

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122121\
 Data File : BF126301.D
 Acq On : 21 Dec 2021 17:27
 Operator : JU/CG
 Sample : PB141610BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB141610BL

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-BF121521.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126301.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.416	392	396	404	rBV	402121	432396	8.65%	1.177%
2	5.046	496	503	518	rBV	1601001	2457593	49.17%	6.688%
3	5.445	565	571	574	rBV	4177635	4966545	99.37%	13.517%
4	5.834	634	637	643	rBV	255917	207271	4.15%	0.564%
5	6.445	735	741	744	rBV	3977169	4970888	99.46%	13.528%
6	6.816	800	804	807	rBV	1371343	1124225	22.49%	3.060%
7	7.381	894	900	903	rBV	3040401	3473775	69.51%	9.454%
8	8.098	1017	1022	1036	rBV	1613590	1593353	31.88%	4.336%
9	9.175	1199	1205	1209	rBV	4223424	4997854	100.00%	13.602%
10	9.851	1315	1320	1337	rBV	1603940	1687968	33.77%	4.594%
11	10.639	1449	1454	1472	rBV	2548154	3079467	61.62%	8.381%
12	11.339	1568	1573	1589	rBV	1524312	1612618	32.27%	4.389%
13	12.927	1838	1843	1846	rBV	4109274	4363841	87.31%	11.876%
14	13.974	2017	2021	2033	rBV	796110	960706	19.22%	2.615%
15	15.421	2262	2267	2286	rBV	426079	815413	16.32%	2.219%

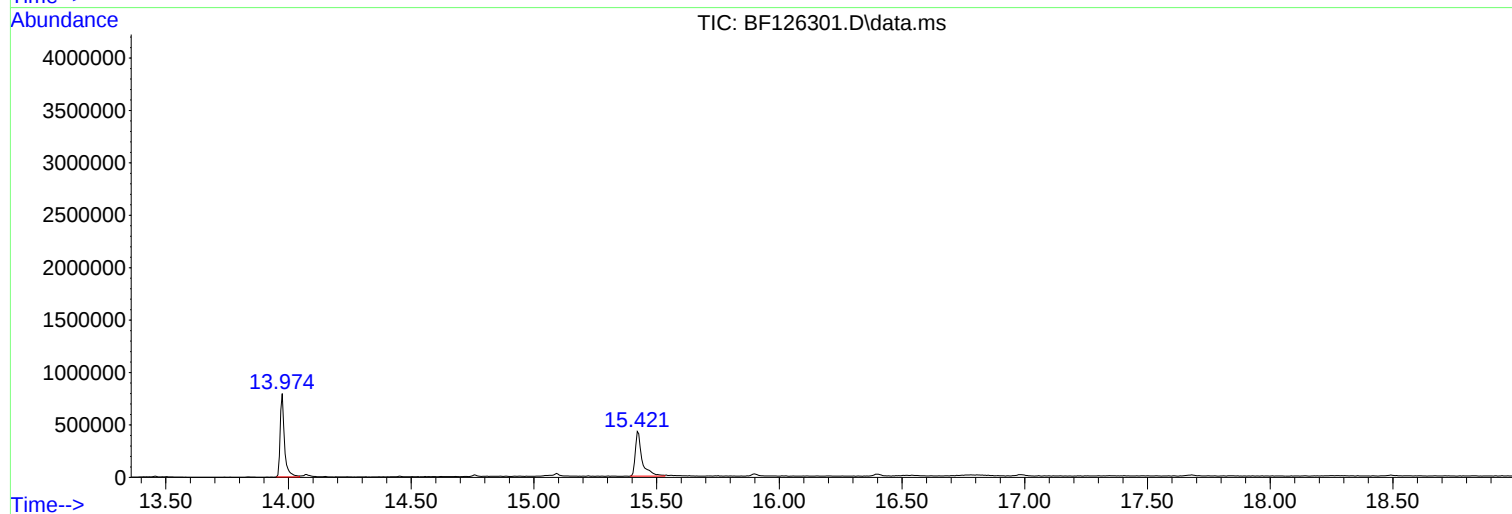
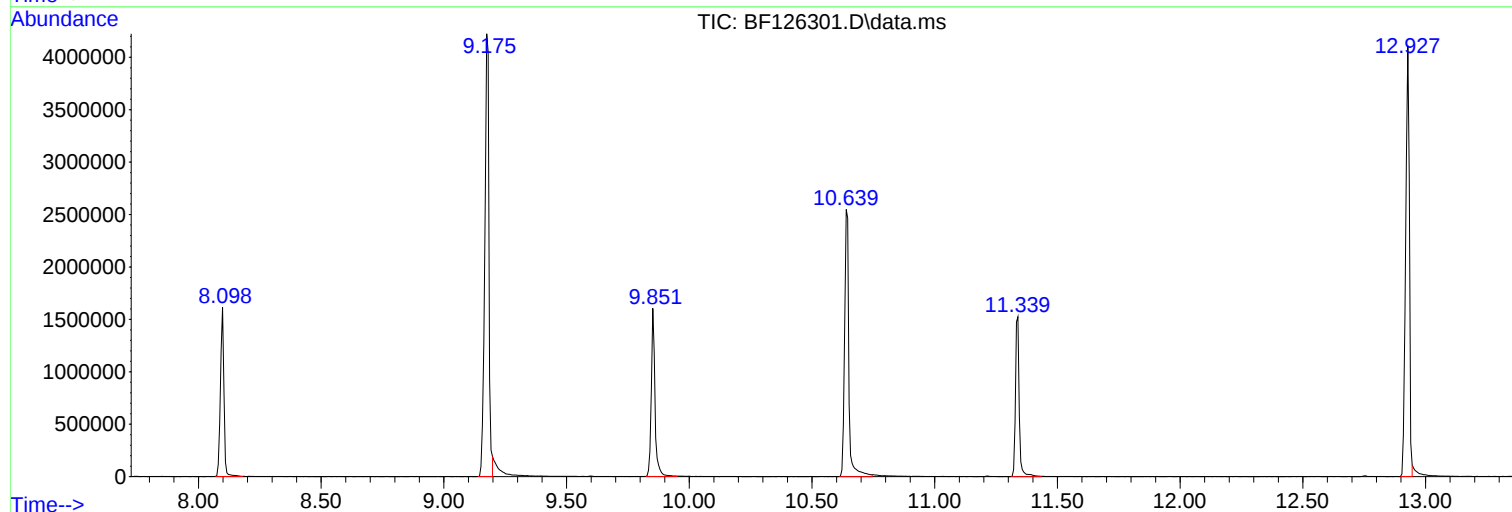
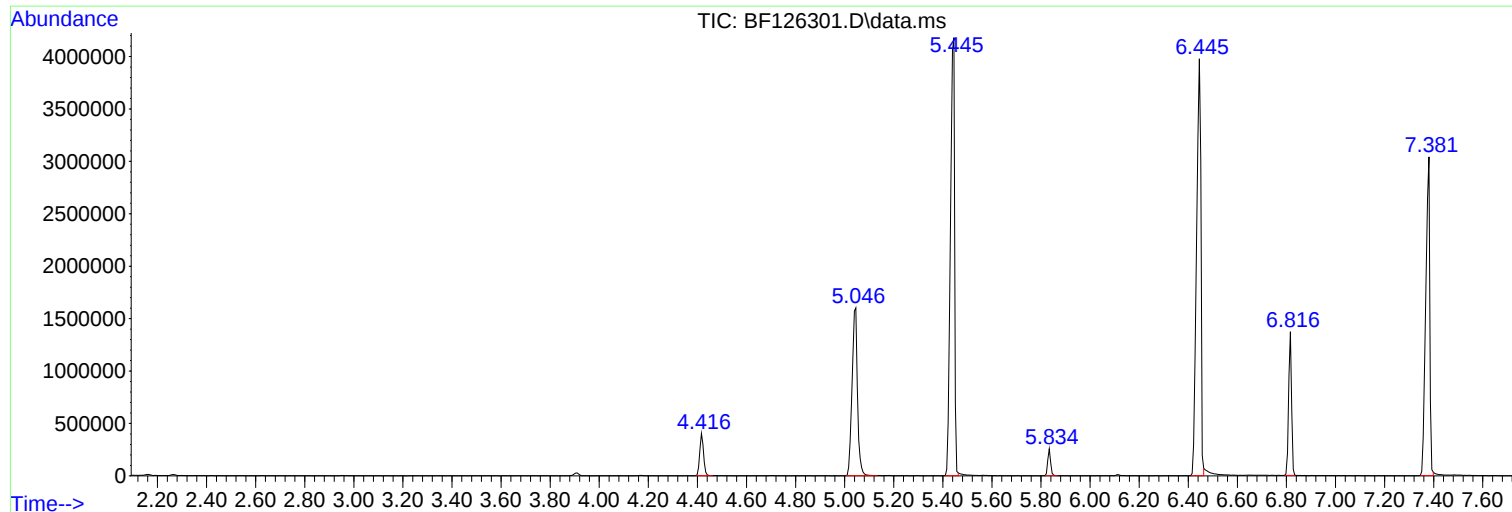
Sum of corrected areas: 36743913

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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.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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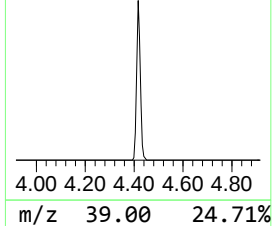
