

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031523\
 Data File : BF132798.D
 Acq On : 15 Mar 2023 12:25
 Operator : CG\JU
 Sample : PB151405BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB151405BL

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-BF022223.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132798.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.610	341	344	354	rBV	215644	262526	3.40%	0.565%
2	5.216	441	447	460	rBV	1882279	2820668	36.58%	6.068%
3	5.610	509	514	517	rBV	5004195	5399303	70.03%	11.615%
4	6.604	677	683	686	rBV	4666405	5509239	71.45%	11.851%
5	6.963	741	744	748	rBV	1529286	1235082	16.02%	2.657%
6	7.534	835	841	844	rBV	3775084	3797044	49.24%	8.168%
7	8.245	959	962	966	rBV	1653349	1515371	19.65%	3.260%
8	9.328	1139	1146	1149	rBV	6883189	6600319	85.60%	14.199%
9	10.010	1258	1262	1265	rBV	2325975	2010848	26.08%	4.326%
10	10.804	1392	1397	1400	rBV	4578375	4466730	57.93%	9.609%
11	11.504	1512	1516	1519	rBV	2407963	2177478	28.24%	4.684%
12	12.892	1748	1752	1755	rBV	158690	118618	1.54%	0.255%
13	13.092	1781	1786	1789	rBV	7005408	7710521	100.00%	16.587%
14	13.598	1869	1872	1876	rBV	146041	126586	1.64%	0.272%
15	14.157	1963	1967	1971	rBV	1754068	1584113	20.54%	3.408%
16	15.686	2222	2227	2235	rBV	699772	961831	12.47%	2.069%
17	17.733	2565	2575	2576	rBV3	76661	189564	2.46%	0.408%

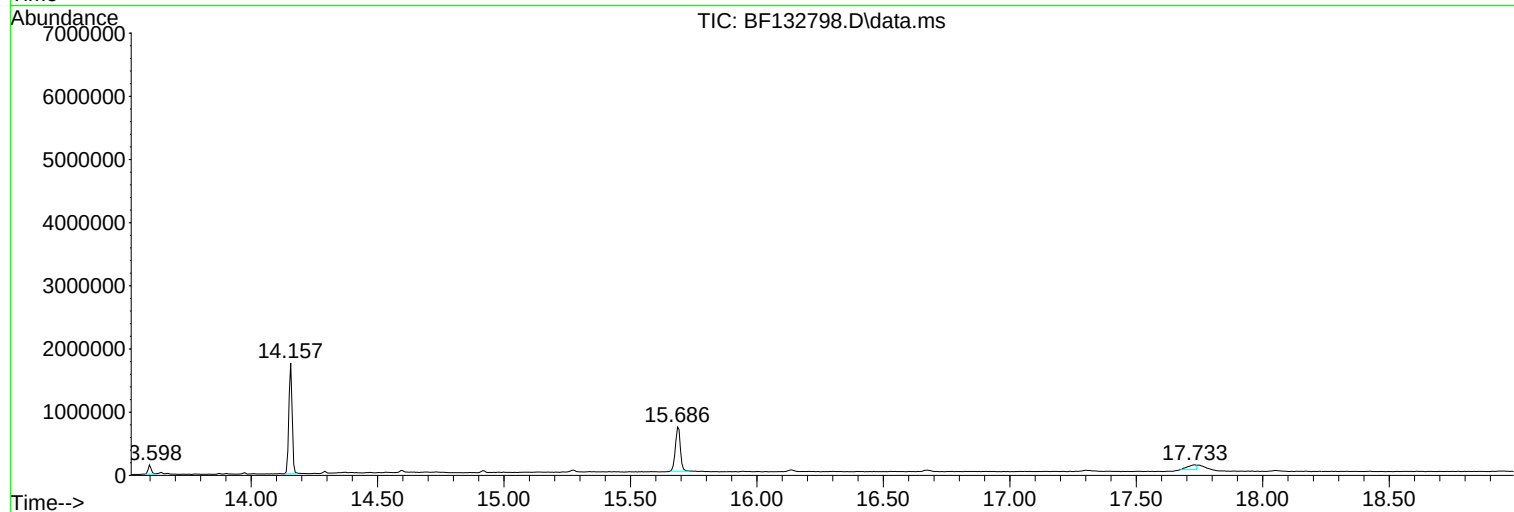
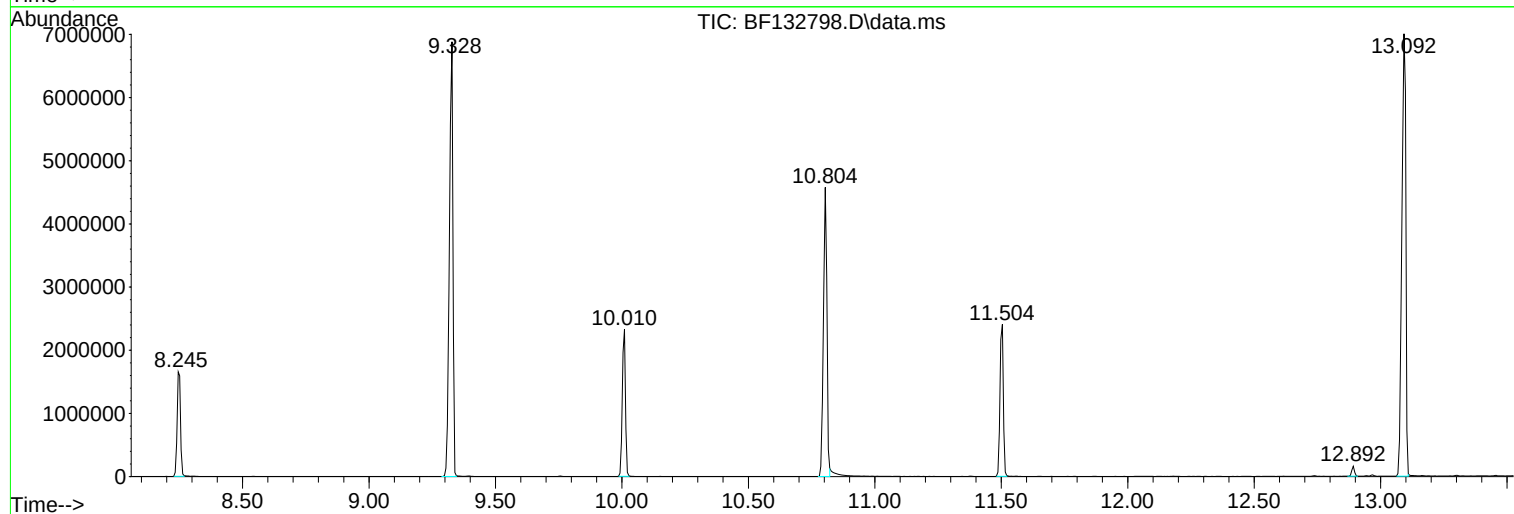
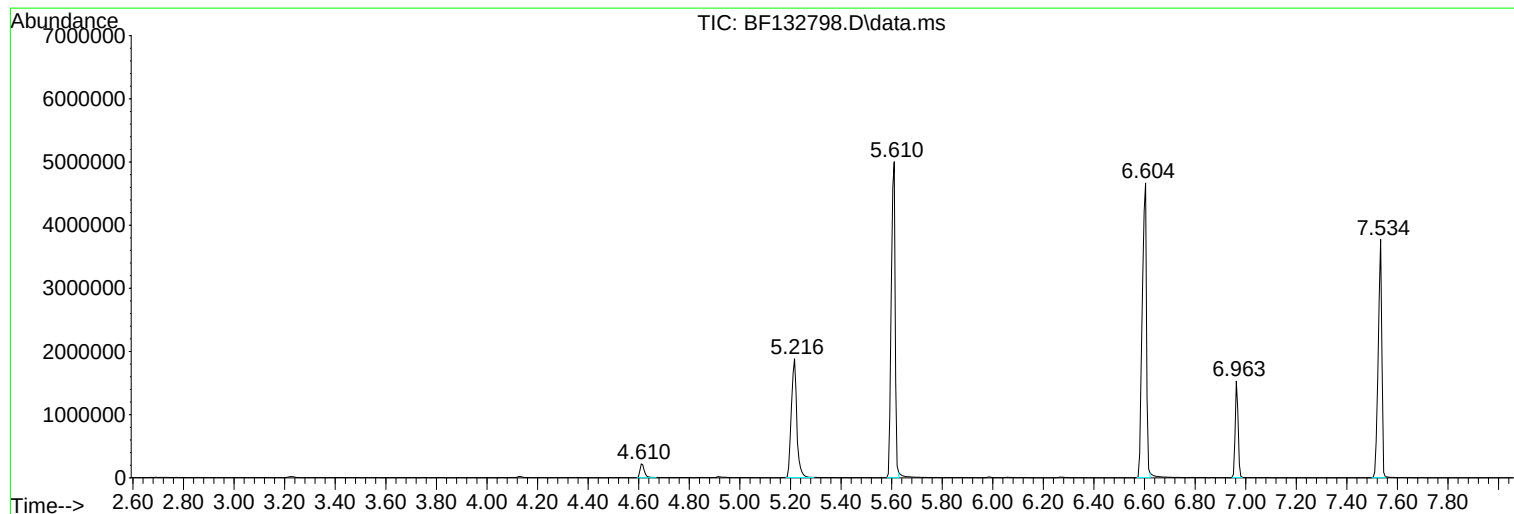
Sum of corrected areas: 46485841

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.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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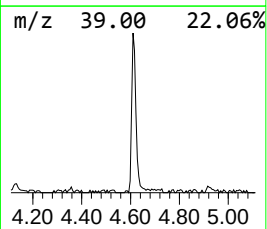
