Electronic Supporting Information

Insight into the internal structure of amyloid-β oligomers by isotope-edited Fourier transform infrared spectroscopy

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Table S1. Band positions and band areas of the component bands of the fits to the amide I spectra of $A\beta_{40}$ and $A\beta_{42}$. Three independent samples of each peptide were measured and co-fitted with Savitzky-Golay windows of 9, 13, and 17 data points, which gave in total nine fits for each peptide. All results were averaged and the standard deviations determined. The total area assigned to β-sheets is 28% for $A\beta_{40}$ and 39% for $A\beta_{42}$. The bands assigned to β-sheets are indicated by bold print.

	Band position ± standard deviation / cm^{-1}	Band area ± standard deviation /%
$A\beta_{40}$	**1685.0 ± 0.1**	**2.1 ± 0.6**
	1677.0 ± 1.9	7.5 ± 3.0
	1661.3 ± 2.2	24.4 ± 3.7
	1642.1 ± 1.1	39.7 ± 4.4
	1624.3 ± 0.4	**22.0 ± 2.0**
	1622.1 ± 0.1	**4.2 ± 0.8**
$A\beta_{42}$	**1685.4 ± 0.2**	**1.4 ± 0.5**
	1679.8 ± 1.2	4.0 ± 1.6
	1665.5 ± 3.9	18.4 ± 4.5
	1644.2 ± 3.2	38.6 ± 4.7
	1626.5 ± 0.9	**32.9 ± 5.9**
	1624.6 ± 0.2	**4.6 ± 1.3**

Table S2. PDB files and residues used to create β-barrel models

PDB file	Type of structure	Number of strands	Residues
1QJP	Barrel	8	A6-A15; A36-A45: A48-A57; A77-A86; A91-A100; A122-A131; A134-A143; A161-A170
1I78	Barrel	10	A11-A20; A50-A59; A63-A72; A111-A120; A126-A135: A180-A189; A191-A200; A232-A241; A244-A253; A288-A297
1K24	Barrel	10	A10-A19; A32-A41; A50-A59; A88-A97; A110-A119; A135-A144; A157-A166; A187-A196; A209-A218; A242-A251
1UYN	Barrel	12	X819-X828; X845-X854; X857-X866; X884 X893; X897-X906; X931-X940; X948-X957; X986-X995; X1000-X1009; X1043-X1052; X1057-X1066; X1074-X1083
1QD6	Barrel	12	C38-C46; C64-C73; C90-C99; C110-C119; C136-C145; C154-C163; C170-C179; C194-C203; C206-C215; C220-C229; C236-C245; C256-C265
1T16	Barrel	14	A43-A52; A79-A88; A91-A99; A126-A135; A139-A148; A208-A217; A220-A229; A274-A283; A286-A295; A326-A335; A338-A347; A368-A377; A380-A389; A412-A421
1OPF	Barrel	16	A11-A23; A36-A48; A57-A67; A80-A89; A94-A100; A135-A143; A150-A159; A172-A182; A184-A193; A213-A222; A224-A233; A255-A264; A268-A278; A292-A303; A307-A317; A331-A340
1OPF	Barrel	16	A12-A21; A38-A47; A58-A67; A80-A89; A94-A100; A134-A143; A150-A159; A173-A182; A184-A193; A213-A222; A224-A233; A255-A264; A269-A278; A293-A302; A307-A316; A331-A340
1A06	Barrel	18	P74-P84; P117-P126; P135-P144; P159-P168; P180-P186; P208-P215; P222-P230; P244-P253; P255-P264; P286-P296; P306-P317; P335-P345; P352-P362; P373-P383; P390-P400; P416-P426; P439-P449; P472-P483
1FEP	Barrel	22	A154-A163; A172-A181; A188-A197; A230-A238; A246-A255; A286-A295; A302-A311; A344-A353; A362-A371; A409-A418; A425-A434; A441-A450; A457-A466; A507-A516; A522-A531; A563-A572; A579-A588; A604-A613; A620-A629; A655-A664; A669-A678; A715-A724
1NQE	Barrel	22	A137-A146; A149-A158; A165-A174; A199-A208; A215-A224; A247-A256; A262-A271; A295-A304; A310-A319; A337-A346; A352-A361; A368-A377; A384-A393; A415-A424; A429-A438; A461-A470; A476-A485; A500-A509; A515-A524; A544-A553; A558-A567; A585-A594

