J. Braz. Chem. Soc., Vol. 19, No. 7, S1-S9, 2008.
Printed in Brazil - ©2008 Sociedade Brasileira de Química
0103 - 5053 $6.00+0.00

Synthesis of Ferrocenyl Oxindole Compounds with Potential Anticancer Activity

Bárbara V. Silva,[a] Núbia M. Ribeiro,[a] Angelo C. Pinto,[a] Maria D. Vargas[b] and Luiz C. Dias[c]

[a]Instituto de Química-CT, Bloco A, Universidade Federal do Rio de Janeiro, Cidade Universitária, 21945-970 Rio de Janeiro-RJ, Brazil

[b] Instituto de Química, Universidade Federal Fluminense, Campus do Valonguinho, Centro, 24020-150 Niterói-RJ, Brazil

[c]Institute of Chemistry, University of Campinas, UNICAMP, P.O. Box 6154, 13084-971 Campinas-SP, Brazil

Table S1. ^{1}H NMR data for compounds **2a**-**2b** to **10a**-**10b**

Carbon	^{1}H chemical shifts (δ/ppm, 250 MHz, $CDCl_3$)							
	2a	**2b**	**3a***	**3b***	**4a***	**4b***	**5a**	**5b**
1	9.28 (s)	7.97 (s)	8.32 (s)	7.89 (s)	8.54 (s)	7.84 (s)	8.21 (s)	8.41(s)
2	-	-	-	-	-	-	-	-
3	-	-	-	-	-	-	-	-
4	7.54 (d, *J* 7.5Hz)	7.49 (d, *J* 7.5Hz)	8.31 (br, s)	7.77 (d, *J*1.6Hz)	7.17 (d, *J* 8.0Hz)	7.19 (d, *J* 8.0Hz)	7.21 (d, *J* 1.6Hz)	7.52 (d, *J* 1.4Hz)
5	7.10 (td, *J* 7.5, 1.0Hz)	7.21 (td, *J* 7.5, 1.1Hz)	-	-	6.89 (t, *J* 8.0Hz)	6.96 (t, *J* 8.0Hz)	-	-
6	6.86 (dd, *J* 7.5, 1.0Hz)	7.02 (td, *J* 7.5, 1.1Hz)	6.69 (d, *J* 8.2Hz)	7.50 (dd, *J* 8.0, 1.6Hz)	7.83 (d, *J* 8.0Hz)	7.37 (d, *J* 8.0Hz)	7.88 (d, *J* 1.6 Hz)	7.48 (d, *J* 1.4Hz)
7	6.81 (d, *J* 7.5Hz)	6.84 (d, *J* 7.5Hz)	7.53 (d, *J* 8.2Hz)	6.63 (d, *J* 8.0Hz)	-	-	-	-
8	7.54 (s)	7.41 (s)	7.71 (s)	7.39 (s)	7.71 (s)	7.43 (s)	7.79 (s)	7.44 (s)
9	-	-	-	-	-	-	-	-
10	-	-	-	-	-	-	-	-
1'	-	-	-	-	-	-	-	-
2'-5'	4.68 (t, *J* 1.7Hz)	5.34 (t, *J* 1.9Hz)	4.75 (br, s)	5.33 (t, *J* 1.9Hz)	4.74 (br, s)	5.34 (t, *J* 1.9Hz)	4.75 (t, *J* 1.7Hz)	4.81 (t, *J* 1.6Hz)
3'-4'	4.49 (t, *J* 1.7Hz)	4.60 (t, *J* 1.9Hz)	4.66 (br, s)	4.64 (t, *J* 1.9Hz)	4.60 (br, s)	4.64 (t, *J* 1.9Hz)	4.69 (t, *J* 1.7Hz)	4.62 (t, *J* 1.6Hz)
Cp	4.14 (s)	4.20 (s)	4.26 (s)	4.21 (s)	4.21 (s)	4.20 (s)	4.26 (s)	4.28 (s)
	6a	**7a***	**7b***	**8a***	**9a**	**9b**	**10a**	**10b**
1	8.44 (s)	8.06 (br, s)	7.71 (s)	9.91 (s)	-	-	8.87 (s)	8.21 (s)
2	-	-	-	-	-	-	-	-
3	-	-	-	-	-	-	-	-
4	-	8.06 (br, s)	7.20 (d, *J* 1.4Hz)	-	7.99 (d, *J* 7.6Hz)	7.50 (d, *J* 7.0Hz)	7.82 (d, *J* 2.0Hz)	7.34 (d, *J* 7.4Hz)
5	7.08 (d, *J* 7.9Hz)	-	-	7.15 (d, *J* 1.4Hz)	7.15 (t, *J* 7.6Hz)	7.15 (td, *J* 7.0, 1.0Hz)	6.91-7.06 (br, m)	6.95(t, *J* 7.4Hz)
6	6.95 (d, *J* 7.9Hz)	7.49 (s)	7.36 (d, *J* 1.4Hz)	-	6.95 (t, *J* 7.6Hz)	7.00 (td, *J* 7.0, 1.0Hz)	6.91-7.06 (br, m)	7.04 (d, *J* 7.4Hz)
7	-	-	-	6.85 (d, *J* 1.4Hz)	6.72 (d, *J* 7.6Hz)	6.72 (d, *J* 7.0Hz)	-	-
8	8.40 (s)	7.76 (s)	7.43 (s)	8.34 (s)	7.76 (s)	7.30 (s)	7.67 (br, s)	7.39 (s)
9	-	-	-	-	5.00 (s)	5.00	2.35 (s)	2.30 (s)
10	-	-	-	-	7.32 (m)	7.32 (m)	-	-
1'	-	-	-	-	-	-	-	-
2'-3'	5.39 (m)	4.66 (m)	5.34 (t, *J* 1.6Hz)	5.11 (t, *J* 1.9Hz)	4.77 (t, *J* 1.7Hz)	5.36 (t, *J* 1.9Hz)	4.80 (br, s)	5.34 (t, *J* 1.8Hz)
4'-5'	4.69 (m)	4.66 (m)	4.68 (t, *J* 1.6Hz)	4.49 (t, *J* 1.9Hz)	4.58 (t, *J* 1.7Hz)	4.58 (t, *J* 1.9Hz)	4.59 (br, s)	4.49 (t, *J* 1.8Hz)
Cp	4.22 (s)	4.25 (s)	4.21 (s)	4.07 (s)	4.25 (s)	4.21 (s)	4.24 (s)	4.19 (s)

* $CDCl_3$ + DMSO.

