

**SIXTH FRAMEWORK PROGRAMME**

**Structuring the European Research Area Specific Programme**

**RESEARCH INFRASTRUCTURES ACTION**

Contract for an:

**INTEGRATING ACTIVITY**

**implemented as**

**COORDINATION ACTION**

*Annex I - "Description of Work"*

Project acronym: **MAX-INF2**

Project full title: **European Macromolecular  
Crystallography Infrastructure Network 2**

Proposal/Contract no.: **505977**

Date of preparation of Annex I:

Operative commencement date of contract: *1-12-2004*

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## **1. Project Summary**

The main goal of MAX-INF2 is to achieve long-term integration of the infrastructure for macromolecular crystallography (MX) in Europe. The network will act to disseminate knowledge concerning the development of the hardware and software required by the MX community. Crystal structure determination of proteins, nucleic acids and their complexes relies heavily on research infrastructures such as synchrotron radiation (SR) facilities, as well as hardware and software development projects. The network will have a forum for identifying areas of cooperation centred around the exploitation of SR, hardware and software development in life science crystallography. It will also extend the model for software coordination currently centred on the highly successful British CCP4 project to a European base. MAX-INF2 brings together large-scale facilities, hardware and software developers, academic and commercial users to reflect the current requirements of high throughput macromolecular structure determination in the post-genomic era.

A second approach, tightly integrated with the first, will be to organise workshops and schools for the European MX user community, in particular for young scientists (Ph.D. students and postdocs). MX is essentially a physical science, and since more and more research groups with a biological or medical background are embarking on crystallography experiments, the need for teaching the basic principles of protein crystallography, e.g. X-ray data collection and structure determination, analysis and exploitation, is growing. This will ensure the development of good common practice in the MX user community.

Many macromolecular crystallographers, in academia and the pharmaceutical industry, support the network described in the current application, and it can be seen as the successor of the highly successful Human Potential network MAX-INF (record number 19468).

## **2. Overall description and fundamental objectives of the CA**

### **2.1 Description of how the CA will enhance the services provided**

MX is a significant and expanding component of the European biological and medical research programme. Structural genomics, i.e. the high-throughput determination of crystal structures of biological macromolecules on an organism- or disease-wide basis, is a new and rapidly expanding area of MX. The large number of structural genomics projects currently in operation world-wide clearly shows the interest in and importance of structural biology, in particular MX. Of paramount importance for future success in the public and private sector is expanding the knowledge and skills base of the next generation of macromolecular crystallographers. MAX-INF2 will provide a mechanism for organising and funding meetings, workshops and schools in MX in Europe. It is aimed to promote cooperation on infrastructure, hardware and software development, and to act as a focus to attract research groups and individuals moving into this area of research by disseminating the appropriate knowledge.

The network will provide a solid basis for MX in Europe firstly by promoting good common practice among MX infrastructure providers and stakeholders in the infrastructure, secondly by serving as an information and integration network. The emphasis of the network is on the coordination of ongoing research efforts rather than the actual funding of research. MAX-INF2 will thus organise a series of meetings and workshops, as well as setting up a website for information exchange. These will enhance the contacts between the different software and hardware developers (many of whom are based at synchrotron radiation sites). However it will, equally importantly, enhance interactions between the developers, the SR sites and the user community. Implementing these activities and assessing their success will involve extensive consultation with users, both informally through workshops and schools and more formally through the Web site. Such contacts will ensure that software and hardware developments at different sites proceed synergistically and without wasteful duplication of effort. The overall goal is thus long-term integration of the MAX infrastructure in Europe.

One major deliverable of the integrating activities is a more cohesive user-friendly research environment, which will improve access to the SR infrastructures for the MX community. The existence of an increasing number of SR beam lines for MX data collection means that better coordination of the software available at those sites (e.g. graphical user interfaces for data acquisition and MX software to take the user ever closer to on-line analysis of the structure at the SR site), requires systems that are common to the sites or at least make the differences more transparent to the user. It is important to have an integrated approach between hardware, data collection facilities at synchrotrons and software, as well as to take account of feedback from user groups, especially when the automated structure determination protocols required by structural genomics efforts become more prevalent. The SR providers will benefit enormously from the educational aspects of the network, since a community of well-trained and well-informed users will be created. Currently SR providers face a heavy workload of user support when user groups visit their facilities, due to the non-standard nature of the user interfaces. Much of this workload will be relieved by the integration activities to be undertaken by the network and by the aforementioned training of users.

Integration of software under the GUI as provided by the CCP4 suite is a further means to integration. This aim is dependent on the willingness of network members to integrate their software under the umbrella of a GUI, but there are big benefits to users if cooperation can be agreed.

In summary this network will spread *good practice, common protocols and collaboration* within the field of crystallography in Europe, in particular for the infrastructure providers such as the synchrotron sources. This has clear benefits for the EU as a whole. Industrial practitioners of MX, in the pharmaceutical and biotechnology sectors, will for example see a significantly reduced time lag between the discovery of a lead compound against a certain disease and the production of a marketable drug, with obvious health and economical benefits for society. Academic researchers will increase the quantity and quality of their research by more effective use of the infrastructures provided by some of the MAX-INF2 members. Since academics frequently carry out basic research on biological macromolecules that later become important drug targets, rendering their research more effective has a "knock-on effect" on industry.

**2.2 Ethical and gender issues**

No special ethical or gender issues are raised by the proposed CA.

