

Data Path : Z:\HPCHEM1\BNA F\DATA\BF111015\
 Data File : BF082887.D
 Acq On : 10 Nov 2015 23:40
 Operator : UM/IZ
 Sample : G4246-02
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 T-14C

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-BF110715.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	4.990	250	254	260	rVB	2013004	3014404	45.93%	4.714%
2	5.424	289	292	294	rBV	5463575	5821727	88.71%	9.105%
3	6.453	379	382	385	rBV	4786109	5347704	81.48%	8.363%
4	6.579	391	393	396	rBV	4097050	5723586	87.21%	8.951%
5	6.819	411	414	416	rBV	1218327	1538248	23.44%	2.406%
6	6.967	425	427	430	rVB	3453169	4049697	61.71%	6.333%
7	7.379	460	463	465	rBV	3796044	3971474	60.51%	6.211%
8	8.099	524	526	529	rVB	2227589	2003262	30.52%	3.133%
9	9.185	618	621	623	rBV	6842620	6562812	100.00%	10.264%
10	9.573	653	655	658	rBV	1844944	1640433	25.00%	2.565%
11	9.859	677	680	682	rBV	2404947	2443242	37.23%	3.821%
12	10.282	714	717	720	rVB3	161093	290026	4.42%	0.454%
13	10.648	746	749	751	rBV	3263639	4119033	62.76%	6.442%
14	10.774	758	760	764	rVB	157319	183737	2.80%	0.287%
15	11.219	797	799	801	rBV	161908	140501	2.14%	0.220%
16	11.334	807	809	812	rBV	2443979	2296933	35.00%	3.592%
17	11.642	835	836	839	rVB	52140	70004	1.07%	0.109%
18	11.882	854	857	859	rBV	311204	344367	5.25%	0.539%
19	12.054	868	872	874	rBV2	48440	83961	1.28%	0.131%
20	12.202	882	885	887	rVB	69860	68431	1.04%	0.107%
21	12.545	913	915	917	rBV	81607	76661	1.17%	0.120%
22	12.659	922	925	928	rVV2	74707	124304	1.89%	0.194%
23	12.762	932	934	936	rVV2	774860	743668	11.33%	1.163%
24	12.831	936	940	943	rVB2	102319	162571	2.48%	0.254%
25	12.934	946	949	951	rVV	4256511	5876155	89.54%	9.190%
26	13.174	966	970	971	rBV2	66054	84028	1.28%	0.131%
27	13.471	993	996	998	rBV	399554	514991	7.85%	0.805%
28	13.517	998	1000	1001	rBV	81175	86907	1.32%	0.136%
29	13.711	1013	1017	1024	rBV3	76153	202279	3.08%	0.316%
30	13.837	1024	1028	1031	rBV	400452	617839	9.41%	0.966%
31	13.974	1037	1040	1042	rBV	2298355	2229556	33.97%	3.487%
32	14.157	1054	1056	1059	rBV	129010	134590	2.05%	0.210%
33	14.465	1081	1083	1086	rBV	212365	289857	4.42%	0.453%
34	14.762	1107	1109	1113	rVB	114621	116180	1.77%	0.182%

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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

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35	15.083	1135	1137	1139	rBV	155299	197548	3.01%	0.309%
36	15.391	1161	1164	1167	rBV	1370463	1645425	25.07%	2.573%
37	15.448	1167	1169	1172	rVB	67296	90773	1.38%	0.142%
38	15.860	1202	1205	1207	rBV	85528	121267	1.85%	0.190%
39	15.905	1207	1209	1213	rBV2	49092	120384	1.83%	0.188%
40	16.328	1244	1246	1250	rVB	43547	88663	1.35%	0.139%
41	16.888	1292	1295	1300	rBV2	39074	95677	1.46%	0.150%
42	17.334	1331	1334	1338	rBV4	64701	173966	2.65%	0.272%
43	17.540	1350	1352	1358	rVB2	41170	97374	1.48%	0.152%
44	18.329	1418	1421	1426	rVB3	34013	99323	1.51%	0.155%
45	19.254	1498	1502	1509	rVB3	41117	128566	1.96%	0.201%
46	20.363	1595	1599	1607	rVB3	28411	111049	1.69%	0.174%

