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

Phytic acid-modified Graphene/Cobalt oxide nanocomposite; Synthesis, characterization, theoretical studies, antiproliferative properties, and catalytic activity

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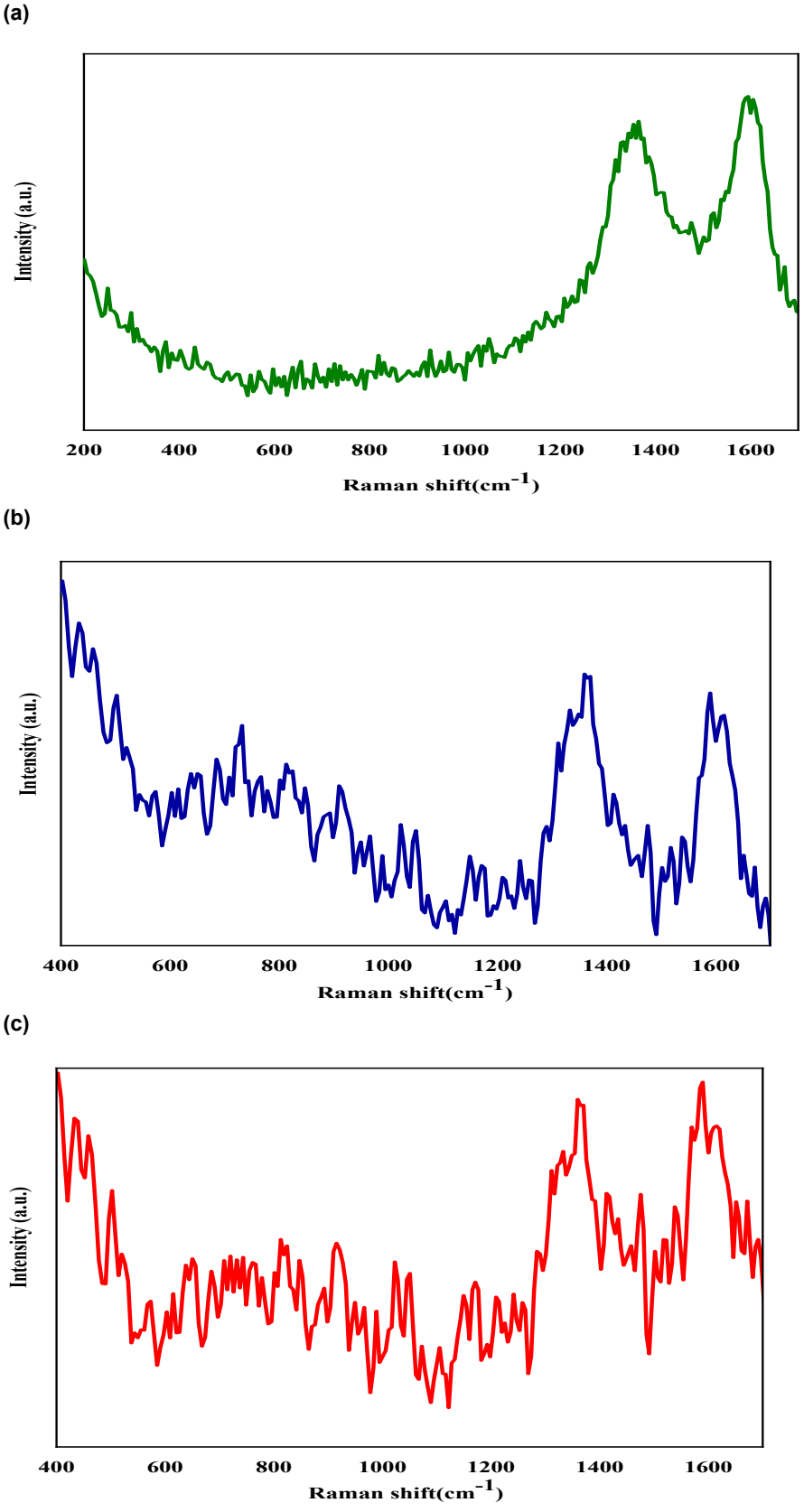

Fig. S1. Raman spectrum of GO **(a)**, GO-Co_3O_4 **(b)**, and GO-Co_3O_4-PA **(c)**.

