Supplementary Information

Table S1. ^{13}C and ^{15}N enrichments of various tissues of *Jatropha curcas.* ^{13}C and ^{15}N enrichments were means of three measurements of IR-MS.

	day	**δ_{13C}/%**	**(S.D.)**	**δ_{15N}/%**	**(S.D.)**
Leaves	5	1.57	(0.009)	3.75	(0.066)
	10	3.05	(0.024)	10.60	(0.010)
	15	4.64	(0.008)	13.26	(0.130)
Stems	5	3.10	(0.016)	8.28	(0.027)
	10	6.67	(0.009)	13.15	(0.055)
	15	7.52	(0.025)	14.49	(0.060)
Roots	5	15.36	(0.124)	19.12	(0.142)
	10	22.77	(0.578)	33.10	(0.042)
	15	28.57	(0.355)	41.45	(0.046)

Table S2. List of chemical shifts assigned to water-soluble metabolites.

Compounds	**Position**	**δ_{1H}/ppm**	**δ_{13C}/ppm**
Glu	α	3.75	56.9
Gln	β	2.44	33.6
Gln	γ	2.13	29.1
Arg	α	3.75	56.9
Arg	β	1.91	30.4
Arg	γ	1.64	26.5
Arg	γ	1.72	26.5
Arg	δ	3.24	43.3
Thr	α	3.58	63.4
Thr	β	4.24	68.9
Thr	γ	1.31	22.3
Val	α	3.58	63.4
Val	β	2.27	31.7
Val	γ	0.99	19.4
Val	γ	1.03	20.7
Ala	α	3.77	53.4
Ala	β	1.47	18.8
Pro	α	4.11	64.1
Pro	β	2.05	31.7
Pro	β	2.33	31.7
Pro	γ	2.00	26.5
Pro	δ	3.41	48.8
Pro	δ	3.33	48.8
Gly	α	3.55	44.3
Ser	α	3.83	59.2
Ser	β	3.96	63.1
Asn	α	3.99	54.0
Asn	β	2.86	37.2
Asn	β	2.94	37.2
Asp	α	3.88	55.0

Table S2. *Cont.*

Compounds	Position	δ_{1H}/ppm	δ_{13C}/ppm
Asp	β	2.66	39.1
Asp	β	2.78	39.1
Glu	α	3.75	56.9
Glu	β	2.05	29.8
Glu	β	2.11	29.8
Glu	γ	2.34	36.2
Lys	α	3.75	56.9
Lys	β	1.90	32.4
Lys	γ	1.44	24.4
Lys	γ	1.50	24.4
Lys	δ	1.71	28.9
Lys	ζ	3.03	41.6
Leu	α	3.75	56.9
Leu	β	1.69	42.4
Leu	γ	1.72	26.5
Leu	δ	0.94	23.6
Leu	δ	0.95	24.9
GABA	2	2.28	37.2
GABA	3	1.91	26.5
GABA	4	3.00	42.0
Choline	1	4.05	58.2
Choline	2	3.50	70.2
Choline	Me	3.19	56.6
Ethanolamine	1	3.82	60.8
Ethanolamine	2	3.13	44.0
Malate	2	4.29	73.1
Malate	3	2.36	45.3
Malate	3	2.66	45.3
Succinate	2	2.39	36.9
Lactate	2	4.10	71.5
Lactate	3	1.31	22.3
Acetate	2	1.90	25.6
Sucrose	G1	5.40	94.8
Sucrose	G2	3.55	73.8
Sucrose	G3	3.75	75.4
Sucrose	G4	3.46	72.1
Sucrose	G5	3.83	75.1
Sucrose	G6	3.80	62.8
Sucrose	F1	3.66	64.1
Sucrose	F3	4.21	79.3
Sucrose	F4	4.04	76.7
Sucrose	F5	3.88	84.1
Sucrose	F6	3.80	65.0
Glucose	α1	5.23	94.8

