SUPPLEMENTARY INFORMATION

New approach to synthesis of functional derivatives of *nido*-carborane: Alkylation of [9-MeS-*nido*-7,8-$C_2B_9H_{11}$]$^-$

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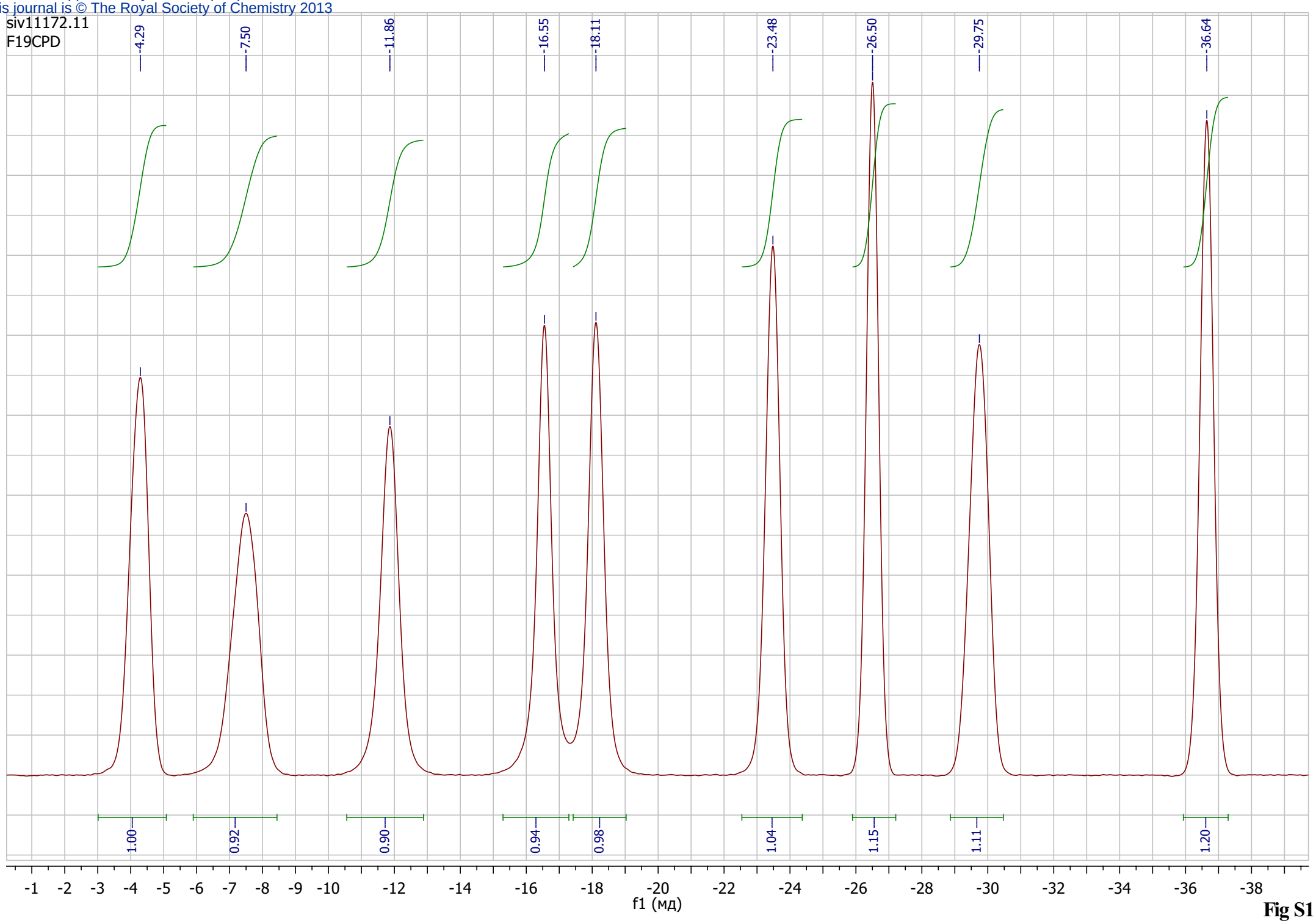

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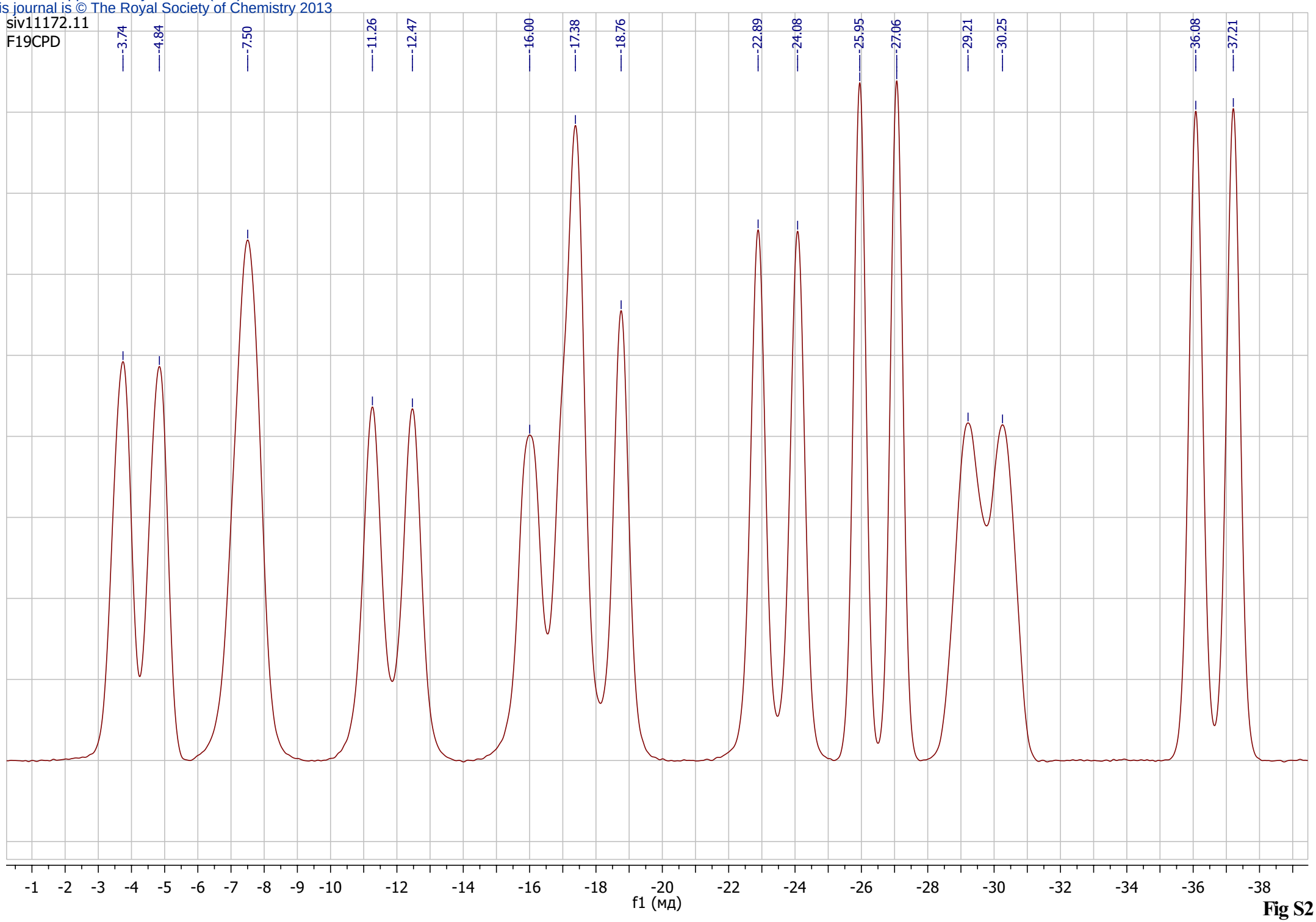

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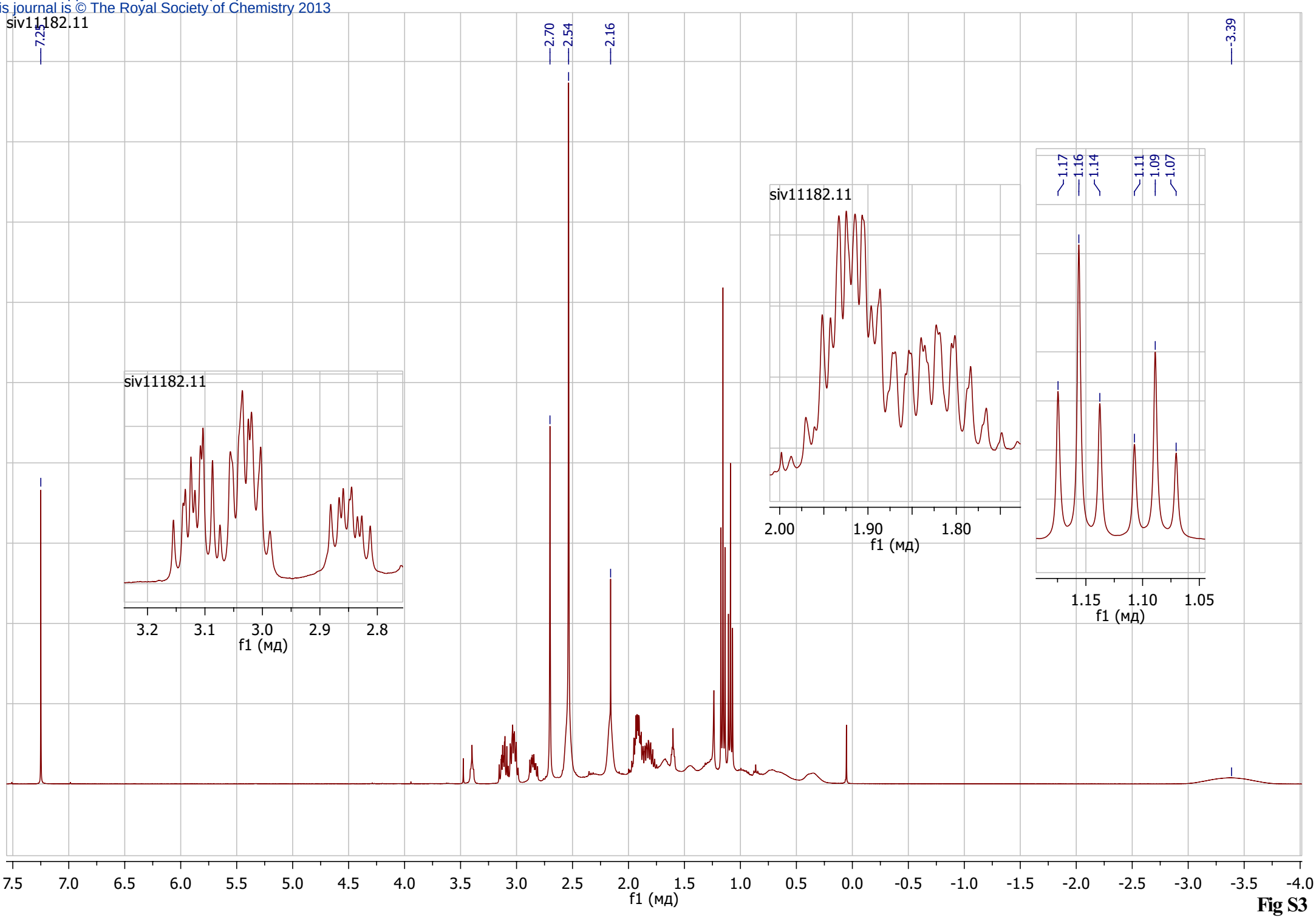

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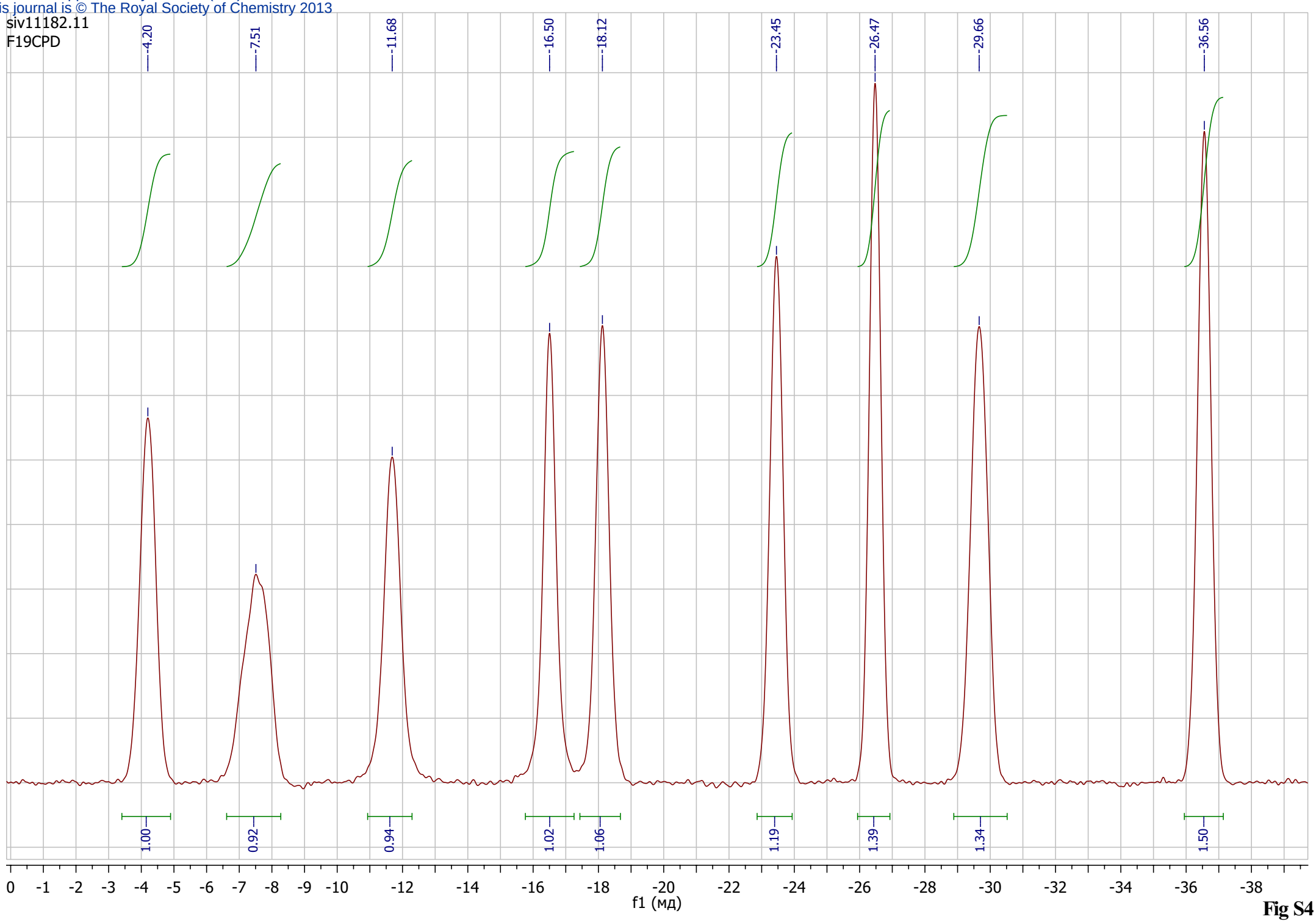

