

Tessema F, Gonfa Y H, Asfaw T B, Tadesse M G, Bachheti A, Singab A N, Bachheti R K. Dehydrocostus lactone from the root of *Ajuga integrifolia* Buch.-Ham.: Quantitative determination and *in silico* study for anti-breast cancer activity. Plant Science Today (Early Access). <https://doi.org/10.14719/pst.2344>

Supplementary Figures

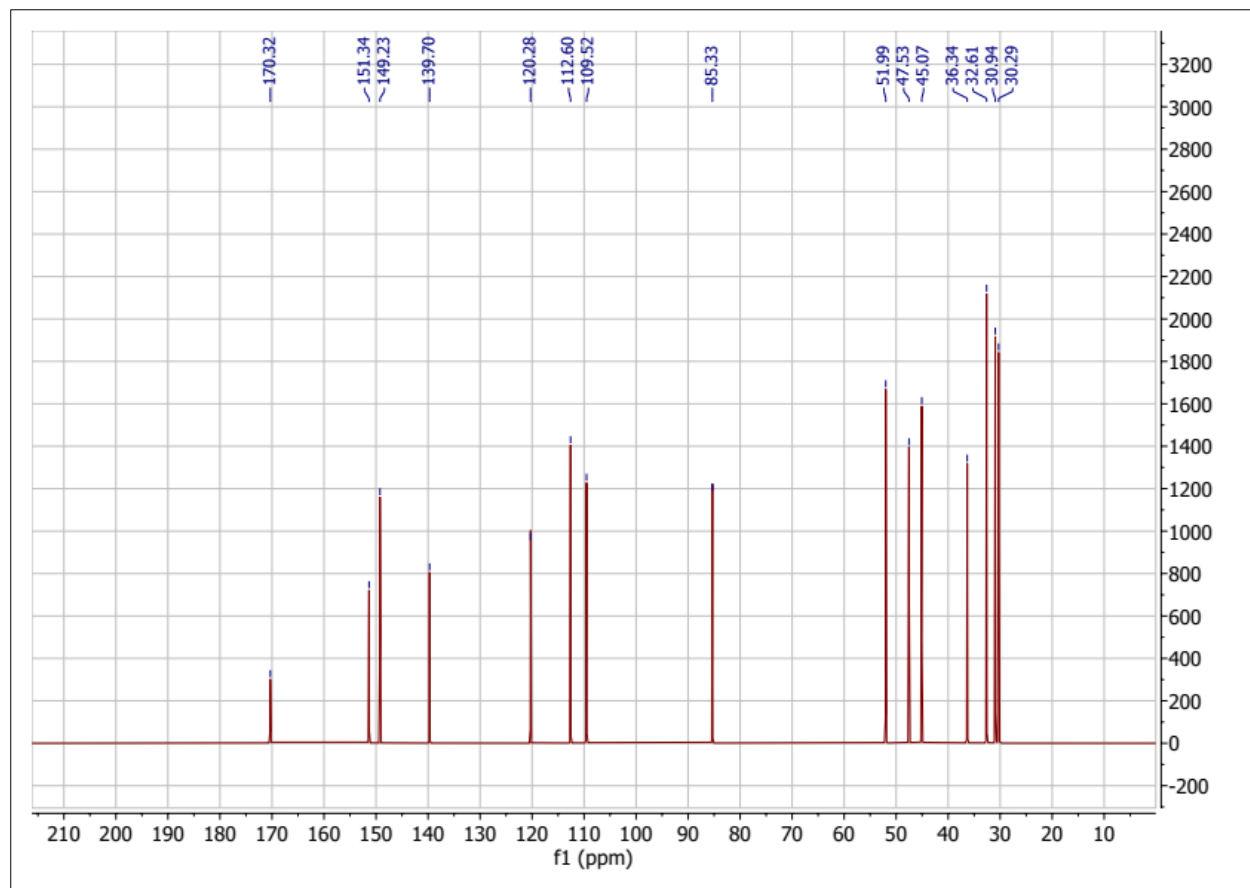


Fig. 1S. ¹³C NMR for Compound 1

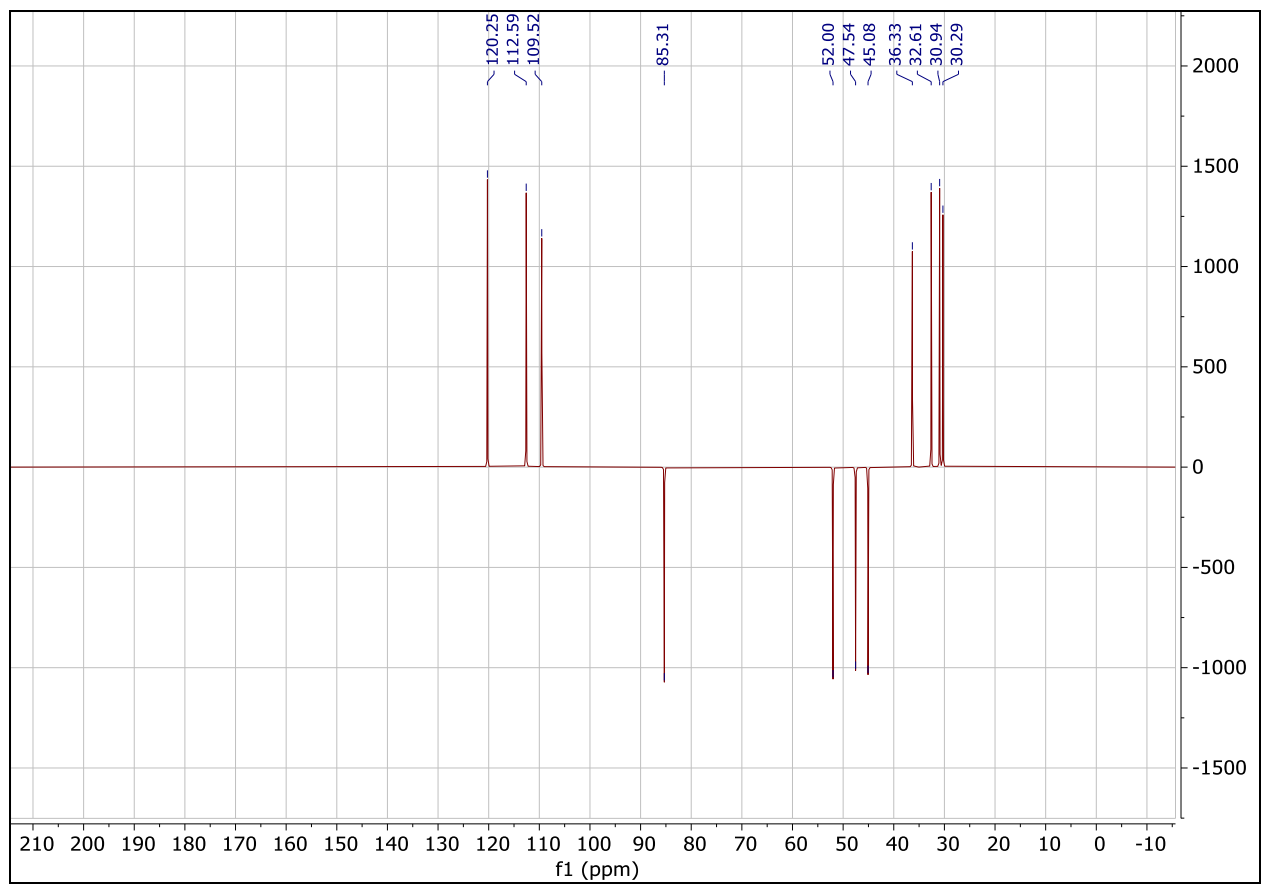
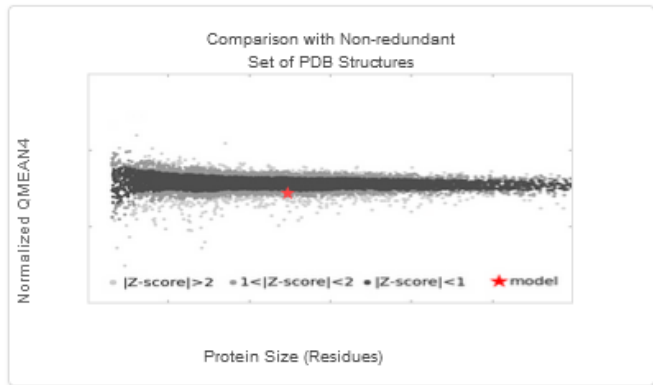
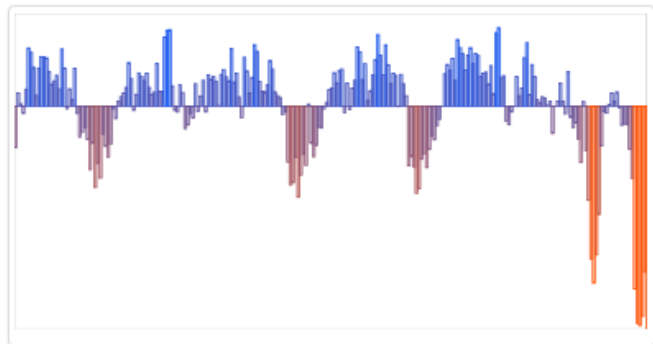
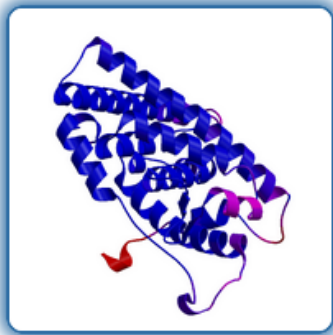


