

# Resource Summary Report

Generated by [RRID](#) on Aug 11, 2026

## [sietraj](#)

RRID:SCR\_018021

Type: Tool

### Proper Citation

sietraj (RRID:SCR\_018021)

### Resource Information

**URL:** [https://www2.bri.nrc.ca/ccb/pub/sietraj\\_main.php](https://www2.bri.nrc.ca/ccb/pub/sietraj_main.php)

**Proper Citation:** sietraj (RRID:SCR\_018021)

**Description:** Software tool for binding free energies from Amber-generated MD trajectories. Alternative to MM-PBSA software provided by AMBER distribution. Virtual alanine mutations are also possible. Solvated interaction energies are calculated using parameters that have been fitted to reproduce binding free energies of data set of 99 protein-ligand complexes.

**Resource Type:** simulation software, software application, software resource

**Keywords:** Binding free energy, Amber, MD trajctory, MM-PBSA, virtual alanine mutation, solvated interaction energy, calculation, parameter, protein-ligand complex

**Availability:** Restricted

**Resource Name:** sietraj

**Resource ID:** SCR\_018021

**Record Creation Time:** 20220129T080338+0000

**Record Last Update:** 20260810T040727+0000

### Ratings and Alerts

No rating or validation information has been found for sietraj.

No alerts have been found for sietraj.

### Data and Source Information

**Source:** [SciCrunch Registry](#)

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## Usage and Citation Metrics

We found 2 mentions in open access literature.

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

Yan FF, et al. (2021) Comparison of the binding characteristics of SARS-CoV and SARS-CoV-2 RBDs to ACE2 at different temperatures by MD simulations. *Briefings in bioinformatics*, 22(2), 1122.

Martin ER, et al. (2020) In vivo crystals reveal critical features of the interaction between cystic fibrosis transmembrane conductance regulator (CFTR) and the PDZ2 domain of Na<sup>+</sup>/H<sup>+</sup> exchange cofactor NHERF1. *The Journal of biological chemistry*, 295(14), 4464.