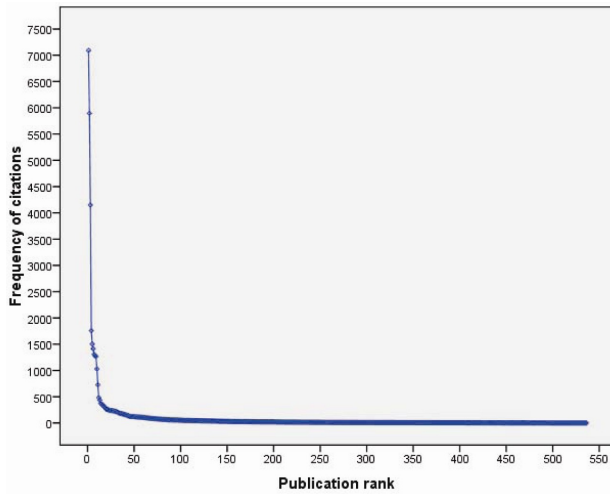
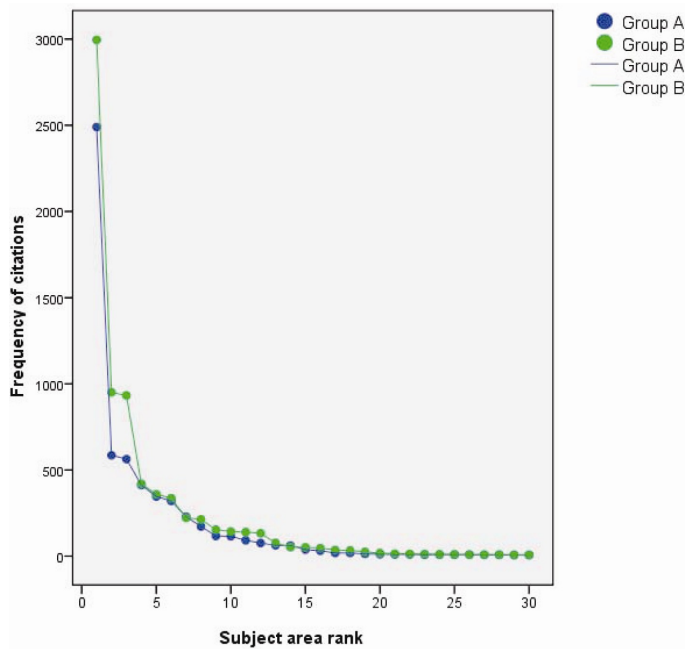


Supplementary Figure A. Citation rank-frequency plot for 536 CCDC publications.



Supplementary Figure B. Subject area rank-frequency plot for the 30 areas with the most citations to the group-A and group-B target articles.



Supplementary Table A. Different journals citing each group-A target article in 2005-08.

Target article	Unique journals	Citations	Mean citations/journal
TAB1	118	2,682	22.73
RES1	97	277	2.86
TAB2	58	247	4.26
CSD1	53	88	1.66
CSD2	64	134	2.09
LS1	174	762	4.38
RES2	39	78	2.00
RES3	19	55	2.89
RES4	39	175	4.49
RES5	68	26	0.38
Total	343	4,524	4.77

Supplementary Table B. Different journals citing each group-B target article in 2005-08.

Target article	Unique journals	Citations	Mean citations/journal
CSD3	253	3,043	12.03
CSD4	112	793	7.08
CSD5	74	584	7.89
LS2	98	273	2.79
CSD6	10	221	22.10
RES6	41	109	2.66
RES7	70	145	2.07
RES8	44	115	2.61
RES9	43	97	2.26
LS3	49	127	2.59
Total	362	5,507	6.41

Supplementary Table C. The thirty journals that cited the group-A target articles most frequently in 2005-08.

