Supplementary Materials

GC-MS Phytochemical Profiling, Pharmacological Properties, and In Silico Studies of *Chukrasia velutina* Leaves: A Novel Source for Bioactive Agents

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Table S1. Phytochemical screening of MECVL.

Test Name	Observation
Resin	+
Flavonoids	-
Saponins	-
Phenol	++
Tannin	++
Alkaloid	+
Carbohydrate	++
Steroid	-
Cholesterol	-
Polyphenol	-
Glycoside	++
Lencoanthocyanin	-

(+) = moderately present; (++) = highly present; (-) = absent.

Table S2. Binding interactions of the selected compounds against human serotonin receptor (pdb: 5I6X) for antidepressant activity.

Compound Name	Hydrogen Bond Interactions	Hydrophobic Bond Interactions
1,2,4 Benzenetriol	Gyl 476, Gyl 476, Ser 174	Leu 492 (Pi-Sigma), Val 479 (Pi- Alkyl)
3-Methyl-2-furoic acid	Tyr 171	Val 488 (Alkyl), Ile 581 (Alkyl), Leu 492 (Alkyl), Leu 492 (Pi- Alkyl), Val 479 (Pi- Alkyl)
2,4-Octadienoic acid, 7-hydroxy-6-methyl	Lue 248, Lue 248, Lue 245	Lue 248 (Alkyl), Gly 249 (Carbon)
Diethyl mercaptal of d-mannose	-	-
dl-Allo-cystathionine	-	-
Phloroglucinol	Ser 174, Gly 476	Val 429 (Pi- Alkyl), Tyr 171 (Pi-Pi-T Shaped)
Acetoacetic acid, 1,3-dithio-, S-ethyl ester	-	Ile 581 (Alkyl)
.beta.-D-Glucopyranose, 1,6-anhydro-	-	-
D-Allose	Try 171	-
Germacrene D	-	-
Cis-muurola-3,5-diene	-	-
.beta.-copaene	-	-
Decanal	Gln 246 Gln 246	Trp 573 (Pi- Alkyl), Trp 573 (Pi- Alkyl)
Dodecanoic acid, 3-hydroxy-	-	Val 479 (Alkyl), Val 488 (Alkyl)
Butanoic acid, octyl ester	-	Trp 573 (Pi- Alkyl), Trp 573 (Pi- Alkyl)
Quinic acid	-	-
1-Heptanol, 2,4-dimethyl-, (R,R)-(+)-	-	-
d-Mannitol, 1-decylsulfonyl-	-	-
d-Mannitol, 1-thiohexyl-1-deoxy-	-	-
4-Diazodamantanone	Tyr 171	Val 479 (Alkyl), Leu 492 (Alkyl)
3-Nonyn-2-ol	Gln 246	Gln 246 (Carbon) Leu 245 (Carbon) Leu 244 (Alkyl) Val 479 (Alkyl) Val 488 (Alkyl)
Chlorozotocin	-	-
Sparsomycin	-	-
9-Dodecen-1-ol, acetate, (Z)-	-	-
Cis-7-Tetradecen-1-ol	-	-

3-Chloropropionic acid, 10-undecenyl ester	-	Leu 245 (Alkyl) Leu 491 (Alkyl) Leu 577 (Alkyl) Val 488 (Alkyl) Val 479 (Alkyl) Val 488 (Alkyl)
Levomenthol	-	Val 488 (Alkyl) Leu 245 (Alkyl) Leu 577 (Alkyl) Leu 577 (Alkyl) Trp 573 (Pi- Alkyl) Trp 573 (Pi- Alkyl)
Dimethylmuconic acid	Tyr 171	Leu 577 (Alkyl) Ile 581 (Alkyl) Phe 170 (Pi-Alkyl)
1,5-Hexadien-3-ol, trifluoroacetate	-	-
Tridecanoic acid, 12-methyl-, methyl ester	-	Leu 248 (Alkyl) Val 479 (Alkyl) Gly 476 (Carbon) Gly 476 (Carbon)
13-Tetradece-11-yn-1-ol	-	-
Undecanal	Gln 246 Trp 573	Trp 573 (Pi-Alkyl) Trp 573 (Pi-Alkyl) Trp 573 (Pi-Sigma) Ile 576 (Alkyl)
Dodecanal	Gln 246 Trp 573	Trp 573 (Pi-Alkyl) Trp 573 (Pi-Alkyl) Leu 245 (Alkyl)
5-Butyl-1,3-oxathiolan-2-one	Tyr 171	Leu 248 (Alkyl) Val 479 (Alkyl) Val 488 (Alkyl) Tyr 171 (Pi-Sulfur)
Glycerol 1-palmitate	-	Leu 245 (Alkyl) Leu 491 (Alkyl) Leu 577 (Alkyl) Val 488 (Alkyl) Ala 580 (Carbon)
Reference drug (Imipramine)	Tyr 171	Val 479 (Pi-Alkyl) Val 479 (Pi-Alkyl) Val 479 (Alkyl) Leu 492 (Alkyl) Ile 581 (Alkyl)

Table S3. Binding interactions of the selected compounds against potassium channel receptor (pdb: 4UUJ) for anxiolytic activity.

