**Antiproliferative activities of 2-hydroxyethyl substituted benzimidazolium salts and their palladium complexes against human cancerous cell lines**

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**Characterization of compounds**

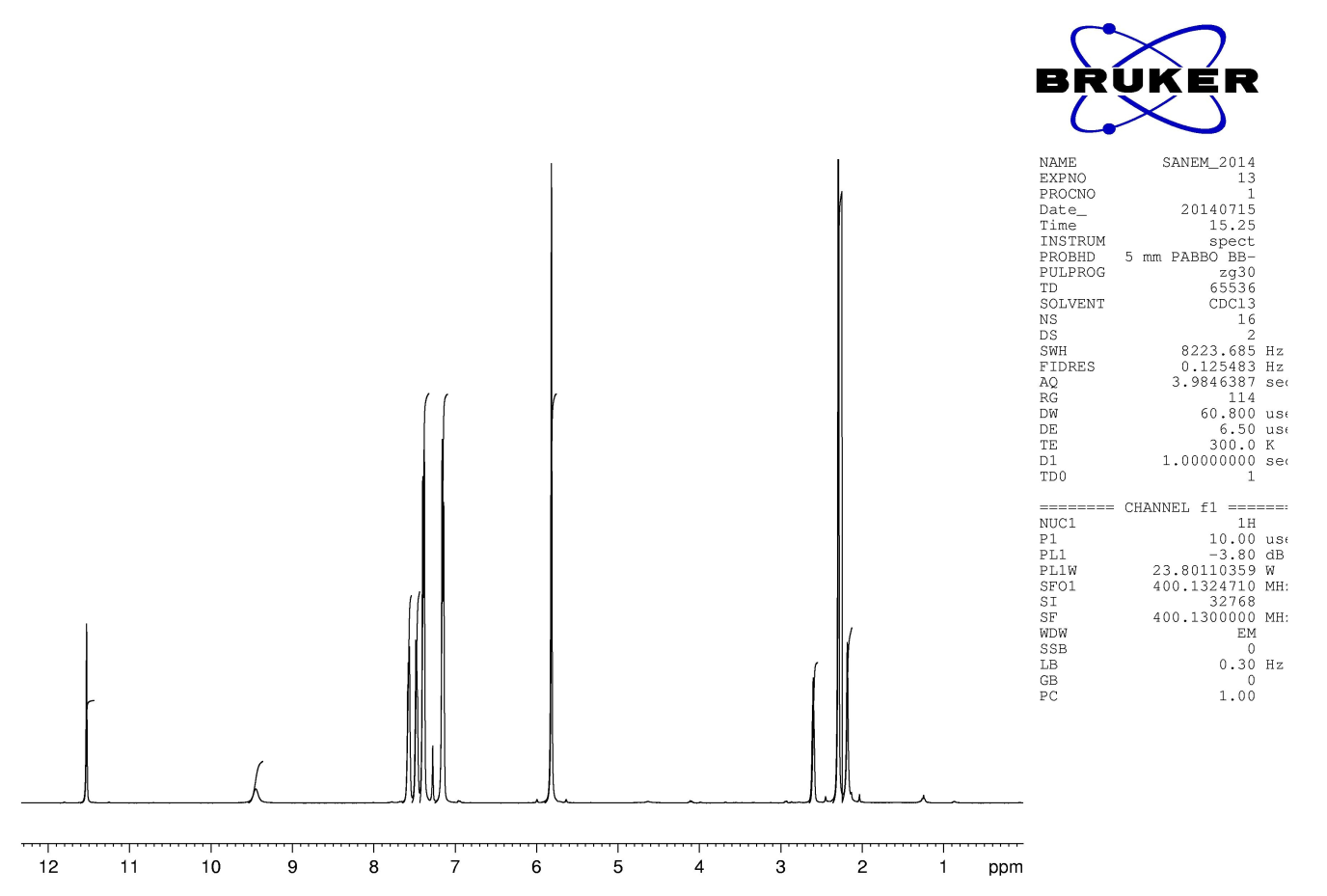
*1-(2-Hydroxyethyl)-3-(2,3,4,5,6-pentamethylbenzyl)-1H-benzo[d]imidazol-3-ium bromide,* ***1b***

