

Supporting information for:

Excited-state intramolecular proton transfer in substituted 4-(2-hydroxyphenyl)imidazole

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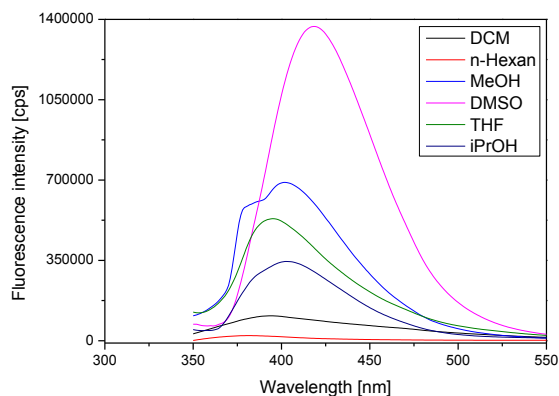


Figure S-1. Fluorescence emission spectra ($\lambda_{\text{ex}}=340$ nm) taken for compound **6** in various solvents

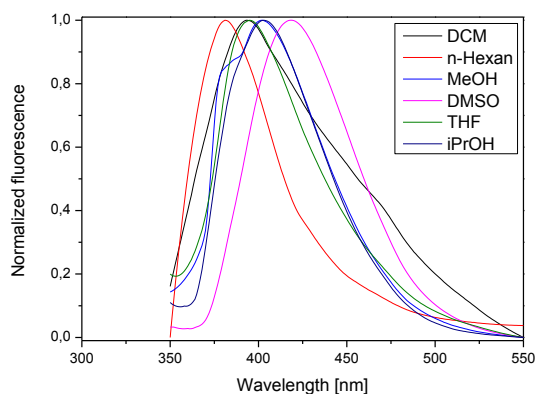


Figure S-2. Normalized fluorescence emission spectra ($\lambda_{\text{ex}}=340$ nm) for compound **6** in various solvents

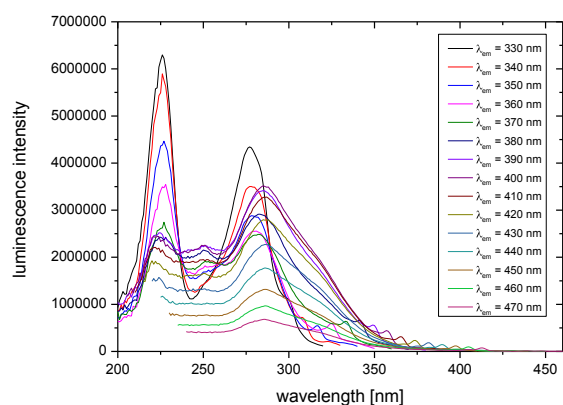


Figure S-3. Fluorescence excitation spectra taken for compound **6** in MeOH at different emission wavelengths from 330 nm to 470 nm.

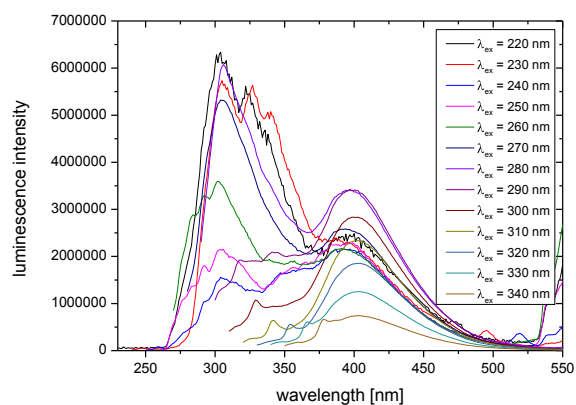


Figure S-4. Fluorescence emission spectra taken for compound **6** in MeOH with different excitation wavelengths from 220 nm to 340 nm.

