

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100815\
 Data File : BF082124.D
 Acq On : 8 Oct 2015 13:12
 Operator : UM/IZ
 Sample : G3927-03
 Misc :
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 OS-SB-28(85-87)

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-BF092815.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.040	252	254	264	rVB	632668	1105880	39.34%	4.662%
2	5.463	288	291	293	rBV	1776583	2189043	77.86%	9.228%
3	6.491	378	381	384	rBV	1608719	2036422	72.43%	8.584%
4	6.629	390	393	395	rBV	2307116	2231241	79.36%	9.406%
5	6.857	411	413	422	rBV	325399	418829	14.90%	1.766%
6	7.017	425	427	430	rBV	1894043	1677621	59.67%	7.072%
7	7.429	460	463	466	rBV	1138563	1230881	43.78%	5.189%
8	8.057	515	518	524	rBV	21700	40765	1.45%	0.172%
9	8.149	524	526	535	rVV	637754	590221	20.99%	2.488%
10	9.097	606	609	611	rBV	50127	52931	1.88%	0.223%
11	9.223	618	620	623	rBV	2059043	2475514	88.05%	10.435%
12	9.623	653	655	657	rBV	452284	398800	14.19%	1.681%
13	9.909	677	680	682	rBV	522245	673761	23.97%	2.840%
14	10.309	713	715	719	rBV2	30197	58680	2.09%	0.247%
15	10.698	746	749	751	rBV	1595695	1728577	61.48%	7.287%
16	10.800	757	758	763	rVB	35484	52038	1.85%	0.219%
17	11.395	807	810	812	rBV	518035	647307	23.02%	2.729%
18	12.435	900	901	903	rBV	29421	32658	1.16%	0.138%
19	12.503	906	907	910	rVB	50178	44910	1.60%	0.189%
20	12.789	931	932	934	rBV	21780	30702	1.09%	0.129%