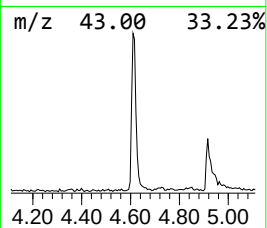
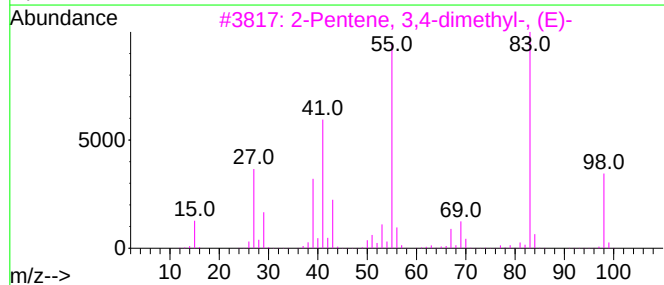
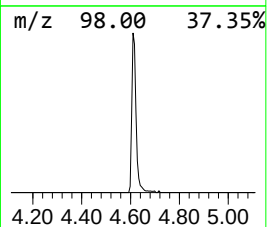
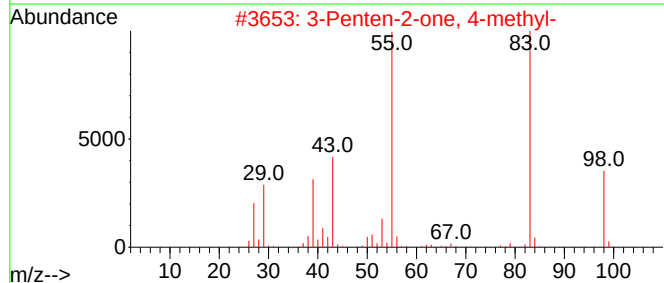
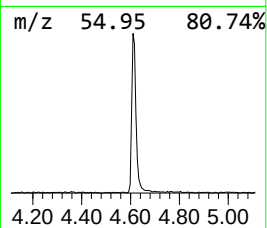
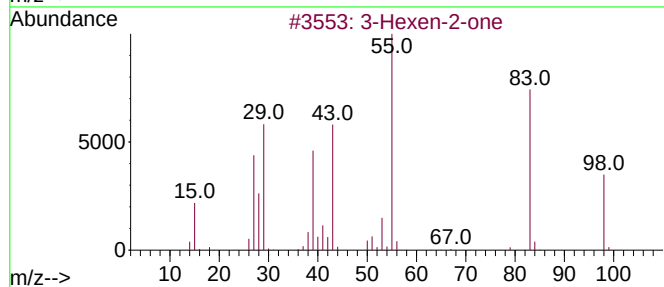
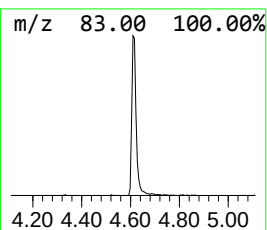
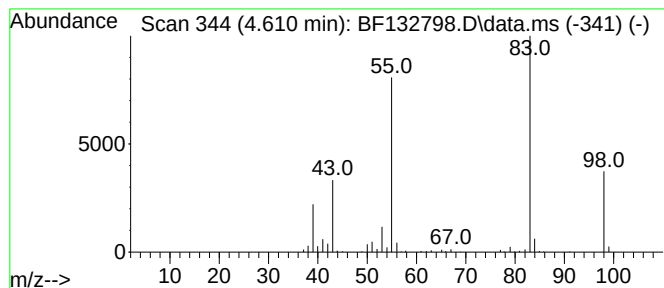
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.610	4.25 ng	262526	1,4-Dichlorobenzene-d4	6.963

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, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86



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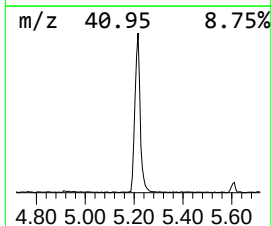
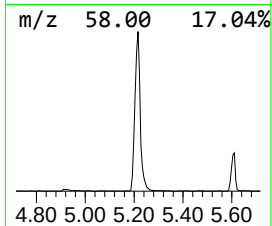
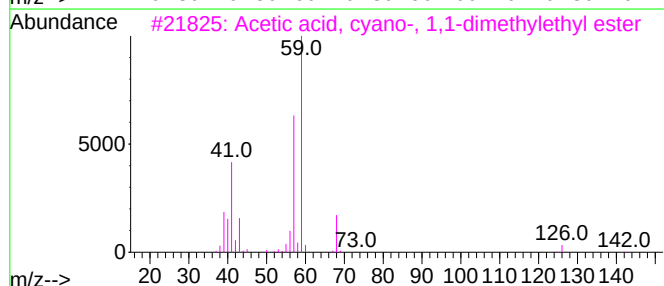
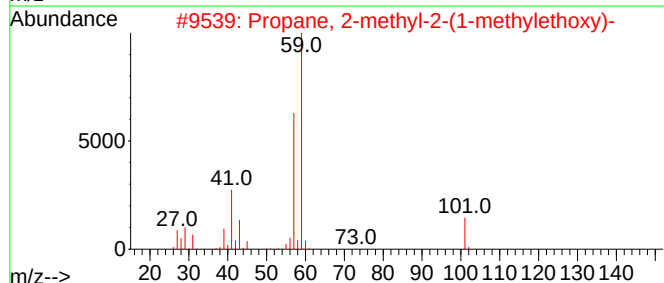
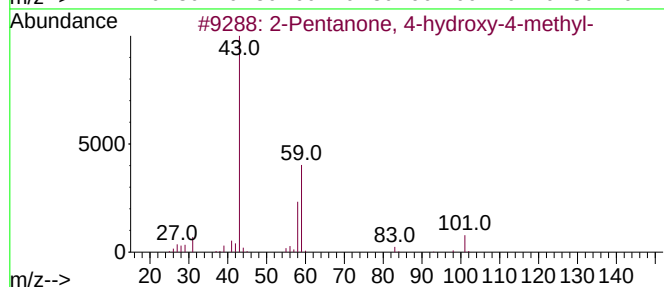