*e-mail: barbara.iq@gmail.com

Table S2. ^{13}C NMR data for compounds **2a-2b** to **10a-10b**

	^{13}C chemical shifts (δ/ppm, 62.5 MHz, $CDCl_3$)
2a	170.2, 141.1, 137.3, 128.2, 123.3, 122.4, 122.3, 121.1, 109.8, 78.3, 71.1, 69.6
2b**	168.2, 138.8, 138.4, 127.4, 125.7, 121.5, 118.2, 109.3, 104.7, 73.6, 72.4, 68.9
3a*	
3b	
4a*	169.4, 140.2, 138.1, 127.9, 124.1, 122.6, 122.3, 120.8, 115.2, 71.9, 71.5, 70.0
4b	
5a	168.9, 142.3, 136.4, 127.2, 127.2, 125.0, 121.4, 120.9, 115.4, 72.6, 71.8, 70.2
5b	
6a	
7a	
7b	
8a*	167.6, 143.2, 142.1, 128.0, 121.4, 120.5, 119.7, 115.4, 111.7, 74.0, 72.8, 70.1
9a	168.4, 142.3, 138.3, 136.3, 128.7, 128.3, 127.4, 127.3, 122.7, 122.5, 122.1, 121.6, 108.9, 108.9, 73.1, 71.3, 69.9
9b	
10a	
10b	

* * $CDCl_3$ + DMSO; ** 125 MHz.

Table S3. Infrared data for compounds **2a-2b** to **10a-10b**

	IR (KBr) ν_{max}/cm^{-1}
2a	3362, 3122, 3066, 3020, 2902, 2838, 1693, 1621, 1608, 1465, 1338, 1220
2b	3434, 3133, 3064, 3021, 2923, 2850, 1695, 1619, 1600, 1473, 1211
3a	3435, 3145, 3101, 8248, 1697, 1618, 1600, 1442, 1223
3b	3447, 3141, 3097, 2918, 1688, 1615, 1596, 1473, 1201
4a	3367, 3170, 3135, 3079, 3002, 2879, 2802, 1695, 1623, 1602, 1481, 1438, 1330, 1205, 1187
4b	3446, 3161, 3003, 2880, 1685, 1260, 1586, 1481, 1439, 1369, 1189
5a	3445, 3132, 3073, 2971, 1688, 1594, 1577, 1468, 1208, 1162
5b	3419, 3112, 2921, 2850, 1697, 1600, 1573, 1448, 1301, 1151
6a	3481, 3135, 2921, 2850, 1692, 1614, 1578, 1466, 1323, 1146
7a	3441, 3135, 3066, 2956, 2848, 1697, 1621, 1599, 1584, 1447, 1227, 1132
7b	3357, 3127, 3005, 2924, 2854, 1709, 1689, 1591, 1463, 1443, 1207, 1155
8a	3428, 3114, 3081, 2958, 2921, 2852, 1689, 1604, 1581, 1178
9a	3442, 3130, 3137, 3079, 1695, 1623, 1604, 1604, 1483, 1330, 1187, 1130
9b	3442, 3128, 3052, 2956, 2917, 1695, 1616, 1604, 1484, 1168
10a	3461, 3357, 3144, 2918, 2833, 1690, 1608, 1594, 1336, 1218, 1189
10b	3466, 3419, 3138, 2917, 2849, 1686, 1626, 1596, 1369, 1206, 1044

