

Bases de données internes

Sommaire

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- Quels sont les intérêts d'une base de données interne ?

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- Comment créer sa propre base ?

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- Quels sont les intérêts d'une base de données interne ?
- Comment créer sa propre base ?
- Comment interroger sa propre base ?

Quels sont les intérêts d'une base de données interne ?

- Base pouvant regrouper l'ensemble des structures réalisées dans le laboratoire

- Base pouvant regrouper l'ensemble des structures réalisées dans le laboratoire
 - Structures publiées,

- Base pouvant regrouper l'ensemble des structures réalisées dans le laboratoire
 - Structures publiées,
 - Structures en attente,

- Base pouvant regrouper l'ensemble des structures réalisées dans le laboratoire
 - Structures publiées,
 - Structures en attente,
 - Structures qui ne seront pas publiées, ...

- Base pouvant regrouper l'ensemble des structures réalisées dans le laboratoire
 - Structures publiées,
 - Structures en attente,
 - Structures qui ne seront pas publiées, ...

- Recherche d'une structure facilitée

- Base pouvant regrouper l'ensemble des structures réalisées dans le laboratoire
 - Structures publiées,
 - Structures en attente,
 - Structures qui ne seront pas publiées, ...

- Recherche d'une structure facilitée

- Recherche par maille permettant d'éviter les doublons

Comment créer sa propre base ?

➤ INIST

- CSD (Cambridge Structural Database)

➤ INIST

- CSD (Cambridge Structural Database)
 - En ligne

➤ INIST

- CSD (Cambridge Structural Database)
 - En ligne
 - Sur DVD

X-PreQuest: chally@ccdc.org

File PubliCSD.aser.ind Entry 87 of 218 Current MELSAY PreQuest

Refcode: MELSAY Reference: 1090,17,1969,2006

Author: A.Pernet-Poll-Chevrier, F.Cantagrel, K.Le Jeune, C.Philouze, P.Y.Chavant

Compound: C18 H24 N2 O2

Formula: C18 H24 N2 O2

Qualifier: *TEMP: at 293.0 K *PRESSURE: *RADIATION: *POWDER: *REFINEMENT: *AB S-CONFIG: *POLYMORPH: *BIOACTIVITY: *CONFORMER: *ISOMER: *STER EOMER: *RACEMATE: *REINT-SEE: *REINT-OF: *CONTRIB: *OTHER-EXP: *OTHER-DIFF:

Remarks: tampon\archive\ArchiveLEDSS97-06\Archive06\Y_Vallee\PY_Chavant\FCA393 "CCDC: CCDC 605990 "XREF: "REMARK: "DOI:

Info: Disorder: Errors: Properties: "COLOR: colorless "HABIT: prism "MP: "SOURCE-CHEM: "SOURCE-NAT: "SE NS: "ISO: "OTHER-CELL: "PHASE-T:

Class: a 8.314(1) b 14.10(2) c 14.97(2)

alpha beta gamma

z 4 sp gr P212121 vol.

R-factor 0.0573 density 1.138 form wt.

Rotation Translation

56 5.0 0.20

Set 3D Display

MELSAY

- JRNL journal-Tetrahedron:Asymm.
- REMARKS Bad character: "
- REMARKS Bad character: "
- Checks Calc.vol= 175489; Calc.form.wt= 300.40; Calc.dens.= 1.14

CCDC ConQuest (1) : search [Search]

File Edit Options View Databases Results Help

Build Queries Combine Queries Manage Hitlists View Results

All Text Author/Journal Chemical Crystal Experimental Diagram 3D Visualiser CSD Internals Search Overview

Refcode: GANMAK CSD version 5.31 (November 2009)

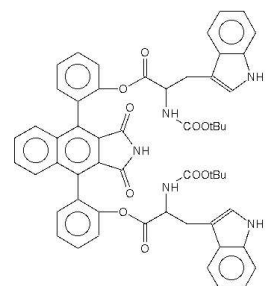
GANMAK

Analyse Hitlist

- ✓ AH0VUO
- ✓ AH0WAV
- ✓ AH0WEZ
- ✓ AH0WID
- ✓ AH0WJO
- ✓ BAPCF
- ✓ BAPCOL
- ✓ BAZCOV
- ✓ BAZCUB
- ✓ DREVYGB
- ✓ ECKOWK
- ✓ EFAZAM
- ✓ EFAZEQ
- ✓ EGOREY
- ✓ EGORIC
- ✓ ESEMUK
- ✓ ETLIUM
- ✓ FERGEP
- ✓ FERGIT
- ✓ FIKHEN
- ✓ FIKHIR
- ✓ GANMAK
- ✓ GHRPAJ
- ✓ GUPVOL
- ✓ HOCPLZ
- ✓ HOKWEJ

122 hits 100% Stop Search

Use as Query... Detach



GANMAK (P221)

File Edit Selection Display View Calculate Search Databases Help

Style Wireframe Colour: by Element Manage Styles Work Picking Mode Select Atoms Clear Measurements

Default view: b a b c a' b' c' x-x' y-y' z-z' x-90 x+90 y-90 y+90 z-90 z+90

Show Labels for: with Atom Labels Atom selections:

Structure Navigator

GANMAK P1gd

Crystal Structures Spacegroup

Databases

- CSD 5.31
 - Feb10
 - Nov09
 - Structures
 - Refcode Lists
 - ConQuest Hits
- search
 - FIKHEN P21/c
 - FIKHIR P-1
 - FIKJOL P21/c
 - MAVVEL P21/a
 - MAVVP P-1
 - NAJMUH P6cn
 - NAJNAO P21/m
 - OPPSAQ P21c121
 - GAVTEO C2/c
 - RAVRUP P21/m
 - SAGGAN P-1
 - SAGHAI P21/c
 - SAGHEY P21/c
 - VARPR P21212
 - Mercury Files

Display Options

Display

- Packing
- Auto centre
- Short Contact (sum of vdW radii)
- H-Bond Default definition
- Contacts...
- More Info
- Powder...

Options

- Show hydrogens
- Depth cue
- Show cell axes
- Z-Clipping
- Label atoms
- Stereo

Press the left mouse button and move the mouse to rotate the structure

X-Vista: led045@csd

VISTA v.2.1 TABLE SPREADSHEET

Quest File: /c:/home/led045/csd_data/searches/temp/cq_temp1

Test: 1 of 1

Parameters	Total	Selected	Suppressed
Refcodes	27	0	n/a
Fragments	122	0	0

REFCOD	PARAMS	11	12	13	14	15	16	17	CVOL
9	BACZUB	11.370	14.110	21.250	74.850	75.860	87.520	3190.194	
10	DIRVGD	9.553	12.583	34.140	90.000	97.100	90.000	4072.344	
11	ECKOWK	9.009	9.009	12.210	90.000	90.000	90.000	850.889	
12	EFAZAM	8.857	10.552	12.859	104.610	93.080	111.210	1024.679	
13	EFAZEQ	8.972	9.116	12.990	97.400	104.030	60.580	867.781	
14	EFAZIU	8.812	13.897	14.728	90.000	90.210	90.000	1803.584	
15	EGOREY	7.463	10.978	17.009	90.000	90.000	90.000	1383.527	
16	EGORIC	18.507	7.374	10.893	90.000	90.593	90.000	1486.425	
17	ESBWH	9.711	12.549	20.893	90.000	92.218	90.000	2292.980	
18	ETLIUM	9.677	21.777	10.190	90.000	107.090	90.000	1026.036	
19	FERGIT	11.854	7.974	23.221	90.000	102.390	90.000	2140.926	
20	FERGEP	11.842	7.891	23.221	90.000	102.480	90.000	2160.846	
21	FIKHEN	21.322	10.920	23.131	90.000	115.410	90.000	4964.721	
22	FIKHIR	12.695	13.213	21.692	74.500	96.800	67.600	3214.422	
23	GANMAK	14.478	14.478	21.310	90.000	90.000	120.000	3867.330	
24	GHRPAJ	7.440	7.070	15.429	90.000	102.480	90.000	792.401	
25	GUPVOL	8.848	12.843	21.551	90.000	90.000	90.000	2448.945	
26	HOCPLZ	7.316	8.426	22.832	90.000	90.000	90.000	1408.973	
27	HOKWEJ	10.164	10.122	14.168	90.000	93.460	90.000	1454.711	
28	KAGAV	22.766	11.719	11.343	90.000	112.100	90.000	2803.671	
29	KGEKEL	15.513	12.257	10.165	107.210	108.120	98.500	1694.182	

Miscellaneous: Test size, Refresh, Help, About

CCDC Mogul 1.1.2: C:\Program Files\CCDC\Mogul 1.1.2\examples\tutorials\AABHTZ.mol2

File Searches Help

Build query Results and analysis View structures

Results Navigator

All hits: 6426


Accepted hits: 6426

R-factor: Any Heaviest Element: Any

Exclude: None

Relevance	Number	Contribution
1.00	6426	100.0%

Mogul search - Bond length - C1 O1



Statistics

Total: 6426

Selected: 6426

Mean: 1.732Å

Standard deviation: 0.024Å

Minimum: 1.273Å

Median: 1.725Å

Lower quartile: 1.723Å

Upper quartile: 1.741Å

Maximum: 2.017Å

Iz-score: 0.410

Histogram display

Displayed hits: 6426

Selected hits: 6426

Select all hits in histogram

Deselect all hits in histogram

Help About

IsoStar 2.1.1

Home Ligand Terminal Ligand Acyclic Links Ligand Ring Systems Ligand Solvates Protein Plots Custom Plots Help

Home

Ligand Terminal

- C,H only
- N,C,H only
- O,C,H only
- N,O,C,H only
- S-containing
- P-containing
- S-containing
- Halo-containing

Ring systems

- Phenols
- C,H only
- N,C,H only
- O,C,H only
- N,O,C,H only
- S-containing
- Nucleic acid bases


Solvates, etc:

- Inorganic
- Organic

Protein Terminal

- Links
- Ring systems

Custom Plots



The display and manipulation of the encrypted IsoStar scatterplots available from this server requires use of a fully licensed installation of the IsoStar Client.

IsoStar provides rapid access to knowledge about the intermolecular interactions formed by a wide variety of chemical groups. Not only will IsoStar indicate when specific interactions have a high frequency of occurrence (and their preferred directionalities), it will also indicate when interactions are unlikely to occur.

IsoStar is derived from experimental information in the CSD and PDB and presents a wealth of information to:

- Molecular modellers studying protein-ligand interactions as part of the rational drug design process
- Medicinal chemists interested in identifying bioisosteric replacements
- Protein crystallographers
- Crystal engineers

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Registered in England No.2155347 Registered Charity No.800579

X-PreQuest: cbailly@cecicsgl2

File: PublisCSD.aser.ind Entry: 87 of 218 Current: MELSAY PreQuest

Open Insert... Print... Undo Redo Revert 1D Edit... Check... Preferences... EXIT
 Close Export... Copy... Paste Make 2D 2D Edit... 3D Check... Help...

