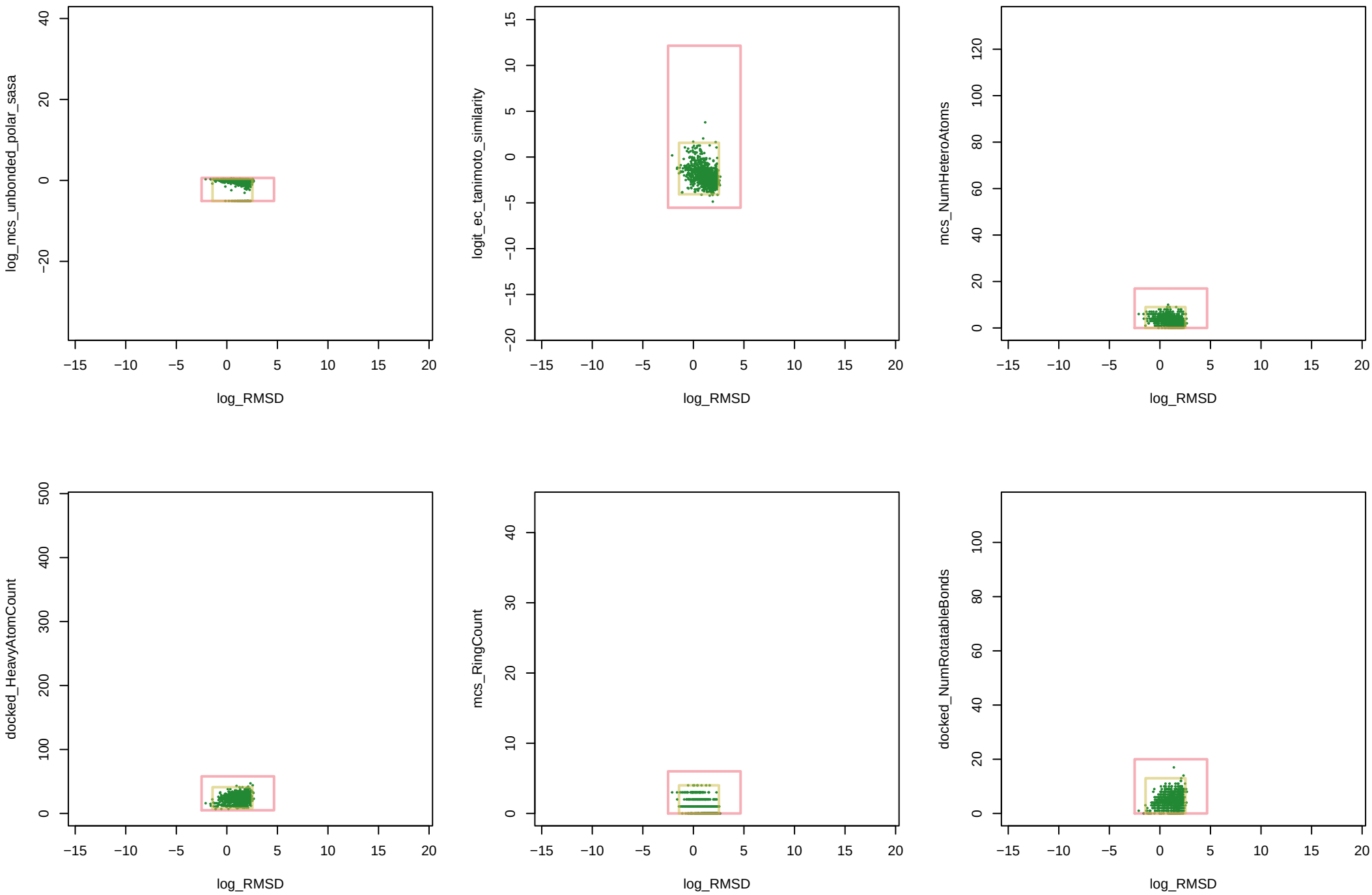
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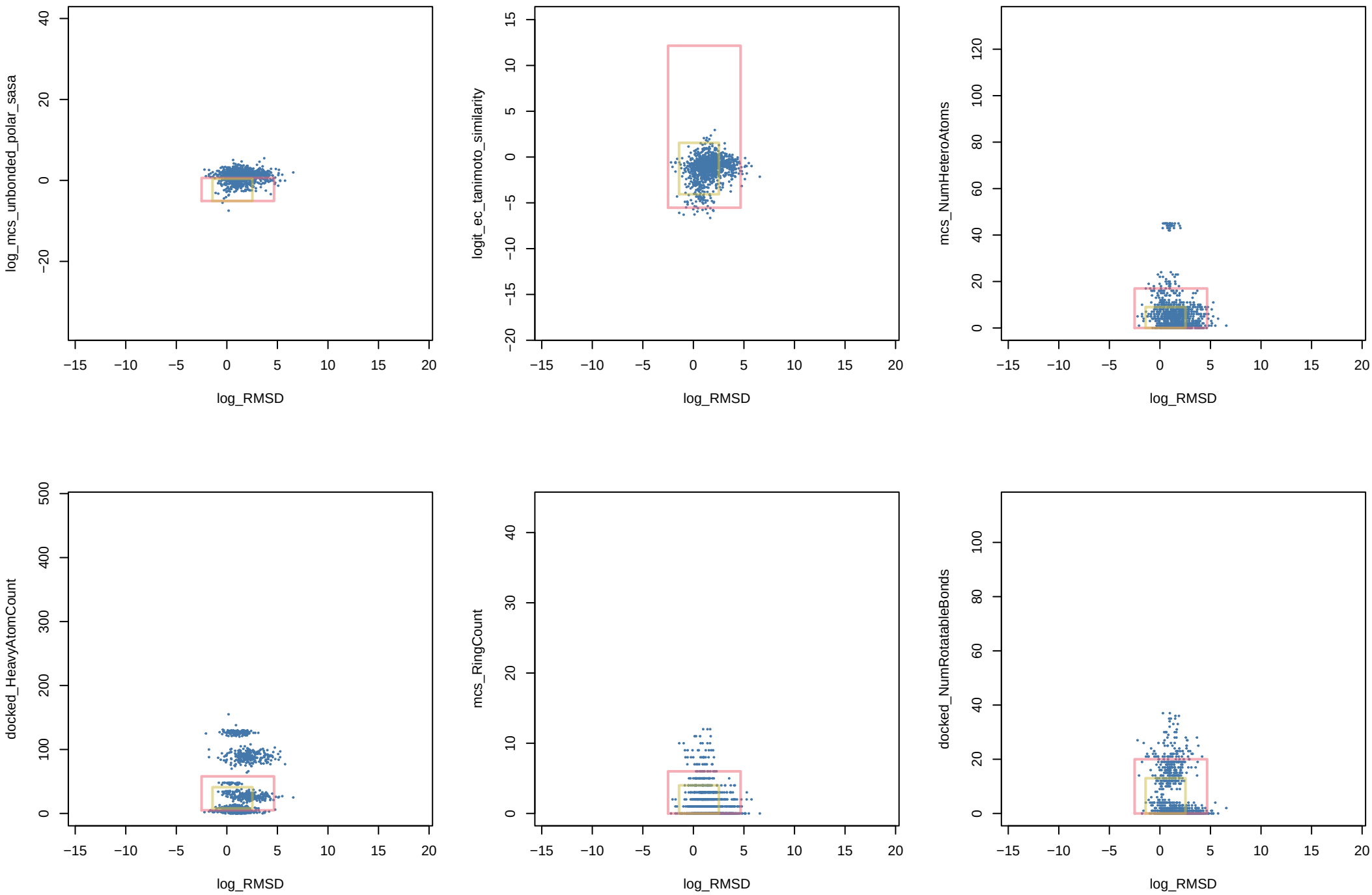
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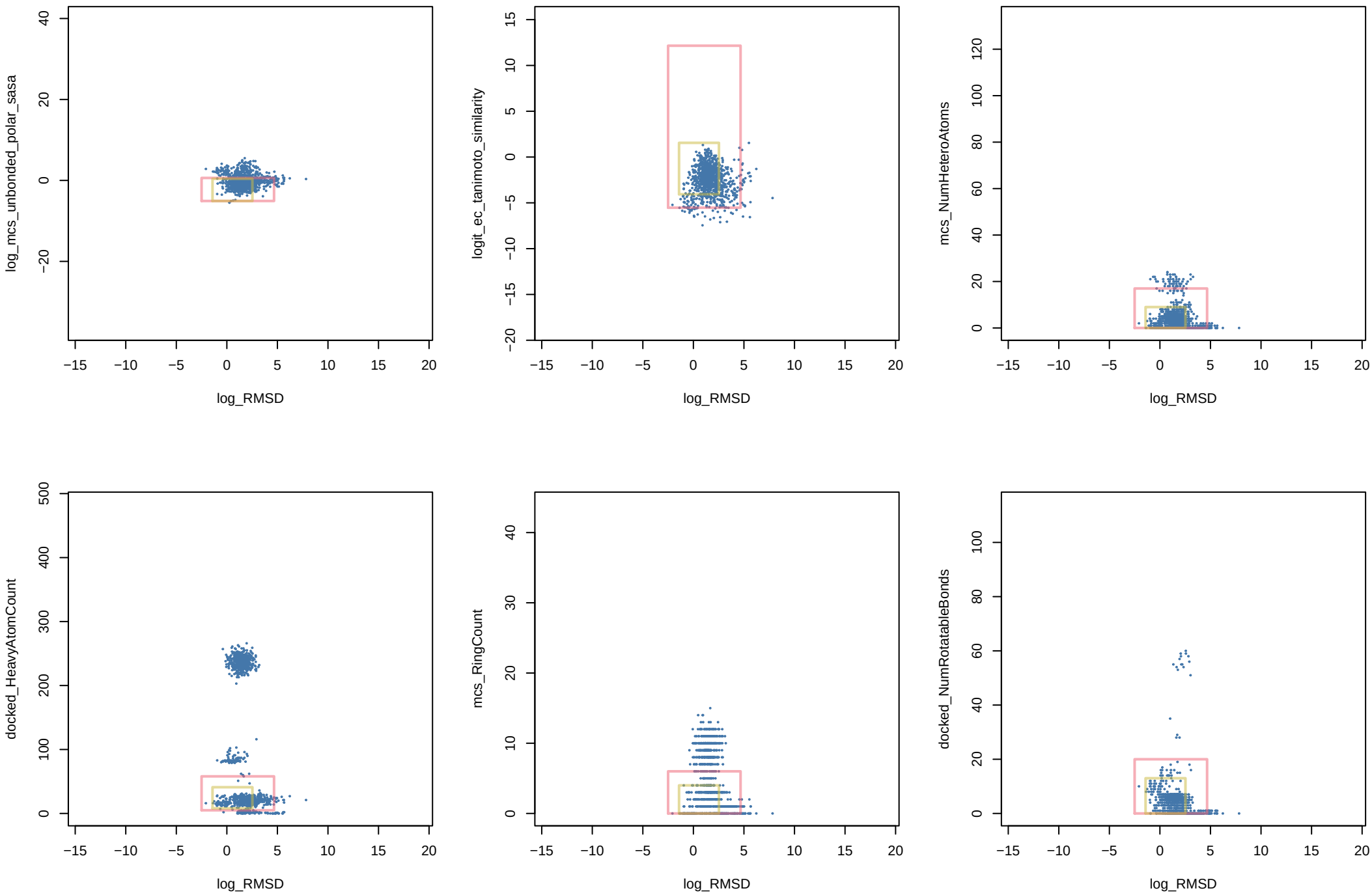
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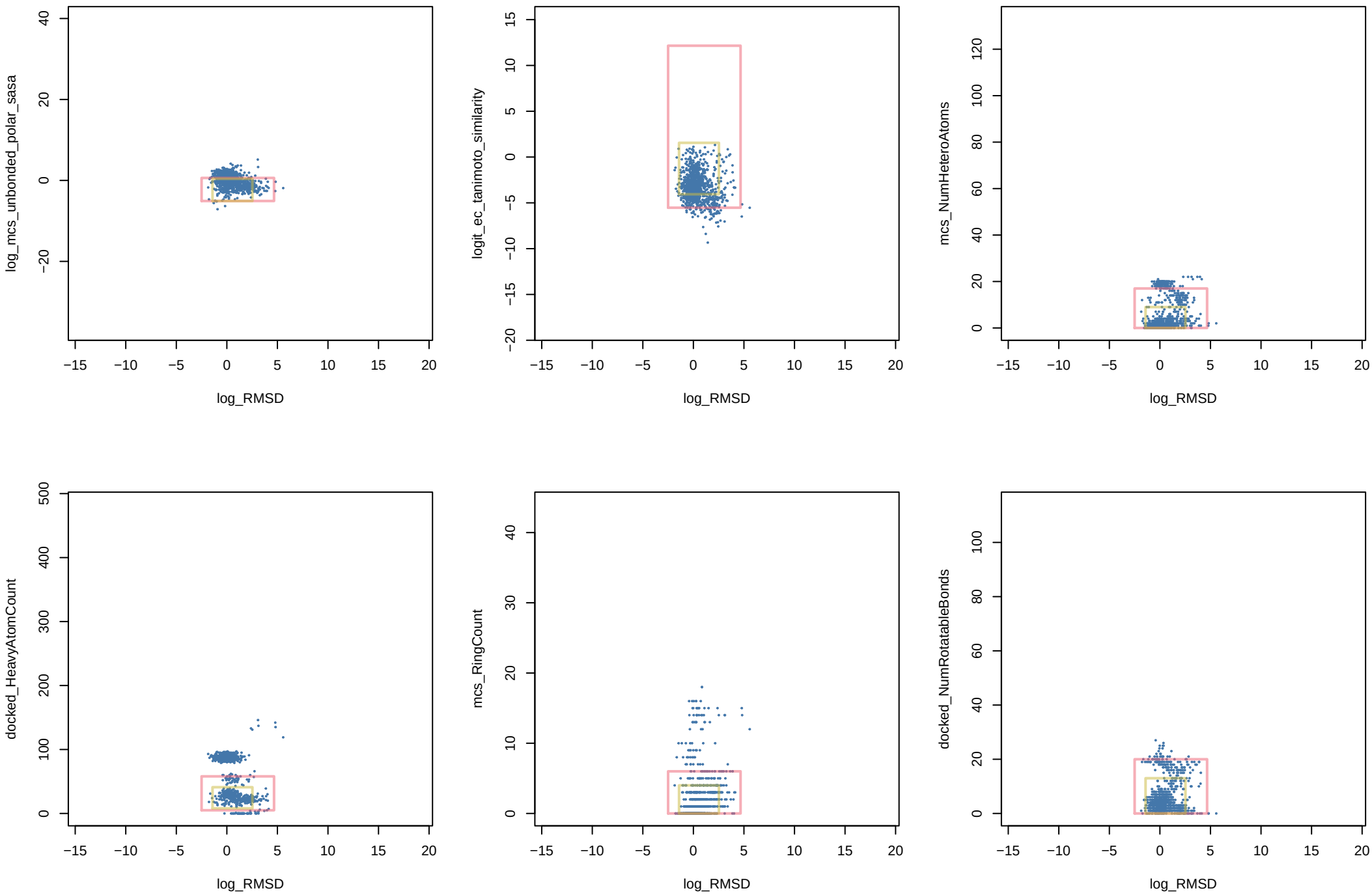
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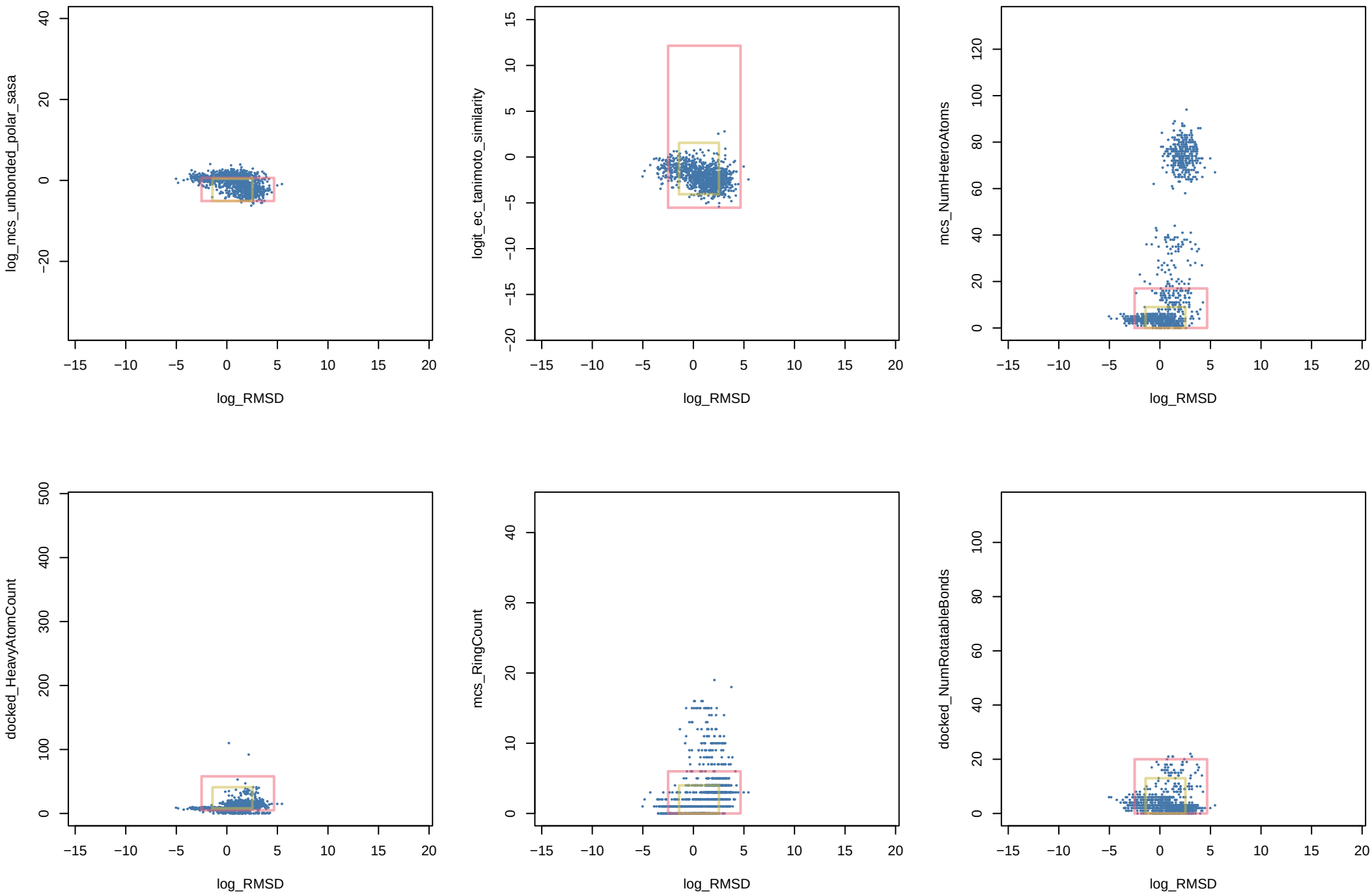
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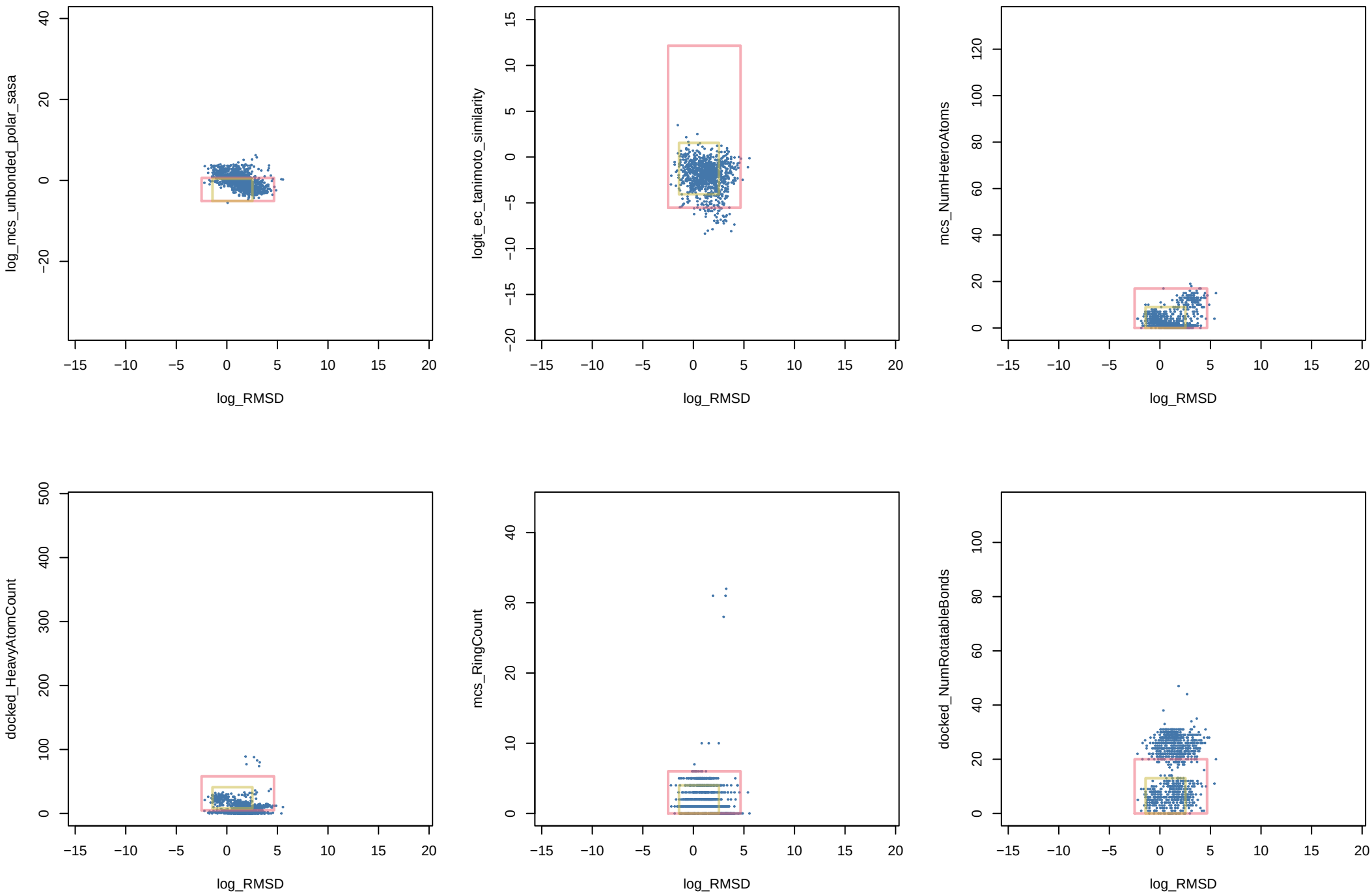
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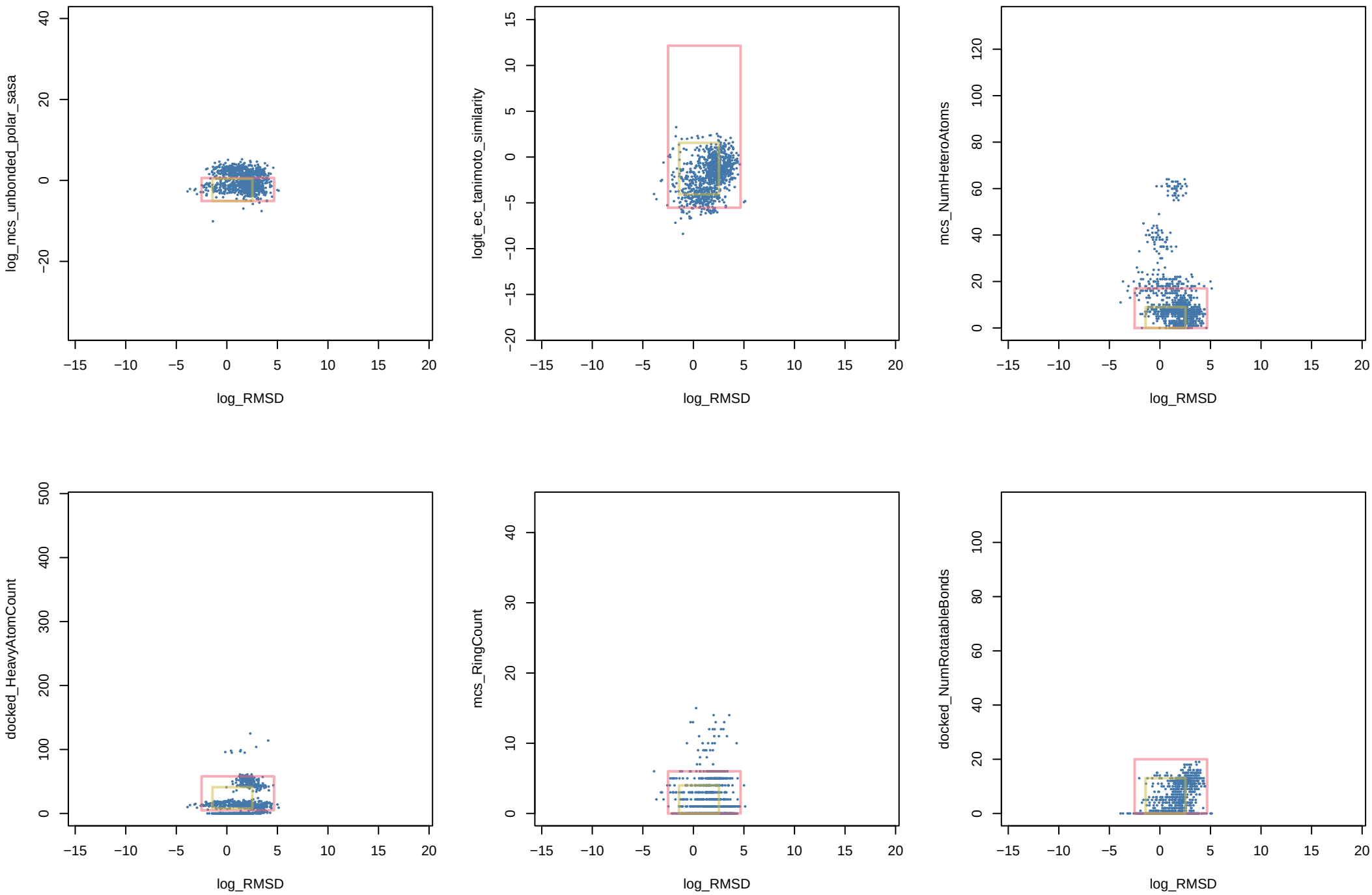
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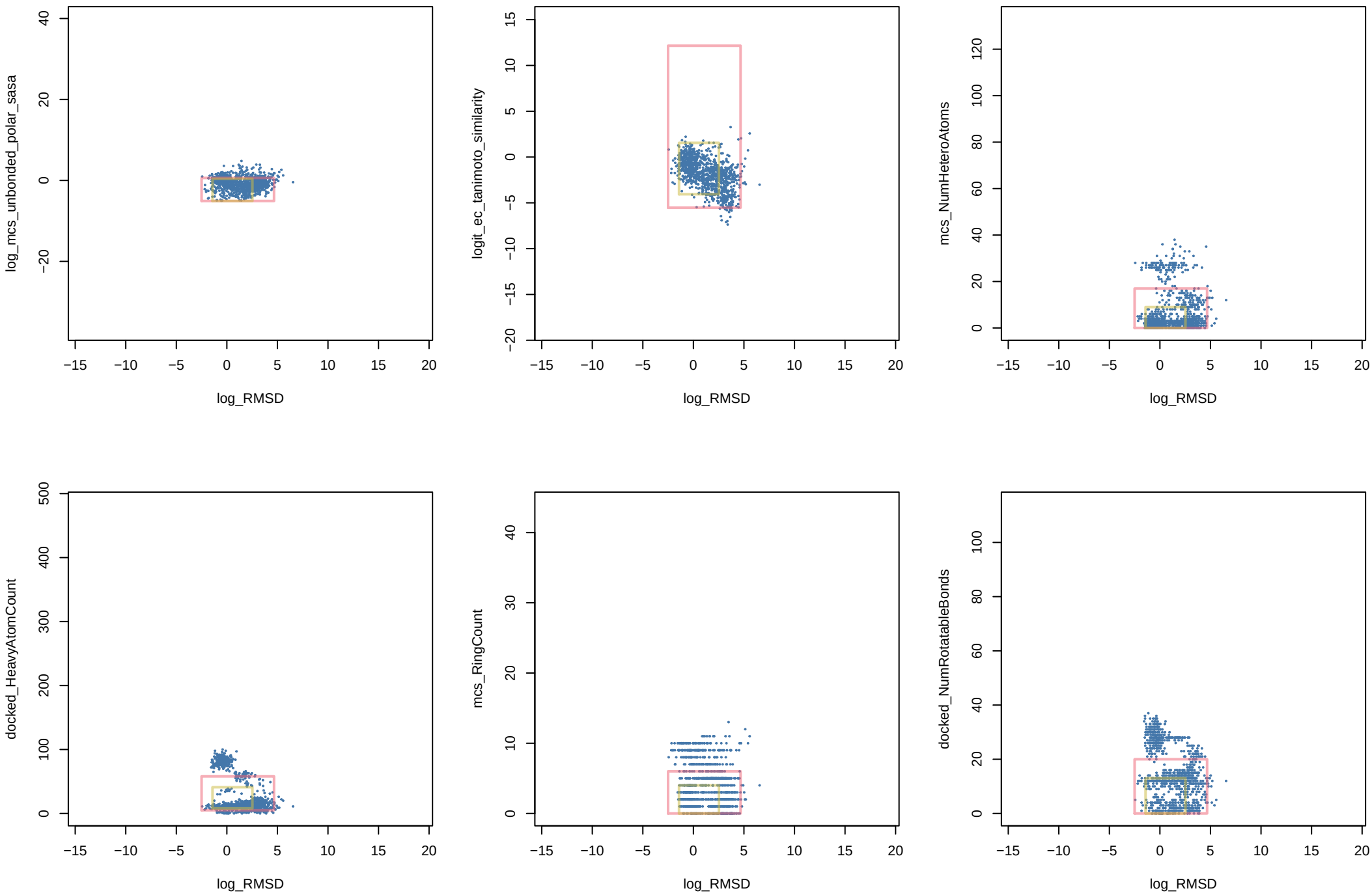
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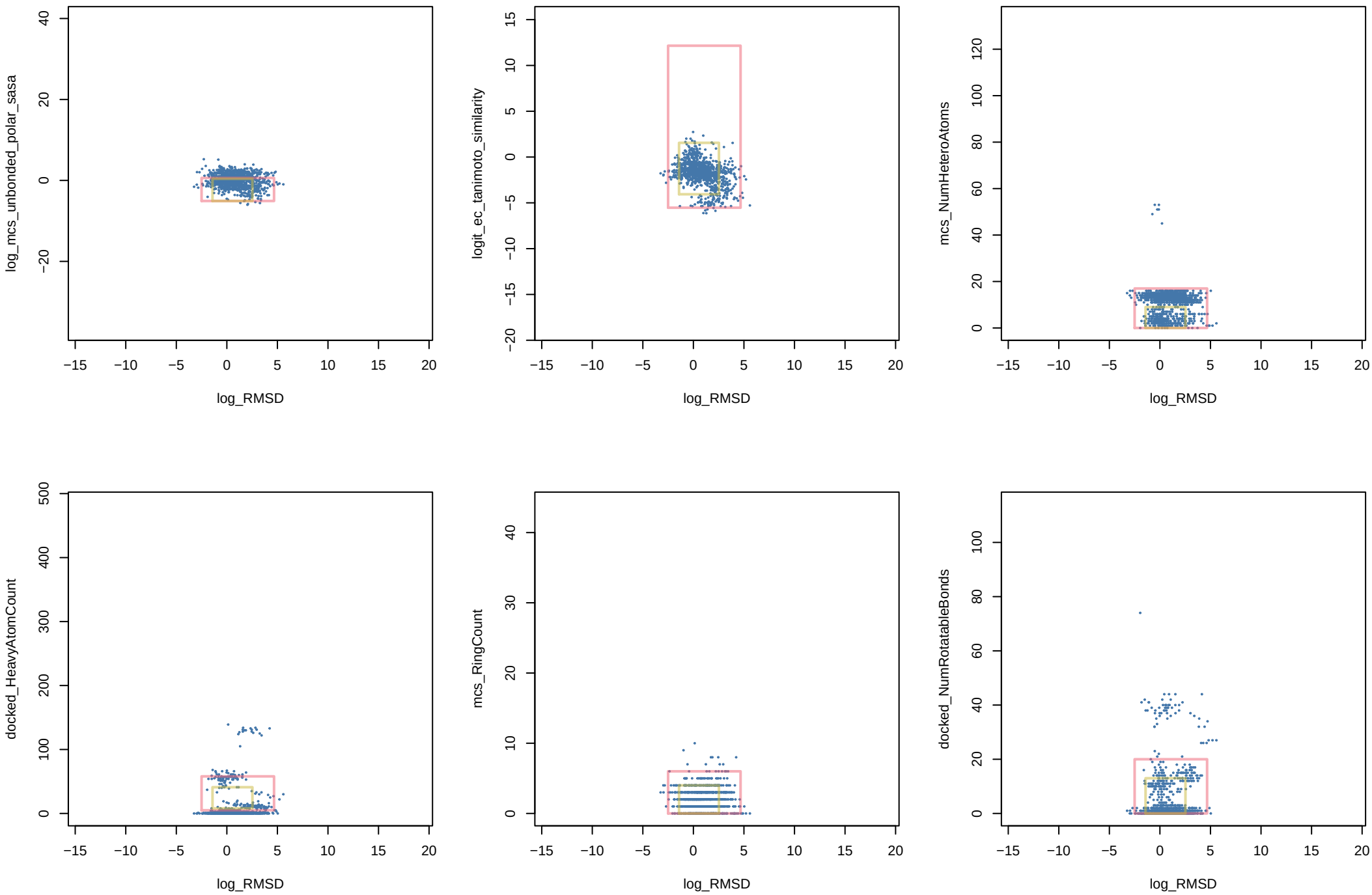
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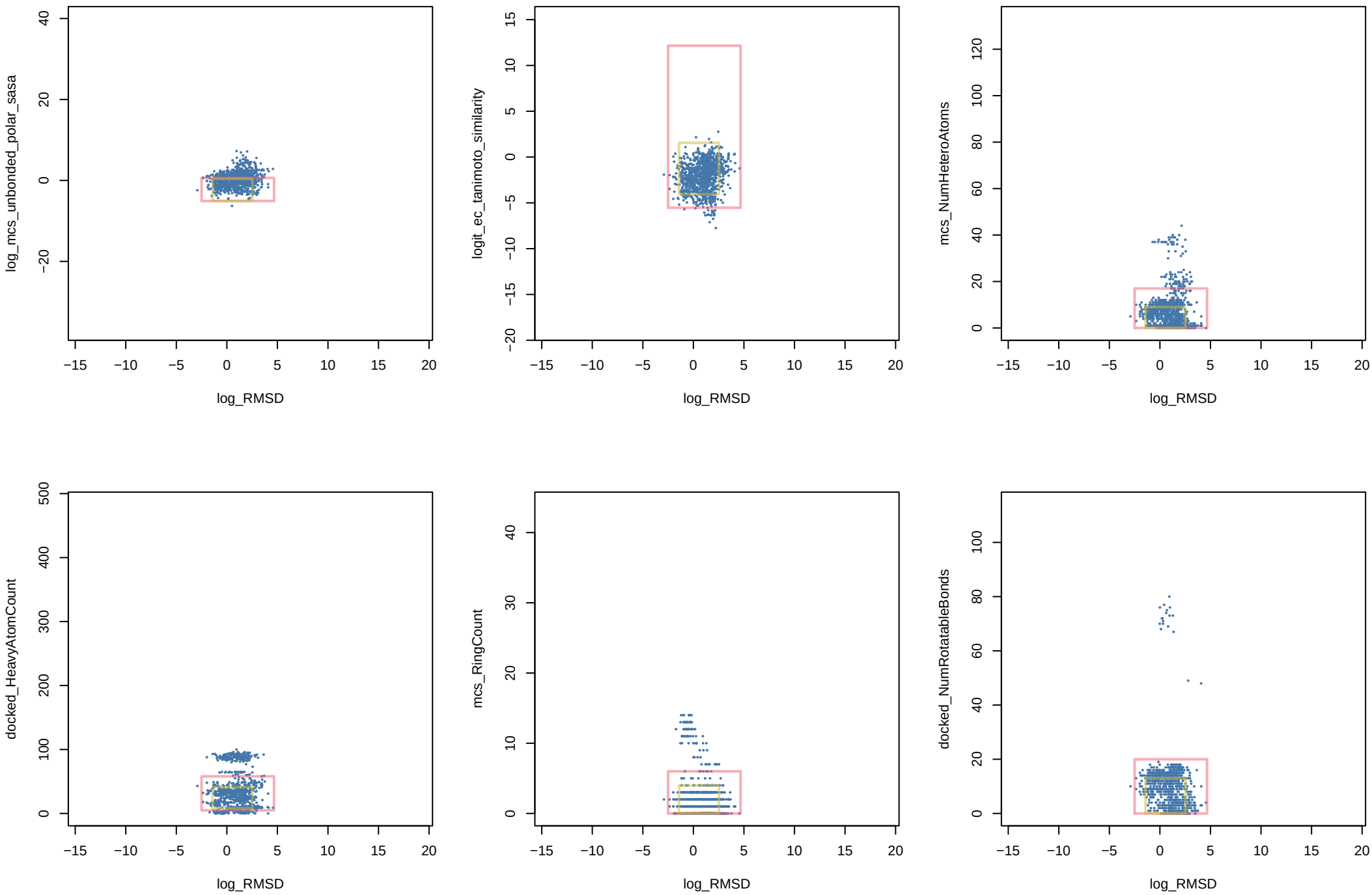
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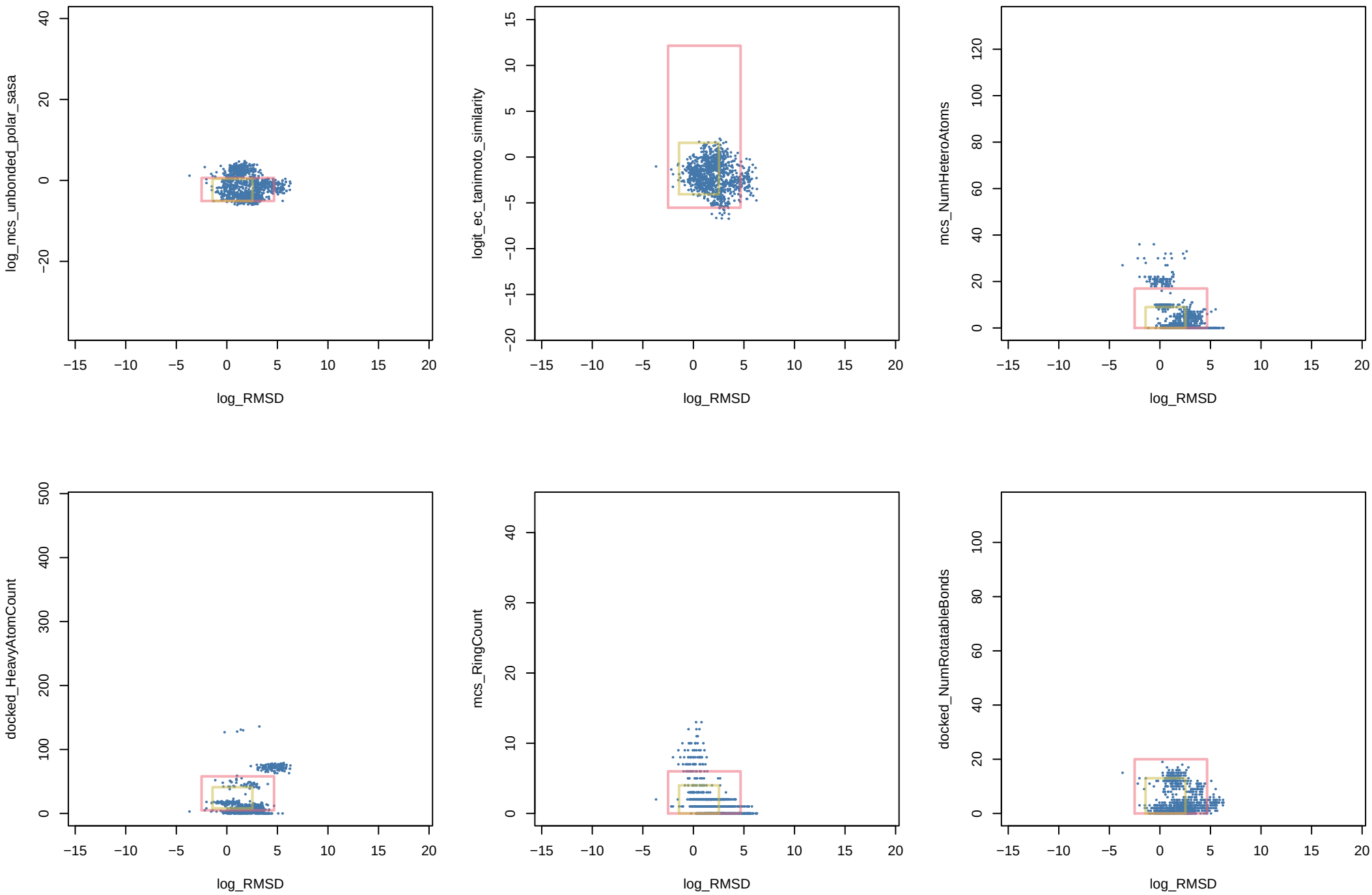
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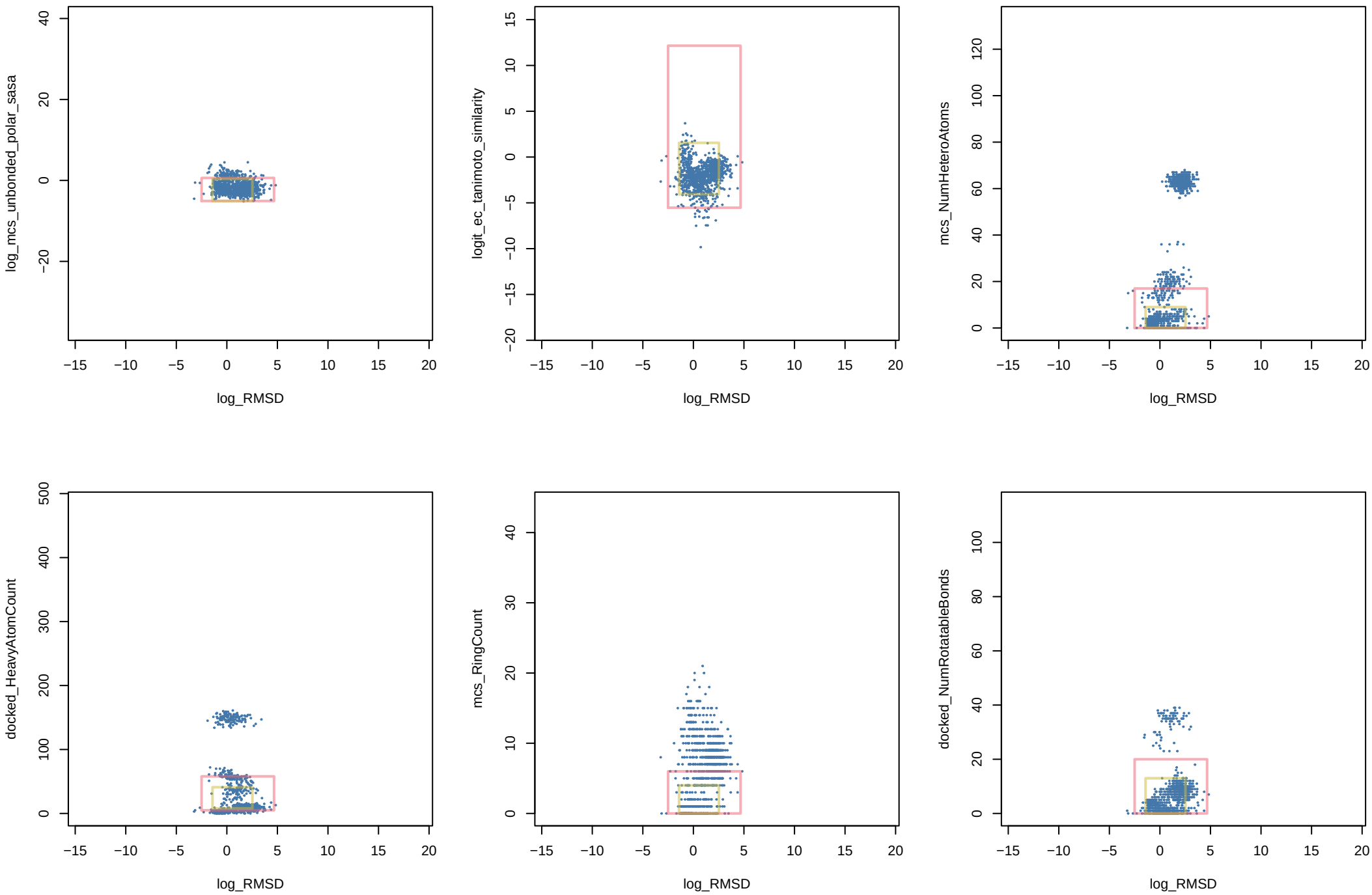
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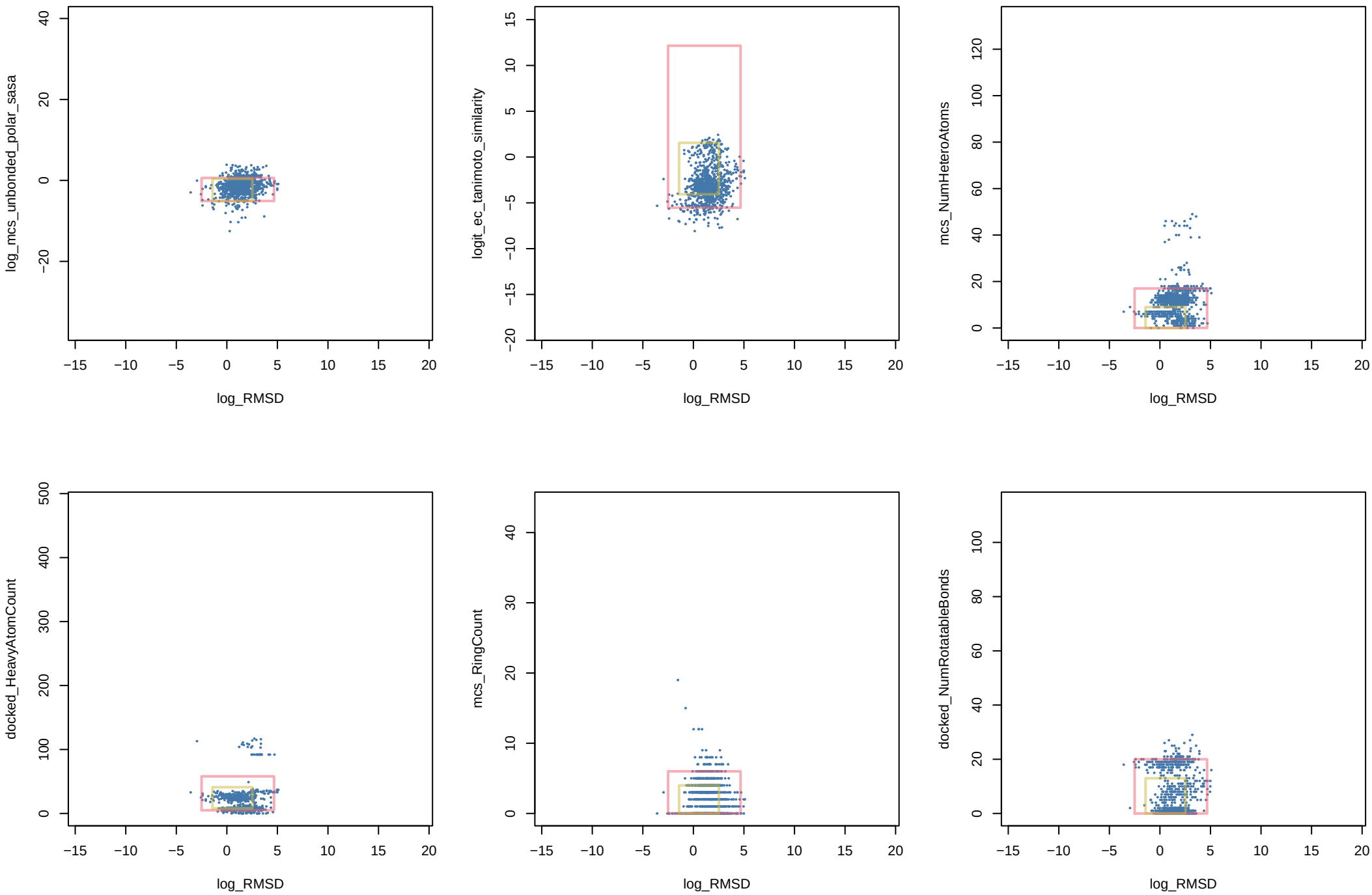
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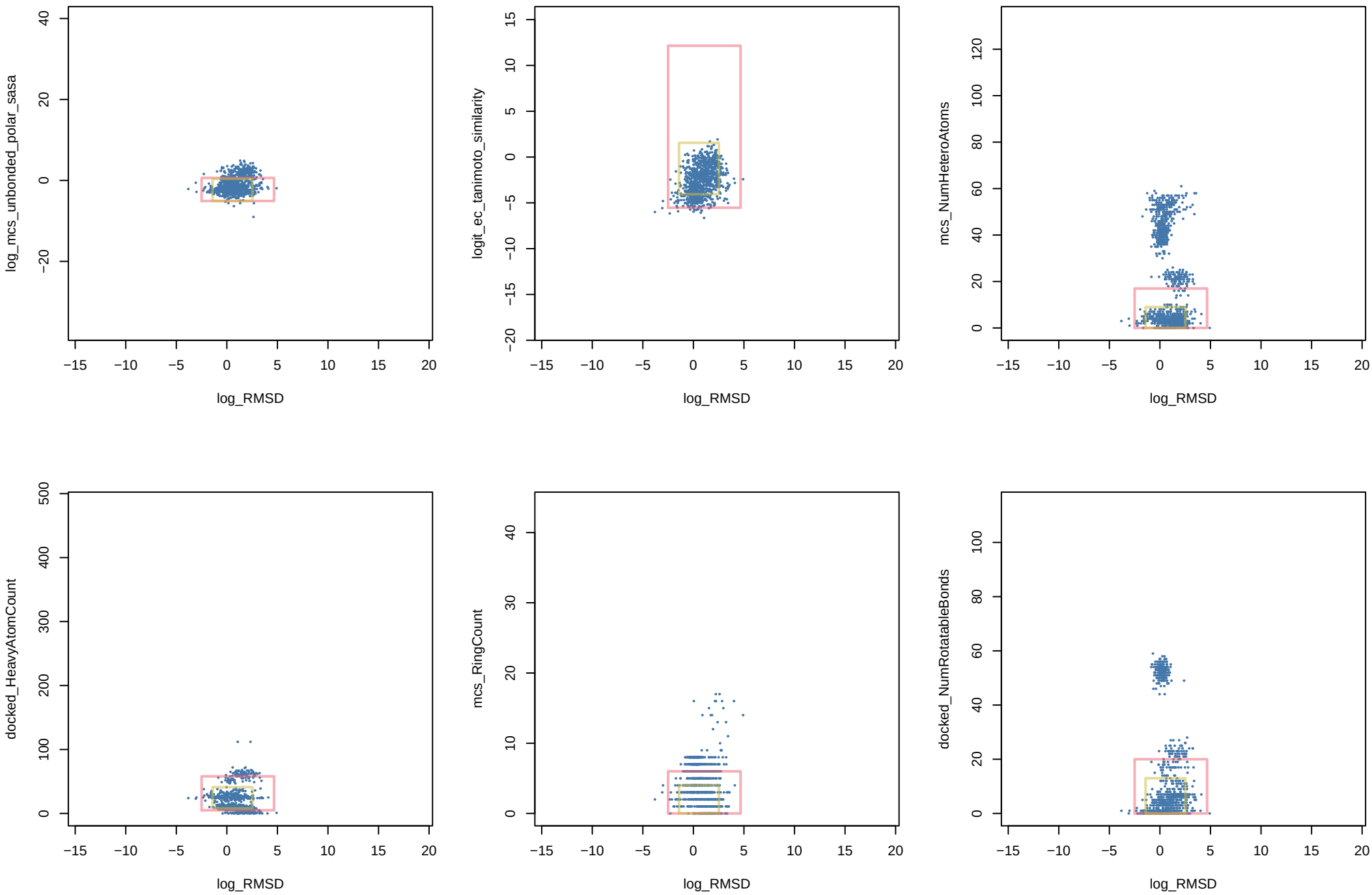
