Research Article

SOHAG JOURNAL OF SCIENCES

https://doi.org/10.21608/sjsci.2022.164408.1033

Synthesis, Characterization, and PASSS Inet Prediction of New Polyesters

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Received: 22nd September 2022, **Revised:** 16th October 2022, **Accepted:** 26th November 2022.
Published online: 1st January 2023

Abstract: The interfacial polycondensation of indazole monomers **3** and **4** with various aromatic and aliphatic acid chlorides, including isophthaloyl-, terephthaloyl-, adipoyl-, and sebacoyl chloride, gave polyesters **5a-d** and **6a-d** containing an indazole moiety. The generated polyesters were categorized using elemental analysis, IR, ^{1}H-NMR, and MS spectra; XRD and Thermal Gravimetry analysis (TGA) examinations. Prediction of inflammatory biological behavior of selected polyesters using PASS Inet at Pa > 0.70, giving a high probability of anti-Gluconate 2-dehydrogenase (acceptor) inhibitor.
Keywords: Polyesters, Interfacial Polycondensation, TGA, PASS Inet, XRD, indazoles.

1. Introduction

Polymers such as polyester are composed of a unit containing two or more acidic groups and a unit containing two or more dihydroxy groups. When they have double bonds in their backbone are known as unsaturated polyesters (UP). Their usage and applications are expanded by their variety, processing flexibility, and low-cost unsaturated polyesters (UP) [1-3]. They have incredible uses, including in composites, polymer concrete, and fiber-reinforced plastics [4]. These uses demand excellent flexibility, thermal properties, and hardness [5-7]. The variety of tailoring polymer monomeric units leads to a wide range of their design. Specific physical characteristics, thermal stability, and high solubility are obtained when the polymer structure incorporates heterocyclic rings [8–11]. The addition of an indazoline ring to the main chain significantly affects the solubility and thermal stability as well as promotes the implementation of optoelectronic properties, including photorefractive and photoconductivity [12].

Our work's goal is to create novel polyesters **5a-d** and **6a-d** using the interfacial polycondensation method using the reaction of dihydroxy monomeric units that contain an indazoline ring, namely: 4-[3-(4-hydroxyphenyl)-2-phenyl-3,3a,4,5,6,7-hexahydro-2*H*-7-indazolylid-enemethyl]-phenol **(3)** and 4-7-[1-(4-hydroxy-3-methoxyphenyl)-methylidene]-2-phenyl-3,3a,4,5,6,7-hexahydro-2*H*-3-indazolyl-2-meth-oxyphenol **(4)** using various acid chlorides beside to examine the impact of the indazoline moiety on the characteristics of the polymer. Selected polyesters were examined for predicting inflammatory biological behavior using PASS Inet at Pa > 0.70, and giving a high probability of anti-Gluconate 2-dehydrogenase (acceptor) inhibitor.

2. Materials and method

2.1. Chemicals

All reagents were obtained from Fluka, Aldrich, and Merck and utilized without additional purification. Using percolated plates of silica gel G/UV-254 with a 0.25 mm thickness (Merck 60 F 254) and UV light (254 nm/365 nm) for viewing, all reactions were seen using thin layer chromatography (TLC). Using a Kofler melting point instrument, melting points were found and corrected. FT-IR-Bruker spectrometer was used to record the infrared spectra presented as cm^{-1} using the attenuated total reflection technique. Nuclear magnetic resonance spectra (^{1}H-NMR) were recorded on a Bruker Bio Spin AG spectrometer at 400 MHz in dimethylsulfoxide (DMSO-d_6) using TMS as an internal reference. XRD Diffraction was obtained at ambient temperature with D8 ADVANCED (BRUKER). XRD diffractometers were obtained by using Ni-filtered Cu Kα radiation. Thermo-gravimetric analyses (TGA) were studied in a nitrogen atmosphere by a thermal analyzer DuPont 2000 with a heating rate of 10.0 °C/min. Sebacoyl dichloride and adipoyl dichloride were freshly bidistilled at 182 °C/16 Torr and 125 °C/11 Torr, respectively, to produce isophthaloyl dichloride and terephthaloyl chloride (Aldrich) from *n*-hexane (m.p. 48 °C) and n-hexane (m.p. 81-82°C), respectively. Analytical grade NaOH. Without further crystallization, 4-hydroxy benzaldehyde, 4-hydroxy-3-methoxy benzalde- hyde, phenyl hydrazine (98%), cyclohexanone (Aldrich), and benzoyl chloride were used. All other materials were refined using standard methods and then used in high purity.

