

Data Path : Z:\HPCHEM1\BNA F\DATA\BF110815\
 Data File : BF082793.D
 Acq On : 7 Nov 2015 6:41
 Operator : UM/IZ
 Sample : G4259-01
 Misc :
 ALS Vial : 31 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-03-110315

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	5.024	254	257	259	rBV	925573	1274357	13.94%	1.836%
2	5.447	291	294	296	rBV	3796121	3488536	38.16%	5.026%
3	6.476	381	384	386	rBV	2452186	2289791	25.05%	3.299%
4	6.613	393	396	399	rBV	5415363	5127970	56.10%	7.389%
5	6.841	414	416	419	rBV	1992833	2656954	29.07%	3.828%
6	7.002	428	430	433	rVB	4250484	5070782	55.47%	7.306%
7	7.413	463	466	468	rBV	4420277	4896466	53.57%	7.055%
8	7.962	508	514	517	rBV2	49361	135737	1.48%	0.196%
9	8.133	526	529	531	rBV	4011428	3675416	40.21%	5.296%
10	9.219	620	624	626	rBV	7238468	9141133	100.00%	13.171%
11	9.607	655	658	659	rVB	339997	343228	3.75%	0.495%
12	9.893	680	683	685	rBV	3620611	4441191	48.58%	6.399%
13	10.042	693	696	698	rBV	103603	116764	1.28%	0.168%
14	10.670	748	751	754	rBV2	4060691	5210877	57.00%	7.508%
15	10.808	760	763	766	rVB	74263	123093	1.35%	0.177%
16	11.253	799	802	804	rBV3	111844	143615	1.57%	0.207%
17	11.368	810	812	815	rBV	3958473	3900754	42.67%	5.620%
18	11.905	857	859	864	rBV2	390674	643250	7.04%	0.927%
19	12.065	871	873	877	rVB2	59174	118471	1.30%	0.171%
20	12.602	918	920	926	rVB5	46640	133204	1.46%	0.192%
21	12.694	926	928	934	rVB	360780	375952	4.11%	0.542%
22	12.785	934	936	939	rVB2	413381	492385	5.39%	0.709%
23	12.865	942	943	945	rVV	94072	96168	1.05%	0.139%
24	12.956	948	951	954	rVB	5993932	6797038	74.36%	9.793%
25	13.494	996	998	1001	rBV	555919	525577	5.75%	0.757%
26	13.871	1029	1031	1039	rBV	398149	532000	5.82%	0.767%
27	14.008	1040	1043	1045	rBV	3396189	3419332	37.41%	4.927%
28	14.191	1057	1059	1063	rVB	134855	241019	2.64%	0.347%
29	14.374	1073	1075	1078	rBV3	52030	113300	1.24%	0.163%
30	14.511	1083	1087	1089	rVV2	58365	114417	1.25%	0.165%
31	14.797	1110	1112	1113	rVB	80047	103388	1.13%	0.149%
32	15.437	1164	1168	1170	rBV	1798943	2637040	28.85%	3.800%
33	15.482	1170	1172	1176	rVB3	111367	204237	2.23%	0.294%
34	15.745	1193	1195	1201	rVB3	71983	216238	2.37%	0.312%

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ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-03-110315

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-BF110715.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.894	1206	1208	1211	rVB2	42114	92503	1.01%	0.133%
36	15.985	1211	1216	1217	rBV4	65303	156551	1.71%	0.226%
37	16.420	1252	1254	1267	rVB	89427	355349	3.89%	0.512%