### 3. List of participants

Table 1a - List of participants of the CA

Participant number	Organisation (name, city, country)	Short name	Date enter project	Date exit project	Short description (i.e. fields of excellence) and specific roles in the consortium
1	Max-Lab, Lund, Sweden	Max-Lab	Start of project	End of project	Synchrotron site, (hardware development). Coordinator. Organiser of one practical workshop (PW), one theoretical school (TS) and one integration workshop (IW).
2	SRS, Daresbury, UK	SRS	Start of project	End of project	Synchrotron site (hardware development), CCP4 software development, website development. Organiser of one PW and responsible for activity N4.
3/5	EMBL Hamburg, D EMBL Grenoble, F <sup>1</sup>	EMBL-HH	Start of project	End of project	Synchrotron sites (hardware & software development). Organiser of four PWs and one IW.
4	ESRF, Grenoble, F	ESRF	Start of project	End of project	Synchrotron site (hardware development). Organiser of two PWs and one IW.
6	University of Vienna, Vienna, Austria	Vienna	Start of project	End of project	MX laboratory, methods development, user. Organiser of two PWs.
7	Paul Scherrer Institut, Villigen, CH	PSI	Start of project	End of project	Synchrotron site (hardware development). Organiser of one PW.

<sup>1</sup> Participant 5 in the initial application (EMBL Grenoble) is merged with participant 3 (EMBL Hamburg). Therefore participant 3 will manage all the funds for these two participants.

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8	Soleil, Gif-sur-Yvette, F	Soleil	Start of project	End of project	Synchrotron site (hardware development). Organiser of two PWs.
9	Diamond, Chilton, UK	Diamond	Start of project	End of project	Synchrotron site (hardware development). Organiser of one PW.
10	Freie Universität Berlin, Berlin, D	FUB	Start of project	End of project	Synchrotron site (hardware development). Organiser of one PW.
12	York University, York, UK	York	Start of project	End of project	MX laboratory, Software development. Organiser of one TS and one PW.
13	Universiteit Leiden, Leiden, NL	Leiden	Start of project	End of project	MX laboratory, Software development. Organiser of two PWs.
15	Georg-August-Universität Göttingen, D	UNIGOE	Start of project	End of project	MX laboratory, Software development. Organiser of one PW.
17	CERBM-GIE, Strasbourg, F <sup>2</sup>	CERBM-GIE	Start of project	End of project	MX laboratory, Software development. Organiser of one PW.
18	MRC, Cambridge, UK	MRC-LMB	Start of project	End of project	MX laboratory, Software development, user. Organiser of one PW.
19	ITQB, Lisbon, P	ITQB	Start of project	End of project	MX laboratory, User. Organiser of one PW.
20	Universita di Pavia, I	Pavia	Start of project	End of project	MX laboratory, User. Organiser of one TS.

<sup>2</sup> The CERBM-GIE is a "Groupement d'Intérêt Economique" consisting of three equal partners: CNRS, INSERM and Université Louis Pasteur, Strasbourg. However the CERBM is a self-managing unit and the CNRS has no scientific or administrative management rôle.

**Table 1b - Composition of the Scientific Advisory Group (see section 7)**

<b>Organisation (name, city, country)</b>	<b>Short name</b>	<b>Date enter project</b>	<b>Date exit project</b>	<b>Short description (i.e. fields of excellence) and specific roles in the consortium</b>
Anka, Karlsruhe, D	Anka	Start of project	End of project	Synchrotron site (hardware development)
Nederlands Kanker Instituut, Amsterdam, NL	NKI	Start of project	End of project	MX laboratory, Software development.
Uppsala Universitet, Uppsala, SE	Uppsala	Start of project	End of project	MX laboratory, Software development.
FORTH, Heraklion, GR	FORTH	Start of project	End of project	MX laboratory, User.
A. Mickiewics University, Poznan, PL	AMU	Start of project	End of project	MX laboratory, User.
University of Copenhagen, Copenhagen, DK	UKBH	Start of project	End of project	MX laboratory, User.
Biovitrum, Stockholm, SE	Biovitrum	Start of project	End of project	MX laboratory, Industrial user.
AstraZeneca, Macclesfield, UK	AstraZeneca	Start of project	End of project	MX laboratory, Industrial user.
IRBM, Pomezia, I	IRBM	Start of project	End of project	MX laboratory, Industrial user.

**4. List of activities****Table 2 - List of activities of CA**

<b>Activity Number</b>	<b>Descriptive Title</b>	<b>Short description and specific objectives of the activity</b>
1	Management of <i>CA</i>	
2	Coordination meetings (CM)	Organisation of the activities of the network, ensuring that the work of the network is disseminated to the scientific community.
N1	Theoretical Schools (TS)	Biannual methods-based Schools with around 200 participants, including presentations by many students and young scientists. Talks will be based around methods development.
N2	Practical Workshops (PW)	A series of small practical workshops, with around 25-40 participants, mainly students and young scientists providing hands-on experience in defined topics of methodology, including data collection, refinement, molecular replacement, MAD, automated model building etc.
N3	Integration Workshops (IW)	Forum for coordination, information and discussion between hardware/software developers and users at the senior scientist level and to allow further integration of synchrotron data collection facilities, detectors and software for structure determination..
N4	Website	Repository for network-related documents, and to provide the community with a single point of reference for schools and workshops organised by the network

