

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011317\
 Data File : BF092261.D
 Acq On : 14 Jan 2017 00:17
 Operator : UM/SJ
 Sample : I1031-07
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMP-0024

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-BF122116.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	4.701	252	255	270	rBV	1405473	2430881	44.53%	5.188%
2	5.170	294	296	313	rVB	4248937	4783681	87.63%	10.209%
3	6.130	377	380	387	rBV	67541	119334	2.19%	0.255%
4	6.244	387	390	392	rBV	4577641	5458814	100.00%	11.650%
5	6.347	396	399	401	rBV	5104340	4848978	88.83%	10.348%
6	6.576	417	419	421	rBV	938507	1012648	18.55%	2.161%
7	6.724	430	432	435	rBV	2836203	3268797	59.88%	6.976%
8	7.147	466	469	471	rBV	2796938	2891955	52.98%	6.172%
9	7.856	529	531	534	rBV	1265947	1364937	25.00%	2.913%
10	8.942	623	626	628	rBV	4591713	4593368	84.15%	9.803%
11	9.342	659	661	663	rBV	732115	626630	11.48%	1.337%
12	9.605	682	684	687	rBV	1405826	1479420	27.10%	3.157%
13	10.028	715	721	722	rBV	53843	62115	1.14%	0.133%
14	10.062	722	724	725	rVB	93182	100618	1.84%	0.215%
15	10.393	751	753	756	rBV2	2145469	2788429	51.08%	5.951%
16	10.530	763	765	769	rVB	151976	186303	3.41%	0.398%
17	10.976	802	804	805	rBV	158814	151870	2.78%	0.324%
18	11.079	811	813	816	rBV	1080918	1472365	26.97%	3.142%
19	11.399	839	841	843	rBV	147873	126153	2.31%	0.269%
20	11.639	860	862	866	rVB2	197927	196169	3.59%	0.419%
21	12.291	917	919	921	rBV	112534	100788	1.85%	0.215%
22	12.508	935	938	941	rVB2	162627	229256	4.20%	0.489%
23	12.668	949	952	955	rBV	3406062	3890151	71.26%	8.302%
24	13.582	1029	1032	1041	rBV2	275548	437503	8.01%	0.934%
25	13.708	1041	1043	1048	rVV	1345032	1379358	25.27%	2.944%
26	14.211	1085	1087	1093	rVB2	71579	125252	2.29%	0.267%
27	14.622	1121	1123	1125	rBV	73389	69442	1.27%	0.148%
28	14.702	1128	1130	1135	rVB	49135	89253	1.64%	0.190%
29	14.782	1135	1137	1138	rBV	69982	83964	1.54%	0.179%
30	15.068	1159	1162	1164	rBV	724686	964724	17.67%	2.059%
31	15.102	1164	1165	1169	rVB	53525	61955	1.13%	0.132%
32	15.468	1194	1197	1199	rBV	89762	132029	2.42%	0.282%
33	15.514	1199	1201	1204	rVV2	34422	61871	1.13%	0.132%
34	15.880	1230	1233	1237	rVB	40427	67408	1.23%	0.144%

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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-BF122116.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	16.108	1251	1253	1260	rVB6	27402	54934	1.01%	0.117%
36	16.302	1265	1270	1272	rBV2	37309	86763	1.59%	0.185%
37	16.360	1272	1275	1276	rVV	52298	99264	1.82%	0.212%
38	16.405	1276	1279	1284	rVV4	83645	221289	4.05%	0.472%
39	16.497	1284	1287	1288	rVV	69754	133208	2.44%	0.284%
40	16.542	1288	1291	1297	rVB	106066	232811	4.26%	0.497%
41	16.760	1306	1310	1315	rBV5	56939	140643	2.58%	0.300%
42	16.920	1321	1324	1330	rVB2	22878	60192	1.10%	0.128%
43	17.263	1352	1354	1357	rBV3	33963	84730	1.55%	0.181%
44	17.583	1380	1382	1388	rVB4	26837	88258	1.62%	0.188%

