



1 Supporting Information

## 2 Inhibitors of SARS-CoV-2 Main Protease from a

## 3 Library of Marine Natural Products: A Virtual

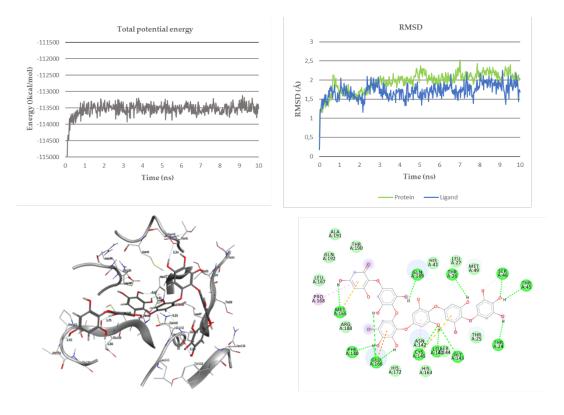
## 4 Screening and Molecular Modeling Study

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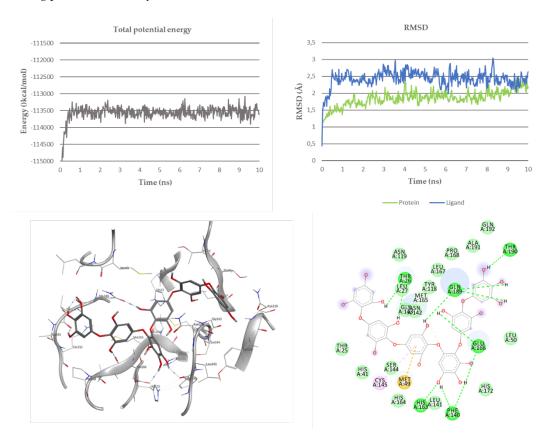
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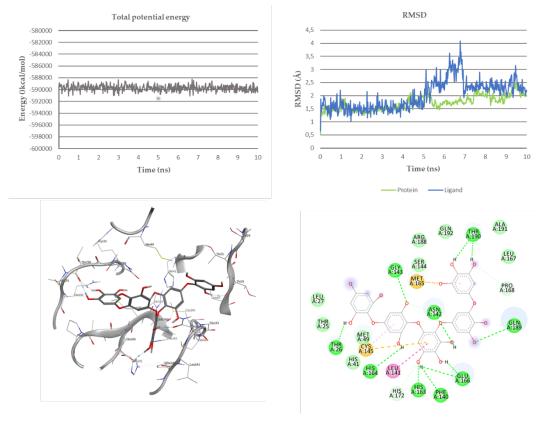
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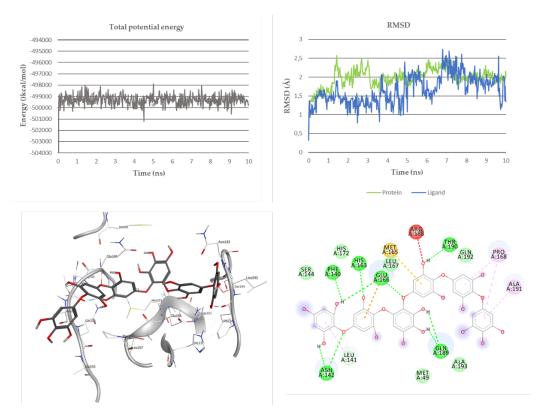
**Figure S1. MNP ID 76265-30-0.** Total energy (up-left) and RMSDs (up-right) of  $M^{pro}$  enzyme and its complexes with ligand. Docking binding pose (down-left) and Interaction (down-right) inside the binding pocket of  $M^{pro}$  enzyme.