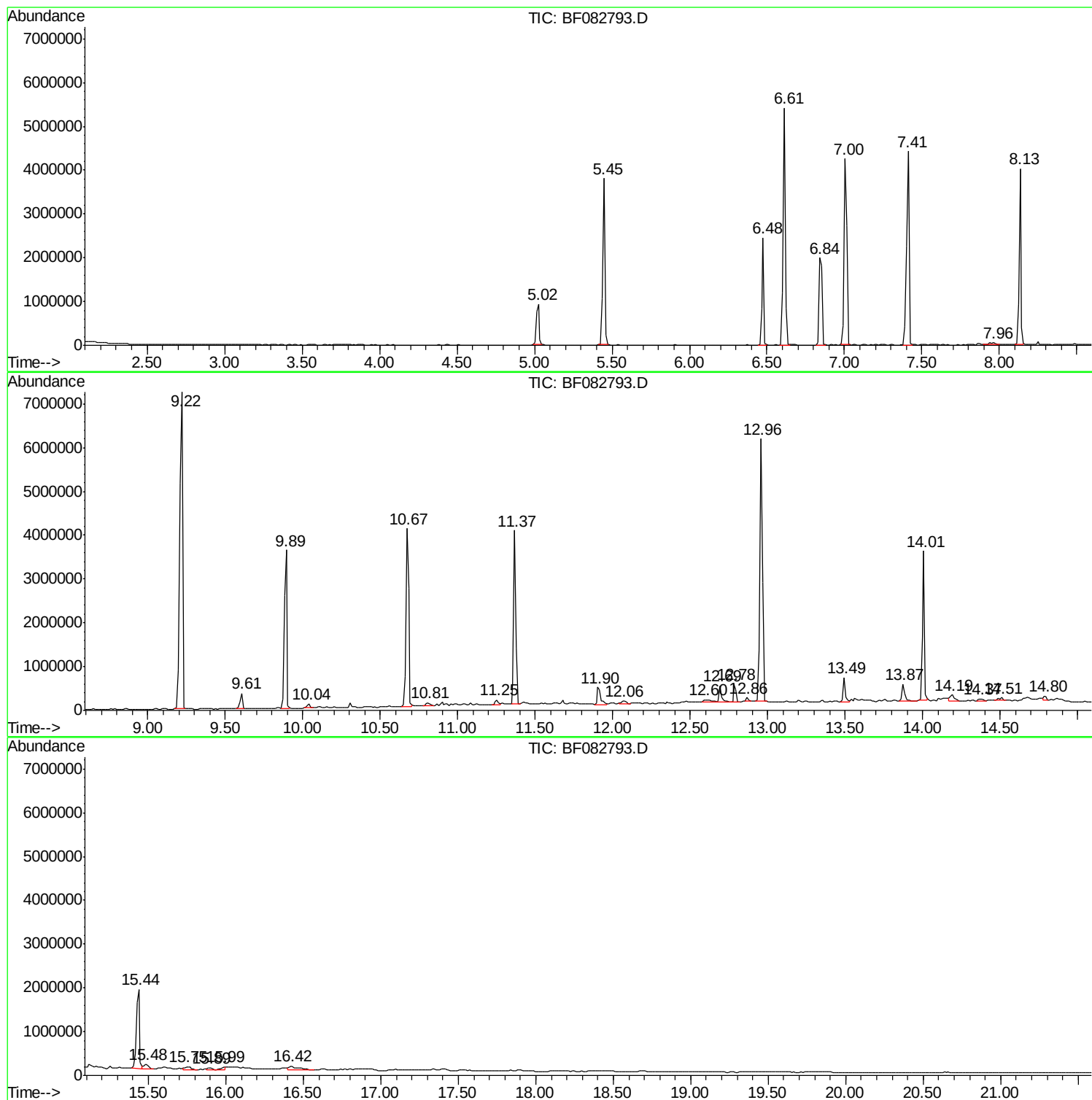
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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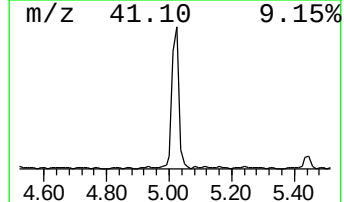
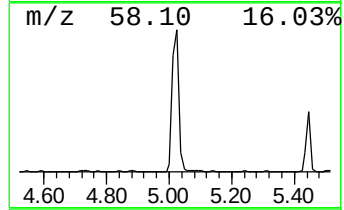
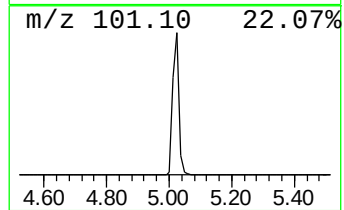
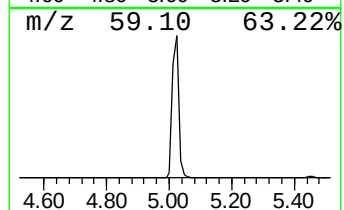
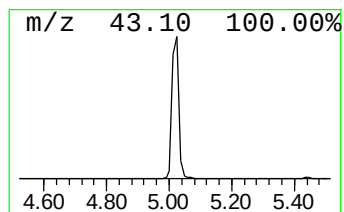
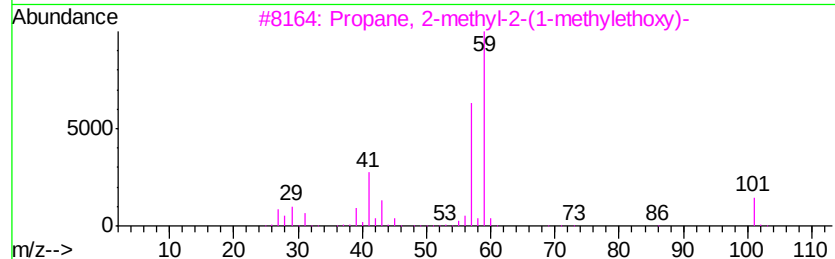
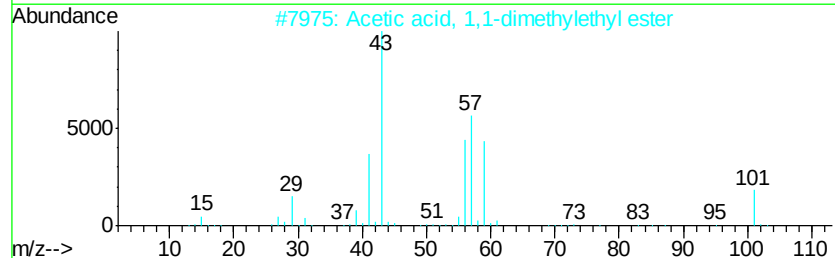
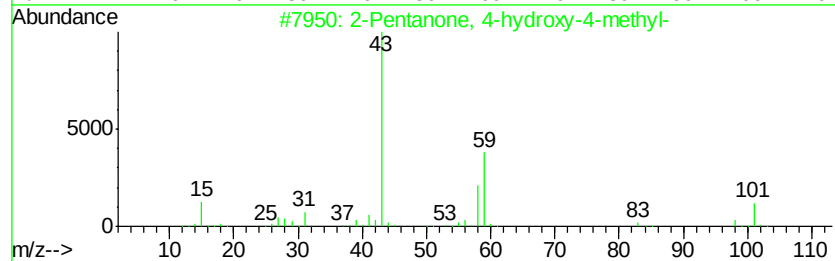
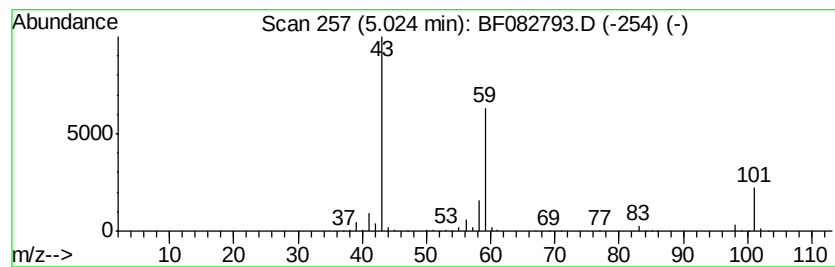
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.02	9.59 ng	1274360	1,4-Dichlorobenzene-d4	6.85

