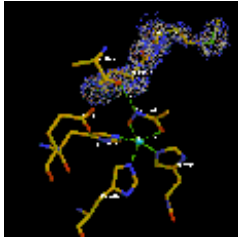
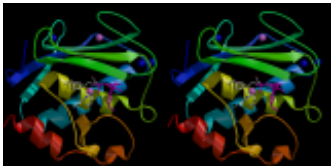

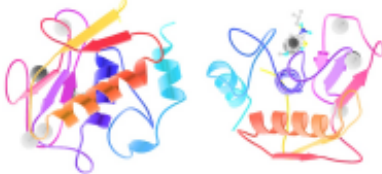
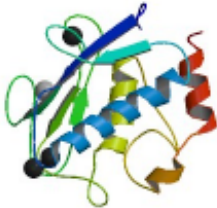
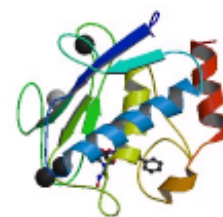


MATRIX METALLOPROTEINASES

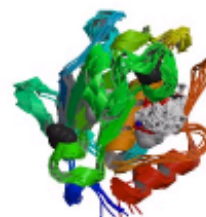
<p>Bertini, I., Calderone, V., Fragai, M., Luchinat, C., Mangani, S., Terni, B. X-Ray structures of binary and ternary enzyme-product-inhibitor complexes of matrix metalloproteinases <i>Angew.Chem.Int.Ed.</i>, 42: 2673-2676, 2003</p>	 <p>PDB code: 1OS2, 1OS9</p>
<p>Bertini, I., Calderone, V., Fragai, M., Luchinat, C., Mangani, S., Terni, B. Crystal structure of the catalytic domain of human matrix metalloproteinase 10 <i>J.Mol.Biol.</i>, 336: 707-716, 2004</p>	 <p>PDB code: 1Q3A</p>
<p>Bertini, I., Calderone, V., Cosenza, M., Fragai, M., Lee, Y. M., Luchinat, C., Mangani, S., Terni, B., Turano, P. Conformational variability of matrix metalloproteinases: beyond a single 3D structure <i>Proc.Natl.Acad.Sci.USA</i>, 102: 5334-5339, 2005</p>	 <p>PDB code: 1YCM, 1Z3J</p>
<p>Bertini, I., Calderone, V., Cosenza, M., Fragai, M., Lee, Y.-M., Luchinat, C., Mangani, S., Terni, B., Turano, P. Conformational variability of matrix metalloproteinases: beyond a single 3D structure <i>Proc.Natl.Acad.Sci.USA</i>, 102: 5334-5339, 2005</p>	 <p>PDB code: 1Y93, 1RMZ</p>
<p>Bertini, I., Calderone, V., Fragai, M., Luchinat, C., Maletta, M., Yeo, K.J. Snapshots of the reaction mechanism of matrix metalloproteinases <i>Angew.Chem.Int.Ed.Engl.</i>, 45: 7952-7955, 2006</p>	 <p>PDB code: 20XU, 20XW, 20XZ, 20Y2, 20Y4</p>

Mannino, C., Nievo, M., Machetti, F., Papakyriakou, A., Calderone, V., Fragai, M., Guarna, A.
Synthesis of bicyclic molecular scaffolds (BTAA): an investigation towards new selective MMP-12 inhibitors
Bioorg.Med.Chem. 14: 7392-7403, 2006



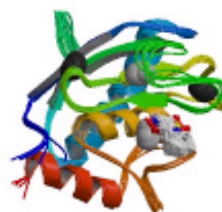
PDB code: 2HU6

Alcaraz, L.A., Banci, L., Bertini, I., Cantini, F., Donaire, A., Gonnelli, L.
Matrix metalloproteinase-inhibitor interaction: the solution structure of the catalytic domain of human matrix metalloproteinase-3 with different inhibitors
J.Biol.Inorg.Chem. 12: 1197-1206, 2007



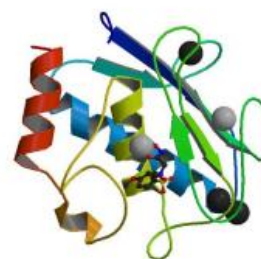
PDB code: 2JNP, 2JT5, 2JT6

Arendt, Y., Banci, L., Bertini, I., Cantini, F., Cozzi, R., Del Conte, R., Gonnelli, L.
Catalytic domain of MMP20 (Enamelysin) – the NMR structure of a new matrix metalloproteinase
FEBS Lett., 581: 4723-4726, 2007



PDB code: 2JSD

Bertini, I., Calderone, V., Fragai, M., Giachetti, A., Loconte, M., Luchinat, C., Maletta, M., Nativi, C., Yeo, K.J.
Exploring the subtleties of drug-receptor interactions: the case of matrix metalloproteinases
J.Am.Chem.Soc., 129: 2466-75, 2007



