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Data Article

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

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ABSTRACT

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* 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, $3CL^{pro}$, 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 σ and ε 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
FDA			**Non-FDA and Investigational**		
ZINC000072318121	Abemaciclib	AMB	ZINC000003922429	Adozelesin	AZL
ZINC000003976838	Afatinib	AFB	ZINC000003780800	Amrubicin	ARC
ZINC000011677837	Apixaban	APX	ZINC000006717782	BMS-599626	BMS
ZINC000000897240	Azelastine	ALT	ZINC000001542916	Carmofur	CMF
ZINC000014210642	Azilsartan	AZT	ZINC000254071113	Ciluprevir	CPV
ZINC000003782818	Candesartan	CDT	ZINC000001714738	Cinanserin	CNS
ZINC000085537017	Cangrelor	CGL	ZINC000004215648	Dihydroergocornine	DHC
ZINC000001552174	Cilostazol	CLT	ZINC000014880002	Dihydroergotoxine	DHE
ZINC000060325170	Cobimetinib	COB	CID3194	Ebselen	EBS
ZINC000012503187	Conivaptan	CVT	ZINC000004215770	Elsamitrucin	ETC
ZINC000035902489	Crizotinib	CZB	ZINC000098208742	Entospletinib	EPB
ZINC000001530788	Cromolyn	CML	ZINC000001494900	Enzastaurin	EZS
ZINC000003986735	Dasatinib	DSB	ZINC000019899628	Fenoverine	FNV
ZINC000001481815	Deferasirox	DFX	ZINC000059185874	GDC-0834	GDC
ZINC000003827556	Delafloxacin	DFC	ZINC000003780340	Hypericin	HPC
ZINC000001529266	Disulfiram	DSR	ZINC000003781738	Lestaurtinib	LTB
ZINC000058581064	Dolutegravir	DLV	ZINC000003950115	Lonafarnib	LFB
ZINC000003932831	Dutasteride	DUS	ZINC000003817327	Ly2090314	LY2
ZINC000222731806	Enasidenib	ESB	ZINC000043203371	MK-3207	MK3
ZINC000052955754	Ergotamine	ETM	ZINC000100001820	PF-00477736	PF0
ZINC000003918453	Ertapenem	EPN	ZINC000013209429	PX-12	P12
ZINC000003938684	Etoposide	ETP	ZINC000038576002	R-343	NI3
ZINC000003860453	Fluorescein	FRC	ZINC000059749972	Radotinib	RDB
ZINC000100001976	Glimepiride	GLP	ZINC000063933734	Rebastinib	RBB
ZINC000035328014	Ibrutinib	IRB	CID121304016	Remdesivir	RDV
ZINC000003920266	Idarubicin	IRC	ZINC000003812168	Ruboxistaurin	RXS
ZINC000013986658	Idelalisib	IDB	ZINC000095535868	Rwj-58259	RWJ
ZINC000008101127	Indocyanine	IDC	ZINC000003973984	Sotrastaurin	STS
ZINC000022448696	Indinavir	IDV	ZINC000003975327	Telomestatin	TMS
ZINC000019632618	Imatinib	IMB	ZINC000028827350	Telcagepant	TCG
ZINC000027990463	Lomitapide	LTP	ZINC000013985228	Tideglusib	TDG
ZINC000064033452	Lumacaftor	LMC	ZINC000043133316	Tirilazad	TAD
ZINC000003927822	Lurasidone	LRD	ZINC000084726167	TMC647055	TMC

(*continued on next page*)

Table 1 (*continued*)