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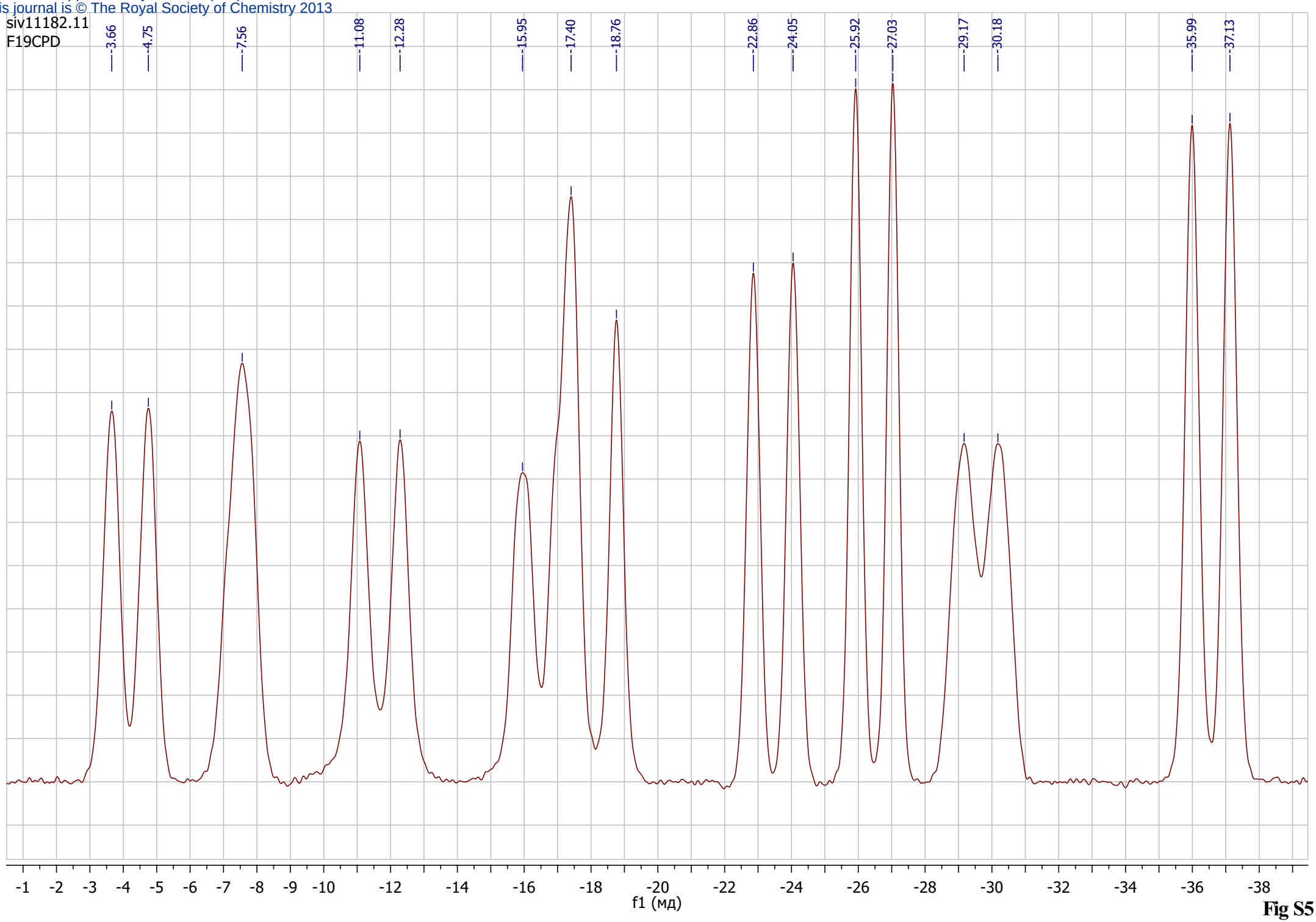

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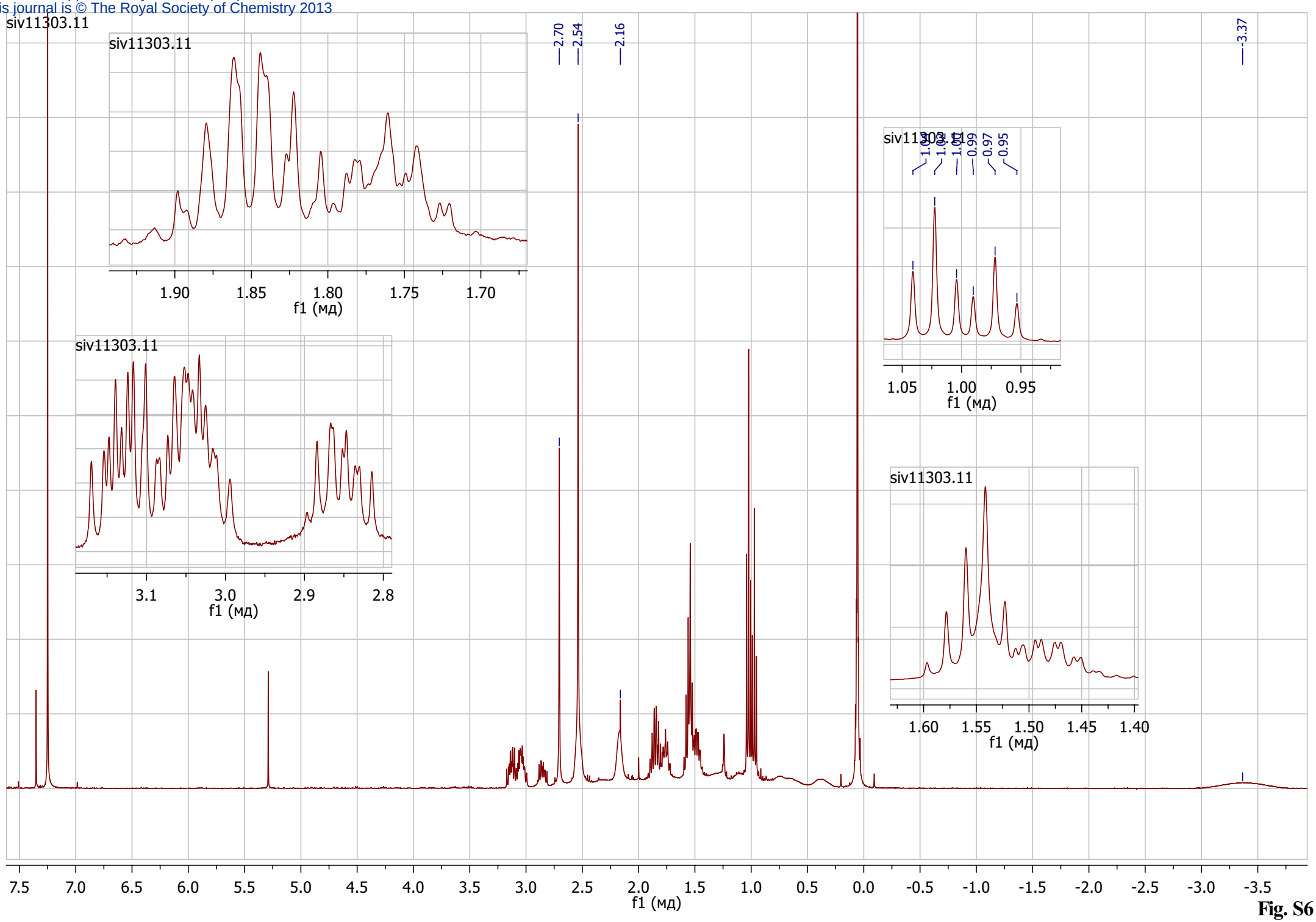

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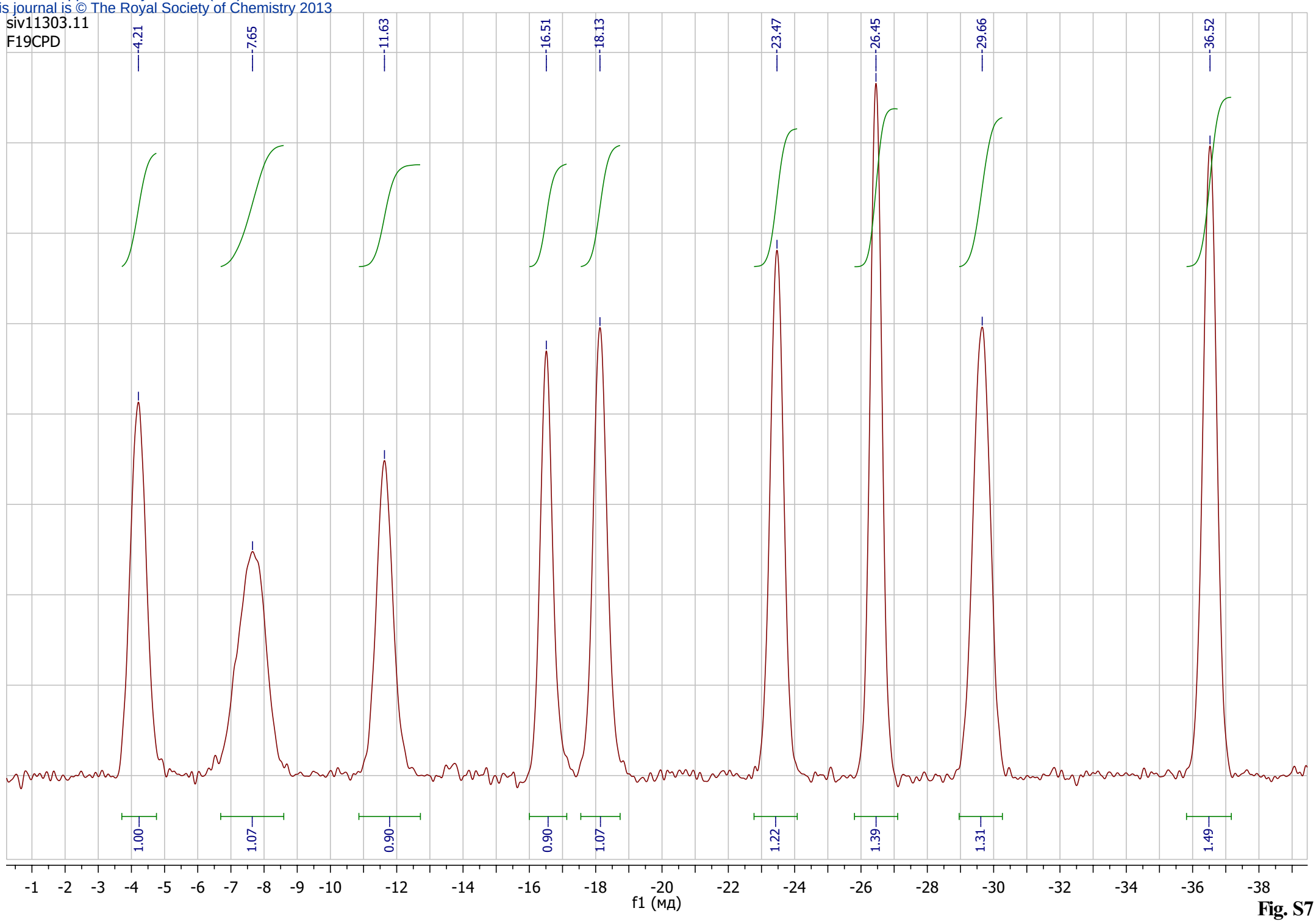

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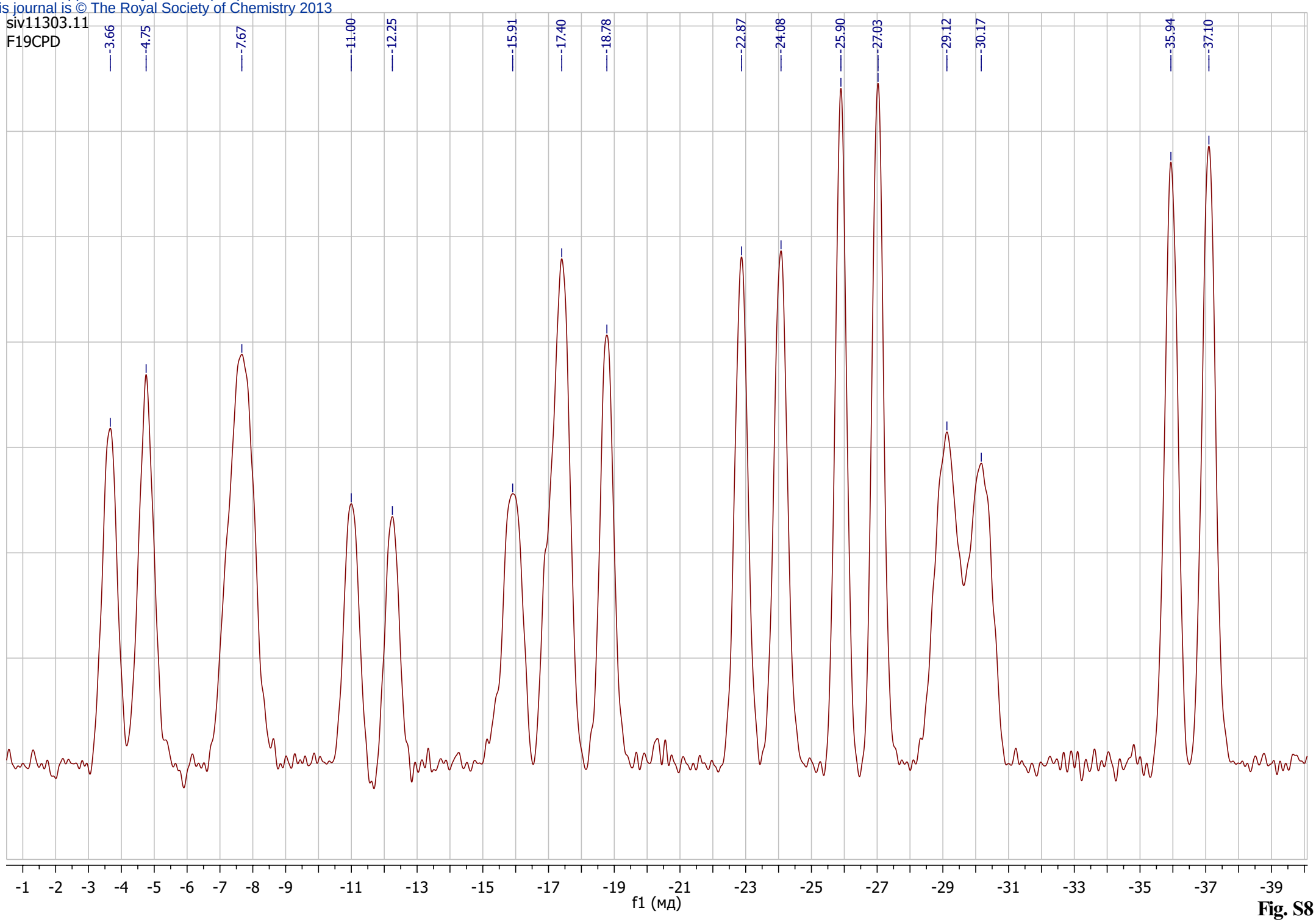

