

Supporting Information

# Putative Inhibitors of SARS-CoV-2 Main Protease from A Library of Marine Natural Products: A Virtual Screening and Molecular Modeling Study

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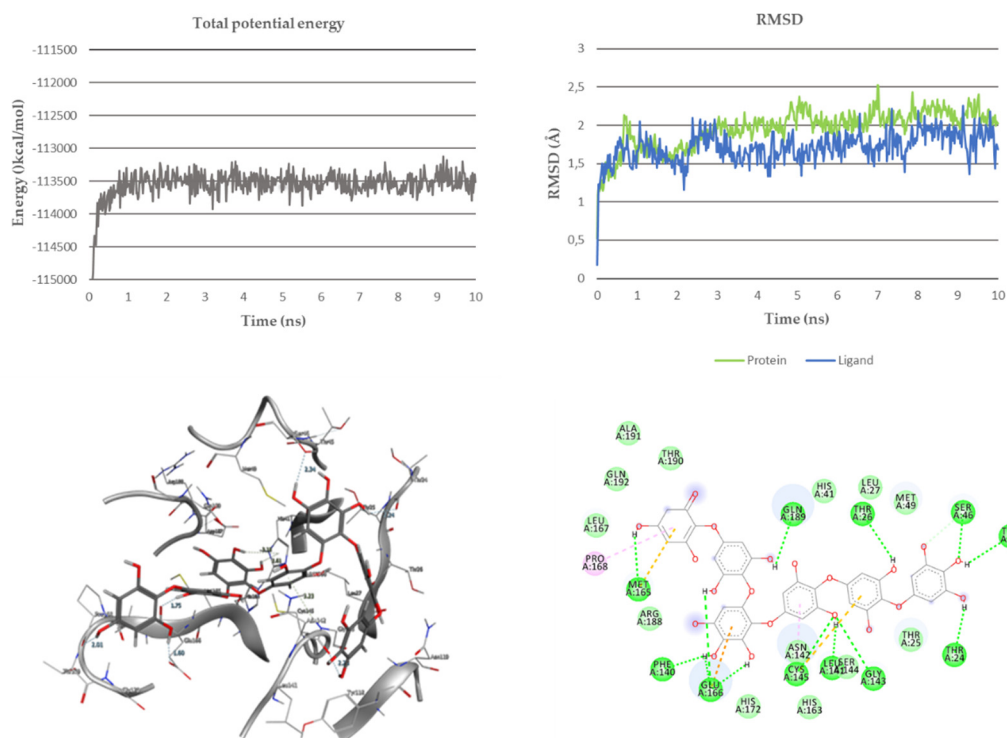
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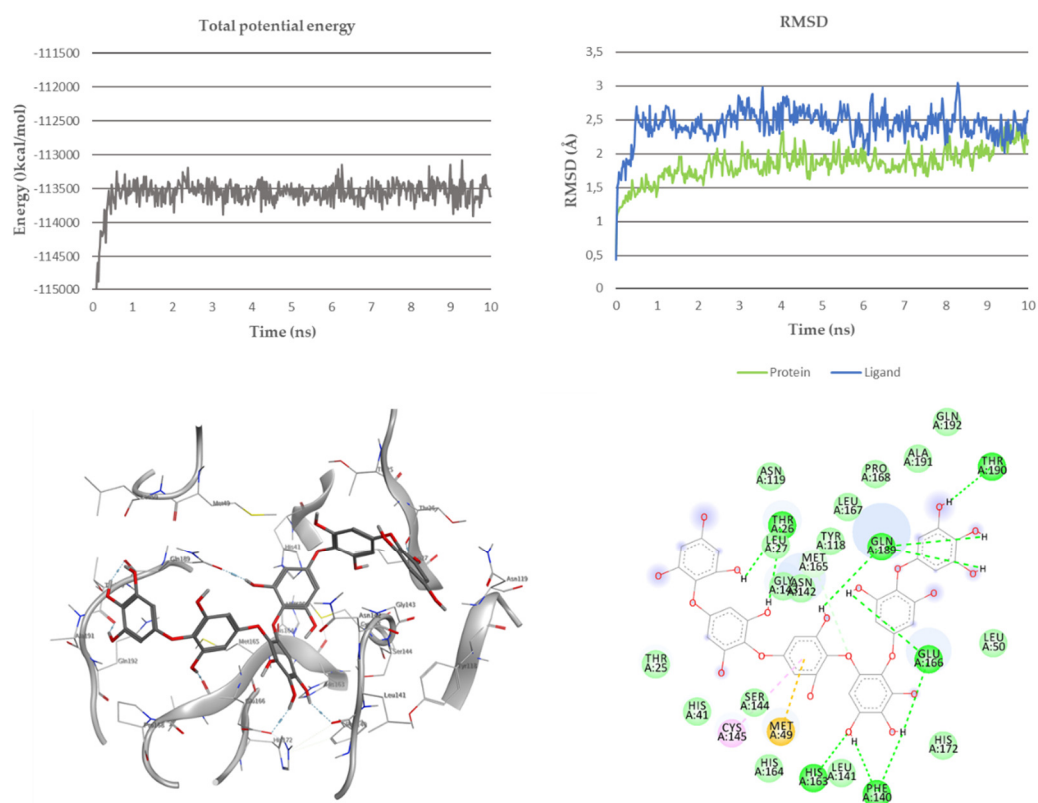
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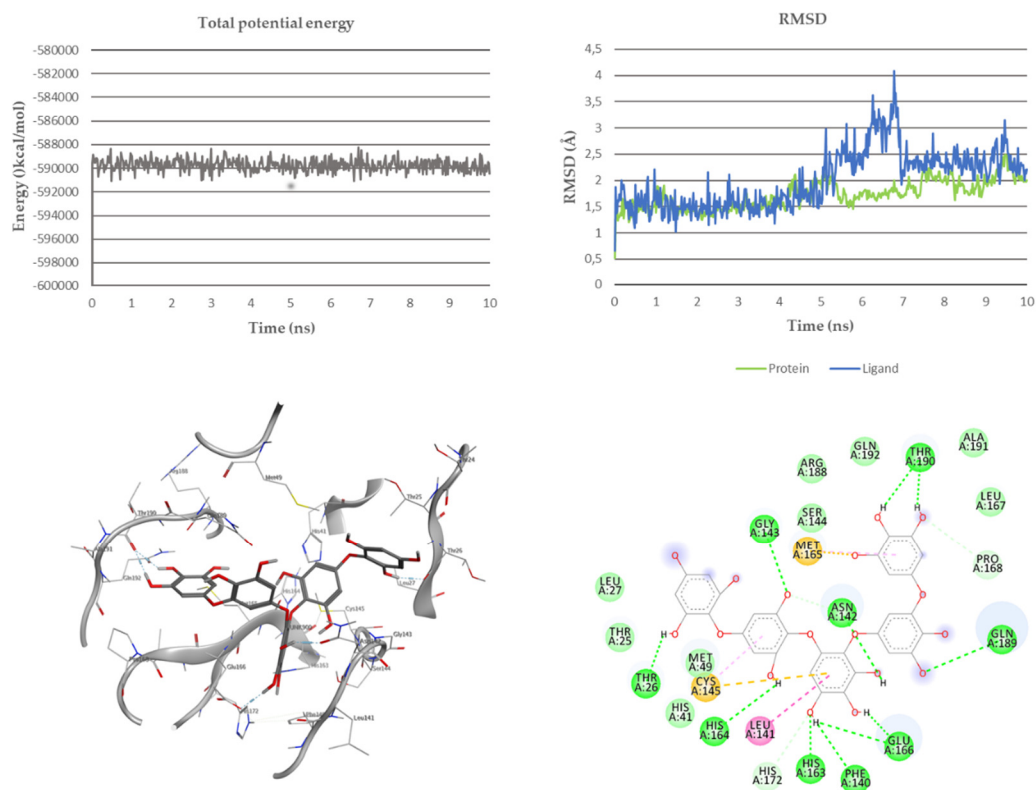
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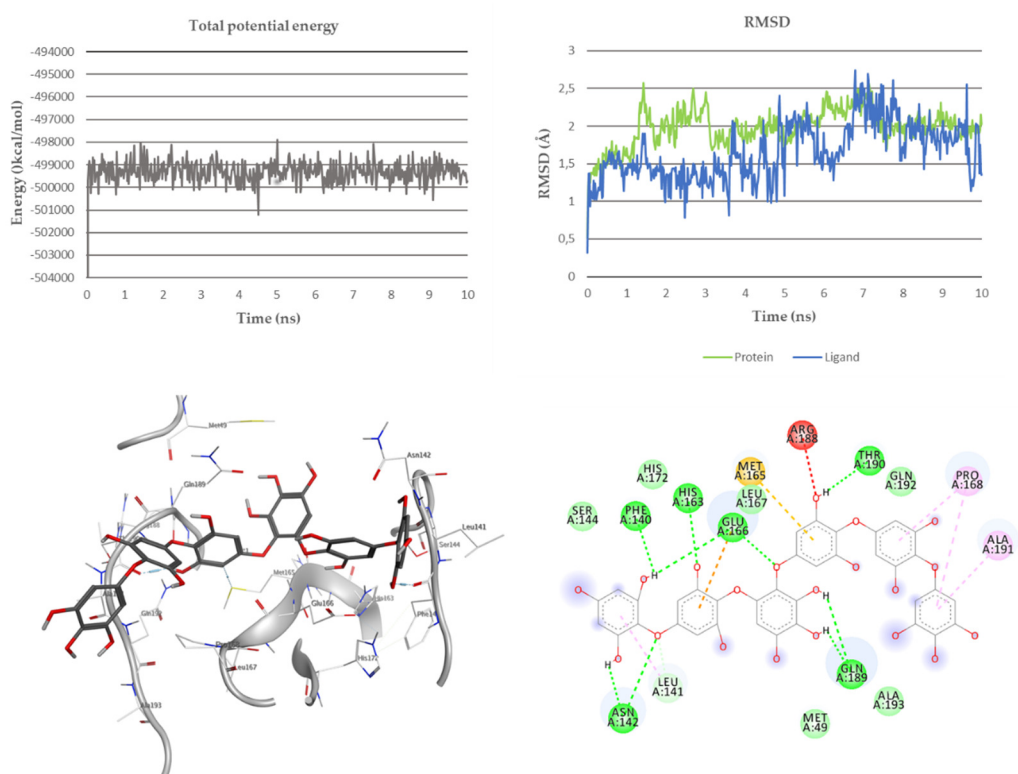
**Figure S1.** MNP ID 76265-30-0. Total energy (up-left) and RMSDs (up-right) of M<sup>Pro</sup> enzyme and its complexes with ligand. Docking binding pose (down-left) and Interaction (down-right) inside the binding pocket of M<sup>Pro</sup> enzyme.



