Supplementary Material

Synthesis, Cytotoxicity and Molecular Docking of New Hybrid Compounds by Combination of Curcumin with Oleanolic Acid

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[2] Department of Clinical Chemistry and Molecular Diagnostics, Poznan University of Medical Sciences, Rokietnicka 3 Str., 60-806 Poznań, Poland; etoton@ump.edu.pl (E.T.)
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* Correspondence: kasik@ump.edu.pl (K.S.K.)

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KS1

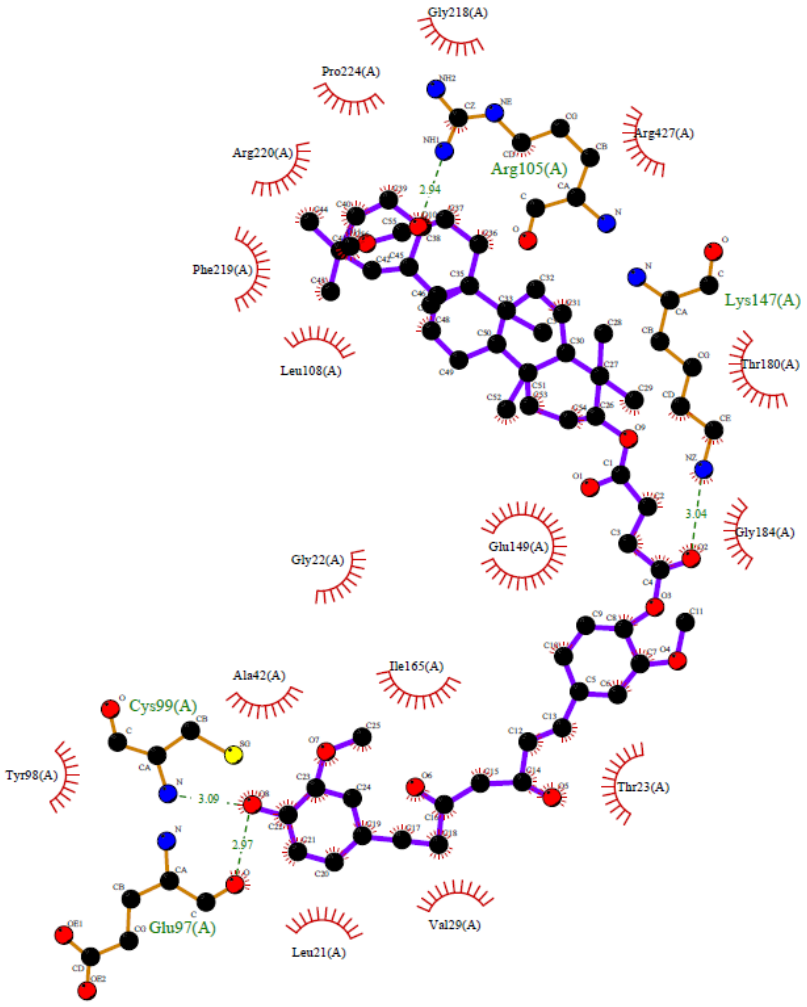

Figure S1 The first poses of the docked ligands to compound **KS1**; hydrogen atoms are omitted; 4kik.pdb protein (LigPlot+ v.2.2 software).

KS2_keto

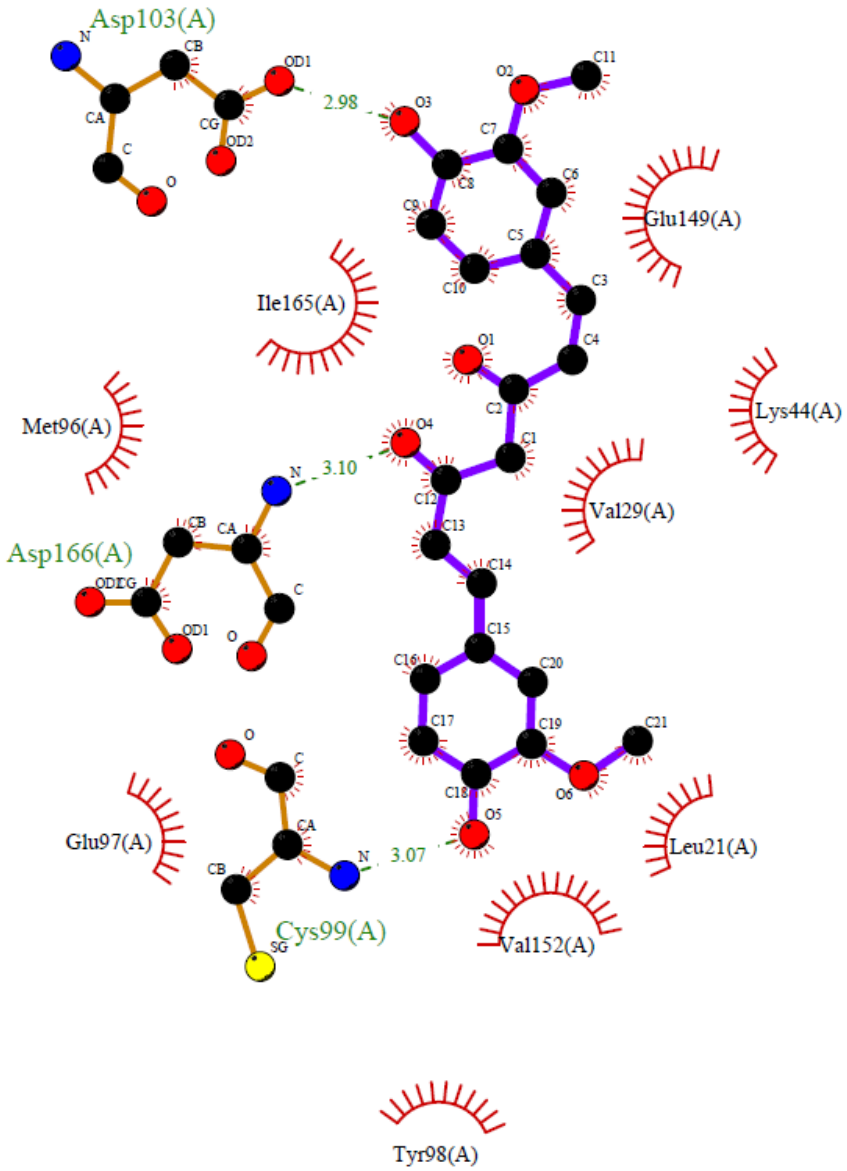

Figure S2 The first poses of the docked ligands to compound **KS2_keto**; hydrogen atoms are omitted; 4kik.pdb protein (LigPlot+ v.2.2 software).

KS2_enol

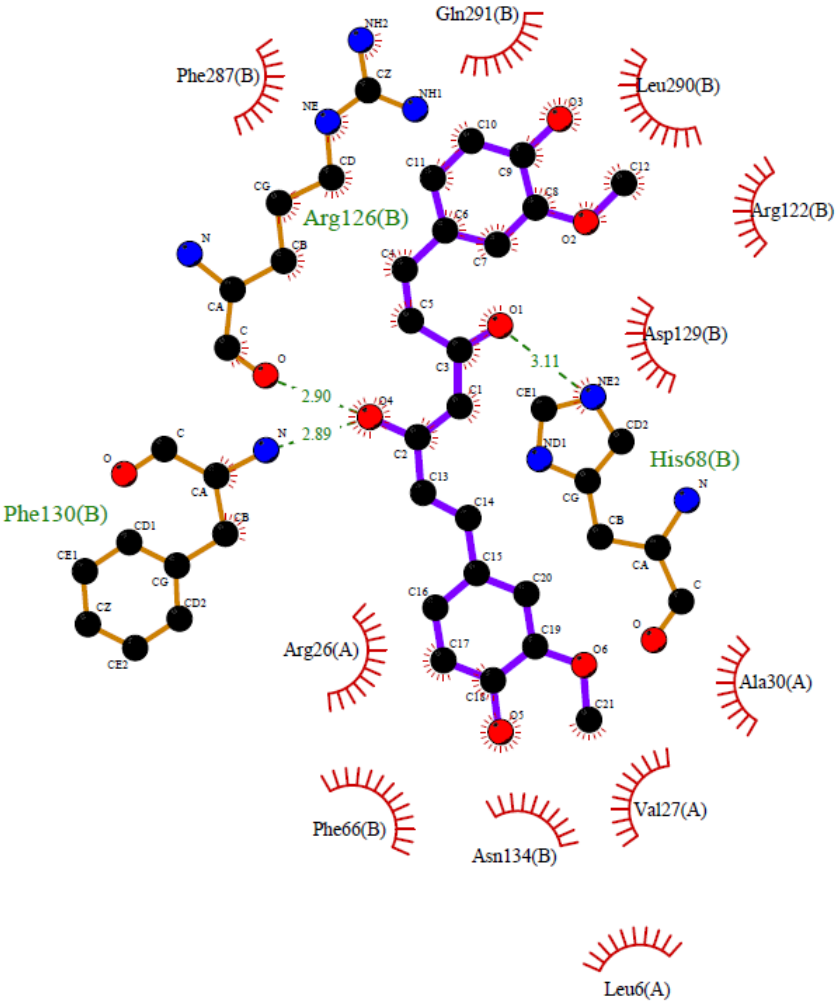

Figure S3 The first poses of the docked ligands to compound **KS2_enol**; hydrogen atoms are omitted; 4kik.pdb protein (LigPlot+ v.2.2 software).

KS3

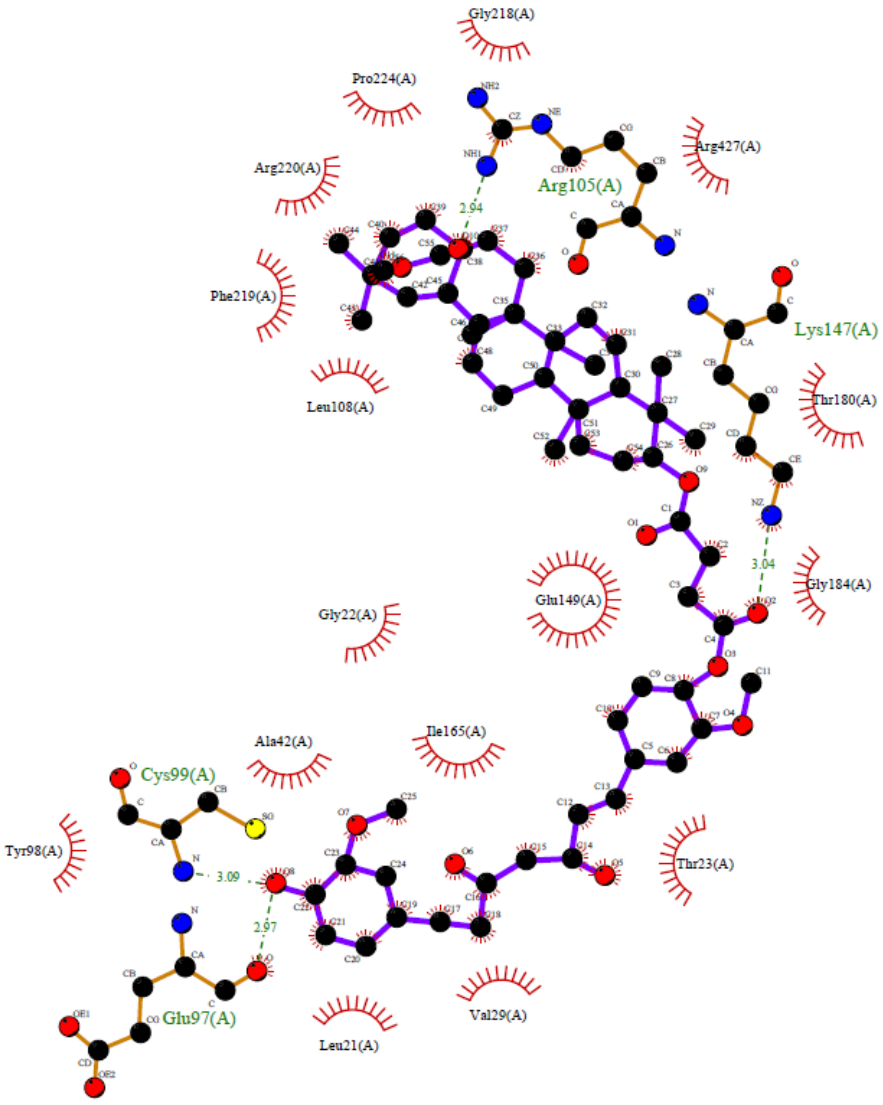

Figure S4 The first poses of the docked ligands to compound **KS3**; hydrogen atoms are omitted; 4kik.pdb protein (LigPlot+ v.2.2 software).

KS4

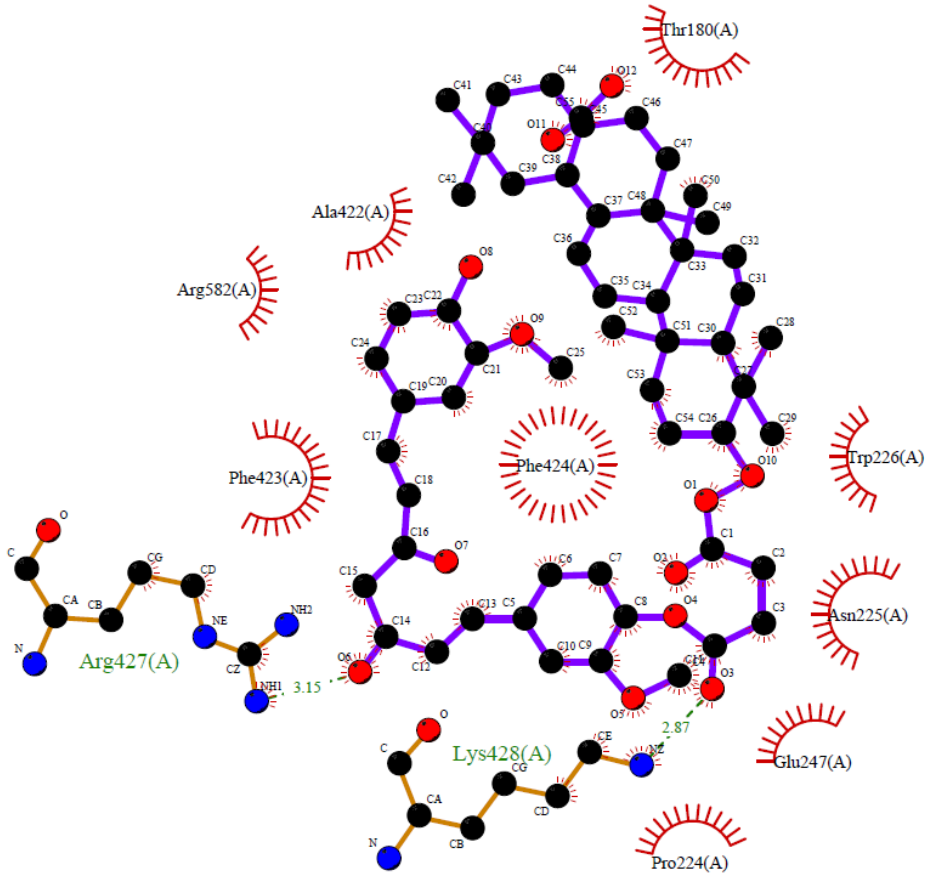

Figure S5 The first poses of the docked ligands to compound **KS4**; hydrogen atoms are omitted; 4kik.pdb protein (LigPlot+ v.2.2 software).

KS5

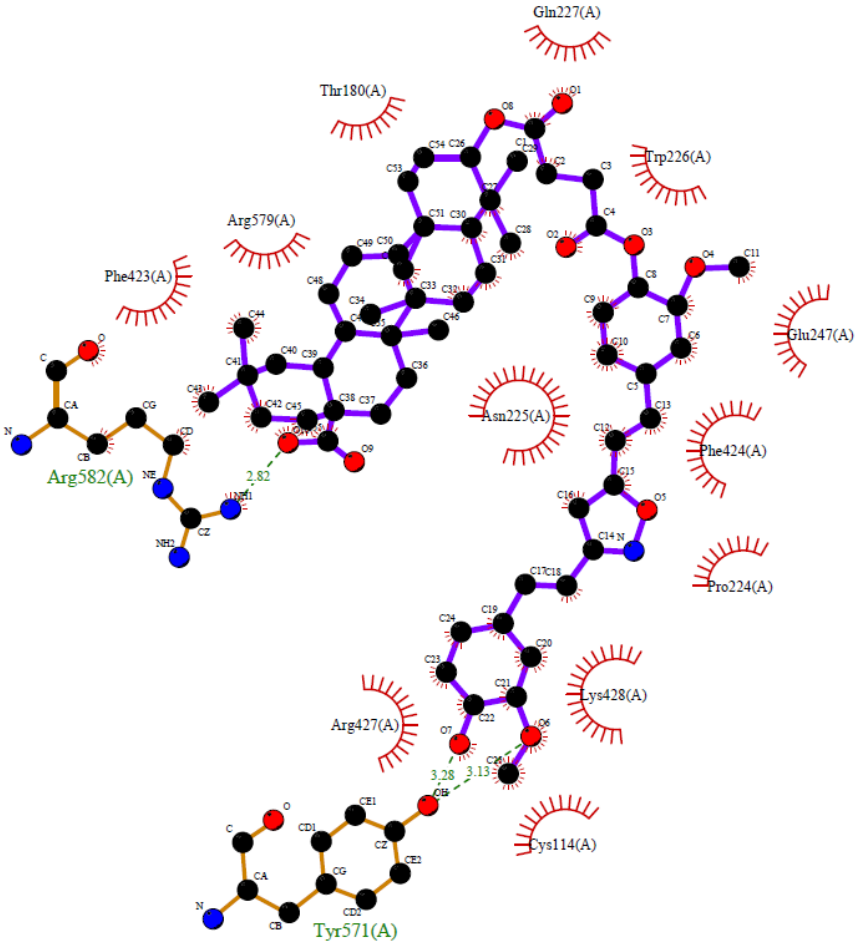

Figure S6 The first poses of the docked ligands to compound **KS5**; hydrogen atoms are omitted; 4kik.pdb protein (LigPlot+ v.2.2 software).

