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POSITIONS & AFFILIATIONS

- 2018- *Associate Professor*, Zernike Institute for Advanced Materials, University of Groningen, Groningen, The Netherlands.
- 2018- *Adjunct Associate Professor*, Department of Structural Biology, University of Pittsburgh School of Medicine, Pittsburgh, PA, USA
- 2016-2018 *Associate Professor (tenured)*, Department of Structural Biology, University of Pittsburgh School of Medicine, Pittsburgh, PA, USA
- 2016- *Affiliated Faculty*, Center for Protein Conformational Diseases, University of Pittsburgh, Pittsburgh, PA, USA
- 2016- *Affiliated Faculty*, Brain Institute, University of Pittsburgh, Pittsburgh, PA, USA
- 2008-2018 *Affiliated Faculty*, Physician Scientist Training Program (PSTP), University of Pittsburgh School of Medicine, Pittsburgh PA, USA
- 2008-2018 *Teaching Faculty*, Medical Scientist Training Program (MD/PhD), University of Pittsburgh and Carnegie Mellon University, Pittsburgh, PA, USA
- 2008-2018 *Teaching Faculty*, Molecular Biophysics & Structural Biology Graduate Program, University of Pittsburgh and Carnegie Mellon University, Pittsburgh, PA, USA
- 2008-2016 *Assistant Professor*, Department of Structural Biology, University of Pittsburgh School of Medicine, Pittsburgh, PA, USA
- 2003-2008 *Postdoctoral Associate*, Francis Bitter Magnet Laboratory, Massachusetts Institute of Technology (Principal Investigator: Prof. Robert G. Griffin), Cambridge MA, USA

EDUCATION

- 1997-2002 Ph.D., Biochemistry, University of Arkansas, Fayetteville, AR, USA
Thesis: 'Structure, orientation, dynamics, hydrophobic matching and lipid interactions of designed tryptophan-anchored membrane-spanning peptides.'
Adviser: Prof. Roger E. Koeppe, II
- 1991-1997 B.Sc./M.Sc., Chemistry, Utrecht University, Utrecht, the Netherlands
Thesis: 'The effect of model peptides on lipid phase behavior, the influence of hydrophobic mismatch and the positioning of tryptophans.'
Adviser: Prof. J. Antoinette Killian

HONORS

2013 Eastern Analytical Symposium New Faculty Award in NMR Spectroscopy, Somerset, NJ

PUBLICATIONS

= (co)corresponding author; * = shared first author

Google Scholar URL: <https://scholar.google.com/citations?user=970EC5QAAAAJ>

1. Matlahov, I., & Van der Wel, P.C.A. *Conformational Studies of Pathogenic Expanded Polyglutamine Protein Deposits from Huntington's Disease*. Exp. Biol. Med. 2019; in press. (invited review)
2. Li, M., Mandal, A., Tyurin, V.A., DeLucia, M., Ahn, J., Kagan, V.E., & Van der Wel, P.C.A. # *Surface-binding to cardiolipin nanodomains triggers cytochrome c pro-apoptotic peroxidase activity via localized dynamics*. Structure. 2019; 27(5):806-815.e4.
3. Smith, A.N., Märker, K., Piretra, T., Boatz, J.C., Matlahov, I., Kodali, R., Hediger, S., Van der Wel, P.C.A. #, & De Paëpe, G. # *Structural Fingerprinting of Protein Aggregates by Dynamic Nuclear Polarization-Enhanced Solid-State NMR at Natural Isotopic Abundance*. J. Am. Chem. Soc. 2018; 140(44): 14576-80.
4. Matlahov, I., & Van der Wel, P.C.A. *Hidden motions and motion-induced invisibility: dynamics-based spectral editing in solid-state NMR*. Methods 2018; 148: 123-135. (invited review)
5. Van der Wel, P.C.A. *New applications of solid state NMR in structural biology*. Emerg. Top. Life Sci. 2018; 2(1): 57-67. (invited review)
6. Witkowski, A., Chan, G.K.L., Boatz, J.C., Li, N.J., Inoue, A.P., Wong, J.C., Van der Wel, P.C.A., Cavigiolio, G. *Methionine oxidized apolipoprotein A-I at the crossroads of HDL biogenesis and amyloid formation*. FASEB J. 2018; 32: 3149-3165.
7. Periole, X., Huber, T., Bonito-Oliva, A., Aberg, K.C., Van der Wel, P.C.A., Sakmar, T.P., & Marrink, S.J. *Energetics Underlying Twist Polymorphisms in Amyloid Fibrils*. J. Phys. Chem. B 2018; 122(3): 1081-1091.
8. Van der Wel, P.C.A. *Insights into protein misfolding and aggregation enabled by solid-state NMR spectroscopy*. Solid State Nucl. Magn. Reson. 2017; 88: 1-14. (invited review)
9. Lin, H.K., Boatz, J.C., Krabbendam, I.E., Kodali, R., Hou, Z., Wetzel, R., Dolga, A.M., Poirier, M.A., and Van der Wel, P.C.A. # *Fibril polymorphism affects immobilized non-amyloid flanking domains of huntingtin exon1 rather than its polyglutamine core*. Nature Commun. 2017; 8: 15462.
10. Boatz, J.C., Whitley, M.J., Li, M., Gronenborn, A.M., and Van der Wel, P.C.A. # *Cataract-associated P23T γ D-crystallin retains a native-like fold in amorphous-looking aggregates formed at physiological pH*. Nature Commun. 2017; 8: 15137.
11. Mandal, A., Boatz, J.C., Wheeler, T., and Van der Wel, P.C.A. # *On the use of ultracentrifugal devices for routine sample preparation in biomolecular magic-angle-spinning NMR*. J. Biomol. NMR 2017; 67(3): 165-178.
12. Kar, K., Baker, M.A., Lengyel, G.A., Hoop, C.L., Kodali, R., Byeon, I.-J., Horne, W.S., Van der Wel, P. C. A., and Wetzel, R. # *Backbone engineering within a latent β -hairpin structure to design inhibitors of polyglutamine amyloid formation*. J. Mol. Biol. 2017; 429(2): 308-323.

