Supplementary Information

July 27, 2015

1 Computational methods

The communicability angles between every pair of nodes can be obtained from the communicability angles matrix, which is given by

$$An = \cos^{-1}\left\{G \oslash \left[\left(\vec{s}\cdot\vec{1}\right)\odot\left(\vec{1}\cdot\vec{s}\right)\right]\right\}^{\odot(1/2)}, \tag{1}$$

where $\oslash$ stands for the entrywise division, $\odot$ for the Hadamard product (entrywise product) of two matrices, and $\cdot$ for the inner product of two vectors. Here, $\vec{s} = diag\,(G)$, $G = \exp\,(A)$ and $\vec{1}$ is an all-ones vector.

In a similar way the communicability distance matrix can be obtained as

$$X = \left(\vec{s}\cdot\vec{1} + 1\vec{\cdot}\vec{s} - 2G\right)^{\odot(1/2)}. \tag{2}$$

From the computationa point of view it is clear that everything rests on the calculation of the matrix exponential. The matrix exponentail can be defined by considering the Taylor series expansion of the matrix as [1]

$$\exp\,(A) = I + A + \frac{A^2}{2!} + \cdots = \sum_{k=0}^{\infty}\frac{A^k}{k!}. \tag{3}$$

However, it is not recommended under any circunstances to use the Taylor series expansion to compute the matrix exponential. There are many ways of doing this computation more efficiently and the reader is directed to the classic papers of Moler and Van Loan for many examples [2, 3]. From those papers it is clear that there are three or four methods that display the best performance. Among them we selected the *scaling and squaring method*, which is implemented in Matlab® and which has become by far the most widely used method for computing $\exp\,(A)$. In brief, the scaling and squaring method scales the matrix A by a power of 2 to reduce the norm to order 1, computes a Padé approximant to the matrix exponential, and then repeatedly squares to undo the effect of the scaling. In Matlab, it is done by using the **expm** function. For an excellent review of the method, its error and accuracy the reader is referred to the classic papers by Higham [4, 5]. The time and complexity of the calculation of matrix exponential do not only depend on the matrix size, but also on the structure of such matrices. A clearer idea of the complexity and timing for adjacency matrices of netowks can be obtained from the recent paper by Benzi and Klymko [6]. The reader should also be aware of excellent bounds existing for the individual entries of the communicability matrix. For instance, using quadrature rule methods Benzi and Boito [7] have obtained bounds for G_{pq} and G_{pp}. Also Estrada and Arrigo [8]have obtained bounds for the communicability distance. Such bound can be easily implemented in cases where the size and complexity of the network impedes the use of the scaling and squaring method for the direct computation of the matrix exponential. A Matlab code is given below for computing both the communicability angle and distance matrices.

Algorithm 1 Matlab function for obtaining the communicability angle and distance matrices.

```
function [An, X]=communicability_geom(A, beta)

%Communicability_angle
%         Generates the matrices An and X of communicability angles
%         and distances of a network.
%         The (i,j) entry of the matrix An corresponds to the
%         communicability angle between the position vectors of the nodes
%         i and j in a hyperspherical embedding of the graph.
%
%        The entry (i,j) of the matrix X corresponds to the
%         communicability distance between the nodes i and j in the graph.
%
%   Input         A: adjacency matrix
%              beta: inverse temperature. Defaults to 1
%
%
%   Output      An: n by n symmetric hollow matrix of communicability angles.
%                X: n by n symmetric hollow matrix of communicability
%                   distances.
%
%   Reference:   Estrada, Ernesto, and Naomichi Hatano.
%                "Communicability Angle and the Spatial Efficiency
%                of Networks." arXiv preprint arXiv:1412.7388 (2014).
%
%   Example: [An, X] = communicability_angle(A,1);

if nargin <= 1
   beta = 1;
end;

% Precalculations
    A=max(A,A')-diag(diag(A));
    n=length(A);
    u=ones(n,1);

% Communicability

     G=expm(beta*A);           % Communicability matrix
     sc=diag(G);               % Vector of self-communicabilities

% Comunicability angles matrix

      An=acosd(G./((sc*u').*(u*sc')).^0.5);

% Communicability distance matrix
     CD=(sc*u'+u*sc'-2*G);            %Squared Communicability distance matrix
     X=CD.^0.5;                       %Communicability distance matrix
```

2 Datasets

Here we give a brief description of the networks used for the tests throughout the paper.

