**PIC Table 2**:

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  |  | Types of inter-molecular interactions | | | | |
| S. No | Complex | Hydrogen bonds | Hydrophobic interactions | Aromatic-aromatic interactions | Cation-π interactions | Total number |
| 1 | G446V- Adenoregulin | 4 | 18 | 0 | 2 | 24 |
| 2 | G446V- Amolopin-1a | 11 | 13 | 2 | 1 | 27 |
| 3 | G446V- Opiod | 24 | 7 | 3 | 2 | 36 |
| 4 | G446V- Amurin-1 | 38 | 21 | 2 | 1 | 62 |
| 5 | G446V- Antimicrobial peptide | 3 | 13 | 1 | 1 | 18 |
| 6 | G446V- Antioxidant peptide 1 |  |  |  |  |  |
| 7 | G446- ARP-AC1 | 6 | 9 | 1 | 1 | 17 |
| 8 | G446V- Ascaphin-1 | 25 | 17 | 2 | 1 | 45 |
| 9 | G446V- Aurein-1 | 7 | 12 | 1 | 0 | 20 |
| 10 | G446V- Bombesin | 31 | 6 | 2 | 1 | 40 |
| 11 | G446V- Bombinin | 19 | 15 | 0 | 0 | 34 |
| 12 | G446V- Brevinin-1BYa | 16 | 18 | 1 | 2 | 37 |
| 13 | G446V- Chunganensisin-A1 | 14 | 14 | 4 | 3 | 35 |
| 14 | G446V- Dermadistinctin-K | 7 | 10 | 2 | 2 | 21 |
| 15 | G446V- Esculentin-1-OG10 | 11 | 12 | 2 | 4 | 29 |
| 16 | G446V- Fallaxidin-3.1.1 | 7 | 11 | 0 | 1 | 19 |
| 17 | G446V- Gaegurin-6-RN | 5 | 18 | 1 | 1 | 25 |
| 18 | G446V- Granulosusin-A1 | 13 | 14 | 3 | 1 | 31 |
| 19 | G446V- Guentherin | 44 | 2 | 0 | 2 | 48 |
| 20 | L452R- Adenoregulin | 5 | 19 | 1 | 3 | 28 |
| 21 | L452R- Amolopin-1a | 22 | 12 | 3 | 1 | 26 |
| 22 | L452R- Opiod | 18 | 6 | 4 | 2 | 30 |
| 23 | L452R- Amurin-1 | 37 | 20 | 2 | 2 | 61 |
| 24 | L452R- Antimicrobial peptide | 13 | 15 | 1 | 0 | 29 |
| 25 | L452R- Antioxidant peptide 1 |  |  |  |  |  |
| 26 | L452R- ARP-AC1 | 10 | 12 | 0 | 0 | 22 |
| 27 | L452R- Ascaphin-1 | 21 | 17 | 1 | 1 | 40 |
| 28 | L452R- Aurein-1 | 10 | 8 | 2 | 0 | 20 |
| 29 | L452R- Bombesin | 33 | 10 | 1 | 0 | 44 |
| 30 | L452R- Bombinin | 19 | 15 | 0 | 0 | 34 |
| 31 | L452R- Brevinin-1BYa | 28 | 16 | 3 | 1 | 48 |
| 32 | L452R- Chunganensisin-A1 | 15 | 12 | 4 | 0 | 31 |
| 33 | L452R- Dermadistinctin-K | 9 | 3 | 0 | 4 | 16 |
| 34 | L452R- Esculentin-1-OG10 | 15 | 11 | 2 | 3 | 31 |
| 35 | L452R- Fallaxidin-3.1.1 | 8 | 14 | 0 | 0 | 22 |
| 36 | L452R- Gaegurin-6-RN | 6 | 16 | 1 | 3 | 26 |
| 37 | L452R- Granulosusin-A1 | 6 | 12 | 4 | 1 | 23 |
| 38 | L452R- Guentherin | 4 | 12 | 0 | 4 | 20 |
| 39 | Y453F- Adenoregulin | 11 | 9 | 1 | 1 | 22 |
| 40 | Y453F- Amolopin-1a | 9 | 12 | 3 | 1 | 25 |
| 41 | Y453F- Opiod | 30 | 7 | 1 | 1 | 39 |
| 42 | Y453F- Amurin-1 | 34 | 20 | 2 | 1 | 57 |