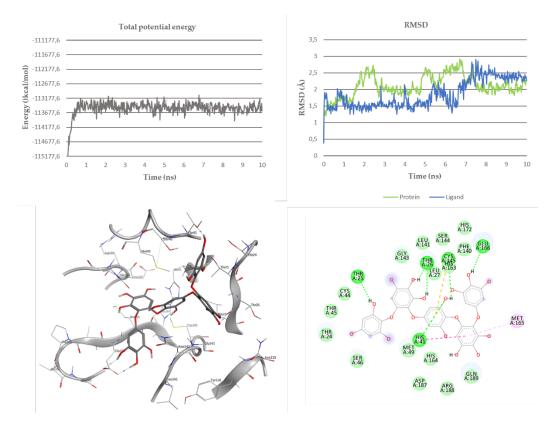
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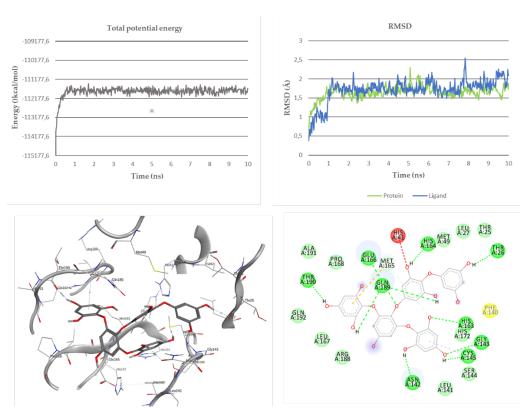
**Figure S3. MNP ID 202211-82-3**. Total energy (up-left) and RMSDs (up-right) of M<sup>pro</sup> enzyme and its complexes with ligand. Docking binding pose (down-left) and Interaction (down-right) inside the binding pocket of M<sup>pro</sup> enzyme.



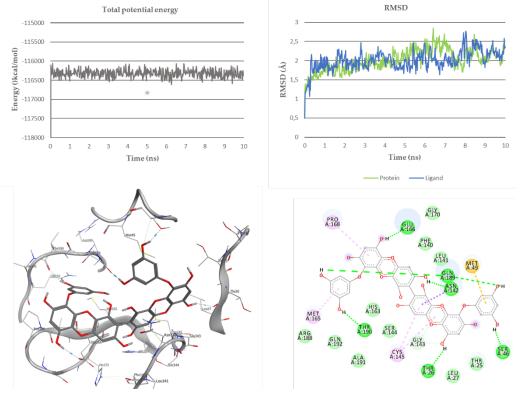
**Figure S4. MNP ID 138529-06-3**. Total energy (up-left) and RMSDs (up-right) of M<sup>pro</sup> enzyme and its complexes with ligand. Docking binding pose (down-left) and Interaction (down-right) inside the binding pocket of M<sup>pro</sup> enzyme.



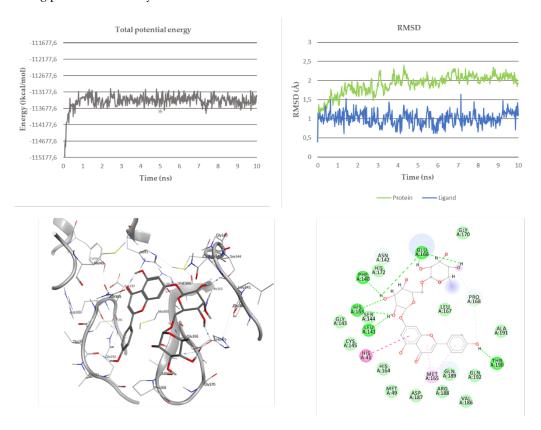
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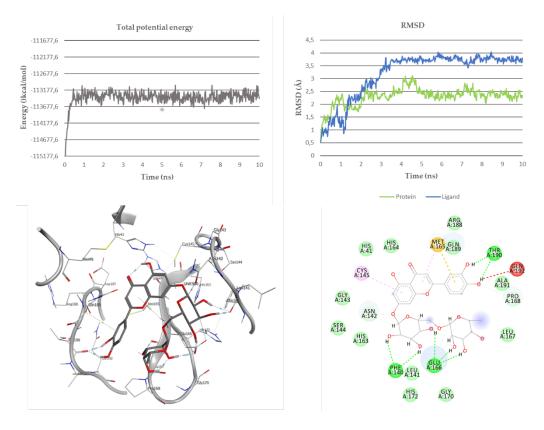
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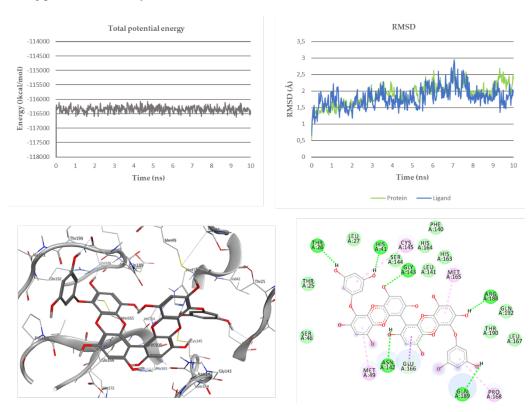
**Figure S7. MNP ID 89445-12-5**. Total energy (up-left) and RMSDs (up-right) of M<sup>pro</sup> enzyme and its complexes with ligand. Docking binding pose (down-left) and Interaction (down-right) inside the binding pocket of M<sup>pro</sup> enzyme.