21	12.983	946	949	951	rBV	2461396	2811382	100.00%	11.851%
22	13.875	1024	1027	1035	rBV	100261	207500	7.38%	0.875%
23	14.001	1035	1038	1039	rVV	201811	317900	11.31%	1.340%
24	14.035	1039	1041	1051	rVB	458701	694132	24.69%	2.926%
25	14.481	1076	1080	1093	rBV4	35811	163729	5.82%	0.690%
26	14.789	1104	1107	1110	rBV2	15190	30970	1.10%	0.131%
27	14.869	1110	1114	1117	rVV2	57309	98068	3.49%	0.413%
28	15.269	1145	1149	1152	rBV	69286	116548	4.15%	0.491%
29	15.475	1164	1167	1178	rBV	358638	535193	19.04%	2.256%
30	15.738	1186	1190	1201	rVB	113407	199166	7.08%	0.840%
31	16.287	1234	1238	1245	rBV	111933	238567	8.49%	1.006%
32	16.961	1290	1297	1304	rBV	89096	229301	8.16%	0.967%
33	17.773	1361	1368	1377	rBV	54724	166752	5.93%	0.703%
34	18.778	1449	1456	1463	rBV2	30065	110841	3.94%	0.467%

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Integration Parameters: rteint.p
Integrator: RTE
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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	20.024	1555	1565	1574	rVB4	18187	85704	3.05%	0.361%
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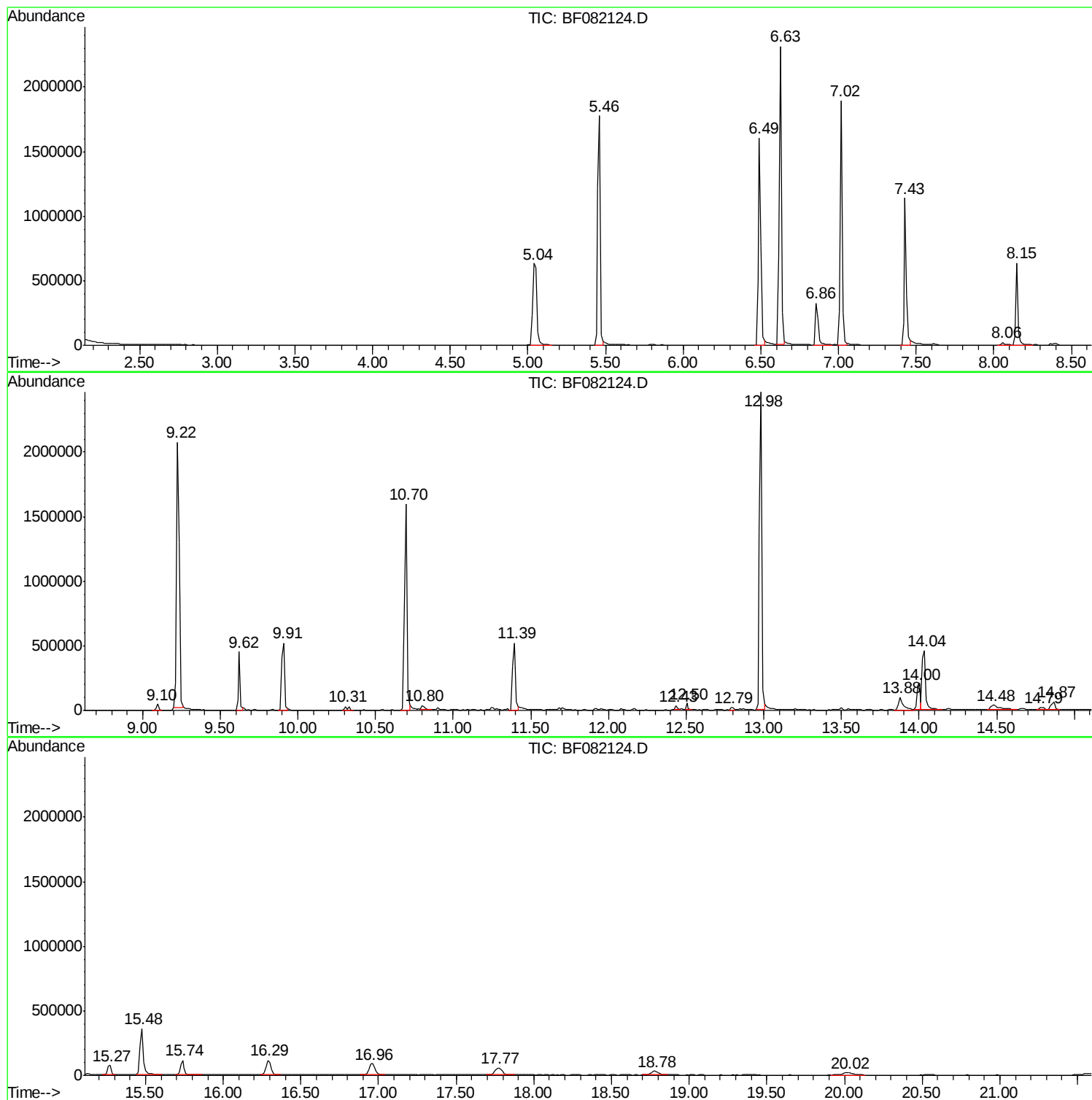
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092815.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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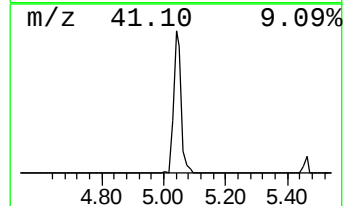
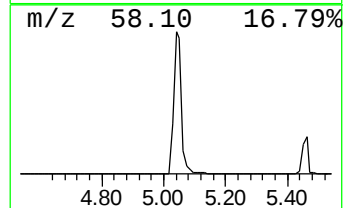
