

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091216\
 Data File : BF090065.D
 Acq On : 12 Sep 2016 16:03
 Operator : UM/SJ
 Sample : H4744-01
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-1A

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-BF083116.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	1.713	9	11	70	rVB	6060722	17413656	100.00%	31.453%
2	4.684	269	271	281	rBV	610724	916546	5.26%	1.656%
3	5.153	309	312	314	rBV	3094133	3898378	22.39%	7.041%
4	6.227	403	406	408	rBV	3406142	3676282	21.11%	6.640%
5	6.342	413	416	419	rVV	3851541	3755119	21.56%	6.783%
6	6.570	434	436	439	rBV	769829	953556	5.48%	1.722%
7	6.730	447	450	453	rBV	3180485	2905646	16.69%	5.248%
8	7.142	483	486	489	rBV	2122917	2184465	12.54%	3.946%
9	7.279	494	498	506	rVB	129762	235188	1.35%	0.425%
10	7.862	547	549	551	rBV	1479019	1309261	7.52%	2.365%
11	8.936	641	643	646	rBV	2795254	4097617	23.53%	7.401%
12	9.336	676	678	681	rBV	1059944	1253430	7.20%	2.264%
13	9.610	699	702	704	rBV	1118331	1341920	7.71%	2.424%
14	10.388	767	770	773	rBV	2172104	2281173	13.10%	4.120%
15	11.073	828	830	834	rBV	1199341	1294489	7.43%	2.338%
16	11.325	850	852	856	rBV	262651	290081	1.67%	0.524%
17	12.502	953	955	957	rBV	144656	190870	1.10%	0.345%
18	12.662	966	969	971	rBV	3242583	3448763	19.80%	6.229%
19	13.565	1046	1048	1052	rBV	138434	193913	1.11%	0.350%
20	13.691	1056	1059	1063	rBV	1178486	1505530	8.65%	2.719%
21	14.468	1125	1127	1128	rBV	162178	212734	1.22%	0.384%
22	15.028	1174	1176	1179	rBV	667815	804863	4.62%	1.454%
23	18.377	1464	1469	1474	rVB2	435209	1199697	6.89%	2.167%

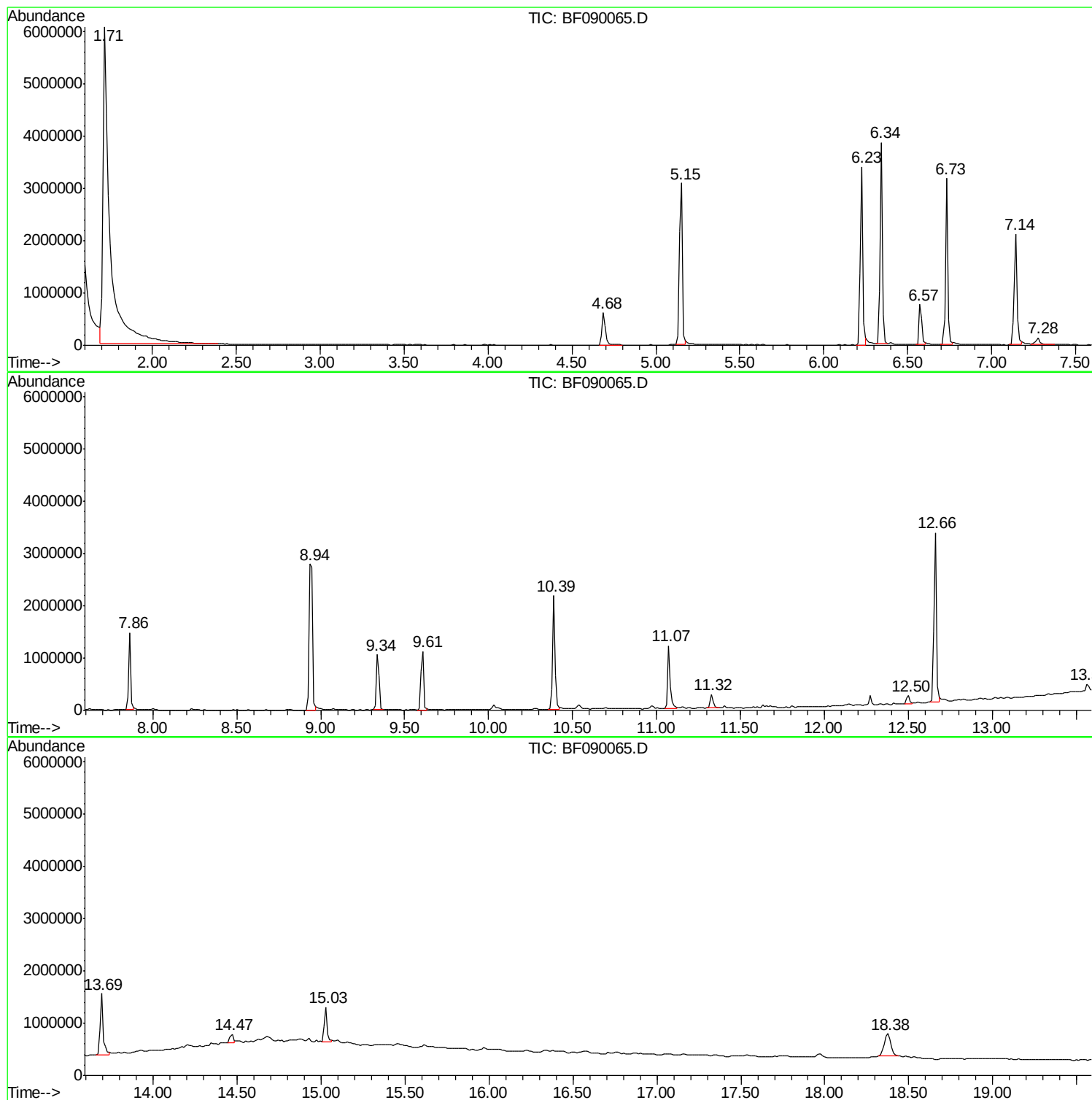
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF083116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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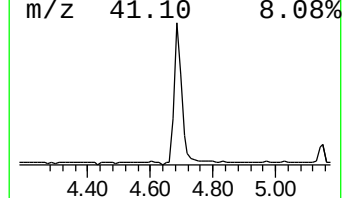
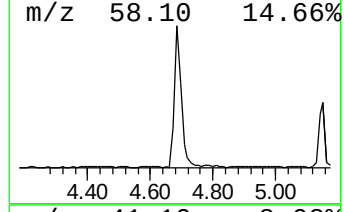
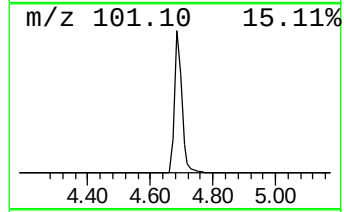
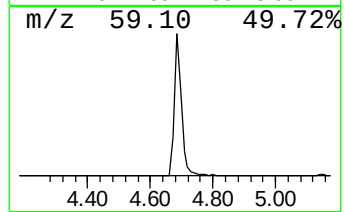
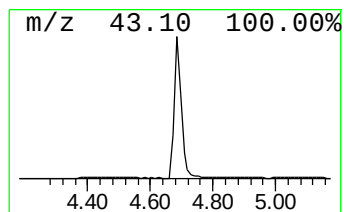
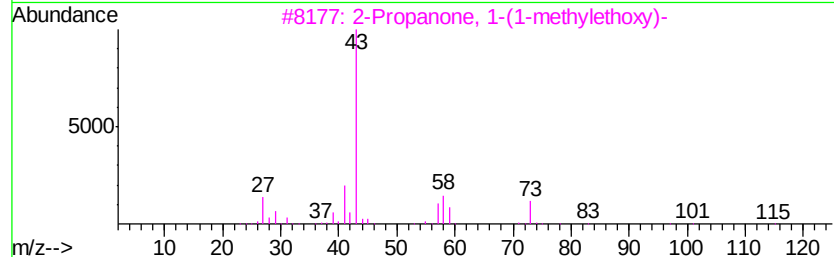
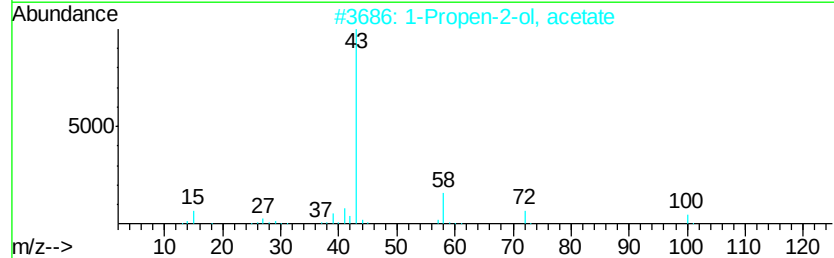
