

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101823\
 Data File : BF135839.D
 Acq On : 18 Oct 2023 10:57
 Operator : CG\JU
 Sample : PB156392BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB156392BL

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-BF101323.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135839.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.340	379	383	404	rBV	819000	1041896	29.01%	3.944%
2	4.981	485	492	514	rBV	1591420	2916734	81.20%	11.041%
3	5.393	558	562	587	rBV	3363219	3591668	99.99%	13.596%
4	5.763	621	625	637	rVB	97652	97289	2.71%	0.368%
5	6.404	729	734	759	rBV	3120422	3508047	97.66%	13.279%
6	6.740	787	791	803	rBV	669073	576086	16.04%	2.181%
7	7.310	884	888	891	rBV	2275642	2255758	62.80%	8.539%
8	8.016	1005	1008	1025	rBV	708346	658731	18.34%	2.494%
9	9.098	1188	1192	1195	rBV	3404032	3362877	93.62%	12.730%
10	9.775	1304	1307	1321	rBV	819942	731035	20.35%	2.767%
11	10.580	1439	1444	1447	rBV	2184057	2100613	58.48%	7.951%
12	11.275	1558	1562	1570	rBV	895308	788461	21.95%	2.985%
13	12.880	1829	1835	1838	rBV	3260159	3591967	100.00%	13.597%
14	13.939	2012	2015	2024	rBV	648459	650701	18.12%	2.463%
15	15.421	2262	2267	2278	rBV	395794	545988	15.20%	2.067%