Refcode: MELSAY Reference: 1090,17,1969,2006

Author: A.Pernet-Poil-Chevrier, F.Cantagrel, K.Le Jeune, C.Philouze, P.Y.Chavant

Compound:
 Synonym:
 Formula: C18 H24 N2 O2

Qualifier: "TEMP: at 293.0 K "PRESSURE: "RADIATION: "POWDER: "REFINEMENT: "ABS-CONFIG: "POLYMORPH: "BIOACTIVITY: "CONFORMER: "ISOMER: "STEREOMER: "RACEMATE: "REINT-SEE: "REINT-OF: "CONTRIB: "OTHER-EXP: "OTHER-DIFF:]

Remarks: tampon/archive/ArchiveLEDSS97-06/Archive06/Y_Vallee/PY_Chavant/FCA393 "CCDC: CCDC 605990 "XREF: "REMARK: "DOI:

Info:
 Disorder:
 Errors:
 Properties: "COLOR: colorless "HABIT: prism "MP: "SOURCE-CHEM: "SOURCE-NAT: "SENS: "ISO: "OTHER-CELL: "PHASE-T:

Class:
 a: 8.314(1) b: 14.10(2) c: 14.97(2)
 alpha: beta: gamma:
 z: 4 sp.grp: P212121 vol:
 R-fact: 0.0573 density: 1.138 form.wt:

MEJKIV 0
 MELRUR 205
MELSAY 13
 MELSEC 0
 MERHIA 0

Rotation: 56 Translation: 0.20

----- MELSAY -----

- JRNL journal=Tetrahedron:Asymm.
- RMARKS Bad character: " _ "
- RMARKS Bad character: " _ "
- Checks Calc.vol= 1754.89; Calc.form.wt= 300.40; Calc.dens.= 1.14

Set 3D Display... Reset

Structure Navigator

Crystal Structures Spacegroup

GANMAK

- Crystal Structures
 - CD 531
 - Feb10
 - May10
 - Nov02
 - Structures
 - Refcode List
 - ConQuest Hits
 - SEARCH
 - FRIEN P21/c
 - FKHR P-1
 - FRYD P21/c
 - MAVVEL P21/a
 - MAVIP P-1
 - NAAMUH Pbcn
 - NAJNAC P21/m
 - GAPGAG P212121
 - GAWTED C2/c
 - BAVRUP P21/m
 - SADGUN P-1
 - SAGHUL P21/c
 - SAGHEY Pbcn
 - VARPR P21212
 - Mercury Files

Tree View

Multiple Structures

Structures

Structure Navigator Searches

X-Vista: led045@csd

VISTA v.2

Quest File: /c/home/led045/csds_d

Test: 1 of 1

Parameters Refcodes Fragments

REFCOD	PARAMS	IT
9	BAZCUB	11.370
10	DIRVGD	9.553
11	ECDKOV	9.009
12	EPAZAM	8.857
13	EPAZEL	8.972
14	EPAZU	8.812
15	EGOREY	7.463
16	EGORC	18.507
17	ESBML	9.711
18	ETUJN	9.077
19	YFQDF	11.854
20	FEROF	11.542
21	FRHEN	21.322
22	FKHR	12.695
23	GANMAK	14.478
24	GIRPAL	7.440
25	GURVQ	8.848
26	HOCPI	7.316
27	HORWE	10.164
28	ICAGV	22.796
29	IGEKEL	15.513

Protein Plots Custom Plots

Available from this server

ions formed by a wide
 stions have a high
 te when interactions are

sents a wealth of

rational drug design

X-PreQuest: chally@ccdc.org

File PubliCSD.aser.ind Entry 87 of 218 Current MELSAY PreQuest

Refcode: MELSAY Reference: 1090,17,1969,2006

Author: A.Pernet-Poll-Chevrier, F.Cantagrel, K.Le Jeune, C.Philouze, P.Y.Chavant

Compound: C18 H24 N2 O2

Formula: C18 H24 N2 O2

Qualifier: *TEMP: at 293.0 K *PRESSURE: *RADIATION: *POWDER: *REFINEMENT: *AB S-CONFIG: *POLYMORPH: *BIOACTIVITY: *CONFORMER: *ISOMER: *STER EOMER: *RACEMATE: *REINT-SEE: *REINT-OF: *CONTRIB: *OTHER-EXP: *OTHER-DIFF:

Remarks: tampon\archive\ArchiveLEDSS97-06\Archive06\Y_Vallee\PY_Chavant\FCA393 "CCDC: CCDC 605990 "XREF: "REMARK: "DOI:

Info: Disorder: Errors: Properties: "COLOR: colorless "HABIT: prism "MP: "SOURCE-CHEM: "SOURCE-NAT: "SE NS: "ISO: "OTHER-CELL: "PHASE-T:

Class: a 8.314(1) b 14.10(2) c 14.97(2)

alpha beta gamma

z 4 sp gr P212121 vol.

R-factor density 0.0573 1.138 form wt

----- MELSAY -----

- JRNL journal-Tetrahedron:Asymm.
- RMARKS Bad character: "
- RMARKS Bad character: "
- Checks Calc.vol= 175488; Calc.form.wt= 300.40; Calc.dens.= 1.14

Rotation Translation

56 5.0 0.20

Set 3D Display

CCDC ConQuest (1) : search [Search]

File Edit Options View Databases Results Help

Build Queries Combine Queries Manage Hitlists View Results

All Text Author/Journal Chemical Crystal Experimental Diagram 3D Visualiser CSD Internals Search Overview

Refcode: GANMAK CSD version 5.31 (November 2009)

GANMAK

Analyse Hitlist

- ✓ AH0VUO
- ✓ AH0WAV
- ✓ AH0WEZ
- ✓ AH0WID
- ✓ AH0WJO
- ✓ BAPCF
- ✓ BAPCOL
- ✓ BAZCOV
- ✓ BAZCUB
- ✓ BIKVYGBI
- ✓ ECKOKW
- ✓ EFAZAM
- ✓ EFAZEQ
- ✓ EGOREY
- ✓ EGORIC
- ✓ ESEMUK
- ✓ ETLIUM
- ✓ FERGEP
- ✓ FERGIT
- ✓ FIKHEN
- ✓ FIKHIR
- ✓ GANMAK
- ✓ GHRPAJ
- ✓ GUPVOL
- ✓ HOCPLZ
- ✓ HOKWEJ

122 hits 100% Stop Search

Use as Query... Detach

GANMAK (P221)

File Edit Selection Display View Calculate Search Databases Help

Style Wireframe Colour: by Element Manage Styles Work Picking Mode Select Atoms Clear Measurements

Default view: b a b c a' b' c' x-x' y-y' z-z' x-90 x+90 y-90 y+90 z-90 z+90

Show Labels for: with Atom Labels Atom selections:

Structure Navigator

GANMAK P1gd

Crystal Structures Spacegroup

Databases

- CSD 5.31
- Feb10
- Nov09
- Structures
- Refcode Lists
- ConQuest Hits
- search
- FIKHEN P21/c
- FIKHIR P-1
- GHRPAJ P21/a
- MAVVEL P-1
- MAVVIP P-1
- NAMUMH P-1
- NAJNAO P-1
- OQPSAQ P21/c121
- GAWTEO C2/c
- BAVRUP P21/m
- SAGQAN P-1
- SAGHAI P21/c
- SAGHEY P-1
- YARPR P-1
- Mercurry Files P21/c121

Display Options

Display

- Packing
- Auto centre
- Short Contact <sum of vdW radii>
- H-Bond Default definition
- Contacts...
- More Info
- Powder...

Options

- Show hydrogens
- Depth cue
- Show cell axes
- Z-Clipping
- Label atoms
- Stereo

Press the left mouse button and move the mouse to rotate the structure

X-Vista: led045@csd

TABLE SPREADSHEET

Quest File: /c:/home/led045/csd_data/searches/temp/cq_temp1

Test: 1 of 1

Parameters	Total	Selected	Suppressed
Refcodes	27	0	n/a
Fragments	122	n/a	0

Data Visualization: Histogram Scattergram Polar Histogram Polar Scatter View REF CODs Correlation/Covariance View Quest Fragment

Parameters: Generate P.O. Scores Create Transform Search Re-name Export Swap Select Pars Clear Pars Select Pars

Refcodes: Select Refs Clear Refs Invert Delete Refs Suppress Unselected Suppress Selected Restore Save Coords

Miscellaneous: Test size Refresh Help About

REFCOD	PARAMS	11	12	13	14	15	16	17	CVOL
9	BACZUB	11.370	14.110	21.250	74.850	75.860	87.520	3190.194	
10	DIRVGD	9.553	12.583	34.140	90.000	97.100	90.000	4072.344	
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16	EGORIC	18.507	7.374	10.893	90.000	90.593	90.000	1486.425	
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19	FERGIT	11.854	7.974	23.221	90.000	102.390	90.000	2140.926	
20	FERGEP	11.842	7.891	23.580	90.000	102.480	90.000	2160.846	
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28	KAGAW	22.766	11.719	11.343	90.000	112.100	90.000	2803.671	
29	KGEKEL	15.513	12.257	10.165	107.210	108.120	98.500	1694.182	

CCDC Mogul 1.1.2: C:\Program Files\CCDC\Mogul 1.1.2\examples\tutorials\AABHTZ.mol2

File Searches Help

Build query Results and analysis View structures

Results Navigator

All hits: 6426

Accepted hits: 6426

R-factor: Any Heaviest Element: Any

Exclude: None

Relevance Number Contribution

1.00 6426 100.0%

View diagrams... More hits...

Statistics

Total: 6426

Selected: 6426

Mean: 1.732Å

Standard deviation: 0.024Å

Minimum: 1.273Å

Median: 1.725Å

Lower quartile: 1.713Å

Upper quartile: 1.741Å

Maximum: 2.017Å

Iz-score: 0.410

Histogram display

Displayed hits: 6426

Selected hits: 6426

Select all hits in histogram

Deselect all hits in histogram

Others...

Click to (d)eselect bars; click and drag to (d)eselect a range

IsoStar 2.1.1

Home Ligand Terminal Ligand Acyclic Links Ligand Ring Systems Ligand Solvates Protein Plots Custom Plots Help

Home

Ligand Terminal C,H only N,C,H only O,C,H only N,O,C,H only S-containing P-containing S-containing Halo-containing

Acyclic links C,H only N,C,H only O,C,H only N,O,C,H only S-containing Nucleic acid bases

Solvates, etc: Inorganic Organic

Protein Terminal Links Ring systems Custom Plots

The display and manipulation of the encrypted IsoStar scatterplots available from this server requires use of a fully licensed installation of the IsoStar Client.

