Supplementary Material

ChemMaps: Towards an Approach for Visualizing the Chemical Space Based on Adaptative Satellite Compounds

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Contents

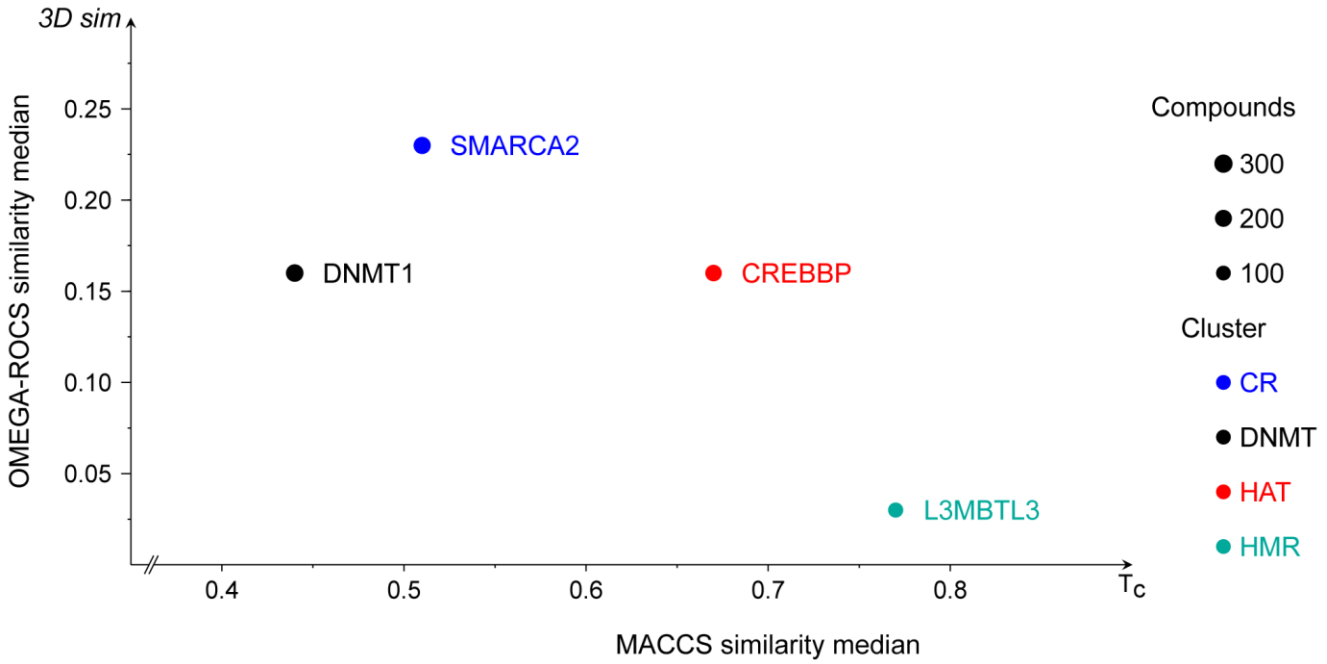

Figure S1. 3D-Consensus Diversity Plot depicting the diversity of the datasets used for the backwards approach. The higher the median similarity either 2D or 3D, the lower diversity of the dataset. The size of the points is proportional to the size of the dataset. The color shows the function of the target. CR: chromatin remodeller; DNMT: DNA-methyltransferase; HAT: histone acetyltransferase; HMR: histone methylation reader.

