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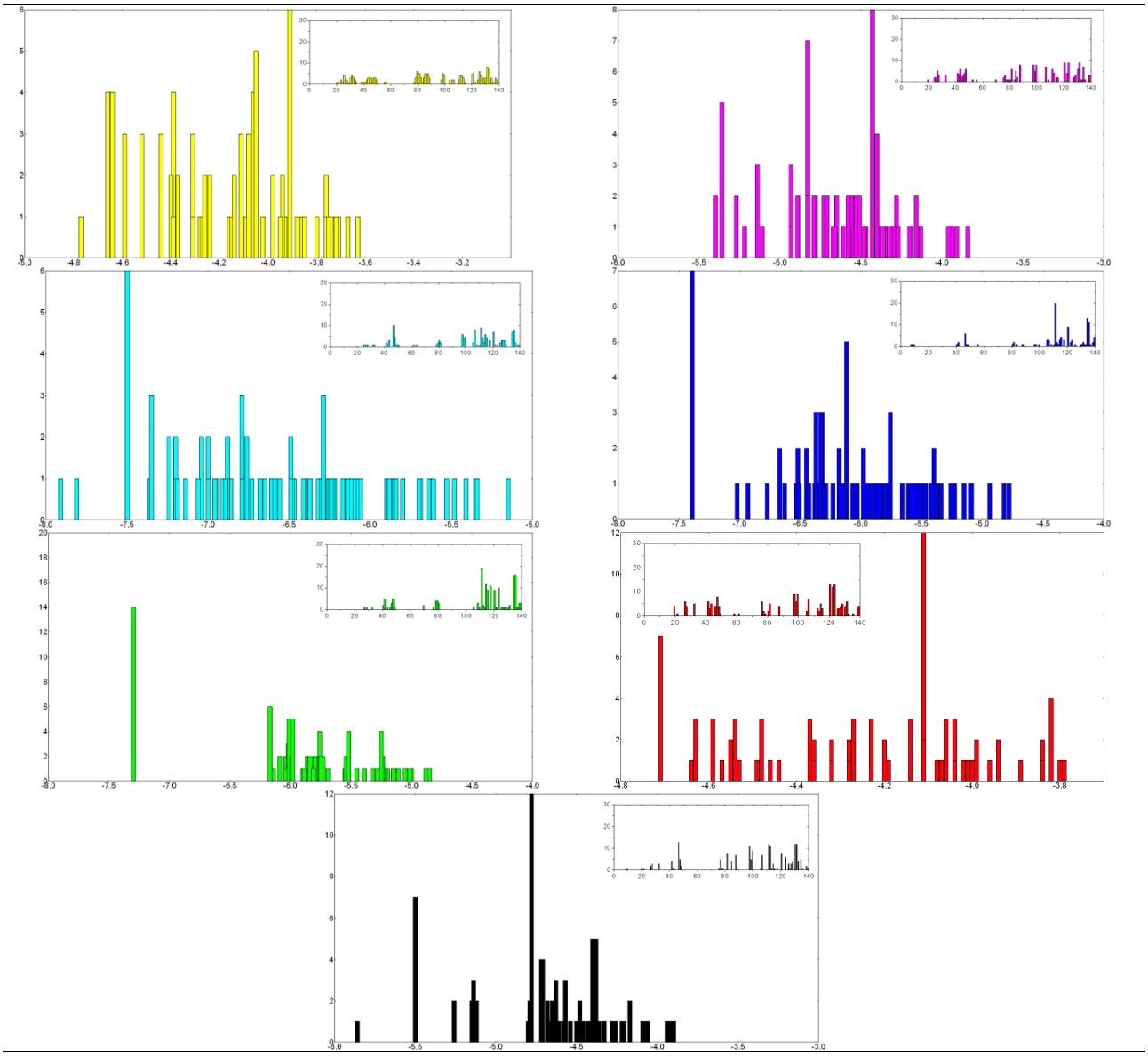

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