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Article

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Supplementary Information

***In Silico* Toxicology Data Resources to Support Read-Across and (Q)SAR**

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References pertaining to each database under different categories

I. Chemistry Databases

1. CFam (C. Zhang et al., 2015)
2. CCDS (Groom & Allen, 2014)
3. ChemAgora Portal (Zanzi & Wittwehr, 2017)
4. ChemSpider (Pence & Williams, 2010)
5. CompTox Chemistry Dashboard (A. J. Williams et al., 2017)
6. ChEBI (Hastings et al., 2015)
7. The Chemical Space Project (Reymond, 2015)
8. COD (Grazulis et al., 2012)
9. ChemIDplus (Tomasulo, 2002)
10. SciFinder (Gabrielson, 2018)
11. ChemDB (J. H. Chen, Linstead, Swamidass, Wang, & Baldi, 2007)
12. ChEMBL (Gaulton et al., 2017)
13. DOCK Blaster (Irwin et al., 2009)
14. Danish QSAR (Pradeep, Povinelli, White, & Merrill, 2016)
15. eChemPortal (de Marcellus, 2014)
16. e-Drug3D (Pihan, Colliandre, Guichou, & Douguet, 2012)
17. eQuilibrator (Flamholz, Noor, Bar-Even, & Milo, 2012)
18. FDB-17 (Visini, Awale, & Reymond, 2017)
19. FilTer Base (Kolte, Londhe, Solanki, Gacche, & Meshram, 2018)

20. GDB-17 (Ruddigkeit, van Deursen, Blum, & Reymond, 2012)
21. HDACiDB (Murugan et al., 2015)
22. IUCLID (Heidorn, Hansen, & Nørager, 1996)
23. JRC-QSAR Model Db (M. Pavan & Worth, 2008)
24. LipidBank (Arita, Yasugi, Seyama, & Nishijima, 2007)
25. Lipidomics Gateway (M. Sud, Fahy, Cotter, Dennis, & Subramaniam, 2012)
26. NCI- DIS-3D Database (Milne, Nicklaus, Driscoll, Wang, & Zaharevitz, 1994)
27. NMRShift DB (S. Kuhn & Schlörer, 2015)
28. OCHEM (Sushko et al., 2011)
29. OSDDChem (Årdal & Røttingen, 2012)
30. PubChem (Hähnke, Kim, & Bolton, 2018)
31. Protein pKa Db (C. P. Toseland, McSparron, Davies, & Flower, 2006)
32. PCDDb (Whitmore, Miles, Mavridis, Janes, & Wallace, 2017)
33. Probes and Drugs Portal (Skuta et al., 2017)
34. Probe Miner (Antolin et al., 2018)
35. SDBS (Saito & Kinugasa, 2011)
36. ZINC 15 (Sterling & Irwin, 2015)

II. Toxicological Databases

1. ACToR (Judson et al., 2008)
2. AcuteTox (Clemmedson, 2008)
3. CPDB (Gold, Manley, Slone, & Rohrbach, 1999)
4. COSMOS (Cronin MTD, 2012)
5. CTD (Davis et al., 2011)
6. CEBS (Lea, Gong, Paleja, Rashid, & Fostel, 2017)
7. ChemTunes & ToxGPS (Fioravanzo et al., 2015; C. Yang et al., 2018)
8. CCRIS (P. Cameron, M. Stump, & Schofield, 2019)
9. DSSTox (Williams-DeVane, Wolf, & Richard, 2009)
10. diXa (Hendrickx et al., 2014)
11. DevTox (Solecki et al., 2010)
12. Drug Matrix (Ganter, Snyder, Halbert, & Lee, 2006)
13. eTox (Cases et al., 2014; Sanz et al., 2017)
14. EADB (J. Shen et al., 2013)
15. EDKB (Ding et al., 2010)
16. HESS Database (Abe et al., 2012)
17. ISSTOX (Benigni, Battistelli, Bossa, Tcheremenskaia, & Crettaz, 2013)
18. Lhasa Carcinogenicity Db (Marchant, 1996; Roberts, Myatt, Johnson, Cross, & Blower, 2000)
19. LiverTox (Yu et al., 2014)
20. LTKB (M. Chen et al., 2013)
21. NCI-60 (DTP) (Close et al., 2018)
22. NCTRlodb (Beger, Young, & Fang, 2004)
23. Open TG-GATEs (Igarashi et al., 2015)

24. pCEC (Sone et al., 2010)
25. ProTox (Priyanka Banerjee, Eckert, Schrey, & Preissner, 2018)
26. SuperToxic (U. Schmidt et al., 2009)
27. ToxLine (Schultheisz, 1981)
28. ToxDB (Hardt et al., 2016)
29. Toxygates (Natsume-Kitatani, Nyström-Persson, Igarashi, Satoh, & Mizuguchi, 2017)
30. Toxbank (Kohonen et al., 2013)
31. Tox21 (R. Huang et al., 2016)
32. Toxcast (Richard et al., 2016)
33. ToxRefDB (M. T. Martin et al., 2009)
34. T3DB (D. Wishart et al., 2015)

III. ADME Databases

1. ADME-AP (L. Z. Sun, Ji, Chen, Wang, & Chen, 2002)
2. ADMET SAR (F. Cheng et al., 2012)
3. ADMETlab (J. Dong et al., 2018)
4. ADMETNet (Q. Xu et al., 2017)
5. AMED Cardiotoxicity (Sato, Yuki, Ogura, & Honma, 2018)
6. BBB/ HIA database (Jie Shen, Cheng, Xu, Li, & Tang, 2010)
7. CYP-DI table (DA., 2007)
8. CYP-450 Inhibitors (Feixiong Cheng et al., 2011)
9. DIDB (Hachad, Ragueneau-Majlessi, & Levy, 2010)
10. e-pk Gene (Hachad et al., 2011)
11. EDETOX Db (F. Williams, 2004)
12. FINDbase (P. Papadopoulos et al., 2014)
13. IDAAPM (Legehar, Xhaard, & Ghemtio, 2016)
14. Metrabase (Mak et al., 2015)
15. OI-DDI (Yeung et al., 2015)
16. PDSP-Ki (Roth, Lopez, Patel, & Kroeze, 2000)
17. Tox-database.net (Polak, Wiśniewska, Glinka, & Polak, 2012)
18. TransportDB (Elbourne, Tetu, Hassan, & Paulsen, 2017)
19. TCDB (Saier et al., 2016)
20. TP-Search (Ozawa et al., 2004)
21. TTD (Y. H. Li et al., 2018)
22. Transformer (Hoffmann et al., 2014)
23. UCSF-P'genetics (Kroetz, Yee, & Giacomini, 2009)
24. UCSF-FDA Transportal (Morrissey et al., 2012)
25. X-MetDB (Spjuth, Rydberg, L. Willighagen, Evelo, & Jeliazkova, 2016)

