Roadmap of 3D-BioInfo-PT, the BioData.pt community of computational structural biology researchers

BioData.pt · **elixir PORTUGAL**

1st **BioData.pt** elixir **All Hands**
3rd **Technical Meeting**
CCMAR, 28-30/09/2022

Roadmap

Inception: the 3D-BioInfo-PT project is born, partially as a re-branding under Biodata.pt of the community involved in the EJIBCE meetings – *Encontros de Jovens Investigadores em Biologia Computacional Estrutural.*
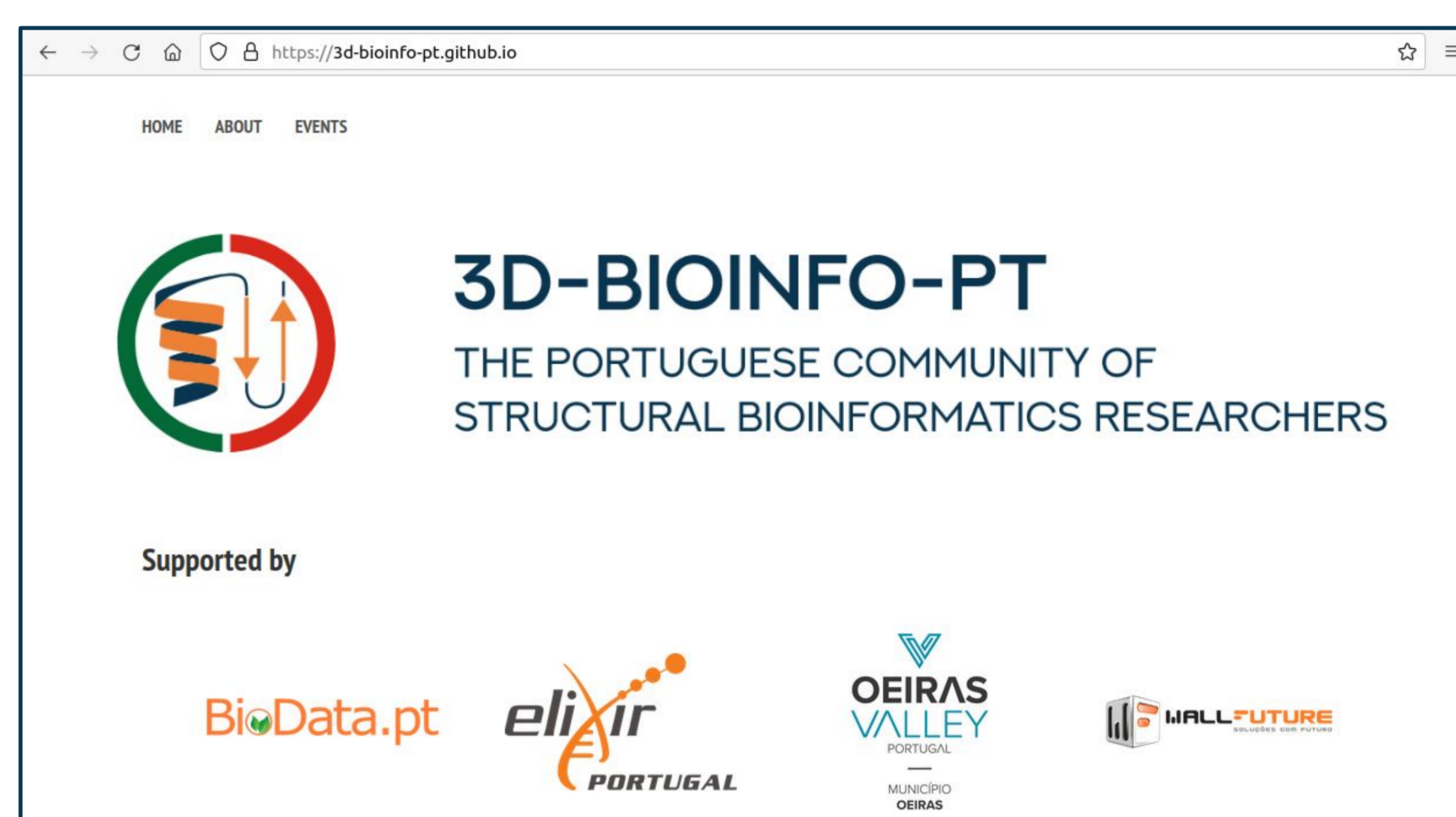
Dec '21

Materialization: Planned roadmap presented and debated at the Biodata.pt Technical Meeting.