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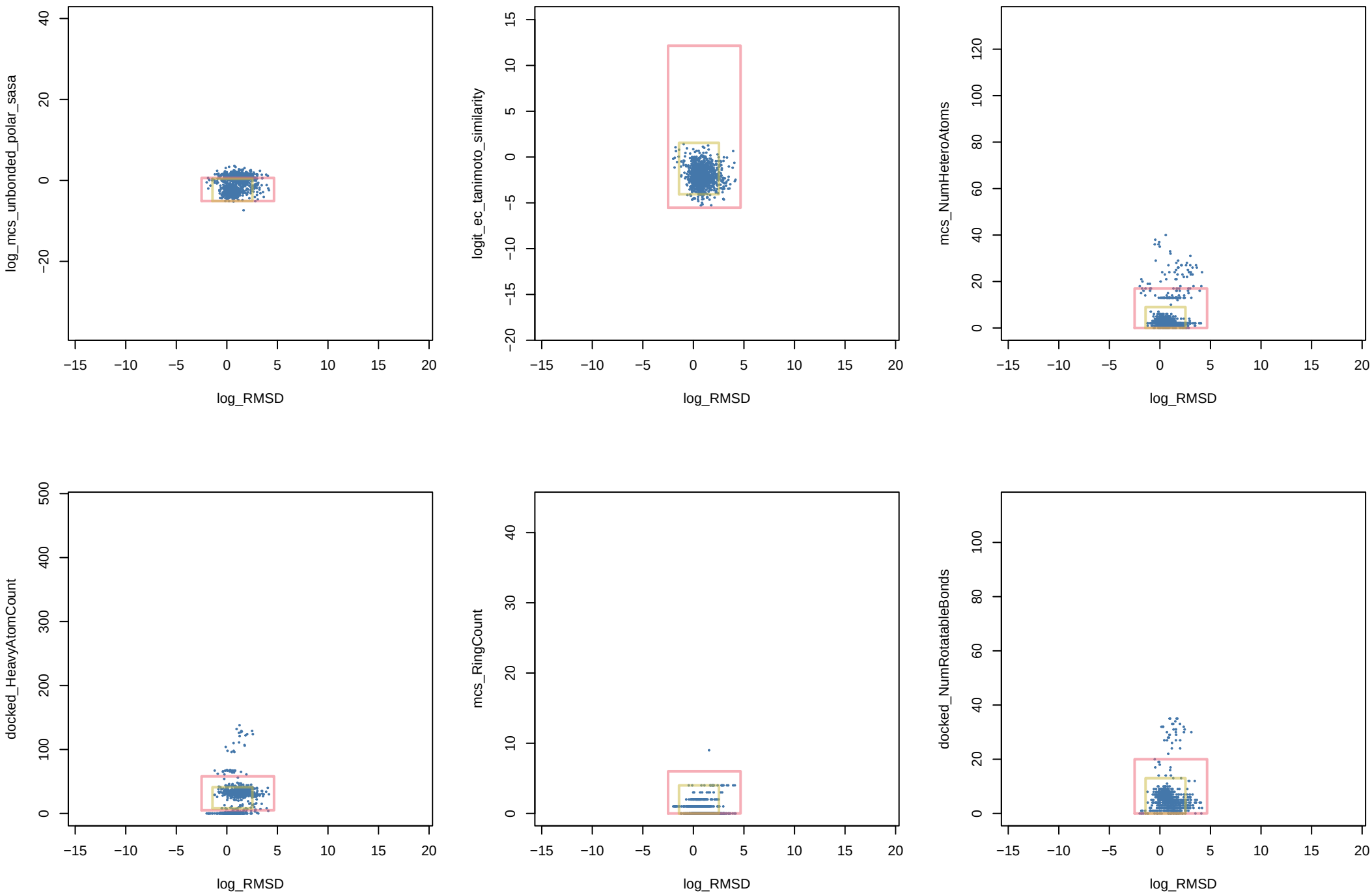
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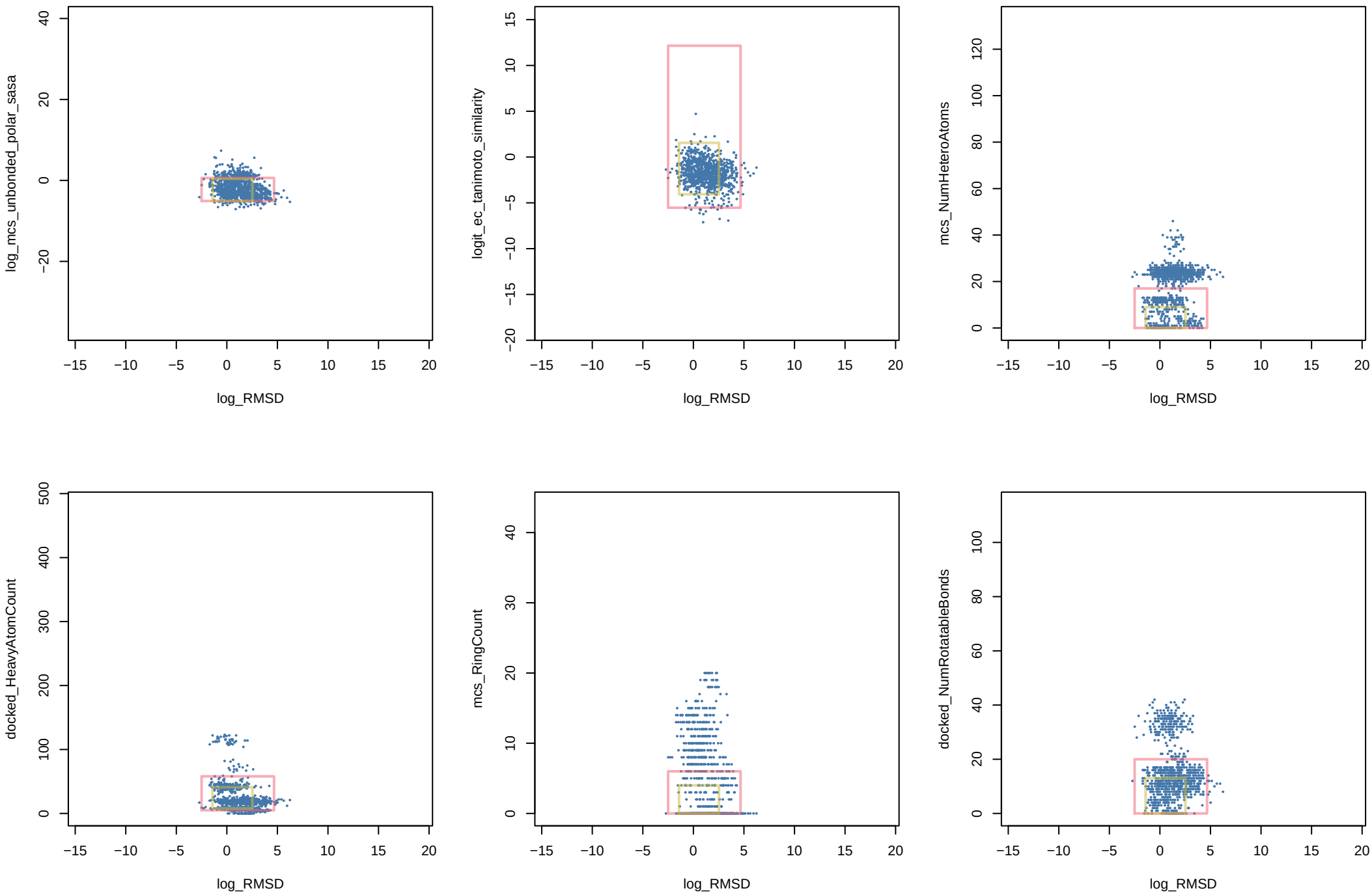
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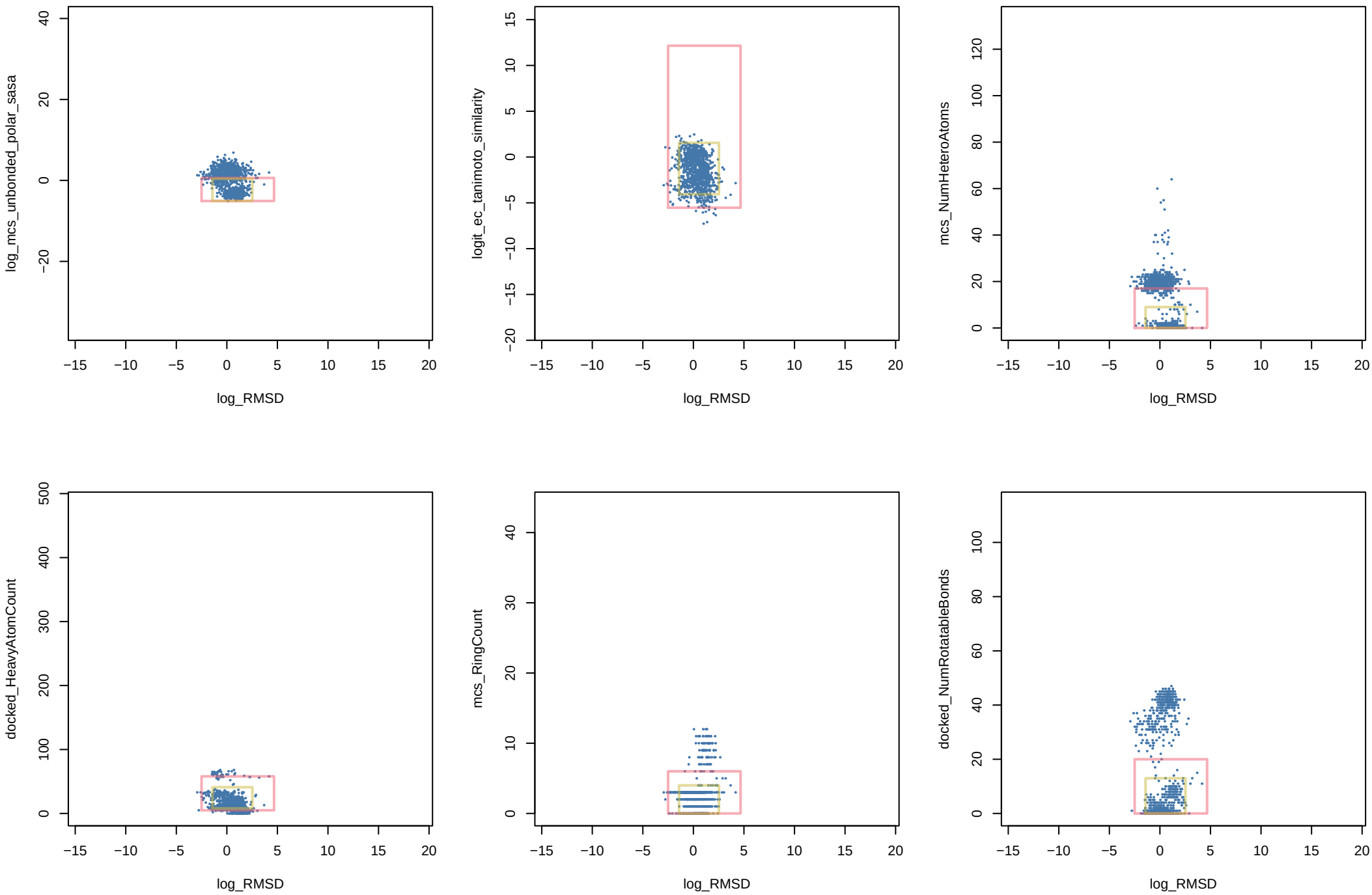
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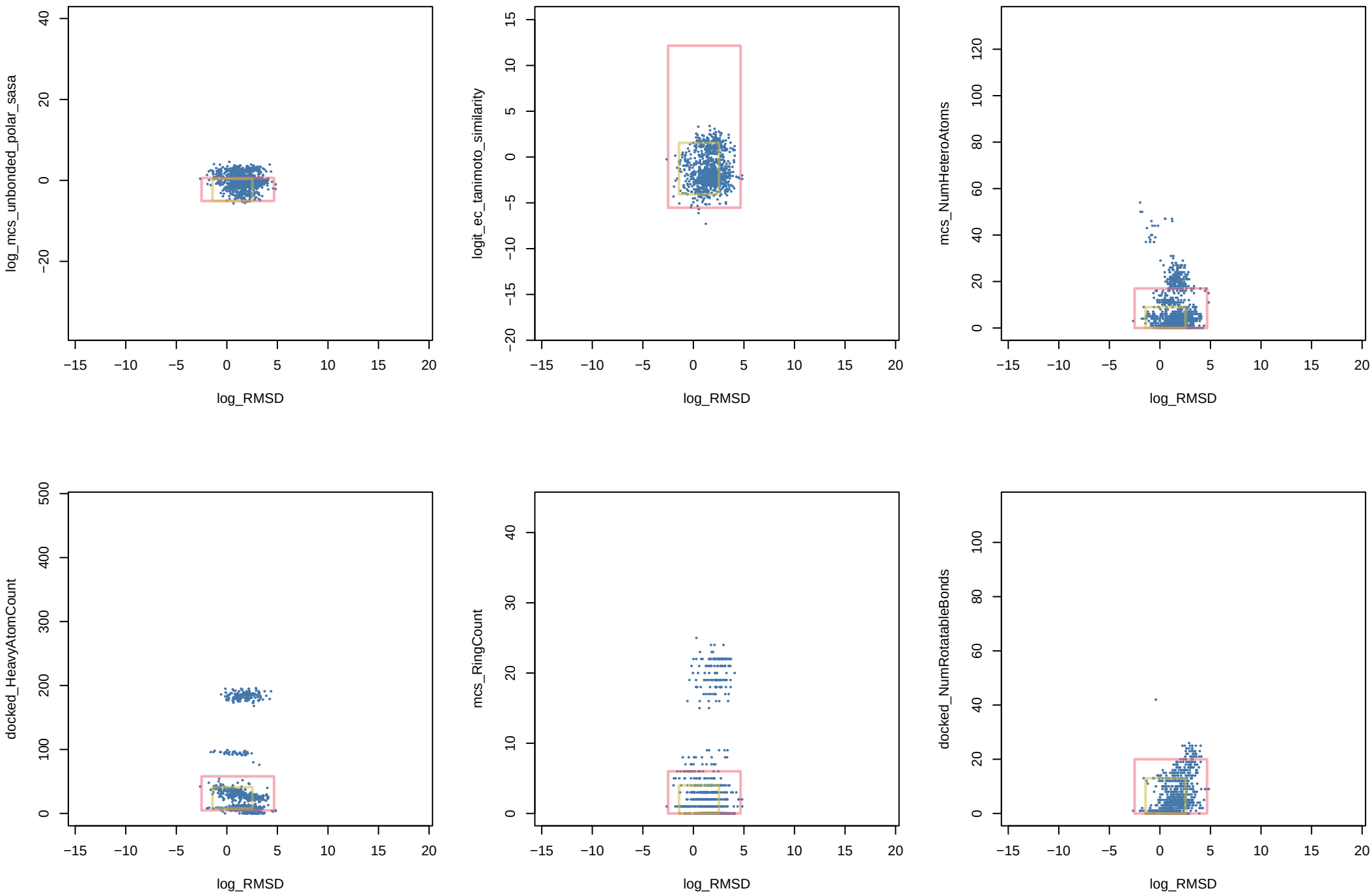
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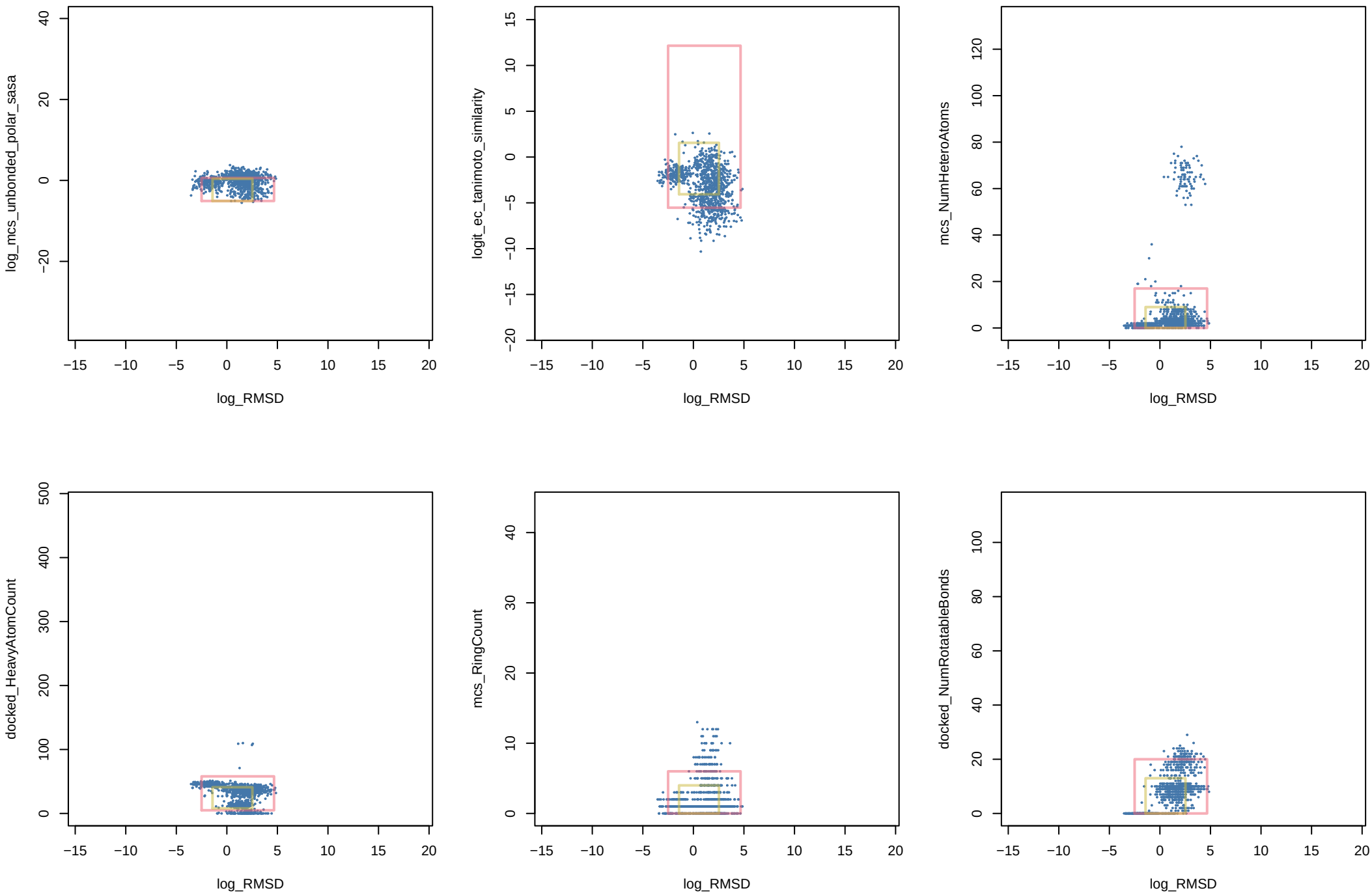
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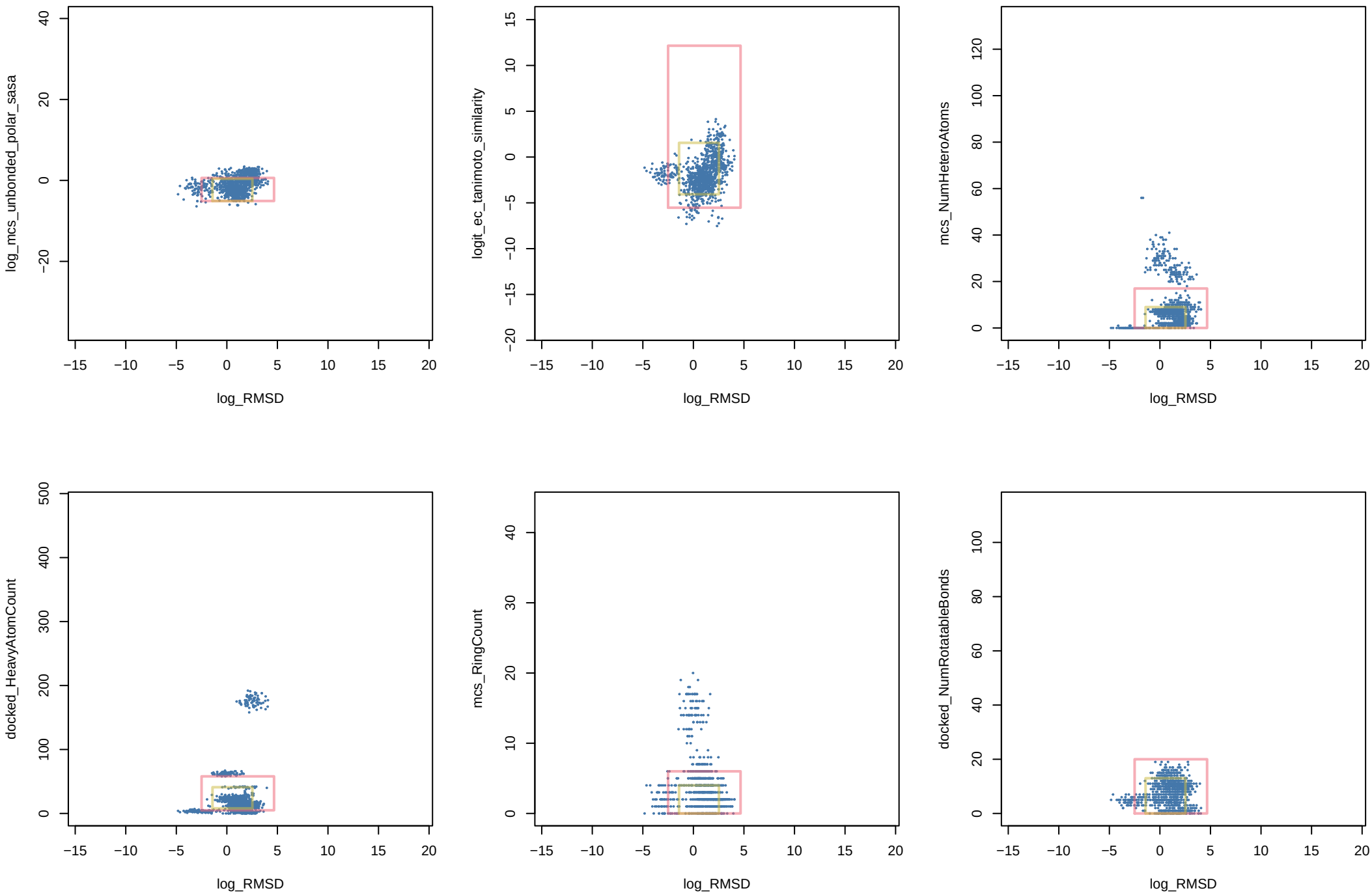
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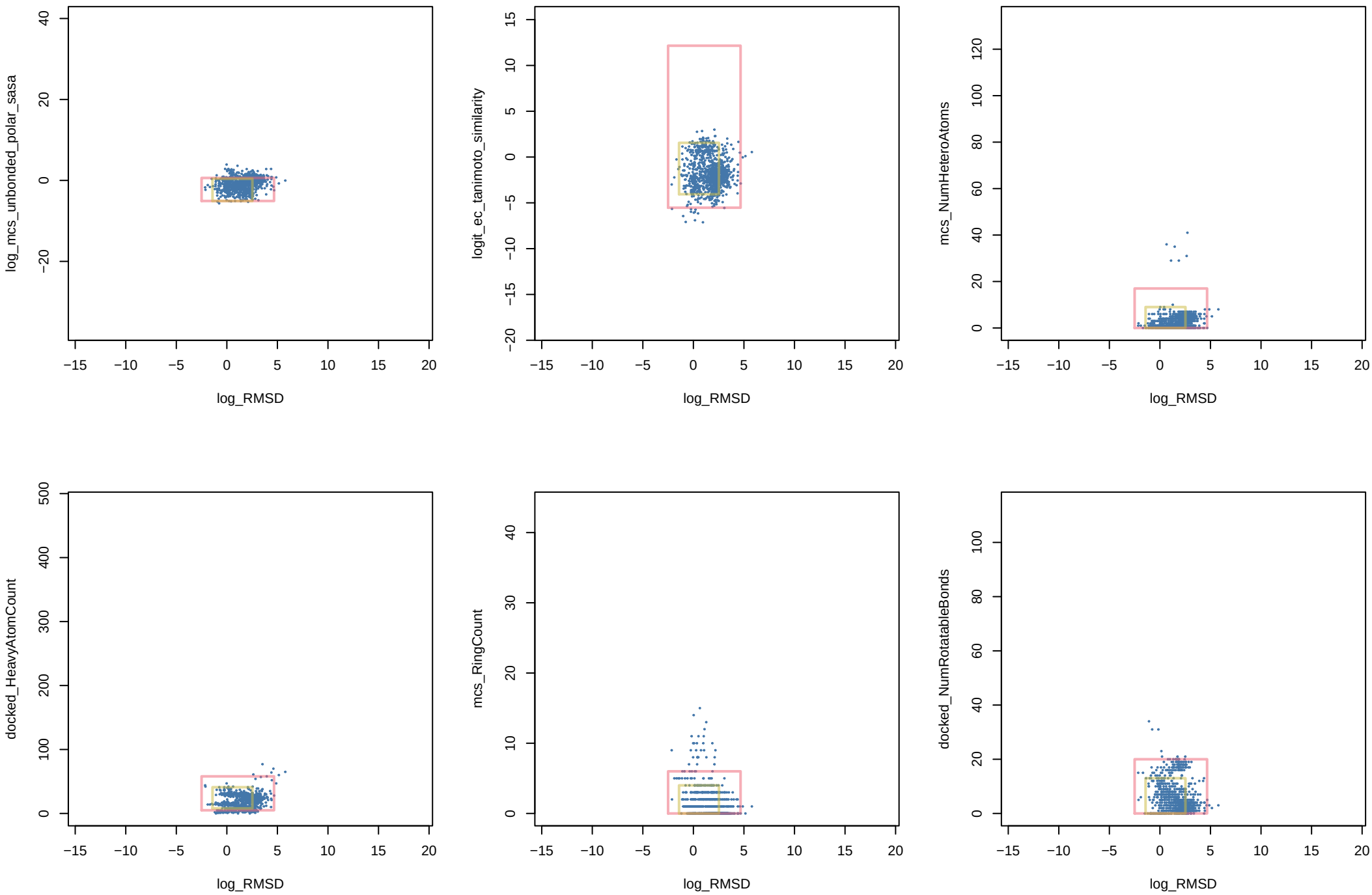
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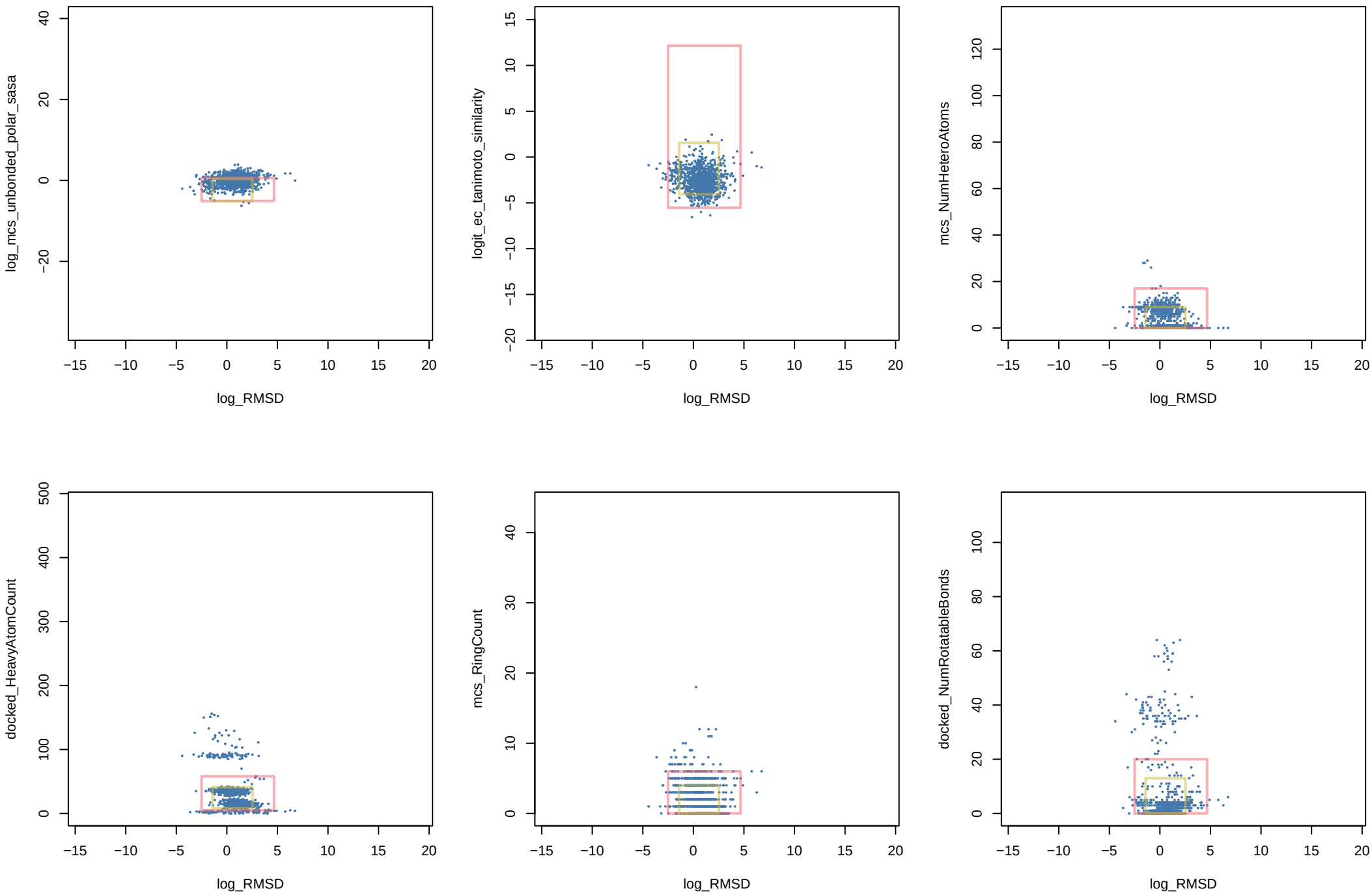
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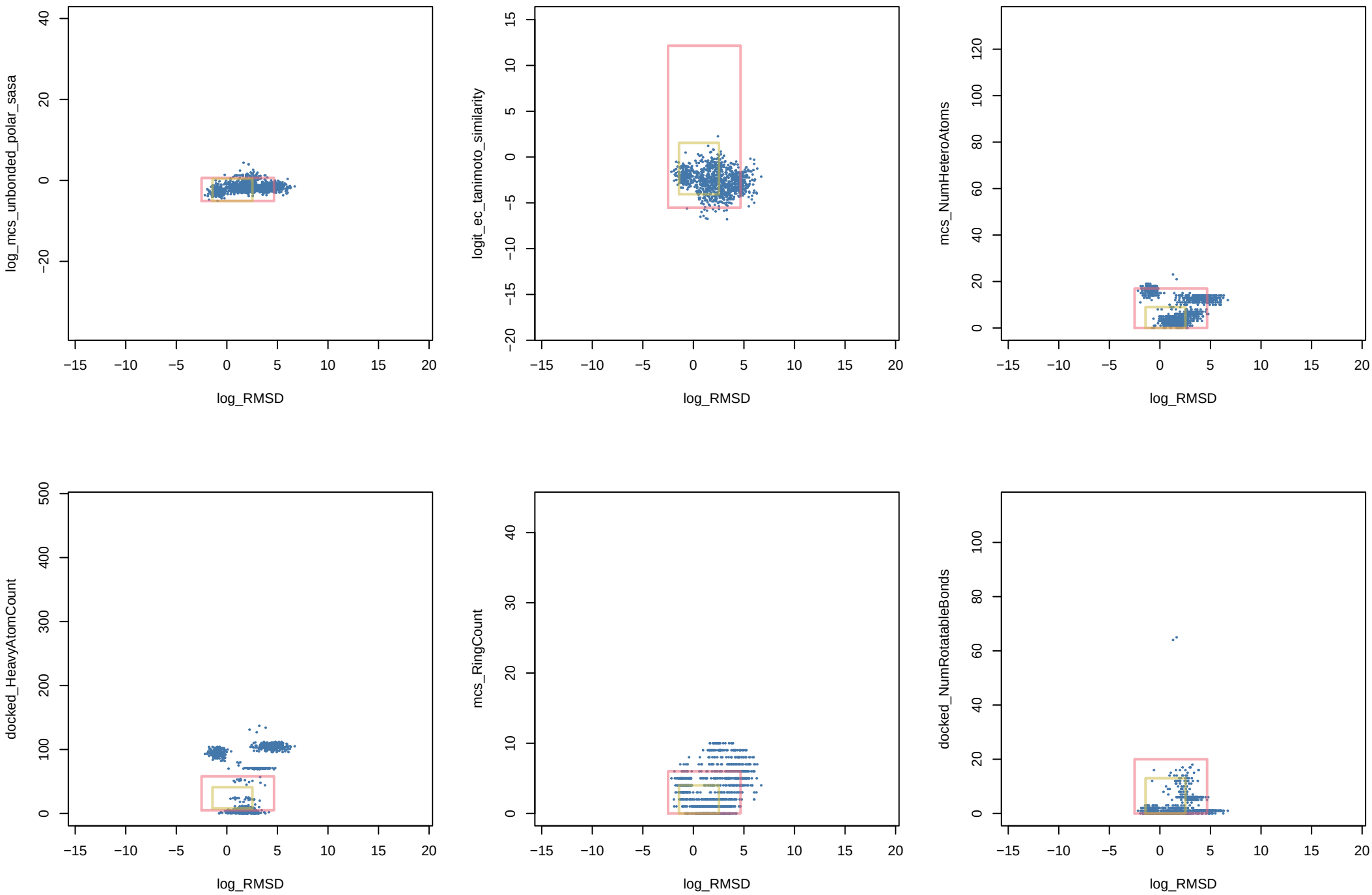
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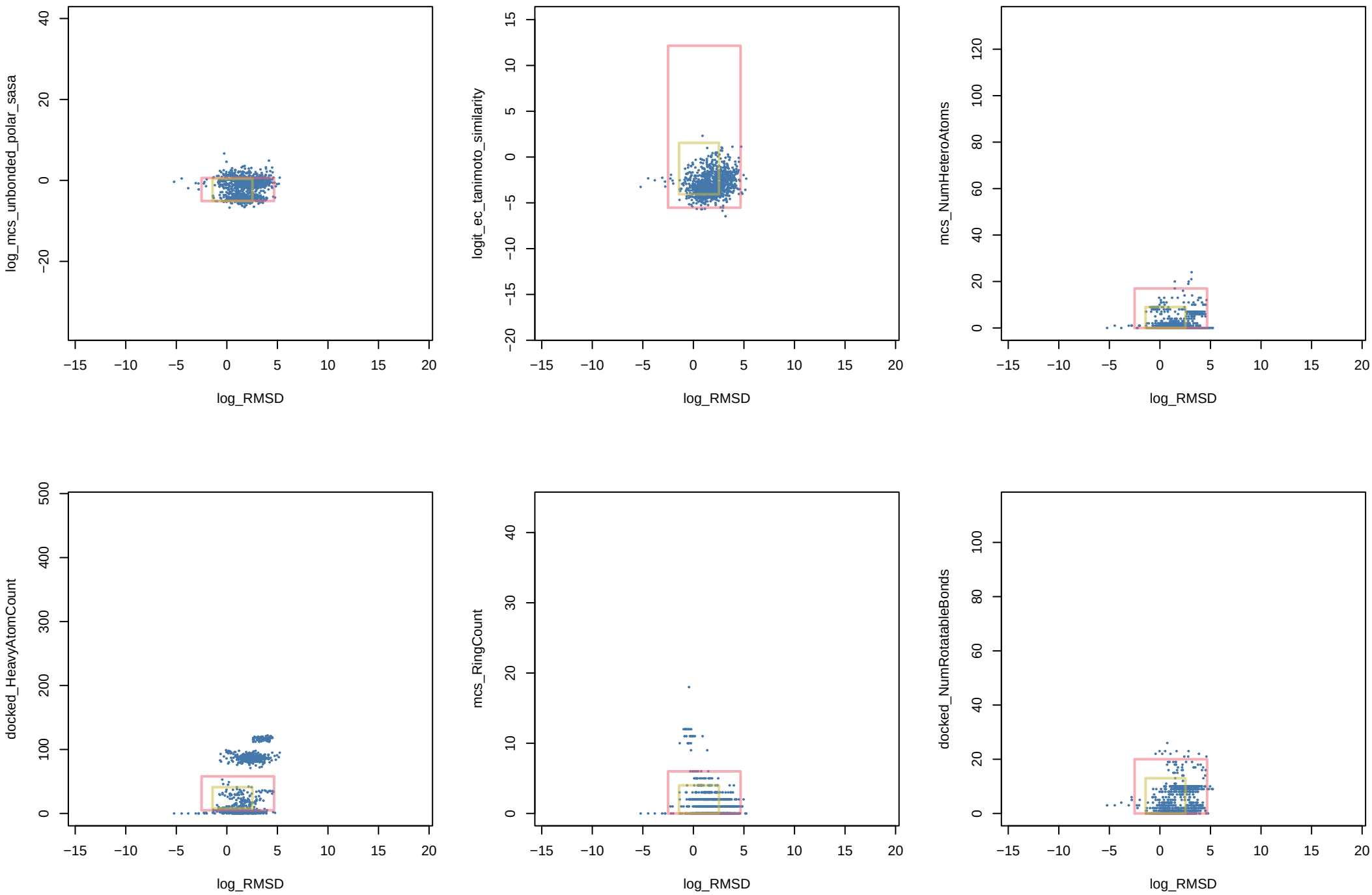
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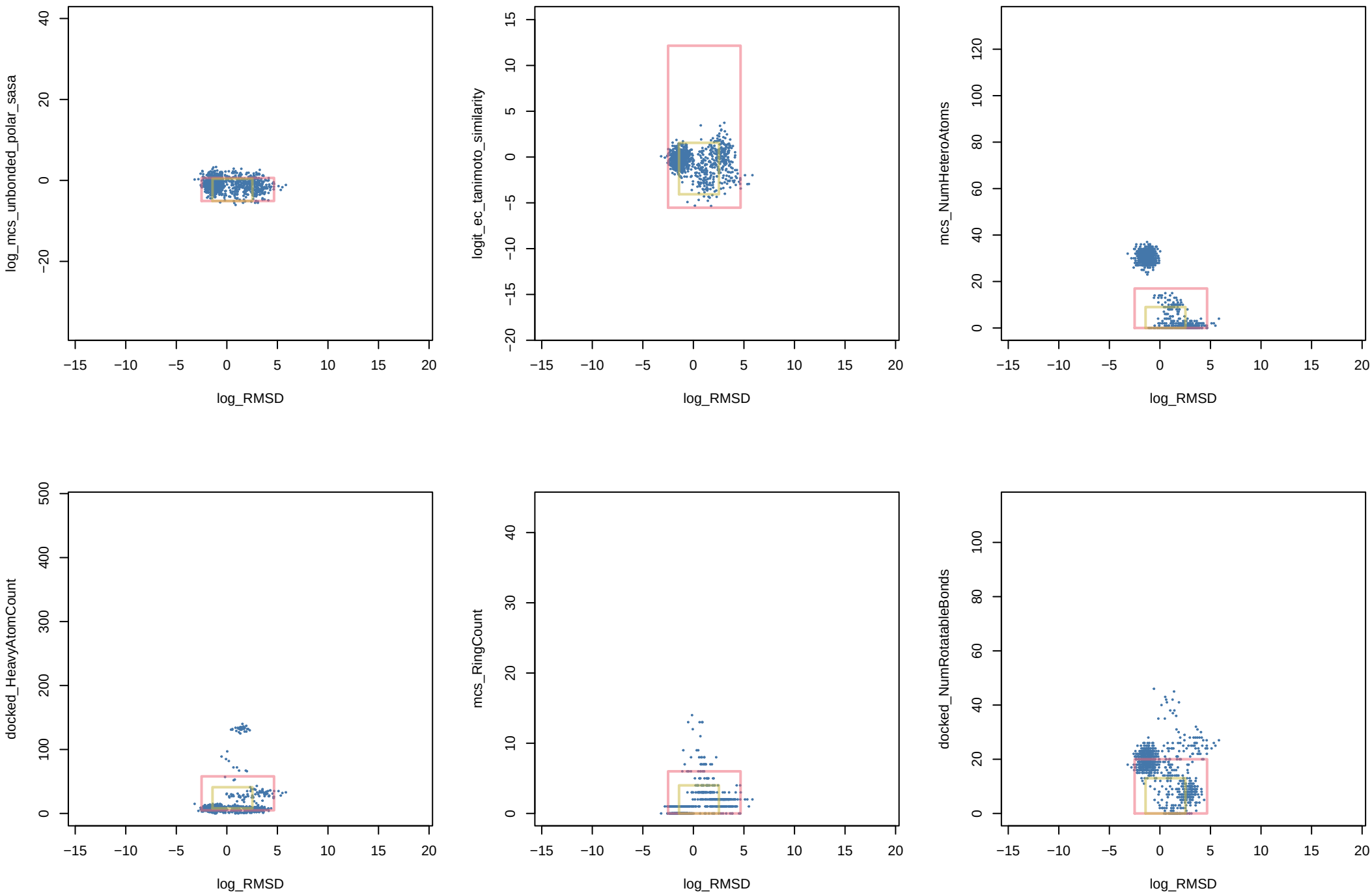
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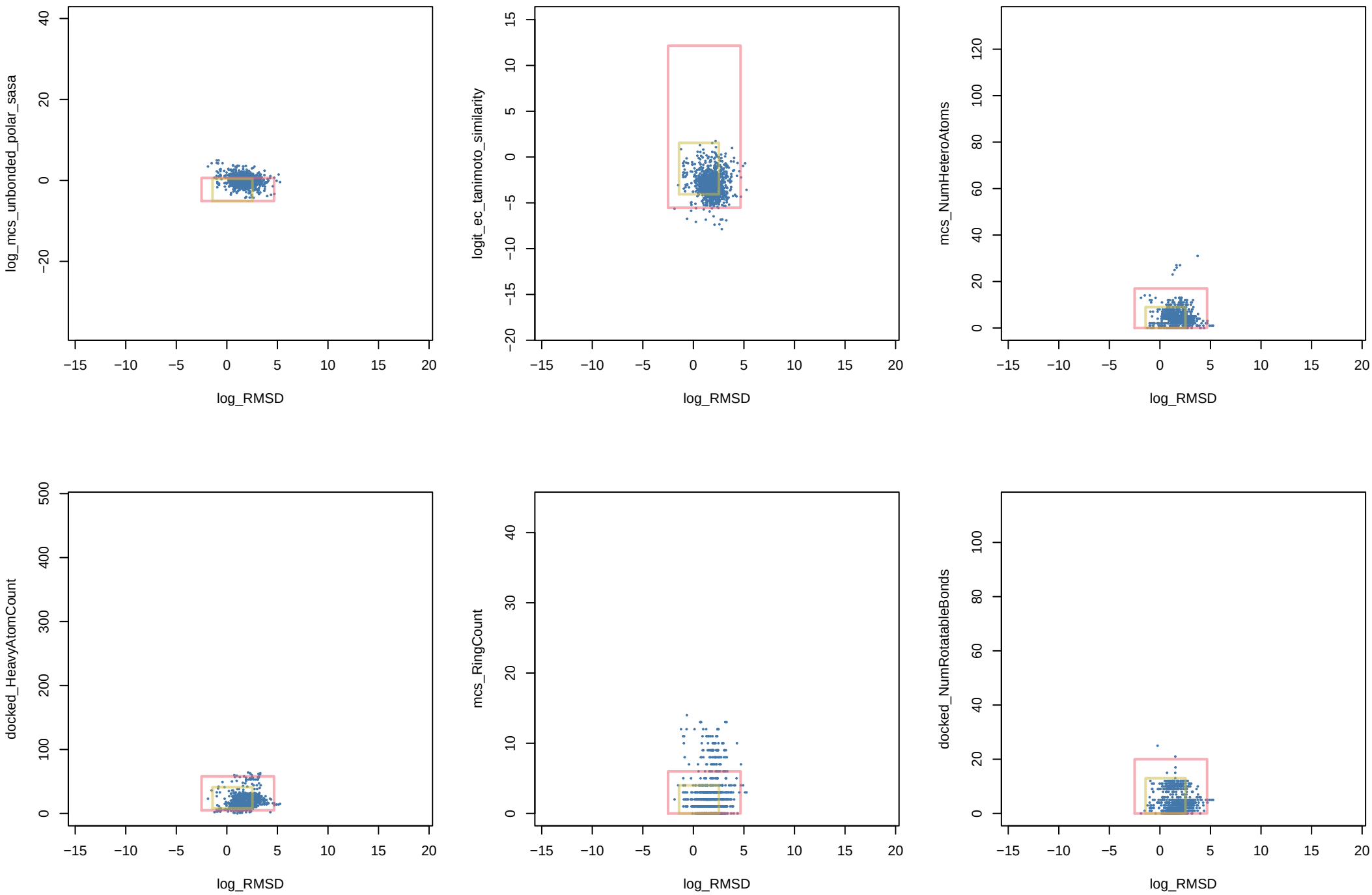
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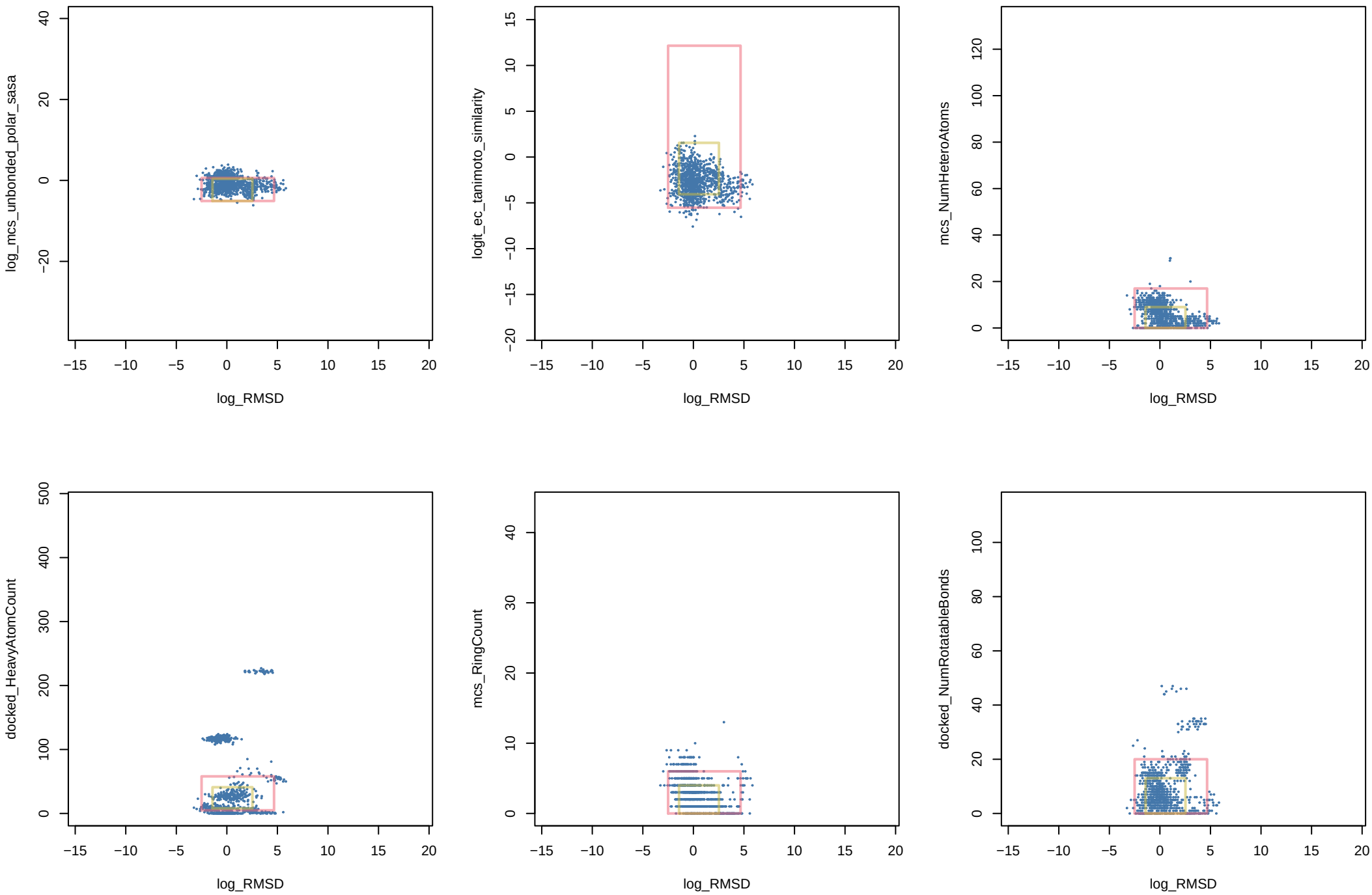
