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SUPPLEMENTARY MATERIAL OPEN ACCESS

In Silico Evaluation of Anthraquinone Derivatives as Potential α-amylase and α-glucosidase Inhibitors in Diabetes Mellitus

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Table S1. List of selected anthraquinone compounds and their canonical smiles used for molecular docking with α-amylase and α-glucosidase enzymes.

Compound	Chemical Name	SMILES
AQ1	1-(methylamino)anthraquinone	CNC1=CC=CC2=C1C(=O)C3=CC=CC=C3C2=O
AQ2	1,4-diaminoanthraquinone	C1=CC=C2C(=C1)C(=O)C3=C(C=CC(=C3C2=O)N)N
AQ3	1,5-dichloroanthraquinone	C1=CC2=C(C(=C1)Cl)C(=O)C3=C(C2=O)C(=CC=C3)Cl
AQ4	1-chloroanthraquinone	C1=CC=C2C(=C1)C(=O)C3=C(C2=O)C(=CC=C3)Cl
AQ5	2-chloroanthraquinone	C1=CC=C2C(=C1)C(=O)C3=C(C2=O)C=C(C=C3)Cl
AQ6	1,8-dichloroanthraquinone	C1=CC2=C(C(=C1)Cl)C(=O)C3=C(C2=O)C=CC=C3Cl
AQ7	2-hydroxyanthraquinone	C1=CC=C2C(=C1)C(=O)C3=C(C2=O)C=C(C=C3)O
AQ8	1,4-dihydroxyanthraquinone (quinizarin)	C1=CC=C2C(=C1)C(=O)C3=C(C=CC(=C3C2=O)O)O
AQ9	1,2-dihydroxyanthraquinone (alizarin)	C1=CC=C2C(=C1)C(=O)C3=C(C2=O)C(=C(C=C3)O)O
AQ10	Anthraquinone	C1=CC=C2C(=C1)C(=O)C3=CC=CC=C3C2=O
AQ11	2-methylanthraquinone	CC1=CC2=C(C=C1)C(=O)C3=CC=CC=C3C2=O
AQ12	2-tert-butylanthraquinone	CC(C)(C)C1=CC2=C(C=C1)C(=O)C3=CC=CC=C3C2=O
AQ13	Anthraquinone-2-carboxylic acid	C1=CC=C2C(=C1)C(=O)C3=C(C2=O)C=C(C=C3)C(=O)O
AQ14	Sodium anthraquinone-2-sulfonate	C1=CC=C2C(=C1)C(=O)C3=C(C2=O)C=C(C=C3)S(=O)(=O)[O-].[Na+]

