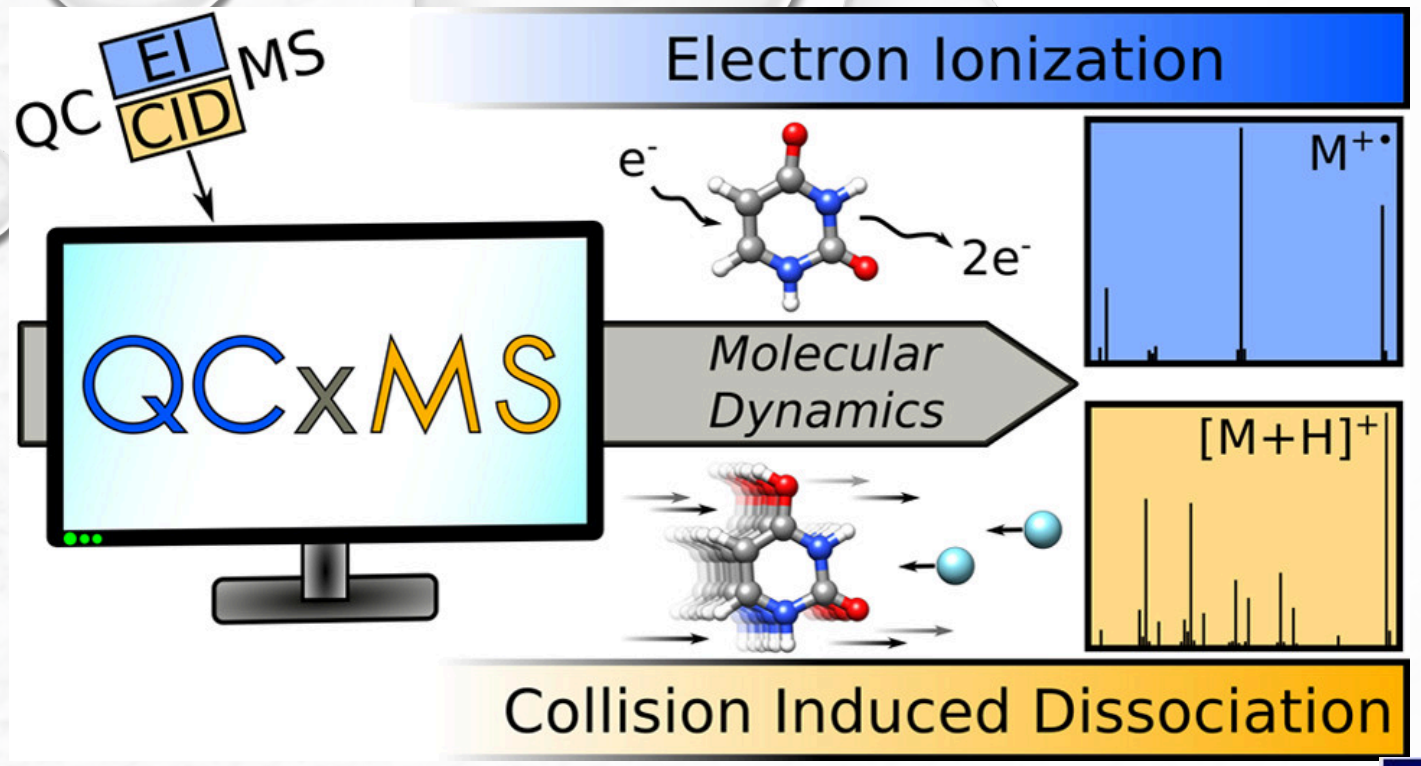
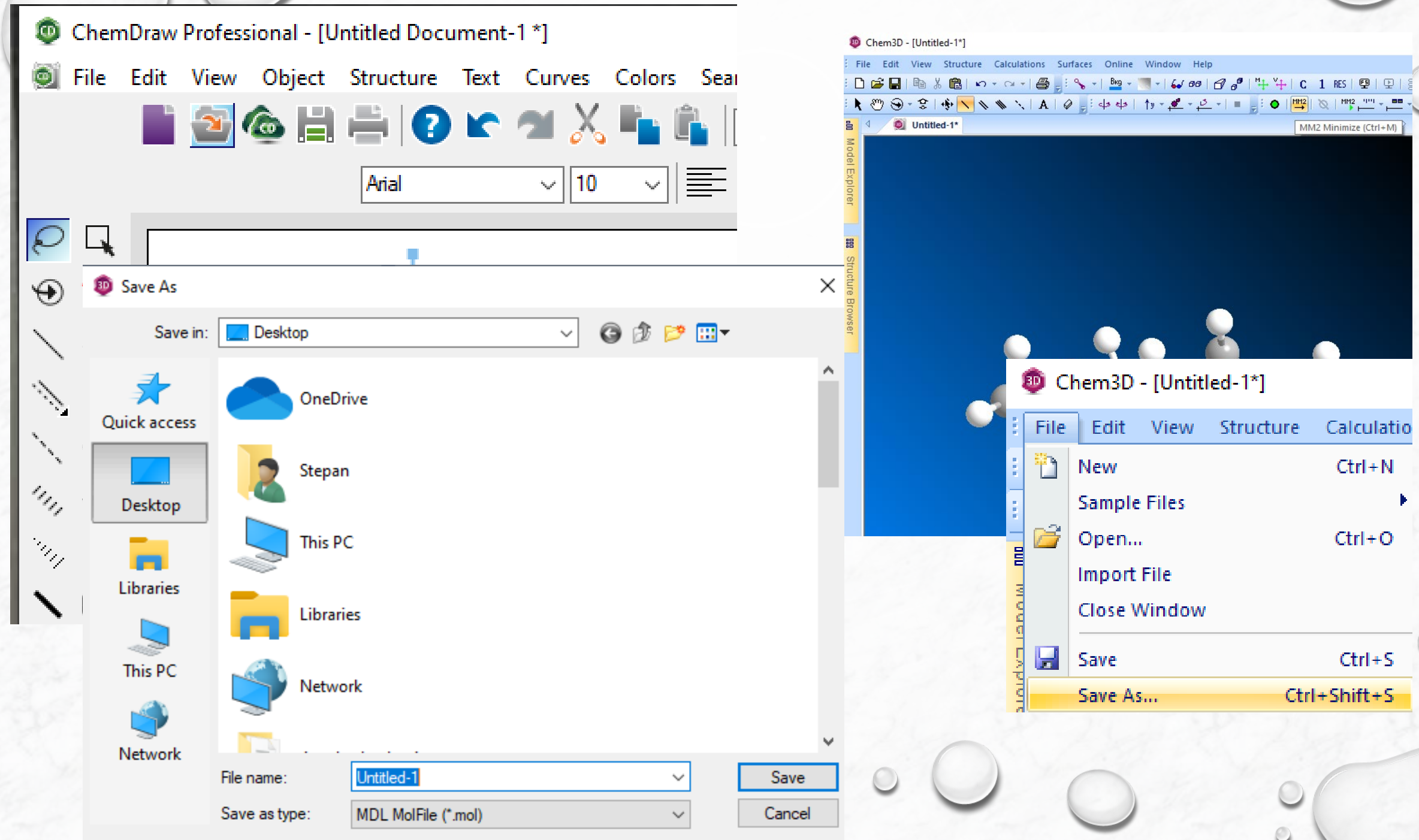
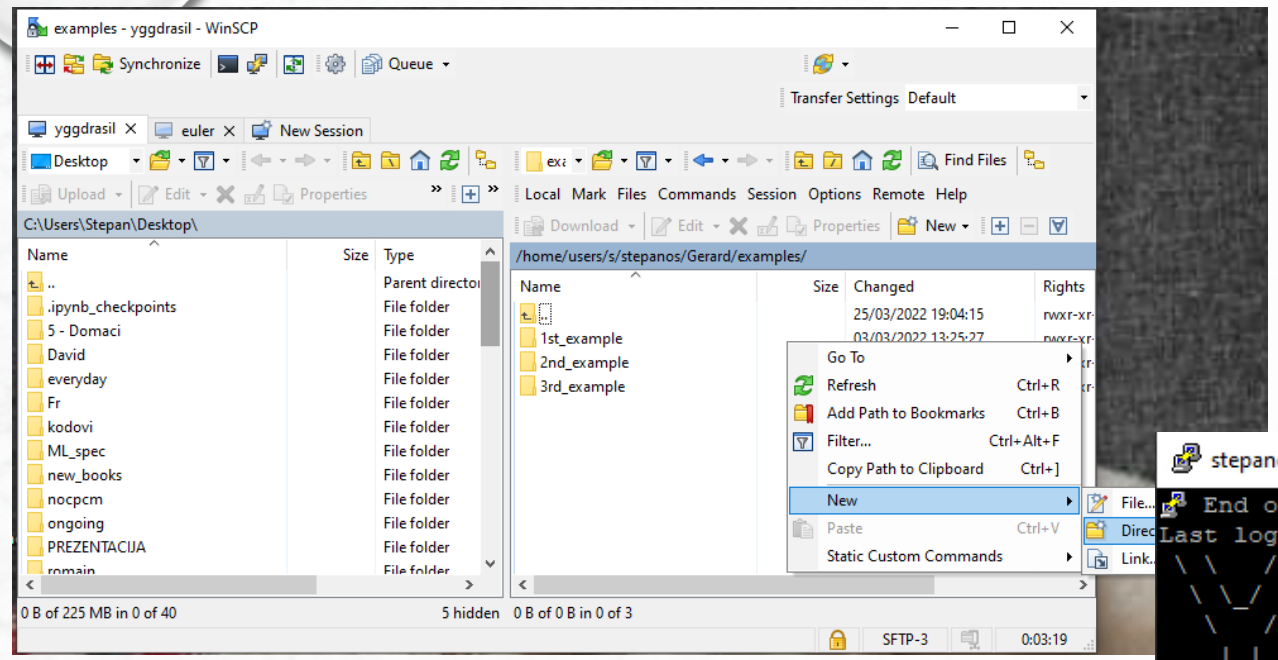
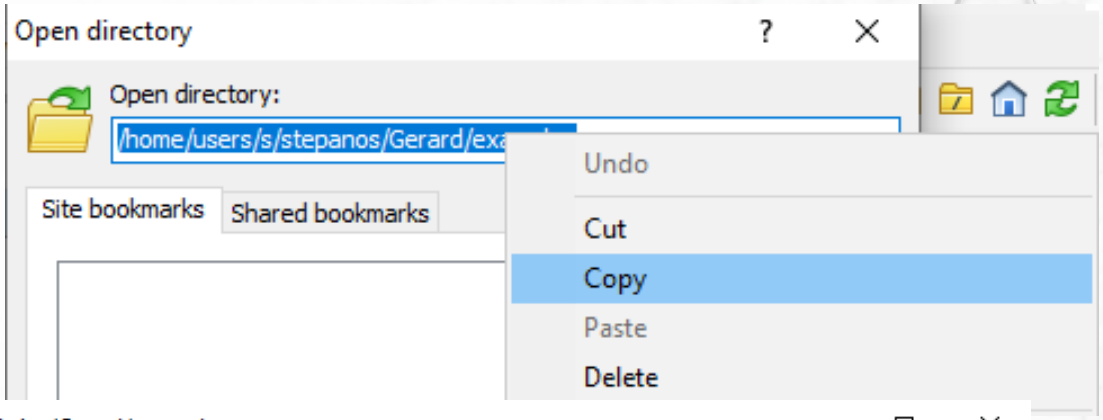
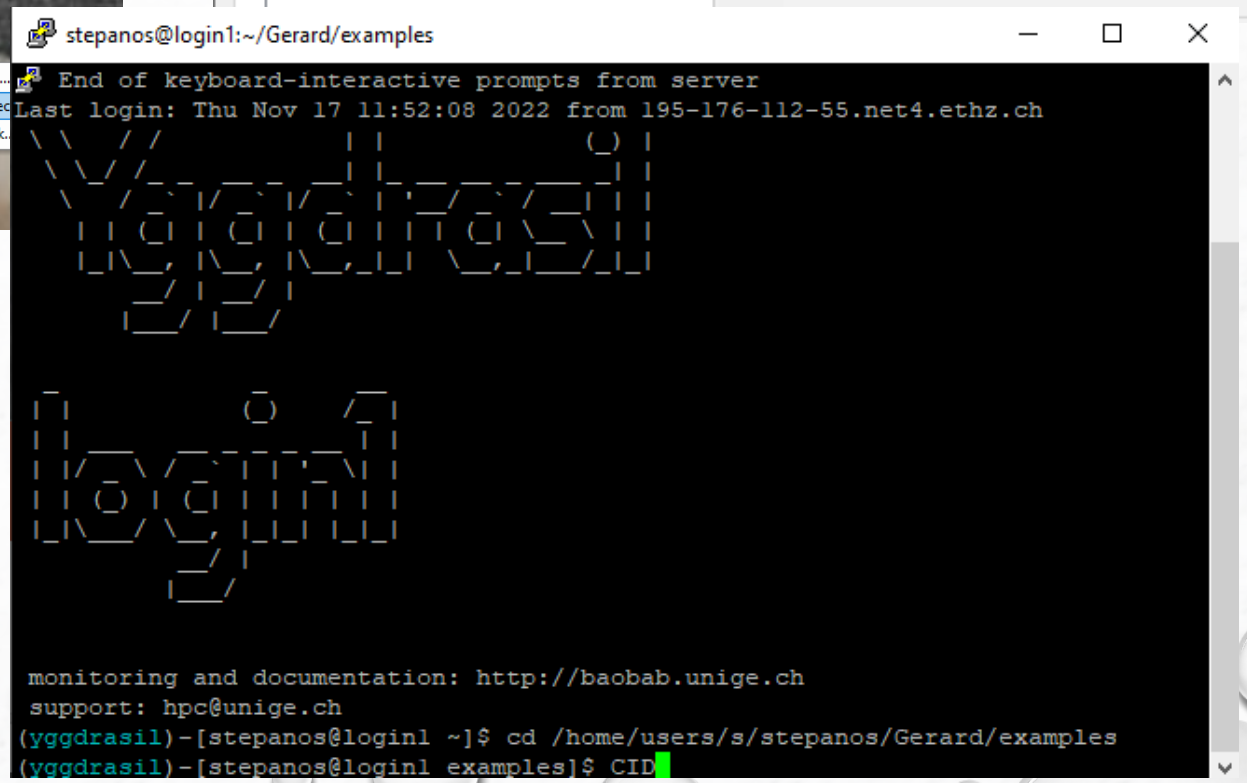


