

Supporting Information

Linking Molecular Structure to Plant Conditions: Advanced Analysis of a Systematic Set of Mini-Plant Scale Low Density Polyethylenes

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¹³C-NMR measurements

Peak assignment is performed according to literature (Axelson et al. 1979; Bovey et al. 1975; Striegel und Krejsa 2000). The chemical shifts observed with the respective peak assignments is given in table S1. xB_y refers to the carbon atom x on a side branch with length y . The methyl-carbon at the end of a branch is always denoted as 1, the second last as 2 and so on. xB_6^+ refers to all branches with chain length 6 or more and thus also includes the contribution of all chain ends (EOC, end of chain). br is the tertiary carbon atom of a branch point, α , β and γ refer to the carbon atoms of the backbone next to a branch point. The peaks used for calculation of the branching densities are displayed with a grey background. Not all peaks were observed in the measurements performed. The spectra are given in figures S1-S6. D1 time should be chosen three to five times of the spin-lattice relaxation time of the carbon atom with the slowest relaxation. Zhou et al. found a spin-lattice relaxation time of around 2 s for the carbon nuclei $3B_6^+$ at a $Cr(acac)_3$ concentration of 0.025 M. (Zhou et al. 2013) As this peak is used to calculate the LCB frequency, a D1 time of at 10 s as used here ensures quantitative conditions.

Table S1. Chemical shifts for LDPE samples observed in ¹³C-NMR spectrum with peak assignment.

chemical shift / ppm	peak assignment
10.9	1B ₂
13.8	1B ₄ , 1B ₅ , 1B ₆ ⁺
22.4	2B ₅ , 2B ₆ ⁺
22.9	2B ₄
26.3	4B ₅
26.7	β B ₄ , β B ₅ , β B ₆ ⁺
28.9	4B ₆ ⁺
29.0	3B ₄
29.4	backbone
29.9	γ B ₄ , γ B ₅ , γ B ₆ ⁺
31.6	3B ₆ ⁺
32.7	3B ₅
33.5	4B ₄
33.9	α B ₄ , α B ₅ , α B ₆ ⁺ , 5B ₅
37.4	brB ₄ , brB ₅ , brB ₆ ⁺

38.3 brB₂

Figure S1:
¹³C-NMR spectrum obtained for sample 03-1. Peak assignment according to