KS6

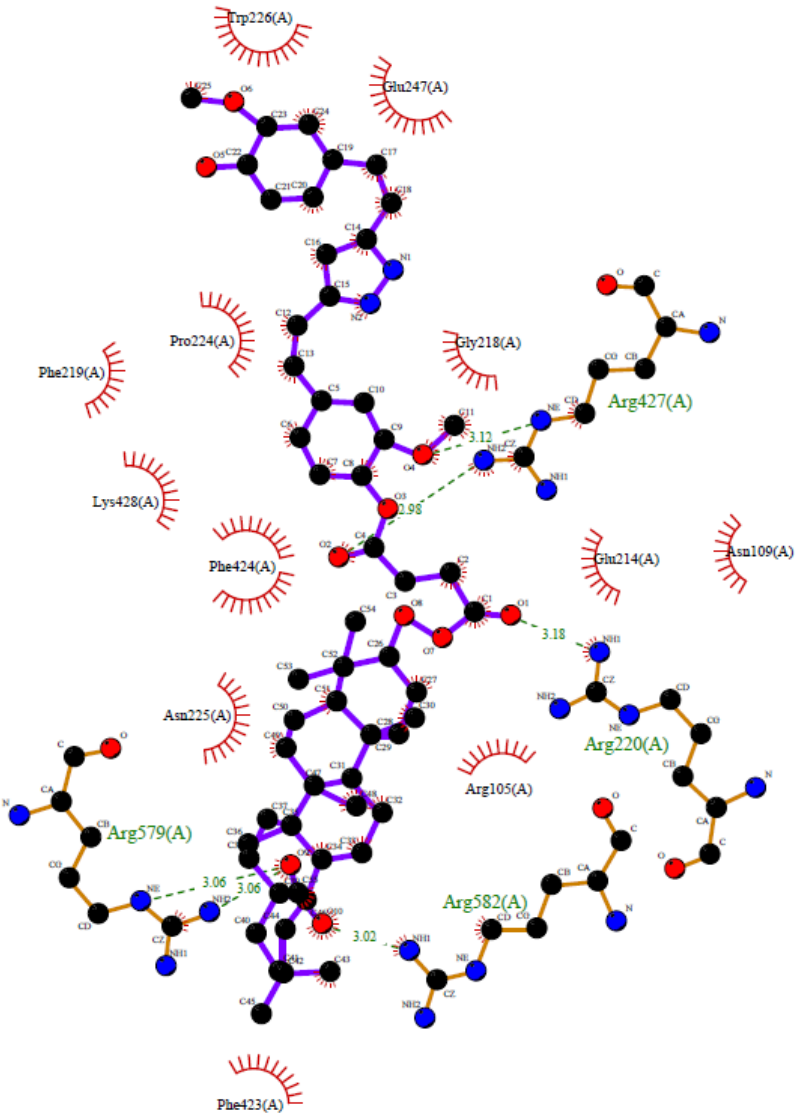

Figure S7 The first poses of the docked ligands to compound **KS6**; hydrogen atoms are omitted; 4kik.pdb protein (LigPlot+ v.2.2 software).

KS7

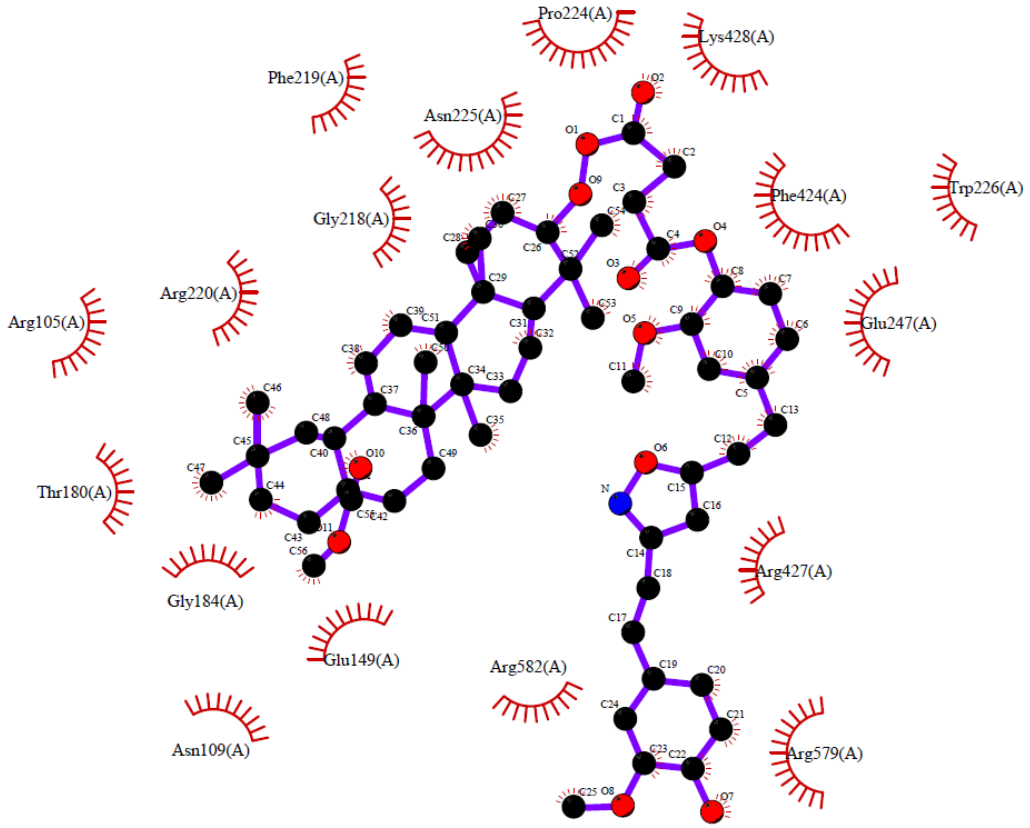

Figure S8 The first poses of the docked ligands to compound **KS7**; hydrogen atoms are omitted; 4kik.pdb protein (LigPlot+ v.2.2 software).

KS8

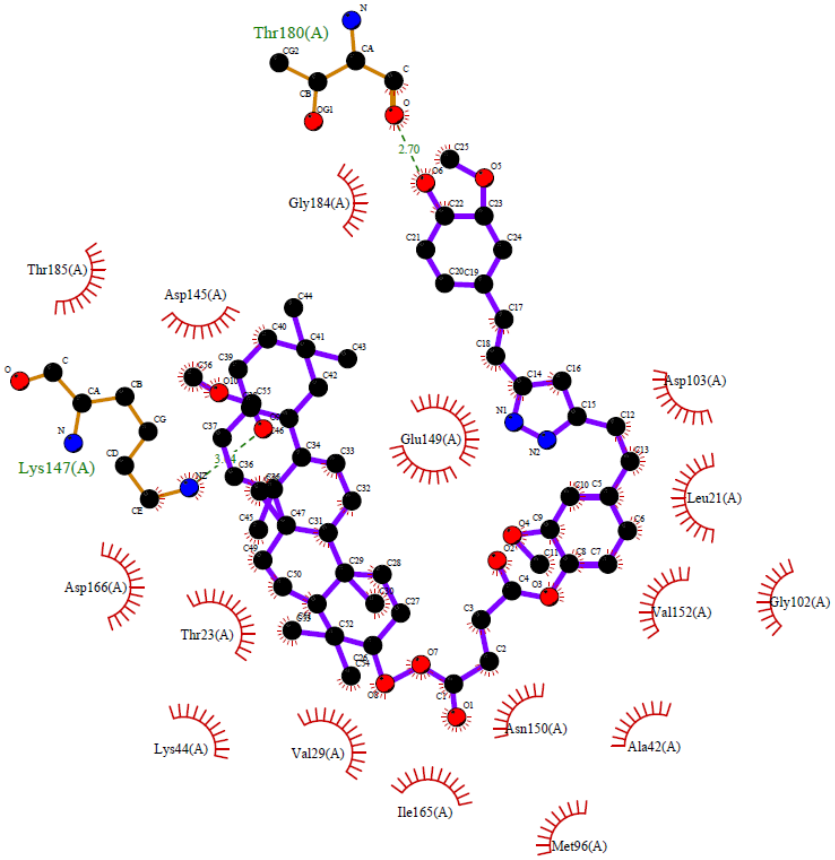

Figure S9 The first poses of the docked ligands to compound **KS8**; hydrogen atoms are omitted; 4kik.pdb protein (LigPlot+ v.2.2 software).

KS1

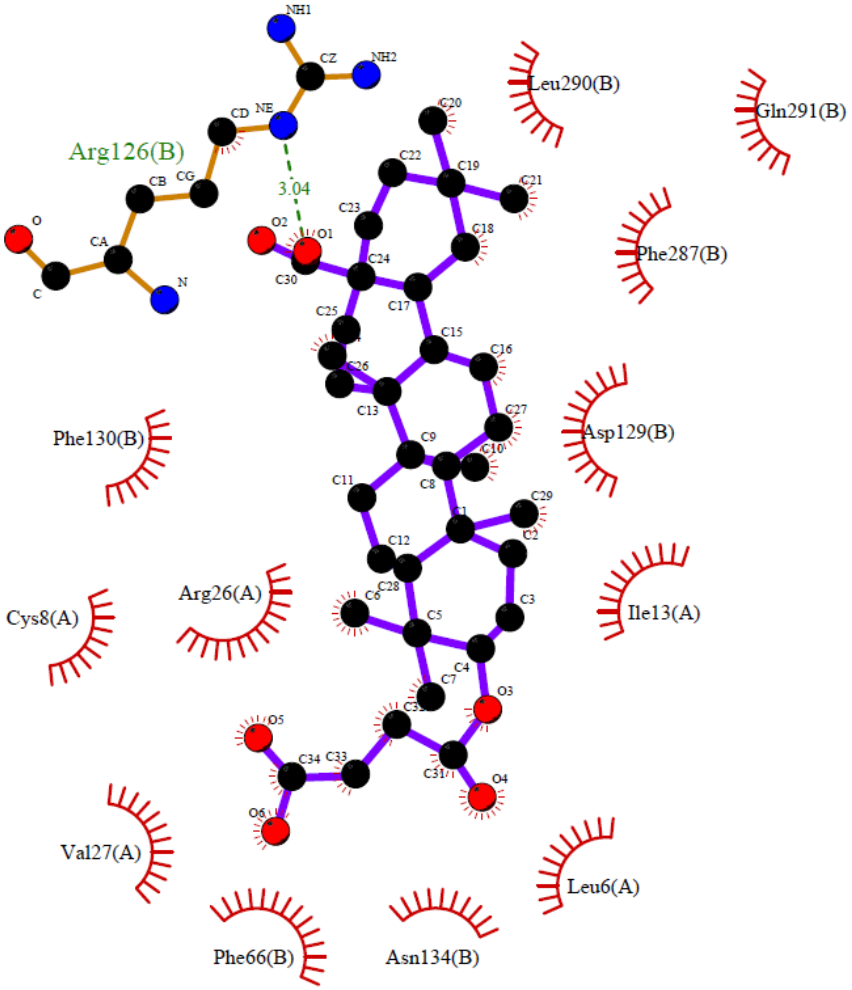

Figure S10 The first poses of the docked ligands to compound **KS1**; hydrogen atoms are omitted; 2w96.pdb protein (LigPlot+ v.2.2 software).

KS2_keto

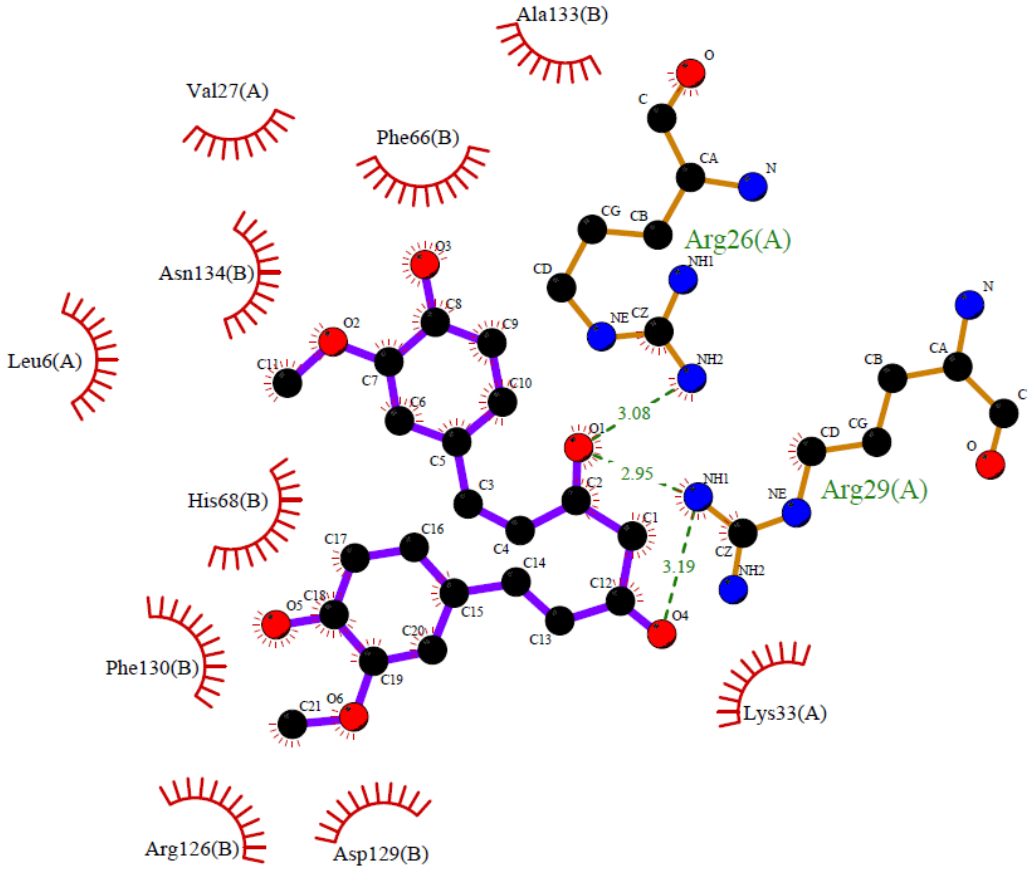

Figure S11 The first poses of the docked ligands to compound **KS2_keto**; hydrogen atoms are omitted; 2w96.pdb protein (LigPlot+ v.2.2 software).

KS2_enol

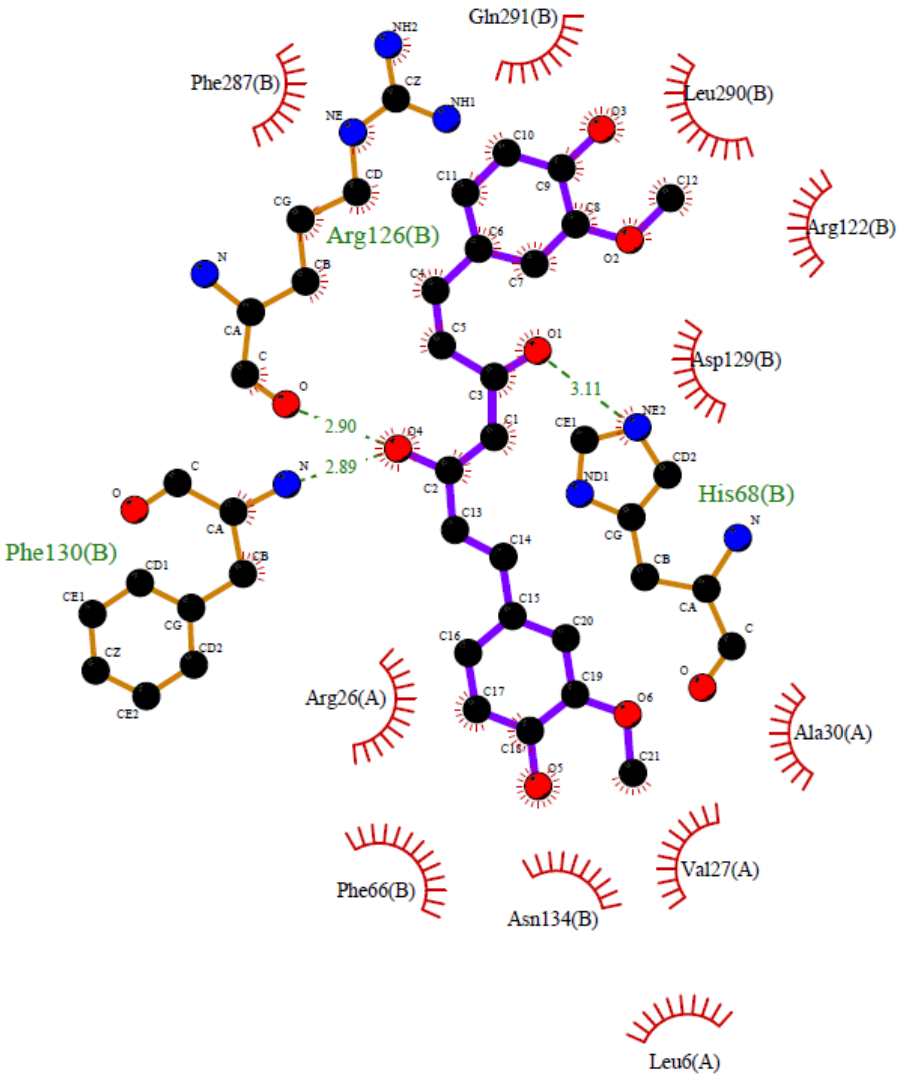

Figure S12 The first poses of the docked ligands to compound **KS2_enol**; hydrogen atoms are omitted; 2w96.pdb protein (LigPlot+ v.2.2 software).

KS3

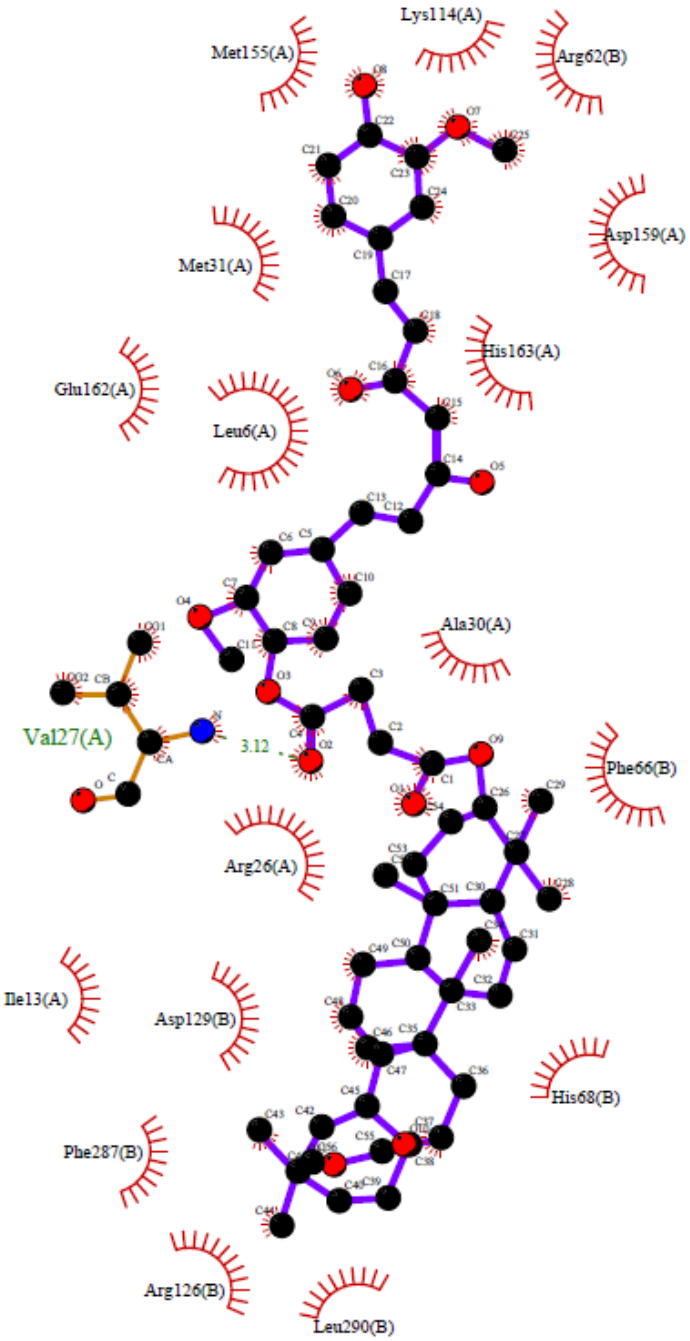

Figure S13. The first poses of the docked ligands to compound **KS3**; hydrogen atoms are omitted; 2w96.pdb protein (LigPlot+ v.2.2 software).

