

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080417\
 Data File : BF097362.D
 Acq On : 4 Aug 2017 18:14
 Operator : SJ/JU
 Sample : PB101226BL
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB101226BL

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-BF072517.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	3.875	351	355	363	rBV	48714	99459	3.05%	0.377%
2	4.587	471	476	502	rBV	629458	1151025	35.32%	4.367%
3	5.045	550	554	573	rBV	2776448	3258436	100.00%	12.362%
4	6.110	730	735	748	rBV	2659543	3079447	94.51%	11.683%
5	6.210	748	752	762	rVB	2689505	2959555	90.83%	11.228%
6	6.439	787	791	802	rVB	610525	615484	18.89%	2.335%
7	6.592	813	817	829	rBV	2323304	2301608	70.64%	8.732%
8	7.010	883	888	907	rBV	1781035	1862242	57.15%	7.065%
9	7.716	1005	1008	1020	rBV	854236	912303	28.00%	3.461%
10	8.798	1186	1192	1195	rBV	2702848	2996534	91.96%	11.368%
11	9.457	1300	1304	1318	rBV	864157	868516	26.65%	3.295%
12	10.251	1434	1439	1454	rBV	1457802	1603106	49.20%	6.082%
13	10.933	1551	1555	1565	rBV	887311	819076	25.14%	3.107%
14	12.515	1819	1824	1827	rBV2	2338006	2553290	78.36%	9.687%
15	13.551	1996	2000	2009	rBV	795642	731018	22.43%	2.773%
16	14.886	2223	2227	2233	rBV	469626	547707	16.81%	2.078%

