

# Isolation and Structure Elucidation of Natural Pentacyclic Triterpenoids and Phytochemical Investigation of Different Fractions of *Ziziphus spina-christi* (L.) Stem Bark Using LCHRMS Analysis

Essam N. Ads <sup>1,\*</sup>, Syed I. Hassan <sup>2</sup>, Saravanan Rajendrasozhan <sup>3</sup>, Mona H. Heta <sup>4</sup>, Shaza H. Aly <sup>5,\*</sup> and Mohamed A. Ali <sup>6</sup>

<sup>1</sup> Department of Chemistry, Faculty of Science, Zagazig University, Zagazig 44519, Egypt; [essam.adss@yahoo.com](mailto:essam.adss@yahoo.com)

<sup>2</sup> Department of Chemistry, College of Science, Sultan Qaboos University, P.O. Box 50, Muscat P.C. 123, Oman; [s.hasan@squ.edu.om](mailto:s.hasan@squ.edu.om)

<sup>3</sup> Department of Chemistry, College of Sciences, University of Ha'il, Ha'il 55476, Saudi Arabia; [s.rajendrasozhan@uoh.edu.sa](mailto:s.rajendrasozhan@uoh.edu.sa)

<sup>4</sup> Department of Pharmacognosy, Faculty of Pharmacy, Fayoum University, Fayoum 63514, Egypt; [mhm07@fayoum.edu.eg](mailto:mhm07@fayoum.edu.eg)

<sup>5</sup> Department of Pharmacognosy, Faculty of Pharmacy, Badr University in Cairo (BUC), Badr City 11829, Egypt; [shaza.husseiny@buc.edu.eg](mailto:shaza.husseiny@buc.edu.eg)

<sup>6</sup> School of Biotechnology, Badr University in Cairo (BUC), Badr City 11829, Egypt; [mohamed.ahmed\\_ali@buc.edu.eg](mailto:mohamed.ahmed_ali@buc.edu.eg)

\* Correspondence: [essam.adss@yahoo.com](mailto:essam.adss@yahoo.com) (E.N.A.); [shaza.husseiny@buc.edu.eg](mailto:shaza.husseiny@buc.edu.eg) (S.H.A.);  
Tel.: +20-15-5551-2497 or +20-10-9957-6833 or +20-50-4037-366 (E.N.A.)