Journal source	Citations	IF	CI
<i>Acta Crystallographica Section E-Structure Reports Online</i>	2,059	0.367	2.11
<i>Acta Crystallographica Section C-Crystal Structure Communications</i>	156	0.561	0.24
<i>Journal of Medicinal Chemistry</i>	149	4.898	2.04
<i>Organometallics</i>	89	3.815	0.95
<i>Journal of Chemical Information and Modeling</i>	87	3.643	0.89
<i>Inorganic Chemistry</i>	82	4.147	0.95
<i>Journal of Organometallic Chemistry</i>	74	1.866	0.39
<i>Journal of the American Chemical Society</i>	52	8.091	1.18
<i>Journal of Chemical Crystallography</i>	50	0.574	0.08
<i>Bioorganic & Medicinal Chemistry</i>	48	3.075	0.41
<i>Dalton Transactions</i>	45	3.580	0.45
<i>Inorganica Chimica Acta</i>	43	1.940	0.23
<i>Polyhedron</i>	43	1.801	0.22
<i>Crystal Growth & Design</i>	42	4.215	0.49
<i>European Journal of Inorganic Chemistry</i>	41	2.694	0.31
<i>Proteins-Structure Function and Bioinformatics</i>	36	3.419	0.34
<i>Journal of Molecular Structure</i>	35	1.594	0.16
<i>Journal of Physical Chemistry A</i>	35	2.871	0.28
<i>Chemistry-A European Journal</i>	33	5.454	0.50
<i>Journal of Structural Chemistry</i>	29	0.579	0.05
<i>Russian Journal of Inorganic Chemistry</i>	28	0.417	0.03
<i>CrystEngComm</i>	27	3.535	0.27
<i>Bioorganic & Medicinal Chemistry Letters</i>	26	2.531	0.18
<i>ChemMedChem</i>	26	3.150	0.23
<i>Journal of Computer-Aided Molecular Design</i>	26	3.620	0.26
<i>Acta Crystallographica Section B-Structural Science</i>	24	2.341	0.16
<i>Angewandte Chemie-International Edition</i>	24	10.87	0.73
	9		
<i>Journal of Physical Chemistry B</i>	24	4.189	0.28
<i>Journal of Molecular Graphics & Modelling</i>	21	2.347	0.14
<i>Russian Chemical Bulletin</i>	21	0.469	0.03
<i>All other journals</i>	1,049	-	-
Total	4,524	-	-

Supplementary Table D. The thirty journals that cited the group-B target articles most frequently in 2005-08.

Journal source	Citations	IF	CI
<i>Acta Crystallographica Section E-Structure Reports Online</i>	1,504	0.367	1.28
<i>Acta Crystallographica Section C-Crystal Structure Communications</i>	618	0.561	0.80
<i>Acta Crystallographica Section B-Structural Science</i>	181	2.341	0.98
<i>Crystal Growth & Design</i>	172	4.215	1.68
<i>CrystEngComm</i>	162	3.535	1.33
<i>Inorganic Chemistry</i>	141	4.147	1.36
<i>Polyhedron</i>	138	1.801	0.58
<i>Journal of Medicinal Chemistry</i>	102	4.898	1.16
<i>Dalton Transactions</i>	95	3.580	0.79
<i>Inorganica Chimica Acta</i>	89	1.940	0.40
<i>European Journal of Inorganic Chemistry</i>	81	2.694	0.51
<i>Journal of Molecular Structure</i>	78	1.594	0.29
<i>Journal of Organometallic Chemistry</i>	75	1.866	0.32
<i>Organometallics</i>	66	3.815	0.58
<i>Journal of Physical Chemistry A</i>	65	2.871	0.43
<i>Journal of Physical Chemistry B</i>	61	4.189	0.59
<i>Chemistry-A European Journal</i>	59	5.454	0.75
<i>Journal of the American Chemical Society</i>	59	8.091	1.11
<i>Proteins-Structure Function and Bioinformatics</i>	48	3.419	0.38
<i>Journal of Chemical Information and Modeling</i>	45	3.643	0.38
<i>Inorganic Chemistry Communications</i>	42	1.854	0.18
<i>Chemical Communications</i>	41	5.340	0.51
<i>Angewandte Chemie-International Edition</i>	36	10.87	0.91
		9	
<i>Journal of Chemical Crystallography</i>	36	0.574	0.05
<i>Journal of Applied Crystallography</i>	34	3.212	0.25
<i>Zeitschrift für Anorganische und Allgemeine Chemie</i>	31	1.102	0.08
<i>Russian Journal of Inorganic Chemistry</i>	30	0.417	0.03
<i>Chemical Physics Letters</i>	29	2.169	0.15
<i>Crystallography Reports</i>	29	0.481	0.03
<i>New Journal of Chemistry</i>	29	2.942	0.20
<i>All other journals</i>	1,331	-	-
Total	5,507	-	-

Supplementary Table E. Different subject areas citing each group-A target article in 2005-08

Target article	Unique subjects	Citations	Mean citations/subject
TAB1	27	2,916	108.0
RES1	23	398	17.3
TAB2	20	364	18.2
CSD1	21	125	6.0
CSD2	23	227	9.9
LS1	52	1,445	27.8
RES2	19	121	6.4
RES3	13	70	5.4
RES4	15	227	15.1
RES5	12	43	3.6
Total	66	5,936	21.8

Supplementary Table F. Different subject areas citing each group-B target article in 2005-08

Target article	Unique subjects	Citations	Mean citations/subject
CSD3	53	4,013	75.7
CSD4	31	1,099	35.5
CSD5	29	689	23.8
LS2	38	499	13.1
CSD6	7	227	32.4
RES6	16	189	11.8
RES7	23	230	10.0
RES8	18	195	10.8
RES9	27	159	5.9
LS3	24	271	11.3
Total	69	7,571	23.0

Supplementary Table G. The thirty subject areas that cited the group-A target articles most frequently in 2005-08.

