Bases de données internes

Sommaire

Sommaire

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

Sommaire

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

Sommaire

- 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

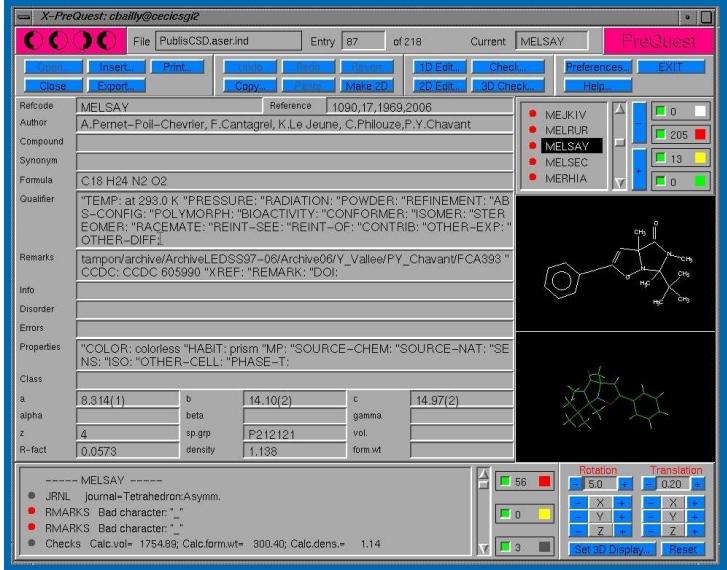
- Base pouvant regrouper l'ensemble des structures réalisées dans le laboratoire
  - Structures publiées,
  - Structures en attente,
  - Structures qui ne seront pas publiées, …
- Recherche d'une structure facilitée
- Recherche par maille permettant d'éviter les doublons

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: cbailly@cecicsgi2
PreQuest
MELSAY
Author
A.Pernet–Poil–Chevrier, F.Cantagrel, K.Le Jeune, C.Philouze,P.Y.Chavant
Compound
Synonym
Formula
C18 H24 N2 O2
Qualifier
Remarks
Info
Disorder
Errors
Properties
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
MELSAY
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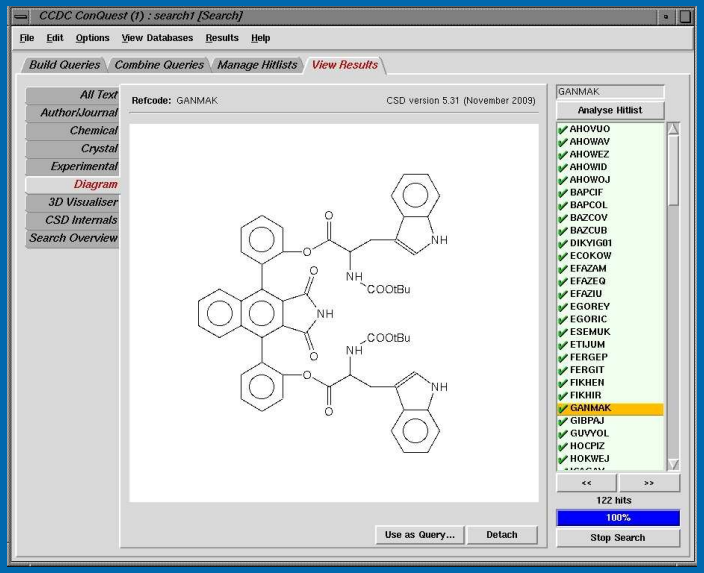
RMARKS Bad character: "_"
RMARKS Bad character: "_"
Checks Calc.vol= 1754.89; Calc.form.wt= 300.40; Calc.dens.= 1.14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Combine Queries
Manage Hitlists
View Results
All Text
Author/Journal
Chemical
Crystal
Experimental
Diagram
3D Visualiser
CSD Internals
Search Overview
Refcode: GANMAK
CSD version 5.31 (November 2009)
Analyse Hitlist
AHOVUO
AHOWAV
AHOWEZ
AHOWID
AHOWOJ
BAPCIF
BAPCOL
BAZCOV
BAZCUB
DIKYIG01
ECOKOW
EFAZAM
EFAZEQ
EFAZIU
EGOREY
EGORIC
ESEMUK
ETIJUM
FERGEP
FERGIT
FIKHEN
FIKHIR
GANMAK
GIBPAJ
GUVVOL
HOCPIZ
HOKWEJ
122 hits
100%
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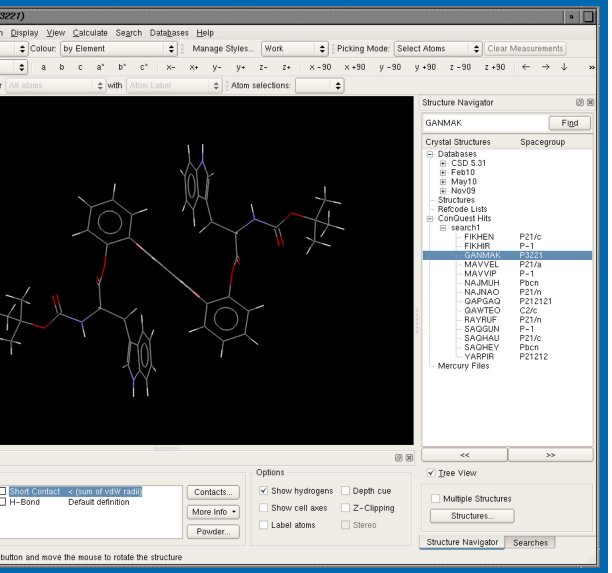
Use as Query...
Detach


GANMAK (P3221)
Structure Navigator
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
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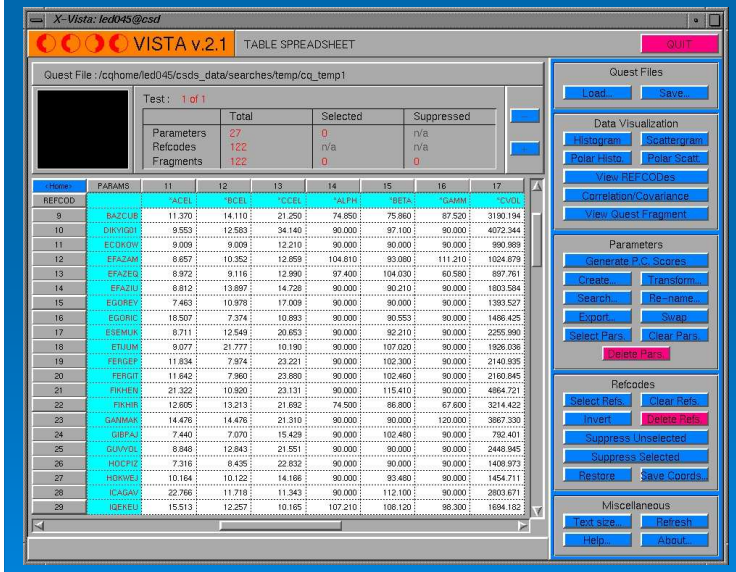
Mercury Files
Display Options
Structure Navigator
Searches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VISTA v.2.1
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Selected
Suppressed
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Refcodes 122 n/a n/a
Fragments 122 0 0
Quest Files
Load...
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.
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Invert
Delete Refs.
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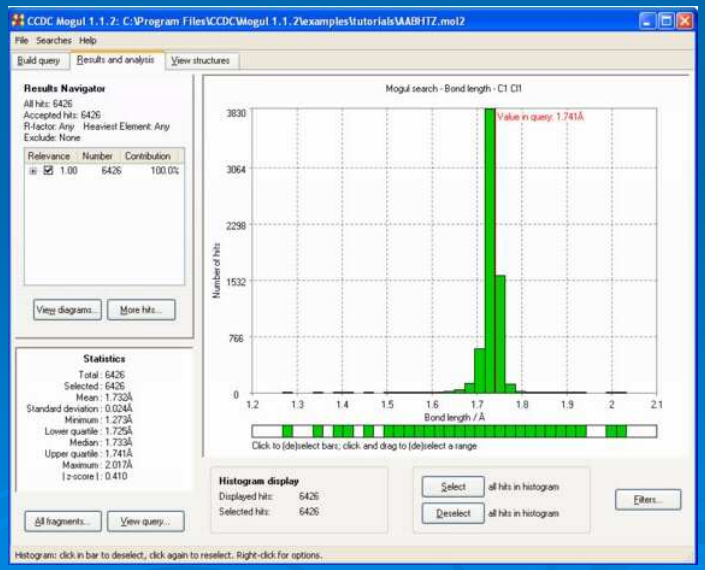
Suppress Selected
Restore
Save Coords...
Miscellaneous
Text size...
Refresh
Help...
About...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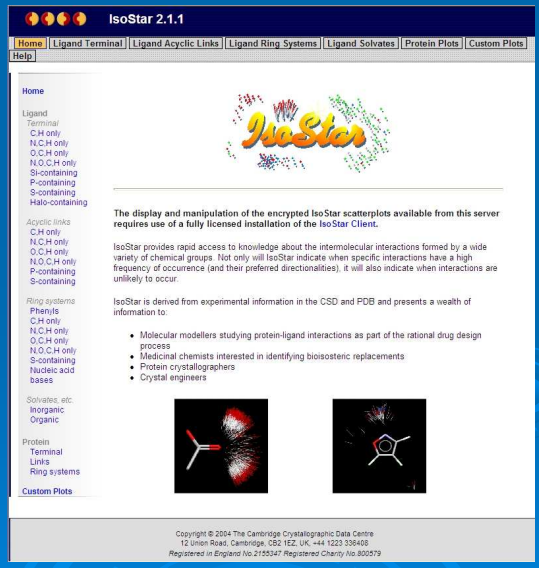
Results Navigator
Mogul search - Bond length - C1 C11
Value in query: 1.741Å
Bond length / Å
Number of hits
Statistics
Histogram display
Select
Deselect
Filters...
Histogram: click in bar to deselect, click again to reselect. Right-click for options.


IsoStar 2.1.1
Home
Ligand Terminal
Ligand Acyclic Links
Ligand Ring Systems
Ligand Solvates
Protein Plots
Custom Plots
Help
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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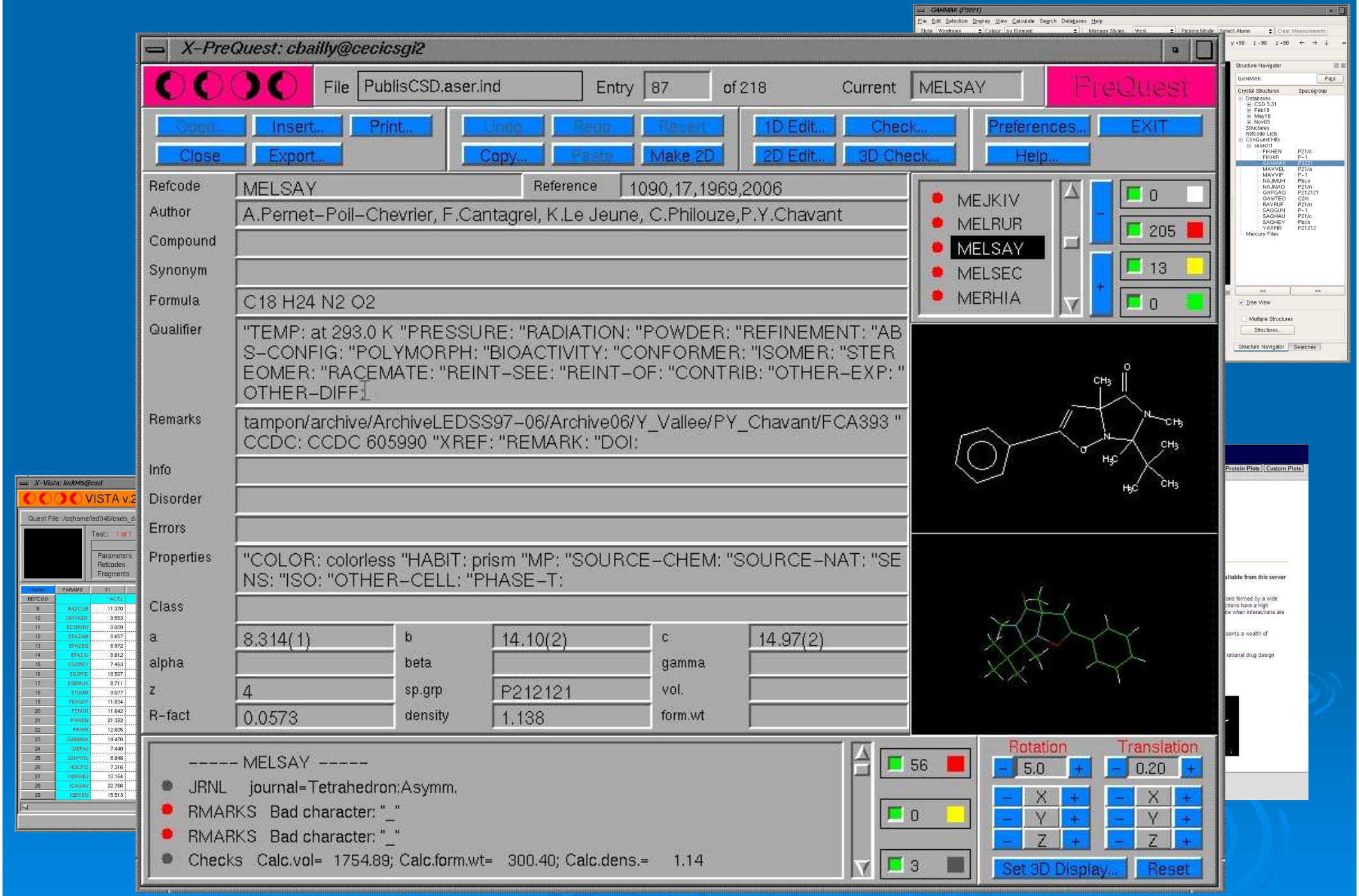
Crystal engineers


X-PreQuest: chailly@cecicsgi2
File PublisCSD.aser.ind
Entry 87
of 218
Current MELSAY
PreQuest
Open...
Insert...
Print...
Close
Export...
Undo
Redo
Revert
Copy...
Paste
Make 2D
1D Edit...
Check...
2D Edit...
3D Check...
Preferences...
EXIT
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:
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Info
Disorder
Errors
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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
MELRUR
MELSAY
MELSEC
MERHIA
0
205
13
0
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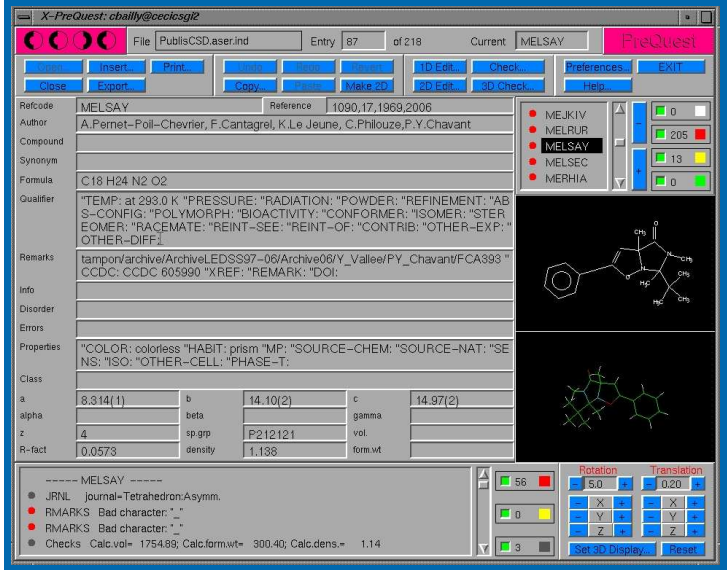
JRNL journal=Tetrahedron:Asymm.
RMARKS Bad character: "_"
RMARKS Bad character: "_"
Checks Calc.vol= 1754.89; Calc.form.wt= 300.40; Calc.dens.= 1.14
56
0
3
Rotation
5.0
Translation
0.20
X
Y
Z
Set 3D Display...
Reset
GANMAK (P3221)
Structure Navigator
Crystal Structures
Spacegroup
Databases
Refcode Lists
ConQuest Hits
Structures
Mercury Files
Tree View
Multiple Structures
Structures...
Structure Navigator
Searches
X-Vista: led045@csd
VISTA v.2
Quest File : /cqhome/led045/csds_d
Test : 1 of 1
Parameters
Refcodes
Fragments
Protein Plots
Custom Plots