IV. Drug Discovery Databases

1. Allosteric Database (Q. Shen et al., 2016)
2. ASDCD (Xing Chen et al., 2014)
3. AffinDB (Block, A Sottriffer, Dramburg, & Klebe, 2006)

4. APD (G. Wang, Li, & Wang, 2016)
5. AutoBind (Darby Tien-Hao Chang, Ke, Lin, & Chiang, 2012)
6. ARDB (B. Liu & Pop, 2009)
7. aBiofilm (Rajput, Thakur, Sharma, & Kumar, 2018)
8. Autosome Chromosome Rearrangement Db (Jie, Lonnie, Peter, & Stephen, 2004)
9. ADHD gene Db (L. Zhang et al., 2012)
10. Allergome Db (Mari, Mari, & Ronconi, 2005)
11. Autism KB (L.-M. Xu et al., 2012)
12. Binding DB (Gilson et al., 2016)
13. Binding MOAD (M. L. Benson et al., 2008)
14. Brenda (Placzek et al., 2017)
15. BioModels (Chelliah, Laibe, & Le Novere, 2013)
16. BCNTB bioinformatics (Gadaleta, Pirrò, Dayem Ullah, Marzec, & Chelala, 2018)
17. BARD (Howe et al., 2015)
18. Big Data Center ("Database Resources of the BIG Data Center in 2019," 2018)
19. BD-gene (S. H. Chang et al., 2013)
20. CLiBE (X. Chen, Ji, Zhi, & Chen, 2002)
21. CTD² (Aksoy et al., 2017)
22. Cancer Resource (Gohlke, Nickel, Otto, Dunkel, & Preissner, 2016)
23. canSAR (Coker et al., 2018)
24. CARLSBAD (Mathias et al., 2013)
25. CCGD (Abbott et al., 2015)
26. Chemical Probes (Frye, 2010)
27. CARD (B. Jia et al., 2017)
28. cBioPortal (J. Gao et al., 2013)
29. CREDO (Schreyer & Blundell, 2013)
30. CCDB (Agarwal, Raghav, Singh, & Raghava, 2011)
31. CS-DEGs (L. Guo, Du, Chang, Zhang, & Wang, 2014)
32. CAMPR3 (Waghu, Barai, Gurung, & Idicula-Thomas, 2016)
33. Cyclonet (Kolpakov et al., 2007)
34. Cancer DR (R. Kumar et al., 2013)
35. Cell Image Library (Orloff, Iwasa, Martone, Ellisman, & Kane, 2013)
36. DART (Ji et al., 2003)
37. DT-Web (Alaimo et al., 2015)
38. DTome (Jingchun Sun, Wu, Xu, & Zhao, 2012)
39. DRH (Corsello et al., 2017)
40. DTC (Tanoli et al., 2018)
41. Drug Miner (Jamali et al., 2016)
42. DCDB (Y. Liu et al., 2014)
43. DrugBank (David S. Wishart, Knox, et al., 2008)
44. DSigDB (M. Yoo et al., 2015)
45. Drug Central (Ursu et al., 2016)
46. D3R (Gaieb et al., 2018)
47. DBAASP (Pirtskhalava et al., 2016)

48. Drug2Gene (Roider et al., 2014)
49. DGIdb (Cotto et al., 2018)
50. DNASU (Seiler et al., 2014)
51. Driver DBv2 (Chung et al., 2016)
52. DiseaseMeth (Lv et al., 2012)
53. EUPath DB (Aurrecochea et al., 2017)
54. Ensembl (Kersey et al., 2018)
55. ExCAPE-DB (Jiangming Sun et al., 2017)
56. e-Drug3D (Pihan et al., 2012)
57. e-HOMD (Fernández Escapa et al., 2018)
58. FaCD Online (Rainville & Garber, 2008)
59. Flow Repository (Spidlen, Breuer, Rosenberg, Kotecha, & Brinkman, 2012)
60. GenomeCRISPR (Rauscher, Heigwer, Breinig, Winter, & Boutros, 2017)
61. GOLD (Mukherjee et al., 2018)
62. Gene DB (Hertz-Fowler et al., 2004)
63. GLIDA (Okuno, Yang, Taneishi, Yabuuchi, & Tsujimoto, 2006)
64. GDSC (W. Yang et al., 2013)
65. HMDC (J. Eppig, 2017)
66. Human/ Animal TFDB (Hu et al., 2018)
67. IntSide (Juan-Blanco, Duran-Frigola, & Aloy, 2015)
68. ICGC (J. Zhang et al., 2011)
69. KDBI (P. Kumar et al., 2009)
70. KinMutBase (Ortutay, Valiaho, Stenberg, & Vihinen, 2005)
71. KLIFS (Kooistra et al., 2016)
72. LigDig (Fuller et al., 2015)
73. Liver Atlas (Y. Zhang et al., 2013)
74. MetaADEDDB (Feixiong Cheng et al., 2013)
75. MetaBase (Bolser et al., 2012)
76. MOSAIC (Nelson et al., 2018)
77. MEdock (Darby Tien-Hau Chang, Oyang, & Lin, 2005)
78. MICAD (Chopra et al., 2012)
79. MTB Db (Krupke et al., 2017)
80. mSignatureDB (P. J. Huang et al., 2018)
81. mutLBSgeneDB (P. Kim, Zhao, Lu, & Zhao, 2017)
82. MK4MDD (L. Guo et al., 2012)
83. Methy Cancer (X. He et al., 2008)
84. NPASS (X. Zeng et al., 2018)
85. NLDB (Murakami, Omori, & Kinoshita, 2016)
86. NCCN (Wood, 2004)
87. NeuroMorpho.Org (Ascoli, Donohue, & Halavi, 2007)
88. NIF (A. Gupta et al., 2008)
89. NPACT (Mangal, Sagar, Singh, Raghava, & Agarwal, 2013)
90. NCG (Kuppili Venkata et al., 2018)
91. Neuron DB (Marenco, Nadkarni, Skoufos, Shepherd, & Miller, 1999)