2.2. Synthesis of monomers

2.2.1. Synthesis of 4-[3-(4-hydroxyphenyl)-2-phenyl-3,3a,4,5,6,7-hexahydro-2*H*-7-indazolylidenmethyl]- phenol (3).

A mixture of phenylhydrazine (1.08 g, 0.01 mole) and 2,6-bis(4-hydroxybenzylidene) cyclohexanone (**1**) (3.06 g, 0.01 mole) methanol (100 ml) was stirred under reflux for 7 hrs. The

mixture was permitted to cool and was reserved at 0°C for 24 hrs. The formed product was filtered, washed with methanol, then with Petroleum-benzene 60-80°, and crystallized from dioxane. Yellow precipitated was obtained, yielding 88%, m.p. 260-262 °C. FT-IR (KBr, ν cm^{-1}); 3531 cm^{-1} (OH), 1605 cm^{-1} (C=N), 1590 cm^{-1} (C=C). ^{1}H-NMR (δ/ DMSO); 9.57- 9.54 (s, 2H, 2OH), 7.56 - 7.46 (m, 13H, Ar-H), 5.97 (s, 1H, C=CH), 3.57 (s, 1H, CH_a), 3.31 (s, 1H, CH_b), 2.82 (s, 2H, $2CH_{2e}$), 2.72 (s, 2H, $2CH_{2\ c}$), 1.83 (s, 2H, $CH_{2\ d}$. The mass spectrum exhibited a molecular weight at 396, which in matched with its molecular structure ($C_{26}H_{24}N_2O_2$). Anal. Calcd (Mol. Weight 396.49): H, 6.11 %, C, 78.75 %, N, 7.06 %. Found: H, 6.07 %,C, 78.73 %, N, 7.04 %.

2.2.2. Synthesis of 4-7-[1-(4-hydroxy-3 methoxyphenyl)-methylidene]-2-phenyl-3,3a,4,5,6,7-hexahydro-2*H*-3-indazolyl-2-methoxyphenol (4).

From 2,6-bis(4-hydroxy-3-methoxybenzylidene)-cyclohexanone (2), crystallized from methanol, yellow ppt., m.p 174-176 °C, yield 92%, FT-IR (KBr, ν cm^{-1}) 3531 (OH), 1590 (C=N) and 1516 cm^{-1} (C=C). ^{1}H-NMR (δ /DMSO): 8.93 (s, 2H, 2OH), 7.53- 6.53 (m, 11H, Ar-H), 6.02(s,1H, C=CH), 4.22 (s,1H, CH_a), 3.83-3.73 (s, 6H, $2OCH_3$), 3.46 (s, 1H, CH_b), 2.85 (s, 2H, $2CH_{2e}$), 2.76 (s, 2H, $2CH_{2\ c}$), 1.85(s, 2H, $CH_{2\ d}$). IR,). Anal. Calcd for ($C_{28}H_{24}N_2O_2$) (456.54): C, 73.66%, H, 6.17 %, N, 6.13 %. Found: C, 73.80 %, H, 6.30 %, N, 6.20.

2.3. Synthesis of Model polymers

2.3.1 General Method

A mixture of 4-[3-(4-hydroxyphenyl)-2-phenyl-3,3a,4,5,6,7-hexahydro-2*H*-7 indazolyliden-methyl]phenol **(3)** or 4-7-[1-(4-hydroxy-3-methoxyphenyl) methylidene]-2-phenyl-3,3a,4,5,6,7-hexahydro-2*H*-3-indazolyl-2-methoxyphenol **(4)** (5 mmol) in sod. hydroxide solution (10 mmol, 10 ml) was stirred at 25 °C for 2 hrs. Benzoyl chloride (10 mmol) was added carefully within 20 min. With continuous stirring for an additional 1.0 hr. The precipitated product was composed by filtration, washed with H_2O, dried, and recrystallization from the suitable solvent.

