

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010616\
 Data File : BF084291.D
 Acq On : 6 Jan 2016 16:02
 Operator : SJ/UM
 Sample : H1010-03
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TEP-MW2-26

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-BF123115.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	3.813	147	151	154	rVB	126996	197185	2.45%	0.299%
2	5.036	256	258	263	rVB	468805	675436	8.38%	1.025%
3	5.470	293	296	298	rBV	4065797	3619294	44.88%	5.492%
4	5.722	316	318	321	rBV	190495	162482	2.01%	0.247%
5	6.499	384	386	389	rBV	2489161	2150557	26.67%	3.263%
6	6.636	395	398	400	rBV	6492683	6075085	75.33%	9.218%
7	6.865	416	418	420	rBV	2056939	1651506	20.48%	2.506%
8	7.025	429	432	434	rBV	6636835	5895816	73.11%	8.946%
9	7.436	465	468	470	rBV	5189146	5479683	67.95%	8.315%
10	8.156	528	531	533	rVB	2211945	2236488	27.73%	3.394%
11	9.185	620	621	623	rBV	83416	107973	1.34%	0.164%
12	9.231	623	625	628	rVB	8233670	8024662	99.50%	12.177%
13	9.619	657	659	662	rBV	238252	252640	3.13%	0.383%
14	9.836	675	678	682	rBV2	43408	84059	1.04%	0.128%
15	9.905	682	684	687	rVB	2813670	2445749	30.33%	3.711%
16	10.293	715	718	719	rBV	134190	152047	1.89%	0.231%
17	10.339	719	722	724	rVV2	126423	152335	1.89%	0.231%
18	10.648	745	749	750	rBV	130170	142693	1.77%	0.217%
19	10.694	750	753	756	rBV	5106976	5568541	69.05%	8.450%
20	10.819	762	764	768	rVB3	97390	199772	2.48%	0.303%
21	11.014	778	781	783	rBV2	49287	83751	1.04%	0.127%
22	11.059	783	785	787	rVB2	87944	97985	1.21%	0.149%
23	11.094	787	788	790	rBV	100849	99285	1.23%	0.151%
24	11.265	800	803	804	rBV	90656	115875	1.44%	0.176%
25	11.391	811	814	816	rBV	2710173	2453517	30.42%	3.723%
26	12.979	950	953	955	rBV	7972908	8064765	100.00%	12.238%
27	13.471	990	996	998	rBV2	70214	113503	1.41%	0.172%
28	13.540	998	1002	1004	rBV4	35944	89444	1.11%	0.136%
29	13.814	1024	1026	1027	rBV	485914	413809	5.13%	0.628%
30	13.837	1027	1028	1030	rVV	699942	918716	11.39%	1.394%
31	13.882	1030	1032	1038	rVB	113526	169364	2.10%	0.257%
32	14.020	1042	1044	1047	rBV	2244478	2257500	27.99%	3.426%
33	14.797	1109	1112	1114	rBV2	68102	114289	1.42%	0.173%
34	14.877	1117	1119	1122	rBV2	57992	90169	1.12%	0.137%

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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-BF123115.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.448	1166	1169	1172	rBV	1345265	1733657	21.50%	2.631%
36	15.825	1200	1202	1204	rBV3	58384	86433	1.07%	0.131%
37	15.871	1204	1206	1208	rVV2	130519	269699	3.34%	0.409%
38	15.974	1211	1215	1218	rVV2	107969	253767	3.15%	0.385%
39	16.031	1218	1220	1224	rVB	112167	179442	2.23%	0.272%
40	16.145	1227	1230	1240	rVB	896678	1824876	22.63%	2.769%
41	16.340	1244	1247	1248	rBV	72748	154182	1.91%	0.234%
42	16.534	1261	1264	1272	rVB2	68683	164293	2.04%	0.249%
43	16.671	1272	1276	1284	rBV	431323	879133	10.90%	1.334%

