



Top: EDICT partners at the kick-off meeting in Dusseldorf, Germany
Bottom-left: Scientific Coordinator, Professor P J F Henderson, Bottom-right: Project Manager, Mrs H Inman



Publishable summary supporting information

Partners Involved

No	Institution	Country	Academic Contact
1	University of Leeds	UK	Peter Henderson Stephen Baldwin Colin Fishwick & Peter Johnson
2	Lausanne University	Switzerland	Bernard Thorens & Frederic Preitner
3	Goteborg University	Sweden	Richard Neutze
4	Aston University	UK	Roslyn Bill
5	University of Basel	Switzerland	Andreas Engel
6	Max-Planck Institute		Hartmut Michel Bert de Groot Werner Kühlbrandt
7	FMP Berlin	Germany	Hartmut Oschkinat
8	Goethe-University Frankfurt am Main	Germany	Robert Tampe Volker Dötsch & Frank Bernhard
9	University of Zurich	Switzerland	Raimund Dutzler
10	ETH Zurich	Switzerland	Kaspar Locher
11	Heinrich-Heine University Dusseldorf	Germany	Lutz Schmitt
12	University of Groningen	Netherlands	Bert Poolman & Dirk Slotboom
13	Commissariat a l'Energie Atomique	France	Eva Pebay-Peyroula
14	Medical Research Council	UK	John Walker Edmund Kunji Chris Tate
16	Aarhus University	Denmark	Poul Nissen
17	Imperial College London	UK	So Iwata Bernadette Byrne Alex Cameron
18	Astra Zeneca	Sweden	Arjan Snijder
19	Oxford University	UK	Frances Ashcroft Mark Sansom
20	Stockholm University	Sweden	Arne Elofsson, Gunnar von Heijne & Erik Lindahl
21	Moscow State University	Russia	Olga Sokolova
22	Hebrew University Jerusalem	Israel	Baruch Kanner Etana Padan
23	University of Milan	Italy	Anna Moroni
24	Fundacio Privada Institut Recerca Biomedica	Spain	Manuel Palacín
25	Helsinki University	Finland	Adrian Goldman
26	Karolinska Institute	Sweden	Par Nordlund
27	Copenhagen University	Denmark	Ulrik Gether
28	Xention Ltd	UK	David Madge
29	Freiburg University	Germany	Carola Hunte

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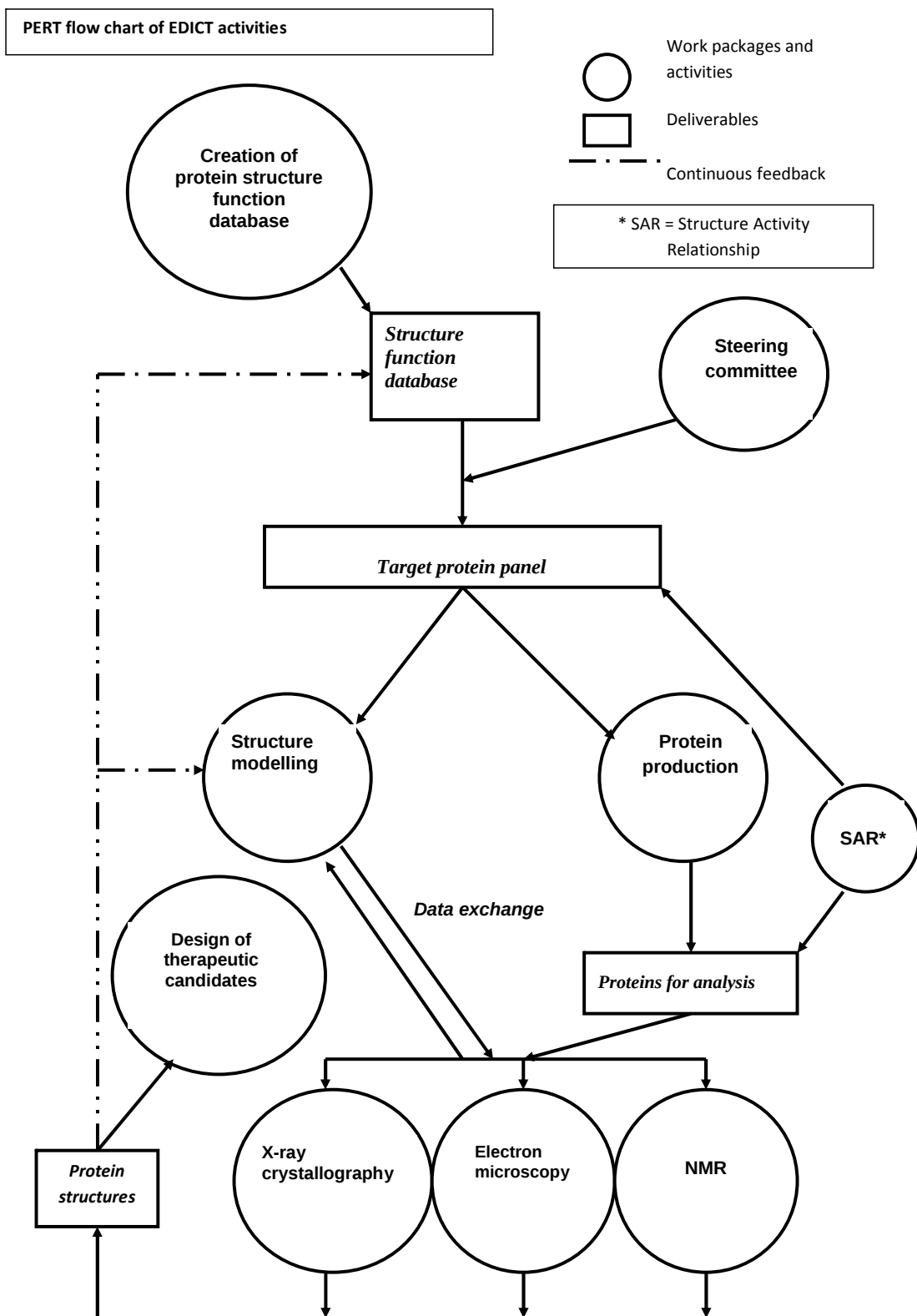