| 43 | Y453F- Antimicrobial peptide | 5 | 15 | 1 | 1 | 22 |
| 44 | Y453F- Antioxidant peptide 1 |  |  |  |  |  |
| 45 | Y453F- ARP-AC1 | 7 | 9 | 3 | 2 | 21 |
| 46 | Y453F- Ascaphin-1 | 2 | 17 | 5 | 1 | 25 |
| 47 | Y453F- Aurein-1 | 6 | 12 | 0 | 0 | 18 |
| 48 | Y453F- Bombesin | 28 | 9 | 3 | 1 | 41 |
| 49 | Y453F- Bombinin | 14 | 13 | 0 | 0 | 27 |
| 50 | Y453F- Brevinin-1BYa | 29 | 19 | 0 | 1 | 48 |
| 51 | Y453F- Chunganensisin-A1 | 10 | 13 | 2 | 0 | 25 |
| 52 | Y453F- Dermadistinctin-K | 5 | 15 | 1 | 2 | 23 |
| 53 | Y453F- Esculentin-1-OG10 | 11 | 9 | 1 | 4 | 25 |
| 54 | Y453F- Fallaxidin-3.1.1 | 15 | 4 | 0 | 0 | 19 |
| 55 | Y453F- Gaegurin-6-RN | 7 | 17 | 1 | 2 | 27 |
| 56 | Y453F- Granulosusin-A1 | 8 | 12 | 5 | 1 | 26 |
| 57 | Y453F- Guentherin | 9 | 8 | 0 | 1 | 18 |
| 58 | S477G- Adenoregulin | 3 | 7 | 2 | 0 | 12 |
| 59 | S477G- Amolopin-1a | 18 | 12 | 2 | 1 | 33 |
| 60 | S477G- Opiod | 12 | 6 | 4 | 2 | 24 |
| 61 | S477G- Amurin-1 | 32 | 16 | 2 | 0 | 50 |
| 62 | S477G- Antimicrobial peptide | 5 | 13 | 0 | 1 | 19 |
| 63 | S477G- Antioxidant peptide 1 |  |  |  |  |  |
| 64 | S477G- ARP-AC1 | 6 | 8 | 1 | 0 | 15 |
| 65 | S477G- Ascaphin-1 | 7 | 15 | 1 | 0 | 23 |
| 66 | S477G- Aurein-1 | 8 | 12 | 3 | 0 | 23 |
| 67 | S477G- Bombesin | 40 | 7 | 2 | 1 | 70 |
| 68 | S477G- Bombinin | 8 | 8 | 1 | 0 | 17 |
| 69 | S477G- Brevinin-1BYa | 15 | 16 | 0 | 0 | 31 |
| 70 | S477G- Chunganensisin-A1 | 18 | 5 | 2 | 4 | 29 |
| 71 | S477G- Dermadistinctin-K | 9 | 9 | 3 | 2 | 23 |
| 72 | S477G- Esculentin-1-OG10 | 15 | 10 | 2 | 3 | 30 |
| 73 | S477G- Fallaxidin-3.1.1 | 23 | 17 | 0 | 0 | 40 |
| 74 | S477G- Gaegurin-6-RN | 8 | 19 | 0 | 2 | 29 |
| 75 | S477G- Granulosusin-A1 | 9 | 11 | 5 | 2 | 27 |
| 76 | S477G- Guentherin | 26 | 10 | 0 | 4 | 40 |
| 77 | S477N-Adenoregulin | 5 | 7 | 1 | 1 | 14 |
| 78 | S477N-Amolopin-1a | 13 | 13 | 4 | 2 | 32 |
| 79 | S477N-Opiod | 59 | 5 | 1 | 2 | 67 |
| 80 | S477N-Amurin-1 | 36 | 19 | 2 | 1 | 58 |
| 81 | S477N-Antimicrobial peptide | 4 | 15 | 1 | 1 | 21 |
| 82 | S477N-Antioxidant peptide 1 |  |  |  |  |  |
| 83 | S477N-ARP-AC1 | 6 | 10 | 1 | 0 | 17 |
| 84 | S477N-Ascaphin-1 | 13 | 12 | 2 | 4 | 31 |
| 85 | S477N-Aurein-1 | 14 | 11 | 2 | 0 | 27 |
| 86 | S477N-Bombesin | 26 | 4 | 1 | 0 | 31 |
| 87 | S477N-Bombinin | 8 | 13 | 0 | 1 | 21 |
| 88 | S477N-Brevinin-1BYa | 28 | 14 | 3 | 1 | 46 |
| 89 | S477N-Chunganensisin-A1 | 29 | 10 | 0 | 0 | 39 |
| 90 | S477N-Dermadistinctin-K | 10 | 8 | 0 | 1 | 19 |
