Supporting Information

Iron-Catalyzed Aryl-Aryl Cross Coupling Route for the synthesis of 1-(2-amino)-phenyl)dibenzo[b,d]furan-2-ol Derivatives and their Biological Evaluation

BarreddiChiranjeevi^{a,1}, Ganesh Koyyada^a, S. Prabusreenivasan^b, Vanaja Kumar ^b, PombalaSujitha^c, C. Ganesh Kumar ^c, B. Sridhar ^d, SaidaShaik^e, MalapakaChandrasekharam^{a, *}

^aInorganic and Physical Chemistry Division ^cMedicinal Chemistry and Phormacology Division ^dCenter for X-ray Crystallography ^cAnalytical Division CSIR-Indian Institute of Chemical Technology, Uppal Road, Tarnaka, Hyderabad-500 007, India

^bTuberculosis Research Centre, V.R. Ramanathan Road, Chennai 600 031, India

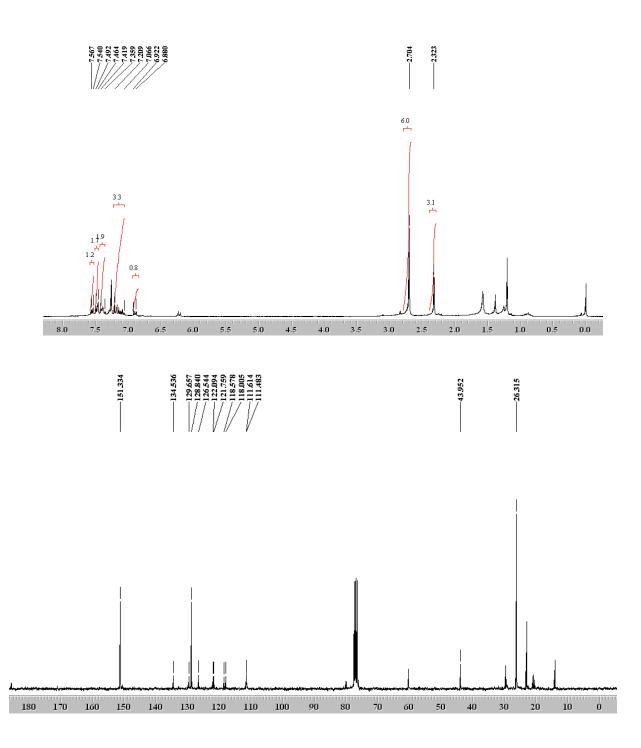
List of Contents

1.¹H and ¹³C NMR spectra of the compounds _____ S2-S15