92. OBO Foundry (B. Smith et al., 2007)
93. OCGD (Gadewal & Zingde, 2011)
94. Open Target (Koscielny et al., 2017)
95. Open PHACTS (A. J. Williams et al., 2012)
96. Orphanet Db (S. Pavan et al., 2017)
97. PDBbind-CN Database (Z. Liu et al., 2015)
98. PoSSuM (Ito, Tabei, Shimizu, Tsuda, & Tomii, 2011)
99. PICKLES (Lenoir, Lim, & Hart, 2018)
100. PhID (Deng, Tu, Deng, & Hu, 2017)
101. PHAROS (Nguyen et al., 2017)
102. PharmGKB (Thorn, Klein, & Altman, 2013)
103. PROMISCUOUS (von Eichborn et al., 2011)
104. PathogenBox (Jeong et al., 2018)
105. RepurposeDB (Shameer et al., 2018)
106. repoDB (Brown & Patel, 2017)
107. RxNav (K. Zeng, Bodenreider, Kilbourne, & Nelson, 2006)
108. Sc-PDB (Desaphy, Bret, Rognan, & Kellenberger, 2015)
109. Super Drug 2.0 (Goede, Dunkel, Mester, Frommel, & Preissner, 2005)
110. Super Target (Hecker et al., 2012)
111. SM2miR (Xinyi Liu et al., 2013)
112. SuperPred/target/toxic (Nickel et al., 2014)
113. Super Natural II (P. Banerjee et al., 2015)
114. Super Pain (Gohlke, Preissner, & Preissner, 2014)
115. Swiss Bioisostere (Wirth, Zoete, Michielin, & Sauer, 2012)
116. SIMAP (Arnold, Goldenberg, Mewes, & Rattei, 2014)
117. Swiss Dock (Grosdidier, Zoete, & Michielin, 2011)
118. Swiss SideChain (Gfeller, Michielin, & Zoete, 2012)
119. SFARI Gene (Banerjee-Basu & Packer, 2010)
120. TDR Targets (Magarinos et al., 2012)
121. TDBTBD (Rosenthal et al., 2017)
122. THPdb (Usmani et al., 2017)
123. TCMID (Xue et al., 2013)
124. TPDB (Hanzlik, Koen, Theertham, Dong, & Fang, 2007)
125. TTDB (Y. H. Li et al., 2018)
126. TAG (J. S. Chen, Hung, Chan, Tsai, & Sun, 2013)
127. TCMID (Xue et al., 2013)
128. TADB (Hanzlik et al., 2007)
129. TissGDB (P. Kim et al., 2018)
130. VKCDB (Gallin & Boutet, 2011)
131. ViPR (Pickett et al., 2012)

V. Drug Information/Clinical Trials/ Pharmacovigilance Databases

1. ATC-DDD (Natsch et al., 1998)

2. ALFRED (Rajeevan et al., 2005)
3. AFND (Gonzalez-Galarza, Christmas, Middleton, & Jones, 2011)
4. AutDB (S. N. Basu, Kollu, & Banerjee-Basu, 2009)
5. BmDR (M. Martin, 2012)
6. BioPortal (Whetzel et al., 2011)
7. BRCA Exchange (Cline et al., 2018)
8. BioLINCC (Ross et al., 2016)
9. BioProject (Barrett et al., 2011)
10. Colorectal Cancer Atlas (Chisanga et al., 2016)
11. CKB (Patterson, Statz, Yin, & Mockus, 2017)
12. Cancer PPD (Tyagi et al., 2015)
13. CVRG (Winslow et al., 2011)
14. CPRD (Herrett et al., 2015)
15. CPIC (Relling & Klein, 2011)
16. Clinical Trials.gov (Schwartz, Woloshin, Zheng, Tse, & Zarin, 2016)
17. COSMIC (Forbes et al., 2008)
18. CTRP (A. Basu et al., 2013)
19. ChemDB (J. Chen, Swamidass, Dou, Bruand, & Baldi, 2005)
20. DAAB (Sircar et al., 2015)
21. DECIPHER (Firth et al., 2009)
22. Drug Trials Snapshots (Whyte, Woodcock, & Wang, 2017)
23. Drug Consumption Db (Ferrer et al., 2012)
24. Disease Ontology (Bello et al., 2018)
25. ENCePP (Kurz, Perez-Gutthann, & Group, 2018)
26. EudraVigilance (Postigo et al., 2018)
27. EAHD -CF-DB (Rallapalli, Kembball-Cook, Tuddenham, Gomez, & Perkins, 2013)
28. FAERS (Fang et al., 2014)
29. GePaRD (Ohlmeier et al., 2015)
30. GHR (Spatz, 2004)
31. HC-SC (MedEffect) (Lexchin, 2014)
32. HPO (Köhler et al., 2018)
33. HEROD (Xian Zeng et al., 2017)
34. ICD-10 (Weatherspoon & Chattopadhyay, 2013)
35. iSAEC (Contreras, Floratos, & Holden, 2013)
36. IDA (Crawford, Neu, & Toga, 2016)
37. LOINC (Khan et al., 2006)
38. Lareb (Scholl, van Hunsel, Hak, & van Puijenbroek, 2018)
39. MedDRA (J. Harrison & Mozzicato, 2009)
40. Micromedex (Chatfield, 2015)
41. MedWatch (Craigle, 2007)
42. MeSH (J. Nelson, Douglas Johnston, & L. Humphreys, 2001)
43. NDF-RT (Zhu, Freimuth, Pathak, Durski, & Chute, 2013)
44. NAPDI (Paine, Shen, & McCune, 2018)
45. Ontobee (Ong et al., 2017)