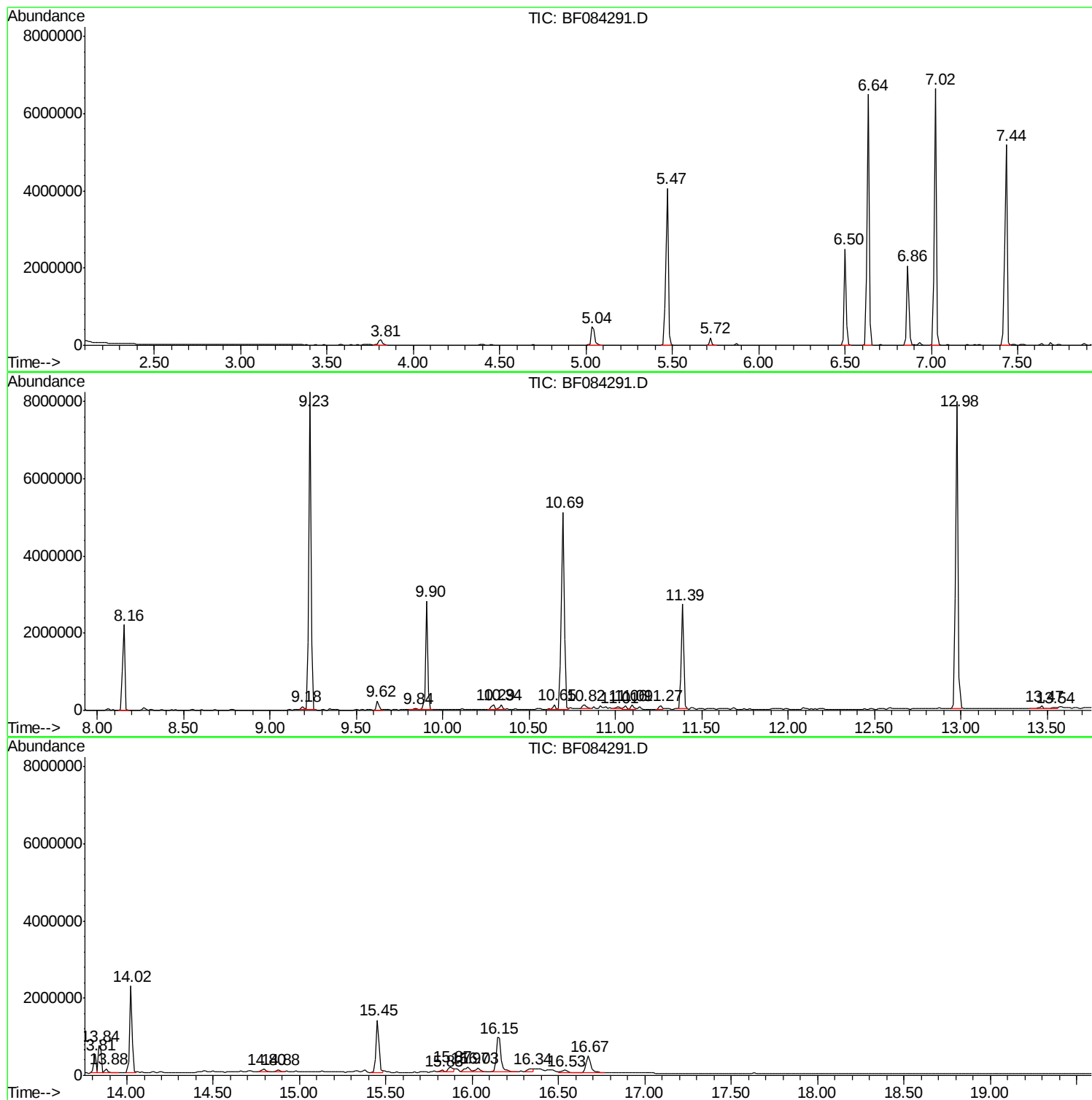
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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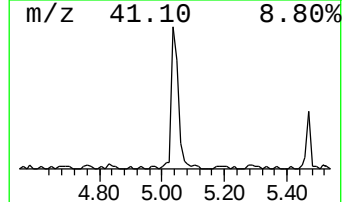
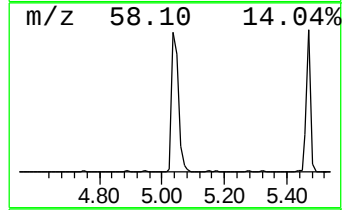
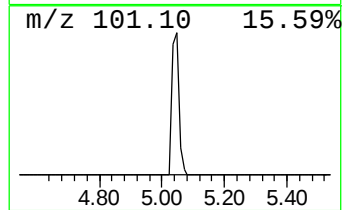
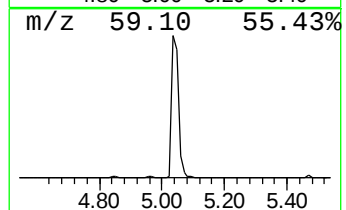
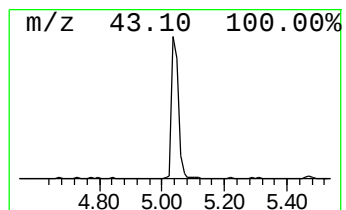
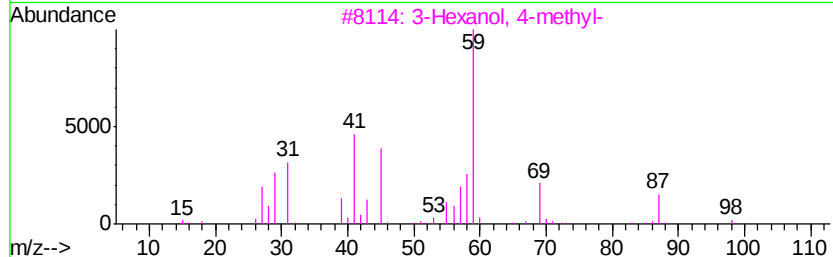
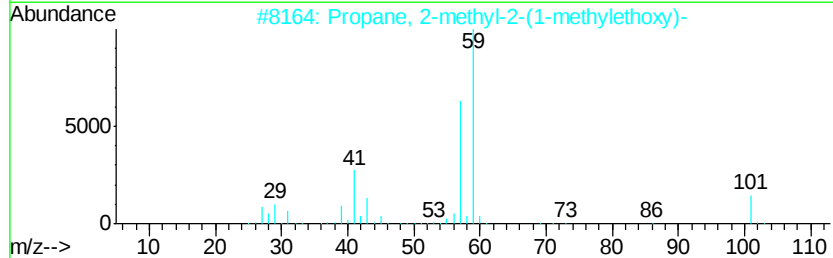
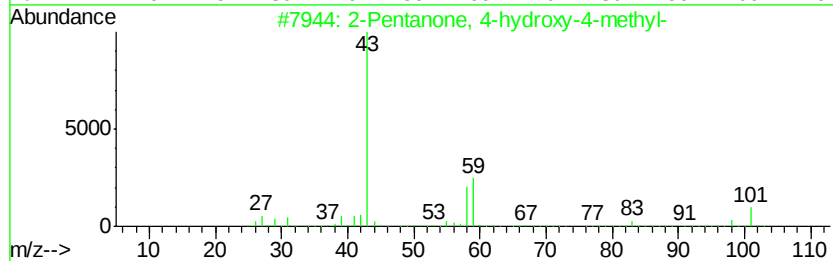
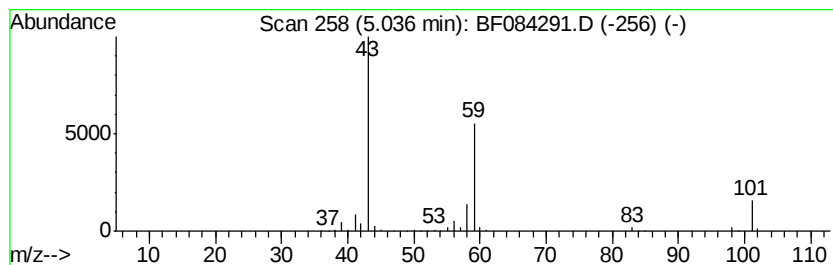
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	8.18 ng	675436	1,4-Dichlorobenzene-d4	6.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			3-Hexanol	102	C6H14O	000623-37-0	33
5			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28



