Supplementary material: Coordinates in PCA space and bibliographical sources for the listed green solvents.

NAME	CAS	F1	F2	F3	F4	Sources
Cluster II: Weak electron pair donor bases						
Acetone	67-64-1	-1.7	-3.2	-3.4	-2.4	A, B
N,N-Dimethyloctanamide	1118-92-9	-0.4	-5.4	1.6	-0.1	C1
Methyl 5-(dimethylamino) 2-methyl-oxopentanoate	1174627-68-9	-1.4	-3.6	-1.5	-1.2	C2
2-Pyrrolidone	616-45-5	-5.4	-1.8	-2.9	-0.6	A, B
Cluster III: Aprotic dipolar						
Acetyltributyl citrate	77-90-7	2.1	-1.6	-0.2	-0.1	A, B
Benzyl benzoate	120-51-4	3.0	-0.3	-0.6	-0.7	A, B
Butylacetate	123-86-4	1.7	-2.3	-0.1	-0.4	D
Butyl laurate	106-18-3	4.1	-1.7	1.4	1.8	E
1,4-Cineol	470-67-7	1.8	-4.3	2.3	1.7	C3
1,8-Cineol	470-82-6	1.6	-4.5	2.7	2.5	C3
Cyclopentyl methyl ether	5614-37-9	1.7	-4.1	1.9	0.9	F
Dibutyl sebacate	109-43-3	2.3	-3.0	1.1	0.5	A, B
Diethyl adipate	141-28-6	1.1	-2.0	-1.1	-0.8	C2
Diethyl glutarate	818-38-2	1.2	-1.6	-1.3	-0.8	C2
Diethyl phthalate	84-66-2	1.7	-0.9	-1.2	-0.7	A, B
Diethyl succinate	123-25-1	1.4	-1.3	-1.4	-0.9	C2
Diisoamylsuccinate	818-04-2	3.1	-1.1	0.1	0.4	C4
Diisobutyl adipate	141-04-8	2.2	-2.3	0.3	0.0	C2
Diisobutyl glutarate	71195-64-7	2.4	-1.9	0.2	0.1	C2
Diisobutyl succinate	925-06-4	2.4	-1.9	0.2	-0.1	C2
Diisooctylsuccinate	2915-57-3	3.8	-1.4	0.8	1.2	C4
Dimethyl adipate	627-93-0	0.4	-1.5	-2.1	-1.1	D, E
Dimethyl glutarate	1119-40-0	0.2	-1.1	-2.5	-1.2	D, E
Dimethyl phthalate	131-11-3	0.9	-0.2	-2.1	-1.0	A, B
Dimethyl succinate	106-65-0	-0.3	-0.8	-3.2	-1.3	D, E
N,N-Dimethyldecanamide	14433-76-2	0.1	-5.3	1.9	0.3	C1
Dimethylisosorbide	5306-85-4	-1.0	-2.7	-2.1	-1.4	A, B, C5
Dioctylsuccinate	14491-66-8	3.8	-1.3	0.9	1.1	C4
1,3-Dioxolane	646-06-0	-1.1	-2.0	-3.0	-1.6	A, B
Ethyl acetate	141-78-6	0.8	-2.1	-1.4	-1.0	A, B, D
Ethyl laurate	106-33-2	4.0	-1.7	1.3	1.5	E
Ethyl linoleate	544-35-4	4.0	-1.5	1.0	1.1	D, E
Ethyl linolenate	1191-41-9	3.8	-1.5	0.9	0.7	D, E
Ethyl myristate	124-06-1	4.1	-1.6	1.3	1.7	D, E
Geranyl acetate	105-87-3	2.7	-1.8	0.4	0.1	C3
Glycerol triacetate	102-76-1	-0.6	-0.5	-3.4	-1.2	A, B, D
Glycerol-1,2,3-tributyl ether	131570-29-1	2.9	-3.0	1.7	1.7	C6
Glycerol-1,2,3-triethyl ether	162614-45-1	0.1	-4.8	1.3	0.2	C6
Glycerol-1,2,3-trimethyl ether	20637-49-4	0.5	-3.4	-0.2	-0.8	C6
Glycerol-1,3-Dibutyl ether	2216-77-5	0.2	-1.7	2.7	0.5	C6
Isoamyle acetate	123-92-2	1.9	-2.3	0.2	0.0	E
Isobutyl acetate	110-19-0	1.9	-2.3	0.0	-0.2	D
Isopropylacetate	108-21-4	1.3	-2.5	-0.7	-1.0	D
Isopropyl myristate	110-27-0	4.3	-1.6	1.5	2.1	A, B
Isosorbide dioctanoate	64896-70-4	2.6	-1.4	0.3	0.3	C5
Methyl abietate	127-25-3	3.8	-1.6	1.1	1.1	C3
Methyl acetate	79-20-9	-0.3	-1.7	-2.9	-1.5	D
Methyl laurate	111-82-0	3.6	-1.7	1.1	1.2	D, E