46. Open FDA (Kass-Hout et al., 2016)
47. OSB (Gleeson et al., 2018)
48. PanDrugs (Piñeiro-Yáñez et al., 2018)
49. PharmVar (Gaedigk et al., 2018)
50. PillBox (Yaniv et al., 2016)
51. PPMI (Marek et al., 2018)
52. PDX- Finder (Conte et al., 2018)
53. PedAM (J. Jia et al., 2018)
54. RxNorm (Freimuth, Wix, Zhu, Siska, & Chute, 2014)
55. SIDER 4.1 (M. Kuhn, Letunic, Jensen, & Bork, 2016)
56. SNOMED-CT (D. Lee, Cornet, Lau, & de Keizer, 2013)
57. Swiss-Var (Mottaz, David, Veuthey, & Yip, 2010)
58. STRIDE (STARR) (Lowe, Ferris, Hernandez, & Weber, 2009)
59. STEP (Salunke & Tuleu, 2015)
60. SUSARs (Pietraszkiewicz, Firlag-Burkacka, Horban, & Kowalska, 2014)
61. TCIA (Prior et al., 2017)
62. Trialtrove (Stergiopoulos, Getz, & Blazynski)
63. Uberon (Mungall, Torniai, Gkoutos, Lewis, & Haendel, 2012)
64. UMLS (Bodenreider, 2004)
65. VarCards (J. Li et al., 2018)
66. VAERS (Singleton, Lloyd, Mootrey, Salive, & Chen, 1999)
67. Vigibase (Lindquist, 2008)
68. WHO ICTRP (Lindquist, 2008)
69. WITHDRAWN (Siramshetty et al., 2016)

VI. Biological Databases

1. AbMiner (Major et al., 2006)
2. AntiJen (Christopher P. Toseland et al., 2005)
3. AlzhCPI (J. Fang et al., 2017)
4. Allen Brain Map Atlas (Sunkin et al., 2013)
5. ABCdb (Fichant, Basse, & Quentin, 2006)
6. AHTPDB (R. Kumar et al., 2015)
7. ADPriboDB (Vivelo, Wat, Agrawal, Tee, & Leung, 2017)
8. AntigenDB (Ansari, Flower, & Raghava, 2010)
9. AAindex (Kawashima et al., 2008)
10. AVPdb (Qureshi, Thakur, Tandon, & Kumar, 2014)
11. Addgene (Kamens, 2015)
12. AlloMAPS (Tan, Tee, Guarnera, Booth, & Berezovsky, 2018)
13. ArrayMap (Tan et al., 2018)
14. AH-DB (Darby Tien-Hao Chang, Yao, Fan, Chiang, & Bai, 2012)
15. ACLAME (Darby Tien-Hao Chang, Yao, et al., 2012)
16. ADHDgene (L. Zhang et al., 2012)
17. BioDBnet (Mudunuri, Che, Yi, & Stephens, 2009)

18. BUSCO (Simao, Waterhouse, Ioannidis, Kriventseva, & Zdobnov, 2015)
19. BrainTranscriptome (Keil, Qalieh, & Kwan, 2018)
20. Broad Bioimage (Ljosa, Sokolnicki, & Carpenter, 2012)
21. BioMuta (Dingerdissen et al., 2018)
22. BDB (B. He et al., 2016)
23. CPDB (Kamburov, Stelzl, Lehrach, & Herwig, 2013)
24. CASBAH (Lüthi & Martin, 2007)
25. CAMEO (Haas et al., 2018)
26. CanEvolve (Samur et al., 2013)
27. CHOPIN (Ochoa-Montano, Mohan, & Blundell, 2015)
28. Cangem (Scheinin et al., 2008)
29. CATH (Dawson et al., 2017)
30. Candidate Cancer Gene (Abbott et al., 2015)
31. CRISPRInc (W. Chen et al., 2018)
32. CirGRDB (X. Li et al., 2018)
33. CCDS (Farrell et al., 2014)
34. DisProt (D. Piovesan et al., 2017)
35. DDBJ (Mashima et al., 2016)
36. dbPTM (K. Y. Huang et al., 2016)
37. Directory of CYP 450 (Fábién & Degtyarenko, 1997)
38. dbSNP (Smigielski, Sirotkin, Ward, & Sherry, 2000)
39. dbGAP (Tryka et al., 2014)
40. dbVar (Ilkka Lappalainen et al., 2012)
41. dbNP (Evelo, van Bochove, & Saito, 2011)
42. DBTSS (Suzuki et al., 2018)
43. DIDA (Gazzo et al., 2016)
44. DDMGD (Raies, Mansour, Incitti, & Bajic, 2015)
45. DEPOD (Duan, Li, & Kohn, 2015)
46. D²P² (Oates et al., 2013)
47. ExoCarta (Keerthikumar et al., 2016)
48. ENCODE ("The ENCODE (ENCyclopedia Of DNA Elements) Project," 2004)
49. ExAC (Lek et al., 2016)
50. EnzymePortal (de Matos et al., 2013)
51. EMDb (Patwardhan, 2017)
52. Eidogen-Sertanty- KKB (Brooijmans, Chang, Mobilio, Denny, & Humblet, 2010)
53. ECO (Chibucos et al., 2014)
54. Ensembl (Zerbino et al., 2018)
55. Enzyme (Bairoch, 2000)
56. EGA (Ilkka Lappalainen et al., 2015)
57. ENA (P. W. Harrison et al., 2018)
58. EMPAIR (Bolasco, Weinhard, Boissonnet, Neujahr, & Gross, 2018)
59. eyeGENE (Blain, Goetz, Ayyagari, & Tumminia, 2013)
60. EuMMCR (Schick et al., 2016)
61. Ebola/ HVF (Kuiken, Thurmond, Dimitrijevic, & Yoon, 2012)

