

## **Supplementary File**

### ***A detailed in vitro characterization of some underrated plant species and in silico drug interaction mechanism validation: A possible horizon of new therapeutic gateway***

<sup>1</sup>Suryasarathi Kumar, <sup>2</sup>Debarati Jana, <sup>3</sup>Sanaya Mukherjee, <sup>3</sup>Chitra Dutta, <sup>4</sup>S Sharda, <sup>5</sup>Adeepa Banerjee, <sup>6</sup>Resmi Khatun, <sup>7</sup>Shreya Gupta, <sup>8</sup>Anuraj Kar, <sup>3</sup>Palash Dey, <sup>9</sup>Baisakhi Mukherjee, <sup>10</sup>Durba Roy, <sup>11</sup>Somdatta Banerjee, <sup>12</sup>Deepayan Samanta, <sup>13</sup>Subhamoy Banerjee, <sup>14</sup>Chinmoyee Pramanik, <sup>15</sup>Anuska Ghosh, <sup>15</sup>Isha Dey, <sup>15</sup>Niladri Choudhury, <sup>3</sup>Sneha Sarkar, <sup>7</sup>Priyanka Talukdar, <sup>7</sup>Somnath Das

<sup>1</sup>School of Biological Sciences & Technology, Department of Applied Biology, Maulana Abul Kalam Azad University of Technology-Main Campus, NH-12 (Old NH-34), Simhat, Haringhata, Nadia, West Bengal 741249, India

<sup>2</sup>School of Life Science, Department of Biotechnology, Babasaheb Bhimrao Ambedkar University, Vidya Vihar Raibareli Road, Babasaheb Bhim Rao Ambedkar University, Lucknow, Uttar Pradesh 226025

<sup>3</sup>Department of Microbiology, Swami Vivekananda Institute of Modern Science Sonarpur Station Rd, Karbala More, Kumarkhali, Narendrapur, Kolkata, West Bengal, India

<sup>4</sup>Department of biotechnology, Dr. Hari Singh Gaur Vishvavidyalaya, Sagar (M.P.), University Road, Sagar, Madhya Pradesh 470003, India

<sup>5</sup>Department of Industrial Biotechnology, Gujarat Biotechnology University, Gujarat International Finance Tec-City, Gandhinagar, Gujarat 382355

<sup>6</sup>Department of Microbiology, Bidhannagar College City Center, 3rd Ave, EB-2, Sector 1, Bidhannagar, Kolkata, West Bengal 700064, India

<sup>7</sup>The Institute of Science Culture and Social Studies, Belgharia, Kolkata, West Bengal 700056, India

<sup>8</sup>IQ City United World School of Business, MBA in Marketing, Vidyasagar University, 10th Floor, Infinity Benchmark, Plot- G1, Block- EP & GP Sector- V, Saltlake, Kolkata 700091

<sup>9</sup>Department of Biotechnology, Institute of Genetic Engineering, 30, Thakurhat Road, Badu, Madhyamgram, Kolkata, West Bengal 700128

<sup>10</sup>Department of Biotechnology, Guru Nanak Institute of Pharmaceutical Science and Technology, 157/F, Nilgunj Rd, Sahid Colony, Panihati, Kolkata, Khardaha, West Bengal 700114

<sup>11</sup>Department of Microbiology, Lady Brabourne College, University of Calcutta, P-1/2, Suhrawardy Ave, Beniapukur, Kolkata, West Bengal 700017

<sup>12</sup>Department of Biotechnology, Jis University, 81, Nilgunj Rd, Jagarata Pally, Deshpriya Nagar, Agarpara, Kolkata, West Bengal 700109

<sup>13</sup>School of Biological Sciences & Technology, Department of Life Science-Microbiology, Maulana Abul Kalam Azad University of Technology, West Bengal-Main Campus, NH-12 (Old NH-34), Simhat, Haringhata, Nadia, West Bengal 741249, India

<sup>14</sup>School of Biological Sciences & Technology, Department of Life Science-Genetics, Maulana Abul Kalam Azad University of Technology, West Bengal-Main Campus, NH-12 (Old NH-34), Simhat, Haringhata, Nadia, West Bengal 741249, India

<sup>15</sup>Department of Microbiology, Swami Vivekananda Institute of Modern Science Sonarpur Station Rd, Karbala More, Kumarkhali, Narendrapur, Kolkata, West Bengal, India

