

Transformation and visualisation of high quantities of analytical data made easy



The challenge

High throughput process development to optimise a chiral synthetic step requires enantiomeric purity, achiral assay and related substances data from two different chromatographic systems. This leads to the following bottlenecks:

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- Sample processing using analytical software can take a long time with impure samples
- Data transformation
- Collation of separate data sets
- Generation of custom reports



How?

CatSci's analytical team employed Knime, a data analytics open source software to automate the transformation, visualisation and reporting of analytical data retrieved from the high throughput process development of a chiral synthetic step.



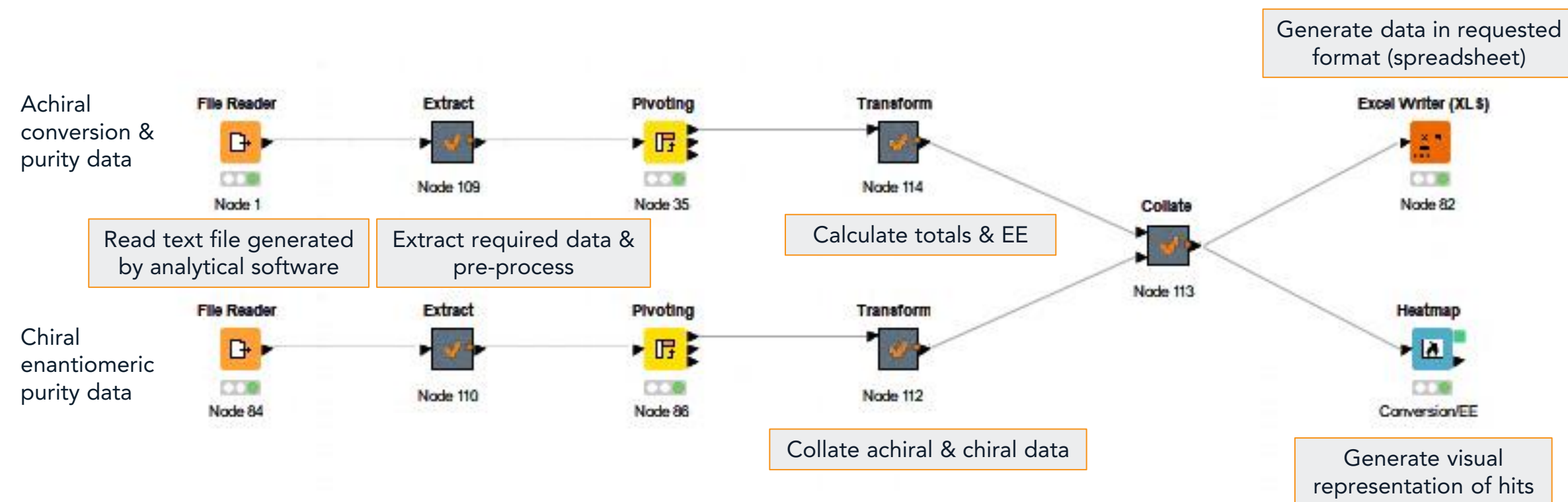
The achievement

A Knime workflow was quickly designed and optimised to address the data manipulation and processing to remove the bottleneck in the workflow. The results were automatically exported to excel for the customer to use.