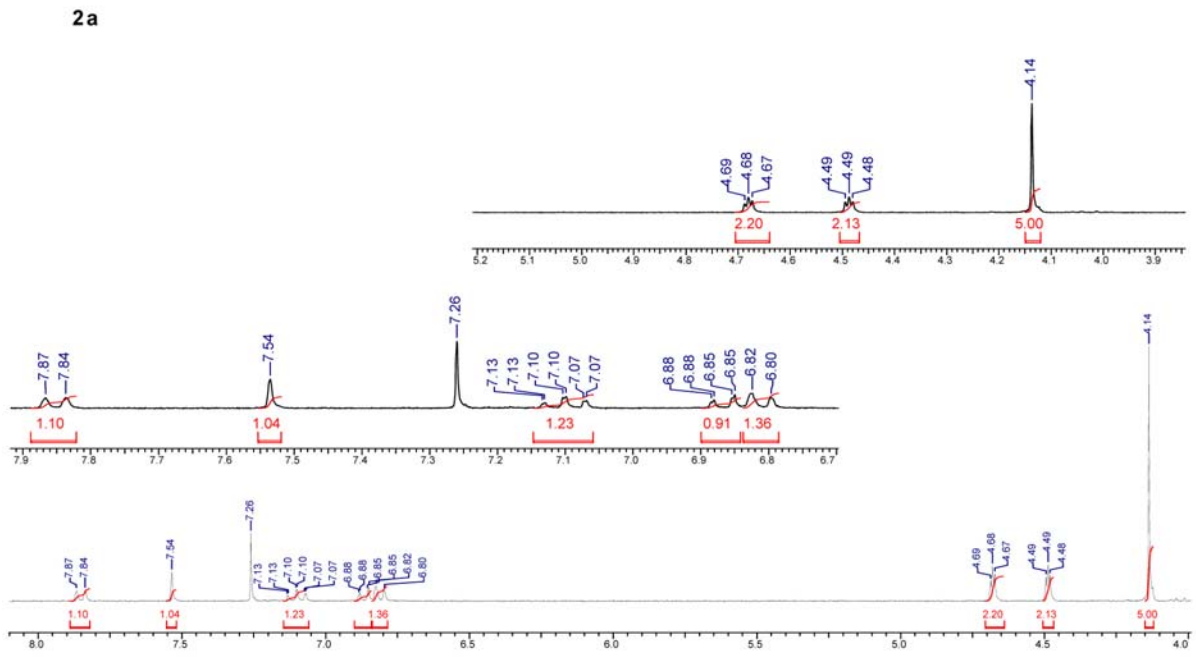

Figure S1. ^1H NMR of **2a.**

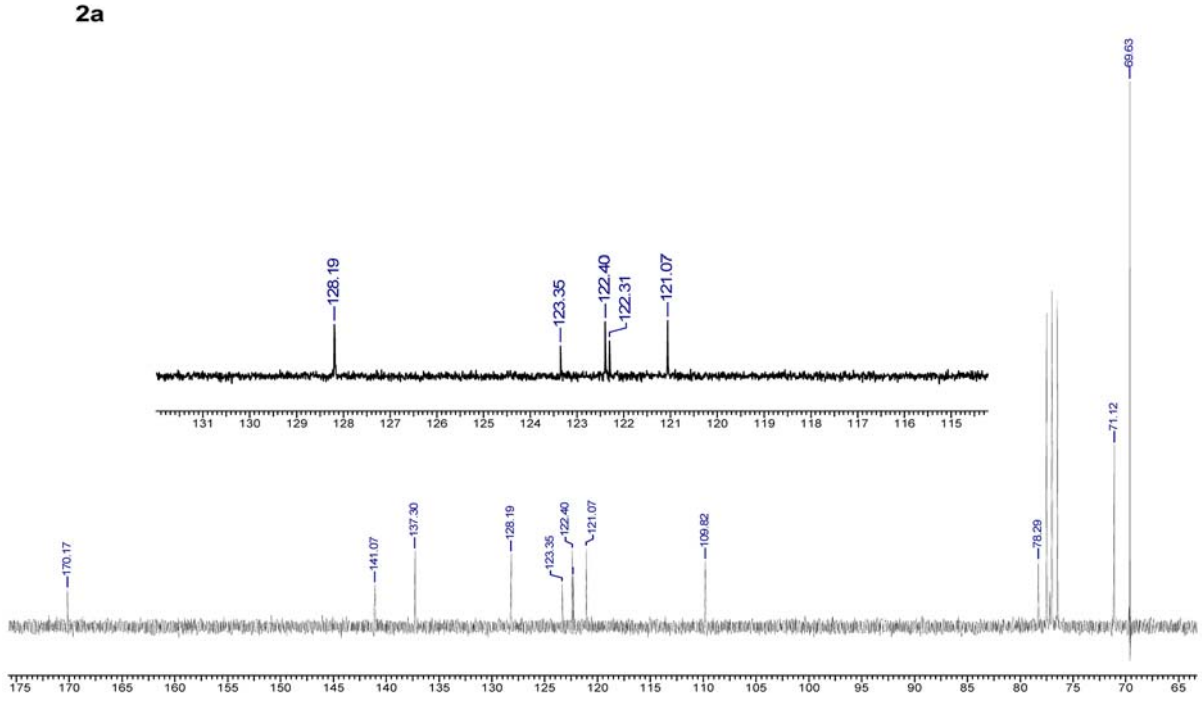

Figure S2. ^{13}C NMR of **2a**.

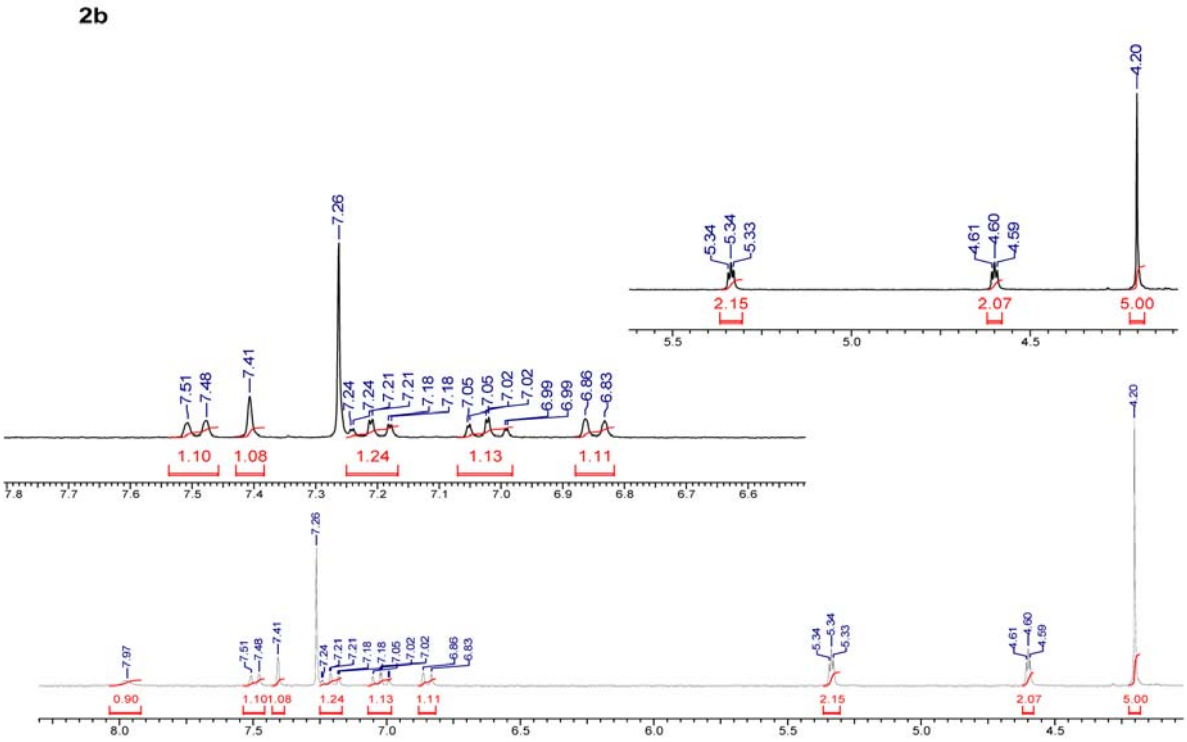

Figure S3. ^{1}H NMR of **2b**.