Figure 4. PERT flow diagram of EDICT activities

Work Package	Acronym	Structures	Organism type	PI's	Function		
WP2 Channels	ELIC	Closed protein pentamer by XRC	Bacterium	Dutzler	Ligand-gated cation channel	1	
	GLIC	Open protein pentamer by XRC	Bacterium	Dutzler	Ligand-gated cation channel	1	
	HCN1	cNMP binding site by XRC	Human	Moroni	K ⁺ /Na ⁺ hyper-polarization-activated cNMP-gated channel	1	
	HCN4	cNMP binding site by XRC	Human	Moroni	K ⁺ /Na ⁺ hyper-polarization-activated cNMP-gated channel	1	
	Kv2.1	Protein complex and deletion mutant by EM and modelling	Rat	Sokolova	Voltage-gated K ⁺ channel	2	
	Kv10.2	Protein complex by EM	Human	Sokolova	Voltage-gated K ⁺ channel	1	
	ChR2	Protein dimer by EM	Green alga	Kühlbrandt	Light-gated ion channel	1	
	Proteorhodopsin	Protein by NMR	Bacterium	Dötsch, Bernhard	Light-driven H ⁺ pump	1	
	Presenilin1	C-terminal fragment by NMR	Human	Dötsch, Bernhard	Gamma-secretase protease	1	
WP3 Transporters	Mhp1	Open-out, occluded, open-in, part occluded, 4 complexes by XRC	Bacterium	Cameron, Beckstein Iwata, Henderson	Na ⁺ -hydantoin symporter	7	
	AdiC	Protein with ligand and mutants by XRC	Bacterium	Palacin	Arginine/agmatine antiporter and mutants	3	
	Transporter	Protein by XRC	Human	Cameron, Iwata	Antiporter	1	
	NhaA	Protein by XRC	Bacterium	Padan	Na ⁺ /H ⁺ antiporter	1	
		Protein dimer by XRC	Bacterium	Cameron	Na ⁺ /H ⁺ antiporter	1	

	NhaP1	Protein dimer, deletion mutant, different conformations by EM	Archaea	Kühlbrandt	Na ⁺ /H ⁺ antiporter	2	
	UraABc	Protein hexamer by EM	Bacterium	Baldwin	Urea channel/transporter	1	
WP4 Aquaporins	AQP4, AQP5, MIP	Proteins by XRC	Human	Neutze	Aquaporin	3	
	AQPY1	Protein by XRC	Yeast	Neutze	Aquaporin	1	
WP5	ThiT	Protein by XRC Protein with (pyri)thiamine	Bacterium	Poolman, Slotbloom	ECF component ABC transporters	2	
	BioY	Protein by XRC Protein with biotin	Bacterium	Poolman, Slotbloom	ECF component ABC transporters	2	
	OppA	Protein by XRC Protein with ligand	Bacterium	Poolman, Slotbloom	Binding protein of ABC transporter	2	
	OpuAC	Protein by XRC Protein with ligand	Bacterium	Poolman, Slotbloom	ABC transporter	2	
	OpuBC	Protein by XRC	Bacterium	Schmitt	Binding protein of ABC transporter	1	
	HlyB	Protein by XRC	Bacterium	Schmitt	Haemolysin exporter	1	
	HmuT	Protein by XRC Protein with ligand	Bacterium	Locher	Binding protein of haem ABC transporter	2	
	ArtMP	Interfacial domains of protein complex by NMR	Bacterium	Oschkinat	Arginine transport system	2	

WP6 F-, P- and PP- ATPases	Fo-F1 ATPase by XRC	Protein by XRC	Bovine	Walker	ATP synthesis	1	
		Protein by XRC	Yeast	Walker	ATP synthesis	1	
		Protein by XRC	Bacterium	Walker	ATP synthesis	1	
	P~Pase	Protein by XRC Protein with ligand	Bacterium	Goldman, Nissen	Generation of Na ⁺ gradient	2	
	P-ATPase	Protein with ligand by XRC	Pig	Nissen	Generation of Na ⁺ gradient in animals	1	
	P-ATPase	Protein with ligand by XRC	Yeast	Nissen	Generation of H ⁺ gradient in fungi	1	
WP7 Mitochondrial transporters	TspO	Protein by EM	Bacterial	Tate	Homologue of mitochondrial outer membrane protein	1	
		43 by XRC, 6 by EM, 3 by NMR	32			52	