Table S2. *Cont.*

Compounds	Position	δ_{1H}/ppm	δ_{13C}/ppm
Glucose	α2	3.54	74.1
Glucose	α3	3.70	75.4
Glucose	α4	3.40	72.5
Glucose	α5	3.82	74.1
Glucose	β1	4.63	98.7
Glucose	β2	3.24	77.0
Glucose	β3	3.46	78.6
Glucose	β4	3.40	72.5
Glucose	β5	3.46	78.6
Glucose	β6	3.72	63.4
Glucose	β6	3.88	63.4
Fructose	α1	3.55	66.6
Fructose	α2	3.70	66.6
Fructose	α3	4.10	78.3
Fructose	α4	4.10	77.1
Fructose	α5	3.81	83.9
Fructose	α6	3.69	66.1
Fructose	α6	4.01	66.1
Fructose	β1	3.55	65.3
Fructose	β1	3.65	65.3
Fructose	β3	3.79	70.2
Fructose	β4	3.88	72.5
Fructose	β5	3.99	71.8
Fructose	β6	3.66	65.1
Fructose	β6	3.81	65.1
Myo-inositol	1	3.54	74.1
Myo-inositol	2	4.05	75.1
Myo-inositol	3	3.54	74.1
Myo-inositol	4	3.61	75.1
Myo-inositol	5	3.24	77.0
Myo-inositol	6	3.61	75.1

Figure S1. PCA sore plots and lading plots of NIR analyses. (**a**), (**b**) 3D score plots of NIR analyses. 2D score plots of NIR analyses. (**c**), (**d**) PC1-PC2, and (**e**), (**f**) PC1-PC3. Coloring of score plots were based on varieties ((**a**), (**c**) and (**e**)) and germination rate ((**b**), (**d**) and (**f**)). Loading plots of PC1, PC2, and PC3.

