

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051915\
 Data File : BF079342.D
 Acq On : 19 May 2015 15:20
 Operator : TP/IZ
 Sample : PB83467BL
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB83467BL

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-BF043015.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	1.278	6	8	11	rVB	1217159	1230863	19.94%	5.781%
2	1.644	38	40	48	rBV	1502840	2662777	43.15%	12.506%
3	1.758	48	50	93	rVB	2816888	6171361	100.00%	28.984%
4	4.879	320	323	332	rVB	287022	347640	5.63%	1.633%
5	5.416	367	370	372	rBV	841906	1065857	17.27%	5.006%
6	6.696	480	482	485	rBV	1011190	1016325	16.47%	4.773%
7	6.833	492	494	497	rBV	923490	1100984	17.84%	5.171%
8	7.130	517	520	522	rBV	244817	252331	4.09%	1.185%
9	7.313	534	536	538	rBV	973068	869011	14.08%	4.081%
10	7.816	578	580	583	rBV	498703	634111	10.28%	2.978%
11	8.708	655	658	660	rBV	330590	342718	5.55%	1.610%
12	10.056	773	776	778	rBV	1088312	1319383	21.38%	6.196%
13	10.879	845	848	850	rVB	360082	391940	6.35%	1.841%
14	11.851	931	933	936	rBV2	692734	891715	14.45%	4.188%
15	12.720	1006	1009	1011	rBV	360761	414705	6.72%	1.948%
16	14.708	1181	1183	1186	rBV	1171959	1622801	26.30%	7.621%
17	16.023	1295	1298	1300	rBV	434554	463340	7.51%	2.176%
18	17.840	1455	1457	1460	rBV	330365	494658	8.02%	2.323%

