| ESRF | **Experiment title:** BAG Barcelona-<br>The C2 domain of PKCe; Hg and Au derivatives | **Experiment number:**<br>LS1522 |
|---|---|---|
| **Beamline:**<br>ID14.2 | **Date of experiment:**<br>from: 13-Feb-00 to: 15-Feb-00 | **Date of report:**<br>2-Aug-00 |
| **Shifts:** | **Local contact(s):**<br>Laurence Dumon | *Received at ESRF:* |

**Names and affiliations of applicants** (* indicates experimentalists):

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## Report:

PKCε is a member of the novel protein kinase Cs which are activated by acidic phospholipids, diacylglycerol (DAG) and phorbol esters but lack the $Ca^{2+}$-dependence of the classical PKC isotypes.

The structure of the calcium independent C2 domain of the novel PKCε was solved by Multiple Isomorphous Replacement. One native data set and two (Hg, Au) heavy atom derivatives were collected at the beam line ID14-2. The structure is now refined (Table 1) and the manuscript submited for publication (1; and see the report: The C2 domain of PKCε in complex with acidic phospholipids)

### References

1.- W.F.Ochoa, S. Corbalan-Garcia, I.Fita, J.C. Gomez-Fernandez, N. Verdaguer "Structure of the C2 domain of Protein Kinase Cε: a membrane binding model for $Ca^{2+}$ independent PKCs." (2000, submited).

**Data collection, phasing and refinement statistics.**

| | PKCE C2 | Hg-derivative | Au-derivative |
|---|---|---|---|
| Cell parameters (Å) | 39.3,57.9,58.7 | 39,8, 56.5, 59.3 | 39.6, 57.1, 58.9 |
| Space group | P212121 | P212121 | P212121 |
| Resolution range (Å) | 20-2.1 | 20-2.3 | 20-3.0 |
| Completeness overall (%) | 98 | 96 | 96 |
| Rmerge overall (%) | 8.6 | 9.0 | 8.8 |
| Average I/σ I | 7.2 | 9.1 | 6.5 |
| | | | |
| Riso(%) | | 49.5 | 32.4 |
| Heavy atom concentration (mM) | | 0.5 | 0.3 |
| Soaking time (hours) | | 24 | 18 |
| Rcullis centric (%) | | 81 | 65 |
| Rcullis acentric (%) | | 81 | 68 |
| Rcullis anomalous (%) | | 85 | 76 |
| Phasing power centric | | 1.08 | 1.55 |
| Phasing power acentric | | 1.34 | 1.85 |
| | | | |
| Rfactor/Rfree | 21.6/26.7 | | |
| Solvent (%) | 44 | | |
| Rms desviations | | | |
| bond lengths (Å) | 0.007 | | |
| angles (°) | 1.531 | | |
| Number solvent molecules | 74 | | |
| Average thermal factor ( $Å^2$) | | | |
| protein main sidechain | 22.6 | | |
| water | 28.9 | | |
| ions | 23.5 | | |