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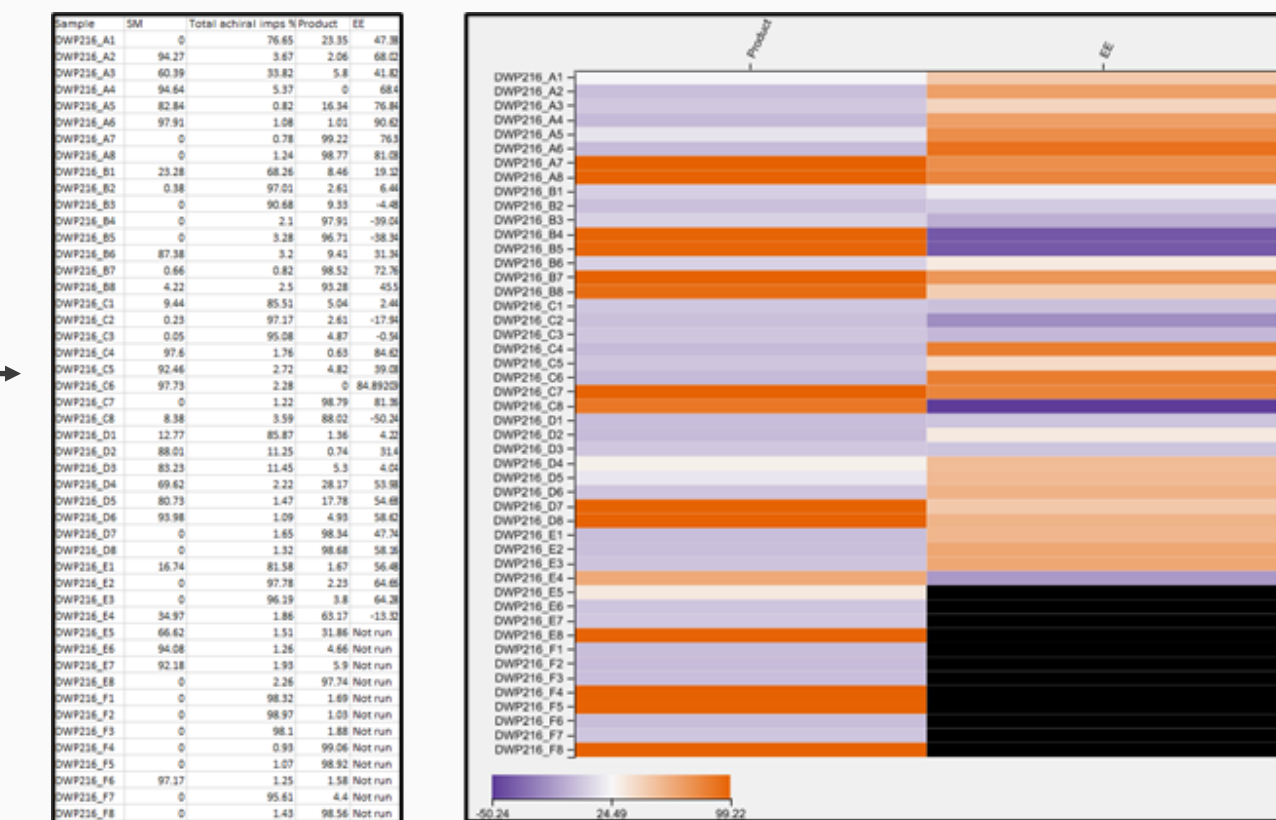
The Knime workflow



Input data (HPLC software)

Sample	SM	Total achiral impgs %	Product	EE
DWP216_A1	0	78.65	23.35	47.38
DWP216_A2	94.27	3.67	2.06	68.02
DWP216_A3	60.39	33.82	5.8	41.82
DWP216_A4	94.84	5.37	0	68.4
DWP216_A5	82.84	0.82	16.34	78.86
DWP216_A6	97.81	1.08	1.01	90.62
DWP216_A7	0	0.78	99.22	76.5
DWP216_A8	0	1.24	98.77	81.08
DWP216_B1	23.28	68.26	8.46	19.32
DWP216_B2	0.38	97.01	2.61	6.46
DWP216_B3	0	99.68	0.33	-4.48
DWP216_B4	0	2.1	97.91	-39.04
DWP216_B5	0	3.28	96.71	-88.34
DWP216_B6	87.38	3.2	9.43	81.36
DWP216_B7	0.66	0.82	98.52	72.78
DWP216_B8	4.22	2.5	93.28	45.5
DWP216_C1	9.44	89.51	5.04	2.46
DWP216_C2	0.23	97.17	2.61	-17.76
DWP216_C3	0.05	99.08	4.87	-0.34
DWP216_C4	97.6	2.76	0.63	84.42
DWP216_C5	92.46	2.72	4.82	99.08
DWP216_C6	97.73	2.28	0	84.89209
DWP216_C7	0	1.22	98.79	81.36
DWP216_C8	8.58	3.59	88.02	-50.24
DWP216_D1	12.77	89.87	1.36	4.22
DWP216_D2	88.01	11.25	0.74	31.4
DWP216_D3	83.23	11.45	5.3	4.05
DWP216_D4	69.62	2.22	28.17	53.98
DWP216_D5	80.73	1.47	17.78	54.48
DWP216_D6	93.58	1.09	4.93	58.62
DWP216_D7	0	1.65	98.34	47.74
DWP216_D8	0	1.22	98.68	81.36
DWP216_E1	16.74	83.58	1.67	54.48
DWP216_E2	0	97.78	2.23	64.48
DWP216_E3	0	99.19	0.8	64.28
DWP216_E4	34.97	1.86	63.17	-13.32
DWP216_E5	66.62	1.51	31.86	Not run
DWP216_E6	94.08	1.26	4.68	Not run
DWP216_E7	82.38	1.93	5.9	Not run
DWP216_E8	0	2.26	97.74	Not run
DWP216_F1	0	98.32	1.68	Not run
DWP216_F2	0	98.97	1.03	Not run
DWP216_F3	0	98.1	1.88	Not run
DWP216_F4	0	0.93	99.04	Not run
DWP216_F5	0	1.07	98.92	Not run
DWP216_F6	97.17	1.25	1.58	Not run
DWP216_F7	0	99.81	4.4	Not run
DWP216_F8	0	1.43	98.54	Not run

Output data (Knime workflow)



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