

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112817\
 Data File : BF100954.D
 Acq On : 29 Nov 2017 1:16
 Operator : SJ/JU
 Sample : I6579-06
 Misc :
 ALS Vial : 31 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 HAR-5-E(7-8)

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-BF110817.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	5.081	505	509	518	rBV	116828	145905	13.73%	1.532%
2	5.475	572	576	580	rBV	1055399	1021291	96.13%	10.727%
3	6.487	743	748	751	rBV	1106162	1035049	97.42%	10.871%
4	6.628	768	772	775	rBV	1279289	1062443	100.00%	11.159%
5	6.857	808	811	815	rBV	450497	346555	32.62%	3.640%
6	7.016	834	838	841	rBV	934861	780430	73.46%	8.197%
7	7.422	902	907	910	rBV	746226	612964	57.69%	6.438%
8	8.139	1025	1029	1032	rBV	527875	410889	38.67%	4.316%
9	8.692	1120	1123	1127	rBV	52895	41290	3.89%	0.434%
10	9.216	1208	1212	1215	rBV	1054431	950991	89.51%	9.988%
11	9.604	1275	1278	1285	rBB	33183	25851	2.43%	0.272%
12	9.892	1324	1327	1331	rBV	430928	375933	35.38%	3.948%
13	10.604	1445	1448	1452	rBV	197429	156654	14.74%	1.645%
14	10.680	1458	1461	1471	rBV	520031	468173	44.07%	4.917%
15	11.380	1577	1580	1583	rBV	392543	319228	30.05%	3.353%
16	12.821	1821	1825	1828	rBV	11920	13610	1.28%	0.143%
17	12.963	1845	1849	1852	rBV	913785	748555	70.46%	7.862%
18	13.857	1998	2001	2008	rBV2	30545	41379	3.89%	0.435%
19	14.021	2025	2029	2038	rBV	453794	404887	38.11%	4.252%
20	14.451	2098	2102	2103	rBV4	10708	13390	1.26%	0.141%
21	15.062	2203	2206	2212	rVB6	13609	19744	1.86%	0.207%
22	15.115	2212	2215	2218	rBV5	17703	17681	1.66%	0.186%
23	15.427	2265	2268	2273	rBV7	13854	23053	2.17%	0.242%
24	15.492	2274	2279	2284	rBV	255959	323952	30.49%	3.402%
25	15.709	2312	2316	2319	rBV6	7646	12601	1.19%	0.132%
26	15.933	2351	2354	2358	rBV4	13127	16907	1.59%	0.178%
27	16.186	2394	2397	2406	rVB10	24202	47664	4.49%	0.501%
28	16.439	2437	2440	2443	rVB4	12287	15059	1.42%	0.158%
29	16.627	2466	2472	2476	rVB5	20444	33286	3.13%	0.350%
30	17.021	2536	2539	2541	rBV4	10873	14875	1.40%	0.156%
31	17.198	2566	2569	2576	rVB8	12645	20868	1.96%	0.219%

