

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021417\
 Data File : BF092940.D
 Acq On : 14 Feb 2017 13:32
 Operator : SJ/MA
 Sample : I1799-02
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SW-1

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-BF013017.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	5.047	257	259	269	rBV	501152	526980	10.67%	1.562%
2	5.470	294	296	299	rBV	1494349	1799525	36.42%	5.335%
3	6.510	385	387	389	rBV	1309704	1251621	25.33%	3.711%
4	6.647	396	399	401	rBV	3077991	3482512	70.48%	10.325%
5	6.876	416	419	421	rBV	1039805	915668	18.53%	2.715%
6	7.036	430	433	435	rBV	2957577	3368628	68.18%	9.988%
7	7.436	465	468	471	rBV	1951618	2820734	57.09%	8.363%
8	7.550	476	478	483	rVV	54598	77898	1.58%	0.231%
9	8.156	529	531	534	rBV	1193142	1184162	23.97%	3.511%
10	8.499	559	561	563	rBV2	66969	92304	1.87%	0.274%
11	9.242	623	626	628	rBV	3876547	4940929	100.00%	14.649%
12	9.630	658	660	662	rBV	106195	85867	1.74%	0.255%
13	9.916	682	685	687	rVB	1220939	1370709	27.74%	4.064%
14	10.339	718	722	724	rBV3	60698	104355	2.11%	0.309%
15	10.705	751	754	756	rBV	2444672	2601630	52.65%	7.714%
16	10.808	762	763	768	rVB	50909	85422	1.73%	0.253%
17	11.265	801	803	808	rVB	50731	76871	1.56%	0.228%
18	11.391	812	814	817	rBV2	1158377	1309599	26.51%	3.883%
19	12.796	934	937	939	rBV	1762568	1704431	34.50%	5.053%
20	12.979	950	953	956	rBV	3564432	3894895	78.83%	11.548%
21	13.871	1029	1031	1035	rBV	45950	77226	1.56%	0.229%
22	14.031	1042	1045	1047	rBV	1129414	1137224	23.02%	3.372%
23	15.460	1167	1170	1173	rBV	581530	818593	16.57%	2.427%

