Electronic Supplementary Material (ESI) for Green Chemistry.

Supplementary Information

Cumulative complexity meta-metrics as an efficiency measure and predictor of PMI during synthetic route design

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1. Dataset compilation

The dataset used for analysis and model generation is shown in section 6 (120 compounds). Due to commercial limitations, we are unable to provide structures or structural identifiers.

A small number of datapoints were added (new data became available) or removed (found to be erroneous) after the model was generated and during the preparation of the manuscript. Based on this, there are some minor discrepancies between the graphs presented here (section 3) and those in the main manuscript.

Step count

Longest linear sequence and total steps have been generated using the guidance and criteria outlined in the main manuscript.

As discussed in the main manuscript, step count (either longest linear sequence [LLS] or total) was not included as a parameter for modelling due to the requirement for continuous values. Using ordinal step count values, test analyses showed a tendency for each individual step number to be assessed independently and assigned unique coefficients, ultimately resulting in highly complex models. Additionally, any predictive model developed using step count as a parameter would not be applicable in cases where the step count is a previously unseen value.

Step count was used solely for the calculation of linearity (L, see below) and data comparison/visualisation during analysis.

Linearity

Calculated using:

$$Linearity\ L = \frac{steps\ (LLS)}{steps\ (total)}$$

Ideality

Calculated manually for each datapoint and may be subject to interpretation in a small number of cases.[1]

Convergence

Calculated manually for each datapoint and may be subject to interpretation in a small number of cases.[2]

PMI

Used as the primary response for modelling and calculated using:

$$PMI = \frac{\sum m(input\ materials\ including\ water)}{m(product)}$$

[1] T. Gaich, P. S. Baran, *J. Org. Chem.*, **2010**, 75, 14, 4657.
[2] J. B. Hendrickson, *J. Am. Chem. Soc.*, **1977**, 99, 16, 5439.

ACS PMI Predicted values

Calculated using the online tool.[3] Assignment of reaction type is required which may be open to interpretation in some cases.

SCScore and ΣC_{SCS}

Individual SCScores were generated using the code provided by the authors.[4] Cumulative values for each compound were generated by summation of SCScores for the target compound and all preceding species along the longest linear sequence including the eventual starting material.

C_{M*} and ΣC_{M*}

A text file providing python code for the conversion of SMILES strings into C_{M*} values is provided in the supplementary information section. This code will also calculate other complexity metrics (C_M, C_{SE}) from the original paper by Proudfoot.[5] Cumulative values for each compound were generated by summation of C_{M*} values for the target compound and all preceding species along the longest linear sequence including the eventual starting material.

FMW

Calculated from the target molecular structure (using Chemdraw or BioviaDraw) excluding associated salts and solvates etc.

2. Approach to statistical modelling

Penalised regression methods were selected based on the following:

- Better suitability to small datasets (as in this case) than more popular machine learning methods, neural networks and decision trees
- Simpler interpretation of the effect of descriptor parameters on responses (PMI)
- Compatible with correlated descriptor parameters
- Effectively maximise influential parameters and remove non-influential parameters, ultimately leading to simpler models
- Implementation of resultant models into software systems is typically straightforward

Parameters from section 1 were modelled against PMI using JMP Pro 16.1. After reviewing earlier modelling output including all parameters from section 1, L, Σ_{CM*}, Σ_{CSCS}, and FMW were selected for inclusion in the model fitting. Many of the options and settings for this type of analysis are software specific but the following general points may be useful:

- Two model fitting personalities were investigated (main parameters only and main parameters with 2-parameter interactions)
- A random seed (9) was specified to allow repeat analysis in JMP to output the same statistical results
- Various response distributions were investigated - Normal, Cauchy, t[5], exponential, LogNormal, Gamma and Weibull.
- Various estimation methods were investigated - Lasso, Elastic Net and Double Lasso

[3] A. Borovika, J. Albrecht, J. Li, A. S. Wells, C. Briddell, B. R. Dillon, L. J. Diorazio, J. R. Gage, F. Gallou, S. G. Koenig, M. E. Kopach, D. K. Leahy, I. Martinez, M. Olbrich, J. L. Piper, F. Roschangar, E. C. Sherer, M. D. Eastgate, *Nat. Sustain.*, **2019**, 2, 1034.

[4] C. W. Coley, L. Rogers, W. H. Green, K. F. Jensen, *J. Chem. Inf. Model.*, **2018**, 58, 2, 252.

[5] J. R. Proudfoot, *Bioorg. Med. Chem. Lett.* **2017**, 27, 2014.