13. Mandal, A., and Van der Wel, P.C.A.[#] *Magic-angle-spinning proton NMR probes the suppression of water's freezing point and liquid-gel phase transitions in lipid vesicles.* Biophys. J. 2016; 111(9): 1965-73.
14. Merg, A.D., Boatz, J.C., Mandal, A., Zhao, G., Mokashi-Punekar, S., Liu, C., Wang, X., Zhang, P., Van der Wel, P.C.A.[#], and Rosi, N.L.[#] *Peptide-directed assembly of single-helical gold nanoparticle superstructures exhibiting intense chiroptical activity.* J. Am. Chem. Soc. 2016; 138(41): 13655-63. (Cited >40 times)
15. Hoop, C.L., Lin, H.-K., Kar, K., Magyarfalvi, G., Lamley, J. M., Boatz, J. C., Mandal, A., Lewandowski, J.R., Wetzel, R., & Van der Wel, P.C.A.[#] *Huntingtin exon 1 fibrils feature an interdigitated β -hairpin-based polyglutamine core.* Proc. Natl. Acad. Sci. USA 2016; 113(6): 1546-51. (Cited >50 times; Recognized as "Highly Cited Paper" on Web of Science)
16. Mandal, A., Hoop, C.L., DeLucia, M., Kodali, R., Kagan, V., Ahn, J., and Van der Wel, P.C.A.[#] *Structural changes and pro-apoptotic peroxidase activity of cardiolipin-bound mitochondrial cytochrome c.* Biophys. J. 2015; 109(9): 1873-1884. (Cited >30 times)
17. Hoop, C., Lin, H.-K.; Kar, K.; Hou, Z., Poirier, M., Wetzel, R., and Van der Wel, P.C.A.[#] *Polyglutamine amyloid core boundaries and flanking domain dynamics in huntingtin fragment fibrils determined by solid-state NMR.* Biochemistry 2014; 53(42): 6653-6666. (Cited 30 times)
18. Kar, K., Arduini, I., Drombosky, K. W., Van der Wel, P. C. A.[#], and Wetzel, R. [#] *D-polyglutamine amyloid recruits L-polyglutamine monomers and kills cells.* J. Mol. Biol. 2014; 426(4): 816–29. (Cited >15 times)
19. Lin, H.-K., and Van der Wel P.C.A.[#] *How amyloid precursor protein protects itself from cleavage.* Structure 2014; 22: 361–362. (invited)
20. Van der Wel, P.C.A. *Lipid Dynamics and Protein-Lipid Interactions in Integral Membrane Proteins: Insights from Solid-State NMR.* eMagRes (Encycl. Magn. Reson.) 2014; 3: 111–8 (invited review)
21. Li, J., and Van der Wel, P. C. A.[#] *Spinning-rate encoded chemical shift correlations from rotational resonance solid-state NMR experiments.* J. Magn. Reson. 2013, 230, 117-124.
22. Kar, K., Hoop, C. L., Drombosky, K. W., Baker, M. A., Kodali, R., Arduini, I., Van der Wel, P. C. A., Horne, W. S., and Wetzel, R. *β -hairpin-mediated nucleation of polyglutamine amyloid formation.* J. Mol. Biol. 2013, 425(7): 1-45. (Cited >50 times)
23. Mishra, R., Hoop, C.L., Kodali, R., Sahoo, B., Van der Wel, P.C.A., and Wetzel, R. *Serine phosphorylation suppresses huntingtin amyloid accumulation by altering protein aggregation properties.* J. Mol. Biol. 2012; 424(1–2): 1-14 (Cited >30 times)
24. Van der Wel, P.C.A. *Domain swapping and amyloid fibril conformation.* Prion. 2012; 6(3): 211-216 (Cited 18 times) (invited perspective)
25. Eddy, M.T., Ong, T.-C., Clark, L., Teijido, O., Van der Wel, P.C.A., Garces, R., Wagner, G., Rostovtseva, T.K., and Griffin, R.G. *Lipid dynamics and protein-lipid interactions in 2D crystals formed with the β -barrel integral membrane protein VDAC1.* J. Am. Chem. Soc. 2012; 134(14): 6375-6387 (Cited >40 times)
26. Hoop, C. L., Sivanandam, V. N., Kodali, R., Srnc, M. N., and Van der Wel, P. C. A.[#] *Structural characterization of the caveolin scaffolding domain in association with cholesterol-rich membranes,* Biochemistry 2012; 51: 90–99 (Cited >30 times)

