

New Molecule Profiling Instructions for authors

AstraZeneca uses ChemAxon as its secure, third party service provider to perform cheminformatics evaluation of compounds for their novelty and properties.

<http://www.chemaxon.com/>

External investigators should contact ChemAxon once they have approval to do so by their institution and have signed the legal document, available on the web portal, between themselves and ChemAxon. As described in the legal document, compounds submitted for evaluation by ChemAxon must be available as solids (2 to 5 μ moles) or 10mM DMSO solutions (200 to 500 μ l) and supplied in AstraZeneca's standard vessels, which will be provided later if compounds are accepted for screening. All structures submitted must have a unique ID, from which structure information cannot be derived.

Please email the signed legal document and the chemical structures, in the form of either SMILES or sdf files, to ChemAxon: azoi-submit@chemaxon.com

Each submission of structures will be unique and will require a new legal document to be signed. Alternatively, external investigators may send the legal document and the structure file(s) combined in a password protected zip file and make the password available for ChemAxon separately from the zip file by any channel they deem secure. ChemAxon will check the signed legal document and validate the compound structures and ID's. External investigators may be required to further clarify, amend or modify the files sent.

Please provide the following information on the signature page of the legal document:

1. Your contact details

- Name
- Title
- Address
- Phone
- Email

2. Contact details of your institution

- Name of the institution
- Country
- Address and lab address
- Web address
- Phone number
- Email address

Also include the following information in your e-mail to ChemAxon:

- Any relevant details of your library e.g. purpose, property space.
- The number of compounds to be evaluated if >1000.

On receipt and acceptance of the signed legal document and validation of the SMILES or sdf files, the cheminformatics evaluation will be performed within ten working days. The resulting report will be shared with AstraZeneca for review against the company's desirability criteria. The report and outcome of this review will be made available to the external investigator through the Open Innovation web portal.

Checklist for external investigators contacting ChemAxon

Signed legal document	
Compound structures are in SMILES or sdf files	
A unique ID has been supplied for each structure submitted	
Compounds are available in format and quantity required for screening at AstraZeneca	
Compounds can be supplied in AstraZeneca's standard vessels	
Details of your library e.g. purpose, property space	
Number of compounds indicated if >1000	
Your contact details provided: name, title, address, phone, e-mail	
Contact details of your institution provided: institution name, country, address, lab address, web address phone, e-mail	