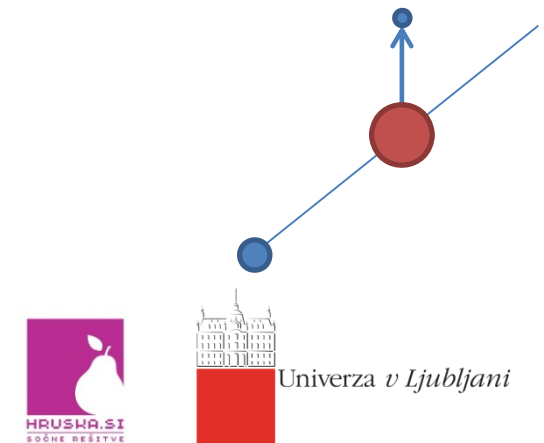


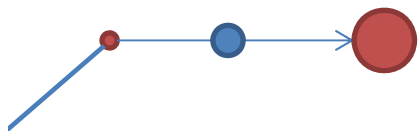
# Network Analysis of Publications on Topological Indices from Web of Science

Computers in Scientific Discovery 6

Jernej Bodlaj,  
Vladimir Batagelj

Ljubljana, 25<sup>th</sup> August, 2012





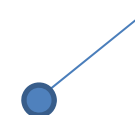
# Presentation Outline

- Motivation
  - To obtain data for testing our new algorithm
  - To explore scientific community behind *topological indices*<sup>1</sup>
    - scientometric analysis
- Preparation of bibliographic data
  - Web of Science<sup>2</sup>
  - *Wos2Pajek*<sup>3</sup> tool
- Analysis results
  - citations between authors
  - citation path
  - journals
  - keywords
  - ...
- net.Plexor
  - network analysis and visualization tool

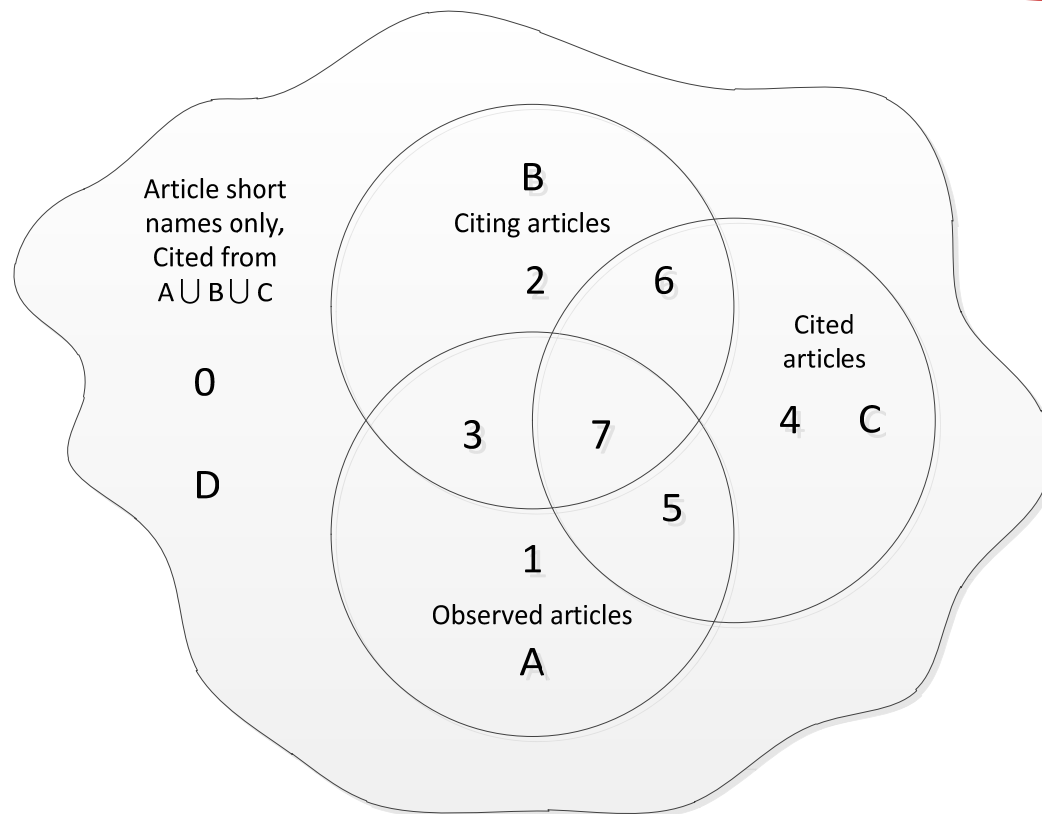
<sup>1</sup> W. R. Mueller, K. Szymanski, J. V. Knop, N. Trinajstić, *Molecular Topological Index*, J. Chem. Inf. Comput. Sci. 30, pp. 160-163, 1990.

