

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040816\
 Data File : BF086185.D
 Acq On : 8 Apr 2016 23:13
 Operator : UM/SJ
 Sample : H2366-02
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B-4PCOMP

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-BF040216.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	4.898	244	246	258	rBV	294184	629807	18.73%	2.073%
2	5.321	281	283	286	rBV	2097295	2880599	85.68%	9.480%
3	5.733	314	319	328	rBV	38671	61638	1.83%	0.203%
4	6.373	373	375	378	rBV	2024789	3083078	91.70%	10.147%
5	6.498	383	386	388	rBV	3066854	3062668	91.09%	10.080%
6	6.727	404	406	409	rBV	810680	749043	22.28%	2.465%
7	6.887	417	420	422	rBV	1840412	2507464	74.58%	8.252%
8	7.299	454	456	458	rBV	2032888	1998849	59.45%	6.578%
9	7.413	463	466	471	rVB3	19388	48508	1.44%	0.160%
10	8.007	516	518	521	rBV	891634	995998	29.62%	3.278%
11	9.093	610	613	615	rBV	3162273	3362230	100.00%	11.065%
12	9.173	617	620	621	rBV	58367	51767	1.54%	0.170%
13	9.482	646	647	650	rBV	315550	403702	12.01%	1.329%
14	9.699	664	666	668	rVB	133777	105297	3.13%	0.347%
15	9.756	669	671	674	rVV	701121	954347	28.38%	3.141%
16	9.927	683	686	688	rBV2	20244	39951	1.19%	0.131%
17	10.019	692	694	696	rVV2	35489	36611	1.09%	0.120%
18	10.202	708	710	711	rVB	99499	132567	3.94%	0.436%
19	10.419	725	729	732	rBV	51989	86533	2.57%	0.285%
20	10.556	738	741	743	rBV	1710731	1868831	55.58%	6.150%
21	10.670	749	751	755	rVB	143071	194070	5.77%	0.639%
22	10.865	765	768	769	rBV3	23735	35291	1.05%	0.116%
23	11.116	788	790	791	rBV	96864	89034	2.65%	0.293%
24	11.139	791	792	796	rVB2	40489	52658	1.57%	0.173%
25	11.242	799	801	805	rBV	1019014	1013224	30.14%	3.335%
26	11.539	825	827	829	rVB	59299	46137	1.37%	0.152%
27	11.779	846	848	853	rBV2	284276	309254	9.20%	1.018%
28	11.950	861	863	864	rBV	30881	40250	1.20%	0.132%
29	12.293	891	893	895	rBV	35223	45500	1.35%	0.150%
30	12.328	895	896	900	rVB	41530	53518	1.59%	0.176%
31	12.453	906	907	909	rBV	123313	159036	4.73%	0.523%
32	12.556	914	916	919	rBV	82369	144329	4.29%	0.475%
33	12.682	925	927	931	rVB2	134025	195021	5.80%	0.642%
34	12.831	937	940	942	rBV	2303059	2355845	70.07%	7.753%

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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

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35	13.059	958	960	961	rBV	74768	63514	1.89%	0.209%
36	13.311	980	982	985	rBV4	29460	35790	1.06%	0.118%
37	13.402	988	990	991	rBV	65838	62760	1.87%	0.207%
38	13.882	1029	1032	1034	rBV	602204	745582	22.18%	2.454%
39	14.042	1044	1046	1050	rBV	68310	95947	2.85%	0.316%
40	14.351	1071	1073	1074	rBV	50325	60039	1.79%	0.198%
41	14.625	1095	1097	1101	rBV2	332212	439181	13.06%	1.445%
42	15.277	1152	1154	1157	rBV	507337	629992	18.74%	2.073%
43	15.871	1204	1206	1213	rVB	89018	202276	6.02%	0.666%
44	16.259	1238	1240	1245	rVB	66404	138640	4.12%	0.456%
45	16.637	1270	1273	1277	rVV2	51214	118674	3.53%	0.391%

