

Sparingly fluorinated maltoside-based surfactants for membrane-protein stabilization

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¹H NMR, ¹⁹F NMR, and ¹³C NMR spectra for all compounds

Figure S1: Superposition of selected experimental and fitted sedimentation velocity profiles

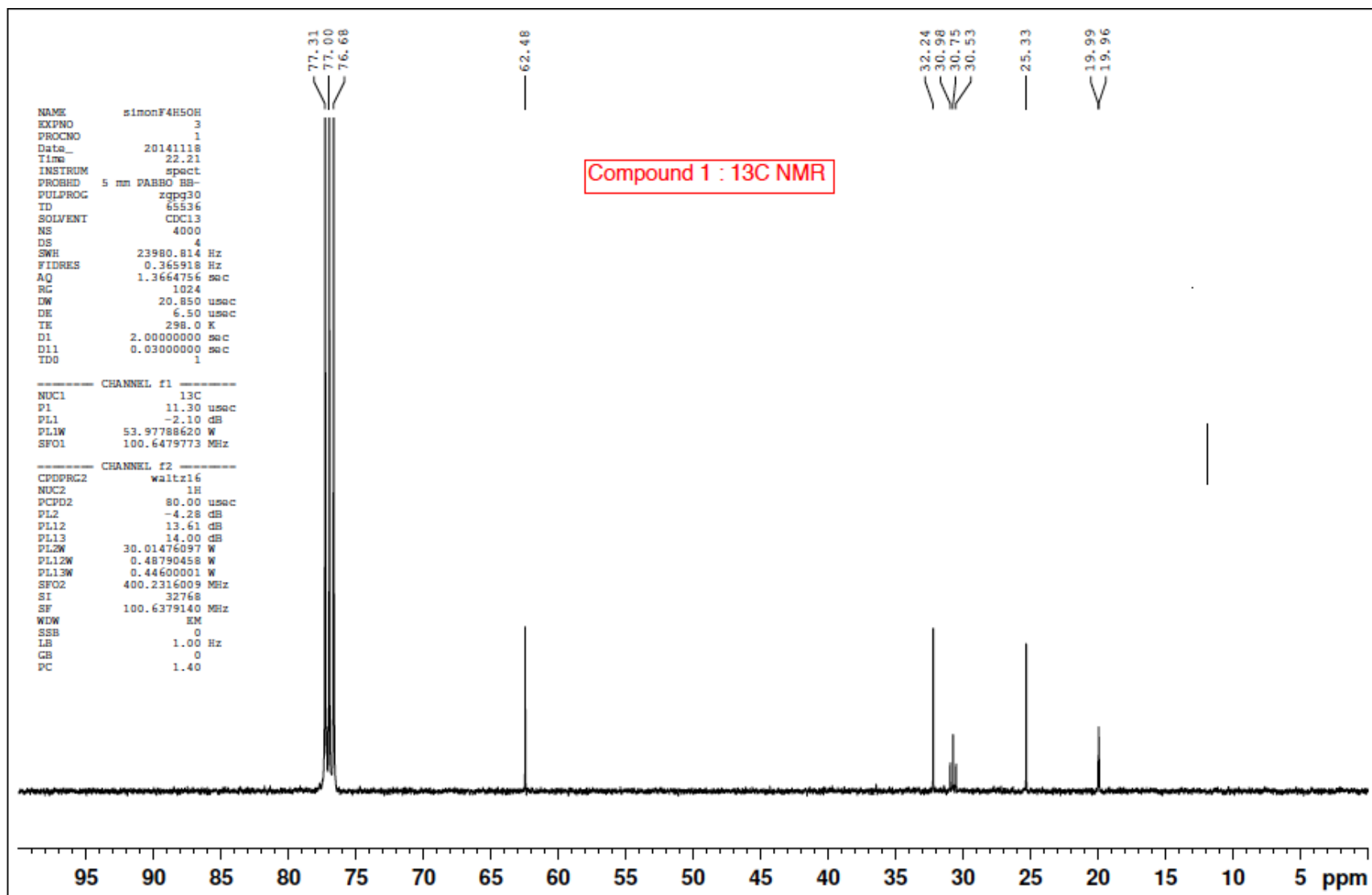
Figure S2: Autocorrelation functions $G(t)$ and size distributions weighted by intensity or volume for F₂H₉βM, F₄H₅βM, and F₆H₂βM in water

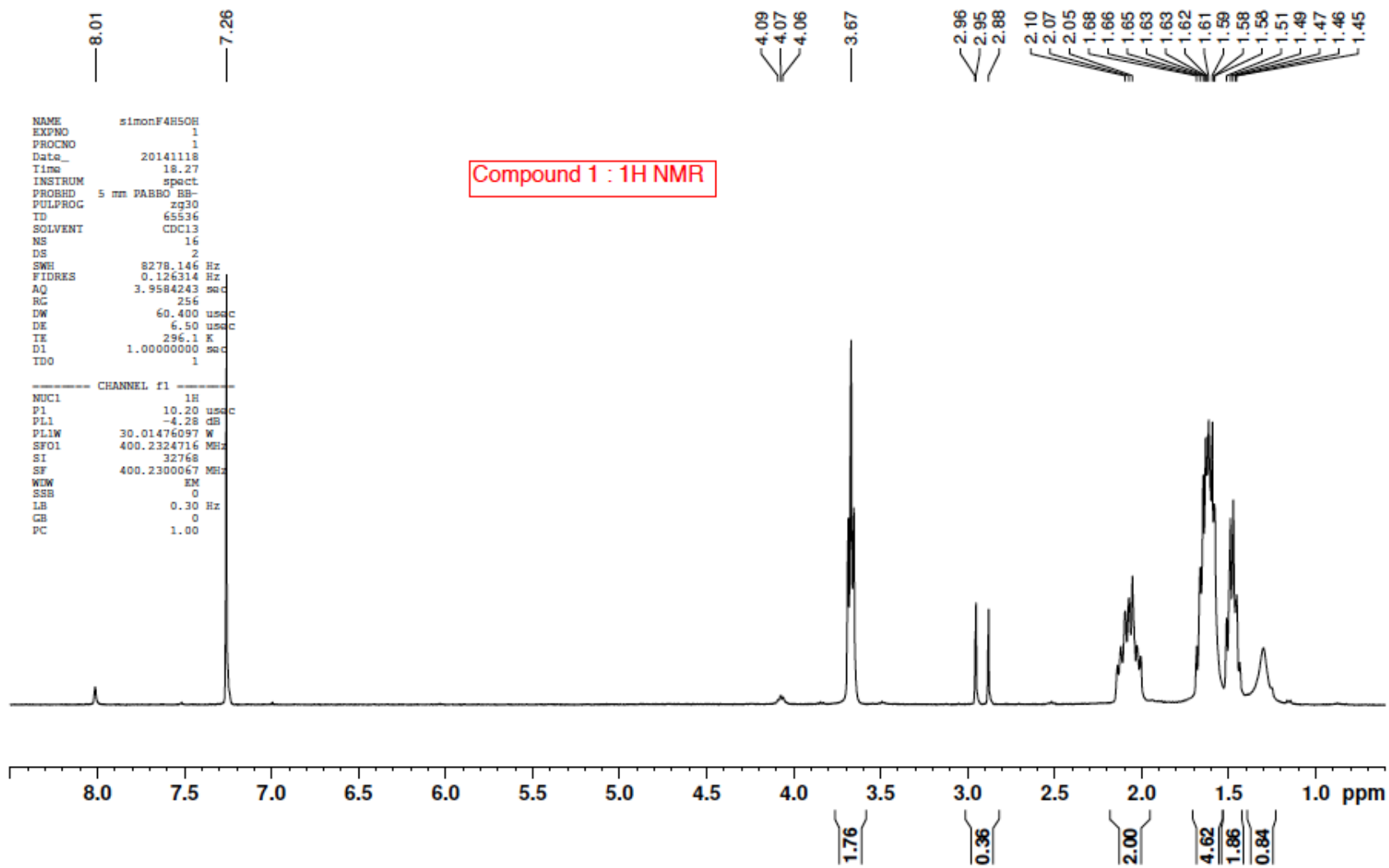
Figure S3: SAXS patterns and pair distribution functions for F₂H₉βM, F₄H₅βM, and F₆H₂βM in water

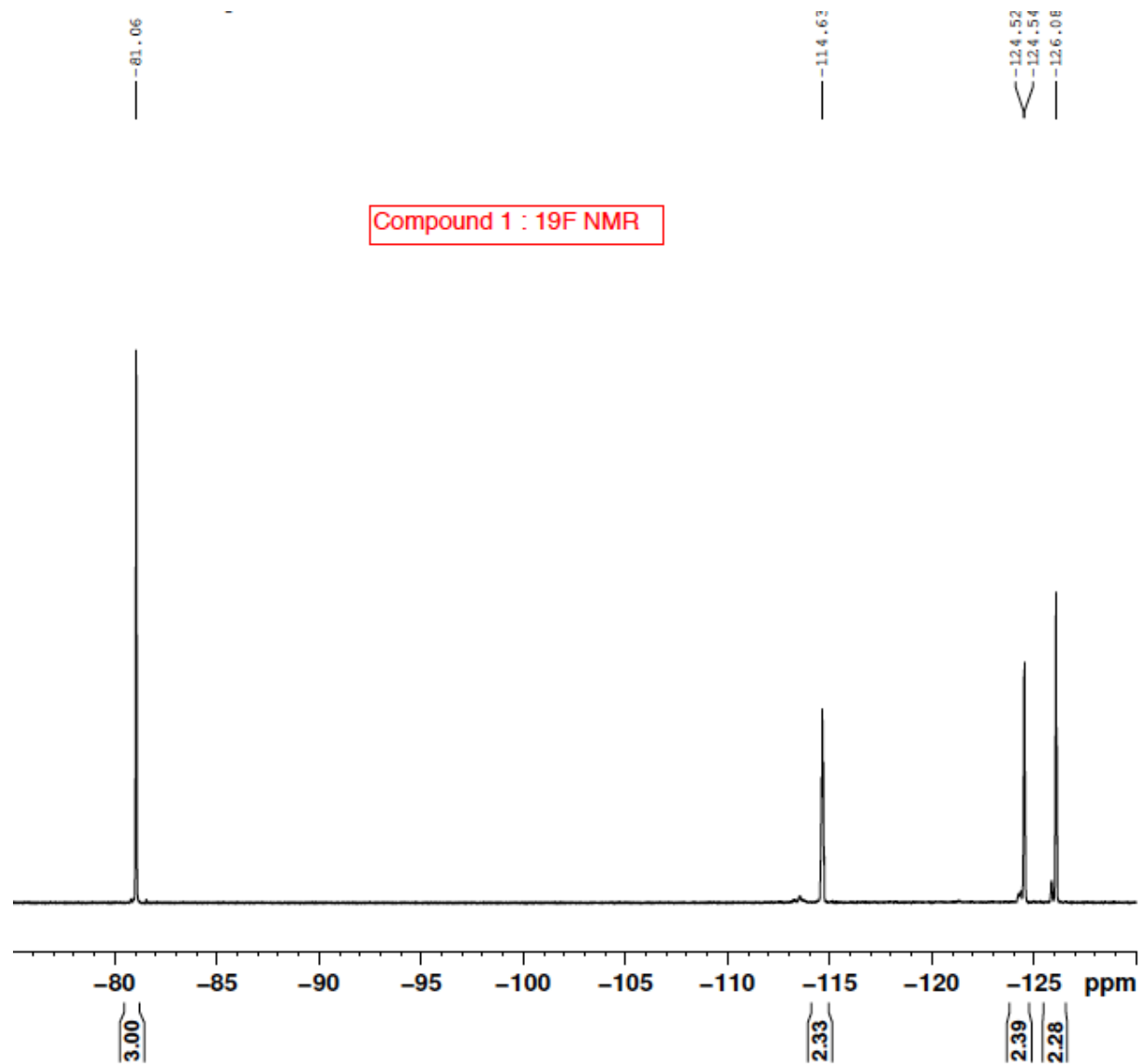
Figure S4: Forward intensity $I(0)$ as a function of total surfactant concentration for F₂H₉βM, F₄H₅βM, and F₆H₂βM for CMC determination

