

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091517\
 Data File : BF098570.D
 Acq On : 15 Sep 2017 15:33
 Operator : SJ/JU
 Sample : I5188-03
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RL-6-11-22

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-BF091117.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	3.540	239	247	258	rBV	791759	1305516	34.22%	3.758%
2	4.828	462	466	482	rBV	249812	398330	10.44%	1.147%
3	5.198	524	529	535	rBV2	32707	51773	1.36%	0.149%
4	5.257	535	539	557	rVV	3517225	3625764	95.03%	10.437%
5	6.304	712	717	728	rBV	2568814	3815456	100.00%	10.983%
6	6.422	732	737	740	rVV	3921345	3695720	96.86%	10.638%
7	6.481	742	747	751	rVB2	89183	118750	3.11%	0.342%
8	6.645	771	775	781	rVB	957347	908317	23.81%	2.615%
9	6.798	797	801	808	rBV	3020406	2783736	72.96%	8.013%
10	7.092	848	851	860	rVB	79695	117034	3.07%	0.337%
11	7.216	867	872	875	rBV	2386878	2195198	57.53%	6.319%
12	7.245	875	877	881	rVB2	104428	87644	2.30%	0.252%
13	7.698	950	954	957	rVB2	35155	42356	1.11%	0.122%
14	7.745	957	962	967	rVB9	19483	41524	1.09%	0.120%
15	7.928	986	993	995	rBV	1365786	1234146	32.35%	3.552%
16	7.951	995	997	1003	rVB2	319478	299525	7.85%	0.862%
17	8.310	1055	1058	1061	rVB4	46703	52708	1.38%	0.152%
18	8.428	1075	1078	1081	rBV4	35470	41936	1.10%	0.121%
19	8.463	1081	1084	1086	rBV3	40947	40929	1.07%	0.118%
20	8.522	1091	1094	1097	rVV	82827	67779	1.78%	0.195%
21	8.639	1112	1114	1117	rBV	168896	129928	3.41%	0.374%
22	8.739	1128	1131	1136	rVB	112190	115846	3.04%	0.333%
23	8.804	1139	1142	1145	rBV4	44371	50821	1.33%	0.146%
24	8.916	1158	1161	1163	rBV	48201	49583	1.30%	0.143%
25	8.951	1164	1167	1171	rVB2	69221	78464	2.06%	0.226%
26	9.004	1171	1176	1179	rBV	3736093	3573587	93.66%	10.287%
27	9.086	1185	1190	1192	rBV3	135231	156007	4.09%	0.449%
28	9.275	1218	1222	1225	rBV3	51607	67818	1.78%	0.195%
29	9.339	1230	1233	1236	rBV3	60564	68804	1.80%	0.198%
30	9.404	1241	1244	1247	rVB	506954	413437	10.84%	1.190%
31	9.539	1264	1267	1273	rBV2	121279	166857	4.37%	0.480%
32	9.586	1273	1275	1278	rVB2	92108	74504	1.95%	0.214%
33	9.616	1278	1280	1283	rBV	130204	111169	2.91%	0.320%
34	9.680	1285	1291	1294	rVV	1217440	1132137	29.67%	3.259%

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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 >
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35	9.880	1323	1325	1327	rBV3	40898	40733	1.07%	0.117%
36	9.904	1327	1329	1331	rVB	72748	57965	1.52%	0.167%
37	10.116	1362	1365	1367	rBV	111267	100974	2.65%	0.291%
38	10.339	1400	1403	1408	rVB2	79569	96988	2.54%	0.279%
39	10.469	1422	1425	1429	rBV	1546752	1447088	37.93%	4.165%
40	10.586	1442	1445	1454	rVB2	229311	377324	9.89%	1.086%
41	11.033	1519	1521	1524	rBV3	107201	121764	3.19%	0.350%
42	11.163	1540	1543	1545	rBV	1071037	898657	23.55%	2.587%
43	11.186	1545	1547	1551	rVB	225280	196280	5.14%	0.565%
44	12.374	1746	1749	1752	rVB	260083	200787	5.26%	0.578%
45	12.604	1785	1788	1790	rBV	252398	218657	5.73%	0.629%
46	12.751	1809	1813	1816	rBV	2457556	2183933	57.24%	6.286%
47	13.804	1988	1992	1995	rBV	888558	920512	24.13%	2.650%
48	15.209	2228	2231	2238	rVB2	627990	765643	20.07%	2.204%