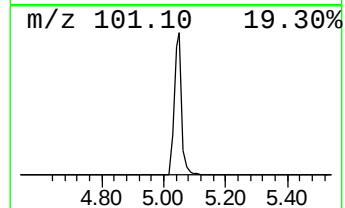
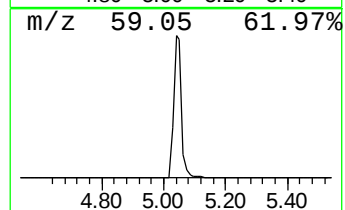
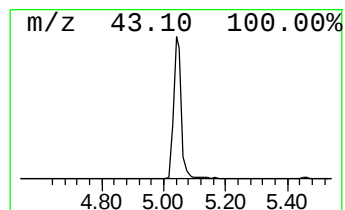
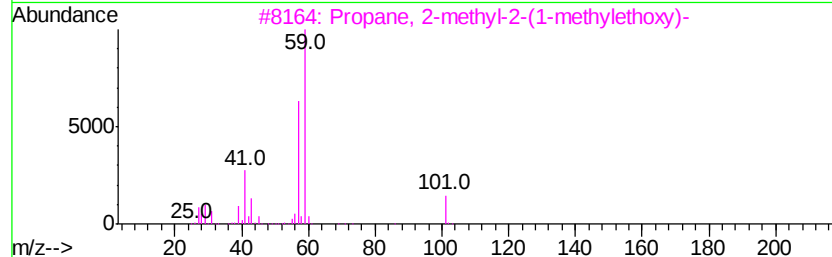
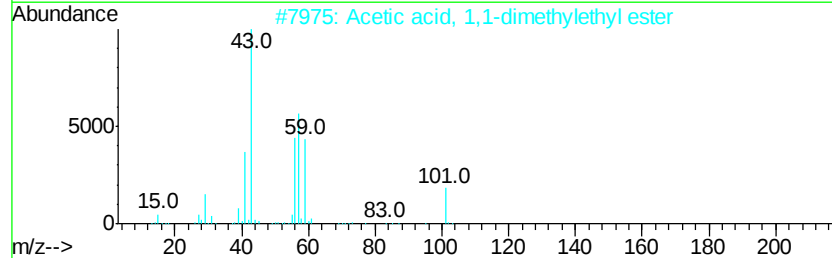
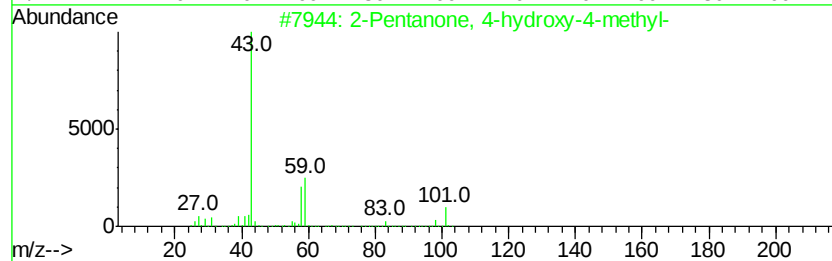
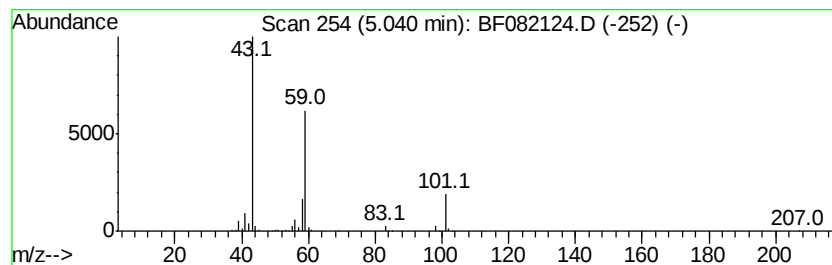
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	52.81 ng	1105880	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
4		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23



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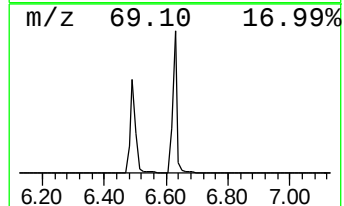
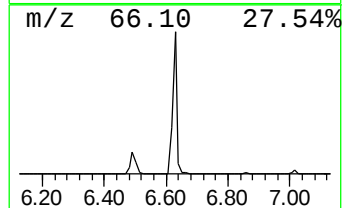
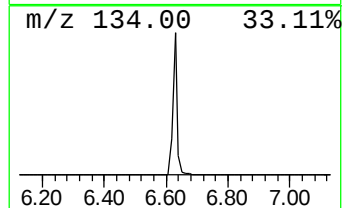
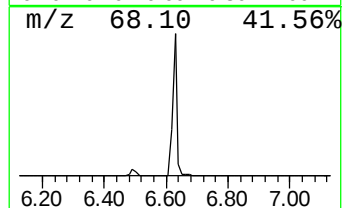
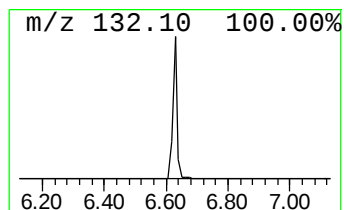
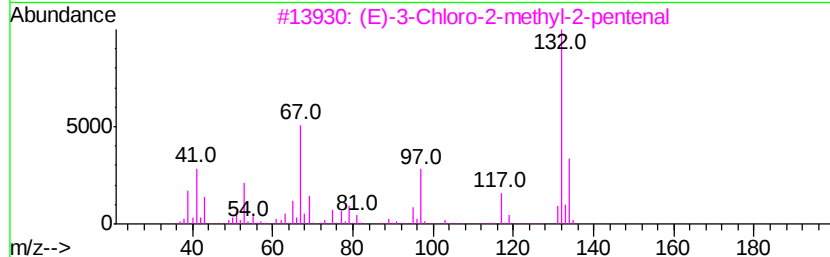
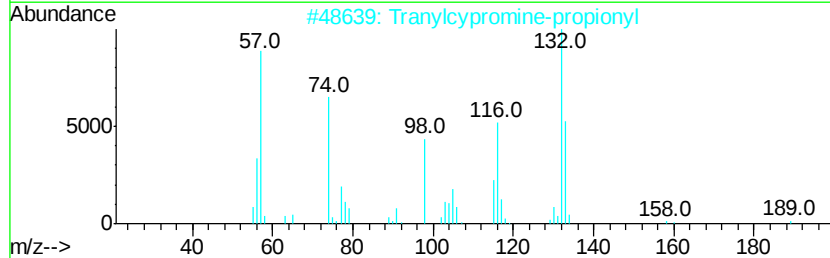
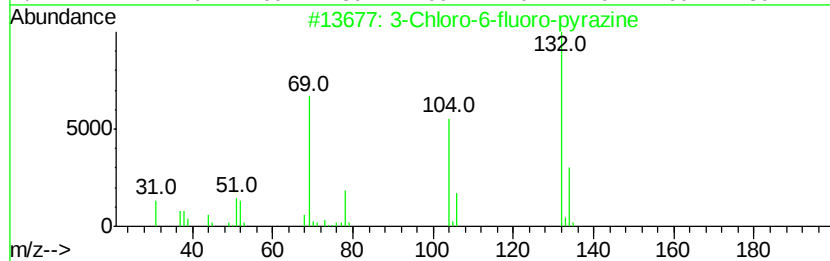
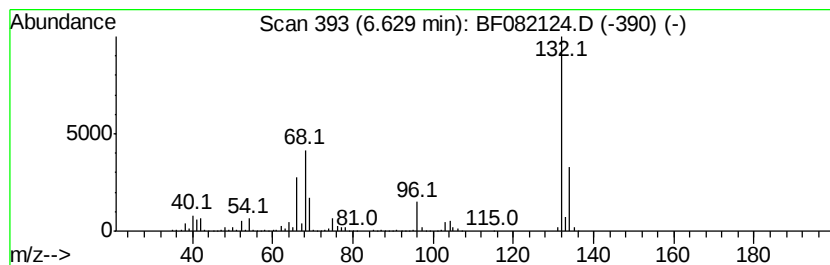
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	106.55 ng	2231240	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	35
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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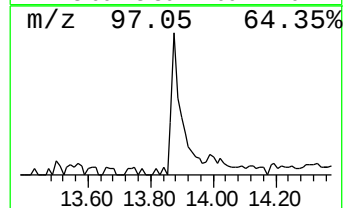
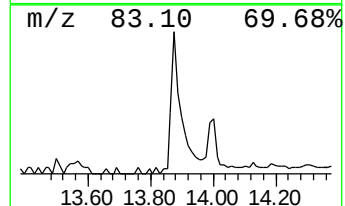
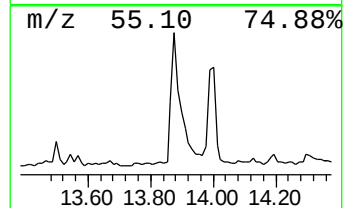
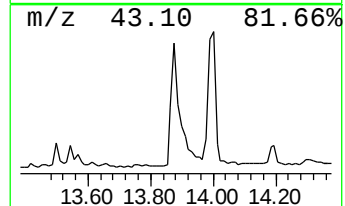
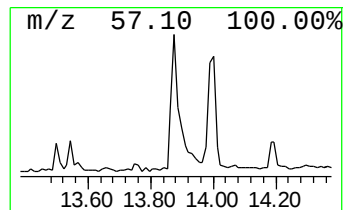
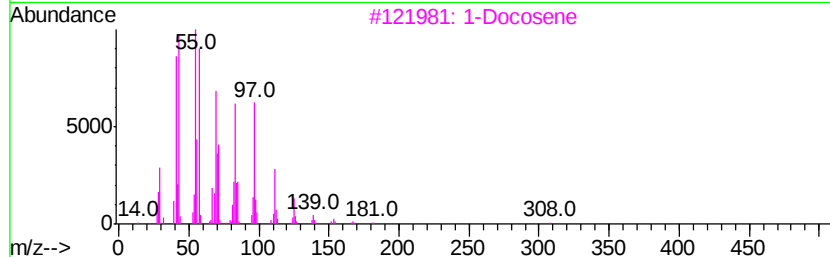
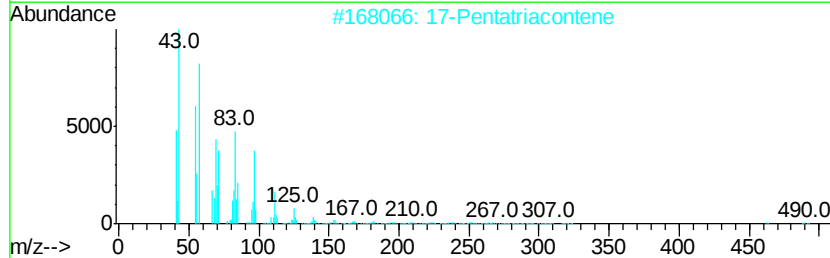