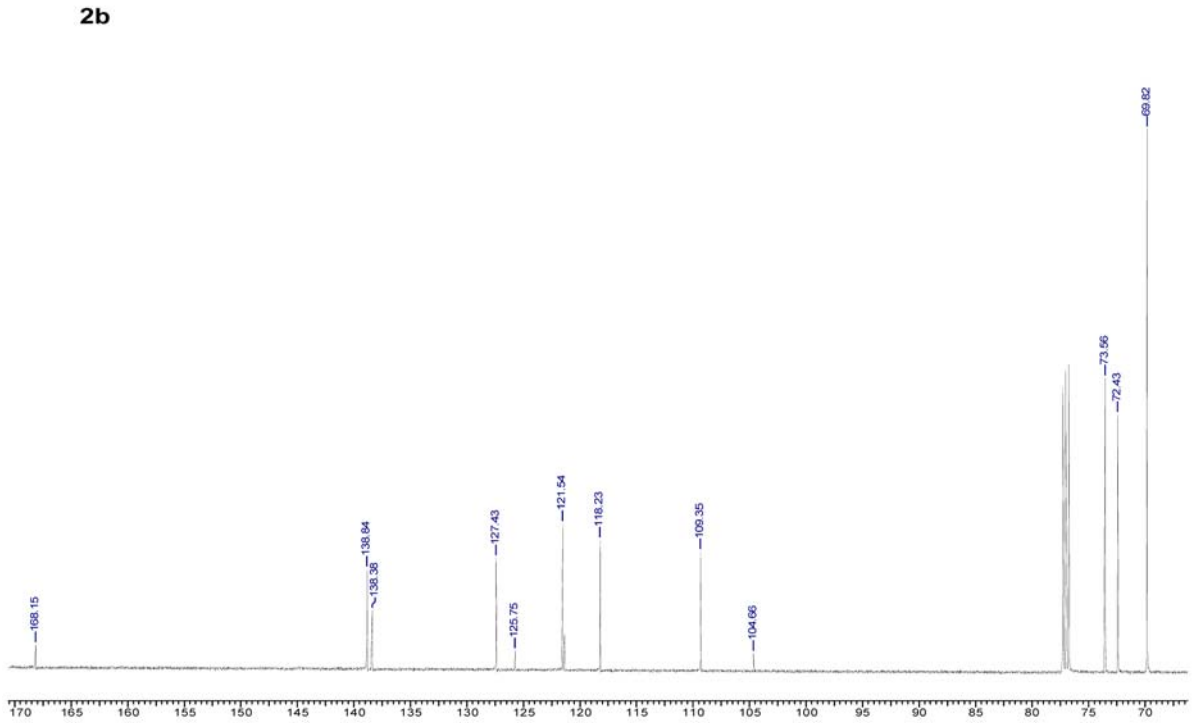

Figure S4. ^{13}C NMR of **2b**.

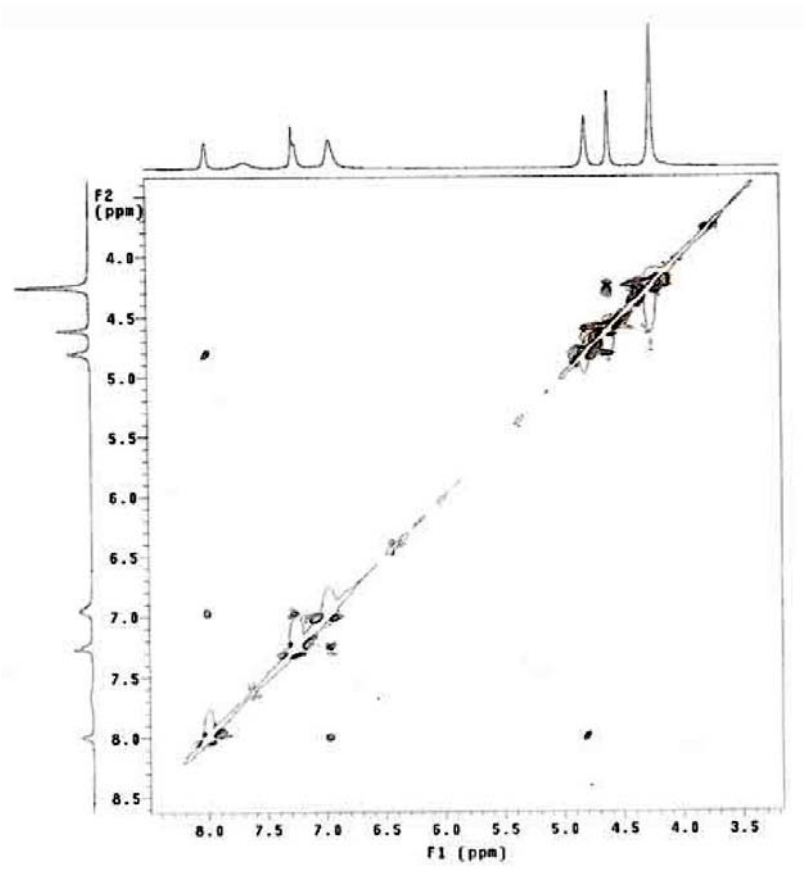

Figure S5. NOESY of **2a**.