A similar compound namely 1-pentamethylbenzyl-3-hydroxyethylbenzimidazolium iodide was prepared by Akkoç et al. [1]. However, in this study, the objective compound **1b** was synthesized from 1-(2,3,4,5,6-pentamethylbenzyl)-1*H*-benzo[*d*]imidazole (0.70 g, 1 mmol) and 2-hydroxyethylbromide (0.32 g, 1 mmol). The yellow colored compound was initially washed with diethyl ether. Yield: 57%, m.p.: 194-196 ºC, color: yellow. IR: 1193.8 (C-O); 1550.7 (C=N); 2867.9, 2920.0 and 3006.8 (C-H); 3211.2 cm-1 (OH). 1H NMR (400 MHz, CDCl3, 298 K), δ: 2.15-2.31 [m, 16 H, NCH2CH2O*H*; NCH2C6(C*H*3)5-2,3,4,5,6]; 4.04 (t, 2 H, NCH2C*H*2OH); 4.75 (t, 2 H, NC*H*2CH2OH); 5.70 [s, 2 H, NC*H*2C6(CH3)5-2,3,4,5,6]; 7.28-8.02 (m, 4 H, Ar-*H*); 9.77 (s, 1 H, NC*H*N). 13C NMR (100 MHz, CDCl3, 298 K), δ: 16.90, 17.02, 17.14, 17.31 and 34.64 [NCH2C6(*C*H3)5-2,3,4,5,6]; 47.51, 49.86 and 58.88 [N*C*H2*C*H2OH and N*C*H2C6(CH3)5-2,3,4,5,6]; 113.20, 113.59, 124.41, 127.27, 127.35, 131.55, 131.95, 133.68, 134.19 and 137.66 (Ar-*C*); 141.34 (N*C*HN). Elemental analysis for C21H27N2OBr (403.36 g/mol) %: Found C: 62.37; H: 6.99; N: 6.92. Anal. Calc. C: 62.53; H: 6.75; N: 6.95.

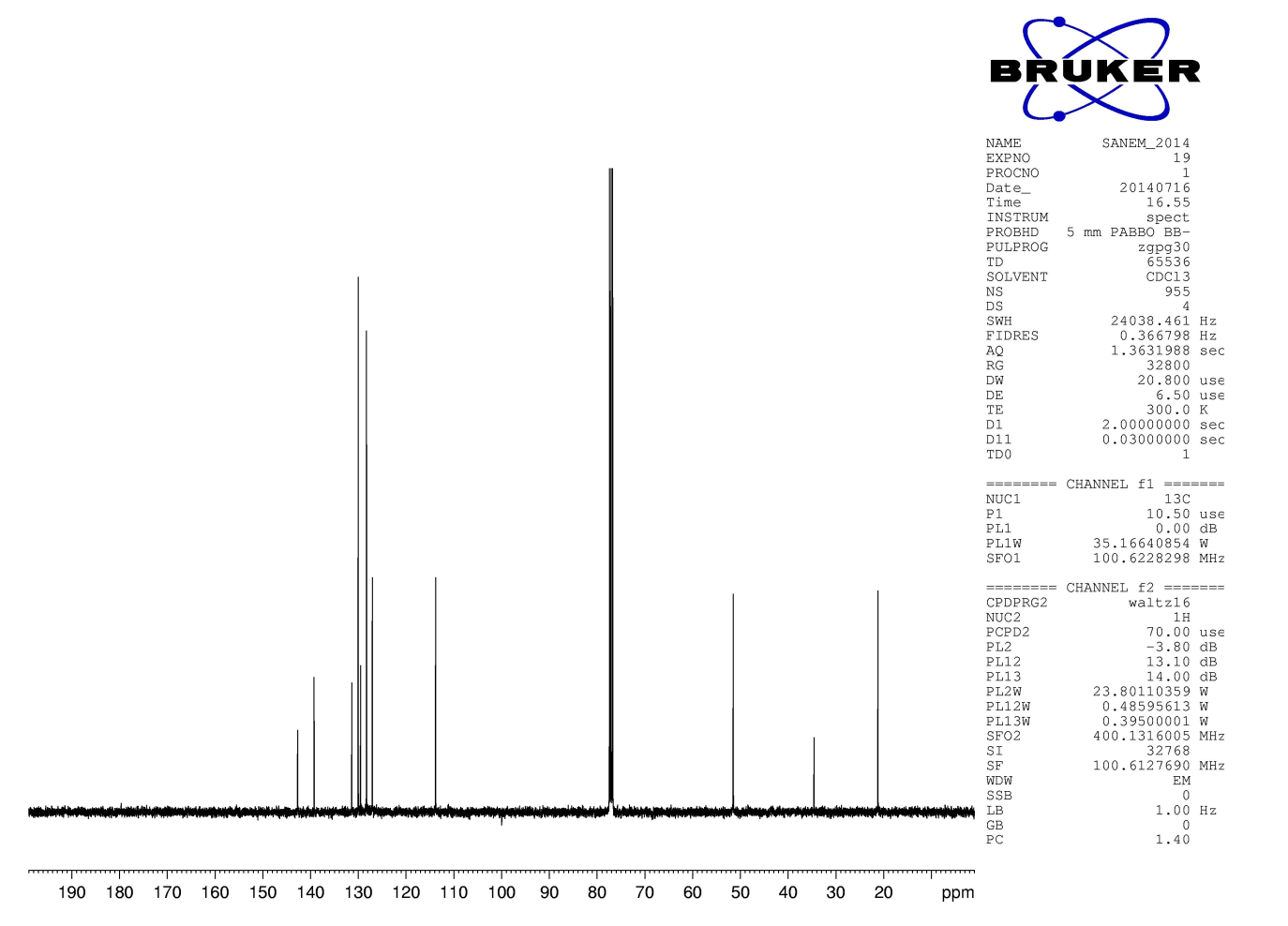
*Dibromo-[1-(2-hydroxyethyl)-3-(2,3,4,5,6-pentamethylbenzyl)benzimidazol-2-ylidene]-N-(3-chloropyridine) palladium (II) complex,* ***2b***