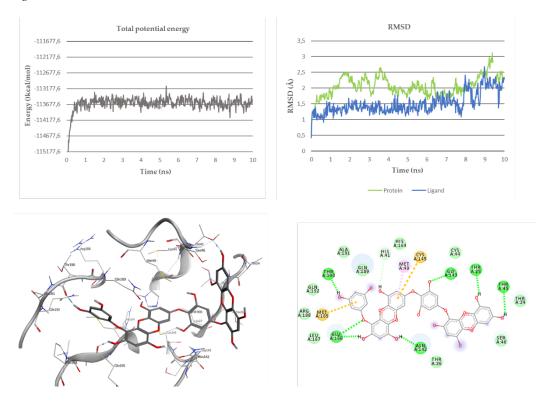
**Figure S8. MNP ID 36790-49-5**. Total energy (up-left) and RMSDs (up-right) of  $M^{\rm pro}$  enzyme and its complexes with ligand. Docking binding pose (down-left) and Interaction (down-right) inside the binding pocket of  $M^{\rm pro}$  enzyme.



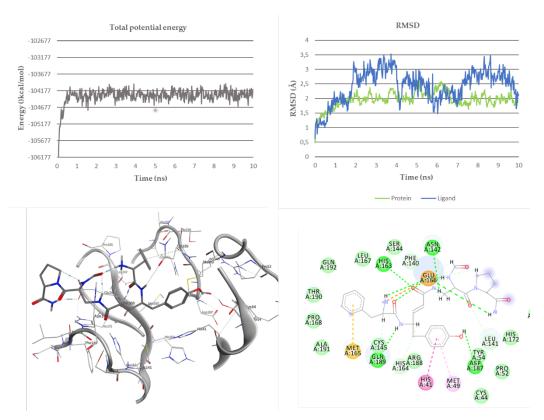
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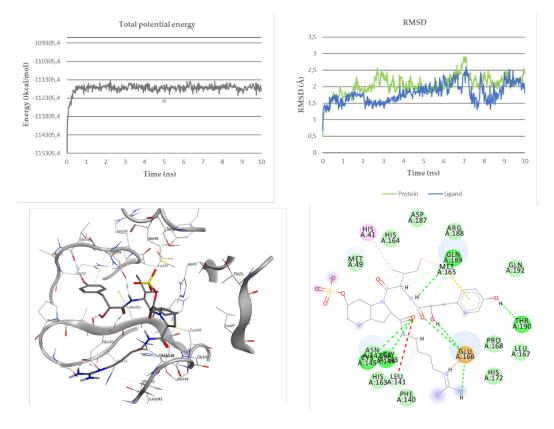
**Figure S10. MNP ID 88095-81-2.** Total energy (up-left) and RMSDs (up-right) of  $M^{pro}$  enzyme and its complexes with ligand. Docking binding pose (down-left) and Interaction (down-right) inside the binding pocket of  $M^{pro}$  enzyme.



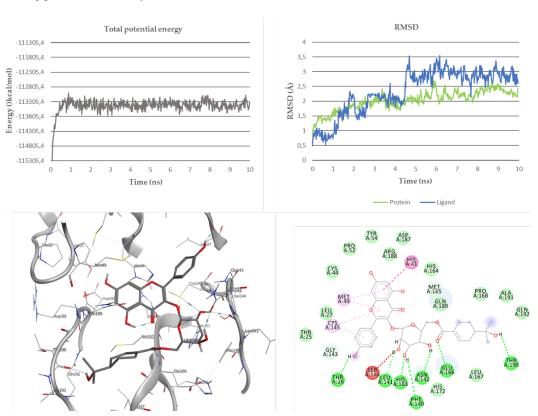
**Figure S11. MNP ID 88095-81-2**. Total energy (up-left) and RMSDs (up-right) of  $M^{pro}$  enzyme and its complexes with ligand. Docking binding pose (down-left) and Interaction (down-right) inside the binding pocket of  $M^{pro}$  enzyme.