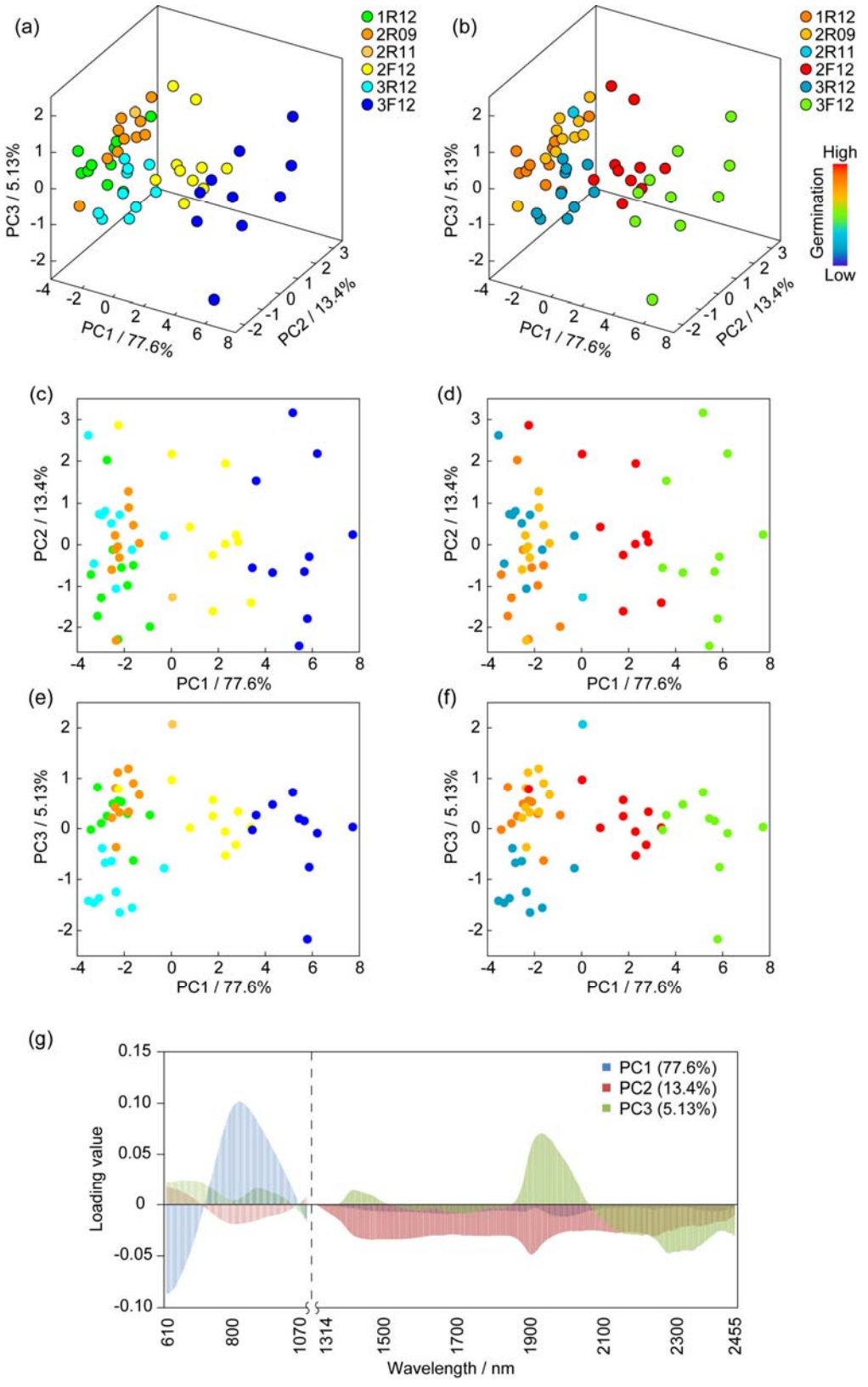


Figure S2. PCA sore plots (PC1-PC3) of NIR analysis (**a**) before and (**b**) after removing outlier. An ellipse in score plot was represented the Hotelling's T2 95% confidence.

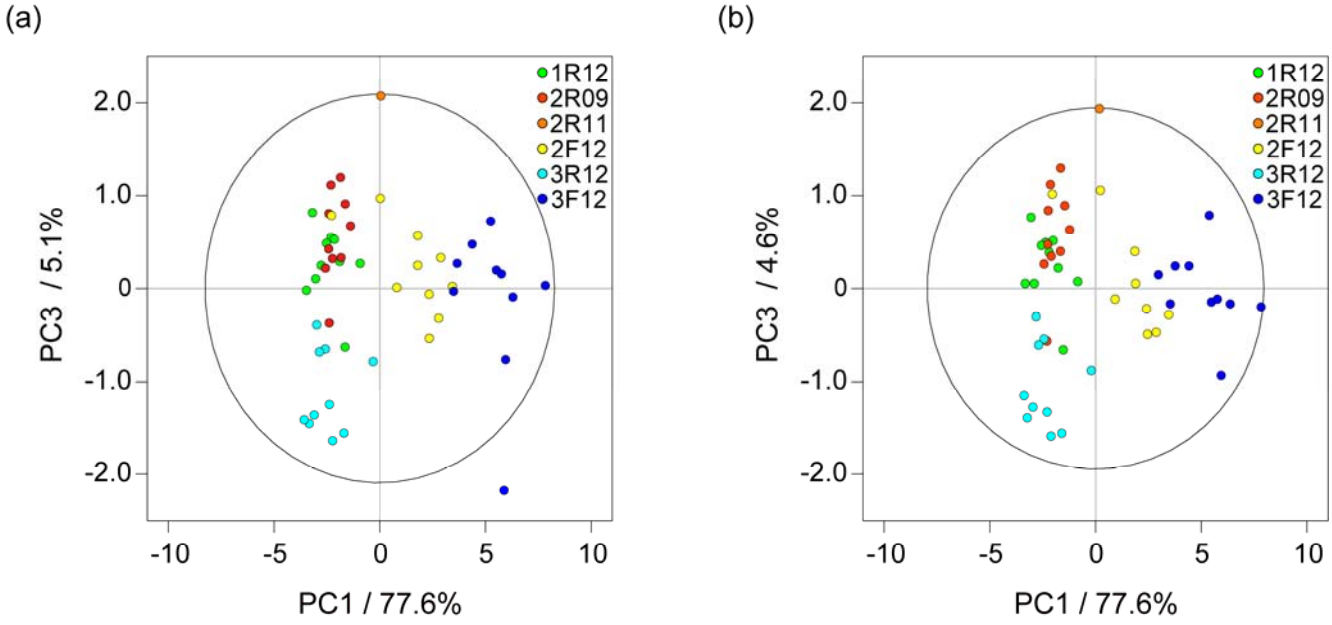


Figure S3. ^{13}C and ^{15}N enrichments of tissues of *Jatropha curcas* as measured by IR-MS. ^{13}C and ^{15}N enrichments were means of three measurements ± S.D.