NAME	CAS	F1	F2	F3	F4	Sources
Cluster III: Aprotic dipolar continued						
Methyl Linoleate	112-63-0	3.8	-1.4	0.9	0.8	E
Methyl linolenate	301-00-8	3.7	-1.3	0.7	0.6	E
Methyl myristate	124-10-7	3.9	-1.6	1.3	1.6	E
Methyl oleate	112-62-9	4.1	-1.4	1.1	1.2	E
Methyl palmitate	112-39-0	4.0	-1.5	1.3	1.8	E
Dimethyl 2-methylglutarate	14035-94-0	1.2	-1.0	-1.6	-0.8	C2
2-Methyltetrahydrofuran	96-47-9	0.0	-5.5	1.7	-0.1	F
Menthanyl acetate	58985-18-5	2.9	-2.6	1.4	1.1	C3
n-Propyl acetate	109-60-4	1.3	-2.2	-0.6	-0.6	D
Terpineol acetate	8007-35-0	2.7	-2.5	1.0	0.6	C3
Tributyl citrate	77-94-1	1.7	-1.4	-0.1	-0.2	A, B
Triethyl citrate	77-93-0	0.0	-1.1	-2.0	-1.0	A, B
Cluster IV: Aprotic highly dipolar						
Dimethyl sulfoxide	67-68-5	-7.9	-4.3	-8.3	-3.3	A,B
2-Furfuraldehyde	98-01-1	-2.5	0.8	-3.2	-0.5	G
Propylene carbonate	108-32-7	-2.6	1.3	-6.0	-1.0	A, B
γ-Valerolactone	108-29-2	-1.7	-1.7	-4.6	-2.3	F
Cluster V: Apolar						
Butyl myristate	110-36-1	4.2	-1.6	1.5	2.1	E
Butyl palmitate	111-06-8	4.2	-1.7	1.5	2.1	E
Butyl stearate	123-95-5	4.5	-1.4	1.5	2.3	E
Cyclohexane	110-82-7	8.4	1.8	0.6	3.5	J
p-Cymene	99-87-6	6.8	1.3	0.0	0.6	C3
β-Myrcene	123-35-3	6.7	1.2	0.1	0.6	C3
Decamethylcyclo-pentasiloxane	541-02-6	4.9	-0.7	0.9	1.8	F
Dipropyleneglycol	110-98-5	-5.6	0.7	0.4	1.2	
Ethyl oleate	111-62-6	4.2	-1.5	1.3	1.6	A, B, D, E
Ethyl palmitate	628-97-7	4.2	-1.5	1.4	2.0	E
Isopropyl palmitate	142-91-6	4.2	-1.7	1.4	1.8	A, B, E
d-Limonene	5989-27-5	7.2	1.1	0.3	1.5	D, E, F
Methyl stearate	112-61-8	4.2	-1.4	1.4	2.0	E
Isododecane	31807-55-3	8.3	1.8	0.6	3.6	A, B
Perfluorooctane	307-34-6	8.2	2.2	0.3	4.4	F
α-Pinene	80-56-8	7.9	1.5	0.5	2.6	C3, D, E, F
β-Pinene	127-91-3	7.1	1.1	0.4	1.3	C3, D, E, F
Terpinolene	586-62-9	7.4	1.1	0.6	2.0	C3
Cluster VII: Amphiprotic						
Benzyl alcohol	100-51-6	-3.4	4.3	2.7	-1.3	A, B
1-Butanol	71-36-3	-2.8	1.9	3.6	1.1	D
Cyclademol	25225-09-6	-1.0	1.4	4.2	1.2	C3
1-Decanol	112-30-1	-1.1	1.7	4.5	1.4	C1
Dihydromyrcenol	18479-58-8	-1.0	0.9	4.0	0.9	C3
1,3-Dioxolane-4-methanol	5660-53-7	-1.5	0.7	2.6	-0.3	C2
Ethanol	64-17-5	-4.6	2.4	2.2	1.5	A, B, D, E, F
EthylHexyllactate	6283-86-9	-0.7	1.0	2.8	-0.2	F
Ethyl lactate	97-64-3	-2.2	0.6	0.8	-1.0	A, B, D, E, F
Geraniol	106-24-1	-1.4	1.2	3.6	0.0	A, B
Glycerol-1,3-diethyl ether	4043-59-8	-2.4	-0.1	2.2	-0.5	C6