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56	
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	28	
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17	
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9	



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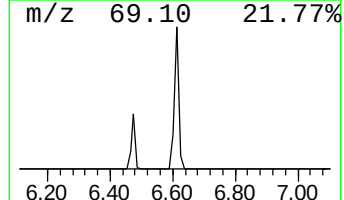
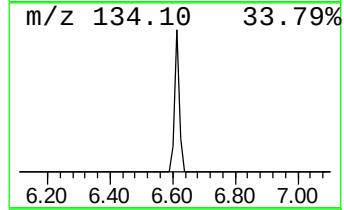
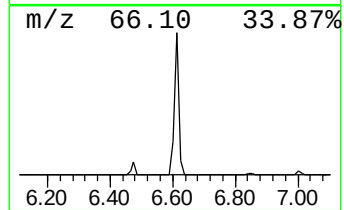
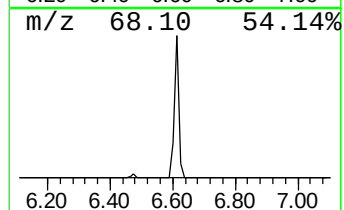
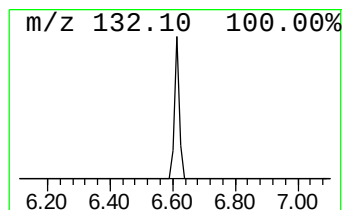
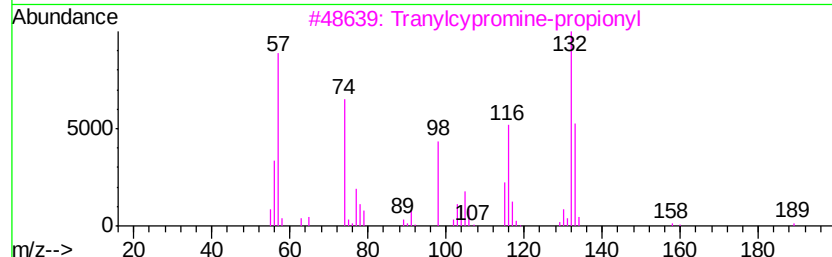
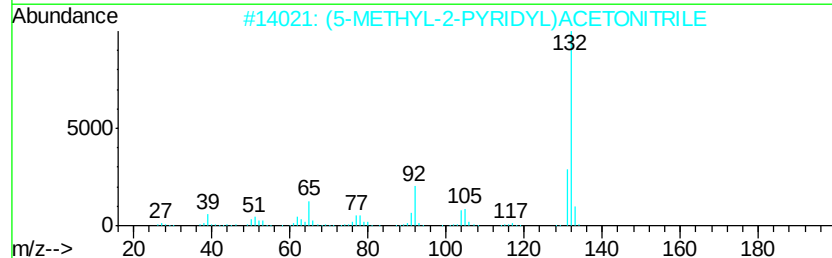
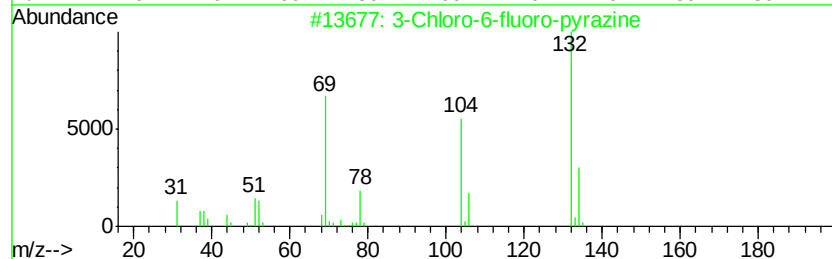
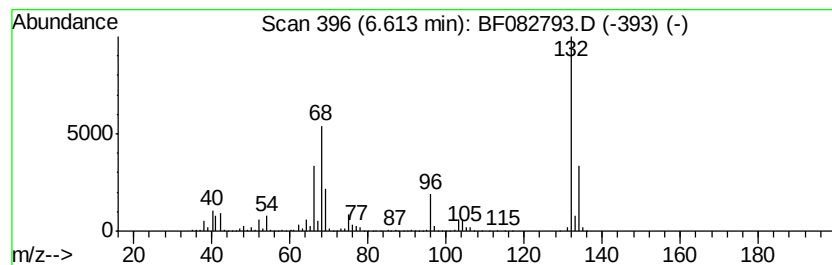
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	38.60 ng	5127970	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
3		Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
4		2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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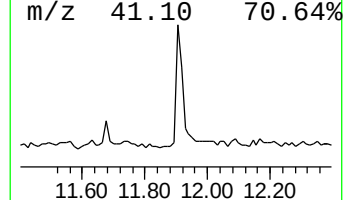
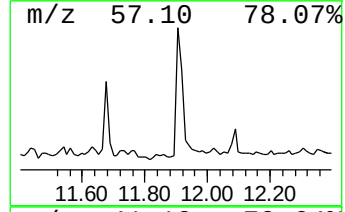
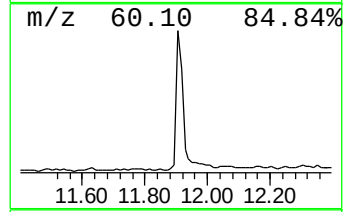
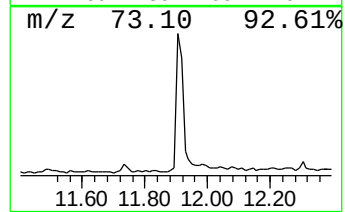
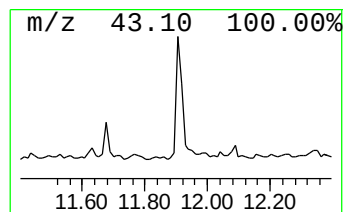
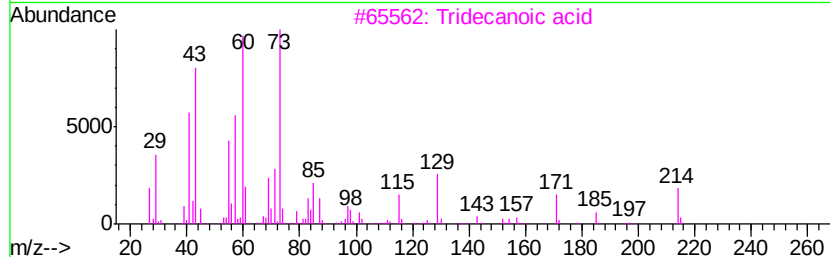
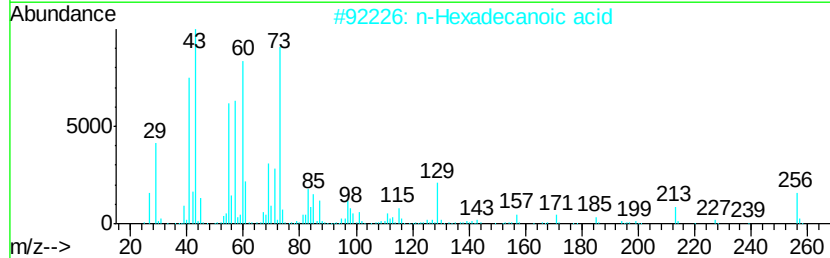
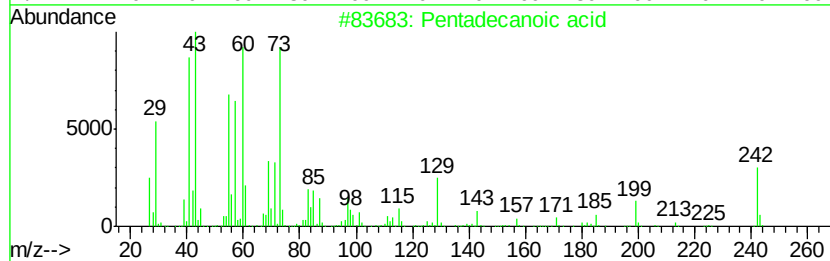
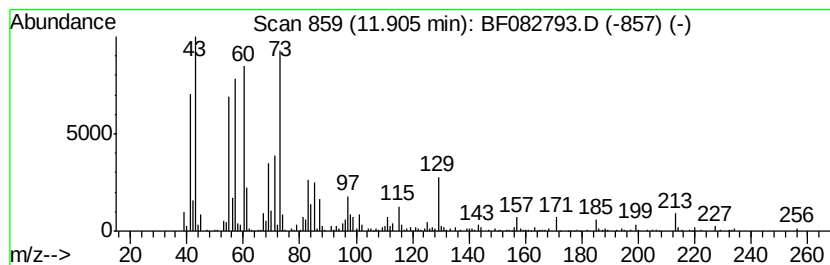
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Pentadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.90	3.30 ng	643250	Phenanthrene-d10	11.37

