United States Environmental Protection Agency

ACToR – Aggregated Computational Toxicology Resource

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Office of Research and Development
National Center for Computational Toxicology

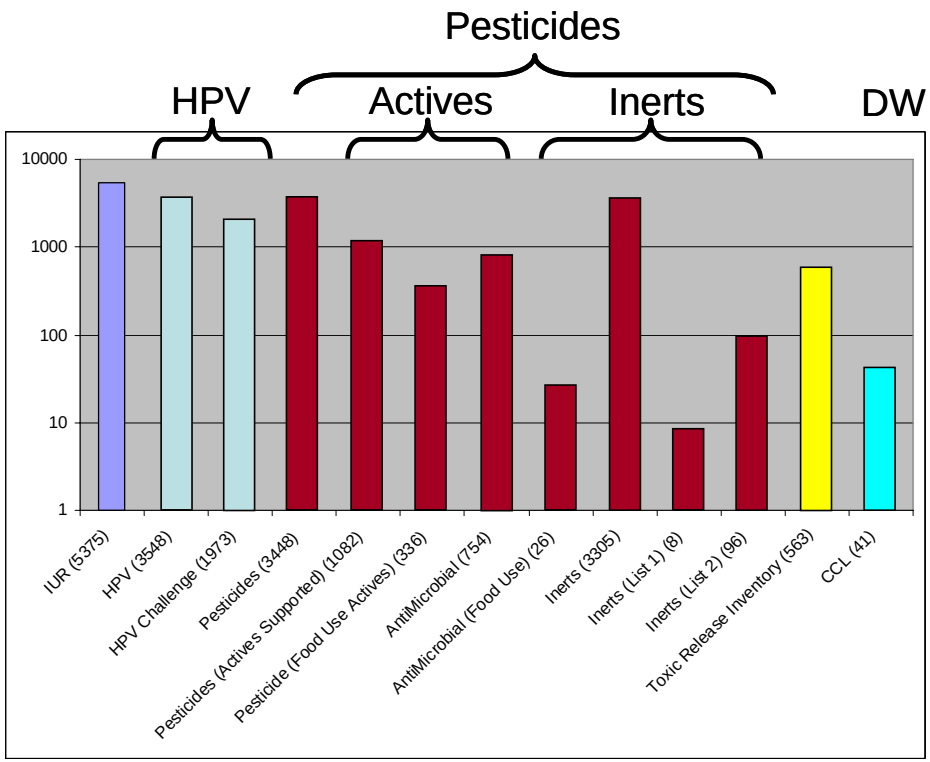
United States Environmental Protection Agency

"…to integrate modern computing and information technology with molecular biology to improve Agency prioritization of data requirements and risk assessment of chemicals"

