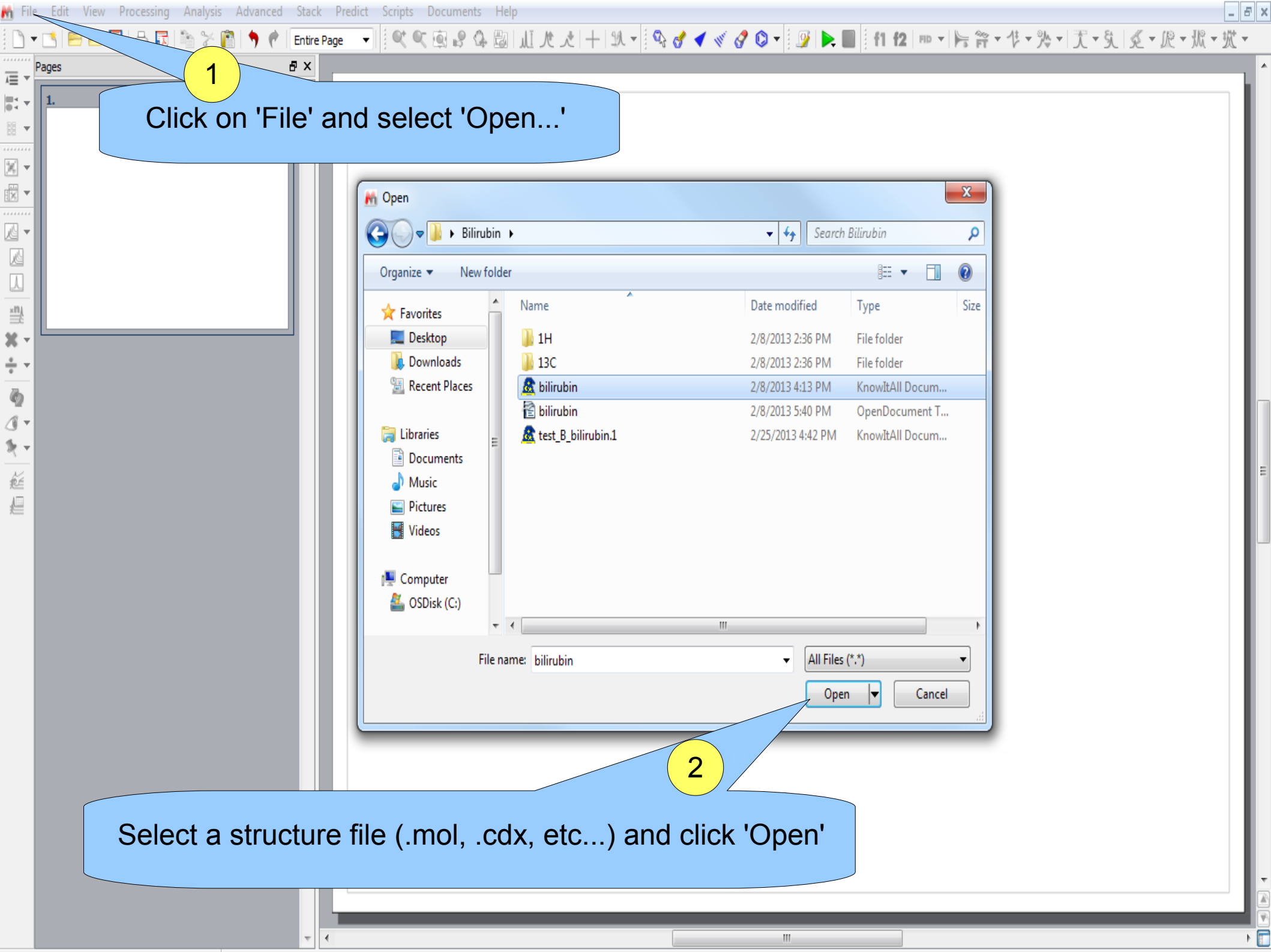
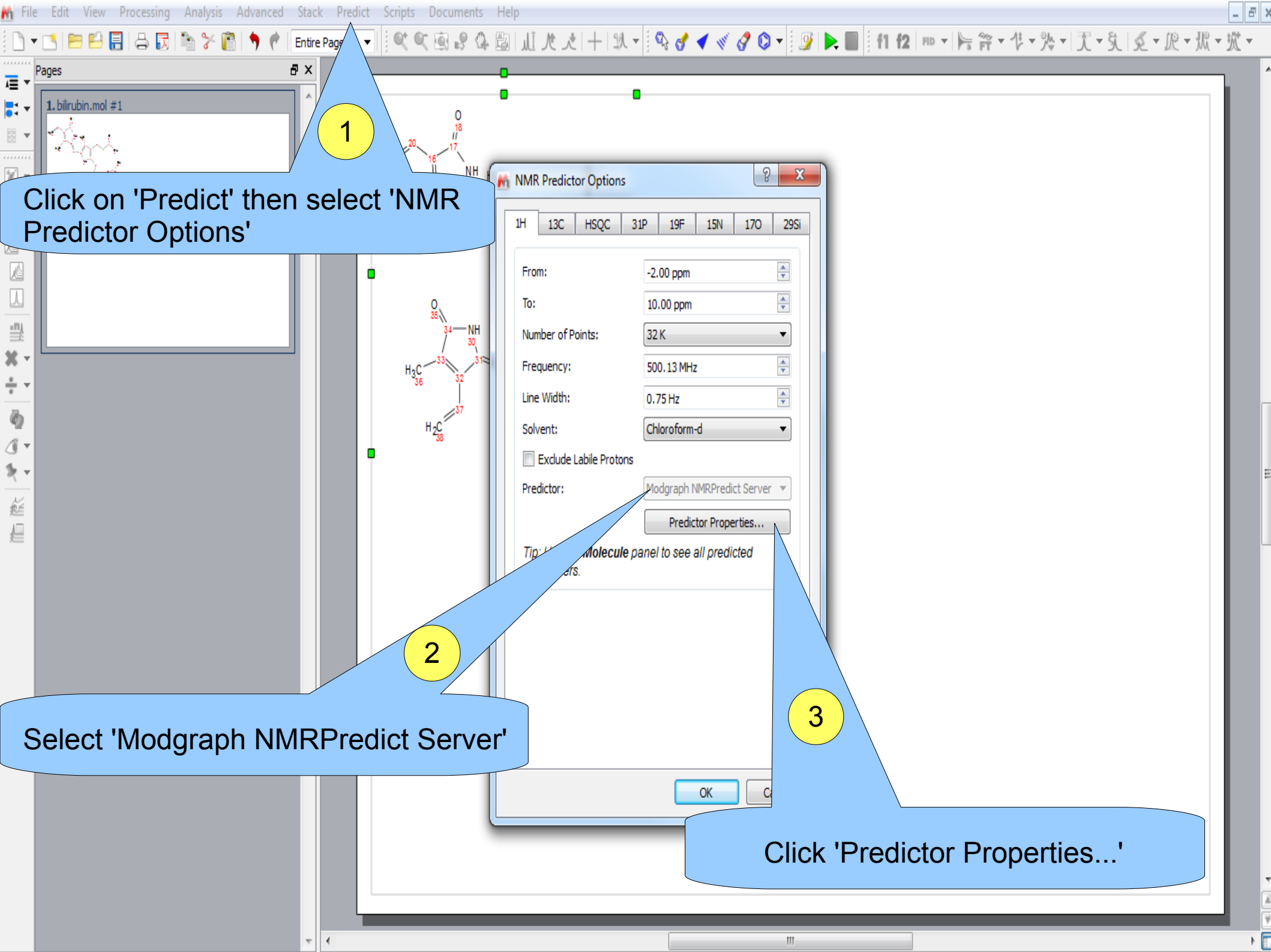

File Edit View Processing Analysis Advanced Stack Predict Scripts Documents Help
Entire Page
Pages
1.
1
Click on 'File' and select 'Open...'
Open
Bilirubin
Search Bilirubin
Organize
New folder
Favorites
Desktop
Downloads
Recent Places
Libraries
Documents
Music
Pictures
Videos
Computer
OSDisk (C:)
Name
Date modified
Type
Size
1H
2/8/2013 2:36 PM
File folder
13C
2/8/2013 2:36 PM
File folder
bilirubin
2/8/2013 4:13 PM
KnowItAll Docum...
bilirubin
2/8/2013 5:40 PM
OpenDocument T...
test_B_bilirubin.1
2/25/2013 4:42 PM
KnowItAll Docum...
