

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020316\
 Data File : BF084811.D
 Acq On : 4 Feb 2016 3:40
 Operator : SJ/IZ
 Sample : H1312-05
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SUP-B005(5-7)

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	4.133	176	179	182	rBV	1584330	2435145	21.91%	5.023%
2	4.876	237	244	246	rBV	4544056	11113463	100.00%	22.922%
3	6.327	369	371	374	rBV	2014072	1760089	15.84%	3.630%
4	6.453	380	382	384	rBV	354396	340508	3.06%	0.702%
5	6.681	400	402	405	rBV	1301069	1123806	10.11%	2.318%
6	6.841	413	416	418	rBV	3804790	3388723	30.49%	6.989%
7	7.253	449	452	455	rBV	2566232	2556630	23.00%	5.273%
8	7.973	512	515	516	rBV	1752411	1623514	14.61%	3.349%
9	7.996	516	517	520	rVB	205817	164998	1.48%	0.340%
10	8.682	575	577	579	rBV	119321	112680	1.01%	0.232%
11	9.059	606	610	612	rBV	4434903	5296028	47.65%	10.923%
12	9.447	642	644	646	rVV	756451	847674	7.63%	1.748%
13	9.722	666	668	670	rVV	1853121	1696316	15.26%	3.499%
14	10.168	706	707	709	rVB	173309	124978	1.12%	0.258%
15	10.636	746	748	752	rVB	190101	221871	2.00%	0.458%
16	11.082	786	787	793	rVB	122362	232897	2.10%	0.480%
17	11.196	795	797	801	rVV	1156149	2374762	21.37%	4.898%
18	11.276	801	804	806	rVB	234192	223583	2.01%	0.461%
19	11.448	816	819	823	rBV2	234019	421951	3.80%	0.870%
20	11.505	823	824	831	rVB4	70835	149890	1.35%	0.309%
21	11.733	842	844	845	rVB	117284	121159	1.09%	0.250%
22	11.813	849	851	855	rVB2	157700	258823	2.33%	0.534%
23	11.996	865	867	872	rVB2	122899	159125	1.43%	0.328%
24	12.408	901	903	905	rVV	846270	722114	6.50%	1.489%
25	12.636	920	923	925	rBV	626812	831017	7.48%	1.714%
26	12.785	934	936	939	rVB	3195584	4571300	41.13%	9.428%
27	12.968	949	952	954	rVB	80079	118773	1.07%	0.245%
28	13.025	954	957	959	rBV	82838	137134	1.23%	0.283%
29	13.276	975	979	982	rVV	1207389	1174965	10.57%	2.423%
30	13.356	982	986	992	rVB4	90714	204775	1.84%	0.422%
31	13.699	1013	1016	1023	rVB3	176323	346420	3.12%	0.715%
32	13.825	1024	1027	1032	rBV2	1164420	1796489	16.16%	3.705%
33	14.591	1092	1094	1100	rBV2	167375	211058	1.90%	0.435%
34	14.831	1112	1115	1119	rBV	147598	298122	2.68%	0.615%

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ClientSampleId :
SUP-B005(5-7)

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	15.151	1141	1143	1145	rVV	118328	141862	1.28%	0.293%
36	15.208	1145	1148	1157	rVB	834618	1068766	9.62%	2.204%
37	18.774	1455	1460	1464	rBV5	38317	112756	1.01%	0.233%