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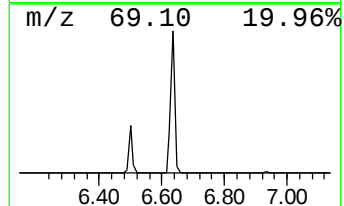
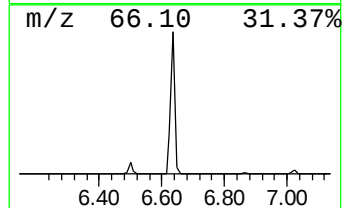
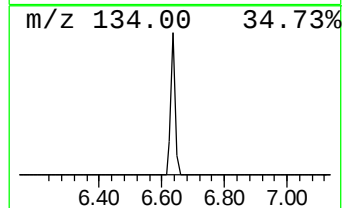
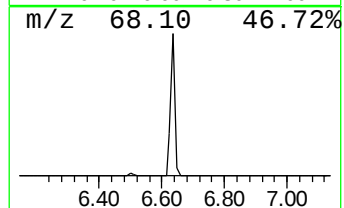
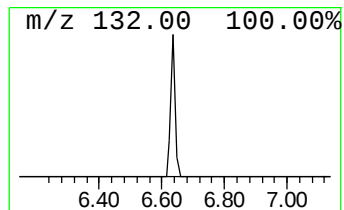
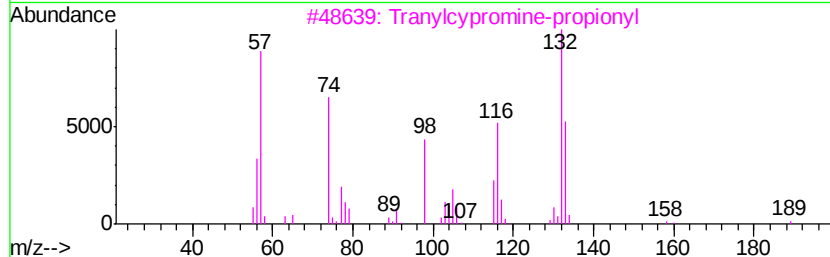
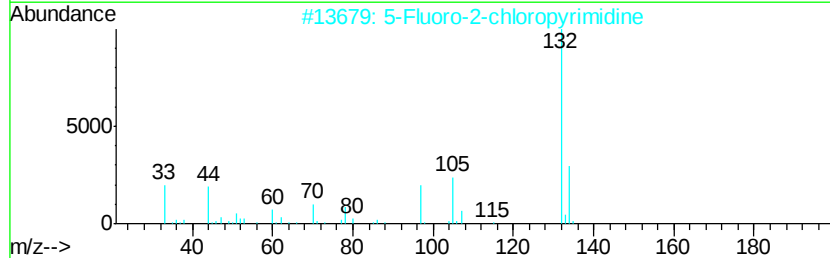
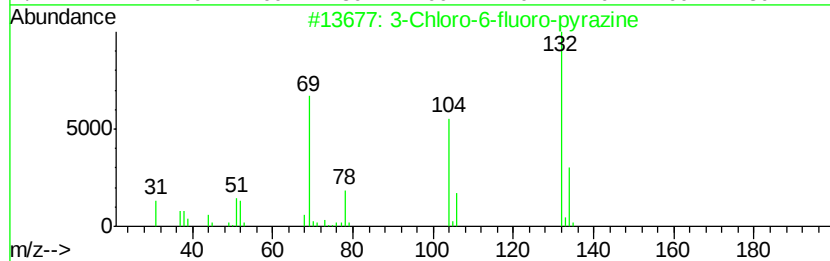
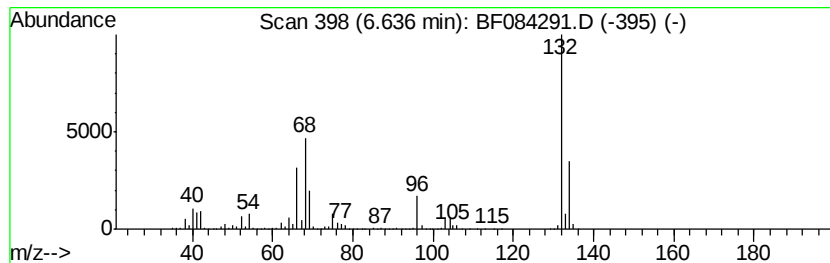
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Peak Number 3 unknown6.64 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.64	73.57 ng	6075090	1,4-Dichlorobenzene-d4	6.86

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	16
3		Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
4		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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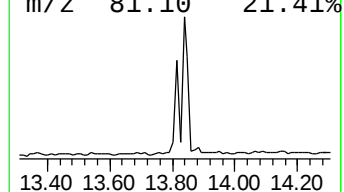
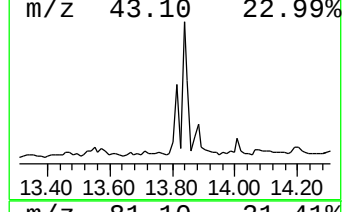
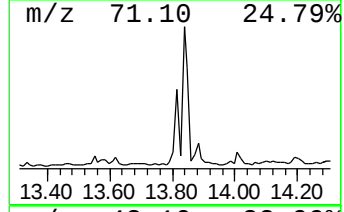
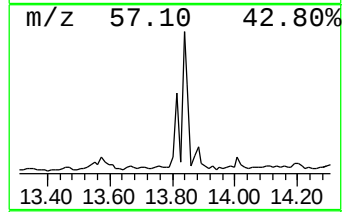
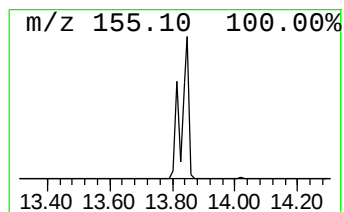
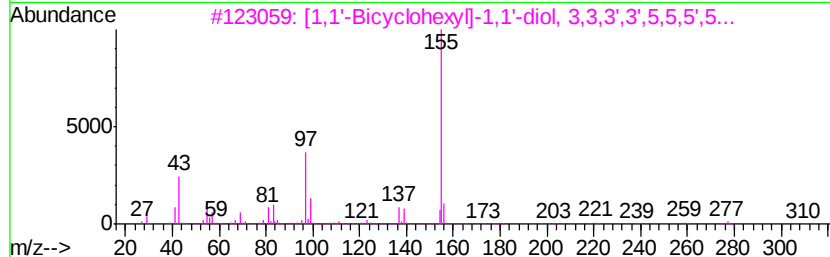
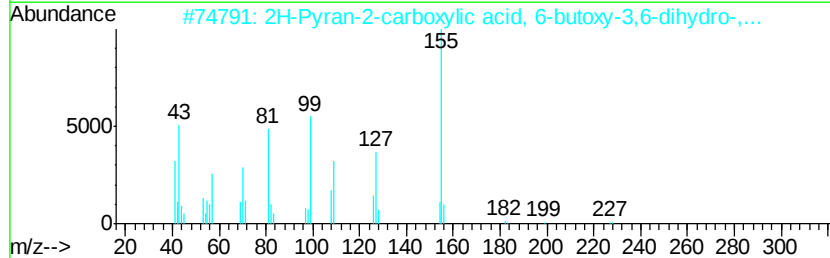
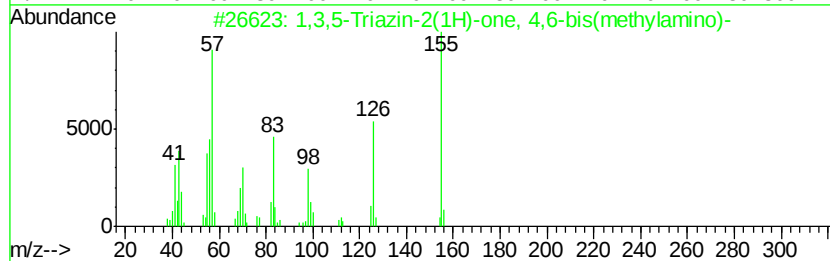
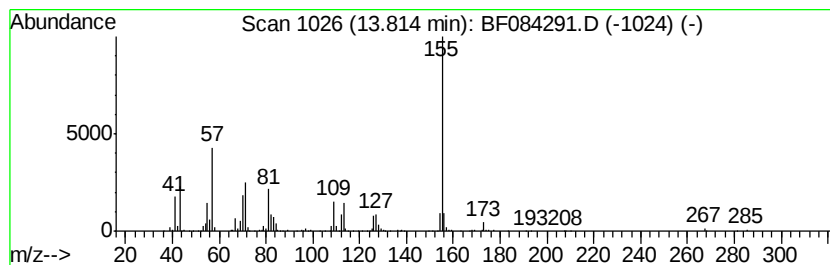
Instrument :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 1,3,5-Triazin-2(1H)-one, 4,... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.81	3.67 ng	413809	Chrysene-d12	14.02	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,5-Triazin-2(1H)-one, 4,6-bis...	155	C5H9N5O	055702-52-8	50
2	2H-Pyran-2-carboxylic acid, 6-bu...	228	C12H20O4	026457-97-6	45
3	[1,1'-Bicvclohexvll]-1,1'-diol, 3...	310	C20H38O2	068525-22-4	38
4	Benzaldehyde, 4-chloro-2-nitro-	185	C7H4ClNO3	005551-11-1	38
5	6-Amino-1,3-dimethyluracil	155	C6H9N3O2	006642-31-5	37