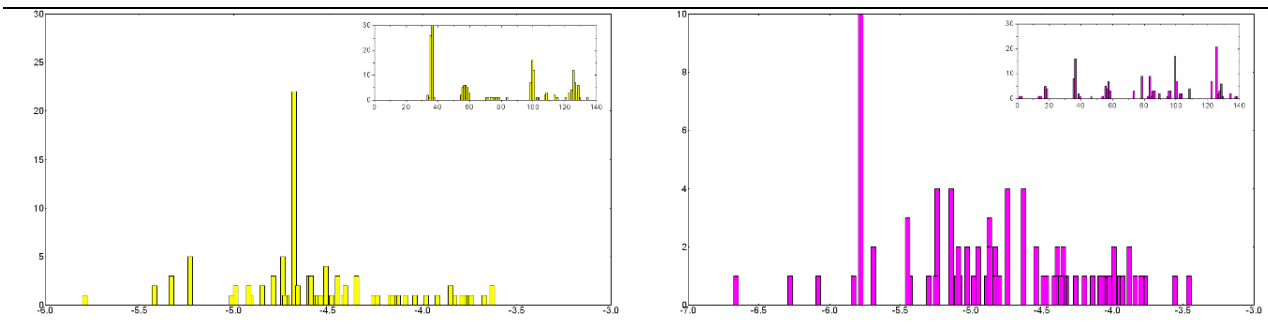

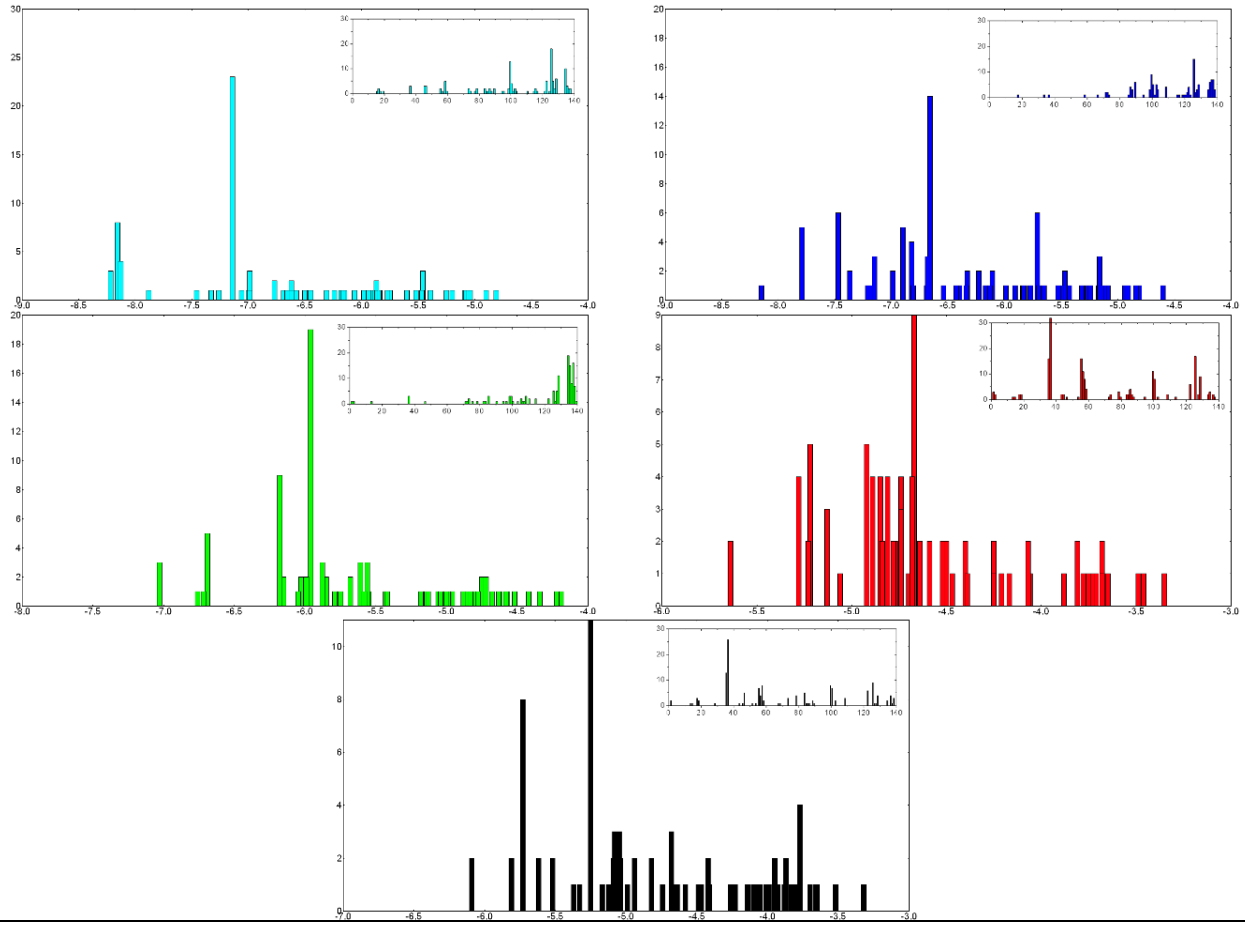

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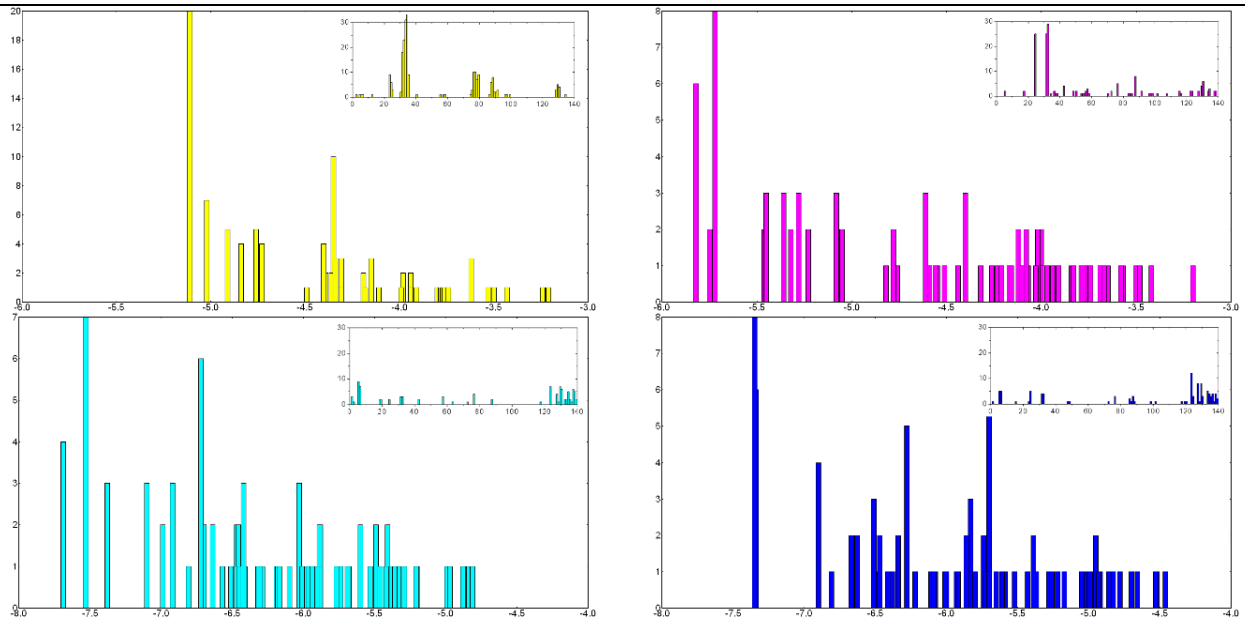