KS4

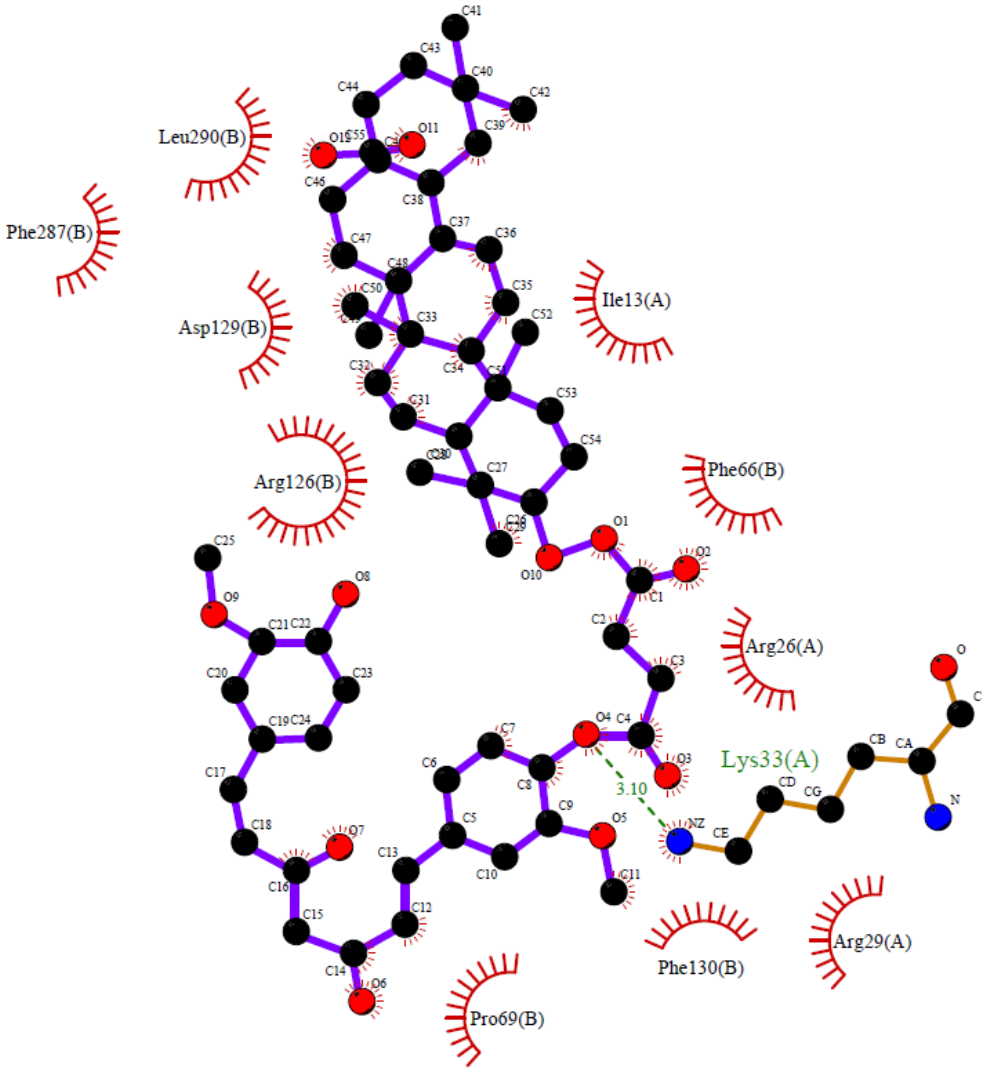

Figure S14 The first poses of the docked ligands to compound **KS4**; hydrogen atoms are omitted; 2w96.pdb protein (LigPlot+ v.2.2 software).

KS5

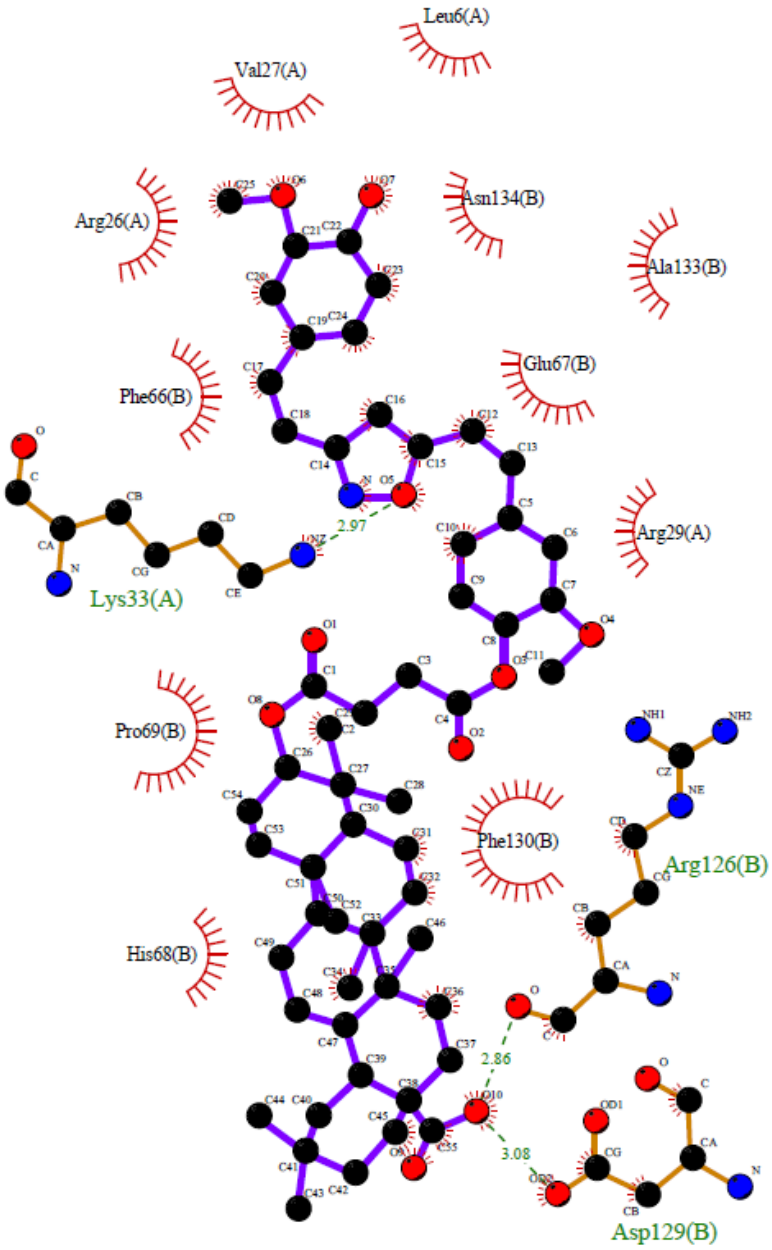

Figure S15 The first poses of the docked ligands to compound **KS5**; hydrogen atoms are omitted; 2w96.pdb protein (LigPlot+ v.2.2 software).

KS6

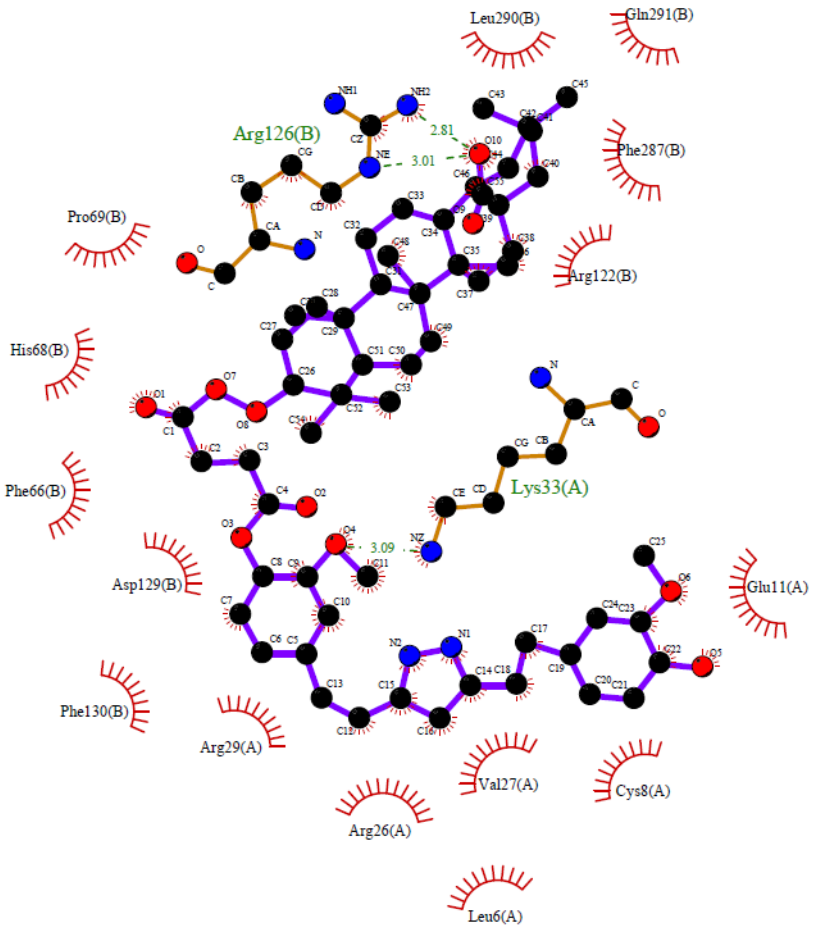

Figure S16 The first poses of the docked ligands to compound **KS6**; hydrogen atoms are omitted; 2w96.pdb protein (LigPlot+ v.2.2 software).

KS7

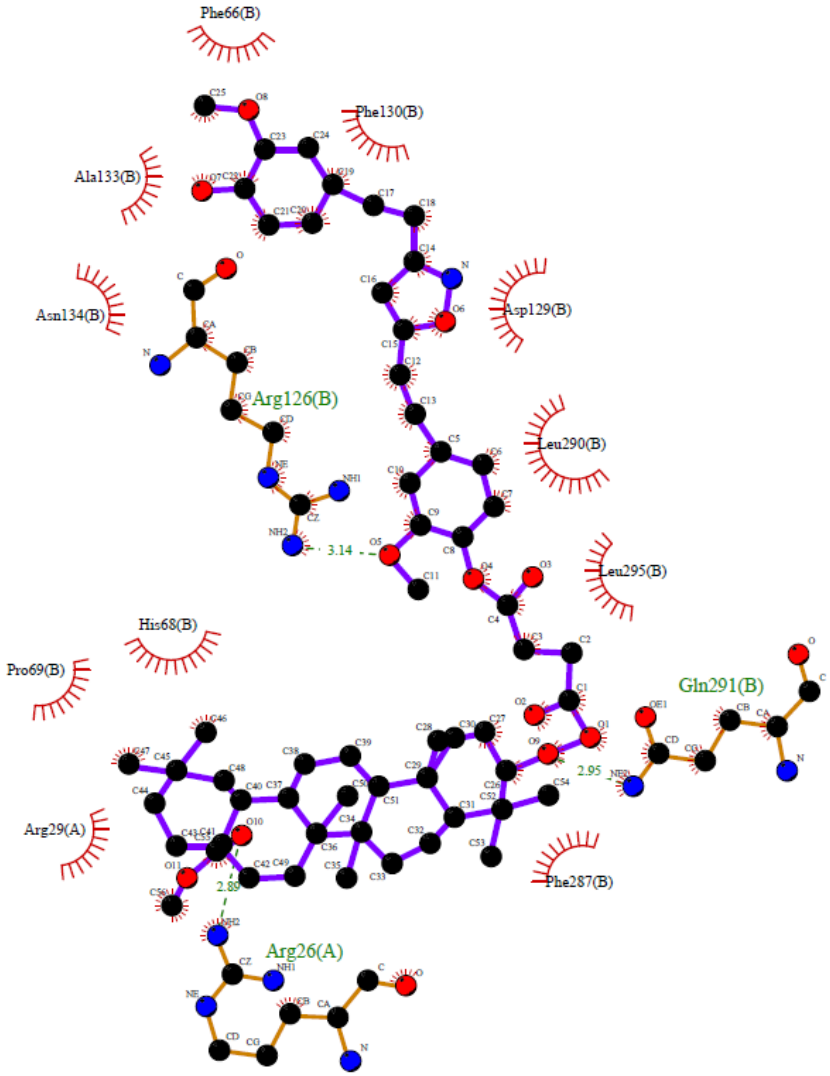

Figure S17 The first poses of the docked ligands to compound **KS7**; hydrogen atoms are omitted; 2w96.pdb protein (LigPlot+ v.2.2 software).

KS8

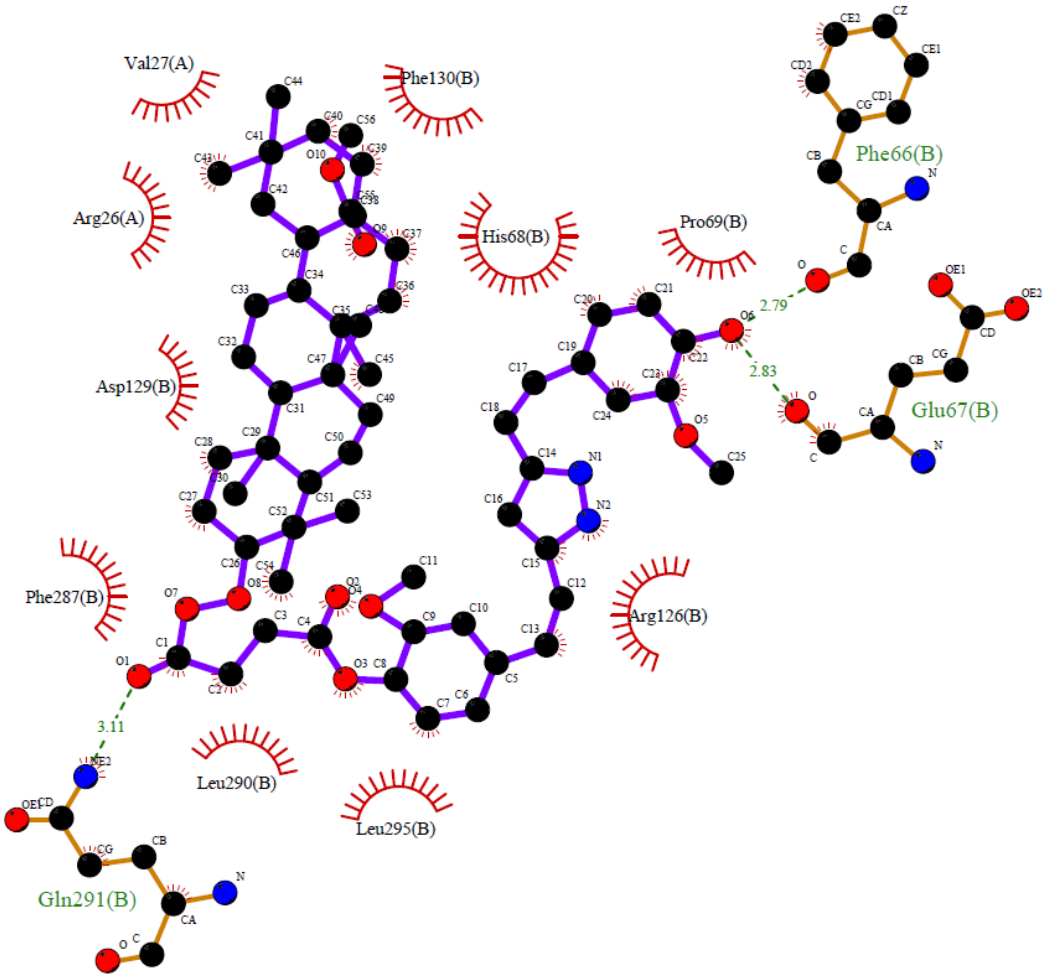

Figure S18 The first poses of the docked ligands to compound **KS8**; hydrogen atoms are omitted; 2w96.pdb protein (LigPlot+ v.2.2 software).

