Electronic Supplementary Material (ESI) for Green Chemistry.

SUPPORTING INFORMATION

Solvents for solid-phase synthesis

Stefan Lawrenson, Michael North*, Fanny Peigneguy and Anne Routledge*

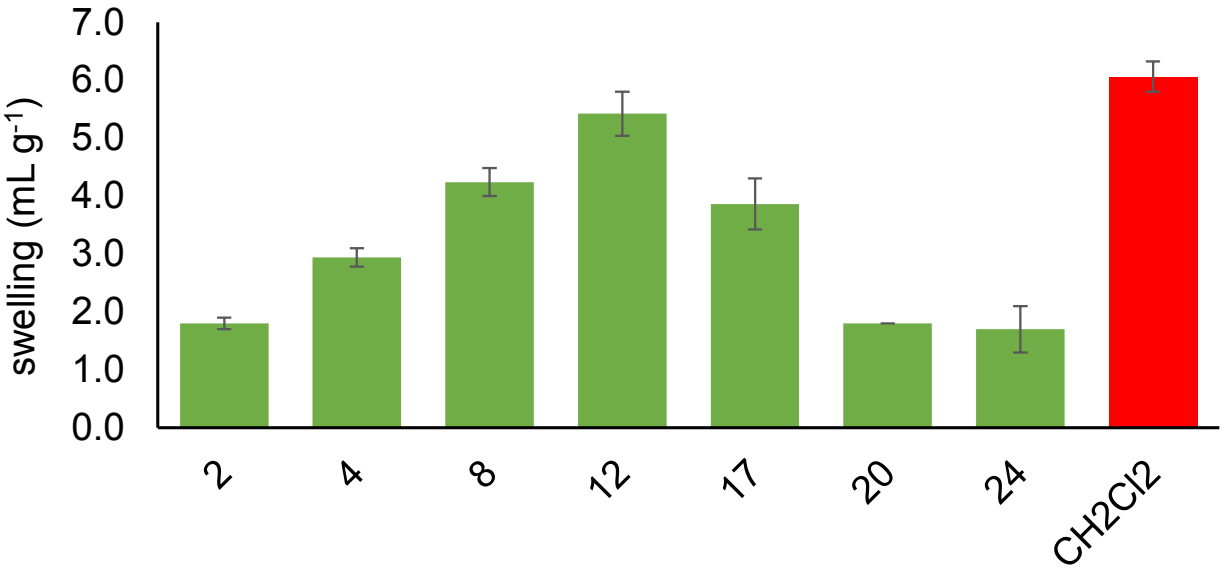
Department of chemistry, University of York, York, UK, Y10 5DD.

Contents

Reproducibility of resin swelling

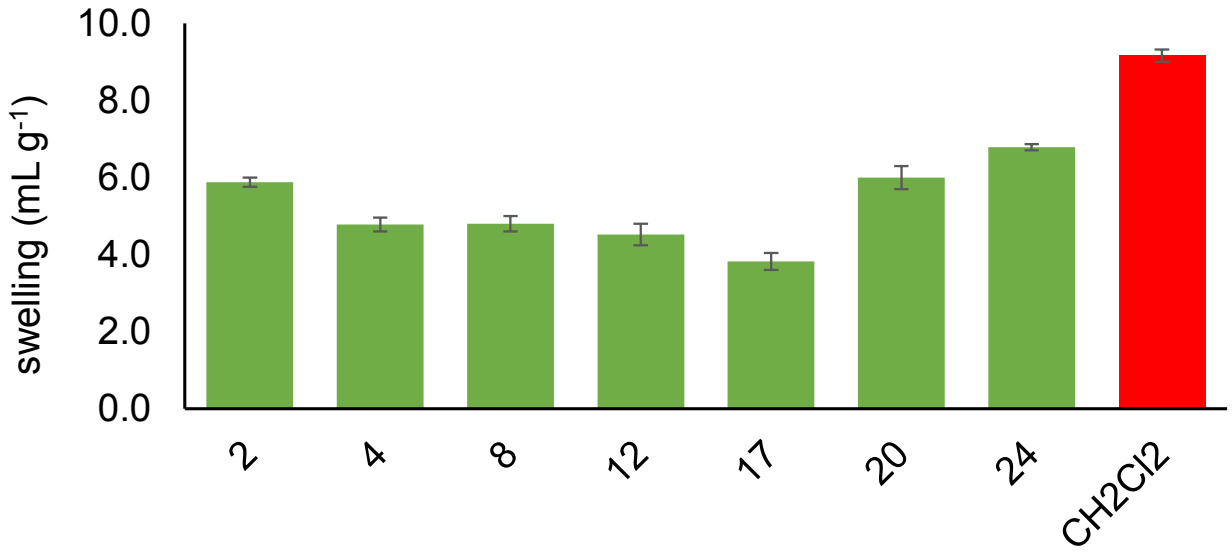
Merrifield resin

Solvent	Run 1	Run 2	Run3	Run 4	Run 5	Average Swelling (mL g^{-1})	Error
2	1.80	1.90	1.70	1.80	1.80	1.80	0.10
4	2.80	3.10	3.00	2.80	3.00	2.94	0.16
8	4.30	4.00	4.30	4.20	4.40	4.24	0.24
12	5.10	5.30	5.50	5.80	5.40	5.42	0.38
17	3.80	3.60	3.90	3.70	4.30	3.86	0.44
20	1.80	1.80	1.80	1.80	1.80	1.80	0.00
24	1.80	1.80	1.80	1.80	1.30	1.70	0.40
CH_2Cl_2	5.90	5.80	6.20	6.10	6.30	6.06	0.26



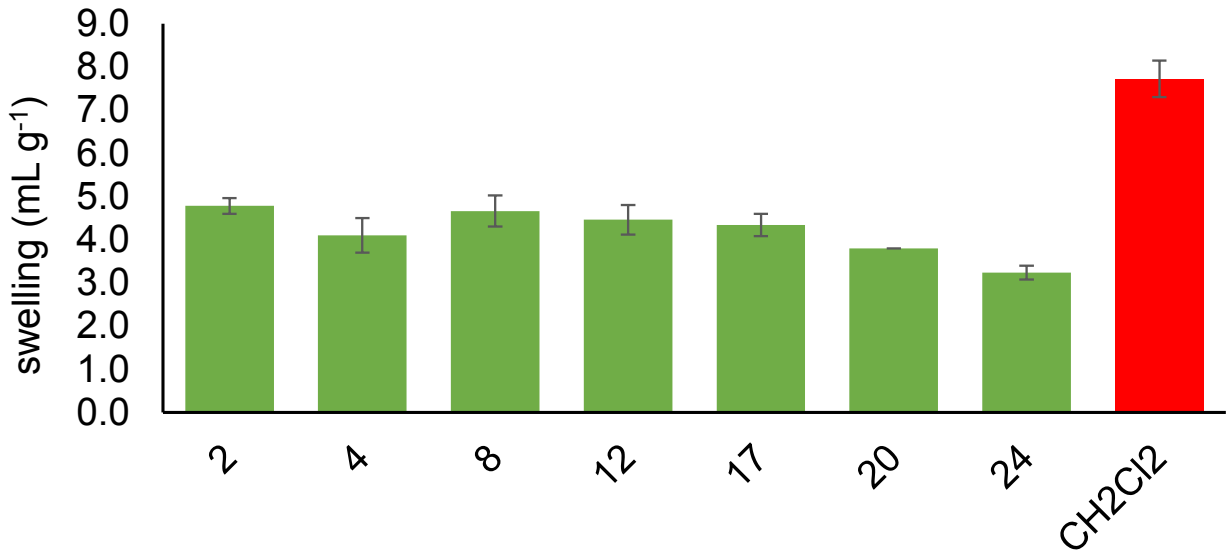
ChemMatrix resin

Solvent	Run 1	Run 2	Run3	Run 4	Run 5	Average Swelling (mL g^{-1})	Error
2	5.80	5.80	5.80	6.00	6.00	5.88	0.12
4	4.90	4.60	4.80	4.80	4.80	4.78	0.18
8	4.60	4.70	4.80	4.90	5.00	4.80	0.20
12	4.60	4.30	4.80	4.30	4.60	4.52	0.28
17	3.80	3.60	3.80	4.00	3.90	3.82	0.22
20	6.00	5.80	6.30	5.90	6.00	6.00	0.30
24	6.80	6.80	6.80	6.70	6.80	6.78	0.08
CH_2Cl_2	9.30	9.10	9.10	9.00	9.30	9.16	0.16



ArgoGel resin

Solvent	Run 1	Run 2	Run3	Run 4	Run 5	Average Swelling (mL g^{-1})	Error
2	4.80	4.60	4.80	4.90	4.80	4.78	0.18
4	4.50	4.30	3.90	4.00	3.80	4.10	0.40
8	4.80	4.80	4.30	4.60	4.80	4.66	0.36
12	4.30	4.40	4.50	4.30	4.80	4.46	0.34
17	4.30	4.60	4.10	4.40	4.30	4.34	0.26
20	3.80	3.80	3.80	3.80	3.80	3.80	0.00
24	3.30	3.10	3.10	3.30	3.40	3.24	0.16
CH_2Cl_2	7.70	7.80	7.30	7.80	8.00	7.72	0.42



Allocation of training set solvents to groups

Merrifield resin

Maximum swelling 6.3 mL g^{-1}; minimum swelling 1.8 mL g^{-1}

6 groups

Swelling range		Solvents	Rank
1.80	2.55	ethylene carbonate (**1**), propylene carbonate (**2**), cyrene (**3**), acetone (**4**), D-limonene (**18**), p-cymene (**19**), MeOH (**20**), EtOH (**21**), isopropanol (**22**)	6
2.55	3.30	γ-valerolactone (**11**), dimethyl carbonate (**16**), diethyl carbonate (**17**)	5
3.30	4.05	EtOAc (**8**)	4
4.05	4.80		3
4.80	5.55	DMF	2
5.55	6.30	cyclopentanone (**7**), 2-MeTHF (**12**), NMP, CH_2Cl_2	1

5 groups

Swelling range		Solvents	Rank
1.80	2.70	ethylene carbonate (**1**), propylene carbonate (**2**), cyrene (**3**), acetone (**4**), D-limonene (**18**), p-cymene (**19**), MeOH (**20**), EtOH (**21**), isopropanol (**22**)	5
2.70	3.60	γ-valerolactone (**11**), dimethyl carbonate (**16**), diethyl carbonate (**17**)	4
3.60	4.50	EtOAc (**8**)	3
4.50	5.40	DMF	2
5.40	6.30	cyclopentanone (**7**), 2-MeTHF (**12**), NMP, CH_2Cl_2	1

4 groups

Swelling range		Solvents	Rank
1.80	2.93	ethylene carbonate (**1**), propylene carbonate (**2**), cyrene (**3**), acetone (**4**), dimethyl carbonate (**16**), D-limonene (**18**), p-cymene (**19**), MeOH (**20**), EtOH (**21**), isopropanol (**22**)	4
2.93	4.05	EtOAc (**8**), γ-valerolactone (**11**), diethyl carbonate (**17**)	3
4.05	5.18	DMF	2
5.18	6.30	cyclopentanone (**7**), 2-MeTHF (**12**), NMP, CH_2Cl_2	1

ParaMax resin

Maximum swelling 7.8 mL g^{-1}; minimum swelling 1.8 mL g^{-1}

6 groups

Swelling range		Solvents	Rank
1.80	2.80	ethylene carbonate (**1**), propylene carbonate (**2**), cyrene (**3**), D-limonene (**18**), p-cymene (**19**), MeOH (**20**), EtOH (**21**), isopropanol (**22**)	6
2.80	3.80		5
3.80	4.80	dimethyl carbonate (**16**)	4
4.80	5.80	acetone (**4**), EtOAc (**8**), γ-valerolactone (**11**), diethyl carbonate (**17**)	3
5.80	6.80		2
6.80	7.80	cyclopentanone (**7**), 2-MeTHF (**12**), NMP, DMF, CH_2Cl_2	1

5 groups

Swelling range		Solvents	Rank
1.80	3.00	ethylene carbonate (**1**), propylene carbonate (**2**), cyrene (**3**), D-limonene (**18**), p-cymene (**19**), MeOH (**20**), EtOH (**21**), isopropanol (**22**)	5
3.00	4.20		4
4.20	5.40	acetone (**4**), EtOAc (**8**), γ-valerolactone (**11**), dimethyl carbonate (**16**), diethyl carbonate (**17**)	3
5.40	6.60		2
6.60	7.80	cyclopentanone (**7**), 2-MeTHF (**12**), NMP, DMF, CH_2Cl_2	1

4 groups

Swelling range		Solvents	Rank
1.80	3.30	ethylene carbonate (**1**), propylene carbonate (**2**), cyrene (**3**), D-limonene (**18**), p-cymene (**19**), MeOH (**20**), EtOH (**21**), isopropanol (**22**)	4
3.30	4.80	dimethyl carbonate (**16**),	3
4.80	6.30	acetone (**4**), EtOAc (**8**), γ-valerolactone (**11**), diethyl carbonate (**17**)	2
6.30	7.80	cyclopentanone (**7**), 2-MeTHF (**12**), NMP, DMF, CH_2Cl_2	1

JandaJel resin

Maximum swelling 8.8 mL g^{-1}; minimum swelling 1.8 mL g^{-1}

6 groups

Swelling range		Solvents	Rank
1.80	2.97	ethylene carbonate (**1**), propylene carbonate (**2**), cyrene (**3**), acetone (**4**), diethyl carbonate (**17**), MeOH (**20**), EtOH (**21**), isopropanol (**22**)	6
2.97	4.13	dimethyl carbonate (**16**)	5
4.13	5.30	D-limonene (**18**)	4
5.30	6.47	EtOAc (**8**), p-cymene (**19**), DMF	3
6.47	7.63		2
7.63	8.80	cyclopentanone (**7**), γ-valerolactone (**11**), 2-MeTHF (**12**), NMP, CH_2Cl_2	1

5 groups

Swelling range		Solvents	Rank
1.80	3.20	ethylene carbonate (**1**), propylene carbonate (**2**), cyrene (**3**), acetone (**4**), diethyl carbonate (**17**), MeOH (**20**), EtOH (**21**), isopropanol (**22**)	5
3.20	4.60	dimethyl carbonate (**16**)	4
4.60	6.00	EtOAc (**8**), D-limonene (**18**), p-cymene (**19**)	3
6.00	7.40	DMF	2
7.40	8.80	cyclopentanone (**7**), γ-valerolactone (**11**), 2-MeTHF (**12**), NMP, CH_2Cl_2	1

4 groups

Swelling range		Solvents	Rank
1.80	3.55	ethylene carbonate (**1**), propylene carbonate (**2**), cyrene (**3**), acetone (**4**), diethyl carbonate (**17**), MeOH (**20**), EtOH (**21**), isopropanol (**22**)	4
3.55	5.30	dimethyl carbonate (**16**), D-limonene (**18**)	3
5.30	7.05	EtOAc (**8**), p-cymene (**19**), DMF	2
7.05	8.80	cyclopentanone (**7**), γ-valerolactone (**11**), 2-MeTHF (**12**), NMP, CH_2Cl_2	1

TentaGel resin

Maximum swelling 5.5 mL g^{-1}; minimum swelling 1.8 mL g^{-1}

6 groups

Swelling range		Solvents	Rank
1.80	2.42	p-cymene (**19**), EtOH (**21**), isopropanol (**22**)	6
2.42	3.03	diethyl carbonate (**17**), D-limonene (**18**), MeOH (**20**)	5
3.03	3.65	propylene carbonate (**2**), acetone (**4**), 2-MeTHF (**12**)	4
3.65	4.27	ethylene carbonate (**1**), cyrene (**3**), EtOAc (**8**), γ-valerolactone (**11**), dimethyl carbonate (**16**), NMP, DMF	3
4.27	4.88	cyclopentanone (**7**)	2
4.88	5.50	CH_2Cl_2 (Note only one solvent in group 1)	1

5 groups

Swelling range		Solvents	Rank
1.80	2.54	p-cymene (**19**), EtOH (**21**), isopropanol (**22**)	5
2.54	3.28	diethyl carbonate (**17**), D-limonene (**18**), MeOH (**20**)	4
3.28	4.02	ethylene carbonate (**1**), propylene carbonate (**2**), cyrene (**3**), acetone (**4**), EtOAc (**8**), γ-valerolactone (**11**), 2-MeTHF (**12**), dimethyl carbonate (**16**), NMP, DMF	3
4.02	4.76		2
4.76	5.50	cyclopentanone (**7**), CH_2Cl_2	1

4 groups

Swelling range		Solvents	Rank
1.80	2.73	diethyl carbonate (**17**), D-limonene (**18**), p-cymene (**19**), EtOH (**21**), isopropanol (**22**)	4
2.73	3.65	propylene carbonate (**2**), acetone (**4**), 2-MeTHF (**12**), MeOH (**20**)	3
3.65	4.58	ethylene carbonate (**1**), cyrene (**3**), EtOAc (**8**), γ-valerolactone (**11**), dimethyl carbonate (**16**), NMP, DMF	2
4.58	5.50	cyclopentanone (**7**), CH_2Cl_2	1

ArgoGel resin

Maximum swelling 7.7 mL g^{-1}; minimum swelling 1.8 mL g^{-1}

6 groups

Swelling range		Solvents	Rank
1.80	2.78	p-cymene (**19**), EtOH (**21**), isopropanol (**22**)	6
2.78	3.77		5
3.77	4.75	ethylene carbonate (**1**), propylene carbonate (**2**), acetone (**4**), 2-MeTHF (**12**), diethyl carbonate (**17**), D-limonene (**18**), MeOH (**20**)	4
4.75	5.73	cyrene (**3**), EtOAc (**8**), γ-valerolactone (**11**), dimethyl carbonate (**16**), NMP, DMF	3
5.73	6.72	cyclopentanone (**7**)	2
6.72	7.70	CH_2Cl_2 (Note only one solvent in group 1)	1

5 groups

Swelling range		Solvents	Rank
1.80	2.98	p-cymene (**19**), EtOH (**21**), isopropanol (**22**)	5
2.98	4.16	ethylene carbonate (**1**), acetone (**4**), MeOH (**20**)	4
4.16	5.34	propylene carbonate (**2**), cyrene (**3**), EtOAc (**8**), γ-valerolactone (**11**), 2-MeTHF (**12**), dimethyl carbonate (**16**), diethyl carbonate (**17**), D-limonene (**18**), NMP, DMF	3
5.34	6.52	cyclopentanone (**7**)	2
6.52	7.70	CH_2Cl_2 (Note only one solvent in group 1)	1