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentadecanoic acid	242	C15H30O2	001002-84-2	91
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81
3		Tridecanoic acid	214	C13H26O2	000638-53-9	64
4		N-Cyclooct-4-enylacetamide	167	C10H17NO	170952-69-9	25
5		Silane, trichlorodocosyl-	442	C22H45Cl3Si	007325-84-0	25



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Misc :
ALS Vial : 31 Sample Multiplier: 1

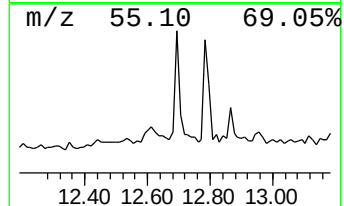
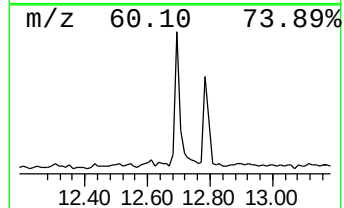
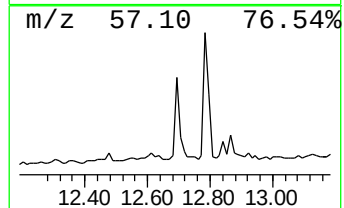
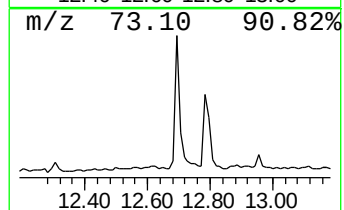
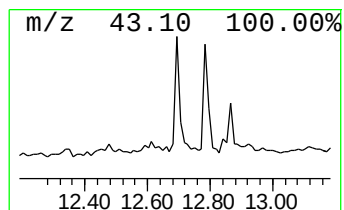
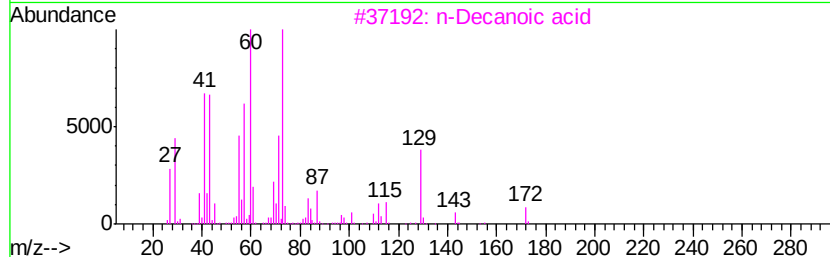
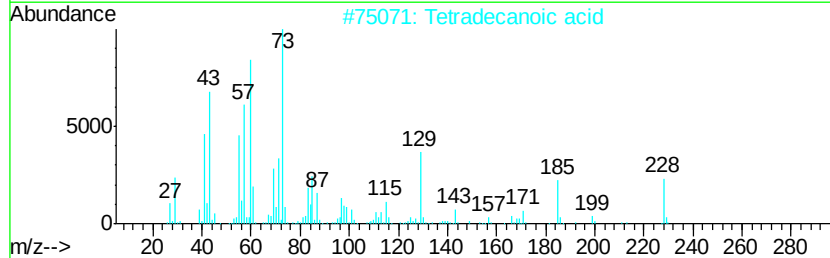
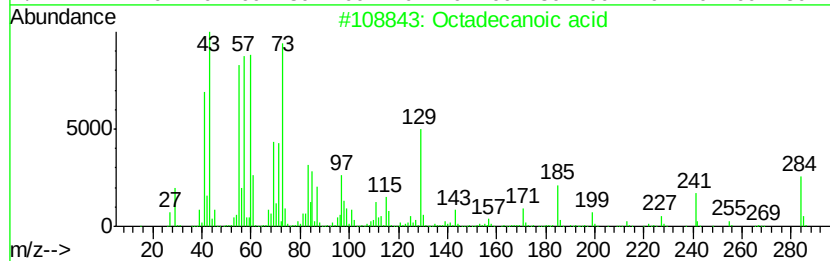
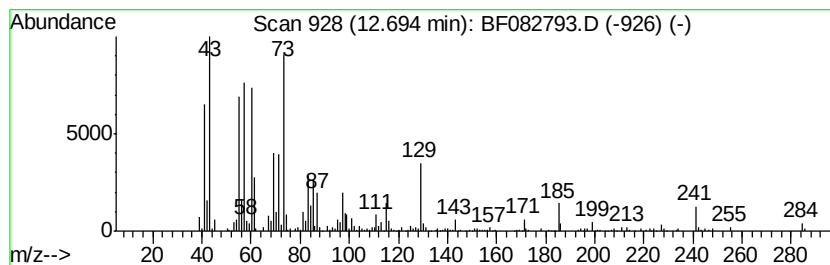
Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.69	2.20 ng	375952	Chrysene-d12	14.01	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	93
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
3	n-Decanoic acid	172	C10H20O2	000334-48-5	76