KS1

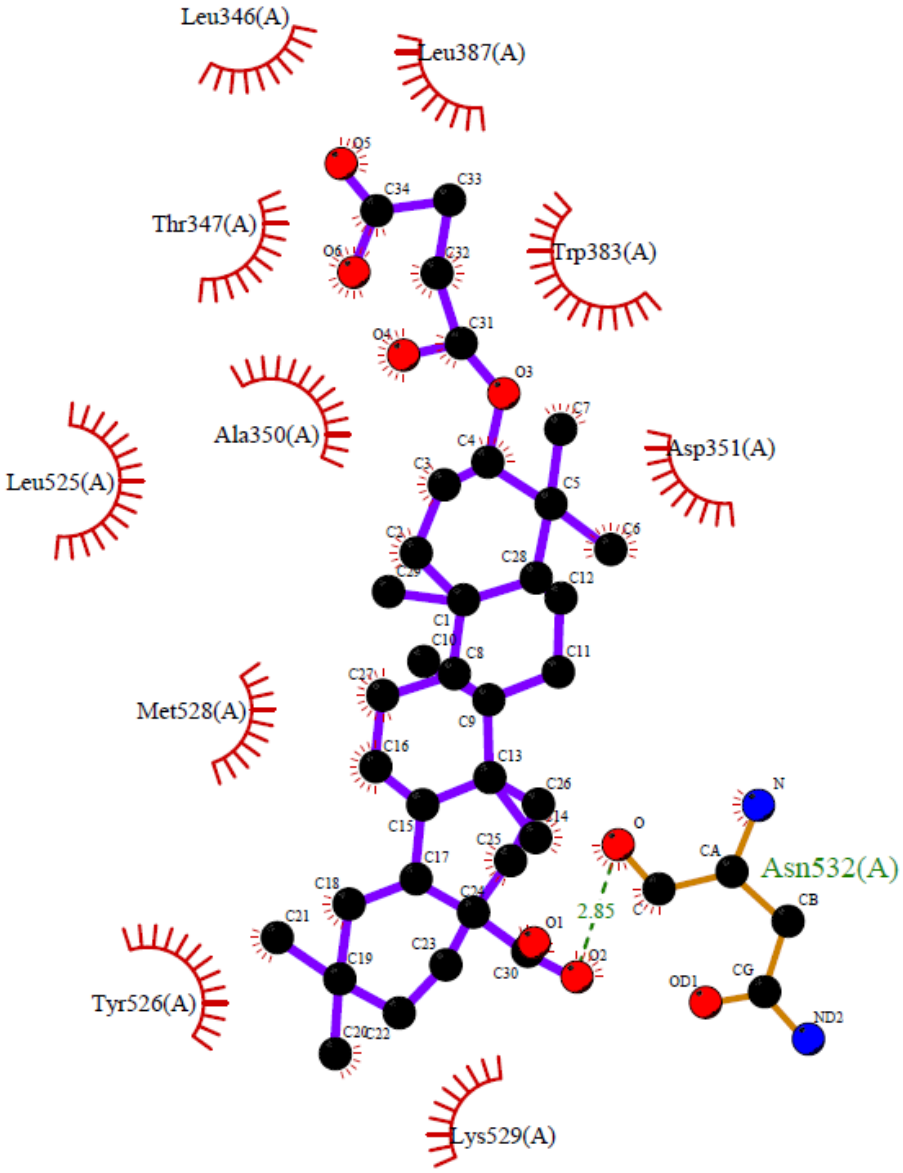

Figure S19 The first poses of the docked ligands to compound **KS1**; hydrogen atoms are omitted; 3dt3.pdb protein (LigPlot+ v.2.2 software).

KS2_keto

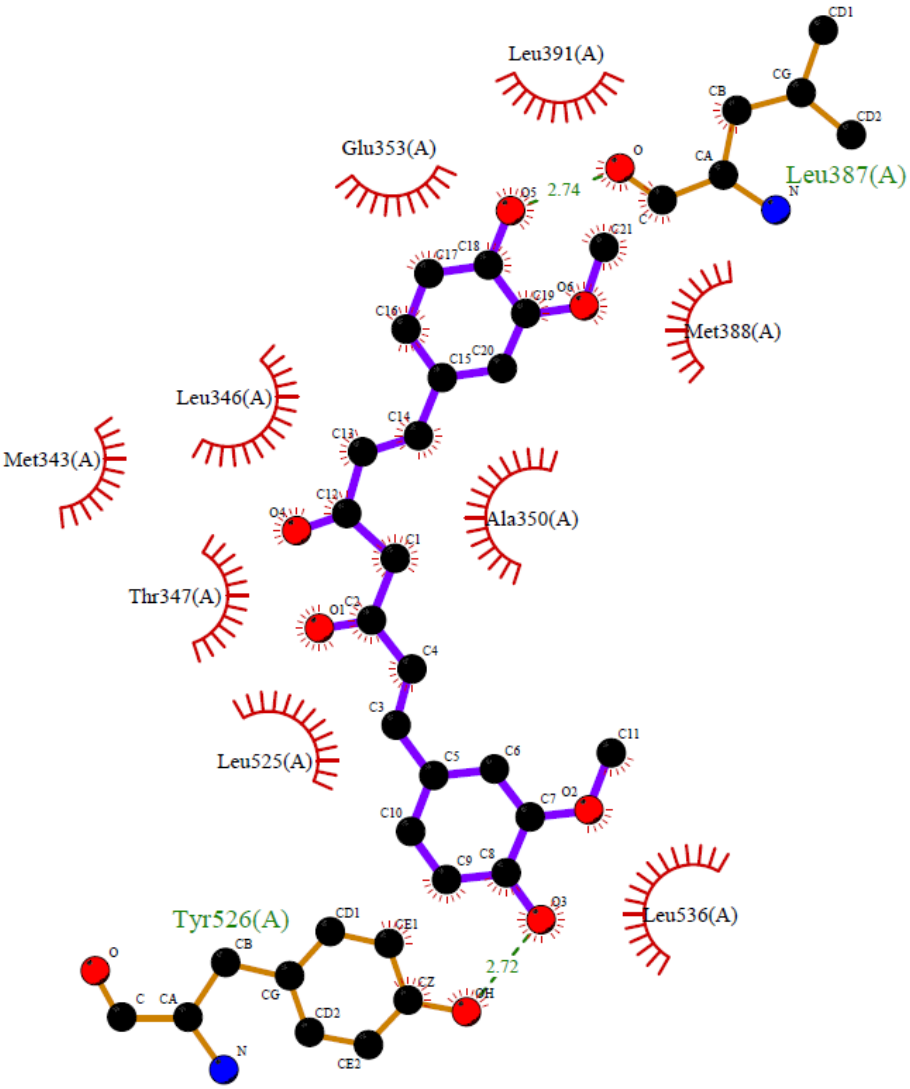

Figure S20a The first poses of the docked ligands to compound **KS2_keto**; hydrogen atoms are omitted; 3dt3.pdb protein (LigPlot+ v.2.2 software).

KS2_enol

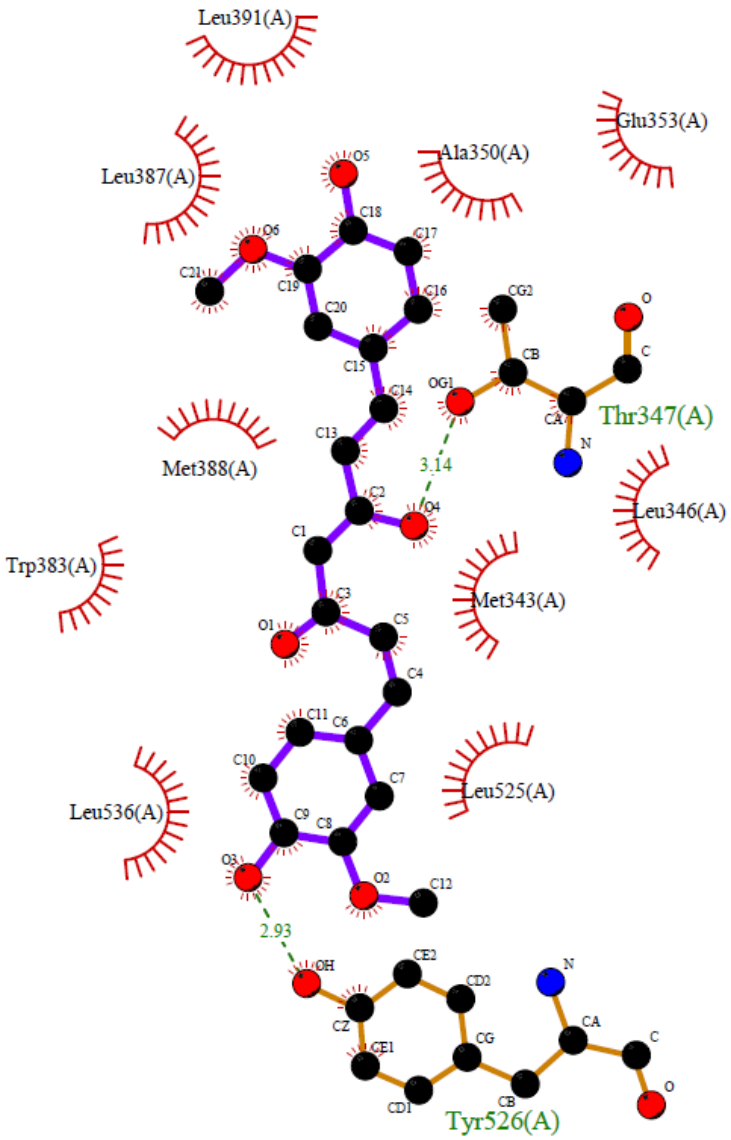

Figure S20b The first poses of the docked ligands to compound **KS2_enol**; hydrogen atoms are omitted; 3dt3.pdb protein (LigPlot+ v.2.2 software).

KS3

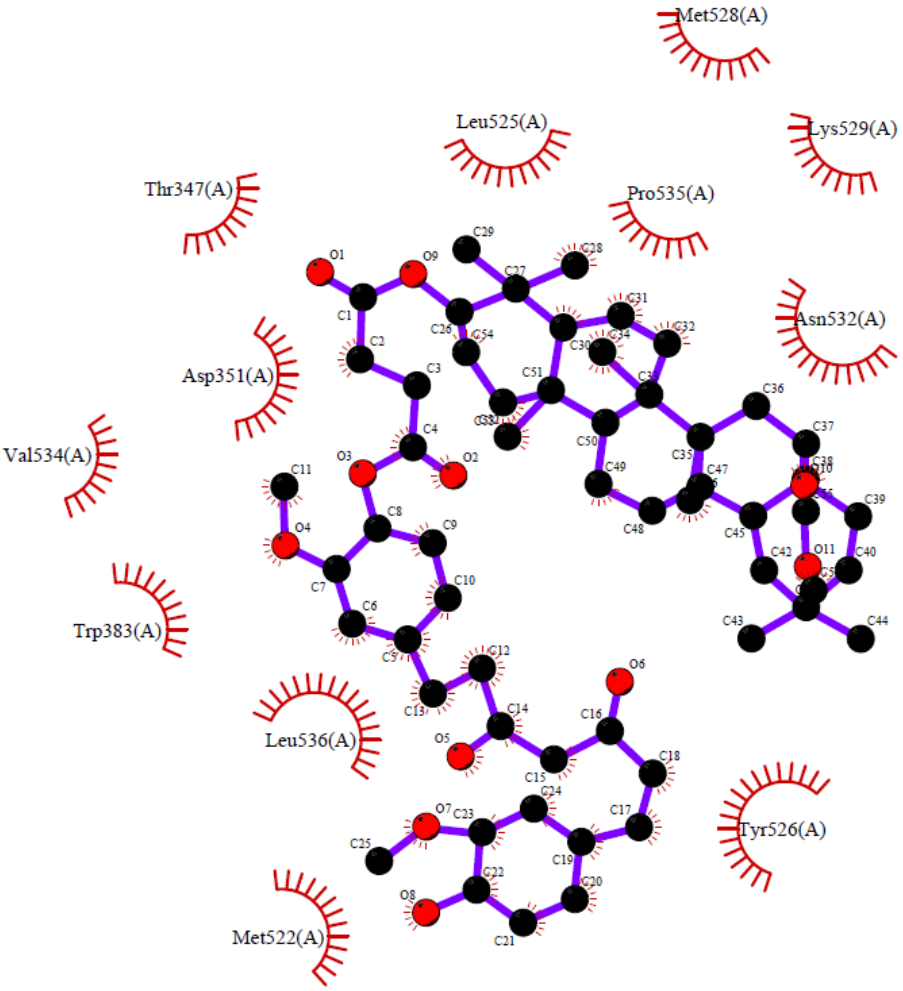

Figure S21 The first poses of the docked ligands to compound **KS3**; hydrogen atoms are omitted; 3dt3.pdb protein (LigPlot+ v.2.2 software).

KS4

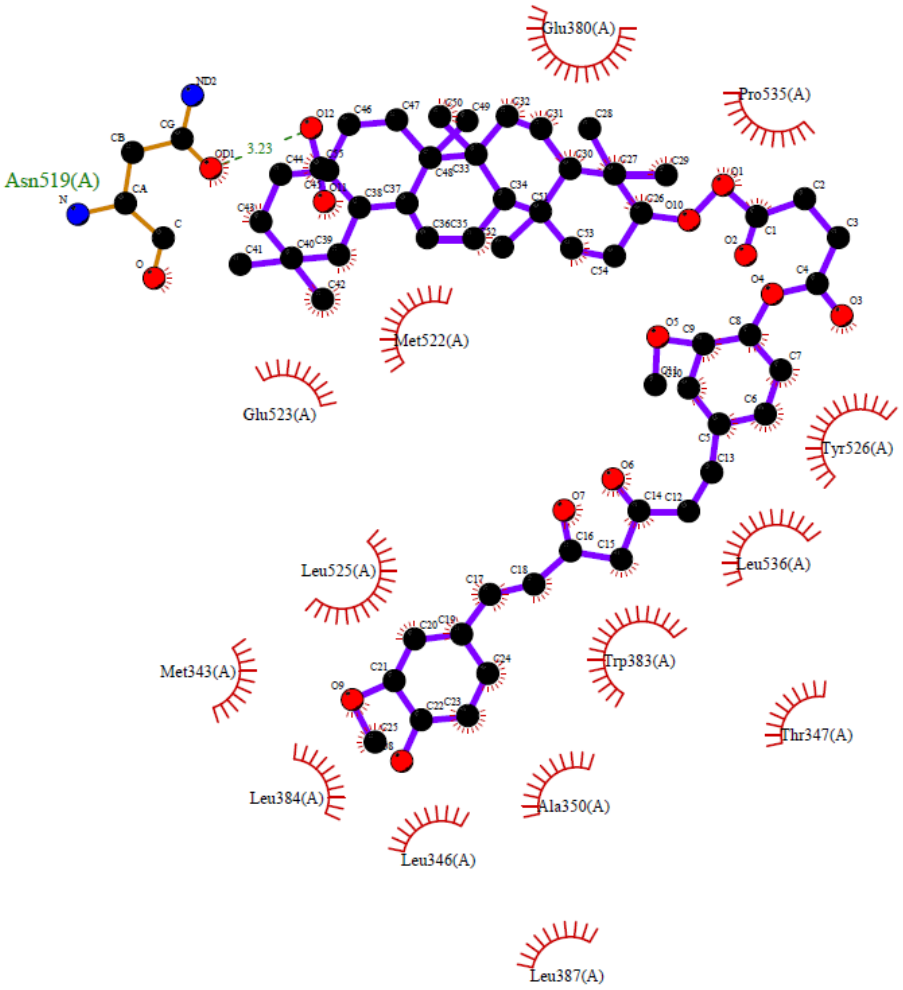

Figure S22 The first poses of the docked ligands to compound **KS4**; hydrogen atoms are omitted; 3dt3.pdb protein (LigPlot+ v.2.2 software).

KS5

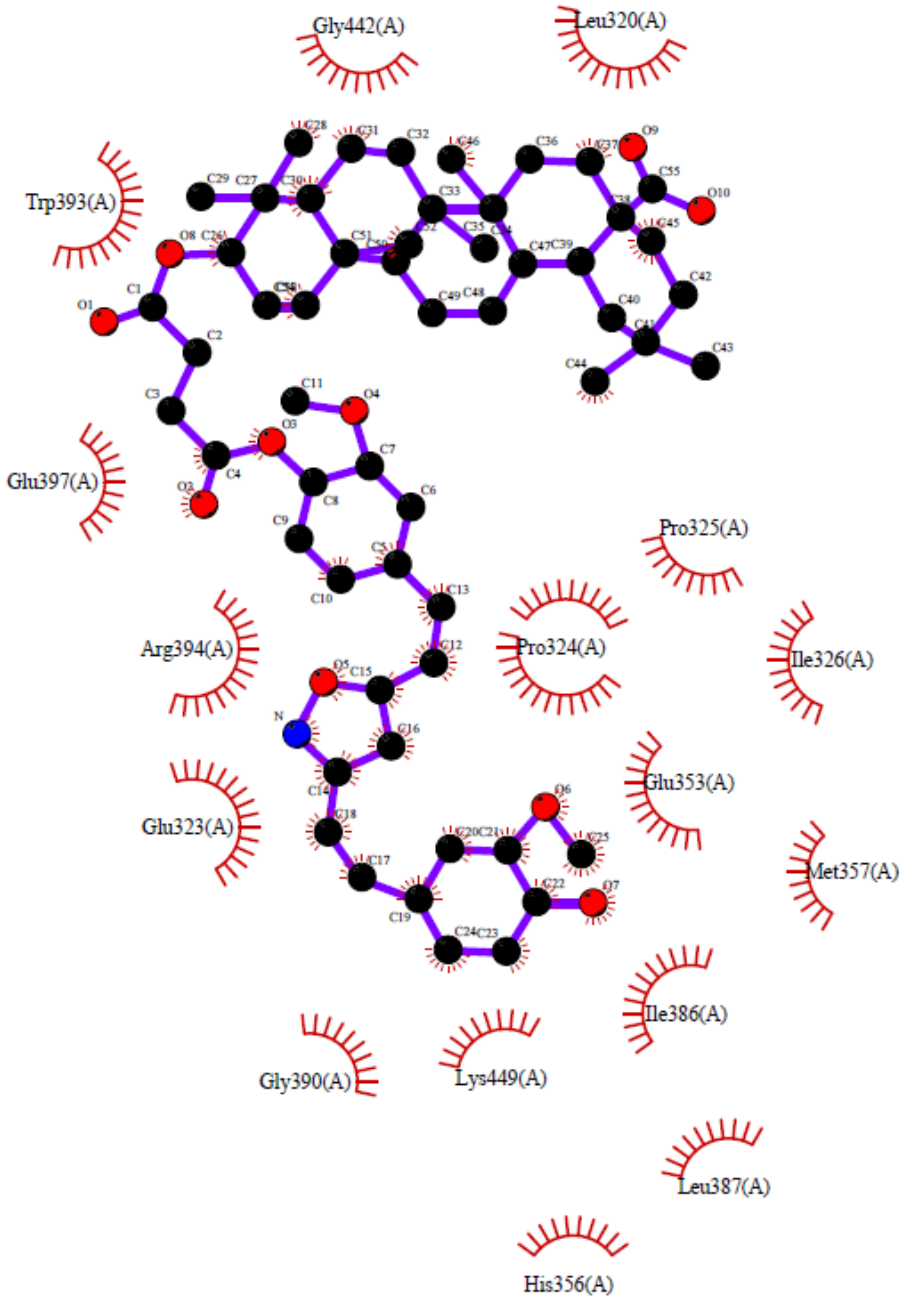

Figure S23 The first poses of the docked ligands to compound **KS5**; hydrogen atoms are omitted; 3dt3.pdb protein (LigPlot+ v.2.2 software).