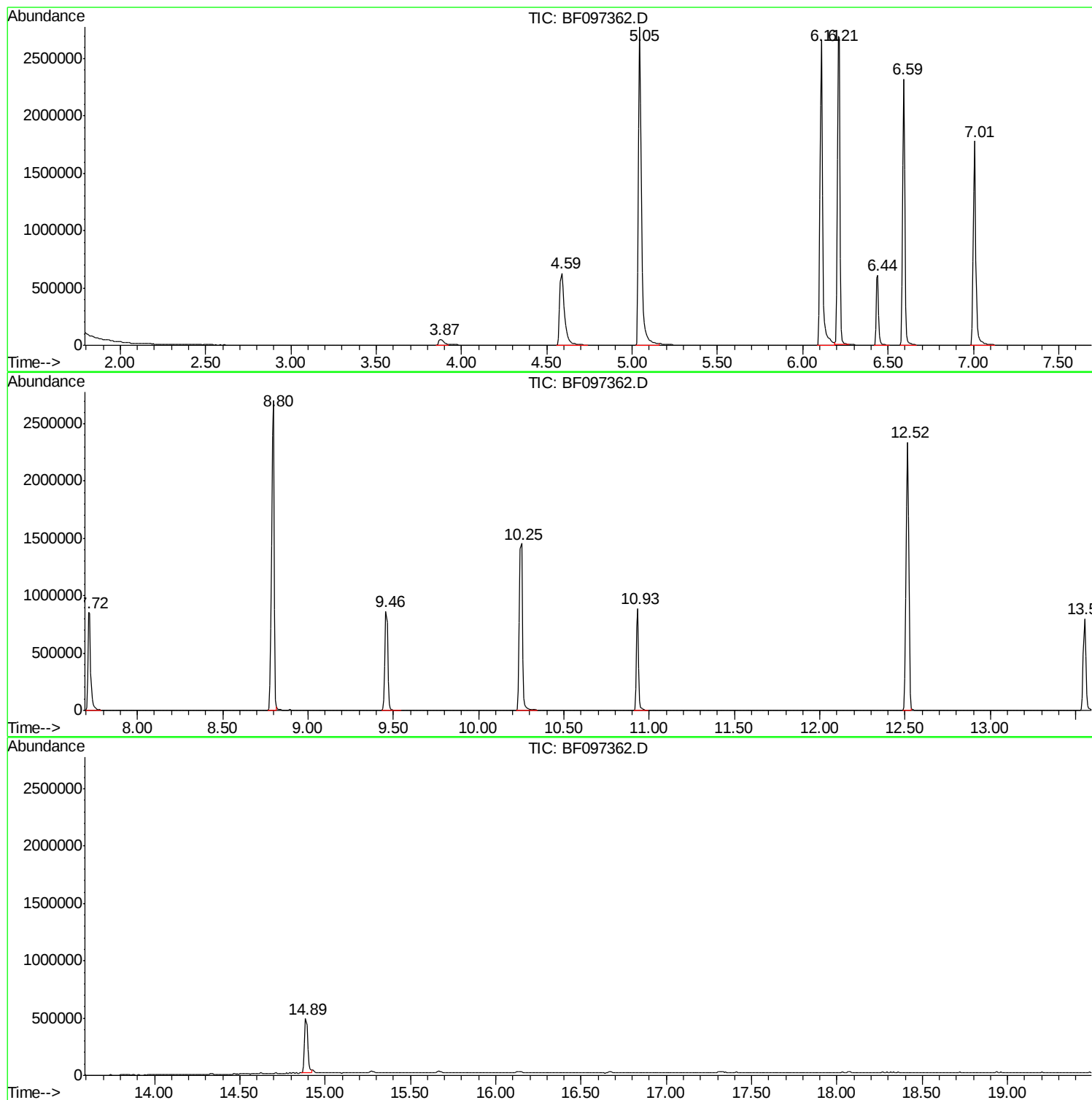
Sum of corrected areas: 26358806

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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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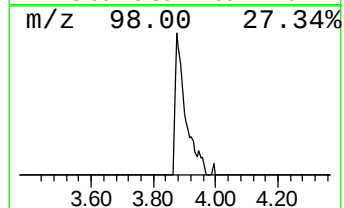
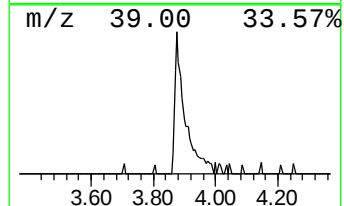
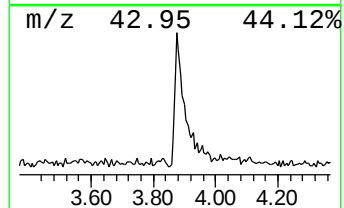
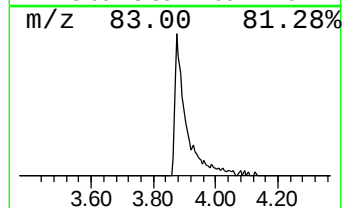
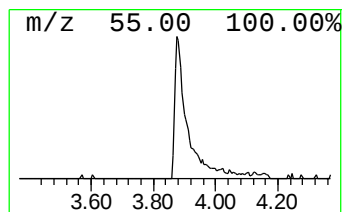
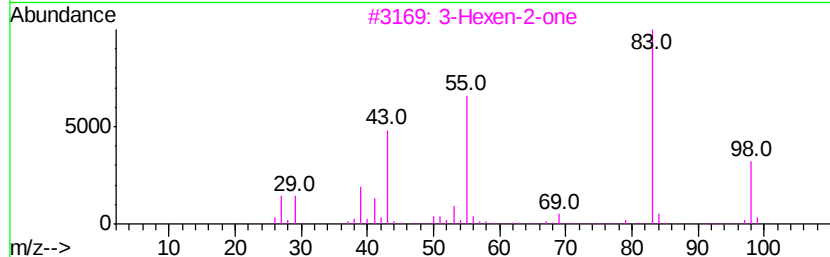
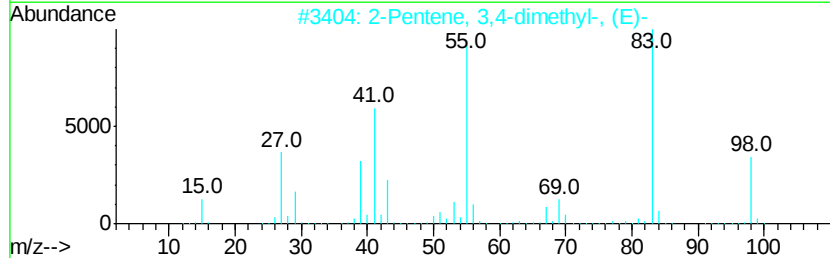
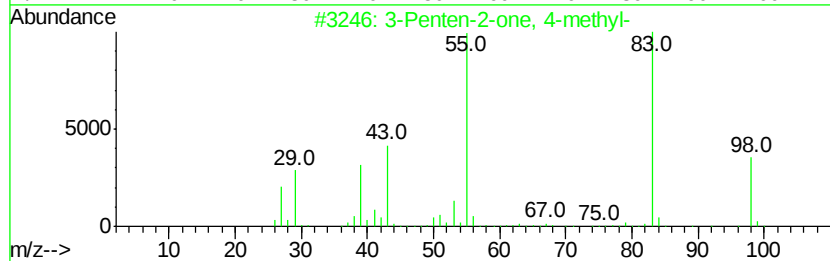
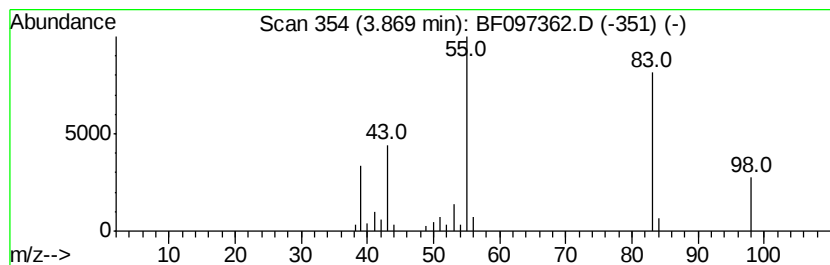
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.87	3.23 ng	99459	1,4-Dichlorobenzene-d4	6.44