Table S1: Summary of surfactant properties

^1H NMR, ^{19}F NMR and ^{13}C NMR of compound 1

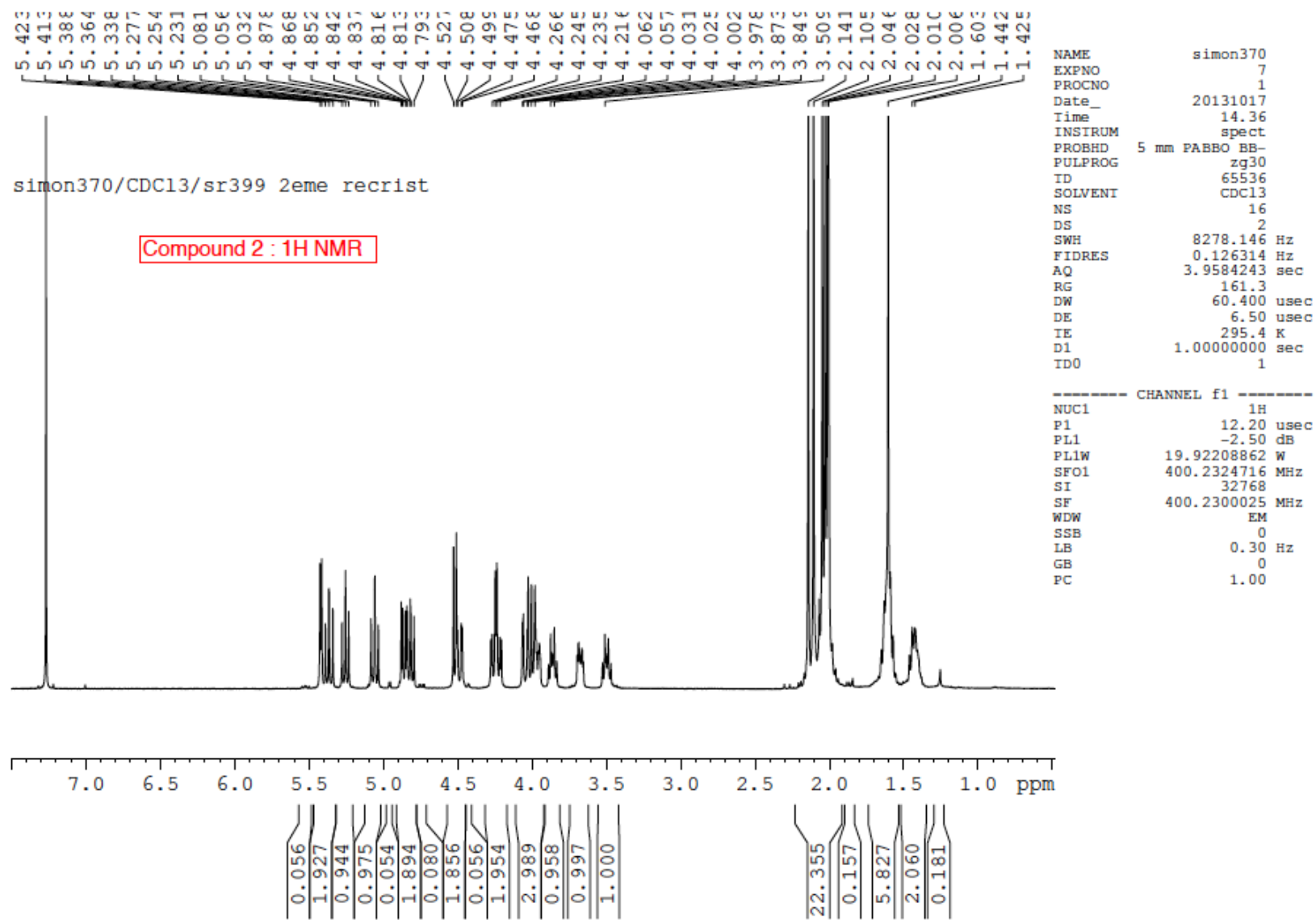


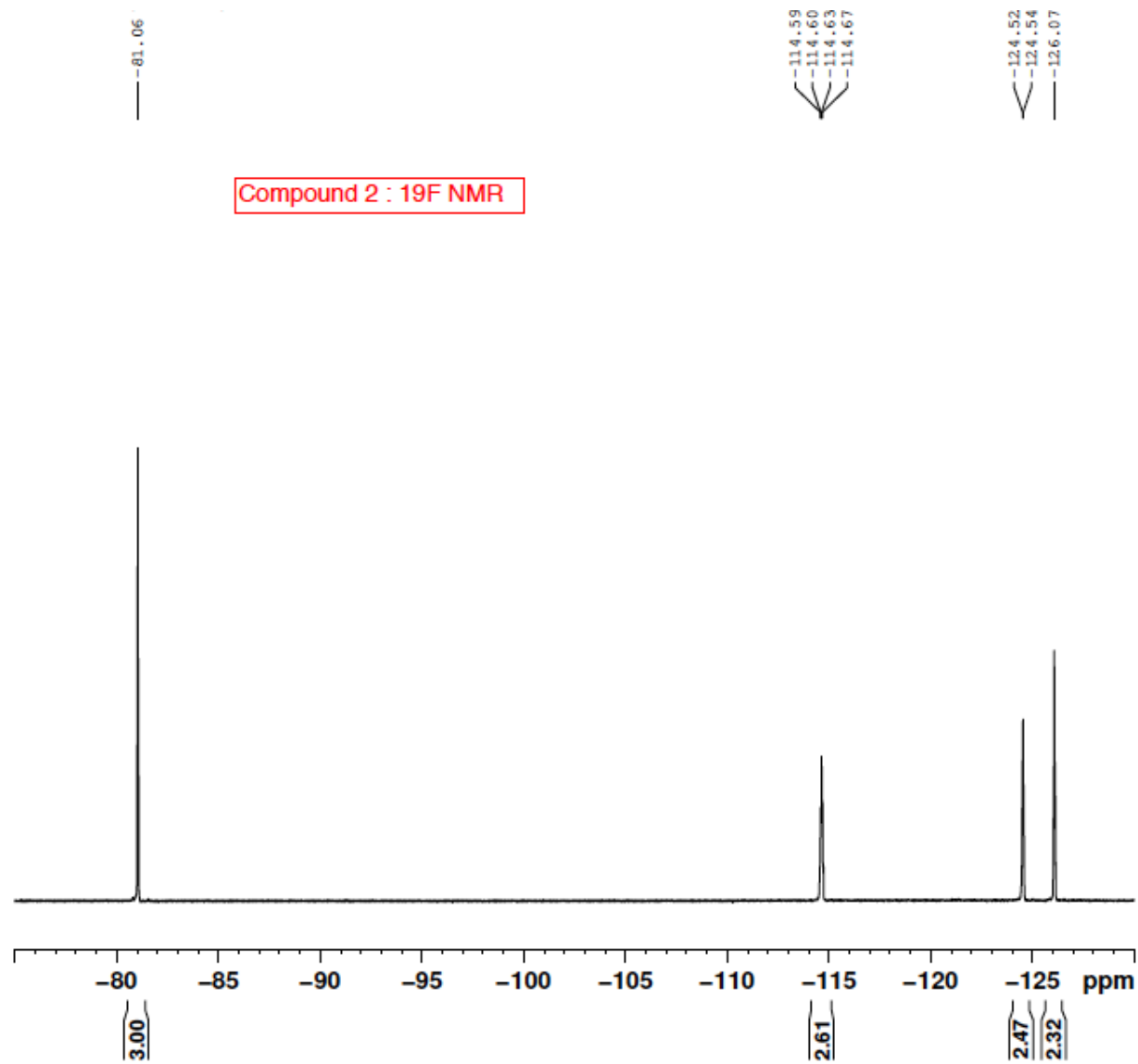




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FIDRES    0.573639 Hz
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RG        574.7
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DE        6.50 usec
TE        296.1 K
D1        1.00000000 sec
ID0       1
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SI        65536