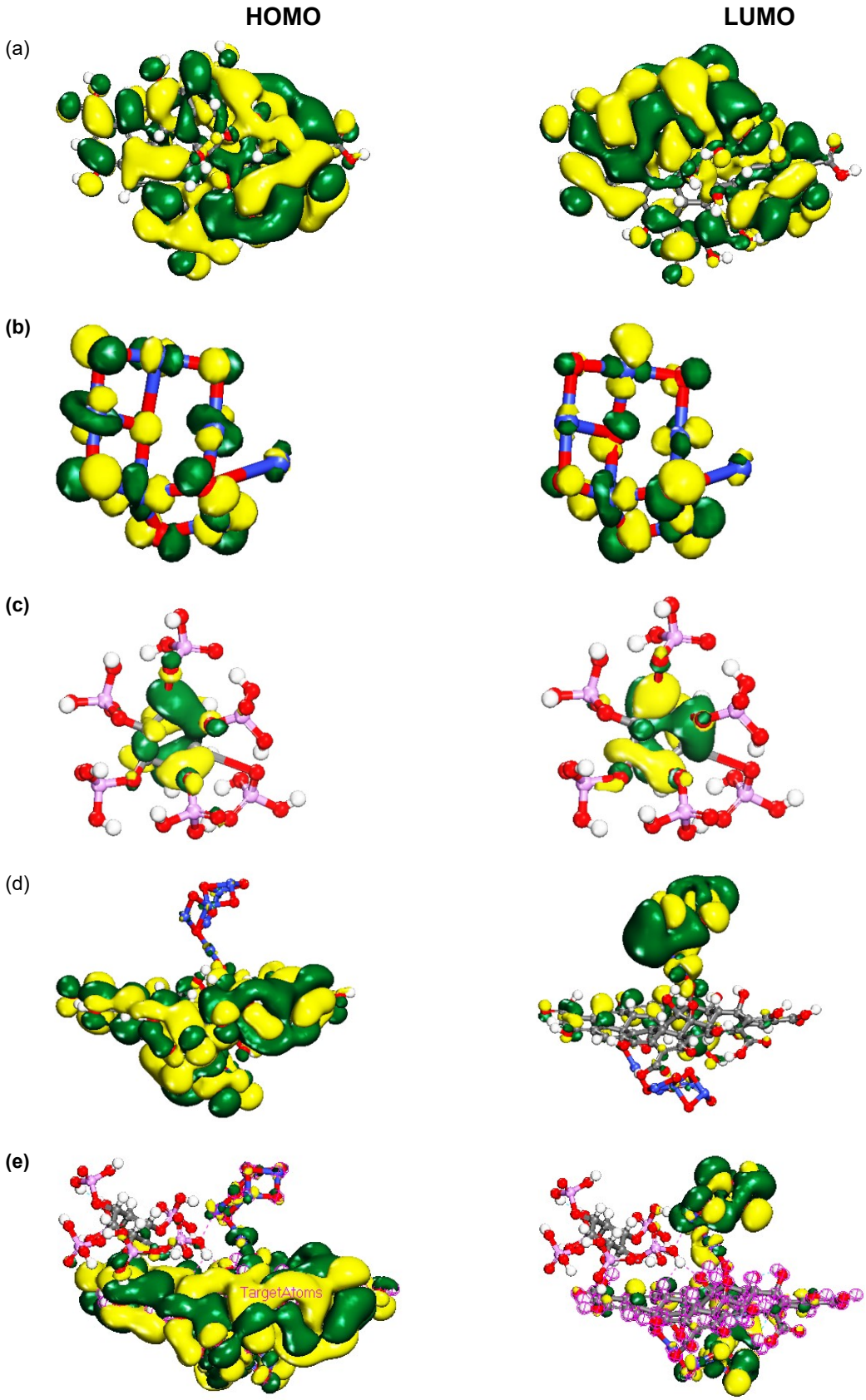

Fig. S2. HOMO and LUMO orbitals of **(a)**; GO, **(b)**; Co_3O_4, **(c)**; PA, **(d)**; GO-Co_3O_4, and **(e)**; GO-Co_3O_4-PA structures after optimization obtained by DMol^3 based on DFT-D in Material Studio 2017.