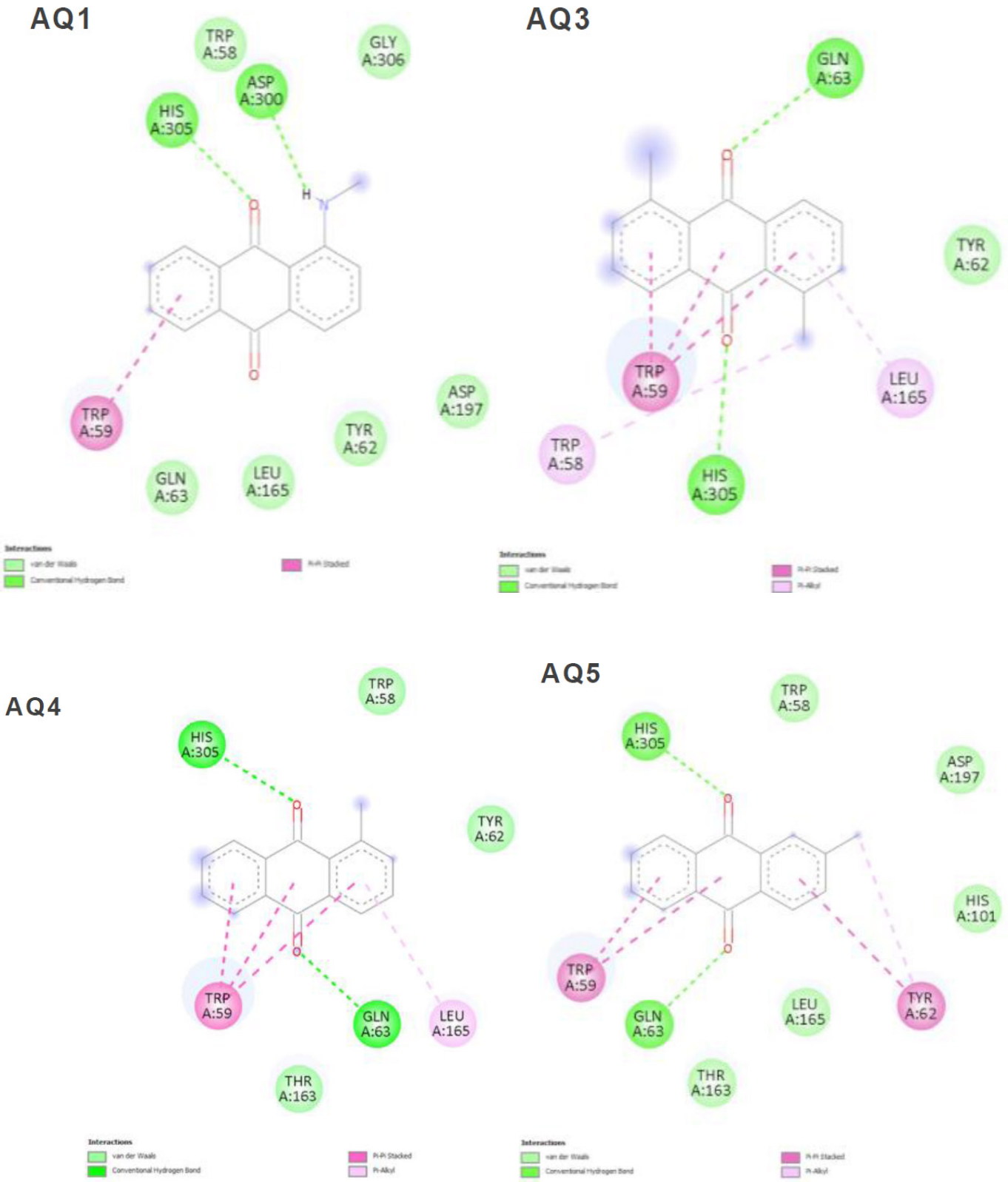
AQ1
TRP A:58
GLY A:306
ASP A:300
HIS A:305
TRP A:59
ASP A:197
TYR A:62
GLN A:63
LEU A:165
AQ3
GLN A:63
TYR A:62
TRP A:59
LEU A:165
TRP A:58
HIS A:305
AQ4
TRP A:58
HIS A:305
TYR A:62
TRP A:59
GLN A:63
LEU A:165
THR A:163
AQ5
TRP A:58
HIS A:305
ASP A:197
HIS A:101
TRP A:59
GLN A:63
LEU A:165
TYR A:62
THR A:163

Fig. S1 contd.....