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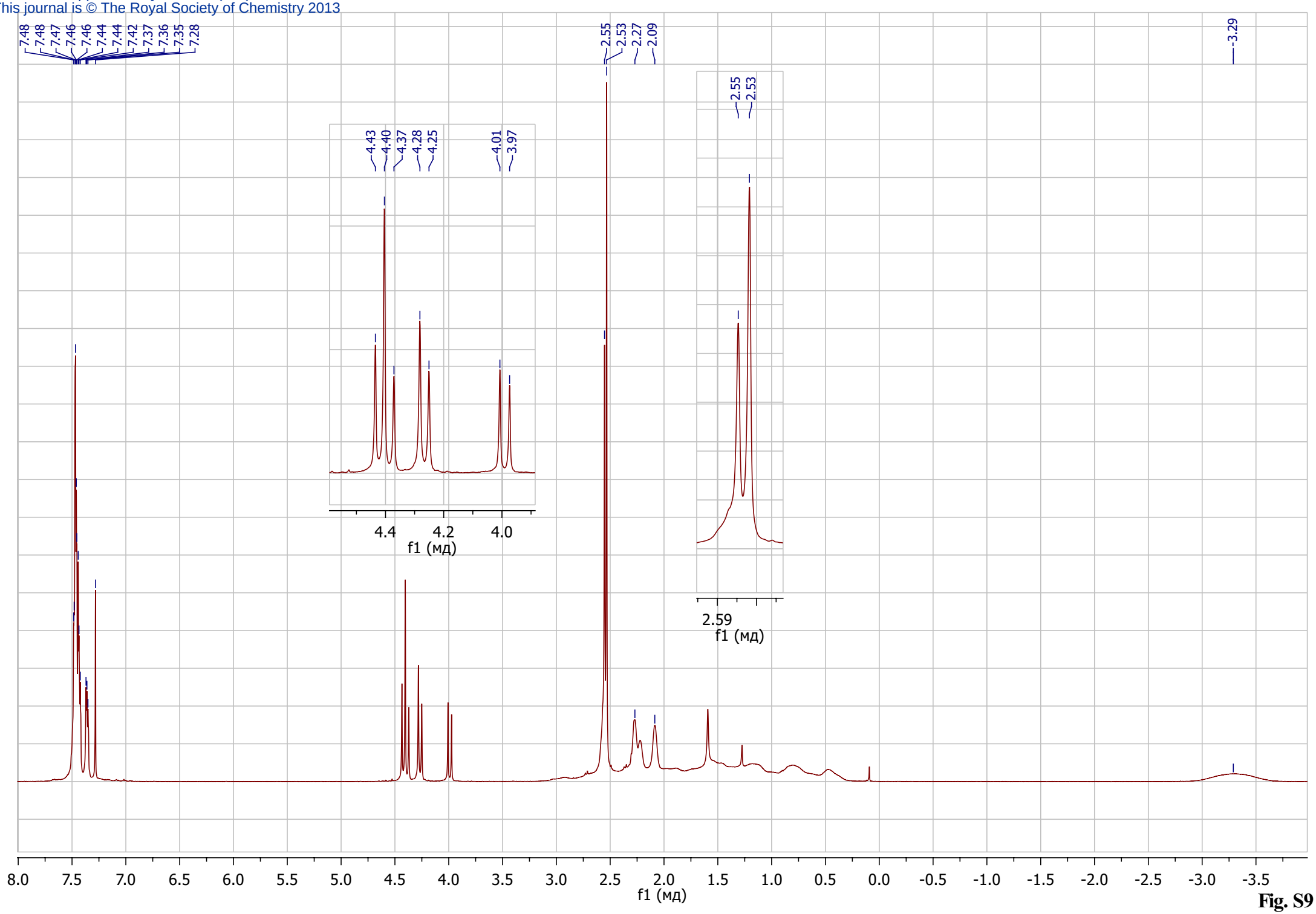

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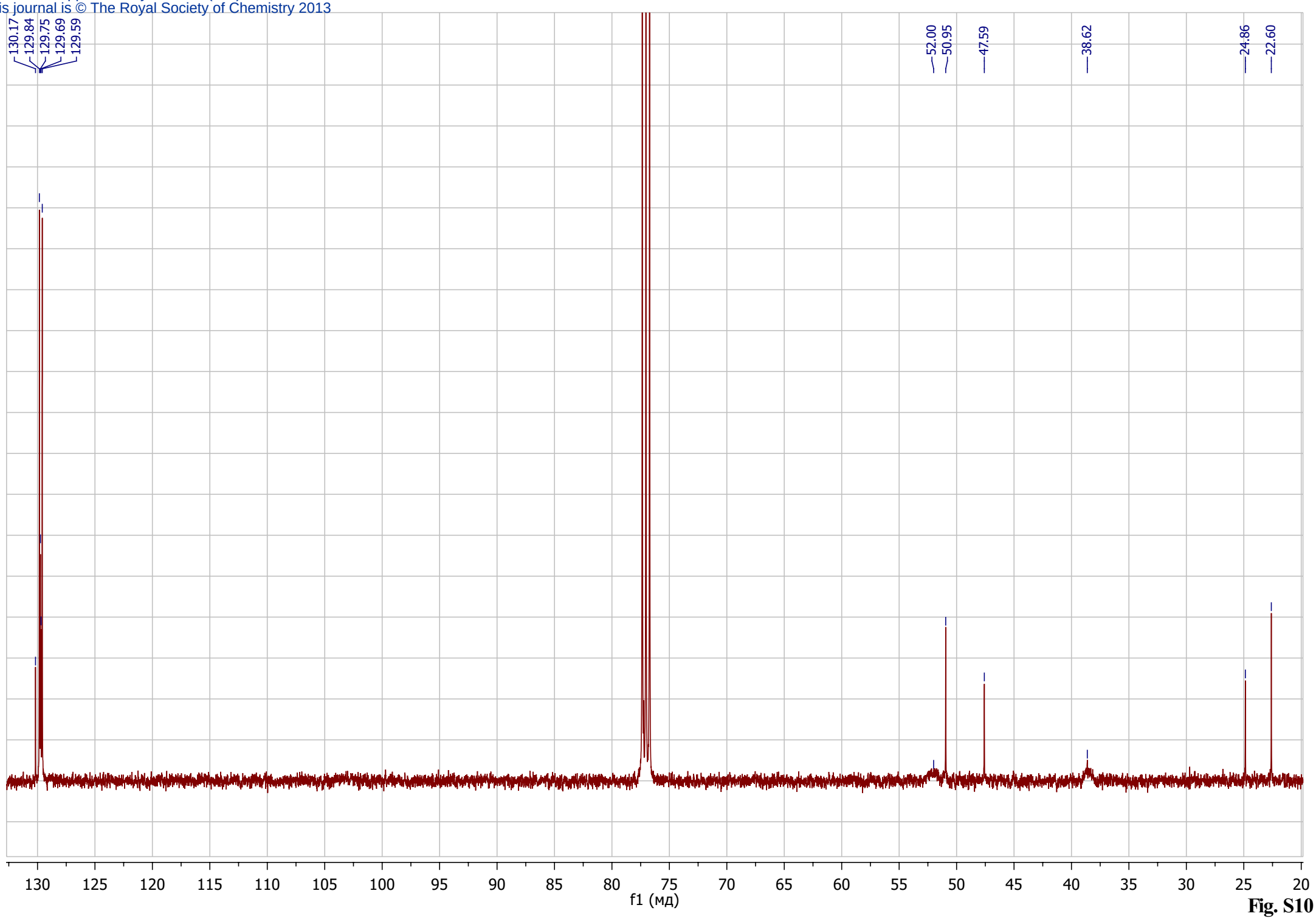

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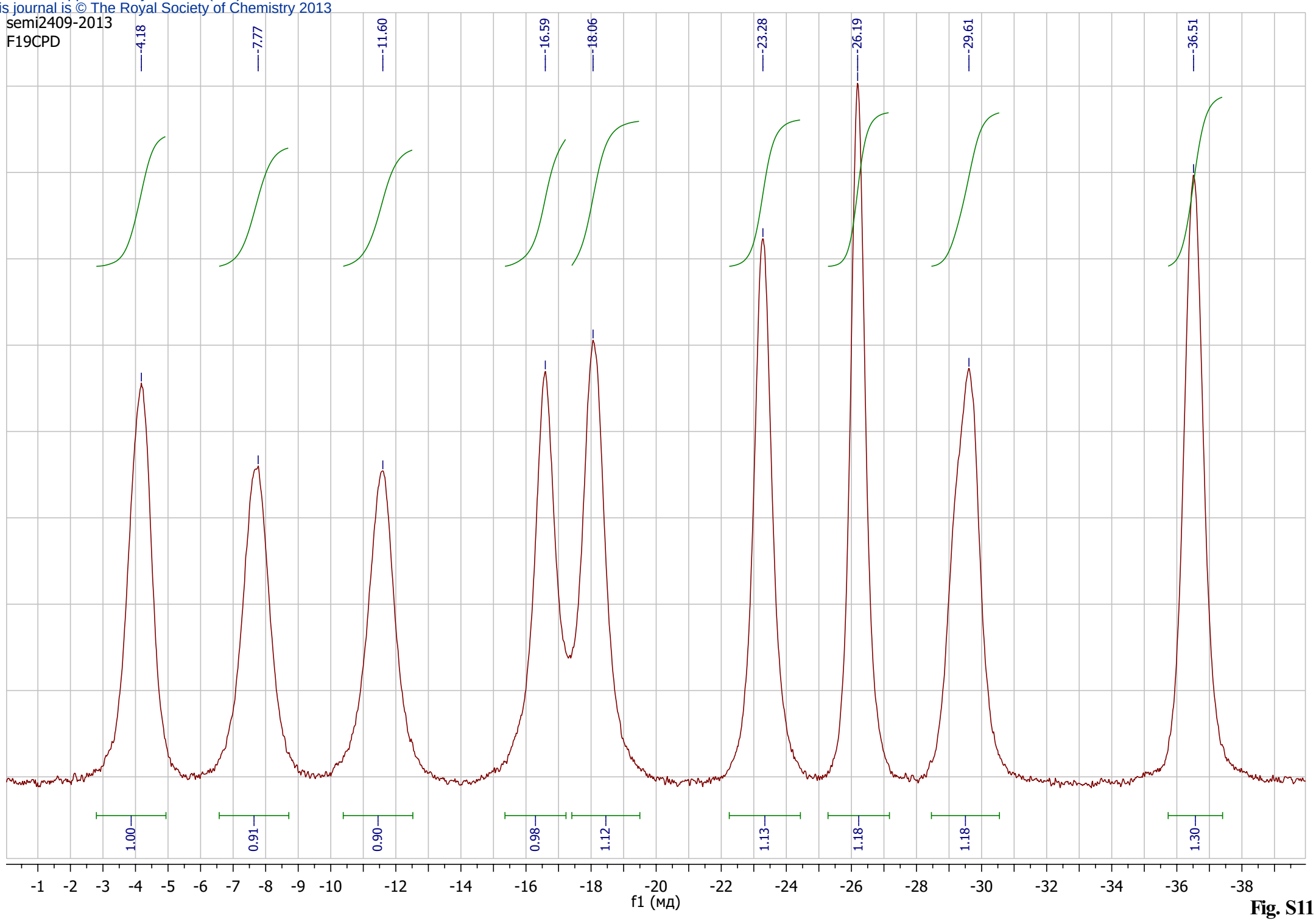

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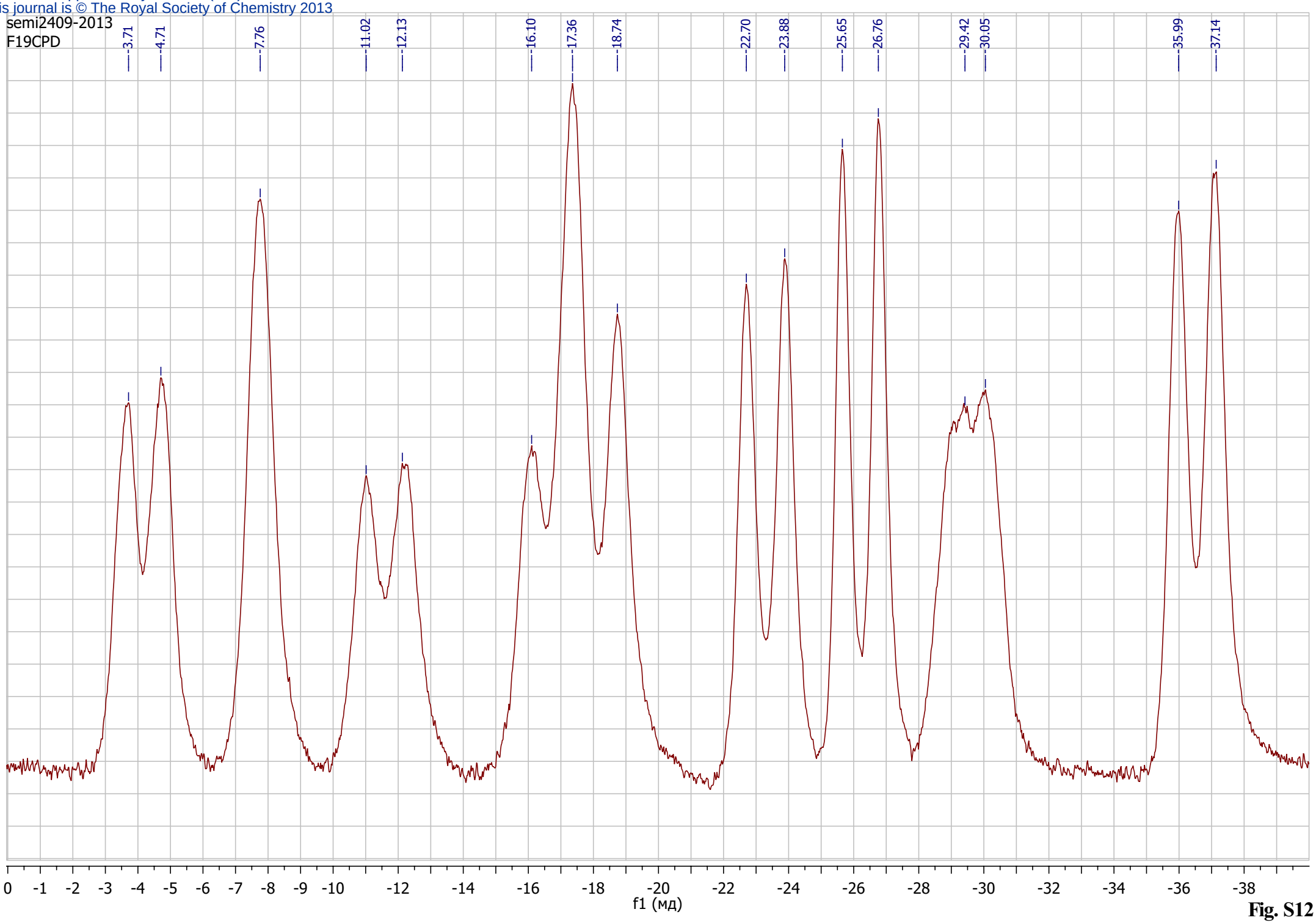

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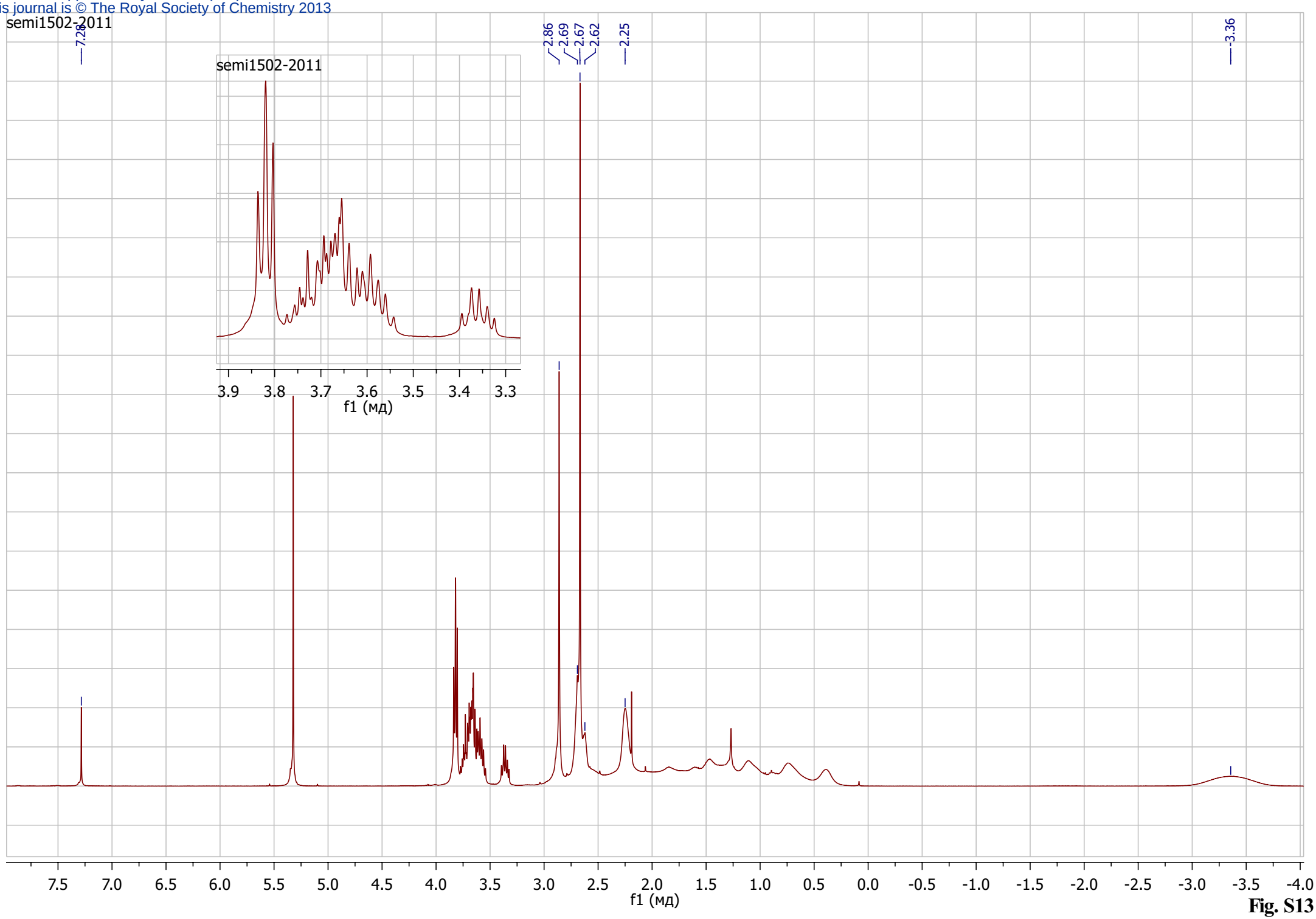

