Supplementary Information

A non-covalent complex based on catechol-benzoxazole moieties: Electrochemical Synthesis and Characterization

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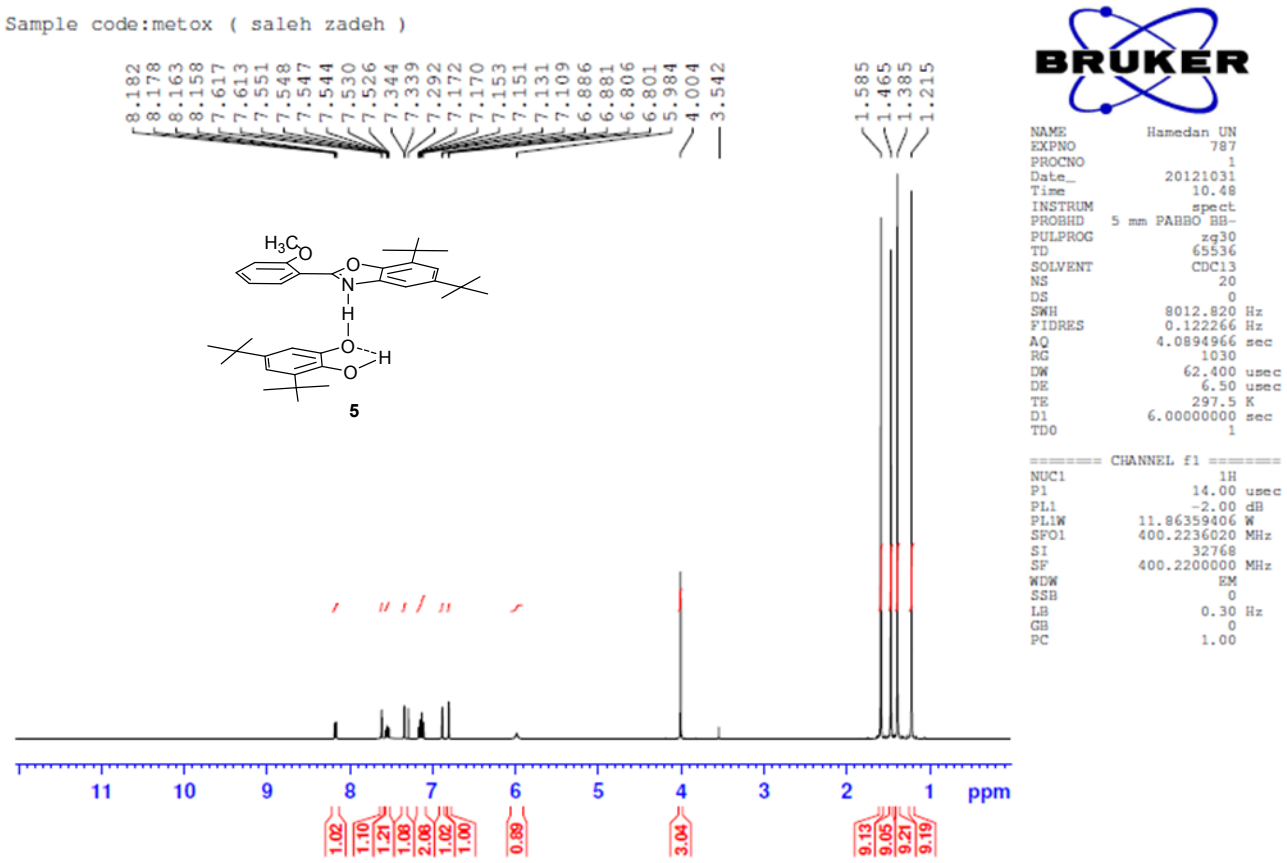
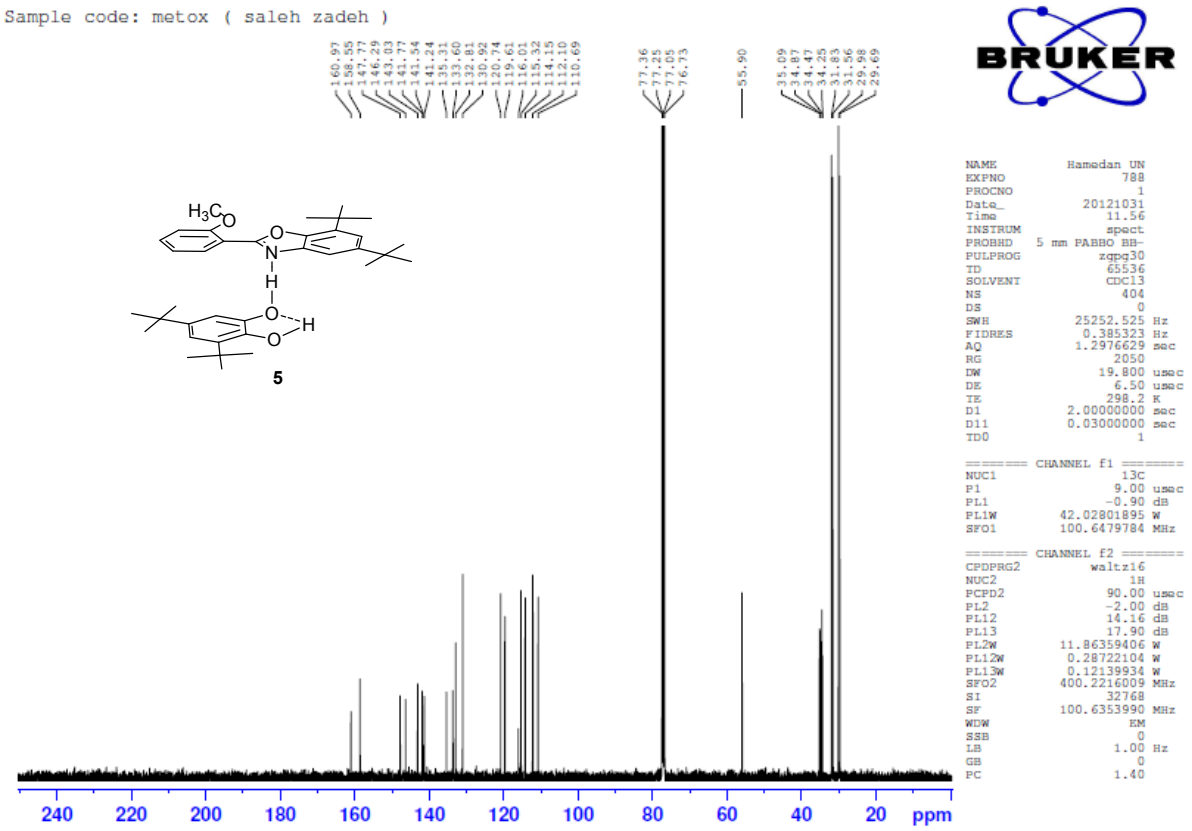
1. ^{1}H NMR spectrum of **5**