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^1H NMR, ^{19}F NMR and ^{13}C NMR of compound 2



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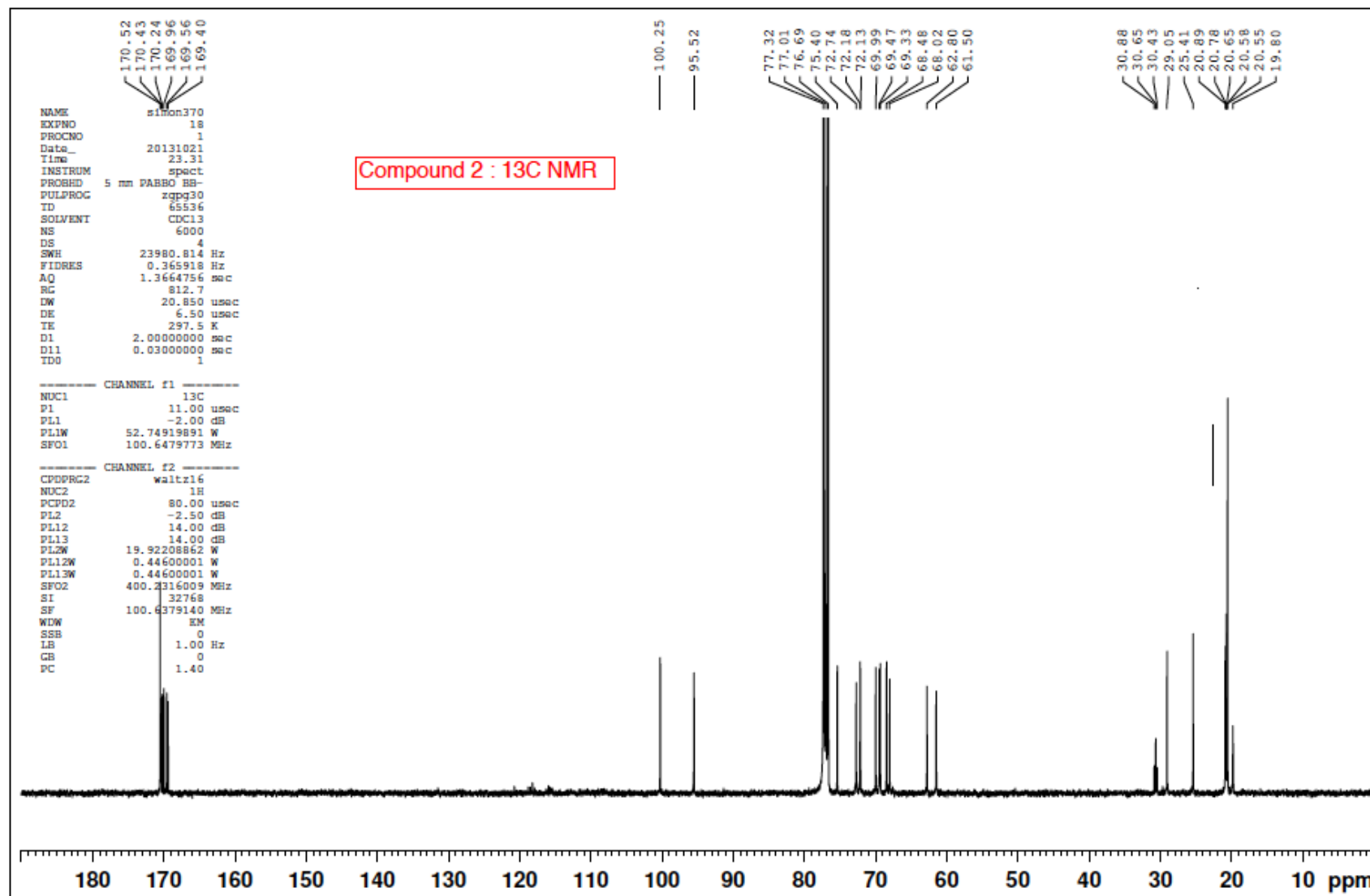
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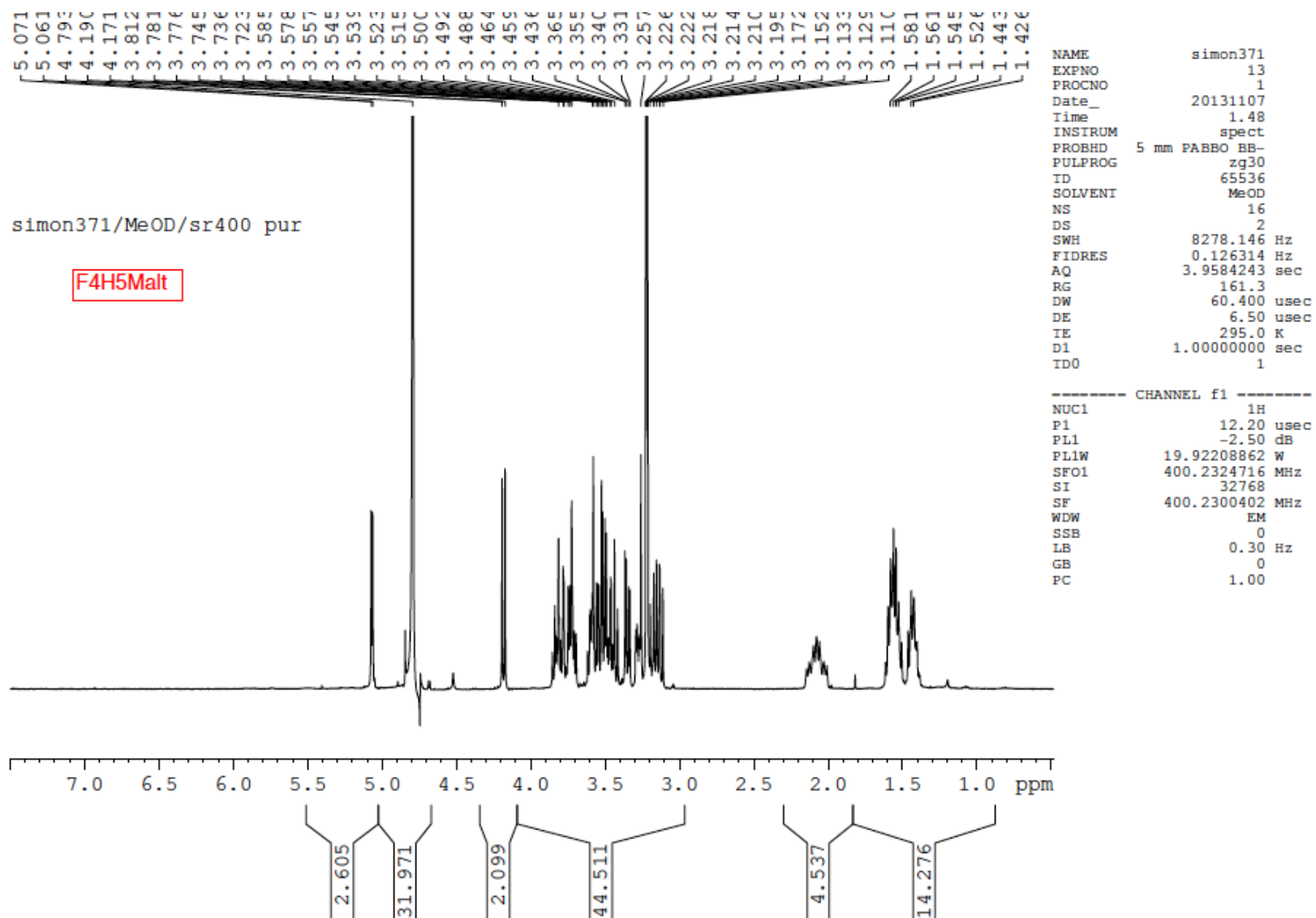
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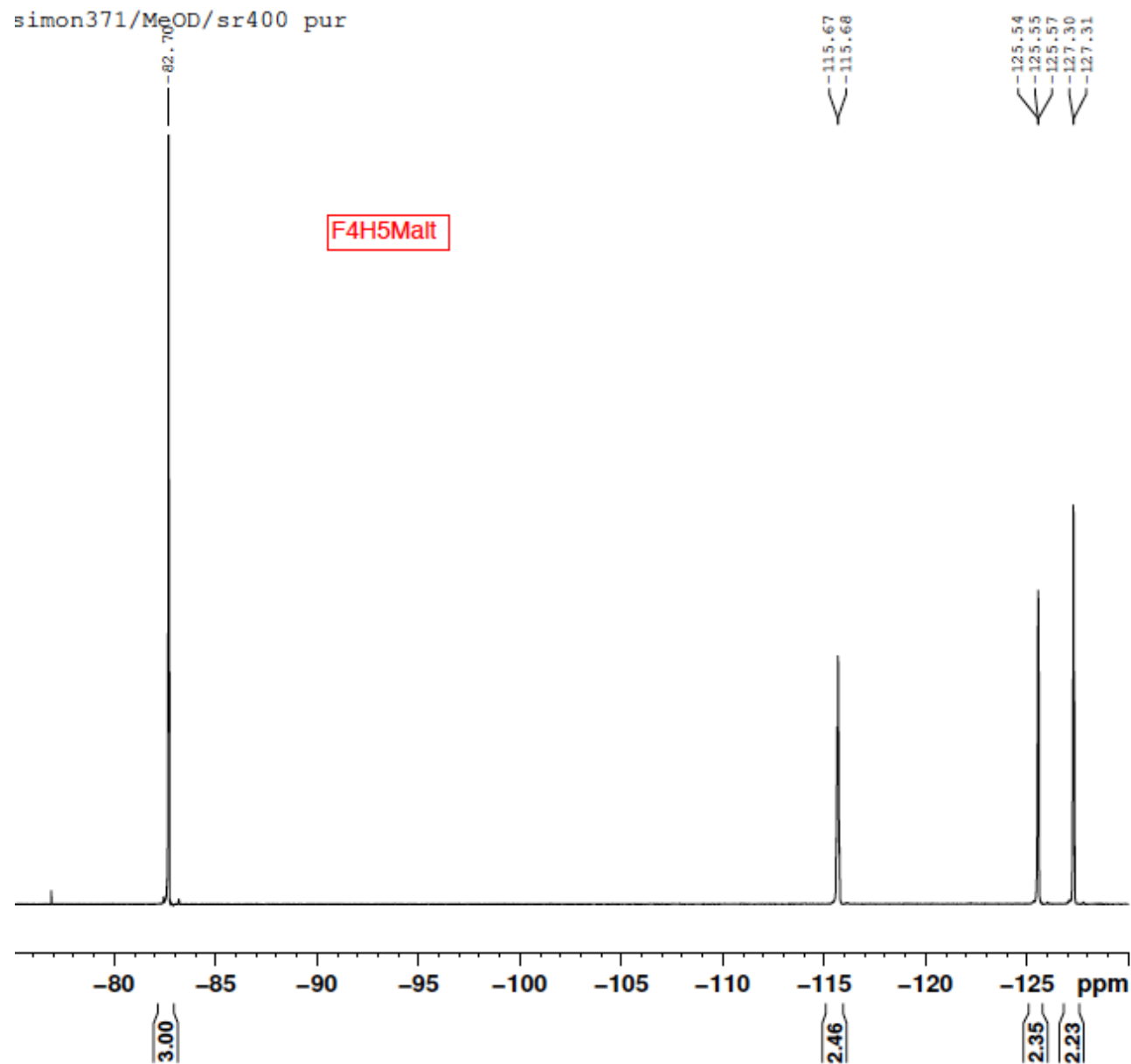
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^1H NMR, ^{19}F NMR and ^{13}C NMR of F4H5Malt