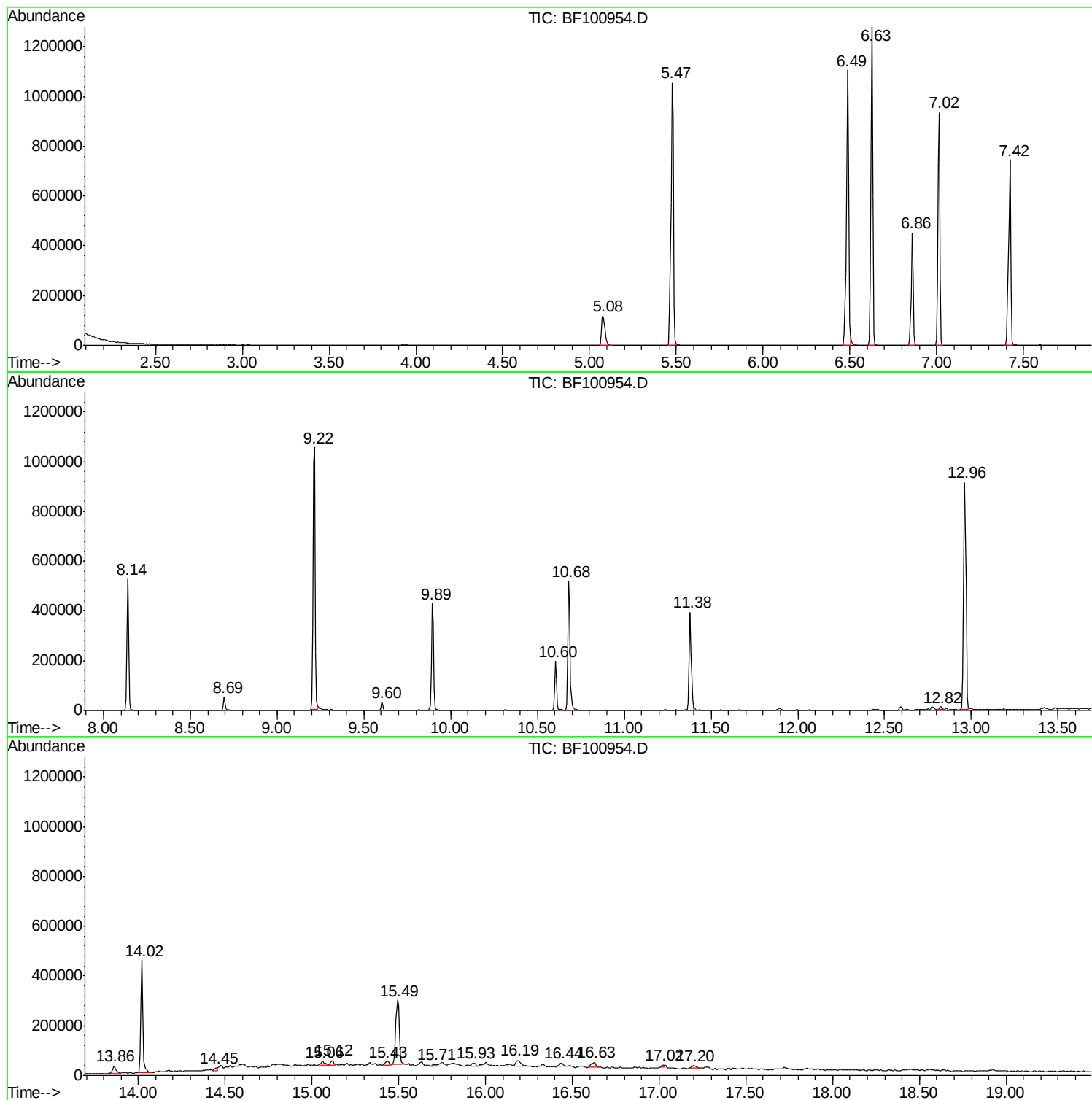
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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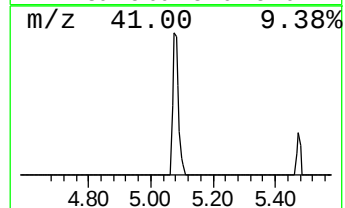
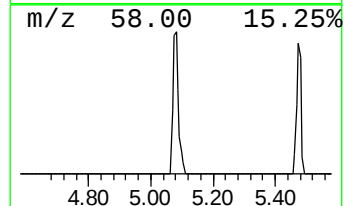
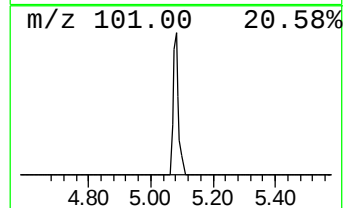
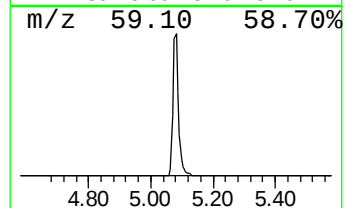
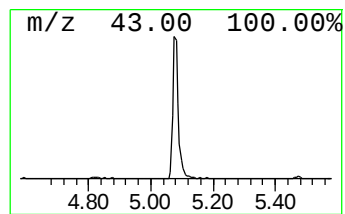
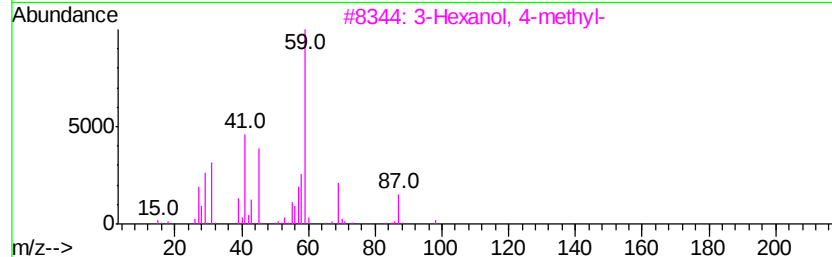
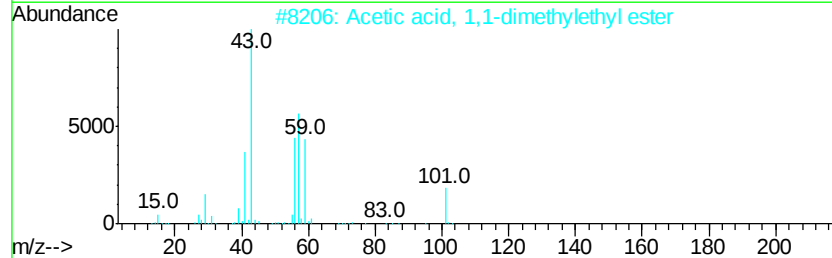
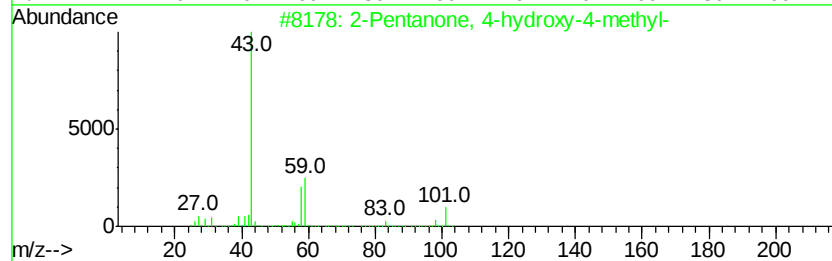
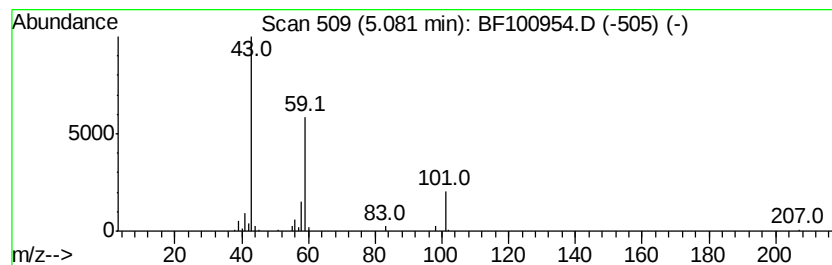
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.08	8.42 ng	145905	1,4-Dichlorobenzene-d4	6.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5			4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9