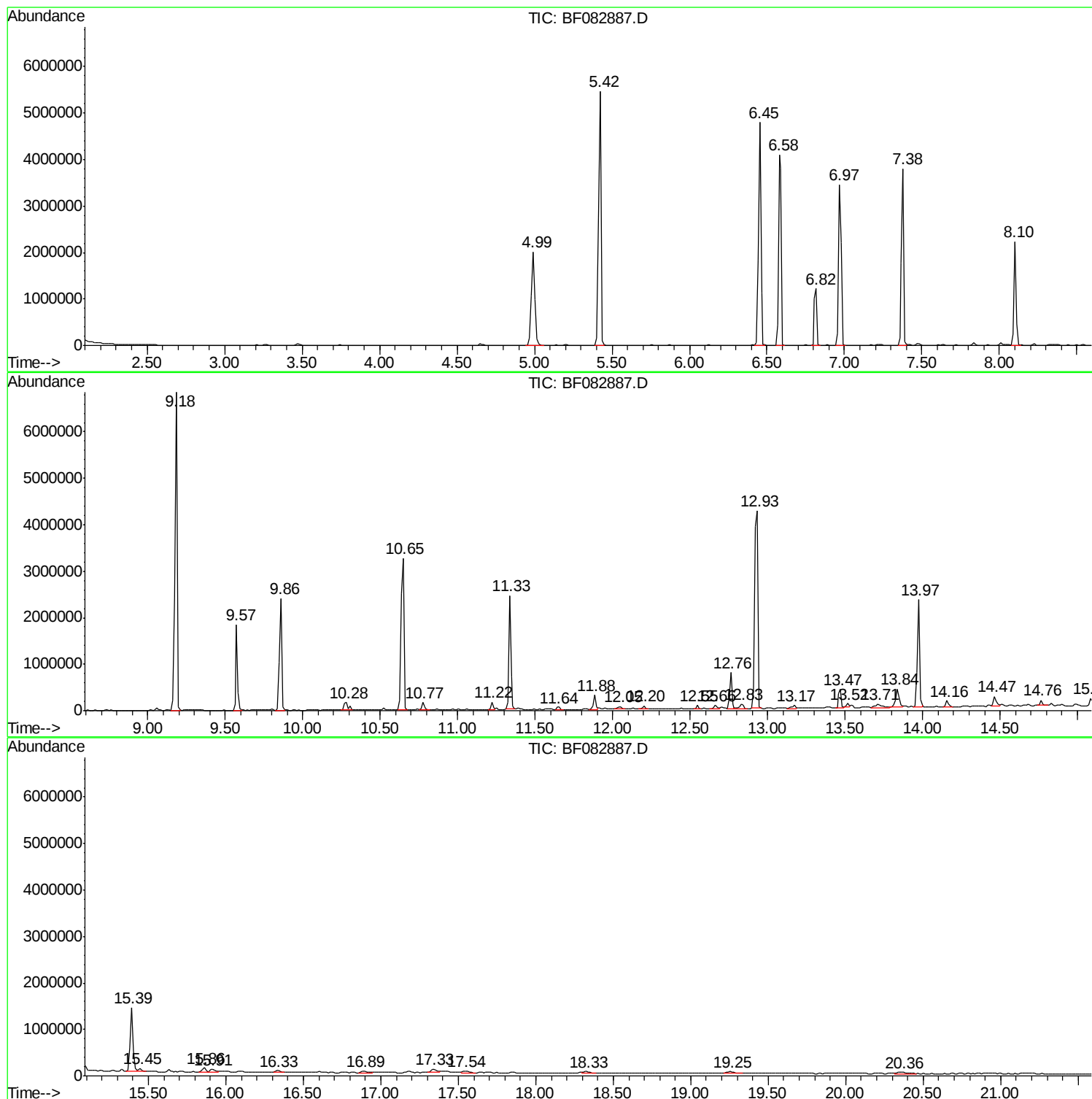
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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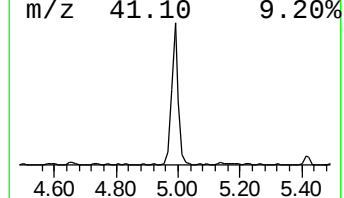
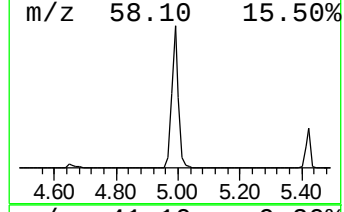
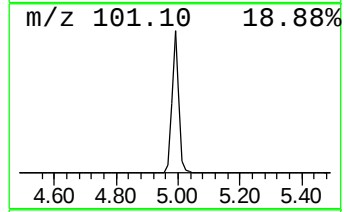
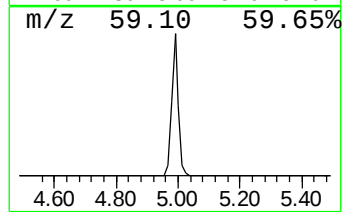
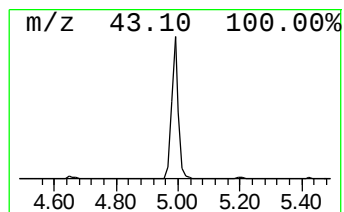
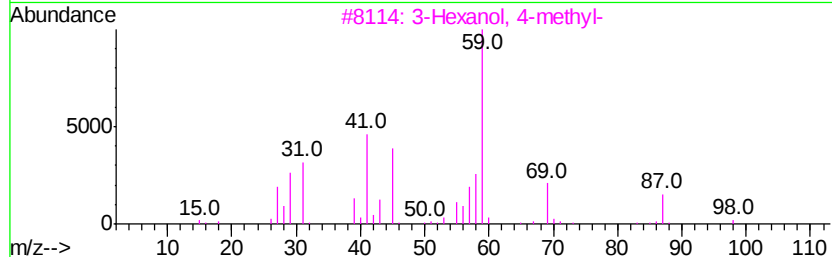
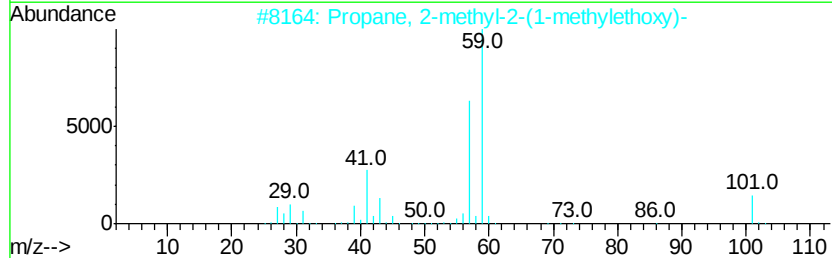
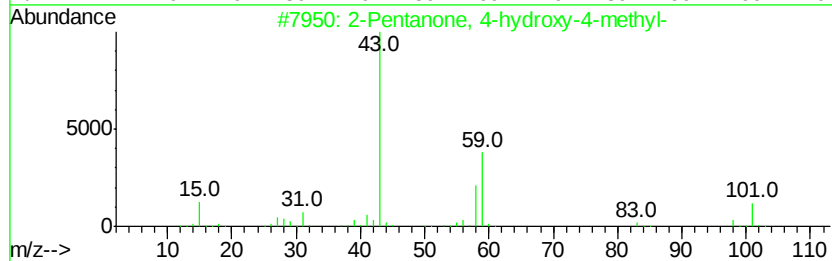
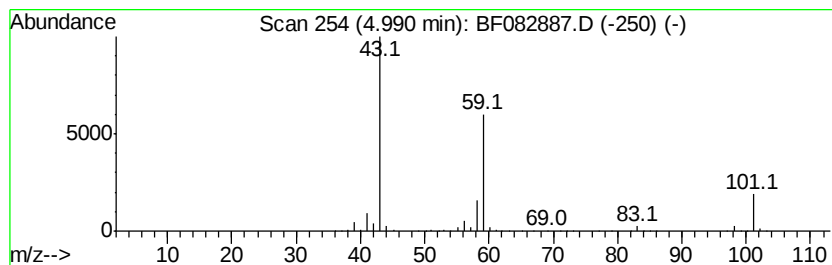
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.99	39.19 ng	3014400	1,4-Dichlorobenzene-d4	6.82

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	36
3	3-Hexanol, 4-methyl-	116	C7H16O		000615-29-2	33
4	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2		001116-98-9	32
5	Morpholine, 4-methyl-	101	C5H11NO		000109-02-4	9