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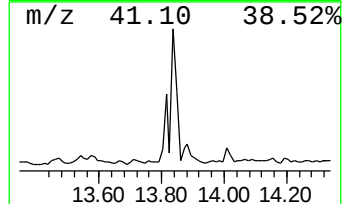
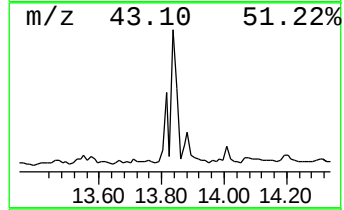
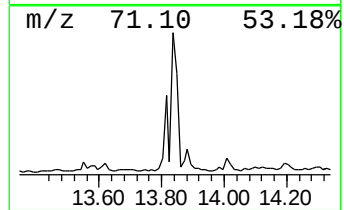
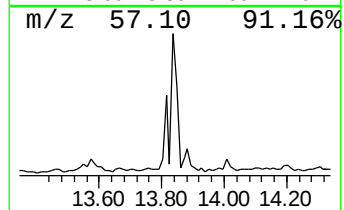
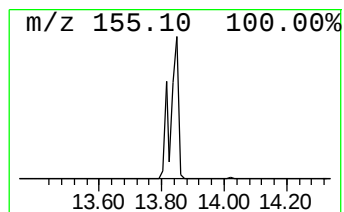
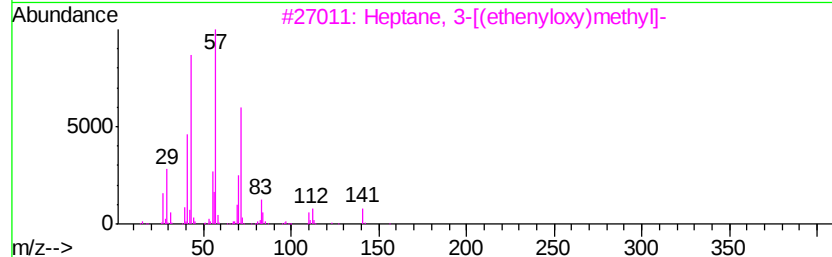
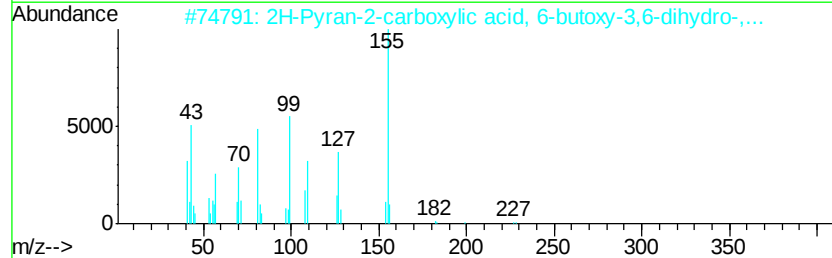
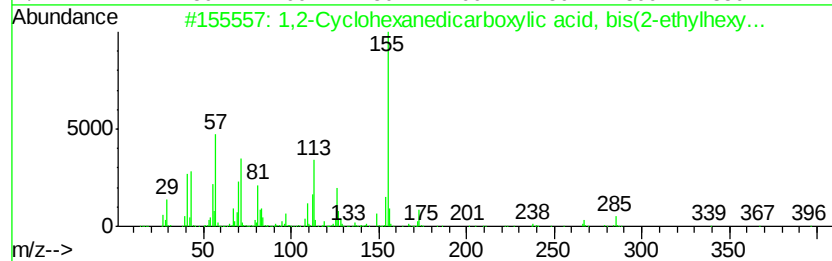
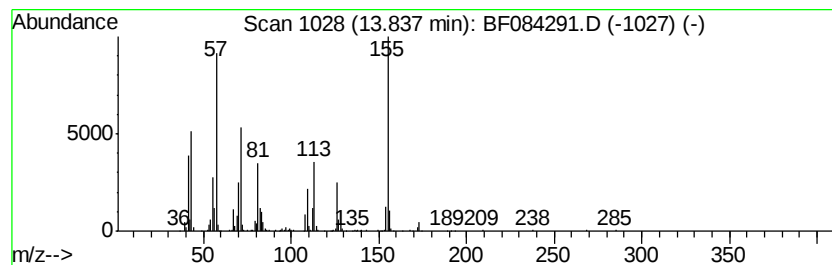
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1,2-Cyclohexanedicarboxylic... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.84	8.14 ng	918716	Chrysene-d12	14.02