KS6

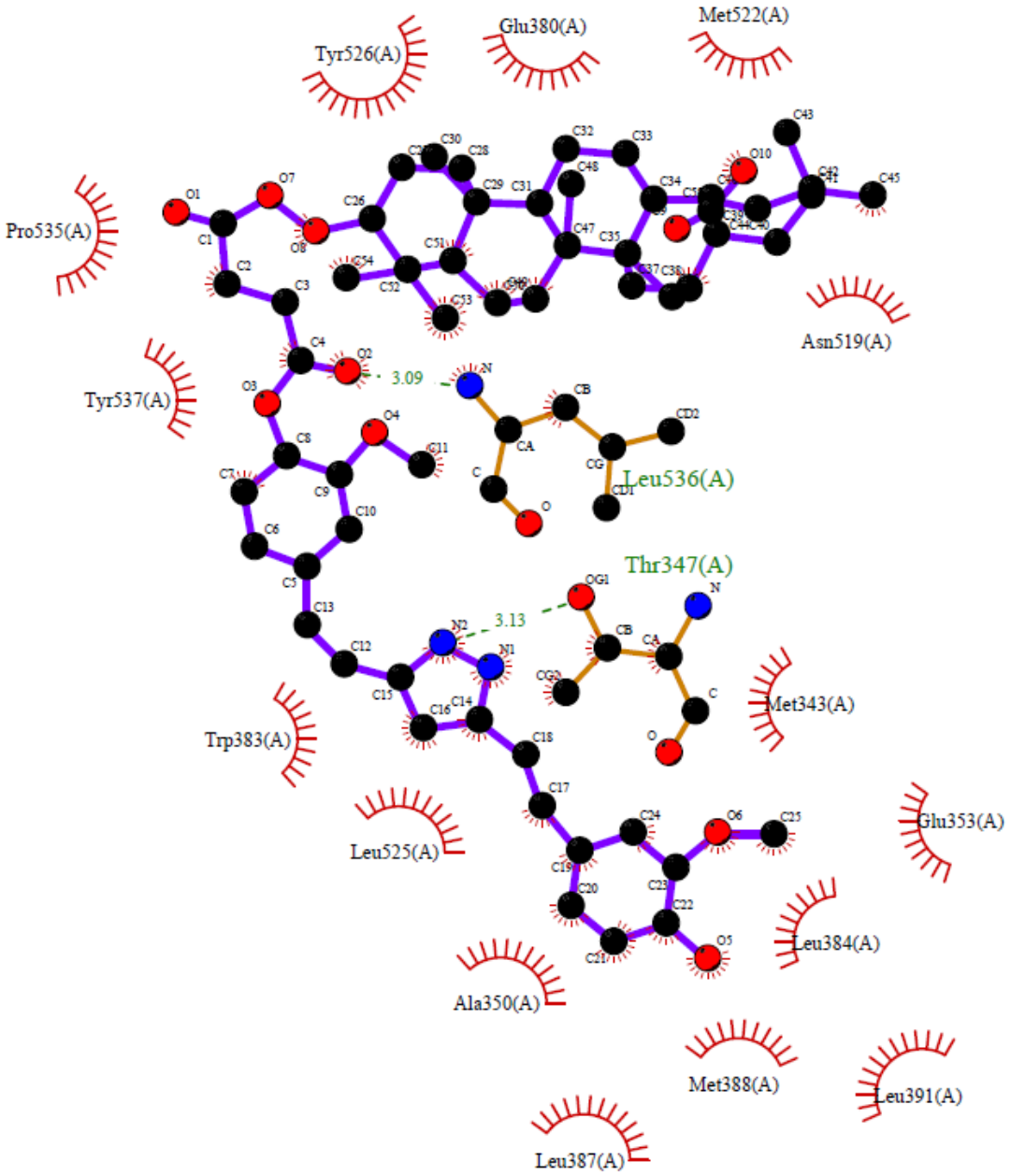

Figure S24 The first poses of the docked ligands to compound **KS6**; hydrogen atoms are omitted; 3dt3.pdb protein (LigPlot+ v.2.2 software).

KS7

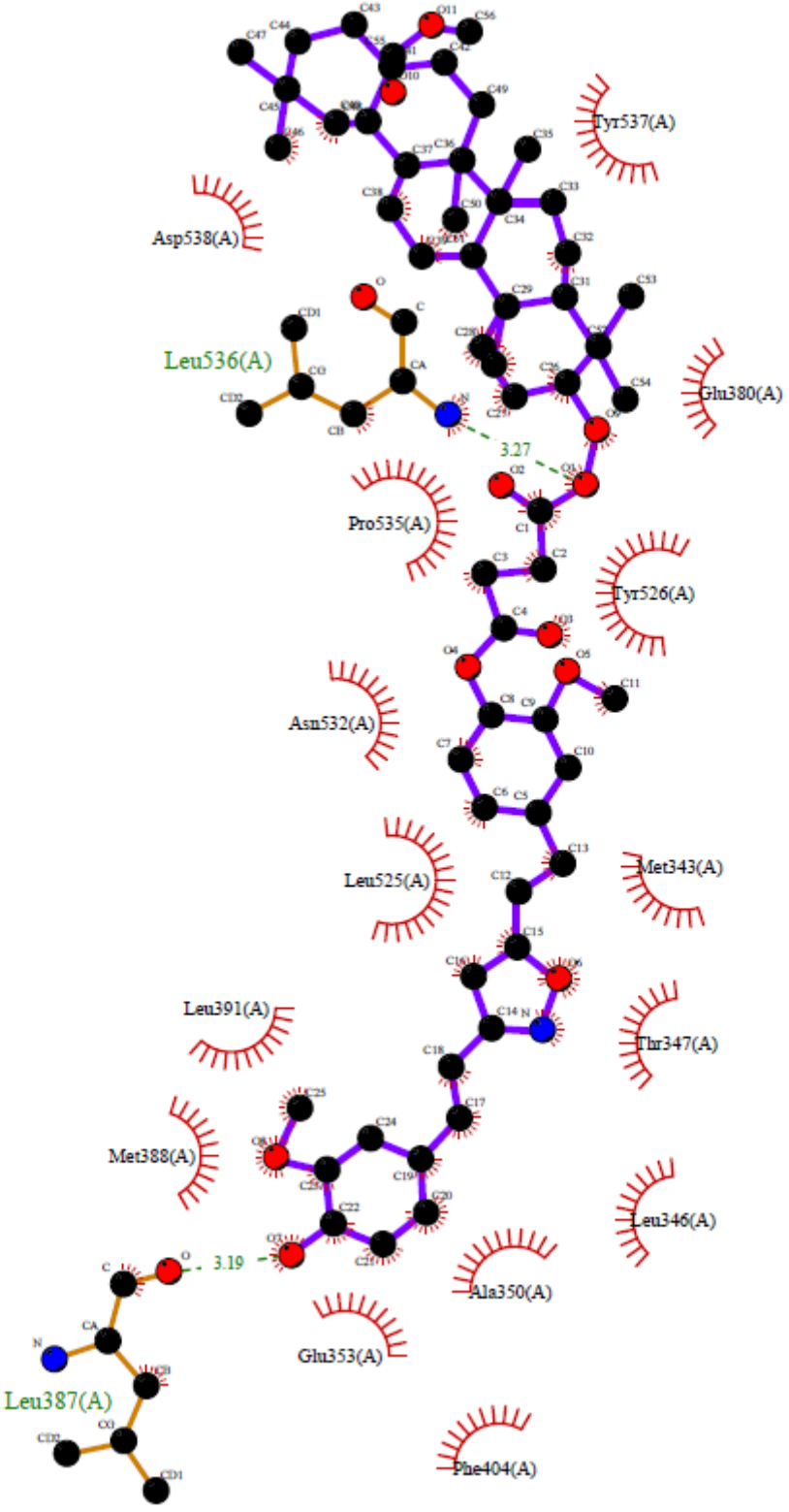

Figure S25 The first poses of the docked ligands to compound **KS7**; hydrogen atoms are omitted; 3dt3.pdb protein (LigPlot+ v.2.2 software).

KS8

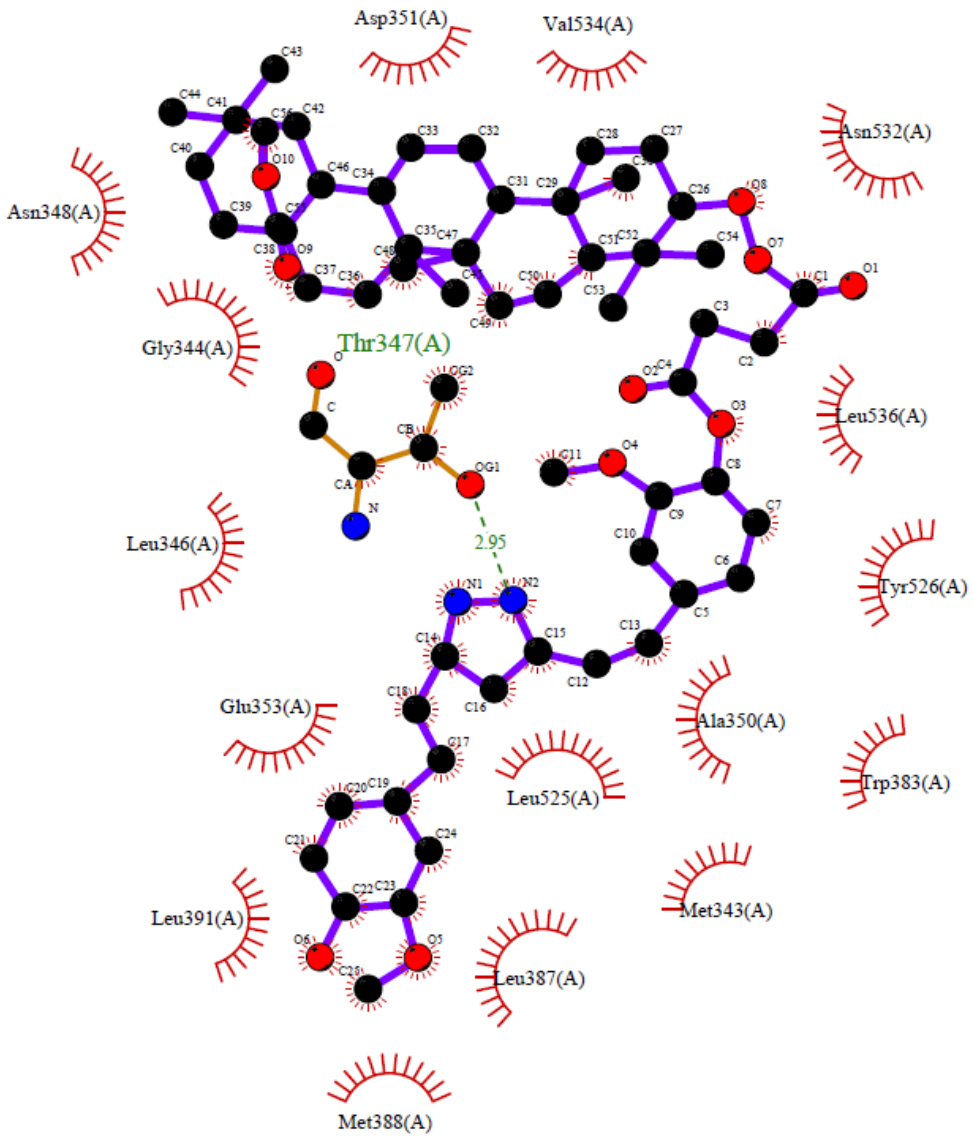

Figure S26 The first poses of the docked ligands to compound **KS8**; hydrogen atoms are omitted; 3dt3.pdb protein (LigPlot+ v.2.2 software).

KS1

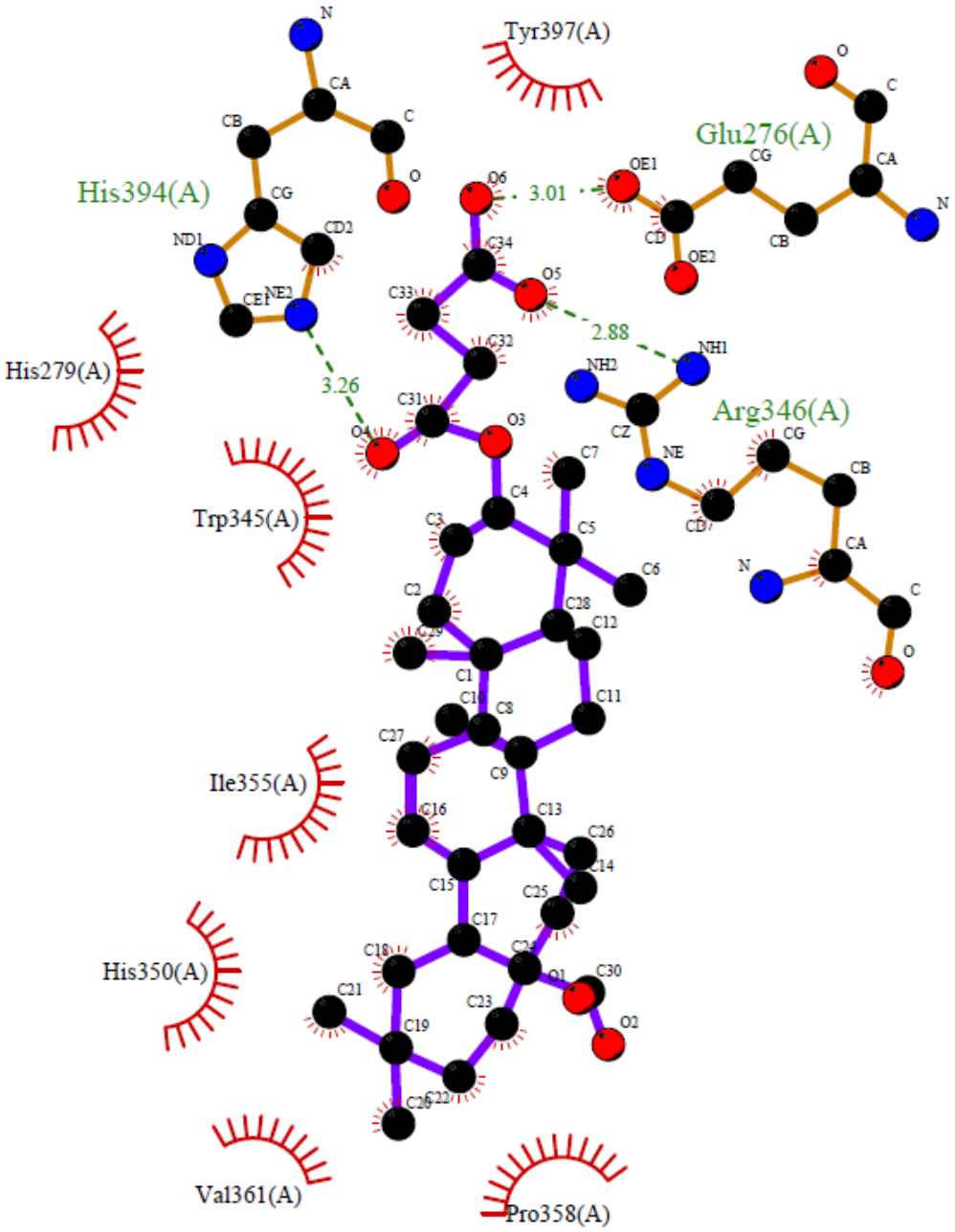

Figure S27 The first poses of the docked ligands to compound **KS1**; hydrogen atoms are omitted; 1l2j.pdb protein (LigPlot+ v.2.2 software).

KS2_keto

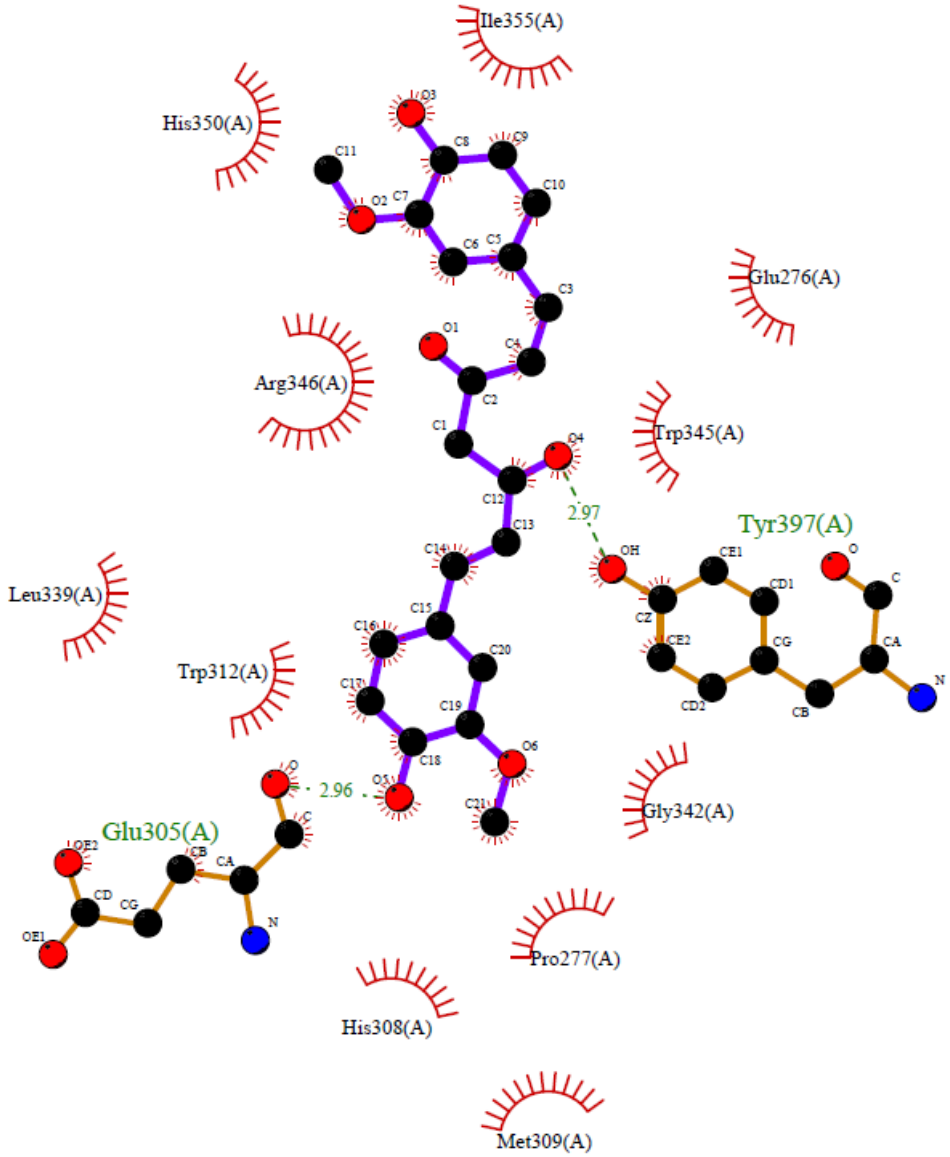

Figure S28 The first poses of the docked ligands to compound **KS2_keto**; hydrogen atoms are omitted; 1l2j.pdb protein (LigPlot+ v.2.2 software).