Compound Name	Hydrogen Bond Interactions	Hydrophobic Bond Interactions
1,2,4 Benzenetriol	Thr 72 Gly 79 Leu 81	Gly 79 (Carbon)
3-Methyl-2-furoic acid	Trp 68 Leu 81	Met 96 (Alkyl) Gly 77 (Carbon) Tyr 82 (Carbon)
2,4-Octadienoic acid, 7-hydroxy-6-methyl	-	Tyr 82 (Carbon) Trp 68 (Pi-Alkyl)
Diethyl mercaptal of d-mannose	-	-
dl-Allo-cystathionine	-	-
Phloroglucinol	Glu 71 Thr 72 Gly 79	-
Acetoacetic acid, 1,3-dithio-, S-ethyl ester	-	Trp 68 (Pi-Alkyl)
.beta.-D-Glucopyranose, 1,6-anhydro-	Trp 68 Thr 72 Leu 81	Gly 77 (Carbon) Gly 79 (Carbon)
D-Allose	Thr 75	Gly 77 (Carbon) Gly 77 (Carbon)
Germacrene D	-	-
Cis-muurola-3,5-diene	-	-
.beta.-copaene	-	-
Decanal	-	Pro 83 (Alkyl) Met 96 (Alkyl) Ala 92 (Alkyl) Trp 68 (Pi-Alkyl)
Dodecanoic acid, 3-hydroxy-	Trp 68	Trp 68 (Pi-Alkyl) Pro 83 (Carbon) Tyr 82 (Pi-Alkyl)
Butanoic acid, octyl ester	-	Ala 92 (Alkyl) Pro 82 (Alkyl)
Quinic acid	Trp 68 Gly 77	Gly 77 (Carbon) Gly 77 (Carbon) Pro 83 (Carbon) Tyr 82 (Carbon)
1-Heptanol, 2,4-dimethyl-, (R,R)-(+)-	-	-
d-Mannitol, 1-decylsulfonyl-	-	-
d-Mannitol, 1-thiohexyl-1-deoxy-	-	-
4-Diazodamantanone	-	Leu 81 (Pi-Alkyl)
3-Nonyn-2-ol	-	Met 96 (Alkyl)
Chlorozotocin	-	-

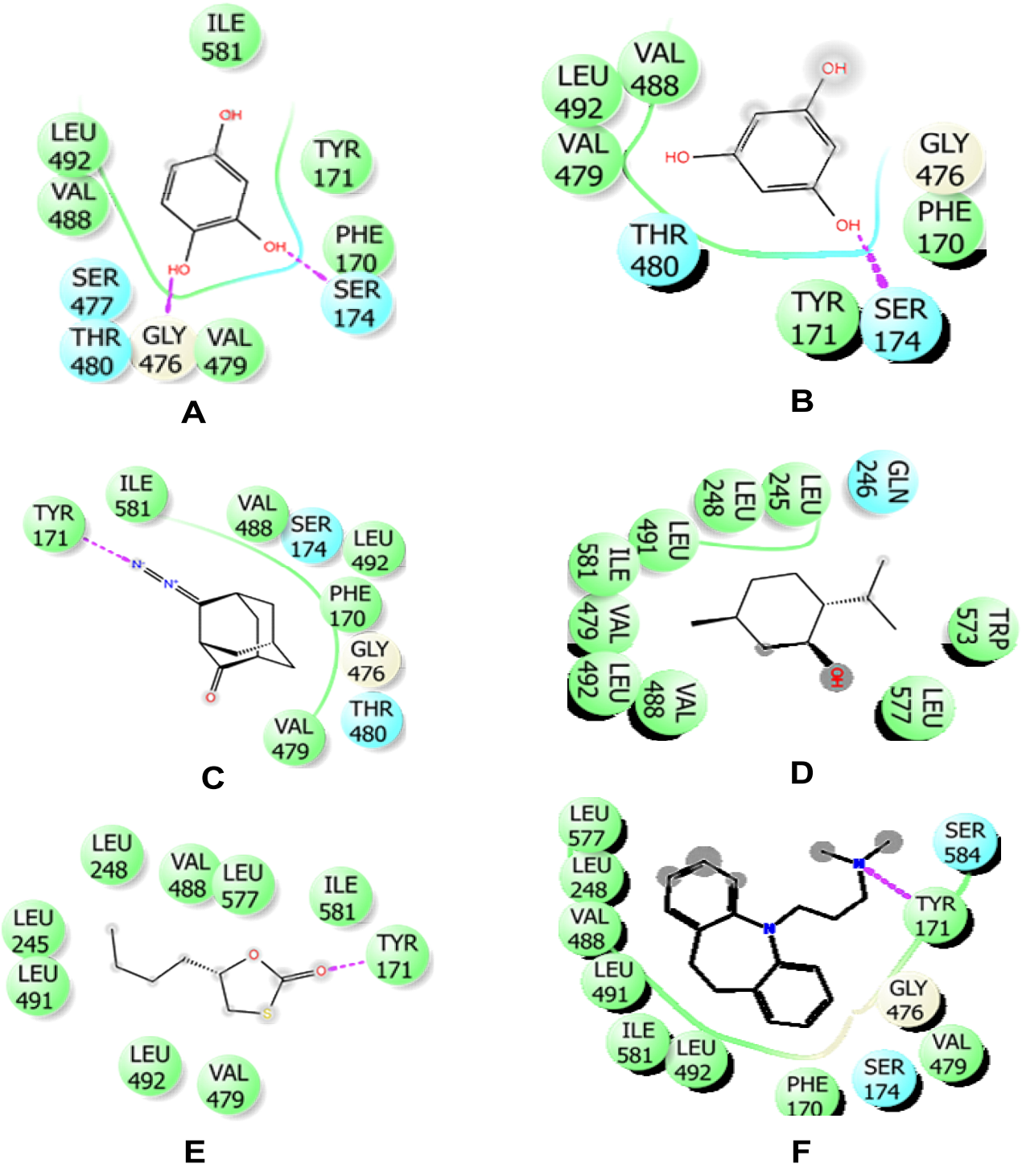
Sparsomycin	-	-
9-Dodecen-1-ol, acetate, (Z)-	-	-
cis-7-Tetradecen-1-ol	-	-
3-Chloropropionic acid, 10-undecenyl ester	-	Tyr 82 (Pi- Sigma)
Levomenthol	Leu 81	Met 96 (Alkyl) Met 96 (Alkyl) Ala 92 (Alkyl) Pro 83 (Alkyl) Trp 68 (Pi-Alkyl) Trp 68 (Pi-Alkyl) Tyr 82 (Pi-Alkyl) Tyr 82 (Pi-Alkyl)
Dimethylmuconic acid	Thr 72 Trp 68	Gly 77 (Carbon) Gly 77 (Carbon) Gly 77 (Carbon)
1,5-Hexadien-3-ol, trifluoroacetate	-	-
Tridecanoic acid, 12-methyl-, methyl ester	-	Trp 68 (Pi-Alkyl) Trp 68 (Pi-Alkyl) Ala 92 (Pi-Alkyl) Met 96 (Alkyl) Pro 83 (Alkyl)
13-Tetradece-11-yn-1-ol	-	Ala 92 (Alkyl) Pro 83 (Alkyl) Arg 89 (Alkyl) Gly 77 (Carbon)
Undecanal	-	Trp 68 (Pi-Alkyl) Trp 68 (Pi-Alkyl) Pro 83 (Alkyl) Ala 92 (Alkyl) Met 96 (Alkyl)
Dodecanal	-	Gly 79 (Carbon) Arg 89 (Alkyl) Pro 83 (Carbon)
5-Butyl-1,3-oxathiolan-2-one	Trp 68	Pro 83 (Carbon) Trp 68 (Pi-Alkyl)
Glycerol 1-palmitate	Trp 78	Trp 78 (Pi-Alkyl) Trp 78 (Pi-Sigma) Gly 79 (Carbon)
Reference drug (Diazepam)	-	Trp 163 (Pi-Pi-Stacked) Trp 163 (Pi-Pi-Stacked) Trp 163 (Pi-Pi-T Shaped) Trp 163 (Pi-Pi-T Shaped) Asp 165 (Carbon) Thr 164 (Carbon) Lys 142 (Pi-Alkyl) Asp 143 (Pi-Anion)

