

Data Path : Z:\HPCHEM1\BNA F\DATA\BF070316\
 Data File : BF088669.D
 Acq On : 4 Jul 2016 1:45
 Operator : UM/SJ
 Sample : H3817-11
 Misc :
 ALS Vial : 31 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 BS-4A-9.5-10FT

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-BF063016.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	1.850	21	23	35	rVV	38702	54473	1.69%	0.188%
2	2.021	35	38	41	rVB	66149	78392	2.43%	0.270%
3	3.016	123	125	139	rBV	72593	151191	4.68%	0.522%
4	4.959	292	295	300	rBV	194418	269105	8.33%	0.928%
5	5.382	329	332	334	rBV	2765619	2941915	91.04%	10.149%
6	6.422	419	423	425	rBV	2824764	3231391	100.00%	11.148%
7	6.547	431	434	437	rBV	2503530	3085912	95.50%	10.646%
8	6.787	452	455	456	rBV	515095	686982	21.26%	2.370%
9	6.936	466	468	471	rVB	1996720	2131616	65.97%	7.354%
10	7.348	501	504	506	rBV	2052291	2092176	64.75%	7.218%
11	8.068	564	567	569	rBV	1171840	1025040	31.72%	3.536%
12	9.142	658	661	664	rBV	2781347	2781069	86.06%	9.594%
13	9.542	693	696	698	rVB	256790	351813	10.89%	1.214%
14	9.816	717	720	722	rBV	1295544	1124484	34.80%	3.879%
15	10.605	786	789	791	rBV	2069488	2245629	69.49%	7.747%
16	10.731	798	800	804	rVB	52045	53251	1.65%	0.184%
17	11.176	837	839	841	rBV	105626	95784	2.96%	0.330%
18	11.291	847	849	852	rVV	1288933	1095659	33.91%	3.780%
19	11.359	852	855	859	rVB2	28248	65532	2.03%	0.226%
20	12.708	971	973	975	rBV	78056	76744	2.37%	0.265%
21	12.879	985	988	990	rBV	2763459	2660008	82.32%	9.177%
22	13.360	1028	1030	1032	rBV	67067	86017	2.66%	0.297%
23	13.417	1033	1035	1038	rVB	45606	53494	1.66%	0.185%
24	13.794	1066	1068	1076	rBV	233946	398003	12.32%	1.373%
25	13.920	1076	1079	1081	rVV	847101	950805	29.42%	3.280%
26	14.434	1123	1124	1131	rVB	65082	109062	3.38%	0.376%
27	15.017	1172	1175	1177	rBV	43080	47150	1.46%	0.163%
28	15.303	1197	1200	1203	rBV	498145	728170	22.53%	2.512%
29	15.851	1243	1248	1254	rBV5	12097	47000	1.45%	0.162%
30	17.691	1402	1409	1415	rVB4	67739	178119	5.51%	0.614%
31	19.063	1524	1529	1539	rVB3	28733	90524	2.80%	0.312%