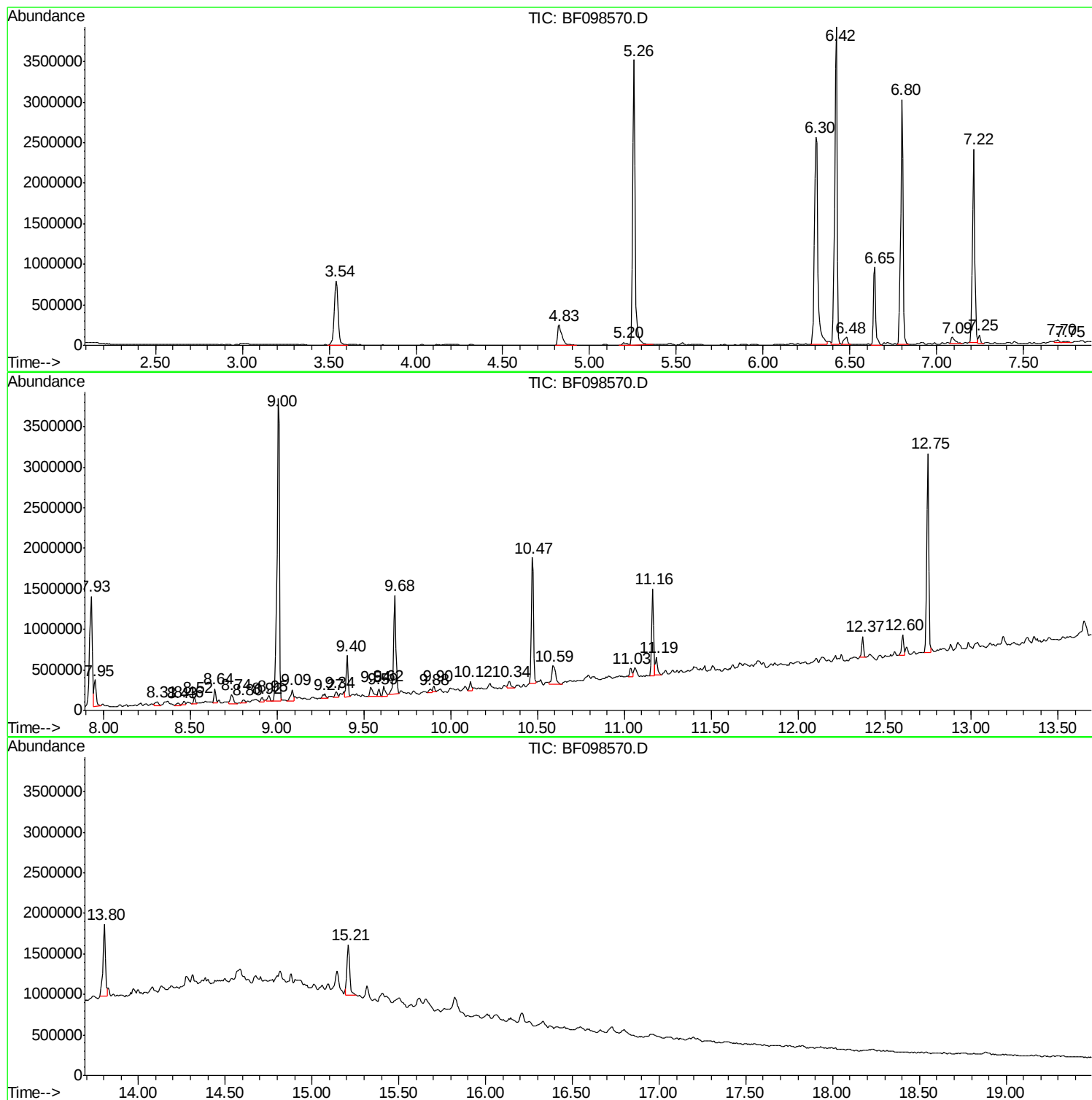
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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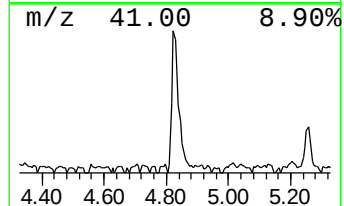
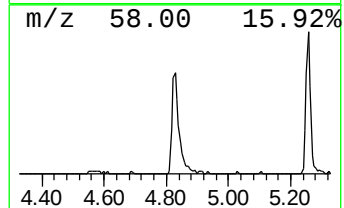
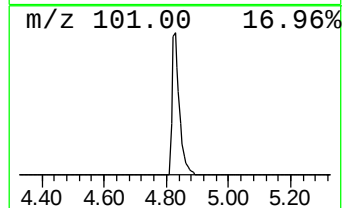
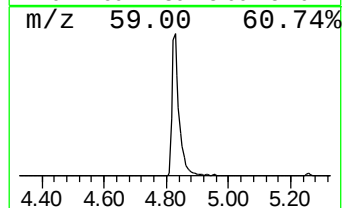