Brain networks

- Neurons: Neuronal synaptic network of the nematode *C. elegans*. Included all data except muscle cells and using all synaptic connections [9]; Cat and macaque visual cortices: the brain networks of macaque visual cortex and cat cortex, after the modifications introduced by Sporn and Kötter [18].

Ecological networks

- Benguela: Marine ecosystem of Benguela off the southwest coast of South Africa [30]; Bridge Brook: Pelagic species from the largest of a set of 50 New York Adirondack lake food webs [20]; Canton Creek: Primarily invertebrates and algae in a tributary, surrounded by pasture, of the Taieri River in the South Island of New Zealand [21]; Chesapeake Bay: The pelagic portion of an eastern U.S. estuary, with an emphasis on larger fishes [22]; Coachella: Wide range of highly aggregated taxa from the Coachella Valley desert in southern California [23]; El Verde: Insects, spiders, birds, reptiles and amphibians in a rainforest in Puerto Rico [24]; Grassland: all vascular plants and all insects and trophic interactions found inside stems of plants collected from 24 sites distributed within England and Wales [25]; Little Rock: Pelagic and benthic species, particularly fishes, zooplankton, macroinvertebrates, and algae of the Little Rock Lake, Wisconsin, U.S. [26]; Reef Small: Caribbean coral reef ecosystem from the Puerto Rico-Virgin Island shelf complex [27]; Scotch Broom: Trophic interactions between the herbivores, parasitoids, predators and pathogens associated with broom, Cytisus scoparius, collected in Silwood Park, Berkshire, England, UK [28]; Shelf: Marine ecosystem on the northeast US shelf [29]; Skipwith: Invertebrates in an English pond [19]; St. Marks: Mostly macroinvertebrates, fishes, and birds associated with an estuarine seagrass community, Halodule wrightii, at St. Marks Refuge in Florida [31]; St. Martin: Birds and predators and arthropod prey of Anolis lizards on the island of St. Martin, which is located in the northern Lesser Antilles [32]; Stony Stream: Primarily invertebrates and algae in a tributary, surrounded by pasture, of the Taieri River in the South Island of New Zealand in native tussock habitat [33]; Ythan_1: Mostly birds, fishes, invertebrates, and metazoan parasites in a Scottish Estuary [34] ;Ythan_2: Reduced version of Ythan1 with no parasites [35].
- Termite: The networks of three-dimensional galleries in termite nests [66]; Ant: The network of galleries created by ants [67]; Dolphins: social network of frequent association between 62 bottlenose dolphins living in the waters off New Zealand [56];

Informational networks

- Centrality: Citation network of papers published in the field of Network Centrality [36, 37]; GD: Citation network of papers published in the Proceedings of Graph Drawing during the period 1994-2000 [38]; ODLIS: Vocabulary network of words related by their definitions in the Online Dictionary of Library and Information Science. Two words are connected if one is used in the definition of the other [39]; Roget: Vocabulary network of words related by their definitions in Roget's Thesaurus of English. Two words are connected if one is used in the definition of the other [40]; Small World: Citation network of papers that cite S. Milgram's 1967 Psychology Today paper or use Small World in title [41].