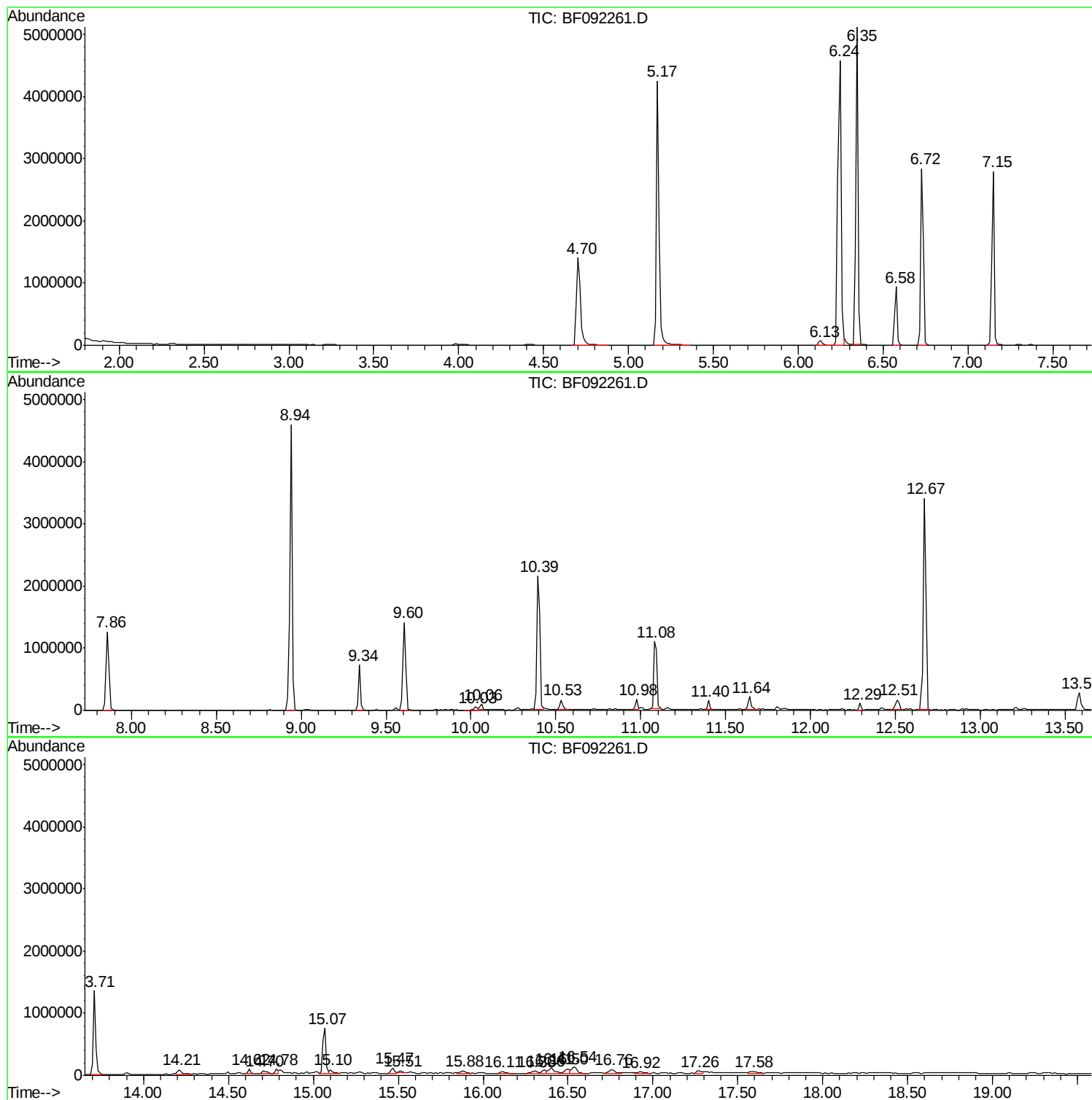
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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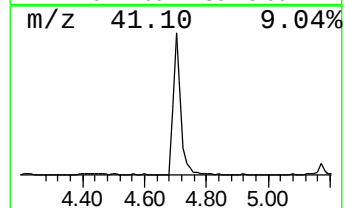
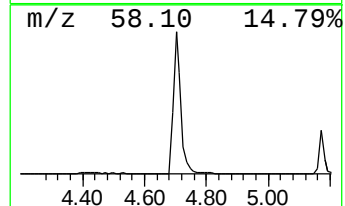
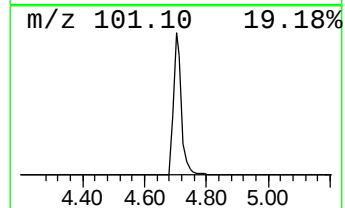
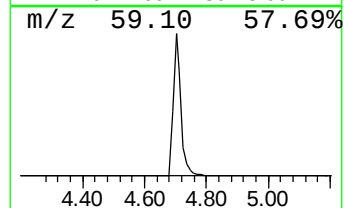
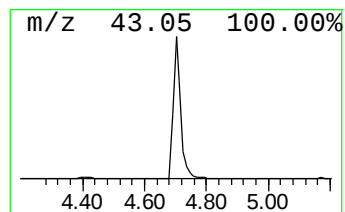
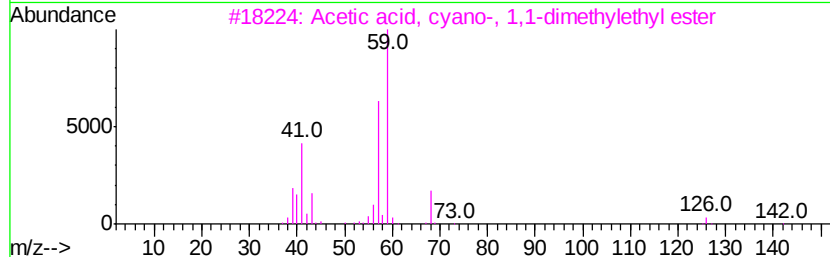
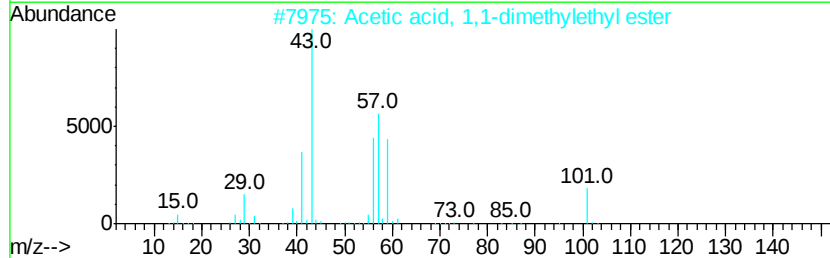
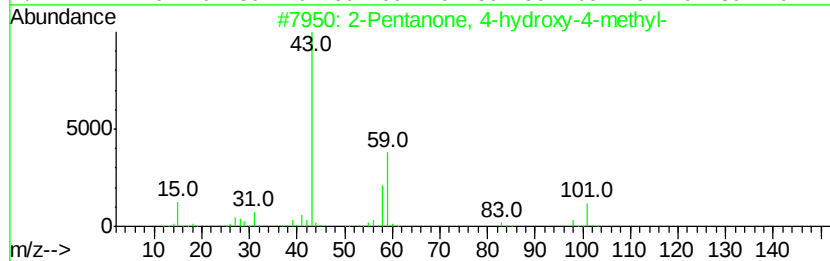
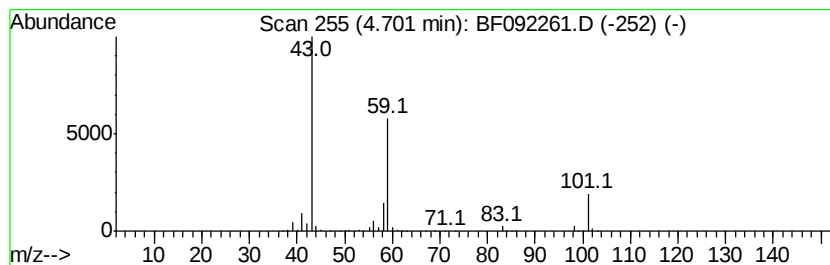
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.70	48.01 ng	2430880	1,4-Dichlorobenzene-d4	6.58

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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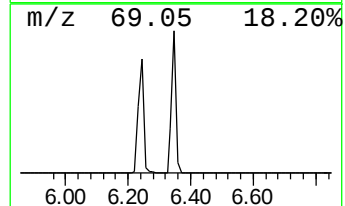
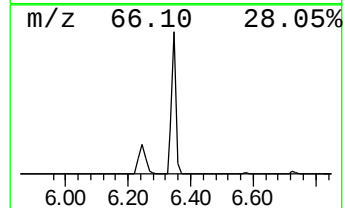
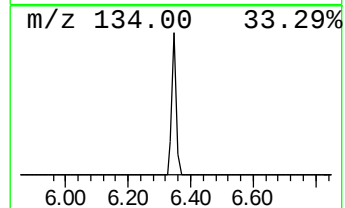
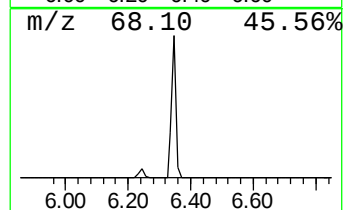
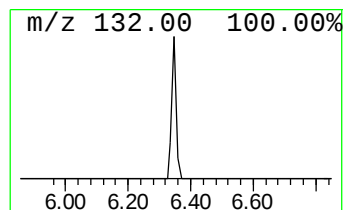
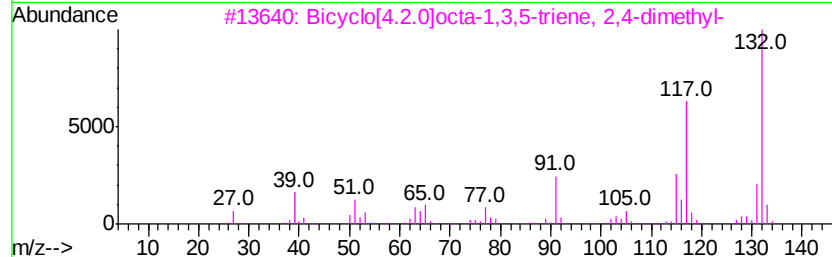
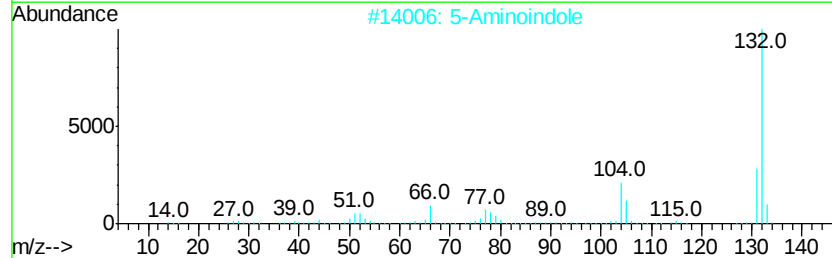
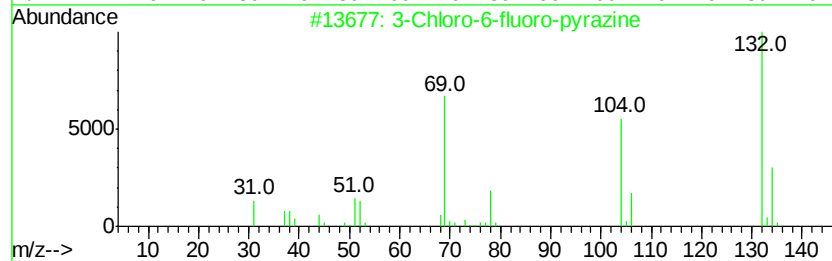
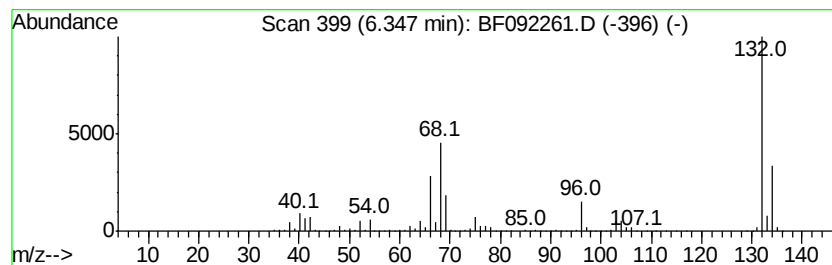
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Peak Number 2 unknown6.35 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.35	95.77 ng	4848980	1,4-Dichlorobenzene-d4	6.58

