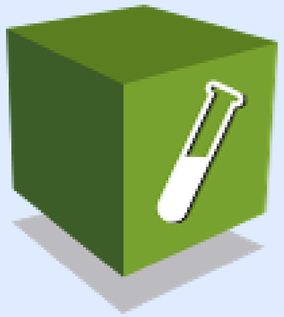
AUTOMATED NMR CHEMICAL SHIFT CALCULTION USING NWCHEM:



Report

Friedrich Schiller University Jena

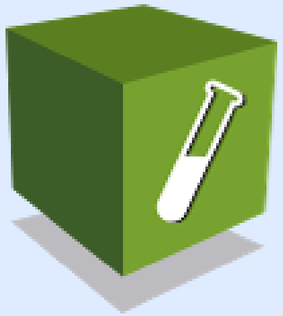
Raj Singh

UNDERSTANDING NWCHEM ?

- Installation on Linux OS
- Reading Documentation
- DFT Calculations
- NMR Chemical Shift Calculation

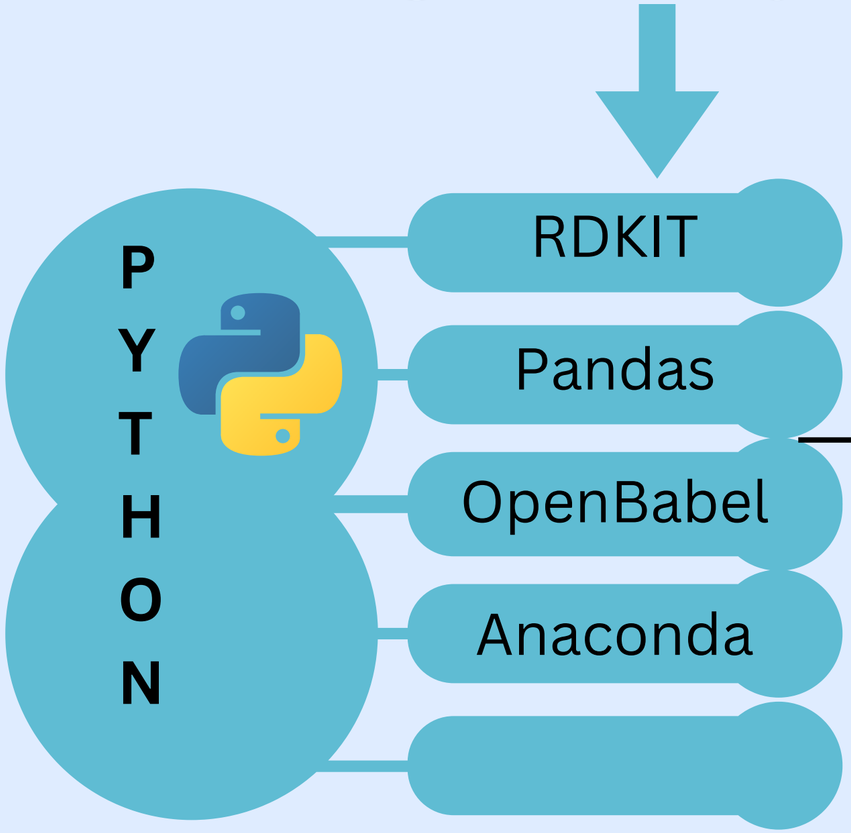
- DFT Functionals
- Basis Set
- Geometry Optimization
- Property Calculations
  a. Shielding
  b. SCF Energy

- NMR Chemical Shift ?
- Learning Isotropic Shielding Tensor
- Reference Molecules
- COSMO Solvent Model
- Shielding and De Shielding Effects
- Taking Small hypothetical molecules



LET'S AUTOMATE NWCHEM

- **Learning Python Libraries**
- **Building a New Python Module**



Take SMILES for Building Molecule Optimising Geometry

Generates 3D Coordinate and Create NWChem Input File as template

Runs the NWChem File

Compare the Result with Reference Molecule and gives the result

CAFFEINE ! BETTER TO START WITH

SMILES : Cn1cnc2c1c(=O)n(C)c(=O)n2C

1H-NMR Chemical Shift

DFT FUNCTIONALS

PBEO

Atom Name / Atom Nos.	Chemical Shift - (Cluster midpoint)
H / 1,2,3	4.46
H / 4	8.20
H/ 5,6,7	3.87
H / 8,9,10	4.01

B3LYP

Atom Name / Atom Nos.	Chemical Shift - Cluster midpoint)
H / 1,2,3	4.18
H / 4	7.91
H/ 5,6,7	3.59
H / 8,9,10	3.76