Examples of structures determined by the EDICT project

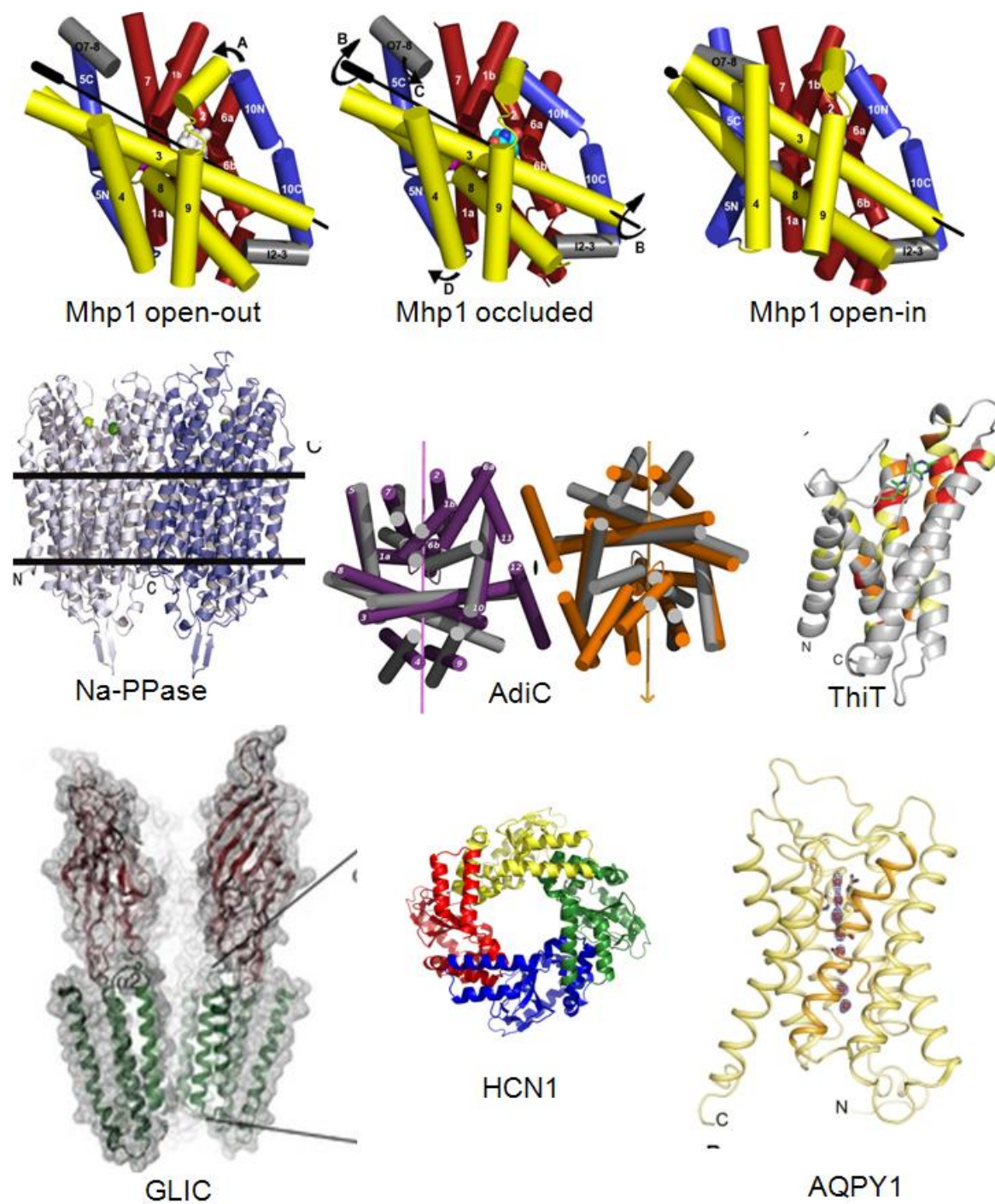


Figure 5. Some examples of structures determined by X-ray crystallography

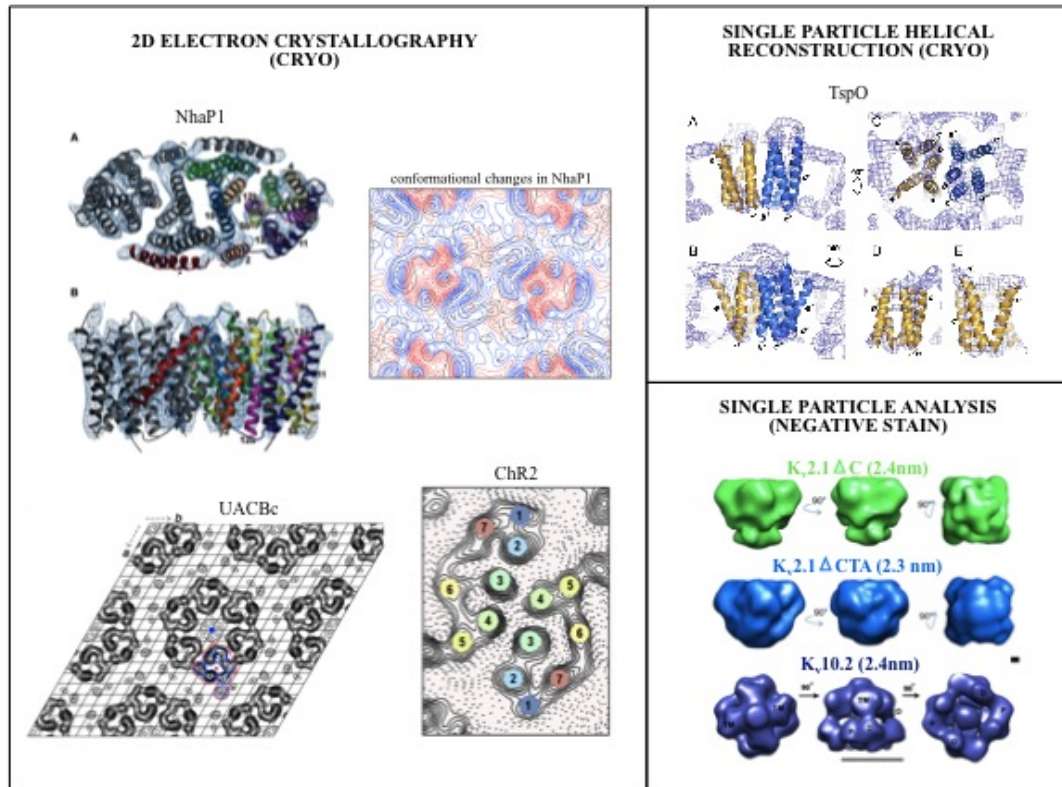


Figure 6. Examples of structures determined by electron microscopy

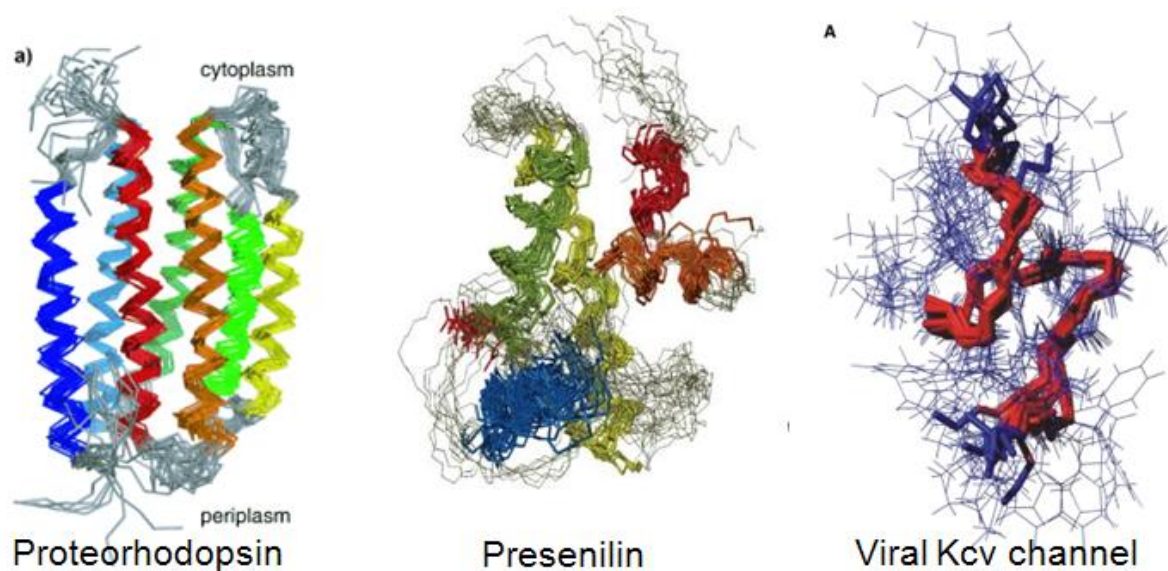


Figure 7. Examples of structures determined by nuclear magnetic resonance

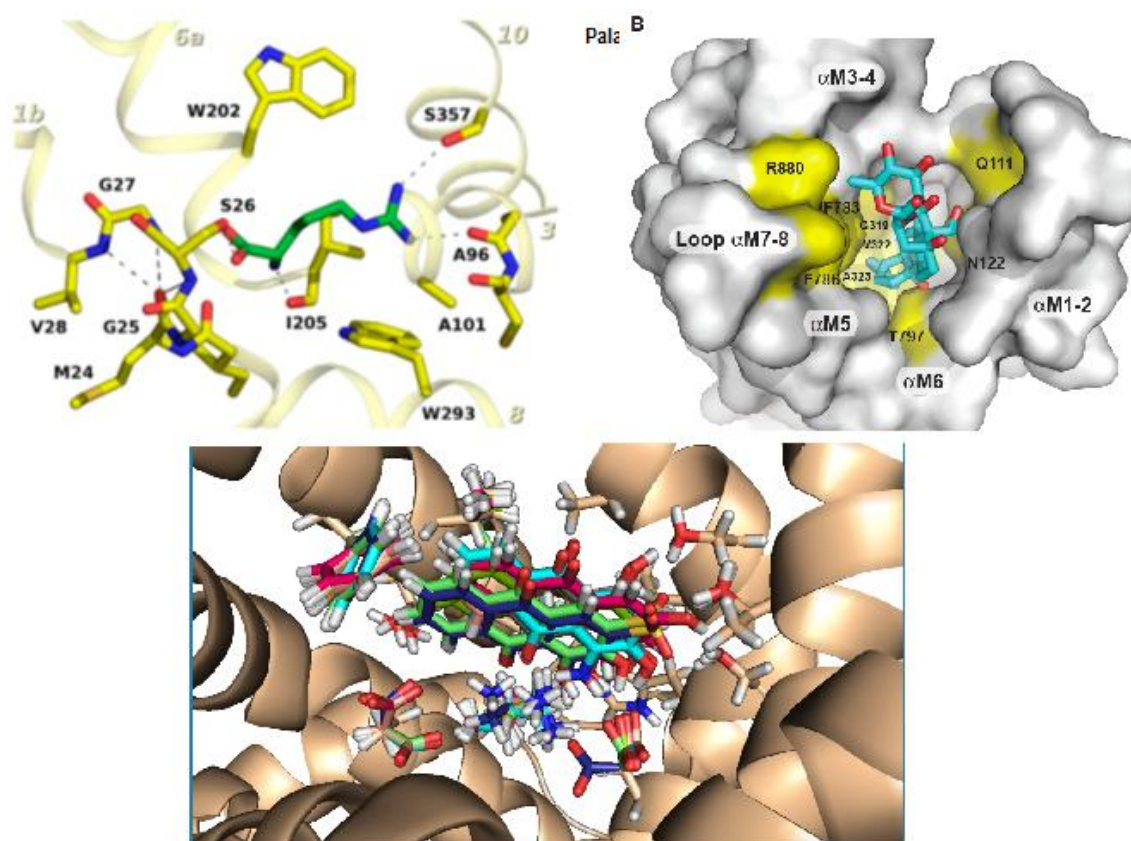


Figure 8. Examples of docking of ligands in EDICT target proteins

Table 2. Examples of dissemination at a Scientific Conference (Period 3 only)

Date	Conference Title	Place	EDICT PI
15/08/2010 – 20/08/2010	Gordon Research Conference, Membrane Transport Proteins	Maine, USA	Ulrik Gether (Chair) Peter Henderson Baruch Kanner Alex Cameron Poul Nissen Oliver Beckstein Robert Tampe
05/01/2011 – 07/01/2011	Biochemical Society, Recent Advances in Membrane Biochemistry	Cambridge, UK	Roslyn Bill Chris Tate Werner Kuhlbrandt Mark Sansom Gunnar von Heijne Peter Henderson Frances Ashcroft
16/05/2011 – 20/05/2011	Cold Spring Harbor Asia Conference, Membrane Proteins: Structure & Function	Suzhou, China	Carola Hunte (organiser), Gunnar von Heijne (keynote) Peter Henderson Werner Kuhlbrandt Hartmut Oschkinat Bert Poolman Chris Tate

19/06/2011 – 24/06/2011	Gordon Research Conference, Mechanisms of Membrane Transport	Maine, USA	Poul Nissen Dirk Slotboom Robert Tampe Kasper Locher
26/6/2010 – 1/7/2010	35 th FEBS Congress,	Goeborg, Sweden	Richard Neutze John Walker Raimund Dutzler Bert Poolman
14/08/2011- 19/08/2011	FASEB Summer research Conferences	Aspen, USA	Frédéric Preitner Bernard Thorens Peter Henderson
15/01/2012 – 20/01/2012	Gordon Research Conference, Ligand Recognition & Molecular Gating	Ventura, USA	Dirk Slotboom (vice chair) Chris Tate

Table 3. Publications of the European Drug Initiative for Channels and transporters
(Arranged in chronological order for each Work Package – see also the EDICT web site)