simon371/MeOD/sr400 pur

F4H5Malt



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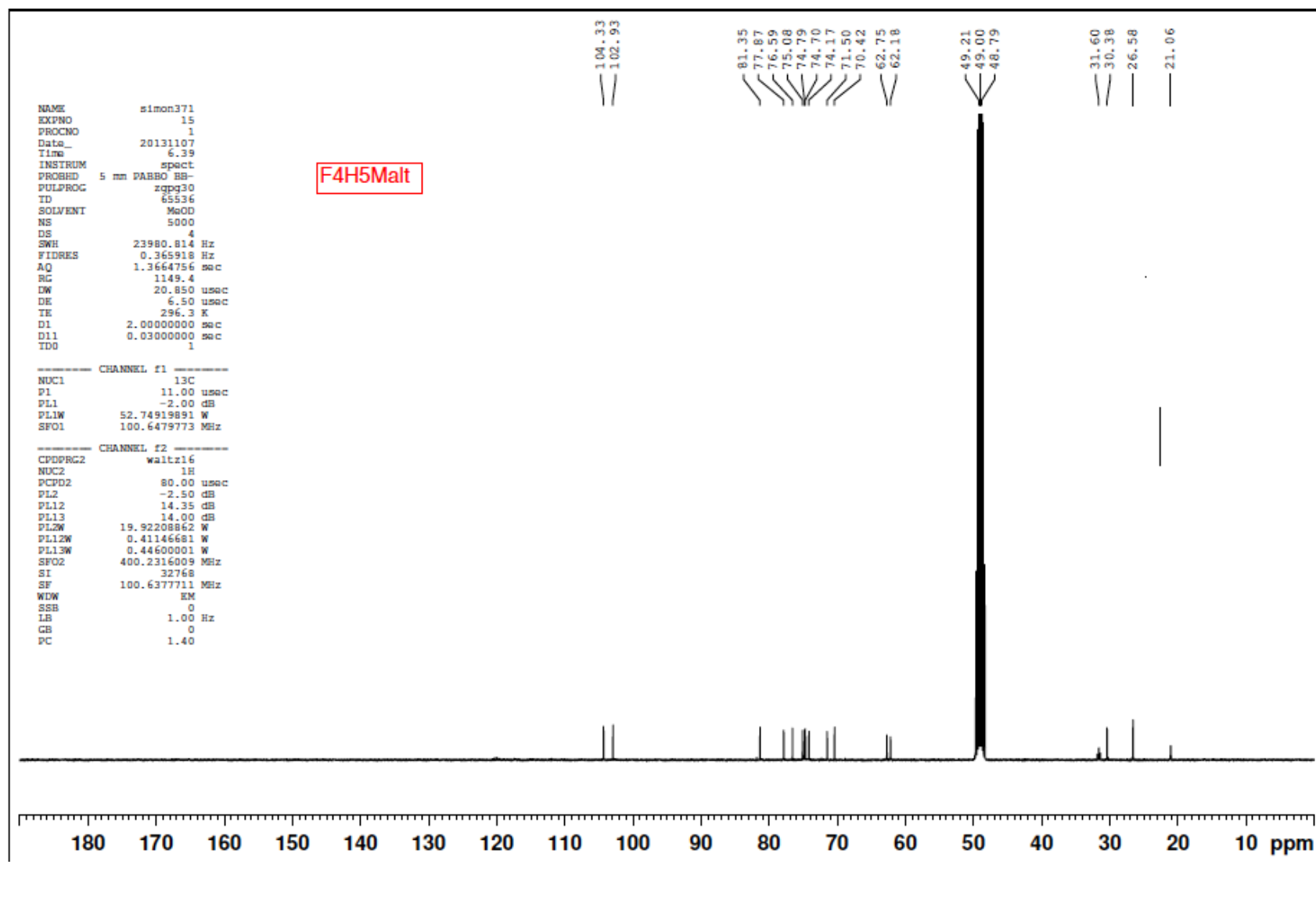
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FIDRES        0.573639 Hz
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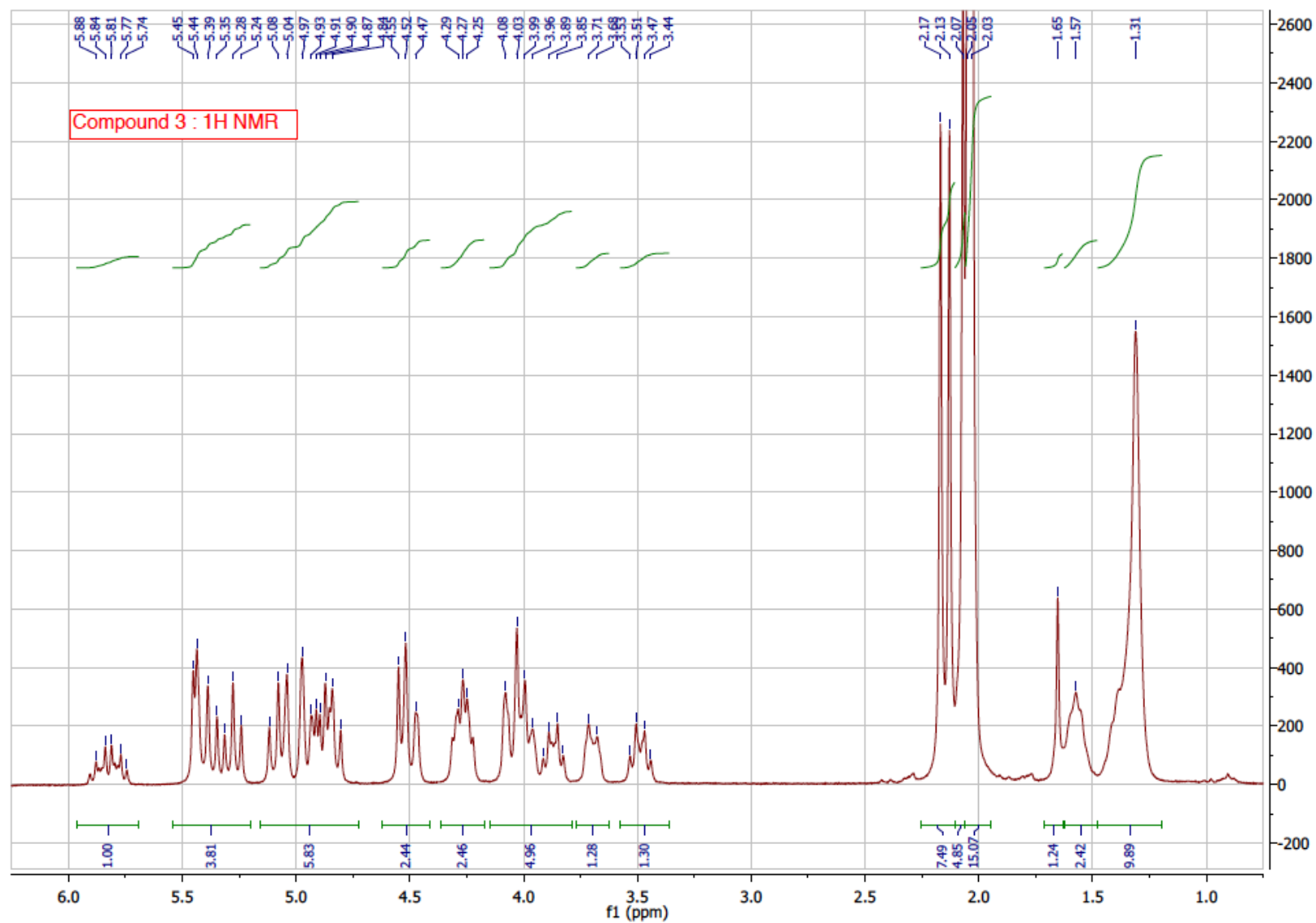
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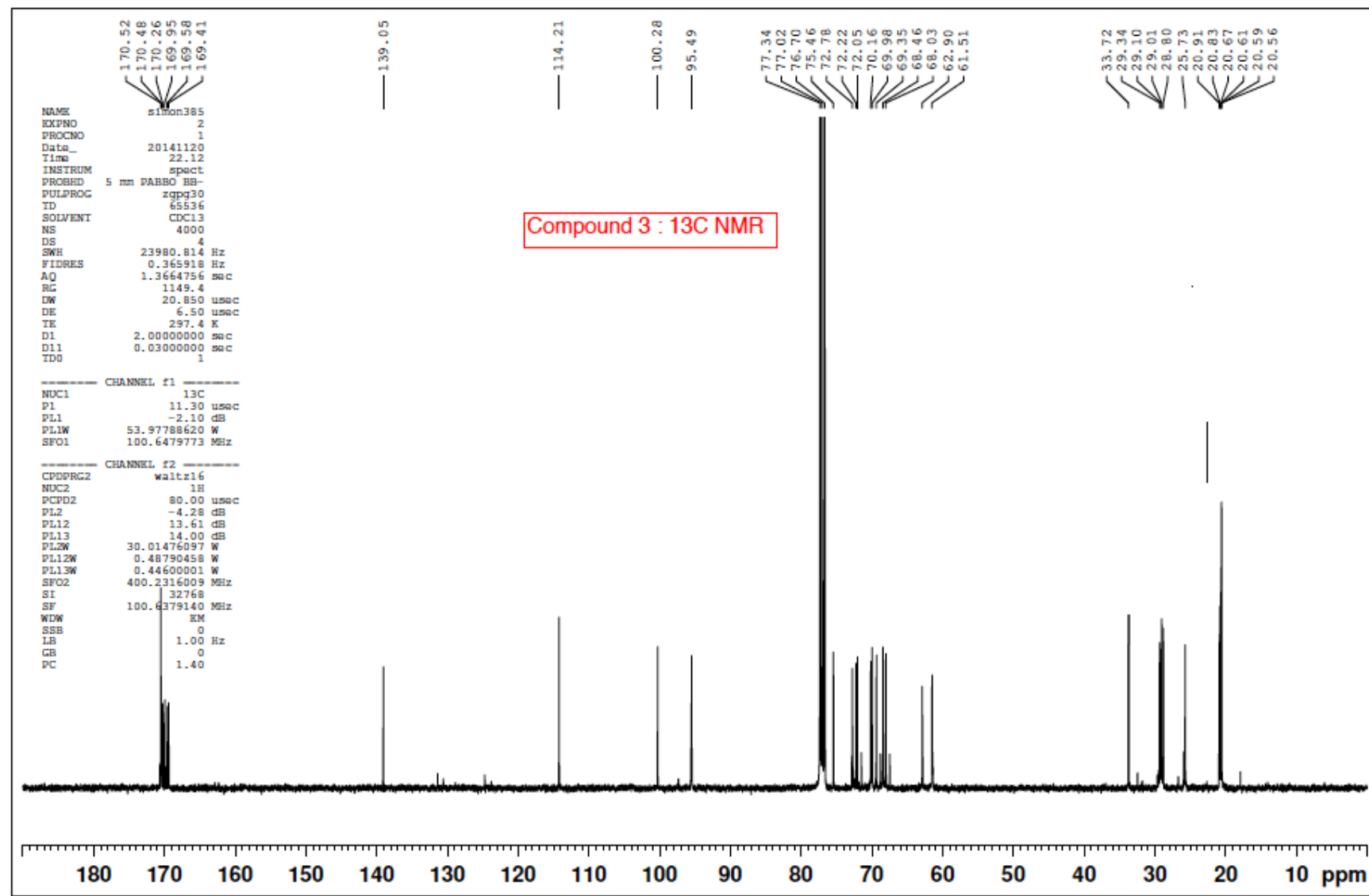
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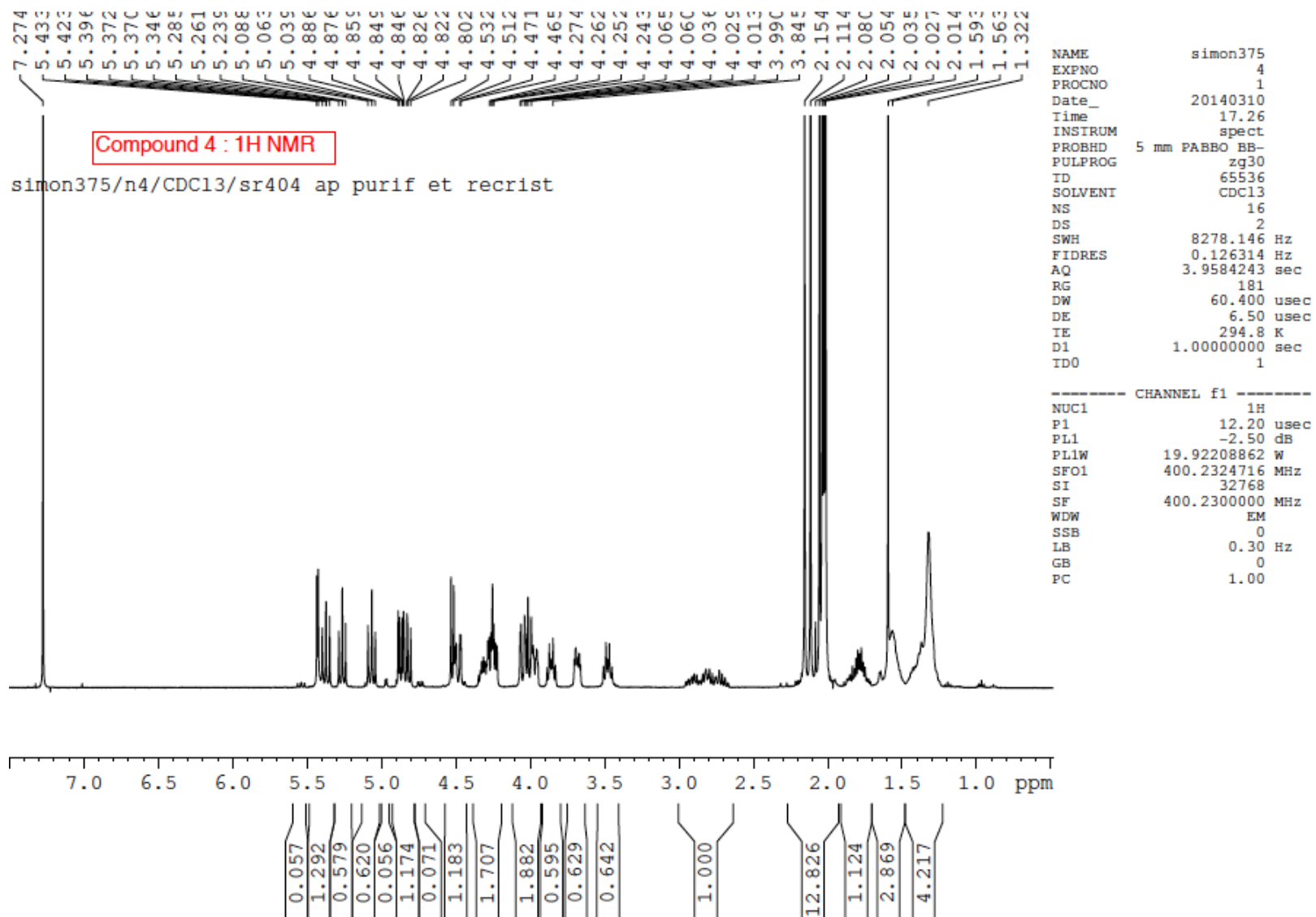
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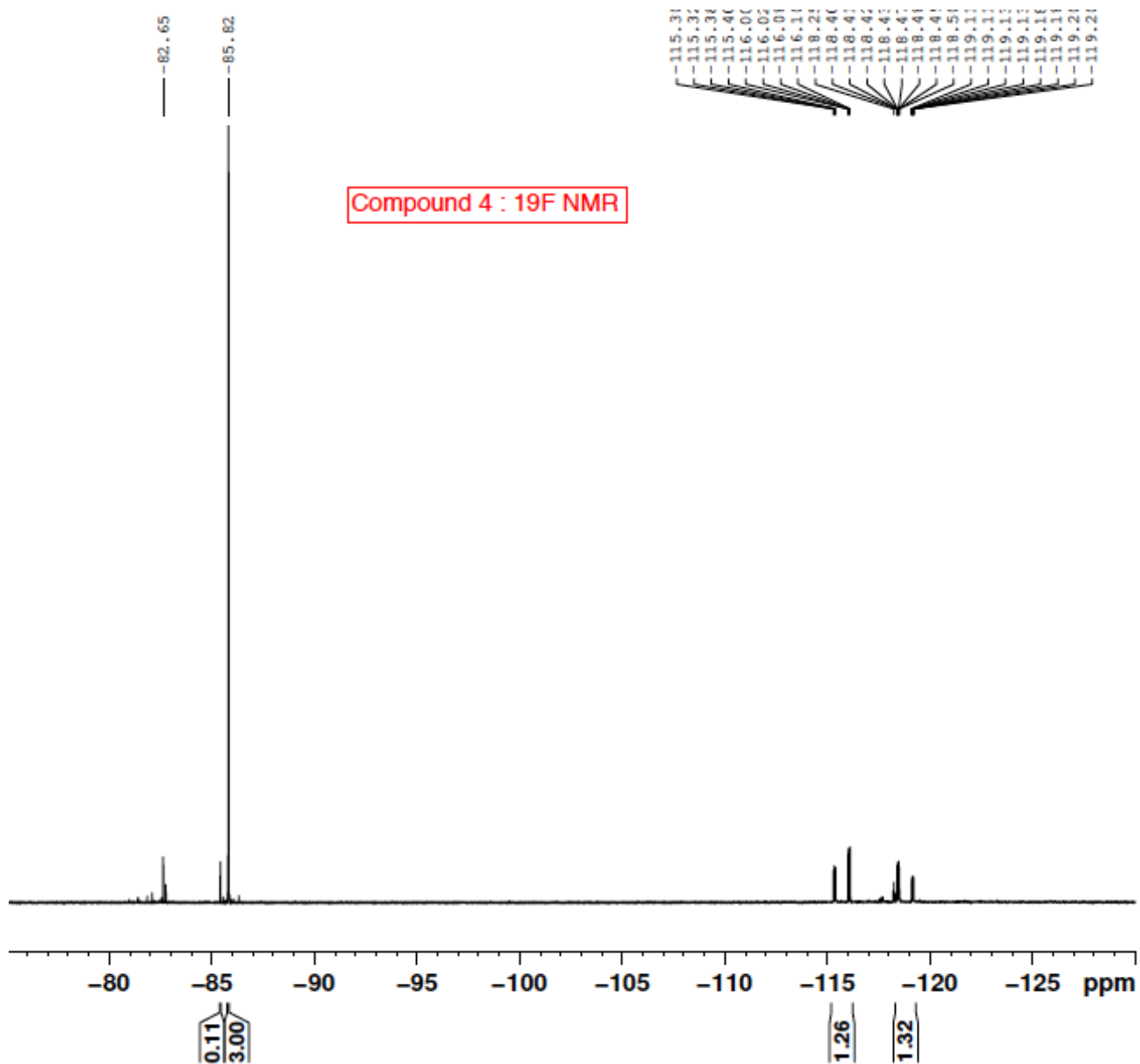
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^1H NMR and ^{13}C NMR of compound 3