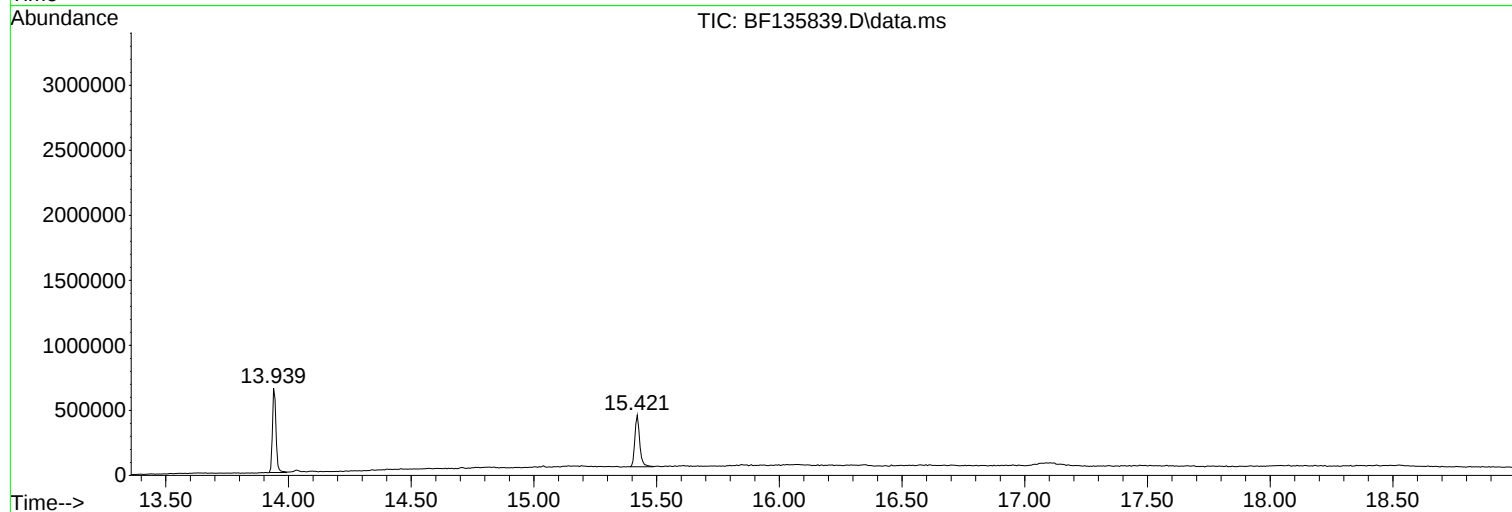
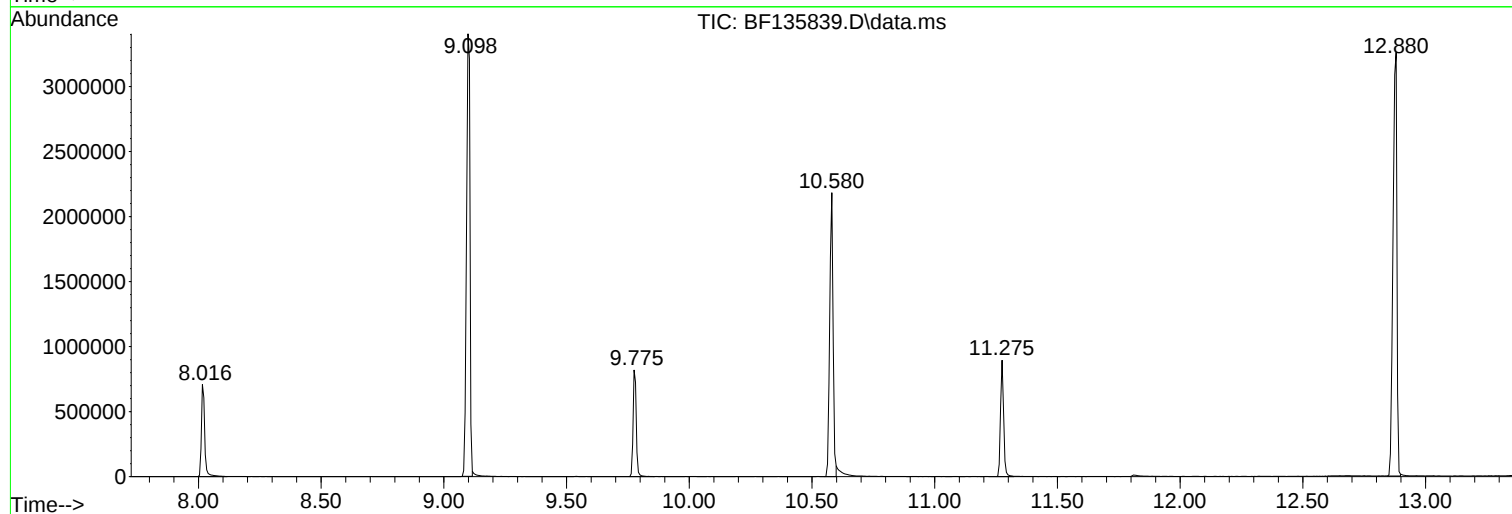
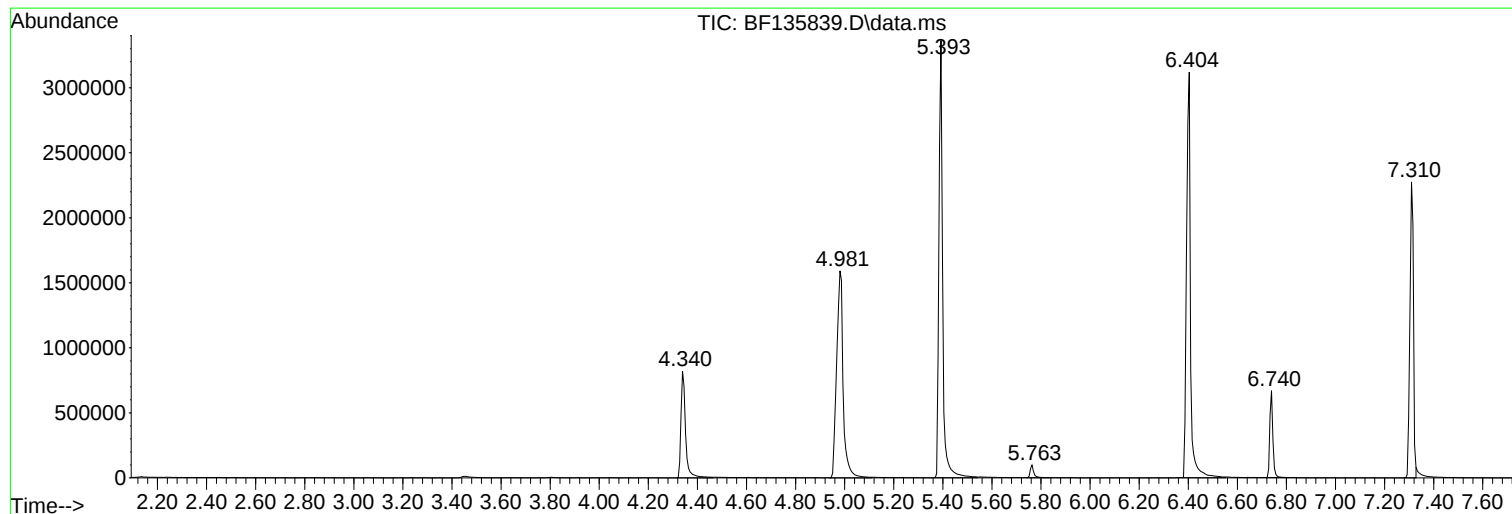
Sum of corrected areas: 26417851