WP1 - Database, annotations and structural modelling
1. Light, S., Sagit, R., Ithychanda, S.S., Qin, J. and Elofsson, A. (Epub 2012) The evolution of filamin - A protein domain repeat perspective. <i>J Struct Biol</i> (Epub ahead of print). 2. Hedin, L.E., Illergard, K. and Elofsson, A. (2011) An introduction to membrane proteins. <i>J Proteome Res</i> 10 (8) : 3324-3331. 3. Shu, N. and Elofsson, A. (2011) KalignP: improved multiple sequence alignments using position specific gap penalties in Kalign2. <i>Bioinformatics</i> 27 (12) : 1702-1703. 4. Hennerdal, A. and Elofsson, A. (2011) Rapid membrane protein topology prediction. <i>Bioinformatics</i> 27 (9) : 1322-1323. 5. Larsson, P., Skwark, M.J., Wallner, B. and Elofsson, A. (2011) Improved predictions by Pcons.net using multiple templates. <i>Bioinformatics</i> 27 (3) : 426-427. 6. Hennerdal, A., Falk, J., Lindahl, E. and Elofsson, A. (2010) Internal duplications in alpha-helical membrane protein topologies are common but the nonduplicated forms are rare. <i>Protein Sci</i> 19 (12) : 2305-2318. 7. Runesson, J., Sollenberg, U.E., Jurkowski, W., Yazdi, S., Eriksson, E.E., Elofsson, A. and Langel, U. (2010) Determining receptor-ligand interaction of human galanin receptor type 3. <i>Neurochem Int</i> 57 (7) : 804-811. 8. Hedin, L.E., Ojemalm, K., Bernsel, A., Hennerdal, A., Illergard, K., Enquist, K., Kauko, A., Cristobal, S., von Heijne, G., Lerch-Bader, M., Nilsson, I. and Elofsson, A. (2010) Membrane insertion of marginally hydrophobic transmembrane helices depends on sequence context. <i>J Mol Biol</i> 396 (1) : 221-229. 9. Bernsel, A., Viklund, H., Hennerdal, A. and Elofsson, A. (2009) TOPCONS: consensus prediction of membrane protein topology. <i>Nucleic Acids Res</i> 37 (Web Server issue) : W465-8 10. Hayat, S. and Elofsson, A. (2012) Ranking models of transmembrane beta-barrel proteins using Z-coordinate predictions. <i>Bioinformatics</i> 28 (12) : i90-6. 11. Tsirigos, K.D. and Hennerdal, A. and Kall, L. and Elofsson, A. (2012) A guideline to proteome-wide alpha-helical membrane protein topology predictions. <i>Proteomics</i>
WP2 - Ion channels and secondary active ion transporters
1. Wohri, A.B., Hillertz, P., Eriksson, P.O., Mueller, J., Dekker, N. and Snijder, A. (Epub 2012) Thermodynamic studies of ligand binding to the human homopentameric glycine receptor using isothermal titration calorimetry. <i>Mol Membr Biol</i> (Epub ahead of print) 2. Hamacher, K., Greiner, T., Ogata, H., Van Etten, J.L., Gebhardt, M., Villarreal, L.P., Cosentino, C., Moroni, A. and Thiel, G. (2012) Phycodnavirus potassium ion channel proteins question the virus molecular piracy hypothesis. <i>PLoS One</i> 7 (6) : e38826* 3. Ben-Yona, A. and Kanner, B.I. (Epub 2012) An acidic amino acid transmembrane helix 10 residue conserved in the neurotransmitter:sodium:symporters is essential for the formation of the extracellular gate of the gamma-aminobutyric acid (GABA) t <i>J Biol Chem</i> (Epub ahead of print) 287 (10) : 7159-7168. 4. Lolicato, M., Nardini, M., Gazzarrini, S., Moller, S., Bertinetti, D., Herberg, F.W., Bolognesi, M.,

- Martin, H., Fasolini, M., Bertrand, J.A., Arrigoni, C., Thiel, G. and Moroni, A. (2011) Tetramerization Dynamics of C-terminal Domain Underlies Isoform-specific cAMP Gating in Hyperpolarization-activated Cyclic Nucleotide-gated Channels. *J Biol Chem* 286 (52) : 44811-44820
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9. Hilf, R.J. and Bertozzi, C. and Zimmermann, I. and Reiter, A. and Trauner, D. and Dutzler, R. (2010) Structural basis of open channel block in a prokaryotic pentameric ligand-gated ion channel. *Nat Struct Mol Biol* 17 (11) : 1330-1336
10. Domanski, J. and Stansfeld, P.J. and Sansom, M.S. and Beckstein, O. (2010) Lipidbook: a public repository for force-field parameters used in membrane simulations. *J Membr Biol* 236 (3) : 255-258
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WP3 - Human metabolite/ion transporters and their homologues

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- Bill, R.M., Henderson, P.J., Iwata, S., Kunji, E.R., Michel, H., Neutze, R., Newstead, S., Poolman, B., Tate, C.G. and Vogel, H. (2011) Overcoming barriers to membrane protein structure determination. *Nat Biotechnol* 29 (4) : 335-340
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WP4 - Structural, functional and computational analyses of human aquaporins

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WP5 - Structural and functional analysis of ABC transporters

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WP6 - Structural, functional and computational analyses of P-type, F-type and PP-ATPases

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WP7 - Structural, functional and computational analyses of mitochondrial transport proteins

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WP8 - X-ray crystallography methods for structure analysis of membrane channels and transporters

N.B. These publications are duplicates from other Work Packages

1. Lolicato, M., Nardini, M., Gazzarrini, S., Moller, S., Bertinetti, D., Herberg, F.W., Bolognesi, M., Martin, H., Fasolini, M., Bertrand, J.A., Arrigoni, C., Thiel, G. and Moroni, A. (2011) Tetramerization Dynamics of C-terminal Domain Underlies Isoform-specific cAMP Gating in Hyperpolarization-activated Cyclic Nucleotide-gated Channels. *J Biol Chem* 286 (52) : 44811-44820

