

**CEFIC LRI Workshop
on AMBIT and READ-ACROSS
21 Jan 2016**

AMBIT Demonstration



1. Basic function of AMBIT



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Log in

Search structures and associated data

Search substances by identifiers

Search substances by endpoint data

Import&Export

Toxtree predictions

2: Assessment Workflow Read Across

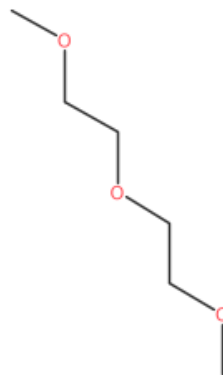


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Ambit assessment:

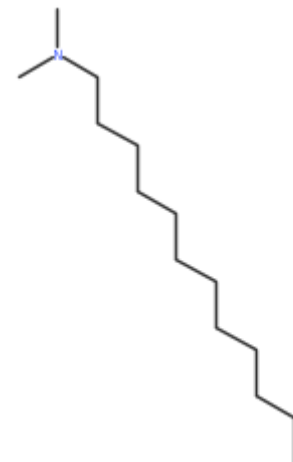
1. Category Glymes

- Initial target: diglyme
- CAS: 111-96-6
- EC: 203-924-4
- SMILES: COCCOCCOC



2. Category Dimethyl Amines

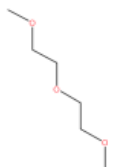
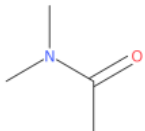
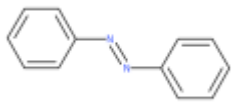
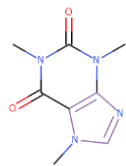
- Initial target: N,N-dimethyldodecan-1-amine
- CAS: 112-18-5
- EC: 203-943-8
- SMILES: CCCCCCCCCCCCN(C)C



Structure examples



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	CAS	Name	SMILE	Remark
	111-96-6	diglyme	COCCOCCOC	With substance data
	127-19-5	dimethylacetamide	CC(=O)N(C)C	With derek data
	103-33-3	Diphenyldiazene	C1=CC=CC=C1N=NC=C2C=CC=CC=2	Azo compound, for structure draw, similarity and substructure search
	58-08-2	Caffeine	CN1C=NC2=C1C(=O)N(C)C(=O)N2C	EPA FHM, DEREK

Substance examples



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Substance Name	UUID	Public Name	Composition
Glymes_Diethylene glycol dimethyl ether_(DEGDME, Diglyme)_ICS_MSe_DE71	IUC5-a438545b-3c6c-403f-83e6-5cd2756d77d6	Diglyme	Monoconstituent substance Containing diglyme (CAS 111-96-6) as constituent
Glymes_Ethylene glycol dimethyl ether_(EGDME, Monoglyme)_ICS_MSe_DE71	IUC5-eb8957ab-538b-48b6-a024-e9875fbd48b1	Monoglyme	Monoconstituent substance Containing monoglyme (CAS 110-71-4) as constituent
CLN_N,N-dimethyl-C12-14-(even numbered)-alkyl-1-amines	IUC5-03298b59-d29b-4670-a92a-c70f2bceec52	N,N-dimethyl-C12-14-(even numbered)-alkyl-1-amines	UVCB Containing: CAS112-18-5; 112-69-6 etc. as constituent