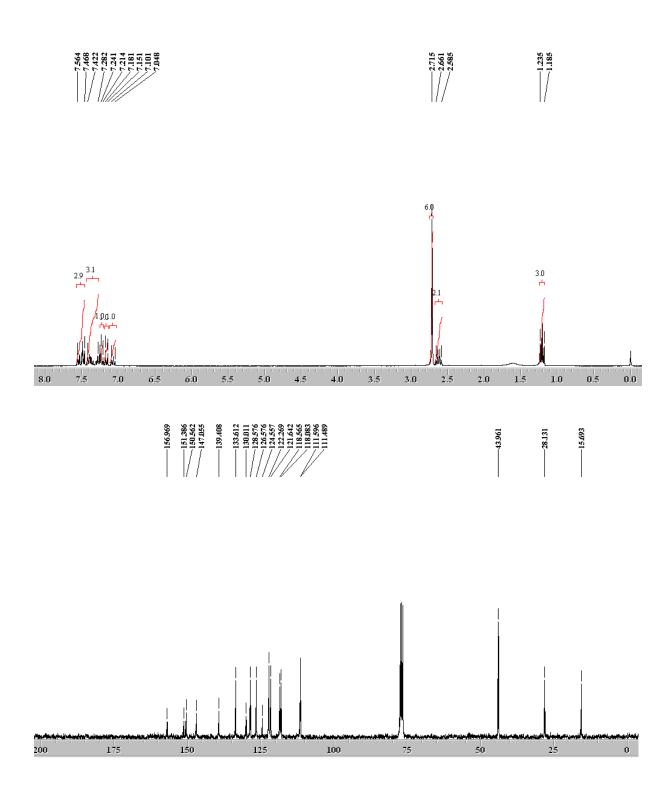
2. HPLC analysis S16-S29

¹H and ¹³C NMR spectra of the compounds

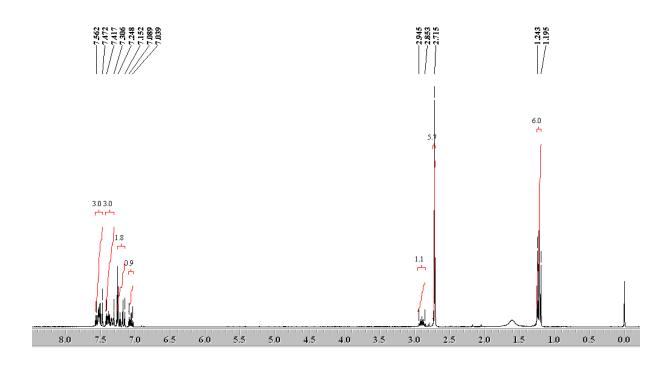
¹H & ¹³C NMR spectra of DBF-3

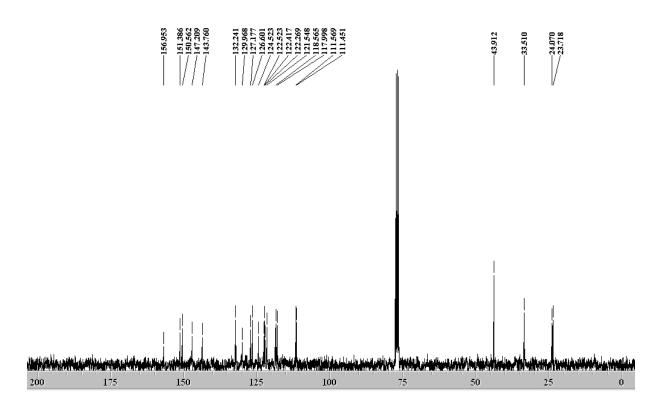


 1 H $\&^{13}$ C NMR spectra of DBF-7

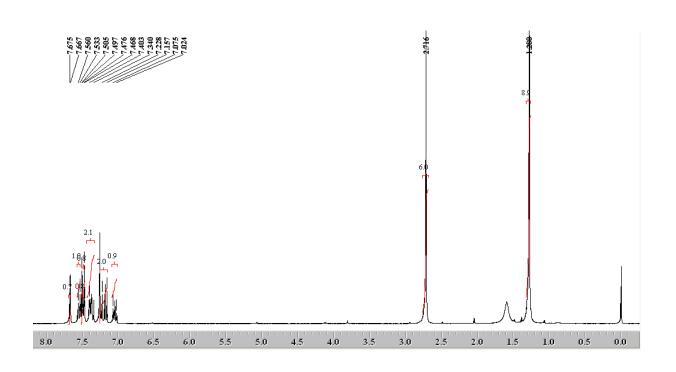


¹H & ¹³C NMR spectra of DBF-4

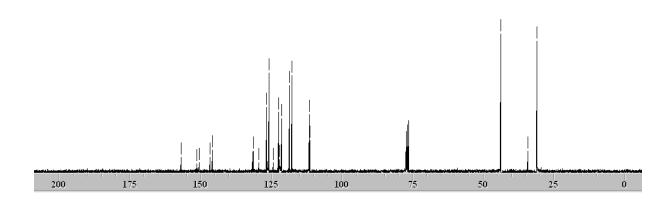




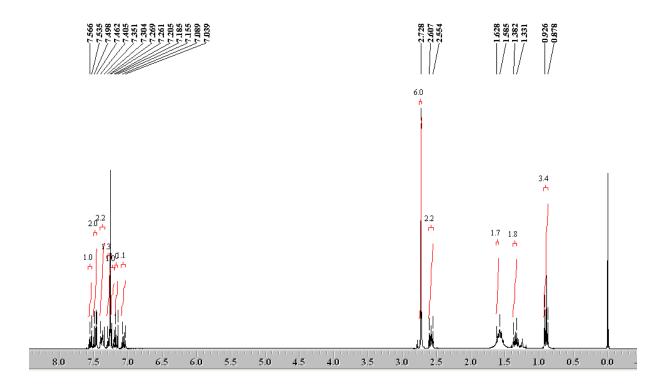
 1 H & 13 C NMR spectra of DBF-5

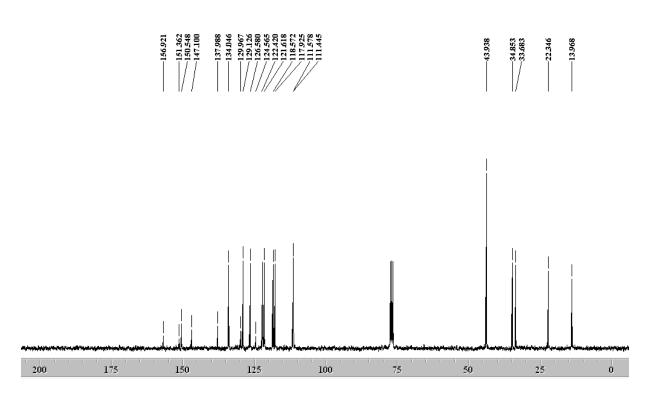




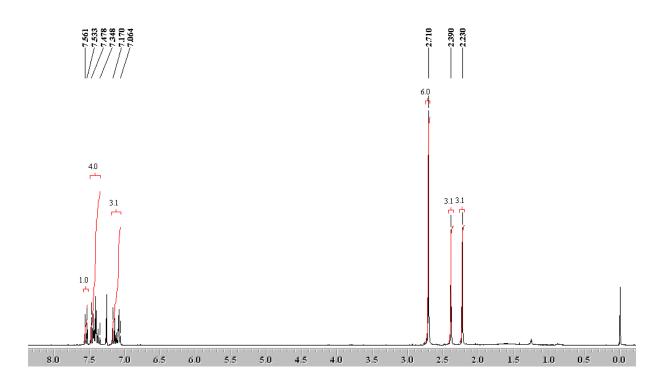


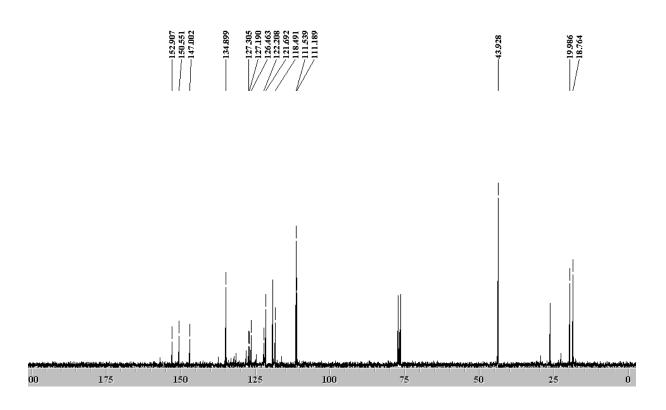
 1 H & 13 C NMR spectra of DBF-8



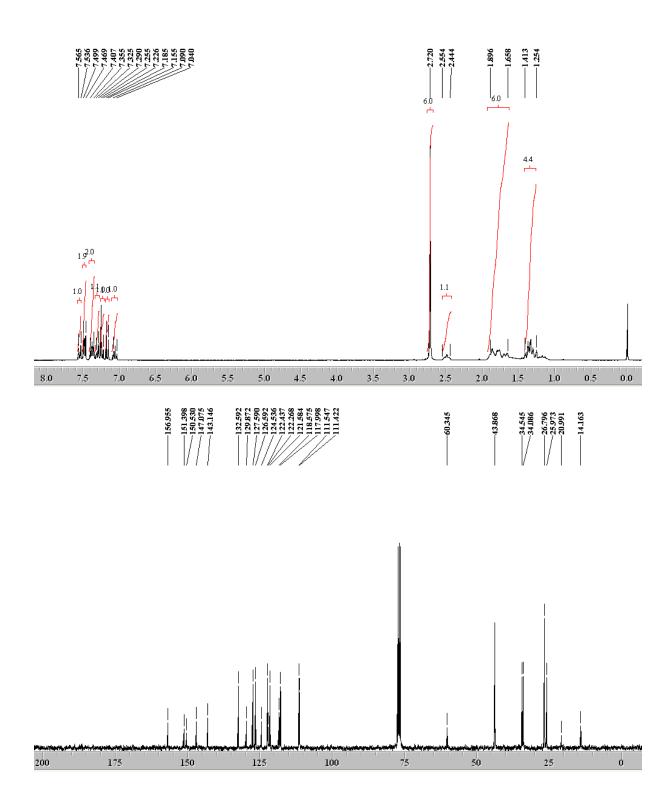


¹H & ¹³C NMR spectra of DBF-14

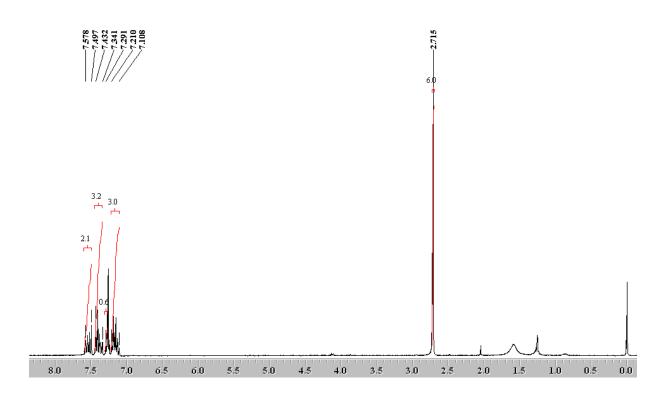


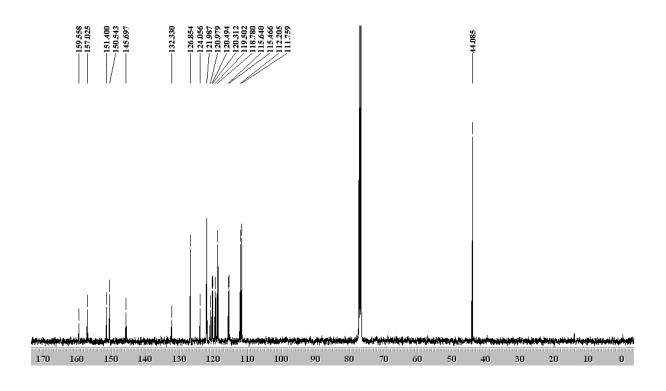


 1 H & 13 C NMR spectra of DBF-13