<sup>2</sup> <http://isiknowledge.com/>

<sup>3</sup> <http://pajek.imfm.si/doku.php?id=wos2pajek>

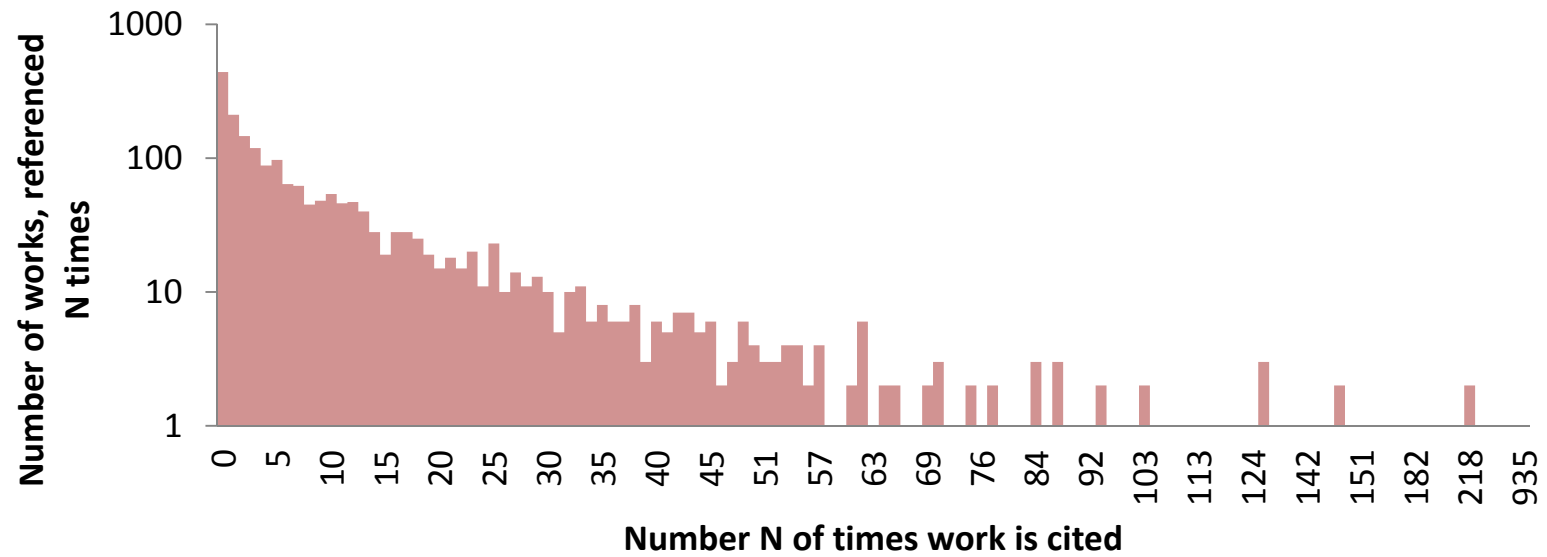
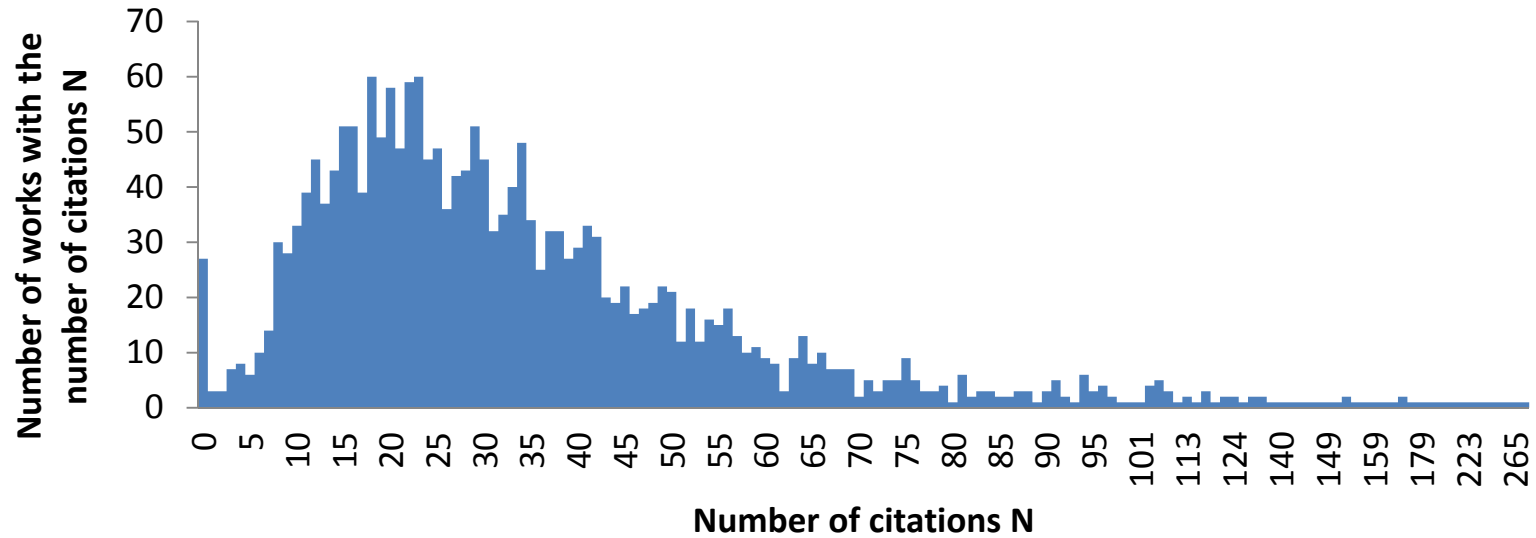


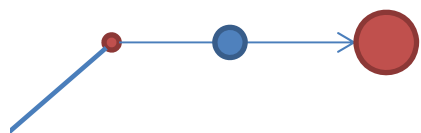
# Dataset



- Boundary problem
  - we remove works, which do not cite any further work, being cited less than 3 times
- Descriptions of works
  - $|A| = 1993$ ,  $|B| = 10787$ ,  $|C| = 2225$ ,  $|D| = 3011$

# Citing Distribution





# The Most Cited Works

**935x HOSOYA\_H(1971)44:2332**

**Topological index - newly proposed quantity characterizing topological nature of structural isomers of saturated hydrocarbons**

Bulletin of the chemical society of Japan

**647x BALABAN\_A(1982)89:399**

**Highly discriminating distance-based topological index**

Chemical physics letters

**314x BALABAN\_A(1983)114:21**

**Topological indexes for structure-activity correlations**

Topics in current chemistry

**259x DOBRYNIN\_A(2001)66:211**

**Wiener index of trees: Theory and applications**

Acta applicandae mathematicae

**226x BALABAN\_A(1983)55:199**

**Topological indexes based on topological distances in molecular graphs**

Pure and applied chemistry

**218x MACCHI\_P(2003)238:383**

**Chemical bonding in transition metal carbonyl clusters: complementary analysis of theoretical and experimental electron densities**

Coordination chemistry reviews

**218x RANDIC\_M(1991)31:311**

**Resolution of ambiguities in structure - property studies by use of orthogonal descriptors**

Journal of chemical information and computer sciences

**215x MIHALIC\_Z(1992)69:701**

**A graph-theoretical approach to structure property relationships**

Journal of chemical education

**209x RANDIC\_M(1991)15:517**

**Orthogonal molecular descriptors**

New journal of chemistry

**193x SCHULTZ\_H(1989)29:227**

**Topological organic-chemistry .1. Graph-theory and topological indexes of alkanes**

Journal of chemical information and computer sciences

**190x SABLJIC\_A(1981)31:189**

**182x GUTMAN\_I(1993)32:651**

**176x KATRITZK\_A(1993)33:835**

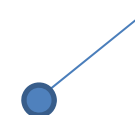
**165x KATRITZK\_A(1996)100:10400**

**156x DOBRYNIN\_A(2002)72:247**

**152x NIKOLIC\_S(2003)76:113**

**151x GALVEZ\_J(1995)35:272**

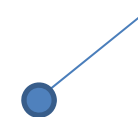
**149x ESTRADA\_E(2001)8:1573**



# SPC → Strongest Citation Path



- ..1975
  - molecular graph theory
- ..1980
  - the molecular structure and their chemical properties
  - term “topological index”
- ..early nineties
  - development of quantitative structure–activity relationships

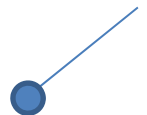


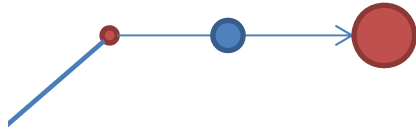


# SPC → Strongest Citation Path



- nineties
  - study of topological descriptors
  - development of predictive models
- the topic mostly evolved by the middle of nineties





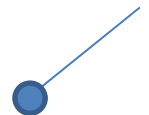
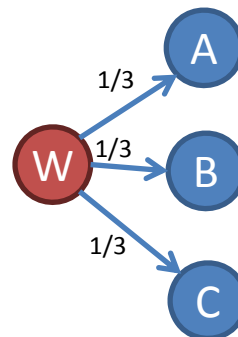
# Number of Works / Author

- Normalized number of articles per individual author:

NA	Author
233,85	RANDIC_M
226,38	GUTMAN_I
136,39	BALABAN_A
103,88	DIUDEA_M
92,89	BASAK_S
90,28	TRINAJST_N
88,40	IVANCIUC_O
77,13	KIER_L
71,54	ESTRADA_E
67,83	CHOU_K
66,44	BONCHEV_D
59,65	ASHRAFI_A