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		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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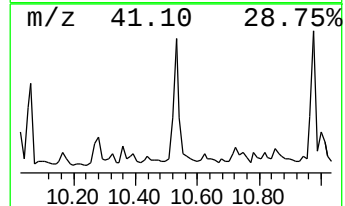
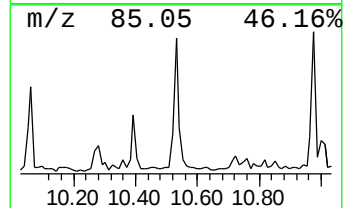
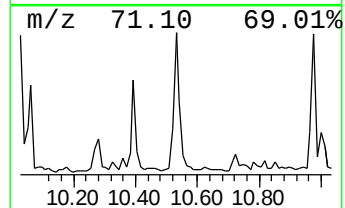
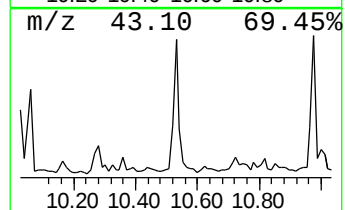
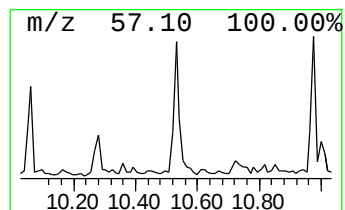
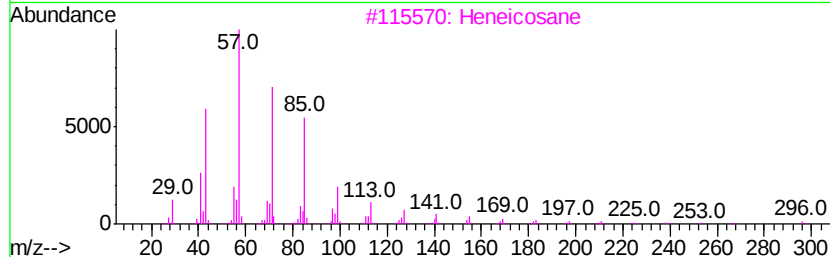
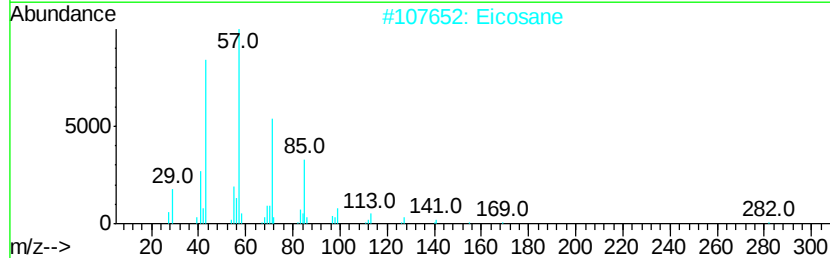
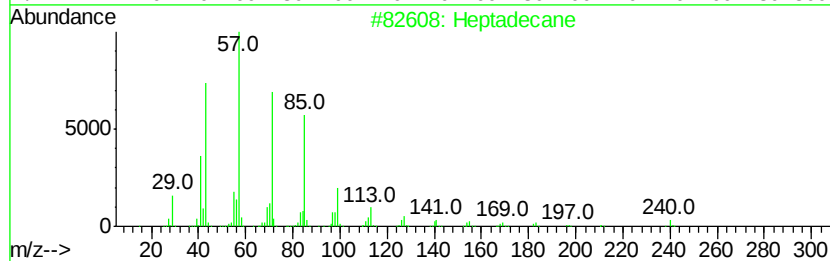
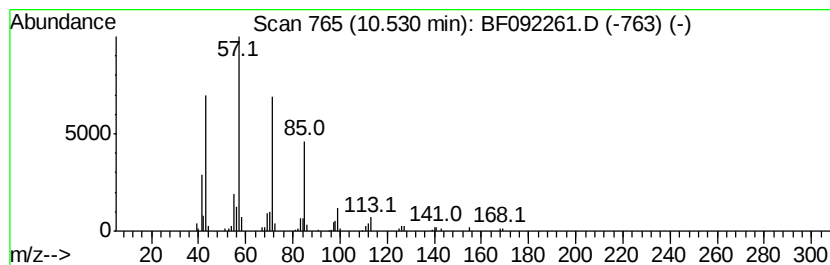
Instrument :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Heptadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD		R.T.	
10.53	2.53 ng	186303	Phenanthrene-d10		11.09	
Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecane	240	C17H36	000629-78-7	91
2		Eicosane	282	C20H42	000112-95-8	91
3		Heneicosane	296	C21H44	000629-94-7	90
4		Heptacosane	380	C27H56	000593-49-7	90
5		Tetradecane	198	C14H30	000629-59-4	87



