Supplementary Materials

for

Chemical composition of various *Nepeta cataria* plant organs' methanol extracts associated with the *in vivo* hepatoprotective and antigenotoxic features, and molecular modeling investigations

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Content

Figure S1. The bioactive conformations of protocatechuic acid (A), *p*-hydroxybenzoic acid (B), caffeic acid (C), and syringic acid (D) within the *r*CATCmpd I. Amino acid residues are depicted in white, hem containing the oxoferryl porphyrin π-cation radical is colored green. For the clarity of presentation, only polar hydrogen atoms were presented within the naturally occurring compounds.

Figure S2. The bioactive conformations of *p*-coumaric acid (A), ferulic acid (B), luteolin-7-*O*-glucoside (C), and quercetin-3-*O*-glucoside (D) within the *r*CATCmpd I. Amino acid residues are depicted in white, hem containing the oxoferryl porphyrin π-cation radical is colored green. For the clarity of presentation, only polar hydrogen atoms were presented within the naturally occurring compounds.

Figure S3. The bioactive conformations of quercetin-3-*O*-rutinoside (A), kaempferol-3-*O*-glucoside (B), quercitrin (C), luteolin (D), kaempferol (E), and isorhamnetin (F) within the *r*CATCmpd I. Amino acid residues are depicted in white, hem containing the oxoferryl porphyrin π-cation radical is colored green. For the clarity of presentation, only polar hydrogen atoms were presented within the naturally occurring compounds.

Figure S4. The bioactive conformations of protocatechuic acid (A), *p*-hydroxybenzoic acid (B), caffeic acid (C), and syringic acid (D) within the *r*DNA binding and cleavage domain of *r*TopIIα. All of the obtained bioactive conformations were superimposed to MDA illustrated in yellow. The sense strand was depicted in green, the antisense strand was colored purple. The nucleotides of interest are depicted in white, whereas the remaining ones were displayed by blue nucleotides objects. For the clarity of presentation, the *C*-terminal domain of *r*TopIIα, nesting the targeted compounds, was illustrated by pink sphere, whereas the non-targeted *C*-terminal domain was denoted by pink ribbons.

Figure S5. The bioactive conformations of *p*-coumaric acid (A), ferulic acid (B), luteolin-7-*O*-glucoside (C), and quercetin-3-*O*-glucoside (D) within the *r*DNA binding and cleavage domain of *r*TopIIα. All of the obtained bioactive conformations were superimposed to MDA illustrated in yellow. The sense strand was depicted in green, the antisense strand was colored purple. The nucleotides of interest are depicted in white, whereas the remaining ones were displayed by blue nucleotides objects. For the clarity of presentation, the *C*-terminal domain of *r*TopIIα, nesting the targeted compounds, was illustrated by pink sphere, whereas the non-targeted *C*-terminal domain was denoted by pink ribbons.

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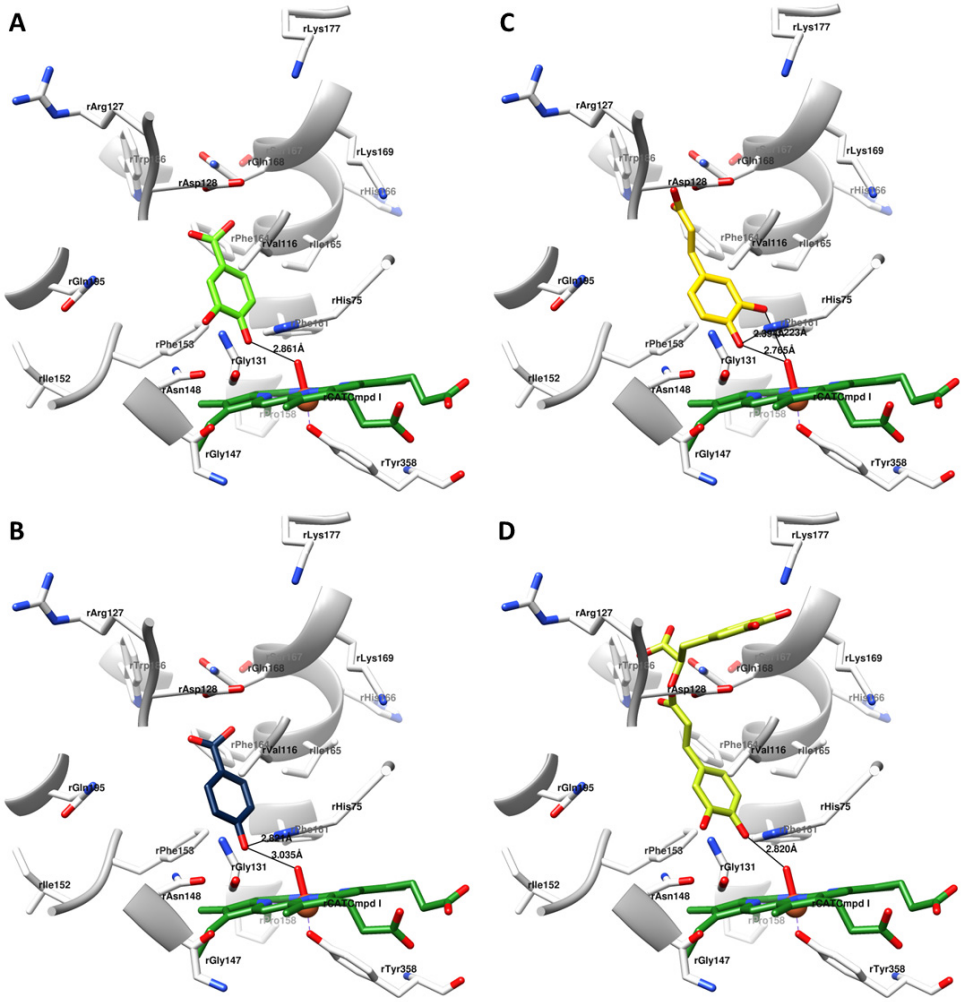