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# A3.1

Proposal Number 505977

Proposal Acronym MAX-INF2

## Financial information - whole duration of the project

Participant n°	Organisation short name	Cost model used	Estimated eligible costs and requested EC contribution (whole duration of the project)		Costs and EC contribution per type of activity		Total (3)=(1)+(2)	Total receipts
					Coordination activities (1)	Consortium Management activities (2)		
1	Lund	AC	Eligible costs	Direct Costs (a)	84,542.00	25,750.00	110,292.00	.00
				of which subcontracting	.00	.00	.00	
				Indirect costs (b)	16,908.00	5,150.00	22,058.00	
				Total eligible costs (a)+	101,450.00	30,900.00	132,350.00	
				Requested EC contribution	101,450.00	30,900.00	132,350.00	
2	CCLRC	FC	Eligible costs	Direct Costs (a)	16,330.00	1,800.00	18,130.00	.00
				of which subcontracting	.00	.00	.00	
				Indirect costs (b)	3,270.00	.00	3,270.00	
				Total eligible costs (a)+	19,600.00	1,800.00	21,400.00	
				Requested EC contribution	19,600.00	1,800.00	21,400.00	
3	EMBL	AC	Eligible costs	Direct Costs (a)	68,750.00	900.00	69,650.00	.00
				of which subcontracting	.00	.00	.00	
				Indirect costs (b)	13,750.00	.00	13,750.00	
				Total eligible costs (a)+	82,500.00	900.00	83,400.00	
				Requested EC contribution	82,500.00	900.00	83,400.00	
4	ESRF	AC	Eligible costs	Direct Costs (a)	40,580.00	900.00	41,480.00	.00
				of which subcontracting	.00	.00	.00	
				Indirect costs (b)	8,120.00	.00	8,120.00	
				Total eligible costs (a)+	48,700.00	900.00	49,600.00	
				Requested EC contribution	48,700.00	900.00	49,600.00	
6	UNIVIE	AC	Eligible costs	Direct Costs (a)	40,580.00	900.00	41,480.00	.00
				of which subcontracting	.00	.00	.00	
				Indirect costs (b)	8,120.00	.00	8,120.00	
				Total eligible costs (a)+	48,700.00	900.00	49,600.00	
				Requested EC contribution	48,700.00	900.00	49,600.00	
7	PSI	FC	Eligible costs	Direct Costs (a)	16,330.00	900.00	17,230.00	.00
				of which subcontracting	.00	.00	.00	
				Indirect costs (b)	3,270.00	.00	3,270.00	
				Total eligible costs (a)+	19,600.00	900.00	20,500.00	
				Requested EC contribution	19,600.00	900.00	20,500.00	

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# A3.1

Proposal Number 505977

Proposal Acronym MAX-INF2

## Financial information - whole duration of the project

Participant n°	Organisation short name	Cost model used	Estimated eligible costs and requested EC contribution (whole duration of the project)				Total (3)=(1)+(2)	Total receipts
			Costs	Coordination activities (1)	Consortium Management activities (2)	Requested EC contribution		
8	SOLEIL	FCF	Eligible costs	Direct Costs (a)	29,670.00	900.00	30,570.00	.00
				of which subcontracting	.00	.00	.00	
				Indirect costs (b)	5,930.00	.00	5,930.00	
				Total eligible costs (a)+	35,600.00	900.00	36,500.00	
			Requested EC contribution	35,600.00	900.00	36,500.00		
9	Diamond	FC	Eligible costs	Direct Costs (a)	16,330.00	1,800.00	18,130.00	.00
				of which subcontracting	.00	.00	.00	
				Indirect costs (b)	3,270.00	.00	3,270.00	
				Total eligible costs (a)+	19,600.00	1,800.00	21,400.00	
			Requested EC contribution	19,600.00	1,800.00	21,400.00		
10	FUB	AC	Eligible costs	Direct Costs (a)	16,330.00	900.00	17,230.00	.00
				of which subcontracting	.00	.00	.00	
				Indirect costs (b)	3,270.00	.00	3,270.00	
				Total eligible costs (a)+	19,600.00	900.00	20,500.00	
			Requested EC contribution	19,600.00	900.00	20,500.00		
12	UOY	AC	Eligible costs	Direct Costs (a)	62,660.00	1,800.00	64,460.00	.00
				of which subcontracting	.00	.00	.00	
				Indirect costs (b)	12,540.00	.00	12,540.00	
				Total eligible costs (a)+	75,200.00	1,800.00	77,000.00	
			Requested EC contribution	75,200.00	1,800.00	77,000.00		
13	LEIDENUNIV	AC	Eligible costs	Direct Costs (a)	40,622.00	900.00	41,522.00	.00
				of which subcontracting	.00	.00	.00	
				Indirect costs (b)	8,128.00	.00	8,128.00	
				Total eligible costs (a)+	48,750.00	900.00	49,650.00	
			Requested EC contribution	48,750.00	900.00	49,650.00		
15	UNIGOE	AC	Eligible costs	Direct Costs (a)	16,330.00	900.00	17,230.00	.00
				of which subcontracting	.00	.00	.00	
				Indirect costs (b)	3,270.00	.00	3,270.00	
				Total eligible costs (a)+	19,600.00	900.00	20,500.00	
			Requested EC contribution	19,600.00	900.00	20,500.00		

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# A3.1

Proposal Number 505977

Proposal Acronym MAX-INF2

## Financial information - whole duration of the project

Participant n°	Organisation short name	Cost model used	Estimated eligible costs and requested EC contribution (whole duration of the project)		Costs and EC contribution per type of activity		Total (3)=(1)+(2)	Total receipts
					Coordination activities (1)	Consortium Management activities (2)		
17	CERBM-GIE	AC	Eligible costs	Direct Costs (a)	16,330.00	900.00	17,230.00	.00
				of which subcontracting	.00	.00	.00	
				Indirect costs (b)	3,270.00	.00	3,270.00	
				Total eligible costs (a)+	19,600.00	900.00	20,500.00	
				Requested EC contribution	19,600.00	900.00	20,500.00	
18	MRC-LMB	FC	Eligible costs	Direct Costs (a)	16,330.00	900.00	17,230.00	.00
				of which subcontracting	.00	.00	.00	
				Indirect costs (b)	3,270.00	.00	3,270.00	
				Total eligible costs (a)+	19,600.00	900.00	20,500.00	
				Requested EC contribution	19,600.00	900.00	20,500.00	
19	IQTB	AC	Eligible costs	Direct Costs (a)	29,670.00	900.00	30,570.00	.00
				of which subcontracting	.00	.00	.00	
				Indirect costs (b)	5,930.00	.00	5,930.00	
				Total eligible costs (a)+	35,600.00	900.00	36,500.00	
				Requested EC contribution	35,600.00	900.00	36,500.00	
20	UNIPV	AC	Eligible costs	Direct Costs (a)	49,330.00	900.00	50,230.00	.00
				of which subcontracting	.00	.00	.00	
				Indirect costs (b)	9,870.00	.00	9,870.00	
				Total eligible costs (a)+	59,200.00	900.00	60,100.00	
				Requested EC contribution	59,200.00	900.00	60,100.00	
TOTAL			Eligible costs	672,900.00	47,100.00	720,000.00	.00	
			Requested EC contribution	672,900.00	47,100.00	720,000.00		