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- Molecular modellers studying protein-ligand interactions as part of the rational drug design process
- Medicinal chemists interested in identifying bioisosteric replacements
- Protein crystallographers
- Crystal engineers

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PublisCSD.asee.rind

File Edit Options View Databases Results Help

Build Queries Combine Queries Manage Hitlists View Results

Refcode: MELSA
 Author: A.Pernet-Poll-Chevrier, F.Cantagrel
 Compound:
 Synonym:
 Formula: C18 H24 N2 O2
 Qualifier: *TEMP: at 293.0 K *PRESSURE: 101325 Pa *S-CONFIG: *POLYMORPH: *BIODIVERSITY: *RACEMATE: *REINTEGRATION: *OTHER-DIFF:
 Remarks: tampon/archiv/ArchiveLEDSS97-CCDC: CCDC 605990 *XREF: *RI
 Info:
 Disorder:
 Errors:
 Properties: *COLOR: colorless *HABIT: prism *NS: *ISO: *OTHER-CELL: *PHAS
 Class:
 a: 8.314(1) b: 14
 alpha: beta
 z: 4 sp.gr: P2
 R-fact: 0.0573 density: 1.13

----- MELSA -----

- JRNL journal-Tetrahedron:Asymm.
- RMARKS Bad character: " "
- RMARKS Bad character: " "
- Checks Calc.vol= 175489; Calc.form.wt= 36

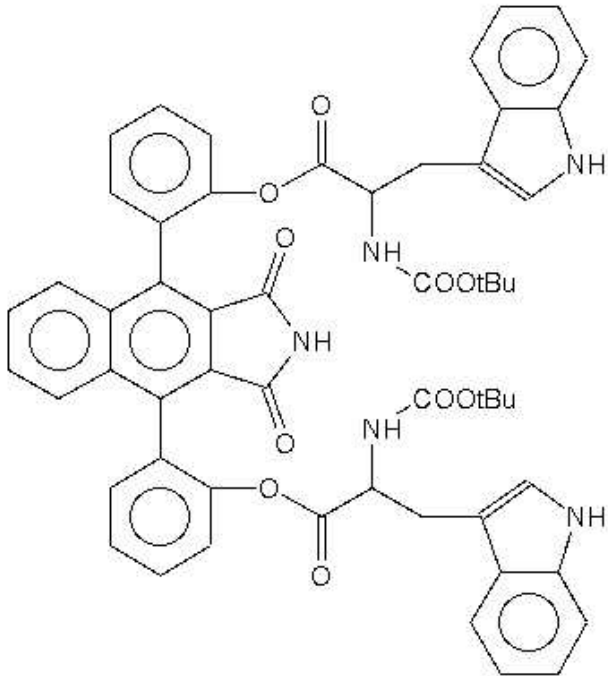
CCDC ConQuest (1) : search1 [Search]

File Edit Options View Databases Results Help

Build Queries Combine Queries Manage Hitlists View Results

Refcode: GANMAK CSD version 5.31 (November 2009)

All Text
 Author/Journal
 Chemical
 Crystal
 Experimental
 Diagram
 3D Visualiser
 CSD Internals
 Search Overview



Use as Query... Detach

Structure Navigator

GANMAK

Crystal Structures Spacegroup

- GANMAK P1
- search1 P21/c
- FIKHEN P-1
- MAVVEL P21/a
- MAVIP P-1
- NAJMUH P6cn
- NAJNAO P21/m
- OPPSAO P21c121
- GAWTED C2/c
- BAVIRP P21/m
- SAGUN P-1
- SAGHAI P21/c
- SAGHEY P6cn
- VARPR P21212
- Mercury Files

Structure Navigator Searches

X-Vista: led045@csd

VISTA v.2.1

Quest File: /c:/home/led045/csds_data/search1

Test: 1 of 1

	Parameters	Total
	Refcodes	27
	Fragments	122

REFCODE	PARAMS	11	12
9	BAZCUB	11.370	14.110
10	DIRYGD	9.553	12.583
11	ECOKOV	9.009	9.009
12	EFAZAM	8.857	10.352
13	EFAZED	8.972	9.116
14	EFAZIU	8.812	13.897
15	EGOREY	7.463	10.978
16	EGORIC	18.507	7.374
17	ESBWEI	9.711	12.543
18	ETIJUM	9.677	2.777
19	TERGEP	11.894	7.974
20	FERGIT	11.642	7.891
21	FIKHEN	21.322	10.920
22	FIKHIR	12.695	13.213
23	GANMAK	14.478	14.478
24	GIBPAJ	7.440	7.070
25	GUVYOL	8.848	12.843
26	HOCPIZ	7.316	8.426
27	HOKWEJ	10.164	10.122
28	ICAGAV	22.766	11.719
29	IGEKEL	15.513	12.357

Protein Plots Custom Plots

Available from this server

ions formed by a wide range of interactions are

resents a wealth of

rational drug design

X-PreQuest: chally@ccdc.org

File PubliCSD.aser.ind Entry 87 of 218 Current MELSAY PreQuest

Refcode: MELSAY Reference: 1090,17,1969,2006

Author: A.Pernet-Poll-Chevrier, F.Cantagrel, K.Le Jeune, C.Philouze, P.Y.Chavant

Compound: C18 H24 N2 O2

Formula: C18 H24 N2 O2

Qualifier: *TEMP: at 293.0 K *PRESSURE: *RADIATION: *POWDER: *REFINEMENT: *AB S-CONFIG: *POLYMORPH: *BIOACTIVITY: *CONFORMER: *ISOMER: *STER EOMER: *RACEMATE: *REINT-SEE: *REINT-OF: *CONTRIB: *OTHER-EXP: *OTHER-DIFF:

Remarks: tampon\archive\ArchiveLEDSS97-06\Archive06\Y_Vallee\PY_Chavant\FCA393 "CCDC: CCDC 605990 "XREF: "REMARK: "DOI:

Info: Disorder: Errors: Properties: "COLOR: colorless "HABIT: prism "MP: "SOURCE-CHEM: "SOURCE-NAT: "SE NS: "ISO: "OTHER-CELL: "PHASE-T:

Class: a 8.314(1) b 14.10(2) c 14.97(2)

alpha beta gamma

z 4 sp gr P212121 vol.

R-factor density 0.0573 1.138 form wt.

Rotation Translation

56 5.0 0.20

0 0

3 Set 3D Display

MELSAY

- JRNL journal-Tetrahedron:Asymm.
- REMARKS Bad character: "
- REMARKS Bad character: "
- Checks Calc.vol= 175489; Calc.form.wt= 300.40; Calc.dens.= 1.14

CCDC ConQuest (1) : search [Search]

File Edit Options View Databases Results Help

Build Queries Combine Queries Manage Hitlists View Results

All Text Author/Journal Chemical Crystal Experimental Diagram 3D Visualiser CSD Internals Search Overview

Refcode: GANMAK CSD version 5.31 (November 2009)

ANALYSE HITLIST

- ✓ AH0VUO
- ✓ AH0WAV
- ✓ AH0WEZ
- ✓ AH0WID
- ✓ AH0WJO
- ✓ BAPCF
- ✓ BAPCOL
- ✓ BAZCOV
- ✓ BAZCUB
- ✓ DIRVYGB
- ✓ ECKOKW
- ✓ EFAZAM
- ✓ EFAZEQ
- ✓ EFAZIU
- ✓ EGOREY
- ✓ EGORIC
- ✓ ESEMUK
- ✓ ETLIUM
- ✓ FERGEP
- ✓ FERGIT
- ✓ FIKHEN
- ✓ FIKHIR
- ✓ GANMAK
- ✓ GHRPAJ
- ✓ GUPVOL
- ✓ HOCPLZ
- ✓ HOKWEJ

122 hits 100% Stop Search

Use as Query... Detach

GANMAK (P221)

File Edit Selection Display View Calculate Search Databases Help

Style Wireframe Colour: by Element Manage Styles Work Picking Mode Select Atoms Clear Measurements

Default view: b a b c a' b' c' x-x' y-y' z-z' x-90 x+90 y-90 y+90 z-90 z+90

Show Labels for: with Atom Labels Atom selections:

Structure Navigator

GANMAK P1gd

Crystal Structures Spacegroup

Databases

- CCDC 5.31
- Feb10
- Nov09
- Structures
- Refcode Lists
- ConQuest Hits
- search
- FIKHEN P21/c
- FIKHIR P-1
- GH0303 P21/c
- MAVVEL P21/a
- MAVVP P-1
- NAJMUH Pcn
- NAJNAO P21/m
- OPPSAQ P21c121
- GAWTEO C2/c
- RAVRUP P21/m
- SAGGAN P-1
- SAGHAI P21/c
- SAGHEY P21/c
- VARPR P21212
- Mercury Files

Display Options

Display

- Packing
- Auto centre
- Short Contact (sum of vdW radii)
- H-Bond Default definition
- Contacts...
- More Info
- Powder...

Options

- Show hydrogens
- Depth cue
- Show cell axes
- Z-Clipping
- Label atoms
- Stereo

Press the left mouse button and move the mouse to rotate the structure

X-Vista: led045@csd

VISTA v.2.1 TABLE SPREADSHEET

Quest File: /c:/home/led045/csd_data/searches/temp/cq_temp1

Test: 1 of 1

Parameters	Total	Selected	Suppressed
Refcodes	27	0	n/a
Fragments	122	0	0

REFCOD	PARAMS	11	12	13	14	15	16	17	CVOL
9	BACUB	11.370	14.110	21.250	74.850	75.860	87.520	3190.194	
10	DIRVYG	9.553	12.583	34.140	90.000	97.100	90.000	4072.344	
11	ECKOKW	9.009	9.009	12.210	90.000	90.000	90.000	890.889	
12	EFAZAM	8.857	10.522	12.859	104.610	93.080	111.210	1024.678	
13	EFAZEQ	8.972	9.116	12.990	97.400	104.030	60.580	867.781	
14	EFAZIU	8.812	13.897	14.728	90.000	90.210	90.000	1803.584	
15	EGOREY	7.463	10.978	17.009	90.000	90.000	90.000	1383.527	
16	EGORIC	18.507	7.374	10.893	90.000	90.593	90.000	1486.425	
17	ESBWH	8.711	12.549	20.893	90.000	92.218	90.000	2292.983	
18	ETLIUM	9.677	21.777	10.190	90.000	107.090	90.000	1026.036	
19	FERGIT	11.854	7.974	23.221	90.000	102.390	90.000	2140.926	
20	FERGEP	11.942	7.891	23.590	90.000	102.480	90.000	2160.845	
21	FIKHEN	21.322	10.920	23.131	90.000	115.410	90.000	4964.721	
22	FIKHIR	12.695	13.213	21.692	74.500	96.800	67.600	3214.422	
23	GANMAK	14.478	14.478	21.310	90.000	90.000	120.000	3867.330	
24	GHRPAJ	7.440	7.070	15.429	90.000	102.480	90.000	792.401	
25	GUPVOL	8.848	12.843	21.551	90.000	90.000	90.000	2448.945	
26	HOCPLZ	7.316	8.426	22.832	90.000	90.000	90.000	1408.973	
27	HOKWEJ	10.164	10.122	14.168	90.000	93.460	90.000	1454.711	
28	KAGAW	22.766	11.719	11.343	90.000	112.100	90.000	2803.671	
29	KGEKEL	15.513	12.257	10.165	107.210	108.120	98.500	1694.182	

Miscellaneous: Test size, Refresh, Help, About

CCDC Mogul 1.1.2: C:\Program Files\CCDC\Mogul 1.1.2\examples\tutorials\AABHTZ.mol2

File Searches Help

Build query Results and analysis View structures

Results Navigator

All hits: 6426
Accepted hits: 6426
R-factor: Any Heaviest Element: Any
Exclude: None

Relevance	Number	Contribution
1.00	6426	100.0%

Mogul search - Bond length - C1 Cl1

Statistics

Total: 6426
Selected: 6426
Mean: 1.732Å
Standard deviation: 0.024Å
Minimum: 1.273Å
Median: 1.725Å
Upper quartile: 1.741Å
Maximum: 2.017Å
Iz-score: 0.410

Histogram display

Displayed hits: 6426
Selected hits: 6426

Click to (d)eselect bars; click and drag to (d)eselect a range

Click to (d)eselect; click again to (d)eselect a range

Click to (d)eselect; click and drag to (d)eselect a range

Click to (d)eselect; click and drag to (d)eselect a range

IsoStar 2.1.1

Home Ligand Terminal Ligand Acyclic Links Ligand Ring Systems Ligand Solvates Protein Plots Custom Plots Help

Home

Ligand Terminal

- C,H only
- N,C,H only
- O,C,H only
- N,O,C,H only
- S-containing
- P-containing
- S-containing
- Halo-containing

Ring systems

- Phenols
- C,H only
- N,C,H only
- O,C,H only
- N,O,C,H only
- S-containing
- Nucleic acid bases

Solvates, etc:

- Inorganic
- Organic

Protein Terminal Links Ring systems Custom Plots

The display and manipulation of the encrypted IsoStar scatterplots available from this server requires use of a fully licensed installation of the IsoStar Client.