Following a similar procedure to that of mentioned in the section of compound **2a**, compound **2b** was synthesized from 1-(2-hydroxyethyl)-3-(2,3,4,5,6-pentamethylbenzyl)-1*H*-benzo[*d*]imidazol-3-ium bromide **1b** (1 mmol), PdCl2 (1 mmol), 3-chloropyridine (3 mL) and K2CO3 (5 mmol) as a base. Yield: 21%, m.p.: 174-175 ºC, color: light yellow. IR: 1255.6 (C-O); 1456.2 (C=N); 2964.4 and 3014.5 (C-H); 3473.6 cm-1 (OH). 1H NMR (600 MHz, CDCl3, 298 K), δ: 2.21-2.28 [m, 16 H, NCH2CH2O*H*; NCH2C6(C*H*3)5-2,3,4,5,6]; 3.40 (t, *J*: 7.2 Hz, 2 H, NCH2C*H*2OH); 4.43 (t, *J*: 5.4 Hz, 2 H, NC*H*2CH2OH); 6.04 [s, 2 H, NC*H*2C6(CH3)5-2,3,4,5,6]; 6.89-8.88 (m, 8 H, Ar-*H*). 13C NMR (100 MHz, CDCl3, 298 K), δ: 14.14, 16.95 and 17.71 [NCH2C6(*C*H3)5-2,3,4,5,6]; 51.87, 61.18 and 65.87 [N*C*H2*C*H2OH and N*C*H2C6(CH3)5-2,3,4,5,6]; 110.56, 111.58, 122.86, 123.29, 124.92, 127.58, 132.66, 133.26, 134.76, 135.05, 135.44, 136.20, 138.09, 149.92, 150.47, 150.95 and 151.48 (Ar-*C*); 161.13 (N*C*N). Elemental analysis for C26H30Br2ClN3OPd (702.22 g/mol) %: Found C: 44.40; H: 4.46; N: 5.99. Anal. Calc. C: 44.47; H: 4.31; N: 5.98.

