

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
 Data File : BF085255.D
 Acq On : 8 Mar 2016 14:59
 Operator : UM/SJ
 Sample : PB88757BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB88757BL

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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	5.167	249	252	258	rBV	696379	847697	18.93%	2.429%
2	5.567	284	287	290	rBV	3195087	3231194	72.16%	9.260%
3	6.584	373	376	378	rBV	3341026	3619285	80.83%	10.373%
4	6.721	386	388	391	rBV	2816919	3531144	78.86%	10.120%
5	6.961	407	409	411	rBB	1014554	899472	20.09%	2.578%
6	7.122	420	423	425	rBV	2364411	2937582	65.61%	8.419%
7	7.522	455	458	460	rBV	2336711	2423118	54.12%	6.945%
8	8.242	518	521	524	rBV	1268113	1170236	26.14%	3.354%
9	9.316	612	615	618	rBV	3009342	4231776	94.51%	12.128%
10	10.002	672	675	677	rBV	1358932	1295532	28.93%	3.713%
11	10.790	741	744	746	rBV	2493776	2549913	56.95%	7.308%
12	11.488	802	805	807	rBV	1486496	1387140	30.98%	3.975%
13	13.076	941	944	946	rBV	3840851	4477535	100.00%	12.832%
14	14.116	1033	1035	1038	rBV	1129760	1168628	26.10%	3.349%
15	15.591	1160	1164	1171	rBV	583057	893484	19.95%	2.561%
16	16.540	1242	1247	1248	rBV3	32155	52748	1.18%	0.151%
17	16.608	1249	1253	1257	rVB4	46344	126009	2.81%	0.361%
18	19.248	1482	1484	1485	rVB	38262	49865	1.11%	0.143%