Table S4. Binding interactions of the selected compounds against human gabaa receptor (pdb: 4COF) for sedative activity.

Compound Name	Hydrogen Bond Interactions	Hydrophobic Bond Interactions
1,2,4 Benzenetriol	Glu 155	Tyr 62 (Pi-Pi- stacked)
	Glu 155	Tyr 205 (Pi-Pi-T- Shaped)
	Gln 64	
3-Methyl-2-furoic acid	Trp 68	Met 96 (Alkyl)
	Leu 81	Gly 77 (Carbon)
		Tyr 82 (Carbon)
2,4-Octadienoic acid, 7-hydroxy-6-methyl	Gln 64	Asp 43 (Carbon)
		Tyr 157 (Carbon)
		Tyr 157 (Pi-Alkyl)
		Tyr 97 (Pi-Alkyl)
		Tyr 62 (Pi-Alkyl)
		Phr 200 (Pi-Alkyl)
Diethyl mercaptal of d-mannose	-	-
dl-Allo-cystathionine	-	-
Phloroglucinol	Gln 64	Tyr 157 (Pi-Pi-T- Shaped)
	Thr 202	Phe 200 (Pi-Pi-T- Shaped)
	Glu 155	
	Tyr 97	
Acetoacetic acid, 1,3-dithio-, S-ethyl ester	Gln 64	Tyr 97 (Pi-Alkyl)
	Gln 64	Tyr 205 (Pi-Alkyl)
.beta.-D-Glucopyranose, 1,6-anhydro-	Gln 64	Glu 155 (Carbon)
	Thr 202	Glu 155 (Carbon)
	Glu 155	Tyr 157 (Carbon)
	Tyr 97	
	Tyr 157	
D-Allose	Glu 155	Tyr 157 (Carbon)
Germacrene D	-	-
Cis-muurola-3,5-diene	-	-
.beta.-copaene	-	-
Decanal	Gln 64	Phe 200 (Pi-Alkyl)
Dodecanoic acid, 3-hydroxy-	Tyr 157	Tyr 62 (Pi-Alkyl)
	Tyr 157	Leu 99 (Alkyl)
	Gln 64	Tyr 157 (Carbon)
Butanoic acid, octyl ester	Gln 64	Ala 45 (Alkyl)
		Leu 99 (Alkyl)
		Met 115 (Alkyl)
		Tyr 205 (Pi-Alkyl)
Quinic acid	Gln 64	Tyr 157 (Carbon)
	Tyr 157	
	Tyr 205	
	Thr 202	
	Glu 155	

