

Model-based inference and classification of immunological control mechanisms from TKI cessation and dose reduction in CML patients

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Supplementary tables

| Patient ID | $Y(0)$ | p_{yx} (months ⁻¹) | p_{xy} (months ⁻¹) | TKI (months ⁻¹) | p_z (cells/months) | K_z (cells) | cessation time (months) | clinical trial or local registry |
|------------|---------|----------------------------------|----------------------------------|-----------------------------|----------------------|---------------|-------------------------|----------------------------------|
| Patient 1 | 742834 | 0.01 | 0.05 | 13.90 | 2210.00 | 362.00 | 85.90 | Bordeaux |
| Patient 2 | 109001 | 0.00 | 0.05 | 1.95 | 1940.00 | 508.00 | 85.70 | STIM2 (Bordeaux) |
| Patient 3 | 33678 | 0.88 | 0.18 | 6.48 | 0.00 | 4.29 | 72.90 | STIM2 (Bordeaux) |
| Patient 4 | 217698 | 0.00 | 0.00 | 2.31 | 53800.00 | 9570.00 | 95.20 | STIM2 (Bordeaux) |
| Patient 5 | 312895 | 0.00 | 0.01 | 2.38 | 176.00 | 28.70 | 60.30 | STIM2 (Bordeaux) |
| Patient 6 | 2740 | 0.70 | 0.21 | 2.07 | 311000.00 | 6480.00 | 53.00 | EUROSKI (Bordeaux) |
| Patient 7 | 11949 | 0.00 | 0.00 | 1.86 | 0.01 | 26.30 | 108.00 | EUROSKI (Bordeaux) |
| Patient 8 | 61731 | 0.00 | 0.00 | 1.86 | 696.00 | 74.70 | 84.70 | EUROSKI (Bordeaux) |
| Patient 9 | 739824 | 0.00 | 0.07 | 2.56 | 325.00 | 85.70 | 60.70 | EUROSKI (Bordeaux) |
| Patient 10 | 559804 | 0.00 | 0.04 | 2.77 | 473.00 | 115.00 | 70.50 | EUROSKI (Bordeaux) |
| Patient 11 | 878259 | 0.00 | 0.00 | 2.57 | 2820.00 | 318.00 | 50.10 | STIM (Bordeaux) |
| Patient 12 | 863636 | 0.04 | 0.00 | 4.30 | 19800.00 | 462.00 | 141.00 | Mannheim |
| Patient 13 | 975440 | 0.11 | 0.00 | 3.23 | 132000.00 | 2120.00 | 145.00 | Mannheim |
| Patient 14 | 1045239 | 0.01 | 0.00 | 2.13 | 54000.00 | 1430.00 | 165.00 | Mannheim |
| Patient 15 | 599823 | 0.59 | 0.06 | 3.62 | 82600.00 | 1300.00 | 131.00 | Mannheim |
| Patient 16 | 546945 | 0.59 | 0.00 | 17.70 | 57600.00 | 1550.00 | 60.70 | Munich |
| Patient 17 | 996734 | 0.00 | 0.05 | 2.36 | 26800.00 | 5700.00 | 95.60 | Munich |
| Patient 18 | 1630508 | 0.00 | 0.05 | 3.32 | 0.00 | 6.84 | 81.30 | Munich |
| Patient 19 | 637927 | 0.00 | 0.00 | 1.86 | 14.70 | 1740.00 | 92.60 | Munich |
| Patient 20 | 628117 | 0.01 | 0.04 | 2.38 | 4420.00 | 419.00 | 99.00 | Munich |
| Patient 21 | 309978 | 0.02 | 0.04 | 7.01 | 2530.00 | 212.00 | 69.30 | EUROSKI (Poitiers) |

Table S1: Individual parameter estimations and clinical trial/local registry of each patient

Initial condition $Y(0)$ and individual parameter estimations for the 21 patients obtained by using the immune model and fitting strategy III. The following fixed parameter values are used for all patients: $K_Y=1e+06$, $m=1e-04$, $r_z=200$, $p_y=1.658$, $a=2$. Given a constant cell number Y , the initial conditions for X and Z are initialized in a quasi-steady state condition. We also report the corresponding clinical trial or local registry from which we obtained the clinical data of each patient.

| Patient ID | treatment duration (clinical data, months) | predicted minimal treatment time to achieve TFR (months and percentage of clinical treatment duration) |
|-------------------|---|---|
| Patient 6 | 53.0 | 0.8 (1.5 %) |
| Patient 12 | 140.8 | 56.5 (40.1 %) |
| Patient 13 | 144.7 | 9.1 (6.3 %) |
| Patient 14 | 164.6 | 10.4 (6.3 %) |
| Patient 15 | 130.6 | 33.2 (25.4 %) |
| Patient 16 | 60.7 | 5.7 (9.4 %) |
| Patient 20 | 99.0 | 38.2 (38.6 %) |
| Patient 21 | 69.3 | 9.9 (14.3 %) |

Table S2 estimated minimal required treatment time of patients with a strong immune response (class B)

Comparison of the treatment duration applied in the clinical trials with the predicted minimal treatment time required to achieve TFR in our simulations using the immune model and fitting strategy III. This concept applies only to class B patients (i.e. with a strong immune response).