(short) summary so far...
Protein Data Bank

- Retrieve structures
  - missing portions and resolution
  - ligands and substrates
Crystal structure of the complex of human neutrophil elastase with 1/2SLPI
Authors: Takimoto-Kamimura, M., Fukushima, K.
Release Date: 2008-08-26
Classification: Hydrolase/hydrolase Inhibitor
Experiment: X-RAY DIFFRACtION with resolution of 1.70 Å
Compound: 2 Polymers [Display Full Polymer Details | Display for All Results]
          2 Ligands [Display Full Ligand Details | Display for All Results]
Citation: Complex of human neutrophil elastase with 1/2SLPI
          (2008) J.SYNCHROTRON RADIAT. 15: 308-311 [Display Full Abstract | Display for All Results]
Molecule of the Month: Thrombin, Trypsin, Serpins, Tissue Factor, Fibrin

Covalent complex structure of elastase
Authors: Huang, W., Yamamoto, Y.
Release Date: 2008-07-01
Classification: Hydrolase
Experiment: X-RAY DIFFRACtION with resolution of 1.80 Å
Compound: 1 Polymer [Display Full Polymer Details | Display for All Results]
          3 Ligands [Display Full Ligand Details | Display for All Results]
Citation: X-ray snapshot of the mechanism of inactivation of human neutrophil elastase by 1,2,5-thiadiazolidin-3-one 1,1-
          dioxid derivatives.
Molecule of the Month: Thrombin, Trypsin, Serpins, Tissue Factor, Fibrin

CRYSTAL STRUCTURE OF HUMAN NEUTROPHIL ELASTASE COMPLEXED WITH AN INHIBITOR (GW475151)
          Fleetwood, G., Humphreys, D.C., Molloy, C.R., Dixon, M., Godward, R.E., Wonacott, A.J., Singh, O.M.P.,
          Hodgson, S.T., Hardy, G.W.
Release Date: 2002-08-29
Classification: Hydrolase
Experiment: X-RAY DIFFRACtION with resolution of 2.00 Å
Compound: 1 Polymer [Display Full Polymer Details | Display for All Results]
          3 Ligands [Display Full Ligand Details | Display for All Results]
Citation: Discovery of Further Pyrrolidine Trans-Lactams as Inhibitors of Human Neutrophil Elastase (Hne) with Potential as
          Development Candidates and the Crystal Structure of Hne Complexed with an Inhibitor (Gw475151)
Molecule of the Month: Thrombin, Trypsin, Serpins, Tissue Factor, Fibrin
charges and pKa values
Software

- PDB: www.pdb.org
- PyMOL: www.pymol.org
  - Mac / Windows / Linux
- propKa and PDB2PQR
- APBS (pymol plugin)
- PSIPRED and Swiss-Model