X-PreQuest: cbailly@cecicsgi2
PreQuest
Refcode MELSAY
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:
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Disorder
Errors
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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
MELSAY
JRNL journal=Tetrahedron:Asymm.
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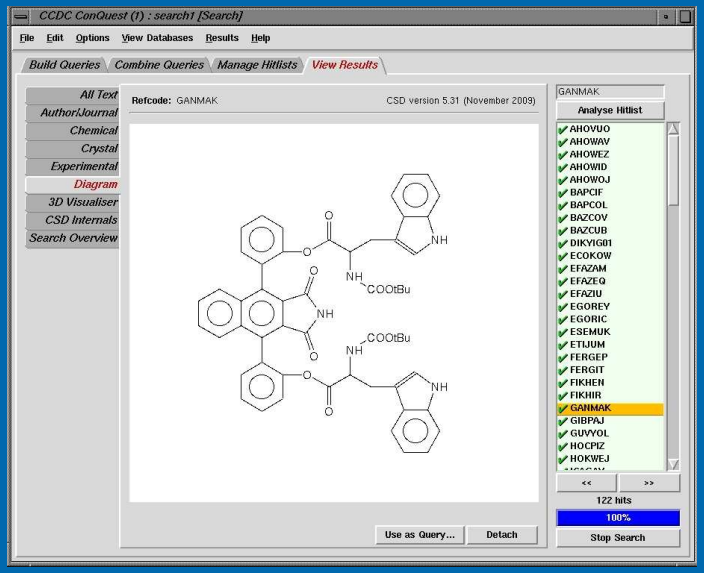
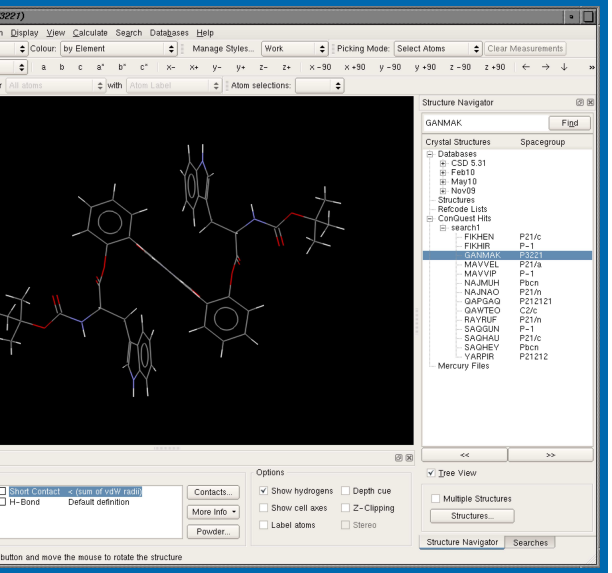
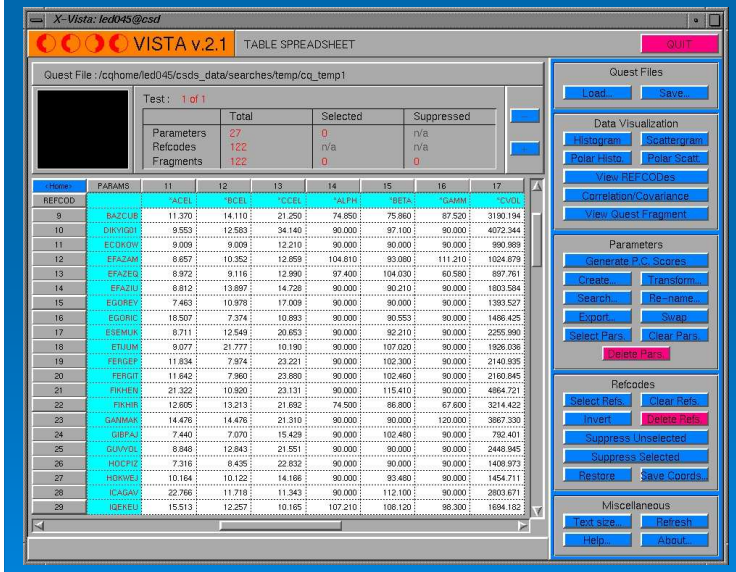
RMARKS Bad character: "_"
Checks Calc.vol= 1754.89; Calc.form.wt= 300.40; Calc.dens.= 1.14


CCDC ConQuest (1) : search1 [Search]
Build Queries
Combine Queries
Manage Hitlists
View Results
Refcode: GANMAK
CSD version 5.31 (November 2009)
Analyse Hitlist
122 hits
100%
Stop Search
Use as Query...
Detach


GANMAK (P3221)
Structure Navigator
Display Options


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
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Selected
Suppressed
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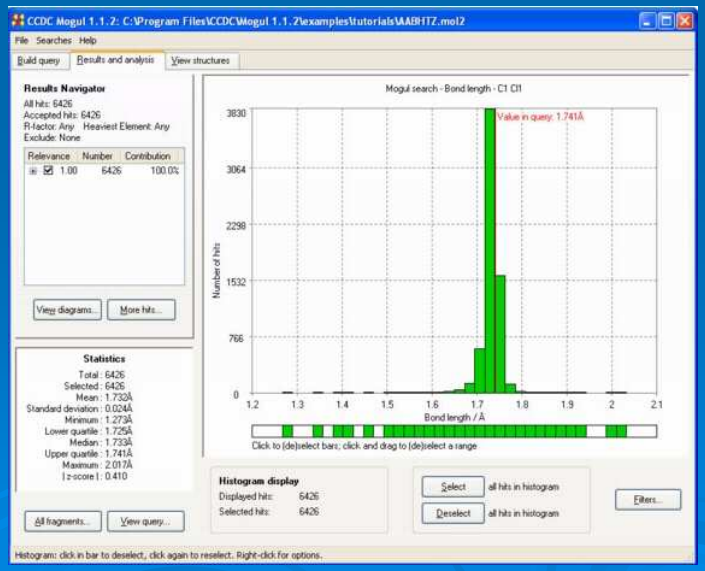
Quest Files
Data Visualization
Parameters
Refcodes
Miscellaneous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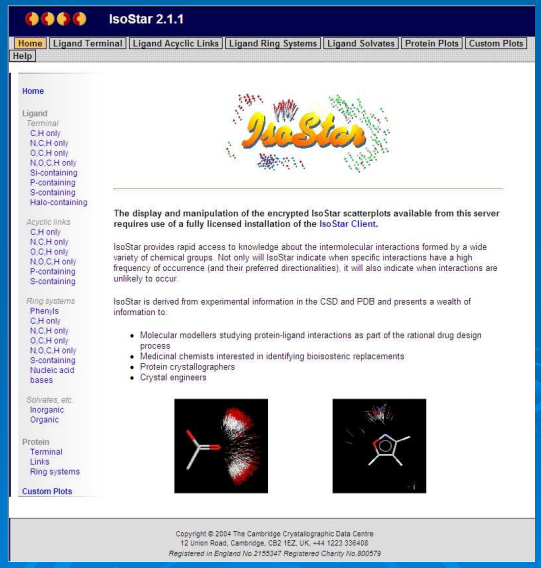
Results Navigator
Statistics
Mogul search - Bond length - C1 Cl1
Bond length / Å
Number of hits
Histogram display


IsoStar 2.1.1
Home
Ligand Terminal
Ligand Acyclic Links
Ligand Ring Systems
Ligand Solvates
Protein Plots
Custom Plots
Help
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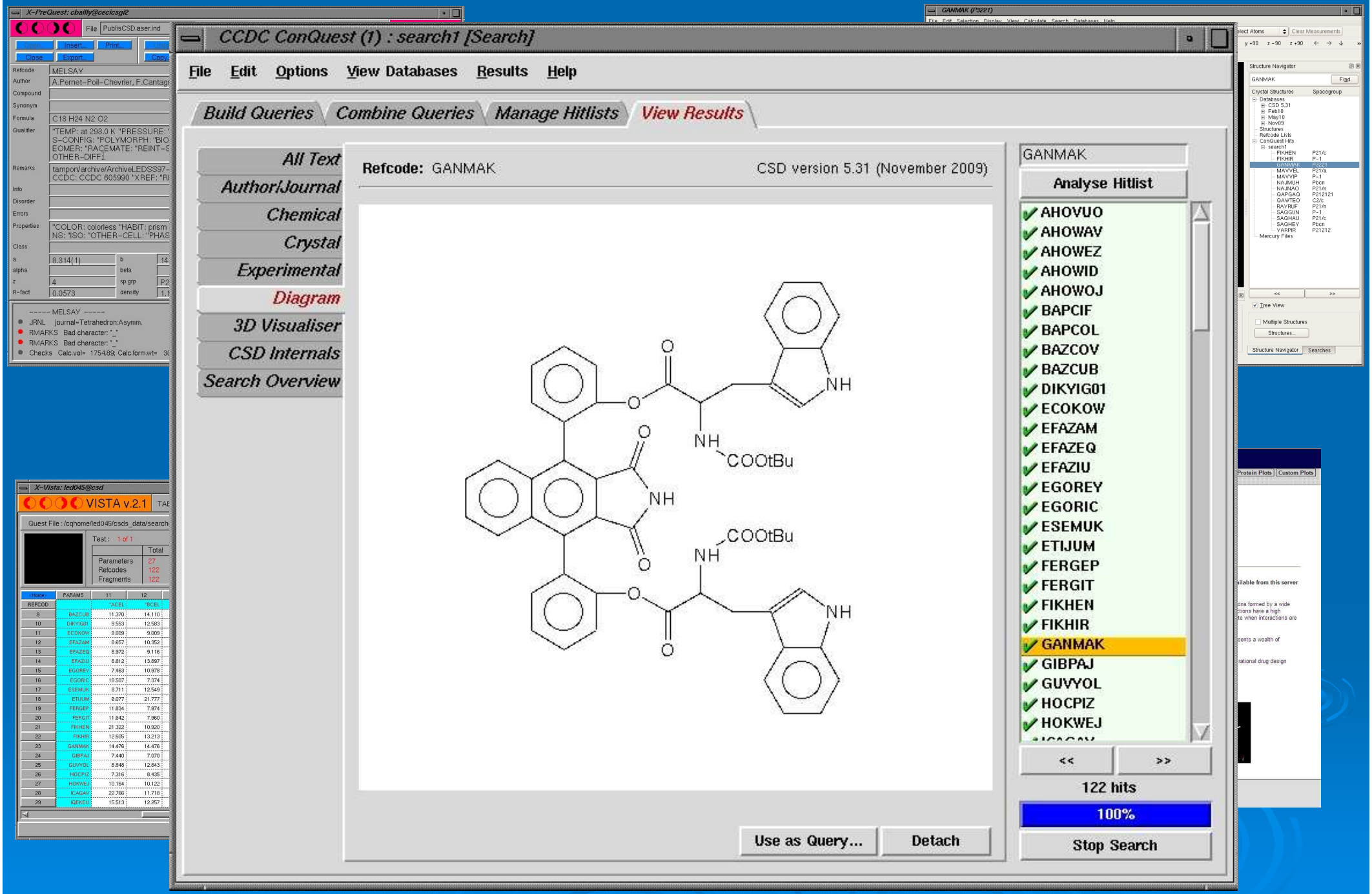
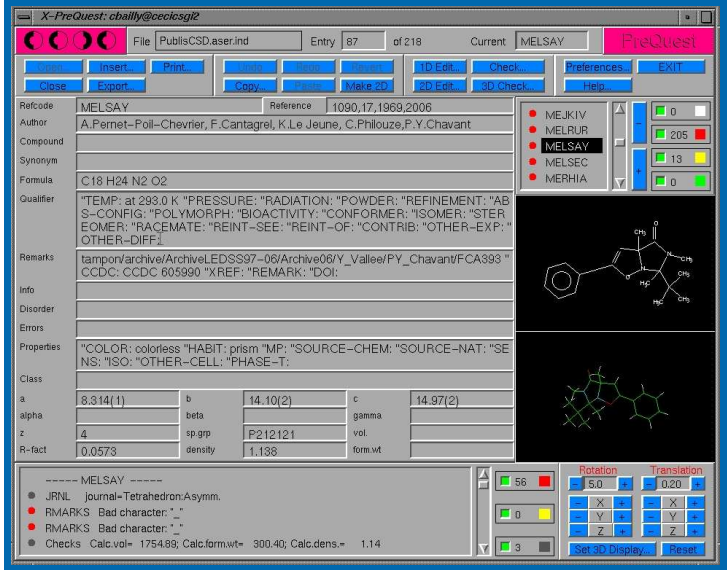

CCDC ConQuest (1) : search1 [Search]
File Edit Options View Databases Results Help
Build Queries Combine Queries Manage Hitlists View Results
All Text
Author/Journal
Chemical
Crystal
Experimental
Diagram
3D Visualiser
CSD Internals
Search Overview
Refcode: GANMAK
CSD version 5.31 (November 2009)
NH
COOtBu
GANMAK
Analyse Hitlist
AHOVUO
AHOWAV
AHOWEZ
AHOWID
AHOWOJ
BAPCIF
BAPCOL
BAZCOV
BAZCUB
DIKYIG01
ECOKOW
EFAZAM
EFAZEQ
EFAZIU
EGOREY
EGORIC
ESEMUK
ETIJUM
FERGEP
FERGIT
FIKHEN
FIKHIR
GANMAK
GIBPAJ
GUVYOL
HOCPIZ
HOKWEJ
<<
>>
122 hits
100%
Stop Search
Use as Query...
Detach
VISTA v.2.1


X-PreQuest: cbailly@cecicsgi2
PreQuest
Refcode MELSAY
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
MELSAY
JRNL journal=Tetrahedron:Asymm.
RMARKS Bad character: "_"
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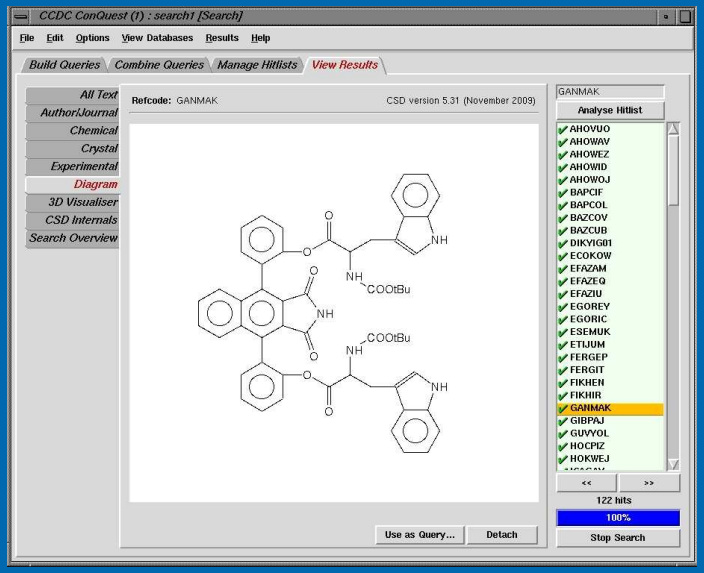
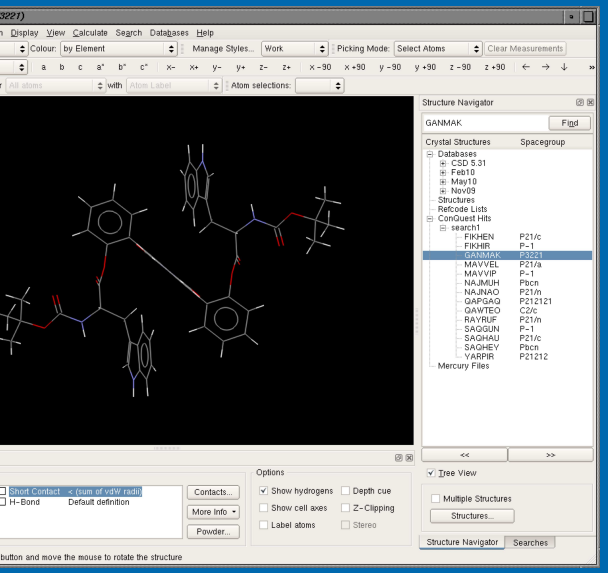
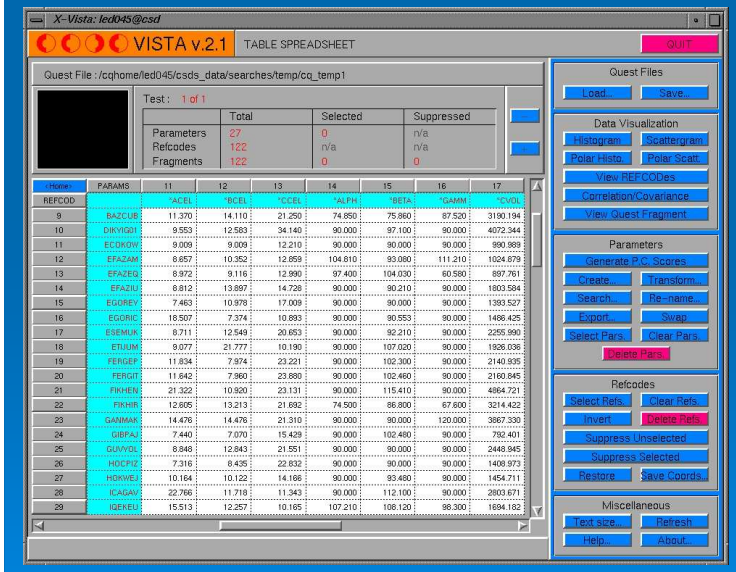