27. Li, J., Hoop, C.L., Kodali, R., Sivanandam, V.N., and Van der Wel, P.C.A. [#] *Amyloid-like fibrils from a domain-swapping protein feature a parallel, in-register conformation without native-like interactions.* J. Biol. Chem. 2011; 286(33): 28988-95 (Cited 20 times)
28. Lewandowski, J.R.* , Van der Wel, P.C.A.* , Rigney, M., Grigorieff, N., and Griffin, R.G. *Structural complexity of a composite amyloid fibril.* J. Am. Chem. Soc. 2011; 133(37): 14686-14698 (Cited >60 times)
29. Sivanandam, V.N, Jayaraman, M., Hoop, C.L., Kodali, R., Wetzel, R., and Van der Wel, P.C.A. [#] *The aggregation-enhancing huntingtin N-terminus is helical in amyloid fibrils.* J. Am. Chem. Soc. 2011; 133(12): 4558–4566 (Cited 90 times)
30. Van der Wel, P.C.A., Lewandowski, J.R., and Griffin, R.G. *Structural characterization of GNNQQNY amyloid fibrils by magic angle spinning NMR.* Biochemistry 2010; 49(44): 9457–9469 (Cited >40 times)
31. Debelouchina, G.T., Bayro, M. J., Van der Wel, P. C. A., Caporini, M. A., Barnes, A. B., Rosay, M., Maas, W. E., and Griffin, R. G. *Dynamic Nuclear Polarization-Enhanced Solid-State NMR Spectroscopy of GNNQQNY Nanocrystals and Amyloid Fibrils.* Phys. Chem. Chem. Phys. 2010; 12(22): 5911-5919 (cited >70 times)
32. De Gortari, I, Portella, G., Salvatella, X., Bajaj, V.S.; Van der Wel, P.C.A., Yates, J., Segall, M., Pickard, C., Payne, M., and Vendruscolo, M. *Time averaging of NMR chemical shifts in the MLF peptide in the solid state* J. Am. Chem. Soc. 2010; 132 (17): 5993–6000 (Cited >50 times)
33. Barnes, A.B., Andreas, L., Huber, M., Ramachandran, R., Van der Wel, P.C.A., Veshtort, M., Griffin, R.G., and Mehta, M.A. *High-resolution solid-state NMR structure of Alanyl-Prolyl-Glycine.* J. Mag. Reson. 2009; 200(1), 95-100 (Cited 10 times)
34. Van der Wel, P.C.A., Eddy, M.T., Ramachandran, R., and Griffin, R.G. *Targeted ¹³C–¹³C distance measurements in a microcrystalline protein via J-decoupled rotational resonance width measurements.* ChemPhysChem 2009; 10: 1656-63 (Cited 10 times)
35. Bajaj, V.S., Van der Wel, P.C.A., and Griffin, R.G. *Observation of a low-temperature, dynamically driven structural transition in a polypeptide by solid state NMR spectroscopy.* J. Am. Chem. Soc. 2009; 131(1): 118-128 (Cited >50 times)
36. Barnes, A. B., Mak-Jurkauskas, M. L., Matsuki, Y., Bajaj, V. S., Van der Wel, P. C. A., DeRocher, R.; Bryant, J., Sirigiri, J. R., Temkin, R. J., Lugtenburg, J., Herzfeld, J., and Griffin, R. G. *Cryogenic sample exchange NMR probe for magic angle spinning dynamic nuclear polarization.* J. Mag. Reson. 2009; 198(2): 261-270 (Cited >70 times)
37. Barnes, A.B., De Paëpe, G., Van der Wel, P.C.A., Hu, K.-N., Joo, C.-G., Bajaj, V.S., Mak-Jurkauskas, M.L., Herzfeld, J., and Griffin, R.G. *High field dynamic nuclear polarization for solid and solution biological NMR.* Appl. Magn. Reson. 2008; 34(3-4): 237-263 (Cited 200 times)
38. Maly, T., Debelouchina, G.T., Bajaj, V.S., Hu, K.-N., Joo, C.-G., Mak-Jurkauskas, M.L., Sirigiri, J.R., Van der Wel, P.C.A., Herzfeld, J. Temkin, R.J., and Griffin, R.G. *Dynamic nuclear polarization at high magnetic fields.* J. Chem. Phys. 2008; 128(5): 052211 (Cited >420 times) (Recognized as “Highly Cited Paper” on Web of Science)
39. Daily, A.E., Greathouse, D.V., Van der Wel, P.C.A., and Koeppe, R.E., II *Helical distortion in tryptophan and lysine anchored membrane-spanning α -helices as a function of hydrophobic mismatch: a solid-state deuterium NMR investigation using the GALA method.* Biophys. J. 2007; 94(2): 480-491 (Cited >30 times)

40. Van der Wel, P.C.A., Lewandowski, J.R., and Griffin, R.G. *Solid state NMR study of amyloid nanocrystals and fibrils formed by the peptide GNNQQNY from yeast prion protein Sup35p*. J. Am. Chem. Soc. 2007; 129(16): 5117-5130 (Cited >120 times)
41. Van der Wel, P.C.A.[#], Reed, N.D., Greathouse, D.V., and Koeppe, R.E., II *Orientation and motion of tryptophan interfacial anchors in membrane-spanning peptides*. Biochemistry 2007; 46(25): 7514-24 (Cited >35 times)
42. Van der Wel, P.C.A., Hu, K.-N., Lewandowski, J.R., and Griffin, R.G. *Dynamic nuclear polarization of amyloidogenic peptide nanocrystals: GNNQQNY, a core segment of the yeast prion protein Sup35p*. J. Am. Chem. Soc. 2006; 128(33):10840-10846 (Recommended on Faculty of 1000 website; cited >170 times)
43. Ramachandran, R., Lewandowski, J.R., Van der Wel, P.C.A., and Griffin, R.G. *Multipole-multimode Floquet theory of rotational resonance width experiments: ^{13}C - ^{13}C distance measurements in uniformly labeled solids*. J. Chem. Phys. 2006; 124(21): 214107 (Cited >20 times)
44. Pulay, P., Scherer, E.M., Van der Wel, P.C.A., and Koeppe, R.E., II *Importance of tensor asymmetry for the analysis of ^2H -NMR spectra from deuterated aromatic rings*. J. Am. Chem. Soc. 2005; 127(49):17488-93. (Cited >10 times)
45. Sceats, E.L., Figueroa, J.S., Cummins, C.C., Loening, N.M., van der Wel, P.C.A., and Griffin, R.G. *Complexes obtained by electrophilic attack on a dinitrogen-derived terminal molybdenum nitride: electronic structure analysis by solid state CP/MAS ^{15}N NMR in combination with DFT calculations*. Polyhedron 2004; 23: 2751-2768 (Cited >50 times)
46. Strandberg, E., Ozdirekcan, S., Rijkers, D.T., Van der Wel, P.C.A., Koeppe, R.E., II, Liskamp, R.M., and Killian, J.A. *Tilt angles of transmembrane model peptides in oriented and non-oriented lipid bilayers as determined by ^2H solid-state NMR*. Biophys. J. 2004; 86: 3709-3721 (Cited >140 times)
47. Koeppe, R.E., II, Sun, H., Van der Wel, P.C.A., Scherer, E.M.; Pulay, P., and Greathouse, D.V. *Combined experimental/theoretical refinement of indole ring geometry using deuterium magnetic resonance and ab initio calculations*. J. Am. Chem. Soc. 2003; 125: 12268-12276 (Cited >20 times)
48. Weiss, T.M., Van der Wel, P.C.A., Killian, J.A., Koeppe, R.E., II, and Huang, H.W. *Hydrophobic mismatch between helices and lipid bilayers*. Biophys. J. 2003; 84: 379-385 (Cited >110 times)
49. Van der Wel, P.C.A.[#], Strandberg, E., Killian, J.A., and Koeppe, R.E., II. *Geometry and intrinsic tilt of a tryptophan anchored membrane spanning peptide by ^2H NMR*. Biophys. J. 2002; 83(3): 1479-1488 (Cited >130 times)
50. Strandberg, E., Morein, S., Rijkers, D.T.S., Liskamp, R.M.J., Van der Wel, P.C.A., and Killian, J.A. *Lipid dependence of membrane anchoring properties and snorkeling behaviour of aromatic and charged residues in transmembrane peptides*. Biochemistry 2002; 41: 7190-7198 (Cited >80 times)
51. Greathouse, D.V., Goforth, R.L., Crawford, T., Van der Wel, P.C.A., and Killian, J.A. *Optimized aminolysis conditions for cleavage of N-protected hydrophobic peptides from solid-phase resins*. J. Peptide Res. 2001; 57: 519-527 (Cited 18 times)
52. Van der Wel, P.C.A., Pott, T., Morein, S., Greathouse, D.V., Koeppe, R.E., II, and Killian, J.A. *Tryptophan-anchored transmembrane peptides promote formation of nonlamellar phases in phosphatidylethanolamine model membranes in a mismatch-dependent manner*. Biochemistry. 2000; 39: 3124-3133 (Cited >40 times)