- Hereditary parameters were not enforced meaning parameters found in 2-parameter interactions were not required to be present as main parameters (FMW in this case).
- KFold(10) analysis was used to generate average tuning parameters allowing subsequent model refinement

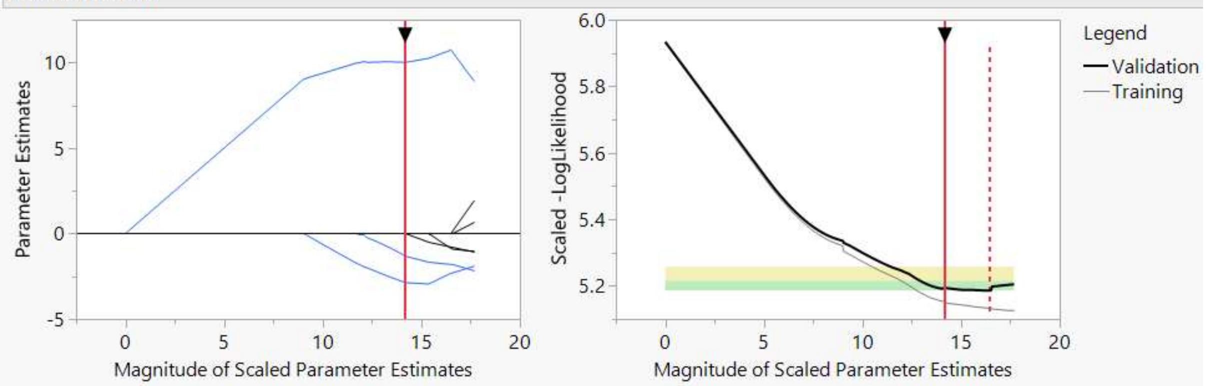
3. Model for PMI prediction

A large number of models were generated using the approach above. The eventual model for PMI prediction (below) was selected based on:

- Minimal estimate bias shown by a relatively even distribution of datapoints above and below the observed/predicted line
- Good estimate precision (density of datapoints close to the observed/predicted line)
- Subsequent analysis of the entire dataset showed a high coefficient of determination (R^2) as discussed in the main manuscript
- Simplicity of the model using only L, FMW and ΣC_{M*}

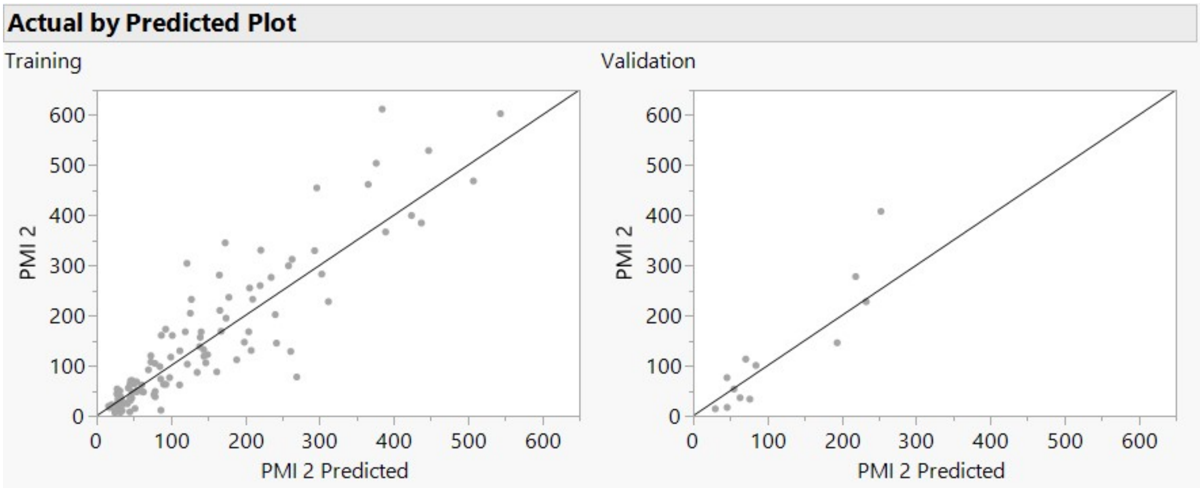
Weibull Adaptive Double Lasso with KFold Validation			
Model Summary		**Estimation Details**	
Response	PMI	**Number of Grid Points**	150
Distribution	Weibull	**Minimum Penalty Fraction**	0
Estimation Method	Adaptive Double Lasso	**Grid Scale**	Square Root
Validation Method	KFold		

