

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030223\
 Data File : BF132614.D
 Acq On : 02 Mar 2023 18:42
 Operator : CG\JU
 Sample : 01760-03
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 72-11998

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:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132614.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.234	445	450	461	rVB	1563470	1943193	47.53%	5.126%
2	5.628	512	517	520	rBV	4045600	3755944	91.86%	9.908%
3	6.628	682	687	690	rBV	3519231	3713587	90.83%	9.796%
4	6.998	747	750	754	rBV	1544823	1297856	31.74%	3.424%
5	7.563	842	846	849	rBV	2712419	2499795	61.14%	6.594%
6	8.286	965	969	972	rBV	2275123	1796474	43.94%	4.739%
7	9.363	1148	1152	1155	rBV	4792434	4088677	100.00%	10.786%
8	9.904	1241	1244	1247	rBV	51095	49576	1.21%	0.131%
9	10.045	1262	1268	1271	rBV	2164982	1838143	44.96%	4.849%
10	10.080	1271	1274	1277	rVB	82691	73633	1.80%	0.194%
11	10.251	1299	1303	1306	rBV2	61397	57396	1.40%	0.151%
12	10.457	1333	1338	1342	rVB4	38689	53009	1.30%	0.140%
13	10.598	1358	1362	1368	rVB	93332	98330	2.40%	0.259%
14	10.680	1371	1376	1379	rVV2	81058	90212	2.21%	0.238%
15	10.757	1386	1389	1392	rVB	329641	281053	6.87%	0.741%
16	10.839	1399	1403	1407	rBV	2542528	2215433	54.18%	5.844%
17	10.951	1418	1422	1429	rBV	316281	323207	7.90%	0.853%
18	11.274	1474	1477	1479	rBV3	37190	48069	1.18%	0.127%
19	11.345	1486	1489	1492	rBV	67416	56205	1.37%	0.148%
20	11.416	1498	1501	1504	rBV	146781	148465	3.63%	0.392%
21	11.545	1519	1523	1525	rBV	1602530	1500089	36.69%	3.957%
22	11.568	1525	1527	1530	rVV	652783	506696	12.39%	1.337%
23	11.616	1532	1535	1538	rVB	176125	156610	3.83%	0.413%
24	11.692	1546	1548	1554	rBV	58696	72794	1.78%	0.192%
25	11.768	1558	1561	1565	rBV	150544	172322	4.21%	0.455%
26	12.057	1606	1610	1612	rBV2	204467	259965	6.36%	0.686%
27	12.163	1624	1628	1630	rBV2	113595	116344	2.85%	0.307%
28	12.339	1656	1658	1661	rBV	71221	69198	1.69%	0.183%
29	12.368	1661	1663	1666	rVB	109820	91571	2.24%	0.242%
30	12.598	1699	1702	1705	rBV	62807	60779	1.49%	0.160%
31	12.686	1714	1717	1721	rBV2	94395	93717	2.29%	0.247%
32	12.763	1727	1730	1734	rBV	1180539	1070714	26.19%	2.824%
33	12.857	1743	1746	1750	rBV4	54860	63192	1.55%	0.167%
34	12.974	1763	1766	1767	rBV	152729	135913	3.32%	0.359%
35	12.998	1767	1770	1775	rVV	981011	857110	20.96%	2.261%
36	13.045	1775	1778	1782	rVB2	60499	63082	1.54%	0.166%

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37	13.133	1787	1793	1796	rBV	3155282	2801422	68.52%	7.390%
38	13.215	1803	1807	1811	rBV3	58532	87332	2.14%	0.230%
39	13.298	1818	1821	1823	rBV4	59697	78888	1.93%	0.208%
40	13.327	1823	1826	1828	rVB	112379	112789	2.76%	0.298%
41	13.392	1834	1837	1840	rVB	90110	73956	1.81%	0.195%
42	13.427	1840	1843	1846	rBV2	82402	92236	2.26%	0.243%
43	13.557	1862	1865	1872	rBV2	58785	70904	1.73%	0.187%
44	13.839	1910	1913	1918	rVB	84805	94058	2.30%	0.248%
45	13.951	1929	1932	1935	rBV3	86503	81741	2.00%	0.216%
46	14.004	1939	1941	1943	rBV	55458	59302	1.45%	0.156%
47	14.045	1946	1948	1953	rVB	134716	148403	3.63%	0.391%
48	14.162	1966	1968	1970	rBV	84339	69810	1.71%	0.184%
49	14.204	1970	1975	1978	rVV2	1384414	1621565	39.66%	4.278%
50	14.227	1978	1979	1987	rVB	441259	365761	8.95%	0.965%
51	14.592	2039	2041	2044	rVB	82870	65497	1.60%	0.173%
52	14.827	2079	2081	2084	rBV	68431	62886	1.54%	0.166%
53	15.292	2156	2160	2164	rBV	361320	565472	13.83%	1.492%
54	15.409	2178	2180	2183	rBV	50509	45791	1.12%	0.121%
55	15.621	2213	2216	2223	rVB	203063	258809	6.33%	0.683%
56	15.692	2224	2228	2234	rVB	205987	276766	6.77%	0.730%
57	15.756	2235	2239	2244	rBV	751453	1047217	25.61%	2.763%
58	16.233	2317	2320	2325	rVB	72956	109332	2.67%	0.288%

