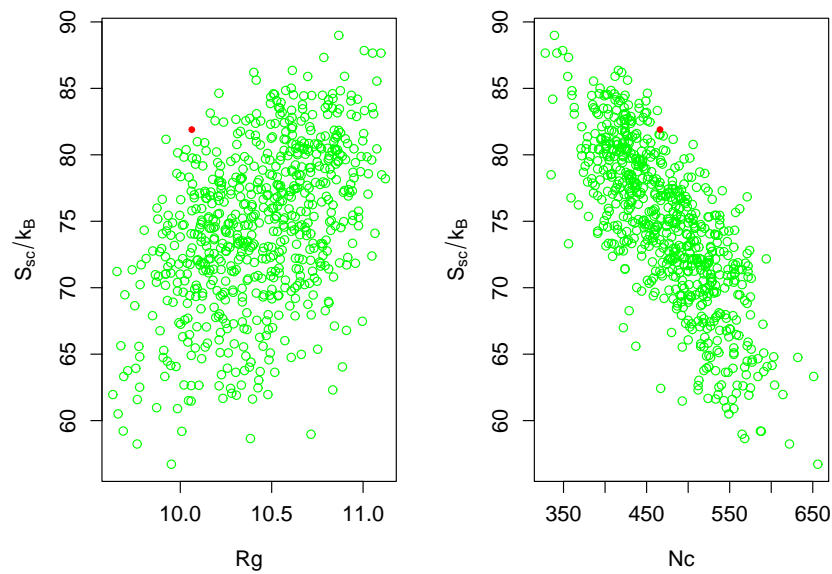


Supplementary material for the paper
On side-chain conformational entropy of proteins
Jinfeng Zhang and Jun S. Liu

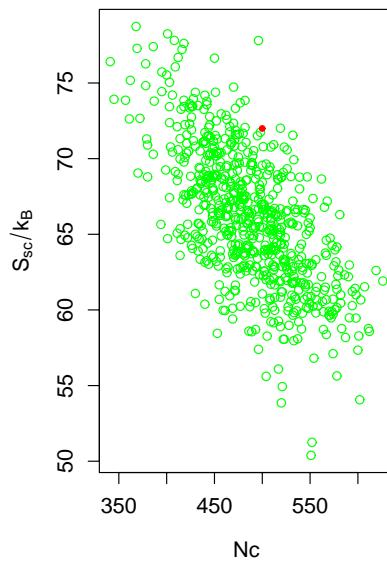
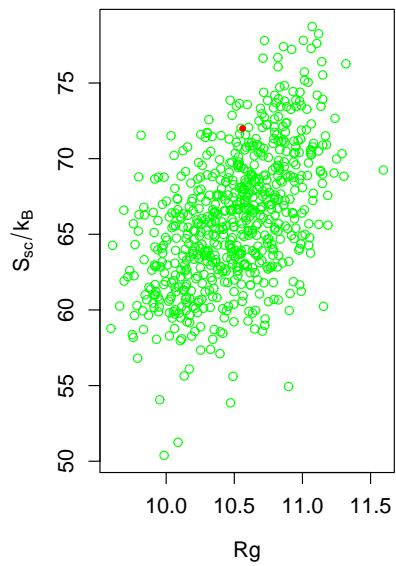
I. Side-chain entropy versus radius of gyration (R_g) and number of contacts (N_c) for X-ray protein structures and their decoys of monomeric proteins. Structures with no self-avoiding side-chain conformation are omitted. Natives are represented by red dots and decoys empty green circles. Y-axis is side-chain entropy and x-axis is R_g and N_c .

1. 4state_reduced decoy set

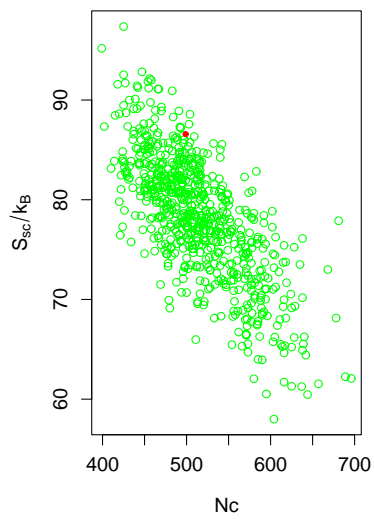
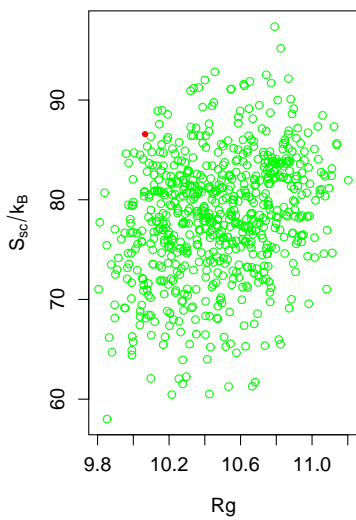
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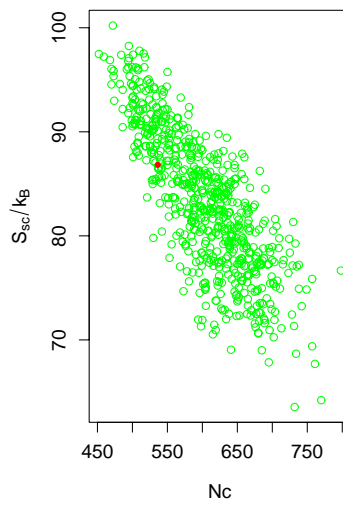
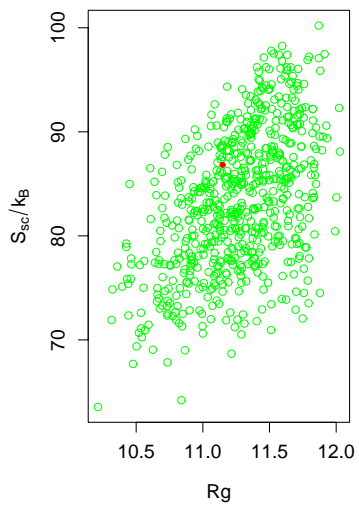
1sn3



