Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supplementary Material

A Green Approach for the Synthesis of Bis (Substituted Sulfabenzamide) *para*-Benzoquinone Based on the Reaction of Sulfabenzamide with Electrochemically Generated *para*-Benzoquinone

Sadegh Khazalpour and Davood Nematollahi*

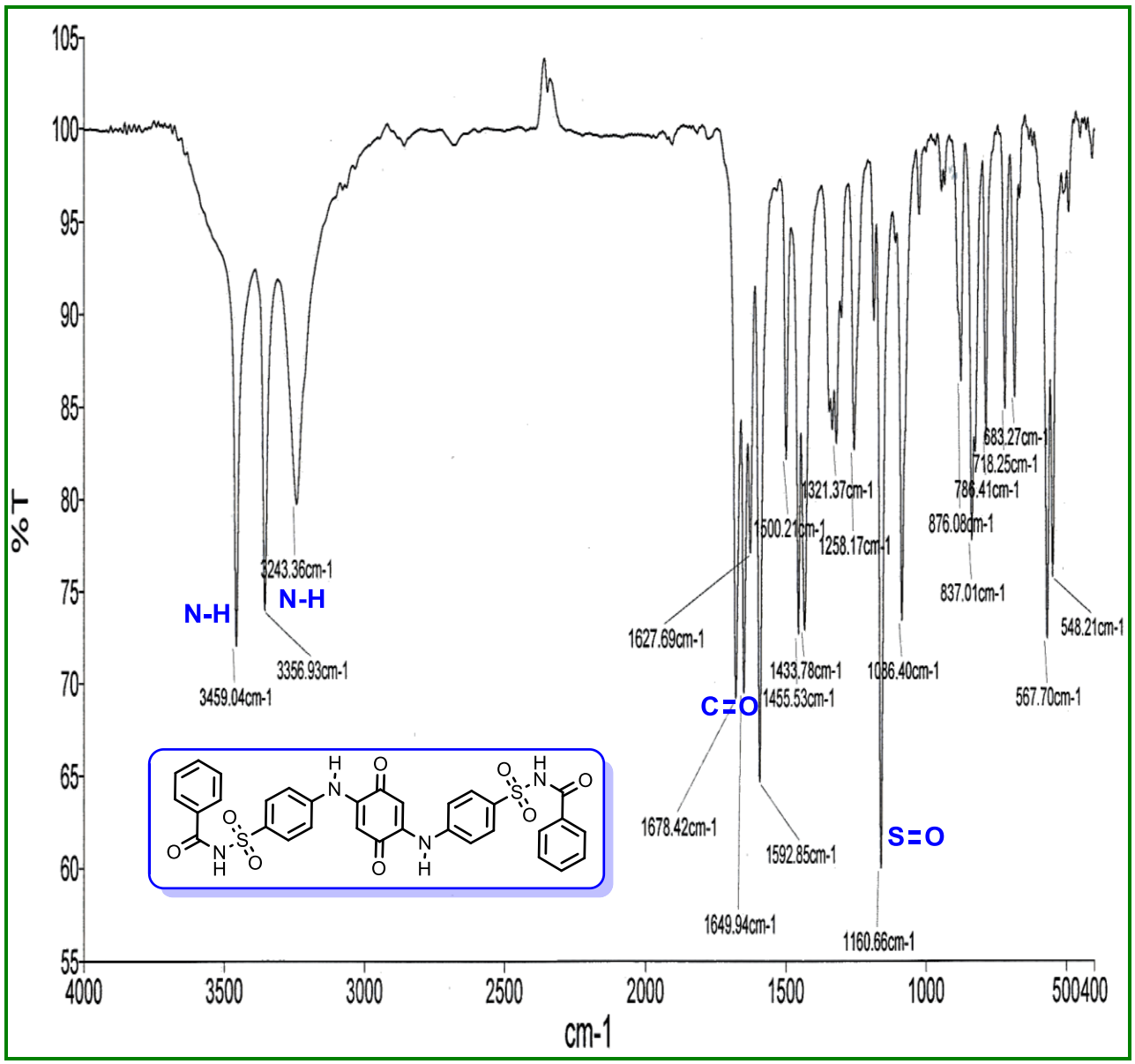
Faculty of Chemistry, Bu-Ali Sina University, Hamedan, Iran, Zip Code: 65178-38683. E-mail: nemat@basu.ac.ir, Fax:+98-811-8257407

Table of Contents:

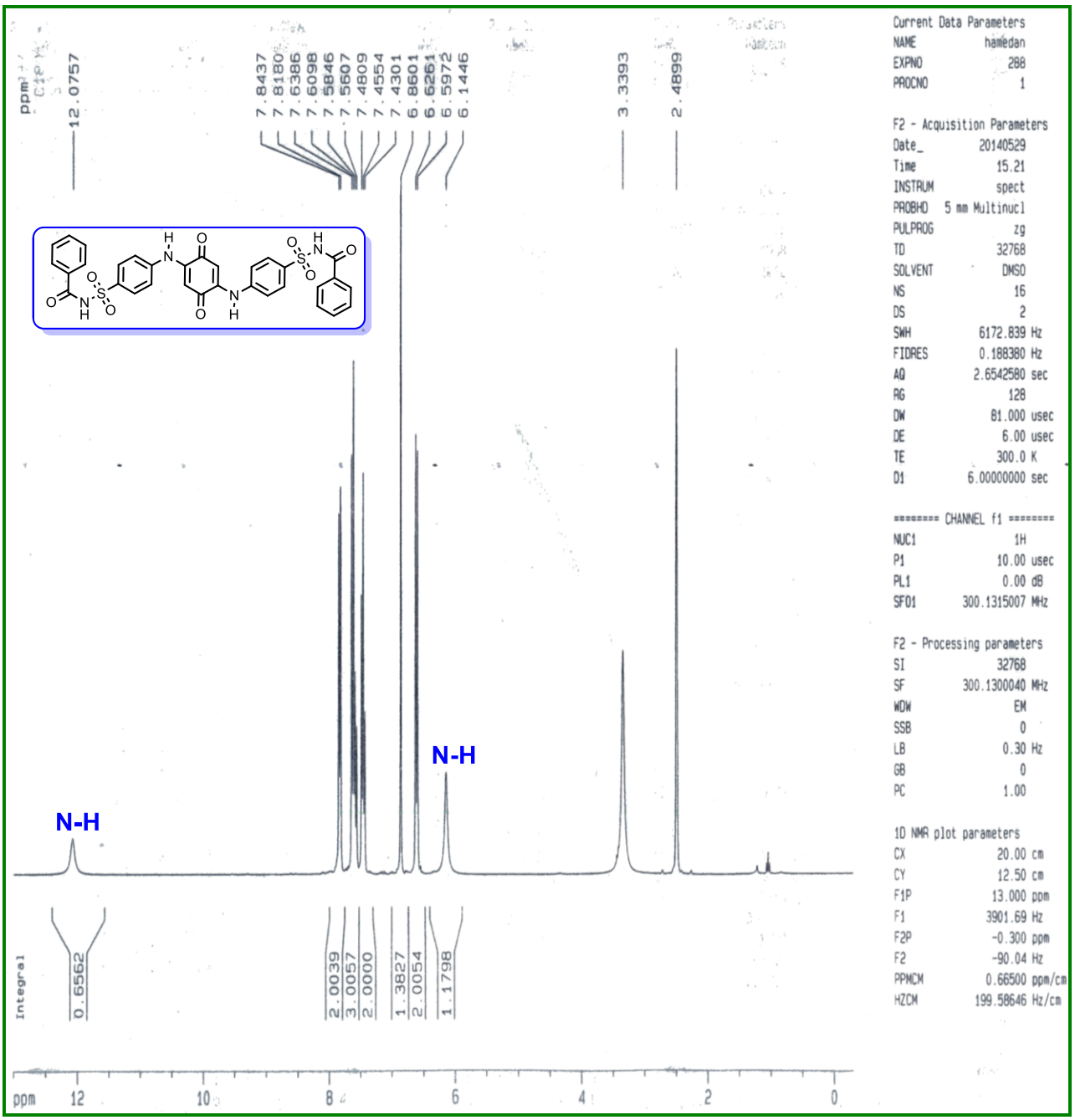
Electroorganic synthesis of *N,N'*-(4,4'-((3,6-dioxocyclohexa-1,4-diene-1,4-diyl)bis (azanediyl))bis(4,1-phenylenesulfonyl))dibenzamide (5) ($C_{32}H_{24}N_4O_8S_2$).

