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- Copper Technical Reference Library
- Corrosion Abstracts
- Engineered Materials Abstracts
- Materials Business File
- METADEX

Subject Coverage

- Steel
- Non-ferrous metals
- Intermetallic compounds
- Ceramics
- Composites
- Polymers
- Plastics
- Rubber
- Adhesive bonding
- Glass
- Casting and molding
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- Technology Terms

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Ligand placement based on prior structures: the guided ligand-replacement method

Klei, Herbert E; Moriarty, Nigel W; Echols, Nathaniel; Terwilliger, Thomas C; Baldwin, Eric T; et al. *Acta Crystallographica Section D* 70.1 (Jan 1, 2014): 134-143.

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AB

Abstract (summary) Translate

The process of iterative structure-based drug design involves the X-ray crystal structure determination of upwards of 100 ligands with the same general scaffold (i.e. chemotype) complexed with very similar, if not identical, protein targets. In conjunction with insights from computational models and assays, this collection of crystal structures is analyzed to improve potency, to achieve better selectivity and to reduce liabilities such as absorption, distribution, metabolism, excretion and toxicology. Current methods for modeling ligands into electron-density maps typically do not utilize information on how similar ligands bound in related structures. Even if the electron density is of sufficient quality and resolution to allow de novo placement, the process can take considerable time as the size, complexity and torsional degrees of freedom of the ligands increase. A new module, Guided Ligand Replacement (GLR), was developed in Phenix to increase the ease and success rate of ligand placement when prior protein-ligand complexes are available. At the heart of GLR is an algorithm based on graph theory that associates atoms in the target ligand with analogous atoms in the reference ligand. Based on this correspondence, a set of coordinates is generated for the target ligand. GLR is especially useful in two situations: (i) modeling a series of large, flexible, complicated or macrocyclic ligands in successive structures and (ii) modeling ligands as part of a refinement pipeline that can automatically select a reference structure. Even in those cases for which no reference structure is available, if there are multiple copies of the bound ligand per asymmetric unit GLR offers an efficient way to complete the model after the first ligand has been placed. In all of these applications, GLR leverages prior knowledge from earlier structures to facilitate ligand placement in the current structure.

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Indexing (details) Cite

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Author	Klei, Herbert E ¹ ; Moriarty, Nigel W; Echols, Nathaniel; Terwilliger, Thomas C; Baldwin, Eric T; Pokross, Matt; Posy, Shana; Adams, Paul D
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	Database	ProQuest Materials Research Professional (1965 - current)

SEARCH FIELDS

Field Name ¹	Field Code	Example	Description and Notes
Abstract	AB	ab("modeling ligands")	Use adjacency and/or Boolean operators to narrow search results.
Abstract present	ABANY	"protein targets " AND abany(yes)	Add: <i>AND ABANY(YES)</i> to a query to limit retrieval to records with abstracts.
Accession number	AN	an(19016986)	A unique document identification number assigned by the information provider. A record can display multiple accession numbers – depending on the products within which it is stored.
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All fields + text	--	"reinforced concrete" N/5 carbon	Same as ALL field code: searches all fields in bibliographic files.
Author ²	AU	au("posy, shana")	Includes all authors. See also First author.
Author affiliation	AF	af(Physical Biosciences Division, Lawrence Berkeley National Laboratory, Berkeley)	
Cited author	CAU	cau(thomas harris)	Authors of cited works.
Cited document title	CTI	cti("lithium titanate")	
Cited publication date	CYR	cyr(2009)	
Cited publication title	CPUB	cpub("biotechnology for biofuels")	
Classification code ²	CC	cc("electrical properties")	Not currently displayed
Conference information	CF	cf("offshore structures ") cf(glasgow) cf(sweden) cf(2008)	Includes conference title, location, number, date.
Corporate author	CA	ca(hoechst or schering)	
Date revised	DREV	drev(20140101) drev(>20111231)	Date that the Information provider revised the record. Note that not all Providers identify a date of revision.
DOI	DOI	doi("10.1007/s00707-013-0941-z")	Digital Object Identifier. Search the portion of the DOI that comes after http://dx.doi.org/ .
Document feature	DF	df(graphs)	Indicates presence in original article of availability of graphics, tabular data, illustrations, etc.
Document title	TI	ti("ligand placement based on prior structures")	Includes Title, Alternate Title, Original Title, and Subtitle but not Publication Title (PUB).

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Alternate title	OTI	oti(federleicht)	Usually the original, non-English title
Document type	DTYPE	dtype("journal article")	
First author	FAU	fau("klei, Herbert e")	First name listed in Author field. It is included in Author browse, but its position cannot be specified in the Author browse. See also Author.
First available	FAV	fav(20140312) fav(>20121231) fav(20120101-20120630)	Indicates the first time a document was loaded in a specific database on PQD. It will not change regardless of how many times the record is subsequently reloaded, as long as the accession number does not change.
From database ³	FDB	ti(ligand?) AND fdb(materialsresearchprof) ti(ligand?) AND fdb(10000201)	Useful in multi-file searches to isolate records from a single file. FDB cannot be searched on its own; specify at least one search term then AND it with FDB.
Identifier (keyword)	IF	if(irrigation OR drainage)	
ISBN	ISBN	isbn(9780877035527)	
ISSN	ISSN	issn(1399-0047) issn(13990047)	Also retrieves electronic ISSN.
Issue	ISS	iss(1)	Also searchable via the Look Up Citation tool.
Journal title	JN, PUB	jn(" acta crystallographica section d ")	Journal names only. For complete Publication name types, use PUB. Displays in Publication title. Also searchable via the Look Up Citation tool for Publication name.
Language	LA	la(english)	The language in which the document was originally published.
Notes	NT	nt(reprint*)	
Number of pages	PCT	pct(10)	
Pagination	PG	pg(134-143)	See also Start page.
Patent application date	PAD	pad(20040501) pad(2004-05-01) pad(>20101231) pad(20110101-20110630)	Displays in Patent information
Patent application number	PA, PAT	pa("10/840183")	Displays in Patent information
Patent assignee	AP, PAT	ap(tata)	Displays in Patent information
Patent publication country	PC, PAT	pc(us)	Displays in Patent information
Patent publication number	PN, PAT	pn(us7249222)	Patent publication number
Publication title ²	PUB	pub("acta crystallographica")	Title of publication where document originally appeared. Also searchable via the Look Up Citation tool.
Publication type	PT, STYPE	pt("scholarly journals")	
Publication year	YR, PY	yr(2015) yr(>2011) yr(2013-2014)	Single year or a range of years may be searched. Displays in Publication date.
Publisher	PB	pb("wiley blackwell")	
References	RF	rf(Krause AND "climate protection")	
Source type	PT, STYPE	stype("conference papers & proceedings")	Searches references cited in the original document.
Start page	PAGE	page(134)	Also searchable on the Look Up Citation page. Displays in Pagination.
Subfile	SFL	sfl(metadex)	The individual database(s) in which the record appears.

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Field Name ¹	Field Code	Example	Description and Notes
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Updates	UD	ud(>20121231) ud(20130101-20130630)	The date(s) the record was loaded as a result of an update provided by the supplier.
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