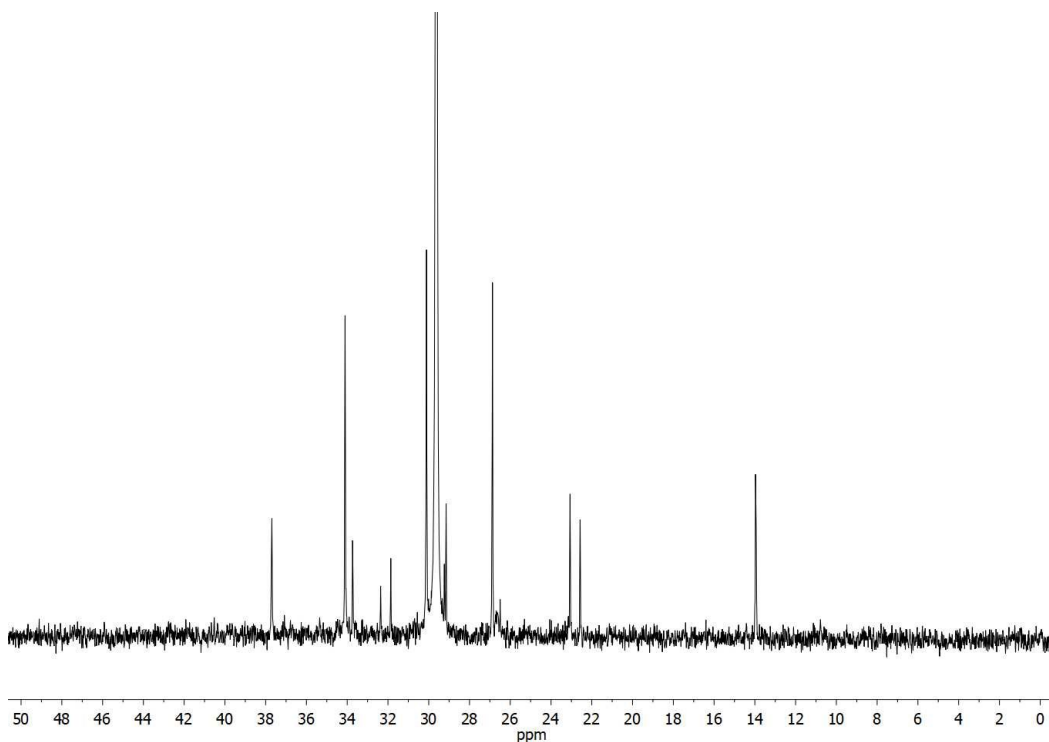


table S1, for experimental details see experimentals of original paper.

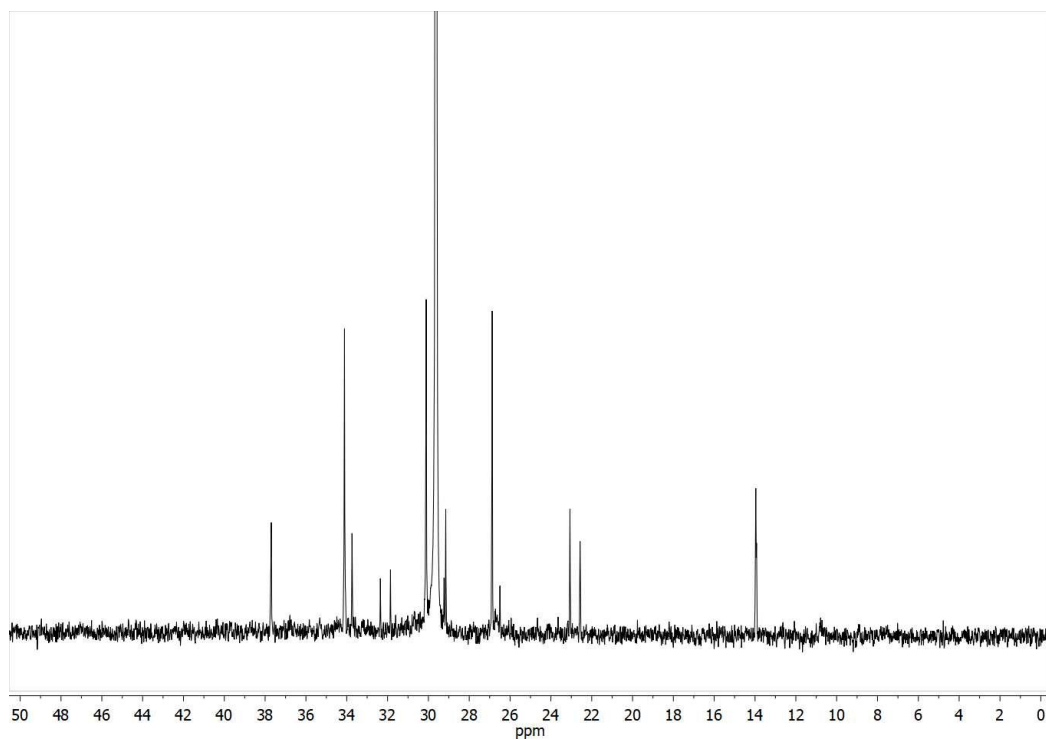


Figure S2: ¹³C-NMR spectrum obtained for sample 03-3. Peak assignment according to table S1, for experimental details see experimentals of original paper.