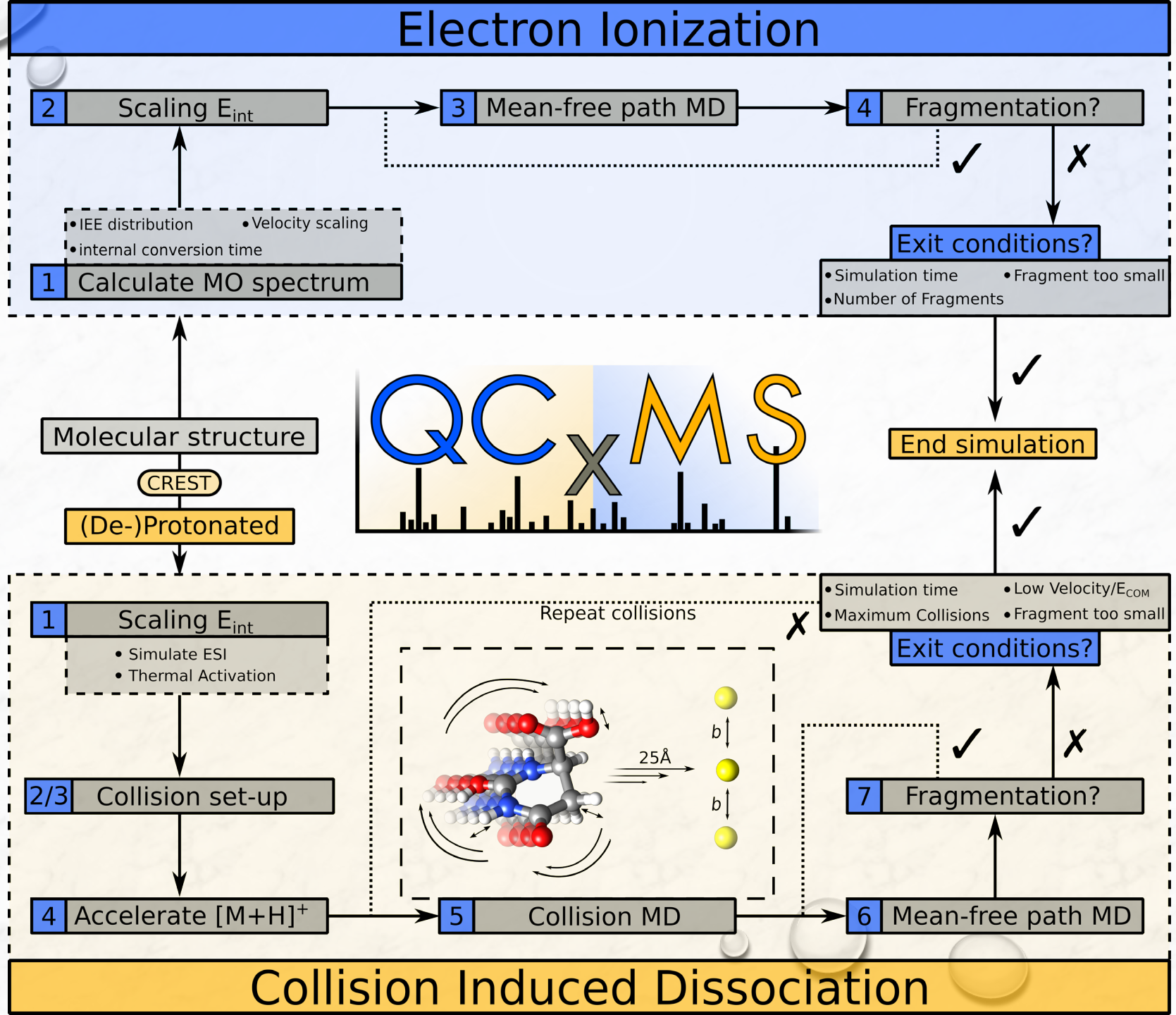
SIRIUS+CSI:FingerID

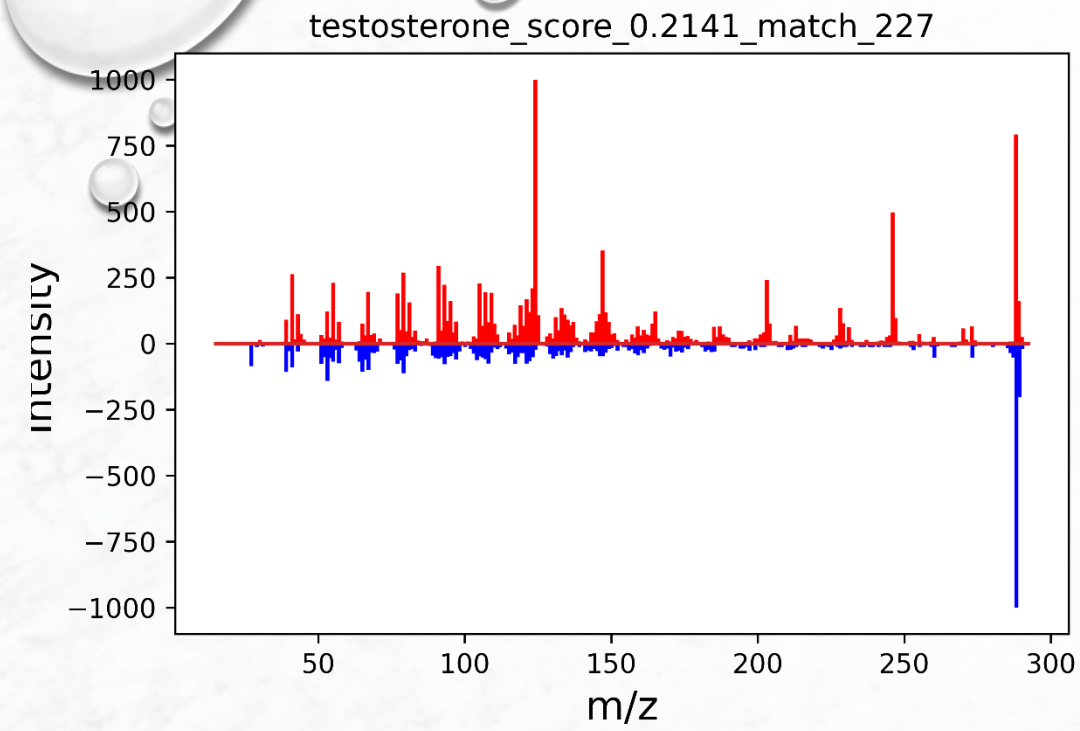

ChemDraw Professional - [Untitled Document-1 *]
File Edit View Object Structure Text Curves Colors Sear
Arial
10
Save As
Save in: Desktop
Quick access
Desktop
Libraries
This PC
Network
OneDrive
Stepan
This PC
Libraries
Network
File name: Untitled-1
Save as type: MDL MolFile (*.mol)
Save
Cancel
Chem3D - [Untitled-1*]
File Edit View Structure Calculations Surfaces Online Window Help
Untitled-1*
MM2 Minimize (Ctrl+M)
Model Explorer
Structure Browser
Chem3D - [Untitled-1*]
File Edit View Structure Calculatio
New Ctrl+N
Sample Files
Open... Ctrl+O
Import File
Close Window
Save Ctrl+S
Save As... Ctrl+Shift+S