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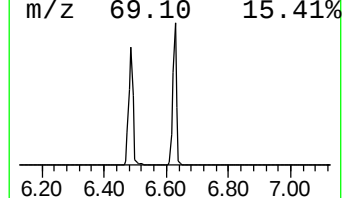
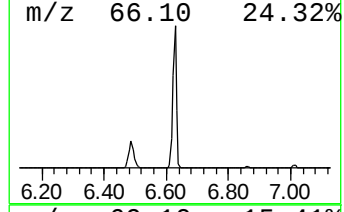
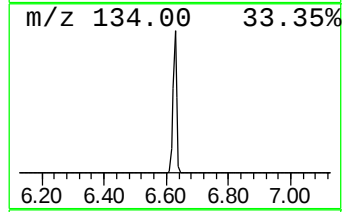
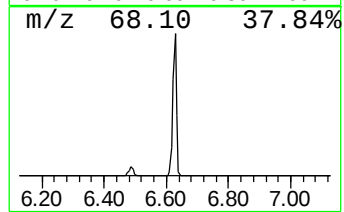
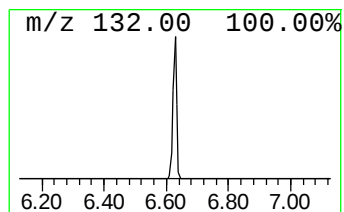
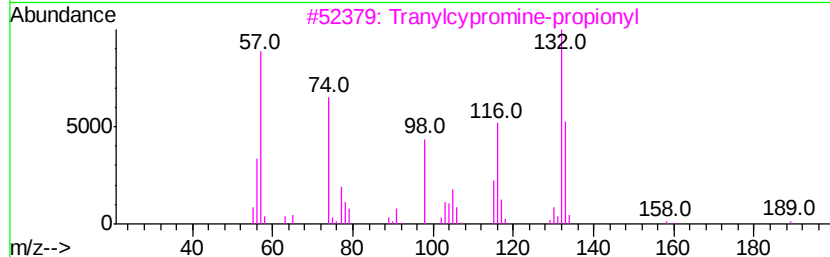
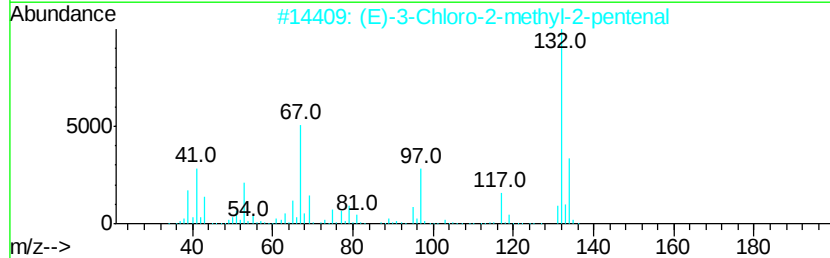
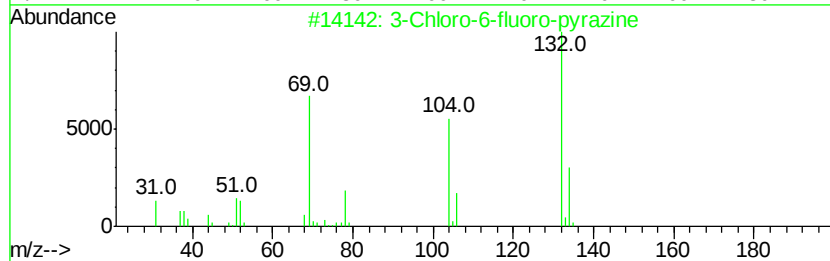
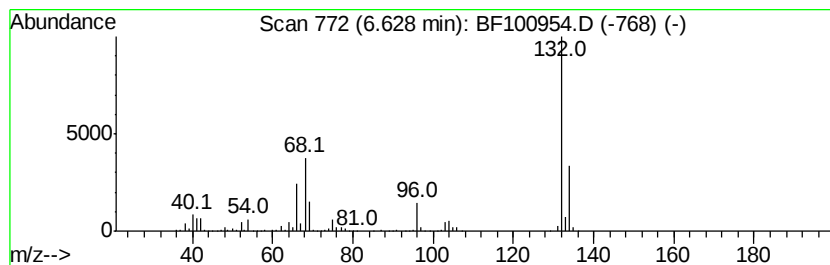
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Peak Number 2 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	61.31 ng	1062440	1,4-Dichlorobenzene-d4	6.86