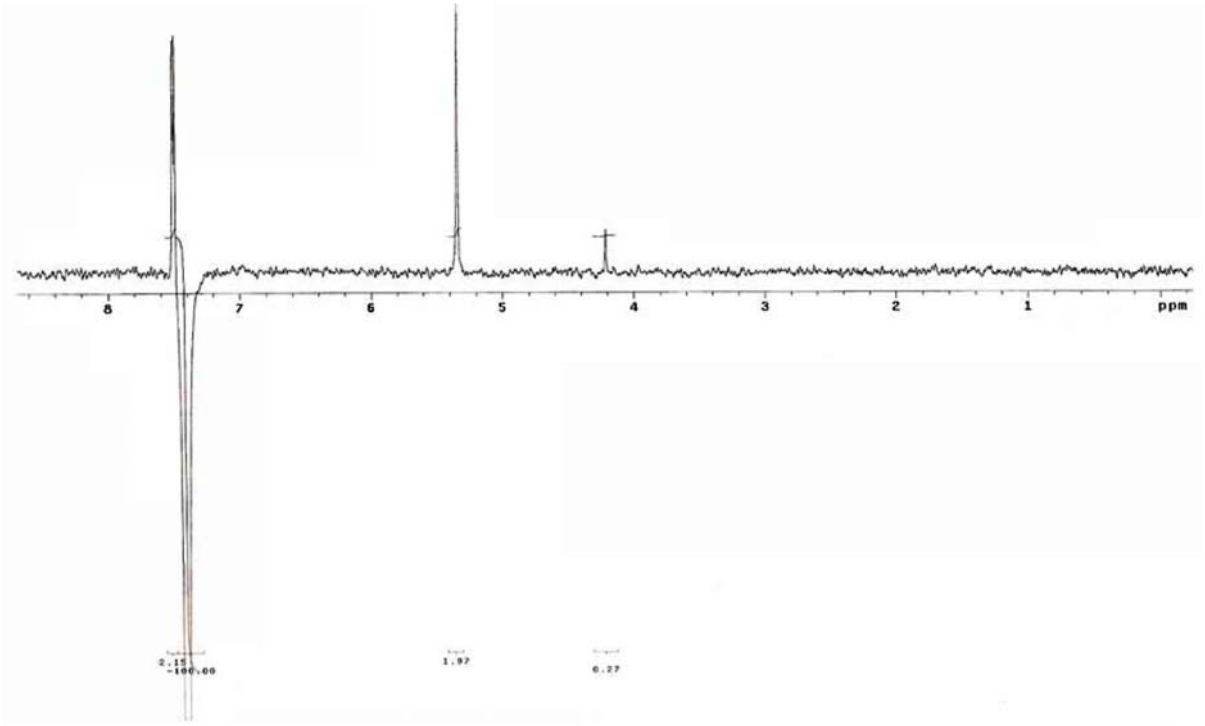

Figure S6. nOe of **2b**.

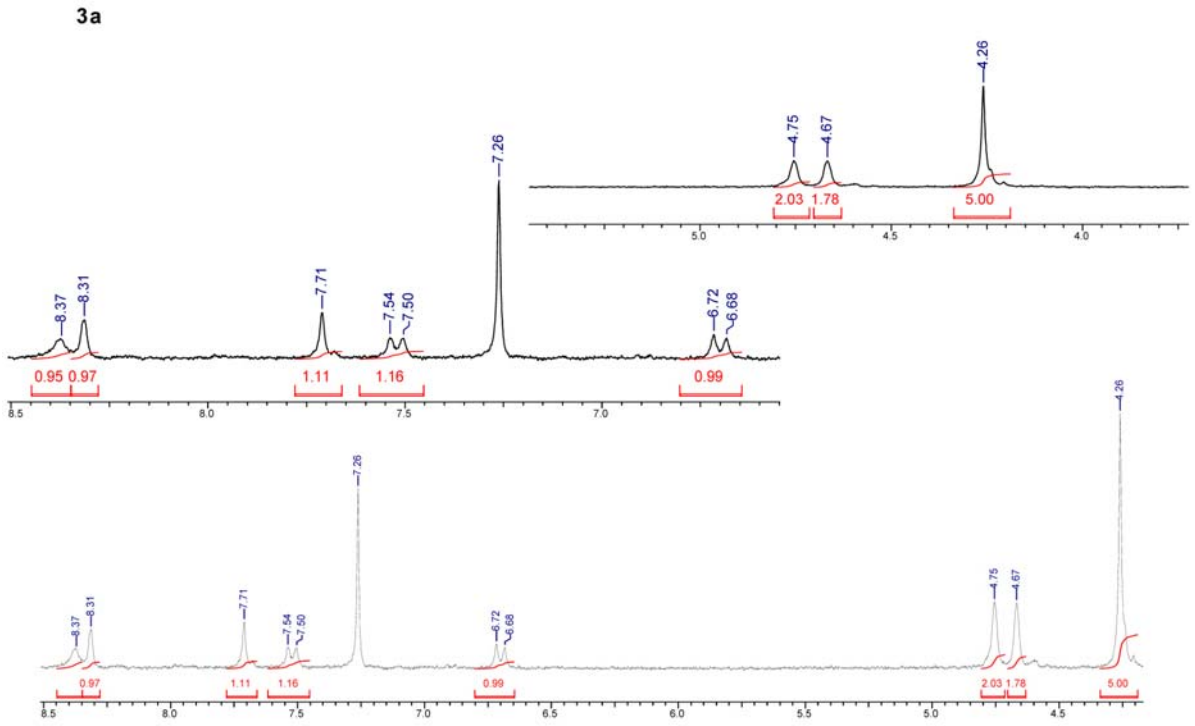

Figure S7. ^{1}H NMR of **3a**.