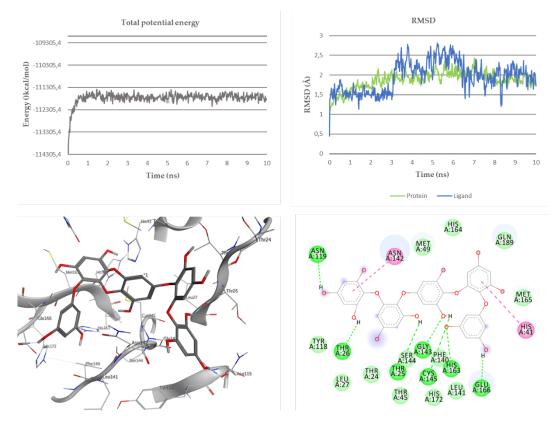
**Figure S12. MNP ID 224577-36-0**. Total energy (up-left) and RMSDs (up-right) of M<sup>pro</sup> enzyme and its complexes with ligand. Docking binding pose (down-left) and Interaction (down-right) inside the binding pocket of M<sup>pro</sup> enzyme.



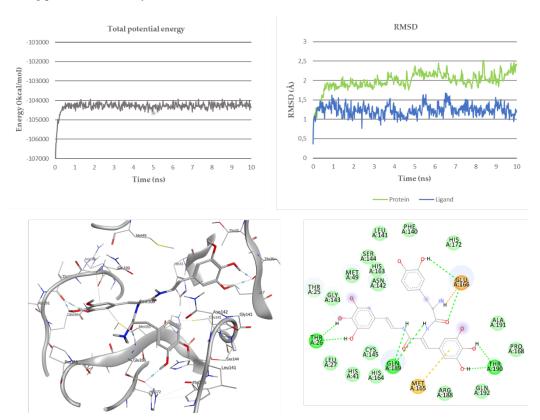
**Figure S13. MNP ID 167228-01-5**. Total energy (up-left) and RMSDs (up-right) of M<sup>pro</sup> enzyme and its complexes with ligand. Docking binding pose (down-left) and Interaction (down-right) inside the binding pocket of M<sup>pro</sup> enzyme.



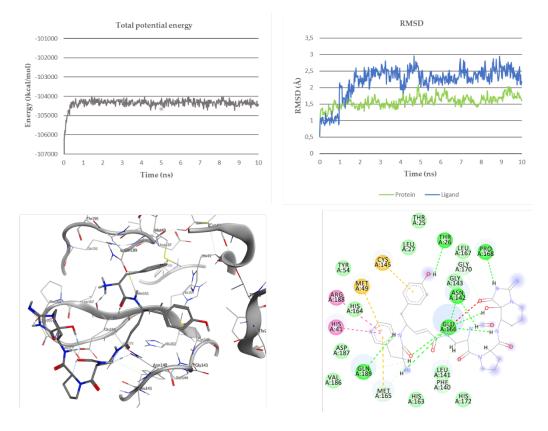
**Figure S14. MNP ID 144027-79-2.** Total energy (up-left) and RMSDs (up-right) of  $M^{pro}$  enzyme and its complexes with ligand. Docking binding pose (down-left) and Interaction (down-right) inside the binding pocket of  $M^{pro}$  enzyme.



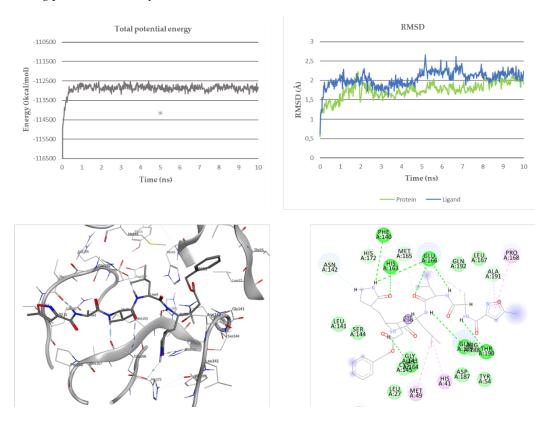
**Figure S15. MNP ID 164176-23-2.** Total energy (up-left) and RMSDs (up-right) of M<sup>pro</sup> enzyme and its complexes with ligand. Docking binding pose (down-left) and Interaction (down-right) inside the binding pocket of M<sup>pro</sup> enzyme.



**Figure S16. MNP ID 115982-31-5**. 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 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.