IsoStar provides rapid access to knowledge about the intermolecular interactions formed by a wide variety of chemical groups. Not only will IsoStar indicate when specific interactions have a high frequency of occurrence (and their preferred directionalities), it will also indicate when interactions are unlikely to occur.

IsoStar is derived from experimental information in the CSD and PDB and presents a wealth of information to:

- Molecular modellers studying protein-ligand interactions as part of the rational drug design process
- Medicinal chemists interested in identifying bioisosteric replacements
- Protein crystallographers
- Crystal engineers

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GANMAK (P3221)

File Edit Selection Display View Calculate Search Databases Help

Style: Wireframe Colour: by Element Manage Styles... Work Picking Mode: Select Atoms Clear Measurements

Default view: b a b c a* b* c* x- x+ y- y+ z- z+ x-90 x+90 y-90 y+90 z-90 z+90

Show Labels for All atoms with Atom Label Atom selections:

Structure Navigator

GANMAK Find

Crystal Structures Spacegroup

Databases

- CSD 5.31
- Feb10
- May10
- Nov09

Structures

Refcode Lists

ConQuest Hits

- search1
 - FIKHEN P21/c
 - FIKHIR P-1
 - GANMAK P3221**
 - MAVVEL P21/a
 - MAVVIP P-1
 - NAJMUH Pbcn
 - NAJNAO P21/n
 - QAPGAQ P212121
 - QAWTEO C2/c
 - RAYRUF P21/n
 - SAQGUN P-1
 - SAQHAU P21/c
 - SAQHEY Pbcn
 - YARPIR P21212

Mercury Files

Display Options

Display

- Packing
- Auto centre
- Short Contact < (sum of vdW radii)
- H-Bond Default definition

Options

- Show hydrogens
- Show cell axes
- Label atoms
- Depth cue
- Z-Clipping
- Stereo

Tree View

- Multiple Structures

Structure Navigator Searches

Press the left mouse button and move the mouse to rotate the structure

X-Vista: led045@csd

VISTA v.2.1

Quest File: /c/home/led045/csds_data/see

Test: 1 of 1

	Parameters	Refcodes	Fragments	Tot
				27
				122
				122

REFCOD	PARAMS	11	12
9	BACUB	11.370	14.114
10	DIRYGD	9.953	12.588
11	ECDKOV	9.009	9.000
12	EPAZAM	8.857	10.352
13	EPAZED	8.972	9.116
14	EPAZIU	8.812	13.889
15	EGOREV	7.463	10.976
16	EGORIC	18.507	7.371
17	ESBMCZ	9.711	12.544
18	ETUDR	9.977	2.777
19	ETUDR	11.854	7.937
20	FERQZ	11.942	7.861
21	FIKHEN	21.322	10.920
22	FIKHIR	12.695	13.211
23	GANMAK	14.478	14.478
24	GIRPAL	7.440	7.071
25	GURVGL	8.848	12.841
26	HDCPIS	7.316	8.428
27	HORWEL	10.164	10.122
28	ICAGAV	22.766	11.711
29	IGEKEL	15.913	12.351

Plots available from this server

or interactions formed by a wide
spheric interactions have a high
also indicate when interactions are

DB and presents a wealth of

part of the rational drug design
placements

X-PreQuest: chally@ccdc.org

File PubliCSD.aser.ind Entry 87 of 218 Current MELSAY PreQuest

Refcode: MELSAY Reference: 1090,17,1969,2006

Author: A.Pernet-Poll-Chevrier, F.Cantagrel, K.Le Jeune, C.Philouze, P.Y.Chavant

Compound: C18 H24 N2 O2

Formula: C18 H24 N2 O2

Qualifier: *TEMP: at 293.0 K *PRESSURE: *RADIATION: *POWDER: *REFINEMENT: *ABS-CONFIG: *POLYMORPH: *BIOACTIVITY: *CONFORMER: *ISOMER: *STEREOMER: *RACEMATE: *REINT-SEE: *REINT-OF: *CONTRIB: *OTHER-EXP: *OTHER-DIFF:

Remarks: tampon\archive\ArchiveLEDSS97-06\Archive06\Y_Vallee\PY_Chavant\FCA393 "CCDC: CCDC 605990 "XREF: "REMARK: "DOI:

Info: Disorder: Errors: Properties: "COLOR: colorless "HABIT: prism "MP: "SOURCE-CHEM: "SOURCE-NAT: "SE NS: "ISO: "OTHER-CELL: "PHASE-T:

Class: a 8.314(1) b 14.10(2) c 14.97(2)

alpha: beta gamma

z 4 sp gr P212121 vol.

R-factor: density 1.138 form wt.

Rotation Translation

56 5.0 0.20

0 0

3 Set 3D Display

MELSAY

- JRNL journal-Tetrahedron:Asymm.
- REMARKS Bad character: "
- REMARKS Bad character: "
- Checks Calc.vol= 175489; Calc.form.wt= 300.40; Calc.dens.= 1.14

CCDC ConQuest (1) : search [Search]

File Edit Options View Databases Results Help

Build Queries Combine Queries Manage Hitlists View Results

All Text Author/Journal Chemical Crystal Experimental Diagram 3D Visualiser CSD Internals Search Overview

Refcode: GANMAK CSD version 5.31 (November 2009)

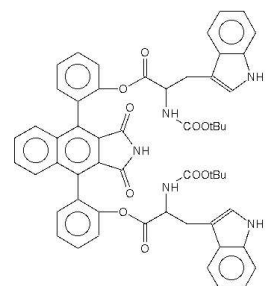
GANMAK

Analyse Hitlist

- ✓ AH0VUO
- ✓ AH0WAV
- ✓ AH0WEZ
- ✓ AH0WID
- ✓ AH0WJO
- ✓ BAPCF
- ✓ BAPCOL
- ✓ BAZCOV
- ✓ BAZCUB
- ✓ DREVYGB
- ✓ ECKOWK
- ✓ EFAZAM
- ✓ EFAZEQ
- ✓ EFAZIU
- ✓ EGOREY
- ✓ EGORIC
- ✓ ESEMUK
- ✓ ETLIUM
- ✓ FERGEP
- ✓ FERGIT
- ✓ FIKHEN
- ✓ FIKHIR
- ✓ FIKHJ
- ✓ GANMAK
- ✓ GIBPAJ
- ✓ GUPVOL
- ✓ HOCPLZ
- ✓ HOKWEJ

122 hits 100% Stop Search

Use as Query... Detach



GANMAK (P221)

File Edit Selection Display View Calculate Search Databases Help

Style Wireframe Colour: by Element Manage Styles Work Picking Mode Select Atoms Clear Measurements

Default view: b a b c a' b' c' x-x' y-y' z-z' x-90 x+90 y-90 y+90 z-90 z+90

Show Labels for: with Atom Labels Atom selections:

Structure Navigator

GANMAK P1gd

Crystal Structures Spacegroup

Databases

- CCDC 5.31
- Feb10
- May10
- Nov09
- Structures
- Refcode Lists
- ConQuest Hits
- search
- FIKHEN P21/c
- FIKHIR P-1
- FIKJ P21/c
- MAVVEL P-1
- MAVVP P-1
- NAJMUH P6cn
- NAJNAO P21/m
- OPPSAQ P21c121
- GAVTEO C2/c
- RAVRUP P21/m
- SAGGAN P-1
- SAGHAI P21/c
- SAGHEY P21/c
- VARPR P21212
- Mercury Files

Display Options

Display

- Packing
- Auto centre
- Short Contact (sum of vdW radii)
- H-Bond Default definition
- Contacts...
- More Info
- Powder...

Options

- Show hydrogens
- Depth cue
- Show cell axes
- Z-Clipping
- Label atoms
- Stereo

Press the left mouse button and move the mouse to rotate the structure

X-Vista: led045@csd

VISTA v.2.1 TABLE SPREADSHEET

Quest File: /c/home/led045/csd_data/searches/temp/cq_temp1

Test: 1 of 1

Parameters	Total	Selected	Suppressed
Refcodes	122	0	n/a
Fragments	122	0	0

Data Visualization: Histogram Scattergram Polar Histogram Polar Scatter View REF CODs Correlation/Covariance View Quest Fragment

Parameters: Generate P.O. Scores Create Transform Search Re-name Export Swap Select Pars Clear Pars Select Pars

Refcodes: Select Refs Clear Refs Invert Delete Refs Suppress Unselected Suppress Selected Restore Save Coords

Miscellaneous: Test size Refresh Help About

REFCOD	PARAMS	11	12	13	14	15	16	17	CVOL
9	BACUB	11.370	14.110	21.250	74.850	75.860	87.520	3190.194	
10	DIRVGD	9.553	12.583	34.140	90.000	97.100	90.000	4072.344	
11	ECKOWK	9.009	9.009	12.210	90.000	90.000	90.000	890.889	
12	EFAZAM	8.857	10.522	12.859	104.610	93.080	111.210	1024.678	
13	EFAZEL	8.972	9.116	12.990	97.400	104.030	60.580	867.781	
14	EFAZIU	8.812	13.897	14.728	90.000	90.210	90.000	1803.584	
15	EGOREY	7.463	10.978	17.009	90.000	90.000	90.000	1383.527	
16	EGORIC	18.507	7.374	10.893	90.000	90.593	90.000	1486.425	
17	ESBWH	9.711	12.549	20.893	90.000	92.218	90.000	2292.980	
18	ETLIUM	9.677	21.777	10.190	90.000	107.090	90.000	1026.036	
19	FERGEP	11.854	7.974	23.221	90.000	102.390	90.000	2140.926	
20	FERGIT	11.842	7.891	23.221	90.000	102.480	90.000	2160.846	
21	FIKHEN	21.322	10.920	23.131	90.000	115.410	90.000	4964.721	
22	FIKHIR	12.695	13.213	21.692	74.590	96.800	67.600	3214.422	
23	GANMAK	14.478	14.478	21.310	90.000	90.000	120.000	3867.330	
24	GIBPAJ	7.440	7.070	15.429	90.000	102.480	90.000	792.401	
25	GUPVOL	8.848	12.843	21.551	90.000	90.000	90.000	2448.945	
26	HOCPLZ	7.316	8.426	22.832	90.000	90.000	90.000	1408.973	
27	HOKWEJ	10.164	10.122	14.168	90.000	93.460	90.000	1454.711	
28	KAGAV	22.766	11.719	11.343	90.000	112.100	90.000	2803.671	
29	KGEKEL	15.513	12.257	10.165	107.210	108.120	98.300	1694.182	

CCDC Mogul 1.1.2: C:\Program Files\CCDC\Mogul 1.1.2\examples\tutorials\AABHTZ.mol2

File Searches Help

Build query Results and analysis View structures

Results Navigator

All hits: 6426


Accepted hits: 6426

R-factor: Any Heaviest Element: Any

Exclude: None

Relevance	Number	Contribution
1.00	6426	100.0%

Mogul search - Bond length - C1 Cl



Statistics

Total: 6426

Selected: 6426

Mean: 1.732Å

Standard deviation: 0.024Å

Minimum: 1.279Å

Median: 1.725Å

Upper quartile: 1.741Å

Maximum: 2.017Å

Iz-score: 0.410

Histogram display

Displayed hits: 6426

Selected hits: 6426

Select all hits in histogram

Deselect all hits in histogram

Help About

IsoStar 2.1.1

Home Ligand Terminal Ligand Acyclic Links Ligand Ring Systems Ligand Solvates Protein Plots Custom Plots Help

Home

Ligand Terminal C,H only N,C,H only O,C,H only N,O,C,H only S-containing P-containing S-containing Halo-containing

Acyclic links C,H only N,C,H only O,C,H only N,O,C,H only S-containing Nucleic acid bases

Solvates, etc: Inorganic Organic

Protein Terminal Links Ring systems Custom Plots

The display and manipulation of the encrypted IsoStar scatterplots available from this server requires use of a fully licensed installation of the IsoStar Client.