**Figure S2.** MNP ID 138551-15-2. Total energy (up-left) and RMSDs (up-right) of M<sup>Pro</sup> enzyme and its complexes with ligand. Docking binding pose (down-left) and Interaction (down-right) inside the binding pocket of M<sup>Pro</sup> enzyme.

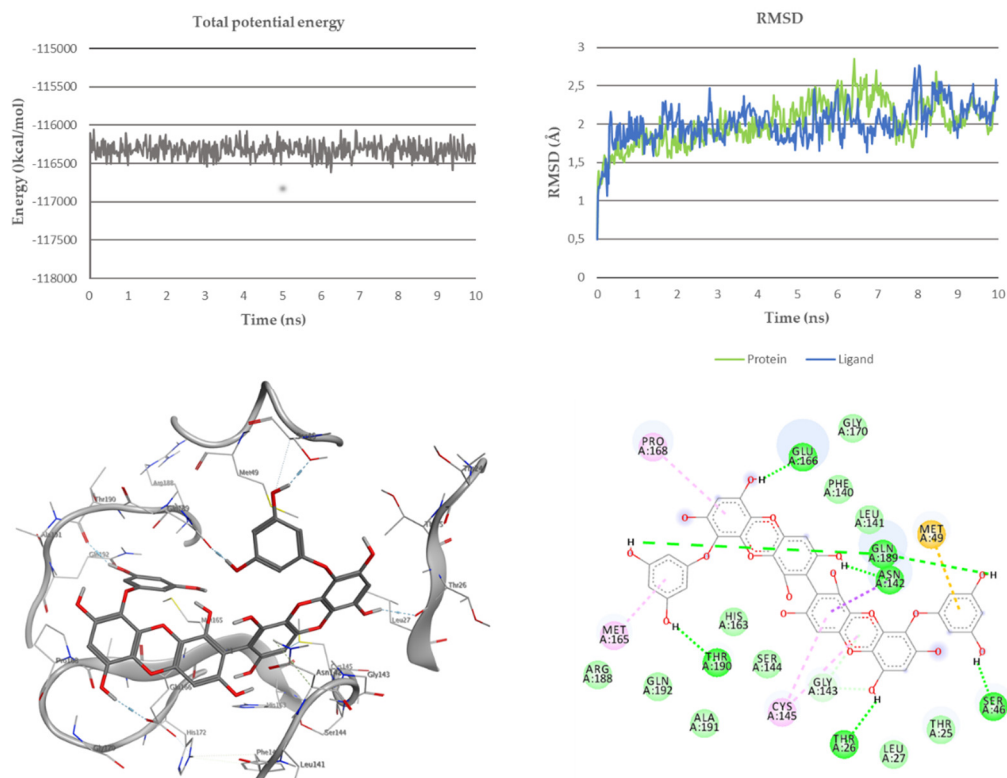


**Figure S3.** MNP ID 202211-82-3. Total energy (up-left) and RMSDs (up-right) of M<sup>PRO</sup> enzyme and its complexes with ligand. Docking binding pose (down-left) and Interaction (down-right) inside the binding pocket of M<sup>PRO</sup> enzyme.

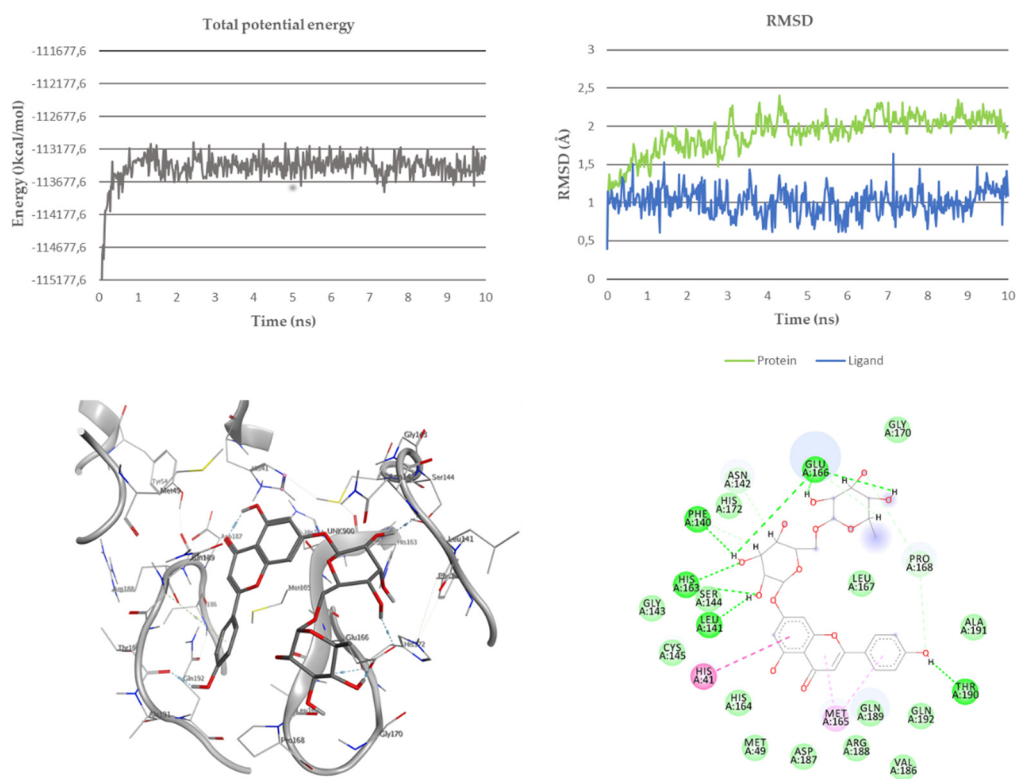


**Figure S4.** MNP ID 138529-06-3. Total energy (up-left) and RMSDs (up-right) of M<sup>PRO</sup> enzyme and its complexes with ligand. Docking binding pose (down-left) and Interaction (down-right) inside the binding pocket of M<sup>PRO</sup> enzyme.