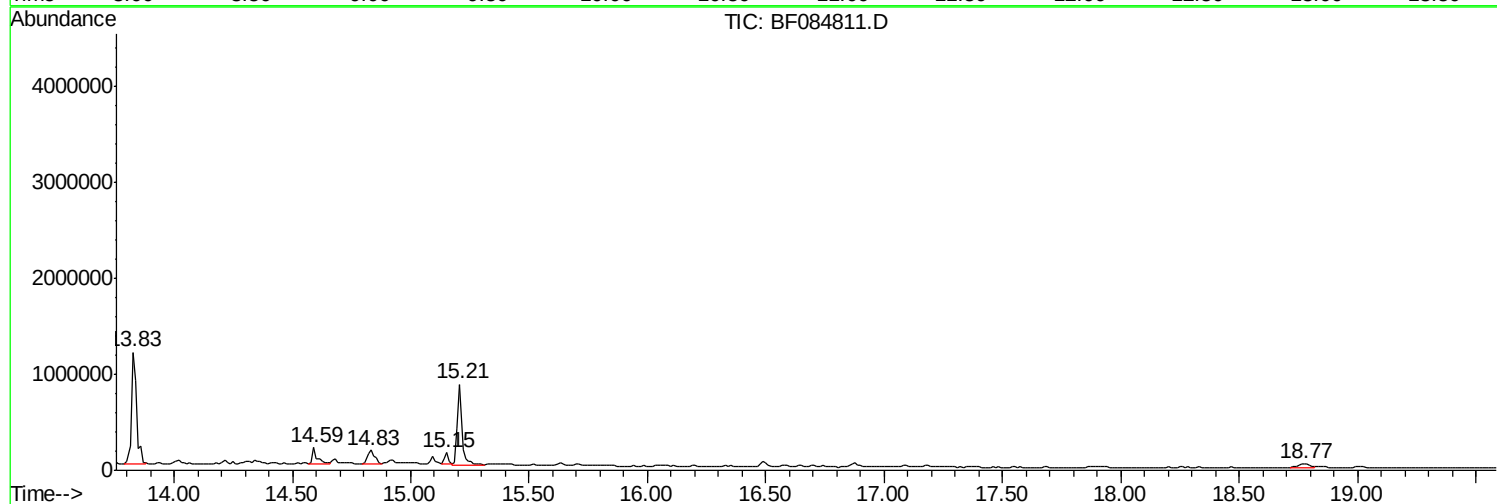
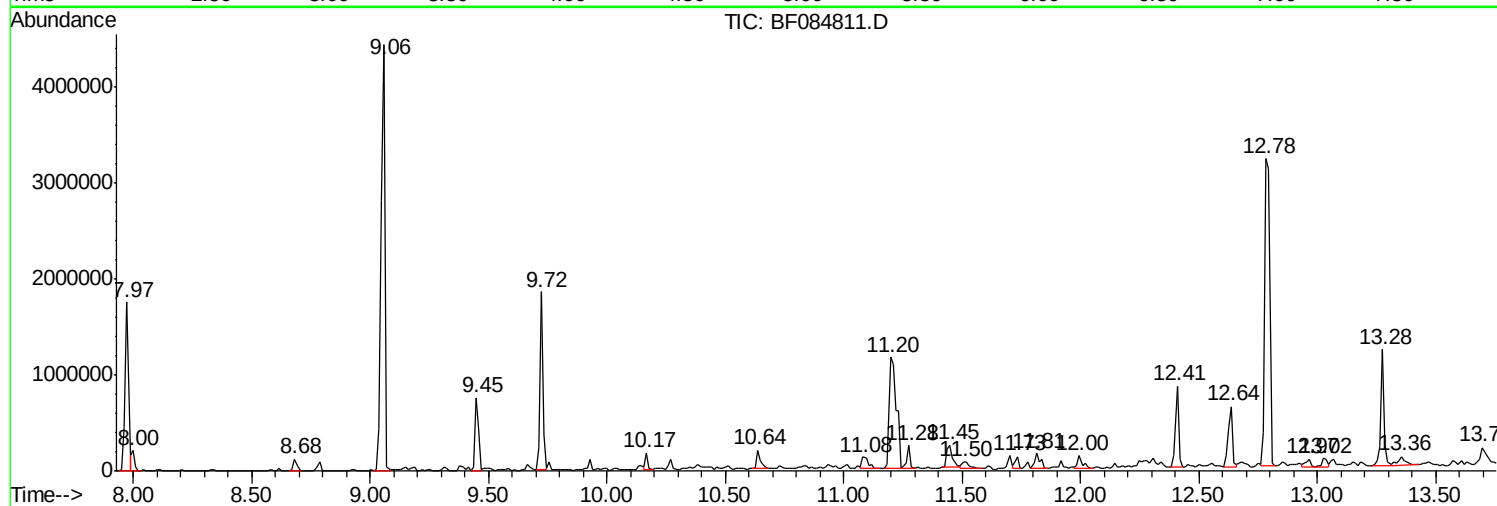
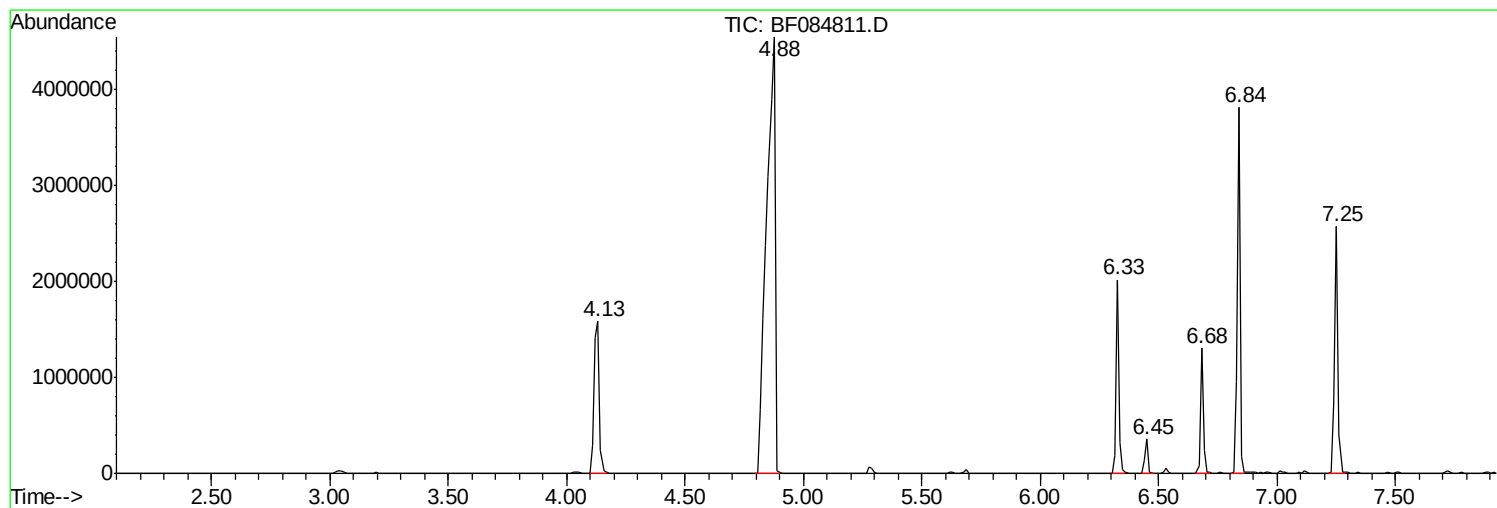
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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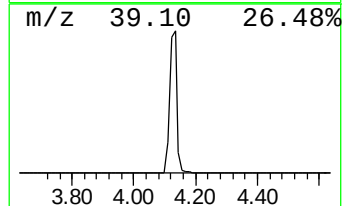
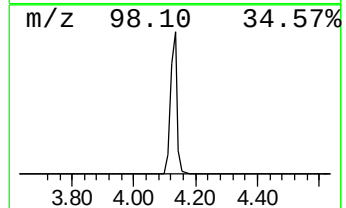
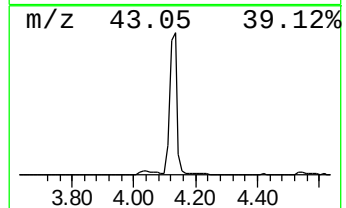
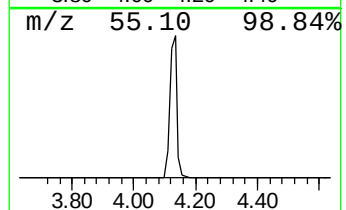
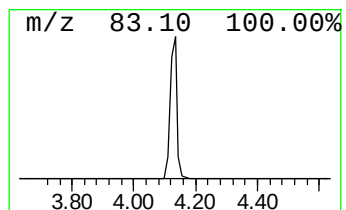
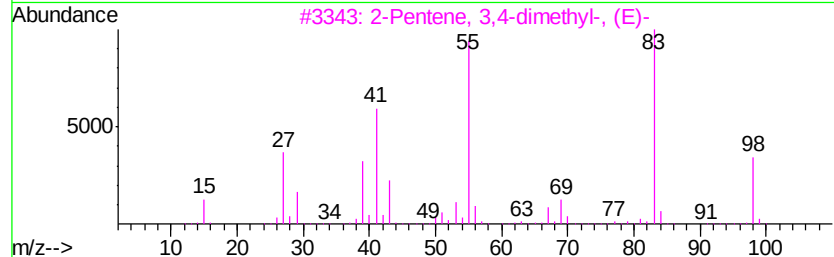
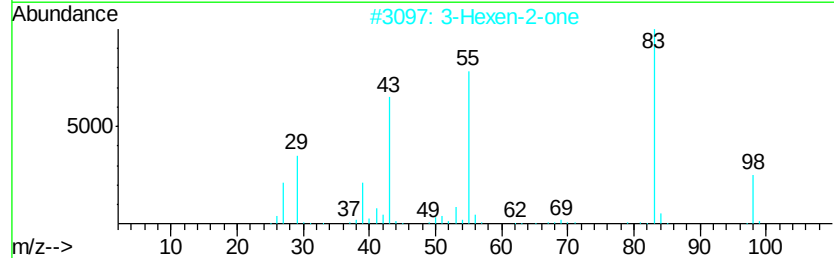
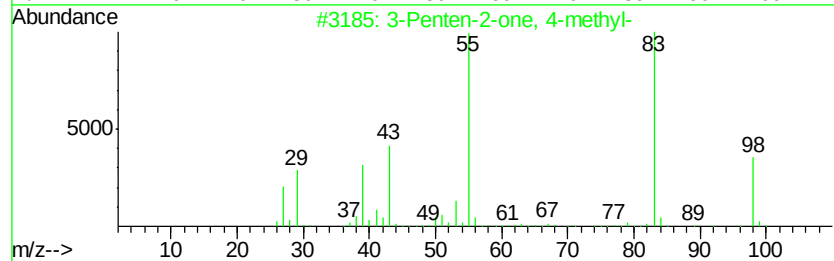
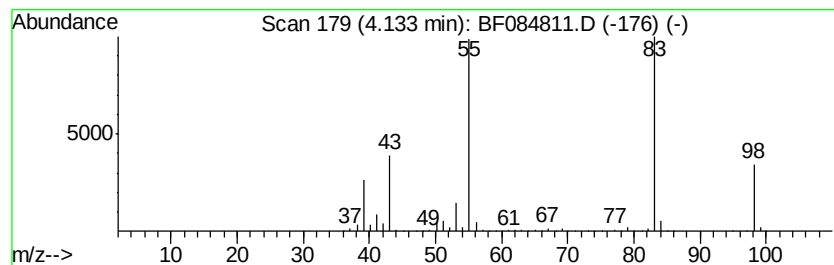
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.13	43.34 ng	2435150	1,4-Dichlorobenzene-d4	6.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2		3-Hexen-2-one	98	C6H10O	000763-93-9	91
3		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86