examples - yggdrasil - WinSCP
Synchronize
Queue
Transfer Settings Default
yggdrasil
euler
New Session
Desktop
Find Files
Upload
Edit
Properties
Local Mark Files Commands Session Options Remote Help
Download
Edit
Properties
New
C:\Users\Stepan\Desktop\
/home/users/s/stepanos/Gerard/examples/
Name
Size
Type
Changed
Rights
..
.ipynb_checkpoints
5 - Domaci
David
everyday
Fr
kodovi
ML_spec
new_books
nocpcm
ongoing
PREZENTACIJA
1st_example
2nd_example
3rd_example
Go To
Refresh Ctrl+R
Add Path to Bookmarks Ctrl+B
Filter... Ctrl+Alt+F
Copy Path to Clipboard Ctrl+]
New
Paste Ctrl+V
Static Custom Commands
0 B of 225 MB in 0 of 40
5 hidden
0 B of 0 B in 0 of 3
SFTP-3
0:03:19


Open directory
Open directory:
/home/users/s/stepanos/Gerard/ex
Site bookmarks
Shared bookmarks
Undo
Cut
Copy
Paste
Delete


stepanos@login1:~/Gerard/examples
End of keyboard-interactive prompts from server
Last login: Thu Nov 17 11:52:08 2022 from 195-176-112-55.net4.ethz.ch
monitoring and documentation: http://baobab.unige.ch
support: hpc@unige.ch
(yggdrasil)-[stepanos@login1 ~]$ cd /home/users/s/stepanos/Gerard/examples
(yggdrasil)-[stepanos@login1 examples]$ CID


Electron Ionization
2 Scaling E_{int}
3 Mean-free path MD
4 Fragmentation?
✓
✗
• IEE distribution
• Velocity scaling
• internal conversion time
1 Calculate MO spectrum
Exit conditions?
• Simulation time
• Fragment too small
• Number of Fragments
✓
Molecular structure
CREST
(De-)Protonated
QCxMS
End simulation
✓
✓
• Simulation time
• Low Velocity/E_{COM}
• Maximum Collisions
• Fragment too small
Exit conditions?
Repeat collisions
✗
1 Scaling E_{int}
• Simulate ESI
• Thermal Activation
b
25Å
b
✓
✗
2/3 Collision set-up
7 Fragmentation?
4 Accelerate $[M+H]^+$
5 Collision MD
6 Mean-free path MD
Collision Induced Dissociation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Intensity
m/z
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750
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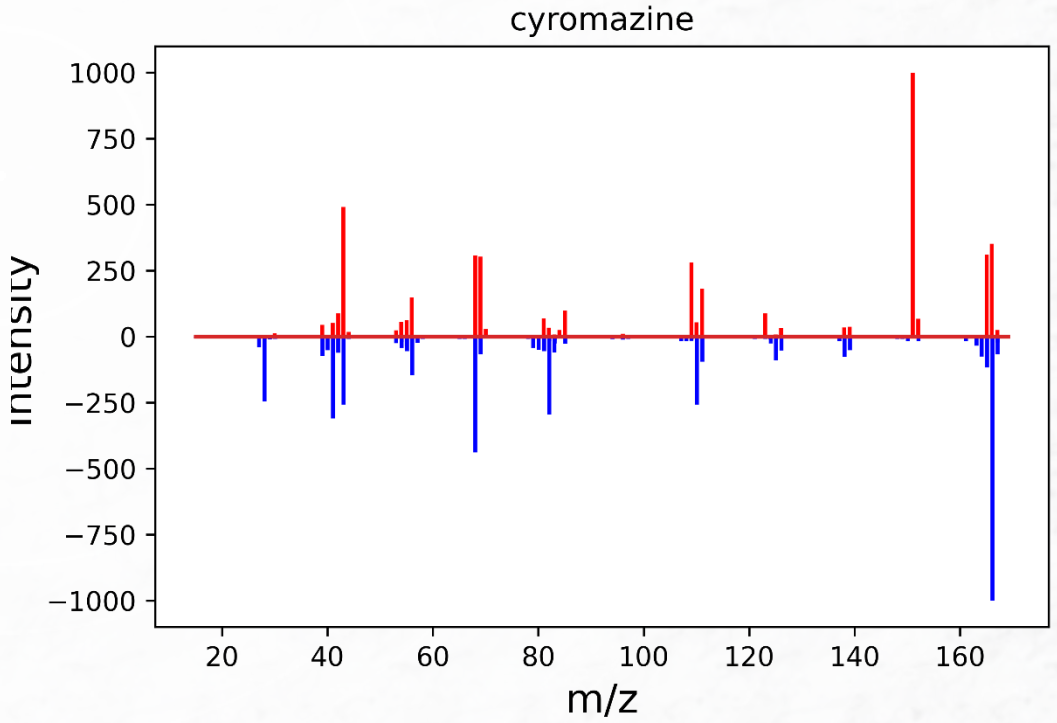
0
−250
−500
−750
−1000
50
100
150
200
250
300


cyromazine
Intensity
m/z
1000
750
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−250
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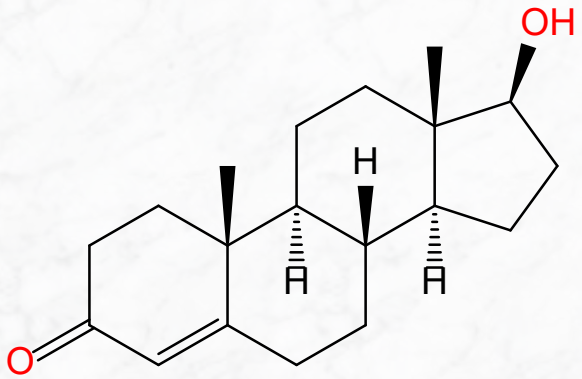
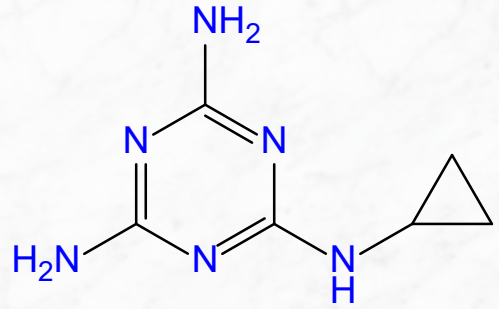
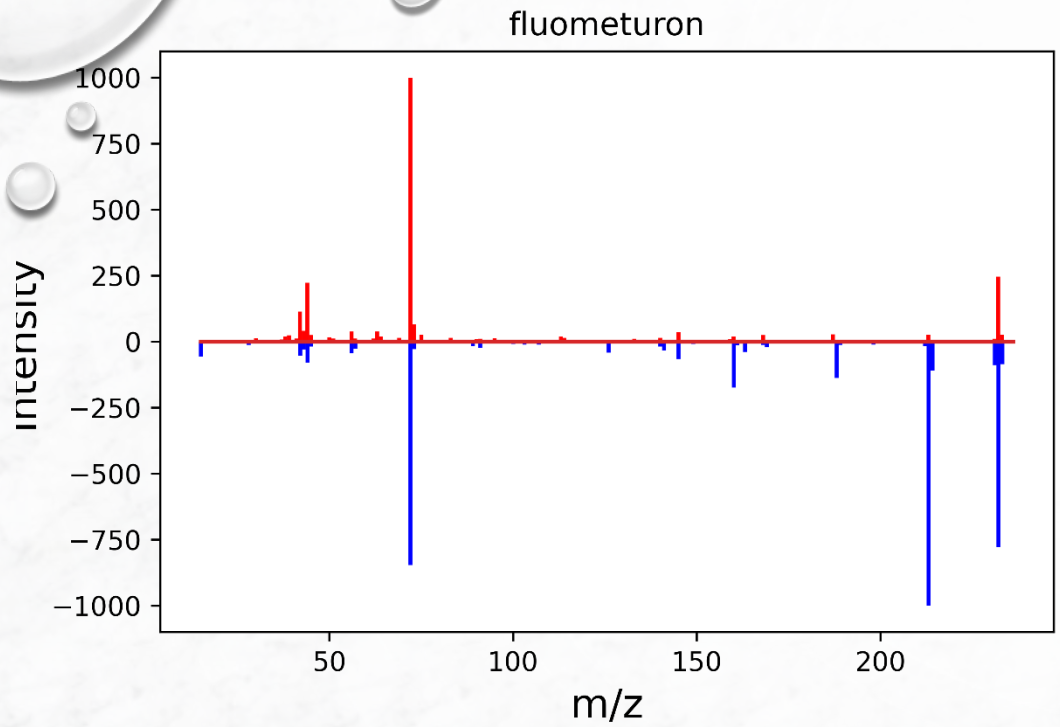
−750
−1000
20
40
60
80
100
120
140
160


