

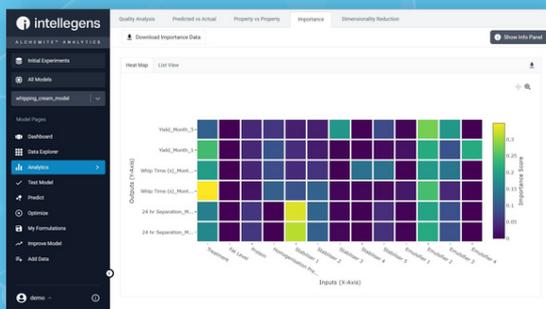
Machine learning for foods, beverages, and FMCG

Design and optimise formulated products, faster

Find solutions you may otherwise miss

Reduce the number of experiments by up to 90%

Innovate to meet market, regulatory, and sustainability requirements



Example analytic - understanding which ingredients impact key target properties

For foods, drinks, and fast moving consumer goods, such as cosmetics and personal care products, formulation development is critical. The success of a product and its cost, safety, and sustainability all depend on getting the right combination of ingredients and processing steps.

This presents formulation teams with a complex optimisation problem in which they need to balance the impact of formulation changes on varied outputs such as taste, texture, rheology, stability, appearance, and the costs and energy usage associated with raw materials and processing. Getting this right usually relies on costly, time-consuming experimental programs. Data often has gaps (is 'sparse') or is noisy, making it hard to analyse with conventional machine learning methods.

Alchemite™ is advanced machine learning software that can build models from real-world, sparse, noisy experimental and process data, where other machine learning methods fail. Identify vital relationships in the data. Design new chemistries and formulations. Propose optimal process parameters. And guide planning of experimental projects to dramatically reduce cost and time.

Emulsifier 3	Emulsifier 4	24 hr Separation_Month_1	24 hr Separation_Month_5	Whip Time (s)_Month_1	Whip Time (s)_Month_5	Yield_Month_1	Yield_Month_5
0.2000	0	Not Separated	Not Separated	406.0	405.0	3.320	2.860
0.2000	0	Not Separated	Not Separated (71%)	280.0	280.9 ± 44.8	2.800	2.695 ± 0.31
0	0	Not Separated (77%)	Not Separated (82%)	100.0	194.2 ± 32.5	1.690	2.161 ± 0.225
0	0	Not Separated	Not Separated	408.0	281.0	2.940	2.510
0.2000	0	Separated	Separated (79%)	413.0	334.6 ± 32	3.040	3.033 ± 0.182
0.2000	0	Not Separated	Not Separated (99%)	269.0	276.9 ± 36.5	2.710	2.953 ± 0.123
0.2000	0	Separated	Separated (92%)	201.0	296.5 ± 51.5	2.430	2.970 ± 0.115
0	0	Not Separated (85%)	Not Separated (88%)	135.0	186.7 ± 25.8	2.040	2.205 ± 0.184
0.2000	0	Not Separated	Not Separated (99%)	290.0	281.3 ± 41.5	2.600	2.932 ± 0.139
0.2000	0	Not Separated (73%)	Not Separated (73%)	202.0 ± 44	248.4 ± 53.5	2.412 ± 0.239	2.446 ± 0.354
0	0	Not Separated	Separated	245.0	211.0	2.400	2.370
0.2000	0	Separated (98%)	Separated (99%)	132.0	231.9 ± 45.9	2.450	2.350 ± 0.181
0.2000	0	Separated	Separated (93%)	211.0	266.0 ± 50.1	2.540	2.519 ± 0.266
0	0	Not Separated	Separated	337.0	300.0	3.210	2.900

The Alchemite™ Analytics platform provides scientists with quick, easy access to advanced machine learning and powerful graphical analytics via a web browser user interface. Here, the machine learning has predicted missing values in a food formulation dataset.

Case studies and white papers

Global dairy products leader, Yili used Alchemite™ to better understand their UHT whipped cream formulations. "We relatively quickly could drop out a number of the ingredients we had been testing... This wasn't obvious if you just looked at them one-by-one, because you always have some cross-interactions. This was a big learning and helped speed up development." intellegens.com/yili

Flavours and fragrances producer, IFF used the Alchemite™ method to study the sensory properties of compounds by analysing physicochemical and sensory data. "Its reliable uncertainty estimates gave us confidence to make critical project decisions". *J Comp-Aided Molecular Design* **35**, 1125-1140 (2021).

Adaptive design of experiments – As well as proposing optimal candidate formulations, Alchemite™ is used iteratively within experimental programs to suggest which set of experiments should be done next in order to most efficiently explore parameter space. This adaptive design of experiments has been shown to reduce experimental workloads by up to 90%. White paper at intellegens.com/experiment

Alchemite™ for formulated products

With the Alchemite™ software, formulators, chemists, and data scientists can:

- Gap-fill and validate sparse, noisy data from suppliers, experiment, simulation, and production
- Auto-generate models that identify key ingredient-property-process relationships
- Quantify uncertainty to support a rational business case for key decisions
- Design experimental programs, reducing the number of experiments by up to 90%
- Identify new or improved formulations and optimise process parameters
- Capture knowledge of formulation recipes as models for sharing and re-use.

Next steps

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