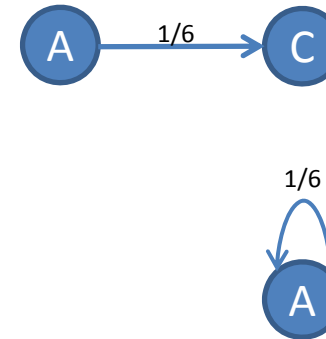
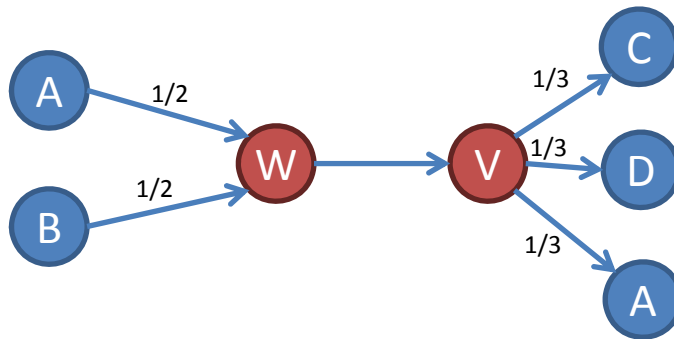
NA	Author
59,40	KHADIKAR_P
55,07	PYKA_A
54,20	TORRENS_F
49,92	HOSOYA_H
48,98	ZHOU_B
45,59	TOROPOV_A
44,98	KLEIN_D
44,57	GONZALEZ_H
44,57	HALL_L
43,47	ROUVRAY_D
40,59	POGLIANI_L

NA	Author
38,39	DOBRYNIN_A
38,28	MEKENYAN_O
38,03	VUKICEVI_D
36,74	LUKOVITS_I
36,38	ROY_K
35,87	KATRITZK_A
35,33	AIHARA_J
34,72	XU_L
33,66	AGRAWAL_V
32,80	HANSCH_C
32,36	BALASUBR_K
31,60	GHOORBANI_M



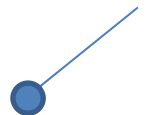


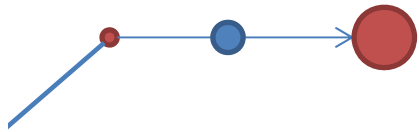
# Author citing another Author



Author	Cited author	Times cited
IVANCIUC_O	BALABAN_A	223,94
RANDIC_M	BALABAN_A	211,68
RANDIC_M	TRINAJST_N	177,37
ESTRADA_E	RANDIC_M	176,91
BALABAN_A	RANDIC_M	176,02
TRINAJST_N	RANDIC_M	168,81
IVANCIUC_O	DIUDEA_M	164,97
ASHRAFI_A	DIUDEA_M	164,44
POGLIANI_L	RANDIC_M	147,93
RANDIC_M	KIER_L	141,41

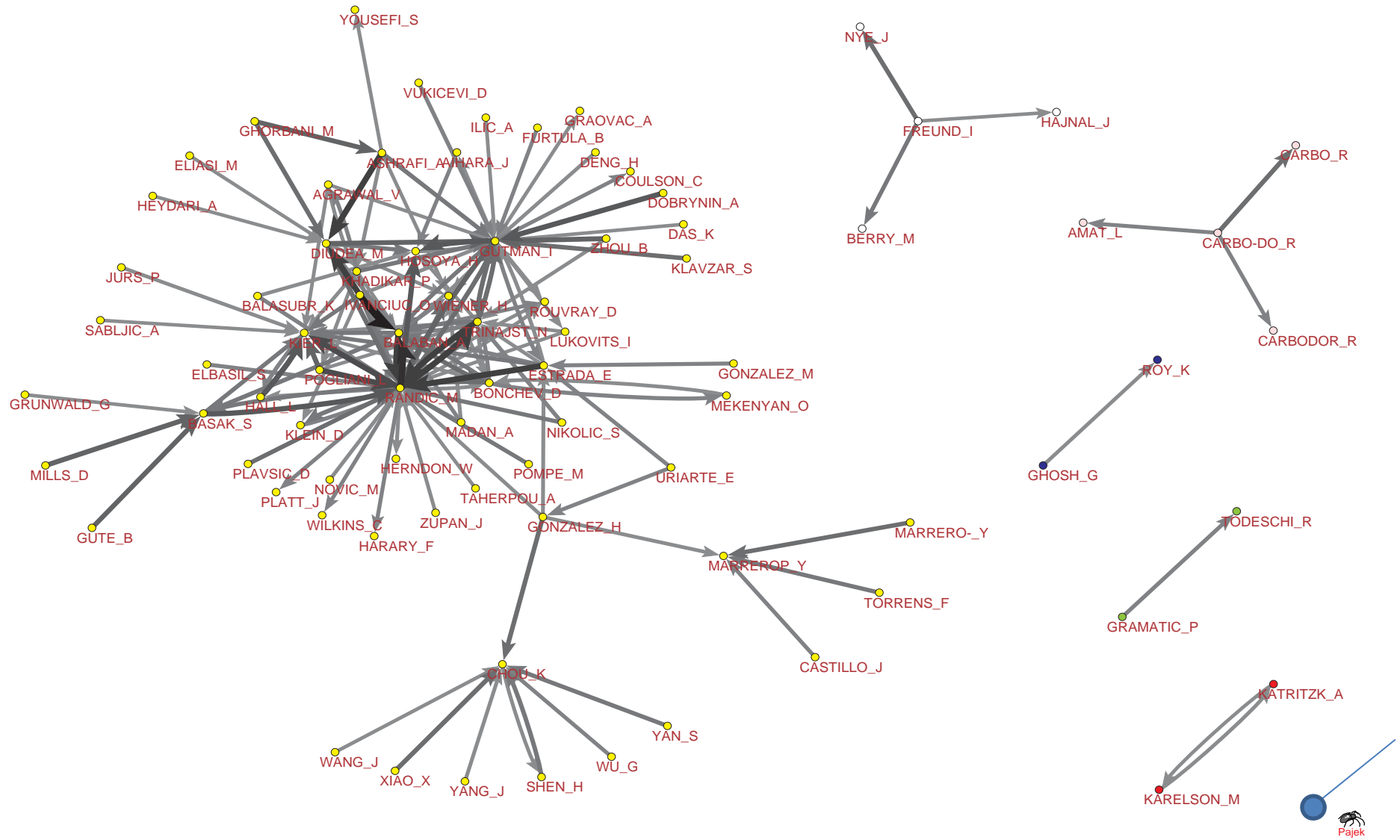
Author	Cited author	Times cited
GUTMAN_I	HOSOYA_H	132,52
HALL_L	KIER_L	131,91
BASAK_S	RANDIC_M	128,98
DOBRYNIN_A	GUTMAN_I	126,13
RANDIC_M	HOSOYA_H	113,96
MILLS_D	BASAK_S	111,15
ZHOU_B	GUTMAN_I	108,43
POGLIANI_L	KIER_L	103,95
DIUDEA_M	GUTMAN_I	99,39
GUTE_B	BASAK_S	97,10