Mar '22

Outreach: the 3D Biotalks are established as a monthly Biodata.pt Talks seminar cycle.

Image: the 3D-BioInfo-PT site is launched at *https://3d-bioinfo-pt.github.io/*

BioData.pt TALKS
3D BioTalks | Session 2:
An overview of mutations distribution within GPCR sub-family A17 in one database - MUG database
Ana Beatriz Caniceiro
Data-Driven Molecular Design - Irina Moreira Lab, UC-Biotech, CNC, University of Coimbra
May 4th, 2022 | 11:00 am | via Zoom
BioData.pt

BioData.pt TALKS
3D BioTalks | Session 3:
Recent Artificial Intelligence tools and architectures for Structural Biology
Francisco Fernandes
Researcher at the Graphics & Interaction group, INESC-ID, Lisboa
June 1st, 2022 | 11:00 am | via Zoom
BioData.pt

BioData.pt TALKS
3D BioTalks | Session 4:
Faster protein pKa predictions with deep learning
Pedro Reis
Ph.D. Student at the Molecular Modeling & Simulation Lab (Machuqueiro Lab), FCUL, Lisboa
July 6th, 2022 | 11:00 am | via Zoom
BioData.pt

BioData.pt TALKS
3D BioTalks | Session 5:
Overview of the Structure-Based Molecular Modelling group @ FCUL
Bruno Victor
Principal Investigator of the Structure-Based Molecular Modelling Lab, FCUL, Lisboa
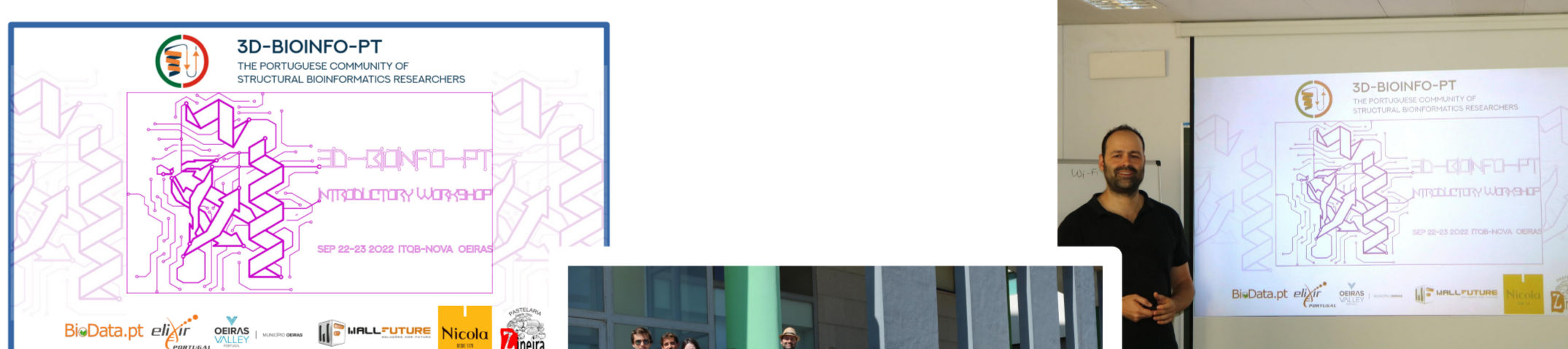September 14th, 2022 | 11:00 am | via Zoom
BioData.pt