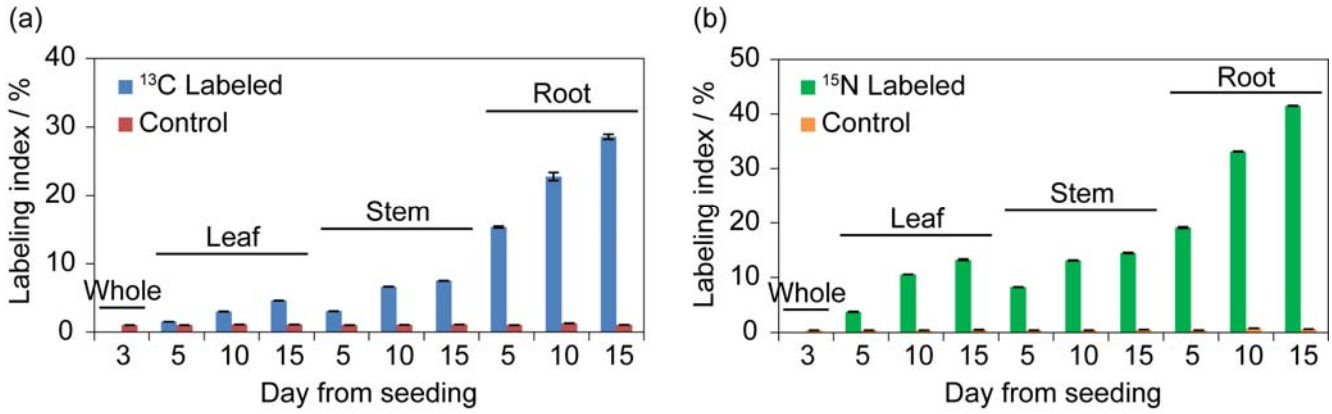


Figure S4. Possible splitting patterns in ^{1}H and ^{13}C NMR spectra in various $^{13}C/^{12}C$ bondomers. This figure was constructed according to Massou *et al.* [1].

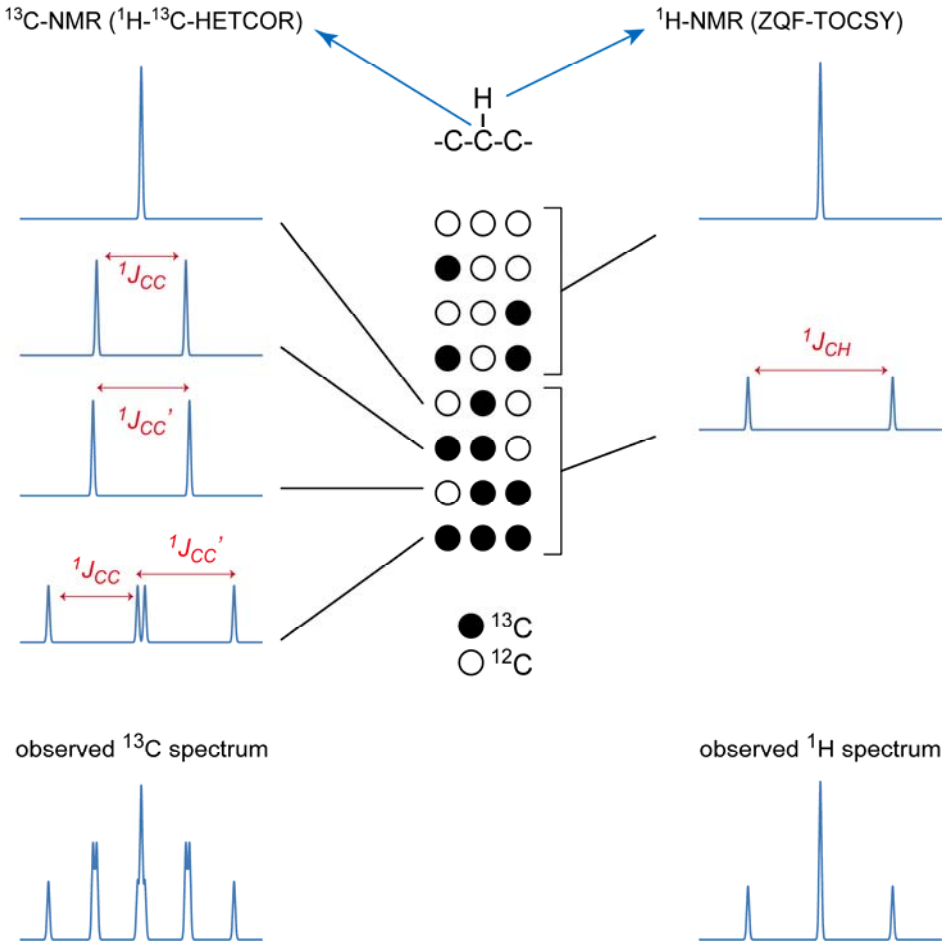


Figure S5. ^{1}H-^{13}C HSQC spectra of water-soluble metabolites in different tissues of *Jatropha curcas* seedlings (2R09). (**a**) Overview; (**b**) Aliphatic region (δ_{1H}: 0.5–4.5 ppm, δ_{13C}: 10–60 ppm); (**c**) Primary alcoholic region (δ_{1H}: 3.0–4.5 ppm, δ_{13C}: 60–90 ppm); (**d**) Anomeric sugar region (δ_{1H}: 4.25–5.5 ppm, δ_{13C}: 90–115 ppm). MI: myo-inositol; MD: maltodextrin; Suc: sucrose; Glc: glucose; Fru: fructose; EA: ethanolamine.