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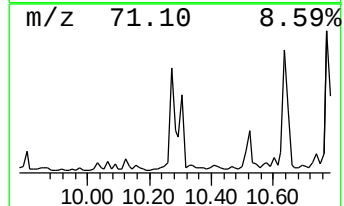
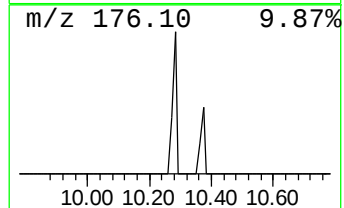
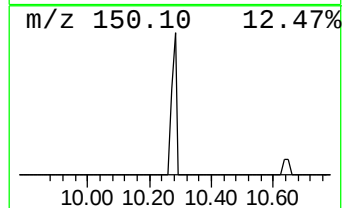
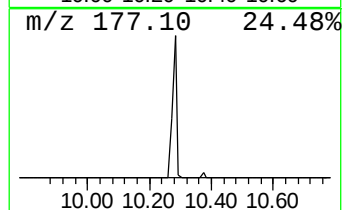
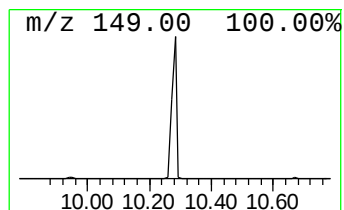
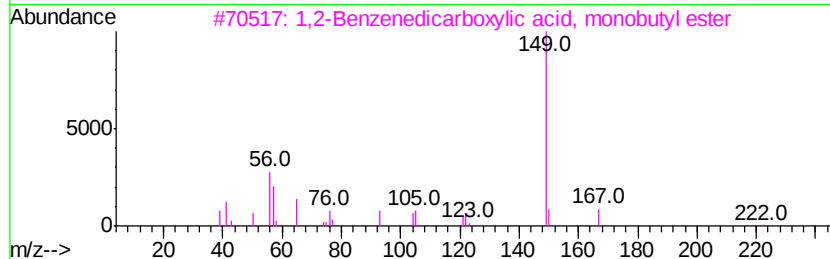
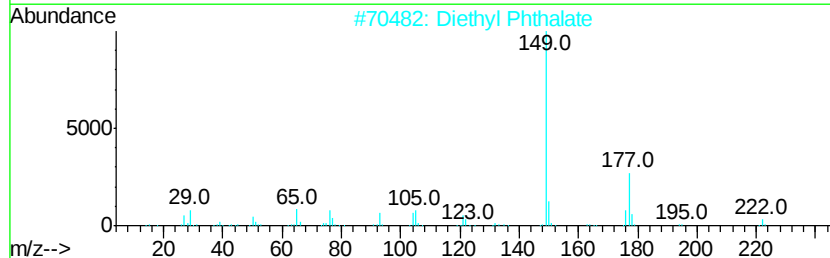
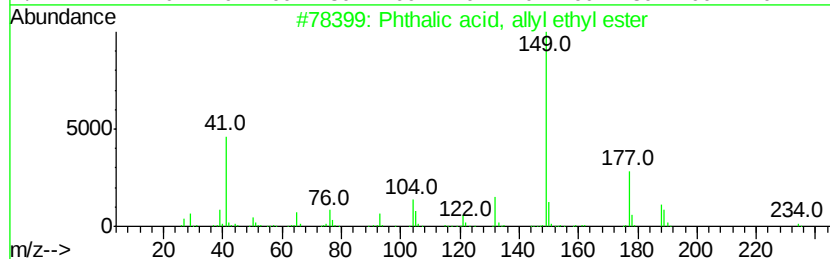
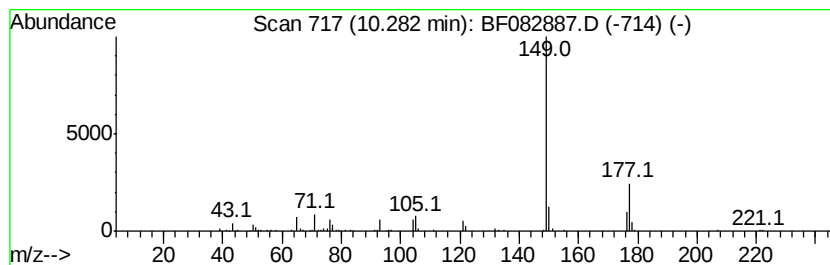
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Peak Number 4 Phthalic acid, allyl ethyl ... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.28	2.37 ng	290026	Acenaphthene-d10	9.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phthalic acid, allyl ethyl ester	234	C13H14O4	033672-94-5	72
2		Diethyl Phthalate	222	C12H14O4	000084-66-2	62
3		1,2-Benzenedicarboxylic acid, mono...	222	C12H14O4	000131-70-4	59
4		1,2-Benzenedicarboxylic acid, di...	250	C14H18O4	000131-16-8	53
5		Phthalic acid, 2-hexyl ester	250	C14H18O4	079107-80-5	53



