

Data Path : Z:\HPCHEM1\BNA F\DATA\BF113016\
 Data File : BF091357.D
 Acq On : 30 Nov 2016 16:33
 Operator : UM/SJ
 Sample : H5767-01
 Misc :
 ALS Vial : 36 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 112216-DSDC-E-D-B

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-BF112916.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	5.041	238	241	244	rBV	604927	636383	9.57%	1.667%
2	5.464	275	278	280	rBV	1279526	1695121	25.49%	4.441%
3	6.481	365	367	371	rBV	1381348	1238731	18.63%	3.245%
4	6.630	377	380	382	rBV	3305236	3094364	46.53%	8.106%
5	6.859	398	400	403	rBV	1073681	1200546	18.05%	3.145%
6	7.019	412	414	417	rVB	4182654	4411415	66.34%	11.556%
7	7.430	446	450	452	rBV	3920500	4143669	62.31%	10.855%
8	8.150	510	513	515	rBV	1832646	1620695	24.37%	4.246%
9	9.225	604	607	610	rBV	4824017	6649734	100.00%	17.420%
10	9.613	639	641	644	rBV	153093	166884	2.51%	0.437%
11	9.899	664	666	669	rVB	1818923	1563538	23.51%	4.096%
12	10.688	732	735	737	rBV	2174280	2102445	31.62%	5.508%
