

Resource Summary Report

Generated by [RRID](#) on Aug 15, 2026

QCxMS

RRID:SCR_026928

Type: Tool

Proper Citation

QCxMS (RRID:SCR_026928)

Resource Information

URL: <https://github.com/qcxms/QCxMS>

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Description: Software application as quantum chemical based program that enables users to calculate mass spectra using Born-Oppenheimer Molecular Dynamics. Quantum mechanic mass spectrometry calculation program.

Resource Type: source code, software application, software resource

Defining Citation: [PMID:23630109](#)

Keywords: Quantum mechanic mass spectrometry calculation, calculate mass spectra, Born-Oppenheimer Molecular Dynamics,

Availability: Free, Available for download, Freely available,

Resource Name: QCxMS

Resource ID: SCR_026928

License: GNU GPL v3

Record Creation Time: 20250513T055331+0000

Record Last Update: 20260815T183256+0000

Ratings and Alerts

No rating or validation information has been found for QCxMS.

No alerts have been found for QCxMS.

Data and Source Information

Source: [SciCrunch Registry](#)

Usage and Citation Metrics

We found 1 mentions in open access literature.

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

Rojas WY, et al. (2025) Galaxy QCxMS for straightforward semi-empirical quantum mechanical EI-MS prediction. GigaByte (Hong Kong, China), 2025, gigabyte160.