| 91 | S477N-Esculentin-1-OG10 | 13 | 10 | 3 | 4 | 30 |
| 92 | S477N-Fallaxidin-3.1.1 | 19 | 12 | 0 | 1 | 32 |
| 93 | S477N-Gaegurin-6-RN | 8 | 18 | 1 | 2 | 29 |
| 94 | S477N-Granulosusin-A1 | 19 | 19 | 3 | 1 | 36 |
| 95 | S477N-Guentherin | 8 | 8 | 0 | 3 | 19 |
| 96 | S477R- Adenoregulin | 5 | 8 | 1 | 1 | 15 |
| 97 | S477R- Amolopin-1a | 10 | 12 | 2 | 1 | 25 |
| 98 | S477R- Opiod | 13 | 7 | 3 | 0 | 23 |
| 99 | S477R- Amurin-1 | 13 | 19 | 1 | 2 | 35 |
| 100 | S477R- Antimicrobial peptide | 9 | 17 | 2 | 1 | 29 |
| 101 | S477R- Antioxidant peptide 1 |  |  |  |  |  |
| 102 | S477R- ARP-AC1 | 12 | 10 | 2 | 3 | 27 |
| 103 | S477R- Ascaphin-1 | 8 | 17 | 3 | 0 | 28 |
| 104 | S477R- Aurein-1 | 14 | 12 | 3 | 0 | 29 |
| 105 | S477R- Bombesin | 40 | 5 | 2 | 0 | 47 |
| 106 | S477R- Bombinin | 7 | 13 | 3 | 0 | 23 |
| 107 | S477R- Brevinin-1BYa | 12 | 17 | 1 | 0 | 30 |
| 108 | S477R- Chunganensisin-A1 | 12 | 12 | 3 | 1 | 28 |
| 109 | S477R- Dermadistinctin-K | 6 | 8 | 3 | 2 | 19 |
| 110 | S477R- Esculentin-1-OG10 | 22 | 11 | 1 | 1 | 35 |
| 111 | S477R- Fallaxidin-3.1.1 | 6 | 13 | 0 | 1 | 20 |
| 112 | S477R- Gaegurin-6-RN | 3 | 16 | 1 | 2 | 22 |
| 113 | S477R- Granulosusin-A1 | 21 | 20 | 2 | 1 | 44 |
| 114 | S477R- Guentherin | 7 | 8 | 0 | 3 | 18 |
| 115 | E484K- Adenoregulin | 11 | 3 | 1 | 4 | 19 |
| 116 | E484K- Amolopin-1a | 13 | 14 | 3 | 1 | 31 |
| 117 | E484K- Opiod | 20 | 6 | 3 | 2 | 31 |
| 118 | E484K- Amurin-1 | 24 | 18 | 1 | 3 | 46 |
| 119 | E484K- Antimicrobial peptide | 17 | 16 | 1 | 1 | 35 |
| 120 | E484K- Antioxidant peptide 1 |  |  |  |  |  |
| 121 | E484K- ARP-AC1 | 8 | 9 | 3 | 2 | 22 |
| 122 | E484K- Ascaphin-1 | 29 | 17 | 6 | 2 | 54 |
| 123 | E484K- Aurein-1 | 9 | 14 | 0 | 0 | 23 |
| 124 | E484K- Bombesin | 32 | 9 | 1 | 0 | 42 |
| 125 | E484K- Bombinin | 8 | 14 | 1 | 1 | 24 |
| 126 | E484K- Brevinin-1BYa | 11 | 19 | 3 | 2 | 35 |
| 127 | E484K- Chunganensisin-A1 | 17 | 13 | 5 | 3 | 38 |
| 128 | E484K- Dermadistinctin-K | 9 | 4 | 0 | 3 | 16 |
| 129 | E484K- Esculentin-1-OG10 | 33 | 10 | 0 | 1 | 44 |
| 130 | E484K- Fallaxidin-3.1.1 | 14 | 14 | 0 | 1 | 29 |
| 131 | E484K- Gaegurin-6-RN | 6 | 14 | 3 | 1 | 24 |
| 132 | E484K- Granulosusin-A1 | 8 | 13 | 4 | 1 | 26 |
| 133 | E484K- Guentherin | 9 | 10 | 0 | 4 | 23 |
| 134 | E484A- Adenoregulin | 15 | 11 | 1 | 4 | 31 |
| 135 | E484A- Amolopin-1a | 15 | 13 | 3 | 1 | 30 |
| 136 | E484A- Opiod | 17 | 10 | 2 | 1 | 30 |
