ÚOCHB AV ČR
IOCB PRAGUE

MAGNETIC RESONANCE DAY

NOVA

Tips & Tricks

NMR SPECTROSCOPY
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What is today's objective?

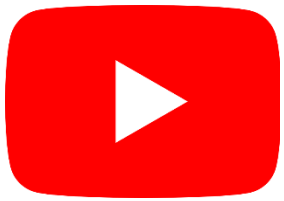
- to introduce possibilities of Mnova@IOCB
- to simplify your Mnova workflow
- to show some features of Mnova program you might not be aware of
- to find your demand for Mnova workshops

866 pages

MestReNova Manual

Last Revision: 3-May-2021

https://www.youtube.com/Mestrelab



tutorials, webinars, tips

Where to download?

https://mestrelab.com/download/mnova/

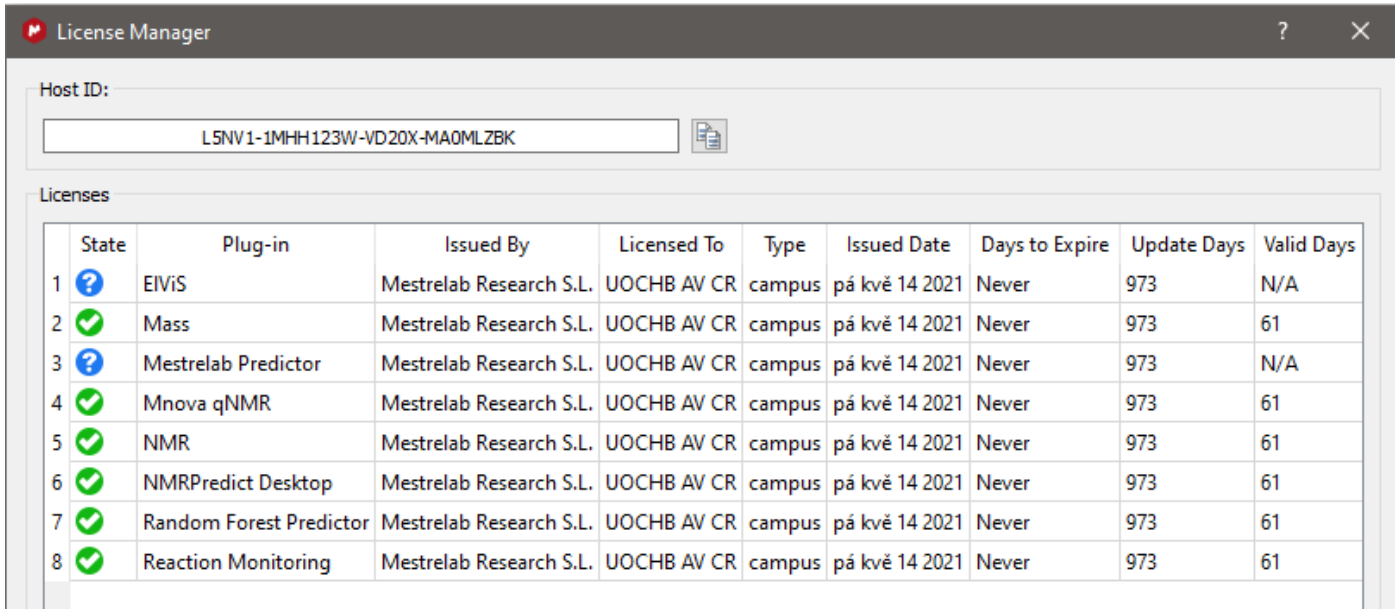
Licenses

Samba server: 147.231.122.7/nmruser/MestrecLic

- IOCB holds unlimited number of licenses for NMR, MS and UV/Vis plugins
- You can install Mnova on your laptop – works 90 days outside IOCB