CCDC ConQuest (1) : search1 [Search]
Build Queries
Combine Queries
Manage Hitlists
View Results
Refcode: GANMAK
CSD version 5.31 (November 2009)
Analyse Hitlist
122 hits
100%
Stop Search
Use as Query...
Detach


GANMAK (P3221)
Structure Navigator
Display Options


X-Vista: led045@csd
VISTA v.2.1
TABLE SPREADSHEET
QUIT
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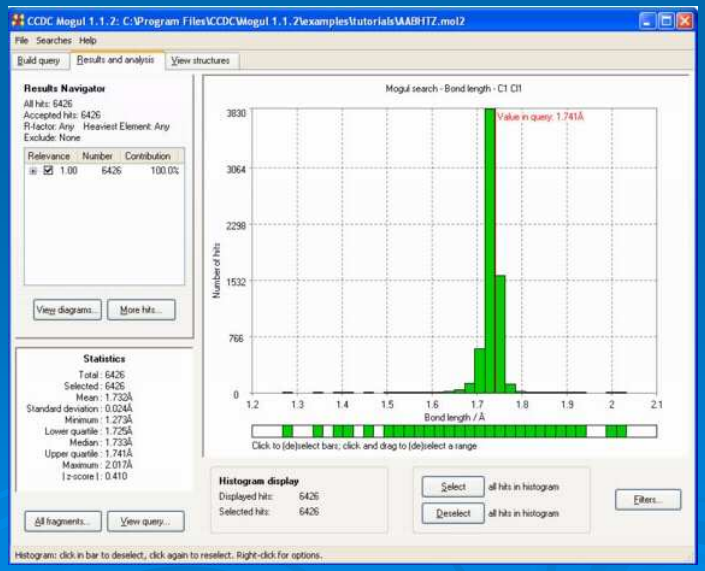
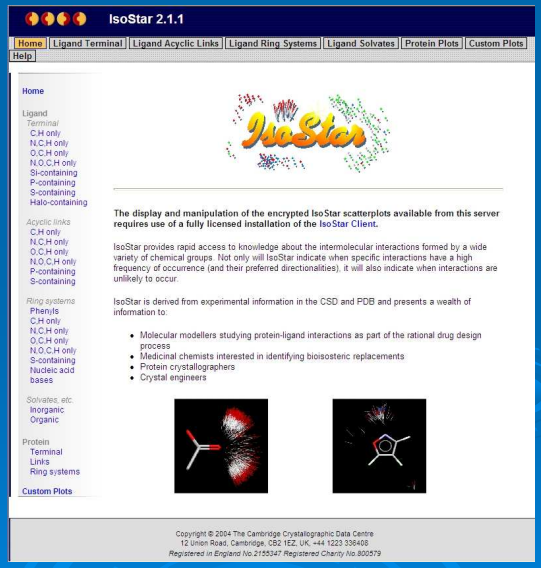
Test : 1 of 1
Total
Selected
Suppressed
Parameters 27 0 n/a
Refcodes 122 n/a n/a
Fragments 122 0 0
Quest Files
Data Visualization
Parameters
Refcodes
Miscellaneous


CCDC Mogul 1.1.2: C:\Program Files\CCDC\Mogul 1.1.2\examples\tutorials\AABHTZ.mol2
Results Navigator
Mogul search - Bond length - C1 C1
Value in query: 1.741Å
Bond length / Å
Statistics
Histogram display


IsoStar 2.1.1
Home
Ligand Terminal
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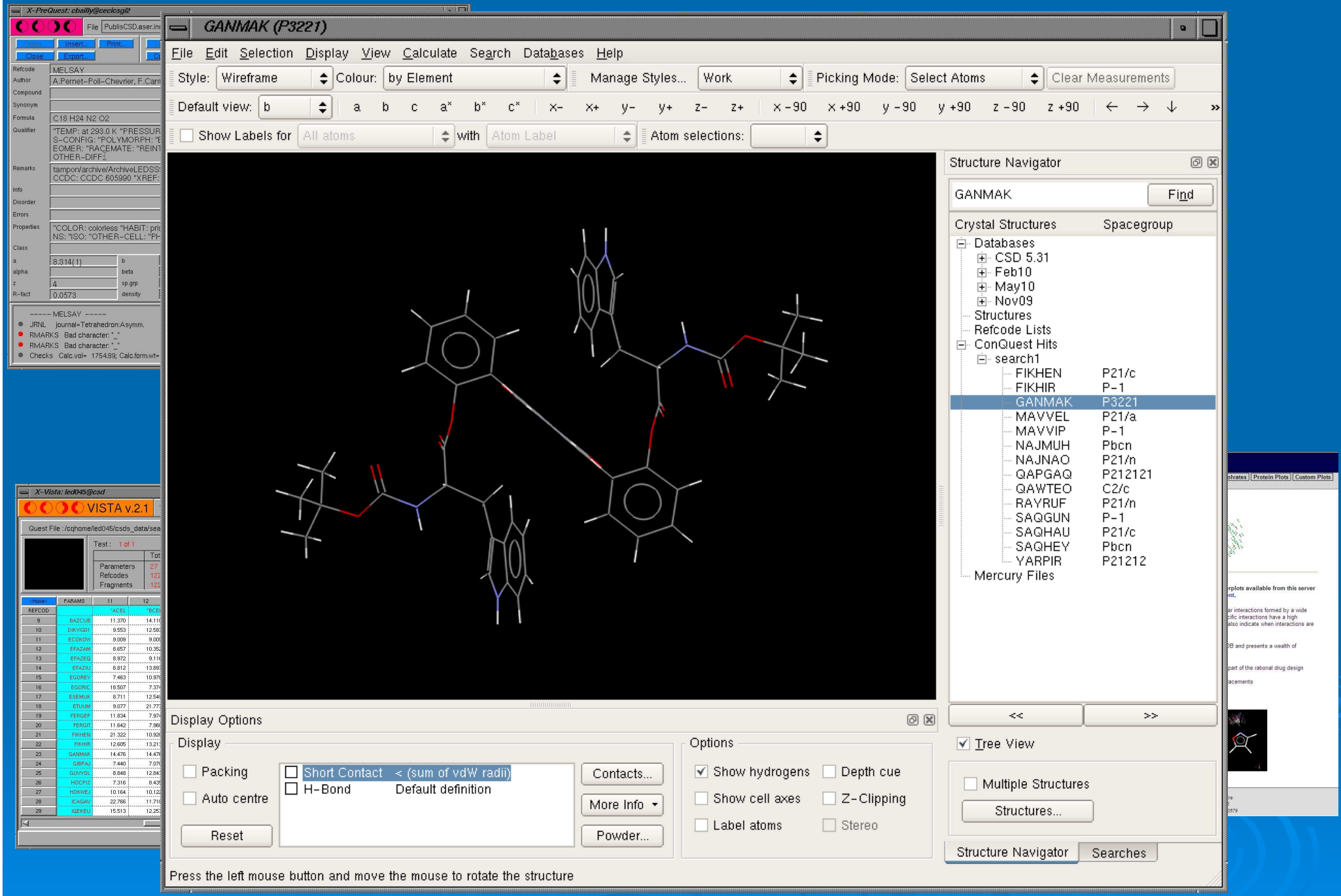
GANMAK (P3221)
File Edit Selection Display View Calculate Search Databases Help
Style: Wireframe
Colour: by Element
Manage Styles...
Work
Picking Mode: Select Atoms
Clear Measurements
Default view: b
Show Labels for All atoms with Atom Label
Atom selections:
Structure Navigator
GANMAK
Find
Crystal Structures
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
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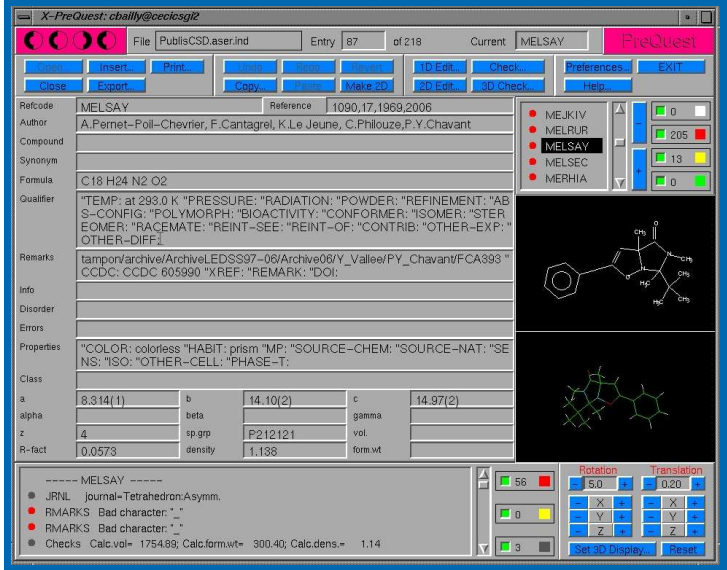
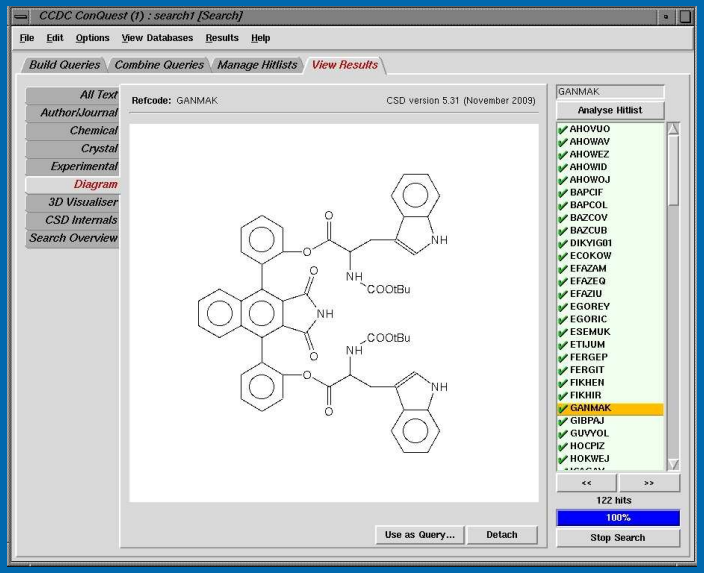
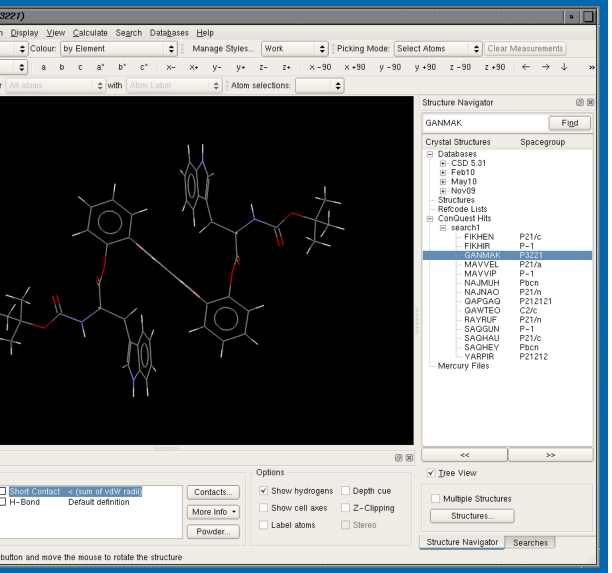
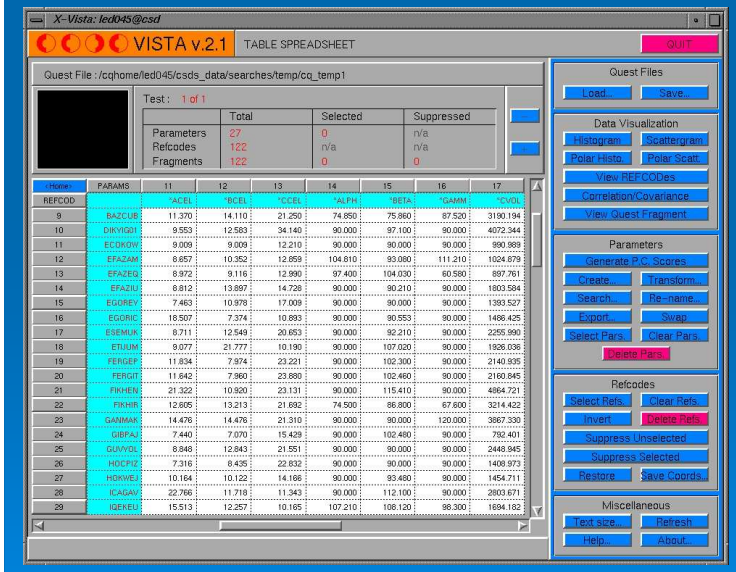
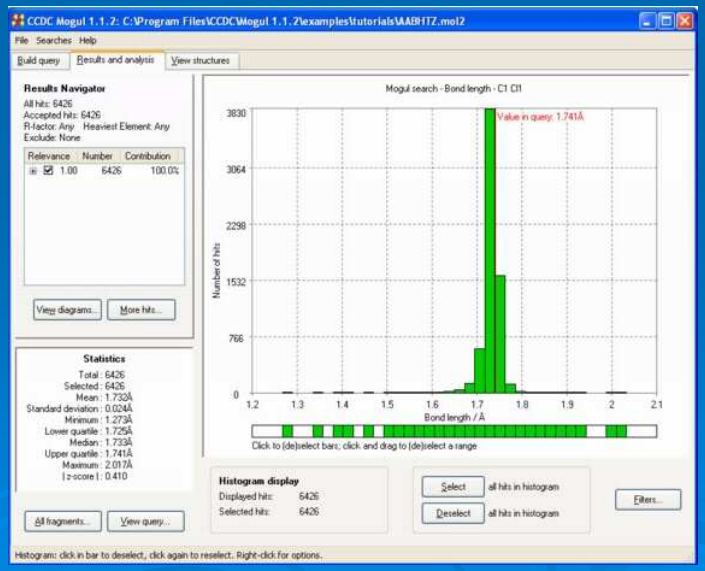
QAWTEO C2/c
RAYRUF P21/n
SAQGUN P-1
SAQHAU P21/c
SAQHEY Pbcn
YARPIR P21212
Mercury Files
Display Options
Display
Packing
Auto centre
Reset
Short Contact < (sum of vdW radii)
H-Bond Default definition
Contacts...
More Info
Powder...
Options
Show hydrogens
Depth cue
Show cell axes
Z-Clipping
Label atoms
Stereo
Tree View
Multiple Structures
Structures...
Structure Navigator
Searches
Press the left mouse button and move the mouse to rotate the structure
VISTA v.2.1

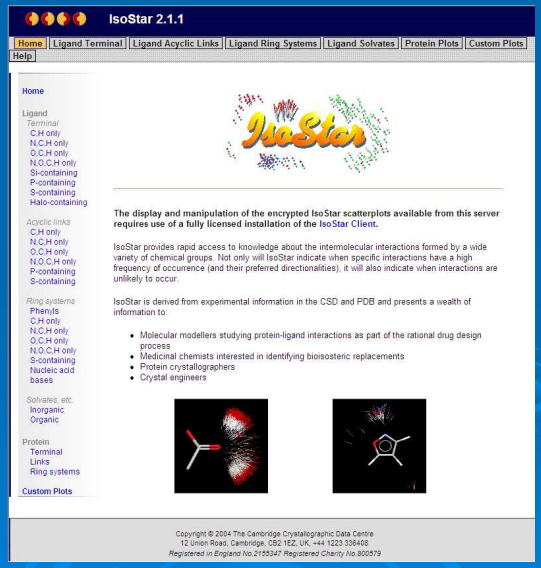

X-PreQuest: cbailly@cecicsgi2
PreQuest
Refcode MELSAY
Author A.Pernet-Poil-Chevrier, F.Cantagrel, K.Le Jeune, C.Philouze,P.Y.Chavant
Compound
Synonym
Formula C18 H24 N2 O2
Qualifier "TEMP: at 293.0 K "PRESSURE: "RADIATION: "POWDER: "REFINEMENT: "ABS-CONFIG: "POLYMORPH: "BIOACTIVITY: "CONFORMER: "ISOMER: "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
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


CCDC ConQuest (1) : search1 [Search]
Build Queries
Combine Queries
Manage Hitlists
View Results
Refcode: GANMAK
CSD version 5.31 (November 2009)
Analyse Hitlist
122 hits
100%
Stop Search
Use as Query...
Detach


GANMAK (P3221)
Structure Navigator
Display Options


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
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...