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



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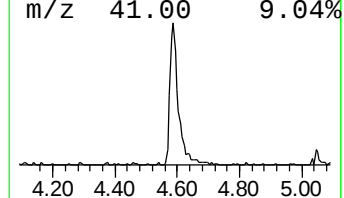
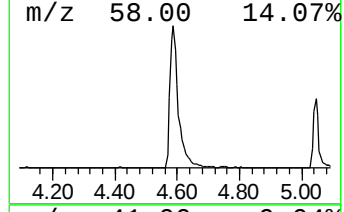
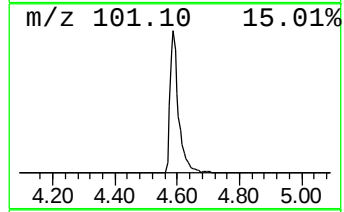
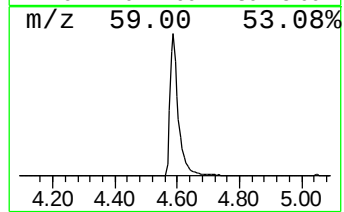
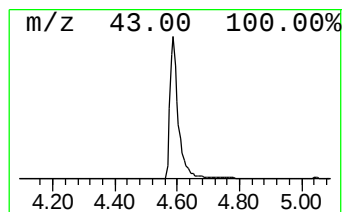
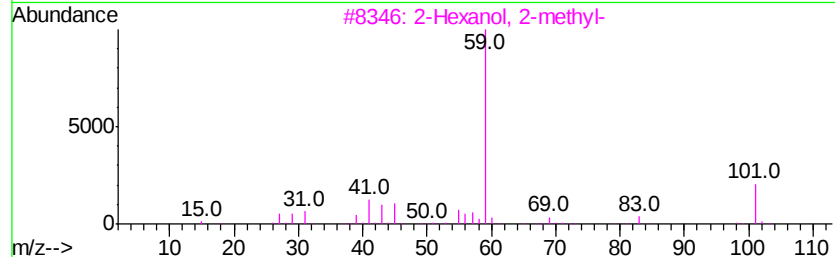
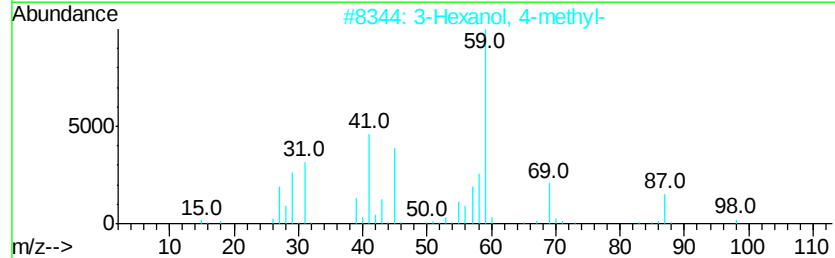
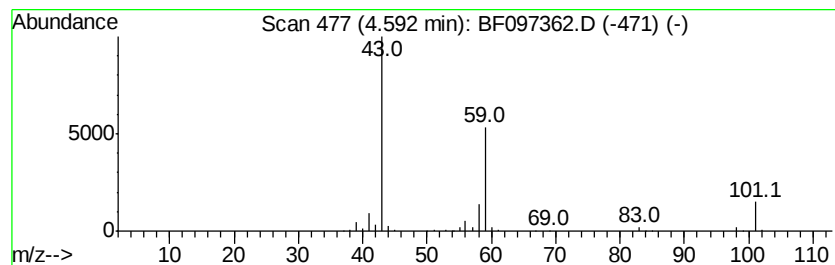
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.59	37.40 ng	1151030	1,4-Dichlorobenzene-d4	6.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9