Available plugins/licenses

→ *Help/License Manager*



	State	Plug-in	Issued By	Licensed To	Type	Issued Date	Days to Expire	Update Days	Valid Days
1	?	ElViS	Mestrelab Research S.L.	UOCHB AV CR	campus	pá kvě 14 2021	Never	973	N/A
2	✓	Mass	Mestrelab Research S.L.	UOCHB AV CR	campus	pá kvě 14 2021	Never	973	61
3	?	Mestrelab Predictor	Mestrelab Research S.L.	UOCHB AV CR	campus	pá kvě 14 2021	Never	973	N/A
4	✓	Mnova qNMR	Mestrelab Research S.L.	UOCHB AV CR	campus	pá kvě 14 2021	Never	973	61
5	✓	NMR	Mestrelab Research S.L.	UOCHB AV CR	campus	pá kvě 14 2021	Never	973	61
6	✓	NMRPredict Desktop	Mestrelab Research S.L.	UOCHB AV CR	campus	pá kvě 14 2021	Never	973	61
7	✓	Random Forest Predictor	Mestrelab Research S.L.	UOCHB AV CR	campus	pá kvě 14 2021	Never	973	61
8	✓	Reaction Monitoring	Mestrelab Research S.L.	UOCHB AV CR	campus	pá kvě 14 2021	Never	973	61

Setting up the Mnova workspace

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Edit/Preferences

General: large icons, vertical tabs

NMR: import parameters (e.g. appodization, zero filling)