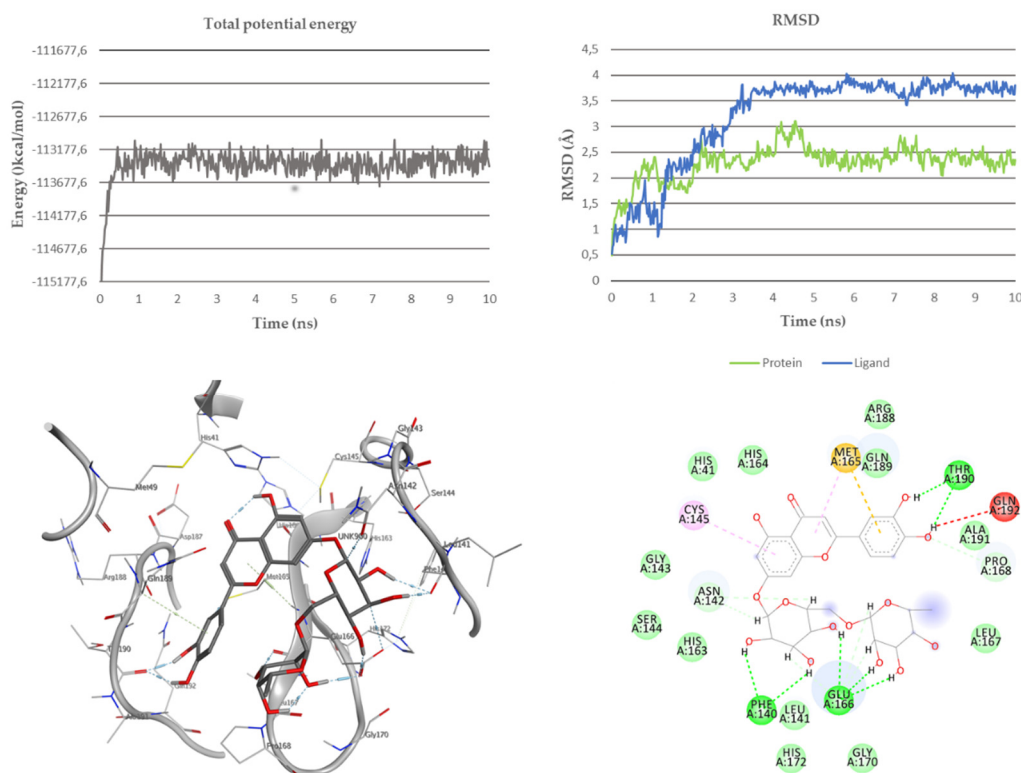




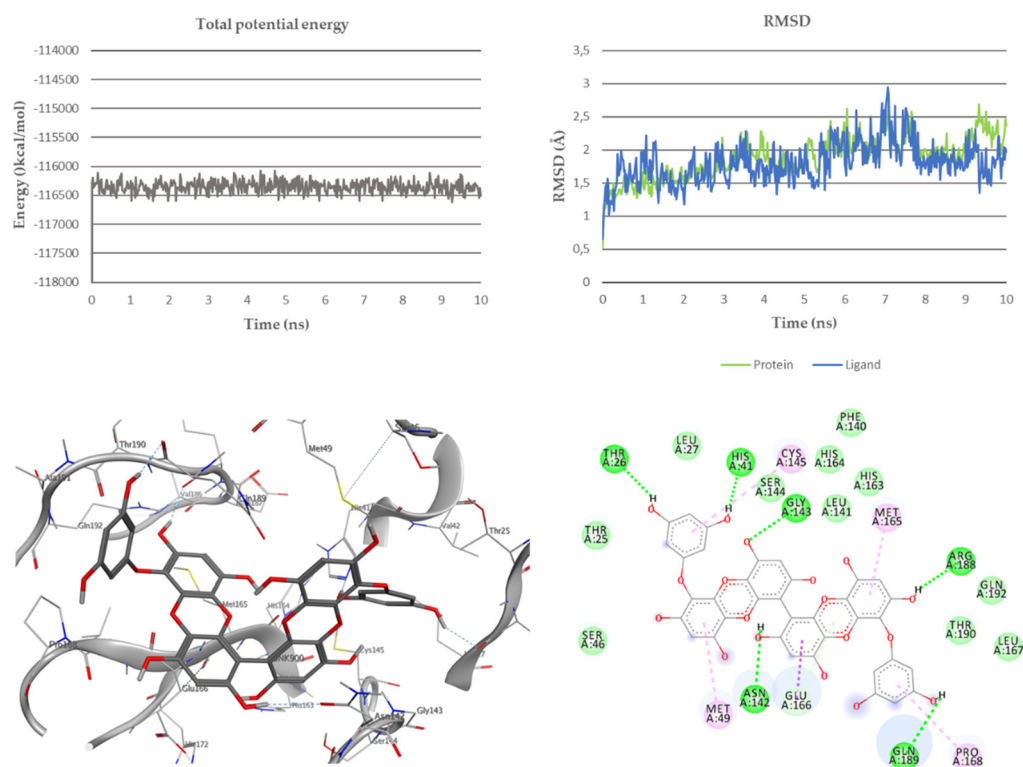
**Figure S7.** MNP ID 89445-12-5. Total energy (up-left) and RMSDs (up-right) of M<sup>Pro</sup> enzyme and its complexes with ligand. Docking binding pose (down-left) and Interaction (down-right) inside the binding pocket of M<sup>Pro</sup> enzyme.



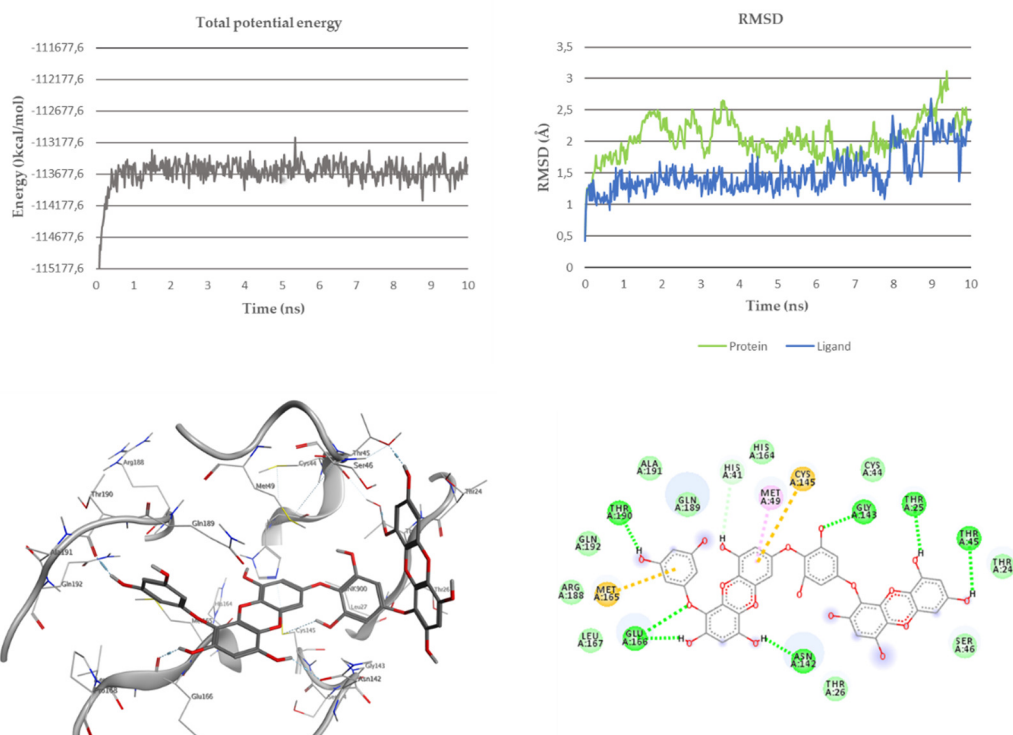
**Figure S8.** MNP ID 36790-49-5. Total energy (up-left) and RMSDs (up-right) of M<sup>Pro</sup> enzyme and its complexes with ligand. Docking binding pose (down-left) and Interaction (down-right) inside the binding pocket of M<sup>Pro</sup> enzyme.



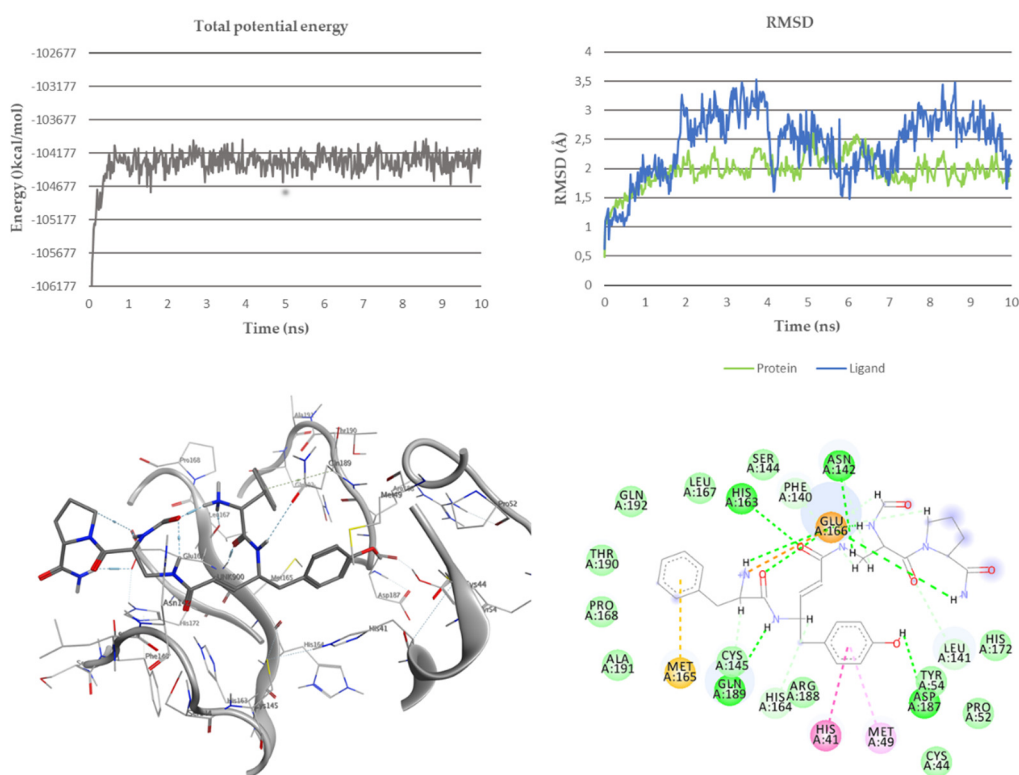
**Figure S9.** MNP ID 20633-84-5. Total energy (up-left) and RMSDs (up-right) of M<sup>Pro</sup> enzyme and its complexes with ligand. Docking binding pose (down-left) and Interaction (down-right) inside the binding pocket of M<sup>Pro</sup> enzyme.