53. Killian, J.A., Morein, S., Van der Wel, P.C.A., de Planque, M.R.R., Greathouse, D.V. and Koeppe, R.E., II. *Peptide influences on lipids*. Novartis Found. Symp. 1999; 225: 170-187 (Cited 2 times)
54. Killian, J.A., de Planque, M.R.R., Van der Wel, P.C.A., Salemink, I., de Kruijff, B., Greathouse, D.V., and Koeppe, R.E., II. *Modulation of membrane structure and function by hydrophobic mismatch between proteins and lipids*. Pure & Appl. Chem. 1998; 70: 75-82 (Cited >20 times)

RESEARCH PRESENTATIONS

Oral seminars at international conferences

FASEB Summer Research Conference (SRC) on Protein Aggregation in Health and Disease, June 9-14 2019, Snowmass, CO, USA: Van der Wel, P.C.A. "TBD" (invited; forthcoming)

3rd Ulm meeting on the Biophysics of Amyloid Formation, Feb. 19-21st 2019, Ulm, Germany: Van der Wel, P.C.A. "Solid-state NMR of misbehaving polyglutamine proteins and chaperones that control them"

29th Faltertage on "Protein Folding, Dynamics and Stability", Oct. 26-28 2018, Halle, Germany: Van der Wel, P.C.A. "Solid-state NMR studies of protein misfolding and self-assembly in Huntington's disease." (invited keynote)

EUROMAR 2018, July 1-5th, 2018, Nantes, France: Van der Wel, P.C.A. 'Magic-angle-spinning NMR of pivotal protein-lipid interactions implicated in programmed cell death.' (invited)

EMBO Workshop Challenges for magnetic resonance in life sciences, May 27-31th, 2018, Grosseto, Italy: Van der Wel, P.C.A. 'Balancing order and disorder in solid-state NMR studies of mobile protein-lipid complexes.'

The 10th Alpine Conference on Solid-State NMR, Sept. 10-14th, 2017, Chamonix Mont-Blanc, France: Van der Wel, P.C.A. 'Revealing order and disorder in polymorphic disease-associated protein aggregates.'

2017 ISMAR (International Society for Magnetic Resonance) meeting, July 23-28, 2017, Québec City, Canada: 'Amyloidogenic self-assembly in peptide-based materials and biology: ssNMR methods and applications.' (invited)

FASEB Summer Research Conference (SRC) on Protein Aggregation in Health and Disease, Jun 11-16th, 2017, Steam Boat Springs, CO, USA: Van der Wel, P.C.A. 'Structural differences of polymorphic and cytotoxic huntingtin exon1 aggregates.' (invited)

5th Dutch Huntington Symposium "From cell to man", November 11th, 2016, Maastricht, The Netherlands: 'The misfolding and aggregation mechanism of mutant huntingtin exon 1 and other polyglutamine proteins.'

58th Rocky Mountain Conference on Magnetic Resonance, July 17-21th, 2016, Breckenridge, CO: 'Solid-state NMR studies of peroxidase-active membrane-bound cytochrome c involved in mitochondrial apoptosis.' (invited)

57th Experimental NMR Conference (ENC), April 10-15th, 2016, Pittsburgh, PA: 'New structural, motional, and mechanistic insights into disease-relevant protein aggregates that cause Huntington's Disease.' (plenary seminar)

International conference on Biophysics of Proteins at Surfaces: Assembly, Activation, Signaling, Oct. 13-15th, 2015, Madrid, Spain: Van der Wel, P.C.A. 'Peripheral binding to cardiolipin-containing membranes causes cytochrome c to gain a peroxidase activity required for mitochondrial apoptosis.'

The 9th Alpine Conference on Solid-State NMR, Sept. 13-17th, 2015, Chamonix Mont-Blanc, France: Van der Wel, P.C.A. 'Challenging structural studies of a simple sequence: polyglutamine studies by solid-state NMR.'

FASEB Science Research Conference (SRC) on Molecular Mechanisms and Physiological Consequences of Protein Aggregation, Jun 21-26th, 2015, West Palm Beach, FL: Van der Wel, P.C.A. 'Structure and dynamics of huntingtin exon 1 fibrils and other polyglutamine aggregates.'

VIth Meeting on the "Molecular Mechanisms of Neurodegeneration, May 28-30th, 2015, Milan, Italy: Mandal, A., Hoop, C.L., DeLucia, M., Kodali, R., Kagan, V.E., Ahn, J., and Van der Wel, P.C.A. 'Mitochondrial lipid peroxidation and membrane disruption in apoptosis and neuronal degradation.'

XXVIth International Conference on Magnetic Resonance in Biological Systems (ICMRBS), August 24-29, 2014, Dallas, TX: 'Magic-angle-spinning NMR studies of the structural and motional features of polyglutamine-based amyloid-like aggregates.' (invited)

55th Experimental NMR Conference (ENC), March 23-28th, 2014, Boston, MA: 'Polymorphism and intrinsic structural heterogeneity in amyloid-like fibrils of polyglutamine and beyond.' (invited)

Eastern Analytical Symposium 2013, Nov., 2013, Somerset, NJ: 'Insights into the structure and formation of polyglutamine amyloid from solid-state NMR spectroscopy.' (EAS New Faculty in NMR Award Lecture; invited).