Supplementary material

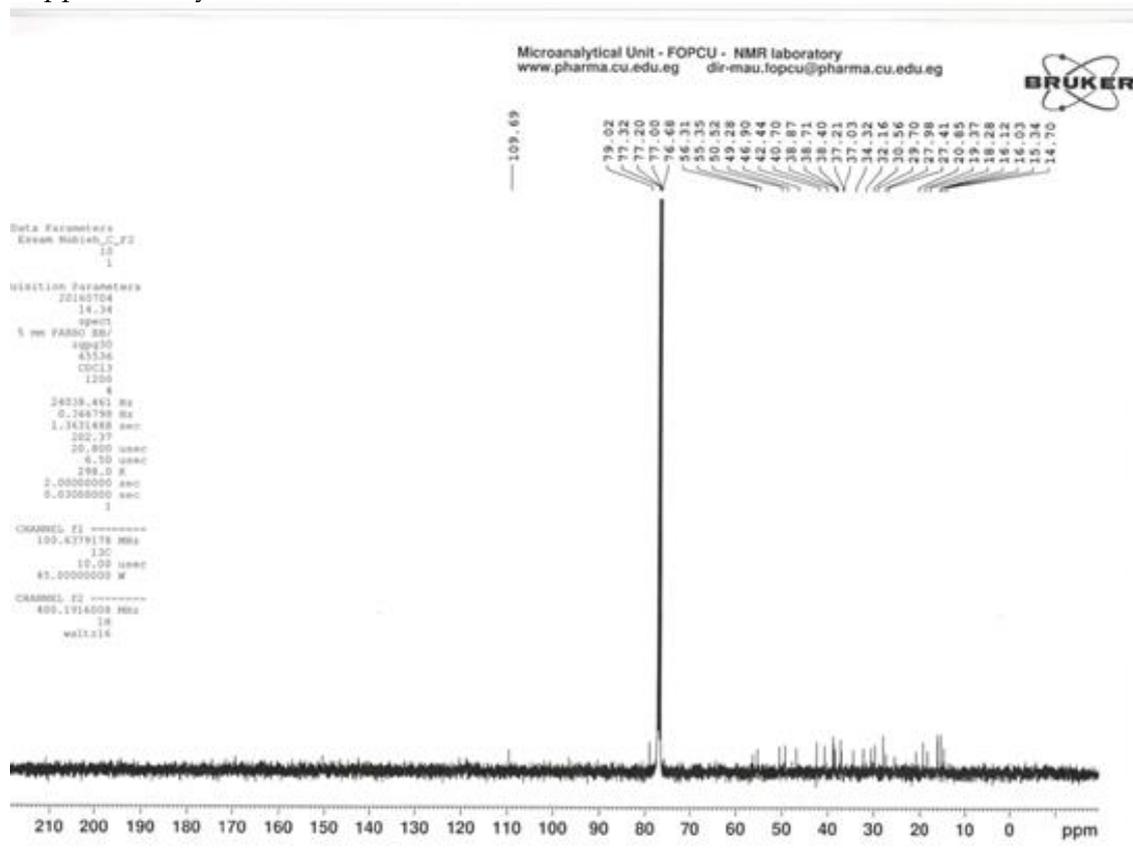


Figure S1. <sup>13</sup>C-NMR Spectra of betulinic acid

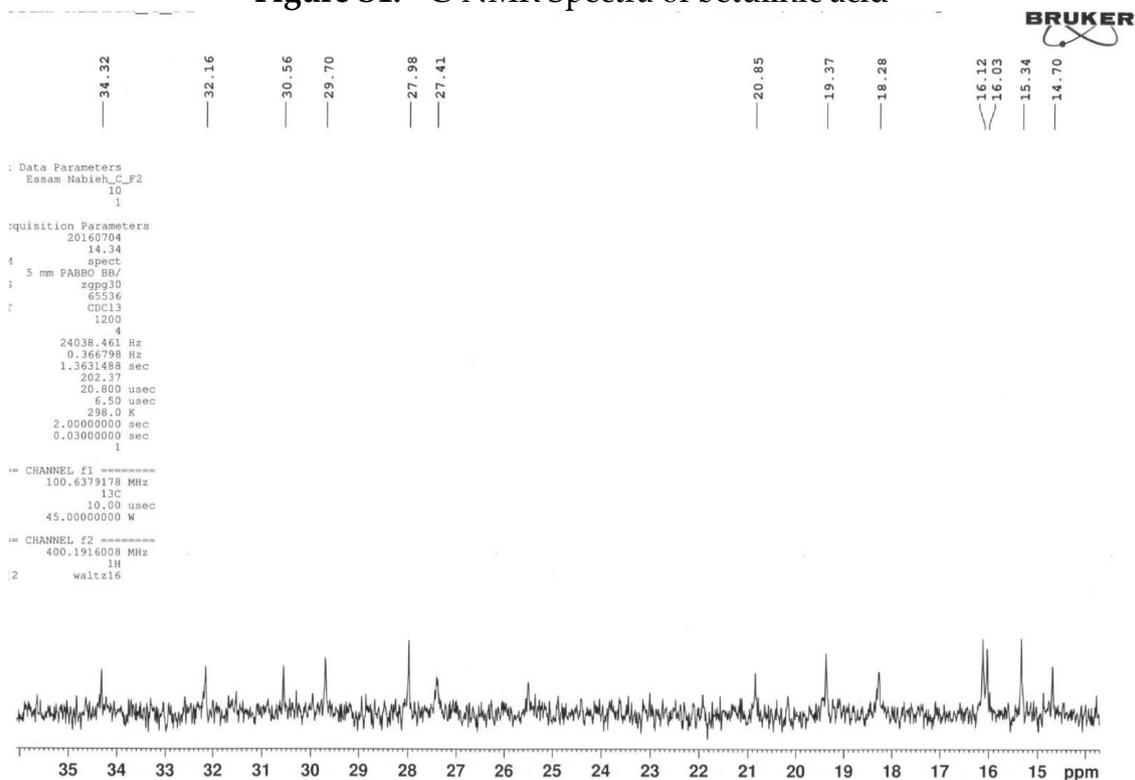


Figure S2. <sup>13</sup>C-NMR Spectra of betulinic acid (enlarged)