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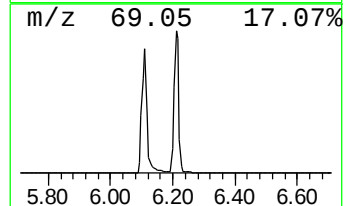
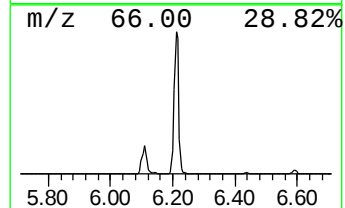
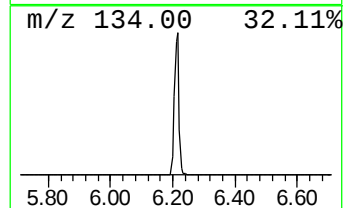
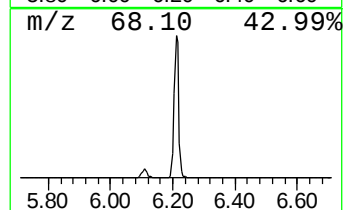
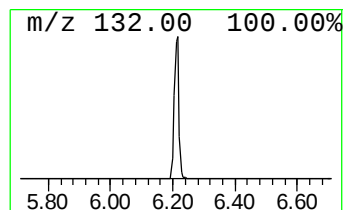
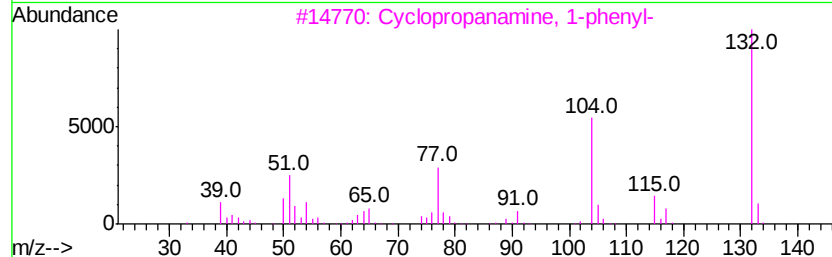
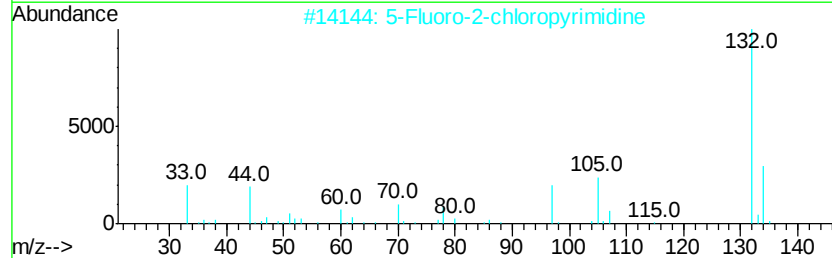
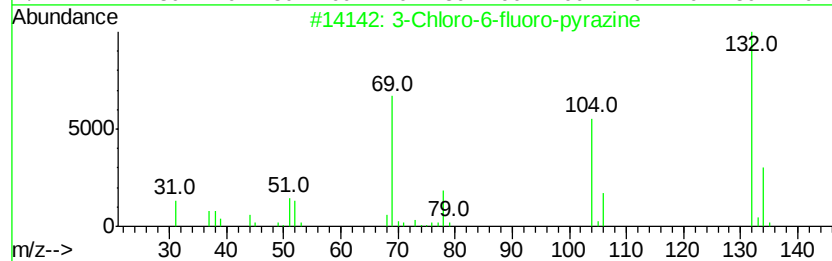
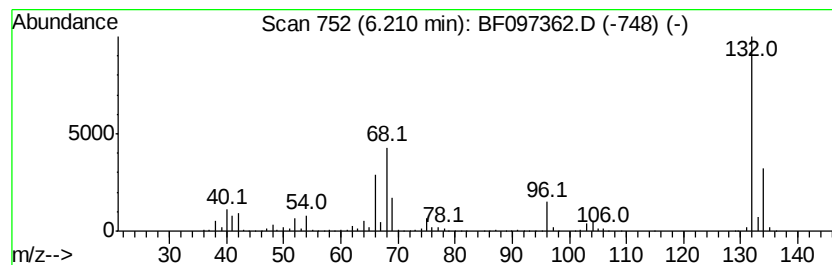
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Peak Number 3 unknown6.21 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.21	96.17 ng	2959560	1,4-Dichlorobenzene-d4	6.44

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	16		
3	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	14		
4	5-Aminoindole	132	C8H8N2	005192-03-0	12		
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10		



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	3.87	3.2	ng	99459	1	6.44	615484	20.0
2-Pentanone, 4-hy...	4.59	37.4	ng	1151030	1	6.44	615484	20.0
unknown6.21	6.21	96.2	ng	2959560	1	6.44	615484	20.0