Subject area	Citations	IF	CI
Crystallography	2,490	1.046	5.13
Chemistry, Inorganic & Nuclear	585	2.247	2.59
Chemistry, Multidisciplinary	563	3.626	4.02
Chemistry, Organic	412	2.75	2.23
Chemistry, Medicinal	346	2.582	1.76
Biochemistry & Molecular Biology	320	4.236	2.67
Chemistry, Physical	229	2.828	1.28
Computer Science, Interdisciplinary Applications	172	1.552	0.53
Pharmacology & Pharmacy	117	2.934	0.68
Biophysics	115	3.124	0.71
Computer Science, Information Systems	92	1.633	0.30
Physics, Atomic, Molecular & Chemical	76	2.446	0.37
Materials Science, Multidisciplinary	62	2.206	0.27
Spectroscopy	61	1.806	0.22
Biochemical Research Methods	38	3.271	0.25
Mathematical & Computational Biology	31	2.835	0.17
Cell Biology	18	5.696	0.20
Chemistry, Applied	18	1.947	0.07
Polymer Science	13	2.235	0.06
Endocrinology & Metabolism	11	4.01	0.09
Engineering, Chemical	10	1.583	0.03
Toxicology	10	2.485	0.05
Biotechnology & Applied Microbiology	8	2.93	0.05
Chemistry, Analytical	8	2.608	0.04
Environmental Sciences	8	2.228	0.04
Oncology	8	4.64	0.07
Mathematics, Interdisciplinary Applications	7	1.587	0.02
Physics, Condensed Matter	7	2.089	0.03
Computer Science, Artificial Intelligence	6	2.011	0.02
Materials Science, Textiles	6	0.914	0.01
All other subject areas	89	-	-
Total	5,936	-	-

Supplementary Table H. The thirty subject areas that cited the group-B target articles most frequently in 2005-08.

Subject area	Citations	<i>IF</i>	<i>CI</i>
Crystallography	2,996	1.046	4.65
Chemistry, Multidisciplinary	950	3.626	5.11
Chemistry, Inorganic & Nuclear	932	2.247	3.11
Chemistry, Physical	419	2.828	1.76
Chemistry, Organic	359	2.75	1.47
Biochemistry & Molecular Biology	336	4.236	2.11
Chemistry, Medicinal	222	2.582	0.85
Materials Science, Multidisciplinary	213	2.206	0.70
Physics, Atomic, Molecular & Chemical	153	2.446	0.56
Computer Science, Interdisciplinary Applications	143	1.552	0.33
Biophysics	139	3.124	0.64
Pharmacology & Pharmacy	133	2.934	0.58
Computer Science, Information Systems	76	1.633	0.18
Biochemical Research Methods	52	3.271	0.25
Spectroscopy	51	1.806	0.14
Chemistry, Applied	46	1.947	0.13
Mathematical & Computational Biology	35	2.835	0.15
Chemistry, Analytical	33	2.608	0.13
Physics, Condensed Matter	25	2.089	0.08
Physics, Applied	17	2.169	0.05
Biotechnology & Applied Microbiology	14	2.93	0.06
Cell Biology	12	5.696	0.10
Multidisciplinary Sciences	12	8.741	0.16
Computer Science, Theory & Methods	10	1.341	0.02
Physics, Multidisciplinary	10	2.793	0.04
Engineering, Chemical	9	1.583	0.02
Food Science & Technology	9	1.717	0.02
Statistics & Probability	9	1.164	0.02
Engineering, Biomedical	8	2.597	0.03
Nanoscience & Nanotechnology	8	3.069	0.04
All other subject areas	140	-	-
Total	7,571	-	-

Supplementary Table I. Citations to group-A target articles from different types of institution during 2008.