| 137 | E484A- Amurin-1 | 21 | 16 | 1 | 3 | 41 |
| 138 | E484A- Antimicrobial peptide | 3 | 15 | 4 | 1 | 23 |
| 139 | E484A- Antioxidant peptide 1 |  |  |  |  |  |
| 140 | E484A- ARP-AC1 | 5 | 19 | 0 | 0 | 24 |
| 141 | E484A- Ascaphin-1 | 4 | 18 | 4 | 1 | 27 |
| 142 | E484A- Aurein-1 | 9 | 14 | 1 | 0 | 24 |
| 143 | E484A- Bombesin | 37 | 8 | 1 | 0 | 46 |
| 144 | E484A- Bombinin | 23 | 15 | 0 | 0 | 38 |
| 145 | E484A- Brevinin-1BYa | 16 | 21 | 2 | 1 | 40 |
| 146 | E484A- Chunganensisin-A1 | 14 | 12 | 3 | 2 | 31 |
| 147 | E484A- Dermadistinctin-K | 21 | 7 | 0 | 3 | 31 |
| 148 | E484A- Esculentin-1-OG10 | 21 | 7 | 0 | 1 | 29 |
| 149 | E484A- Fallaxidin-3.1.1 | 2 | 19 | 0 | 1 | 22 |
| 150 | E484A- Gaegurin-6-RN | 7 | 17 | 1 | 2 | 27 |
| 151 | E484A- Granulosusin-A1 | 4 | 12 | 4 | 1 | 21 |
| 152 | E484A- Guentherin | 9 | 8 | 0 | 0 | 17 |
| 153 | E484D- Adenoregulin | 6 | 12 | 1 | 0 | 19 |
| 154 | E484D- Amolopin-1a | 19 | 14 | 2 | 2 | 37 |
| 155 | E484D- Opiod | 13 | 8 | 2 | 1 | 24 |
| 156 | E484D- Amurin-1 | 29 | 20 | 2 | 1 | 52 |
| 157 | E484D- Antimicrobial peptide | 9 | 17 | 2 | 0 | 28 |
| 158 | E484D- Antioxidant peptide 1 |  |  |  |  |  |
| 159 | E484D- ARP-AC1 | 12 | 17 | 0 | 3 | 32 |
| 160 | E484D- Ascaphin-1 | 23 | 25 | 2 | 1 | 51 |
| 161 | E484D- Aurein-1 | 3 | 10 | 3 | 2 | 18 |
| 162 | E484D- Bombesin | 19 | 9 | 2 | 0 | 30 |
| 163 | E484D- Bombinin | 10 | 10 | 0 | 0 | 20 |
| 164 | E484D- Brevinin-1BYa | 16 | 17 | 3 | 3 | 39 |
| 165 | E484D- Chunganensisin-A1 | 16 | 13 | 3 | 1 | 33 |
| 166 | E484D- Dermadistinctin-K | 6 | 8 | 1 | 2 | 17 |
| 167 | E484D- Esculentin-1-OG10 | 18 | 12 | 0 | 0 | 30 |
| 168 | E484D- Fallaxidin-3.1.1 | 5 | 11 | 0 | 1 | 17 |
| 169 | E484D- Gaegurin-6-RN | 10 | 18 | 2 | 1 | 31 |
| 170 | E484D- Granulosusin-A1 | 6 | 12 | 5 | 1 | 24 |
| 171 | E484D- Guentherin | 6 | 12 | 0 | 4 | 22 |
| 172 | E484G- Adenoregulin | 5 | 16 | 0 | 0 | 21 |
| 173 | E484G- Amolopin-1a | 15 | 17 | 3 | 1 | 36 |
| 174 | E484G- Opiod | 17 | 10 | 0 | 1 | 28 |
| 175 | E484G- Amurin-1 | 22 | 19 | 2 | 2 | 45 |
| 176 | E484G- Antimicrobial peptide | 4 | 14 | 4 | 1 | 23 |
| 177 | E484G- Antioxidant peptide 1 |  |  |  |  |  |
| 178 | E484G- ARP-AC1 | 6 | 16 | 0 | 0 | 22 |
| 179 | E484G- Ascaphin-1 | 7 | 14 | 2 | 1 | 24 |
| 180 | E484G- Aurein-1 | 9 | 11 | 0 | 0 | 20 |
| 181 | E484G- Bombesin | 21 | 6 | 2 | 0 | 29 |
| 182 | E484G- Bombinin | 22 | 7 | 0 | 0 | 29 |