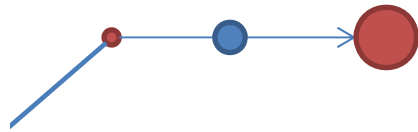
# Citing another Author - Visual

- Generalized cores (log scale):  $t=2.2$



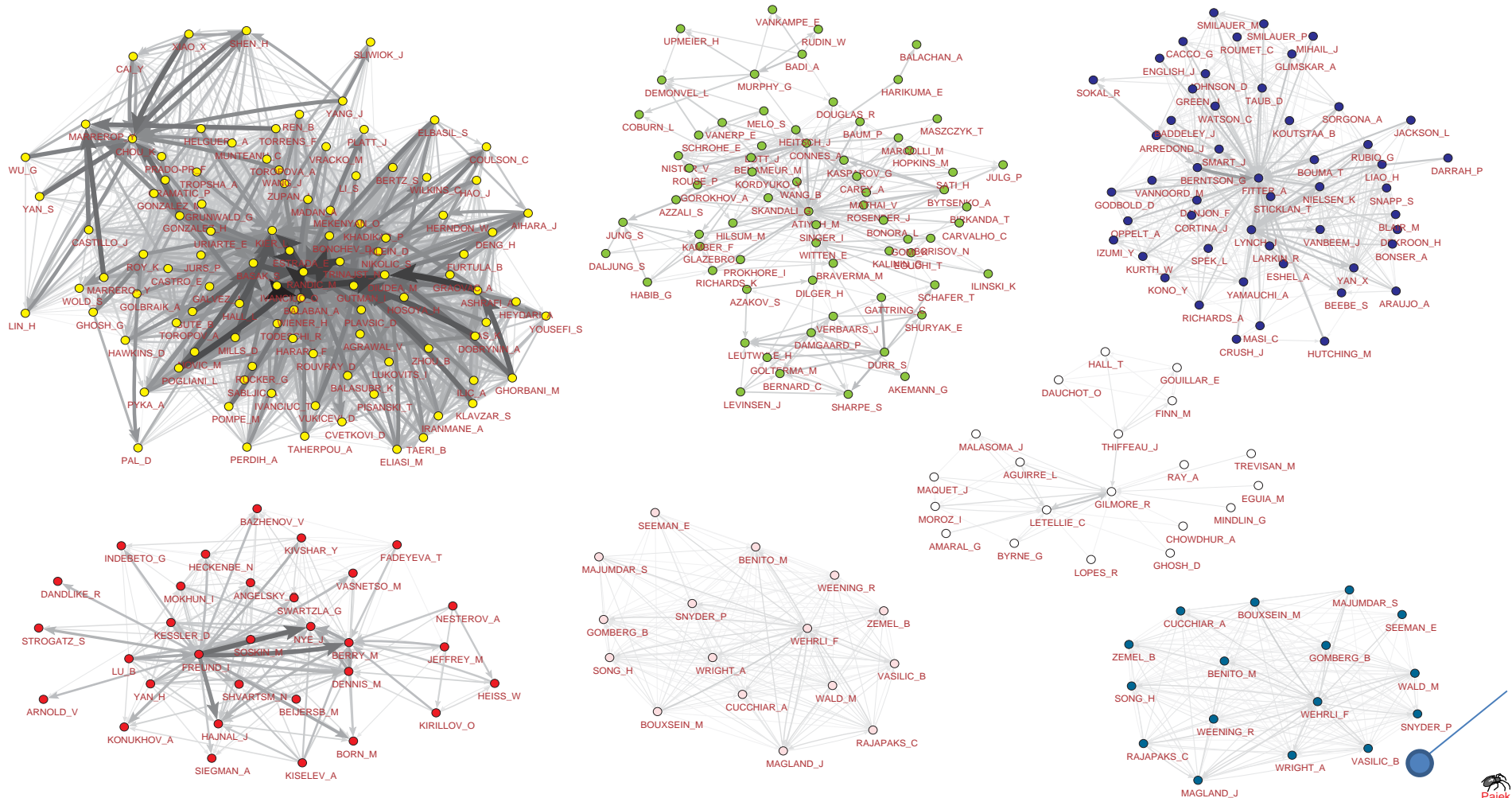
# Self Citing

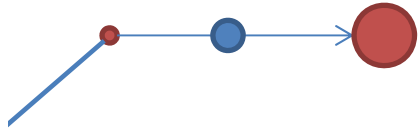
Number of self-citations (NS)	Number of articles (NA)	Author	NS/NA
1687,89	233,85	RANDIC_M	7,22
266,12	40,59	POGLIANI_L	6,56
189,33	35,33	AIHARA_J	5,36
66,68	13,92	GHARAGHE_F	4,79
302,54	67,83	CHOU_K	4,46
375,87	88,40	IVANCIUC_O	4,25
132,51	31,35	FREUND_I	4,23
300,95	71,54	ESTRADA_E	4,21
49,13	12,16	REN_B	4,04
100,13	25,51	SABLJIC_A	3,92
51,60	13,20	PERDIH_A	3,91
509,75	136,39	BALABAN_A	3,74
126,39	36,38	ROY_K	3,47
172,12	49,92	HOSOYA_H	3,45
184,69	54,20	TORRENS_F	3,41
60,90	17,92	BADER_R	3,40
344,91	103,88	DIUDEA_M	3,32
138,39	44,57	GONZALEZ_H	3,10
281,08	92,89	BASAK_S	3,03
164,85	55,07	PYKA_A	2,99
46,22	15,75	RAOS_N	2,93
194,59	66,44	BONCHEV_D	2,93
91,34	31,60	GHORBANI_M	2,89
46,90	17,87	TAHERPOU_A	2,63



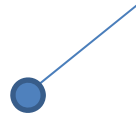
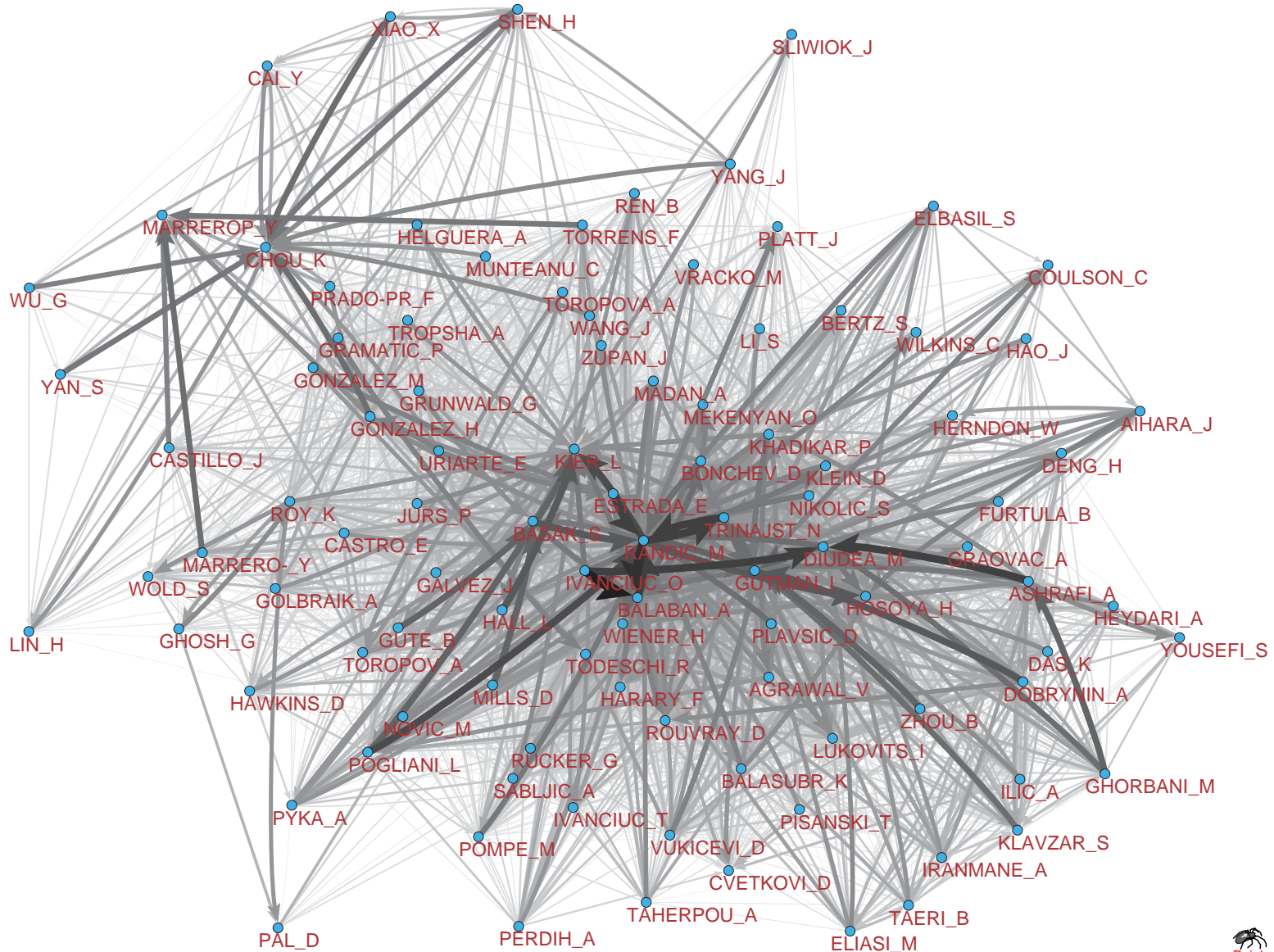
# Islands of Authors