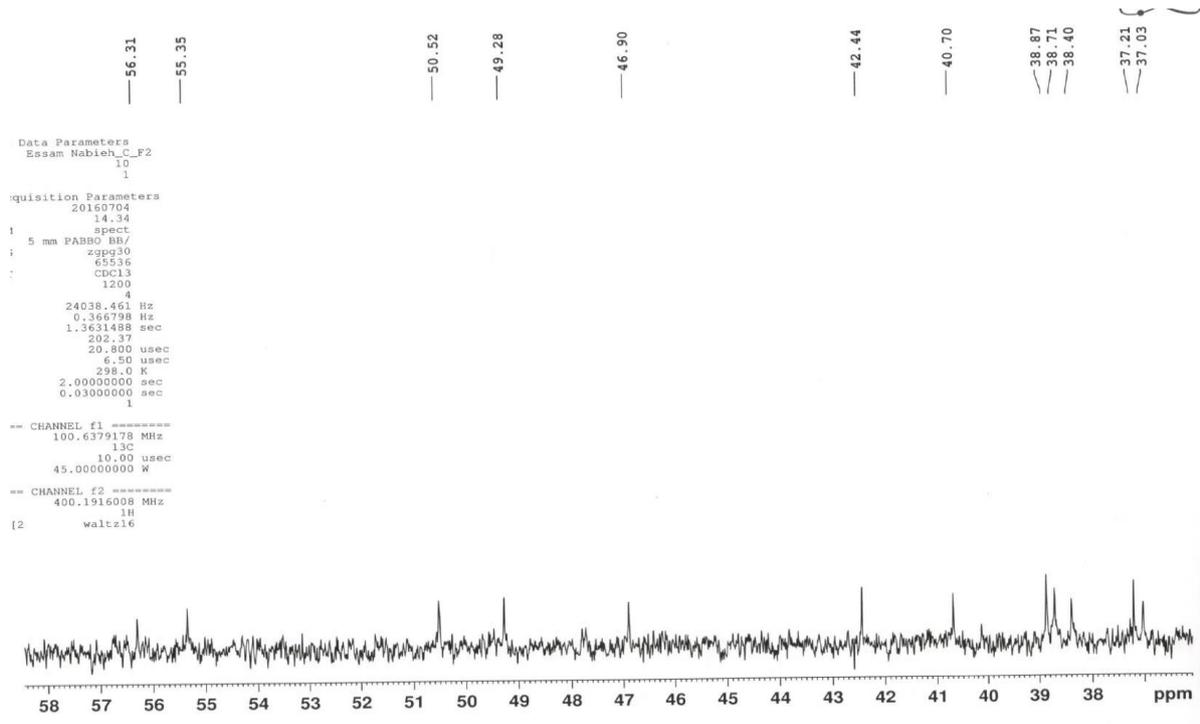


Figure S3.  $^{13}\text{C}$ -NMR Spectra of betulinic acid (enlarged)

