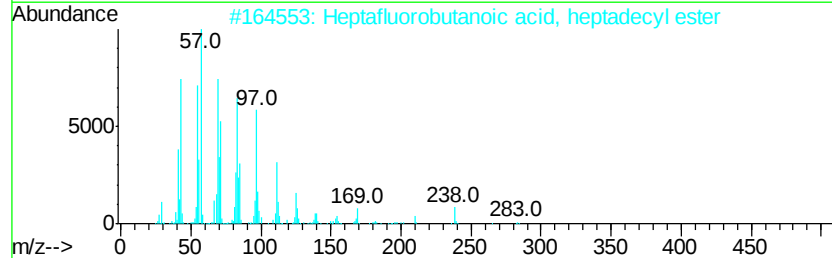
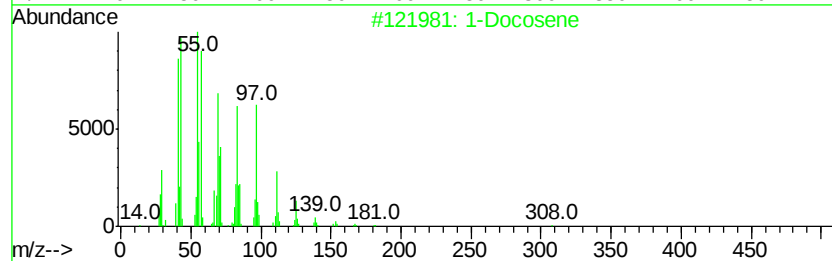
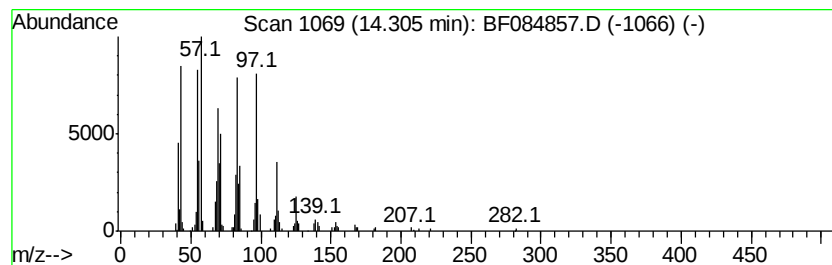
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1-Docosene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.31	7.09 ng	443634	Chrysene-d12	13.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Docosene	308	C22H44	001599-67-3	91
2		Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	91
3		17-Pentatriacontene	491	C35H70	006971-40-0	91
4		Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	91
5		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020516\
Data File : BF084857.D
Acq On : 5 Feb 2016 14:04
Operator : SJ/IZ
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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
S4-B006(17-19)

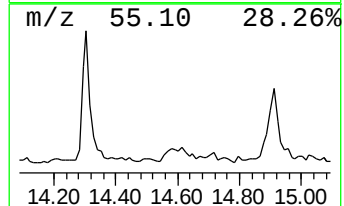
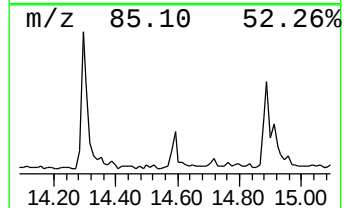
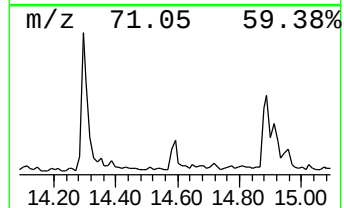
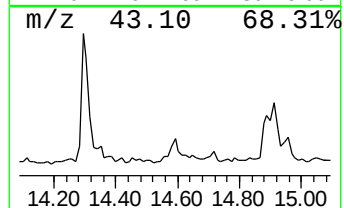