Biological networks

- Protein-protein interaction networks in: *Kaposi sarcoma herpes virus* (KSHV) [42]; *P. falciparum* (malaria parasite) [43]; *human* [44]; *S. cerevisiae* (yeast) [45, 46]; *A. fulgidus* [47]; *H. pylori* [48]; *C. elegans* [49]; *E. coli* [50] and *B. subtilis* [51].
- Trans_E.coli: Direct transcriptional regulation between operons in *Escherichia coli* [52, 53]; Trans_sea_urchin: Developmental transcription network for sea urchin endomesoderm development. [52]; Trans_yeast: Direct transcriptional regulation between genes in *Saccaromyces cerevisae*. [9, 52].

Social and economic networks

- Corporate: American corporate elite formed by the directors of the 625 largest corporations that reported the compositions of their boards selected from the Fortune 1000 in 1999 [54]; Geom: Collaboration network of scientists in the field of Computational Geometry [41]; Prison: Social network of inmates in prison who chose "What fellows on the tier are you closest friends with?" [55]; Drugs: Social network of injecting drug users (IDUs) that have shared a needle in the last six months [57]; Zachary: Social network of friendship between members of the Zachary karate club [58]; College: Social network among college students in a course about leadership. The students choose which three members they wanted to have in a committee [59]; ColoSpring: The risk network of persons with HIV infection during its early epidemic phase in Colorado Spring, USA, using analysis of community wide HIV/AIDS contact tracing records (sexual and injecting drugs partners) from 1985-1999 [60]; Galesburg: Friendship ties among 31 physicians [37]; High_Tech: Friendship ties among the employees in a small high-tech computer firm which sells, installs, and maintain computer systems [61, 37]; Saw Mills: Social communication network within a sawmill, where employees were asked to indicate the frequency with which they discussed work matters with each of their colleagues [62, 37]; MMM: World trade network of miscellaneous manufacture of metals (MMM) in 1994 [37].

Protein residue networks

- Nodes represent amino acids and two nodes are connected if the corresponding amino acids are separated at less than 7Å in the crystallographic structure deposited in the Protein Data Bank (PDB). The proteins considered were transformed to protein residue networks in [12] and the ones selected here have codes: 1lfb; 9rnt; 1aep; 1jpc; 1vls; 1klo; 2aak; 1xjo; 1amm; 1mla; 1ad2; 1nox; 1akz; 1xsm; 1ako; 1han; 1air; 1gnd; 1aa6; 1alo; 1kit.

Urban street networks

- Nodes represent the intersections between two streets in a city and the edges represent segments of streets between two intersections [65]. The networks represent the following cities from the ones studied in [65]: Barcelona; Rio Grande; Yuliang; Chegkan; Atlanta; Berlin; Rotterdam; Hong Kong; Mecca; Cambridge; Oxford; Ahmedabad; Milton Keynes.

Technological and infrastructural networks

- Electronic: Three electronic sequential logic circuits parsed from the ISCAS89 benchmark set, where nodes represent logic gates and flip-flop [9]; USAir97: Airport transportation network between airports in US in 1997 [41]; Internet: The internet at the Autonomous System (AS) level as of September 1997 and of April 1998 [63]; Power Grid: The power grid network of the Western USA [64].

Software networks

- Collaboration networks associated with six different open-source software systems, which include collaboration graphs for three Object Oriented systems written in C++, and call graphs for three procedural systems written in C. The class collaboration graphs are from version 4.0 of the VTK visualization library; the CVS snapshot dated 4/3/2002 of Digital Material (DM), a library for atomistic simulation of materials; and version 1.0.2 of the AbiWord word processing program. The call graphs are from version 2.4.19 of the kernel of the Linux operating system, version 3.23.32 of the MySQL relational database system, and version 1.2.7 of the XMMS multimedia system. Details of the construction and/or origin of these networks are provided in Myers [10].