**Supplementary Table 1:** Detailed FTIR functional group analysis.

Functional Groups	<i>Areca catechu</i>		<i>Graptophyllum pictum</i>		<i>Tradescantia pallida</i>		<i>Chrysogonum peruvianum</i>		<i>Cocos nucifera</i>	
	<i>E. coli</i>	<i>Staphylococcus</i> sp.	<i>E. coli</i>	<i>Staphylococcus</i> sp.	<i>E. coli</i>	<i>Staphylococcus</i> sp.	<i>E. coli</i>	<i>Staphylococcus</i> sp.	<i>E. coli</i>	<i>Staphylococcus</i> sp.
Aliphatic Ester, Acetate	+	+	-	+	-	+	+	+	-	-
Linear Bromo Compound	+	+	-	-	+	-	+	+	+	+

Unsaturated Hydrocarbon, Cis Alkene	+	+	-	-	-	+	-	-	-	+
Unsaturated Hydrocarbon, Vinyl	+	-	-	-	-	+	-	-	-	-
Aliphatic Acid Halide, Linear	+	+	+	+	+	+	+	+	+	+
CHF2	+	-	-	+	-	-	-	-	-	+
Ethoxy Silane	+	+	+	+	+	+	+	+	+	+
Aliphatic Nitrile	+	+	-	-	+	-	+	+	-	-
Furan, 2 subst.	+		-	-	-	-	-	-	-	+
Unsaturated Hydrocarbon, Vinylidene	+	-	-	-	-	+	-	-	-	+
Aliphatic Acid Halide, Long Chain Linear	+	-	-	-	-	-	-	-	-	-
Aliphatic Primary Amide	+	+	-	+	-	-	+	-	-	-
Aliphatic Tertiary	+	-	-	+	-	-	-	-	-	-
Unsaturated Hydrocarbon, Trisubstituted	+	+	-	-	-	-	-	-	-	-
3-Substituted Phenol	+	-	-	-	-	-	-	-	-	-
4-Subst Pyridine	+	-	-	-	-	-	-	-	-	+
Aliphatic Amido,	+	-	-	+	-	-	-	-	-	+









Aryl Strained Ring or Activated Carbonyl	+	-	-	-	-	-	-	-	-	+
Carbonyl, Possibly 2-Hydroxy Acid	+	-	-	-	-	-	-	-	-	-
Carbonyl, Possibly Conjugated Acid	+	-	-	-	-	-	-	-	-	-
Carboxylic Acid, Diacid	+	-	-	-	-	-	-	-	-	-
Carboxylic Acid, General	+	-	-	-	-	-	-	-	-	+
Carboxylic Acid, Linear Chain	+	-	-	-	-	-	-	-	-	-
Cyclic Anhydride, Five Membered	+	-	-	+	-	-	-	-	-	+
Cyclic Anhydride, Six Membered	+	-	-	+	-	-	-	-	-	+
Diaryl Phosphite	+	-	-	-	-	-	-	-	-	-
Epoxy Substituent	+	-	-	-	-	-	-	-	-	+
Hydroxy Compound	+	-	-	+	-	-	-	-	-	+





Secondary Alcohol, In Chain OH	+	-	-	-	-	-	-	-	-	-
Substituted Allene	+	-	-	-	-	-	-	-	-	-
Terminal Allene	+	-	-	-	-	-	-	-	-	+
Tertiary Alcohol	+	+	+	+	+	+	+	+	+	+
Tertiary Alcohol, Possibly 2-OH and Methyl	+	+	-	-	-	-	-	-	-	-
Tetraethyl Ammonium Salt	+	-	-	+	-	+	+	-	-	+
Tetramethyl Ammonium Salt	+	+	-	+	-	+	-	+	-	+
Triaryl Phosphate	+	-	-	-	-	-	-	-	-	+
Unsaturated Hydrocarbon, Cis-Trans Alkene	+	+	-	-	-	+	-	-	-	+
Unsaturated Hydrocarbon, Cyclic, >C5	+	+	+	+	+	+	+	+	+	+
Unsaturated Hydrocarbon, Generic, Isolated	+	-	-	+	-	-	-	-	-	+