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	17
3		Tranvlcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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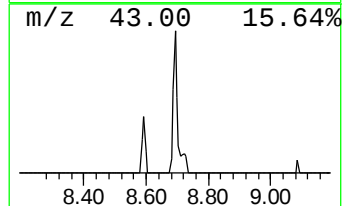
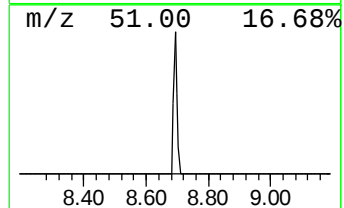
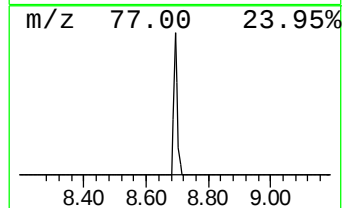
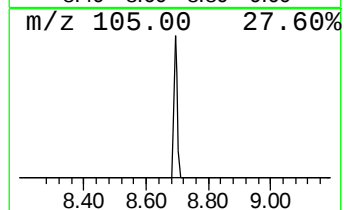
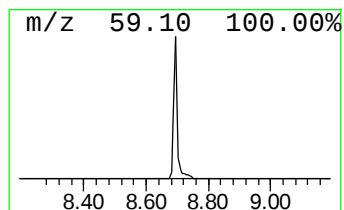
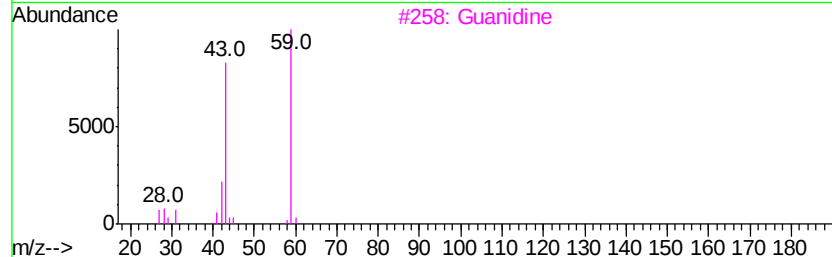
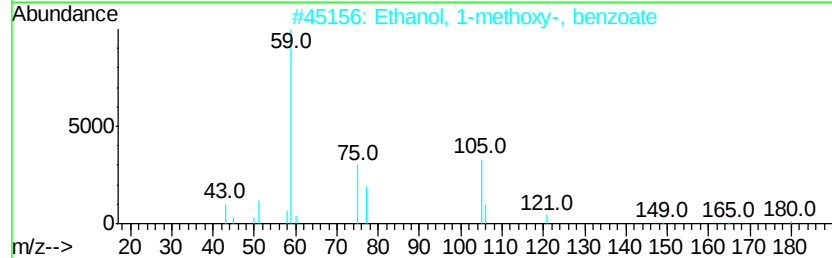
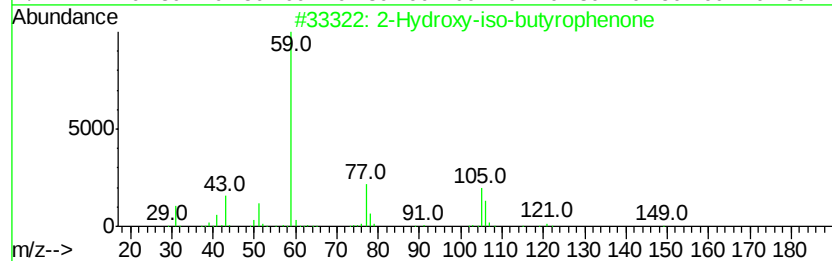
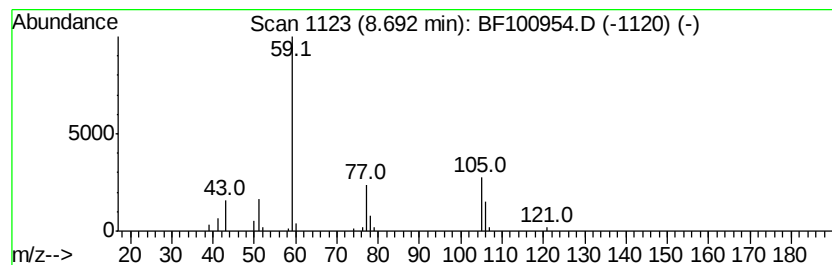
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Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.69	2.01 ng	41290	Napthalene-d8	8.14

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	90
2		Ethanol, 1-methoxy-, benzoate	180	C10H12O3	051835-44-0	64
3		Guanidine	59	CH5N3	000113-00-8	7
4		Acetamide	59	C2H5NO	000060-35-5	5
5		2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	4