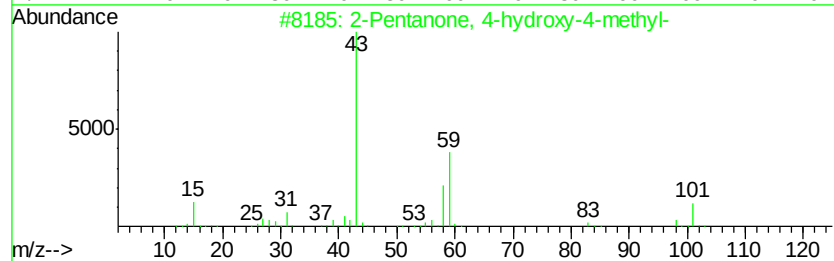
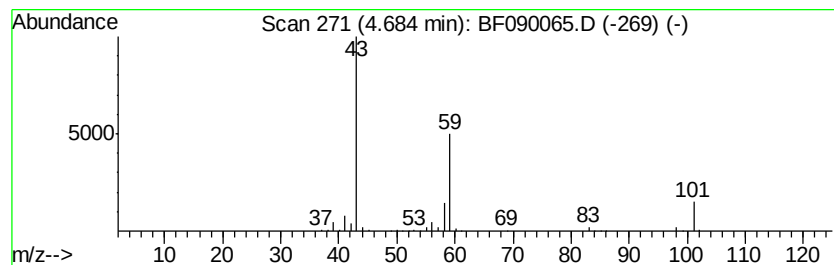
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.68	19.22 ng	916546	1,4-Dichlorobenzene-d4	6.57

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3		2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9
4		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
5		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	7



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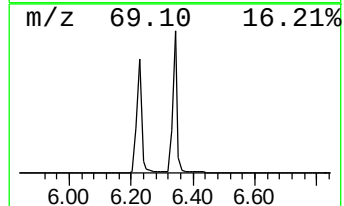
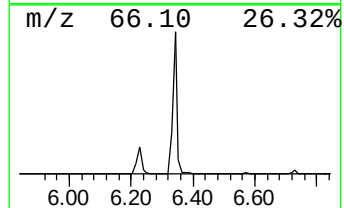
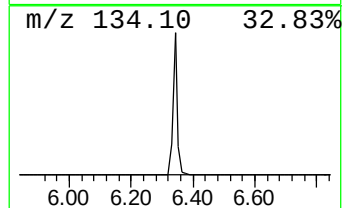
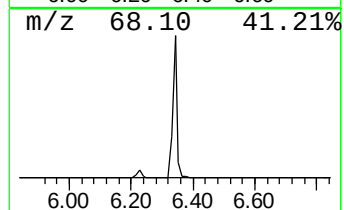
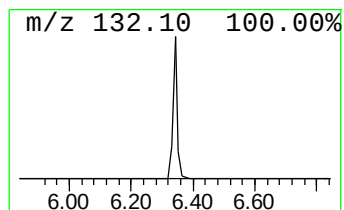
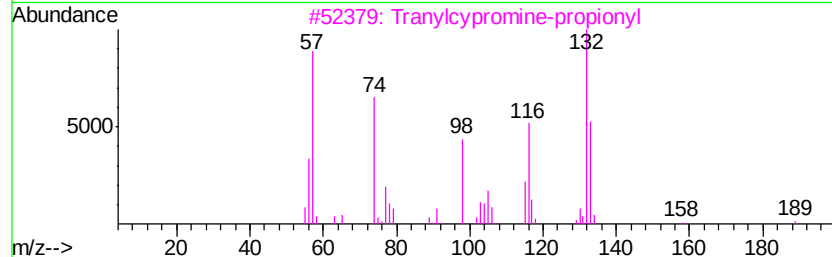
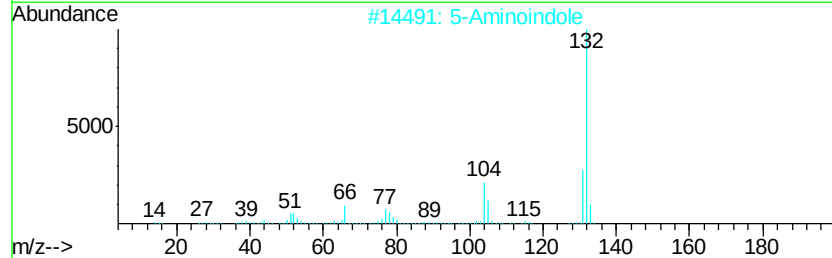
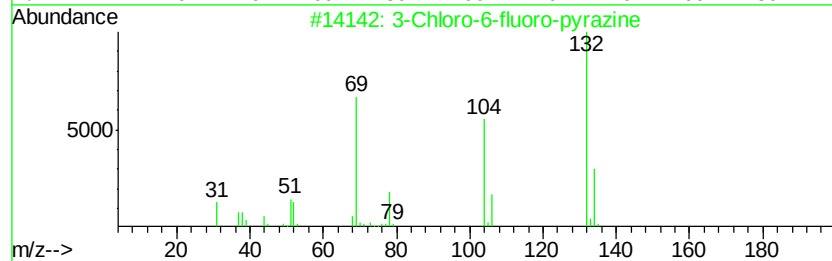
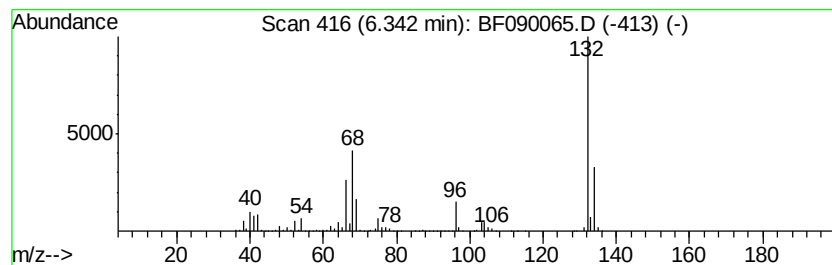
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Peak Number 3 unknown6.34 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.34	78.76 ng	3755120	1,4-Dichlorobenzene-d4	6.57