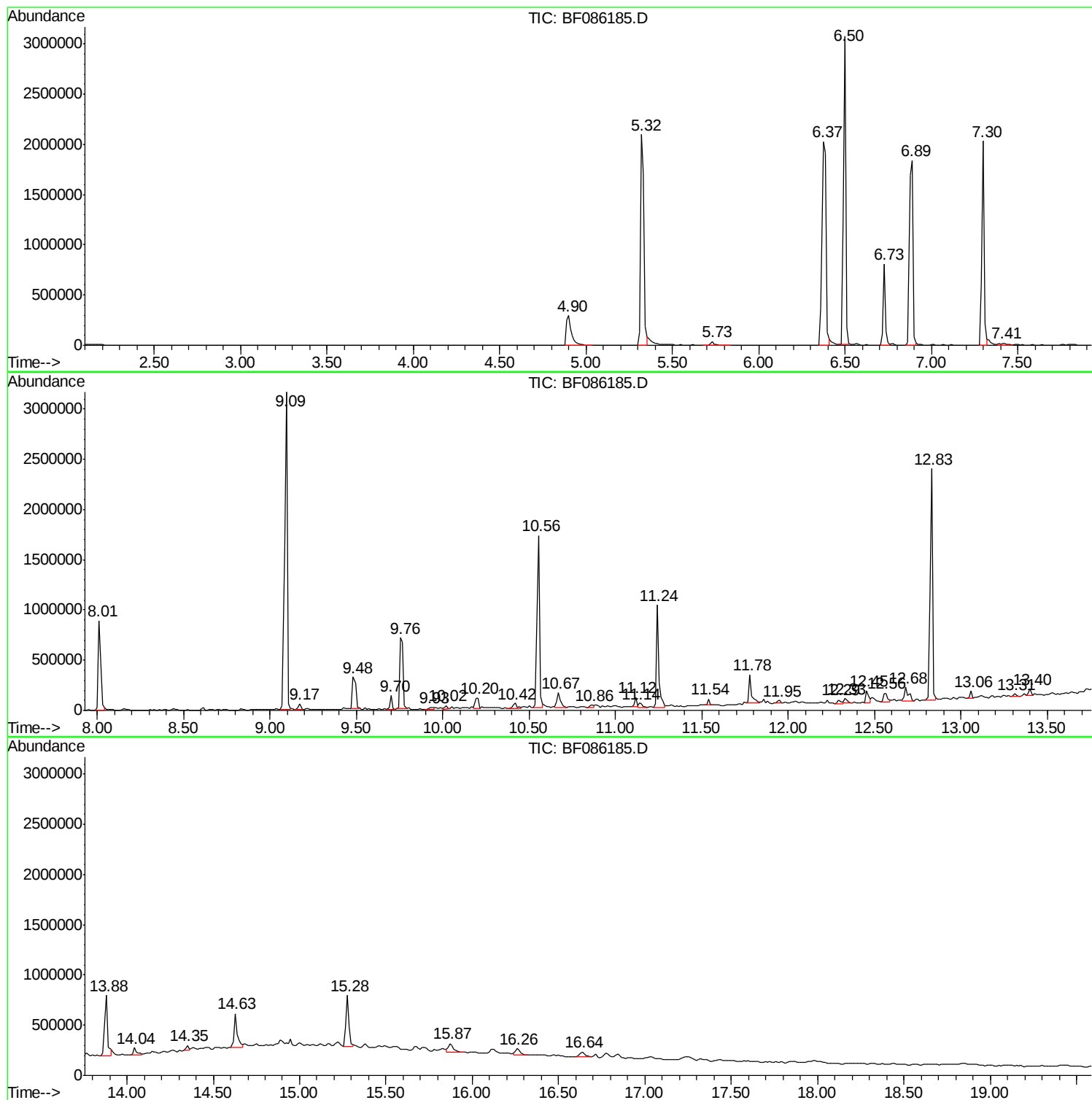
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040216.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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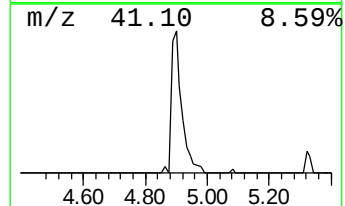
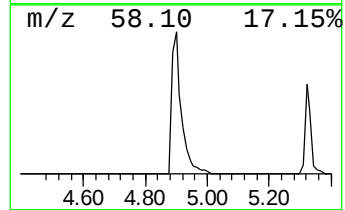
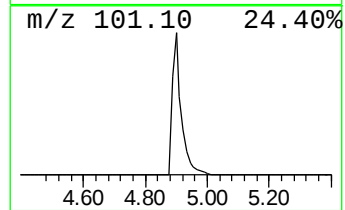
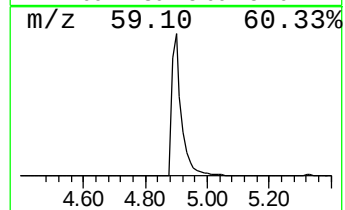
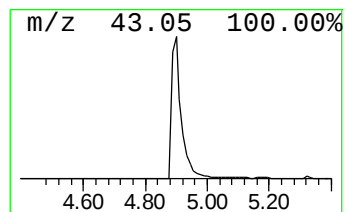
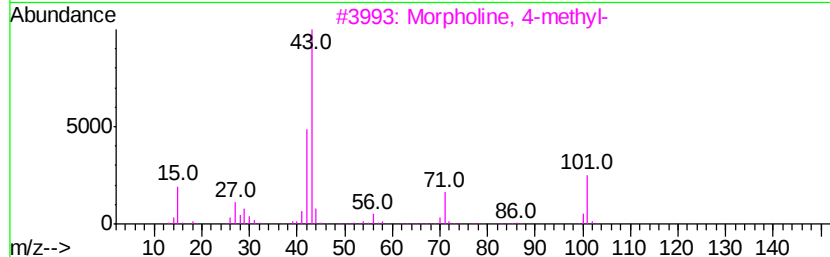
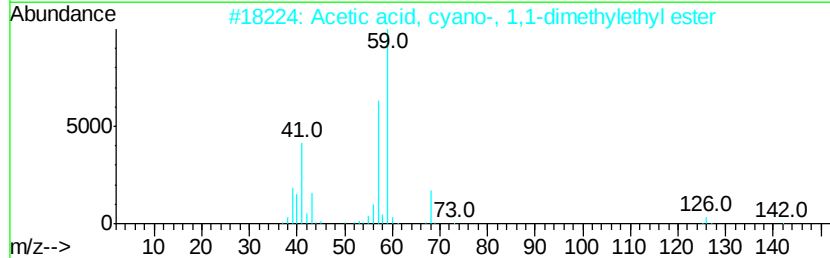
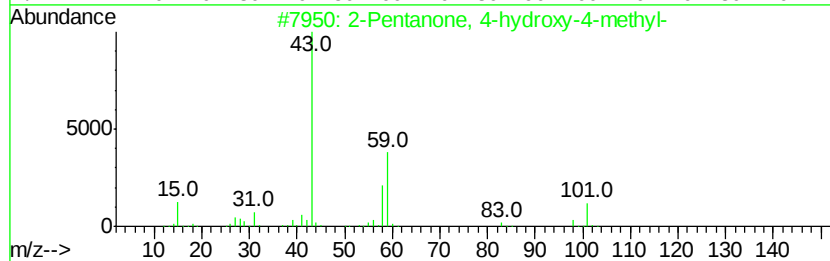
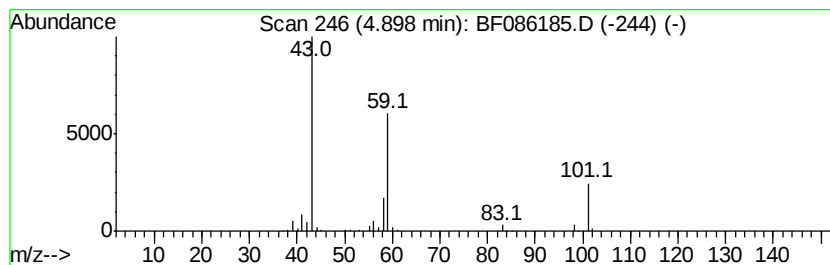
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040216.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.90	16.82 ng	629807	1,4-Dichlorobenzene-d4	6.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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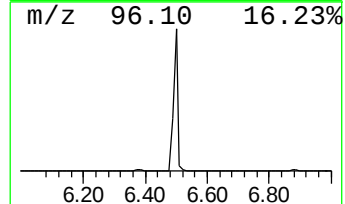
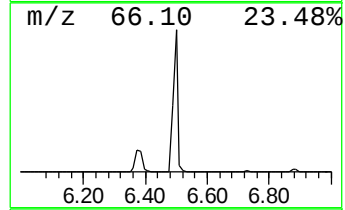
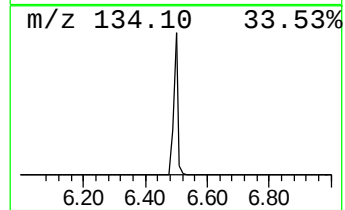
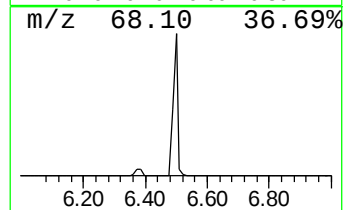
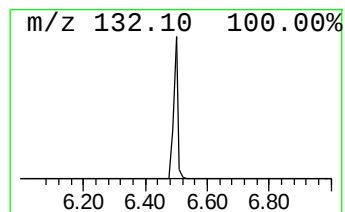