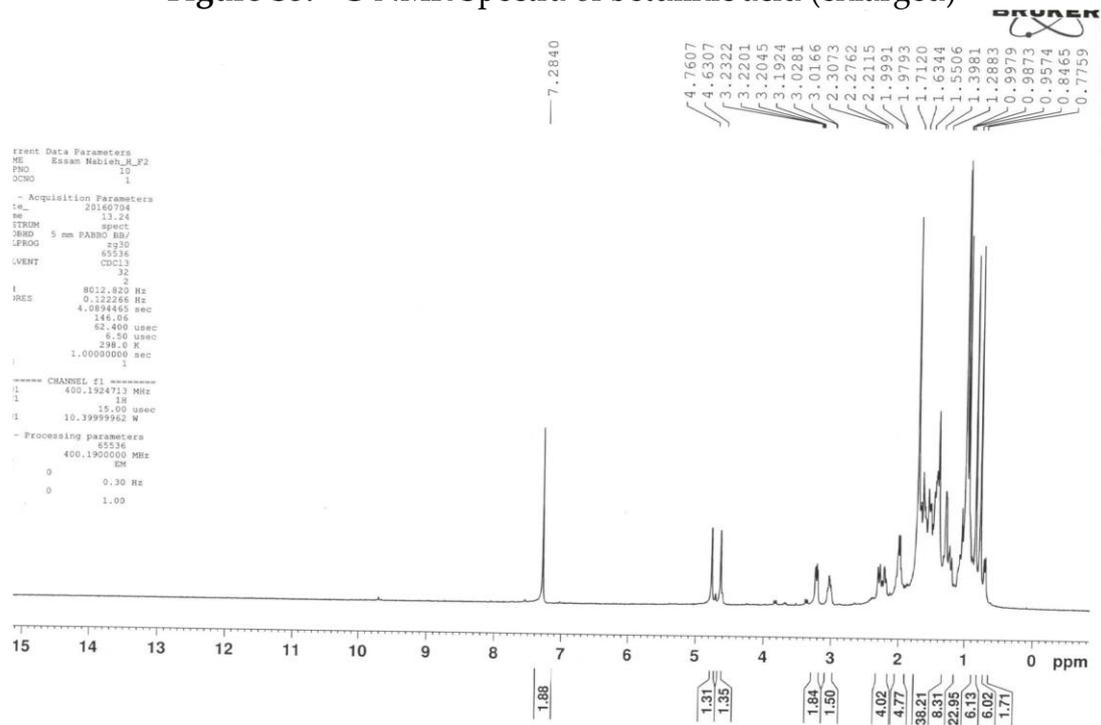


Figure S4.  $^1\text{H}$ -NMR Spectra of betulinic acid

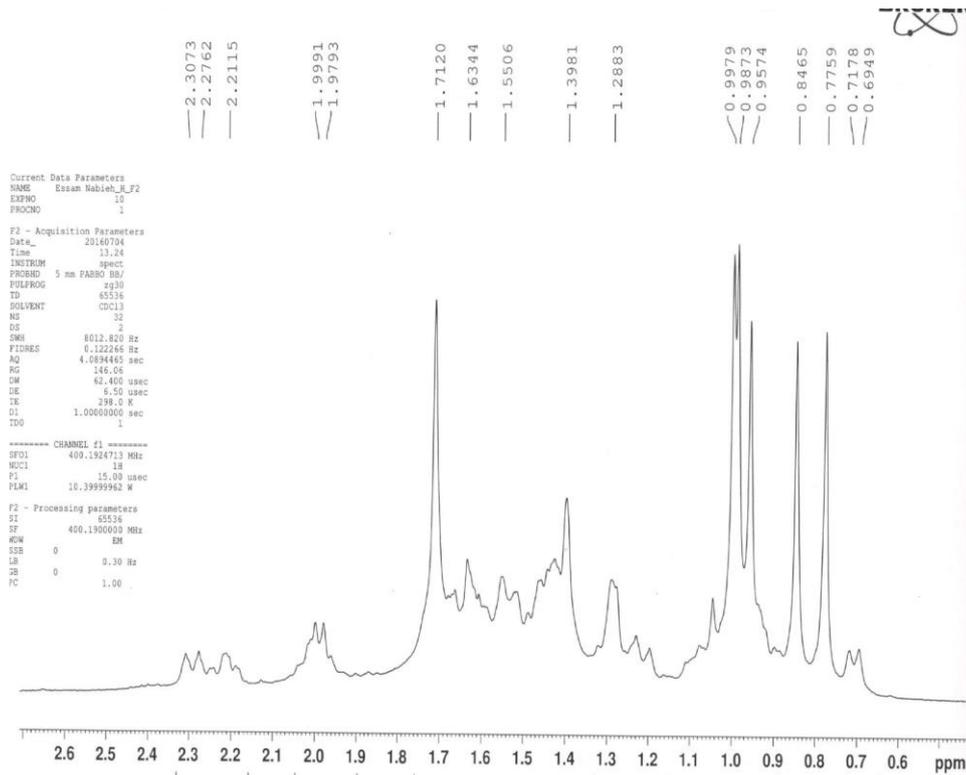


Figure S4. <sup>1</sup>H-NMR Spectra of betulinic acid (enlarged)

