

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031116\
 Data File : BF085395.D
 Acq On : 12 Mar 2016 3:25
 Operator : UM/SJ
 Sample : PB88821BL
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB88821BL

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	5.144	247	250	256	rBV	180826	235862	5.66%	0.825%
2	5.544	282	285	287	rBV	3376650	3523219	84.53%	12.330%
3	6.562	371	374	376	rBV	2996437	3150904	75.59%	11.027%
4	6.699	383	386	389	rBV	3143471	3329632	79.88%	11.652%
5	6.939	404	407	409	rBV	600500	821128	19.70%	2.874%
6	7.087	418	420	423	rBV	2326809	2548734	61.15%	8.919%
7	7.499	453	456	458	rBV	2184498	2184388	52.41%	7.644%
8	8.219	517	519	521	rBV	1249651	1053536	25.28%	3.687%
9	9.305	611	614	616	rBV	3078201	4168196	100.00%	14.587%
10	9.979	670	673	675	rBV	1350630	1178427	28.27%	4.124%
11	10.768	739	742	744	rBV	1936884	1801293	43.22%	6.304%
12	11.465	800	803	805	rBV	923889	788390	18.91%	2.759%
13	13.054	939	942	944	rBV	2618999	2445305	58.67%	8.557%
14	14.105	1031	1034	1036	rBV	595631	573516	13.76%	2.007%
15	15.568	1159	1162	1165	rBV	444630	539839	12.95%	1.889%
16	16.540	1240	1247	1259	rBV	54693	232696	5.58%	0.814%

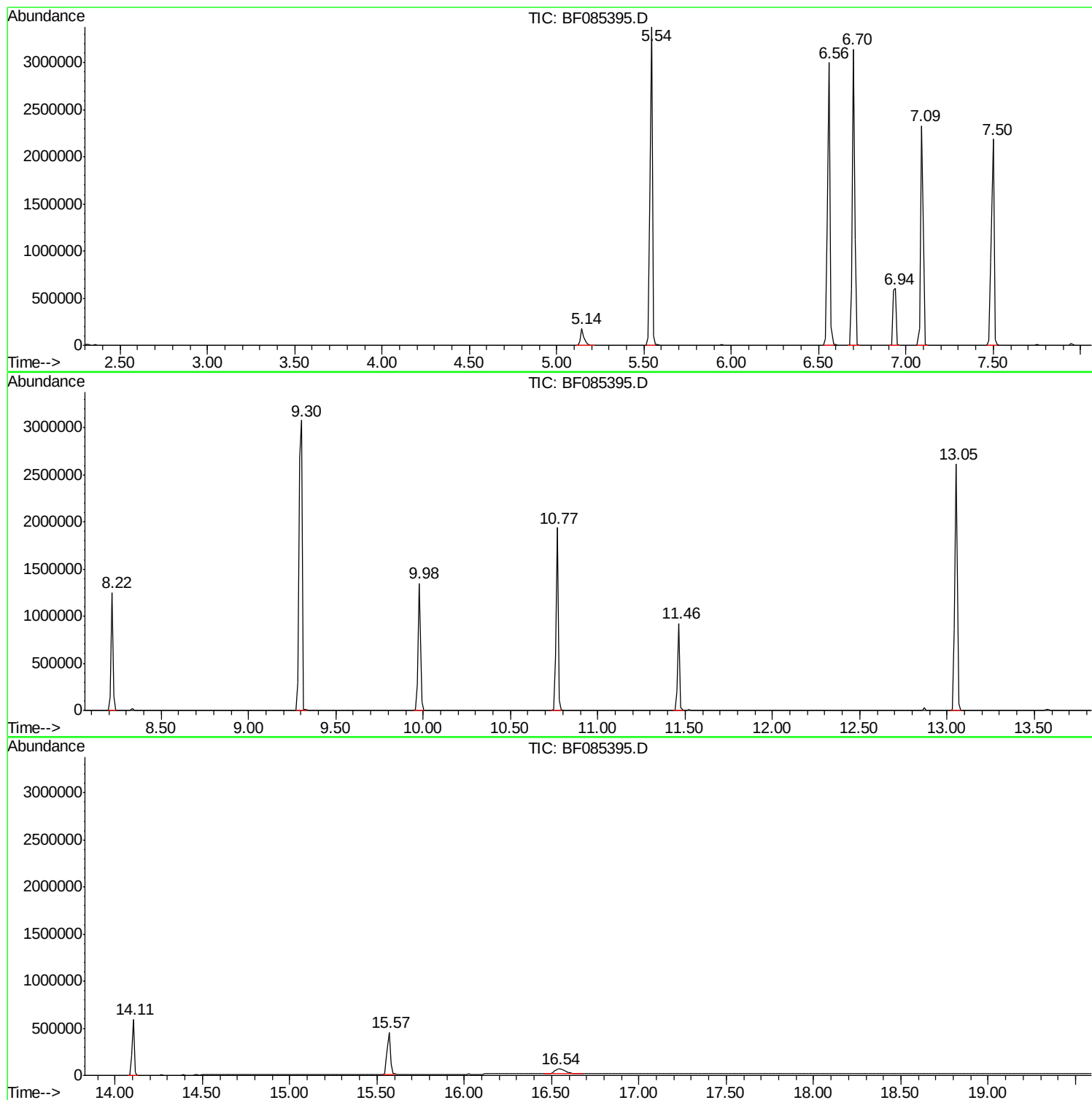
Sum of corrected areas: 28575065

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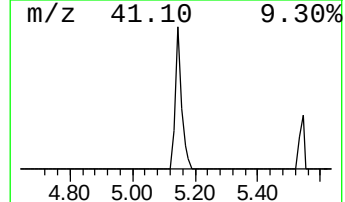
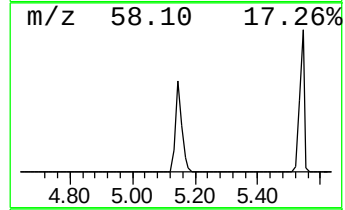
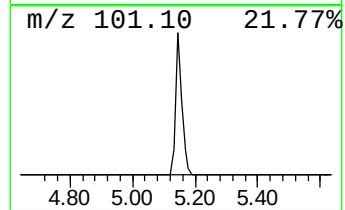
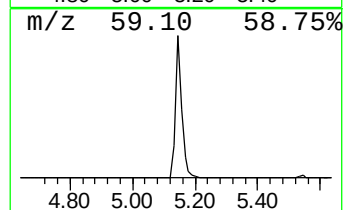
