

# AUGMENTED ANALYTICS

First simple-to-use AI innovating compounds, mixtures and processes









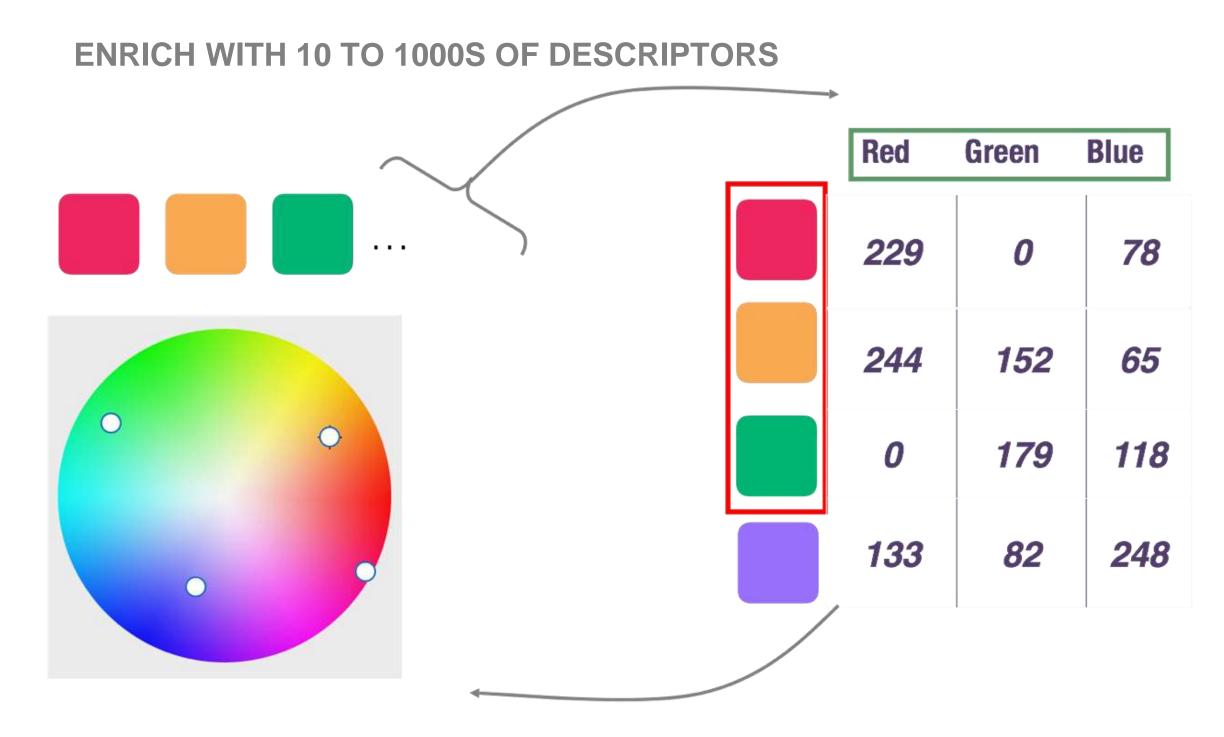




# HOW TO FIGHT THE COMBINATORIAL EXPLOSION?

# 

MAKE PREDICTIONS
FOR UNKNOWN
COMPOUNDS,
PRODUCTS,
SERVICES, ...

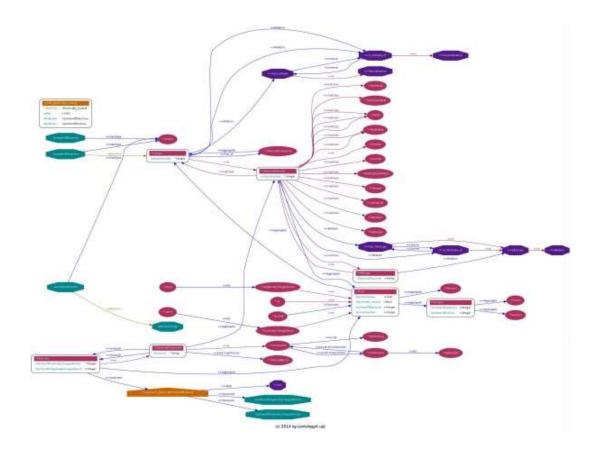


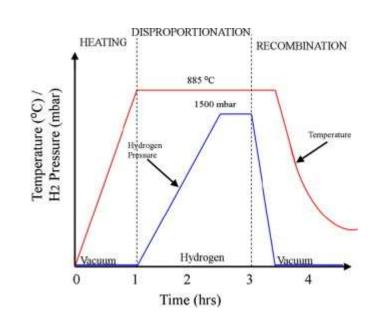
FROM CATEGORICAL TO CONTINUOUS SPACE

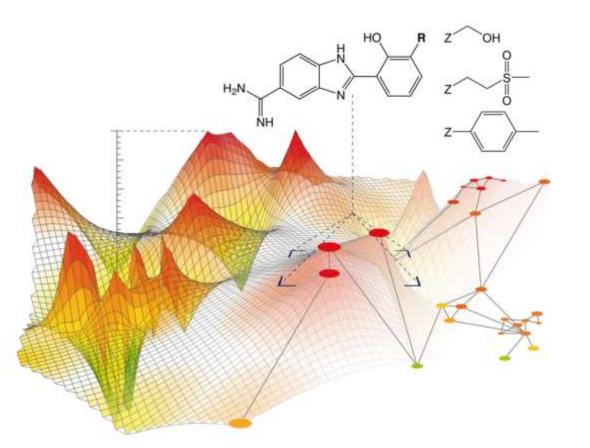


## DATASTORIES loves thousands of variables

- PROCESSING CONDITIONS
- COMPOUND INFORMATION
- Calculated properties
- Ontologies
- Formulations
- Spectra
- Chemical Spaces
- WEATHER CONDITIONS