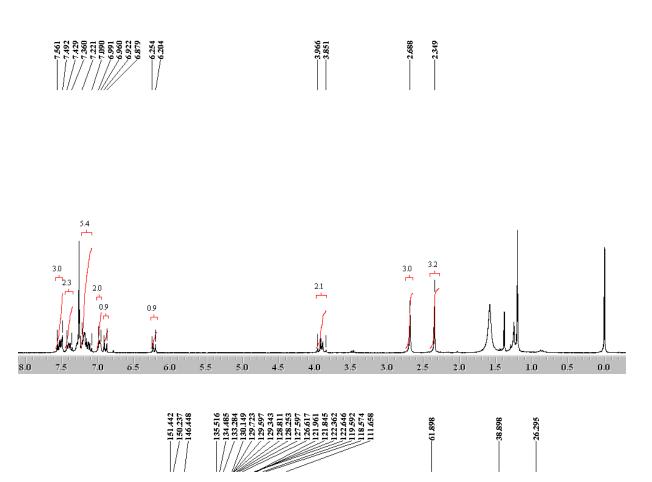


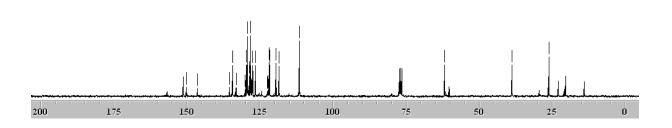
¹H & ¹³C NMR spectra of DBF-20



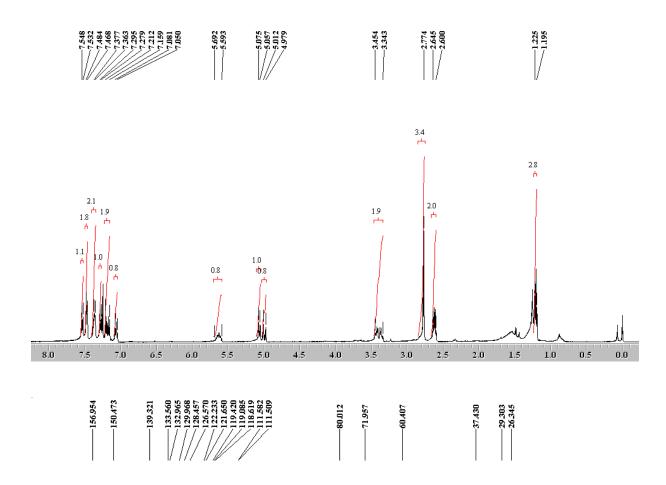


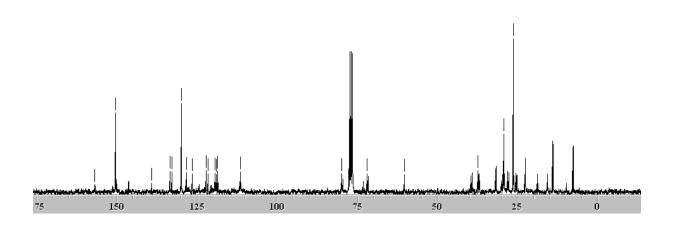
¹H & ¹³C NMR spectra of DBF-15



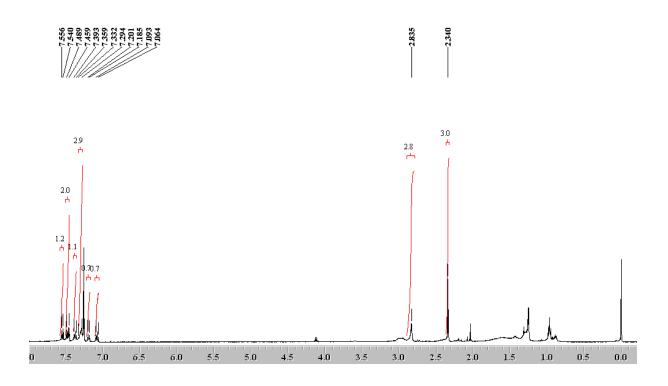


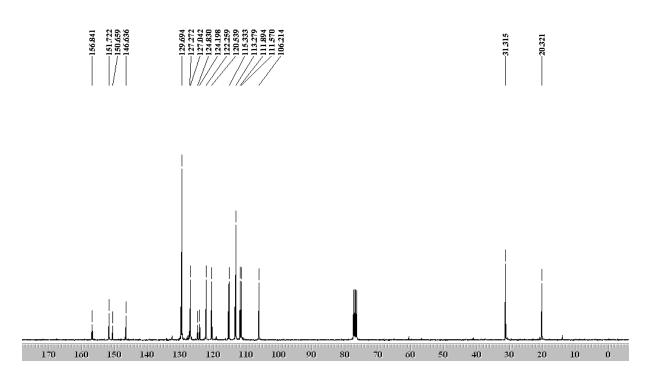
 1 H & 13 C NMR spectra of DBF-16



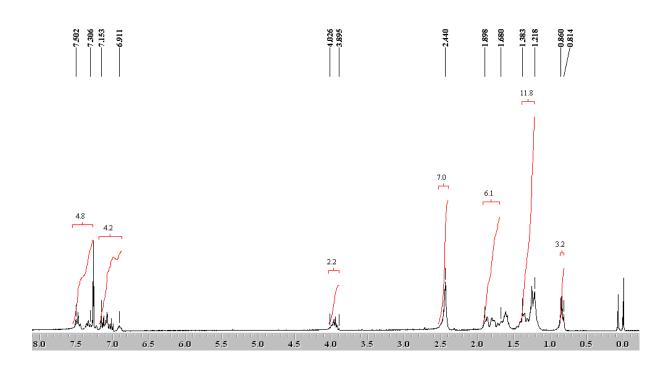


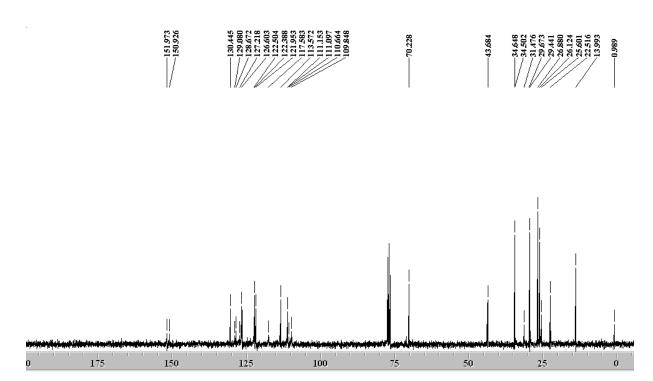
 1 H & 13 C NMR spectra of DBF-18



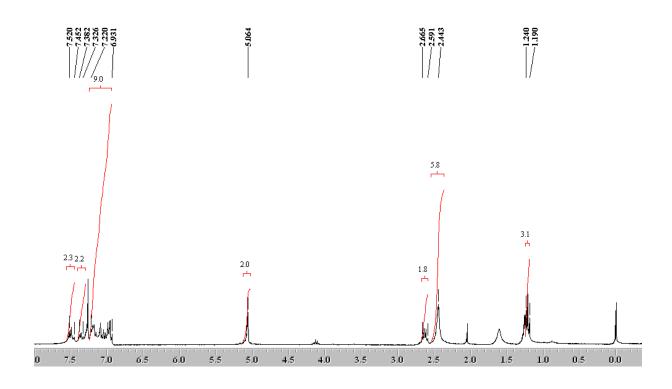


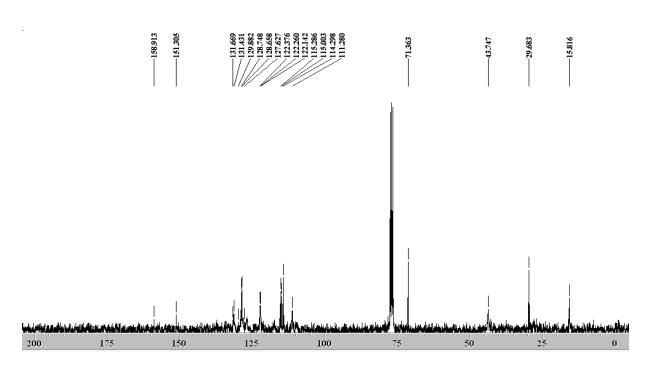
¹H & ¹³C NMR spectra of DBF-19



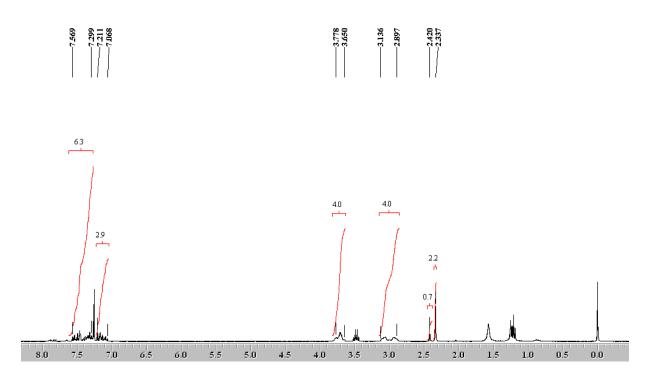


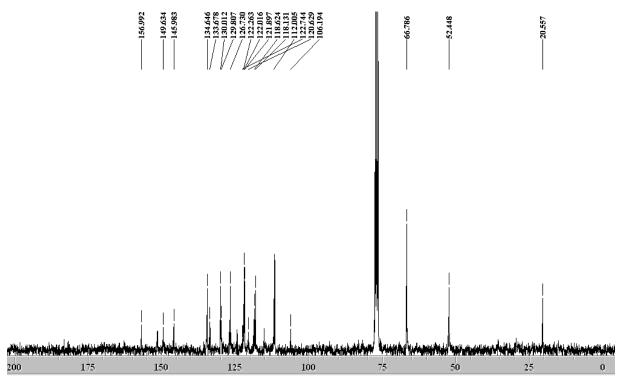
 1 H & 13 C NMR spectra of DBF-21





¹H & ¹³C NMR spectra of DBF-9





HPLC REPORT

Sample Information