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- Molecular modellers studying protein-ligand interactions as part of the rational drug design process
- Medicinal chemists interested in identifying bioisosteric replacements
- Protein crystallographers
- Crystal engineers

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Registered in England No.2155347 Registered Charity No.800579

X-PreQuest: chally@cecosg2

File PublisCSD.aser.ind

Close Insert Print

Class Export Copy

Refcode MELSAY

Author A.Pernet-Poll-Chevrier, F.Cantagrel

Compound

Synonym

Formula C18 H24 N2 O2

Qualifier *TEMP: at 293.0 K *PRESSURE: "PZ S-CONFIG: "POLYMORPH: "BIOAC EOMER: "RACEMATE: "REINT-SEE OTHER-DIFF:

Remarks tampon/archive/ArchiveLEDSS97-06; CCDC: CCDC 605990 *XREF: "REM

Info

Disorder

Errors

Properties *COLOR: colorless *HABIT: prism *M NS: "ISO: "OTHER-CELL: "PHASE-

Class

a 8.314(1) b 14.10

alpha beta

z 4 sp.grp P212

R-fact 0.0573 density 1.138

----- MELSAY -----

- JRNL Journal-Tetrahedron:Asymm.
- RMARKS Bad character: ""
- RMARKS Bad character: ""
- Checks Calc.vol= 175489; Calc.form.wt= 300.4

X-Vista: led045@csd

VISTA v.2.1 TABLE SPREADSHEET

Quit

Quest File : /cqhome/led045/csds_data/searches/temp/cq_temp1

Test: 1 of 1

	Total	Selected	Suppressed
Parameters	27	0	n/a
Refcodes	122	n/a	n/a
Fragments	122	0	0

<Home>	PARAMS	11	12	13	14	15	16	17
REFCOD		*ACEL	*BCEL	*CCEL	*ALPH	*BETA	*GAMM	*CVOL
9	BAZCUB	11.370	14.110	21.250	74.850	75.860	87.520	3190.194
10	DIKYIGDI	9.553	12.583	34.140	90.000	97.100	90.000	4072.344
11	ECDKOW	9.009	9.009	12.210	90.000	90.000	90.000	990.989
12	EFAZAM	8.657	10.352	12.859	104.810	93.080	111.210	1024.879
13	EFAZEQ	8.972	9.116	12.990	97.400	104.030	60.580	897.761
14	EFAZIU	8.812	13.897	14.728	90.000	90.210	90.000	1803.584
15	EGOREY	7.463	10.978	17.009	90.000	90.000	90.000	1393.527
16	EGORIC	18.507	7.374	10.893	90.000	90.553	90.000	1486.425
17	ESEMUK	8.711	12.549	20.653	90.000	92.210	90.000	2255.990
18	ETIJUM	9.077	21.777	10.190	90.000	107.020	90.000	1926.036
19	FERGEP	11.834	7.974	23.221	90.000	102.300	90.000	2140.935
20	FERGIT	11.642	7.960	23.890	90.000	102.460	90.000	2160.845
21	FIKHEN	21.322	10.920	23.131	90.000	115.410	90.000	4864.721
22	FIKHIR	12.605	13.213	21.692	74.500	86.800	67.600	3214.422
23	GANMAK	14.476	14.476	21.310	90.000	90.000	120.000	3867.330
24	GIBPAJ	7.440	7.070	15.429	90.000	102.480	90.000	792.401
25	GUVDL	8.848	12.843	21.551	90.000	90.000	90.000	2448.945
26	HOCPIZ	7.316	8.435	22.832	90.000	90.000	90.000	1408.973
27	HOKWEJ	10.164	10.122	14.166	90.000	93.480	90.000	1454.711
28	ICAGAV	22.766	11.718	11.343	90.000	112.100	90.000	2803.671
29	IQEKEU	15.513	12.257	10.165	107.210	108.120	98.300	1694.182

Quest Files

Load... Save...

Data Visualization

Histogram Scattergram

Polar Histo. Polar Scatt.

View REFCODEs

Correlation/Covariance

View Quest Fragment

Parameters

Generate P.C. Scores

Create... Transform...

Search... Re-name...

Export... Swap

Select Pars. Clear Pars.

Delete Pars.

Refcodes

Select Refs. Clear Refs.

Invert Delete Refs

Suppress Unselected

Suppress Selected

Restore Save Coords...

Miscellaneous

Text size... Refresh

Help... About...

X-PreQuest: chally@ccdc.org

File PubliCSD.aser.ind Entry 87 of 218 Current MELSAY PreQuest

Refcode: MELSAY Reference: 1090,17,1969,2006

Author: A.Pernet-Poll-Chevrier, F.Cantagrel, K.Le Jeune, C.Philouze, P.Y.Chavant

Compound: C18 H24 N2 O2

Formula: C18 H24 N2 O2

Qualifier: *TEMP: at 293.0 K *PRESSURE: *RADIATION: *POWDER: *REFINEMENT: *AB S-CONFIG: *POLYMORPH: *BIOACTIVITY: *CONFORMER: *ISOMER: *STER EOMER: *RACEMATE: *REINT-SEE: *REINT-OF: *CONTRIB: *OTHER-EXP: *OTHER-DIFF:

Remarks: tampon\archive\ArchiveLEDSS97-06\Archive06\Y_Vallee\PY_Chavant\FCA393 "CCDC: CCDC 650590 "XREF: "REMARK: "DOI:

Info: Disorder: Errors: Properties: "COLOR: colorless "HABIT: prism "MP: "SOURCE-CHEM: "SOURCE-NAT: "SE NS: "ISO: "OTHER-CELL: "PHASE-T:

Class: a 8.314(1) b 14.10(2) c 14.97(2)

alpha beta gamma

z 4 sp gr P212121 vol.

R-factor 0.0573 density 1.138 form wt.

Rotation Translation

56 5.0 0.20

Set 3D Display

----- MELSAY -----

- JRNL journal-Tetrahedron:Asymm.
- RMARKS Bad character: "
- RMARKS Bad character: "
- Checks Calc.vol= 175488; Calc.form.wt= 300.40; Calc.dens.= 1.14

CCDC ConQuest (1) : search [Search]

File Edit Options View Databases Results Help

Build Queries Combine Queries Manage Hitlists View Results

All Text Author/Journal Chemical Crystal Experimental Diagram 3D Visualiser CSD Internals Search Overview

Refcode: GANMAK CSD version 5.31 (November 2009)

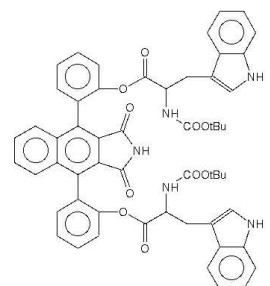
GANMAK

Analyse Hitlist

- ✓ AH0VUO
- ✓ AH0WAV
- ✓ AH0WEZ
- ✓ AH0WID
- ✓ AH0WJO
- ✓ BAPCF
- ✓ BAPCOL
- ✓ BAZCOV
- ✓ BAZCUB
- ✓ DREVYGBI
- ✓ ECKOKW
- ✓ EFAZAM
- ✓ EFAZEQ
- ✓ EFAZIU
- ✓ EGOREY
- ✓ EGORIC
- ✓ ESEMUK
- ✓ ETLIUM
- ✓ FERGEP
- ✓ FERGIT
- ✓ FIKHEN
- ✓ FIKHIR
- ✓ FIKHJ
- ✓ GANMAK
- ✓ GIBPAJ
- ✓ GUPVOL
- ✓ HOCPLZ
- ✓ HOKWEJ

122 hits 100% Stop Search

Use as Query... Detach



GANMAK (P221)

File Edit Selection Display View Calculate Search Databases Help

Style Wireframe Colour: by Element Manage Styles Work Picking Mode Select Atoms Clear Measurements

Default view: b a b c a' b' c' x-x' y-y' z-z' x-90 x+90 y-90 y+90 z-90 z+90

Show Labels for Atom Labels With Atom Labels Atom selections

Structure Navigator

GANMAK P1gd

Crystal Structures Spacegroup

Databases

- CCDC 5.31
- Feb10
- May10
- Nov09
- Structures
- Refcode Lists
- ConQuest Hits
- search
- FIKHEN P21/c
- FIKHIR P-1
- FIKJ P21/c
- MAVVEL P21/a
- MAVIP P-1
- NAJMUH P6cn
- NAJNAO P21/m
- OPPSAQ P21c121
- GAVTEO C2/c
- RAVRUP P21/m
- SAGQAN P-1
- SAGHAI P21/c
- SAGHEY P21/c
- VARPR P21212
- Mercury Files

Display Options

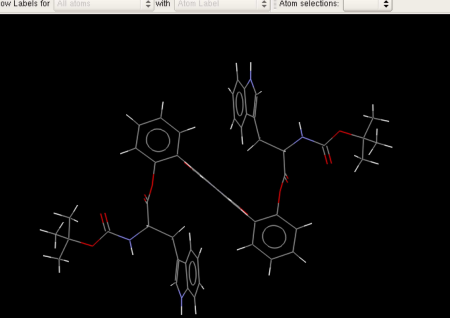
Display

- Packing
- Auto centre
- Short Contact (sum of vdW radii)
- H-Bond Default definition
- Contacts...
- More Info
- Powder...