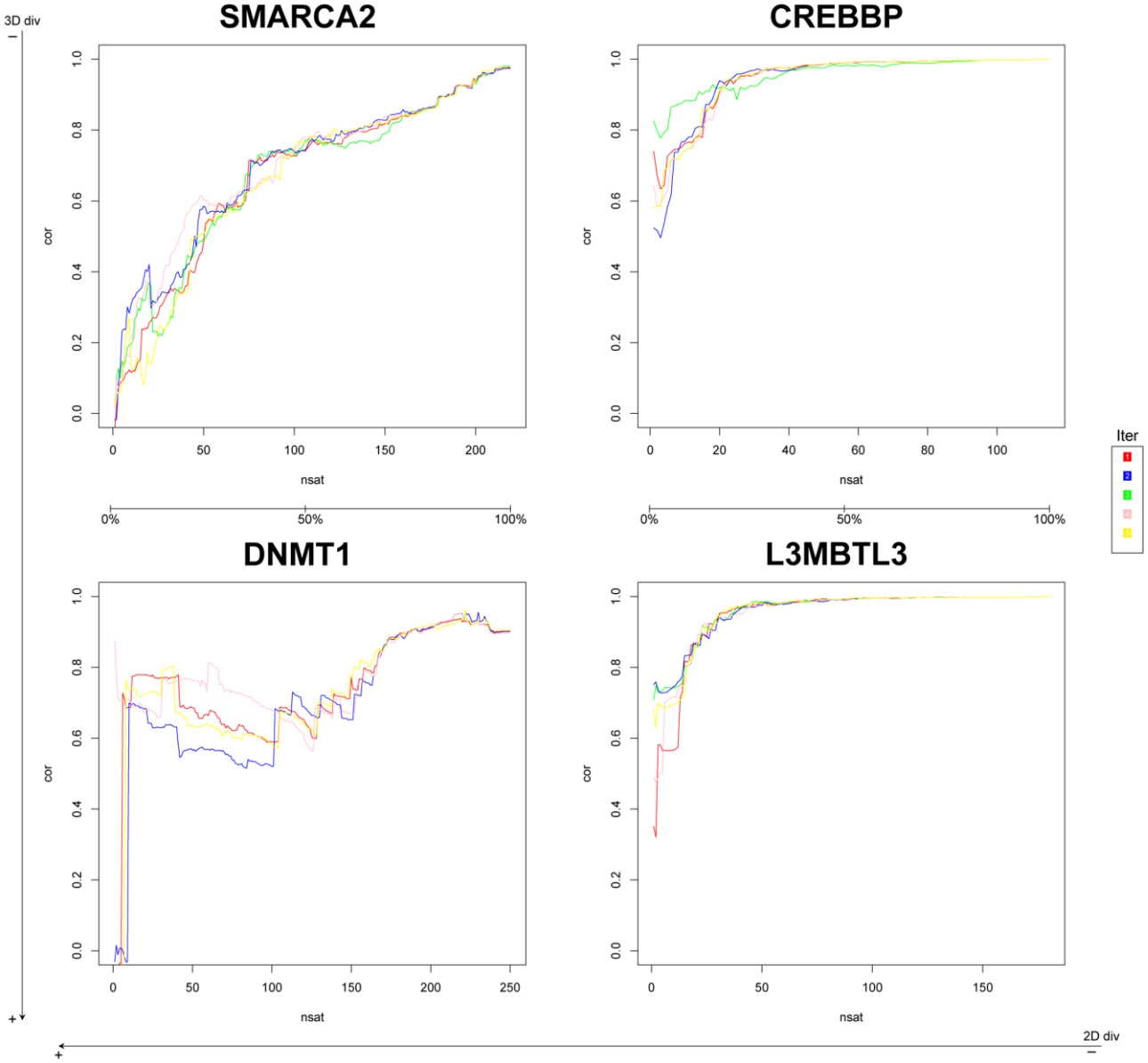

Figure S2. Backwards analysis with 3PCs picking satellites by diversity. The correlation with the results from the whole matrix was calculated with increasing numbers of satellites. Each colored line represents one of the five random sets.