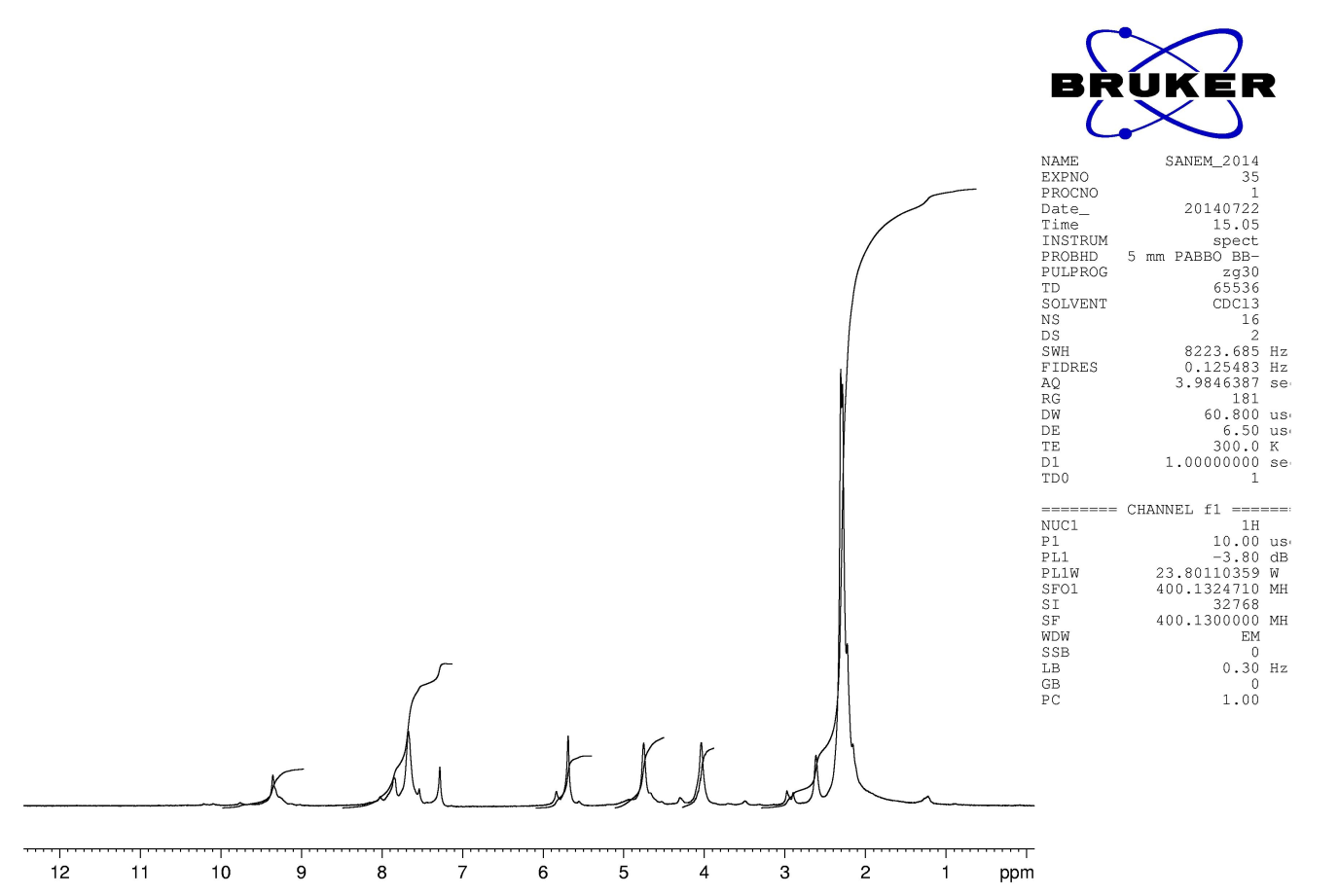
**Spectra of synthesized compounds**