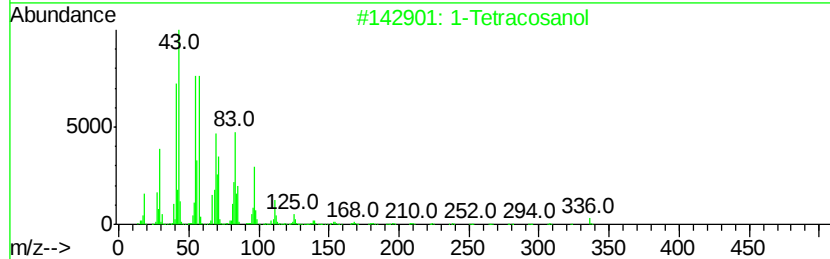
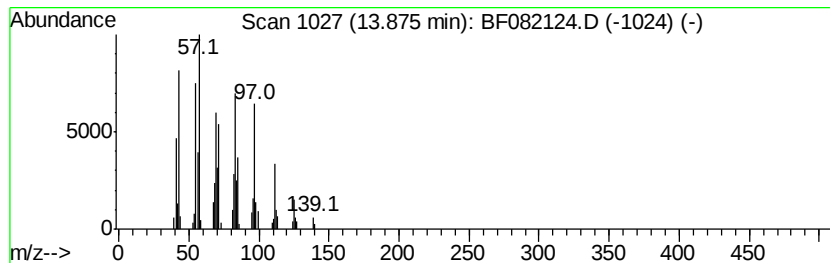
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 4 1-Tetracosanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.88	5.98 ng	207500	Chrysene-d12	14.04

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tetracosanol		354	C24H50O	000506-51-4	91
2	17-Pentatriacontene		491	C35H70	006971-40-0	91
3	1-Docosene		308	C22H44	001599-67-3	90
4	Pentafluoropropionic acid, octadec...		416	C21H37F5O2	1000280-07-7	87
5	3-Chloropropionic acid, heptadec...		346	C20H39ClO2	1000283-05-1	83



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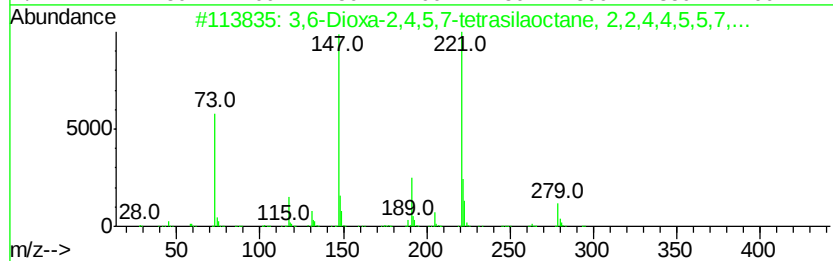
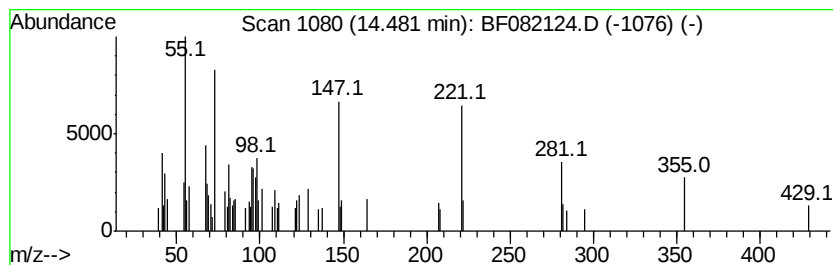
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown14.48 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.48	4.72 ng	163729	Chrysene-d12	14.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	38
2		Carbamic acid, N-(2,3-dimethylph...	221	C12H15NO3	339273-79-9	35
3		Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	27
4		Trisiloxane, 1,1,1,5,5,5-hexamet...	384	C12H36O4Si5	003555-47-3	27
5		N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	22



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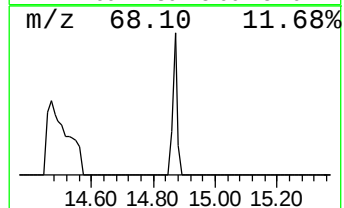
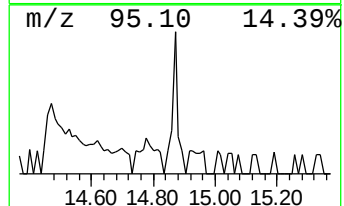
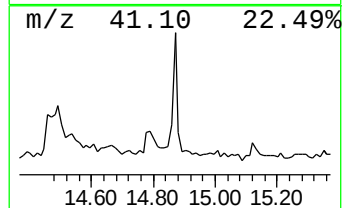
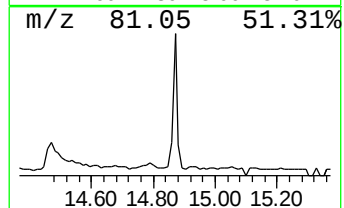