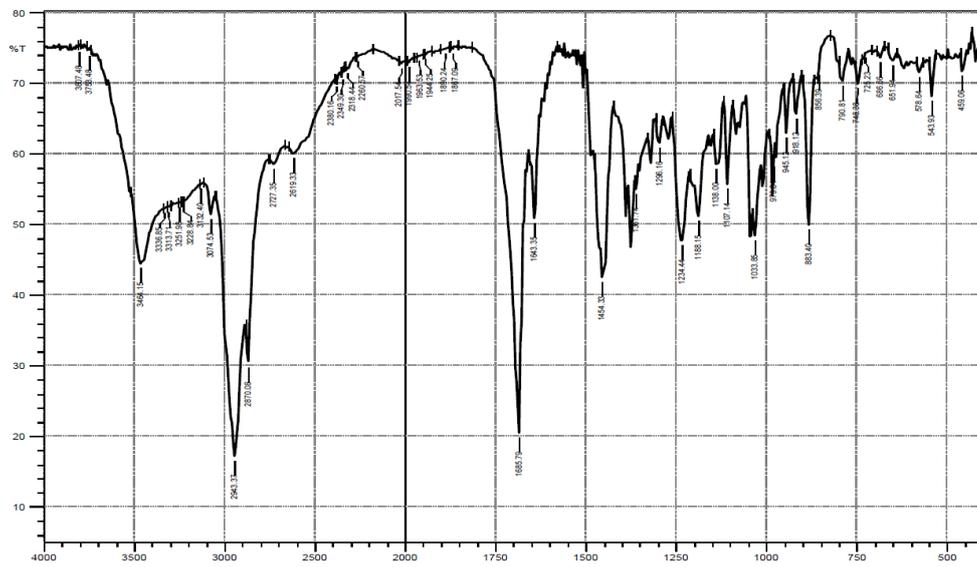
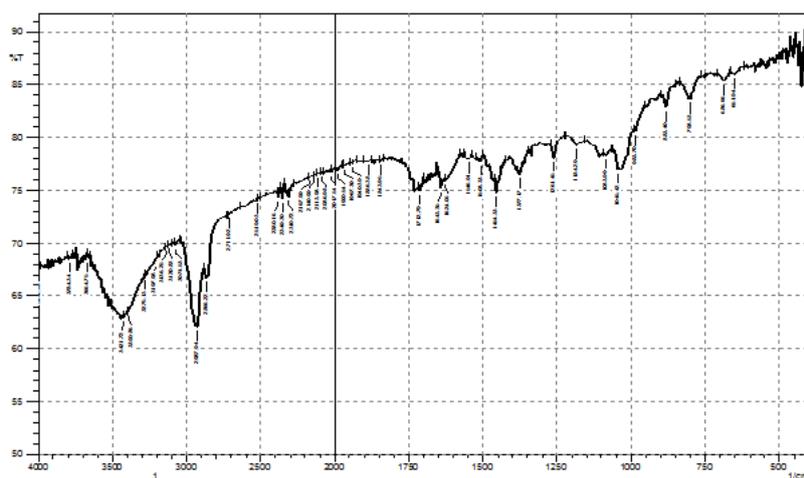


Figure S5. IR Spectrum of betulinic acid



**Figure S6.** IR Spectrum of betuline

**Table S1.** Docking validation results

Protein	Control for RMSD	RMSD
<i>Aspergillus Fumigatus</i>	Voriconazole	1.2
<i>C. Albicans</i>	(1-Methyl-1H-Imidazol-2-yl)-(3-Methyl-4-{3-[(Pyridin-3-yl-methyl)-Amino]-Propoxy}-Benzofuran-2-yl)-Methanone	0.7
<i>E.coli</i>	[7,8-Dihydro-Pterin-6-yl Methanyl]-Phosphonophosphate	0.9
<i>Pseudomonas aeruginosa</i>	Thymidine-5'-Diphosphate	0.8
<i>S. aureus</i>	6-Hydroxymethylpterin-Diphosphate	0.6
<i>Streptococcus pneumoniae</i>	Pterin-6-yl-Methyl-Monophosphate	0.7