Options

- Show hydrogens
- Depth cue
- Show cell axes
- Z-Clipping
- Label atoms
- Stereo

Press the left mouse button and move the mouse to rotate the structure



X-Vista: led045@csd

TABLE SPREADSHEET

Quest File: /c:/home/led045/csd_data/searches/temp/cq_temp1

Test: 1 of 1

Parameters	Total	Selected	Suppressed
Refcodes	27	0	n/a
Fragments	122	n/a	0

Data Visualization: Histogram Scattergram Polar Histogram Plot Scatter

View REF CODs Correlation/Covariance View Quest Fragment

Parameters: Generate P.O. Scores Create Transform Search Re-name Export Swap Select Pars Clear Pars Select Pars

Refcodes: Select Refs Clear Refs Invert Delete Refs Suppress Unselected Suppress Selected Restore Save Coords

Miscellaneous: Test size Refresh Help About

REFCOD	PARAMS	11	12	13	14	15	16	17	CVOL
9	BACUB	11.370	14.110	21.250	74.850	75.860	87.520	3190.194	
10	DIRVGD	9.553	12.583	34.140	90.000	97.100	90.000	4072.344	
11	ECKOKW	9.009	9.009	12.210	90.000	90.000	90.000	850.889	
12	EFAZAM	8.857	10.522	12.859	104.610	93.080	111.210	1024.678	
13	EFAZEL	8.972	9.116	12.990	97.400	104.030	60.580	867.781	
14	EFAZIU	8.812	13.897	14.728	90.000	90.210	90.000	1803.584	
15	EGOREY	7.463	10.978	17.009	90.000	90.000	90.000	1383.527	
16	EGORIC	18.507	7.374	10.893	90.000	90.593	90.000	1486.425	
17	ESBMH	8.911	12.543	20.833	90.000	92.218	90.000	2292.983	
18	ETLIUM	9.677	21.777	10.190	90.000	107.090	90.000	1026.036	
19	FERGIT	11.854	7.974	23.221	90.000	102.390	90.000	2140.926	
20	FERGEP	11.842	7.891	23.221	90.000	102.480	90.000	2160.846	
21	FIKHEN	21.322	10.920	23.131	90.000	115.410	90.000	4864.721	
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29	KGEKEL	15.513	12.257	10.165	107.210	108.120	98.500	1694.182	

CCDC Mogul 1.1.2: C:\Program Files\CCDC\Mogul 1.1.2\examples\tutorials\AABHTZ.mol2

File Searches Help

Build query Results and analysis View structures

Results Navigator

All hits: 6426


Accepted hits: 6426

R-factor: Any Heaviest Element: Any

Exclude: None

Relevance	Number	Contribution
1.00	6426	100.0%

Mogul search - Bond length - C1 O1



Statistics

Total: 6426

Selected: 6426

Mean: 1.732A

Standard deviation: 0.024A

Minimum: 1.273A

Median: 1.725A

Upper quartile: 1.741A

Maximum: 2.017A

Iz-score: 0.410

Histogram display

Displayed hits: 6426

Selected hits: 6426

Select all hits in histogram

Deselect all hits in histogram

Help About

IsoStar 2.1.1

Home Ligand Terminal Ligand Acyclic Links Ligand Ring Systems Ligand Solvates Protein Plots Custom Plots Help

Home

Ligand Terminal C,H only N,C,H only O,C,H only N,O,C,H only S-containing P-containing S-containing Halo-containing

Acyclic links C,H only N,C,H only O,C,H only N,O,C,H only S-containing Nucleic acid bases

Solvates, etc: Inorganic Organic

Protein Terminal Links Ring systems Custom Plots


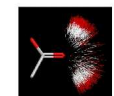

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IsoStar is derived from experimental information in the CSD and PDB and presents a wealth of information to:

- Molecular modellers studying protein-ligand interactions as part of the rational drug design process
- Medicinal chemists interested in identifying bioisosteric replacements
- Protein crystallographers
- Crystal engineers

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Registered in England No.2155347 Registered Charity No.800579

X-PreQuest: chally@ccciscg2

File PublsCSD

Close Export

Refcode: MELSAY
 Author: A.Pernet-Poll-Chevrier,
 Compound:
 Synonym:
 Formula: C18 H24 N2 O2
 Qualifier: *TEMP: at 293.0 K *PRE S-CONFIG: *POLYMOR EOMER: *RACEMATE: *OTHER-DIFF:
 Remarks: tampon/archive/ArchiveL CCDC: CCDC 605990 *)
 Info:
 Disorder:
 Errors:
 Properties: *COLOR: colorless *HAB NS: *ISO: *OTHER-CEL
 Class:
 a: 8.314(1) b:
 alpha: beta:
 z: 4 sp gr:
 R-fact: 0.0573 densit:

----- MELSAY -----

- JRNL journal-Tetrahedron:Asym
- RMARKS Bad character: " "
- RMARKS Bad character: " "
- Checks Calc.vol= 175489; Calc.f

CCDC Mogul 1.1.2: C:\Program Files\CCDC\Mogul 1.1.2\examples\tutorials\MAABHTZ.mol2

File Searches Help

Build query Results and analysis View structures

Results Navigator

All hits: 6426
 Accepted hits: 6426
 R-factor: Any Heaviest Element: Any
 Exclude: None

Relevance	Number	Contribution
<input checked="" type="checkbox"/> 1.00	6426	100.0%

View diagrams... More hits...

Statistics

Total: 6426
 Selected: 6426
 Mean: 1.733Å
 Standard deviation: 0.024Å
 Minimum: 1.273Å
 Lower quartile: 1.725Å
 Median: 1.733Å
 Upper quartile: 1.741Å
 Maximum: 2.017Å
 |z-score|: 0.410

All fragments... View query...

Mogul search - Bond length - C1 C11

Number of hits

Bond length / Å

Value in query: 1.741Å

Click to (de)select bars; click and drag to (de)select a range

Histogram display

Displayed hits: 6426
 Selected hits: 6426

Select all hits in histogram
 Deselect all hits in histogram

Filters...

Histogram: click in bar to deselect, click again to reselect. Right-click for options.

Structure Navigator

GANMAK P1221

Crystal Structures Spacegroup

- Databases
 - CSD 5.31
 - Feb10
 - May10
 - Nov09
 - Structures
 - Refcode Lists
 - ConQuest Hits
- search
 - FRHEN P21/c
 - FRHEN P-1
 - FRHEN P21/a
 - FRHEN P-1
 - FRHEN P2/c
 - FRHEN P21/m
 - FRHEN P21/c121
 - FRHEN C2/c
 - FRHEN P21/m
 - FRHEN P-1
 - FRHEN P21/c
 - FRHEN P2/c
 - FRHEN P21212
- Mercury Files

Structure Navigator Searches

X-Vista: led045@csd

VISTA v.2

Quest File: /c:/home/led045/csds_d

Test: 1 of 1

Parameters Refcodes Fragments

REFCOD	PARAMS	IT
9	BACUB	11,370
10	DIRVIG	9,553
11	ECOKOV	9,009
12	EPAZAM	8,857
13	EPAZED	8,972
14	EPAZIU	8,812
15	EGOREY	7,463
16	EGORIC	18,507
17	ESBNU	9,711
18	ETUDU	9,677
19	YENDE	11,854
20	FEROT	11,542
21	FRHEN	21,322
22	FRHE	12,656
23	GANMAK	14,478
24	DIRPA	7,440
25	GURVIG	8,848
26	HOCFID	7,316
27	HORWE	10,164
28	ICAGU	22,766
29	IGEKEL	15,513

Solvates Protein Plots Custom Plots

Protein Plots

Protein Plots available from this server

Protein interactions formed by a wide range of interactions have a high degree of specificity and also indicate when interactions are important for the function of the protein. The Protein Plots database presents a wealth of information on the interactions between the protein and its ligands, as part of the rational drug design process.

Protein Plots

X-PreQuest: chally@ccdc.org

File PubliCSD.aser.ind Entry 87 of 218 Current MELSAY PreQuest

Refcode: MELSAY Reference: 1090,17,1969,2006

Author: A.Pernet-Poll-Chevrier, F.Cantagrel, K.Le Jeune, C.Philouze, P.Y.Chavant

Compound: C18 H24 N2 O2

Formula: C18 H24 N2 O2

Qualifier: *TEMP: at 293.0 K *PRESSURE: *RADIATION: *POWDER: *REFINEMENT: *AB S-CONFIG: *POLYMORPH: *BIOACTIVITY: *CONFORMER: *ISOMER: *STER EOMER: *RACEMATE: *REINT-SEE: *REINT-OF: *CONTRIB: *OTHER-EXP: *OTHER-DIFF:

Remarks: tampon\archive\ArchiveLEDSS97-06\Archive06\Y_Vallee\PY_Chavant\FCA393 "CCDC: CCDC 605990 "XREF: "REMARK: "DOI:

Info: Disorder: Errors: Properties: "COLOR: colorless "HABIT: prism "MP: "SOURCE-CHEM: "SOURCE-NAT: "SE NS: "ISO: "OTHER-CELL: "PHASE-T:

Class: a 8.314(1) b 14.10(2) c 14.97(2)

alpha beta gamma

z 4 sp gr P212121 vol.

R-factor 0.0573 density 1.138 form wt.

Rotation Translation

56 5.0 0.20

0 0

3 Set 3D Display

MELSAY

- JRNL journal-Tetrahedron:Asymm.
- RMARKS Bad character: "
- RMARKS Bad character: "
- Checks Calc.vol= 175489; Calc.form.wt= 300.40; Calc.dens.= 1.14

CCDC ConQuest (1) : search [Search]

File Edit Options View Databases Results Help

Build Queries Combine Queries Manage Hitlists View Results

All Text Author/Journal Chemical Crystal Experimental Diagram 3D Visualiser CSD Internals Search Overview

Refcode: GANMAK CSD version 5.31 (November 2009)

GANMAK

Analyse Hitlist

- ✓ AH0VUO
- ✓ AH0WAV
- ✓ AH0WEZ
- ✓ AH0WID
- ✓ AH0WJO
- ✓ BAPCF
- ✓ BAPCOL
- ✓ BAZCOV
- ✓ BAZCUB
- ✓ DREVYGB
- ✓ ECKOKW
- ✓ EFAZAM
- ✓ EFAZEQ
- ✓ EFAZIU
- ✓ EGOREY
- ✓ EGORIC
- ✓ ESEMUK
- ✓ ETLIUM
- ✓ FERGEP
- ✓ FERGIT
- ✓ FIKHEN
- ✓ FIKHIR
- ✓ GANMAK
- ✓ GHRPAJ
- ✓ GUYVOL
- ✓ HOCPIZ
- ✓ HOKWEJ

122 hits 100% Stop Search

Use as Query... Detach

GANMAK (P221)

File Edit Selection Display View Calculate Search Databases Help

Style Wireframe Colour: by Element Manage Styles Work Picking Mode Select Atoms Clear Measurements

Default view: b a b c a' b' c' x-x' y-y' z-z' x-90 x+90 y-90 y+90 z-90 z+90

Show Labels for Atom types With Atom types Atom selections

Structure Navigator

GANMAK P1gd

Crystal Structures Spacegroup

Databases

- CSD 5.31
- Feb10
- Nov09
- Structures
- Refcode Lists
- ConQuest Hits
- search
- FIKHEN P21/c
- FIKHIR P-1
- GH0303 P21/c
- MAVVEL P21/a
- MAVVP P-1
- NAJMUH P6cn
- NAJNAO P21/m
- OPPSAQ P21c121
- GAVTEO C2/c
- RAVRUP P21/m
- SAGGAN P-1
- SAGHAI P21/c
- SAGHEY P21/c
- VARPR P21212
- Mercury Files

Display Options

Display

- Packing
- Auto centre
- Short Contact (sum of vdW radii)
- H-Bond Default definition
- Contacts...
- More info
- Powder...