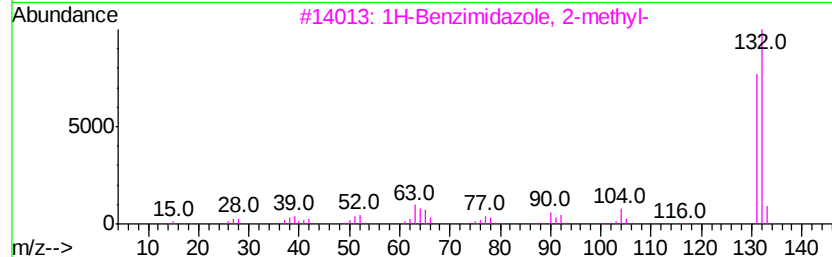
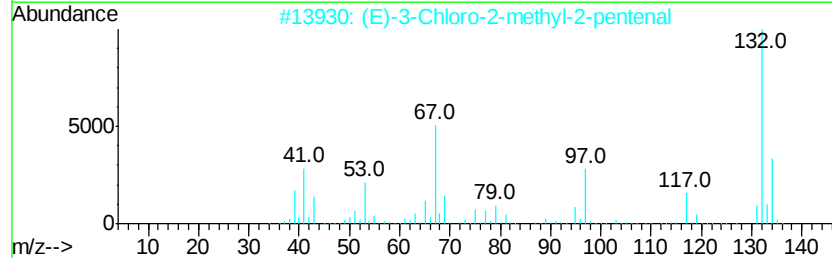
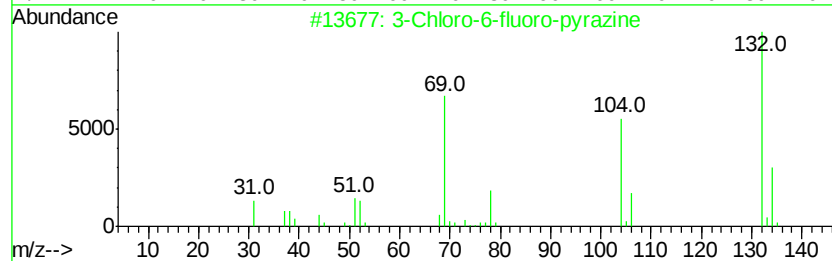
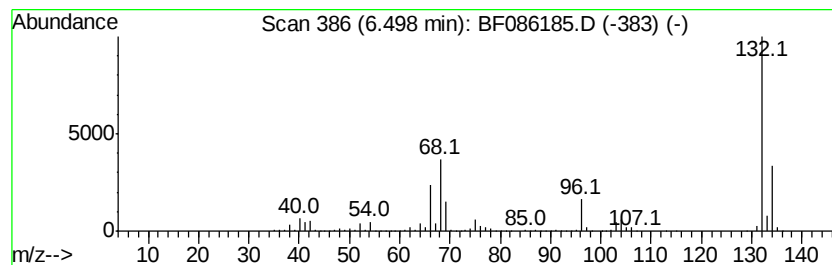
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Peak Number 2 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	81.78 ng	3062670	1,4-Dichlorobenzene-d4	6.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
4		Imidazole, 4,5-dicvano-1-methyl-	132	C6H4N4	019485-35-9	9
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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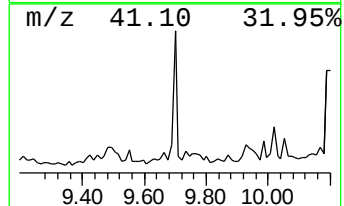
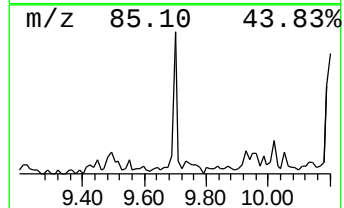
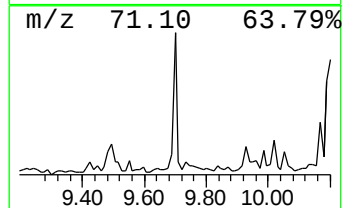
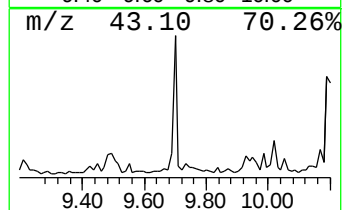
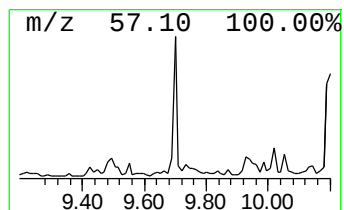
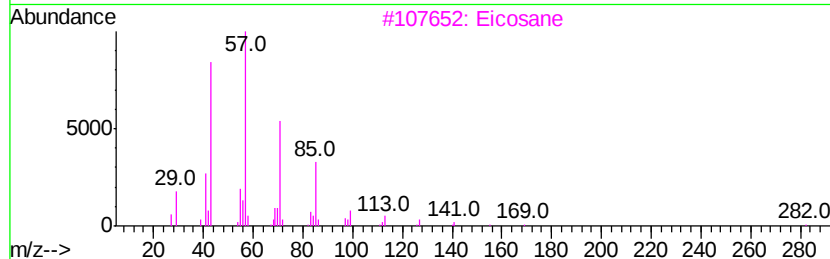
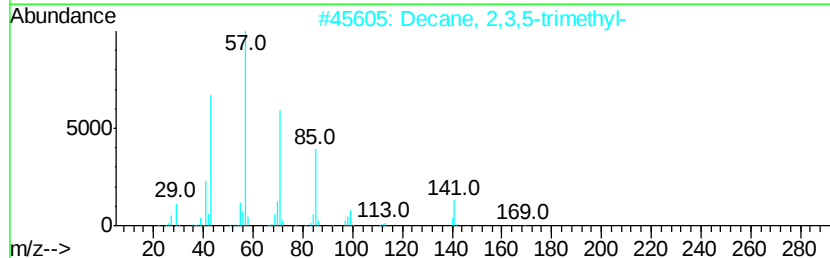
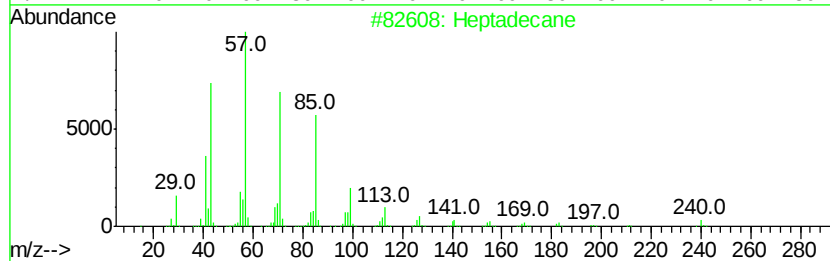
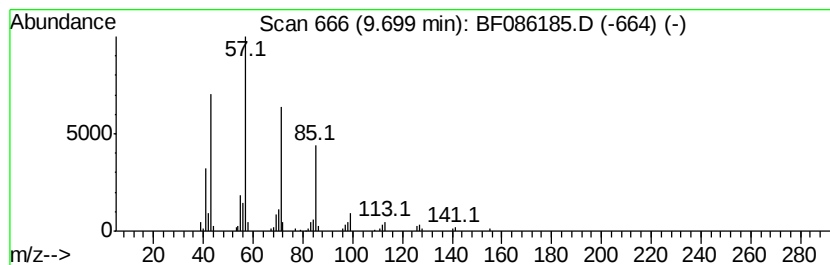
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Heptadecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.70	2.21 ng	105297	Acenaphthene-d10	9.76