^1H NMR, ^{19}F NMR and ^{13}C NMR of compound 4

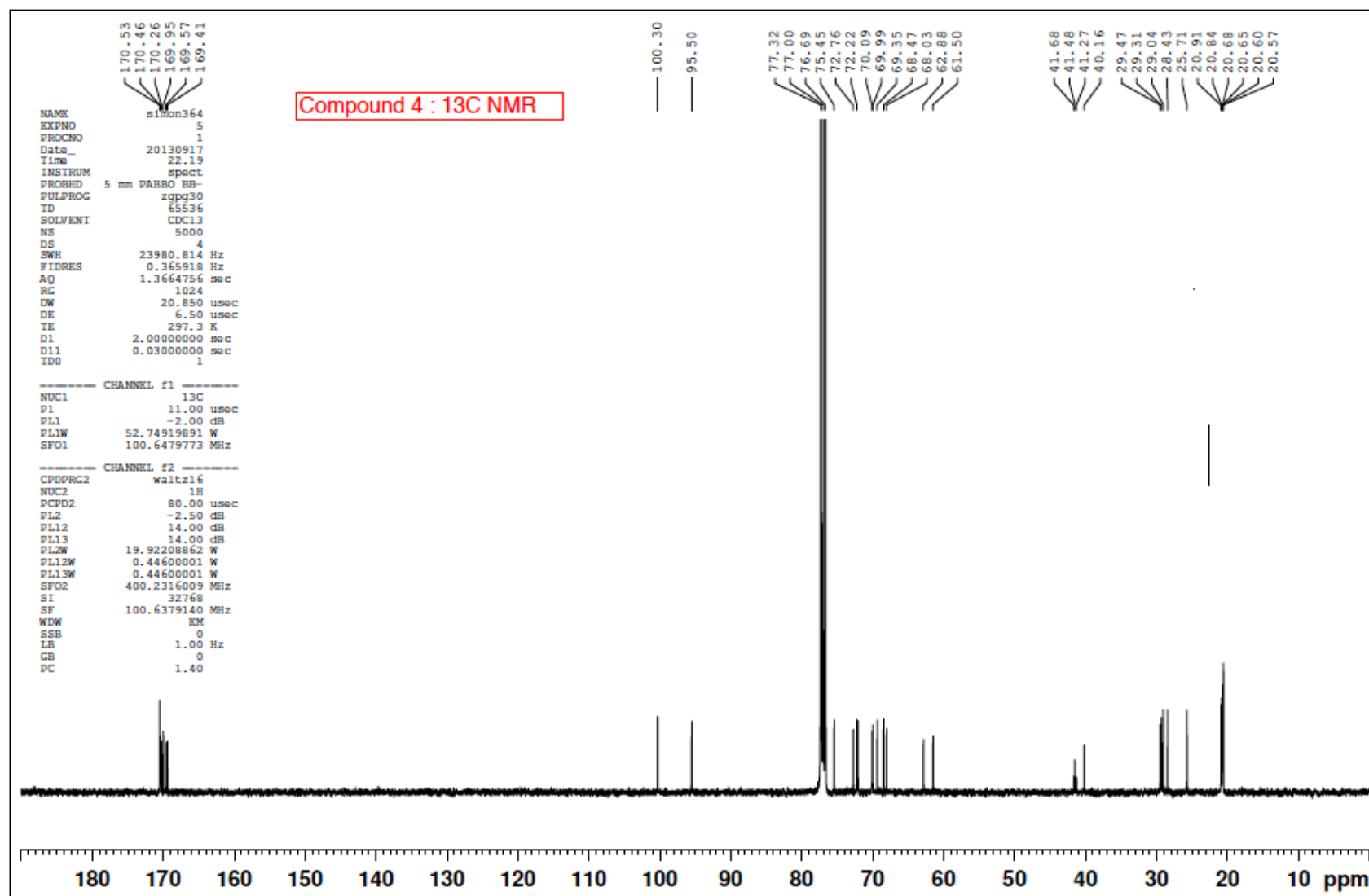


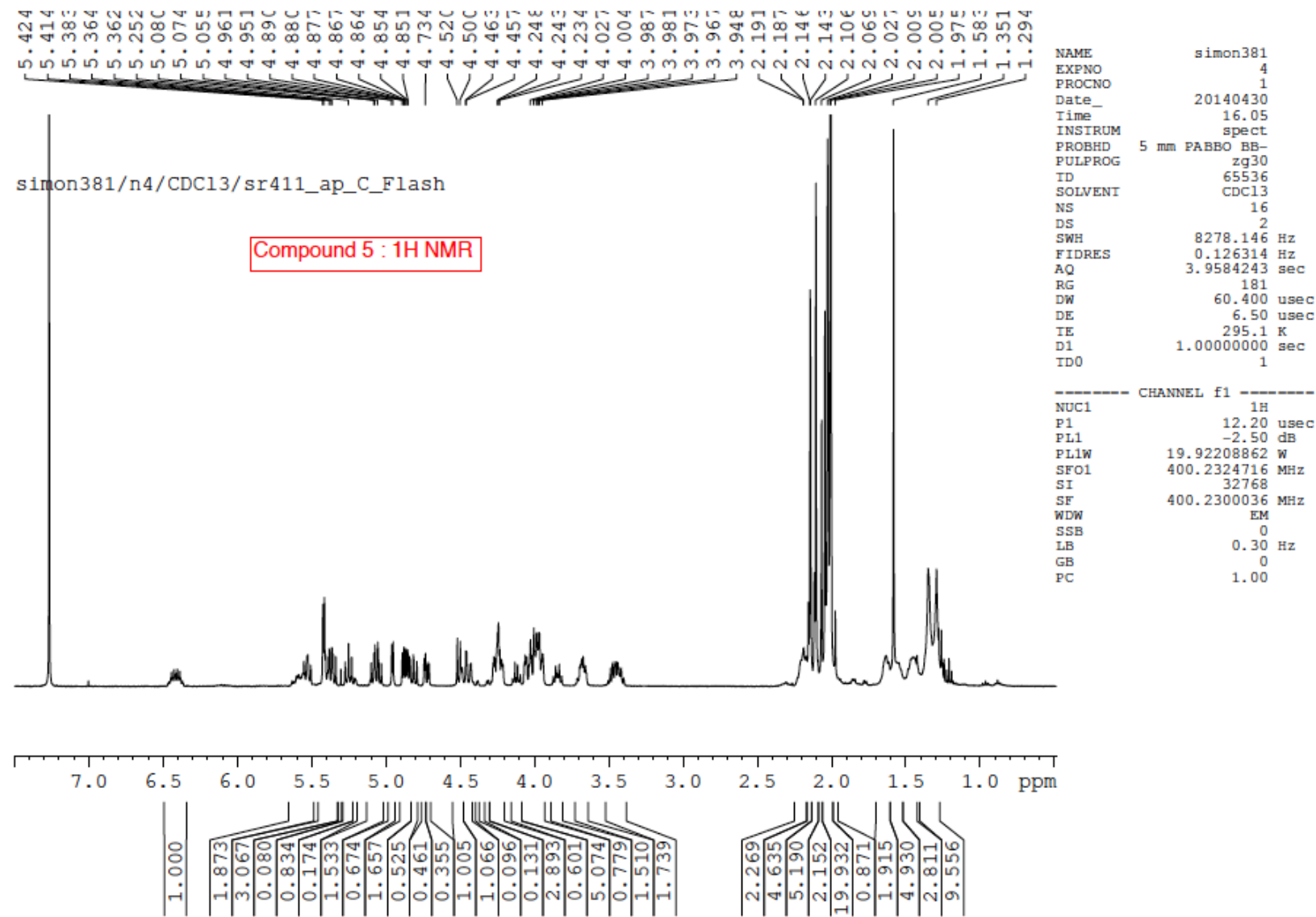
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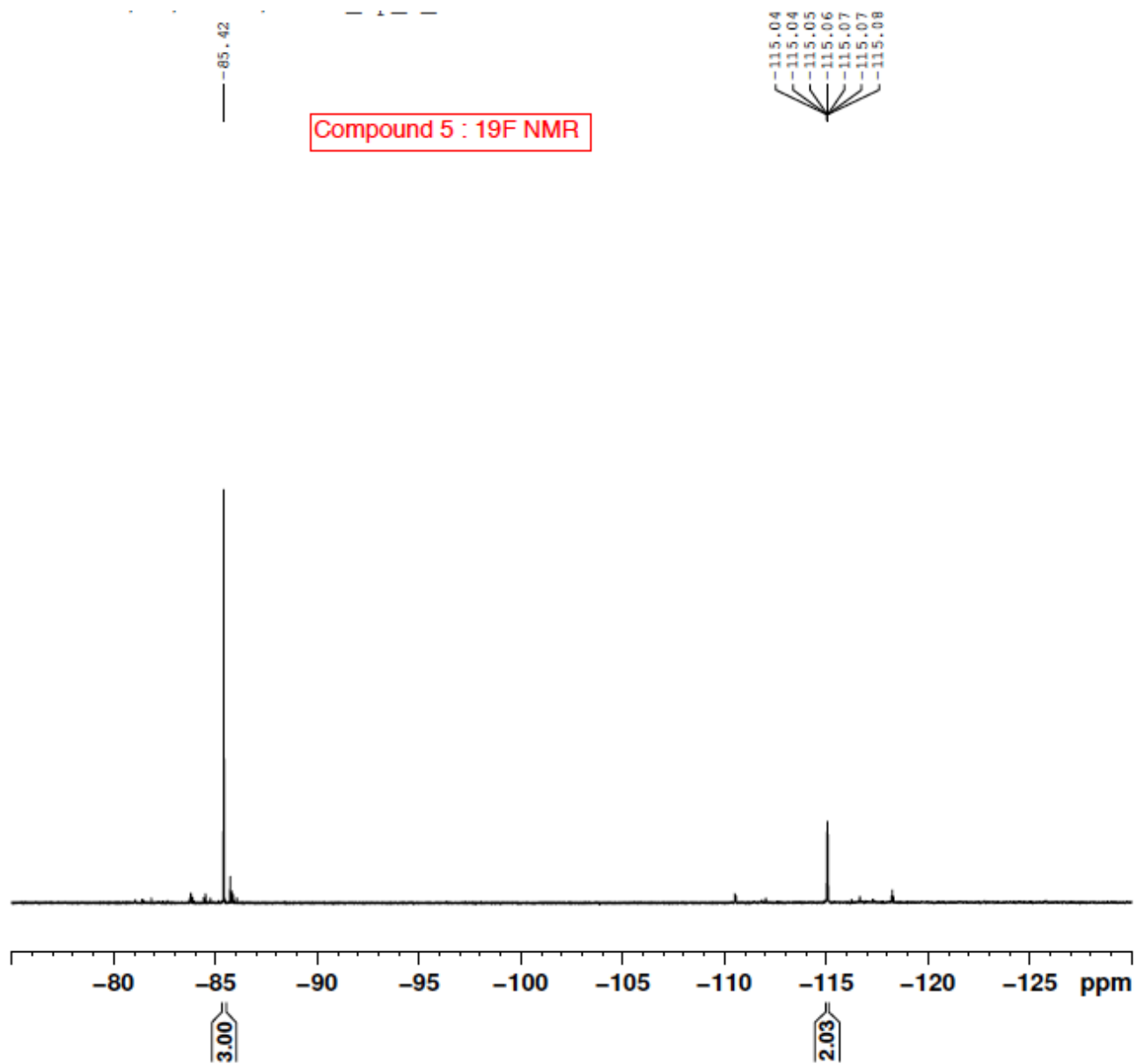
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SOLVENT       CDC13
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FIDRES        0.573639 Hz
AQ            0.8716788 sec
RG            574.7
DW            6.650 usec
DE            6.50 usec
TE            294.7 K
D1            1.00000000 sec
ID0           1
  
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```

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SFO1          376.5548010 MHz
SI            65536
SF            376.5924600 MHz
WDW           EM
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LB            0.30 Hz
GB            0
PC            1.00
  
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^1H NMR, ^{19}F NMR and ^{13}C NMR of compound 5



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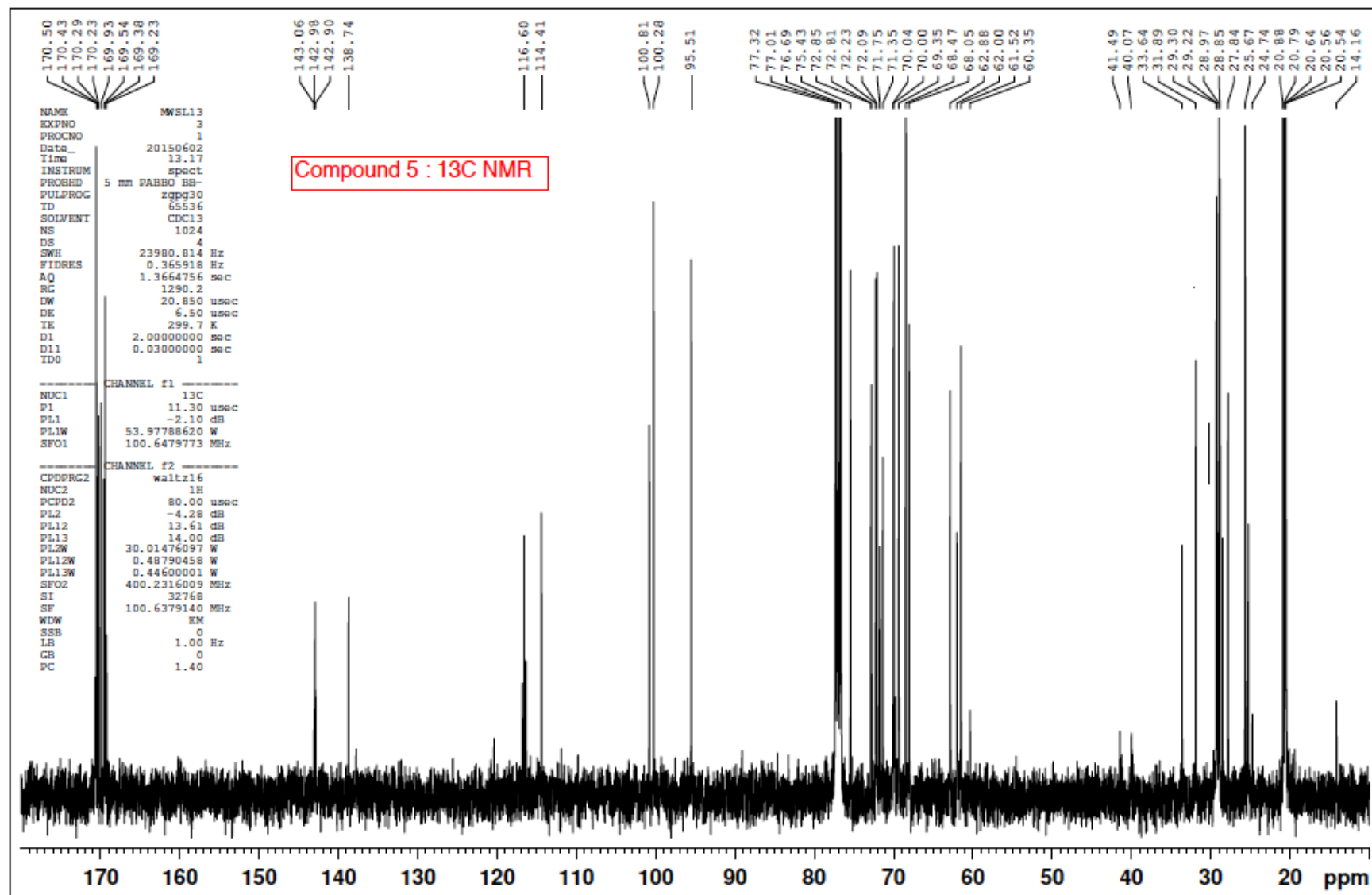
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ID           131072
SOLVENT      CDC13
NS           16
DS           4
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FIDRES       0.573639 Hz
AQ           0.8716788 sec
RG           574.7
DW           6.650 usec
DE           6.50 usec
TE           295.0 K
D1           1.00000000 sec
ID0          1