Solution Path



Term	**Estimate**	**Std Error**	**Wald ChiSquare**	**Prob > ChiSquare**	**Lower 95%**	**Upper 95%**
Intercept	3.8791	0.2602	222.2912	<0.0001*	3.3691	4.3890
L	-0.8252	0.2406	11.7610	0.0006*	-1.2968	-0.3536
ΣC_{SCS}	0	0	0	1.0000	0	0
ΣC_{M*}	0.04581	0.0026	321.8488	<0.0001*	0.0408	0.0508
FMW	0	0	0	1.000	0	0
(L - 0.9173)*(ΣC_{SCS} - 11.9107)	0	0	0	1.000	0	0
(L - 0.9173)*(ΣC_{M*} - 37.4275)	0	0	0	1.000	0	0
(L - 0.9173)*(FMW - 311.2910)	0	0	0	1.000	0	0
(ΣC_{SCS} - 11.9107)*(ΣC_{M*} - 37.4275)	0	0	0	1.000	0	0
(ΣC_{SCS} - 11.9107)*(FMW - 311.2910)	0	0	0	1.000	0	0

(ΣC_{M^*} - 37.4275)*(FMW - 311.2910)	-0.0001	2.4 x 10^{-5}	30.4399	<0.0001*	-0.0002	-0.0009
Weibull dist. Parameters (scale)	0.4279	0.0348	150.9741	<0.0001*	0.3597	0.4962



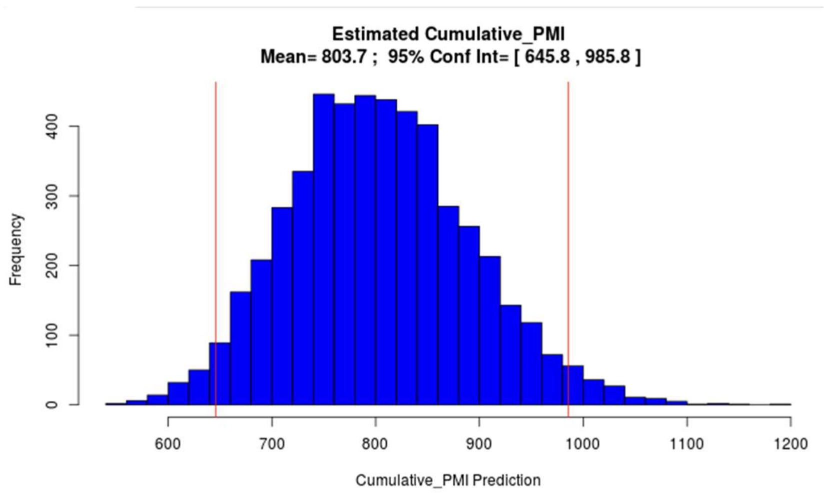
Prediction Expression

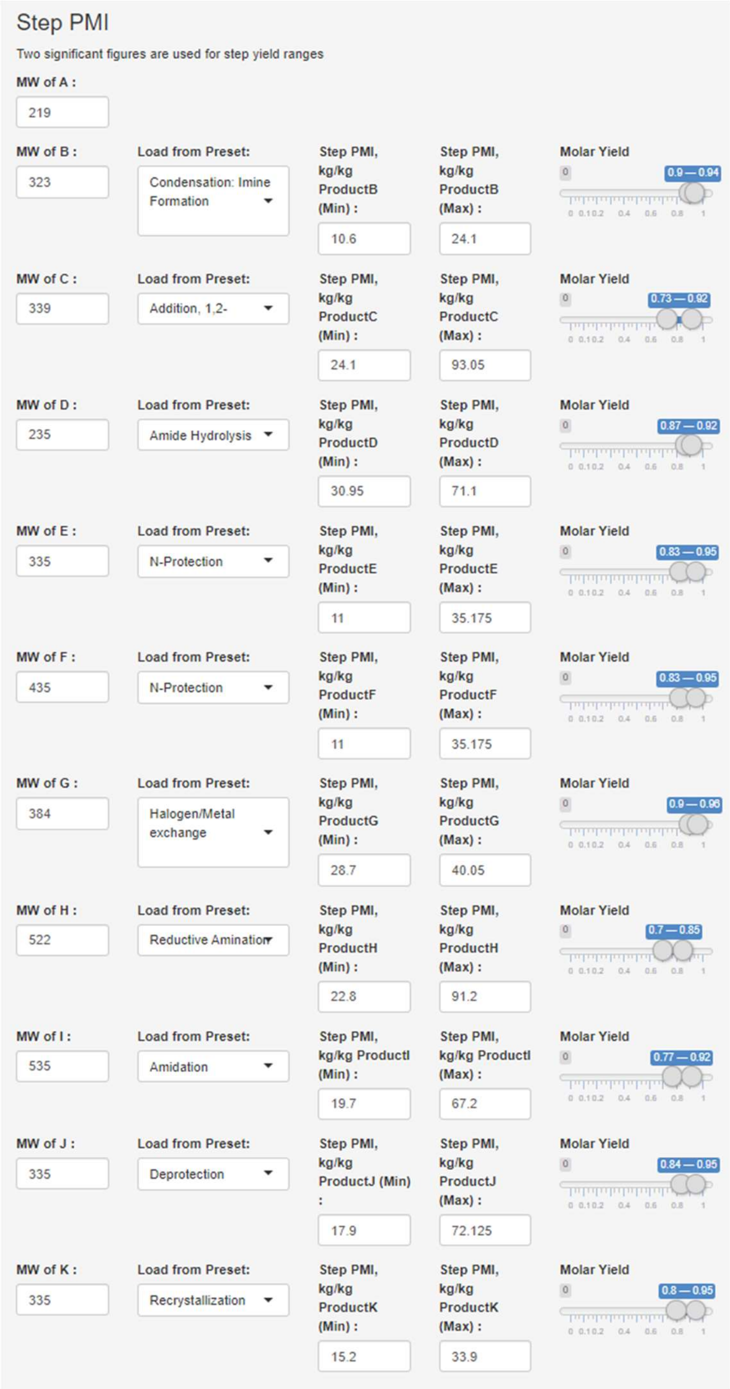
$$\mathrm{Exp}\left(\begin{array}{l}3.8790745637\\ +-0.825211216\cdot \mathrm{Lin2}\\ +0.0458106703\cdot \mathrm{cCM^*}\\ +\left(\mathrm{cCM^*}-37.42752\right)\cdot\left(\left(\mathrm{MW}-311.29096\right)\cdot -0.000131784\right)\end{array}\right)\cdot \mathrm{Gamma}\left(1+0.4279294041\right)$$