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	55
5	Amyl Nitrite	117	C5H11NO2	000110-46-3	27



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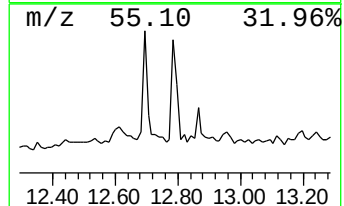
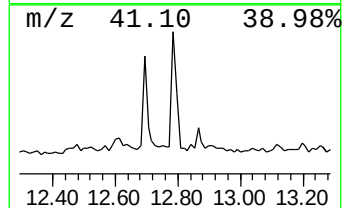
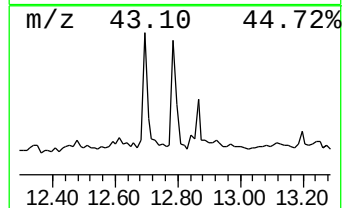
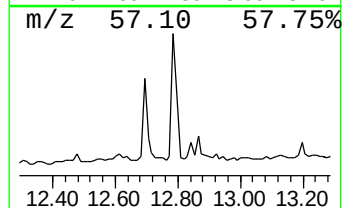
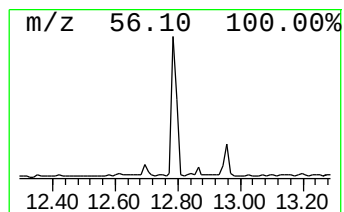
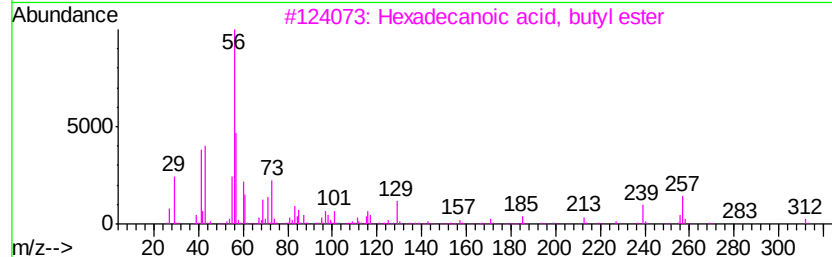
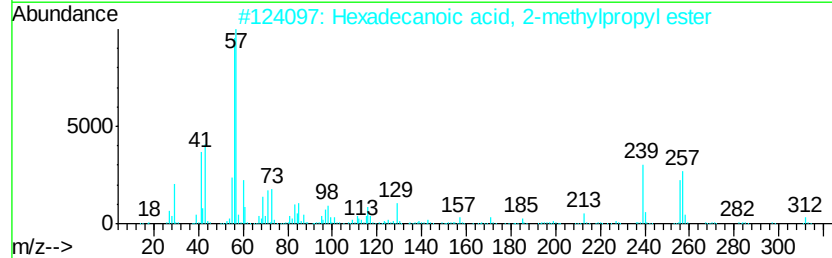
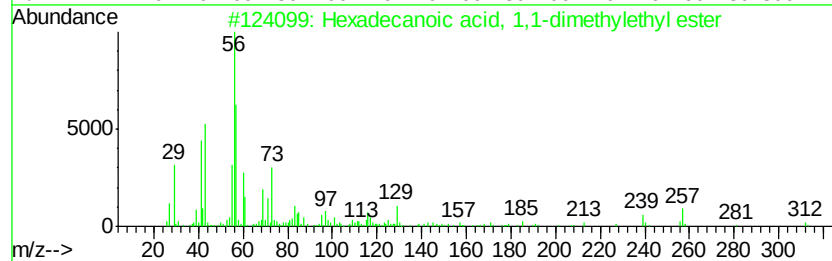
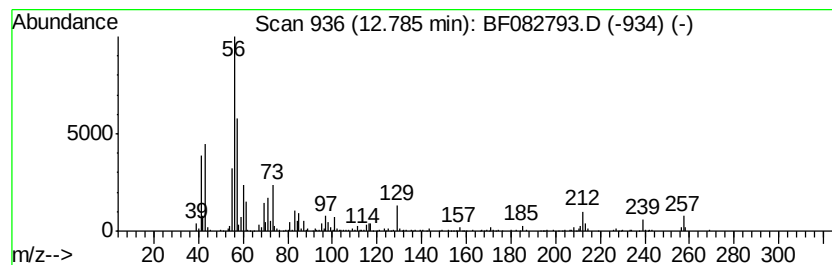
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Hexadecanoic acid, 1,1-dime... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.79	2.88 ng	492385	Chrysene-d12	14.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	91
2		Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	64
3		Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	46
4		Myristic acid isobutyl ester	284	C18H36O2	025263-97-2	45
5		Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	38