Unsaturated Hydrocarbon, Trans Conjugated	+	+	-	-	-	+	-	-	-	+
Aliphatic Acid or Carbonyl Compound	+	-	-	-	-	-	-	-	-	+
Aliphatic Aldehyde	+	-	-	-	-	-	-	-	-	-
Aliphatic Amino Acid - Carbonyl Compound	+	-	-	-	-	+	-	-	-	-
Carbonyl, Alpha Methylene	+	-	-	+	-	-	-	-	-	+
Strained Ring or Activated Carbonyl	+	-	-	+	-	-	-	-	-	+
t-Butoxy Substituent	+	-	-	-	-	-	-	-	-	-
Aliphatic Primary Amide, Linear	+	-	-	-	-	-	-	-	-	-
Aliphatic Amine, Primary, Possibly Methoxy Substituted	+	-	-	-	-	-	-	-	-	-
N-Methyl Amino,	+	+	+	+	-	+	+	+	-	+

Tertiary, Aliphatic										
Nitrile, Phenyl Substituted	+	-	-	+	-	-	-	-	-	+
Phenyl Subs. Isocyanate	+	-	-	+	-	-	-	-	-	+
Phenyl Subs. Isothiocyanate	+	-	-	-	-	-	-	-	-	+
Alkene Conjugated Ketone	+	-	-	-	-	-	-	-	-	-
Aliphatic Sulfonic Acid	+	-	-	-	-	-	-	-	-	+
Phenyl Substituent	+	+	+	+	+	+	+	+	+	+
Linear Chloro Compound	+	+	-	+	+	+	+	+	+	+
Methoxy Substituent	+	-	-	-	-	-	-	-	-	-
Silanol	+	-	-	+	-	-	-	-	-	+
Unsaturated Hydrocarbon, Ether Conjugated	+	+	+	+	+	+	-	+	+	+
Aliphatic Alkoxy, Methoxy	+	+	+	+	+	+	+	+	+	+
CF <sub>3</sub> group	+	+	+	+	+	+	+	+	+	+
Long Chain Halogen Compound	-	+	-	-	-	+	-	+	-	-

Tetrapropyl Ammonium Salt	-	+	-	+	-	-	+	-	-	-
Long Chain Alkyl, Crystalline	-	+	-	+	+	+	-	+	+	+
Long Chain Substituent	-	+	-	+	+	+	-	-	+	+
Aliphatic Mercapto Group	-	-	-	-	+	-	-	-	-	-
Aliphatic Nitrile, Conjugated	-	-	-	-	+	-	-	-	-	-
Aliphatic Isonitrile	-	-	-	-	+	-	-	-	-	-
Aliphatic Mercaptan, Branched, Methyl	-	-	-	-	+	-	-	-	-	-
Aliphatic Thiocyanate	-	-	-	-	+	-	-	-	-	-
Aliphatic Amine, Primary	-	-	-	-	-	-	-	-	-	-
Aliphatic Amine Salt, Secondary	-	-	-	-	+	-	-	-	-	-
Branched, Gem Dimethyl	-	-	-	-	+	-	-	-	-	-
N-MethylAmino Substituent	-	-	-	-	-	-	+	-	-	-





Alcohol, Long Chain										
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**Supplementary Table 2:** Molecular docking analysis of the target and pathogenic proteins of *E. coli* and *Staphylococcus* sp.

Proteins	Antibiotics	Vina score (kcal/mol)	Cavity volume (Å <sup>3</sup> )	Centre	Docking size	Contact residues
3DW0 - Carbapenemase	Penicillin	-7.3	448	9, -25, 30	22, 22, 22	<b>Chain B:</b> CYS69 SER70 LYS73 TRP105 SER106 PRO107 TYR129 SER130 ASP131 ASN132 GLU166 LEU167 LEU169 ASN170 THR215 THR216 GLY217 HIS219 ARG220 LYS234 THR235 GLY236 THR237 CYS238 GLY239 HIS274 GLU276
	Ampicillin	-7.4	448	9, -25,30	21,21,21	<b>Chain B:</b> CYS69 SER70 LYS73 TRP105 PRO107 TYR129 SER130 ASP131 ASN132 GLU166 LEU167 GLU168 LEU169 ASN170 SER171 THR215 THR216 GLY217 HIS219 ARG220 LYS234 THR235 GLY236 THR237 CYS238 GLY239 HIS274 GLU276
	Tetracycline	-8.3	286	-7,17,24	21,21,21	<b>Chain A:</b> SER70 LYS73 PRO104 TRP105 SER106 PRO107 GLN128 TYR129 SER130 ASP131 ASN132 GLU166 LEU167 ASN170 THR215 THR216 GLY217 ARG220 LYS234