13	10.813	744	746	751	rVB	62039	73007	1.10%	0.191%
14	11.259	783	785	787	rBV	74340	67228	1.01%	0.176%
15	11.385	793	796	798	rVB	1381560	1358454	20.43%	3.559%
16	11.911	840	842	844	rBV	171009	204284	3.07%	0.535%
17	12.699	909	911	918	rBV	206239	257661	3.87%	0.675%
18	12.802	918	920	922	rVV	175126	183398	2.76%	0.480%
19	12.974	932	935	937	rBV	4501684	4884008	73.45%	12.794%
20	13.499	979	981	984	rBV	136226	144118	2.17%	0.378%
21	13.877	1012	1014	1019	rBV	58588	80749	1.21%	0.212%
22	14.014	1023	1026	1028	rBV	1156928	1149613	17.29%	3.012%
23	14.494	1066	1068	1075	rBV3	20920	68987	1.04%	0.181%
24	15.442	1148	1151	1154	rBV	860143	1039452	15.63%	2.723%
25	15.500	1154	1156	1165	rVB	46279	139207	2.09%	0.365%

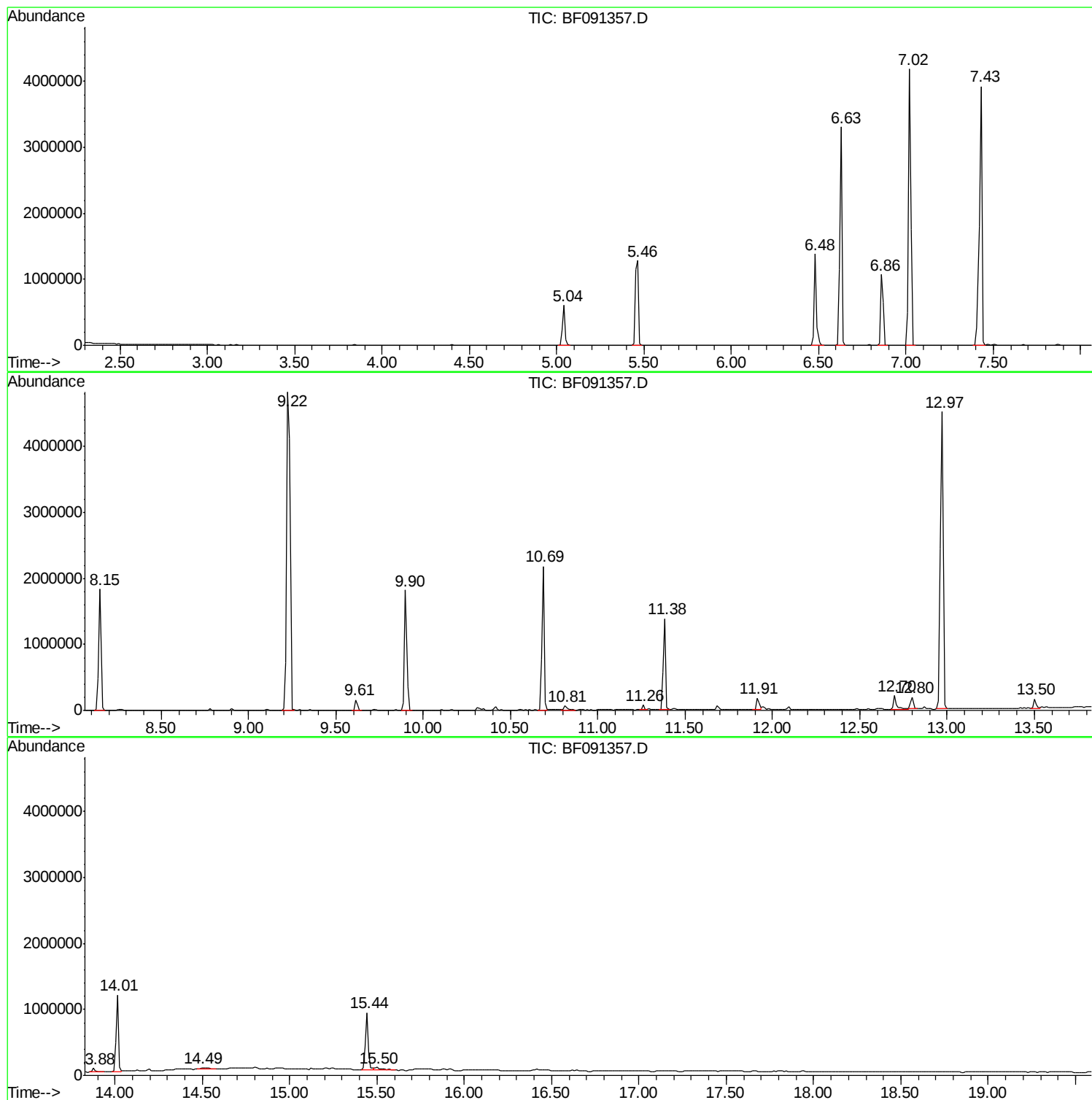
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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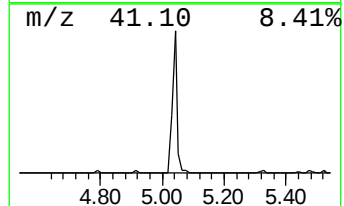
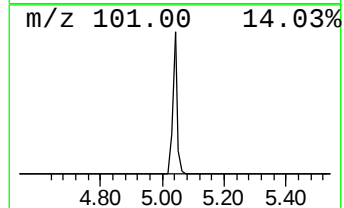
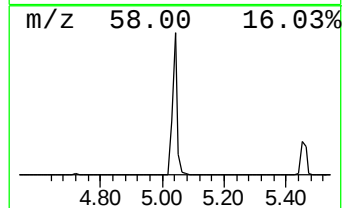
