

Resource Summary Report

Generated by SPARC SAWG on Aug 9, 2026

PyContact

RRID:SCR_025066

Type: Tool

Proper Citation

PyContact (RRID:SCR_025066)

Resource Information

URL: <https://pycontact.github.io/>

Proper Citation: PyContact (RRID:SCR_025066)

Description: Software tool for analysis of non-covalent interactions in molecular dynamics trajectories. Implemented in Python and is universally applicable to any kind of MD trajectory supported by MDAnalysis package.

Resource Type: software resource, software application, data analysis software, data processing software

Defining Citation: [PMID:29414703](https://pubmed.ncbi.nlm.nih.gov/29414703/)

Keywords: non-covalent interactions, molecular dynamics trajectories,

Funding: German Research Foundation ;
NIGMS P41 GM104601;
NSF

Availability: Free, Available for download, Freely available,

Resource Name: PyContact

Resource ID: SCR_025066

Alternate URLs: <https://github.com/maxscheurer/pycontact>

License: GNU GPL v3

Record Creation Time: 20240305T200904+0000

Record Last Update: 20260808T190717+0000

Ratings and Alerts

No rating or validation information has been found for PyContact.

No alerts have been found for PyContact.

Data and Source Information

Source: [SciCrunch Registry](#)

Usage and Citation Metrics

We found 3 mentions in open access literature.

Listed below are recent publications. The full list is available at [SPARC SAWG](#).

Cesaro S, et al. (2025) A crucial active site network of titratable residues guides catalysis and NAD⁺ binding in human succinic semialdehyde dehydrogenase. Protein science : a publication of the Protein Society, 34(1), e70024.

Omar MH, et al. (2024) Discovery of a Cushing's syndrome protein kinase A mutant that biases signaling through type I AKAPs. Science advances, 10(8), ead1258.

Ubbiali D, et al. (2021) An anti-HER2 nanobody binds to its antigen HER2 via two independent paratopes. International journal of biological macromolecules, 182, 502.