

b)

Exhaustive search

Exhaustive search

Figure S3 An exhaustive search was performed to find an initial estimate of the solubility (C_s) . The cost function (sum of squares) was evaluated firstly using a) a broad search space $(10^2 \le C_s \le 10^5 \text{ nM})$, which was followed by b) a confined search space in the proximity to the best solution, obtained from the first exhaustive search.