Institutional type	CSD1-2	TAB1-2	LS1	RES1-5	Total
University	78	1,202	376	187	1,843
Institute	4	19	14	11	48
Academy	0	68	11	28	107
Commercial	2	12	85	14	113
CCDC	0	0	2	1	3
Other	8	15	27	6	56
Unknown	0	2	5	1	8
Total	92	1,318	520	248	2,178

Supplementary Table J. Citations to group-B target articles from different types of institution during 2008.

Institutional type	CSD3-6	LS2-3	RES6-9	Total
University	1,574	178	180	1,932
Institute	50	19	9	78
Academy	94	9	7	110
Commercial	71	30	20	121
CCDC	16	2	7	25
Other	110	20	28	158
Unknown	11	4	2	17
Total	1,926	262	253	2,441

Supplementary Table K. The thirty journals that cited the group-C target articles most frequently since publication.

Journal source	Citations	IF	CI
<i>Acta Crystallographica Section E-Structure Reports Online</i>	1,499	0.367	0.59
<i>Acta Crystallographica Section C-Crystal Structure Communications</i>	1,045	0.561	0.62
<i>Journal of the American Chemical Society</i>	555	8.091	4.78
<i>Crystal Growth & Design</i>	517	4.215	2.32
<i>CrystEngComm</i>	430	3.535	1.62
<i>Inorganic Chemistry</i>	345	4.147	1.52
<i>Journal of Molecular Structure</i>	335	1.594	0.57
<i>Chemical Communications</i>	328	5.340	1.86
<i>Acta Crystallographica Section B-Structural Science</i>	300	2.341	0.75
<i>Chemistry-A European Journal</i>	274	5.454	1.59
<i>Angewandte Chemie-International Edition</i>	265	10.87	3.07
		9	
<i>Dalton Transactions</i>	262	3.580	1.00
<i>New Journal of Chemistry</i>	240	2.942	0.75
<i>Journal of Physical Chemistry A</i>	218	2.871	0.67
<i>Journal of Organic Chemistry</i>	212	3.952	0.89
<i>Inorganica Chimica Acta</i>	181	1.940	0.37
<i>Polyhedron</i>	176	1.801	0.34
<i>Organometallics</i>	147	3.815	0.60
<i>European Journal of Inorganic Chemistry</i>	141	2.694	0.40
<i>Journal of Organometallic Chemistry</i>	138	1.866	0.27
<i>Tetrahedron</i>	121	2.897	0.37
<i>Tetrahedron Letters</i>	110	2.538	0.30
<i>Journal of Chemical Crystallography</i>	109	0.574	0.07
<i>Journal of Physical Chemistry B</i>	108	4.189	0.48
<i>Inorganic Chemistry Communications</i>	106	1.854	0.21
<i>Chemistry of Materials</i>	100	5.046	0.54
<i>Zeitschrift fur Naturforschung Section B</i>	100	0.852	0.09
<i>Zeitschrift fur Anorganische und Allgemeine Chemie</i>	98	1.102	0.11
<i>Helvetica Chimica Acta</i>	87	1.396	0.13
<i>Journal of the Chemical Society-Perkin Transactions 2</i>	80	-	-
<i>All other journals</i>	3,415	-	-
Total	12,042	-	-

Supplementary Table L. The thirty journals that cited the group-D target articles most frequently since publication.

Journal source	Citations	IF	CI
<i>Journal of Molecular Biology</i>	439	4.146	3.16
<i>Journal of the American Chemical Society</i>	266	8.091	3.73
<i>Inorganic Chemistry</i>	245	4.147	1.76
<i>Biochemistry</i>	242	3.379	1.42
<i>Acta Crystallographica Section D-Biological Crystallography</i>	223	2.943	1.14
<i>Acta Crystallographica Section C-Crystal Structure Communications</i>	208	0.561	0.20
<i>Journal of Biological Chemistry</i>	186	5.520	1.78
<i>Crystal Growth & Design</i>	178	4.215	1.30
<i>Acta Crystallographica Section E-Structure Reports Online</i>	172	0.367	0.11
<i>CrystEngComm</i>	159	3.535	0.98
<i>Structure</i>	154	5.397	1.44
<i>Dalton Transactions</i>	140	3.580	0.87
<i>Inorganica Chimica Acta</i>	134	1.940	0.45
<i>Chemistry-A European Journal</i>	131	5.454	1.24
<i>European Journal of Inorganic Chemistry</i>	115	2.694	0.54
<i>Chemical Communications</i>	111	5.340	1.03
<i>Polyhedron</i>	108	1.801	0.34
<i>Inorganic Chemistry Communications</i>	107	1.854	0.34
<i>Angewandte Chemie-International Edition</i>	100	10.87	
		9	1.89
<i>Protein Science</i>	93	3.115	0.50
<i>Journal of Computer-Aided Molecular Design</i>	89	3.620	0.56
<i>Journal of Molecular Structure</i>	86	1.594	0.24
<i>Zeitschrift Fur Anorganische und Allgemeine Chemie</i>	85	1.102	0.16
<i>Organometallics</i>	80	3.815	0.53
<i>Proceedings of the National Academy of Sciences</i>	79	9.380	1.29
<i>Acta Crystallographica Section B-Structural Science</i>	73	2.341	0.30
<i>EMBO Journal</i>	73	8.295	1.05
<i>Journal of Organic Chemistry</i>	73	3.952	0.50
<i>Journal of Medicinal Chemistry</i>	72	4.898	0.61
<i>New Journal of Chemistry</i>	70	2.942	0.36
<i>All other journals</i>	2,987	-	-
Total	7,278	-	-