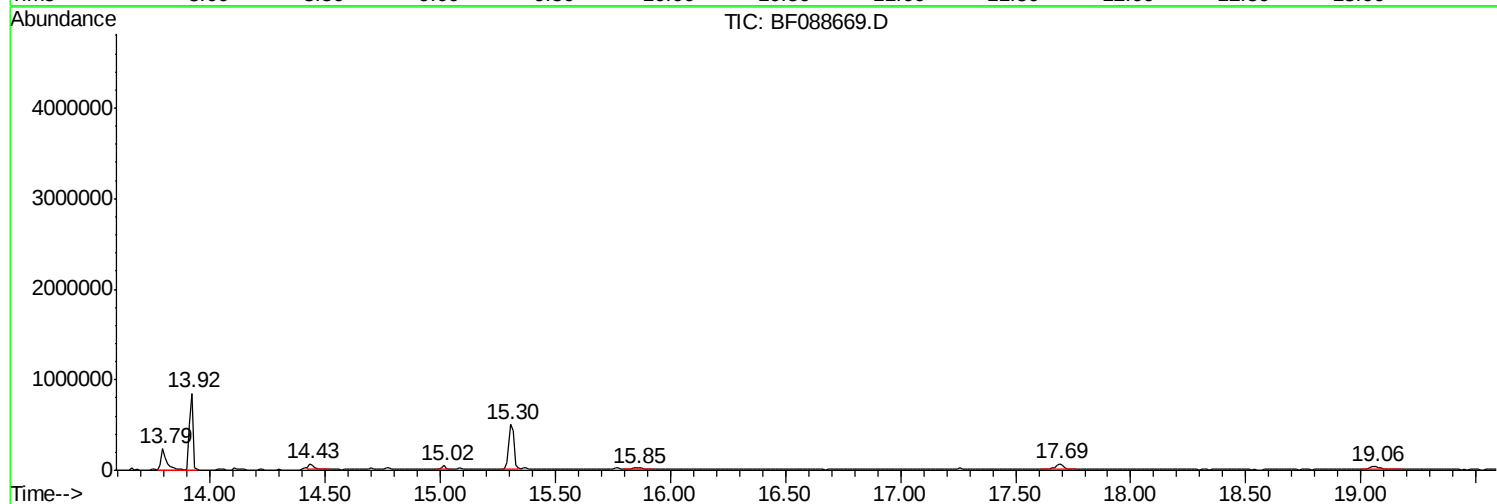
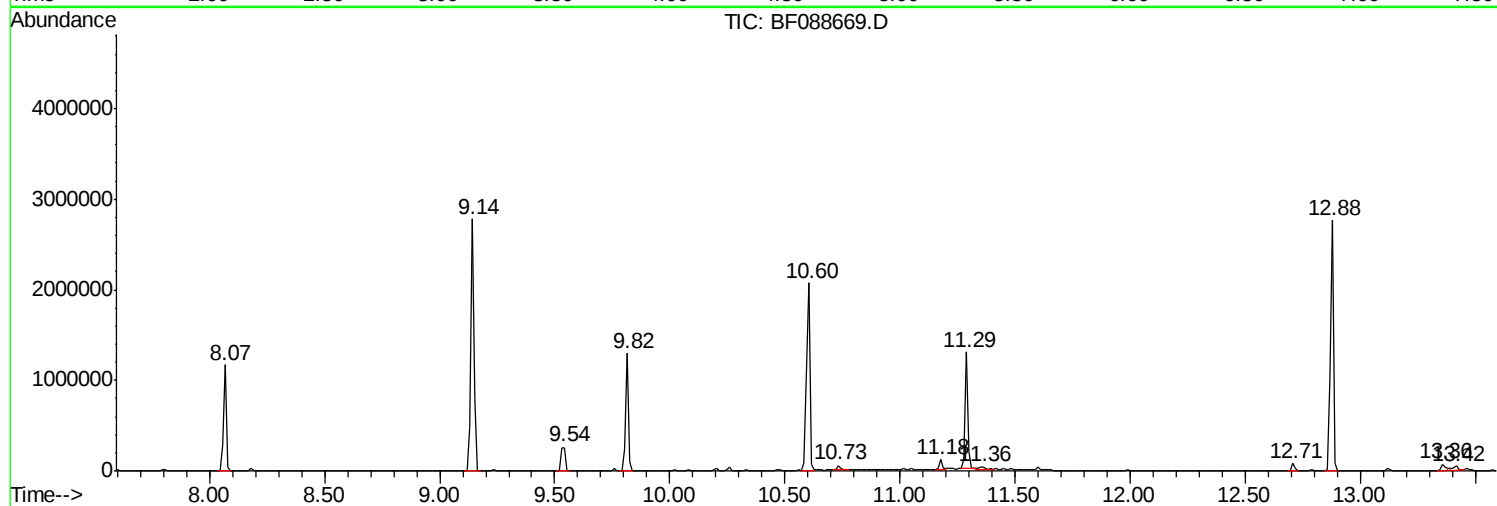
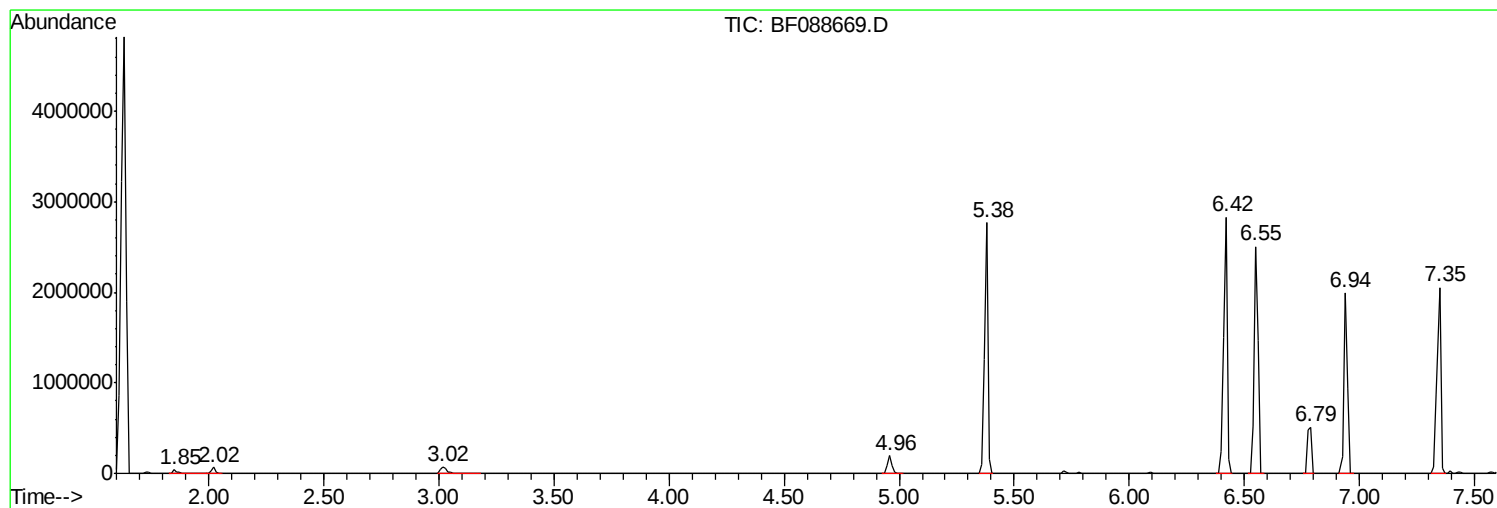
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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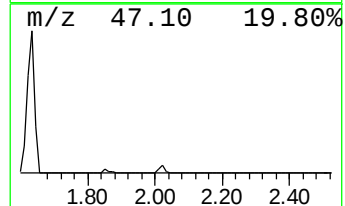
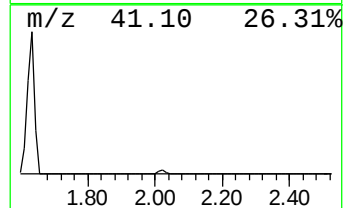
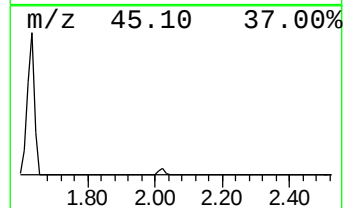
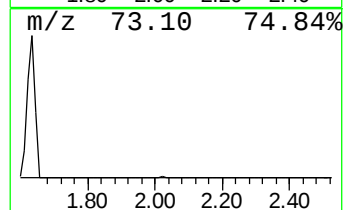
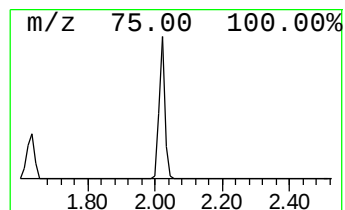
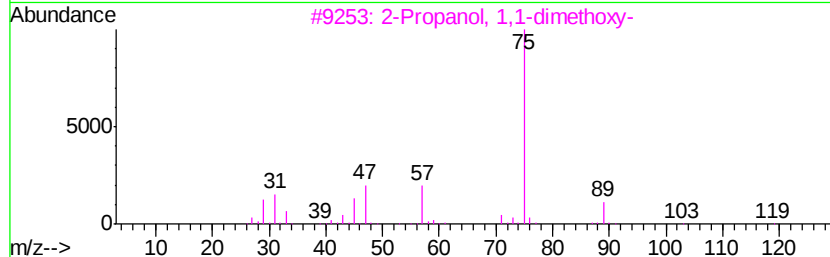
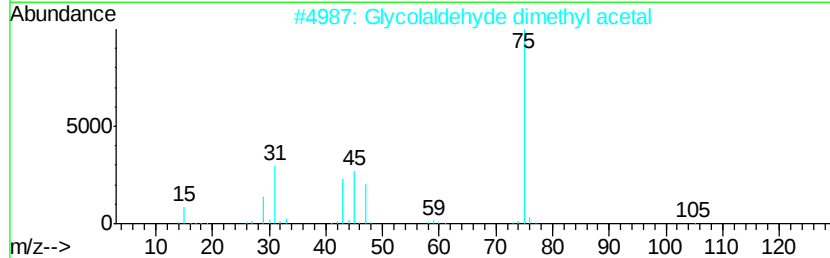
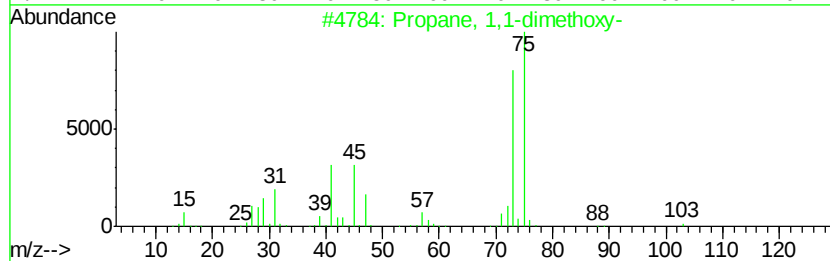
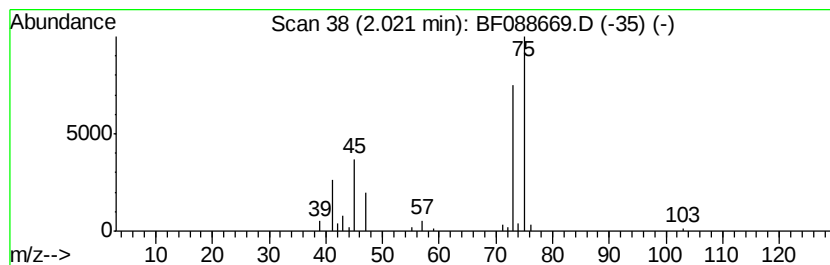
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TIC Library : C:\Database\NIST11.L
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Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.02	2.28 ng	78392	1,4-Dichlorobenzene-d4	6.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	74
2		Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	50
3		2-Propanol, 1,1-dimethoxy-	120	C5H12O3	042919-42-6	38
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	14
5		1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	10