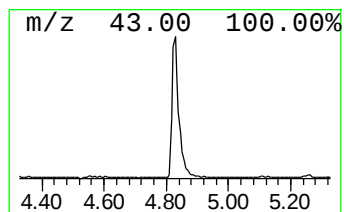
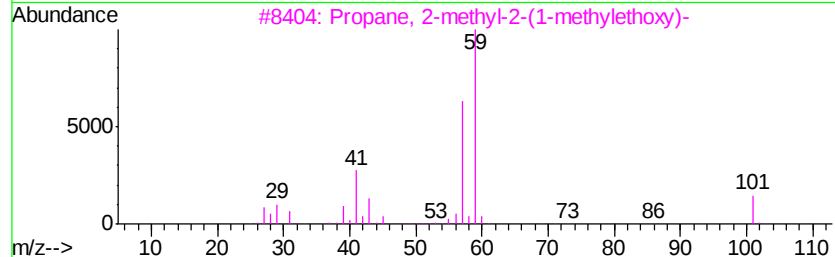
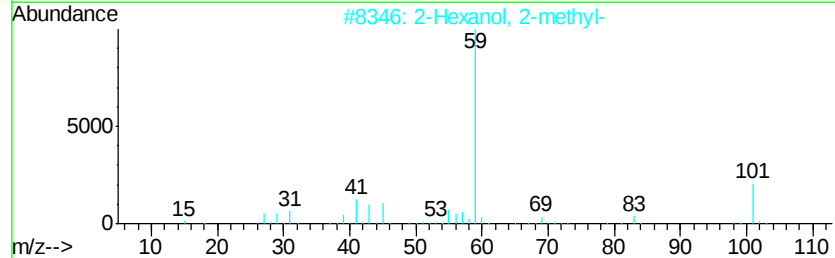
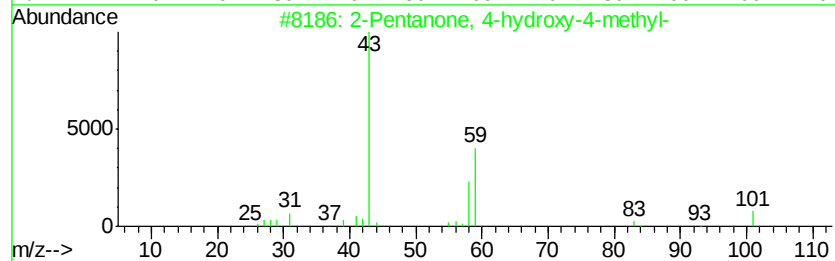
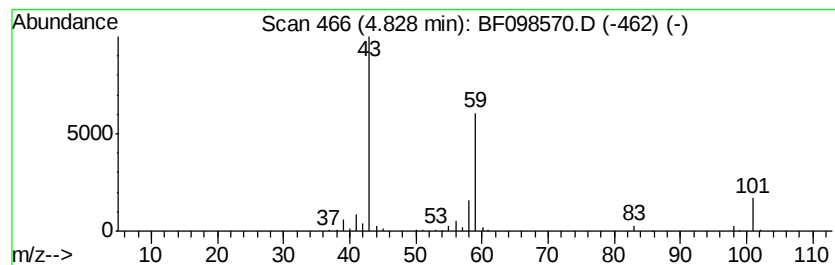
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.83	8.77 ng	398330	1,4-Dichlorobenzene-d4	6.65