2.3.2. Synthesis of 1-phenylcarbonyloxy-4-[2-phenyl-3-(4-phenylcarbonyl-oxyphenyl)-3,3a,4,5,6,7-hexahydro-2*H*-7-indazol-ylidenmethyl]benzene (A)

The precipitate that formed was crystallization from benzene, yellow ppt, 87.07%, m.p. 200 °C, FT-IR (KBr, ν cm^{-1}): 1723 cm^{-1} (C=O (s) $_{ester}$), 1662 cm^{-1} (C=N), 1595 cm^{-1} (C=C). ^{1}H-NMR (δ/DMSO); 8.16 – 7.38 (m, 24 H, Ar + =CH), 4.48 - 4.42 (d,1H,Ha), 3.78- 3.43 (m,1H, Hb), 2.32-2.21 (t , 2H, He), 1.42-1.32 (m, 2H,Hc), 1.26-1.20 (m, 2H, Hd).

2.3.3. Synthesis of 2-methoxy-4-[3-(3-methoxy-4-phenylcarbonyl-oxyphenyl)-2-phenyl-3,3a,4,5,6,7-hexahydro-2*H*-7-indazolylidene-methyl]-1-phenylcarbonyloxybenzene (B)

The precipitate that formed was crystallization from benzene, yellow ppt, 87.07%, m.p. 200 °C, FT-IR (KBr, ν cm^{-1}):1735 cm^{-1} (C=O $_{(s)ester}$), 1596 cm^{-1} (C=N), 1515 cm^{-1} (C=C). ^{1}H-NMR (δ / DMSO); 8.4 (s,1H, =CH), 8.13 (s,2H, CH aromatic anisyl), 7.75 -7.11 (m,4H, Ar-H aromatic $_{anisyl}$), 7.13-6.70 (m,15H, Ar-H aromatic), 3.84 (S, 6H, $2OCH_3$), 4.52-4.43 (d,1H,Ha), 3.79-3.4 (m,1H, Hb), 2.30-2.23 (t , 2H, He), 1.40-1.32 (m, 2H,Hc), 1.24-1.18 (m, 2H, Hd).

2.4. Synthesis of Polymers 5a-d and 6a-d.

In a 3-necked flask containing a desiccated N_2 inlet-outlet, and condenser, dropping funnel, a mixture of 4-[3-(4-hydroxyphenyl)-2-phenyl-3,3a,4,5,6,7-hexahydro-2*H*-7-indazolyliden-methyl]phenol **(3)** (0.01 mol, 3.97g) or 4-7-[1-(4-hydroxy-3-methoxy-phenyl)methylidene]-2-phenyl-3,3a,4,5,6,7-hexahydro-2*H*-3-indazolyl-2-methoxy-phenol **(4)** (0.01 mol, 4.56 g), methylene chloride (25 ml) and sodium hydroxide solution (0.02 mol, 0.8 g in water 100 ml) was mechanically stirred at room temperature for 1 hr. The selective acid chloride (0.01 mol); isophthaloyl– (2.03 g), terephthaloyl- (2.03 g), adipoyl- (1.46 g), and sebacoyl dichloride (2.1 ml) in methylene chloride (5 ml) was added over a period of 120 s. at ambient temperature with strongly stirred. The precipitated polymer generated during the churning was filtered, washed with hot water, hot methanol, then hot acetone, and dried under condensed pressure. The results are summarised as follows:

Polymer 5_a:

FT-IR (KBr, ν cm^{-1}): 1596 (C=N), 1498 (C=C), 1735 (C=O), 2928 ($CH_{aliphatic}$), 3020 (CH- aromatic). ^{1}H-NMR (DMSO-d_6) : 7.24 – 6.71 (m, 17 H, 13H, Ar- H + 4H , Ar-H of isophthalate), 6.02 (s, 1H, C = CH), 3.60 (broad signale, 1H, CH_a), 2.31 (broad signale, 1H, CH_b), 1.88 (broad signal, 2H, CH_{2e}) , 1.64 (broad signale, 2H , CH_{2C}), 1.25 (broad signale, 2H, CH_{2d}) .