Python code for the calculation of pPMI using the model above is provided in the supplementary information section.

4. Worked example AZD4831

The predicted PMI for Route A using the ACS PMI Calculator was generated using the information below:





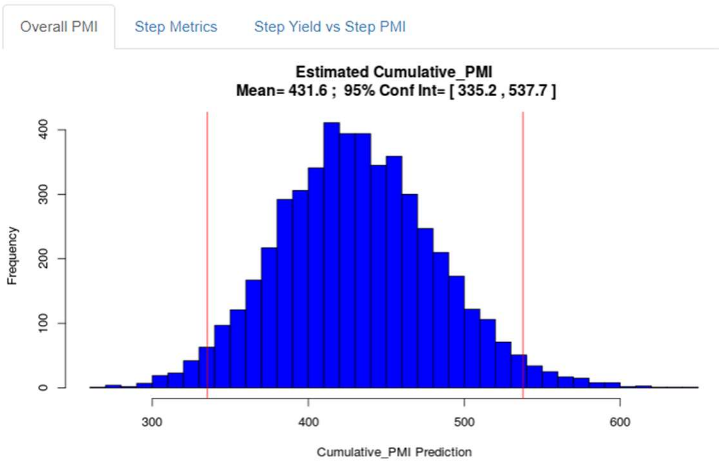
We are unable to disclose information regarding Route B due to commercial reasons.

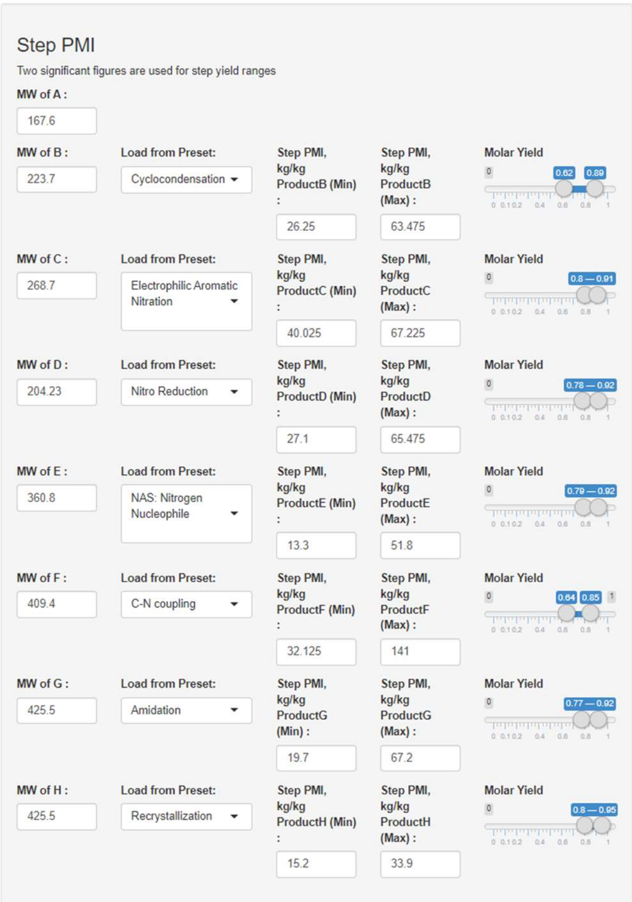
5. Literature examples

Synthetic routes are provided by the references stated in the main manuscript (Tables 4 and 5).

