Supporting Information

C,C-Diacetylenic Phosphaalkenes in Palladium-Catalyzed Cross-Coupling Reactions

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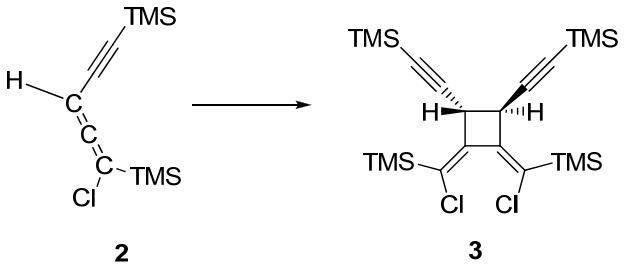
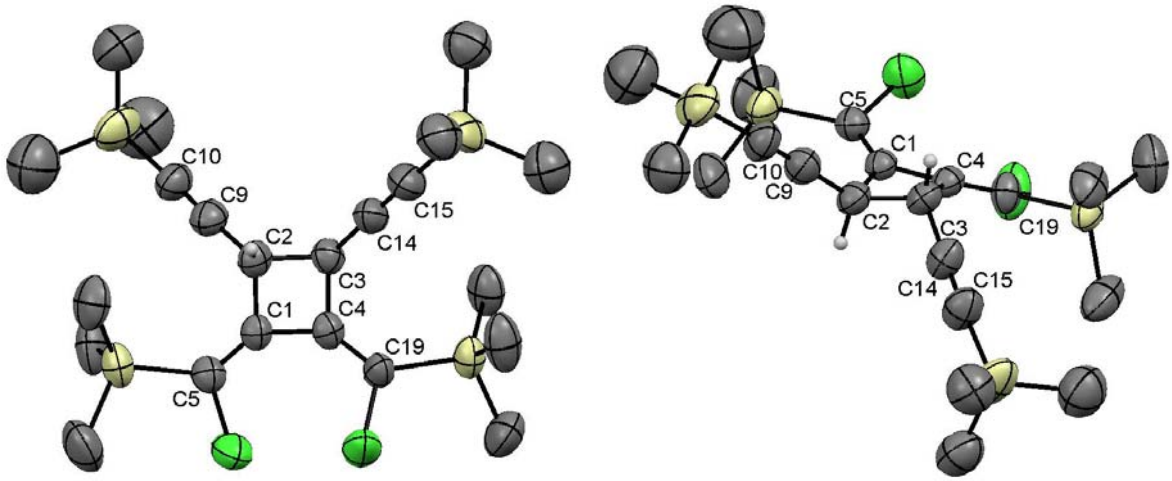
Experimental



2 **3**

SCHEME 1. Dimerization of **2**.