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	38
3			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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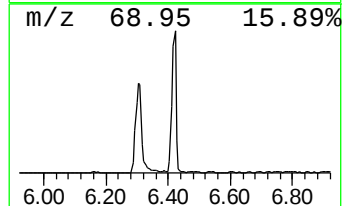
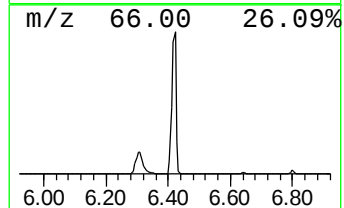
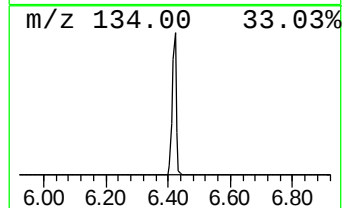
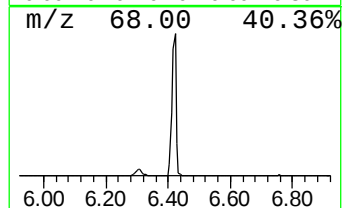
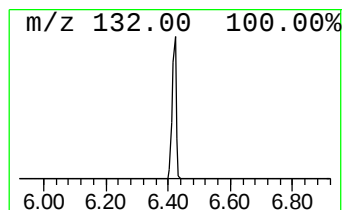
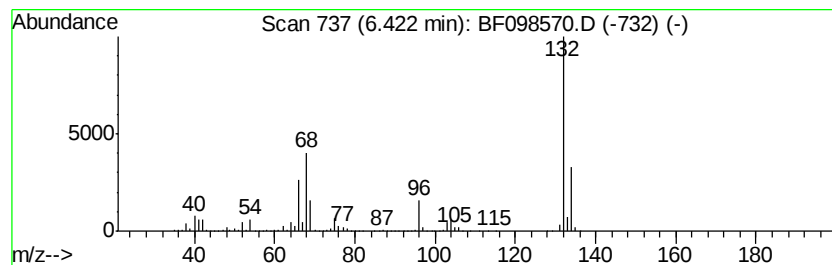
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.42 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.42	81.38 ng	3695720	1,4-Dichlorobenzene-d4	6.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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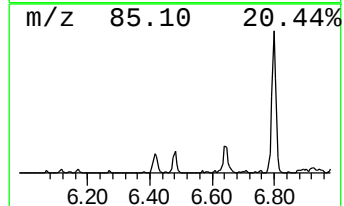
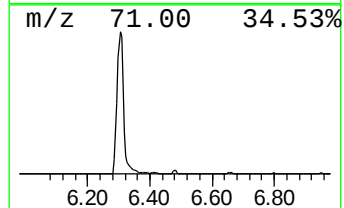
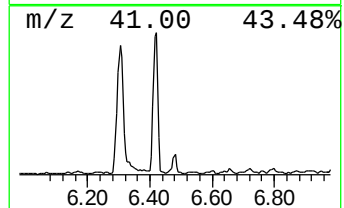
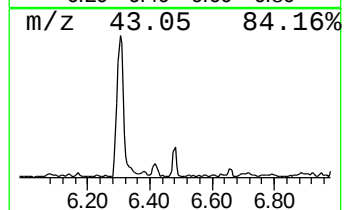
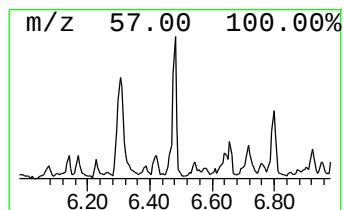
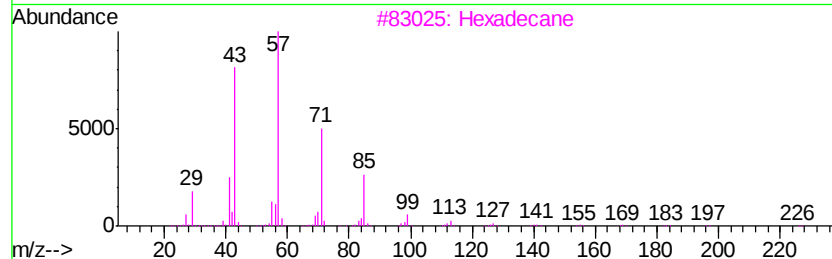
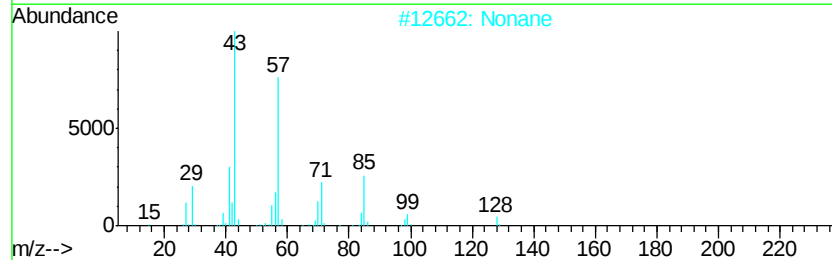
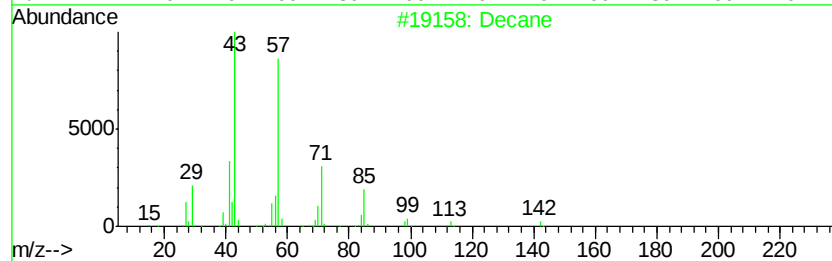
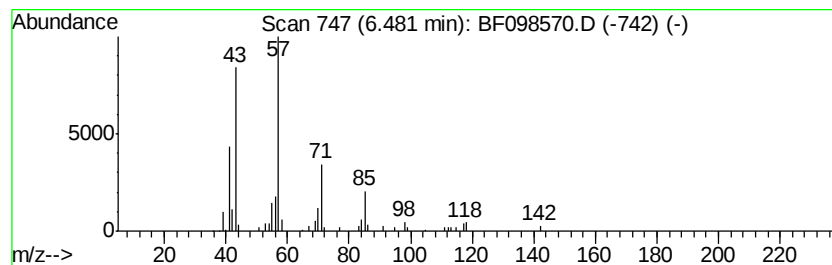
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Decane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	2.61 ng	118750	1,4-Dichlorobenzene-d4	6.65