Predicted PMIs from the ACS PMI Calculator are as referenced,[6] with the exception of compounds **19** and **25** which are provided below.

Deucravacitinib **19**

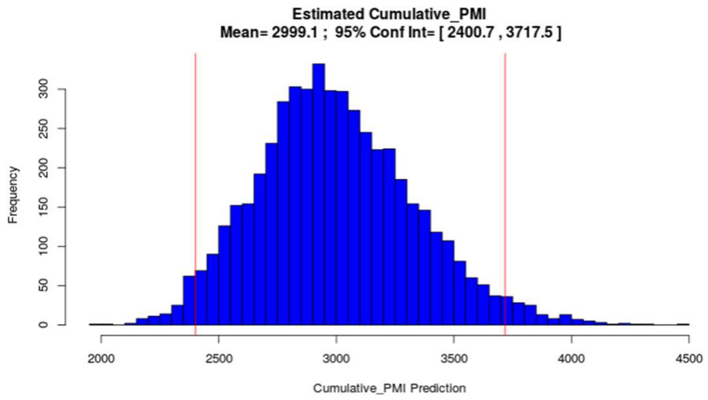




[6] A. Borovika, J. Albrecht, J. Li, A. S. Wells, C. Briddell, B. R. Dillon, L. J. Diorazio, J. R. Gage, F. Gallou, S. G. Koenig, M. E. Kopach, D. K. Leahy, I. Martinez, M. Olbrich, J. L. Piper, F. Roschangar, E. C. Sherer, M. D. Eastgate, *Nat. Sustain.*, **2019**, 2, 1034.

BMS-741672 **25**

Overall PMI | Step Metrics | Step Yield vs Step PMI



Step PMI

Two significant figures are used for step yield ranges

MW of A : 156.2

MW	Load from Preset	Step PMI, kg/kg Product (Min)	Step PMI, kg/kg Product (Max)	Molar Yield
MW of B : 228.2	Alpha Acylation	17	28.5	0.73 – 0.95
MW of C : 331.4	Reductive Amination	22.8	91.2	0.7 — 0.85
MW of D : 331.4	Salt Formation	9	29.275	0.83 — 0.94
MW of E : 229.3	Deprotection	17.9	72.125	0.84 — 0.95
MW of F : 494.6	Amidation	19.7	67.2	0.77 — 0.92
MW of G : 509.6	Methylation	20.475	57.8	0.79 — 0.95
MW of H : 446.5	Cycloalkylation	26.65	58.5	0.72 — 0.91
MW of I : 402.4	Deprotection	17.9	72.125	0.84 — 0.95
MW of J : 459.6	Reductive Amination	22.8	91.2	0.7 — 0.85

MW of	MW	Load from Preset:	Step PMI, kg/kg Product (Min) :	Step PMI, kg/kg Product (Max) :	Molar Yield
MW of K :	431.5	Ester Hydrolysis	15.2	68.375	0.79 — 0.96
MW of L :	502.7	Other Rearrangement	17.825	37.25	0.76 — 0.88
MW of M :	444.6	Deprotection	17.9	72.125	0.84 — 0.95
MW of N :	310.4	Deprotection	17.9	72.125	0.84 — 0.95
MW of T :	232.6	Chlorodehydration	18.05	44.425	0.82 — 0.93
MW of P :	161.1				
MW of Q :	287	Oxidative Iodination	17.2	31.7	0.83 — 0.95
MW of R :	186.1	NAS: Carbon Nucleophile	23.5	35.2	0.78 — 0.9
MW of S :	241.2	Cyclocondensation	26.25	63.475	0.62 — 0.89
MW of O :	232.6	NAS: Nitrogen Nucleophile	13.3	51.8	0.79 — 0.92