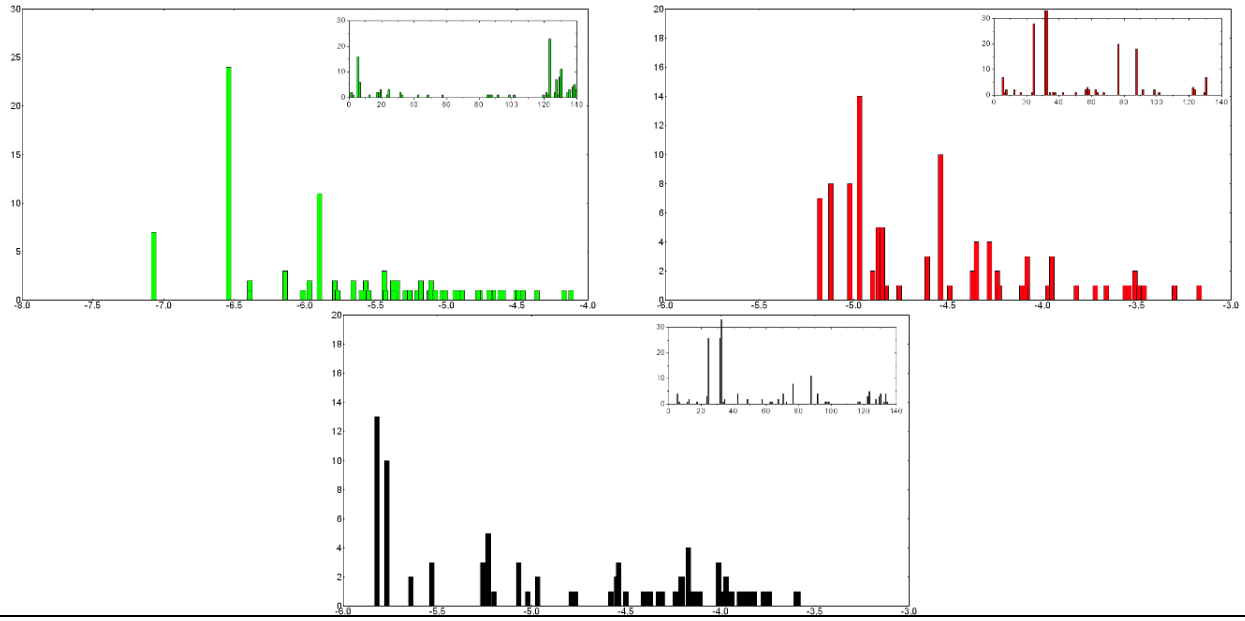

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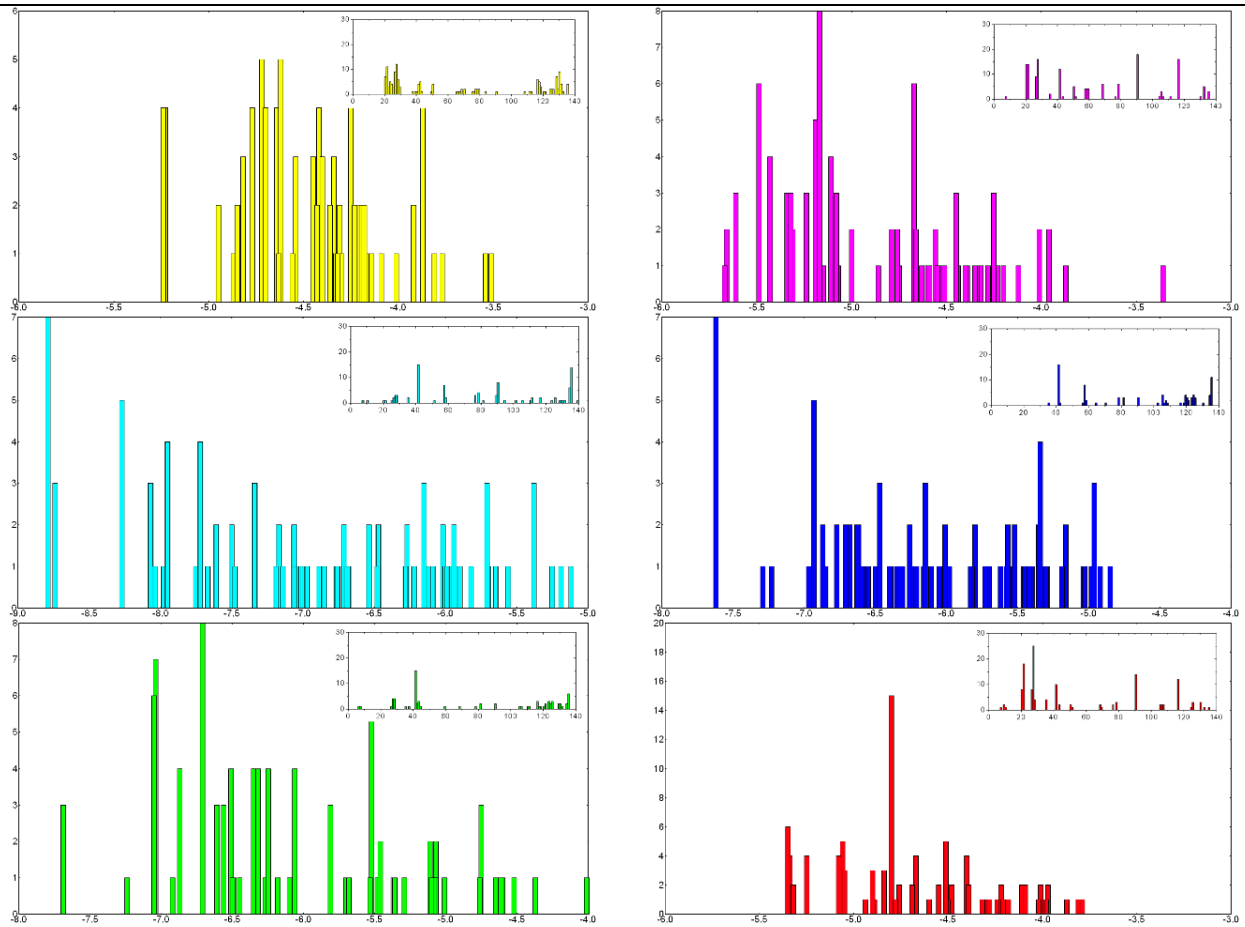