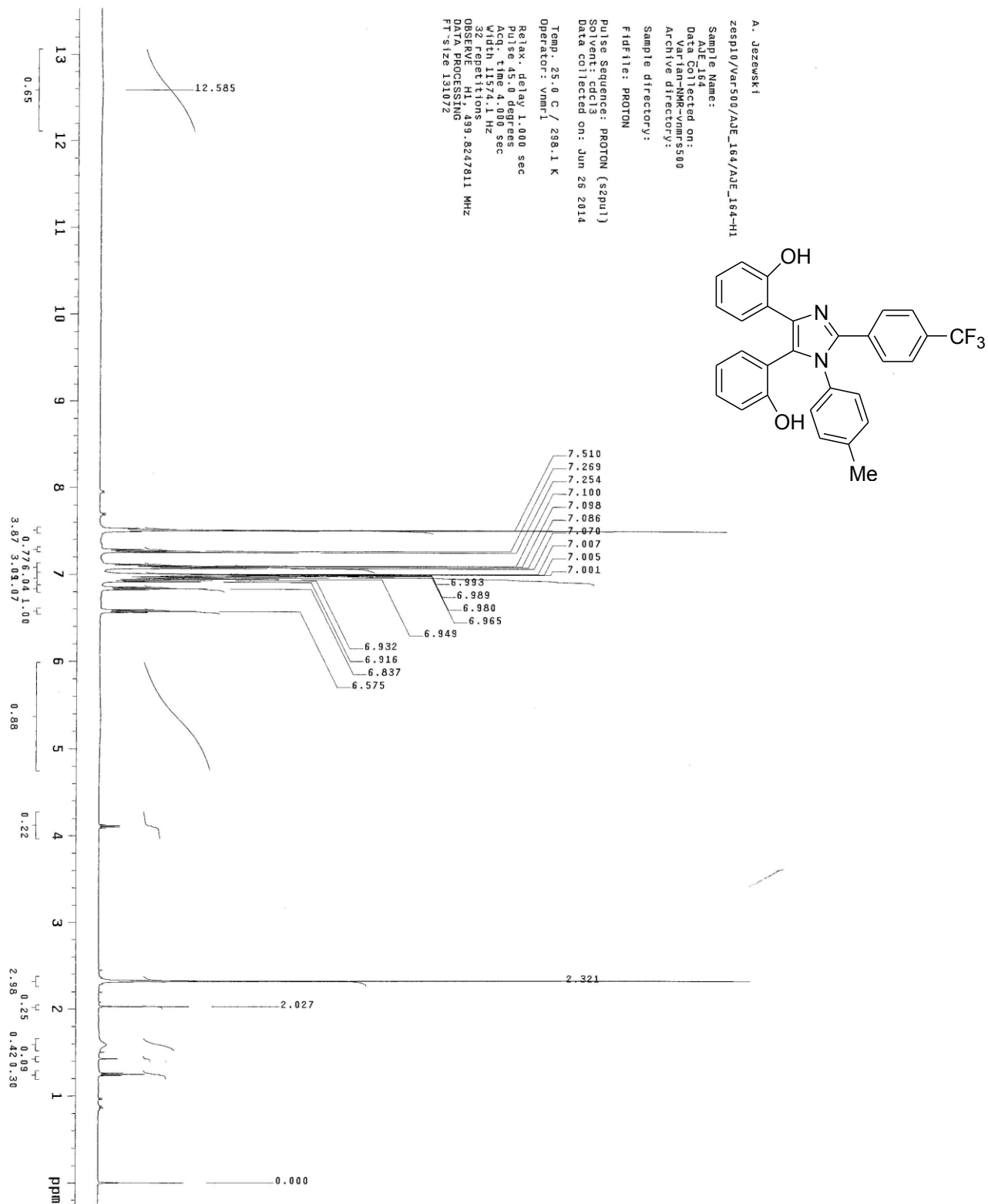


Fig. S-5. ^1H NMR spectrum of compound **6**.