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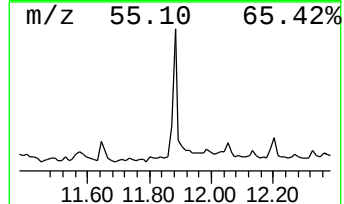
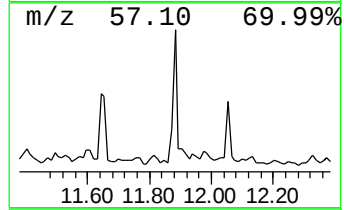
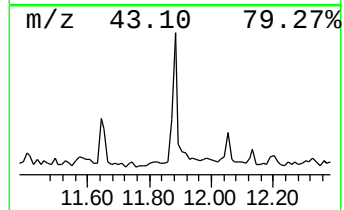
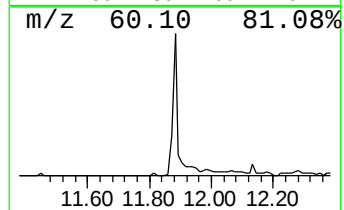
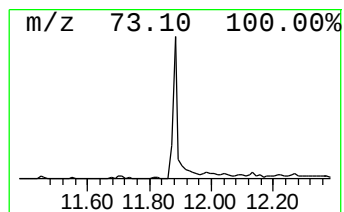
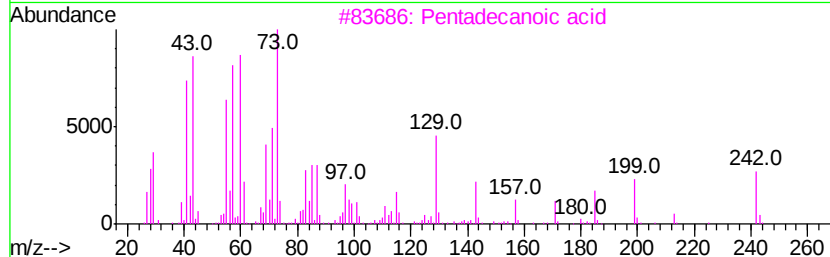
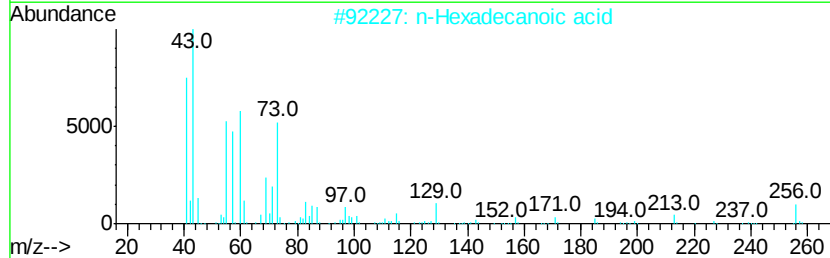
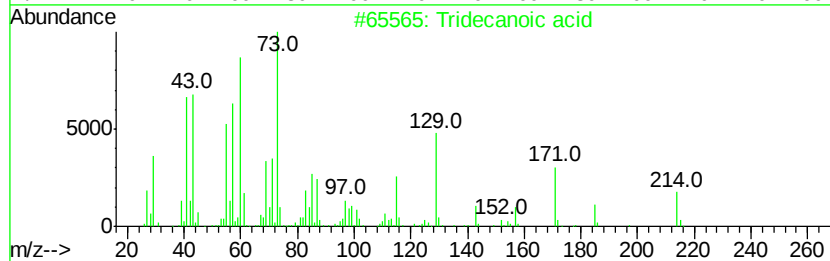
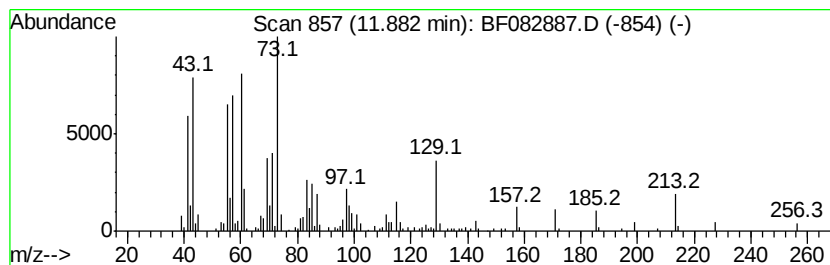
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 Tridecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.88	3.00 ng	344367	Phenanthrene-d10	11.33

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tridecanoic acid	214	C13H26O2	000638-53-9	93
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5		6-Methyl(pentamethylene)silyloxy...	326	C20H42OSi	1000278-79-4	14



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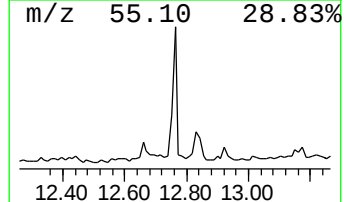
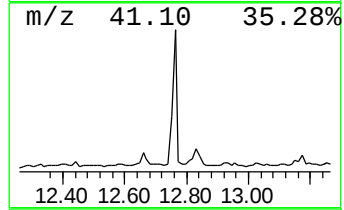
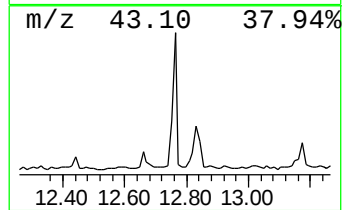
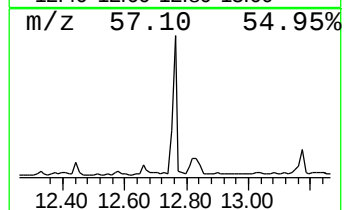
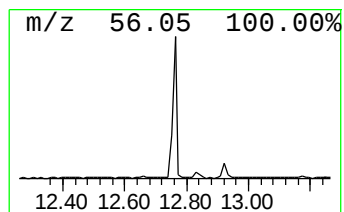
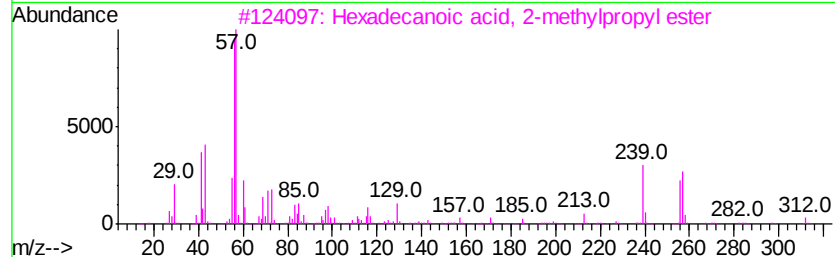
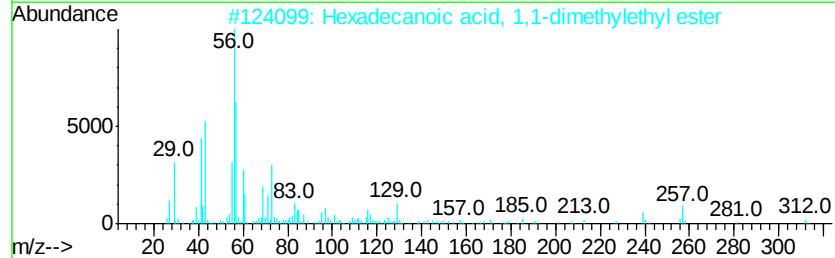
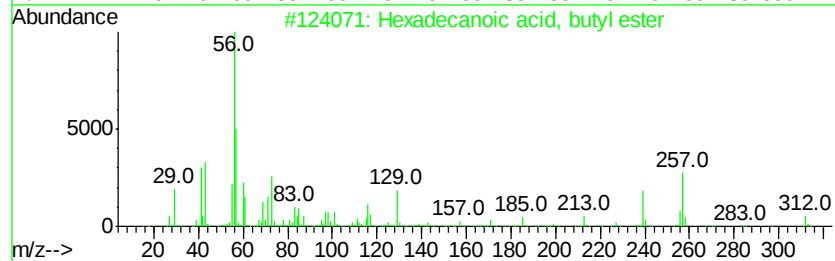
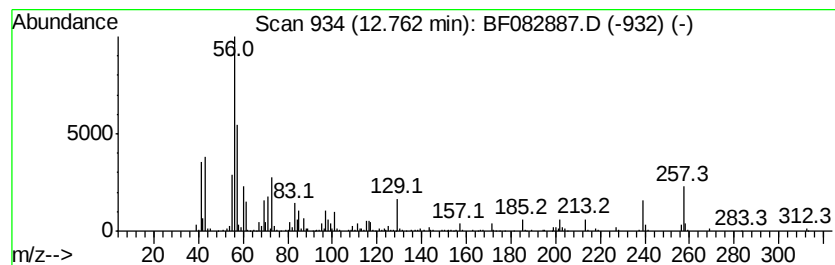
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.76	6.67 ng	743668	Chrysene-d12	13.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	80
3		Hexadecanoic acid, 2-methylpropyl...	312	C20H40O2	000110-34-9	72
4		Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	35
5		Pentadecane, 8-methylene-	224	C16H32	055668-09-2	32