	Glu 155	
1-Heptanol, 2,4-dimethyl-, (R,R)-(+)-	-	-
d-Mannitol, 1-decylsulfonyl-	-	-
d-Mannitol, 1-thiohexyl-1-deoxy-	Gln 64	Tyr 62 (Pi-Sulfur)
	Tyr 205	Phe 200 (Pi-Sulfur)
		Leu 99 (Pi-Alkyl)
		Thr 202 (Carbon)
		Thr 202 (Carbon)
		Tyr 157 (Carbon)
		Tyr 205 (Carbon)
4-Diazodamantanone	-	Tyr 155 (Pi-Cation)
		Tyr 62 (Pi-Alkyl)
		Tyr 205 (Pi-Alkyl)
		Phe 200 (Pi-Alkyl)
3-Nonyn-2-ol	Glu 155	Met 155 (Pi-Alkyl)
		Tyr 205 (Pi-Alkyl)
		Glu 155 (Carbon)
Chlorozotocin	-	-
Sparsomycin	-	-
9-Dodecen-1-ol, acetate, (Z)-	-	-
Cis-7-Tetradecen-1-ol	-	-
3-Chloropropionic acid, 10-undecenyl ester	Gln 64	Met 115 (Cl, Br, I))
Levomenthol	Gln 64	Tyr 62 (Pi-Alkyl)
		Tyr 97 (Pi-Alkyl)
		Tyr 205 (Pi-Alkyl)
		Tyr 205 (Pi-Alkyl)
		Phe 200 (Pi-Alkyl)
Dimethylmuconic acid	Gln 64, Glu 155, Tyr 157 (2)	Tyr 92 (Pi-Alkyl)
		Tyr 157 (Pi-Alkyl)
		Phe 200 (Pi-Alkyl)
		Gly 127 (Pi-Alkyl)
1,5-Hexadien-3-ol, trifluoroacetate	-	-
Tridecanoic acid, 12-methyl-, methyl ester	Ala 201	Tyr 97 (Pi-Alkyl)
		Tyr 205 (Pi-Alkyl)
		Tyr 205 (Pi-Alkyl)
		Phe 200 (Pi-Alkyl)
		Phe 200 (Pi-Sigma)
		Ala 201 (Alkyl)
13-Tetradece-11-yn-1-ol	-	Tyr 62 (Pi-Sigma)
		Tyr 157 (Pi-Alkyl)
		Met 115 (Alkyl)
Undecanal	Gln 64	Ala 45 (Pi-Alkyl)
		Tyr 62 (Pi-Alkyl)
Dodecanal	Tyr 157	Tyr 62 (Pi-Alkyl)
		Gly 127 (Carbon)
5-Butyl-1,3-oxathiolan-2-one	Gln 64	Tyr 62 (Pi-Alkyl)