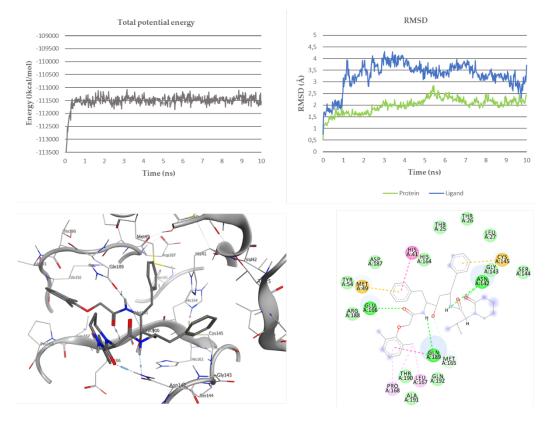
**Figure S18. PRD\_002214**. Total energy (up-left) and RMSDs (up-right) of M<sup>pro</sup> enzyme and its complexes with ligand. Docking binding pose (down-left) and Interaction (down-right) inside the binding pocket of M<sup>pro</sup> enzyme.

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**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	-10.18
	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	
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	-10.00
	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	
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	-9.95
	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	
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	-9.62
	A MET 165 A GLU 166 A LEU 167 A PRO 168 A GLN 189 A THR 190	
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	-9.61
	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	

0.790-75-4   A PHE 140 A LEU 141 A ASS 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A   -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 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 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 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 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 THS 165 A GLU 166 A LEU 167 A PRO 168 A HIS 172 A ARG 188 A GLN 189 THS 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 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 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 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  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  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 163 A MET 165 A GLU 166 A HIS 172 A GLN 189  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 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  151458-0-7-7-7-7-7-7-7-7-7-7-7-7-7-7-7-7-7-7-	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	-9.61
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  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  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 183 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A HIS 172 A ARG 188 A GLN 189  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  58990-46-6  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  147716-81-2  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 LEU 167 A PRO 168 A ARG 188 A GLN 189 A THR 190  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  151379-39-4  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  134458-00-7  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 ARG 188 A GLN 189 A THR 190 A ALA 191 A GLN 192  134458-00-7  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 HIS 172 A GLN 189  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		MET 165 A GLU 166 A LEU 167 A PRO 168 A GLN 189 A THR 190	
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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  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  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  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  -9.00  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  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  -8.94	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	-9.22
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  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  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  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 -9.00 143 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  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 -8.94		MET 165 A GLU 166 A LEU 167 A PRO 168 A ARG 188 A GLN 189 A THR 190 A GLN 192	
166 A HIS 172 A GLN 189  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  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  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 -9.00 143 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  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 -8.94 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A PRO 168 A GLN	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	-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  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  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  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  -8.94  143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A PRO 168 A GLN		141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU	
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  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  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  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  -8.94		166 A HIS 172 A GLN 189	
ASP 187 A ARG 188 A GLN 189 A THR 190 A ALA 191  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  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  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	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	-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  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  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		SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A PRO 168 A HIS 172 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  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  -9.00 143 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  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		ASP 187 A ARG 188 A GLN 189 A THR 190 A ALA 191	
ASP 187 A ARG 188 A GLN 189 A THR 190 A ALA 191  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 -9.00  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  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 -8.94  143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A PRO 168 A GLN	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	-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  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		SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A PRO 168 A HIS 172 A	
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  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		ASP 187 A ARG 188 A GLN 189 A THR 190 A ALA 191	
186 A ASP 187 A ARG 188 A GLN 189 A THR 190 A ALA 191 A GLN 192  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	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	-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		143 A SER 144 A CYS 145 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A VAL	
143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A PRO 168 A GLN		186 A ASP 187 A ARG 188 A GLN 189 A THR 190 A ALA 191 A GLN 192	
	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	-8.94
189 A THR 190 A ALA 191		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	

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	-8.92
	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	
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	-8.91
	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	
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	-8.91
	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	
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	-8.91
	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	
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	-8.87
	PRO 168 A HIS 172 A ARG 188 A GLN 189 A THR 190 A ALA 191 A GLN 192	
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	-8.85
	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	
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	-8.84
	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	
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	-8.84
	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	
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	-8.82
	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	
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	-8.81
	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	
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	-8.81
	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	
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	-8.80
	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	
52645-09-7	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	-8.79
	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	

