Data Article

Structural and antitumoral characteristic dataset of the chitosan based magnetic nanocomposite

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ABSTRACT

The evaluation on the characteristic dataset and figures presented here, are related to our latest research data entitled “Fabrication of chitosan based magnetic nanocomposite by click reaction strategy; evaluation of nanometric and Cytotoxic characteristics” [1]. FTIR, Vibrating Sample Magnetometer (VSM) measurements, Xray diffraction (XRD) information and the resulted figures for structural confirmation of the prepared chitosan based nanocomposite are presented in this article. The morphological changes of the Fibroblast, Saos, MCF7 and Hela cell lines after treatment with the mention compound were displayed. The additional adsorption data for the synthesized nanobiocomposite were also demonstrated with graphs.

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IR spectra were recorded on a Perkin-Elmer FT-IR-1710 spectrophotometer with the samples in KBr pellets. Fig. 1 displays the FT-IR spectra of the prepared samples and the characteristic peaks data were introduced as Table 1. Vibrating Sample Magnetometer (VSM) measurements were performed by using a vibrating sample magnetometer (LDJ Electronics Inc., Model 9600) and the data was inserted as Table 2 and the resulted pattern was displayed in Fig. 2. The X-ray powder diffraction (XRD) of the catalyst was carried out on a Philips PW 1830 X-ray diffractometer with CuKα source (λ = 1.5418 Å) in a range of Bragg’s angles (5–80°) at room temperature and demonstrated in Fig. 3. The crystal planes of Fe₃O₄ which confirm the existence of magnetic nanoparticles in the composite were assigned in Table 3.

Brunauer–Emmett–Teller (BET) analysis were performed using automatic sorption analyzer ASAP 2020, Micromeritics, USA. The Isotherm Linear Absolute Plot and isotherm Pressure Composition...

Fig. 1. FT-IR spectra of a) azidated chitosan, b) chitosan-silane composite, c) chitosan-silane clicked @ Fe₃O₄.
Table 1
FT-IR analysis data of a) Azidated chitosan, b) Chitosan-silane composite, c) Chitosan-silane clicked @ Fe₃O₄.

| FT-IR Analysis | Wavenumber (cm⁻¹) |
|----------------|------------------|
| Azidated chitosan (a) | 910, 1090, 1160, 1270, 1395, 1540, 1625, 2100, 2895, 3430 (br) |
| Chitosan-silane composite (b) | 1070, 1150, 1420, 1650, 2945, 3265, 3450 |
| Chitosan-silane clicked @ Fe₃O₄ (c) | 570, 1018, 1107, 1400, 1620, 2925, 3400 |

Table 2
The detailed magnetization data versus applied field of MNC.