Polymer 5_b:

FT-IR (KBr, ν cm^{-1}): 1597 (C=N), 1497 (C=C), 1733 (C=O), 2932 ($CH_{aliphatic}$), 3060 (CH- aromatic).

Polymer 5_c:

FT-IR (KBr, ν cm^{-1}): at 1597 (C=N), at 1500 (C=C), at 1750 (C=O), 3051 (Ar-H stretch). at 2928 (CH $_{aliphatic}$), ^{1}H-NMR (DMSO-d_6) : 7.78 – 7.06 (m, 13 H, Ar- H) , 6.07 (s, 1H, C = CH), 2.89 (broad signal, 7H, (CH_{2e} +2 CH_2CO + CH_a), 2.64 (broad signal, 3H, CH_{2c} + CH_b), 1.79 (broad signal, 6H, CH_{2d} + 2 CH_2CO).

Polymer 5_d:

FT-IR (KBr, ν cm^{-1}): 1598 (C=N), 1498 (C=C), 1750 (C=O), at 3059 (Ar-H stretch), 2934 (CH $_{aliphatic}$),.^{1}H-NMR (DMSO-d_6): 7.77 – 7.05 (m, 13 H, Ar- H) 6.05 (s, 1H, C = CH), 2.85 (broad signal, 4H, $2CH_2CO$), 2.60 (broad signal, 3H, CH_{2e} + CH_a), 2.10 (broad signal, 3H, CH_{2c} + CH_b), 1.66 (broad signal, 6H , CH_{2d} + 2 CH_2CO) , 1.39 (broad signal, 8H, 4 CH_2CO).

Polymer 6_a:

FT-IR (KBr, ν cm^{-1}): 1597 (C=N), 1499 (C=C), 1740 (C=O), 3062 (Ar-H stretch), 2932 (CH $_{aliphatic}$). ^{1}H-NMR (DMSO-d_6): 7.87 – 6.82 (m, 15 H, 11H Ar- H + 4H, Ar-H of isophthalate), 6.14 (s, 1H, C = CH), 3.93 (broad signal, 1H, CH_a), 3.83-3.76 (6H, $2OCH_3$), 2.17 (broad signal, 1H, CH_b), 1.73 (broad signal, 2H, CH_{2e}) , 1.51 (broad signal, 2H, CH_{2C}), 1.24 (broad signal, 2H, CH_{2d}).

Polymer 6b:

FT-IR (KBr, ν cm^{-1}): 1595 (C=N), 1499 (C=C), 1738 (C=O), 3063 (Ar-H stretch), 2930 ($CH_{aliphatic}$).

Polymer 6c:

FT-IR (KBr, ν cm^{-1}): 1596 (C=N), at 1498 (C=C), at 1754 (C=O), 3051 (Ar-H stretch), 2932 ($CH_{aliphatic}$),^{1}H-NMR (DMSO-d_6) : 7.55 – 6.80 (m, 11 H, Ar- H) , 6.06 (s, 1H, C = CH), 3.80- 3.72 (6H, 2OCH_3), 2.64 (broad signal, 7H, CH_{2e} + 2CH_2CO+ CH_a), 2.08 (broad signal, 3H, CH_{2C} + CH_b), 1.79 (broad signal, 6H , CH_{2d} + 2 CH_2CO) .

