Data Article

Dataset of AMBER force field parameters of drugs, natural products and steroids for simulations using GROMACS

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\textbf{A B S T R A C T}

We provide general AMBER force field (GAFF) parameters for 160 organic molecules including drugs, natural products, and steroids, which can be employed without further processing in molecular dynamics (MD) simulations using GROMACS. We determined these parameters based on quantum mechanical (QM) calculations involving geometry optimization at the HF6-31G\textsuperscript{*} level of theory. For each molecule we provide a coordinate file of the three-dimensional molecular structure, the topology and the parameter file. The applicability of these parameters was demonstrated by MD simulations of these molecules bound to the active site of the main protease of the coronavirus SARS-CoV-2, 3CL\textsuperscript{pro}, which is a main player during viral replication causing COVID-19.

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Specifications Table

| Subject | Physical and Theoretical Chemistry |
|---------|-----------------------------------|
| Specific subject area | Computational biochemistry, Drug discovery, Computer-aided drug design |
| Type of data | PDB files, topology and parameter files in GROMACS format, Gaussian 09 and GROMACS code used for generating the data |
| How data were acquired | Quantum mechanics (QM) at the HF6-31G* level of theory, explicit-solvent molecular dynamics (MD) simulations |
| Data format | Raw |
| Parameters for data collection | Software used: Gaussian 09 for QM, GROMACS 2018 for MD |
| Description of data collection | Force field parameters were derived from QM calculations and assembled in the required files for MD simulations with GROMACS. |
| Data source location | Institute of Biological Information Processing: Structural Biochemistry (IBI-7), Forschungszentrum Jülich, 52428 Jülich, Germany |
| Data accessibility | Dataset is uploaded on Mendeley Data: https://doi.org/10.17632/phxtv76n5s.3 |
| Related research article | Olubiyi et al., Molecules 25, 3193 (2020) [1] |

Value of the Data

- GAFF parameters of 160 organic molecules ready for use in MD simulations employing GROMACS.
- The parameters given here are compatible with AMBER force fields, allowing to study the interactions of these molecules with proteins.
- Easy identification of the molecules via their ZINC or PubChem accession identifiers and, if available, their trivial names.

1. Data Description

In Table 1, the 160 molecules for which GAFF parameters were derived are listed. The compounds include 62 drugs approved by the FDA (U.S. Food and Drug Administration), 44 drugs approved by other countries’ national regulatory agencies (non-FDA) and investigational drugs, 39 natural products, 10 steroids, and 5 other molecules. Most of these molecules are included in the ZINC database [2–4], which is a curated collection of more than 230 million commercially available chemical compounds prepared for virtual screening. The molecules in Table 1 are therefore denoted by their ZINC database accession identifier (ID). For the few cases where a ZINC accession ID is not available, we provide the one from PubChem (starting with CID), which is a database of chemical molecules and their activities against biological assays. For the five molecules which are not yet found in the ZINC or the PubChem database, the reference where information about the molecule in question can be found is provided. In addition to the respective database accession ID we provide, if available, the trivial names of the compounds. For an easy identification of the molecules in MD simulations, we invented a 3-letter code for each molecule, that is also shown in Table 1 and is used as molecular identifier in the PDB and GROMACS files provided here.

For each of the molecules, we supply four files containing the raw data, which are compatible with the GROMACS format and allow the performance of MD simulations without further processing:

1. A PDB file containing three-dimensional coordinates of the molecule.
2. A top file containing the topology of the molecule.
3. An itp file containing the force field parameters, including the atomic charges as well as the \( \sigma \) and \( \varepsilon \) values.
4. An itp file with position restraints involving the heavy atoms as needed by an equilibration MD run.
Table 1
Identification details of the 160 molecules parameterized in this work.