Accession ID	Trivial Name	3-Letter Code
ZINC000100003902	Maraviroc	MVC
ZINC000003831151	Montelukast	MTL
ZINC000100378061	Naldemedine	NMD
ZINC000005844788	Nebivolol	NBL
ZINC000006716957	Nilotinib	NLB
ZINC000043206370	Niraparib	NPB
ZINC000040430143	Olaparib	OPB
ZINC000003812865	Olsalazine	OSZ
ZINC000003938686	Palbociclib	PBB
ZINC000004214700	Paliperidone	PLP
ZINC000011617039	Pazopanib	PZB
ZINC000030691797	Perampanel	PRP
ZINC000004175630	Pimozide	PMZ
ZINC000013831130	Raltegravir	RTV
ZINC000013818943	Regadenoson	RDS
ZINC000003944422	Ritonavir	RNV
ZINC000003816514	Rolapitant	RLT
ZINC000029416466	Saquinavir	SQV
ZINC000019796168	Sildenafil	SDF
ZINC000253632968	Simeprevir	SPV
ZINC000001489478	Sitagliptin	STG
ZINC000049036447	Suvorexant	SVX
ZINC000003993855	Tadalafil	TDF
ZINC000001530886	Telmisartan	TMT
ZINC000004099008	Teniposide	TNP
ZINC000001530948	Thalidomide	THD
ZINC000100016058	Tipranavir	TPV
ZINC000043100709	Trametinib	TMB
ZINC000018324776	Vardenafil	VDF
	Steroids	
ZINC000003815419	2-Hydroxyestradiol	HED
ZINC000004096681	2-Hydroxyestrone	HES
CID91451	17-α-hydroxypregnenolone	AHP
ZINC000003978083	Tubocurarine	TBC
ZINC000068250462	Tucatinib	TCB
ZINC000095539256	UK-432,097	UK4
ZINC000001490807	–	NI5
ZINC000001539348	–	NI4
ZINC000003930598	–	NI7
ZINC000018710085	–	TFB
ZINC000021290045	–	NI1
ZINC000049888572	–	NI2
ZINC000095092808	–	NI6
ZINC000100029945	Zosuquidar	ZSQ
	Natural Products	
ZINC000003984030	Amentoflavone	AMF
CID5321811	Bavacoumestan A	BCA
ZINC000004098612	Corilagin	CRG
ZINC000018847034	Daidzein	DDZ
CID12443227	Epitaraxerol	ETX
ZINC000003870412	Epigallocatechin gallate	EGC
ZINC000001531664	Ginkgetin	GKT
ZINC000100777667	Glabrolide	GBL
ZINC000004098322	Homoeriodictyol	HMR
CID10077799	Isocorilagin	ICL
ZINC000003197535	Isoginkgetin	IGK
ZINC000100828606	Neodiosmin	NDS
ZINC000044351169	Proanthocyanidin A1	PA1
ZINC000004098619	Proanthocyanidin A2	PA2
ZINC000095619717	Proanthocyanidin A5'	PA5
ZINC000003978800	Rhoifolin	RHL
ZINC000002015152	Shikonin	SKN
ZINC000150352420	Theacitrin A	TCA
ZINC000230071666	Theacitrin C	TCC
ZINC000003978446	Theaflavin	TFV
ZINC000169372863	Theasinensin A	TSA

(*continued on next page*)

Table 1 (*continued*)

Accession ID	Trivial Name	3-Letter Code	Accession ID	Trivial Name	3-Letter Code
ZINC000004081043	Allopregnanolone	APG	ZINC000008214976	Theasinensin B	TSB
ZINC000004428526	Androstenedione	ASD	ZINC000169333962	Theasinensin F	TSF
ZINC000004340309	Cortisol	CTS	ZINC000002107922	–	N14
ZINC000003807917	Dehydroepiandrosterone	DHE	ZINC000002114470	–	N09
CID5757	Estradiol	ESD	ZINC000002125422	–	N10
CID27125	Estetrol	ESO	ZINC000002147804	–	N02
ZINC000118912393	Testosterone	TST	ZINC000002148919	–	N01
	Others		ZINC000002158857	–	N13
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
			ZINC000008789992	–	N03
			ZINC000011865175	–	N06
			ZINC000012296408	–	N04
			ZINC000012881832	–	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 $3CL^{pro}$ 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 *gcrt* 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 ACPYPE [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 ACPYPE 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 $R_{\min} = 2.12$ Å and $\varepsilon = 0.2910$ kcal/mol and can be converted into the GROMACS format using

$$\sigma_{\text{GROMACS}}\,[\text{nm}] = 2 \cdot R_{\min}\,[\mathring{\text{A}}] \cdot 2^{-\frac{1}{6}} \cdot 0.1 = 3.77741 \times 10^{-1}\ \text{nm}$$

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

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 $3CL^{pro}$ [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 $3CL^{pro}$ 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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