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane		240	C17H36	000629-78-7	90
2	Decane, 2,3,5-trimethyl-		184	C13H28	062238-11-3	83
3	Eicosane		282	C20H42	000112-95-8	83
4	Hexadecane		226	C16H34	000544-76-3	80
5	Tridecane		184	C13H28	000629-50-5	72



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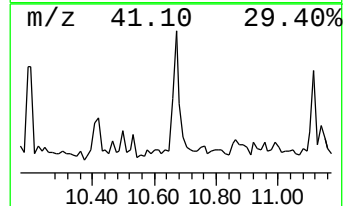
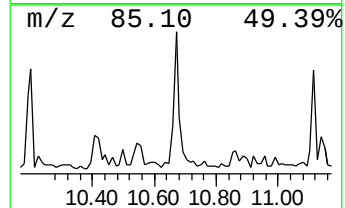
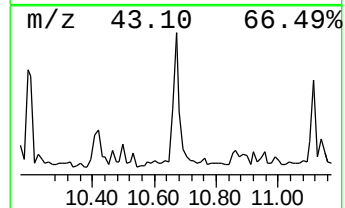
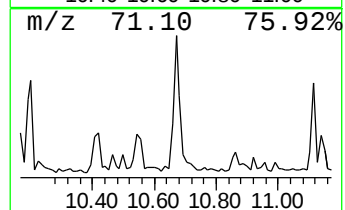
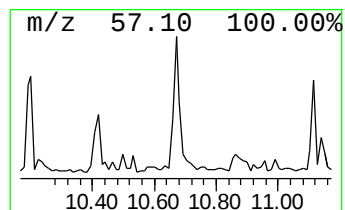
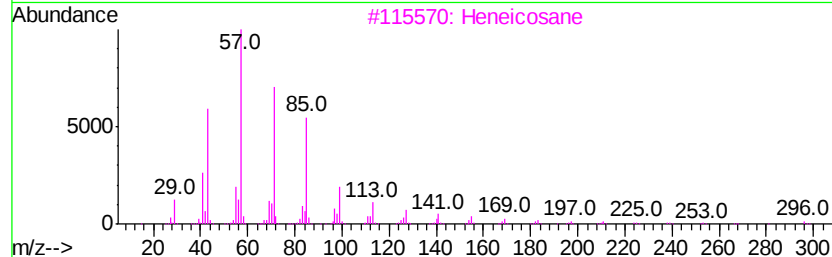
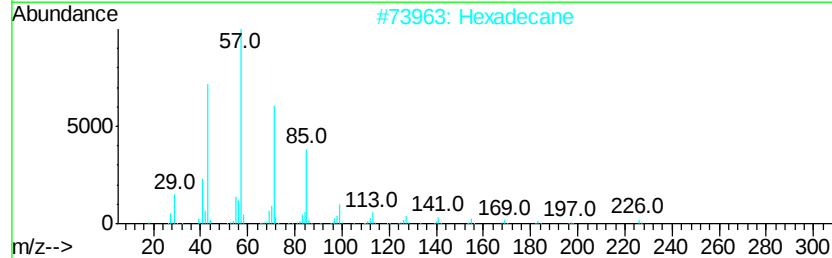
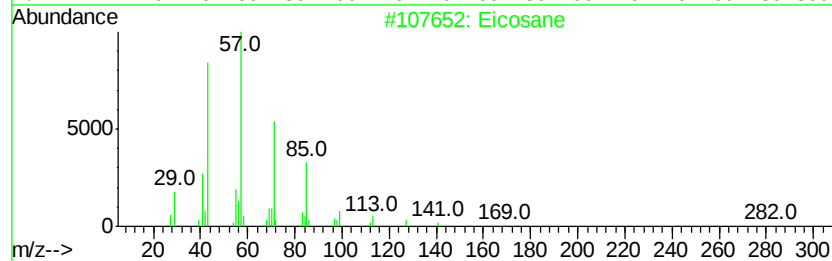
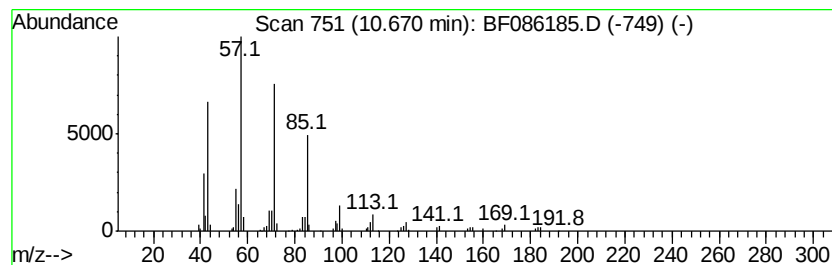
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.67	3.83 ng	194070	Phenanthrene-d10	11.24

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	91
2	Hexadecane		226	C16H34	000544-76-3	91
3	Heneicosane		296	C21H44	000629-94-7	91
4	Tridecane, 7-hexyl-		268	C19H40	007225-66-3	90
5	Tridecane, 1-iodo-		310	C13H27I	035599-77-0	90



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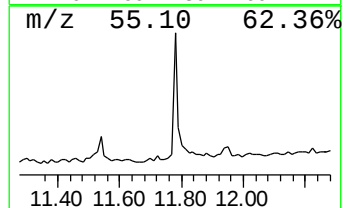
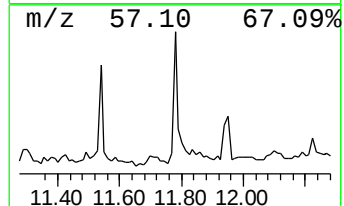
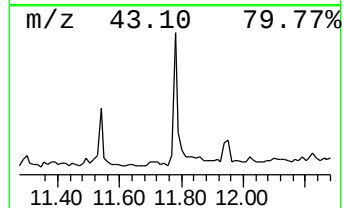
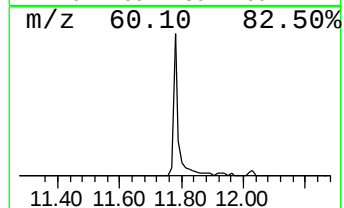
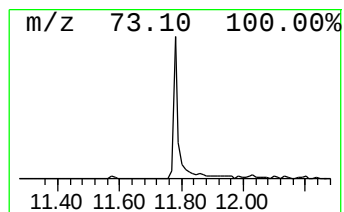
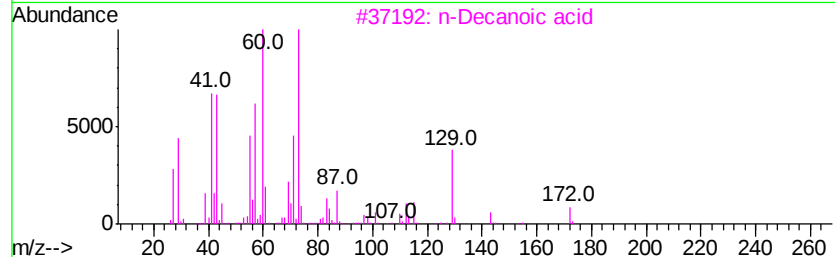
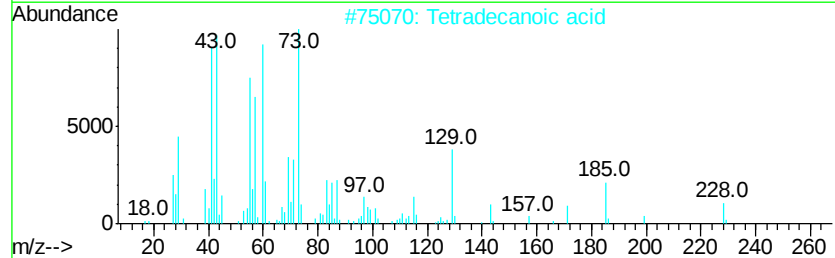
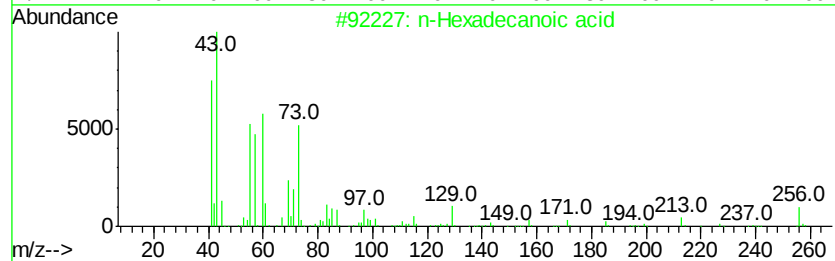
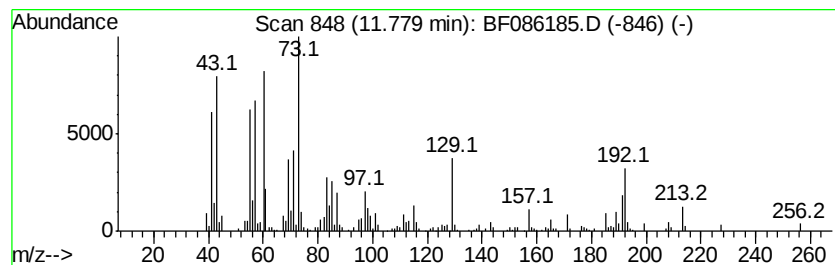
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 7 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.78	6.10 ng	309254	Phenanthrene-d10	11.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
3	n-Decanoic acid	172	C10H20O2	000334-48-5	76
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
5	Undecane	156	C11H24	001120-21-4	11



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040816\
Data File : BF086185.D
Acq On : 8 Apr 2016 23:13
Operator : UM/SJ
Sample : H2366-02
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-4PCOMP