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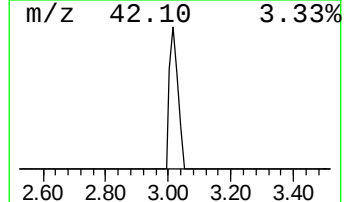
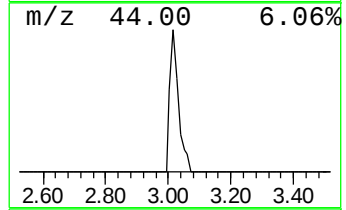
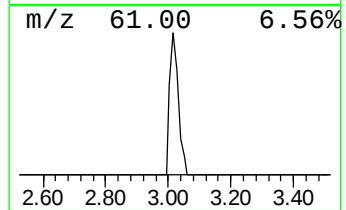
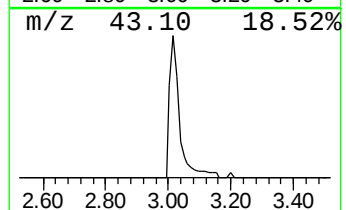
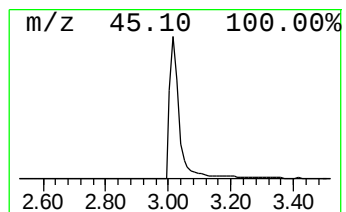
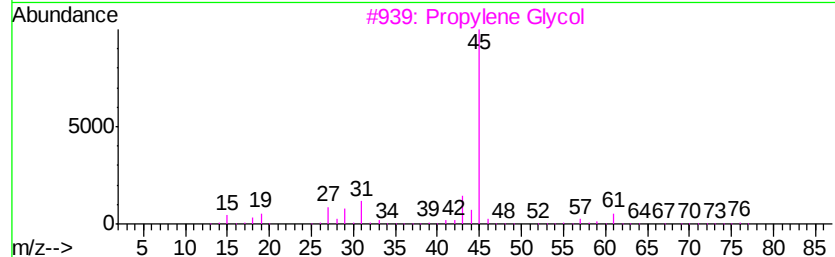
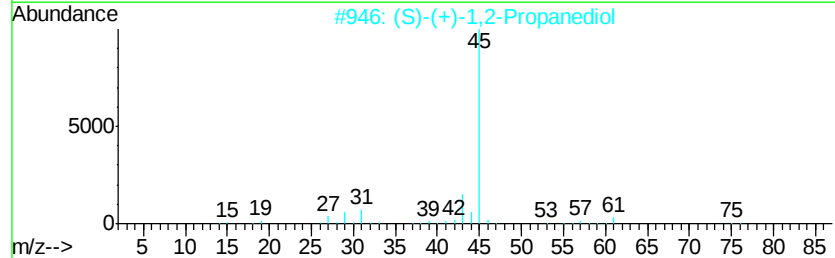
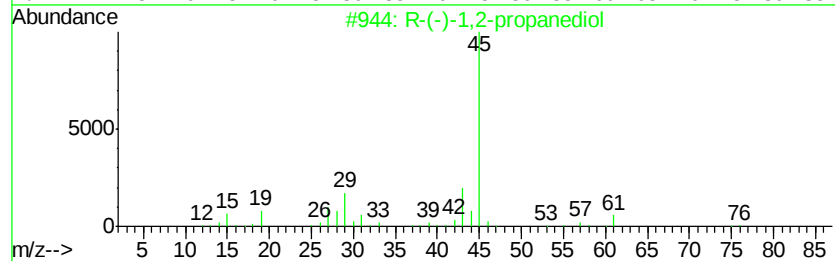
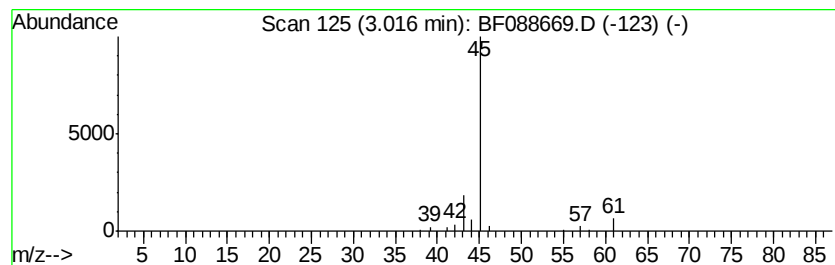
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Peak Number 2 R-(-)-1,2-propanediol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.02	4.40 ng	151191	1,4-Dichlorobenzene-d4	6.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	64
2		(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
3		Propylene Glycol	76	C3H8O2	000057-55-6	9
4		Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5		Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	002155-30-8	9