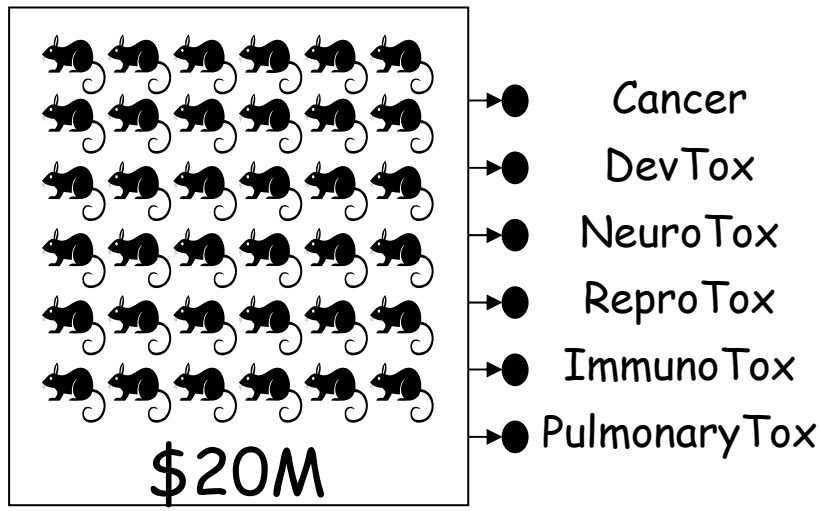
www.epa.gov/ncct

ToxCast Addresses the Critical Need for Prioritization

Too Many Chemicals



Too High a Cost



Limited Data is Available on Chemicals of Interest to the EPA

List	**TOXCAST1 (408)**	SIDS1 (507)	NTPBSI2carc (659)	NTPBSI2dev (61)	NTPBSI2repro (101)	AcuteTox1 (103)	ATSDR_CERCLA1 (275)	EPADNT1 (79)	GRADN1 (72)	IMMTOX1 (87)	IRISSI1 (536)	REPDOSE1_ID (422)	REPROTECT1_ID (56)	TCNCGC1 (367)	ZEBET1 (359)	NTPBSI2genotox (2071)	AREXCH1 (153)	CPDBAS1 (1445)	CSTARC1 (133)	CTEPPS1 (60)
HPV (2843)	1	14	6	1	1	1	2	0	0	1	6	9	0	1	4	19	1	8	1	0
HPV Challenge (1973)	1	17	9	1	2	1	3	1	0	1	8	12	0	1	4	24	1	10	1	0
IUR (5375)	1	8	4	1	1	1	2	0	0	0	3	5	0	1	2	14	0	6	0	0
TRI (577)	20	9	31	2	4	5	21	5	4	3	49	26	3	18	14	54	3	45	3	2
OPPIN Pesticide (3448)	10	2	6	1	1	2	3	2	1	1	9	4	1	9	4	12	1	9	1	1
OPPN Food Use Actives (336)	53	0	7	0	0	2	5	13	4	1	32	2	1	49	4	12	2	12	1	2
OPPN Antimicrobial (754)	5	4	10	1	2	3	6	2	2	2	9	8	2	5	9	21	2	13	1	0
OPPN Antimicrobial Food Use (26)	65	0	19	0	0	8	15	27	15	0	46	4	8	65	19	42	4	46	0	4
OPPN Inerts (3305)	1	5	5	1	1	1	1	0	0	0	3	5	0	1	3	12	1	7	1	0
INERTS List 1 (8)	25	38	100	13	25	13	50	0	0	0	100	100	0	25	38	100	13	75	0	0
INERTS List (96)	3	27	26	6	8	2	10	1	0	5	27	26	1	2	11	35	0	20	1	3
CCL (49)	31	6	37	2	2	0	43	14	10	2	67	20	2	29	18	51	0	41	4	8
EPA DWC (71)	27	14	58	6	8	15	75	7	10	11	92	37	4	21	31	63	10	65	6	10