						THR235 GLY236 THR237 CYS238 GLY239 HIS274 GLU276
	Metronidazole	-5.4	448	9, -25,30	17,17,17,	<b>Chain B:</b> CYS69 SER70 LYS73 TRP105 SER106 PRO107 TYR129 SER130 ASP131 ASN132 GLU166 LEU167 ASN170 THR216 GLY217 ARG220 LYS234 THR235 GLY236 THR237 CYS238 GLY239 HIS274 GLU276
1QOH - Shiga toxin	Penicillin	-8.4	3259	-21, -1, 115	22, 29, 32	<b>Chain F:</b> GLU116 ASN118 TRP134 <b>Chain J:</b> TRP530 THR531 ASN532 ARG533 TRP534 ASN535 SER554 ASN555 THR556 GLY562 PHE563 ALA564 <b>Chain K:</b> ASN118 ASN132 TRP134 ASN135 PRO138 LEU139 <b>Chain L:</b> TRP234 ASN235 GLN237 PRO238 LEU239 <b>Chain M:</b> TRP334 ASN335 GLN337 PRO338 <b>Chain N:</b> TRP434 ASN435 GLN437 PRO438 <b>Chain O:</b> TRP534 ASN535 PRO538
	Ampicillin	-8.6	3259	-21, -1,115	27,29,32	<b>Chain F:</b> TYR114 GLU116 ASN118 TRP134 <b>Chain J:</b> TRP530 THR531 ASN532 ARG533 TRP534 ASN535 SER554 ASN555 THR556 GLY560 SER561 GLY562 PHE563 ALA564 <b>Chain K:</b> TYR114 ASP117 ASN118 ASN132 ARG133 TRP134 ASN135 GLN137 PRO138 <b>Chain L:</b> ASN218 TRP234 ASN235

						PRO238 LEU239 <b>Chain M:</b> TRP334 ASN335 LEU336 GLN337 PRO338 LEU339 <b>Chain N:</b> TRP434 ASN435 GLN437 PRO438 <b>Chain O:</b> TRP534 ASN535 PRO538
	Tetracycline	-9.3	1310	-20,4,110	27,21,21	<b>Chain F:</b> TYR114 GLU116 ASN118 TRP134 <b>Chain J:</b> ASN532 ARG533 TRP534 ASN535 <b>Chain K:</b> TRP134 PRO138 <b>Chain L:</b> TRP234 ASN235 PRO238 LEU239 <b>Chain M:</b> TRP334 ASN335 LEU336 GLN337 PRO338 LEU339 <b>Chain N:</b> TRP434 ASN435 LEU436 GLN437 PRO438 <b>Chain O:</b> TRP534 ASN535 GLN537 PRO538
	Metronidazole	-5.2	1360	16,12,71	17,28,34	<b>Chain A:</b> ASN115 GLU116 ASP117 <b>Chain E:</b> GLU565 <b>Chain H:</b> ALA301 ASP303 CYS304 ALA305 LYS306 SER325 ARG327 CYS357 <b>Chain Q:</b> ASP217 ASN218 TRP230 THR231 ASN232 ARG233 TRP234 GLN237 SER254 ASN255 THR256 SER261 GLY262 PHE263 ALA264 <b>Chain R:</b> GLU316
1AZZ - Collagenase		-8.0	3165	0,63,116	35,22,35	<b>Chain B:</b> TYR94 ASN95 SER96 PHE97 <b>Chain C:</b> GLU33 SER34 LYS37 GLU39 LEU40 LEU41 ASN61 TYR72 ALA99