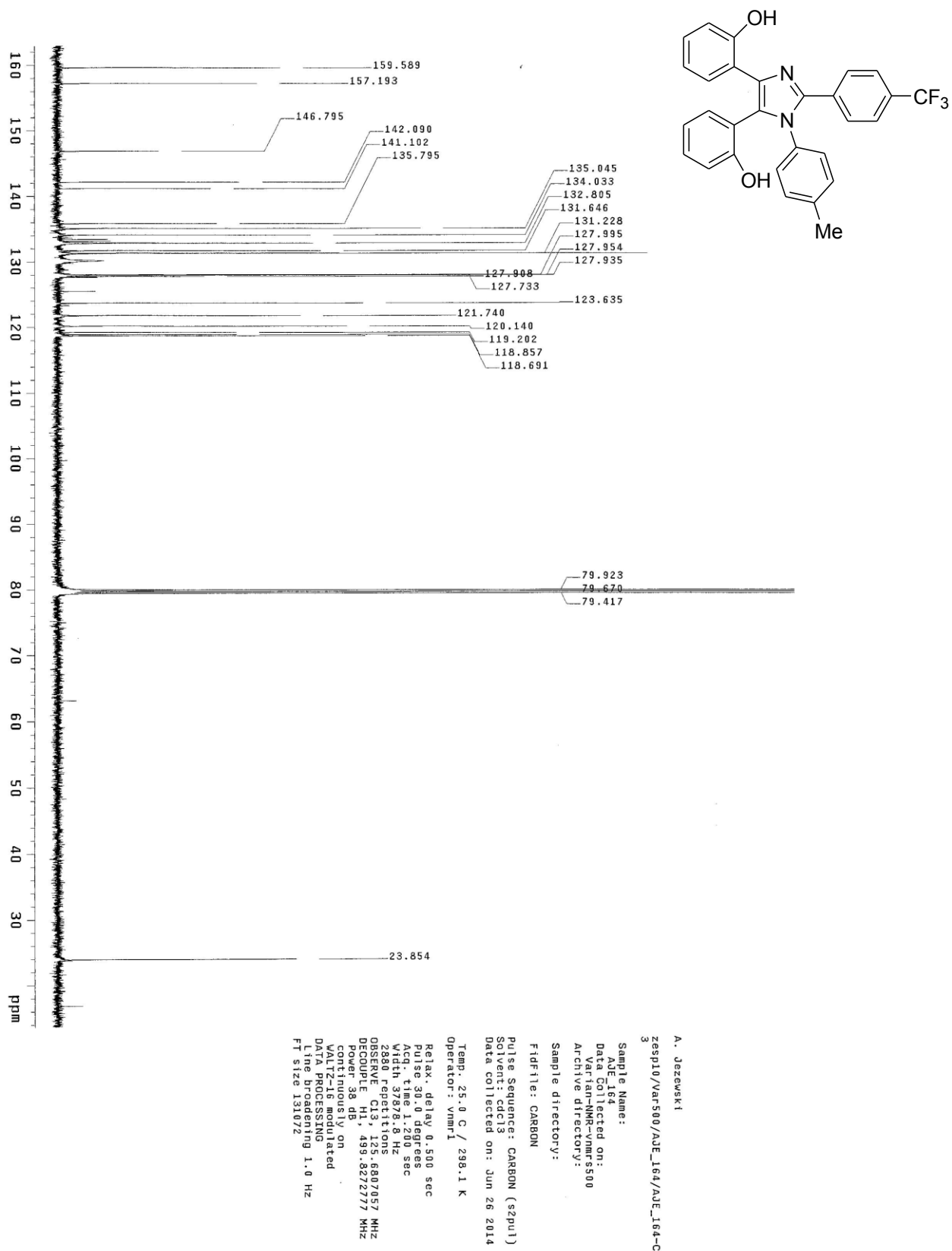
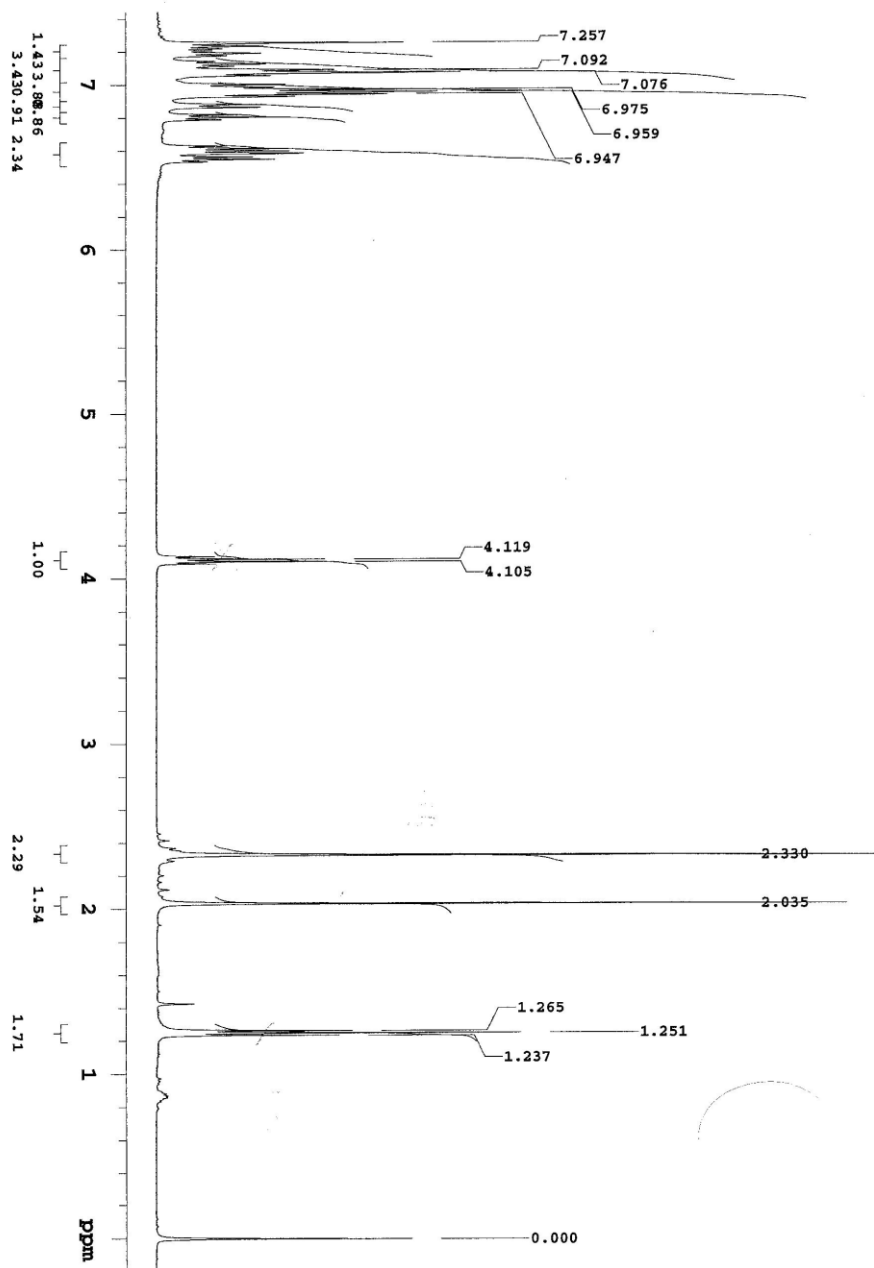
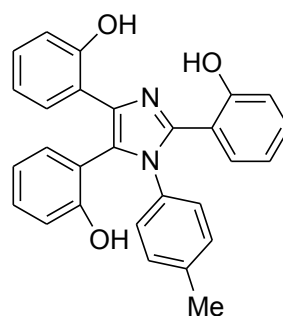