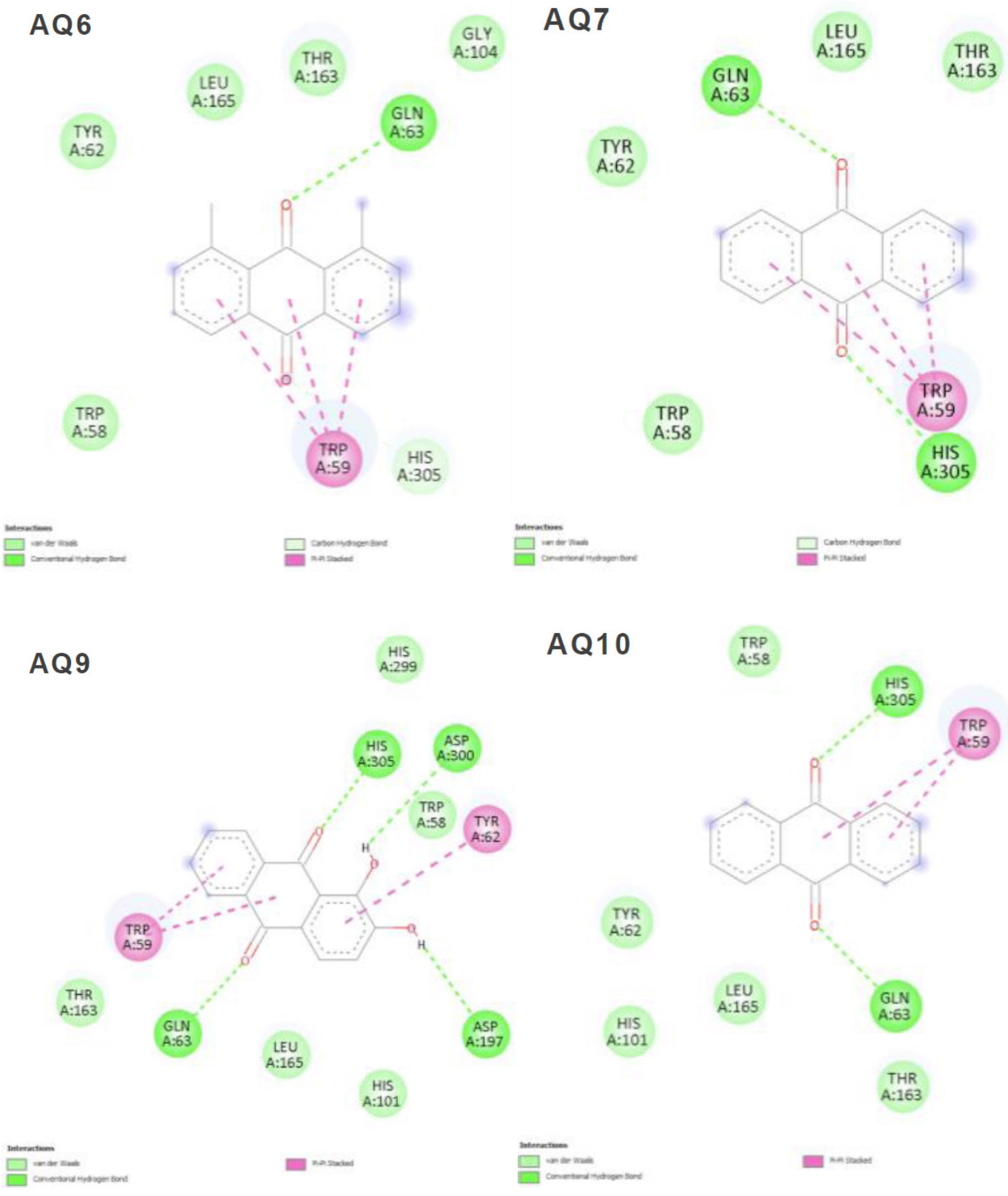
AQ6
GLY A:104
THR A:163
LEU A:165
GLN A:63
TYR A:62
TRP A:58
TRP A:59
HIS A:305
AQ7
LEU A:165
THR A:163
GLN A:63
TYR A:62
TRP A:59
TRP A:58
HIS A:305
AQ9
HIS A:299
HIS A:305
ASP A:300
TRP A:58
TYR A:62
TRP A:59
THR A:163
GLN A:63
LEU A:165
ASP A:197
HIS A:101
AQ10
TRP A:58
HIS A:305
TRP A:59
TYR A:62
LEU A:165
GLN A:63
HIS A:101
THR A:163

Fig. S1 contd.....