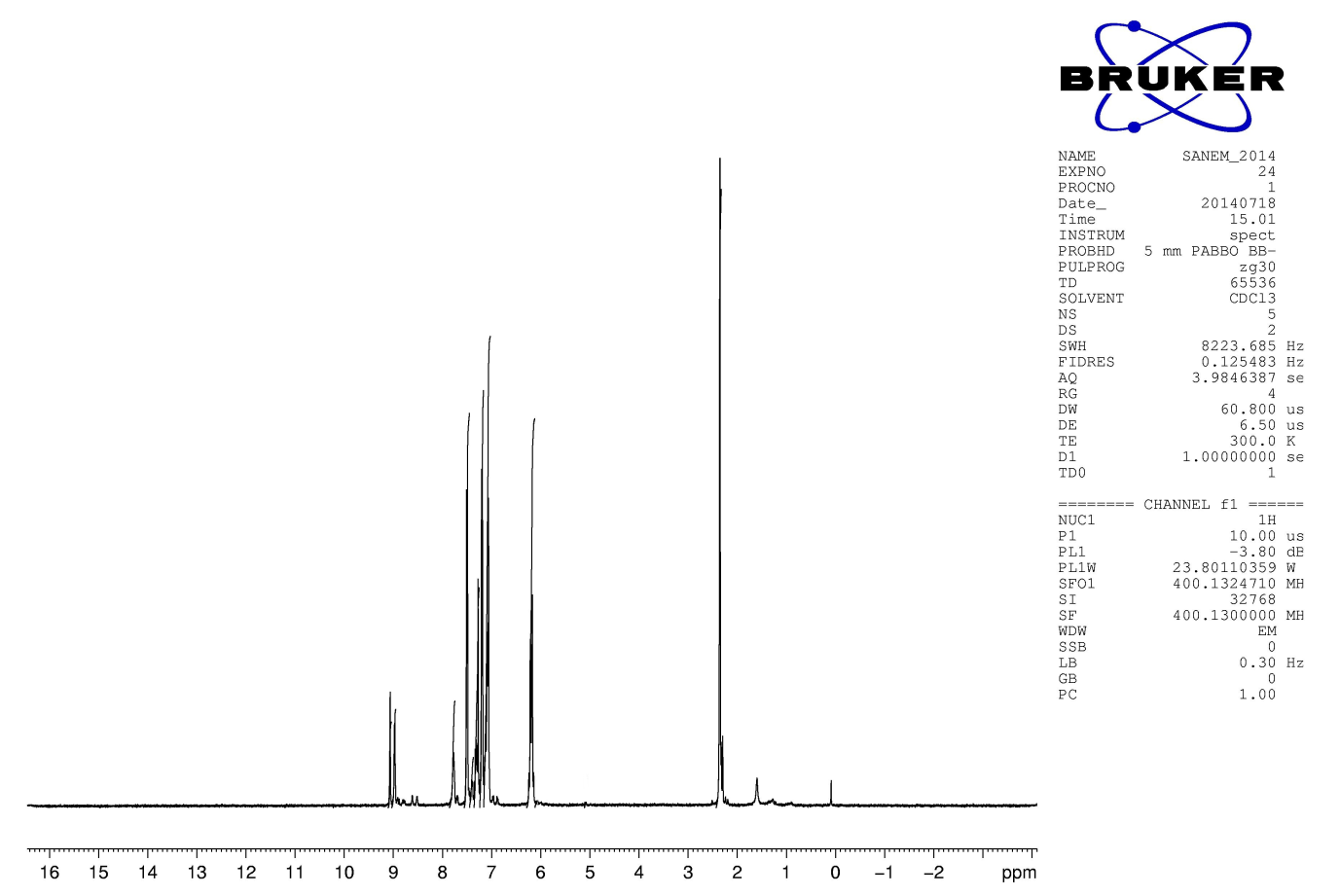
**Scheme 1.** 1H NMR spectra of compound **1a**.