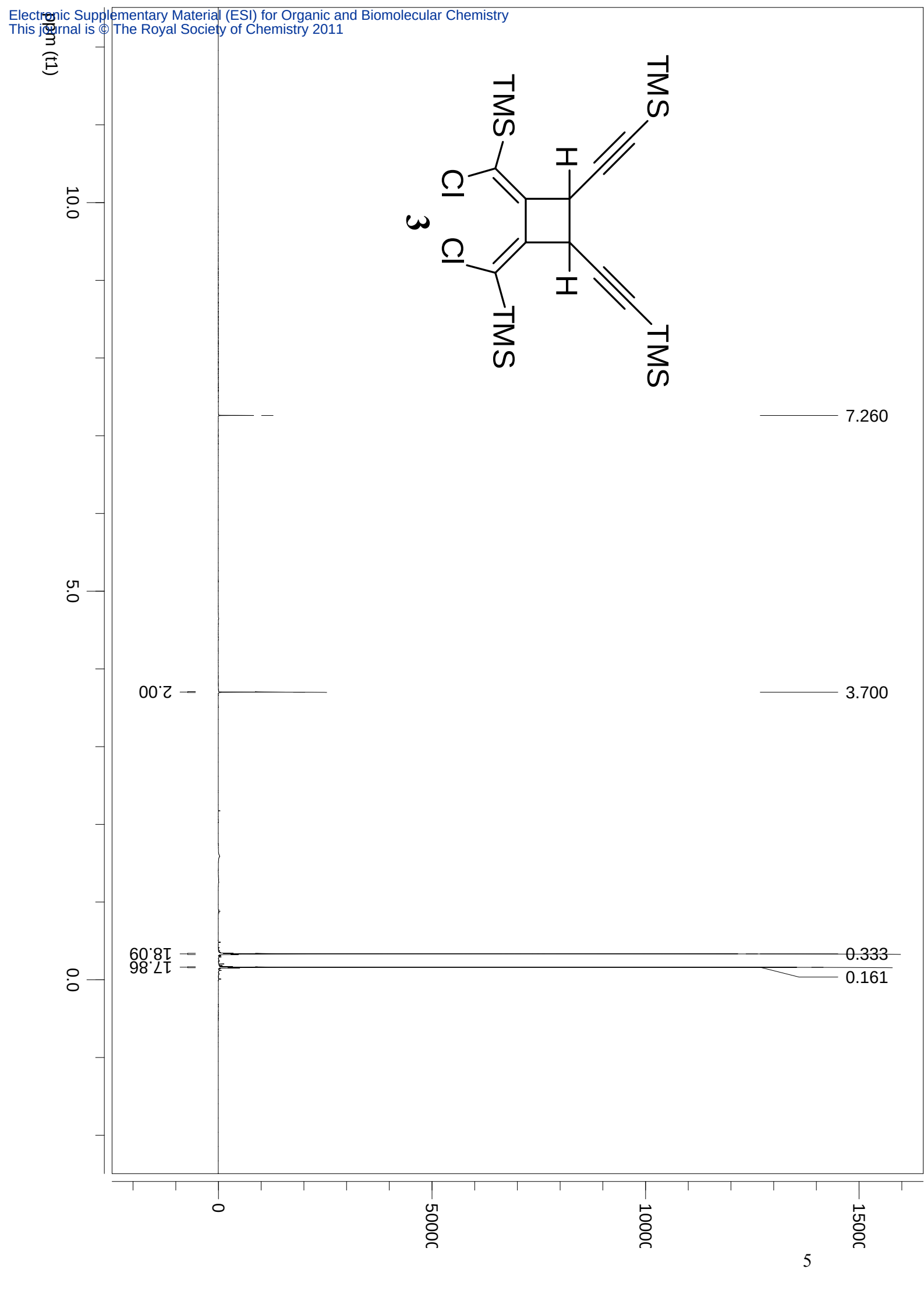


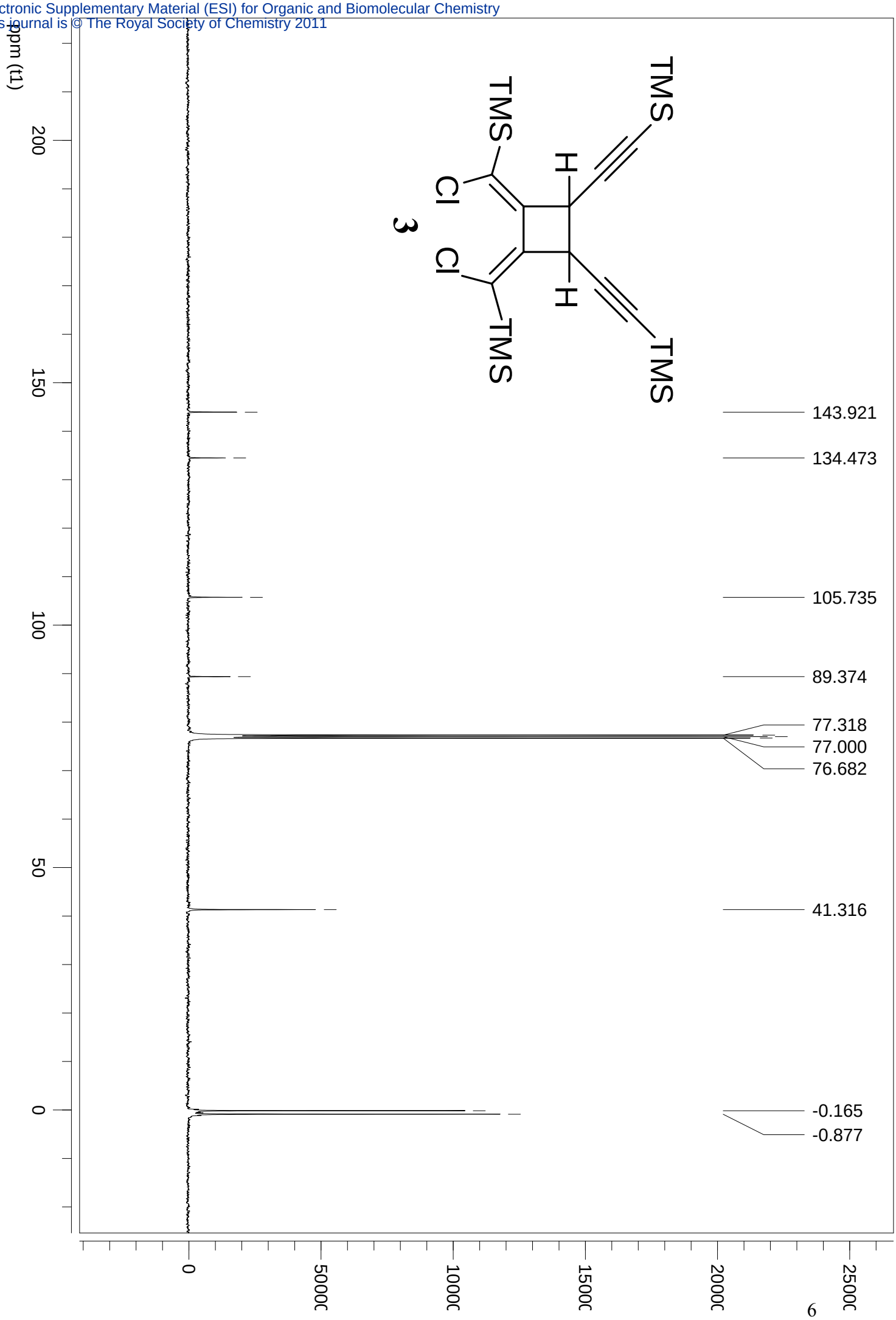
front view **side view**

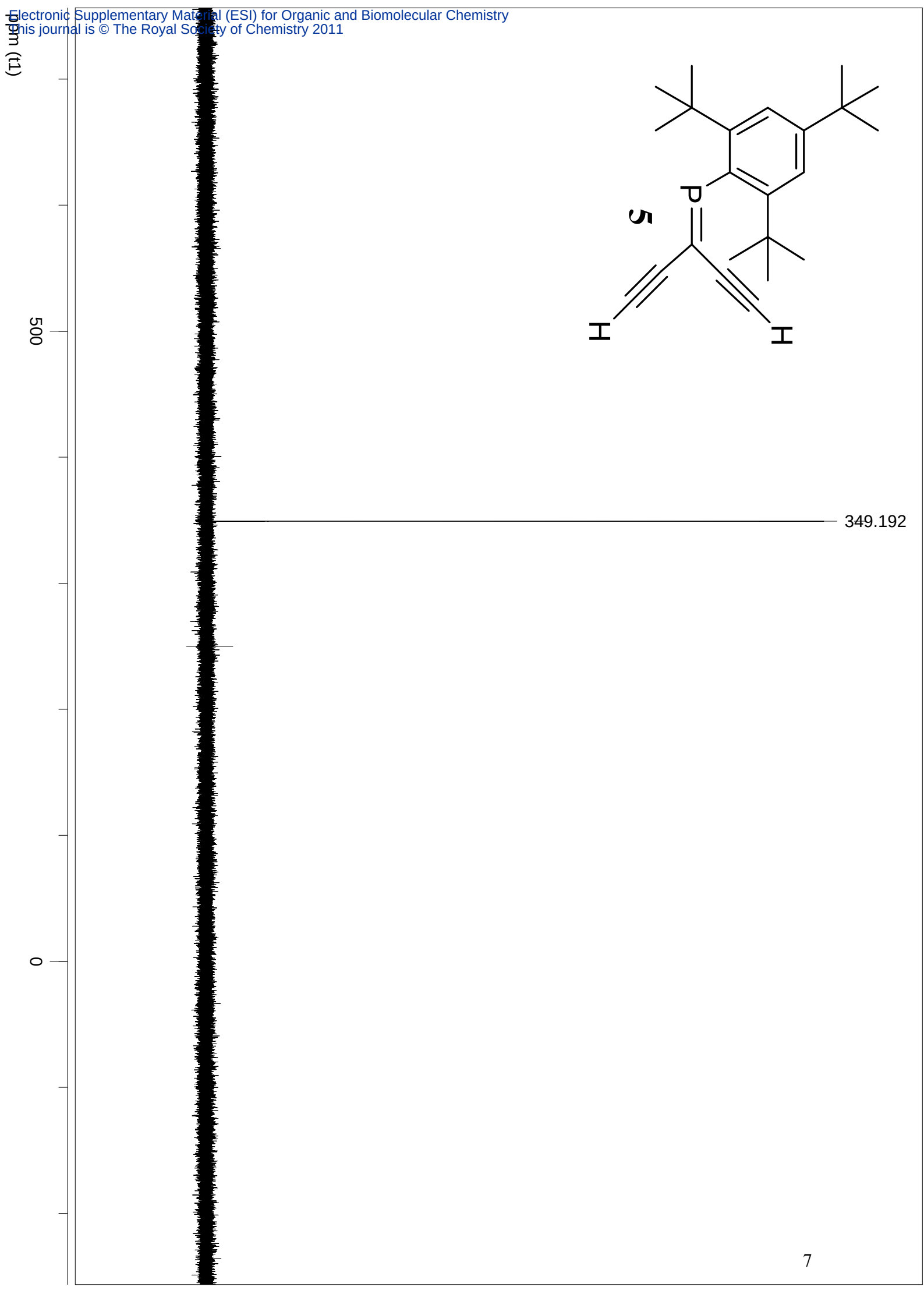
FIGURE 1. ORTEP drawing (at 50% probability level) of **3**. Hydrogen atoms and disordered methyl groups are omitted for clarity. Chloride atoms and silicon atoms are depicted in green and light yellow, respectively. Selected bond lengths (Å) and angles (deg). C1-C2 1.528(9), C2-C3 1.572(9), C3-C4 1.537(9), C1-C4 1.484(9), C1-C5 1.351(9), C4-C19 1.350(9), C14-C15 1.215(10), C9-C10 1.204(10). Angles C1-C2-C3 88.3(5), C2-C3-C4 86.5(5), C1-C4-C3 91.3(5), C2-C1-C4 90.0(5).

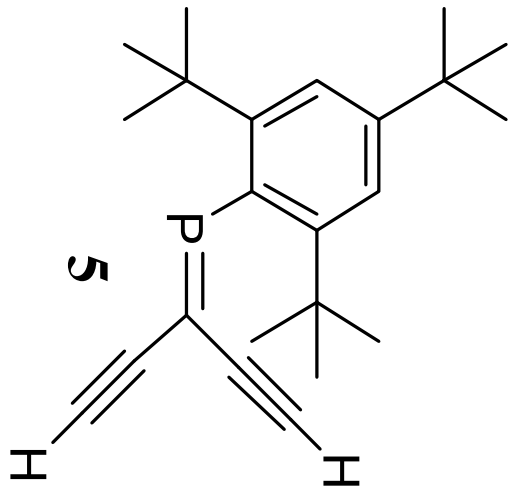
TABLE 1. Crystallographic data for **3.**

Compound	**3**
Formula	$C_{22}H_{38}Cl_2Si_4$
M_w (g/mol); F(000)	485.78 ; 1040
T (K); wavelength (Å)	293 ; 0.71073
Crystal System	Monoclinic
Space Group	P21/c
Unit Cell: a (Å)	11.502(2)
b (Å)	11.404(2)
c (Å)	23.465(5)
β (°)	93.20(3)
V (Å^3); Z; ; $d_{calcd.}$ (g/cm^3)	3073.2(11) ; 4 ; 1.050
θ range (°); completeness	1.74 to 25.02 ; 0.980
collected reflections; R_σ	17333 ; 0.1273
unique reflections; R_{int}	5326 ; 0.1208
μ (mm^{-1}); Abs. Corr.	0.374;Semi-empirical from equivalents
$R_1(F)$; w$R(F^2)$ [$I > 2\sigma(I)$]	0.1168 ; 0.3644
$R_1(F)$; w$R(F^2)$ (all data)	0.1575 ; 0.3912
GoF(F^2)	1.025
Residual electron density (e$^-$/Å^3)	0.494 and -0.467