		Tyr 205 (Pi-Alkyl)
		Phe 200 (Pi-Alkyl)
Glycerol 1-palmitate	Ala 45	Asp 43 (Carbon)
	Ile 44	Asp 43 (Acceptor-Acceptor)
	Arg 207	Phe 200 (Pi-Sigma)
Reference drug (Diazepam)	-	Tyr 157 (Carbon)
		Tyr 157 (Carbon)
		Tyr 157 (Carbon)
		Tyr 205 (Pi-Alkyl)
		Ala 201 (Pi-Alkyl)
		Asp 43 (Pi-Anion)
		Tyr 62 (Pi-Pi-Stacked)
		Phe 200 (Pi-Pi-Stacked)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PHE 170
SER 174
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THR 480
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VAL 479
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GLY 476
PHE 170
THR 480
TYR 171
SER 174
B
TYR 171
ILE 581
VAL 488
SER 174
LEU 492
PHE 170
GLY 476
THR 480
VAL 479
C
GLN 246
LEU 245
LEU 248
LEU 491
ILE 581
VAL 479
TRP 573
LEU 492
VAL 488
LEU 577
D
LEU 248
VAL 488
LEU 577
ILE 581
LEU 245
TYR 171
LEU 491
LEU 492
VAL 479
E
LEU 577
SER 584
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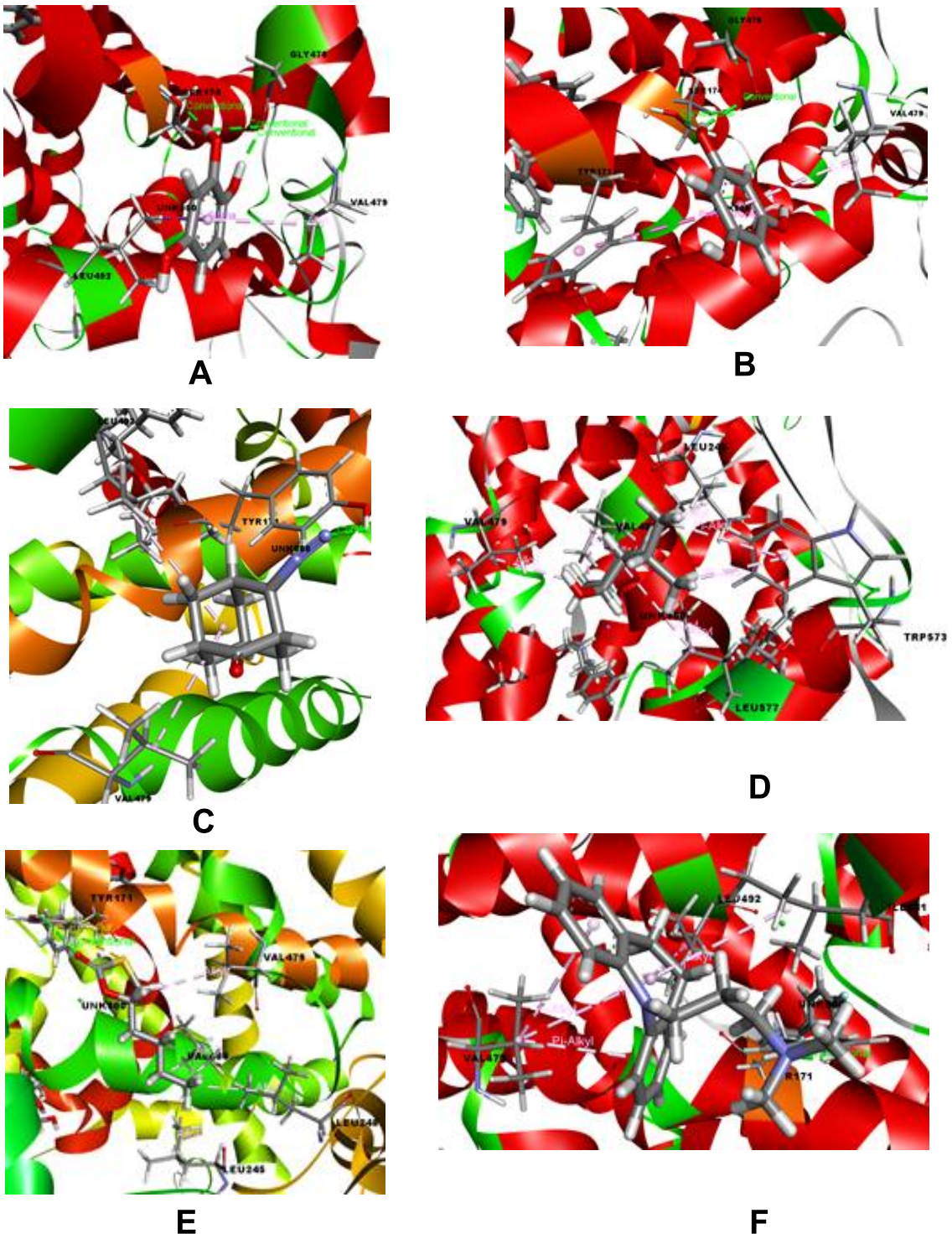
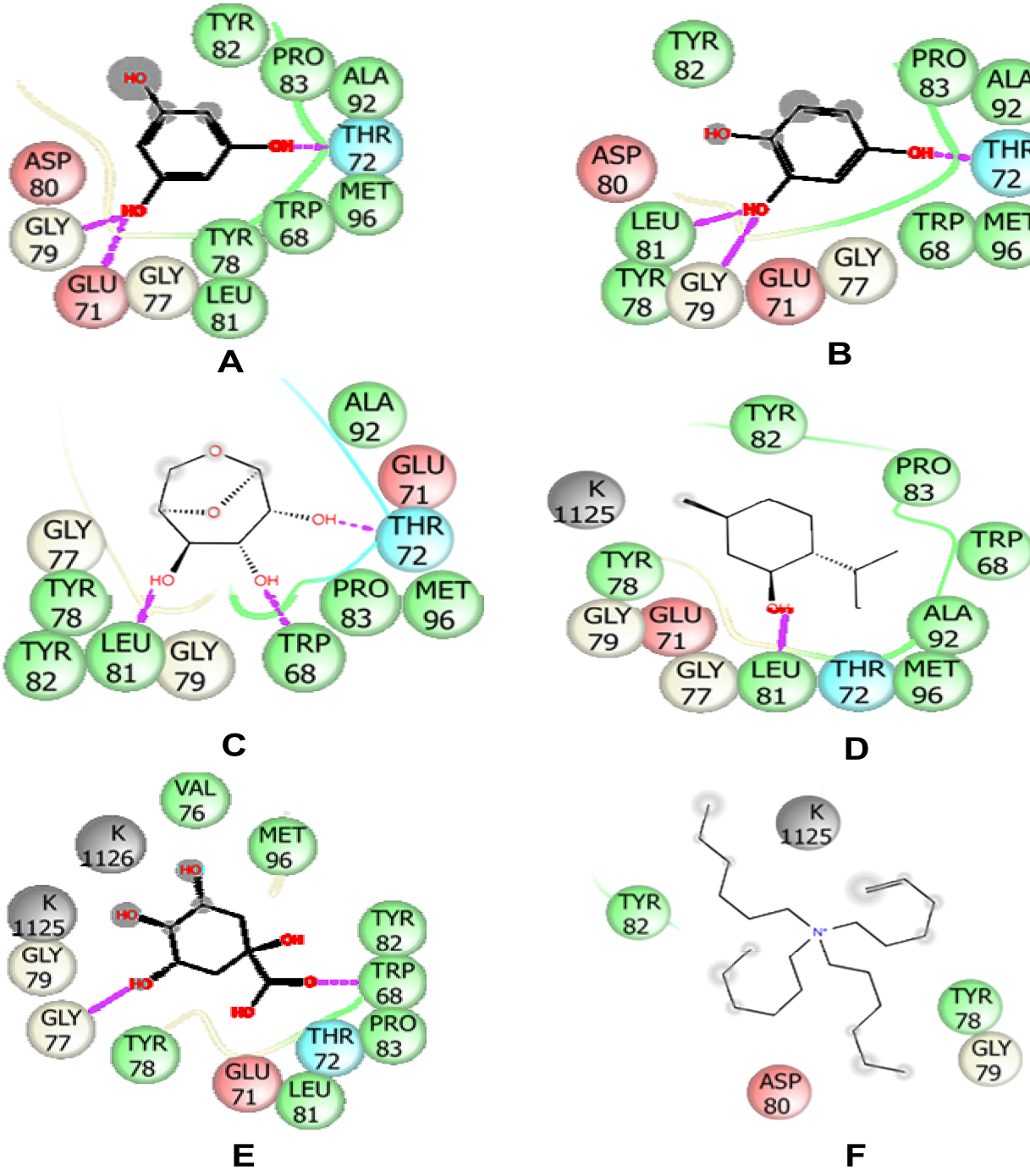
ILE 581
LEU 492
VAL 479
SER 174
PHE 170
F

