

List of (some) revisions

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Various minor textual changes have been made throughout the thesis, which are ignored here. The numbering of all equations, figures, pages, etc. refer to that in the corrected version.

Front matter

- Corrected term of submission on front page
- Reworded parts of acknowledgements

1 NMR theory

- Added missing punctuation to equations where necessary
- Corrected explanation of rotating frame and resonance condition (p. 7) (ω_{rf} symbol was unnecessary)
- Corrected caption of fig. 1.2 (p. 13) (the π symbol was not rendered correctly)
- Reworked explanation of fig. 1.8 to improve clarity (p. 30)

2 Pure shift NMR

- Added an example of a pure shift spectrum in the introduction (fig. 2.1; p. 36)
- Corrected pulse sequence in fig. 2.3a (p. 42) (caption described a NOESY experiment but there was no mixing time)
- Removed unnecessary colour from fig. 2.17 (p. 67)
- Additionally labelled the two ‘special optima’ in fig. 2.20 with different shapes (p. 75)
- Added conclusion section (pp. 87–89)

3 POISE

- Fixed incorrect labels in fig. 3.3 pp. 105)
- Inserted missing factor of $1/2$ in eq. 3.21 (p. 117)
- Improved explanation of POISE source code locations (p. 110)
- Reworked § 3.4.2 so as to bring table 3.4 before tables 3.5 and 3.6 (pp. 122–123)
- Added labels quantifying post-optimisation NOESY sensitivity enhancements in fig. 3.11 (p. 128)
- Reworded discussion on gramicidin NOESY optimisation to avoid implying that results were *accurate* (they are merely *reproducible*) (p. 128)
- Removed unnecessary colour in figs. 3.24, 3.26, and 3.27 (pp. 146–152)
- Explicitly disambiguated cost functions in eqs. 3.34 and 3.35 (p. 148) (previously they were implied to be the same)
- Added conclusion section (pp. 162–163)

4 NOAH

- Added missing y -axis labels in various figures
- Standardised captions where necessary
- Added missing diagram in fig. 4.64a (p. 262)
- Extended explanation of symmetrisation procedure in covariance spectra (pp. 270–271)
- Added conclusion section (p. 272)