A mixture of phosphate buffer solution (*c* = 0.2 M, pH = 8.0)/ethanol mixture (50/50, v/v) containing hydroquinone (0.25 mmol) and sulfabenzamide (0.5 mmol) was subjected to electrolysis in a divided cell at 0.20 V versus Ag/AgCl. The electrolysis was terminated when the current decayed to 5% of its original value. At the end of electrolysis the precipitated solid was collected by filtration and was washed with *n*-hexane. The precipitated solid was recrystallized from methanol to give the compound **5** (isolated yield, 74%) as an orange solid, m.p: 184-185 ºC.^{1}H NMR (300 MHz, DMSO-d_6)δ/ppm: 6.14 (br, 2H, NH, D_2O exchangeable), 6.61 (d, *J* = 8.7 Hz, 4H, aromatic), 6.86 (s, 2H, quinone), 7.46 (t, *J* = 7.6 Hz, 4H, aromatic), 7.60 (m, 6H, aromatic), 7.83 (d, *J* = 7.7 Hz, 4H, aromatic), 12.0 (br, ~2H, NH, D_2O exchangeable). ^{13}C NMR (75 MHz, DMSO-d_6) δ/ppm:112.2, 123.7, 128.2, 128.5, 130.1, 131.9, 132.9, 136.6, 153.7, 165, 187.7 (C=O). IR (KBr) *v*/cm^{-1}: 3459 (NH), 3357 (NH), 3243 (NH), 1678 (C=O), 1628, 1650, 1592, 1500, 1455, 1434, 1321, 1258, 1161, 1086, 876, 837, 786, 718, 683, 568, 548. MS (EI, 70 eV); *m/z* (relative intensity): 658 (M + 2H) (3), 505 (22), 503 (23), 428 (100), 426 (100), 347 (14), 276 (94).

