BEILSTEIN JOURNAL OF ORGANIC CHEMISTRY

Supporting Information

for

A proposed sustainability index for synthesis plans based on input provenance and output fate: application to academic and industrial synthesis plans for vanillin as a case study

John Andraos

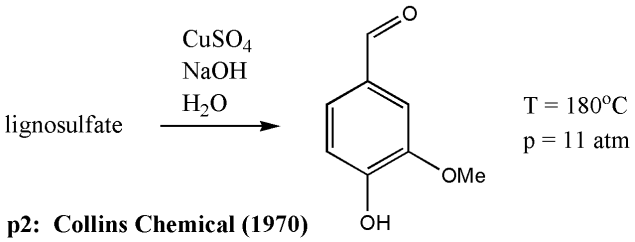
Beilstein J. Org. Chem. **2020,** *16,* 2346–2362. doi:10.3762/bjoc.16.196

Figure S1 comprising 22 vanillin synthesis plans, data for vanillin synthesis plans on production of 1 kg vanillin, Borda count results, and Poset analysis

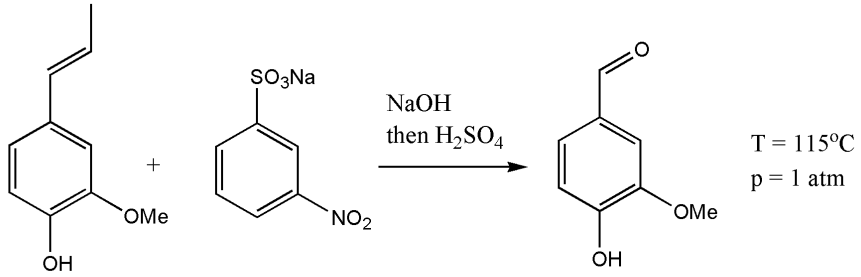
Table of Contents

Part 1: Figure S1. List of 22 vanillin synthesis plans showing reaction conditions in each reaction step.

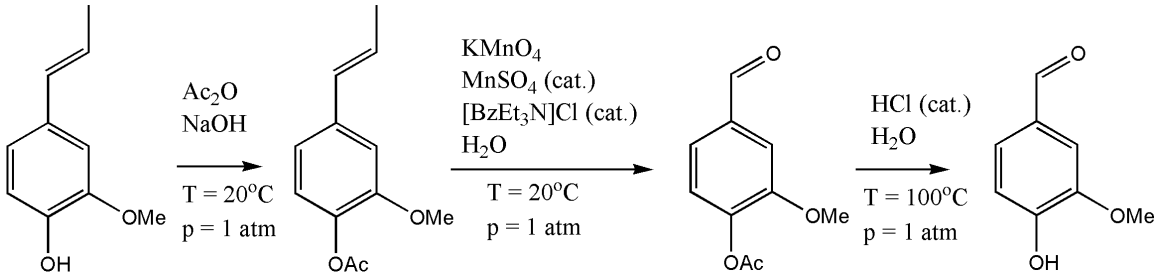
p1: Borregaard (1999)



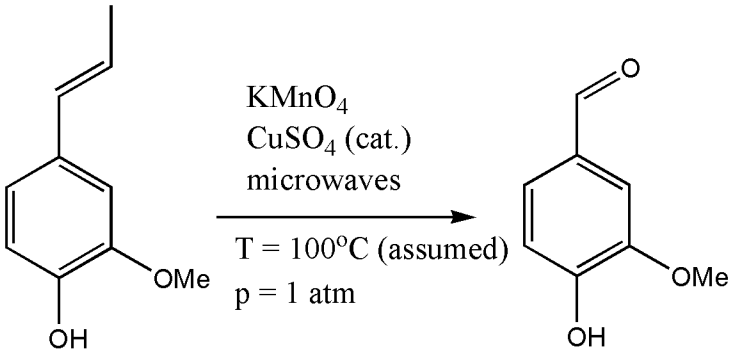
p2: Collins Chemical (1970)



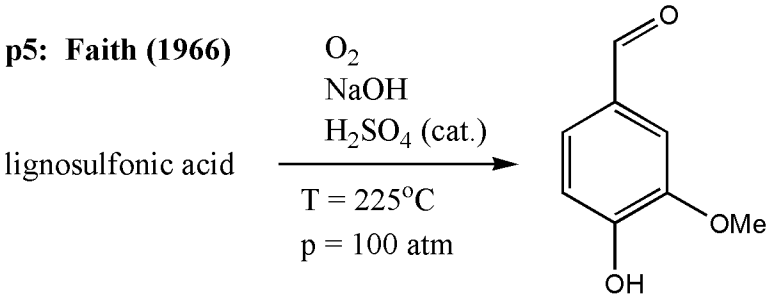
p3: Eilks - Pt 1 (2016)



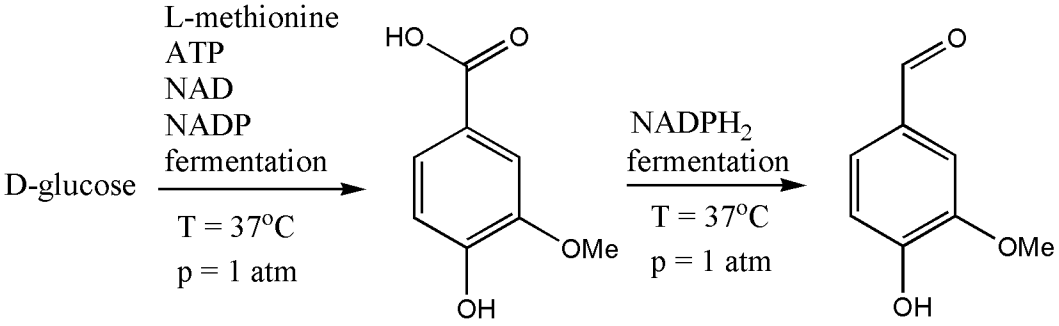
p4: Eilks - Pt 2 (2016)



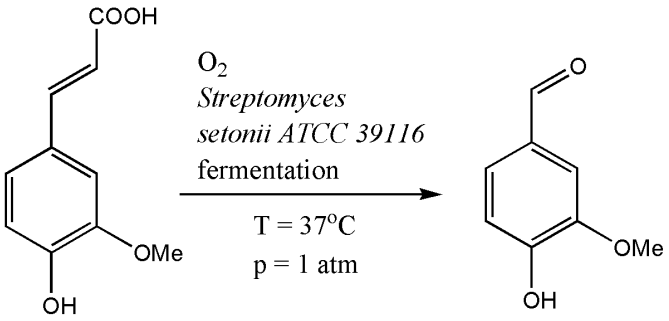
p5: Faith (1966)



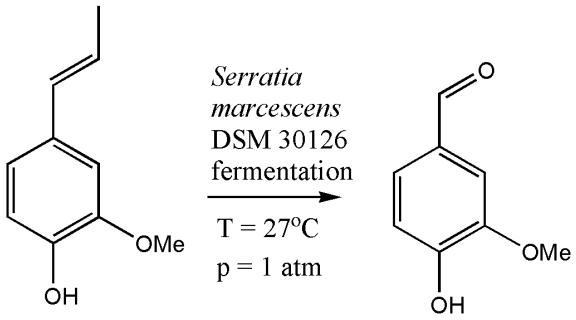
p6: Frost (1998)



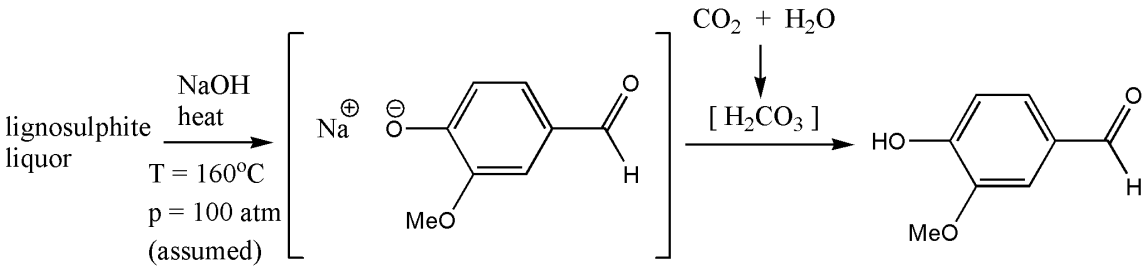
p7: Givaudan-Roure (1998)



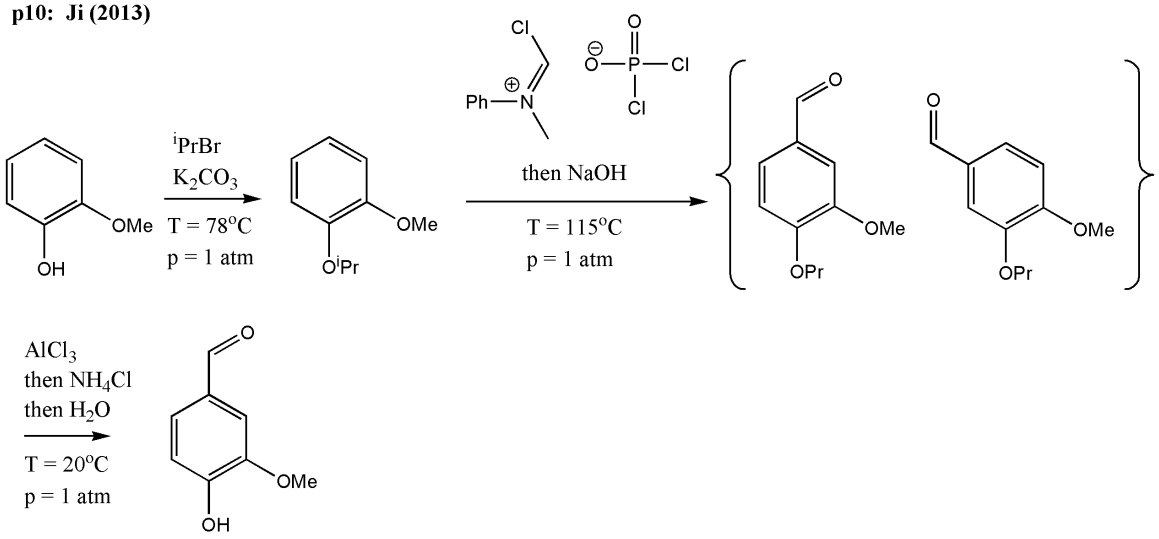
p8: Haarmann-Reimer (1991)