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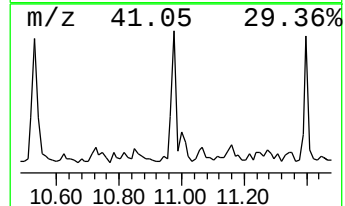
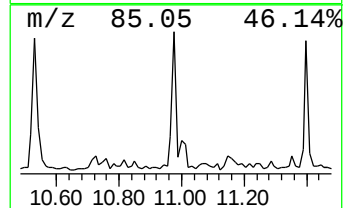
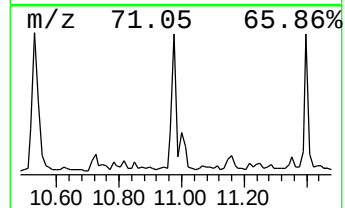
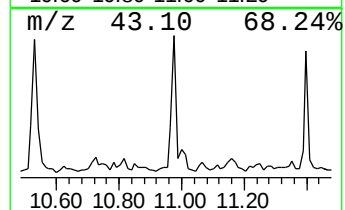
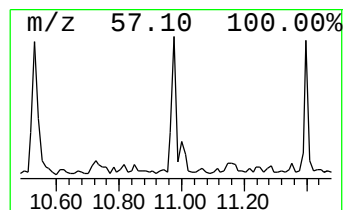
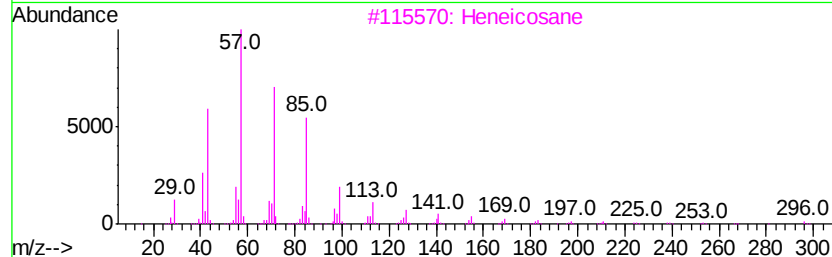
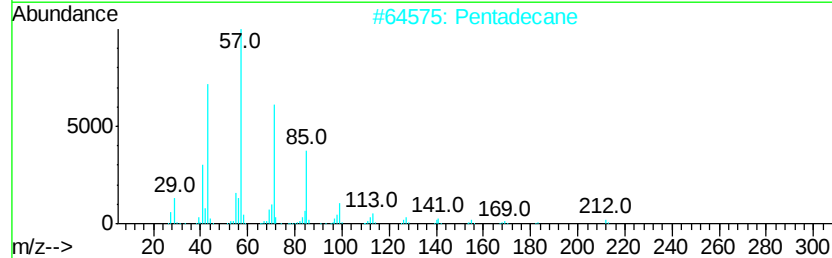
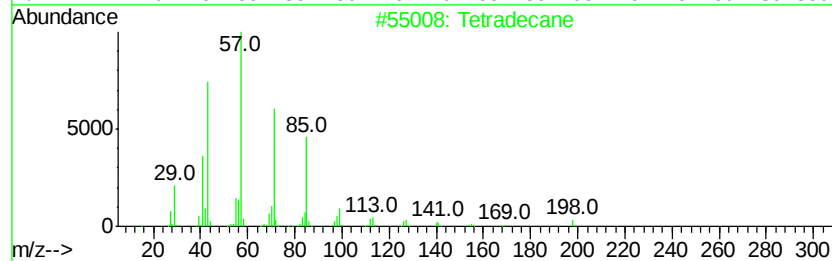
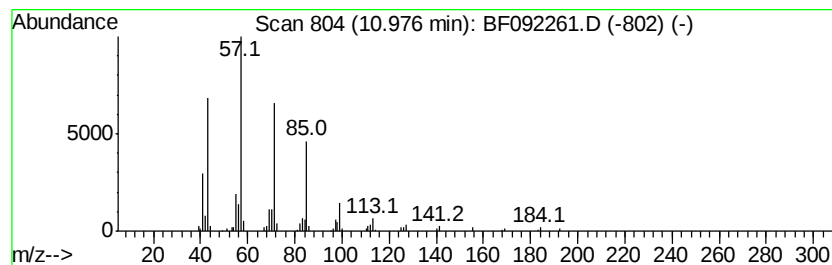
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Tetradecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.98	2.06 ng	151870	Phenanthrene-d10	11.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetradecane	198	C14H30	000629-59-4	91
2		Pentadecane	212	C15H32	000629-62-9	90
3		Heneicosane	296	C21H44	000629-94-7	90
4		Nonadecane	268	C19H40	000629-92-5	87
5		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	87



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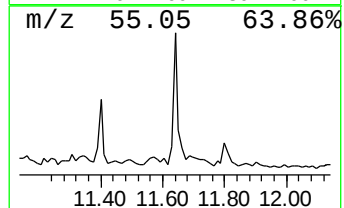
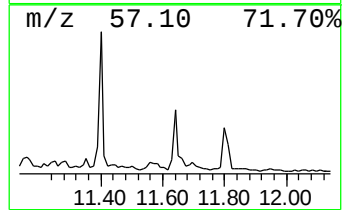
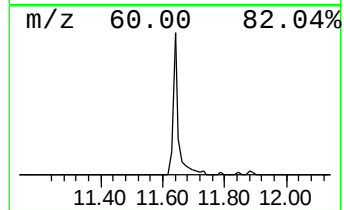
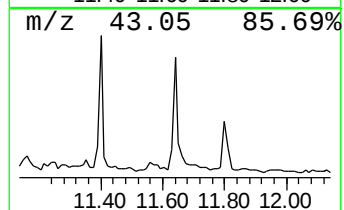
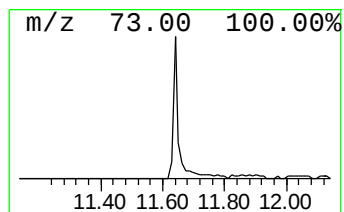
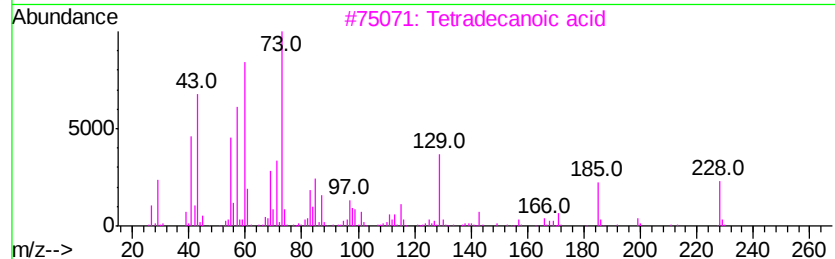
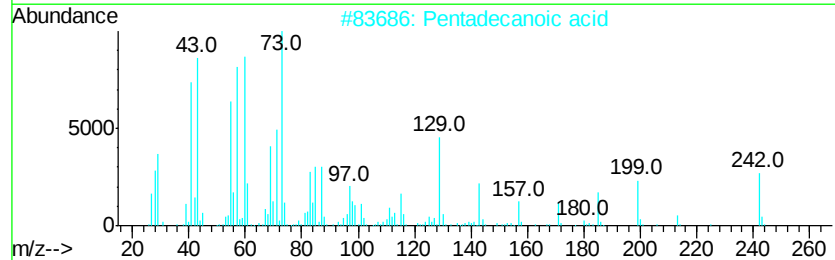
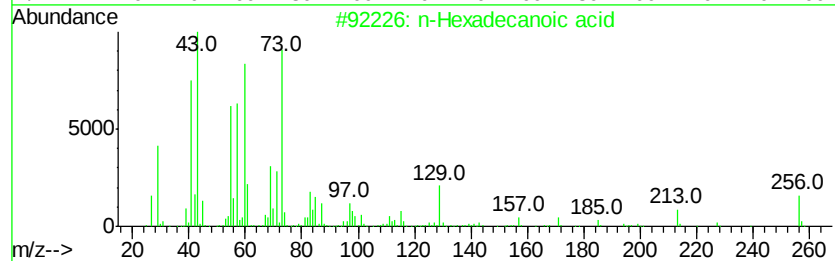
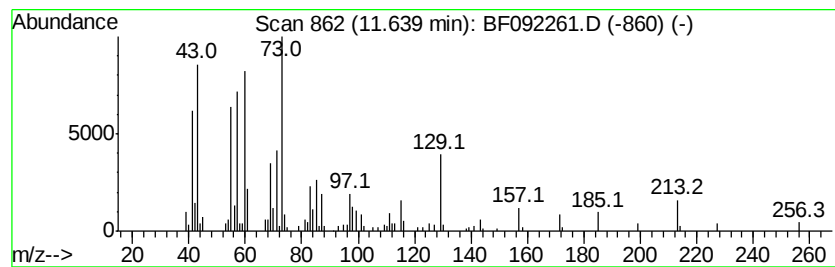
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Peak Number 6 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.64	2.66 ng	196169	Phenanthrene-d10		11.09
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
4	Tridecanoic acid	214	C13H26O2	000638-53-9	81
5	n-Decanoic acid	172	C10H20O2	000334-48-5	81



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011317\
Data File : BF092261.D
Acq On : 14 Jan 2017 00:17
Operator : UM/SJ
Sample : I1031-07
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-0024