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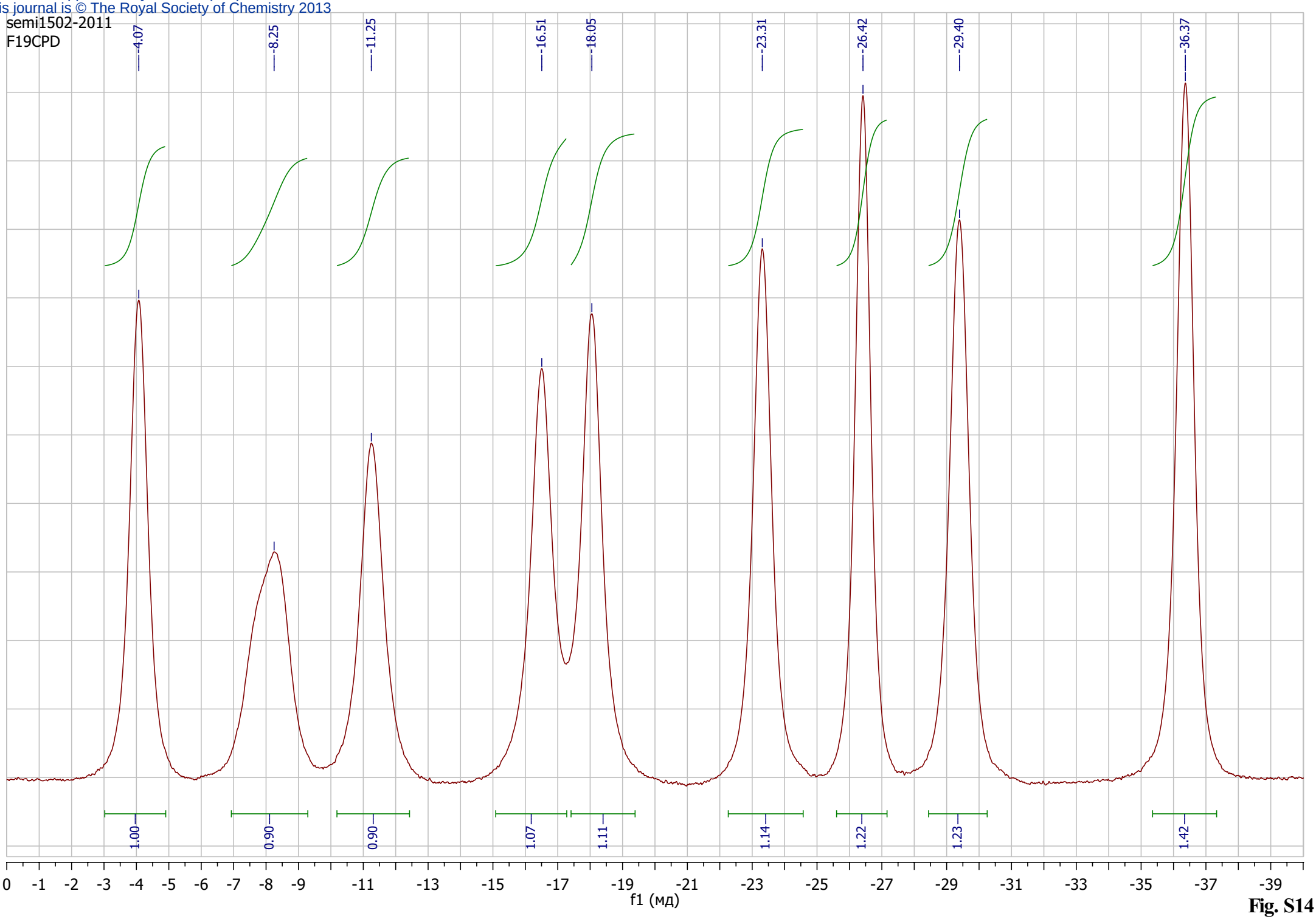

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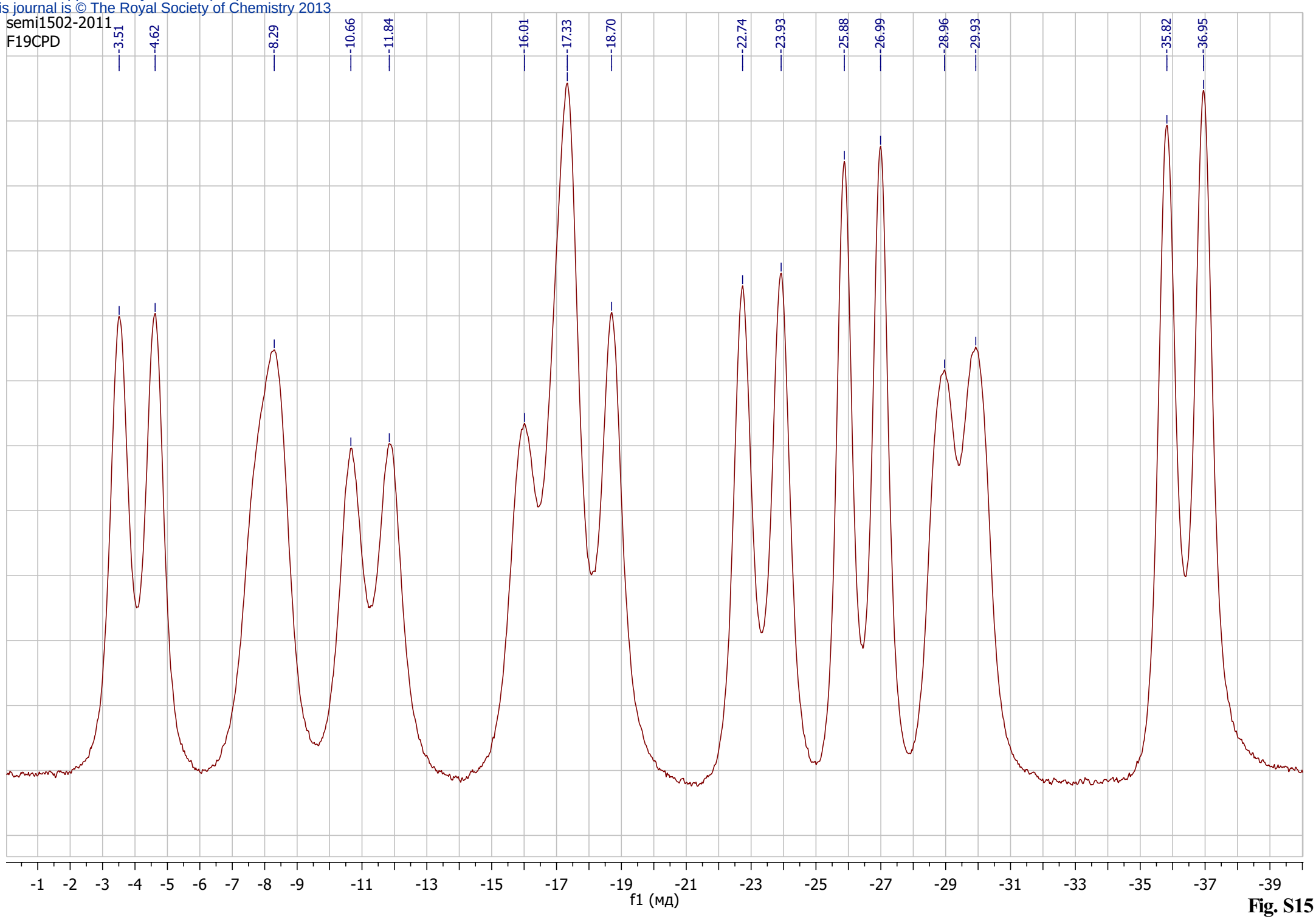

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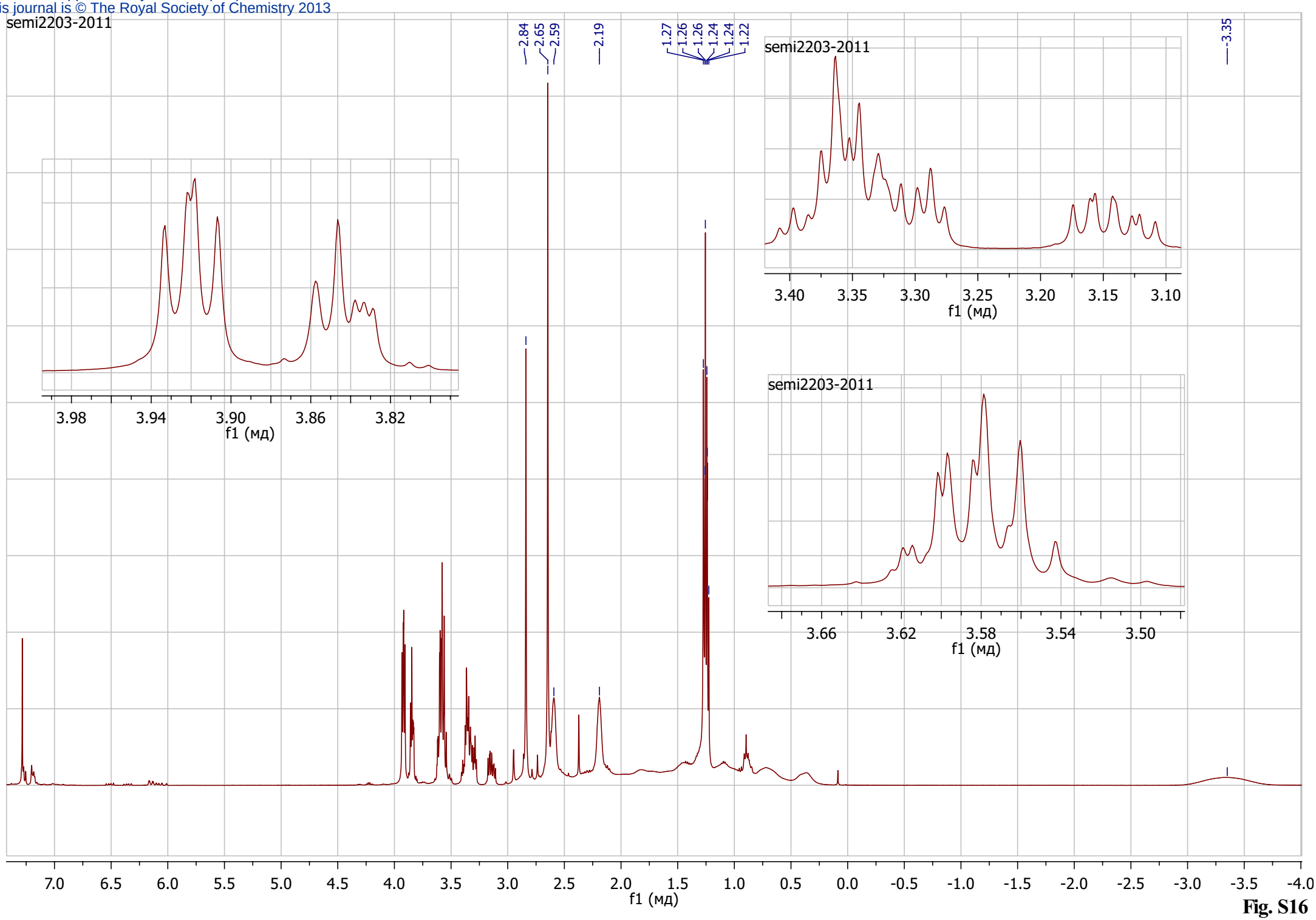

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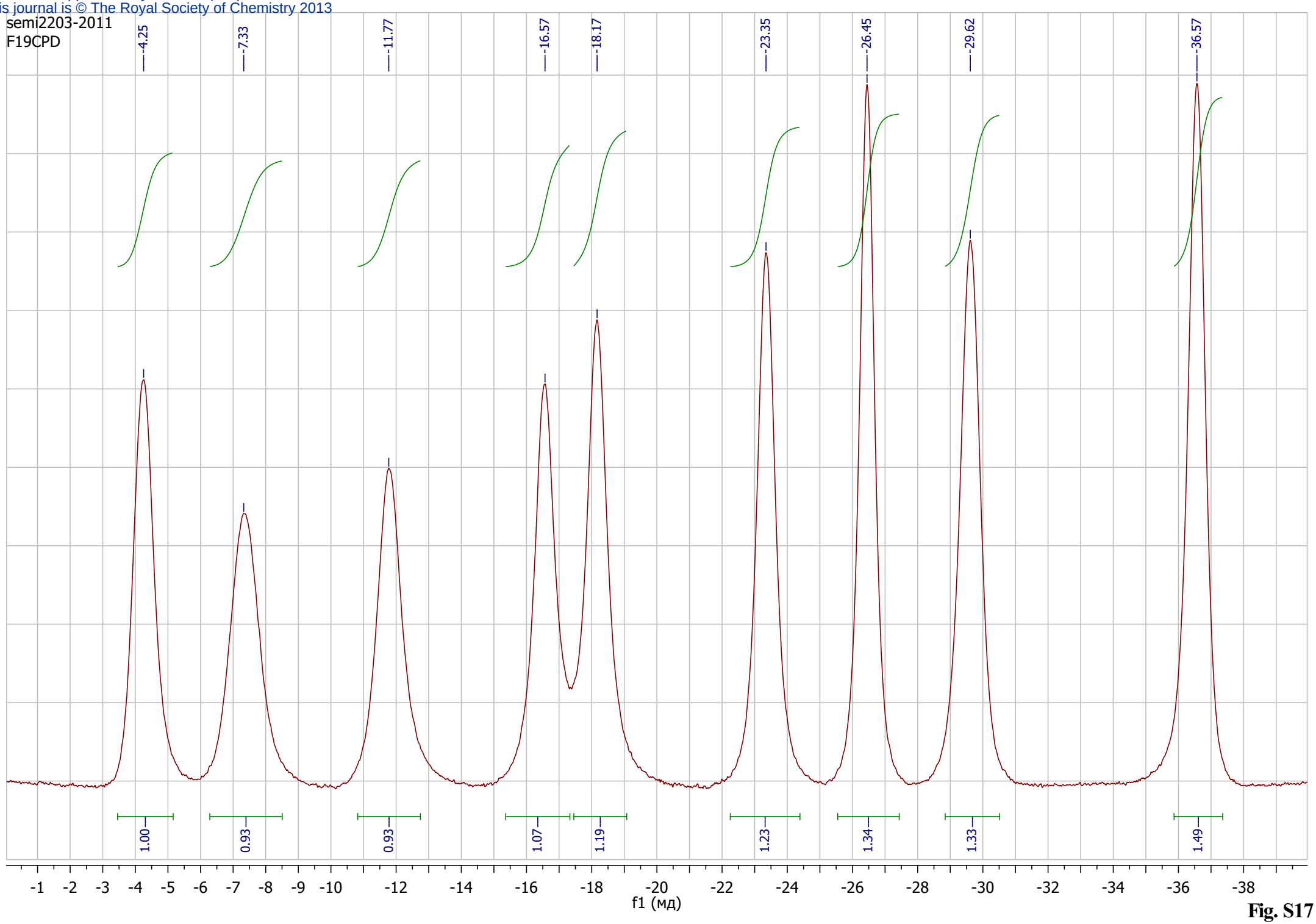