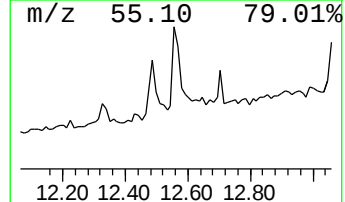
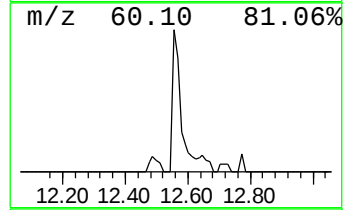
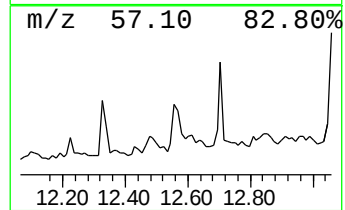
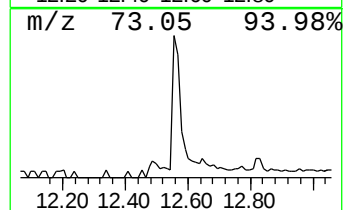
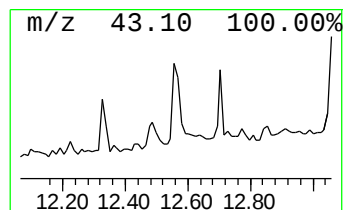
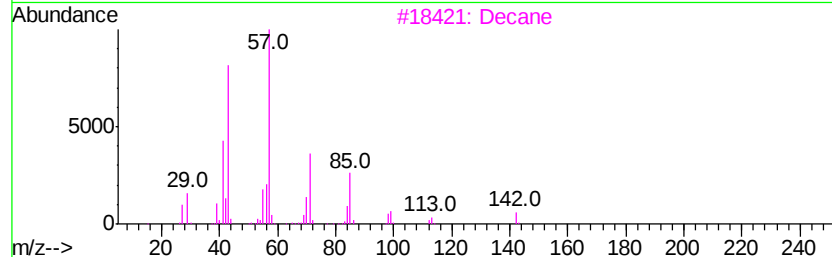
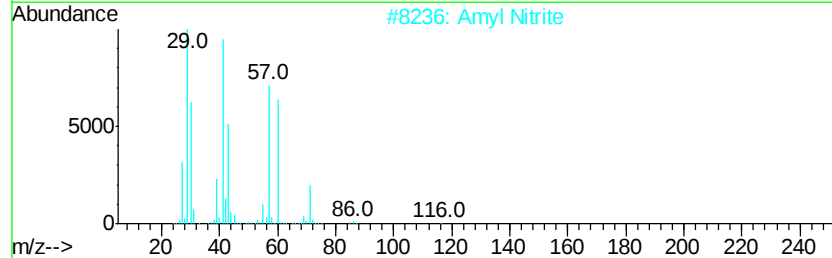
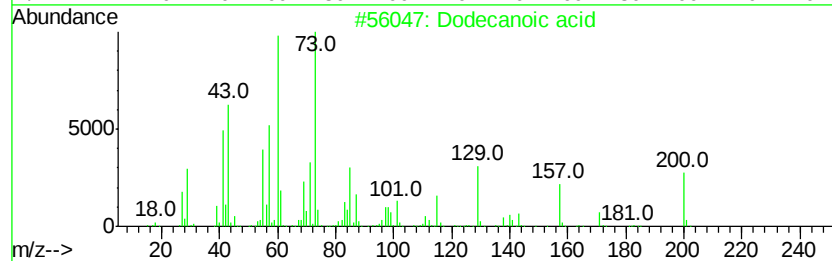
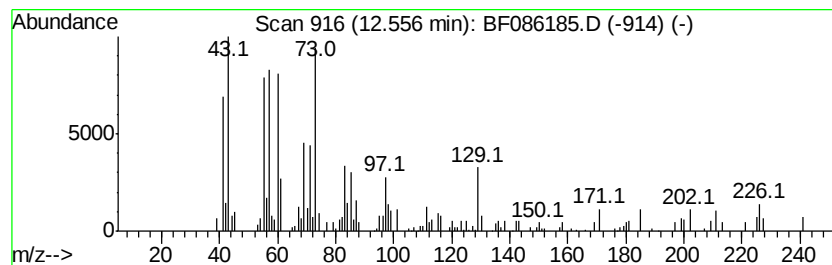
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Dodecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.56	2.85 ng	144329	Phenanthrene-d10	11.24

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Dodecanoic acid	200	C12H24O2	000143-07-7	53
2		Amyl Nitrite	117	C5H11NO2	000110-46-3	35
3		Decane	142	C10H22	000124-18-5	25
4		2,3,4,5-Tetrahydroxypentanal	150	C5H10O5	053106-52-8	22
5		Pentafluoropropionic acid, penta...	374	C18H31F5O2	1000280-07-5	11



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040816\
Data File : BF086185.D
Acq On : 8 Apr 2016 23:13
Operator : UM/SJ
Sample : H2366-02
Misc :
ALS Vial : 24 Sample Multiplier: 1

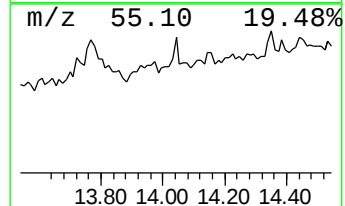
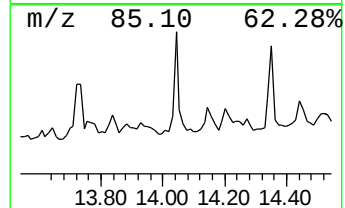
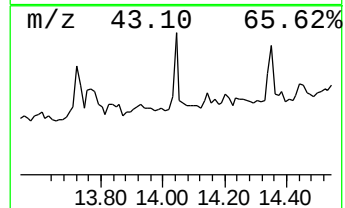
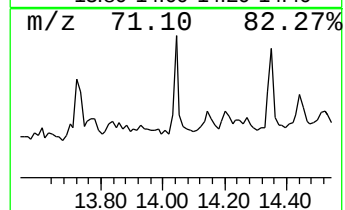
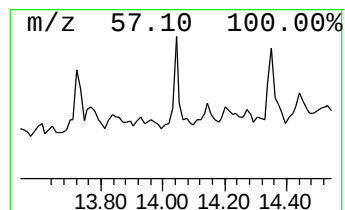
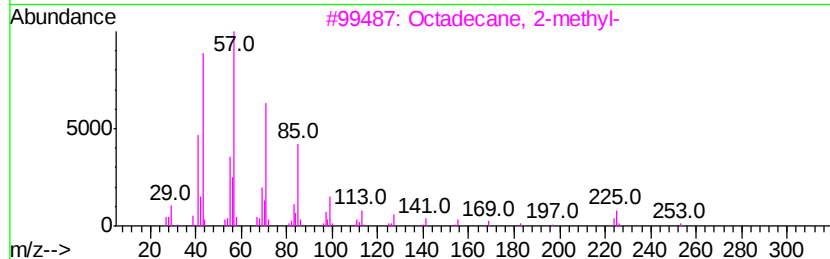
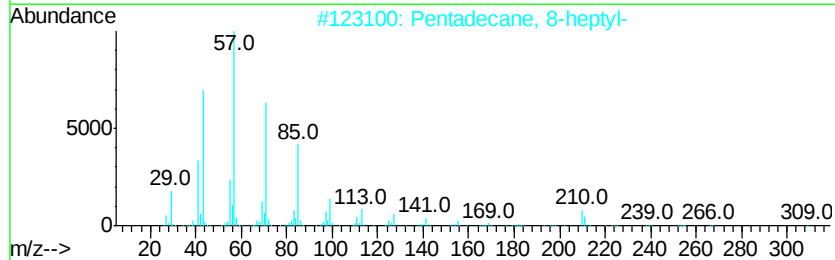
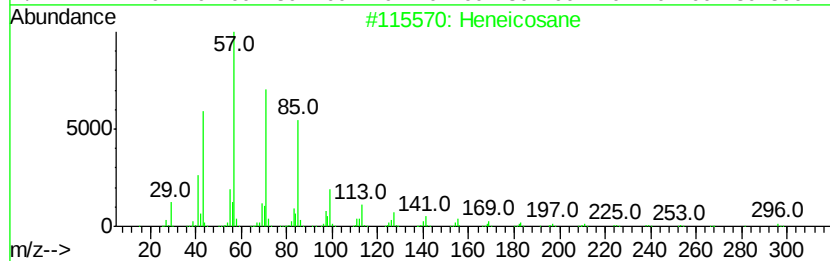
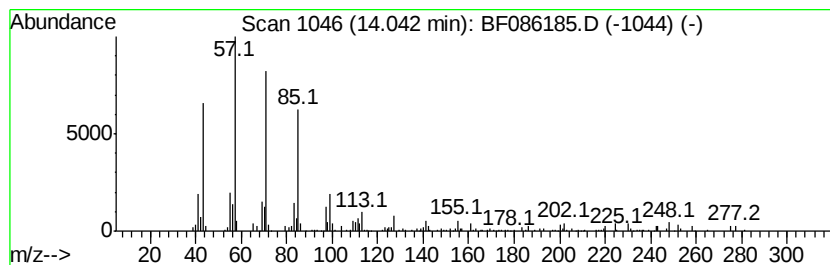
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heneicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.04	2.57 ng	95947	Chrysene-d12	13.88
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heneicosane	296 C21H44	000629-94-7	90
2	Pentadecane, 8-heptyl-	310 C22H46	071005-15-7	87
3	Octadecane, 2-methyl-	268 C19H40	001560-88-9	86
4	Heptadecane, 9-octyl-	352 C25H52	007225-64-1	80
5	Tetracosane	338 C24H50	000646-31-1	80