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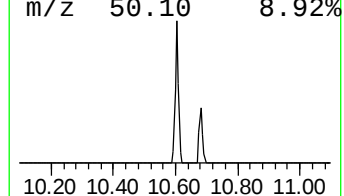
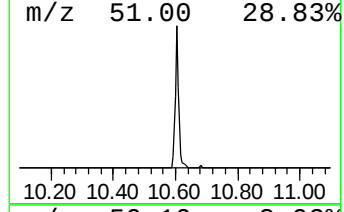
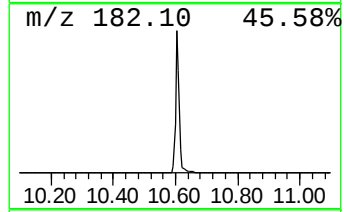
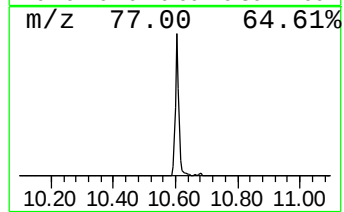
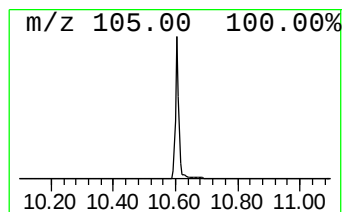
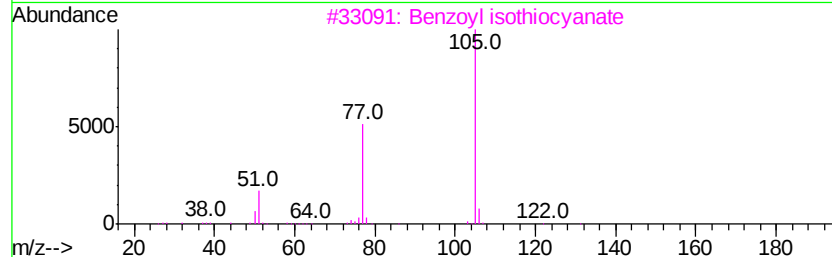
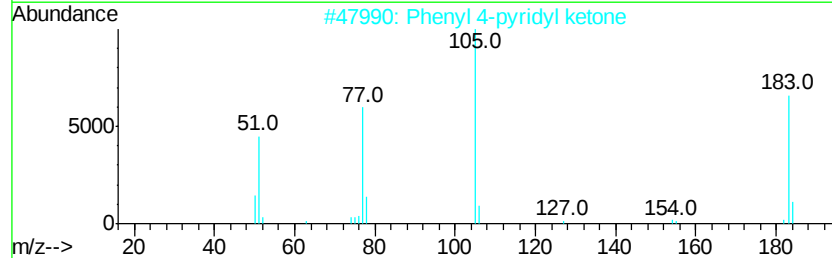
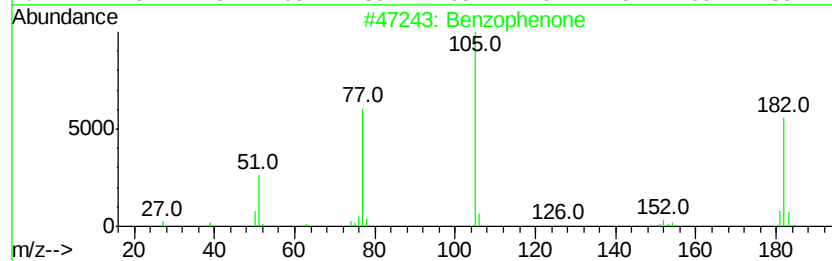
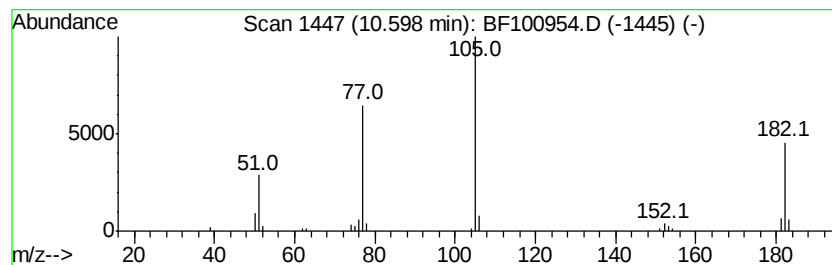
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Peak Number 5 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.60	8.33 ng	156654	Acenaphthene-d10	9.89

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzophenone	182	C13H10O	000119-61-9	96
2		Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	58
3		Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	47
4		Benzilamide	227	C14H13NO2	004746-87-6	47
5		Benzenecarbothioic acid	138	C7H6OS	000098-91-9	47



