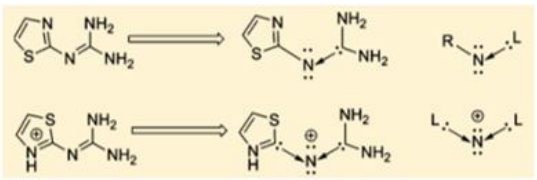
Contributions in Theoretical Organic Chemistry

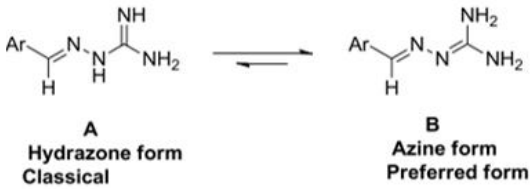
Chemical bonding

Chem. Eur. J.	*2015*		accepted
J. Org. Chem.	*2014*	*79*	4852
J. Phys. Chem. A	*2012*	*116*	9071
J. Phys. Chem. A	*2011*	*115*	7645
J. Org. Chem.	*2011*	*76*	2558
Chem. Commun.	*2009*		1064
J. Med. Chem.	*2005*	*48*	7615



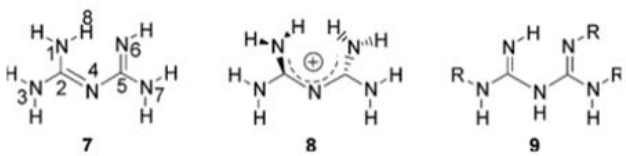
Tautomerism

RSC Advances	*2015*	*5*	55938
RSC Advances	*2013*	*3*	25268
J. Comput. Chem.	*2013*	*34*	1577
Int. J. Quant. Chem.	*2008*	*108*	1277
J. Org. Chem.	*2000*	*65*	4622
J. Am. Chem. Soc.	*1994*	*116*	642
J. Am. Chem. Soc.	*1993*	*115*	2348



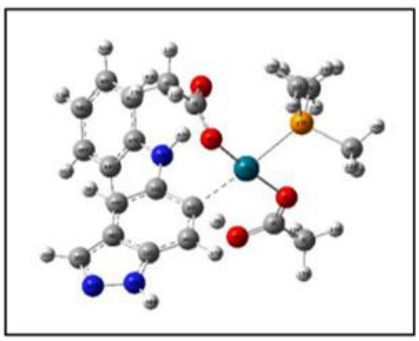
Electron delocalization / resonance

RSC Advances	*2014*	*4*	4533
J. Org. Chem.	*2014*	*79*	4852
J. Comput. Chem.	*2010*	*31*	1259
J. Comput. Chem	*2006*	*27*	334
J. Phys. Chem. A	*2004*	*108*	10509
J. Phys. Chem. A	*2003*	*107*	1627
J. Org. Chem.	*2000*	*65*	4622
Chem. Phys. Lett.	*1997*	*276*	31



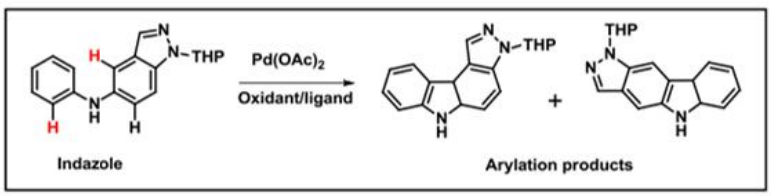
C-H bond activation

Org. Letts.	*2015*	*17*	3742
Org. Biomol. Chem.	*2015*	*13*	7790
Tetrahedron Letts	*2015*	*56*	4057
Org. Biomol. Chem.	*2015*	*13*	5235
J. Org. Chem.	*2015*	*80*	1746
Org. Biomol. Chem.	*2015*	*13*	1481
Chem. Commun.	*2014*		12076
J. Org. Chem.	*2012*	*77*	8321