View/Toolbars

View/Tables – parameters, compounds, multiplets, peaks

View/Panels – data browser, cursor info

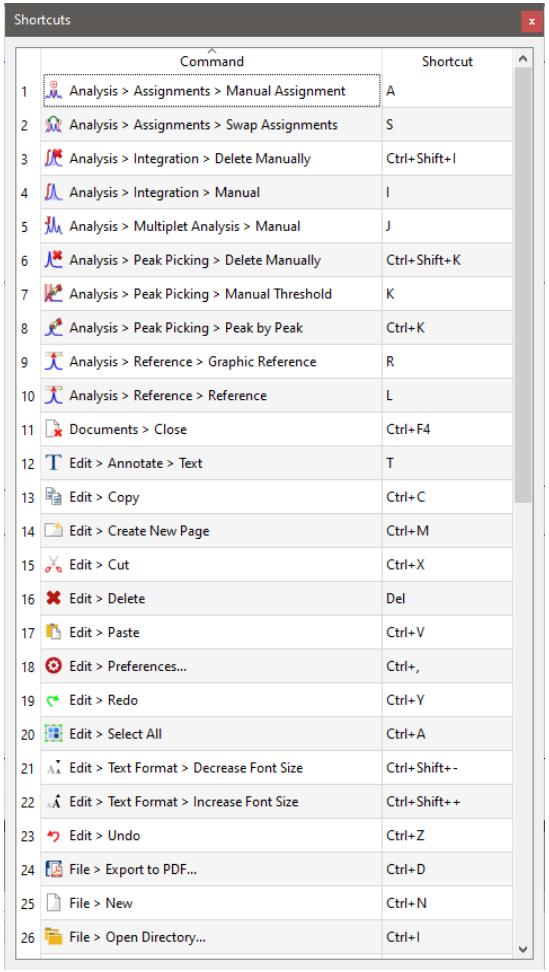
View/Pages **Ctrl+F2**

Shortcuts

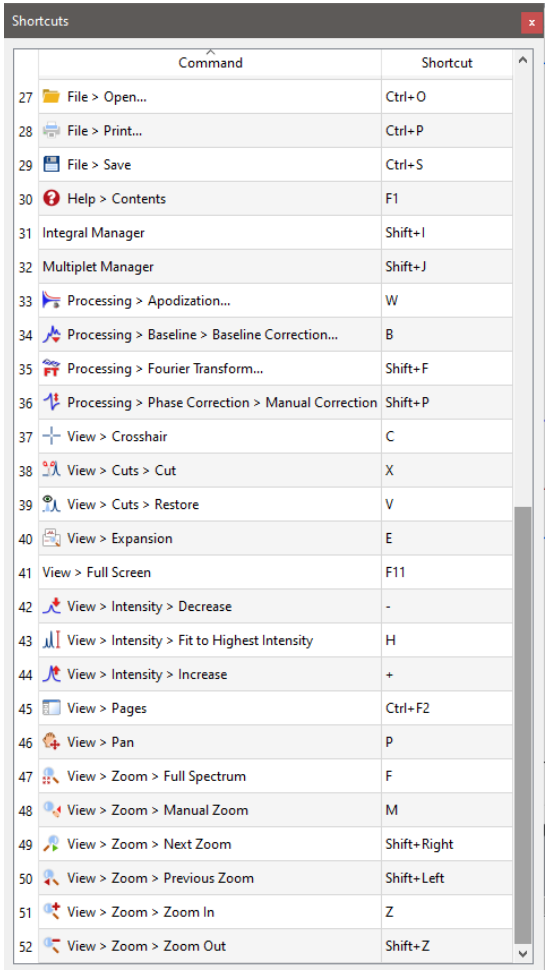
to see them go to: *Help/Shorcuts*

Important shortcuts for NMR:

I – manual integration
J – manual multiplet analysis
K – manual threshold for peak picking
Ctrl+K – peak picking peak by peak
L – reference
R – graphic reference
W – apodization
B – baseline correction
Shift+P – phase correction
C – crosshair
E – expansion
– – decrease intensity
+ – increase intensity
F – full spectrum
Z – zoom



	Command	Shortcut
1	Analysis > Assignments > Manual Assignment	A
2	Analysis > Assignments > Swap Assignments	S
3	Analysis > Integration > Delete Manually	Ctrl+Shift+I
4	Analysis > Integration > Manual	I
5	Analysis > Multiplet Analysis > Manual	J
6	Analysis > Peak Picking > Delete Manually	Ctrl+Shift+K
7	Analysis > Peak Picking > Manual Threshold	K
8	Analysis > Peak Picking > Peak by Peak	Ctrl+K
9	Analysis > Reference > Graphic Reference	R
10	Analysis > Reference > Reference	L
11	Documents > Close	Ctrl+F4
12	Edit > Annotate > Text	T
13	Edit > Copy	Ctrl+C
14	Edit > Create New Page	Ctrl+M
15	Edit > Cut	Ctrl+X
16	Edit > Delete	Del
17	Edit > Paste	Ctrl+V
18	Edit > Preferences...	Ctrl+,
19	Edit > Redo	Ctrl+Y
20	Edit > Select All	Ctrl+A
21	Edit > Text Format > Decrease Font Size	Ctrl+Shift+-
22	Edit > Text Format > Increase Font Size	Ctrl+Shift++
23	Edit > Undo	Ctrl+Z
24	File > Export to PDF...	Ctrl+D
25	File > New	Ctrl+N
26	File > Open Directory...	Ctrl+I



	Command	Shortcut
27	File > Open...	Ctrl+O
28	File > Print...	Ctrl+P
29	File > Save	Ctrl+S
30	Help > Contents	F1
31	Integral Manager	Shift+I
32	Multiplet Manager	Shift+J
33	Processing > Apodization...	W
34	Processing > Baseline > Baseline Correction...	B
35	Processing > Fourier Transform...	Shift+F
36	Processing > Phase Correction > Manual Correction	Shift+P
37	View > Crosshair	C
38	View > Cuts > Cut	X
39	View > Cuts > Restore	V
40	View > Expansion	E
41	View > Full Screen	F11
42	View > Intensity > Decrease	-
43	View > Intensity > Fit to Highest Intensity	H
44	View > Intensity > Increase	+
45	View > Pages	Ctrl+F2
46	View > Pan	P
47	View > Zoom > Full Spectrum	F
48	View > Zoom > Manual Zoom	M
49	View > Zoom > Next Zoom	Shift+Right
50	View > Zoom > Previous Zoom	Shift+Left
51	View > Zoom > Zoom In	Z
52	View > Zoom > Zoom Out	Shift+Z

NMR data processing

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Dataset opening:

1. *File/Open* (**Ctrl+O**) or *File/OpenDirectory* (**Ctrl+I**)
2. Drag and drop the folder with NMR data (the folder can contain structure in *.mol file - will be open automatically)
3. Data browser panel – selection of location containing data

Customizing the spectrum appearance (graphical properties) – *Edit/Properties* or right mouse button click on spectrum and then *Properties*

Essential steps in 1D NMR data processing (in *Processing*):