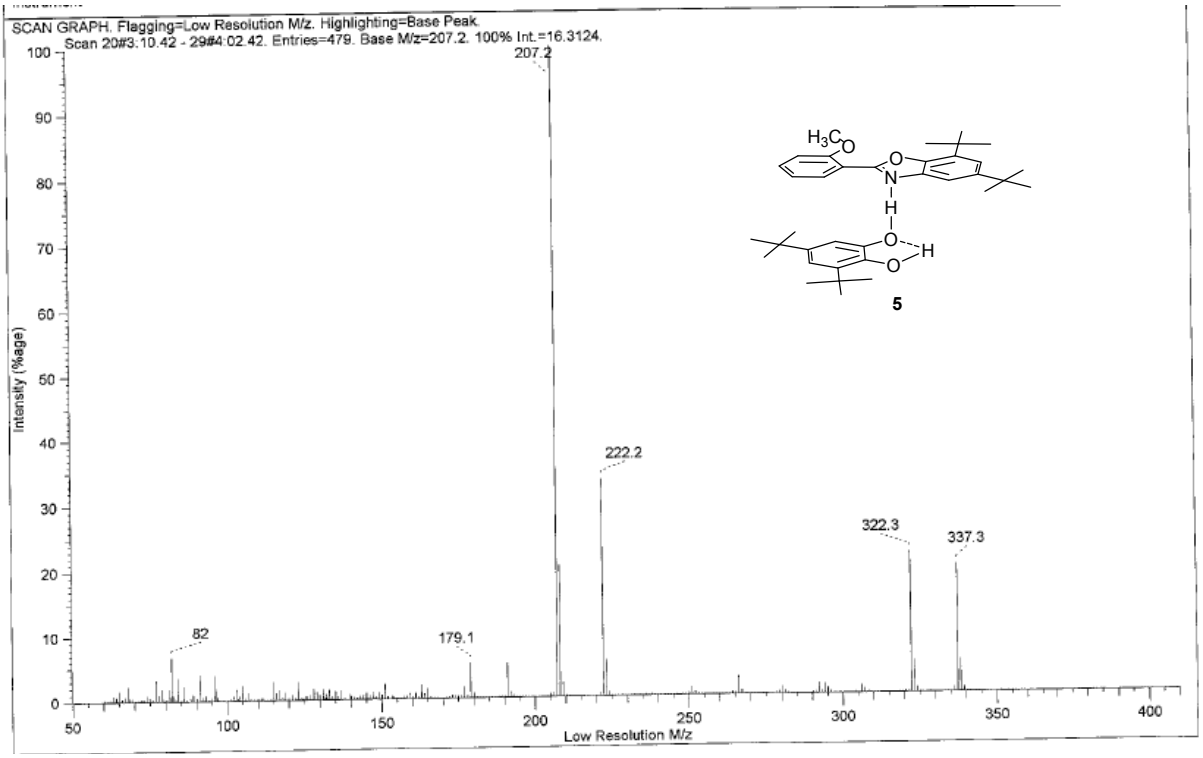


2. ^{13}C NMR spectrum of **5**

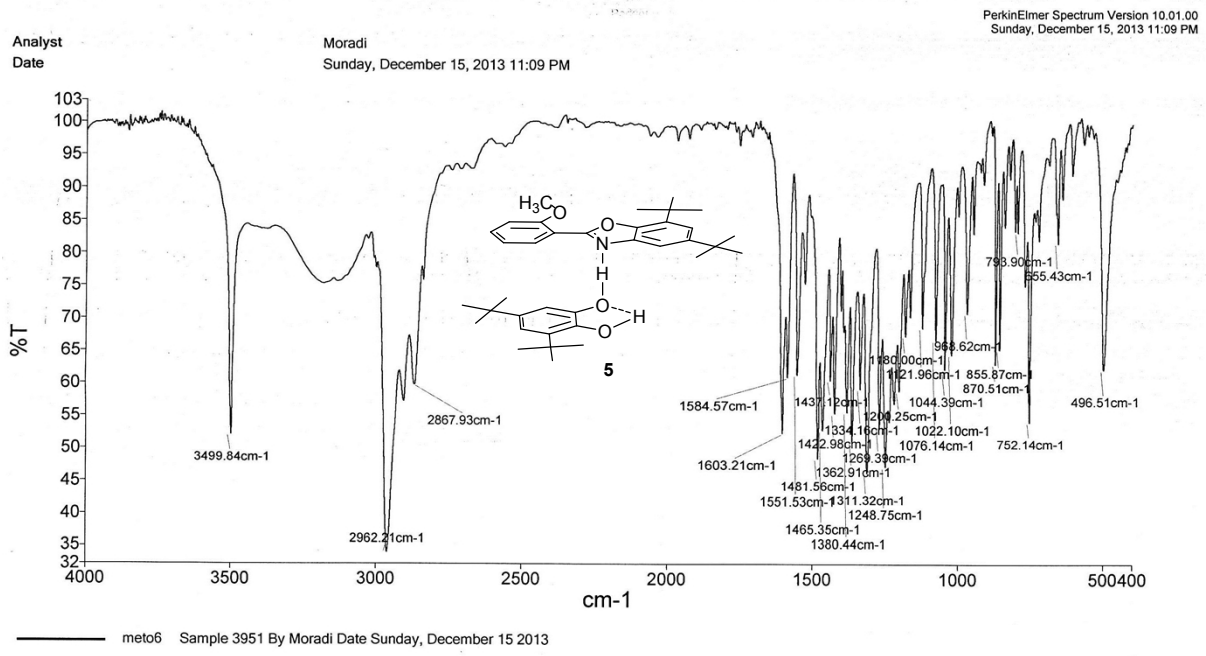


NAME	Hamedan UN
EXPNO	788
PROCNO	1
Date_	20121031
Time	11.56
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	404
DS	0
SWH	25252.525 Hz
FIDRES	0.385323 Hz
AQ	1.2976629 sec
RG	2050
DW	19.800 usec
DE	6.50 usec
TE	298.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.00 usec
PL1	-0.90 dB
PL1W	42.02801895 W
SFO1	100.6479784 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.00 dB
PL12	14.16 dB
PL13	17.90 dB
PL2W	11.86359406 W
PL12W	0.28722104 W
PL13W	0.12139934 W
SFO2	400.2216009 MHz
SI	32768
SF	100.6353990 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

3. M.S spectrum of **5**



4. FT-IR spectrum of **5**



5. X-Ray crystal data for **5**

(C_{36} H_{49} N_1O_4), M = 559.76, Monoclinic, a = 14.9211(6) Å, b = 9.5163(2) Å, c = 23.0981(9) Å, α = 90.00 °, β = 99.446(3) °, γ = 90.00 °, V = 3235.31(19) Å^3 ,T = 120(2) K, Space group P21/c, Z = 4, 18503 reflections measured, 7019 independent