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.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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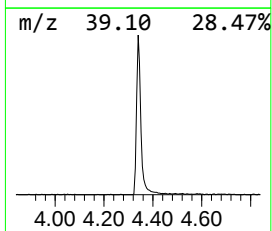
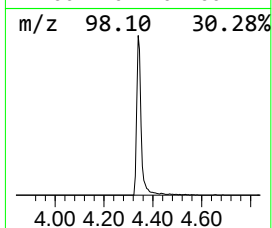
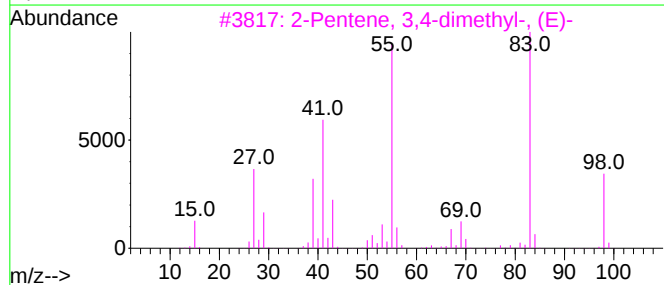
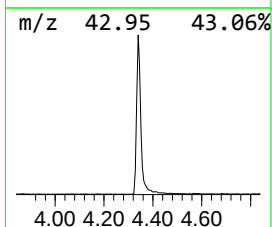
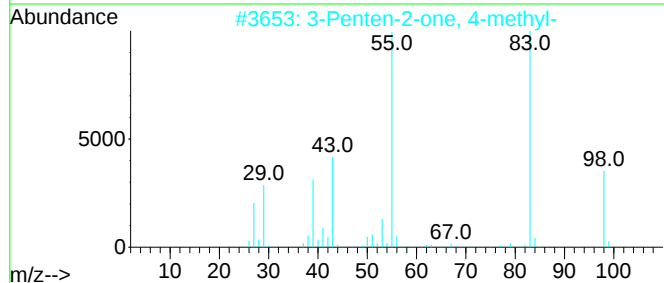
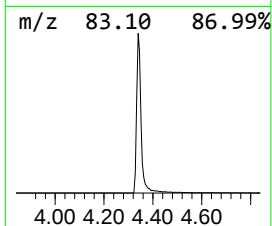
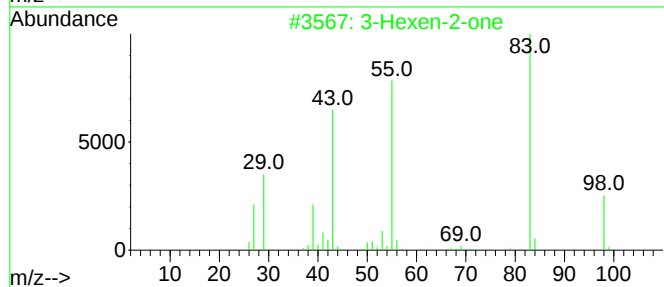
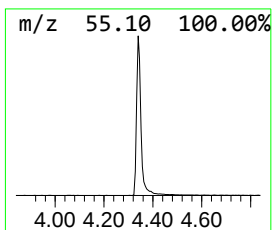
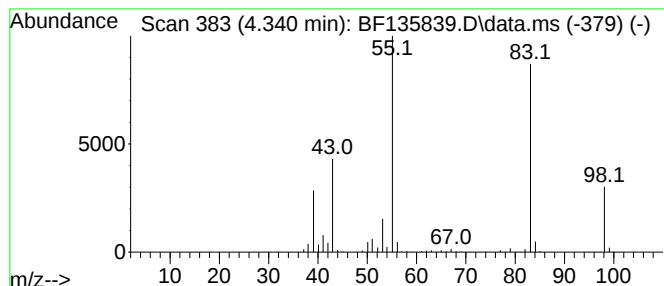
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Hexen-2-one Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.340	36.17 ng	1041900	1,4-Dichlorobenzene-d4	6.739

