

Evolutione dynamiky proteinů

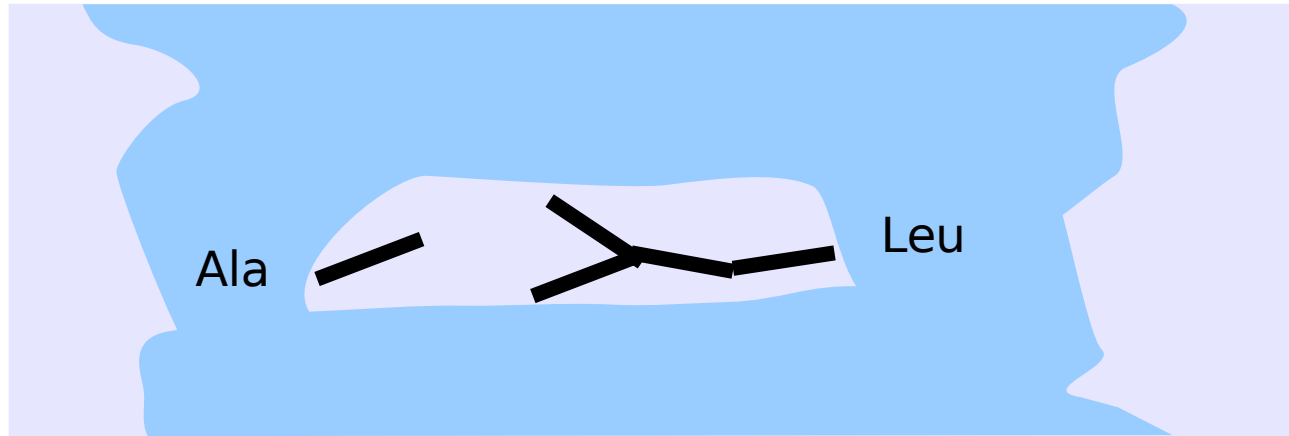
Vojtěch Spiwok

Koevoluce:

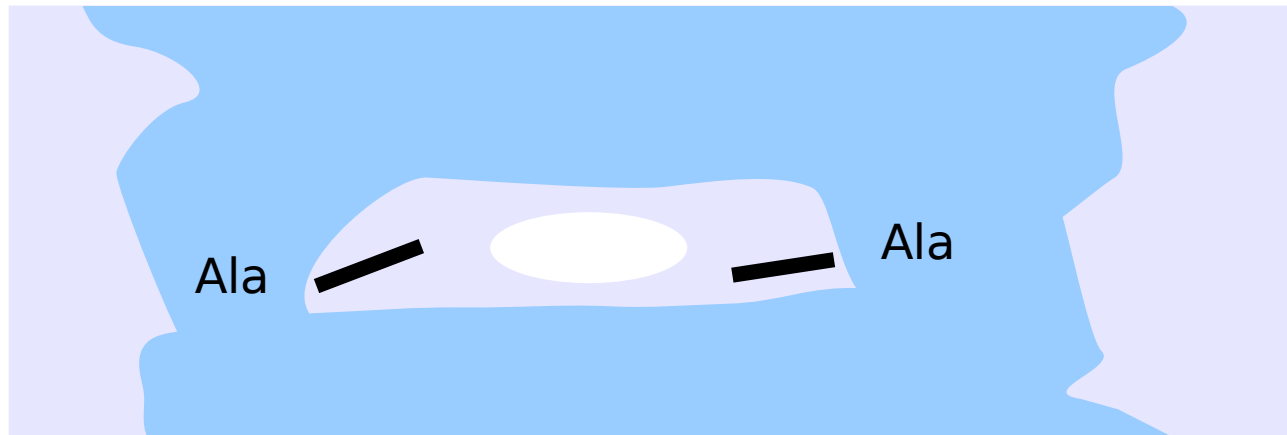
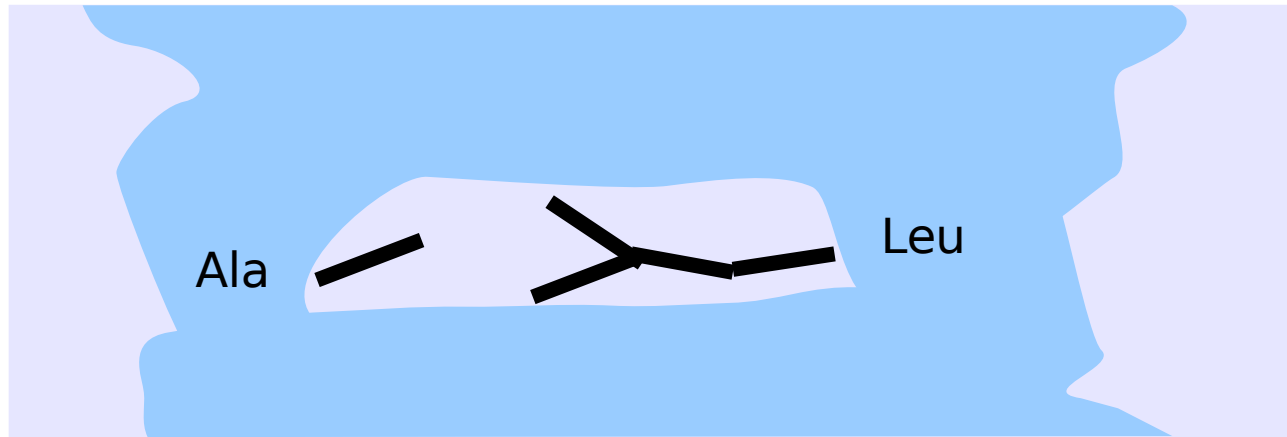
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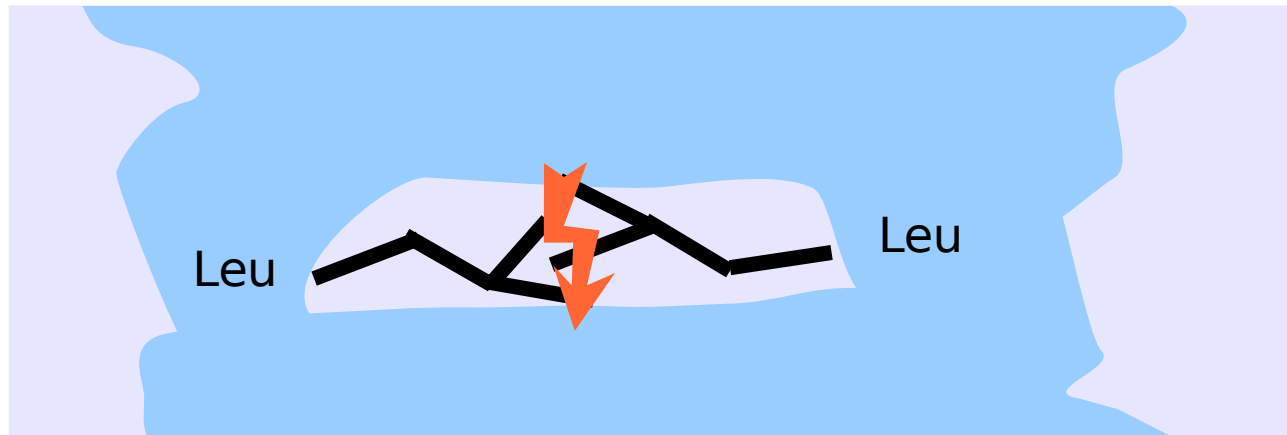
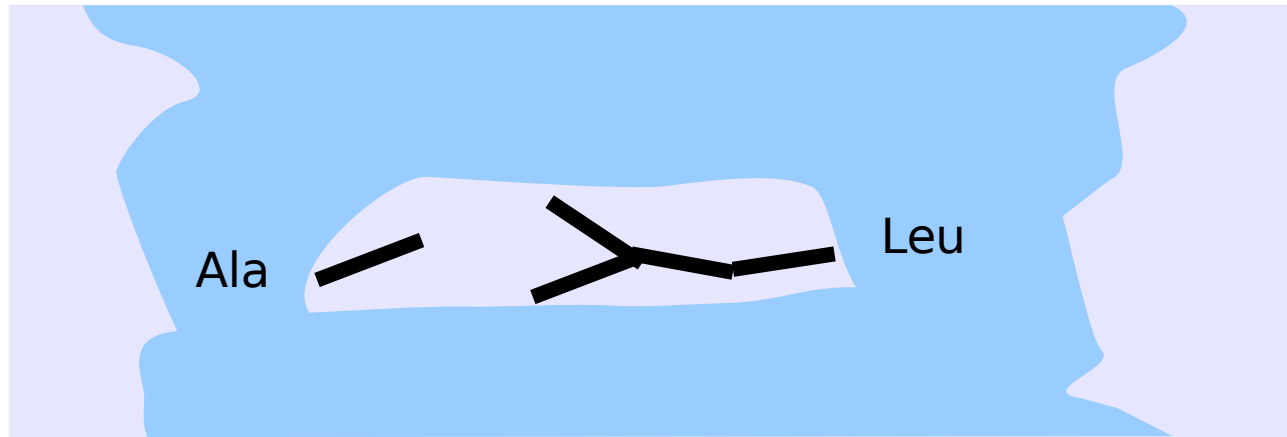
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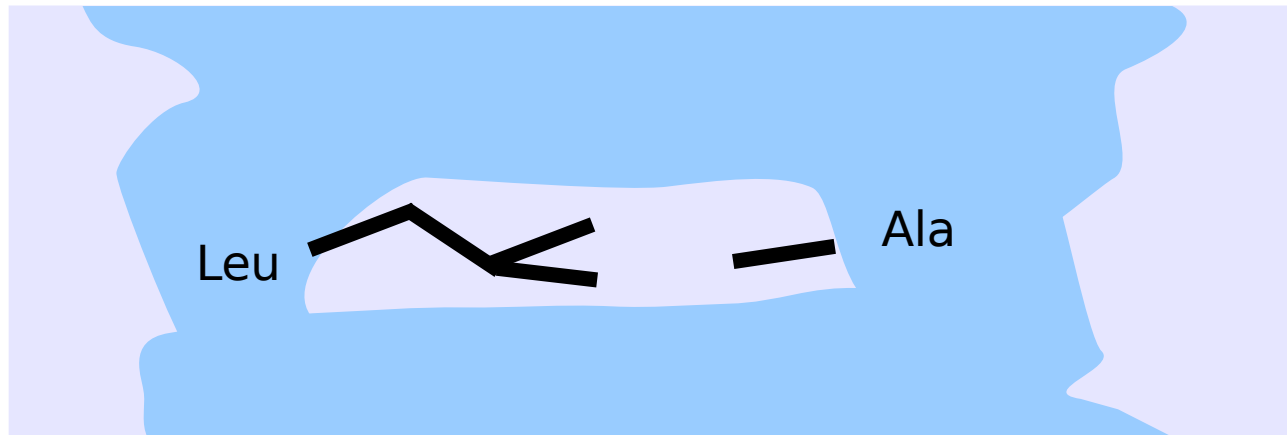
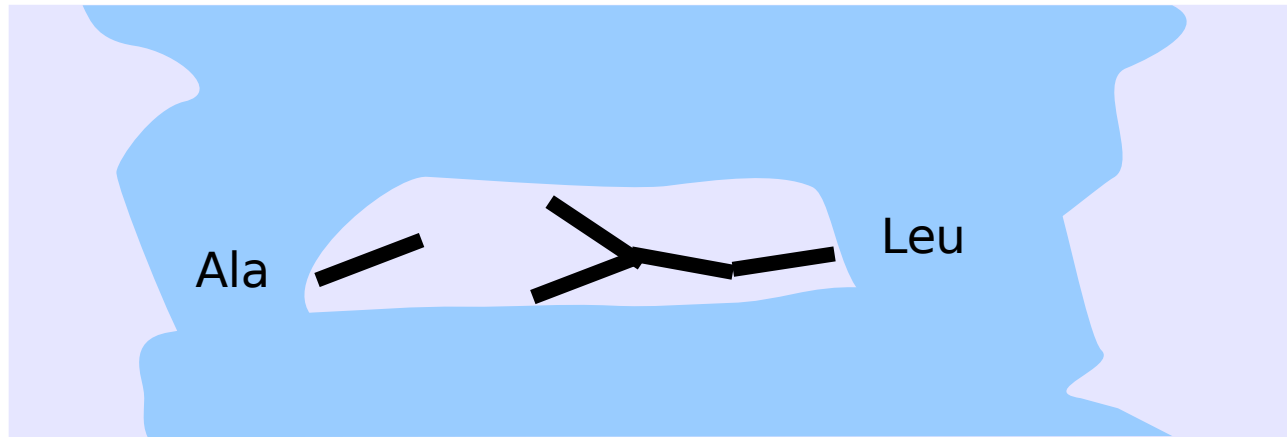
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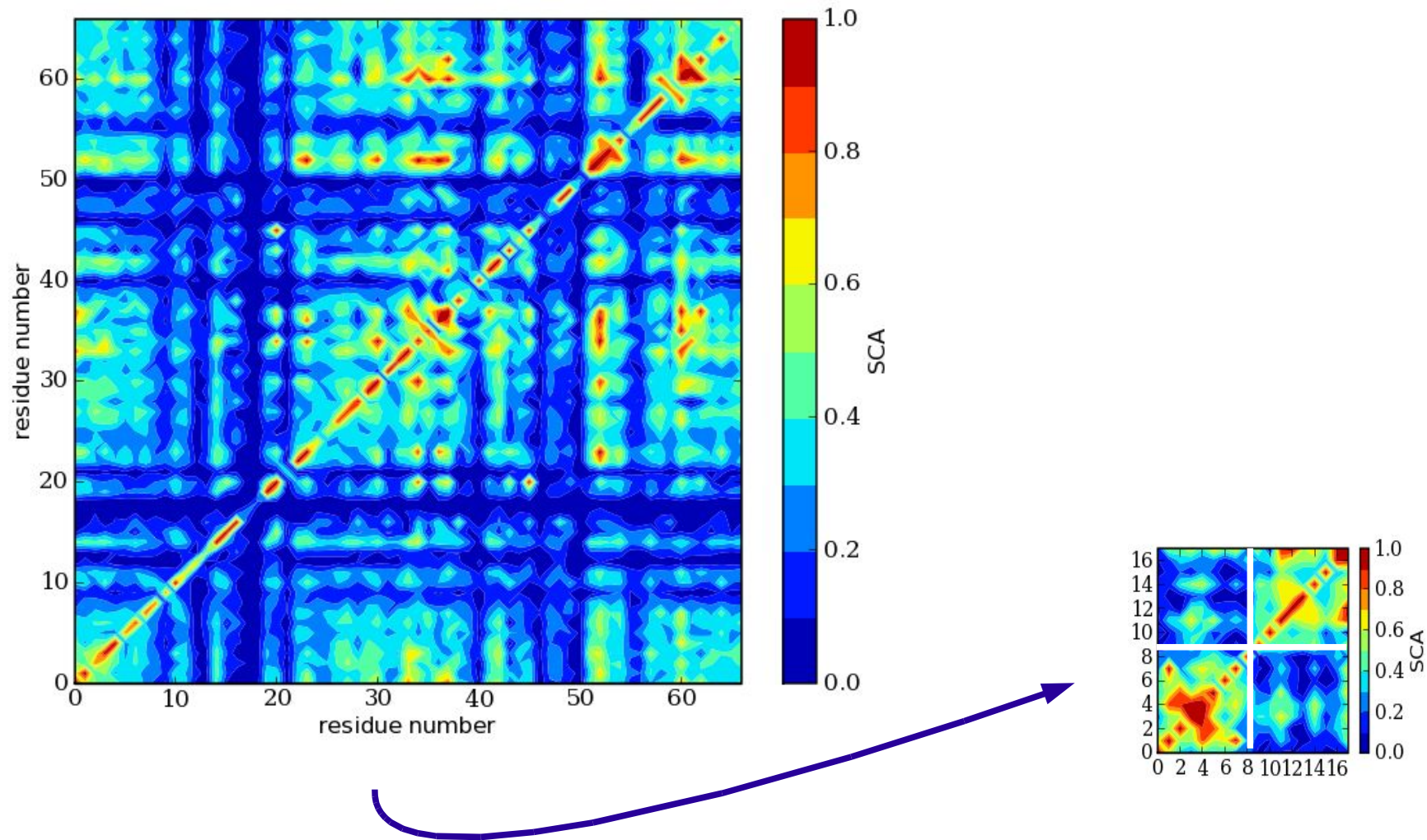
Koevoluce:



Koevoluce:

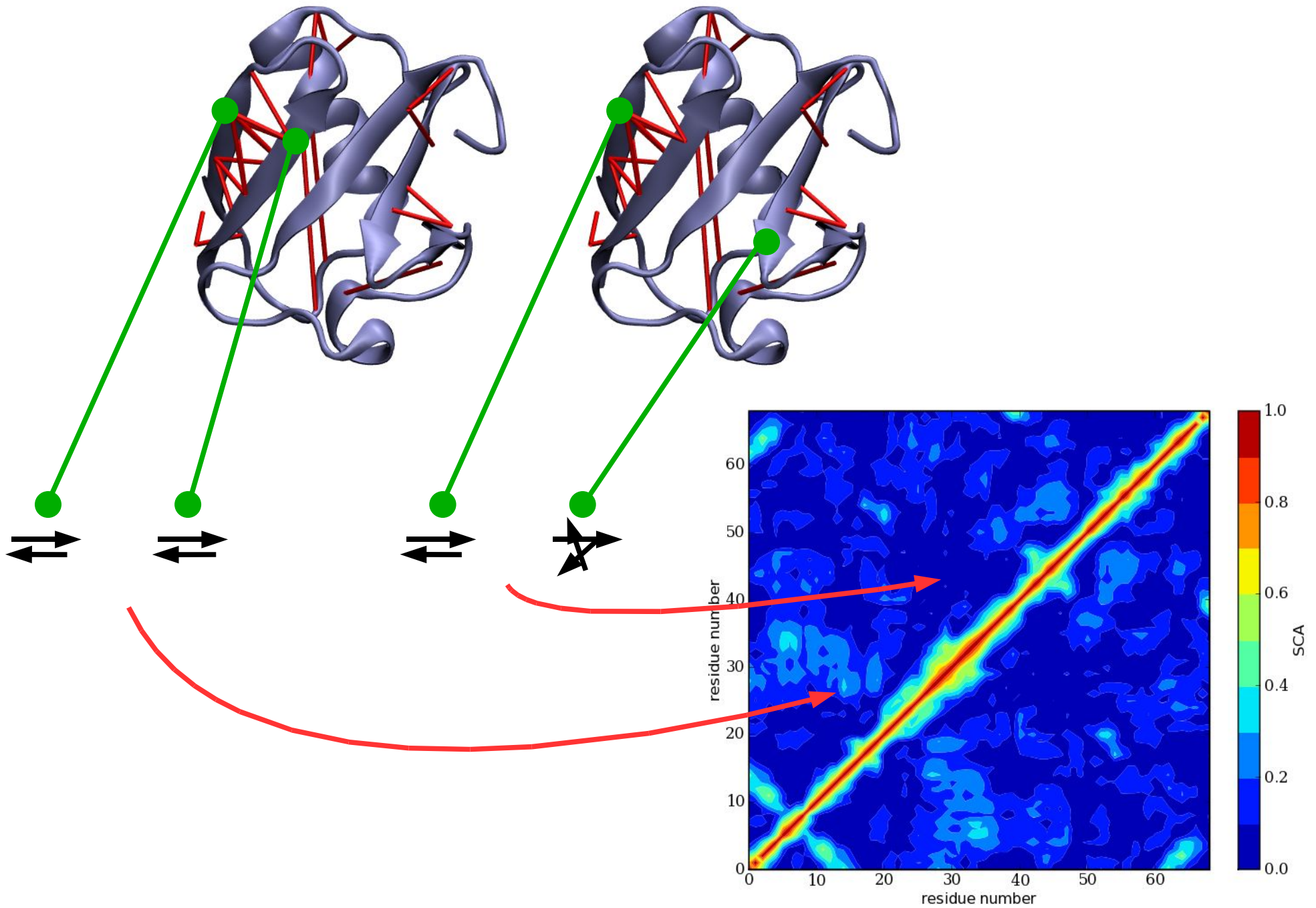


Proteinové sektory:

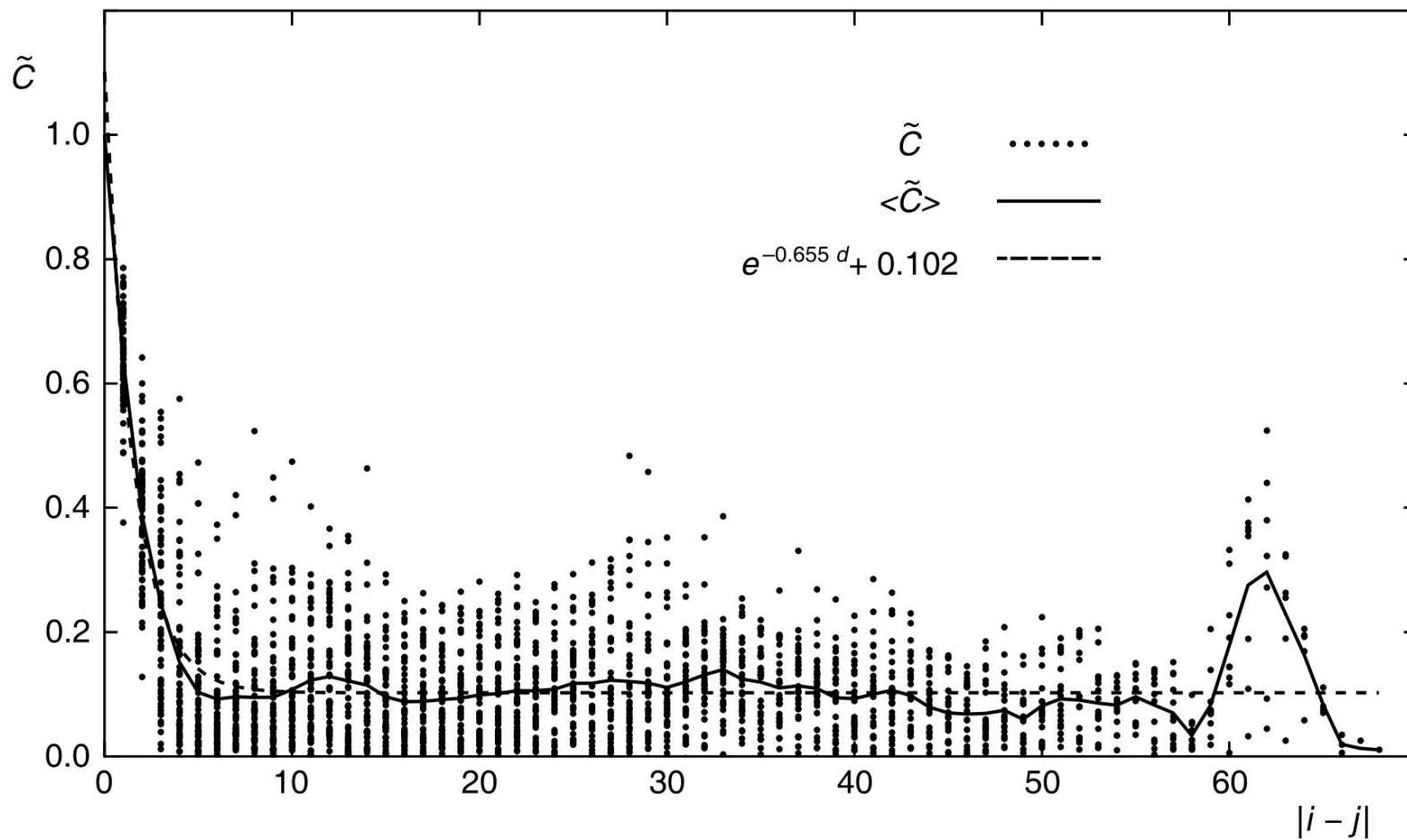


N Halabi, O Rivoire, S Leibler, R Ranganathan: Protein Sectors: Evolutionary Units of Three-Dimensional Structure. *Cell* (2009) **138**, 774.

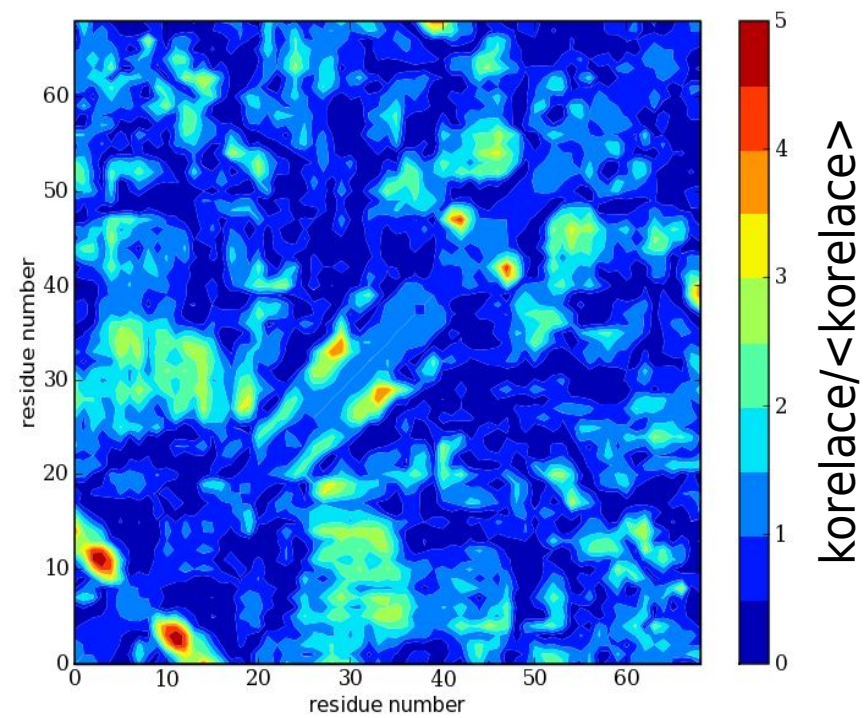
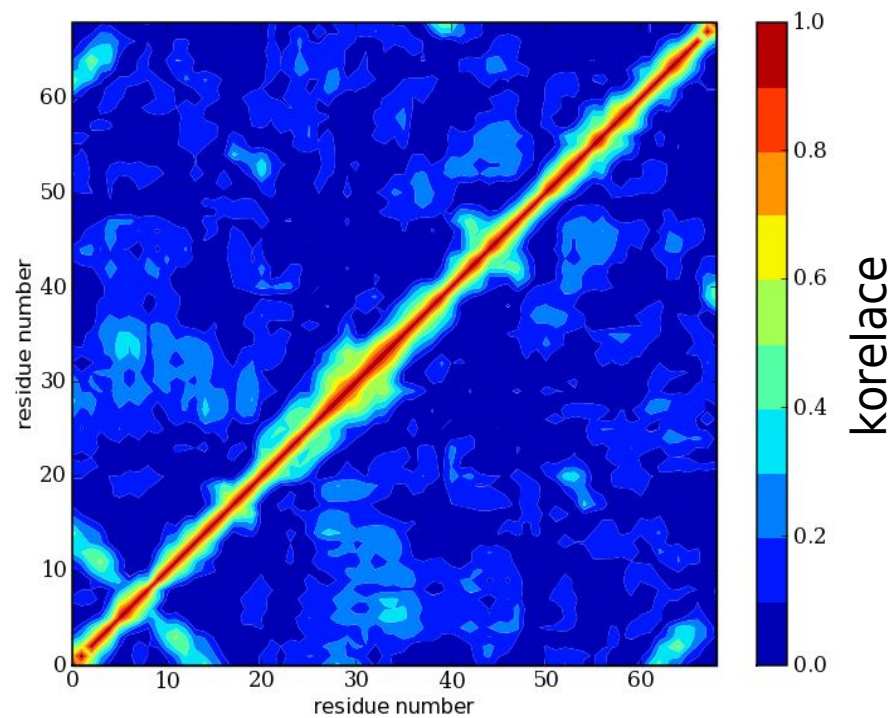
Kolektivní pohyby v molekulách:



Kolektivní pohyby v molekulách:



Kolektivní pohyby v molekulách:



Evoluce dynamiky:

Statistical coupling analysis:

844 sekvencí ubiquitinové rodiny (mnohočetné přiřazení PFAM)

identita < 95 %

67 pozic

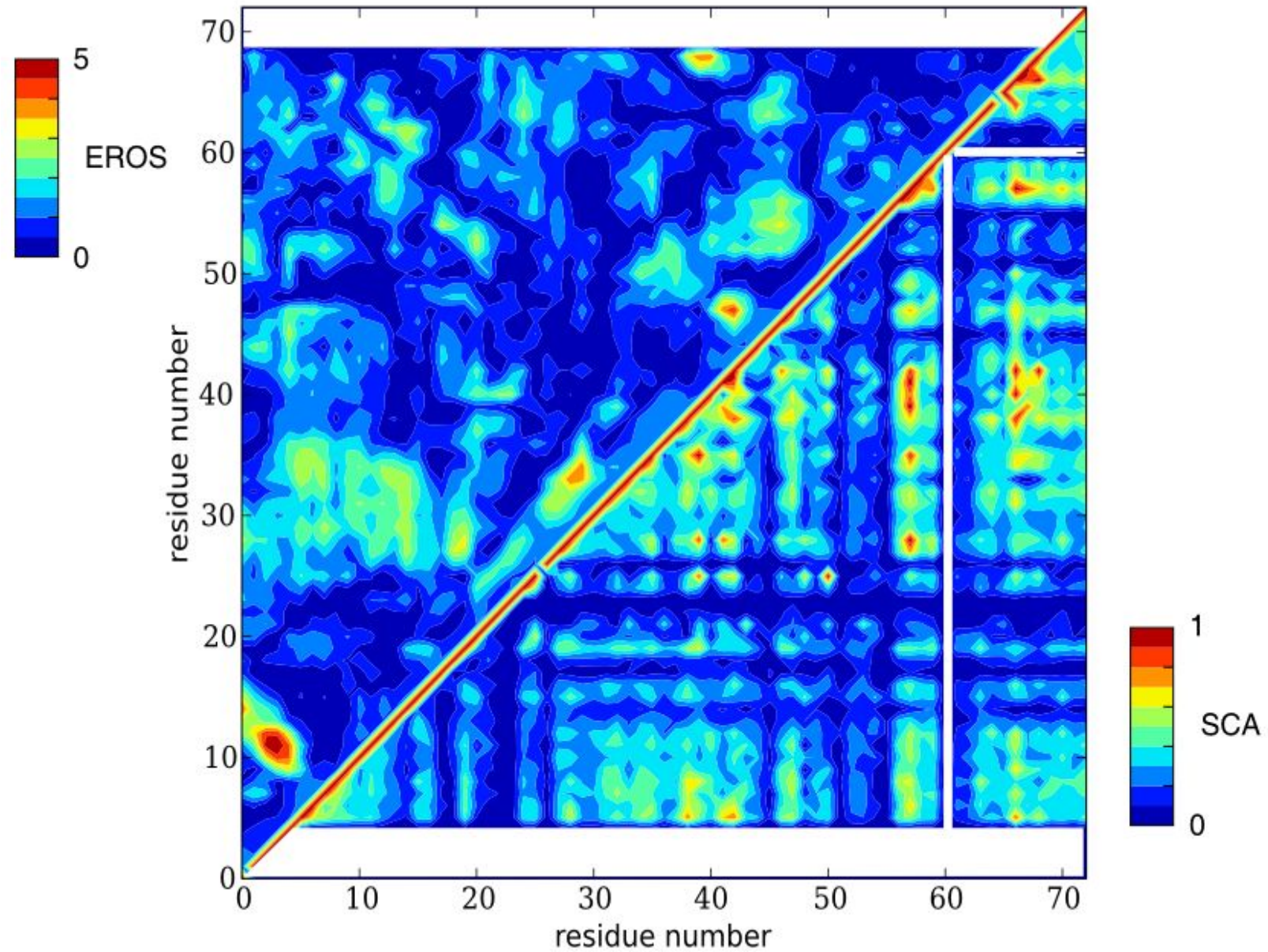
Analýza kolektivních pohybů:

EROS ensemble (PDB-ID: 2K39), 116 struktur

OF Lange, N-A Lakomek, C Farès, GF Schröder, KFA Walter, S Becker, J Meiler, H Grubmüller, C Griesinger, BL de Groot: Recognition Dynamics Up to Microseconds Revealed from an RDC-Derived Ubiquitin Ensemble in Solution. *Science* (2008) **320**, 1471.