	Penicillin					TYR100 LEU101 GLY102 ASP103 ALA104 MET106 LEU107 ARG108 TYR109 ARG128 TRP130 <b>Chain D:</b> GLU33 SER34 LEU36 LYS37 GLU39 LEU40 LEU41 ASN61 TYR72 THR98 ALA99 TYR100 LEU101 GLY102 ASP103 ALA104 GLY105 MET106 LEU107 ARG108 TYR109 ASN110 PRO114 ILE115
	Ampicillin	-7.9	3165	0,63,116	35,21,35	<b>Chain B:</b> ASN95 SER96 PHE97 <b>Chain C:</b> GLU33 SER34 LYS37 GLU39 LEU40 LEU41 ASN61 TYR72 ALA99 TYR100 LEU101 GLY102 ASP103 ALA104 GLY105 MET106 LEU107 ARG108 TYR109 ARG128 TRP130 <b>Chain D:</b> GLU33 SER34 THR35 LEU36 LYS37 GLU39 LEU40 LEU41 ASN61 TYR72 THR98 ALA99 TYR100 LEU101 GLY102 ASP103 ALA104 GLY105 MET106 LEU107 ARG108 TYR109 ASN110 PRO114 ILE115 ARG128
	Tetracycline	-9.2	386	6,57,137	21,21,21	<b>Chain B:</b> ASP60 VAL90 HIS91 GLU92 ASN93 TYR94 ASN95 SER96 PHE97 VAL98 <b>Chain C:</b> PRO29 GLN30 GLU31 ASP32 GLU33 SER34 THR35 LEU36 ARG108 TYR109 ASN110 SER111 LYS112 <b>Chain D:</b> ARG54 ARG128
						<b>Chain B:</b> ASN93 ASN95 VAL98 SER100 ASN101 THR177 ASP178 GLY179 TYR233

	Metronidazole	-5.6	1561	2,66,136	17,17,17	<b>Chain C:</b> TYR13 LEU27 ASN61 LYS62 THR63 GLY68 TYR69 ASP70 TYR71 TYR72 LEU107 ARG108 TYR109 ASN110 LEU113 PRO114 ILE115 VAL116
<b><i>Staphylococcus aureus</i> - Pathogenic Proteins</b>						
1C76 - Coagulase	Penicillin	-7.1	9314	21,50,55	35,22,35	<b>Chain B:</b> VAL17 GLU18 LEU41 CYS42 CYS58 ASN143 ARG145 GLU146 THR147 TRP148 THR149 SER149 VAL149 ALA149 ARG187 CYS191 GLU192 GLY193 ASP194 SER195 SER214 TRP215 GLY216 GLU217 GLY219 CYS220 ASP221 ARG221 ASP222 GLY223 LYS224 <b>Chain D:</b> ASP5 TYR6 SER7 GLN71 LEU74 GLU75 LYS77 LYS78 TYR81 GLU82 LYS85 THR104 PHE105 ASP106 GLN107 TYR108 THR109 ILE110
	Ampicillin	-7.2	9551	51,13,15	35,28,35	<b>Chain F:</b> MET32 PHE34 PRO37 GLN38 GLU39 LEU40 TRP60 ARG67 LYS70 ARG73 THR74 ARG75 ASN143 ARG145 GLU146 THR147 TRP148 THR149 SER149 VAL149 ALA149 GLU149 VAL150 GLN151 GLU192 GLY193 <b>Chain H:</b> GLU46 THR47 TYR48 LEU194 GLY197 ASP198 LYS201 PRO202 HIS203

	Tetracycline	-8.4	9551	51,13,15	35,28,35	<b>Chain F:</b> GLU39 LEU40 LEU41 HIS57 TYR60 TRP60 LYS60 LEU99 ASN143 ARG145 GLU146 THR147 TRP148 THR149 THR149 SER149 VAL149 ALA149 GLU149 VAL150 ILE174 CYS191 GLU192 GLY193 SER195 SER214 TRP215 GLY216 GLU217 GLY219 CYS220 ARG221 <b>Chain H:</b> LEU74 LYS77 PHE105 ASP106
	Metronidazole	-4.9	9551	51,13,15	35,28,35	<b>Chain F:</b> VAL17 GLN20 ASP21 MET32 PHE34 GLN38 GLU39 LEU40 ARG67 LYS70 ARG73 THR74 ARG75 ASN143 ARG144 ARG145 GLU146 THR147 THR149 THR149 VAL149 ALA149 VAL150 GLN151 PRO152 SER153 VAL154 GLN156 CYS191 GLU192 CYS220 ASP221 <b>Chain H:</b> GLU46 TYR48 LYS56 LYS59 ASP60 MET63 GLN71 LEU194 HIS203
1QY6 - Protease	Penicillin	-5.9	88	14, 23, 40	22, 22, 22	<b>Chain A:</b> LYS50 HIS51 ASP54 TYR88 GLU91 GLY92 ASP93 TYR152 LYS154 GLY155 GLU156 ALA157 MET158 GLN159 TRP185 VAL188 PHE192 ASN193 GLY194 ALA195 VAL196 PHE197