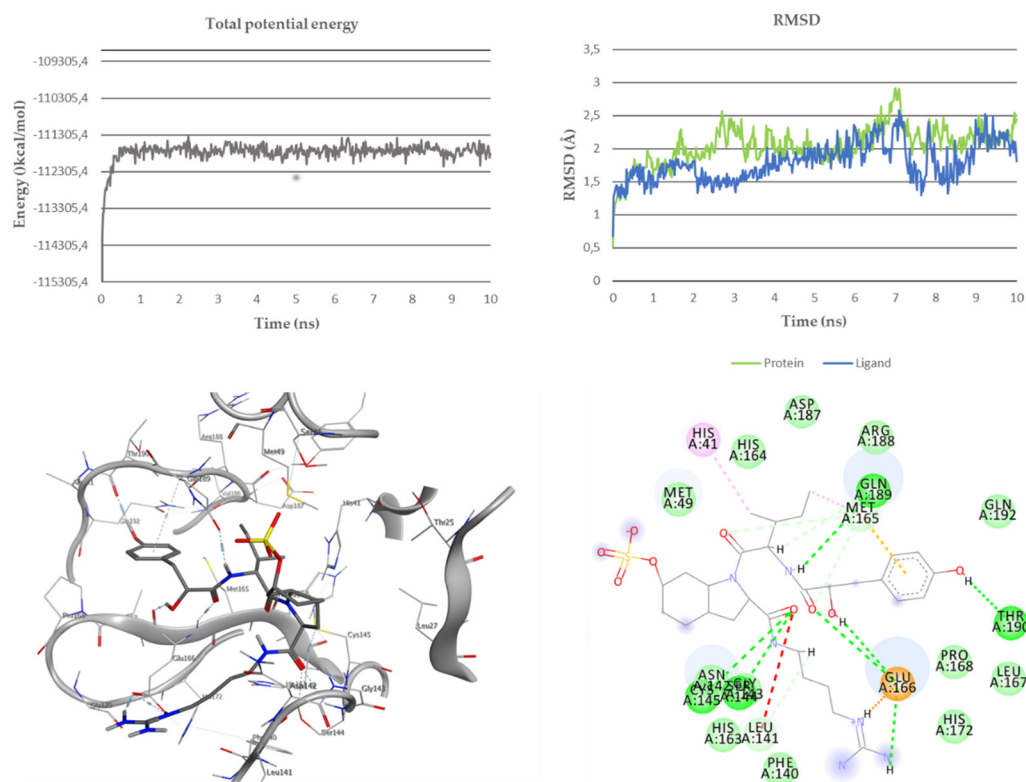
**Figure S10.** MNP ID 88095-81-2. Total energy (up-left) and RMSDs (up-right) of M<sup>Pro</sup> enzyme and its complexes with ligand. Docking binding pose (down-left) and Interaction (down-right) inside the binding pocket of M<sup>Pro</sup> enzyme.



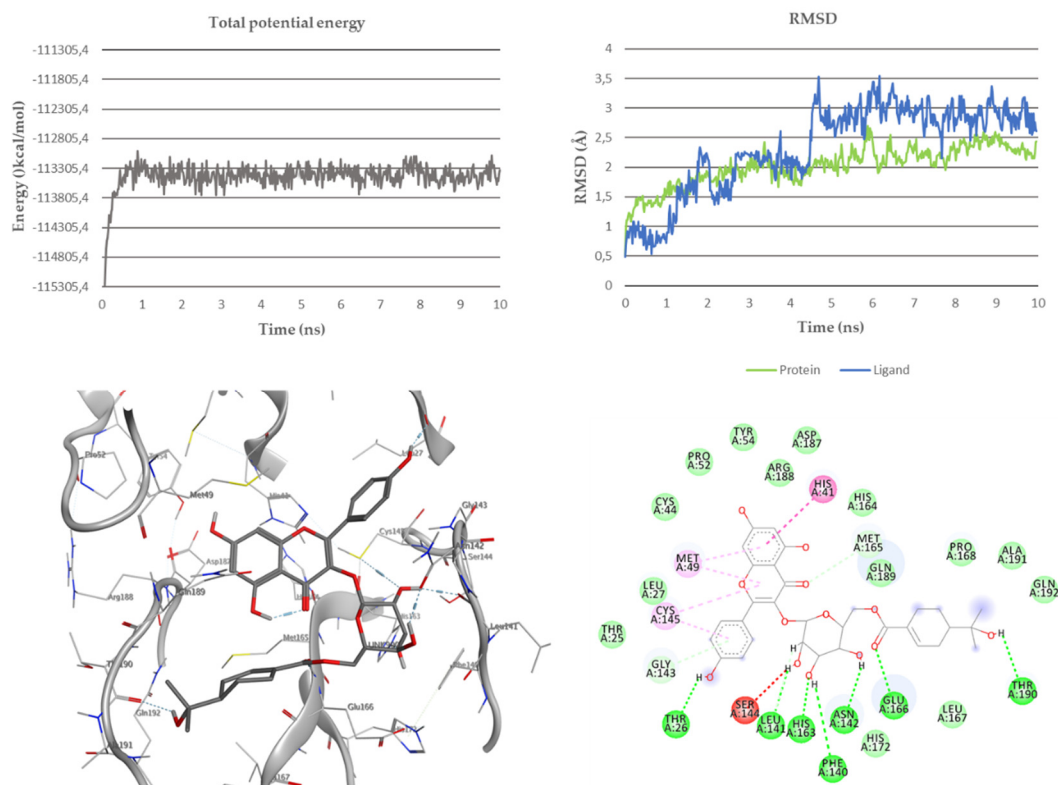
**Figure S11.** MNP ID 88095-81-2. Total energy (up-left) and RMSDs (up-right) of M<sup>Pro</sup> enzyme and its complexes with ligand. Docking binding pose (down-left) and Interaction (down-right) inside the binding pocket of M<sup>Pro</sup> enzyme.



**Figure S12.** MNP ID 224577-36-0. Total energy (up-left) and RMSDs (up-right) of M<sup>Pro</sup> enzyme and its complexes with ligand. Docking binding pose (down-left) and Interaction (down-right) inside the binding pocket of M<sup>Pro</sup> enzyme.



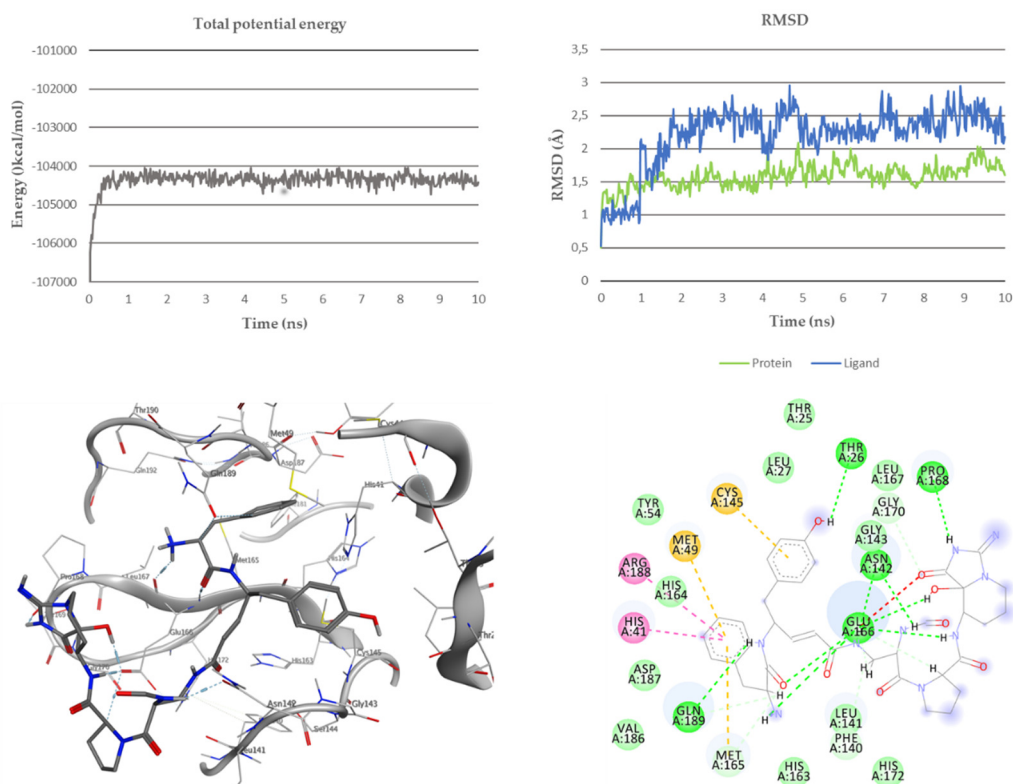
**Figure S13.** MNP ID 167228-01-5. Total energy (up-left) and RMSDs (up-right) of M<sup>Pro</sup> enzyme and its complexes with ligand. Docking binding pose (down-left) and Interaction (down-right) inside the binding pocket of M<sup>Pro</sup> enzyme.



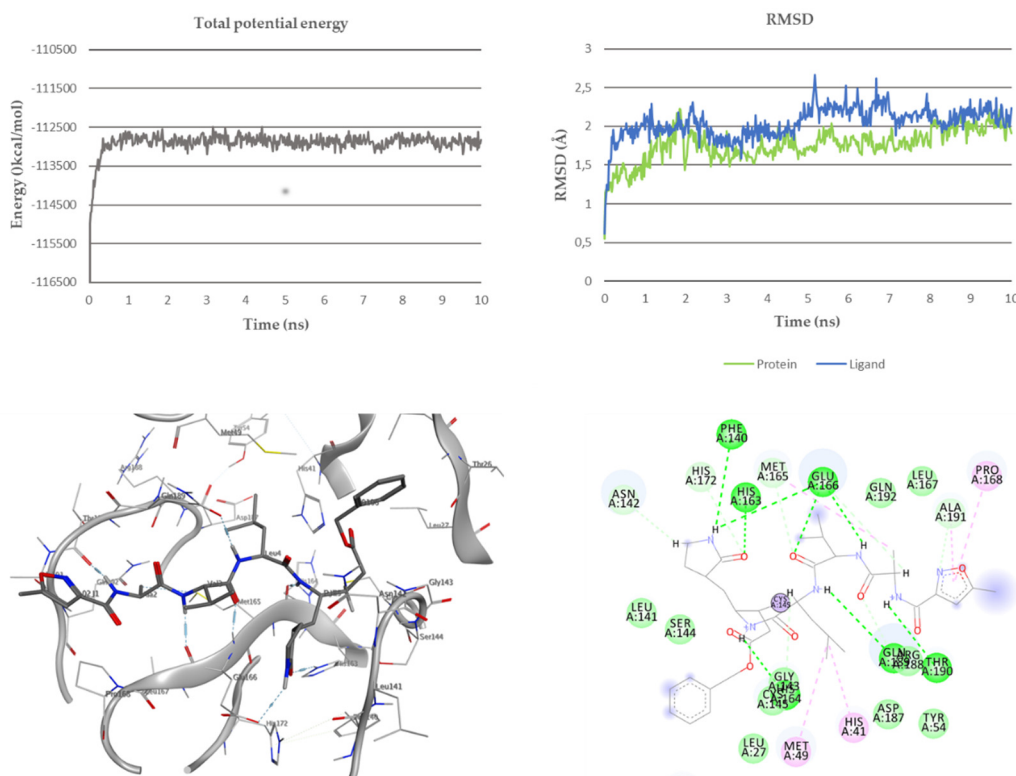
**Figure S14.** MNP ID 144027-79-2. Total energy (up-left) and RMSDs (up-right) of M<sup>Pro</sup> enzyme and its complexes with ligand. Docking binding pose (down-left) and Interaction (down-right) inside the binding pocket of M<sup>Pro</sup> enzyme.



