

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051421\
 Data File : BF123933.D
 Acq On : 14 May 2021 19:55
 Operator : JU/CG
 Sample : PB136395BL
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB136395BL

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-BF051421.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123933.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.275	26	32	37	rVB	42149	57803	2.85%	0.492%
2	2.381	45	50	55	rVB	37035	48415	2.38%	0.412%
3	5.522	578	584	587	rBV	1547793	1594559	78.52%	13.569%
4	6.516	747	753	756	rBV	1431050	1594944	78.54%	13.572%
5	6.898	815	818	822	rBV	370389	298044	14.68%	2.536%
6	7.463	908	914	917	rBV	990185	1054730	51.94%	8.975%
7	8.181	1032	1036	1040	rVB	411404	378209	18.62%	3.218%
8	9.263	1214	1220	1223	rVB	2141240	1886473	92.90%	16.053%
9	9.939	1330	1335	1338	rVB	564580	439877	21.66%	3.743%
10	10.727	1464	1469	1472	rBV	1449971	1260178	62.06%	10.724%
11	11.421	1584	1587	1591	rVB	515405	438422	21.59%	3.731%
12	13.015	1853	1858	1861	rBV	2335610	2030733	100.00%	17.281%
13	14.062	2032	2036	2039	rBV	432819	352055	17.34%	2.996%
14	15.551	2284	2289	2296	rVB2	231414	282169	13.89%	2.401%
15	17.209	2563	2571	2572	rBV3	22445	34926	1.72%	0.297%

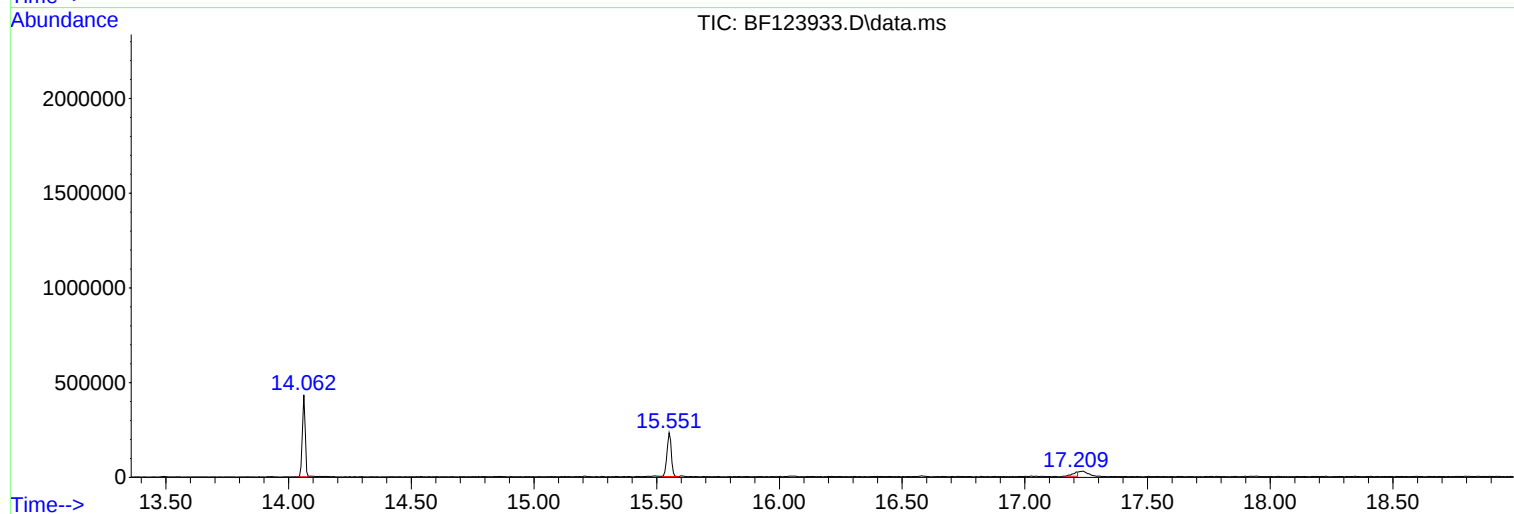
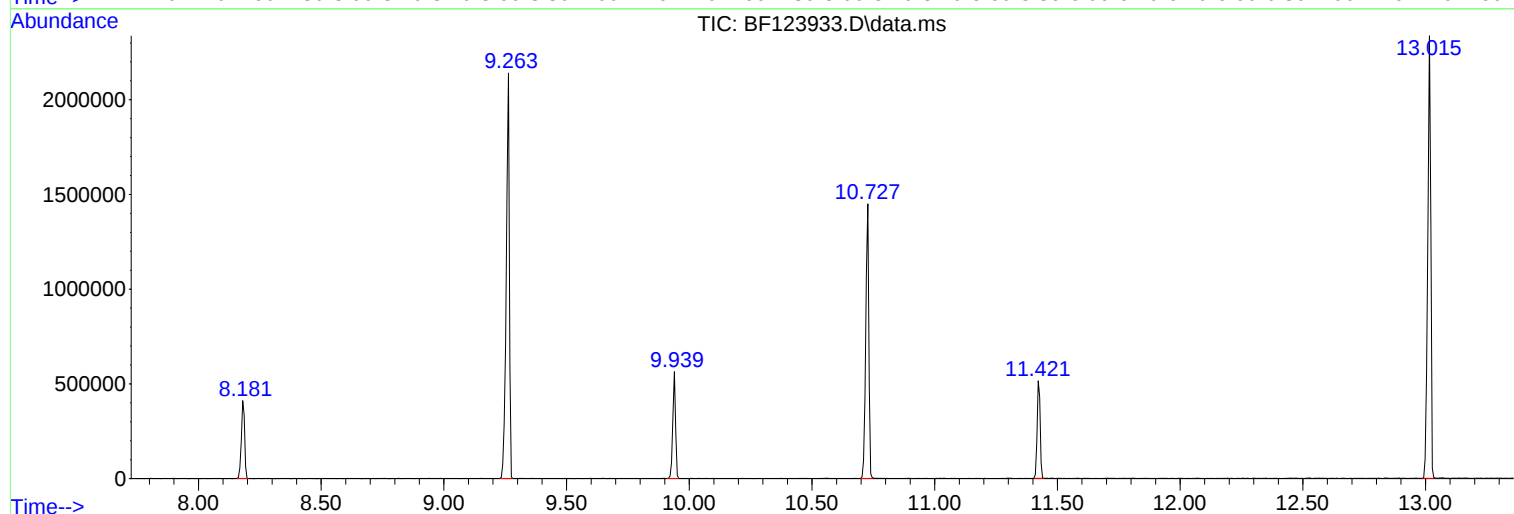
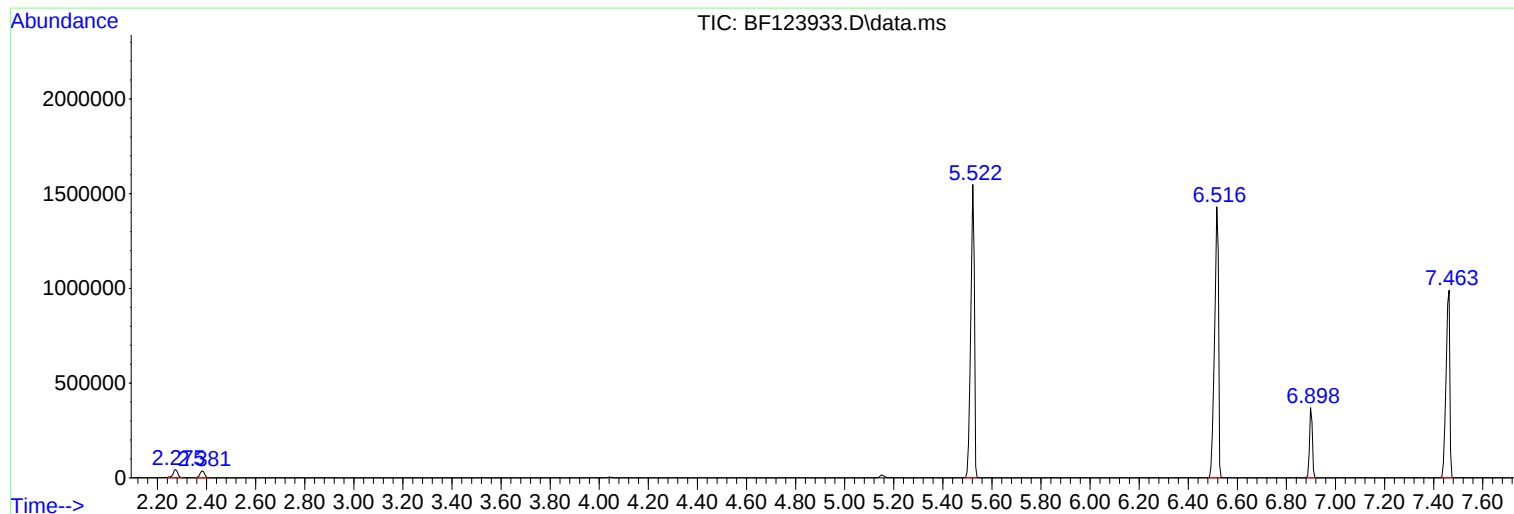
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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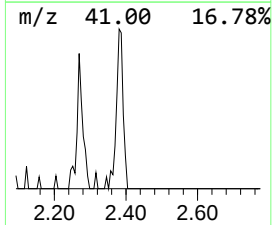
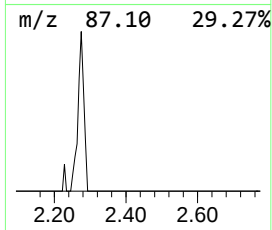
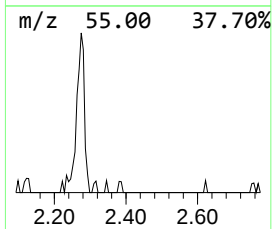
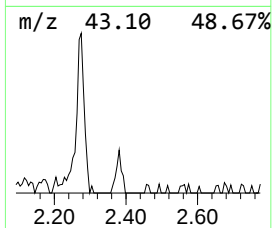
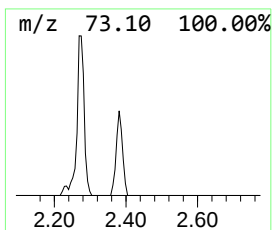
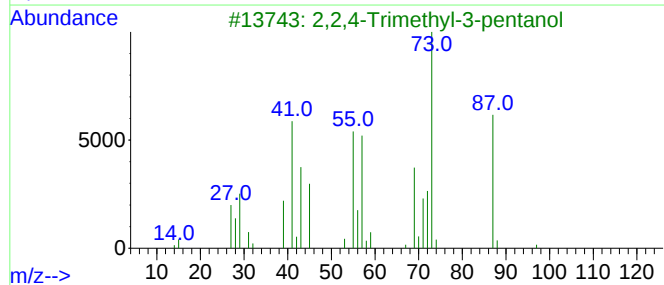