3 Results

In Table 1 we give the values of the network parameters studied in this paper as well as a few others that can give a better idea of the kind of networks we have studied here. They include: the number of nodes n, the number of edges m, the average node degree $\langle k \rangle$, the maximum node degree k_{max}, the average path length $\langle l \rangle$, average Watts and Strogatz clustering coefficient $\bar{C}$, the network efficiency E, average resistance distance $\langle \Omega \rangle$, average communicability distance $\langle \xi \rangle$ and angle $\langle \theta \rangle$. The networks belong to the following classes: biological (1-14), urban street networks (15-27), ecological networks (28-49), social networks (50-64), software networks (65-70), technological and infrastructural networks (71-77).

Table 1. Values of the average communicability angles of all the real-world networks studied except the protein residue networks.

No.	Name	n	m	$\langle k \rangle$	k_{max}	$\langle l \rangle$	$\bar{C}$	E	$\langle \Omega \rangle$	$\langle \xi \rangle$	$\langle \theta \rangle$
1	PIN_yeast	2224	6609	5.94	64	4.38	0.14	0.25	1.27	177.09	38.92
2	PIN_Ecoli	230	695	6.04	36	3.78	0.22	0.31	1.66	147.96	39.76
3	PIN_KSHV	50	114	4.56	16	2.84	0.13	0.42	1.13	5.18	51.59
4	PIN_Malaria	229	604	5.28	35	3.38	0.17	0.33	0.82	8.65	55.04
5	PIN_Human	2783	6007	4.32	129	4.84	0.07	0.22	1.55	36.32	58.79
6	Trans_urchin	45	80	3.56	14	3.22	0.21	0.39	2.02	4.22	61.87
7	PIN_Hpylori	710	1396	3.93	55	4.15	0.02	0.26	1.47	7.13	67.51
8	Trans_Ecoli	328	456	2.78	72	4.83	0.11	0.25	2.54	5.19	77.44
9	PIN_Afulgidus	32	36	2.25	9	3.60	0.06	0.35	2.49	2.18	79.35
10	PIN_Bsubtilis	84	98	2.33	17	4.05	0.04	0.29	2.52	2.52	81.77
11	Trans_yeast	662	1062	3.21	71	5.20	0.05	0.22	2.06	7.16	83.33
12	cat Cortex	52	515	19.81	37	1.64	0.66	0.69	0.13	5792.78	0.22
13	neurons	280	1973	14.09	77	2.63	0.28	0.42	0.26	4575.37	1.57
14	Macaque	32	194	12.13	22	1.66	0.65	0.69	0.24	91.52	3.60
15	Barcelona	5575	16060	5.76	126	7.94	0.19	0.15	1.08	828.39	71.89
16	Rio Grande	855	2702	6.32	57	6.90	0.08	0.18	1.35	67.23	79.68
17	Yuliang	88	129	2.93	7	6.03	0.17	0.23	3.22	2.76	85.84
18	Chegkan	414	1208	5.84	18	8.97	0.16	0.15	0.99	7.98	86.07
19	Atlanta	3234	7319	4.53	65	7.71	0.15	0.15	1.64	12.20	86.47
20	Berlin	4495	12889	5.73	50	9.24	0.20	0.13	1.07	16.46	88.19
21	Rotterdam	1300	2759	4.24	28	9.59	0.14	0.13	1.62	4.69	88.60
22	Hong Kong	916	1613	3.52	23	12.85	0.13	0.11	4.33	3.94	88.91
23	Mecca	1464	2789	3.81	18	13.44	0.21	0.10	1.98	3.79	89.48
24	Cambridge	1509	2190	2.90	31	11.15	0.11	0.11	3.98	3.08	89.49
25	Oxford	1622	2825	3.48	19	12.97	0.17	0.10	3.05	3.43	89.53
26	Ahmedabad	4874	7242	2.97	21	13.41	0.16	0.09	3.60	3.06	89.86
27	Milton Keynes	5581	7261	2.60	25	13.19	0.08	0.09	4.62	2.73	89.89
28	Ants	74	97	2.62	7	5.57	0.04	0.24	2.92	2.50	85.51
29	Termite3	268	437	3.26	12	7.89	0.12	0.18	2.37	3.35	87.16
30	Termite2	260	280	2.15	12	9.11	0.01	0.15	5.22	2.30	88.84
31	Termite1	507	676	2.67	10	8.51	0.04	0.15	2.95	2.64	89.00
32	Dolphins	62	159	5.13	12	3.36	0.26	0.38	0.99	5.98	65.37
33	Shelf	81	1451	35.83	69	1.57	0.59	0.72	0.07	61317050	0.00
34	Elverde	156	1439	18.45	83	2.30	0.21	0.50	0.38	393308.86	0.01
35	Skipwith	35	353	20.17	32	1.42	0.63	0.79	0.11	3327.87	0.02
36	ReefSmall	50	503	20.12	39	1.60	0.61	0.70	0.14	8975.44	0.05
37	LittleRock	181	2318	25.61	105	2.22	0.35	0.51	0.25	37085665	0.05
38	Stony	112	830	14.82	45	2.34	0.07	0.49	0.45	5371.98	0.10
39	Coachella	30	241	16.07	25	1.46	0.71	0.77	0.16	622.10	0.25
40	Canton	108	707	13.09	47	2.35	0.05	0.49	0.48	1103.80	0.46
41	Benguela	29	191	13.17	24	1.62	0.57	0.72	0.26	160.96	1.23
42	BridgeBrook	75	542	14.45	41	2.17	0.20	0.54	0.30	2041.51	2.01