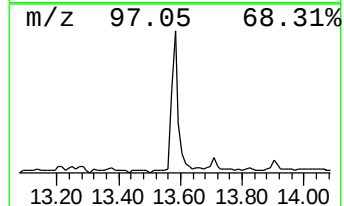
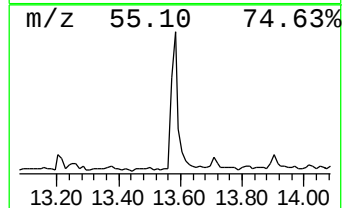
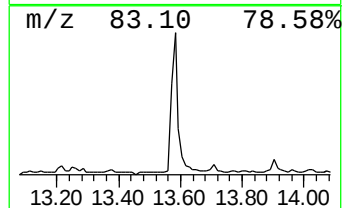
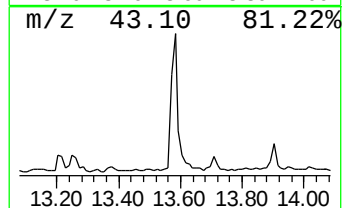
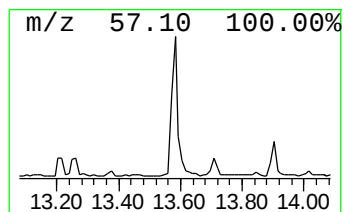
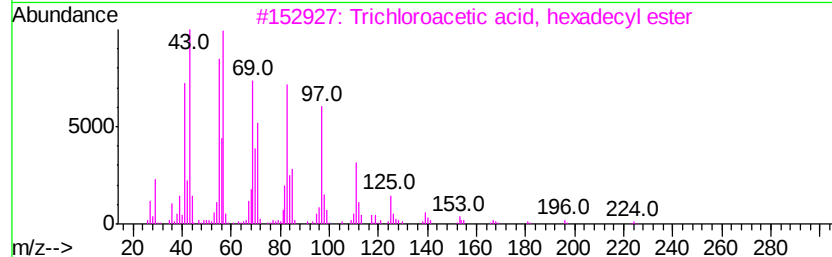
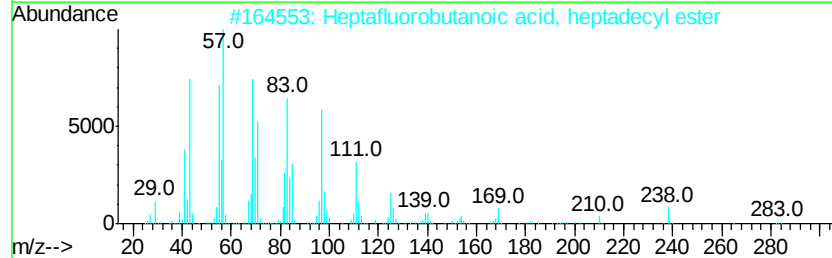
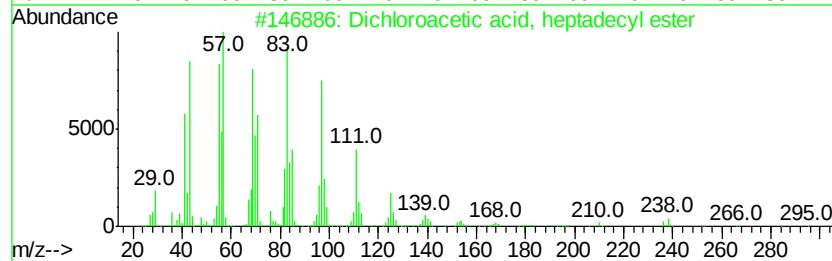
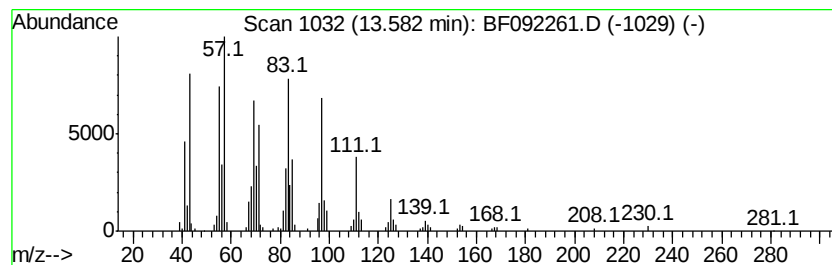
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Dichloroacetic acid, heptad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.58	6.34 ng	437503	Chrysene-d12	13.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
2			Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	94
3			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4			1-Docosene	308	C22H44	001599-67-3	91
5			Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011317\
Data File : BF092261.D
Acq On : 14 Jan 2017 00:17
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Misc :
ALS Vial : 22 Sample Multiplier: 1

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ClientSampleId :
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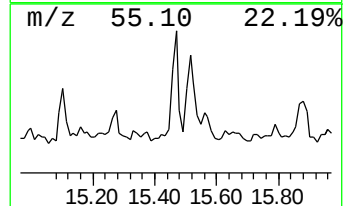
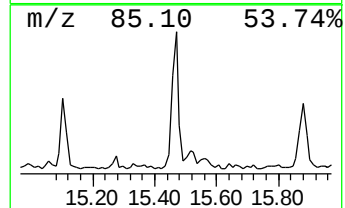
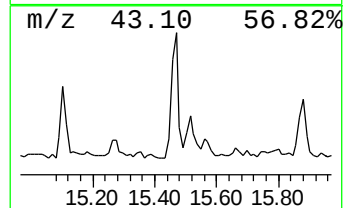
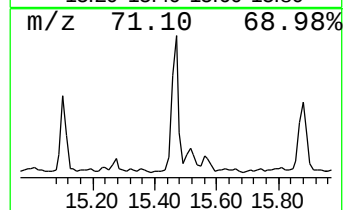
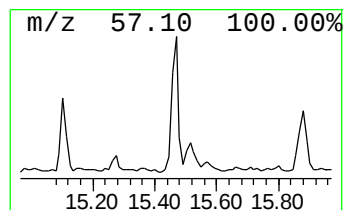
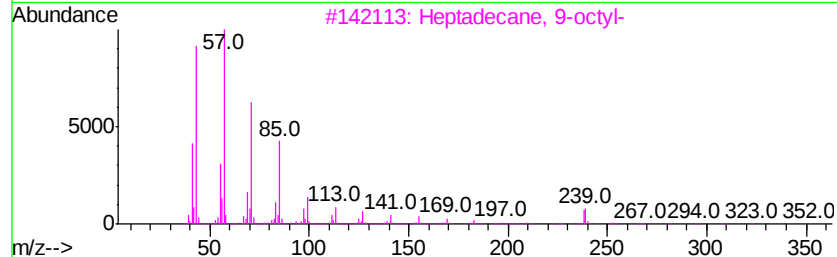
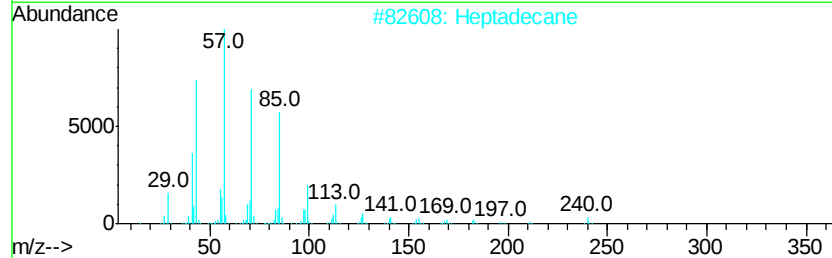
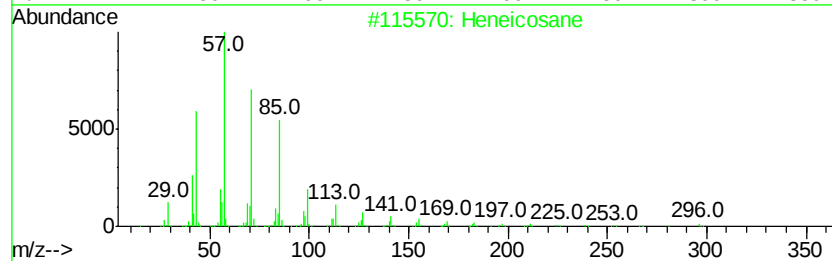
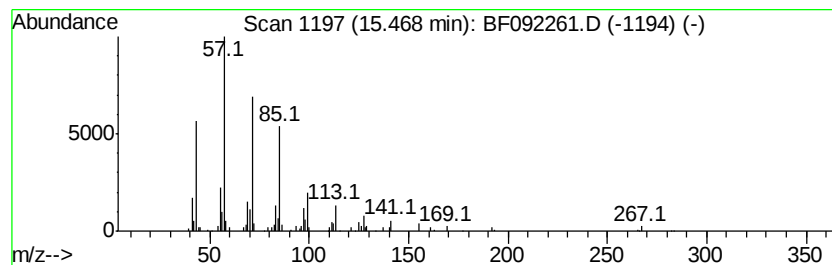
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heneicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.47	2.74 ng	132029	Perylene-d12	15.07