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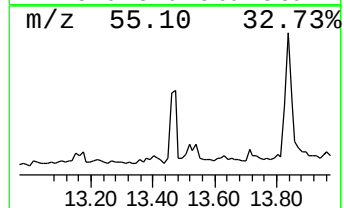
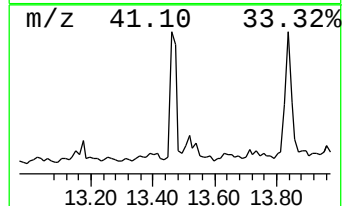
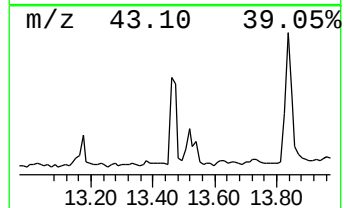
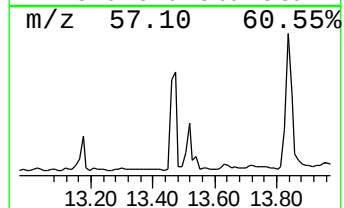
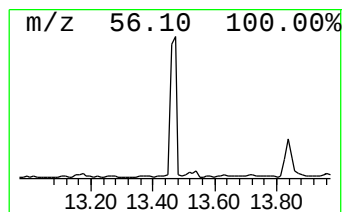
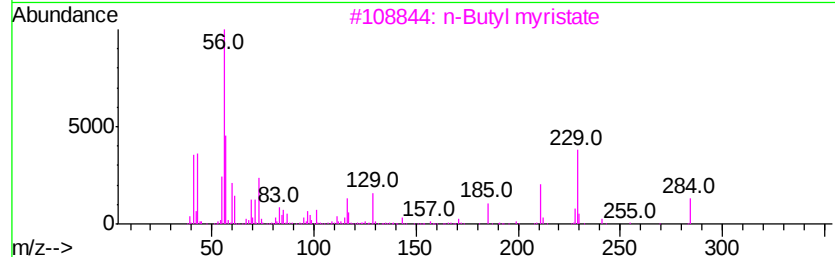
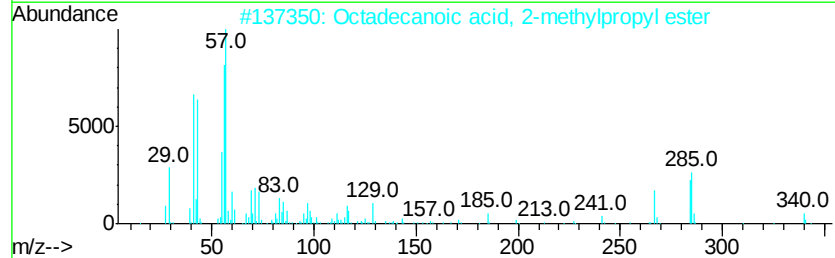
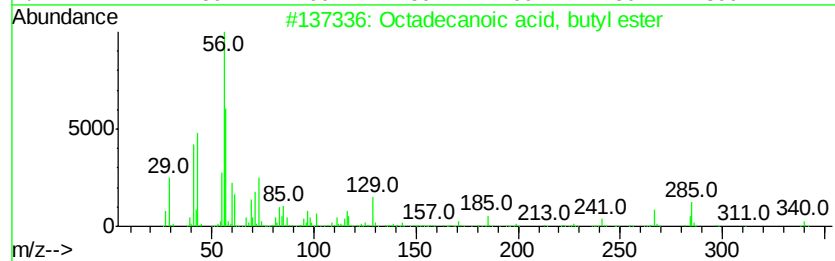
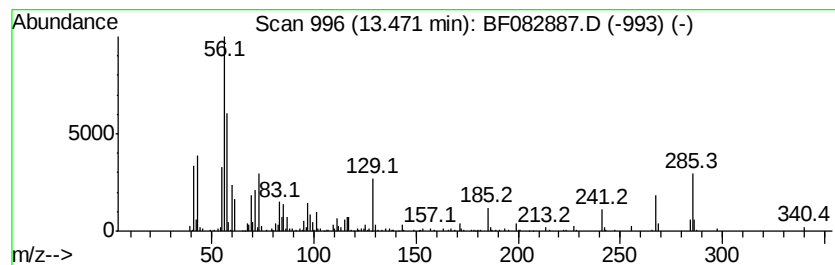
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.47	4.62 ng	514991	Chrysene-d12	13.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	96
2		Octadecanoic acid, 2-methylpropyl ester	340	C22H44O2	000646-13-9	83
3		n-Butyl myristate	284	C18H36O2	000110-36-1	50
4		Nipecotic acid	129	C6H11NO2	000498-95-3	38
5		1,3-Pentanediol, 2,2,4-trimethyl-	146	C8H18O2	000144-19-4	32



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111015\
Data File : BF082887.D
Acq On : 10 Nov 2015 23:40
Operator : UM/IZ
Sample : G4246-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
T-14C