OH
H
O


NH2
N
N
H2N
N
N
H


fluometuron
intensity
m/z
1000
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500
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−750
−1000
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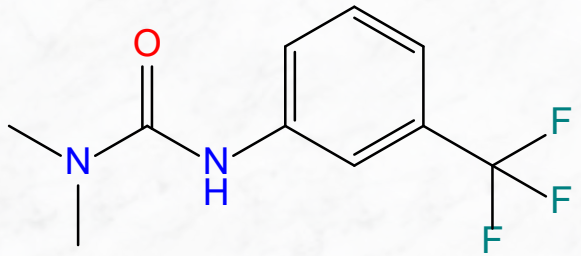
150
200


O
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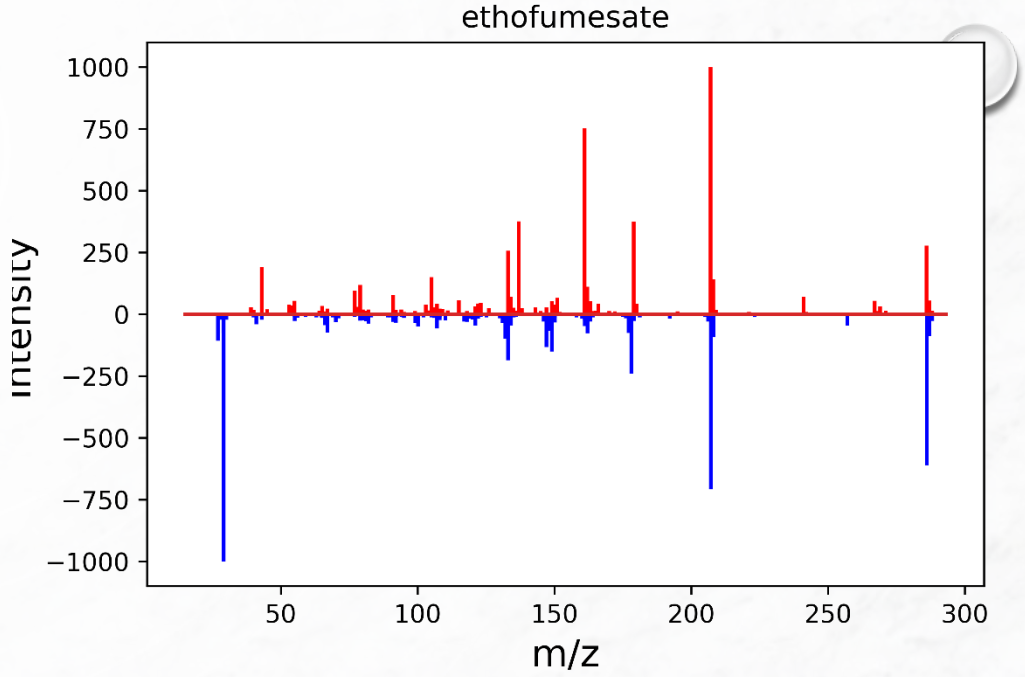
N
H
F
F
F


ethofumesate
intensity
m/z
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−750
−1000
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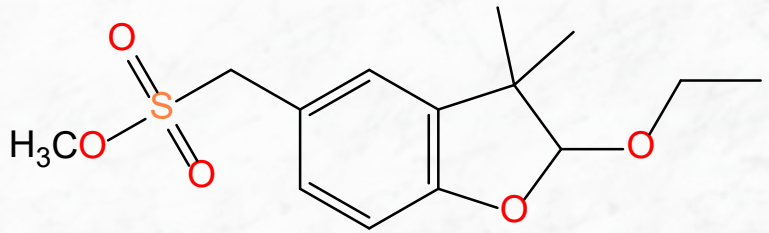
O
S
O
H3CO
O
O

_Caffeine.csv

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3	16.029751 ,	0.005805179623466041
4	26.003074 ,	0.013471860017466511
5	27.000108 ,	0.000053626967610475
6	27.006428 ,	0.000154040727351248
7	27.010899 ,	0.181271276035546991
8	28.003462 ,	0.000000820820902343
9	28.007933 ,	0.000603366892912558
10	28.014253 ,	0.002041881781989936
11	28.017175 ,	0.000022074397541847
12	28.018724 ,	3.961203718690776032
13	29.002739 ,	1.249745959808614026
14	29.011287 ,	0.000014716265027898
15	29.015758 ,	0.013744968930747286
16	29.022078 ,	0.042842506526365377
17	29.025000 ,	0.000964559208845820
18	29.026549 ,	0.013465420863808678
19	30.006093 ,	0.014161642961305622
20	30.006956 ,	0.000278672752237400
21	30.009015 ,	0.000152003314375083
22	30.019112 ,	0.000241139802211455
23	30.023583 ,	0.000054123002236236
24	30.029903 ,	0.000142687923665156
25	30.032825 ,	0.000004373575954353
26	31.006984 ,	0.002356051382030205
27	31.018389 ,	2.202619689798452463
28	31.026937 ,	0.000000820045491441
29	32.021743 ,	0.023352795151260555
30	32.022606 ,	0.000848380766877671
31	32.024665 ,	0.000714425867911729
32	33.022634 ,	0.004956329377416802
33	33.025960 ,	0.000044651616744483
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35	41.002739 ,	0.038343816051383303
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37	42.006093 ,	0.000844785187825894
38	42.006956 ,	0.000010216006603413
39	42.009015 ,	0.000004715079838857
40	42.010564 ,	0.013694210589722757
41	42.023583 ,	0.002696255719681824
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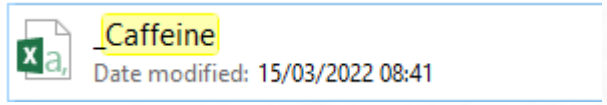
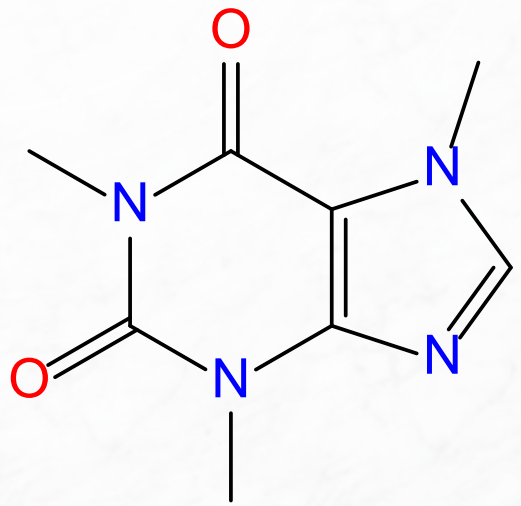
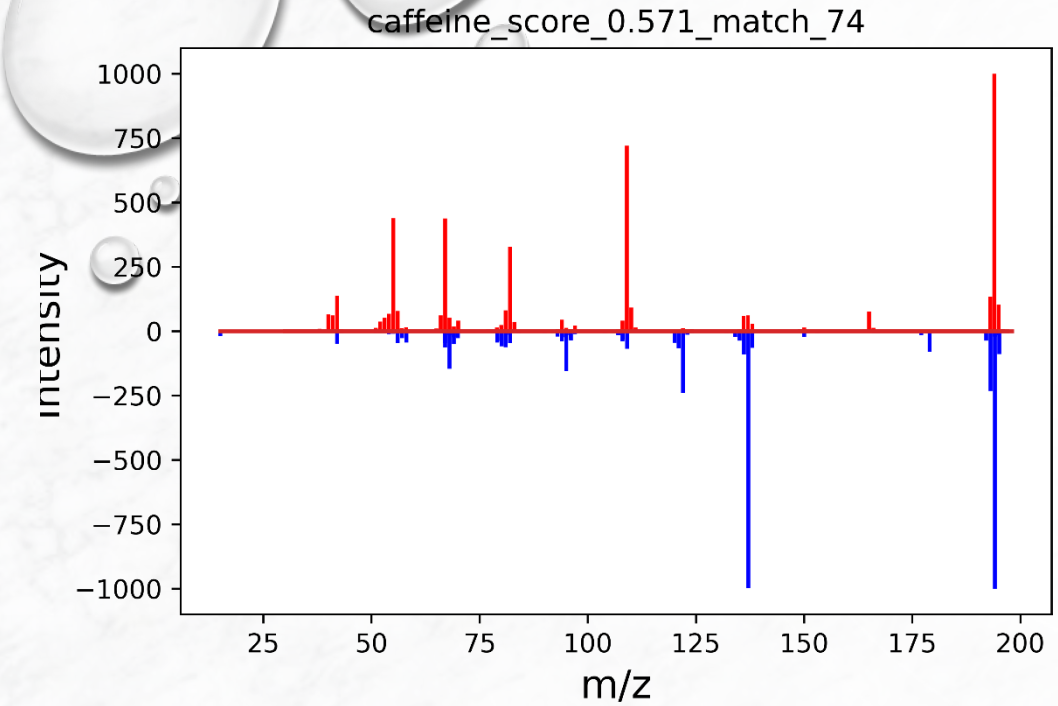
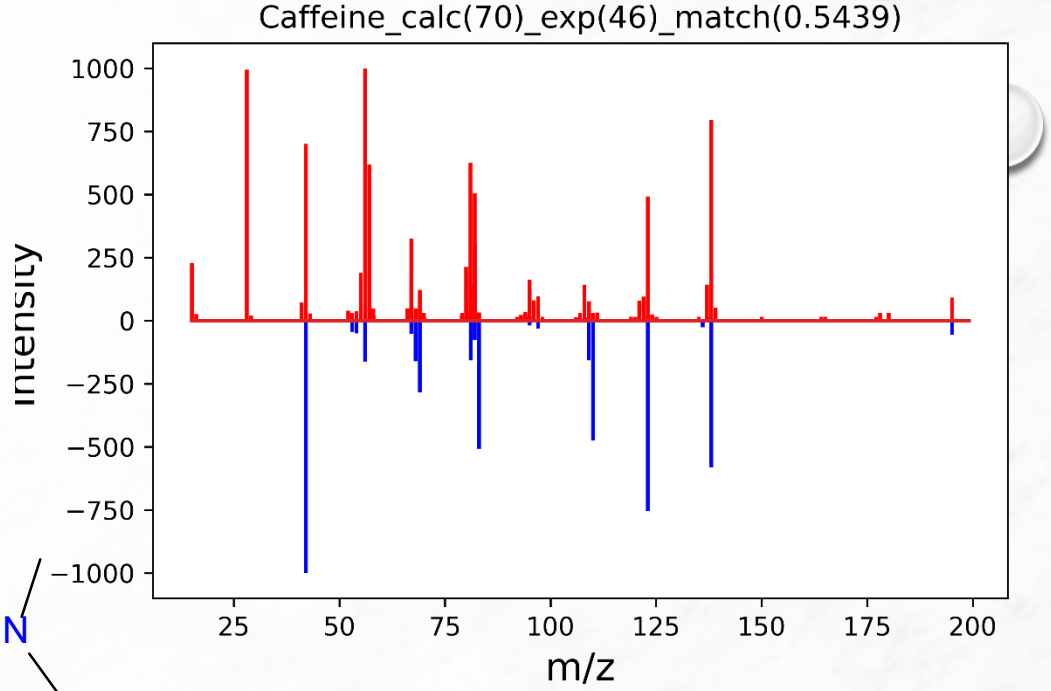
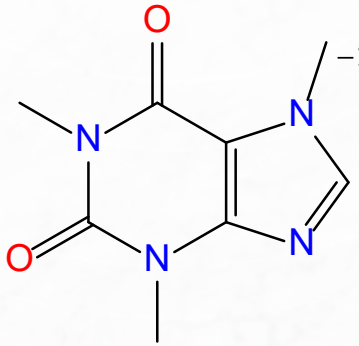
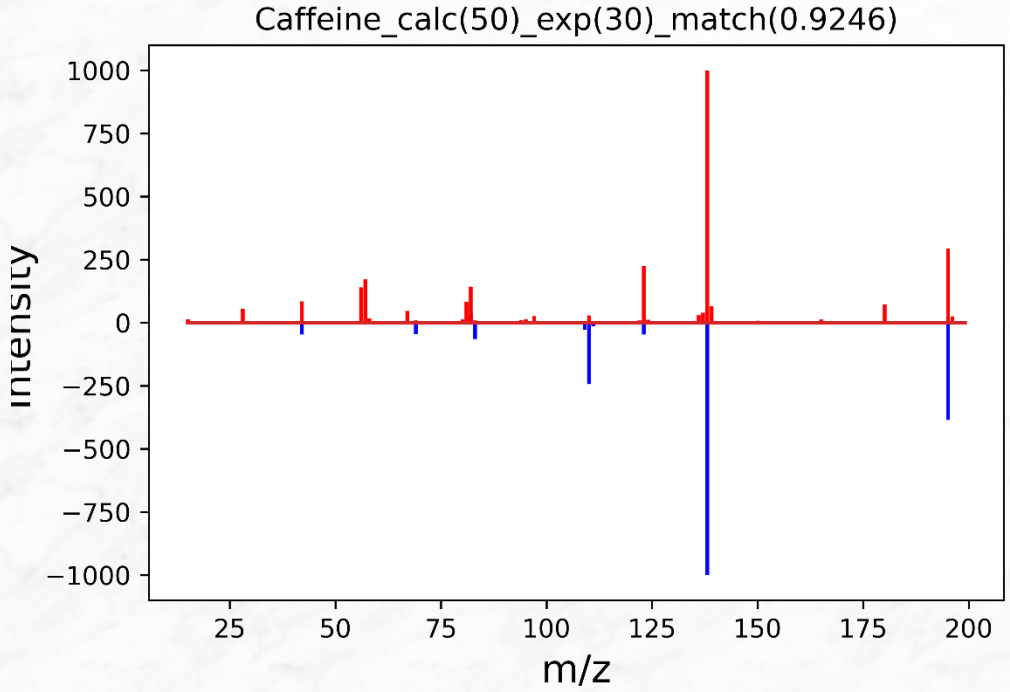