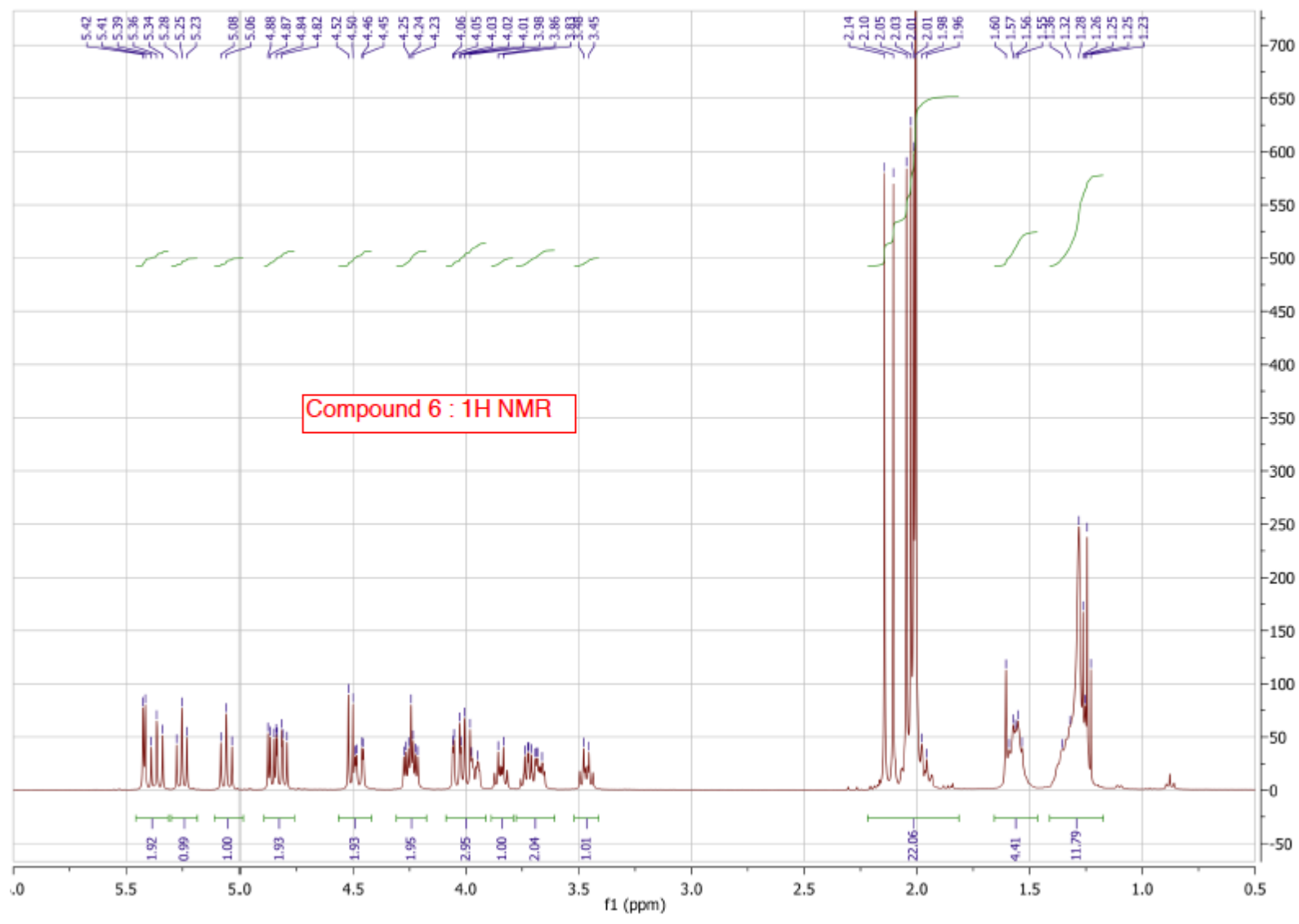
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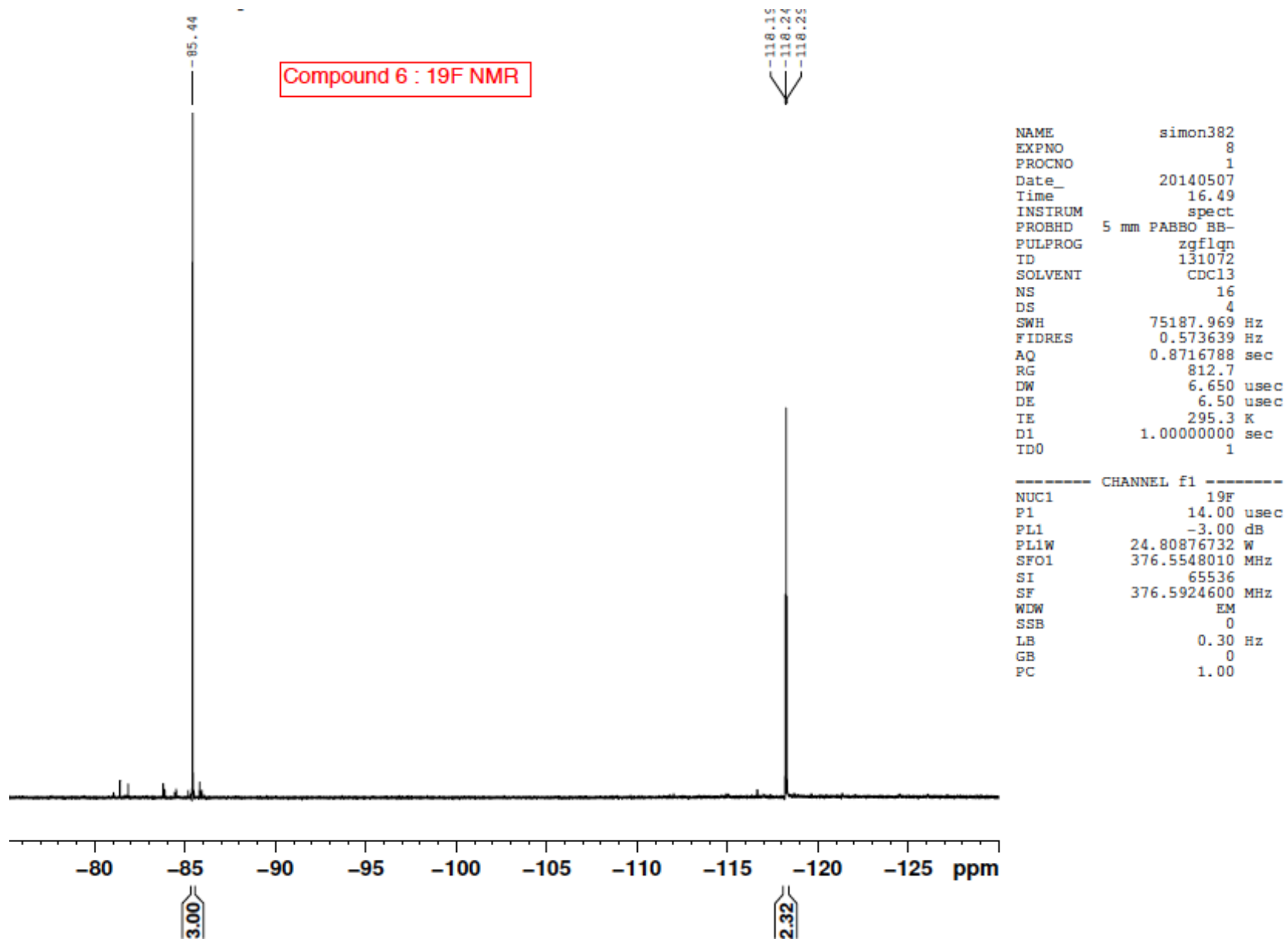
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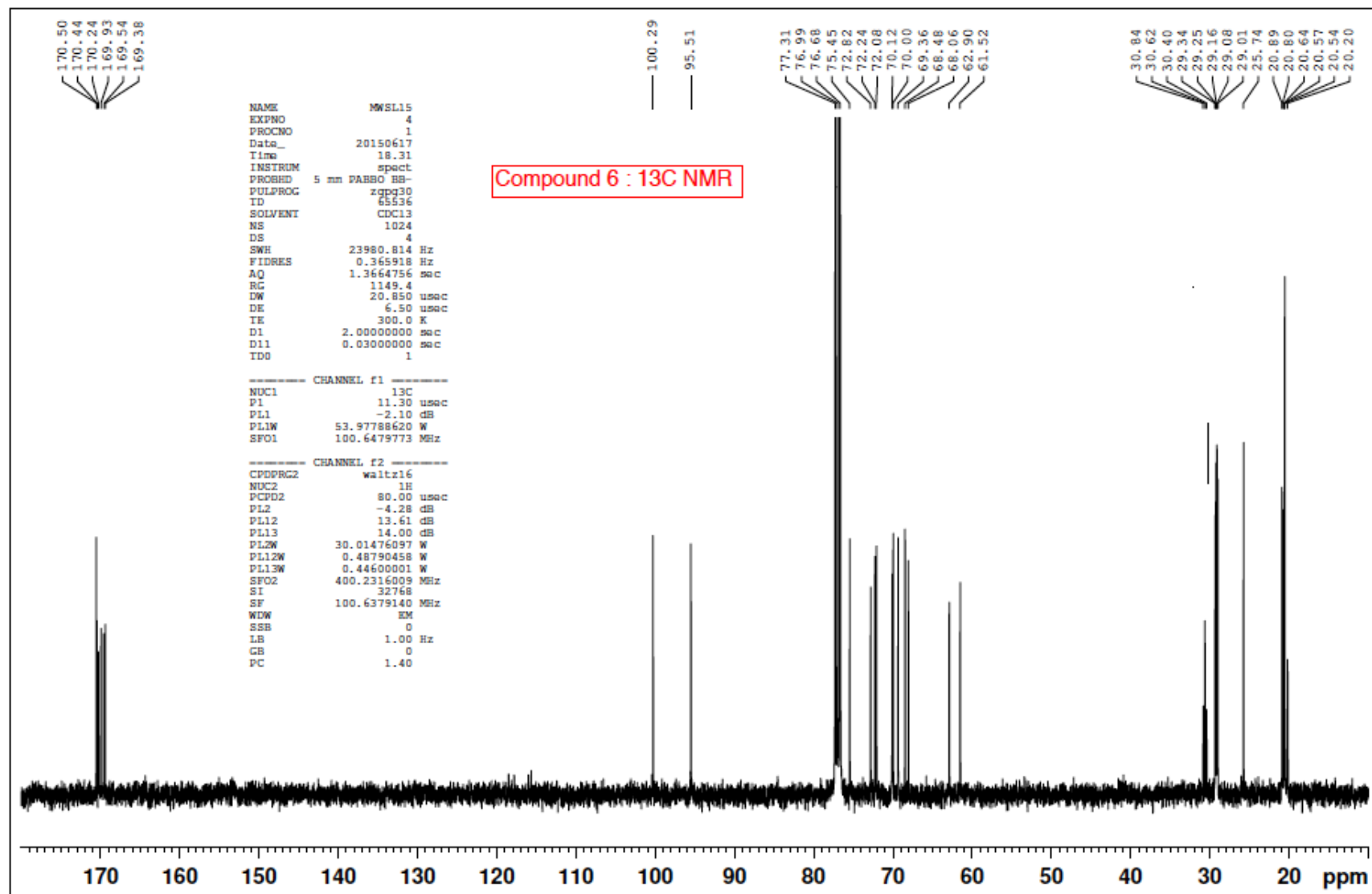
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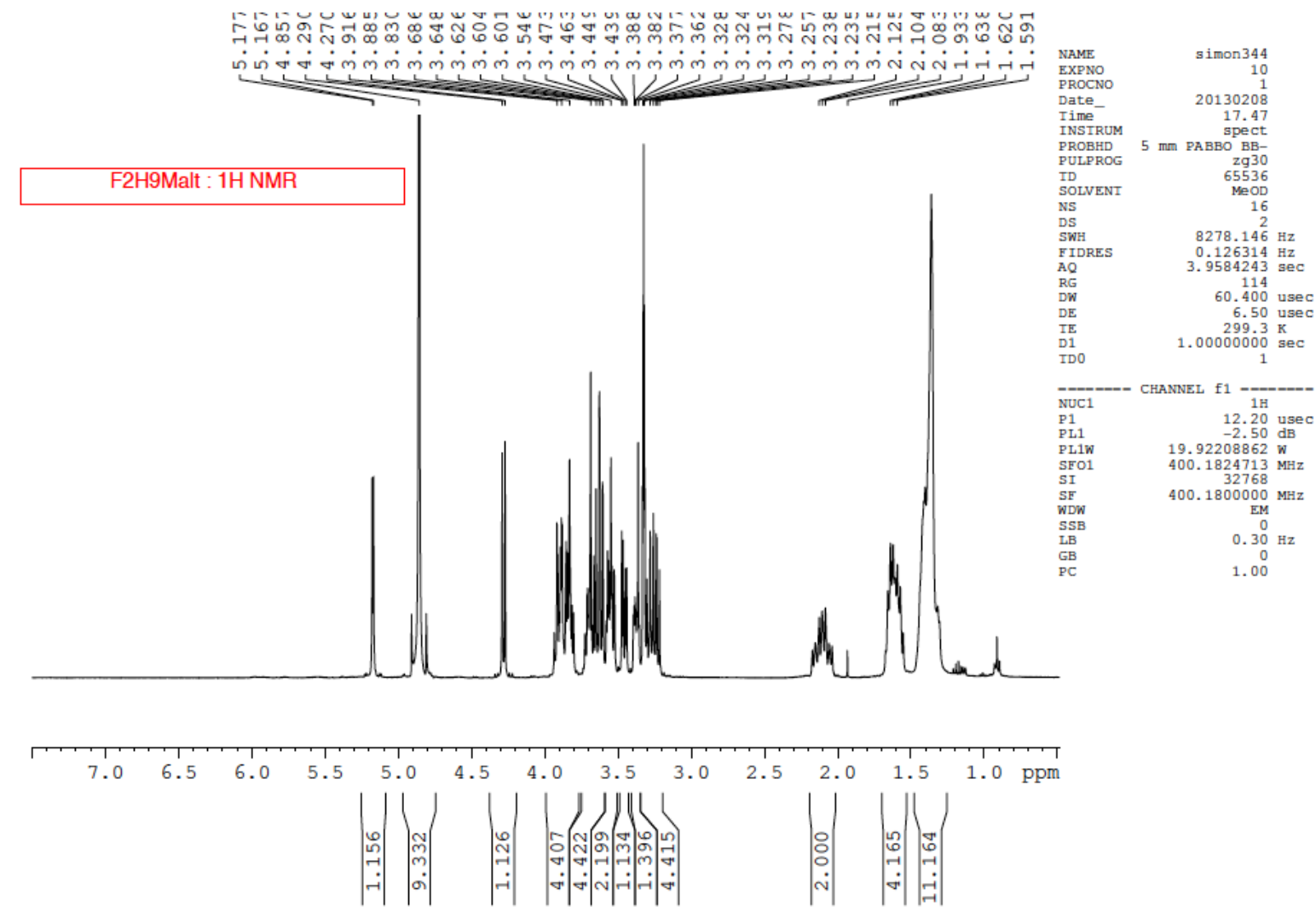
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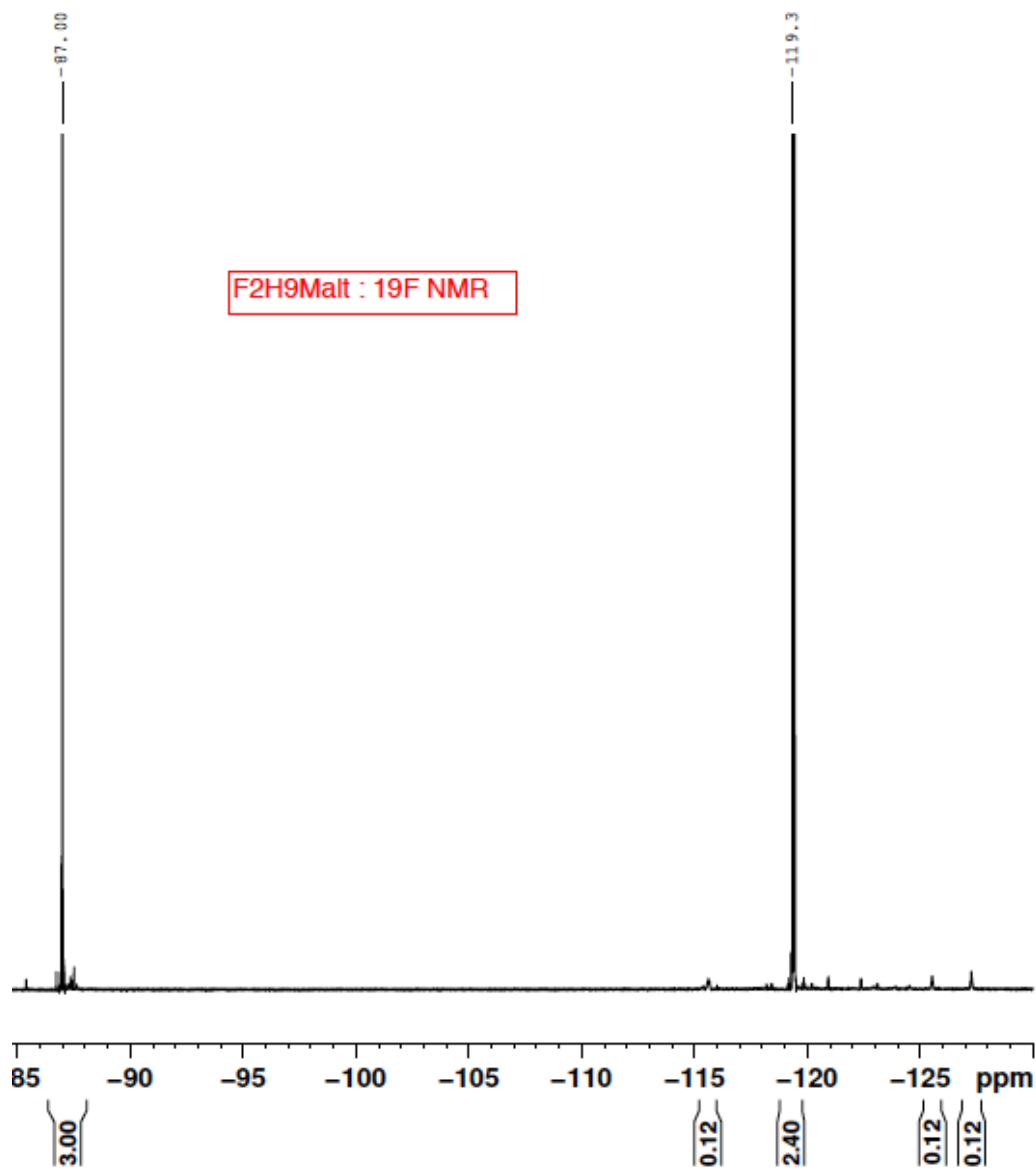