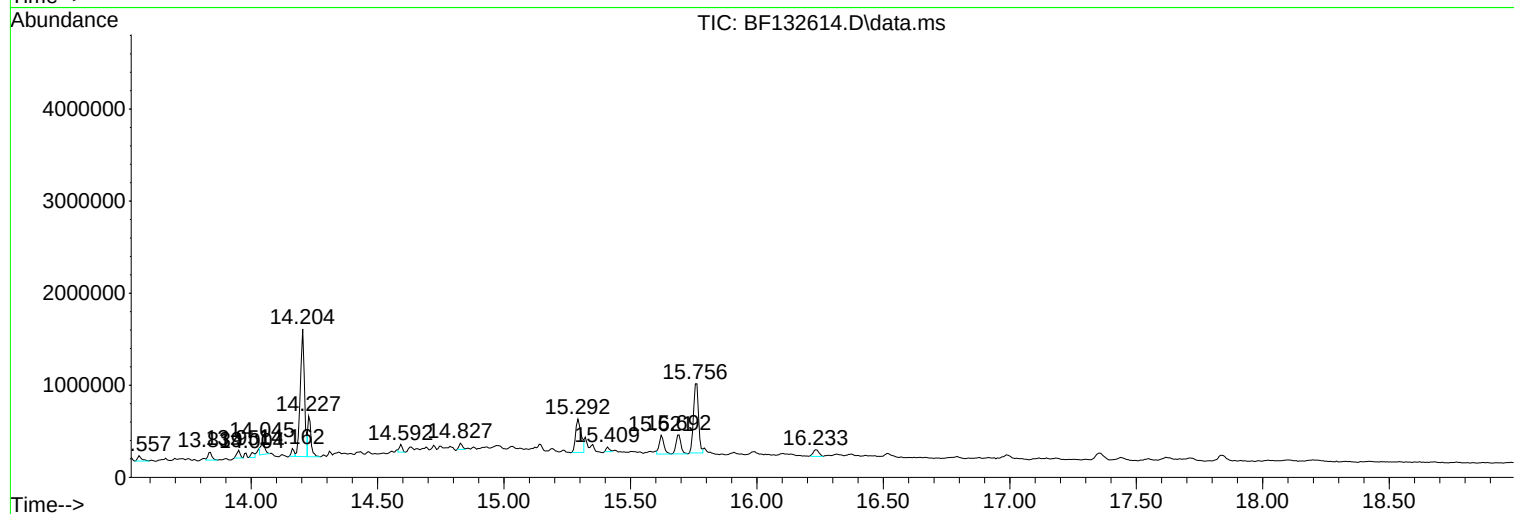
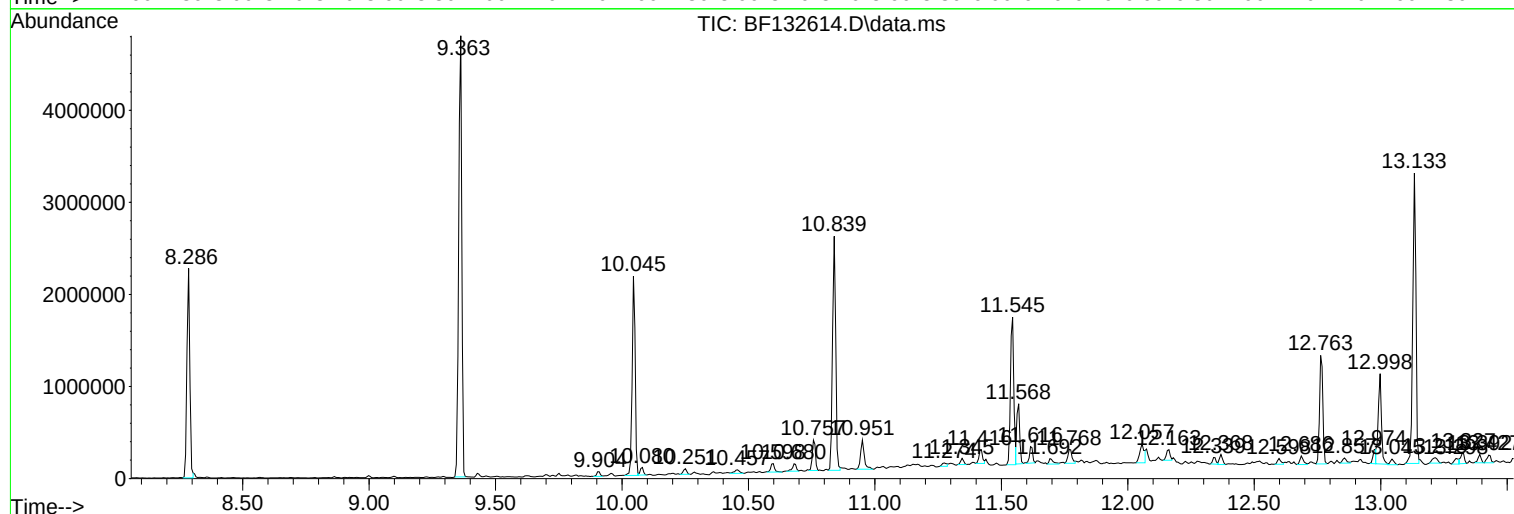
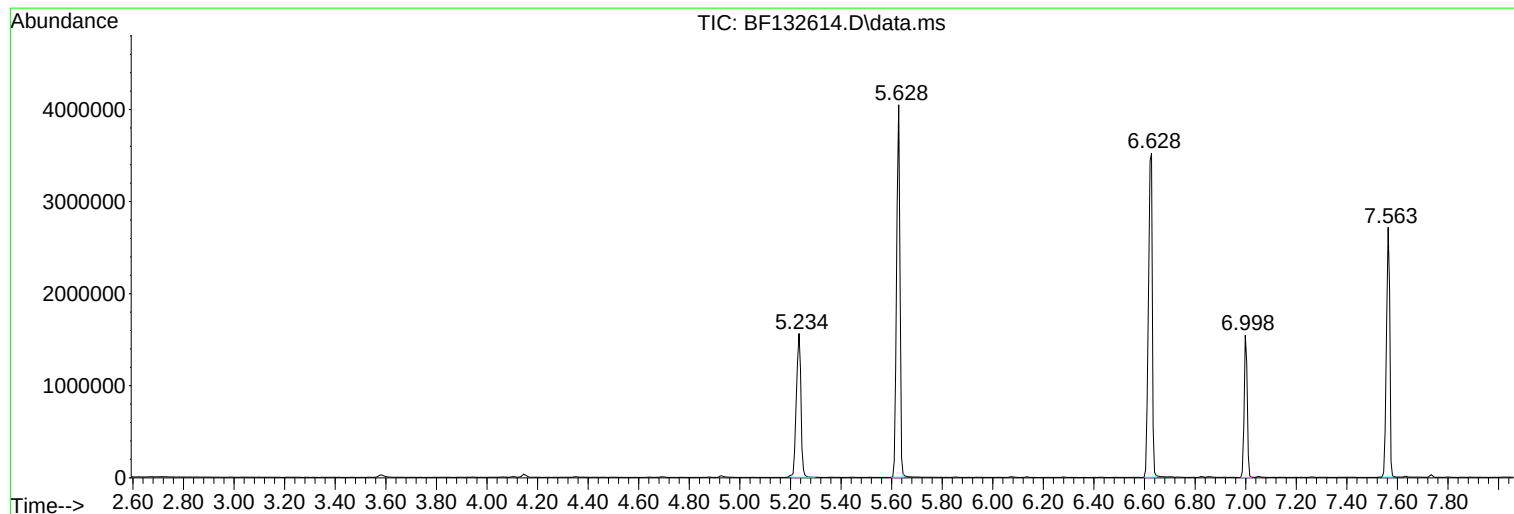
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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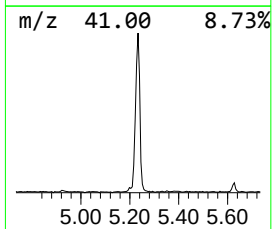
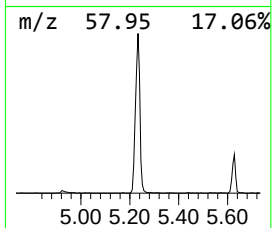
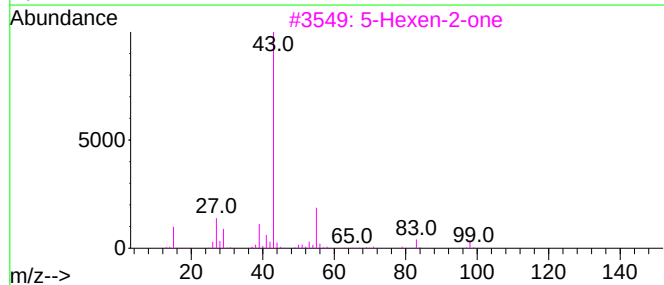