| 183 | E484G- Brevinin-1BYa | 11 | 17 | 1 | 1 | 30 |
| 184 | E484G- Chunganensisin-A1 | 2 | 6 | 1 | 0 | 9 |
| 185 | E484G- Dermadistinctin-K | 5 | 11 | 1 | 2 | 19 |
| 186 | E484G- Esculentin-1-OG10 | 6 | 13 | 1 | 2 | 22 |
| 187 | E484G- Fallaxidin-3.1.1 | 5 | 9 | 0 | 1 | 15 |
| 188 | E484G- Gaegurin-6-RN | 3 | 21 | 2 | 0 | 26 |
| 189 | E484G- Granulosusin-A1 | 5 | 13 | 3 | 1 | 22 |
| 190 | E484G- Guentherin | 6 | 10 | 0 | 2 | 18 |
| 191 | F490S- Adenoregulin | 3 | 7 | 1 | 1 | 12 |
| 192 | F490S- Amolopin-1a | 37 | 14 | 2 | 1 | 54 |
| 193 | F490S- Opiod | 8 | 12 | 0 | 0 | 20 |
| 194 | F490S- Amurin-1 | 30 | 18 | 1 | 1 | 50 |
| 195 | F490S- Antimicrobial peptide | 9 | 8 | 1 | 3 | 21 |
| 196 | F490S- Antioxidant peptide 1 |  |  |  |  |  |
| 197 | F490S- ARP-AC1 | 4 | 11 | 2 | 0 | 17 |
| 198 | F490S- Ascaphin-1 | 29 | 21 | 3 | 0 | 53 |
| 199 | F490S- Aurein-1 | 9 | 12 | 0 | 0 | 21 |
| 200 | F490S- Bombesin | 29 | 7 | 1 | 0 | 36 |
| 201 | F490S- Bombinin | 17 | 15 | 0 | 0 | 32 |
| 202 | F490S- Brevinin-1BYa | 23 | 19 | 0 | 2 | 44 |
| 203 | F490S- Chunganensisin-A1 | 9 | 13 | 4 | 2 | 28 |
| 204 | F490S- Dermadistinctin-K | 9 | 4 | 0 | 5 | 18 |
| 205 | F490S- Esculentin-1-OG10 | 16 | 12 | 2 | 3 | 33 |
| 206 | F490S- Fallaxidin-3.1.1 | 21 | 5 | 0 | 0 | 26 |
| 207 | F490S- Gaegurin-6-RN | 6 | 15 | 0 | 2 | 23 |
| 208 | F490S- Granulosusin-A1 | 17 | 19 | 2 | 1 | 39 |
| 209 | F490S- Guentherin | 37 | 6 | 0 | 4 | 47 |
| 210 | N501Y- Adenoregulin | 9 | 20 | 3 | 3 | 35 |
| 211 | N501Y- Amolopin-1a | 13 | 16 | 3 | 1 | 33 |
| 212 | N501Y- Opiod | 18 | 7 | 5 | 2 | 32 |
| 213 | N501Y- Amurin-1 | 25 | 19 | 1 | 2 | 47 |
| 214 | N501Y- Antimicrobial peptide | 2 | 15 | 3 | 1 | 21 |
| 215 | N501Y- Antioxidant peptide 1 |  |  |  |  |  |
| 216 | N501Y- ARP-AC1 | 8 | 16 | 1 | 2 | 27 |
| 217 | N501Y- Ascaphin-1 | 26 | 16 | 4 | 1 | 47 |
| 218 | N501Y- Aurein-1 | 9 | 11 | 3 | 1 | 24 |
| 219 | N501Y- Bombesin | 37 | 10 | 3 | 1 | 51 |
| 220 | N501Y- Bombinin | 9 | 11 | 1 | 1 | 22 |
| 221 | N501Y- Brevinin-1BYa | 14 | 18 | 0 | 0 | 32 |
| 222 | N501Y- Chunganensisin-A1 | 11 | 8 | 2 | 4 | 25 |
| 223 | N501Y- Dermadistinctin-K | 14 | 7 | 1 | 2 | 24 |
| 224 | N501Y- Esculentin-1-OG10 | 9 | 13 | 1 | 2 | 25 |
| 225 | N501Y- Fallaxidin-3.1.1 | 6 | 11 | 0 | 0 | 17 |
| 226 | N501Y- Gaegurin-6-RN | 1 | 15 | 4 | 1 | 21 |
| 227 | N501Y- Granulosusin-A1 | 12 | 12 | 0 | 0 | 24 |
| 228 | N501Y- Guentherin | 42 | 5 | 0 | 1 | 48 |