62. ERGR (A.-Y. Guo et al., 2009)
63. EPDnew (Dreos, Ambrosini, Cavin Périer, & Bucher, 2013)
64. Fraggile (Ahmed et al., 2011)
65. Fusion GDB (P. Kim & Zhou, 2018)
66. GenBank (D. A. Benson et al., 2013)
67. GlycoEpitope (Okuda, Nakao, & Kawasaki, 2021)
68. GLASS (W. K. B. Chan et al., 2015)
69. GEO (Clough & Barrett, 2016)
70. GPCRdb (Pándy-Szekeres et al., 2018)
71. GTEX portal (Consortium, 2013)
72. Genome 3D (Spielmann, Lupiáñez, & Mundlos, 2018)
73. GENT (G. Shin et al., 2011)
74. GO (Gene Ontology, 2015)
75. GENCODE (Frankish et al., 2018)
76. GlyTouCan (Tiemeyer et al., 2017)
77. GtRNAdb (P. P. Chan & Lowe, 2016)
78. GenomeProperties (Richardson et al., 2018)
79. GeneAtlas (Frezal, 1998)
80. GermOnline (Wiederkehr et al., 2004)
81. GPMdb (Fenyo & Beavis, 2015)
82. GenomeRNAi (E. E. Schmidt et al., 2013)
83. HAMAP (Pedruzzi et al., 2015)
84. HGNC (Braschi et al., 2019)
85. Human Protein Atlas (Uhlen et al., 2010)
86. HPRD (S. Peri et al., 2003)
87. Human Genome Project (Gardiner, 2002)
88. HERvd (Paces, Pavlicek, & Paces, 2002)
89. HORDE (Olender, Nativ, & Lancet, 2013)
90. HAGR (de Magalhaes, Costa, & Toussaint, 2005)
91. HEMD (Z. Huang et al., 2012)
92. HPM (M. S. Kim et al., 2014)
93. HIV molecular immunology Db (Los Alamos National, Theoretical, & Biophysics Group, 1995)
94. hPSCreg (Seltmann et al., 2016)
95. HGVD (Higasa et al., 2016)
96. HlStome (Khare et al., 2012)
97. HEDD (Shao et al., 2018)
98. HGVS (Horaitis & Cotton, 2004)
99. H-InvDB (Takeda et al., 2013)
100. iPTMnet (H. Huang et al., 2018)
101. IEDB (Y. Kim et al., 2012)
102. IUPHAR (Sharman et al., 2013)
103. IID (Kotlyar, Pastrello, Sheahan, & Jurisica, 2016)
104. IMGT (Lefranc et al., 2005)

105. InterPro (Mitchell et al., 2018)
106. iProClass (Wu, Huang, Nikolskaya, Hu, & Barker, 2004)
107. ImmPort (Bhattacharya et al., 2018)
108. InSiGHT variant Db (Plazzer et al., 2013)
109. IntEnz (Fleischmann et al., 2004)
110. IPD (Maccari et al., 2017)
111. IMGT/GENE-Db (Giudicelli, Chaume, & Lefranc, 2005)
112. IMGT/mAb-DB (Poirion et al., 2010)
113. IMOTA (Palmieri et al., 2018)
114. Interferome (Rusinova et al., 2013)
115. IDR (E. Williams et al., 2017)
116. JGI Genome Portal
117. JGA (Kodama et al., 2015)
118. KinWeb (Milanesi et al., 2006)
119. KIDFamMap (Chiu et al., 2013)
120. Labome (Xie, 2017)
121. LGICdb (Le Novere & Changeux, 2001)
122. LIPID MAPS (Fahy et al., 2009)
123. LncRNADisease v2.0 (Z. Bao et al., 2018)
124. LOCATE (Sprenger et al., 2008)
125. MGC (Temple et al., 2009)
126. MITOMAP (Lott et al., 2013)
127. miRWalk (Dweep & Gretz, 2015)
128. MGnify (L Mitchell et al., 2017)
129. MHCBN (Lata, Bhasin, & Raghava, 2009)
130. MitoProteome (Cotter, Guda, Fahy, & Subramaniam, 2004)
131. MEROPS (Rawlings et al., 2018)
132. MultitaskProtDB (Franco-Serrano et al., 2018)
133. MatrixDB (Clerc et al., 2018)
134. MPSTRUC (Stansfeld et al., 2015)
135. miRBase (Kozomara & Griffiths-Jones, 2014)
136. MRMAssayDB (Bhowmick, Mohammed, & Borchers, 2018)
137. MetaGene (Noguchi, Park, & Takagi, 2006)
138. MitoMiner (A. C. Smith & Robinson, 2018)
139. Morphinome (Prokai, Zharikova, & Stevens, 2005)
140. MedReaders (Guohua Wang et al., 2018)
141. MSDD (Yue et al., 2018)
142. MethHC (W.-Y. Huang et al., 2015)
143. miRandola (Russo et al., 2018)
144. MetalPDB (Putignano, Rosato, Banci, & Andreini, 2018)
145. Microbiome DB (Oliveira et al., 2018)
146. Mitocheck (Cai et al., 2018)
147. Membranome (Lomize, Hage, & Pogozheva, 2018)
148. MetaBase (Pedersen & Bongo, 2017)