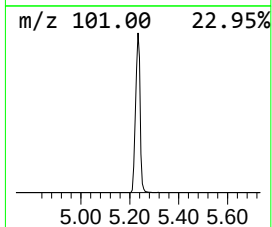
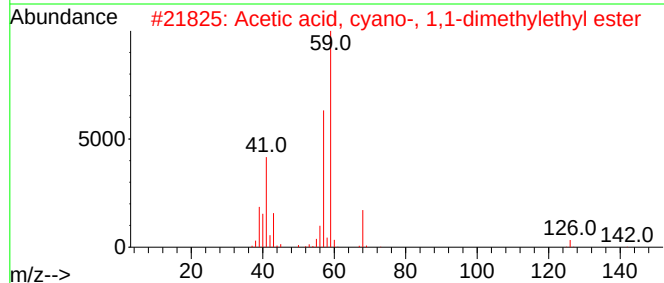
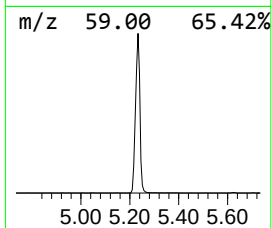
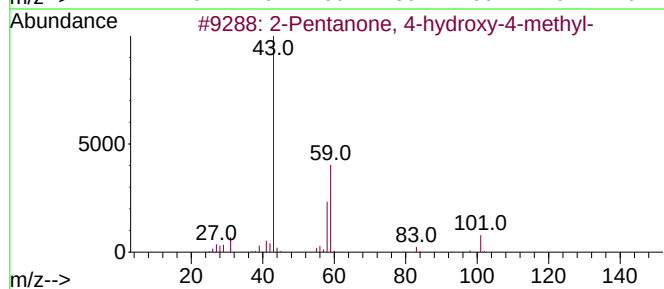
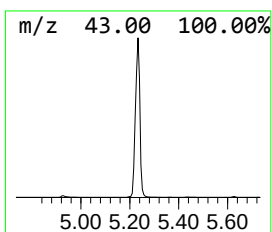
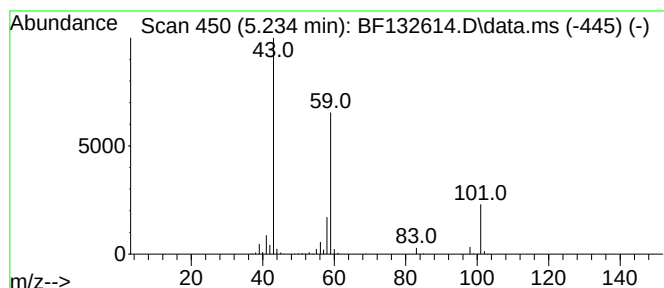
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.234	29.94 ng	1943190	1,4-Dichlorobenzene-d4	6.998