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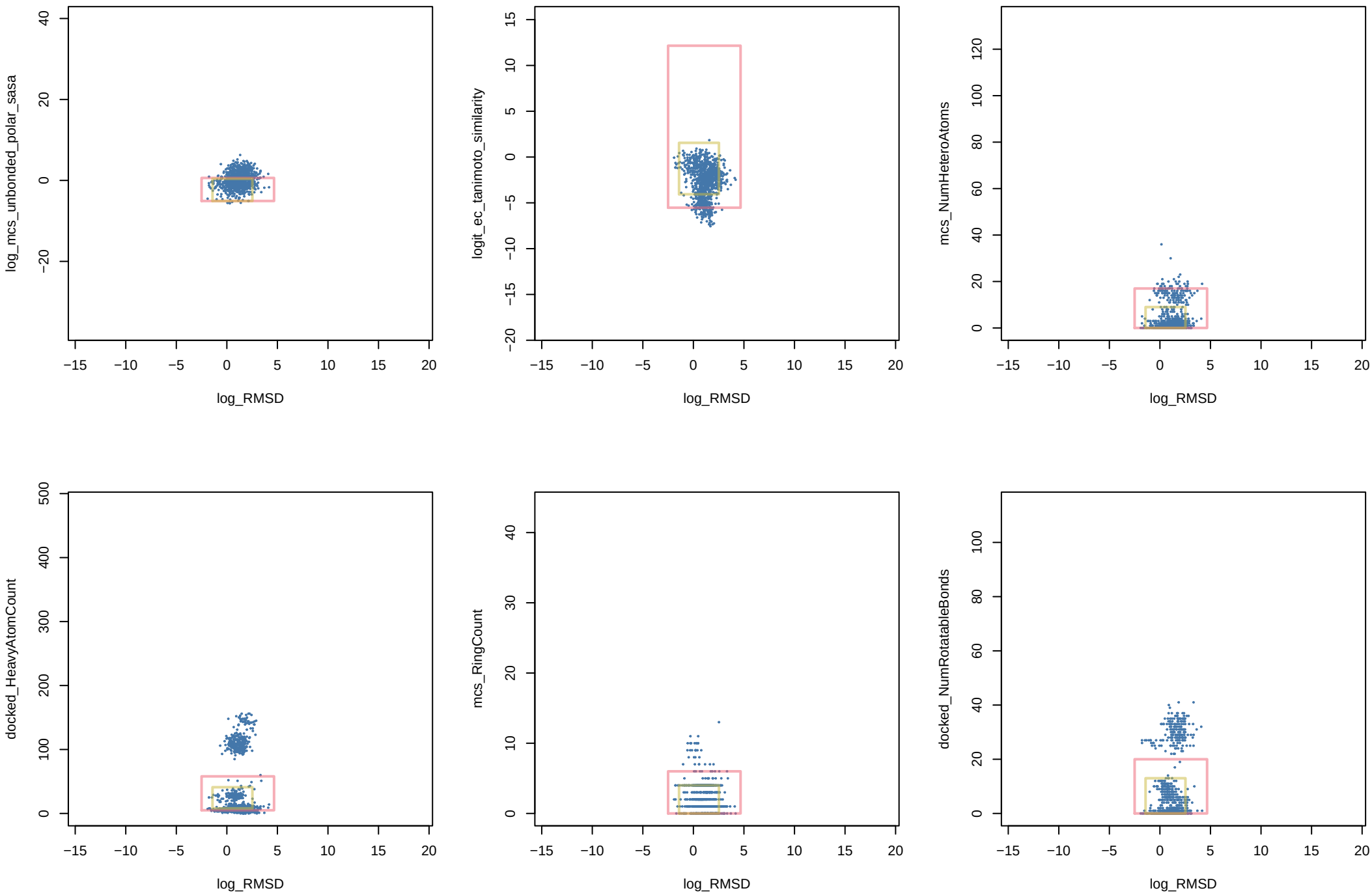
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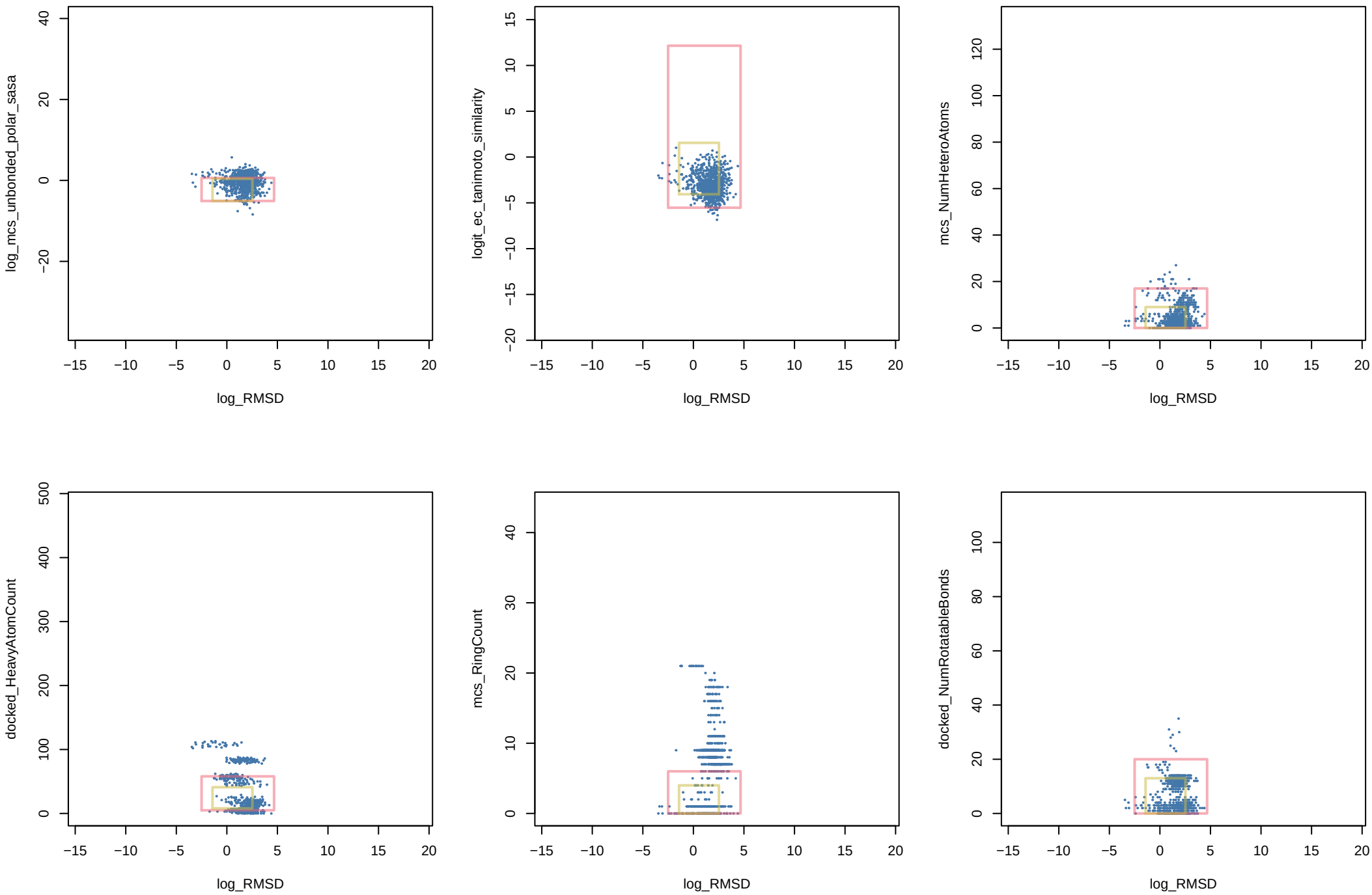
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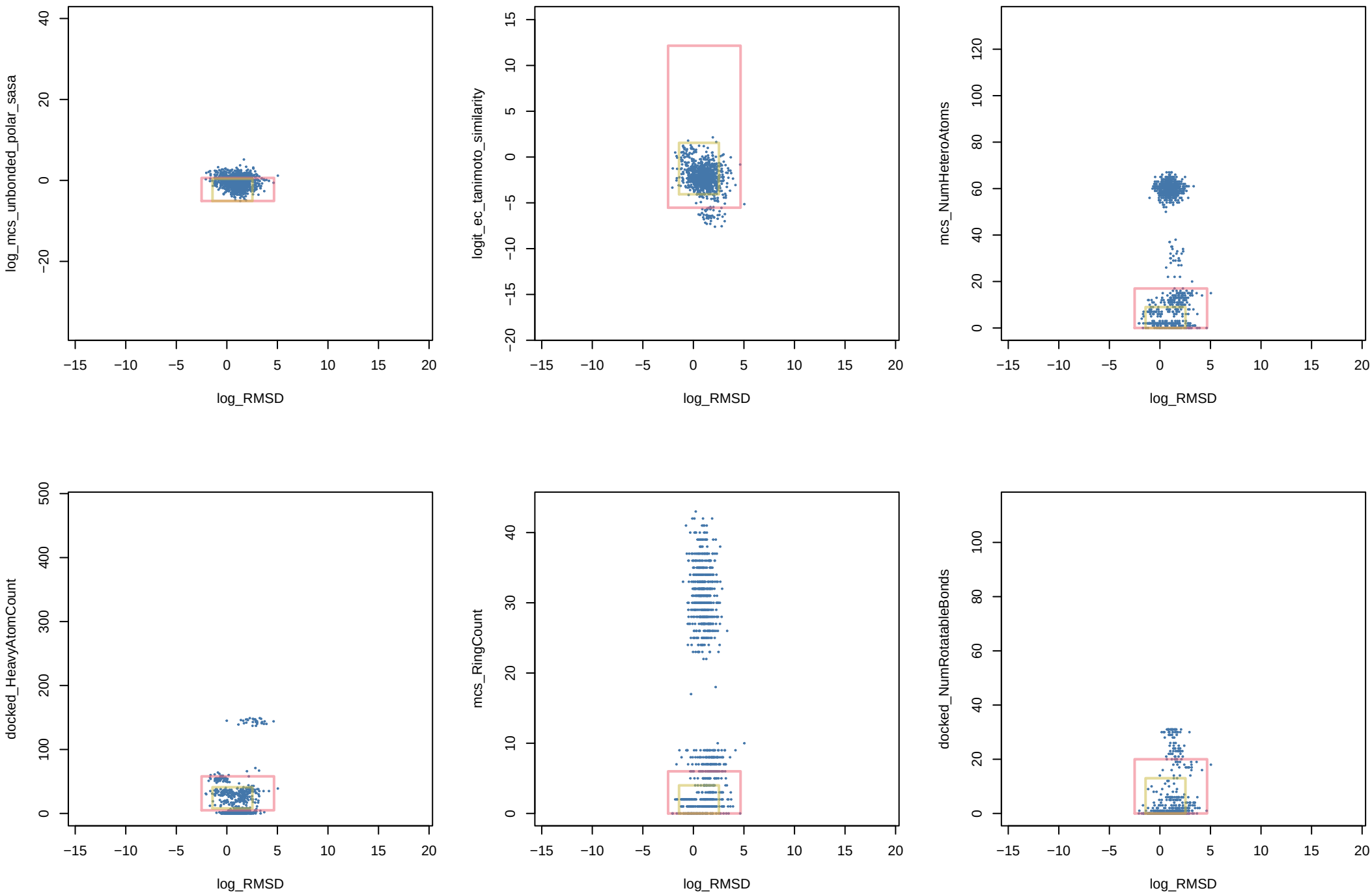
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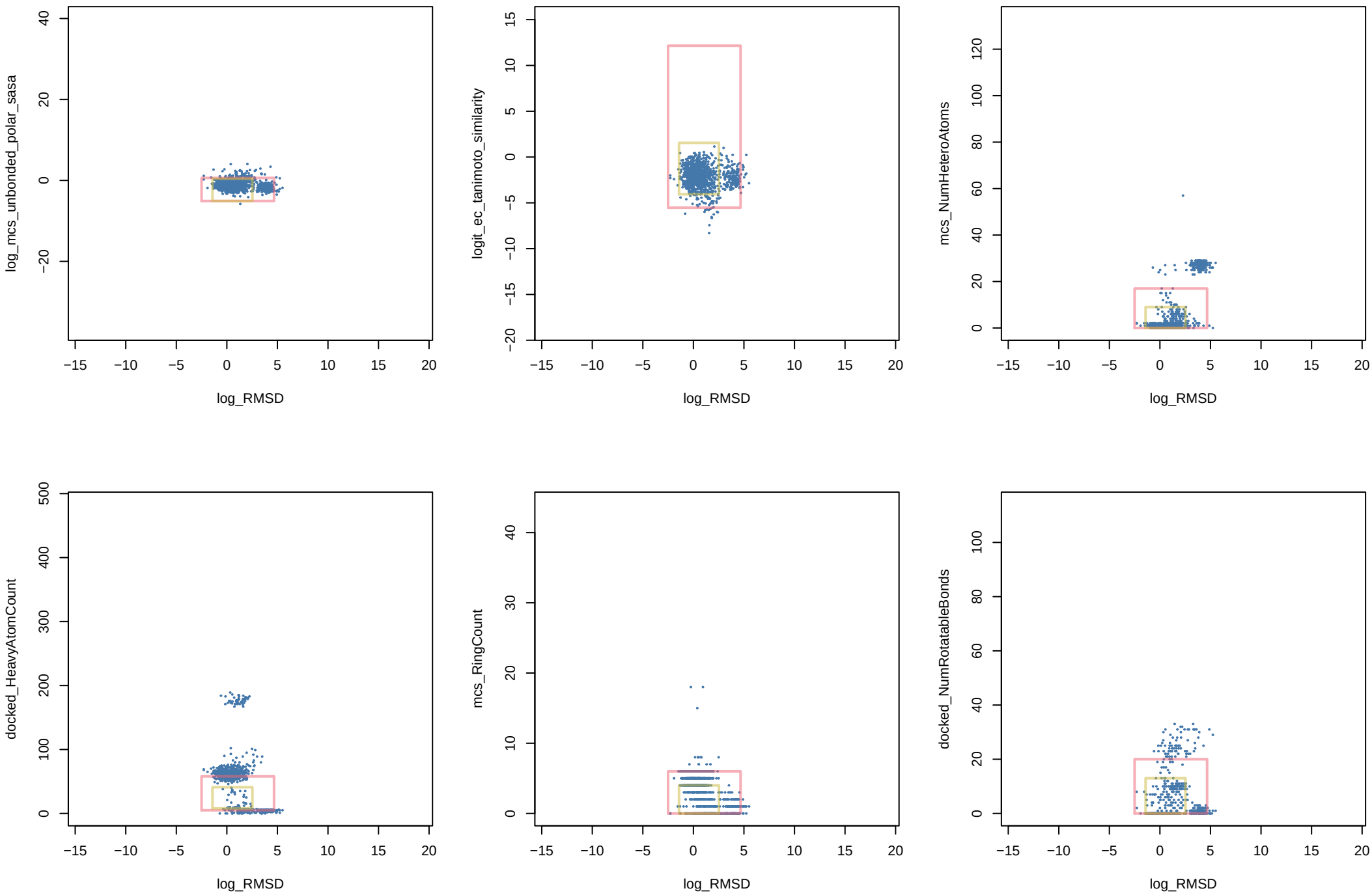
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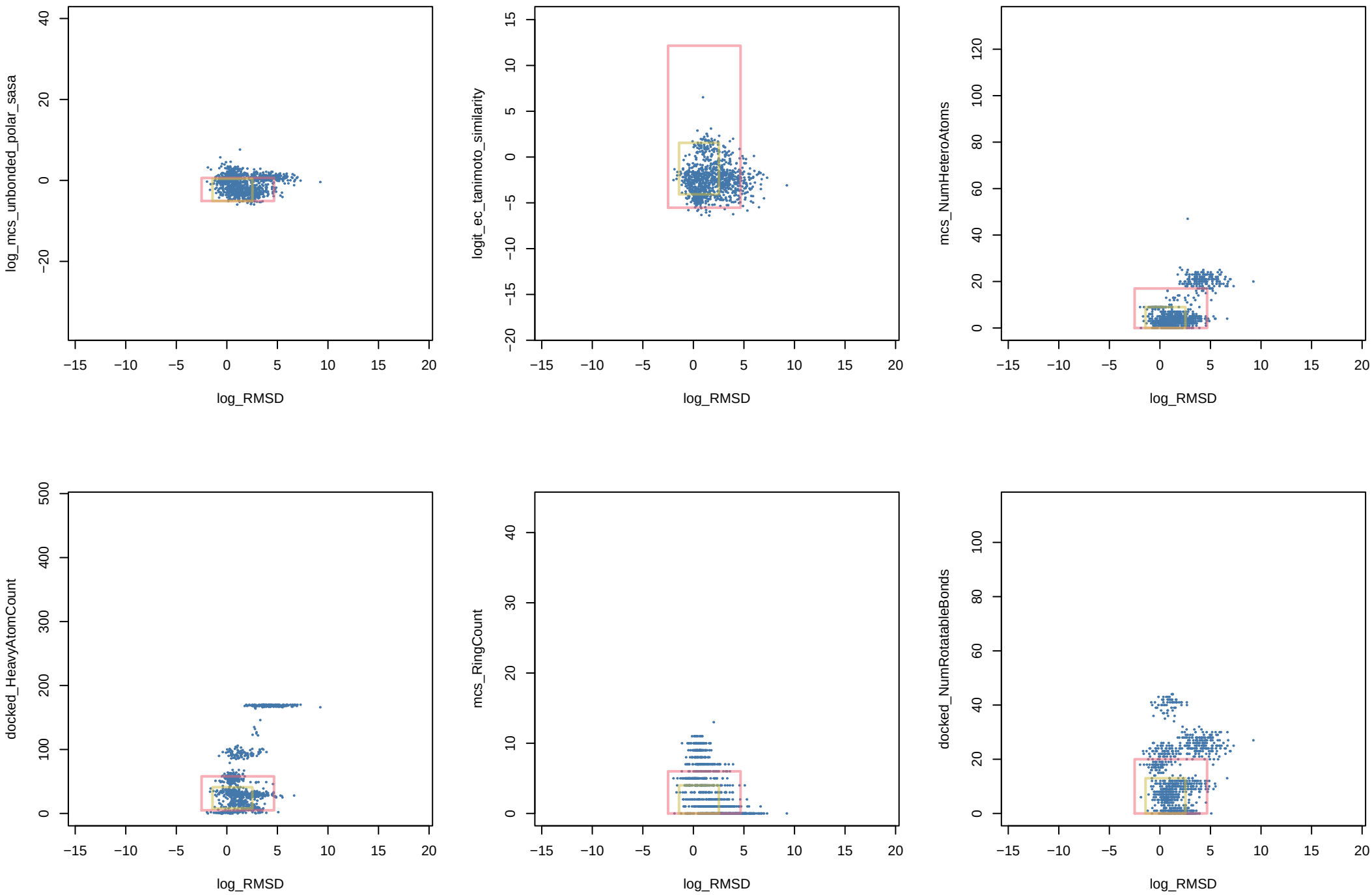
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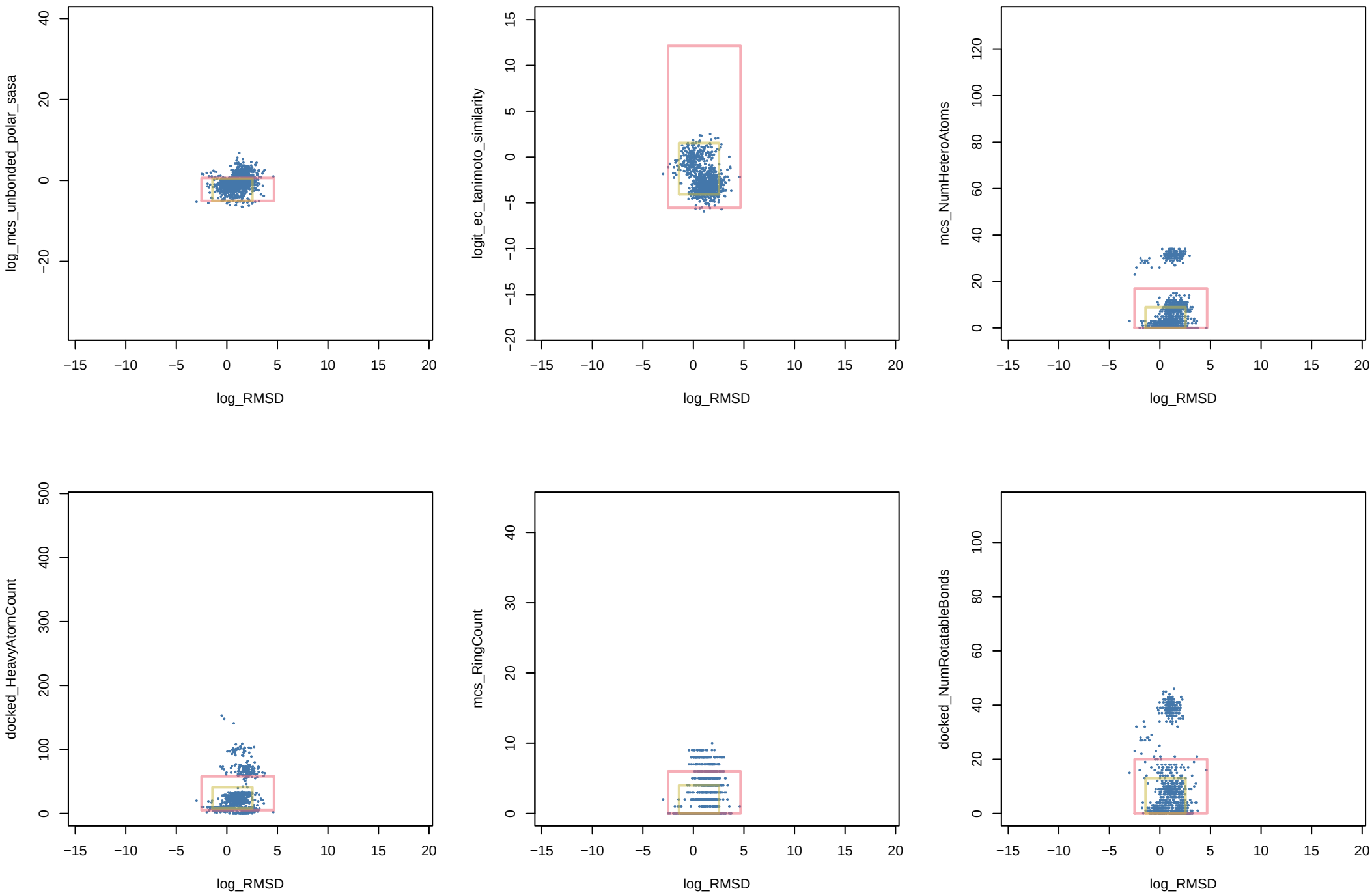
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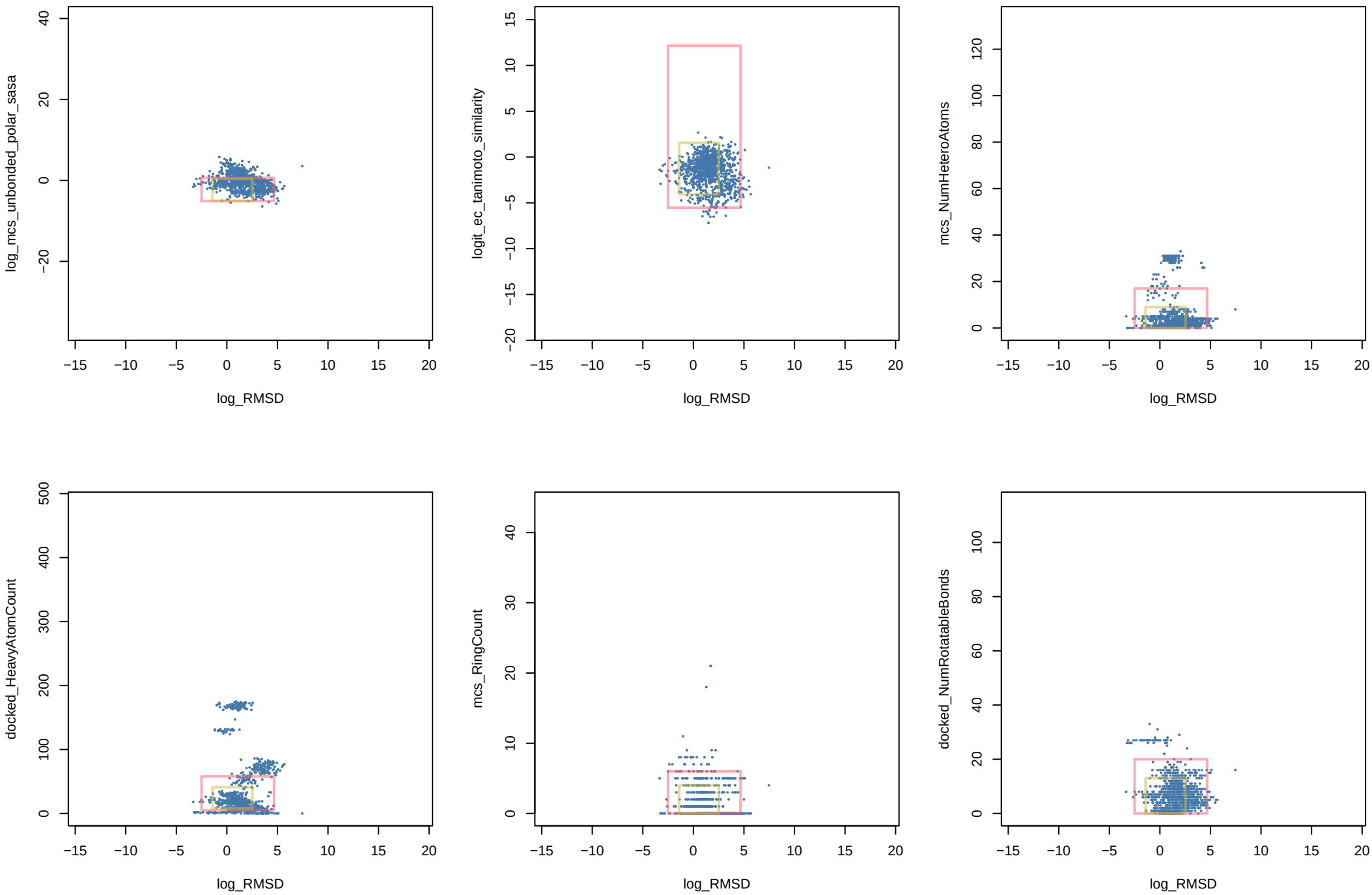
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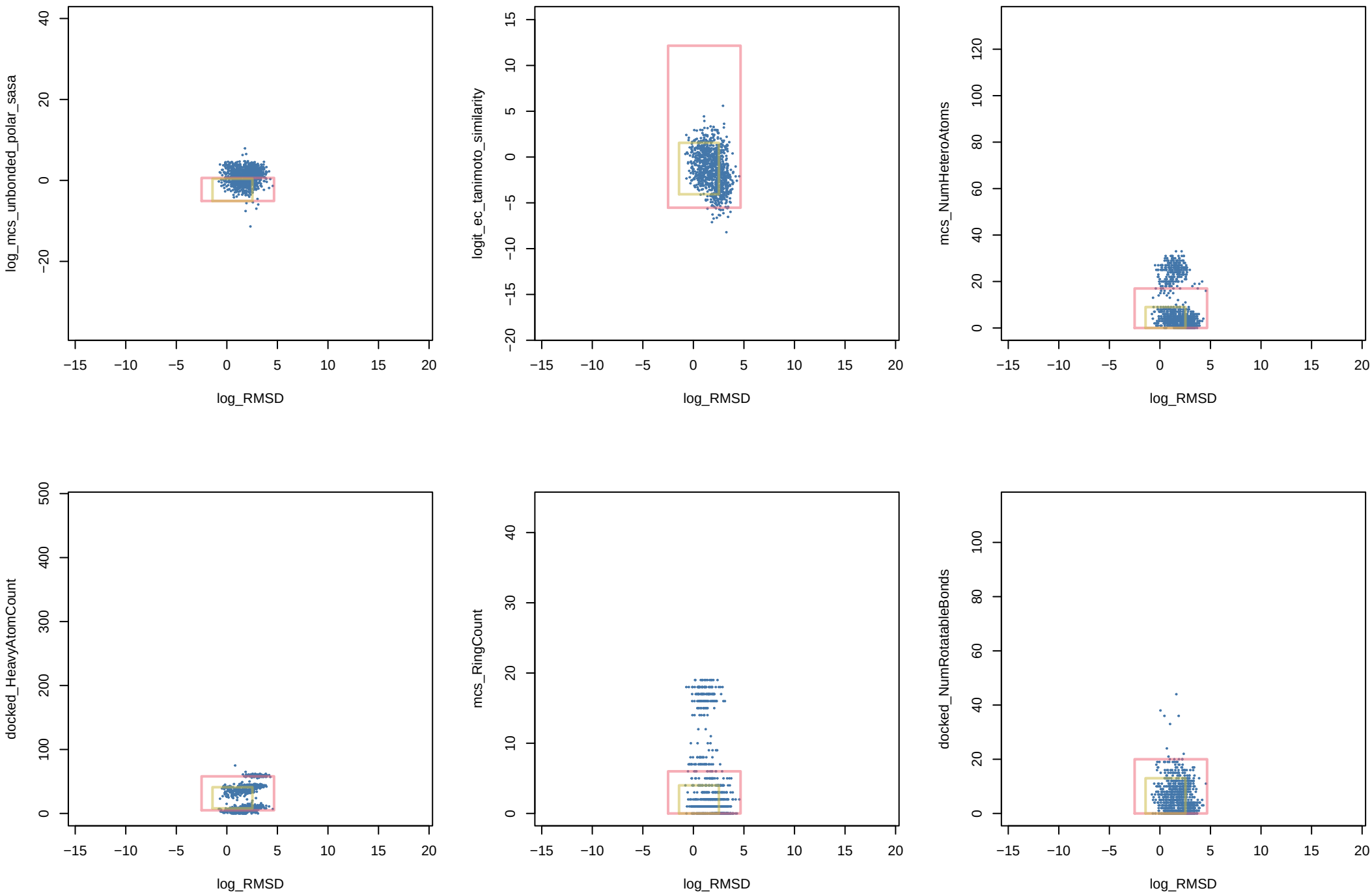
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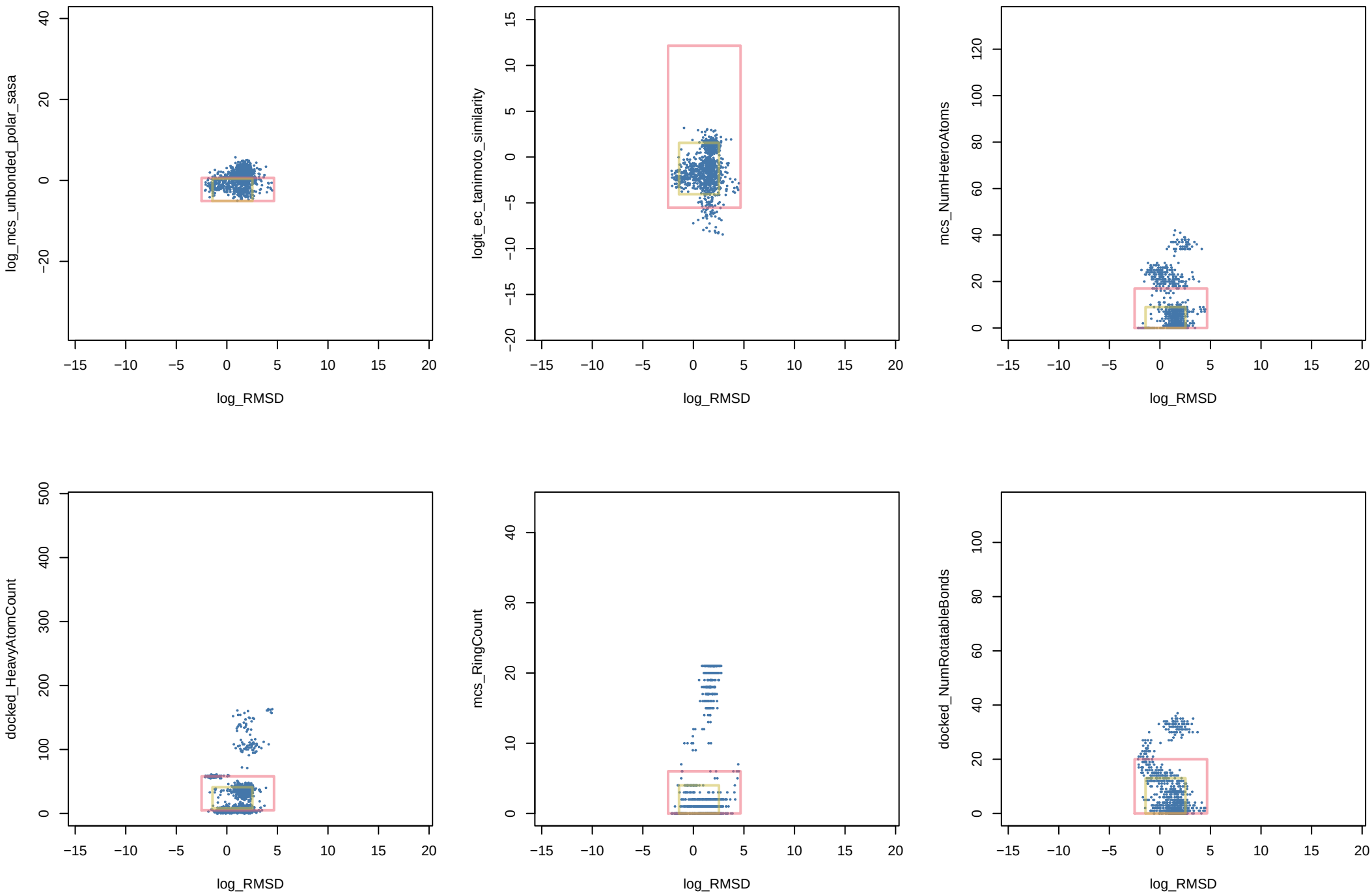
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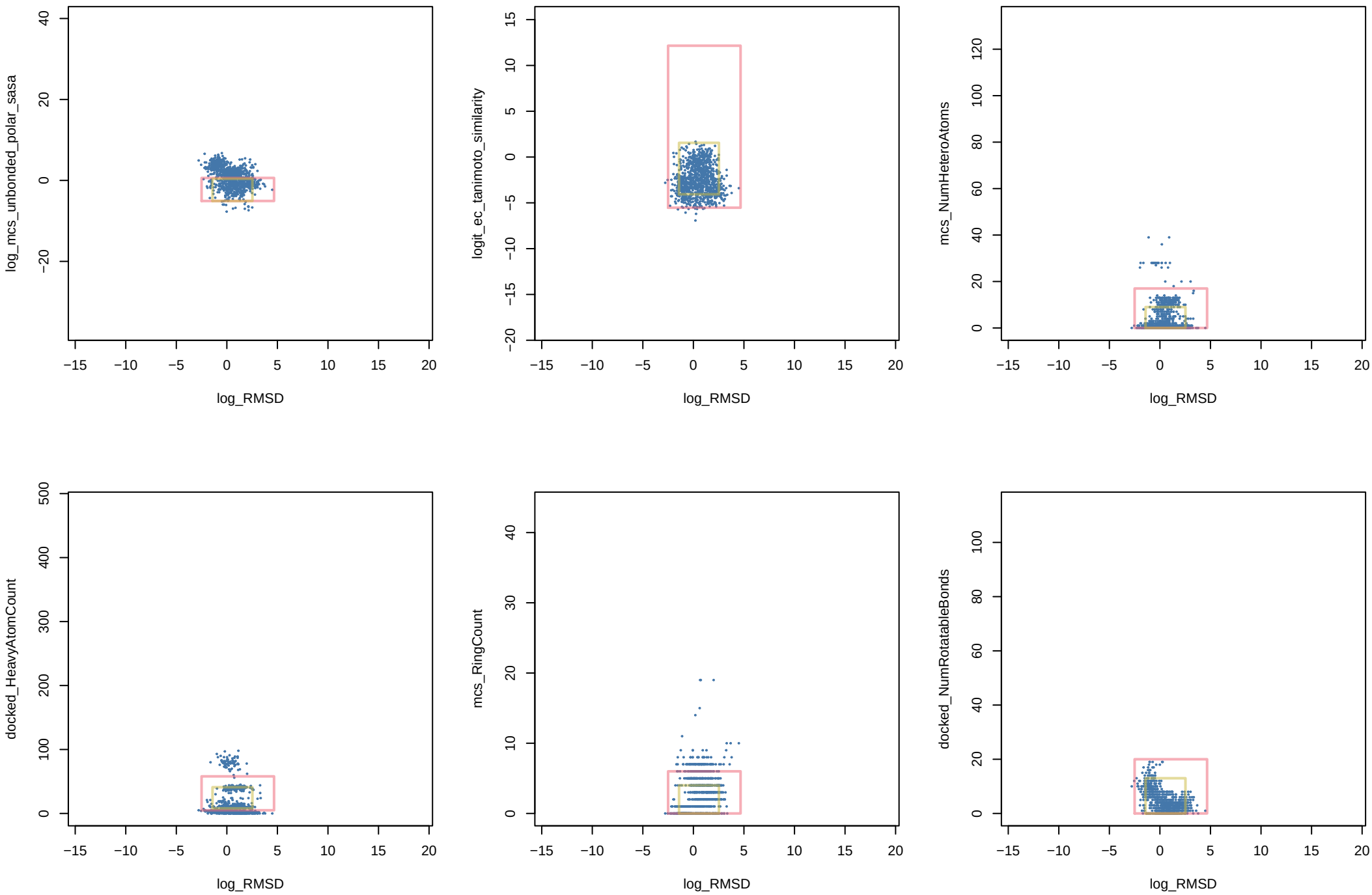
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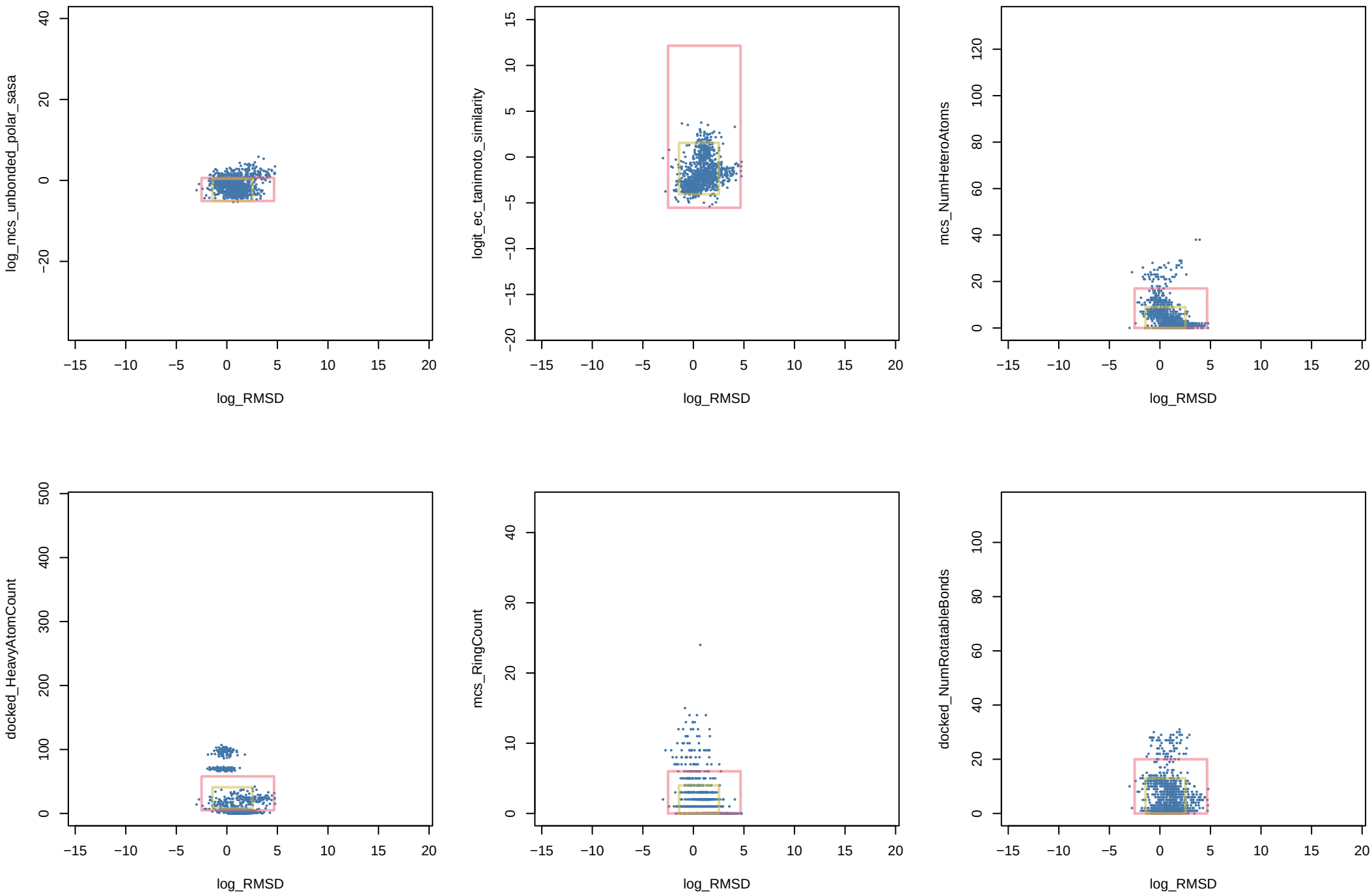
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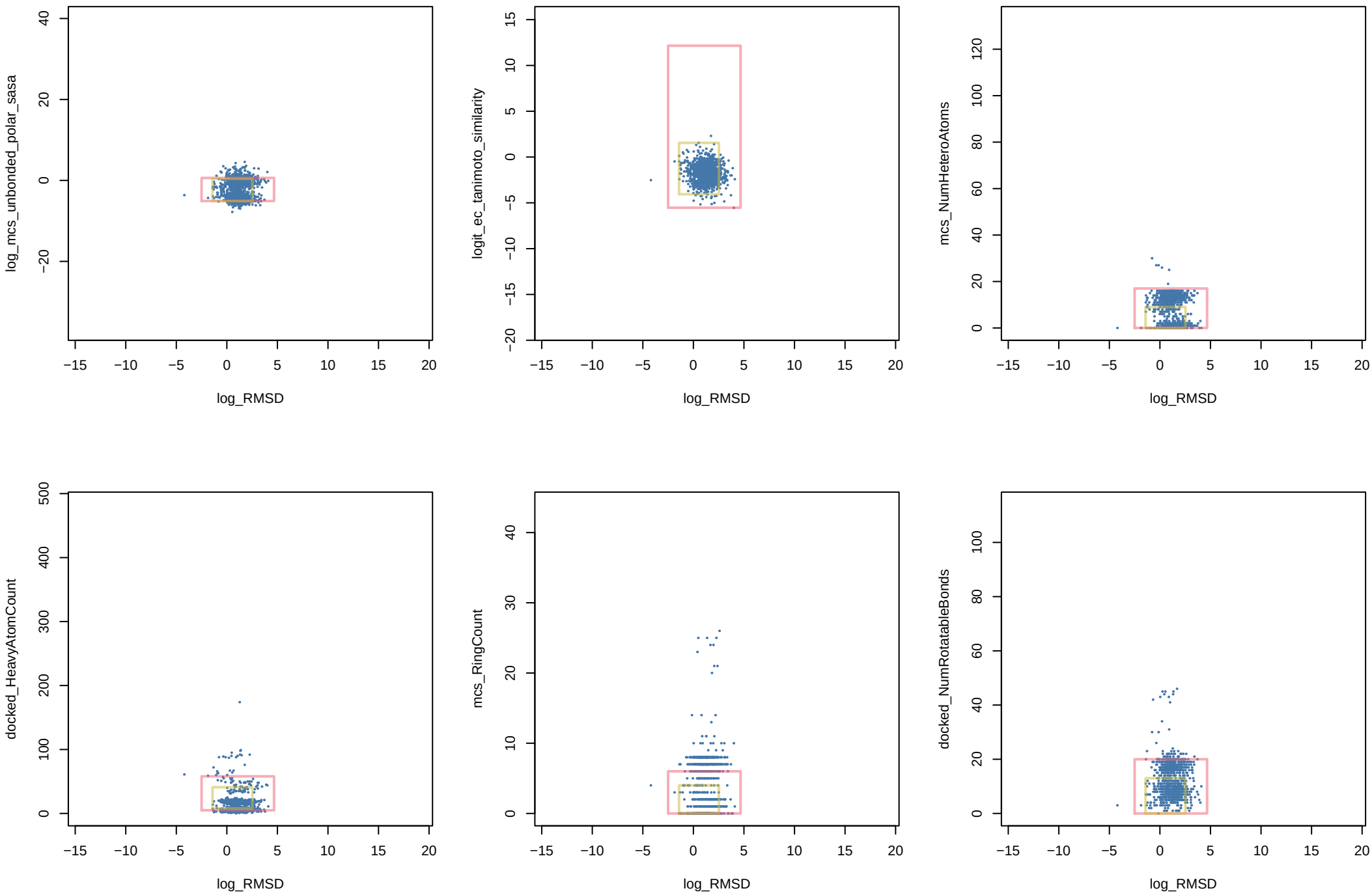
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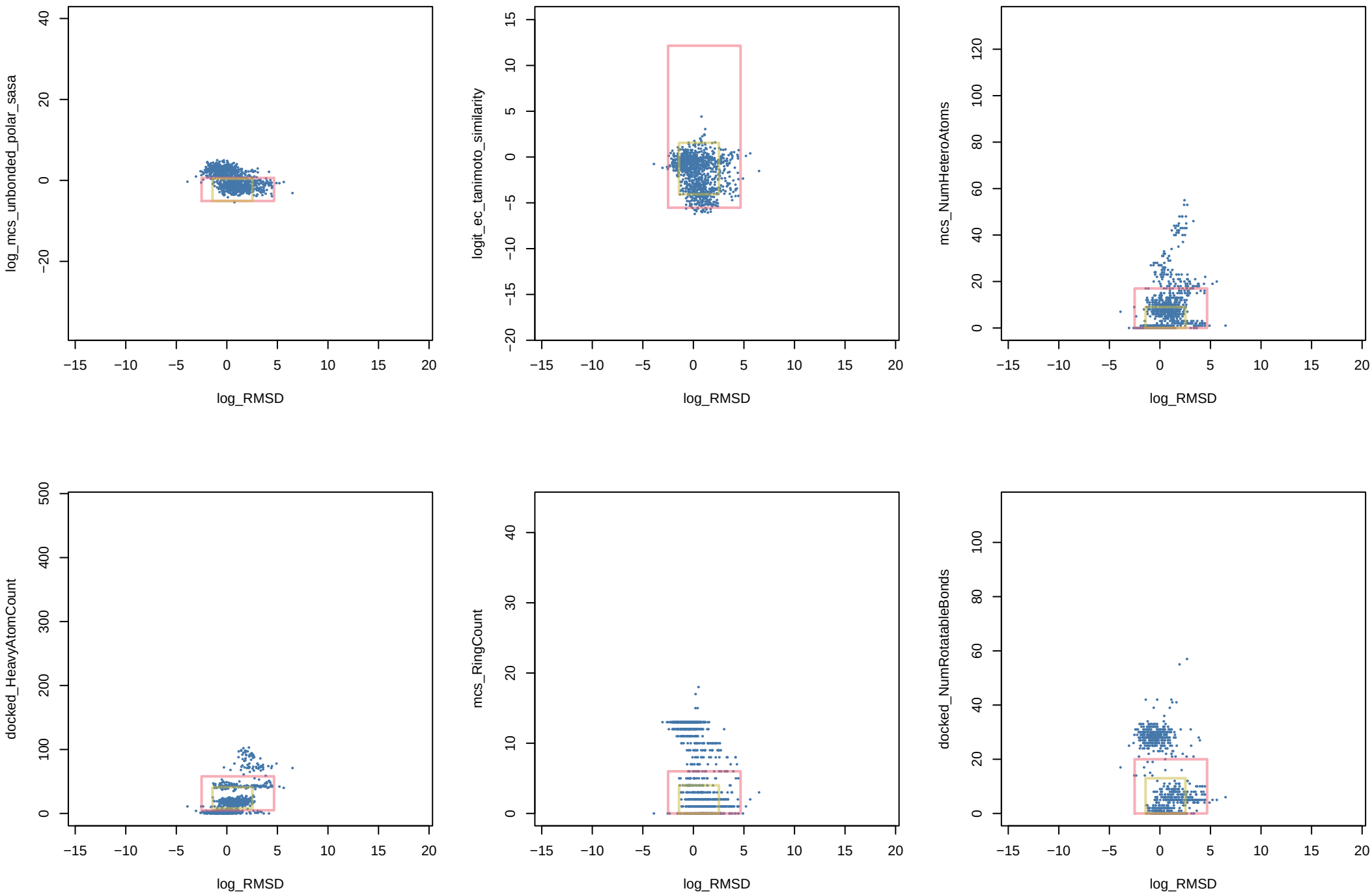