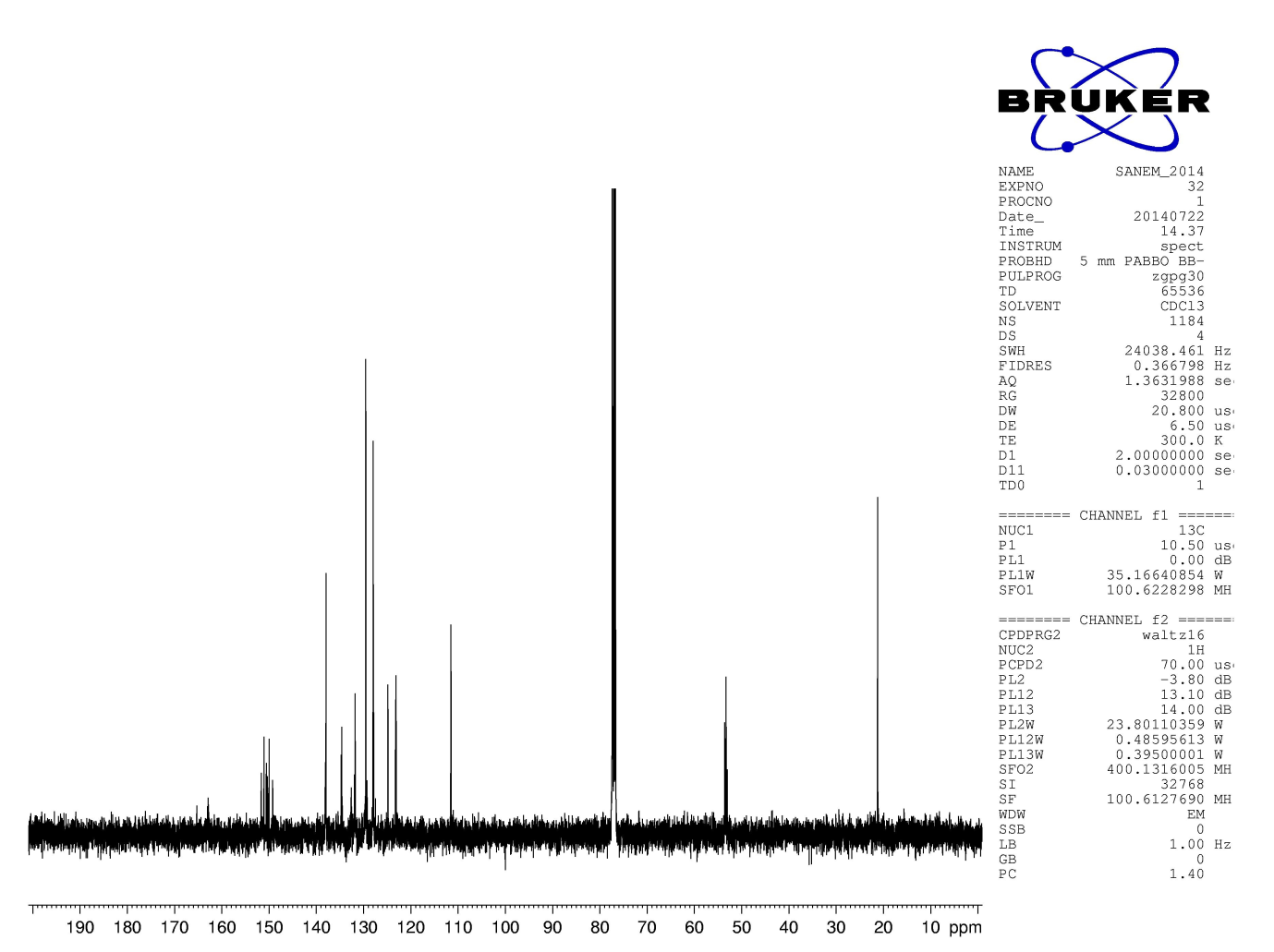
**Scheme 2.** 13C NMR spectra of compound **1a**.



**Scheme 3.** 1H NMR spectra of compound **1b**.



**Scheme 4.** 1H NMR spectra of compound **2a**.



**Scheme 5.** 13C NMR spectra of compound **2a**.

**Scheme 6.** HRMS spectra of **2a**.

**Scheme 7.** HRMS spectra of **2a**.

**Scheme 8.** HRMS spectra of **2a**.

**Scheme 9.** HRMS spectra of **2a**.

**Reference**

[1] Akkoç, M.; Öz, E.; Demirel, S.; Dorcet, V.; Roisnel, T.; Bayri, A.; et al. Investigation of potential hybrid capacitor property of chelated N-Heterocyclic carbene Ruthenium(II) complex. *J. Organomet. Chem.* **2018**, *866*, 214-22. DOI: [https://doi.org/10.1016/j.jorganchem.2018.04.035](https://doi.org/10.1016/j.jorganchem.2018.04.035" \o "Persistent link using digital object identifier" \t "_blank)