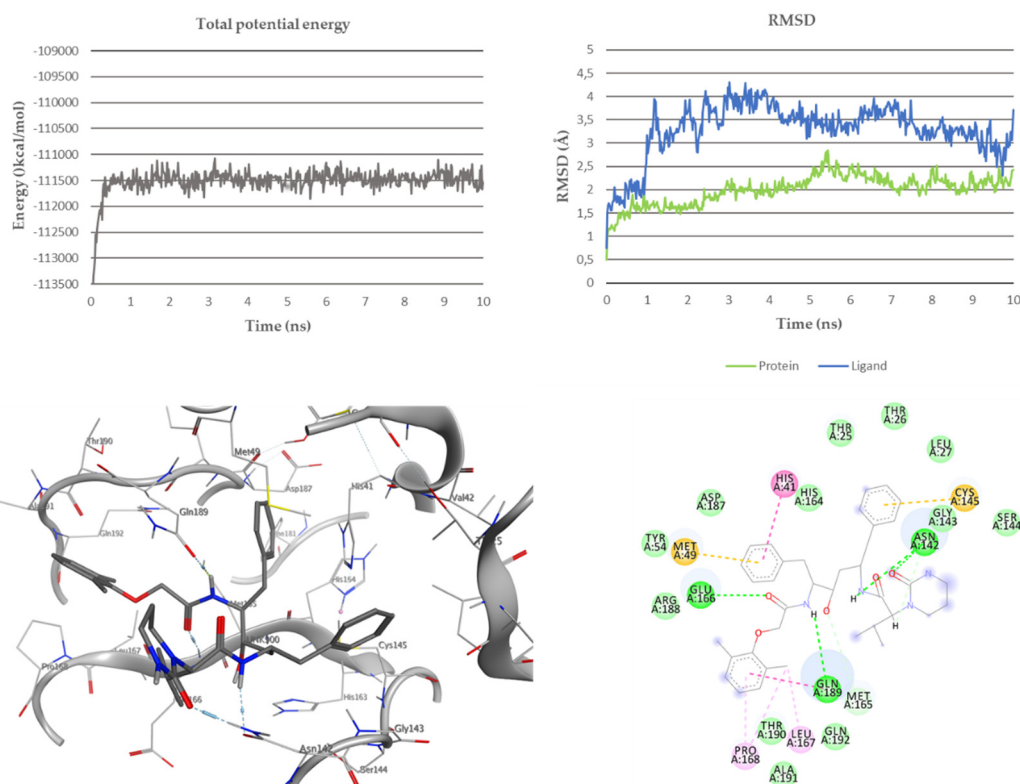




**Figure S17.** MNP ID 224577-35-9. Total energy (up-left) and RMSDs (up-right) of M<sup>Pro</sup> enzyme and its complexes with ligand. Docking binding pose (down-left) and Interaction (down-right) inside the binding pocket of M<sup>Pro</sup> enzyme.



**Figure S18.** PRD\_002214. Total energy (up-left) and RMSDs (up-right) of M<sup>Pro</sup> enzyme and its complexes with ligand. Docking binding pose (down-left) and Interaction (down-right) inside the binding pocket of M<sup>Pro</sup> enzyme.



**Figure S19.** MNP ID 224577-35-9. Total energy (up-left) and RMSDs (up-right) of M<sup>Pro</sup> enzyme and its complexes with ligand. Docking binding pose (down-left) and Interaction (down-right) inside the binding pocket of M<sup>Pro</sup> enzyme.

**Table S1.** Virtual screening of chemical structures of the marine dataset that passed the pharmacophore filter including the contacting receptor residues and binding energy.

MNP ID <sup>a</sup>	Contacting receptor residues	Binding Energy (kcal/mol) Vina
78798-08-0	A THR 25 A THR 26 A LEU 27 A MET 49 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A HIS 172 A ARG 188 A GLN 189 A THR 190 A ALA 191 A GLN 192	-10.18
211686-51-0	A THR 24 A THR 25 A THR 26 A HIS 41 A MET 49 A TYR 118 A ASN 119 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A MET 165 A GLU 166 A LEU 167 A PRO 168 A HIS 172 A GLN 189 A THR 190 A ALA 191	-10.00
40663-80-7	A THR 24 A THR 25 A THR 26 A LEU 27 A HIS 41 A THR 45 A SER 46 A MET 49 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A HIS 172 A GLN 189 A THR 190 A ALA 191 A GLN 192	-9.95
1008752-06-	A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A GLN 189 A THR 190	-9.62
104196-68-1	A HIS 41 A TYR 54 A PHE 140 A LEU 141 A ASN 142 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A PRO 168 A HIS 172 A ASP 187 A ARG 188 A GLN 189 A THR 190 A GLN 192	-9.61

07900-75-4	A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A GLN 189 A THR 190	-9.61
144027-79-2	A THR 25 A THR 26 A LEU 27 A HIS 41 A MET 49 A TYR 54 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A MET 165 A GLU 166 A LEU 167 A PRO 168 A HIS 172 A ASP 187 A ARG 188 A GLN 189 A THR 190 A ALA 191 A GLN 192	-9.56
858950-40-0	A THR 25 A THR 26 A LEU 27 A HIS 41 A MET 49 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A ARG 188 A GLN 189 A THR 190 A ALA 191 A GLN 192	-9.56
18115-90-7	A MET 49 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A HIS 172 A ARG 188 A GLN 189	-9.43
152845-74-4	A THR 25 A THR 26 A LEU 27 A HIS 41 A MET 49 A LEU 141 A ASN 142 A GLY 143 A CYS 145 A MET 165 A GLU 166 A PRO 168 A ARG 188 A GLN 189 A THR 190 A GLN 192	-9.35
58950-46-6	A THR 25 A THR 26 A LEU 27 A HIS 41 A MET 49 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A ARG 188 A GLN 189 A THR 190	-9.31
147716-81-2	A THR 24 A THR 25 A THR 26 A LEU 27 A HIS 41 A THR 45 A SER 46 A MET 49 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A MET 165 A GLU 166 A HIS 172 A GLN 189	-9.29
151379-39-4	A THR 24 A THR 25 A THR 26 A LEU 27 A HIS 41 A THR 45 A SER 46 A MET 49 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A MET 165 A GLU 166 A HIS 172 A GLN 189	-9.28
79849-37-9	A THR 25 A THR 26 A LEU 27 A HIS 41 A VAL 42 A MET 49 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A ARG 188 A GLN 189 A THR 190 A ALA 191 A GLN 192	-9.22
134458-00-7	A THR 25 A LEU 27 A HIS 41 A MET 49 A ASN 142 A GLY 143 A CYS 145 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A ARG 188 A GLN 189 A THR 190 A GLN 192	-9.22
65745-47-3	A THR 24 A THR 25 A THR 26 A LEU 27 A HIS 41 A SER 46 A MET 49 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A HIS 172 A GLN 189	-9.14
514830-04-7	A THR 25 A LEU 27 A HIS 41 A MET 49 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A PRO 168 A HIS 172 A ASP 187 A ARG 188 A GLN 189 A THR 190 A ALA 191	-9.14
113540-81-1	A THR 25 A LEU 27 A HIS 41 A MET 49 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A PRO 168 A HIS 172 A ASP 187 A ARG 188 A GLN 189 A THR 190 A ALA 191	-9.13
97888-14-7	A HIS 41 A CYS 44 A MET 49 A PRO 52 A TYR 54 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A VAL 186 A ASP 187 A ARG 188 A GLN 189 A THR 190 A ALA 191 A GLN 192	-9.00
144587-57-5	A THR 25 A THR 26 A LEU 27 A HIS 41 A MET 49 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A PRO 168 A GLN 189 A THR 190 A ALA 191	-8.94