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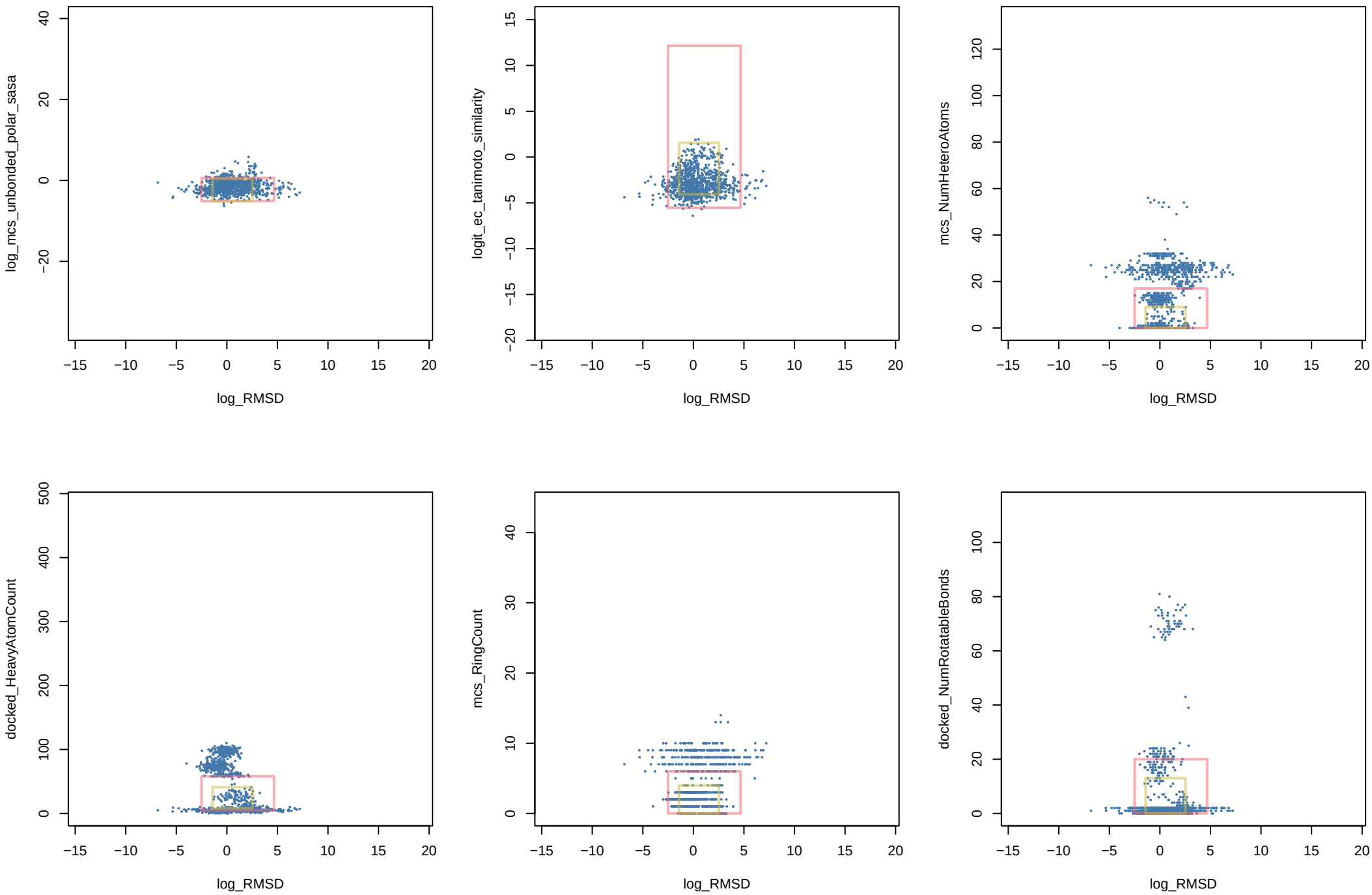
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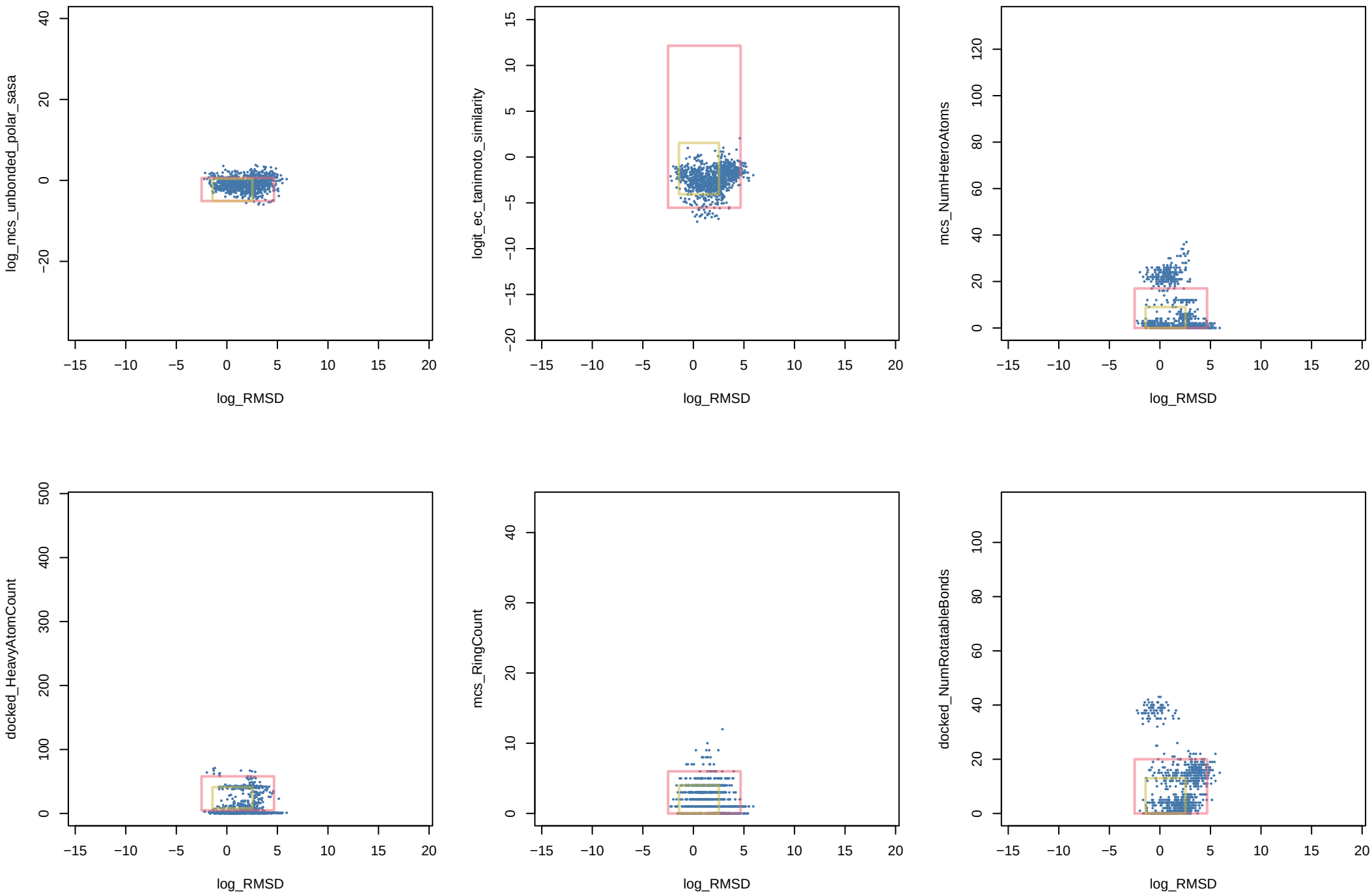
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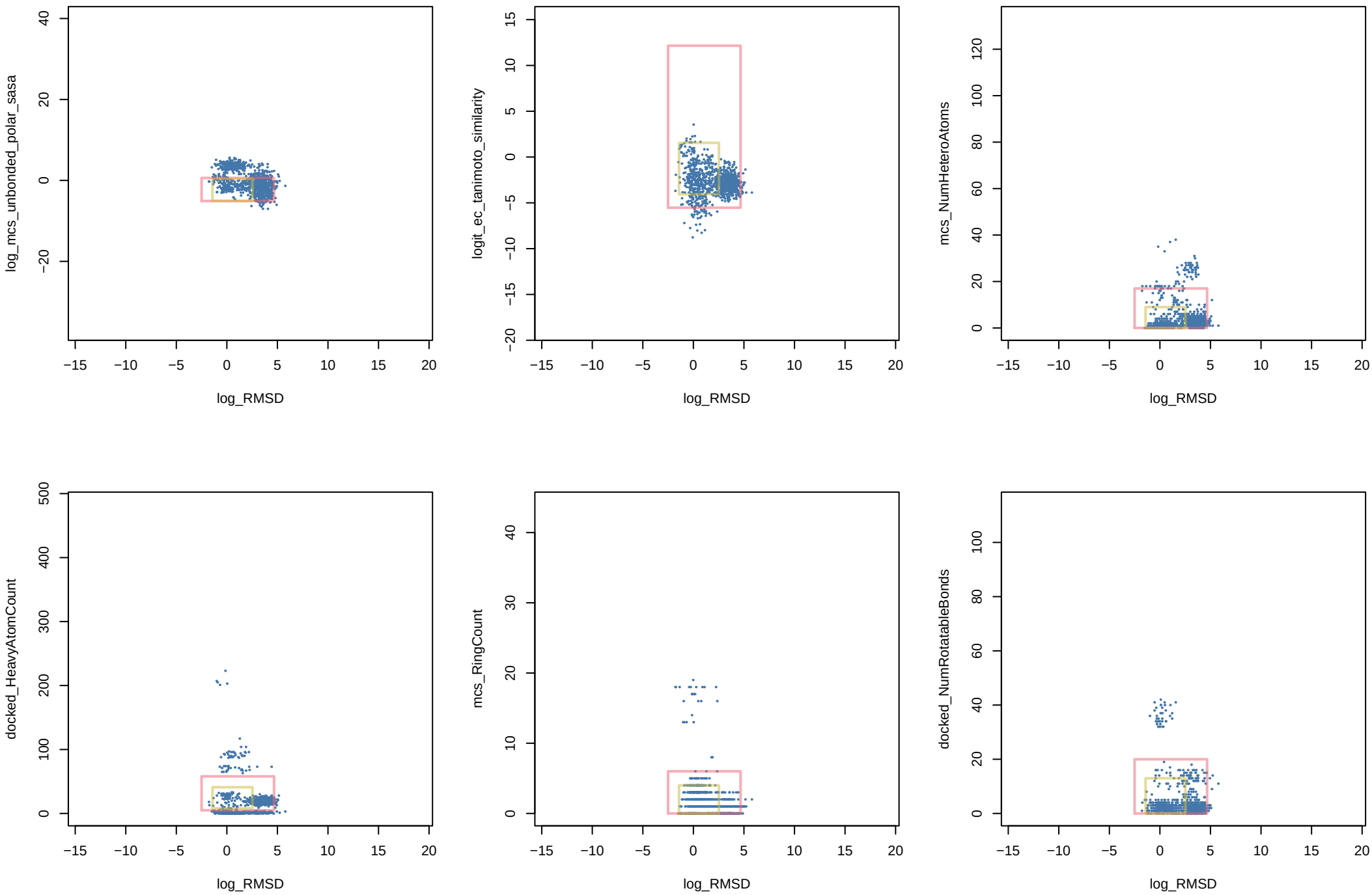
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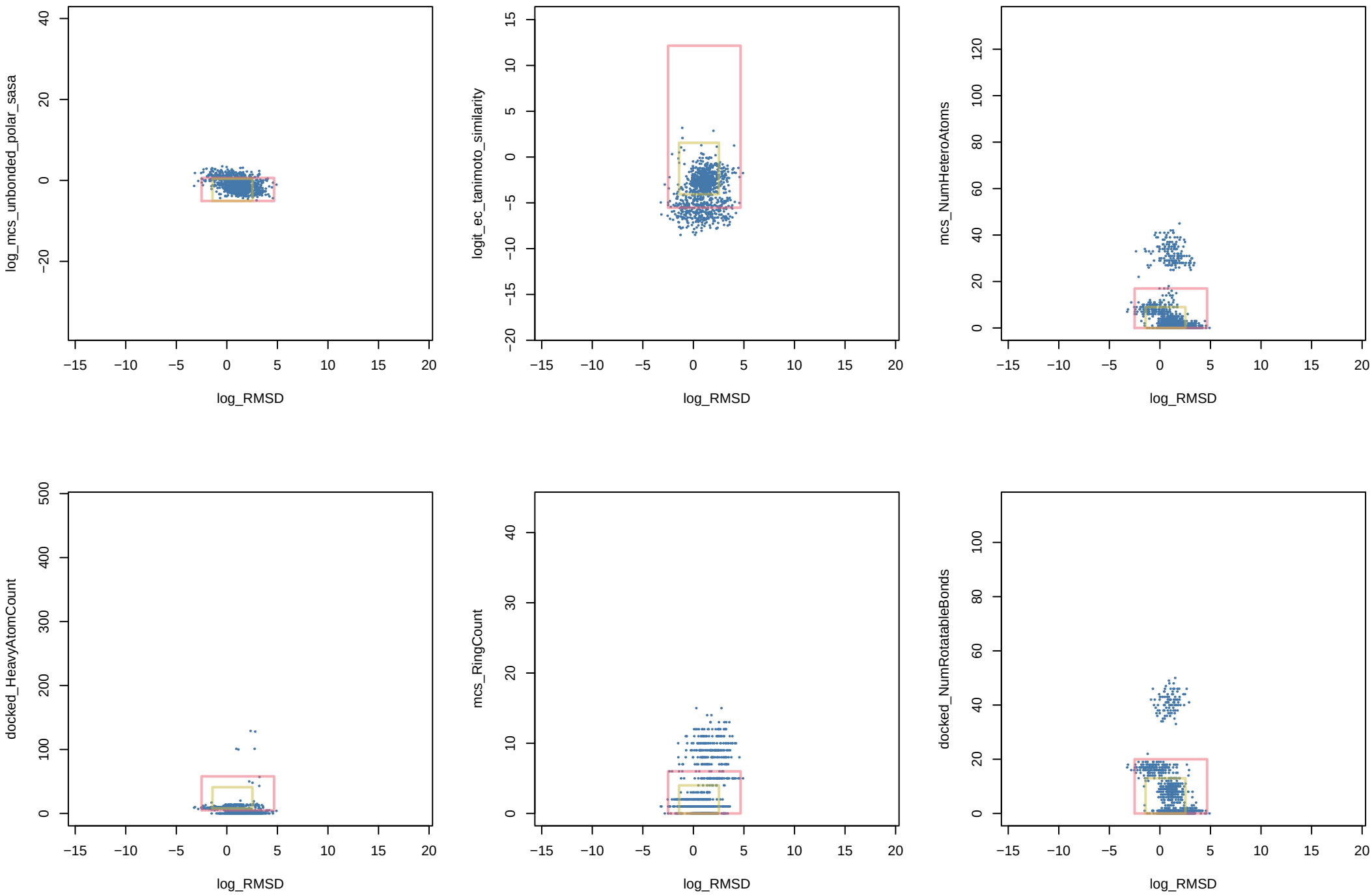
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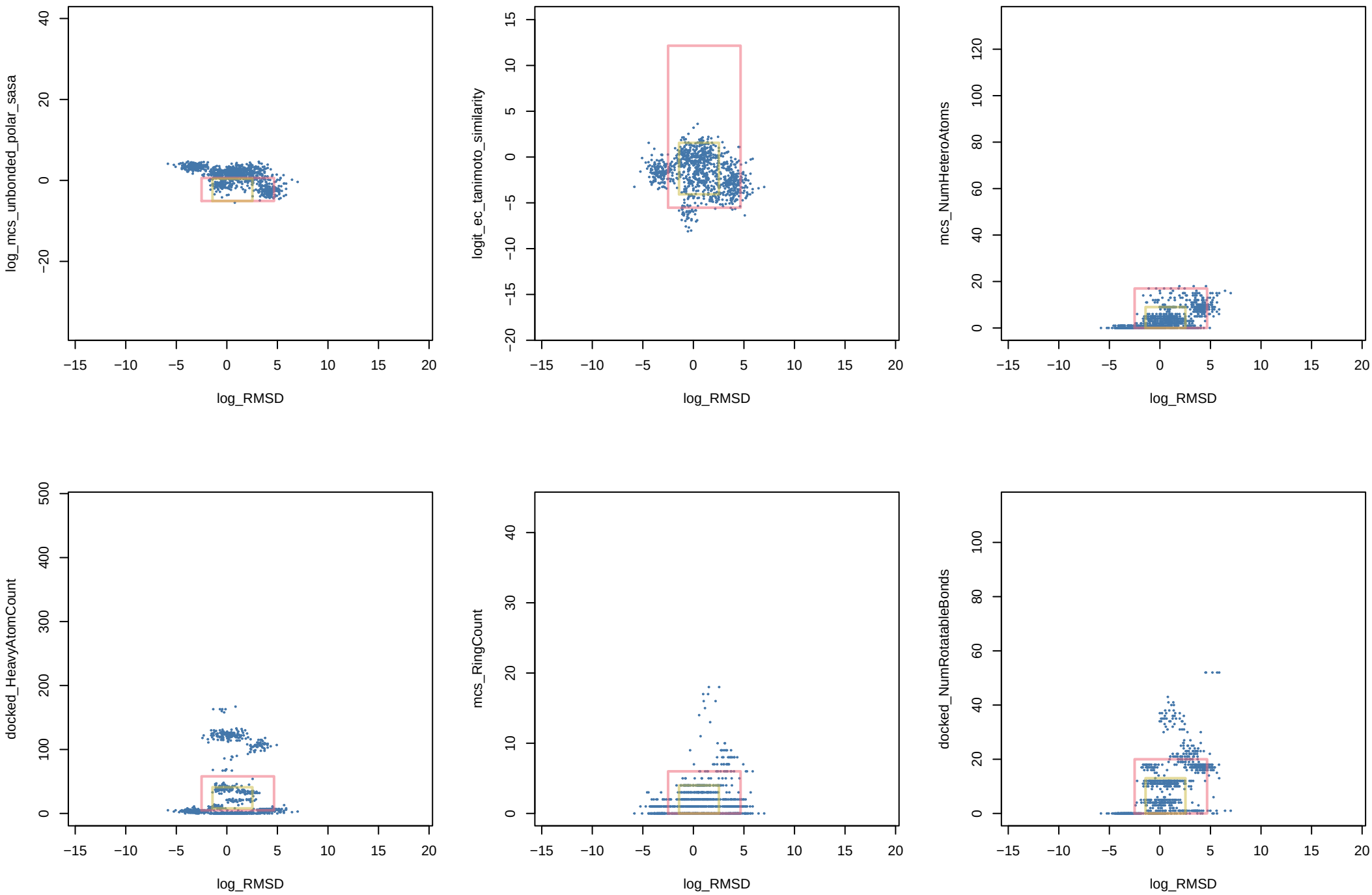
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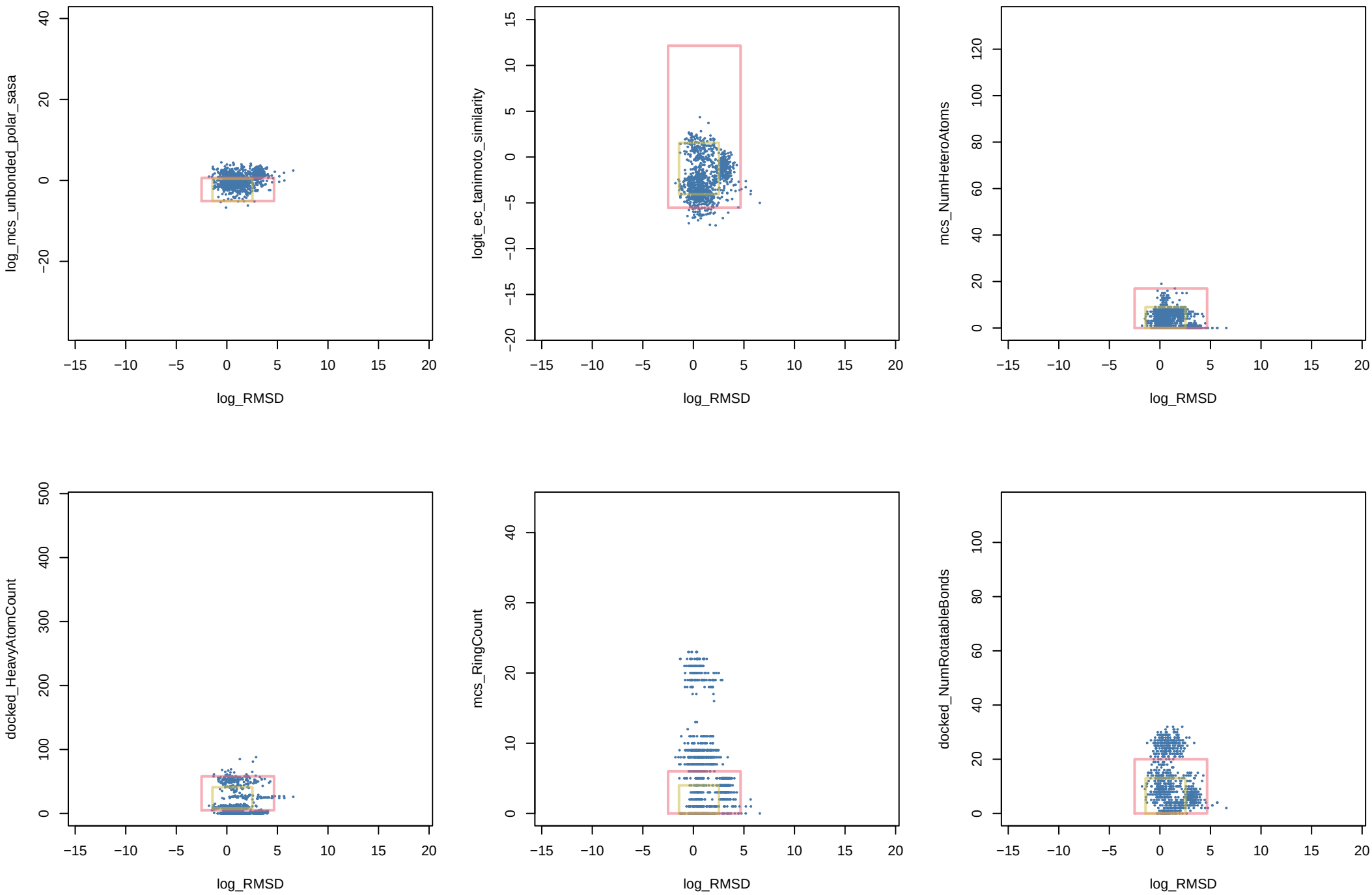
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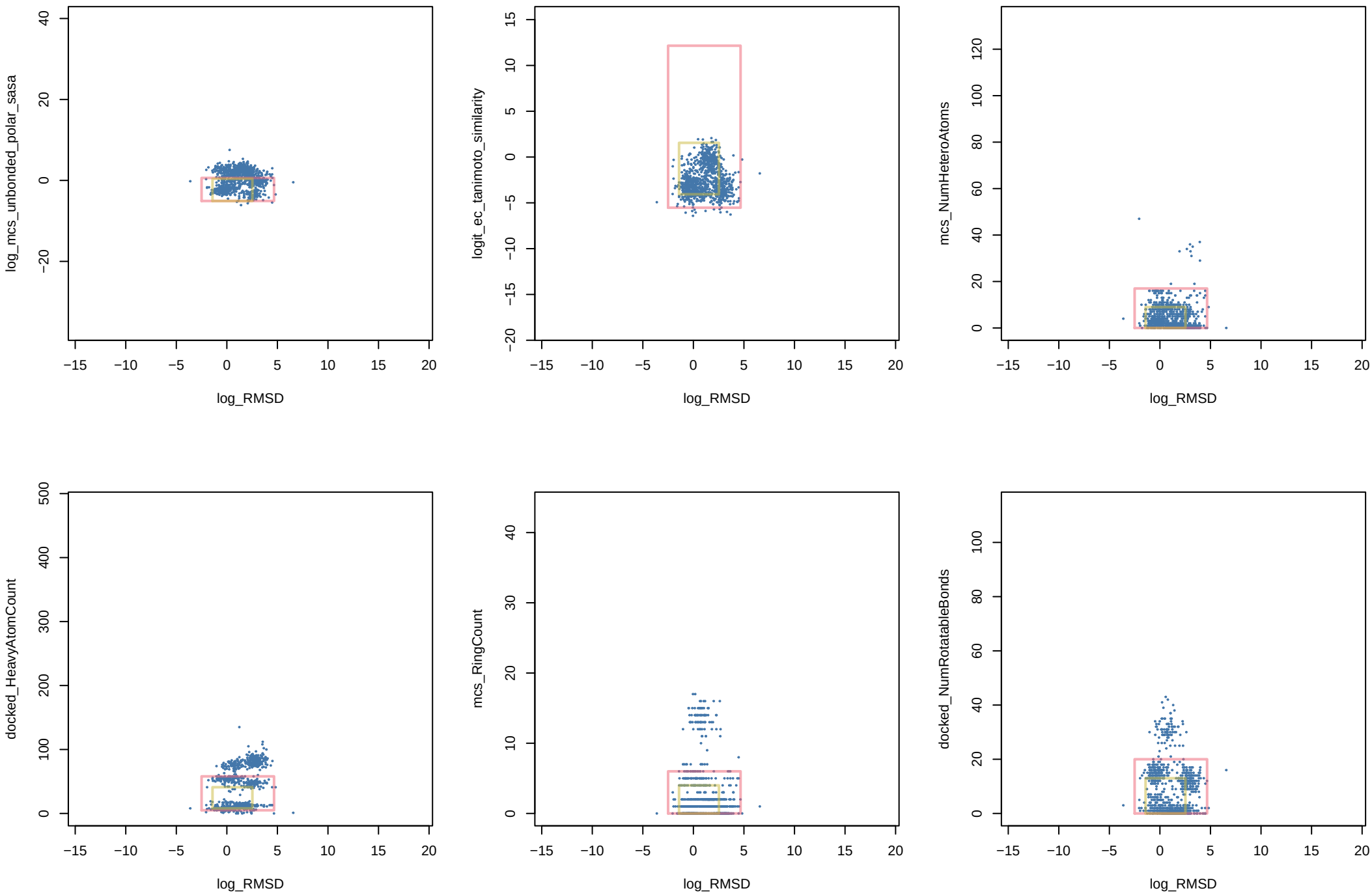
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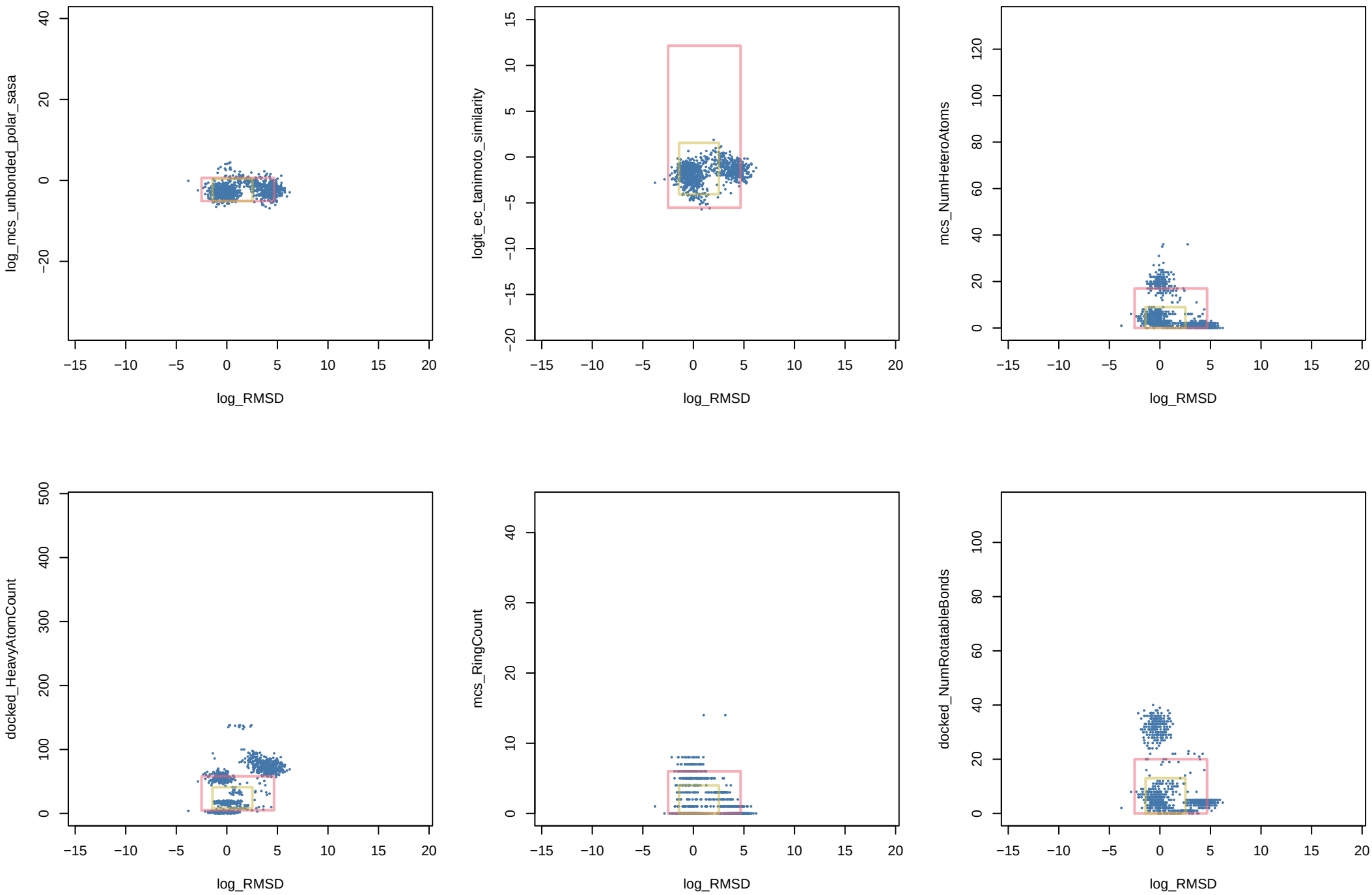
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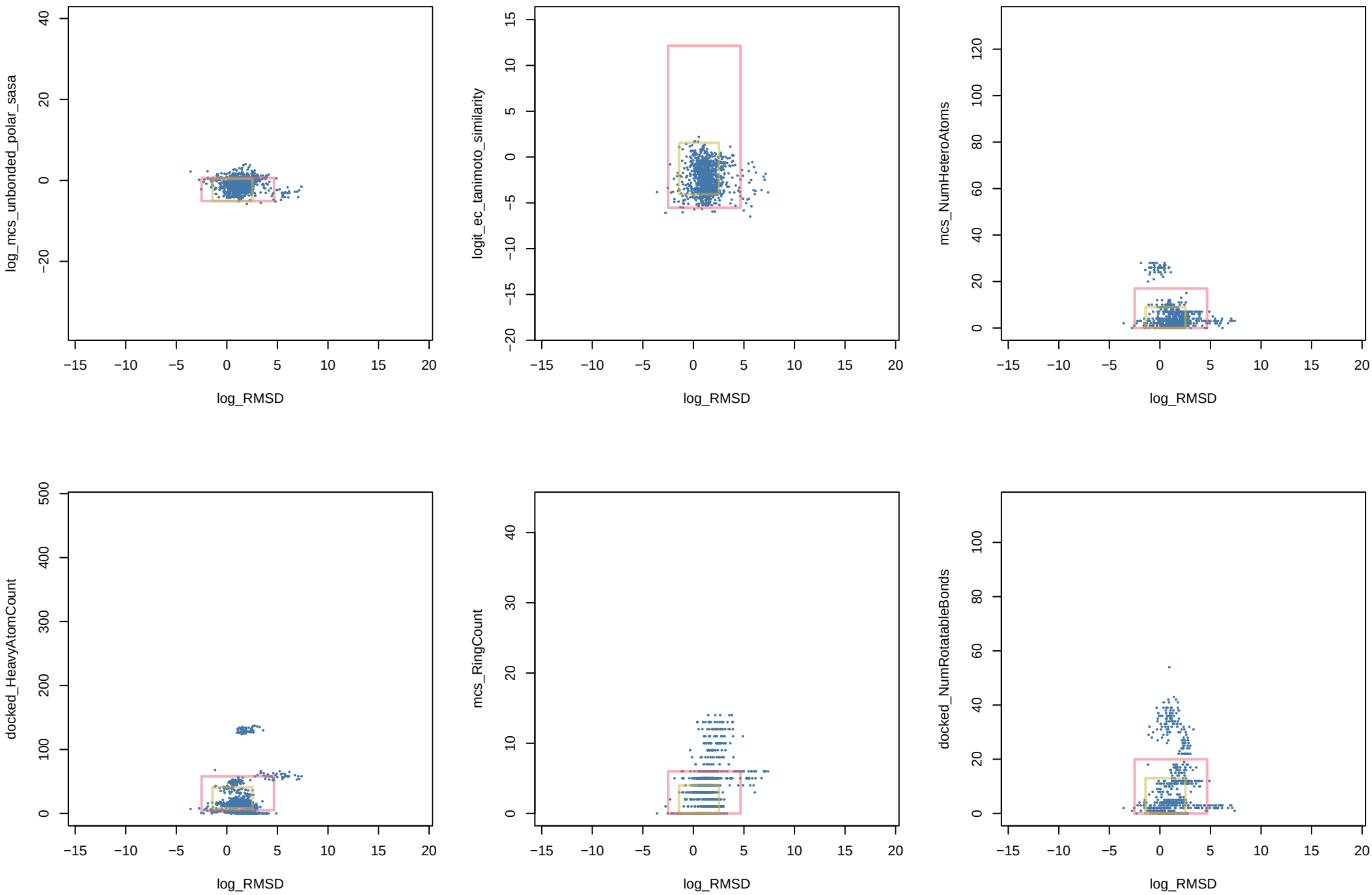
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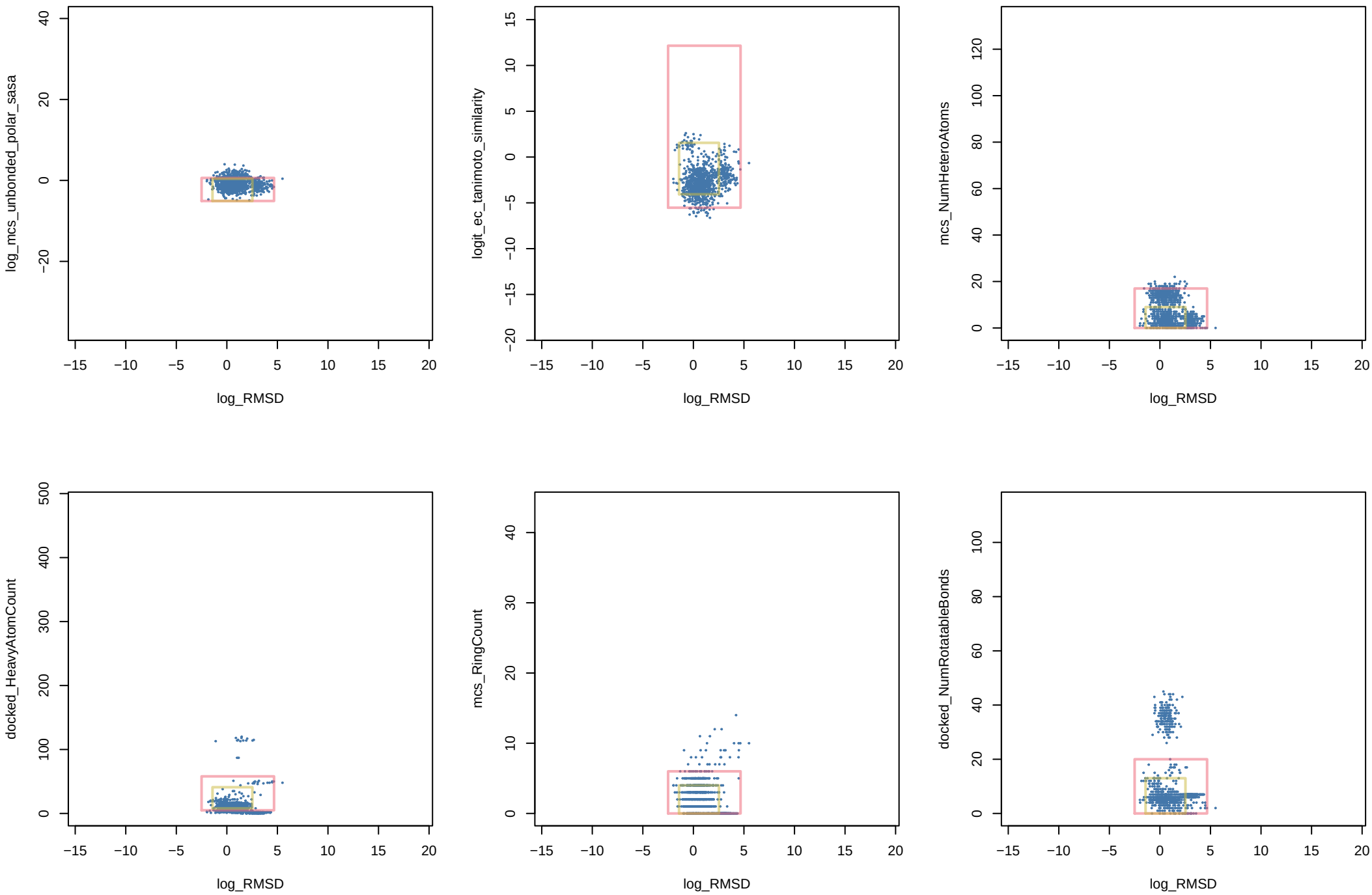
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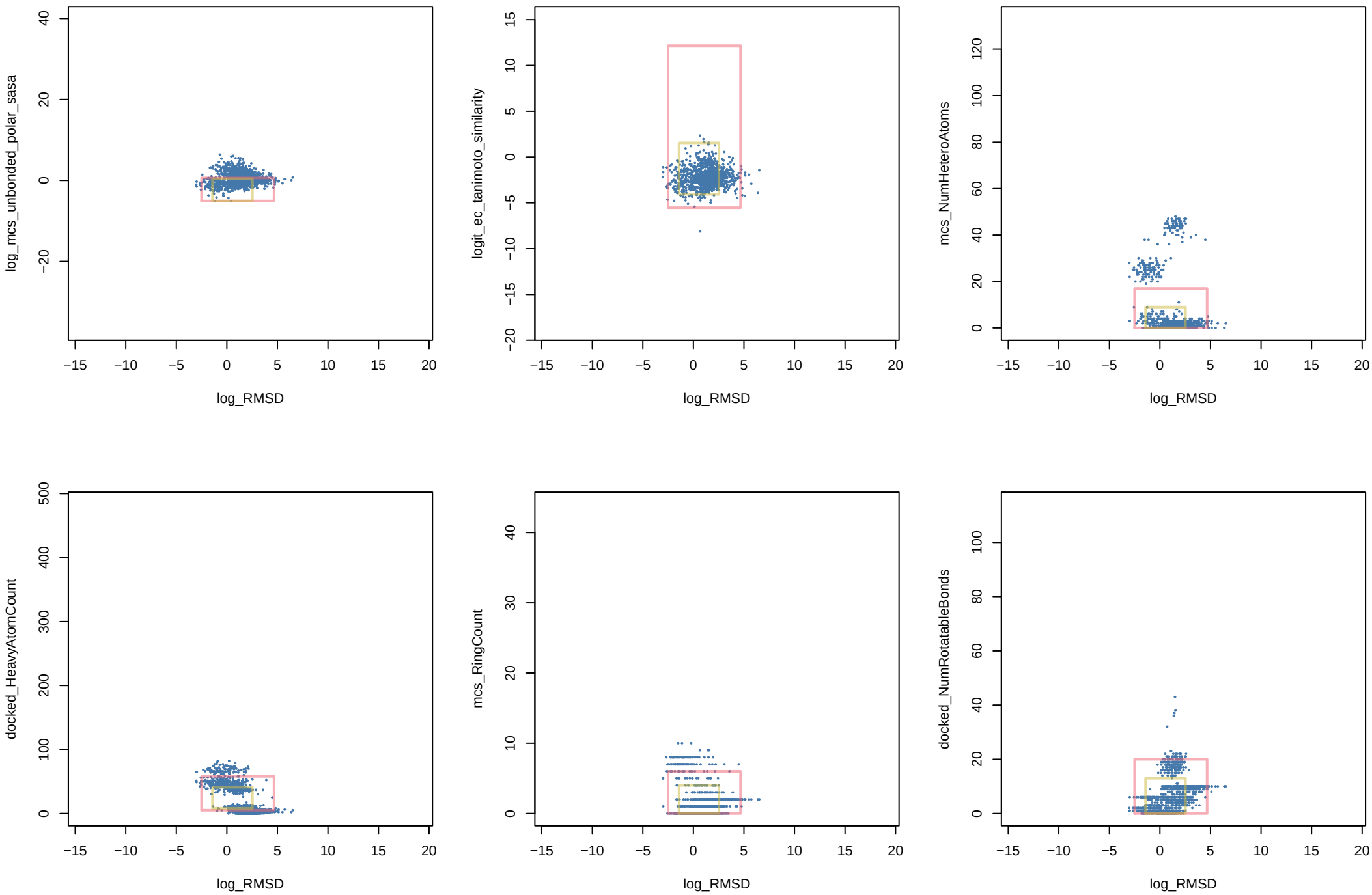
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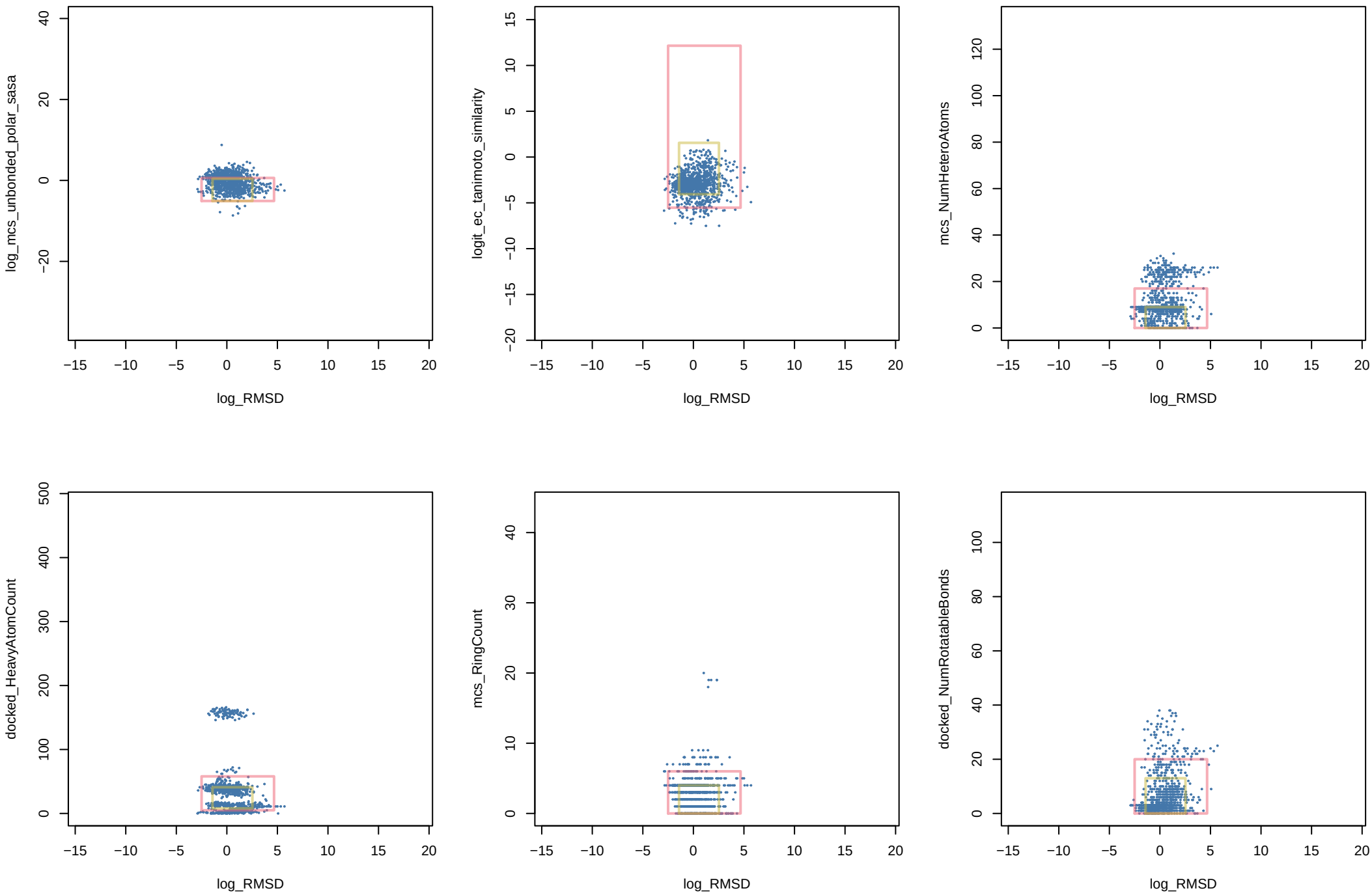
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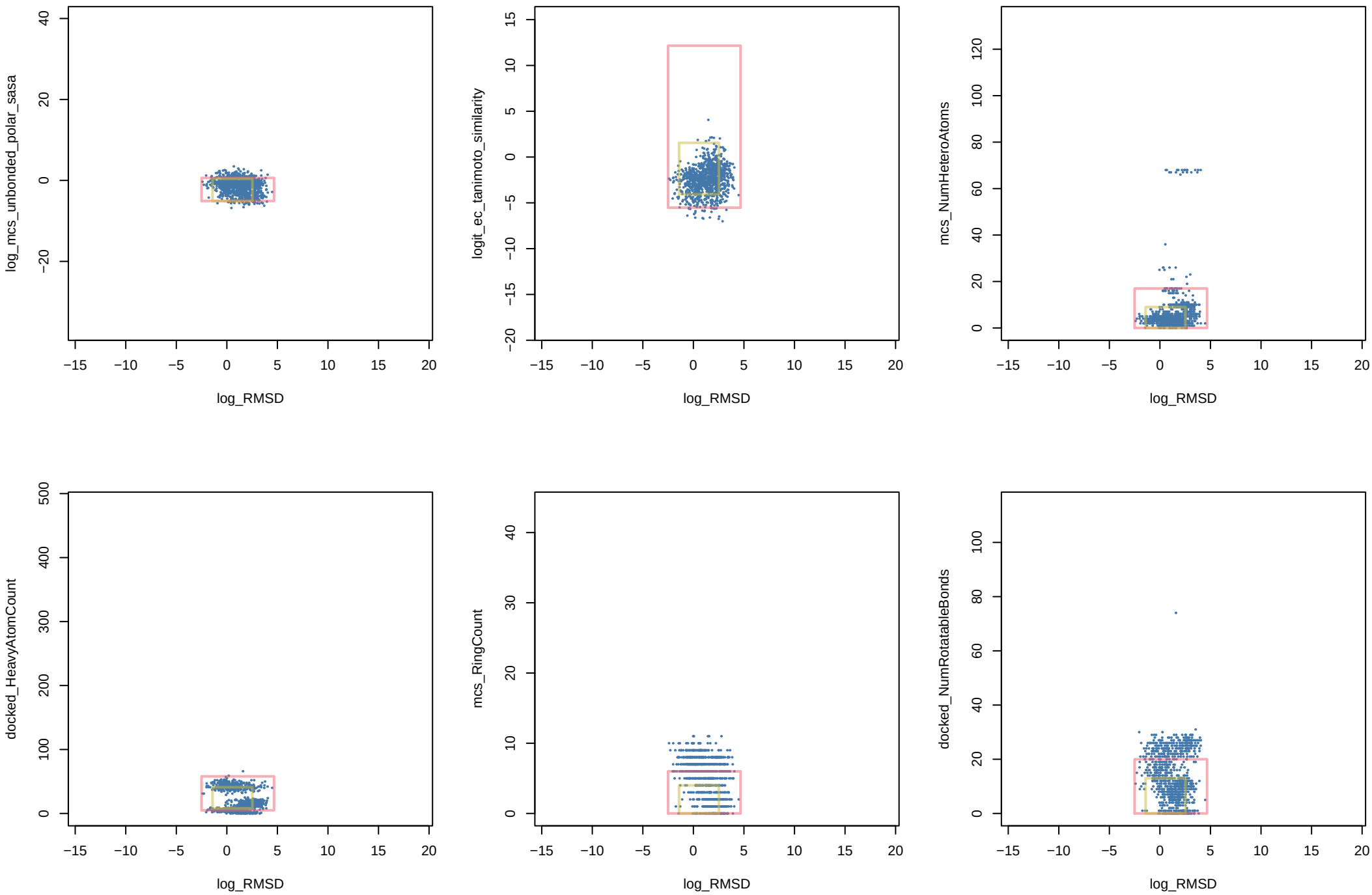