149. MINAS (Schnabl, Suter, & Sigel, 2012)
150. MIPModDB (A. B. Gupta et al., 2012)
151. Modomics (Boccaletto et al., 2018)
152. NRR (Martinez et al., 1997)
153. NPD (Dellaire, Farrall, & Bickmore, 2003)
154. NextProt (Gaudet et al., 2017)
155. NURSA (Margolis, Evans, & W O'Malley, 2005)
156. NC-IUBMB (Lilley et al., 1995)
157. NPIDB (Kirsanov et al., 2013)
158. NIH 3D Print Exchange (McCarthy et al., 2014)
159. NONCODE (C. Liu et al., 2005)
160. NATsDB (Y. Zhang et al., 2007)
161. O-GLYCBASE (R. Gupta, Birch, Rapacki, Brunak, & Hansen, 1999)
162. OrthoDB (Kriventseva et al., 2018)
163. OverGeneDB (Rosikiewicz, Suzuki, & Makatowska, 2018)
164. ORDB (Crasto, Marengo, Miller, & Shepherd, 2002)
165. OncoDB.HCC (W.-H. Su et al., 2007)
166. Organelle DB (Wiwatwattana & Kumar, 2005)
167. OpenSNP (Greshake, Bayer, Rausch, & Reda, 2014)
168. OGEE (W.-H. Chen, Lu, Chen, Zhao, & Bork, 2017)
169. PANTHER (Mi, Muruganujan, Ebert, Huang, & Thomas, 2018)
170. PRINTS (Attwood et al., 1997)
171. PSP (Hornbeck et al., 2015)
172. PRO (Natale et al., 2011)
173. Phospho- ELM (Dinkel et al., 2011)
174. Phospho3D (Dinkel et al., 2011)
175. Plasma Proteome (Schwenk et al., 2017)
176. PDBTM (Kozma, Simon, & Tusnády, 2013)
177. Protein Kinase Resource (Petretti & Prigent, 2005)
178. ProtChemSI (Kalinina, Wichmann, Apic, & Russell, 2011)
179. PHI (Takemoto & Aie, 2017)
180. PDB (Berman et al., 2000)
181. PRIDE (Vizcaino et al., 2016)
182. PROXiMATE (Jemimah, Yugandhar, & Michael Gromiha, 2017)
183. PHOSIDA (Gnad, Gunawardena, & Mann, 2011)
184. PSCDB (Amemiya, Koike, Kidera, & Ota, 2012)
185. Proteome Isoelectric Point (Kozlowski, 2017)
186. PED (Marzec et al., 2018)
187. PlasmID (Zuo et al., 2007)
188. PPT- DB (David S. Wishart, Arndt, et al., 2008)
189. Platinum (Pires, Blundell, & Ascher, 2015)
190. Peroxisome DB (Schluter, Real-Chicharro, Gabaldon, Sanchez-Jimenez, & Pujol, 2010)
191. PDBSum (Laskowski, Jabłońska, Pravda, Vařeková, & Thornton, 2018)

192. Pfam (Finn et al., 2014)
193. Polbase (Langhorst, Jack, Reha-Krantz, & Nichols, 2012)
194. PolymiRTS (L. Bao et al., 2007)
195. ProtoNet (Rappoport, Linial, & Linial, 2013)
196. PrimerBank (X. Wang, Spandidos, Wang, & Seed, 2012)
197. ProtCID (X. Wang et al., 2012)
198. Rhea (Morgat et al., 2017)
199. RoadMapepigenomics (Roadmap Epigenomics et al., 2015)
200. RBPDB (Cook, Kazan, Zuberi, Morris, & Hughes, 2011)
201. RNA Central ("RNAcentral: a hub of information for non-coding RNA sequences," 2018)
202. RegPhos (K.-Y. Huang et al., 2014)
203. REPAIRtoire (Milanowska et al., 2011)
204. RMDB (Cordero, Lucks, & Das, 2012)
205. RAID (Yi et al., 2017)
206. SAGD (Shi et al., 2018)
207. Stanford Tissue Microarray Db (Marinelli et al., 2008)
208. SCDE (Ho Sui et al., 2012)
209. Super Hapten (Günther, Hempel, Dunkel, Rother, & Preissner, 2007)
210. The SystemMHC Atlas (Shao et al., 2018)
211. SNPeffect (De Baets et al., 2012)
212. SiRecords (Ren et al., 2009)
213. SuperFamily (Pandurangan, Stahlhacke, Oates, Smithers, & Gough, 2019)
214. SwissLipids (Aimo et al., 2015)
215. SSDB (Tohsato, Ho, Kyoda, & Onami, 2016)
216. SBCDDb (Newberg, Mann, Mann, Jenkins, & Copeland, 2018)
217. StarBase (J.-H. Li, Liu, Zhou, Qu, & Yang, 2014)
218. SelenoDB (Romagné et al., 2014)
219. SBKB (Gabanyi et al., 2011)
220. SWISS-MODEL (Biasini et al., 2014)
221. SynSysNet (von Eichborn et al., 2013)
222. SynLethDB (J. Guo, Liu, & Zheng, 2016)
223. Sc-PDB (Kellenberger et al., 2006)
224. STRENDA (Swainston et al., 2018)
225. SDAP (Ivanciuc, Schein, & Braun, 2003)
226. SYFPEITHI (Ivanciuc et al., 2003)
227. STRING (Szklarczyk et al., 2017)
228. SM2miR (X. Liu et al., 2013)
229. tRNADB (Jühling et al., 2009)
230. TSgene (Zhao, Sun, & Zhao, 2013)
231. topPTM (M. G. Su et al., 2014)
232. TP53 (Leroy et al., 2017)
233. TCDB (Saier et al., 2016)
234. TubercuList (Lew, Kapopoulou, Jones, & Cole, 2011)

235. tRFdb (P. Kumar, Mudunuri, Anaya, & Dutta, 2015)
236. THPdb (Usmani et al., 2017)
237. Telomerase (Podlevsky, Bley, Omana, Qi, & Chen, 2008)
238. UniProt (UniProt, 2014)
239. UbiProt (Chernorudskiy et al., 2007)
240. UniProbe Db (Newburger & Bulyk, 2009)
241. ValidatorDB (Sehna et al., 2015)
242. ViralZone (Masson et al., 2013)
243. VariO (Vihinen, 2014)
244. VDJdb (Shugay et al., 2018)
245. Wnt Db (Nusse & Varmus, 2012)
246. 1000,000 Genomes Project (Turnbull et al., 2018)
247. 3did (Mosca, Céol, Stein, Olivella, & Aloy, 2014)
248. 5S rRNA (Dinman, 2005)