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2-Cyclohexanedicarboxylic acid...	396	C24H44O4	000084-71-9	53
2			2H-Pyran-2-carboxylic acid, 6-bu...	228	C12H20O4	026457-97-6	22
3			Heptane, 3-[(ethenyl)oxy]methyl-	156	C10H20O	000103-44-6	22
4			2,4-Dimethyl-heptane-3,5-dione	156	C9H16O2	037484-68-7	22
5			4,6-Dihydropyrimidine, 5-amino...	155	C5H5N3O3	001074-97-1	22



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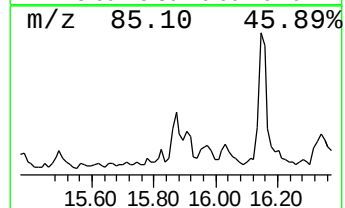
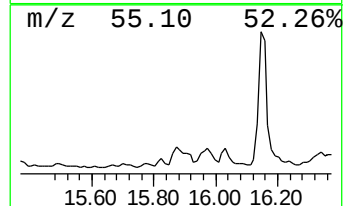
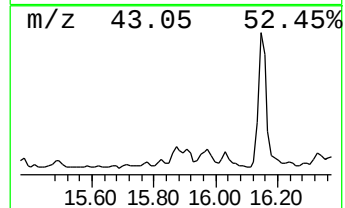
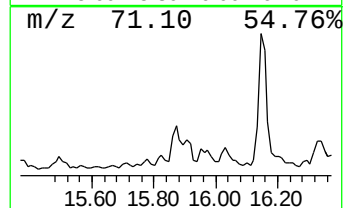
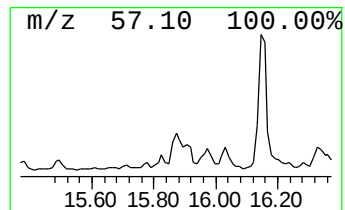
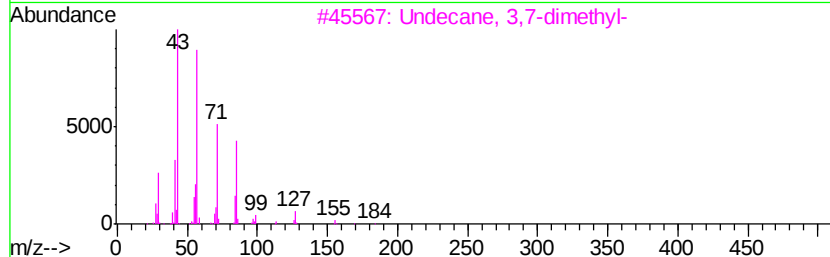
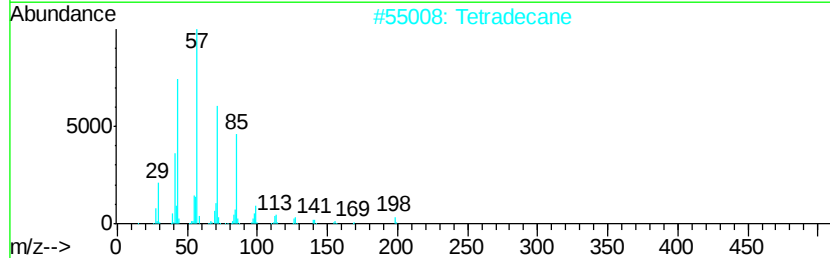
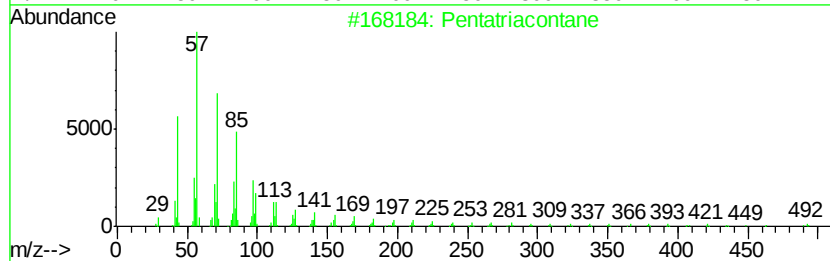
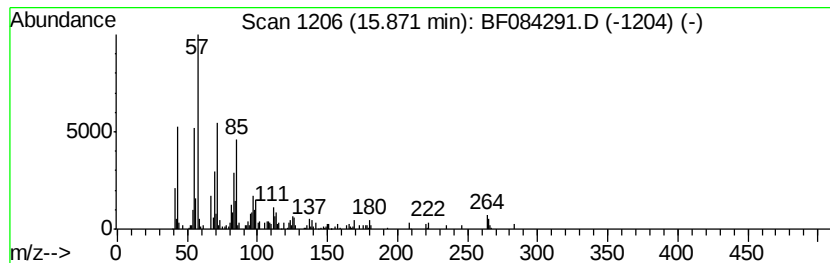
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ClientSampleId :
TEP-MW2-26

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Pentatriacontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.87	3.11 ng	269699	Perylene-d12	15.45	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentatriacontane	493	C35H72	000630-07-9	64
2	Tetradecane	198	C14H30	000629-59-4	47
3	Undecane, 3,7-dimethyl-	184	C13H28	017301-29-0	47
4	Oleic acid, eicosyl ester	563	C38H74O2	022393-88-0	47
5	Undecane, 3-methyl-	170	C12H26	001002-43-3	47