Fig. S-6. ¹³C NMR spectrum of compound 6.



A. Jezewski
 zesp10/Var500/AJE_171/AJE_171-H1
 Sample Name:
 AJE_171
 Data Collected on:
 Varian-NMR-VnmrS500
 Archive directory:
 Sample directory:
 FIDFile: PROTON
 Pulse Sequence: PROTON (a2pul)
 Solvent: cdcl3
 Data collected on: Sep 5 2014
 Temp: 25.0 C / 298.1 K
 Operator: vnmr1
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 4.000 sec
 Width 11574.1 Hz
 32 repetitions
 OBSERVE H1, 499.8247801 MHz
 DATA PROCESSING
 FT size 131072



Fig. S-7. ^1H NMR spectrum of compound 7

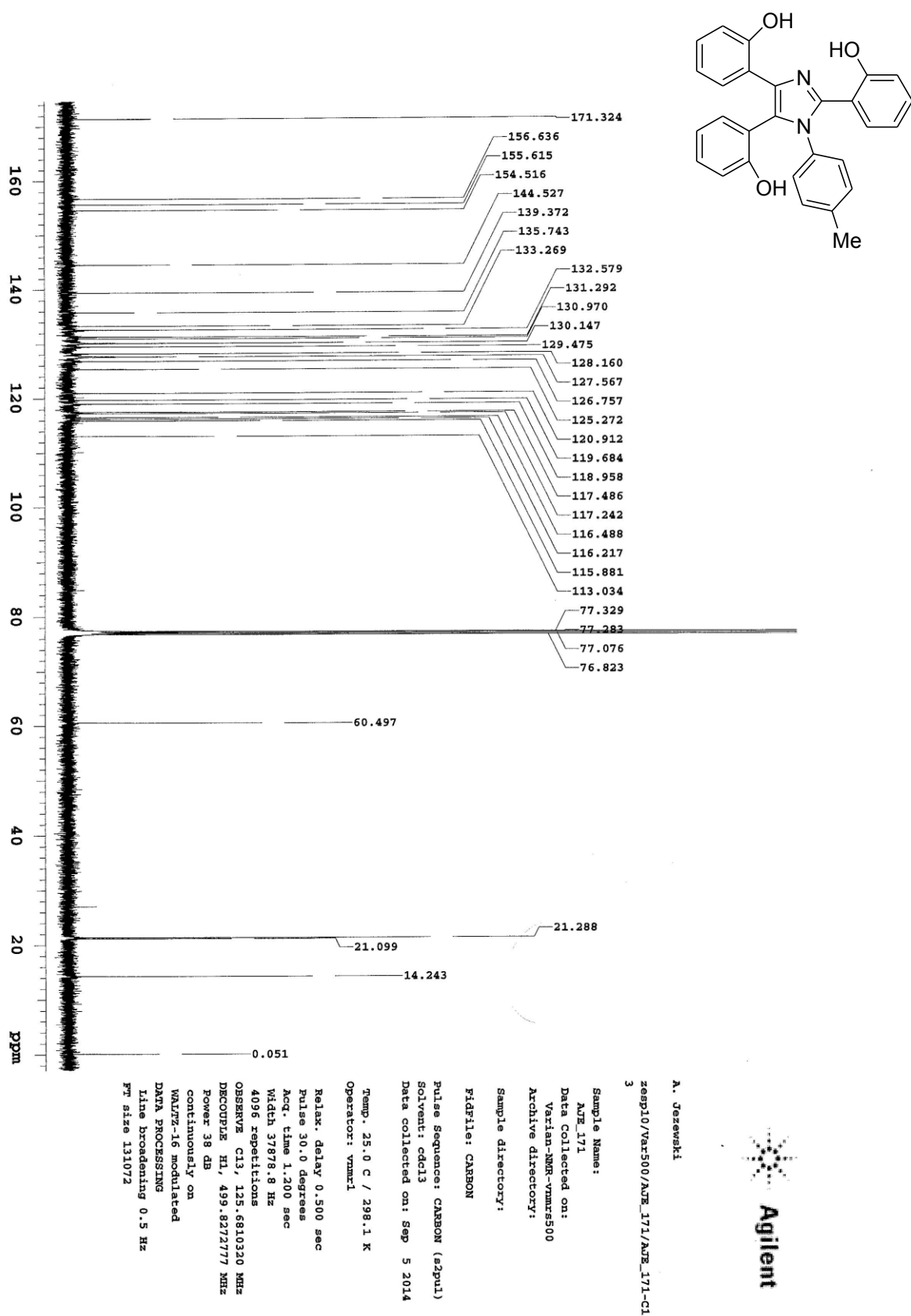


Fig. S-8. ^{13}C NMR spectrum of compound 7.

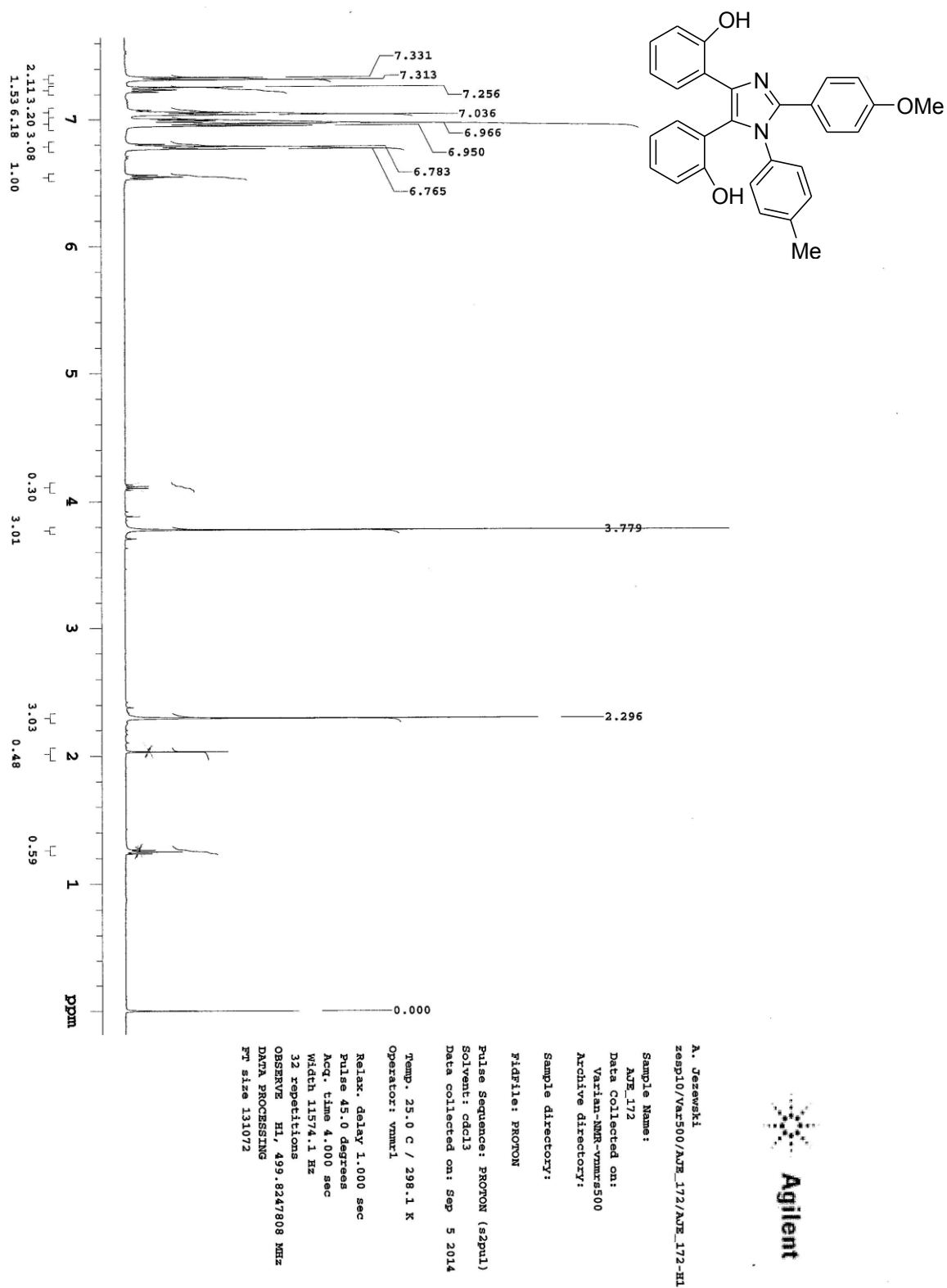


Fig. S-9. ¹H NMR spectrum of compound **8**.