reflections (R_{int} = 0.0464). The final R_1 values were 0.0674 ($I > 2\sigma(I)$).The final $wR(F^2)$ values were 0.1554 ($I > 2\sigma(I)$).The final R_1 values were 0.0843 (all data).The final $wR(F^2)$ values were 0.1631 (all data). Absorption coefficient was 0.073 μ/mm, Radiation type was MoK\α, Goodness of fit on F^2 was 1.190. CCDC number CCDC 992193.

Compound reference	d:\determination\solution\c424\khc424
Chemical formula	C_{36} H_{49} N_1O_4
Formula Mass	559.76
Crystal system	Monoclinic
a/Å	14.9211(6)
b/Å	9.5163(2)
c/Å	23.0981(9)
α/°	90.00
β/°	99.446(3)
γ/°	90.00
Unit cell volume/Å^3	3235.31(19)
Temperature/K	120(2)
Space group	P21/c
No. of formula units per unit cell, Z	4
Radiation type	MoKα
Absorption coefficient, μ/mm^{-1}	0.073
No. of reflections measured	18503
No. of independent reflections	7019
R_{int}	0.0464
Final R_1 values ($I > 2\sigma(I)$)	0.0674
Final $wR(F_2)$ values ($I > 2\sigma(I)$)	0.1554
Final R_1values (all data)	0.0843
Final $wR(F_2)$ values (all data)	0.1631
Goodness of fit on F^2	1.190
CCDC	992193