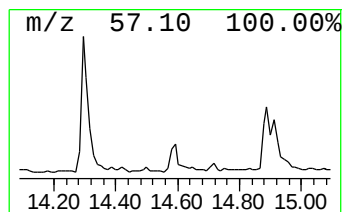
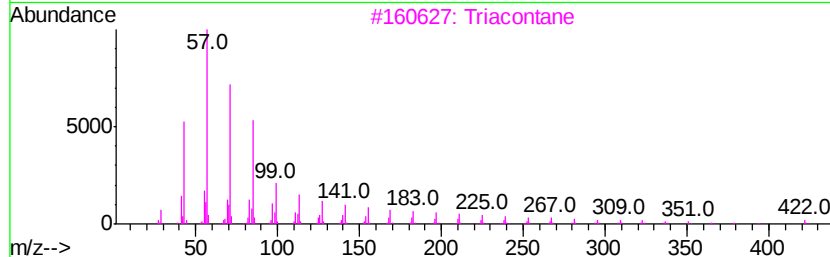
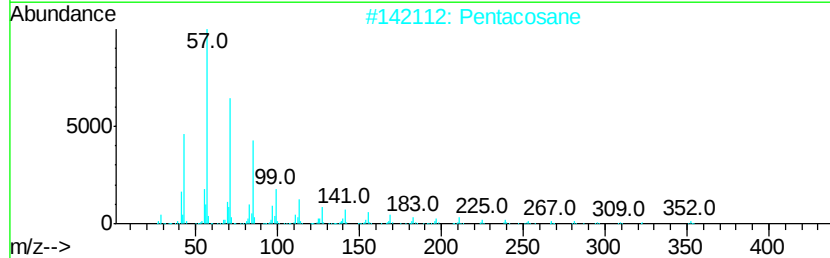
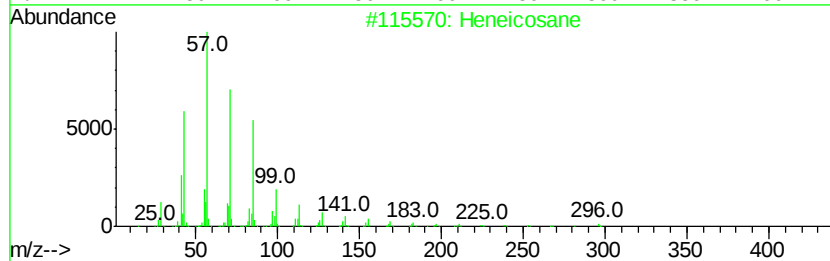
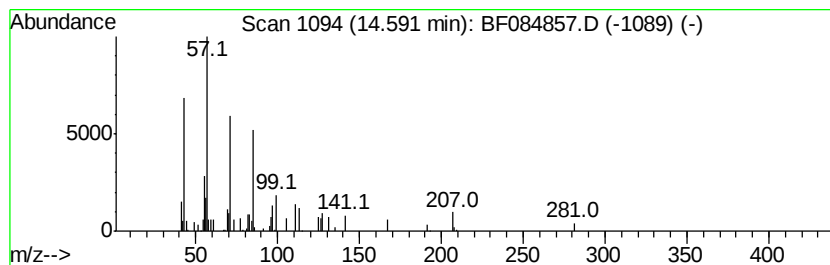
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Heneicosane Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.59	2.14 ng	96226	Perylene-d12	15.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	80
2		Pentacosane	352	C25H52	000629-99-2	80
3		Triacontane	422	C30H62	000638-68-6	72
4		Tetratriacontane	479	C34H70	014167-59-0	72
5		Nonacosane	408	C29H60	000630-03-5	72



Data Path : Z:\HPCHEM1\BNA F\DATA\BF020516\
Data File : BF084857.D
Acq On : 5 Feb 2016 14:04
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ClientSampleId :
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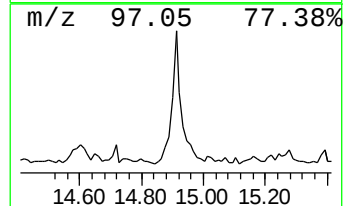
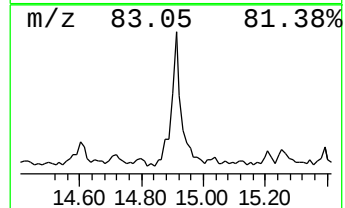
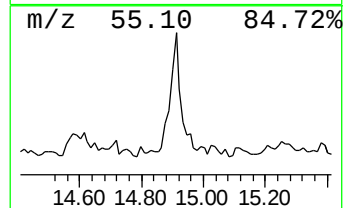