PDB code: 3NX7, 3LK8, 3F15, 3F16, 3F17, 3F18, 3F19, 3F1A

Bertini, I., Calderone, V., Fragai, M., Jaiswal, R., Luchinat, C., Melikian, M., Mylonas, E., Svergun, D.I.
Evidence of reciprocal reorientation of the catalytic and hemopexin-like domains of full-length MMP-12
J.Am.Chem.Soc., 130: 7011-7021, 2008



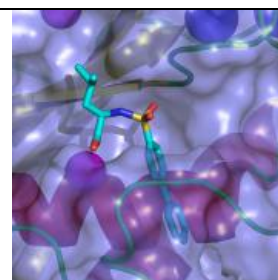
PDB code: 2JXY, 3BA0

Balayssac, S., Bertini, I., Bhaumik, A., Lelli, Luchinat, C.,
Paramagnetic shifts in solid-state NMR of proteins to elicit structural information
Proc.Natl.Acad.Sci.USA, 105: 17284-17289, 2008



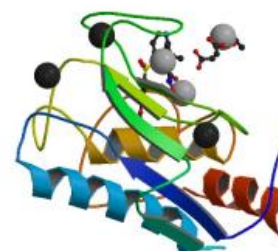
PDB code: 2K9C

Dragoni, E., Calderone, V., Fragai, M., Jaiswal, R.,
Luchinat, C., and Nativi, C.
Biotin-tagged probes for MMP expression and activation: design, synthesis and binding properties
Bioconjug.Chem., 4: 719-727, 2009



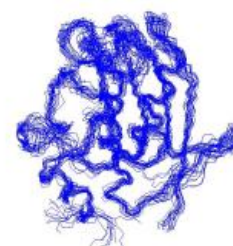
PDB code: 3EHX, 3EHY

Isaksson, J., Nyström, S., Derbyshire, D., Wallberg, H.,
Agback, T., Kovacs, H., Bertini, I., Giachetti, A.,
Luchinat, C.
**Does a fast nuclear magnetic resonance spectroscopy-
and X-ray crystallography hybrid approach provide
reliable structural information of ligand-protein
complexes? A case study of metalloproteinases**
J.Med.Chem., 52: 1712-1722, 2009



PDB code: 2W0D

Bertini, I., Bhaumik, A., De Paepe, G., Griffin, R. G.,
Lelli, M., Lewandowski, J., and Luchinat, C.
**High-resolution solid state NMR structure of a 17.6
kDa protein**
J.Am.Chem.Soc., 132: 1032-1040, 2010



PDB code: 2KRJ

Attolino, E., Calderone, V., Dragoni, E., Fragai, M.,
Richichi, B., Luchinat, C., Nativi, C.
**Structure-based approach to nanomolar, water soluble
matrix metalloproteinases inhibitors (MMPIs)**
Eur.J.Med.Chem., 45: 5919-25, 2010



PDB code: 3N2U, 3N2V

Bertini, I., Calderone, V., Cerofolini, L., Fragai, M., Geraldes, C. F. G. C., Hermann, P., Luchinat, C., Parigi, G., and Teixeira, J. M. C.

The catalytic domain of MMP-1 studied through tagged lanthanides

FEBS Lett., 586: 557-567, 2012

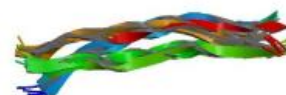


PDB code: 3SHI

Bertini, I., Fragai, M., Luchinat, C., Melikian, M., Toccafondi, M., Lauer, J.L., Fields, G.B.

Structural basis for matrix metalloproteinase 1-catalyzed collagenolysis

J. Am. Chem. Soc., 134: 2100-2110, 2012



PDB code: 2LLP

Mordini, A., Mori, M., Massaro, A., Calderone, V., Fragai, M., Luchinat, C.

Contribution of ligand free energy of solvation to design new potent MMPs inhibitors

To be published



PDB code: 3RTS, 3RTT, 4GUY

Czarny, B., Stura, E.A., Devel, L., Vera, L., Lajeunesse, E., Beau, F., Calderone, V., Fragai, M., Luchinat, C., Dive, V.

Molecular determinants of a selective matrix metalloproteinase-12 inhibitor: Insights from crystallography and thermodynamic studies.

J Med Chem., 56: 1149-1159, 2013

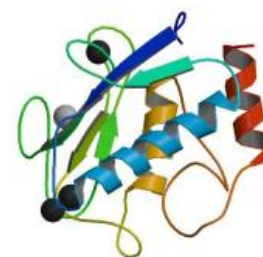


PDB code: 4GQL, 4GR0, 4GR3, 4GR8

Udi, Y., Fragai, M., Grossman, M., Mitternacht, S., Arad-Yellin, R., Calderone, V., Melikian, M., Toccafondi, M., Berezovsky, I.N., Luchinat, C., Sagi, I.

Unraveling hidden regulatory sites in structurally homologous metalloproteases

J. Mol. Biol., 425: 2330-2346, 2013



PDB code: 4IJO