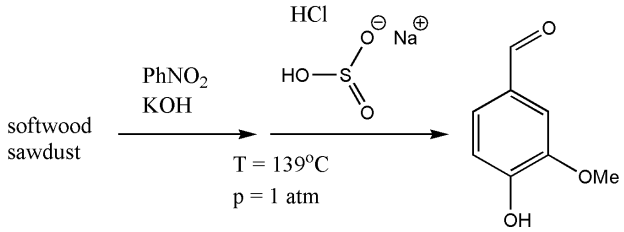
p9: Hibbert (1936)



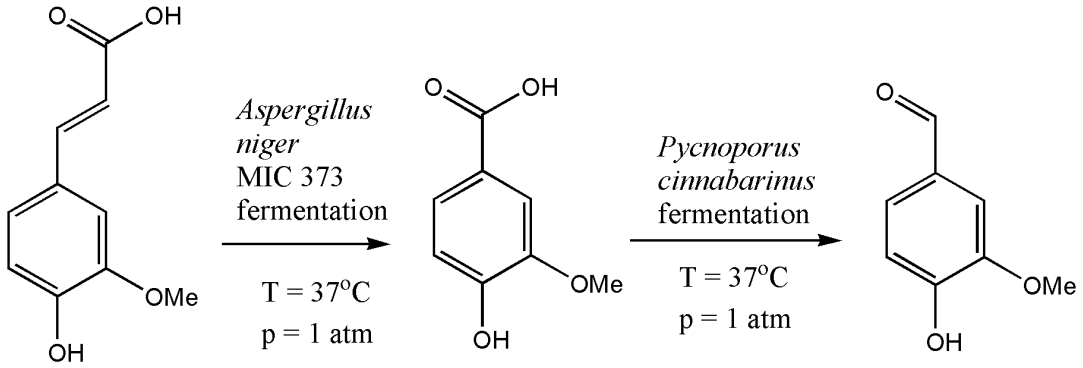
p10: Ji (2013)



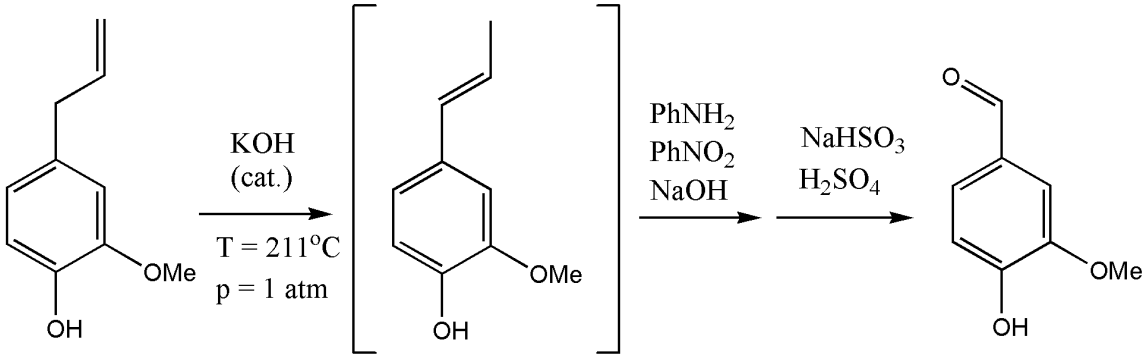
p11: Lampman (1977)



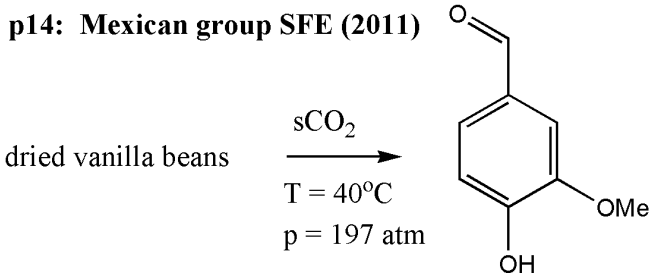
p12: Lesage-Meesen (1996)



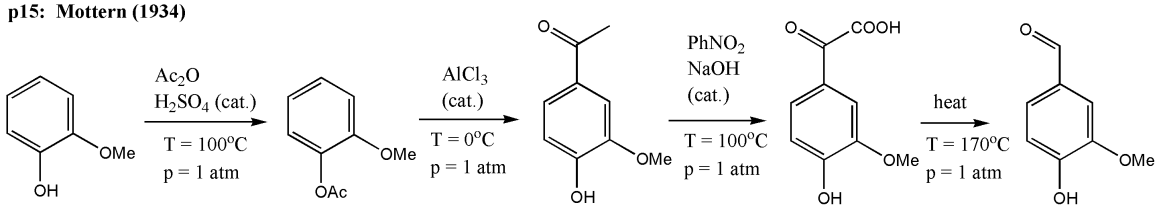
p13: Mayer (1949)



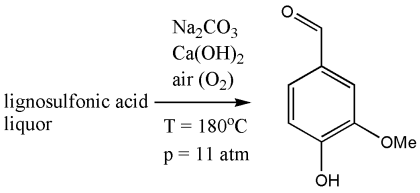
p14: Mexican group SFE (2011)



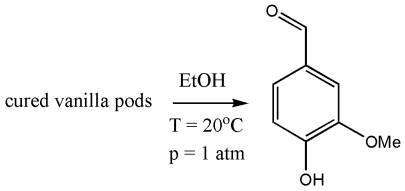
p15: Mottern (1934)



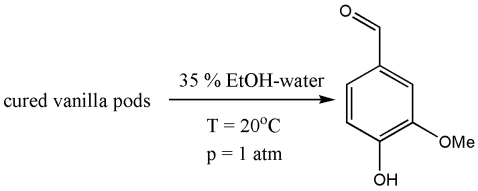
p16: Ontario Paper Co. (1962)



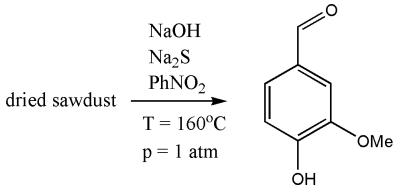
p17: percolation extraction cut (2005)



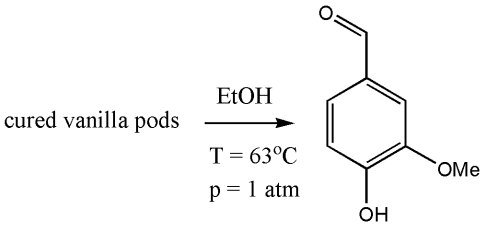
p18: percolation extraction whole (2005)



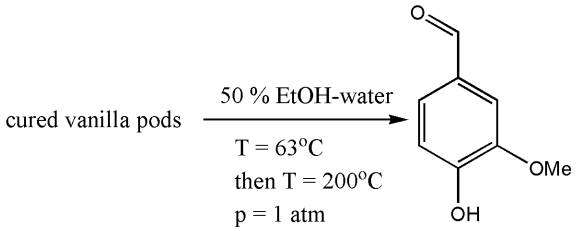
p19: Sorensen-Mehlum (1956)



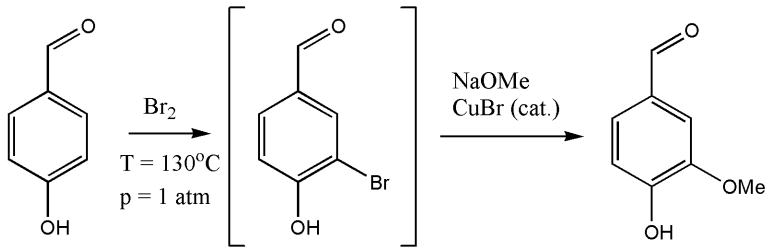
p20: Soxhlet extraction cut (1995)



p21: Soxhlet extraction ground (1995)



p22: Taber (2007)



Part 2: Data for Vanillin Synthesis Plans Based on Production of 1 kg Vanillin

P1: Borregaard

Bjørsvik, H.R. Org. Process Res. Dev. 1999, 3, 330-340. DOI:10.1021/op9900028

Input Materials	
Reagents	
lignosulfate (24 wt%)	12500g
CuSO4 (16.3 wt%)	182.14g
NaOH (50 wt%)	8377.59g
Reaction Solvents	
water from lignosulfate	39583.33g
water from CuSO4 soln.	935.28g
water from NaOH soln.	8377.59g
water	14015.15g
Catalysts	
none	0g
Workup	
none	0g
Purification	
none	0g
SUM	83971.10g
Waste Byproducts	
unidentified	20059.73g
sacrificial reagents	
CuSO4 (16.3 wt%)	182.14g
NaOH (50 wt%)	8377.59g
	8559.73g

P2: Collins Chemical

Fiecchi, A.; Mario, G.; Cabella, P.; Cicognani, G. US3544621 (1970)

Input Materials	
Reagents	
isoeugenol	1199.04g
NaOH	1199.04g
m-NO2-benzenesulfonate Na	2398.08g
H2SO4 (96 wt%)	4834.53g
Reaction Solvents	
water	19184.65g
benzene	3161.87g
water from 96 wt% H2SO4	201.44g
Catalysts	
65 wt% HNO3	1601.50g
Workup Materials	
NaOH	1973.28g
water	1973.28g
Purification	

none	0g
SUM	37726.71g

Waste Byproducts	
water	118.42g
acetaldehyde	289.47g
azobenzene byproduct	1269.74g
NaHSO4	789.47g
unidentified	6163.59g
	8630.70g

sacrificial reagents	
NaOH	1199.04g

P3: Eilks – Pt 1
Garner, N.; Siole, A.; Eilks, I. J. Sci. Educ. 2016, 17, 25-28.