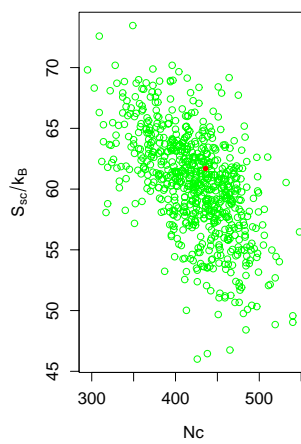
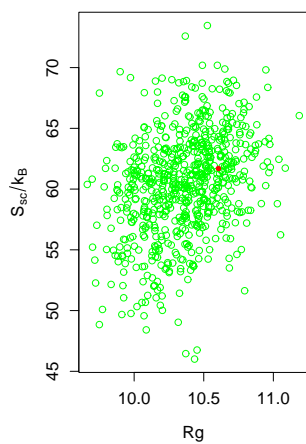
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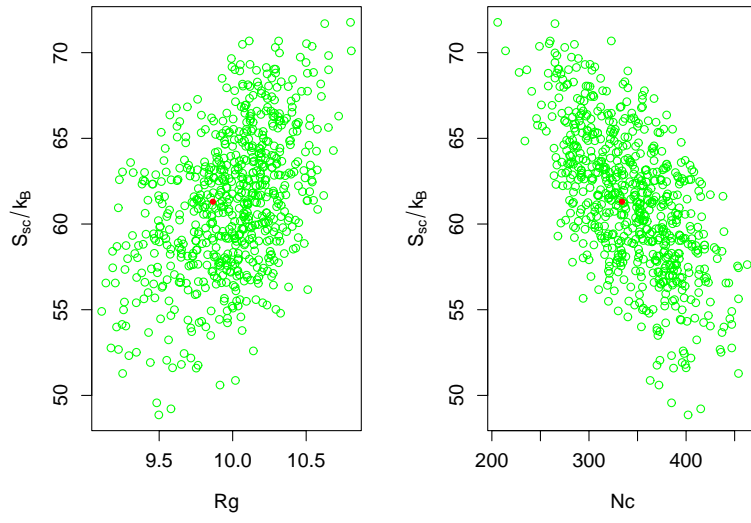
3icb (Metal binding protein)



4pti (Protein with disulfide bonds)

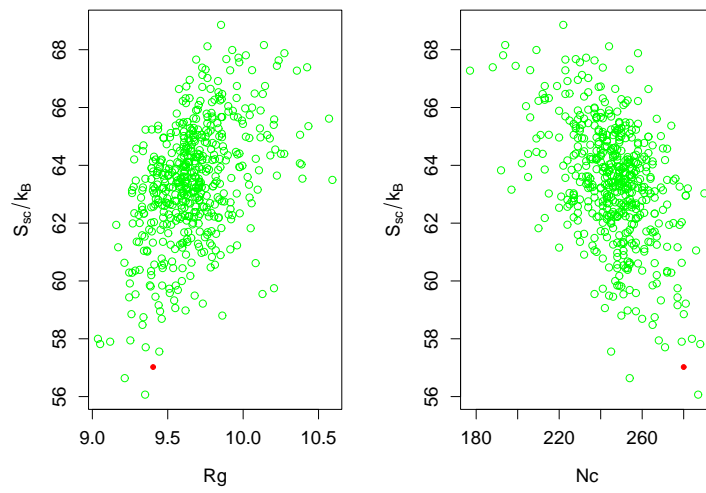


4rxn (Metal binding protein)

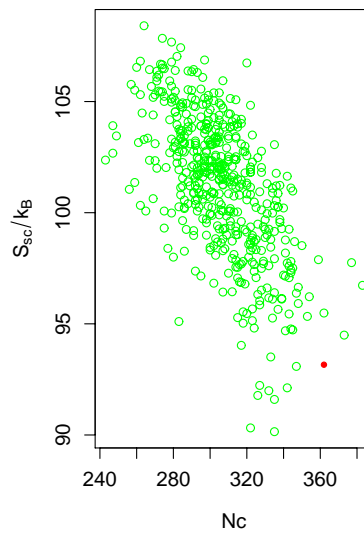
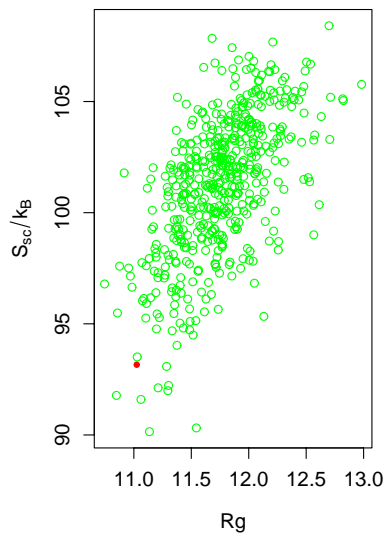


2. fisa

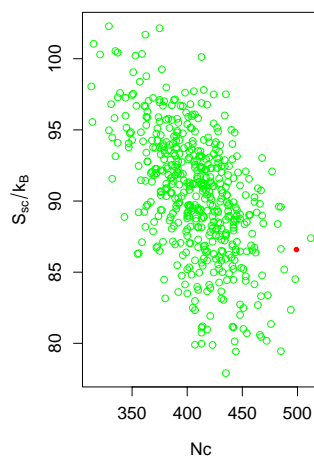
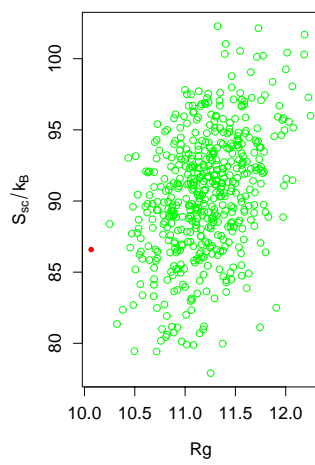
1fc2 (Protein interacting with another protein)



1hdd-C (Protein interacting with another protein)

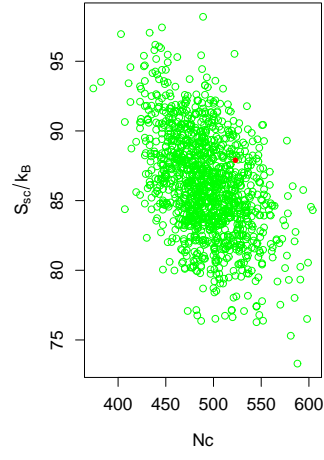
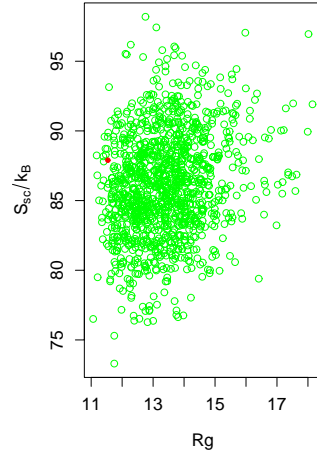