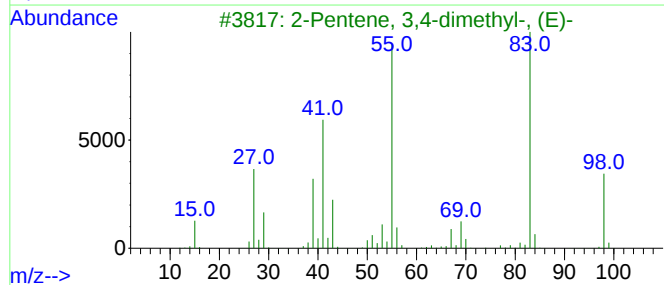
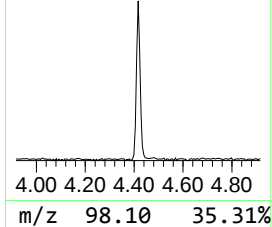
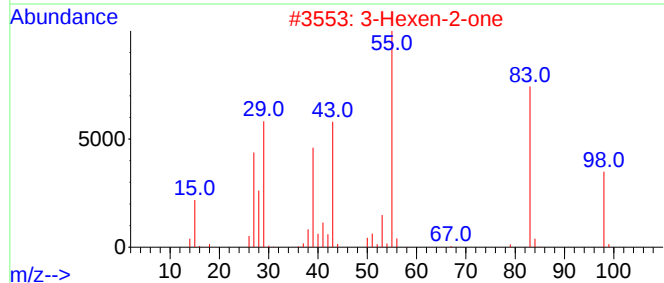
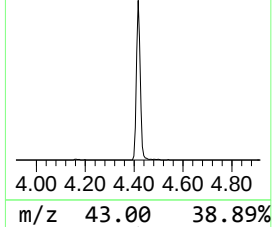
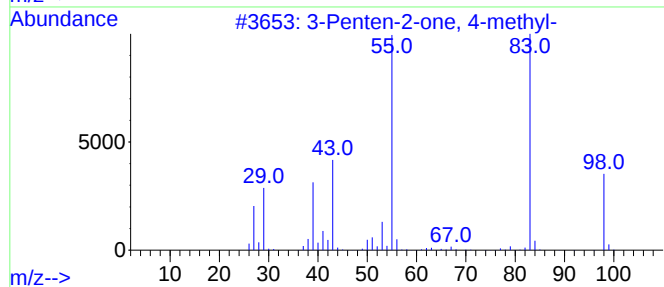
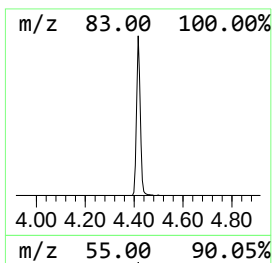
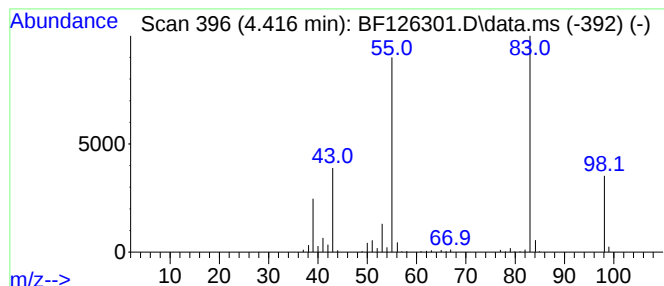
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.416	7.69 ng	432396	1,4-Dichlorobenzene-d4	6.816

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2		3-Hexen-2-one	98	C6H10O	000763-93-9	91
3		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80



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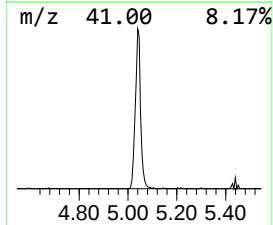
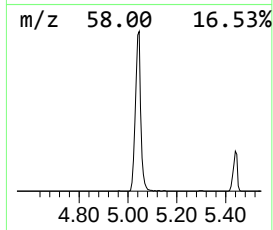
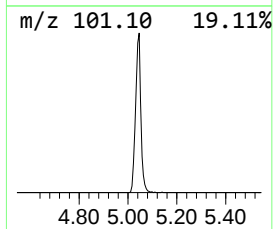