International Symposium "Atomic View of Biomolecular Function", July 11-13th, 2013, University of Michigan, Ann Arbor, MI: 'Studies of polyglutamine amyloid structure and formation.' (invited)

Eastern Analytical Symposium (EAS), Nov. 2012, Somerset, NJ: 'Insights into amyloid formation mechanisms from studying fibrils by solid-state NMR.' (invited)

Eastern Analytical Symposium (EAS), Nov. 2011, Somerset, NJ: 'Insights into the role of the N-terminus in huntingtin amyloid formation from solid-state NMR.' (invited)

International Workshop on Biological and Biophysical Basis of Membrane Dynamics and Organization (BBBMDO), Nov. 5-6th 2010, Pittsburgh, PA: 'Investigations of protein-lipid interactions via solid-state NMR.' (invited)

Hereditary Disease Foundation's Symposium HD2010: "The Milton Wexler Celebration of Life", Aug. 4-7th, 2010, Cambridge, MA: Van der Wel, P.C.A., Jayaraman, M., Natarajan, S., Hoop, C.L., Kodali, R., Wetzel, R. 'Solid-state NMR-based structural characterization of a huntingtin N-terminal fragment in its fibrillar state.'

52nd Annual Rocky Mountain Conference on Analytical Chemistry, Aug. 1-5th, 2010, Snowmass, CO: 'Magic angle spinning studies of fibrillized huntingtin fragments.'

53rd Biophysical Society Annual Meeting, 2009, Boston, MA: Van der Wel, P.C.A., Lewandowski, J.R., and Griffin, R.G. 'Solid state NMR studies of structural and motional complexity in amyloid-like fibrils of the peptide GNNQQNY.'

59th Pittsburgh Conference on Analytical Chemistry and Applied Spectroscopy (PittCon 2008), New Orleans, LA: 'Structure determination of amyloid peptides and proteins.'

51st Biophysical Society Annual Meeting, Mar. 2007, Baltimore, MD: Van der Wel, P.C.A., Lewandowski, J.R., and Griffin, R.G. 'Features of crystal and fibril formation by GNNQQNY, peptide fragment of yeast prion protein Sup35p.'

Other Seminars

Berendsen Center Symposium, Nov. 21st, 2018, Groningen, The Netherlands: 'Probing amyloidogenic self-assembly by solid-state NMR: discovering design principles for functional nano-materials.' (invited lecture)

7th Dutch Huntington Symposium, Nov. 9th, 2018, Amsterdam, The Netherlands: 'Molecular structure and biological activity of protein aggregates associated with Huntington disease.'

University of Groningen Medical Center, Molecular Medicine Seminar Series, Dec 13th 2018: 'Structural investigations of misbehaving polyglutamine proteins and chaperones that control them.' (forthcoming)

53rd NMR-DG Meeting, Oct 5th, 2018, Radboud University, Nijmegen, The Netherlands: 'Solid-State NMR studies of oligomeric chaperones and the amyloidogenic nucleation process that they target'

NMR Summerschool of the COAST MSc+ program 2018, Aug. 23rd 2018, Radboud University, Nijmegen, The Netherlands: 'Biological solid-state NMR' (invited lecture)

2nd Gateway Regional NMR Conference, Nov. 4th 2017, Columbus, OH: 'Solid-state NMR studies of disease-related protein misfolding and aggregation.' (invited)

University of Groningen, Zernike Institute for Advanced Materials, Zernike seminar, Apr. 20th, 2017, Groningen, the Netherlands 'NMR studies of amyloidogenic self-assembly: biological design principles for functional nanomaterials.'

Baylor University, Department of Chemistry, Departmental Seminar, Feb. 3rd, 2017, Waco, TX: 'Cytochrome c as a lipid peroxidase in mitochondrial apoptosis: New insights from solid-state NMR spectroscopy.' (invited)

University of Texas Southwestern, Center for Alzheimer's and Neurodegenerative Diseases, Feb. 2nd, 2017, Waco, TX: 'Misfolding and Aggregation Mechanisms of Expanded Polyglutamine in Huntingtin's Exon 1 and Beyond.'

University of Pittsburgh, Pittsburgh Institute for Neurodegenerative Diseases (PIND) seminar series, Nov. 30th, 2016, Pittsburgh, PA: 'Structural studies of the protein misfolding and deposition mechanisms associated with Huntington's disease' (invited)

University of California, Irvine, Department of Chemistry, Physical Chemistry Seminar, Nov. 15th, 2016, Irvine, CA: 'NMR studies of the misfolding mechanism of mutant huntingtin exon1 and other polyglutamine proteins.' (invited)

University of California, Riverside, Department of Chemistry, Physical Chemistry Seminar, Nov. 14th, 2016, Riverside, CA: 'NMR studies of the misfolding mechanism of mutant huntingtin exon1 and other polyglutamine proteins.' (invited)

Washington & Jefferson College, Department of Chemistry, Oct. 11th 2016, Washington, PA: 'Structural biology of protein aggregation in Huntington's disease and other protein misfolding diseases.' (invited)

Children's Hospital Oakland Research Institute (CHORI), Departmental Seminar Series, March 17th, 2016, Oakland, CA: 'Toxic mechanisms of neurodegeneration in Huntington's Disease and beyond: protein misfolding, aggregation, and pro-apoptotic mitochondrial lipid peroxidation.' (invited)

Case Western Reserve University School of Medicine, Department of Physiology and Biophysics, Nov. 30th, 2015, Cleveland, OH: 'Membrane-mediated activation of the proapoptotic peroxidase function of mitochondrial cytochrome c.' (invited)

University of Binghamton, SUNY, Department of Chemistry, Chemistry Colloquium, Oct. 30th, 2015, Binghamton, NY: 'Mitochondrial cytochrome c's proapoptotic peroxidase function induced by peripheral binding to cardiolipin-containing membranes.' (invited)

University of Minnesota, Department of Biochemistry, Molecular Biology and Biophysics, Departmental Seminar, Oct. 15th 2014, Minneapolis, MN: 'Solid-state NMR studies of protein misfolding and self-assembly in Huntington's Disease.' (invited)

Pennsylvania State University, Chemistry Department, Departmental Seminar, Oct. 14th 2014, University Park, PA: 'Solid-state NMR studies of amyloid formation and mitochondrial protein-lipid interactions implicated in neurodegenerative disease.' (invited)