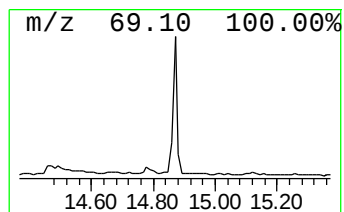
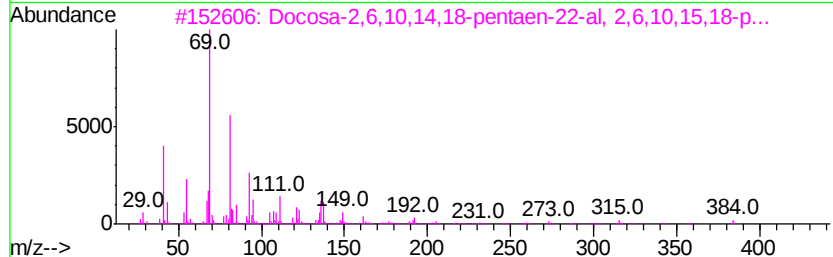
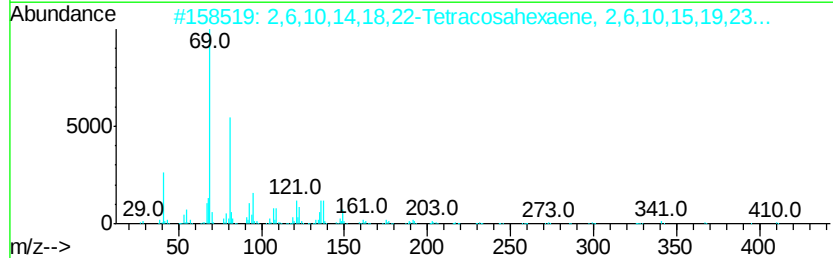
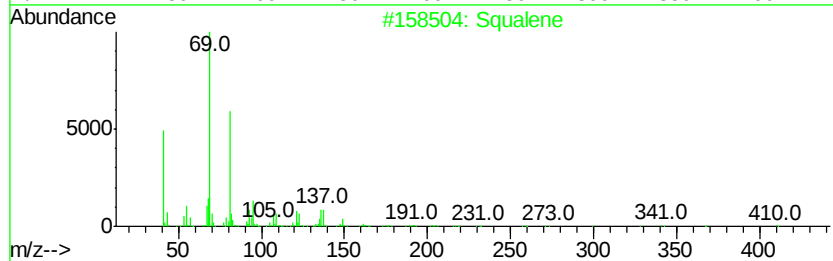
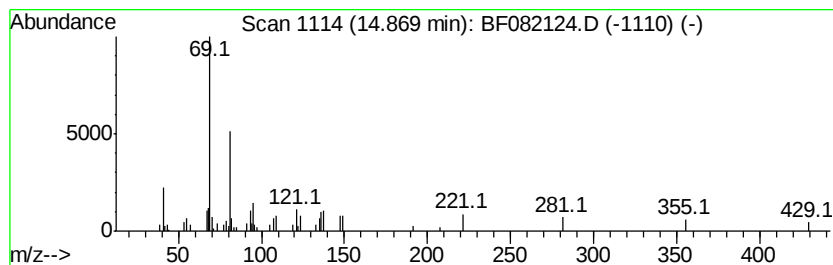
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Squalene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.87	3.66 ng	98068	Perylene-d12	15.48
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Squalene	410 C30H50	007683-64-9	83
2	2,6,10,14,18,22-Tetracosahexaene...	410 C30H50	000111-02-4	83
3	Docosa-2,6,10,14,18-pentaen-22-a...	384 C27H44O	1000163-04-7	80
4	4,9,13,17-Tetramethyl-4,8,12,16-...	316 C22H36O	056882-09-8	72
5	7,11-Dimethyldodeca-2,6,10-trien...	208 C14H24O	125529-10-4	59



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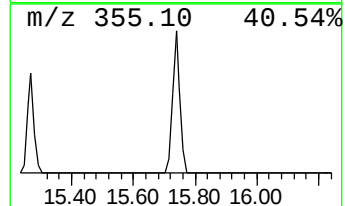
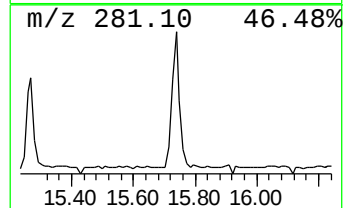
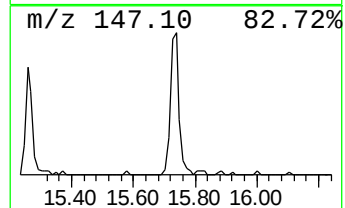
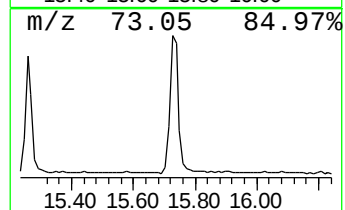
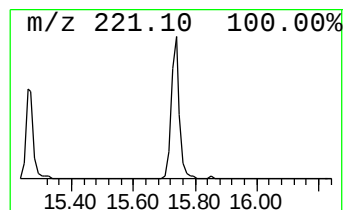
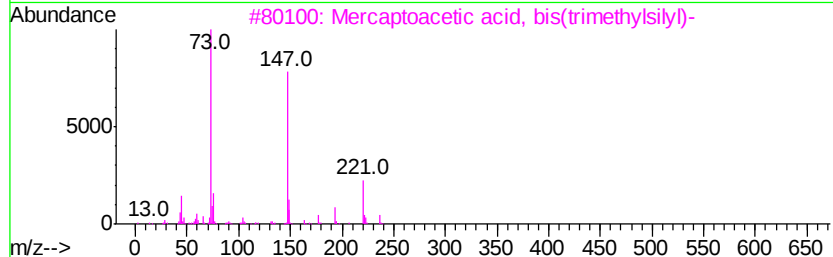
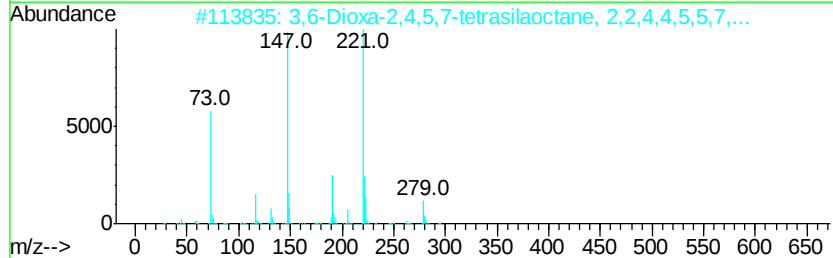
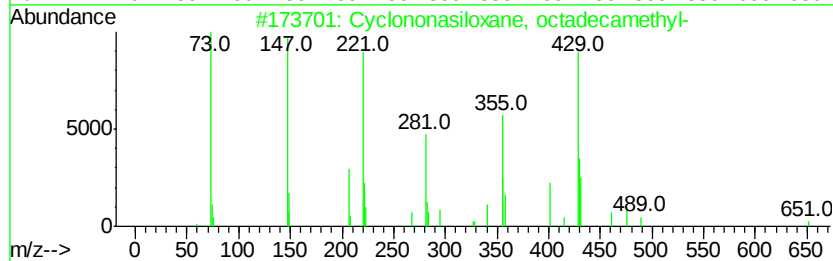
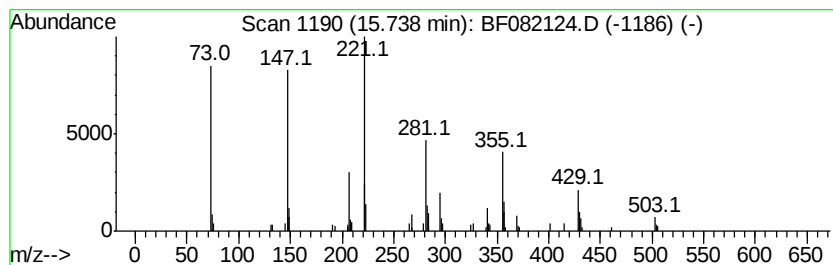
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown15.74 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.74	7.44 ng	199166	Perylene-d12	15.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	90
2		3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	43