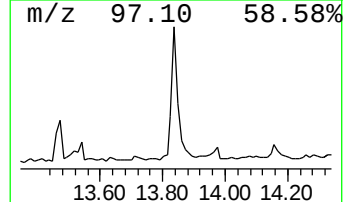
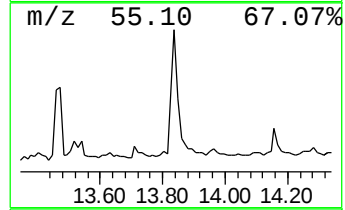
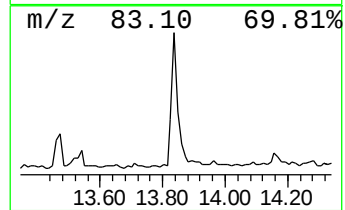
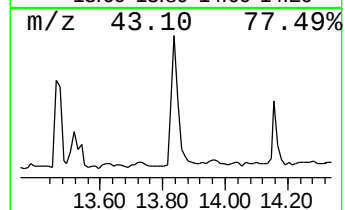
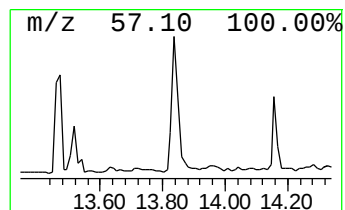
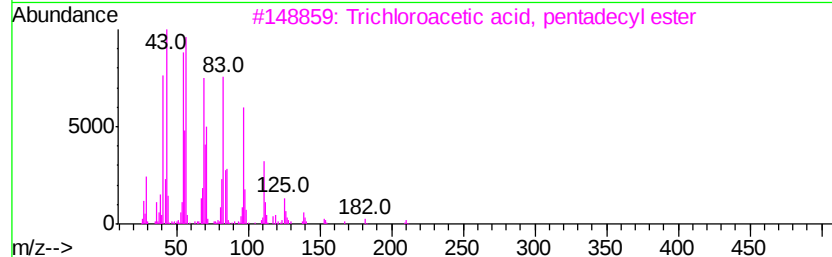
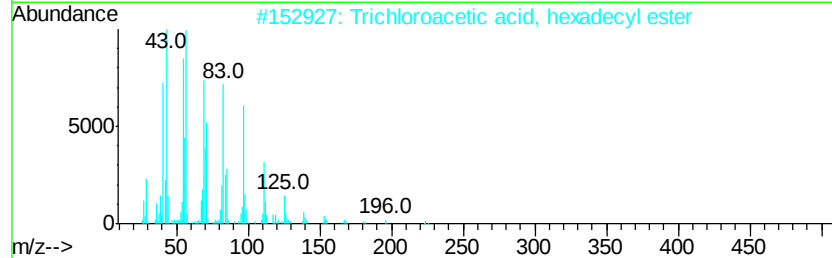
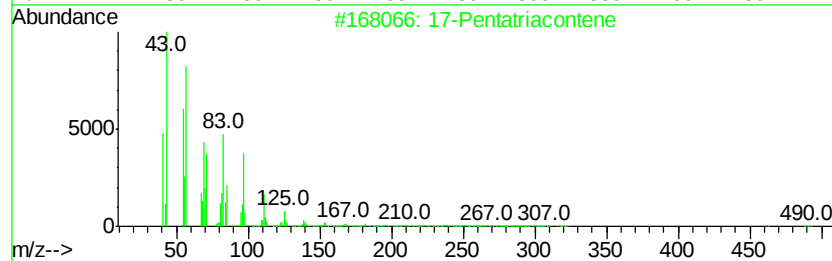
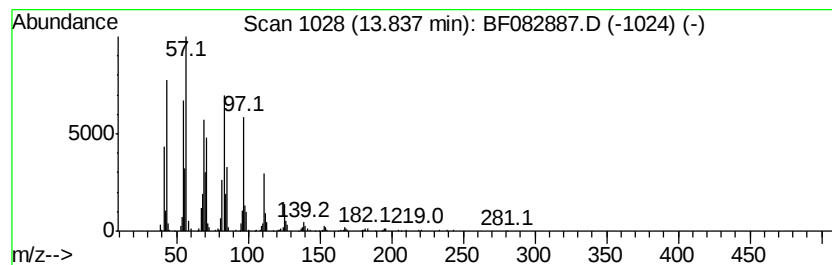
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 17-Pentatriacontene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.84	5.54 ng	617839	Chrysene-d12	13.97

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		17-Pentatriacontene	491	C35H70	006971-40-0	91
2		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
4		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	91
5		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111015\
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Acq On : 10 Nov 2015 23:40
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Sample : G4246-02
Misc :
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Instrument :
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ClientSampleId :
T-14C

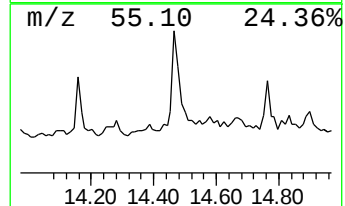
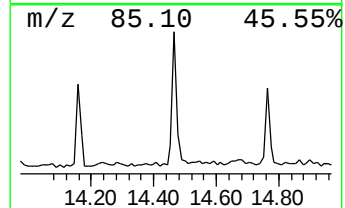
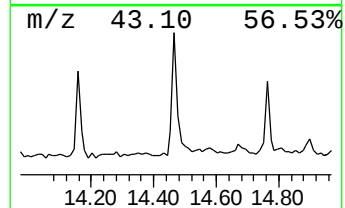
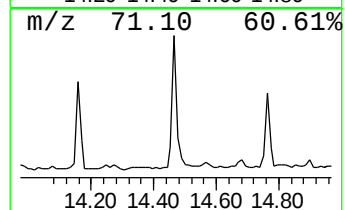
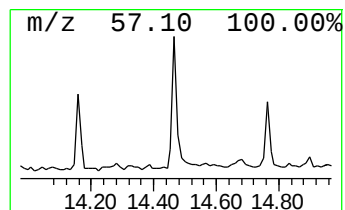
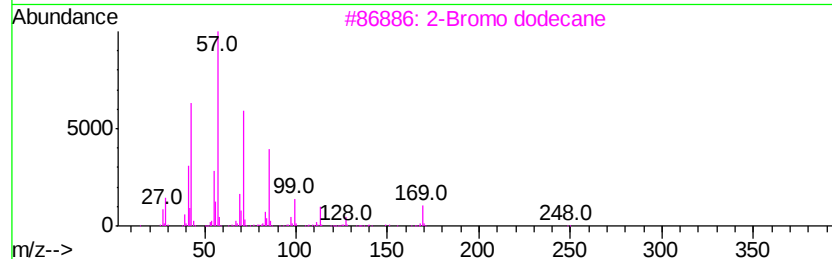
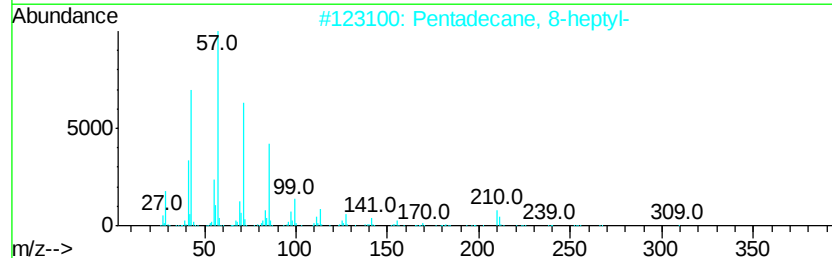
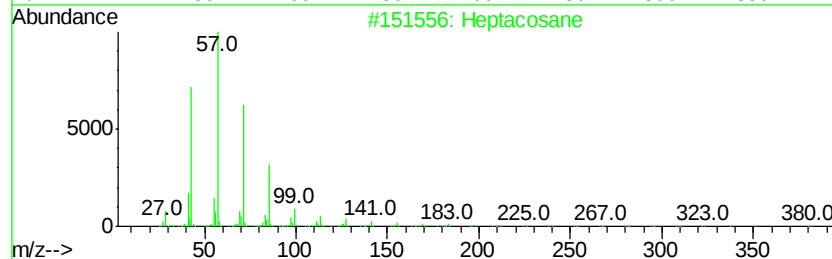
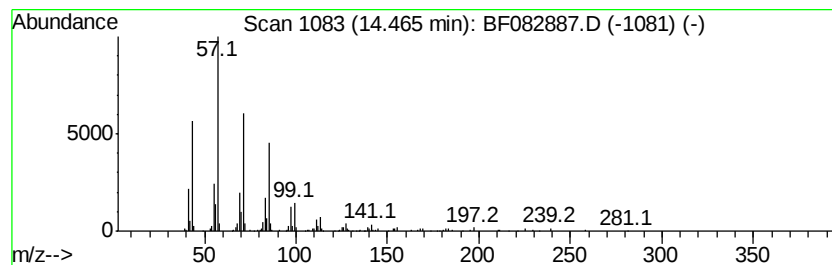
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.47	2.60 ng	289857	Chrysene-d12	13.97