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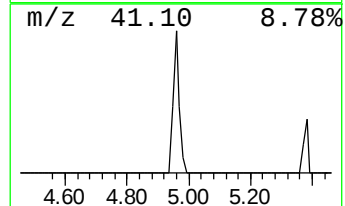
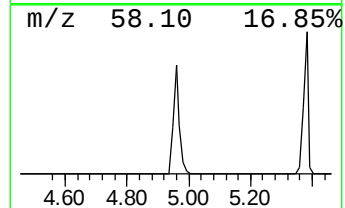
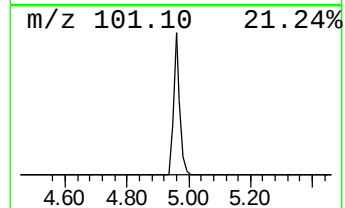
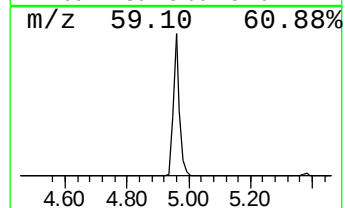
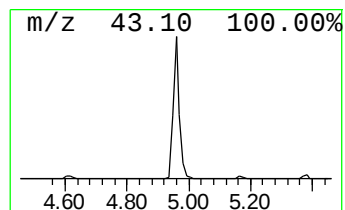
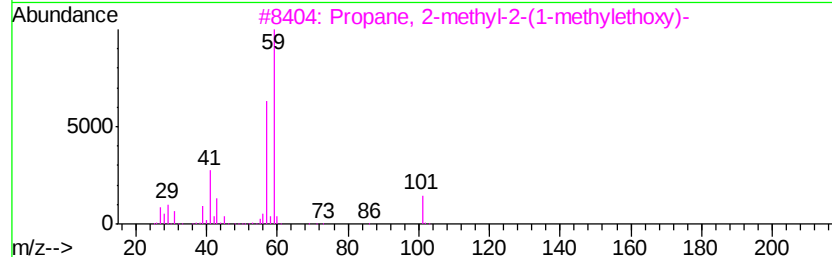
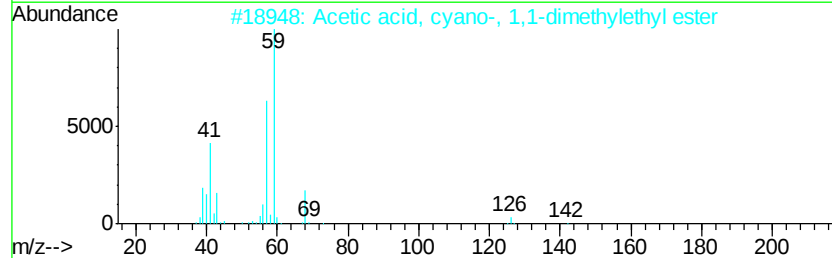
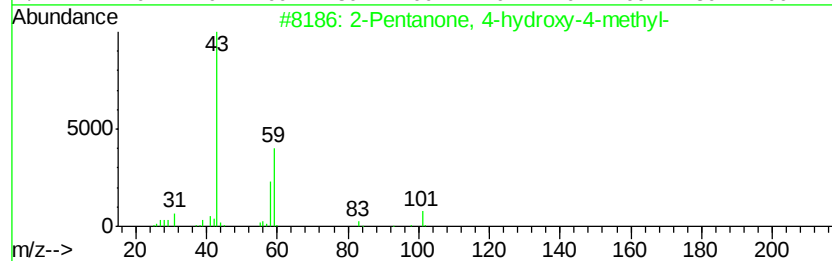
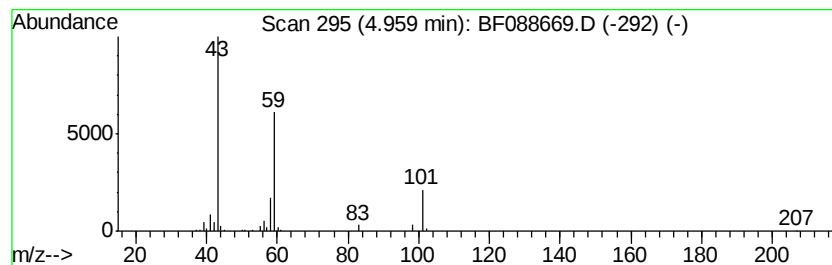
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.96	7.83 ng	269105	1,4-Dichlorobenzene-d4	6.79