3		Mercaptoacetic acid, bis(trimeth...	236	C8H20O2SSi2	006398-62-5	32
4		N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	25
5		Trisiloxane, 1,1,1,5,5,5-hexamet...	384	C12H36O4Si5	003555-47-3	22



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100815\
Data File : BF082124.D
Acq On : 8 Oct 2015 13:12
Operator : UM/IZ
Sample : G3927-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OS-SB-28(85-87)

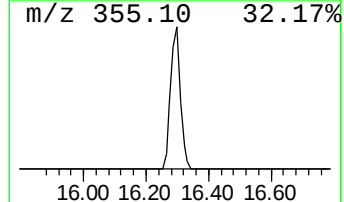
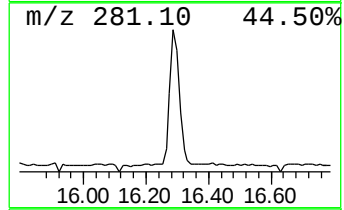
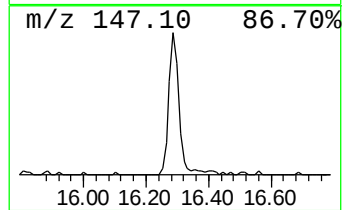
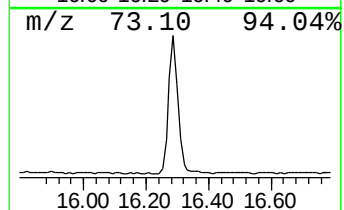
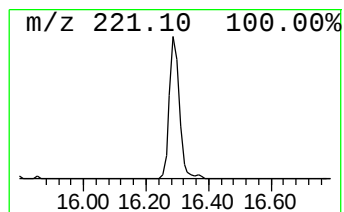
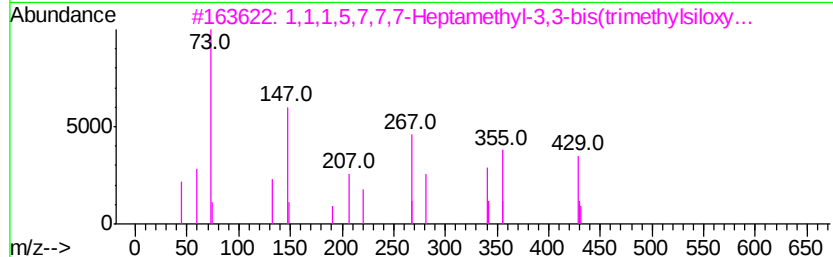
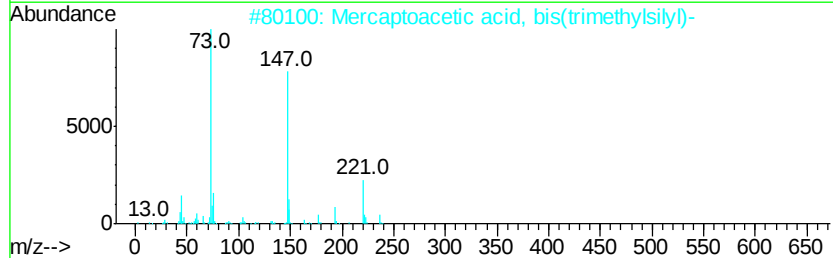
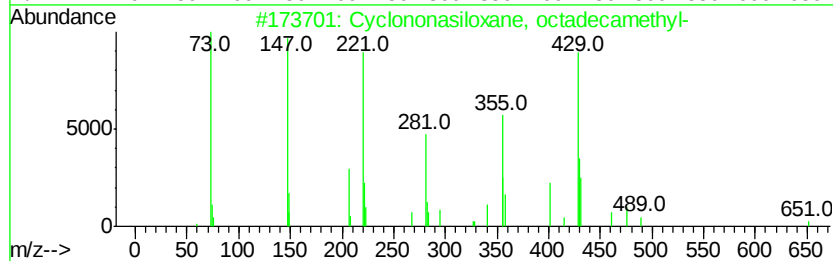
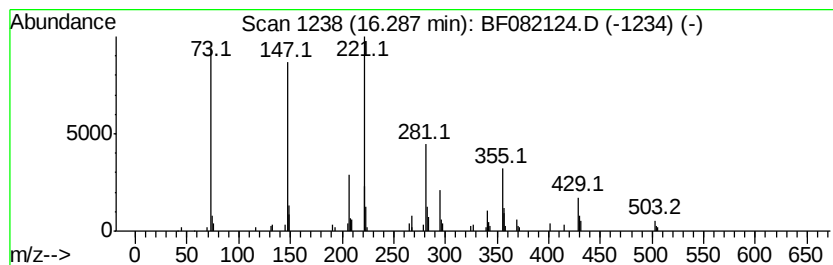
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown16.29 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.29	8.92 ng	238567	Perylene-d12	15.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	90
2		Mercaptoacetic acid, bis(trimeth...	236	C8H20O2SSi2	006398-62-5	40
3		1,1,1,5,7,7,7-Heptamethyl-3,3-bi...	444	C13H40O5Si6	038147-00-1	38
4		N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	30
5		Trisiloxane, 1,1,1,5,5,5-hexamet...	384	C12H36O4Si5	003555-47-3	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100815\
Data File : BF082124.D
Acq On : 8 Oct 2015 13:12
Operator : UM/IZ
