Supplementary Data

Mechanistic modeling as an explanatory tool for clinical treatment of chronic catatonia
Roberts and Conour (2022) Frontiers Pharmacology

Data Selection Filter: After synthetic data was generated, the following sequence of filters were implemented to remove subjects that did not conform to clinical practice or observations.
Remove subjects if pre-treatment includes clozapine.
Remove subjects if pre-treatment includes lamotrigine.
Remove subjects if pre-treatment has olanzapine is greater than 20mg/d.
Remove subjects with pre-treatment includes both clozapine and olanzapine.
Remove subjects if post-treatment of Lamotrigine is less than 400mg of greater than 500mg.
Remove subjects if pre-treatment does not include antipsychotics.
Remove subjects if post-treatment does not include antipsychotics.
Remove subjects if post-treatment includes methylphenidate.
Remove subjects if pre-treatment BFCRS score is less than or equal to post-treatment score.
Remove subjects if their BFCRS score changes less than 9 (for consistency with clinical dataset).
Remove subjects if the number of post-treatment medications is less than 3.
Remove subjects if post-treatment includes both clonazepam and lorazepam.
Remove subjects if pre-treatment has more than 1 mood stabilizer.
Balanced the number of subjects with clozapine post-treatment to 80%.

Pharmacokinetic Parameters: Partial list of the most prominent medications in the study.

| param             | Clozapine | Olanzapine | Lamotrigine | Clonazepam | Lorazepam |
|-------------------|-----------|------------|-------------|------------|-----------|
| bioavailability   | 0.65      | 0.87       | 0.950       | 0.9        | 0.85      |
| clearance (L/hr)  | 31.00     | 21.80      | 2.100       | 2.1        | 4.30      |
| blood/brain ratio | 1.00      | 1.00       | 1.900       | 1.0        | 1.53      |
| mole wt (g/mol)   | 326.82    | 312.43     | 256.091     | 315.7      | 321.20    |

Receptor Affinities: Partial list of the most prominent medications in the study from (Roth and Lopez 2006).

| receptors      | Dopamine | 5-HT | Clozapine | Olanzapine | Lamotrigine | Clonazepam | Lorazepam |
|----------------|----------|------|-----------|------------|-------------|------------|-----------|
| D1             | 130.0    | 9690.0 | 89.0      | 25.00      | 10000       | 10000      | 10000     |
| D2             | 469.43   | 10000 | 28.0      | 3.00       | 10000       | 10000      | 10000     |
| 5-HT1A         | 8248.0   | 2.789 | 104.8     | 610.00     | 10000       | 10000      | 10000     |
| 5-HT2A         | 10000    | 20.80 | 1.0       | 1.48       | 10000       | 10000      | 10000     |
| M1             | 10000    | 10000 | 1.4       | 2.00       | 10000       | 10000      | 10000     |

Roth, B., and Lopez, E. (2006). Psychoactive drug screening program Ki database.
Available at: https://pdsp.unc.edu/databases/kidb.php.