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23. Borshchevskiy, V.I., Round, E.S., Popov, A.N., Buldt, G. and Gordeliy, V.I. (2011) X-ray-radiation-induced changes in bacteriorhodopsin structure. *J Mol Biol* 409 (5) : 813-825
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25. Borshchevskiy, V., Efremov, R., Moiseeva, E., Buldt, G. and Gordeliy, V. (2010) Overcoming merohedral twinning in crystals of bacteriorhodopsin grown in lipidic mesophase. *Acta Crystallogr D Biol Crystallogr* 66 (Pt 1) : 26-32
26. Borshchevskiy V, Moiseeva E, Kuklin A, Buldt G, Hato M. and V Gordeliy (2010) Isoprenoid-chained lipid b-XylOC16+4 - A novel molecule for in meso membrane protein crystallization *Journal of*

WP9 - Electron microscopy methods for structure analysis of membrane channels and transporters

N.B. These publications are duplicates from other Work Packages

1. Korkhov, V.M. and Sachse, C. and Short, J.M. and Tate, C.G. (2010) Three-dimensional structure of TspO by electron cryomicroscopy of helical crystals. *Structure* 18 (6) : 677-687
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Publications in press
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6. Mutations of the mitochondrial ADP/ATP carrier causing genetic diseases impair the transport of nucleotides » S. Ravaud, A. Bidon-Chanal, I. Blesneac, P. Machillot, C. Juillan-Binard, F. Dehez, C. Chipot, E. Pebay-Peyroula (2012) <i>ACS Chem Bio</i>
7. A Virtual High-throughput Screening Approach to the Discovery of Novel Inhibitors of the Bacterial Leucine Transporter, LeuT: Katie J Simmons, Kamil Gotfryd, Christian B Billesbølle, Claus J Loland, Ulrik Gether, Colin W G Fishwick and A Peter Johnson, <i>Molecular Membrane Biology</i>
8. the proton transport and regulation of UCP1 using solid supported membranes» I. Blesneac, S. Ravaud, P. Machillot, S. Masscheylen, B. Miroux, M. Vivaudou and E. Pebay-Peyroula, <i>European Biophysical Journal</i>
9. Peter Paulsen, Wiktor Jurkowski, Rossen Apostolov, Erik Lindahl, Poul Nissen & Hanne Poulsen The C-terminal cavity of the Na,K-ATPase analyzed by docking and electrophysiology <i>Molecular Membrane Biology</i>



Figure 9. Journal front covers featuring EDICT papers

Table 4. Researcher exchange visits

Name	Home Institution	Host Institution	Date from	Date to
Iiulia Blesneac	CEA	Groningen	15/09/2008	21/09/2008
Tommi Kajander	Helsinki	Diamond	10/02/2009	13/02/2009
Christopher Lentes	Leeds	Imperial	08/03/2009	22/03/2009
Kamil Gotfryd	Copenhagen	Aarhus	23 one and two day visits between 18/02/2009 and 29/03/2012	
Wiktor Jurkowski	Stockholm	Leeds	16/11/2009	20/11/2009
Dawid Krenc	Max-Planck	Gothenburg	18/11/2009	21/11/2009
Sören Wacker	Max-Planck	Leeds	21/11/2009	27/11/2009
Constantina Fotinou	Oxford	Aarhus	18/01/2010	20/02/2010
Marco Lolicato	Milan	Zurich	24/06/2010	26/06/2010
Juho Kelloalo	Helsinki	Aarhus	02/08/2010	03/09/2010
Maria Karlova	Moscow	Milan	07/12/2010	21/12/2010
Maike Bublitz	Aarhus	MRC	07/03/2012	31/03/2012

A report on mobility and gender issues (Deliverable D12.10)

The EDICT project involves over 120 people, including academics, PhD students, Postdocs and technicians from twelve different countries. This report is split into various sections covering partner geographic locations, male/female employee ratio and detailed information on the workforce.

Section 1. Partner geographic locations

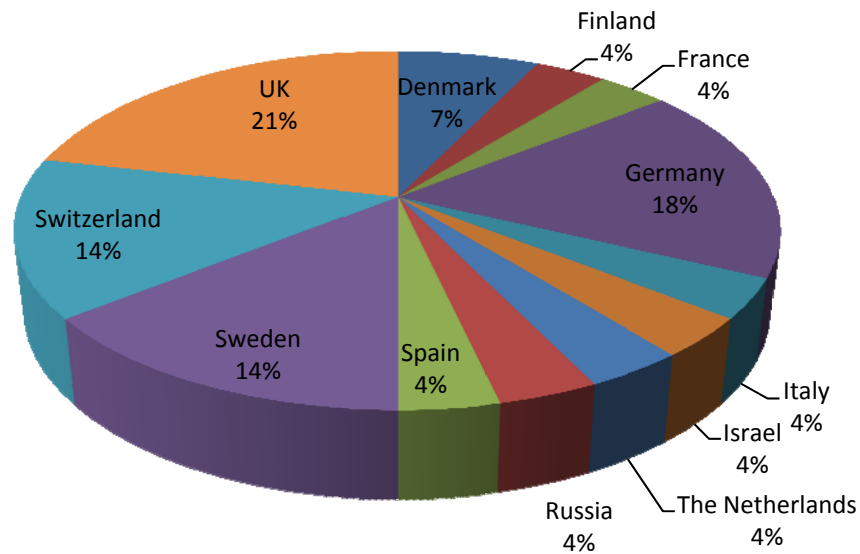
The distribution of partners between countries is illustrated in Figure 1 and their identities are listed in Table 1.

Table 1. The countries involved in the project and their related partner laboratory.