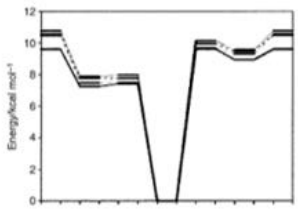
Reaction Mechanisms

Chem. Commun.	*2016*		in print
RSC Advances	*2015*	*5*	88353
J. Phys. Chem. B	*2014*	*118*	9199
J. Org. Chem.	*2014*	*79*	3427
Crystal Growth Design	*2013*	*13*	2004
RSC Advances	*2012*	*2*	11366
J. Org. Chem.	*2012*	*77*	8562
J. Org. Chem.	*2011*	*76*	5999
J. Org. Chem.	*2010*	*75*	5487
Chem. Commun.	*2009*		1067
Angew. Chem. Int. Ed.	*2008*	*47*	4703
J. Am. Chem. Soc.	*2007*	*129*	4506
J. Phys. Chem. A	*2004*	*108*	784
Chem. Commun.	*2003*		1420
Org. Letters	*2000*	*2*	2725

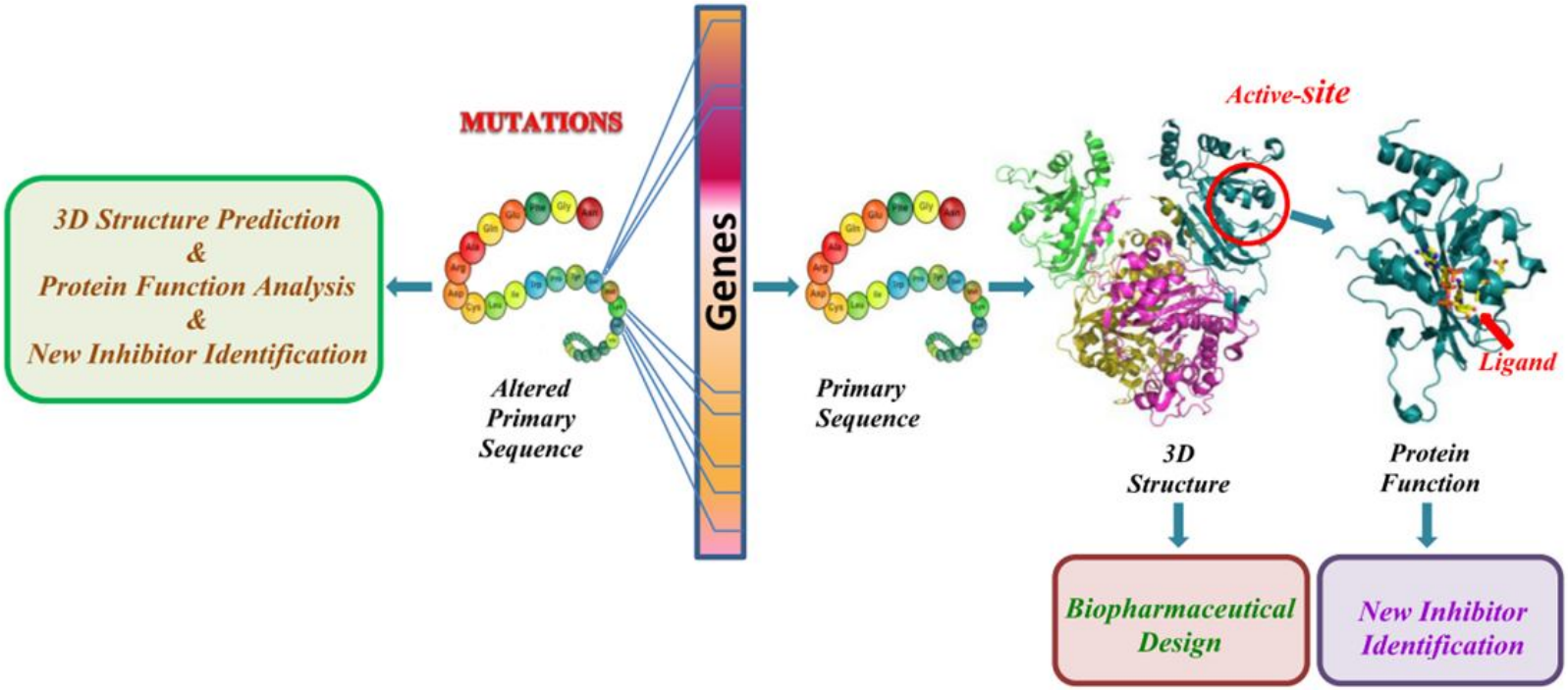


Conformational analysis

J. Phys. Chem. A	*2014*	*118*	187
Tetrahedron	*2005*	*61*	5633
Tet. Lett.	*2002*	*43*	8289
J. Chem. Soc., Perkin Trans.	*2000*		2469
J. Chem. Soc., Perkin Trans.	*2000*		43