43	Ythan2	92	416	9.04	50	2.25	0.22	0.49	0.53	180.70	2.03
44	Ythan1	134	593	8.85	65	2.40	0.23	0.46	0.57	251.88	2.16
45	StMartins	44	218	9.91	27	1.93	0.33	0.59	0.37	41.77	6.15
46	StMarks	48	218	9.08	19	2.09	0.28	0.55	0.35	33.30	8.25
47	ScotchBroom	154	366	4.75	36	3.39	0.14	0.33	1.60	95.26	30.32
48	Chesapeake	33	71	4.30	10	2.80	0.20	0.45	1.09	3.72	60.69
49	SmallW	233	994	8.53	147	2.37	0.56	0.45	0.63	1459.4	5.05
50	ODLIS	2898	16376	11.30	592	3.17	0.30	0.34	0.65	45714627	0.04
51	Roget	994	3640	7.32	28	4.08	0.15	0.27	0.64	14.80	65.74
52	GD	249	635	5.10	20	4.15	0.24	0.28	1.19	8.32	75.65
53	Centrality	118	613	10.39	66	2.37	0.37	0.47	0.56	1025.69	1.01
54	Corporate	1586	11540	14.55	65	3.51	0.50	0.31	0.27	2099.82	15.54
55	Geom	3621	9461	5.23	102	5.32	0.54	0.21	1.66	15960.86	17.22
56	HighTech	33	91	5.52	16	2.36	0.45	0.51	0.79	7.22	39.20
57	Zachary	34	78	4.59	17	2.41	0.57	0.49	0.84	4.60	45.45
58	College	32	80	5.00	13	2.30	0.33	0.51	0.58	3.62	52.10
59	Galesburg	31	67	4.32	10	2.53	0.35	0.47	0.94	3.60	59.71
60	Drugs	616	2012	6.53	58	5.28	0.55	0.23	1.84	245.25	64.02
61	SawMill	36	62	3.44	13	3.14	0.31	0.40	1.40	2.96	71.41
62	Prison	67	142	4.24	11	3.35	0.31	0.36	1.06	3.87	76.54
63	MMM	80	875	21.88	77	1.72	0.75	0.64	0.14	185828.3	0.01
64	Colospg	324	347	2.14	20	8.33	0.03	0.15	5.95	2.48	88.46
65	Linux	5285	11352	4.30	1058	4.66	0.11	0.24	1.44	172348.6	3.47
66	MySQL	1480	4190	5.66	220	5.47	0.16	0.23	1.55	895.51	45.68
67	VTK	771	1357	3.52	83	4.53	0.06	0.24	1.90	9.78	70.11
68	Abi	1035	1719	3.32	89	5.08	0.06	0.22	2.31	9.26	72.86
69	Digital	150	198	2.64	25	4.85	0.05	0.25	3.02	3.25	81.62
70	XMMS	971	1802	3.71	36	6.35	0.05	0.18	2.15	6.50	84.32
71	USAir97	332	2126	12.81	139	2.74	0.63	0.41	0.83	37248593	0.00
72	electronic1	122	189	3.10	10	4.93	0.06	0.25	1.77	2.68	86.18
73	electronic2	252	399	3.17	14	5.81	0.06	0.20	1.84	2.77	87.94
74	electronic3	512	819	3.20	22	6.86	0.05	0.17	1.92	2.83	88.89
75	PowerGrid	4941	6594	2.67	19	18.99	0.08	0.06	5.23	2.74	89.91
76	Internet98	3522	6324	3.59	742	3.77	0.19	0.29	1.65	375932.59	0.42
77	Internet97	3015	5156	3.42	590	3.76	0.18	0.29	1.73	84399.95	0.78

