The Journal of Chemical Physics

Erratum: "AMBER-DYES in AMBER: Implementation of fluorophore and linker parameters into AmberTools" [J. Chem. Phys. 152, 221103 (2020)]

Cite as: J. Chem. Phys. **154**, 109901 (2021); https://doi.org/10.1063/5.0046589
Submitted: 04 February 2021 • Accepted: 17 February 2021 • Published Online: 10 March 2021

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scitation.org/journal/jcp

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Submitted: 4 February 2021 • Accepted: 17 February 2021 •
Published Online: 10 March 2021

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https://doi.org/10.1063/5.0046589

Previously, we adapted the AMBER-DYES parameter set derived by Graen *et al.*[1] into "AMBER-DYES in AMBER" to generate a force field applicable within the AMBER package of molecular simulation codes[2] for commonly used fluorescent dyes and linkers attached to a protein.[3] Recently, we became aware that the chemical structure of Alexa Fluor™ 647 (Alexa 647) available in "AMBER-DYES in AMBER" [Fig. 1(a)], which we took over from Graen *et al.*,[1] differs from the chemical structure generally available and now considered correct for Alexa 647[4] [Fig. 1(b)]. The chemical structure of Alexa 647, now commercially available from Thermo Fisher

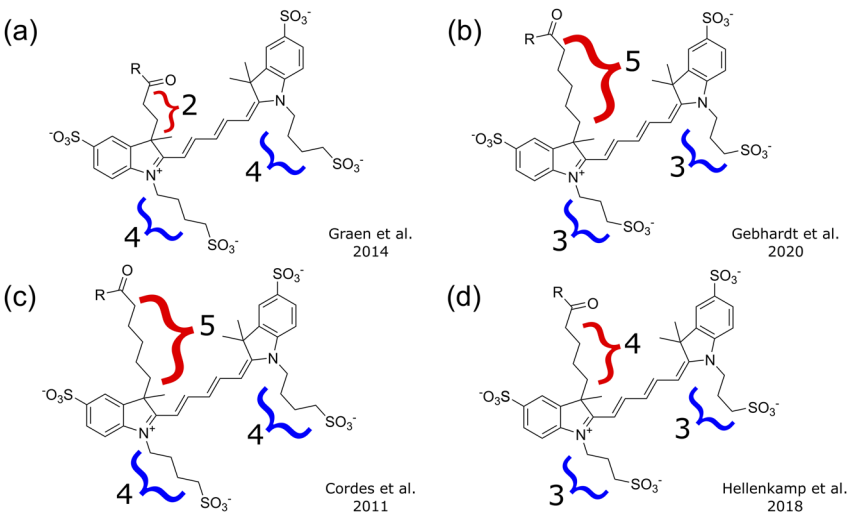

FIG. 1. Structures of Alexa Fluor 647 used in publications. The length of the carbon chain between the carbonyl group and the indolium moiety of the dye is marked by a red bracket; the length of the two carbon chains between the sulfo groups and the indolium moieties is marked by a blue bracket. (a) Structure used by Graen *et al.*[1] to parameterize AMBER-DYES. The structure has a C_2-chain (red) and two C_4-chains (blue) and agrees with that in Ref. 1. (b) Correct structure with a C_5-chain (red) and two C_3-chains (blue) according to Ref. 4. (c) Structure used in Ref. 6 with the correct C_5-chain (red), but wrong C_4-chains (blue). (d) Structure used in Ref. 7 with the wrong C_4-chain (red), but correct C_3-chains (blue).

Scientific,[5] has two differences [Figs. 1(a) and 1(b)]: (I) The length of the carbon chain between the carbonyl group and the indolium moiety of the dye and (II) the length of the two carbon chains between the sulfo groups and the indolium moieties. Note that yet other chemical structures of Alexa 647 were depicted in Ref. 6 [Fig. 1(c)] and Ref. 7 [Fig. 1(d)].

For the correct structure [Fig. 1(b)], we derived partial atomic charges using the restrained electrostatic potential (RESP[8]) procedure following the workflow described for the reparameterization of the cysteine linker in Ref. 3. The longer carbon chain between the indolium moiety and the carbonyl group [Fig. 1(b), red bracket] allows the dye to move more freely and occupy a larger volume around its attachment point.

The updated parameters for the Alexa 647 dye are listed in Texts S1 and S2. A *leaprc.amberdyes* file was created, which, when sourced in LEaP,[9] automatically loads the *lib* and *dat* files for the respective dye/linker combinations (see Table I in Ref. 3). The updated parameters have been made available in AmberTools20.[2]

See the supplementary material containing the new parameters for Alexa 647.

We are grateful for computational support and infrastructure provided by the "Zentrum für Informations- und Medientechnologie" (ZIM) at the Heinrich Heine University Düsseldorf and the computing time provided by the John von Neumann Institute for Computing (NIC) to H.G. on the supercomputers JURECA and JUWELS at the Jülich Supercomputing Centre (JSC, user IDs: HDD201 and schepers1).

The authors declare no competing financial interest.

NOMENCLATURE

Alexa Fluor 647	Alexa 647
T4L	T4 lysozyme

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