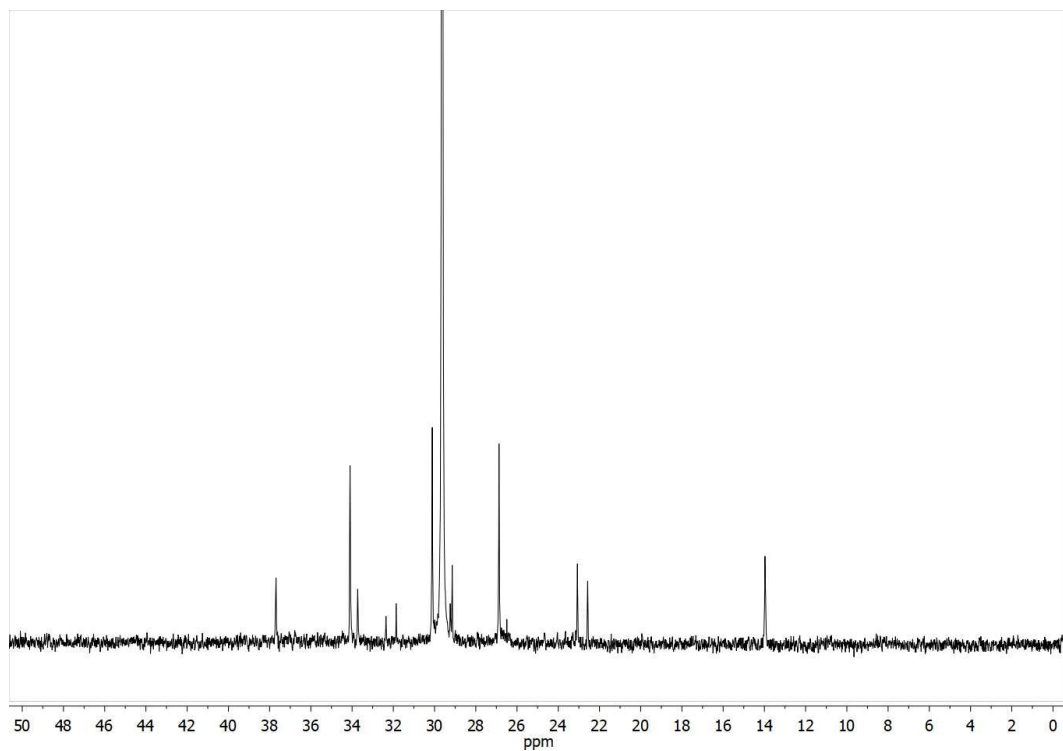


Figure S3: ^{13}C -NMR spectrum obtained for sample 03-4. Peak assignment according to table S1, for experimental details see experimentals of original paper.