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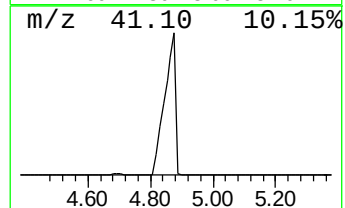
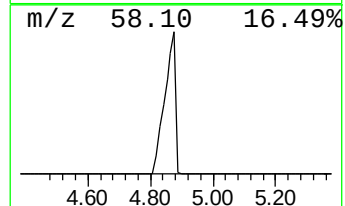
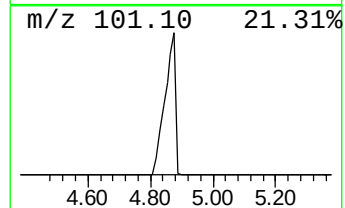
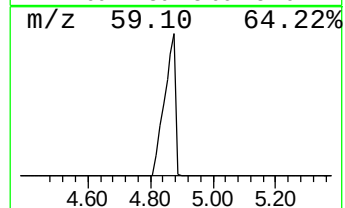
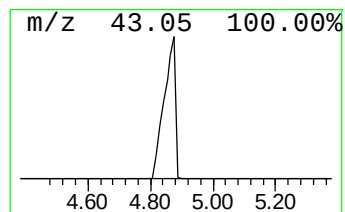
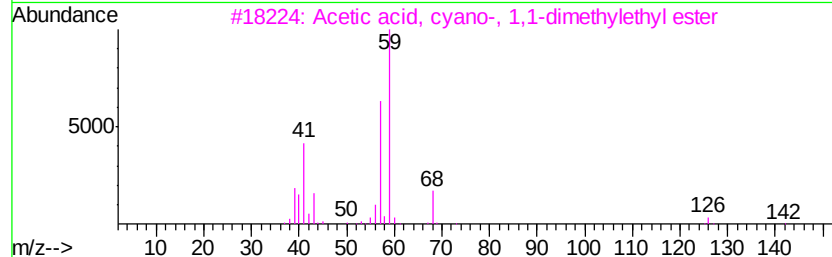
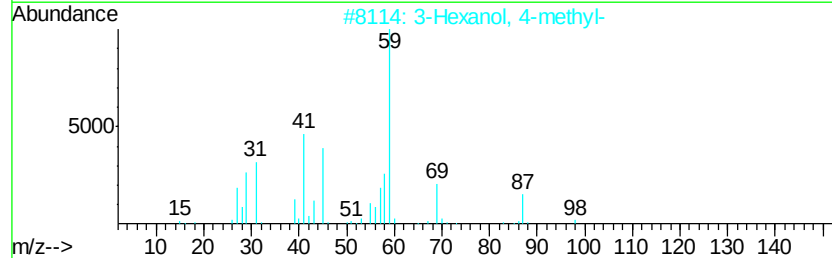
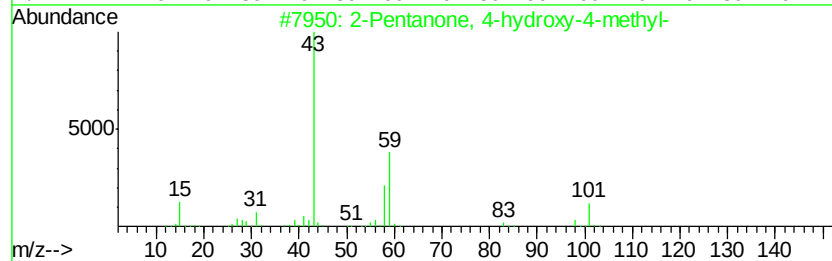
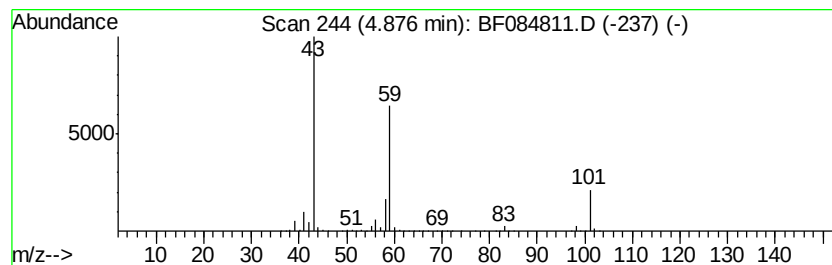
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.88	197.78 ng	11113500	1,4-Dichlorobenzene-d4	6.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	9