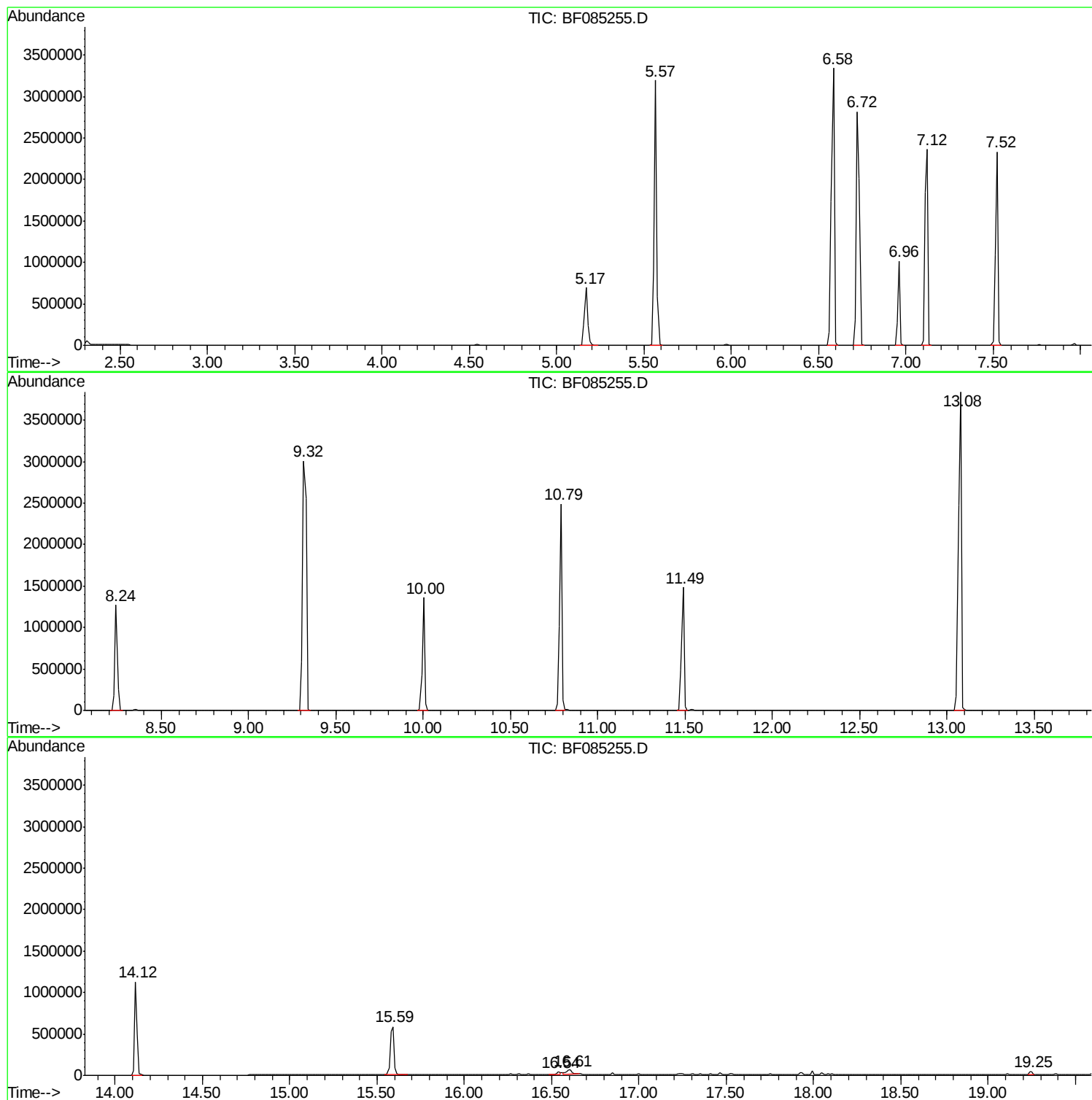
Sum of corrected areas: 34892358

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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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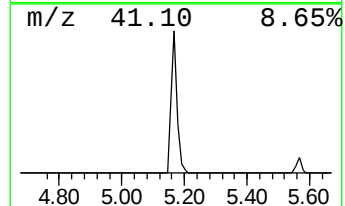
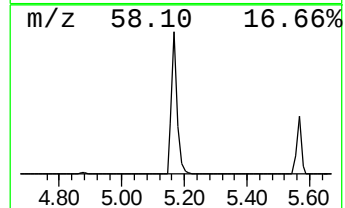