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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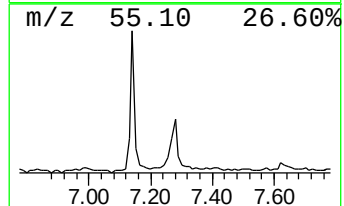
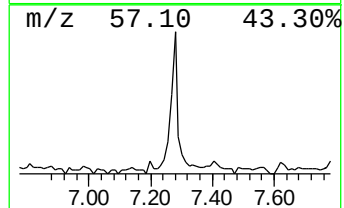
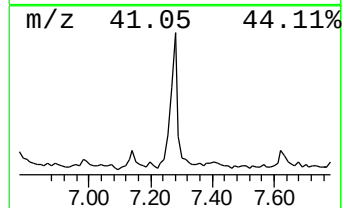
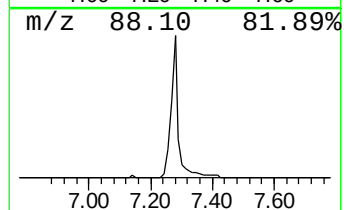
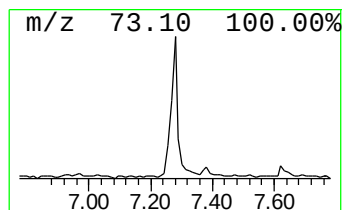
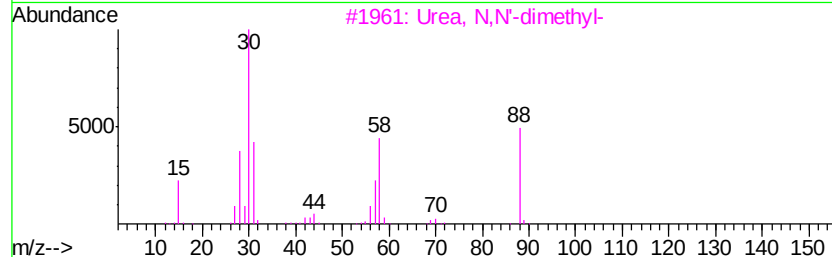
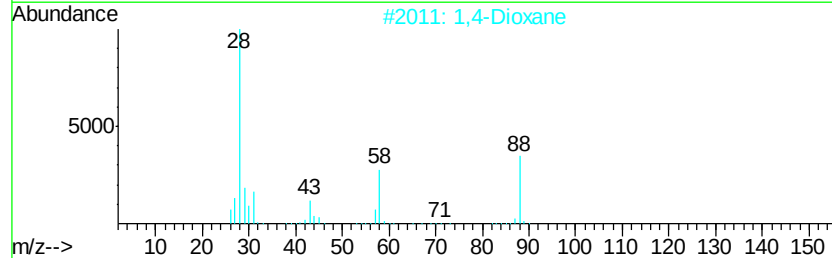
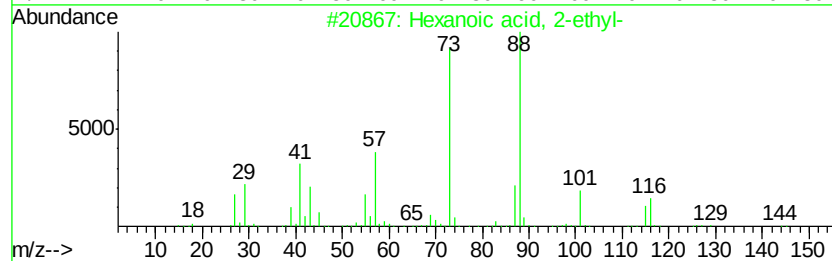
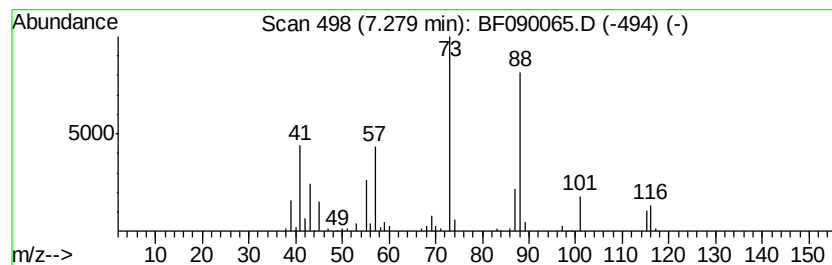
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Peak Number 5 Hexanoic acid, 2-ethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.28	3.59 ng	235188	Naphthalene-d8	7.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2		1,4-Dioxane	88	C4H8O2	000123-91-1	47
3		Urea, N,N'-dimethyl-	88	C3H8N2O	000096-31-1	37
4		Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	36
5		Heptanoic acid, ethyl ester	158	C9H18O2	000106-30-9	36



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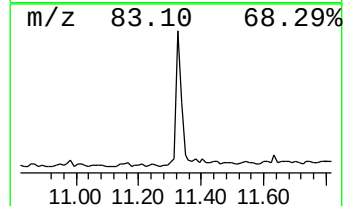
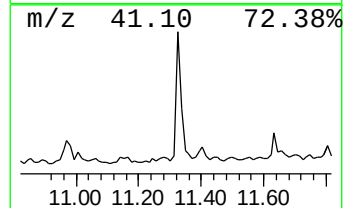
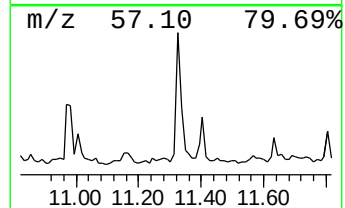