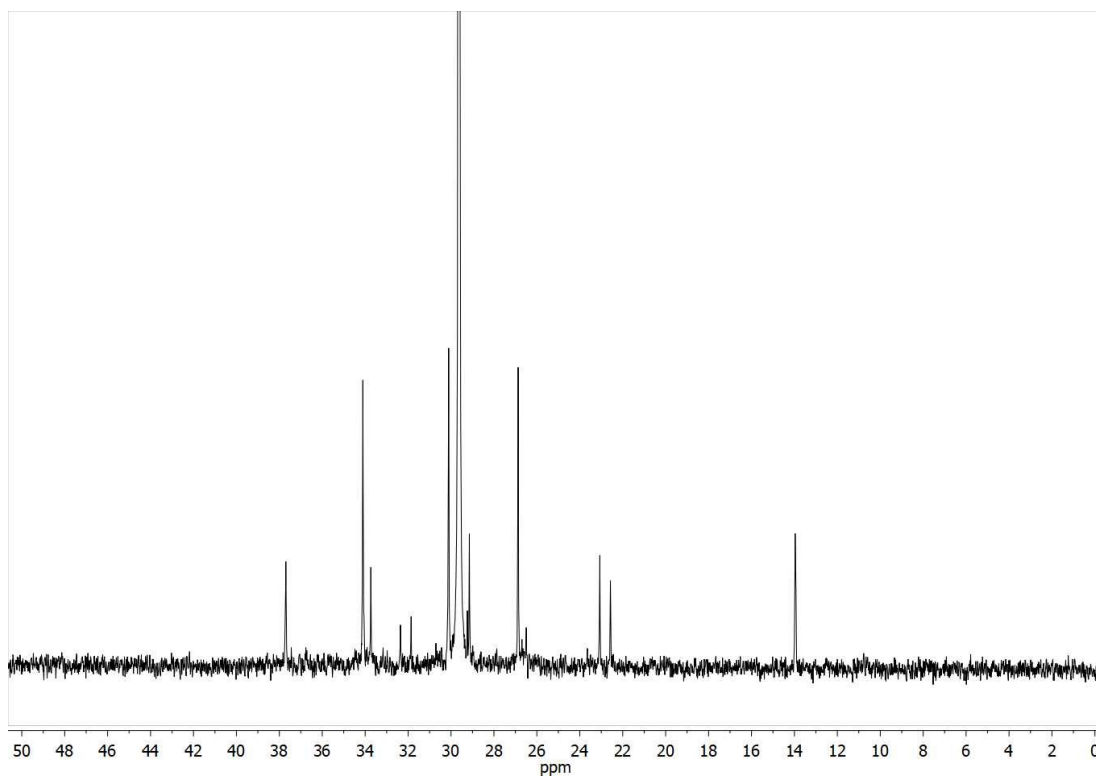


Figure S4: ^{13}C -NMR spectrum obtained for sample 04-2. Peak assignment according to table S1, for experimental details see experimentals of original paper.

