

Modelling and Simulation Core Submission Form

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| **Applicant Details** | | | | | | | | | | | | | | |
| **Name** | |  | | | | | | | | | | | | |
| **Address** | |  | | | | | | | | | | | | |
| **Contact details** | | Telephone | | | | | | | | | | | | |
| Email | | | | | | | | | | | | |
| **Overview/Strategy** | | | | | | | | | | | | | | |
| **Brief description of context and supporting data** (please include the drug name, target disease and use case, and any relevant information relating to special handling or stability). | |  | | | | | | | | | | | | |
| **Route of Administration** | | | | | | | | | | | | | | |
| **Expected route of delivery**  (please tick more than one if relevant) | | * Subcutaneous (please specify): \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_ * Intramuscular (please specify): \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_ * Transdermal (please specify): \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_ * Oral (please specify): \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_ * Other (please specify): \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_ | | | | | | | | | | | | |
| **Device technology**  (please tick more than one if relevant) | | * None: \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_ * Implant (please specify): \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_ * Microneedle patches (please specify): \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_ * Intracellular depot (please specify): \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_ * Other (please specify): \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_ | | | | | | | | | | | | |
| **Formulation** | | | | | | | | | | | | | | |
| **Type of formulation** (please tick more than one if relevant) | | * Inorganic (please specify): \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_ * Lipid-based (please specify): \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_ * Solid drug nanoparticle (please specify):\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_ * Polymeric (please specify): \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_ * In situ forming depot (please specify): \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_ * Aqueous solution: \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_ * Other (please specify): \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_ | | | | | | | | | | | | |
| **Characteristics** | |  | | | | | | | | | | **Not available** | | |
| Chemical composition | |  | | | | | | | | | | € | | |
| Nanoformulation size | |  | | | | | | | | | | € | | |
| Nanoformulation charge | |  | | | | | | | | | | € | | |
| **Drug** **Physicochemical Properties** | | | | | | | | | | | | | | |
| **Properties** | | **Value** | | | | | | | **Notes** | | | **Not available** | | |
| Molecular weight | |  | | | | | | |  | | | € | | |
| logP | |  | | | | | | |  | | | € | | |
| Protein binding | |  | | | | | | |  | | | € | | |
| pKa | |  | | | | | | |  | | | € | | |
| Acid/base | |  | | | | | | |  | | | € | | |
| Blood to plasma ratio | |  | | | | | | |  | | | € | | |
| Solubility (water) | |  | | | | | | |  | | | € | | |
| **Supporting Pharmacology Data** | | | | | | | | | | | | | | |
|  | | | **Value** | | | | | | **Notes** | | | | **Not available** | |
| Target concentration (e.g Ctrough target or PAIC90) | | |  | | | | | |  | | | | €  €  € | |
| Caco-2 cells apparent permeability (cm/s) | | |  | | | | | |  | | | |
| Dissolution/drug release rate | | |  | | | | | |  | | | |
| **Metabolism/Elimination** | | | | | | | | | | | | | | |
| **Please provide a brief description of the metabolism/elimination processes** (if known) | | | |  | | | | | | | | | | |
| **Phase I in vitro metabolism** (indicate the CYP isoform) | | | | | | | | | | | | | | |
| **Enzyme** | | | | **Km** | | | **Vmax** | | | | **Clint** | **Not available** | | |
|  | | | |  | | |  | | | |  | € | | |
|  | | | |  | | |  | | | |  | € | | |
|  | | | |  | | |  | | | |  | € | | |
| **Phase II in vitro metabolism** (indicate the metabolism enzymes) | | | | | | | | | | | | | | |
| **Enzyme** | | | | **Km** | | | **Vmax** | | | | **Clint** | **Not available** | | |
|  | | | |  | | |  | | | |  | € | | |
|  | | | |  | | |  | | | |  | € | | |
|  | | | |  | | |  | | | |  | € | | |
| **Other mechanisms of clearance (e.g. renal, MPS, RES)** | | | | | | | | | | | | | | |
| **Mechanisms** | | | | **Value** | | | | **Notes** | | | | **Not available** | | |
|  | | | |  | | | |  | | | | € | | |
|  | | | |  | | | |  | | | | € | | |
| **Pre-clinical Pharmacokinetic Data** (provide as relevant) | | | | | | | | | | | | | | |
| **Species** | **Route of administration** | | | | **AUC** | **Cmax** | | | | **Clearance** | | | | **Volume of distribution** |
|  |  | | | |  |  | | | |  | | | |  |
|  |  | | | |  |  | | | |  | | | |  |
|  |  | | | |  |  | | | |  | | | |  |
| **Clinical Pharmacokinetic Data** (provide as relevant) | | | | | | | | | | | | | | |
| **Route of administration** | | | | | **AUC** | **Cmax** | | | | **Clearance** | | | | **Volume of distribution** |
|  | | | | |  |  | | | |  | | | |  |
|  | | | | |  |  | | | |  | | | |  |