(a)



(b)

Figure S1. Best scored compounds exert in 2D **(a)** and 3D **(b)** of 1,2,4-Benzenetriol **(A),** Phloroglucinol **(B),** 4-Diazodamantanone **(C),** Levomenthol **(D),** 5-Butyl-1,3-oxathiolan-2-one **(E)** and also **(F)** Imipramine (RSD) when they enclosed with human serotonin receptor (PDB: 5I6X) for antidepressant effect of MECVL.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THR 72
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TRP 68
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GLY 77
LEU 81
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B
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D
E
F
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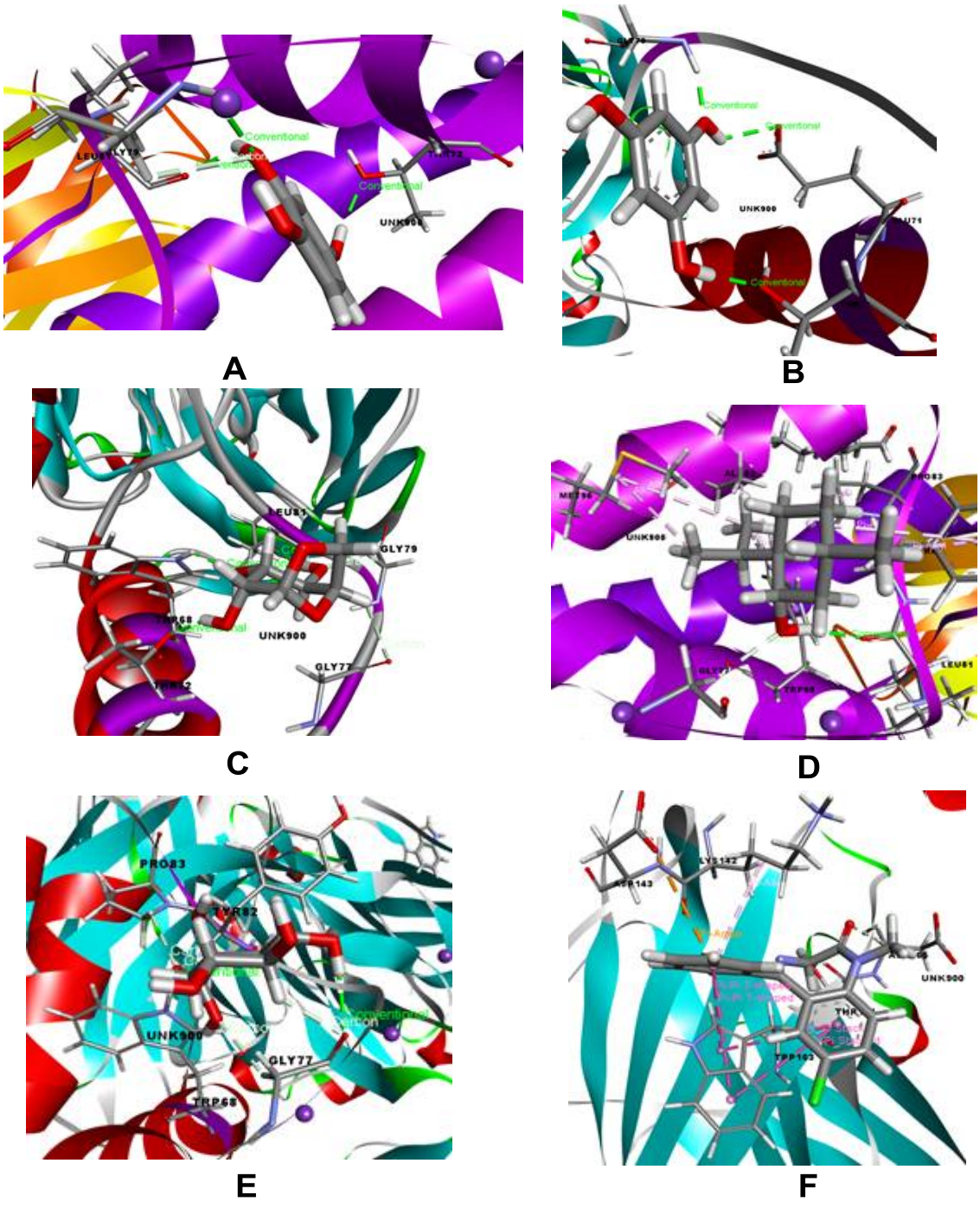
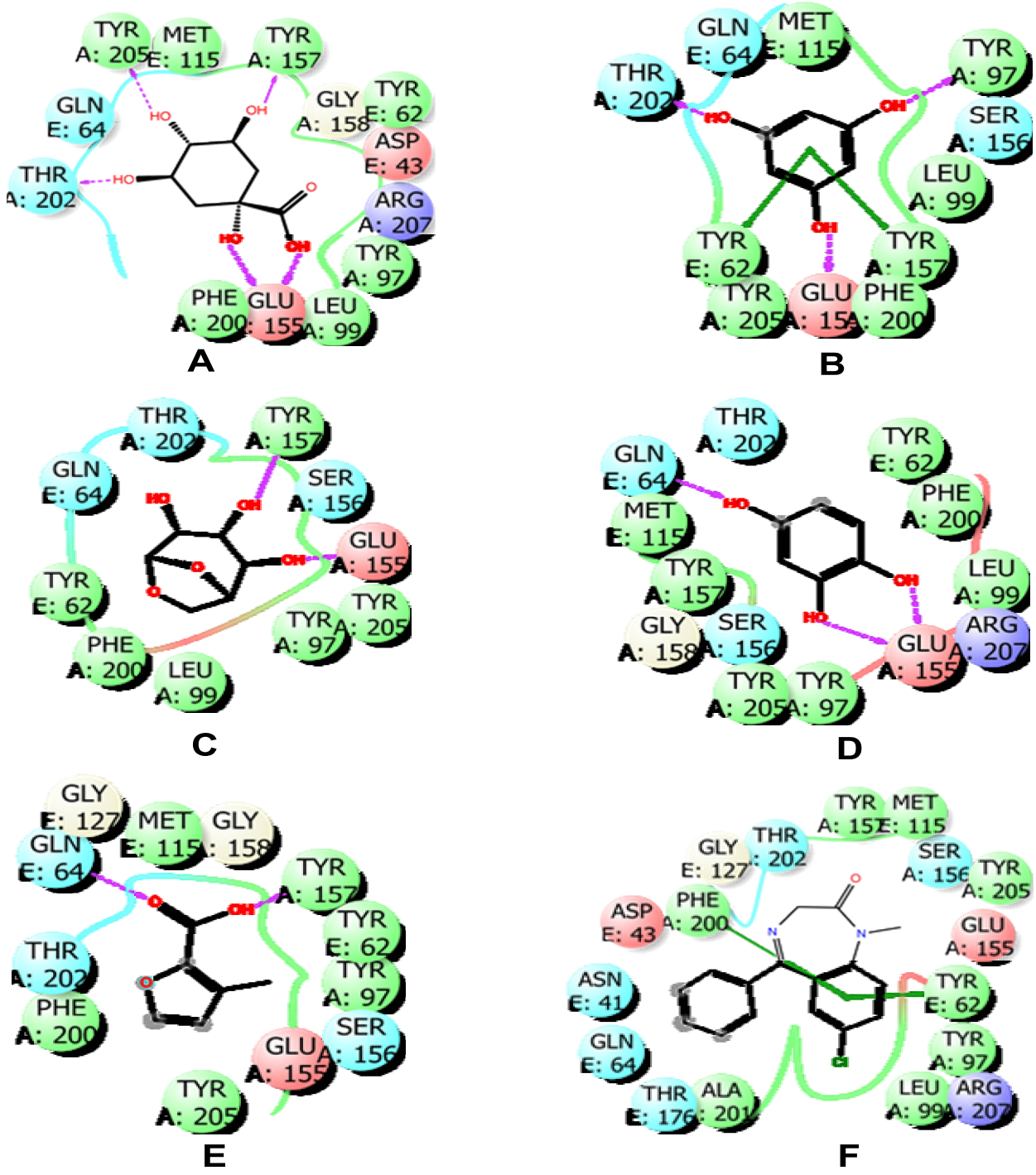
K 1126
VAL 76
HO
OH
O

(a)



(b)