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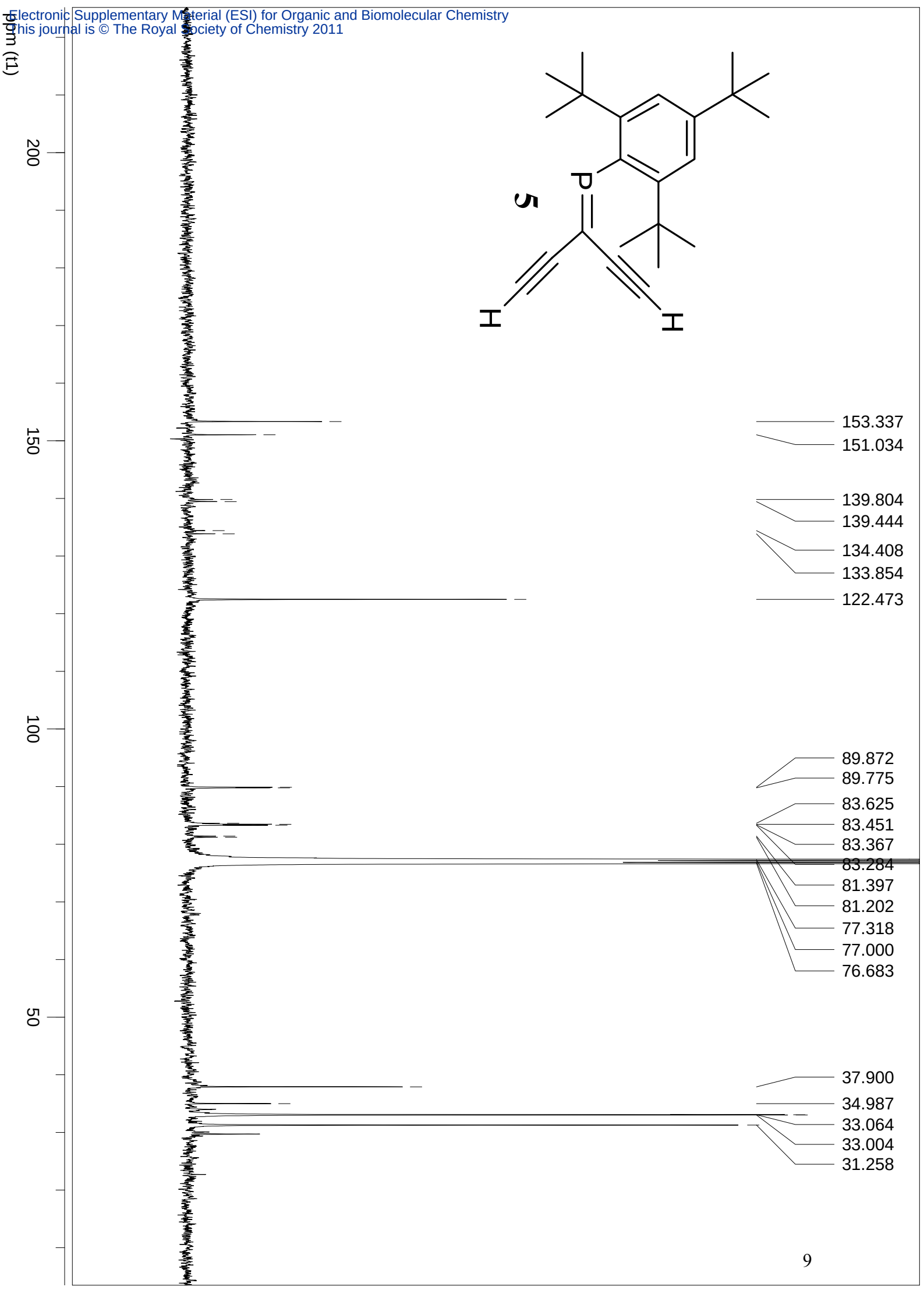