Options

- Show hydrogens
- Depth cue
- Show cell axes
- Z-Clipping
- Label atoms
- Stereo

Press the left mouse button and move the mouse to rotate the structure

X-Vista: led045@csd

VISTA v.2.1 TABLE SPREADSHEET

Quest File: /c:/home/led045/csd_data/searches/temp/cq_temp1

Test: 1 of 1

Parameters	Total	Selected	Suppressed
Refcodes	27	0	n/a
Fragments	122	n/a	0

REFCOD	PARAMS	11	12	13	14	15	16	17	CVOL
9	BACUB	11.370	14.110	21.250	74.850	75.860	87.520	3190.194	
10	DIRVYG	9.553	12.583	34.140	90.000	97.100	90.000	4072.344	
11	ECKOKW	9.009	9.009	12.210	90.000	90.000	90.000	890.889	
12	EFAZAM	8.857	10.522	12.859	104.610	93.080	111.210	1024.678	
13	EFAZEQ	8.972	9.116	12.990	97.400	104.030	60.580	867.781	
14	EFAZIU	8.812	13.897	14.728	90.000	90.210	90.000	1803.584	
15	EGOREY	7.463	10.978	17.009	90.000	90.000	90.000	1383.527	
16	EGORIC	18.507	7.374	10.893	90.000	90.593	90.000	1486.425	
17	ESBWH	8.711	12.543	20.833	90.000	92.218	90.000	2292.983	
18	ETLIUM	9.677	21.777	10.190	90.000	107.090	90.000	1026.036	
19	FERGIT	11.854	7.974	23.221	90.000	102.390	90.000	2140.926	
20	FERGEP	11.842	7.891	23.590	90.000	102.480	90.000	2160.846	
21	FIKHEN	21.322	10.920	23.131	90.000	115.410	90.000	4964.721	
22	FIKHIR	12.695	13.213	21.692	74.500	96.800	67.600	3214.422	
23	GANMAK	14.478	14.478	21.310	90.000	90.000	120.000	3867.330	
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28	KAGAV	22.766	11.719	11.343	90.000	112.100	90.000	2803.671	
29	KGEKEL	15.513	12.257	10.165	107.210	108.120	98.300	1694.182	

Miscellaneous: Test size, Refresh, Help, About

CCDC Mogul 1.1.2: C:\Program Files\CCDC\Mogul 1.1.2\examples\tutorials\AABHTZ.mol2

File Searches Help

Build query Results and analysis View structures

Results Navigator

All hits: 6426

Accepted hits: 6426

R-factor: Any Heaviest Element: Any

Exclude: None

Relevance	Number	Contribution
1.00	6426	100.0%

Mogul search - Bond length - C1 O1

Value in query: 1.741Å

Statistics

Total: 6426

Selected: 6426

Mean: 1.732Å

Standard deviation: 0.024Å

Minimum: 1.273Å

Median: 1.725Å

Lower quartile: 1.723Å

Upper quartile: 1.741Å

Maximum: 2.017Å

Iz-score: 0.410

Histogram display

Displayed hits: 6426

Selected hits: 6426

Select all hits in histogram

Deselect all hits in histogram

Help About

Histogram: click in bar to deselect, click again to reselect. Right-click for options.

IsoStar 2.1.1

Home Ligand Terminal Ligand Acyclic Links Ligand Ring Systems Ligand Solvates Protein Plots Custom Plots Help

Home

Ligand Terminal

- C,H only
- N,C,H only
- O,C,H only
- N,O,C,H only
- S-containing
- P-containing
- S-containing
- Halo-containing

Acyclic links

- C,H only
- N,C,H only
- O,C,H only
- N,O,C,H only
- S-containing
- Nucleic acid bases

Solvates, etc:

- Inorganic
- Organic

Protein Terminal Links Ring systems Custom Plots

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- Crystal engineers

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Registered in England No.2155347 Registered Charity No.800579

X-PreQuest: chailly@ceclsg12

File PublsCSD.aser.ind Entry 87 of 218 Current M

Refcode: MELSAY Reference: 1090,17,1969,2006

Author: A.Pernet-Poll-Chevrier, F.Cantagrel, K.Le Jeune, C.Philouze, P.Y.Chavant

Compound: C18 H24 N2 O2

Formula: C18 H24 N2 O2

Qualifier: *TEMP: at 293.0 K *PRESSURE: "RADIATION"; *POWDER; *REFINEMENT: "AB S-CONFIG"; *POLYMORPH; *BIOACTIVITY: "CONFORMER"; *ISOMER; *STEREOMER; *RACEMATE; *REINT-SEE; *REINT-OF; *CONTRIB; *OTHER-EXP; *OTHER-DIFF.

Remarks: tampon\archive\ArchiveLEDSS97-06\Archive06\Y_Vallee\FY_Chavant\FCA393 "CCDC: CCDC 605990 "XREF:"REMARK: "DOI:

Info: Disorder: Errors: Properties: *COLOR: colorless *HABIT: prism *MP: "SOURCE-CHEM: "SOURCE-NAT: "SE NS; *ISO: *OTHER-CELL: *PHASE-T:

Class: a 8.314(1) b 14.10(2) c 14.97(2)

alpha: beta gamma

z 4 sp.grp P212121 vol.

R-factor: density 1.138 form.vt

----- MELSAY -----

- JRNL journal-Tetrahedron:Asymm.
- RMARKS Bad character: ""
- RMARKS Bad character: ""
- Checks Calc.vol= 175489; Calc.form.vt= 300.40; Calc.dens.= 1.14

IsoStar 2.1.1

Home | Ligand Terminal | Ligand Acyclic Links | Ligand Ring Systems | Ligand Solvates | Protein Plots | Custom Plots

Help

Home

Ligand Terminal

C,H only
N,C,H only
O,C,H only
N,O,C,H only
Si-containing
P-containing
S-containing
Halo-containing

Acyclic links

C,H only
N,C,H only
O,C,H only
N,O,C,H only
P-containing
S-containing

Ring systems

Phenyls
C,H only
N,C,H only
O,C,H only
N,O,C,H only
S-containing
Nucleic acid bases


Solvates, etc.

Inorganic
Organic

Protein

Terminal
Links
Ring systems

Custom Plots



The display and manipulation of the encrypted IsoStar scatterplots available from this server requires use of a fully licensed installation of the IsoStar Client.

IsoStar provides rapid access to knowledge about the intermolecular interactions formed by a wide variety of chemical groups. Not only will IsoStar indicate when specific interactions have a high frequency of occurrence (and their preferred directionalities), it will also indicate when interactions are unlikely to occur.

IsoStar is derived from experimental information in the CSD and PDB and presents a wealth of information to:

- Molecular modellers studying protein-ligand interactions as part of the rational drug design process
- Medicinal chemists interested in identifying bioisosteric replacements
- Protein crystallographers
- Crystal engineers

X-Vista: led045@csd

VISTA v.2.1 TABLE SPREADSHEET

Quest File: /c:/home/led045/csd/s_data/searches/temp/cq_temp1

Test: 1 of 1

Parameters	Total	Selected	Suppressed
Relcodes	27	0	n/a
Fragments	122	n/a	n/a
	0	0	0

REFCODE	PARAMS	11	12	13	14	15	16	17
9	BZCUB	11,370	14,110	21,250	74,850	75,860	87,520	3190,194
10	DIRVGD	9,553	12,583	34,140	90,000	97,100	90,000	4072,344
11	ECDKOV	9,009	9,009	12,210	90,000	90,000	90,000	890,889
12	EPAZAM	8,857	10,352	12,859	104,810	93,080	111,210	1024,678
13	EPAZEL	8,972	9,116	12,990	97,400	104,030	60,580	867,781
14	EPAZU	8,812	13,897	14,728	90,000	90,210	90,000	1803,584
15	EGOREV	7,463	10,978	17,009	90,000	90,000	90,000	1383,527
16	EGORC	18,507	7,374	10,893	90,000	90,553	90,000	1486,425
17	ESBWH	9,714	12,549	20,893	90,000	92,218	90,000	2292,946
18	ETUDM	9,677	21,777	10,190	90,000	107,090	90,000	1828,036
19	FEHDF	11,854	7,974	23,221	90,000	102,340	90,000	2140,925
20	FEROT	11,644	7,891	23,580	90,000	102,460	90,000	2160,845
21	FRHEE	21,322	10,920	23,131	90,000	115,410	90,000	4864,721
22	FRHFR	12,695	13,213	21,692	74,500	86,800	67,600	3214,422
23	GANMAK	14,478	14,478	21,310	90,000	90,000	120,000	3867,330
24	GIRPA	7,440	7,070	15,429	90,000	102,480	90,000	792,401
25	GURVGL	8,848	12,843	21,551	90,000	90,000	90,000	2448,945
26	HDCPZ	7,316	8,426	22,832	90,000	90,000	90,000	1409,973
27	HORWZ	10,164	10,122	14,168	90,000	93,460	90,000	1454,711
28	KAGAV	22,766	11,719	11,343	90,000	112,100	90,000	2803,671
29	IGEKEL	15,513	12,257	10,165	107,210	108,120	98,500	1694,182

Picking Mode Select Atoms Clear Measurements

x -90 x +80 y -90 y +90 z -90 z +90

Structure Navigator

GANMAK

Crystal Structures Spacegroup

- Databases
 - CSD 5.31
 - Feb10
 - May10
 - Nov09
 - Structures
 - Relcode Lists
 - ConQuest Hits
- search
 - FRHEN P21/c
 - FRHFR P-1
 - FRHFR P-1
 - MAVEL P21/a
 - MAVIP P-1
 - NAJMUH Pccn
 - NAJNAO P21/m
 - QPSAQ P212121
 - GAVTED C2/c
 - RAVRUP P21/m
 - SAGGAN P-1
 - SAGHAI P21/c
 - SAGHEY Pccn
 - VARPR P21212
- Mercury Files

Hydrogens Depth cue

Cell axes Z-Clipping

Atoms Stereo

Structure Navigator Searches

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➤ INIST

- CSD (Cambridge Structural Database)
 - En ligne
 - Sur DVD

➤ Configurations requises

➤ INIST

- CSD (Cambridge Structural Database)
 - En ligne
 - Sur DVD

➤ Configurations requises

- Windows (2000, XP, Vista, 7)

➤ INIST

- CSD (Cambridge Structural Database)
 - En ligne
 - Sur DVD

➤ Configurations requises

- Windows (2000, XP, Vista, 7)
- Linux (RedHat, Suse, Debian)

➤ INIST

- CSD (Cambridge Structural Database)
 - En ligne
 - Sur DVD

➤ Configurations requises

- Windows (2000, XP, Vista, 7)
- Linux (RedHat, Suse, Debian)
- MacOSX (10.4, 10.5, 10.6)

➤ INIST

- CSD (Cambridge Structural Database)
 - En ligne
 - Sur DVD

➤ Configurations requises

- Windows (2000, XP, Vista, 7)
- Linux (RedHat, Suse, Debian)
- MacOSX (10.4, 10.5, 10.6)

➤ Licence sous 24 heures

Prequest

Prequest

- Format requis : CIF

Prequest

- Format requis : CIF
- Plusieurs champs peuvent être renseignés

Refcode : N°incrémenté automatiquement / Référence CS D

X-PreQuest: cbailly@cecicsgl2

File PublisCSD.aser.ind Entry 87 of 218 Current MELSAY PreQuest

Open Insert... Print... Undo Redo Repeat 1D Edit... Check... Preferences... EXIT
Close Export... Copy... Paste Make 2D 2D Edit... 3D Check... Help...