File name: bilirubin
All Files (*.*)
Open
Cancel
2
Select a structure file (.mol, .cdx, etc...) and click 'Open'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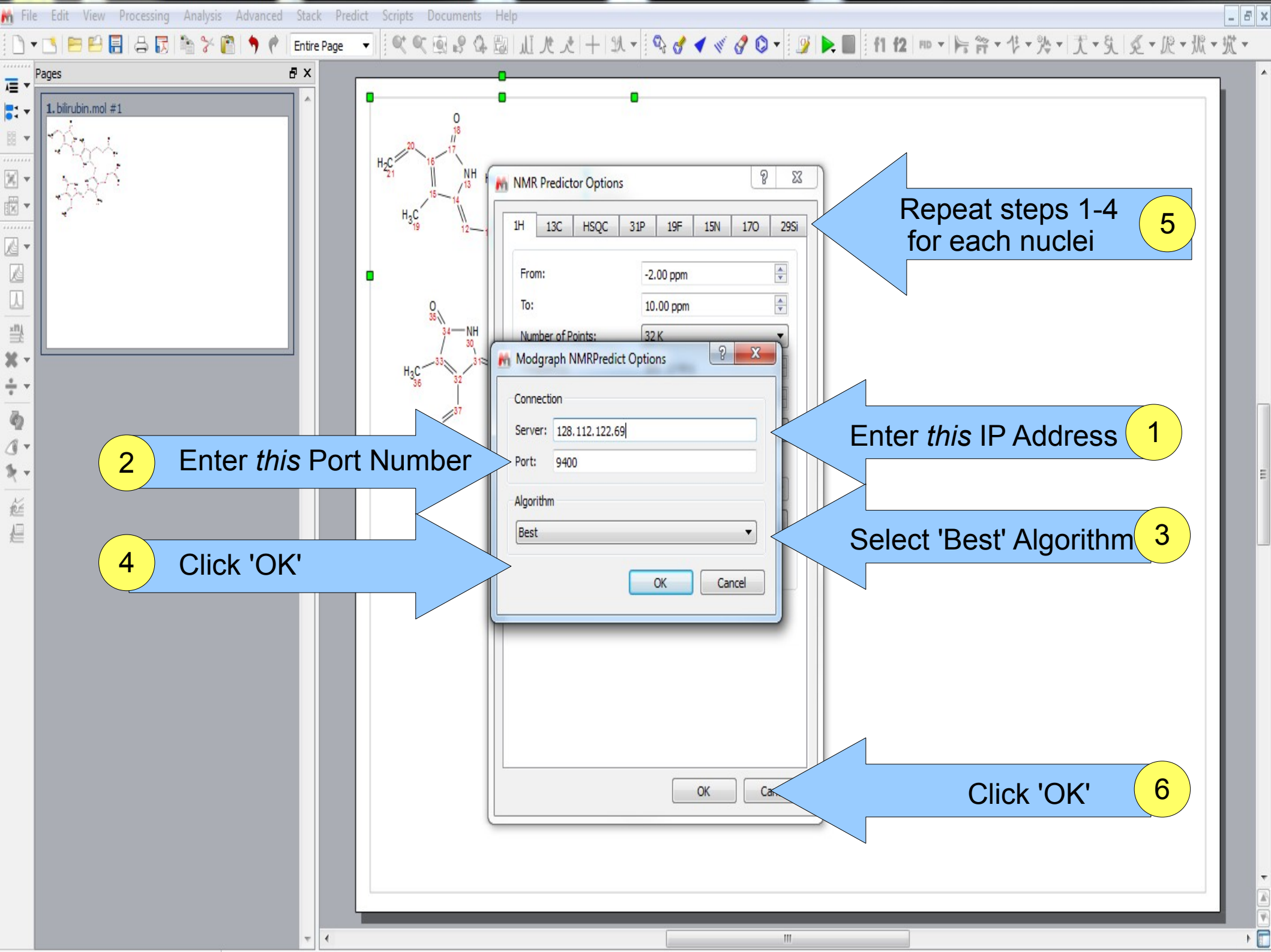
Pages
1. bilirubin.mol #1
1
Click on 'Predict' then select 'NMR Predictor Options'
NMR Predictor Options
1H 13C HSQC 31P 19F 15N 17O 29Si
From: -2.00 ppm
To: 10.00 ppm
Number of Points: 32 K
Frequency: 500.13 MHz
Line Width: 0.75 Hz
Solvent: Chloroform-d
Exclude Labile Protons
Predictor: Modgraph NMRPredict Server
Predictor Properties...