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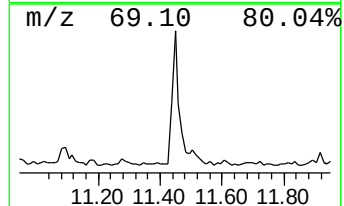
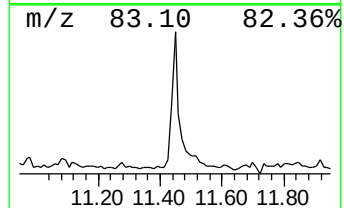
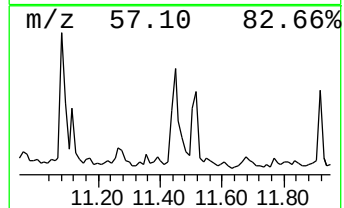
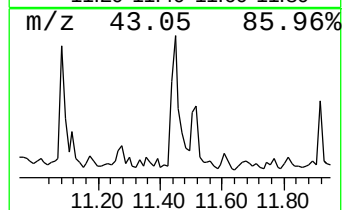
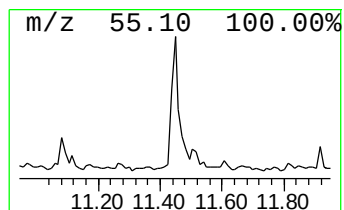
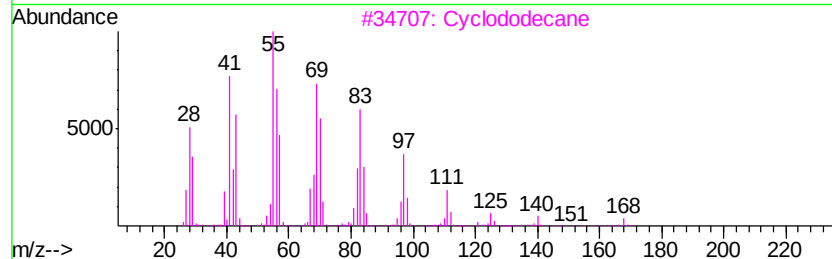
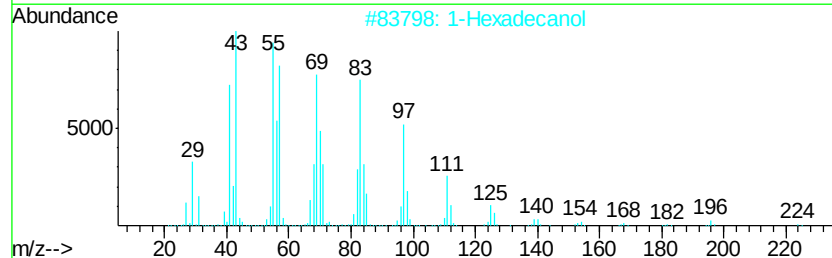
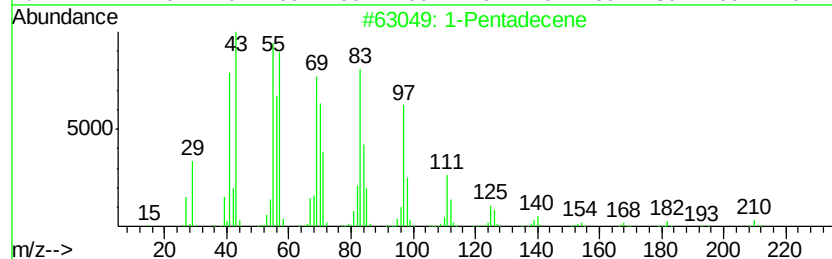
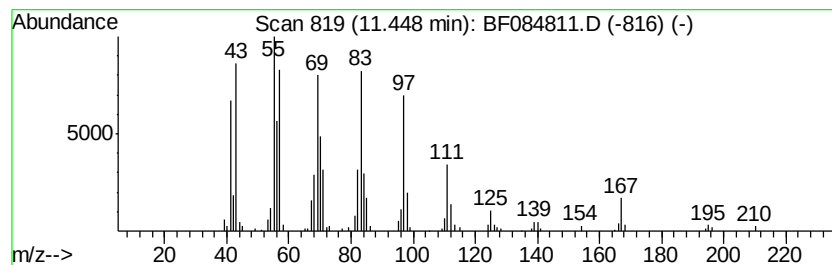
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Pentadecene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.45	3.55 ng	421951	Phenanthrene-d10		11.21
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentadecene	210	C15H30	013360-61-7	98
2	1-Hexadecanol	242	C16H34O	036653-82-4	94
3	Cyclododecane	168	C12H24	000294-62-2	93
4	9-Octadecene, (E)-	252	C18H36	007206-25-9	91
5	5-Octadecene, (E)-	252	C18H36	007206-21-5	91



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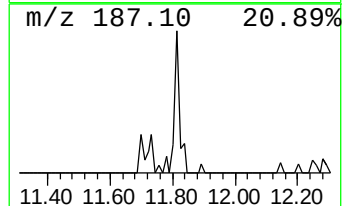
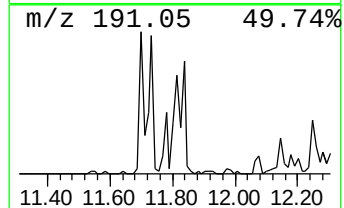
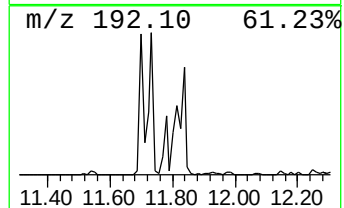
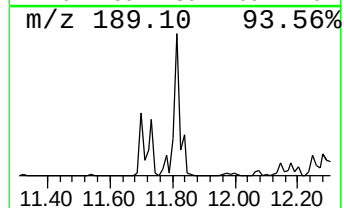
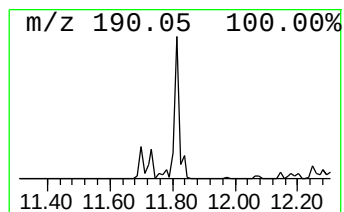
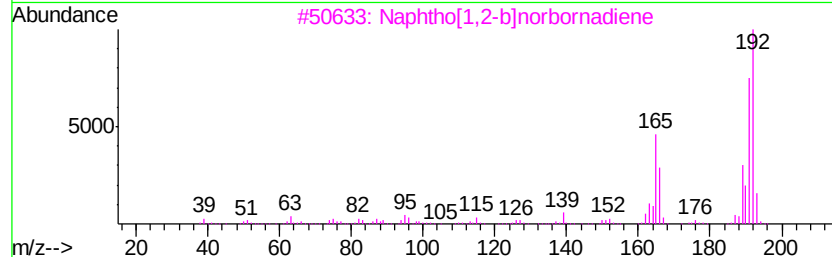
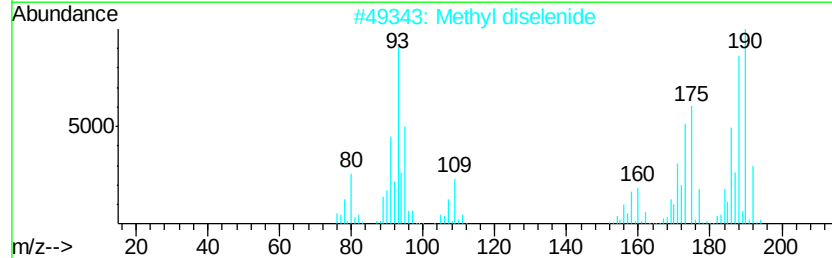
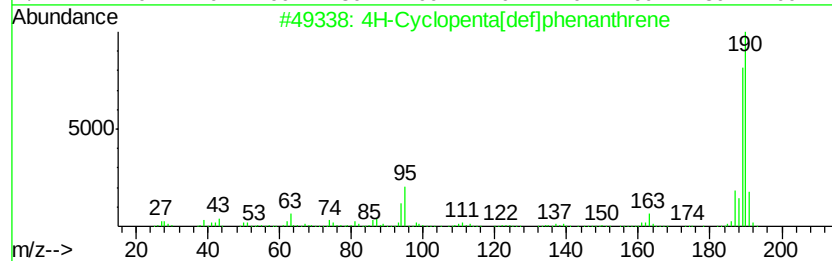
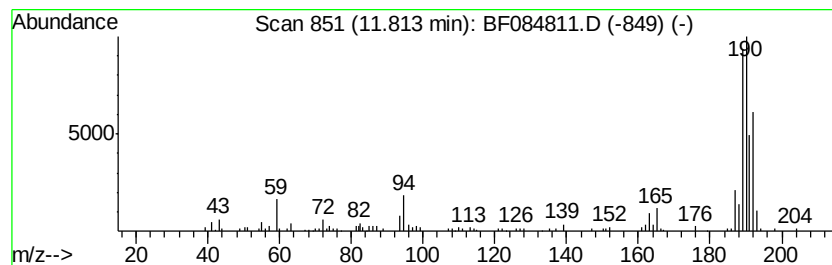
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 4H-Cyclopenta[def]phenanthrene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.81	2.18 ng	258823	Phenanthrene-d10	11.21	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	58
2	Methyl diselenide	190	C2H6Se2	007101-31-7	41
3	Naphtho[1,2-b]norbornadiene	192	C15H12	1000210-14-8	35
4	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	35
5	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	30