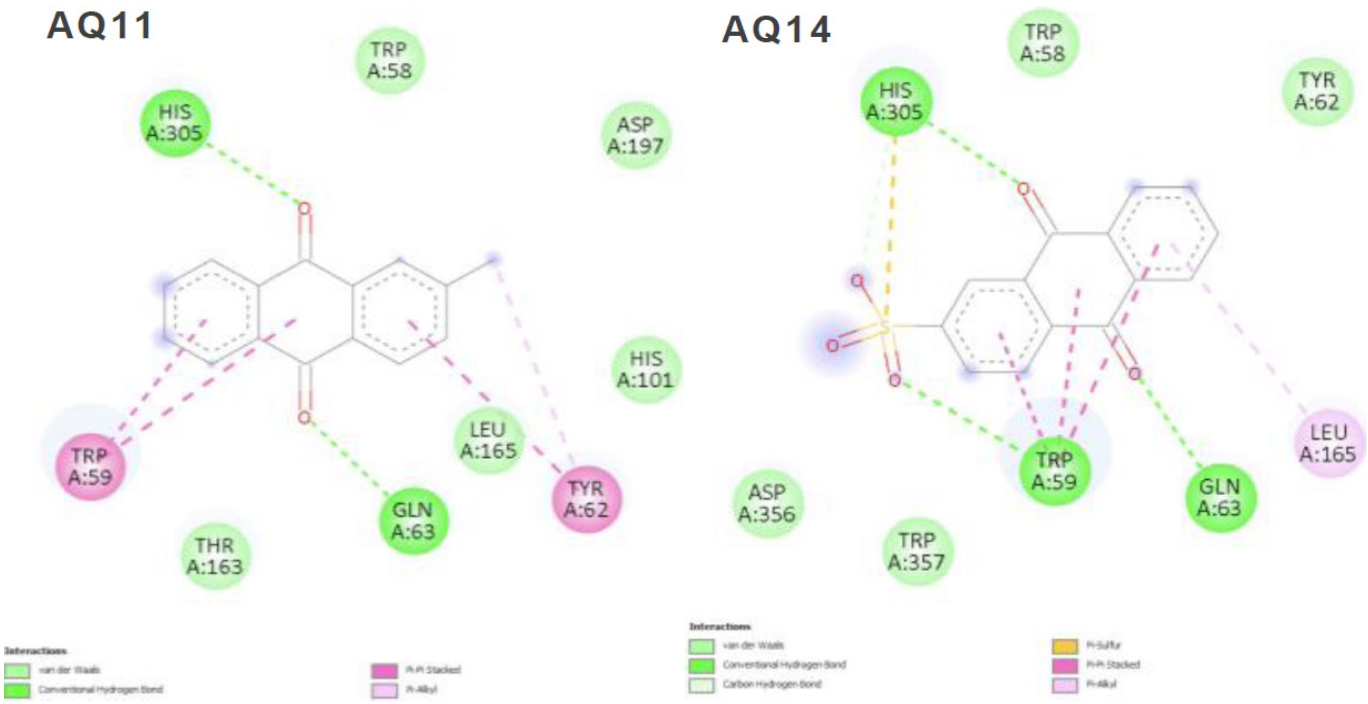

Fig. (S1). The 2D diagrams of binding poses of 10 of the 14 compounds interacting with α-amylase, excluding the top 4 compounds with the highest interactions. Interactions in light and dark green colours represent hydrogen bond; interactions in pink or purple colours represent hydrophobic interactions.