Table S3. 0.1→ 1 ^{13}C-band shifts. The parameters were adjusted so that they matched the spectra of the **$A\beta_{40}$** oligomers. The angle of dipole derivative was **10°**

Structure	Dipole derivative magnitude (D Å^{-1} amu$^{-1/2}$)	Center wavenumber (cm^{-1})	^{13}C shift (cm^{-1}) for building block ± standard deviation (only for average values)
Sheet, 4 strands, 10 residues/strand	3.507	1652.9	Single strand: 15.6
			2-strand block: 7.6
Sheet, 6 strands, 10 residues/strand	3.220	1654.5	Single strand: 16.7
			2-strand block: 10.1
			3-strand block: 6.2
Sheet, 12 strands, 10 residues/strand	2.988	1656.4	Single strand: 18.0
			2-strand block: 12.3
			3-strand block: 9.0
Sheet, 24 strands, 10 residues/strand	2.890	1657.1	Single strand: 18.4
			2-strand block: 13.2
			3-strand block: 10.0
Barrel, 8 strands, 1QJP	3.240	1658.7	Single strand: 18.7
			2-strand block: 11.6
Barrel, 12 strands, 1UYN	3.245	1658.2	Single strand: 19.1
			2-strand block: 11.9
			3-strand block: 7.8
Barrel, 18 strands, 1A06	3.340	1658.8	Single strand: 19.7
			2-strand block: 13.1
			3-strand block: 9.1
Barrel, 22 strands, 1NQE	3.174	1658.2	Single strand: 19.1
			2-strand block: 12.7
Averages			**Single strand: 18.2 ± 1.4**
			2-strand block: 11.6 ± 1.8
			3-strand block: 8.4 ± 1.5

Table S4. 0.1→ 1 ^{13}C-band shifts. The parameters were adjusted so that they matched the spectra of the **Aβ_{40}** oligomers. The angle of dipole derivative was **20°**

Structure	Dipole derivative magnitude (D Å^{-1} amu$^{-1/2}$)	Center wavenumber (cm^{-1})	^{13}C shift (cm^{-1}) for building block ± standard deviation (only for average values)
Sheet, 2 strands, 10 residues/strand (not considered in the average)	4.929	1653.2	Single strand: 12.5
Sheet, 3 strands, 10 residues/strand (not considered in the average)	3.910	1654.1	Single strand: 15.6
Sheet, 4 strands, 10 residues/strand	3.557	1655.4	Single strand: 16.7
			2-strand block: 8.3
			Interlaced model 1: 11.4
Sheet, 6 strands, 10 residues/strand	3.270	1656.7	Single strand: 17.8
			2-strand block: 10.6
			3-strand block: 6.3
			Interlaced model 2: 15.1
Sheet, 6 strands, 6 residues/strand	3.285	1657.4	Single strand: 17.6
Sheet, 6 strands, 4 residues/strand	3.600	1658.2	Single strand: 17.3
Sheet, 12 strands, 10 residues/strand	3.032	1658.3	Single strand: 18.8
			2-strand block: 12.7
			3-strand block: 9.1
			Interlaced model 1: 15.6
			Interlaced model 2: 16.9
Sheet, 12 strands, 6 residues/strand	3.095	1658.5	Single strand: 18.4
Sheet, 24 strands, 10 residues/strand	2.935	1658.3	Single strand: 19.1
			2-strand block: 13.5
			3-strand block: 10.1
			Interlaced model 1: 16.3
			Interlaced model 2: 17.5
Barrel, 8 strands, 1QJP	3.287	1661.2	Single strand: 19.5
			2-strand block: 12.1
			Interlaced model 1: 15.8
Barrel, 10 strands, 1I78	3.330	1660.5	Single strand: 19.6
			2-strand block: 12.1
Barrel, 10 strands, 1K24	3.310	1662.2	Single strand: 19.9
			2-strand block: 12.6
Barrel, 12 strands, 1UYN	3.285	1660.7	Single strand: 19.9
			2-strand block: 12.3
			3-strand block: 7.8
			Interlaced model 1: 15.8
			Interlaced model 2: 18.0
Barrel, 12 strands, 1QD6	3.420	1660.2	Single strand: 20.2
			2-strand block: 12.9
			3-strand block: 8.5
			Interlaced model 1: 16.6
			Interlaced model 2: 18.0
Barrel, 14 strands, 1T16	3.281	1661.3	Single strand: 20.0
			2-strand block: 12.6