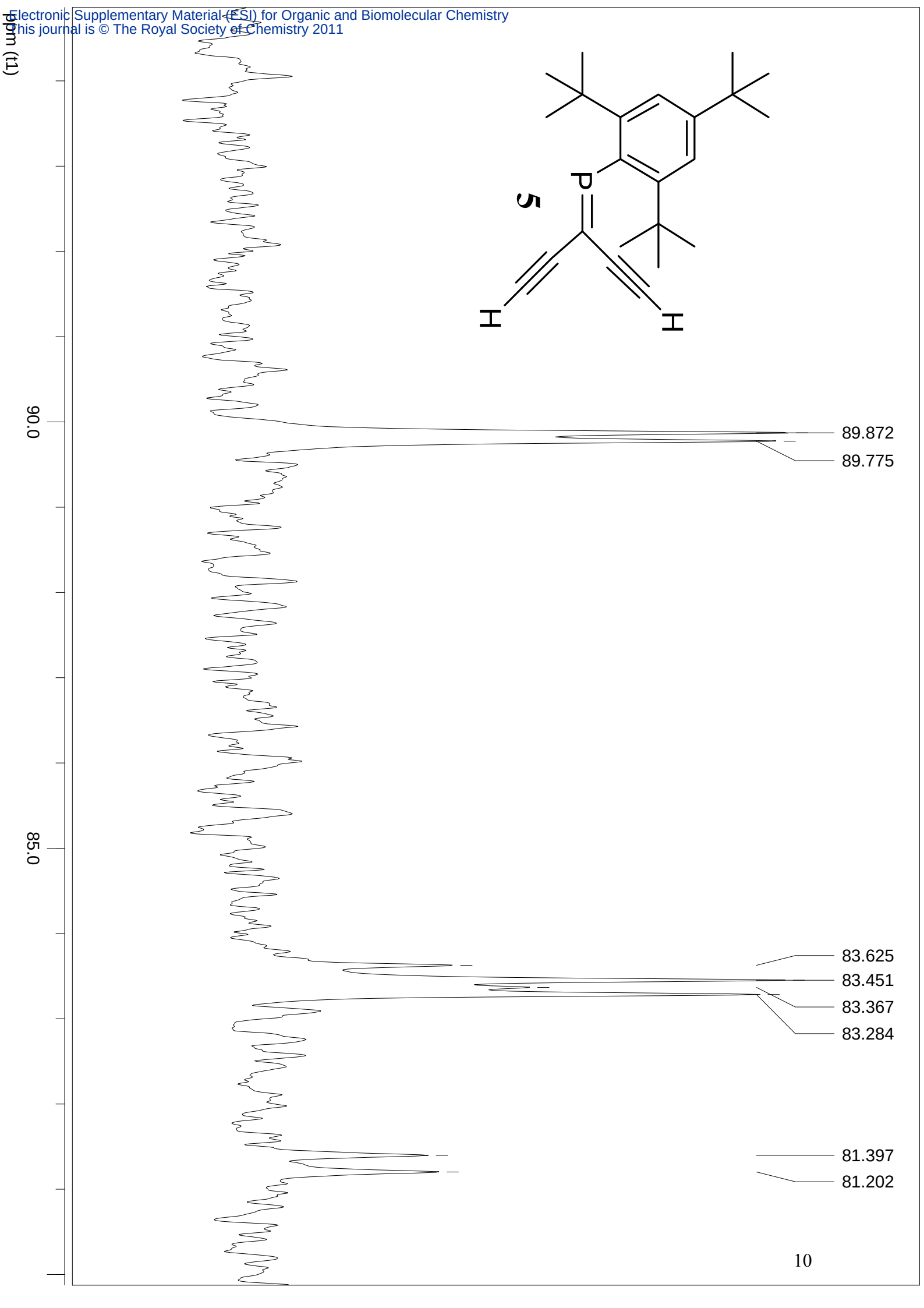

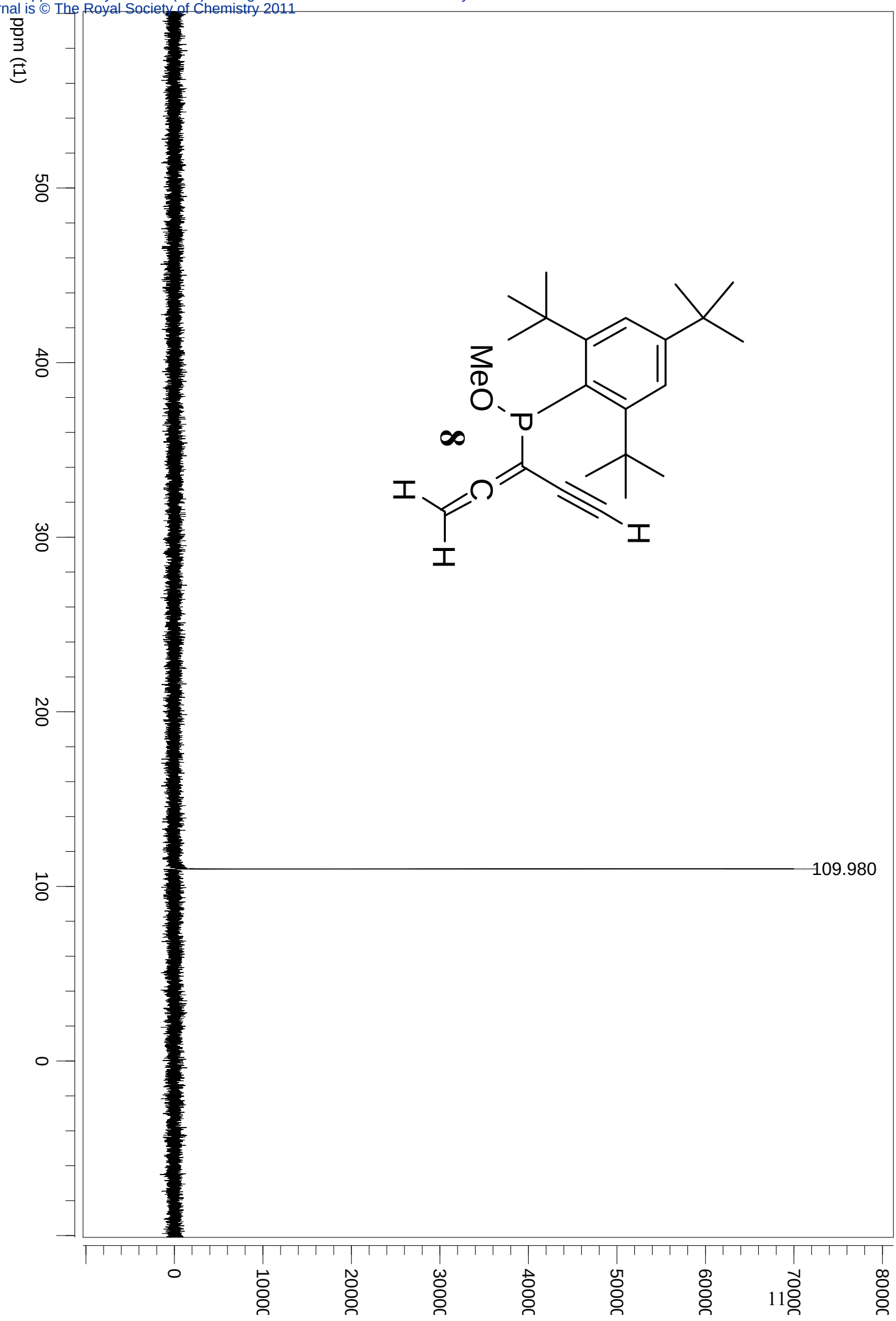