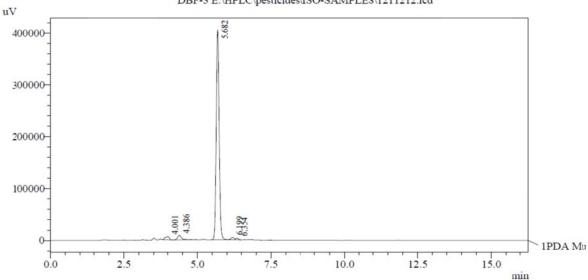
Acquired by : Admin
Sample Name : DBF-3
Sample ID : DBF-3
Injection Volume : 10 uL
Data Filename : 1211212.lcd
Method Filename : 2310200.lcm

Batch Filename

Report Filename : RK.lcr

Date Acquired : 11/14/2012 4:39:59 PM Data Processed : 11/29/2012 12:32:15 PM

$\label{lem:chromatogram} $$ DBF-3 E:\HPLC\pesticides\ISO-SAMPLES\1211212.lcd $$$



1 PDA Multi 1 / 295nm 4nm

PeakTable

Peak#	Ret. Time	Area	Area %	Resolution	Tailing Factor	Theoretical Plate#
1	4.001	62130	2.095	0.000	0.878	3752.987
2	4.386	82925	2.796	1.542	1.434	5447.231
3	5.682	2766710	93.299	5.976	1.143	13429.517
4	6.199	33619	1.134	2.396	0.000	11117.677
5	6.354	20024	0.675	0.615	0.000	8978.507
Total		2965408	100.000			

ativ	e Retention
	0.000
	0.000
	0.000
	0.000
	0.000