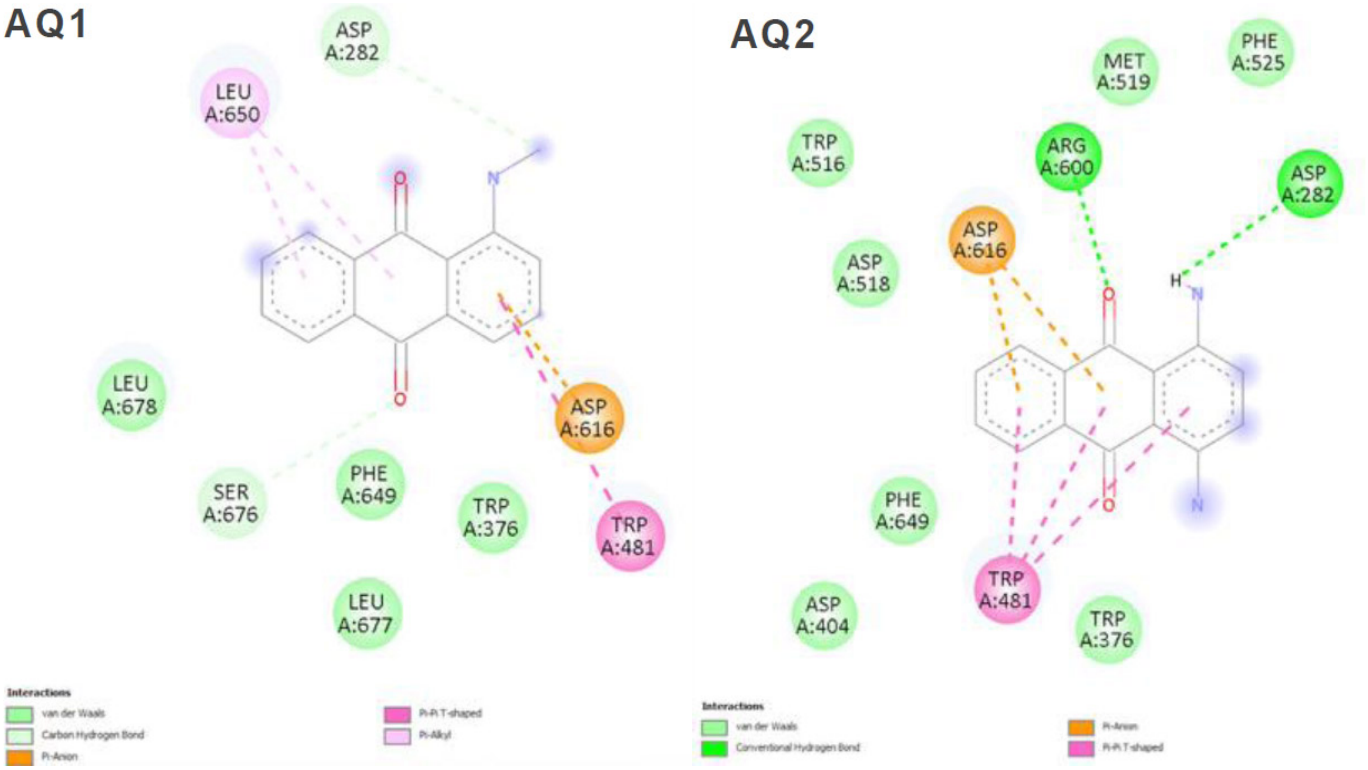

Fig. S2 contd.....