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



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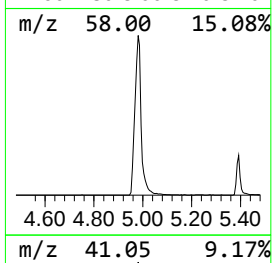
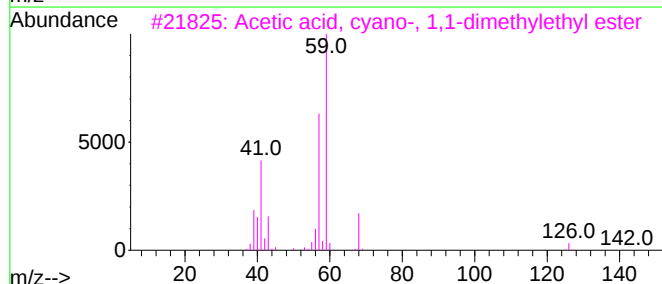
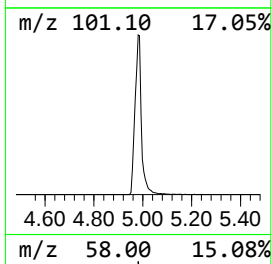
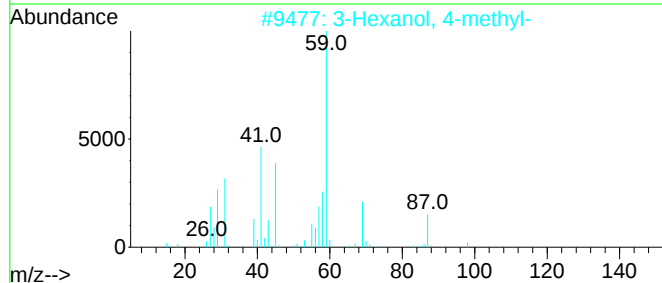
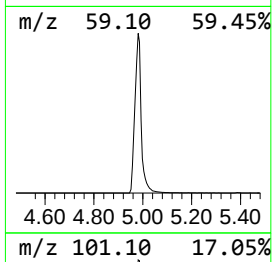
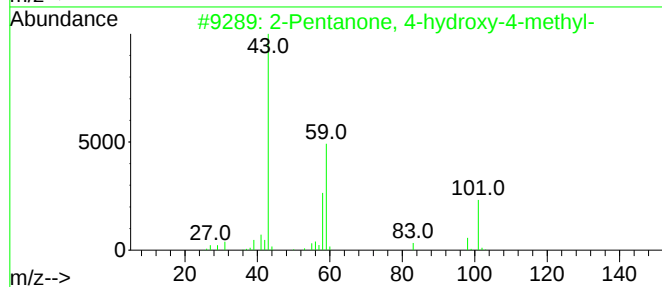
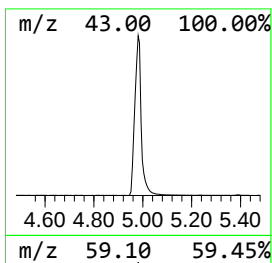
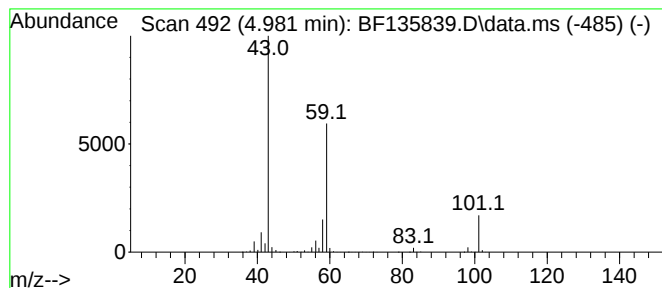
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD			R.T.
4.981	101.26 ng	2916730	1,4-Dichlorobenzene-d4			6.739

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2		000123-42-2	64
2	3-Hexanol, 4-methyl-	116	C7H16O		000615-29-2	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2		001116-98-9	23
4	1-Propen-2-ol, acetate	100	C5H8O2		000108-22-5	12
5	2,3-Butanedione, monooxime	101	C4H7NO2		000057-71-6	9