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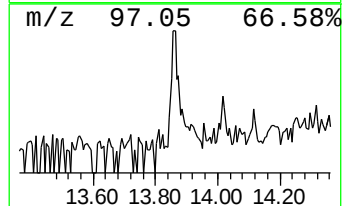
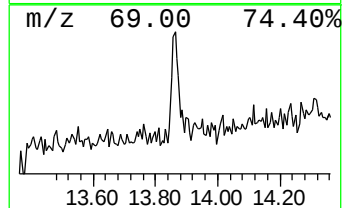
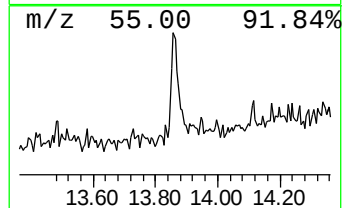
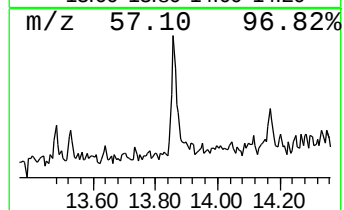
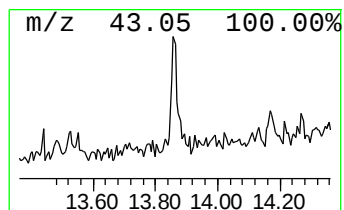
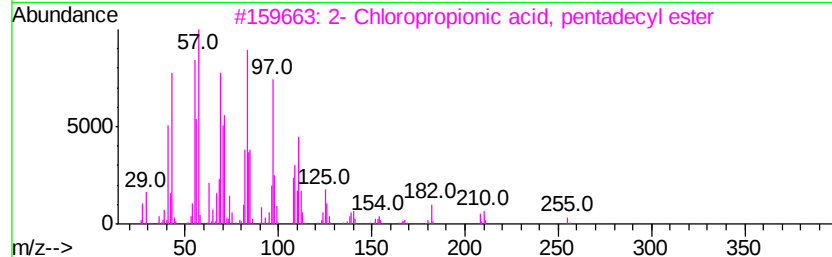
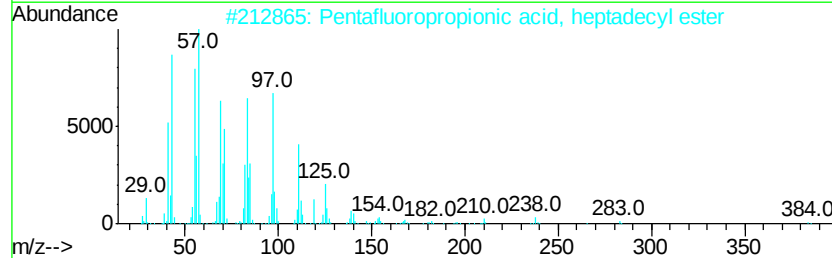
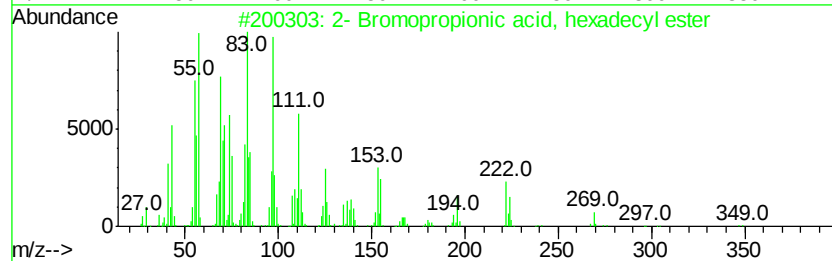
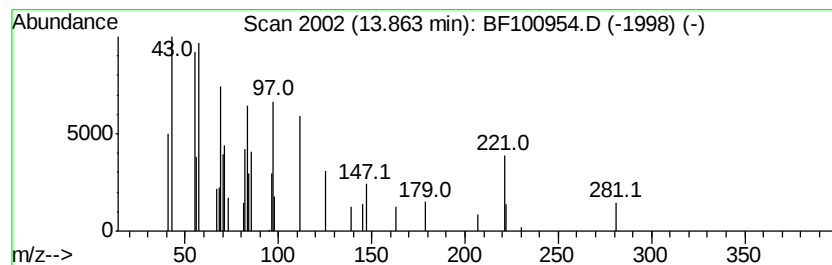
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Peak Number 6 2- Bromopropionic acid, hex... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.86	2.04 ng	41379	Chrysene-d12	14.02

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-	Bromopropionic acid, hexadecyl...	376	C19H37BrO2	063966-83-6	74	
2	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	68		
3	2- Chloropropionic acid, pentade...	318	C18H35ClO2	1000292-44-1	62		
4	Heptadecyl heptafluorobutyrat	452	C21H35F7O2	959085-66-6	62		
5	2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	62		