Apr '22

May '22

Jun '22

Jul '22

Aug '22

Teaching: the first 3D-BioInfo-PT workshop takes place at ITQB NOVA. It is an event with 35 participants (out of 62 applicants) hailing from 7 different institutions. Main support from the Oeiras Valley initiative and Wallfuture Lda.
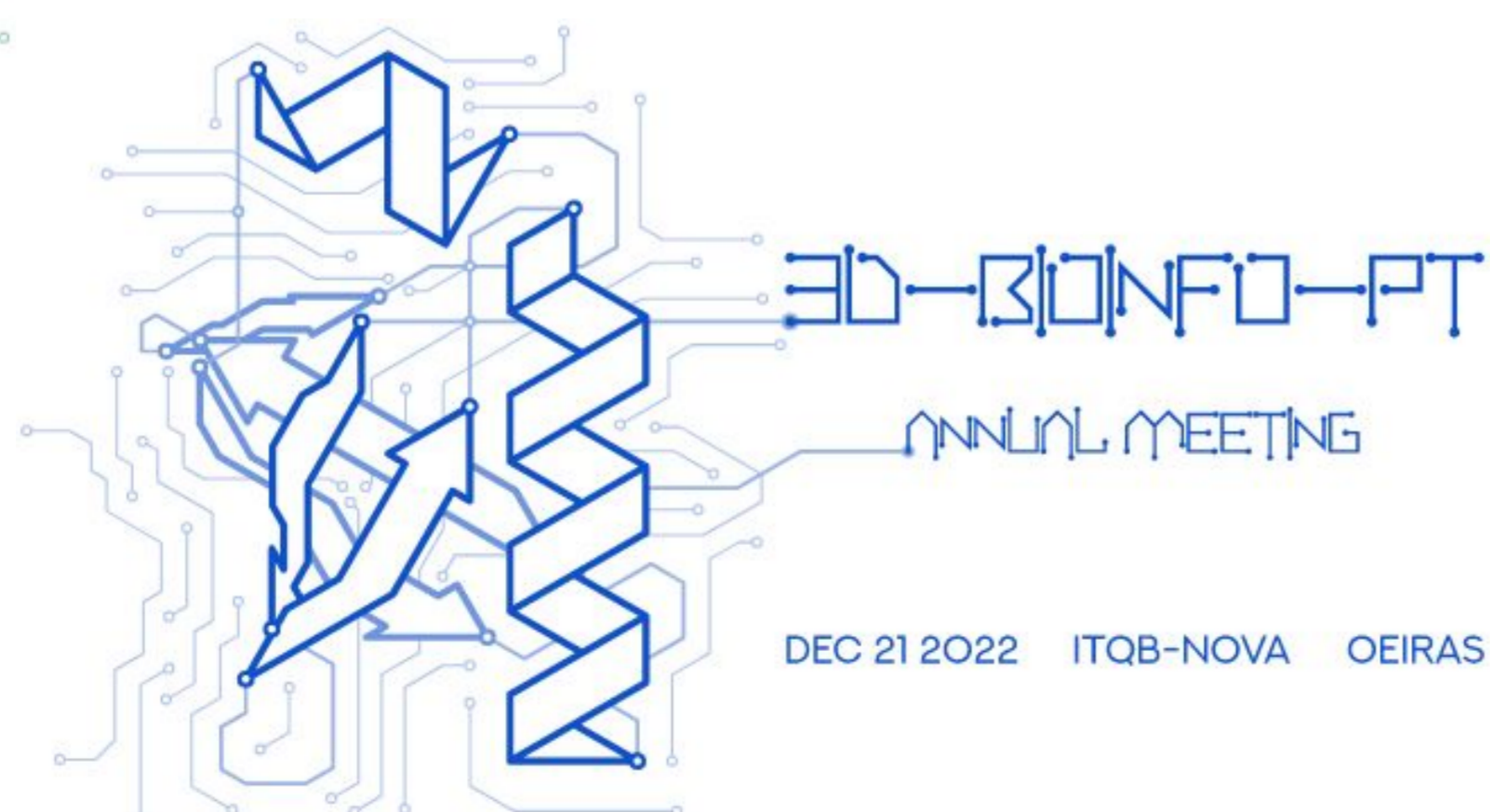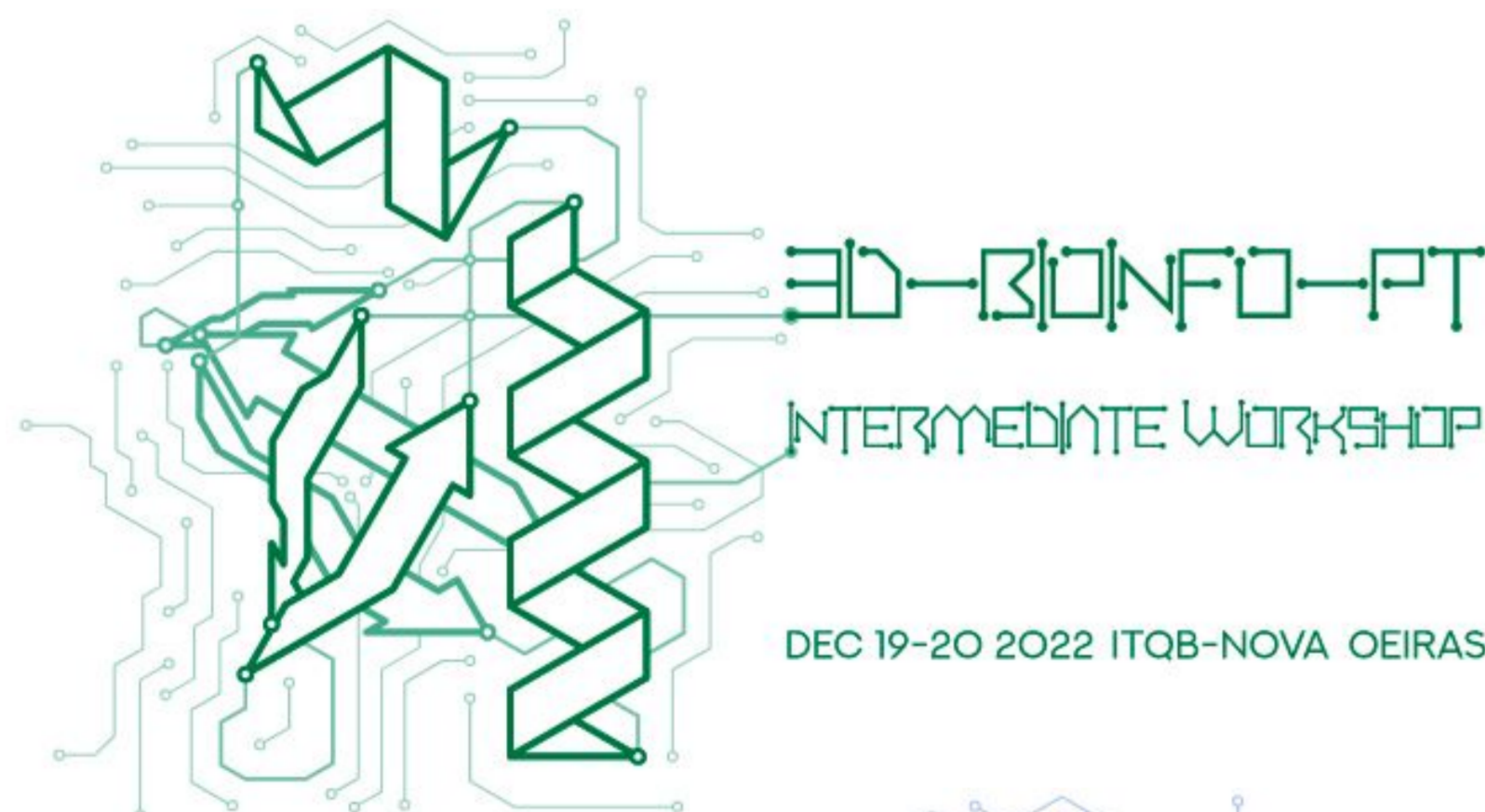
Continuity: maintain the 3D Biotalks seminar cycle and expand its reach.

Sep '22

Networking: maintain the EJIBCE tradition of the annual meeting. Organize a satellite workshop.

Oct '22

Nov '22

3D-BIOINFO-PT
INTERMEDIATE WORKSHOP
DEC 19-20 2022 ITQB-NOVA OEIRAS

Dec '22

3D-BIOINFO-PT
ANNUAL MEETING
DEC 21 2022 ITQB-NOVA OEIRAS

2023

Collaboration: bring together the 3D-BioInfo-PT coordinating groups to write a perspective article on computational structural research in Portugal.

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