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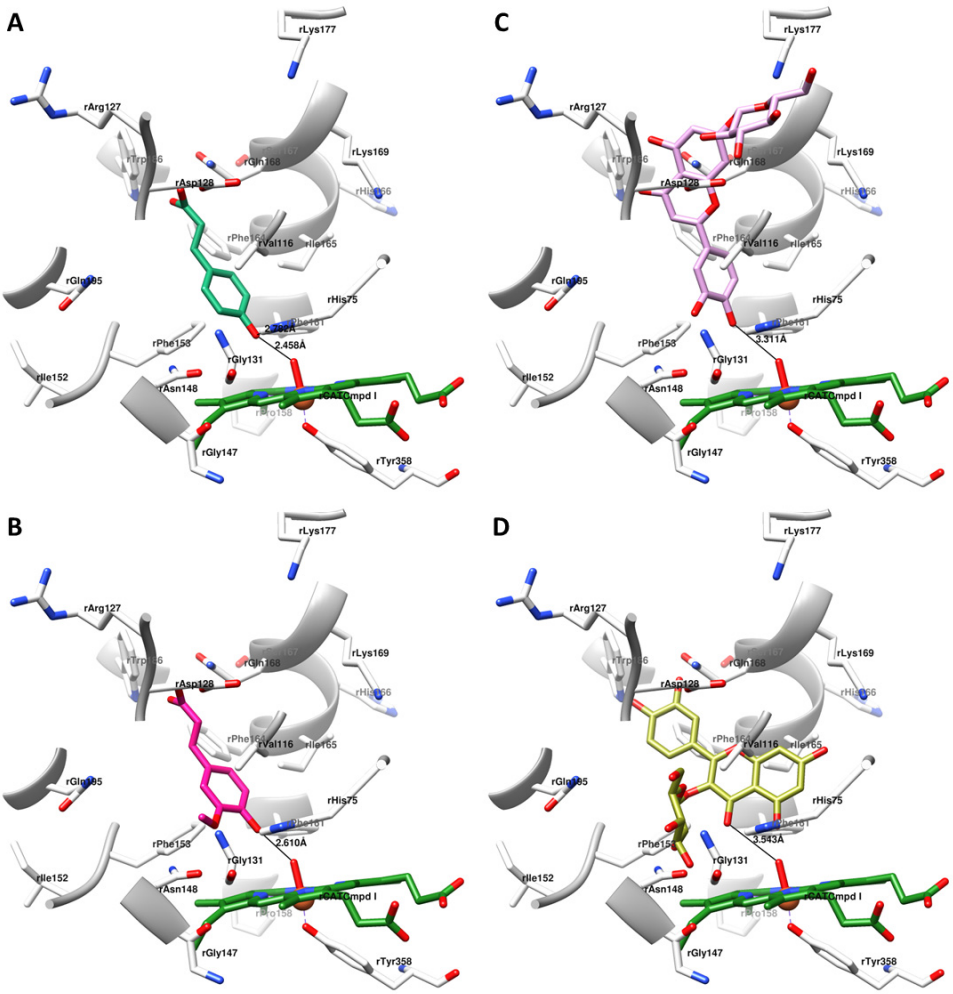