Step 1

Input Materials	
Reagents	
isoeugenol	8902.05g
acetic anhydride	14891.86g
NaOH (1 M, 3.8 wt%)	10815.26g
Reaction Solvents	
water from 1 M NaOH	273796.94g
Catalysts	
none	0g
Workup	
none	
Purification	
EtOH	54346.33g
water	68880.01g
SUM	431632.45g

Waste Byproducts	
water	734.27g
NaOAc	3345.03g
unidentified	22126.51g
	26205.81g

sacrificial reagents	
acetic anhydride	14891.86g
NaOH (1 M, 3.8 wt%)	10815.26g
	25707.12g

Step 2

Input Materials
Reagents

product 2	8403.36g
KMnO4	15966.39g
water	315126.05g
Reaction Solvents	
MTBE	233193.28g
Catalysts	
MnSO4	15966.39g
[BzEt3N]Cl	840.34g
Workup Materials	
MTBE	248739.49g
NaHCO3	4201.68g
water	84033.61g
Purification	
none	0g
SUM	918067.22g

Waste Byproducts	
MnO2	1908.07g
KOH	1229.03g
acetaldehyde	724.25g
unidentified	332441.18g
	336302.52g

sacrificial reagents	
water	315126.05g

Step 3

Input Materials	
Reagents	
product 2	3193.28g
water (as 6 M HCl, 20 wt%)	110823.53g
Reaction Solvents	
none	0g
Catalysts	
HCl	27705.88g
Workup Materials	
MTBE	93277.31g
activated charcoal	4201.68g
Purification	
water	126050.42g
SUM	362058.82g

Waste Byproducts	
HOAc	394.74g
unidentified	112622.07g
	113016.81g

sacrificial reagents	
none	0g

Overall

	mass inputs (g)
step 1	431632.5
step 2	918067.2
step 3	362058.8
SUM	1711758

product	
vanillin	1000g

sacrificial reagents	mass (g)
step 1	25707.12
step 2	315126.1
step 3	0
SUM	340833.2

P4: Eilks – Pt 2
Garner, N.; Siole, A.; Eilks, I. J. Sci. Educ. 2016, 17, 25-28.

Input Materials	
Reagents	
isoeugenol	1687.24g
KMnO4	10823.05g
Reaction Solvents	
none	0.00g
Catalysts	
CuSO4	43621.40g
Workup Materials	
MTBE	91358.02g
Purification	
none	0g
SUM	147489.71g
Waste Byproducts	
KMnO2	649.18g
acetaldehyde	226.80g
unidentified	10634.31g
	11510.29g
sacrificial reagents	
none	0.00g

P5: Faith

Faith, W.L.; Keyes, D.B.; Clark, R.L. Industrial Chemicals, 3rd ed., Wiley: New York, 1966, p. 796

Input Materials	
Reagents	
lignosulfonic acid	6700g
dioxygen	5147.05g
NaOH	20000g
Reaction Solvents	
butanol	1000g
nitrogen	16727.91g
Catalysts	
H2SO4 (66 Be)	400g
Workup	
none	0g
Purification	
none	0g
SUM	49974.96g

Waste Byproducts	
unidentified	30847.05g

sacrificial reagents	
none	0g

P6: Frost

Li, K.; Frost, J.W. J. Am. Chem. Soc. 1998, 120, 10545

Step 1

Input Materials	
Reagents	
L-methionine	2222.22g
D-glucose	111111.11g
ATP	22777.78g
NAD	11111.11g
NADP	45555.56g
Reaction Solvents	
water	11111111.33g
Catalysts	
nutrients	383888.90g
Workup	
none	0g
Purification	
none	0g
SUM	11687778.01g

Waste byproducts	
ADP	12708.33g
NADH2	6736.11g
NADPH2	30119.05g
CO2	873.02g
fructose 6-phosphate	2579.37g
H3PO4	972.22g
2-amino-4-mercapto-butyric acid	1339.29g
dihydroxyacetone phosphate	1686.51g
unidentified	134097.22g
SUM	191111.11g

sacrificial reagents	
ATP	22777.78g
NAD	11111.11g
NADP	45555.56g
SUM	79444.45g

Step 2

Input Materials	
Reagents	
vanillic acid	1666.67g
NADPH2	12666.67g
Reaction Solvents	
fermentation broth	366666.67g
Catalysts	
nutrients	295233.33g
Workup	
EtOAc	901000.00g
water	1373333.33g
CH2Cl2	1336000.00g
Purification	
none	0g
SUM	4284900.00g

Waste byproducts	
NADP	4980.26g
water	118.42g
unidentified	8234.65g
SUM	13333.33g

sacrificial reagents	
NADPH2	12666.67g

Overall

Input materials	
step 1	11687778g
step 2	4284900g

SUM	15972678g

Product

vanillin	1000g

sacrificial reagents

step 1	79444.45
step 2	12666.67
SUM	92111.12g

P7: Givaudan-Roure

Muheim, A.; Müller, B.; Münch, T.; Wetli, M. EP885968 (Givaudan-Roure, 1998)

Input Materials	
Reagents	
ferulic acid (10 wt% in 0.5 M NaOH)	1700g
dioxygen	740.74g
Reaction Solvents	
0.5 M NaOH soln	15300.00g
Catalysts	
nutrients	3038.52g
Workup	
none	0g
Purification	
none	0g
SUM	20779.26g

Waste Byproducts	
glyoxylic acid	486.84g
unidentified	953.90g

sacrificial reagents	
none	0g

P8: Haarmann & Reimer

Rabenhorst, J.; Hopp, R. US5017388 (1991)

Input Materials	
Reagents	
isoeugenol	22222.22g
Reaction Solvents	
water	1111111.11g
Catalysts/Nutrients	
Na2HPO4	3472.22g
KH2PO4	2777.78g
(NH4)2PO4	2777.78g
FeSO4 7 H2O	27.78g
MgSO4 (1 M)	2222.22g
CaCl2 (0.1 M)	3333.33g

glycerol	11111.11g
Workup	
none	0g
Purification	
none	0g
SUM	1159055.56g
Waste Byproducts	
acetaldehyde	289.47g
unidentified	20932.75g
	21222.22g
sacrificial reagents	
none	0g

P9: Hibbert
Hibbert, H.; Tomlinson, G.H. Jr. US 2069185 (1937)

Input Materials	
Reagents	
sulphite liquor	375000g
NaOH	42857.14g
CO2	71428.57g
water	0.00g
Reaction Solvents	
none	0g
Catalysts	
none	0g
Workup Materials	
benzene	313928.57g
Purification Materials	
none	0g
SUM	803214.29g
Waste Byproducts	
unidentified	488285.71g
sacrificial reagents	
CO2	71428.57g

P10: Ji
Huang, W.B.; Du, C.Y.; Jiang, J.A.; Ji, Y.F. Res. Chem. Intermed. 2013, 39, 2849-2856. DOI:10.1007/s11164-012-0804-6

Step 1
Input Materials
Reagents

guaiacol	6877.38g
iPrBr	13632.74g
K2CO3	15307.72g
Reaction Solvents	
EtOH	67355.56g
Catalysts	
KI	1885.73g
Workup	
none	
Purification	
silica gel	0.00g
CH2Cl2	1425649.93g
SUM	1530709.07g

Waste Byproducts	
KBr	5800.00g
KHCO3	4878.05g
unidentified	17042.23g
	27720.28g

sacrificial reagents	
iPrBr	13632.74g
K2CO3	15307.72g
	28940.46g

Step 2

Input Materials	
Reagents	
product 2	8097.56g
O=PCl3	11219.51g
PhNHCHO	9878.05g
NaOH (2 M)	9756.10g
Reaction Solvents	
water from 2 M NaOH	121951.22g
Catalysts	
none	0.00g
Workup Materials	
CH2Cl2	733170.73g
Purification	
none	0g
SUM	885975.61g

Waste Byproducts	
water	735.48g
NaCl	2388.26g
PhNHMe	4372.01g
Na[O=PCl2O]	6410.93g
unidentified	17117.71g
	31024.39g

sacrificial reagents	
O=PCl3	11219.51g
NaOH	4939.02g
	16158.54g

Step 3

Input Materials	
Reagents	
product 2	7926.83g
water as NH4Cl soln.	60975.61g
Reaction Solvents	
CH2Cl2	48878.05g
Catalysts	
AlCl3	2927.20g
NH4Cl (2 M)	6396.34g
Workup Materials	
CH2Cl2	244390.24g
sat'd NaCl soln.	172741.46g
Purification	
silica gel	0.00g
pet.ether	780487.80g
EtOAc	109878.05g
SUM	1426674.76g

Waste Byproducts	
iPrOH	394.74g
unidentified	67507.70g
	67902.44g

sacrificial reagents	
none	0g

Overall

	mass inputs (g)
step 1	1530709
step 2	885975.6
step 3	1426675
SUM	3843359

product	
vanillin	1000g

sacrificial reagents	mass (g)
step 1	28940.46
step 2	16158.54
step 3	0
SUM	45099g

P11: Lampman

Lampman, G.M.; Andrews, J.; Bratz, W.; Hanssen, O.; Kelley, K.; Perry, D.; Ridgeway, A. J. Chem. Educ. 1977, 54, 776

Input Materials	
Reagents	
sawdust	457317.07g
PhNO2	1467073.17g
KOH	579268.29g
HCl (37 wt%)	1948774.39g
NaHSO3 (20 wt%)	7317073.17g
Reaction Solvents	
DMSO	2685365.85g
water	762195.12g
Catalysts	
none	0g
Workup Materials	
water	6097560.98g
Et2O	9713414.63g
MgSO4	609756.10g
Purification Materials	
hot cyclohexane	593750.00g
cyclohexane	308750.00g
SUM	32540298.78g
Waste Byproducts	
unidentified	11768506.10g
sacrificial reagents	
KOH	579268.29g
HCl (37 wt%)	1948774.39g
NaHSO3 (20 wt%)	7317073.17g
SUM	9845115.85g

P12: Lesage-Meesen

Lesage-Meesen, L.; Delattrea, M.; Haona, M.; Asther, M. US 6162637 (Institut National de la Recherche Agronomique, 2000)

Lesage-Meesen, L.; Delattrea, M.; Haona, M.; Thibault, J.F.; Ceccaldi, B.C.; Brunerie, P.; Asther, M. J. Biotechnology 1996, 50, 107

Step 1

Input Materials	
Reagents	
ferulic acid	9698.28g
dioxygen	4105.09g
Reaction Solvents	
water	1436781.61g
Catalysts	

nutrients	57060.76g
Workup	
none	0g
Purification	
none	0g
SUM	1507645.73g
Waste Byproducts	
oxalic acid	2770.94g
unidentified	5860.02g
	8630.95g
sacrificial reagents	
none	0g

Step 2

Input Materials	
Reagents	
vanillic acid	5172.41g
NADPH2	29556.65g
Reaction Solvents	
water	17241379.31g
Catalysts	
nutrients	684729.06g
Workup	
none	0g
Purification	
none	0g
SUM	17955665.02g
Waste Byproducts	
water	118.42g
NADP	4980.26g
unidentified	28630.38g
	33729.06g
sacrificial reagents	
NADPH2	29556.65g

Overall

Input materials	
step 1	1507646g
step 2	17926207g
SUM	19433853g
product	
vanillin	1000g
sacrificial reagents	
step 1	0

step 2	29556.65
SUM	29556.65g

P13: Mayer
Mayer, E. Oesterreichische Chem. Ztg. 1949, 50, 40

Input Materials	
Reagents	
eugenol	1171.43g
PhNH2	5986.00g
PhNO2	4210.50g
NaOH (50 wt%)	1035.03g
H2SO4 (50 wt%)	1993.00g
NaHSO3 (20 wt%)	857.14g
Reaction Solvents	
water	642.86g
water from 50 wt% NaOH	1035.03g
water from 20 wt% NaHSO3	3428.57g
Catalysts	
KOH	607.14g
Workup	
benzene	4897.29g
Purification	
none	0g
SUM	25863.98g

Waste Byproducts	
water	473.68g
PhN=NPh	2394.74g
CH3CHO	289.47g
NaHSO4	1578.95g
SO2	421.05g
unidentified	9095.20g
	14253.10g

sacrificial reagents	
PhNH2	5986.00g
NaOH (50 wt%)	1035.03g
H2SO4 (50 wt%)	1993.00g
NaHSO3 (20 wt%)	857.14g
SUM	9871.17g

P14: Mexican group SFE
Castillo-Ruz, M.C.; Guillermo-Alcocer, C.G.; Bojorquez-Gamboa, R.R.; Rocha-Uribe, J.A. Tecnol. Ciencia Ed. (IMIQ) 2011, 26, 80-84.