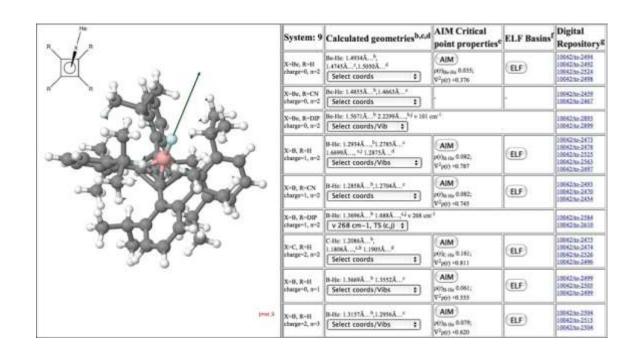




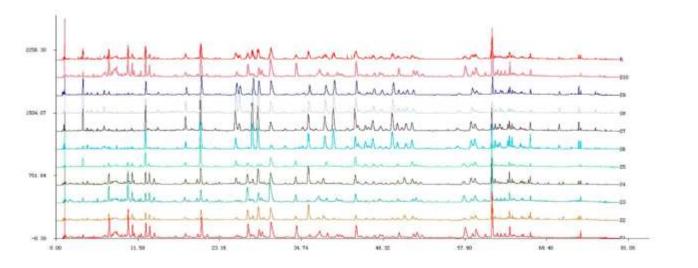




Lactic acid, CH<sub>3</sub>CH(OH)CO<sub>2</sub>H





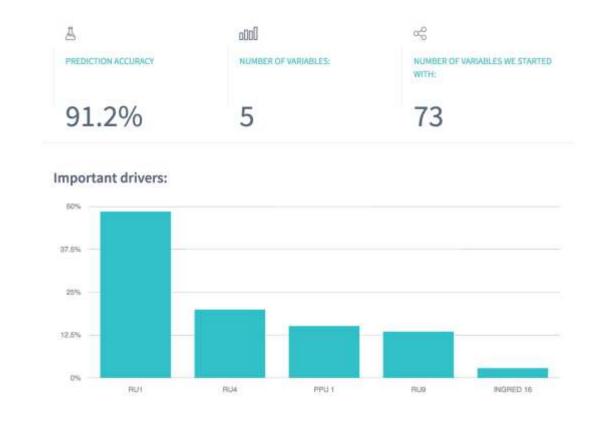




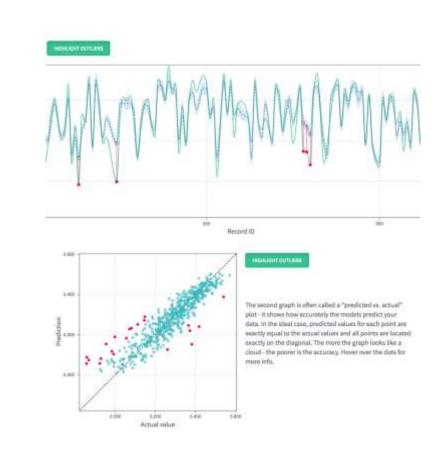




How is everything inter-connected?



From all inputs, which are the dominant ones?



What are the exceptions to the rule?