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane		142	C10H22	000124-18-5	90
2	Nonane		128	C9H20	000111-84-2	86
3	Hexadecane		226	C16H34	000544-76-3	64
4	Tridecane		184	C13H28	000629-50-5	64
5	Heptane, 2,4-dimethyl-		128	C9H20	002213-23-2	59



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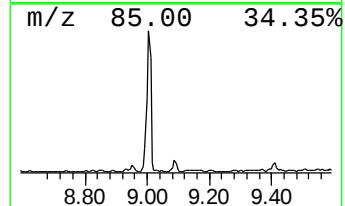
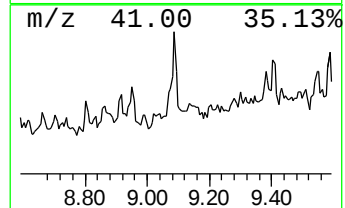
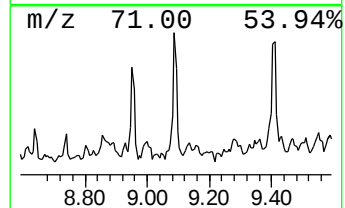
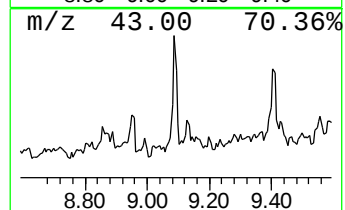
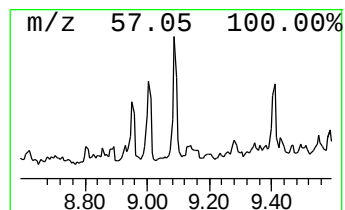
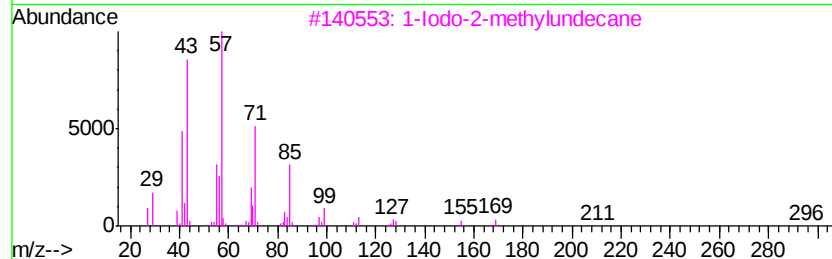
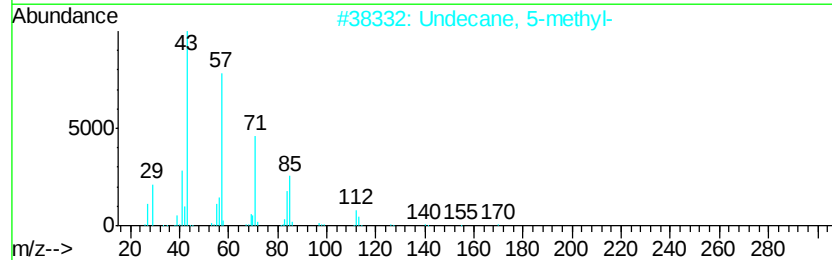
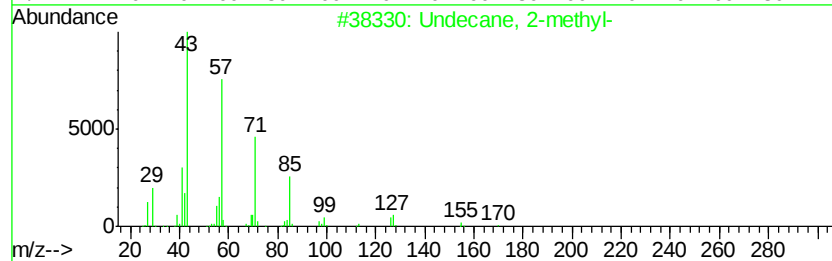
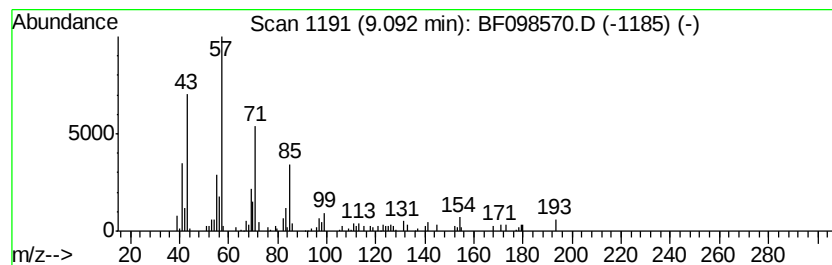
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Undecane, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.09	2.76 ng	156007	Acenaphthene-d10	9.68	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane, 2-methyl-	170	C12H26	007045-71-8	72
2	Undecane, 5-methyl-	170	C12H26	001632-70-8	72
3	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	64
4	Hexadecane	226	C16H34	000544-76-3	58
5	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	53