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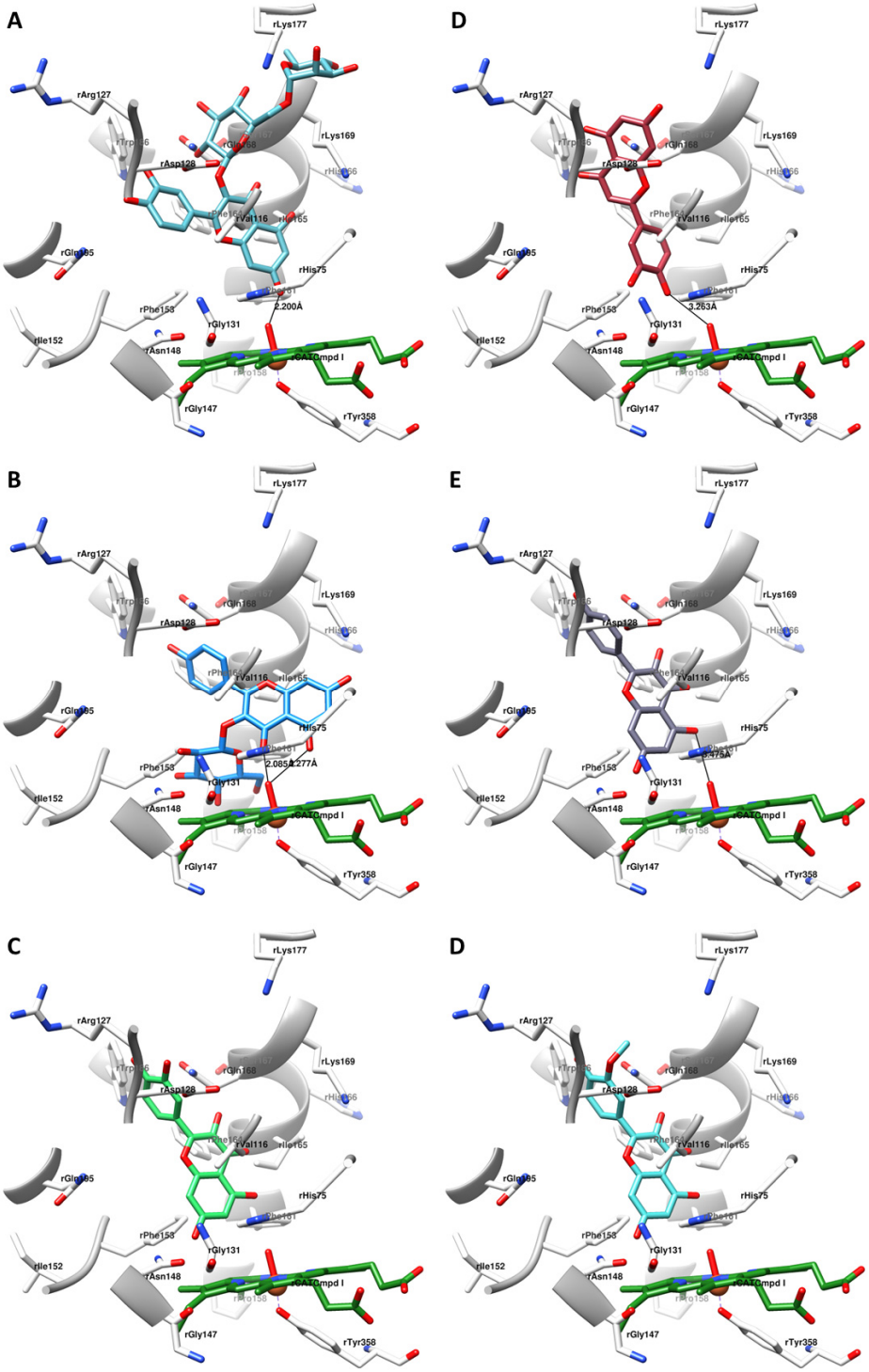