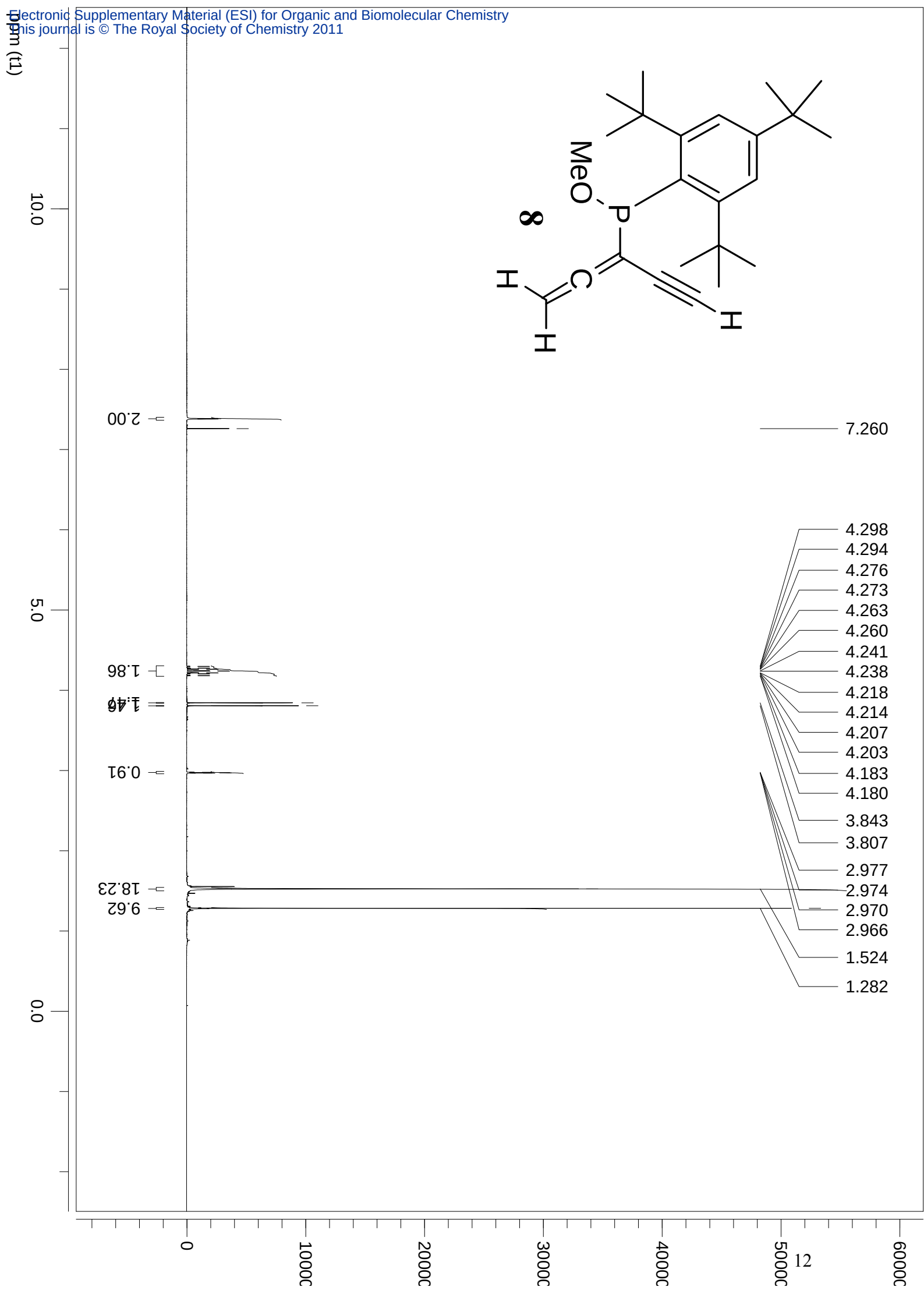

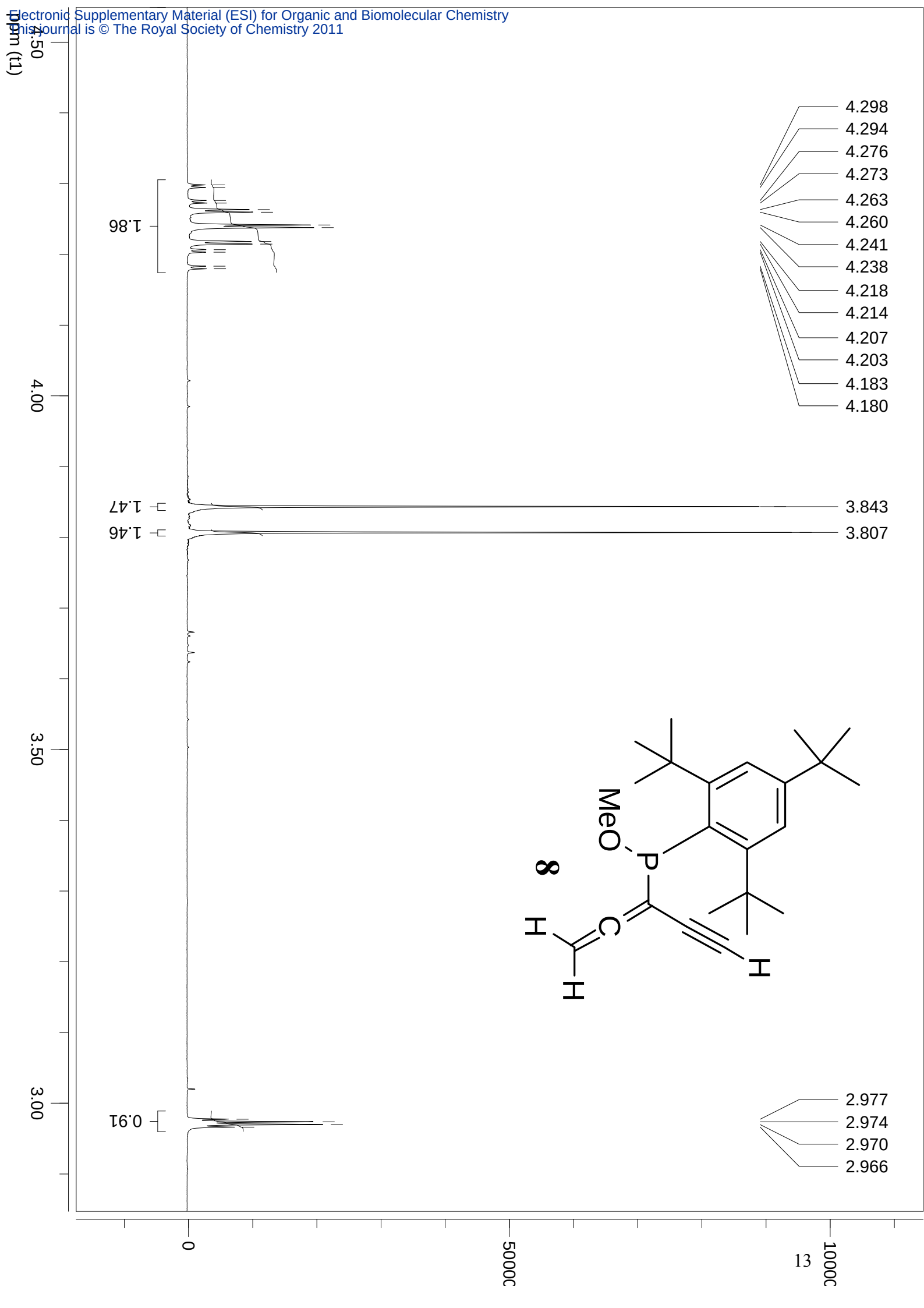

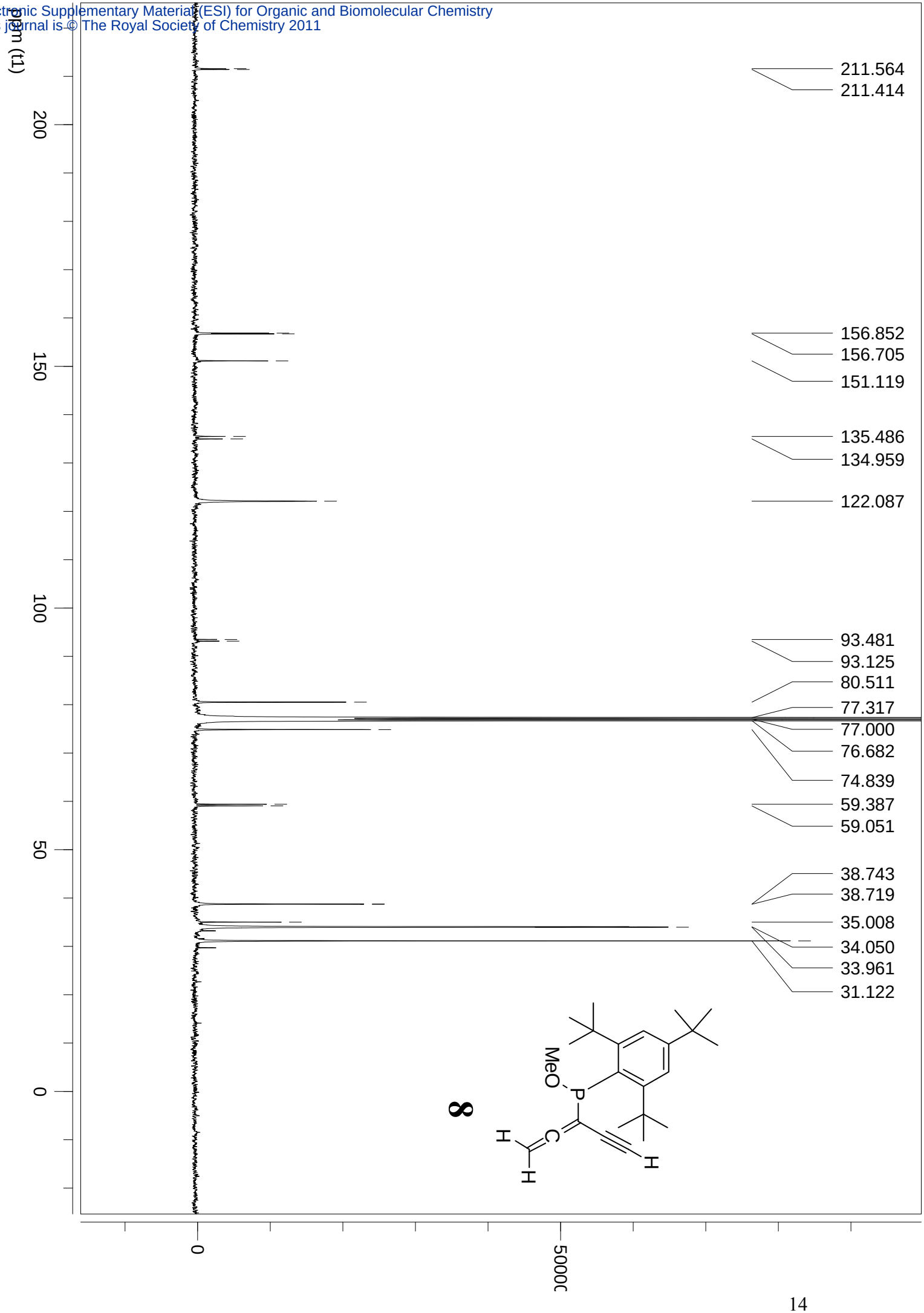