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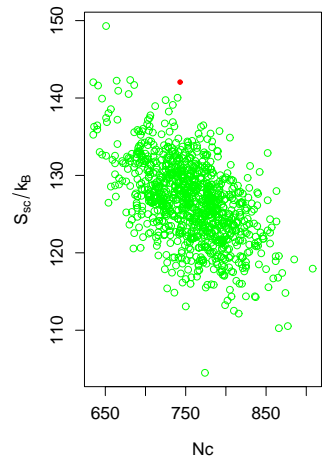
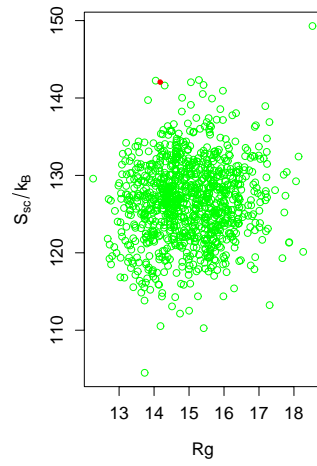


3. fisa_casp3

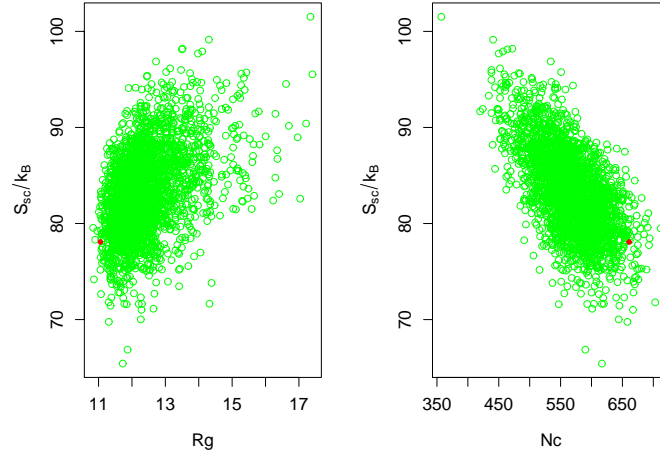
1bg8-A (Protein with Disulfide bonds)



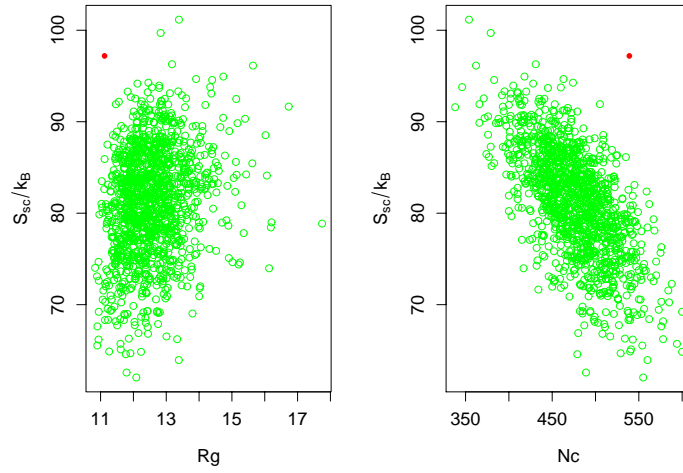
1b10



1eh2 (Metal binding protein)

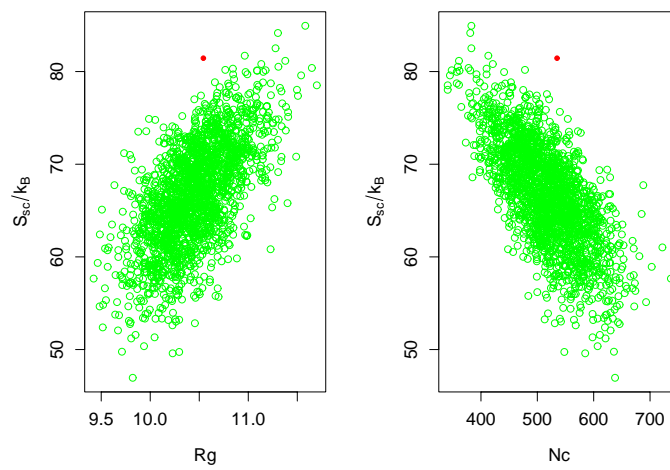


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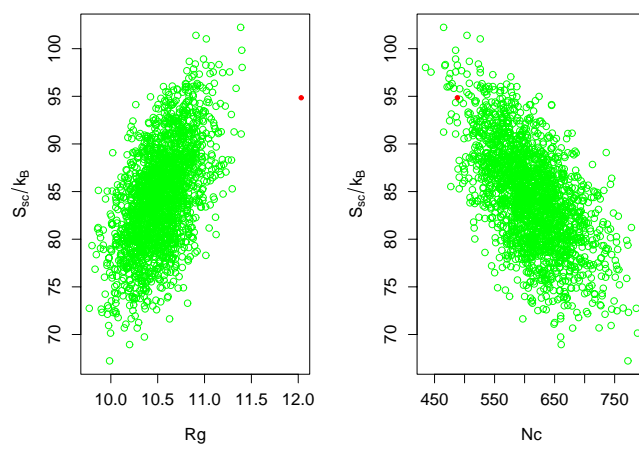