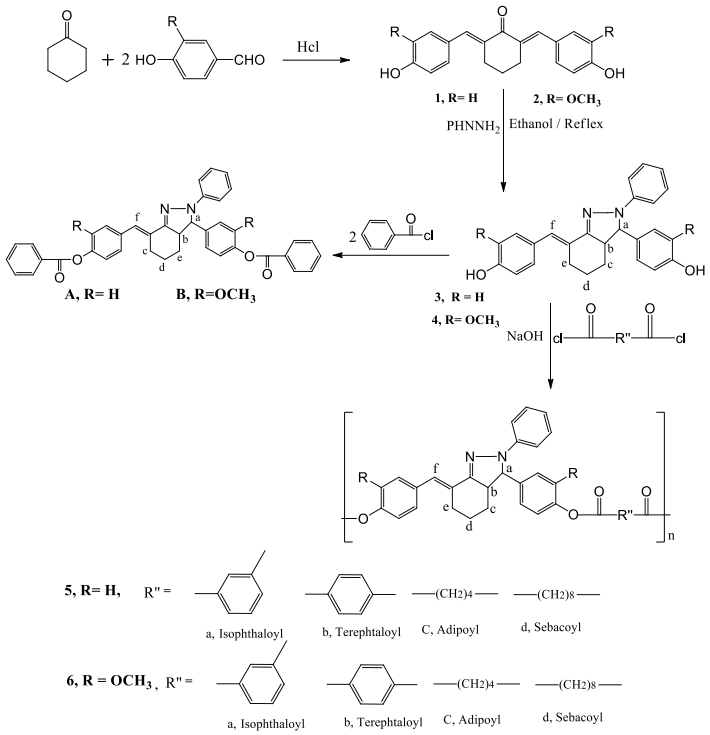
Polymer 6d:

FT-IR (KBr, ν cm^{-1}): at 1598 (C=N), at 1499 (C=C), at 1761 (C=O), at 3051 (Ar-H stretch), 2932 ($CH_{aliphatic}$),^{1}H-NMR (DMSO-d_6) : 7.55 – 6.80 (m, 11 H, Ar- H) 6.07 (s, 1H, C = CH), 3.82- 3.65 (6H, 2OCH_3), 2.55 (broad signal, 7H, CH_{2e} + 2CH_2CO + CH_a), 2.10 (broad signal, 3H, CH_{2c} + CH_b), 1.67 (broad signal, 6H , CH_{2d} + 2 CH_2CO) , 1.37 (broad signal, 8H , 4 CH_2CO).

3. Results and discussion

3.1. Chemistry

Reaction between 4-hydroxybenzaldehyde or 4-hydroxy-3-methoxybenzaldehyde with cyclohexanone (1:2) in ethanol as solvent and passing HCl gas, condensation products: 2,6-bis(4-hydroxybenzylidene) cyclohexanone (**1**) and 2,6-bis(4-hydroxy-3-methoxy-benzylidene) cyclohexanone (2) were given. New monomers 4-[3-(4-hydroxyphenyl)-2-phenyl-3,3a,4,5,6,7-hexa-hydro-2*H*-7- indazolylidenemethyl] phenol **(3)** and 4-7[1-(4-hydroxy-3methoxyphenyl)methyldene]-2-phenyl-3,3a,4,5,6,7-hexahydro-2*H*-3-indazolyl-2-methoxyphenol **(4)** based on indazoline moiety were prepared by condensation of 2,6–bis(4-hydroxybenzylidene) cyclohexane (**1**) or 2,6–bis(4-hydroxyl-3-methoxybenzylidene) cyclohexane **(2)** with phenyl hydrazine in ethanol (Scheme 1). The mass spectrum of compound **3** at 396 is displayed the molecular weight of the molecule formula ($C_{26}H_{24}N_2O_2$). The interaction of 4-[3-(4-hydroxyphenyl)-2-phenyl-3,3a,4,5,6,7-hexahydro-2H-7-indazolylidenmethyl] phenol (**3**), or 4-7-[1-(4-hydroxy-3 methoxyphenyl)methylidene]-2-phenyl-3,3a,4,5,6,7-hexahydro-2H-3-indazolyl-2-methoxyphenol (**4**) with different aromatic and aliphatic diacid chlorides e.g. isophthaloyl-, terephthaloyl-, adipoyl- and sebacoyl chloride using interfacial polycondensation technique in presence of benzyltriethylammonium chloride as base give unsaturated polyesters 5a-d and 6a-d (**13-15**). Model compounds (**A, B**) were synthesized by reaction of the monomer 4-[3-(4-hydroxyphenyl)-2-phenyl-3,3a,4,5,6,7-hexahydro-2*H*-7 indazolylidenmethyl] phenol (3) (1 mol) or 4-7-[1-(4-hydroxy-3methoxyphenyl) methylidene]-2-phenyl-3,3a,4,5,6,7-hexa-hydro-2*H*-3-indazolyl-2-methoxyphenol (4) (1mol) with benzoyl chloride (two moles) in sodium hydroxide solution with stirring at 25 °C. The structure of the resulting polymers was established from elemental and spectral analysis. The FI-IR, and ^{1}H-NMR spectra of all polyesters showed the disappearance of the characteristic absorption band of the OH group and showed the appearance of new bands at 1733- 1762 ($C=O_{ester}$) and 1120 – 1100 cm^{-1} (C – O- C) groups; 1595 – 1597 cm^{-1} for C=C groups and other characteristic absorption bands in various polyesters 5a-d and 6a-d (see experimental).



