# Hyperspectral Raman imaging of neuritic plaques and neurofibrillary tangles in brain tissue from Alzheimer's disease patients

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**Supplementary Table 1**

**Assignments of the Amide I of proteins in Raman spectroscopy and infrared absorption spectroscopy**

| Amide I | Raman spectroscopy in [$cm^{-1}$] | Ref. | Infrared absorption spectroscopy in [$cm^{-1}$] | Ref. |
|---|---|---|---|---|
| α-helix | 1650-1655<br>1645-1655 | 1<br>4 | 1648-1657<br>1650-1657 | 2, 3<br>5 |
| β or extended structures | 1665-1670<br>1668-1673 strong<br>1669 | 1<br>6<br>8 | 1623-1641 strong<br>1674-1695 weak<br>1628-1634 strong<br>1612-1640 antiparallel beta-sheet<br>1670-1690 weak<br>1626-1640 parallel beta-sheet | 2, 3<br>2, 3<br>6<br>5<br>5<br>5 |
| Turn | 1662-1672 | 7 | 1662-1686<br>1655-1675<br>1680-1696 | 2, 3<br>5<br>5 |
| Unordered | 1639 (max)<br>1638 (broad) | 8<br>9 | 1642-1657<br>1640-1651 | 2, 3<br>5 |

For additional information on "turns", we refer to an extensive review by Vass et. al., added as reference 10 below.

References:


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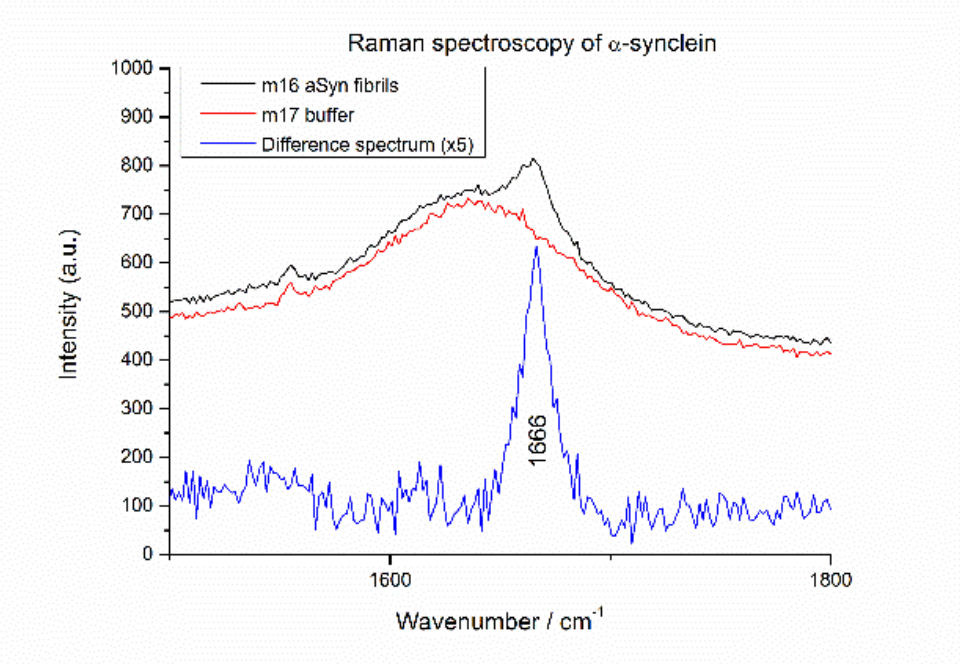
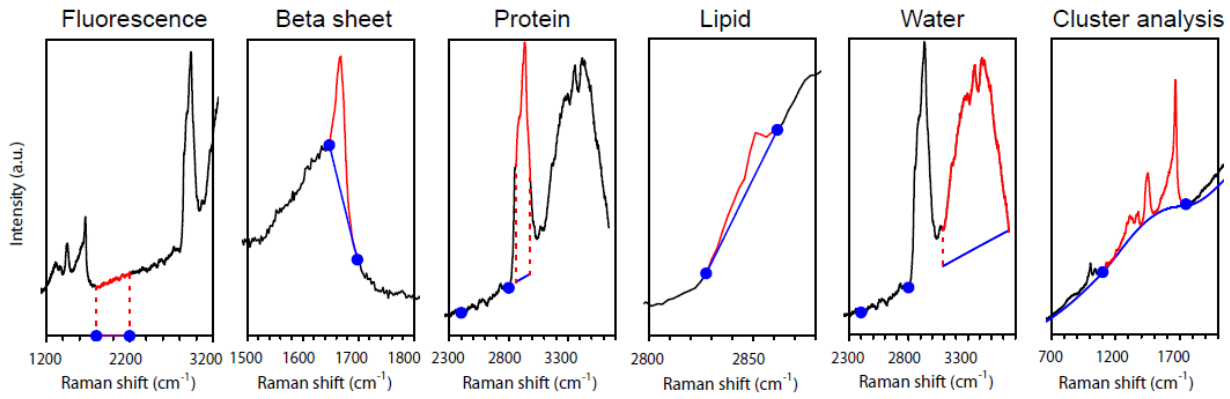
10) E. Vass, M. Hollósi, F. Besson, R. Buchet, (2003) Vibrational spectroscopic detection of beta- and gamma-turns in synthetic and natural peptides and proteins. Chem. Rev. 103, 1917-1954