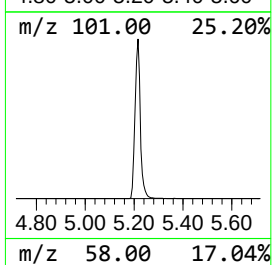
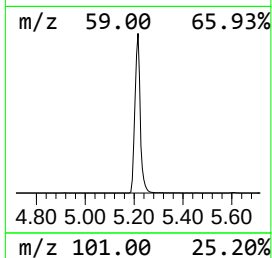
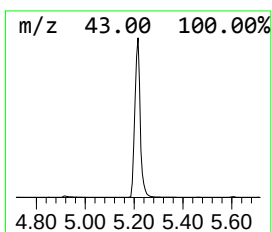
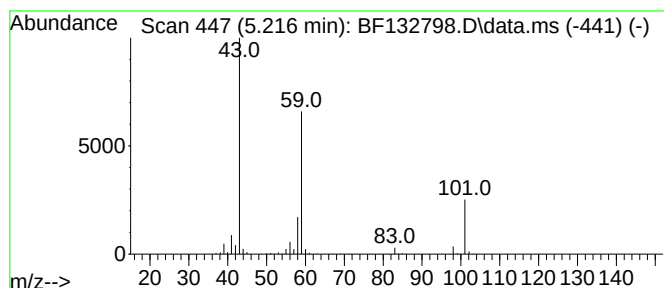
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.216	45.68 ng	2820670	1,4-Dichlorobenzene-d4	6.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	50
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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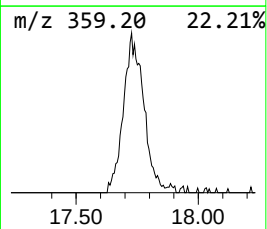
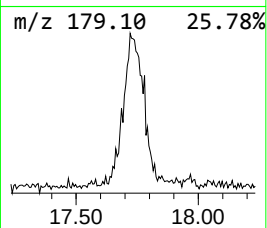
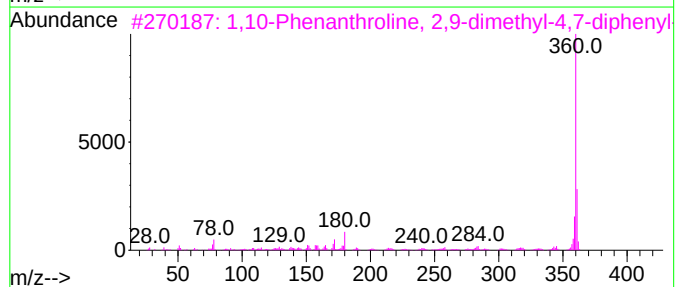
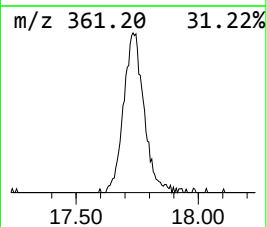
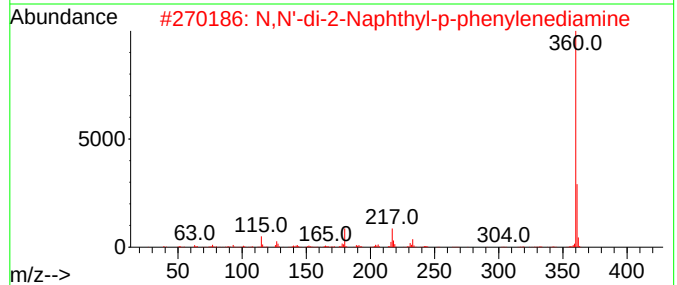
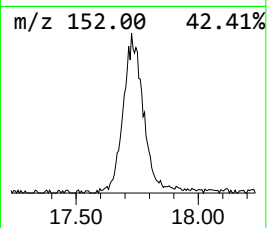
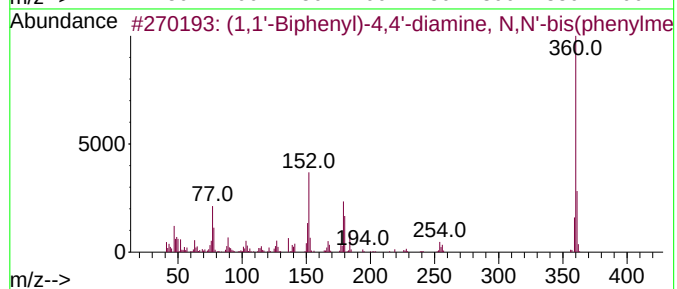
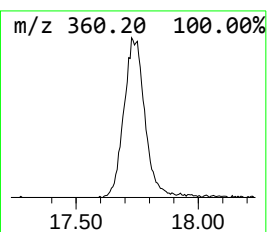
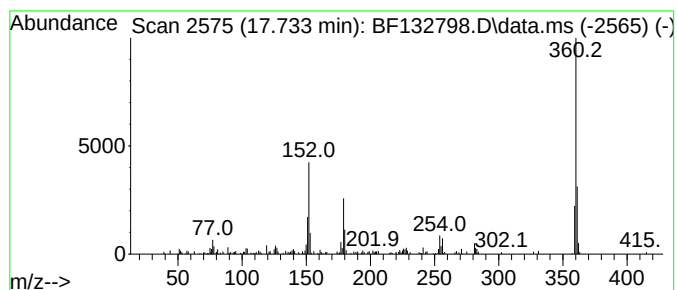
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Peak Number 3 (1,1'-Biphenyl)-4,4'-diamin... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.733	3.94 ng	189564	Perylene-d12	15.686

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(1,1'-Biphenyl)-4,4'-diamine, N,...	360	C26H20N2	006311-48-4	93
2			N,N'-di-2-Naphthyl-p-phenylenedi...	360	C26H20N2	000093-46-9	55
3			1,10-Phenanthroline, 2,9-dimethy...	360	C26H20N2	004733-39-5	49
4			Benzaldehyde, 4-hydroxy-3,5-dime...	360	C18H20N2O6	014414-32-5	49
5			Pentacyclo[18.4.1.1(2,7).1(8,13)...	360	C28H24	101077-60-5	43



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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	4.610	4.3	ng	262526	1	6.963	1235080	20.0
2-Pentanone, 4-...	5.216	45.7	ng	2820670	1	6.963	1235080	20.0
(1,1'-Biphenyl)...	17.733	3.9	ng	189564	6	15.686	961831	20.0