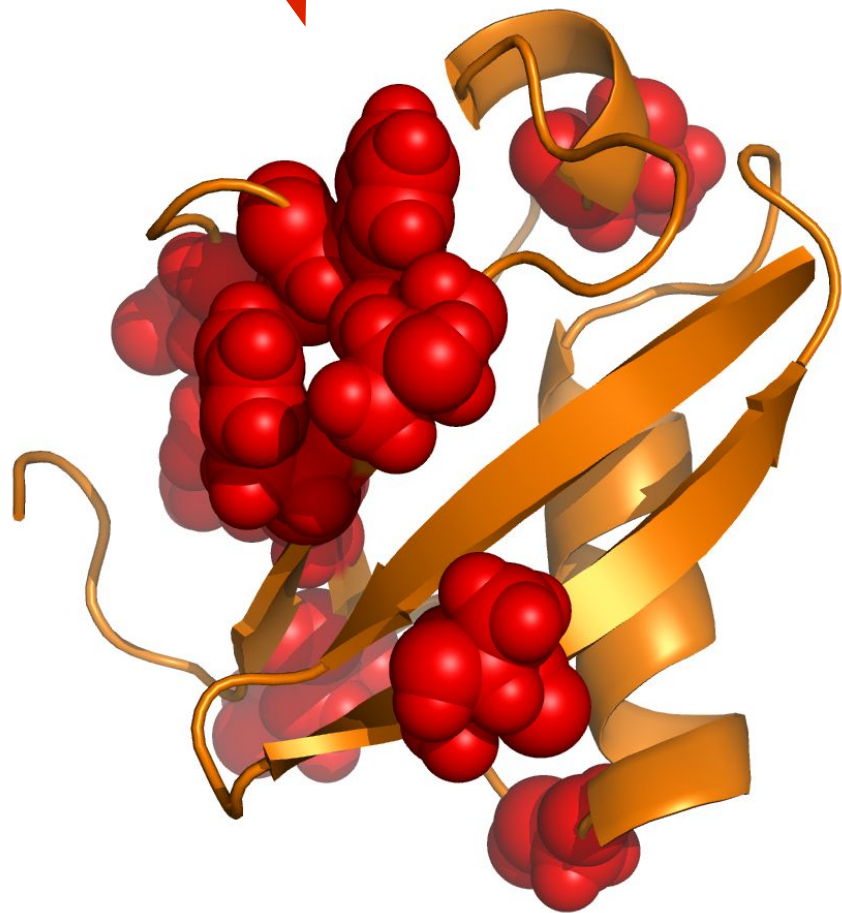
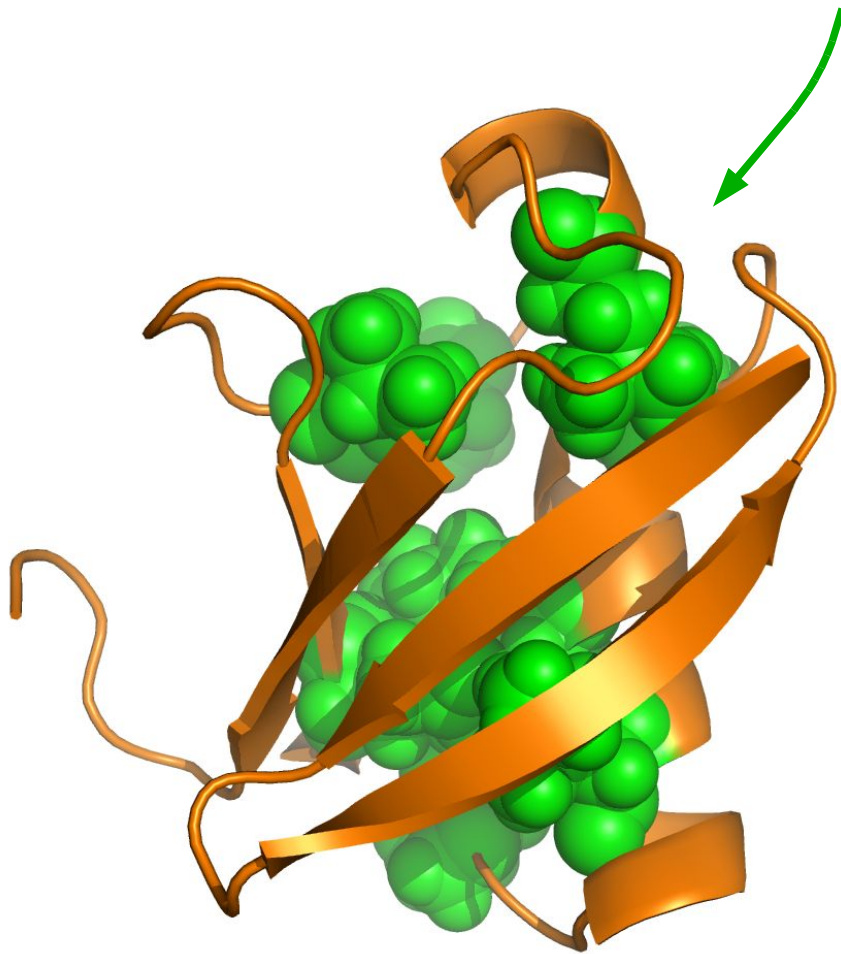
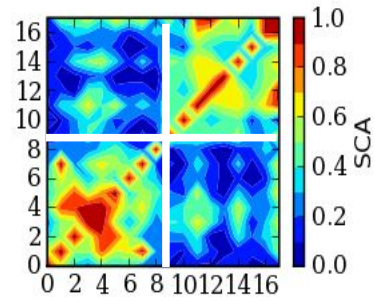
korelace / <korelace>

Evolve dynamiky:



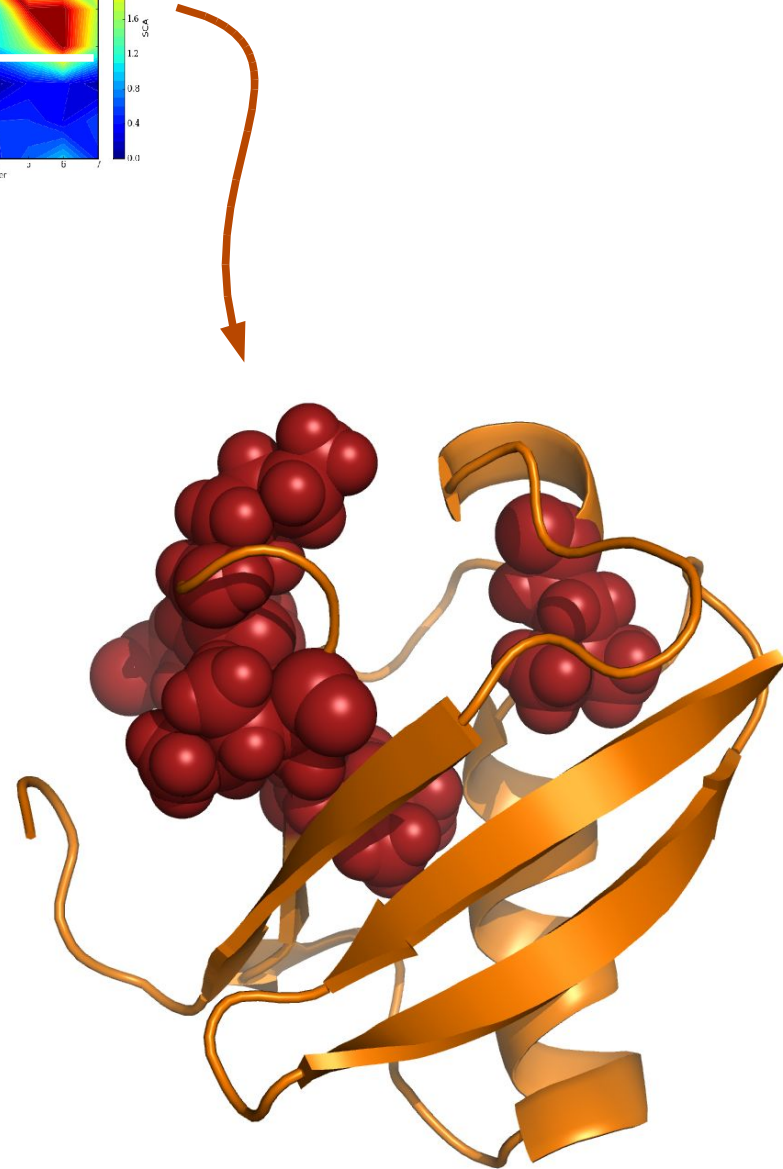
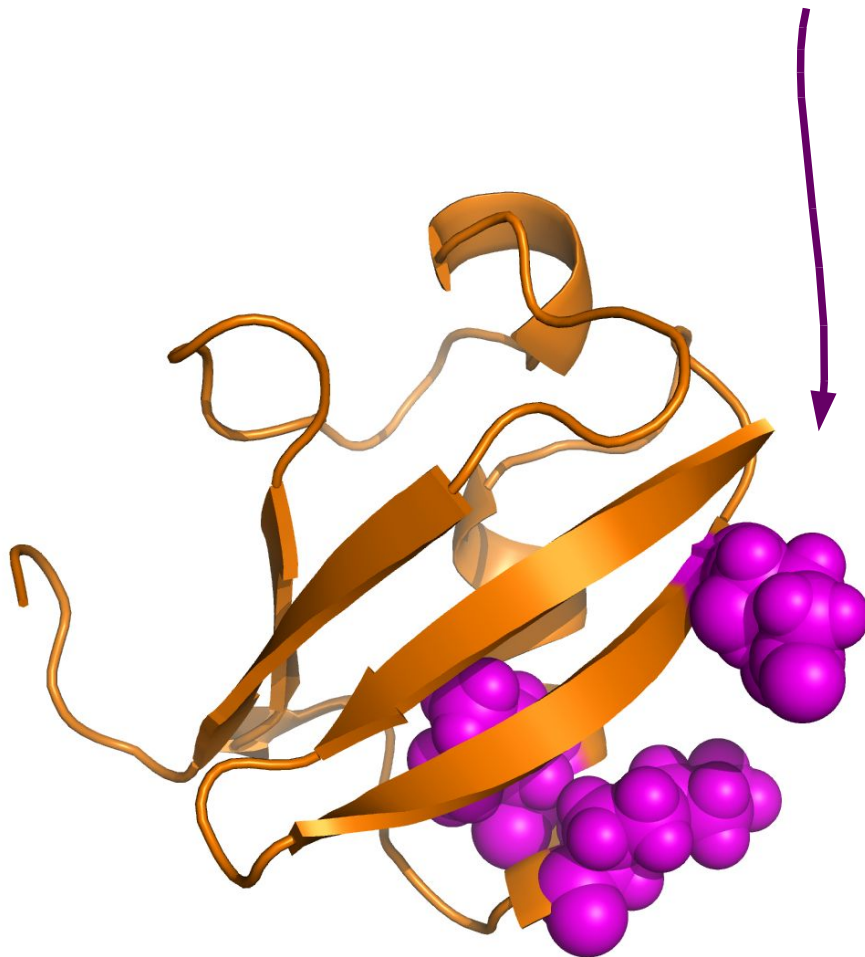
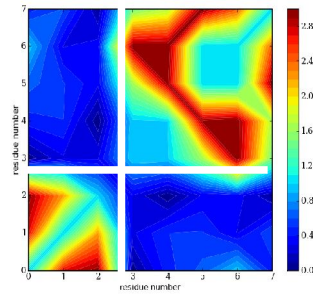
Evolve dynamiky:

SCA sektory



Evoluce dynamiky:

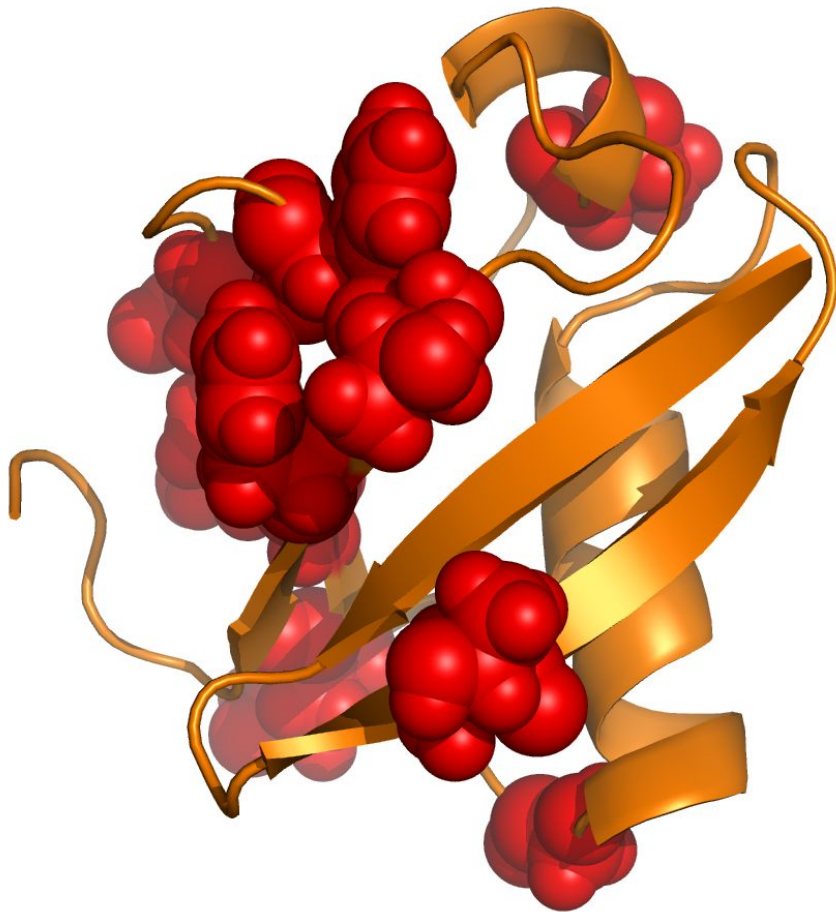
pohybové sektory



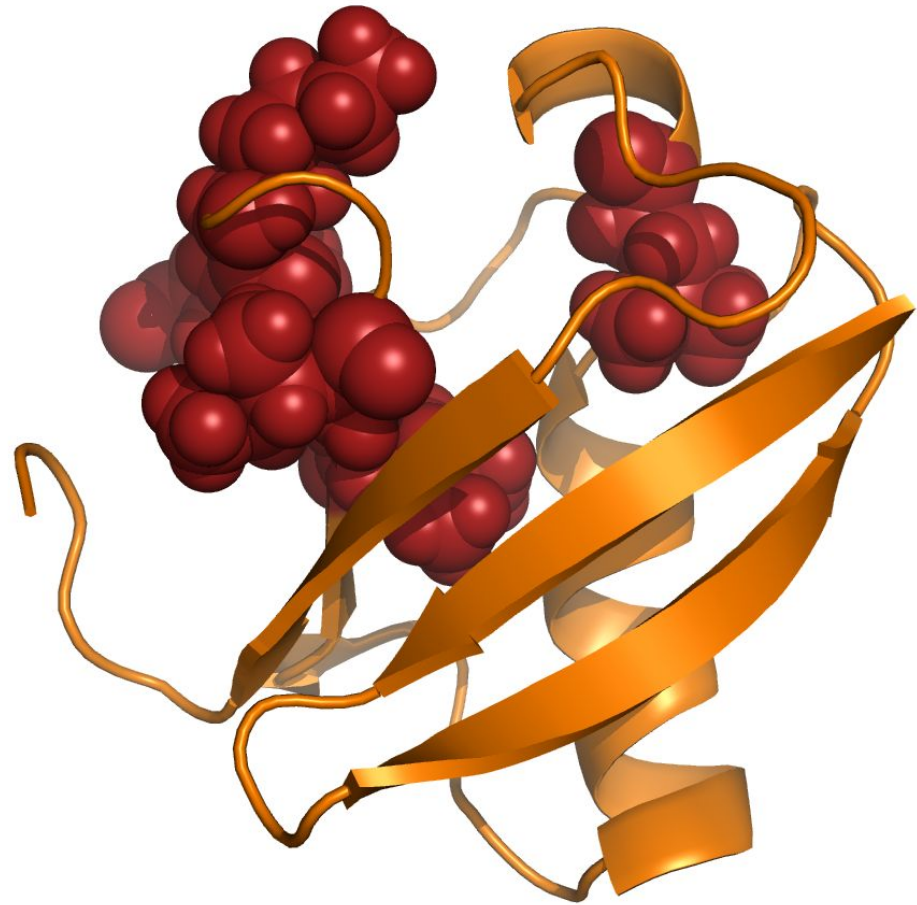
Evoluce dynamiky:

SCA vs. pohybové sektory

SCA



pohyby



Evoluce dynamiky:

-QIFVKTLTGKTITLEVEPSDTIENVKAKIQDKEGIPPDQQRLIFAGKQLEDGRTLSDYNIQKESTLHLV-----

-QIFVKTLTGKTITLEVEPSDTIENVKAKIQDKEGIPPDQQR**LI**FAG**K**QLEDGRT**L**SDYNIQKESTLHLV-----

-----TLTGKTITLEVESSD**T**IENV**KAKI**QDKEGIP**PD**Q**RL**IFAGK**QLED**GRT**L**SDYNI-KESTLHLVLRRLR--

-----TLTGKT**I**TLEVESSDTIENVKAKIQDKE**G**IPPD**Q**RL**I**FAG**K**QLEDGRT**L**SDYNI-KEST**LH**LVLRLR--

MQIFVKTLTGKTITLEVEPSDTIENVKAKIQDKEGIPPDQQRLIFAGKQLEDGRTLSDYNIQKESTLHLVLRRLRGG

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1

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20

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30

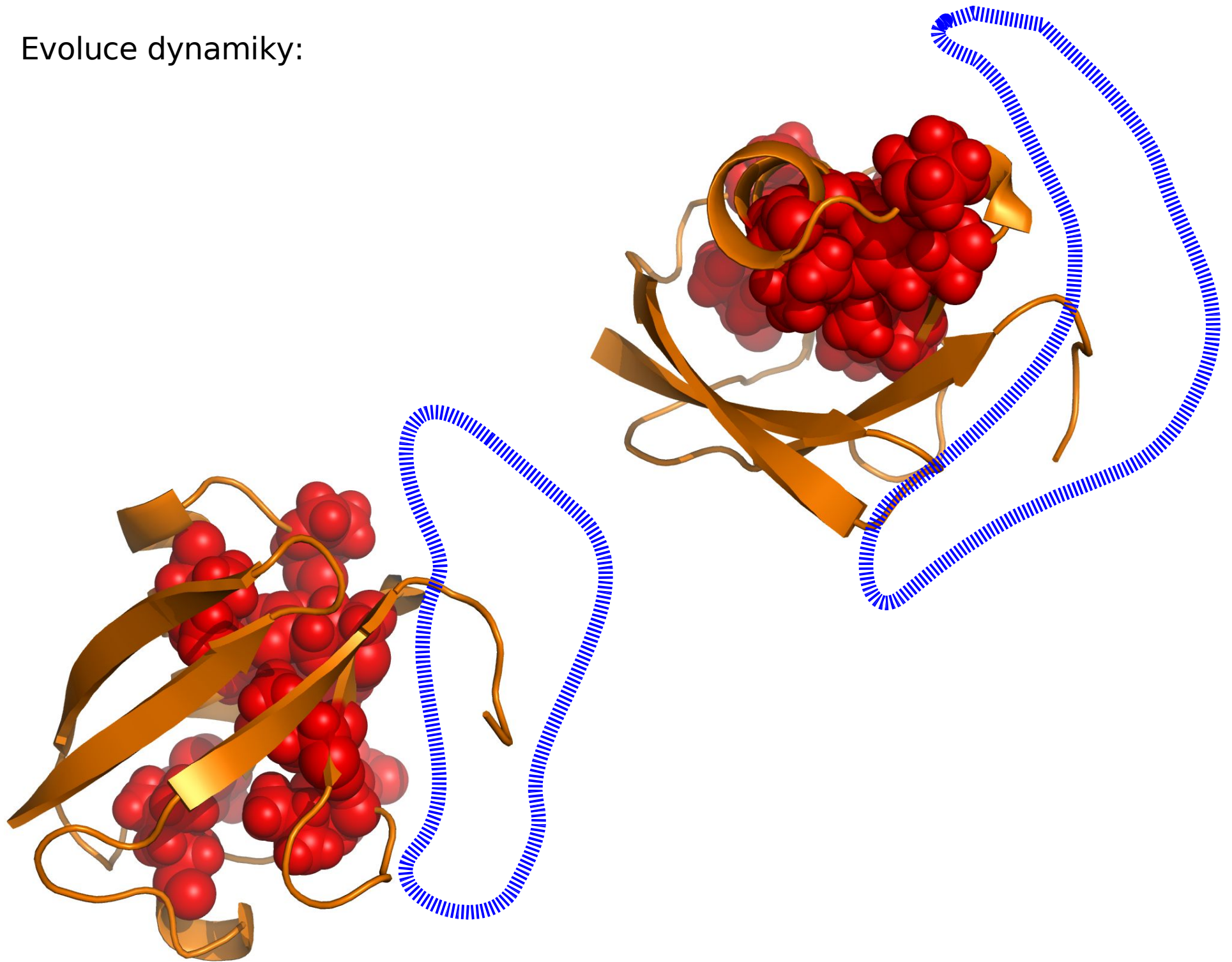
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50

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60

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70

Evolve dynamiky:



Shrnutí

Ko-evoluce aminokyselinových zbytků proteinů probíhá nezávisle na vzdálenosti v polypeptidovém řetězci

Kolektivní pohyby u sekvenčně blízkých zbytků jsou silnější

I přesto je možné vystopovat oblast, v níž je na jedné straně svázána evoluce a na druhé straně svázán pohyb atomů