4. lattice_ssfit

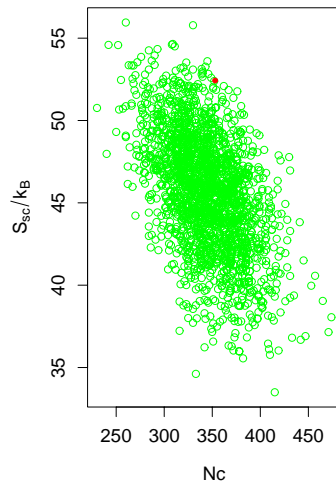
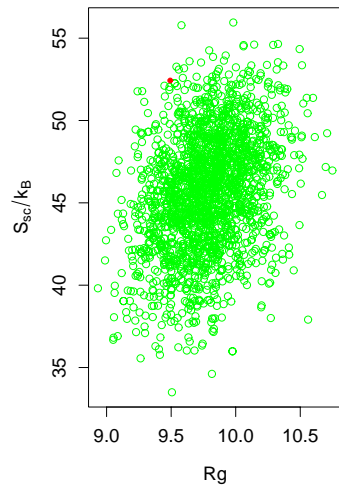
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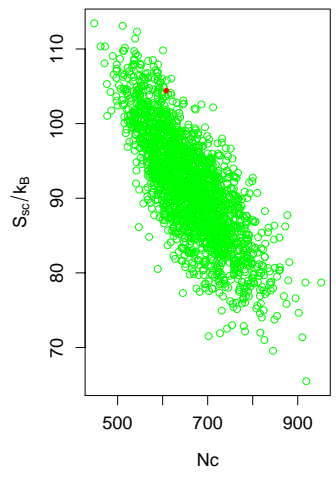
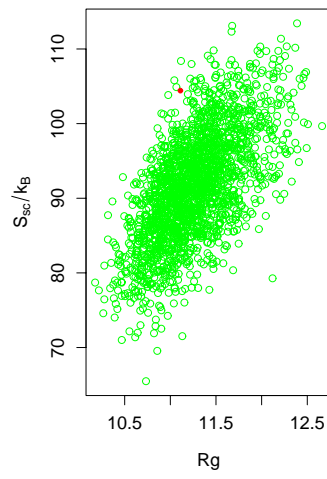
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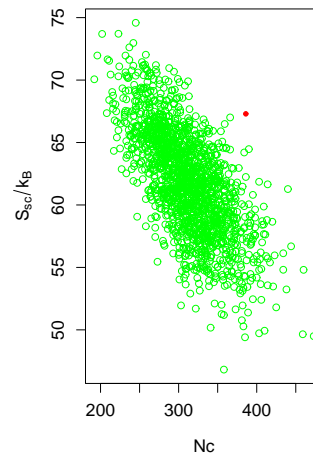
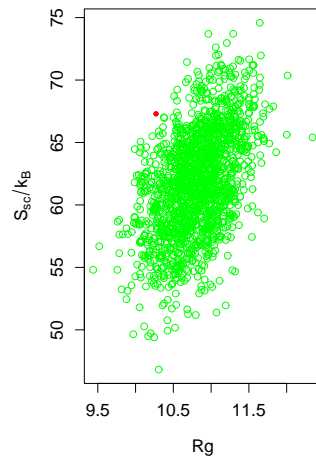
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1nkl

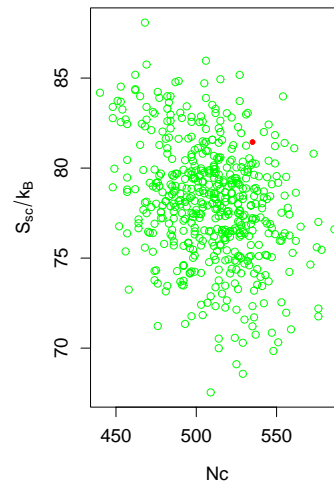
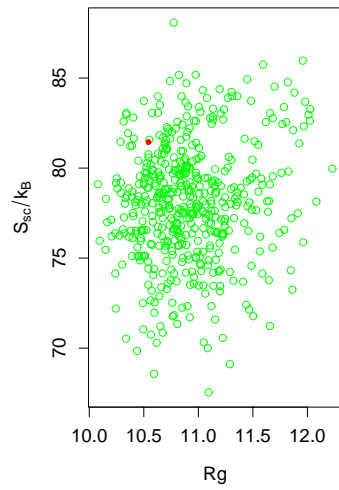


1pgb

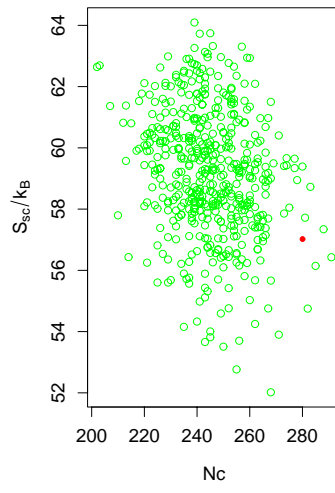
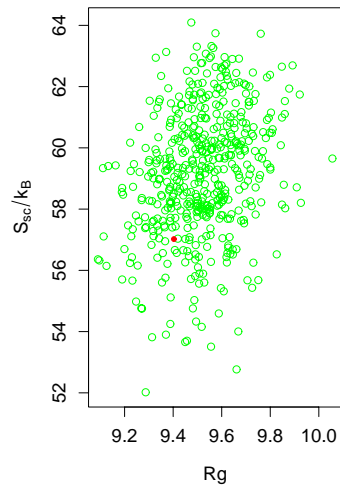


5. lmds

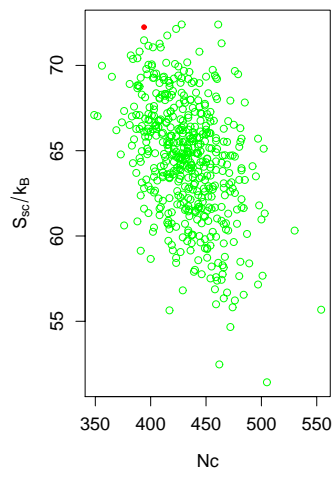
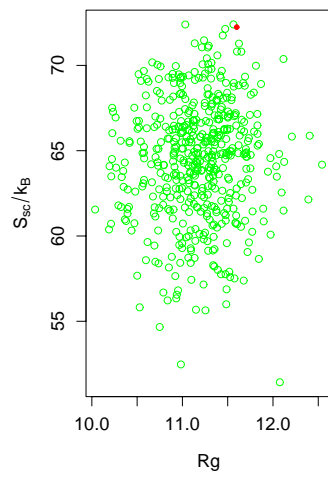
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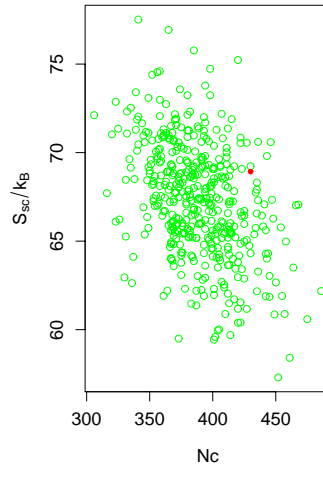
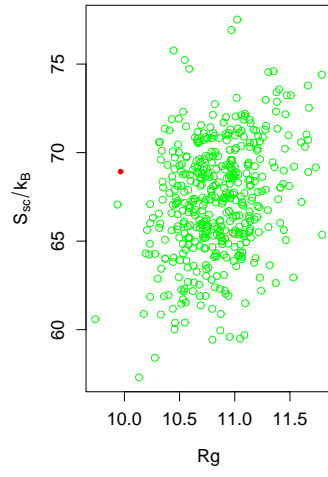
1fc2 (Protein interacting with another protein)