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# A3.2a

Proposal Number	505977	Proposal Acronym	MAX-INF2
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## Estimated breakdown of the EC contribution per reporting period

Reporting Periods	Start month	End month	Estimated Grant to the Budget	
			Total	in which first six months
Reporting Period 1	1	12	140,000.00	.00
Reporting Period 2	13	24	140,000.00	100,000.00
Reporting Period 3	25	36	140,000.00	100,000.00
Reporting Period 4	37	48	140,000.00	100,000.00
Reporting Period 5	49	60	160,000.00	100,000.00
Reporting Period 6			.00	.00
Reporting Period 7			.00	.00

The financial organisation of the network is as follows:

1. The travel costs for attending the CMs and IWs are estimated to be 600€ per participant and meeting. In order to make most efficient use of funds for travel, the four ordinary CMs will be held in conjunction with the IWs; a further two extraordinary meetings will be arranged, if necessary, by participants 1 and 13. The cost of organising an extraordinary CM is estimated to be 10 150€.
2. The cost of organising a TS (activity N1) is estimated to be 55 600€.
3. The cost of organising a PW (activity N2) is estimated to be 16 000€ per meeting. Approximately 23 meetings will be held in total, leading to an estimated total cost of 368 000€, or 73 600 €/year). The particular workshops to be funded and the organisers for each workshop will be decided at the yearly Coordination Meetings. The initial budget is based on wishes to organise workshops expressed by the network participants in October 2004.
4. The cost of organising an IW (activity N3) is estimated to be 10 100€. A further cost of 3 600€ is estimated for the travel costs of the SAG associated with their attendance at these meetings.
5. The auditing costs are estimated at 16 200€. The coordinator will receive 30 900 € as salary costs for coordinating and managing the network during its five-year duration.

In cases 2, 3 and 4 an indicative budget has been provided based on current information on the organisers of each activity and the workshops that have been planned for the first 18 months (see description of activities below).

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Participant	Activity	Item of expenditure	Amount/ year	Amount Total
All participants	1	<b>Management</b>  <i>of which auditing salary + overhead for coordinator</i>	9 420€	47 100€ 16 200€ 30 900€
All participants	2	<b>Extraordinary coordination meetings (2 total)</b>  <i>per meeting:</i>  <i>Travel costs for representatives of all consortium members</i>  <i>Local costs for organiser</i>	9 320€  600€ per participant  10 150€ per meeting	46 700€  19 200€  20 300€
Participants 1, 12 and 20	N1	<b>Theoretical Schools (TS, 3 total)</b>  <b>One School:</b> <i>Travel subsidies for speakers and young scientists</i> <i>Rent Villa Olmo and services</i> <i>Secretarial effort for organising workshop</i>	33 360€  <u>55 600€</u> 25 000€  25 000€  5 600€	166 800€
All participants except 20	N2	<b>Practical Workshops (PW): 23 total, 4–5 per year</b>  <b>One Workshop</b> <i>Travel for tutors and organisers</i> <i>Costs for educational tools (eg. rent computers for tutorials)</i> <i>Specific secretarial effort for organising workshop</i>	73 600€  <u>16 000€</u> 10 000€  4 000€  2 000€	368 000€

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<b>All participants and Scientific Advisory Group</b>	<b>N3</b>	<b>Integration Workshops (IW, 4 total)</b>	<b>18 280€</b>	<b>91 400€</b>
	<i>Of which, per meeting:</i>	<i>Travel costs for representatives of consortium members</i>	<i>600€ per participant*</i>	<i>36 600€</i>
		<i>Travel costs for members of SAG</i>	<i>3 600€</i>	<i>14 400€</i>
		<i>Local costs (hotel, meals, locale, secretarial help), per workshop</i>	<i>10 100€</i>	<i>40 400€</i>
<b>2</b>	<b>N4</b>	<b>Programmer</b>	<b>0€</b>	<b>0€</b>
<b>Totals</b>				<b>720000€</b>

## **7. Management of the activity**

### **7.1 Description of the activity**

#### Management of the Network

The network is modelled on ongoing collaborative efforts within MAX-INF and benefits from the high level of experience gained within that project, which was coordinated by participant 2. Computing support for establishing and updating WWW pages will be provided by a band 5 programmer at Daresbury Laboratory (participant 2).

Participant 1 is the coordinator of the network.

The coordinator will be responsible for:

- The communication with the commission
- The overall financial, administrative and legal management
- Reporting to the commission collecting audit certificates and reports from all partners
- Keep and update the consortium agreement
- Chair the coordination meetings and prepare minutes from them

#### Coordination meetings

Annual coordination meetings (CMs) for the administration of the network will be organised. These meetings are separate from the Integration Workshops in activity N3, as the latter are forums for scientific discussion rather than administration. However to make effective use of time and travel funds the coordination meetings will be held in conjunction with the IWs. There is provision for two extraordinary meetings if the need arises: the latter may comprise relevant subgroups of the total members.

A total of 4 ordinary and 2 extraordinary CMs are planned in the 5 years of the contract. It is important to arrange a meeting early in the first and at approximately equal intervals thereafter. However, the actual timing needs to be flexible, and will aim to address the needs of the network, and to coordinate with other meetings of interest to the members. The date and venue of each meeting will be decided at the previous meeting.