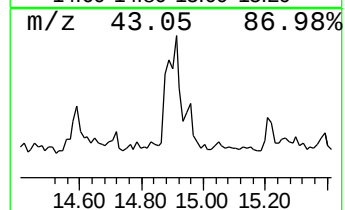
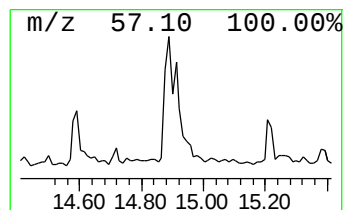
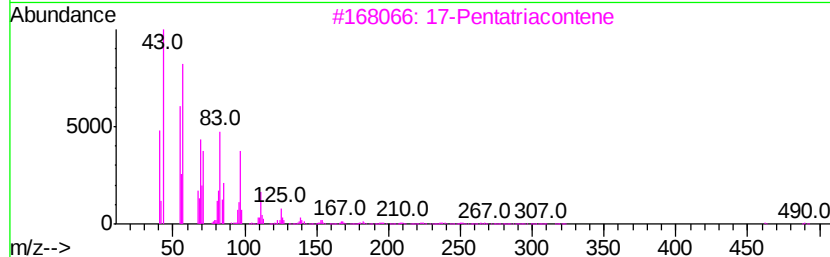
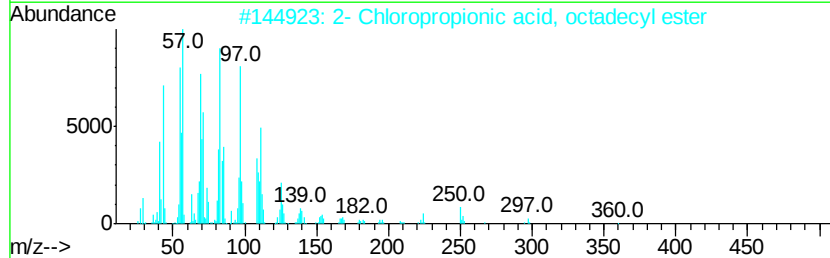
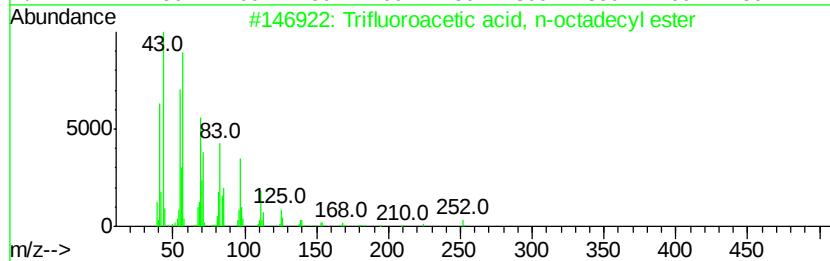
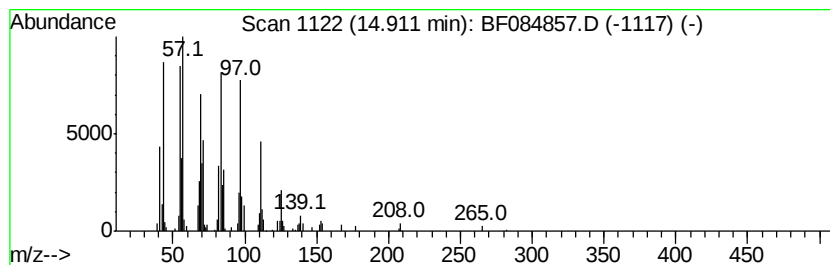
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Trifluoroacetic acid, n-oct... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.91	6.28 ng	282522	Perylene-d12	15.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trifluoroacetic acid, n-octadecyl...	366	C20H37F3O2	079392-43-1	91
2		2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91
3		17-Pentatriacontene	491	C35H70	006971-40-0	90
4		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	90
5		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020516\
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S4-B006(17-19)

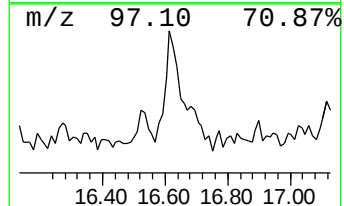
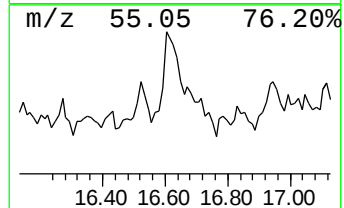