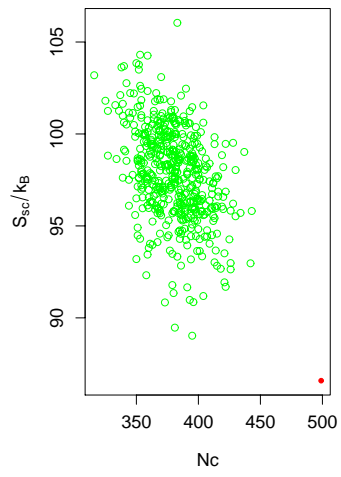
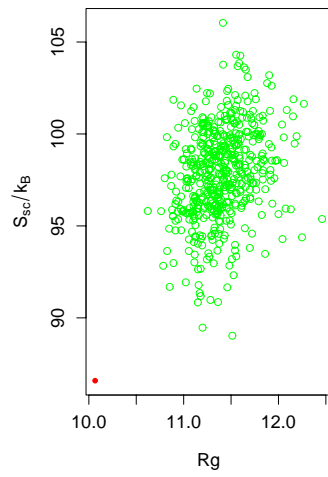
ligd



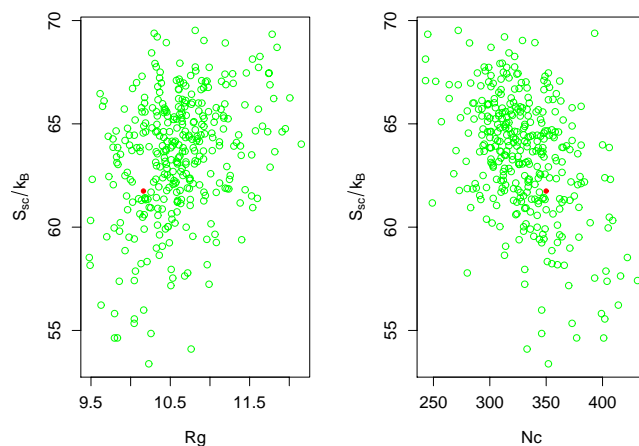
1shf-A



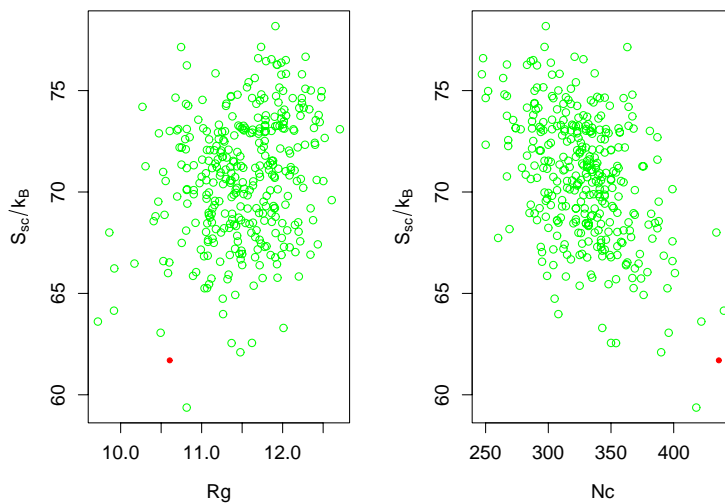
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2ovo

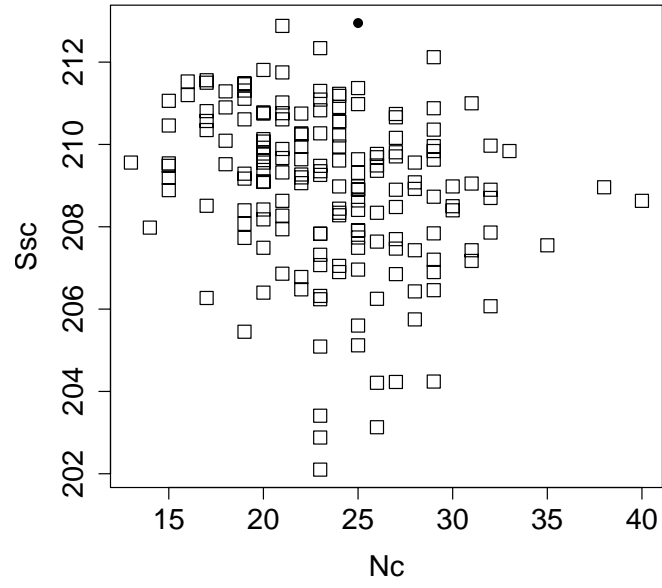


4pti (Protein with disulfide bonds)

