Supplementary Material

Synthesis of some oxazolo[4,5-d]pyrimidine derivatives and evaluation of their antiviral activity and cytotoxicity

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### Table S1. ADMET properties of oxazolo[4,5-d]pyrimidine derivatives predicted by pkCSM online server

| Compd | Water solubility | Caco2 Permeability | Skin Permeability | P-glycoprotein inhibitor | Intrinsic P-glycoprotein inhibitor | Caco2 permeability | Vmax (human) | Fraction unbound (human) | CNS permeability | CYP2B6 substrate | CYP3A4 substrate | CYP2C9 inhibitor | CYP2D6 inhibitor | CYP3A inhibitor | Total Clearance | Renal OAT2 substrates | AKR1B10 toxicity | Max. co-administered dose (human) | hERG inhibitor | hME44 inhibitor | Oral Rat Acute Toxicity (LD50) | Oral Rat Chronic Toxicity (LOAEL) | Hepatotoxicity | Skin Sensitization | Minnow toxicity | 7-Pyridonyl toxicity | Microsome toxicity |
|-------|-----------------|-------------------|------------------|-------------------------|---------------------------------|-----------------|-------------|------------------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|
| 1     | -3.793          | 0.991             | -2.735           | Yes                     | Yes                             | Yes             | 0.135       | 0.245                  | -1.586         | No             | No             | No             | No             | No             | 0.404         | No             | Yes            | 0.693          | No             | No             | 3.098         | 0.793          | Yes            | No             | 0.285         | -1.45         |
| 2     | -3.382          | 1.299             | -2.735           | Yes                     | Yes                             | Yes             | 0.237       | 0.329                  | -1.819         | No             | Yes            | Yes            | Yes            | No             | 0.759         | No             | No             | 0.675          | No             | Yes            | 2.739         | 0.068          | Yes            | No             | 0.285         | -1.626        |
| 3     | -4.085          | 1                 | -2.735           | Yes                     | Yes                             | Yes             | 0.642       | 0.154                  | -1.762         | No             | Yes            | No             | No             | Yes            | 0.718         | No             | Yes            | 0.711          | No             | Yes            | 3.401         | 0.034          | Yes            | No             | 0.285         | -2.737        |
| 4     | -4.08           | 0.976             | -2.735           | Yes                     | Yes                             | Yes             | 0.666       | 0.13                   | -1.928         | No             | Yes            | No             | No             | Yes            | 0.88          | No             | No             | 0.715          | No             | Yes            | 3.371         | 0.191          | Yes            | No             | 0.285         | -1.61         |
| 5     | -3.814          | 0.807             | -2.727           | Yes                     | Yes                             | Yes             | 0.432       | 0.205                  | -2.131         | No             | Yes            | Yes            | Yes            | No             | 0.611         | No             | No             | 0.468          | No             | Yes            | 2.59          | 1.125          | Yes            | No             | 0.289         | 0.22          |
| 6     | -3.629          | 1.121             | -2.731           | No                      | Yes                             | Yes             | 0.447       | 0.232                  | -1.99          | No             | Yes            | Yes            | Yes            | No             | 0.668         | No             | No             | 0.484          | No             | Yes            | 2.683         | 1.179          | Yes            | No             | 0.288         | 0.711         |
| 7     | -3.939          | 1.295             | -2.734           | Yes                     | Yes                             | Yes             | 0.733       | 0.229                  | -1.783         | No             | Yes            | Yes            | Yes            | Yes            | 0.699         | No             | Yes            | 0.445          | No             | Yes            | 2.765         | 1.153          | Yes            | No             | 0.286         | -0.501        |
| 8     | -3.777          | 1.135             | -2.735           | Yes                     | Yes                             | Yes             | 1.097       | 0.248                  | -1.932         | No             | Yes            | No             | No             | Yes            | 0.594         | No             | No             | 0.66           | No             | Yes            | 2.914         | 1.048          | Yes            | No             | 0.285         | -0.436        |
| 9     | -3.846          | 1.202             | -2.735           | Yes                     | Yes                             | Yes             | 1.182       | 0.25                   | -1.845         | No             | Yes            | No             | No             | Yes            | 0.518         | No             | No             | 0.662          | No             | Yes            | 2.868         | 1.084          | Yes            | No             | 0.285         | -0.298        |
| 10    | -3.293          | 0.995             | -2.734           | No                      | Yes                             | Yes             | 0.415       | 0.169                  | -2.389         | No             | Yes            | Yes            | Yes            | No             | 1.02          | No             | No             | 0.458          | No             | Yes            | 2.54          | 0.825          | Yes            | No             | 0.286         | -2.013        |
| 11    | -3.21           | 1.192             | -2.735           | No                      | Yes                             | Yes             | 0.167       | 0.261                  | -2.083         | No             | Yes            | No             | Yes            | Yes            | 1.096         | No             | No             | 0.785          | No             | Yes            | 2.855         | 0.886          | Yes            | No             | 0.285         | -6.516        |
| 12    | -3.252          | 1.111             | -2.735           | No                      | Yes                             | Yes             | 0.209       | 0.267                  | -2.01          | No             | Yes            | No             | Yes            | No             | 1.101         | No             | No             | 0.786          | No             | Yes            | 2.897         | 0.942          | Yes            | No             | 0.285         | -6.497        |
| 13    | -3.632          | 1.095             | -2.735           | No                      | Yes                             | Yes             | -0.042      | 0.258                  | -2.584         | No             | Yes            | No             | No             | No             | 1.016         | No             | No             | 0.778          | No             | Yes            | 2.999         | 0.508          | Yes            | No             | 0.285         | -3.759        |
| 14    | -3.239          | 1.191             | -2.735           | No                      | Yes                             | Yes             | 0.193       | 0.262                  | -1.991         | No             | Yes            | Yes            | Yes            | No             | 1.104         | No             | No             | 0.787          | No             | Yes            | 2.86          | 0.907          | Yes            | No             | 0.285         | -6.633        |
| 15    | -3.261          | 1.11              | -2.735           | No                      | Yes                             | Yes             | 0.236       | 0.268                  | -1.919         | No             | Yes            | No             | Yes            | No             | 1.108         | No             | No             | 0.789          | No             | Yes            | 2.903         | 0.963          | Yes            | No             | 0.285         | -6.615        |