Structural repositioning, *in-silico* molecular modeling, oxidative degradation, and biological screening of linagliptin as adenosine 3 receptor (ADOR3) modulators targeting hepatocellular carcinoma

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**Supporting Data**

Figure S1: $^1$HNMR spectra for Degradation Product (DEG)
Figure S2: C\textsuperscript{13}NMR spectra for Degradation Product (DEG)
Figure S3: DEPT135 spectra for Degradation Product (DEG)
Figure S4: 3D spectrum scan of (a) Linagliptin and (b) the proposed degradation product.

**LC-MS/MS chromatographic and mass spectrometric conditions:**
The column temperature was kept at 25°C, the injection volume used was 10 µL, and the flow rate was 0.3 mL/min with 3 min as the run time. Cone voltage was set at 30 V; source temperature was set at 150°C, and the collision energy was set at 30 eV for both drugs to enable multiple reaction monitoring (MRM) of the transition pairs.
of m/z 473.11 to 420.07 for LIN and m/z 285.05 to 156.93 for DEG in the positive mode utilizing Electro Spray Ionization (ESI). The following parameters were applied: turbo ions spray at 400°C, capillary temperature at 275°C, sheath and auxiliary gas at 15 and 2 psi, respectively, ion spray voltage of 3800 V, capillary voltage of 4 KV, capillary offset of 35 and de-solvating line temperature at 400°C.