757976-67-3	A THR 24 A THR 25 A THR 26 A LEU 27 A HIS 41 A CYS 44 A THR 45 A SER 46 A MET 49 A TYR 54 A ASN 142 A GLY 143 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A ASP 187 A ARG 188 A GLN 189	-8.92
97948-90-8	A HIS 41 A CYS 44 A MET 49 A PRO 52 A TYR 54 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A ASP 187 A ARG 188 A GLN 189 A THR 190 A GLN 192	-8.91
89444-89-3	A THR 25 A THR 26 A LEU 27 A HIS 41 A MET 49 A PHE 140 A LEU 141 A ASN 142 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A PRO 168 A ASP 187 A ARG 188 A GLN 189 A THR 190 A GLN 192	-8.91
97888-13-6	A HIS 41 A CYS 44 A MET 49 A PRO 52 A TYR 54 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A ASP 187 A ARG 188 A GLN 189 A THR 190 A GLN 192	-8.91
131727-01-0	A LEU 50 A PHE 140 A LEU 141 A ASN 142 A HIS 163 A MET 165 A GLU 166 A LEU 167 A PRO 168 A HIS 172 A ARG 188 A GLN 189 A THR 190 A ALA 191 A GLN 192	-8.87
175669-27-9	A HIS 41 A MET 49 A TYR 54 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A HIS 172 A ASP 187 A ARG 188 A GLN 189 A THR 190 A ALA 191	-8.85
24577-34-8	A HIS 41 A CYS 44 A MET 49 A PRO 52 A TYR 54 A PHE 140 A LEU 141 A ASN 142 A CYS 145 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A THR 169 A GLY 170 A ASP 187 A ARG 188 A GLN 189 A THR 190 A ALA 191 A GLN 192	-8.84
194427-76-4	A THR 25 A THR 26 A LEU 27 A HIS 41 A MET 49 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A PRO 168 A HIS 172 A GLN 189 A THR 190 A ALA 191	-8.84
144027-78-1	A THR 25 A THR 26 A LEU 27 A HIS 41 A MET 49 A TYR 54 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A ASP 187 A ARG 188 A GLN 189 A THR 190 A ALA 191 A GLN 192	-8.82
133056-07-2	A THR 25 A THR 26 A LEU 27 A HIS 41 A VAL 42 A MET 49 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A PRO 168 A HIS 172 A ARG 188 A GLN 189 A THR 190 A ALA 191 A GLN 192	-8.81
105239-70-1	A THR 24 A THR 25 A THR 26 A LEU 27 A HIS 41 A CYS 44 A THR 45 A SER 46 A MET 49 A PRO 52 A TYR 54 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A HIS 172 A ASP 187 A ARG 188 A GLN 189	-8.81
345642-84-4	A THR 25 A THR 26 A LEU 27 A HIS 41 A MET 49 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A MET 165 A GLU 166 A LEU 167 A PRO 168 A ARG 188 A GLN 189 A THR 190 A GLN 192	-8.80
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105815-90-5	A HIS 41 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A PRO 168 A HIS 172 A VAL 186 A ASP 187 A ARG 188 A GLN 189 A THR 190	-8.73
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224577-31-5	A HIS 41 A CYS 44 A MET 49 A PRO 52 A TYR 54 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A THR 169 A GLY 170 A ASP 187 A ARG 188 A GLN 189 A THR 190 A ALA 191 A GLN 192	-8.72
224577-33-7	A HIS 41 A CYS 44 A MET 49 A PRO 52 A TYR 54 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A THR 169 A GLY 170 A ASP 187 A ARG 188 A GLN 189 A THR 190 A ALA 191 A GLN 192	-8.72
50335-04-1	A HIS 41 A MET 49 A PHE 140 A LEU 141 A ASN 142 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A HIS 172 A VAL 186 A ASP 187 A ARG 188 A GLN 189 A THR 190 A GLN 192	-8.71
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852872-93-6	A THR 25 A THR 26 A LEU 27 A HIS 41 A VAL 42 A MET 49 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A GLY 170 A ASP 187 A ARG 188 A GLN 189 A THR 190 A ALA 191 A GLN 192	-8.61
104758-18-1	A SER 46 A GLU 47 A MET 49 A LEU 50 A PHE 140 A LEU 141 A ASN 142 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A HIS 172 A ARG 188 A GLN 189 A THR 190 A ALA 191 A GLN 192	-8.58
97915-31-6	A THR 24 A THR 25 A THR 26 A LEU 27 A HIS 41 A THR 45 A MET 49 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A GLY 170 A HIS 172 A VAL 186 A ARG 188 A GLN 189 A THR 190 A ALA	-8.58
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55544-35-9	A THR 25 A THR 26 A LEU 27 A HIS 41 A MET 49 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A MET 165 A GLU 166 A LEU 167 A PRO 168 A ARG 188 A GLN 189 A THR 190 A ALA 191 A GLN 192	-8.56
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273410-51-8	A THR 24 A THR 25 A THR 26 A LEU 27 A HIS 41 A MET 49 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A VAL 186 A ASP 187 A ARG 188 A GLN 189	-8.54
115982-32-6	A THR 24 A THR 25 A THR 26 A HIS 41 A SER 46 A MET 49 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A HIS 172 A VAL 186 A ASP 187 A ARG 188 A GLN 189	-8.50
81657-79-6	A THR 24 A THR 25 A THR 26 A LEU 27 A HIS 41 A SER 46 A MET 49 A TYR 54 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A VAL 186 A ASP 187 A ARG 188 A GLN 189 A GLN 192	-8.50
36119-03-6	A THR 25 A THR 26 A LEU 27 A HIS 41 A CYS 44 A MET 49 A PRO 52 A TYR 54 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A PRO 168 A HIS 172 A ASP 187 A ARG 188 A GLN 189 A THR 190 A GLN 192	-8.47
83481-23-6	A MET 49 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A HIS 172 A ARG 188 A GLN 189 A THR 190 A ALA 191 A GLN 192	-8.47
80680-43-9	A HIS 41 A MET 49 A TYR 54 A ASN 142 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A ASP 187 A ARG 188 A GLN 189 A THR 190 A ALA 191	-8.47
18097-67-1	A THR 25 A THR 26 A LEU 27 A HIS 41 A CYS 44 A MET 49 A PRO 52 A TYR 54 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A ASP 187 A ARG 188 A GLN 189	-8.46
138529-07-4	A THR 24 A THR 25 A THR 26 A LEU 27 A HIS 41 A CYS 44 A THR 45 A SER 46 A GLU 47 A ASP 48 A MET 49 A LEU 50 A TYR 54 A ASN 142 A GLY 143 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A PRO 168 A ASP 187 A ARG 188 A GLN 189 A THR 190 A ALA 191 A	-8.45

61369-27-5	A THR 24 A THR 25 A THR 26 A HIS 41 A CYS 44 A THR 45 A SER 46 A MET 49 A TYR 54 A ASN 142 A GLY 143 A CYS 145 A HIS 164 A MET 165 A GLU 166 A PRO 168 A ASP 187 A ARG 188 A GLN 189 A THR 190 A ALA 191	-8.45
70022-71-8	A THR 25 A LEU 27 A HIS 41 A MET 49 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A ARG 188 A GLN 189 A THR 190 A ALA 191 A GLN 192	-8.45
55482-27-4	A THR 24 A THR 25 A THR 26 A HIS 41 A CYS 44 A THR 45 A SER 46 A MET 49 A PRO 52 A TYR 54 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A ASP 187 A ARG 188 A GLN 189 A THR 190	-8.44
138529-05-2	A THR 24 A THR 25 A THR 26 A LEU 27 A HIS 41 A CYS 44 A THR 45 A SER 46 A MET 49 A ASN 142 A GLY 143 A CYS 145 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A VAL 186 A ASP 187 A ARG 188 A GLN 189 A THR 190 A GLN 192	-8.40
690627-61-3	A THR 24 A THR 25 A THR 26 A LEU 27 A HIS 41 A MET 49 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A HIS 172 A ARG 188 A GLN 189 A THR 190 A ALA 191 A GLN 192	-8.40
213547-25-2	A THR 24 A THR 25 A THR 26 A LEU 27 A HIS 41 A THR 45 A SER 46 A MET 49 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A HIS 172 A GLN 189	-8.40
52796-14-2	A THR 25 A LEU 27 A HIS 41 A MET 49 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A HIS 172 A ARG 188 A GLN 189 A THR 190 A ALA 191 A GLN 192	-8.38
207385-07-7	A THR 25 A LEU 27 A HIS 41 A MET 49 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A HIS 172 A ARG 188 A GLN 189 A THR 190 A ALA 191 A GLN 192	-8.38
102506-55-8	A THR 24 A THR 25 A THR 26 A LEU 27 A HIS 41 A CYS 44 A THR 45 A SER 46 A MET 49 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A MET 165 A GLU 166 A LEU 167 A PRO 168 A ARG 188 A GLN 189 A THR 190 A GLN 192	-8.38
188558-97-6	A THR 24 A THR 25 A THR 26 A HIS 41 A MET 49 A ASN 142 A GLY 143 A CYS 145 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A ASP 187 A ARG 188 A GLN 189 A THR 190 A ALA 191 A GLN 192	-8.36
256649-68-0	A MET 49 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A HIS 172 A ARG 188 A GLN 189 A THR 190 A GLN 192	-8.36
55945-74-9	A HIS 41 A MET 49 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A GLN 189 A THR 190 A ALA 191	-8.34
65773-98-0	A THR 25 A THR 26 A LEU 27 A HIS 41 A MET 49 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A HIS 172 A GLN 189	-8.34