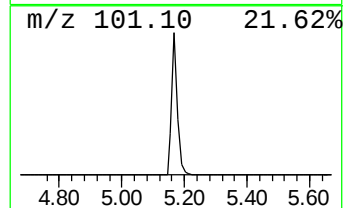
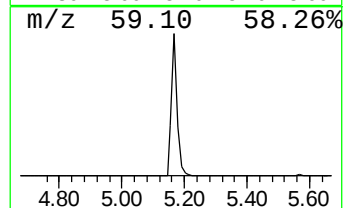
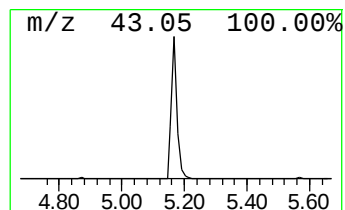
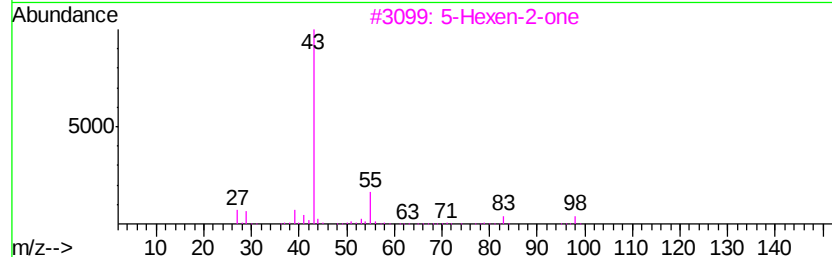
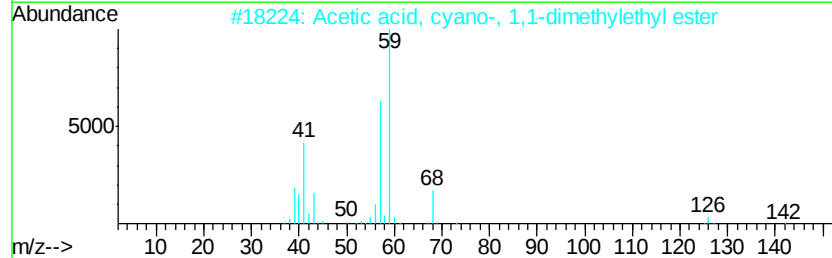
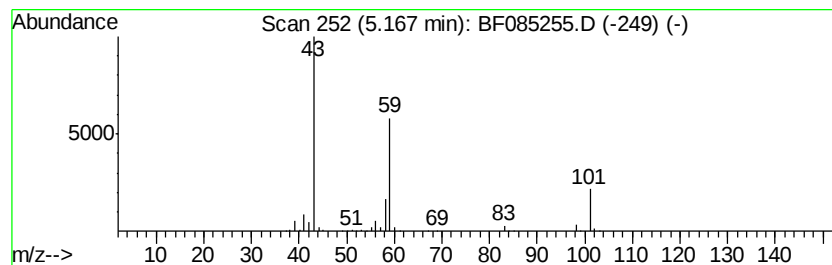
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.17	18.85 ng	847697	1,4-Dichlorobenzene-d4	6.96