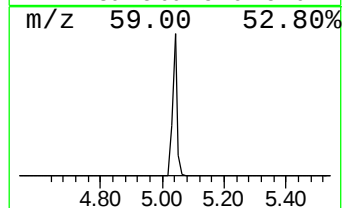
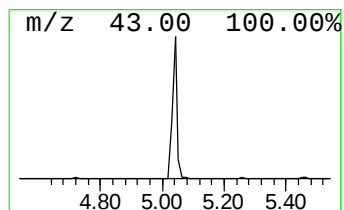
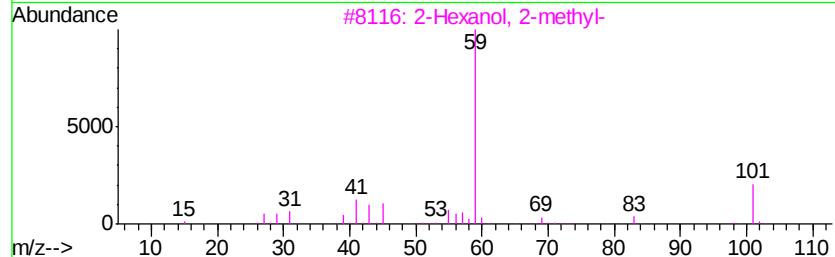
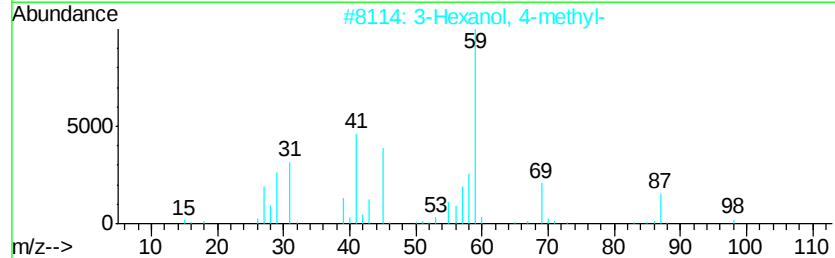
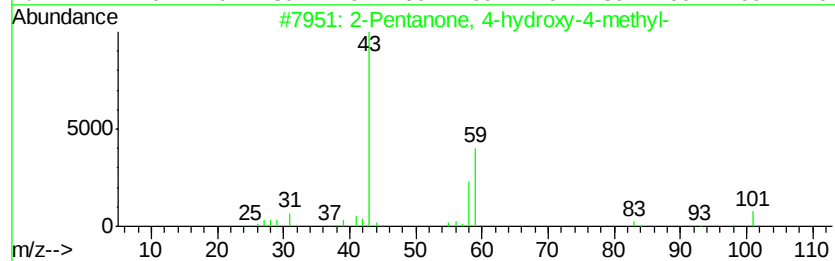
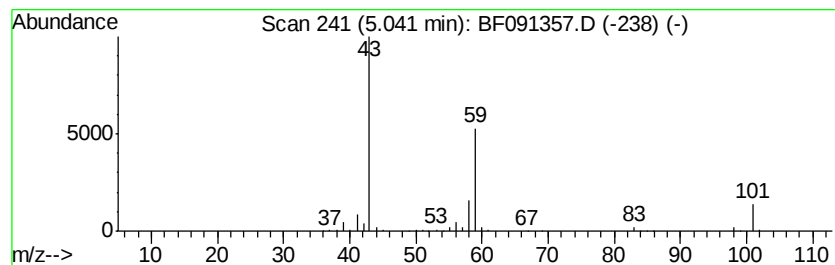
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.04	10.60 ng	636383	1,4-Dichlorobenzene-d4	6.86

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	32
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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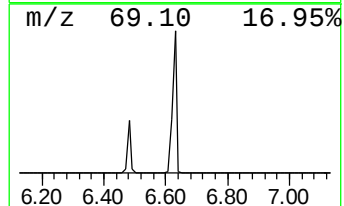
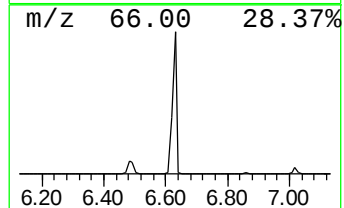
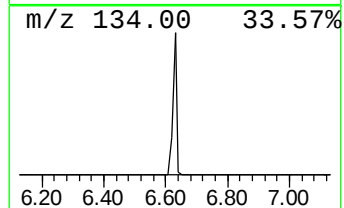
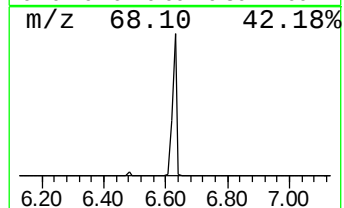
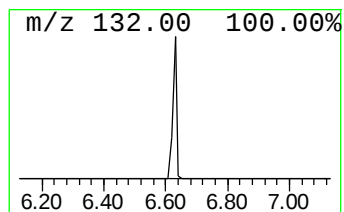
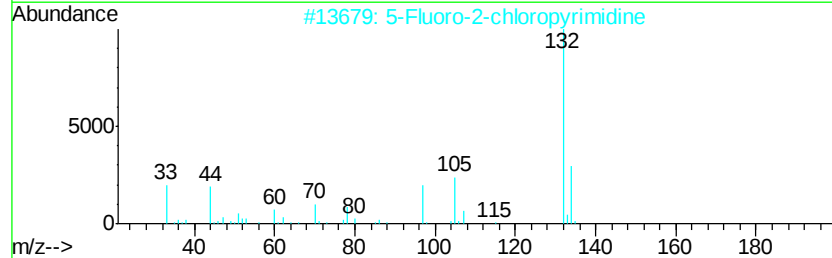
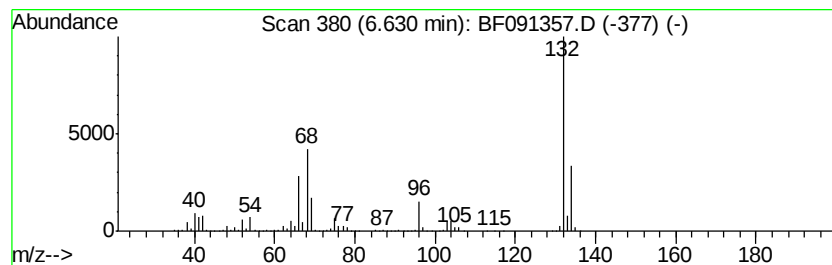
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.63 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	51.55 ng	3094360	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		5-Aminoindole	132	C8H8N2	005192-03-0	