137809-94-0	A THR 24 A THR 25 A THR 26 A LEU 27 A HIS 41 A CYS 44 A MET 49 A LEU 50 A TYR 54 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A GLY 170 A ASP 187 A ARG 188 A GLN 189 A THR 190 A GLN 1	-8.33
137844-97-4	A THR 24 A THR 25 A THR 26 A LEU 27 A THR 45 A SER 46 A MET 49 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A HIS 172 A ARG 188 A GLN 189 A THR 190 A GLN 192	-8.32
36011-19-5	A THR 24 A THR 25 A THR 26 A LEU 27 A HIS 41 A VAL 42 A CYS 44 A THR 45 A SER 46 A MET 49 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A HIS 172 A GLN 189	-8.30
54854-92-1	A THR 25 A THR 26 A LEU 27 A HIS 41 A MET 49 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A HIS 172 A ARG 188 A GLN 189 A THR 190 A GLN 192	-8.29
656250-28-1	A THR 24 A THR 25 A THR 26 A HIS 41 A CYS 44 A THR 45 A SER 46 A MET 49 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A HIS 172 A GLN 189	-8.29
798575-31-2	A THR 24 A THR 25 A THR 26 A HIS 41 A CYS 44 A THR 45 A SER 46 A MET 49 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A HIS 172 A GLN 189	-8.29
128129-56-6	A THR 25 A THR 26 A LEU 27 A HIS 41 A MET 49 A ASN 142 A GLY 143 A CYS 145 A MET 165 A GLU 166 A VAL 186 A ASP 187 A ARG 188 A GLN 189 A THR 190 A GLN 192	-8.28
144587-58-6	A THR 25 A THR 26 A LEU 27 A HIS 41 A MET 49 A ASN 142 A GLY 143 A CYS 145 A MET 165 A GLU 166 A LEU 167 A PRO 168 A GLN 189 A THR 190 A ALA 191 A GLN 192	-8.27
72380-13-3	A THR 25 A THR 26 A LEU 27 A HIS 41 A VAL 42 A MET 49 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A MET 165 A GLU 166 A LEU 167 A PRO 168 A ARG 188 A GLN 189 A THR 190 A GLN 192	-8.24
83903-60-0	A THR 25 A THR 26 A CYS 44 A THR 45 A SER 46 A MET 49 A PHE 140 A LEU 141 A ASN 142 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A HIS 172 A ARG 188 A GLN 189 A THR 190 A ALA 191 A GLN 192	-8.23
50611-86-4	A HIS 41 A CYS 44 A MET 49 A PRO 52 A TYR 54 A PHE 140 A LEU 141 A ASN 142 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A HIS 172 A ASP 187 A ARG 188 A GLN 189	-8.23
164176-22-1	A THR 24 A THR 25 A LEU 27 A HIS 41 A CYS 44 A THR 45 A SER 46 A MET 49 A PRO 52 A TYR 54 A ASN 142 A GLY 143 A CYS 145 A HIS 164 A MET 165 A GLU 166 A PHE 181 A ASP 187 A ARG 188 A GLN 189	-8.23
164176-24-3	A THR 24 A THR 25 A THR 26 A HIS 41 A CYS 44 A THR 45 A SER 46 A MET 49 A PRO 52 A TYR 54 A ASN 119 A ASN 142 A GLY 143 A CYS 145 A HIS 164 A MET 165 A GLU 166 A ASP 187 A ARG 188 A GLN 189	-8.21
70938-59-9	A HIS 41 A MET 49 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A HIS 172 A ASP 187 A ARG 188 A GLN 189 A THR 190 A ALA 191 A GLN 192	-8.21

114-25-0	THR 24 A THR 25 A THR 26 A HIS 41 A CYS 44 A THR 45 A SER 46 A MET 49 A PRO 52 A TYR 54 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A ASP 187 A ARG 188 A GLN 189 A THR 190 A	-8.21
174630-08-1	A THR 24 A THR 25 A THR 26 A LEU 27 A HIS 41 A CYS 44 A THR 45 A SER 46 A MET 49 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A ARG 188 A GLN 189 A THR 190 A ALA 191 A GLN 192	-8.21
72509-61-6	A THR 25 A THR 26 A MET 49 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A ARG 188 A GLN 189	-8.20
184348-39-8	A THR 25 A THR 26 A HIS 41 A MET 49 A TYR 118 A ASN 119 A ASN 142 A GLY 143 A CYS 145 A HIS 164 A MET 165 A GLU 166 A GLN 189	-8.19
137809-89-3	A THR 24 A THR 25 A LEU 27 A HIS 41 A CYS 44 A THR 45 A SER 46 A MET 49 A TYR 54 A PHE 140 A ASN 142 A GLY 143 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A HIS 172 A ASP 187 A ARG 188 A GLN 189	-8.17
111036-40-9	A LEU 27 A HIS 41 A MET 49 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A HIS 172 A ASP 187 A ARG 188 A GLN 189 A THR 190 A ALA 191 A GLN 192	-8.15
164176-23-2	A THR 24 A THR 25 A THR 26 A HIS 41 A CYS 44 A SER 46 A MET 49 A PRO 52 A TYR 54 A ASN 119 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 164 A MET 165 A GLU 166 A PHE 181 A ASP 187 A ARG 188 A GLN 189	-8.15
137824-59-0	A HIS 41 A CYS 44 A MET 49 A PRO 52 A TYR 54 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A HIS 172 A ASP 187 A ARG 188 A GLN 189 A THR 190 A ALA 191 A GLN 192	-8.15
76689-96-8	A THR 24 A THR 25 A LEU 27 A HIS 41 A CYS 44 A THR 45 A SER 46 A MET 49 A PRO 52 A TYR 54 A ASN 142 A GLY 143 A CYS 145 A HIS 164 A MET 165 A GLU 166 A PHE 181 A ASP 187 A ARG 188 A GLN 189	-8.15
142925-51-7	A HIS 41 A CYS 44 A MET 49 A PRO 52 A TYR 54 A PHE 140 A LEU 141 A ASN 142 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A THR 169 A GLY 170 A HIS 172 A ASP 187 A ARG 188 A GLN 189 A THR 190 A ALA 191 A GLN 192	-8.14
172854-77-2	A MET 49 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A HIS 172 A ARG 188 A GLN 189 A THR 190 A GLN 192	-8.14
329050-25-1	A THR 24 A THR 25 A THR 26 A LEU 27 A HIS 41 A VAL 42 A MET 49 A TYR 54 A ASN 142 A GLY 143 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A PHE 181 A ASP 187 A ARG 188 A GLN 189	-8.10
137809-88-2	A HIS 41 A CYS 44 A MET 49 A TYR 54 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A MET 165 A GLU 166 A PRO 168 A HIS 172 A VAL 186 A ASP 187 A ARG 188 A GLN 189 A THR 190 A GLN 192	-8.09

86425-61-8	A THR 24 A THR 25 A THR 26 A LEU 27 A HIS 41 A VAL 42 A SER 46 A MET 49 A ASN 119 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A HIS 172 A ASP 187 A ARG 188 A GLN 189	-8.06
823808-55-5	A THR 25 A LEU 27 A HIS 41 A MET 49 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A HIS 172 A ARG 188 A GLN 189 A THR 190 A ALA 191 A GLN 192	-8.06
145613-82-7	A LEU 27 A HIS 41 A MET 49 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A HIS 172 A ASP 187 A ARG 188 A GLN 189 A THR 190 A ALA 191 A GLN 192	-8.05
858950-52-4	A THR 25 A THR 26 A LEU 27 A HIS 41 A MET 49 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A PRO 168 A GLN 189	-8.05
80442-78-0	A MET 49 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A GLN 189 A THR 190	-8.04
80442-79-1	A MET 49 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A GLN 189 A THR 190	-8.04
115268-43-4	A HIS 41 A MET 49 A LEU 141 A ASN 142 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A ARG 188 A GLN 189	-8.04
364344-14-9	A THR 24 A THR 25 A THR 26 A LEU 27 A HIS 41 A MET 49 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A ARG 188 A GLN 189 A THR 190 A GLN 192	-8.04
105404-85-1	A THR 24 A THR 25 A THR 26 A HIS 41 A CYS 44 A THR 45 A SER 46 A MET 49 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A ARG 188 A GLN 189 A THR 190	-8.04
137824-58-9	A THR 25 A THR 26 A LEU 27 A MET 49 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A PRO 168 A HIS 172 A ARG 188 A GLN 189 A THR 190 A ALA 191 A GLN 192	-8.04
99102-40-6	A THR 24 A THR 25 A THR 26 A LEU 27 A HIS 41 A VAL 42 A THR 45 A SER 46 A MET 49 A TYR 118 A ASN 142 A GLY 143 A CYS 145 A MET 165 A GLU 166 A GLN 189	-8.02
100244-36-8	A THR 24 A THR 25 A THR 26 A LEU 27 A HIS 41 A MET 49 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A GLN 189	-8.02
157207-91-5	A MET 49 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A HIS 172 A ASP 187 A ARG 188 A GLN 189 A THR 190 A ALA 191	-8.02
329197-89-9	A THR 24 A THR 25 A THR 26 A LEU 27 A HIS 41 A MET 49 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A GLN 189	-8.01
2643-02-9	THR 24 A THR 25 A THR 26 A LEU 27 A HIS 41 A THR 45 A SER 46 A MET 49 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A ARG 188 A GLN 189 A GLN 192	-8.01
143346-97-8	A HIS 41 A MET 49 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A ARG 188 A GLN 189 A THR 190 A ALA 191 A GLN 192	-8.01