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010616\
Data File : BF084291.D
Acq On : 6 Jan 2016 16:02
Operator : SJ/UM
Sample : H1010-03
Misc :
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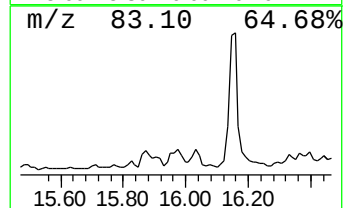
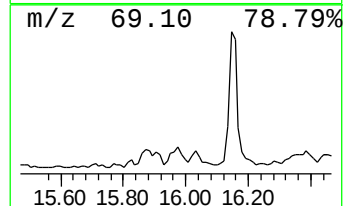
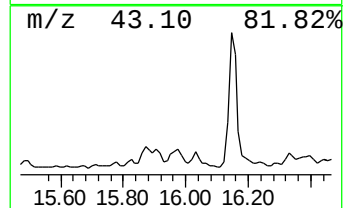
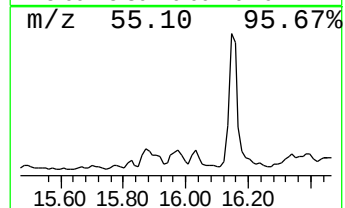
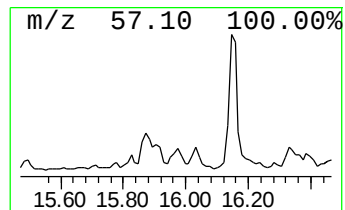
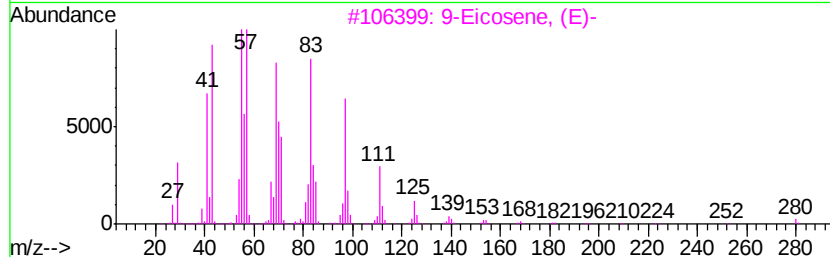
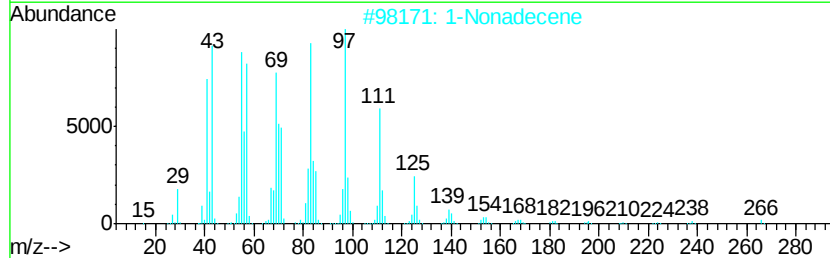
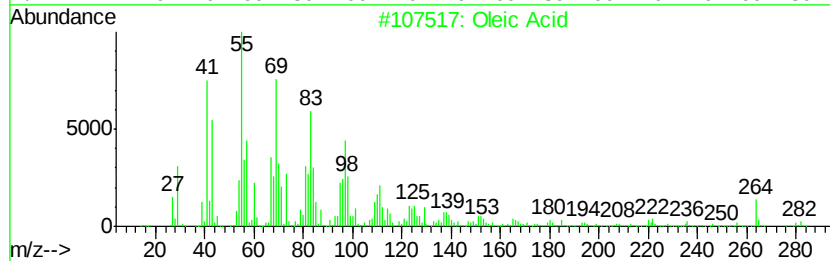
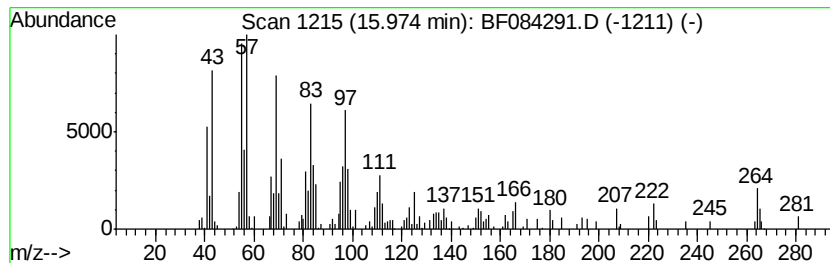
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ClientSampleId :
TEP-MW2-26

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Oleic Acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.97	2.93 ng	253767	Perylene-d12	15.45
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Oleic Acid	282 C18H34O2	000112-80-1	74
2	1-Nonadecene	266 C19H38	018435-45-5	64
3	9-Eicosene, (E)-	280 C20H40	074685-29-3	64
4	Trichloroacetic acid, tetradecyl...	358 C16H29Cl3O2	074339-52-9	64
5	14-Pentadecenoic acid	240 C15H28O2	017351-34-7	62



Data Path : Z:\HPCHEM1\BNA F\DATA\BF010616\
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Acq On : 6 Jan 2016 16:02
Operator : SJ/UM
Sample : H1010-03
Misc :
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Instrument :
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ClientSampleId :
TEP-MW2-26

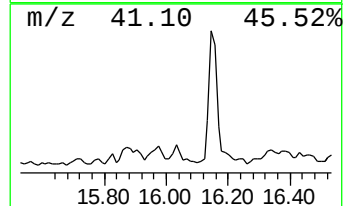
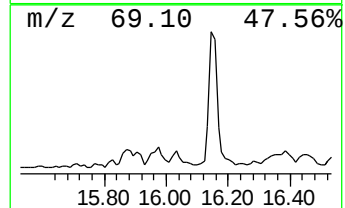
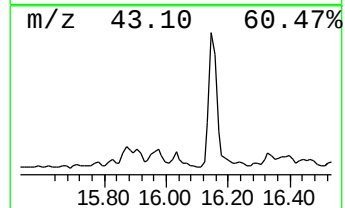
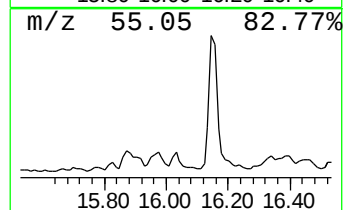
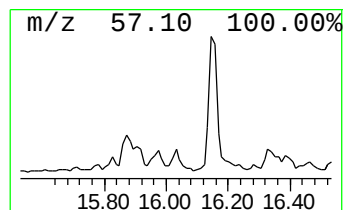
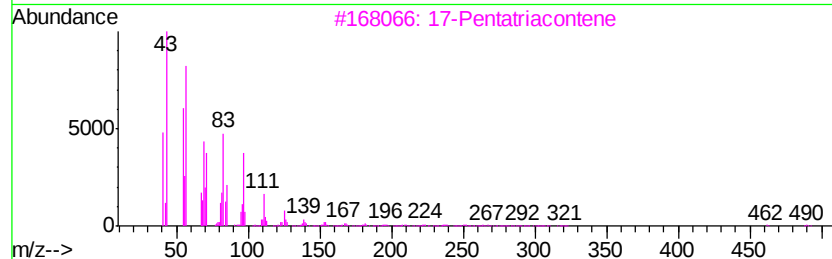
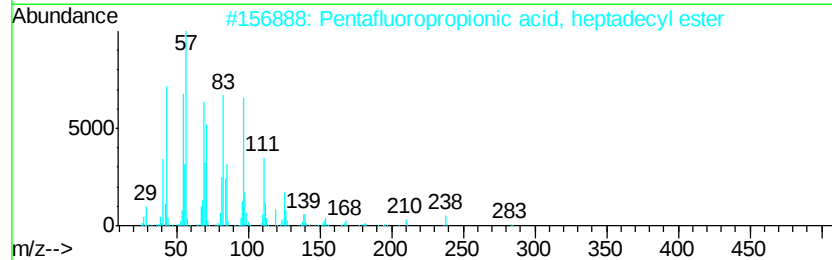
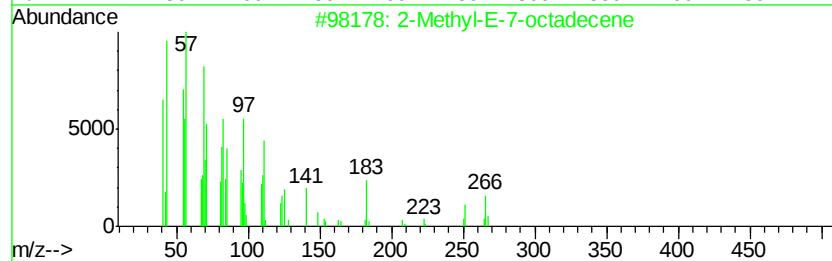
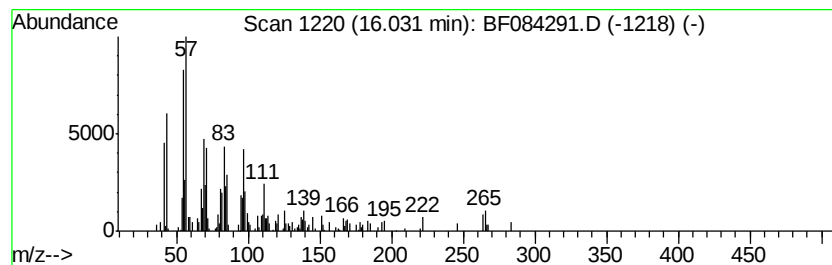
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 2-Methyl-E-7-octadecene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.03	2.07 ng	179442	Perylene-d12	15.45