^1H NMR, ^{19}F NMR and ^{13}C NMR of compound 6





^1H NMR, ^{19}F NMR and ^{13}C NMR of F2H9Malt



```

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Time_         17.50
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SOLVENT       MeOD
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RG            645.1
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TE            299.3 K
D1            1.00000000 sec
ID0           1

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----- CHANNEL f1 -----
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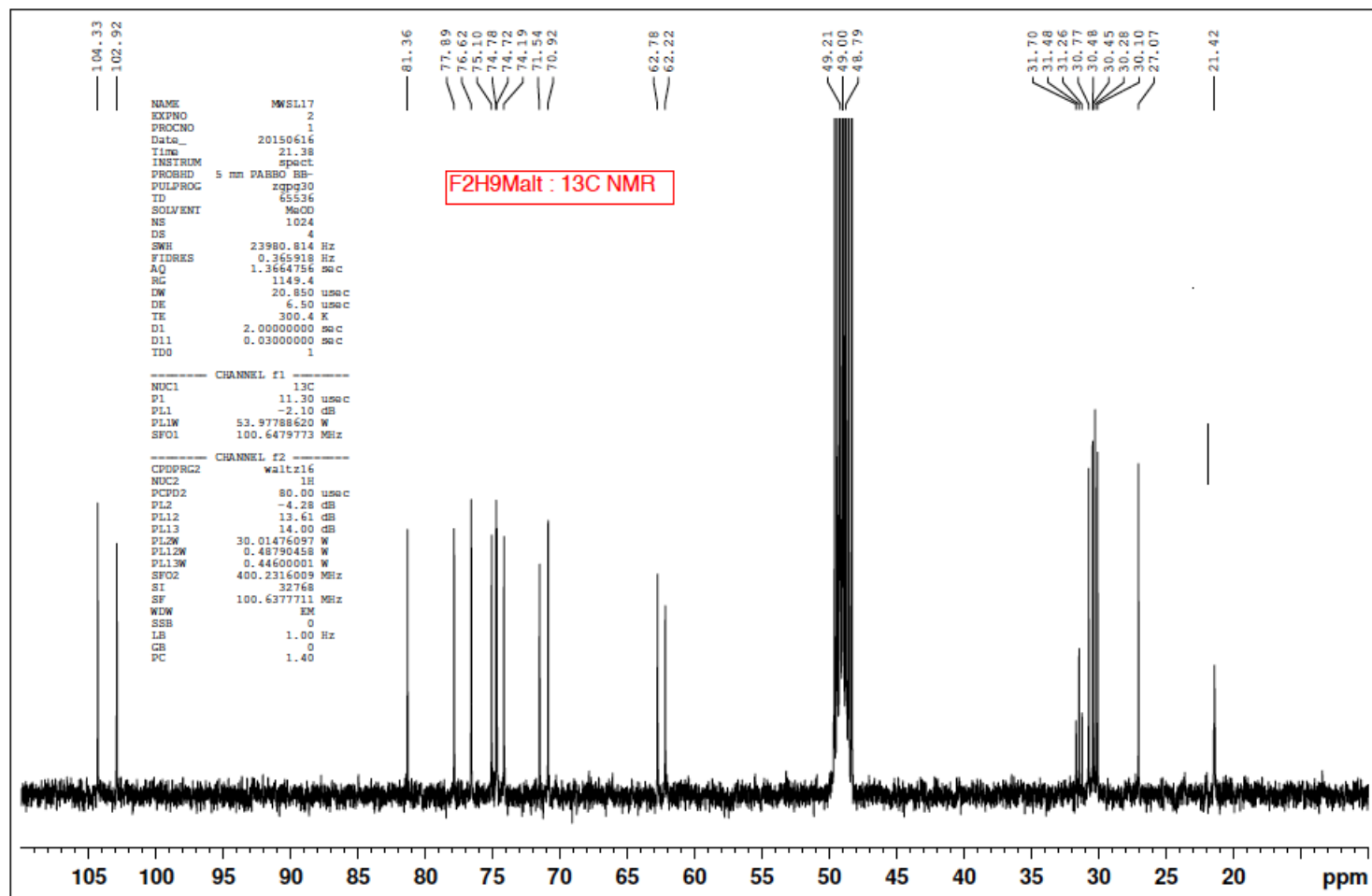


Figure S1. Superposition of selected experimental and fitted sedimentation velocity profiles acquired every ~ 20 min during 4 h at $130'000$ g (top) and residuals (bottom), for of F_2H_9M (A), F_4H_5M (B), and F_6H_2M (C) at 2 g/L in water at $20^\circ C$, using interference optics, after subtraction of the systematic noises and of the $c(s)$ results obtained at the indicated concentrations (D–F).

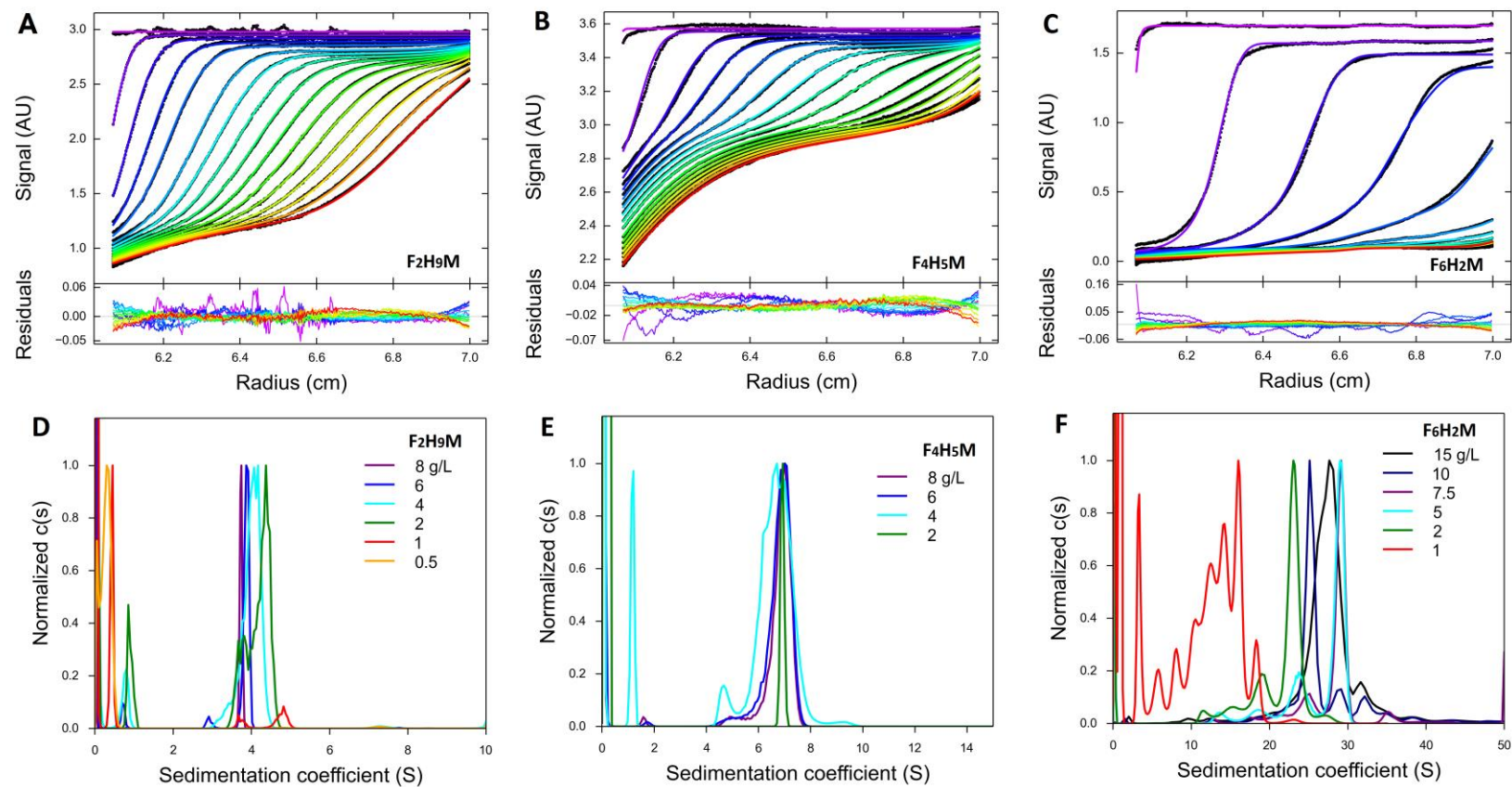


Figure S2. Autocorrelation functions $G(t)$ (A,D,G) and size distributions weighted by intensity (B,E,H) or volume (C,F,I) for $F_2H_9\beta M$, $F_4H_5\beta M$, and $F_6H_2\beta M$ in water.

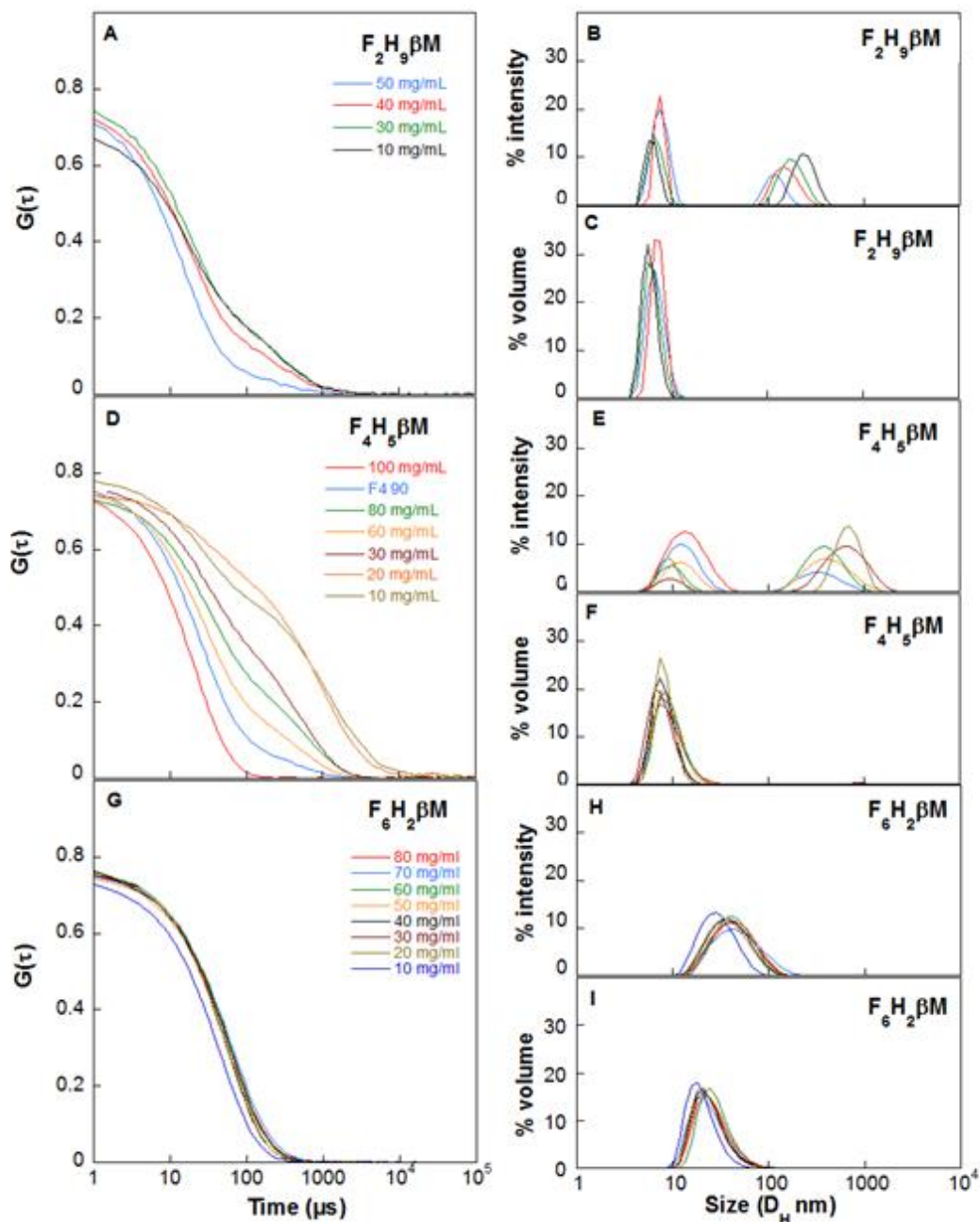


Figure S3. SAXS patterns (top) and pair distribution functions (bottom) for $F_2H_9\beta M$ (A,C), $F_4H_5\beta M$ (B,E), and $F_6H_2\beta M$ (C,F) in water.

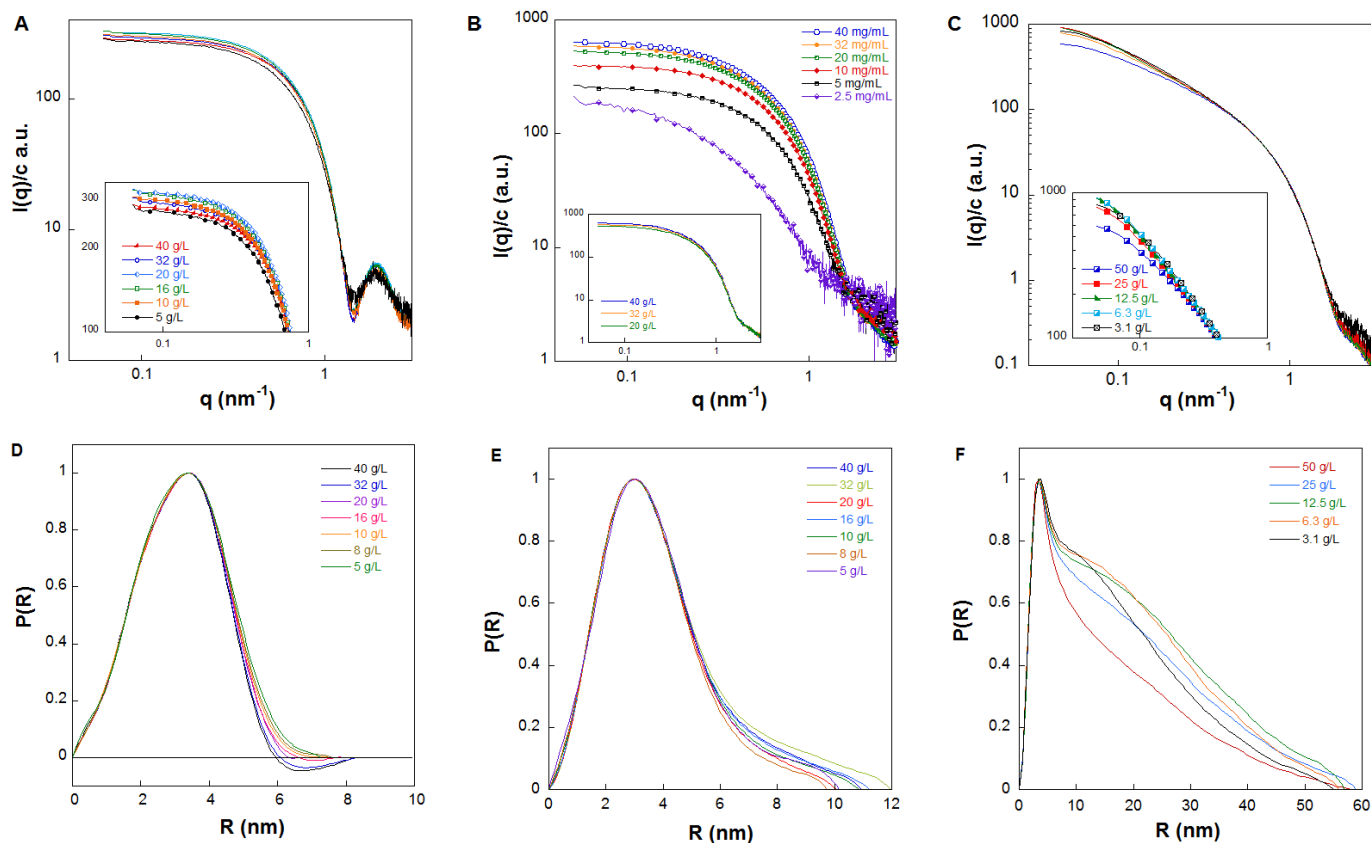


Figure S4. Forward intensity $I(0)$ as a function of total surfactant concentration for $F_2H_9\beta M$, $F_4H_5\beta M$, and $F_6H_2\beta M$ for CMC determination.

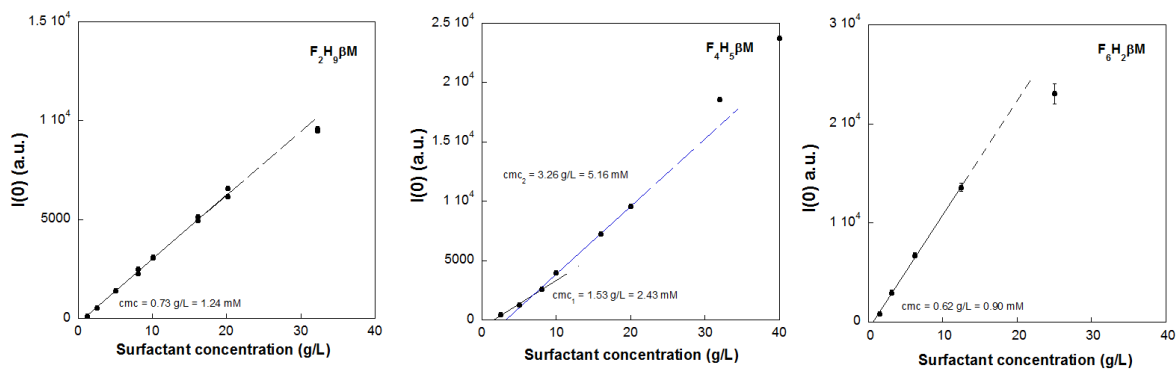


Table S1. Surfactant properties.

| Surfactant (abbreviation) | H ₁₂ βM | F ₂ H ₉ βM | F ₄ H ₅ βM | F ₆ H ₂ βM |
|---|---|--|--|---|
| Formula | C ₂₄ H ₄₆ O ₁₁ | C ₂₃ H ₃₉ F ₅ O ₁₁ | C ₂₁ H ₃₁ F ₉ O ₁₁ | C ₂₀ H ₂₅ F ₁₃ O ₁₁ |