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-dimethy...	141	C7H11NO2	001116-98-9	17
3			5-Hexen-2-one	98	C6H10O	000109-49-9	9
4			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5			Guanidine	59	CH5N3	000113-00-8	9



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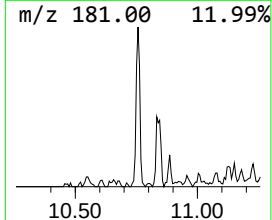
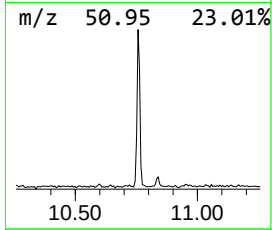
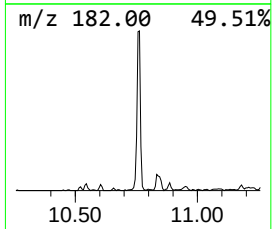
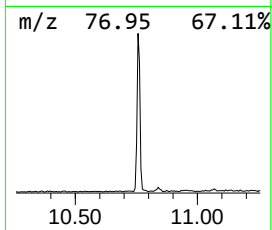
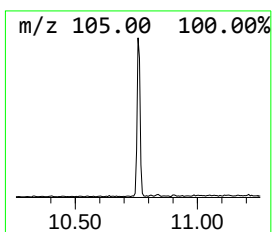
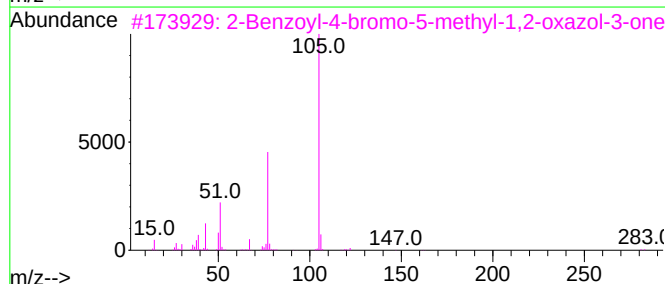
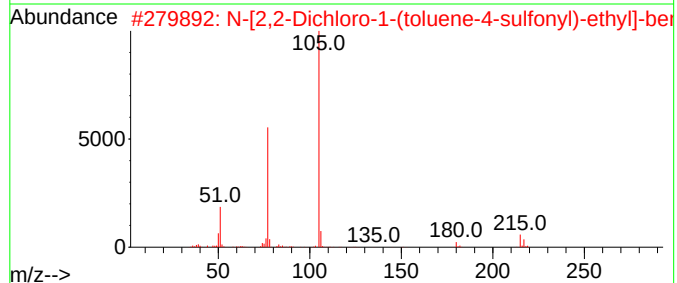
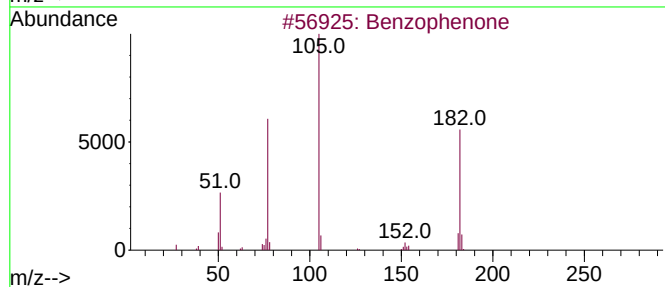
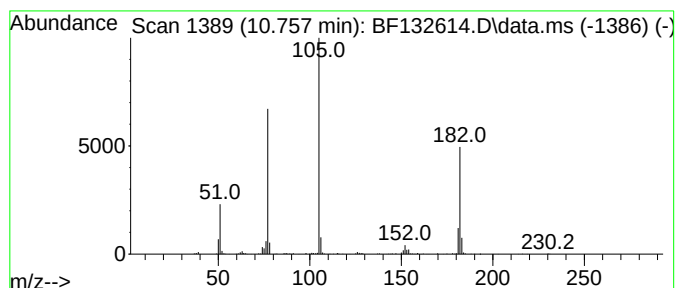
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.757	3.06 ng	281053	Acenaphthene-d10	10.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			N-[2,2-Dichloro-1-(toluene-4-sul...	371	C16H15Cl2NO3S	136800-77-6	47
3			2-Benzoyl-4-bromo-5-methyl-1,2-o...	281	C11H8BrNO3	1000444-92-3	47
4			Methyl benzilate	242	C15H14O3	000076-89-1	47
5			Vinyl benzoate	148	C9H8O2	000769-78-8	47