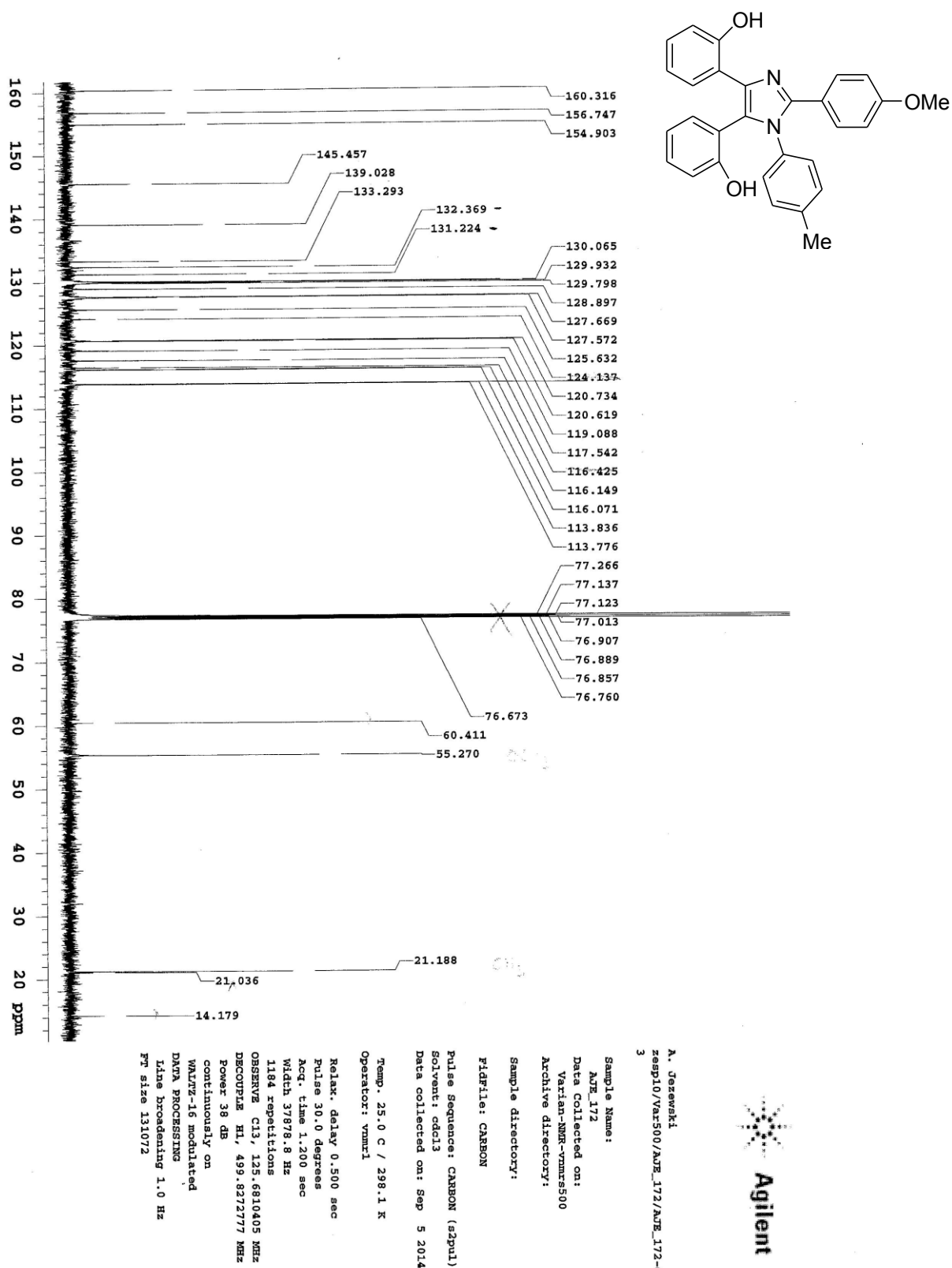


Fig. S-10. ^{13}C NMR spectrum of compound 8.