% target lists covered by source data

ToxCast: Chemical prioritization

ToxCast™

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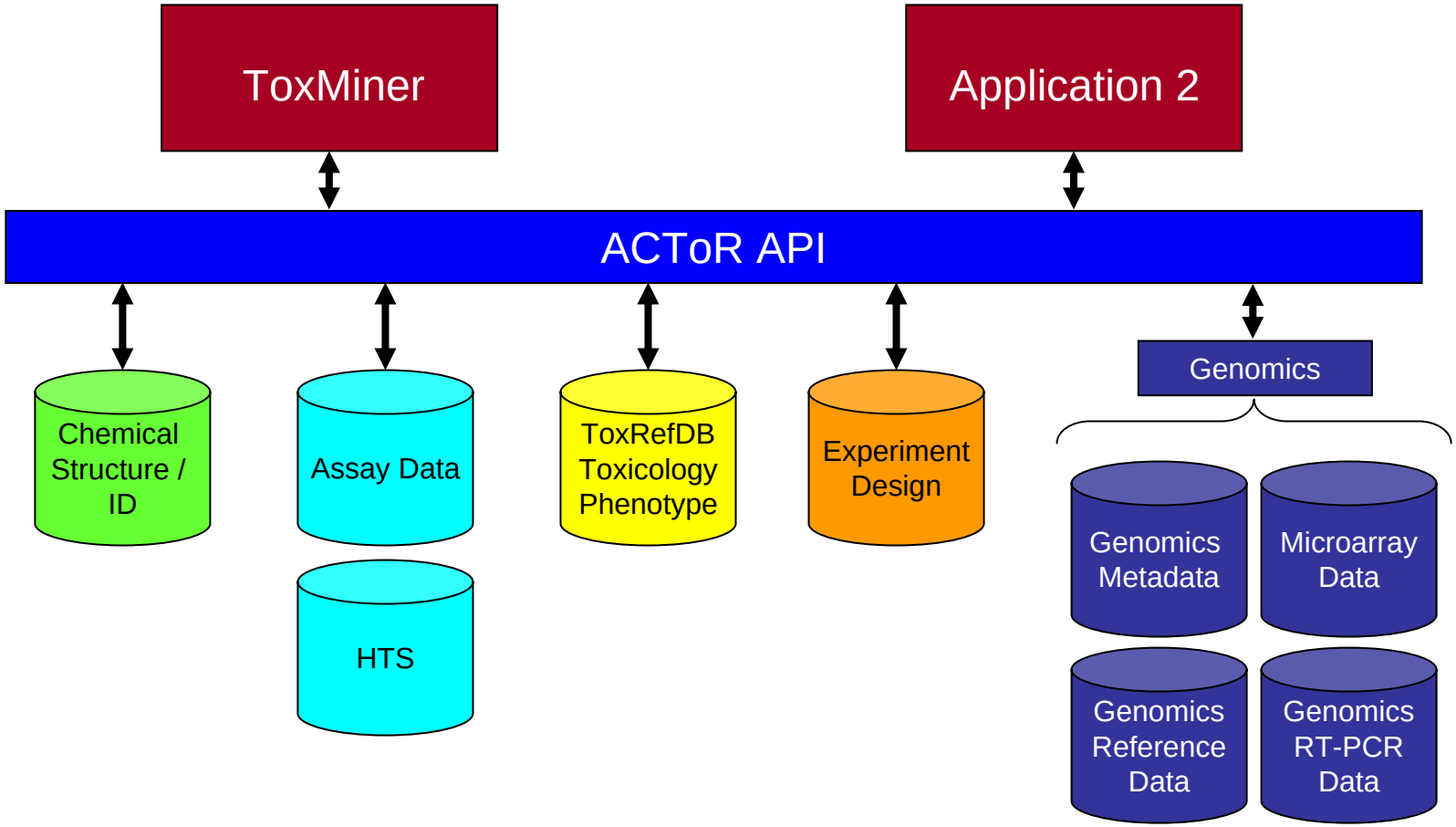
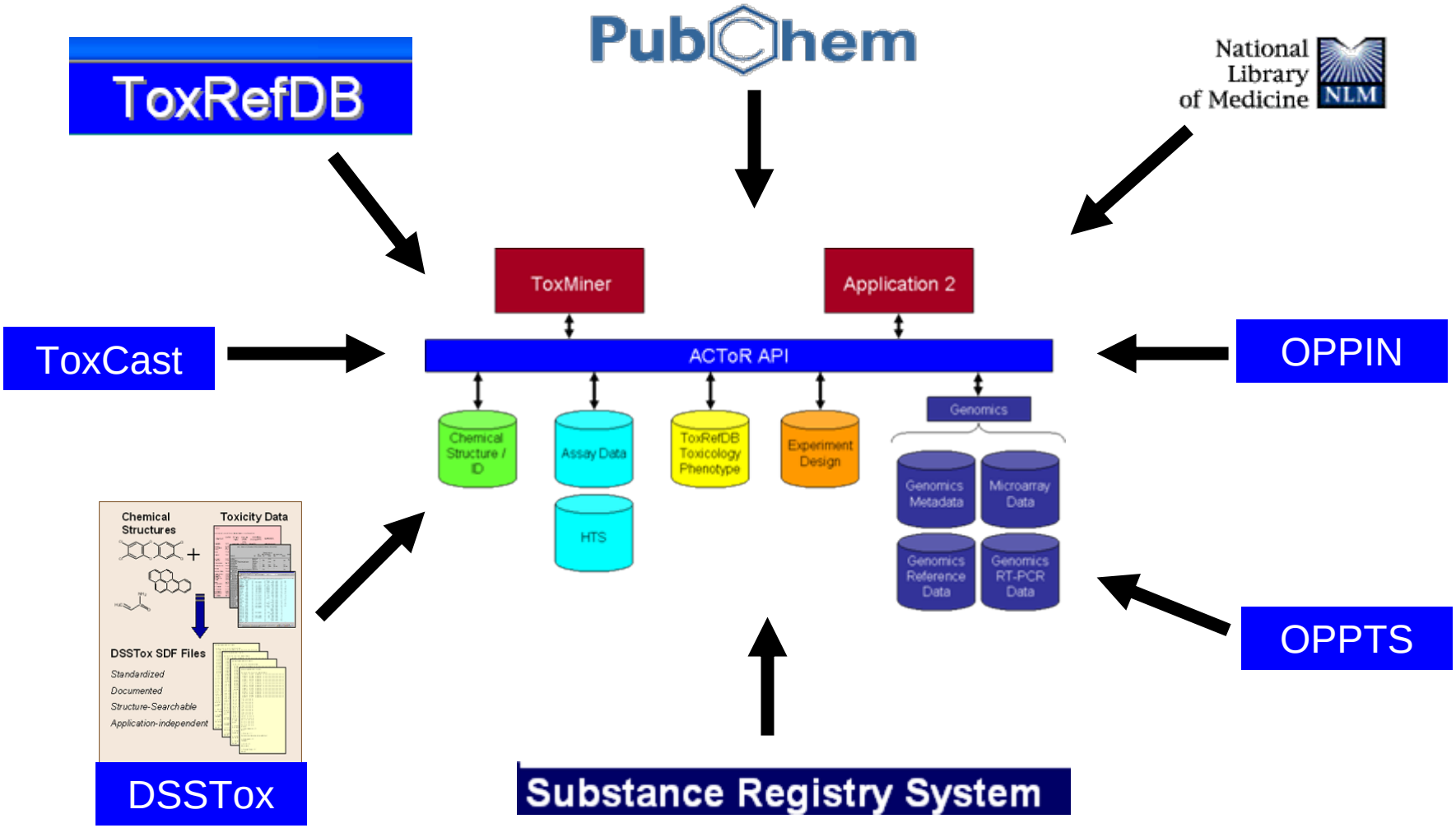
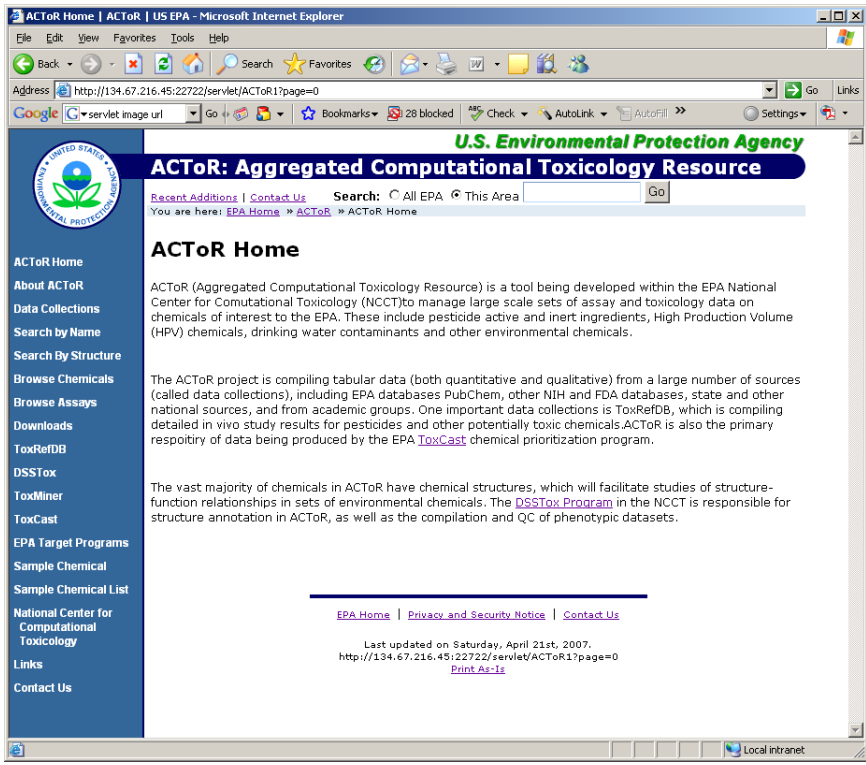


Addresses data needs of ToxCast and other EPA programs

ACToR Draws from Diverse Data Sources



ACToR Status

- Data Sources
  - 135 data sources
  - Many are currently just lists of chemicals
  - Need to retrieve and collate phenotype data
- Chemicals
  - >3 million
  - Most are from PubChem
  - >200,000 have some assay / phenotype data
- Tasks
  - Load existing data
  - Download & collate phenotype data
  - Finish beta version of web site
- Planned intranet beta release: May 21, 2007