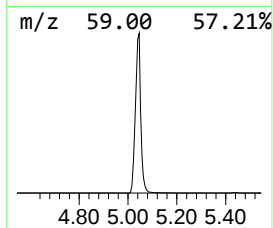
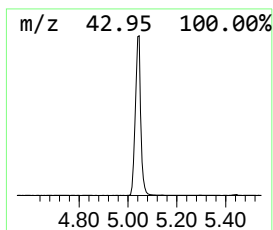
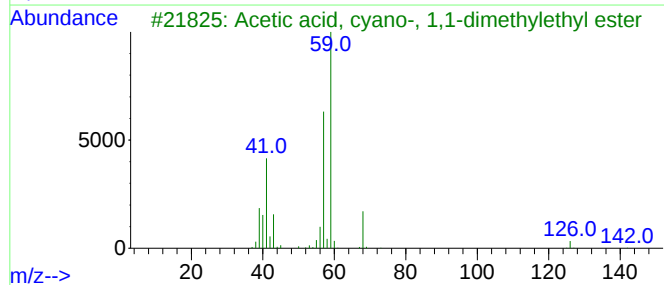
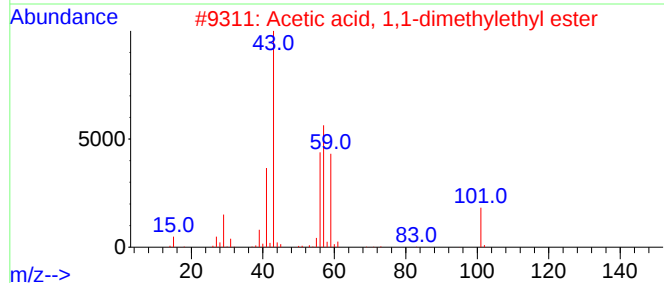
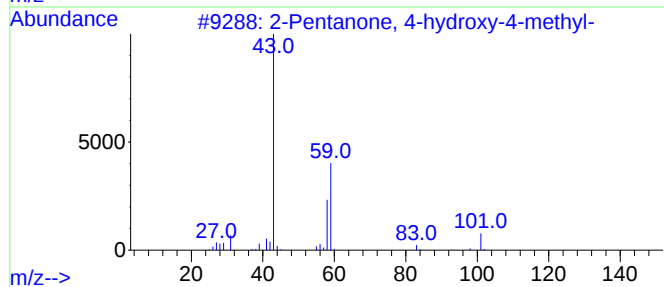
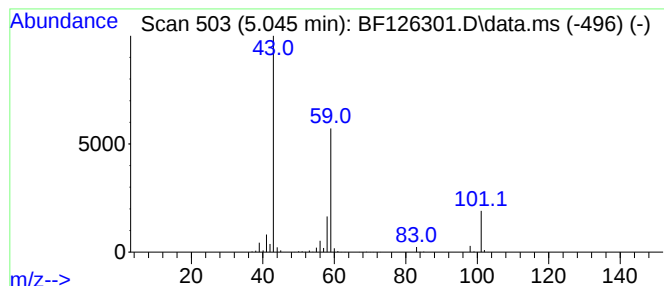
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.045	43.72 ng	2457590	1,4-Dichlorobenzene-d4	6.816

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, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9		
5	Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9		



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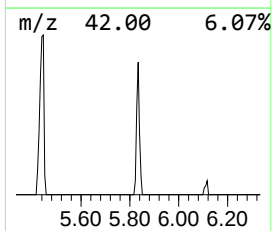
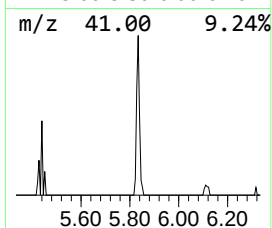
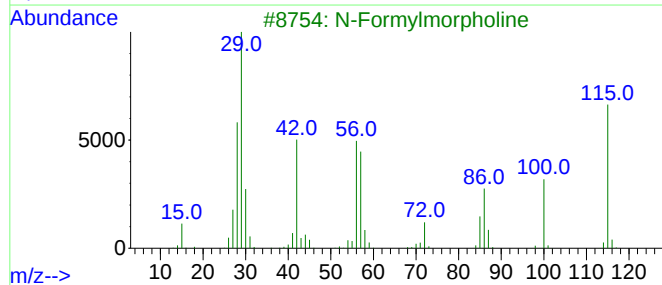
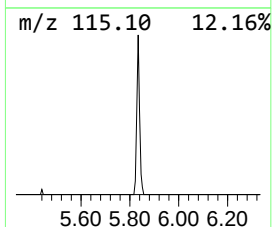
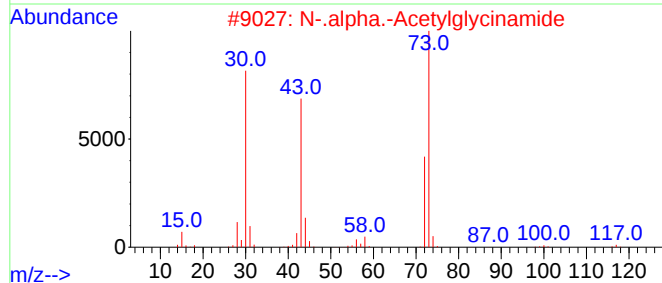