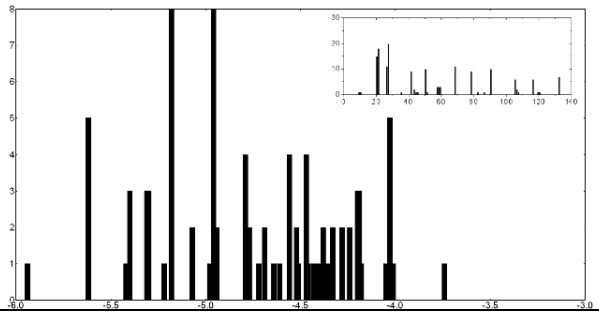

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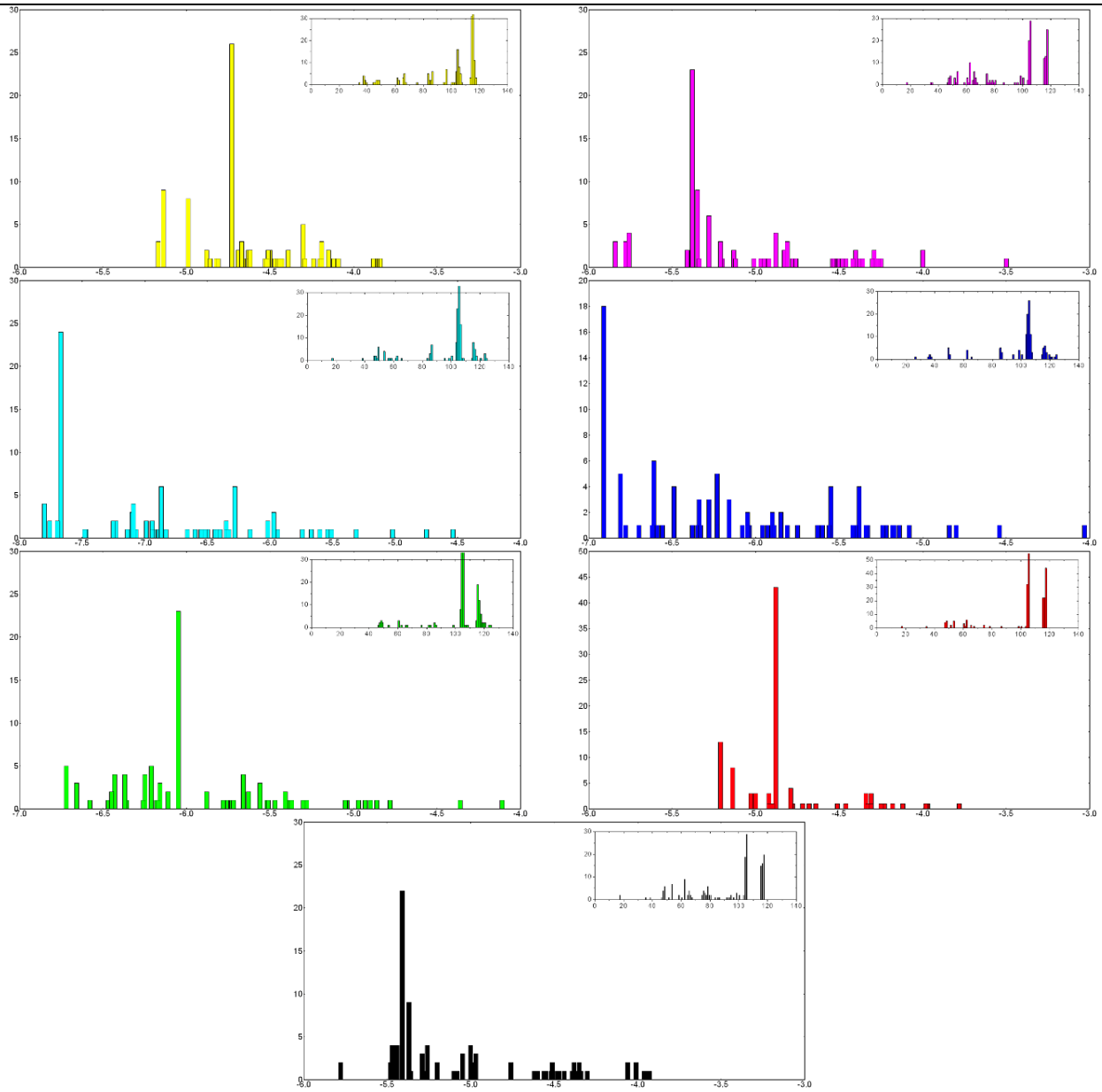

Cluster 6