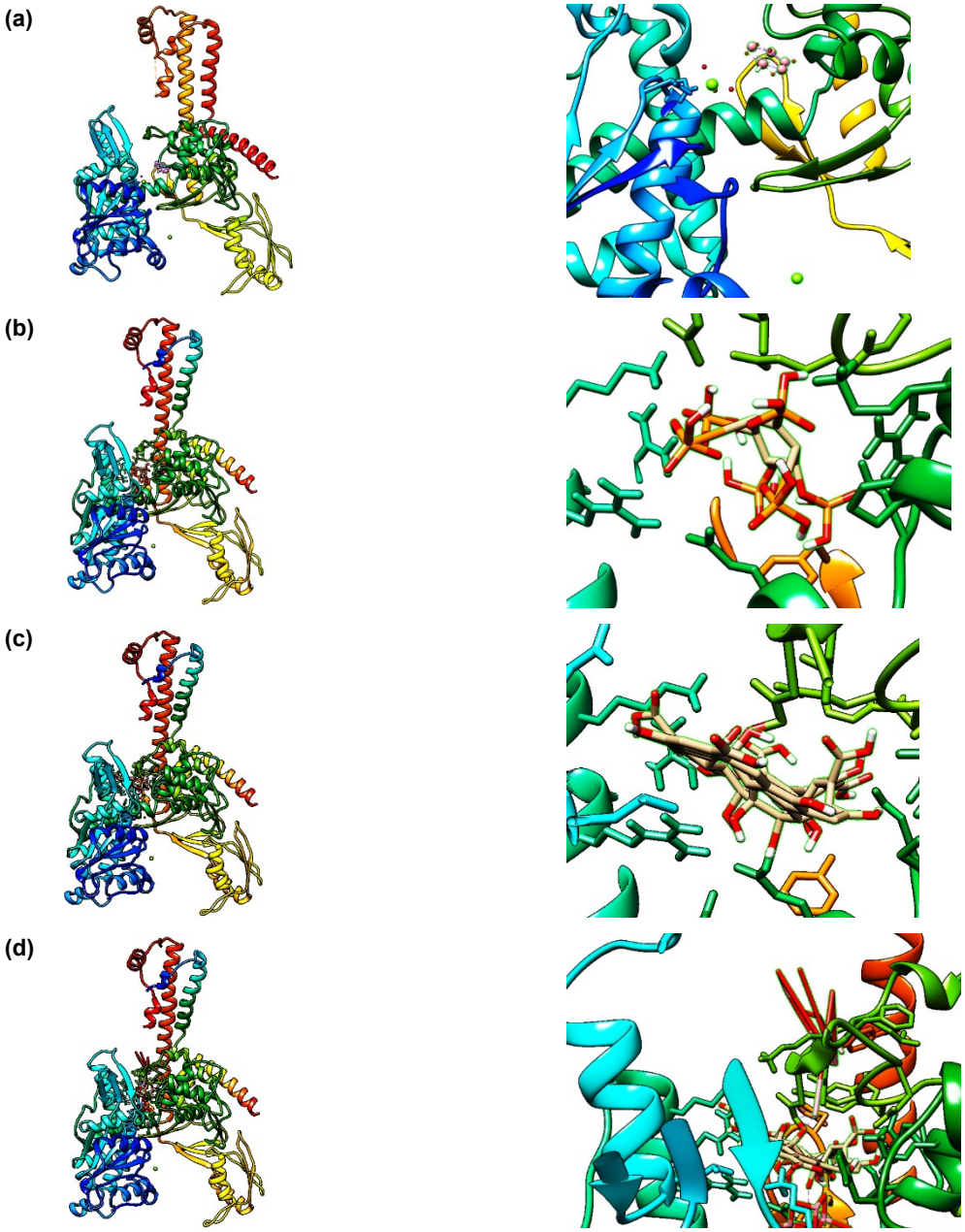

Fig. S3. Docking conformation of **(a)**; Co_3O_4 **(b)**; PA **(c)**; GO and **(d)**; GO-Co_3O_4 with human topoisomerase IIα bound