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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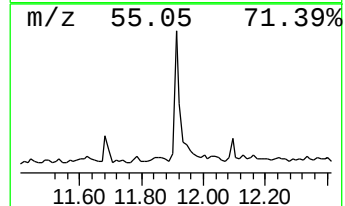
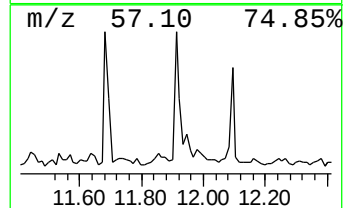
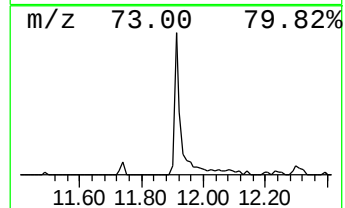
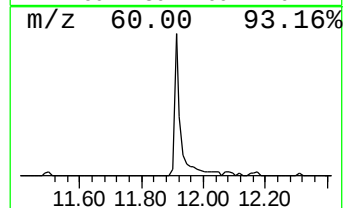
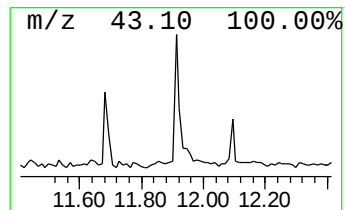
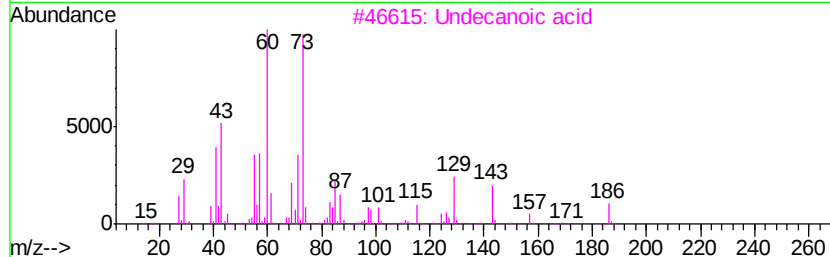
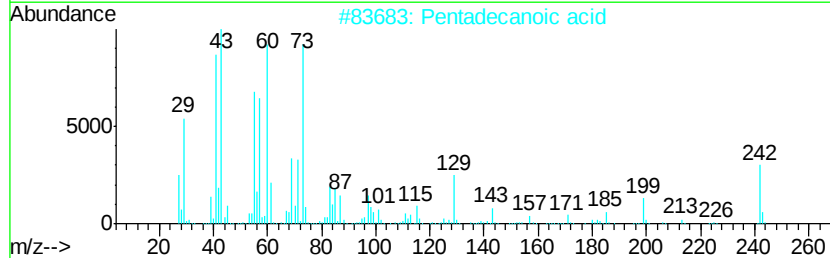
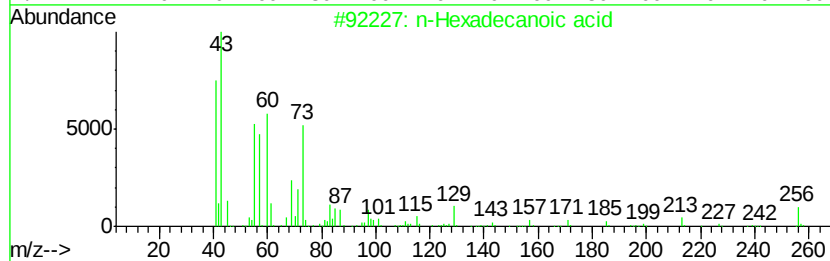
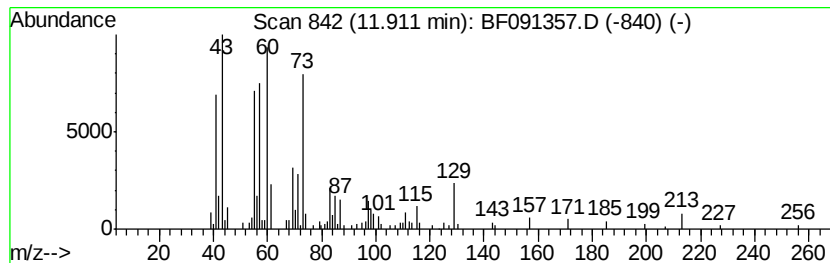
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.91	3.01 ng	204284	Phenanthrene-d10	11.38	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Undecanoic acid	186	C11H22O2	000112-37-8	80
4	Tridecanoic acid	214	C13H26O2	000638-53-9	80
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	72



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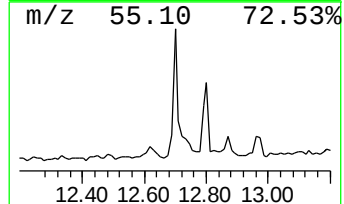
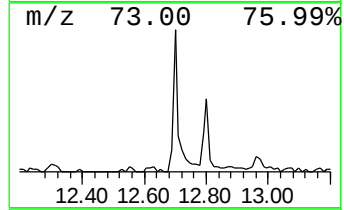
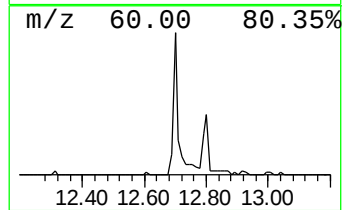
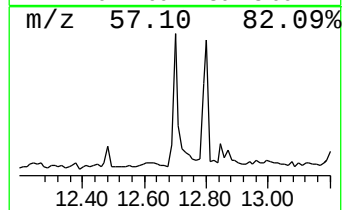