| Accession ID       | Trivial Name   | 3-Letter Code | Accession ID       | Trivial Name   | 3-Letter Code |
|--------------------|----------------|---------------|--------------------|----------------|---------------|
| ZINC000072318121   | Abemaciclib    | AMB           | ZINC00003922429    | Adzelesin      | AZL           |
| ZINC000039768338   | Afatinib       | AFB           | ZINC00003780800    | Amrubcin       | ARC           |
| ZINC00001677837    | Apixaban       | APX           | ZINC00006717782    | BMS-599626     | BMS           |
| ZINC00000897240    | Azelastine     | ALT           | ZINC00001542916    | Carmofur       | CMF           |
| ZINC000014210642   | Azilsartan     | AZT           | ZINC000254071113   | Ciluprevir     | CPV           |
| ZINC000037828121   | Candesartan    | CDT           | ZINC0000174738     | Cinanserin     | CNS           |
| ZINC000085537017   | Cangrelor      | CGL           | ZINC00004215648    | Dihydroergocornine | DHC          |
| ZINC00001552174    | Ciclosporin    | CLT           | ZINC00014880002    | Dihydroergotoxine | DHE          |
| ZINC000060325170   | Cobimetinib    | COB           | CID3194            | Ebselen         | EBS           |
| ZINC00012503187    | Conivaptan     | CVT           | ZINC00004215770    | Elsamitrucin   | ETC           |
| ZINC00035902489    | Crizotinib     | CZB           | ZINC00098208742    | Entosplatinib  | EPB           |
| ZINC00001530788    | Cromolyn       | CML           | ZINC00001494900    | Enzastaurin    | EFS           |
| ZINC00003986735    | Dasatinib      | DSB           | ZINC00019899628    | Fenoverine     | FNV           |
| ZINC00001481815    | Deferasirox    | DFX           | ZINC00059185874    | GDC-0834       | GDC           |
| ZINC00003827556    | Delafloxacin   | DFC           | ZINC0003780340     | Hypericin      | HPC           |
| ZINC00001529268    | Disulfiram     | DSR           | ZINC0003781738     | Lestaurnitbin  | LTB           |
| ZINC00058581064    | Dolutegravir   | DLV           | ZINC0003950115     | Lonafernia     | LFB           |
| ZINC00003932831    | Dutasteride    | DUS           | ZINC0003817327     | Ly2090314      | LY2           |
| ZINC00022733806    | Enasidenib     | ESB           | ZINC00043203371    | MK-3207        | MK3           |
| ZINC00052955754    | Ergotamine     | ETM           | ZINC00100001820    | PF-00477736    | PF0           |
| ZINC00003918453    | Ertapenem      | EPN           | ZINC00013209429    | PX-12          | P12           |
| ZINC00003938684    | Etoposide      | ETP           | ZINC00038576002    | R-343          | NI3           |
| ZINC00003860453    | Fluorescein    | FRC           | ZINC00059749972    | Radotinib      | RDB           |
| ZINC000100001976   | Glimepiride    | GLP           | ZINC00063933734    | Rebastinib     | RBB           |
| ZINC00003532804    | Ibrutinib      | IRB           | CID121304016       | Remdesivir     | RDV           |
| ZINC00003920266    | Idarubicin     | IRC           | ZINC00003812168    | Ruboxistaurin  | RXS           |
| ZINC000013986658   | Idelalisib     | IDB           | ZINC00095533868    | Rwj-58259      | RJW           |
| ZINC000008101127   | Indocyanine    | IDC           | ZINC00003973984    | Sotrastraurin  | STS           |
| ZINC000022448696   | Indinavir      | IDV           | ZINC0003975327     | Telomestatin   | TMS           |
| ZINC000019632618   | Imatinib       | IMB           | ZINC00028827350    | Telcagepant    | TCG           |
| ZINC000027990463   | Lomitapide     | LTP           | ZINC0001385228     | Tideglusib     | TDG           |
| ZINC000064033452   | Lumacaftor     | LMC           | ZINC00043133316    | Tirilazad      | TAD           |
| ZINC00003927822    | Lurasidone     | LRD           | ZINC00084726167    | TMC647055      | TMC           |