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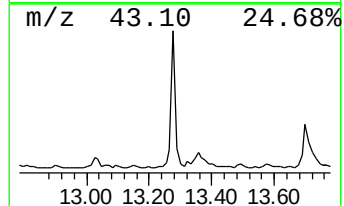
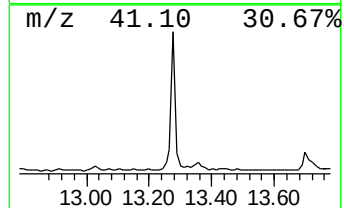
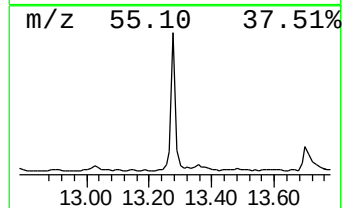
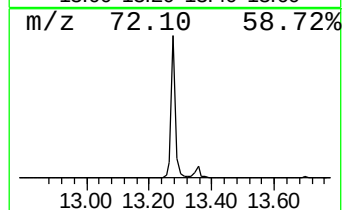
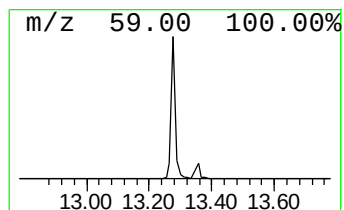
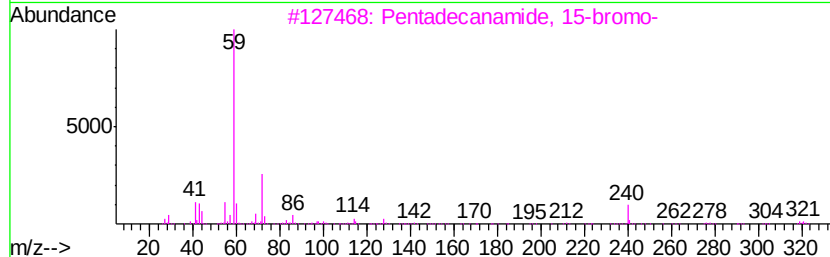
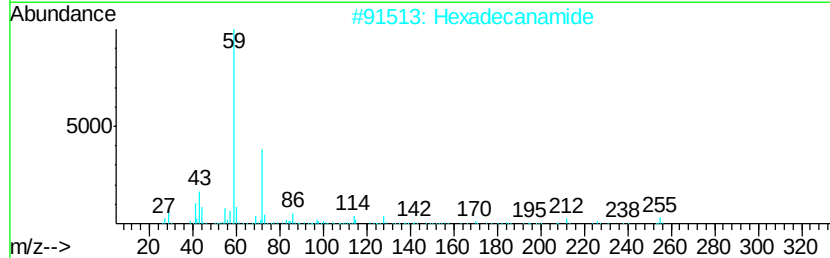
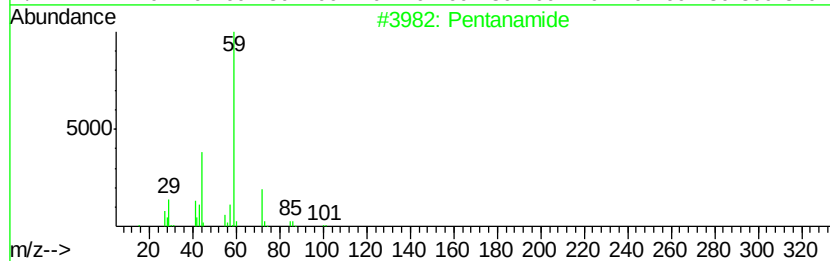
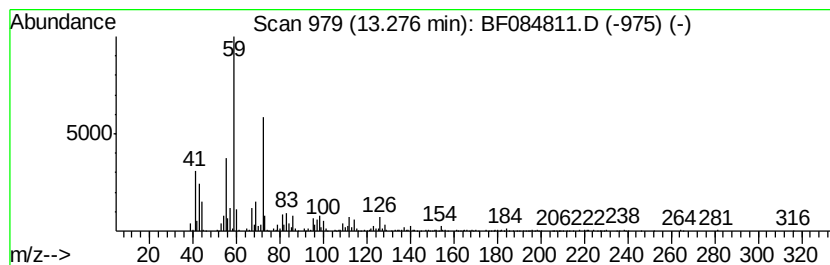
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Pentanamide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.28	13.08 ng	1174970	Chrysene-d12	13.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentanamide	101	C5H11NO	000626-97-1	59
2		Hexadecanamide	255	C16H33NO	000629-54-9	56
3		Pentadecanamide, 15-bromo-	319	C15H30BrNO	1000163-86-1	56
4		Dodecanamide	199	C12H25NO	001120-16-7	53
5		Octanamide	143	C8H17NO	000629-01-6	53



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020316\
Data File : BF084811.D
Acq On : 4 Feb 2016 3:40
Operator : SJ/IZ
Sample : H1312-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SUP-B005(5-7)