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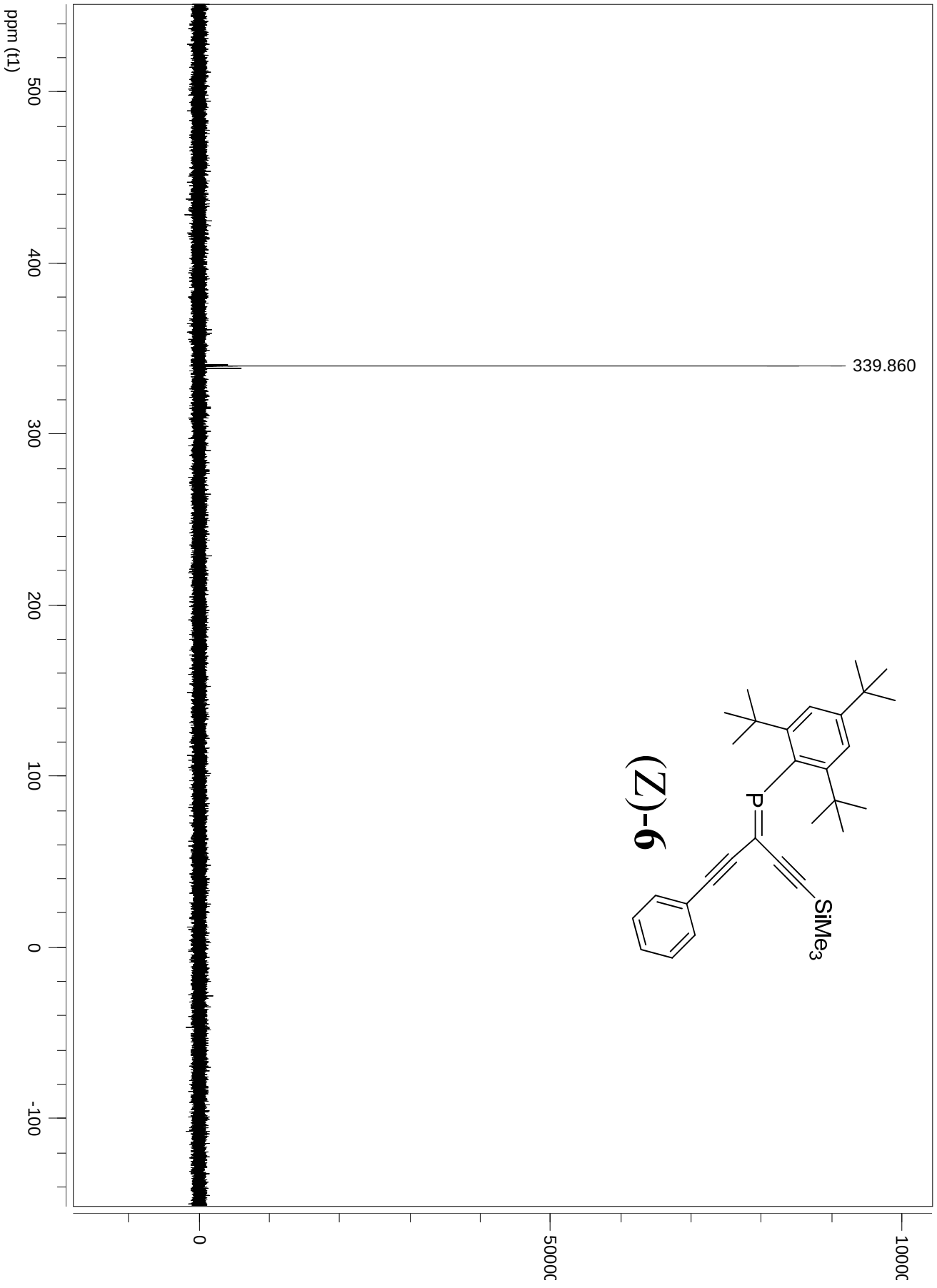