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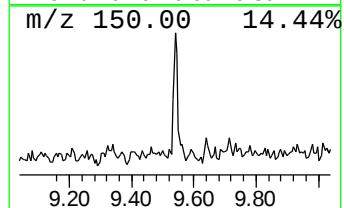
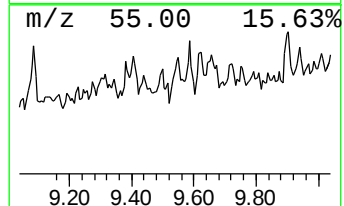
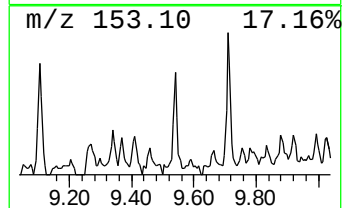
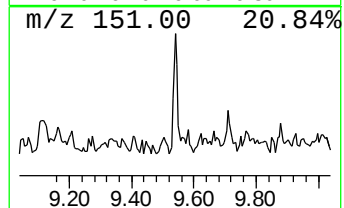
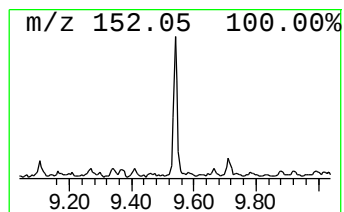
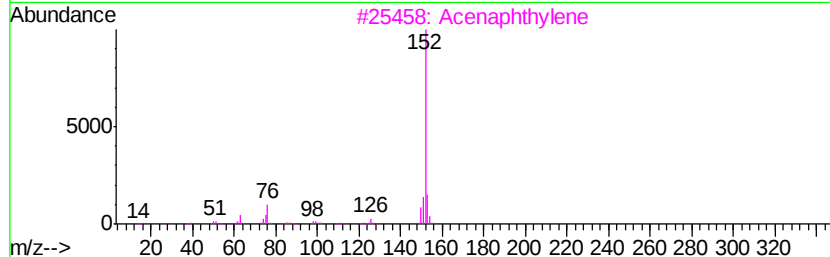
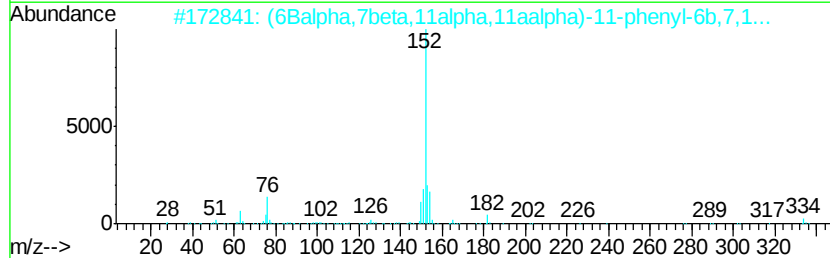
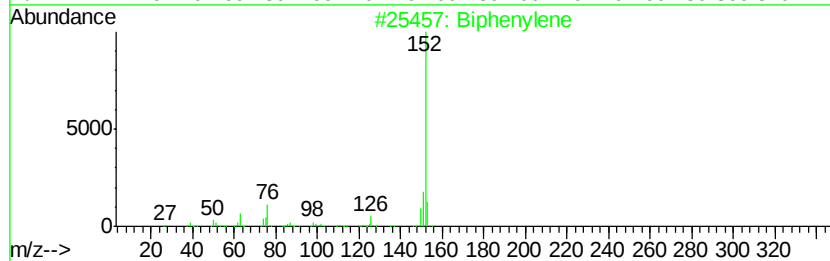
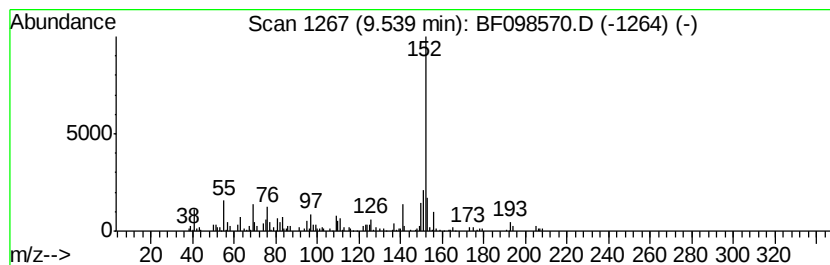
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Biphenylene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.54	2.95 ng	166857	Acenaphthene-d10	9.68

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Biphenylene	152	C12H8	000259-79-0	93
2			(6Balpha,7beta,11alpha,11aalpha)...	334	C25H18O	1000241-69-8	64
3			Acenaphthylene	152	C12H8	000208-96-8	64
4			Benzaldehyde, 2-hydroxy-3-methoxy-	152	C8H8O3	000148-53-8	53
5			5,6-Dihydro-4-methylthieno(2,3-d...	152	C7H8N2S	092204-06-3	53



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091517\
Data File : BF098570.D
Acq On : 15 Sep 2017 15:33
Operator : SJ/JU
Sample : I5188-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