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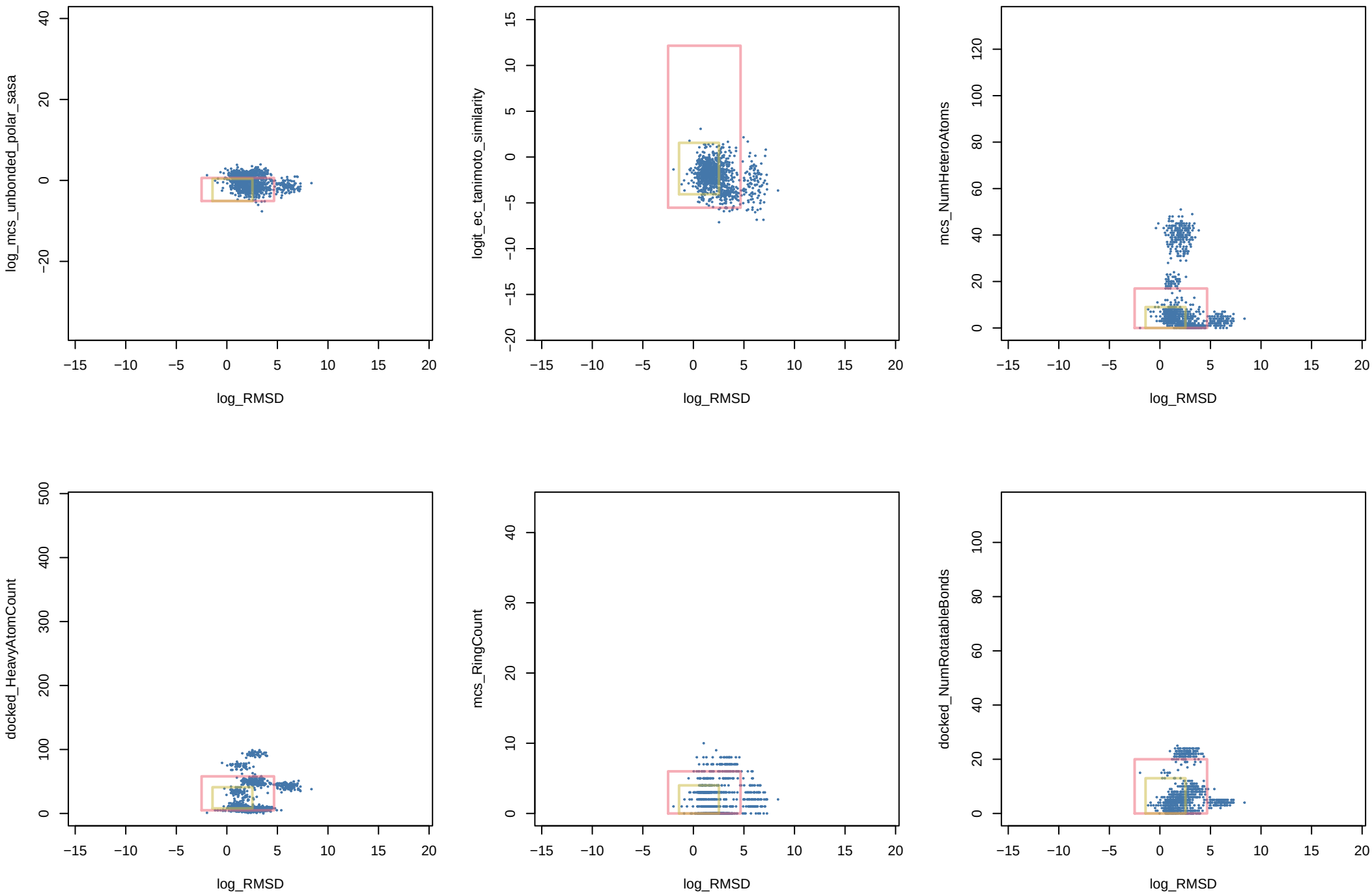
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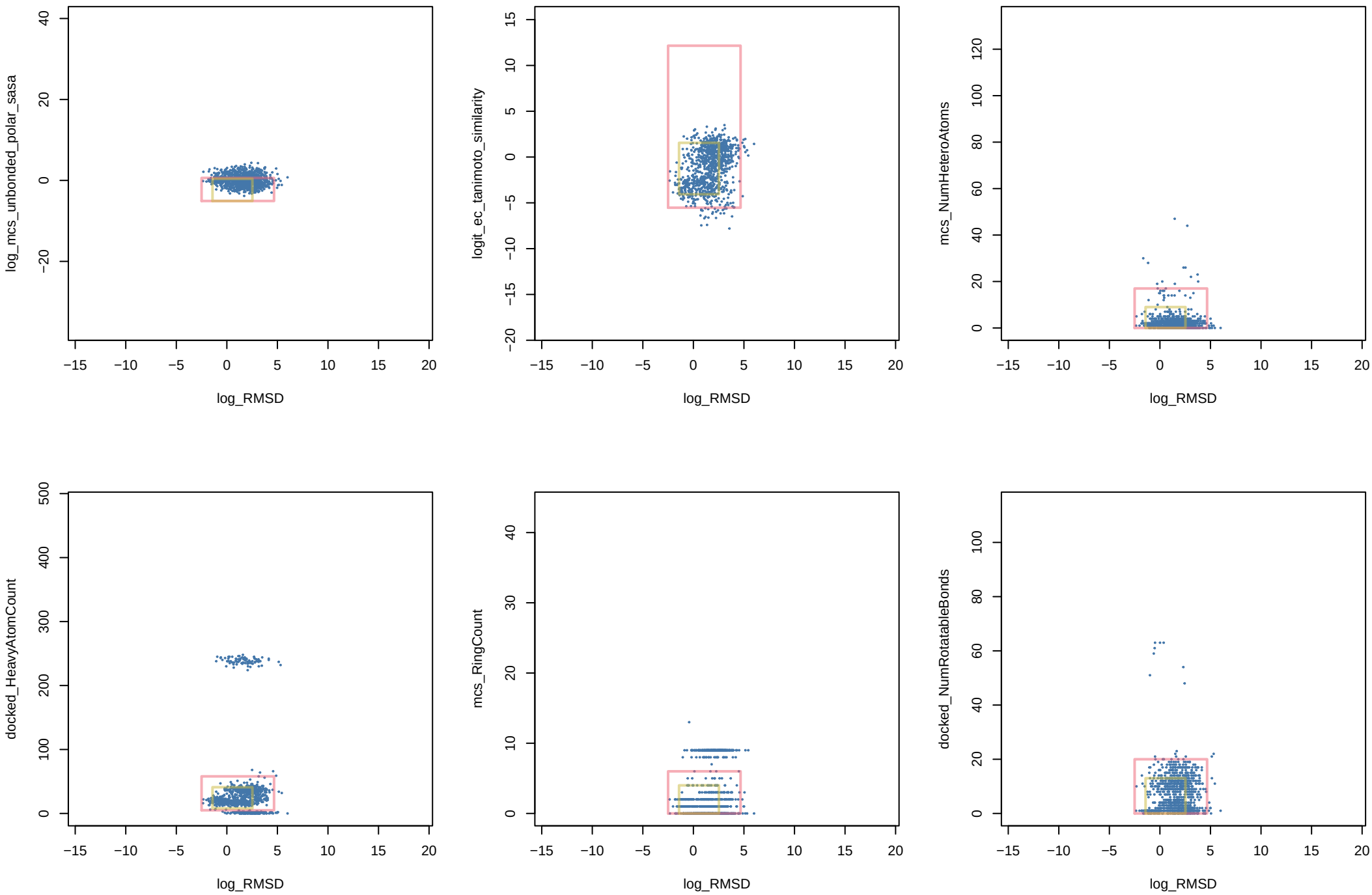
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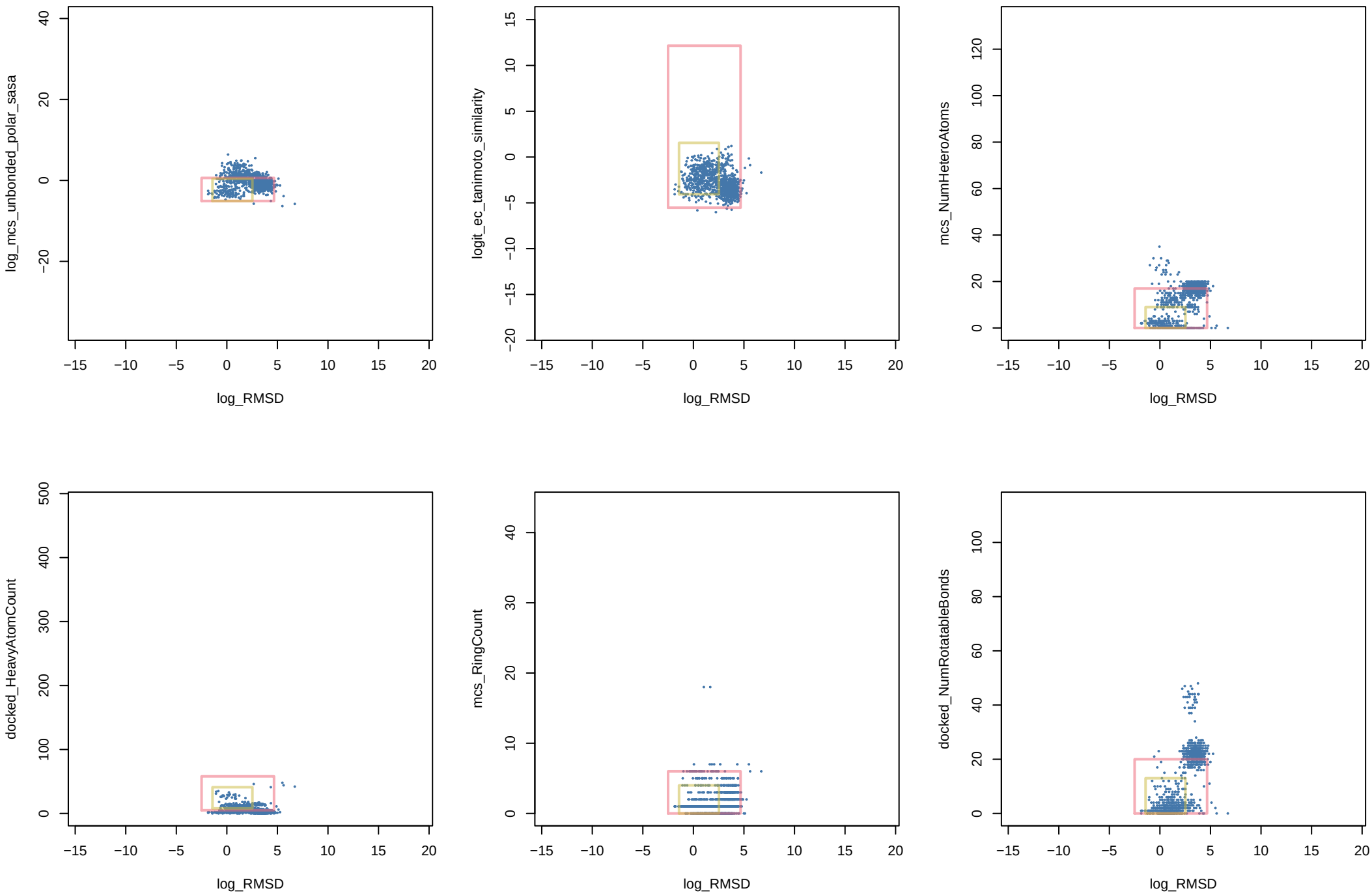
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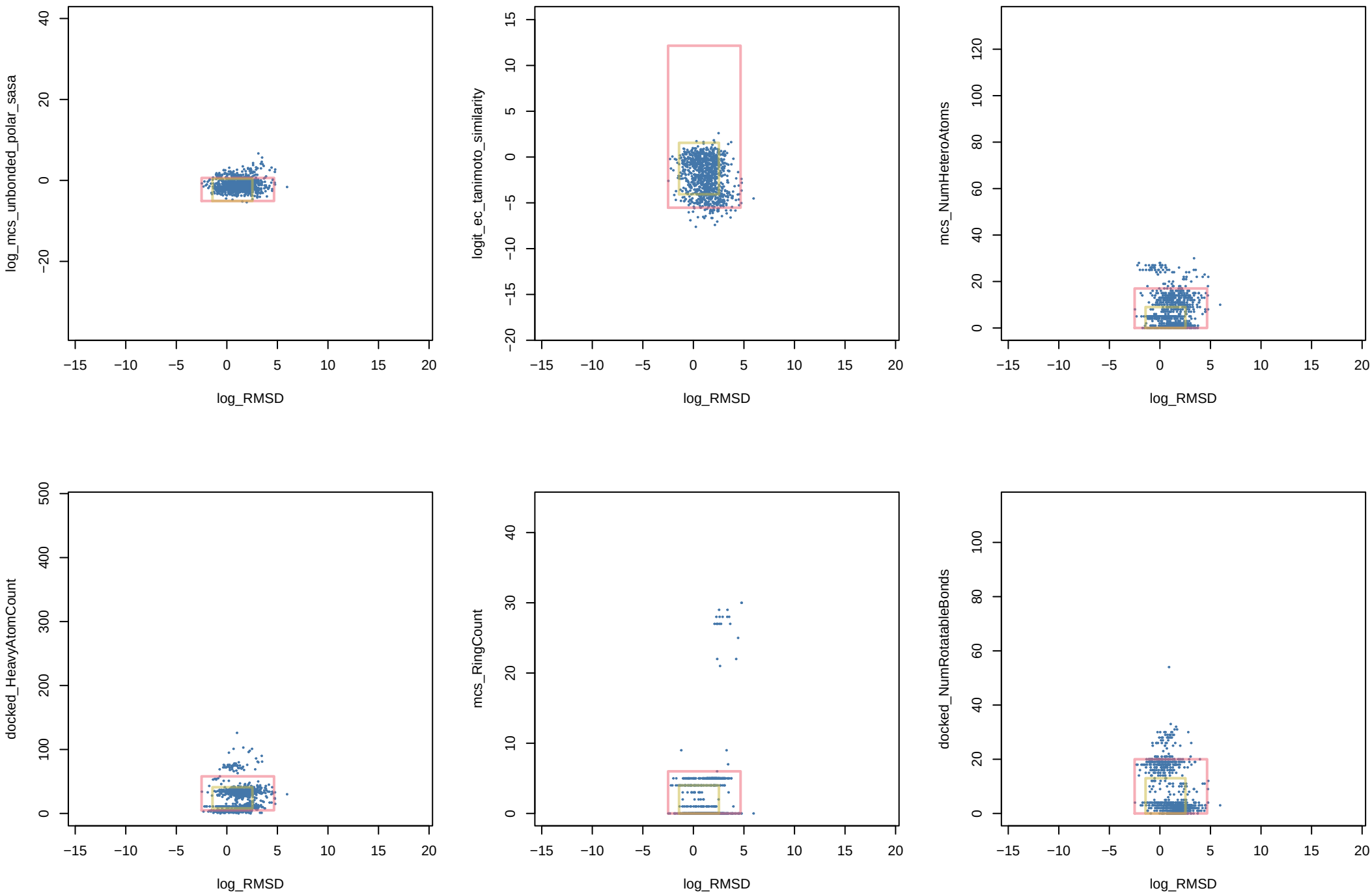
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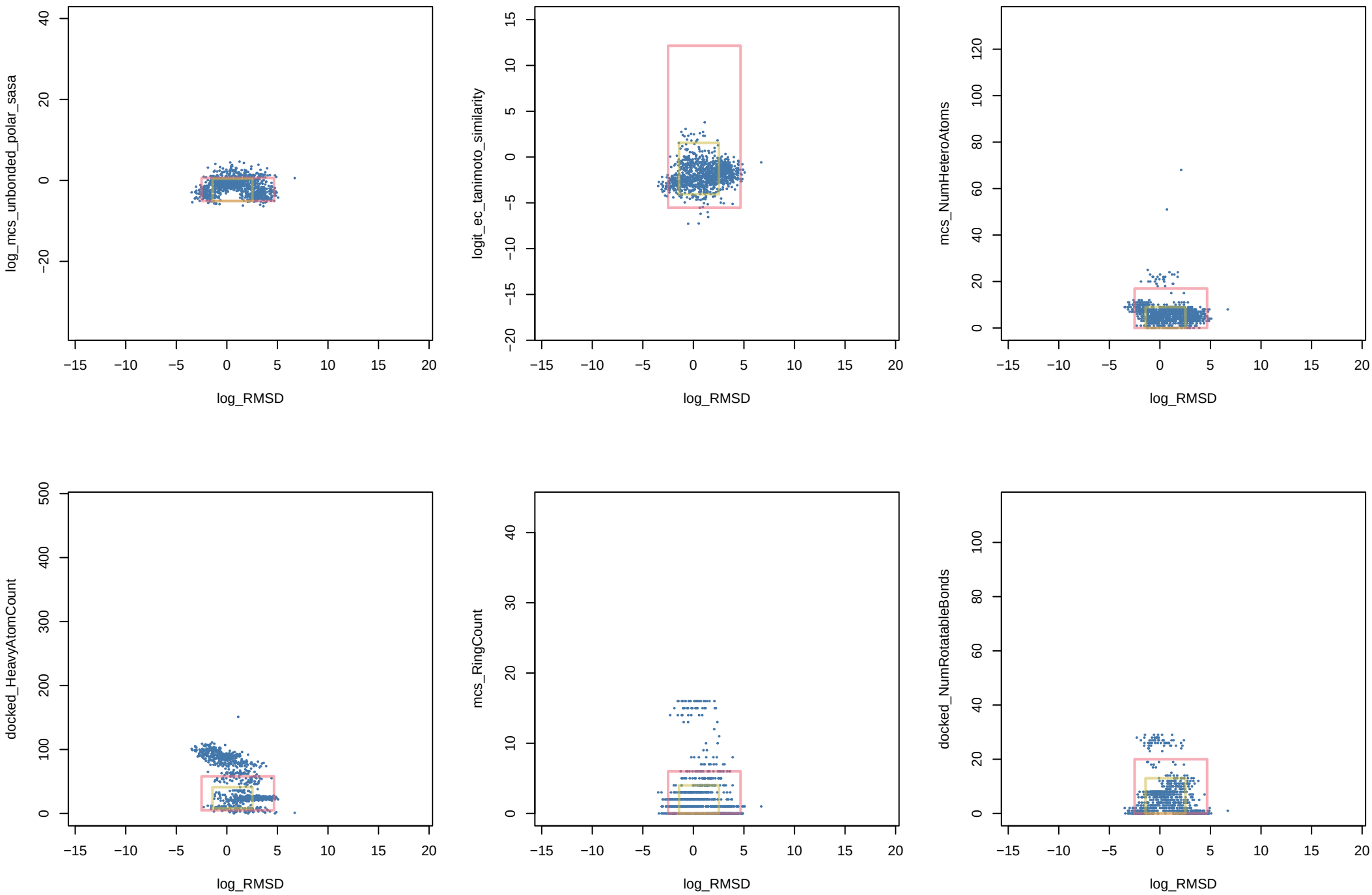
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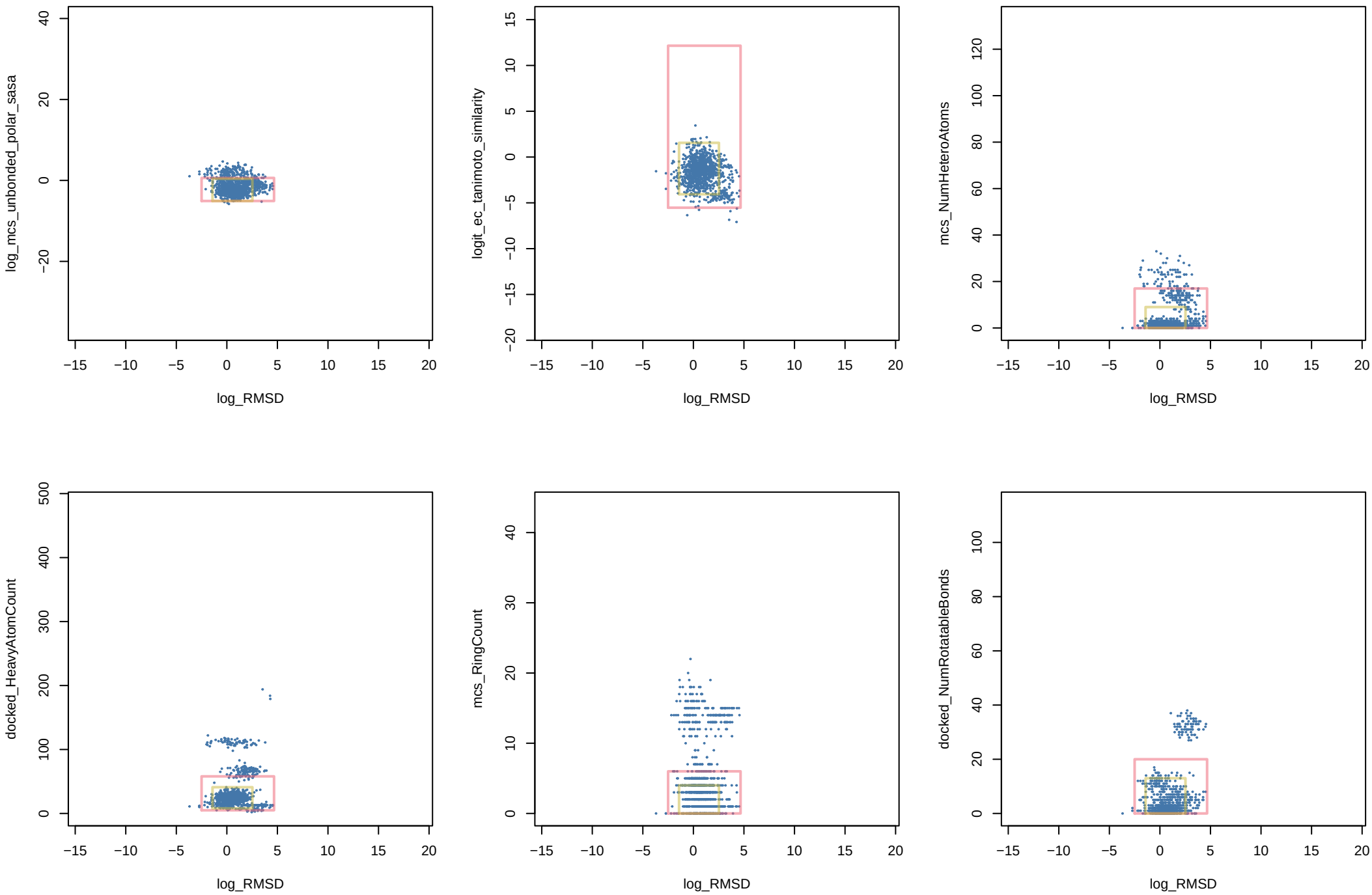
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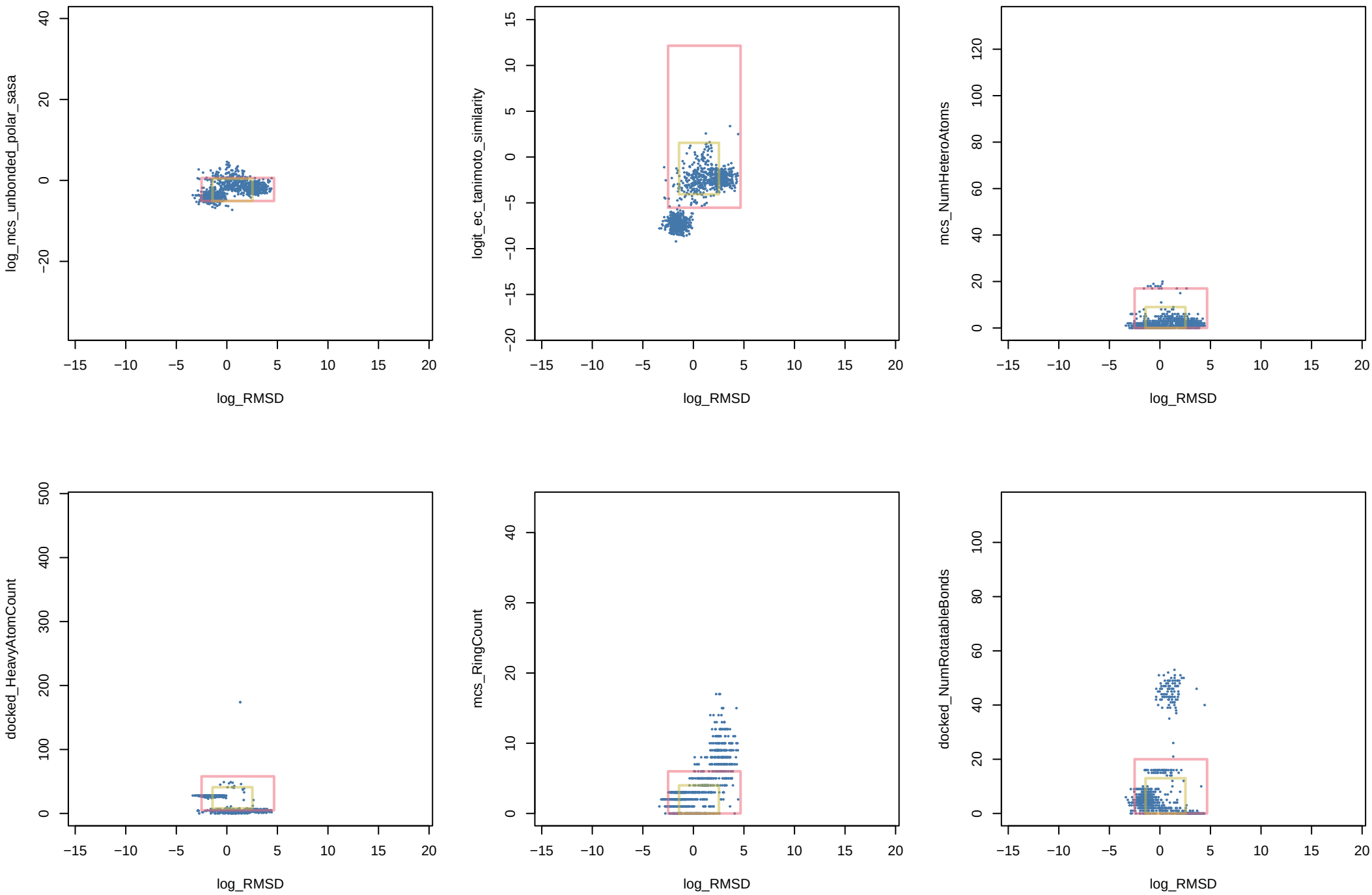
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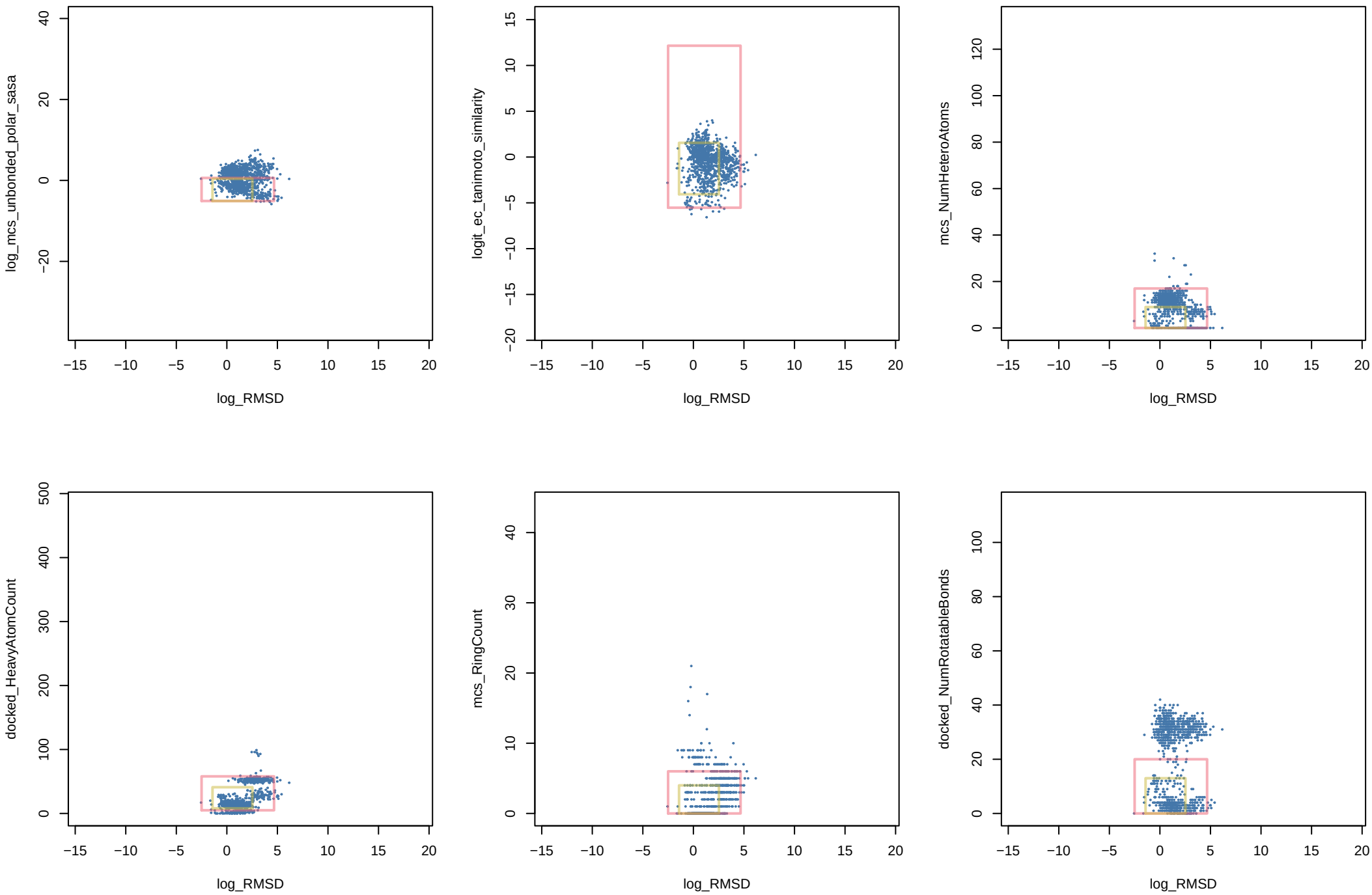
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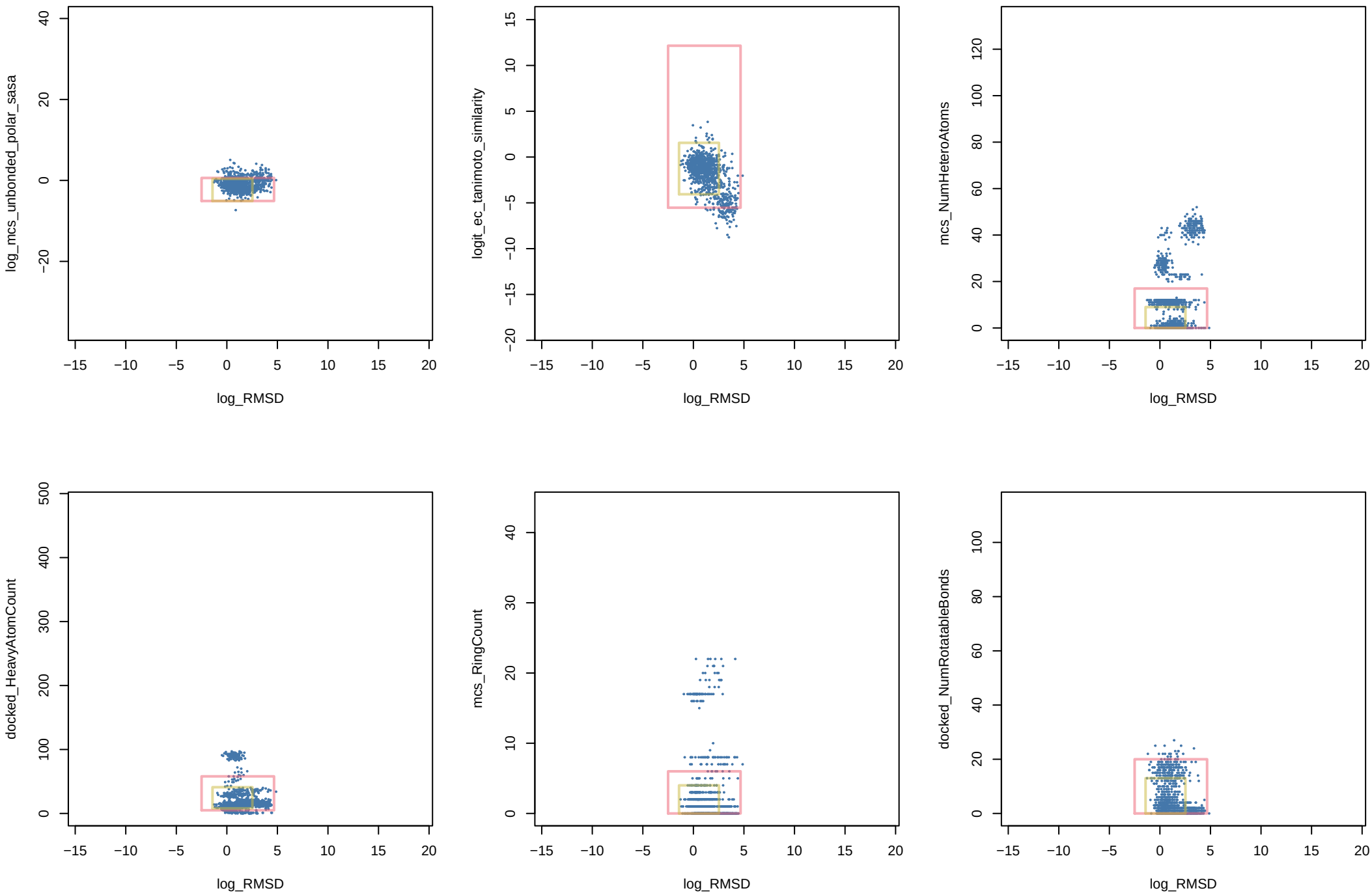
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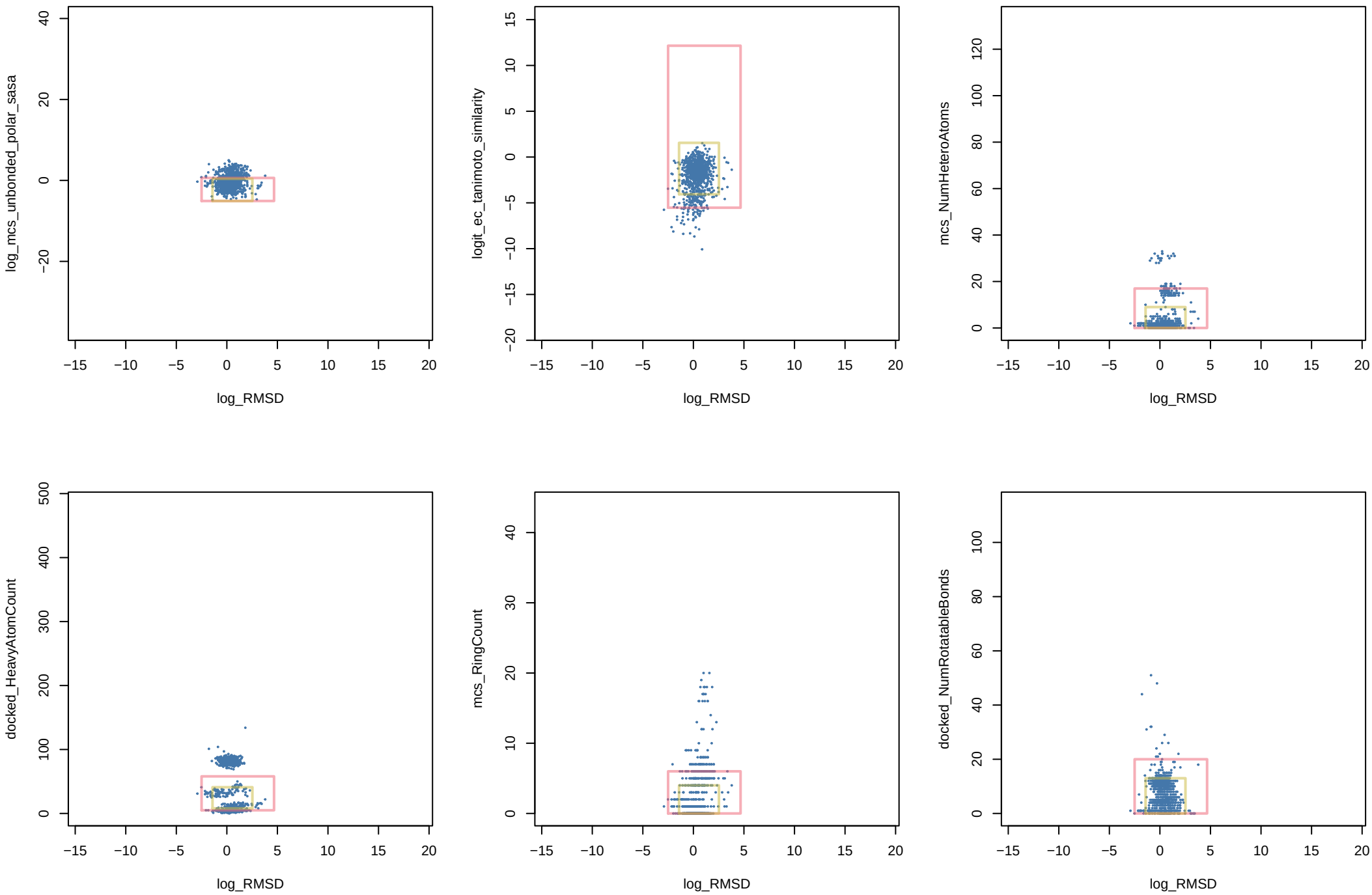
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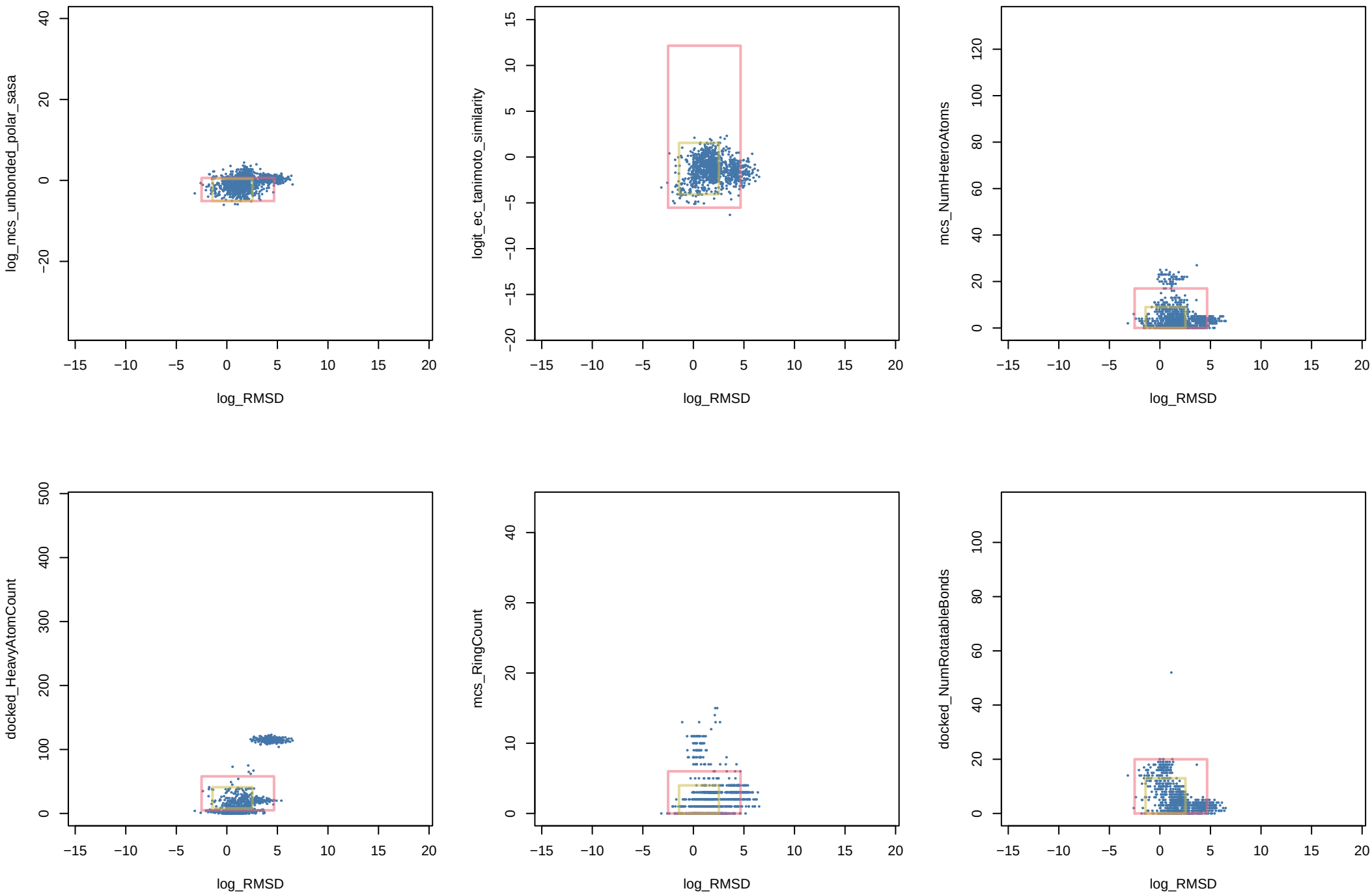
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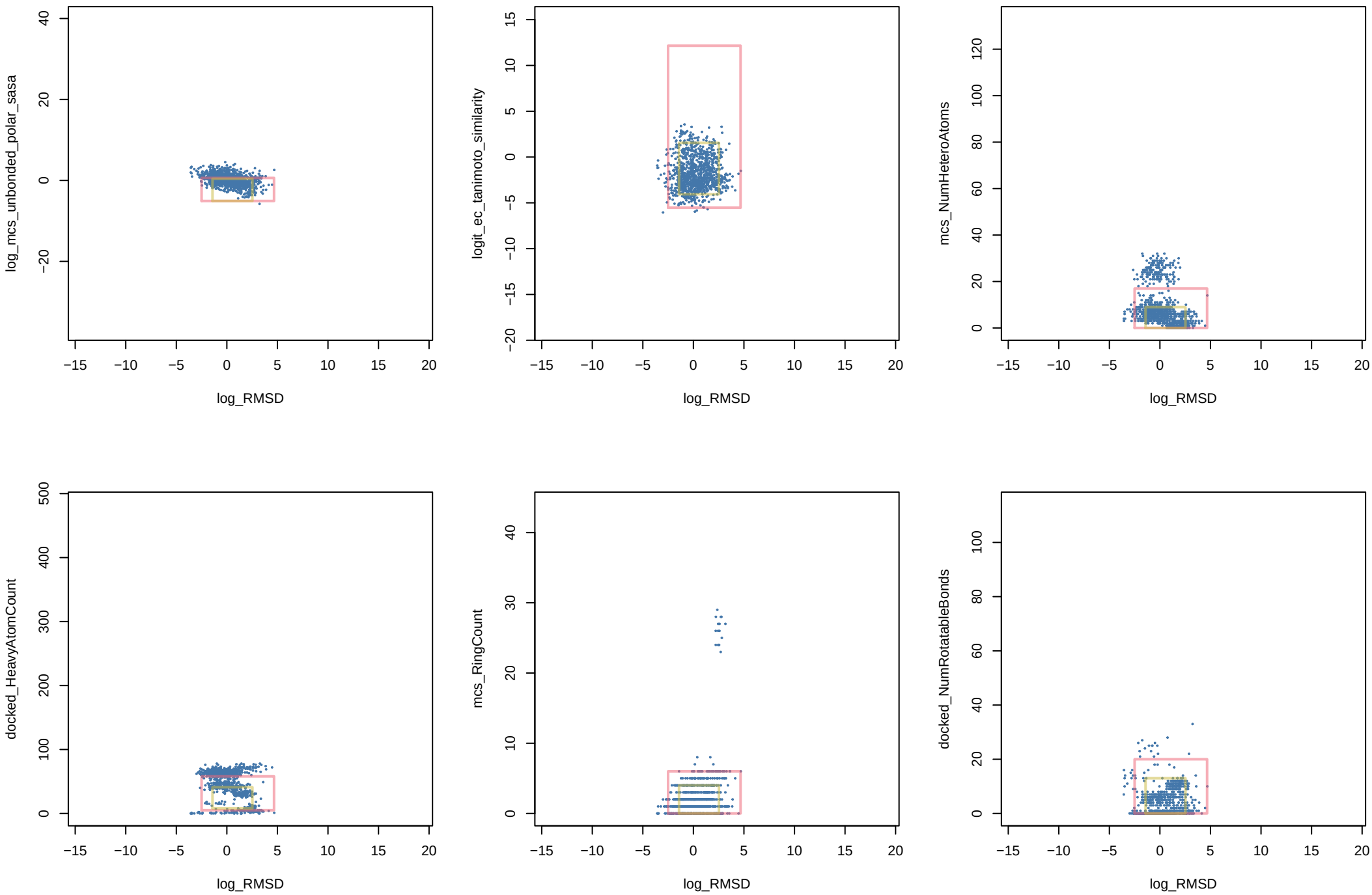
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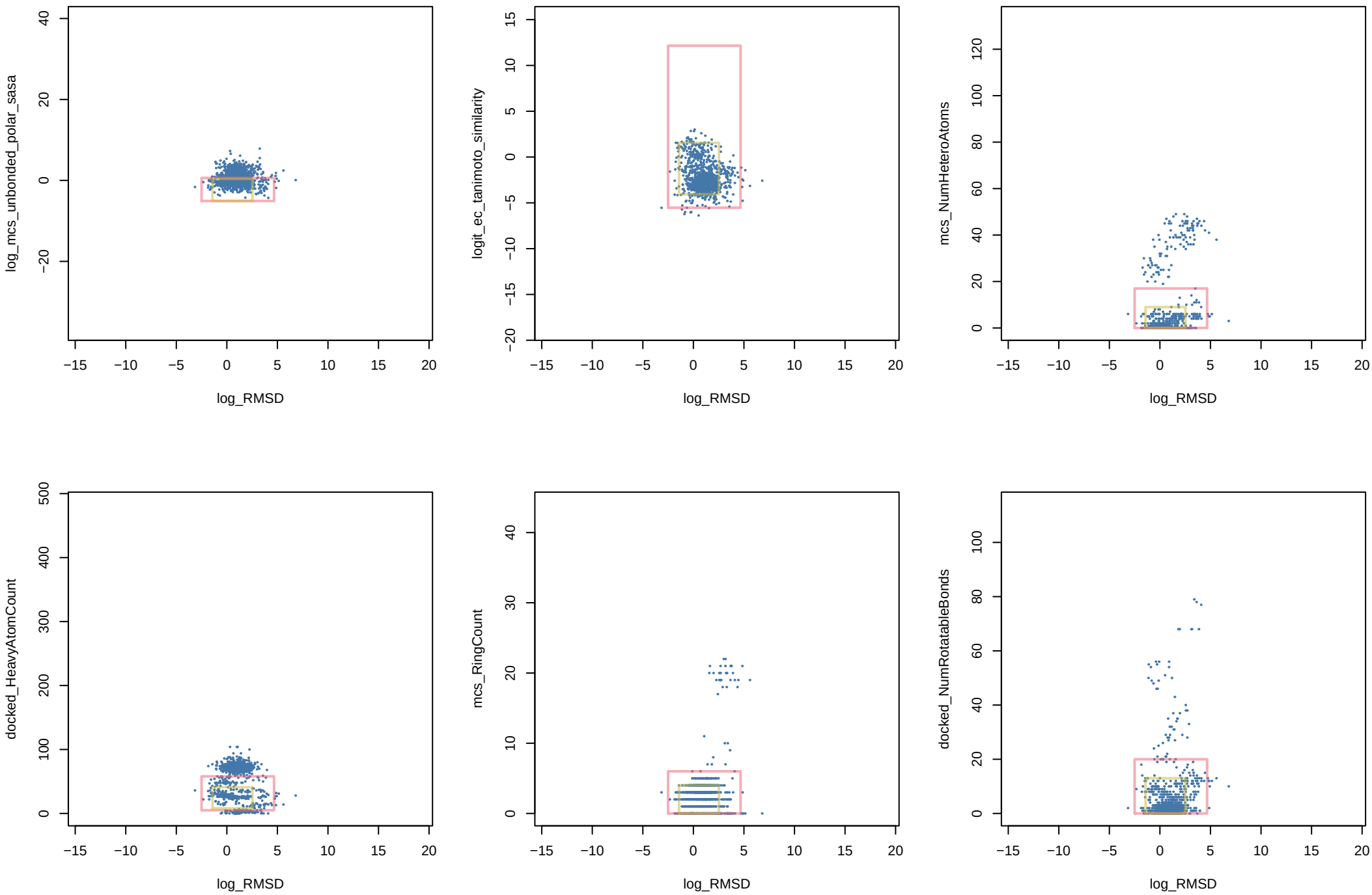
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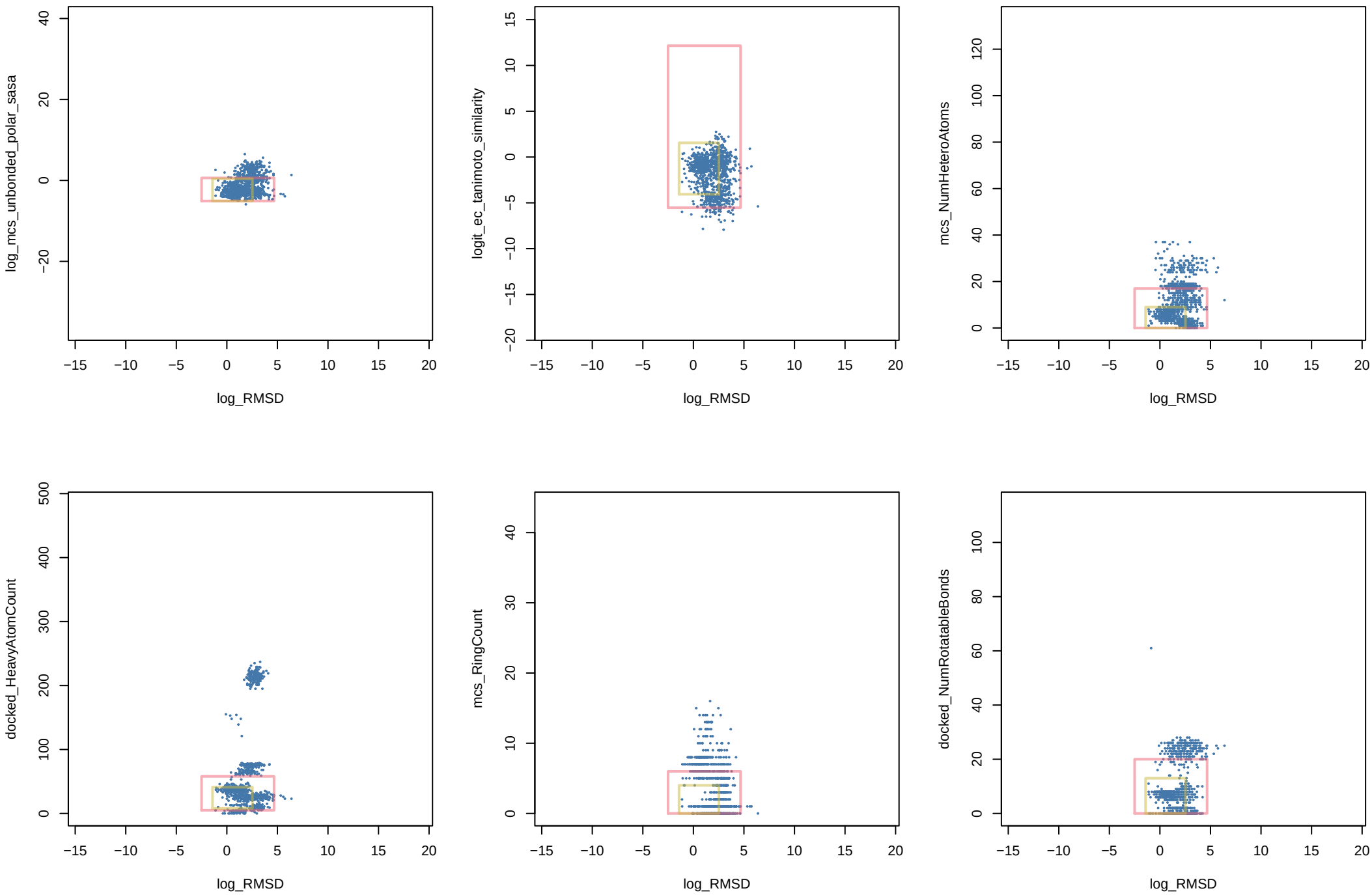