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Heptadecane		240	C17H36	000629-78-7	87
3	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	86
4	Pentacosane		352	C25H52	000629-99-2	86
5	Octacosane		394	C28H58	000630-02-4	86



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011317\
Data File : BF092261.D
Acq On : 14 Jan 2017 00:17
Operator : UM/SJ
Sample : I1031-07
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
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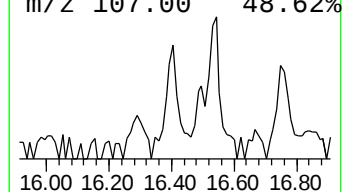
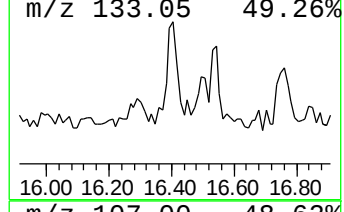
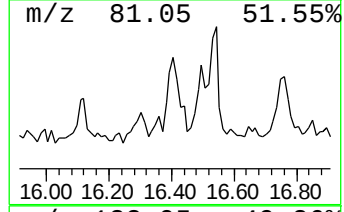
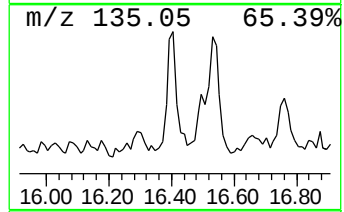
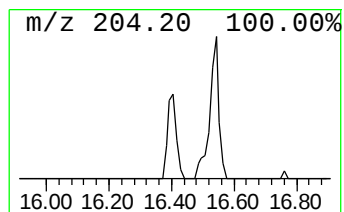
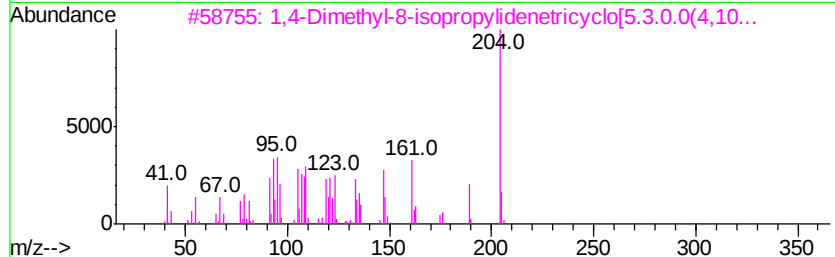
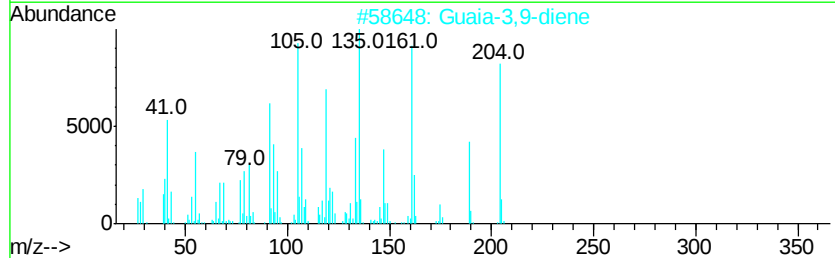
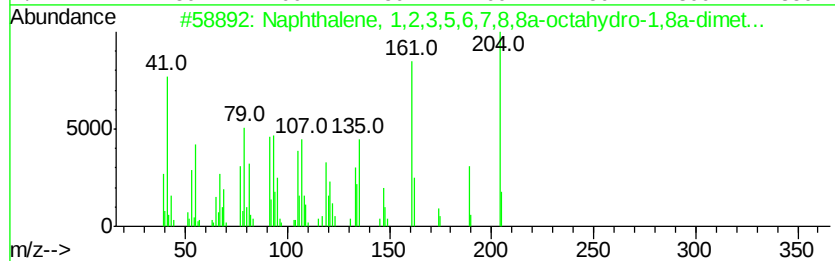
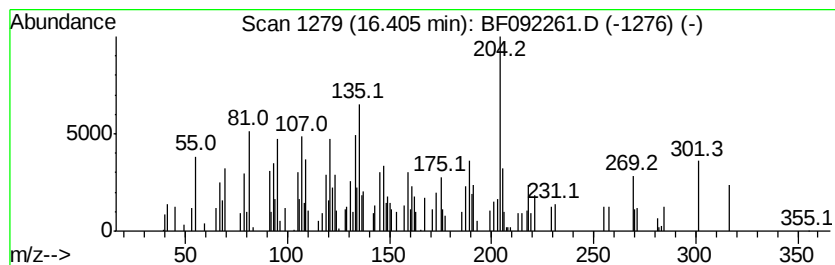
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown16.41 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.41	4.59 ng	221289	Perylene-d12	15.07