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	32
3			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	23
4			Butane	58	C4H10	000106-97-8	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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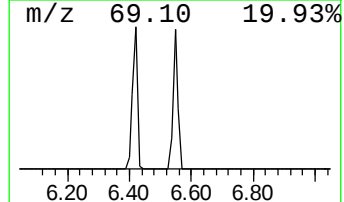
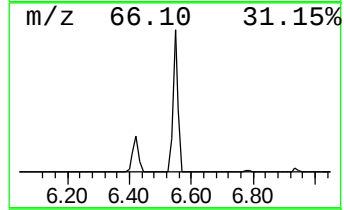
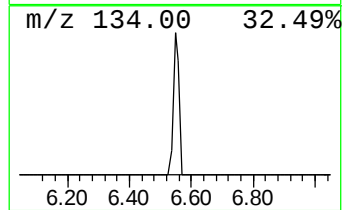
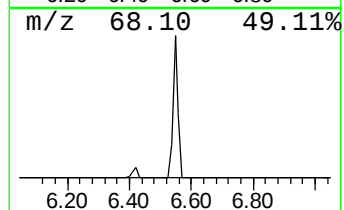
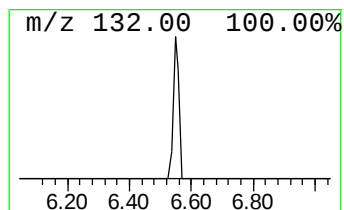
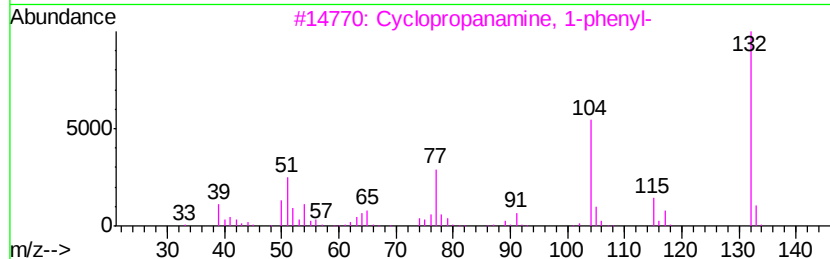
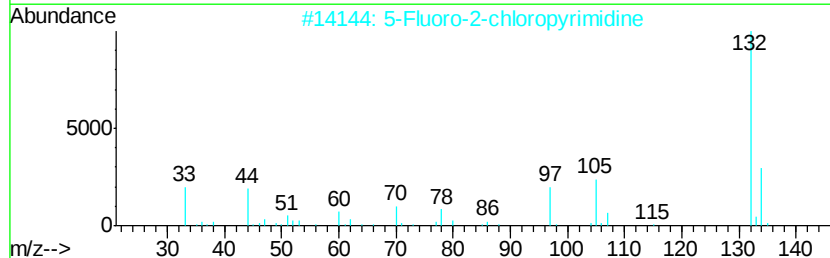
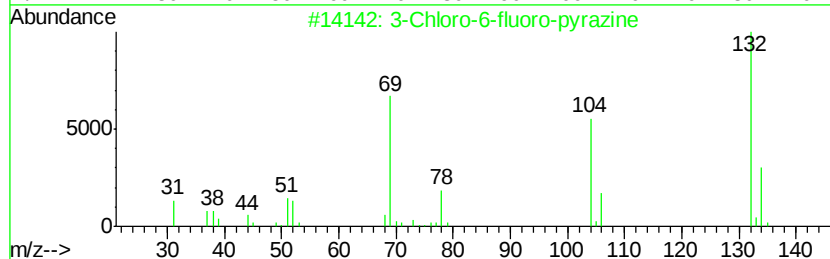
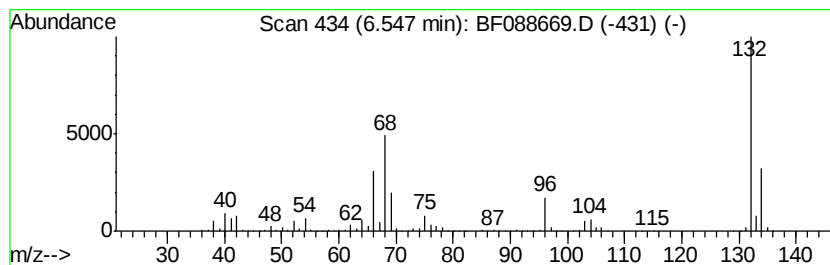
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Peak Number 4 unknown6.55 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.55	89.84 ng	3085910	1,4-Dichlorobenzene-d4	6.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
4		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
5		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10