| (Oe) | emu/g (Oe) | emu/g (Oe) | emu/g (Oe) | emu/g (Oe) | emu/g (Oe) | emu/g (Oe) | emu/g (Oe) |
|------|------------|------------|------------|------------|------------|------------|------------|
| 1.90 | −0.02 | 5501.11 | 24.62 | 321.11 | 13.21 | −828.88 | −18.44 | −2469.45 | −22.66 |
| 19.409 | 1.34 | 6001.11 | 24.78 | 236.11 | 11.40 | −1057.49 | −19.57 | −1935.21 | −21.89 |
| 33.72 | 2.44 | 6501.11 | 24.93 | 191.83 | 10.15 | −1285.17 | −20.37 | −1545.17 | −21.11 |
| 47.11 | 3.44 | 7001.11 | 25.07 | 157.97 | 9.11 | −1545.17 | −21.07 | −1287.70 | −20.42 |
| 62.11 | 4.46 | 7501.11 | 25.18 | 131.71 | 8.20 | −1951.52 | −21.87 | −1051.93 | −19.60 |
| 78.38 | 5.50 | 8001.11 | 25.29 | 111.58 | 7.39 | −2469.45 | −22.64 | −828.88 | −18.47 |
| 91.90 | 6.29 | 8501.11 | 25.40 | 91.11 | 6.49 | −2998.88 | −23.23 | −743.88 | −17.92 |
| 111.96 | 7.26 | 8001.11 | 25.29 | 78.04 | 5.74 | −3498.88 | −23.63 | −658.88 | −17.29 |
| 133.18 | 8.12 | 7501.11 | 25.18 | 61.75 | 4.71 | −3998.88 | −23.94 | −573.88 | −16.53 |
| 158.35 | 9.00 | 7001.11 | 25.06 | 45.95 | 3.68 | −4498.88 | −24.20 | −488.88 | −15.63 |
| 192.15 | 10.07 | 6501.11 | 24.92 | 32.08 | 2.70 | −4998.88 | −24.42 | −403.88 | −14.50 |
| 236.11 | 11.32 | 6001.11 | 24.81 | 17.14 | 1.56 | −5498.88 | −24.62 | −318.88 | −13.08 |
| 321.11 | 13.13 | 5501.11 | 24.63 | 0.50 | 0.20 | −5998.88 | −24.79 | −239.66 | −11.38 |
| 406.11 | 14.54 | 5001.11 | 24.44 | −11.57 | −0.72 | −6498.88 | −24.94 | −175.97 | −9.58 |
| 491.11 | 15.66 | 4501.11 | 24.22 | −27.47 | −1.96 | −6998.88 | −25.06 | −140.75 | −8.38 |
| 576.11 | 16.54 | 4001.11 | 23.96 | −42.01 | −3.01 | −7498.88 | −25.19 | −113.56 | −7.28 |
| 661.11 | 17.31 | 3501.11 | 23.65 | −57.33 | −4.00 | −7998.88 | −25.30 | −91.45 | −6.23 |
| 746.11 | 17.92 | 3001.11 | 23.26 | −73.00 | −4.95 | −8498.88 | −25.40 | −72.20 | −5.17 |
| 831.11 | 18.47 | 2501.11 | 22.75 | −91.45 | −6.01 | −7998.88 | −25.29 | −57.41 | −4.27 |
| 916.11 | 18.94 | 2001.11 | 22.07 | −113.56 | −7.04 | −7498.88 | −25.19 | −40.59 | −3.19 |
| 1178.04 | 20.00 | 1521.03 | 21.08 | −141.48 | −8.19 | −6998.88 | −25.06 | −26.32 | −2.21 |
| 1533.99 | 21.08 | 1173.47 | 20.03 | −176.25 | −9.47 | −6498.88 | −24.93 | −11.81 | −1.08 |
| 2001.11 | 22.04 | 916.11 | 18.97 | −238.94 | −11.30 | −5998.88 | −24.78 | 1.90 | −0.02 |
| 2501.11 | 22.72 | 831.11 | 18.50 | −318.88 | −13.02 | −5498.88 | −24.63 |
| 3001.11 | 23.23 | 746.11 | 17.97 | −403.88 | −14.41 | −4998.88 | −24.43 |
| 3501.11 | 23.62 | 661.11 | 17.35 | −488.88 | −15.62 | −4498.88 | −24.20 |
| 4001.11 | 23.94 | 576.11 | 16.60 | −573.88 | −16.47 | −3998.88 | −23.94 |
| 4501.11 | 24.20 | 491.11 | 15.71 | −658.88 | −17.23 | −3498.88 | −23.63 |
| 5001.11 | 24.42 | 406.11 | 14.60 | −743.88 | −17.89 | −2998.88 | −23.25 |
dataset were inserted in Tables 4 and 5 respectively and the adsorption and desorption graphs were displayed in Fig. 4. The morphology of cancer cells after treatment with different concentrations of nanocomposite were displayed in Fig. 5.