4 groups

Swelling range		Solvents	Rank
1.80	3.28	p-cymene (**19**), EtOH (**21**), isopropanol (**22**)	4
3.28	4.75	ethylene carbonate (**1**), propylene carbonate (**2**), acetone (**4**), 2-MeTHF (**12**), diethyl carbonate (**17**), D-limonene (**18**), MeOH (**20**)	3
4.75	6.23	cyrene (**3**), cyclopentanone (**7**), EtOAc (**8**), γ-valerolactone (**11**), dimethyl carbonate (**16**), NMP, DMF	2
6.23	7.70	CH_2Cl_2 (Note only one solvent in group 1)	1

HypoGel resin

Maximum swelling 4.8 mL g^{-1}; minimum swelling 1.8 mL g^{-1}

6 groups

Swelling range		Solvents	Rank
1.80	2.30	p-cymene (**19**), MeOH (**20**), EtOH (**21**), isopropanol (**22**)	6
2.30	2.80	propylene carbonate (**2**), diethyl carbonate (**17**), D-limonene (**18**)	5
2.80	3.30	ethylene carbonate (**1**), acetone (**4**), EtOAc (**8**), dimethyl carbonate (**16**)	4
3.30	3.80	cyrene (**3**), γ-valerolactone (**11**)	3
3.80	4.30	2-MeTHF (**12**)	2
4.30	4.80	cyclopentanone (**7**), NMP, CH_2Cl_2, DMF	1

5 groups

Swelling range		Solvents	Rank
1.80	2.40	propylene carbonate (**2**), D-limonene (**18**), p-cymene (**19**), MeOH (**20**), EtOH (**21**), isopropanol (**22**)	5
2.40	3.00	ethylene carbonate (**1**), acetone (**4**), EtOAc (**8**), dimethyl carbonate (**16**), diethyl carbonate (**17**)	4
3.00	3.60	cyrene (**3**), γ-valerolactone (**11**)	3
3.60	4.20	2-MeTHF (**12**)	2
4.20	4.80	cyclopentanone (**7**), NMP, CH_2Cl_2, DMF	1

4 groups

Swelling range		Solvents	Rank
1.80	2.55	propylene carbonate (**2**), D-limonene (**18**), p-cymene (**19**), MeOH (**20**), EtOH (**21**), isopropanol (**22**)	4
2.55	3.30	ethylene carbonate (**1**), acetone (**4**), EtOAc (**8**), dimethyl carbonate (**16**), diethyl carbonate (**17**)	3
3.30	4.05	cyrene (**3**), γ-valerolactone (**11**), 2-MeTHF (**12**)	2
4.05	4.80	cyclopentanone (**7**), NMP, CH_2Cl_2, DMF	1

NovaGel resin

Maximum swelling 5.8 mL g^{-1}; minimum swelling 1.8 mL g^{-1}

6 groups

Swelling range		Solvents	Rank
1.80	2.47	D-limonene (**18**), p-cymene (**19**), MeOH (**20**), EtOH (**21**), isopropanol (**22**)	6
2.47	3.13	ethylene carbonate (**1**), propylene carbonate (**2**), diethyl carbonate (**17**)	5
3.13	3.80	acetone (**4**), EtOAc (**8**), γ-valerolactone (**11**), 2-MeTHF (**12**), dimethyl carbonate (**16**)	4
3.80	4.47	cyrene (**3**)	3
4.47	5.13	cyclopentanone (**7**), NMP, DMF	2
5.13	5.80	CH_2Cl_2 (Note only one solvent in group 1)	1

5 groups

Swelling range		Solvents	Rank
1.80	2.60	D-limonene (**18**), p-cymene (**19**), MeOH (**20**), EtOH (**21**), isopropanol (**22**)	5
2.60	3.40	ethylene carbonate (**1**), propylene carbonate (**2**), EtOAc (**8**), dimethyl carbonate (**16**), diethyl carbonate (**17**)	4
3.40	4.20	acetone (**4**), γ-valerolactone (**11**), 2-MeTHF (**12**)	3
4.20	5.00	cyrene (**3**), cyclopentanone (**7**), NMP	2
5.00	5.80	DMF, CH_2Cl_2	1

4 groups

Swelling range		Solvents	Rank
1.80	2.80	ethylene carbonate (**1**), propylene carbonate (**2**), diethyl carbonate (**17**), D-limonene (**18**), p-cymene (**19**), MeOH (**20**), EtOH (**21**), isopropanol (**22**)	4
2.80	3.80	acetone (**4**), EtOAc (**8**), γ-valerolactone (**11**), 2-MeTHF (**12**), dimethyl carbonate (**16**)	3
3.80	4.80	cyrene (**3**), NMP	2
4.80	5.80	cyclopentanone (**7**), DMF, CH_2Cl_2	1

ChemMatrix resin

Maximum swelling 9.8 mL g^{-1}; minimum swelling 1.8 mL g^{-1}

6 groups

Swelling range		Solvents	Rank
1.80	3.13	p-cymene (**19**), isopropanol (**22**)	6
3.13	4.47	acetone (**4**), EtOH (**21**)	5
4.47	5.80	EtOAc (**8**), 2-MeTHF (**12**), diethyl carbonate (**17**), D-limonene (**19**)	4
5.80	7.13	ethylene carbonate (**1**), propylene carbonate (**2**), cyclopentanone (**7**), γ-valerolactone (**11**), dimethyl carbonate (**16**), MeOH (**20**)	3
7.13	8.47	cyrene (**3**),DMF, NMP	2
8.47	9.80	CH_2Cl_2 (Note only one solvent in group 1)	1

5 groups

Swelling range		Solvents	Rank
1.80	3.40	p-cymene (**19**), isopropanol (**22**)	5
3.40	5.00	acetone (**4**), EtOAc (**8**), D-limonene (**18**), EtOH (**21**)	4
5.00	6.60	propylene carbonate (**2**), γ-valerolactone (**11**), 2-MeTHF (**12**), dimethyl carbonate (**16**), diethyl carbonate (**17**),	3
6.60	8.20	ethylene carbonate (**1**), cyclopentanone (**7**), MeOH (**20**), NMP, DMF	2
8.20	9.80	cyrene (**3**), CH_2Cl_2	1

4 groups

Swelling range		Solvents	Rank
1.80	3.80	p-cymene (**19**), EtOH (**21**), isopropanol (**22**)	4
3.80	5.80	acetone (**4**), EtOAc (**8**), diethyl carbonate (**17**), 2-MeTHF (**12**), D-limonene (**18**)	3
5.80	7.80	ethylene carbonate (**1**), propylene carbonate (**2**), cyclopentanone (**7**), γ-valerolactone (**11**), dimethyl carbonate (**16**), MeOH (**20**), NMP, DMF,	2
7.80	9.80	cyrene (**3**), CH_2Cl_2	1

SpheriTide resin

Maximum swelling 5.3 mL g^{-1}; minimum swelling 1.8 mL g^{-1}

6 groups

Swelling range		Solvents	Rank
1.80	2.38	ethylene carbonate (**1**), propylene carbonate (**2**), diethyl carbonate (**17**), D-limonene (**18**), p-cymene (**19**)	6
2.38	2.97	cyrene (**3**), acetone (**4**), EtOAc (**8**), 2-MeTHF (**12**), dimethyl carbonate (**16**), isopropanol (**22**)	5
2.97	3.55	γ-valerolactone (**11**)	4
3.55	4.13	cyclopentanone (**7**), MeOH (**20**), EtOH (**21**)	3
4.13	4.72		2
4.72	5.30	NMP, DMF, CH_2Cl_2	1

5 groups

Swelling range		Solvents	Rank
1.80	2.50	ethylene carbonate (**1**), propylene carbonate (**2**), diethyl carbonate (**17**), D-limonene (**18**), p-cymene (**19**)	5
2.50	3.20	cyrene (**3**), acetone (**4**), EtOAc (**8**), γ-valerolactone (**11**), 2-MeTHF (**12**), dimethyl carbonate (**16**), isopropanol (**22**)	4
3.20	3.90	cyclopentanone (**7**), MeOH (**20**), EtOH (**21**)	3
3.90	4.60		2
4.60	5.30	NMP, DMF, CH_2Cl_2	1

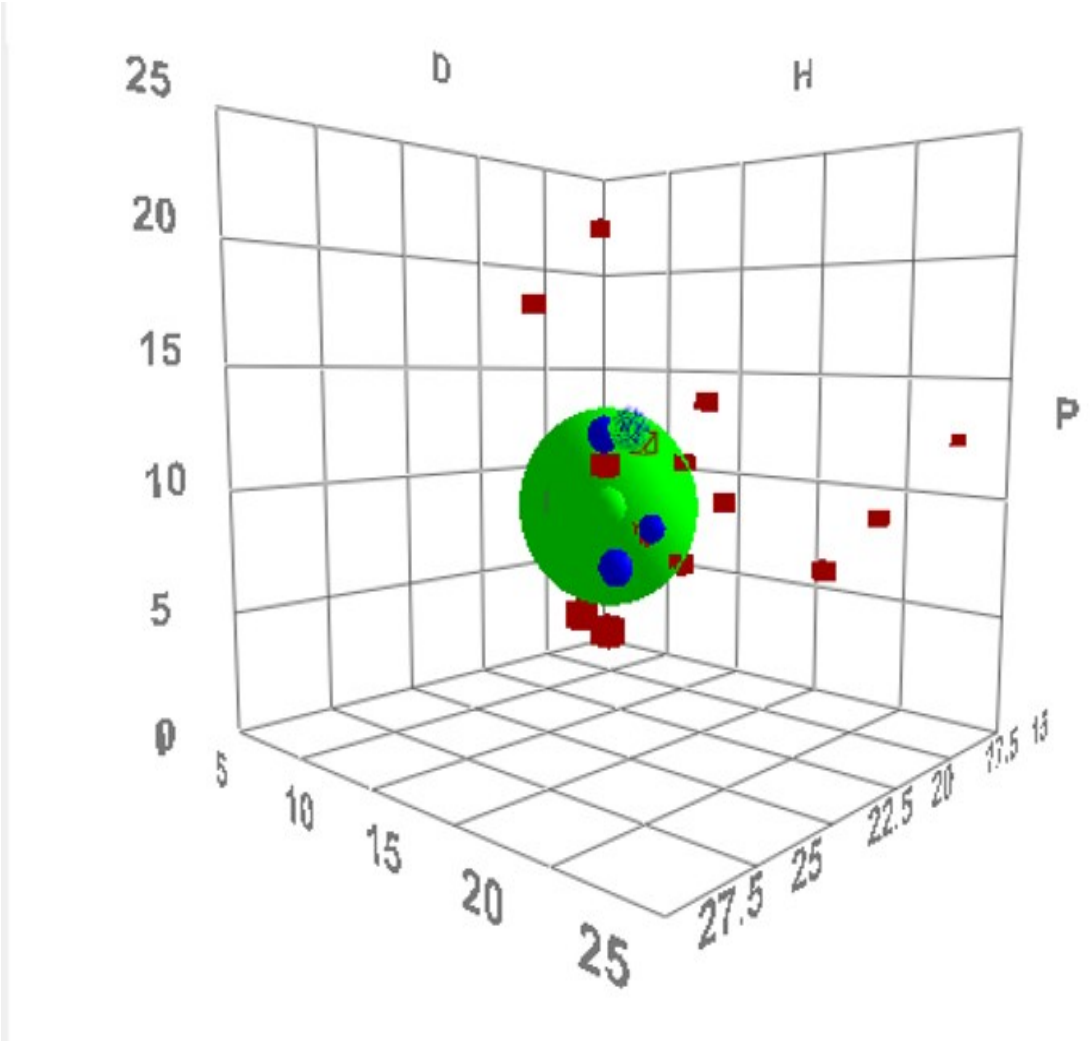
4 groups

Swelling range		Solvents	Rank
1.80	2.68	ethylene carbonate (**1**), propylene carbonate (**2**), EtOAc (**8**), diethyl carbonate (**17**), D-limonene (**18**), p-cymene (**19**)	4
2.68	3.55	cyrene (**3**), acetone (**4**), γ-valerolactone (**11**), 2-MeTHF (**12**), dimethyl carbonate (**16**), isopropanol (**22**)	3
3.55	4.43	cyclopentanone (**7**), MeOH (**20**), EtOH (**21**)	2
4.43	5.30	NMP, DMF, CH_2Cl_2	1