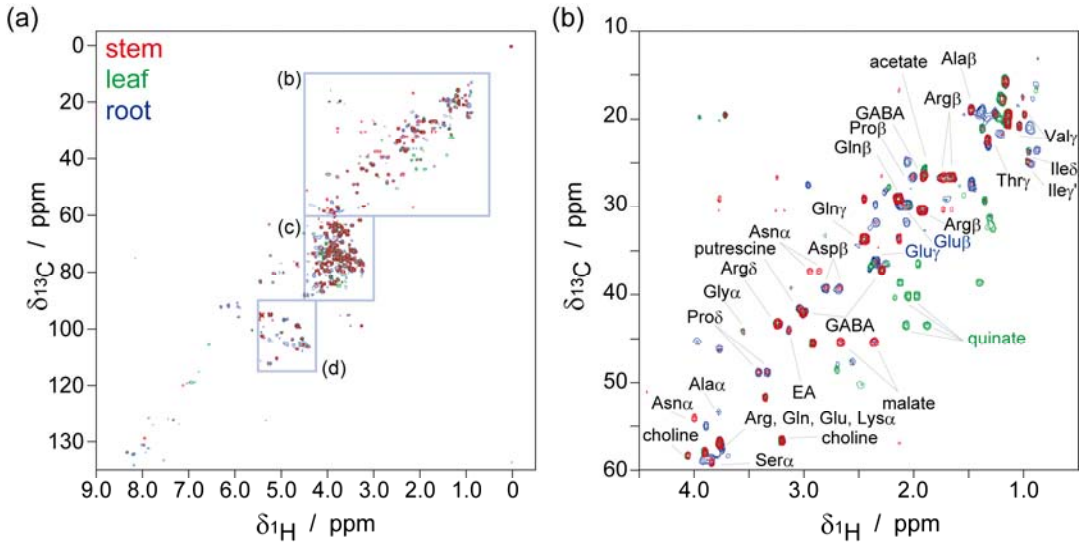
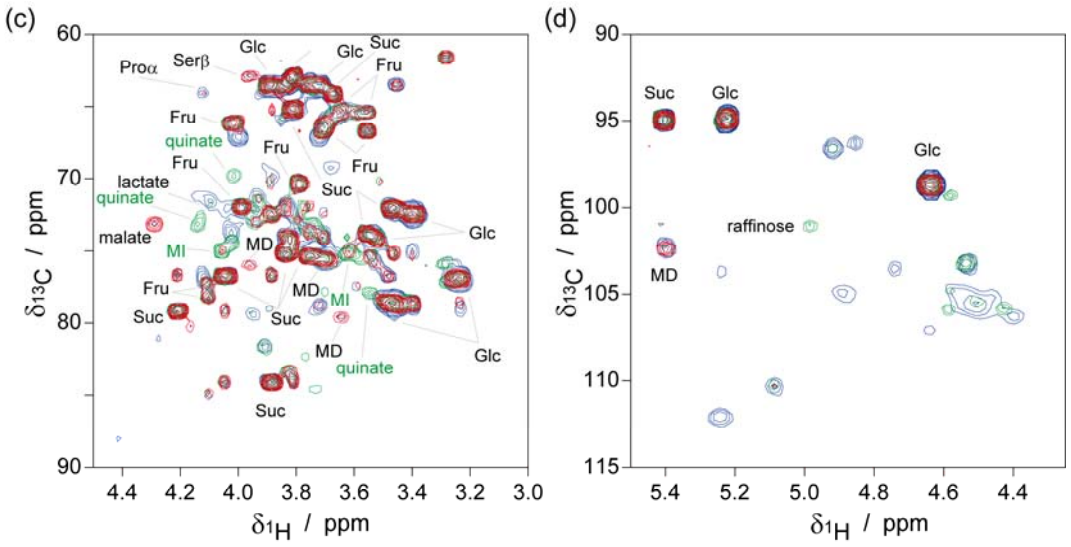


Figure S5. *Cont.*



Reference

1. Massou, S.; Nicolas, C.; Letisse, F.; Portais, J.C. NMR-based fluxomics: Quantitative 2D NMR methods for isotopomers analysis. *Phytochemistry* **2007**, *68*, 2330–2340.