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	004630-07-3	47
2			Guaia-3,9-diene	204	C15H24	000489-83-8	46
3			1,4-Dimethyl-8-isopropylidenetri...	204	C15H24	1000140-07-7	45
4			1,2,4,8-Tetramethylbicyclo[6.3.0...	204	C15H24	137235-51-9	43
5			1H-Cycloprop[e]azulene, 1a,2,3,4...	204	C15H24	000489-40-7	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011317\
Data File : BF092261.D
Acq On : 14 Jan 2017 00:17
Operator : UM/SJ
Sample : I1031-07
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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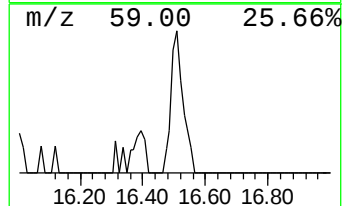
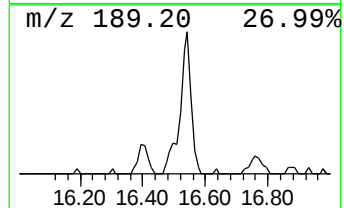
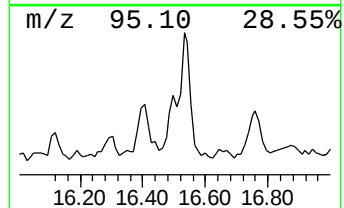
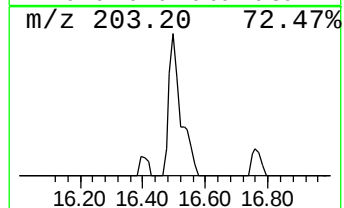
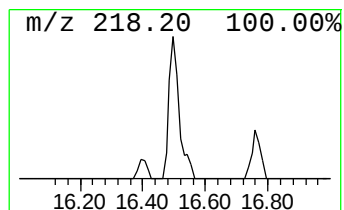
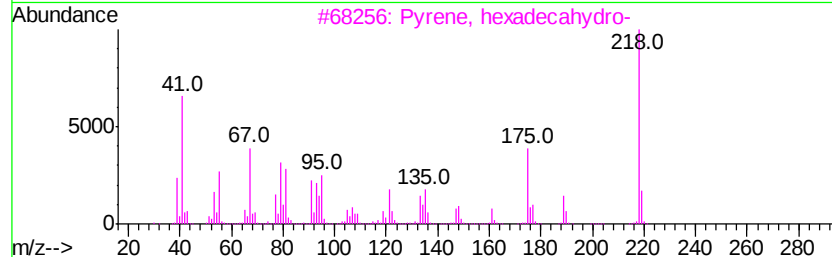
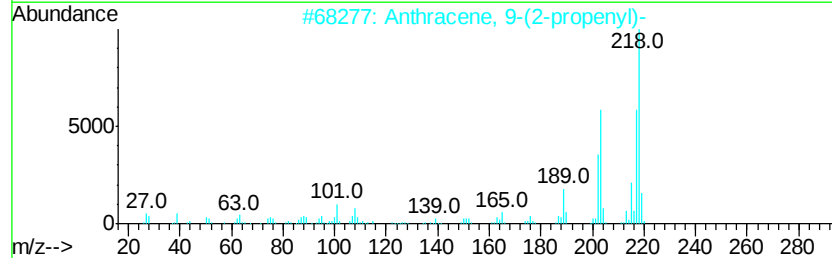
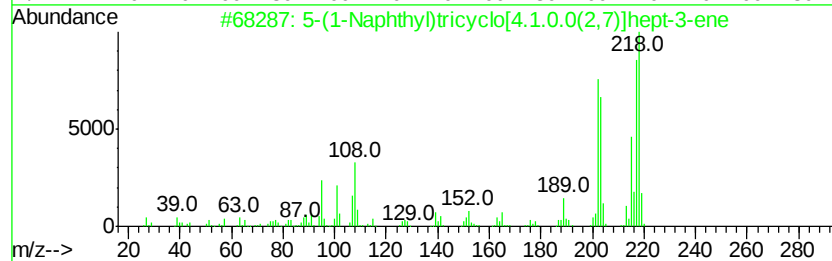
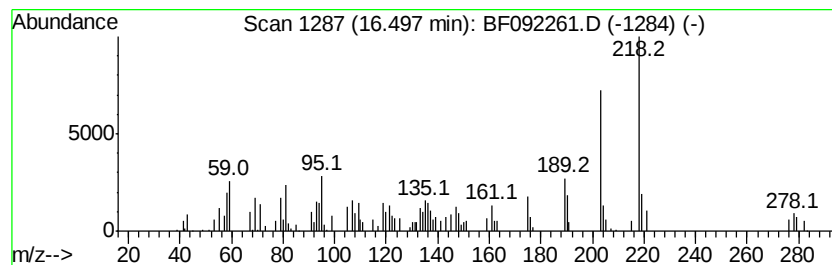
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 5-(1-Naphthyl)tricyclo[4.1.... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.50	2.76 ng	133208	Perylene-d12	15.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-(1-Naphthyl)tricyclo[4.1.0.0(2...]	218	C17H14	107729-05-5	64
2		Anthracene, 9-(2-propenyl)-	218	C17H14	023707-65-5	52
3		Pvrene, hexadecahydro-	218	C16H26	002435-85-0	50
4		9,11-Dimethyltetracyclo[7.3.1.0(...]	218	C16H26	053263-99-3	49
5		Indolizine, 1-acetyl-2-methyl-6-...	218	C11H10N2O3	1000071-33-1	46



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011317\
Data File : BF092261.D
Acq On : 14 Jan 2017 00:17
Operator : UM/SJ
Sample : I1031-07
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-0024

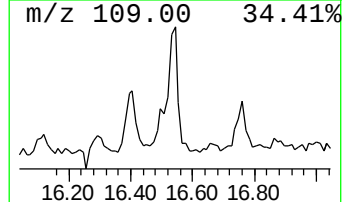
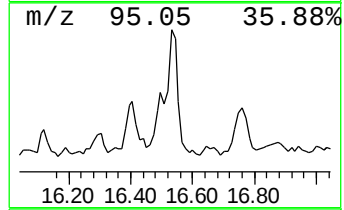
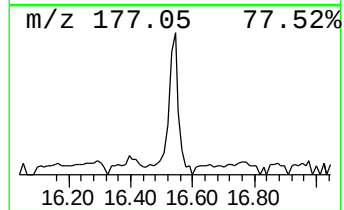
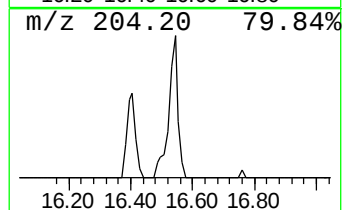
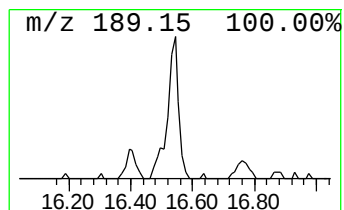
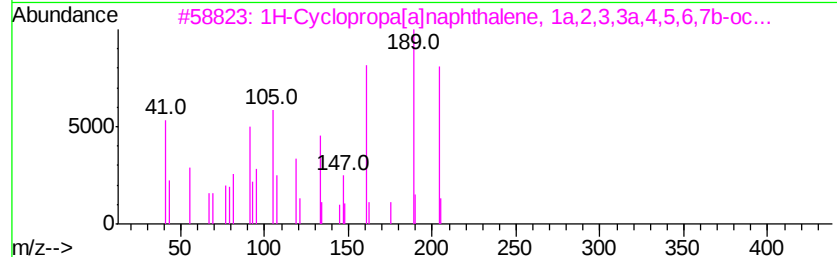
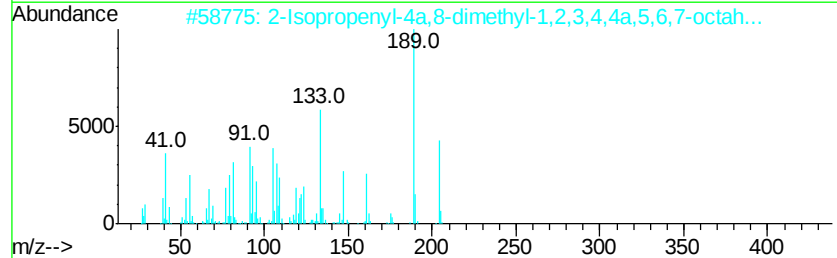
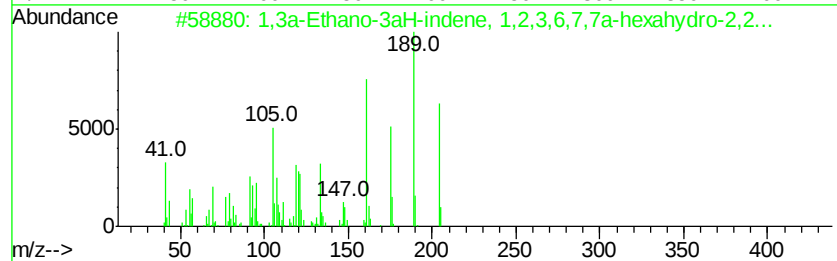
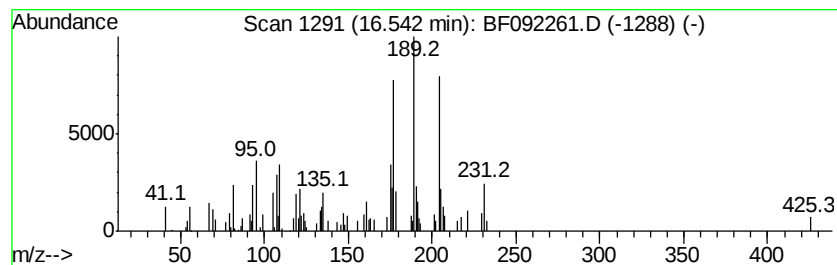
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown16.54 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.54	4.83 ng	232811	Perylene-d12	15.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3a-Ethano-3aH-indene, 1,2,3,6,...	204	C15H24	004545-68-0	45
2		2-Isopropenyl-4a,8-dimethyl-1,2,...	204	C15H24	1000192-43-5	38
3		1H-Cyclopropa[alnaphthalene, 1a,...	204	C15H24	1000147-32-8	38
4		Labda-7,14-dien-13(R)-ol-.alpha....	436	C26H44O5	1000292-93-1	35
5		1H-Cyclopropa[a]naphthalene, 1a,...	204	C15H24	000489-29-2	27