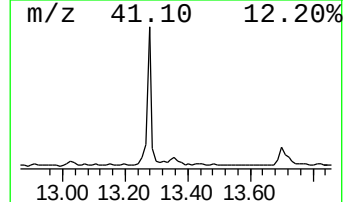
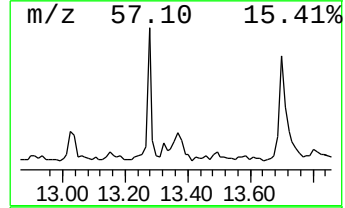
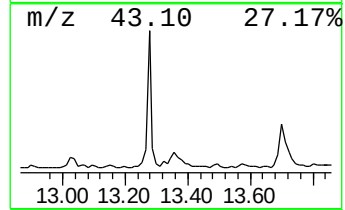
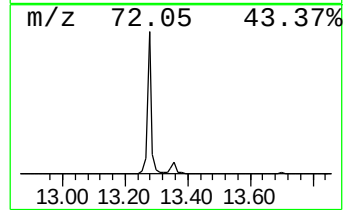
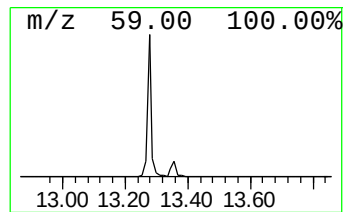
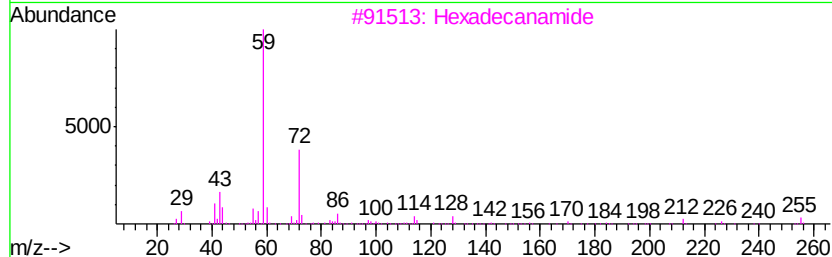
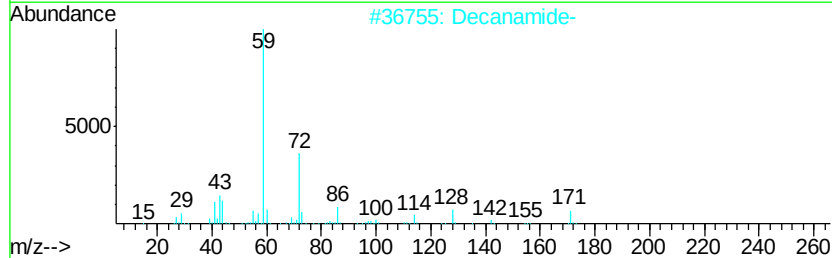
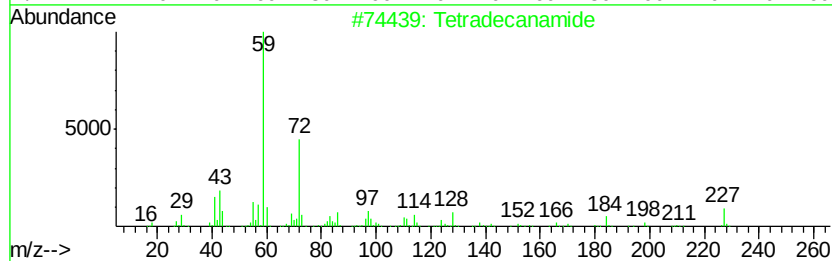
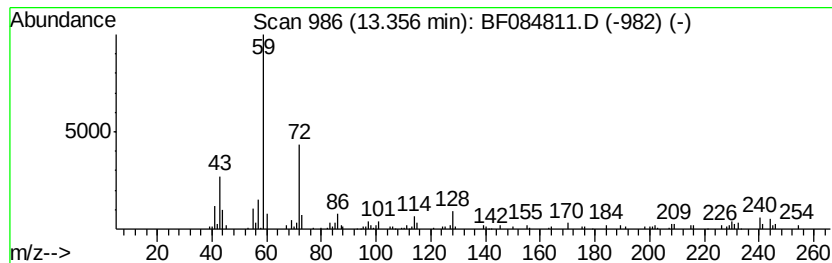
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tetradecanamide Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.36	2.28 ng	204775	Chrysene-d12	13.84

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetradecanamide	227	C14H29NO	000638-58-4	72
2		Decanamide-	171	C10H21NO	002319-29-1	72
3		Hexadecanamide	255	C16H33NO	000629-54-9	72
4		Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	64
5		Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	59



Data Path : Z:\HPCHEM1\BNA F\DATA\BF020316\
Data File : BF084811.D
Acq On : 4 Feb 2016 3:40
Operator : SJ/IZ
Sample : H1312-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SUP-B005(5-7)