6. Dataset

entry	Step(LLS)	Step(total)	Ideality	Linearity	Convergency	Yield	PMI	ACSPMI	pPMI	SCS	ΣC_{SCS}	CM*	ΣC_{M*}
1	1	1	1.00	1.00	1.00	0.66	53.7	34	28	2.27	4.14	8.24	15.04
2	1	1	1.00	1.00	1.00	0.68	33.4	26	33	3.72	5.77	8.44	16.30
3	1	1	1.00	1.00	1.00	0.69	7.25	33	32	1.85	3.08	8.33	15.34
4	1	1	1.00	1.00	1.00	0.70	43.7	46	27	1.61	2.90	7.48	14.57
5	1	1	1.00	1.00	1.00	0.72	32.9	54	29	1.55	2.93	7.57	15.06
6	1	1	1.00	1.00	1.00	0.74	23.2	45	27	2.76	4.37	7.83	15.59
7	1	1	1.00	1.00	1.00	0.78	14.1	33	30	2.47	3.71	8.42	15.65
8	1	1	1.00	1.00	1.00	0.78	16.55	14	17	1.55	2.55	6.66	11.69
9	1	1	1.00	1.00	0.60	0.80	27.4	45	34	2.60	4.25	8.49	15.84
10	1	1	1.00	1.00	1.00	0.83	18.8	19	31	2.45	3.76	8.36	15.44
11	1	1	1.00	1.00	1.00	0.84	23.2	18	31	2.96	5.49	8.23	15.44
12	1	1	1.00	1.00	1.00	0.85	49.8	70	31	1.90	3.78	7.95	16.00
13	1	1	1.00	1.00	1.00	0.87	9.6	33	24	2.52	4.18	7.86	15.23
14	1	1	1.00	1.00	1.00	0.90	30.9	57	45	2.61	4.62	8.77	16.53
15	1	1	1.00	1.00	1.00	0.90	9.2	45	29	2.05	3.59	7.60	15.18
16	1	1	1.00	1.00	0.50	0.92	38.5	43	32	2.82	4.17	8.39	15.96
17	1	1	1.00	1.00	1.00	0.92	10.4	45	25	2.11	3.49	7.89	15.49
18	1	1	1.00	1.00	1.00	0.92	10.4	43	34	2.17	3.86	8.88	17.14
19	1	1	1.00	1.00	1.00	0.93	53.6	31	22	1.97	3.46	7.52	14.94
20	1	1	1.00	1.00	1.00	0.94	23.8	45	36	1.77	3.24	8.86	17.13
21	1	1	1.00	1.00	1.00	0.94	9.2	70	25	2.04	3.53	7.25	14.23
22	1	1	1.00	1.00	1.00	0.95	8	31	45	2.88	4.73	8.97	17.50
23	2	3	0.50	0.67	0.67	0.55	160.4	90	102	3.19	6.61	9.59	27.20
24	2	2	0.50	1.00	0.50	0.60	64.2	70	51	2.84	7.21	7.82	23.41
25	2	2	0.50	1.00	0.50	0.65	47.6	95	63	2.02	6.43	8.94	26.45
26	2	2	1.00	1.00	0.60	0.70	32.65	60	30	2.36	4.91	7.37	19.06
27	2	2	0.50	1.00	0.67	0.77	47.5	70	48	2.74	5.60	8.46	23.34
28	2	3	1.00	0.67	0.50	0.80	63.1	36	90	3.35	8.84	8.94	24.38

entry	Step(LLS)	Step(total)	Ideality	Linearity	Convergency	Yield	PMI	ACSPMI	pPMI	SCS	ΣC_{SCS}	CM*	ΣC_{M*}
29	2	2	0.50	1.00	0.60	0.80	55.7	90	43	2.40	5.99	7.79	22.97
30	2	2	0.50	1.00	0.50	0.81	61.5	53	45	2.11	5.87	8.12	23.57
31	2	2	0.50	1.00	0.60	0.81	76.3	70	45	2.29	5.61	8.18	23.48
32	2	2	1.00	1.00	0.60	0.82	70.2	136	46	2.10	5.03	7.78	22.85
33	2	2	1.00	1.00	0.60	0.85	70.7	74	48	2.96	6.45	8.38	23.87
34	2	2	1.00	1.00	0.60	0.85	33.5	53	76	2.66	7.38	9.25	26.75
35	2	2	0.50	1.00	0.50	0.87	35.7	120	47	2.23	6.09	8.37	25.51
36	2	2	1.00	1.00	0.44	0.88	48.8	96	79	4.42	10.19	9.51	25.81
37	2	2	0.50	1.00	0.50	0.89	16.9	89	46	2.67	6.38	8.39	24.04
38	2	2	1.00	1.00	1.50	0.90	71.2	44	42	2.02	5.48	7.99	22.93
39	2	2	1.00	1.00	0.31	0.90	53.6	70	55	3.14	7.39	8.75	24.59
40	2	2	1.00	1.00	0.44	0.77	113.2	135	71	3.66	8.29	9.26	25.78
41	2	2	0.50	1.00	0.50	0.91	35.2	74	45	2.40	6.59	8.15	23.38
42	2	2	0.50	1.00	0.50	0.94	51	105	54	2.12	5.36	8.65	25.78
43	2	2	1.00	1.00	0.60	0.94	14.6	125	52	2.16	5.69	8.14	22.37
44	3	3	0.33	1.00	0.33	0.39	107.6	121	73	2.53	8.39	8.16	31.72
45	3	3	0.33	1.00	0.50	0.58	38.2	96	79	2.42	7.48	9.24	29.91
46	3	4	0.50	0.75	0.57	0.73	117.2	158	100	3.67	10.88	8.49	31.90
47	3	3	1.00	1.00	0.50	0.78	108.4	86	72	2.42	7.90	8.26	31.19
48	3	4	0.25	0.75	0.33	0.79	232.4	158	128	3.76	10.37	9.75	36.95
49	3	3	0.67	1.00	0.38	0.81	11.3	70	87	2.24	8.72	8.31	33.79
50	3	3	0.67	1.00	0.43	0.82	92	126	70	2.35	8.93	7.92	31.30
51	3	3	0.33	1.00	0.43	0.82	98.3	148	85	2.38	8.29	8.73	33.51
52	3	6	1.00	0.50	0.33	0.82	156.7	175	139	4.41	13.25	9.08	33.47
53	3	3	0.66	1.00	0.40	0.83	42.3	118	77	2.91	8.51	8.61	31.95
54	3	5	0.40	0.60	0.33	0.85	138.4	184	139	3.86	10.29	9.70	36.15
55	3	3	1.00	1.00	0.38	0.85	160.8	180	87	2.81	10.20	7.99	34.74
56	3	3	0.33	1.00	0.40	0.86	62.8	103	93	2.19	7.55	9.02	34.80
57	3	3	0.67	1.00	0.31	0.88	76.4	166	98	4.64	14.82	9.49	35.30
58	3	3	0.67	1.00	0.44	0.91	68.1	74	54	2.74	7.65	7.72	26.78