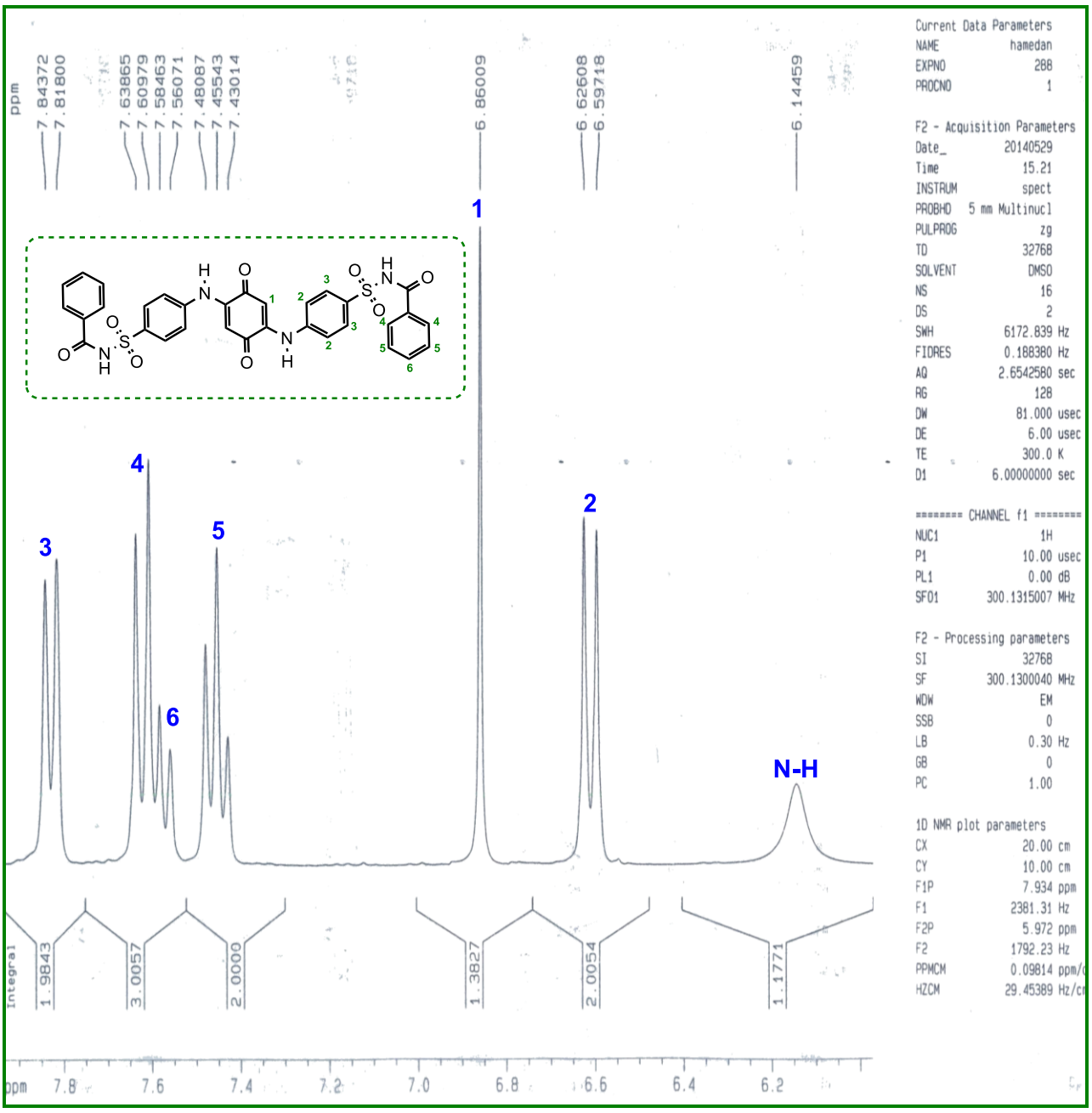
IR spectrum of 5



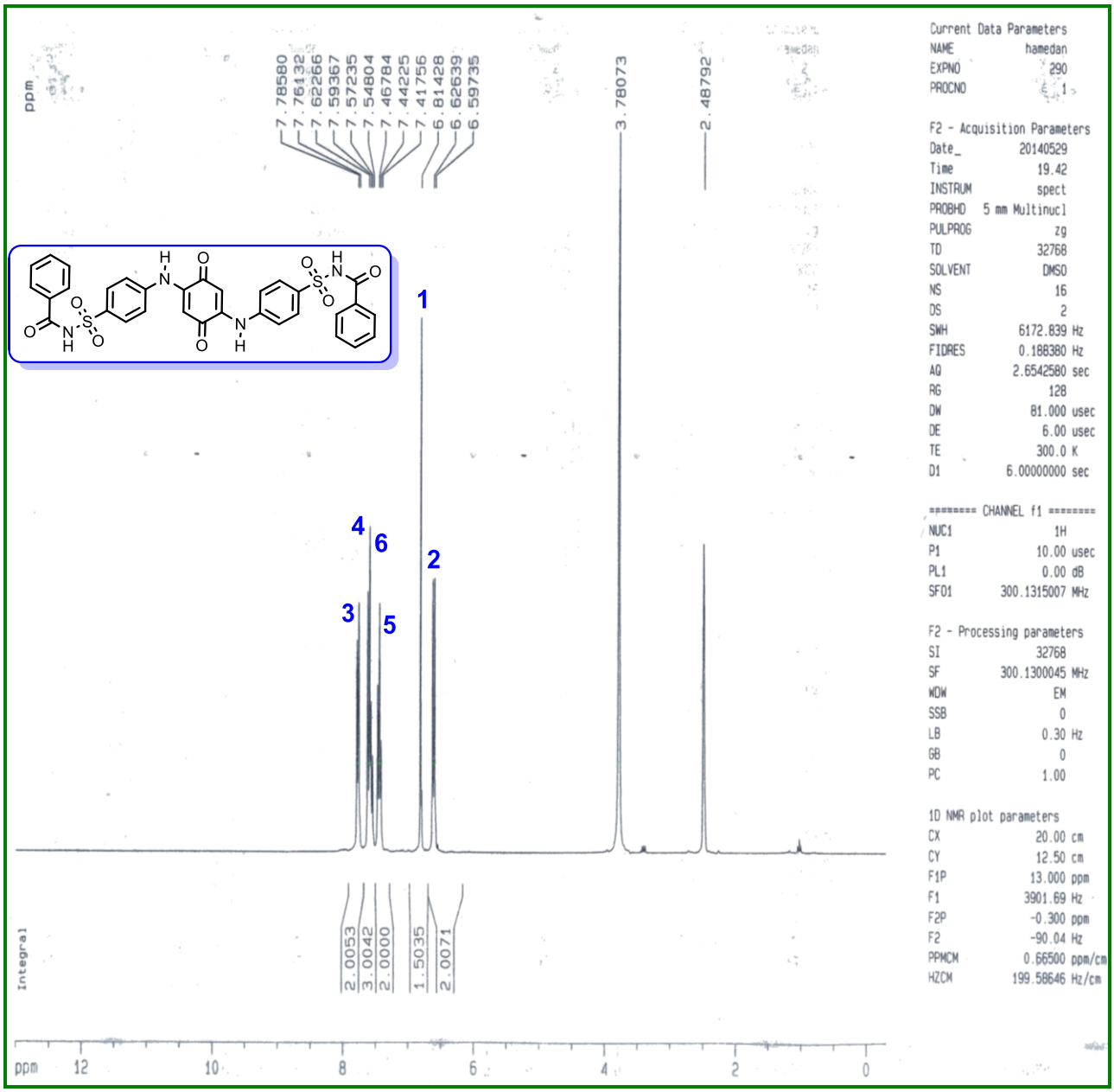
[1]HNMR spectrum of 5