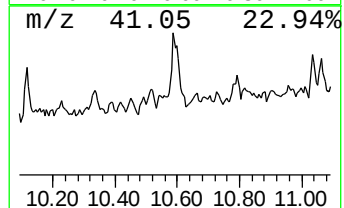
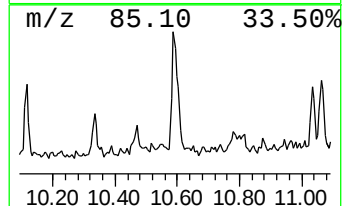
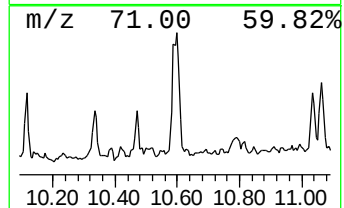
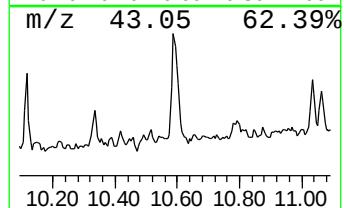
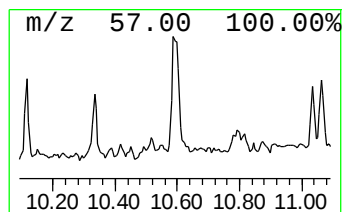
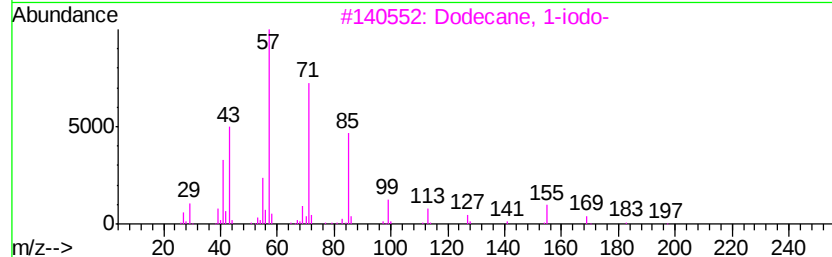
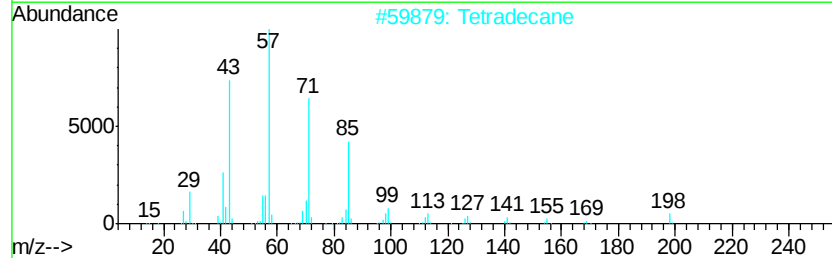
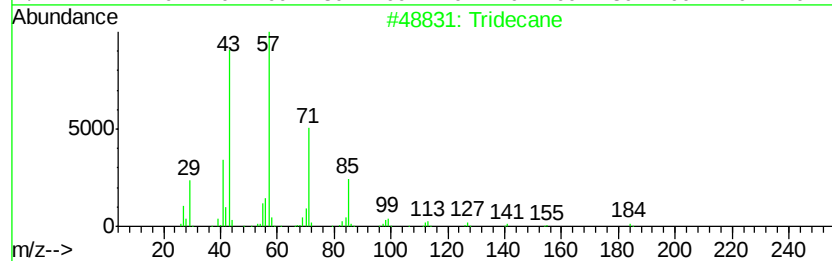
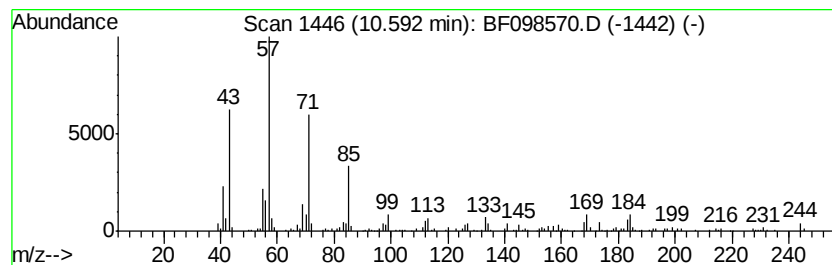
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ClientSampled :
RL-6-11-22

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tridecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.59	8.40 ng	377324	Phenanthrene-d10	11.16	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	87
2	Tetradecane	198	C14H30	000629-59-4	81
3	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	72
4	Tridecane, 6-methyl-	198	C14H30	013287-21-3	72
5	Undecane, 2-methyl-	170	C12H26	007045-71-8	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091517\
Data File : BF098570.D
Acq On : 15 Sep 2017 15:33
Operator : SJ/JU
Sample : I5188-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RL-6-11-22