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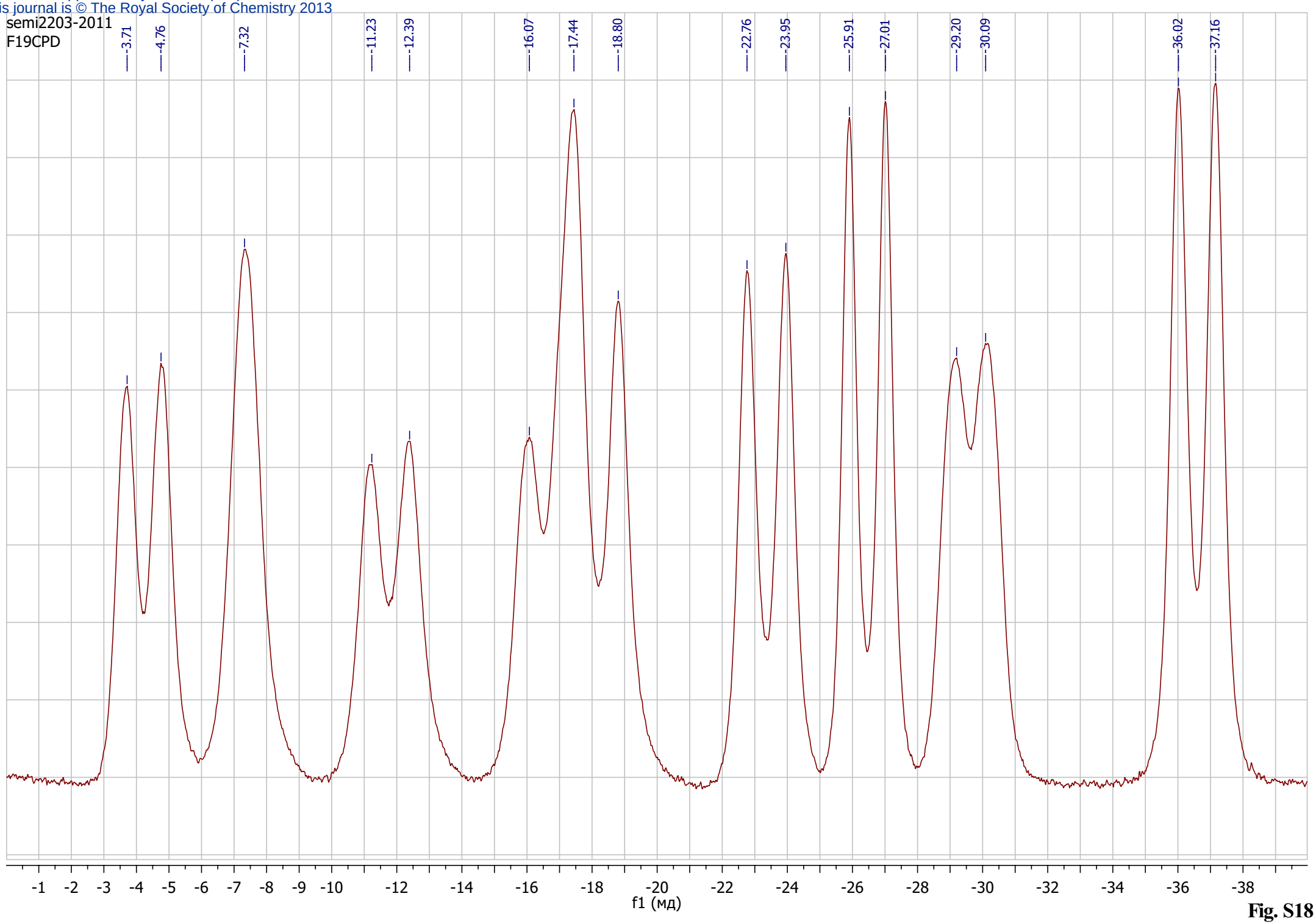

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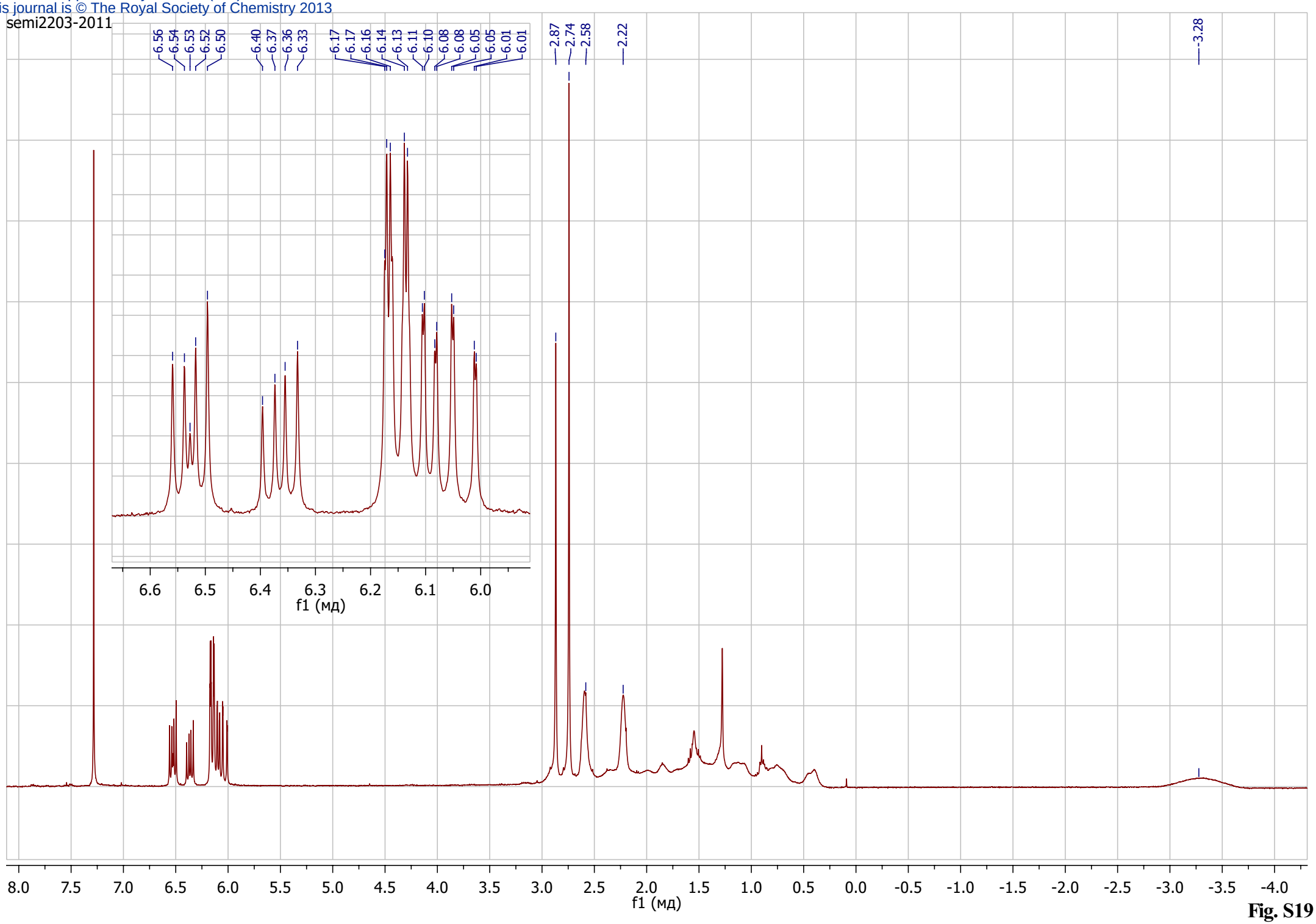

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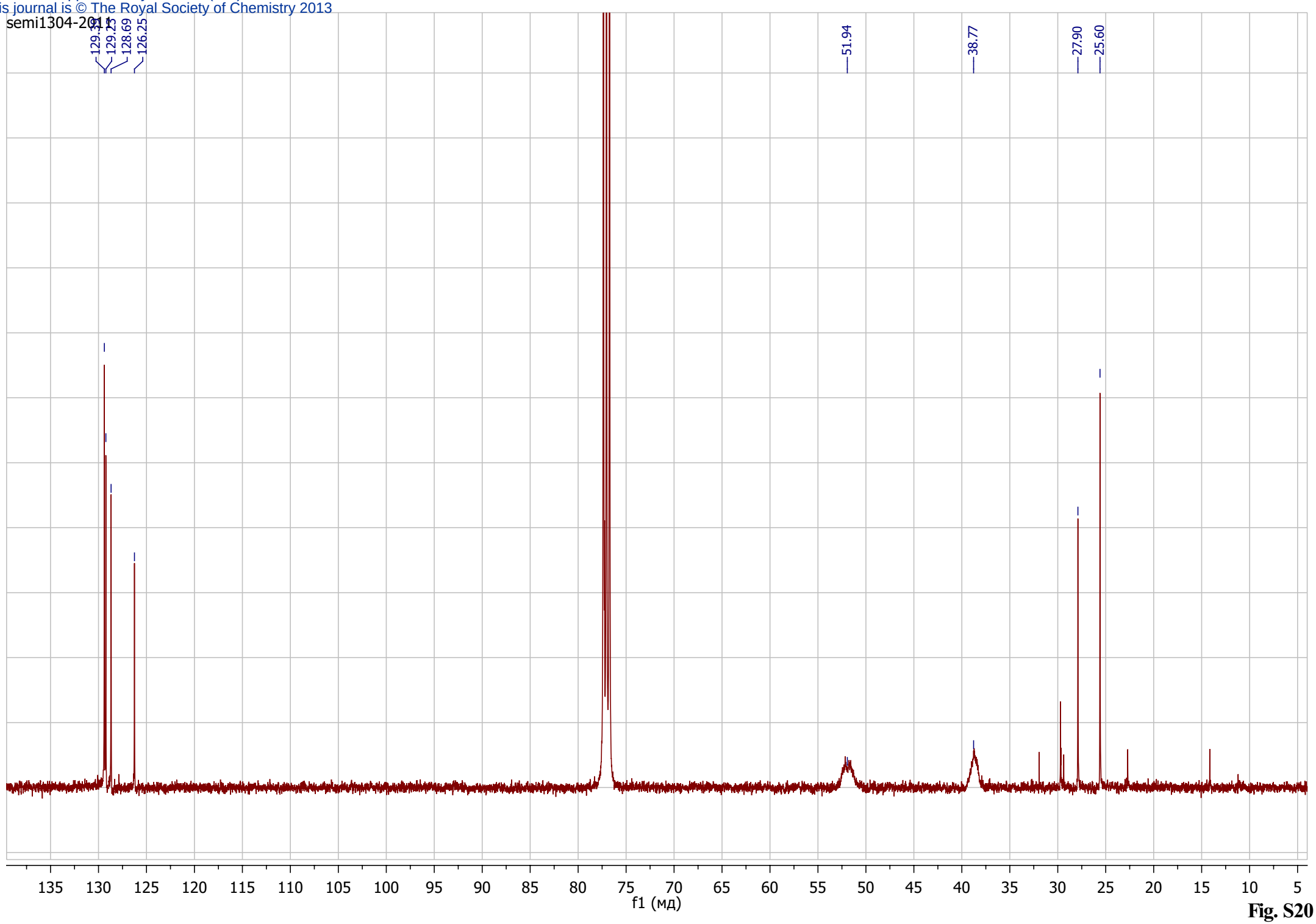

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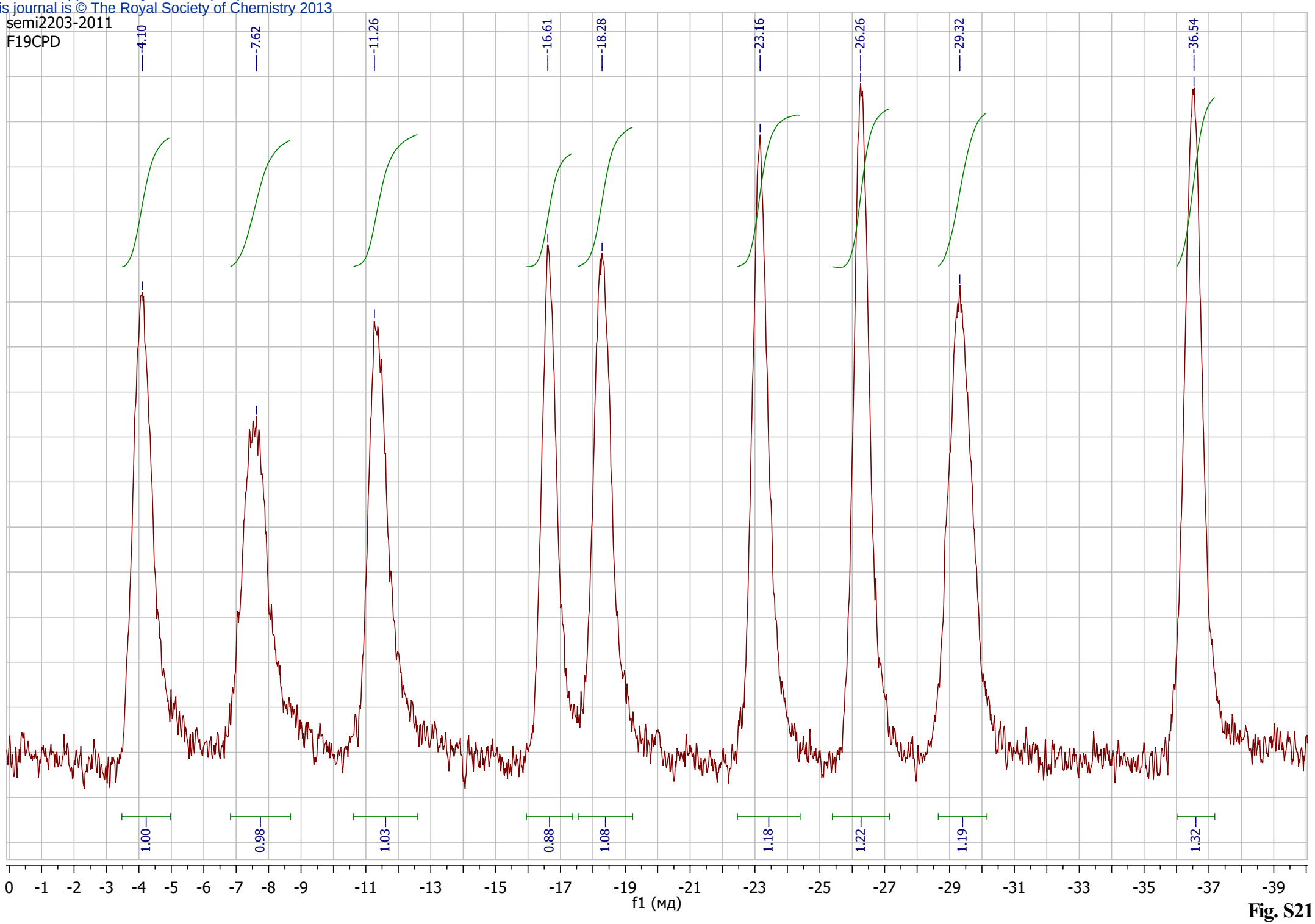