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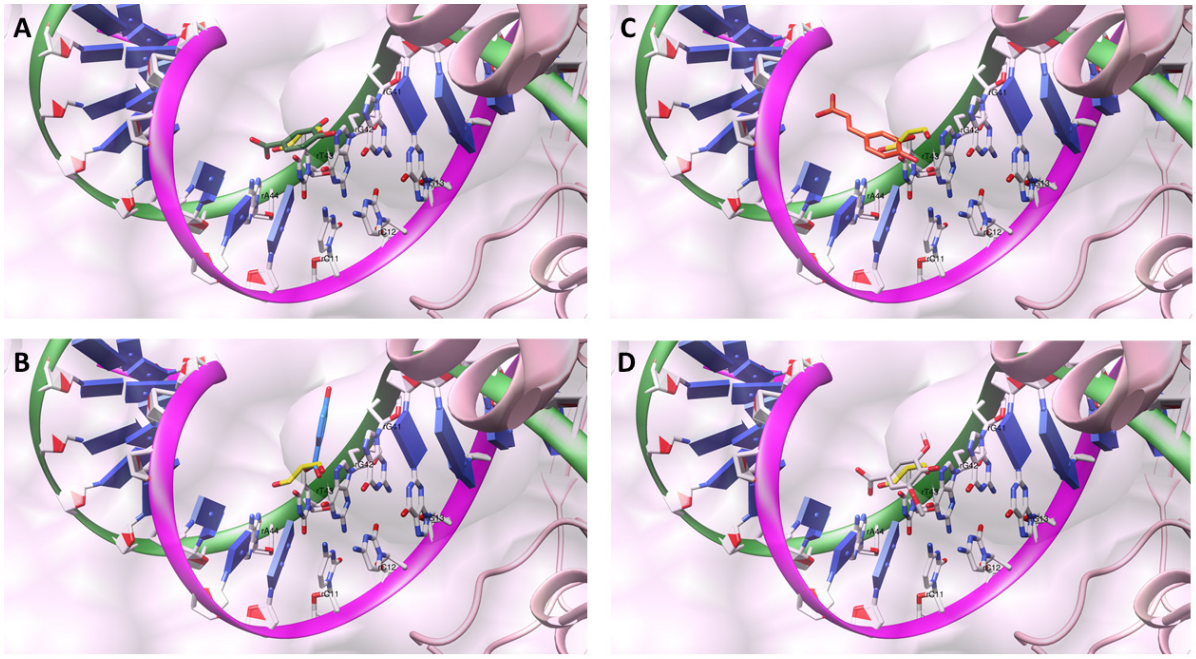

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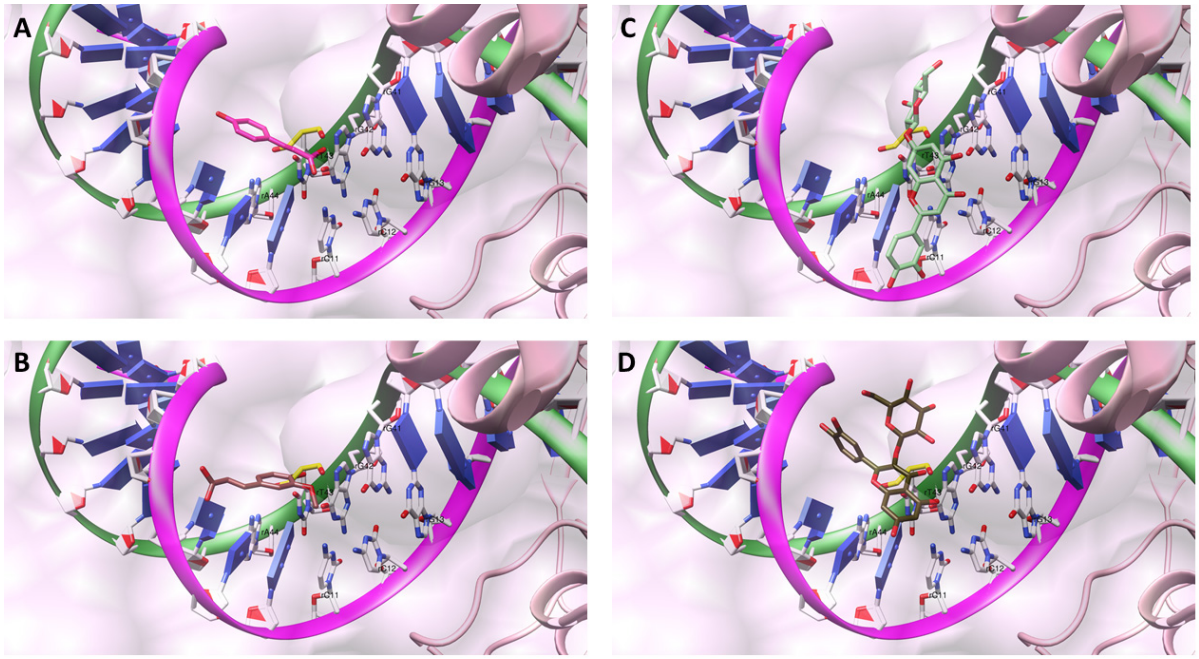