In Fig. (1) we illustrate the scatterplots of the communicability angle versus a few of the network parameters studied in the paper for the 77 real-world networks given in Table 1. Apart from the evident lack of correlation between the pairs of measures it is interesting to notice the fact that there are pairs of networks with the same value of a given parameter, e.g., average degree, average path length, efficiency, etc., but having very different values of the communicability angle. There is one example provided in the main text of the article but many more can be extracted from these plots. Notice the plot between the communicability distance and communicability angle is semi-log scale.

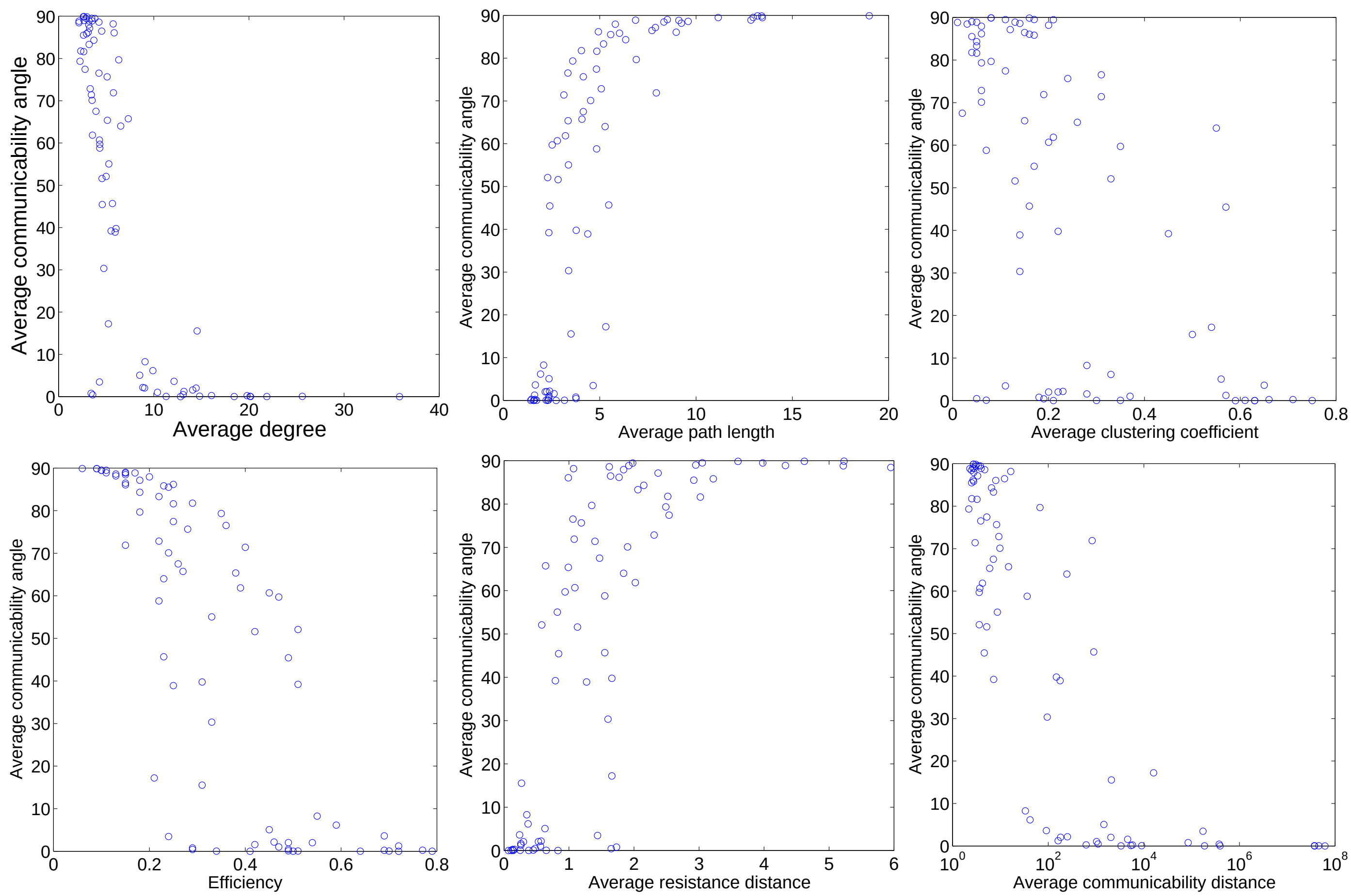

Figure 1: Scatterplots of the average communicability angle vs. a few network metrics.

Table 2. Values of the average communicability angles as well as the real and expected values of the volume of all the protein residue networks studied.

PDB code	$V_o\left(\mathring{A}^3\right)$	$V_e\left(\mathring{A}^3\right)$	$\langle\theta\rangle$
1npoA	9002.4	9566.2	64.75