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane		380	C27H56	000593-49-7	86
2	Pentadecane, 8-heptyl-		310	C22H46	071005-15-7	86
3	2-Bromo dodecane		248	C12H25Br	013187-99-0	86
4	Eicosane		282	C20H42	000112-95-8	80
5	Tetratetracontane		619	C44H90	007098-22-8	74



Data Path : Z:\HPCHEM1\BNA F\DATA\BF111015\
Data File : BF082887.D
Acq On : 10 Nov 2015 23:40
Operator : UM/IZ
Sample : G4246-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
T-14C

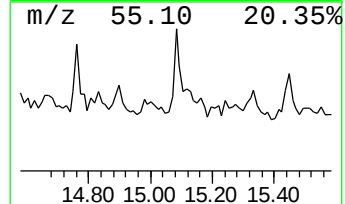
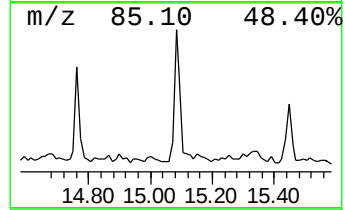
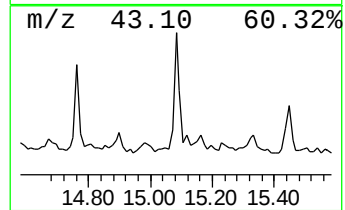
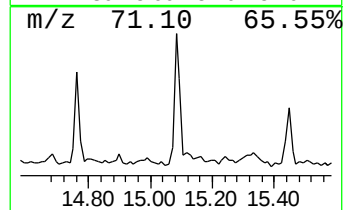
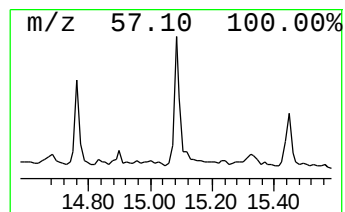
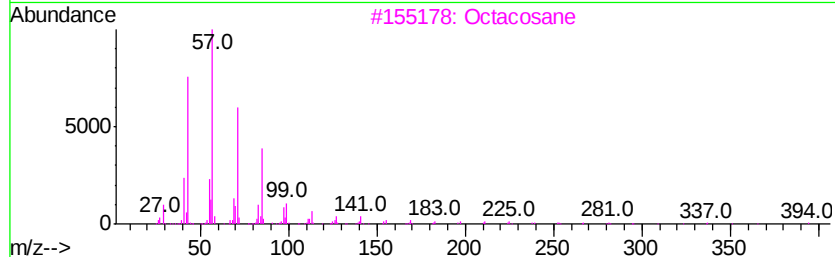
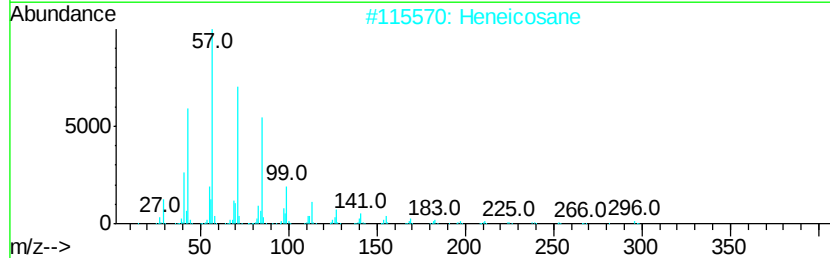
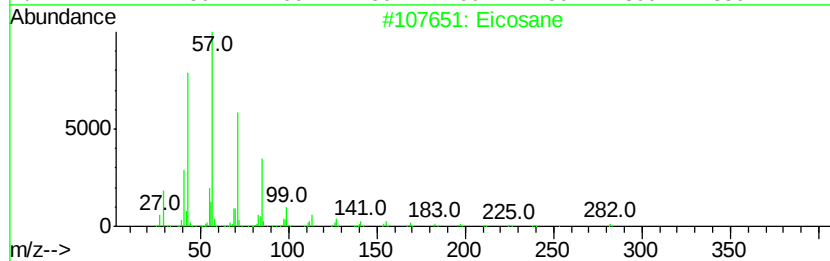
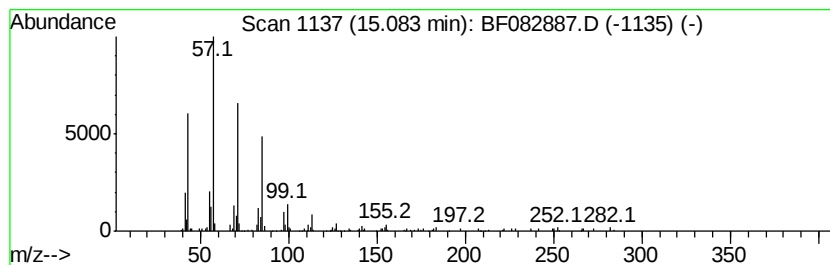
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.08	2.40 ng	197548	Perylene-d12	15.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	93
2		Heneicosane	296	C21H44	000629-94-7	87
3		Octacosane	394	C28H58	000630-02-4	87
4		Tetracosane	338	C24H50	000646-31-1	86
5		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	83