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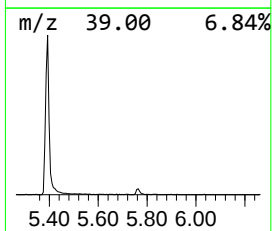
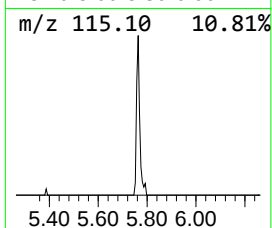
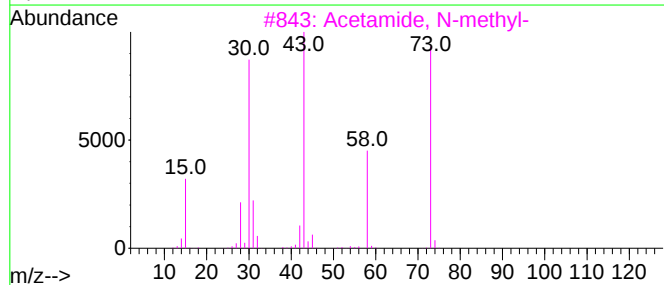
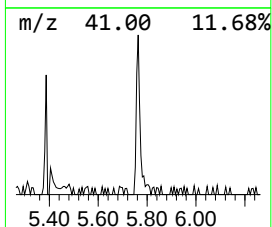
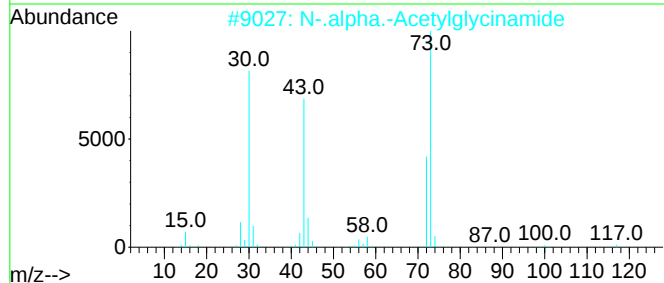
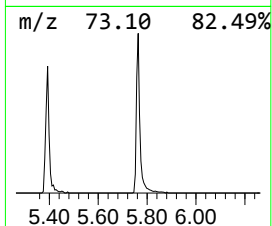
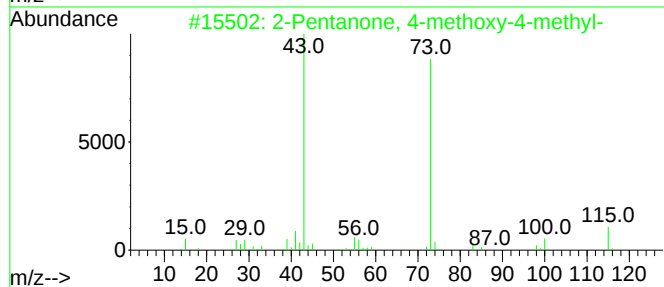
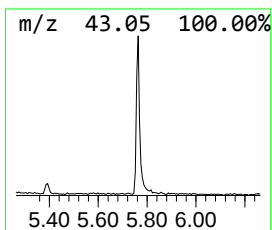
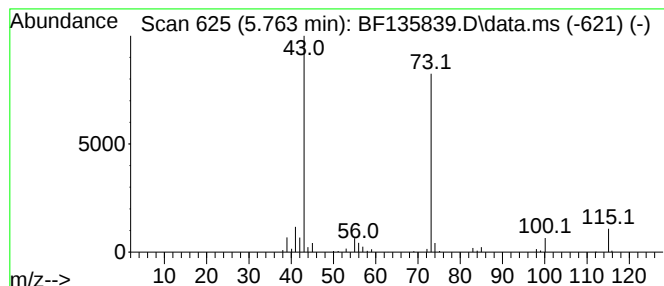
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Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.763	3.38 ng	97289	1,4-Dichlorobenzene-d4	6.739

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			Acetamide, N-methyl-	73	C3H7NO	000079-16-3	32
4			3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	17
5			3,6-Heptanedione	128	C7H12O2	001703-51-1	17



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Hexen-2-one	4.340	36.2	ng	1041900	1	6.739	576086	20.0
2-Pentanone, 4-...	4.981	101.3	ng	2916730	1	6.739	576086	20.0
2-Pentanone, 4-...	5.763	3.4	ng	97289	1	6.739	576086	20.0