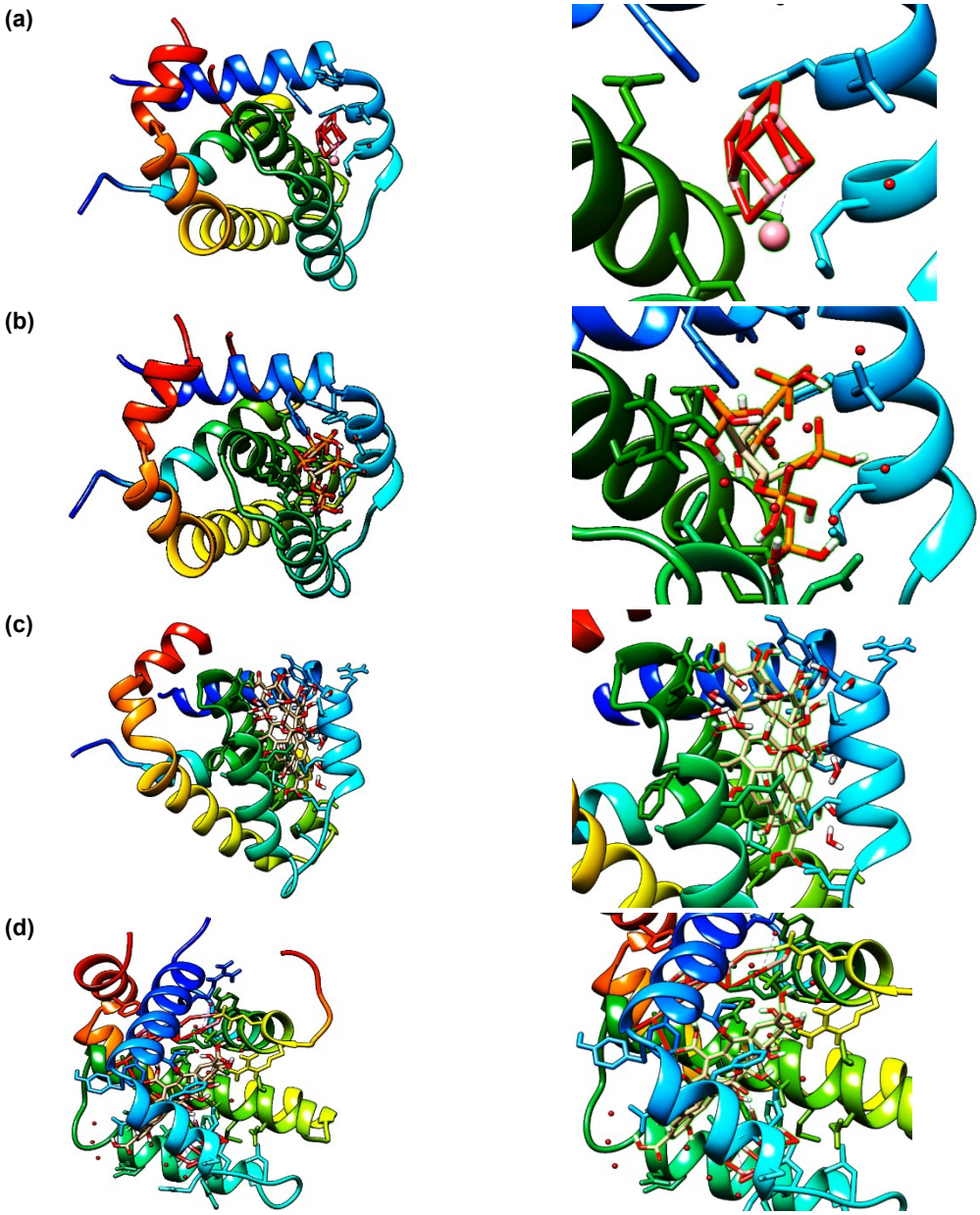

Fig. S4. Docking conformation of **(a)**; Co_3O_4 **(b)**; PA **(c)**; GO and **(d)**; GO -Co_3O_4 in Bcl-2 (4LXD).