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040816\
Data File : BF086185.D
Acq On : 8 Apr 2016 23:13
Operator : UM/SJ
Sample : H2366-02
Misc :
ALS Vial : 24 Sample Multiplier: 1

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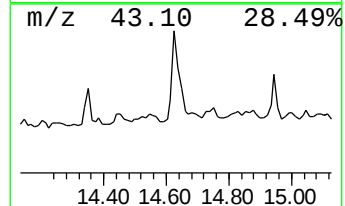
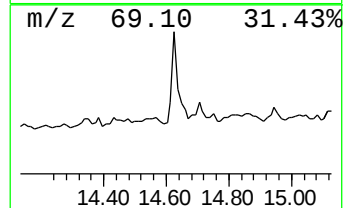
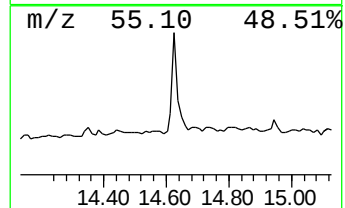
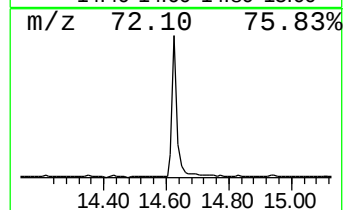
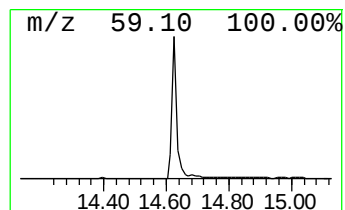
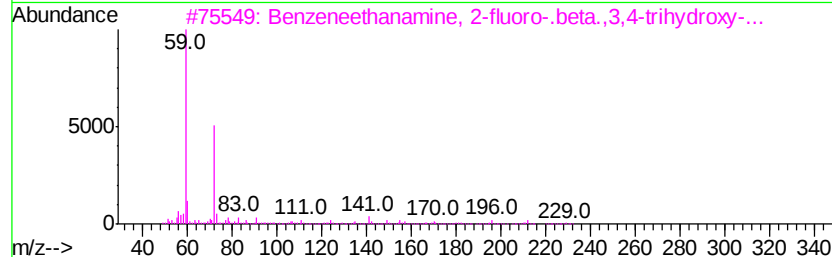
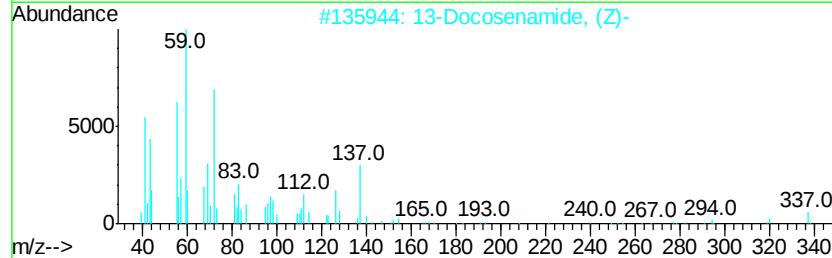
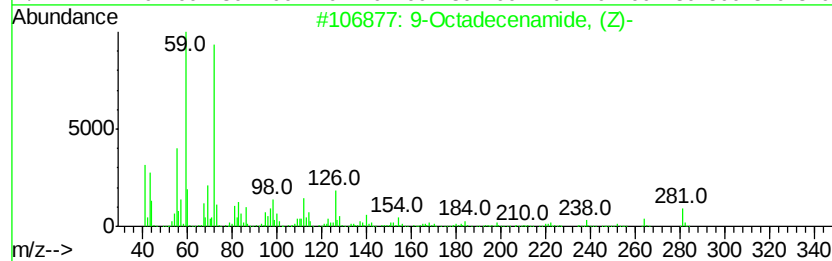
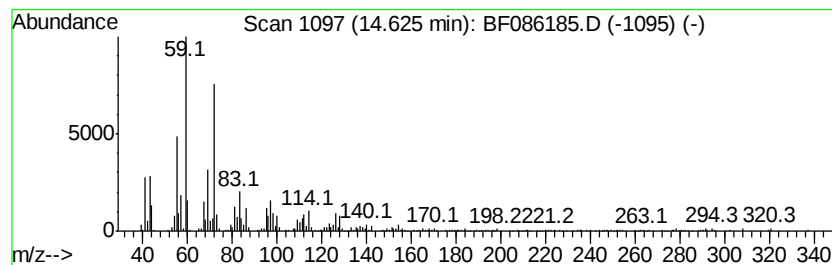
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.63	13.94 ng	439181	Perylene-d12	15.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	90
2		13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	78
3		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	50
4		Octadecanamide	283	C18H37NO	000124-26-5	47
5		1,1,2-Trimethyl-1-silacyclobutane	114	C6H14Si	030681-90-4	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040816\
Data File : BF086185.D
Acq On : 8 Apr 2016 23:13
Operator : UM/SJ
Sample : H2366-02
Misc :
ALS Vial : 24 Sample Multiplier: 1