	Ampicillin	-5.9	88	14,23,40	21,21,21	<b>Chain A:</b> LYS50 HIS51 ASP54 GLU91 GLY92 ASP93 LEU94 TYR152 LYS154 GLY155 GLU156 ALA157 MET158 GLN159 TRP185 VAL188 PHE192 ASN193 GLY194 ALA195 VAL196
	Tetracycline	-6.8	88	14,23,40	21,21,21	<b>Chain A:</b> LYS50 HIS51 GLU91 GLY92 ASP93 TYR152 LYS154 GLY155 GLU156 ALA157 MET158 GLN159 TRP185 VAL188 GLU191 PHE192 GLY194 ALA195 VAL196 PHE197
	Metronidazole	-4.9	206	31,28,46	17,17,17	<b>Chain A:</b> SER118 ASN119 ASN120 ALA121 GLU122 THR123 GLN124 GLN127 ASN128 ILE129 ILE150 ASN175 GLU176 LYS177 GLU179 ILE181 ALA216
2AZD - Staphylokinase	Penicillin	-6.3	73	2, -13,4	22,22,22	<b>Chain A:</b> PHE18 GLU19 PRO20 TYR24 MET26 TYR44 GLU46 GLU88 VAL89 THR90 TYR91 TYR92 LYS94 GLU99 HIS119 ILE120 ASN122 PRO123 GLY124 PHE125 ASN126 ILE128
	Ampicillin	-5.9	82	-4, -3,4	21,21,21	<b>Chain A:</b> ASN28 VAL29 THR30 GLU38 PRO42 ASP82 SER84 ALA85 LYS86 ILE87 GLU88 THR101 SER103 ASN126 LEU127 ILE128 THR129 LYS130

	Tetracycline	-6.9	73	2, -13,4	21,21,21	<b>Chain A:</b> GLU19 PRO20 TYR24 MET26 TYR44 GLU46 GLU88 VAL89 THR90 TYR91 TYR92 ASP93 LYS94 GLU99 HIS119 ILE120 LYS121 ASN122 PRO123 GLY124 PHE125 ASN126 ILE128
	Metronidazole	-4.2	114	6, -16,14	17,17,17	<b>Chain A:</b> SER16 PHE18 GLU19 PRO20 THR21 GLY22 PRO23 TYR24 GLU46 PHE47 PRO48 ILE49 LYS50
<b><i>Escherichia coli</i> – Structural proteins</b>						
<b>3VMA - PBP1b</b>	<b>Penicillin</b>	-8.3	2264	44, 107, - 2	22, 22, 35	<b>Chain A:</b> TYR107 ALA130 THR131 GLN132 ARG157 PRO158 PHE159 ASP160 GLU166 ASP198 PRO199 ARG200 LEU201 ILE202 THR203 MET204 ILE205 SER206 GLN212 LEU214 PHE215 VAL216 PRO217 GLY220 SER319 ASN322 ILE324 PRO328 LEU329 LEU332 TYR333 TYR334 PHE335 GLY336 PRO338 VAL339 GLU340 GLU341 PRO403 ARG404 GLY405 VAL407 ILE408 SER409 PRO410 GLN411 PRO412 MET415 GLN416 ARG419 LYS437 PHE442 SER444 ASP448 GLU451 GLN494
<b>6G9F - PBP2</b>	<b>Penicillin</b>	-8.4	885	43, 71, 42	22, 22, 22	<b>Chain A:</b> PRO63 ILE64 ALA65 PRO66 SER67 ARG68 ASN82 GLN87 GLU89 GLU122 ARG125 SER126 HIS127

