



UNIVERSITY OF MARYLAND | NIST  
**INSTITUTE FOR BIOSCIENCE  
& BIOTECHNOLOGY RESEARCH**

**9600 Gudelsky Dr.  
Rockville, MD 20850  
Tel: (240) 314-6000  
Fax: (240) 314-6225**

Published on *Institute for Bioscience and Biotechnology Research* (<https://ibbr.umd.edu>)

Home > Drude polarizable force field for aliphatic ketones and aldehydes, and their associated acyclic carbohydrates.

---

# Drude polarizable force field for aliphatic ketones and aldehydes, and their associated acyclic carbohydrates.

Title	Drude polarizable force field for aliphatic ketones and aldehydes, a
Publication Type	Journal Article
Year of Publication	2017
Authors	Small, MC, Aytenfisu, AH, Lin, F-Y, He, X, Mackerell, AD
Journal	J Comput Aided Mol Des
Volume	31
Issue	4
Pagination	349-363
Date Published	2017 Apr
ISSN	1573-4951
Keywords	Aldehydes, Fructose, Glucose, Ketones, Molecular Dynamics Simula
Abstract	The majority of computer simulations exploring biomolecular functi
DOI	10.1007/s10822-017-0010-0
Alternate Journal	J. Comput. Aided Mol. Des.
PubMed ID	28190218
PubMed Central ID	PMC5392138
Grant List	R01 GM070855 / GM / NIGMS NIH HHS / United States R01 GM072558 / GM / NIGMS NIH HHS / United States