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3			5-Hexen-2-one	98	C6H10O	000109-49-9	9
4			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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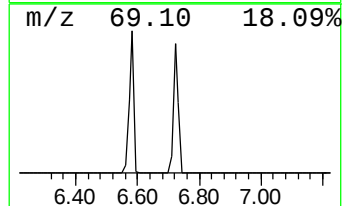
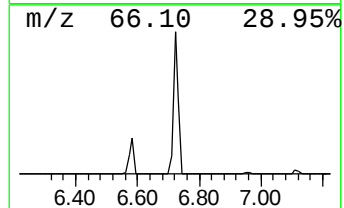
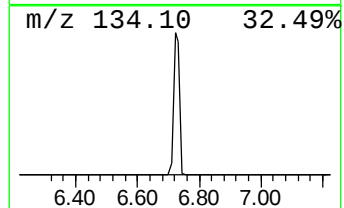
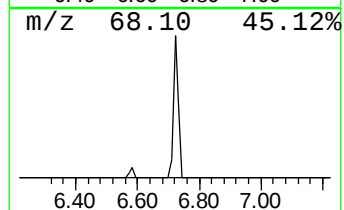
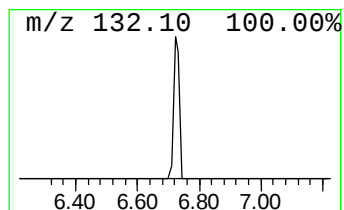
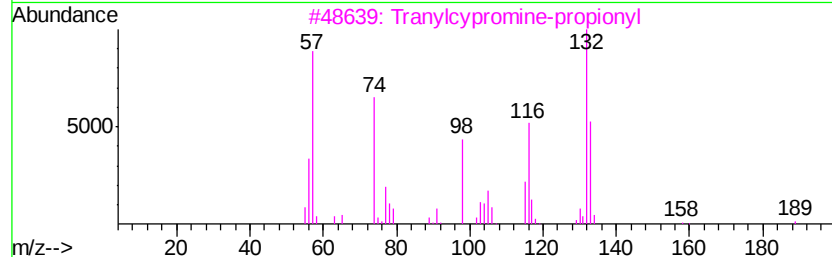
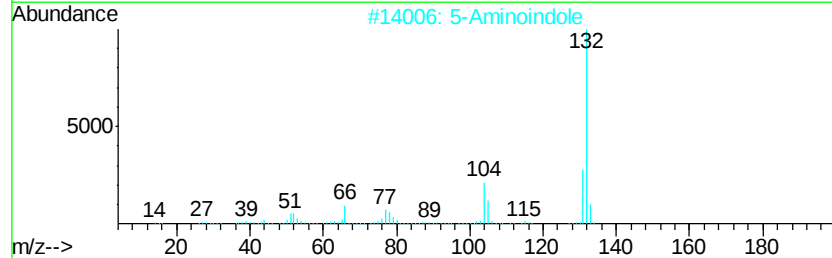
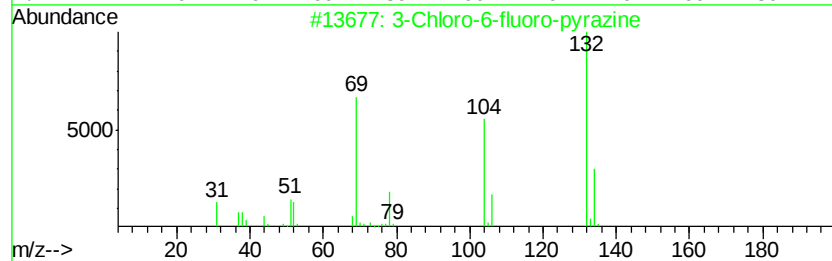
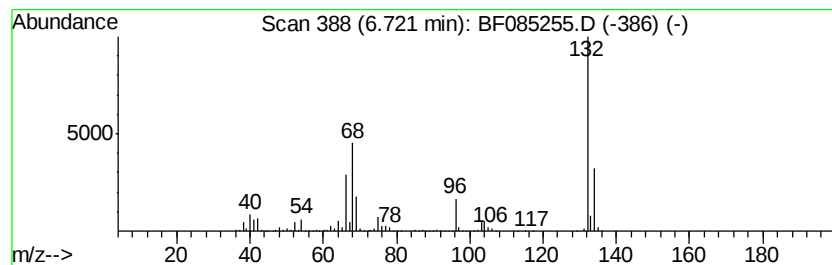
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Peak Number 2 unknown6.72 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.72	78.52 ng	3531140	1,4-Dichlorobenzene-d4	6.96