Input Materials
Reagents

dried vanilla beans	17241.38g
Reaction Solvents	
sCO2	7496251.87g
Catalysts	
none	0g
Workup	
none	0g
Purification	
none	0g
SUM	7513493.25g

sacrificial reagents	
none	0g

Waste Byproducts	
spent vanilla beans	16241.38g

P15: Mottern

Mottern, H.O. J. Am. Chem. Soc. 1934, 56, 2107-2108.

Step 1

Input Materials	
Reagents	
guaiacol	2046.26g
acetic anhydride	1848.23g
Reaction Solvents	
none	0g
Catalysts	
H2SO4 (98 wt%)	30.30g
Workup Materials	
water	33004.12g
Na2CO3	3300.41g
Purification	
none	0g
SUM	40229.32g

Waste Byproducts	
HOAc	966.27g
unidentified	254.89g
	1221.15g

sacrificial reagents	
none	0g

Step 2

Input Materials	
Reagents	
product 1	2673.33g
Reaction Solvents	
none	0g

Catalysts	
AlCl3	2744.62g
Workup Materials	
ice	35644.45g
Et2O	25236.27g
Na2SO4	3564.45g
Purification	
none	0g
SUM	67189.79g

Waste Byproducts	
unidentified	1318.84g

sacrificial reagents	
none	0g

Step 3

Input Materials	
Reagents	
product 2	1354.49g
PhNO2	1044.89g
Reaction Solvents	
water	2902.48g
Catalysts	
NaOH	967.49g
Workup Materials	
HCl	967.49g
charcoal	967.49g
Purification	
none	0g
SUM	6849.85g

Waste Byproducts	
aniline	624.33g
unidentified	459.26g
	1083.59g

sacrificial reagents	
none	0g

Step 4

Input Materials	
Reagents	
product 3	1315.79g
Reaction Solvents	
p-Me2N-C6H4-CH3	1315.79g
Catalysts	
none	0g
Workup Materials	

Et2O	3726.32g
dilute HCl	5368.42g
Purification	
none	0g
SUM	10410.53g

Waste Byproducts	
CO2	289.47g
unidentified	26.32g
	315.79g
sacrificial reagents	
none	0g

Overall

Input materials	
step 1	40229.32g
step 2	67189.79g
step 3	6849.85g
step 4	10410.53g
SUM	124679.5g

product	
vanillin	1000g

sacrificial reagents	
step 1	0g
step 2	0g
step 3	0g
step 4	0g
SUM	0g

P16: Ontario Paper Co.
Craig, D.; Logan, C.D. US3054659 (1962)

Input Materials	
Reagents	
lignosulfonic acid liquor	245542.23g
Na2CO3	18833.33g
Ca(OH)2	13666.67g
air (oxygen)	49600.43g
Reaction Solvents	
nitrogen	161201.41g
Catalysts	
none	0g
Workup	
H2SO4	35491.50g
toluene	206830.32g
Purification	

none	0g
SUM	731165.90g
Waste Byproducts	
solids	26333.19g
lignin	5249.97g
acetovanillone	83.33g
calcium oxalate	500.00g
sodium sulfate	25166.53g
unidentified	269309.64g
	326642.66g
sacrificial reagents	
Na2CO3	18833.33g
Ca(OH)2	13666.67g
	32500.00g

P17: Percolation extraction cut
Sujalmi, S.; Suharso; Supriyanto, R.; Buchari Indo. J. Chem. 2005, 5, 7-10.

Input Materials	
Reagents	
cured vanilla pods	49504.95g
Reaction Solvents	
none	0g
Catalysts	
none	0g
Workup	
EtOH	781188.12g
Purification Materials	
none	0g
SUM	830693.07g
Waste Byproducts	
spent vanilla pods	48504.95g
sacrificial reagents	
none	0g

P18: Percolation extraction whole
Sujalmi, S.; Suharso; Supriyanto, R.; Buchari Indo. J. Chem. 2005, 5, 7-10.

Input Materials	
Reagents	
vanilla pods	83252.57g
Reaction Solvents	
35 wt% EtOH-water	944932.33g
Catalysts	
none	0g

Workup	
none	0g
Purification	
none	0g
SUM	1028184.90g
Waste Byproducts	
spent vanilla pods	82253g
sacrificial reagents	
none	0g

P19: Sorensen-Mehlum
Sorensen, N.A.; Mehlum, J. US2752394 (1956)

Input Materials	
Reagents	
dried sawdust	11382.11g
NaOH	22926.83g
Na2S	6585.37g
PhNO2	48902.44g
Reaction Solvents	
water	243902.44g
Catalysts	
none	0g
Workup	
H2SO4	56170.73g
Et2O	172682.93g
Purification	
none	0g
SUM	562552.85g
Waste Byproducts	
unidentified	88796.75g
sacrificial reagents	
NaOH	22926.83g
Na2S	6585.37g
	29512.20g

P20: Soxhlet extraction cut
Sujalmi, S.; Suharso; Supriyanto, R.; Buchari Indo. J. Chem. 2005, 5, 7-10.

Input Materials	
Reagents	
cured vanilla pods	28089.89g
Reaction Solvents	
none	0g
Catalysts	

none	0g
Workup	
EtOH	554073.03g
Purification Materials	
none	0g
SUM	582162.92g

Waste Byproducts	
spent vanilla pods	27089.89g

sacrificial reagents	
none	0g

P21: Soxhlet extraction ground
Voisine, R.; Carmichael, L.; Chalier, P.; Cormier, F.; Morin, A. J. Agr. Food Chem. 1995, 43, 2658-2661. DOI:10.1021/jf00058a019

Input Materials	
Reagents	
cured vanilla pods	56000g
Reaction Solvents	
none	0g
Catalysts	
none	0g
Workup	
50 % (v/v) EtOH	3924480g
Et2O	708000g
95 % (v/v) EtOH	204025g
silica gel	17500g
water	250000g
methanol	59400g
47.5 % (v/v) EtOH	18783.2g
Purification	
47.5 % (v/v) EtOH	93916g
SUM	5332104.2g

Waste Byproducts	
spent vanilla pods	55000g

sacrificial reagents	
none	0g

P22: Taber
Taber, D.F.; Patel, S.; Hambleton, T.M.; Winkel, E.E. J. Chem. Educ. 2007, 84, 1158. DOI:10.1021/ed084p1158

Input Materials	
Reagents	
4-hydroxybenzaldehyde	1084.60g

bromine	1420.65g
NaOMe	480.07g
Reaction Solvents	
methanol	25770.07g
EtOAc	977.22g
Catalysts	
CuBr	867.68g
Workup Materials	
3 M HCl soln.	68329.72g
EtOAc	146583.51g
Na2SO4	10845.99g
Purification Materials	
silica gel	59652.93g
Et2O	230368.76g
pet. Ether	1180043.38g
water	216919.74g
SUM	1943344.32g

Waste Byproducts	
HBr	532.24g
NaBr	676.97g
unidentified	776.10g
	1985.31g

sacrificial reagents	
bromine	1420.65g

Part 3: Borda Count Results

Plan	PMI (kg/kg)	Points
Givaudan-Roure	21	22
Mayer	26	21
Faith	50	20
Collins Chemical	38	19
Borregaard Synthesis	84	18
Mottern	125	17
Eilks Pt 2	147	16
Sorensen-Mehlum	563	15
Soxhlet extraction cut	582	14
Ontario Paper Co.	730	13
Hibbert	803	12
percolation extraction cut	831	11
percolation extraction whole	1028	10
Haarmann & Reimer	1159	9
Eilks Pt 1	1712	8
Taber	1943	7
Ji	3843	6
Soxhlet extraction ground	5332	5
Mexican group SFE	7513	4
Frost	15973	3
Lesage-Meesen	19434	2
Lampman	32540	1

Plan	SR (kg/kg)	Points
Faith	0	22
Givaudan-Roure	0	22
Mottern	0	22
Eilks Pt 2	0	22
Haarmann & Reimer	0	22
percolation extraction cut	0	22
percolation extraction whole	0	22
Soxhlet extraction cut	0	22
Soxhlet extraction ground	0	22
Mexican group SFE	0	22
Collins Chemical	1.2	21
Taber	1.4	20
Borregaard Synthesis	8.6	19
Mayer	10	18
Sorensen-Mehlum	29.5	17
Lesage-Meesen	30	16
Ontario Paper Co.	32.5	15
Ji	45	14
Hibbert	71	13
Frost	92	12
Eilks Pt 1	341	11

Lampman	9845	10

Plan	IEE (kJ/kg)	Points
percolation extraction cut	0	22
percolation extraction whole	0	22
Givaudan-Roure	795	21
Mottern	2189	20
Eilks Pt 2	2881	19
Haarmann & Reimer	9388	18
Eilks Pt 1	17309	17
Mayer	20989	16
Faith	29286	15
Taber	28138	14
Soxhlet extraction cut	50219	13
Collins Chemical	50440	12
Borregaard Synthesis	169046	11
Ji	325200	10
Frost	578763	9
Sorensen-Mehlum	653838	8
Ontario Paper Co.	688521	7
Soxhlet extraction ground	676694	6
Lesage-Meesen	939475	5
Hibbert	1005329	4
Mexican group SFE	1678005	3
Lampman	2398980	2