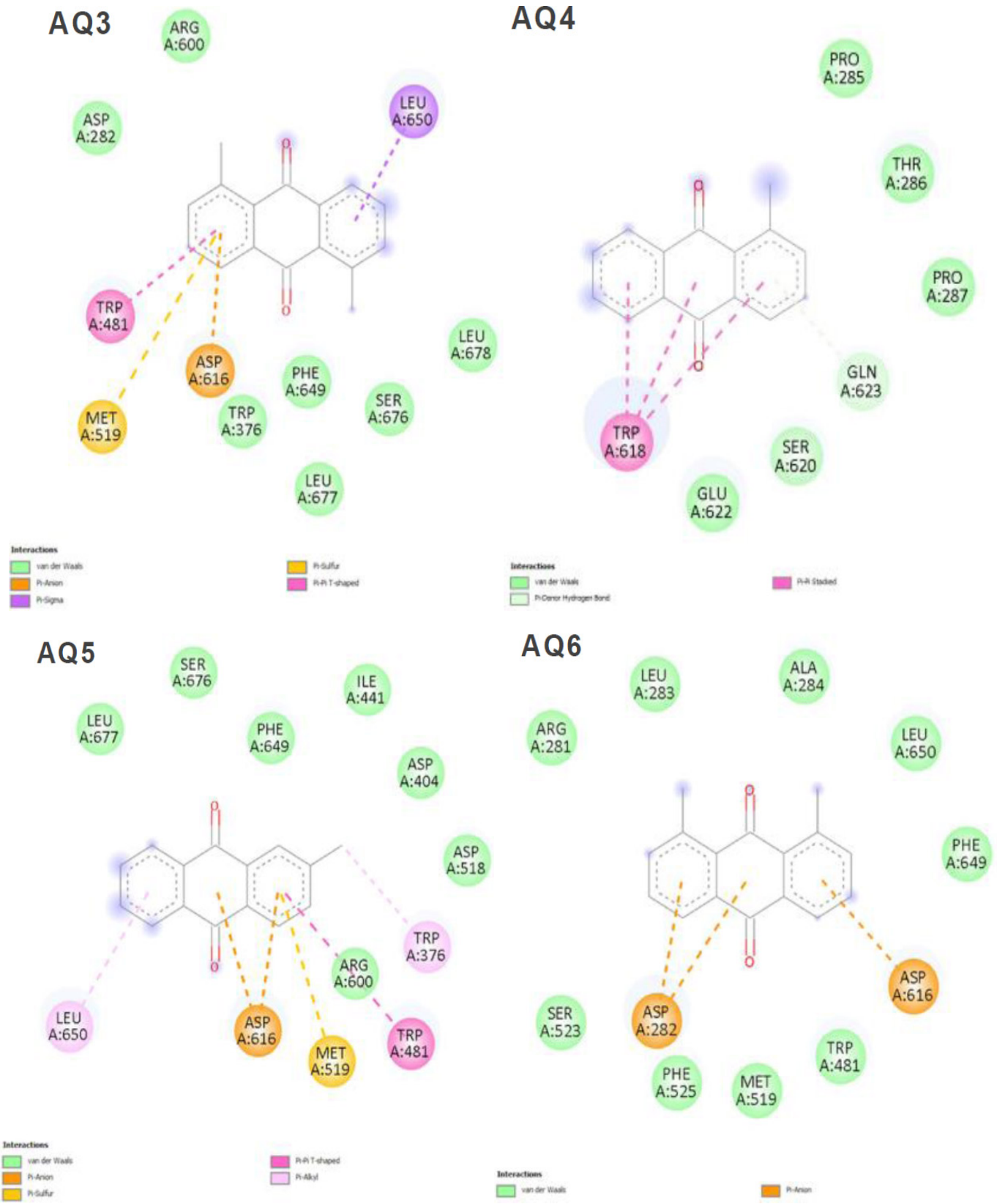
AQ3
ARG A:600
LEU A:650
ASP A:282
TRP A:481
ASP A:616
PHE A:649
LEU A:678
SER A:676
MET A:519
TRP A:376
LEU A:677
Interactions
van der Waals
Pi-Anion
Pi-Sigma
Pi-Sulfur
Pi-Pi T-shaped
AQ4
PRO A:285
THR A:286
PRO A:287
GLN A:623
TRP A:618
SER A:620
GLU A:622
Interactions
van der Waals
Pi-Donor Hydrogen Bond
Pi-Pi Stacked
AQ5
SER A:676
ILE A:441
LEU A:677
PHE A:649
ASP A:404
ASP A:518
TRP A:376
ARG A:600
LEU A:650
ASP A:616
MET A:519
TRP A:481
Interactions
van der Waals
Pi-Anion
Pi-Sulfur
Pi-Pi T-shaped
Pi-Alkyl
AQ6
LEU A:283
ALA A:284
ARG A:281
LEU A:650
PHE A:649
ASP A:616
SER A:523
ASP A:282
TRP A:481
PHE A:525
MET A:519
Interactions
van der Waals
Pi-Anion

Fig. S2 contd.....