Michigan State University, Chemistry Department, Departmental Seminar, Sept. 26th 2014, East Lansing, MI, USA: 'Solid-state NMR studies of amyloid formation by polyglutamine and huntingtin fragments.' (invited)

Washington University, St. Louis, Chemistry Department, Departmental Seminar, May. 1st 2014, St Louis, MO: 'Solid-state NMR characterization of the amyloid core and flanking regions of polyglutamine-containing aggregates.' (invited)

West-Virginia University, Department of Chemistry, Departmental Seminar, Sep. 2013, Morgantown, WV: 'Insights into amyloid formation and structure from magic-angle-spinning solid-state NMR.' (invited)

University of Delaware, Chemistry Department, Departmental Seminar, May 13th 2013, Newark, DE: 'Insights into amyloid formation mechanisms from studying fibrils by solid-state NMR.' (invited)

University of California, Berkeley, Department of Chemistry and Alexander Pines Research Group seminar, Mar. 15th 2013, Berkeley, CA: 'Insights into amyloid formation mechanisms from studying fibrils by solid-state NMR.' (invited)

University of Pittsburgh Science 2012 Symposium, Oct. 4th 2012, Pittsburgh, PA: ‘Structural studies of biological nano-assemblies.’ (invited)

American Chemical Society (ACS) Central Regional Meeting, Jun. 2012, Dearborn, MI: ‘Structural studies of amyloid fibril formation by solid-state NMR.’

Ursinus College, Chemistry Department, Departmental Seminar, Oct. 24th 2011, Collegeville, PA: ‘Structural insights into amyloid fibril formation from solid-state NMR.’

Carnegie Mellon University, Department of Physics, Departmental Seminar, Feb. 10th 2011, Pittsburgh, PA: ‘Insights into the role of the N-terminus in huntingtin amyloid formation from solid-state NMR.’ (invited)

University of Arkansas, Department of Chemistry & Biochemistry, Departmental Seminar, Oct. 11th 2010, Fayetteville, AR: ‘Magic-angle-spinning solid-state NMR studies into the structure and formation of amyloid fibril aggregates.’ (invited)

University of Pittsburgh Science 2010 Symposium, Oct. 7th 2010, Pittsburgh, PA: ‘Studying Troublesome Solids: How magic (angles) and high RPMs allow a molecular view of aggregated proteins.’ (invited)

TEACHING

Courses

- Instructor in Biophysics course (University of Groningen; 2019-)
- Member of the curriculum committee for the Life Science & Technology Bachelor’s program (University of Groningen; 2018-)
- Instructor in the Introduction to Biomedical Sciences (iBMS) course (University of Groningen; 2018-)
- Co-director of the Molecular Biophysics II graduate course of the Molecular Biophysics & Structural Biology graduate program (University of Pittsburgh & Carnegie Mellon University) (2013-2018)
- Co-director of the Advanced NMR Spectroscopy graduate course of the Molecular Biophysics & Structural Biology graduate program (University of Pittsburgh & Carnegie Mellon University) (2015)
- Teaching faculty for Molecular Biophysics & Structural Biology graduate program at the University of Pittsburgh School of Medicine (University of Pittsburgh & Carnegie Mellon University) (2008-2018)
- Instructor in the Molecular Biophysics I: Structure graduate course of the Molecular Biophysics & Structural Biology graduate program (University of Pittsburgh & Carnegie Mellon University) (2008-2017)
- Instructor in the Molecular Biophysics II graduate course of the Molecular Biophysics & Structural Biology graduate program (University of Pittsburgh & Carnegie Mellon University) (2010-2018)
- Instructor in the Advanced NMR Spectroscopy graduate course of the Molecular Biophysics & Structural Biology graduate program (University of Pittsburgh & Carnegie Mellon University) (2010, 2013)
- Small group supervisor/instructor in the Professional Development II graduate course of the Medical Scientist Training Program (MSTP) MD/PhD program of the University of Pittsburgh School of Medicine (2013-2018)

- Preceptor in the Foundations Colloquium graduate course of the Medical Scientist Training Program (MD/PhD) program of the University of Pittsburgh School of Medicine (2014)
- Invited guest lecturer in the Advanced Topics in Nuclear Magnetic Resonance course (CHM285) of Carlow University's Department of Chemistry (Pittsburgh, PA; Fall 2015)

Supervision

- Current PhD supervisor of Mustapha El Hariri El Nokab at the Zernike Institute for Advanced Materials of the University of Groningen.
- Past PhD supervisor for Dr. Jennifer Boatz of the Molecular Biophysics and Structural Biology graduate program (University of Pittsburgh and Carnegie Mellon University).
- Past PhD supervisor for Dr Abhishek Mandal, who graduated with PhD in Dec 2016 from the Molecular Biophysics and Structural Biology graduate program of the University of Pittsburgh and Carnegie Mellon University. (Currently at Highmark Corporation, Pittsburgh, PA).
- Past PhD supervisor for Dr Cody Hoop, who graduated with PhD in Nov 2014 from the Molecular Biophysics and Structural Biology graduate program of the University of Pittsburgh and Carnegie Mellon University. (Currently a research associate at Rutgers University).
- Supervisor of postdoctoral research associates:
 - Dr. V.N. Sivanandam (2008-2010)
 - Dr. Jun Li (2009-2011)
 - Dr. Hsiang-Kai (Kyle) Lin (2013-2015)
 - Dr. Irina Matlahov (2016-)
 - Dr. Mingyue Li (2016-)
- First-year advisor for Pitt MBSB graduate students (2009-2013).
- Rotation project supervisor for Pitt MBSB student rotation projects (2009-2016).
- Lab mentor for undergraduate researchers Sara Lewandowski (2010), George Alvarez (2012), Marissa Di (2015), Lexi Wivell (2016), Ricardo Capeles (2017) in the Summer Undergraduate Research Program (SURP) of the University of Pittsburgh School of Medicine.
- Research advisor for undergraduate student James Nassur (Spring 2016), and Talia Piretra (Summer 2017)
- Undergraduate research mentor in the University of Pittsburgh's First Experience in Research program, for Audrey Valentine (Spring 2016) and Talia Piretra (Spring 2017)
- Career Advisor for student Ananya Mukundan in the University of Pittsburgh School of Medicine MD/PhD Medical Scientist Training Program (MSTP) (2016-2018).