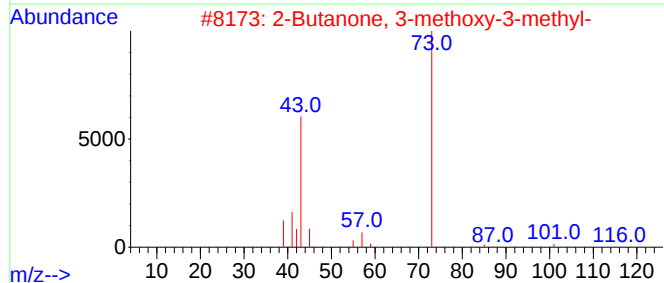
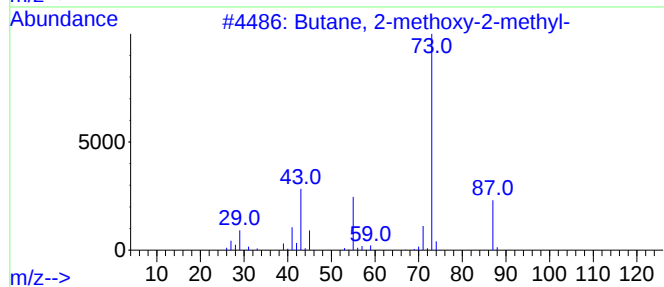
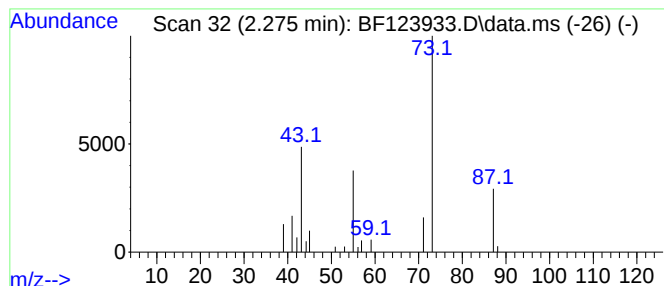
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.275	3.88 ng	57803	1,4-Dichlorobenzene-d4	6.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	50
2			2-Butanone, 3-methoxy-3-methyl-	116	C6H12O2	036687-98-6	25
3			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	17
4			1,4-Butanediamine	88	C4H12N2	000110-60-1	10
5			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	9



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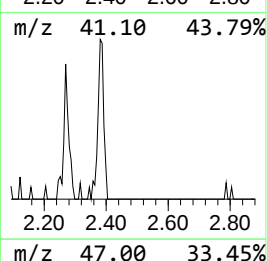
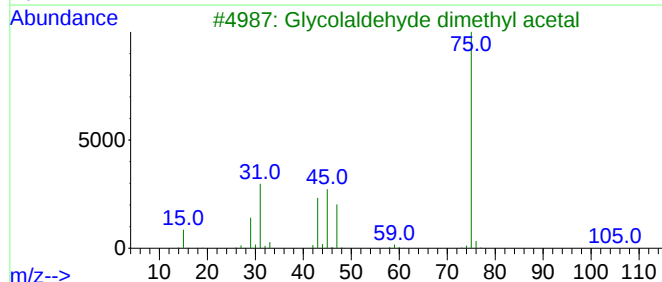
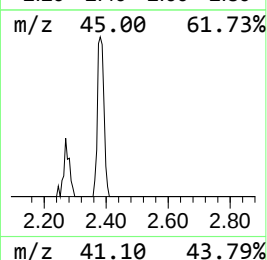
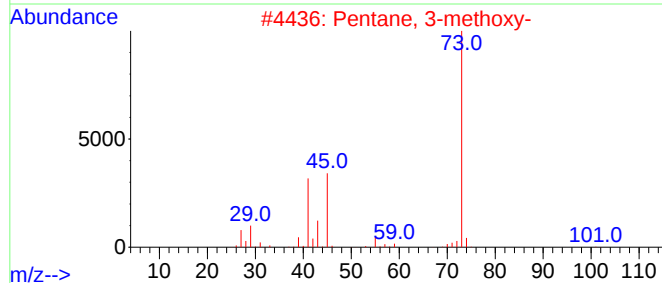
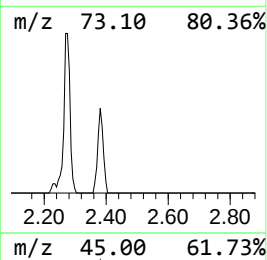
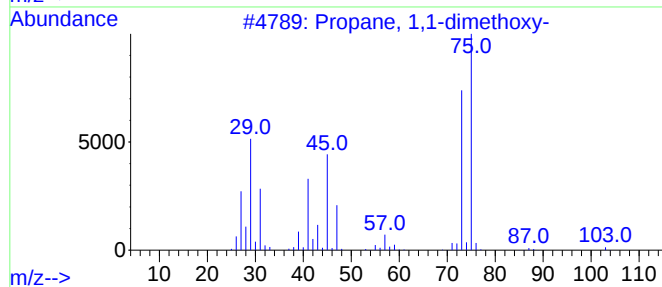
