Electronic Supplementary Information (ESI)

Green Electrochemical Strategy for One-step Synthesis of New Catechol Derivatives

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Spectroscopic characterizations of the electro- synthesized products (6, 7, and 8):

After purifications, all the electrochemical synthesized organic products were characterized by using FT-IR (Shimadzu FT-IR 8101 PC). \textsuperscript{1}H and \textsuperscript{13}C NMR spectra were recorded in DMSO-d\textsubscript{6} at 25 \textdegree C using a 300 MHz and 75 MHz Varian Mercury VX “NMR300” spectrometer, respectively. All chemical shifts for NMR spectra were measured in form of ppm with \( \delta \) units relative to TMS in DMSO-d\textsubscript{6} as an internal standard. Electron impact mass spectra were obtained at 70 eV using a GCMS-QP 1000 EX Shimadzu spectrometer. Both elemental analysis using elemental C,H,N,S Analyzer- Vario EL III Germany, mass (MS) and NMR spectra were carried out at the Microanalytical Center of Cairo University. Melting points (uncorrected) were recorded on melting point apparatus SMP 10. The results indicate that the formed electro-synthesized organic products are mainly depending on the nature of the nucleophilic reagent (3, 4, or 5) used. The spectroscopic data of the electrosynthesized products 6, 7 or 8 via Michael addition reaction are summarized as the following:
Product number 6:

Name: 4-(4-Amino-5-benzyl-4H-[1,2,4]triazol-3-ylsulfanyl)-benzene-1,2-diol

Data: Yellowish white crystals Yield: 0.26 g, 82.8 %, mp: 159 oC. IR spectrum (KBr) , ν, cm⁻¹: 3400 (br. OH), 3287, 3238 (NH₂), 3085 (CH-aromatic), 2935 (CH₂), 1624 (C=N); ¹H NMR (DMSO-d6) (δ ppm): 9.4 (br.s, 1H, OH), 9.1 (s, 1H, OH), 7.36-7.21 (m, 8H, Ar'H), 5.54 (s, 2H, NH₂), 4.02 (s, 2H, CH₂); ¹³C NMR spectrum (75 MHz, DMSO-d6) (δ, ppm): 28.55 (CH₂), 115.27, 120.72, 127.05, 127.19, 128.58, 128.88, 134.00, 134.12 (Ar-C), 144.01 (Ar-OH), 146.95 (Ar-OH), 151.53 (C=N), 160.91 (C=N); Ms: m/z 314 (M⁺). Anal. Calcd for C15H14N4O2S; C, 57.31; H, 4.49; N, 17.82; S, 10.20. Found: C, 57.92; H, 4.71; N, 17.16; S, 10.03.
FT-IR results for the product number 6.

![FT-IR Spectrum](image)

**Peak Find - S**

| No. | Position | Intensity | No. | Position | Intensity | No. | Position | Intensity |
|-----|----------|-----------|-----|----------|-----------|-----|----------|-----------|
| 1   | 3287.07  | 69.2151   | 2   | 3236.86  | 41.555    | 3   | 3150.15  | 42.7087   |
| 4   | 3085.55  | 38.0285   | 5   | 2935.13  | 43.8449   | 6   | 2769.28  | 77.87     |
| 7   | 1624.73  | 54.7206   | 8   | 1568.81  | 44.5516   | 9   | 1485.53  | 29.1785   |
| 10  | 1452.14  | 62.2401   | 11  | 1418.39  | 55.826    | 12  | 1336.43  | 63.7843   |
| 15  | 1294.07  | 51.3988   | 14  | 1048.12  | 71.4458   | 16  | 958.52   | 61.983    |
| 16  | 795.48   | 72.1685   | 17  | 755.959  | 53.242    | 18  | 730.889  | 39.2643   |
| 19  | 714.467  | 55.6365   | 20  | 694.248  | 35.1965   | 21  | 635.43   | 71.1816   |
| 22  | 567.534  | 75.892    | 23  | 542.863  | 69.7093   | 24  | 482.117  | 61.0154   |
MS results for the product number 6.
$^1$H NMR results for the product number 6.
$^{13}$C NMR results for the product number 6.
Product number 7:

Name: 5,6-(Diphenyl-[1,2,4]triazin-3-ylsulfanyl)-benzene-1,2-diol

Data: Pale yellow crystals, Yield: 0.23 g, 61.6 %, mp: 175 oC. IR spectrum (KBr), ν, cm⁻¹: 3430 (br. OH), 3050 (CH-aromatic), 1596 (C=N); ¹H NMR (DMSO-d6) (δ ppm): 9.04 (br.s, 2H, 2OH), 7.46-7.29 (m, 13H, Ar'H); ¹³C NMR spectrum (75 MHz, DMSO-d6) (δ, ppm): 113.88, 120.52, 121.00, 126.86, 128.47, 128.67, 132.12, 135.05 (Ar-C), 144.38 (Ar-OH), 147.17 (Ar-OH), 153.18 (C=N), 153.83 (C=N), 157.84 (N=C-S); Ms: m/z 373 (M⁺). Anal. Calcd for C21H15N3O2S; C, 67.54; H, 4.05; N, 11.25; S, 8.59. Found: C, 67.17; H, 4.86; N, 11.34; S, 8.06.
FT-IR results for the product number 7.
MS results for the product number 7.
$^1$H NMR results for the product number 7.
$^{13}$C NMR results for the product number 7.
Product number 8:

Name: 6-(3,4-Dihydroxy-phenylsulfanyl)-1H-pyrimidine-2,4-dione

Data: Brown crystals Yield: 0.2 g, 79.3 %, mp: 193 oC. IR spectrum (KBr), $\nu$, cm$^{-1}$: 3443 (br. OH), 1703 (C=O); $^1$H NMR (DMSO-d6) ($\delta$ ppm): 11.71 (br.s, 2H, 2OH), 11.08 (s, 1H, NH), 6.96-6.55 (m, 3H, Ar'H), 1.90 (s, 2H, CH$_2$); $^{13}$C NMR spectrum (75 MHz, DMSO-d6) ($\delta$, ppm): 31.83 (CH$_2$), 116.20, 120.72, 122.33, 127.69 (Ar-C), 145.32 (Ar-OH), 147.65 (Ar-OH), 162.36 (S-C=N), 166.55 (C=O), 167.98 (C=O); Ms: m/z 252 (M$^+$). Anal. Calcd for C$_{10}$H$_8$N$_2$O$_4$S; C, 47.61; H, 3.20; N, 11.11; S, 12.71. Found: C, 47.56; H, 3.13; N, 11.45; S, 12.49.
FT-IR results for the product number 8.
MS results for the product number 8.
$^1$H NMR results for the product number 8.
13C NMR results for the product number 8.