Plan	RSGI (kg)	Points
Givaudan-Roure	0	22
Lesage-Meesen	0	22
Borregaard Synthesis	0	22
Haarmann & Reimer	0	22
Faith	6	21
Collins Chemical	38	20
Mayer	163	19
Mottern	277	18
Eilks Pt 2	673	17
percolation extraction whole	1579	16
Sorensen-Mehlum	1952	15
Ontario Paper Co.	2101	14
Soxhlet extraction cut	2644	13
percolation extraction cut	3727	12
Hibbert	3768	11
Eilks Pt 1	4492	10
Taber	12327	9
Frost	16369	8
Soxhlet extraction ground	16828	7
Ji	24670	6
Mexican group SFE	27578	5

Lampman	112106	4

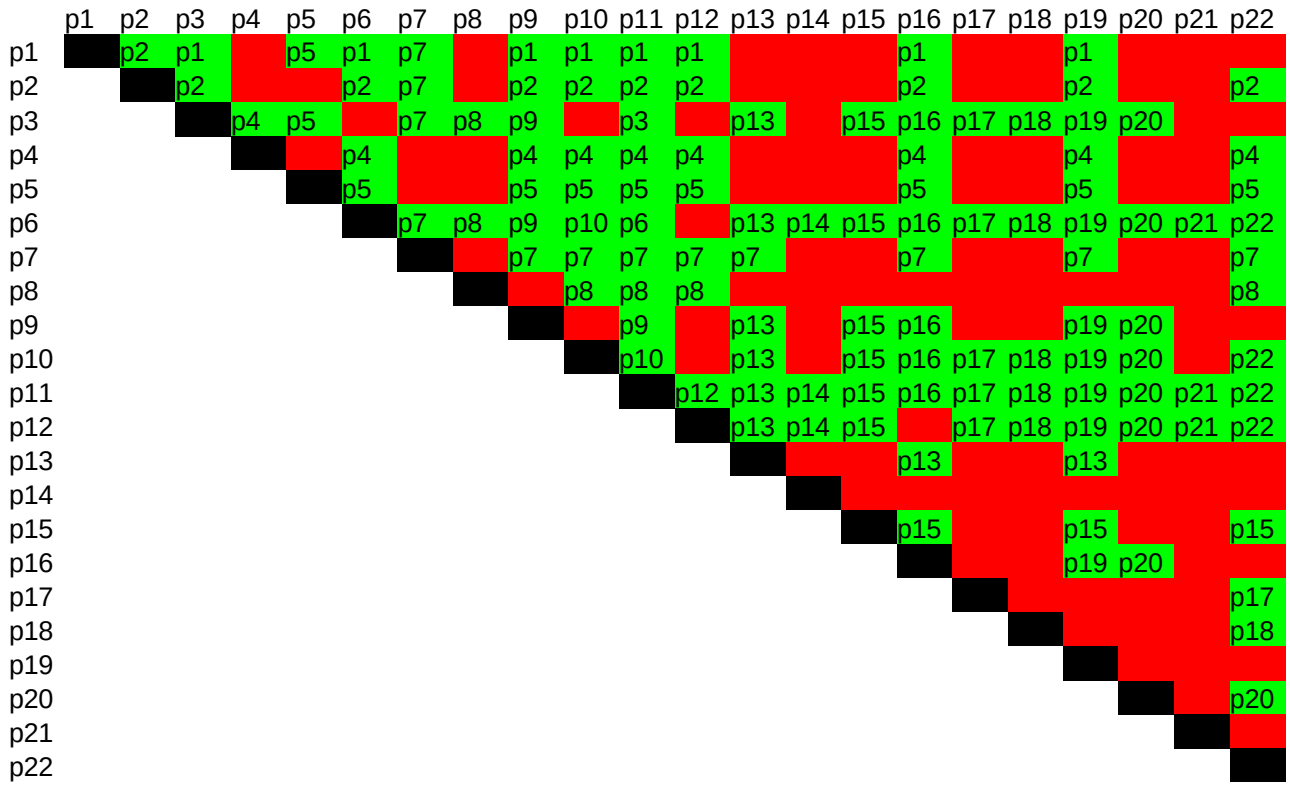
Plan	SI	Points
Lesage-Meesen	0.8072	22
Haarmann & Reimer	0.7762	21
percolation extraction whole	0.7272	20
Frost	0.6725	19
percolation extraction cut	0.6391	18
Soxhlet extraction cut	0.6385	17
Mexican group SFE	0.6345	16
Givaudan-Roure	0.5956	15
Borregaard Synthesis	0.5756	14
Eilks Pt 1	0.4866	13
Ontario Paper Co.	0.4689	12
Mottern	0.4603	11
Faith	0.4551	10
Collins Chemical	0.4519	9
Soxhlet extraction ground	0.4246	8
Hibbert	0.4207	7
Sorensen-Mehlum	0.4171	6
Taber	0.3946	5
Ji	0.3914	4
Eilks Pt 2	0.3907	3
Lampman	0.3704	2
Mayer	0.3676	1

Part 4: Poset Analysis

Green-coloured entries indicate comparable pairs. Dominant plan is specified.
Red-coloured entries indicate incomparable pairs.
For each attribute order, plans enclosed in boxes have the same high rank.

PMI versus SR

PMI order	SR order
p7	p4
p13	p5
p2	p7
p5	p8
p1	p14
p15	p15
p4	p17
p19	p18
p20	p20
p16	p21
p9	p2
p17	p22
p18	p1
p8	p13
p3	p19
p22	p12
p10	p16
p21	p10
p14	p9
p6	p6
p12	p3
p11	p11

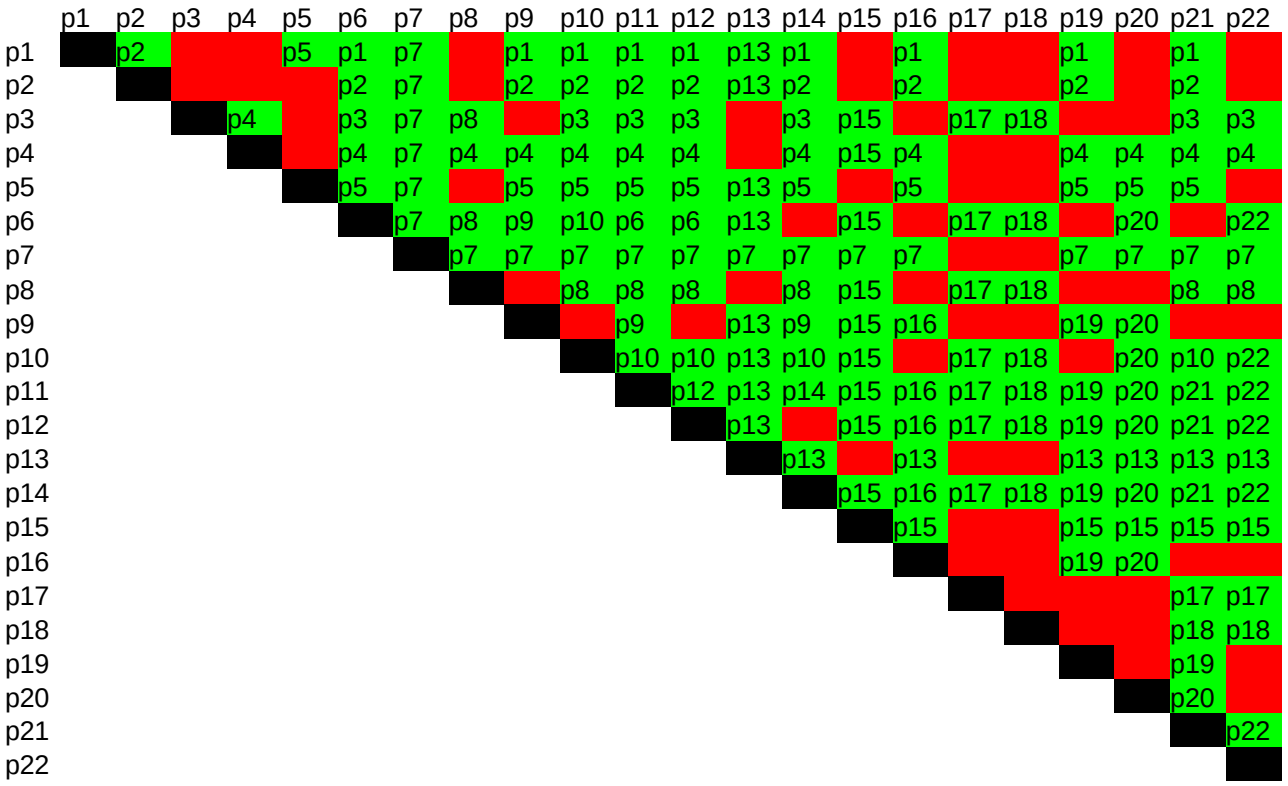


	p1	p2	p3	p4	p5	p6	p7	p8	p9	p10	p11	p12	p13	p14	p15	p16	p17	p18	p19	p20	p21	p22
PMI vs SR	8	10	1	9	10	1	12	6	3	2	0	1	8	3	9	5	6	6	7	8	3	4