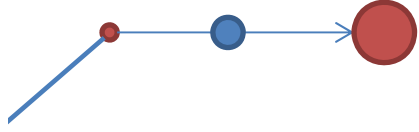
- We identified 29 islands in normalized collaboration network, sized from 5 to 100 authors.
- 7 islands is composed of more than 10 authors:





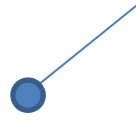
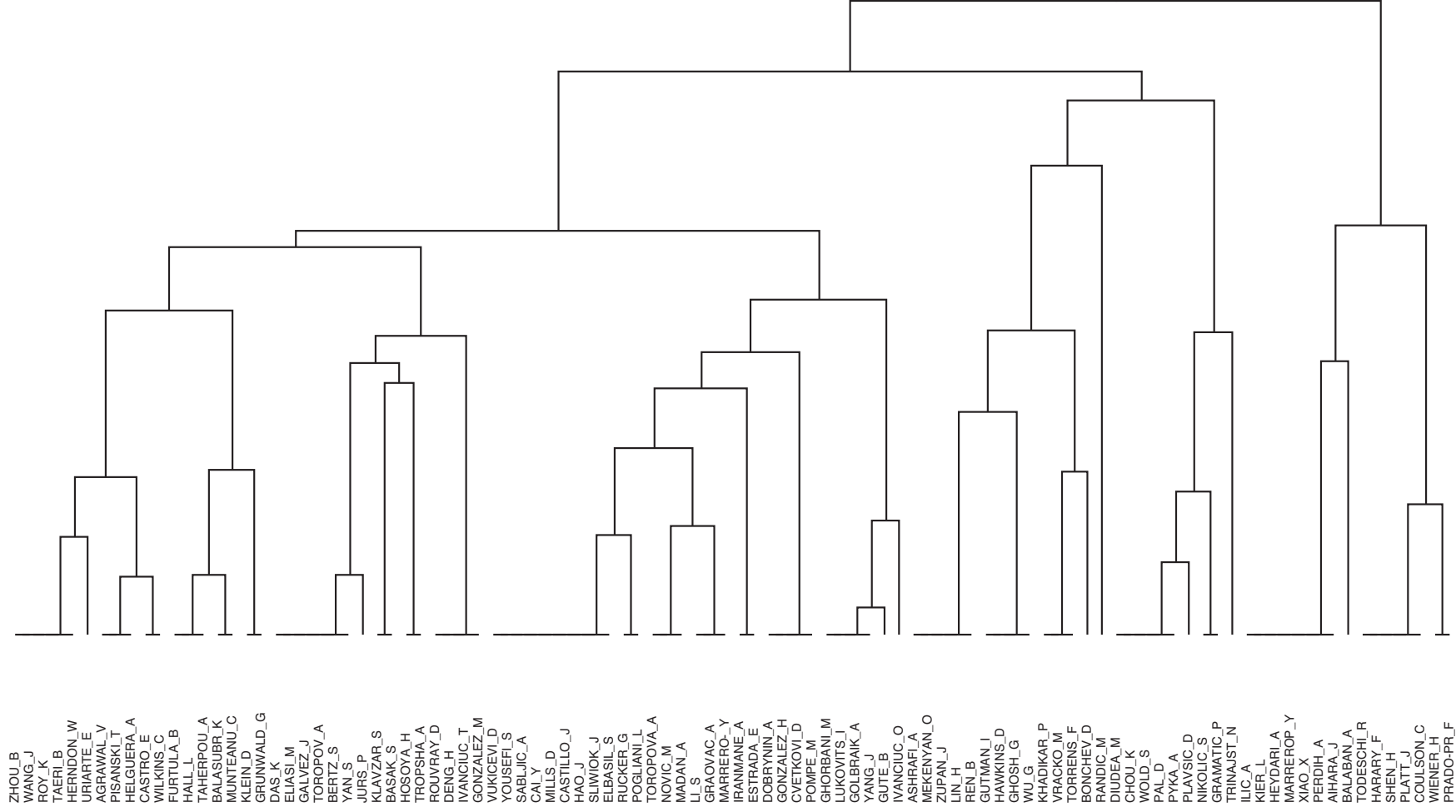
# The Largest Island of Authors

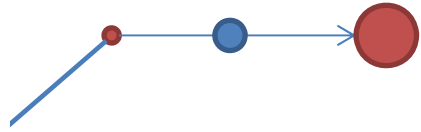




# The Largest Island – Hierarchy

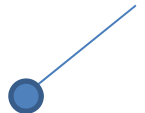
Pajek - Ward [0.00,5.59]