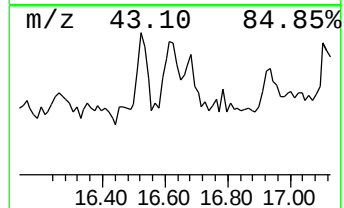
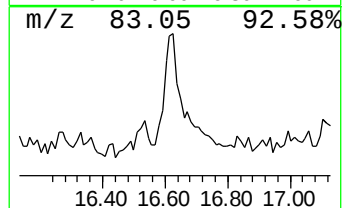
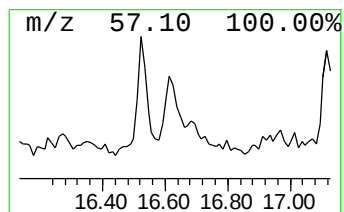
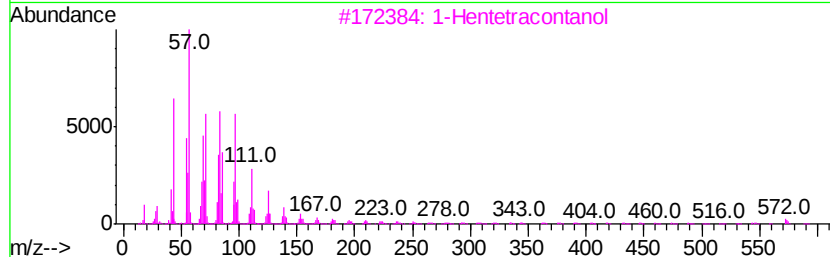
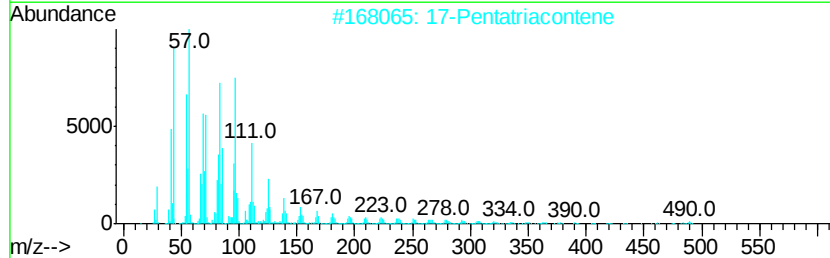
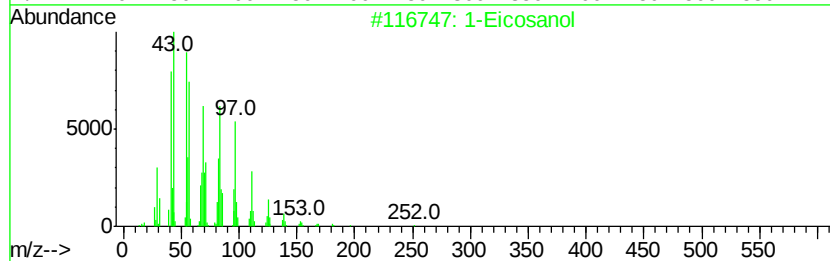
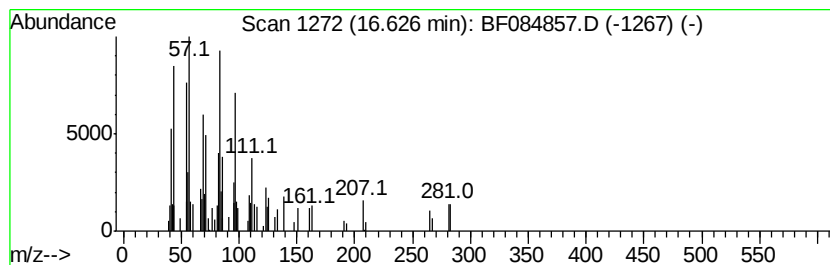
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 1-Eicosanol Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.63	2.58 ng	116104	Perylene-d12	15.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Eicosanol	298	C20H42O	000629-96-9	64
2		17-Pentatriacontene	491	C35H70	006971-40-0	64
3		1-Hentetracontanol	593	C41H84O	040710-42-7	58
4		Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	47
5		Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	47



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020516\
Data File : BF084857.D
Acq On : 5 Feb 2016 14:04
Operator : SJ/IZ
Sample : H1329-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S4-B006(17-19)

