

GSRS Beyond Substances that Invitro Pharmacology

Version 3.1

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OFFICE OF DATA, ANALYTICS, AND RESEARCH

ORGANIZING INFORMATION

FDA has the most important/valuable repository of human biological and product data but limited integration though rapidly improving.

Submission process

- Paper
- PDFs

Organizational

- Different Centers
- Different Contractors
- Business Process
- Lack of Data Standardization/Digitization

ORGANIZING INFORMATION

- **Substances are one of the key lynchpins for organizing information**
 - To accomplish this, substances need to be defined in a consistent and unambiguous manner
 - The identifier should stay with the substance throughout its entire regulatory lifespan
 - The identifier can be used to tie substances to products, applications, clinical trials, and adverse events, etc.

BEYOND SUBSTANCES

- Names, Identifiers and Classification
- Relationships
- Products
- Applications
- Clinical Trials
- Adverse Events
- Impurities
- Manufacturing Module
- Invitro Pharmacology

NAMES, IDENTIFIERS AND CLASSIFICATION

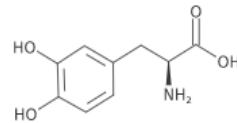
- Extensive list of Curated Names (company codes, common names and systematic names). (Over 1 million)
- Identifiers and Classification Codes (Over 1 million)
- Many Identifiers and Classification IDs have Linkouts
- Identifiers
 - Inxight, Pubchem, EPA CompTox, ECHA, Wikipedia, Drug Bank
- Classification
 - ATC, NCI Thesaurus, FDA Orphan Drug

BEYOND SUBSTANCES

- ATC Level 1
- Record Status
- Substance Type
- Source Tag
- Domain
- Code System
- ATC Level 2
- ATC Level 3
- ATC Level 4
- WHO-SDG Level 1
- WHO-SDG Level 2
- Application Center
- Application Type

LEVODOPA

ABSOLUTE



Names: LEVODOPA ✓
 (-)-3-(3,4-DIHYDROXYPHENYL)-L-ALANINE
 (-)-L-AMINO-.BETA.-(3,4-HYDROXYBENZENE) PROPIONIC ACID
 ADVANCED CARE/MULTICARE INTERVENTION (ACP/MCP) COMPONENT LEVODOPA
[See 51 More](#)

Codes: **BDNUM** : 0010264AA
CAS : [59-92-7](#)
WHO-ATC : [N04BA01](#), [N04BA03](#), [N04BA02](#)
EVMPD : SUB08468MIG
LIVERTOX : [NBK548734](#)
[See 33 More](#)

Relationships: 35
Mol. Weight: 197.19
Formula: C₉H₁₁NO₄

Substance Hierarchy

> [LEVODOPA](#)

Application Count:
[CDER GSRS: 315](#)
[CDER Integrity: 253](#)

Product Count:
[HEALTH CANADA: 31](#)
[SPL \(Active\) : 425](#)

Clinical Trial Count:
[223](#)

Adverse Event Case Count:
[77571](#)

466270600J

[Inight Drugs](#)

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Validated By: DJS
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466270600J
 {ACTIVE MOIETY}

SINGLE SUBSTANCE DATA

- Overview >
- Products, Applications, Clinical Trials, Adverse Events, Impurities Specs >
- Substance Hierarchy >
- Chemical Structure >
- Names And Synonyms 55 >
- Codes - Classifications 22 >
- Codes - Identifiers 29 >
- Relationships Visualization >
- Relationships: Active Moiety 1 >
- Relationships: Metabolites 9 >
- Relationships: Impurities 16 >
- Relationships: Constituents 1 >
- Relationships 8 >

Definitional Access [Public definition](#)

Products, Applications, Clinical Trials, Adverse Events, Impurities Specs ^

< Product (31)		Application (327)		Clinical Trial (230)		Clinical Trial Europe (5)		Adverse Event PT (55) >	
HEALTH CANADA		SPL							
HEALTH CANADA		Export All Products							
Product ID	Product Name	Labeler Name	Country	Status	Product Type	Ingredient Type	Application Number		
98863 	SANDOZ LEVODOPA-CARBIDOPA-ENTACAPONE	SANDOZ CANADA INCORPORATED		APPROVED		Active Ingredient			
98862 	SANDOZ LEVODOPA-CARBIDOPA-ENTACAPONE	SANDOZ CANADA INCORPORATED		APPROVED		Active Ingredient			
98861 	SANDOZ LEVODOPA-CARBIDOPA-ENTACAPONE	SANDOZ CANADA INCORPORATED		APPROVED		Active Ingredient			
98860 	SANDOZ LEVODOPA-CARBIDOPA-ENTACAPONE	SANDOZ CANADA INCORPORATED		APPROVED		Active Ingredient			
98859 	SANDOZ LEVODOPA-CARBIDOPA-ENTACAPONE	SANDOZ CANADA INCORPORATED		APPROVED		Active Ingredient			