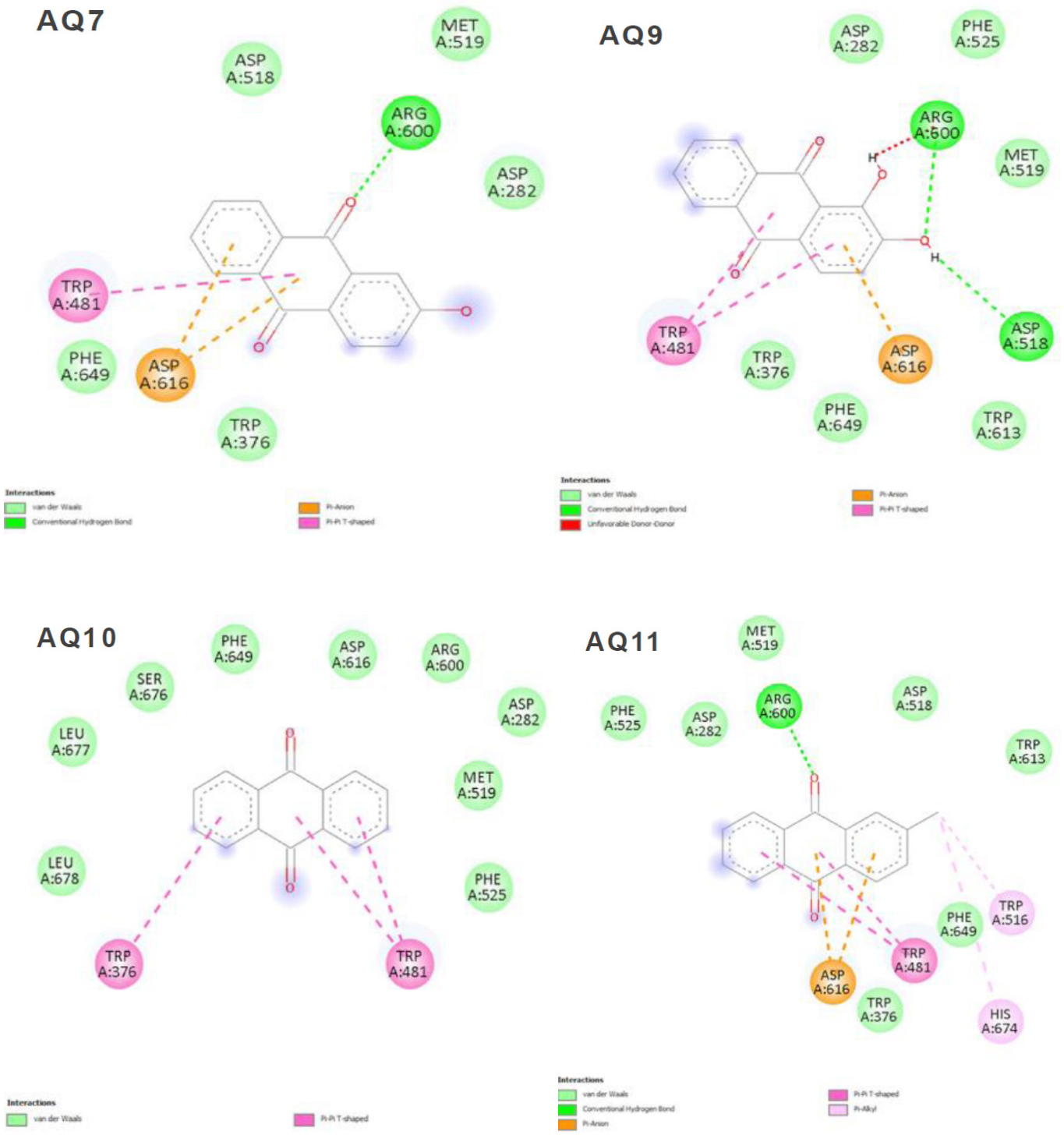

Fig. (S2). The 2D diagrams of binding poses of 10 of the 14 compounds interacting with α-glucosidase, excluding the top 4 compounds with the highest interactions. Interactions in light and dark green colours represent hydrogen bond; interactions in pink or purple colours represent hydrophobic interaction.