Mcule - 'High Solubility Fragments' library

The library was created from Mcule's database with the following physicochemical property restrictions:

Property	Min	Max
Molar mass	80	275
H-bond acceptors	1	6
H-bond donors	0	3
Rotatable bonds	0	3
LogP	-1.7	4.5
Solubility in DMSO (mM)*	200	-
Solubility in PBS (mM)*	1	-

*Based on experimental data of chemical suppliers.

It was further filtered by substructure filters Including PAINS[1,2] to avoid promiscuous functional groups.

It contains the molecules in SDF format with fields regarding the solubility data of the molecules.
If you would prefer another molecular format or further filtering - feel free to contact us at support@mcule.com.

1, Baell, J. B. & Holloway, G. A. New Substructure Filters for Removal of Pan Assay Interference Compounds (PAINS) from Screening Libraries and for Their Exclusion in Bioassays. J. Med. Chem. 2719–2740 (2010).
2, Saubern, S., Guha, R. & Baell, J. B. KNIME Workflow to Assess PAINS Filters in SMARTS Format . Comparison of RDKit and Indigo Cheminformatics Libraries. Mol. Inform. 30, 847–850 (2011).

mcule.com Kft. ● H-1115 Budapest, Bartok Bela ut 105-113. Building II/A, Hungary, EU ● 535 Everett Ave #410, Palo Alto, CA 94301, USA ● www.mcule.com

Our professional laboratory services include

- Transferring samples to plates/vials as solid or DMSO solution
- Solubility characterization
- Temperature controlled shipping
- Quality control via LC-MS & NMR (on demand)

Please also reach out to our cheminformatics experts with projects related to

- Screening library building/expansion
- Generation of synthetically feasible chemical spaces based on your building blocks
- Filtering the Mcule database based on your criteria

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