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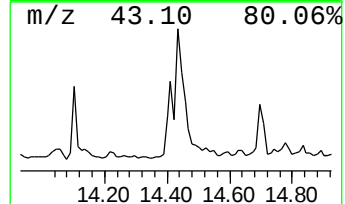
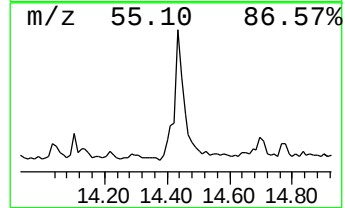
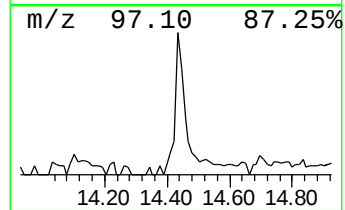
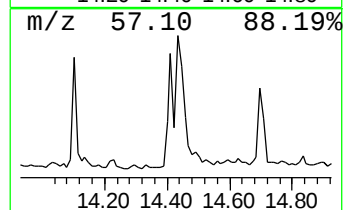
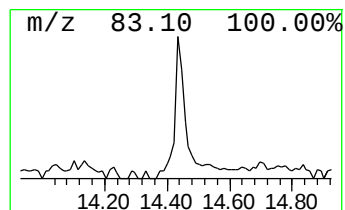
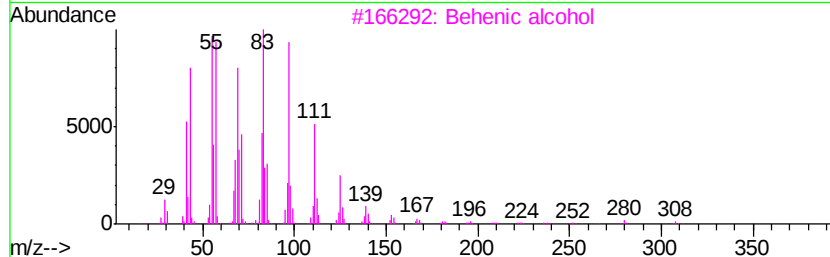
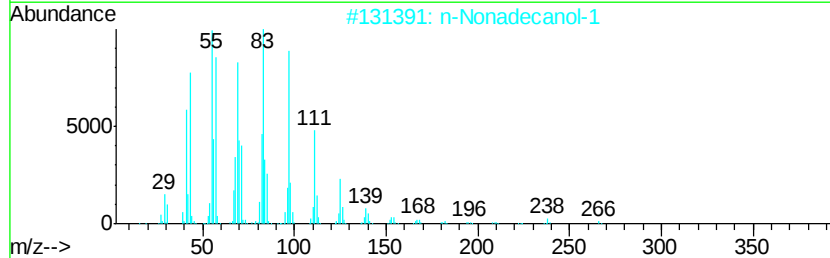
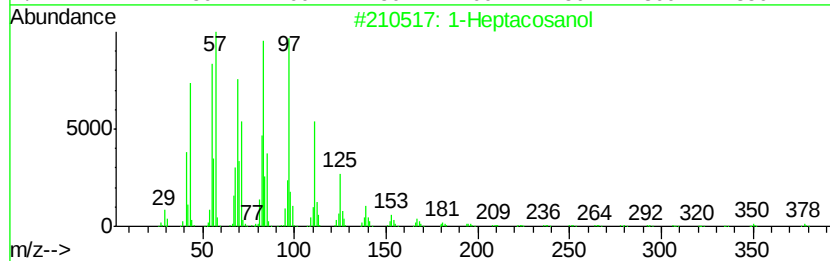
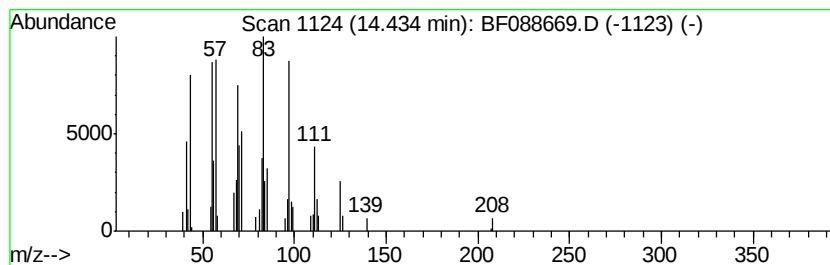
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Peak Number 7 1-Heptacosanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.43	2.29 ng	109062	Chrysene-d12	13.92	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	93
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	90
3	Behenic alcohol	326	C22H46O	000661-19-8	90
4	1-Heneicosanol	312	C21H44O	015594-90-8	90
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	87