Acquired by : Admin
Sample Name : dbf-4
Sample ID : dbf-4
Injection Volume : 5 uL
Data Filename : 2310200.lcm
Batch Filename : 2310200.lcm

Report Filename : RK.lcr

uV

3000000-

2500000

2000000-

1500000

1000000

500000

0-

0.0

Date Acquired : 11/1/2012 4:24:25 PM
Data Processed : 11/29/2012 11:39:21 AM

Chromatogram dbf-4 E:\HPLC\pesticides\data compar\1111202.lcd

10.0

1PDA Mult

12.5

1 PDA Multi 1 / 305nm 4nm

2.5

PeakTable

7.5

6.224

5.0

DA Ch1 305nm 4nm				
Peak#	Ret. Time	Area	Area %	Resolution
1	6.224	196652	1.427	0.000
2	7.174	13144803	95.387	6.683
3	7.379	439009	3.186	1.267
Total		13780464	100.000	

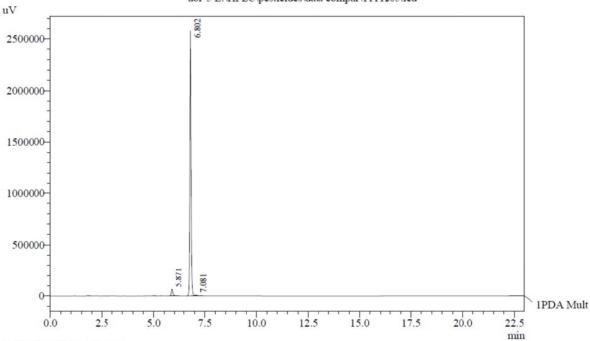
Acquired by Sample Name : Admin : DBF-5 Sample ID
Injection Volume
Data Filename : DBF-5 : 5 uL : 1111205.lcd Method Filename : 2310200.lcm