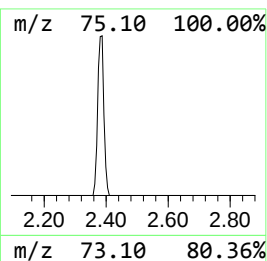
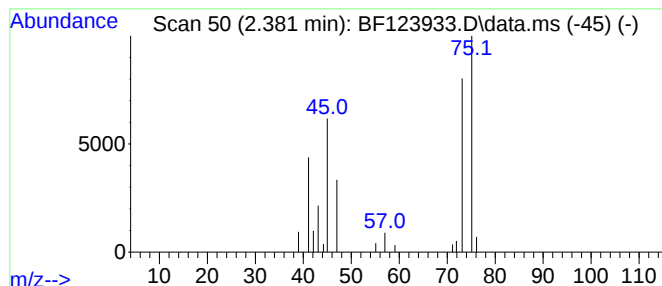
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Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.381	3.25 ng	48415	1,4-Dichlorobenzene-d4	6.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	78
2			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	35
3			Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	9
4			N-Ethylformamide	73	C3H7NO	000627-45-2	5
5			Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	4



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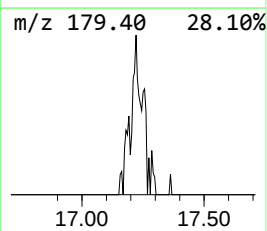
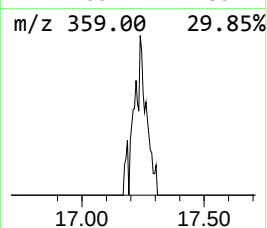
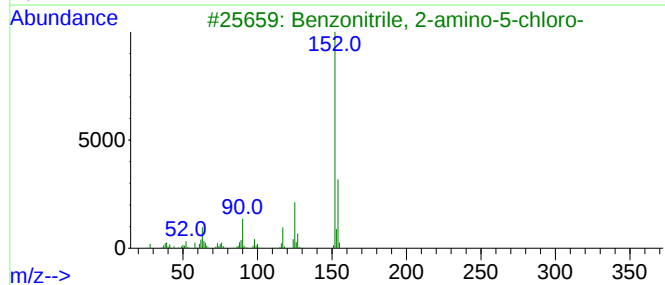
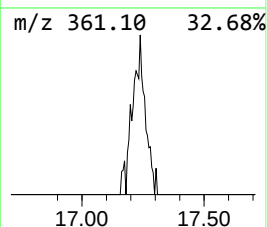
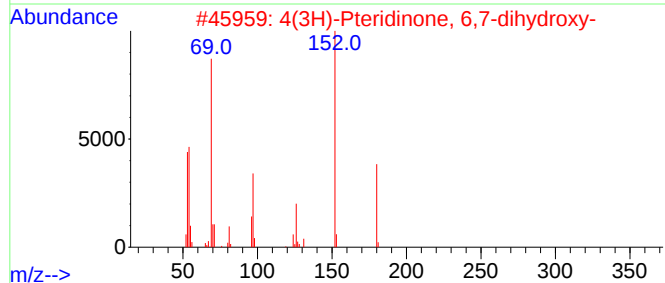
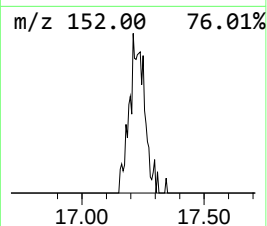
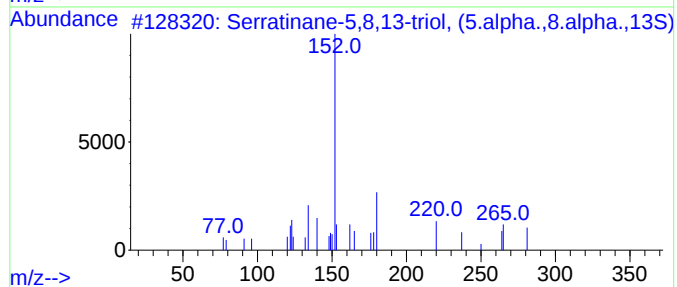