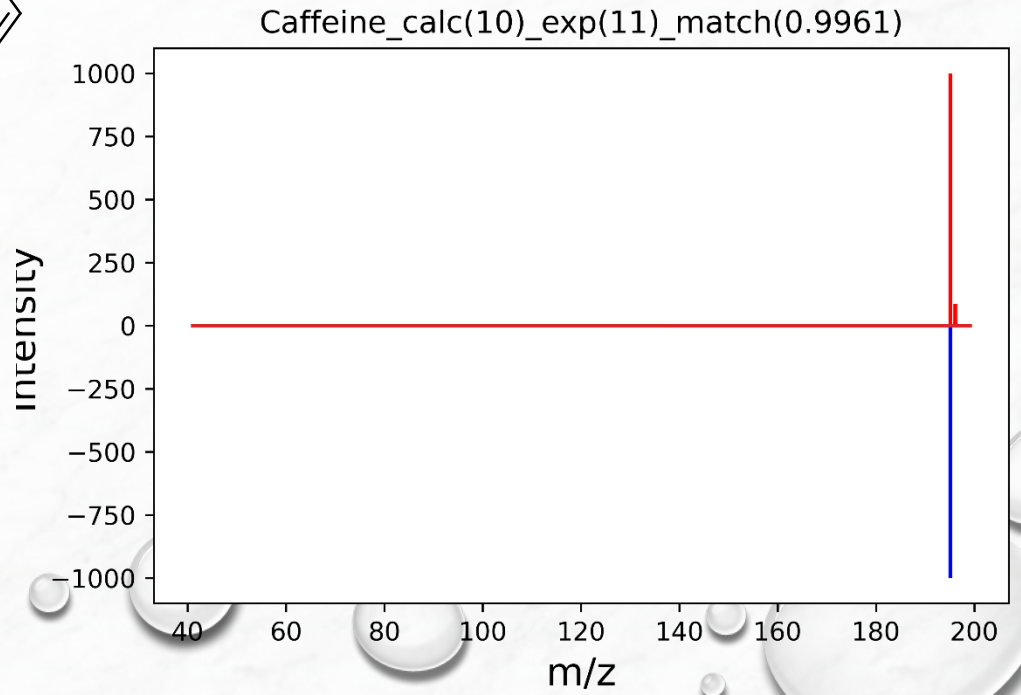


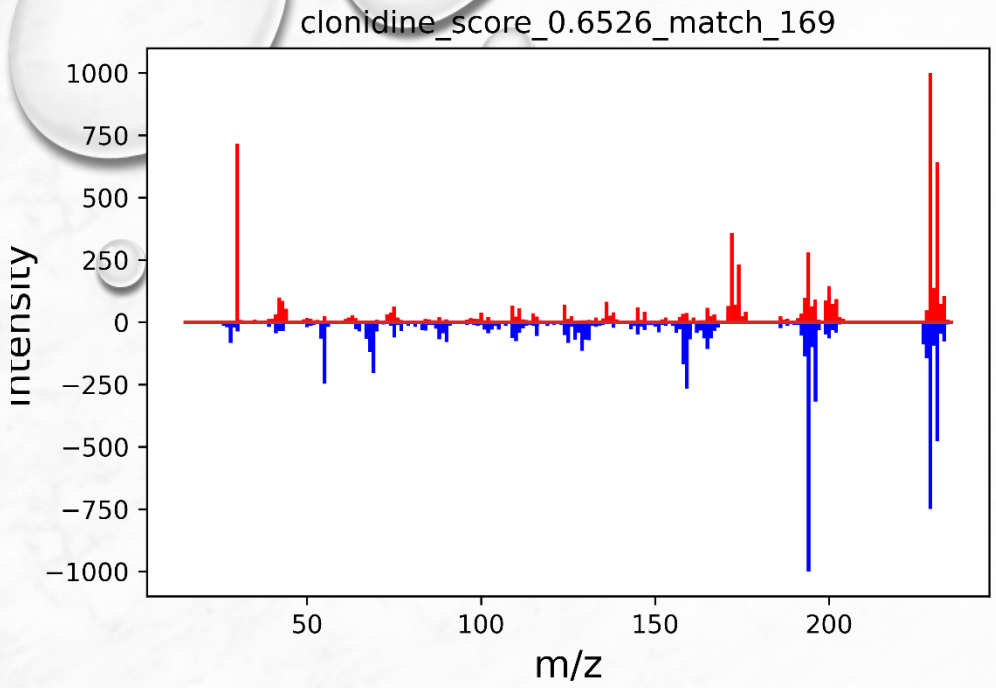

caffeine_score_0.571_match_74
Intensity
m/z

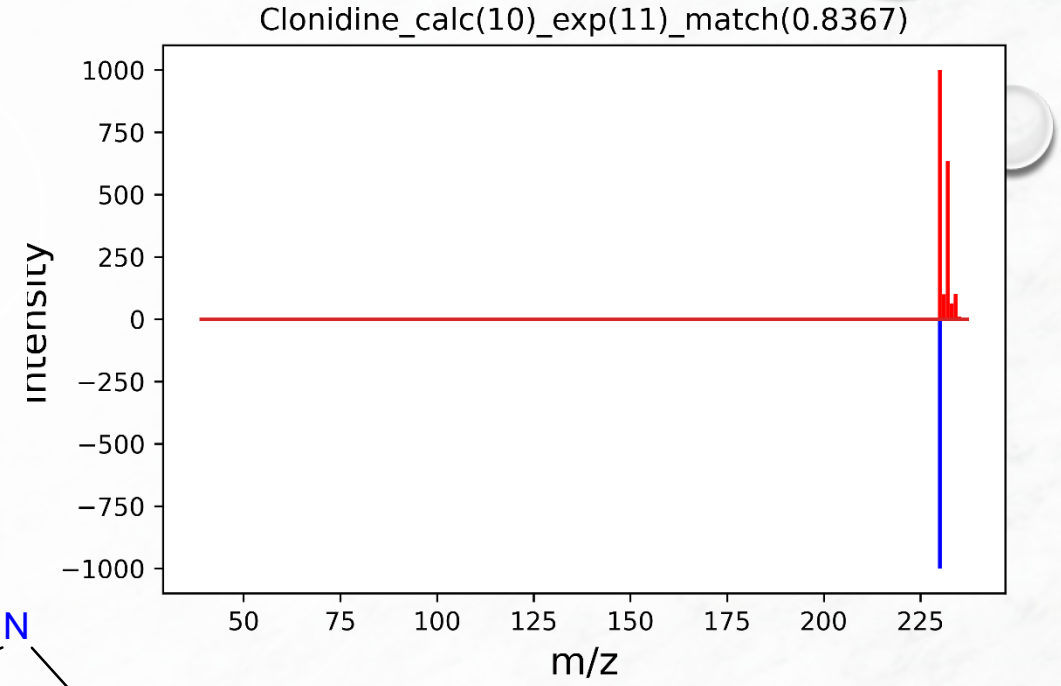

Caffeine_calc(70)_exp(46)_match(0.5439)
Intensity
m/z

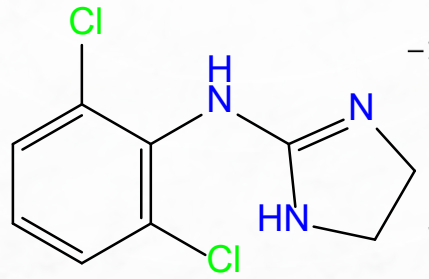

O
N
N
O
N
N


Caffeine_calc(50)_exp(30)_match(0.9246)
Intensity
m/z


Caffeine_calc(10)_exp(11)_match(0.9961)
Intensity
m/z


clonidine_score_0.6526_match_169
intensity
m/z


Clonidine_calc(10)_exp(11)_match(0.8367)
intensity