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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	-8.73
	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	
17991-67-2	A THR 24 A THR 25 A THR 26 A LEU 27 A MET 49 A PHE 140 A LEU 141 A ASN 142 A	-8.72
	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	
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	-8.72
	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	
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	-8.72
	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	
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	-8.71
	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	
445430-65-9	A THR 24 A THR 25 A THR 26 A LEU 27 A HIS 41 A MET 49 A TYR 118 A ASN 119 A PHE	-8.68
	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 GLN	
	192	
935841-71-7	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	-8.66
	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	
136024-80-1	A THR 24 A THR 25 A THR 26 A HIS 41 A MET 49 A PHE 140 A LEU 141 A ASN 142 A GLY	-8.62
	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	
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	-8.61
	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	
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	-8.58
	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	
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	-8.58
	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	
35906-51-5	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	-8.57
	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	

208927-15-5	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	-8.56
	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	
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	-8.56
	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	
194234-73-6	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	-8.56
	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 HIS 172 A VAL 186 A ASP 187 A ARG 188 A GLN 189	
104759-19-5	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	-8.55
	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	
133613-77-1	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	-8.55
	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	
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	-8.54
	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	
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	-8.50
	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	
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	-8.50
	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	
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	-8.47
	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	
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	-8.47
	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	
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	-8.47
	GLU 166 A LEU 167 A PRO 168 A ASP 187 A ARG 188 A GLN 189 A THR 190 A ALA 191	
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	-8.46
	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	
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	-8.45
	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	

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	-8.45
	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	
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	-8.45
	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	
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	-8.44
	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	
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	-8.40
	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	
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	-8.40
	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	
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	-8.40
	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	
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	-8.38
	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	
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	-8.38
	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	
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	-8.38
	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	
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	-8.36
	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	
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	-8.36
	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	
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	-8.34
	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	
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	-8.34
	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	
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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	-8.33
	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	
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	-8.32
	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	
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	-8.30
	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	
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	-8.29
	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	
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	-8.29
	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	
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	-8.29
	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	
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	-8.28
	165 A GLU 166 A VAL 186 A ASP 187 A ARG 188 A GLN 189 A THR 190 A GLN 192	
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	-8.27
	165 A GLU 166 A LEU 167 A PRO 168 A GLN 189 A THR 190 A ALA 191 A GLN 192	
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	-8.24
	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	
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	-8.23
	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	
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	-8.23
	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	
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	-8.23
	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	
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	-8.21
	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	
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	-8.21
	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	

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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	-8.21
	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	
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	-8.21
	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	
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	-8.20
	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	
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	-8.19
	CYS 145 A HIS 164 A MET 165 A GLU 166 A GLN 189	
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	-8.17
	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	
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	-8.15
	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	
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	-8.15
	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	
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	-8.15
	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	
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	-8.15
	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	
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	-8.14
	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	
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	-8.14
	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	
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	-8.10
	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	
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	-8.09
	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	

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	-8.06
	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	
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	-8.06
	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	
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	-8.05
	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	
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	-8.05
	145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A PRO 168 A GLN 189	
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	-8.04
	MET 165 A GLU 166 A LEU 167 A PRO 168 A GLN 189 A THR 190	
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	-8.04
	MET 165 A GLU 166 A LEU 167 A PRO 168 A GLN 189 A THR 190	
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	-8.04
	GLU 166 A LEU 167 A PRO 168 A ARG 188 A GLN 189	
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	-8.04
	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	
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	-8.04
	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	
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	-8.04
	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	
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	-8.02
	A TYR 118 A ASN 142 A GLY 143 A CYS 145 A MET 165 A GLU 166 A GLN 189	
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	-8.02
	143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A GLN 189	
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	-8.02
	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	
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	-8.01
	143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A GLN 189	
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	-8.01
	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	
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	-8.01
	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	