NAME	CAS	F1	F2	F3	F4	Sources
Cluster VII: Amphiprotic continued						
Glycerol-1,2-dibutyl ether	91337-36-9	-0.3	-1.4	2.8	0.4	C6
Glycerol-1,2-diethyl ether	4756-20-1	-2.1	-0.5	2.3	-0.5	C6
Glycerol-1,2-dimethyl ether	40453-77-8	-2.6	-0.7	0.7	-1.0	C6
Glycerol-1,3-dimethyl ether	623-69-8	-2.6	-0.1	1.2	-0.8	C6
Glycerol-1-butyl monoether	624-52-2	-1.7	0.0	1.9	0.2	C6
Glycerol-1-ethyl monoether	1874-62-0	-3.7	1.8	1.8	0.0	C6
Glycerol-2-butyl monoether	100078-36-2	-3.6	1.6	2.5	0.3	C6
Glycerol-2-ethyl monoether	22598-16-9	-4.3	1.6	1.2	-0.2	C6
Glycofurol (n=2)	52814-38-7	-2.5	-1.0	1.5	-0.7	C6
N,N-Diethylolcapramide	136-26-5	-2.9	0.1	3.4	0.0	C1
Caprylic acid diethanolamide	3077-30-3	-3.1	-0.2	2.7	-0.1	C1
Isoamyl alcohol	123-51-3	-2.5	1.9	3.7	1.0	D, E
Isopropyl alcohol	67-63-0	-3.5	1.6	2.9	1.2	A, B
Methyl ricinoleate	141-24-2	-0.5	1.0	3.4	0.1	E
Menthanol	498-81-7	-0.9	1.1	4.3	1.4	C3
Nopol	128-50-7	-1.1	0.5	4.0	1.0	C3
1-Octanol	111-87-5	-1.5	1.7	4.3	1.3	C1
Oleic acid	112-80-1	-1.9	7.2	5.9	-1.6	A, B
Oleyl alcohol	143-28-2	-0.3	1.7	4.5	1.3	A, B, F
PolyEthyleneGlycol 600	25322-68-3	-2.7	0.9	1.5	-1.0	F
Solketal	100-79-8	-3.1	1.1	1.1	-0.8	C2
Ricinoleic acid	141-22-0	-2.5	5.3	5.1	-0.8	A, B
α-Terpineol	98-55-5	-0.9	0.9	3.7	0.5	C3
β-Terpineol	138-87-4	-1.1	1.7	3.8	0.4	C3
Tetrahydrofurfurylic alcohol	97-99-4	-4.0	1.1	1.5	-0.1	H
Cluster VIII: Polar protic						
1,3-Dioxan-5-ol	4740-78-7	-5.5	3.5	-0.7	-0.9	A, B
1,3-Dioxolane-4-methanol	5464-28-8	-5.0	2.6	-1.0	-1.0	A, B
Ethylene glycol	107-21-1	-7.6	5.2	-0.9	2.6	D
β-Farnesen	18794-84-8	6.9	1.2	0.1	0.9	C7
Furfurylic alcohol	98-00-0	-4.5	4.8	1.6	-0.9	D
Glycerol	56-81-5	-7.2	5.4	-0.4	1.8	E, F
Glycerol carbonate	931-40-8	-8.3	7.6	-2.9	0.5	D, E, F
Glycerol-1-methyl monoether	623-39-2	-3.9	1.0	-0.1	-0.6	C6
Glycerol-2-methyl monoether	761-06-8	-5.2	2.4	0.3	0.0	C6
5-(Hydroxymethyl)furfural	67-47-0	-6.0	4.9	-0.6	-0.7	G
3-Hydroxypropionic acid	503-66-2	-8.6	7.8	-0.2	0.8	G
3-Methoxy-3-methyl-1-butanol	56539-66-3	-5.9	4.9	-0.4	-0.7	D
PolyEthyleneGlycol 200	112-60-7	-4.7	-0.7	-1.3	-1.2	A, B, F
1,3-Propanediol	504-63-2	-5.7	2.0	1.1	1.1	D, F
Propylene glycol	57-55-6	-5.5	3.9	1.3	1.4	A, B, D, F
Cluster IX: Organic acidic compounds						
Acetic acid	64-19-7	-7.2	8.5	2.3	-0.8	G
Propionic acid	79-09-4	-5.6	8.0	4.1	-1.4	G
Cluster X: Polar structured						
Water	7732-18-5	-16.7	17.2	-5.3	15.8	A, B, F
Ionic liquids						
Choline acetate	14586-35-7	-15.8	-3.3	-18.7	-6.7	I
3-Butyl-1-methylimidazolium tetrafluoroborate	174501-65-6	-6.1	2.6	-7.6	-1.6	F

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C1 Cognis
C2 Rhodia
C3 DRT
C4 ARD
C5 Roquette
C6 Novance
C7 Amyris

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