m/z


Cl
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N
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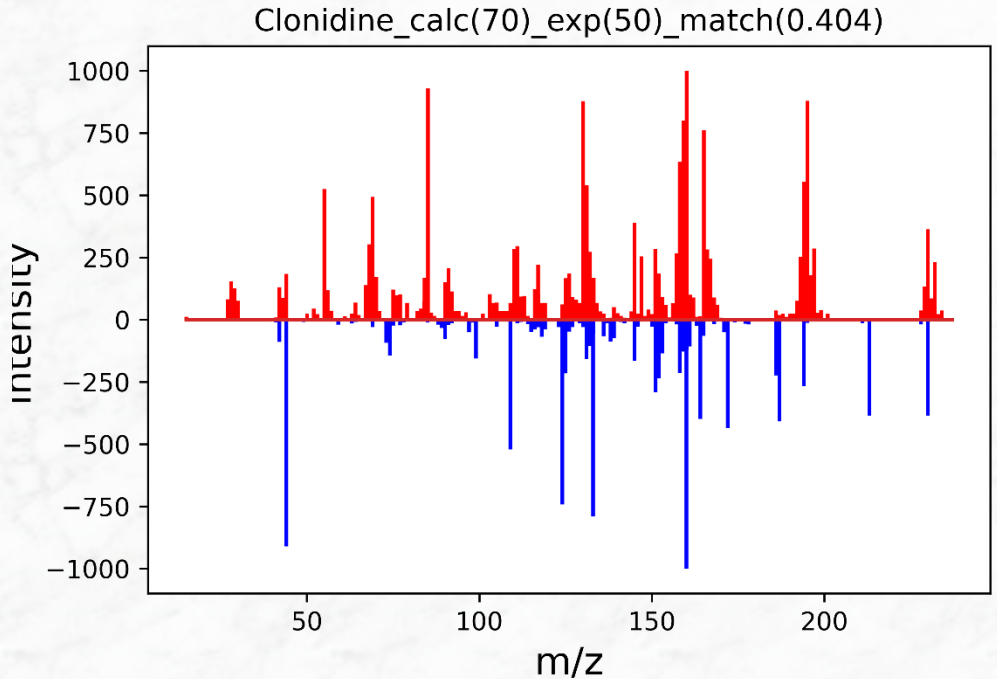
HN
Cl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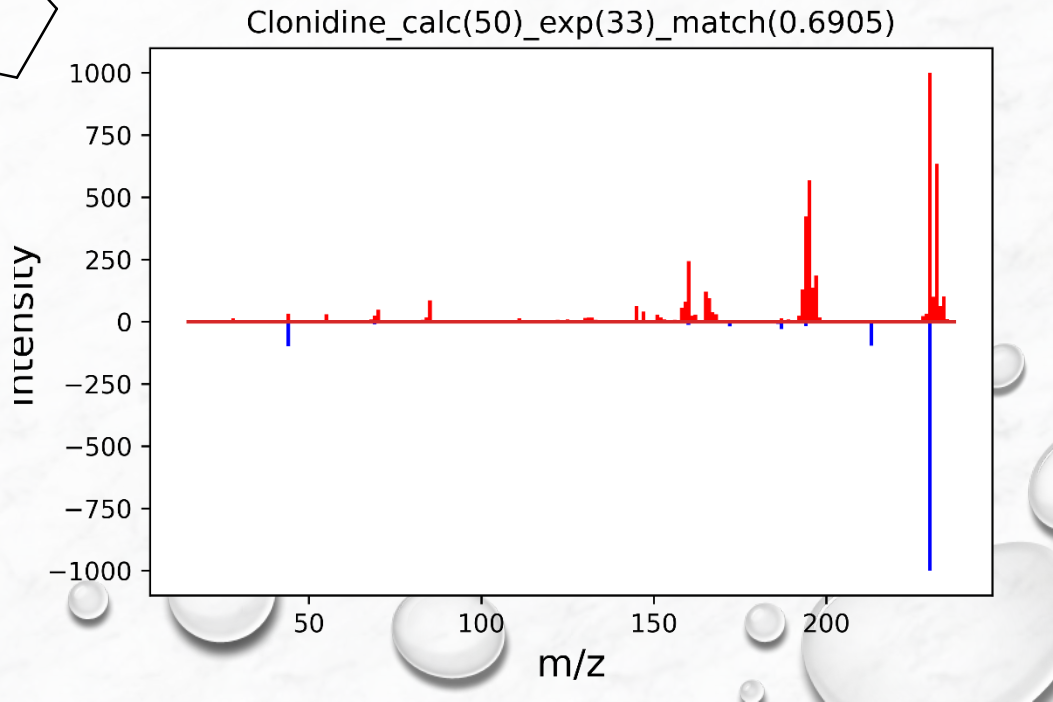
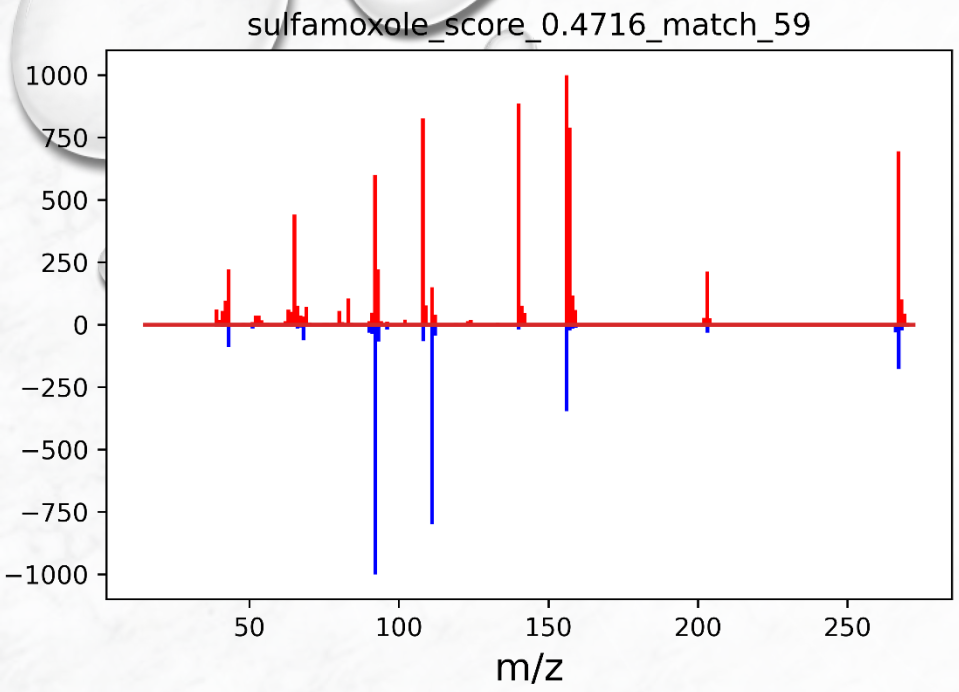
intensity
m/z


Clonidine_calc(50)_exp(33)_match(0.6905)
intensity
m/z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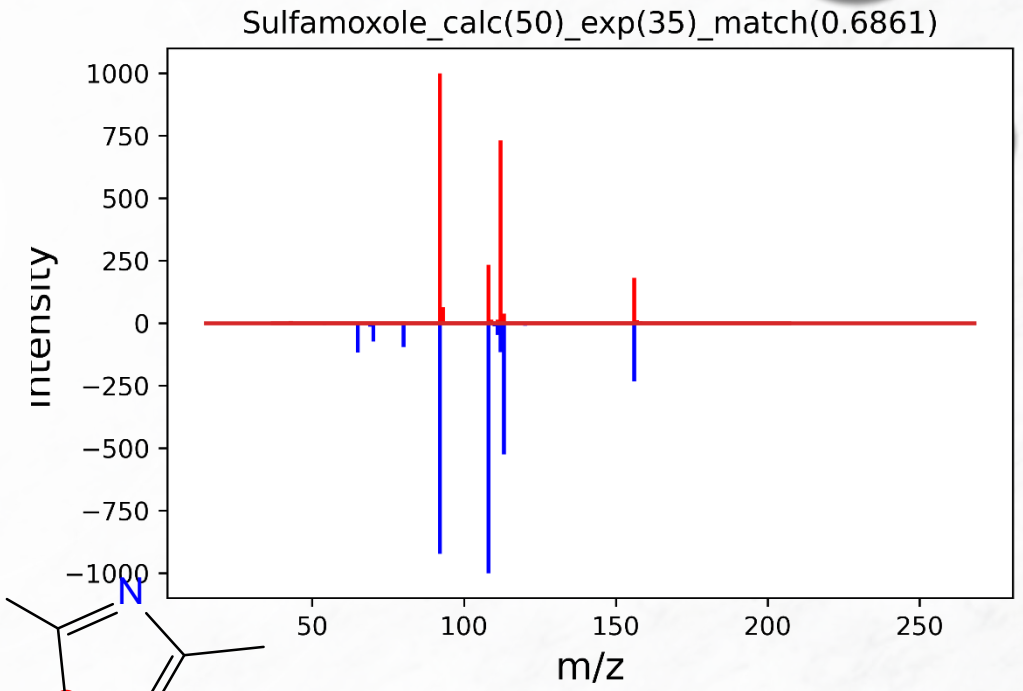
−750
−1000
50
100
150
200
250
m/z