1. Fourier transformation
2. Zero filling – improves digital resolution
3. Appodization (**W**) – enhances sensitivity (exponential function) or resolution (exponential function + Gaussian function); in order to see the FID+function click on *View/FullView*
4. Phase correction (**Shift+P**)
5. Baseline correction (**B**), multipoint baseline correction
6. Referencing (**L**)
7. Peak picking (**K** – setting threshold, **Ctrl+K** – peak by peak), *PeakPicking/Options*
8. Integration (**I**)

How to streamline your NMR data processing

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1. use **Data Browser** for storing of your NMR data
2. create your favorite **graphical properties** of spectra and save it
3. create your favorite **Processing Template** for each type of spectrum (^{1}H, ^{13}C, ^{31}P…) and save it

Other "tricks":

- several types of spectra on single page
- expanding of spectrum - *View/Expansion* or **E**
- finding experiment parameters – *View/Tables/Parameters*
- chemical structure (supported format of chemical structures: *.mol *.cdx *.sdf)
- signal suppression - *Processing/Signal Suppression*

NMR data reporting

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MestReNova enables easy creation of Supporting Info:

1. Pasting a spectrum into MSWord- possibility of later formatting the spectrum
2. Export to PDF – *File/Export to PDF* or **Ctrl+D**
3. Copy as a picture - *Edit/Copy Special/Copy as Image*

Peaks report generation:

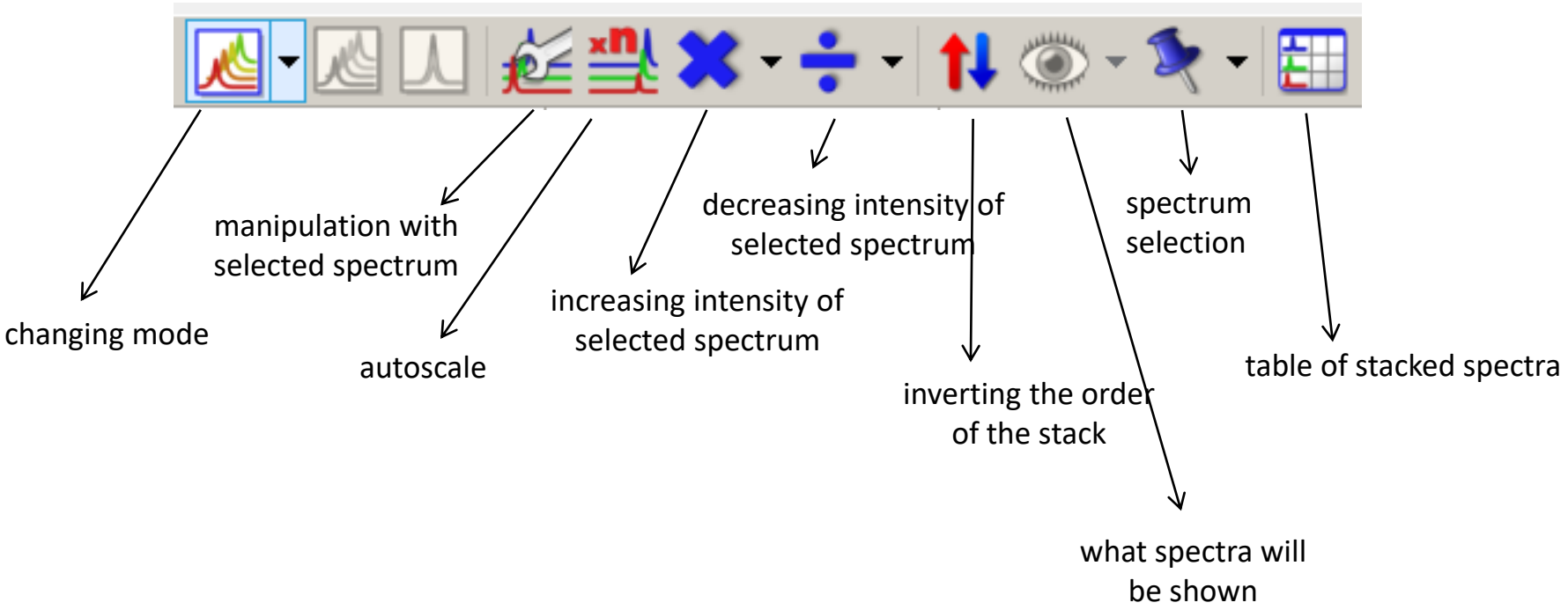
1. Creating of peak list by peak picking
2. Peak report generation *Scripts/Report/Peaks* or in Peaks Table *Report Peaks*
3. Changing style of peak report in Peaks Table *Setup Report*