Contributions in Computational Biology



Computational mutational analysis

Science Reporter (Nature)	***2016***	DOI 10.1038/srep20600	

Macromolecular structure and function prediction

J. Biomol. Struct. Dyn.	***2015***		1
J. Biomol. Struct. Dyn.	***2015***	DOI 10.1080/07391102.2015.1005137.	
Appl. Biochem. Biotech.	***2013***	*171*	417
Curr. Protein & Peptide Sci.	***2007***	*8*	352
Enzyme and Microbial Tech.	***2005***	*36*	232

Biopharmaceutical design

PLOS One	***2016***	11	e0150764

Computer Programming and Pharmacoinformatics Tool Development

Drug likeness

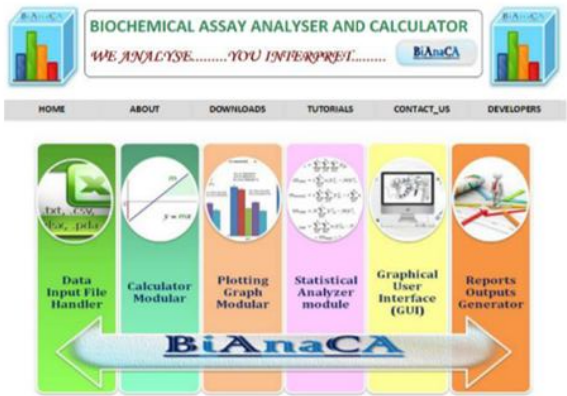
http://www.niper.gov.in/pi_dev_tools/DruLiToWeb/DruLiTo_index.html