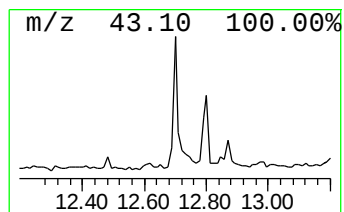
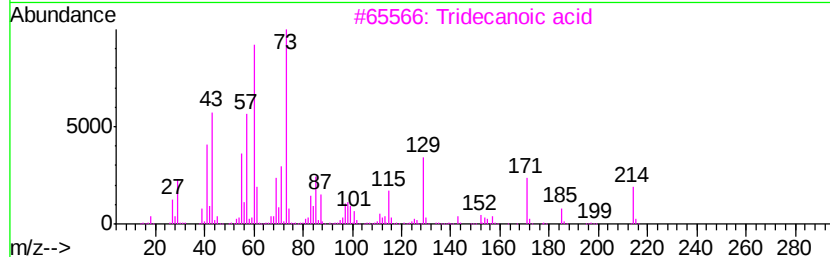
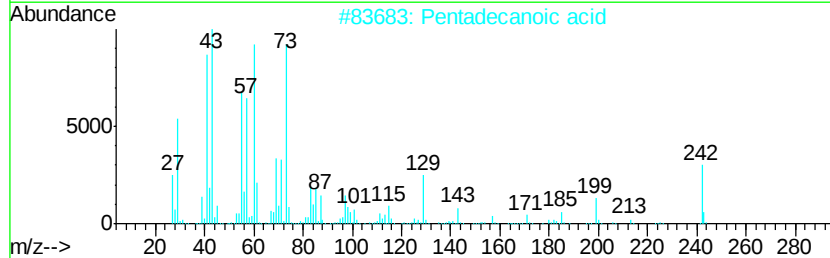
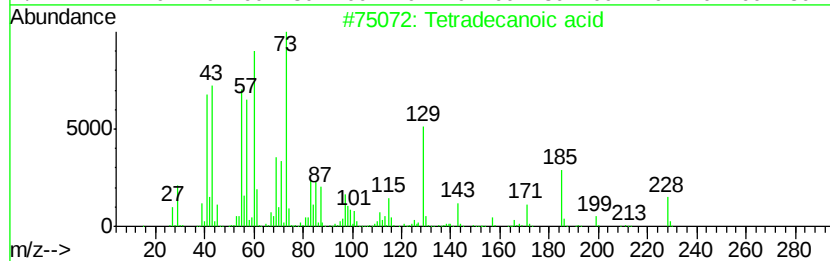
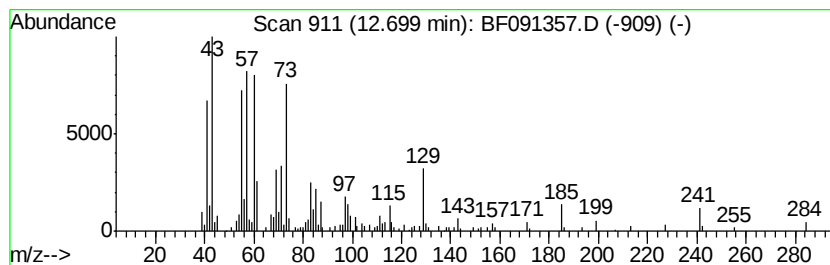
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Peak Number 5 Tetradecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.70	4.48 ng	257661	Chrysene-d12	14.01

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetradecanoic acid	228	C14H28O2	000544-63-8	83
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	80
3		Tridecanoic acid	214	C13H26O2	000638-53-9	80
4		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
5		Undecanoic acid	186	C11H22O2	000112-37-8	62



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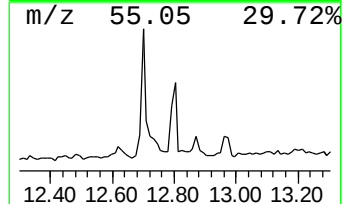
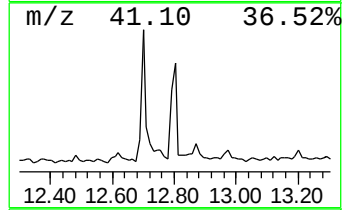
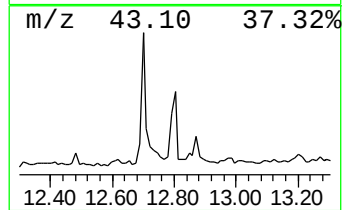
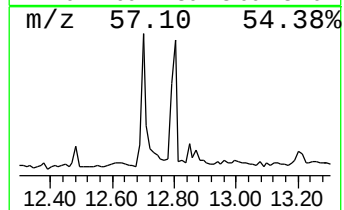
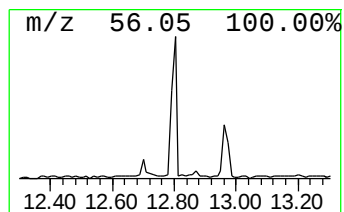
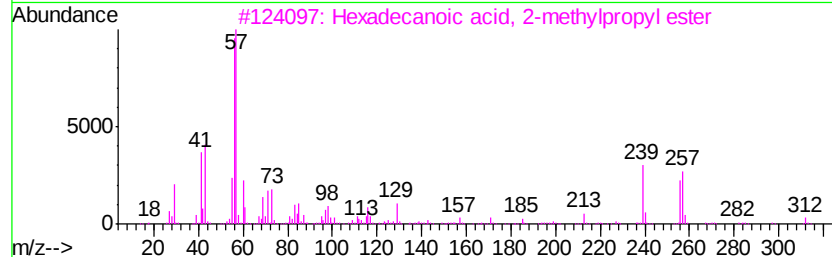