PMI versus IEE

PMI order	IEE order
p7	p17
p13	p18
p2	p7
p5	p15
p1	p4
p15	p8
p4	p3
p19	p13
p20	p22
p16	p5
p9	p20
p17	p2
p18	p1
p8	p10
p3	p6
p22	p19
p10	p21
p21	p16
p14	p12

p6	p9
p12	p14
p11	p11

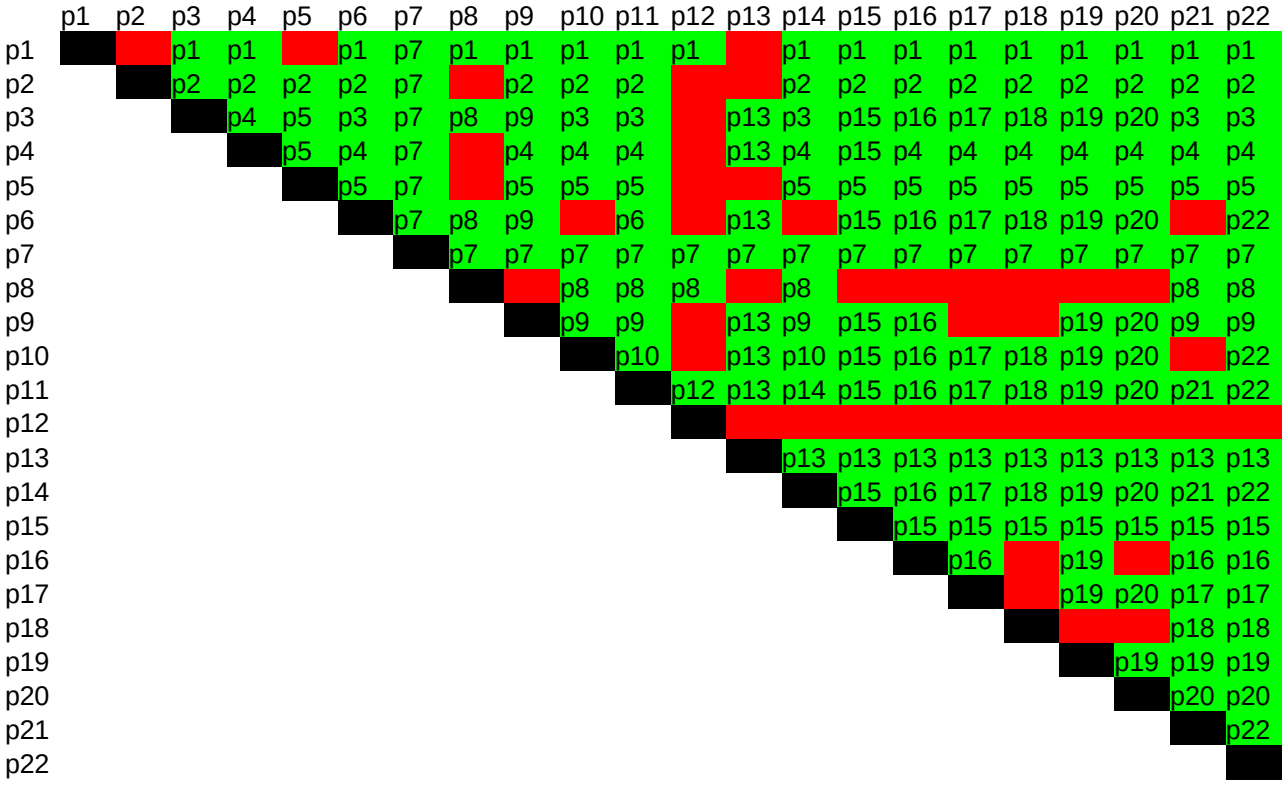


	p1	p2	p3	p4	p5	p6	p7	p8	p9	p10	p11	p12	p13	p14	p15	p16	p17	p18	p19	p20	p21	p22
PMI vs IEE	9	10	7	13	11	8	19	2	3	5	0	1	14	1	9	4	9	9	6	8	3	6

PMI versus RSGI

PMI order	RSGI order
p7	p1
p13	p7
p2	p8
p5	p12
p1	p5
p15	p2
p4	p13
p19	p15
p20	p4
p16	p18
p9	p19
p17	p16

p18	p20
p8	p17
p3	p9
p22	p3
p10	p22
p21	p6
p14	p21
p6	p10
p12	p14
p11	p11

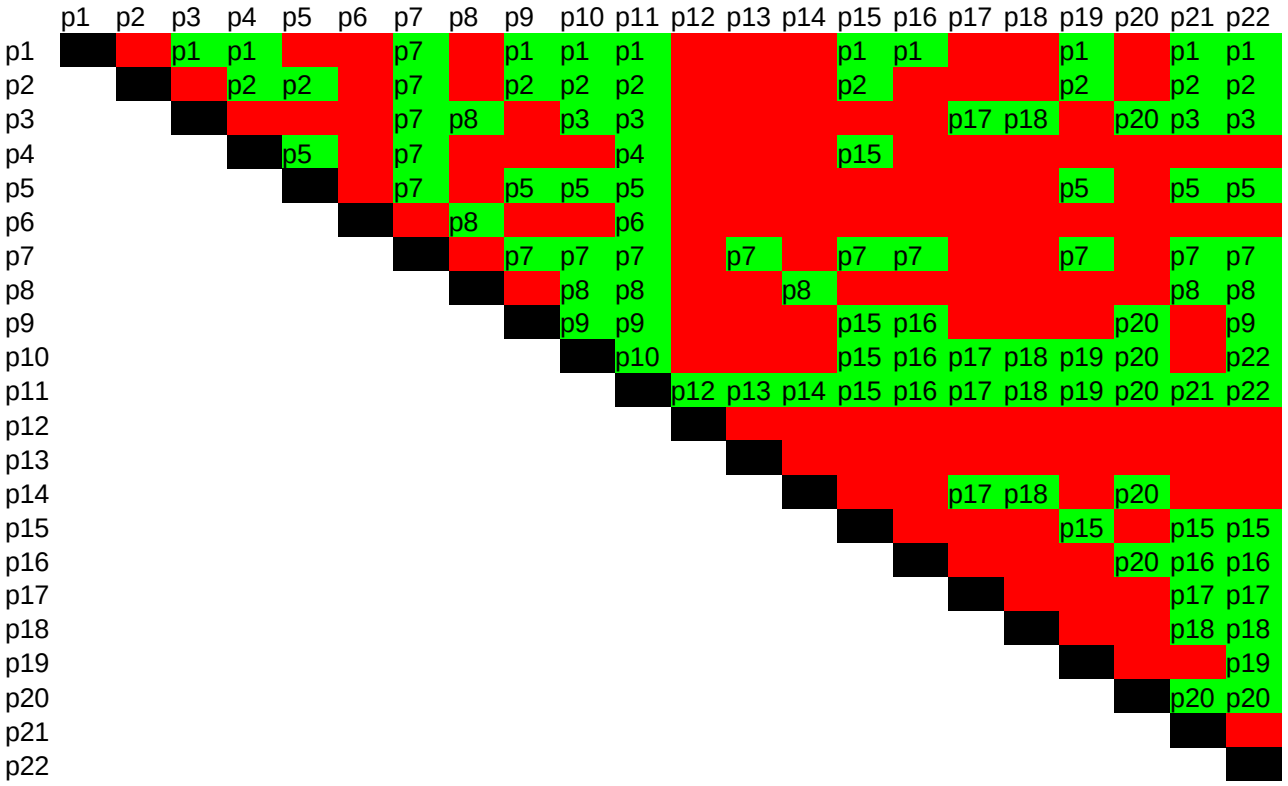


	p1	p2	p3	p4	p5	p6	p7	p8	p9	p10	p11	p12	p13	p14	p15	p16	p17	p18	p19	p20	p21	p22
PMI vs RSGI	17	16	5	12	15	1	21	8	7	2	0	1	15	1	14	9	7	7	11	9	2	5

PMI versus SI

PMI order	SI order
p7	p12
p13	p8
p2	p18
p5	p6
p1	p17
p15	p20
p4	p14

p19	p7
p20	p1
p16	p3
p9	p16
p17	p2
p18	p15
p8	p5
p3	p21
p22	p9
p10	p19
p21	p22
p14	p10
p6	p4
p12	p13
p11	p11

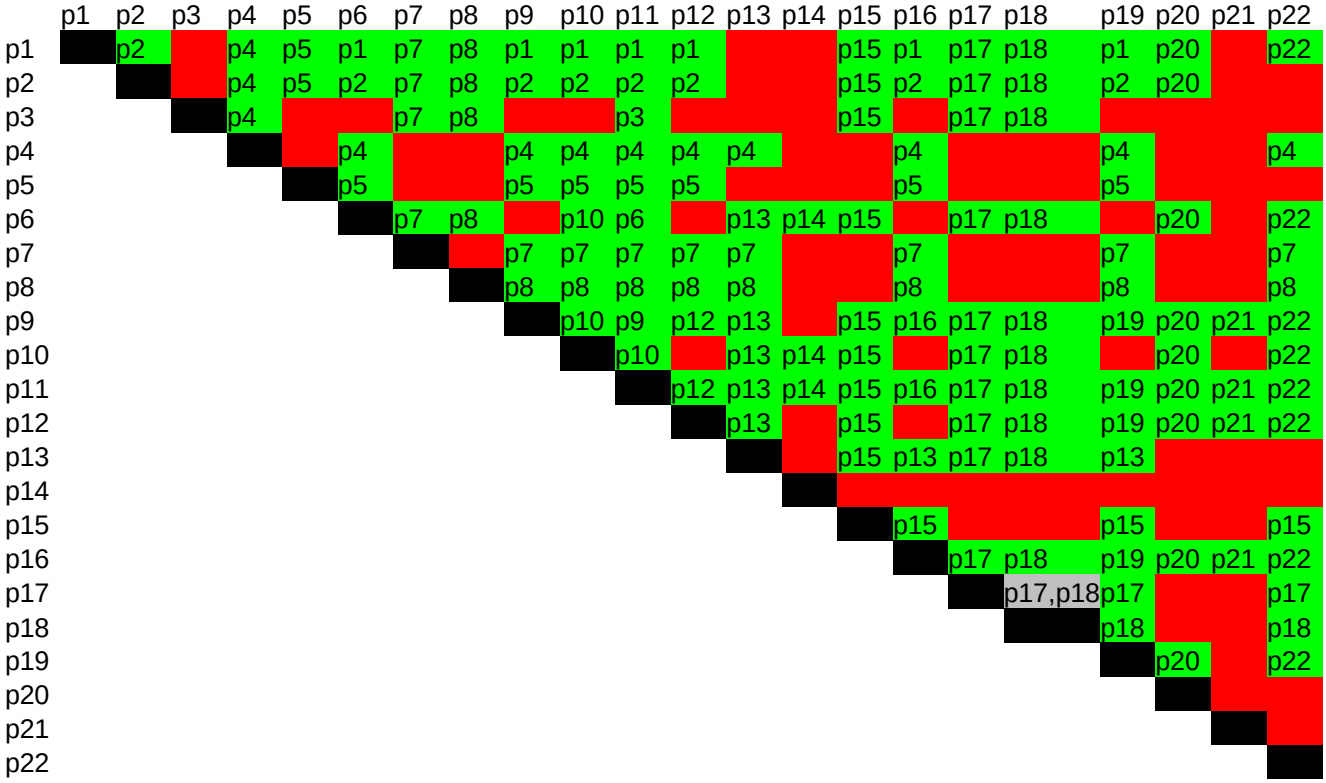


	p1	p2	p3	p4	p5	p6	p7	p8	p9	p10	p11	p12	p13	p14	p15	p16	p17	p18	p19	p20	p21	p22
PMI vs SI	10	9	4	1	7	1	14	7	3	1	0	1	1	1	7	5	6	6	3	7	1	2