CCDC Mogul 1.1.2: C:\Program Files\CCDC\Mogul 1.1.2\examples\tutorials\AABHTZ.mol2
Results Navigator
Statistics
Mogul search - Bond length - C1 C1
Bond length / Å
Number of hits
Histogram display
Displayed hits: 6426
Selected hits: 6426
Select all hits in histogram
Deselect all hits in histogram
Filters...
All fragments...
View query...
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
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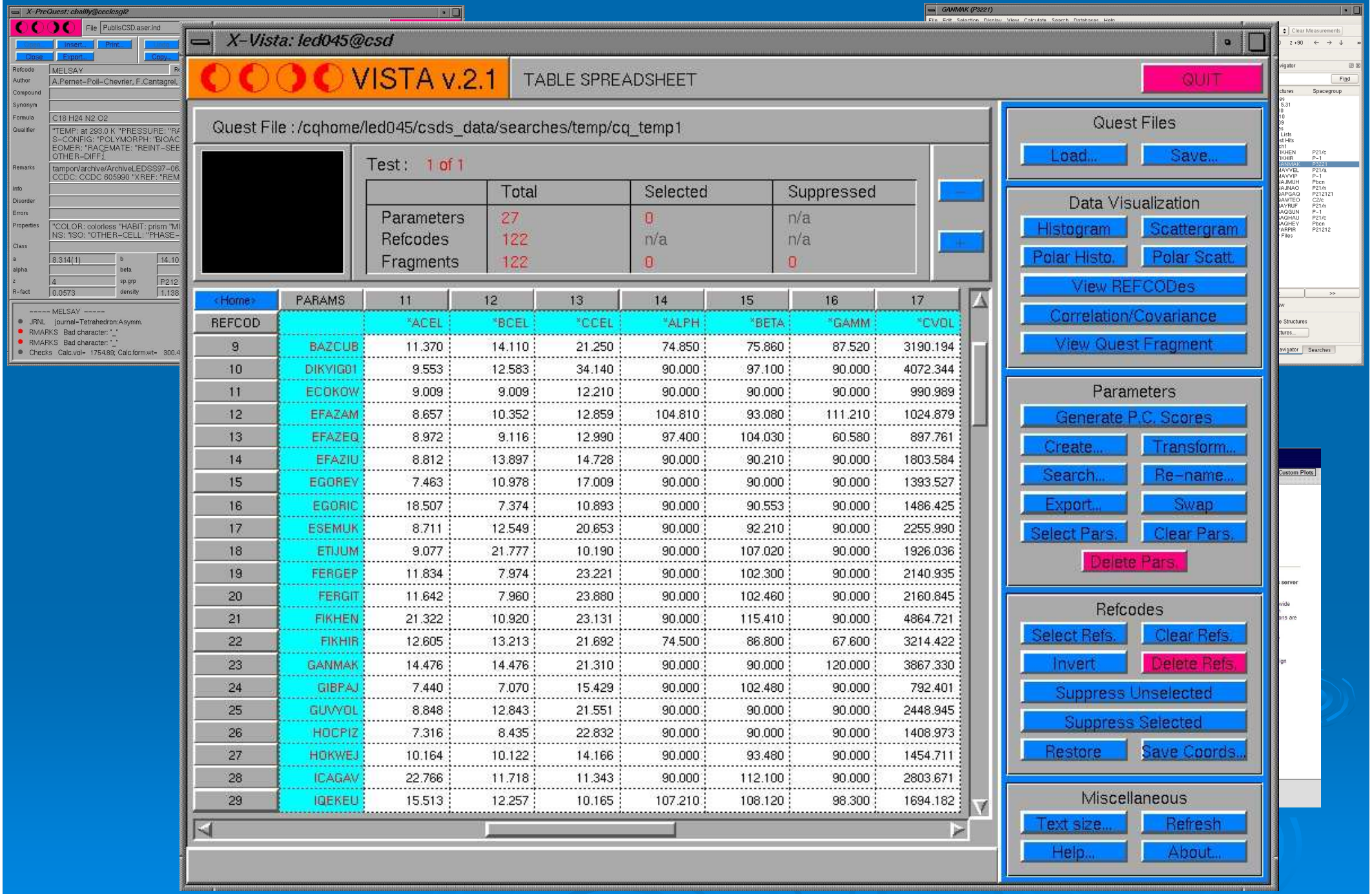
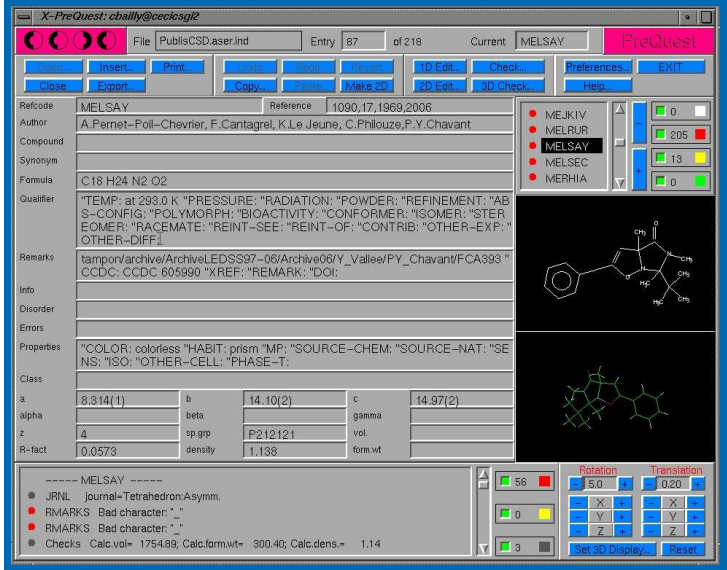
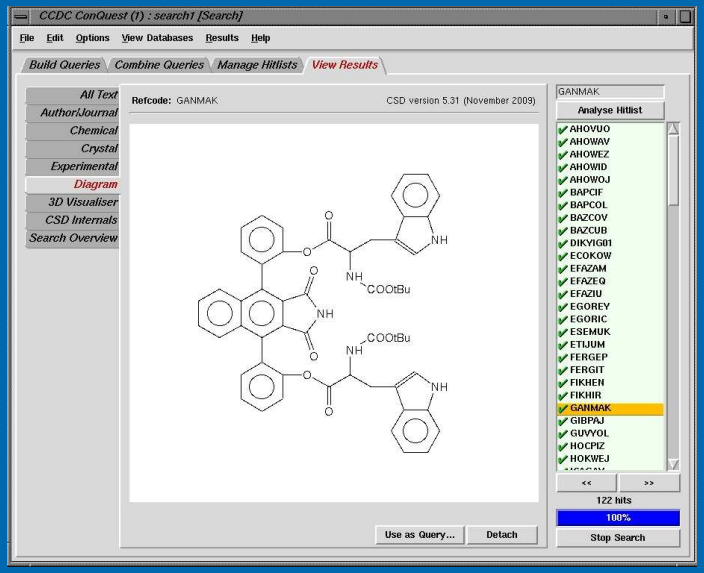
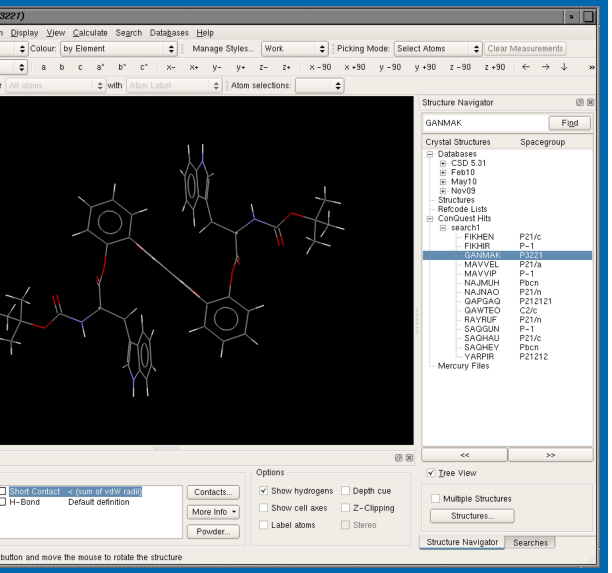
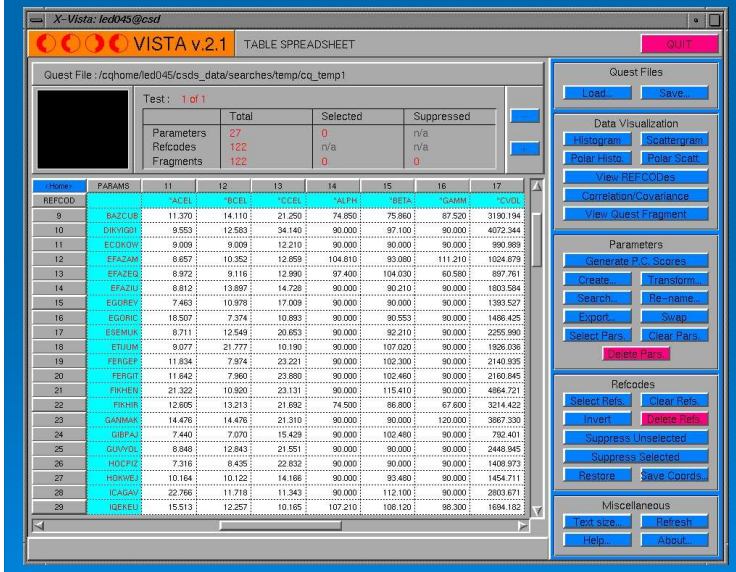


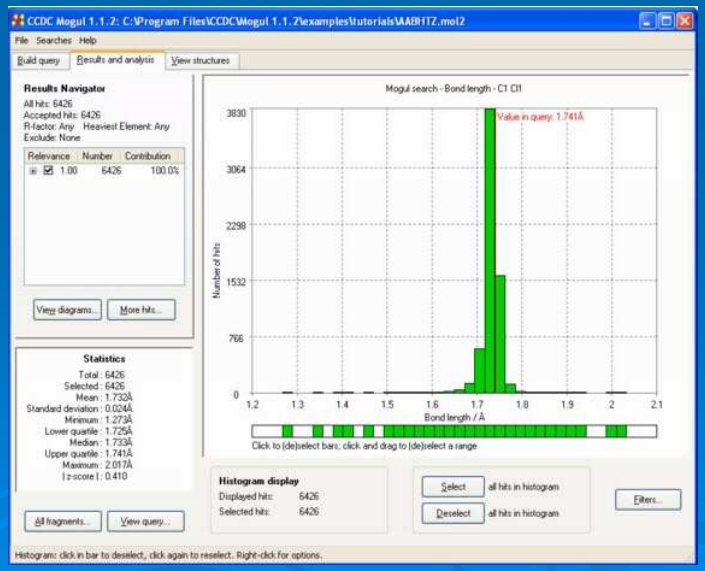
<Home>	PARAMS	11	12	13	14	15	16	17
REFCOD		*ACEL	*BCEL	*CCEL	*ALPH	*BETA	*GAMM	*CVOL
9	BAZCUB	11.370	14.110	21.250	74.850	75.860	87.520	3190.194
10	DIKVIG01	9.553	12.583	34.140	90.000	97.100	90.000	4072.344
11	ECOKOW	9.009	9.009	12.210	90.000	90.000	90.000	990.989
12	EFAZAM	8.657	10.352	12.859	104.810	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	23.880	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	GUVVOL	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

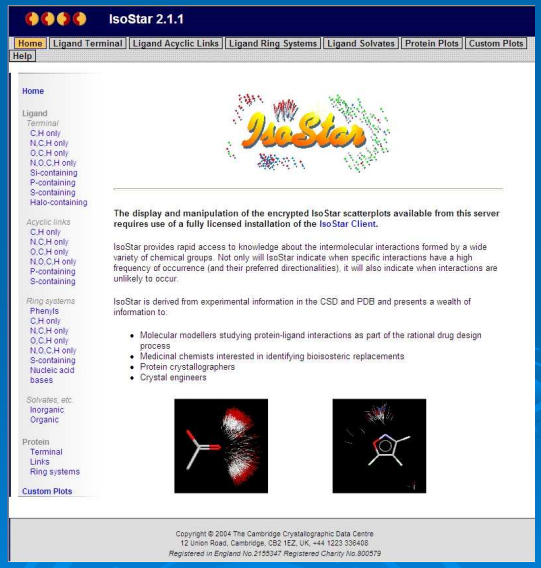

X-PreQuest: cbailly@cecicsgi2
PreQuest
MELSAY
Reference
1090,17,1969,2006
A.Pernet-Poil-Chevrier, F.Cantagrel, K.Le Jeune, C.Philouze,P.Y.Chavant
C18 H24 N2 O2
8.314(1)
14.10(2)
14.97(2)
4
P212121
0.0573
1.138
JRNL journal=Tetrahedron:Asymm.
RMARKS Bad character: "_"
RMARKS Bad character: "_"
Checks Calc.vol= 1754.89; Calc.form.wt= 300.40; Calc.dens.= 1.14


CCDC ConQuest (1) : search1 [Search]
Build Queries
Combine Queries
Manage Hitlists
View Results
Refcode: GANMAK
CSD version 5.31 (November 2009)
Analyse Hitlist
122 hits
100%
Stop Search
Use as Query...
Detach


GANMAK (P3221)
Structure Navigator
Display Options


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


CCDC Mogul 1.1.2: C:\Program Files\CCDC\Mogul 1.1.2\examples\tutorials\AAEHTZ.mol2
Results Navigator
Statistics
Mogul search - Bond length - C1 C1
Bond length / Å
Histogram display