Table 3
Data resulted from XRD pattern of MNC.

| Crystal planes (2-Theta) | Fe3O4 | Chitosan/SiO2 Broad Peak (15–30°) | Unassigned |
|--------------------------|-------|----------------------------------|------------|
| 2 0 0 (30.4°)            | 3 1 1 (35.7°) | 4 2 2 (53.6°) | 5 1 1 (57°) | 4 4 0 (63.0°) |
| 3 1 1 (35.7°)            | 4 0 0 (43.4°) | 5 1 1 (57°) | 4 4 0 (63.0°) |
| 4 0 0 (43.4°)            | 4 2 2 (53.6°) | 5 1 1 (57°) | 4 4 0 (63.0°) |
| 5 1 1 (57°)              | 4 4 0 (63.0°) |
| 4 2 2 (53.6°)            | 5 1 1 (57°) |
| 5 1 1 (57°)              | 4 4 0 (63.0°) |

Table 4
Quantity of MNC-adsorption and desorption versus absolute pressure.

| No. | MNC-Adsorption Quantity (cm³/g STP) | Absolute Pressure (kPa) | MNC-Desorption Quantity (cm³/g STP) | Absolute Pressure (kPa) |
|-----|-----------------------------------|--------------------------|-------------------------------------|--------------------------|
| 1   | 0.0155                            | 3.9491                   | 3.1219                              | 10.2207                  |
| 2   | 0.0308                            | 4.5614                   | 6.2336                              | 11.3728                  |
| 3   | 0.0533                            | 5.0750                   | 11.0299                             | 12.4181                  |
| 4   | 0.0775                            | 5.4451                   | 15.8141                             | 13.1678                  |
| 5   | 0.1012                            | 5.7218                   | 20.6030                             | 13.8167                  |
| 6   | 0.1165                            | 5.8714                   | 30.1617                             | 15.0107                  |
| 7   | 0.5385                            | 7.7433                   | 37.9474                             | 16.0667                  |
| 8   | 0.9008                            | 8.4642                   | 47.5964                             | 17.7131                  |
| 9   | 1.1723                            | 8.8480                   | 57.5541                             | 20.1034                  |
| 10  | 2.8142                            | 10.1713                  | 68.1428                             | 24.9174                  |
| 11  | 4.5636                            | 10.9367                  | 76.8254                             | 34.0477                  |
| 12  | 6.3321                            | 11.4933                  | 87.8111                             | 75.9624                  |
| 13  | 8.1536                            | 11.9367                  | 90.7318                             | 79.2349                  |
| 14  | 9.9705                            | 12.3060                  | 95.2962                             | 82.0726                  |
| 15  | 14.1124                           | 13.0277                  | 97.0361                             | 83.6500                  |
| 16  | 18.3035                           | 13.6566                  | 99.0819                             | 86.1214                  |
| 17  | 22.4814                           | 14.2307                  |                                     |                          |
| 18  | 30.8083                           | 15.3401                  |                                     |                          |
| 19  | 39.1600                           | 16.5298                  |                                     |                          |
| 20  | 47.4831                           | 17.9148                  |                                     |                          |
| 21  | 51.6722                           | 18.7439                  |                                     |                          |
### 2. Experimental design, materials and methods

The magnetic nanocomposite was prepared using chitosan. To prepare functionalized chitosan, the chitosan was azidated using chloroacetyl chloride and sodium azide. Then click reaction which has been incorporated in our recent studies \[2,3\] and also employed in some biological researches \[4,5\] was performed between functionalized chitosan and trimethoxy(3-(prop-2-yn-1-ylthio)propyl)silane. Then magnetization was done using ferric and ferrous chloride solution. The characteristic peaks for azidated at around 2100 cm$^{-1}$, C–H bond of triazole rings and Si–O–Si bonds at 3265 cm$^{-1}$ and 1150 cm$^{-1}$ respectively. The resulted FT-IR spectra and the corresponding data of the synthesized products were presented in Fig. 1 and Table 1. Also, the detailed FT-IR data including the transmittances at each wavenumbers for the compounds a, b, and c were provided as a supplementary file.

### Table 4 (continued)

| No. | MNC-Adsorption | MNC-Desorption |
|-----|----------------|----------------|
|     | Quantity (cm$^3$/g STP) | Absolute Pressure (kPa) | Quantity (cm$^3$/g STP) | Absolute Pressure (kPa) |
| 22  | 59.9826 | 20.7978 |
| 23  | 68.2312 | 23.8461 |
| 24  | 72.5367 | 26.2876 |
| 25  | 80.4382 | 33.3906 |
| 26  | 89.6708 | 54.5202 |
| 27  | 94.0723 | 73.1871 |
| 28  | 97.0785 | 80.9530 |
| 29  | 99.0819 | 86.1214 |