Dendrimer builder

J. Comp. Chem.	***2012***	*33*	1997

http://www.physics.iisc.ernet.in/~maiti/dbt/home.html

BiAnaca

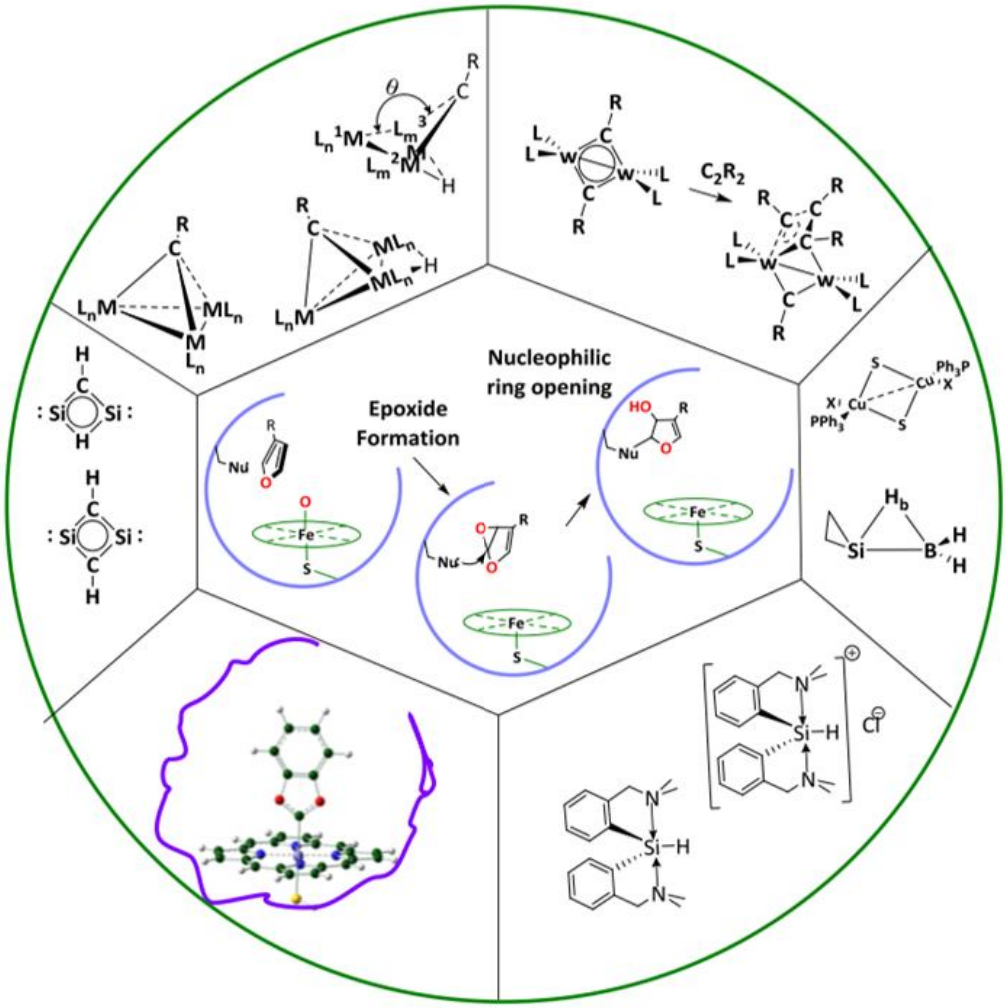


http://www.niper.ac.in/pi_dev_tools/BiAnaCA/ABOUT.html

Descriptor calculations

Int. J. Chem. Mod.	***2016***	accepted.	
Internet Ele. J. Mol. Design	***2015***	accepted.	
Lett. Drug Design Disc.	***2015***	*11*	844
ACS Comb. Sci.	***2014***	*16*	101
Int. J. Comput. Biol. Drug Des.	***2014***	*7*	295
Int. J. Comp. Biol. Drug Des.	***2012***	*5*	335