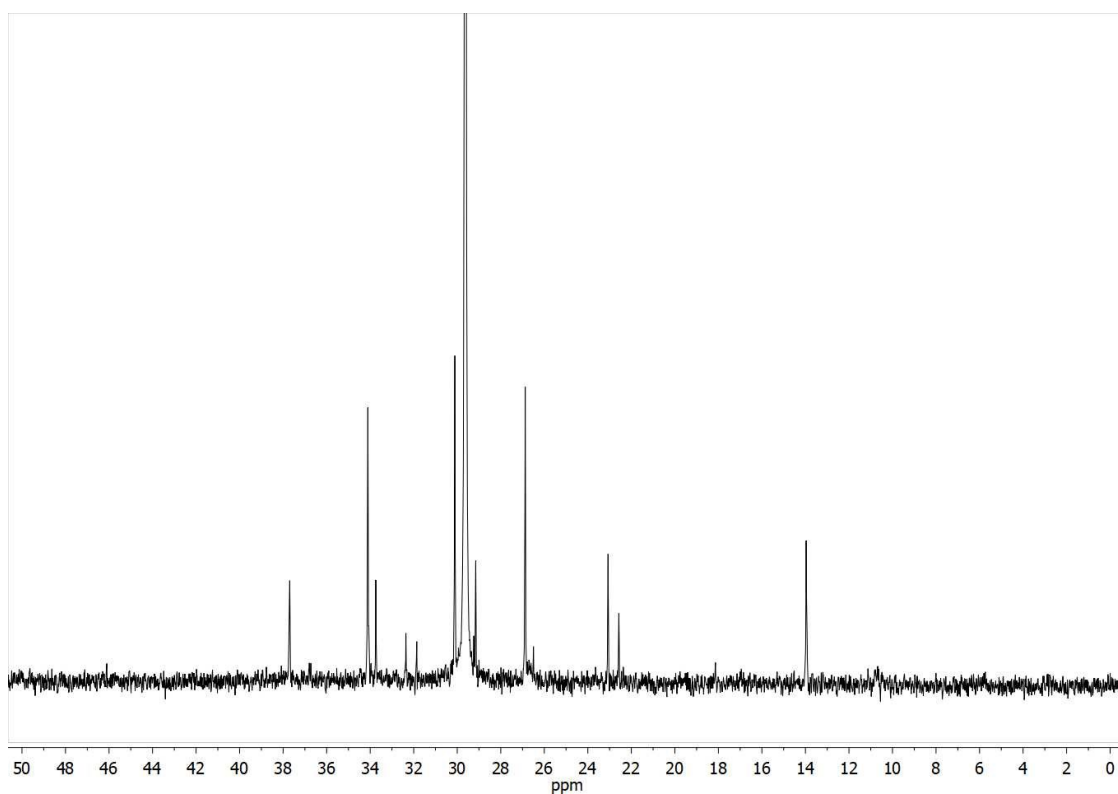


Figure S5: ^{13}C -NMR spectrum obtained for sample 05-1. Peak assignment according to table S1, for experimental details see experimentals of original paper.

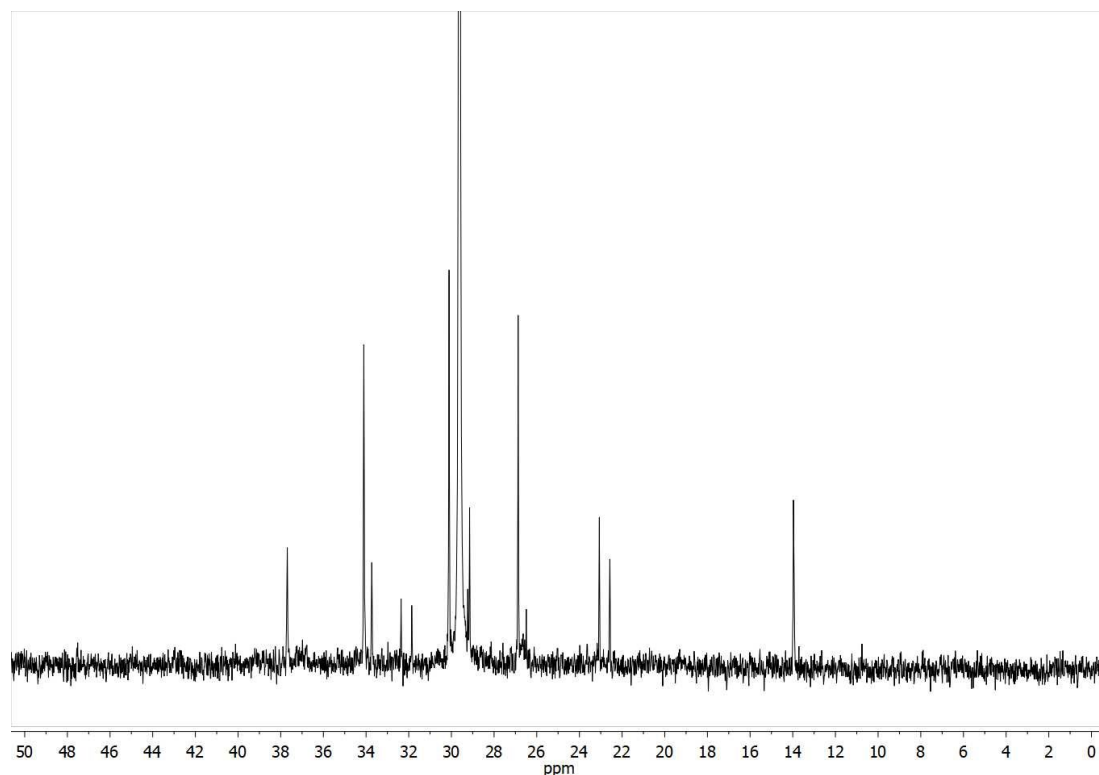


Figure S6: ^{13}C -NMR spectrum obtained for sample 06-3. Peak assignment according to table S1, for experimental details see experimentals of original paper.

References

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