# Minor corrections

* Section 1.1, page 1: “focusing on SFs” should read: “focusing on **scoring functions (SFs)**”
* Section 2.4, page 3: “see section 3.C.1” should read: “see section **3.3.1**”
* Section 2.4, page 4: “complexes by performing dockings,” has an extras “s” and should read: “complexes by performing **docking**,”
* Section 3.1, page 4: “see section 3.C” should read: “see section **3.3**”
* Section 3.1, page 4: “ with CASF is conductedin a” is missing a space and should read: “with CASF is **conducted in** a”
* Section 3.3.4, page 6: “in section 2.D” should read: “in section **2.4**”
* Section 3.3.4, page 6: “this regression is performedwith” has a missing space, and should read: “this regression is **performed with**”
* Section 3.3.4, page 6: “from the databases mentioned in section 3. A, such as” should read: “from the databases mentioned in section **3.1**, such as”
* Section 3.3.4, page 6: “see section 3.C.1” should read: “see section **3.3.1**”
* Section 3.3.4, page 6: “As mentioned in section 3.C.2” should read: “As mentioned in section **3.3.2**”
* Section 3.3.4, page 7: “because when docking the comparison” has a missing comma, and should read “because when **docking, the** comparison”
* Section 3.3.4, page 9: “ As the iterations proceed,”, the word “the” can be eliminated, and should read “**As iterations proceed**,”
* Section 3.3.4, page 9: “can spuriously improve the performance”, can be improved in clarity, and should read “**can lead to spurious improvements in the performance**”

# Major corrections

* Change all the instances of “**an SF**” to “**a SF**”. There are six scattered in the text.
* The last two paragraphs of section 3.3.4 are actually Fig1 and Fig2 captions and should be deleted from the section text.
* Fig1 caption is “Fig. (1). Schematic binding affinity landscapes for a given protein-ligand complex for two scoring functions.” and should read: “**Fig. (1). Schematic binding affinity landscapes for a given protein-ligand complex for two scoring functions.The plot shows the binding energy estimates (scores) corresponding to two different scoring functions (SF1 in light blue and SF2 in orange) across all possible generalized coordinates values of a protein-ligand complex. The point in black is located at the experimental binding energy (dotted black line) and at the experimentally determined coordinate (full black line). The plot shows a putative case where the error of both SFs in the scoring task is very low, but the local and global minima of each scoring function correspond to different areas. With SF1, performing either minimization of the experimental structure or docking should result in a similar pose, while performing docking with SF2 will result in a completely different binding mode.”**
* Fig2 caption is ”Fig. (2). Schematic binding affinity landscapes for active and inactive compounds on the same target for two scoring functions.” and should read: “**Fig. (2). Schematic binding affinity landscapes for active and inactive compounds on the same target for two scoring functions. Each line represents the binding landscape of a molecule to the same protein target, with the active compound in a solid line and inactive compounds in dashed and dotted lines. Two different theoretical SFs are represented in each panel. Dots indicate protein-ligand complex structures used for training/evaluation of ranking power (see section 3.3.3), positioned at the same generalized coordinates in each panel. For the active molecule, the coordinates correspond to the experimental structure; for inactive compounds, coordinates are either experimentally determined or generated through molecular docking. Panel A: A self-consistent SF (light blue) where each training pose represents the global minimum, correctly ranking the active compound as the best binding candidate. Panel B: A non-self-consistent SF (orange). Though this SF ranks the active compound as the best candidate using the given poses, a complete energy landscape exploration would reveal both decoys ranking higher than the active com- pound.**