SR versus IEE

SR order	IEE order
p4	p17
p5	p18

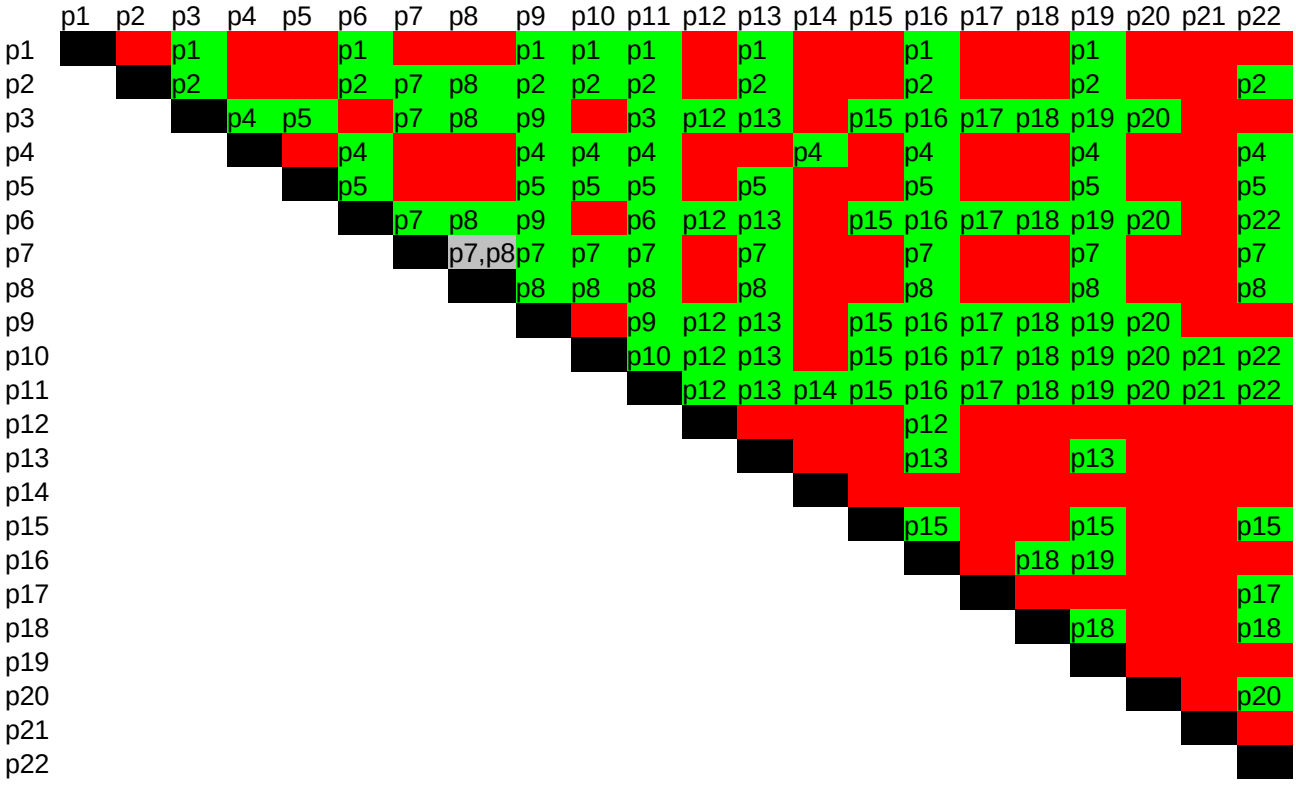
p7	p7
p8	p15
p14	p4
p15	p8
p17	p3
p18	p13
p20	p22
p21	p5
p2	p20
p22	p2
p1	p1
p13	p10
p19	p6
p12	p19
p16	p21
p10	p16
p9	p12
p6	p9
p3	p14
p11	p11



	p1	p2	p3	p4	p5	p6	p7	p8	p9	p10	p11	p12	p13	p14	p15	p16	p17	p18	p19	p20	p21	p22
SR vs IEE	7	8	1	12	9	1	12	12	1	3	0	2	7	3	12	2	13	13	4	9	4	8

SR versus RSGI

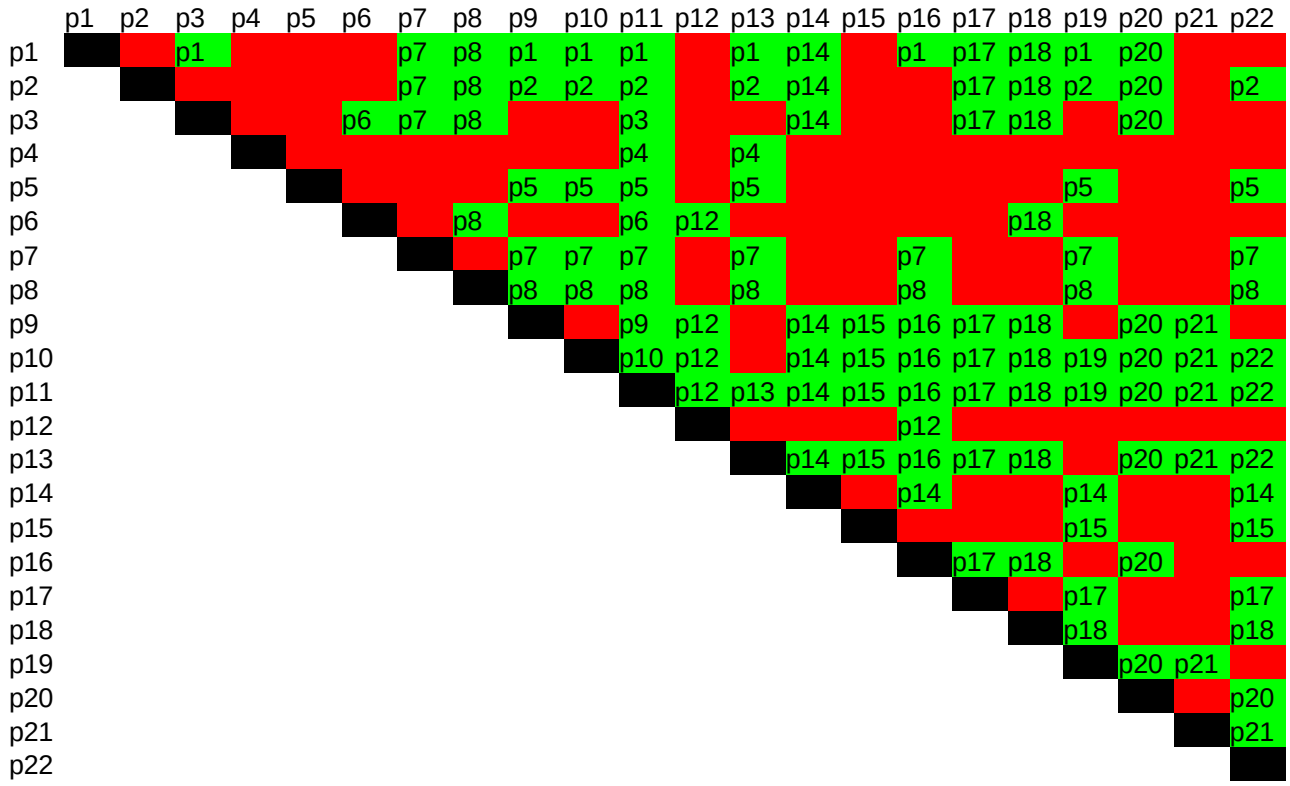
SR order	RSGI order
p4	p1
p5	p7
p7	p8
p8	p12
p14	p5
p15	p2
p17	p13
p18	p15
p20	p4
p21	p18
p2	p19
p22	p16
p1	p20
p13	p17
p19	p9
p12	p3
p16	p22
p10	p6
p9	p21
p6	p10
p3	p14
p11	p11



	p1	p2	p3	p4	p5	p6	p7	p8	p9	p10	p11	p12	p13	p14	p15	p16	p17	p18	p19	p20	p21	p22
SR vs RSGI	8	9	1	9	9	1	11	11	3	1	0	6	7	1	8	5	6	8	6	6	2	3

SR versus SI

SR order	SI order
p4	p12
p5	p8
p7	p18
p8	p6
p14	p17
p15	p20
p17	p14
p18	p7
p20	p1
p21	p3
p2	p16
p22	p2
p1	p15
p13	p5
p19	p21
p12	p9
p16	p19
p10	p22
p9	p10
p6	p4
p3	p13
p11	p11