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Definitional Access [Public definition](#)

Products, Applications, Clinical Trials, Adverse Events, Impurities Specs ^

		Application (327)	Clinical Trial (230)	Clinical Trial Europe (5)	Adverse Event PT (5549)	Adverse
Adverse Event PT		Export		Analysis by Substance		
PT Term	Prim SOC ↑	Case Count	PT Count ↓	PRR		
DYSKINESIA	NERVOUS SYSTEM DISORDERS	77571	6515 <small>FAERS Public Dashboard</small>	48.74		
DEATH	GENERAL DISORDERS AND ADMINISTRATION SITE CONDITIONS	77571	5020 <small>FAERS Public Dashboard</small>	1.55		
PARKINSON'S DISEASE	NERVOUS SYSTEM DISORDERS	77571	4011 <small>FAERS Public Dashboard</small>	81.66		
HALLUCINATION	PSYCHIATRIC DISORDERS	77571	3780 <small>FAERS Public Dashboard</small>	12.97		
HALLUCINATION	PSYCHIATRIC DISORDERS	77571	3780 <small>FAERS Public Dashboard</small>	12.97		

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RELATIONSHIPS

- Active Moiety, Salt/Solvate, Impurities
- Targets and Target Organisms
 - Inhibitors, Agonists, Inverse Agonist etc.
- Off-Target
 - Safety (HERG)
 - Plasma Protein Binding
- Metabolism, Transporters and Metabolites
 - Inhibitors, Substrates and Inducers
 - Active Metabolites, Prodrugs, Presence (Plasma, Urine, Feces etc)

PRODUCT MODULE (MICROSERVICE)

Register New Product

Product Overview ^

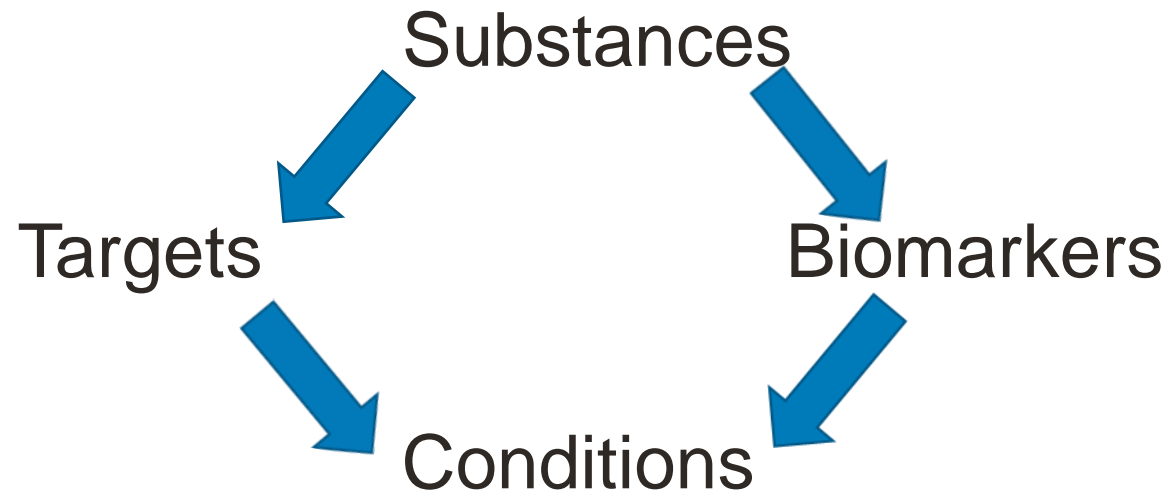
Administravail Pharmaceutical Dosage Form CAPSULE ▼	Route of Administration BUCCAL ▼	Unit of Presentation ▼
Country Code ▼	Language ▼	Shelf Life
Number of Manufacture Item ▼	Manufacturer Name	Manufacturer Code
		Manufacturer Code Type ▼
		Storage Conditions

Product Provenance 0 + ADD NEW ^

Manufacture Item 0 → Lot → Ingredient + ADD NEW ^

FUTURE MODULES (MICROSERVICES)

- In-Vitro Preclinical Pharmacology
- Toxicology
- Biomarkers
- Conditions (Clinical Particulars)



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