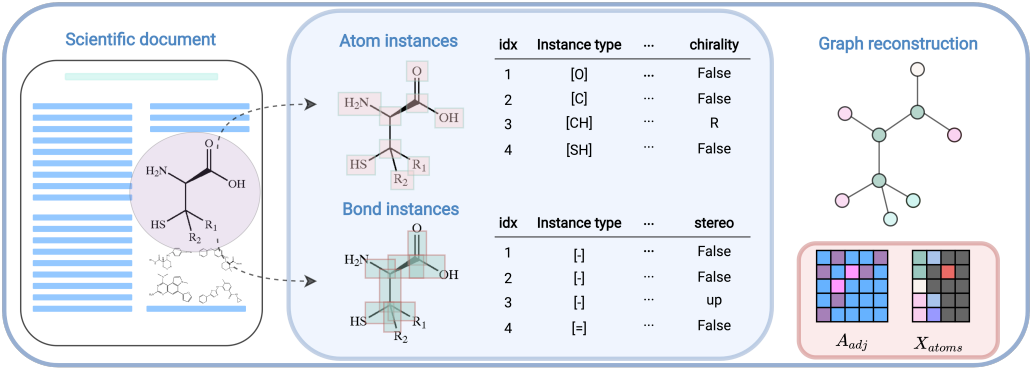

Scientific document
Atom instances
Bond instances
idx
Instance type
...
chirality
1
[O]
...
False
2
[C]
...
False
3
[CH]
...
R
4
[SH]
...
False
idx
Instance type
...
stereo
1
[-]
...
False
2
[-]
...
False
3
[-]
...
up
4
[=]
...
False
Graph reconstruction
A_{adj}
X_{atoms}