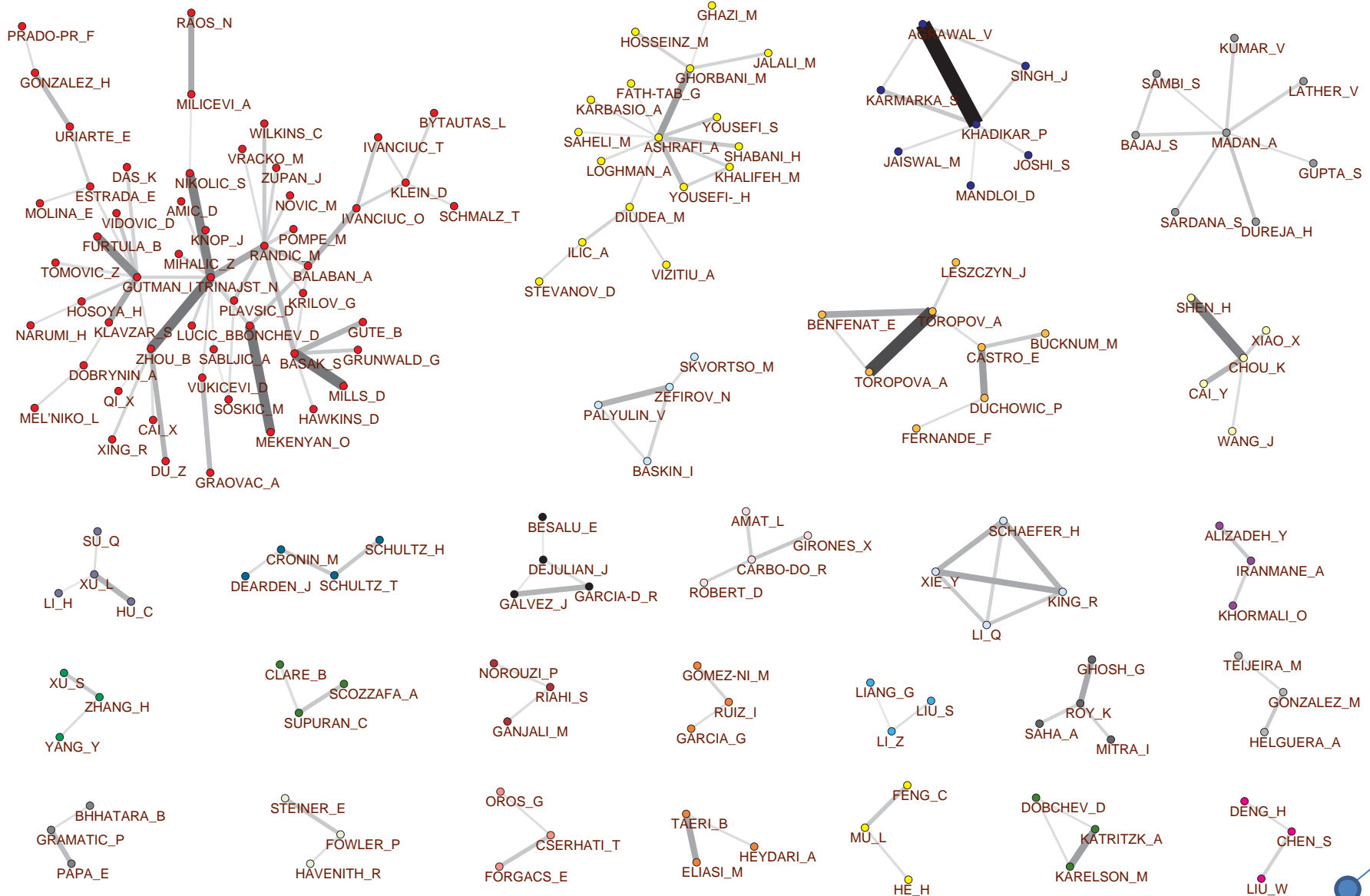
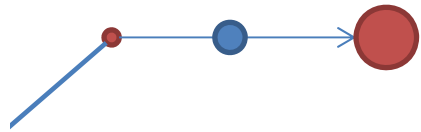


# Co-authorship

- Co-authorship connected components:
  - 1365 components of 2 or more authors,
  - 939 of 3 or more,
  - 574 of 4 or more,
  - ...
  - 1, the largest component consist of 11363 authors.
- Valued cores on the largest component
  - 67 groups of collaborating authors on at least 1.0 works,  $t=11$
  - Largest group: 53 authors