IsoStar 2.1.1
Home
Ligand Terminal
Ligand Acyclic Links
Ligand Ring Systems
Ligand Solvates
Protein Plots
Custom Plots
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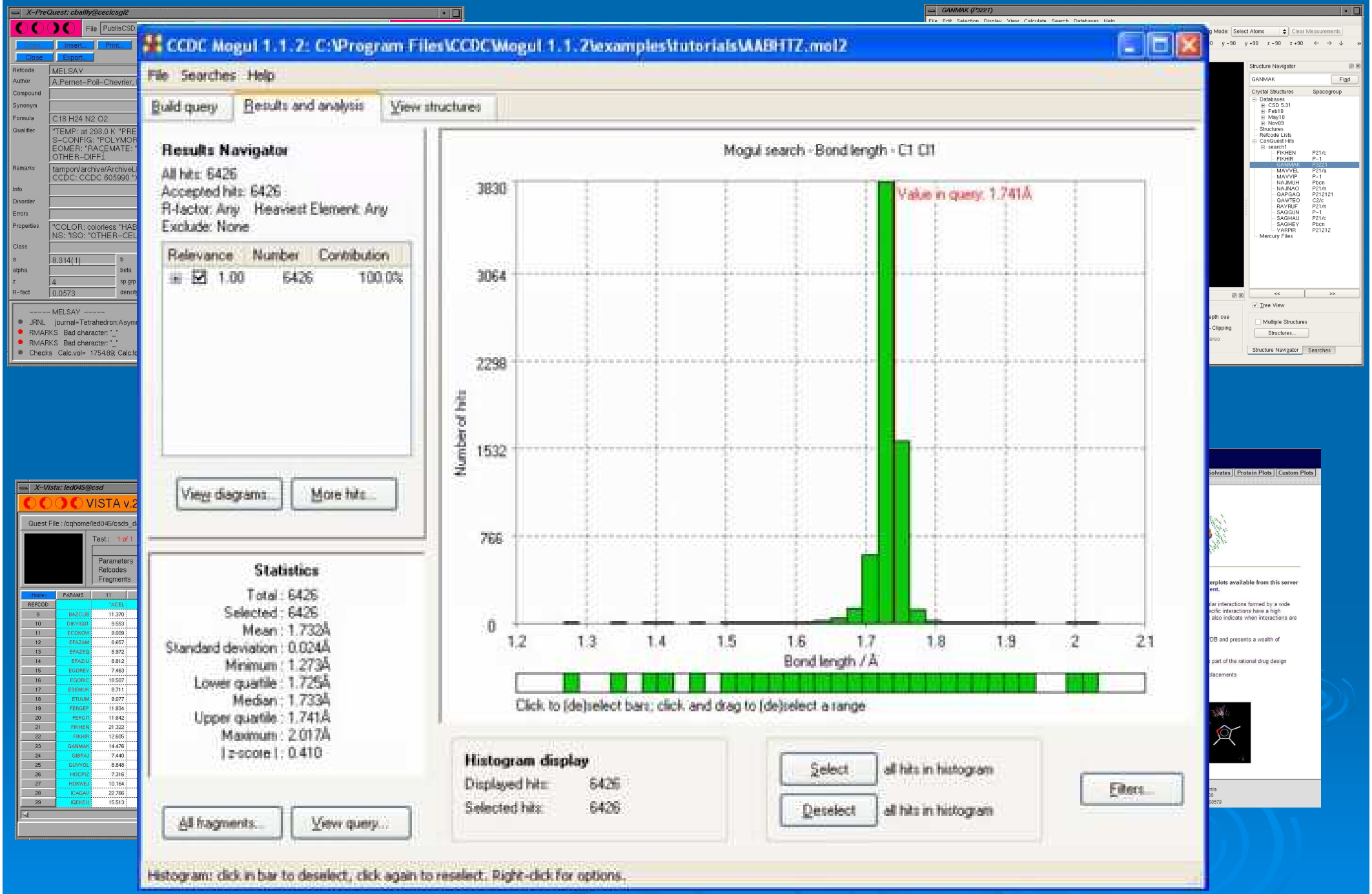
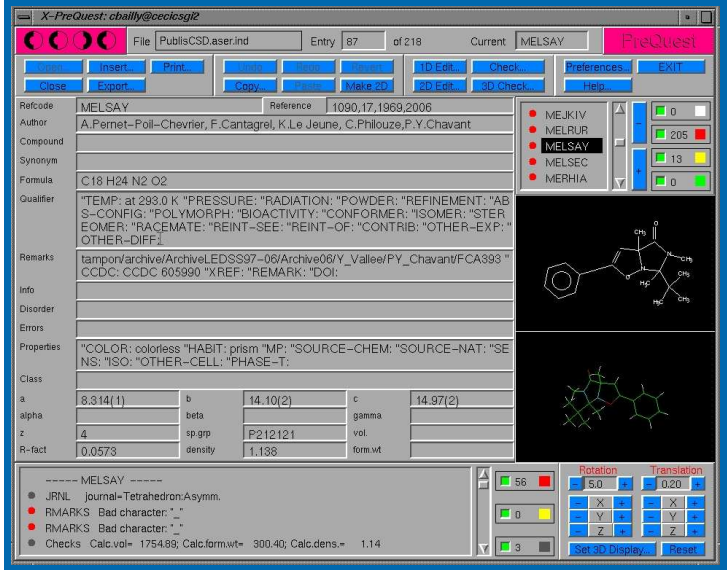

CCDC Mogul 1.1.2: C:\Program Files\CCDC\Mogul 1.1.2\examples\tutorials\AABHTZ.mol2
File Searches Help
Build query
Results and analysis
View structures
Results Navigator
All hits: 6426
Accepted hits: 6426
R-factor: Any Heaviest Element: Any
Exclude: None
Relevance Number Contribution
1.00 6426 100.0%
View diagrams...
More hits...
Statistics
Total : 6426
Selected : 6426
Mean : 1.732Å
Standard deviation : 0.024Å
Minimum : 1.273Å
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
Value in query: 1.741Å
Number of hits
3830
3064
2298
1532
766
0
1.2
1.3
1.4
1.5
1.6
1.7
1.8
1.9
2
2.1
Bond length / Å
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.


X-PreQuest: cbailly@cecicsgi2
PreQuest
MELSAY
A.Pernet–Poil–Chevrier, F.Cantagrel, K.Le Jeune, C.Philouze,P.Y.Chavant
C18 H24 N2 O2
8.314(1)
14.10(2)
14.97(2)
0.0573
1.138
P212121
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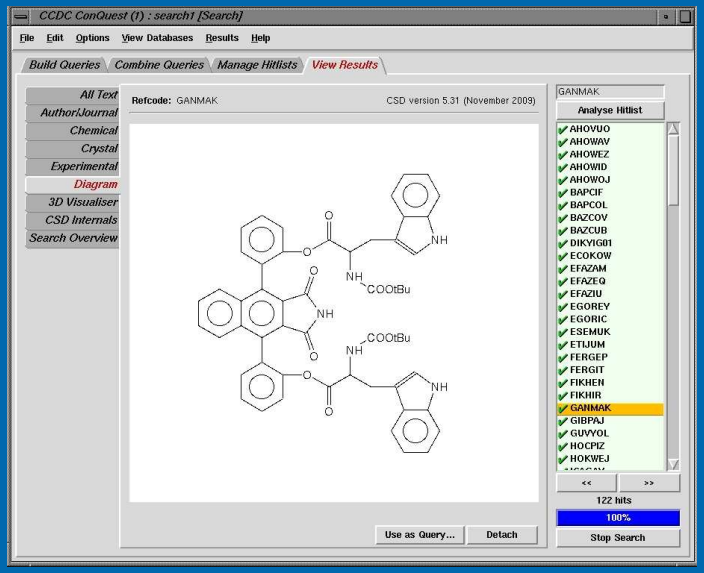
Checks Calc.vol= 1754.89; Calc.form.wt= 300.40; Calc.dens.= 1.14


CCDC ConQuest (1) : search1 [Search]
Build Queries
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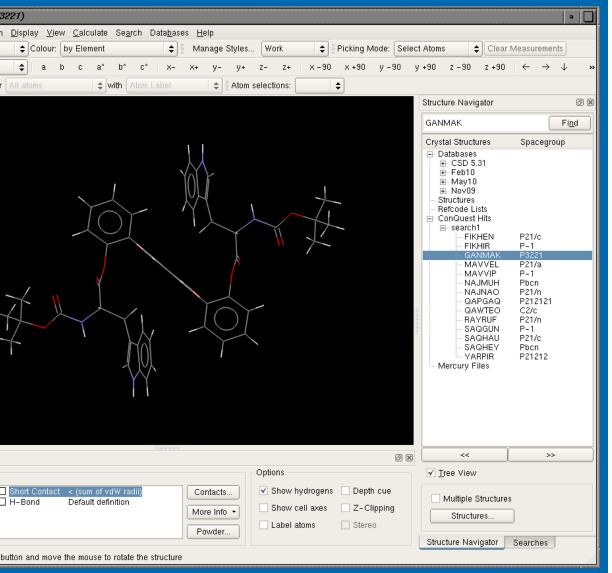
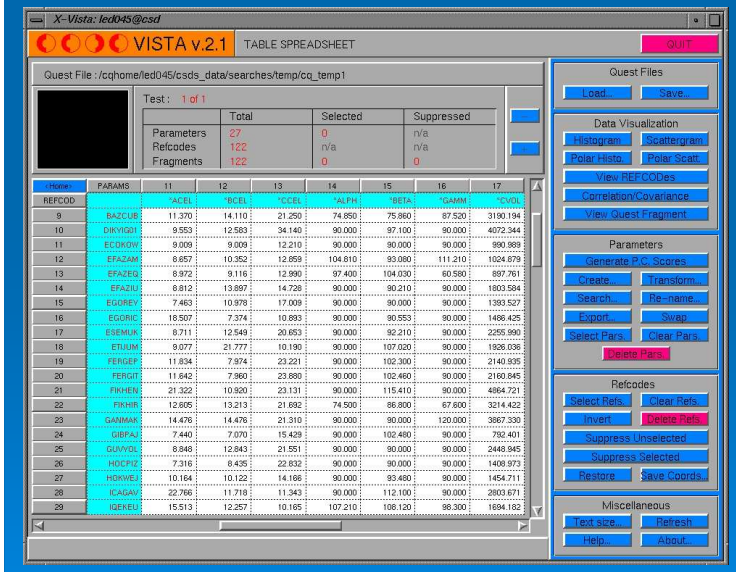
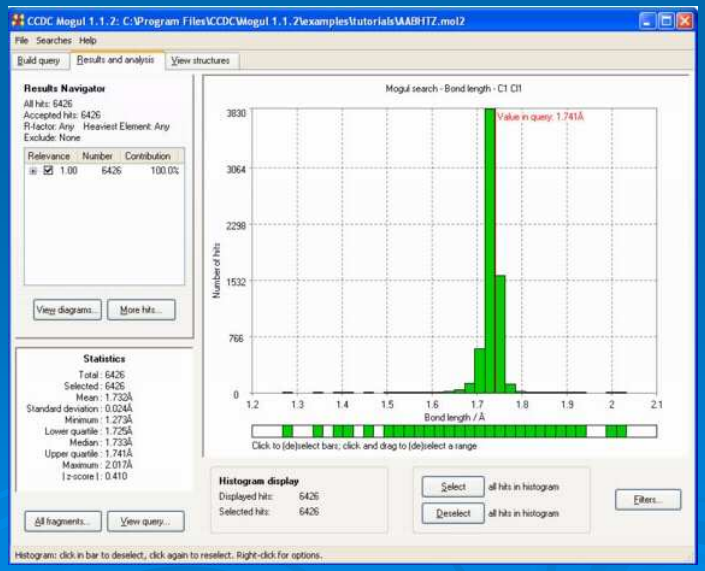
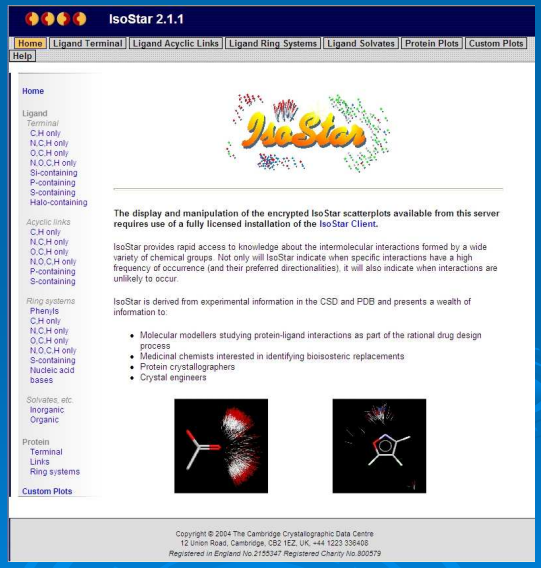
View Results
Refcode: GANMAK
CSD version 5.31 (November 2009)
Analyse Hitlist
122 hits
100%
Stop Search
Use as Query...
Detach


GANMAK (P3221)
Structure Navigator
Display Options


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
Quest Files
Data Visualization
Parameters
Refcodes
Miscellaneous


CCDC Mogul 1.1.2: C:\Program Files\CCDC\Mogul 1.1.2\examples\tutorials\AABHTZ.mol2
Results Navigator
Mogul search - Bond length - C1 C11
Bond length / Å
Statistics
Histogram display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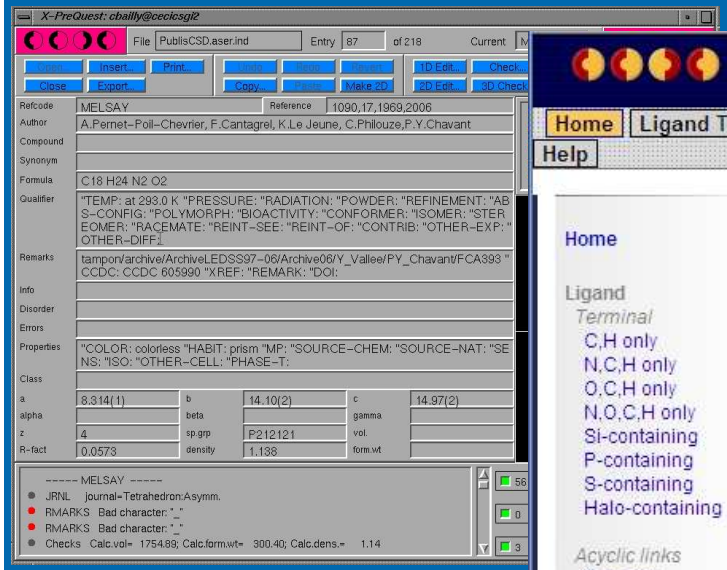

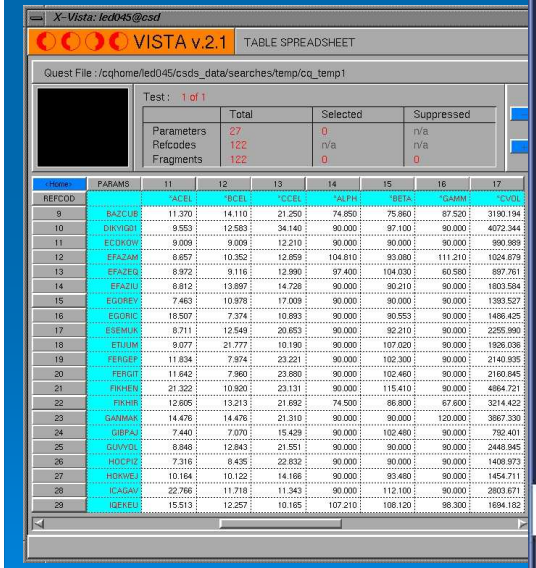

<Home>	PARAMS	11	12	13	14	15	16	17
REFCOD		*ACEL	*BCEL	*CCEL	*ALPH	*BETA	*GAMM	*CVOL
9	BAZCUB	11.370	14.110	21.250	74.850	75.860	87.520	3190.194
10	DIKYIG01	9.553	12.583	34.140	90.000	97.100	90.000	4072.344
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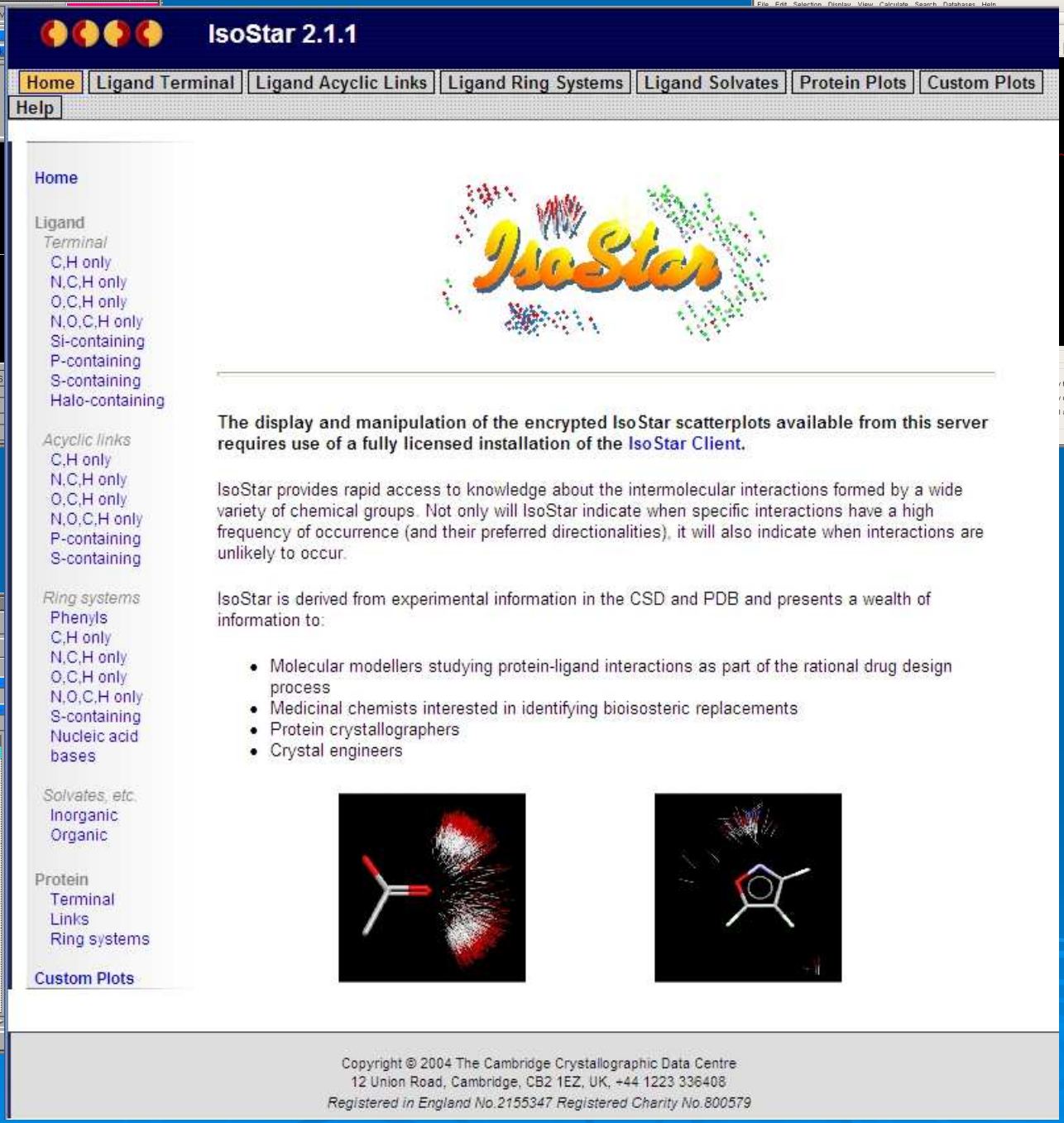
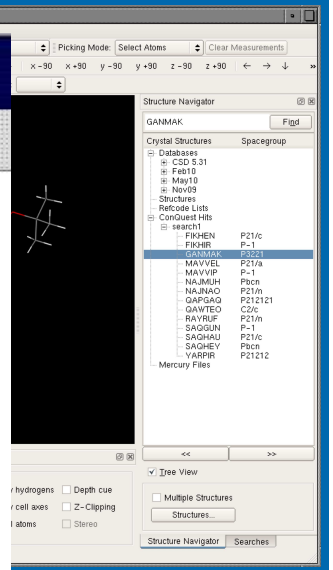
28	ICAGAY	22.766	11.718	11.343	90.000	112.100	90.000	2803.671
29	IQEKEU	15.513	12.257	10.165	107.210	108.120	98.300	1694.182