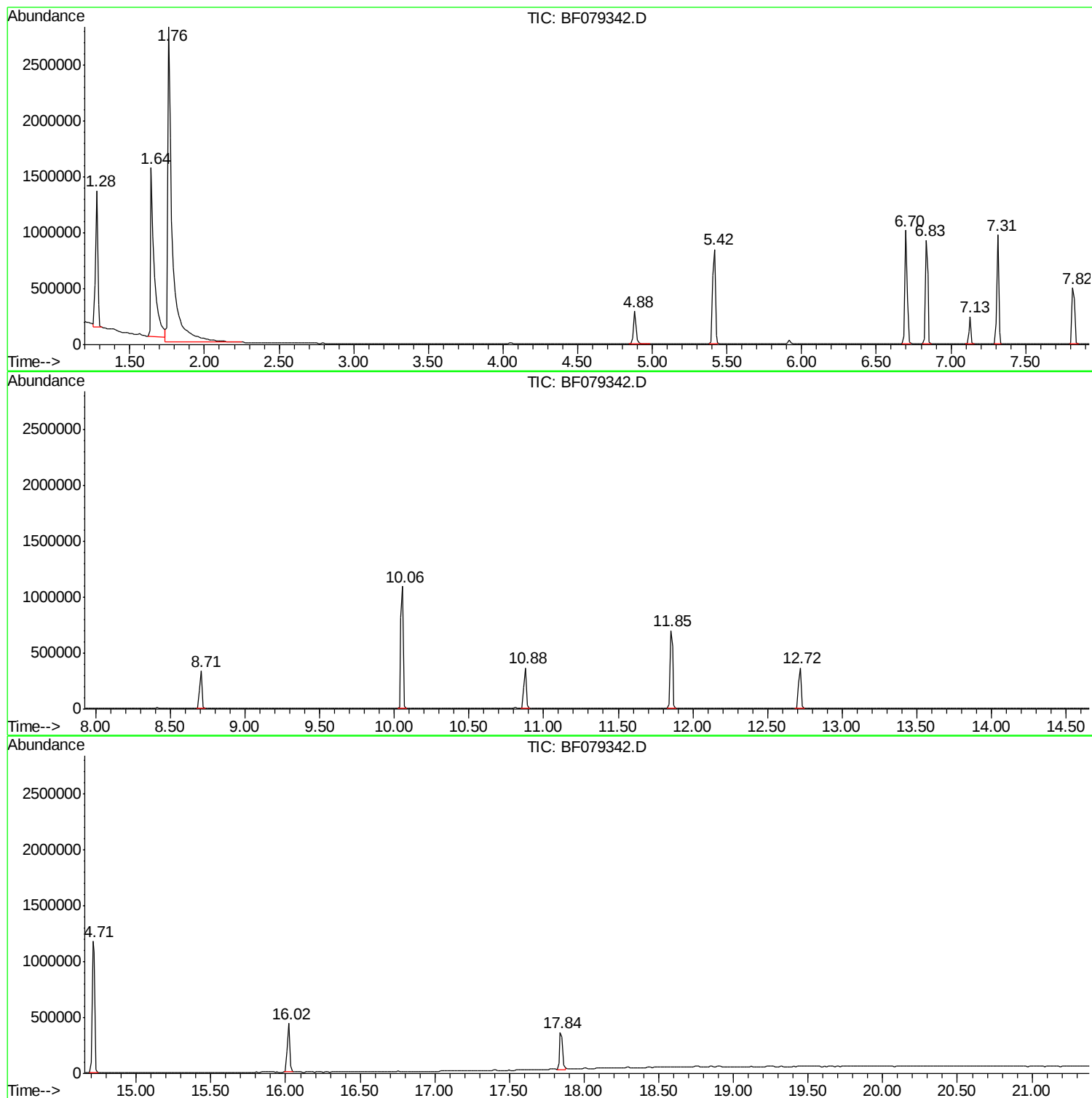
Sum of corrected areas: 21292520

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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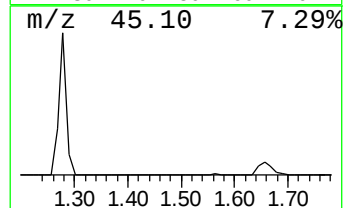
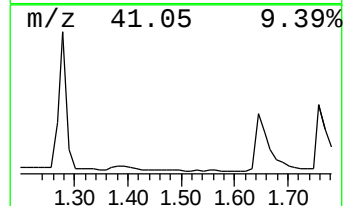
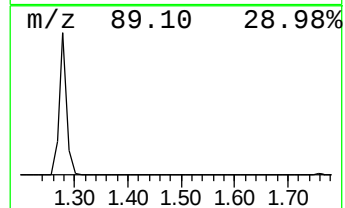
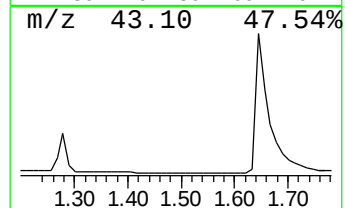
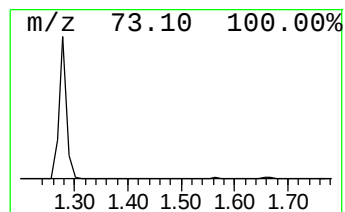
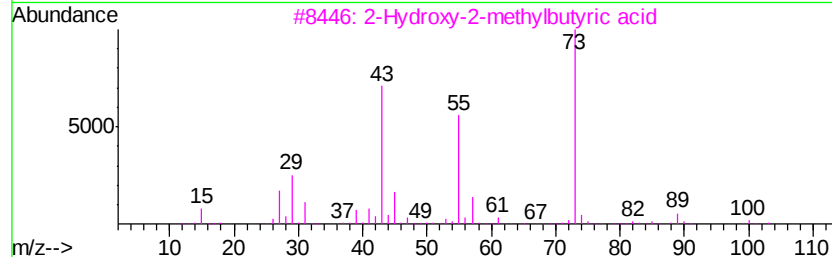
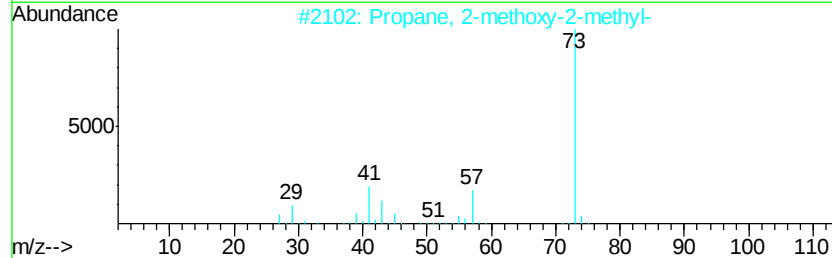
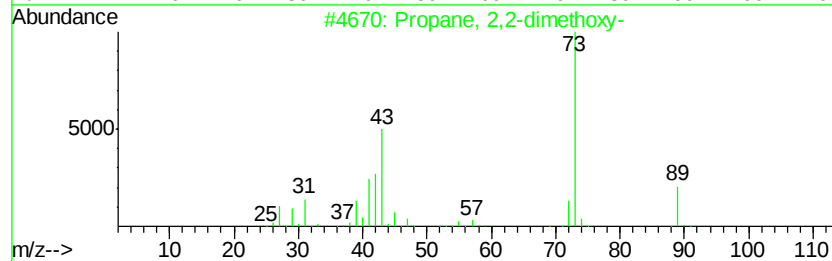
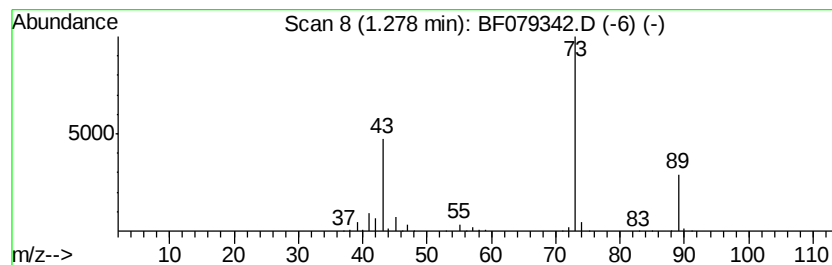
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.28	97.56 ng	1230860	1,4-Dichlorobenzene-d4	7.13