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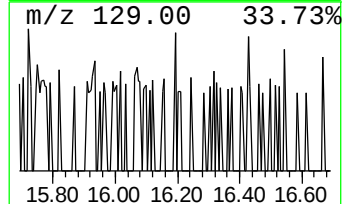
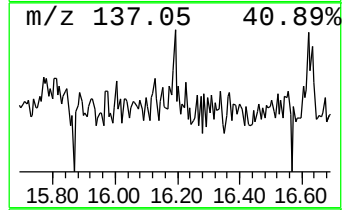
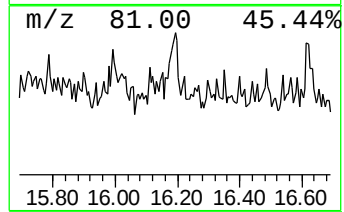
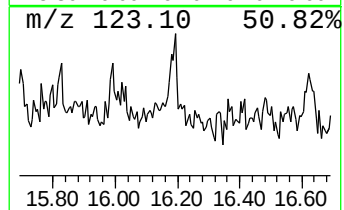
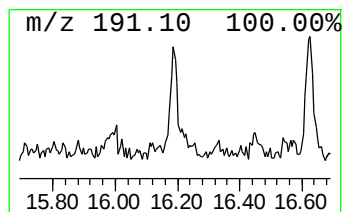
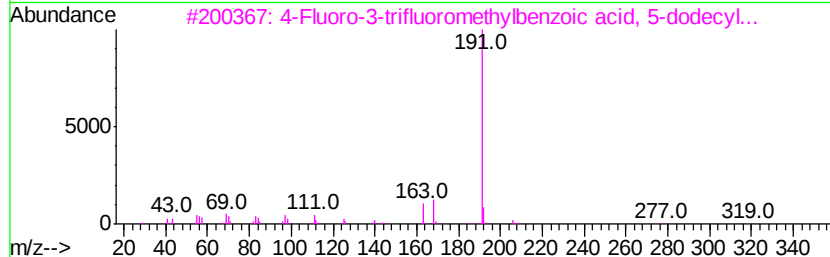
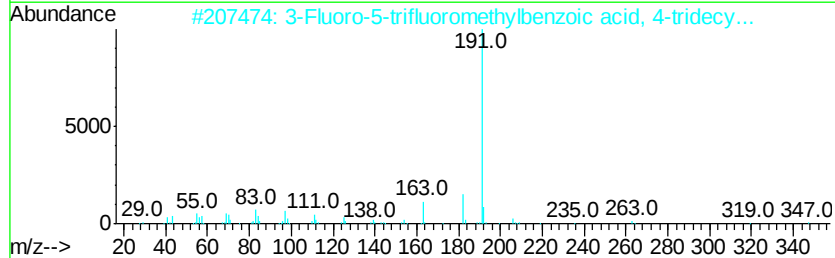
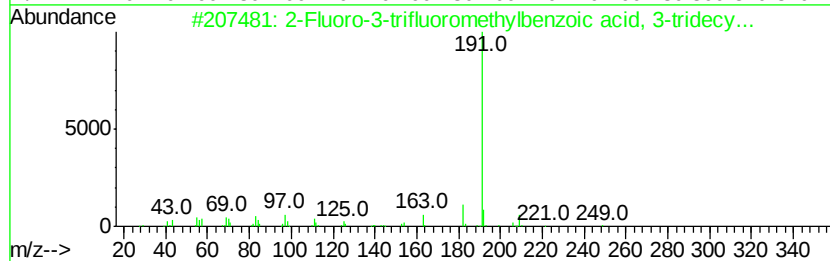
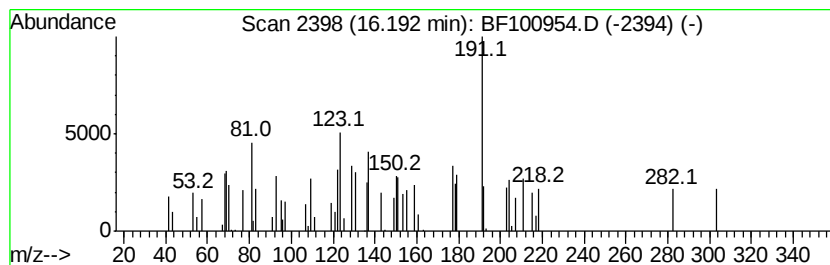
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown16.19 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.19	2.94 ng	47664	Perylene-d12	15.49

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Fluoro-3-trifluoromethylbenzoi...	390	C21H30F4O2	1000338-51-5	22		
2	3-Fluoro-5-trifluoromethylbenzoi...	390	C21H30F4O2	1000338-66-2	22		
3	4-Fluoro-3-trifluoromethylbenzoi...	376	C20H28F4O2	1000338-67-5	22		
4	N,N'-di-sec-Butyl-p-phenylenedia...	220	C14H24N2	000101-96-2	22		
5	4-Fluoro-2-trifluoromethylbenzoic...	390	C21H30F4O2	1000338-49-6	22		



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112817\
Data File : BF100954.D
Acq On : 29 Nov 2017 1:16
Operator : SJ/JU
Sample : I6579-06
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HAR-5-E(7-8)