d l	A	В	C	D	E	F	G	Н	1	1	К	L	M	N	0	P	Q	R	S	T	U	٧	w	
	TR-1	TR-2	TR-3	TR-4	TR-5	TR-6	TR-7	TR-8	TR-9	TR-10	TR-11	TR-12	TR-13	TR-14	TR-15	TR-16	TR-17	TR-18	TR-19	TR-20	TR-21	TR-22	TR-23	
37	,76826	0	10,72934	0	0	0	0	0	0	10,25688	0	0	0	4,102712	10,25428	0	15,76425	0	0	0	0	0		0
34	,95269	0	0	S 194846	0	0	0	0	0	13,76054	0	0	0	0	15,82367	0	7,150036	0	0	.0	7,738014	0		0
34	,55571	0	0	0	8,750768	0	0	0	0	16,11571	0	0	0	0	13,09145	0	15,70946	0	0	4,029879	0	0		0
28	,82497	0	0	7,635113	0	0	0	0	0	7,703272	0	0	0	35,38289	0	0	9,053304	0	0	3,706599	0	0		0
45	,48735	0	0	0	5,725948	0	0	0	0	0	0	0	0	10,38714	5,767717	0	25,38208	0	0	0	0	0		0
7 2	0,3436	0	7,000182	0	0	0	0	0	0	27,55418	0	0	0	24,85957	11,73996	0	0	0	0	0	0	0		0
3 31	,11202	0	5,220457	0	0	0	0	0	0	34,54729	0	0	0	0	14,63688	0	4,95252	0	0	0	0	0		0
32	,37367	0	0	0	12,12199	0	0	0	0	11,27032	0	0	0	0	17,04875	0	0	0	0	5,883745	0	0	8,3629	1
0 21	,08679	0	0	12,0013	D	0	0	0	0	39,11747	0	0	0	2,547448	16,09833	0	0	0	0	0	0	0		0
1 34	,04005	0	0	9,913737	0	0	0	0	0	10,49266	0	0	0	0	12,77843	0	9,564582	0	0	1,822931	0	0	6,84469	7
2 36	,87246	0	0	0	9,72228	0	0	0	0	0	0	0	0	0	11,65103	0	11,62069	0	0	0	11,75469	0		0
3 25	,65631	0	13,09147	0	0	0	0	0	0	22,20215	0	0	0	4,224551	10,02183	0	0	0	0	0	11,2843	0		0
4 22	,40442	0	8,783758	0	0	0	0	0	0	18,69243	0	0	0	33,04642	0	0	0	0	0	0	1,065661	0		0
5 34	,90682	0	0	12,90205	0	0	0	0	.0	7,474624	0	0	0	7,646666	0	0	4,598522	0	0	4,478193	8,636207	0		0
6 46	,17838	0	.0	8,227612	0	0	0	0	0	8,160793	0	0	0	0	4,116057	0	28,16221	0	0	0	0	0		0
7 4	3,4119	0	0	3,1644	0	0	0	0	0	0	0	0	0	0	0	0	29,1443	0	0	0	0	0		0
8 25	,68776	0	0	0	13,32756	0	0	0	0	1,712921	0	0	0	40,98206	0	0	8,509068	0	0	2,264378	0	0		0
9 22	,17325	0	0	0	15,51469	0	0	0	0	0	0	0	0	0	0	0	11,47414	0	0	36,63111	0	0	4,99163	7
0 44	,54397	0	0	2,907071	0	0	0	0	0	3,53224	0	0	0	0,920674	29,78012	0	0	0	0	1,827625	1,919983	0	1,54924	9
1 47	,52828	0	0	0	3,514452	0	0	0	0	0	0	0	0	0	0	0	10,74762	0	0	0	32,61489	0		0
2 32	,83928	0	0	4,120787	0	0	0	0	0	0	0	0	0	8,571727	43,62387	0	2,653173	0	0	0	0	0	2,83682	5
3 43	,98922	0	0	8,906335	0	0	0	0	0	1,80919	0	0	0	2,28944	0	0	3,211237	0	0	0	0	0	21,1252	2
4 44	,62924	0	0	12,16238	0	0	0	0	0	0	0	0	0	0	1,366464	0	3,985396	0	0	15,2404	0	0	1,40426	3
5 35	,54513	0	11,37611	0	0	0	0	0	0	0	0	0	0	4,709295	35,95016	0	0	0	0	1,819234	2,2117	0	2,10402	5
6 43	,85994	0	7,674158	0	0	0	0	0	0	3,437808	0	0	0	2,73932	0	0	3,013572	0	0	0	0	0	26,3539	2
7 47	,91409	0	3,122331	0	0	0	0	0	0	5,497414	0	0	0	2,203527	0	0	4,032631	0	0	0	0	0	31,9243	4
8 45	,80616	0	0	6,82948	0	0	0	0	0	0	0	0	0	0	0	0	9,056673	0	0	25,54012	0	0	2,24799	13
9 43	,13861	0	0	0	9,647631	.0	0	0	0	0	0	0	0	0	2,058998	0	5,899411	0	0	0	0	0	24,9353	1
0 43	,88031	0	4,496614	0	0	0	0	0	0	0	0	0	0	1,154935	0	0	6,648952	0	0	24,33565	0	0	3,21065	3
1 38	,72733	0	13,00038	0	0	0	0	0	0	2,672408	0	0		1,83461	0	0	2,974023	0	0	0	0	0	20,9206	14
2 4	5,6319	0	3,118648	0	0	0	0	0	0	1,63725	0	0	0	1,885133	0	0	4,721086	0	0	0	0,988732	0	27,8897	7
3 4	2,9275	0	0	7,7325	0	0	0	0	0	0	0	0	.0	0	0	0	27,5641	0	0	0	0	0		0
4 42	,61154	0	0	0	10,5919	0	0	0	0	0	0	0	0	0	0		29,56291	0	0	0	0	0		0
-01	7,1598	0	0	5,4685	0	0	0	0	0	0	0	0	0	0	0		21,0023	0	0	0	0	0		0
	,74313	0	0	9,770785	0	0	0	0	0	0	0	0	0	1,758895	0		5,565318	0	0	2,603289	33,21929	0		0
	52258	-0	15,04078	0	0	0	0	-0	0	3,423076	0	0		38,16451	11		9,450287	0	0	0	0	0		0