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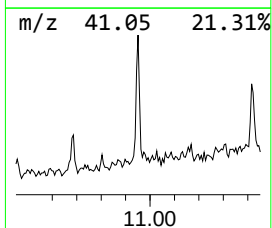
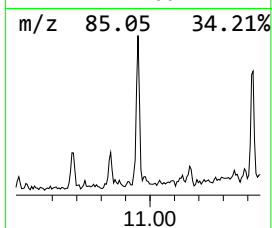
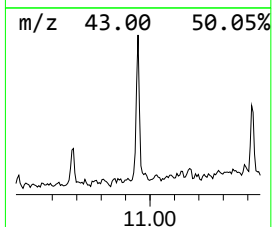
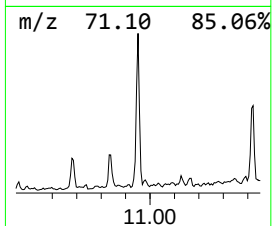
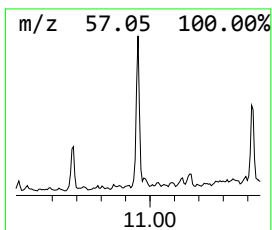
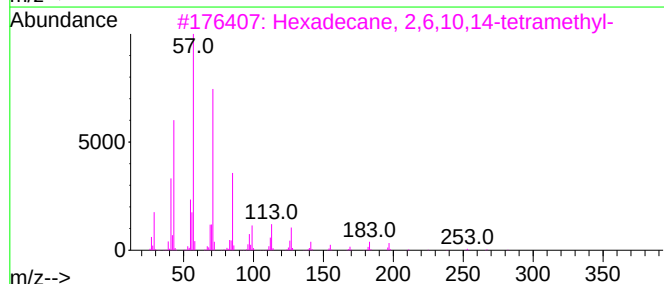
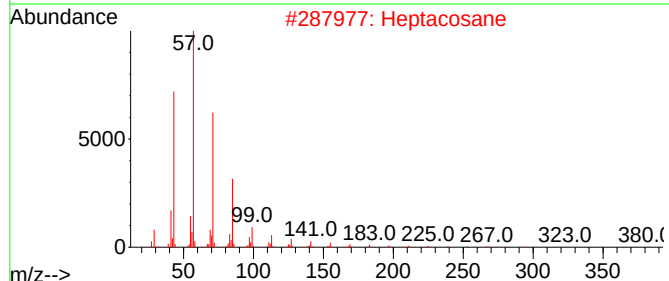
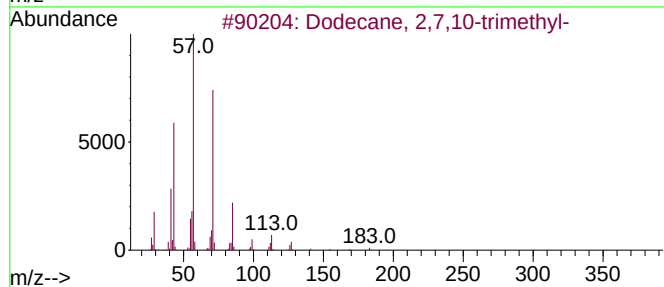
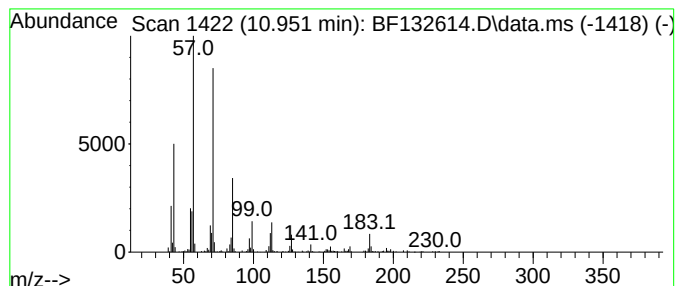
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Dodecane, 2,7,10-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.951	4.31 ng	323207	Phenanthrene-d10	11.545	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	86
2	Heptacosane	380	C27H56	000593-49-7	86
3	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	83
4	Sulfurous acid, 2-ethylhexyl non...	320	C17H36O3S	1010309-19-2	72
5	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	72