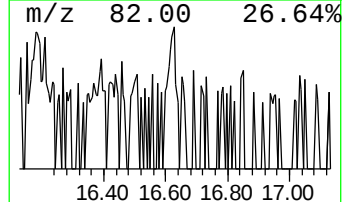
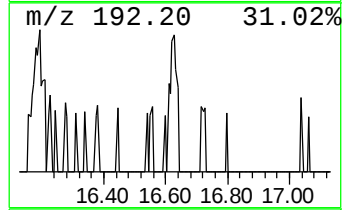
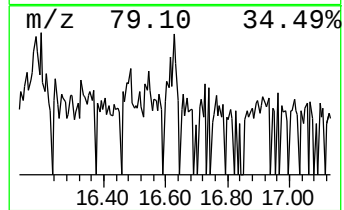
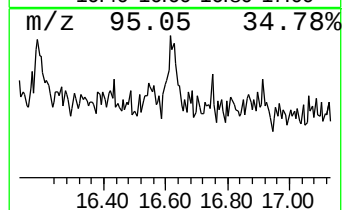
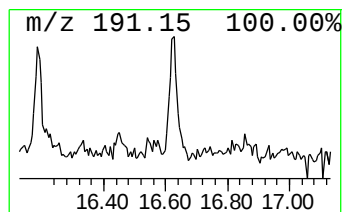
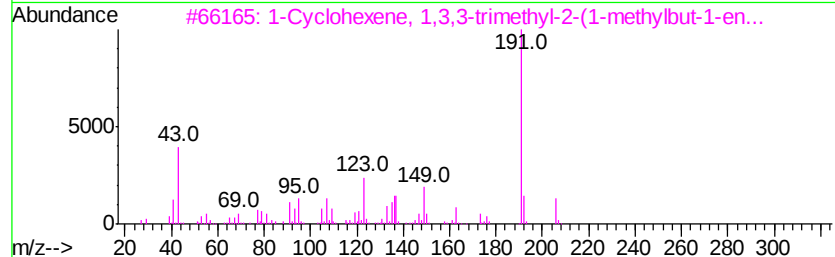
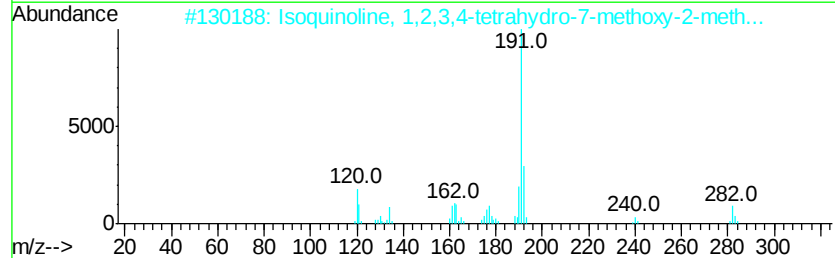
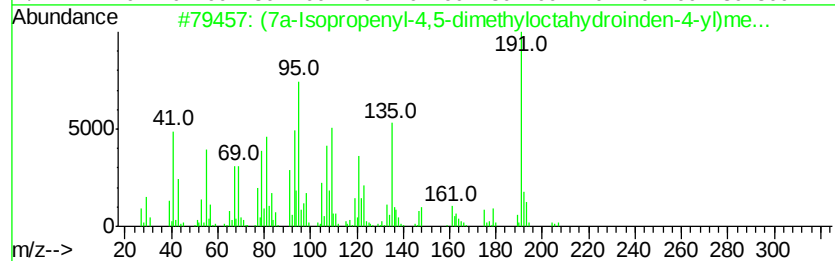
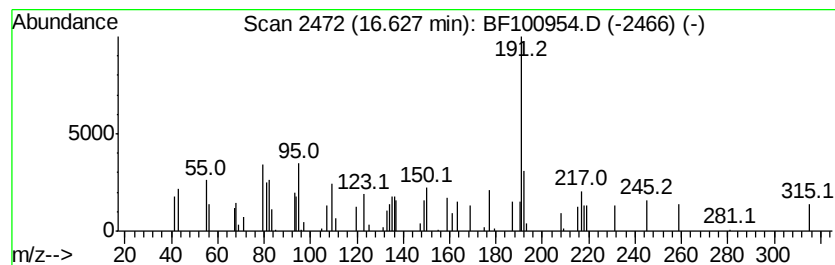
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown16.63 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.63	2.06 ng	33286	Perylene-d12	15.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(7a-Isopropenyl-4,5-dimethylocta...	222	C15H26O	1000187-02-9	37
2		Isoquinoline, 1,2,3,4-tetrahydro...	283	C18H21NO2	036646-87-4	37
3		1-Cyclohexene, 1,3,3-trimethyl-2...	206	C14H22O	1000197-08-4	35
4		Piperidine, N-[3-methoxyphenyl]-	191	C12H17NO	032040-06-5	35
5		N-Methyl-9-phenanthrenemethanamine	221	C16H15N	076532-36-0	32



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112817\
Data File : BF100954.D
Acq On : 29 Nov 2017 1:16
Operator : SJ/JU
Sample : I6579-06
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HAR-5-E(7-8)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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...	5.08	8.4	ng	145905	1	6.86	346555	20.0
unknown6.63	6.63	61.3	ng	1062440	1	6.86	346555	20.0
2-Hydroxy-iso-but...	8.69	2.0	ng	41290	2	8.14	410889	20.0
Benzophenone	10.60	8.3	ng	156654	3	9.89	375933	20.0
2- Bromopropionic...	13.86	2.0	ng	41379	5	14.02	404887	20.0
unknown16.19	16.19	2.9	ng	47664	6	15.49	323952	20.0
unknown16.63	16.63	2.1	ng	33286	6	15.49	323952	20.0