Batch Filename

: RK.lcr

Report Filename Date Acquired : 11/1/2012 5:30:02 PM Data Processed : 11/20/2012 12:12:15 PM

Chromatogram dbr-5 E:\HPLC\pesticides\data compar\1111205.lcd



1 PDA Multi 1 / 254nm 4nm

PeakTable

Peak#	Ret. Time	Area	Area %	Resolution
1	5.871	327481	3.092	0.000
2	6.802	10214742	96.434	7.131
3	7.081	50290	0.475	1.675
Total		10592512	100.000	

Acquired by : Admin Sample Name : DBF-7 Sample ID : DBF-7 Injection Volume : 5 uL

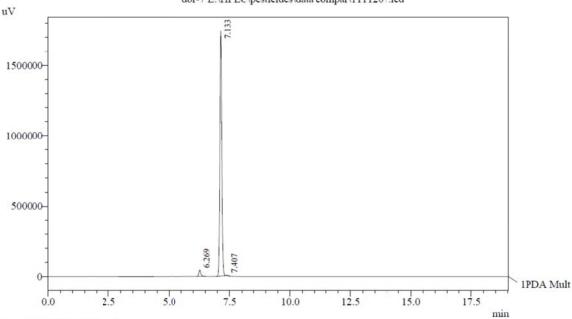
Data Filename : 1111207.lcd Method Filename : 2310200.lcm

Batch Filename

Report Filename : RK.lcr

Date Acquired : 11/1/2012 6:12:22 PM
Data Processed : 11/29/2012 11:46:25 AM

$Chromatogram \\ dbr-7 E:\HPLC\pesticides\data compar\1111207.lcd$



1 PDA Multi 1 / 254nm 4nm

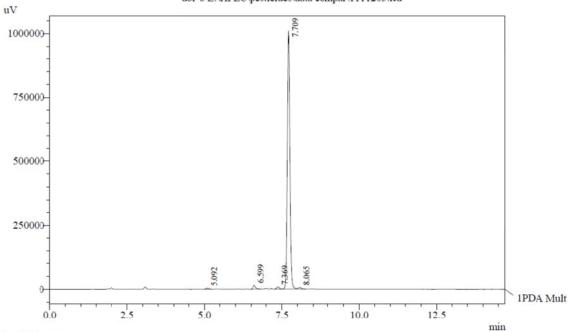
DA Ch1 25	54nm 4nm		•	Cilitation
Peak#	Ret. Time	Area	Area %	Resolution
1	6.269	251685	2.562	0.000
2	7.133	9549479	97.202	5.177
3	7.407	23168	0.236	1.737
Total		9824332	100.000	

Acquired by Sample Name : Admin : dbr-8 Sample ID : dbr-8 Injection Volume :5 uL Data Filename :1111203.lcd Method Filename : 2310200.lcm

Batch Filename

Report Filename Date Acquired : RK.lcr : 11/1/2012 4:47:09 PM : 11/29/2012 11:44:49 AM Data Processed

Chromatogram dbr-8 E:\HPLC\pesticides\data compar\1111203.lcd



1 PDA Multi 1 / 305nm 4nm

PDA Ch1 305nm 4nm

Peak#	Ret. Time	Area	Area %	Resolution
1	5.092	23769	0.397	0.000
2	6.599	87283	1.457	9.029
3	7.369	47516	0.793	4.646
4	7.709	5786349	96.587	2.070
5	8.065	45911	0.766	1.852
Total		5990828	100.000	

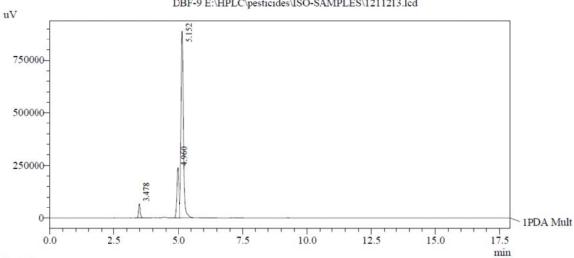
Acquired by : Admin
Sample Name : DBF-9
Sample ID : DBF-9
Injection Volume : 10 uL
Data Filename : 1211213.lcd
Method Filename : 2310200.lcm

Batch Filename

Report Filename : RK.lcr

Date Acquired : 11/14/2012 4:57:38 PM
Data Processed : 11/29/2012 12:33:48 PM

$\label{lem:chromatogram} $$ DBF-9 E:\HPLC\pesticides\ISO-SAMPLES\I211213.lcd $$$



1 PDA Multi 1 / 295nm 4nm

PeakTable

The second was						
Peak#	Ret. Time	Area	Area %	Resolution	Tailing Factor	Theoretical Plate#
1	3.478	306209	3.989	0.000	1.267	10471.542
2	4.960	1455283	18.957	9.296	0.000	11742.620
3	5.152	5915353	77.054	1.035	0.000	12078.227
Total		7676846	100.000			

Retention '
0.000
0.000
0.000

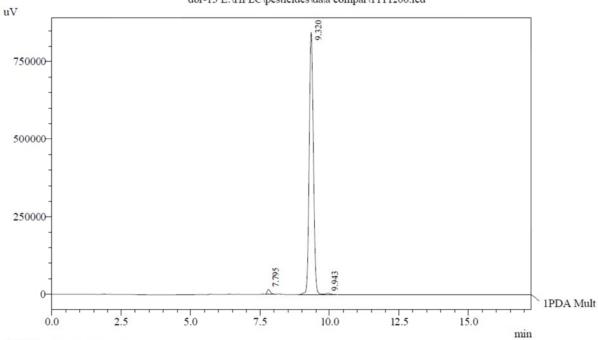
Acquired by : Admin Sample Name : DBF-13 Sample ID : DBF-13 Injection Volume : 5 uL : 1111206.lcd Data Filename Method Filename : 2310200.lcm