(continued on next page)
| Accession ID   | Trivial Name | 3-Letter Code | Accession ID   | Trivial Name | 3-Letter Code |
|---------------|--------------|---------------|---------------|--------------|---------------|
| ZINC00000003902 | Maraviroc   | MVC           | ZINC00000397803 | Tubocurarine | TBC           |
| ZINC000000381151 | Montelukast | MTL           | ZINC000068250462 | Tucatinib   | TCB           |
| ZINC0000010378061 | Naldemedine | NMD           | ZINC0000095539256 | UK-432,097  | UK4           |
| ZINC000005844788 | Nebivolol   | NBL           | ZINC000001490807 | —           | N15           |
| ZINC000006769597 | Nilotinib   | NLI           | ZINC000001539348 | —           | N14           |
| ZINC0000043206370 | Niraparib  | NPB           | ZINC000003930598 | —           | N17           |
| ZINC0000040430143 | Olaparib   | OPB           | ZINC000018710085 | —           | TFB           |
| ZINC000003812865 | Olsalazine  | OSZ           | ZINC000021290045 | —           | N11           |
| ZINC000003938686 | Palbociclib | PBB           | ZINC000049888572 | —           | N12           |
| ZINC000004214700 | Paliperidone | PLP          | ZINC000095092808 | —           | N16           |
| ZINC000011617039 | Pazopanib   | PZB           | ZINC000100029945 | Zosuquidar   | ZSQ           |
| ZINC0000030691797 | Perampanel | PRP           |               |              |               |
| ZINC000004175630 | Pimozide    | PMZ           | ZINC000003984030 | Amentoflavone | AMF           |
| ZINC000013831130 | Raltegravir  | RTV           | CID5321811     | Bavacoumestan A | BCA         |
| ZINC000003818943 | Regadenoson | RDS           | ZINC000004098612 | Corilagin   | CRG           |
| ZINC000003944422 | Ritonavir   | RNV           | ZINC00018847034 | Daidzein    | DDZ           |
| ZINC000003816514 | Rolapitant  | RLT           | CID12443227    | Epitaraxerol | ETX           |
| ZINC000029416466 | Saquinavir  | SQV           | ZINC00003870412 | Epigallocatechin gallate | EGC     |
| ZINC000019796168 | Sildenafil  | SDF           | ZINC00001531664 | Ginkgetin   | GKT           |
| ZINC000253632686 | Simprevir  | SPP           | ZINC0001077667 | Glabrolide   | GBL           |
| ZINC00000489478 | Sitagliptin | STG           | ZINC00004098322 | Homoeriodictyol | HMR     |
| ZINC000049036447 | Suvorexant | SVX           | CID10077799    | Isocorilagin | ICL           |
| ZINC000003938355 | Tadalafil   | TDF           | ZINC000003197535 | Isoginkgetin | IGK           |
| ZINC000001530886 | Telmisartan | TMT           | ZINC000100828606 | Neodiosmin   | NDS           |
| ZINC000004099008 | Teniposide | TNP           | ZINC000044351169 | Proanthocyanidin A1 | PA1   |
| ZINC000001530948 | Thalidomide | THD           | ZINC00004098619 | Proanthocyanidin A2 | PA2   |
| ZINC0000100016058 | Tipranavir | TFP           | ZINC000095619717 | Proanthocyanidin A5' | PA5   |
| ZINC000043100709 | Trametinib | TMB           | ZINC00000978800 | Rhodofolin   | RHL           |
| ZINC000018324776 | Vardenafil | VDF           | ZINC00002015152 | Shikonin     | SKN           |
| ZINC000003815419 | 2-Hydroxyestradiol | HED | ZINC0000230071666 | Theacitrin A | TCA   |
| ZINC000004096681 | 2-Hydroxyestrone | HES | ZINC000003978446 | Theacitrin C | TCC   |
| CID91451      | 17-α-hydroxyprogrenolone | AHP | ZINC000169372863 | Theasinensin A | TSA   |

(continued on next page)
| Accession ID   | Trivial Name          | 3-Letter Code | Accession ID   | Trivial Name          | 3-Letter Code |
|---------------|-----------------------|---------------|---------------|-----------------------|---------------|
| ZINC0000004081043 | Allopregnanolone      | APG           | ZINC0000008214976 | Theasinensin B    | TSB           |
| ZINC0000004428526 | Androstenedione       | ASD           | ZINC0000169333962 | Theasinensin F    | TSB           |
| ZINC0000004340309 | Cortisol              | CTS           | ZINC000002107922 | —                   | N14           |
| ZINC0000003807917 | Dehydroepiandrosterone | DHE            | ZINC000002114470 | —                   | N09           |
| CID5757       | Estradiol             | ESD           | ZINC000002125422 | —                   | N10           |
| CID27125      | Estetrol              | ESO           | ZINC000002147804 | —                   | N02           |
| ZINC000118912393 | Testosterone          | TST           | ZINC000002148919 | —                   | N01           |
| PDB 6LU7[19] | N3                    | N3P           | ZINC000002161217 | —                   | N08           |
| α-Ketoamide [20] | Inhibitor 11R        | 11R           | ZINC000004235306 | —                   | N15           |
| α-Ketoamide [20] | Inhibitor 13A        | 13A           | ZINC000006624329 | —                   | N12           |
| α-Ketoamide [20] | Inhibitor 13B        | 13B           | ZINC000008297065 | —                   | N16           |
| α-Ketoamide [20] | Inhibitor 14B        | 14B           | ZINC000008764269 | —                   | N11           |
|               | Other                 | Others        | ZINC000008789992 | —                   | N03           |
|               |                       |               | ZINC000011865175 | —                   | N06           |
|               |                       |               | ZINC00012296408  | —                   | N04           |
|               |                       |               | ZINC00012881832  | —                   | N05           |
|               |                       |               | ZINC000014887561 | Zeylanone           | ZYL           |
All files are assembled into one zip file, which is supplied via Mendeley Data, https://doi.org/10.17632/phxtv76n5s.3. Unpacking the zip file yields five folders: FDA, Non-FDA_and_Investigational, Natural_Products, Steroids, and Others. In each of them, one finds further directories, which are named according to the accession ID listed in Table 1. In these subdirectories there are the four files per molecule located, which all start with the 3-letter code as listed in the Table.