Scheme **1**. Synthesis of polymers 5a-d, 6a-d

3.2. Polymers characterization

3. 2.1. XRD measurements

The produced polymers' crystallinity grade is identified using the XRD diffraction method . Figs. **1A** and **1B** The XRD of 5a-d & 6a-d has few reflection peaks with an intermediate crystalline/amorphous structure, and 6a-d polyesters have more amorphous structure overall. The broad range of orientation in these structures, which are transitional between the ordered crystalline states (marked long-range order) in the organization of their atoms as well as molecules, is what causes the interference that has been seen in the area 2 θ = 5-60°. Additionally, the presence of polar groups like C=O, N-N, and C=N as well as high C=C bond heights impart some order to polymer chains. Additionally, the presence of polar groups like C=O, N-N, and C=N as well as high C=C bond heights, lend some order to polymer chains. In particular, the polymer's indazoline ring confers some stiffness and tends to promote.
More specifically, compared to polyesters based on diarylidenecycloalkanones, the polymer's indazoline ring provides some rigidity and seems to facilitate the packing of the material to build crystalline forms. [**16**]. The less dense packing of the unsymmetrical polymer units in its backbone causes the amorphous appearance. Additionally, the methoxy groups found in polyesters 6a-d influence the structure's orientation, resulting

in a degree of space between the units, a decrease in crystallinity, and a widened peak in the hologram. $(CH_2)_8$ are found in **5d** and **6d** polymers, which raise their flexibility, mutual attraction, and random coiling of adjacent chains that result in tiny crystalline peaks. An additional characteristic is shown within each group of **5a-d** and **6a-d**, where higher ordering is seen in the polymers 5b and 6b, including terephthaloyl moiety; this, thanks to its geometrical structure, is once more helping with the arranging and packing. [17].

3.2.2. Thermal Gravimetric Analysis (TGA):

TGA was used to evaluate the thermal behaviour of the polyesters 5a-d and 6a-d while heating them at a rate of 10°C per minute in nitrogen. The temperatures for various percent weight losses are provided by the thermographs of these samples (form 0 to 600C^0). When the temperature ranges from 70 °C to 240 °C, the loss of moisture and entrapped solvents occurs first, resulting in a smaller weight loss of 2.0- 5.0%. The temperature at which these polymers begin to break down (10% loss) is known as the polymer decomposition temperature (PDT). For all samples, the temperature range between ~272 °C and ~370 °C corresponds to these substances' initial (10% loss) break down . Similar decomposition patterns were shown by all of the produced polymeric compounds. For polyester 5a, it has been found that slow mass-loss occurs between ~ 276.8 °C and ~377.5 °C (-13.03%) in the initial. and quick mass loss (-57.32%) between ~408.4 and 600 °C (-57.32%) in the second Polyester 5b experiences mass loss between ~82.8 °C and ~138.6 °C (-6.05%) in the initial area and between ~182.4 °C and ~285.7 °C (-9.2%) in the second region. The quick mass loss in the third region is between ~ 302.88 °C and 600 °C (-41.06%). Polymer 5c is seen to be rapid between ~238.31 and ~331.55 °C (-37.37 %). In the first region, between ~351.37 and 510.52 °C (- 62.5%), polymer 5d, there was a slow mass loss between ~270.8 and 385.8 °C (-12.63 %), and there was a rapid mass loss between ~408.5 and 600°C (-70.4%) in the second area. Table **1** and Fig. **2** show that the polymers made from aromatic diacid chloride 5a,b are more thermally stable than those made from aliphatic diacid chloride 5c,d.