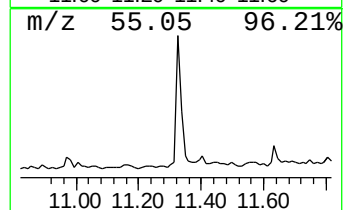
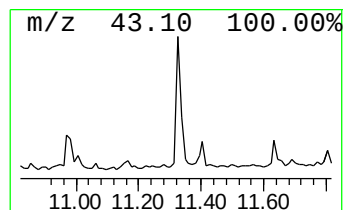
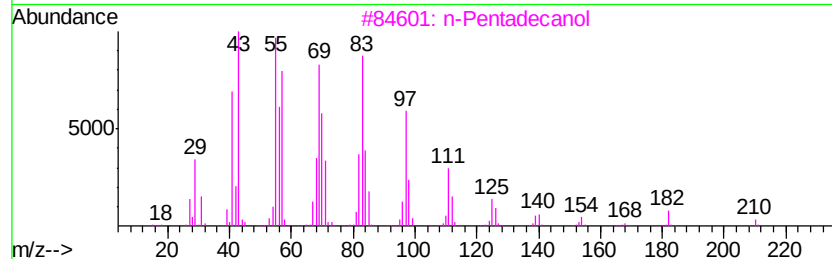
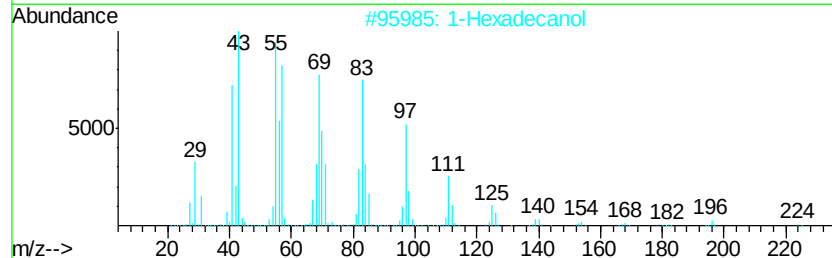
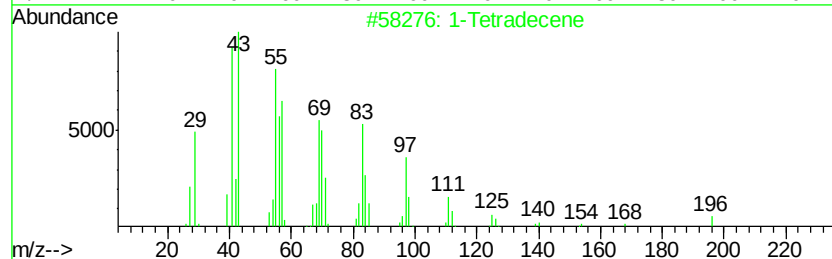
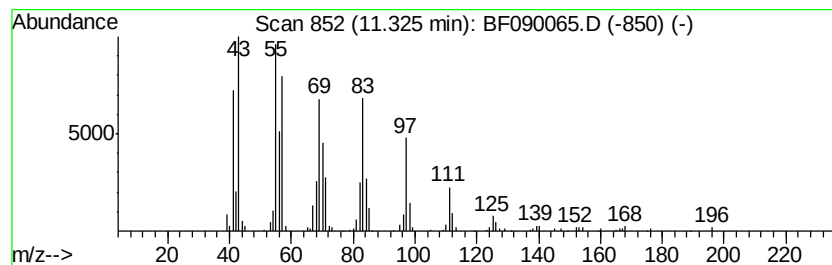
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Peak Number 6 1-Tetradecene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.32	4.48 ng	290081	Phenanthrene-d10		11.07
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tetradecene	196	C14H28	001120-36-1	96
2	1-Hexadecanol	242	C16H34O	036653-82-4	94
3	n-Pentadecanol	228	C15H32O	000629-76-5	91
4	1-Tetradecanol	214	C14H30O	000112-72-1	91
5	n-Tridecan-1-ol	200	C13H28O	000112-70-9	91



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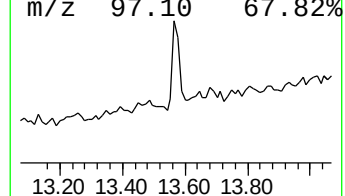
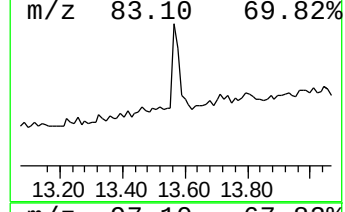
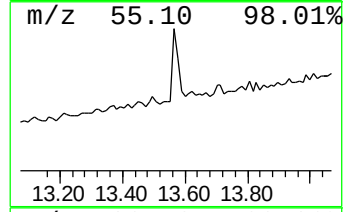
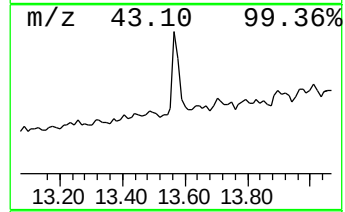
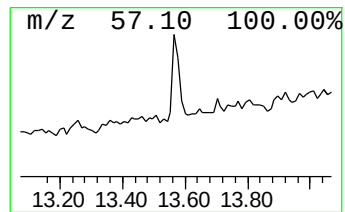
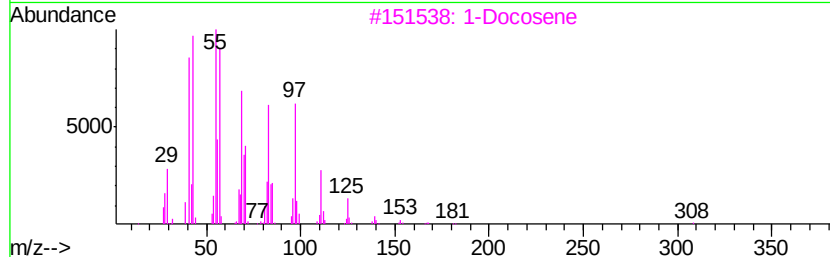
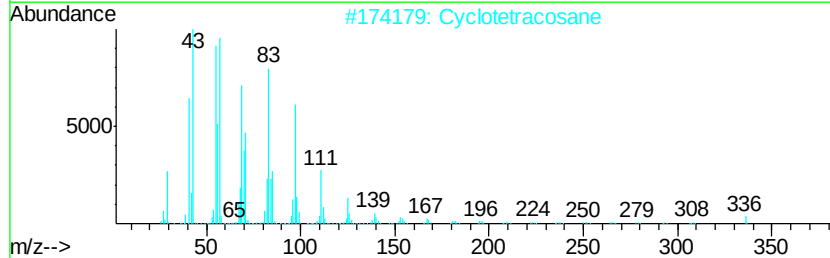