140774 22 2	A THE 41 A MEET 40 A LEH 50 A PURE 440 A LETT 441 A JOSEPH CONTROL OF THE CONTROL	0.00
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	-8.00
	CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A HIS 172 A	
440415	GLN 189 A THR 190 A ALA 191 A GLN 192	
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	-7.99
	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	
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	-7.99
	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	
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	-7.98
	MET 165 A GLU 166 A PRO 168 A HIS 172 A GLN 189 A THR 190 A ALA 191 A GLN 192	
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	-7.98
	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	
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	-7.97
	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	
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	-7.96
	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	
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	-7.92
	141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A GLU 166 A GLN 189	
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	-7.90
	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	
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	-7.90
	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	
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	-7.90
	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	
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	-7.89
	143 A CYS 145 A HIS 164 A MET 165 A GLU 166 A ASP 187 A ARG 188 A GLN 189	
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	-7.89
	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	
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	-7.88
	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	
858950-36-4  79206-71-6  724462-47-9  2122-98-7    79067-75-7  603125-81-1  134985-04-9  94513-77-6  92679-03-3  65604-87-7	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  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  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  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  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  A THR 24 A THR 25 A THR 26 A LEU 27 A HIS 41 A MET 49 A LEU 141 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  A THR 25 A THR 26 A LEU 27 A HIS 41 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  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  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  A THR 24 A THR 25 A THR 26 A LEU 27 A HIS 41 A MET 49 A TYR 54 A SN 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 HIS 172 A ASP 187 A ARG 188 A GLN 189 A THR 190 A ALA 191  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  A THR 24 A THR 25 A THR 26 A LEU 167 A PRO 168	-7.98 -7.98 -7.97 -7.96 -7.90 -7.90 -7.89 -7.89

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	-7.87
	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	
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	-7.87
	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	
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	-7.86
	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	
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	-7.86
	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	
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	-7.85
	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	
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	-7.84
	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	
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	-7.84
	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	
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	-7.84
	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	
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	-7.83
	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	
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	-7.83
	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	
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	-7.83
	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	
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	-7.83
	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	
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	-7.83
303123-00-0	145 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A ARG 188 A GLN 189 A THR	7.00
	190 A ALA 191 A GLN 192	