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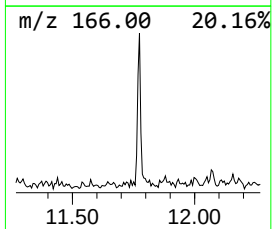
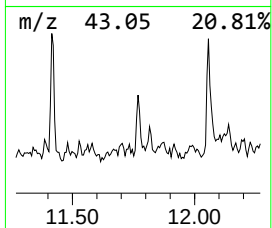
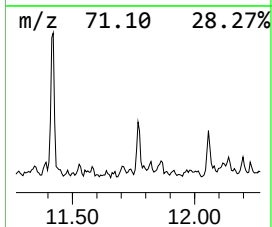
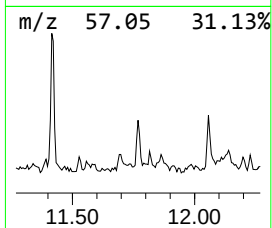
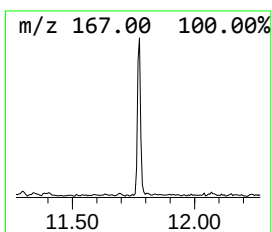
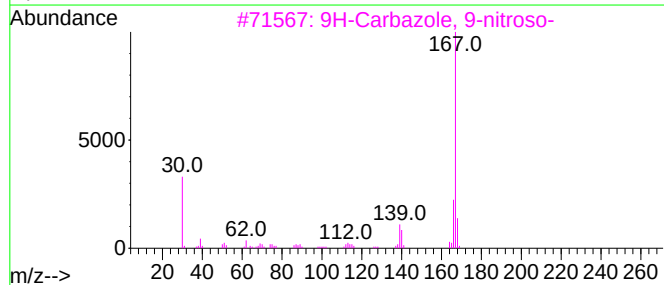
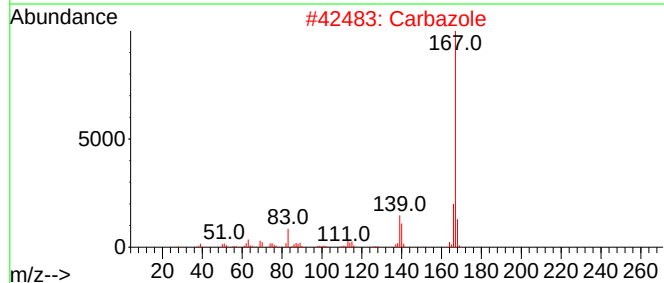
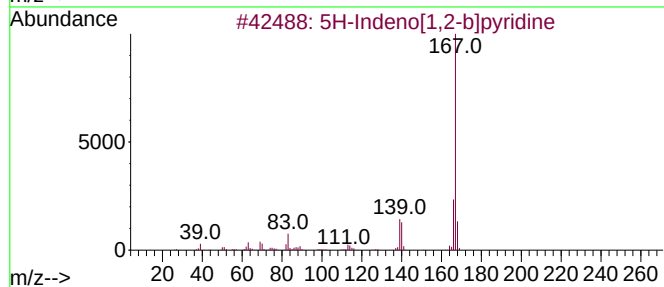
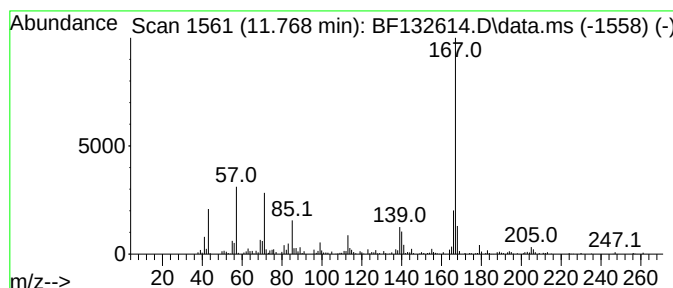
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 5H-Indeno[1,2-b]pyridine Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.769	2.30 ng	172322	Phenanthrene-d10	11.545

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5H-Indeno[1,2-b]pyridine	167	C12H9N	000244-99-5	76
2			Carbazole	167	C12H9N	000086-74-8	76
3			9H-Carbazole, 9-nitroso-	196	C12H8N2O	002788-23-0	59
4			Thiazolo[3,2-a]pyridinium, 2,3-d...	167	C8H9NOS	023003-43-2	53
5			9H-Carbazole-9-methanol	197	C13H11NO	002409-36-1	53



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ALS Vial : 11 Sample Multiplier: 1

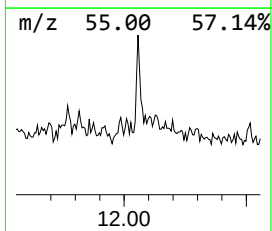
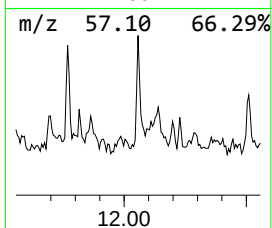
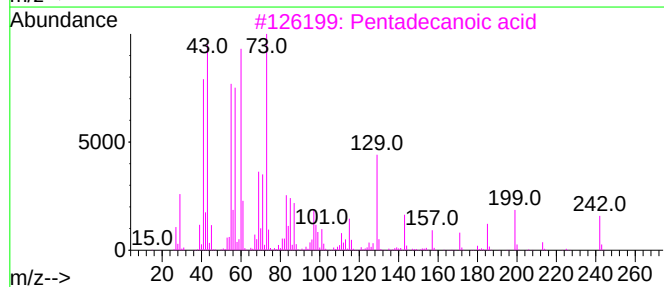
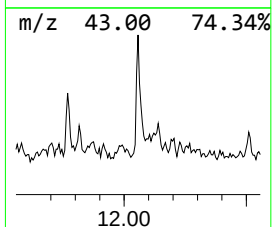
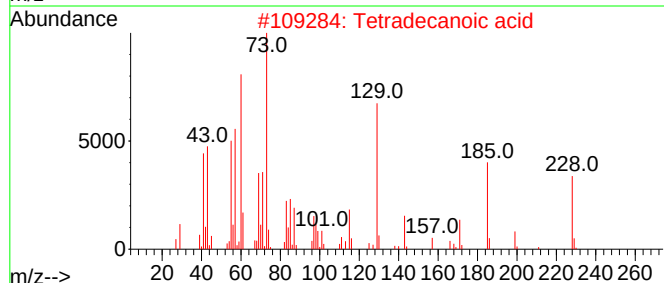
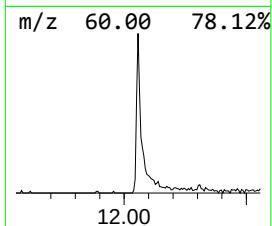
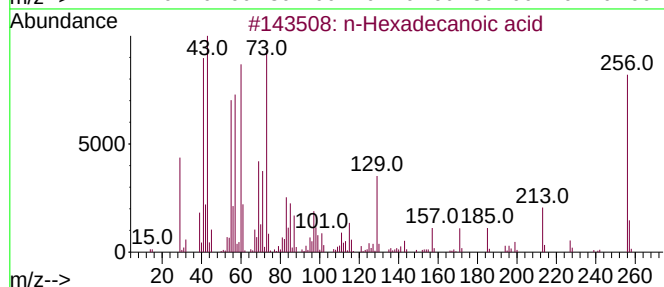
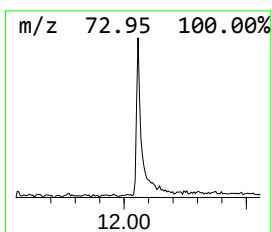
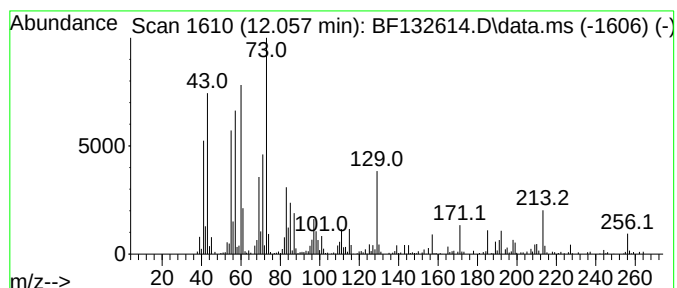
Instrument :
BNA_F
ClientSampleId :
72-11998