entry	Step(LLS)	Step(total)	Ideality	Linearity	Convergency	Yield	PMI	ACSPMI	pPMI	SCS	ΣC_{SCS}	CM*	ΣC_{M*}
59	3	3	0.33	1.00	0.40	0.93	120	121	73	2.40	8.02	8.12	31.60
60	3	3	0.67	1.00	0.38	0.95	104.7	103	79	3.19	9.64	8.19	32.06
61	3	3	0.75	1.00	0.31	0.97	172.9	227	93	3.53	11.82	8.94	34.72
62	3	3	0.67	1.00	0.19	0.97	73.6	124	86	3.21	10.59	8.83	33.42
63	4	4	0.50	1.00	0.31	0.74	100.7	129	84	2.74	10.38	7.55	34.33
64	4	6	0.67	0.67	0.31	0.75	168.9	316	168	3.47	11.76	8.85	42.36
65	4	4	0.75	1.00	0.36	0.79	167.8	217	119	3.20	12.13	8.18	39.47
66	4	5	0.40	0.80	0.36	0.79	167.6	197	141	3.67	14.55	8.49	40.40
67	4	4	0.75	1.00	0.22	0.79	103.2	260	122	5.00	19.82	9.63	44.93
68	4	4	0.75	1.00	0.33	0.81	129.7	250	112	3.19	10.51	8.09	38.67
69	4	5	0.20	0.80	0.29	0.82	345.3	334	173	3.23	13.57	8.38	42.78
70	4	4	0.75	1.00	0.40	0.83	158.4	130	118	2.84	10.75	8.23	39.42
71	4	4	0.75	1.00	0.27	0.85	86.8	139	135	3.02	11.73	8.16	41.95
72	4	4	0.25	1.00	0.29	0.89	119	206	144	2.45	10.01	8.58	43.38
73	4	6	0.67	0.67	0.19	0.89	87.8	193	162	4.34	14.93	9.63	43.05
74	4	9	0.56	0.44	0.25	0.90	232.7	303	209	4.87	15.16	9.80	45.94
75	4	7	0.86	0.57	0.25	0.90	195	216	174	4.41	17.65	9.08	42.55
76	4	4	0.25	1.00	0.25	0.91	304.3	362	122	2.53	10.92	8.16	39.88
77	4	4	0.50	1.00	0.33	0.96	61.8	177	112	3.00	10.48	9.24	39.15
78	4	4	0.80	1.00	0.28	0.91	204.7	270	126	3.81	15.62	9.20	43.93
79	5	8	0.63	0.63	0.28	0.68	259.9	258	221	4.78	16.90	9.36	50.34
80	5	5	0.80	1.00	0.31	0.70	210.4	155	166	3.50	15.64	8.77	48.24
81	5	6	0.67	0.83	0.25	0.84	167.8	149	204	3.35	15.08	8.91	50.87
82	5	5	0.60	1.00	0.29	0.84	206.7	170	182	2.48	13.22	7.99	47.41
83	5	7	0.57	0.71	0.24	0.84	227.8	376	232	3.47	15.23	8.85	51.21
84	5	8	0.63	0.63	0.25	0.85	236.6	117	179	4.24	14.63	8.94	43.28
85	5	10	0.50	0.50	0.20	0.85	312.3	388	263	4.87	20.03	9.80	55.74
86	5	5	0.60	1.00	0.18	0.87	122.3	313	149	5.00	24.82	9.63	54.55
87	5	7	0.57	0.71	0.16	0.88	130.5	237	207	4.34	19.27	9.63	52.68
88	5	5	0.40	1.00	0.26	0.89	112	194	189	3.37	13.38	9.15	52.53