Sample : G3927-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OS-SB-28(85-87)

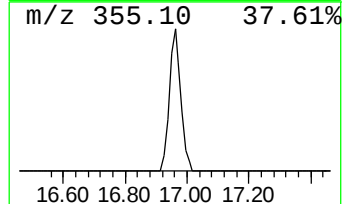
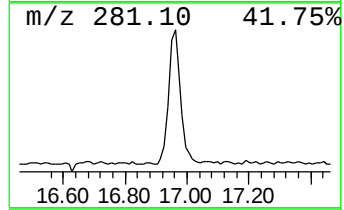
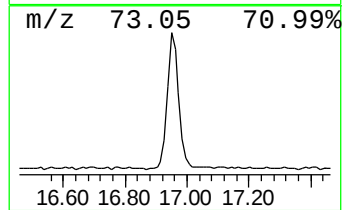
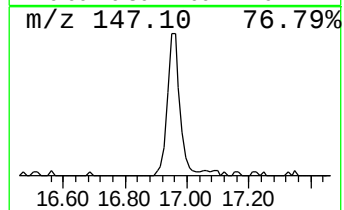
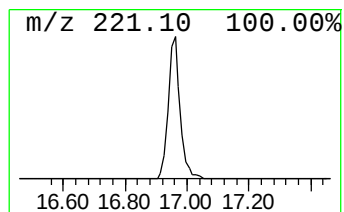
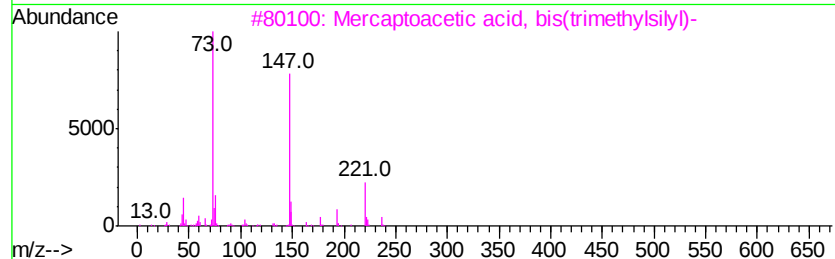
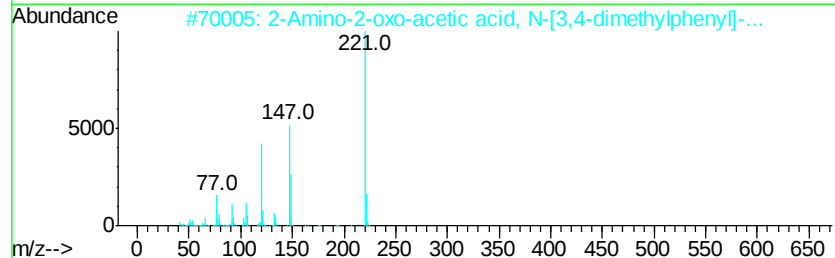
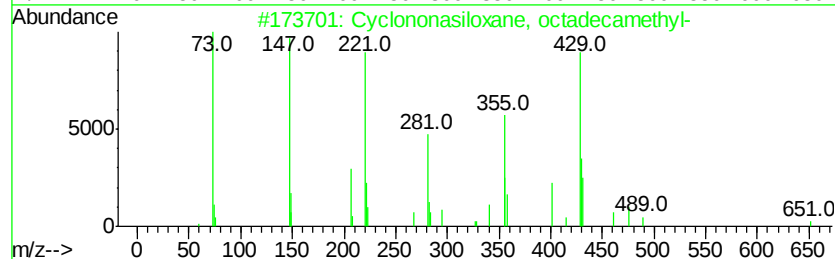
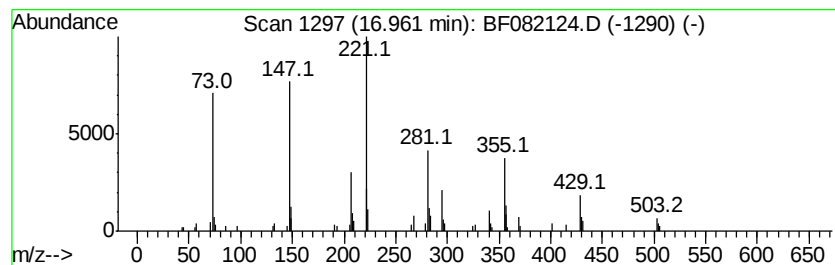
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown16.96 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.96	8.57 ng	229301	Perylene-d12	15.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	87
2		2-Amino-2-oxo-acetic acid, N-[3,...	221	C12H15N03	024451-17-0	47
3		Mercaptoacetic acid, bis(trimeth...	236	C8H20O2SSi2	006398-62-5	38
4		2-(2',4',4',6',6',8',8'-Heptamet...	652	C16H48O10Si9	145344-72-5	32
5		N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	30



Data Path : Z:\HPCHEM1\BNA F\DATA\BF100815\
Data File : BF082124.D
Acq On : 8 Oct 2015 13:12
Operator : UM/IZ
Sample : G3927-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OS-SB-28(85-87)

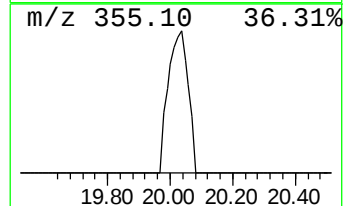
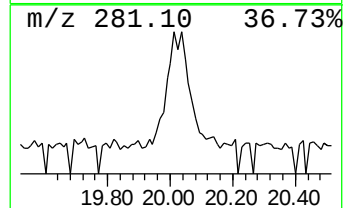
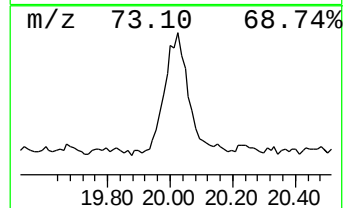
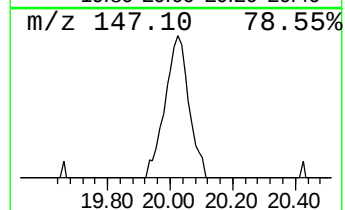
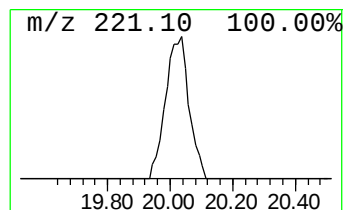
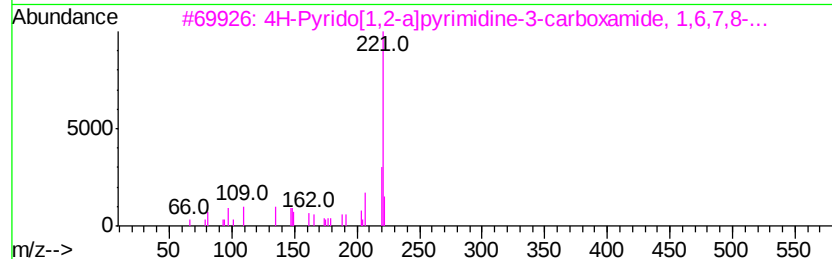
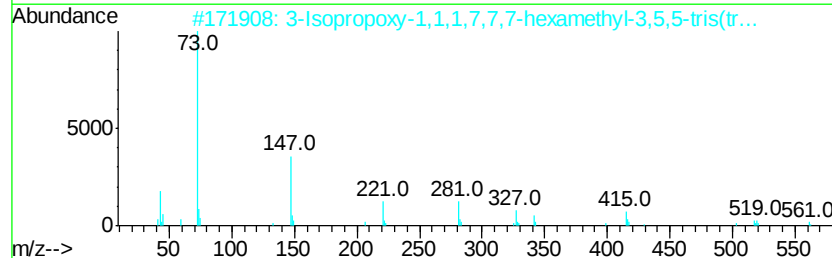