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011317\
Data File : BF092261.D
Acq On : 14 Jan 2017 00:17
Operator : UM/SJ
Sample : I1031-07
Misc :
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ClientSampleId :
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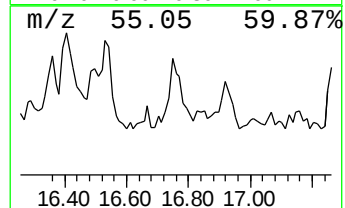
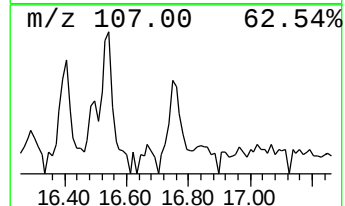
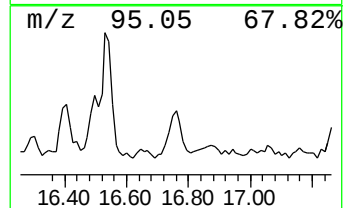
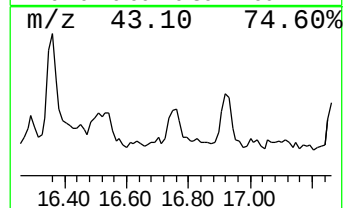
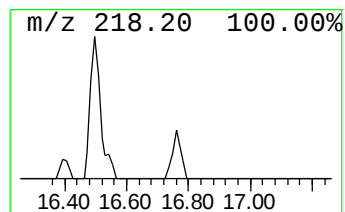
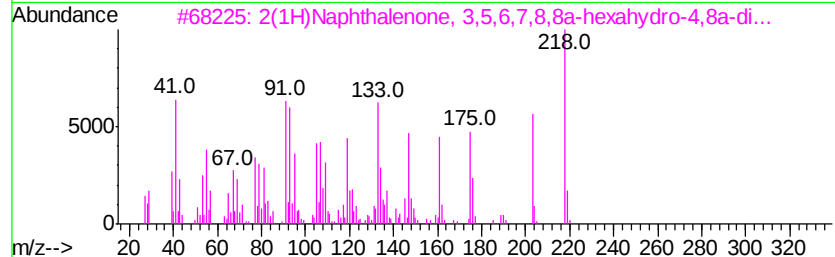
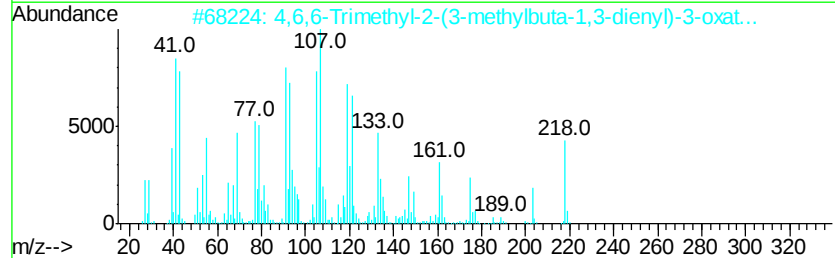
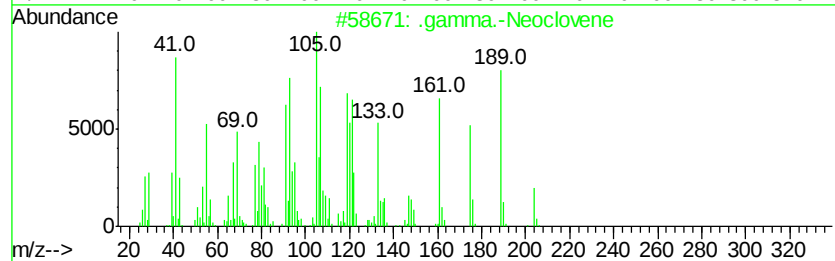
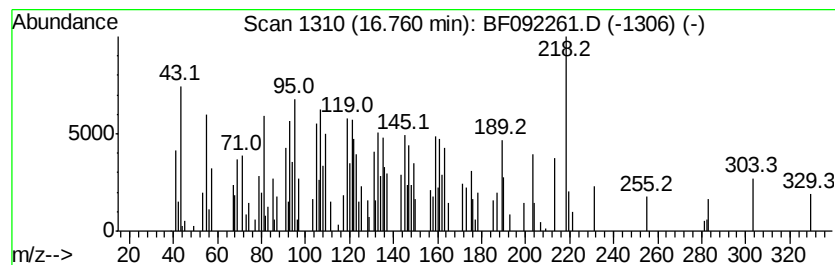
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 .gamma.-Neoclovene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.76	2.92 ng	140643	Perylene-d12	15.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	.gamma.-Neoclovene	204	C15H24	1000156-11-7	59
2		4,6,6-Trimethyl-2-(3-methylbuta-...	218	C15H22O	1000190-22-2	46
3		2(1H)Naphthalenone, 3,5,6,7,8,8a...	218	C15H22O	1000188-66-5	46
4		2H-Cyclopropafalnaphthalen-2-one...	218	C15H22O	006831-17-0	42
5		7-Oxabicyclo[4.1.0]heptane, 2,2,...	218	C15H22O	070038-20-9	41



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011317\
 Data File : BF092261.D
 Acq On : 14 Jan 2017 00:17
 Operator : UM/SJ
 Sample : I1031-07
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMP-0024

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.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...	4.70	48.0	ng	2430880	1	6.58	1012650	20.0
unknown6.35	6.35	95.8	ng	4848980	1	6.58	1012650	20.0
Heptadecane	10.53	2.5	ng	186303	4	11.09	1472370	20.0
Tetradecane	10.98	2.1	ng	151870	4	11.09	1472370	20.0
n-Hexadecanoic acid	11.64	2.7	ng	196169	4	11.09	1472370	20.0
Dichloroacetic ac...	13.58	6.3	ng	437503	5	13.71	1379360	20.0
Heneicosane	15.47	2.7	ng	132029	6	15.07	964724	20.0
unknown16.41	16.41	4.6	ng	221289	6	15.07	964724	20.0
5-(1-Naphthyl)tri...	16.50	2.8	ng	133208	6	15.07	964724	20.0
unknown16.54	16.54	4.8	ng	232811	6	15.07	964724	20.0
.gamma.-Neoclovene	16.76	2.9	ng	140643	6	15.07	964724	20.0