GOT THE RESULT - FOR CAFFEINE

Experimental and Theoretical Calculations - Found a Match

1H-NMR Chemical Shift

More Accurate Result with B3LYP

B3LYP

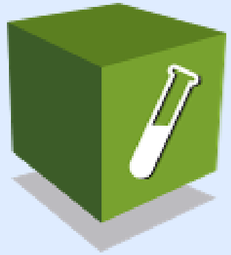
Atom Name / Atom Nos.	Chemical Shift - (Cluster midpoint)
H / 1,2,3	4.18
H / 4	7.91
H/ 5,6,7	3.59
H / 8,9,10	3.76

Calculated Values

Experimental

HMDB Database

Atom Name / Atom Nos.	Chemical Shift - Cluster midpoint)
H / 1,2,3	4.00
H / 4	7.51
H/ 5,6,7	3.41
H / 8,9,10	3.59



- **Approach to Integrate NWChem NMR Chemical Shift to COCONUT Library**
- **Documented the Report and Next Step to COCONUT**

COllecTion of Open Natural ProdUcTs

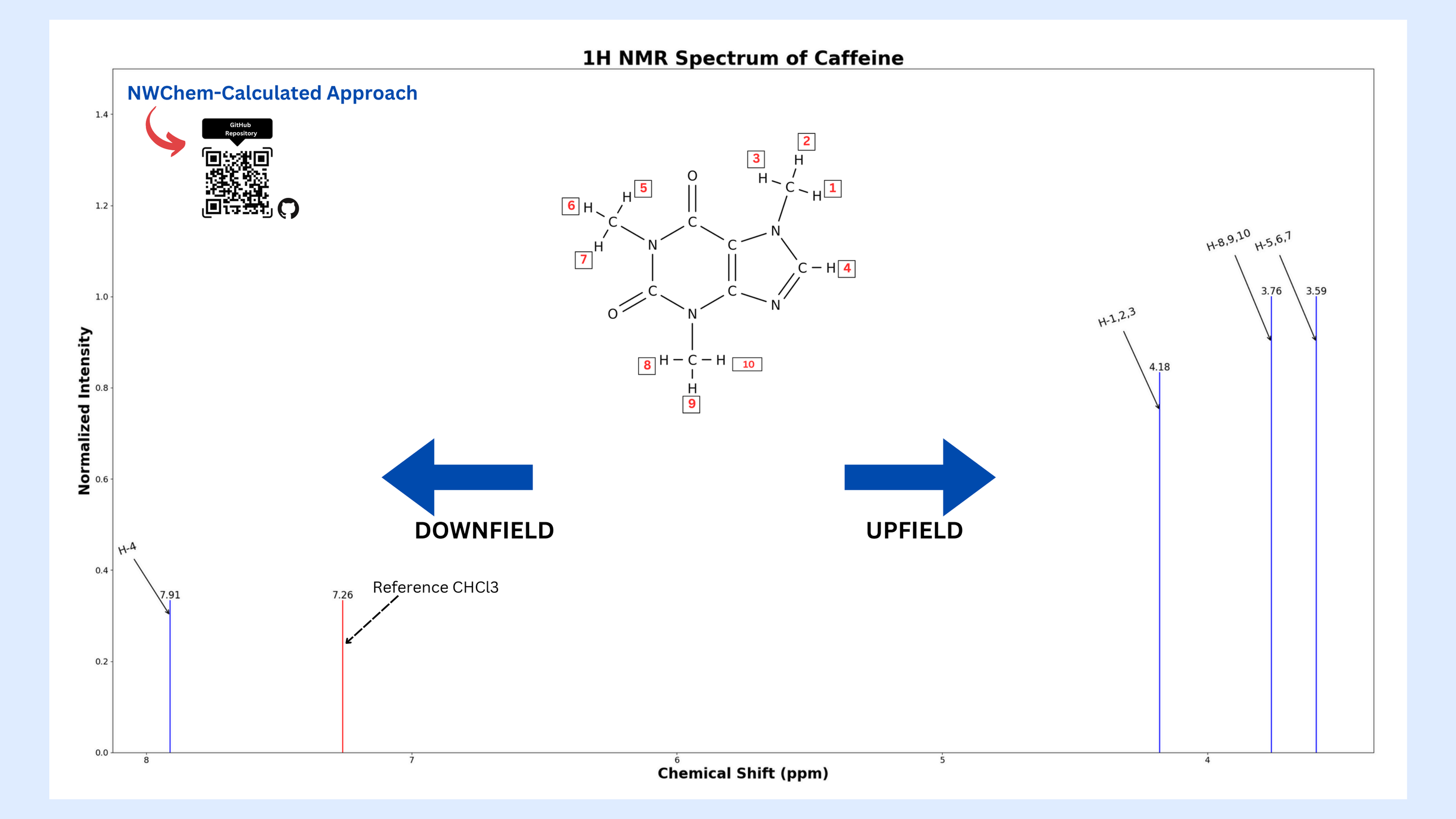
Automated NWChem NMR Shift Calculations with B3LYP/6-311G Basis Set Produce More Accurate ^1H Chemical Shifts for Caffeine in $CDCl_3$ Compared to PBE0