Sulfamoxole_calc(50)_exp(35)_match(0.6861)
Intensity
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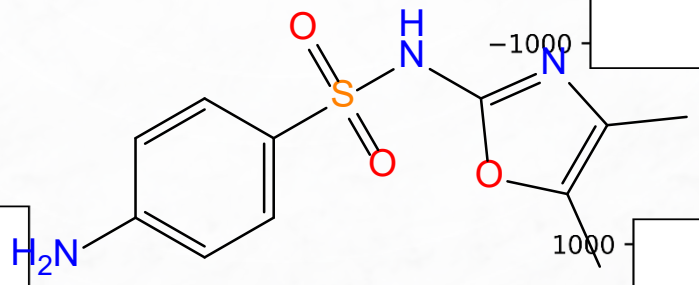
−1000
50
100
150
200
250
m/z


O
H
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S
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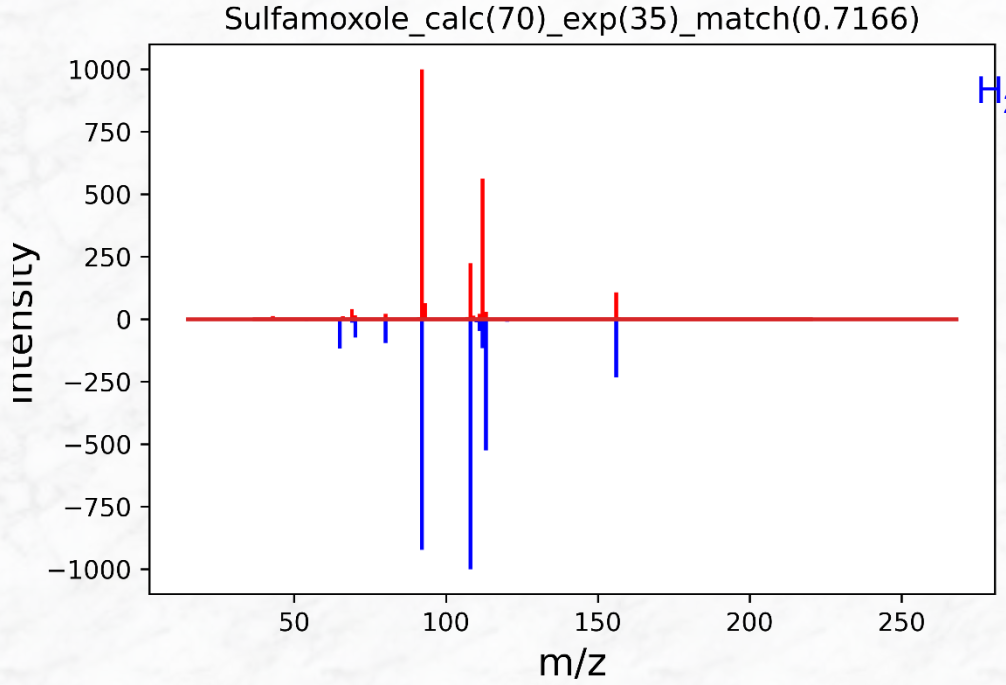
O
O
H_2N


Sulfamoxole_calc(70)_exp(35)_match(0.7166)
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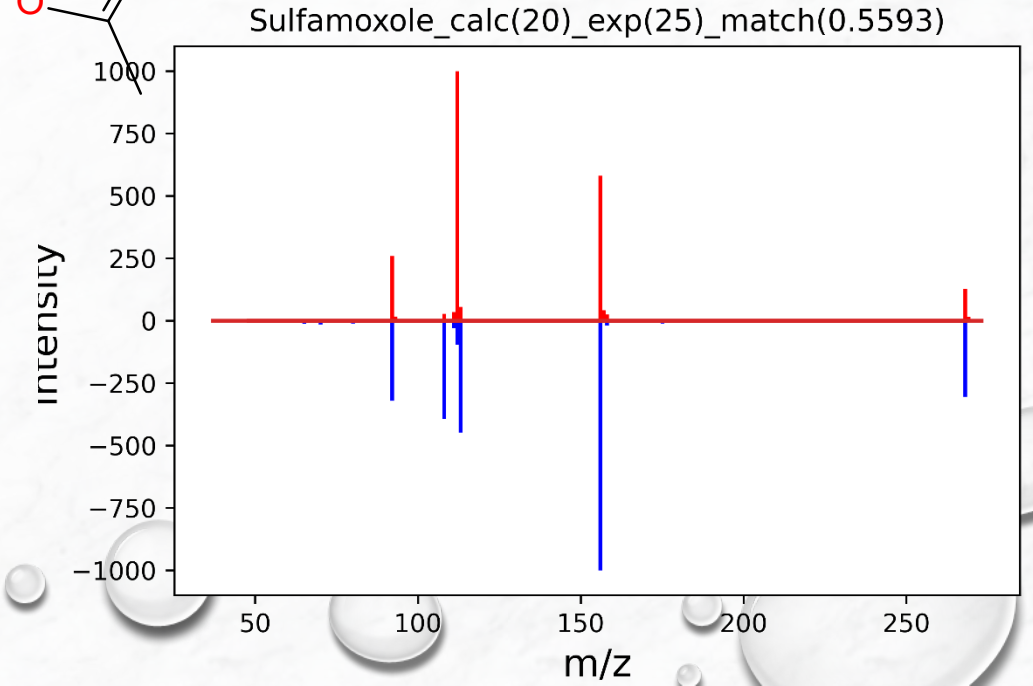
200
250
m/z


Sulfamoxole_calc(20)_exp(25)_match(0.5593)
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−1000
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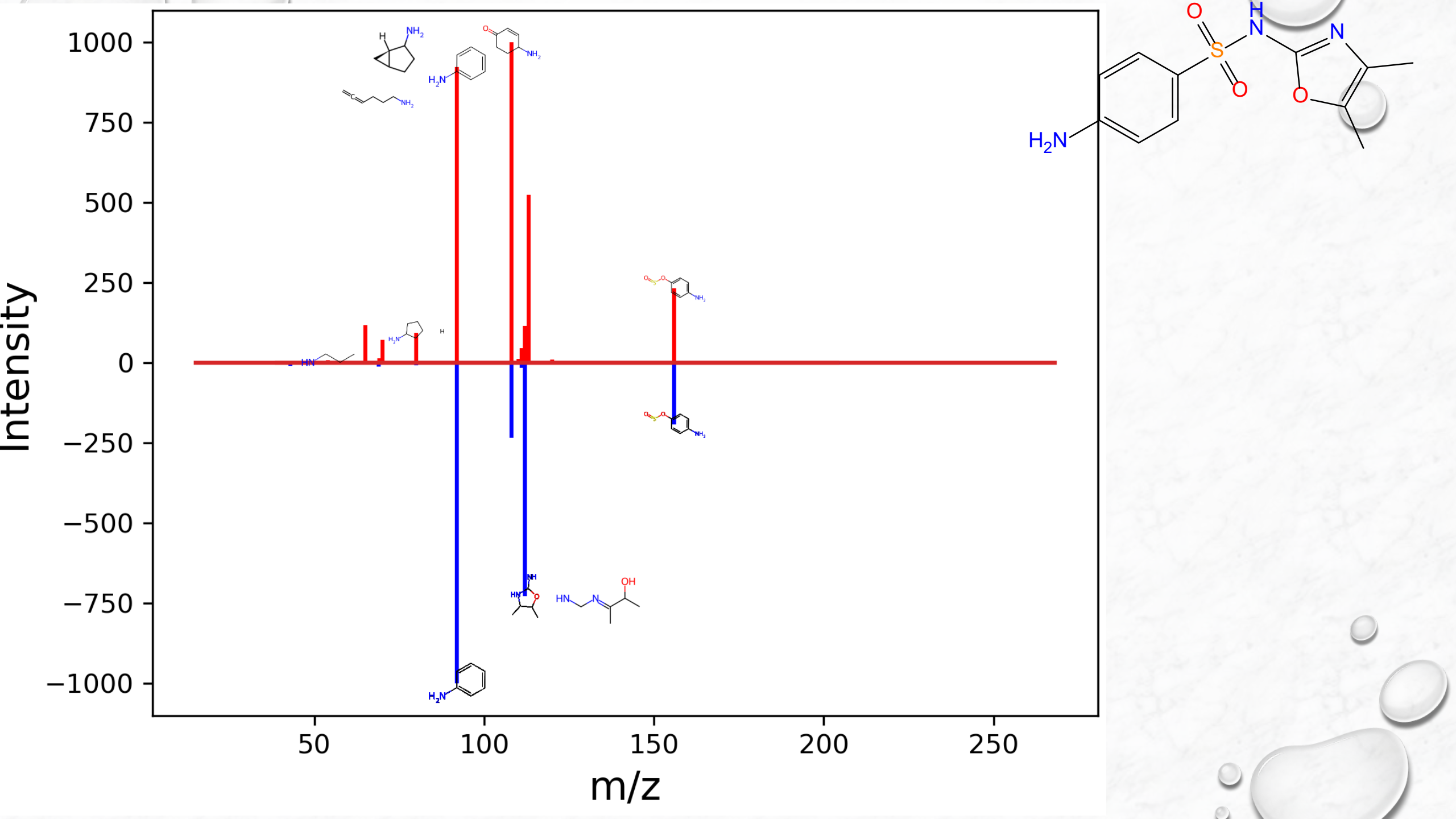
100
150
200
250
m/z


Intensity
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−250
−500
−750
−1000
50
100
150
200
250
m/z
H_2N
O
S
N
H
O
O
N
O
H_2N

Download Links

Documentation

- Online Documentation
- Video tutorials
- Bookchapter on using SIRIUS 4 (Preprint) -- does not cover the new LC-MS/MS processing option
- Demo data

SIRIUS+CSI:FingerID GUI and CLI - Version 5.6.2 (2022-11-03)

These versions include the Java Runtime Environment, so there is no need to install Java separately! Just execute.