Multiplets report generation:

1. Creating of multiplet list by multiplet analysis (**J**)
2. Peak report generation *Scripts/Report/Multiplets* or in Multiplets Table *Report Multiplets*
3. Changing style of multiplet report Multiplets Table *Setup Report*

Working with multiple NMR spectra

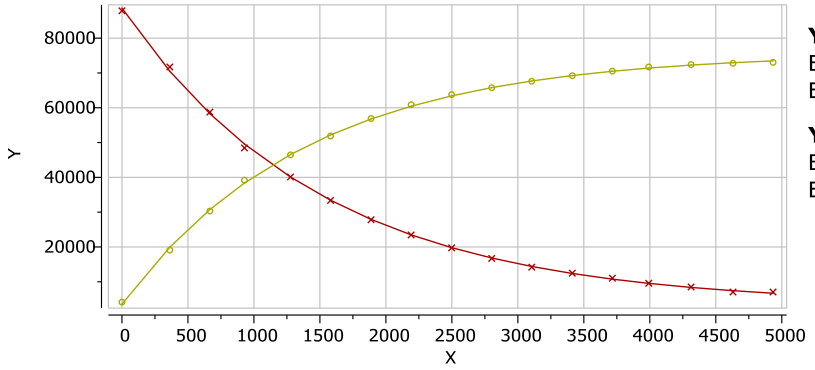
1. select spectra in Pages Table
2. Go to *Stack/Stack Spectra*
3. To work with stacked spectra → activate toolbar *Stacked*



Graphical properties of the stacked spectra → *Properties/Stacked*

Reaction kinetics monitoring

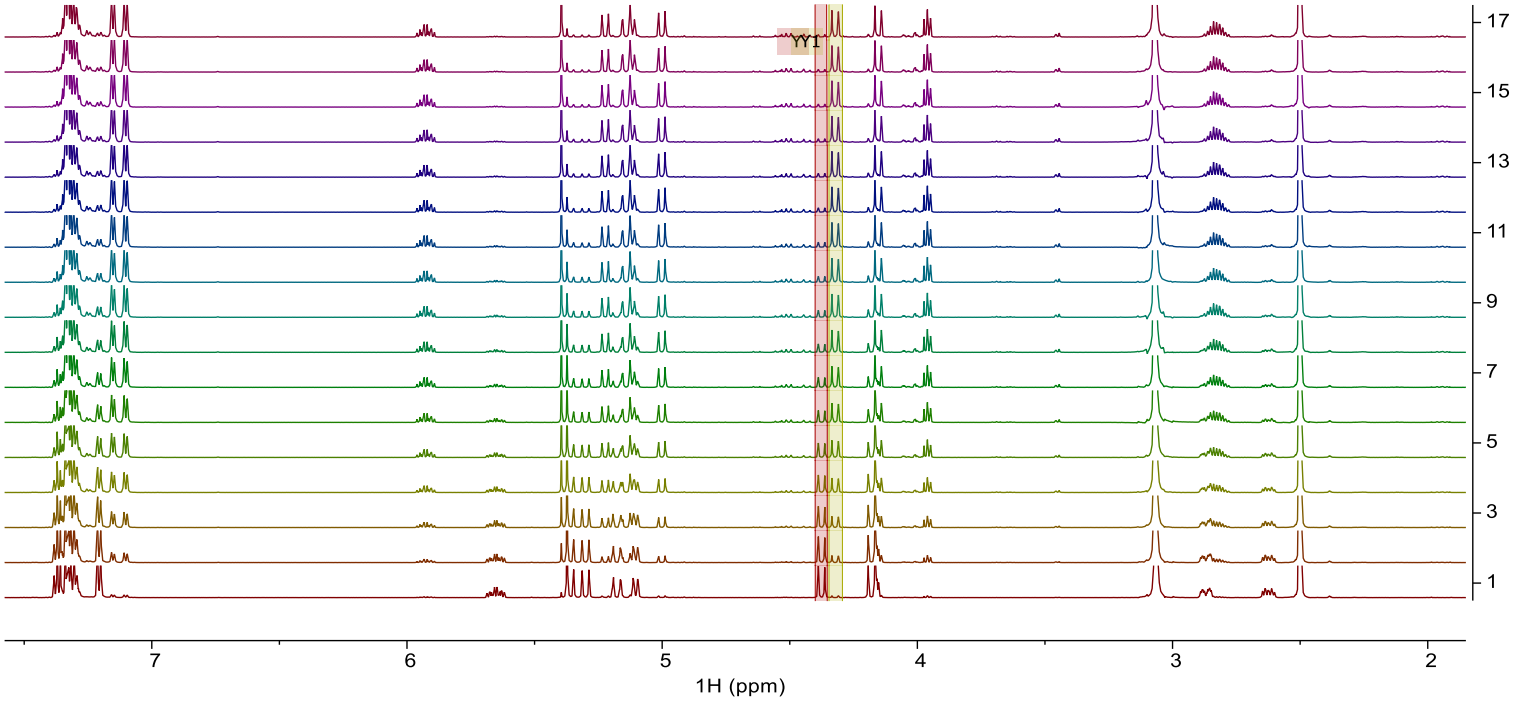
In stacked mode: *Advanced/Data Analysis/Create/Integrals Graph*