						THR130 SER131 ILE132 PRO133 THR136 LYS159 GLY160 TYR161 LYS162 ARG163 ARG164 VAL179 LYS181 ALA201 THR202 HIS203 ASP204 ILE205 HIS219 VAL298 ASP299 GLY300
<b>6UMK - FtsZ</b>	<b>Penicillin</b>	-8.0	2725	19, -6, 23	22, 33, 22	<b>Chain A:</b> VAL18 GLY19 GLY20 GLY21 GLY22 GLY23 ASN24 ALA25 GLU27 ASN43 THR44 ASP45 ALA48 LYS51 THR52 ALA53 GLY71 GLY103 MET104 GLY105 GLY106 GLY107 THR108 GLY109 THR132 PRO134 PHE135 PHE137 GLU138 ARG142 ASN165 GLU178 LEU179 PHE182 ALA185 ASN186
<b>3VMA - PBP1b</b>	<b>Ampicillin</b>	-8.1	2264	44, 107, - 2	21, 21, 35	<b>Chain A:</b> TYR107 ALA130 GLN132 ARG157 PRO158 PHE159 ASP198 PRO199 ARG200 LEU201 ILE202 THR203 MET204 ILE205 SER206 SER207 GLN212 LEU214 VAL216 PRO217 SER219 GLY220 PHE221 SER319 ASN322 GLU323 ILE324 PRO328 LEU329 LEU332 TYR333 TYR334 PHE335 GLY336 ARG337 PRO338 VAL339 GLU340 GLU341 PRO403 ARG404 GLY405 VAL407 ILE408 SER409 PRO410 GLN411 PRO412 MET415 GLN416 ARG419 PHE442 SER444 GLN447 ASP448
<b>FtsZ(6UMK)</b>	<b>Ampicillin</b>	-7.9	2725	19, -6, 23	21, 33, 21	<b>Chain A:</b> VAL18 GLY19 GLY20 GLY21 GLY22 GLY23 ASN24 ALA25 GLU27 ASN43 THR44 ASP45 ALA48



						LYS51 THR52 GLY63 ILE64 THR65 ALA70 GLY71 ALA72 VAL76 GLY103 MET104 GLY105 GLY106 GLY107 THR108 GLY109 THR110 THR132 LYS133 PRO134 PHE135 GLU138 ARG142 ASN165 GLU178 LEU179 PHE182 ALA185 ASN186
<b>UVRB(1QOJ)</b>	<b>Metronidazole</b>	-5.4	146	13, 43, 5	17, 17, 17	<b>Chain A:</b> LEU639 GLU640 GLY641 LEU642 GLN645 HIS646 ALA647 GLN648 GLU654 ALA655 ALA656 ILE658 ARG659 ASP660 LEU662 <b>Chain B:</b> ALA647 LEU650 PHE652
<b>EXCINUCLEASE ABC SUBUNIT(1E52)</b>	<b>Metronidazole</b>	-40.1	2113	13, -9, -1	26, 27, 17	<b>Chain B:</b> HIS27 GLU28 LEU29 GLY31 LEU32 MET34 GLN35 HIS27 GLU28 LEU29 GLU30 GLY31 LEU32 MET34 GLN35 HIS27 GLU28 LEU29 GLY31 LEU32 MET34 GLN35 HIS27 GLU28 LEU29 GLY31 LEU32 MET34 GLN35 HIS27 GLU28 LEU29 GLY31 LEU32 MET34 HIS27 GLU28 LEU29 GLY31 LEU32 MET34 GLN35 GLN38 HIS27 GLU28 LEU29 GLY31 LEU32 MET34 HIS27 GLU28 LEU29 GLY31 LEU32 GLN35 HIS27 GLU28 GLY31 LEU32 GLN35 HIS27 GLU28 LEU29 GLY31 LEU32 HIS27 GLU28 LEU29 GLY31 LEU32 MET34 GLN35 HIS27 GLU28 LEU29 GLU30 GLY31 LEU32 MET34 GLN35 GLN38 HIS27 GLU28 LEU29 GLY31 LEU32 MET34 GLN35 HIS27 GLU28 LEU29 GLY31 LEU32 HIS27 GLU28 LEU29 GLY31 LEU32 GLN35