- 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)

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  - 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

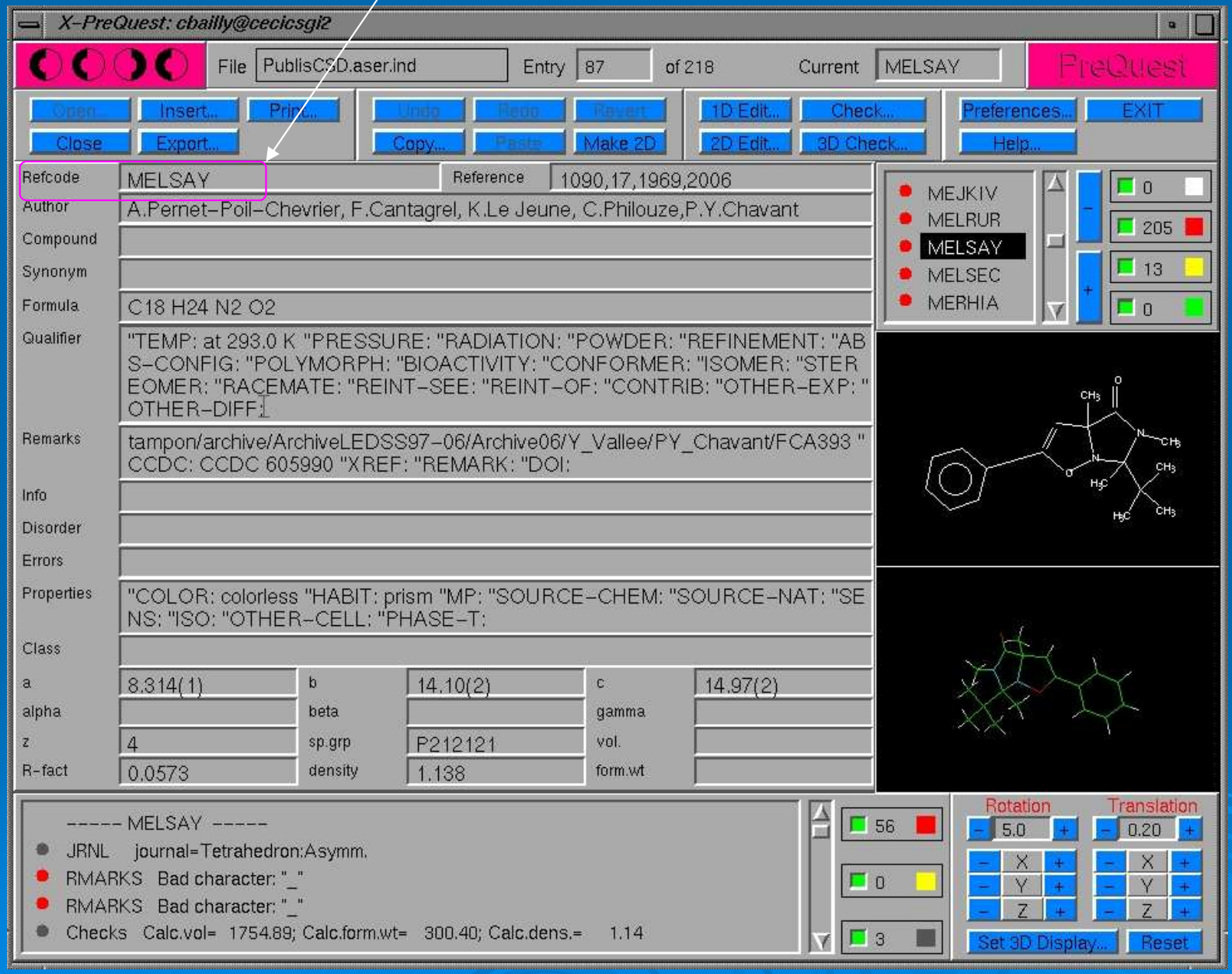
Prequest

- Format requis : CIF

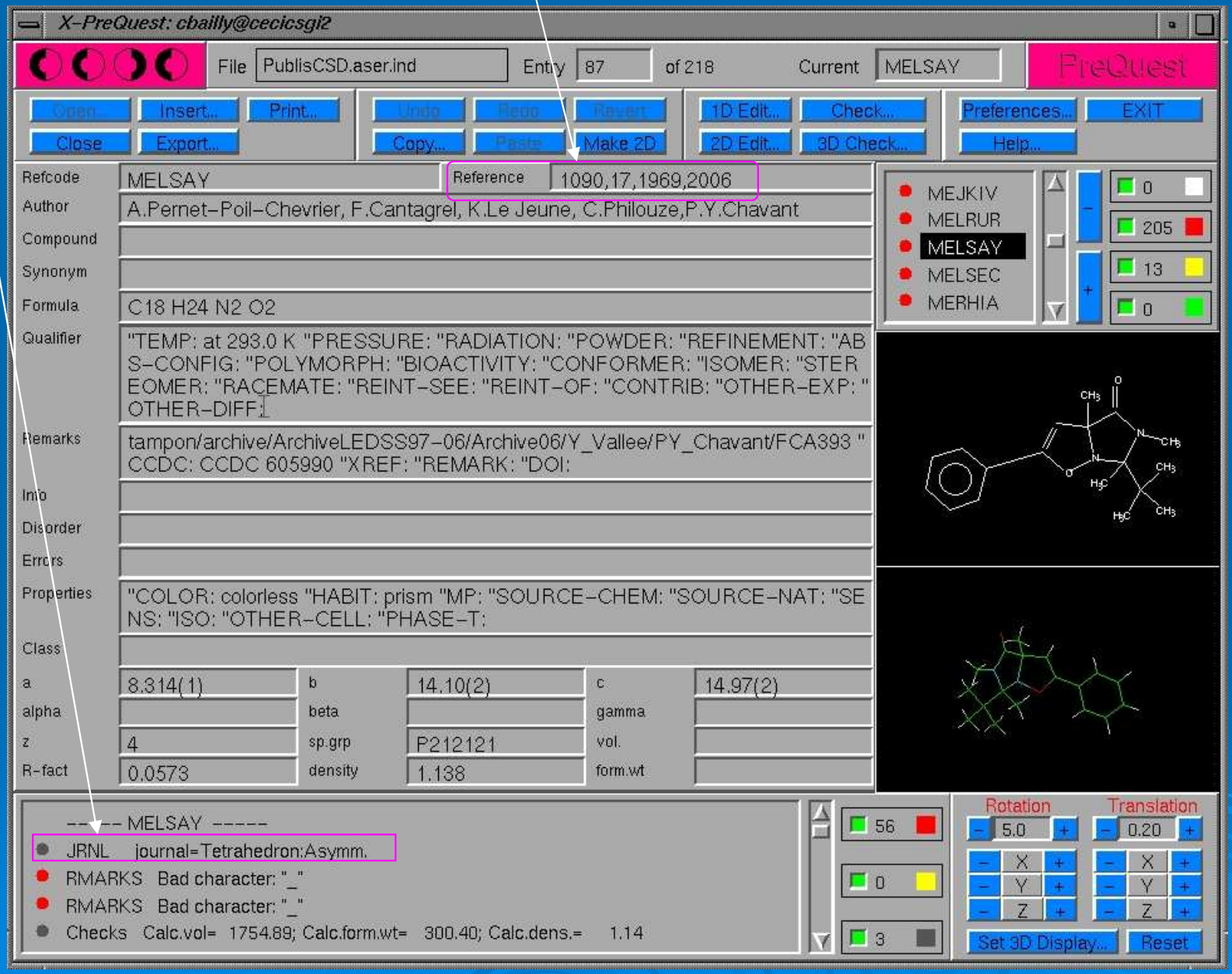
Prequest

- Format requis : CIF
- Plusieurs champs peuvent être renseignés

Refcode : N°incrémenté automatiquement / Référence CS D

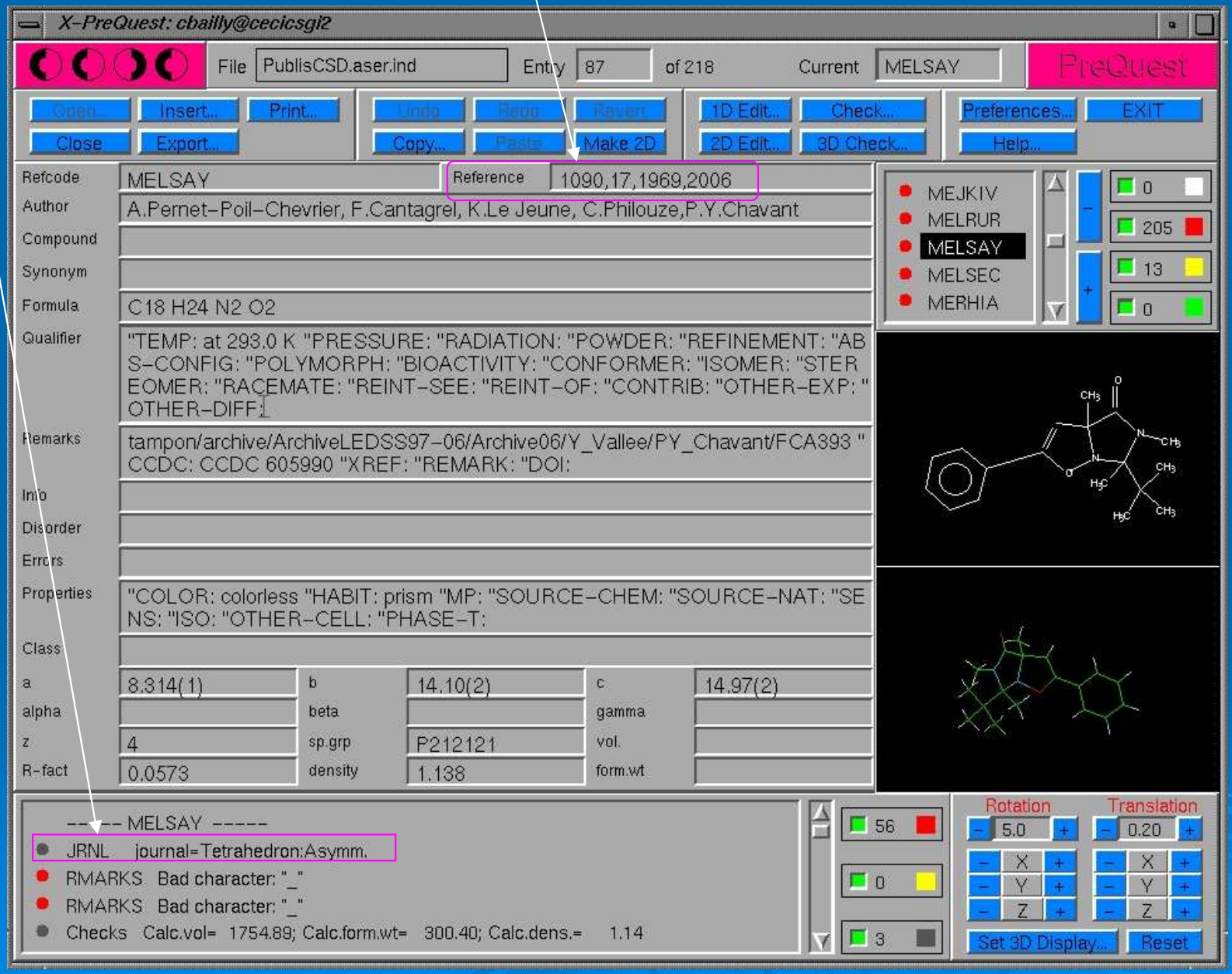


Référence du Journal : Nom, Volume, Page, Année

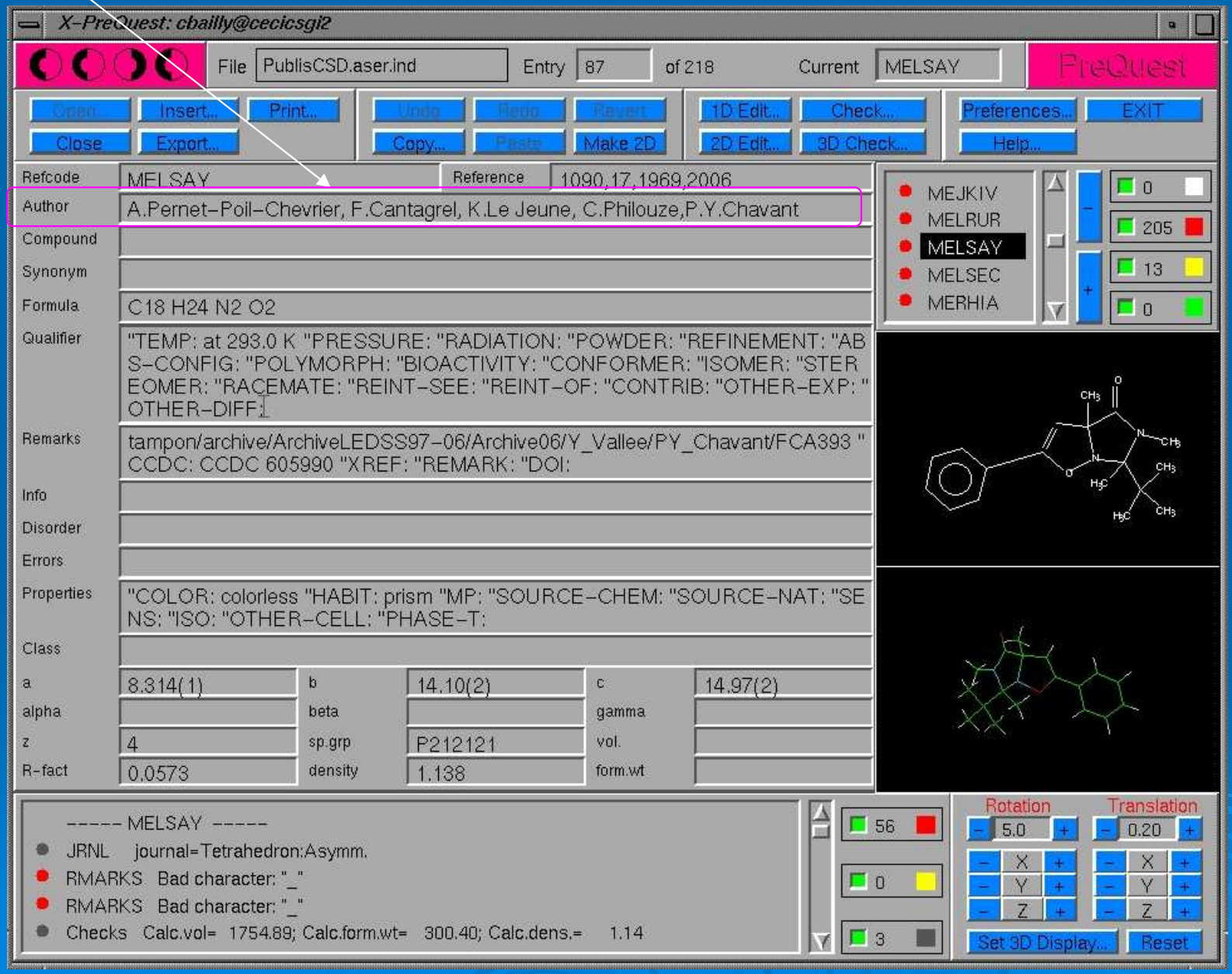


http://www.ccdc.cam.ac.uk/support/documentation/quest/volume3/z304.html

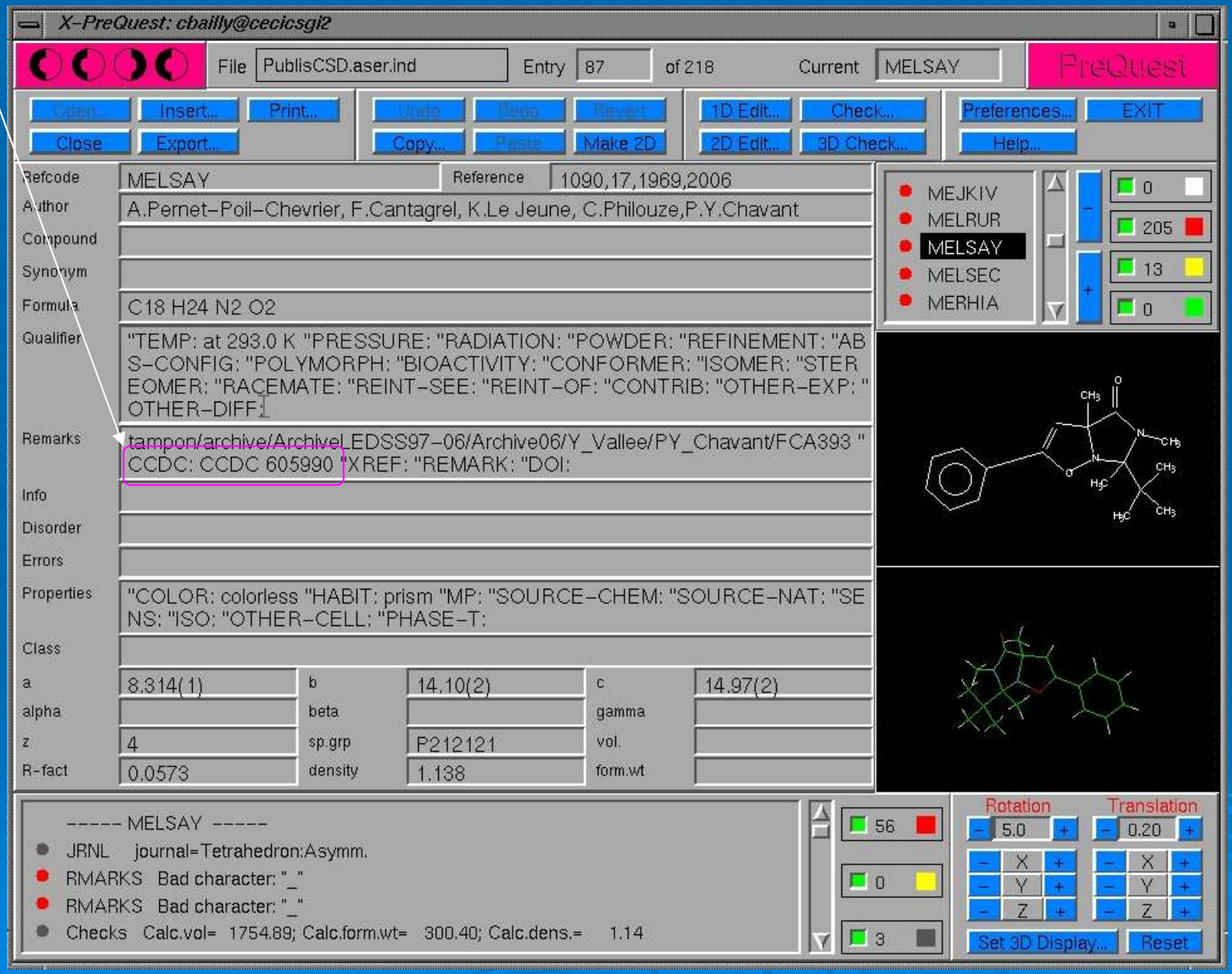
Référence du Journal : Nom, Volume, Page, Année



Auteurs


X-PreQuest: cbailly@cecicsgi2
File PublisCSD.aser.ind
Entry 87
of 218
Current MELSAY
PreQuest
Open
Insert...
Print...
Close
Export...
Undo
Redo
Revert
Copy...
Paste
Make 2D
1D Edit...
Check...
2D Edit...
3D Check...
Preferences...
EXIT
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
MELRUR
MELSAY