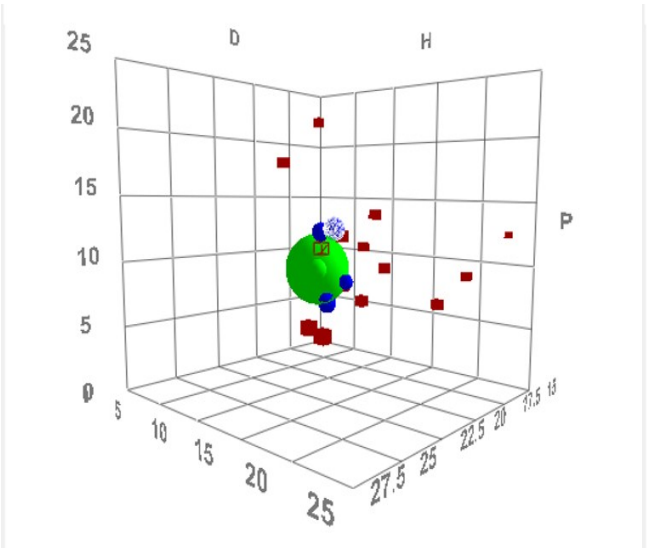
3D plots of HSPiP predictions

Merrifield resin

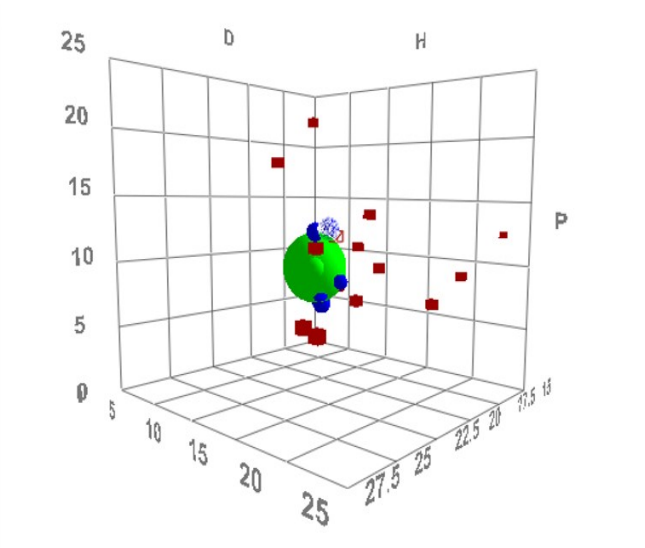
5 Groups



4 Groups

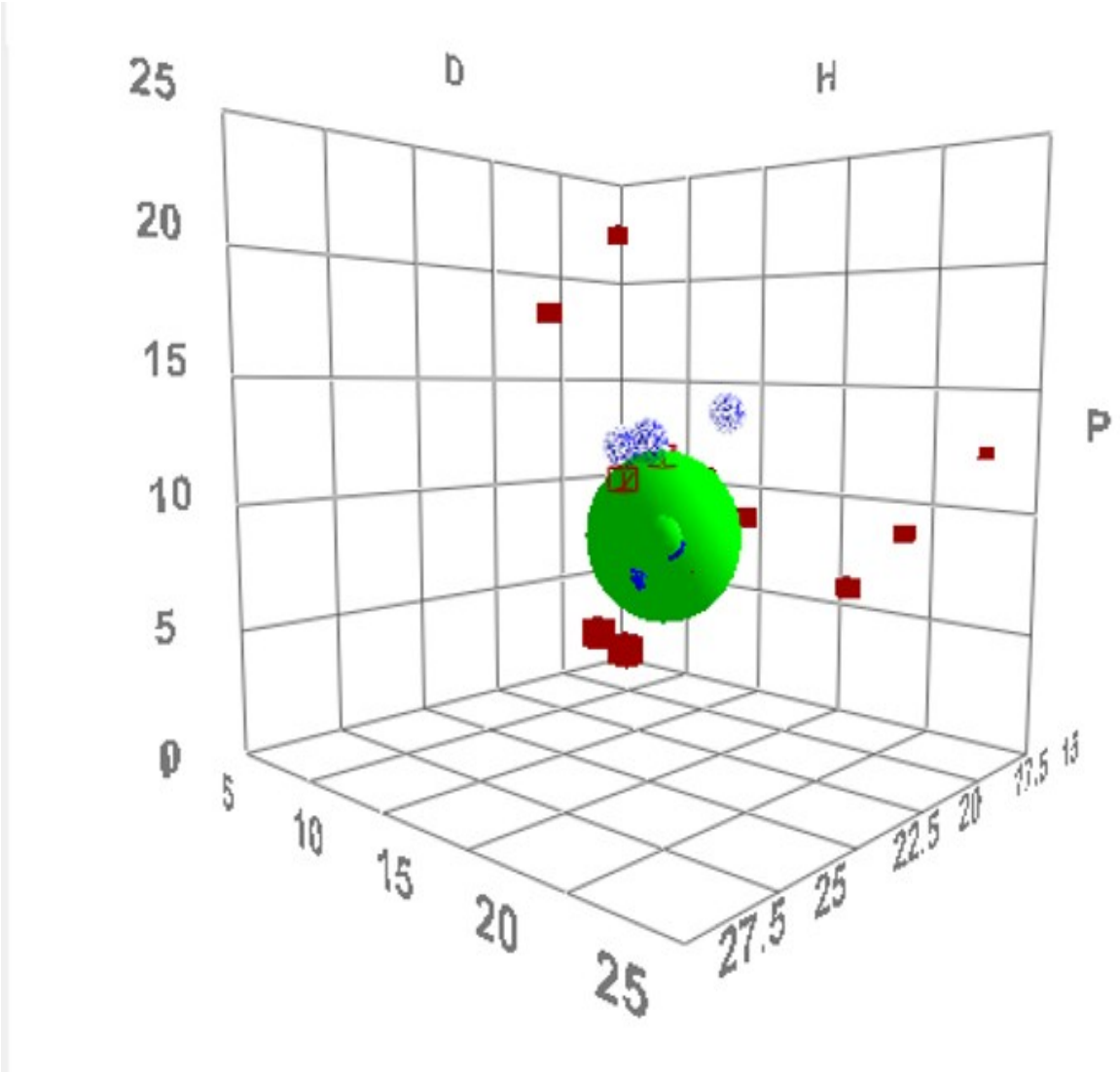


6 Groups

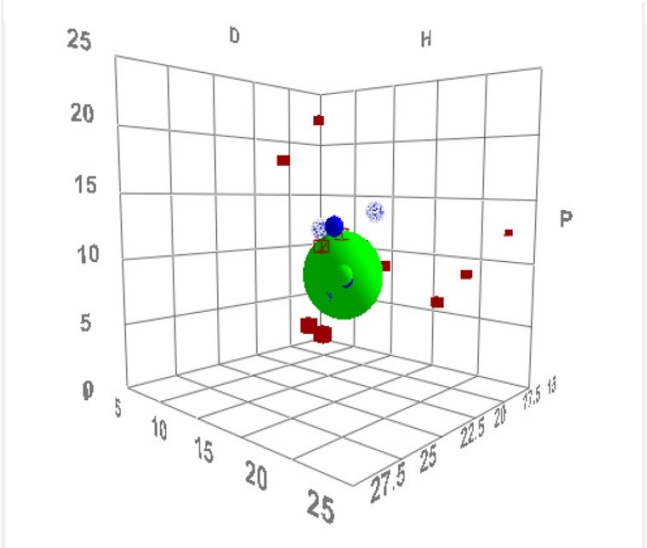


ParaMax resin

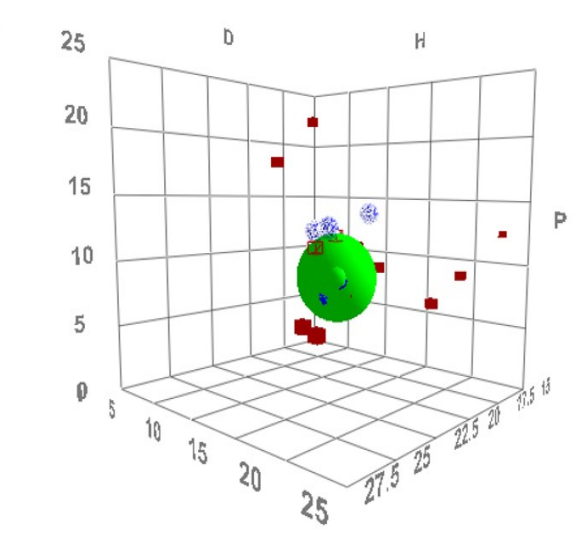
5 Groups



4 Groups

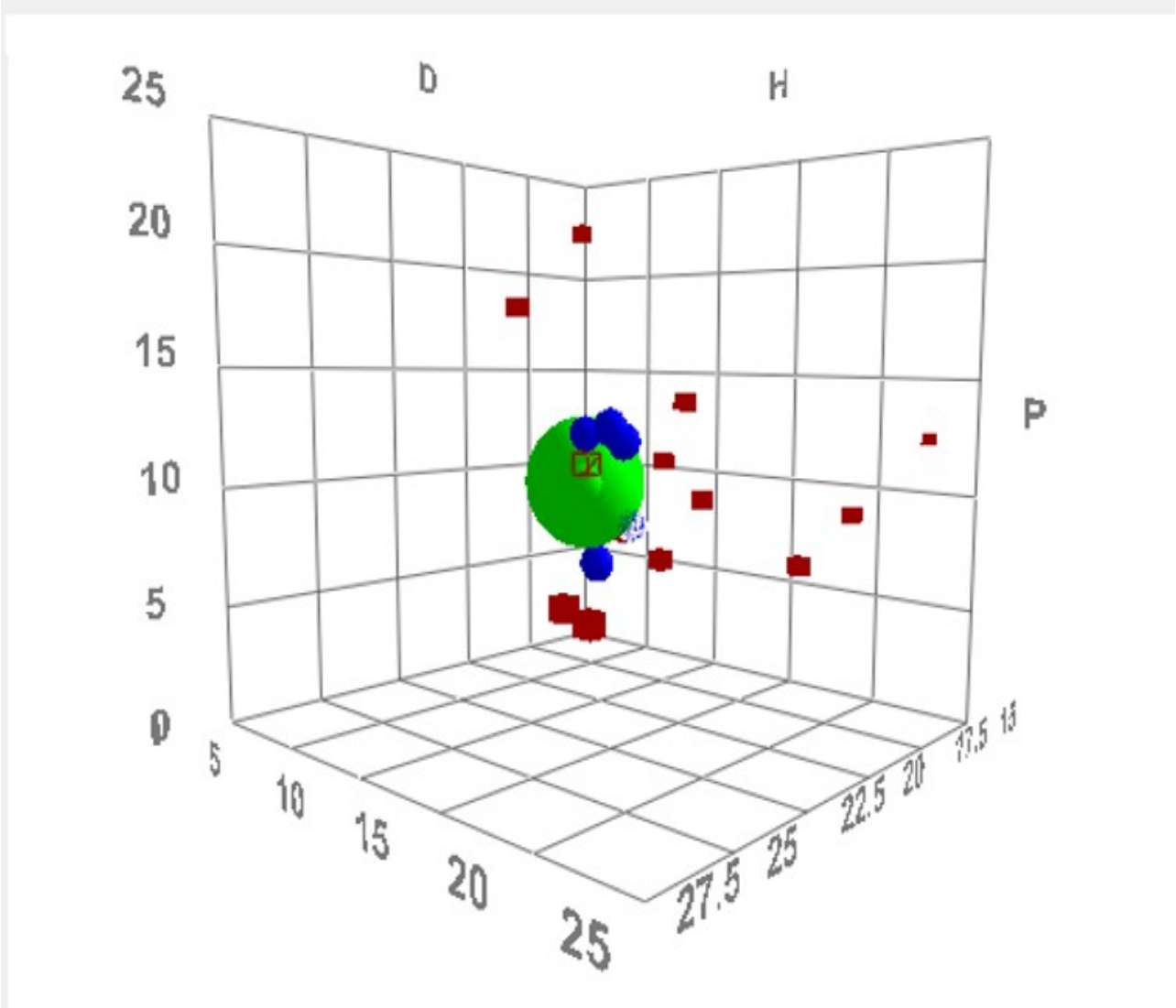


6 Groups

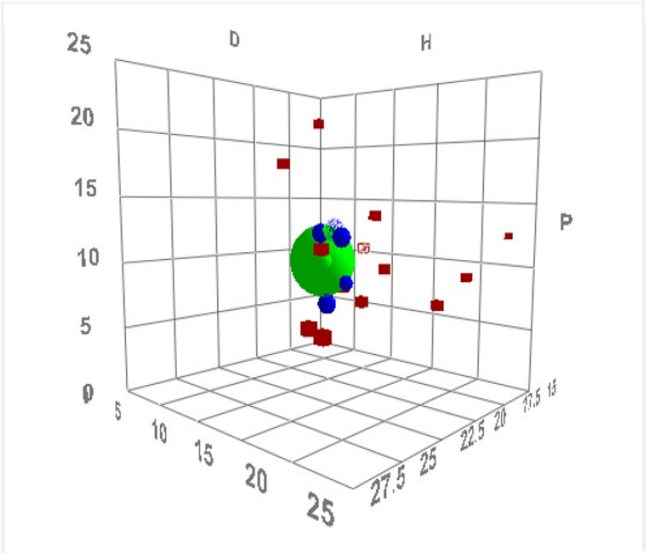


JandaJel resin

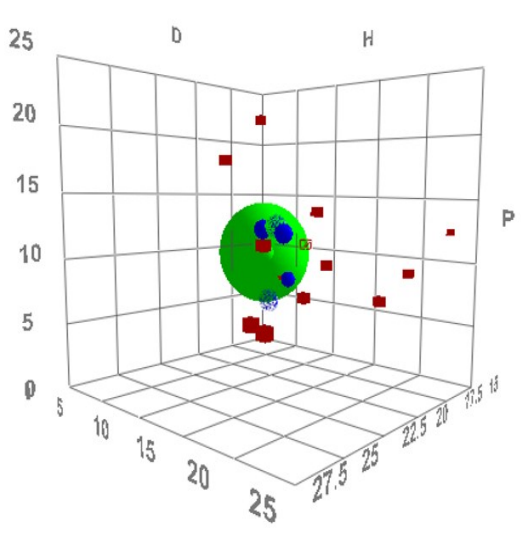
5 Groups



4 Groups

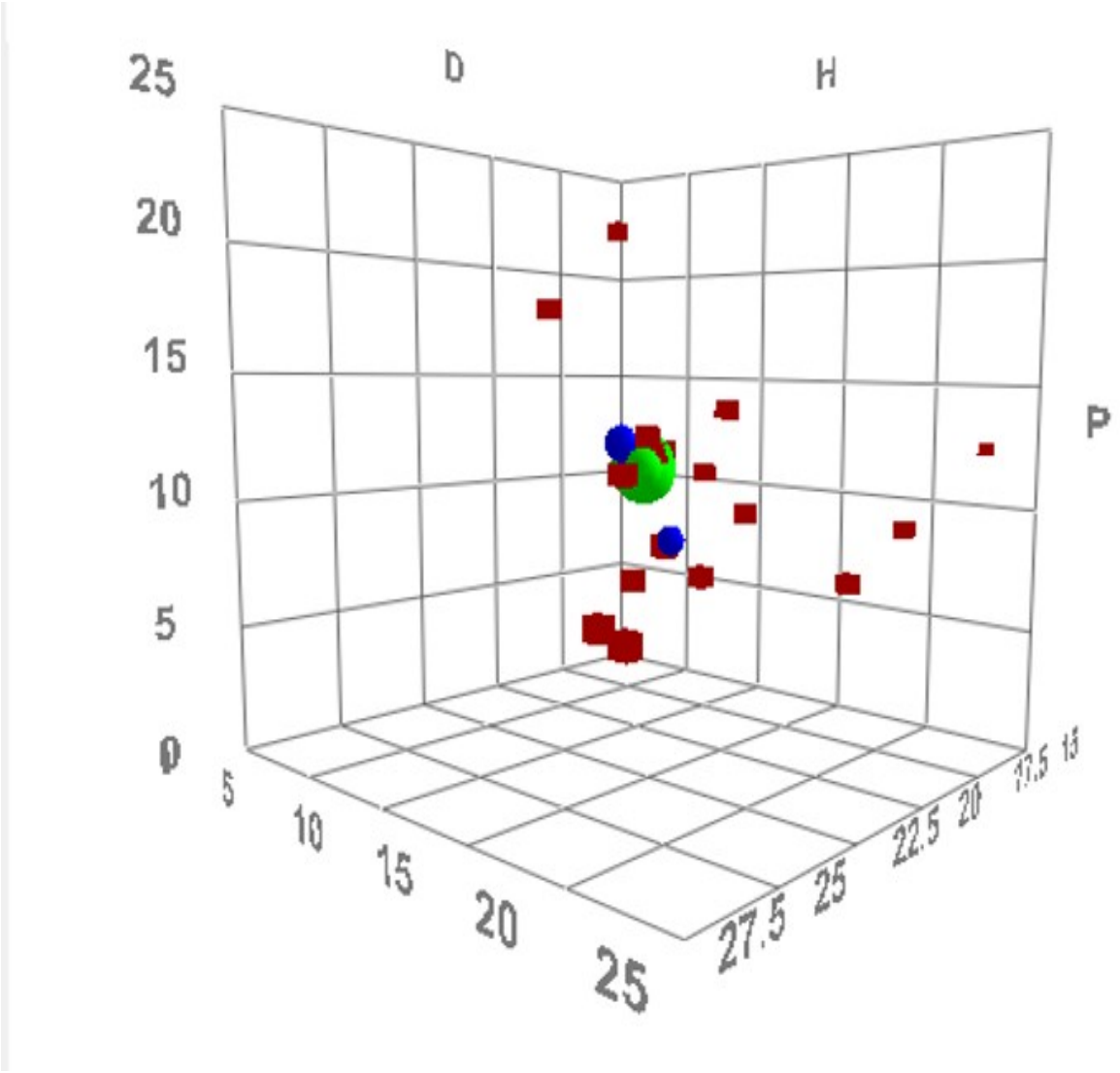


6 Groups

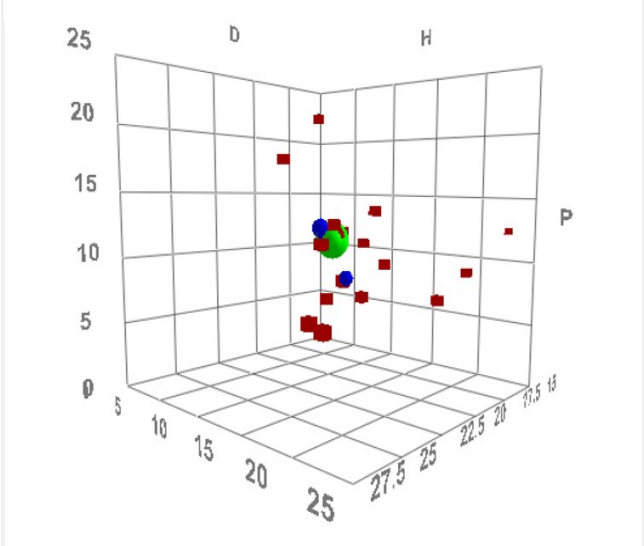


TentaGel resin

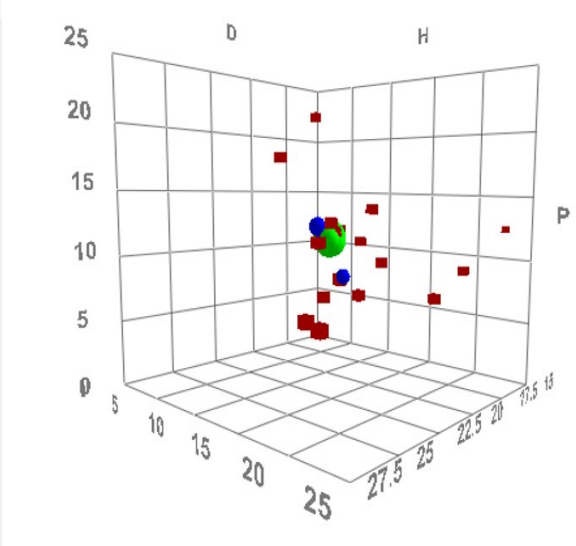
5 Groups



4 Groups

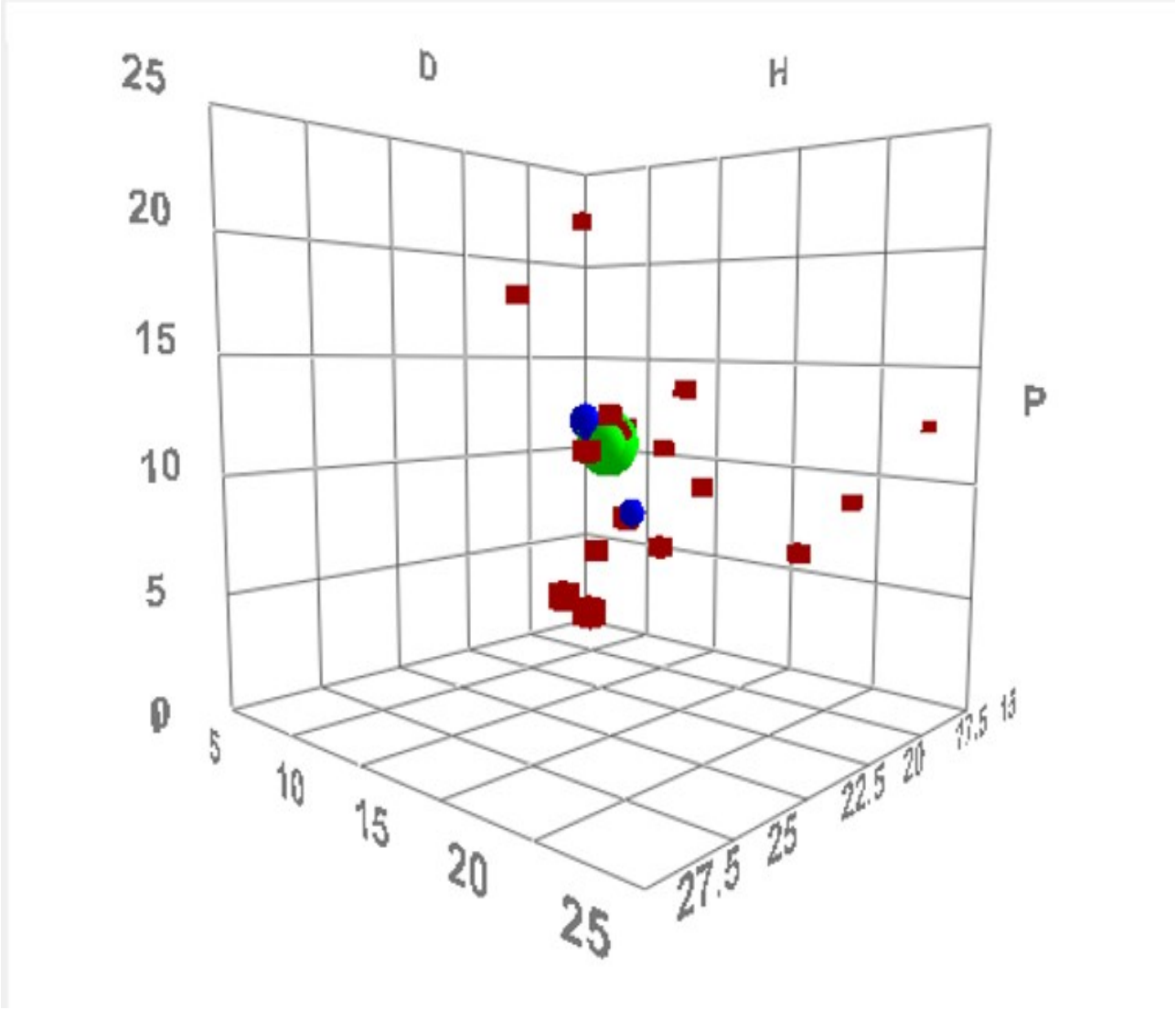


6 Groups

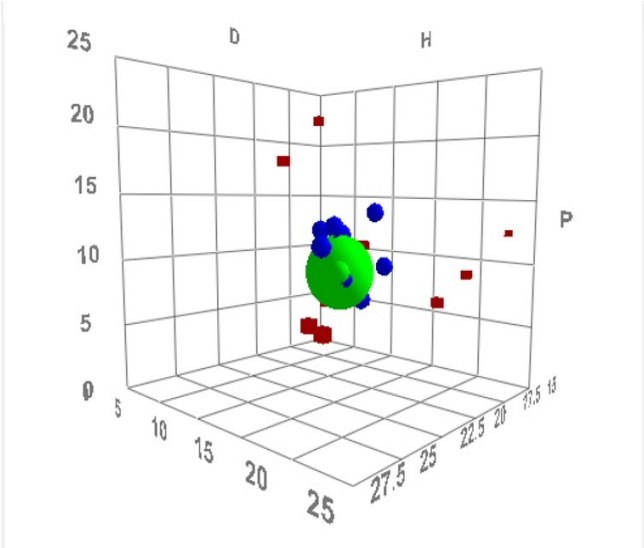


ArgoGel resin

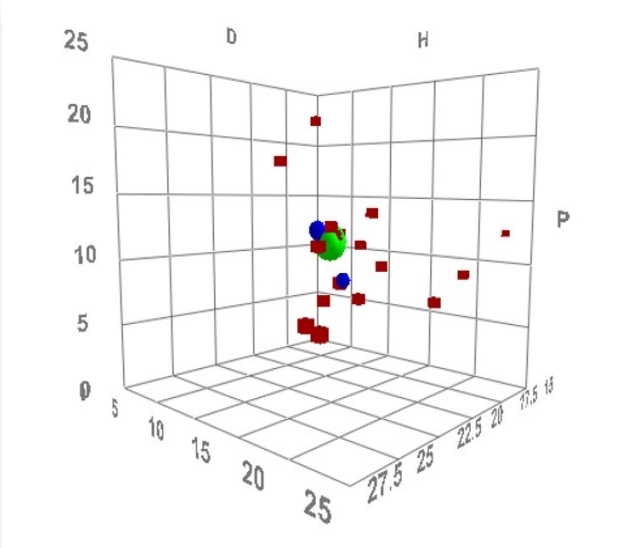
5 Groups



4 Groups

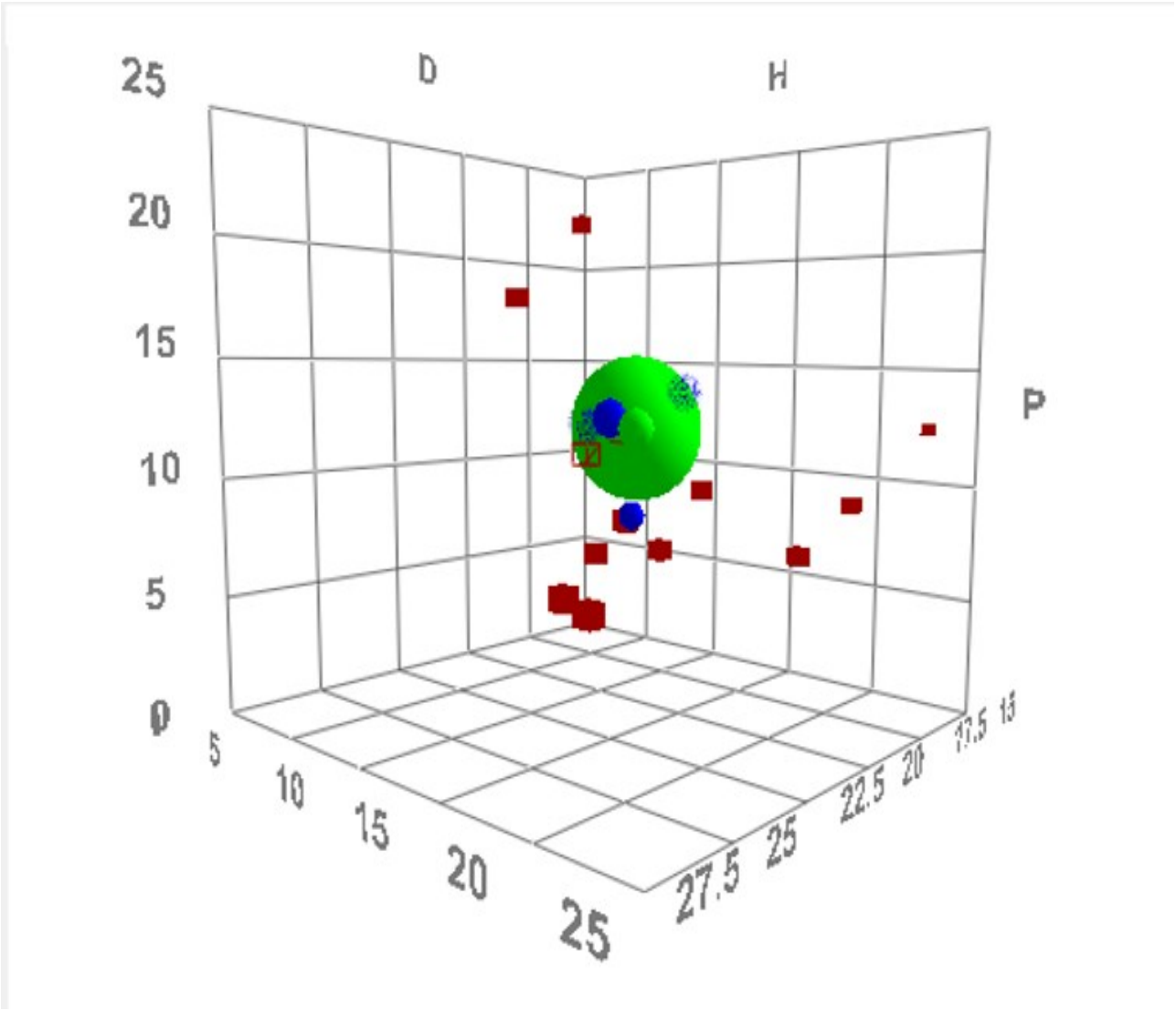


6 Groups

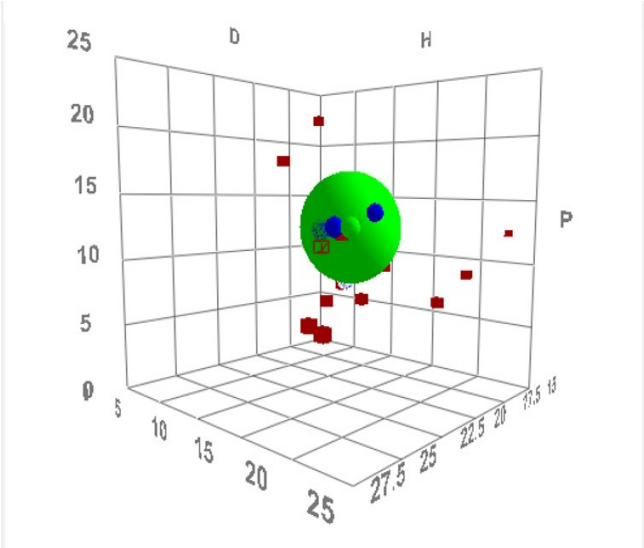


HypoGel resin

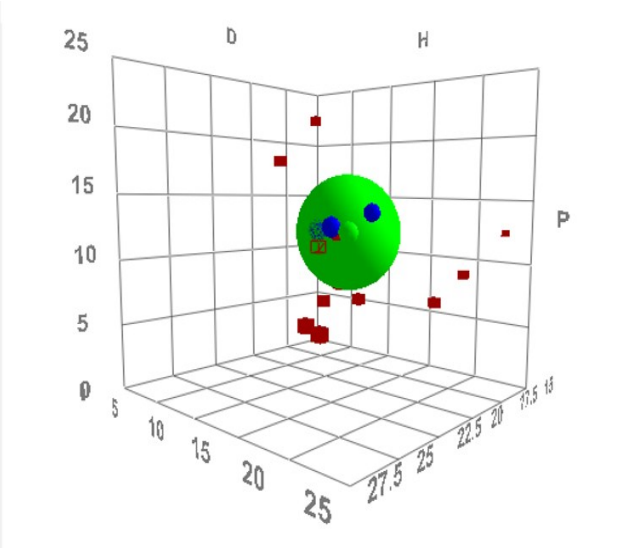
5 Groups



4 Groups

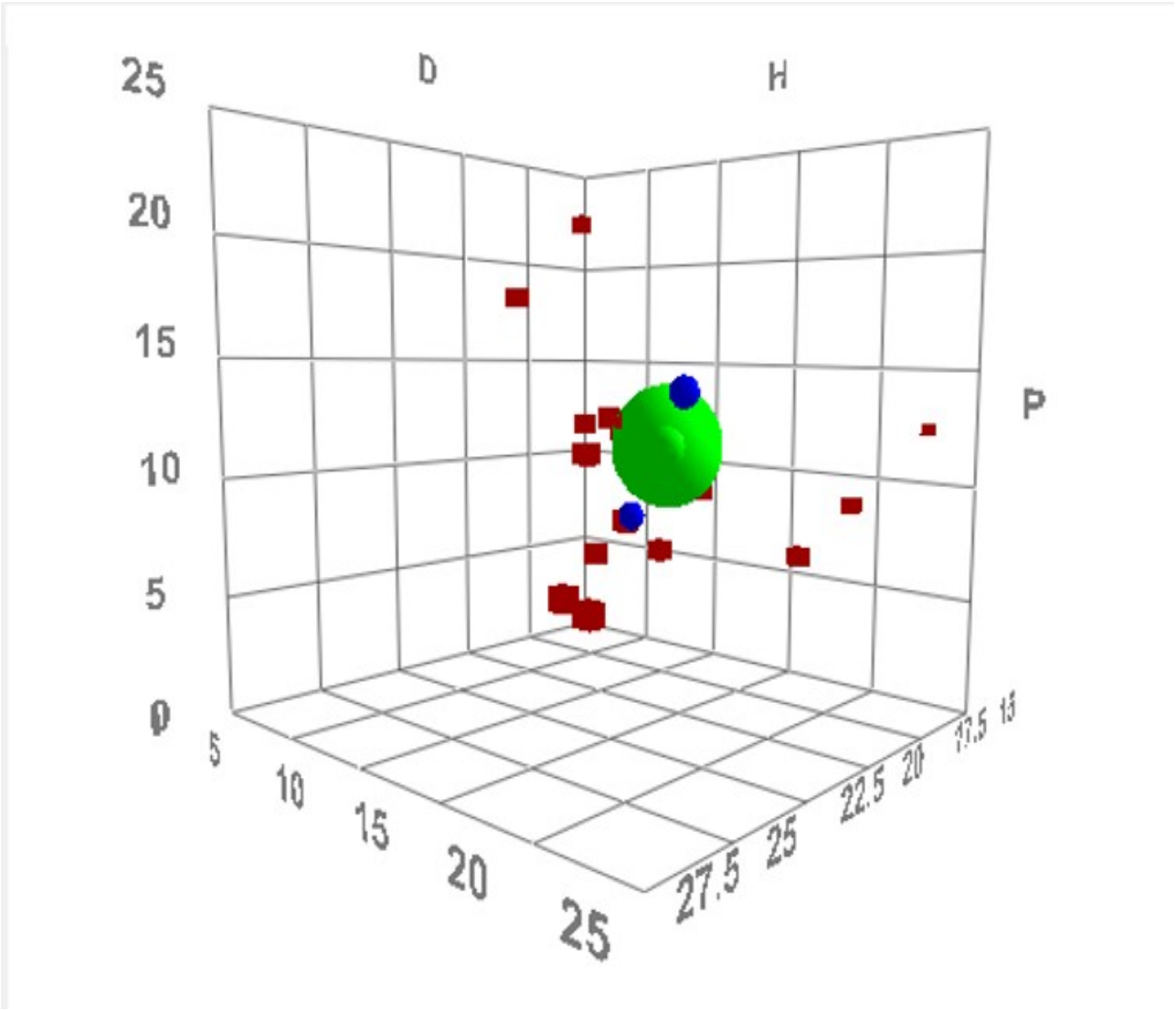


6 Groups

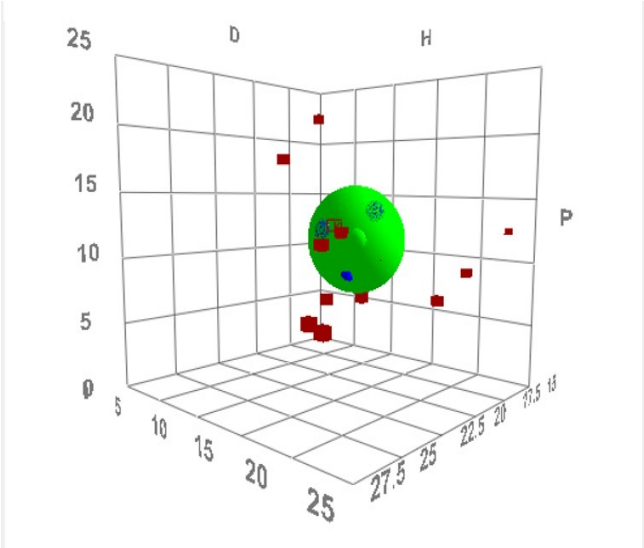


NovaGel resin

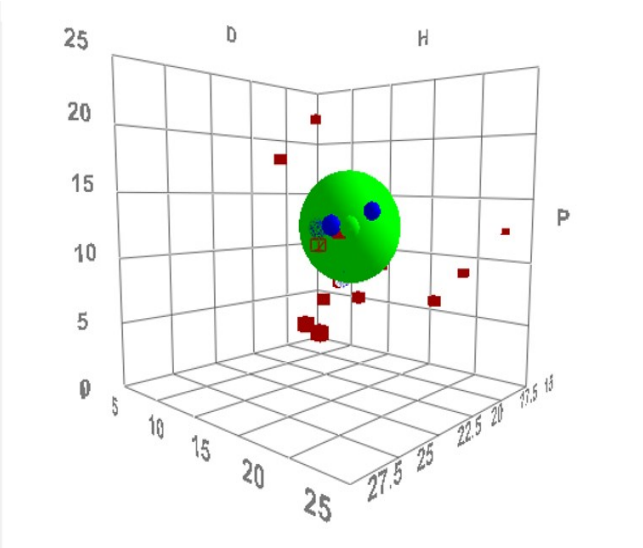
5 Groups



4 Groups

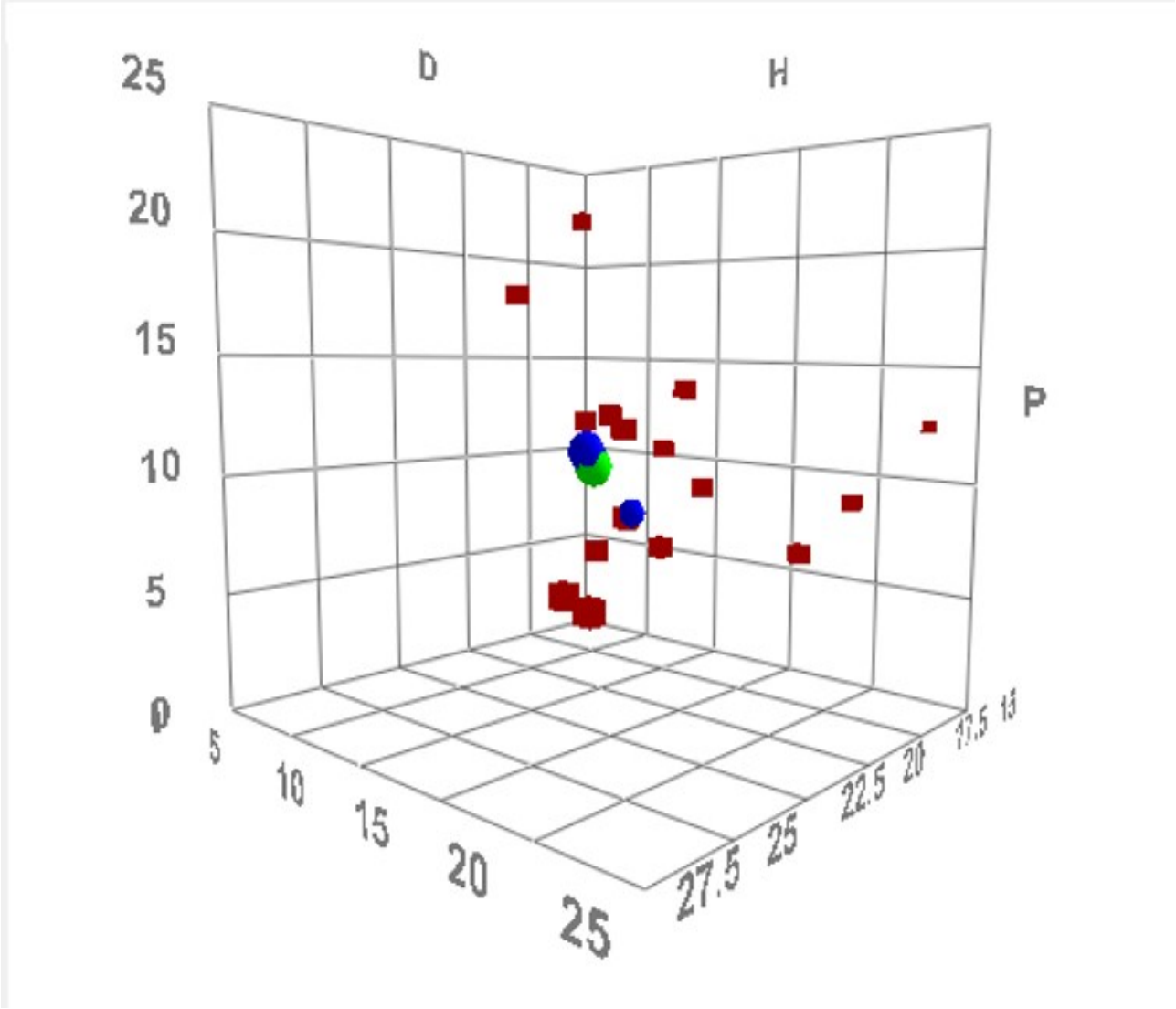


6 Groups

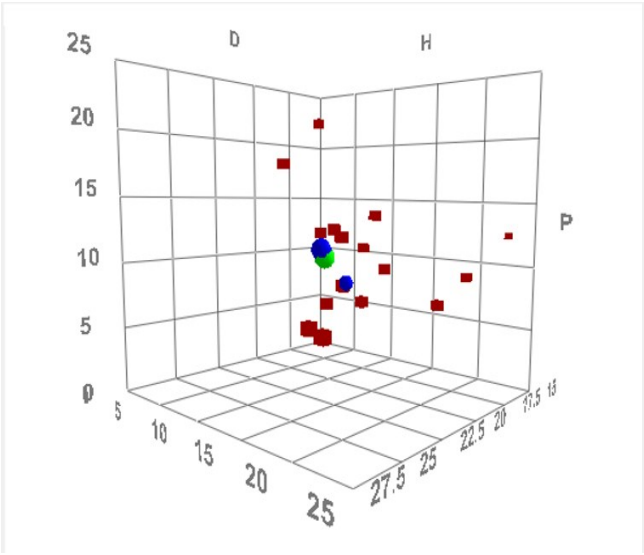


ChemMatrix resin

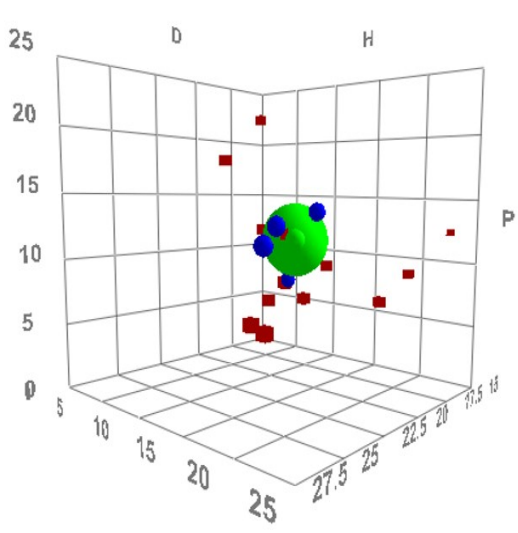
5 Groups



4 Groups

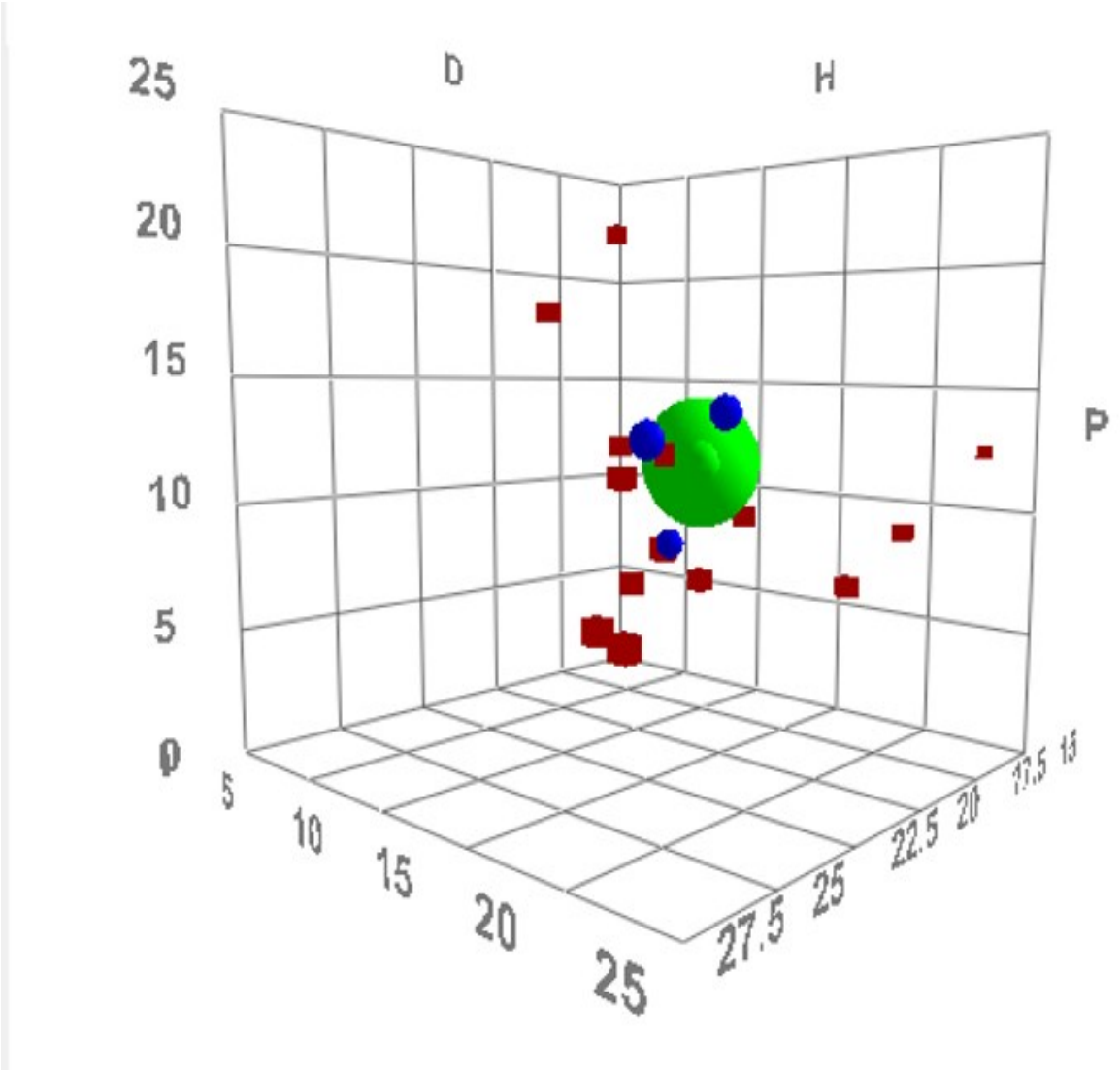


6 Groups

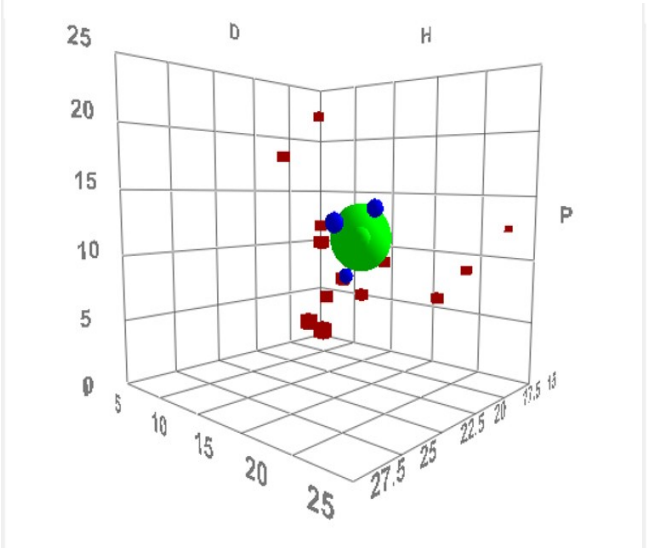


SpheriTide resin

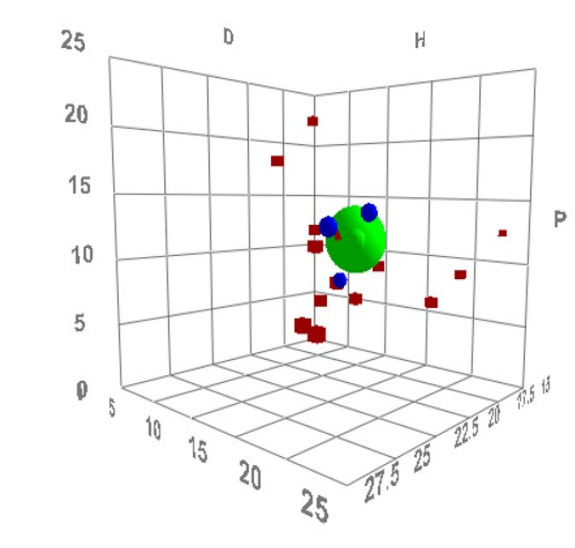
5 Groups



4 Groups



6 Groups



Predictions of solvents to swell each resin

The following pages list the HSPiP predictions of good solvents to swell each resin.

The solvents are listed in order of increasing distance from the ideal solvent parameters (D, P and H) for that resin to a lower cut off of a solvent which was in the training set and gave swelling of the resin of less than 4.0 mL g^{-1}. Solvents are colour coded as:

Black: solvent that was in the training set.

Green, orange or red corresponding to the recommendations in the latest version of the Glaxo green solvents guide (Green Chem., 2016, 18, 3879–3890).

Blue: solvent that is not in the Glaxo green solvents guide.

The columns in the tables correspond to:

Distance:	distance from the ideal solvent parameters
D:	dispersion energy
P:	dipolar energy
H:	hydrogen bonding energy
BPt:	boiling point
FPt:	flash point
VP@25	vapour pressure at 25 ^{o}C
MPt:	melting point

Merrifield resin

Ideal parameters: D, 17.5; P, 8.5; H, 4.3

Solvents	Distance	D	P	H	BPt	FPt	VP@25	MPt
Cyclohexanone	0.75	17.8	8.4	5.1	155	44	3.73	-31
Isophorone	1	17	8	5	215	90	0.309	-8
Dichloromethane	2.69	17	7.3	7.1	40	-4	435	-95