Denmark	University of Aarhus (partner 16)	Nissen
Denmark	University of Copenhagen (partner 27)	Gether
Finland	Helsinki University (partner 25)	Goldman
France	CEA (partner 13)	Pebay-Peyroula
Germany	Max-Planck Institute (partner 6)	Michel, de Groot, Kühlbrandt
Germany	FMP Berlin (partner 7)	Oschkinat
Germany	Goethe-University Frankfurt (partner 8)	Tampe, Dötsch & Bernhard
Germany	Heinrich-Heine University Dusseldorf (partner 11)	Schmitt
Germany	University of Freiburg (partner 29)	Hunte
Italy	University of Milan (partner 23)	Moroni
Israel	Hebrew University of Jerusalem (partner 22)	Kanner & Padan
The Netherlands	University of Groningen (partner 12)	Poolman & Slotboom
Russia	Moscow State University (partner 21)	Sokolova
Spain	IRB (partner 24)	Palacin
Sweden	Goteborg University (partner 3)	Neutze
Sweden	AstraZeneca (partner 18)	Snijder
Sweden	Stockholm University (partner 20)	Elofsson, von Heijne & Lindahl
Sweden	Karolinska Institute (partner 26)	Nordlund
Switzerland	University of Lausanne (partner 2)	Thorens & Preitner
Switzerland	University of Basel (partner 5)	Engel
Switzerland	University of Zurich (partner 9)	Dutzler
Switzerland	ETH Zurich (partner 10)	Locher
UK	University of Leeds (partner 1)	Henderson, Baldwin, Fishwick & Johnson
UK	Aston University (partner 4)	Bill
UK	Medical Research Council (partner 14)	Walker, Kunji, Tate
UK	Imperial College (partner 17)	Iwata, Byrne, Cameron
UK	University of Oxford (partner 19)	Ashcroft, Sansom
UK	Xention (partner 28)	Madge

The participation of ten European countries and Israel and Russia has resulted in at least 25 of the PI's participating in joint publications and ingoing joint projects with their staff.

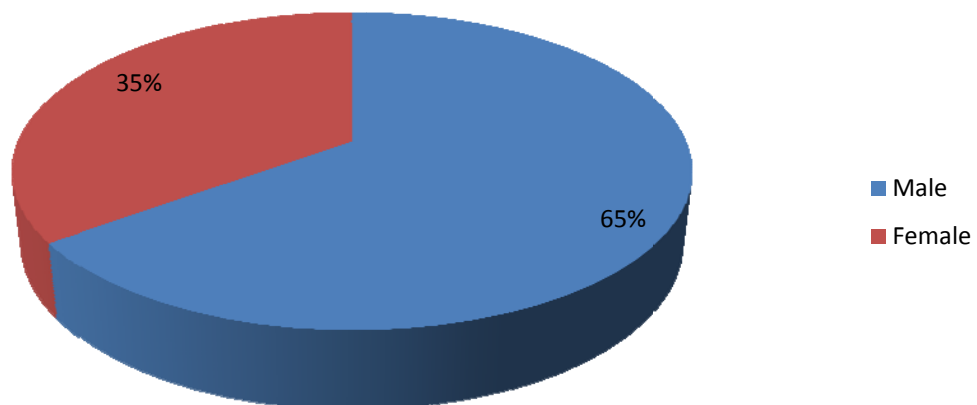
Figure 1. EDICT Partner Country Distribution

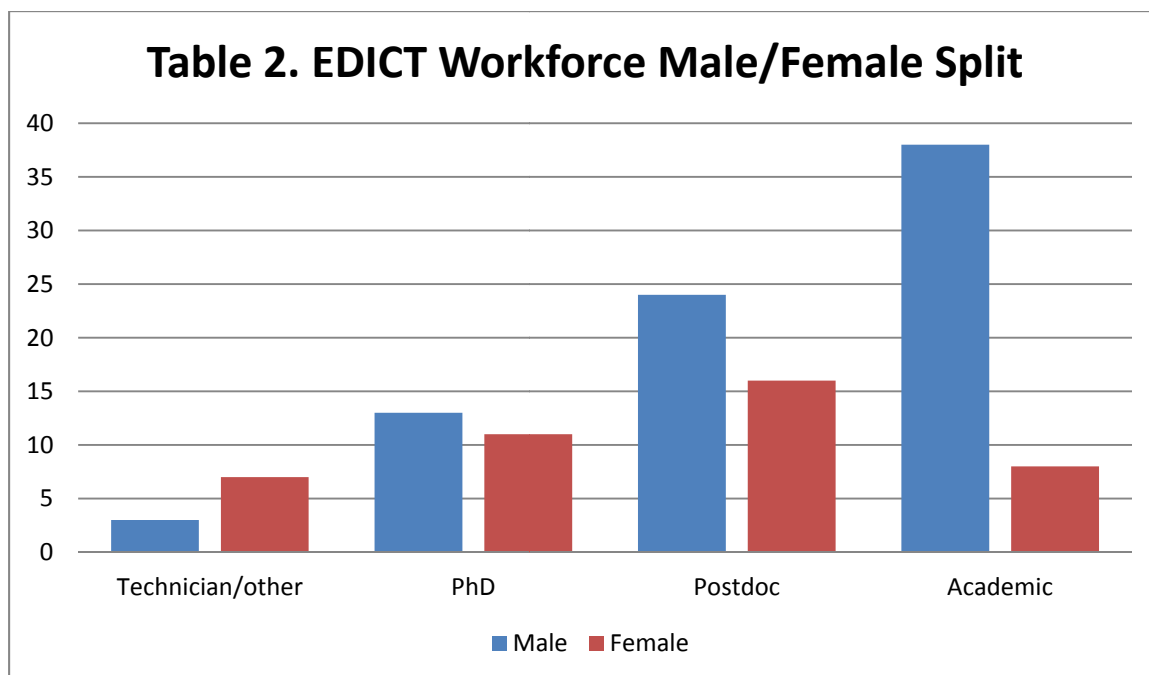


Section 2. Male/Female Split

The EDICT workforce overall has a healthy male to female split (35% male, 65% female). At PhD level the split is almost equal, this falls at Postdoc level and then a dramatic fall at Academic level (Table 2). To the best of our knowledge these observations reflect the general experience amongst European projects.