For polymer 6a, the mass loss is between ~293.5 and 422.02 °C (-39.27%) in the initial area and between ~436.6 and 600 °C (-55.3%) in the second district. In the first section of polymer 6b Fig. **2**, the mass loss is between ~272.24 °C and 412.60 °C (-26.83%), while in the second region, it is between ~439.78 °C and 600 °C (-91.63 %).

For polymer 6c, the mass loss is quick between ~233.20 and 392.60 °C (-50.49 %) in the first zone and ~424.72 and 600°C (-63.72%) in the second region. Polymer 6d shows the mass loss between ~ 316.32 and 427.43 °C (-47.02 %) in the first area and between ~ 455.55 and 519.76 °C (-59.2 %) in the second. In the third region, between ~ 551.94 °C and 600 °C (- 67.67%), there is a quick mass loss.

These polyesters exhibit high thermal stability and have a high char yield at 600 °C due to side reactions, such as double addition during pyrolysis, which increase chain linking. Polyesters 6a-d that contain (OCH_3) also exhibit better thermal stability because the (OCH_3) functions as a barrier, promotes crosslinking, and delays the chain's breakdown. [18, 19].

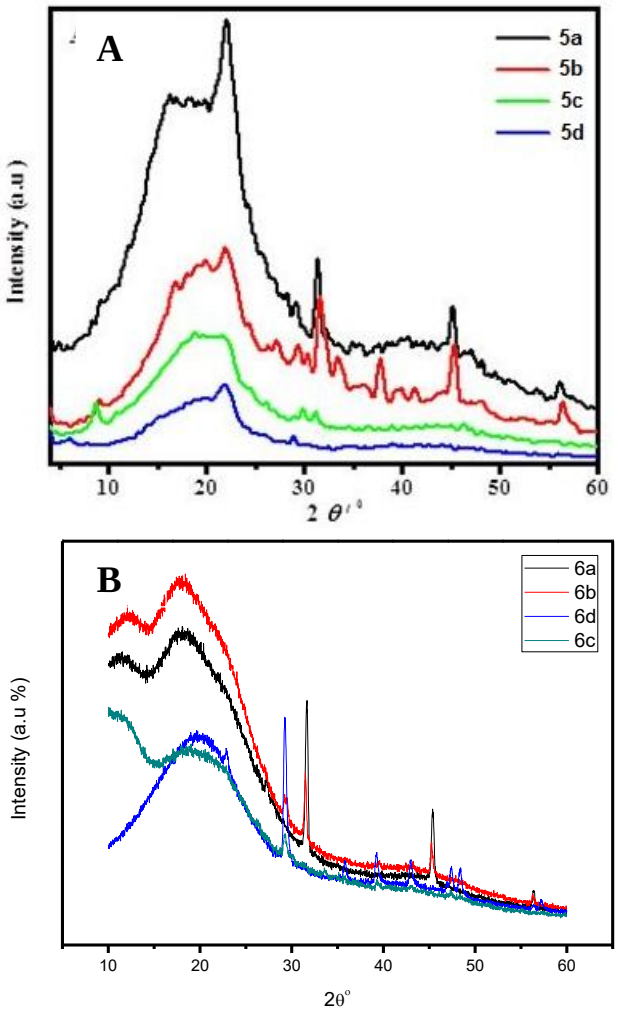


Fig. **1**. XRD of polymer (A) 5a-d & (B) 6a-d.

3.2.3. Biological behavior

The biological behavior of 10 compounds was achieved via the PASS database internet site [20]. The Biological behavior prediction using the PASS database was based on an analysis of a training set containing about 46.000 drugs as a reference. It estimates the probability of the molecule being active Pa and inactive Pi for all compounds. The consideration of Pa [21-22] values helps in the interpretation of prediction results.

When Pa > 0.70 is predicted high, their experimental activity and the compounds are close analogs of known pharmaceutical drugs. From their data (table **2**), anti-inflammatory and Gluconate 2-dehydrogenase (acceptor) inhibitor are their biological activity.