entry	Step(LLS)	Step(total)	Ideality	Linearity	Convergency	Yield	PMI	ACSPMI	pPMI	SCS	ΣC_{SCS}	CM*	ΣC_{M*}
89	5	6	0.33	0.83	0.26	0.89	408	309	252	3.91	17.49	8.72	51.50
90	5	6	0.17	0.83	0.18	0.90	330.6	359	220	3.89	18.15	9.50	55.96
91	5	5	0.40	1.00	0.25	0.91	132.4	206	144	3.22	13.69	9.22	48.37
92	5	5	0.80	1.00	0.29	0.94	105.9	251	147	3.81	14.33	8.76	47.42
93	5	5	0.83	1.00	0.22	0.96	280.9	360	165	3.79	19.41	9.38	53.30
94	6	9	0.66	0.67	0.26	0.68	313.7	229	336	3.52	16.74	8.92	56.33
95	6	6	0.83	1.00	0.27	0.78	276.4	241	235	3.41	19.05	8.76	57.00
96	6	7	0.43	0.86	0.23	0.85	202	298	241	4.43	21.92	9.31	60.80
97	6	9	0.56	0.67	0.22	0.85	329.6	327	294	4.78	21.69	9.36	59.71
98	6	9	0.67	0.67	0.22	0.89	255.1	208	207	4.89	19.51	9.32	52.60
99	6	7	0.71	0.86	0.25	0.90	145.9	358	194	4.37	18.70	9.02	56.44
100	6	6	0.50	1.00	0.20	0.95	147	284	199	3.57	17.26	9.24	57.61
101	6	6	0.71	1.00	0.18	0.95	282.9	612	303	4.07	23.48	9.10	62.40
102	7	11	0.27	0.64	0.18	0.72	367	486	390	4.13	21.11	9.58	71.06
103	7	8	0.75	0.88	0.23	0.77	504	372	378	4.37	23.42	9.09	66.09
104	7	7	0.43	1.00	0.17	0.83	384.9	512	437	4.08	21.34	8.68	66.29
105	7	10	0.60	0.70	0.19	0.83	128.6	251	261	4.99	23.75	9.68	69.59
106	7	10	0.50	0.70	0.21	0.83	454.9	375	296	5.00	26.92	9.77	70.57
107	7	10	0.70	0.70	0.20	0.86	277.9	258	219	5.00	24.51	9.56	62.16
108	7	8	0.63	0.88	0.20	0.88	145.2	423	243	4.37	23.06	9.02	65.45
109	7	10	0.70	0.70	0.21	0.88	449.5	310	472	3.42	20.16	9.01	65.34
110	7	7	0.63	1.00	0.22	0.96	529.2	495	447	4.07	27.55	9.10	71.50
111	8	11	0.64	0.73	0.17	0.75	299.4	310	259	5.00	29.51	9.56	71.72
112	8	9	0.67	0.89	0.18	0.79	602.9	439	544	4.37	27.79	9.09	75.19
113	8	11	0.73	0.73	0.17	0.80	673.4	426	649	3.66	23.82	9.15	74.50
114	8	12	0.25	0.67	0.16	0.81	468.6	568	509	4.13	25.24	9.58	80.63
115	8	9	0.56	0.89	0.22	0.82	399.8	529	424	4.80	26.14	9.49	75.78
116	8	11	0.55	0.73	0.17	0.86	228	302	313	4.99	28.73	9.68	79.27
117	8	11	0.45	0.73	0.17	1.00	461.8	443	366	5.00	31.92	9.77	80.34
118	9	13	0.69	0.69	0.17	1.00	715.3	566	612	4.33	28.15	9.61	84.11

entry	*Step(LLS)*	*Step(total)*	*Ideality*	*Linearity*	*Convergency*	*Yield*	*PMI*	*ACSPMI*	*pPMI*	*SCS*	ΣC_{SCS}	*CM**	ΣC_{M*}
119	9	10	0.60	0.90	0.21	-	612	581	385	5.00	31.14	9.60	85.37
120	10	14	0.64	0.71	0.15	0.67	930.9	671	822	4.33	32.48	9.61	93.72