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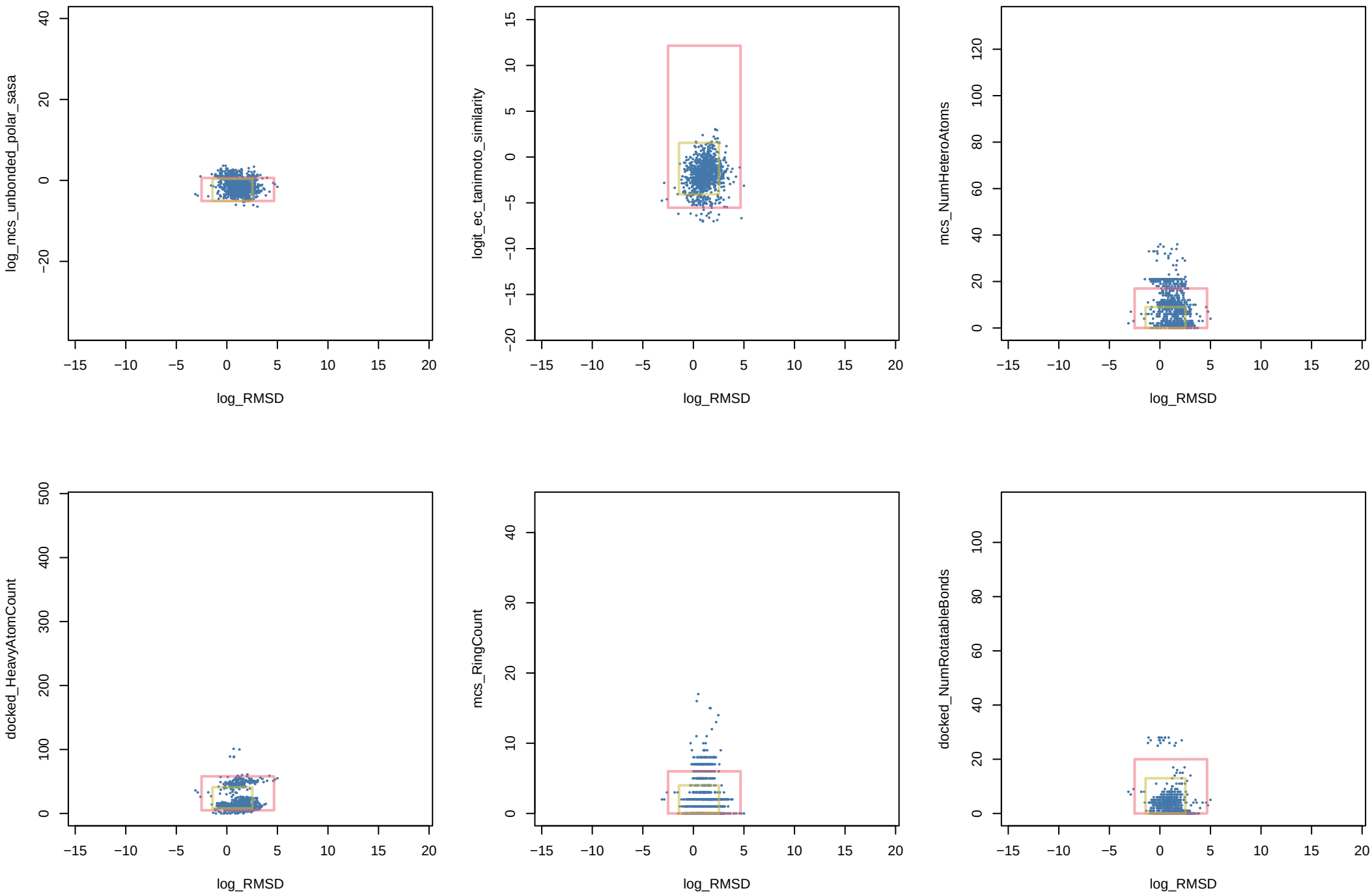
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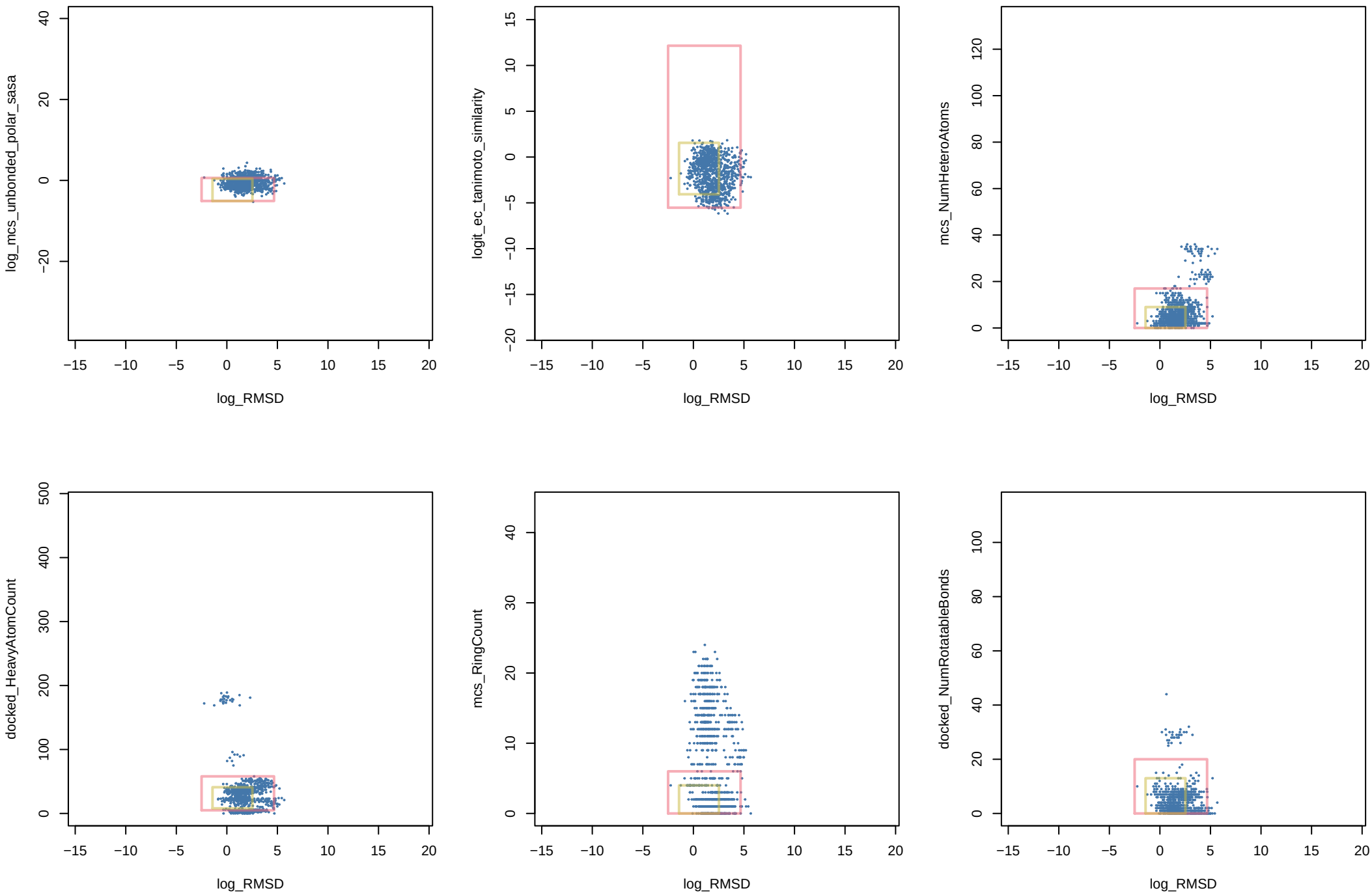
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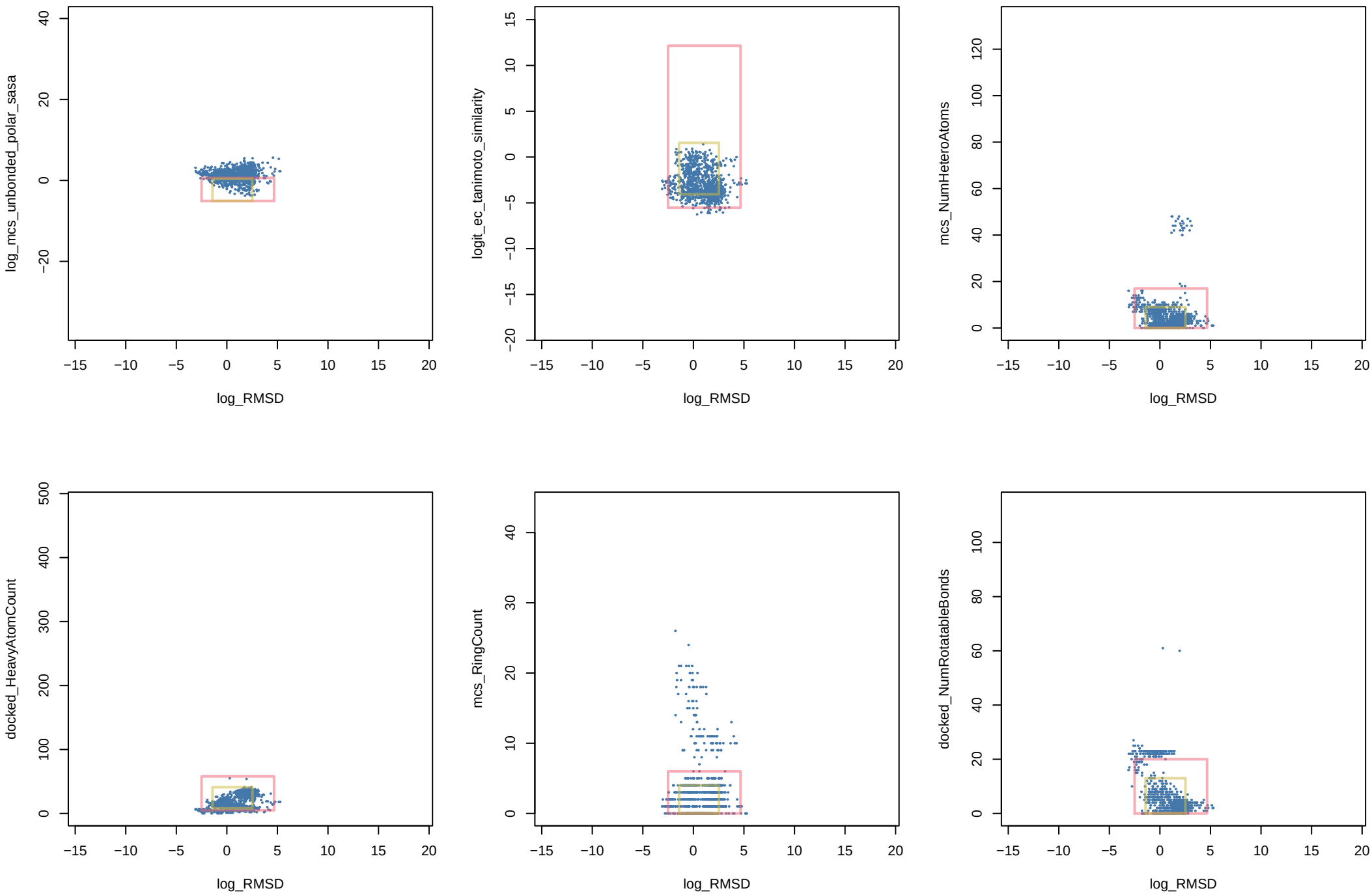
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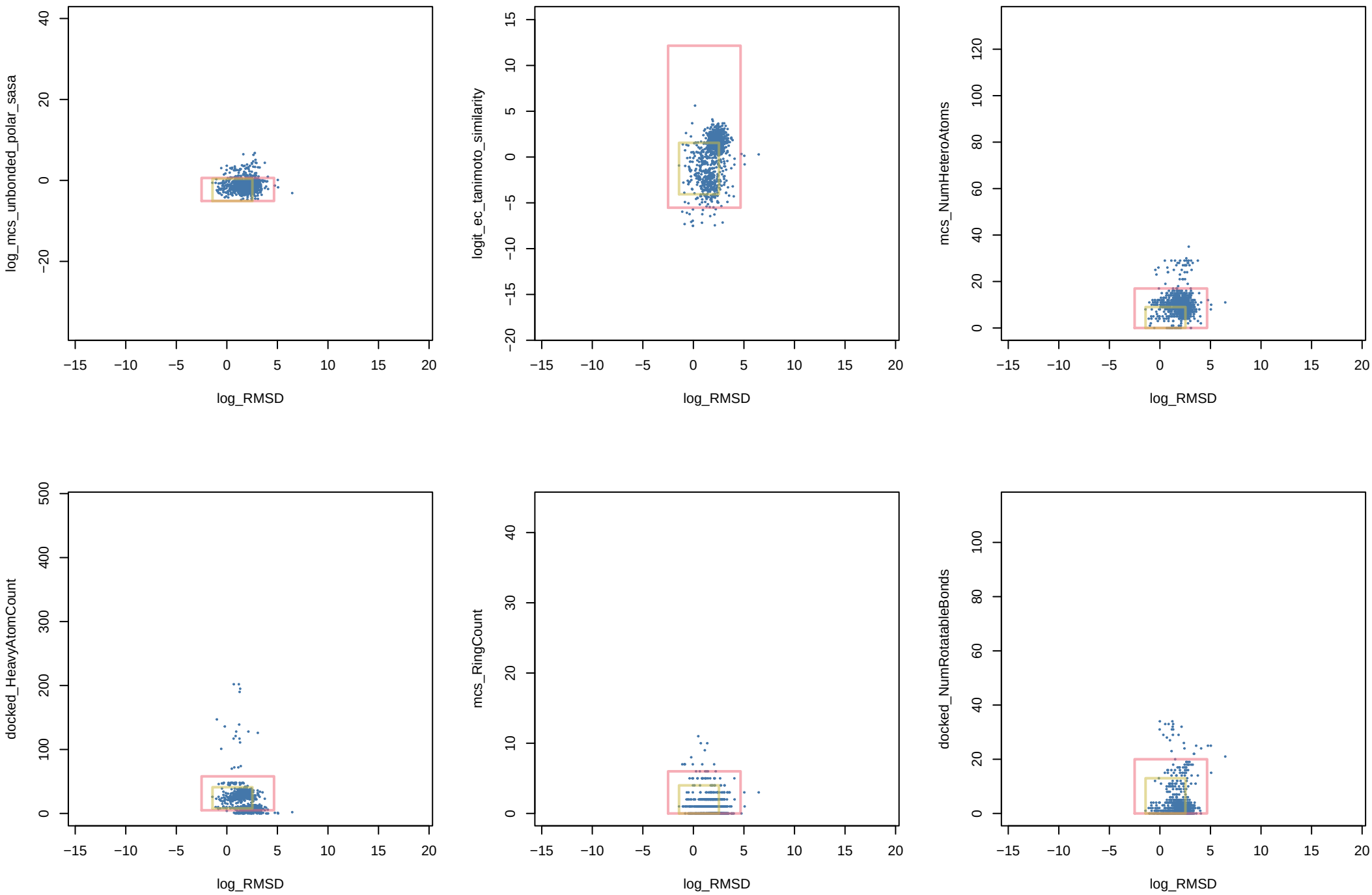
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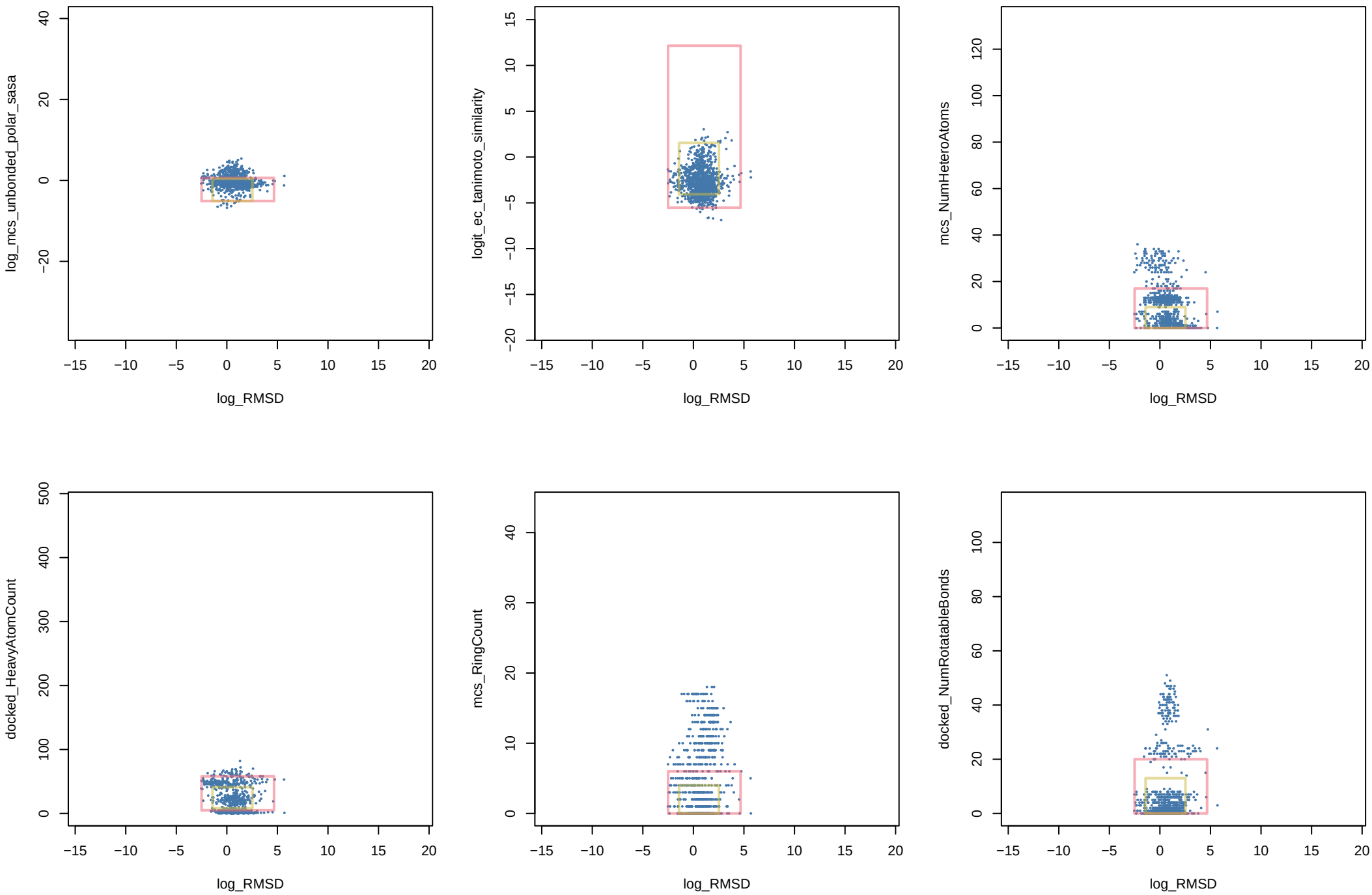
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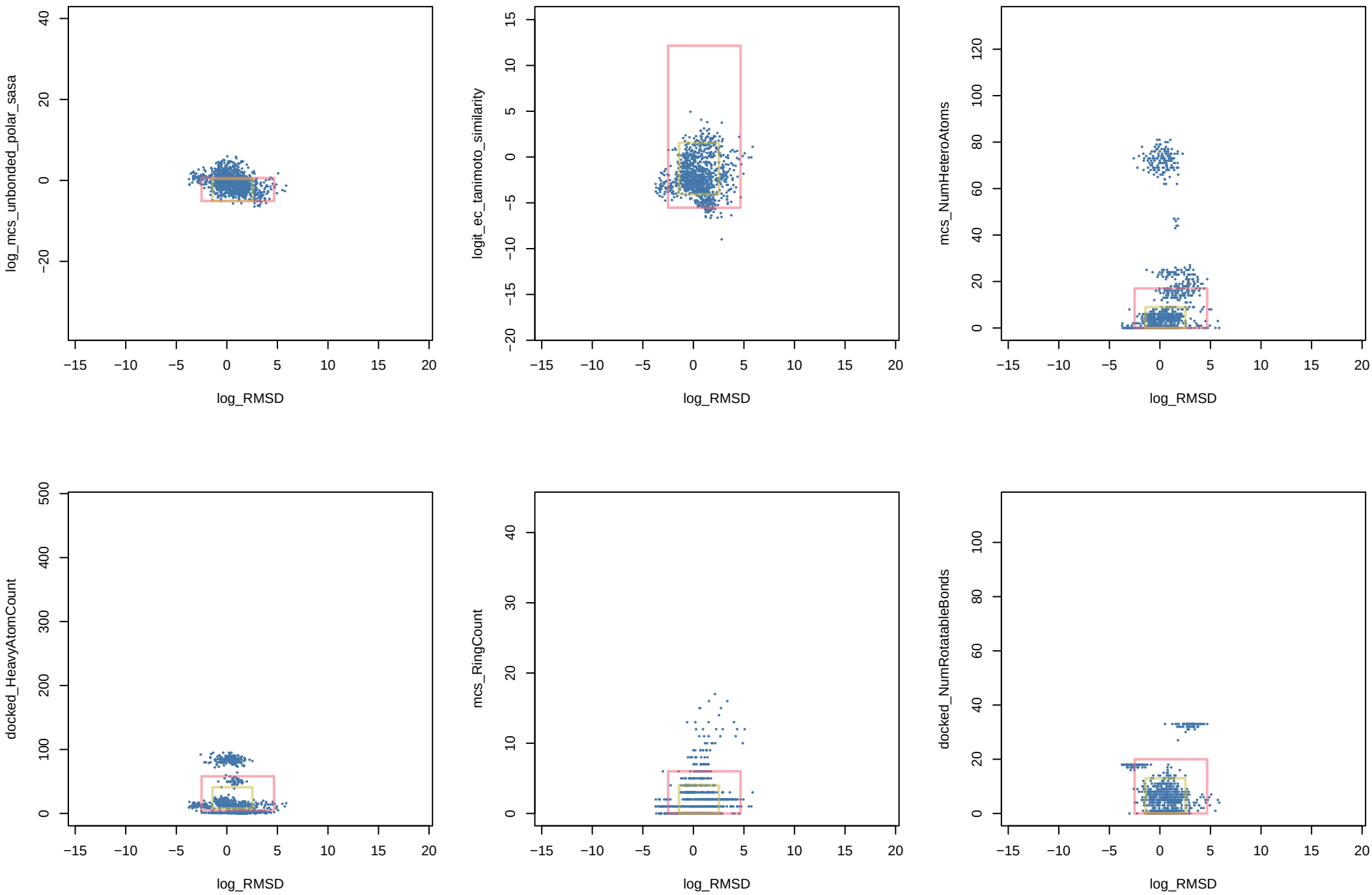
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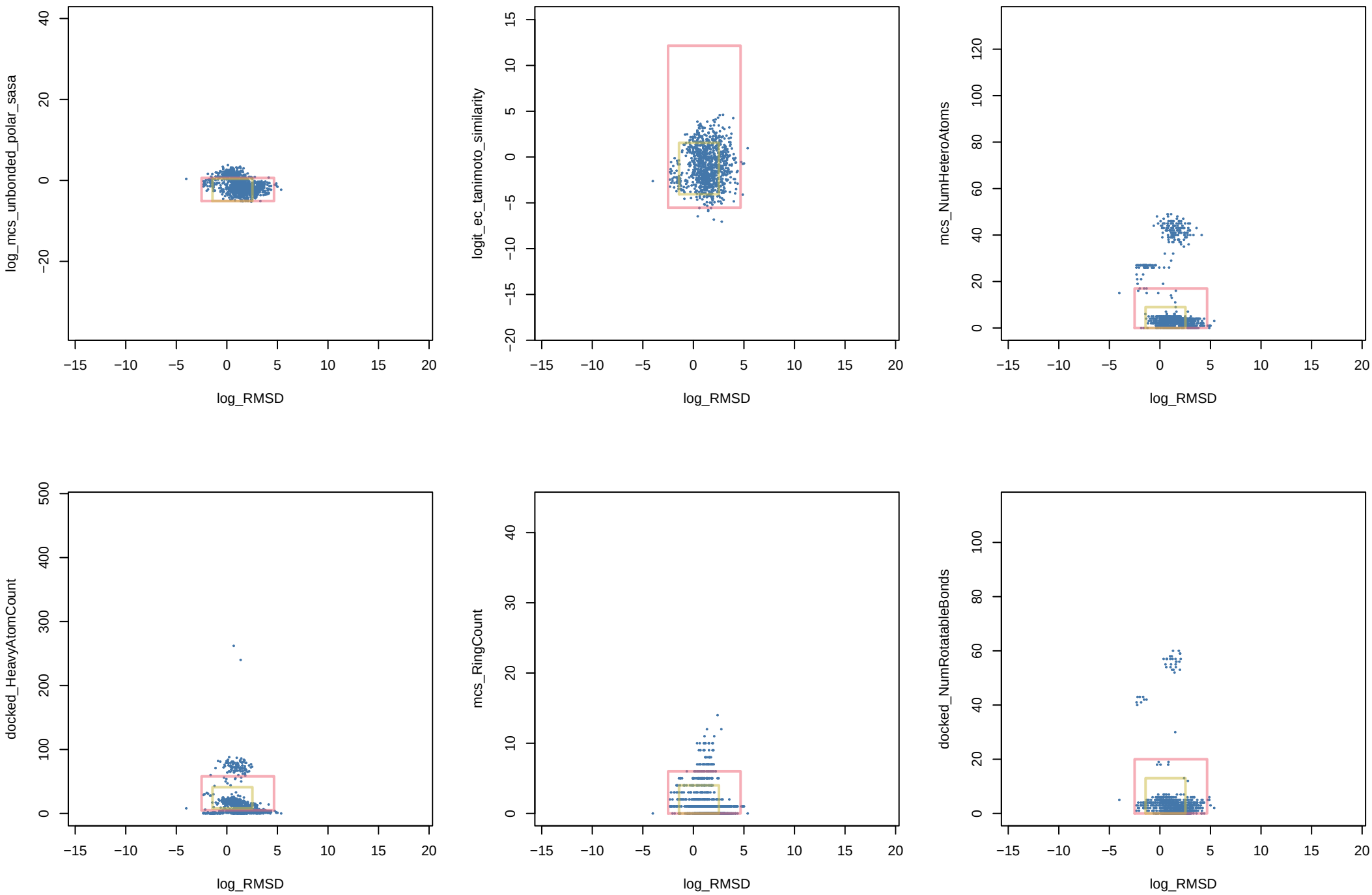
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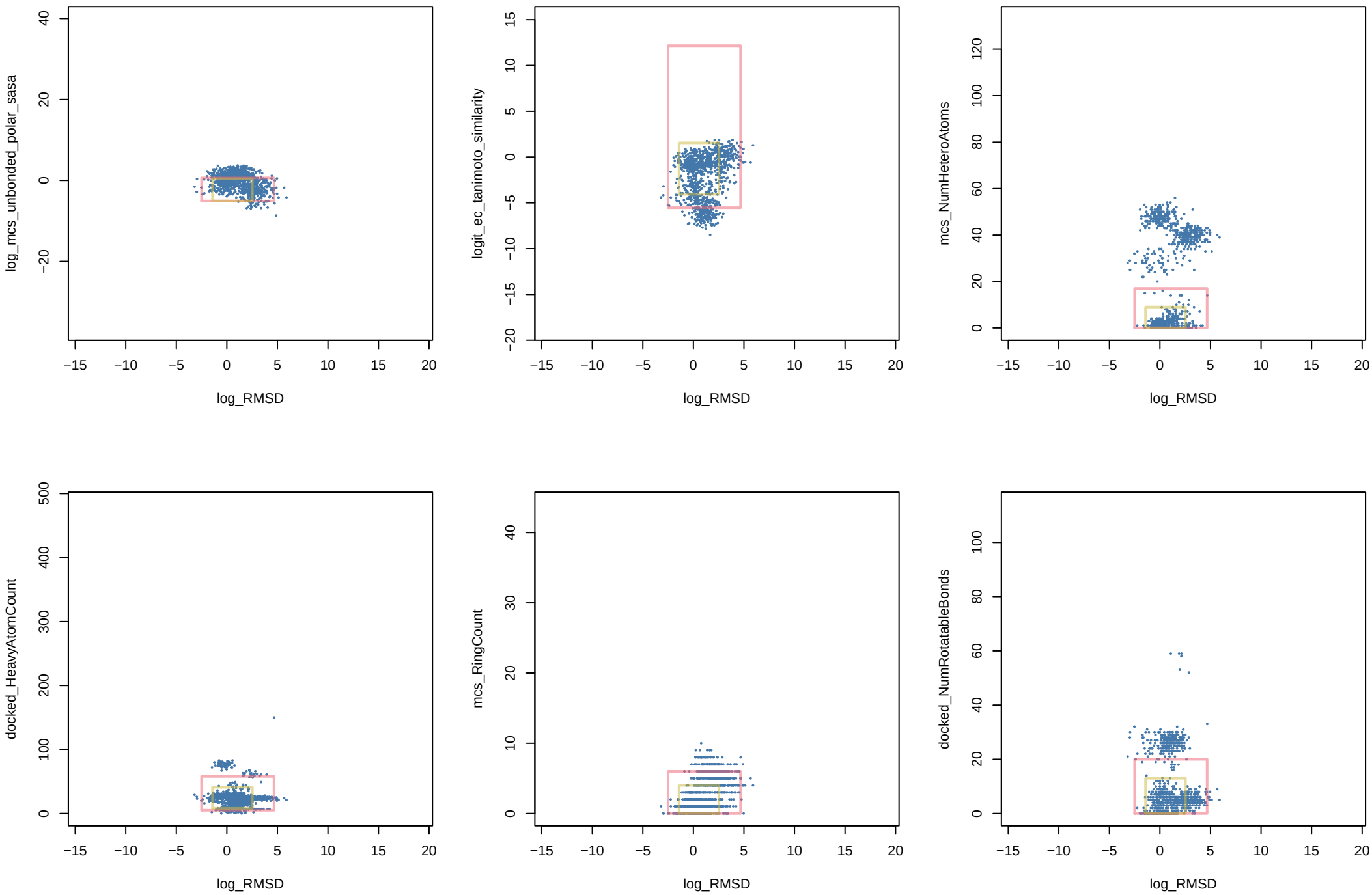
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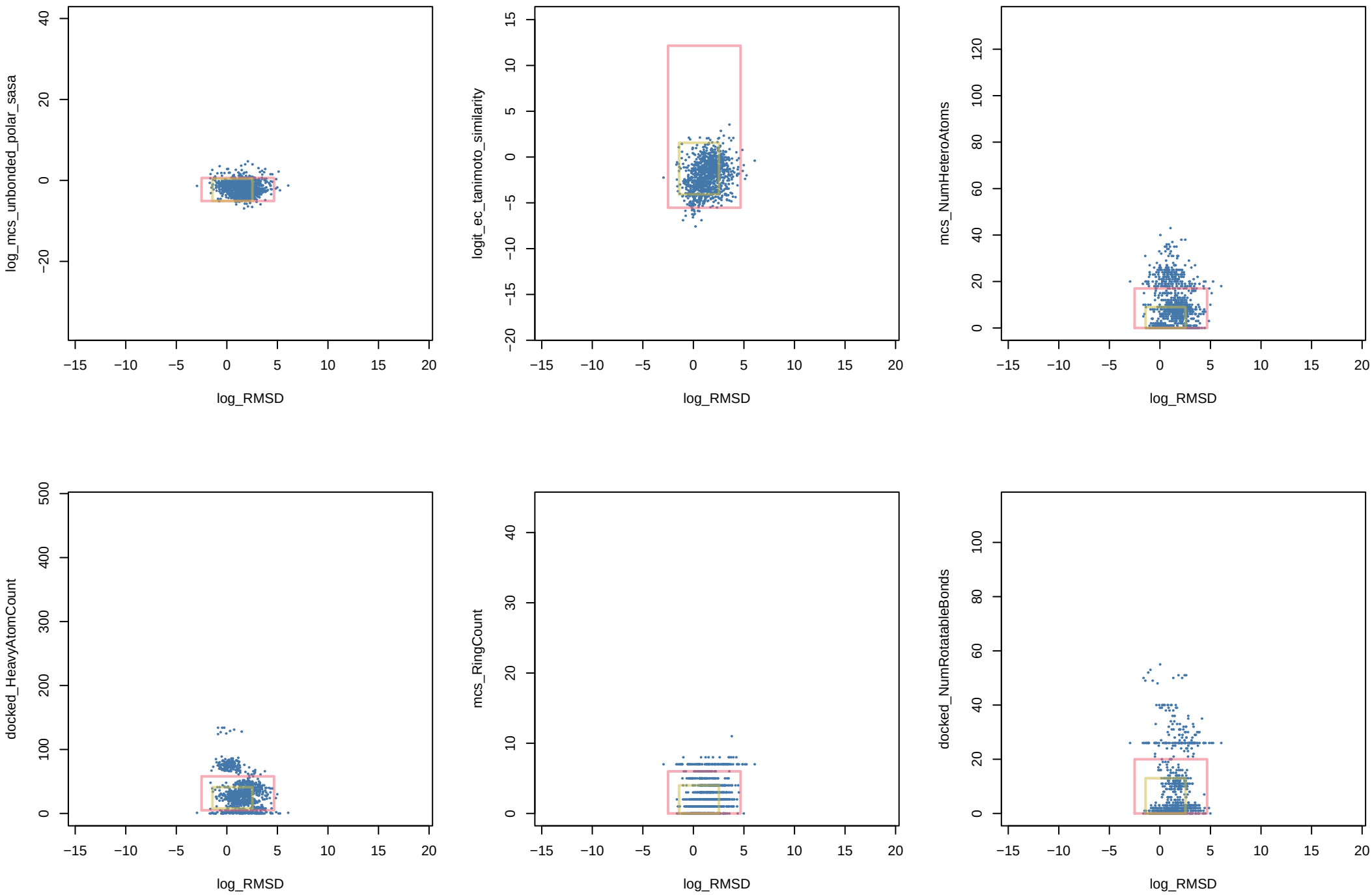
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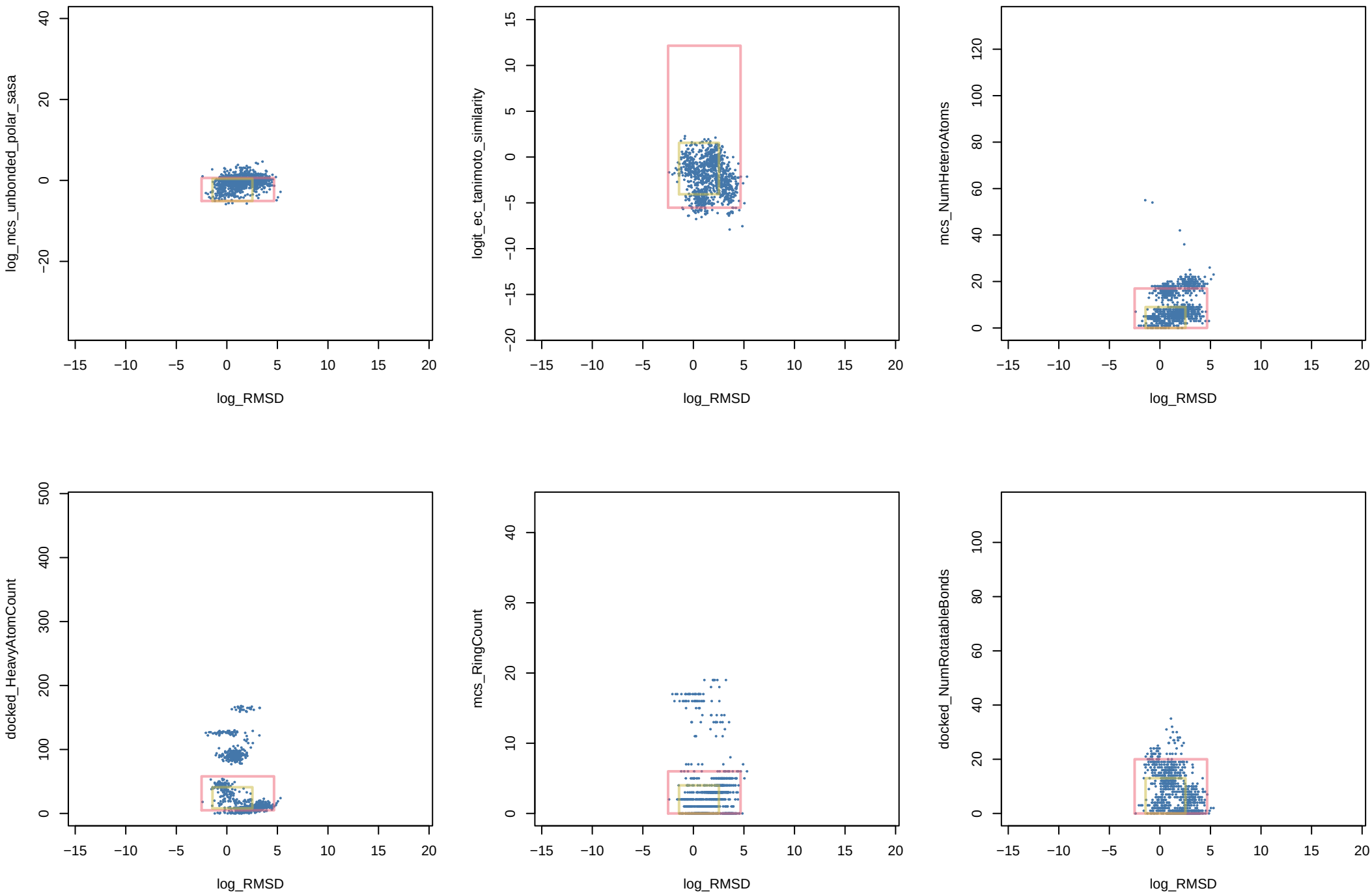
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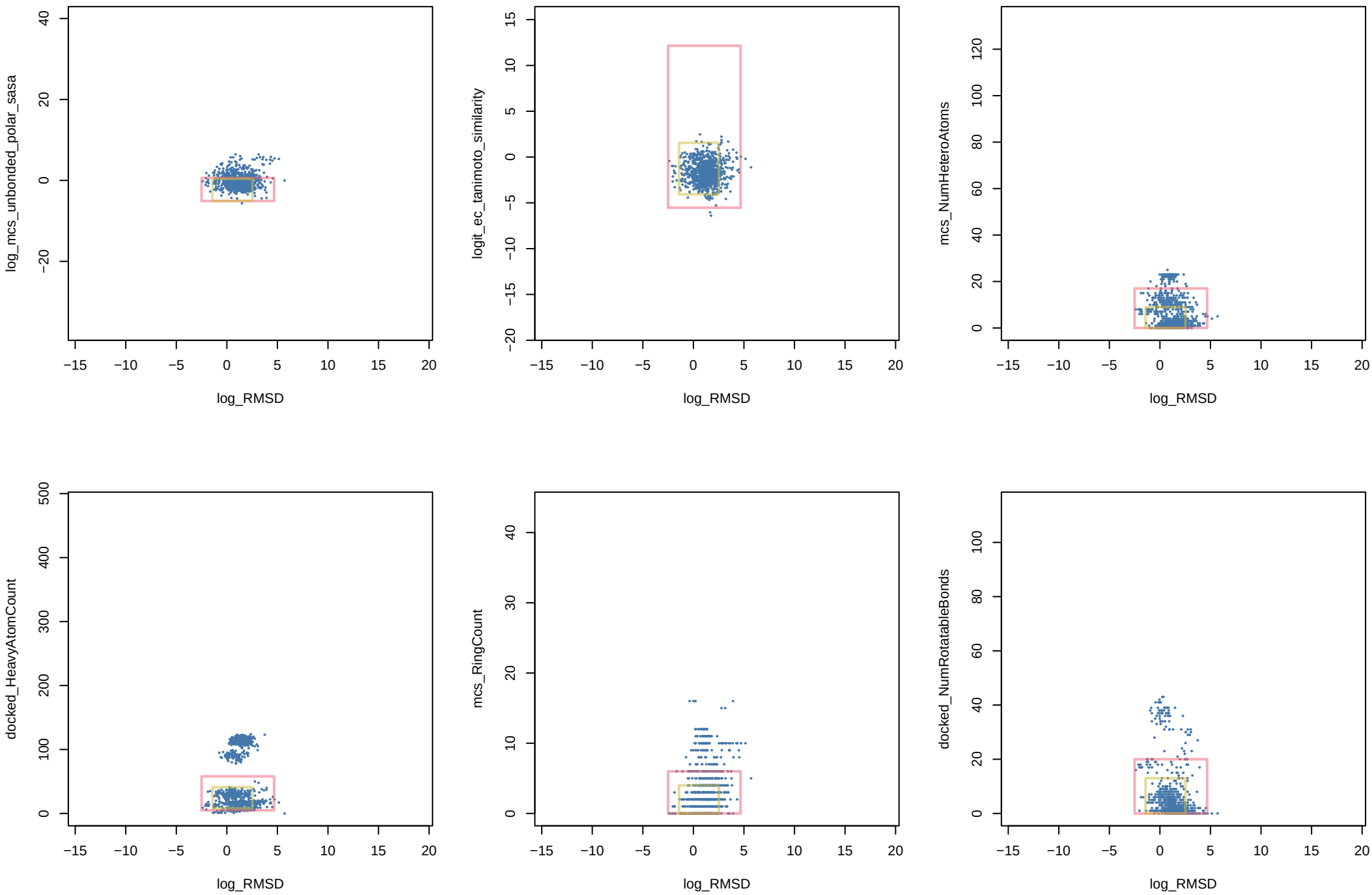
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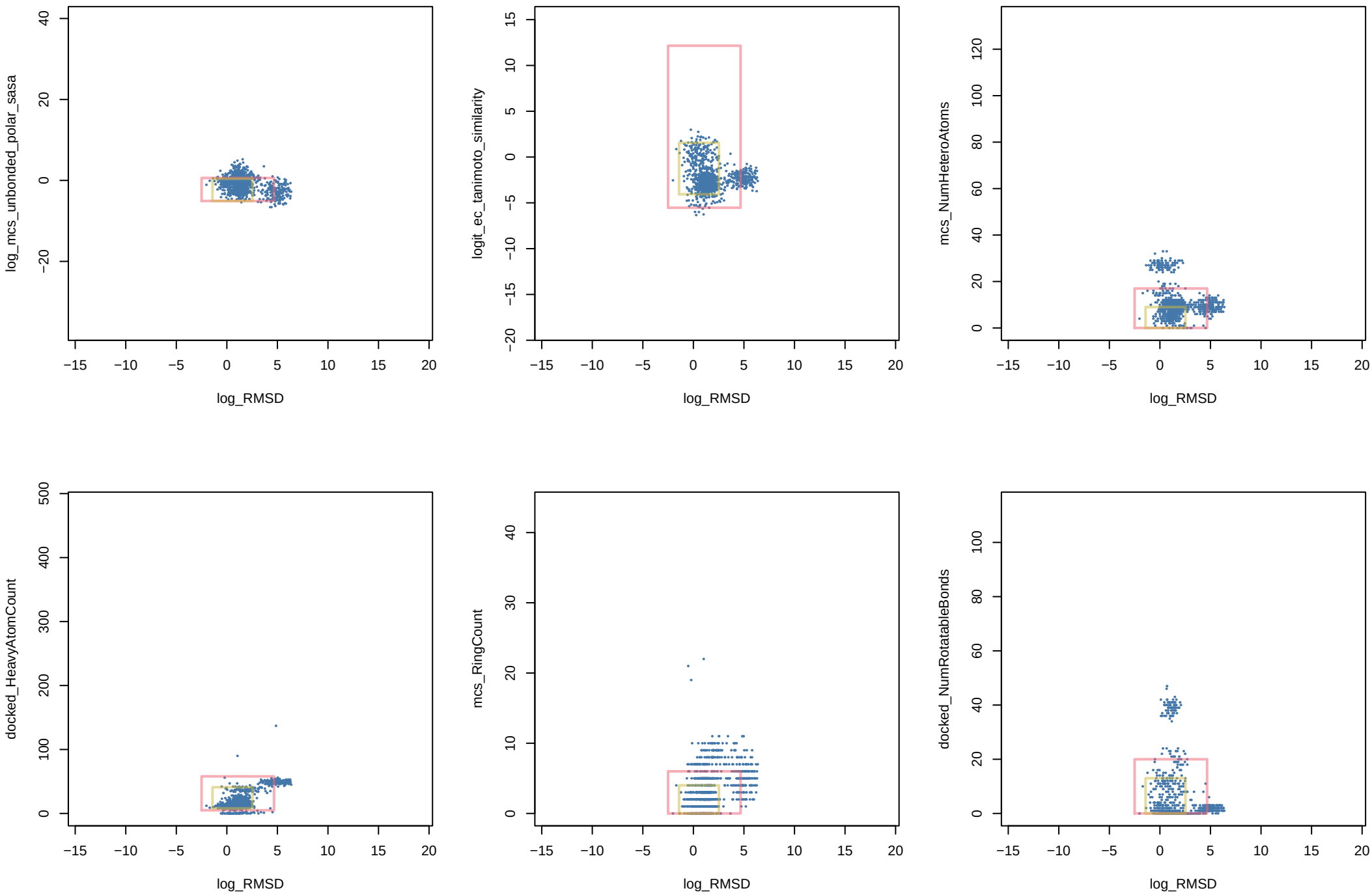
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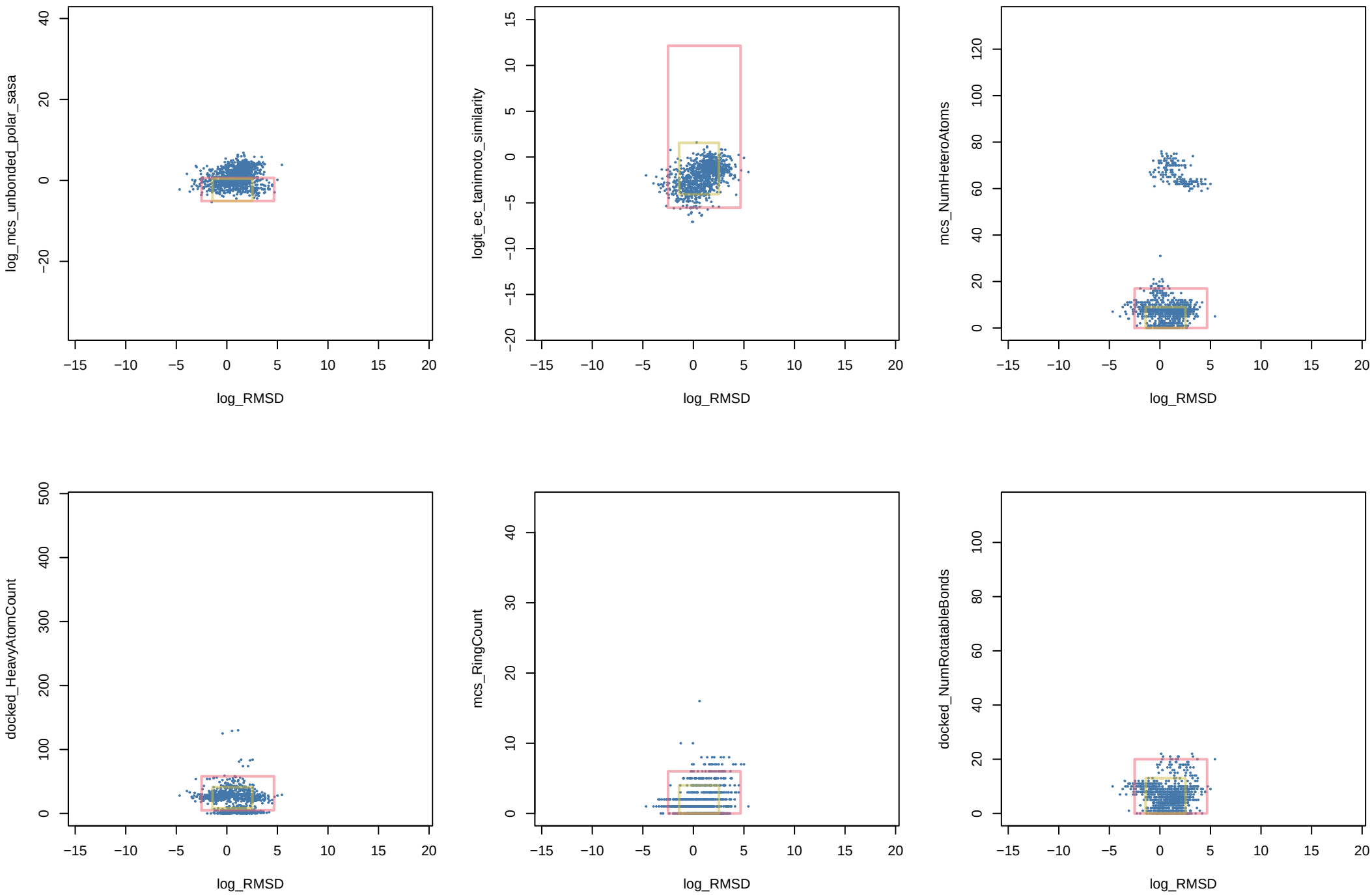