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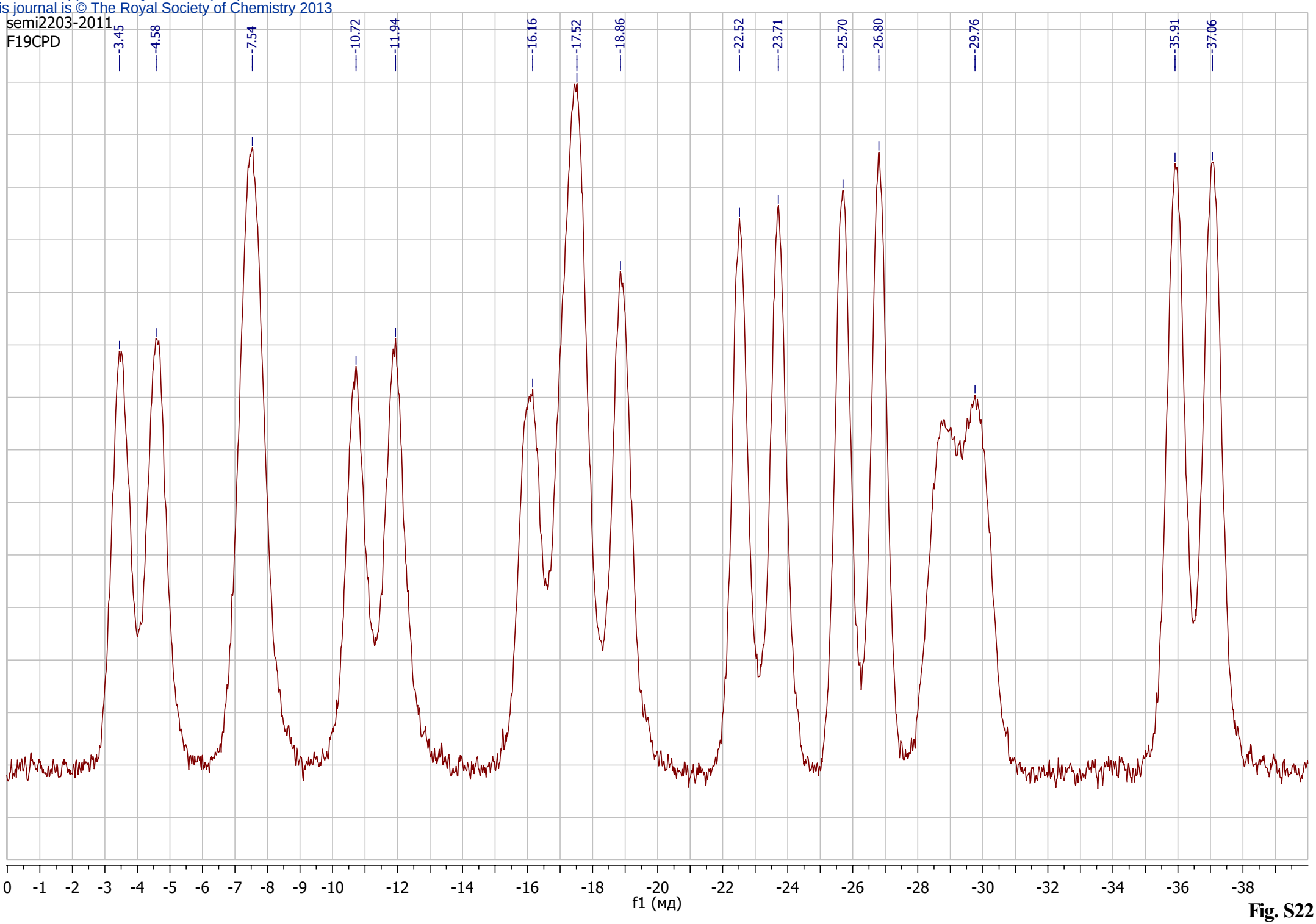

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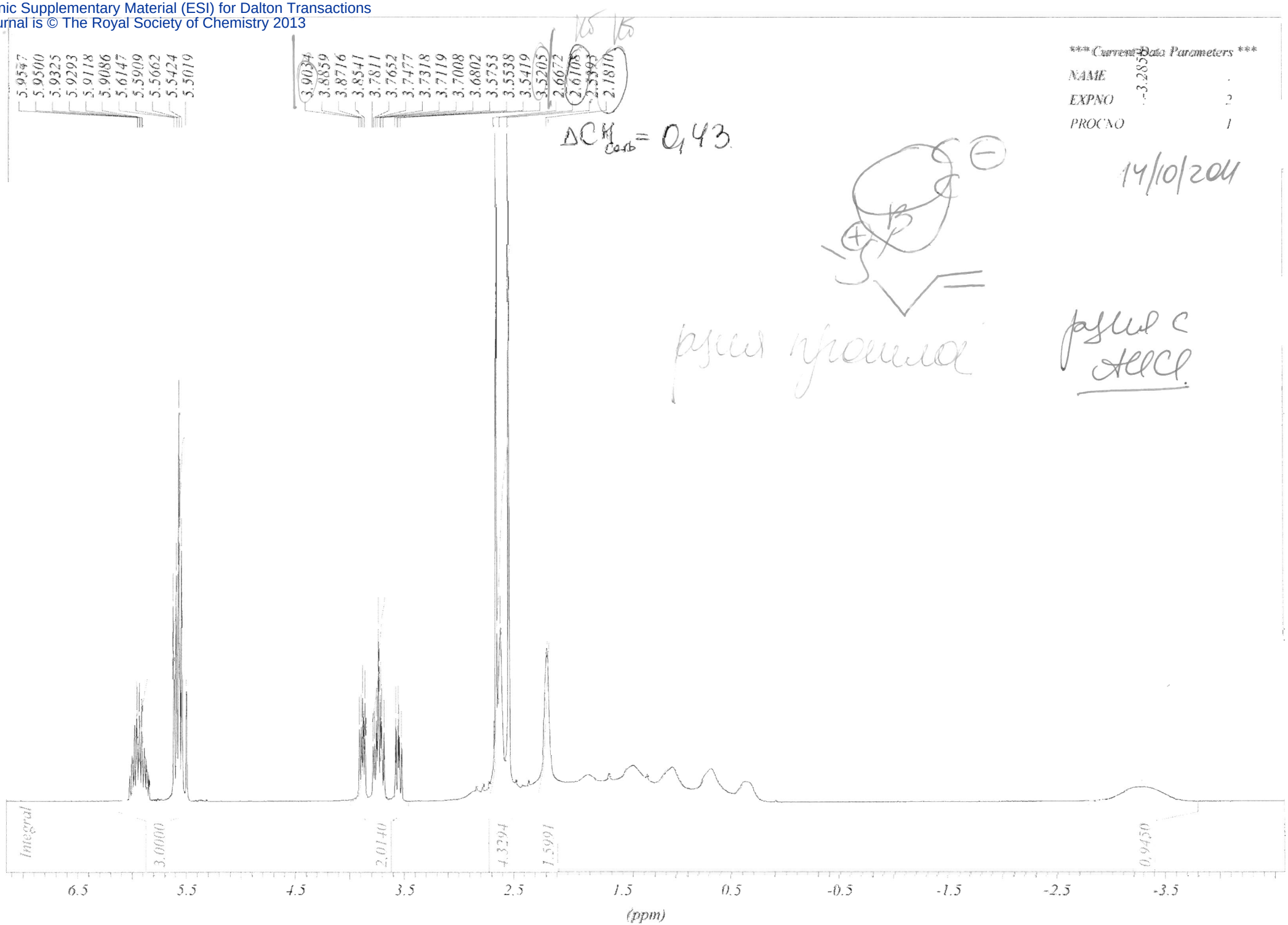