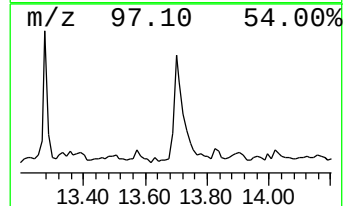
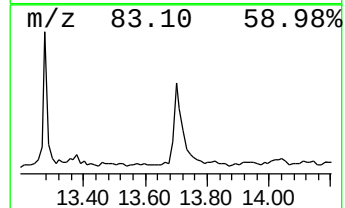
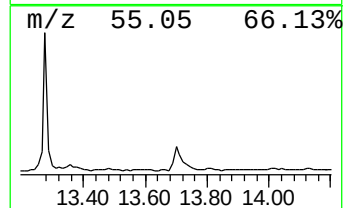
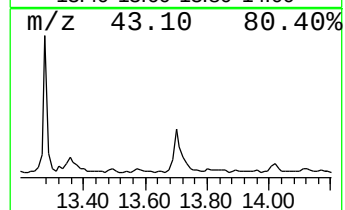
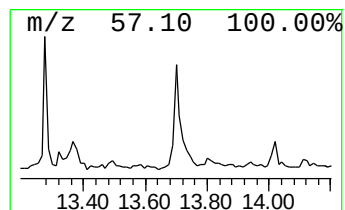
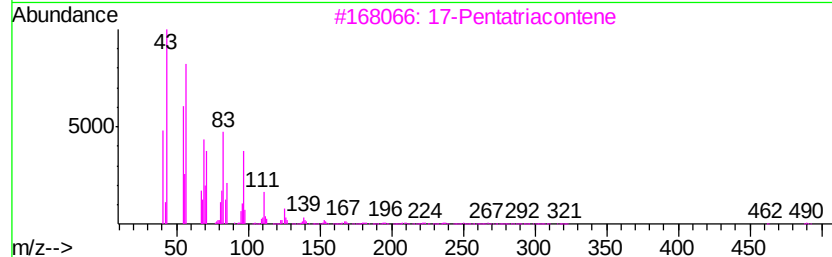
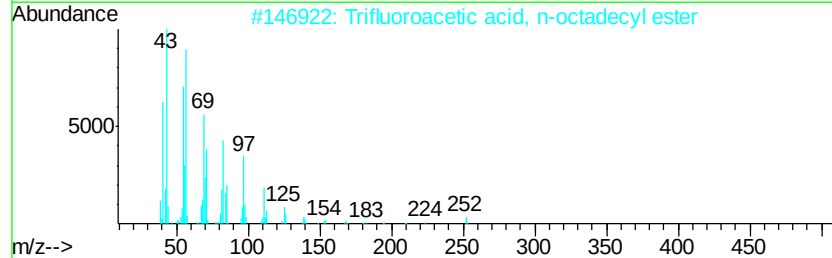
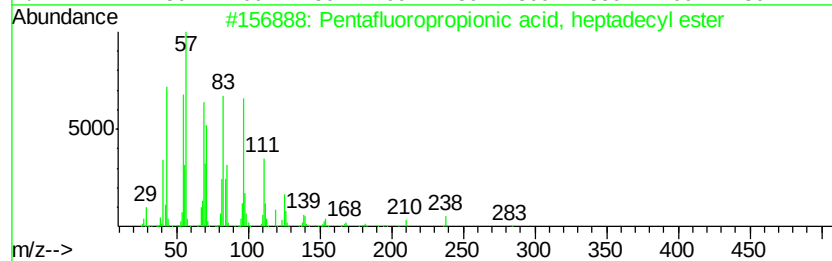
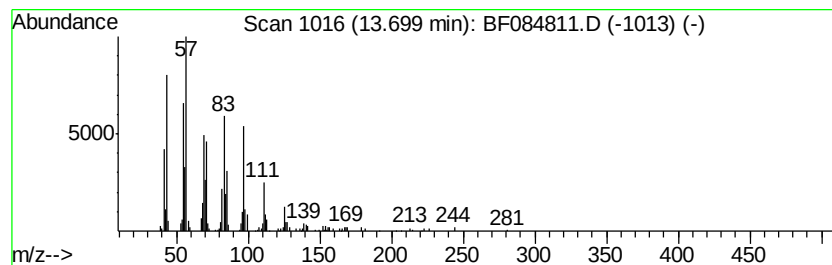
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Pentafluoropropionic acid, ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.70	3.86 ng	346420	Chrysene-d12	13.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	91
2		Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	91
3		17-Pentatriacontene	491	C35H70	006971-40-0	91
4		1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	91
5		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020316\
Data File : BF084811.D
Acq On : 4 Feb 2016 3:40
Operator : SJ/IZ
Sample : H1312-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SUP-B005(5-7)

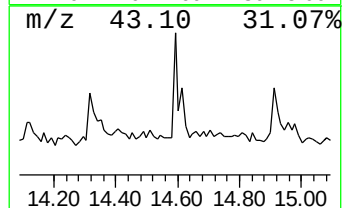
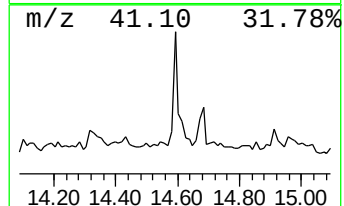
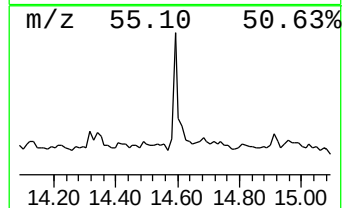
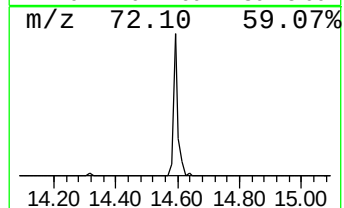
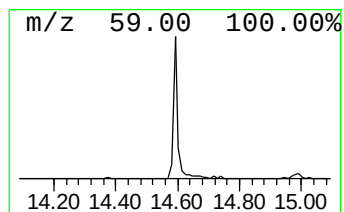
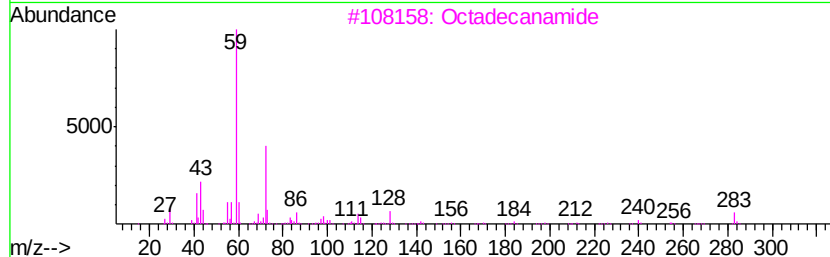
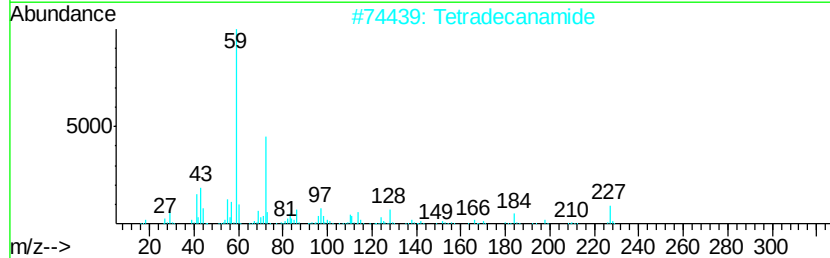
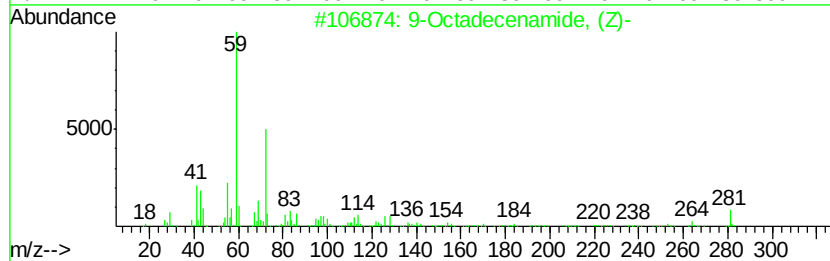
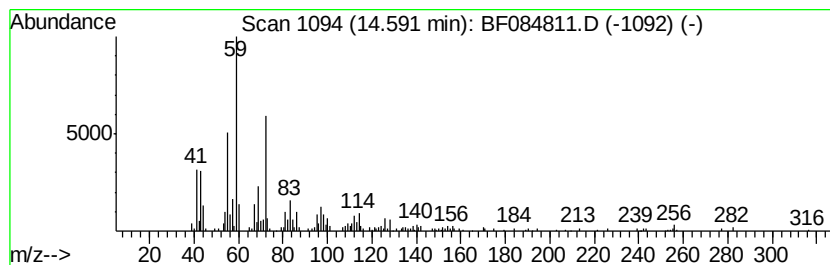
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 9-Octadecenamide, (Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.59	3.95 ng	211058	Perylene-d12	15.21