Contributions in Theoretical Inorganic Chemistry



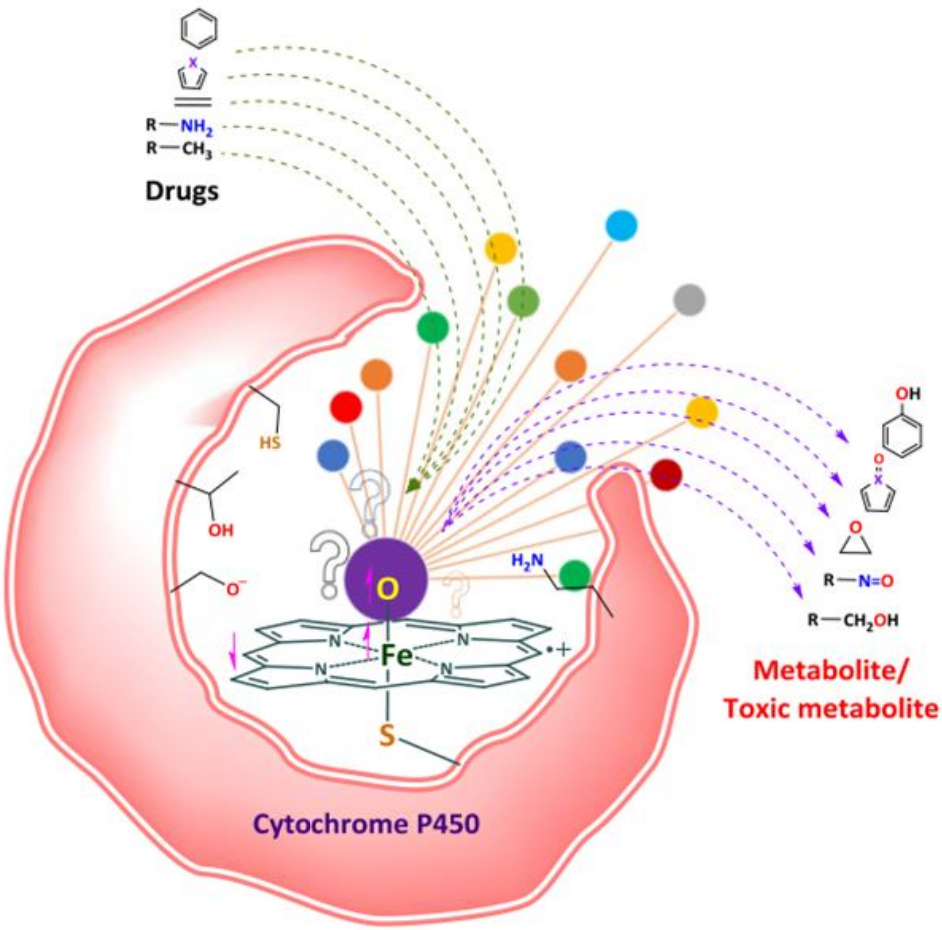
Organometallic chemistry

Inorg. Chem.	***2006***	*45*	1535
Inorg. Chem.	***2003***	*42*	4743
Organometallics	***2002***	*21*	3683
Inorg. Chem.	***1994***	*33*	2046
Chem. Phys. Lett.	***1994***	*217*	296
Organometallics	***1993***	*12*	4267
Angew. Chem., Int. Ed. Engl.	***1993***	*32*	865
Organometallics	***1991***	*10*	3613
Organometallics	***1992***	*11*	2528
J. Phys. Chem.	***1990***	*94*	5530
Inorg. Chim. Acta	***1989***	*162*	281
Polyhedron	***1988***	*7*	871
J. Organomet. Chem.	***1988***	*347*	401
J. Am. Chem. Soc.	***1987***	*109*	2560

Bioinorganic Catalysis

Chem. Res. Tox.	***2016***	*28*	2364
J. Bio. Inorg. Chem.	***2015***	*142*	84
Inorg. Chem.	***2013***	*52*	13496
Inorg. Chem.	***2013***	*52*	5097

Contributions in Pharmaceutical Sciences



Drug Metabolism

J. Comput. Chem.	***2014***	*35*	2047
Eur. J. Med. Chem.	***2014***	*71*	15
Inorg. Chem.	***2013***	*52*	13496
Drug Metabolism Letters	***2013***	*6*	221
Inorg. Chem.	***2013***	*52*	5097
J. Phys. Chem. A	***2012***	*116*	10441
J. Comp. Chem.	***2012***	*33*	1740
J. Mol. Mod.	***2012***	*18*	709
J. Phys. Chem. A	***2011***	*115*	891
Chem. Res. Tox.	***2011***	*24*	1113
Theochem	***2010***	*962*	97
J. Phys. Chem. A	***2004***	*108*	3784.

Drug toxicity

Chem. Res. Tox.	***2015***	28	2364.
Drug Metabolism Letters	***2013***	*6*	221
Chem. Res. Tox.	***2011***	*24*	1113

Drug delivery

J. Chem. Phys.	***2016***		*in print*
Nanoscale	***2014***	*6*	2476
Soft Matter	***2013***	*9*	6492
Structural Chem.	***2012***	*23*	1857
J. Phys. Org. Chem.	***2012***	*25*	649
J. Nanosci. Nanotechnol.	***2006***	*6*	3277

Contributions in Medicinal Chemistry

Anti-diabetic agent design and synthesis

Anti-malarial agent design and synthesis

Eur. J. Med. Chem.	*2016*		*in print*
Eur. J. Med. Chem.	*2009*	*44*	3488
Eur. J. Med. Chem.	*2009*	*44*	42
Bioorg. Med. Chem. Letts.	*2008*	*18*	4959
Eur. J. Med. Chem.	*2008*	*43*	2784
Eur. J. Med. Chem.	*2008*	*43*	949
Bioorg. Med. Chem.	*2007*	*15*	3728
Eur. J. Med. Chem.	*2007*	*42*	1014
Bioorg. Med. Chem.	*2007*	*15*	1547
J. Med. Chem.	*2005*	*48*	7615
J. Med. Chem.	*2005*	*48*	3015
Bioorg. Med. Chem.	*2005*	*13*	2331
Bioorg. Med. Chem.	*2004*	*12*	2709

J. Biomol. Struct. Dyn.	*2015*	*33*	1913
Bioorg. Med. Chem. Letts.	*2014*	*24*	613
J. Mol. Mod.	*2011*	*17*	657
J. Enzy. Inhib Med. Chem.	*2010*	*25*	635
Chem. Biol. Drug Design	*2010*	*75*	15
J. Mol. Graph. Mod.	*2009*	*28*	357
Curr. Med. Chem.	*2008*	*15*	1522
J. Med. Chem.	*2005*	*48*	7615