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			5-Aminoindole	132	C8H8N2	005192-03-0	12
3			Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4			Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5			Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9



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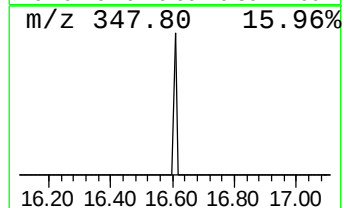
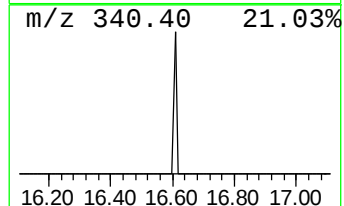
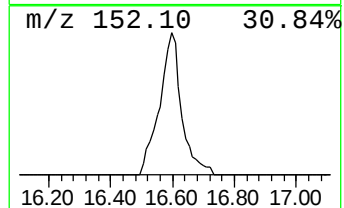
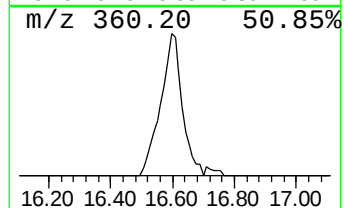
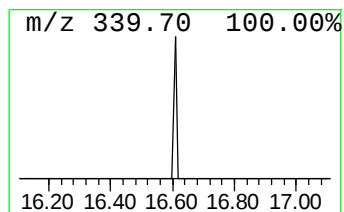
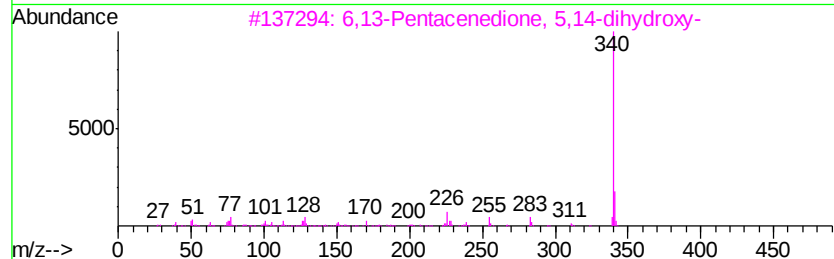
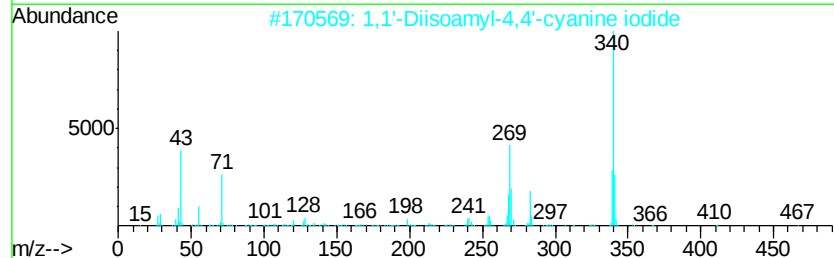
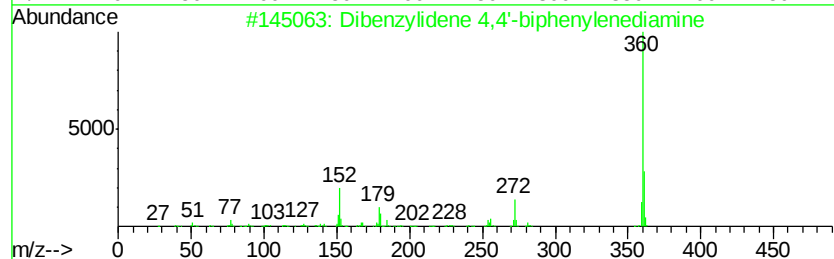
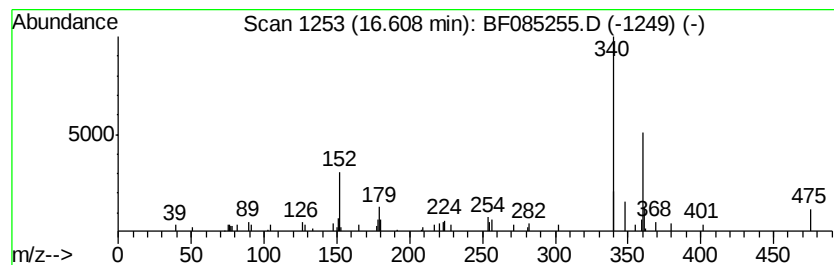
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Peak Number 4 unknown16.61 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.61	2.82 ng	126009	Perylene-d12	15.59

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dibenzylidene 4,4'-biphenylenedi...	360	C26H20N2	006311-48-4	30
2		1,1'-Diisoamyl-4,4'-cyanine iodide	538	C29H35IN2	000523-42-2	16
3		6,13-Pentacenedione, 5,14-dihydr...	340	C22H12O4	068970-90-1	16
4		[2-(4-Methoxy-phenyl)-2H-benzo[g...	360	C22H20N2O3	1000188-59-8	11
5		2-Cyclohexylamino-3-methyl(pheny...	360	C23H24N2O2	134614-17-8	10



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.17	18.9	ng	847697	1	6.96	899472	20.0
unknown6.72	6.72	78.5	ng	3531140	1	6.96	899472	20.0
unknown16.61	16.61	2.8	ng	126009	6	15.59	893484	20.0