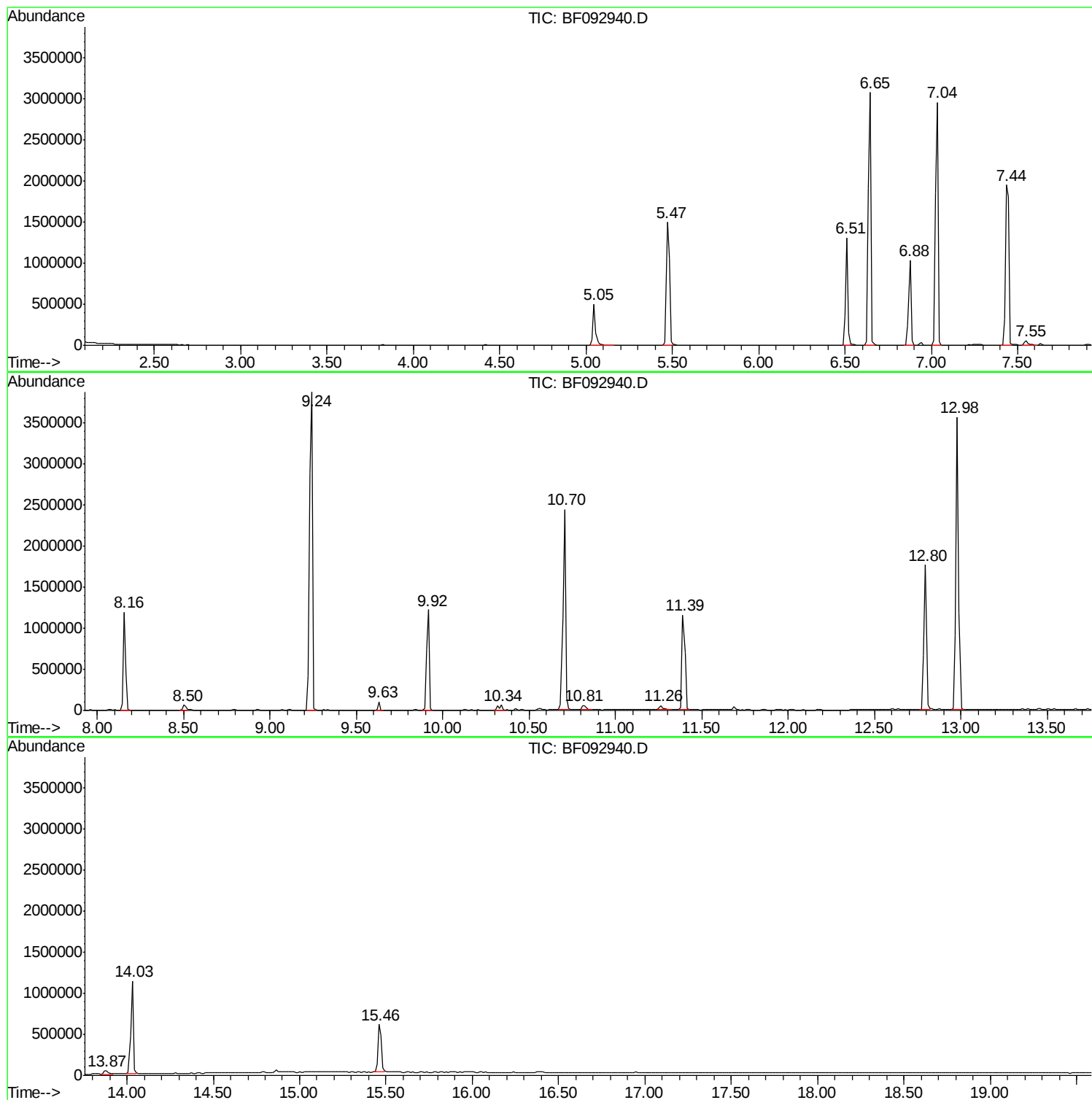
Sum of corrected areas: 33727783

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.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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Instrument :
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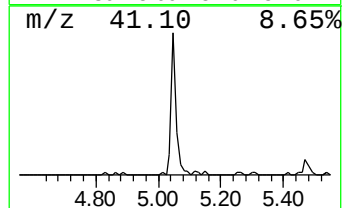
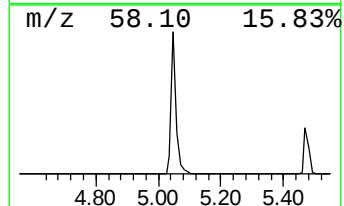
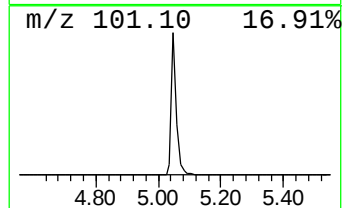
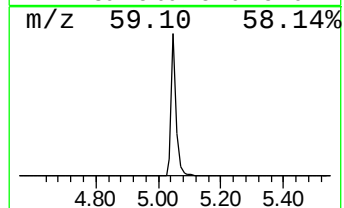
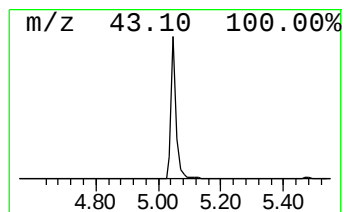
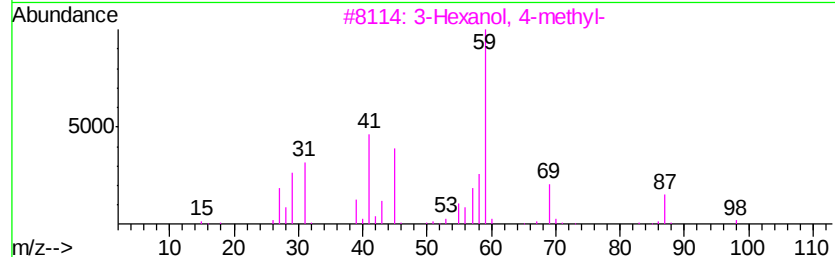
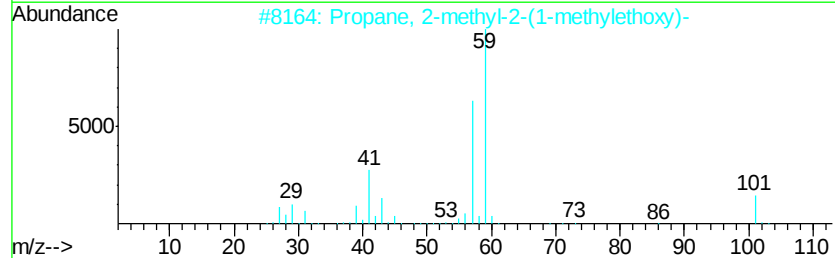
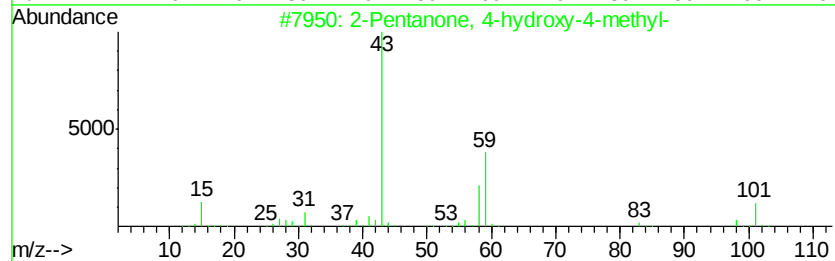
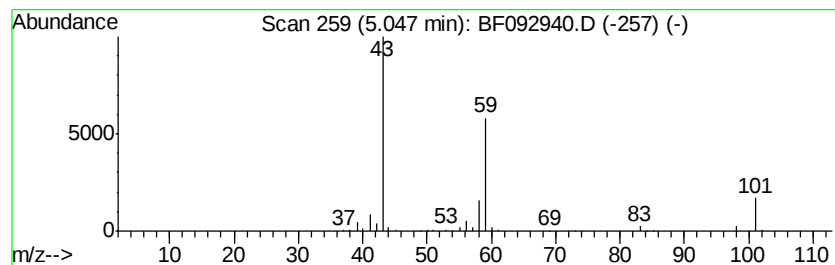
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	11.51 ng	526980	1,4-Dichlorobenzene-d4	6.88