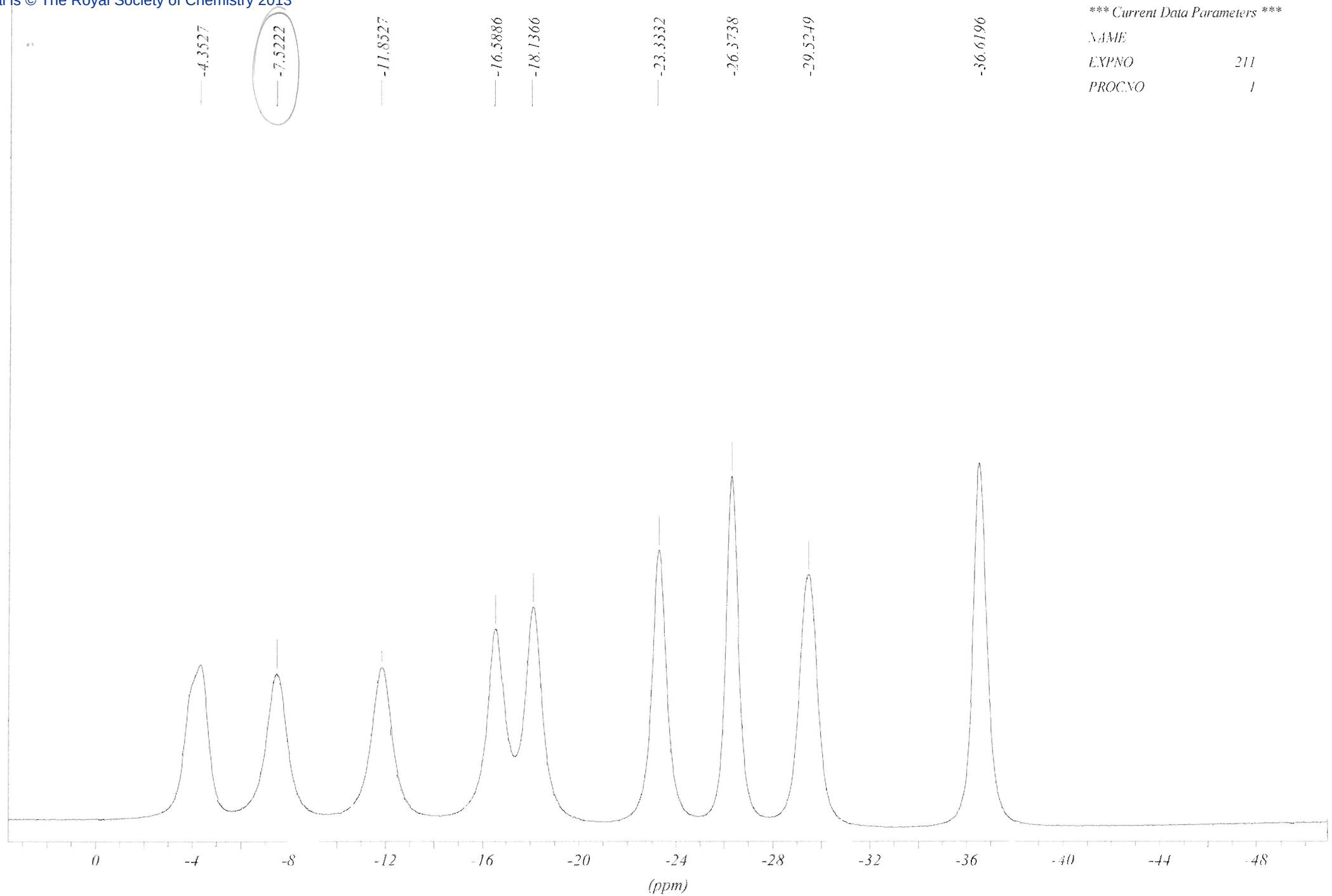

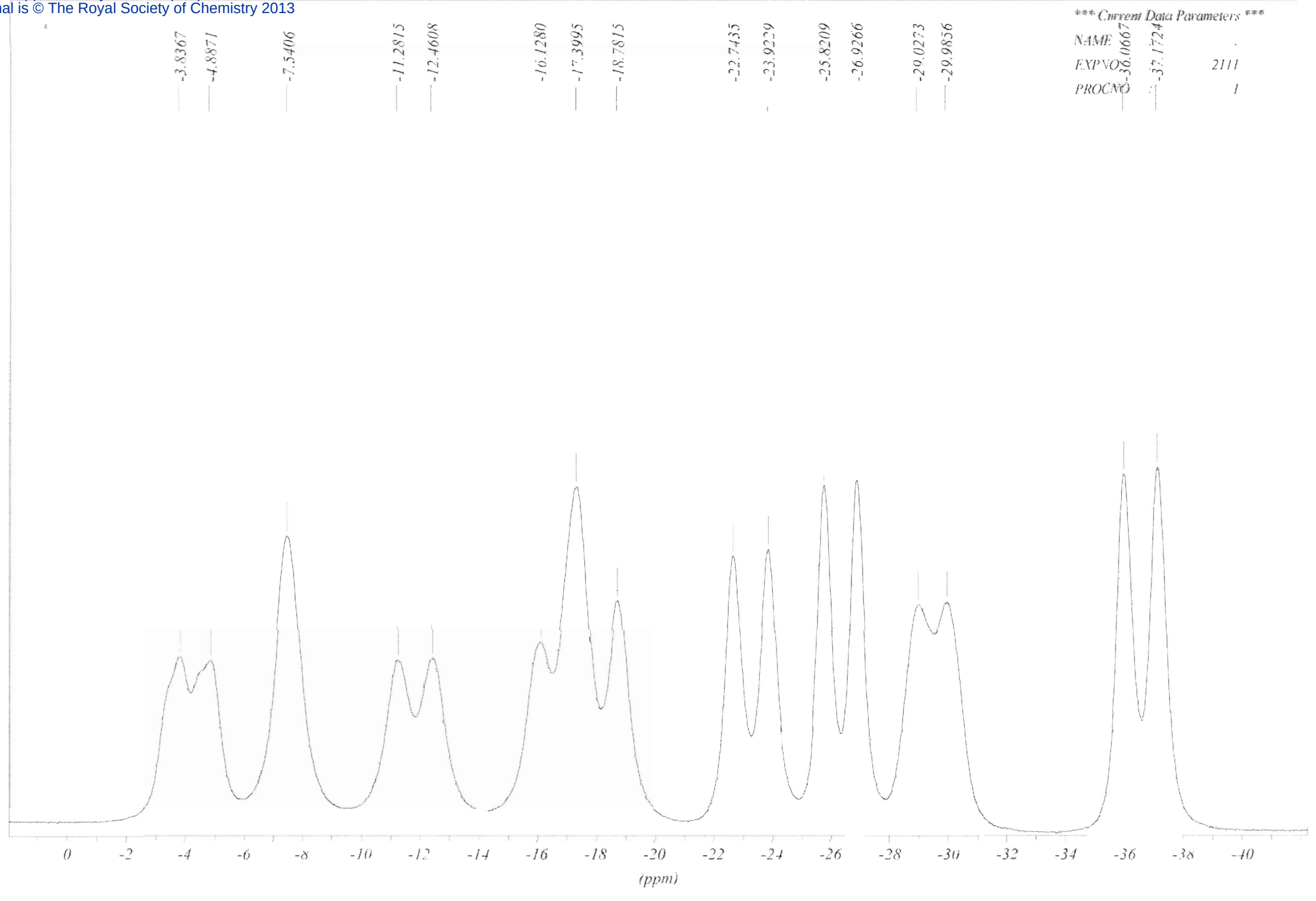

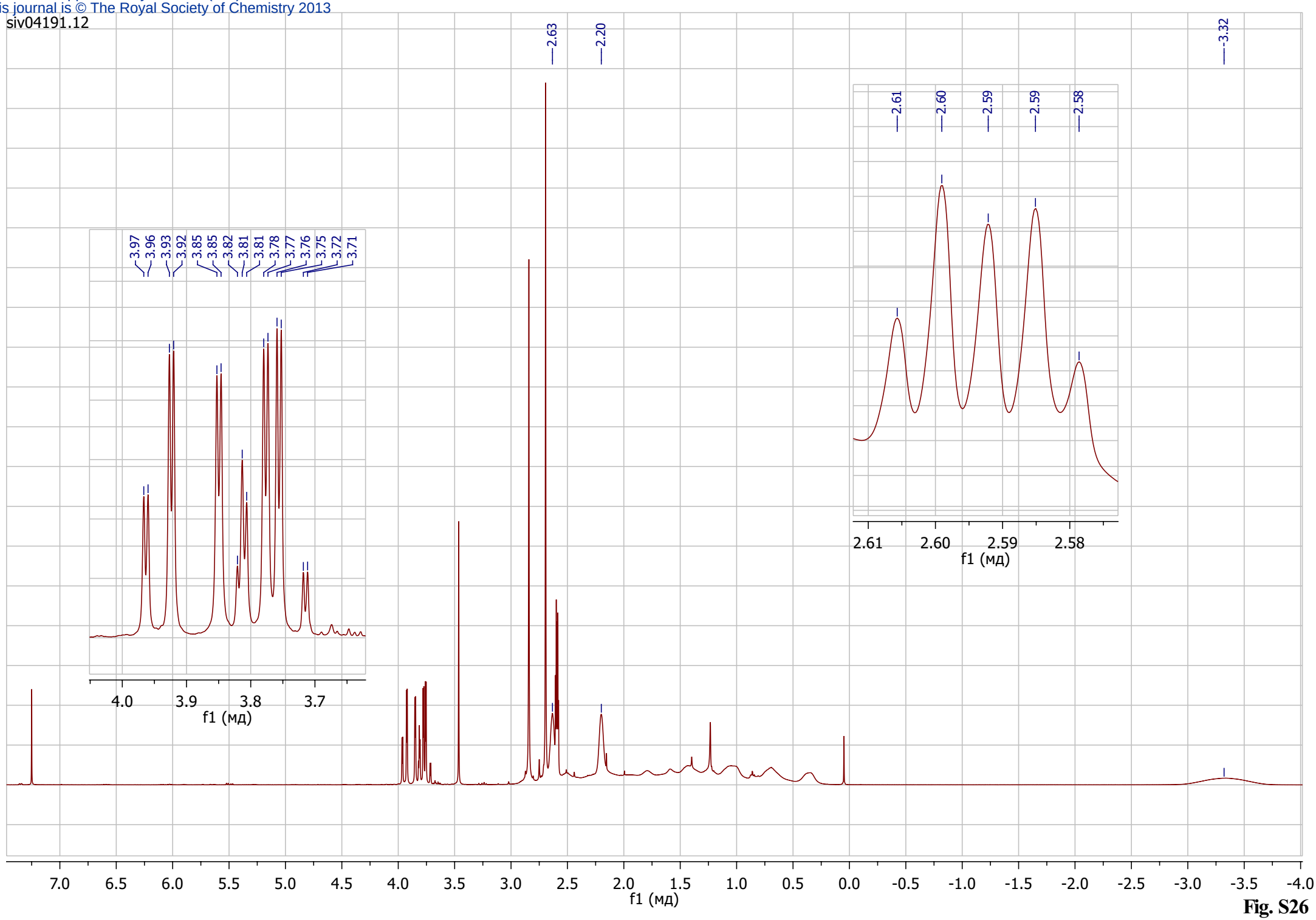

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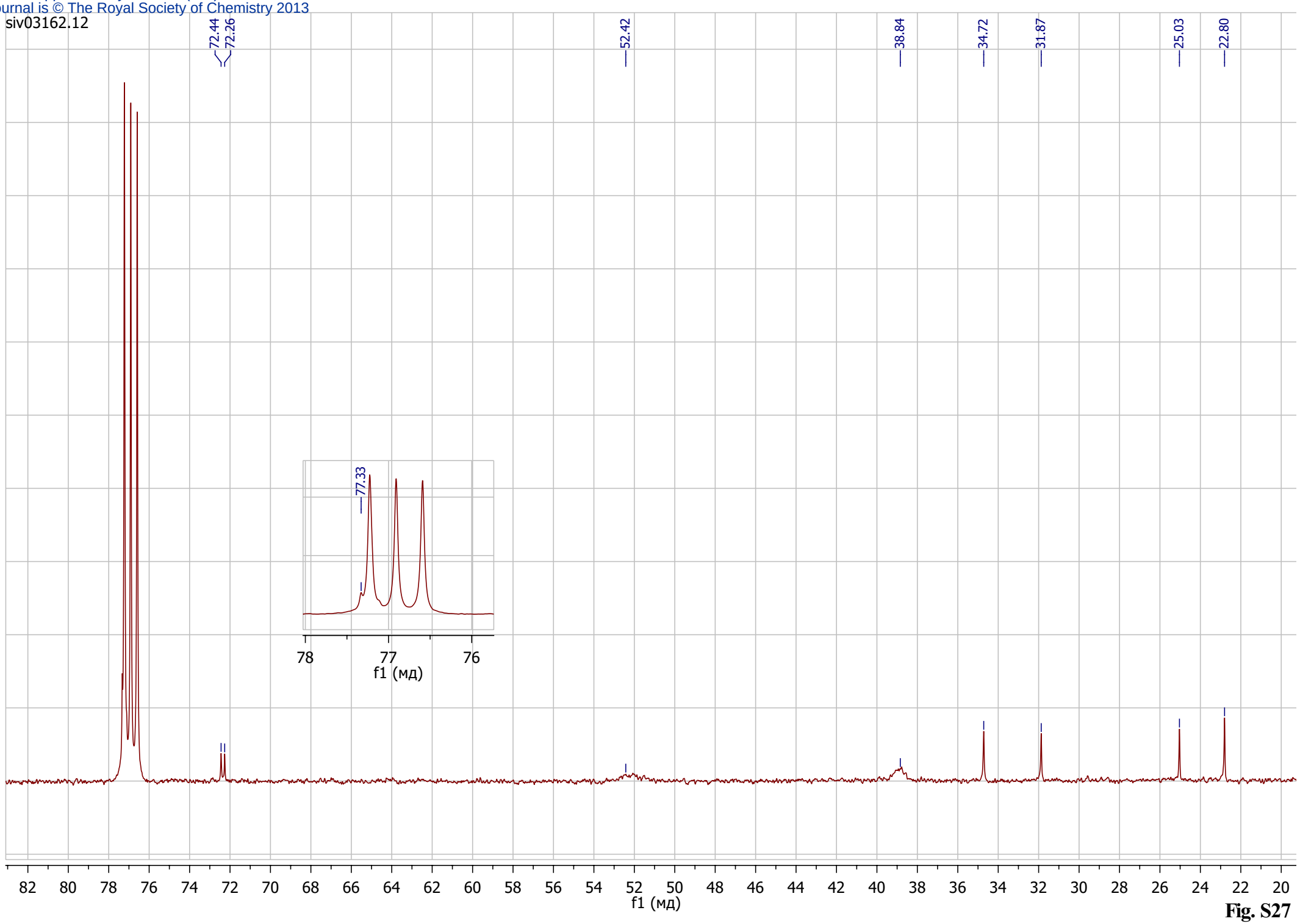

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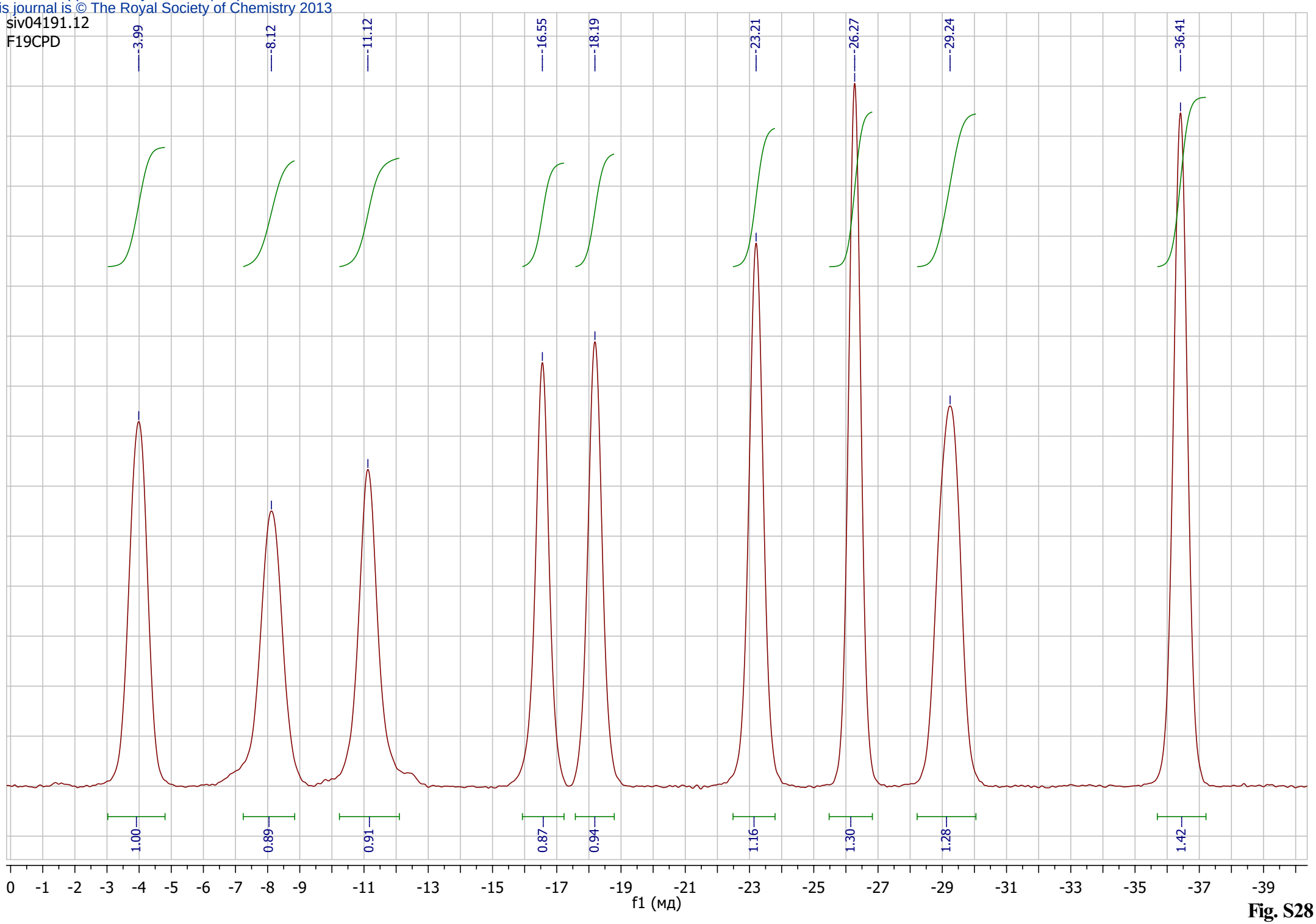

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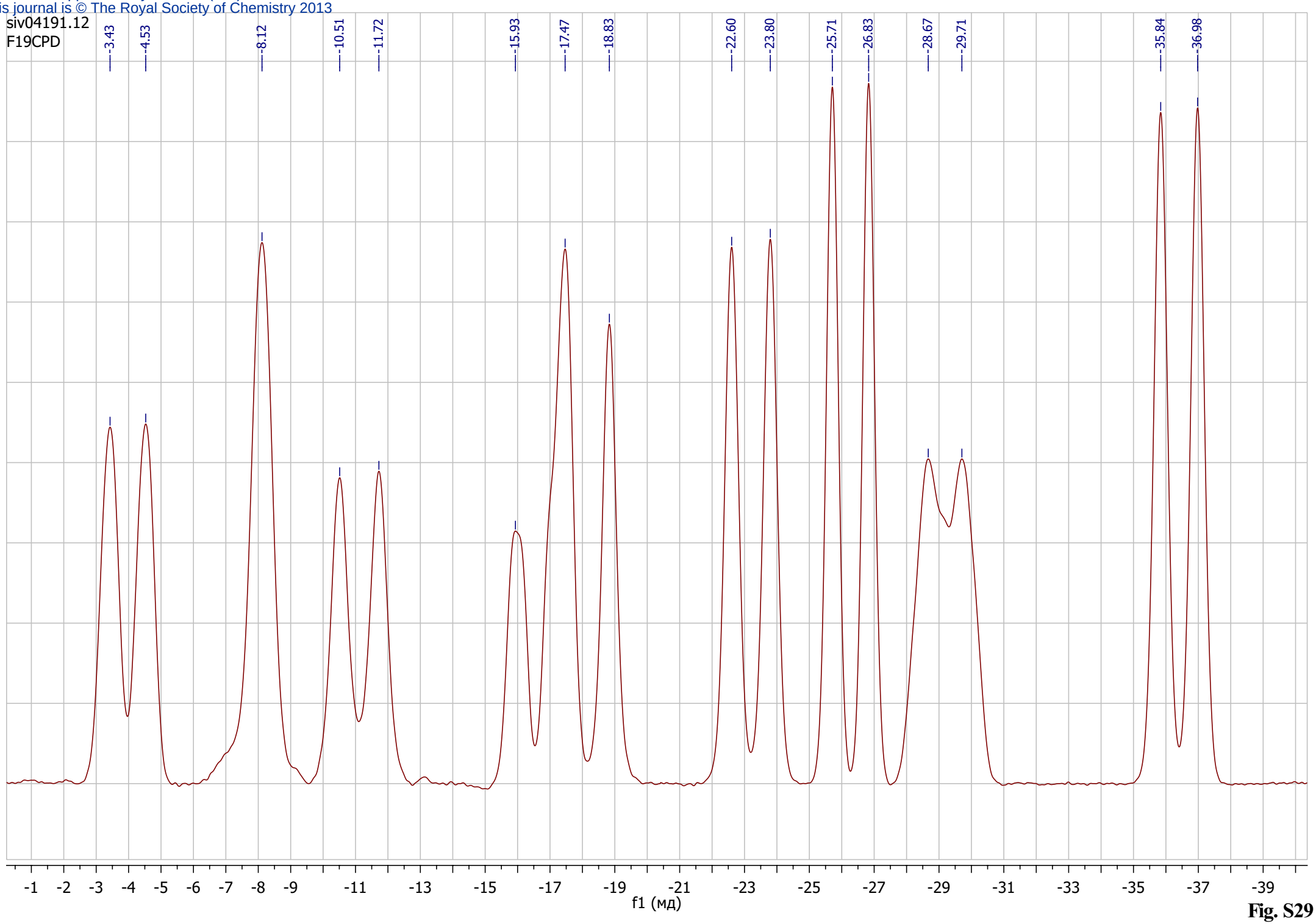

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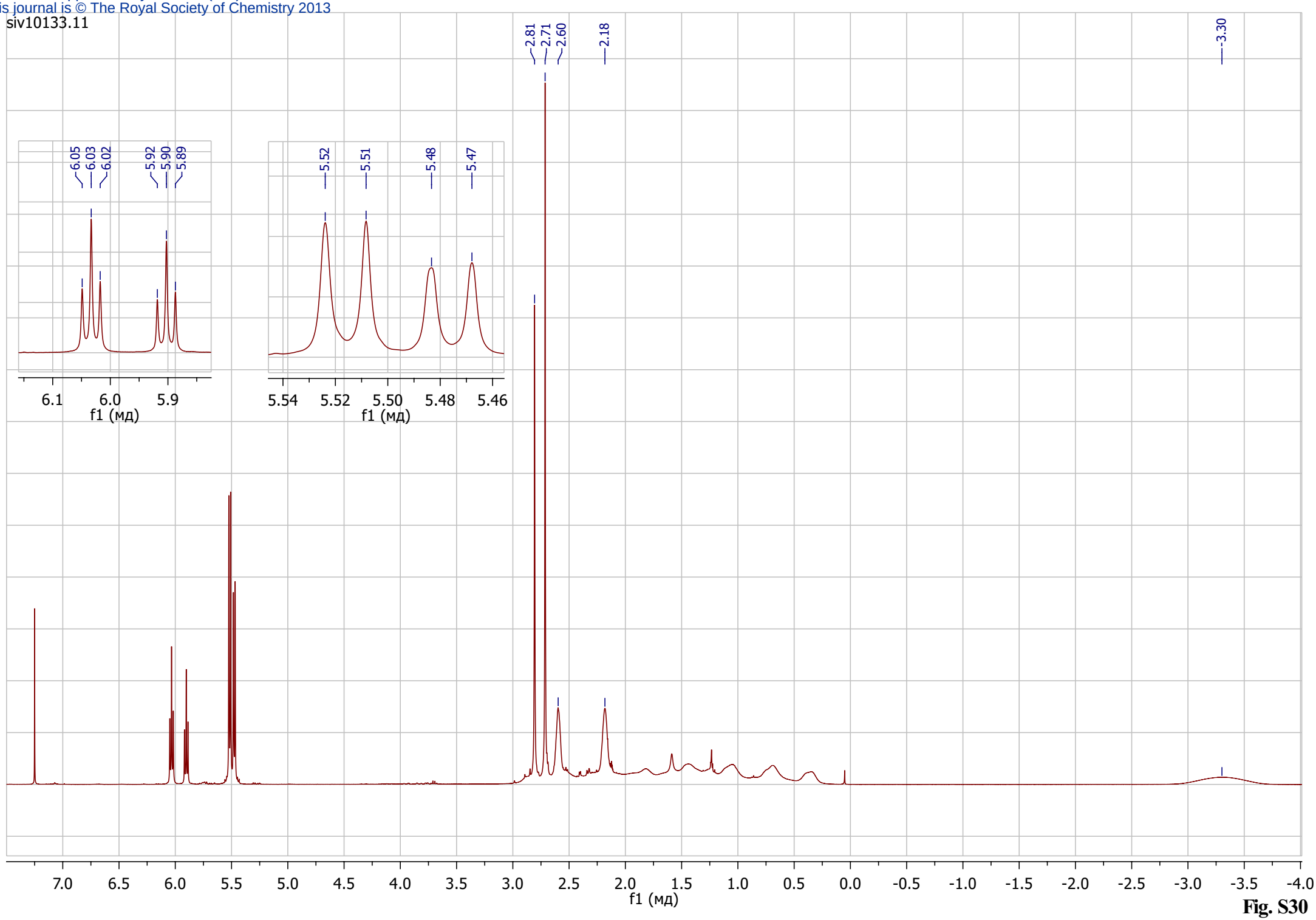