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methyl-E-7-octadecene	266	C19H38	1000130-92-3	87	
2	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	80	
3	17-Pentatriacontene	491	C35H70	006971-40-0	68	
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	64	
5	Acetic acid, chloro-, octadecyl ...	346	C20H39ClO2	005348-82-3	62	



Data Path : Z:\HPCHEM1\BNA F\DATA\BF010616\
Data File : BF084291.D
Acq On : 6 Jan 2016 16:02
Operator : SJ/UM
Sample : H1010-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TEP-MW2-26

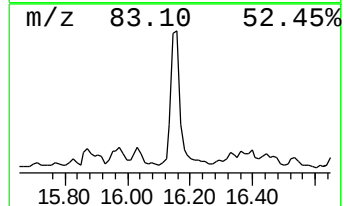
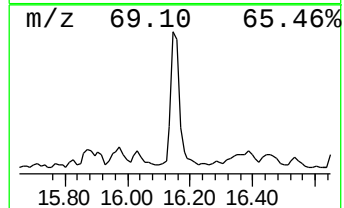
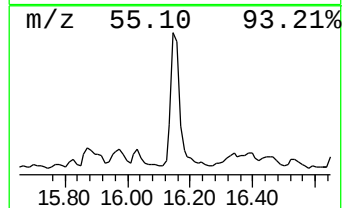
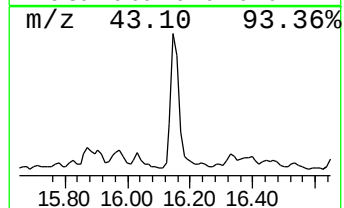
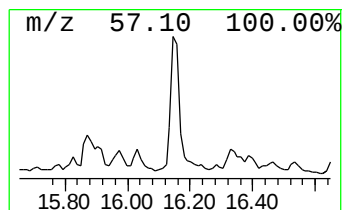
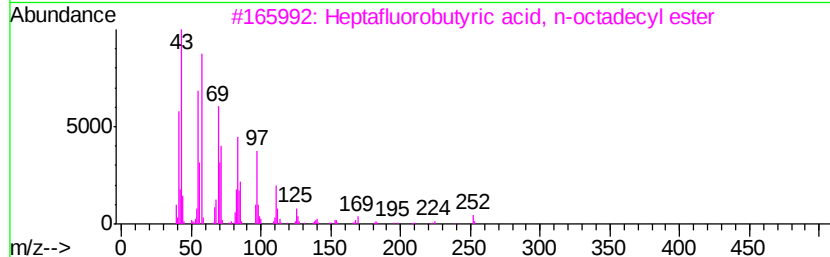
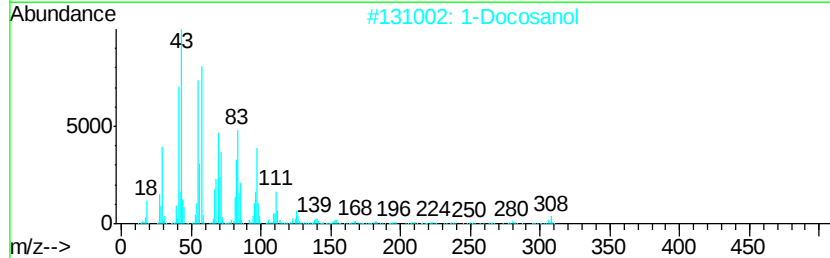
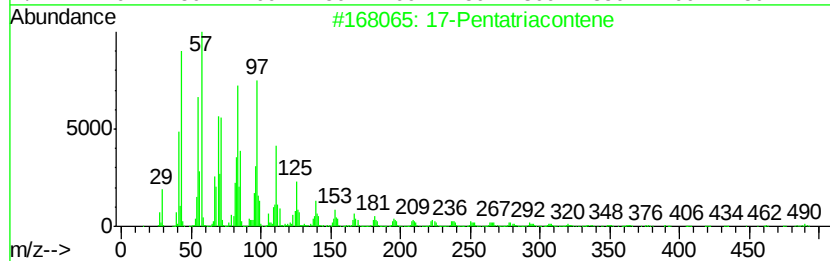
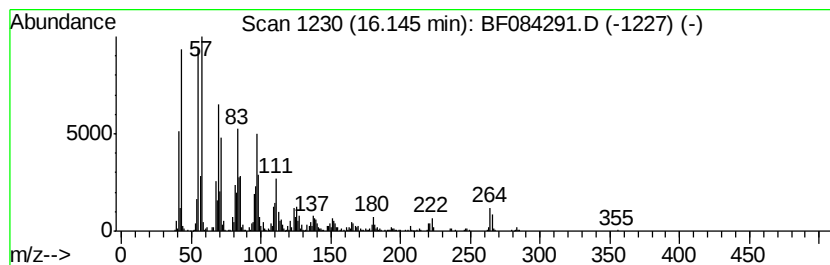
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 17-Pentatriacontene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.15	21.05 ng	1824880	Perylene-d12	15.45

