

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022417\
 Data File : BF093148.D
 Acq On : 24 Feb 2017 16:51
 Operator : SJ/MA
 Sample : PB97158BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB97158BL

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-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	5.001	252	255	265	rBV	1198575	1759646	37.11%	4.445%
2	5.436	290	293	295	rBV	2943476	4159743	87.74%	10.509%
3	6.476	381	384	386	rBV	3784286	4266755	90.00%	10.779%
4	6.602	392	395	397	rBV	4039566	4085121	86.16%	10.320%
5	6.830	413	415	417	rBV	1051629	872858	18.41%	2.205%
6	6.990	426	429	431	rBV	3270157	3198529	67.46%	8.080%
7	7.402	462	465	467	rBV	2516273	2469981	52.10%	6.240%
8	8.122	526	528	530	rBV	1333894	1171291	24.71%	2.959%
9	9.208	619	623	625	rBV	3903119	4741101	100.00%	11.977%
10	9.813	673	676	679	rBV	28351	60676	1.28%	0.153%
11	9.882	679	682	684	rVB	1085473	1297000	27.36%	3.277%
12	10.671	748	751	753	rBV	2434186	2636995	55.62%	6.662%
13	11.356	809	811	814	rBV2	1213674	1306192	27.55%	3.300%
14	12.568	911	917	922	rBV2	18598	52550	1.11%	0.133%
15	12.945	947	950	953	rBV	3236887	4622343	97.50%	11.677%
16	13.448	990	994	998	rBV4	22077	62726	1.32%	0.158%
17	13.871	1028	1031	1033	rVB	44878	61627	1.30%	0.156%
18	13.997	1040	1042	1045	rVB	1396298	1296307	27.34%	3.275%
19	14.637	1095	1098	1102	rBV3	34174	94142	1.99%	0.238%
20	14.957	1118	1126	1130	rBV	55078	236353	4.99%	0.597%
21	15.425	1164	1167	1170	rBV	891698	1131923	23.87%	2.860%

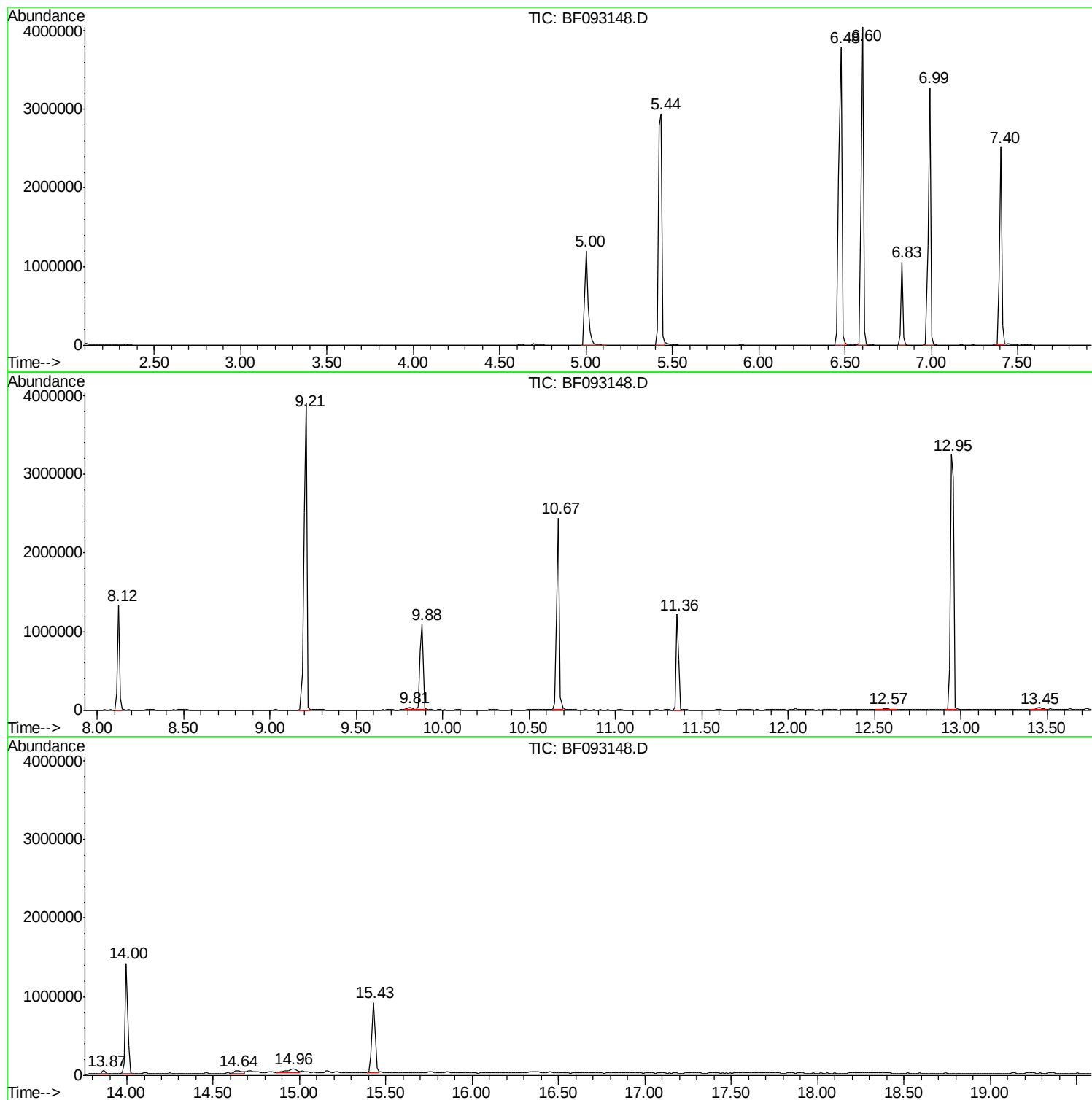
Sum of corrected areas: 39583859

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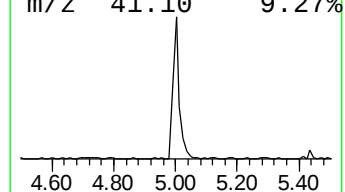
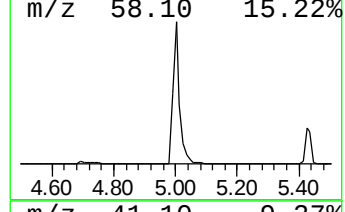
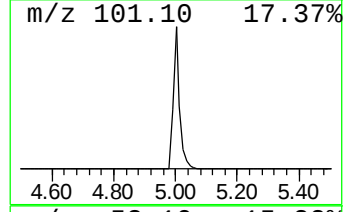