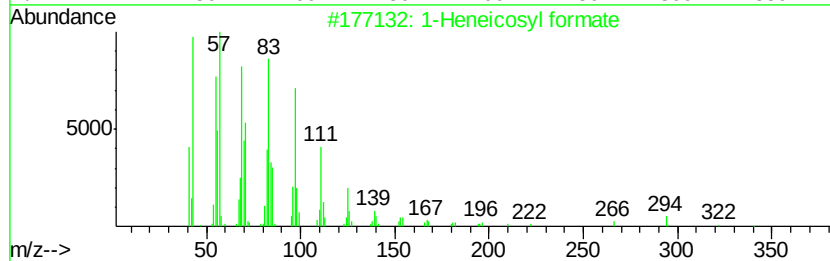
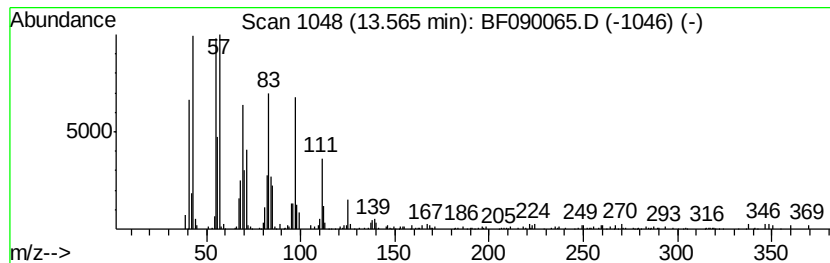
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Peak Number 7 1-Heneicosyl formate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.57	2.58 ng	193913	Chrysene-d12	13.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosyl formate	340	C22H44O2	077899-03-7	96
2	Cyclotetracosane	336	C24H48	000297-03-0	94
3	1-Docosene	308	C22H44	001599-67-3	94
4	Z-12-Pentacosene	350	C25H50	1000131-09-4	93
5	E-15-Heptadecenal	252	C17H32O	1000130-97-9	93



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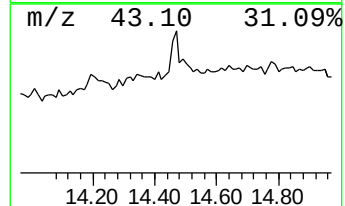
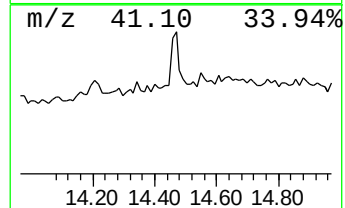
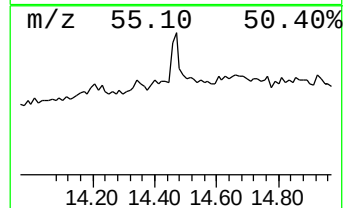
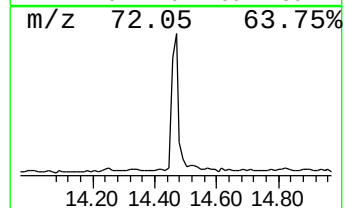
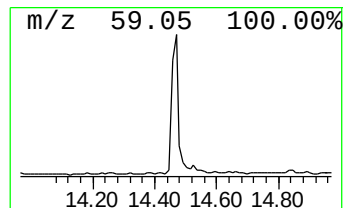
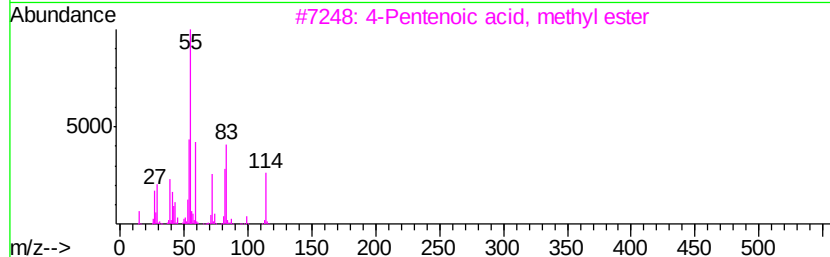
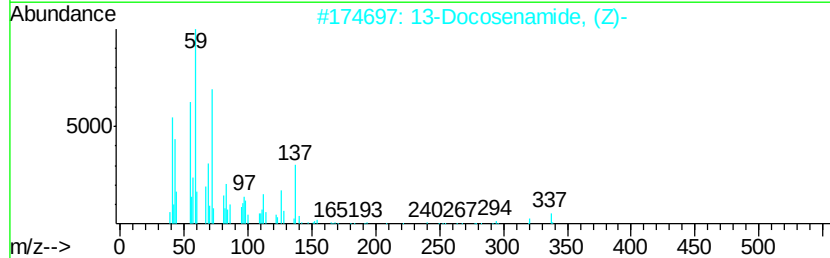
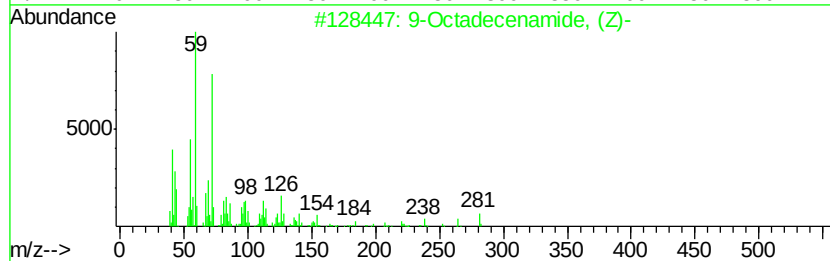
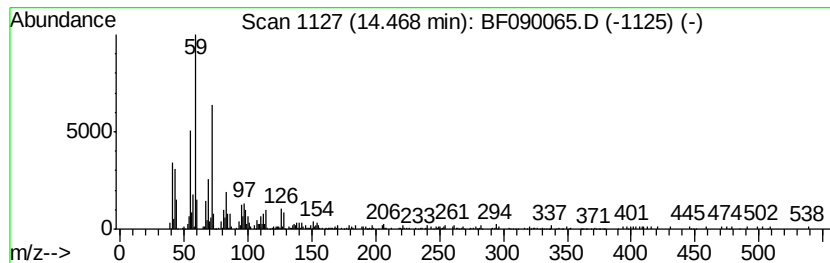
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 9-Octadecenamide, (Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.47	5.29 ng	212734	Perylene-d12	15.03