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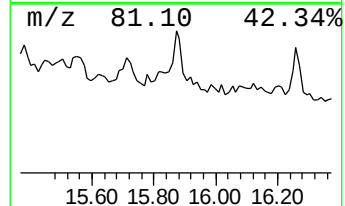
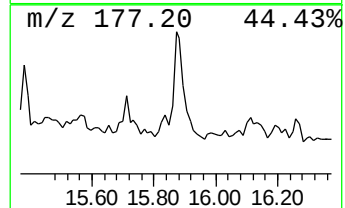
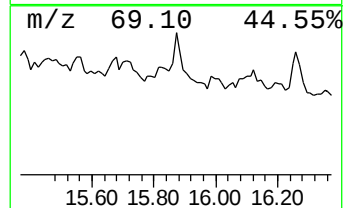
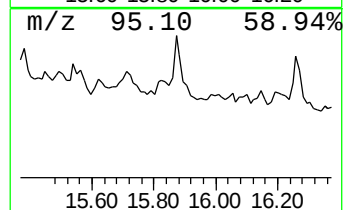
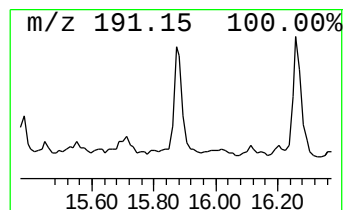
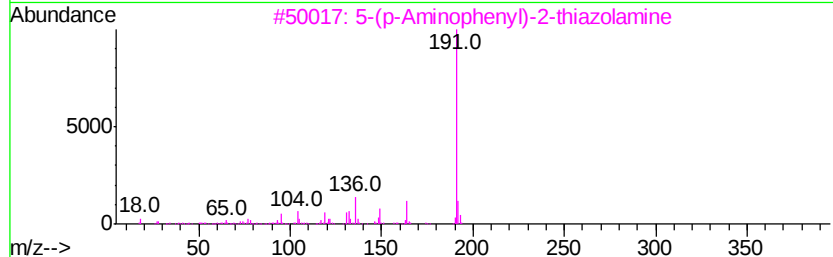
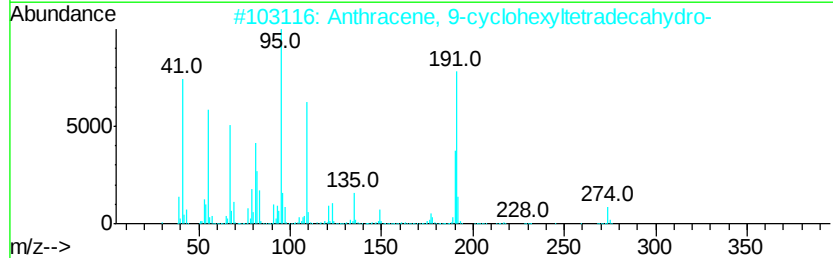
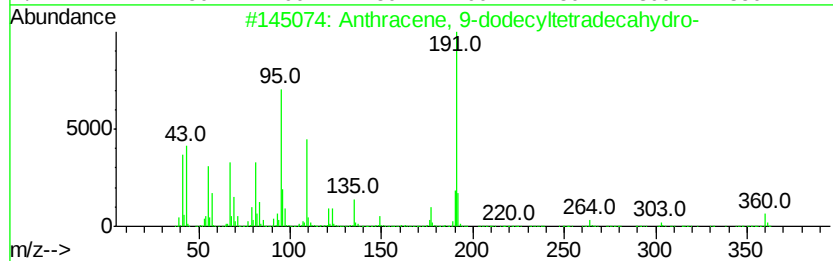
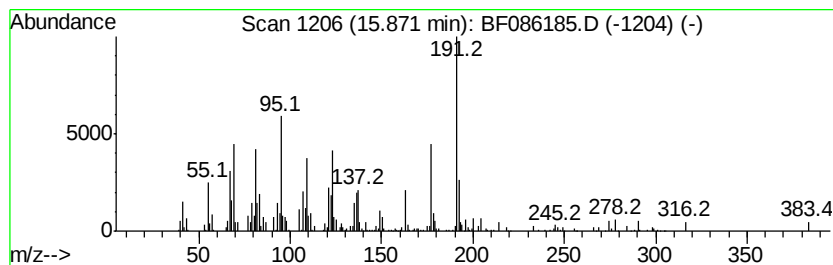
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown15.87 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.87	6.42 ng	202276	Perylene-d12	15.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Anthracene, 9-dodecyltetradeca...	360	C26H48	055401-75-7	32
2		Anthracene, 9-cyclohexyltetradec...	274	C20H34	055255-70-4	30
3		5-(p-Aminophenyl)-2-thiazolamine	191	C9H9N3S	090349-87-4	25
4		4H-1,3-Benzodioxin-4-one, 2-(1,1...	266	C16H26O3	124899-18-9	14
5		Divinylbis(cyclopropyl)silane	164	C10H16Si	1000109-95-2	14



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040816\
Data File : BF086185.D
Acq On : 8 Apr 2016 23:13
Operator : UM/SJ
Sample : H2366-02
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
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ClientSampled :
B-4PCOMP

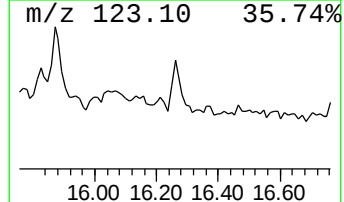
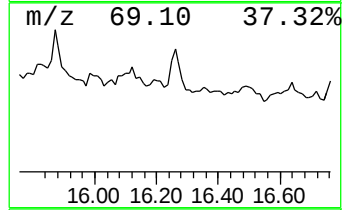
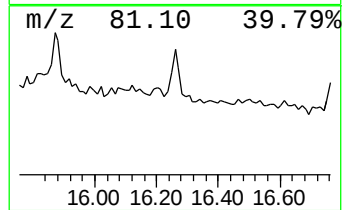
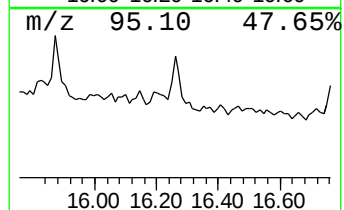
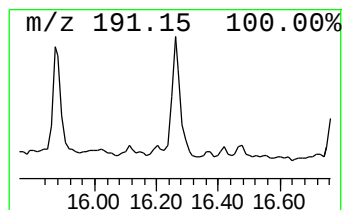
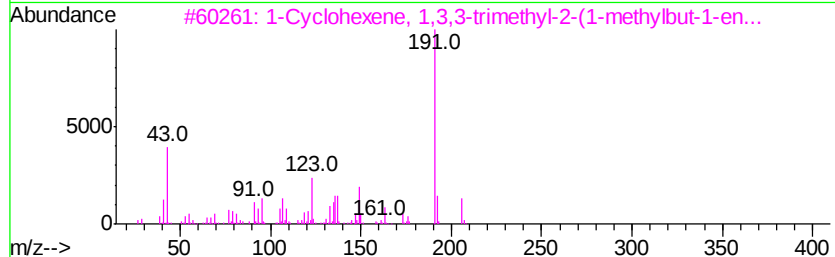
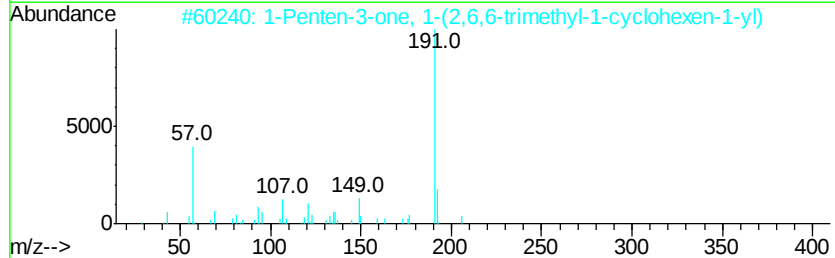
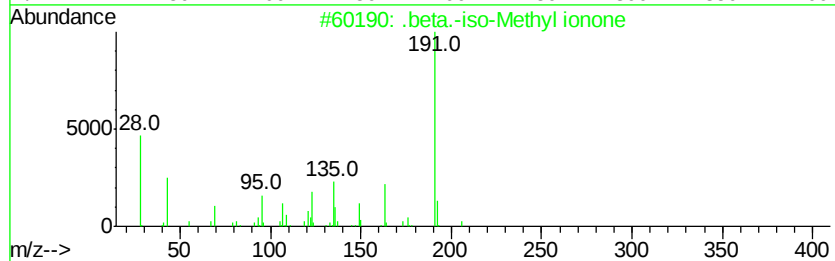
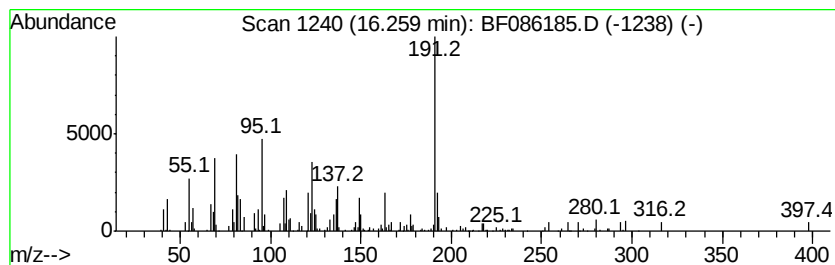
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 .beta.-iso-Methyl ionone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.26	4.40 ng	138640	Perylene-d12	15.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	50
2		1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	42
3		1-Cyclohexene, 1,3,3-trimethyl-2...	206	C14H22O	1000197-08-4	38
4		4,5-Dihydrothiazol-4-one, 2-(2-m...	222	C10H10N2O2S	022476-61-5	35
5		4-(3H-Imidazo[4,5-b]pyridin-2-yl...	342	C15H18N8S	1000276-08-2	32