**Supplementary Figure S1**




The Raman spectrum of alpha-synuclein in β-sheet structure in aqueous solution.
(Previously unpublished data by ME van Raaij, I. Segers-Nolten, C. Otto, V. Subramaniam).

**Supplementary Figure S2**




Raman intensity integration for broad-band autofluorescence background (1800-2200 cm-1), β-sheet (1649-1698 cm-1), protein (2860-2980 cm-1), lipid (2830-2860 cm-1) and water (3088-3648 cm-1). The baseline removal before the combined cluster analysis is shown on the right. The spectral band used for integration are shown in red. The blue dots indicate the points used for baseline estimation and the blue lines the estimated baseline which was subtracted from the spectral band intensity. The prominent peaks inside the Raman bands are visible for β-sheet at 1666 cm-1, for protein at 2935 cm-1 and for lipid at 2850 cm-1.

**Supplementary Figure S3**

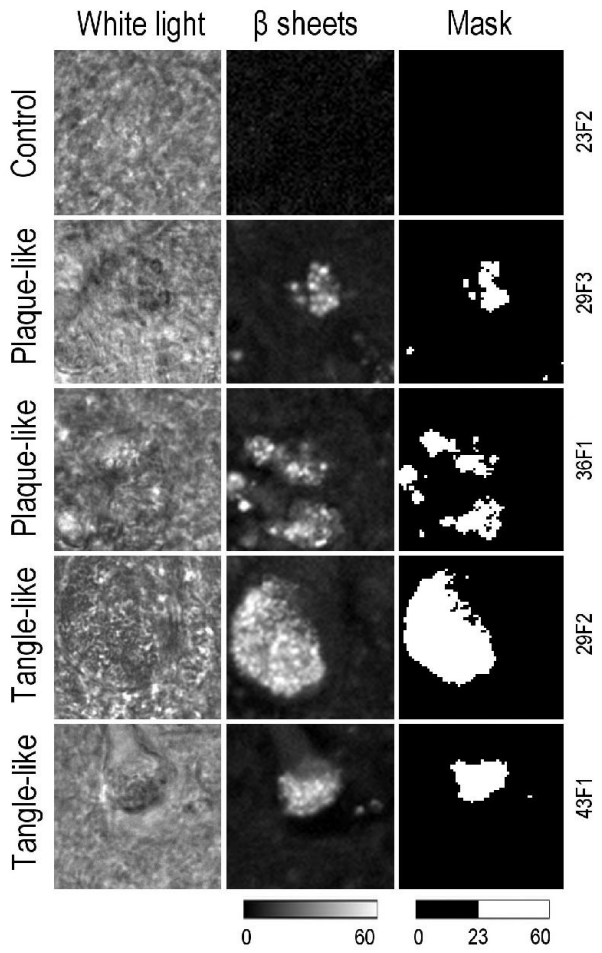



Illustration that shows the creation of the image mask used for separation of the areas of the features from that of the surrounding tissue. Maximum entropy thresholding was applied to the β-sheet intensity results (Fig 2). White light images from the bright field video mode of the Raman microscope are given for reference on the left. Tissue ID numbers are given on the right; image size is of 30 x 30 µm. First row shows a control sample, below two samples with plaque-like features and two samples with tangle-like features. Grey scale bar below show the range of the Raman intensities displayed.