

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): \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_
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| **Device technology**(please tick more than one if relevant) | * None: \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_
* Implant (please specify): \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_
* Microneedle patches (please specify): \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_
* Intracellular depot (please specify): \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_
* Other (please specify): \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_
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| **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): \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_
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| **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** |
|  |  |  |  |  |
|  |  |  |  |  |