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	56
2			Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
3			2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9
4			N-Ethylformamide	73	C3H7NO	000627-45-2	5
5			1,3,5-Trioxane	90	C3H6O3	000110-88-3	4



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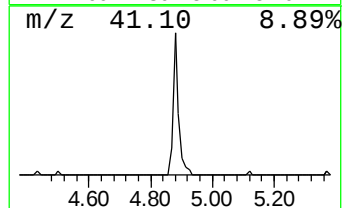
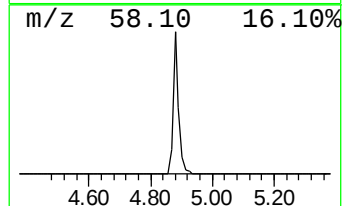
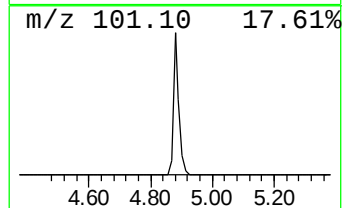
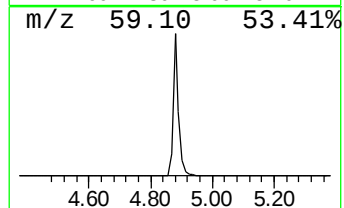
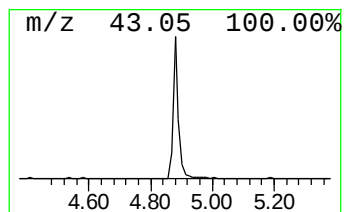
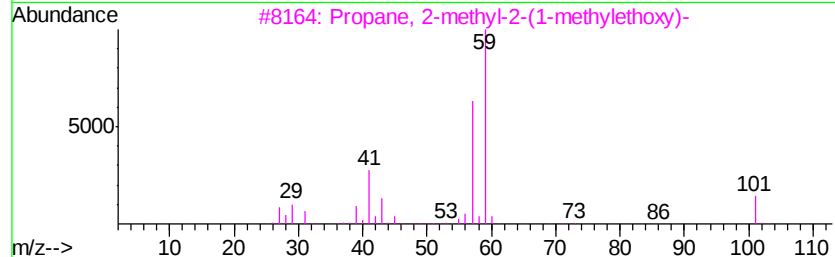
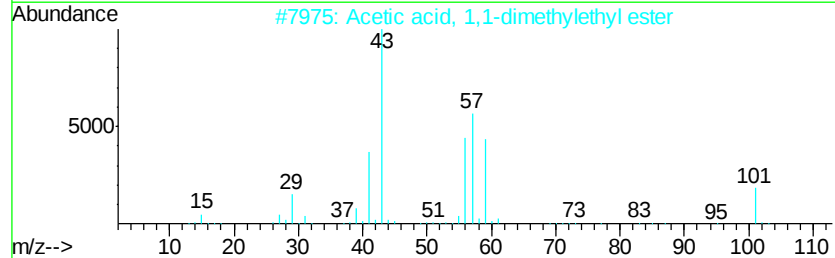
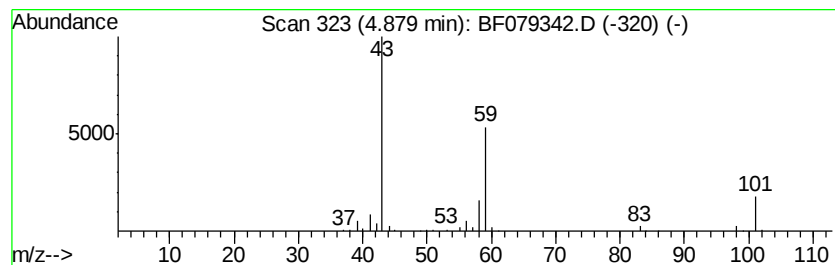
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Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.88	27.55 ng	347640	1,4-Dichlorobenzene-d4	7.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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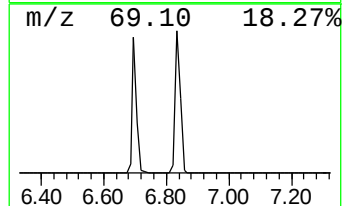
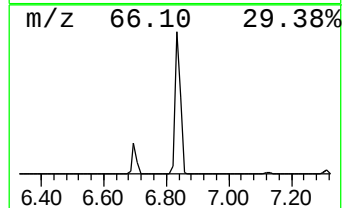