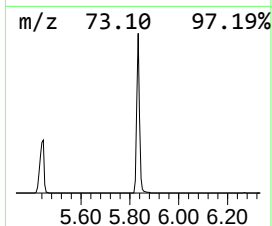
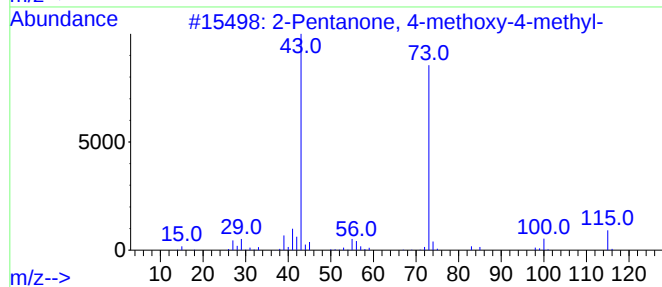
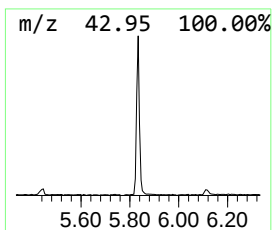
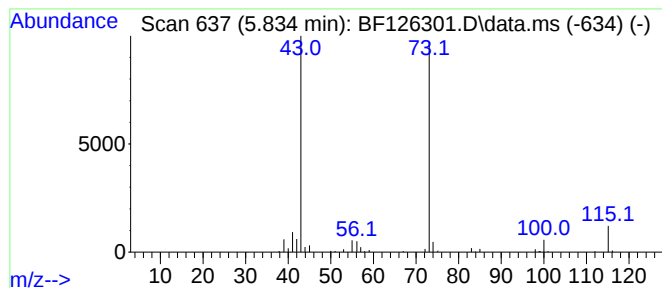
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Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.834	3.69 ng	207271	1,4-Dichlorobenzene-d4	6.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2			N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	38
3			N-Formylmorpholine	115	C5H9NO2	004394-85-8	10
4			1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	10
5			Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one,...	4.416	7.7	ng	432396	1	6.816	1124230	20.0
2-Pentanone, 4-...	5.045	43.7	ng	2457590	1	6.816	1124230	20.0
2-Pentanone, 4-...	5.834	3.7	ng	207271	1	6.816	1124230	20.0