MELSEC
MERHIA
0
205
13
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
56
0
3
Rotation
5.0
Translation
0.20
X
Y
Z
Set 3D Display...
Reset

N° de dépôt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File PublisCSD.aser.ind
Entry 87
of 218
Current MELSAY
PreQuest
Open
Insert...
Print...
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Redo
Revert
Copy...
Paste
Make 2D
1D Edit...
Check...
2D Edit...
3D Check...
Preferences...
EXIT
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/Archive_EDSS97-06/Archive06/Y_Vallee/PY_Chavant/FCA393 "CCDC: CCDC 605990 "XREF: "REMARK: "DOI:
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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
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MEJKIV
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MELSAY
MELSEC
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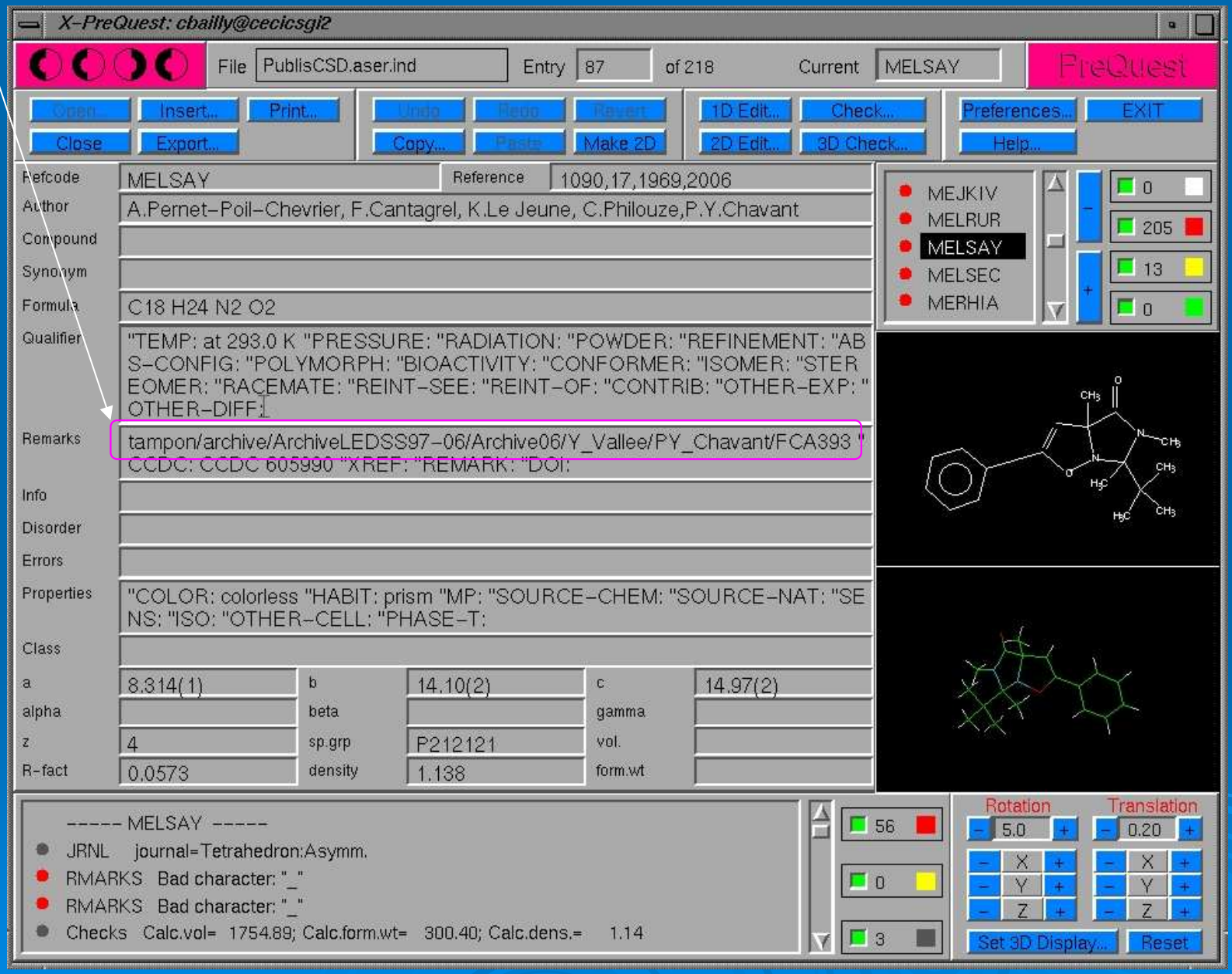
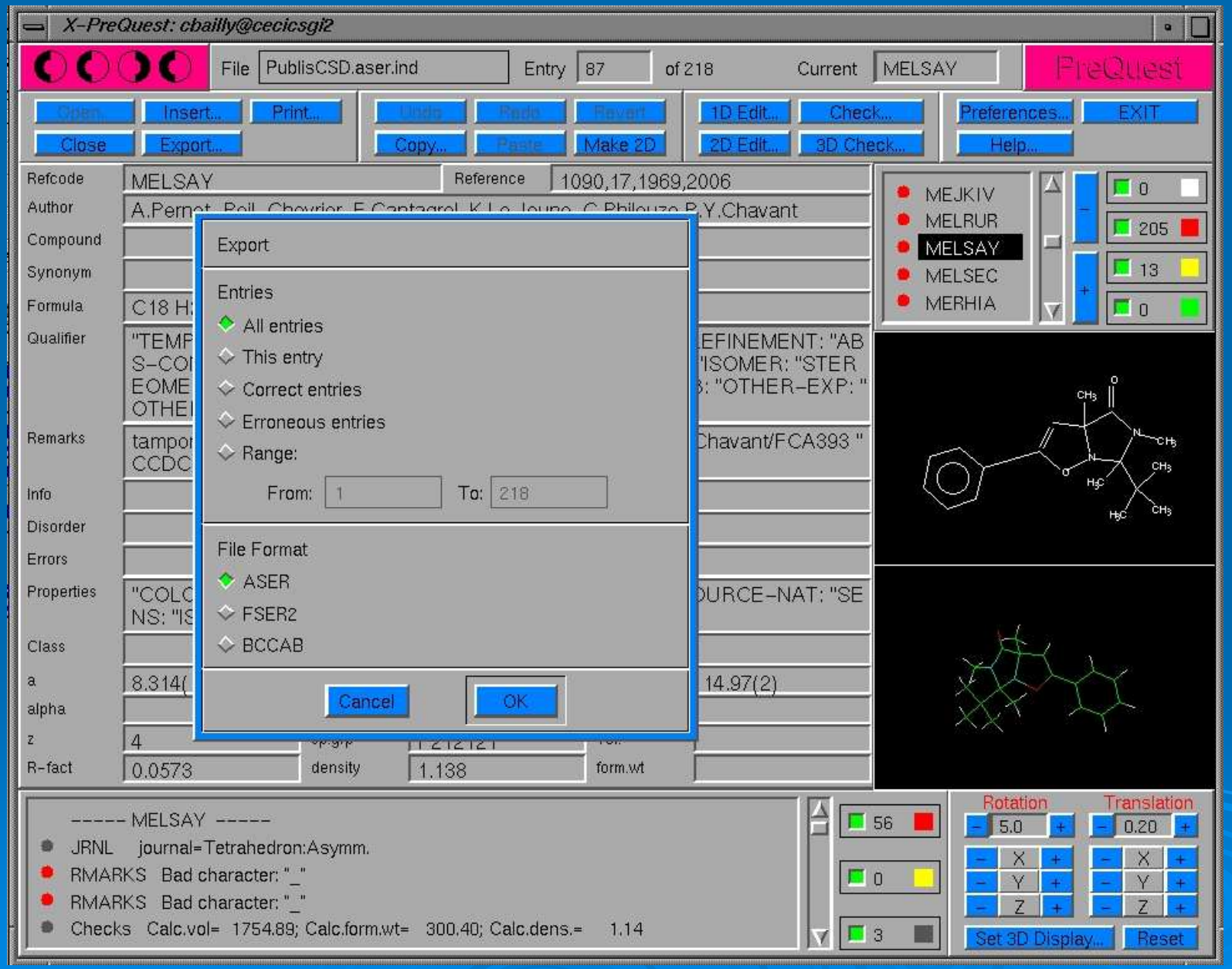
3
Rotation
5.0
Translation
0.20
X
Y
Z
Set 3D Display...
Reset