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  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 GLN 192  137571-30-3 A THR 24 A THR 25 A THR 26 A LEU 167 A PRO 168 A HIS 172 A ARG 188 A GLN 189 A THR 190 A GLN 192  137671-30-3 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  79005-82-6 A THR 24 A THR 25 A THR 26 A LEU 27 A HIS 41 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A HIS 172 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 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  64108-8-5-6 A THR 24 A THR 25 A THR 26 A LEU 27 A HIS 41 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  64108-8-5-6 A THR 24 A THR 25 A THR 26 A LEU 27 A HIS 41 A CYS 145 A GLU 166 A ASP 187 A ARG 188 A GLN 180  123154-33-6 A THR 25 A LEU 27 A HIS 41 A MET 49 A PHB 140 A LEU 141 A ASN 142 A GLY 143 A ARG 188 A GLN 180  123154-33-6 A THR 25 A LEU 27 A HIS 41 A MET 49 A PHB 140 A LEU 141 A ASN 142 A GLY 143 A ARG 188 A GLN 180  123154-33-6 A THR 26 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  136019-24-7 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  137809-87-1 A HIS 24 A THR 25 A THR 26 A HIS 172 A ARG 188 A GLN 189 A THR 190 A ALA 191 A GLN 192  137809-87-1 A THR 24 A THR 25 A THR 26 A HIS 172 A ARG 188 A GLN 189 A THR 190 A ALA 191 A GLN 191 A GLU 166 A HIS 172 A A H			
188 A GLN 189 A THR 190 A GLN 192  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  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 -7.82  188 A GLN 189 A THR 190  79005-82-6  A THR 24 A THR 25 A THR 26 A LEU 27 A HIS 41 A SER 146 A MET 165 A GLU 166 A ARG 188 A GLN 189 A THR 190  A PHE 140 A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 163 A HIS 164 A MET 165 A GLU 166 A HIS 172 A GLN 189  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  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  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 165 A GLU 166 A LEU 167 A PRO 168 A HIS 172 A ARG 188 A GLN 189 A THR 190 A GLU 170 A ASP 187 A ARG 188 A GLN 189 A THR 190 A GLU 167 A PRO 168 A HIS 163 A HIS 164 A CYS 145 A HIS 163 A HIS 164 A CYS 145 A HIS 163 A HIS 164 A CYS 145 A HIS 163 A HIS 164 A CYS 145 A HIS 163 A HIS 164 A CYS 145 A HIS 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  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 ALA 191 A GLN 192  128733-01-0  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  128733-01-0  A MET 165 A GLU 166 A HIS 172  A RES 144 A CYS 145 A HIS 163 A HIS 164 A HIS 163 A HIS 164 A MET 165 A GLU 166 A HIS 172  128733-01-0  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 HIS 172  128733-01-	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	-7.83
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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  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 -7.82  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  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 -7.81  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  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 -7.79  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  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 -7.78  A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A -7.78  MET 165 A GLU 166 A HIS 172  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 -7.78  MET 165 A GLU 166 A HIS 172  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 -7.78  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  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 -7.77  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 GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A HIS 172 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 GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A HIS 172 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 GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A HIS 172 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 161 A HIS 172 A GLY 143 A		GLN 192	
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  -7.82  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  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  GLN 192  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  GLN 192  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  -7.78  A LEU 141 A ASN 142 A GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A  -7.78  MET 165 A GLU 166 A HIS 172  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  -7.78  MET 165 A GLU 166 A HIS 172  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  -7.78  MET 165 A GLU 166 A HIS 172  A THR 25 A HIS 41 A MET 49 A THR 54 A GLN 189 A THR 190 A ALA 191 A GLN 192  80764-19-8  A THR 25 A HIS 163 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  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  -7.77  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  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  -7.77  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  133056-09-4  A THR 24 A THR 25 A THR 26 A LEU 27 A HIS 41 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A HIS 172 A GLN 189	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	-7.82
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GLY 170 A ASP 187 A ARG 188 A GLN 189 A THR 190 A ALA 191 A GLN 192  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  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  —7.79  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  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  —7.78  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  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  —7.78  MET 165 A GLU 166 A HIS 172 A ARG 188 A GLN 189 A THR 190 A ALA 191 A GLN 192  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  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  —7.77  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 GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A  GLU 166 A HIS 172 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 GLY 143 A SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A  GLU 166 A HIS 172 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  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  —7.77	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	-7.82
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GLN 192  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  —7.78  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  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  —7.78  MET 165 A GLU 166 A HIS 172 A ARG 188 A GLN 189 A THR 190 A ALA 191 A GLN 192  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  —7.78  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  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  —7.77  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  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  —7.77	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	-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		MET 165 A GLU 166 A PRO 168 A HIS 172 A ARG 188 A GLN 189 A THR 190 A ALA 191 A	
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  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  —7.78  MET 165 A GLU 166 A HIS 172 A ARG 188 A GLN 189 A THR 190 A ALA 191 A GLN 192  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  —7.78  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  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  —7.77  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  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  —7.77		GLN 192	
GLU 166 A HIS 172  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 -7.78  MET 165 A GLU 166 A HIS 172 A ARG 188 A GLN 189 A THR 190 A ALA 191 A GLN 192  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 -7.78  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  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 -7.77  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  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 -7.77	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	-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 -7.78  MET 165 A GLU 166 A HIS 172 A ARG 188 A GLN 189 A THR 190 A ALA 191 A GLN 192  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 -7.78  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  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 -7.77  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  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 -7.77		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	
MET 165 A GLU 166 A HIS 172 A ARG 188 A GLN 189 A THR 190 A ALA 191 A GLN 192  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  -7.78  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  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  -7.77 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  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  -7.77		GLU 166 A HIS 172	
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 -7.78  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  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 -7.77  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  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 -7.77	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	-7.78
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  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 -7.77  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  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 -7.77		MET 165 A GLU 166 A HIS 172 A ARG 188 A GLN 189 A THR 190 A ALA 191 A GLN 192	
HIS 172 A ASP 187 A ARG 188 A GLN 189 A THR 190 A ALA 191 A GLN 192  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 -7.77  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  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 -7.77	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	-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 -7.77  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  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 -7.77		SER 144 A CYS 145 A HIS 163 A HIS 164 A MET 165 A GLU 166 A LEU 167 A PRO 168 A	
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  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 -7.77		HIS 172 A ASP 187 A ARG 188 A GLN 189 A THR 190 A ALA 191 A GLN 192	
GLU 166 A HIS 172 A GLN 189  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 -7.77	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	-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 -7.77		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	
142 A GLY 143 A CYS 145 A MET 165 A GLU 166 A LEU 167 A PRO 168 A GLN 189	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	-7.77
		142 A GLY 143 A CYS 145 A MET 165 A GLU 166 A LEU 167 A PRO 168 A GLN 189	

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	-7.76
	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	
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	-7.76
	GLU 166 A PRO 168 A ARG 188 A GLN 189 A THR 190 A ALA 191 A GLN 192	
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	-7.76
	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	
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	-7.75
	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	
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	-7.75
	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	
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	-7.75
	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	
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	-7.74
	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	
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	-7.74
	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	