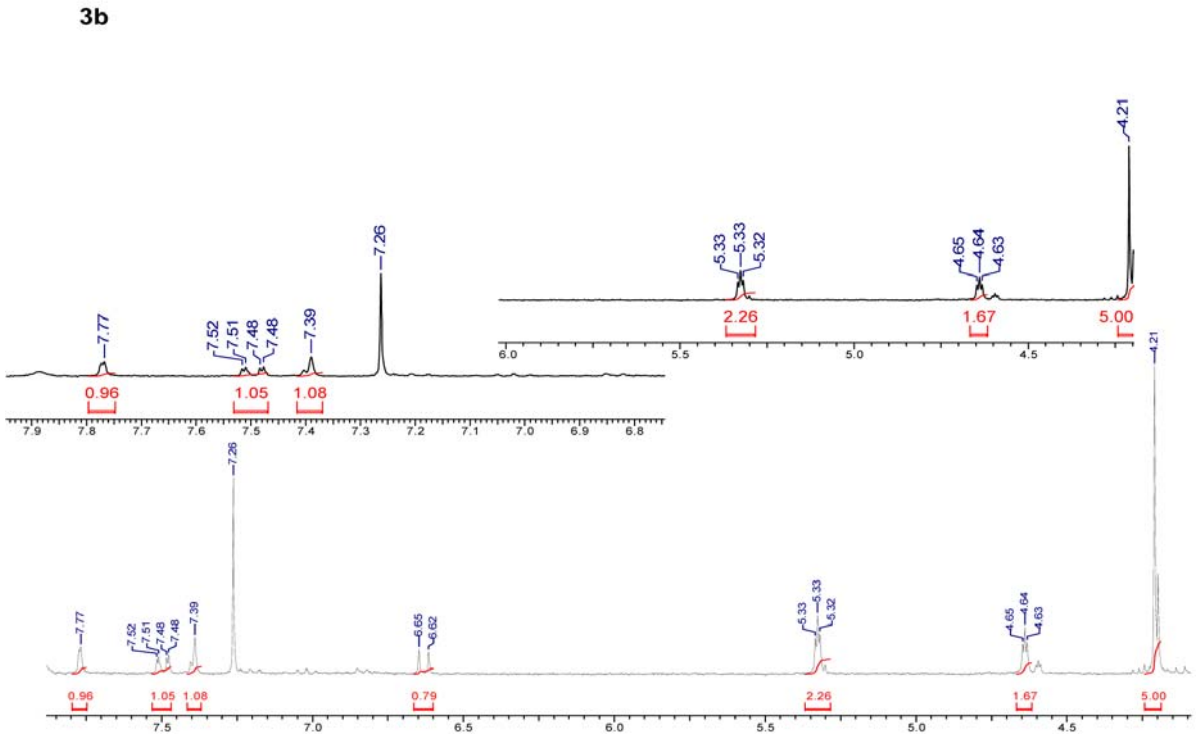

Figure S8. ^{1}H NMR of **3b**.

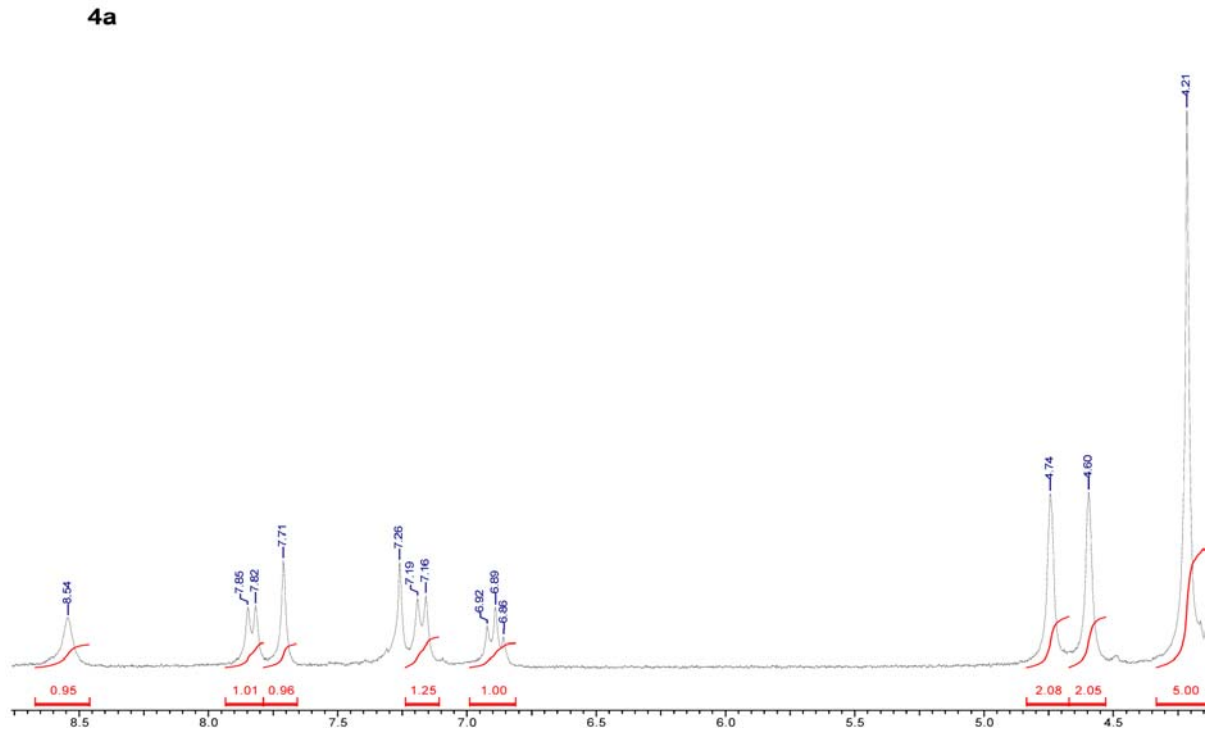

Figure S9. ^{1}H NMR of **4a**.