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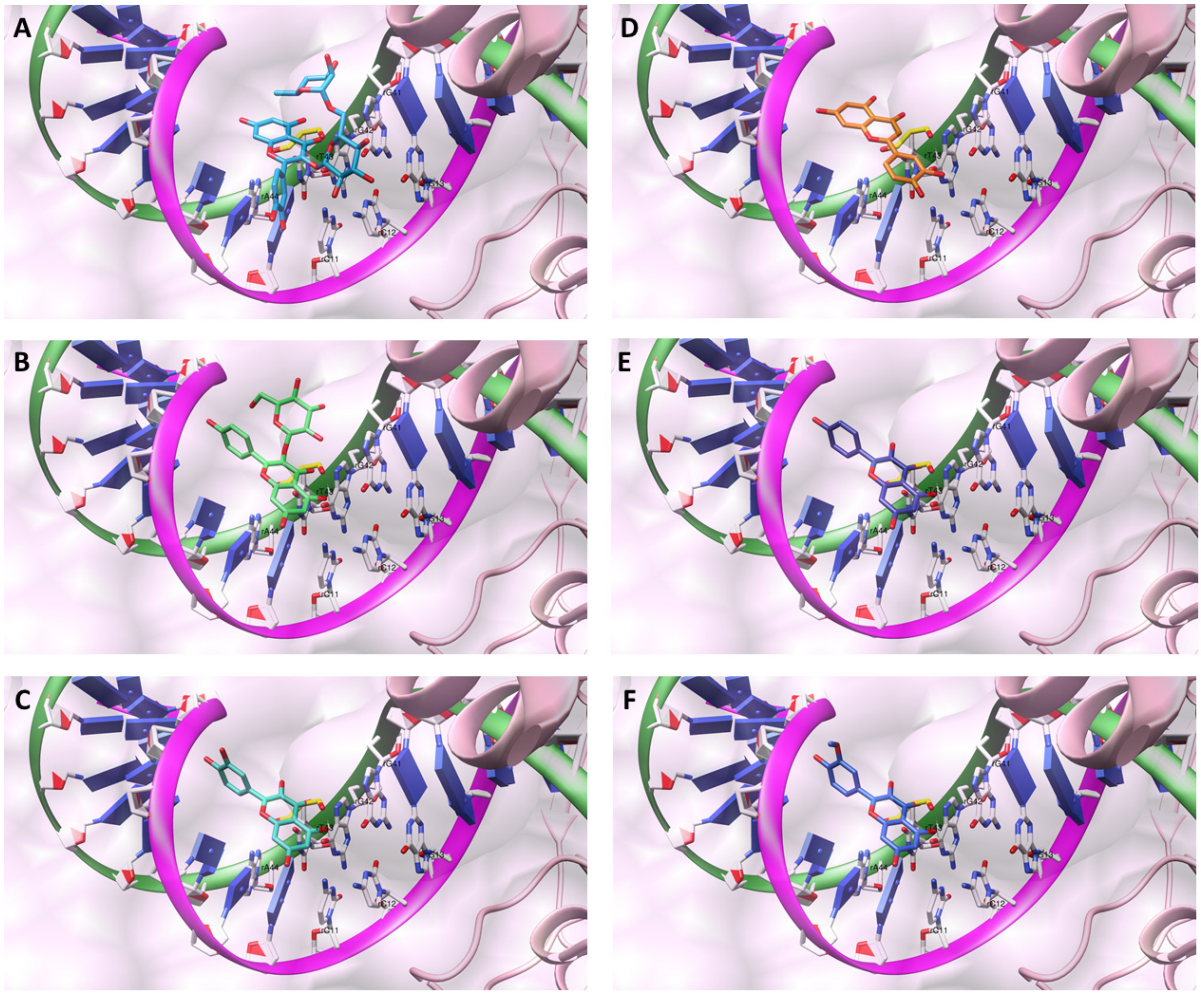

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