PhD committees

- PhD committee member for PhD students at the University of Groningen: Wei Chen (PhD, 2019).
- PhD committee member for PhD students within the University of Pittsburgh/CMU MBSB PhD graduate program: Rakesh Mishra (PhD, graduated 2012), Saketh Chemuru (PhD, graduated 2014), Naima Sharaf (PhD, graduated in 2016), and Rebecca Eells (PhD, graduated in 2018).
- External PhD committee member for PhD students at the University of Pittsburgh: Hyo Soon Cho (PhD, graduated 2011; Chemistry Dept), Keith Callenberg (PhD, graduated 2013; Pitt/CMU Computational Biology Graduate Program), Bocheng Yin (Chemistry Dept), Kulakulasooriyagei I Silva (PhD, graduated 2014; Chemistry Dept), Dariush Mohammadyani (PhD, graduated 2015, Bioengineering), Andrea Merg (Chemistry Dept.), and Ryan Jakubek (Sept 2016-present; Chemistry Dept.).
- External PhD committee member for PhD student Changmiao Guo at the University of Delaware Chemistry Department (2013-2017).
- External Thesis Examiner for the Department of Chemical Sciences, Indian Institute of Science Education and Research (IISER) Mohali, Chandigarh (India).

- Chair for comprehensive examination committee for graduate student David Punihaole (2011) in the MBSB PhD graduate program (Pitt/CMU).

Other

- Training and mentoring of graduate and undergraduate students at the Massachusetts Institute of Technology Francis Bitter Magnet Lab (as postdoctoral associate).
- As a graduate student: mentor of undergraduate honors students; teaching assistant in several chemistry and biochemistry lab courses to undergraduate students; teaching assistant for biochemistry and physical chemistry lectures; instructor of selected lectures in an undergraduate Biochemistry course.

SERVICE

Editing

- Academic Editor for the journal PLOS ONE (2013-present).

Reviewing

- Invited grant reviewer for the National Institutes of Health (NIH) Biophysics of Neural Systems Study Section (BPNS) study section
- Invited grant reviewer for the National Science Foundation (NSF)
- Invited grant reviewer for the National Institutes of Health (NIH) SBIR/STTR review panel
- Invited grant reviewer for the National Institutes of Health (NIH) special interest panel (2018)
- Invited external reviewer for other international funding agencies:
 - German Research Foundation (Deutsche Forschungsgemeinschaft, DFG), Life Sciences division
 - Medical Research Council (UK), Molecular and Cellular Medicine Board
 - Danish Council for Independent Research, Section Natural Sciences (Denmark)
 - Human Frontier Science Program (HFSP; France)
 - Agence Nationale de la Recherche (ANR; France)
 - NWO (Netherlands Organization for Scientific Research), Netherlands.
 - Wellcome Trust, Grants Programme (UK)
- Invited grant reviewer for various internal funding programs of the University of Pittsburgh, including the Competitive Medical Research Fund (CMRF), and the Pittsburgh Alzheimer Disease Research Center (ADRC) pilot program.
- Reviewer for journals: Accounts of Chemical Research, ACS Chemical Biology, ACS Chemical Neuroscience, Acta Biomaterialia, Archives of Biochemistry and Biophysics; Biochemistry, Biochimica et Biophysica Acta (BBA), Biomacromolecules, the Biophysical Journal, ChemComm, Chem. Phys. Lipids, Diabetes, the FEBS Journal, Journal of the American Chemical Society (JACS), Journal of Biological Chemistry (JBC), Journal of Biomolecular NMR, Journal of Magnetic Resonance, Journal of Membrane Biology, Journal of Molecular Biology, Journal of Molecular Graphics and Modelling, Journal of Physical Chemistry, Journal of Physical Chemistry Letters, Journal of the Royal Society Interface, Journal of Structural Biology, Langmuir, Magnetic Resonance in Chemistry, Nature Communications, Organic & Biomolecular Chemistry, Physical Chemistry Chemical Physics (PCCP), PLOS Biology, Proceedings of the National Academy of Science (PNAS), Protein Expression and Purification, Protein Science, Scientific Reports, Seminars in Cell and Developmental Biology, and Solid State Nuclear Magnetic Resonance.

Conferences

- Chair of magnetic resonance oral seminar sessions at the 2013 Eastern Analytical Symposium (EAS); Nov 2013; Somerset, NJ

- Chair of magnetic resonance oral seminar sessions at the 2014 Eastern Analytical Symposium (EAS); Nov. 2014; Somerset, NJ
- Organizer and chair of seminar session at the Central Regional American Chemical Society (ACS) meeting (CERM) in Pittsburgh, on the topic of structural biology (Oct 2014)
- Chair of a solid-state NMR oral seminar session at the 2014 ICMRBS international conference in Dallas, TX (Aug 2014)
- Web coordinator for the first US/Canada Biological Solid State NMR Winter School in Stowe, VT (2008)

Other

- Lecturer in the *Imagination at Work* program of the Centrum JongerenCommunicatie Chemie (C³); 2019-
- Contributing Faculty Member for F1000Prime (Faculty of 1000), in the section Cellular Death & Stress Responses (2016 – present).
- Lecturer in the Biennial NMR Summer School of the COAST MSc+ program, hosted at Radboud University, Nijmegen (2018).
- Chair and member of recruitment committee of Molecular Biophysics & Structural Biology graduate program (University of Pittsburgh/Carnegie Mellon University) (2010-2016).
- University of Pittsburgh and Carnegie Mellon University Molecular Biophysics & Structural Biology graduate program website coordinator (2010-2018).
- Liaison for the Molecular Biophysics & Structural Biology graduate program and the University of Pittsburgh School of Medicine's MD/PhD program (MSTP; Medical Scientist Training Program) (2015-2018).
- Member of the Faraday Lecture Committee of the Spectroscopy Society of Pittsburgh, which organizes an annual scientific lecture and demo directed at local middle- and high-school students (2012-2018).
- Member of the Educational Networking Committee of the Spectroscopy Society of Pittsburgh (SSP), charged with informing local schools of funding opportunities offered by the SSP (2013-2016).
- Member of the Elementary School Science Olympiad Program Committee (ESSOP) of the Spectroscopy Society of Pittsburgh (SSP) (2016-2018).
- Host of annual departmental tours for summer course directed at female high school students (organized by Carlow University, Pittsburgh, PA) (2014-2018).
- Co-host of departmental demos/visits for local undergraduate students from Washington & Jefferson College, Indiana University of Pennsylvania and the Community College of Allegheny County (2008, 2009, 2010).
- Co-host of facility tour in continuing education for the Spectroscopy Society of Pittsburgh, in Oct 2013, on the topic of Structural Biology.
- Lab mentor for undergraduate research projects for students from Washington & Jefferson College (Washington, PA; Jan. 2010).
- Volunteer activities for local and regional American Chemical Society (ACS) activities.