KS2_enol

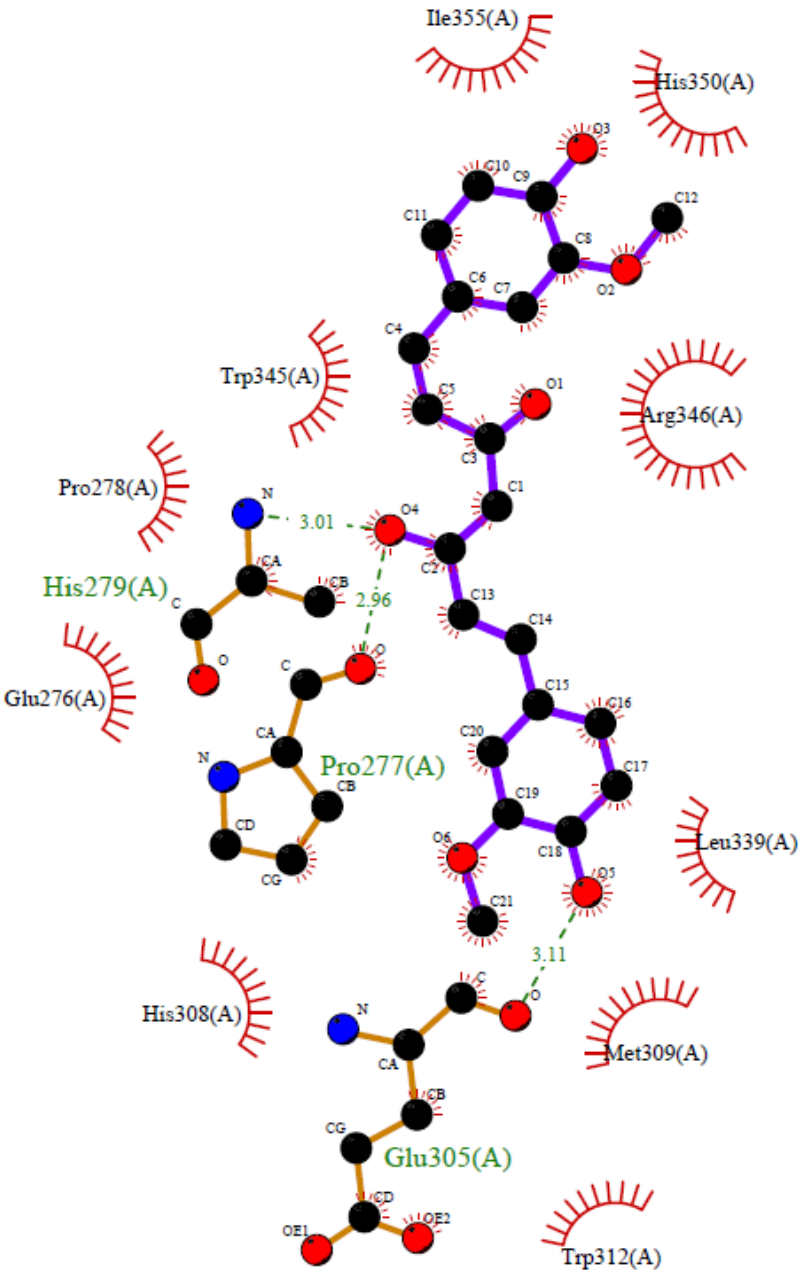

Figure S29 The first poses of the docked ligands to compound **KS2_enol**; hydrogen atoms are omitted; 1l2j.pdb protein (LigPlot+ v.2.2 software).

KS3

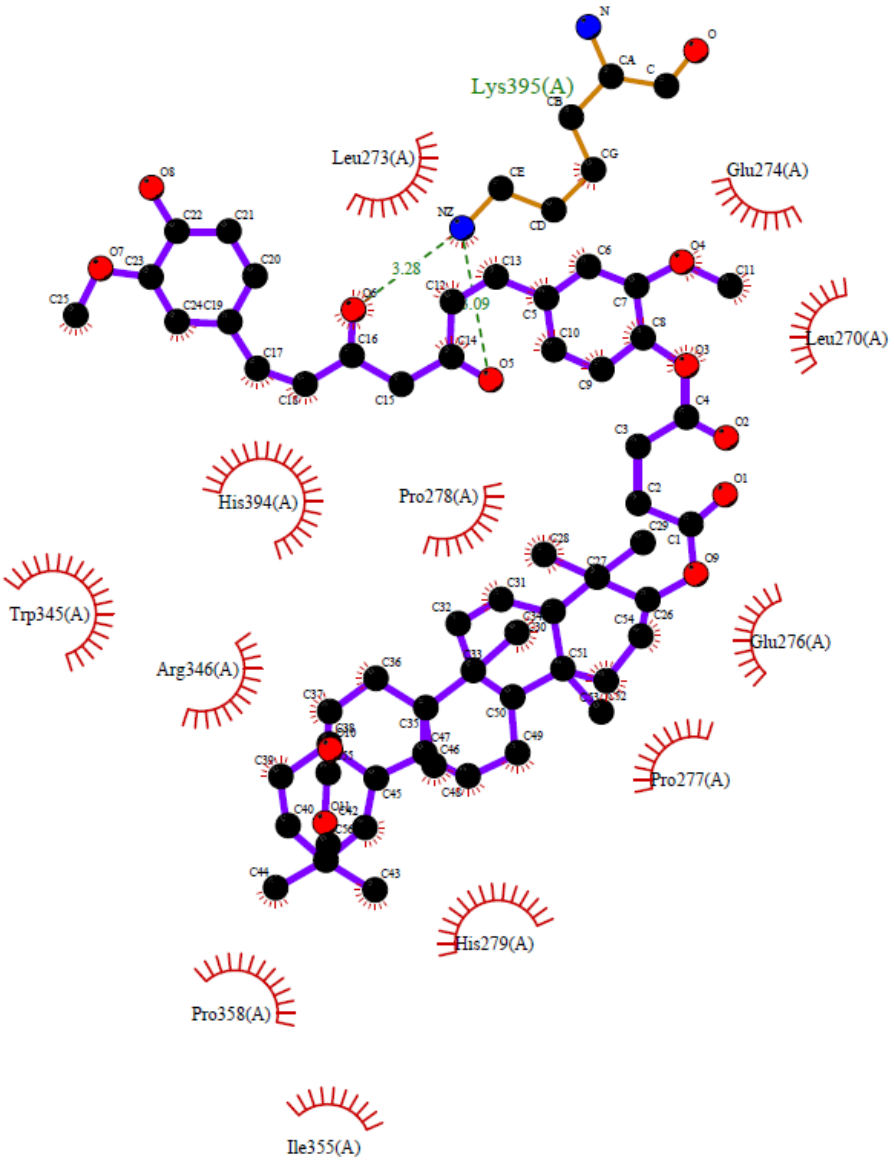

Figure S30 The first poses of the docked ligands to compound **KS3**; hydrogen atoms are omitted; 1l2j.pdb protein (LigPlot+ v.2.2 software).

KS4

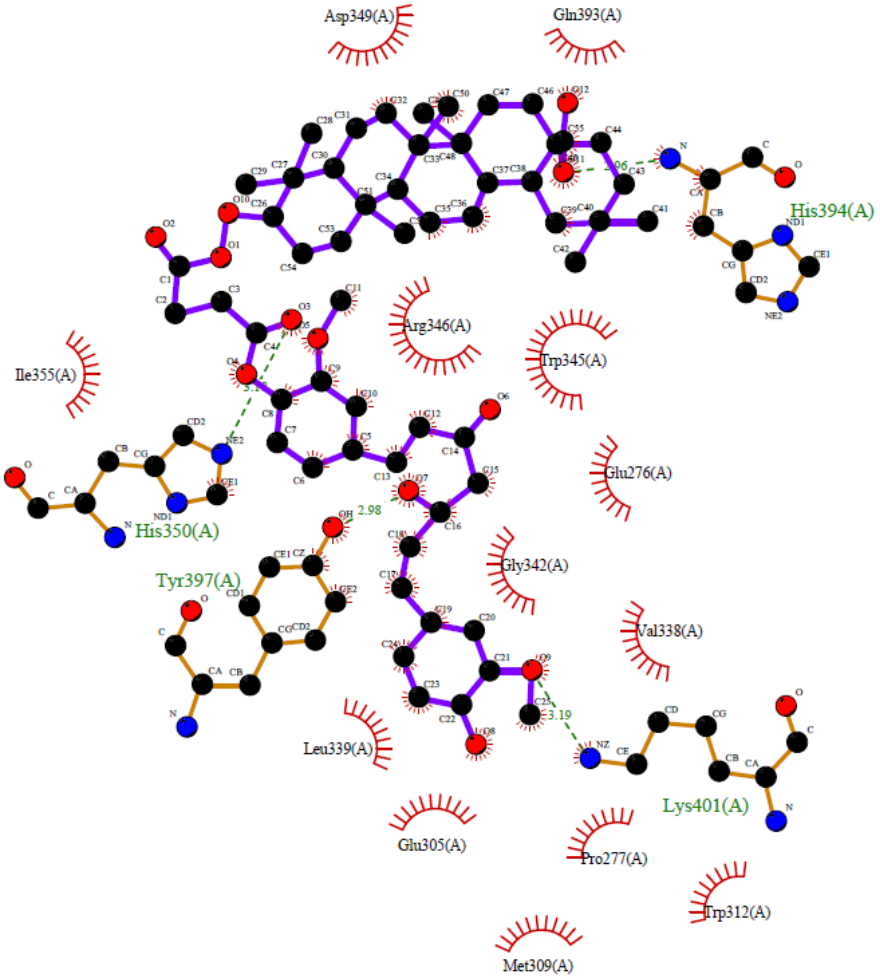

Figure S31 The first poses of the docked ligands to compound **KS4**; hydrogen atoms are omitted; 1l2j.pdb protein (LigPlot+ v.2.2 software).

KS5

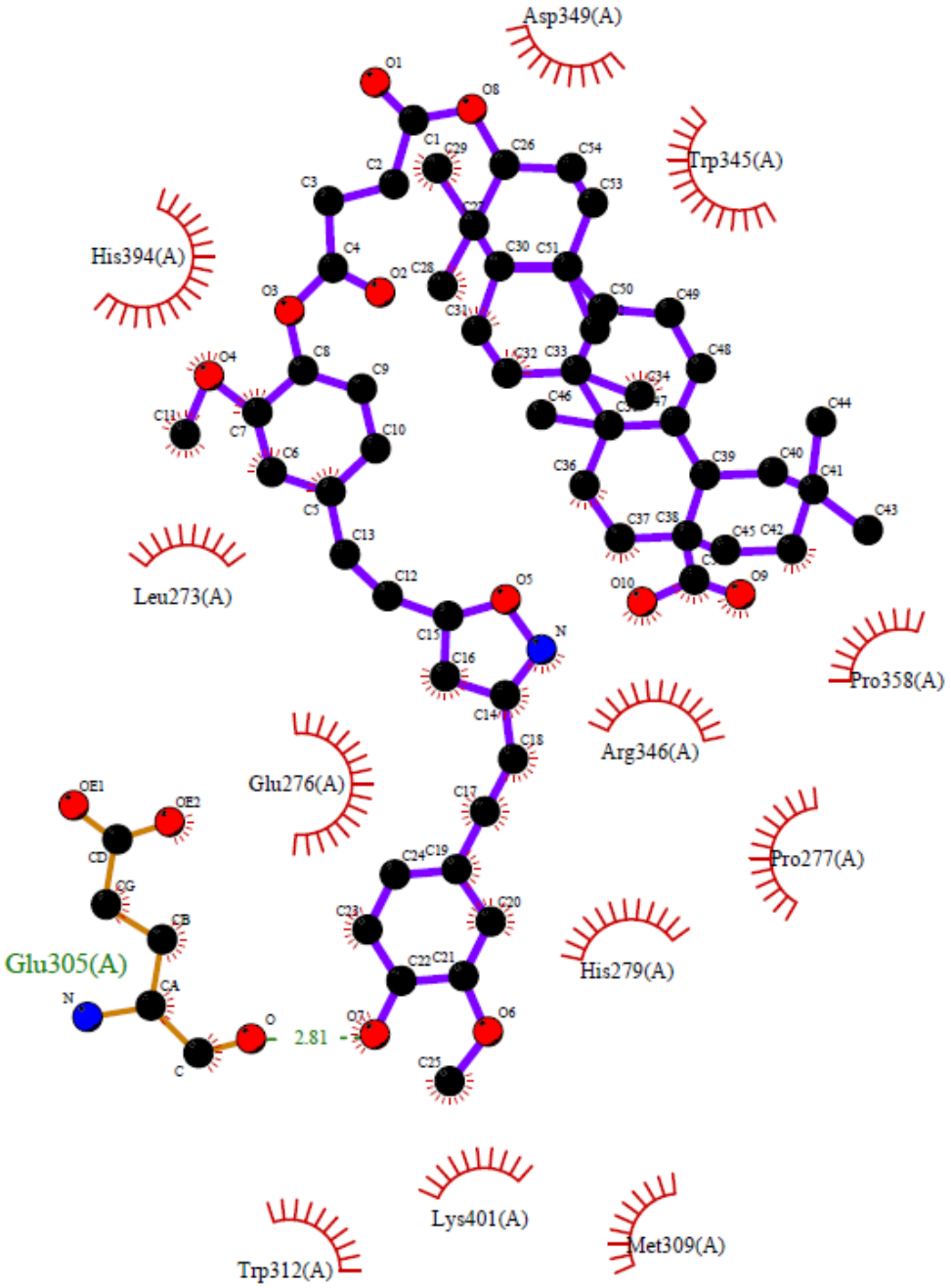

Figure S32 The first poses of the docked ligands to compound **KS6**; hydrogen atoms are omitted; 1l2j.pdb protein (LigPlot+ v.2.2 software).

KS6

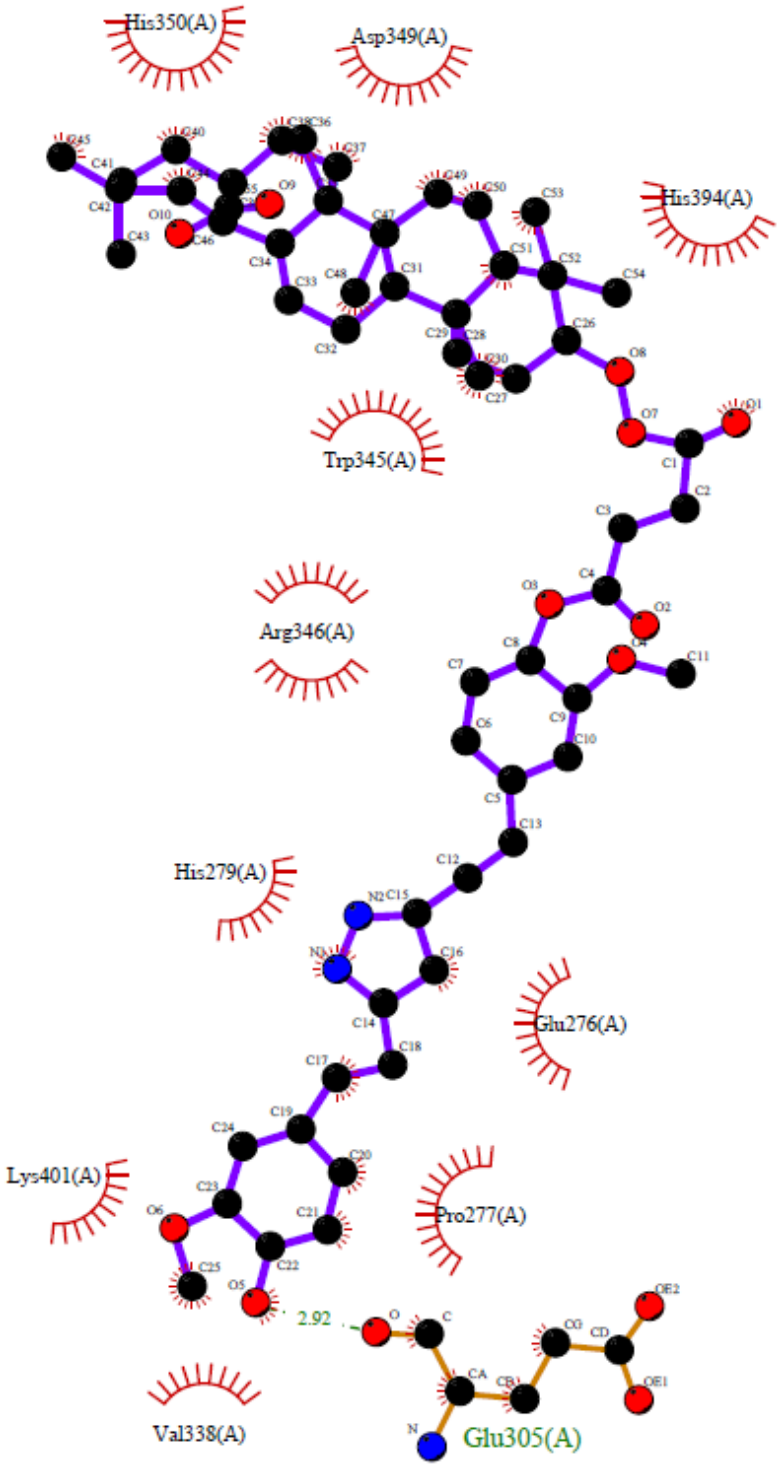

Figure S33 The first poses of the docked ligands to compound **KS6**; hydrogen atoms are omitted; 1l2j.pdb protein (LigPlot+ v.2.2 software).