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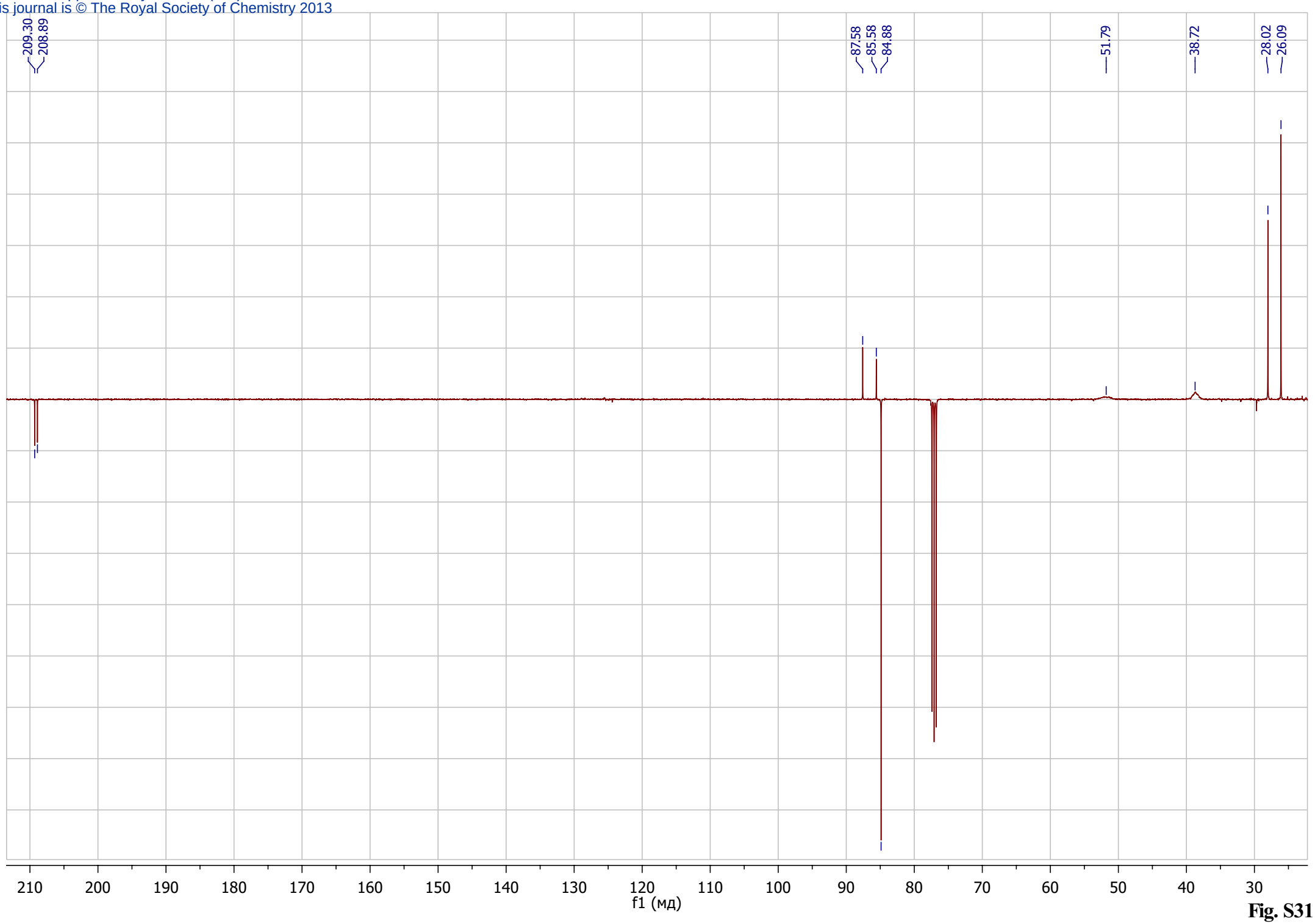

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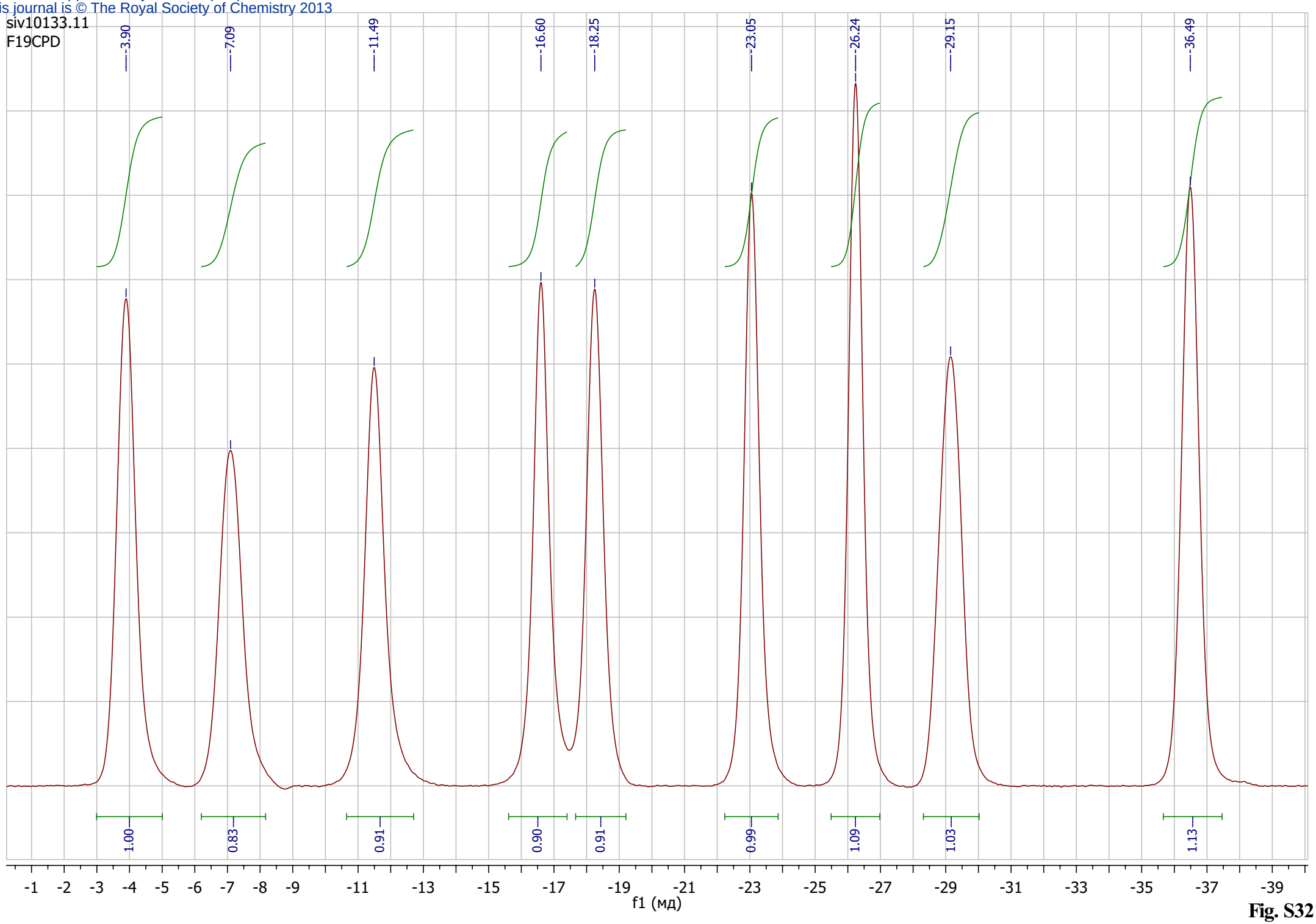

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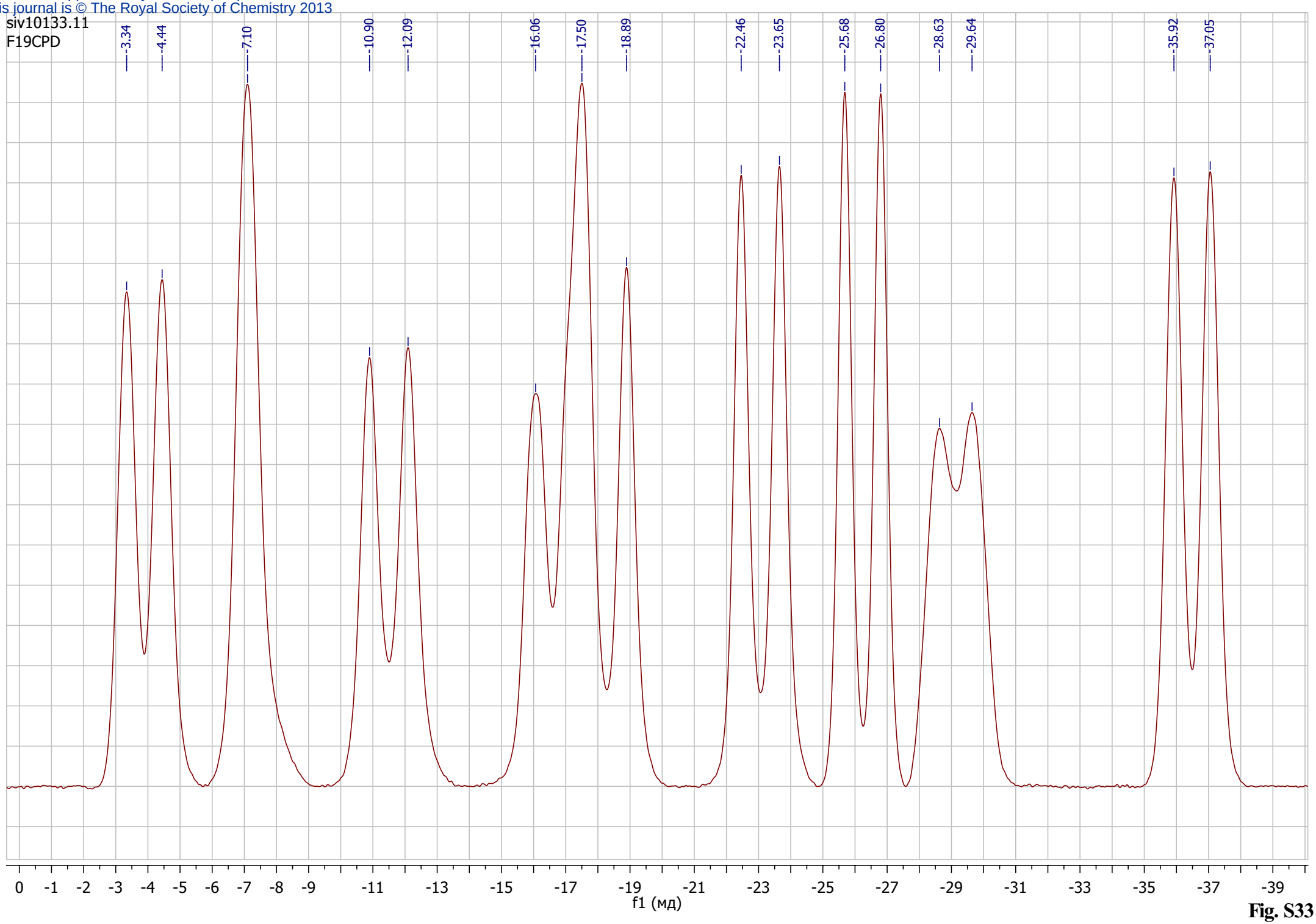

Fig. S33

Table S1. Bond lengths distribution in [9-RMeS-*nido*-7,8-$C_2B_9H_{11}$] derivatives in comparison with [*nido*-7,8-$C_2B_9H_{12}$]$^-$ anion

Bond	anion[a]	anion[b]	SMe_2-derivative[c] first molecule	SMe_2-derivative[c] second molecule	Compound **7**	Compound **5**
B1-B2	1.761	1.757	1.740(5)	1.724(5)	1.755(3)	1.759(2)
B1-B3	1.773	1.777	1.778(5)	1.769(5)	1.774(3)	1.782(2)
B1-B4	1.767	1.775	1.774(4)	1.777(5)	1.774(3)	1.769(2)
B1-B5	1.793	1.795	1.777(4)	1.768(5)	1.787(3)	1.782(2)
B1-B6	1.799	1.798	1.795(4)	1.793(5)	1.811(3)	1.809(2)
B2-B3	1.755	1.758	1.740(5)	1.728(6)	1.756(3)	1.757(2)
B3-B4	1.762	1.770	1.769(5)	1.768(5)	1.778(3)	1.775(2)
B4-B5	1.756	1.747	1.767(4)	1.771(5)	1.763(2)	1.771(2)
B5-B6	1.823	1.820	1.797(4)	1.790(5)	1.811(3)	1.811(2)
B6-B2	1.758	1.763	1.762(5)	1.757(5)	1.775(3)	1.773(2)
B2-C7	1.716	1.715	1.690(5)	1.679(5)	1.698(2)	1.699(2)
B3-C7	1.712	1.715	1.712(5)	1.704(5)	1.704(2)	1.707(2)
B3-C8	1.718	1.731	1.740(5)	1.738(5)	1.725(2)	1.737(2)
B4-C8	1.719	1.738	1.752(4)	1.744(5)	1.735(2)	1.736(2)
B4-B9	1.795	1.796	1.749(4)	1.757(4)	1.759(3)	1.769(2)
B5-B9	1.764	1.764	1.736(4)	1.736(4)	1.748(3)	1.741(2)
B5-B10	1.782	1.781	1.779(4)	1.776(4)	1.796(3)	1.801(2)
B6-B10	1.779	1.782	1.785(4)	1.788(5)	1.791(3)	1.795(2)
B6-B11	1.779	1.768	1.775(5)	1.777(5)	1.800(3)	1.795(2)
B2-B11	1.803	1.804	1.800(5)	1.796(5)	1.808(3)	1.812(2)
C7-C8	1.555	1.564	1.525(4)	1.531(4)	1.550(2)	1.549(2)
C8-B9	1.607	1.622	1.571(4)	1.582(4)	1.594(2)	1.591(2)
B9-B10	1.831	1.813	1.775(4)	1.773(4)	1.780(3)	1.788(2)
B10-B11	1.853	1.841	1.843(5)	1.851(5)	1.861(3)	1.863(2)
B11-C7	1.614	1.621	1.623(5)	1.613(5)	1.637(2)	1.637(2)

[a] [*nido*-7,8-$C_2B_9H_{12}$]$^-$ anion, refcode CENBUS[1]; [b] [*nido*-7,8-$C_2B_9H_{12}$]$^-$ anion, refcode GUNHUS01[1]; [c] [9-Me_2S-*nido*-7,8-$C_2B_9H_{11}$], refcode VYUHIG[1], there are two independent molecules in the asymmetric unit cell

References

1. F.H. Allen, *Acta Crystallogr*., **2002**, *B58*, 380; (b) *Cambridge Structural Database*, **2012**, Version 5.34