Each coordination meeting will follow an agenda typically including the following items:

- Presentations by the coordinator followed by discussion
- Report on Integration Workshops (IWs, activity N3)
- Proposition of Practical Workshops (PWs, activity N2) that participants would like to organise
- Appointment of organisers for the PWs and Theoretical Schools (TSs, activity N1) if this deviates from the original budget.
- Discussion of network-supported operative initiatives such as PWs and TSs.
- Debate of general issues concerning the development and future needs of the MX community.
- Other issues arising that are deemed to be within the scope of this network.
- Financial overview of the network's expenses and proposition of a preliminary budget for the next 18 months.

The organisation of each meeting will comply with the following rules:

- All attendees will be notified of the date and place at least four months in advance.
- The programme management will be represented at each meeting.
- The agenda and documentation for each meeting will be circulated to the members at least two weeks before the meeting. All business will be conducted by e-mail.
- The minutes of each meeting will be the responsibility of the coordinator and will be distributed to all network members within one month.

The meeting will decide

- Which PWs will be organised in the following year
- The financial contribution of the network to the approved PWs, if this deviates from the scheme in the initial budget.
- Which participant will have responsibility for organising the next TS
- Which of the synchrotron sites will organise the next IW.

Decisions will be taken on a simple majority basis. Any changes to the above organisation of the coordination meetings or to any other aspects of the network organisation will have to be approved by a 75% majority. Every participant has one vote.

Details of the consortium management will be finalized in the consortium agreement, which will be signed by all participants.

## **7.2 Plan for using and disseminating knowledge**

The goals for MAX-INF2 are twofold. The first goal is to coordinate research efforts in European laboratories involved in developing methods for MX. This connects the European synchrotrons that provide facilities for data collection with laboratories involved in hardware and software technologies. In order to guarantee a feedback to the user community several different user groups will have access to MAX-INF2 through membership in the Scientific Advisory Group (SAG). The potential benefits of the integration activities are very high, both for participating infrastructure facilities and for others. Contact between providers and users is enhanced, as is contact between those concerned primarily with hardware developments at the facilities with those working in software developments to exploit the resulting data.

The first part involves the dissemination of good common practice for MX in Europe by organising Practical Workshops and Theoretical Schools. The importance of these is clear. The MX community is expanding fast, leading to an increasing number of inexperienced infrastructure stakeholders who require training at a state-of-the-art level. Previous experience has shown that SR infrastructure operators gain immensely from organising and teaching at the workshops and schools, since in the end they benefit from well-trained users who can carry out optimised experiments with less supervision. In addition to transfer of knowledge from the experienced to the inexperienced, the workshops bring together the most experienced providers in a field, generating collaboration and discussion at the highest level.

In order to keep informed on further developments within the field of crystallography and infrastructures, MAX-INF2 will keep close contacts with other EC networks or proposals such as BIOXHIT or the I3 IA-SFS ("Integrating Activity on Synchrotron

and Free Electron Laser Science"). As well as the participation of the SAG, MAX-INF2 will keep contact with European scientific societies: for example, members of the MX Special Interest Group of the European Crystallographic Association (ECA) will be informed about the outcome of the coordination meetings in order to facilitate coordination of workshops etc.

The existing website for MAX-INF will be continued and regularly updated. It will act as a repository for network-related documents, and to provide the community with a single point of reference for the MAX-INF2 schools and workshops.

#### Long-term integration

Given the complex technical nature of methods and hardware development for protein crystallography, it can often occur that several infrastructure providers, e.g. synchrotron radiation sources, pursue parallel technical solutions to a common problem. While this is not necessarily harmful, unnecessary parallel developments can be avoided by exchange of information, ideas and protocols. We propose to drive this exchange in two ways: firstly by promoting protein crystallographic education in Europe and secondly by promoting dialogue between software and hardware developers and providers at a senior level. The first of these generates a well-educated, skilful user base that can demand more of the providers: the second enables the providers themselves to offer an improved, streamlined service with as many common aspects as possible. Both of these aspects are vital for long-term integration.

#### Added value for the EU

The specific emphasis on MX in MAX-INF2 will result in significant added value for the EU and associated economic area, as the structural information on biological macromolecules produced by MX in the academic and private sectors is the motor for major economic developments in the pharmaceutical and biotechnology sectors. Many of the skilled MX practitioners in the private sector have extensive academic training to doctoral level and above, and many have participated in and/or benefited directly from the previous network MAX-INF. MAX-INF2 is complementary to the BIOXHIT and I3-SRS networks, which will be ensured by the representation of several of the MAX-INF2 participants in these networks. BIOXHIT revolves around technology development for European structural genomics and the educational component of BIOXHIT is focused on practical workshops in specific aspects of structural genomics rather than the fundamental crystallographic methodology (of benefit to all MX practitioners) to be disseminated within MAX-INF2. I3-IA-SFS covers all aspects of research using synchrotron radiation with little specific emphasis on MX as far as education is concerned. The HERCULES course ("Higher European Research Course For Users Of Large Experimental Systems"), which is partly funded by I3-IA-SFS, also offers a very broad education in all aspects of synchrotron radiation; thus it has negligible overlap with MAX-INF2.