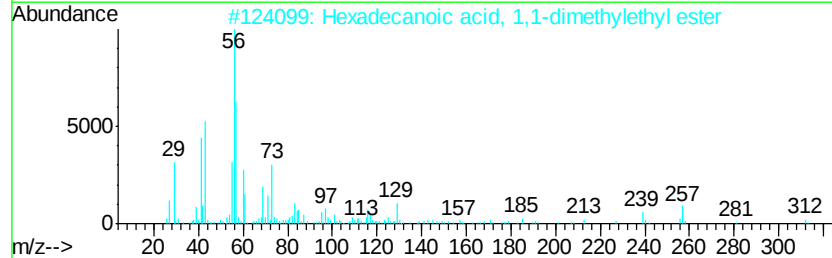
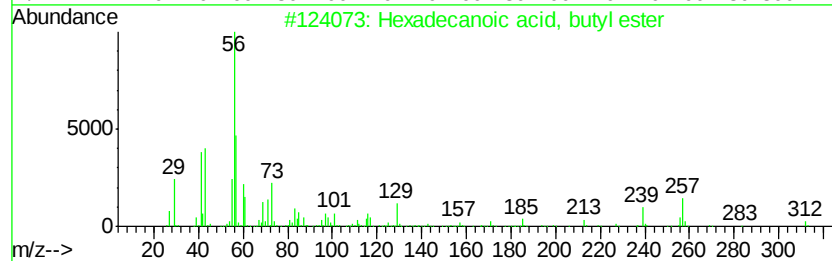
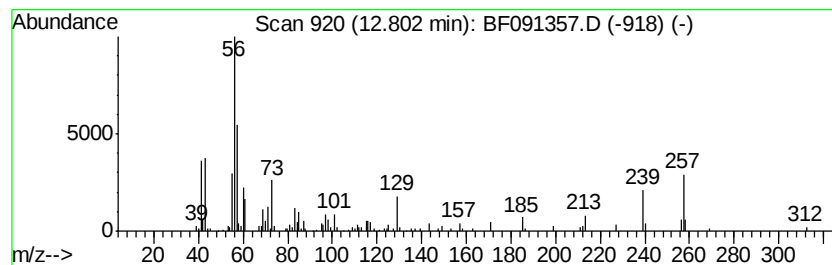
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.80	3.19 ng	183398	Chrysene-d12	14.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	97
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	91
3		Hexadecanoic acid, 2-methylpropyl...	312	C20H40O2	000110-34-9	55
4		Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	38
5		1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	27



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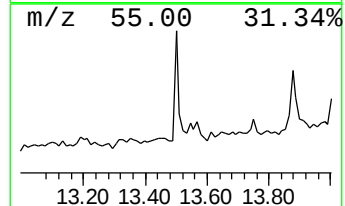
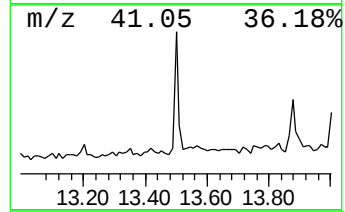
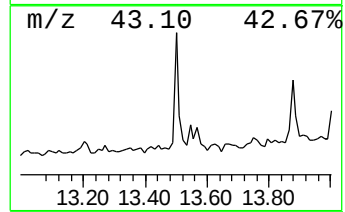
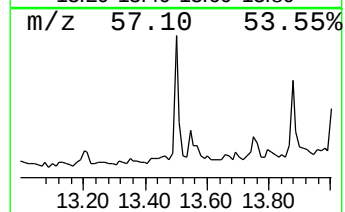
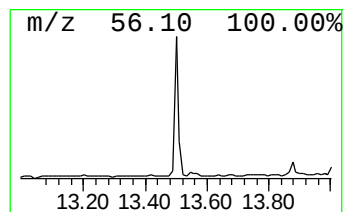
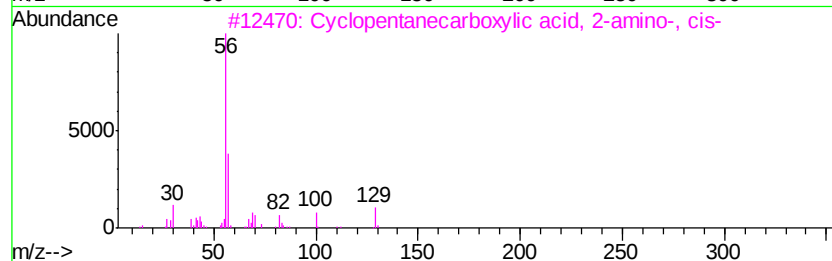
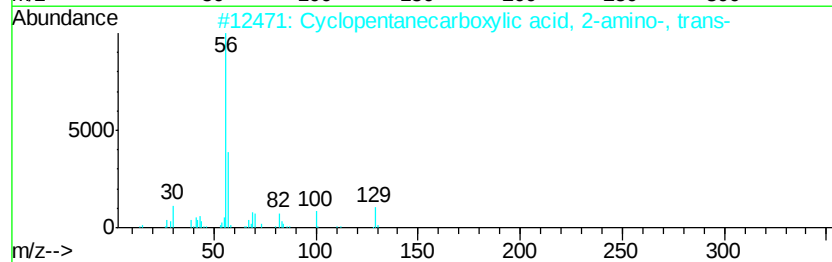
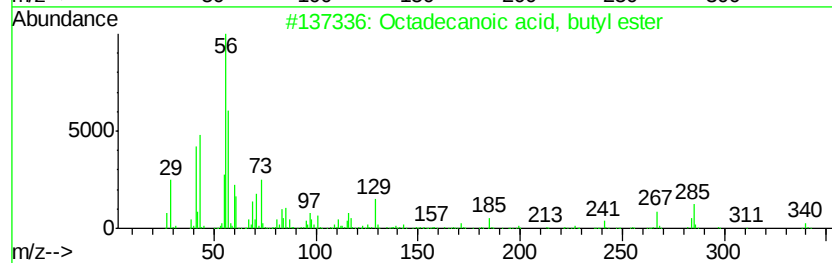
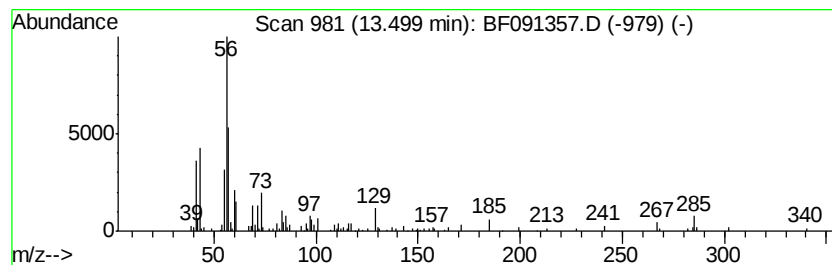