4. Conclusion

Novel polyesters 5_{a-d},6_{a-d} based on indazole moiety in the main chain are prepared by interfacial polycondensation of two indazoline monomers with an acid chloride. Different techniques confirmed and described the producing polyesters, including FTIR, ^{1}H-NMR-, MS spectra, TGA, and XRD analysis. The synthesized polyesters exhibit high thermal stability with a high char yield at 600 °C as a result of side

reactions Also, the polyester compounds have good biological results using PASS Inet at Pa > 0.70 giving a high probability for anti-inflammatory, Gluconate 2-dehydrogenase(acceptor) inhibitor.

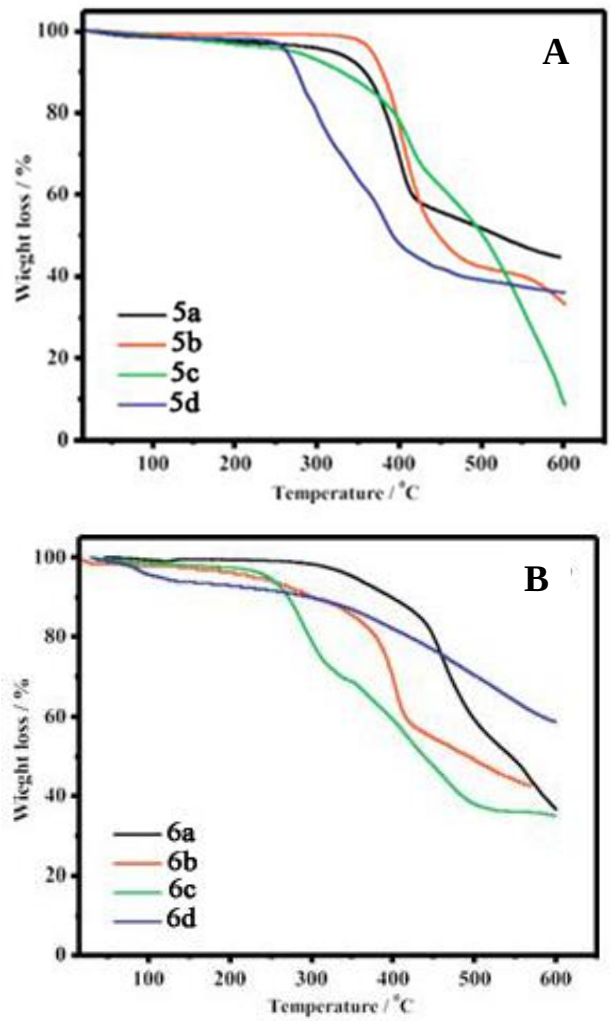


Fig 2. TGA of polymer (A) 5a-d & (B) 6a-d

Table 1. Thermal Properties of Polymers 5_{a-d} and 6_{a-d}

Temperature (C) for various % Decomposition						Char yield at 600 °C
Polymer code	10	20	30	40	50	
5_a	341	416	435	451	528	45%
5_b	297	421	504	585	501	39%
5_c	272	298	338	397	439	36%
5_d	362	418	436	463	512	32%
6_a	365	391	406	424	527	43%
6_b	328	392	418	459	501	58%
6_c	275	299	327	363	391	35%
6_d	370	386	399	412	438	31%

Table 2: Biological Activity predicted by PASS for Pa

Comp. No.	Activities	Pa	Pi
3	Antiinflammatory	0.777	0.008
4	Antiinflammatory	0.749	0.010
5a	Antiinflammatory	0.766	0.009
5b	Antiinflammatory	0.769	0.009
5c	Antiinflammatory, Gluconate2dehydroenase(acceptor)inhibitor.	0.849 0.772	0.008 0.009
5d	Antiinflammatory, Gluconate2dehydroenase(acceptor)inhibitor.	0.849 0.772	0.008 0.009
6a	Antiinflammatory	0.763	0.009
6b	Antiinflammatory	0.766	0.009
6c	Antiinflammatory, Gluconate2dehydroenase(acceptor)inhibitor.	0.840 0.769	0.009 0.009
6d	Antiinflammatory, Gluconate2dehydroenase(acceptor)inhibitor.	0.840 0.769	0.009 0.009

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