**8) Description of the other activities of the CA****Summary:**

<b>Activity Number</b>	<b>Descriptive Title</b>	<b>Short description and specific objectives of the activity</b>
N1	Theoretical Schools (TS)	Approximately biannual methods-based Schools with around 200 participants, including presentations by many students and young scientists. Talks will be based around methods development.
N2	Practical Workshops (PW)	A series of small practical workshops, with around 25-40 participants, mainly students and young scientists providing hands-on experience in defined topics of methodology, including data collection, refinement, molecular replacement, MAD, automated model building etc.
N3	Integration Workshops (IW)	Forum for coordination, information and discussion between hardware/software developers and users at the senior scientist level and to allow further integration of synchrotron data collection facilities, detectors and software for structure determination.
N4	Website	Repository for network-related documents, and to provide the community with a single point of reference for schools and workshops organised by the network

**8.N1 Activity N1: Theoretical Schools****8.N1.1 Description and objectives of the activity**

The objective of this activity is to spread good common practice in MX techniques at the theoretical level. Theoretical Schools in the methodology of MX will be thus be organised every two years. These will be mainly lecture-based, which differentiates them from the Practical Workshops described in activity N2. The Schools will encourage good practice, common protocols and collaboration by educating the practitioners of MX (stakeholders in the infrastructure) in the latest methods. The schools will be based on a model successfully used in MAX-INF and will be held at Villa Olmo in Como, Italy, continuing a tradition started by the first meeting at this location in 1989. They will involve up to 200 participants, including many students and young scientists (Ph.D. students and postdoctoral fellows). The participants will not be limited to members of the consortium but they will come from EU member states. Lectures will be given by acknowledged experts; young scientists will be given the opportunity to present their work.

The MX community is large, thus these larger-scale meetings are essential to give the opportunity to a significant proportion of the community to hear about advances in techniques and to ensure that European MX groups are operating at an internationally competitive level. Talks will be based around all aspects of methods development in the MX area, and will be presented by a combination of international scientists, infrastructure facility operators and software and hardware developers, mostly members of the consortium. In addition the young scientists will be encouraged to present their results to a wide forum, either orally or in the form of a poster. They will also be encouraged to discuss limitations of the infrastructure and indicate areas in which they feel developments are required, which gives invaluable feedback to the infrastructure providers.

**8.N1.2 Participants in the activity**

At present we plan to have the Theoretical Schools organised by participants 1, 12 and 20; however the final organisers will be decided at a future coordination meeting. The theme and participants are outlined below.

**8.N1.3 Outline implementation for the full duration of the activity (including milestones and deliverables)**

As the deliverable in this case is dissemination of knowledge and techniques in the field of MX, the schools are milestones and deliverables in themselves.

	<b>Year 1</b>	<b>Year 2</b>	<b>Year 3</b>	<b>Year 4</b>	<b>Year 5</b>
deliverable		Theoretical School 1	Theoretical School 2		Theoretical School 3

**Theoretical School 1 (Villa Olmo, Como, Italy, 7–11 May 2006)**

**Title:** 8<sup>th</sup> International School on Crystallography of Biological Macromolecules

**Organisers:** Andrea Carfi (participant 26), Derek Logan & Marjolein Thunnissen (participant 1)

**Invited speakers:** G. Stier, U Shepers, H. Niemann, Arnaud Ducruix, Jan Löwe, Naomi Chayen, Irme Sinning, R. Dutzler, Eva Pebay-Peyroula, Jim Pflugrath, Andrew Leslie (participant 18), Jules Hendrix, Richard Pauptit (participant 25), N. Norkakoti, Andrea Mattevi (participant 20), Vincent Mikol, Jerome Kallen, George Sheldrick (participant 15), Gérard Bricogne, Richard Kahn, Kevin Cowtan, Thomas Schneider, Randy Read, Airlie McCoy, Anastassis Perrakis (participant 14), Garib Murshudov (participant 12), U. Göhlke, Werner Kuhlbrandt, Dmitri Svergun, F. Rey.

**Theoretical School 2 (year 3):** will be arranged by participant 20 together with another non-Italian participant, to be decided at a coordination meeting.

**Theoretical School 3 (year 5):** will be arranged by participants 6 and 12, probably at the same location.

#### **8.N1.4 Expected outcome**

The schools will result in a raised level of education and awareness in the theoretical and methodological aspects of MX. The schools will encourage good practice, common protocols and collaboration. This will produce more skilled practitioners in the discipline, which is of general benefit, ensuring increased competitiveness for European MX research groups. Another outcome is the integration of participants inside and outside the CA due to personal meetings and exchange of ideas.

**8.N2 Activity N2: Practical workshops****8.N2.1 Description and objectives of the activity**

The objective of this activity is to spread good common practice in MX techniques on the practical level. Practical Workshops will allow young scientists to be coached by specialists in the latest techniques and methods. Therefore MAX-INF2 will organise a series of small workshops, with around 20–40 participants, on defined topics in methodology, including, but not limited to:

- data collection
- refinement
- molecular replacement
- multiple wavelength anomalous dispersion methods
- automated model building

The workshops will be organised by members of the consortium, in particular those involved in the development of new methodologies or the synchrotron radiation providers. The workshops will differ from the Schools described in activity N1 by being very much “hands-on”, i.e. practical more than theoretical. Four to five workshops a year will be held, on different topics and at different sites, to cover the needs of the rapidly expanding and widespread MX community. The participants will be young scientists (Ph.D. students and postdoctoral fellows). They will not be limited to members of the consortium but they will come from EU member states. The choice of workshops for a given year is dependent on ongoing developments in the field and will be decided at MAX-INF coordination meetings after application from consortium members to arrange such workshops (see section 7.1). In the first 18 months the CA plans to finance workshops arranged by participants 7, 8 and 19 (see below).

**8.N2.2 Participants in the activity**

All participants are welcome to arrange workshops and to apply for funding for these at the coordination meetings. Those who have done so in the past (i.e. in the framework of MAX-INF) are consortium members 2–10, 12, 15 and 17–19.

**8.N2.3 Outline implementation for the full duration of the activity (including milestones and deliverables)**

	<b>Year 1</b>	<b>Year 2</b>	<b>Year 3</b>	<b>Year 4</b>	<b>Year 5</b>
<b>deliverable</b>	Practical Workshops 1–3 below and 1 additional workshop	4–5 workshops	4–5 workshops	4–5 workshops	4–5 workshops

**Concrete plans for workshops in the first 18 months:**

**Workshop 1:** *Membrane proteins: the rocky road from gene to crystal.* 19–24 September, 2005, Oeiras, Portugal. Organisers participant 19 and Prof. So Iwata, Imperial College, London, UK.