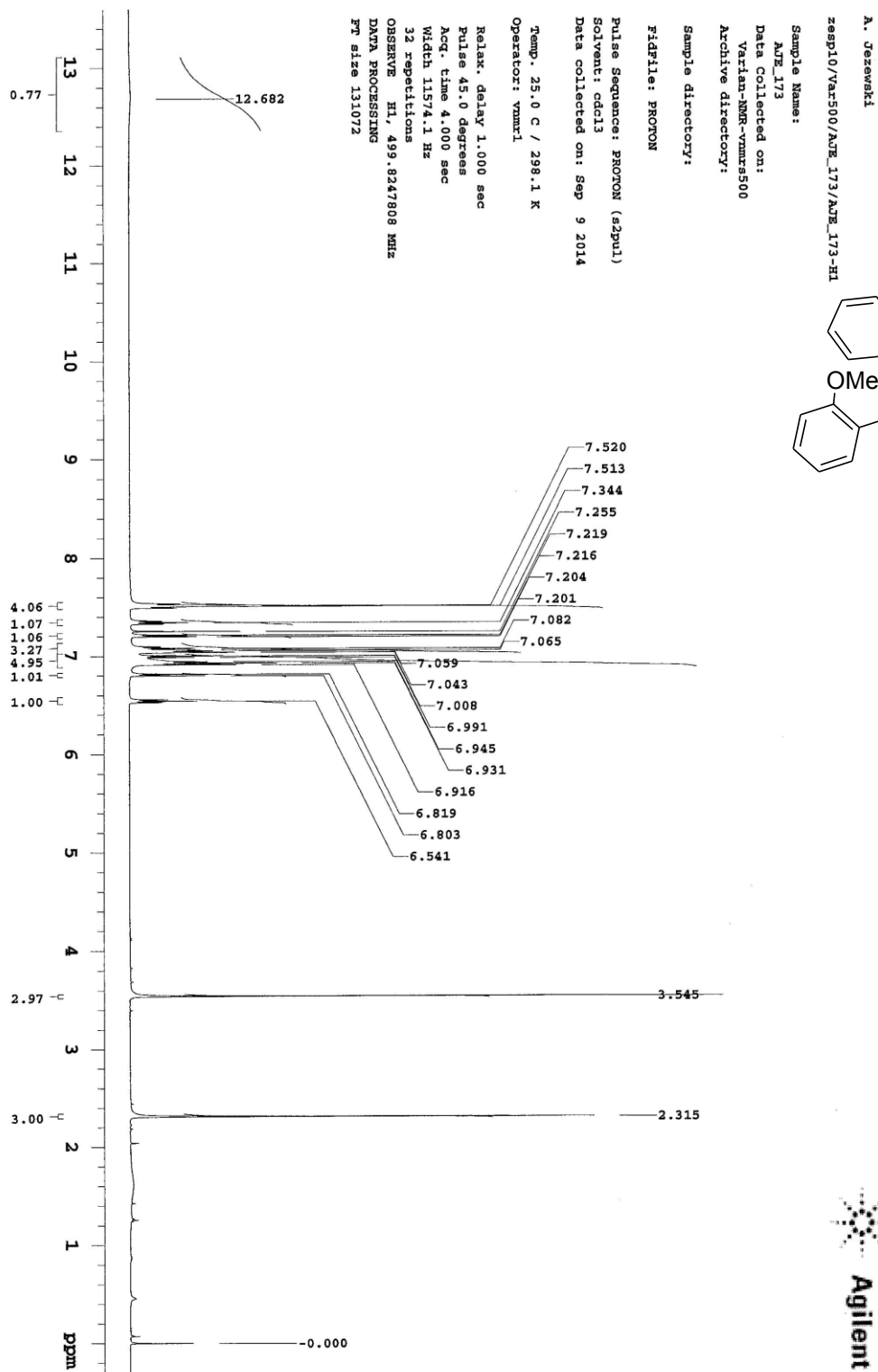


Fig. S-11. ¹H NMR spectrum of compound **9**.

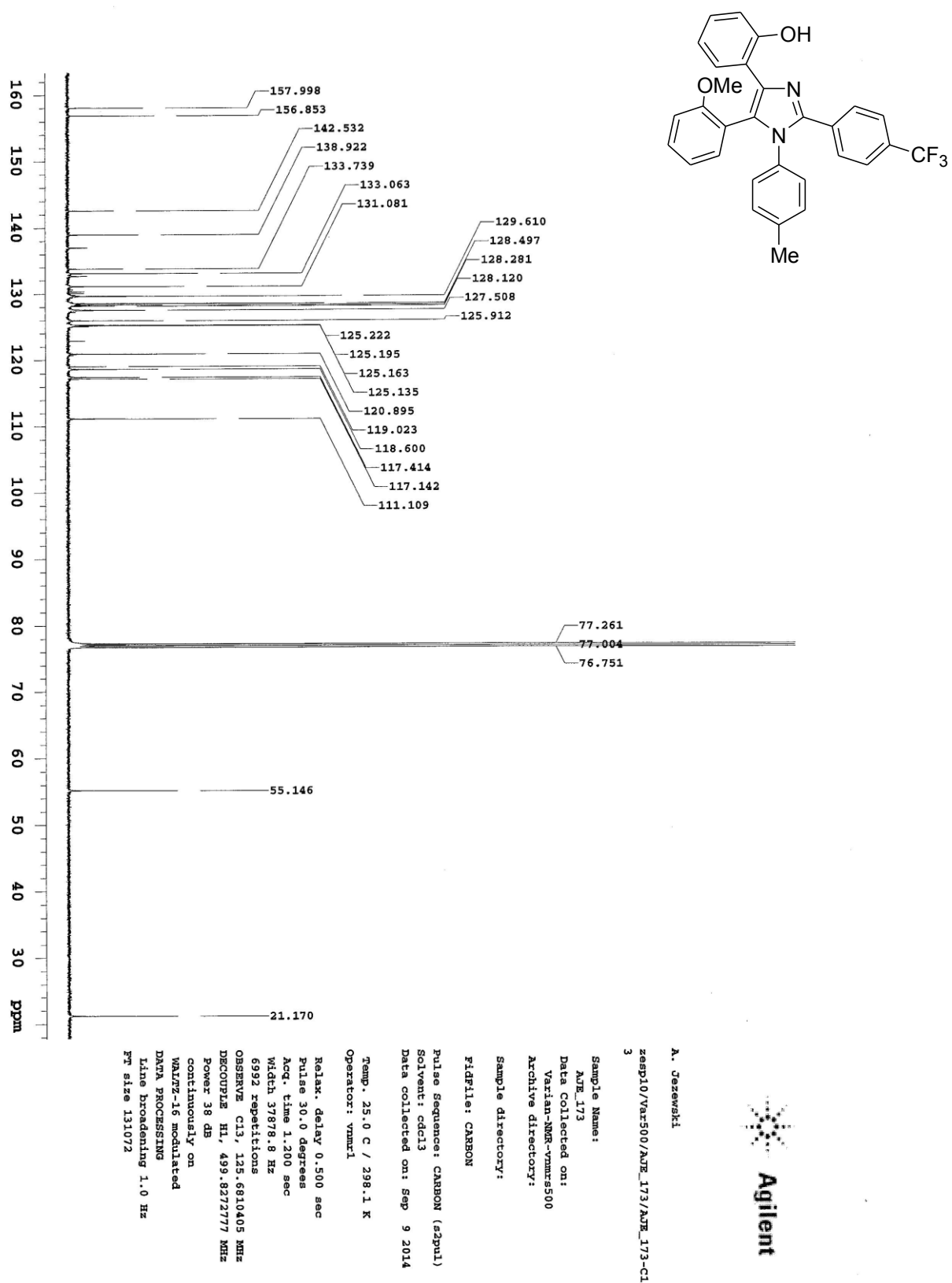


Fig. S-12. ¹³C NMR spectrum of compound 9.