Figure S2. Best scored compounds exert in 2D **(a)** and 3D **(b)** of Phloroglucinol (**A),** 1,2,4 Benzenetriol (**B),** .beta.-D-Glucopyranose, 1,6-anhydro- (**C),** Levomenthol **(D),** Quinic acid **(E)** and also **(F)** Diazepam (RSD) when they enclosed with potassium channel receptor (PDB: 4UUJ) for anxiolytic effect of MECVL.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PHE A: 200
GLU A: 155
LEU A: 99
A
GLN E: 64
MET E: 115
THR A: 202
TYR A: 97
SER A: 156
LEU A: 99
TYR E: 62
TYR A: 157
TYR A: 205
GLU A: 155
PHE A: 200
B
THR A: 202
TYR A: 157
GLN E: 64
SER A: 156
GLU A: 155
TYR E: 62
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TYR A: 97
PHE A: 200
LEU A: 99
C
THR A: 202
TYR E: 62
GLN E: 64
PHE A: 200
MET E: 115
LEU A: 99
TYR A: 157
GLY A: 158
SER A: 156
ARG A: 207
GLU A: 155
TYR A: 205
TYR A: 97
D
GLY E: 127
MET E: 115
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TYR A: 97
PHE A: 200
SER A: 156
GLU A: 155
TYR A: 205
E
TYR A: 157
MET E: 115
GLY E: 127
THR A: 202
SER A: 156
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PHE A: 200
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GLU A: 155
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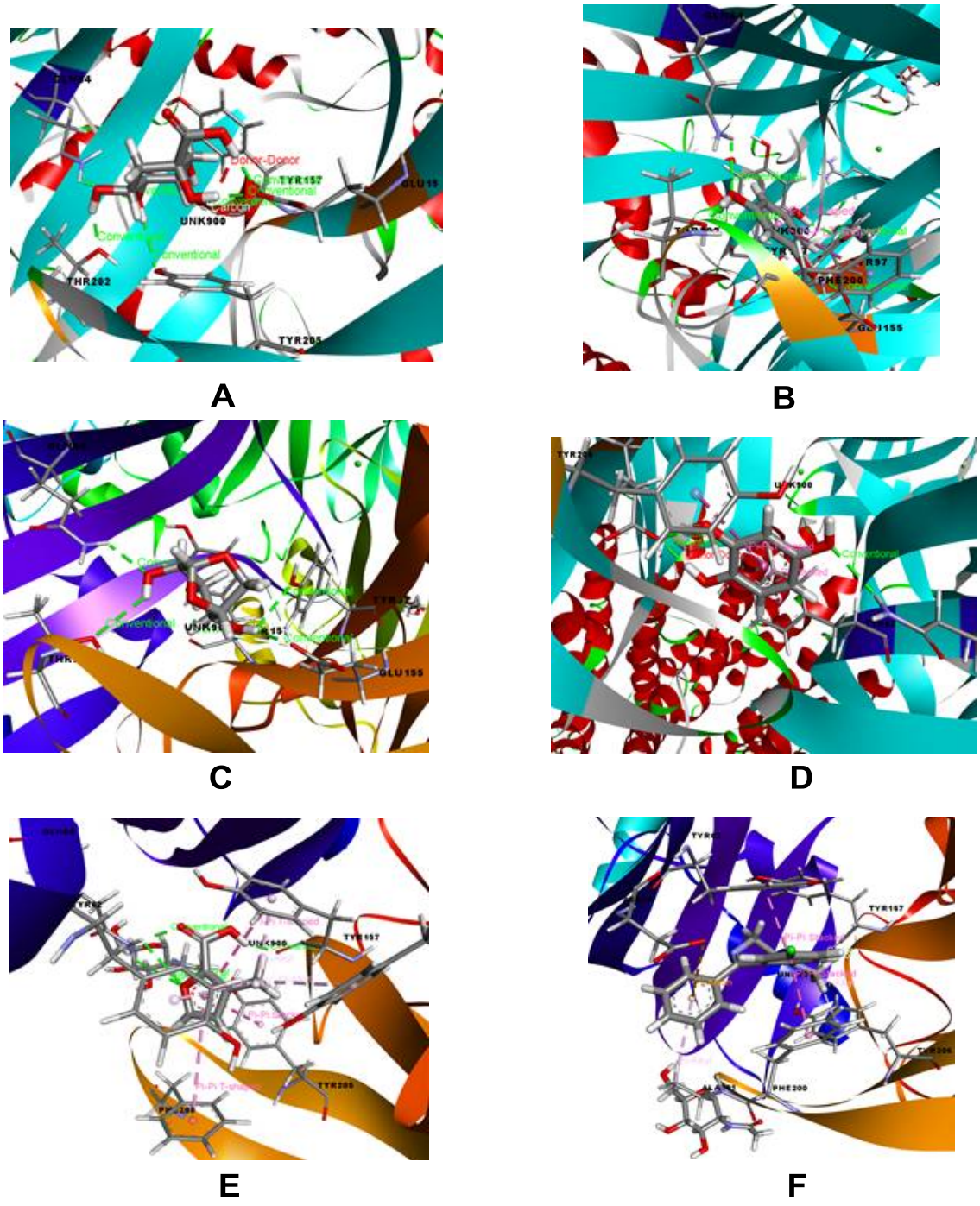
LEU A: 99
ARG A: 207
F

(a)



(b)

Figure S3. Best scored compounds exert in 2D **(a)** and 3D **(b)** of Quinic acid **(A),** Phloroglucinol **(B),** .beta.-D-Glucopyranose, 1,6-anhydro- **(C),** 3-Methyl-2-furoic acid **(D),** 1,2,4 Benzenetriol **(E)** and also **(F)** Diazepam (RSD) when they enclosed with crystal structure of human gabaa receptor (PDB: 4COF) for sedative effect of MECVL.