Force constant files for “FCCP”

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Description

Descriptions for the entry (BMOD0000008537) FCCP from Selleckchem Anti cancer compound Selleckchem.com(Anti cancer compound library). This entry was first introduced in [1].
This entry is aggregated and processed from the following sources[2][3][4][5][6][7][8][9]:

- On 2018-01-09 entry ID: S8276 was downloaded from Anti cancer compound library (Selleckchem Anti cancer compound Selleckchem.com)
- On 2018-08-28 entry ID: S8276 was downloaded from NMR Screening (National Magnetic Resonance Facility At Madison)
- On 2018-08-28 entry ID: S8276 was downloaded from ALATIS (National Magnetic Resonance Facility At Madison)
- On 2018-08-28 entry ID: S8276 was downloaded from RUNER (National Magnetic Resonance Facility At Madison)

Entry contents

There are 1 type of information in the entry (Molecular modeling file set), which are consist of 5 files for RUNER, 4 files for Xplor-NIH, 16 files for AMBER, 4 files for CHARMM. To produce the content of this entry 4 software packages were used;

- TopSpin[7]: provided by Bruker Biospin, which was used for Collection, Processing, Data analysis
- ALATIS[2]: provided by NMRFAM, which was used for Unique atom labeling
- RUNER[2][3]: provided by NMRFAM, which was used for Converting atom names to PDB format, Executing antechamber, Preparing molecular modeling files
- RDKit[9]: provided by RDKit: Open-Source Cheminformatics Software, which was used for Generating canonical SMILES strings

The NMRbox[8] computing platform was utilized in NMRbox to execute these software packages.

Release notes

There are 1 release notes for this entry, as follows:

- Author “NMRFAM” on 2018-08-28 applied the task “original meta data”, that is marked as “original”.

References

[1] TBA, *TBA*, TBA.

[2] Dashti Hesam, Westler William M., Markley John L., Eghbalnia Hamid R., *Unique identifiers for small molecules enable rigorous labeling of their atoms*, Scientific Data, 2017, 4, doi:10.1038/sdata.2017.73, https://www.nature.com/articles/sdata201773, 28534867, https://www.ncbi.nlm.nih.gov/pubmed/28534867, PMC5441290

[3] Dashti Hesam, Wedell Jonathan R., Cornilescu Gabriel, Schwieters Charles D., Westler William M., Markley John L., Eghbalnia Hamid R., *Robust nomenclature and software for enhanced reproducibility in molecular modeling of small molecules*, biorxiv preprint, 2018, https://doi.org/10.1101/429530, https://www.biorxiv.org/content/early/2018/09/27/429530

[4] Selleckchem, http://www.selleckchem.com/

[5] Wang J, Wolf RM, Caldwell JW, Kollman PA, Case DA., *Development and testing of a general amber force field.*, J. Comput Chem., 2004 Jul, 25, 9, doi: 0.1002/jcc.20035, 15116359

[6] Wang Junmei, Wang Wei, Kollman Peter A., Case David A., *Automatic atom type and bond type perception in molecular mechanical calculations.*, Journal of Molecular Graphics and Modelling, 2006, 25, 2, https://doi.org/10.1016/j.jmgm.2005.12.005

[7] TopSpin V.4, Bruker; https://www.bruker.com/products/mr/nmr/nmr-software/nmr-software/topspin/overview.html

[8] Maciejewski, M.W., Schuyler, A.D., Gryk, M.R., Moraru, I.I., Romero, P.R., Ulrich, E.L., Eghbalnia, H.R., Livny, M., Delaglio, F., Hoch, J.C. (2017) NMRbox: A Resource for Biomolecular NMR Computation. Biophysical Journal, 112, 1529-1534. http://dx.doi.org/10.1016/j.bpj.2017.03.011

[9] RDKit: Open-source cheminformatics; http://www.rdkit.org