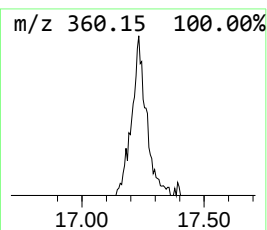
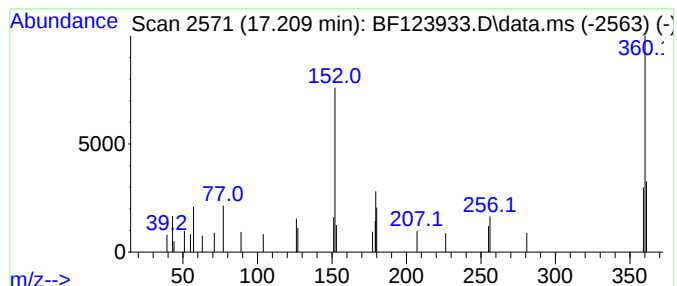
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Peak Number 3 unknown17.209 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.209	2.48 ng	34926	Perylene-d12	15.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Serratinane-5,8,13-triol, (5.alpha...	281	C16H27NO3	005532-22-9	22
2			4(3H)-Pteridinone, 6,7-dihydroxy-	180	C6H4N4O3	1000351-73-1	14
3			Benzonitrile, 2-amino-5-chloro-	152	C7H5ClN2	005922-60-1	9
4			2,4-Dimethoxytoluene	152	C9H12O2	038064-90-3	9
5			Benzenamine, 2-methyl-5-nitro-	152	C7H8N2O2	000099-55-8	9



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.275	3.9	ng	57803	1	6.898	298044	20.0
Propane, 1,1-di...	2.381	3.3	ng	48415	1	6.898	298044	20.0
unknown17.209	17.209	2.5	ng	34926	6	15.551	282169	20.0