Raj Singh

1. Introduction

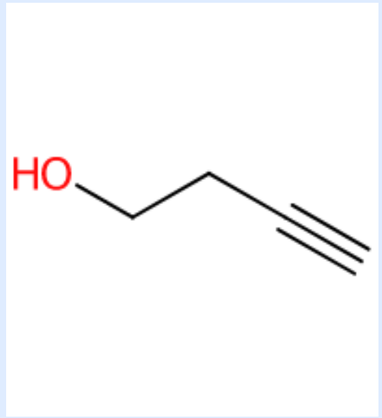
In NMR (Nuclear Magnetic Resonance) spectroscopy, chemical shifts denote the variations in the resonant frequency of a nucleus within a magnetic field, induced by its surrounding chemical environment. These variations arise from the shielding or deshielding effects exerted by the electron cloud around the nucleus. Local electron density variations, influenced by adjacent atoms or functional groups, modify the resonant frequency of the nucleus relative to a reference standard, typically tetramethylsilane (TMS) in organic solvents. This modification, quantified in parts per million (ppm), is termed the chemical shift. TMS, or $(CH_3)_4Si$, serves as the standard reference for chemical shifts, with δTMS defined as 0 ppm. Chemical shift measurements for ^1H nuclei in samples are referenced against the ^1H resonance of TMS

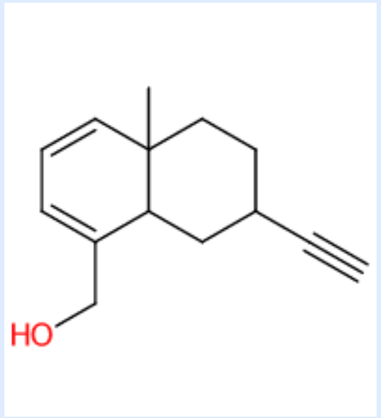
GitHub Repository

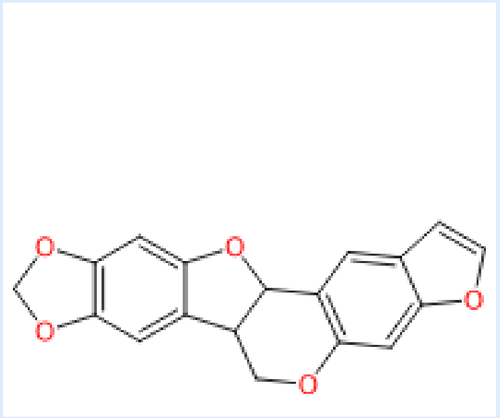

1H NMR Spectrum of Caffeine
NWChem-Calculated Approach
GitHub Repository
Normalized Intensity
Chemical Shift (ppm)
DOWNFIELD
UPFIELD
H-4
7.91
7.26
Reference CHCl3
H-1,2,3
4.18
H-8,9,10
3.76
H-5,6,7
3.59

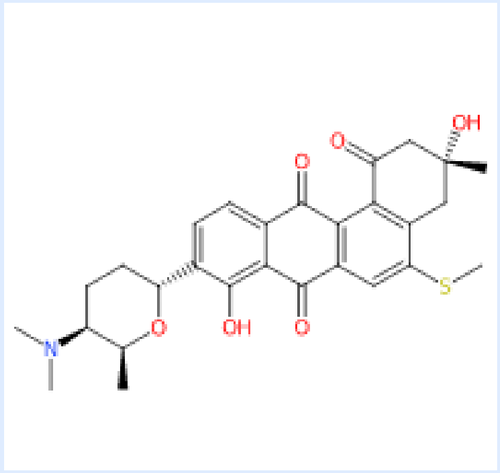
NATURAL PRODUCTS

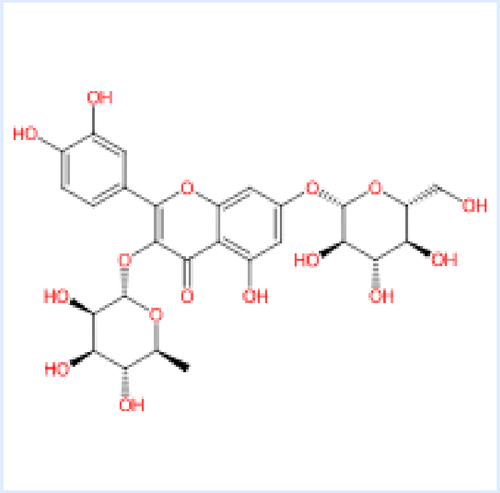
COCONUT
COllecTion of Open Natural ProdUcTs











3-BUTYN-1-OL	657.38 seconds	5	1
(7-ethynyl-4a-methyl-6,7,8,8a-tetrahydro-5H-naphthalen-1-yl)methanol	14492.10 seconds	15	1
Edulin	16381.17 seconds	23	0
Monacyclinone J	241879.78	36	3
17306-45-5	492188.37 seconds	43	6

THANKYOU