VII. Protein-Protein Interactions

1. APID (Alonso-Lopez et al., 2016)
2. BioGRID (Oughtred et al., 2019)
3. BCL2DB (Rech de Laval, Deleage, Aouacheria, & Combet, 2014)
4. CancerNet (Meng et al., 2015)
5. ComPPI (Veres et al., 2015)
6. CAZy (Cantarel et al., 2009)
7. Complex Portal (Meldal et al., 2019)
8. CORUM (Ruepp et al., 2010)
9. Differential Net (Basha, Shpringer, Argov, & Yeager-Lotem, 2018)
10. DynaSIN (Bhardwaj, Abyzov, Clarke, Shou, & Gerstein, 2011)
11. DIP (Salwinski et al., 2004)
12. DOMMINO (Kuang, Dhroso, Han, Shyu, & Korkin, 2016)
13. gpDB (Theodoropoulou, Bagos, Spyropoulos, & Hamodrakas, 2008)
14. GWIDD (Kundrotas, Zhu, & Vakser, 2012)
15. HINT (Das & Yu, 2012)
16. HIP (Rual et al., 2005)
17. HPRD (Suraj Peri et al., 2004)
18. H-Inv DB (Takeda et al., 2013)
19. HCSGD (Q. Dong et al., 2017)
20. Hit Predict (López, Nakai, & Patil, 2015)
21. InnateDB (Breuer et al., 2013)
22. IMEx (Orchard et al., 2012)
23. INstruct (Meyer, Das, Wang, & Yu, 2013)
24. IRView (Fujimori et al., 2012)
25. IntAct (Kerrien et al., 2012)
26. I2D (Kotlyar et al., 2016)
27. IIDB (Tseng et al., 2015)
28. iMOTdb (Pugalenthi, Bhaduri, & Sowdhamini, 2006)

29. iRefWeb (Turner et al., 2010)
30. KBDock (Ghoorah, Devignes, Smaïl-Tabbone, & Ritchie, 2014)
31. miRTarBase (Chou et al., 2018)
32. MIPS (Pagel et al., 2005)
33. Mentha (Calderone, Castagnoli, & Cesareni, 2013)
34. MATADOR (Günther et al., 2008)
35. MINT (Licata et al., 2012)
36. ORTI (Vafaee et al., 2016)
37. PSMDB (Wallach & Lilien, 2009)
38. PrePPI (Q. C. Zhang, Petrey, Garzón, Deng, & Honig, 2013)
39. PiSITE (Higurashi, Ishida, & Kinoshita, 2009)
40. ProtInDB (Jordan, El-Manzalawy, Dobbs, & Honavar, 2012)
41. ProtChemSI (Kalinina, Wichmann, Apic, & Russell, 2012)
42. PINT (M. D. Kumar & Gromiha, 2006)
43. PIMADb (Mathew & Sowdhamini, 2016)
44. PIPs (McDowall, Scott, & Barton, 2009)
45. Peptide Atlas (Deutsch, 2010)
46. SCOPPI (Winter, Henschel, Kim, & Schroeder, 2006)
47. SKEMPI (Jankauskaite, Jimenez-Garcia, Dapkunas, Fernandez-Recio, & Moal, 2018)
48. SNAPPI-View (Jefferson, Walsh, Roberts, & Barton, 2007)
49. TRIP Db (Shin, Shin, So, Kwon, & Jeon, 2011)
50. UniHI (Kalathur et al., 2014)
51. Wiki-PI (Orie & Ganapathiraju, 2012)
52. 2P2ldb (Basse, Betzi, Morelli, & Roche, 2016)

VIII. OMICS databases

1. Angiogenes (Müller et al., 2016)
2. Array Express Db (Rustici et al., 2013)
3. ArrayTrack (H. Fang et al., 2017)
4. BiGG Models (King et al., 2016)
5. BioSample (Gostev et al., 2012)
6. BioStudies (Sarkans et al., 2018)
7. BMRDB (Smelter, Astra, & Moseley, 2017)
8. BML-NMR (Ludwig et al., 2012)
9. BioPlex 2.0 (Huttlin et al., 2017)
10. BioSystems (Geer et al., 2010)
11. BioXpress (Wan et al., 2015)
12. C-MAP (Subramanian et al., 2017)
13. ccmGDB (P. Kim, Cheng, Zhao, & Zhao, 2016)
14. CEGA (Dousse, Junier, & Zdobnov, 2016)

15. CGHub (Wilks et al., 2014)
16. CKDdb (Fernandes & Husi, 2017)
17. CTRP (A. Basu et al., 2013)
18. DepMap (Tsherniak et al., 2017)
19. DISNOR (Lo Surdo et al., 2018)
20. DSigDB (Minjae Yoo et al., 2015)
21. DGVa (I. Lappalainen et al., 2013)
22. DRUGSURV (Amelio et al., 2014)
23. DisGeNet (Piñero et al., 2017)
24. DGIdb (Cotto et al., 2018)
25. Expression Atlas (Papatheodorou et al., 2018)
26. Fiehn Lib Db (Fiehn, 2016)
27. GeneCards (Safran et al., 2010)
28. HMA (Pornputtapong, Nookaew, & Nielsen, 2015)
29. HMDB 4.0 (D. S. Wishart et al., 2018)
30. Incardiome KB (Sharma, Deshpande, Ghatge, & Vangala, 2017)
31. IPD (Robinson, Halliwell, McWilliam, Lopez, & Marsh, 2013)
32. KUPKB (Jupp, Klein, Schanstra, & Stevens, 2011)
33. LOMA (Buchkremer et al., 2010)
34. Metabolomics Workbench (Manish Sud et al., 2016)
35. MutAIT (Avancini et al., 2016)
36. MitoProteome (Cotter et al., 2004)
37. MSigDB (Liberzon et al., 2015)
38. MobiDB (Damiano Piovesan et al., 2018)
39. MBROLE (López-Ibáñez, Pazos, & Chagoyen, 2016)
40. NCI-60 (DTP) (Monga & Sausville, 2002)
41. OMIM (Hamosh, Scott, Amberger, Bocchini, & McKusick, 2005)
42. Omics DI (Perez-Riverol et al., 2017)
43. PACdb (Gamazon et al., 2010)
44. PRIDE (Jones & Cote, 2008)
45. PharmacDB (Smirnov et al., 2018)
46. READDB (Hashemikhabir, Neelamraju, & Janga, 2015)
47. RefSeq (Pruitt, Tatusova, & Maglott, 2007)
48. Rfam (Griffiths-Jones, Bateman, Marshall, Khanna, & Eddy, 2003)
49. RGED (Q. Zhang et al., 2014)
50. Signalink 2 (Fazekas et al., 2013)
51. SIGNOR (Perfetto et al., 2016)
52. TBDRM-db (Sandgren et al., 2009)
53. TCGA (Rau, Flister, Rui, & Auer, 2019)
54. UniCarb-DB (Campbell et al., 2014)
55. UPdb (T. Papadopoulos et al., 2016)