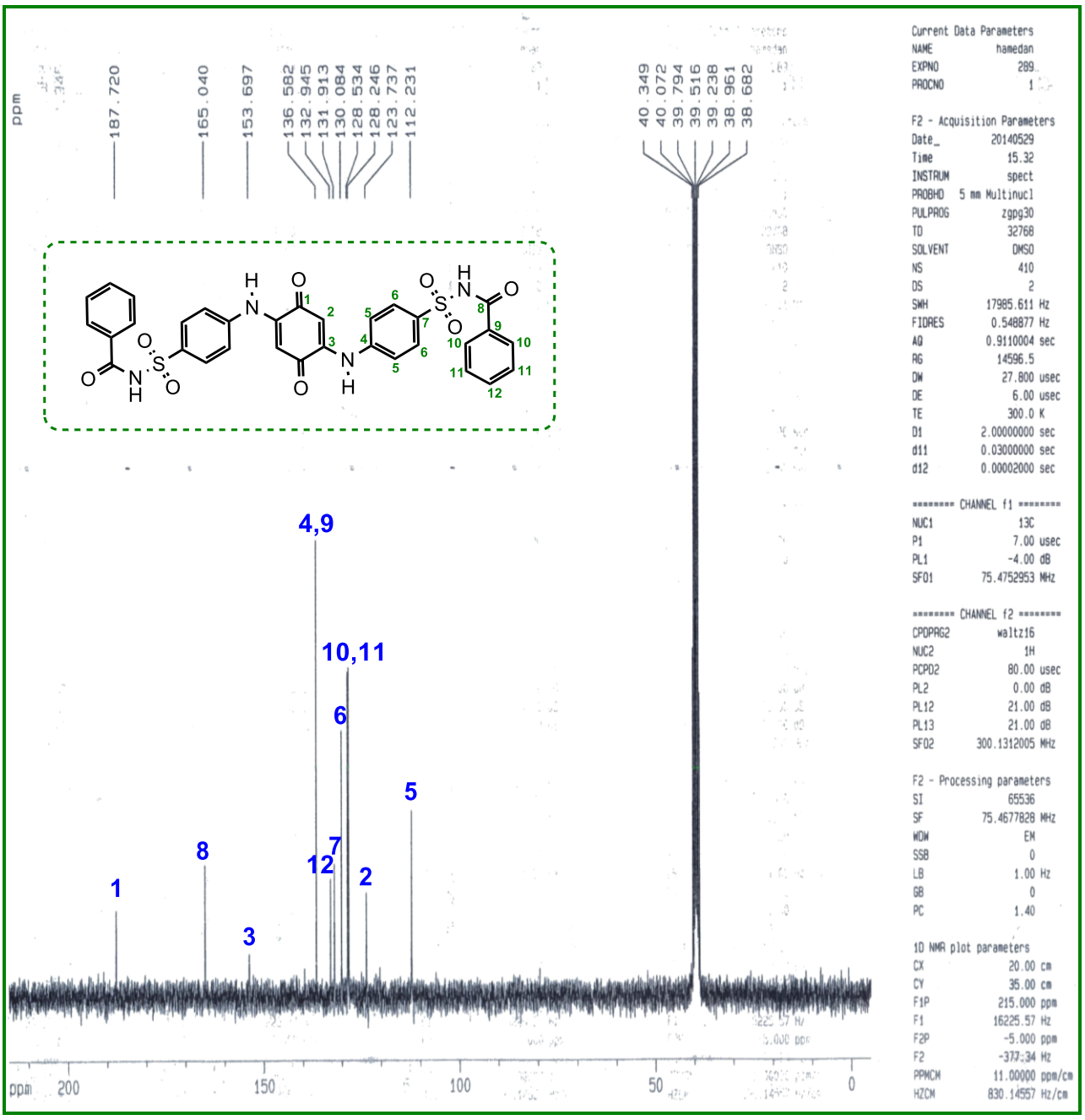
Expanded ^{1}H-NMR spectrum of 5



^{1}HNMR spectrum of 5 with D_2O



^{13}CNMR spectrum of 5



Mass spectrum of 5