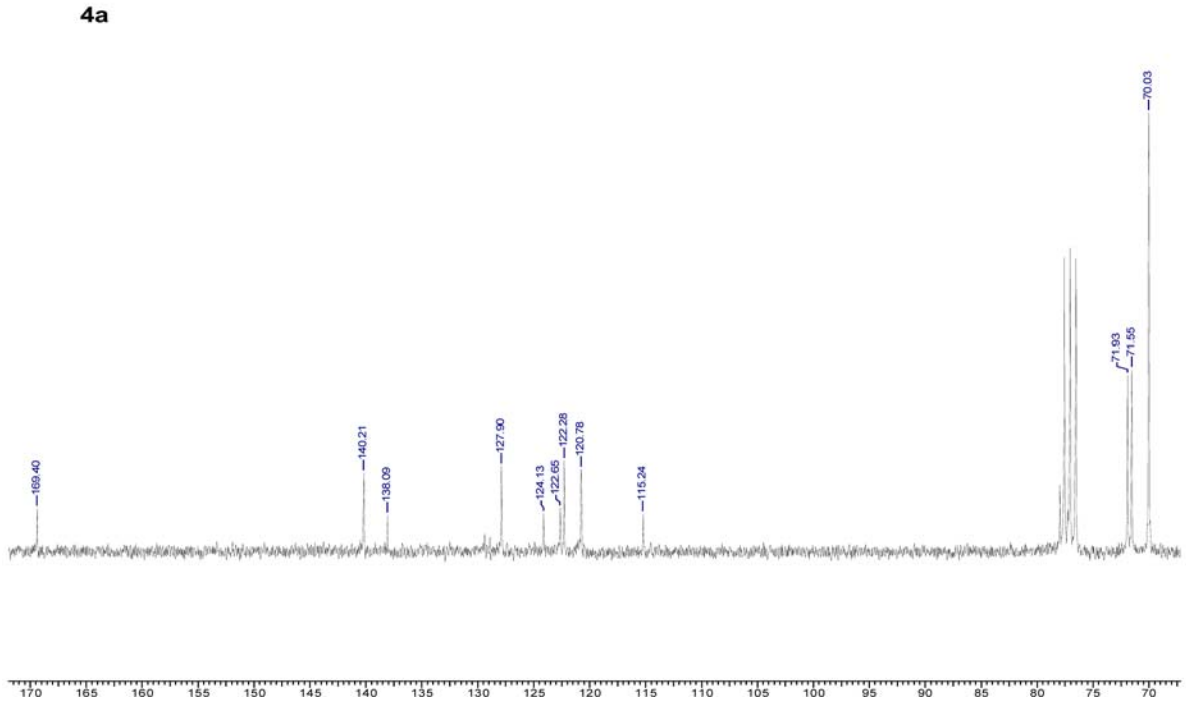

Figure S10. ^{13}C NMR of **4a**.

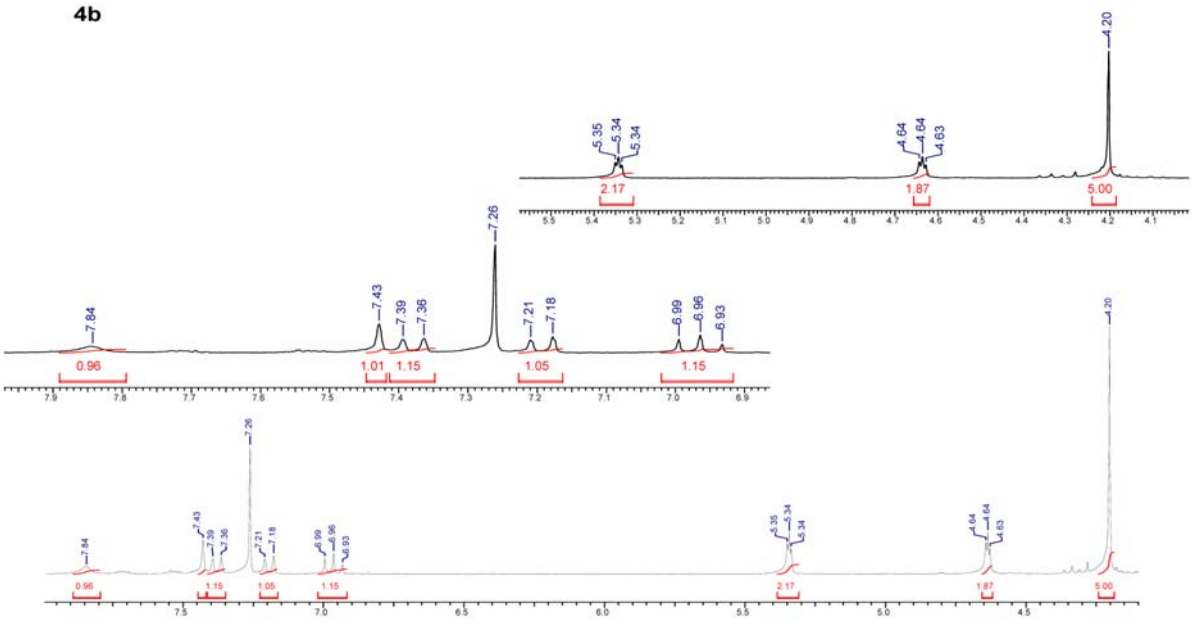

Figure S11. ^{1}H NMR of **4b**.

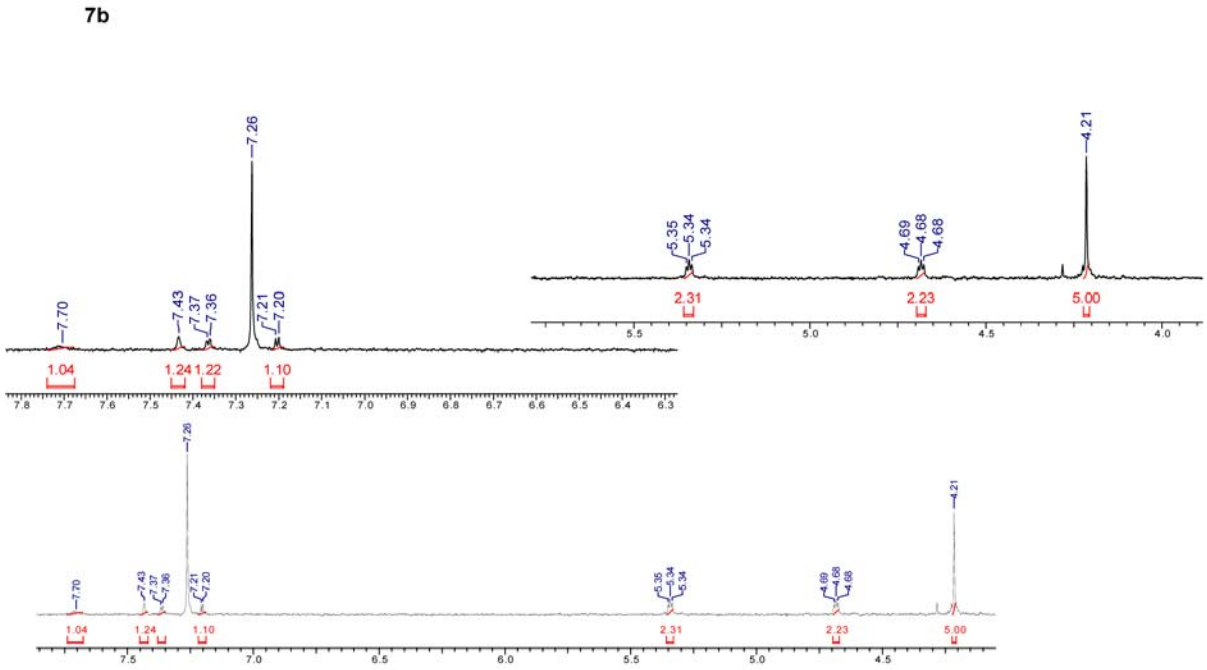

Figure S12. [1]H NMR of **7b**.