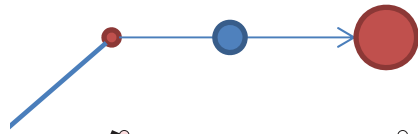


# Valued Cores of Authors





# Valued Cores of Authors



HALL\_L  
R\_L

HANSCH\_C  
VERMA\_R

LUKOVITS\_I  
LINERT\_W

GHASEMI\_J  
SAAIDPOU\_S

CABALLER\_J  
FERNANDE\_M

YUAN\_H  
CAO\_C

BADER\_R  
KEITH\_T

MACCHI\_P  
SIRONI\_A

GOLBRAIK\_A  
TROPASHA\_A

YEH\_Y  
YAN\_W

THAKUR\_A  
THAKUR\_M

KVASNICK\_V  
POSPICHA\_J

BAGCHI\_M  
NANDI\_S

TORRENS\_F  
CASTELLA\_G

YAZDANI\_J  
BAHRAMI\_A

HEMMATEE\_B  
MIRI\_R

LIU\_B  
LIU\_M

NATARAJA\_R  
NIRDOSH\_I

VARNEK\_A  
SOLOV'EV\_V

BAJORATH\_J  
GODDEN\_J

BURDEN\_F  
WINKLER\_D

GUHA\_R  
JURS\_P

BOLBOACA\_S  
JANTSCHI\_L

RUCKER\_G  
RUCKER\_C

FATEMI\_M  
JALALI-H\_M

PYKA\_A  
BOBER\_K

YUNES\_R  
HEINZEN\_V

DJAKOVIC\_T  
PERISIC\_N

SUMPTER\_B  
NOID\_D

FAMINI\_G  
WILSON\_L

LAZZERET\_P  
PELLONI\_S

ARAUJO\_O  
MORALES\_D

PERDIH\_A  
PERDIH\_B

BRENDLE\_E  
PAPIRER\_E

WU\_G  
YAN\_S

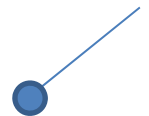
RAKSHIT\_S  
HAZRA\_B

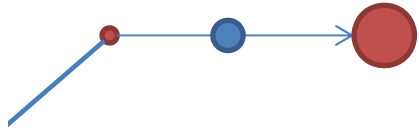
LU\_B  
YAN\_H

KING\_J  
MOLNAR\_S

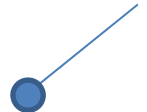
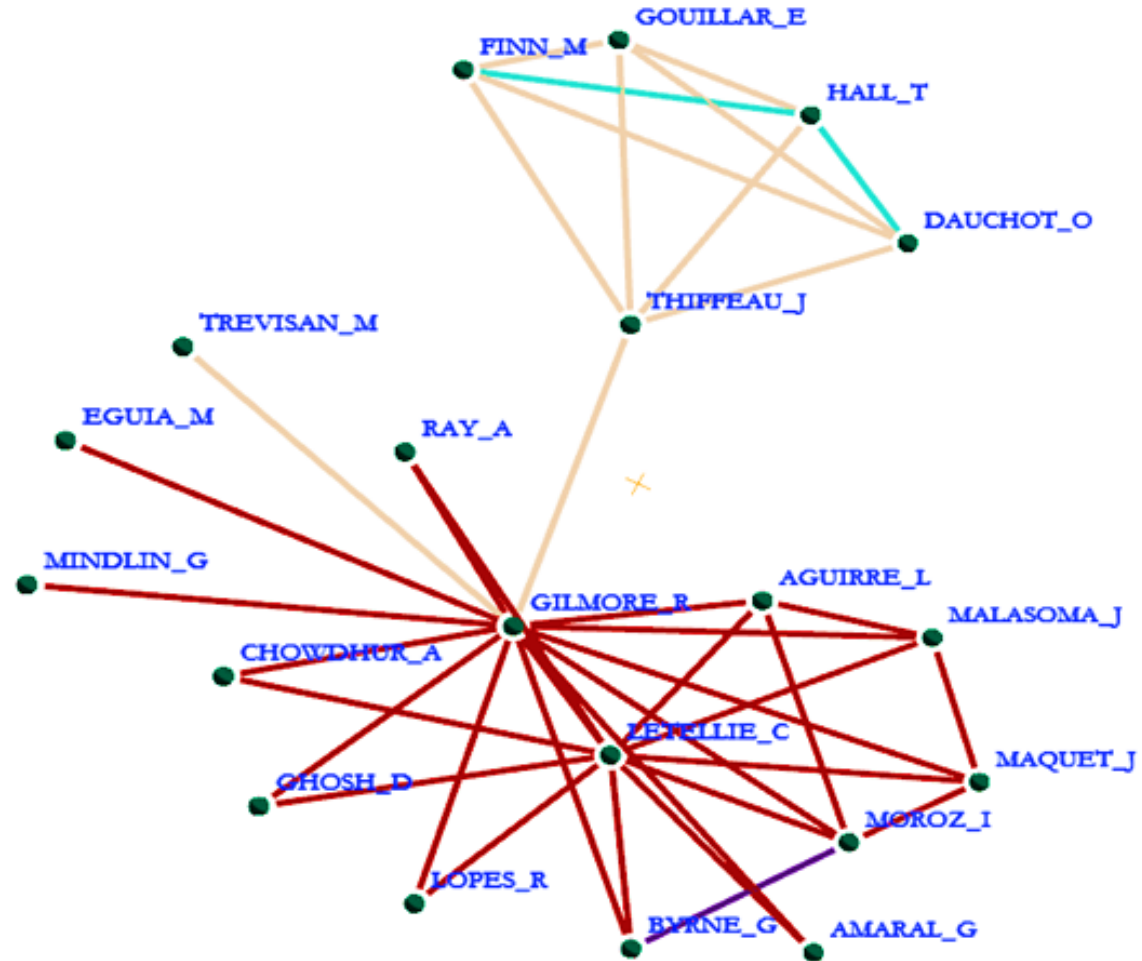
KACHKOV\_S\_A  
DEKHTYAR\_M

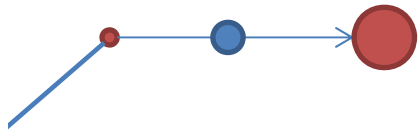
SHARMA\_V  
KUMAR\_S



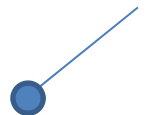
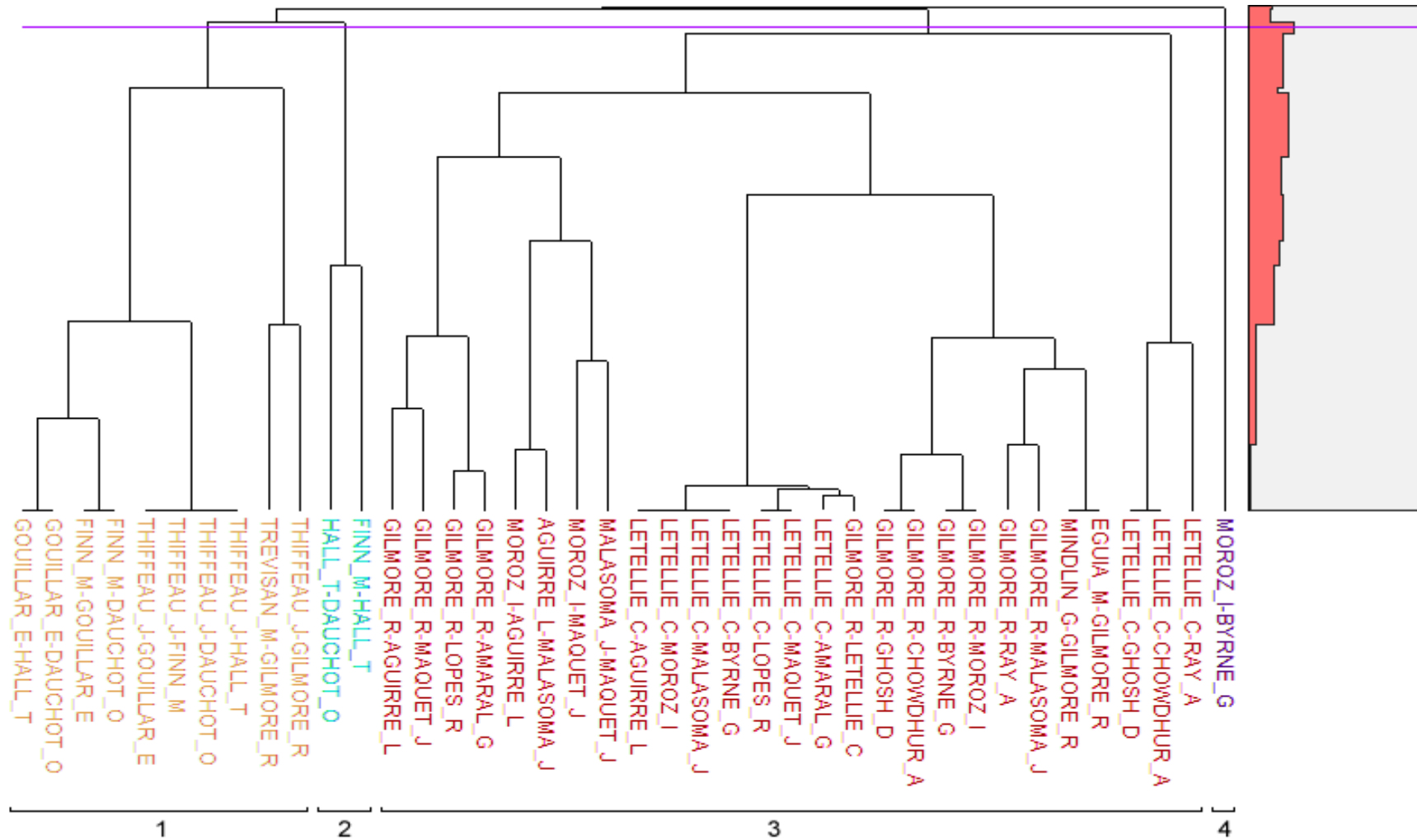


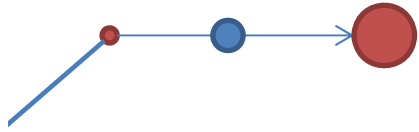
# Structure of *Thifeau J.* Island





# Link Clustering to get Structure

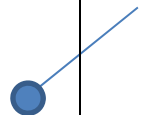




# Thifeau J. Island Keywords

- The most prominent keywords in clusters:

1	2	3	4
1,00 attractor	1,00 attractor	0,96 generate	1,00 advection
1,00 generate	1,00 different	0,88 dynamics	1,00 allow
0,87 dynamics	1,00 generate	0,83 attractor	1,00 braid
0,87 mapping	1,00 image	0,83 symmetry	1,00 chaotic
0,87 topological	1,00 mechanism	0,68 index	1,00 device
0,71 chaotic	1,00 topologically	0,65 equivariant	1,00 entropy
0,71 index	0,66 bound	0,65 strange	1,00 fluid
0,71 strange	0,66 condition	0,60 dynamical	1,00 fluid-mechanics
0,57 motion	0,66 distinguish	0,60 mapping	1,00 line
0,57 present	0,66 enclose	0,55 present	1,00 material
0,43 advection	0,66 establish	0,55 nonlinear	1,00 mixer
0,43 fluid	0,66 flow	0,49 image	1,00 motion
0,43 mixer	0,66 fold	0,49 series	1,00 number
0,43 use	0,66 identical	0,49 study	1,00 possible
0,29 dynamical	0,66 lift	0,47 result	1,00 rod
0,29 flow	0,66 restrict	0,47 distinguish	1,00 stir
0,29 trajectory	0,66 strange	0,47 equation	1,00 stretch
0,29 two-dimensional	0,66 tear	0,47 identical	1,00 topological
0,29 dynamical	0,66 torus	0,47 lift	1,00 use
0,14 entropy	0,33 analysis	0,47 map	0,50 application
0,14 fluid-mechanics	0,33 autonomous	0,47 rotation	0,50 arise
0,14 group	0,33 bar	0,44 topological	0,50 assign
0,14 identical	0,33 behavior	0,42 model	0,50 base





# Important Journals

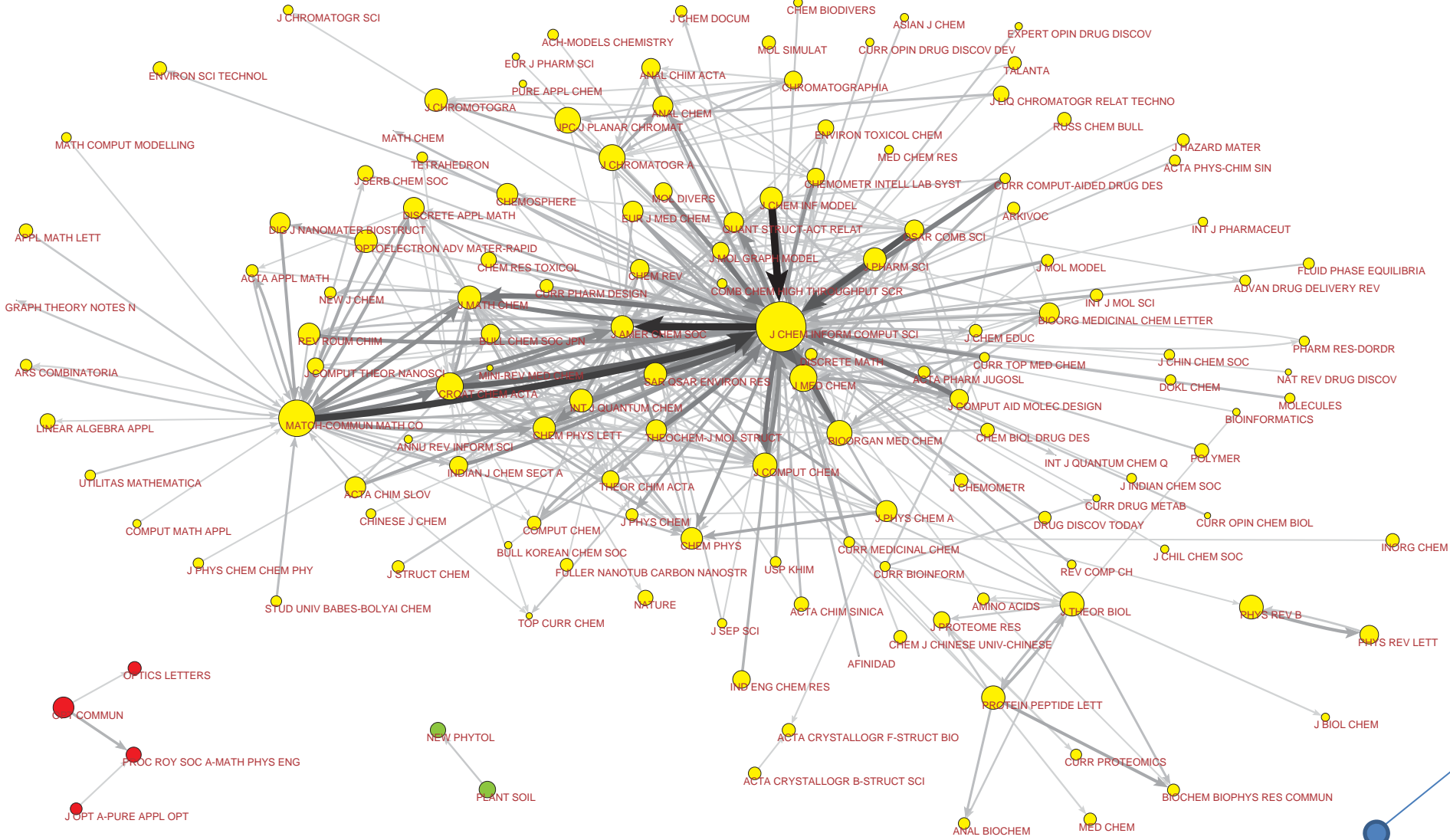
- In top 1% of journals, more than 110 works are published
- 1039 (6,84%) works are published individually in distinct journals

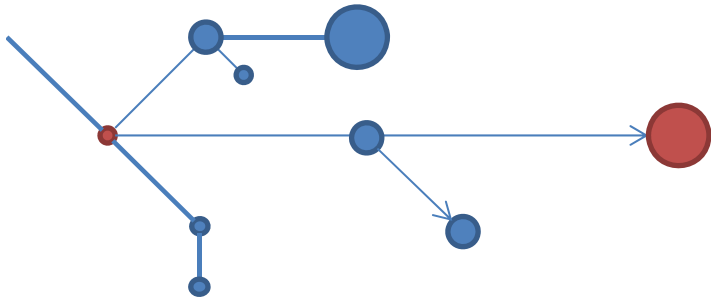
Num. articles	Journal
929	J CHEM INFORM COMPUT SCI
531	MATCH-COMMUN MATH CO
248	J MED CHEM
241	J MATH CHEM
240	J CHEM INF MODEL
222	CROAT CHEM ACTA
202	BIOORGAN MED CHEM
196	THEOCHEM-J MOL STRUCT
182	INT J QUANTUM CHEM
181	CHEM PHYS LETT
181	J AMER CHEM SOC
178	J COMPUT CHEM
169	SAR QSAR ENVIRON RES
167	J CHROMATOGR A
164	QSAR COMB SCI
155	EUR J MED CHEM
139	J PHYS CHEM A
130	CHEM PHYS
118	JPC-J PLANAR CHROMAT
116	J COMPUT AID MOLEC DESIGN

Num. articles	Journal
111	CHEMOMETR INTELL LAB SYST
110	DISCRETE APPL MATH
109	BIOORG MEDICINAL CHEM LETTER
109	QUANT STRUCT-ACT RELAT
108	CHEMOSPHERE
98	J MOL GRAPH MODEL
98	J PHARM SCI
98	J CHROMOTOGRA
96	CHROMATOGRAPHIA
95	ANAL CHIM ACTA
95	ANAL CHEM
87	REV ROUM CHIM
85	INDIAN J CHEM SECT A
77	J THEOR BIOL
75	MOL DIVERS
74	OPTOELECTRON ADV MATER-RAPID
73	PHYS REV B
71	PHYS REV LETT
68	IND ENG CHEM RES
65	DIG J NANOMATER BIOSTRUCT



# Journals Citing





Thank You for your attention...

Jernej Bodlaj  
Vladimir Batagelj

Jernej@hruska.si  
Vladimir.Batagelj@fmf.uni-lj.si