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.057	3.47 ng	259965	Phenanthrene-d10		11.545	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	97
2	Tetradecanoic acid		228	C14H28O2	000544-63-8	90
3	Pentadecanoic acid		242	C15H30O2	001002-84-2	68
4	n-Decanoic acid		172	C10H20O2	000334-48-5	68
5	Tridecanoic acid		214	C13H26O2	000638-53-9	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030223\
Data File : BF132614.D
Acq On : 02 Mar 2023 18:42
Operator : CG\JU
Sample : 01760-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11998

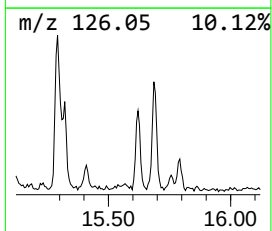
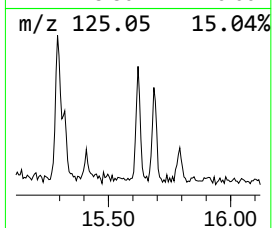
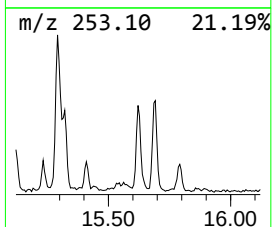
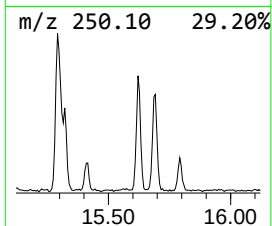
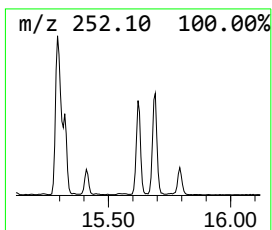
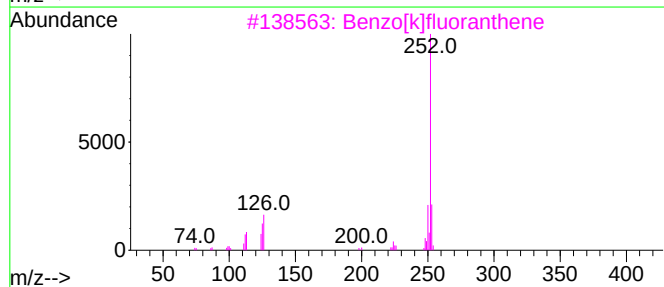
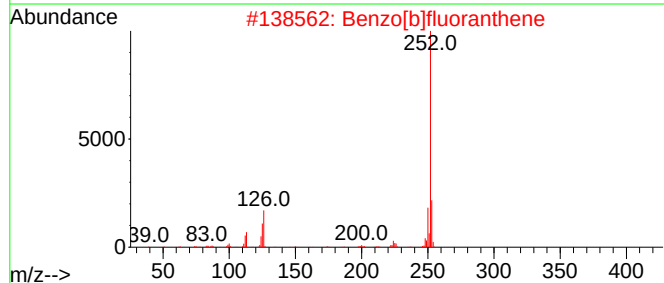
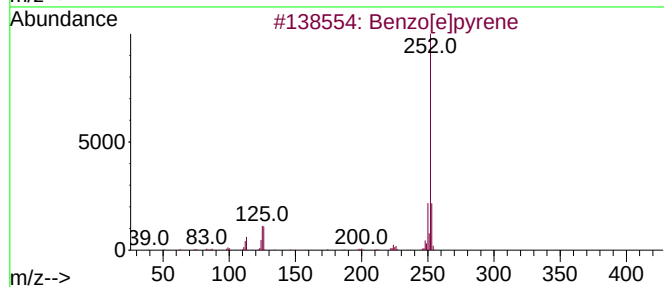
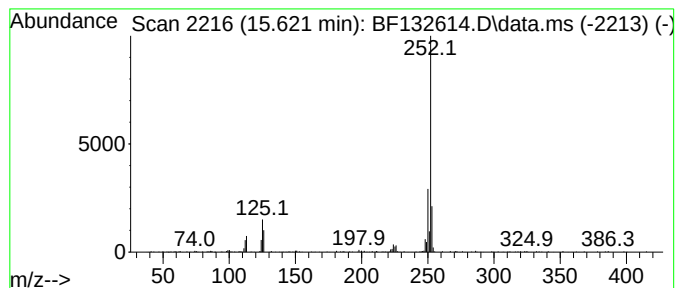
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Benzo[e]pyrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.621	4.94 ng	258809	Perylene-d12	15.762