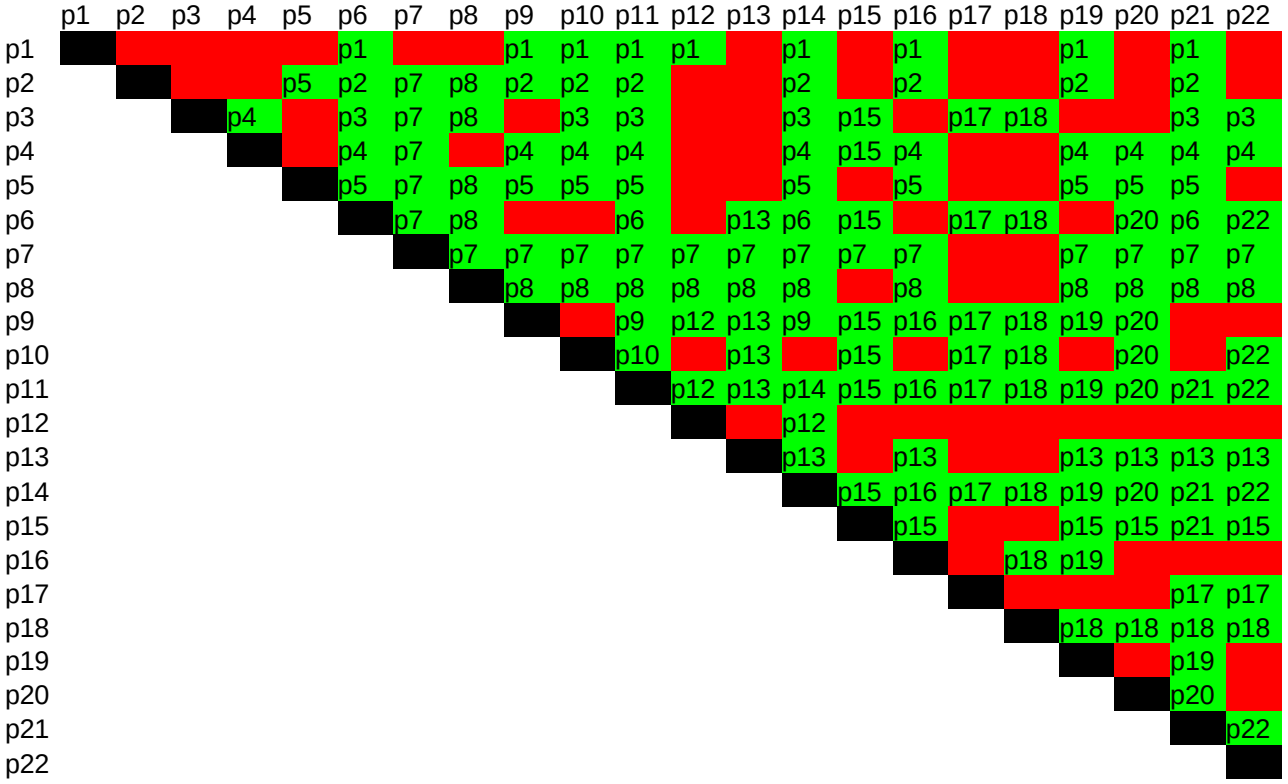


	p1	p2	p3	p4	p5	p6	p7	p8	p9	p10	p11	p12	p13	p14	p15	p16	p17	p18	p19	p20	p21	p22
SR vs SI	7	5	1	2	7	2	10	11	1	1	0	5	1	10	6	4	9	11	2	10	6	3

IEE versus RSGI

IEE order	RSGI order
p17	p1
p18	p7
p7	p8
p15	p12
p4	p5
p8	p2
p3	p13
p13	p15
p22	p4
p5	p18
p20	p19
p2	p16
p1	p20
p10	p17
p6	p9
p19	p3
p21	p22

p16	p6
p12	p21
p9	p10
p14	p14
p11	p11

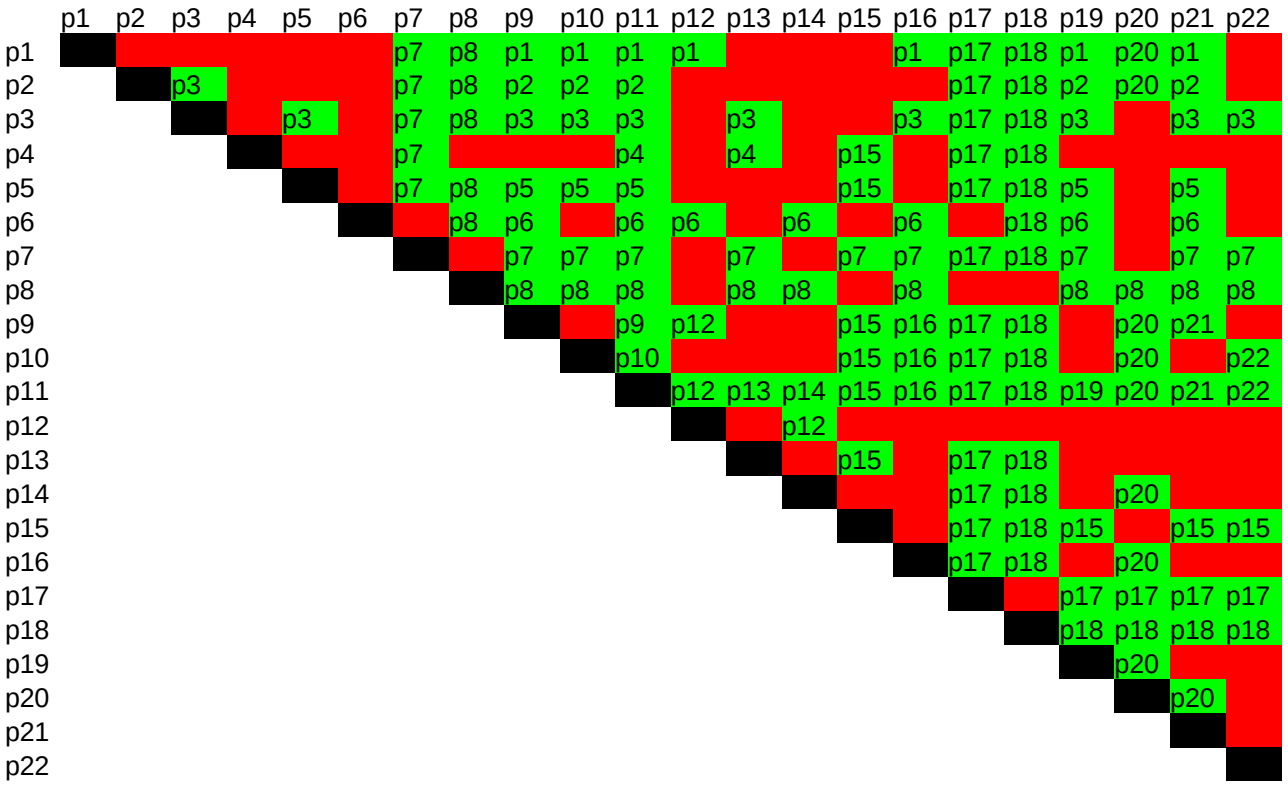


	p1	p2	p3	p4	p5	p6	p7	p8	p9	p10	p11	p12	p13	p14	p15	p16	p17	p18	p19	p20	p21	p22
IEE vs RSGI	9	8	6	11	10	3	18	15	2	1	0	3	10	1	11	3	8	11	5	6	3	5

IEE versus SI

IEE order	SI order
p17	p12
p18	p8
p7	p18
p15	p6
p4	p17
p8	p20
p3	p14
p13	p7
p22	p1
p5	p3
p20	p16

p2	p2
p1	p15
p10	p5
p6	p21
p19	p9
p21	p19
p16	p22
p12	p10
p9	p4
p14	p13
p11	p11

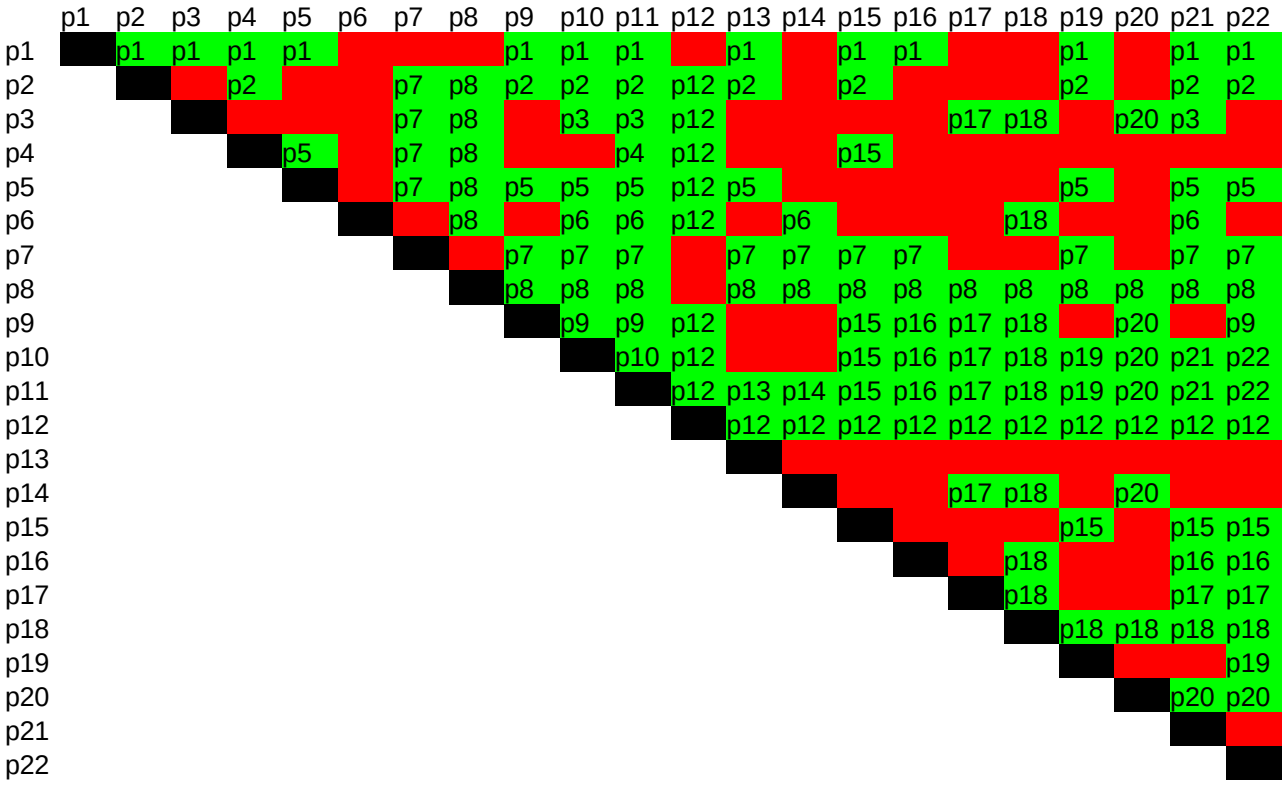


	p1	p2	p3	p4	p5	p6	p7	p8	p9	p10	p11	p12	p13	p14	p15	p16	p17	p18	p19	p20	p21	p22
IEE vs SI	7	5	10	2	5	7	14	15	1	1	0	3	1	1	9	3	17	18	1	9	2	2

RSGI versus SI

RSGI order	SI order
p1	p12
p7	p8
p8	p18
p12	p6
p5	p17
p2	p20

p13	p14
p15	p7
p4	p1
p18	p3
p19	p16
p16	p2
p20	p15
p17	p5
p9	p21
p3	p9
p22	p19
p6	p22
p21	p10
p10	p4
p14	p13
p11	p11



	p1	p2	p3	p4	p5	p6	p7	p8	p9	p10	p11	p12	p13	p14	p15	p16	p17	p18	p19	p20	p21	p22
RSGI vs SI	13	8	3	1	8	4	14	18	3	1	0	18	1	1	8	5	7	12	3	7	2	2