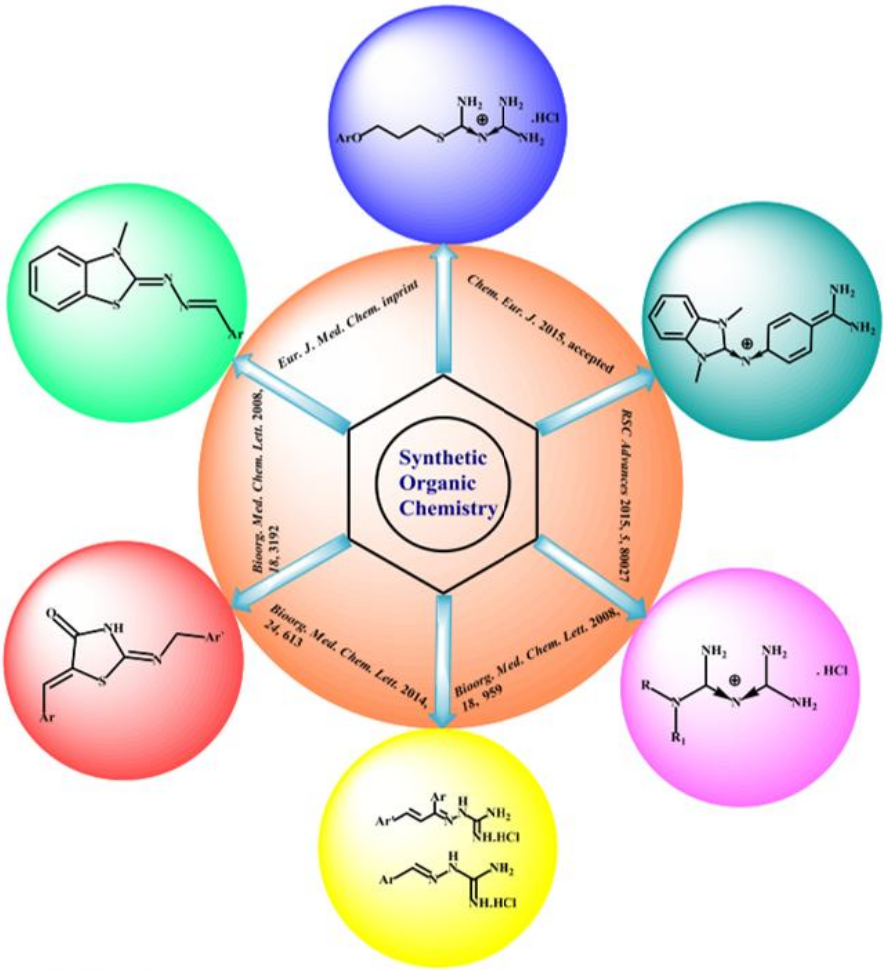
Anti-cancer agent design and synthesis

Other therapeutic areas

Oncotarget	*2016*		in print
Scientific Reports	*2016*		
ACS Med. Chem. Lett.	*2015*	*6*	481
DNA Repair	*2014*	*24*	15
Anticancer Drugs	*2014*	*25*	704
Med. Chem. Comm.	*2014*	*5*	766
ChemMedChem.	*2013*	*8*	1873
MedChemComm	*2013*	*4*	1257
J. Med. Chem.	*2011*	*54*	5013
Eur. J. Med. Chem.	*2006*	*41*	1310

J. Biomol. Struct. Dyn.	*2015*	*33*	1082
RSC Advances	*2015*	*5*	80027
ACS Med. Chem. Letts.	*2015*	*6*	1065
Med. Chem. Res.	*2013*	*23*	1819
Medicinal Chemistry Res.	*2013*	*21*	5654
Eur. J. Med. Chem.	*2012*	*52*	82

Synthesis of Quantum Chemically designed molecules



Divalent N(I) compounds

Chem. Eur. J.	***2015***		accepted.
Eur. J. Med. Chem.	***2015***		accepted.
Bioorg. Med. Chem. Letts.	***2014***	*24*	613
Med. Chem. Res.	***2015***	*24*	1974

Guanylthiourea derivatives

Bioorg. Med. Chem. Letts.	***2014***	*24*	613

Azines

J. Org. Chem.	***2016***		*in print*
RSC Advances	***2015***	*5*	80027

Barbituric acid derivatives

Eur. J. Med. Chem.	***2016***		accepted.
Bioorg. Med. Chem. Letts.	***2008***	*18*	959
Bioorg. Med. Chem. Letts.	***2008***	*18*	3192