Supplementary Table M. The thirty subject areas that cited the group-C target articles most frequently since publication.

Subject area	Citations	<i>IF</i>	<i>CI</i>
Crystallography	4441	1.046	3.20
Chemistry, Multidisciplinary	3838	3.626	9.59
Chemistry, Inorganic & Nuclear	2145	2.247	3.32
Chemistry, Physical	1624	2.828	3.16
Chemistry, Organic	1440	2.75	2.73
Materials Science, Multidisciplinary	875	2.206	1.33
Physics, Atomic, Molecular & Chemical	492	2.446	0.83
Biochemistry & Molecular Biology	337	4.236	0.98
Spectroscopy	166	1.806	0.21
Biophysics	133	3.124	0.29
Chemistry, Medicinal	112	2.582	0.20
Physics, Condensed Matter	98	2.089	0.14
Pharmacology & Pharmacy	96	2.934	0.19
Chemistry, Applied	88	1.947	0.12
Multidisciplinary Sciences	86	8.741	0.52
Polymer Science	80	2.235	0.12
Physics, Applied	70	2.169	0.10
Nanoscience & Nanotechnology	68	3.069	0.14
Chemistry, Analytical	51	2.608	0.09
Biochemical Research Methods	38	3.271	0.09
Engineering, Chemical	30	1.583	0.03
Computer Science, Interdisciplinary Applications	24	1.552	0.03
Mathematics, Interdisciplinary Applications	18	1.587	0.02
Physics, Multidisciplinary	12	2.793	0.02
Cell Biology	10	5.696	0.04
Computer Science, Information Systems	10	1.633	0.01
Materials Science, Textiles	10	0.914	0.01
Biotechnology & Applied Microbiology	9	2.93	0.02
Electrochemistry	9	2.828	0.02
Instruments & Instrumentation	7	1.504	0.01
All other subject areas	67	-	-
Total	16,484	-	-

Supplementary Table N. The thirty subject areas that cited the group-D target articles most frequently.

Subject area	Citations	IF	CI
Biochemistry & Molecular Biology	2263	4.236	8.93
Chemistry, Multidisciplinary	1605	3.626	5.42
Chemistry, Inorganic & Nuclear	1431	2.247	3.00
Crystallography	1358	1.046	1.32
Biophysics	849	3.124	2.47
Chemistry, Organic	588	2.75	1.51
Chemistry, Physical	578	2.828	1.52
Cell Biology	398	5.696	2.11
Biochemical Research Methods	319	3.271	0.97
Materials Science, Multidisciplinary	317	2.206	0.65
Chemistry, Medicinal	251	2.582	0.60
Computer Science, Interdisciplinary Applications	189	1.552	0.27
Physics, Atomic, Molecular & Chemical	184	2.446	0.42
Pharmacology & Pharmacy	140	2.934	0.38
Multidisciplinary Sciences	138	8.741	1.12
Spectroscopy	85	1.806	0.14
Computer Science, Information Systems	59	1.633	0.09
Physics, Condensed Matter	56	2.089	0.11
Biotechnology & Applied Microbiology	47	2.93	0.13
Polymer Science	42	2.235	0.09
Chemistry, Applied	40	1.947	0.07
Chemistry, Analytical	29	2.608	0.07
Physics, Applied	29	2.169	0.06
Mathematical & Computational Biology	28	2.835	0.07
Nanoscience & Nanotechnology	23	3.069	0.07
Mathematics, Interdisciplinary Applications	18	1.587	0.03
Engineering, Chemical	16	1.583	0.02
Plant Sciences	15	2.354	0.03
Hematology	14	5.350	0.07
Microbiology	14	3.341	0.04
All other subject areas	228	-	-
Total	11,351	-	-