Refcode MELSAY Reference 1090,17,1969,2006

Author A.Pernet-Poil-Chevrier, F.Cantagrel, K.Le Jeune, C.Philouze, P.Y.Chavant

Compound

Synonym

Formula C18 H24 N2 O2

Qualifier "TEMP: at 293.0 K "PRESSURE: "RADIATION: "POWDER: "REFINEMENT: "ABS-CONFIG: "POLYMORPH: "BIOACTIVITY: "CONFORMER: "ISOMER: "STEREOMER: "RACEMATE: "REINT-SEE: "REINT-OF: "CONTRIB: "OTHER-EXP: "OTHER-DIFF

Remarks tampon/archive/ArchiveLEDSS97-06/Archive06/Y_Vallee/PY_Chavant/FCA393 "CCDC: CCDC 605990 "XREF: "REMARK: "DOI:

Info

Disorder

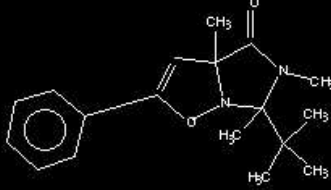

Errors

Properties "COLOR: colorless "HABIT: prism "MP: "SOURCE-CHEM: "SOURCE-NAT: "SENS: "ISO: "OTHER-CELL: "PHASE-T:

Class

a	8.314(1)	b	14.10(2)	c	14.97(2)
alpha		beta		gamma	
z	4	sp.grp	P212121	vol.	
R-factor	0.0573	density	1.138	form.wt	

MEJKIV 0
MELRUR 205
MELSAY 13
MELSEC 0
MERHIA 0

----- MELSAY -----

- JRNL journal=Tetrahedron:Asymm.
- RMARKS Bad character: " _ "
- RMARKS Bad character: " _ "
- Checks Calc.vol= 1754.89; Calc.form.wt= 300.40; Calc.dens.= 1.14

Rotation Translation

56 0 3

5.0 0.20

X Y Z X Y Z

Set 3D Display... Reset

Référence du Journal : Nom, Volume, Page, Année

X-PreQuest: cbailly@cecicsgl2

File PublisCSD.aser.ind Entry 87 of 218 Current MELSAY PreQuest

Open Insert... Print... Undo Redo Repeat 1D Edit... Check... Preferences... EXIT
Close Export... Copy... Paste Make 2D 2D Edit... 3D Check... Help...

Refcode MELSAY Reference 1090,17,1969,2006

Author A.Pernet-Poil-Chevrier, F.Cantagrel, K.Le Jeune, C.Philouze, P.Y.Chavant

Compound

Synonym

Formula C18 H24 N2 O2

Qualifier "TEMP: at 293.0 K "PRESSURE: "RADIATION: "POWDER: "REFINEMENT: "ABS-CONFIG: "POLYMORPH: "BIOACTIVITY: "CONFORMER: "ISOMER: "STEREOMER: "RACEMATE: "REINT-SEE: "REINT-OF: "CONTRIB: "OTHER-EXP: "OTHER-DIFF

Remarks tampon/archive/ArchiveLEDSS97-06/Archive06/Y_Vallee/PY_Chavant/FCA393 "CCDC: CCDC 605990 "XREF: "REMARK: "DOI:

Imb

Disorder

Errors

Properties "COLOR: colorless "HABIT: prism "MP: "SOURCE-CHEM: "SOURCE-NAT: "SENS: "ISO: "OTHER-CELL: "PHASE-T:

Class

a	8.314(1)	b	14.10(2)	c	14.97(2)
alpha		beta		gamma	
z	4	sp.grp	P212121	vol.	
R-factor	0.0573	density	1.138	form.wt	

MEJKIV 0
MELRUR 205
MELSAY 13
MELSEC 0
MERHIA 0

Chemical structure (2D): CN1C(=O)N(C)C1C2=CC=CC=C2

Chemical structure (3D):

--- MELSAY ---
 JRNL journal=Tetrahedron:Asymm.
 RMARKS Bad character: " _"
 RMARKS Bad character: " _"
 Checks Calc.vol= 1754.89; Calc.form.wt= 300.40; Calc.dens.= 1.14

Rotation 56 Translation 0.20
 - 5.0 + - 0.20 +
 - X + - X +
 - Y + - Y +
 - Z + - Z +
 Set 3D Display... Reset

Référence du Journal : Nom, Volume, Page, Année

X-PreQuest: cbailly@cecicsgl2

File PublisCSD.aser.ind Entry 87 of 218 Current MELSAY PreQuest

Open Insert... Print... Undo Redo Repeat 1D Edit... Check... Preferences... EXIT
Close Export... Copy... Paste Make 2D 2D Edit... 3D Check... Help...

Refcode MELSAY Reference 1090,17,1969,2006
Author A.Pernet-Poil-Chevrier, F.Cantagrel, K.Le Jeune, C.Philouze,P.Y.Chavant
Compound
Synonym
Formula C18 H24 N2 O2
Qualifier "TEMP: at 293.0 K "PRESSURE: "RADIATION: "POWDER: "REFINEMENT: "ABS-CONFIG: "POLYMORPH: "BIOACTIVITY: "CONFORMER: "ISOMER: "STEREOMER: "RACEMATE: "REINT-SEE: "REINT-OF: "CONTRIB: "OTHER-EXP: "OTHER-DIFF
Remarks tampon/archive/ArchiveLEDSS97-06/Archive06/Y_Vallee/PY_Chavant/FCA393 "CCDC: CCDC 605990 "XREF: "REMARK: "DOI:
Imb
Disorder
Errors
Properties "COLOR: colorless "HABIT: prism "MP: "SOURCE-CHEM: "SOURCE-NAT: "SENS: "ISO: "OTHER-CELL: "PHASE-T:
Class
a 8.314(1) b 14.10(2) c 14.97(2)
alpha beta gamma
z 4 sp.grp P212121 vol.
R-factor 0.0573 density 1.138 form.wt.

MEJKIV 0
MELRUR 205
MELSAY 13
MELSEC 0
MERHIA 0

--- MELSAY ---
● JRNL journal=Tetrahedron:Asymm.
● RMARKS Bad character: " _ "
● RMARKS Bad character: " _ "
● Checks Calc.vol= 1754.89; Calc.form.wt= 300.40; Calc.dens.= 1.14

Rotation Translation
5.0 0.20
X Y Z X Y Z
Set 3D Display... Reset

Auteurs

X-PreQuest: cbailly@cecicsgl2

File PublisCSD.aser.ind Entry 87 of 218 Current MELSAY PreQuest

Open Insert... Print... Undo Redo Repeat 1D Edit... Check... Preferences... EXIT
Close Export... Copy... Paste Make 2D 2D Edit... 3D Check... Help...

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Compound

Synonym

Formula C18 H24 N2 O2

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Remarks tampon/archive/ArchiveLEDSS97-06/Archive06/Y_Vallee/PY_Chavant/FCA393 "CCDC: CCDC 605990 "XREF: "REMARK: "DOI:

Info

Disorder

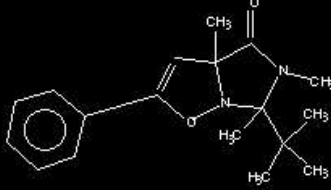

Errors

Properties "COLOR: colorless "HABIT: prism "MP: "SOURCE-CHEM: "SOURCE-NAT: "SENS: "ISO: "OTHER-CELL: "PHASE-T:

Class

a	8.314(1)	b	14.10(2)	c	14.97(2)
alpha		beta		gamma	
z	4	sp.grp	P212121	vol.	
R-factor	0.0573	density	1.138	form.wt	

MEJKIV 0
MELRUR 205
MELSAY 13
MELSEC 0
MERHIA 0

----- MELSAY -----

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- RMARKS Bad character: " _ "
- RMARKS Bad character: " _ "
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Rotation 56 Translation 0.20

-	X	+	-	X	+
-	Y	+	-	Y	+
-	Z	+	-	Z	+

Set 3D Display... Reset

N° de dépôt

X-PreQuest: cbailly@cecicsgl2

File PublisCSD.aser.ind Entry 87 of 218 Current MELSAY PreQuest

Open Insert... Print... Undo Repeat Revert 1D Edit... Check... Preferences... EXIT
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Compound

Synonym

Formula C18 H24 N2 O2

Qualifier "TEMP: at 293.0 K "PRESSURE: "RADIATION: "POWDER: "REFINEMENT: "ABS-CONFIG: "POLYMORPH: "BIOACTIVITY: "CONFORMER: "ISOMER: "STEREOMER: "RACEMATE: "REINT-SEE: "REINT-OF: "CONTRIB: "OTHER-EXP: "OTHER-DIFF

Remarks tampon/archive/ArchiveLEDSS97-06/Archive06/Y_Vallee/PY_Chavant/FCA393 "CCDC: CCDC 605990 "XREF: "REMARK: "DOI:

Info

Disorder


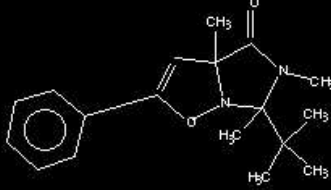
Errors

Properties "COLOR: colorless "HABIT: prism "MP: "SOURCE-CHEM: "SOURCE-NAT: "SENS: "ISO: "OTHER-CELL: "PHASE-T:

Class

a	8.314(1)	b	14.10(2)	c	14.97(2)
alpha		beta		gamma	
z	4	sp.grp	P212121	vol.	
R-factor	0.0573	density	1.138	form.wt	

MEJKIV 0
MELRUR 205
MELSAY 13
MELSEC 0
MERHIA 0



----- MELSAY -----

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Rotation Translation
56 0 3
5.0 0.20
X Y Z X Y Z
Set 3D Display... Reset

Zone d'archivage

X-PreQuest: cbailly@cecicsgl2

File PublisCSD.aser.ind Entry 87 of 218 Current MELSAY PreQuest

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Close Export... Copy... Paste Make 2D 2D Edit... 3D Check... Help...

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Remarks tampon/archive/ArchiveLEDSS97-06/Archive06/Y_Vallee/PY_Chavant/FCA393
CCDC: CCDC 605990 "XREF: "REMARK: "DOI:

Info

Disorder

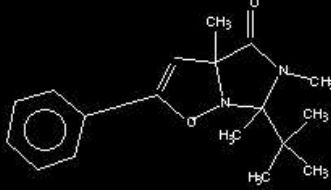

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Rotation Translation
56 0 3
5.0 0.20
X Y Z X Y Z
Set 3D Display... Reset

Comment interroger sa propre base ?

Activation de la base

Prepare Inhouse Database(s) for use in ConQuest

Activating an Inhouse Database for use with ConQuest

Directory containing databases */usr4/people/cbailly/csd_data/Bases-donnees*

Database to activate

Database Name (e.g. 'Inhouse1')

Database Version (e.g. '1.1')

Database Date (e.g. 'April 2001')

Search/Display Order

Activation de la base

Prepare Inhouse Database(s) for use in ConQuest

Activating an Inhouse Database for use with ConQuest

Directory containing databases */usr4/people/cbailly/csd_data/Bases-donnees*

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Database to activate

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Database Version (e.g. '1.1')

Database Date (e.g. 'April 2001')

Search/Display Order

Interrogation via Conquest

➤ Interrogation possible par :

Interrogation via Conquest

- Interrogation possible par :
 - Fragments

Interrogation via Conquest

- Interrogation possible par :
 - Fragments
 - Nom du responsable

Interrogation via Conquest

- Interrogation possible par :
 - Fragments
 - Nom du responsable
 - Noms des auteurs

Interrogation via Conquest

- Interrogation possible par :
 - Fragments
 - Nom du responsable
 - Noms des auteurs
 - Année

Interrogation via Conquest

- Interrogation possible par :
 - Fragments
 - Nom du responsable
 - Noms des auteurs
 - Année
 - Paramètres de maille, ...

Interrogation via Conquest

- Interrogation possible par :
 - Fragments
 - Nom du responsable
 - Noms des auteurs
 - Année
 - Paramètres de maille, ...
- Possibilité de recherche simultanée dans plusieurs bases (CSD + bases internes)