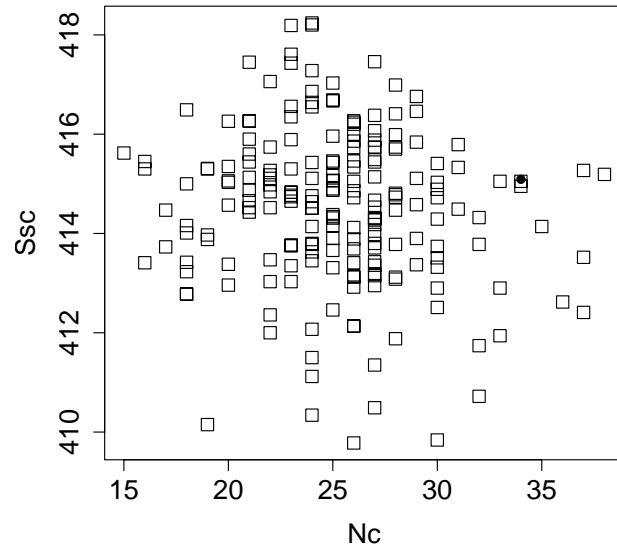


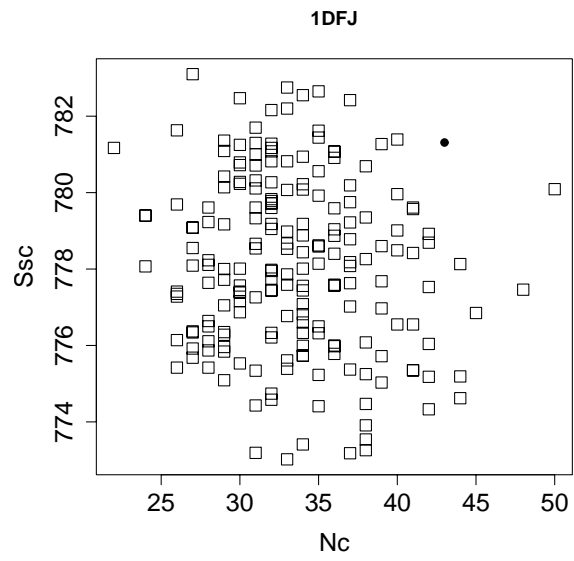
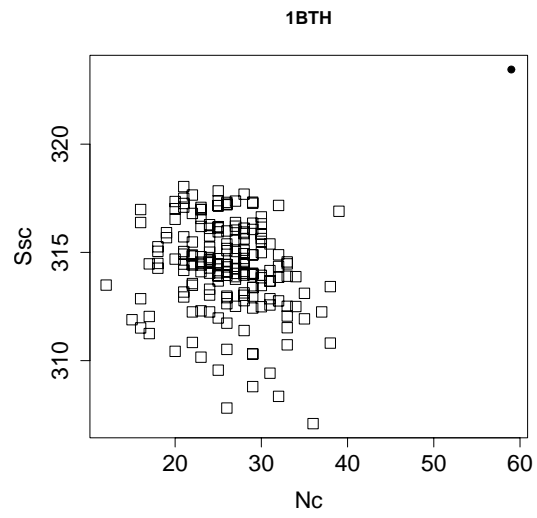
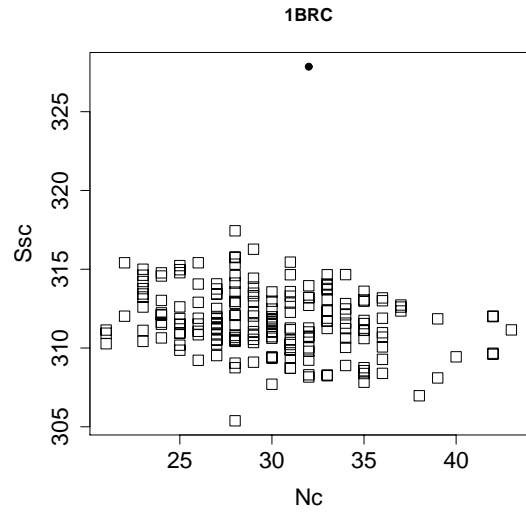
- II. Side-chain entropy versus number of contacts for X-ray structures and their decoys of protein-protein complexes generated by Rosetta program. Native complexes are represented by black dot and decoys empty squares. For some proteins (1bvk, 1cse, 1nmb, 2btf, 3hr), except native complex, all decoy structures have no self-avoiding conformations. Their figures are not shown.

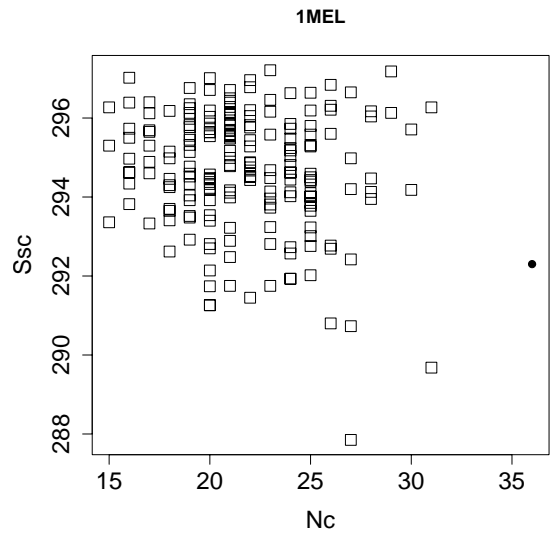
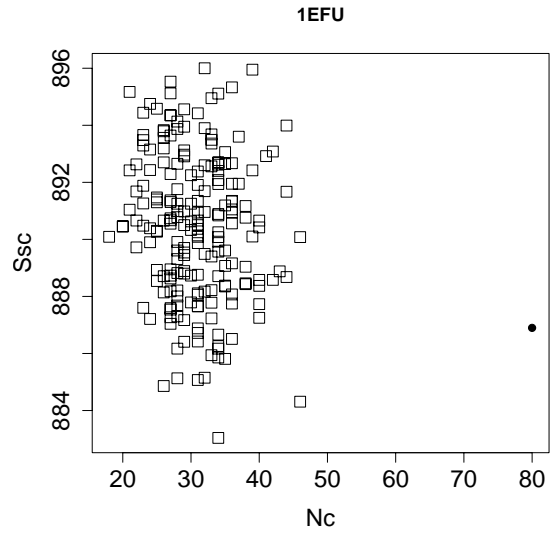
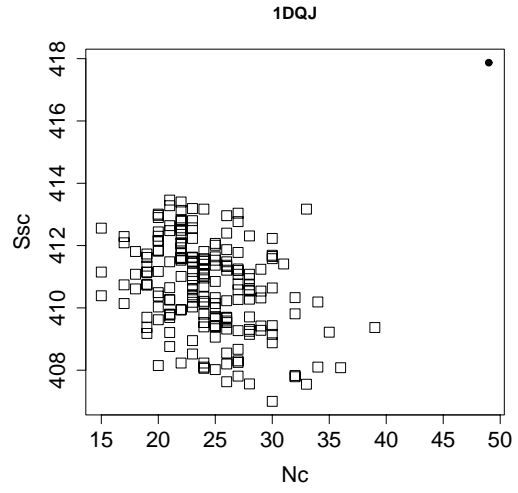
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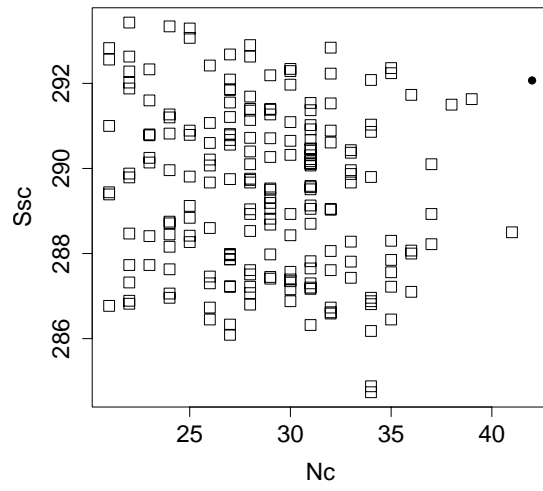
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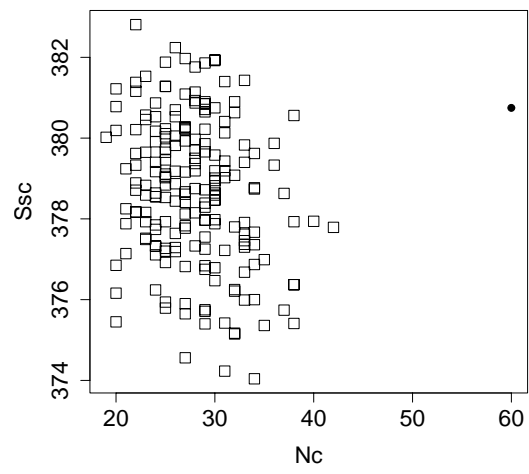