PROFESSIONAL MEMBERSHIPS

- Biophysical Society (IDP and Membrane Biophysics Subgroups)
- American Chemical Society (ACS)
- Koninklijke Nederlandse Chemische Vereniging (KNCV; Royal Dutch Chemical Society)
- Spectroscopy Society of Pittsburgh (SSP)
- International Society for Magnetic Resonance (ISMAR)
- American Society for Biochemistry and Molecular Biology (ASBMB)

- Protein Society

RESEARCH FUNDING

Current/past grant support

Campagne team Huntington (CTH)

1/4/2019 – 31/3/2023

(Principal Investigator)

€250K

Measuring and modulating the structure of toxic misfolded huntingtin exon 1 assemblies.

The major goal of this grant is to determine the atomic structure of the amyloid core of misfolded mutant huntingtin exon 1, using solid-state NMR and complementary techniques. In addition, we will determine how inhibitory small molecules affect the structure and toxicity of the misfolded protein and analyze the role of seeding in mutant huntingtin exon 1 fibril formation.

NIH/NIGMS R01 GM121583-01

18/9/2017 – 17/9/2022

(Co-Investigator; PI: R. Ramachandran, Case Western Univ.)

\$40K/yr (direct)

Molecular Mechanisms of Drp1-catalyzed mitochondrial membrane fission.

The major goal of this proposal is to determine the molecular mechanism by which the Dynamin Related Protein 1 (Drp1) catalyzes mitochondrial membrane fission. The latter process is a critical component of the mitochondrial dynamics that regulate the morphology, size and quality control of mitochondria. Our contribution to this collaborative project is to use advanced solid-state NMR to probe the interaction of the Drp1 membrane-binding domain with membranes and in particular the mitochondrial lipid cardiolipin.

NIH/NIGMS R01 GM113908-01

1/9/2016 – 31/8/2020

(Principal Investigator*)

\$235K/yr (direct)

The molecular basis of cardiolipin-protein interactions implicated in intrinsic apoptosis.

The major goal of this grant is to elucidate pivotal early stages of mitochondrial apoptosis. Mitochondrial dysfunction and intrinsic apoptosis play key roles in the neuronal degradation in Huntington's Disease and other disorders. Lipid peroxidation has been identified as a critical step, that may also present a viable target for the design of mitochondrially targeted drugs. In this project we employ solid-state NMR and an array of complementary structural and functional experiments to probe the pivotal protein-lipid interactions that facilitate the pro-apoptotic peroxidation of cardiolipin lipid species.

** Funded and operated as PI in 2016-2018; transferred PI status to collaborator Valerian Kagan upon move to the Netherlands in Aug. 2018.*

NIH/NIGMS R01 GM112678-01

1/1/2015 – 31/12/2019

(Principal Investigator*)

\$252K/yr (direct)

Structural polymorphism in the misfolding and aggregation of expanded polyglutamine proteins

The major goal of this proposal is to detail the structural heterogeneity and polymorphism within and among different aggregated polyglutamine-containing peptides and multiple disease-related proteins, by solid-state NMR spectroscopy, EM and complementary spectroscopic techniques. This includes the determination of the molecular features of the polyglutamine amyloid core and to elucidate the underpinnings of reported molecular

polymorphism between different kinds of polyglutamine aggregates from huntingtin exon-1 and other disease-related proteins.

** Funded and operated as PI in 2015-2018; transferred PI status to collaborator James Conway upon move to the Netherlands in Aug. 2018.*

NIH/National Institute on Aging R01 AG019322-12 (Co-investigator; Principal Investigator: R. Wetzel)
15/6/2001 – 31/5/2015 \$30K/yr (direct)

Structures and Properties of Polyglutamine Proteins and Their Aggregates

The aim of this grant is to investigate the structure and aggregation mechanism of the polyglutamine-containing huntingtin protein that is the causative agent of Huntington's Disease. An array of complementary biochemical and structural tools is employed to investigate N-terminal fragments of the protein. The Van der Wel group's role is to use solid-state NMR to determine site-specific structural and motional features of the mature aggregates, with a focus on the non-glutamine flanking sequences, which play important roles in the misfolding and aggregation processes that cause Huntington's Disease.

NIH Major Instrumentation S10 1S10RR033477 (Major User; Principal Investigator: A. Gronenborn)
9/2013-30/8/2014 (\$2,000,000)

750MHz Wide Bore NMR Spectrometer

This proposal funded the acquisition of a wide-bore 750 MHz NMR spectrometer for solid-state NMR investigations of membrane proteins, macromolecular assemblies, and protein aggregates. The successful grant proposal, a significant part of which I assembled and co-wrote, addresses the needs of multiple researchers at the University of Pittsburgh and their collaborators across multiple universities. As the primary solid-state NMR group in Pittsburgh, the Van der Wel group is the primary "major user".

Univ. Pittsburgh Schools of the Health Sciences Bridge Funding (Principal Investigator)
1/4/2014-31/3/2015 \$100,000

Structural characterization of misfolding and amyloid formation in Huntington's Disease and other polyglutamine expansion diseases

These funds supported our use of solid-state NMR spectroscopy to determine the internal atomic structure of polyglutamine aggregates, including in particular the misfolded core of the amyloid-like fibrils formed by huntingtin protein's exon-1 domain. The obtained results delineate on a molecular level how the mutant huntingtin protein undergoes conformational changes that lead to neuronal degradation. By our molecular understanding of these pivotal early events, these studies may help inform the design of targeted drugs or treatments against Huntington's disease and related disorders.