Dimethyl Isosorbide	2.98	17.6	7.1	7.5	234	105	0.03	-50
Methyl Propyl Ketone	3.02	16	7.6	4.7	102	7	35	-77
Methyl Ethyl Ketone	3.05	16	9	5.1	80	-5	90.3	-87
Tributyl Phosphate	3.09	16.3	6.3	4.3	289	166	0.001	-80
Butyl Benzoate	3.23	18.3	5.6	5.5	250	105	0.006	-22
1,4-Dioxane	3.45	17.1	6.8	7.8	101	12	36.5	12
Methyl iso-Amyl Ketone	3.96	16	5.7	4.1	145	36	5.1	-74
Cyclopentyl Methyl Ether	4.28	16.7	4.3	4.3	106	0	35.5	-140
Tetrahydrofuran	4.34	16.8	5.7	8	66	-17	181	-109
1-Nitropropane	4.45	16.6	12.3	5.5	131	24	9.84	-104
n-Butyl Propionate	4.63	15.7	5.5	5.9	145	32	4.19	-90
N-Methyl-2-Pyrrolidone	4.82	18	12.3	7.2	204	96	0.088	-24
Butyl Glycol Acetate	4.85	15.3	7.5	6.8	192	84	0.3	-64
n-Propyl Propanoate	4.85	15.5	5.6	5.7	123	19	13.5	-76
Methyl Iso-Butyl Ketone	4.9	15.3	6.1	4.1	116	16	19.8	-84
Methyl Acetate	4.97	15.5	7.2	7.6	57	-10	217	-98
1,3-Dioxolane	4.99	18.1	6.6	9.3	78	-6	110	-95
Acetone	5	15.5	10.4	7	56	-17	232	-95

ParaMax resin

Ideal parameters: D, 17.7; P, 7.9; H, 7.7

Solvents	Distance	D	P	H	BPt	FPt	VP@25	MPt
Dimethyl Isosorbide	0.82	17.6	7.1	7.5	234	105	0.03	-50
1,4-Dioxane	1.58	17.1	6.8	7.8	101	12	36.5	12
Dichloromethane	1.6	17	7.3	7.1	40	-4	435	-95
1,3-Dioxolane	2.19	18.1	6.6	9.3	78	-6	110	-95
Cyclohexanone	2.68	17.8	8.4	5.1	155	44	3.73	-31
Tetrahydrofuran	2.81	16.8	5.7	8	66	-17	181	-109
Isophorone	3.04	17	8	5	215	90	0.309	-8
Butyl Benzoate	3.41	18.3	5.6	5.5	250	105	0.006	-22
Glycerol Triacetate	4.34	16.5	4.5	9.1	259	138	0.001	4
Methyl Ethyl Ketone	4.41	16	9	5.1	80	-5	90.3	-87
Methyl Acetate	4.41	15.5	7.2	7.6	57	-10	217	-98
Propylene Glycol Monoethyl Ether Acetate	4.45	15.6	6.3	7.7	165	54	1.3	-60
N-Methyl-2-Pyrrolidone	4.51	18	12.3	7.2	204	96	0.088	-24
Diethylene Glycol Monobutyl Ether	4.51	16	7	10.6	231	78	0.033	-68
Methyl Propyl Ketone	4.53	16	7.6	4.7	102	7	35	-77
Ethyl Acetate	4.58	15.8	5.3	7.2	77	-3	96.5	-84
Propylene Glycol Phenyl Ether	4.61	17.4	5.3	11.5	243	129	0.002	21
Tributyl Phosphate	4.67	16.3	6.3	4.3	289	166	0.001	-80
N,N-Dimethyl Acetamide	4.74	16.8	11.5	10.2	166	70	1.16	-20
Dipropylene Glycol Mono n-Butyl Ether	4.77	15.7	6.5	10	230	100	0.002	-20
Butyl Glycol Acetate	4.86	15.3	7.5	6.8	192	84	0.3	-64
Diacetone Alcohol	4.87	15.8	8.2	10.8	168	45	1.07	-44
n-Butyl Propionate	4.96	15.7	5.5	5.9	145	32	4.19	-90
Butyl Diglycol Acetate	5.07	16	4.1	8.2	245	105	0.008	-32
Acetone	5.09	15.5	10.4	7	56	-17	232	-95
Propylene Glycol Monomethyl Ether Acetate	5.18	15.6	5.6	9.8	146	50	2.91	-68
Tetrahydrofurfuryl Alcohol	5.2	17.8	8.2	12.9	178	75	0.928	-80

n-Propyl Propanoate	5.31	15.5	5.6	5.7	123	19	13.5	-76
Cyclopentyl Methyl Ether	5.32	16.7	4.3	4.3	106	0	35.5	-140
Methyl iso-Amyl Ketone	5.39	16	5.7	4.1	145	36	5.1	-74
1-Nitropropane	5.41	16.6	12.3	5.5	131	24	9.84	-104
Methyl Carbitol	5.71	16.2	7.8	12.6	194	96	0.17	-65