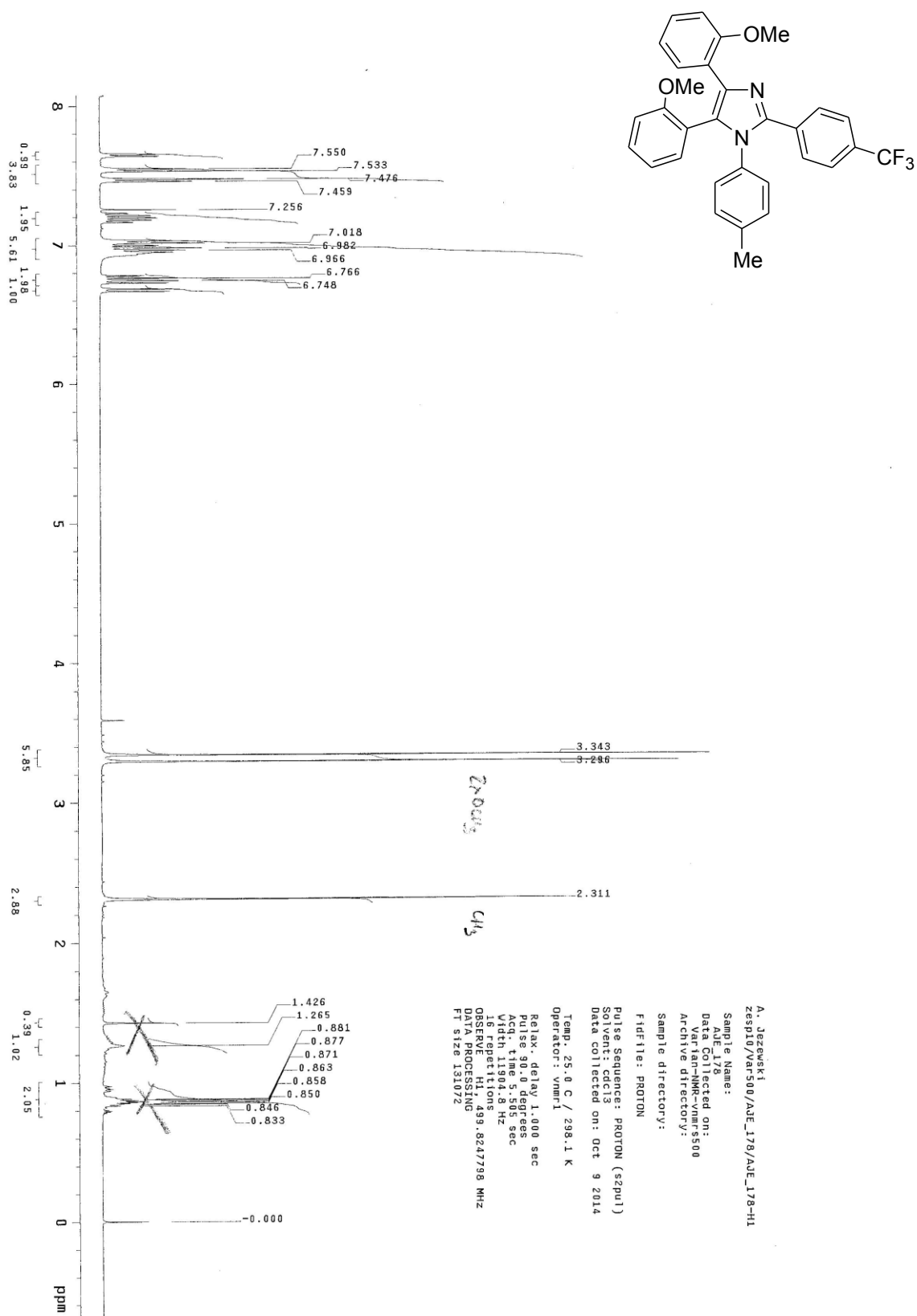


Fig. S-13. ^1H NMR spectrum of compound **11**.