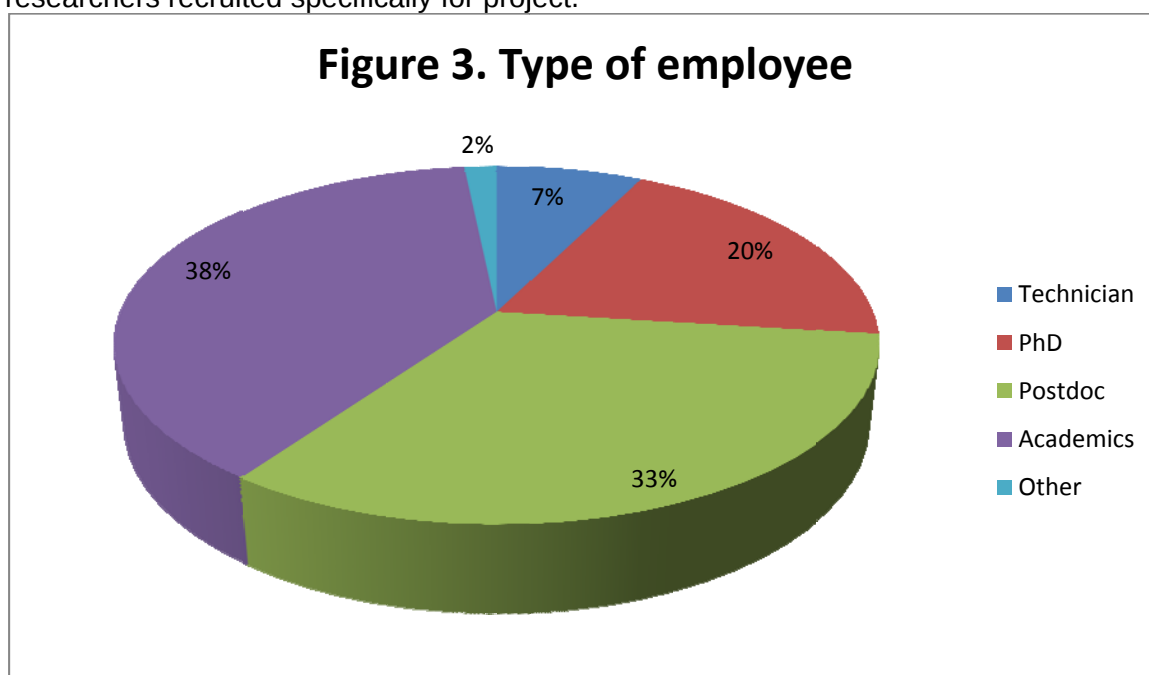
Figure 2. EDICT Overall Workforce Male/Female Split





Section 3. Type of EDICT workforce

The EDICT workforce can be split into five categories: Technicians, PhD students, Postdocs, Academics and other (project manager). The largest group of employees is the Academic staff who were named in the original grant application, followed closely by Postdoctoral researchers recruited specifically for project.



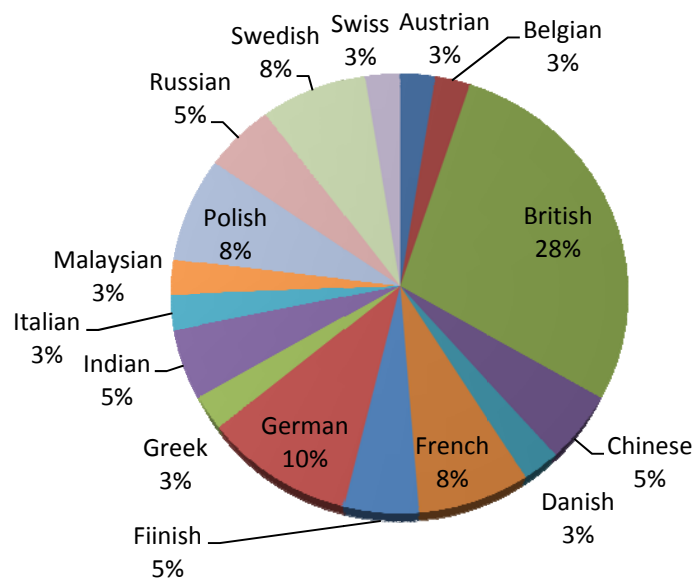
Section 4. Detailed information about employees

A questionnaire was sent out to all employees (technicians, PhD students and Postdocs) to gain a better understanding of the EDICT workforce. From the data collected, the average employee age is 33 years old, with the youngest employee being 25 and oldest being 49. The list of nationalities was also varied; 16 different nationalities recorded.

The majority of employees , 77%, are partnered (including marital partner, civil partner or other live in partner) and of those with partners most of their partner's occupations were also scientific/academic. The occupations included researcher, scientist, software engineer, microbiologist, biochemist, teacher, lecturer, student, architect, professor, accountant and Postdoc.

Of those who are partnered, 40% have children. Only 33% of all employees have children despite 80% of respondents stating that their Institution has family friendly policies e.g. flexible working hours.

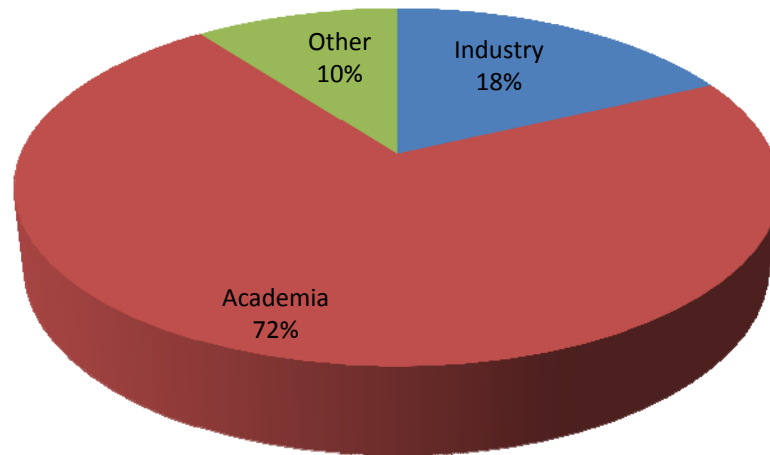
Figure 4. Employee Nationalities



Section 5. Future career plans

The overall majority of employees, 72% stated that they wanted to stay in academia after finishing their EDICT contract. Only 18% wanted to move to industry and 10% wanted to work in other areas.

Figure 5. Breakdown of employment sectors



The mobility of researchers around Europe is interesting, 65% of respondents said they were planning on looking for work in the same country as their current employment. Looking at employee nationality and current geographical location, 59% of employees were the same nationality as the lab they were working in. When asked about future career plans, if respondents secured a job in their desired country of work, 53% would be the same nationality as the country of employment.