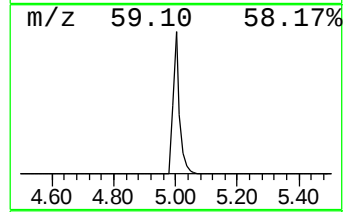
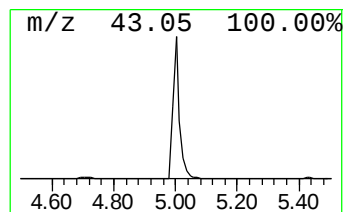
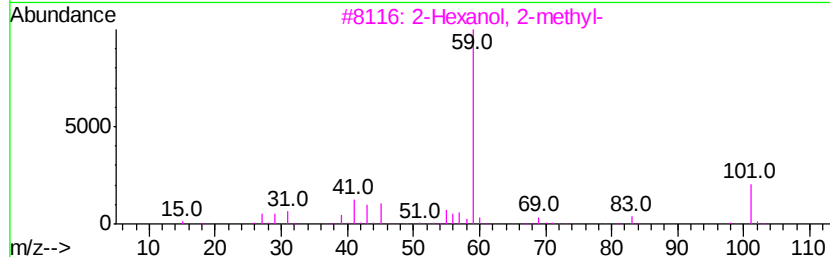
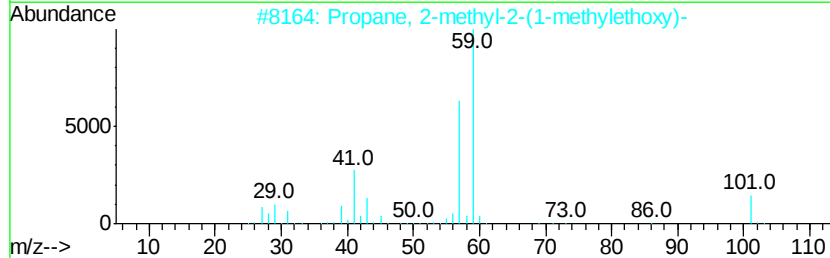
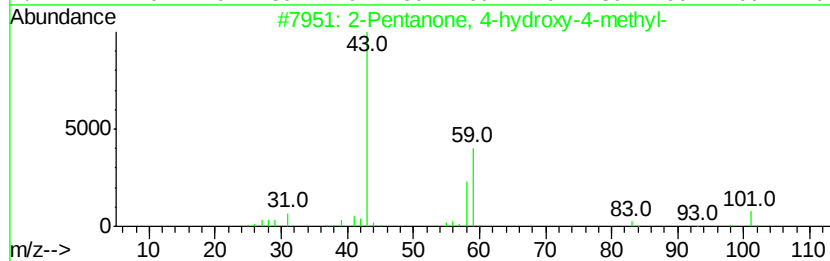
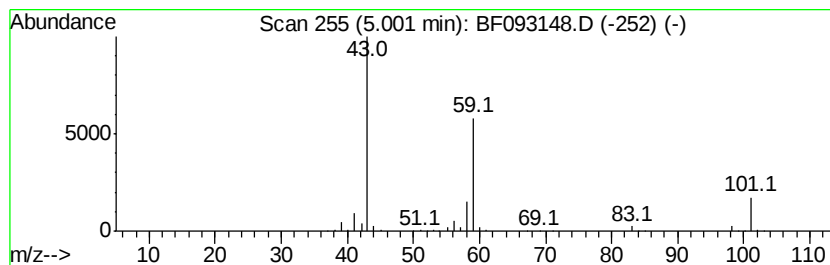
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	40.32 ng	1759650	1,4-Dichlorobenzene-d4	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2		Propane, 2-methyl-2-(1-methylethoxy)-	116	C7H16O	017348-59-3	33
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5		Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	32



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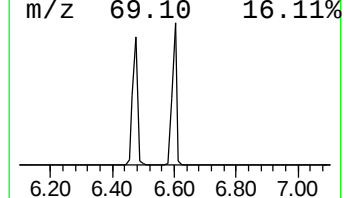
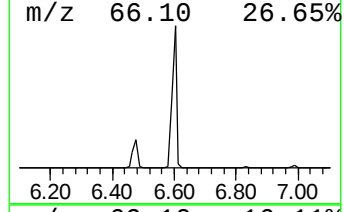
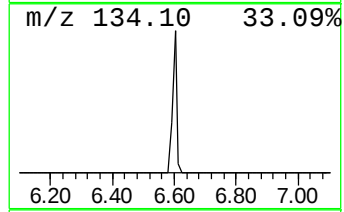
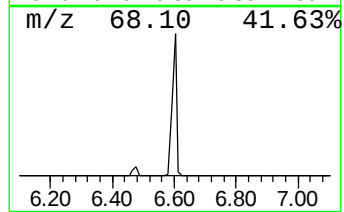
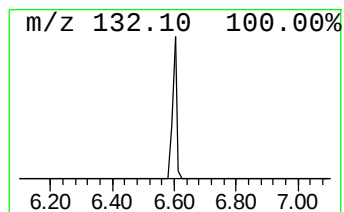