Barrel, 16 strands, 1OPF	3.313	1661.1	Single strand: 20.0
			2-strand block: 13.1
			Interlaced model 1: 16.4
Barrel, 16 strands, 1OPF	3.333	1661.0	Single strand: 19.7
			2-strand block: 12.3
			Interlaced model 1: 16.1
Barrel, 18 strands, 1A06	3.348	1660.2	Single strand: 20.1
			2-strand block: 13.4
			3-strand block: 9.1
Barrel, 22 strands, 1FEP	3.211	1660.2	Single strand: 20.0
			2-strand block: 13.0
			Interlaced model 2: 18.3
Barrel, 22 strands, 1NQE	3.211	1660.6	Single strand: 20.0
			2-strand block: 13.4
Dodecamer, 5HOW	3.660	1678.0	(2-strand block): 10.3
Averages of all barrels and sheets with 4 or more strands			**Single strand: 19.2 ± 1.1**
			2-strand block: 12.3 ± 1.3
			3-strand block: 8.5 ± 1.3
			Interlaced model 1: 15.5 ± 1.8
			Interlaced model 2: 17.3 ± 1.3
Averages using the same structures as for the other angles (Table S3 and S5)			**Single strand: 19.0 ± 1.2**
			2-strand block: 12.0 ± 1.8
			3-strand block: 8.5 ± 1.5
			Interlaced model 1: 15.0 ± 2.0
			Interlaced model 2: 17.2 ± 1.3

Table S5. 0.1→ 1 ^{13}C-band shifts. The parameters were adjusted so that they matched the spectra of the **Aβ_{40}** oligomers. The angle of dipole derivative was **30°**

Structure	Dipole derivative magnitude (D Å^{-1} amu$^{-1/2}$)	Center wavenumber (cm^{-1})	^{13}C shift (cm^{-1}) for building block ± standard deviation (only for average values)
Sheet, 4 strands, 10 residues/strand	3.659	1659.4	Single strand: 17.9
			2-strand block: 8.9
Sheet, 6 strands, 10 residues/strand	3.370	1660.2	Single strand: 18.8
			2-strand block: 11.1
			3-strand block: 6.5
Sheet, 12 strands, 10 residues/strand	3.127	1661.2	Single strand: 19.8
			2-strand block: 13.1
			3-strand block: 9.2
Sheet, 24 strands, 10 residues/strand	3.027	1661.5	Single strand: 20.0
			2-strand block: 13.7
			3-strand block: 10.1
Barrel, 8 strands, 1QJP	3.445	1665.8	Single strand: 20.5
			2-strand block: 12.4
Barrel, 12 strands, 1UYN	3.475	1665.9	Single strand: 21.5
			2-strand block: 13.1
			3-strand block: 8.0
Barrel, 18 strands, 1A06	3.463	1663.5	Single strand: 21.2
			2-strand block: 14.0
			3-strand block: 9.3
Barrel, 22 strands, 1NQE	3.344	1664.6	Single strand: 21.3
			2-strand block: 14.1
Averages			**Single strand: 20.1 ± 1.3**
			2-strand block: 12.5 ± 1.8
			3-strand block: 8.6 ± 1.4

Table S6. 0.1→ 1 ^{13}C-band shifts. The parameters were adjusted so that they matched the spectra of the **$A\beta_{42}$** oligomers. The angle of dipole derivative was **20°**

Structure	Dipole derivative magnitude (D Å^{-1} amu$^{-1/2}$)	Center wavenumber (cm^{-1})	^{13}C shift (cm^{-1}) for building block
Sheet, 12 strands, 10 residues/strand	2.868	1659.0	Single strand: 17.3
			2-strand block: 11.5
			3-strand block: 8.2
Barrel, 12 strands, 1QD6	3.250	1660.8	Single strand: 18.6
			2-strand block: 11.7
			3-strand block: 7.7