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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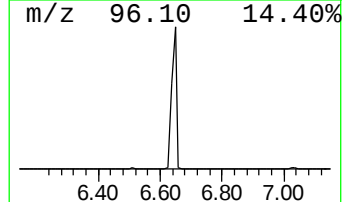
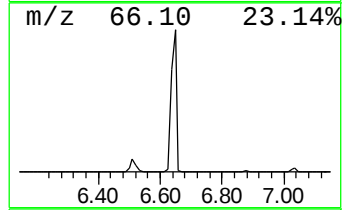
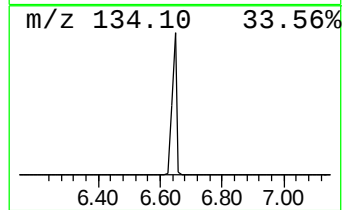
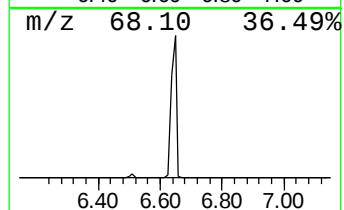
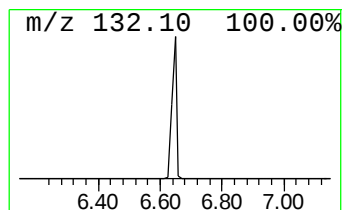
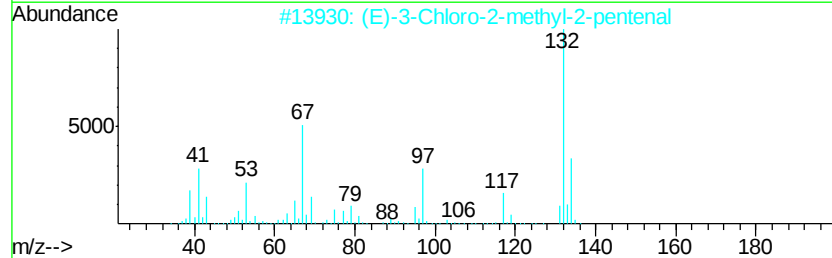
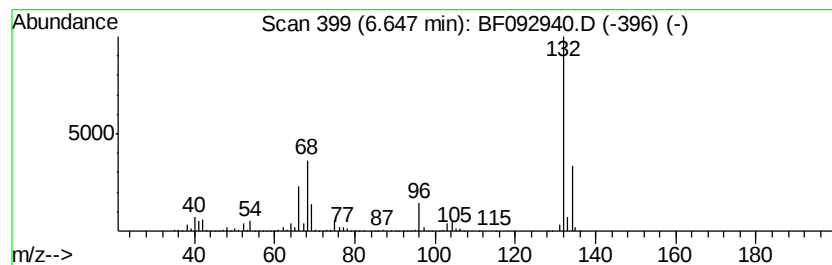
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	76.06 ng	3482510	1,4-Dichlorobenzene-d4	6.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9