KS7

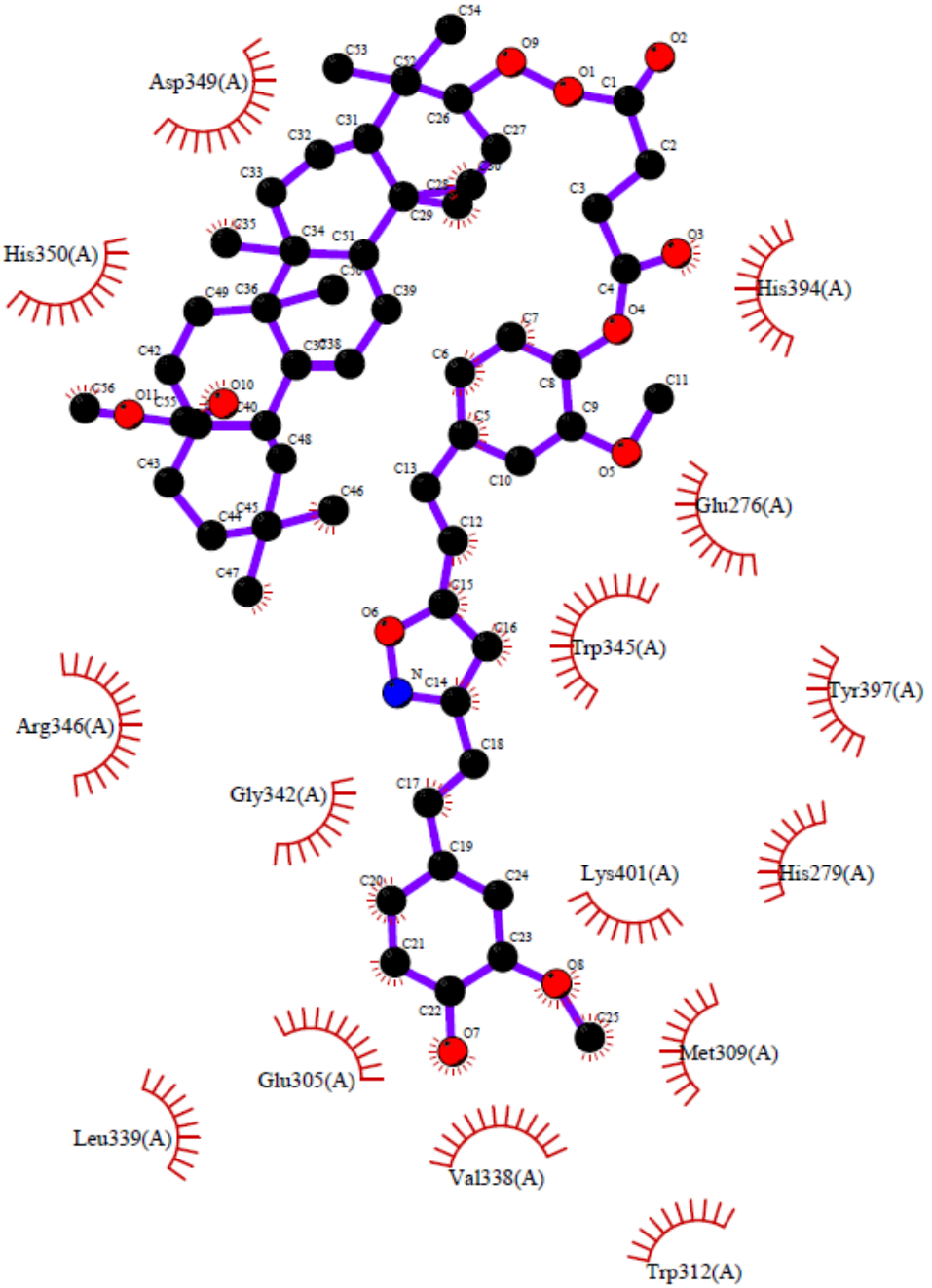

Figure S34 The first poses of the docked ligands to compound **KS7**; hydrogen atoms are omitted; 1l2j.pdb protein (LigPlot+ v.2.2 software).

KS8

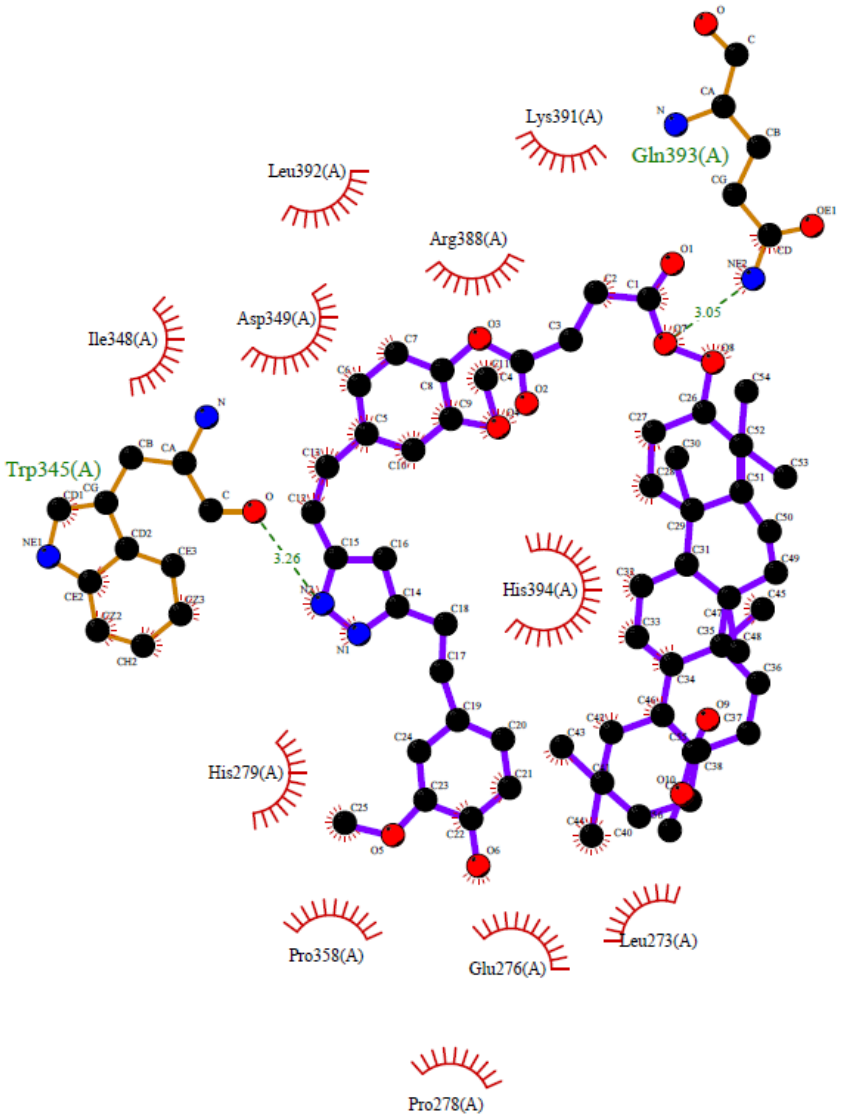

Figure S35 The first poses of the docked ligands to compound **KS8**; hydrogen atoms are omitted; 1l2j.pdb protein (LigPlot+ v.2.2 software).

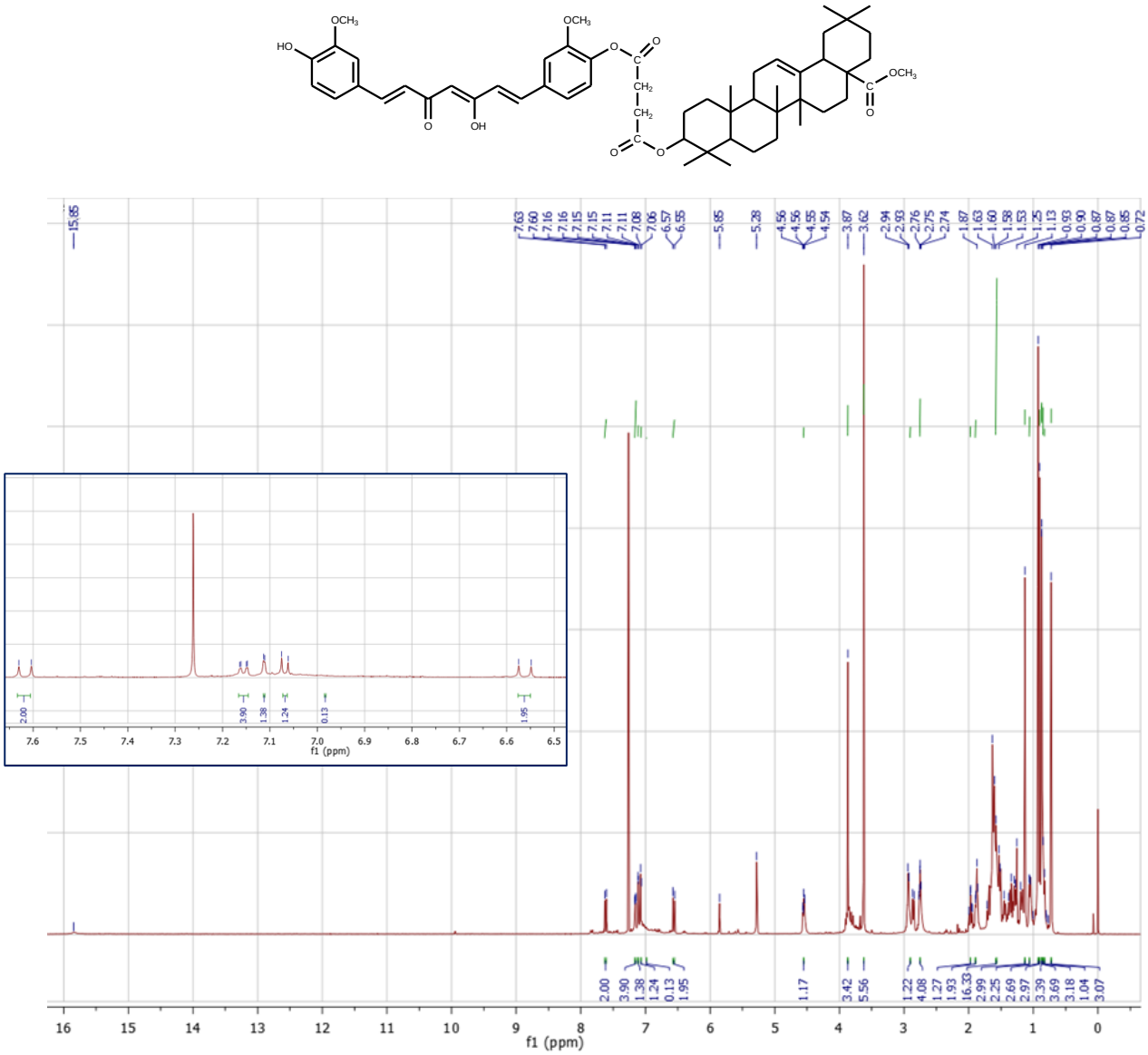

Figure S36 ^{1}H-NMR spectrum of Curcumin mono-oleanoyl hydrogen succinate methyl ester

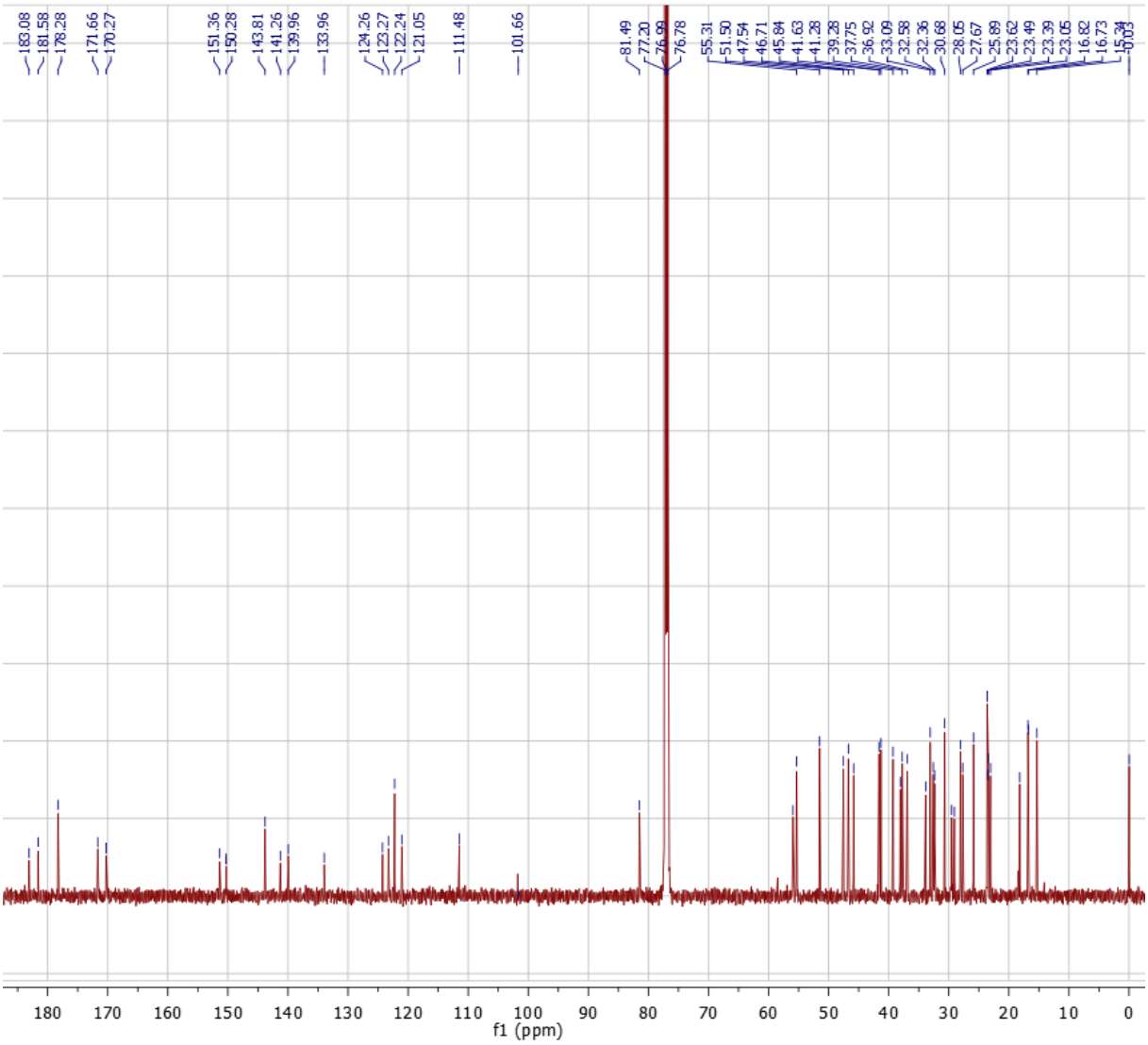

Figure S37 ^{13}C-NMR spectrum of Curcumin mono-oleanoyl hydrogen succinate methyl ester