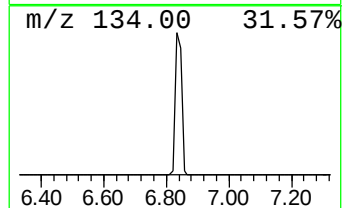
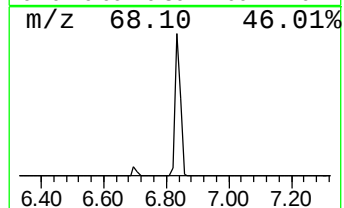
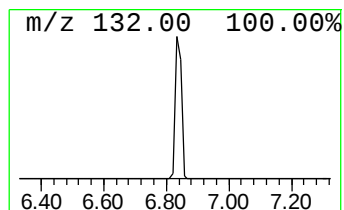
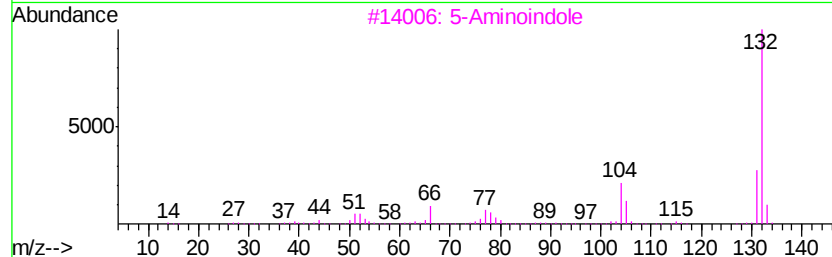
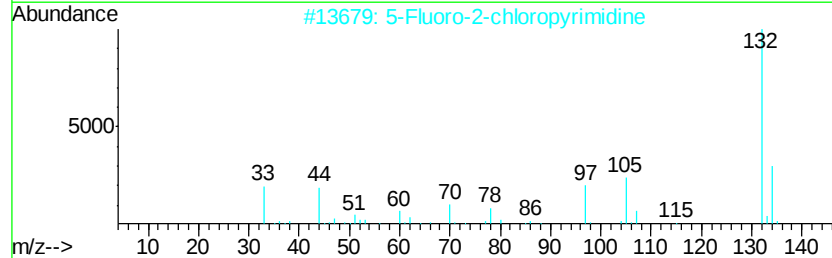
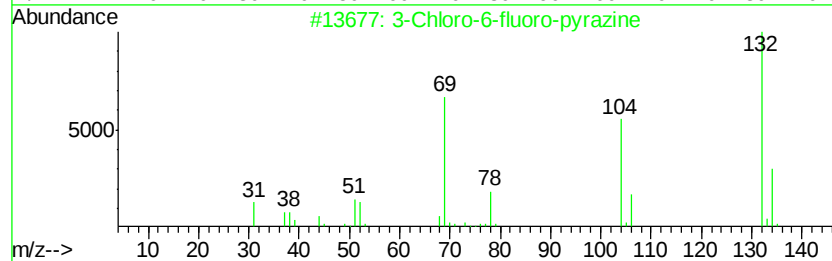
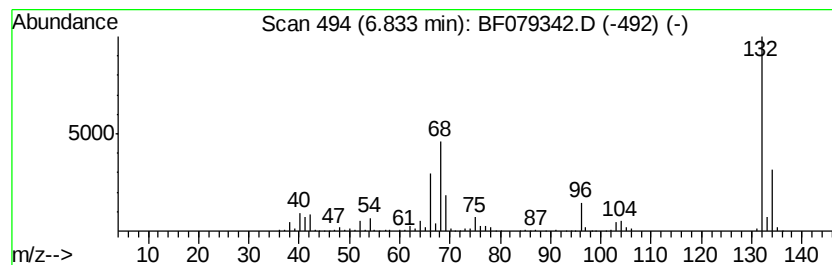
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Peak Number 5 unknown6.83 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.83	87.27 ng	1100980	1,4-Dichlorobenzene-d4	7.13

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine			132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine			132	C4H2ClFN2	062802-42-0	12
3	5-Aminoindole			132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl			189	C12H15NO	1000123-86-3	10
5	Bicyclo[4.2.0]octa-1,3,5-triene, ...			132	C10H12	028749-81-7	9



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 2,2-dime...	1.28	97.6	ng	1230860	1	7.13	252331	20.0
2-Pentanone, 4-hy...	4.88	27.6	ng	347640	1	7.13	252331	20.0
unknown6.83	6.83	87.3	ng	1100980	1	7.13	252331	20.0