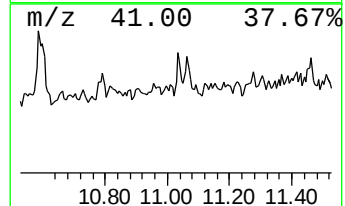
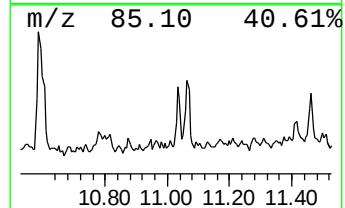
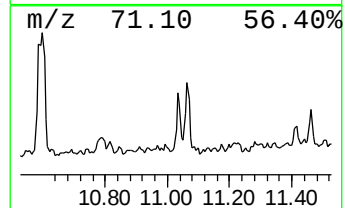
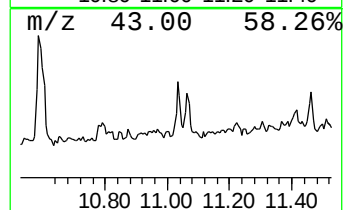
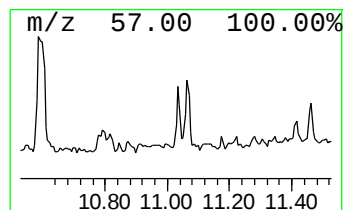
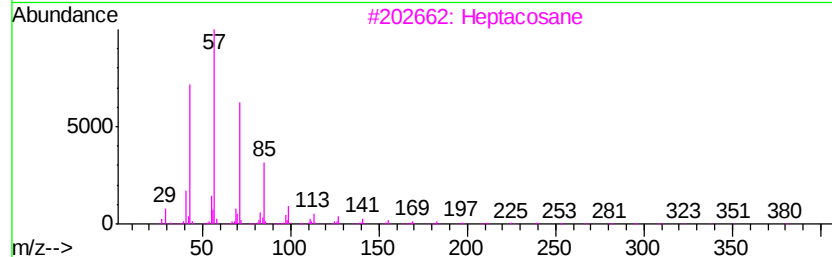
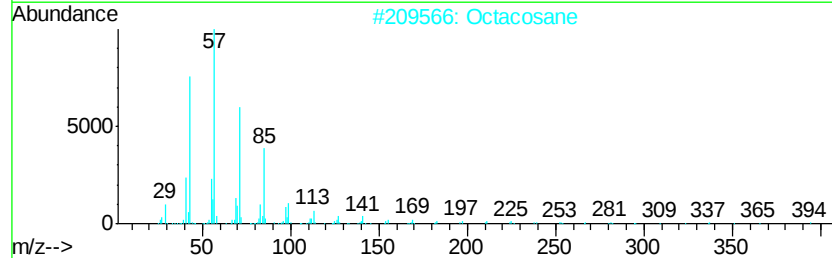
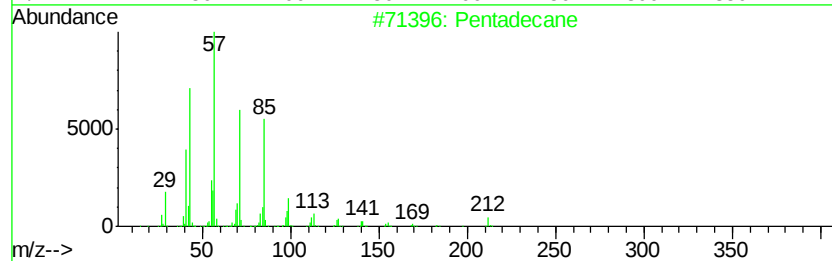
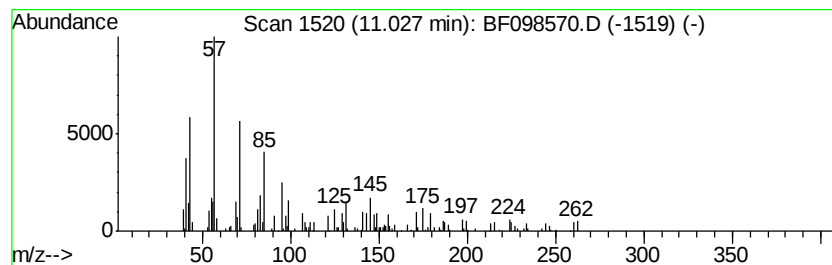
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Pentadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.03	2.71 ng	121764	Phenanthrene-d10	11.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecane	212	C15H32	000629-62-9	70
2		Octacosane	394	C28H58	000630-02-4	70
3		Heptacosane	380	C27H56	000593-49-7	62
4		Eicosane	282	C20H42	000112-95-8	58
5		Hexadecane	226	C16H34	000544-76-3	58



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091517\
Data File : BF098570.D
Acq On : 15 Sep 2017 15:33
Operator : SJ/JU
Sample : I5188-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RL-6-11-22

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.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...	4.83	8.8	ng	398330	1	6.65	908317	20.0
unknown6.42	6.42	81.4	ng	3695720	1	6.65	908317	20.0
Decane	6.48	2.6	ng	118750	1	6.65	908317	20.0
Undecane, 2-methyl-	9.09	2.8	ng	156007	3	9.68	1132140	20.0
Biphenylene	9.54	3.0	ng	166857	3	9.68	1132140	20.0
Tridecane	10.59	8.4	ng	377324	4	11.16	898657	20.0
Pentadecane	11.03	2.7	ng	121764	4	11.16	898657	20.0