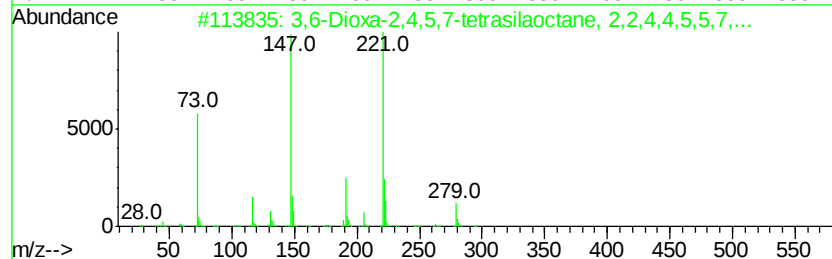
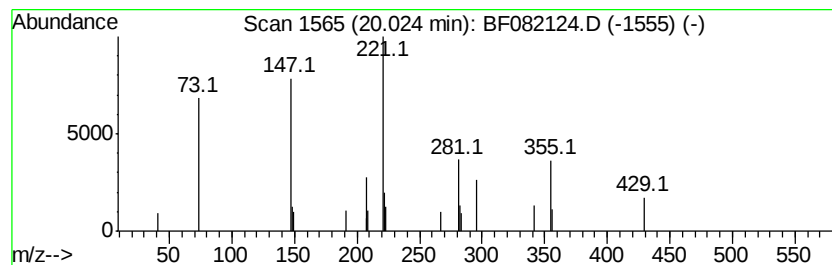
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092815.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown20.02 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.02	3.20 ng	85704	Perylene-d12	15.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	50
2		3-Isopropoxy-1,1,1,7,7,7-hexamet...	576	C18H52O7Si7	071579-69-6	32
3		4H-Pyrido[1,2-a]pyrimidine-3-car...	221	C11H15N3O2	064399-29-7	27
4		N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	27
5		1,3-Benzodioxole, 5-[3-acetamino...	221	C12H15NO3	1000124-33-0	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100815\
Data File : BF082124.D
Acq On : 8 Oct 2015 13:12
Operator : UM/IZ
Sample : G3927-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OS-SB-28(85-87)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092815.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.04	52.8	ng	1105880	1	6.86	418829	20.0
unknown6.63	6.63	106.6	ng	2231240	1	6.86	418829	20.0
1-Tetracosanol	13.88	6.0	ng	207500	5	14.04	694132	20.0
unknown14.48	14.48	4.7	ng	163729	5	14.04	694132	20.0
Squalene	14.87	3.7	ng	98068	6	15.48	535193	20.0
unknown15.74	15.74	7.4	ng	199166	6	15.48	535193	20.0
unknown16.29	16.29	8.9	ng	238567	6	15.48	535193	20.0
unknown16.96	16.96	8.6	ng	229301	6	15.48	535193	20.0
unknown20.02	20.02	3.2	ng	85704	6	15.48	535193	20.0