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2		13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	81
3		4-Pentenoic acid, methyl ester	114	C6H10O2	000818-57-5	80
4		Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	50
5		2-Octanol, 2-methyl-6-methylene-	156	C10H20O	018479-59-9	46



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091216\
Data File : BF090065.D
Acq On : 12 Sep 2016 16:03
Operator : UM/SJ
Sample : H4744-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-1A

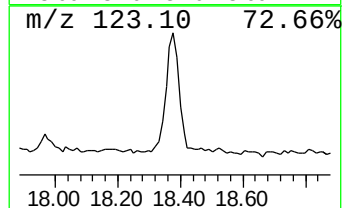
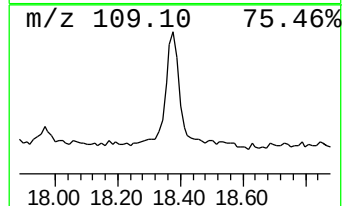
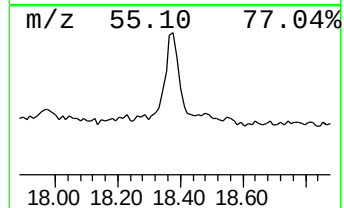
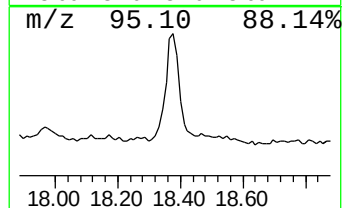
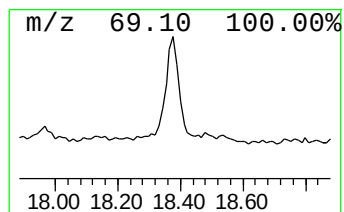
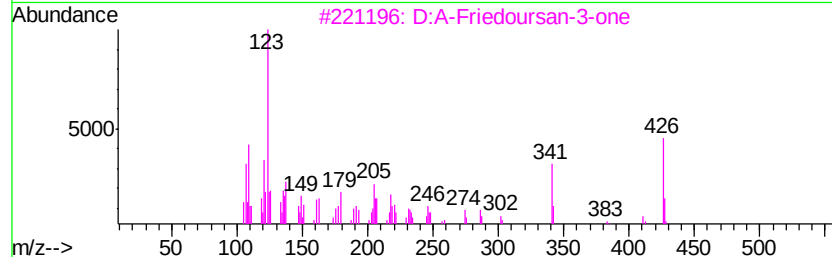
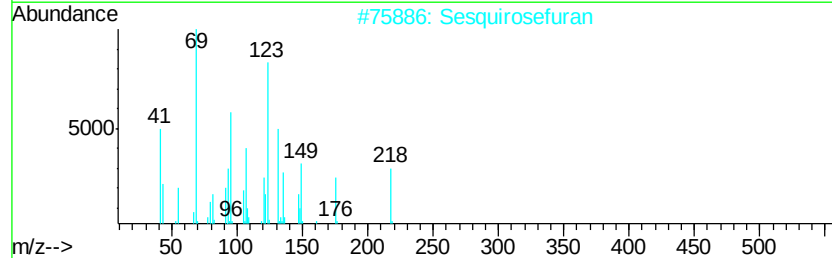
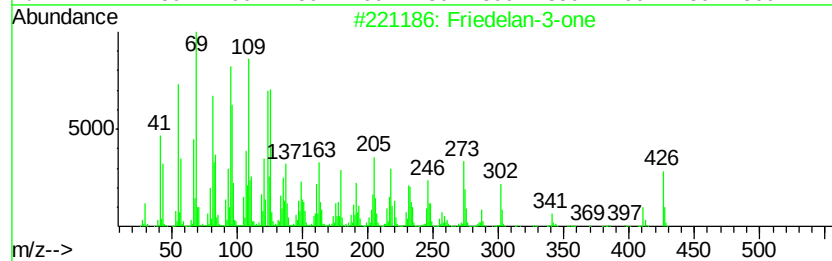
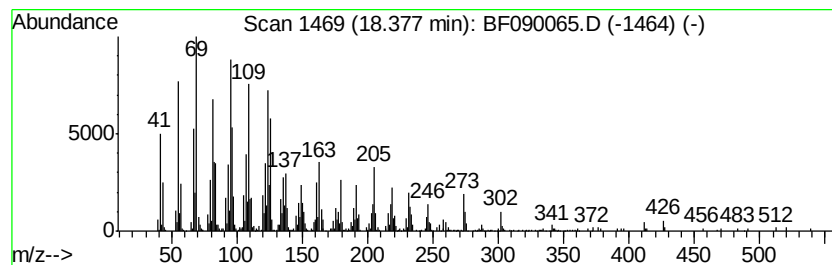
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Friedelan-3-one Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.38	29.81 ng	1199700	Perylene-d12	15.03

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Friedelan-3-one	426	C30H50O	000559-74-0	80
2		Sesquirosefuran	218	C15H22O	039007-93-7	62
3		D:A-Friedoursan-3-one	426	C30H50O	089950-00-5	50
4		7-Tetradecyne	194	C14H26	035216-11-6	50
5		Caparratriene	206	C15H26	1000374-08-7	49



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091216\
Data File : BF090065.D
Acq On : 12 Sep 2016 16:03
Operator : UM/SJ
Sample : H4744-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-1A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF083116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.68	19.2	ng	916546	1	6.57	953556	20.0
unknown6.34	6.34	78.8	ng	3755120	1	6.57	953556	20.0
Hexanoic acid, 2-...	7.28	3.6	ng	235188	2	7.86	1309260	20.0
1-Tetradecene	11.32	4.5	ng	290081	4	11.07	1294490	20.0
1-Heneicosyl formate	13.57	2.6	ng	193913	5	13.69	1505530	20.0
9-Octadecenamide, ...	14.47	5.3	ng	212734	6	15.03	804863	20.0
Friedelan-3-one	18.38	29.8	ng	1199700	6	15.03	804863	20.0