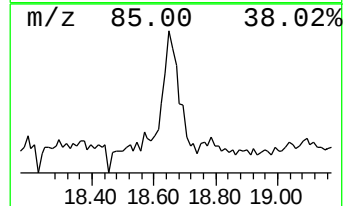
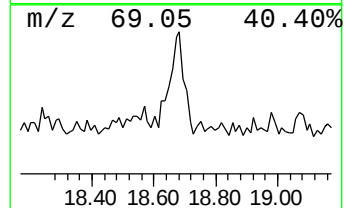
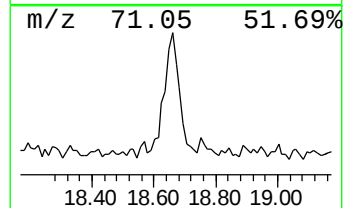
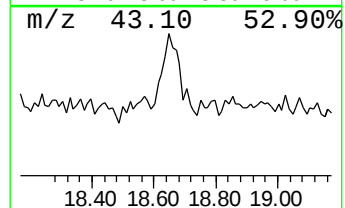
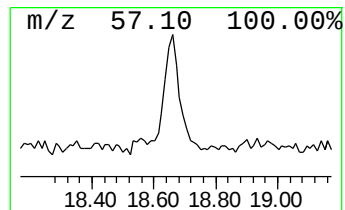
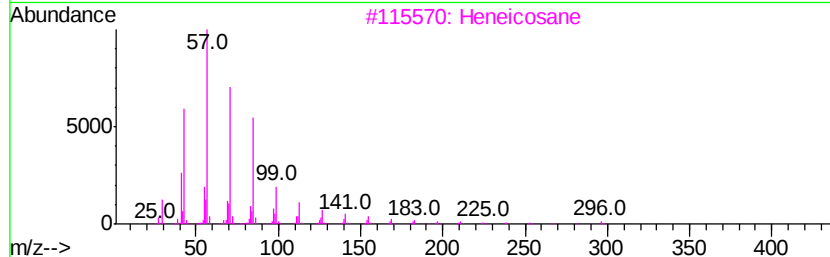
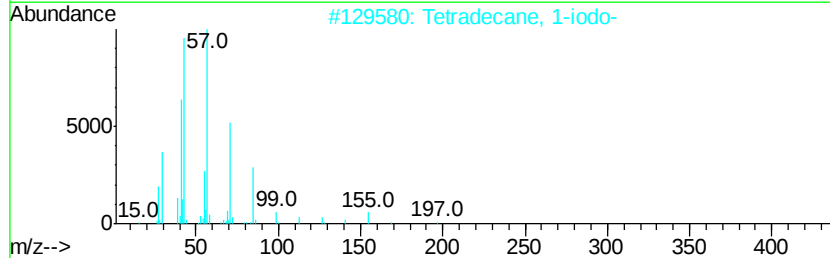
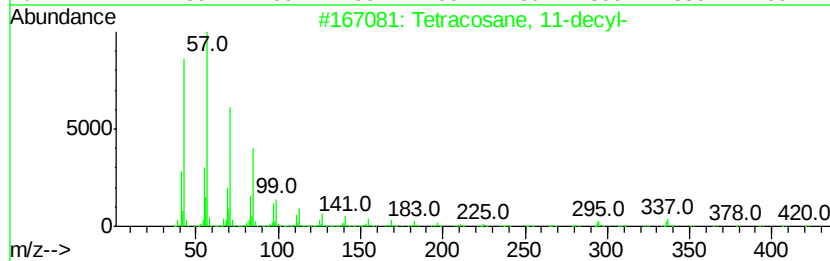
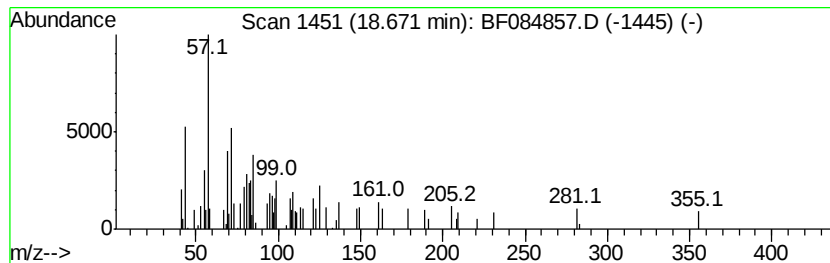
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 unknown18.67 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.67	3.20 ng	143791	Perylene-d12	15.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetracosane, 11-decyl-	479	C34H70	055429-84-0	27
2		Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	27
3		Heneicosane	296	C21H44	000629-94-7	27
4		Triacontane	422	C30H62	000638-68-6	27
5		Eicosane	282	C20H42	000112-95-8	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020516\
 Data File : BF084857.D
 Acq On : 5 Feb 2016 14:04