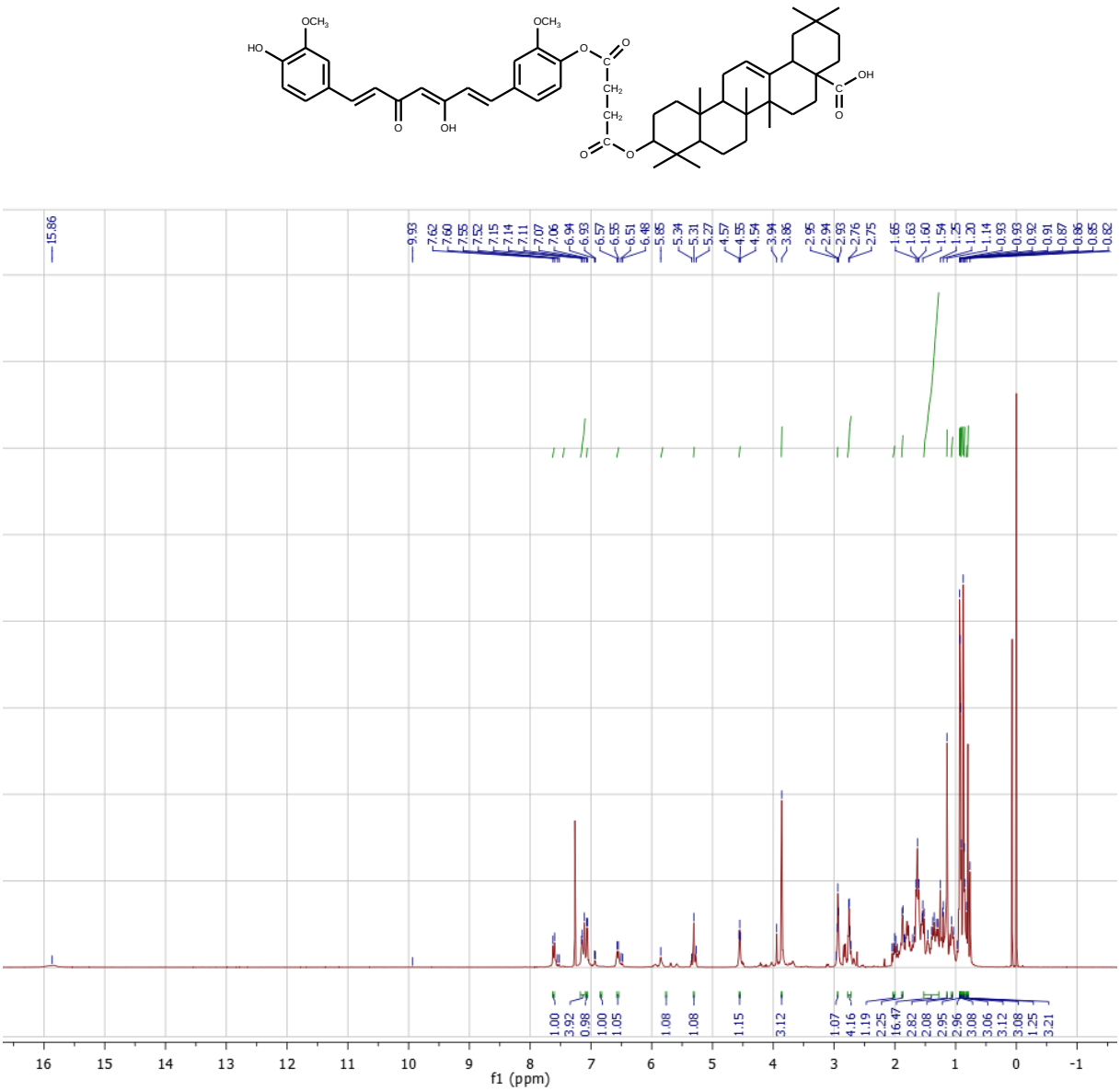

Figure S38 ^{1}H-NMR spectrum of Curcumin mono-oleanoyl hydrogen succinate

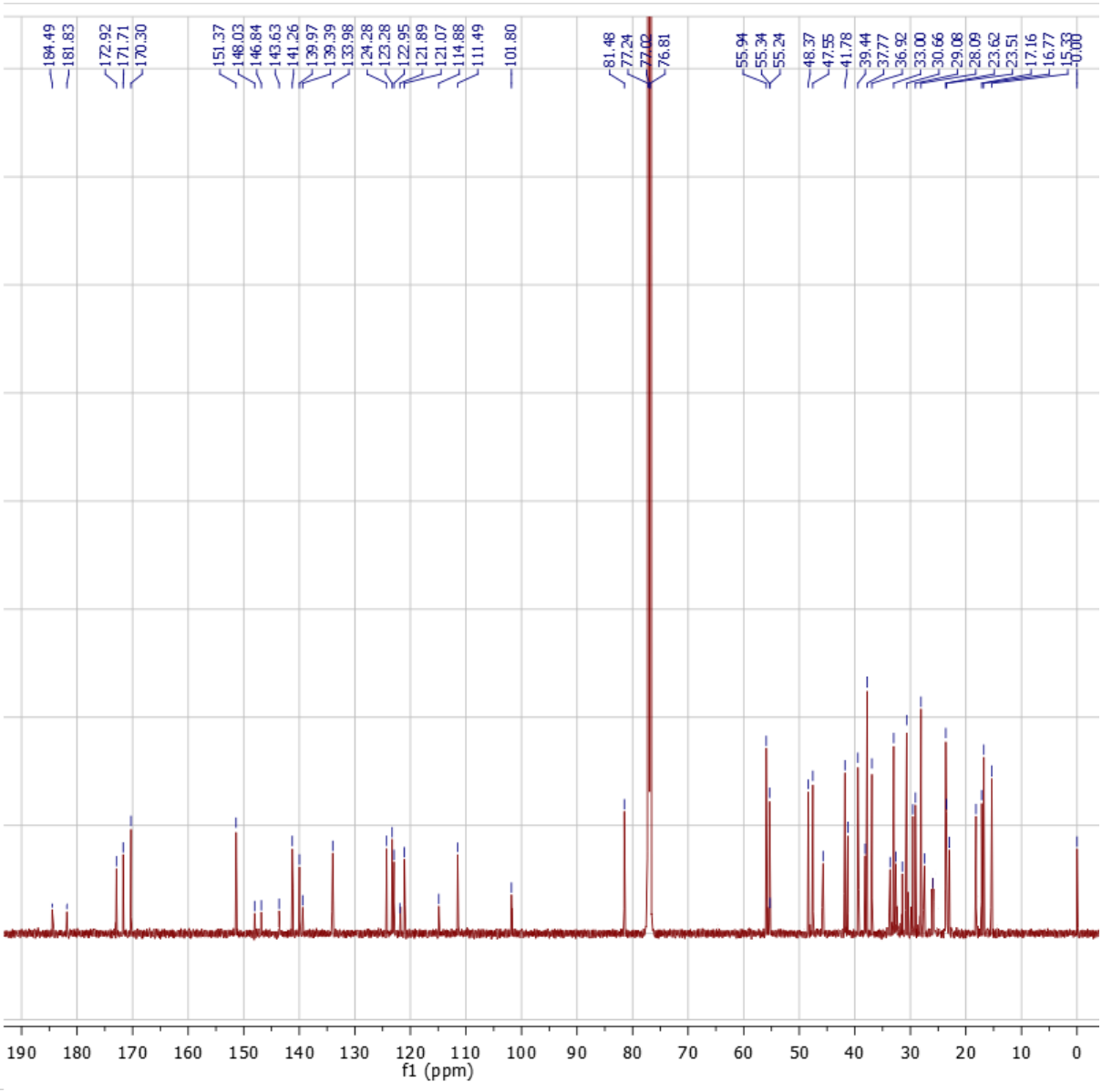

Figure S39 ^{13}C-NMR spectrum of Curcumin mono-oleanoyl hydrogen succinate

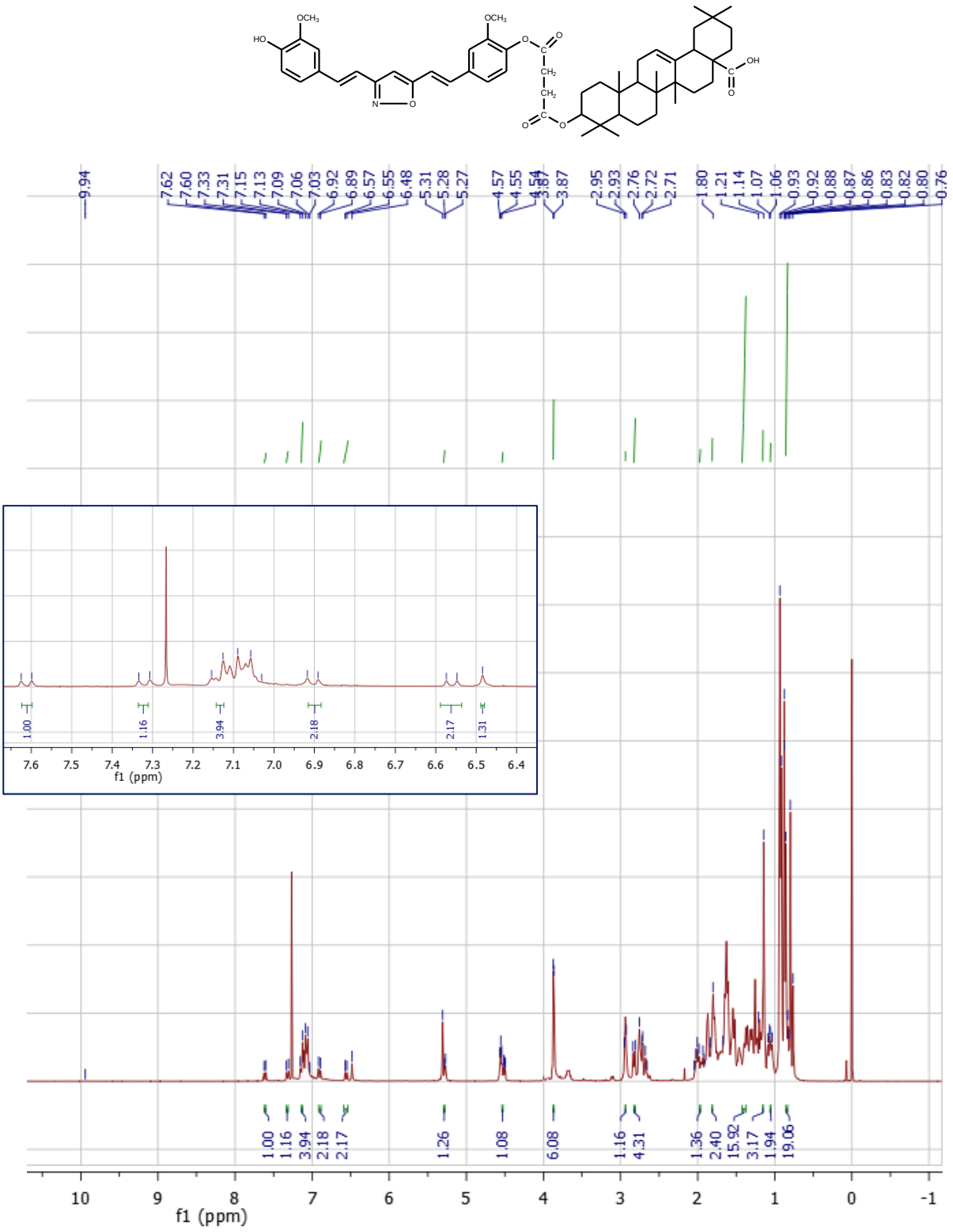

Figure S40 ^{1}H-NMR spectrum of Curcumin isoxazole mono-oleanoyl hydrogen succinate

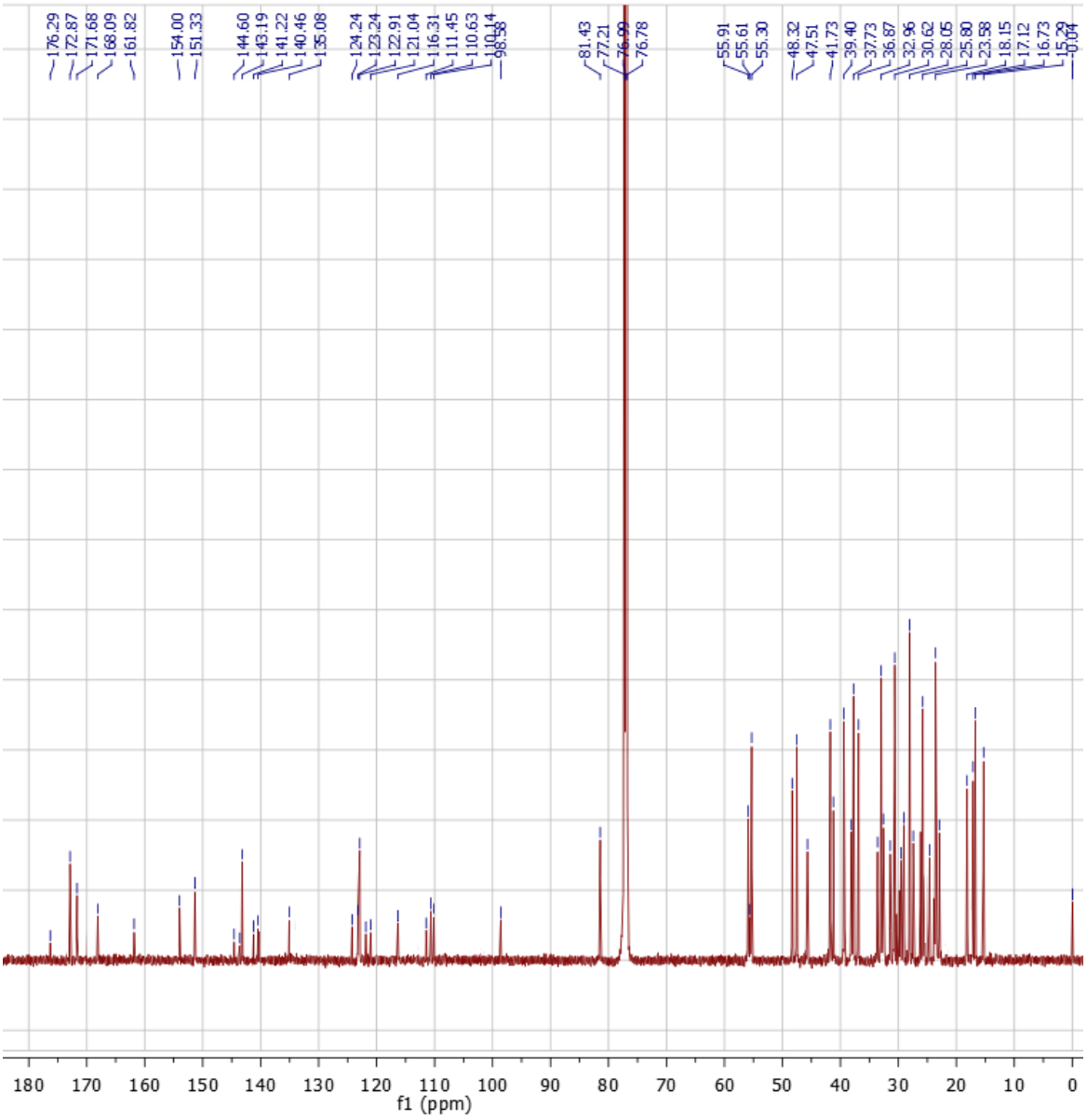

Figure S41 ^{13}C-NMR spectrum of Curcumin isoxazole mono-oleanoyl hydrogen succinate

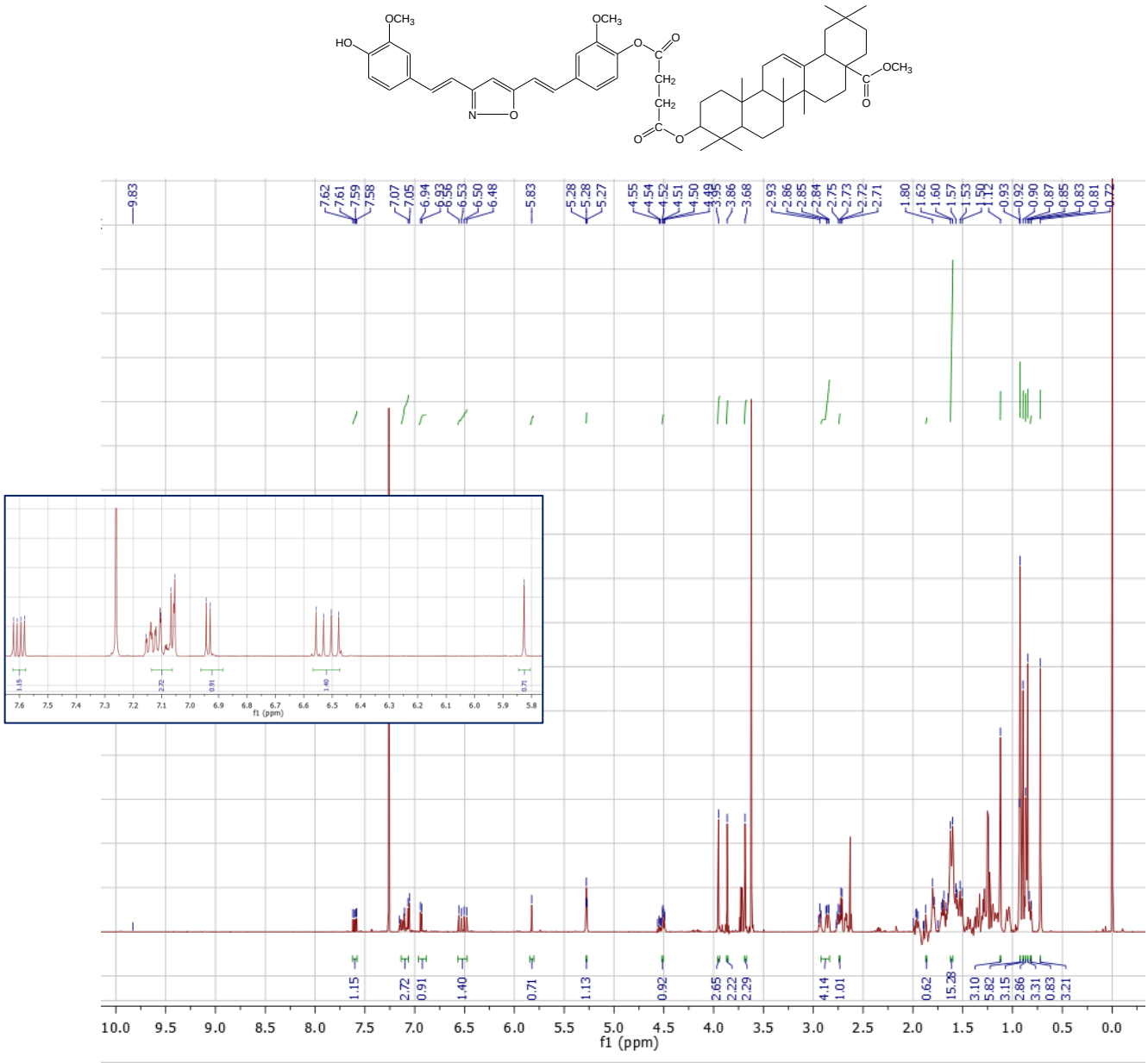

Figure S42 ^{1}H-NMR spectrum of Curcumin isoxazole mono-oleanoyl hydrogen succinate methyl ester

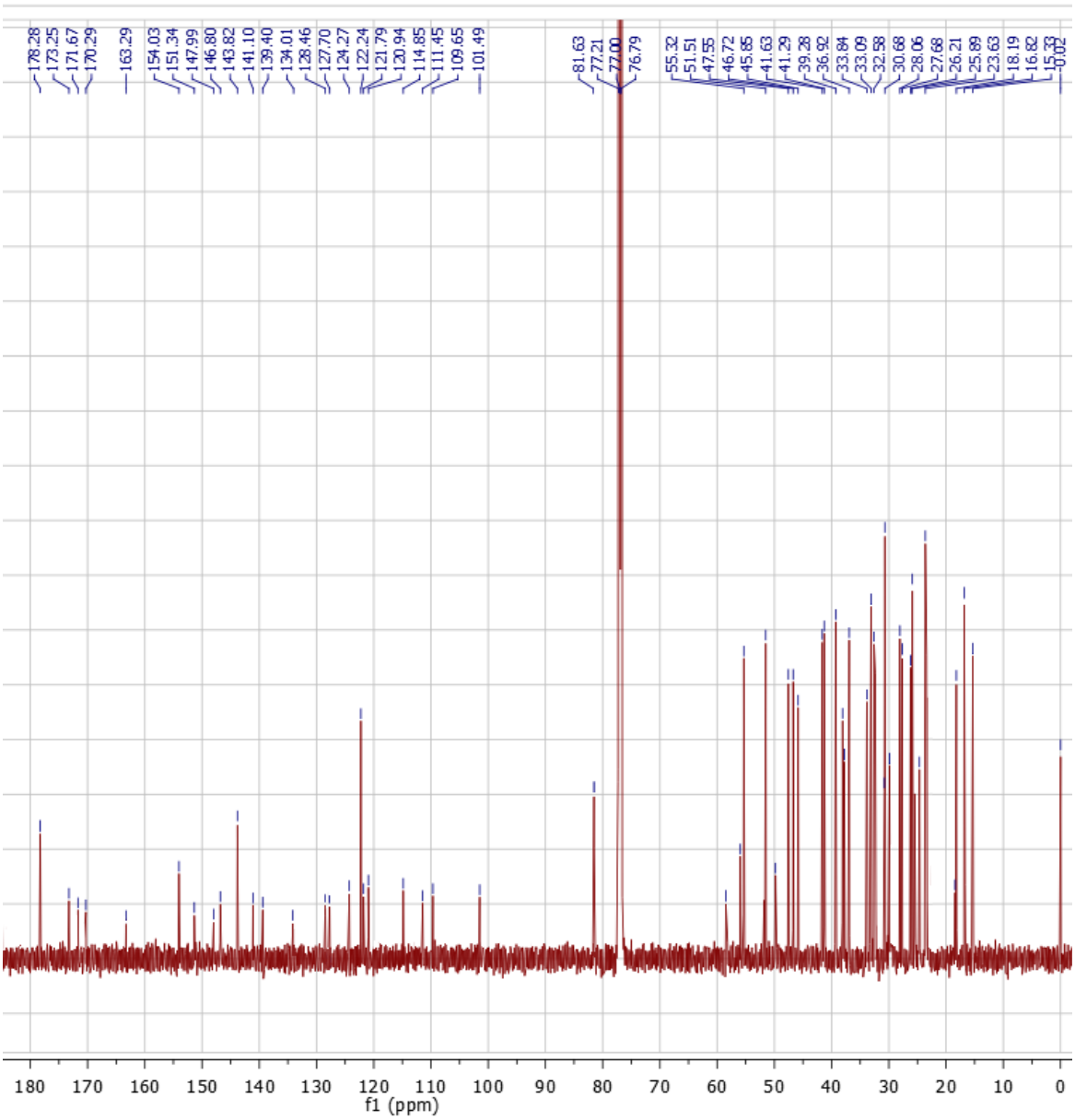

Figure S43 ^{13}C-NMR spectrum of Curcumin isoxazole mono-oleanoyl hydrogen succinate methyl ester