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BS-4A-9.5-10FT

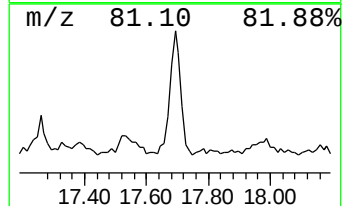
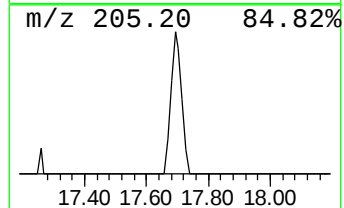
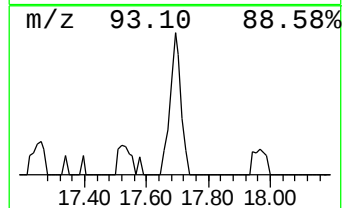
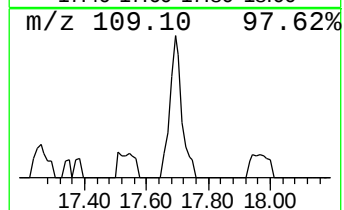
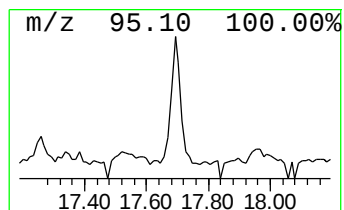
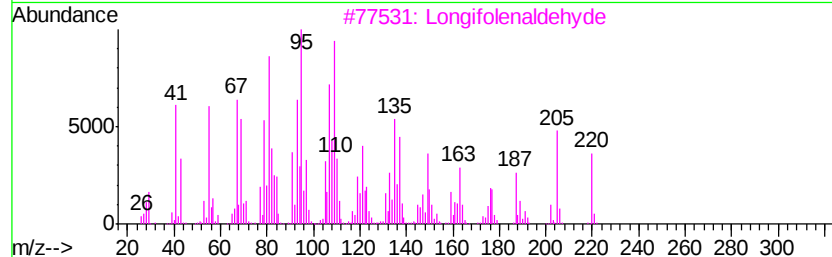
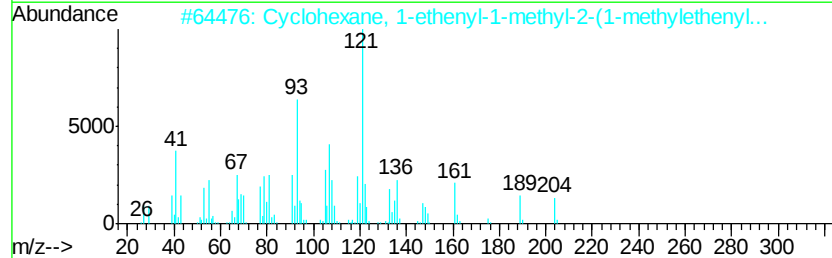
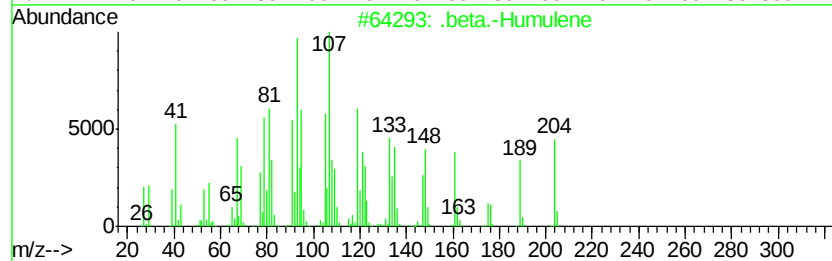
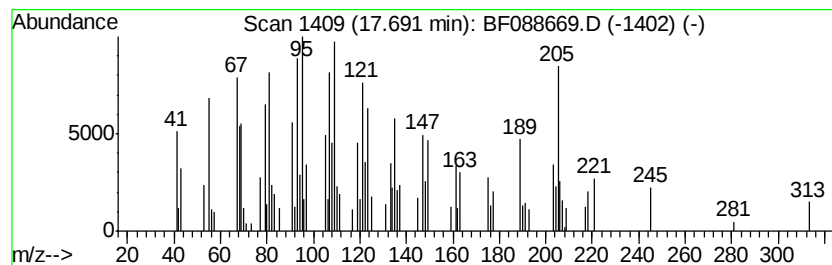
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 .beta.-Humulene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.69	4.89 ng	178119	Perylene-d12	15.31

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	.beta.-Humulene	204	C15H24	000116-04-1	56
2		Cyclohexane, 1-ethenyl-1-methyl-...	204	C15H24	003242-08-8	55
3		Longifolenaldehyde	220	C15H24O	019890-84-7	49
4		Guaia-9,11-diene	204	C15H24	1000374-19-8	47
5		.gamma.-Elemene	204	C15H24	029873-99-2	46



Data Path : Z:\HPCHEM1\BNA F\DATA\BF070316\
Data File : BF088669.D
Acq On : 4 Jul 2016 1:45
Operator : UM/SJ
Sample : H3817-11
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BS-4A-9.5-10FT