Fig. 2S. DEPT – 135 for Compound 1

Quality for 3ert.pdb

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QMEAN4 Value: -1.03

Fig. 3S. Quality comparison for 3ERT.pdb and Qmean value

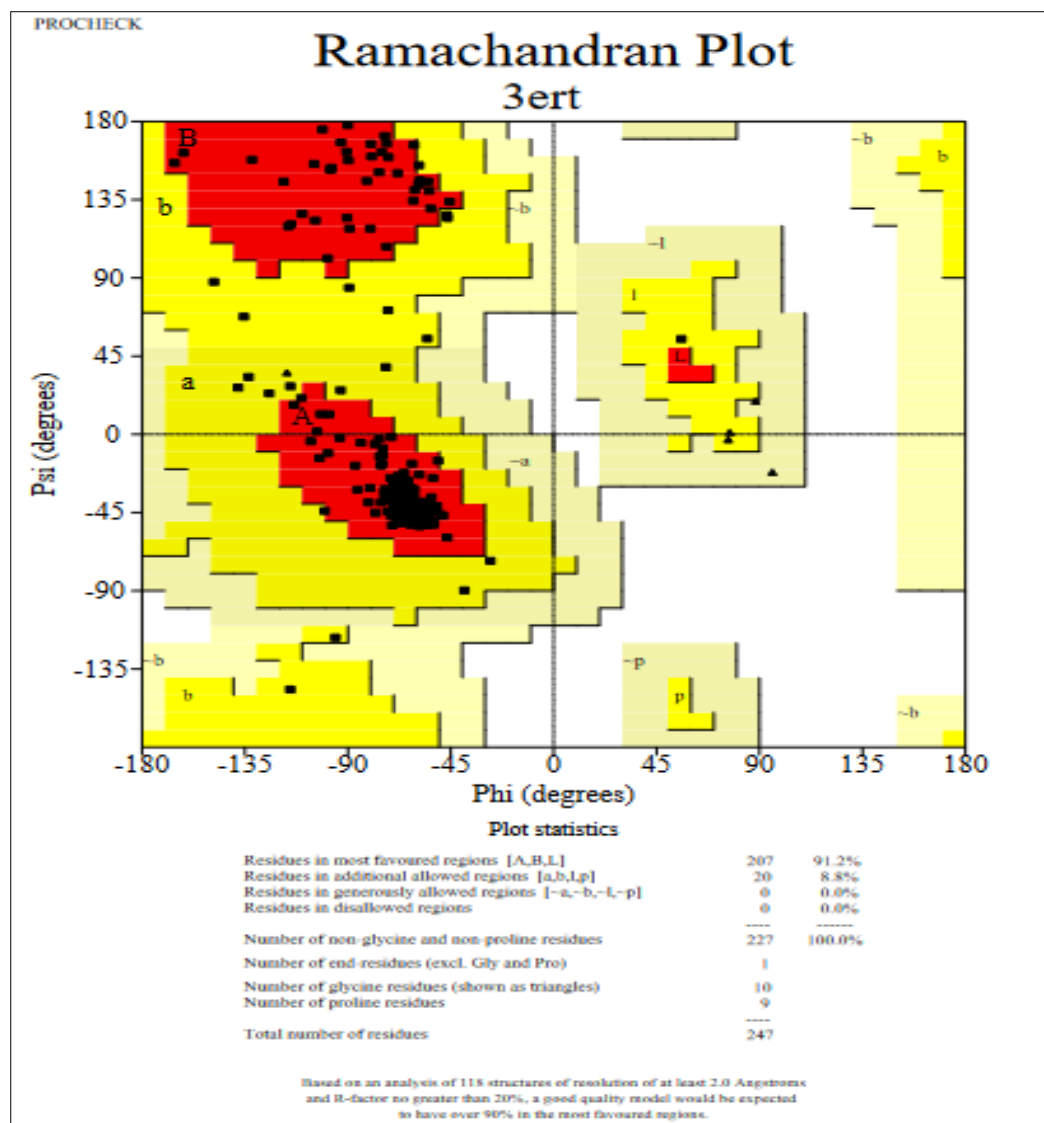


Fig. 4S. Ramachandran Plot for 3ERT. PDB with summary statistics