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ClientSampleId :
MW-03-110315

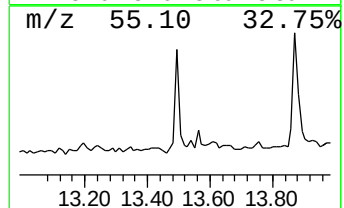
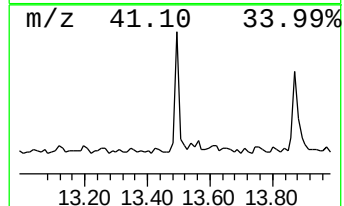
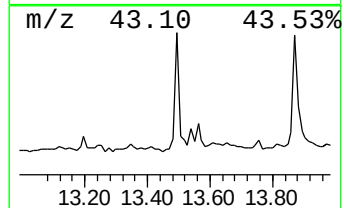
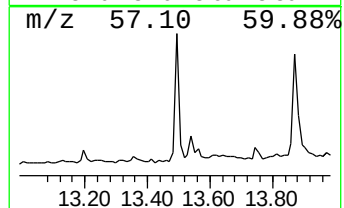
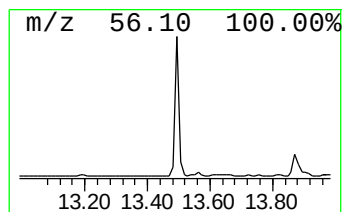
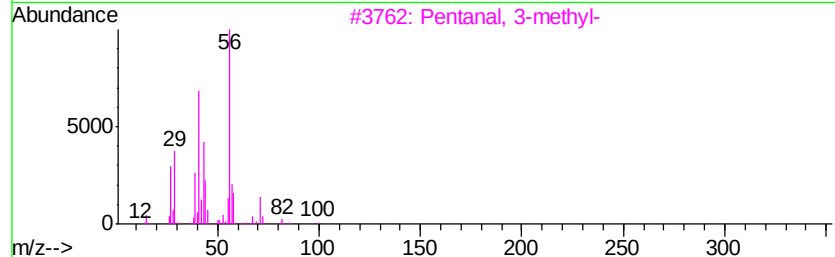
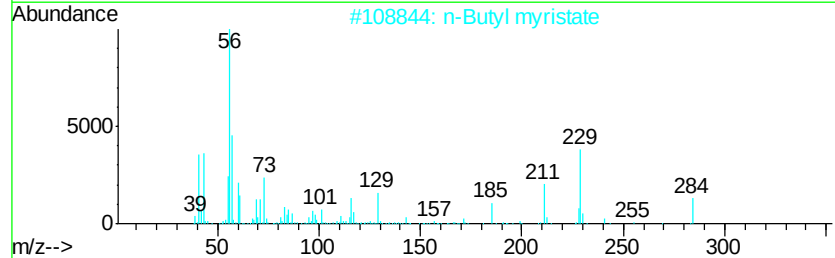
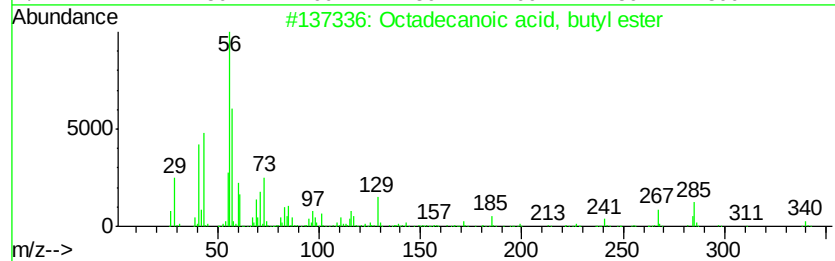
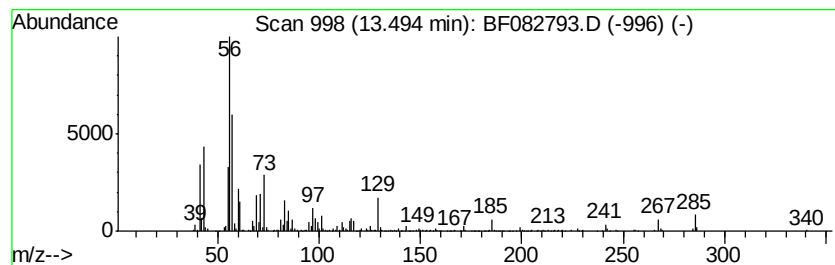
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
13.49	3.07 ng	525577	Chrysene-d12	14.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	93
2		n-Butyl myristate	284	C18H36O2	000110-36-1	80
3		Pentanal, 3-methyl-	100	C6H12O	015877-57-3	43
4		Urea, N,N'-di-2-propenyl-	140	C7H12N2O	001801-72-5	38
5		2,2-Dimethyl-1,3-butanediol	118	C6H14O2	000076-35-7	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110815\
Data File : BF082793.D
Acq On : 7 Nov 2015 6:41
Operator : UM/IZ
Sample : G4259-01
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-03-110315