						HIS27 GLU28 LEU29 GLU30 GLY31 LEU32 MET34 GLN35 HIS27 GLU28 LEU29 GLY31 LEU32 GLN35 HIS27 GLU28 GLU30 GLY31 LEU32 MET34 HIS27 GLU28 LEU29 GLU30 GLY31 LEU32 HIS27 GLU28 LEU29 GLY31 LEU32 MET34 GLN35
<b>Elongation factor EF-Tu (1EFC)</b>	<b>Tetracycline</b>	-7.5	555	50, 29, -9	21, 21, 21	<b>Chain A:</b> ASN13 ALA57 ARG58 THR93 GLY94 ALA95 ALA96 GLN97 MET98 ASP99 VAL125 GLY126 VAL127 PRO128 TYR129 GLU201 PRO202 GLU203 ARG204 ALA205 LYS208 LEU211 PRO213 GLU215 GLU232 ARG233 TYR331 PHE332 ARG333 THR334 ASP369 ASP370 GLY371 LEU372 ARG373 PHE374
<b>ELONGATION FACTOR TU (1DG1)</b>	<b>Tetracycline</b>	-7.1	278	34, 71, - 48	21, 21, 21	<b>Chain H:</b> GLU215 ASP216 PHE218 ILE220 ARG223 VAL226 THR228 GLY229 ARG230 GLU259 MET260 PHE261 ARG262 LYS263 ASN273 VAL274 GLY275 VAL276
<b>Leucine--tRNA ligase (protein) (5ONH)</b>	<b>Tetracycline</b>	-8.5	12469	9, 26, 66	35, 34, 35	<b>Chain A:</b> ALA607 ALA608 <b>Chain D:</b> MET40 LEU41 PRO42 TYR43 PRO44 SER45 GLY46 ARG47 HIS49 HIS52 TYR56 ASP80 PHE82 GLY83 LEU84 PRO85 GLY88 ALA89 LYS92 ASN93 TRP100 ASN104 ALA167 GLU169 TRP177 ARG424 ARG426 ASP491 THR492 PHE493 SER496 GLU532 HIS533 MET568 ARG583 ASN584 TRP585 VAL586

						LYS619 MET620 SER621 LYS622 SER623 LYS624 ASN625
<b><i>Staphylococcus aureus</i> – Structural proteins</b>						
<b>Transpeptidase (1XA1)</b>	<b>Penicillin</b>	-6.9	1245	6, 60, 21	22,22,31	<b>Chain B:</b> GLN18 ILE19 LEU20 ASP21 LYS22 LYS42 TYR46 GLU48 LYS49 GLU248 <b>Chain C:</b> ILE74 ILE75 ASN76 ASN79 SER80 ARG81 MET82 SER83 TRP84 HIS86 GLU97 TRP110 ARG114 ASP117 GLN118
<b>Transpeptidase (1XA1)</b>	<b>Ampicillin</b>	-6.8	1245	6, 60, 21	21,21,31	<b>Chain B:</b> LEU13 HIS14 ASN15 ASP16 TYR17 GLN18 ILE19 LEU20 ASP21 LYS22 LYS42 TYR46 ASN47 GLU48 LYS49 GLU248 <b>Chain C:</b> ASP71 ARG72 HIS73 ILE74 ILE75 ASN76 ASN79 SER80 ARG81 MET82 SER83 TRP84 HIS86 LYS87 TYR89 GLU97 GLN98 TRP110 ARG114 ASP117 GLN118 PRO120 ASN122 TYR123
<b>Methionyl tRNA Synthetase (1FFY)</b>	<b>Tetracyclines</b>	-8.0	7409	31, 69, 66	29,35,35	<b>Chain A:</b> GLY55 PRO56 PRO57 TYR58 ALA59 ASN60 GLY61 HIS64 GLY66 HIS67 ASN70 LYS71 ASP95 LEU99 PRO100 GLN135 LEU193 ALA194 GLU195 ALA196 MET444 ARG448 GLY449 TRP451 VAL452 ARG455 ARG457 ASP526 VAL527 TRP528 GLU554 GLY555 ASP557 GLN558 ARG560 GLY561 TRP562 ASN564 HIS585 PHE587
<b>RecA (6TTY)</b>	<b>Metronidazole</b>	-5.8	2457	-50, 17, 37	17, 33, 17	<b>Chain A:</b> ASN2 LEU3 PRO5 TYR21 MET31 LEU32 GLY33

						SER34 ASN39 VAL40 SER43 ILE44 GLN47 <b>Chain B:</b> ASN2 LEU3 PRO5 <b>Chain F:</b> ASP38 ASN39 VAL40 ASN42 SER43 <b>Chain G:</b> LEU3 ILE4 TYR21 ILE30 MET31 LEU32 GLY33 SER34 ASN39 VAL40 ASN42 SER43 ILE44 GLN47
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