Y' = B+F*exp(-X*G)
B=3428; F=8.518e+4; G=0.0006602;
Error: 0.000007008

Y1' = B+F*exp(-X*G)
B=7.563e+4; F=-7.204e+4; G=0.0007104;
Error: 0.000006999

half-life $t_{1/2}$ = 0.693/G



Prediction of NMR spectra

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- Paste molecular structure or drag and drop file with your structure (*.mol *.cdx *.sdf) to *Compounds* Table and run prediction of ^{1}H, ^{13}C, and other nuclei *Predict/1H Spectrum* or *^{13}C Spectrum*

- You can try also for other nuclei (^{11}B, ^{15}N, ^{19}F, ^{29}Si, and ^{31}P)

- *Predict/Prediction Options* – selection of e.g. solvent, frequency, number of datapoints….

- Compare predicted spectrum with your experimental spectrum

Comparison of your NMR spectra with published data

- paste published spectrum into *Multiplet Report to Spectrum* script and generate spectrum (*Scripts/NMR Tools/Multiplet Report to Spectrum*)

  example for JM040 – 2,6-diamino-2'-deoxyadenosine

2,6-Diamino-2′-deoxyadenosine (2)—Supplied by Raylo Chem. Edmonton, Alberta, Canada. ^{1}H NMR (300 MHz, d_6-DMSO): δ 2.17 (m, J = 2.7, 6.0, −13.2 Hz, 1H), 2.60 (m, J = 5.7, 8.4, −13.5 Hz, 1H), 3.52 (m, 1H), 3.59 (m, 1H), 3.84 (m, 1H), 4.35 (m, 1H), 5.26 (m, 5′-OH, 1H), 5.29 (m, 3′-OH, 1H), 5.76 (br s, 2 NH_2, 2H), 6.17 (dd, J = 6.0, 8.1 Hz, 1H), 6.76 (br s, 6 NH_2, 2H), 7.92 (s, 1H), ^{13}C NMR (75 MHz, d_6-DMSO): δ 39.31, 61.91, 70.94, 83.03, 87.57, 113.39, 135.69, 151.12, 156.08, 159.94. MS: m/e 267 $(M + 1)^+$. UV max: 255, 280 nm.

Journal of Pharmaceutical Sciences **1994**, *83 (4),* 525-531.

- compare with experimental spectrum

Interested in workshops?

NMR SPECTROSCOPY RESEARCH-SERVICE GROUP IOCB PRAGUE offers Mnova workshops covering various topics:

- 1D NMR processing
- 2D NMR processing
- multiplet analysis
- spectra assignment
- presenting NMR data
- reaction monitoring and qNMR
- spin system simulation
- Mnova scripts
- troubleshooting

workshops concept:

- 10 attendees with laptops
- topics will be specified upon demand
- hands-on solving of particular problem

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