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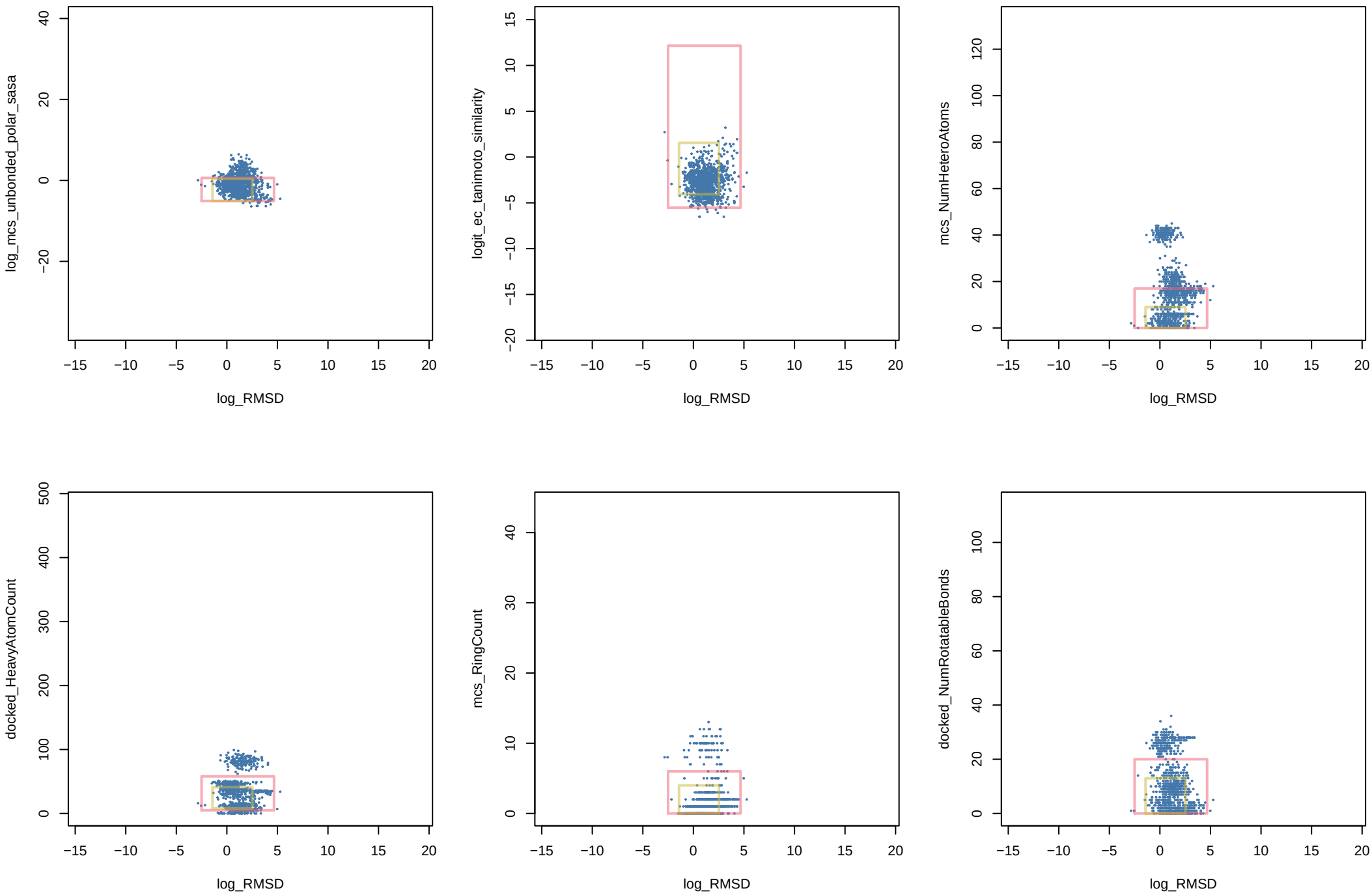
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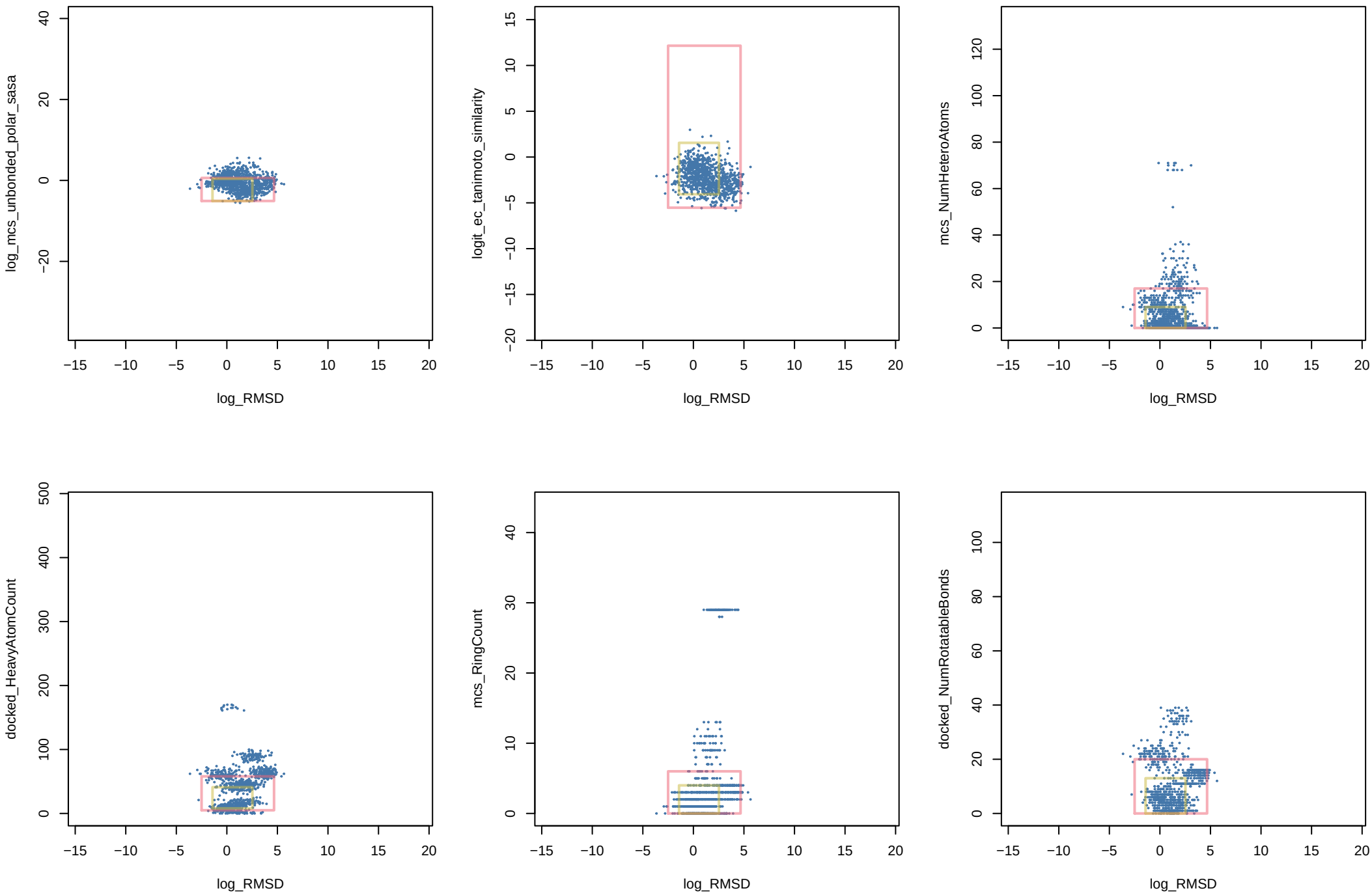
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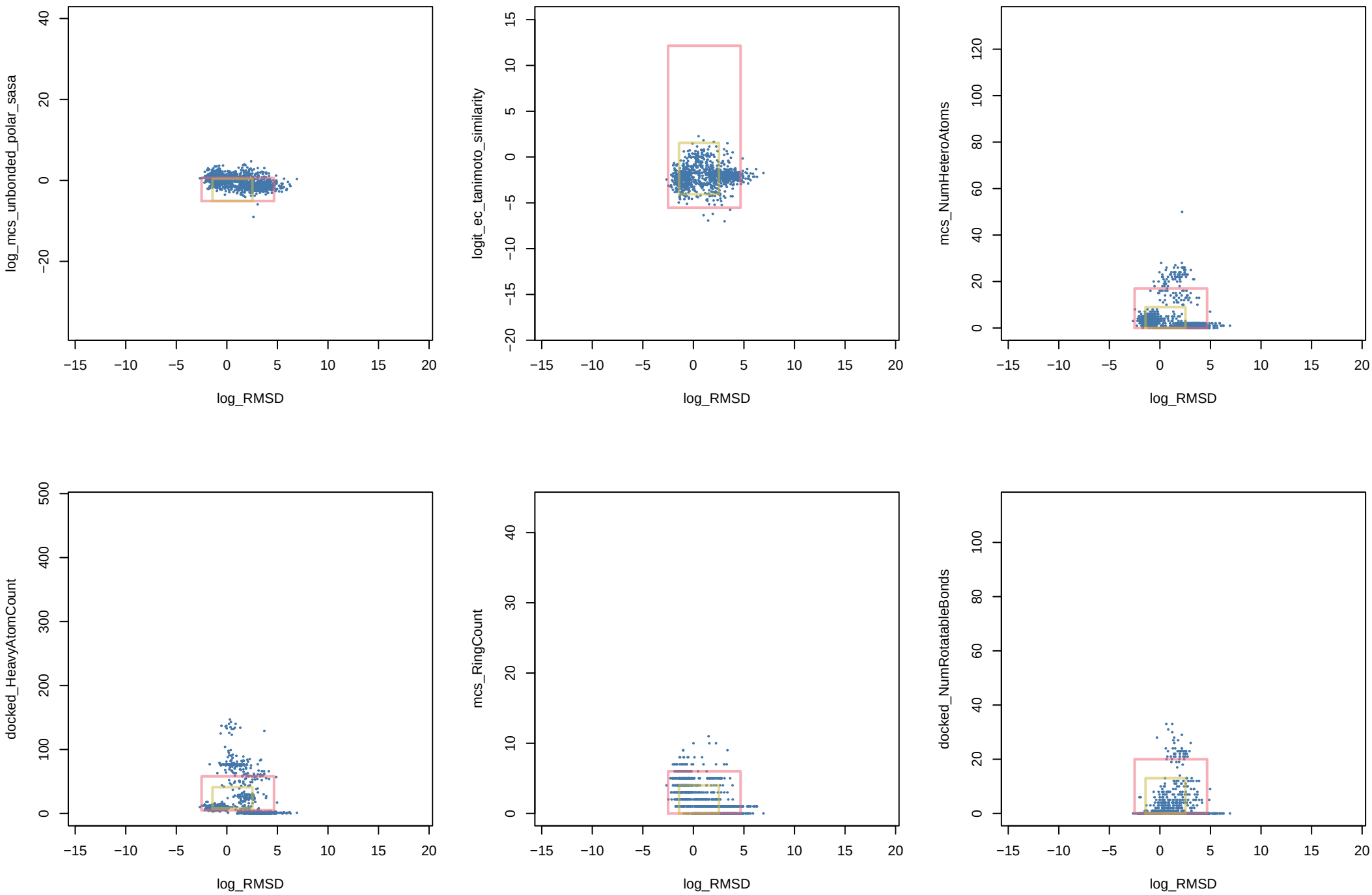
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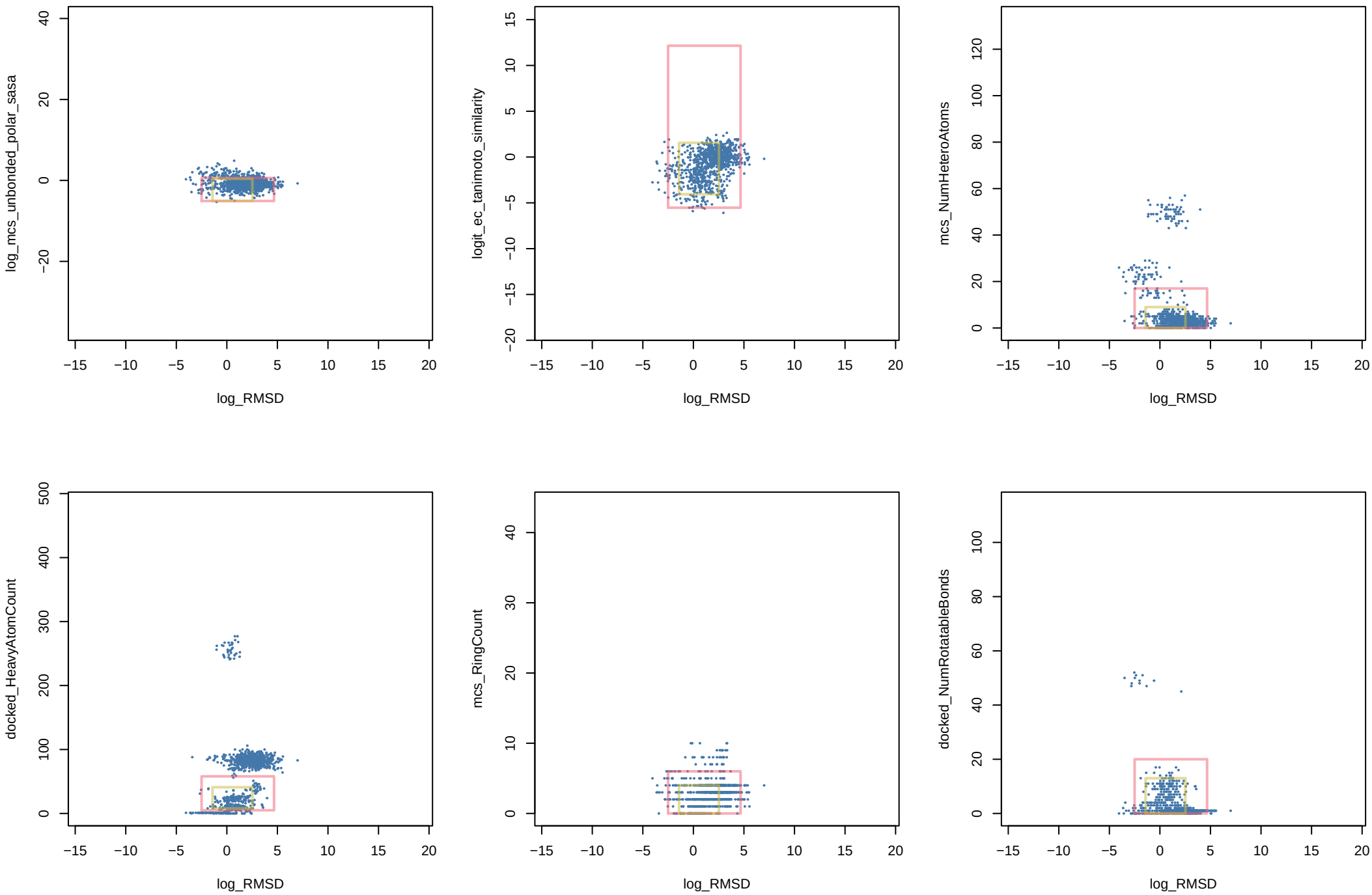
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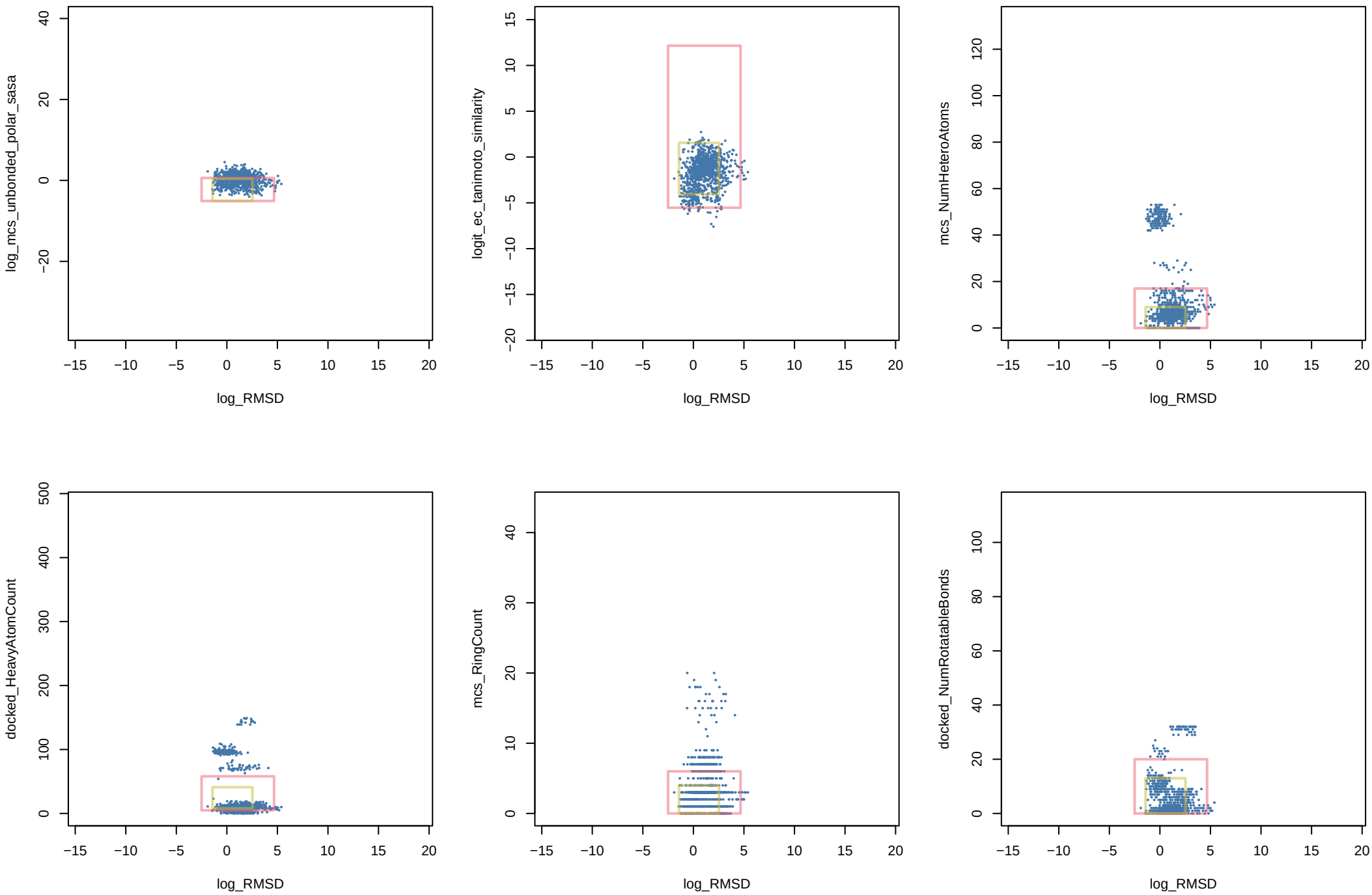
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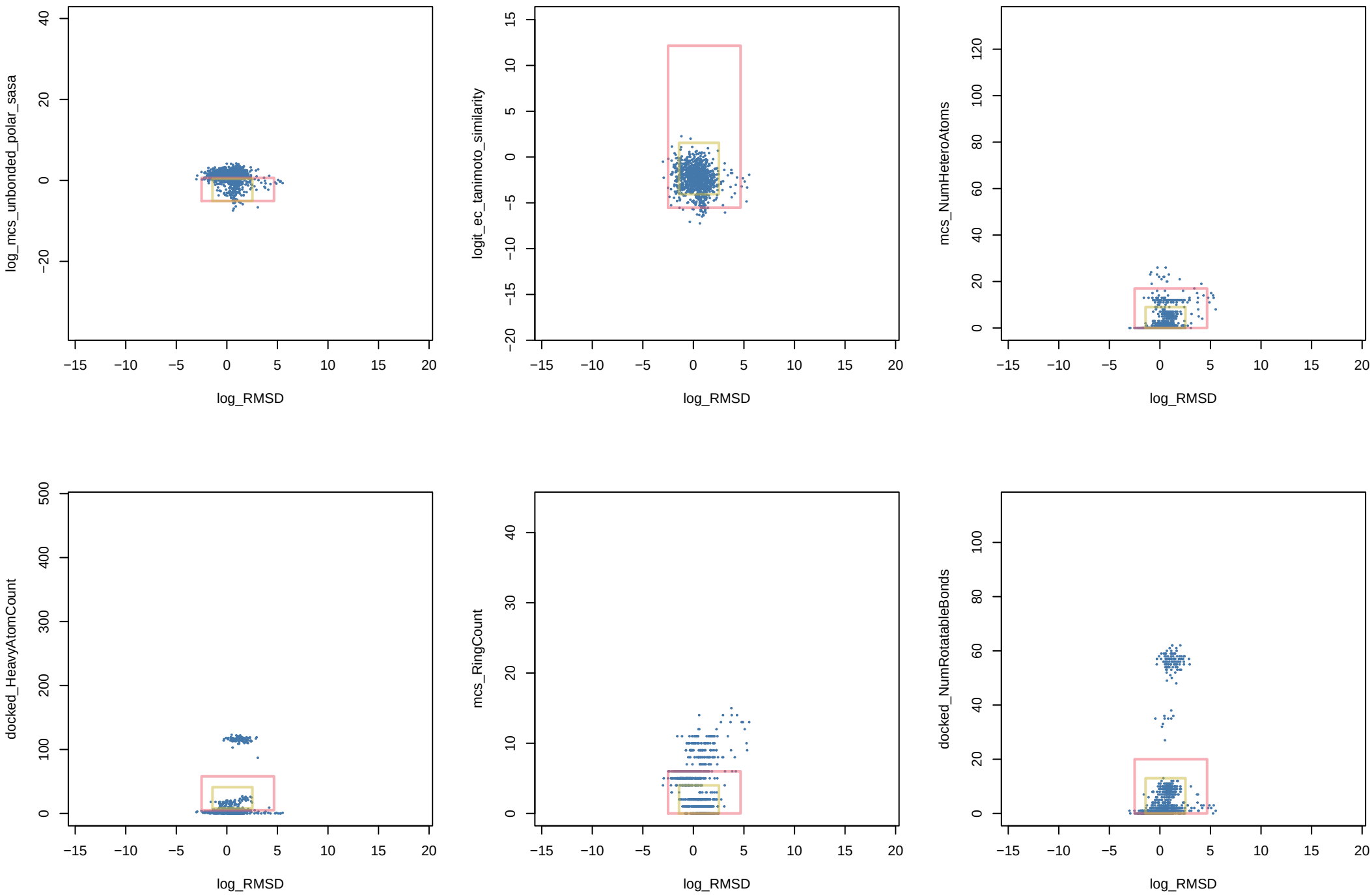
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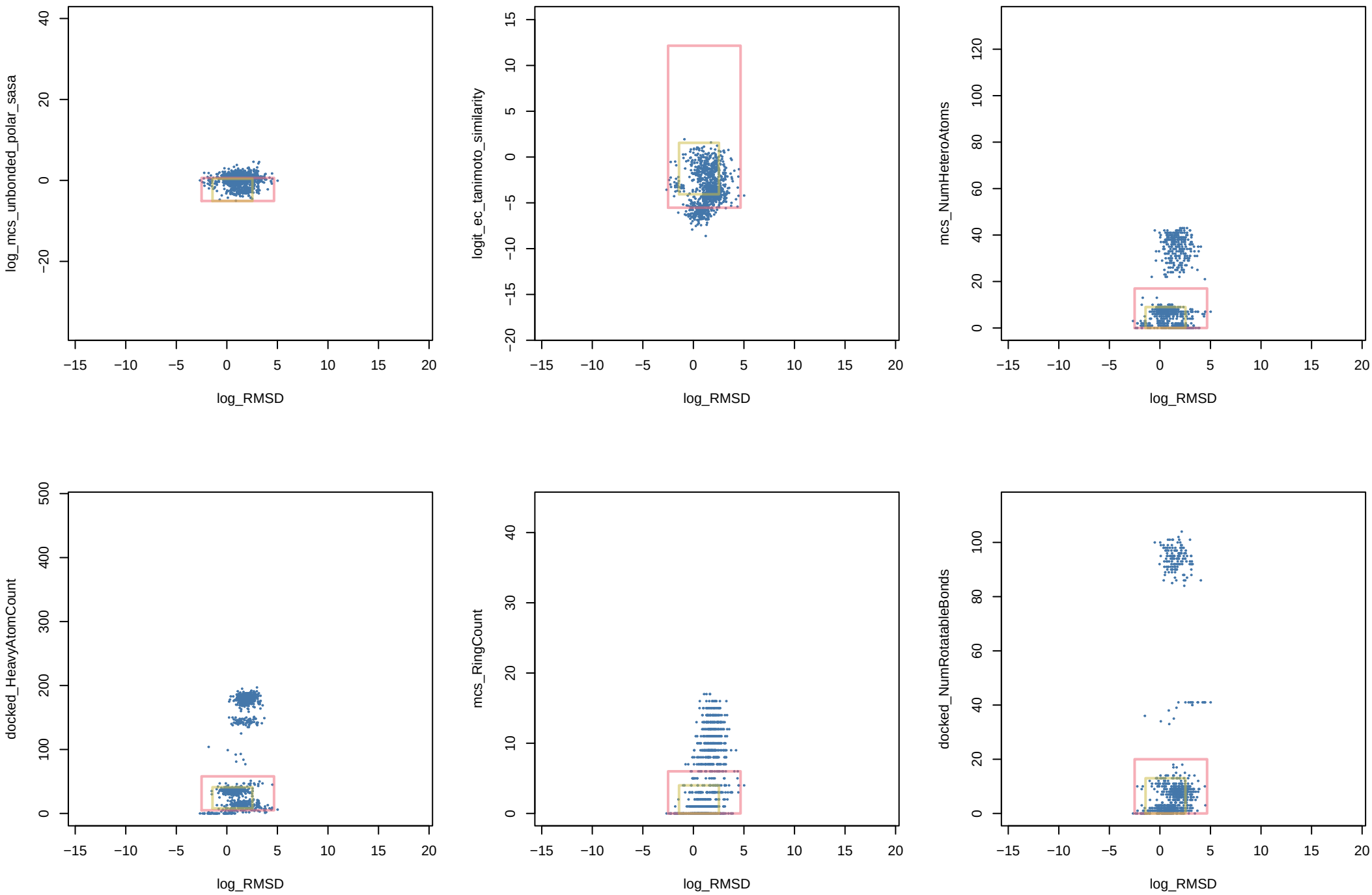
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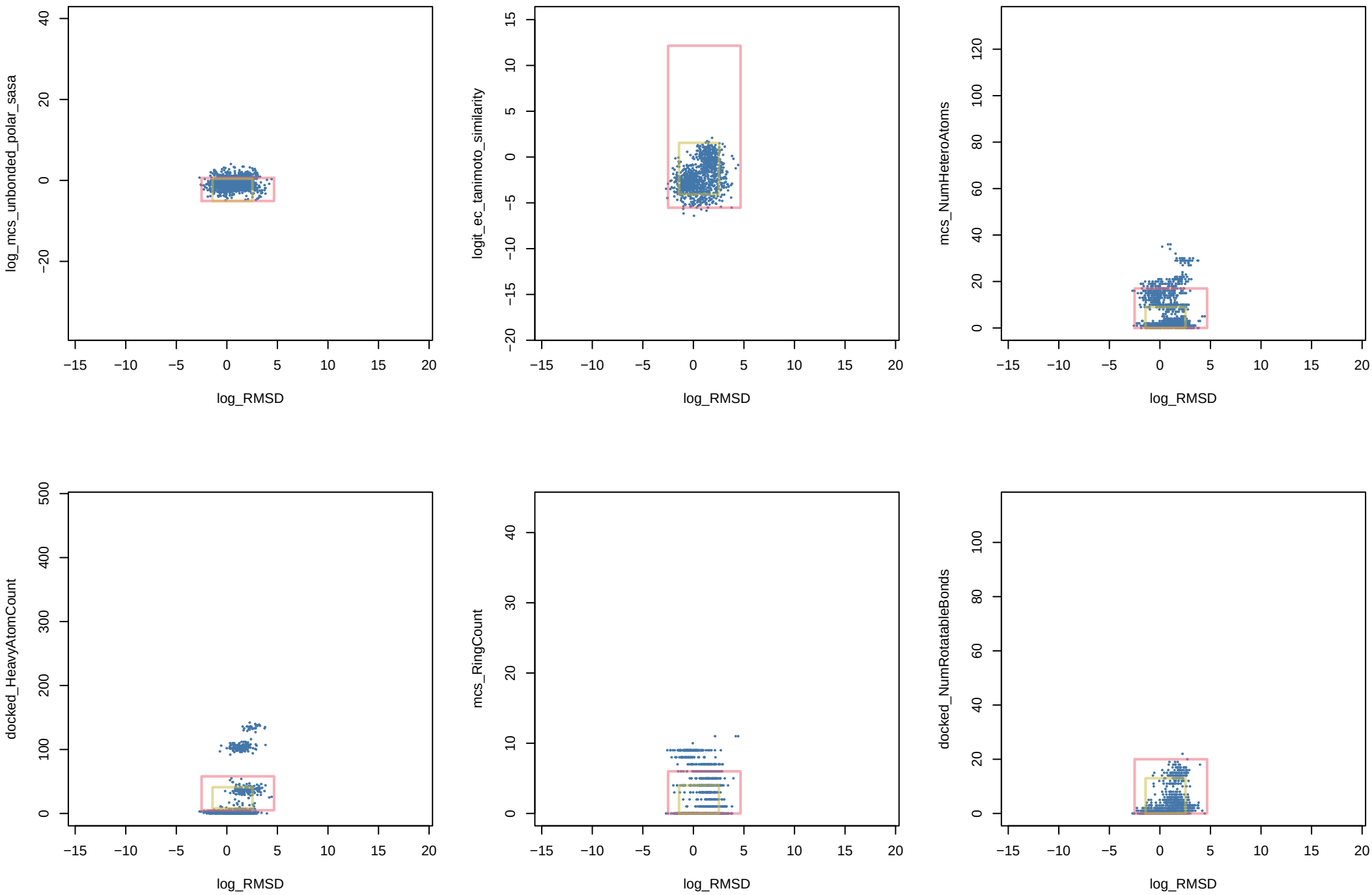
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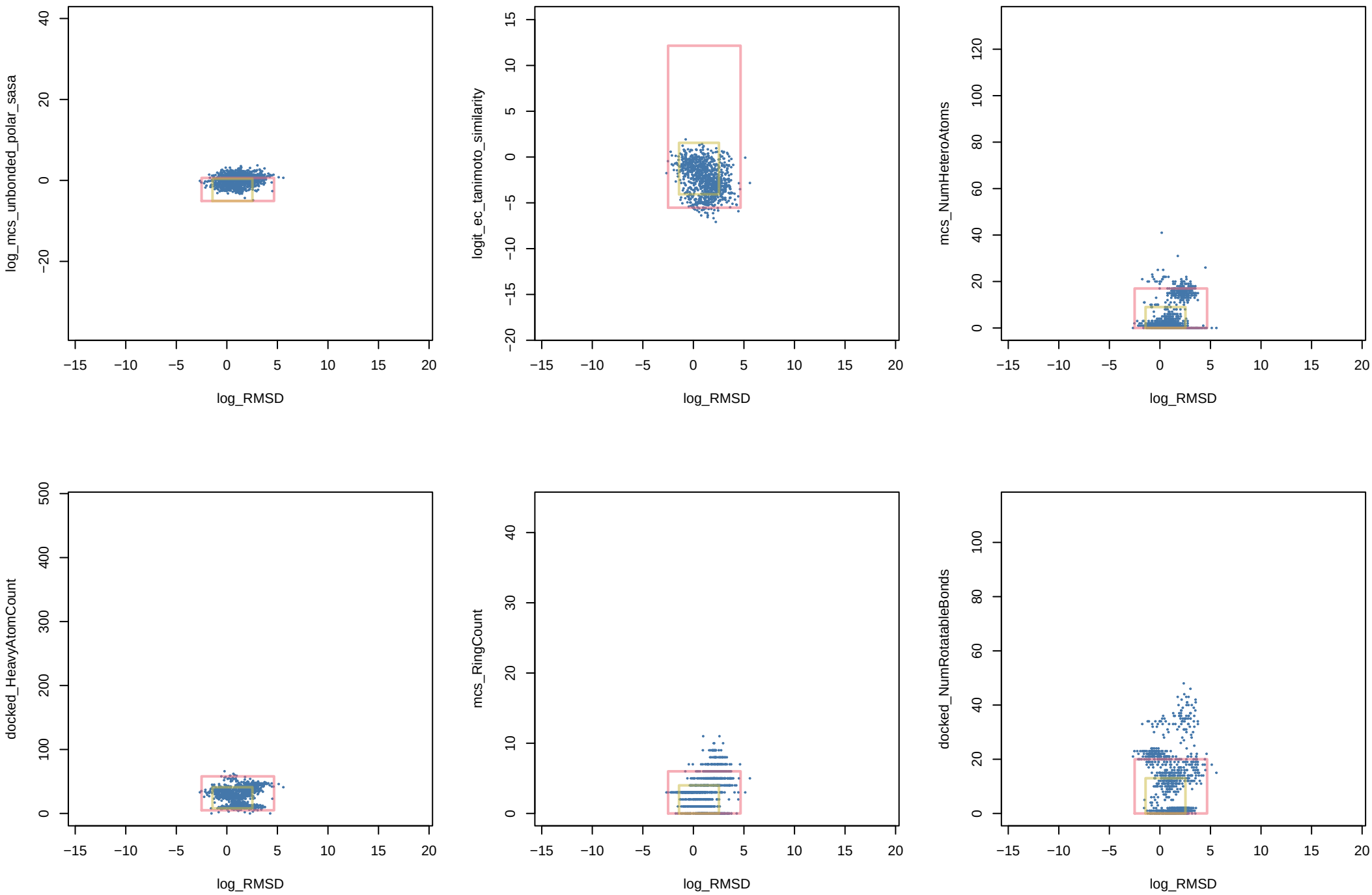
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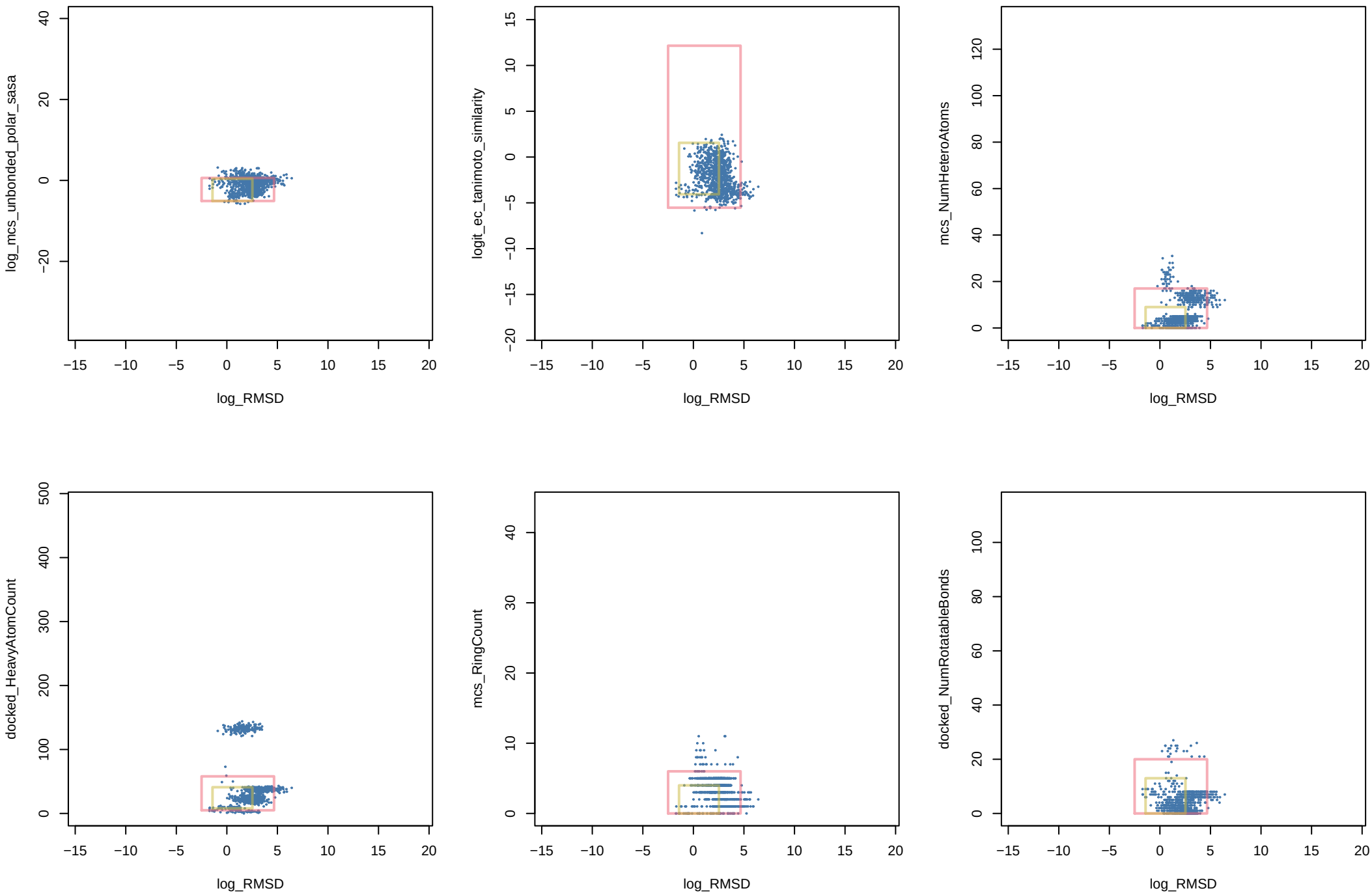
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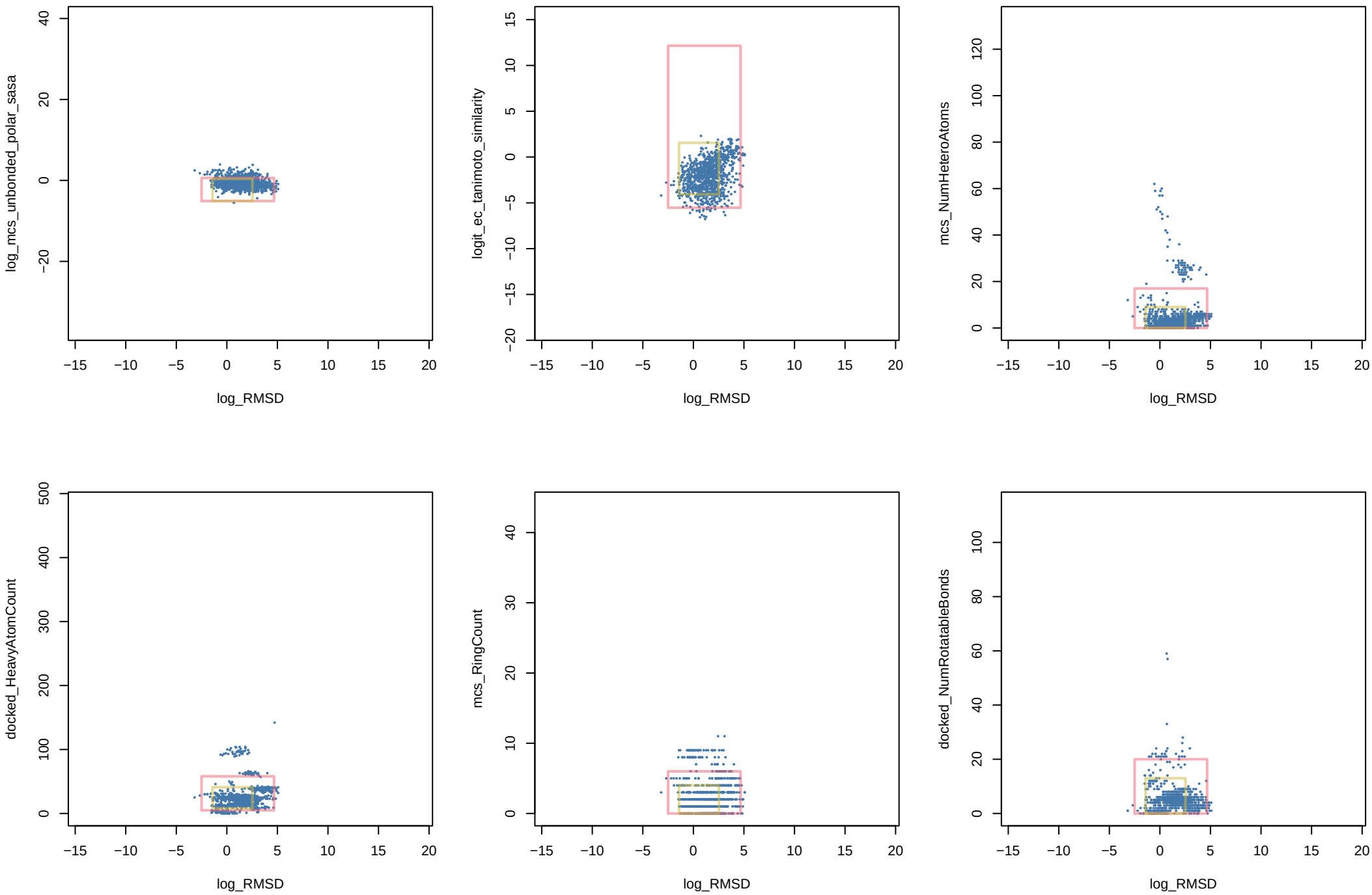
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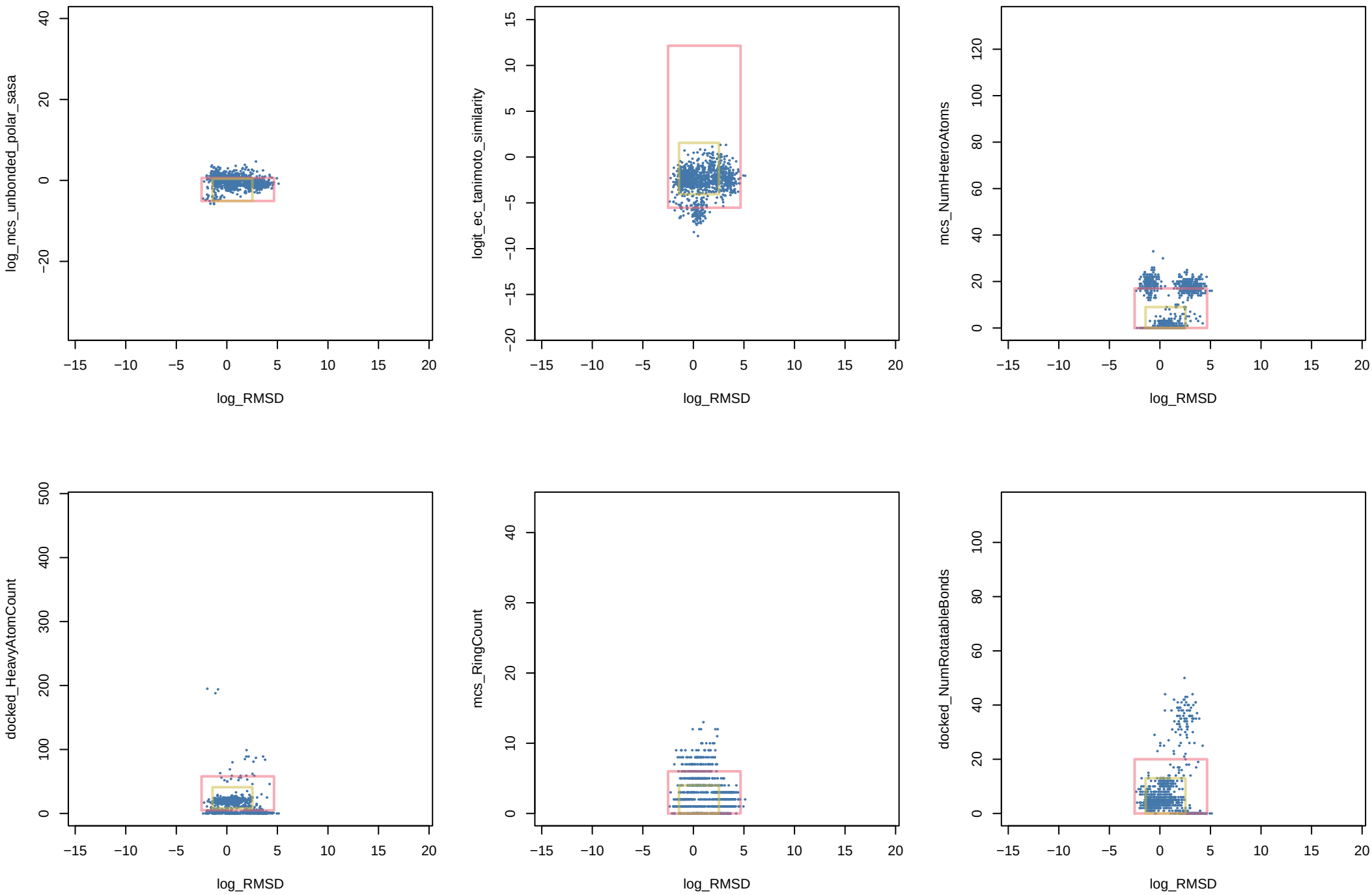
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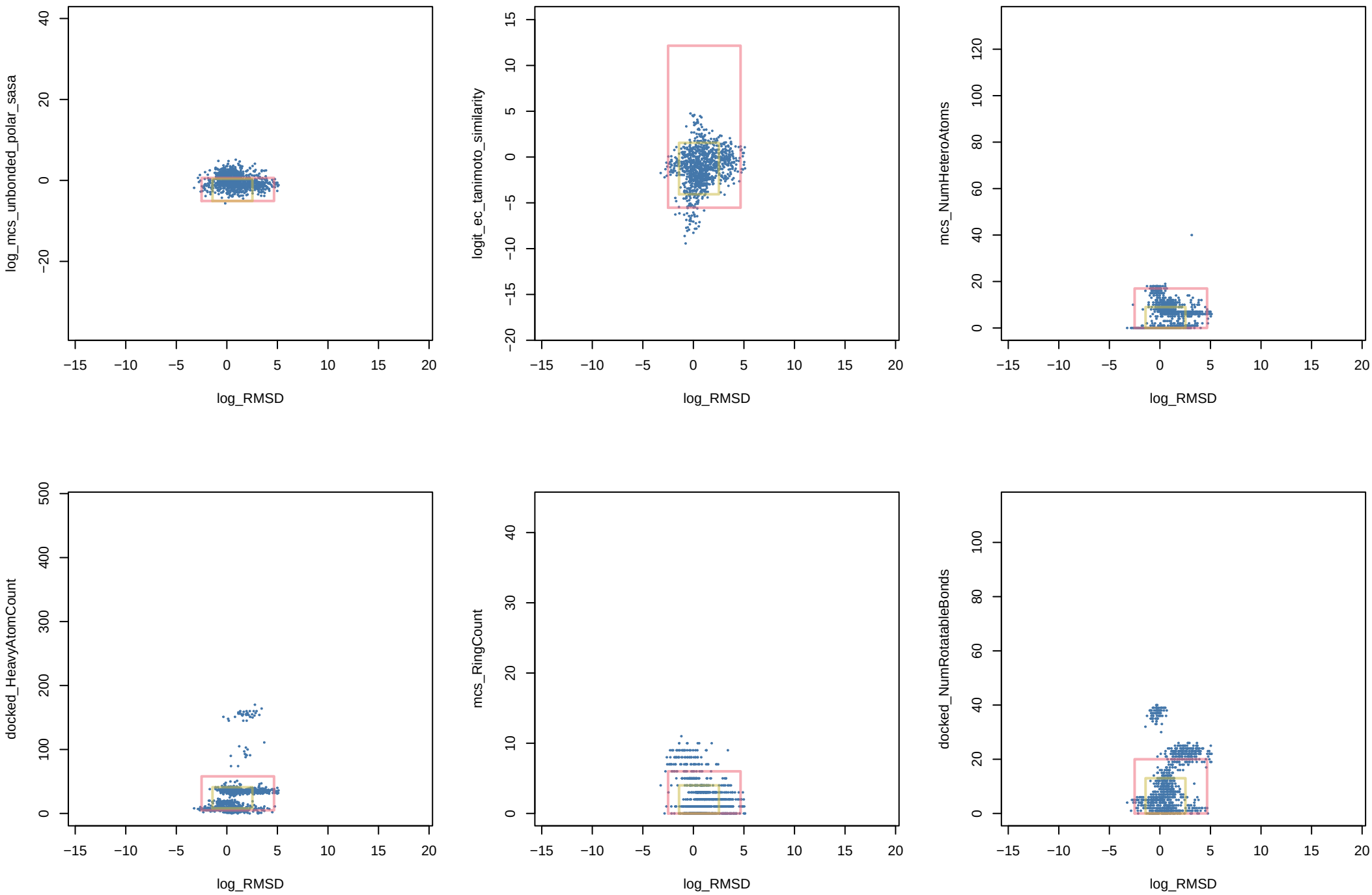