149764-33-0	A HIS 41 A MET 49 A LEU 50 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A HIS 172 A GLN 189 A THR 190 A ALA 191 A GLN 192	-8.00
143113-32-0	A THR 24 A THR 25 A THR 26 A LEU 27 A HIS 41 A THR 45 A SER 46 A MET 49 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A GLY 170 A HIS 172 A GLN 189	-7.99
77658-95-8	A THR 24 A THR 25 A THR 26 A LEU 27 A HIS 41 A CYS 44 A MET 49 A TYR 54 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A HIS 172 A ASP 187 A ARG 188 A GLN 189	-7.99
858950-36-4	A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A PRO 168 A HIS 172 A GLN 189 A THR 190 A ALA 191 A GLN 192	-7.98
79206-71-6	A THR 25 A HIS 41 A MET 49 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A HIS 172 A ARG 188 A GLN 189 A THR 190 A ALA 191 A GLN 192	-7.98
724462-47-9	A THR 25 A THR 26 A LEU 27 A HIS 41 A MET 49 A TYR 54 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A HIS 172 A ASP 187 A ARG 188 A GLN 189	-7.97
2122-98-7	THR 25 A THR 26 A LEU 27 A HIS 41 A MET 49 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A HIS 172 A GLN 189 A THR 190	-7.96
79067-75-7	A THR 24 A THR 25 A THR 26 A LEU 27 A SER 46 A MET 49 A ASN 119 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A GLU 166 A GLN 189	-7.92
603125-81-1	A THR 25 A THR 26 A LEU 27 A HIS 41 A MET 49 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 164 A MET 165 A GLU 166 A PRO 168 A ARG 188 A GLN 189 A THR 190 A GLN 192	-7.90
134985-04-9	A HIS 41 A CYS 44 A MET 49 A LEU 50 A PRO 52 A TYR 54 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A HIS 172 A ASP 187 A ARG 188 A GLN 189 A THR 190 A ALA 191	-7.90
94513-77-6	A THR 24 A THR 25 A THR 26 A LEU 27 A HIS 41 A CYS 44 A THR 45 A SER 46 A MET 49 A LEU 50 A TYR 54 A CYS 145 A HIS 164 A MET 165 A GLU 166 A LEU 167 A ASP 187 A ARG 188 A GLN 189 A THR 190 A ALA 191 A GLN 192	-7.90
92679-03-3	A THR 24 A THR 25 A THR 26 A LEU 27 A HIS 41 A MET 49 A TYR 54 A ASN 142 A GLY 143 A CYS 145 A HIS 164 A MET 165 A GLU 166 A ASP 187 A ARG 188 A GLN 189	-7.89
65604-87-7	A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A GLY 170 A HIS 172 A ASP 187 A ARG 188 A GLN 189 A THR 190 A GLN 192	-7.89
304902-16-7	A HIS 41 A MET 49 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A ARG 188 A GLN 189 A THR 190 A ALA 191 A GLN 192	-7.88

181034-78-6	A HIS 41 A CYS 44 A MET 49 A PRO 52 A TYR 54 A ASN 142 A CYS 145 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A GLY 170 A ASP 187 A ARG 188 A GLN 189 A THR 190 A ALA 191 A GLN 192	-7.87
221290-77-3	A THR 24 A THR 25 A THR 26 A LEU 27 A HIS 41 A MET 49 A TYR 54 A ASN 119 A ASN 142 A GLY 143 A CYS 145 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A ASP 187 A ARG 188 A GLN 189 A THR 190 A ALA 191 A GLN 192	-7.87
76689-97-9	A HIS 41 A MET 49 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A HIS 172 A ASP 187 A ARG 188 A GLN 189 A THR 190 A ALA 191	-7.86
92679-02-2	A THR 24 A THR 25 A THR 26 A LEU 27 A HIS 41 A CYS 44 A MET 49 A PRO 52 A TYR 54 A ASN 142 A GLY 143 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A PHE 181 A ASP 187 A ARG 188 A GLN 189	-7.86
170894-36-7	A THR 25 A THR 26 A LEU 27 A HIS 41 A MET 49 A LEU 50 A ASN 142 A GLY 143 A CYS 145 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A GLN 189 A THR 190 A ALA 191 A GLN 192	-7.85
170894-37-8	A THR 25 A THR 26 A LEU 27 A HIS 41 A MET 49 A ASN 142 A GLY 143 A CYS 145 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A GLN 189 A THR 190 A ALA 191 A GLN 192	-7.84
564-16-9	MET 49 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A HIS 172 A GLN 189 A THR 190 A ALA 191 A GLN 192	-7.84
129602-18-2	A THR 25 A THR 26 A LEU 27 A HIS 41 A VAL 42 A MET 49 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A HIS 172 A GLN 189 A THR 190 A ALA 191 A GLN 192	-7.84
142797-28-2	A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A HIS 172 A ARG 188 A GLN 189 A THR 190 A GLN 192	-7.83
58115-30-3	A THR 25 A THR 26 A LEU 27 A HIS 41 A MET 49 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A MET 165 A GLU 166 A LEU 167 A PRO 168 A ARG 188 A GLN 189 A THR 190 A ALA 191 A GLN 192	-7.83
53755-56-9	A THR 25 A THR 26 A LEU 27 A HIS 41 A MET 49 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A HIS 172 A VAL 186 A ASP 187 A ARG 188 A GLN 189 A THR 190 A ALA 191 A GLN 192	-7.83
123167-01-1	A THR 24 A THR 25 A THR 26 A LEU 27 A HIS 41 A THR 45 A SER 46 A MET 49 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A ARG 188 A GLN 189 A THR 190 A ALA 191 A GLN 192	-7.83
603125-80-0	A THR 25 A THR 26 A LEU 27 A HIS 41 A MET 49 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A ARG 188 A GLN 189 A THR 190 A ALA 191 A GLN 192	-7.83

207683-70-3	A THR 25 A THR 26 A LEU 27 A HIS 41 A SER 46 A MET 49 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A MET 165 A GLU 166 A LEU 167 A PRO 168 A ARG 188 A GLN 189 A THR 190 A GLN 192	-7.83
129893-35-2	A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A HIS 172 A ARG 188 A GLN 189 A THR 190 A GLN 192	-7.83
137571-30-3	A THR 24 A THR 25 A THR 26 A LEU 27 A HIS 41 A SER 46 A MET 49 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A ARG 188 A GLN 189 A THR 190	-7.82
79005-82-6	A THR 24 A THR 25 A THR 26 A LEU 27 A HIS 41 A CYS 44 A THR 45 A SER 46 A MET 49 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A HIS 172 A GLN 189	-7.82
128298-63-5	A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A HIS 172 A ARG 188 A GLN 189 A THR 190 A GLN 192	-7.82
64108-85-6	A THR 24 A THR 25 A THR 26 A LEU 27 A HIS 41 A CYS 44 A SER 46 A MET 49 A PRO 52 A TYR 54 A ASN 142 A GLY 143 A CYS 145 A HIS 164 A MET 165 A GLU 166 A ASP 187 A ARG 188 A GLN 189	-7.82
123154-33-6	A THR 25 A LEU 27 A HIS 41 A MET 49 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A GLY 170 A ASP 187 A ARG 188 A GLN 189 A THR 190 A ALA 191 A GLN 192	-7.82
100019-24-7	A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A HIS 172 A ARG 188 A GLN 189 A THR 190 A GLN 192	-7.81
128733-04-0	A MET 49 A PHE 140 A LEU 141 A ASN 142 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A PRO 168 A HIS 172 A ARG 188 A GLN 189 A THR 190 A ALA 191 A GLN 192	-7.79
137809-87-1	A THR 24 A THR 25 A THR 26 A HIS 41 A CYS 44 A THR 45 A SER 46 A MET 49 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A HIS 172	-7.78
128819-90-9	A MET 49 A PHE 140 A LEU 141 A ASN 142 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A HIS 172 A ARG 188 A GLN 189 A THR 190 A ALA 191 A GLN 192	-7.78
80764-19-8	A THR 25 A HIS 41 A MET 49 A TYR 54 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A HIS 172 A ASP 187 A ARG 188 A GLN 189 A THR 190 A ALA 191 A GLN 192	-7.78
160796-24-7	A THR 25 A THR 26 A LEU 27 A HIS 41 A CYS 44 A THR 45 A SER 46 A MET 49 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A HIS 172 A GLN 189	-7.77
133056-09-4	A THR 24 A THR 25 A THR 26 A LEU 27 A HIS 41 A THR 45 A SER 46 A MET 49 A ASN 142 A GLY 143 A CYS 145 A MET 165 A GLU 166 A LEU 167 A PRO 168 A GLN 189	-7.77

23235-67-8	A HIS 41 A MET 49 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A HIS 172 A ASP 187 A ARG 188 A GLN 189 A THR 190 A GLN 192	-7.76
681260-09-3	A HIS 41 A MET 49 A ASN 142 A GLY 143 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A PRO 168 A ARG 188 A GLN 189 A THR 190 A ALA 191 A GLN 192	-7.76
33579-63-4	A THR 25 A THR 26 A LEU 27 A HIS 41 A VAL 42 A MET 49 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A HIS 172 A ARG 188 A GLN 189	-7.76
648883-31-2	A THR 25 A THR 26 A LEU 27 A HIS 41 A MET 49 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 164 A MET 165 A GLU 166 A PRO 168 A ARG 188 A GLN 189 A THR 190 A GLN 192	-7.75
143572-73-0	A THR 24 A THR 25 A THR 26 A LEU 27 A HIS 41 A MET 49 A TYR 54 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A PHE 181 A ASP 187 A ARG 188 A GLN 189	-7.75
159334-35-7	A HIS 41 A MET 49 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A PRO 168 A HIS 172 A GLN 189 A THR 190 A ALA 191 A GLN 192	-7.75
184885-91-4	A THR 25 A THR 26 A LEU 27 A HIS 41 A CYS 44 A THR 45 A SER 46 A MET 49 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A HIS 172 A GLN 189	-7.74
133883-22-4	A THR 25 A THR 26 A LEU 27 A MET 49 A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A HIS 172 A ARG 188 A GLN 189 A THR 190 A ALA 191 A GLN 192	-7.74