2. Experimental Design, Materials and Methods

To determine the GAFF parameters of the 160 molecules, we used the PDB files that we obtained from docking of these compounds bound to the crystal structure of 3CL\textsuperscript{pro} in our previous study [1] as starting point. We isolated the molecules from the protein in order to have only the ligand in the PDB file, which was processed using the GROMACS tool gmx editconf to enter the CONECT records specifying the connectivity between atoms in the PDB file. This is needed by Open Babel [5], which was applied afterwards to add missing hydrogen atoms. We then utilized Antechamber [6,7] as available in AmberTools 19 [8] to generate the input gcrf file for Gaussian, which contains the coordinates and net charge of the molecule in question. This format was selected since it guarantees that the atom order as present in the PDB file is not changed by Gaussian. These preparatory steps were followed by the QM calculations at the HF6-31G* level of theory, including a geometry optimization and the determination of the electrostatic potential using Gaussian 09 [9]. Antechamber was then employed to extract the force field parameters from the output file called gout, involving bond lengths, bond angles, and torsion angles as well as Lennard-Jones (LJ) interaction parameters. Furthermore, Antechamber also allows to calculate the restrained electrostatic potential (RESP) for determining partial charges [10,11]. Afterwards, we created a mol2 file containing all necessary parameters, which was analyzed by ACYPYE [12] to generate the required GROMACS input files with extensions .gro, .top, and .itp.

To this procedure two exceptions had to be made: (1) In the case that the molecule in question contains an iodine atom, the basis set CEP-31G was used because at the 6-31G* level this atom is not included. This change is automatically accomplished by Antechamber. (2) Since ebselen contains a selenium atom which is not defined in Antechamber, we had to use a workaround. We performed the parameterization with sulfur, which exhibits similar properties like selenium, replacing the selenium atom. After the ACYPYE step, the sulfur atom was converted back to selenium in the affected GROMACS files. In addition, we changed the Se–N bond parameters in the itp file to the ones that were optimized for the MD software AMBER [13,14], which are $R_{\text{min}} = 2.12$ Å and $\varepsilon = 0.2910$ kcal/mol and can be converted into the GROMACS format using

$$
\sigma_{\text{GROMACS}} \text{[nm]} = 2 \cdot R_{\text{min}} \text{[Å]} \cdot 2^{-1/6} \cdot 0.1 = 3.77741 \times 10^{-1} \text{ nm}
$$

$$
\epsilon_{\text{GROMACS}} \text{[kJ/mol]} = 4.184 \cdot \varepsilon_{\text{AMBER}} \text{[kcal/mol]} = 1.21754 \text{ kJ/mol}
$$

To test the reliability of the resulting force field parameters, we applied them in energy minimizations of the 160 molecules using their structures as obtained from docking to 3CL\textsuperscript{pro} [15], which were also used for the force field parameterization as starting structures. These calculations were realized with GROMACS 2018 [16]. The energy minimizations were performed using the steepest descent algorithm until all forces were less than 10 kJ mol\(^{-1}\) nm\(^{-1}\). The resulting energy-minimized structures were compared to the corresponding geometry-optimized conformations from the QM calculations by determining their root mean square deviation (RMSD) after structural superposition using PyMOL [17]. If the RMSD was ≤ 4 Å, then no further checks were applied. If this cutoff was exceeded, which happened for only few of the molecules, the structural reorientations were inspected in more detail. However, in none of the cases severe structural rearrangements had occurred. The increased RMSD values could be explained with local rotations of rings or alkyl groups. Afterwards, we applied the newly derived force field parameters in 20 ns MD simulations of the molecules docked to 3CL\textsuperscript{pro} using GROMACS 2018 and
AMBER14SB [18] as force field for the protein. For 99 of the ligands that fulfilled specific structural requirements for inhibitor design reported in [15], the MD simulations were extended to 100 ns. All MD simulations (whether 20 ns or 100 ns) finished successfully without any stability or incompatibility issues arising.

Via the already mentioned Mendeley dataset (https://doi.org/10.17632/phxtv76n5s.3), a zip file is provided that contains all Gaussian and GROMACS input files used for generating the force field parameters, along with bash scripts for automating the parameterization procedure as much as possible.

CRediT Author Statement

Jennifer Loschwitz: Methodology, Software, Data curation, Validation, Writing - original draft; Anna Jäckering: Formal analysis, Visualization, Writing - original draft; Monika Keutmann: Investigation, Data curation, Validation; Maryam Olagunju: Investigation, Data curation; Olujide O. Olubiyi: Conceptualization, Supervision, Writing - review & editing; Birgit Strodel: Conceptualization, Supervision, Project administration, Resources, Writing - review & editing.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships which have, or could be perceived to have, influenced the work reported in this article.

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