Batch Filename

Report Filename : RK.lcr

Date Acquired : 11/1/2012 5:53:50 PM Data Processed : 11/20/2012 12:11:51 PM

Chromatogram dbr-13 E:\HPLC\pesticides\data compar\1111206.lcd



1 PDA Multi 1 / 254nm 4nm

PeakTable

Peak#	Ret. Time	Area	Area %	Resolution
1	7.795	126474	1.419	0.000
2	9.320	8723796	97.890	6.044
3	9.943	61589	0.691	1.902
Total		8911858	100.000	

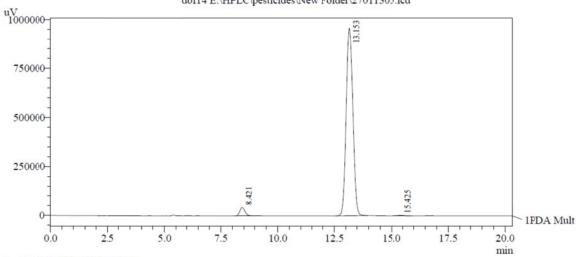
: Admin : DBF-14 Acquired by Sample Name Sample ID : DBF-14 Injection Volume Data Filename : 20 uL : 27011305.lcd : ANALYSIS.lcm Method Filename

Batch Filename

Report Filename : RK.lcr

: 1/28/2013 2:35:40 PM Date Acquired Data Processed : 2/2/2013 5:19:16 PM

Chromatogram dbf14 E:\HPLC\pesticides\New Folder\27011305.lcd



1 PDA Multi 1 / 254nm 4nm

PDA Ch1 2	54nm 4nm		
Peak#	Ret. Time	Area	A
1	8.421	667276	

DIL CHI	- TARRES - TARRES					
Peak#	Ret. Time	Area	Area %	Resolution	Tailing Factor	Theoretical Plate#
1	8.421	667276	3.320	0.000	1.184	6618.971
2	13.153	19372383	96.392	9.864	1.095	9306.630
3	15.425	57748	0.287	3.980	1.168	10704.193
Total		20097408	100.000			

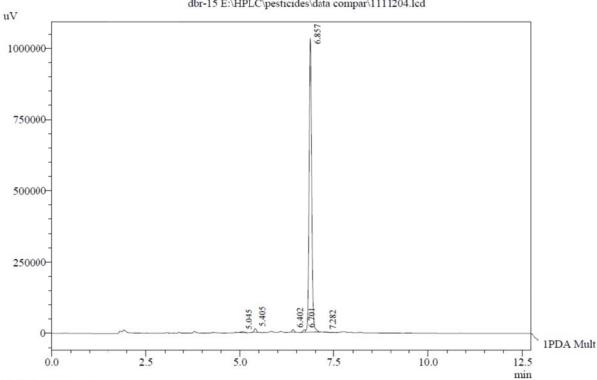
ative	Retention 7
	0.000
	0.000
	0.000

Acquired by Sample Name Sample ID : Admin : DBF-15 : DBF-15 Injection Volume Data Filename : 5 uL : 1111204.lcd Method Filename : 2310200.lcm

Batch Filename

: RK.ler : 11/1/2012 5:05:10 PM : 2/2/2013 5:00:37 PM Report Filename Date Acquired Data Processed

Chromatogram dbr-15 E:\HPLC\pesticides\data compar\1111204.lcd



1 PDA Multi 1 / 254nm 4nm

PeakTable

PDA	Ch1	254nm	4nm
-----	-----	-------	-----

Peak#	Ret. Time	Area	Area %	Resolution
1	5.045	22325	0.443	0.000
2	5.405	53731	1.066	2.286
3	6.402	34665	0.688	8.053
4	6.701	39017	0.774	1.865
5	6.857	4886933	96.930	0.909
6	7.282	5068	0.101	3.169
Total		5041740	100.000	

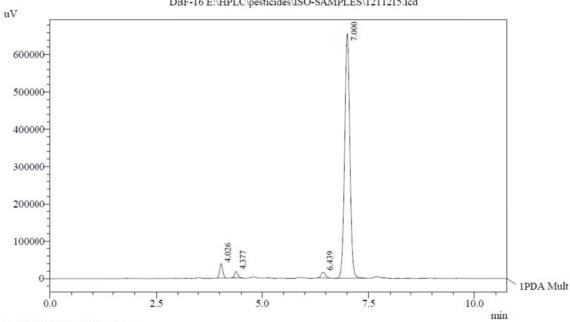
Acquired by : Admin
Sample Name : DBF-16
Sample ID : DBF-16
Injection Volume : 10 uL
Data Filename : 1211215.lcd
Method Filename : 2310200.lcm

Batch Filename :

Report Filename : RK.lcr

Date Acquired : 11/14/2012 5:34:37 PM
Data Processed : 11/29/2012 12:35:21 PM

Chromatogram DBF-16 E:\HPLC\pesticides\ISO-SAMPLES\1211215.lcd



1 PDA Multi 1 / 295nm 4nm

PeakTable

Peak#	Ret. Time	Area	Area %	Resolution	Tailing Factor	Theoretical Plate#
1	4.026	190055	3.218	0.000	1.200	11687.889
2	4.377	89773	1.520	2.289	1.218	12334.311
3	6.439	118820	2.012	10.602	1.028	12392.278
4	7.000	5507269	93.250	2.405	1.062	14211.387
Total		5905917	100.000			

mive i	Retention '
	0.000
	0.000
9	0.000
î .	0.000

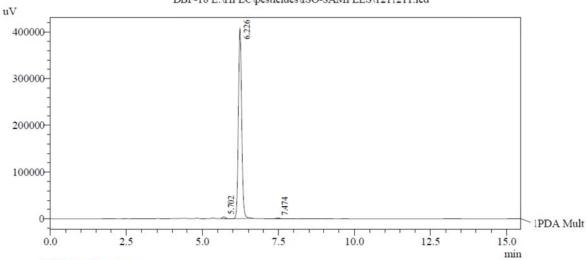
Acquired by : Admin
Sample Name : DBF-18
Sample ID : DBF-18
Injection Volume : 10 uL
Data Filename : 1211211.lcd
Method Filename : 2310200.lcm