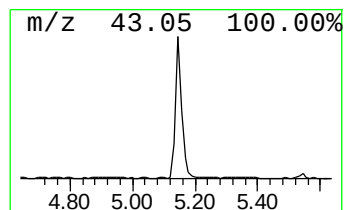
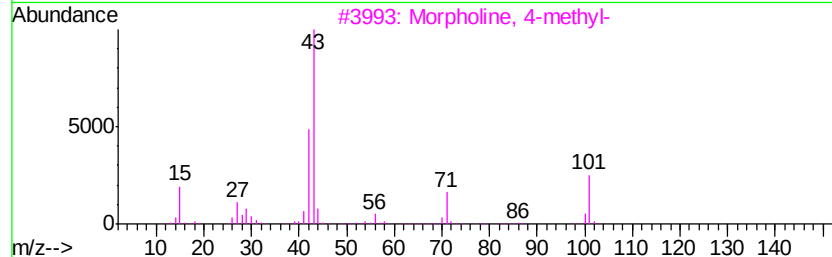
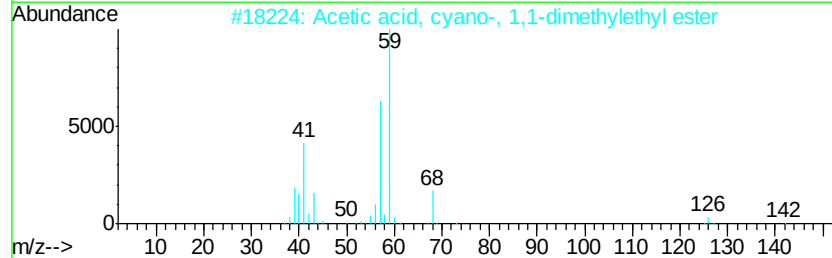
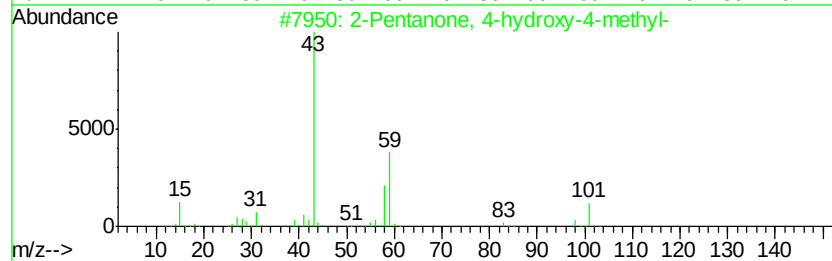
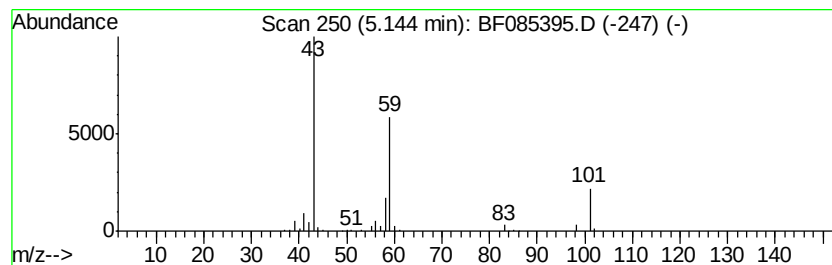
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	5.74 ng	235862	1,4-Dichlorobenzene-d4	6.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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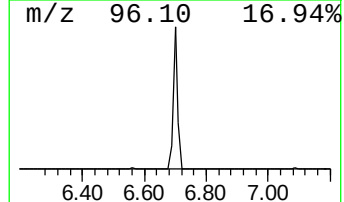
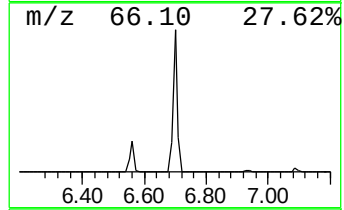
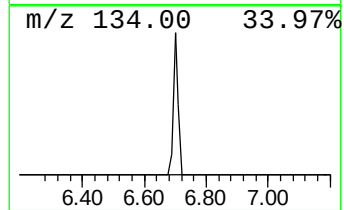
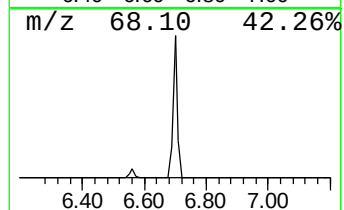
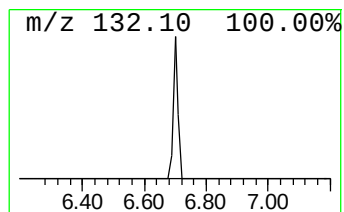
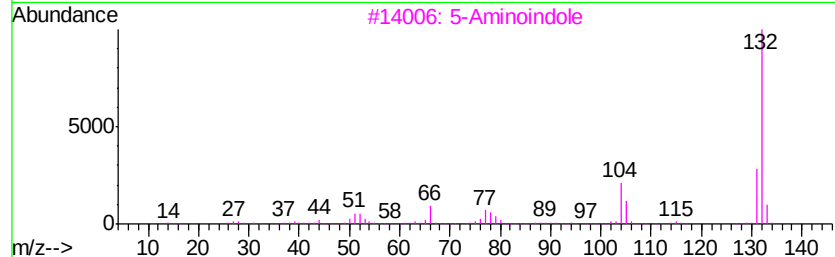
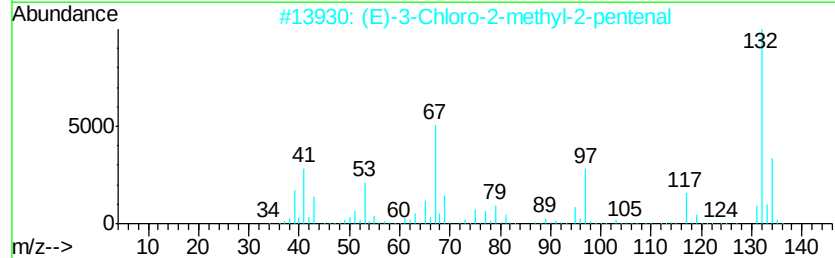
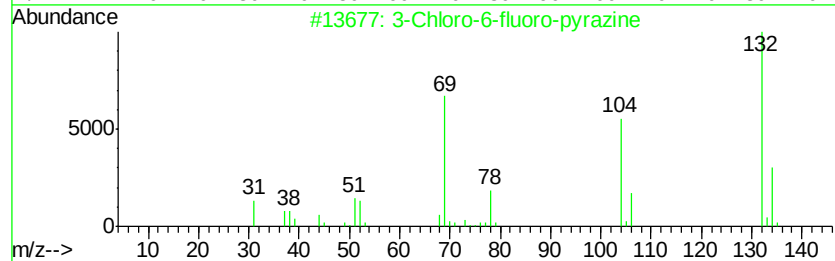