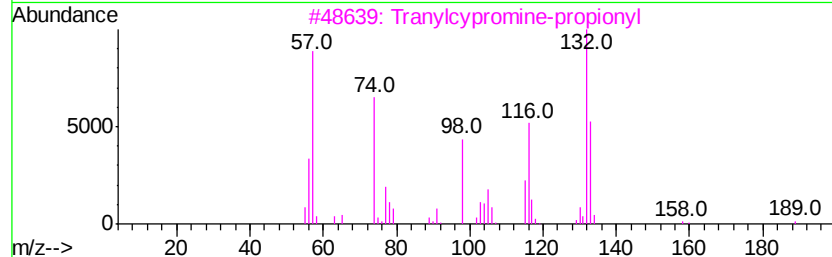
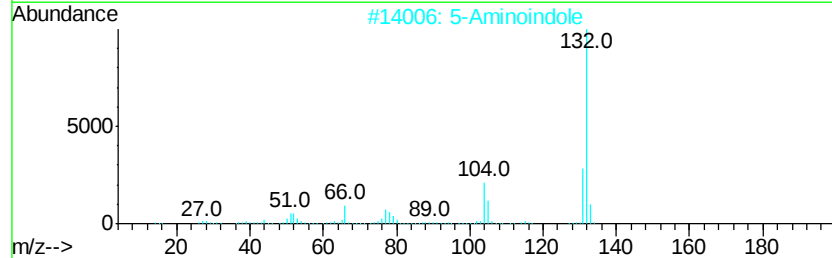
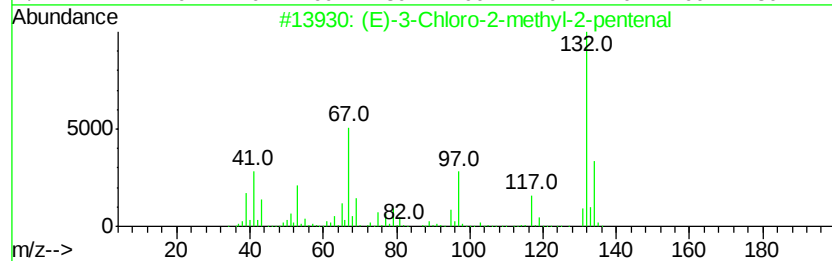
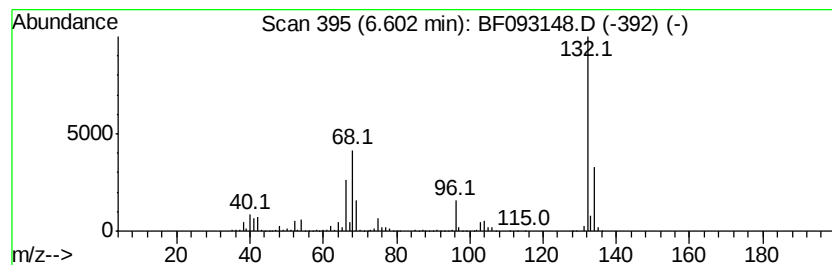
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Peak Number 2 unknown6.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	93.60 ng	4085120	1,4-Dichlorobenzene-d4	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9
5		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9



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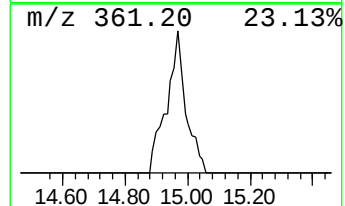
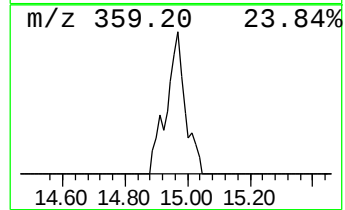
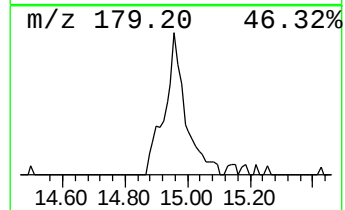
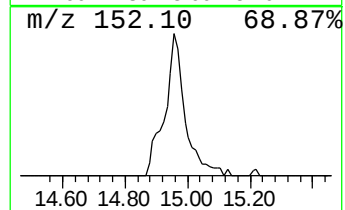
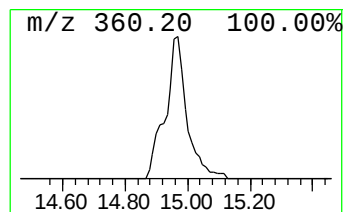
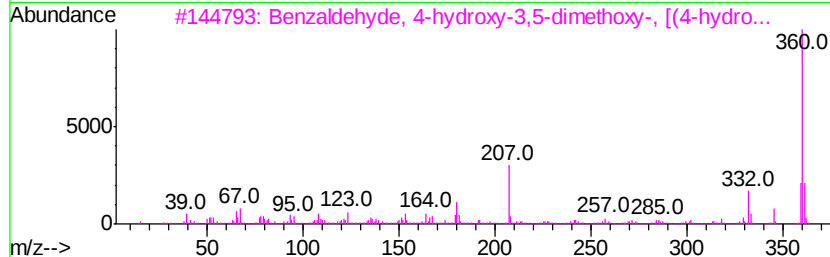
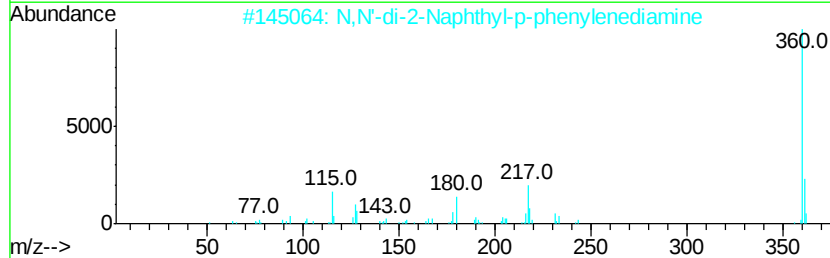
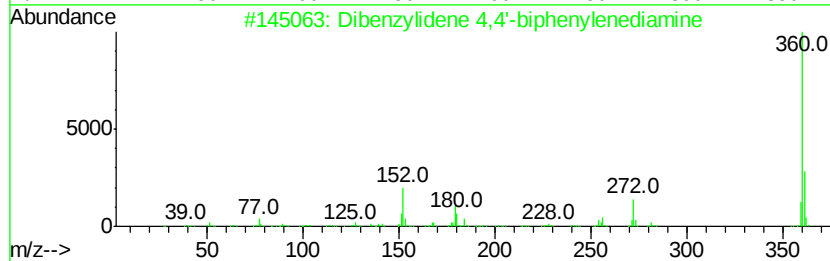
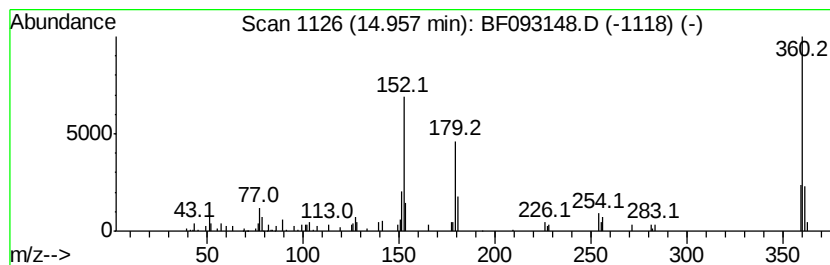
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Peak Number 4 Dibenzylidene 4,4'-biphenyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	4.18 ng	236353	Perylene-d12	15.43

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dibenzylidene 4,4'-biphenylenedi...	360	C26H20N2	006311-48-4	87
2		N,N'-di-2-Naphthyl-p-phenylenedi...	360	C26H20N2	000093-46-9	38
3		Benzaldehyde, 4-hydroxy-3,5-dime...	360	C18H20N2O6	014414-32-5	38
4		1,3,2-Dioxaborolane, bis(spiro[4...	360	C20H13B06	1000150-23-7	38
5		1,10-Phenanthroline, 2,9-dimethy...	360	C26H20N2	004733-39-5	35



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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...	5.00	40.3	ng	1759650	1	6.83	872858	20.0
unknown6.60	6.60	93.6	ng	4085120	1	6.83	872858	20.0
Dibenzylidene 4,4...	14.96	4.2	ng	236353	6	15.43	1131920	20.0