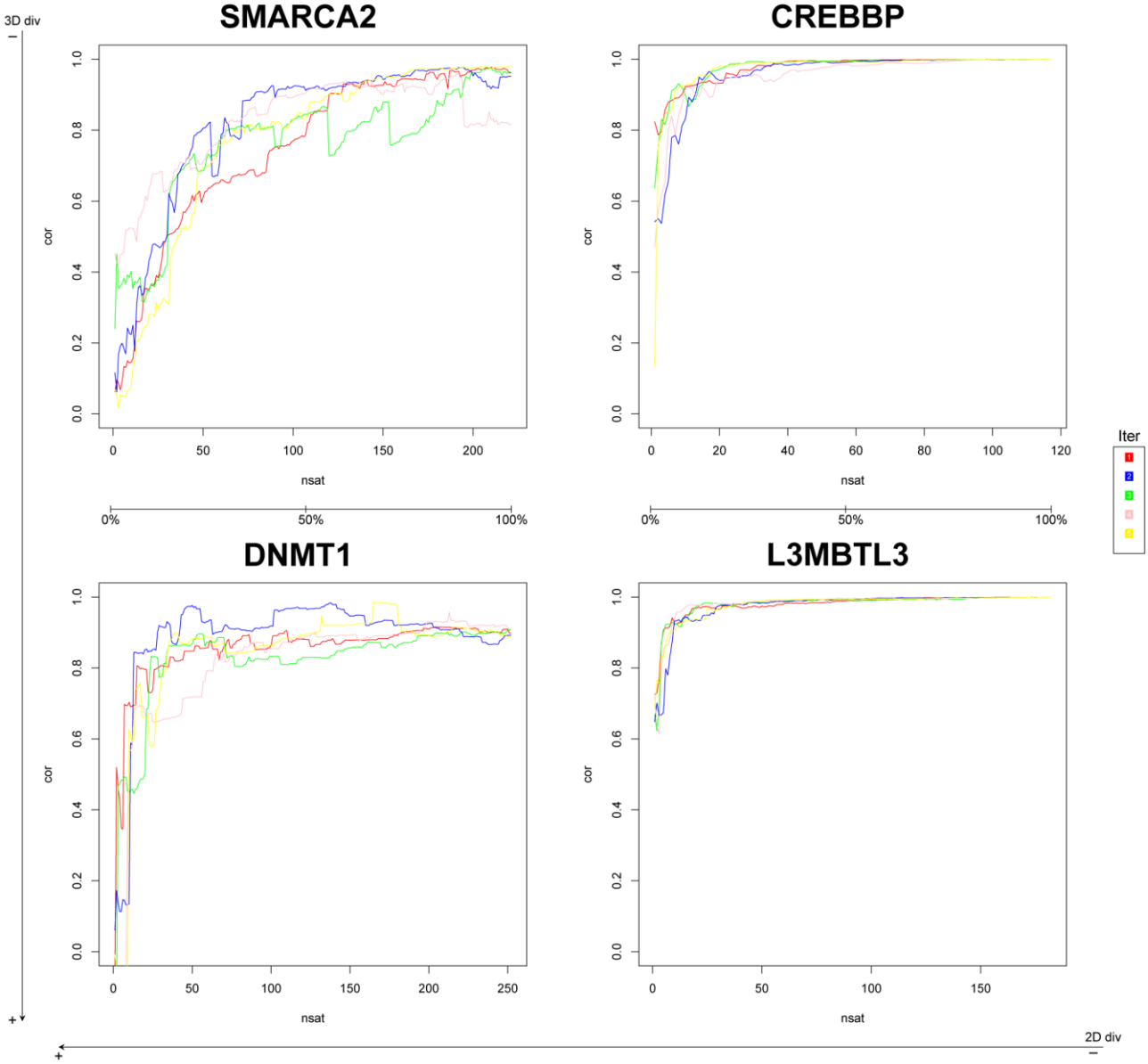

Figure S3. Backwards analysis with 3PCs picking satellites at random. The correlation with the results from the whole matrix was calculated with increasing numbers of satellites. Each colored line represents one of the five random sets.