1tfs	7634.98	7976.8	65.01
1ptx	8010.5	8252.9	65.95
1dtx	7470.9	7873.5	68.27
5rxn	6620.4	6778.5	68.28
1ceaA	9869.9	10508	68.35
2abd	10670.11	11518.2	69.69
1cdr	10144.64	10349.8	71.09
1lfb	10127.9	10658.1	71.78
9rnt	12314.6	12960.6	73.93
2madL	14881.6	15848.1	74.90
2azaA	16295.7	16507	74.97
1fkj	13754.5	13857.3	75.31
1rtp1	14006.2	13826.3	75.32
7rsa	15909.9	16152.8	75.40
1aep	19285	19593.3	76.17
1jpc	13204.3	14075.5	76.34
1vls	18689.3	19421.7	78.91
2aak	20200.5	20330.8	79.75
1xjo	33590.9	34157.4	79.97
1amm	24208	25079.8	80.73
1mla	39239.1	38549.4	81.55
1ad2	29637.1	29160.4	81.63
1nox	27195.8	26599.2	81.64
1akz	30738.2	30650.2	81.76
1xsm	41236.8	40782.6	82.81
1ako	37803.6	37354.7	82.97
1han	37972.1	37900.1	83.41
1air	44558.3	45452.7	83.56
1gnd	61577.9	58899.4	85.72
1aa6	99503.2	94252.3	86.38
1alo	120846.1	118421.6	86.98
1kit	103772.6	101172.2	87.26
8catA	70353.4	68895.4	86.98
1kit	103772.6	101172.2	87.27
1gpb	120845.6	115900.9	87.40
1qba	125154.4	116908.8	87.48
1oacA	102370.8	97918	87.59
2cas	75066.7	74830.9	87.65
1bglA	147042.7	141837.9	88.13

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