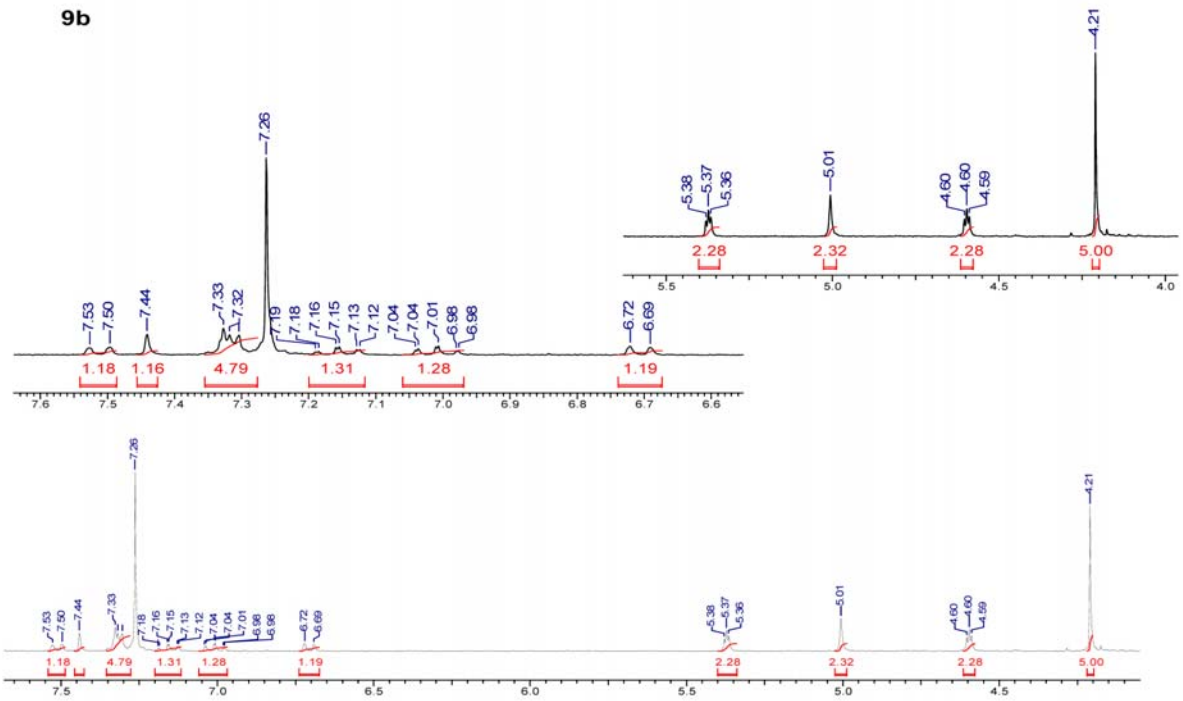

Figure S13. [1]H NMR of **9b**.

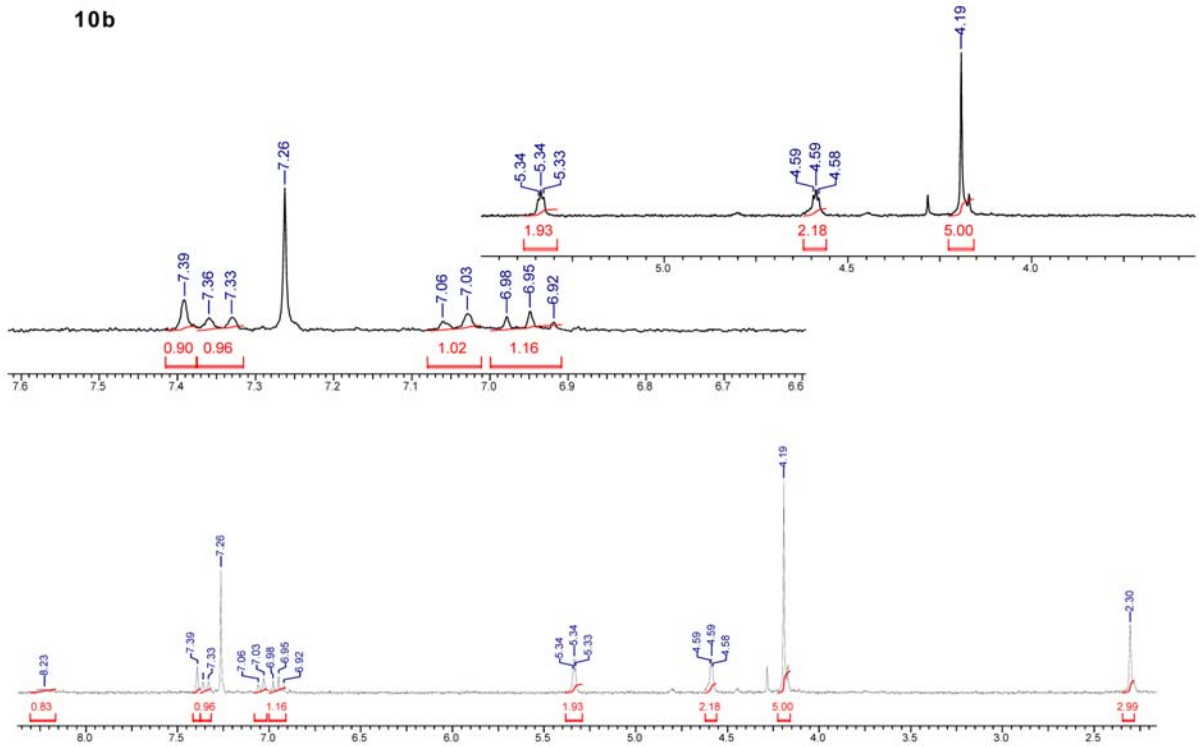

Figure S14. ^{1}H NMR of **10b**.