- for Windows (64bit): msi / zip / msi (signed by Bright Giant)
- for Mac (64bit): pkg / zip / pkg (signed by Bright Giant)
- for Linux (64bit): zip

https://bio.informatik.uni-jena.de/software/sirius/

SIRIUS 5.6.2 on Project: 'C:\Users\stepa\AppData\Local\Temp\.sirius-tmp-project-3a294009-d17f-44f0-bbcb-b7b06627fe54'

New | Open | Save As | Save Copy | Import Compound | Import | Summaries | FBMN Export | Compute All | Databases | Jobs | Log | Settings | Webservice | Account | Help | About

Filter: Hit enter ...

LC-MS | Formulas | Spectra | Trees | Predicted Fingerprint | Structures | Substructure Annotation | Compound Classes

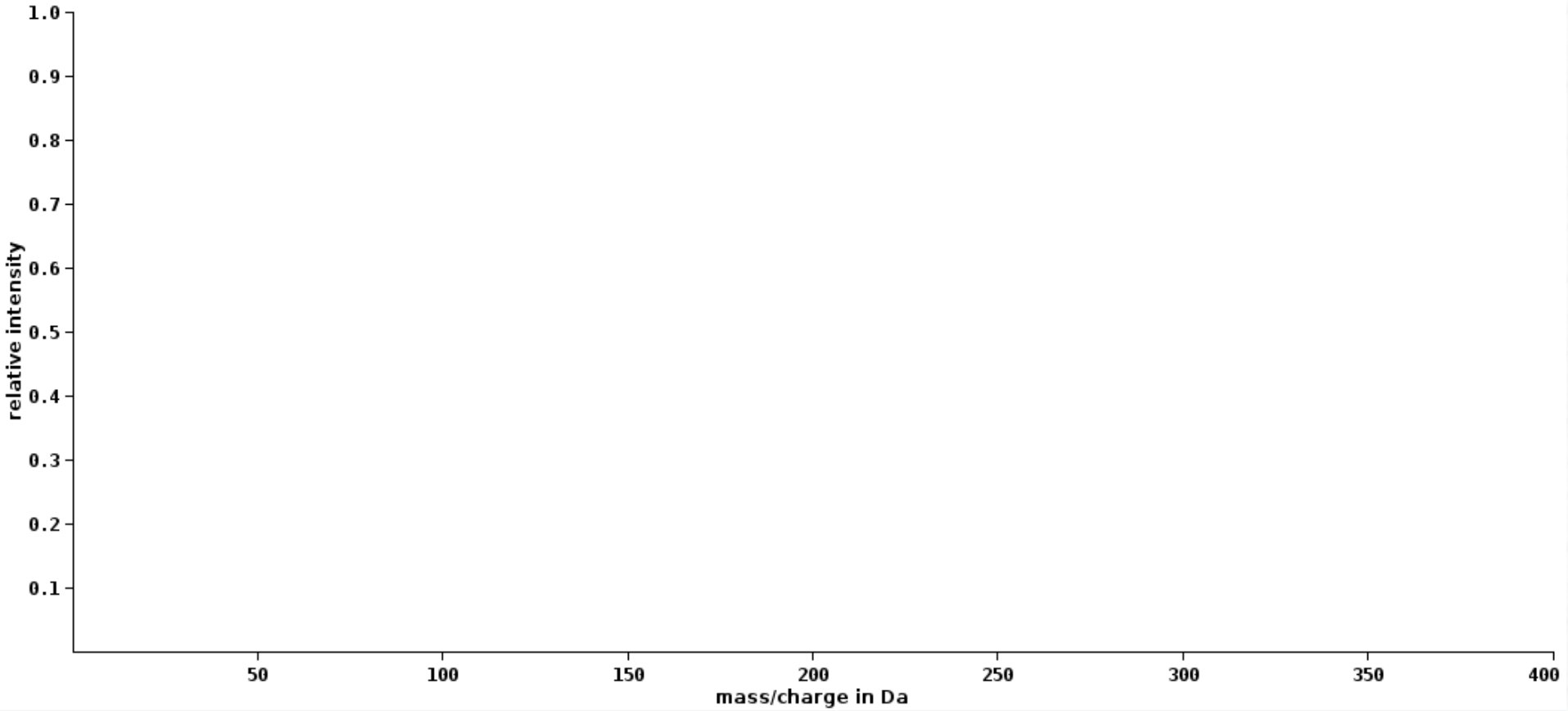
Rank	Molecular Fo...	Adduct	Zodiac Score	Sirius Score	Isotope Score	Tree Score	Explained Pe...	Total Explain...	Median Mas...	Median Abso...	Lipid Class

Mode | Preset: Default | Scale | Customize | Reset

N/A

License: **SIRIUS Community Edition** (Non Commercial) | Compounds: **UNLIMITED** | Jobs: **0**

Import as Single Compound



Name

Precursor mass (m/z)

Most intensive

Adduct

[M + ?]+

Molecular Formula

MS level

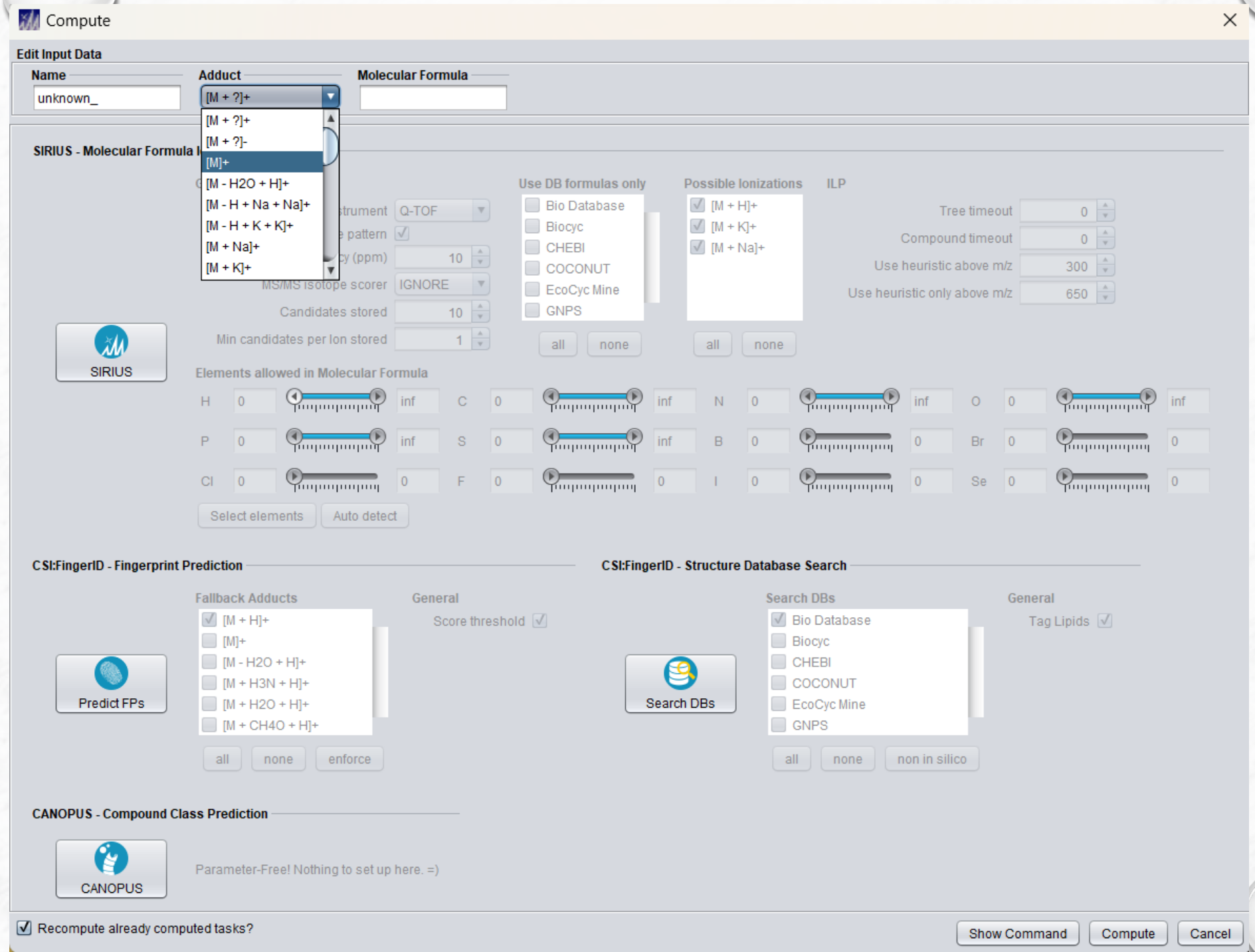
MS 1

Collision energy (eV)

Change

Import

Cancel


Compute
Edit Input Data
Name
unknown_
Adduct
[M + ?]+
Molecular Formula
[M + ?]+
[M + ?]-
[M]+
[M - H2O + H]+
[M - H + Na + Na]+
[M - H + K + K]+
[M + Na]+
[M + K]+
SIRIUS - Molecular Formula I
Use DB formulas only
Bio Database
Biocyc
CHEBI
COCONUT
EcoCyc Mine
GNPS
all
none
Possible Ionizations
[M + H]+
[M + K]+
[M + Na]+
all
none
ILP
Tree timeout
0
Compound timeout
0
Use heuristic above m/z
300
Use heuristic only above m/z
650
Q-TOF
pattern
10
MS/MS isotope scorer
IGNORE
Candidates stored
10
Min candidates per Ion stored
1
SIRIUS
Elements allowed in Molecular Formula
H 0 inf
C 0 inf
N 0 inf
O 0 inf
P 0 inf
S 0 inf
B 0 0
Br 0 0
Cl 0 0
F 0 0
I 0 0
Se 0 0
Select elements
Auto detect
CSI:FingerID - Fingerprint Prediction
Fallback Adducts
[M + H]+
[M]+
[M - H2O + H]+
[M + H3N + H]+
[M + H2O + H]+
[M + CH4O + H]+
all
none
enforce
General
Score threshold
Predict FPs
CSI:FingerID - Structure Database Search
Search DBs
Bio Database
Biocyc
CHEBI
COCONUT
EcoCyc Mine
GNPS
all
none
non in silico
General
Tag Lipids
CANOPUS - Compound Class Prediction
CANOPUS
Parameter-Free! Nothing to set up here. =)
Recompute already computed tasks?
Show Command
Compute
Cancel