Data Path : Z:\HPCHEM1\BNA F\DATA\BF111015\
Data File : BF082887.D
Acq On : 10 Nov 2015 23:40
Operator : UM/IZ
Sample : G4246-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
T-14C

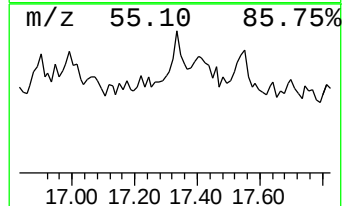
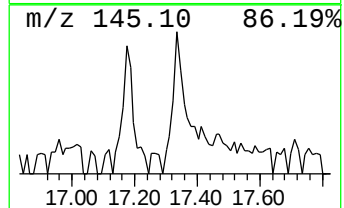
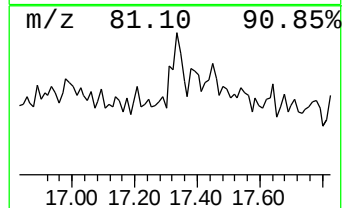
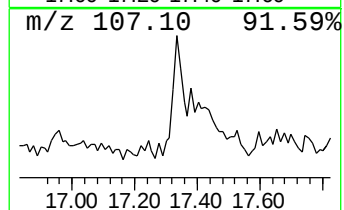
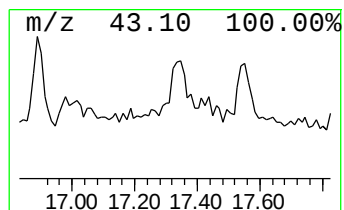
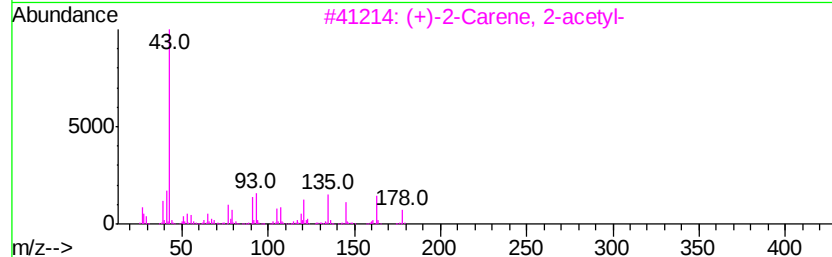
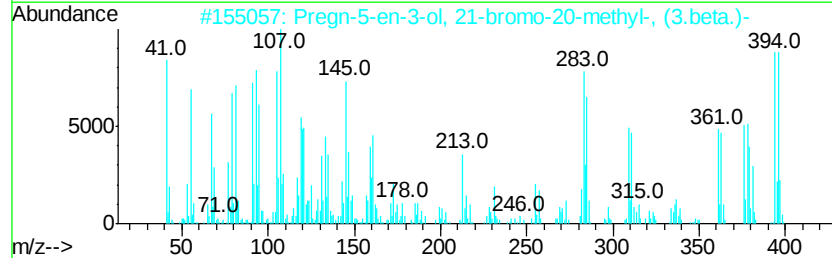
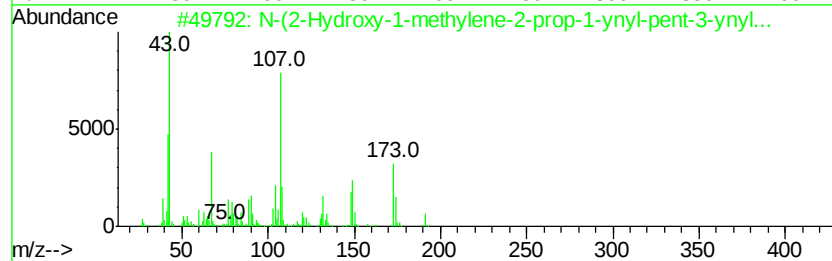
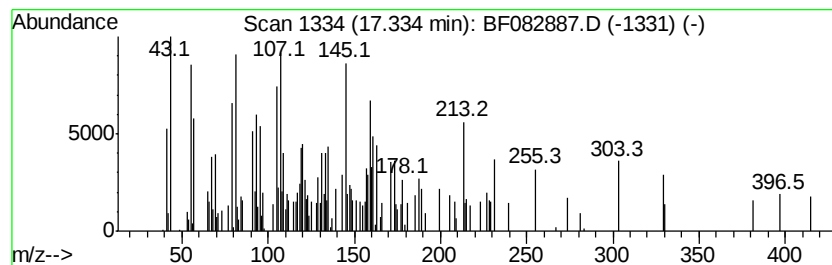
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown17.33 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.33	2.11 ng	173966	Perylene-d12	15.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	N-(2-Hydroxy-1-methylene-2-prop-...	191	C11H13NO2	1000194-35-2	44
2		Pregn-5-en-3-ol, 21-bromo-20-met...	394	C22H35BrO	055103-80-5	43
3		(+)-2-Carene, 2-acetyl-	178	C12H18O	1000151-09-7	14
4		Bronopol	199	C3H6BrNO4	000052-51-7	14
5		1,3,4-Thiadiazol-2-amine, 5-trif...	273	C11H10F3N3S	1000267-89-8	14



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111015\
Data File : BF082887.D
Acq On : 10 Nov 2015 23:40
Operator : UM/IZ
Sample : G4246-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.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...	4.99	39.2	ng	3014400	1	6.82	1538250	20.0
Phthalic acid, al...	10.28	2.4	ng	290026	3	9.86	2443240	20.0
Tridecanoic acid	11.88	3.0	ng	344367	4	11.33	2296930	20.0
Hexadecanoic acid...	12.76	6.7	ng	743668	5	13.97	2229560	20.0
Octadecanoic acid...	13.47	4.6	ng	514991	5	13.97	2229560	20.0
17-Pentatriacontene	13.84	5.5	ng	617839	5	13.97	2229560	20.0
Heptacosane	14.47	2.6	ng	289857	5	13.97	2229560	20.0
Eicosane	15.08	2.4	ng	197548	6	15.39	1645430	20.0
unknown17.33	17.33	2.1	ng	173966	6	15.39	1645430	20.0