n-Butyl Acetate	5.79	15.8	3.7	6.3	126	27	12.1	-74
Ethyl Lactate	5.85	16	7.6	12.5	155	47	2.07	-26
Propylene Glycol Monomethyl Ether	5.9	15.6	6.3	11.6	120	32	4.55	-97
n-Propyl Acetate	5.95	15.3	4.3	7.6	102	14	33	-95
Benzyl Benzoate	5.96	20	5.1	5.2	323	158	0.001	19
Methyl Oleate	5.97	16.2	3.8	4.5	344	180	0	20
Dipropylene Glycol Methyl Ether	5.99	15.5	5.7	11.2	215	75	0.006	-32
Propylene Glycol Monobutyl Ether	6.02	15.3	4.5	9.2	171	63	0.294	-29
n-Amyl Acetate	6.14	15.8	3.3	6.1	148	22	10.5	-71
Methyl Iso-Butyl Ketone	6.24	15.3	6.1	4.1	116	16	19.8	-84
Ethylene Glycol Monobutyl Ether	6.32	16	5.1	12.3	171	100	0.867	-74
Benzyl Alcohol	6.35	18.4	6.3	13.7	205	93	0.08	-15
Di-isoButyl Ketone	6.46	16	3.7	4.1	168	49	1.72	-46
Iso-Propyl Acetate	6.52	14.9	4.5	8.2	81	5	60.4	-73
Iso-Pentyl Acetate	6.78	15.3	3.1	7	142	25	4.6	-79
sec-Butyl Acetate	6.79	15	3.7	7.6	112	17	21.6	-99
N,N-Dimethyl Formamide	6.86	17.4	13.7	11.3	152	58	3.7	-60
Cyclohexanol	6.92	17.4	4.1	13.5	161	68	0.913	23
2-Phenoxy Ethanol	6.93	17.8	5.7	14.3	237	113	0.007	13
Methanol	7	14.7	5	10	65	12	128	-98

JandaJel resin

Ideal parameters: D, 17.1; P, 9.3; H, 4.1

Solvents	Distance	D	P	H	BPt	FPt	VP@25	MPt
Isophorone	1.59	17	8	5	215	90	0.309	-8
Cyclohexanone	1.61	17.8	8.4	5.1	155	44	3.73	-31
Methyl Ethyl Ketone	2.79	16	9	5.1	80	-5	90.3	-87
Methyl Propyl Ketone	3.09	16	7.6	4.7	102	7	35	-77
Tributyl Phosphate	3.5	16.3	6.3	4.3	289	166	0.001	-80
Dichloromethane	3.59	17	7.3	7.1	40	-4	435	-95
1-Nitropropane	3.72	16.6	12.3	5.5	131	24	9.84	-104
Dimethyl Isosorbide	4.03	17.6	7.1	7.5	234	105	0.03	-50
Butyl Benzoate	4.32	18.3	5.6	5.5	250	105	0.006	-22
Methyl iso-Amyl Ketone	4.33	16	5.7	4.1	145	36	5.1	-74
1,4-Dioxane	4.42	17.1	6.8	7.8	101	12	36.5	12
N-Methyl-2-Pyrrolidone	4.64	18	12.3	7.2	204	96	0.088	-24
Acetone	4.79	15.5	10.4	7	56	-17	232	-95
Cyclopentyl Methyl Ether	5.01	16.7	4.3	4.3	106	0	35.5	-140
Methyl Iso-Butyl Ketone	5.04	15.3	6.1	4.1	116	16	19.8	-84
Butyl Glycol Acetate	5.11	15.3	7.5	6.8	192	84	0.3	-64
n-Butyl Propionate	5.19	15.7	5.5	5.9	145	32	4.19	-90
n-Propyl Propanoate	5.31	15.5	5.6	5.7	123	19	13.5	-76
Tetrahydrofuran	5.32	16.8	5.7	8	66	-17	181	-109
Methyl Acetate	5.4	15.5	7.2	7.6	57	-10	217	-98
Propylene Glycol Monoethyl Ether Acetate	5.72	15.6	6.3	7.7	165	54	1.3	-60
Ethyl Acetate	5.79	15.8	5.3	7.2	77	-3	96.5	-84
Methyl Oleate	5.81	16.2	3.8	4.5	344	180	0	20
1,3-Dioxolane	6.02	18.1	6.6	9.3	78	-6	110	-95
Di-isoButyl Ketone	6.05	16	3.7	4.1	168	49	1.72	-46
n-Butyl Acetate	6.61	15.8	3.7	6.3	126	27	12.1	-74
N,N-Dimethyl Acetamide	6.62	16.8	11.5	10.2	166	70	1.16	-20
Benzyl Benzoate	6.85	20	5.1	5.2	323	158	0.001	19
n-Amyl Acetate	6.88	15.8	3.3	6.1	148	22	10.5	-71
Butyl Diglycol Acetate	7.02	16	4.1	8.2	245	105	0.008	-32