 Operator : SJ/IJ
 Sample : H1329-05
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S4-B006(17-19)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.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...	4.82	28.3	ng	1555340	1	6.66	1099860	20.0
unknown6.43	6.43	90.6	ng	4981750	1	6.66	1099860	20.0
n-Hexadecanoic acid	11.72	2.5	ng	196075	4	11.17	1565250	20.0
Tetracosane	12.28	4.1	ng	323422	4	11.17	1565250	20.0
Hexadecanoic acid...	12.59	2.9	ng	182116	5	13.80	1251180	20.0
2-Bromo dodecane	13.00	8.3	ng	521330	5	13.80	1251180	20.0
Octadecanoic acid...	13.30	2.3	ng	144708	5	13.80	1251180	20.0
Trichloroacetic a...	13.67	21.9	ng	1372090	5	13.80	1251180	20.0
1-Docosene	14.31	7.1	ng	443634	5	13.80	1251180	20.0
Heneicosane	14.59	2.1	ng	96226	6	15.17	899129	20.0
Trifluoroacetic a...	14.91	6.3	ng	282522	6	15.17	899129	20.0
1-Eicosanol	16.63	2.6	ng	116104	6	15.17	899129	20.0
unknown18.67	18.67	3.2	ng	143791	6	15.17	899129	20.0