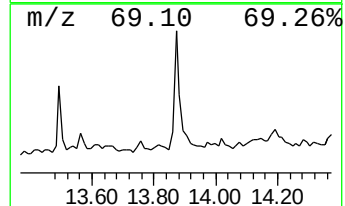
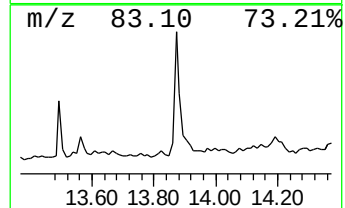
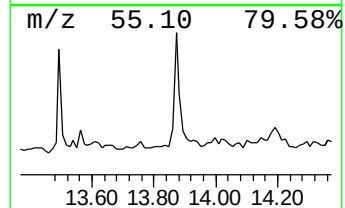
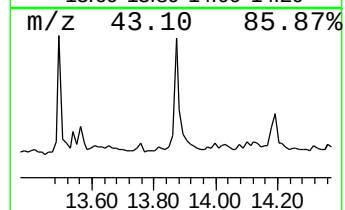
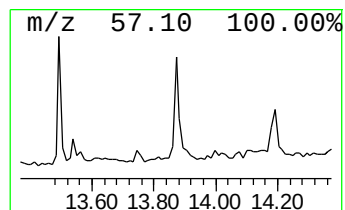
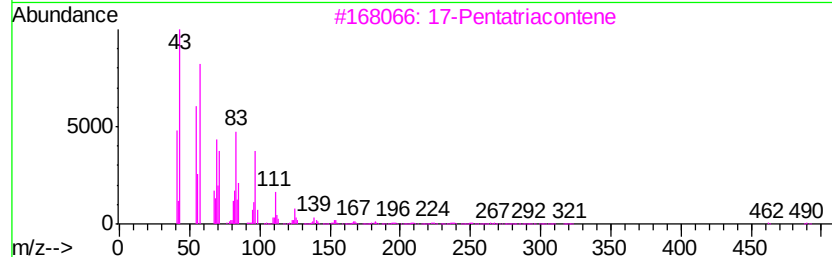
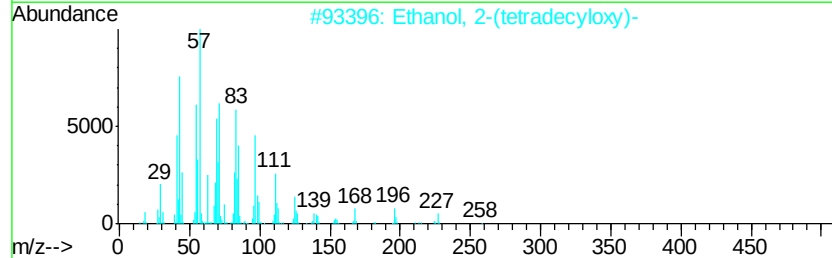
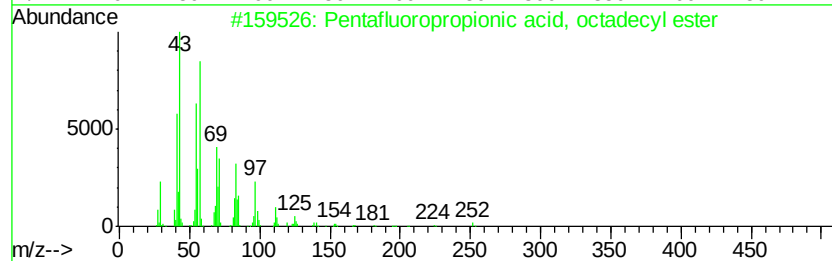
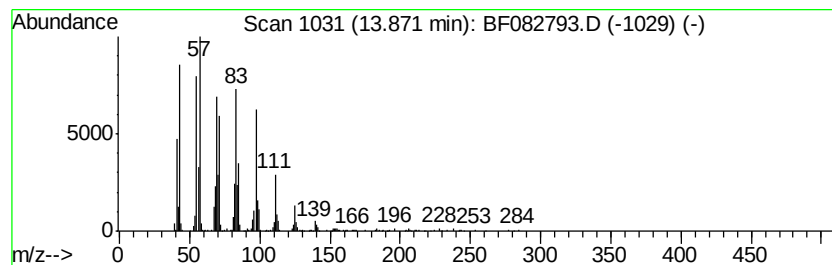
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Pentafluoropropionic acid, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	3.11 ng	532000	Chrysene-d12	14.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentafluoropropionic acid, octad...	416	C21H37F5O2	1000280-07-7	91
2		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
3		17-Pentatriacontene	491	C35H70	006971-40-0	87
4		1-Octadecanol	270	C18H38O	000112-92-5	83
5		1-Nonadecanol	284	C19H40O	001454-84-8	81



Data Path : Z:\HPCHEM1\BNA F\DATA\BF110815\
Data File : BF082793.D
Acq On : 7 Nov 2015 6:41
Operator : UM/IZ
Sample : G4259-01
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-03-110315