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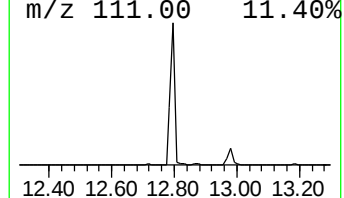
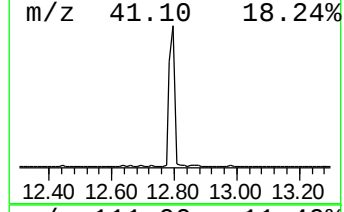
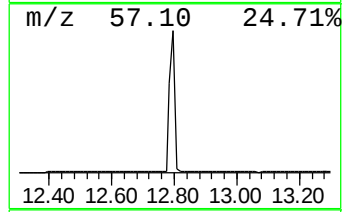
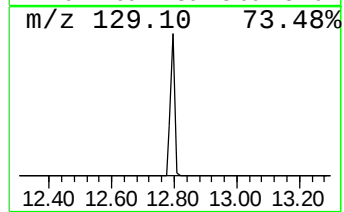
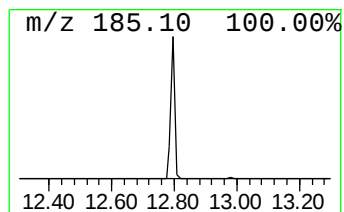
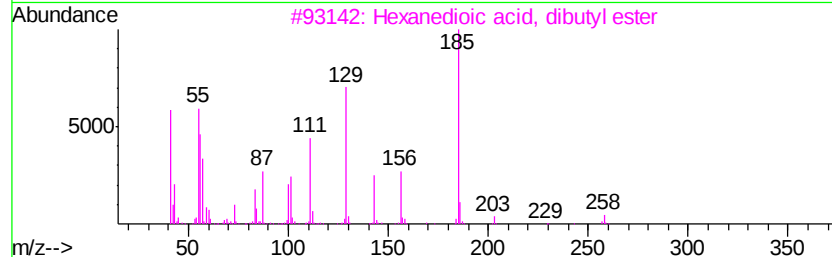
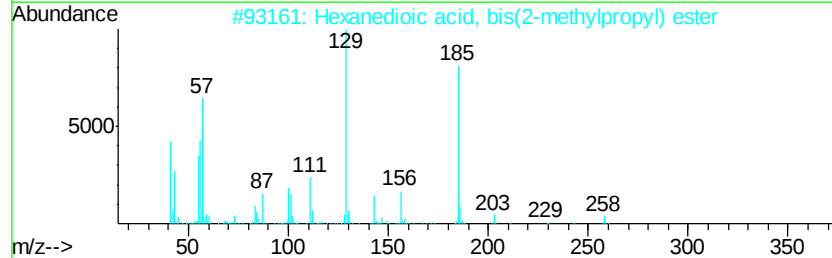
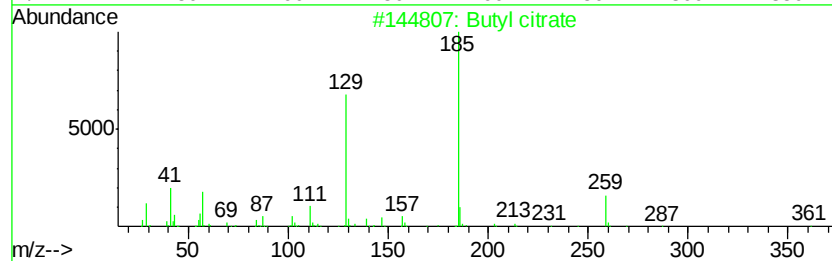
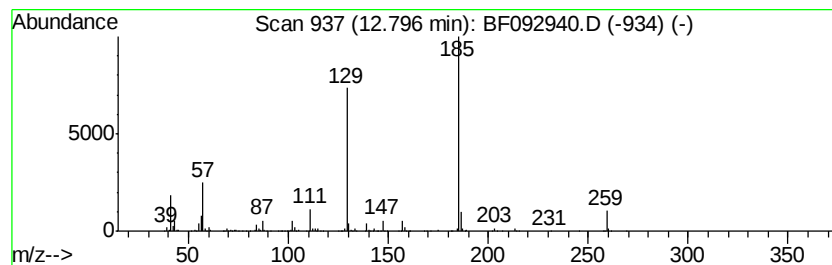
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Peak Number 4 Butyl citrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.80	29.98 ng	1704430	Chrysene-d12	14.03
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Butyl citrate	360 C18H32O7	000077-94-1	91
2	Hexanedioic acid, bis(2-methylpr...	258 C14H26O4	000141-04-8	56
3	Hexanedioic acid, dibutyl ester	258 C14H26O4	000105-99-7	50
4	2-Bromo-3-methylaniline	185 C7H8BrN	1000289-33-5	27
5	8-ALLYLOXYMETHYL-1-NAPHTHALDEHYDE	226 C15H14O2	1000237-19-3	25



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.05	11.5	ng	526980	1	6.88	915668	20.0
unknown6.65	6.65	76.1	ng	3482510	1	6.88	915668	20.0
Butyl citrate	12.80	30.0	ng	1704430	5	14.03	1137220	20.0