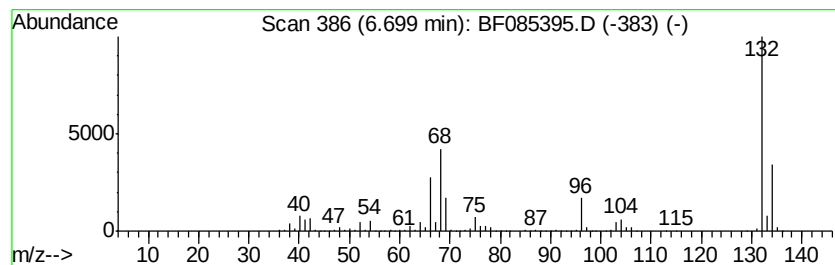
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Peak Number 2 unknown6.70 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	81.10 ng	3329630	1,4-Dichlorobenzene-d4	6.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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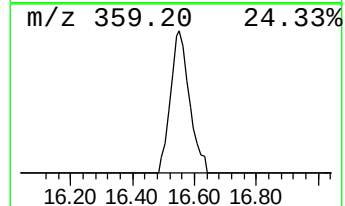
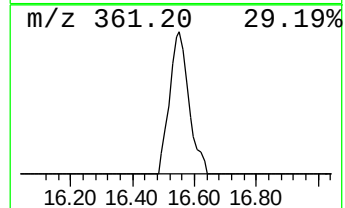
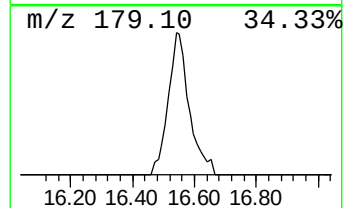
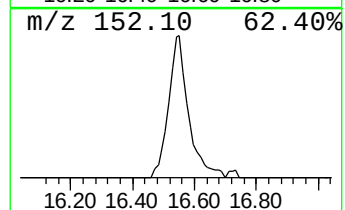
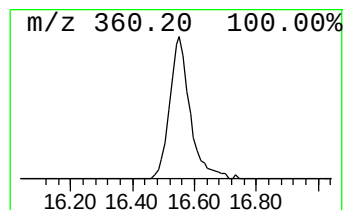
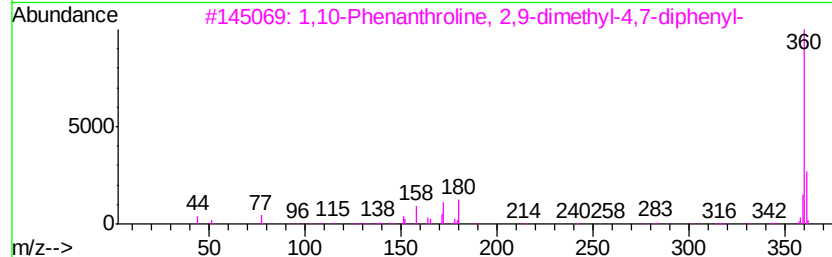
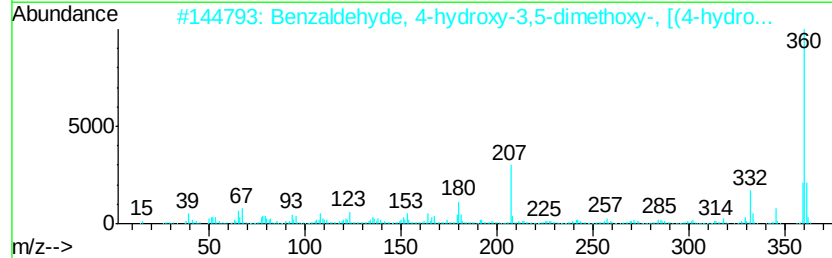
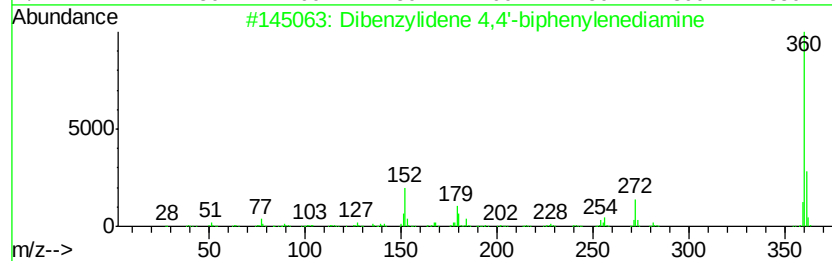
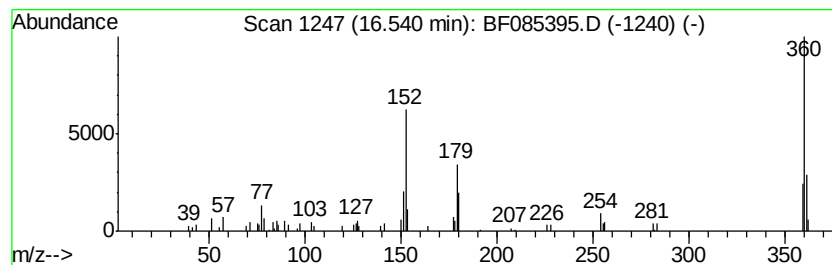
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Peak Number 4 Dibenzylidene 4,4'-biphenyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.54	8.62 ng	232696	Perylene-d12	15.57

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dibenzylidene 4,4'-biphenylenedi...	360	C26H20N2	006311-48-4	90
2		Benzaldehyde, 4-hydroxy-3,5-dime...	360	C18H20N2O6	014414-32-5	43
3		1,10-Phenanthroline, 2,9-dimethy...	360	C26H20N2	004733-39-5	38
4		1,3,2-Dioxaborolane, bis(spiro[4...	360	C20H13B06	1000150-23-7	38
5		N,N'-di-2-Naphthyl-p-phenylenedi...	360	C26H20N2	000093-46-9	35



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.14	5.7	ng	235862	1	6.94	821128	20.0
unknown6.70	6.70	81.1	ng	3329630	1	6.94	821128	20.0
Dibenzylidene 4,4...	16.54	8.6	ng	232696	6	15.57	539839	20.0