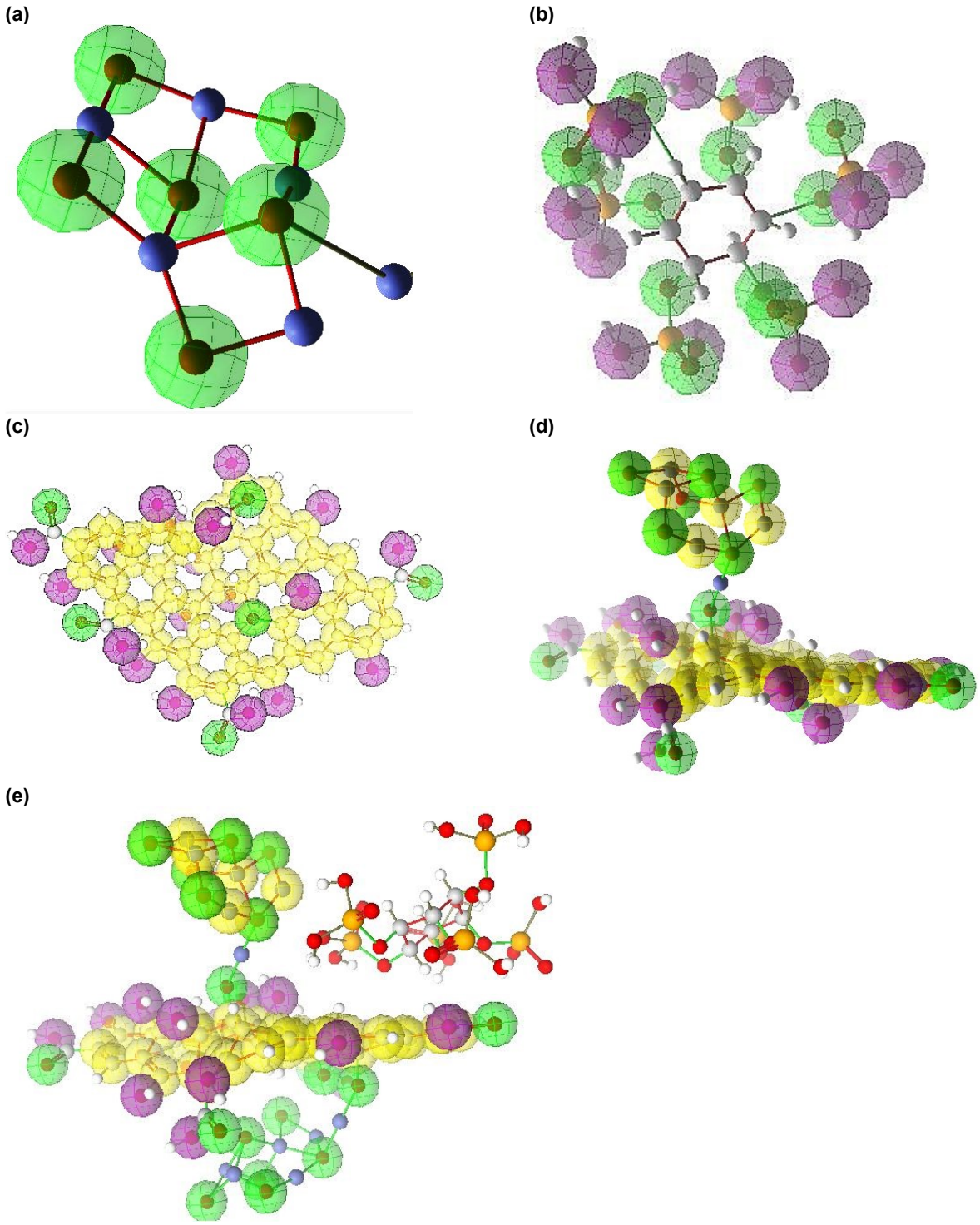

Fig. S5. The pharmacophore chemical features from onto **(a)**; Co_3O_4 **(b)**; PA **(c)**; GO **(d)**; GO-Co_3O_4 and **(e)**; GO-Co_3O_4-PA.

Table S1. The amino acid residues of human topoisomerase IIα bound with compounds.