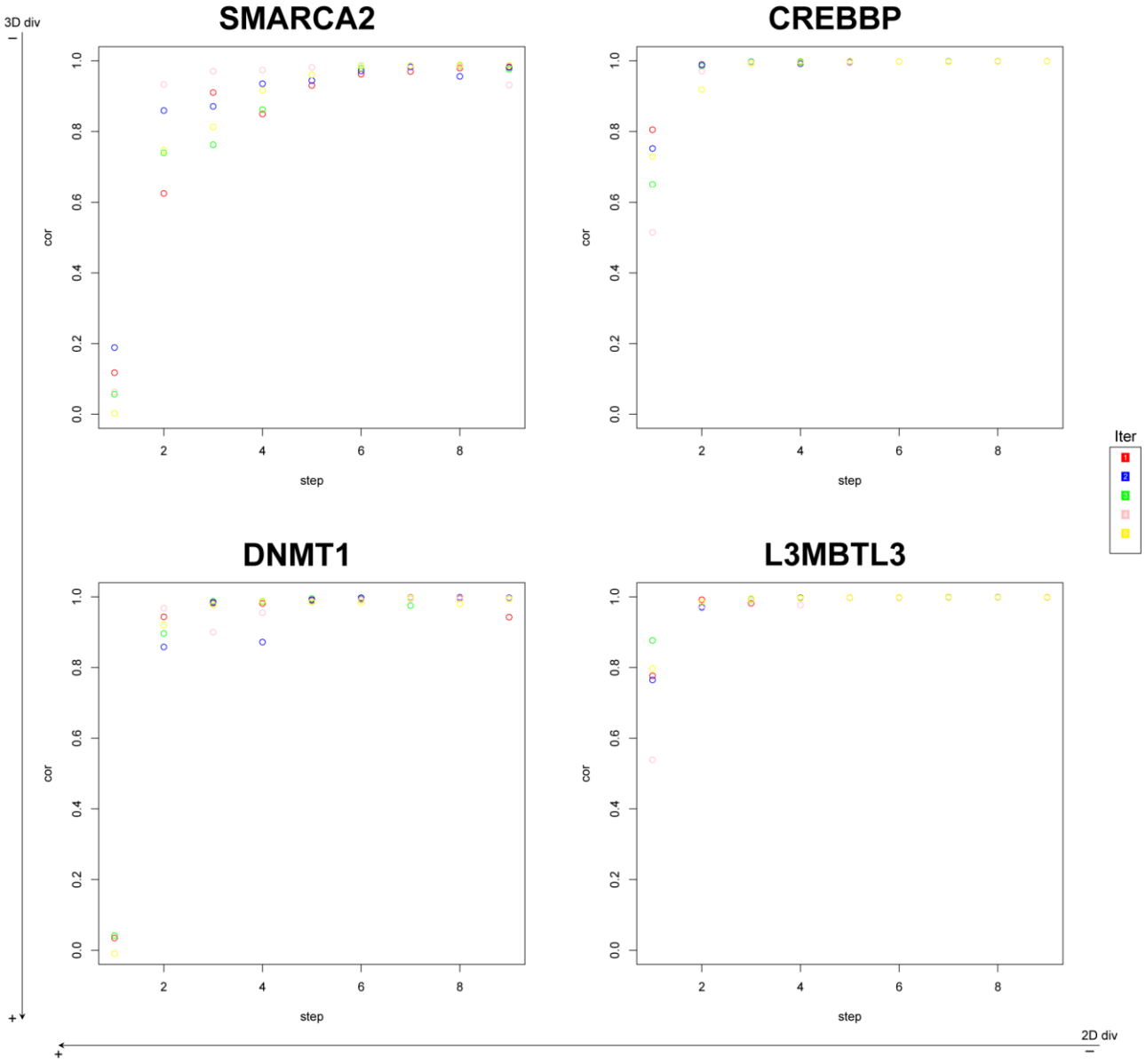

Figure S4. Forward analysis with 2PCs picking satellites at random with step sizes of 10%.