Batch Filename

Report Filename : RK.lcr

Date Acquired : 11/14/2012 4:16:28 PM
Data Processed : 11/29/2012 12:30:40 PM

Chromatogram DBF-18 E:\HPLC\pesticides\ISO-SAMPLES\1211211.lcd



1 PDA Multi 1 / 295nm 4nm

PeakTable

IDA CIII 2	Juni 4mii					
Peak#	Ret. Time	Area	Area %	Resolution	Tailing Factor	Theoretical Plate#
1	5.702	25485	0.822	0.000	1.175	14161.579
2	6.226	3062636	98.769	2.589	1.143	13715.828
3	7.474	12673	0.409	5.440	1.170	14732.618
Total		3100793	100.000			

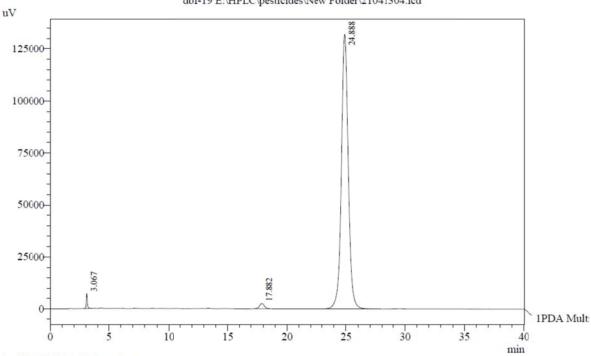
tive Retention		
	0.000	
	0.000	
	0.000	

Acquired by : Admin
Sample Name : dbf-19
Sample ID : dbf-19
Injection Volume : 20 uL
Data Filename : 21041304.lcd
Method Filename : mip.lcm
Batch Filename :

Batch Filename : Report Filename : RK.lcr

Date Acquired : 4/21/2013 1:24:15 PM Data Processed : 4/22/2013 10:38:36 AM

Chromatogram dbf-19 E:\HPLC\pesticides\New Folder\21041304.lcd



1 PDA Multi 1 / 280nm 4nm

PeakTable

PDA Ch1 280nm 4nm

Peak#	Ret. Time	Area	Area %
1	3.067	44967	0.837
2	17.882	69046	1.285
3	24.888	5259478	97.878
Total		5373491	100.000

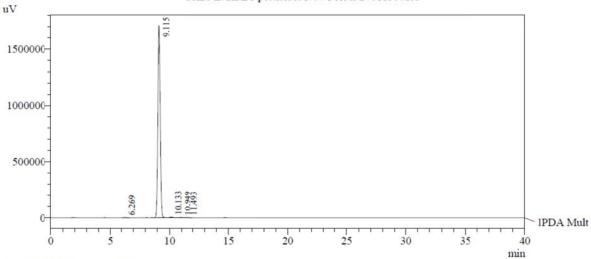
Acquired by Sample Name : Admin : DBF-20 Sample ID : DBF-20 Injection Volume Data Filename Method Filename : 20 uL : 27011304.lcd : ANALYSIS.lcm

Batch Filename

Report Filename

: RK.lcr : 1/28/2013 1:04:59 PM : 1/29/2013 3:27:08 PM Date Acquired Data Processed

Chromatogram dbf20 E:\HPLC\pesticides\New Folder\27011304.lcd



1 PDA Multi 1 / 254nm 4nm

Peak#	Ret. Time	Area	Area %	Resolution	Tailing Factor	Theoretical Plate#
1	6.269	52359	0.223	0.000	1.331	5364.858
2	9.115	23262750	99.020	7.920	1.108	9390.276
3	10.133	89936	0.383	2.601	1.078	9949.893
4	10.949	42193	0.180	2.022	1.088	11935.131
5	11.493	45714	0.195	1.218	1.243	8717.667
Total		23492951	100.000			

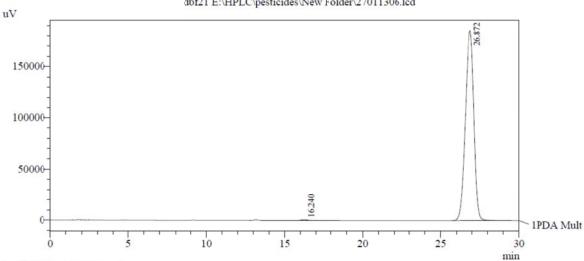
ative I	Retention 7
	0.000
	0.000
	0.000
	0.000
	0.000

Acquired by Sample Name Sample ID : Admin : DBF-21 : DBF-21 Injection Volume : 20 uL : 27011306.lcd Data Filename : ANALYSIS.lcm

Method Filename Batch Filename

Report Filename Date Acquired : RK.lcr : 1/28/2013 2:57:41 PM Data Processed : 2/2/2013 5:25:23 PM

Chromatogram dbf21 E:\HPLC\pesticides\New Folder\27011306.lcd



1 PDA Multi 1 / 295nm 4nm

PeakTable

Peak#	Ret. Time	Area	Area %	Resolution	Tailing Factor	Theoretical Plate#
1	16.240	20583	0.290	0.000	1.133	7823.380
2	26.872	7089297	99.710	12.155	0.940	11215.512
Total		7109880	100.000			

ative	Retention 7
	0.000
	0.000