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	87
2		Tetradecanamide	227	C14H29NO	000638-58-4	64
3		Octadecanamide	283	C18H37NO	000124-26-5	59
4		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	59
5		Hexadecanamide	255	C16H33NO	000629-54-9	59



Data Path : Z:\HPCHEM1\BNA F\DATA\BF020316\
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Acq On : 4 Feb 2016 3:40
Operator : SJ/IZ
Sample : H1312-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SUP-B005(5-7)

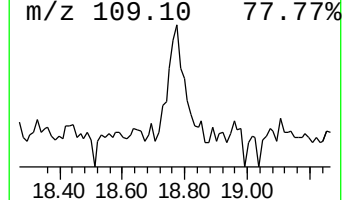
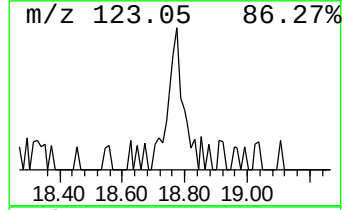
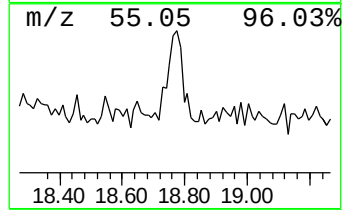
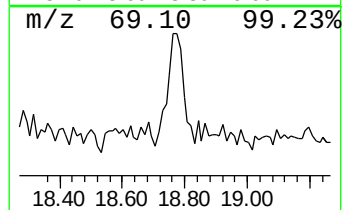
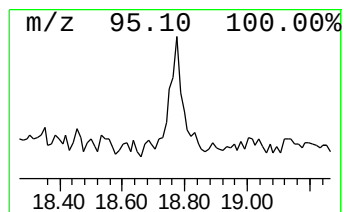
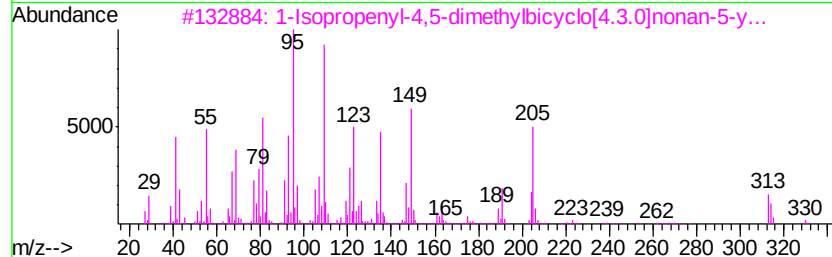
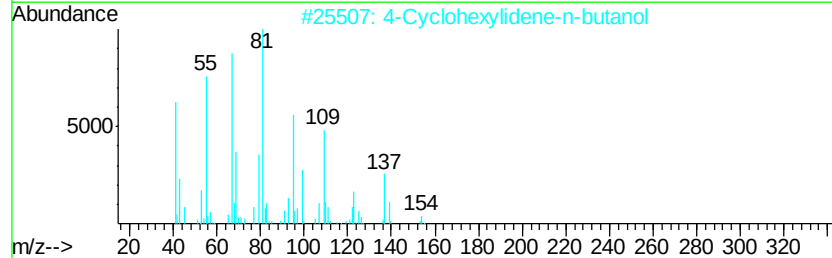
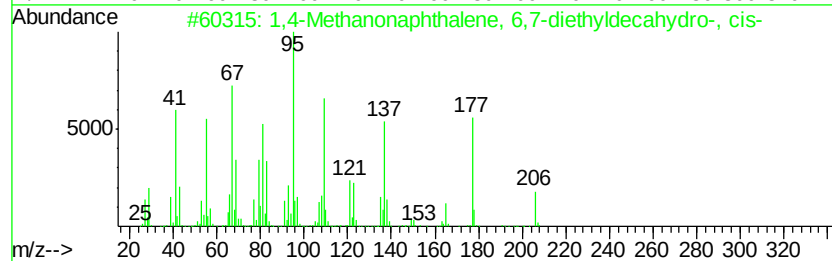
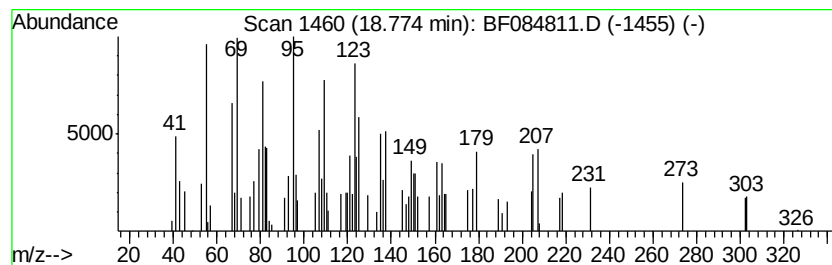
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF020116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown18.77 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.77	2.11 ng	112756	Perylene-d12	15.21

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,4-Methanonaphthalene, 6,7-diet...	206	C15H26	016539-02-9	35
2		4-Cyclohexylidene-n-butanol	154	C10H18O	004441-58-1	22
3		1-Isopropenyl-4,5-dimethylbicycl...	330	C21H30OS	1000195-85-4	22
4		3-Cyclohexene-1-carboxaldehyde, ...	152	C10H16O	040702-26-9	18
5		Carveol	152	C10H16O	1000285-09-9	15



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020316\
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Acq On : 4 Feb 2016 3:40
Operator : SJ/IZ
Sample : H1312-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SUP-B005(5-7)

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
3-Penten-2-one, 4...	4.13	43.3	ng	2435150	1	6.68	1123810	20.0
2-Pentanone, 4-hy...	4.88	197.8	ng	11113500	1	6.68	1123810	20.0
1-Pentadecene	11.45	3.5	ng	421951	4	11.21	2374760	20.0
4H-Cyclopenta[def...	11.81	2.2	ng	258823	4	11.21	2374760	20.0
Pentanamide	13.28	13.1	ng	1174970	5	13.84	1796490	20.0
Tetradecanamide	13.36	2.3	ng	204775	5	13.84	1796490	20.0
Pentafluoropropio...	13.70	3.9	ng	346420	5	13.84	1796490	20.0
9-Octadecenamide,...	14.59	4.0	ng	211058	6	15.21	1068770	20.0
unknown18.77	18.77	2.1	ng	112756	6	15.21	1068770	20.0