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid, butyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.50	2.51 ng	144118	Chrysene-d12	14.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	92
2		Cyclopentanecarboxylic acid, 2-amino-, trans-	129	C6H11NO2	040482-05-1	47
3		Cyclopentanecarboxylic acid, 2-amino-, cis-	129	C6H11NO2	037910-65-9	47
4		n-Butyl myristate	284	C18H36O2	000110-36-1	43
5		1-Hexene, 2-methyl-	98	C7H14	006094-02-6	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF113016\
Data File : BF091357.D
Acq On : 30 Nov 2016 16:33
Operator : UM/SJ
Sample : H5767-01
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
112216-DSDC-E-D-B

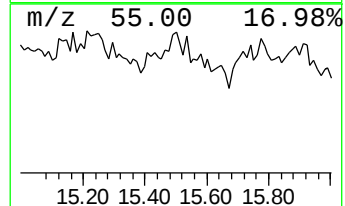
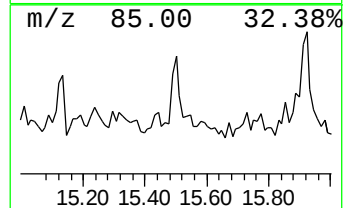
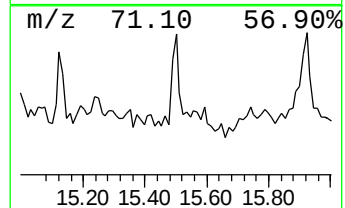
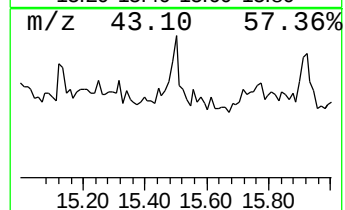
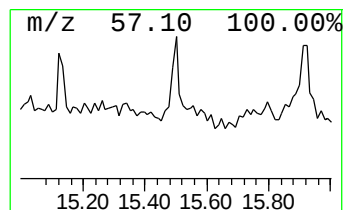
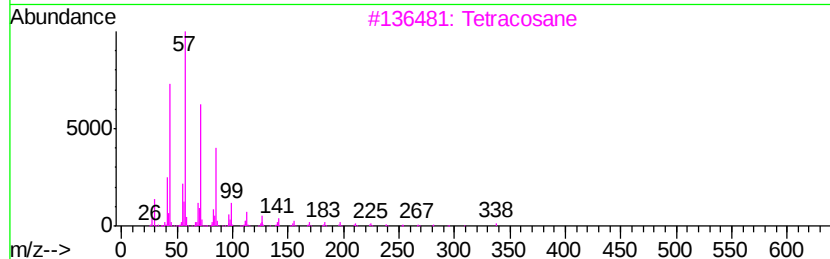
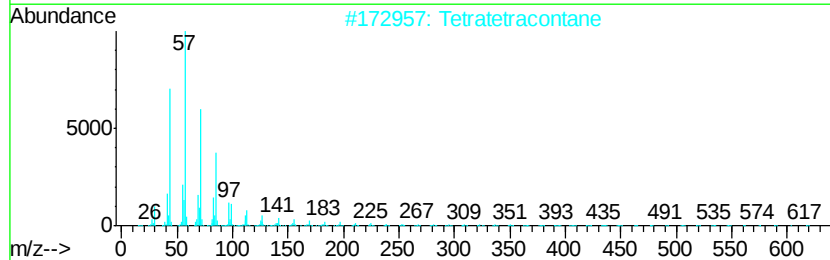
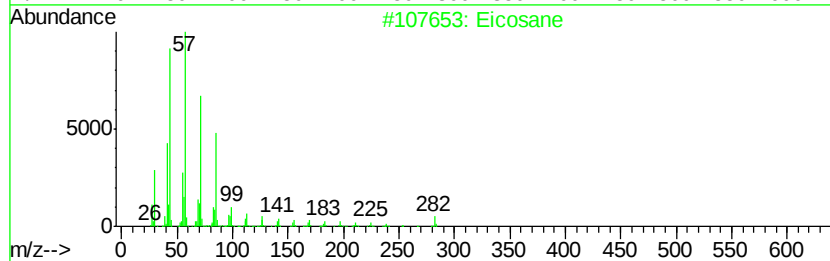
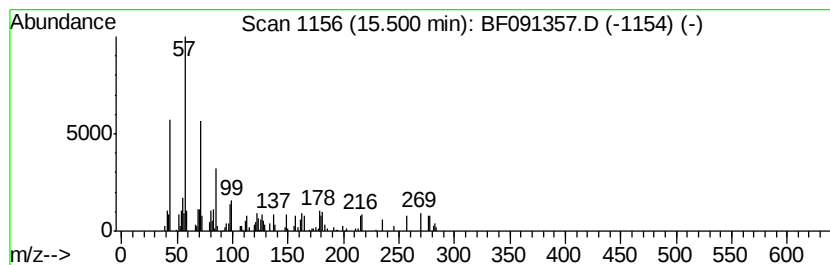
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.50	2.68 ng	139207	Perylene-d12	15.44

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	70
2	Tetratetracontane		619	C44H90	007098-22-8	45
3	Tetracosane		338	C24H50	000646-31-1	43
4	Octacosane		394	C28H58	000630-02-4	43
5	Hexatriacontane		507	C36H74	000630-06-8	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF113016\
Data File : BF091357.D
Acq On : 30 Nov 2016 16:33
Operator : UM/SJ
Sample : H5767-01
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
112216-DSDC-E-D-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.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	10.6	ng	636383	1	6.86	1200550	20.0
unknown6.63	6.63	51.5	ng	3094360	1	6.86	1200550	20.0
n-Hexadecanoic acid	11.91	3.0	ng	204284	4	11.38	1358450	20.0
Tetradecanoic acid	12.70	4.5	ng	257661	5	14.01	1149610	20.0
Hexadecanoic acid...	12.80	3.2	ng	183398	5	14.01	1149610	20.0
Octadecanoic acid...	13.50	2.5	ng	144118	5	14.01	1149610	20.0
Eicosane	15.50	2.7	ng	139207	6	15.44	1039450	20.0