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	97
2			Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
3			Benzo[k]fluoranthene	252	C20H12	000207-08-9	90
4			Benzo[a]pyrene	252	C20H12	000050-32-8	90
5			Perylene	252	C20H12	000198-55-0	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030223\
Data File : BF132614.D
Acq On : 02 Mar 2023 18:42
Operator : CG\JU
Sample : 01760-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11998

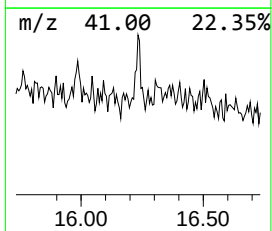
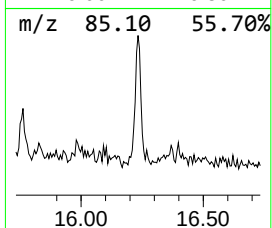
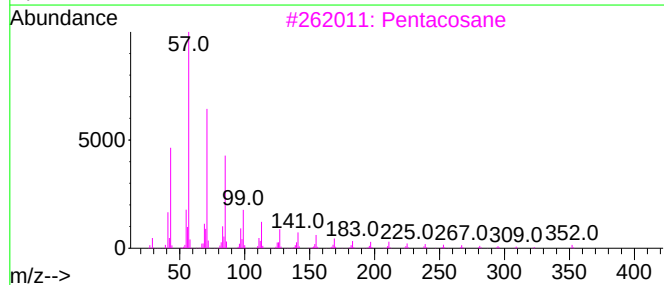
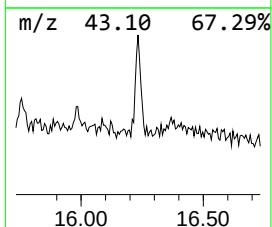
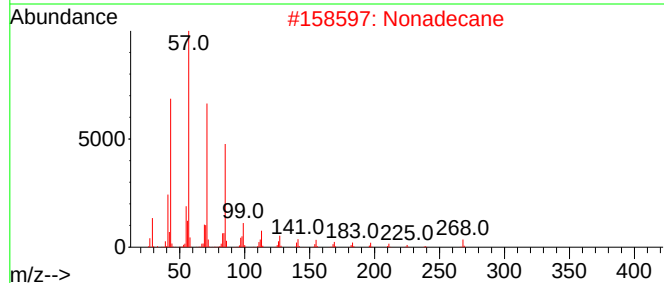
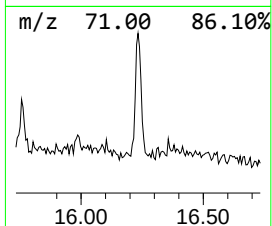
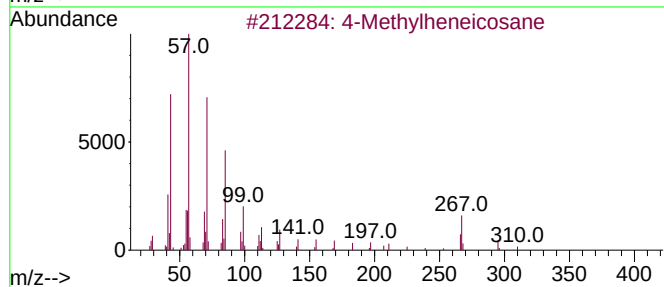
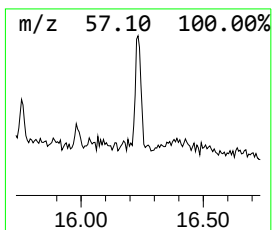
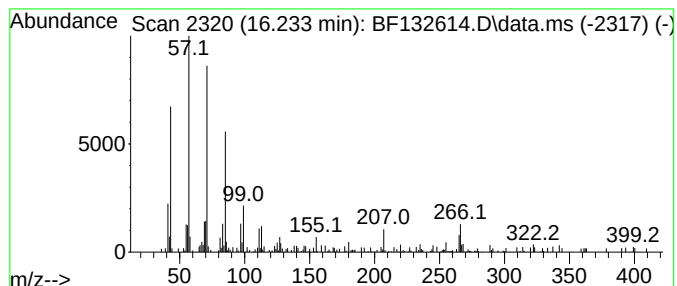
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 4-Methylheneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.233	2.09 ng	109332	Perylene-d12	15.762

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Methylheneicosane	310	C22H46	025117-29-7	86
2			Nonadecane	268	C19H40	000629-92-5	76
3			Pentacosane	352	C25H52	000629-99-2	72
4			Heneicosane	296	C21H44	000629-94-7	72
5			Hexacosane	366	C26H54	000630-01-3	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030223\
Data File : BF132614.D
Acq On : 02 Mar 2023 18:42
Operator : CG\JU
Sample : 01760-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11998

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.234	29.9	ng	1943190	1	6.998	1297860	20.0
Benzophenone	10.757	3.1	ng	281053	3	10.045	1838140	20.0
Dodecane, 2,7,1...	10.951	4.3	ng	323207	4	11.545	1500090	20.0
5H-Indeno[1,2-b...	11.769	2.3	ng	172322	4	11.545	1500090	20.0
n-Hexadecanoic ...	12.057	3.5	ng	259965	4	11.545	1500090	20.0
Benzo[e]pyrene	15.621	4.9	ng	258809	6	15.762	1047220	20.0
4-Methylheneico...	16.233	2.1	ng	109332	6	15.762	1047220	20.0