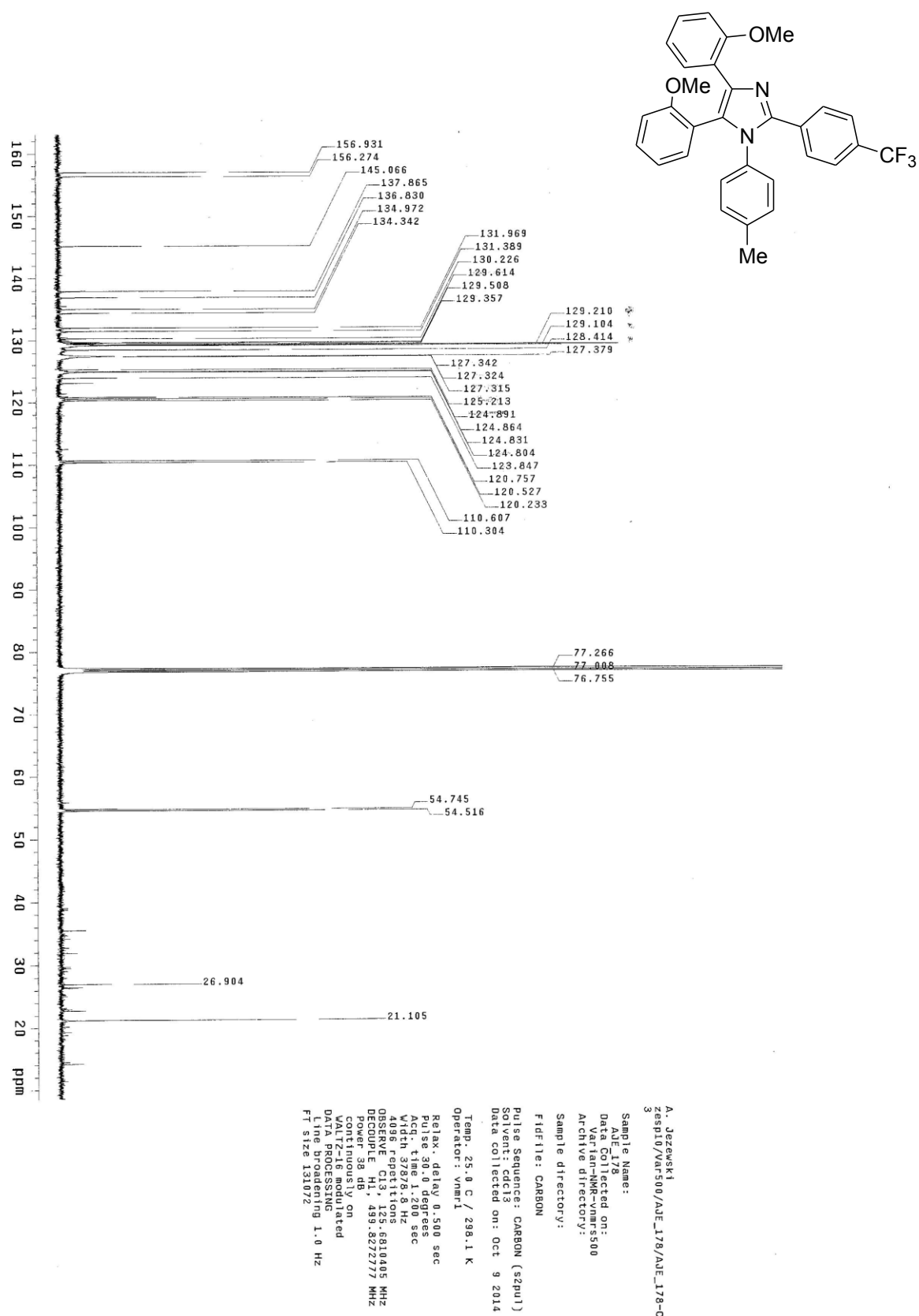


Fig. S-14. ^{13}C NMR spectrum of compound **11**.

X-ray structure determining of 4,5-Bis(2'-hydroxyphenyl)-1-(4-methylphenyl)-2-(4-trifluoromethylphenyl)-imidazole (6) Crystal data and measurement conditions are given in Table S-1. The structure was solved by the SHELXL-2014 (Sheldrick, 2014) program.

Table S-1. Crystal data and measurement conditions for 4,5-Bis(2'-hydroxyphenyl)-1-(4-methylphenyl)-2-(4-trifluoromethylphenyl)-imidazole (6)

Formula	C ₂₉ H ₂₁ F ₃ N ₂ O ₂
Molecular weight g/mol	486.48
Crystal system	monoclinic
a [Å]	16.6424(6)
b [Å]	9.3140(3)
c [Å]	17.8080(7)
β [deg]	99.221(2)
V [Å ³]	2724.70(17)
Molecular multiplicity	Z=4
Calculated density [g/cm ³]	1.242
Space group	P 1 21/n 1
Radiation (graphite monochromated)	Cu Kα
Wavelength [Å]	1.54178
Absorption coefficient [mm ⁻¹]	0.780
F(000)	1060
Crystal size [mm]	0.254 x 0.438 x 0.553
Temperature [K]	296(2)
Scan range (2θ) [deg]	66.593 – 3.967
Number of collected data:	
total measured	4806
unique [with / >2 σ]	3636
R	0.1504

X-ray structure determining of 4-(2'-Hydroxyphenyl)-5-(2'-methoxyphenyl)-1-(*p*-tolyl)-2-(*p*-trifluoromethylphenyl)-1*H*-imidazole (9) Crystal data and measurement conditions are given in Table S-2. The structure was solved by the SHELXL-2014 (Scheldrick 2014) program

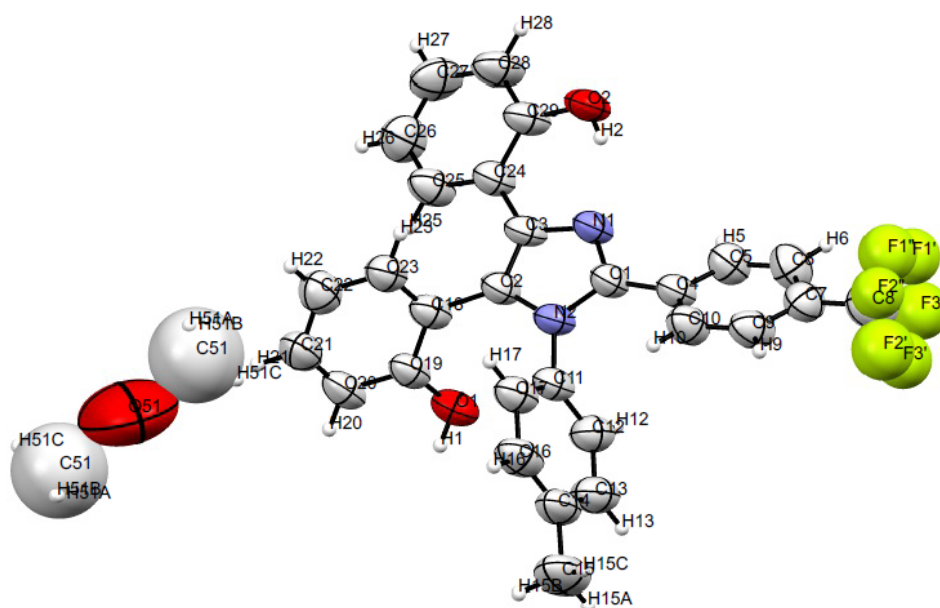


Figure S-5 Molecule structure of compound **6**

Table S-2. Crystal data and measurement conditions for 4-(2'-Hydroxyphenyl)-5-(2'-methoxyphenyl)-1-(p-tolyl)-2-(p-trifluoromethylphenyl)-1H-imidazole (**9**)

Formula	$C_{30}H_{23}F_3N_2O_2$
Molecular weight g/mol	500.51
Crystal system	monoclinic
a [Å]	12.476(2)
b [Å]	8.8085(15)
c [Å]	23.896(4)
β [deg]	103.508(6)
V [Å ³]	2553.4(8)
Molecular multiplicity	Z=4
Calculated density [g/cm ³]	1.302
Space group	P 1 21/c 1
Radiation (graphite monochromated)	Cu K α
Wavelength [Å]	1.54178
Absorption coefficient [mm ⁻¹]	0.808
F(000)	1040
Crystal size [mm]	0.100 x 0.113 x 0.220
Temperature [K]	296(2)
Scan range (2 θ) [deg]	66.578 – 3.644
Number of collected data:	
total measured	2054
unique [with / >2 σ]	440
R	0.0813