Glycerol Triacetate	7.03	16.5	4.5	9.1	259	138	0.001	4
n-Propyl Acetate	7.21	15.3	4.3	7.6	102	14	33	-95
Dipropylene Glycol Mono n-Butyl Ether	7.23	15.7	6.5	10	230	100	0.002	-20
Diethylene Glycol Monobutyl Ether	7.34	16	7	10.6	231	78	0.033	-68
d-Limonene	7.37	17.2	1.8	4.3	177	43	1.61	-74
t-Butyl Acetate	7.39	15	3.7	6	96	1	46.7	-58
Diacetone Alcohol	7.41	15.8	8.2	10.8	168	45	1.07	-44
Propylene Glycol Monomethyl Ether Acetate	7.54	15.6	5.6	9.8	146	50	2.91	-68
Iso-Pentyl Acetate	7.82	15.3	3.1	7	142	25	4.6	-79
Iso-Propyl Acetate	7.85	14.9	4.5	8.2	81	5	60.4	-73
Iso-Butyl Isobutyrate	7.92	15.1	2.8	5.8	148	38	3.7	-81
sec-Butyl Acetate	7.96	15	3.7	7.6	112	17	21.6	-99
Propylene Glycol Monobutyl Ether	7.99	15.3	4.5	9.2	171	63	0.294	-29
Toluene	8.16	18	1.4	2	111	4	28.4	-95
Xylene	8.24	17.6	1	3.1	140	24	7	-15
ε-Caprolactone	8.25	19.7	15	7.4	241	127	0.135	-1
γ-Butyrolactone	8.26	18	16.6	7.4	204	98	0.17	-43
Propylene Glycol Phenyl Ether	8.36	17.4	5.3	11.5	243	129	0.002	21
N,N-Dimethyl Formamide	8.52	17.4	13.7	11.3	152	58	3.7	-60
Dipropylene Glycol Methyl Ether	8.69	15.5	5.7	11.2	215	75	0.006	-32
Propylene Glycol Monomethyl Ether	8.73	15.6	6.3	11.6	120	32	4.55	-97
1,4-Dioxane	8.86	17.5	1.8	9	101	12	36.5	12
Methyl Carbitol	8.89	16.2	7.8	12.6	194	96	0.17	-65
Methanol	8.9	14.7	5	10	65	12	128	-98

TentaGel resin

Ideal parameters: D, 17.8; P, 10.9; H, 6.5

Solvents	Distance	D	P	H	BPt	FPt	VP@25	MPt
N-Methyl-2-Pyrrolidone	1.77	18	12.3	7.2	204	96	0.088	-24
Cyclohexanone	2.76	17.8	8.4	5.1	155	44	3.73	-31
1-Nitropropane	2.83	16.6	12.3	5.5	131	24	9.84	-104
Isophorone	3.47	17	8	5	215	90	0.309	-8
Dichloromethane	3.87	17	7.3	7.1	40	-4	435	-95
Dimethyl Isosorbide	3.88	17.6	7.1	7.5	234	105	0.03	-50
Methyl Ethyl Ketone	4.11	16	9	5.1	80	-5	90.3	-87
N,N-Dimethyl Acetamide	4.27	16.8	11.5	10.2	166	70	1.16	-20
1,4-Dioxane	4.43	17.1	6.8	7.8	101	12	36.5	12
Acetone	4.5	15.5	10.4	7	56	-17	232	-95
Methyl Propyl Ketone	5.01	16	7.6	4.7	102	7	35	-77
1,3-Dioxolane	5.17	18.1	6.6	9.3	78	-6	110	-95
Butyl Benzoate	5.42	18.3	5.6	5.5	250	105	0.006	-22
Tetrahydrofuran	5.67	16.8	5.7	8	66	-17	181	-109
N,N-Dimethyl Formamide	5.71	17.4	13.7	11.3	152	58	3.7	-60
Tributyl Phosphate	5.74	16.3	6.3	4.3	289	166	0.001	-80
ε-Caprolactone	5.84	19.7	15	7.4	241	127	0.135	-1
Methyl Acetate	5.85	15.5	7.2	7.6	57	-10	217	-98
Butyl Glycol Acetate	5.88	15.3	7.5	6.8	192	84	0.3	-64
γ-Butyrolactone	5.89	18	16.6	7.4	204	98	0.17	-43
Propylene Glycol Monoethyl Ether Acetate	6.33	15.6	6.3	7.7	165	54	1.3	-60
Diacetone Alcohol	6.39	15.8	8.2	10.8	168	45	1.07	-44
Methyl iso-Amyl Ketone	6.59	16	5.7	4.1	145	36	5.1	-74
Diethylene Glycol Monobutyl Ether	6.63	16	7	10.6	231	78	0.033	-68
n-Butyl Propionate	6.7	15.7	5.5	5.9	145	32	4.19	-90
Ethyl Acetate	6.77	15.8	5.3	7.2	77	-3	96.5	-84
Dimethyl Sulfoxide (DMSO)	6.88	18.4	16.4	10.2	191	87	0.486	19
n-Propyl Propanoate	6.89	15.5	5.6	5.7	123	19	13.5	-76

Dipropylene Glycol Mono n-Butyl Ether	6.92	15.7	6.5	10	230	100	0.002	-20
Tetrahydrofurfuryl Alcohol	7	17.8	8.2	12.9	178	75	0.928	-80
Methyl Iso-Butyl Ketone	7.14	15.3	6.1	4.1	116	16	19.8	-84
Cyclopentyl Methyl Ether	7.15	16.7	4.3	4.3	106	0	35.5	-140
Glycerol Triacetate	7.29	16.5	4.5	9.1	259	138	0.001	4
Benzyl Benzoate	7.41	20	5.1	5.2	323	158	0.001	19
Methyl Carbitol	7.53	16.2	7.8	12.6	194	96	0.17	-65
Propylene Glycol Monomethyl Ether Acetate	7.53	15.6	5.6	9.8	146	50	2.91	-68
Propylene Glycol Phenyl Ether	7.54	17.4	5.3	11.5	243	129	0.002	21
Ethyl Lactate	7.7	16	7.6	12.5	155	47	2.07	-26
Butyl Diglycol Acetate	7.76	16	4.1	8.2	245	105	0.008	-32
Methyl Oleate	7.88	16.2	3.8	4.5	344	180	0	20
Sulfolane	8	18	18	9.9	287	165	0.002	27
Propylene Glycol Monomethyl Ether	8.08	15.6	6.3	11.6	120	32	4.55	-97
n-Butyl Acetate	8.09	15.8	3.7	6.3	126	27	12.1	-74
n-Propyl Acetate	8.21	15.3	4.3	7.6	102	14	33	-95
Di-isoButyl Ketone	8.24	16	3.7	4.1	168	49	1.72	-46
Dipropylene Glycol Methyl Ether	8.3	15.5	5.7	11.2	215	75	0.006	-32
Propylene Glycol Monobutyl Ether	8.44	15.3	4.5	9.2	171	63	0.294	-29
Glycerol Diacetate	8.45	16.4	8.9	14.2	250	160	0	179
n-Amyl Acetate	8.45	15.8	3.3	6.1	148	22	10.5	-71
Iso-Propyl Acetate	8.66	14.9	4.5	8.2	81	5	60.4	-73
Acetonitrile	8.66	15.3	18	6.1	82	2	86.6	-44
Benzyl Alcohol	8.68	18.4	6.3	13.7	205	93	0.08	-15
Propylene Carbonate	8.81	20	18	4.1	242	135	0.004	-48

ArgoGel resin

Ideal parameters: D, 18.4; P, 8.4; H, 8.4

Solvents	Distance	D	P	H	BPt	FPt	VP@25	MPt
N-Methyl-2-Pyrrolidone	1.71	18	12.3	7.2	204	96	0.088	-24
1-Nitropropane	2.71	16.6	12.3	5.5	131	24	9.84	-104
Cyclohexanone	2.85	17.8	8.4	5.1	155	44	3.73	-31
Isophorone	3.52	17	8	5	215	90	0.309	-8
Dichloromethane	3.94	17	7.3	7.1	40	-4	435	-95
Dimethyl Isosorbide	3.99	17.6	7.1	7.5	234	105	0.03	-50
Methyl Ethyl Ketone	4.09	16	9	5.1	80	-5	90.3	-87
N,N-Dimethyl Acetamide	4.23	16.8	11.5	10.2	166	70	1.16	-20
Acetone	4.43	15.5	10.4	7	56	-17	232	-95
1,4-Dioxane	4.51	17.1	6.8	7.8	101	12	36.5	12
Methyl Propyl Ketone	5.03	16	7.6	4.7	102	7	35	-77
1,3-Dioxolane	5.28	18.1	6.6	9.3	78	-6	110	-95
Butyl Benzoate	5.55	18.3	5.6	5.5	250	105	0.006	-22
N,N-Dimethyl Formamide	5.66	17.4	13.7	11.3	152	58	3.7	-60
Tetrahydrofuran	5.75	16.8	5.7	8	66	-17	181	-109
Tributyl Phosphate	5.78	16.3	6.3	4.3	289	166	0.001	-80
γ-Butyrolactone	5.79	18	16.6	7.4	204	98	0.17	-43
ε-Caprolactone	5.82	19.7	15	7.4	241	127	0.135	-1
Methyl Acetate	5.86	15.5	7.2	7.6	57	-10	217	-98
Butyl Glycol Acetate	5.88	15.3	7.5	6.8	192	84	0.3	-64
Propylene Glycol Monoethyl Ether Acetate	6.36	15.6	6.3	7.7	165	54	1.3	-60
Diacetone Alcohol	6.4	15.8	8.2	10.8	168	45	1.07	-44
Methyl iso-Amyl Ketone	6.63	16	5.7	4.1	145	36	5.1	-74
Diethylene Glycol Monobutyl Ether	6.66	16	7	10.6	231	78	0.033	-68
n-Butyl Propionate	6.74	15.7	5.5	5.9	145	32	4.19	-90
Dimethyl Sulfoxide	6.81	18.4	16.4	10.2	191	87	0.486	19
Ethyl Acetate	6.82	15.8	5.3	7.2	77	-3	96.5	-84
n-Propyl Propanoate	6.92	15.5	5.6	5.7	123	19	13.5	-76
Dipropylene Glycol Mono n-Butyl Ether	6.95	15.7	6.5	10	230	100	0.002	-20

Tetrahydrofurfuryl Alcohol	7.05	17.8	8.2	12.9	178	75	0.928	-80
Methyl Iso-Butyl Ketone	7.16	15.3	6.1	4.1	116	16	19.8	-84
Cyclopentyl Methyl Ether	7.23	16.7	4.3	4.3	106	0	35.5	-140
Glycerol Triacetate	7.36	16.5	4.5	9.1	259	138	0.001	4
Benzyl Benzoate	7.55	20	5.1	5.2	323	158	0.001	19
Methyl Carbitol	7.55	16.2	7.8	12.6	194	96	0.17	-65
Propylene Glycol Monomethyl Ether Acetate	7.57	15.6	5.6	9.8	146	50	2.91	-68
Propylene Glycol Phenyl Ether	7.62	17.4	5.3	11.5	243	129	0.002	21
Ethyl Lactate	7.72	16	7.6	12.5	155	47	2.07	-26
Butyl Diglycol Acetate	7.82	16	4.1	8.2	245	105	0.008	-32
Sulfolane	7.91	18	18	9.9	287	165	0.002	27
Methyl Oleate	7.95	16.2	3.8	4.5	344	180	0	20
Propylene Glycol Monomethyl Ether	8.11	15.6	6.3	11.6	120	32	4.55	-97
n-Butyl Acetate	8.15	15.8	3.7	6.3	126	27	12.1	-74
n-Propyl Acetate	8.25	15.3	4.3	7.6	102	14	33	-95
Di-isoButyl Ketone	8.3	16	3.7	4.1	168	49	1.72	-46
Dipropylene Glycol Methyl Ether	8.33	15.5	5.7	11.2	215	75	0.006	-32
Glycerol Diacetate	8.46	16.4	8.9	14.2	250	160	0	179
Propylene Glycol Monobutyl Ether	8.48	15.3	4.5	9.2	171	63	0.294	-29
n-Amyl Acetate	8.51	15.8	3.3	6.1	148	22	10.5	-71
Acetonitrile	8.53	15.3	18	6.1	82	2	86.6	-44
Iso-Propyl Acetate	8.69	14.9	4.5	8.2	81	5	60.4	-73
Propylene Carbonate	8.76	20	18	4.1	242	135	0.004	-48
Benzyl Alcohol	8.76	18.4	6.3	13.7	205	93	0.08	-15
Ethylene Glycol Monobutyl Ether	8.95	16	5.1	12.3	171	100	0.867	-74
t-Butyl Acetate	9.01	15	3.7	6	96	1	46.7	-58
sec-Butyl Acetate	9.08	15	3.7	7.6	112	17	21.6	-99
Methanol	9.15	14.7	5	10	65	12	128	-98

HypoGel resin

Ideal parameters: D, 17.3; P, 11.7; H, 9.1

Solvents	Distance	D	P	H	BPt	FPt	VP@25	MPt
N-Methyl-2-Pyrrolidone	1.73	18	12.3	7.2	204	96	0.088	-24
N,N-Dimethyl Acetamide	2.23	16.8	11.5	10.2	166	70	1.16	-20
N,N-Dimethyl Formamide	3.13	17.4	13.7	11.3	152	58	3.7	-60
1-Nitropropane	3.74	16.6	12.3	5.5	131	24	9.84	-104
Acetone	4.75	15.5	10.4	7	56	-17	232	-95
γ-Butyrolactone	4.83	18	16.6	7.4	204	98	0.17	-43
Dimethyl Sulfoxide	4.92	18.4	16.4	10.2	191	87	0.486	19
Dimethyl Isosorbide	5.06	17.6	7.1	7.5	234	105	0.03	-50
Cyclohexanone	5.11	17.8	8.4	5.1	155	44	3.73	-31
Dichloromethane	5.11	17	7.3	7.1	40	-4	435	-95
ε-Caprolactone	5.35	19.7	15	7.4	241	127	0.135	-1
1,4-Dioxane	5.38	17.1	6.8	7.8	101	12	36.5	12
1,3-Dioxolane	5.56	18.1	6.6	9.3	78	-6	110	-95
Isophorone	5.57	17	8	5	215	90	0.309	-8
Diacetone Alcohol	5.62	15.8	8.2	10.8	168	45	1.07	-44
Methyl Ethyl Ketone	5.64	16	9	5.1	80	-5	90.3	-87
Tetrahydrofurfuryl Alcohol	5.71	17.8	8.2	12.9	178	75	0.928	-80
Sulfolane	6.16	18	18	9.9	287	165	0.002	27
Diethylene Glycol Monobutyl Ether	6.22	16	7	10.6	231	78	0.033	-68
Methyl Carbitol	6.38	16.2	7.8	12.6	194	96	0.17	-65
Methyl Acetate	6.45	15.5	7.2	7.6	57	-10	217	-98
Tetrahydrofuran	6.54	16.8	5.7	8	66	-17	181	-109
Ethyl Lactate	6.63	16	7.6	12.5	155	47	2.07	-26
Butyl Glycol Acetate	6.68	15.3	7.5	6.8	192	84	0.3	-64
Methyl Propyl Ketone	6.73	16	7.6	4.7	102	7	35	-77
Glycerol Diacetate	6.76	16.4	8.9	14.2	250	160	0	179
Dipropylene Glycol Mono n-Butyl Ether	6.8	15.7	6.5	10	230	100	0.002	-20
Propylene Glycol Monoethyl Ether Acetate	7.01	15.6	6.3	7.7	165	54	1.3	-60

Propylene Glycol Phenyl Ether	7.3	17.4	5.3	11.5	243	129	0.002	21
Butyl Benzoate	7.31	18.3	5.6	5.5	250	105	0.006	-22
Propylene Glycol Monomethyl Ether	7.53	15.6	6.3	11.6	120	32	4.55	-97
Propylene Glycol Monomethyl Ether Acetate	7.62	15.6	5.6	9.8	146	50	2.91	-68
Tributyl Phosphate	7.64	16.3	6.3	4.3	289	166	0.001	-80
Ethyl Acetate	7.74	15.8	5.3	7.2	77	-3	96.5	-84