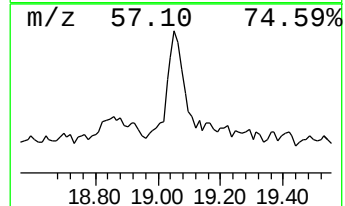
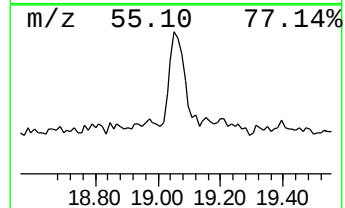
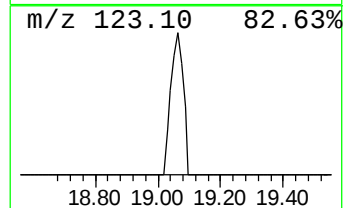
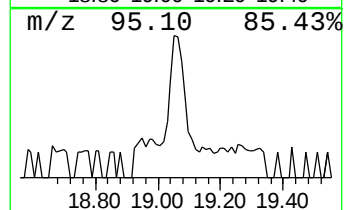
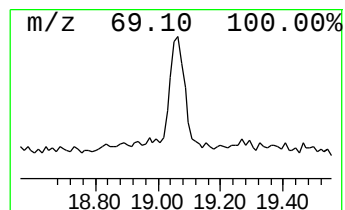
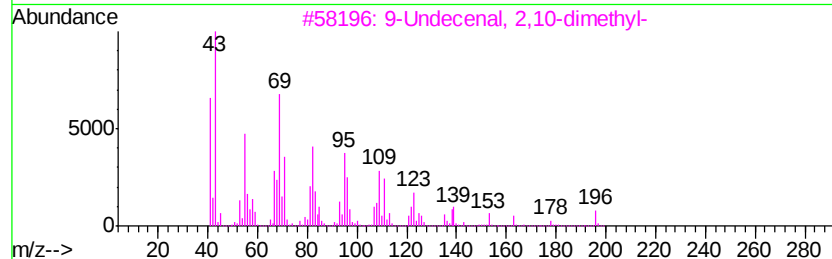
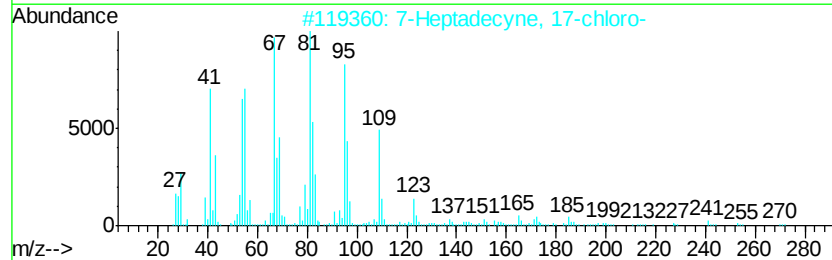
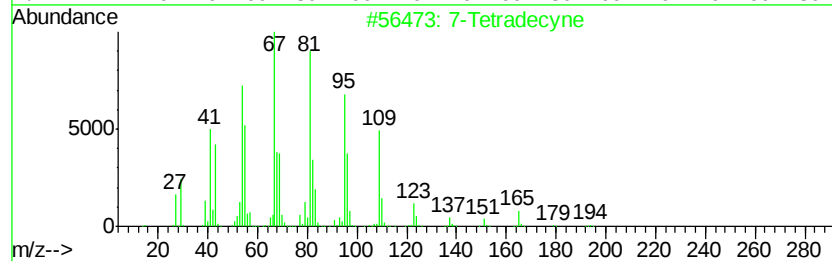
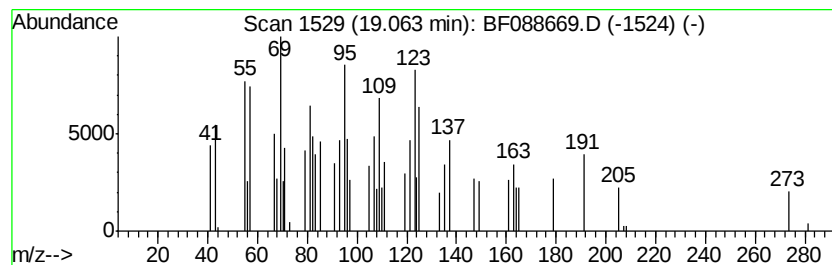
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown19.06 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.06	2.49 ng	90524	Perylene-d12	15.31

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	7-Tetradecyne	194	C14H26	035216-11-6	22
2		7-Heptadecyne, 17-chloro-	270	C17H31Cl	056554-75-7	22
3		9-Undecenal, 2,10-dimethyl-	196	C13H24O	1000131-85-9	22
4		Bicyclo[4.1.0]heptane-7-carboxyl...	258	C16H18O3	1000311-46-7	22
5		Caparratriene	206	C15H26	1000374-08-7	22



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070316\
Data File : BF088669.D
Acq On : 4 Jul 2016 1:45
Operator : UM/SJ
Sample : H3817-11
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BS-4A-9.5-10FT

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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
Propane, 1,1-dime...	2.02	2.3	ng	78392	1	6.79	686982	20.0
R-(-)-1,2-propane...	3.02	4.4	ng	151191	1	6.79	686982	20.0
2-Pentanone, 4-hy...	4.96	7.8	ng	269105	1	6.79	686982	20.0
unknown6.55	6.55	89.8	ng	3085910	1	6.79	686982	20.0
1-Heptacosanol	14.43	2.3	ng	109062	5	13.92	950805	20.0
.beta.-Humulene	17.69	4.9	ng	178119	6	15.31	728170	20.0
unknown19.06	19.06	2.5	ng	90524	6	15.31	728170	20.0