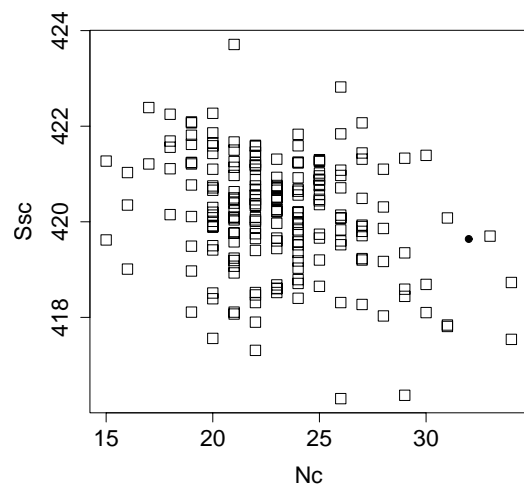
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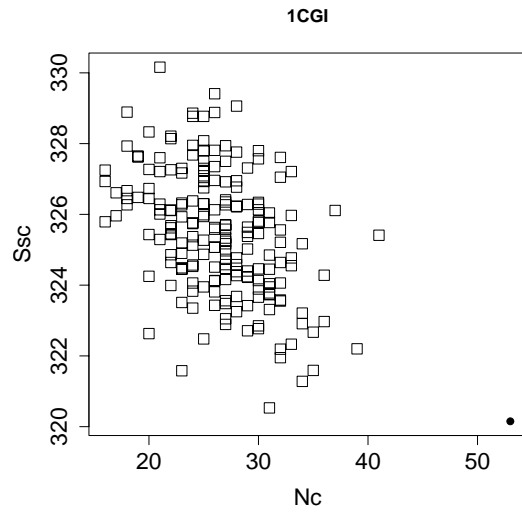
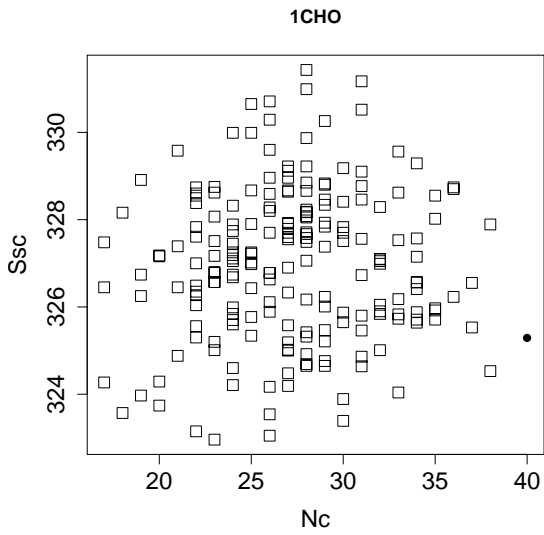
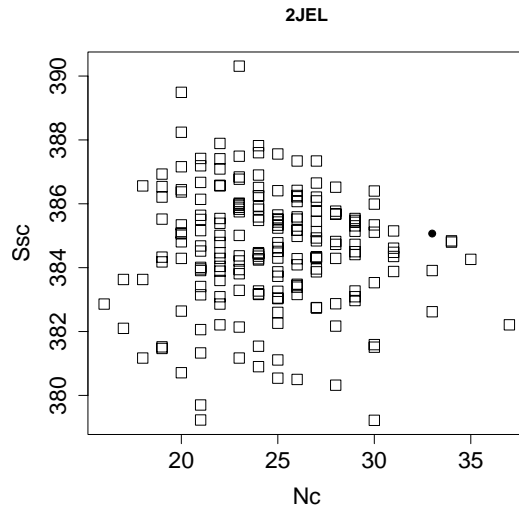
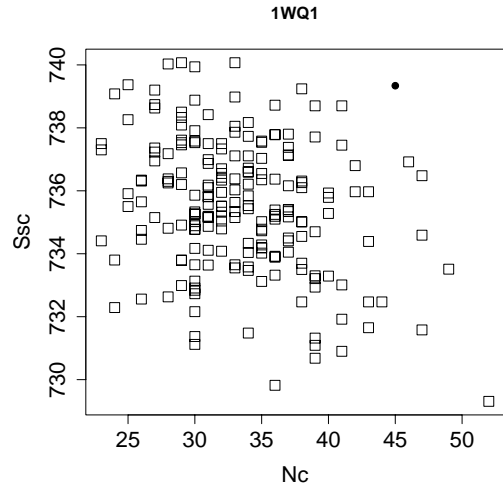