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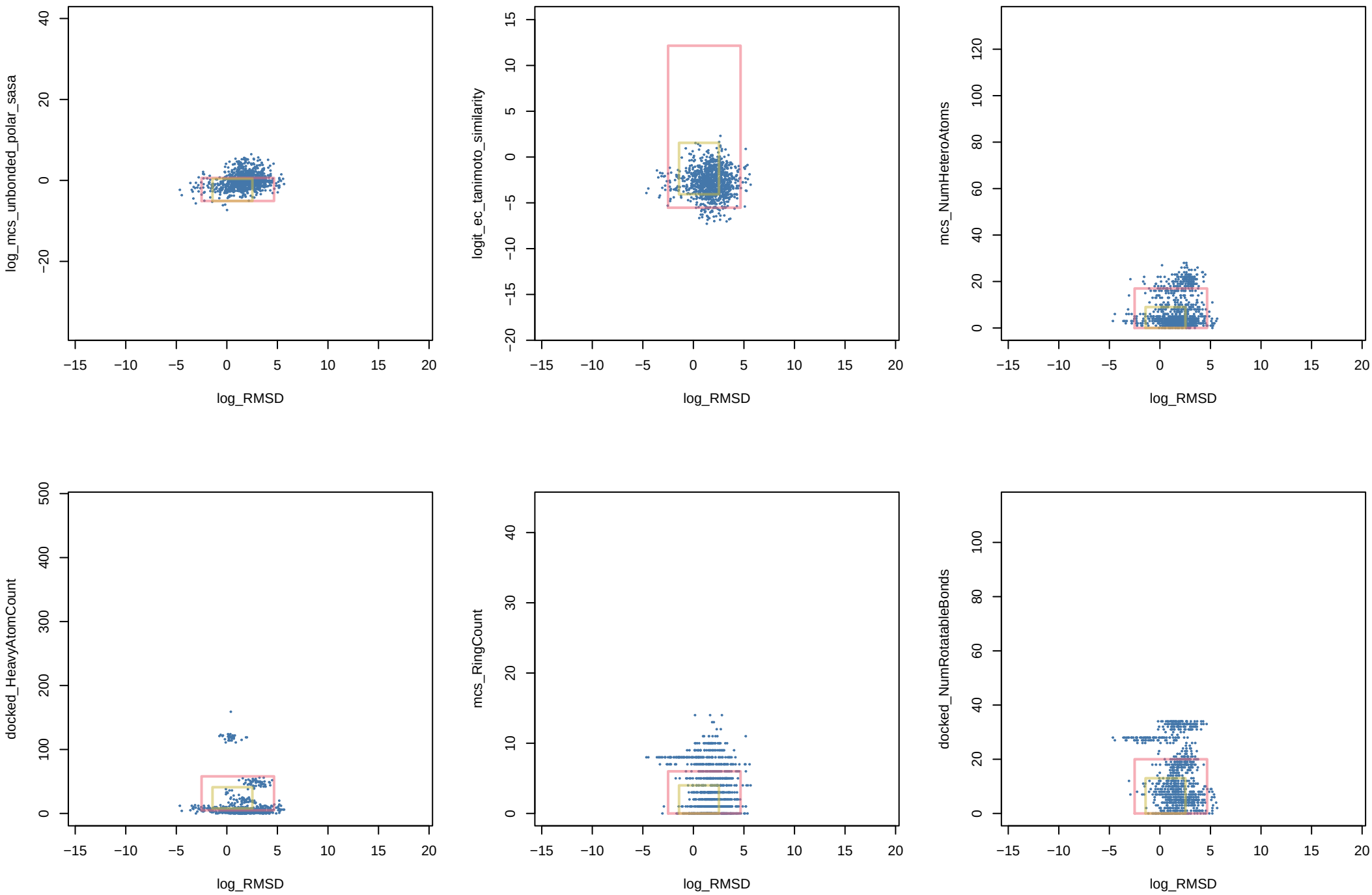
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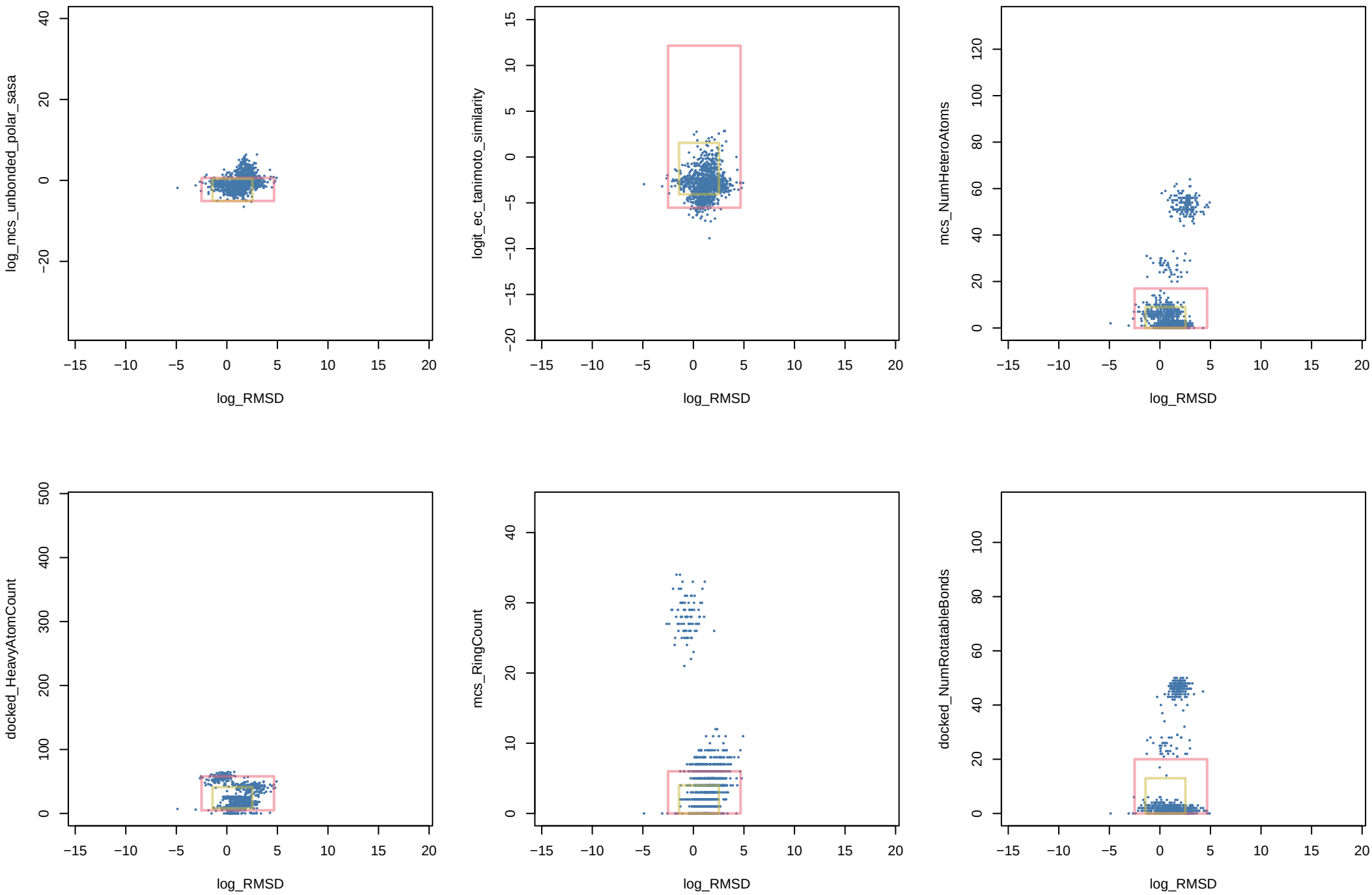
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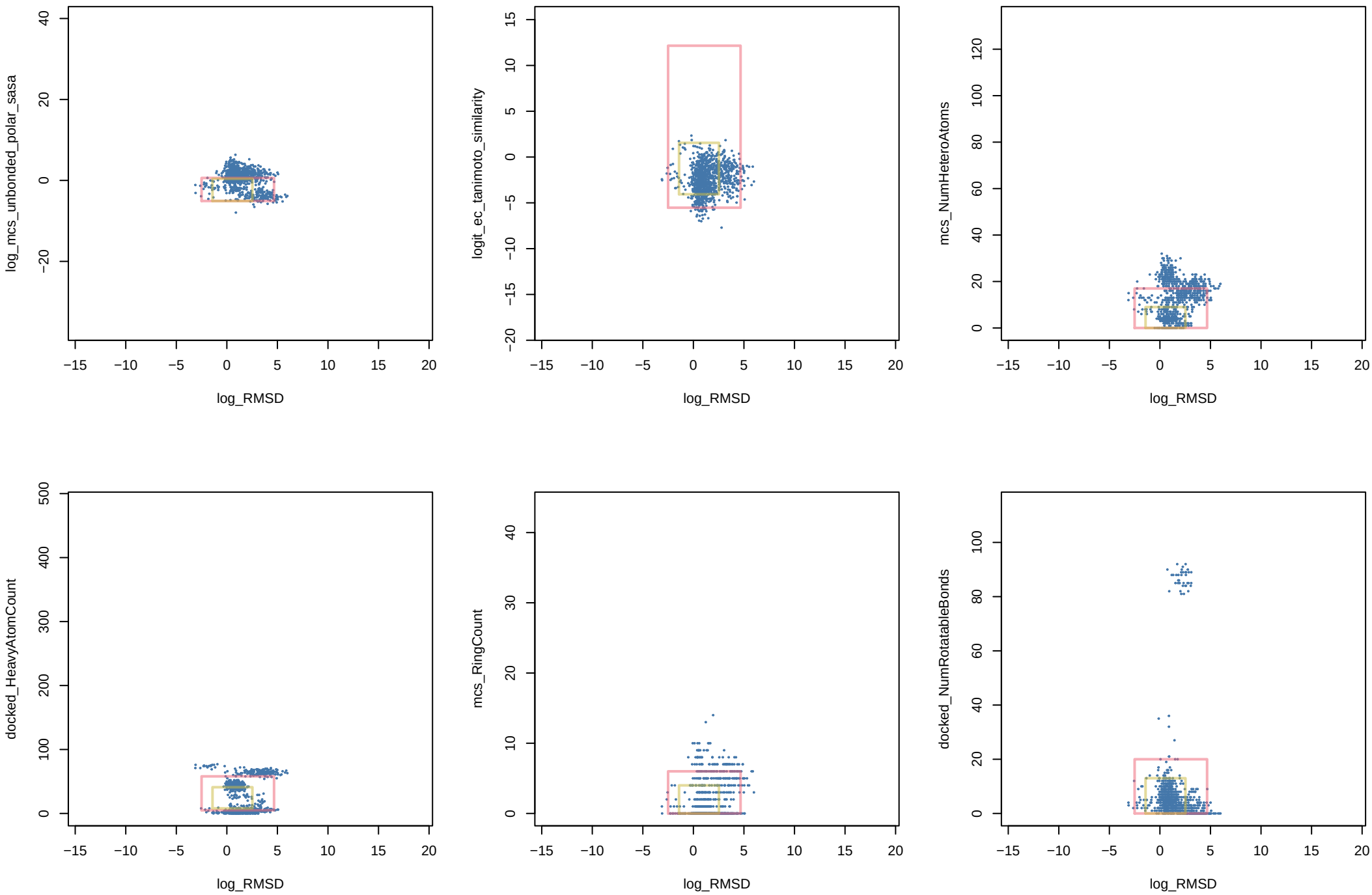
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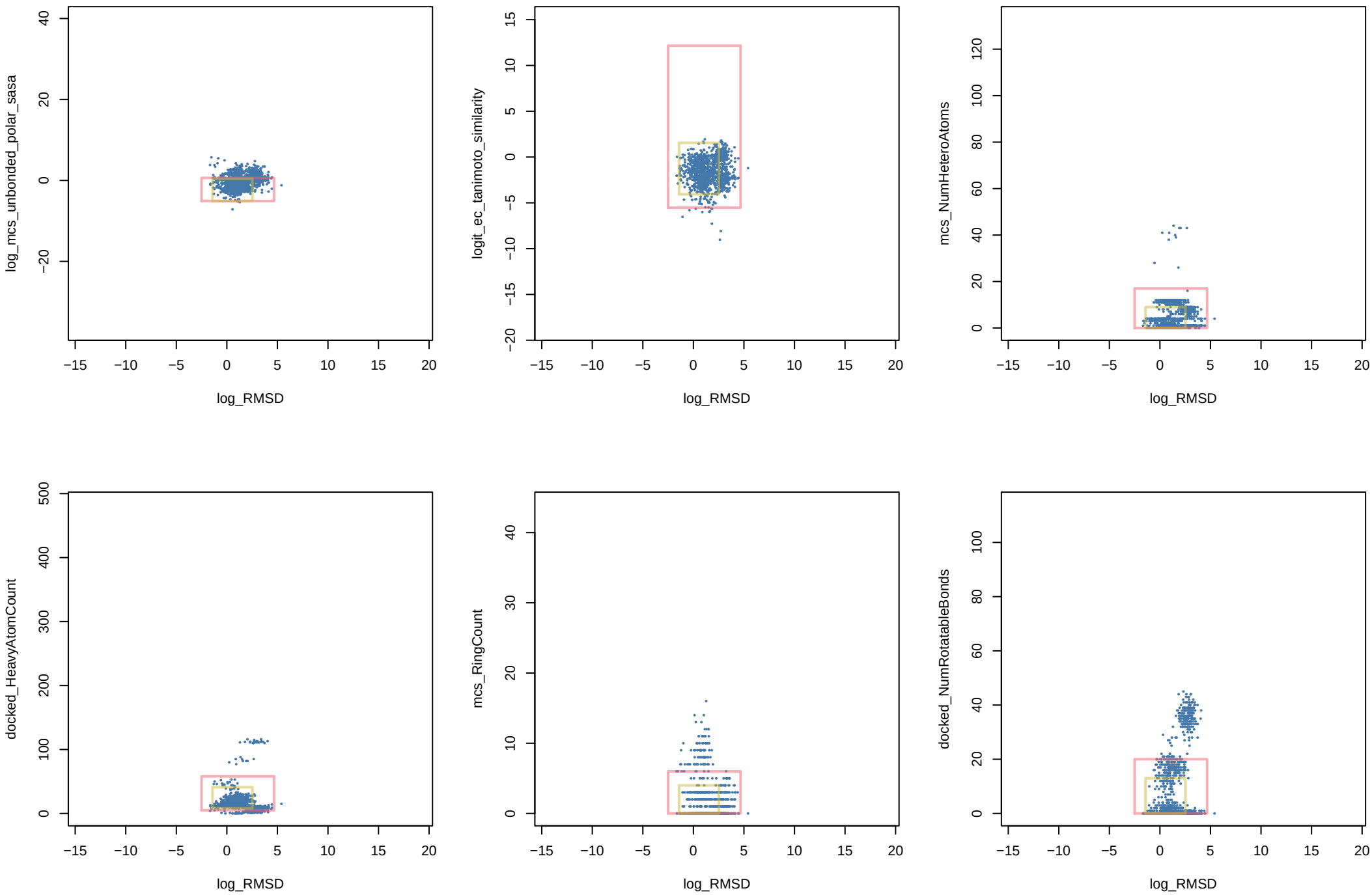
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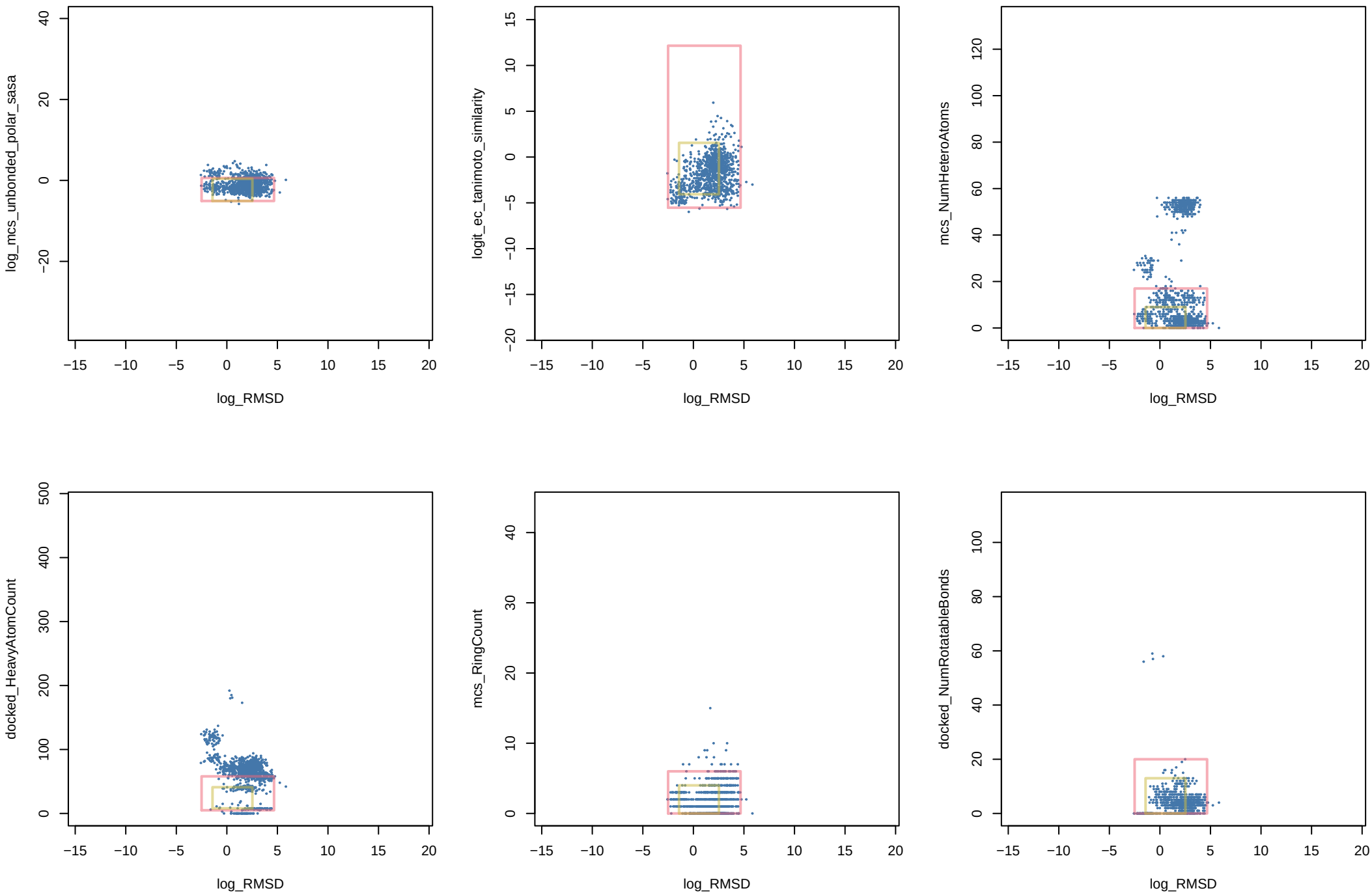
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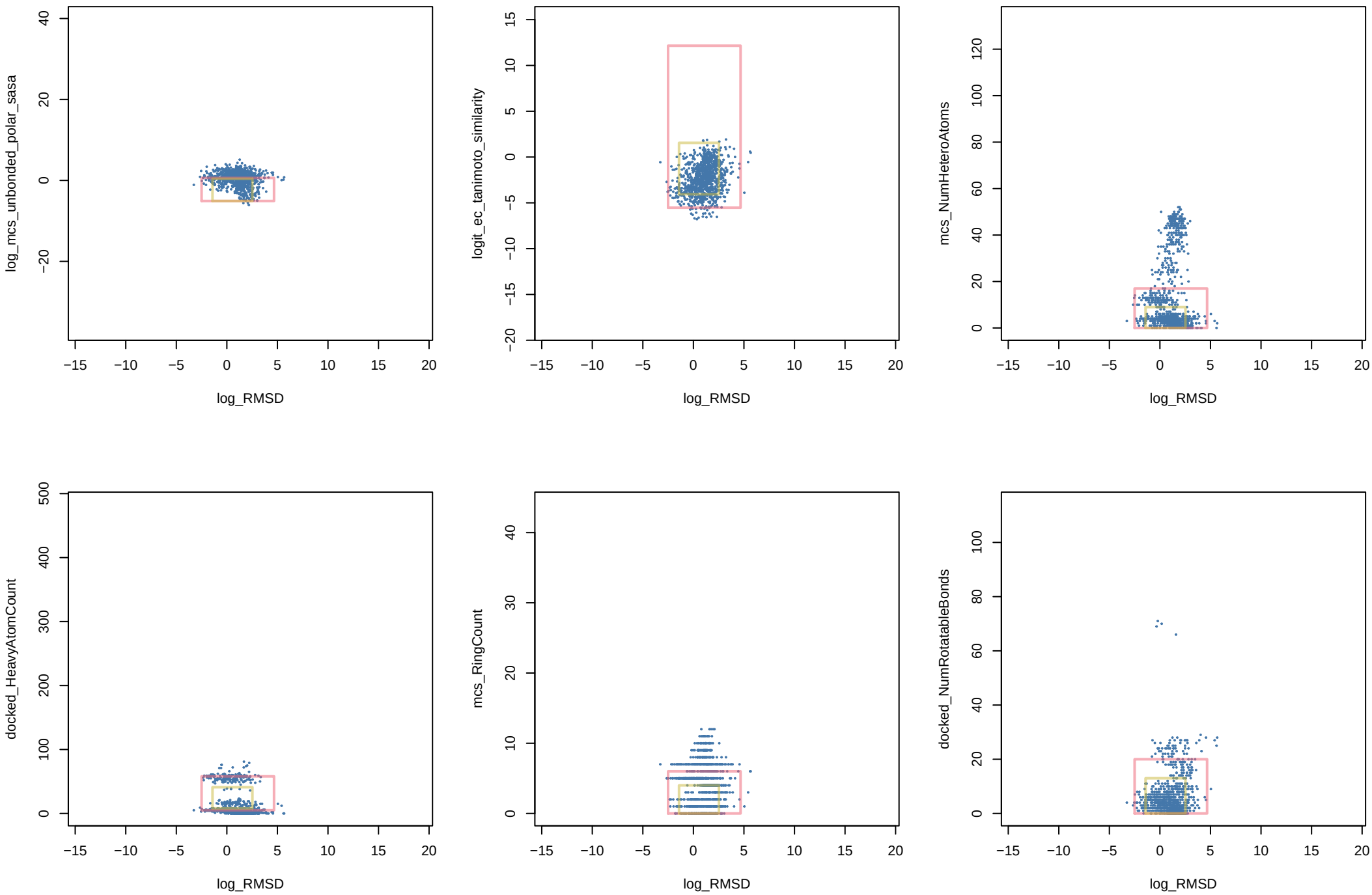
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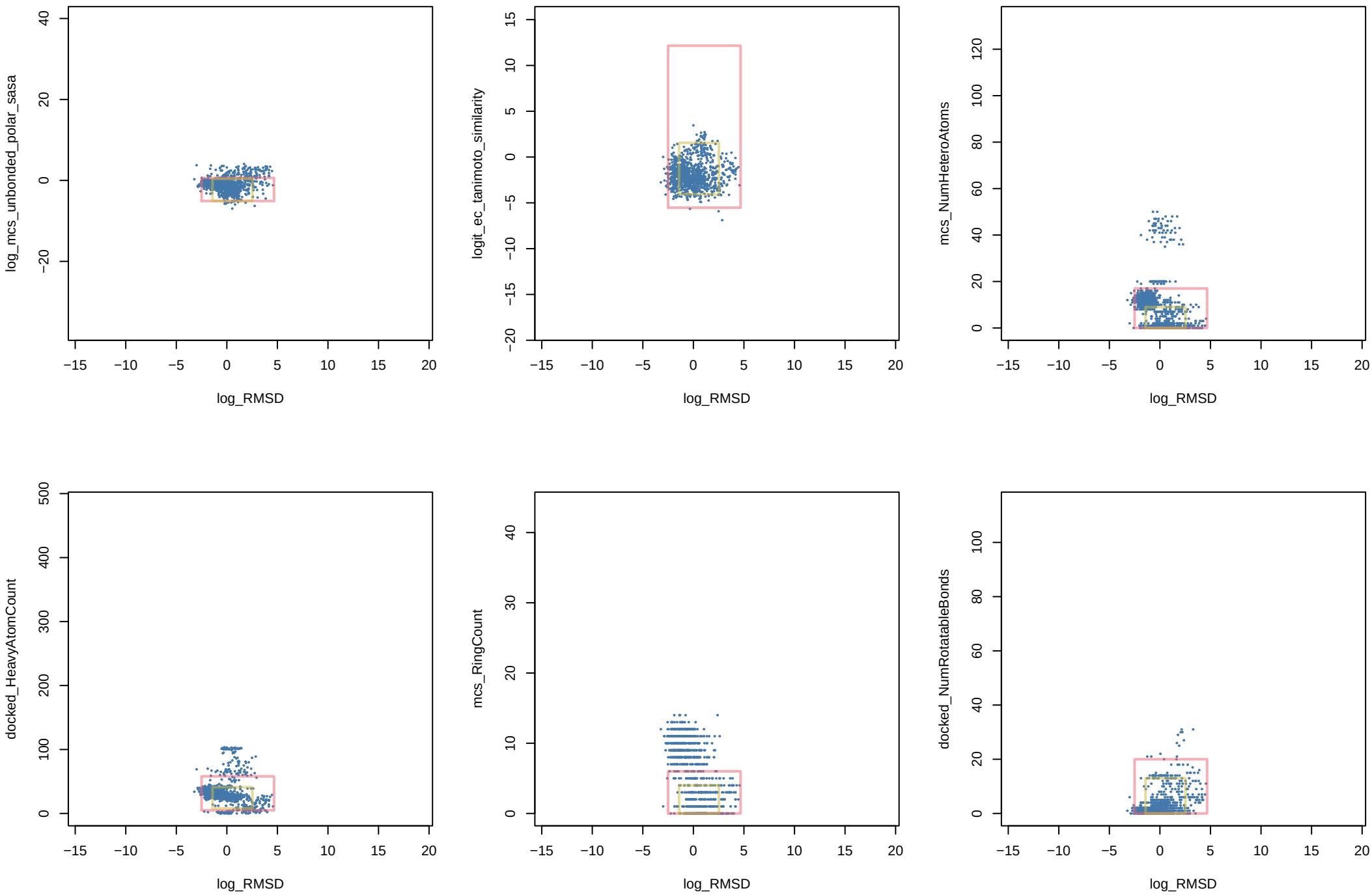
docked_HeavyAtomCount
log_RMSD
mcs_RingCount
log_RMSD
docked_NumRotatableBonds
log_RMSD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log_RMSD
logit_ec_tanimoto_similarity
log_RMSD
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log_RMSD
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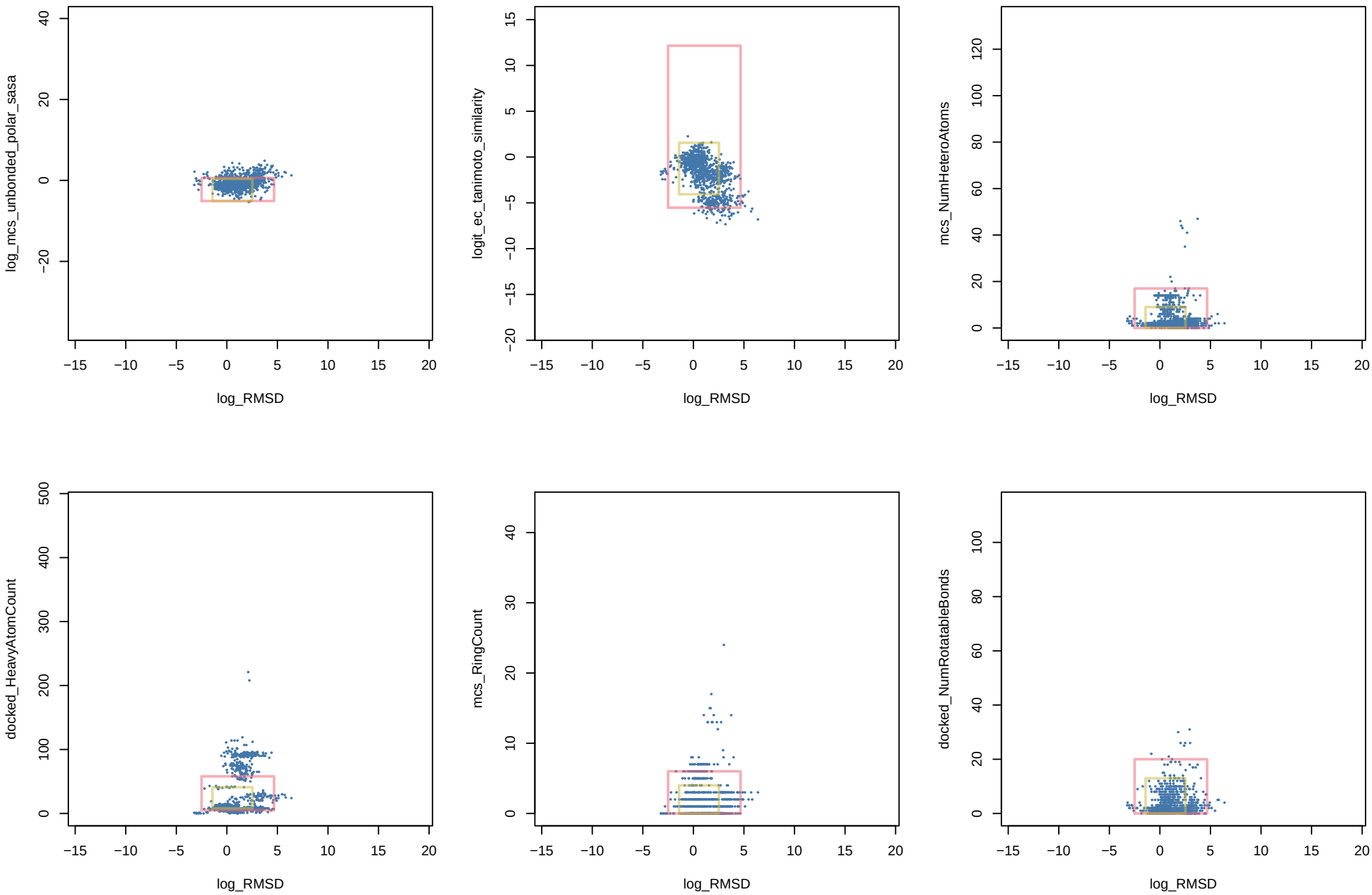
log_RMSD
docked_NumRotatableBonds
log_RMSD


log_mcs_unbonded_polar_sasa
log_RMSD
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log_RMSD
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log_RMSD
mcs_RingCount
log_RMSD
docked_NumRotatableBonds
log_RMSD