### Table 5

Quantity of absolute pressure versus weight %N$_2$.

| No. | MNC-Adsorption | MNC-Desorption |
|-----|----------------|----------------|
|     | Weight % N$_2$ | Absolute Pressure (kPa) | Weight % N$_2$ | Absolute Pressure (kPa) |
| 1   | 0.0352 | 0.0155 | 0.0912 | 3.1219 |
| 2   | 0.0407 | 0.0308 | 0.1014 | 6.2336 |
| 3   | 0.0452 | 0.0533 | 0.1108 | 11.0299 |
| 4   | 0.0485 | 0.0775 | 0.1174 | 15.8141 |
| 5   | 0.0510 | 0.1012 | 0.1232 | 20.6030 |
| 6   | 0.0523 | 0.1165 | 0.1339 | 30.1617 |
| 7   | 0.0690 | 0.5385 | 0.1433 | 37.9474 |
| 8   | 0.0755 | 0.9008 | 0.1580 | 47.5964 |
| 9   | 0.0789 | 1.1723 | 0.1793 | 57.5541 |
| 10  | 0.0907 | 2.8142 | 0.2223 | 68.1428 |
| 11  | 0.0975 | 4.5636 | 0.3038 | 76.8254 |
| 12  | 0.1025 | 6.3321 | 0.6778 | 87.8111 |
| 13  | 0.1065 | 8.1536 | 0.7070 | 90.7318 |
| 14  | 0.1098 | 9.9705 | 0.7323 | 95.2962 |
| 15  | 0.1162 | 14.1124 | 0.7464 | 97.0362 |
| 16  | 0.1218 | 18.3035 | 0.7684 | 99.0819 |
| 17  | 0.1269 | 22.4814 |
| 18  | 0.1368 | 30.8083 |
| 19  | 0.1474 | 39.1600 |
| 20  | 0.1598 | 47.4831 |
| 21  | 0.1672 | 51.6722 |
| 22  | 0.1855 | 59.9826 |
| 23  | 0.2127 | 68.2312 |
| 24  | 0.2345 | 72.5367 |
| 25  | 0.2979 | 80.4382 |
| 26  | 0.4864 | 89.6708 |
| 27  | 0.6530 | 94.0723 |
| 28  | 0.7223 | 97.0785 |
| 29  | 0.7684 | 99.0819 |
Magnetization experiments of the prepared magnetic nanocomposite (MNC) were obtained using VSM technique at room temperature. As can be seen in Fig. 2, this product with saturation magnetization value ($M_s$) of 25.4 (emu/g) has super paramagnetic characteristics. Moreover; the corresponding data were presented in Table 2.

The XRD pattern of the synthesized chitosan nanocomposite (Fig. 3) demonstrated the crosslinking reaction between Si groups and chitosan with the broad peak at $15-30^\circ$. Moreover the existence of magnetic nanoparticles in the structure was confirmed by determining the crystal planes of Fe$_3$O$_4$ nanoparticles (Table 3).

![Isotherm Linear Absolute Plot](image_url)

*Fig. 4.* (a) Isotherm linear absolute plot (b) isotherm pressure composition.

![Morphology of the mentioned cell lines](image_url)

*Fig. 5.* Morphology of the mentioned cell lines after incorporating the prepared nanobiocomposite samples in concentrations of 15.62, 31.5, 62.5 and 125 μg/mL.
To attain adsorption data of the synthesized nanocomposite for further experiments, the samples were outgassed at 60 °C and then experiments according to the Brunauer—Emmett—Teller (BET) theory were performed. The isotherm plots were used to calculate the specific surface area and the average pore diameter of the chitosan/magnetic nanocomposite and the difference between adsorption and desorption steps.

For evaluating the cell cytotoxicity of the prepared sample (MNC) according to the literature [6], some known cell lines were considered including Fibroblast, MCF7, Hela, and Saos. The resulted data were surveyed in the main article and the morphology of the cell lines with treatment of different concentrations of the samples were imaged by microscopic technique and presented here in Fig. 5.

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Conflict of Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.dib.2019.104583.

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