Data Path : Z:\HPCHEM1\BNA F\DATA\BF040816\
Data File : BF086185.D
Acq On : 8 Apr 2016 23:13
Operator : UM/SJ
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Misc :
ALS Vial : 24 Sample Multiplier: 1

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B-4PCOMP

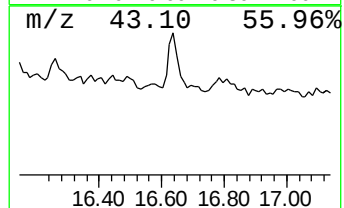
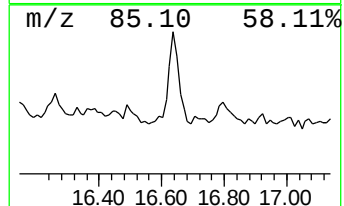
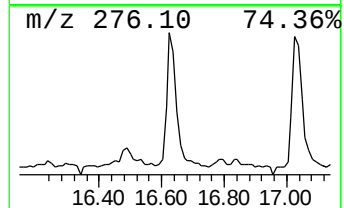
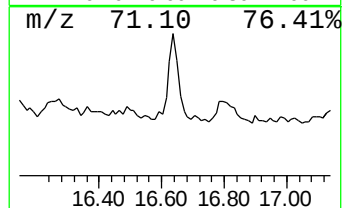
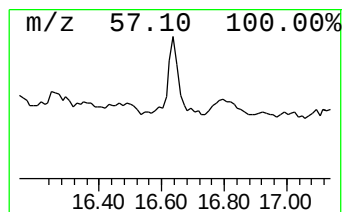
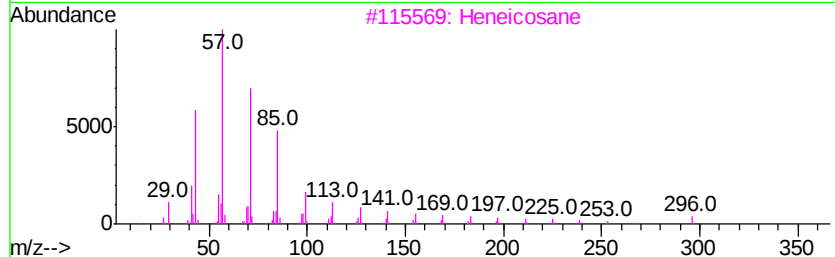
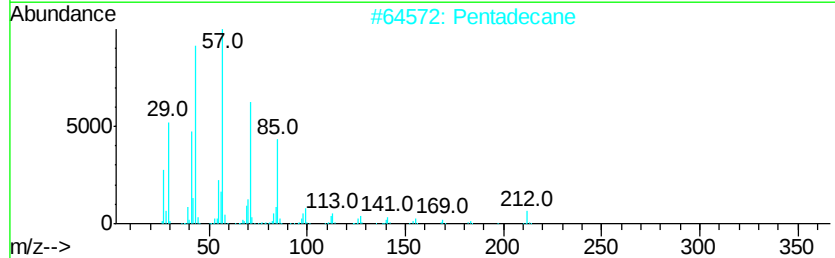
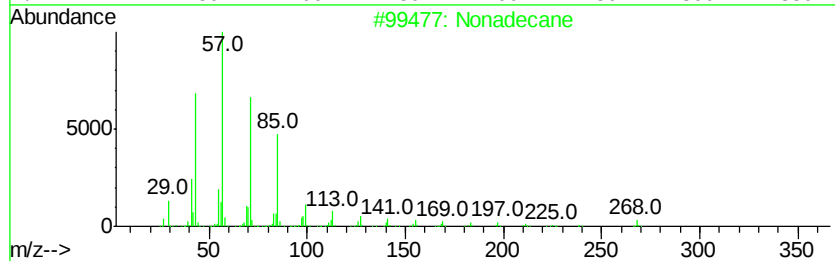
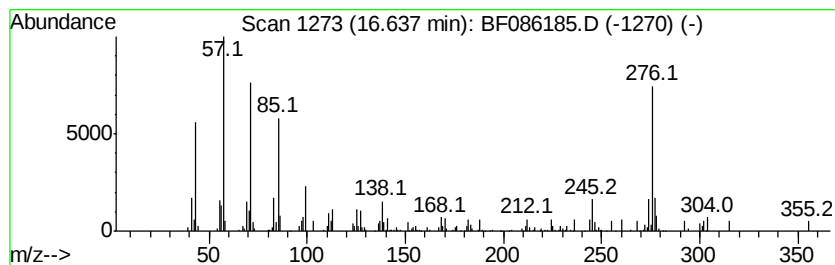
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Nonadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.64	3.77 ng	118674	Perylene-d12	15.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonadecane	268	C19H40	000629-92-5	87
2		Pentadecane	212	C15H32	000629-62-9	52
3		Heneicosane	296	C21H44	000629-94-7	43
4		Tetracosane	338	C24H50	000646-31-1	43
5		Octacosane	394	C28H58	000630-02-4	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040816\
Data File : BF086185.D
Acq On : 8 Apr 2016 23:13
Operator : UM/SJ
Sample : H2366-02
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-4PCOMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040216.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
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unknown6.50	6.50	81.8	ng	3062670	1	6.73	749043	20.0
Heptadecane	9.70	2.2	ng	105297	3	9.76	954347	20.0
Eicosane	10.67	3.8	ng	194070	4	11.24	1013220	20.0
n-Hexadecanoic acid	11.78	6.1	ng	309254	4	11.24	1013220	20.0
Dodecanoic acid	12.56	2.9	ng	144329	4	11.24	1013220	20.0
Heneicosane	14.04	2.6	ng	95947	5	13.88	745582	20.0
9-Octadecenamide, ...	14.63	13.9	ng	439181	6	15.28	629992	20.0
unknown15.87	15.87	6.4	ng	202276	6	15.28	629992	20.0
.beta.-iso-Methyl...	16.26	4.4	ng	138640	6	15.28	629992	20.0
Nonadecane	16.64	3.8	ng	118674	6	15.28	629992	20.0