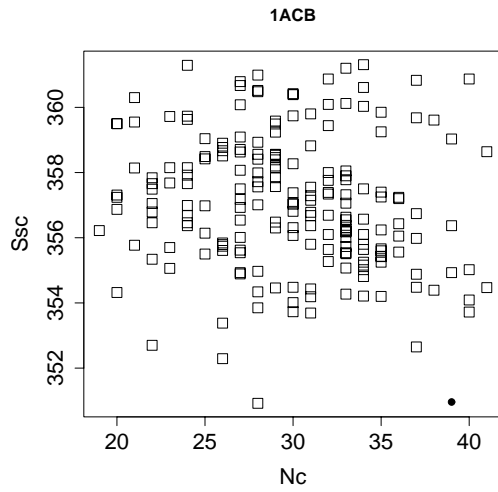
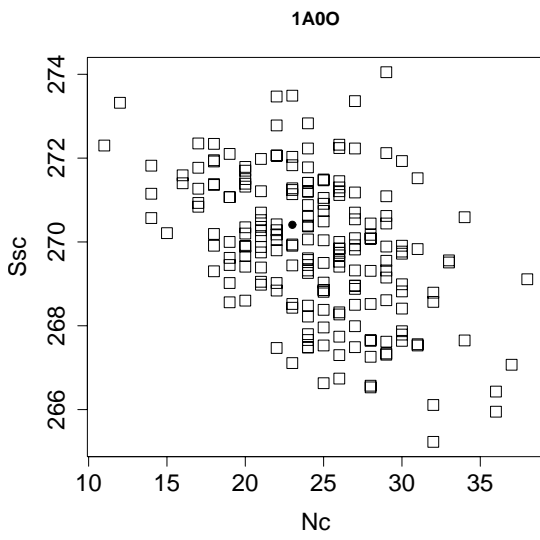
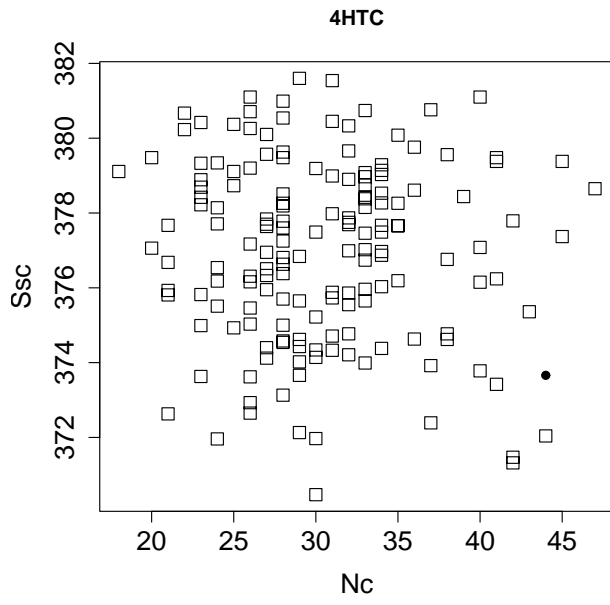
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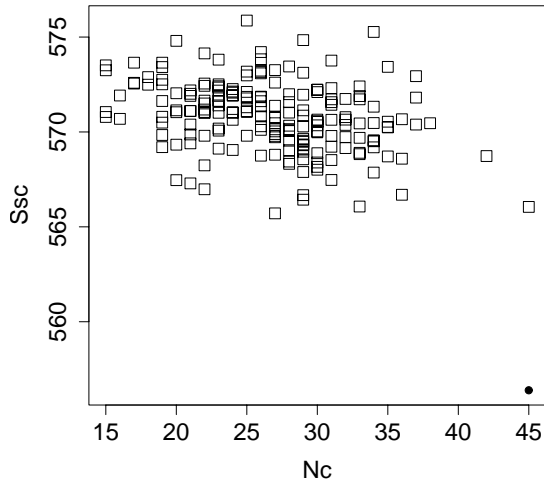
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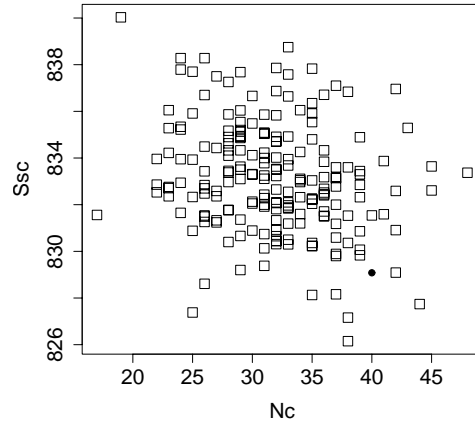




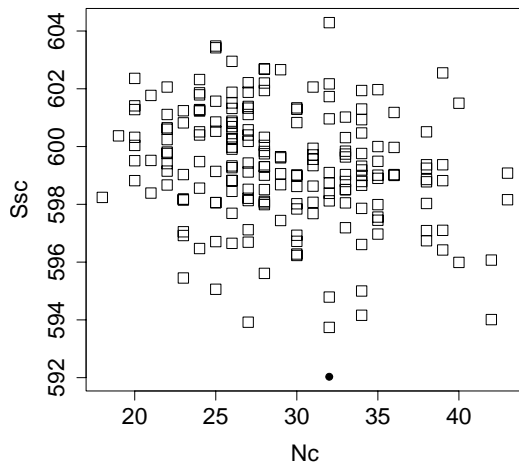
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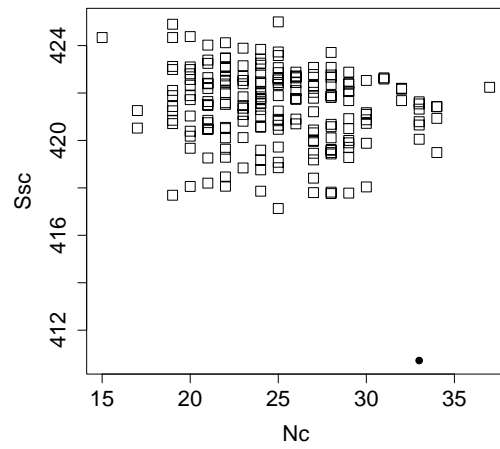
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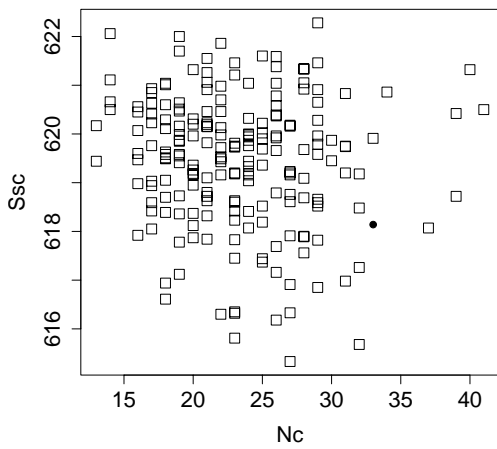
1EO8



1MLC



1QFU



1STF