| Formula molar mass (g/mol) | 510.6 | 586.5 | 630.5 | 688.4 |
| Head formula | C ₁₂ H ₂₁ O ₁₁ | C ₁₂ H ₂₁ O ₁₁ | C ₁₂ H ₂₁ O ₁₁ | C ₁₂ H ₂₁ O ₁₁ |
| Head molar mass (g/mol) | 341.3 | 341.3 | 341.3 | 341.3 |
| Chain formula | C ₁₂ H ₂₅ | C ₁₁ H ₁₈ F ₅ | C ₉ H ₁₀ F ₉ | C ₈ H ₄ F ₁₃ |
| Chain molar mass (g/mol) | 169.3 | 245.2 | 289.2 | 347.1 |
| CMC from TS (mM / gL ⁻¹) | 0.17 / 0.087 | 1.14 / 0.67 | 2.16 / 1.36 | 0.71 / 0.49 |
| ∂n/∂c (mL/g) from AUC | | 0.107 | 0.078 | 0.071 |
| ε _{0.1%} L/(g cm) from AUC | | 0.012 | 0.07 | 0.009 |
| \bar{V} (cm ³ g ⁻¹) from density meas. | 0.819 | 0.749 | 0.632 | 0.578 |
| \bar{V} (cm ³ g ⁻¹) from composition | | 0.718 | 0.629 | 0.564 |
| V _{monomer} (Å ³) from density meas. | 694.4 | 729.4 | 661.5 | 660.6 |
| V _{head} (Å ³) from chem. formula | 348 | 348 | 348 | 348 |
| V _{chain} (Å ³) from chem. formula | 346.5 | 381.4 | 313.5 | 312.6 |
| Total number of electrons | 278 | 310 | 326 | 350 |
| Head number of electrons | 181 | 181 | 181 | 181 |
| Chain number of electrons | 97 | 129 | 145 | 169 |
| ρ ^{elect} (e ⁻ / Å ³) from density meas. | 0.400 | 0.425 | 0.493 | 0.529 |
| ρ ^{elect} (e ⁻ / Å ³) for polar head | 0.520 | 0.520 | 0.520 | 0.520 |
| ρ ^{elect} (e ⁻ / Å ³) for hydrophobic chain | 0.280 | 0.338 | 0.462 | 0.541 |
| ρ ^{elect} (e ⁻ / Å ³) for H ₂ O | 0.334 | 0.334 | 0.334 | 0.334 |
| <i>Data from SAXS</i> | | | | |
| M _w (kDa) | 65 | 38 | 32 | >500 |
| N _{agg} from I(0) | 125 | 65 | 50 | >700 |
| R _G (nm) | 3.2 | 2.5 | 3.2 | 15.8 |
| <i>Data from DLS</i> | | | | |
| D _{max} (nm) | 8.0 | 7.6 | 10.8 | 57 |
| R _H (nm) | 3.6 | 2.7 | 4.6 | 15.6 |
| <i>Data from SV*</i> | | | | |
| k' _s mL/g | | -17 +/- 2 | 0 +/- 3 | |
| S ₀ , S _{max} * S | | 4.20 +/- 0.02 | 6.83 +/- 0.1 | 0.28 +/- 0.1* |
| N _{agg} | | 87 | 154 | 1750* |
| f/f _{min} | | 1.1 | 1.6 | 2.4* |

*N_{agg} and f/f_{min} are derived from the related s and R_H from DLS.