IX. Pathways Based Databases

1. AOP-KB (Ives, Campia, Wang, Wittwehr, & Edwards, 2017)

2. Aging Chart (Moskalev et al., 2016)
3. Biocyc (Paley & Karp, 2017)
4. DIMEdb (O'Shea et al., 2018)
5. Effectopedia (Sachana, 2018)
6. Endonet (Potapov et al., 2006)
7. Human Cyc (Trupp et al., 2010)
8. iPAVS (Sreenivasaiah, Rani, Cayetano, Arul, & Kim, 2012)
9. KEGG (Kanehisa, Sato, Furumichi, Morishima, & Tanabe, 2018)
10. MetaCyc (Caspi et al., 2016)
11. MetaboLights (Kale et al., 2016)
12. MetaMapTox (Kamp et al., 2012)
13. MMMP (Mocellin & Rossi, 2008)
14. Nrf2Ome (Türei et al., 2013)
15. PID (Schaefer et al., 2009)
16. PDID (C. Wang et al., 2016)
17. Pathway Commons (Cerami et al., 2011)
18. PathCards (Belinky et al., 2015)
19. PathDIP (Rahmati, Abovsky, Pastrello, & Jurisica, 2017)
20. Pathways Web (Melott, Weinstein, & Broom, 2016)
21. Pathbase (Schofield et al., 2004)
22. Reactome (Croft et al., 2011)
23. MalaCard (Rappaport et al., 2017)
24. yAPOPTOSIS (Wanichthanarak, Cvijovic, Molt, & Petranovic, 2013)
25. SMPDB (Frolkis et al., 2010)
26. STITCH (M. Kuhn, von Mering, Campillos, Jensen, & Bork, 2008)
27. TIGER (X. Liu, Yu, Zack, Zhu, & Qian, 2008)
28. TRANSPATH (Choi et al., 2004)
29. Tri ForC (Miettinen et al., 2018)
30. TCSBN (S. Lee et al., 2018)
31. WikiPathways (Slenter et al., 2018)
32. XTalkDB (Sam, Teel, Tegge, Bharadwaj, & Murali, 2017)

X. Patent related database

1. SCRIPDB (Heifets & Jurisica, 2012)
2. SureChEMBL (Papadatos et al., 2016)

XI. Environmental Exposure related database

1. ATSDR (Kowalski, Anderson, Moore, & Wilder, 2013)
2. ASTDR MRLs (Selene, Chou, Holler, & T De Rosa, 1998)
3. CEDI/ADI DB (Neltner et al., 2011)
4. EWAG-BBD (Junfeng Gao, Ellis, & Wackett, 2010)
5. Exposome (Neveu et al., 2016)

6. ECOdrug (Verbruggen et al., 2018)
7. EnviPath (Wicker et al., 2016)
8. HeatDB (O'Mahony et al., 2016)
9. HSDB (Fonger, 1995)
10. Household Products DB (Cooney & Figg, 2018)
11. IRIS (Dourson, 2018)
12. IARC (Pearce et al., 2015)
13. LINCS (Koleti et al., 2018)
14. OECD-QSAR (Fitzpatrick, 2007)
15. PHAROS (Friar & Vittori, 2017)
16. RiskIE (Wullenweber et al., 2008)
17. RITA (Morawietz, Rittinghausen, & Mohr, 1992)

XII. Animal Alternatives/ Methods

1. Atlases-Pathology Images (Feit, Kempf, Jedlickova, & Burg, 2005)
2. AnimalTFDB (Hu et al., 2018)
3. Bgee (Bastian et al., 2008)
4. Cellosaurus (Bairoch, 2018)
5. CCLE (Barretina et al., 2012)
6. Cell Line Navigator (Krupp et al., 2013)
7. DB-ALM (Adolphe, 1995)
8. FCS-Free- Db (Gstraunthaler, Lindl, & van der Valk, 2013)
9. Humane Endpoint ("How to determine humane endpoints for research animals," 2015)
10. IMPC (Koscielny et al., 2014)
11. ICLAC (Fusenig, Capes-Davis, Bianchini, Sundell, & Lichter, 2017)
12. Interspecies (Bokkers & Slob, 2007)
13. IMSR (J. T. Eppig, Motenko, Richardson, Richards-Smith, & Smith, 2015)
14. IGRhCellID (Shiau, Gu, Chen, Lin, & Jou, 2011)
15. KERIS (P. Li, Tompkins, Xiao, & the Inflammation and Host Response to Injury Large, 2017)
16. LifeMap Discovery®, Cells & Tiss (Edgar et al., 2013)
17. Mouse Atlas of Gene Expression (Siddiqui et al., 2005)
18. NTP nonneoplastic lesion atlas (C. W. Schmidt, 2014)
19. Organ system heterogeneity DB (Mannil, Vogt, Prinz, & Campillos, 2015)
20. Rat Genome Db (Shimoyama et al., 2015)
21. ZFIN (Sprague et al., 2006)

XIII. Nano Materials Toxicity

1. caNanoLab (Morris, Gaheen, Lijowski, Heiskanen, & Klemm, 2015)
2. DaNa (Krug et al., 2018)
3. Good Nano Guide (Kulinowski & Jaffe, 2009)
4. eNanoMapper (Jeliazkova et al., 2015)

5. NHECD (Maimon & Browarnik, 2010)
6. NanoHub (Madhavan et al., 2013)
7. NECID (Oberbek, 2018)

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