NovaGel resin

Ideal parameters: D, 17.8; P, 11.4; H, 9.6

Solvents	Distance	D	P	H	BPt	FPt	VP@25	MPt
N,N-Dimethyl Acetamide	1.03	16.8	11.5	10.2	166	70	1.16	-20
N,N-Dimethyl Formamide	3.05	17.4	13.7	11.3	152	58	3.7	-60
N-Methyl-2-Pyrrolidone	3.7	18	12.3	7.2	204	96	0.088	-24
Diacetone Alcohol	3.93	15.8	8.2	10.8	168	45	1.07	-44
Tetrahydrofurfuryl Alcohol	3.96	17.8	8.2	12.9	178	75	0.928	-80
Methyl Carbitol	4.38	16.2	7.8	12.6	194	96	0.17	-65
Diethylene Glycol Monobutyl Ether	4.58	16	7	10.6	231	78	0.033	-68
Ethyl Lactate	4.66	16	7.6	12.5	155	47	2.07	-26
Dimethyl Isosorbide	4.71	17.6	7.1	7.5	234	105	0.03	-50
Acetone	4.72	15.5	10.4	7	56	-17	232	-95
1,3-Dioxolane	4.72	18.1	6.6	9.3	78	-6	110	-95
Glycerol Diacetate	4.73	16.4	8.9	14.2	250	160	0	179
1,4-Dioxane	4.74	17.1	6.8	7.8	101	12	36.5	12
Dichloromethane	4.76	17	7.3	7.1	40	-4	435	-95
1-Nitropropane	5.08	16.6	12.3	5.5	131	24	9.84	-104
Dipropylene Glycol Mono n-Butyl Ether	5.32	15.7	6.5	10	230	100	0.002	-20
Methyl Acetate	5.66	15.5	7.2	7.6	57	-10	217	-98
Tetrahydrofuran	5.69	16.8	5.7	8	66	-17	181	-109
Propylene Glycol Phenyl Ether	5.73	17.4	5.3	11.5	243	129	0.002	21
Propylene Glycol Monomethyl Ether	5.76	15.6	6.3	11.6	120	32	4.55	-97
Cyclohexanone	5.81	17.8	8.4	5.1	155	44	3.73	-31
Methyl Ethyl Ketone	5.96	16	9	5.1	80	-5	90.3	-87
Isophorone	5.97	17	8	5	215	90	0.309	-8
Methyl Cellosolve	5.99	16	8.2	15	124	38	10.8	-85
Ethylene Glycol Monomethyl Ether	5.99	16	8.2	15	124	40	10.8	-85
Dimethyl Sulfoxide	6.02	18.4	16.4	10.2	191	87	0.486	19

Propylene Glycol Monoethyl Ether Acetate	6.13	15.6	6.3	7.7	165	54	1.3	-60
Butyl Glycol Acetate	6.14	15.3	7.5	6.8	192	84	0.3	-64
Propylene Glycol Monomethyl Ether Acetate	6.19	15.6	5.6	9.8	146	50	2.91	-68
Benzyl Alcohol	6.22	18.4	6.3	13.7	205	93	0.08	-15
Dipropylene Glycol Methyl Ether	6.28	15.5	5.7	11.2	215	75	0.006	-32
Hexylene Glycol	6.42	16.7	6.7	15	197	93	0.001	-40
γ-Butyrolactone	6.58	18	16.6	7.4	204	98	0.17	-43
Ethylene Glycol Monobutyl Ether	6.59	16	5.1	12.3	171	100	0.867	-74
Glycerol Triacetate	6.62	16.5	4.5	9.1	259	138	0.001	4
2-Phenoxy Ethanol	6.69	17.8	5.7	14.3	237	113	0.007	13
n-Amyl Alcohol	6.72	15.9	5.9	13.9	138	42	6.6	-78
Methyl Propyl Ketone	6.86	16	7.6	4.7	102	7	35	-77
Ethyl Acetate	6.94	15.8	5.3	7.2	77	-3	96.5	-84

ChemMatrix resin

Ideal parameters: D, 18.6; P, 9.9; H, 7.0

Solvents	Distance	D	P	H	BPt	FPt	VP@25	MPt
N-Methyl-2-Pyrrolidone	2.76	18	12.3	7.2	204	96	0.088	-24
Cyclohexanone	2.85	17.8	8.4	5.1	155	44	3.73	-31
Dimethyl Isosorbide	3.42	17.6	7.1	7.5	234	105	0.03	-50
Dichloromethane	4.07	17	7.3	7.1	40	-4	435	-95
1,3-Dioxolane	4.09	18.1	6.6	9.3	78	-6	110	-95
Isophorone	4.18	17	8	5	215	90	0.309	-8
1,4-Dioxane	4.34	17.1	6.8	7.8	101	12	36.5	12
Butyl Benzoate	4.51	18.3	5.6	5.5	250	105	0.006	-22
1-Nitropropane	4.93	16.6	12.3	5.5	131	24	9.84	-104
N,N-Dimethyl Acetamide	5.11	16.8	11.5	10.2	166	70	1.16	-20
Tetrahydrofuran	5.57	16.8	5.7	8	66	-17	181	-109
Methyl Ethyl Ketone	5.59	16	9	5.1	80	-5	90.3	-87
ε-Caprolactone	5.64	19.7	15	7.4	241	127	0.135	-1
Benzyl Benzoate	5.77	20	5.1	5.2	323	158	0.001	19
Methyl Propyl Ketone	6.1	16	7.6	4.7	102	7	35	-77
Acetone	6.23	15.5	10.4	7	56	-17	232	-95

SpheriTide resin

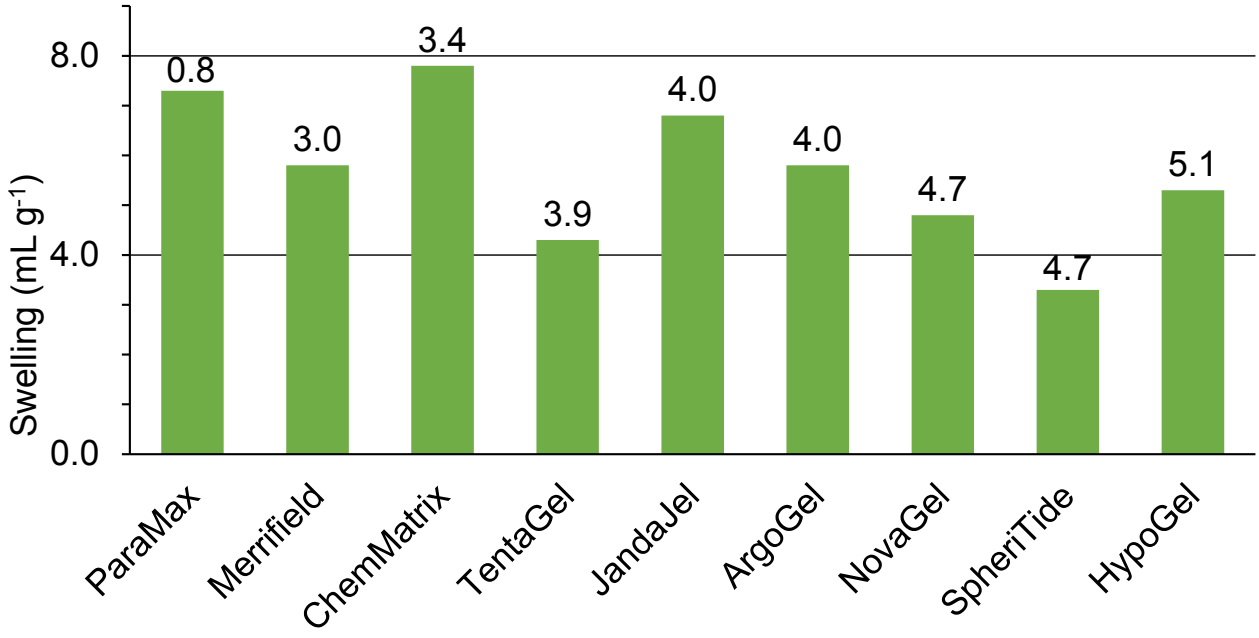
Ideal parameters: D, 17.5; P, 11.1; H, 9.6

Solvents	Distance	D	P	H	BPt	FPt	VP@25	MPt
N,N-Dimethyl Acetamide	1.1	16.8	11.5	10.2	166	70	1.16	-20
N-Methyl-2-Pyrrolidone	2.92	18	12.3	7.2	204	96	0.088	-24
N,N-Dimethyl Formamide	3.11	17.4	13.7	11.3	152	58	3.7	-60
1-Nitropropane	4.11	16.6	12.3	5.5	131	24	9.84	-104
Acetone	4.14	15.5	10.4	7	56	-17	232	-95
Diacetone Alcohol	4.37	15.8	8.2	10.8	168	45	1.07	-44
Dichloromethane	4.62	17	7.3	7.1	40	-4	435	-95
Dimethyl Isosorbide	4.71	17.6	7.1	7.5	234	105	0.03	-50
1,4-Dioxane	4.79	17.1	6.8	7.8	101	12	36.5	12
Tetrahydrofurfuryl Alcohol	4.91	17.8	8.2	12.9	178	75	0.928	-80
Diethylene Glycol Monobutyl Ether	5.05	16	7	10.6	231	78	0.033	-68
1,3-Dioxolane	5.11	18.1	6.6	9.3	78	-6	110	-95
Methyl Carbitol	5.15	16.2	7.8	12.6	194	96	0.17	-65
Cyclohexanone	5.33	17.8	8.4	5.1	155	44	3.73	-31
Methyl Ethyl Ketone	5.36	16	9	5.1	80	-5	90.3	-87
Ethyl Lactate	5.39	16	7.6	12.5	155	47	2.07	-26
Isophorone	5.49	17	8	5	215	90	0.309	-8
Methyl Acetate	5.56	15.5	7.2	7.6	57	-10	217	-98
Glycerol Diacetate	5.62	16.4	8.9	14.2	250	160	0	179
Dipropylene Glycol Mono n-Butyl Ether	5.66	15.7	6.5	10	230	100	0.002	-20
Dimethyl Sulfoxide	5.73	18.4	16.4	10.2	191	87	0.486	19
Tetrahydrofuran	5.83	16.8	5.7	8	66	-17	181	-109
γ-Butyrolactone	5.88	18	16.6	7.4	204	98	0.17	-43
Butyl Glycol Acetate	5.89	15.3	7.5	6.8	192	84	0.3	-64
Propylene Glycol Monoethyl Ether Acetate	6.12	15.6	6.3	7.7	165	54	1.3	-60
Propylene Glycol Monomethyl Ether	6.31	15.6	6.3	11.6	120	32	4.55	-97
Methyl Propyl Ketone	6.38	16	7.6	4.7	102	7	35	-77

Propylene Glycol Phenyl Ether	6.42	17.4	5.3	11.5	243	129	0.002	21
Propylene Glycol Monomethyl Ether Acetate	6.52	15.6	5.6	9.8	146	50	2.91	-68
ε-Caprolactone	6.59	19.7	15	7.4	241	127	0.135	-1
Dipropylene Glycol Methyl Ether	6.77	15.5	5.7	11.2	215	75	0.006	-32
Ethylene Glycol Monomethyl Ether	6.85	16	8.2	15	124	40	10.8	-85
Sulfolane	6.91	18	18	9.9	287	165	0.002	27
Ethyl Acetate	6.94	15.8	5.3	7.2	77	-3	96.5	-84

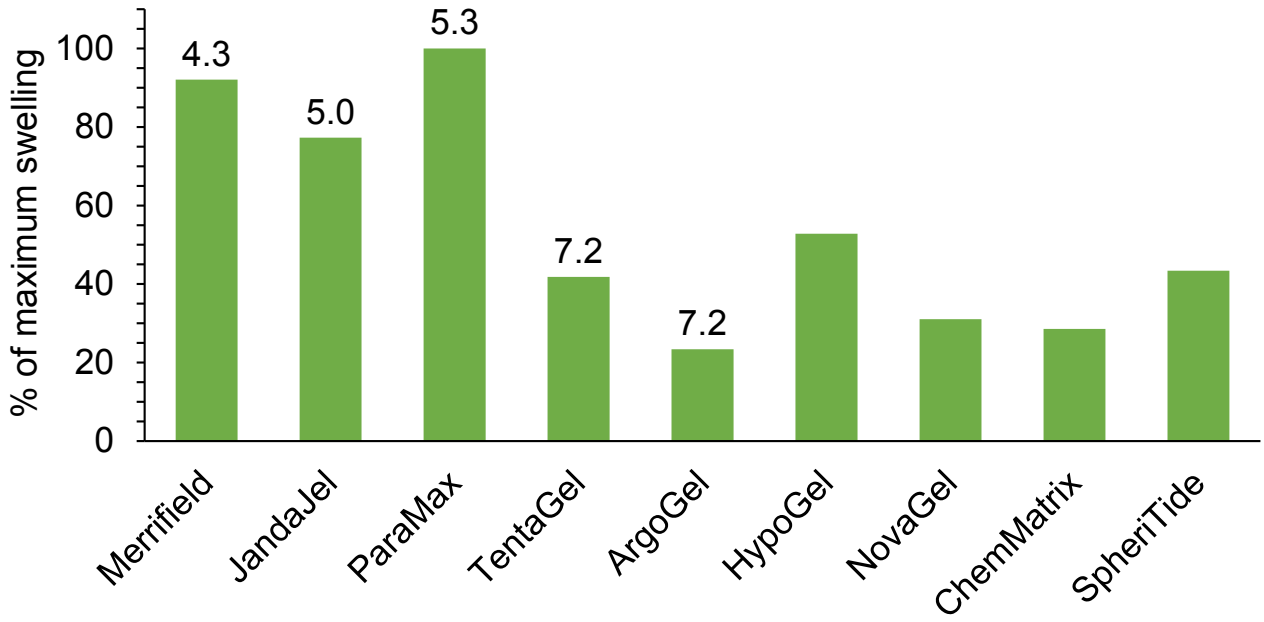
Swelling of resins in dimethyl isosorbide

The graph below is presented as a plot of amount of swelling rather than the % swelling shown in the main manuscript. This is less appropriate for comparison between resins, but does indicate the amount of swelling relative to the 4.0 mL g^{-1} threshold for a good solvent (only SpheriTide did not meet this threshold). Resins are ranked from highest predicted swelling (left) to lowest (right) with the RMS deviation of the solvent parameters for dimethyl isosorbide from those of an ideal solvent given as a number above each bar.



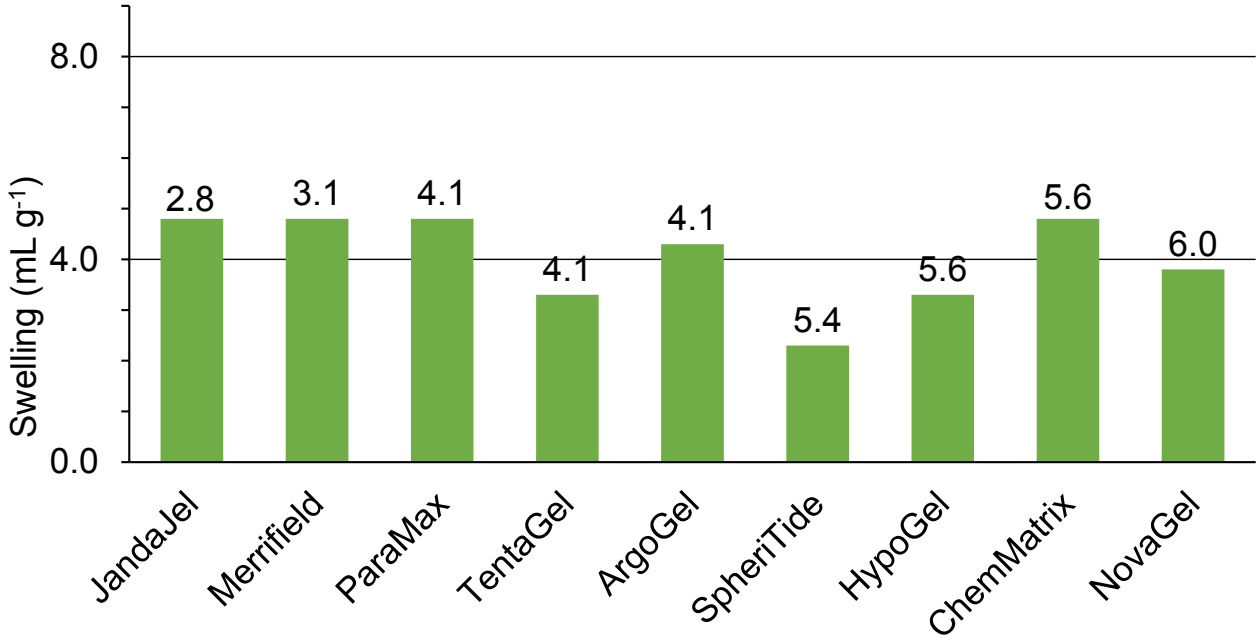
Swelling of resins in cyclopentyl methyl ether

The graph below is presented as a plot of amount of swelling rather than the % swelling shown in the main manuscript. This is less appropriate for comparison between resins, but does indicate the amount of swelling relative to the 4.0 mL g^{-1} threshold for a good solvent. Resins are ranked from highest predicted swelling (left) to lowest (right) with the RMS deviation of the solvent parameters for cyclopentyl methyl ether from those of an ideal solvent given as a number above each bar. Where no number is given, the deviation is so large that the solvent is not in the 'Predictions of solvents to swell each resin' table for that solvent.



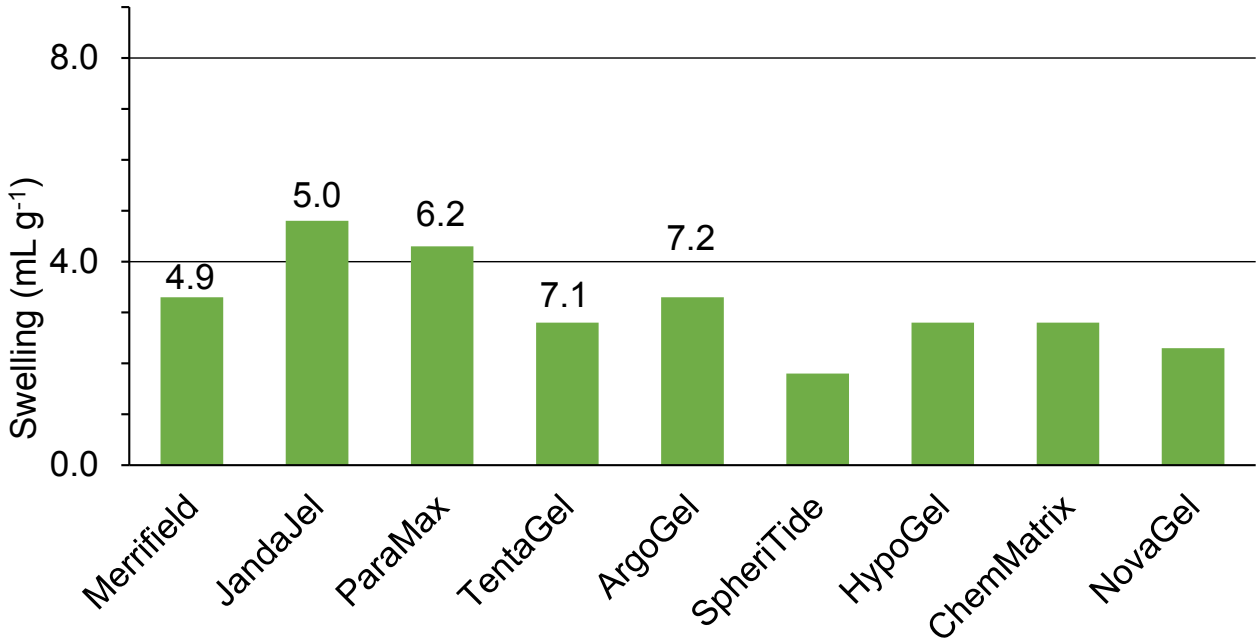
Swelling of resins in butan-2-one

The graph below is presented as a plot of amount of swelling rather than the % swelling shown in the main manuscript. This is less appropriate for comparison between resins, but does indicate the amount of swelling relative to the 4.0 mL g^{-1} threshold for a good solvent. Resins are ranked from highest predicted swelling (left) to lowest (right) with the RMS deviation of the solvent parameters for butan-2-one from those of an ideal solvent given as a number above each bar.