*Provisional list of proposed speakers:*

Prof. So Iwata, London Imperial College of Science, Technology and Medicine, UK  
 Prof. Gunnar von Heijne, Stockholm University, Sweden  
 Prof. Peter Henderson, University of Leeds, UK  
 Dr. Edmund Kunji, MRC Cambridge, UK  
 Prof. Thue W. Schwartz, Panum Institute, Denmark  
 Dr. Bernadette Byrne, London Imperial College of Science, Technology and Medicine, UK  
 Dr. Kaspar Locher, ETH Swiss Federal Institute of Technology Zurich, Switzerland  
 Dr. Carola Hunte, MPI Frankfurt, Germany  
 Prof. Raimund Dutzler, University of Zurich, Switzerland  
 Prof. Eva Pebay-Peyroula, IBS, France  
 Prof. Miguel Teixeira (participant 19)  
 Prof. Herman van Tilbeurgh, IBBMC, France  
 Dr. Richard Neutze, Chalmers University of Technology, Sweden

**Workshop 2:** *Exploiting anomalous scattering in macromolecular structure determination.* 14th-19th June 2005, ESRF, Grenoble, France. Organisers Bill Shepard (participant 4) and Hassan Berhali (participant 3).

Invited speakers:

Dr. P. Adams	Lawrence Berkeley Lab	Patterson methods/Phenix/CNS
Prof. G. Bricogne	Global Phasing Ltd	Phase calculation/autoSHARP
Dr. C. Vonrhein	Global Phasing Ltd	Automated phasing/autoSHARP
Dr. K. Diederichs	University of Konstanz	Radiation damage/XDS
Dr. W. Kabsch	MPI, Heidelberg	Data processing/XDS
Dr. A. Perrakis	NKI, Amsterdam	Map interpretation & tracing
Dr. H. Powell	participant 18	Data processing/Mosflm
Dr. T. Schneider	IFOM, Milano	Direct Methods/SHELX
Prof. G. Sheldrick	participant 15	Substructure determination/ SHELX
Dr. Q. Hao	Los Alamos National Lab	Automated phasing/Solve-Resolve
Dr. C. Weeks	Hauptman-Woodward MRI	Substructure determination/SnB
Prof. R. Read	Cambridge University	PHASER
Dr. E. Garman	Oxford University	Radiation Damage
Dr. Z. Dauter	Brookhaven Nat. Lab.	S, P, Ca-SAD/Data collection
	strategies	
Prof. E. Dodson	University of York	SIR/MIR/SAS/MAD
Dr. G. Evans	participant 9	BL instrumentation / autoSHARP
Dr. L. Duke	participant 9	3 <sup>rd</sup> gen. synchrotrons/BL
	instrumentation	
Dr. K. McAuley	participant 9	High resolution/ACORN
Dr. A. Thompson	participant 8	3 <sup>rd</sup> generation synchrotrons
Prof. C. Giacovazzo	Institute of Crystallography	High resolution / SIRPROT
Dr. James Holton	ALS, Berkley	Automated processing ELVES
Ana Gonzalez	ALS, Berkley	Data collection strategies for
SAD/MAD		

Dr. Stephen Cusack	participant 3	Introduction
Dr. Sine Larsen	participant 4	Introduction
Dr. Jean-Luc Ferrer	IBS	Automatic data processing
Dr. Richard Kahn	IBS	Anom. scattering / Long wavelengths
Dr. Gordon Leonard	participant 4	S & P SAD phasing
Dr. Sean McSweeney	participant 4	Anomalous diffraction methods
Dr. Raimond Ravelli	participant 3	Radiation Damage & Phasing
Dr. Didier Nurizzo	participant 4	BL Scientist
Dr. H. Belrahli	MRC, participant 3	BL Scientist
Dr. M. Walsh	MRC, participant 3	BL Scientist
Dr. Andrew McCarthy	EMBL-Grenoble	BL Scientist
Dr. William Shepard	participant 4	BL Scientist

**Workshop 3:** Future directions in synchrotron radiation bio-crystallography", Synchrotron SOLEIL, St. Aubin, France, 13th-14th December 2004. Organisers: Andrew Thompson, Roger Fourme, Eric Girard, Pierre Legrand (participant 8).

*Invited speakers:*

Mourad Idir (participant 8)  
 Patrice Vachette (IBBMC, Orsay)  
 Thierry Moreno (participant 8)  
 Gérard Bricogne (Global Phasing, Cambridge)  
 Hubert Kettenberger (University of Munich, Munich)  
 Richard Kahn (IBS, Grenoble)  
 Clemens Schulze-Briese (participant 7)  
 Marc Schiltz (EPFL, Lausanne)  
 Colin Nave (participant 2)  
 Lilian Jacquamet (IBS/FIP, Grenoble)  
 Martin Walsh (MRC France, Grenoble)  
 Dominique Bourgeois (IBS, Grenoble)  
 Ian Tickle (Astex Technology, Cambridge)  
 Marcel Knossow (LEBS, Gif sur Yvette)  
 Oleg Chubar (participant 8)  
 Guy Schoen (participant 5)  
 Roger Fourme (participant 8)  
 Eric Girard (participant 8)  
 Felix Rey (VMS, Gif sur Yvette)

**Workshop 4:** "Macromolecular crystallography, from measurements to model" EMBL Hamburg, October–November 2005. Organisers: Dr. Victor Lamzin (participant 3).