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			17-Pentatriacontene	491	C35H70	006971-40-0	72
2			1-Docosanol	326	C22H46O	000661-19-8	68
3			Heptafluorobutyric acid, n-octadecyl ester	466	C22H37F7O2	000400-57-7	68
4			Pentafluoropropionic acid, heptafluorooctyl ester	402	C20H35F5O2	1000283-04-2	62
5			6-Octadecenoic acid, (Z)-	282	C18H34O2	000593-39-5	62



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010616\
Data File : BF084291.D
Acq On : 6 Jan 2016 16:02
Operator : SJ/UM
Sample : H1010-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
TEP-MW2-26

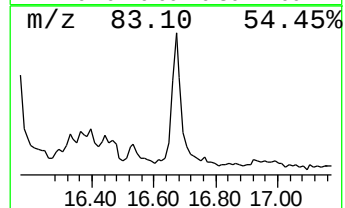
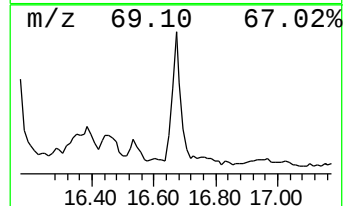
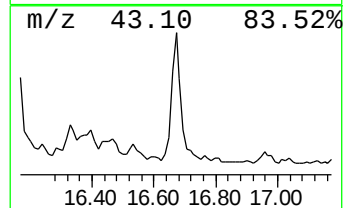
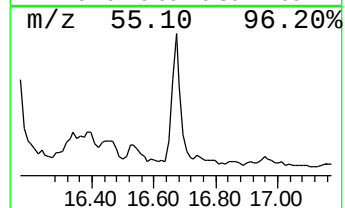
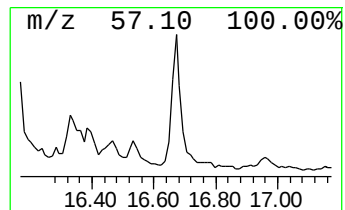
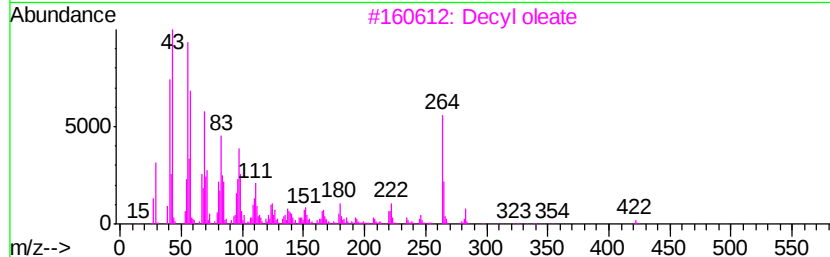
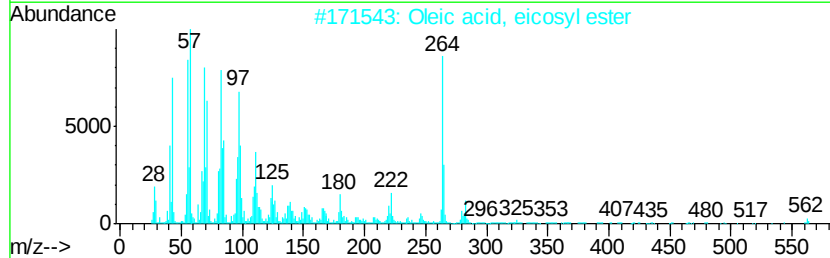
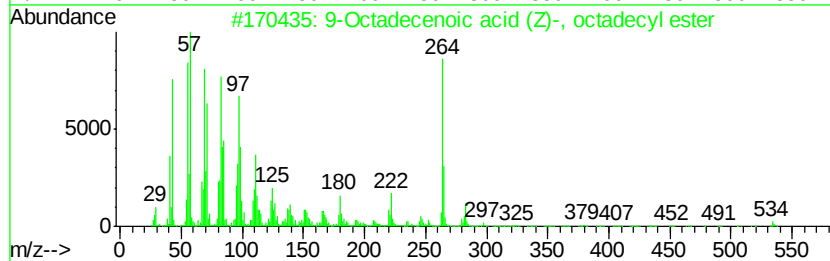
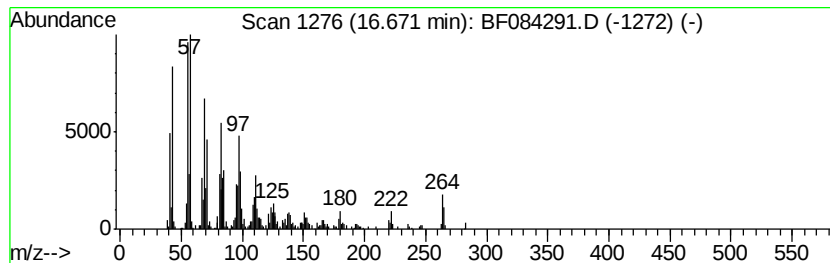
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 9-Octadecenoic acid (Z)-, o... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.67	10.14 ng	879133	Perylene-d12	15.45

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenoic acid (Z)-, octade...	535	C36H70O2	017673-49-3	91
2		Oleic acid, eicosyl ester	563	C38H74O2	022393-88-0	91
3		Decyl oleate	422	C28H54O2	003687-46-5	90
4		17-Pentatriacontene	491	C35H70	006971-40-0	76
5		Z-5-Nonadecene	266	C19H38	1000131-11-8	62



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010616\
 Data File : BF084291.D
 Acq On : 6 Jan 2016 16:02
 Operator : SJ/UM
 Sample : H1010-03
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
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 ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.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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unknown6.64	6.64	73.6	ng	6075090	1	6.86	1651510	20.0
1,3,5-Triazin-2(1...	13.81	3.7	ng	413809	5	14.02	2257500	20.0
1,2-Cyclohexanedi...	13.84	8.1	ng	918716	5	14.02	2257500	20.0
Pentatriacontane	15.87	3.1	ng	269699	6	15.45	1733660	20.0
Oleic Acid	15.97	2.9	ng	253767	6	15.45	1733660	20.0
2-Methyl-E-7-octa...	16.03	2.1	ng	179442	6	15.45	1733660	20.0
17-Pentatriacontene	16.15	21.1	ng	1824880	6	15.45	1733660	20.0
9-Octadecenoic ac...	16.67	10.1	ng	879133	6	15.45	1733660	20.0