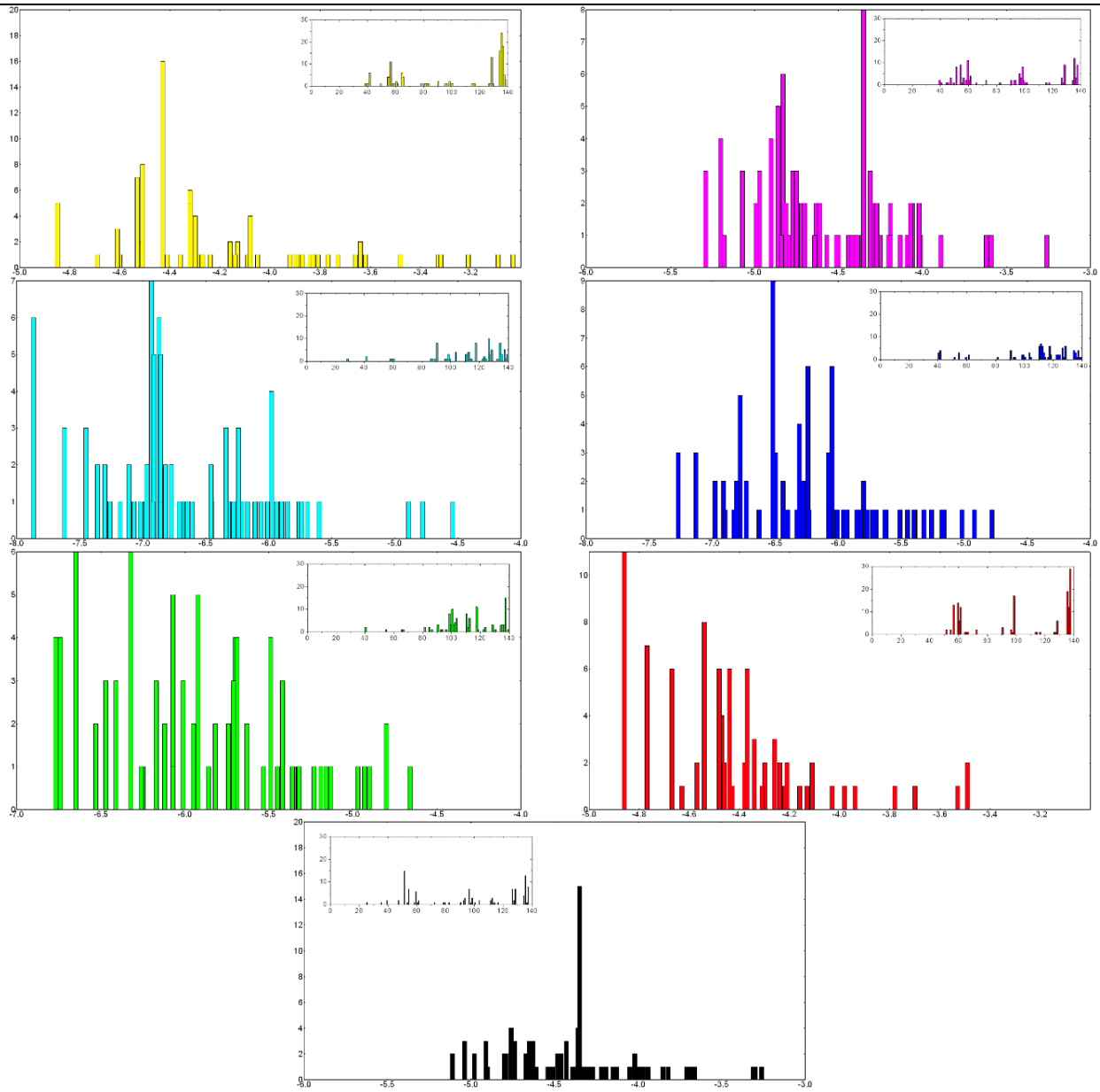

Figure S2. **Molecular docking**: Results for the 100 runs for each of the 6 AS representatives conformations with DCH (yellow), DHI (pink), DOP (light blue), DOP-H (blue), DQ (green), IQ (red) and LEUK (black) (54 complexes). Clustering of the doking results, as implemented in AUTODOCK, plotted as a function of the AUTODOCK scoring function (in Kcal/mol). Inset: The number of hits (defined in Tab. 2SI) between AS and the respective ligand.