Compounds	Amino acids	$\Delta G_{binding}$
Co_3O_4	Arg A727, Asp A1004, Glu A712, Glu A839, Gly A1007, His A1005, Ile A715, Leu A722, Phe A1003, Pro A716, Pro A724, Ser A717, Trp A840, and Val A1006	-73.019
PA	Arg A672, Arg A673, Arg A713, Arg A727, Asp A831, Glu A712, Glu A837, Glu A839, Gly A1007, Ile A715, Leu A722, Leu A829, Lys A676, Lys A723, Lys A728, Phe A1003, Pro A716, Pro A724, Glu A712, Glu A837, Glu A839, Gly A1007, Ile A715, Leu A722, Leu A829, Lys A723, Lys A676, Lys A728, Phen A1003, Pro A716, Pro A724, Pro A838, Ser A709, Ser A717, Val A836 and Val A1006	-131.561
GO	Arg A672, Arg A673, Arg A727, Asp A831, Asp A832, Asp A1004, Glu A596, Glu A712, Glu A837, Glu A839, Gly A1007, His A758, His A1005, Leu A592, Lys A676, Lys A728, Phe A1003, Pro A724, Glu A712, Glu A837, Glu A839, Gly A1007, His A1005, His A758, Leu A592, Lys A676, Lys A728, Phe A1003, Pro A724, Pro A838, Ser A717, Trp A840, Tyr A612, Val A719, Val A836, Val A1006	-66.268
GO-Co_3O_4	Arg A672, Arg A673, Arg A713, Asn A708, Asp A831, Asp A710, Asp A1004, Glu A839, Glu A837, Glu A712, Gly A725, Gly A1007, His A758, His A759, His A1007, Leu A592, Leu A829, Lys A676, Lys A723, Lys A728, Phe A1003, Pro A724, Ser A709, Ser A755, Ser A756, Tyr A757, Val A1006	-84.848
GO-Co_3O_4-PA	Ala A752, Arg A835, Arg A713, Arg A713, Arg A727, Asp A835, Asn A711, Asn A711, Asp A831, Asp A832, Gln A834, Glu A712, Glu A753, Glu A839, Gly A725, Gly A1007, His A758, His A759, His A758, His A759, Ile A715, Leu A592, Leu A722, Leu A829, Lys A676, Lys A723, Lys A728, Lys A827, Met A754, Phe A1003, Phe A731, Phe A828, Pro A716, Pro A724, Pro A838, Ser A709, Ser A714, Ser A717, Ser A755, Ser A756, Ser A763, Tyr A612, Tyr A757, Tyr A830, and Val A836	-732.849

Table S2. The amino acid residues of Bcl-2 (4LXD) with compounds.

Compounds	Amino acids	$\Delta G_{binding}$
Co_3O_4	Ala A146, Asp A108, Glu A149, Leu A134, Met A112, Phe A101, Phe A109, Phe A150, Ser A102, Tyr A105, Val A130, Val A153	-69.135
PA	Ala A146, Asp A108, Glu A149, Leu A134, Met A112, Phe A101, Phe A109, Phe A150, Ser A102, Tyr A105, Val A130, Val A153	-98.200
GO	Ala A110, Ala A146, Arg A143, Arg A103, Arg A104, Arg A106, Asp A108, Glu A149, Glu A133, Glu A157, Gly A142, Gly A98, Gly A151, Gly A152, Leu A134, Leu A118, Leu A116, Met A112, Met A154, Phe A101, Phe A109, Phe A150, Phen A147, Ser A102, Ser A113, Tyr A105, Val A130, Val A131, Val A153	-70.234
GO-Co_3O_4	Ala A97, Ala A110, Ala A146, Arg A143, Arg A126, Arg A107, Arg A106, Arg A95, Arg A24, Asp A108, Gln A115, Gln A96, Gln A23, Glu A149, Glu A133, Glu A157, Glu A132, Glu A111, Glu A115, Glu A157, Gly A151, Gly A152, Gly A142, Gly A98, His A91, Ile A17, Ile A144, Leu A134, Leu A118, Leu A116, Leu A94, Lys A15, Lys A20, Met A112, Met A154, Met A174, Phe A101, Phe A195, Phe A150, Phe A148, Phe A147, Phe A135, Phe A127, Phe A109, Ser A102, Ser A113, Ser A114, Thr A93, Trp A141, Tyr A105, Tyr A19, Tyr A16, Val A130, Val A131, Val A153, Val A156, Val A145	-141.334
GO-Co_3O_4-PA	Ala A110, Ala A146, Ala A171, Arg A24, Arg A103, Arg A104, Arg A106, Arg A126, Gln A169, Asp A108, Asp A100, Asp A99, Cys A155, Gln A23, Glu A111, Glu A133, Glu A149, Glu A157, Glu A149, Glu A157, Gly A98, Gly A151, Gly A152, Ile A17, Ile A12, Ile A170, Leu A21, Leu A94, Leu A116, Leu A118, Leu A134, Leu A166, Lys A15, Lys A20, Met A14, Met A112, Ser A102, Ser A113, Ser A114, Ser A158, Thr A129, Trp A173, Tyr A105, Tyr A19, Tyr A16, Val A153, Val A156, Val A167, Val A131, Val A130, Val A13	-158.297