Zone d’archivage




X-PreQuest: cbailly@cecicsgi2
File PublisCSD.aser.ind
Entry 87
of 218
Current MELSAY
PreQuest
Open...
Insert...
Print...
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Export...
Undo
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Paste
Make 2D
1D Edit...
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2D Edit...
3D Check...
Preferences...
EXIT
Help...
Refcode MELSAY
Reference 1090,17,1969,2006
Author A.Pernot, Poil, Chevrier, F.Cantagrel, K.Le Jeune, C.Philouze,P.Y.Chavant
Compound
Synonym
Formula C18 H
Qualifier "TEMP S-CO EOME OTHE
Remarks tampo CCDC
Info
Disorder
Errors
Properties "COLC NS: "IS
Class
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alpha
z 4
R-fact 0.0573
density 1.138
form.wt
14.97(2)
Chavant/FCA393 "
Export
Entries
All entries
This entry
Correct entries
Erroneous entries
Range:
From: 1
To: 218
File Format
ASER
FSER2
BCCAB
Cancel
OK
MEJKIV
MELRUR
MELSAY
MELSEC
MERHIA
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205
13
0
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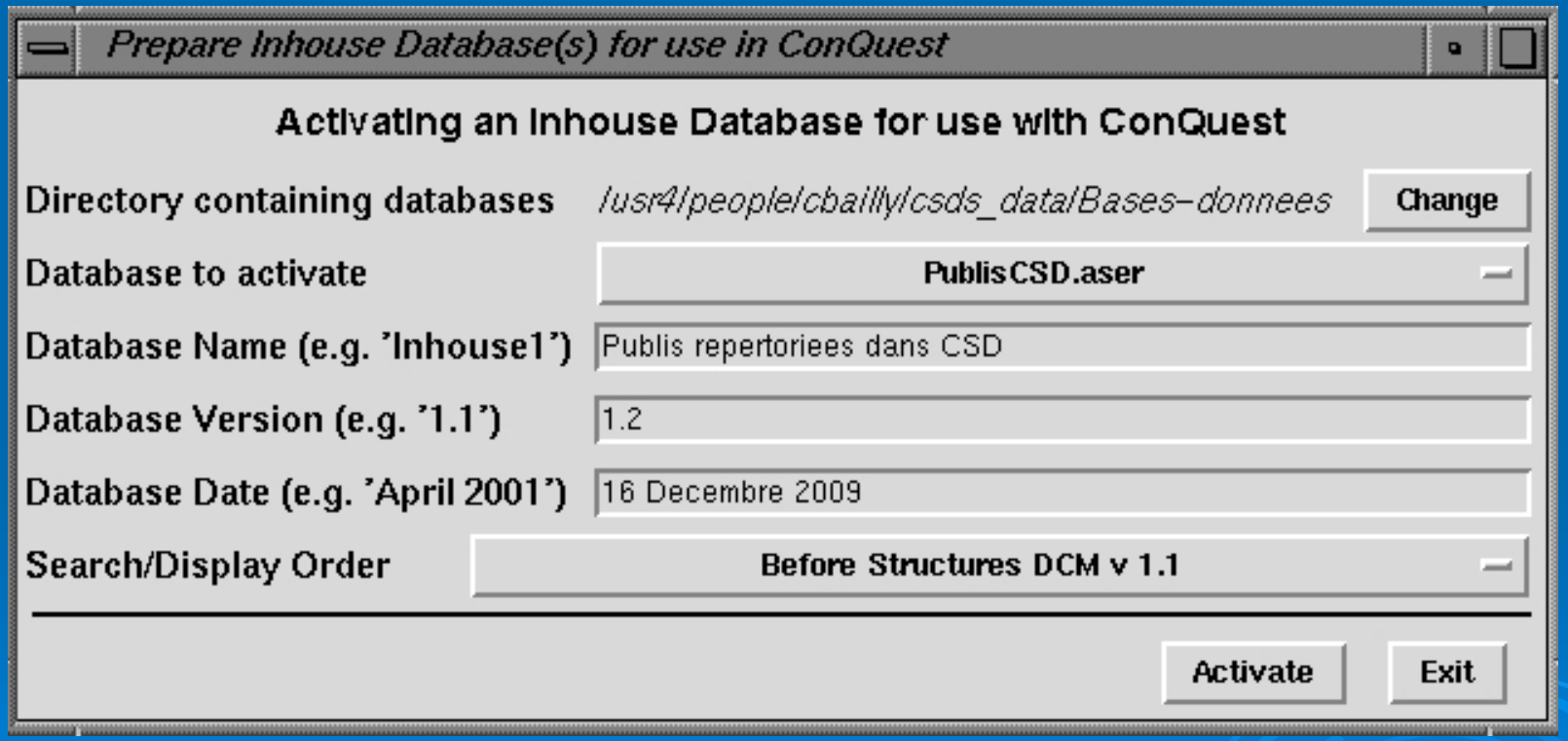
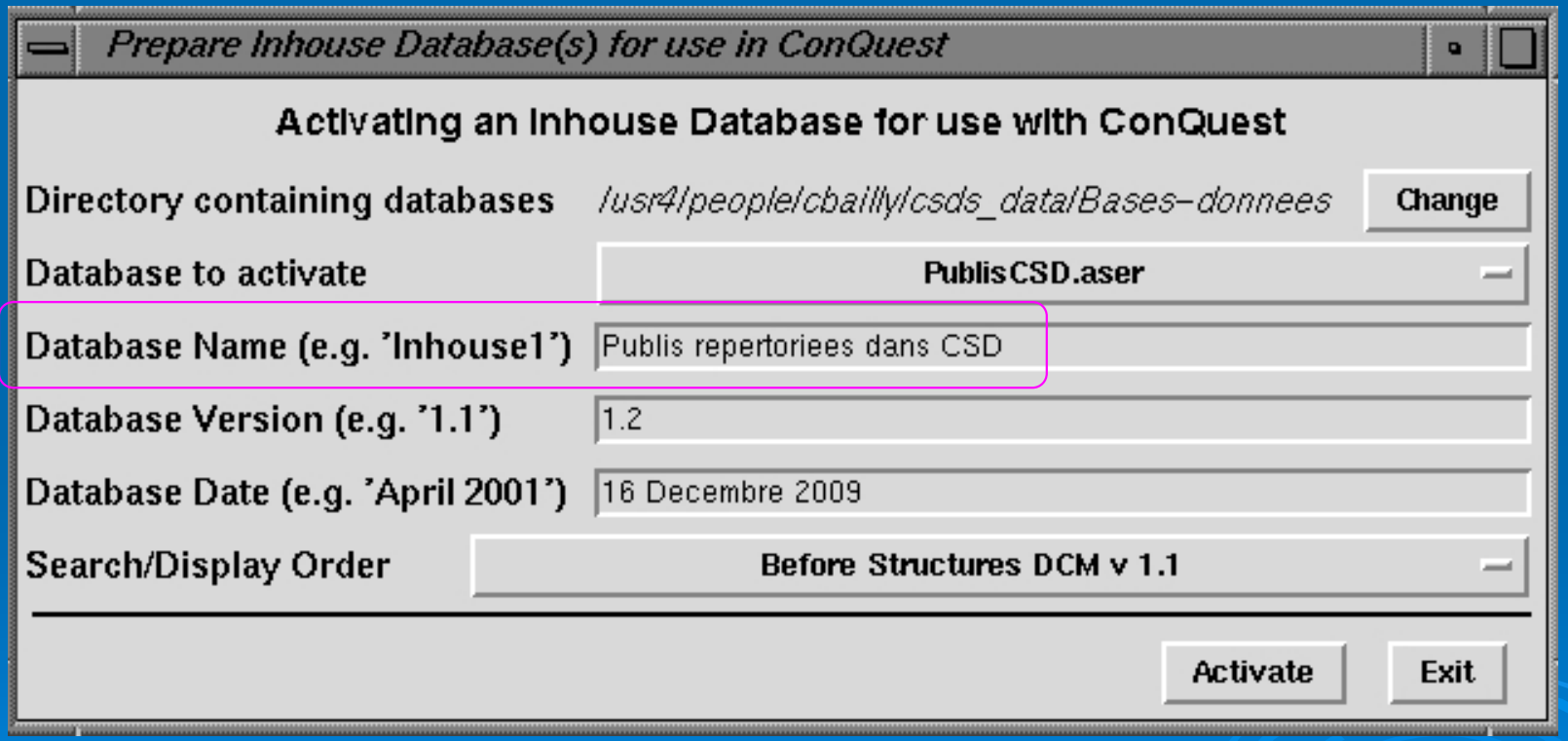
56
0
3
Rotation
5.0
Translation
0.20
X
Y
Z
Set 3D Display...
Reset

Comment interroger sa propre base ?

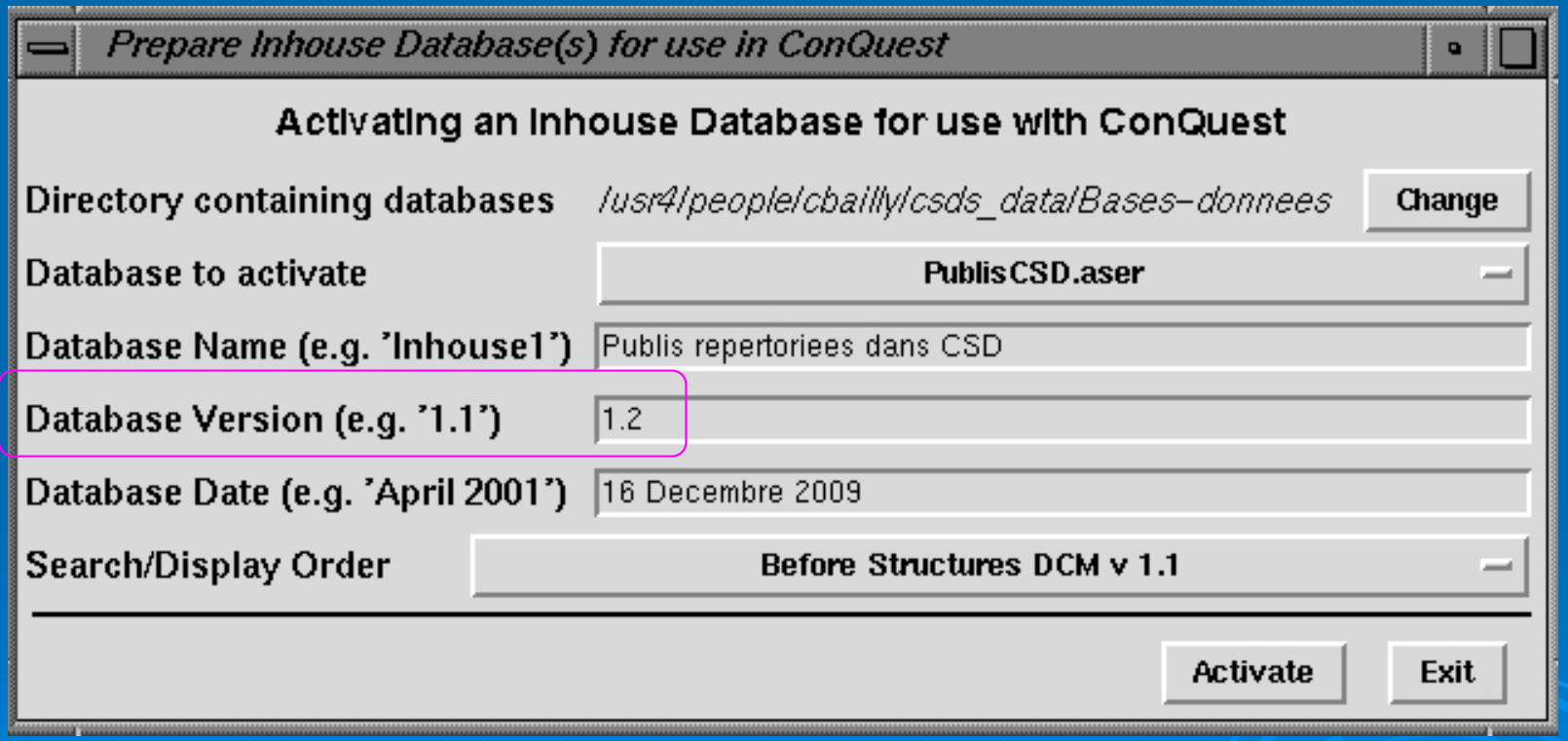
Activation de la base



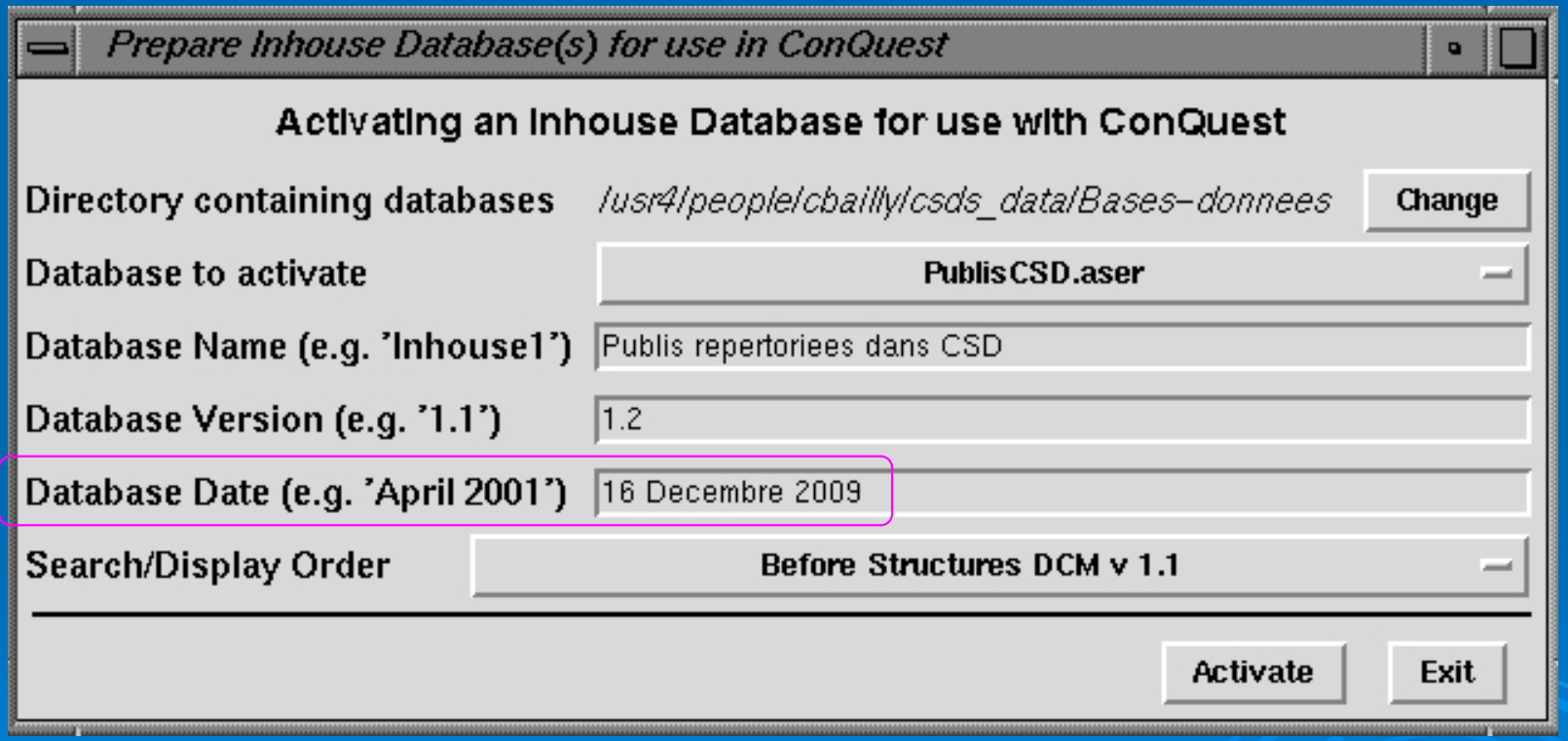
Activation de la base



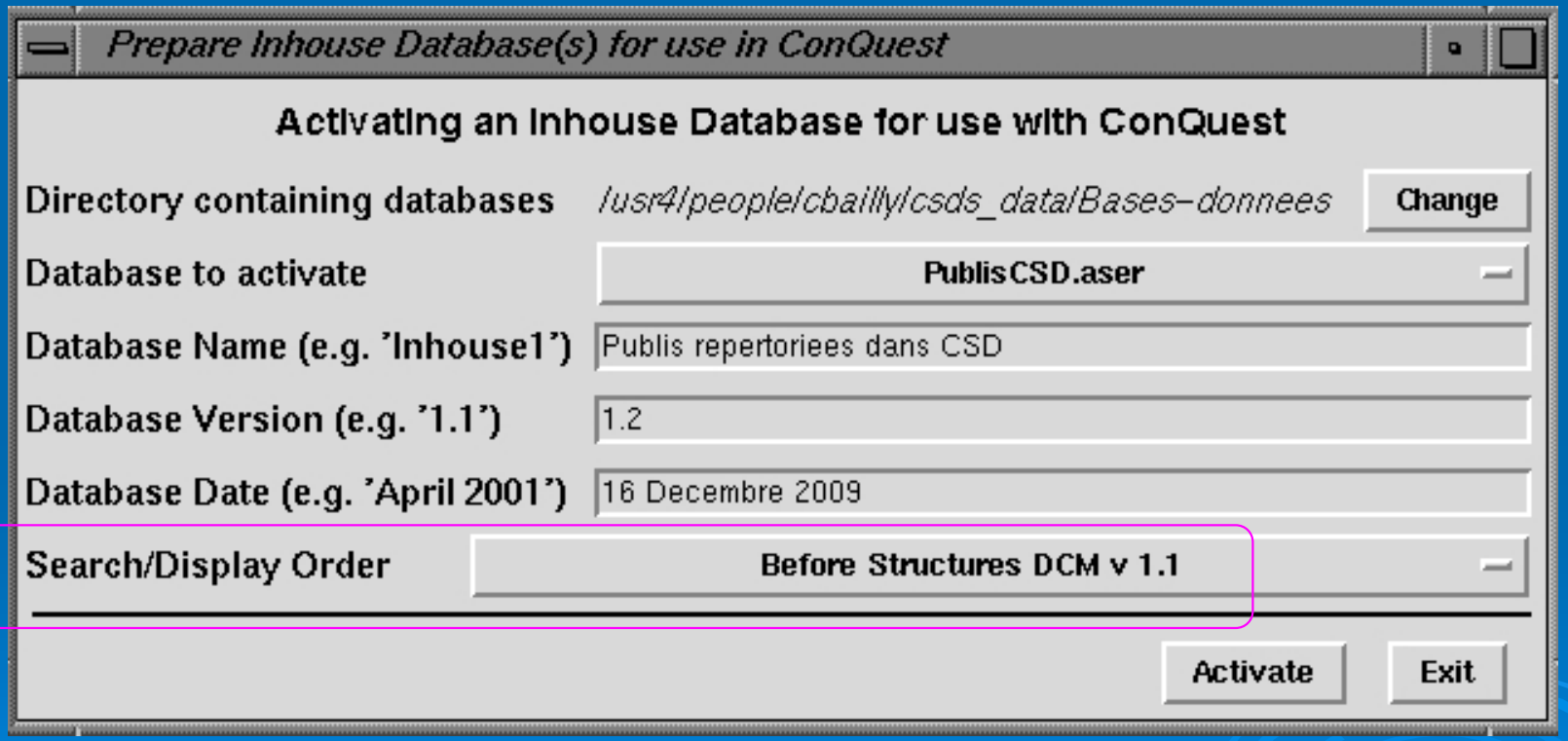
Activation de la base



Activation de la base



Activation de la base



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)