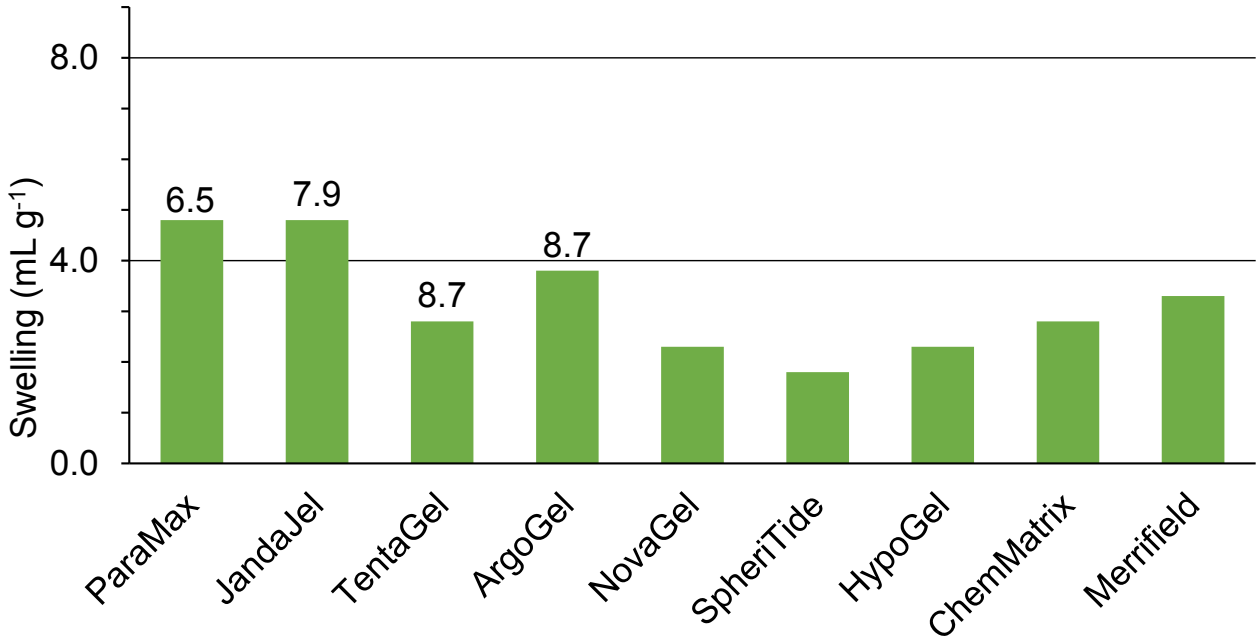
Swelling of resins in 4-methylpentan-2-one

The graph below is presented as a plot of amount of swelling rather than the % swelling shown in the main manuscript. This is less appropriate for comparison between resins, but does indicate the amount of swelling relative to the 4.0 mL g^{-1} threshold for a good solvent. Resins are ranked from highest predicted swelling (left) to lowest (right) with the RMS deviation of the solvent parameters for 4-methylpentan-2-one from those of an ideal solvent given as a number above each bar. Where no number is given, the deviation is so large that the solvent is not in the 'Predictions of solvents to swell each resin' table for that solvent.



Swelling of resins in isopropyl acetate

The graph below is presented as a plot of amount of swelling rather than the % swelling shown in the main manuscript. This is less appropriate for comparison between resins, but does indicate the amount of swelling relative to the 4.0 mL g^{-1} threshold for a good solvent. Resins are ranked from highest predicted swelling (left) to lowest (right) with the RMS deviation of the solvent parameters for isopropyl acetate from those of an ideal solvent given as a number above each bar. Where no number is given, the deviation is so large that the solvent is not in the 'Predictions of solvents to swell each resin' table for that solvent.

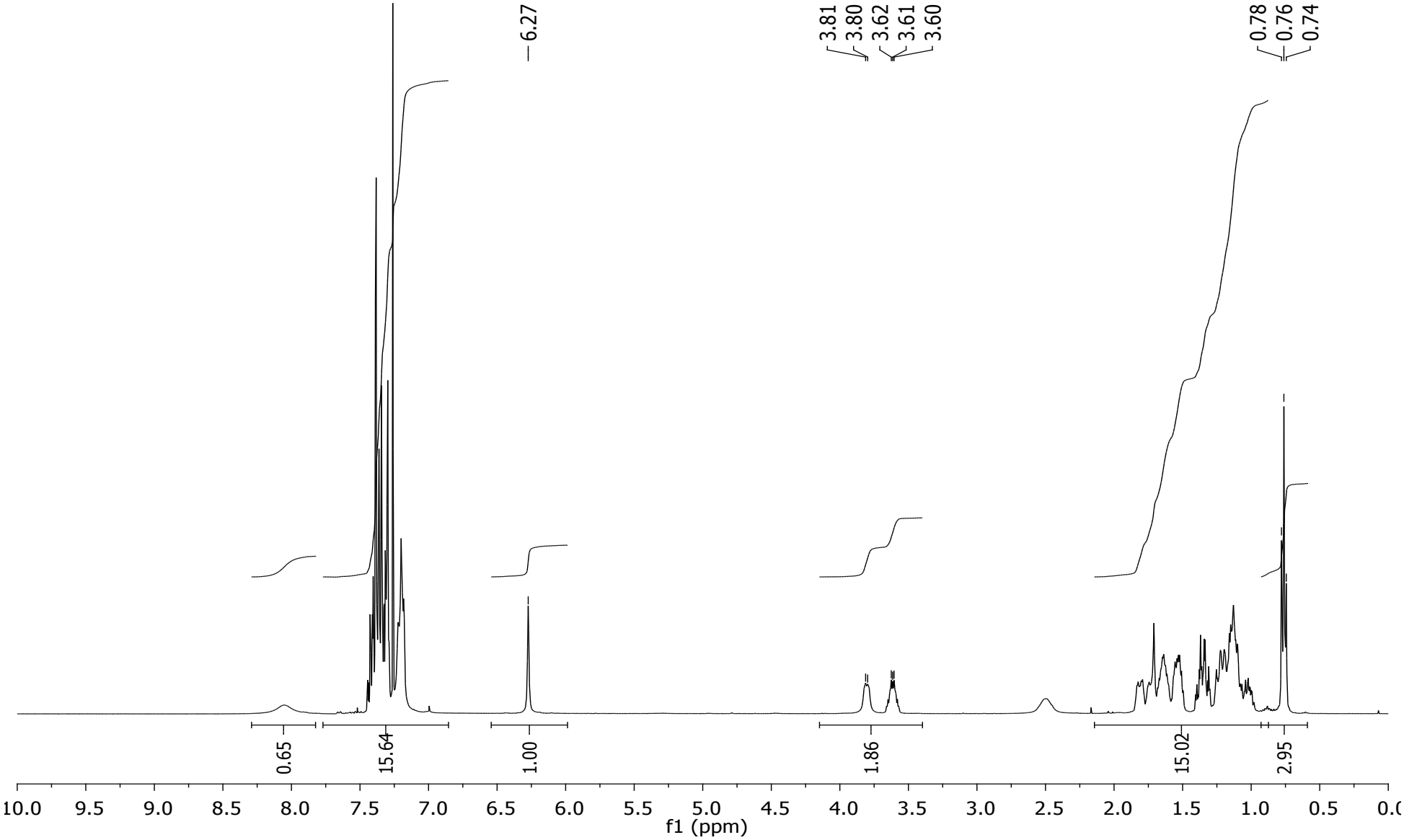


Solvent list and parameters used for mixed solvent study

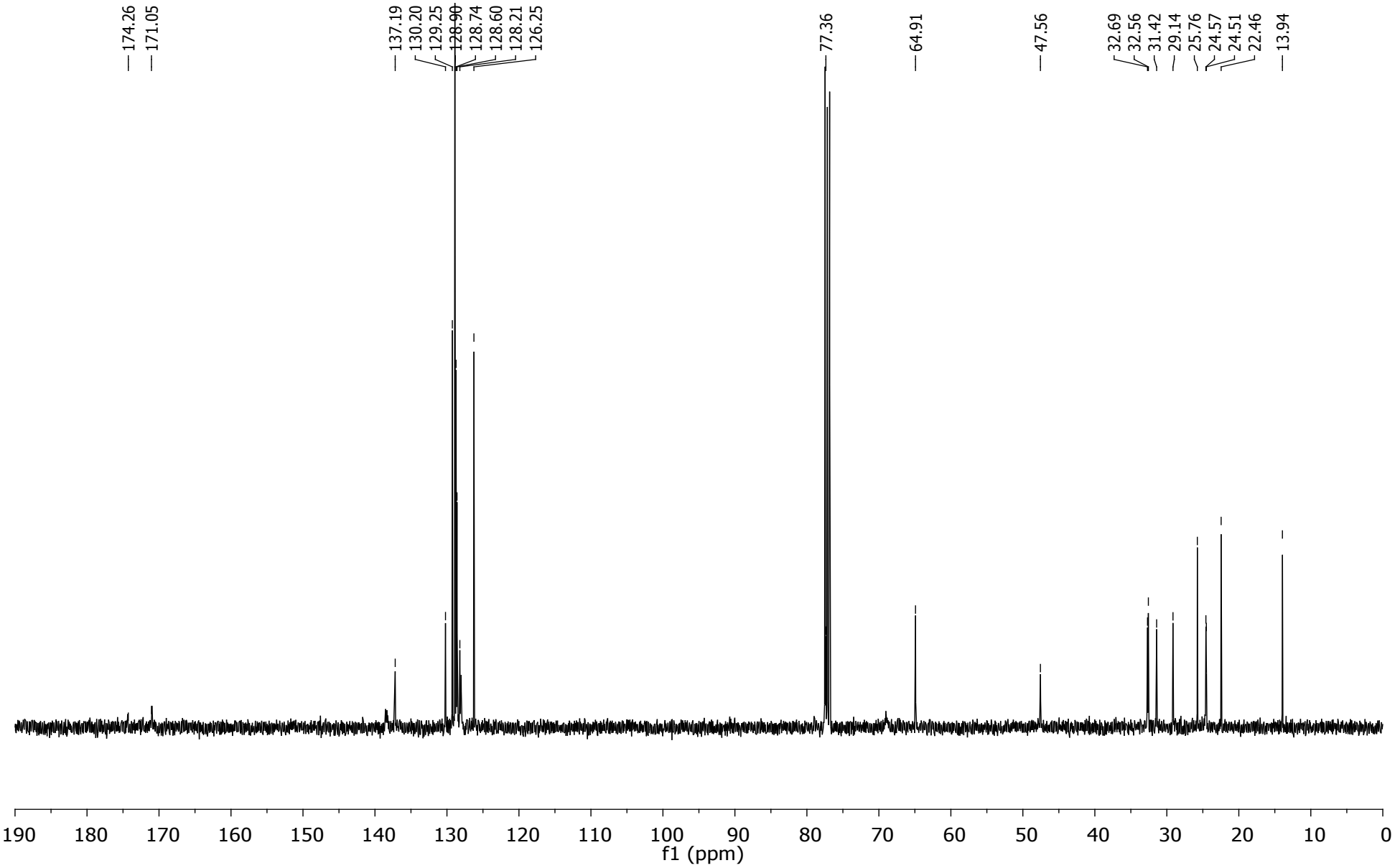
Solvent	D	P	H	BPt	FPt	V@25	MPt
Ethylene Carbonate **1**	18	21.7	5.1	248	143	0.009	36
Propylene Carbonate **2**	20	18	4.1	242	135	0.004	-48
Cyrene **3**	18.8	10.6	6.9	-	-	-	-
Acetone **4**	15.5	10.4	7	56	-17	232	-95
Methyl Ethyl Ketone **5**	16	9	5.1	80	-5	90.3	-87
Methyl Iso-Butyl Ketone **6**	15.3	6.1	4.1	116	16	19.8	-84
Cyclopentanone **7**	17.9	11.9	5.2	131	-	10.3	-51
Ethyl Acetate **8**	15.8	5.3	7.2	77	-3	96.5	-84
Isopropyl Acetate **9**	14.9	4.5	8.2	89	-	60.4	-73
i-Butyl Acetate **10**	15.1	3.7	6.3	117	-	17.2	-99
g-Valerolactone **11**	16.9	11.5	6.3	186.5	72.4	0.549	-29.4
2-Methyl Tetrahydrofuran **12**	16.9	5	4.3	79	-	96.1	-137
Anisole **13**	17.8	4.4	6.9	154	-	3.4	-38
Dimethyl Isosorbide **14**	17.6	7.1	7.5	234	105	0.03	-50
Cyclopentyl Methyl Ether **15**	16.7	4.3	4.3	106	0	35.5	-140
Dimethyl Carbonate **16**	15.5	8.6	9.7	90	-	50	0
Diethyl Carbonate **17**	15.1	6.3	3.5	127	-	10	-43
d-Limonene **18**	17.2	1.8	4.3	177	43	1.61	-74
para-Cymene **19**	17.3	2.4	2.4	182.7	55.5	0.914	-45.1
Methanol **20**	14.7	12.3	22.3	65	12	128	-98
Ethanol **21**	15.8	8.8	19.4	78	13	59.1	-114
2-Propanol **22**	15.8	6.1	16.4	82	14	43.4	-88
1-Heptanol **23**	16	5.3	11.7	176	-	0.308	-34
Water **24**	15.5	16	42.3	100	-	21.8	0

NMR spectra of compounds 28 and 29

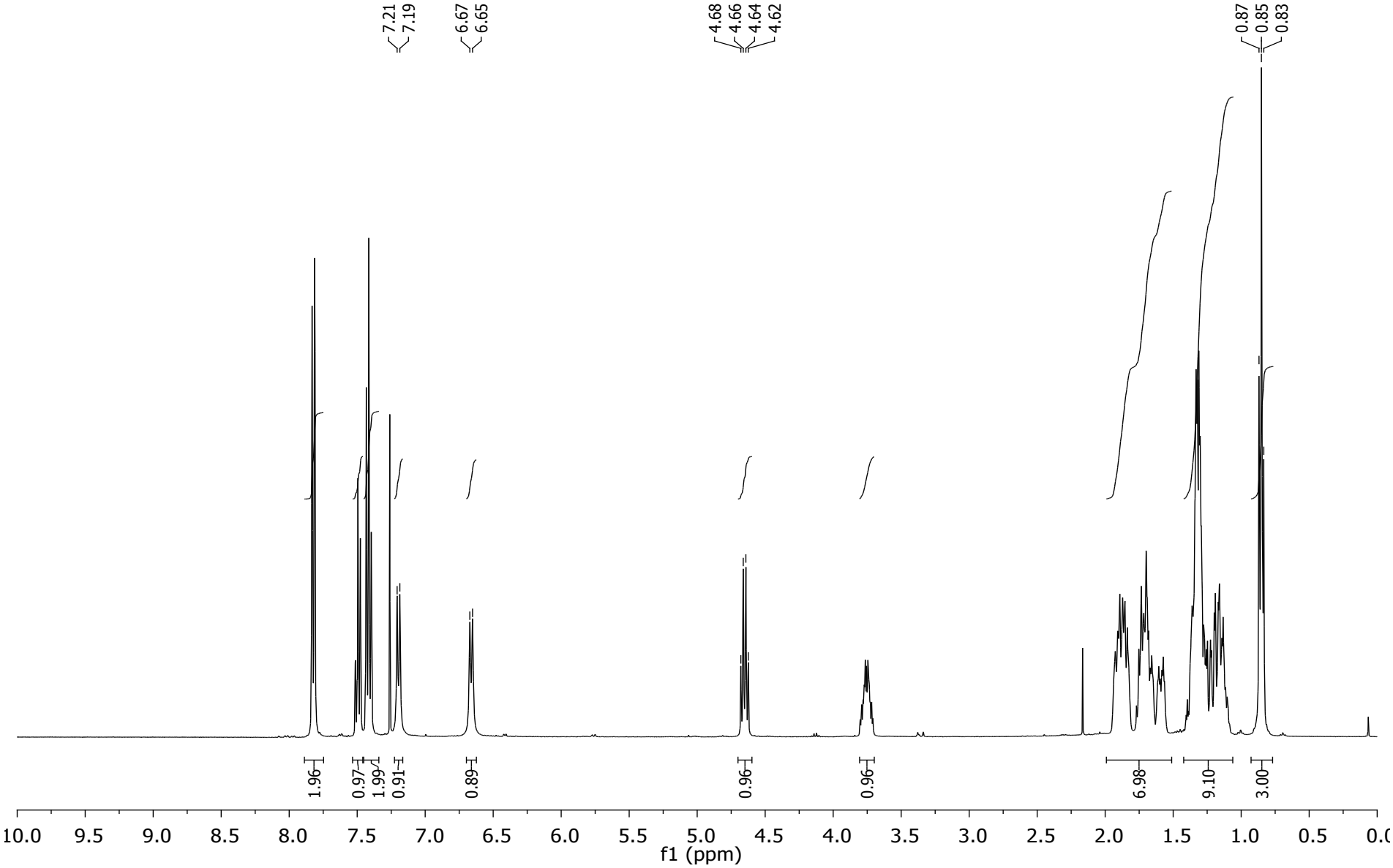
^{1}H NMR spectrum of compound **28**



^{13}C NMR spectrum of compound **28**



^{1}H NMR spectrum of compound **29**



^{13}C NMR spectrum of compound **29**