OK
2
Select 'Modgraph NMRPredict Server'
3
Click 'Predictor Properties...'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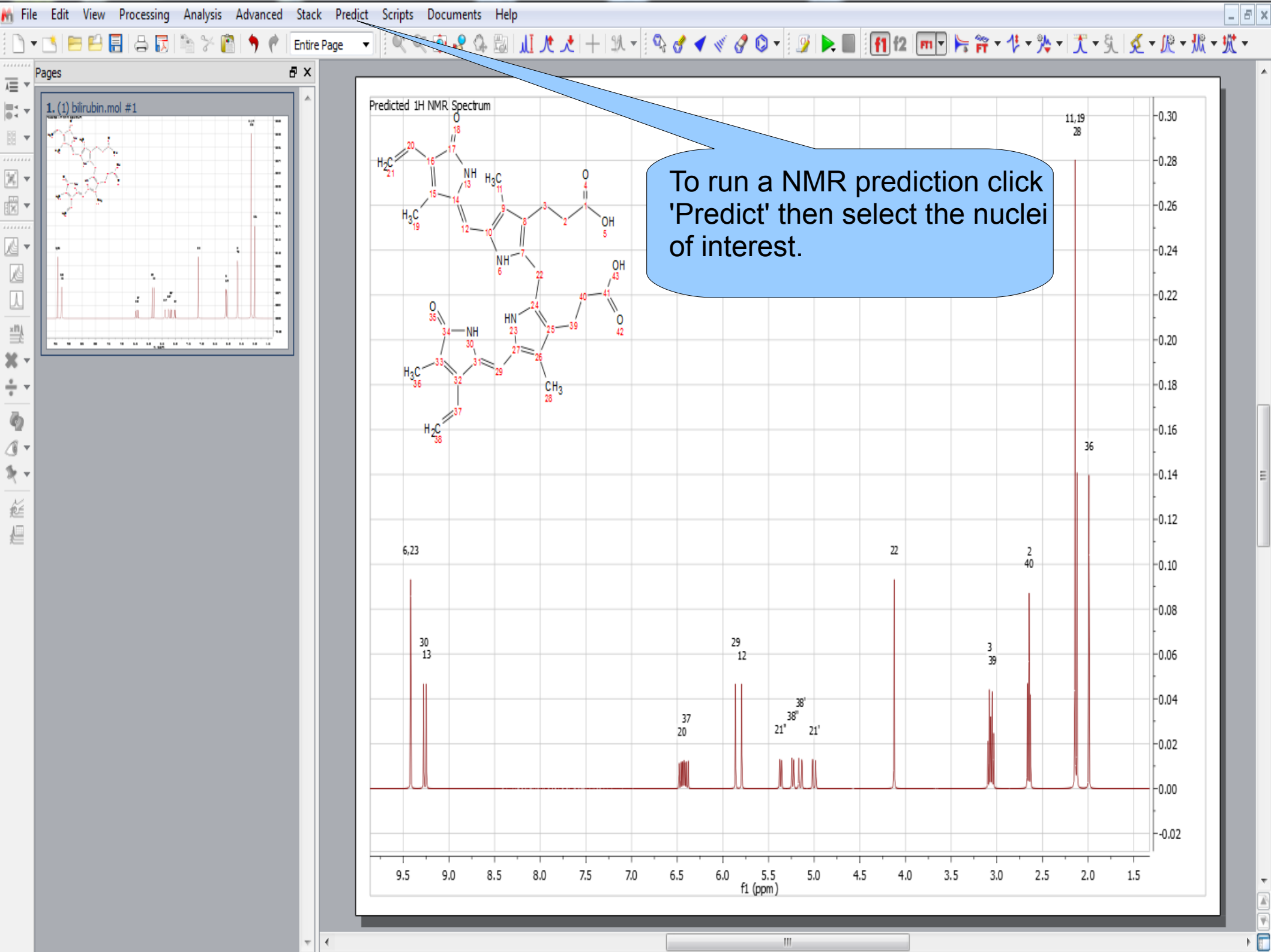
Pages
1. bilirubin.mol #1
NMR Predictor Options
1H 13C HSQC 31P 19F 15N 17O 29Si
From: -2.00 ppm
To: 10.00 ppm
Number of Points: 32 K
Modgraph NMRPredict Options
Connection
Server: 128.112.122.69
Port: 9400
Algorithm
Best
OK
Cancel
OK
Repeat steps 1-4 for each nuclei
5
Enter this IP Address
1
Enter this Port Number
2
Select 'Best' Algorithm
3
Click 'OK'
4
Click 'OK'
6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Pages
1. (1) bilirubin.mol #1
Predicted 1H NMR Spectrum
To run a NMR prediction click 'Predict' then select the nuclei of interest.
11,19
28
36
6,23
30
13
37
20
29
12
22
3
39
2
40
38'
38"
21"
21'
f1 (ppm)