Workshops for following periods will be decided at coordination meetings in the interim. Some suggestions from network participants follow:

*Tools and techniques to design the ideal construct for protein expression, Vienna, Austria.* Organiser Kristina Djinovic (participant 6)

*Phasing with soft X-rays, Vienna, Austria.* Organiser Kristina Djinovic (participant 6)

#### **8.N2.4 Expected outcome**

The workshops will have a very similar outcome to N1 (Theoretical Schools), except that here the emphasis is on practical skills, thus the workshops will have particular importance for the synchrotron service providers, where practical abilities in data collection and structure solution are of prime importance in an era where these processes can be carried out in hours rather than months or years as previously. In this respect such workshops are of particular importance for the integration of MX activities in Europe. In addition the workshops provide valuable feedback to the organisers and tutors on how well their methodological and practical solutions work in the hands of the user community. Thus information is disseminated both "downwards" from developers and providers to users and "upwards" from users to developers and providers.

## **8.N3 Activity N3: Integration Workshops**

### **8.N3.1 Description and objectives of the activity**

The competitiveness of MX in Europe in relation to e.g. the USA is crucially dependent on the exchange of scientific ideas between methods developers, synchrotron radiation providers and representatives of the user community, which is the objective of activity N3. There are many aspects of infrastructure provision for MX that will benefit from a culture of cooperation. The integration workshops are a good starting point for collaborations and exchange of ideas, which in this case is lateral rather than vertical in the cases of the Theoretical Schools (activity N1) and Practical Workshops (activity N2).

These workshops will take place over approximately one and a half days. The venue for meetings will be one of the participating infrastructure facilities (participants 1–4, 7–10), on a rotating basis. All attendees will be notified of the date and place at least four months in advance. Presentations on new developments from hardware and software developers will be given. Furthermore there will be presentations of the activities at *all* synchrotrons, with sufficient time for discussion and questions. There will be approximately 40–50 participants at each Integration Workshop. One or two delegates will represent each of the consortium members. In addition the Scientific Advisory Group, representing the user community, will be invited to participate in order to speed outward communication of the latest developments within MAX-INF2 and inward communication of the developing needs of the users. Invited speakers from outside the network will always be invited, in order for the network to obtain information on important developments elsewhere. The majority of participants will be at the group leader/senior researcher level, providing a wealth of expertise. These workshops will be used to identify additional common developments and MAX-INF2 will ensure that these developments progress, e.g. by providing infrastructure to facilitate communication (e.g. activity N4). This aspect has been highly successful in MAX-INF, e.g. with the developments in the DNA project.

Another aim of the Integration Workshops will be to extend the UK-based CCP4 model of cooperation to MX software development in general within the EU. There is already a critical mass of software development as represented by the CCP4 suite of programs, which is used extensively around the world. The CCP4 suite is a collection of programs donated by many people working on methods and code development. A Graphical User Interface (GUI) has been developed within CCP4 which provides the opportunity for further integration of software from the perspective of the user, without removing the independence of individual software suppliers. The GUI provides an excellent framework within which further cooperation between European software developers can take place, and wider development and exploitation of the GUI will be addressed by the network, directed at high throughput MX.

### **8.N3.2 Participants in the activity**

The meetings will be organised by participants 1, 3, 4 and 6. All participants will attend, with particular roles as described in 8.N3.1.

**8.N3.3 Outline implementation for the full duration of the activity (including milestones and deliverables)**

	<b>Year 1</b>	<b>Year 2</b>	<b>Year 3</b>	<b>Year 4</b>	<b>Year 5</b>
<b>deliverable</b>		Integration Workshop 1	Integration Workshop 2	Integration Workshop 3	Integration Workshop 4

**8.N3.4 Expected outcome**

This activity will produce a heightened awareness of the activities of other network participants, lead to a high degree of integration of hardware and software development, this avoiding unnecessary duplication of effort due to ignorance of current trends. The presence of user representatives (both academic and industrial) in the form of the Scientific Advisory Group will ensure that the information is quickly disseminated to the user community, as well as enabling rapid feedback into the development process.

**8.N4 Activity N4: Web site****8.N4.1 Description and objectives of the activity**

Macromolecular crystallographers already use the Internet and electronic communication extensively, and these are the chosen media for dissemination of information in MAX-INF2. The MAX-INF web site was set up ([www.ccp4.ac.uk/maxinf](http://www.ccp4.ac.uk/maxinf)) to act as a repository for network-related documents, and to provide the community with a single point of reference for schools and workshops organised by the network. An email distribution list has also been set up to coordinate network activities. These activities will be continued and developed in MAX-INF2. The web pages are generated by PHP scripts which allow a degree of automation. In particular, network members can upload information to the web site through simple form-based interfaces. New interfaces will be added as required. The web site will act as a forum for integration activities. If there is sufficient demand, a "Wiki" will be set up for discussion of integration activities, as has been done for other projects ([www.ytbl.york.ac.uk/ehtpx](http://www.ytbl.york.ac.uk/ehtpx)). Specific links to the home pages of the participating members will be established and the outcome will be a network of centres, or a "virtual centre", a resource easily accessible by all macromolecular crystallographers in Europe. Programming support will be provided by existing CCP4 staff at Daresbury Laboratory (participant 2).

**8.N4.2 Participants in the activity**

Participant 2

**8.N4.3 Outline implementation for the full duration of the activity (including milestones and deliverables)**

	<b>Year 1</b>	<b>Year 2</b>	<b>Year 3</b>	<b>Year 4</b>	<b>Year 5</b>
<b>Deliverable</b>	Functioning web site	Maintenance of web site	Maintenance of web site	Maintenance of web site	Maintenance of web site

**8.N4.4 Expected outcome**

The web site will smooth the functioning of the coordinating activity and will therefore enhance the productivity and expected outcomes of activities N1–N3. It will also function as an information point for the whole MX community in Europe, informing about the latest technical and methodological developments as well as the currently available workshops and schools.