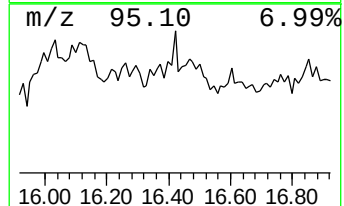
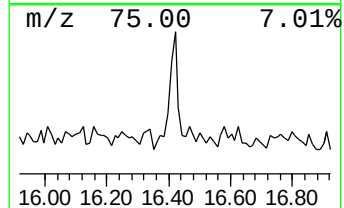
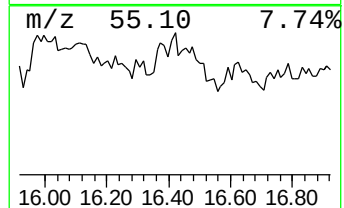
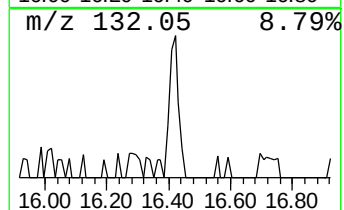
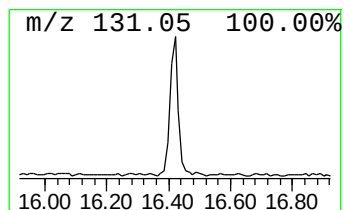
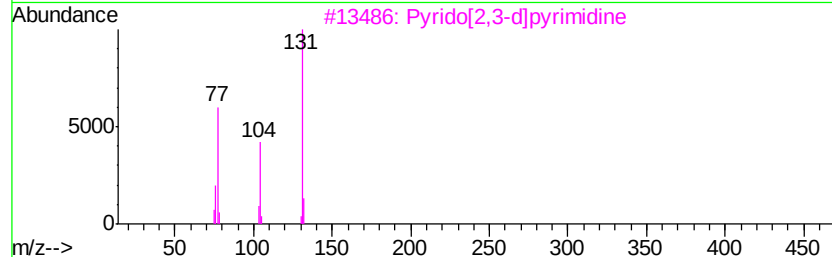
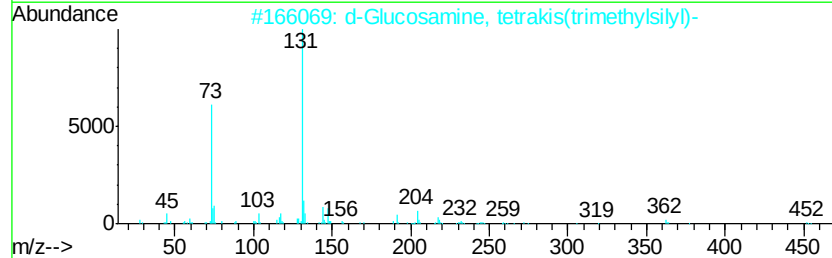
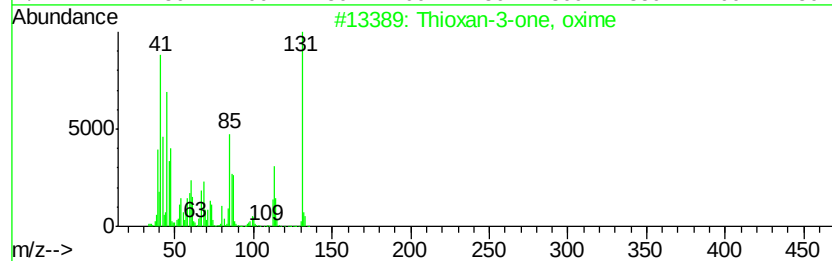
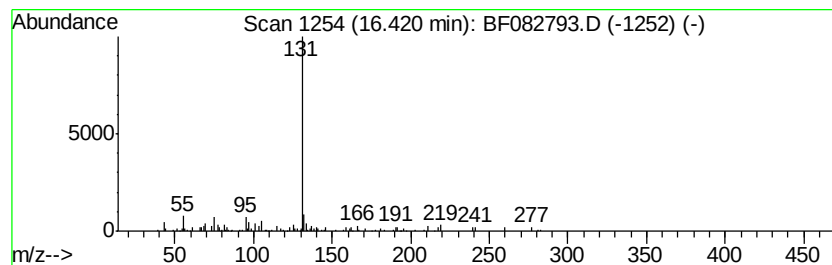
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF110715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Thioxan-3-one, oxime Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.42	2.70 ng	355349	Perylene-d12	15.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Thioxan-3-one, oxime	131	C5H9NOS	058230-51-6	53
2		d-Glucosamine, tetrakis(trimethy...	467	C18H45N05Si4	1000079-26-2	12
3		Pyrido[2,3-d]pyrimidine	131	C7H5N3	000254-61-5	9
4		Hydrazinecarbothioamide, 2-(1-me...	131	C4H9N3S	001752-30-3	9
5		N-(p-Vinylbenzoyl)-l-alanine	219	C12H13N03	139184-60-4	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110815\
Data File : BF082793.D
Acq On : 7 Nov 2015 6:41
Operator : UM/IZ
Sample : G4259-01
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-03-110315

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...	5.02	9.6 ng		1274360	1	6.85	2656950	20.0
unknown6.61	6.61	38.6 ng		5127970	1	6.85	2656950	20.0
Pentadecanoic acid	11.90	3.3 ng		643250	4	11.37	3900750	20.0
Octadecanoic acid	12.69	2.2 ng		375952	5	14.01	3419330	20.0
Hexadecanoic acid...	12.79	2.9 ng		492385	5	14.01	3419330	20.0
Octadecanoic acid...	13.49	3.1 ng		525577	5	14.01	3419330	20.0
Pentafluoropropio...	13.87	3.1 ng		532000	5	14.01	3419330	20.0
Thioxan-3-one, oxime	16.42	2.7 ng		355349	6	15.44	2637040	20.0