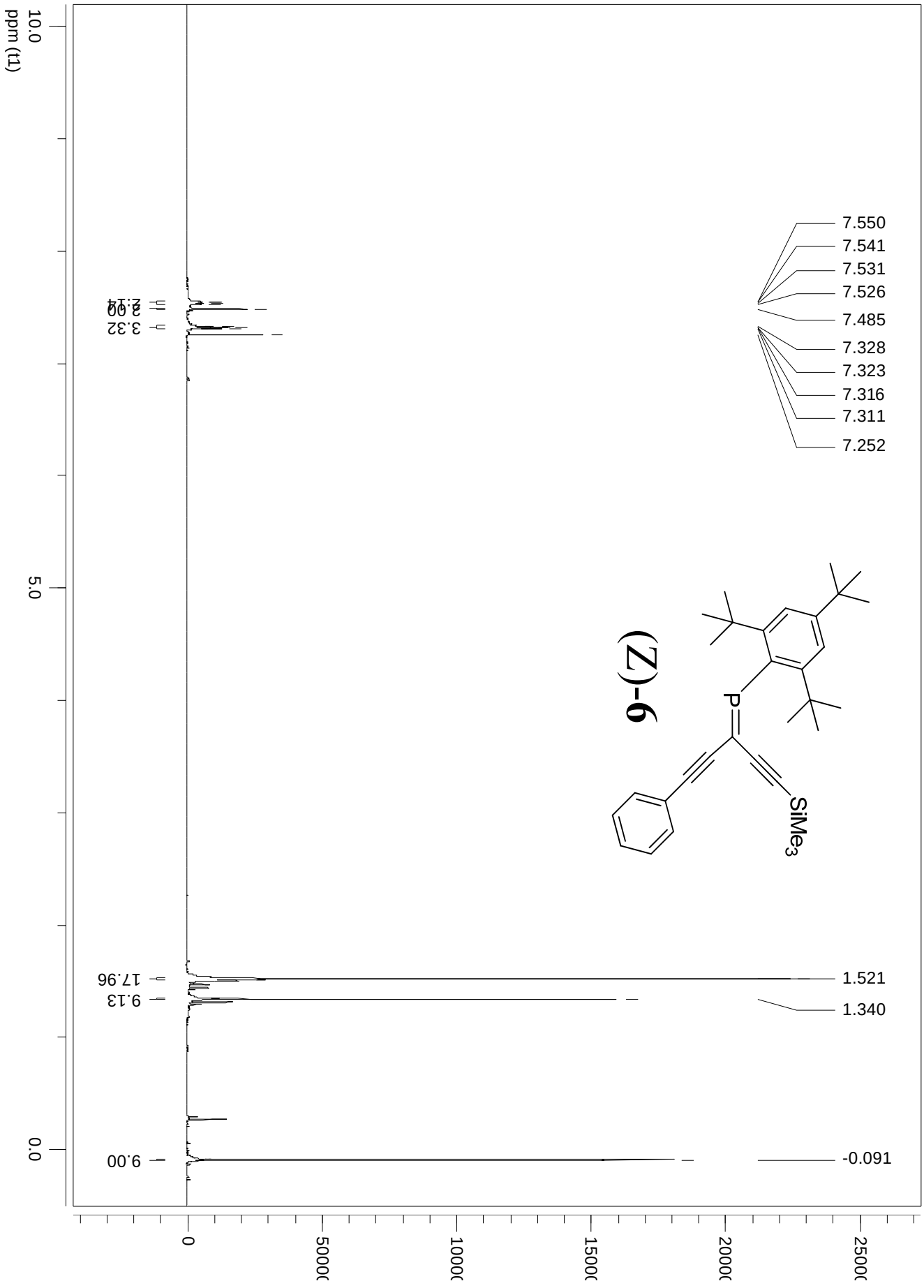

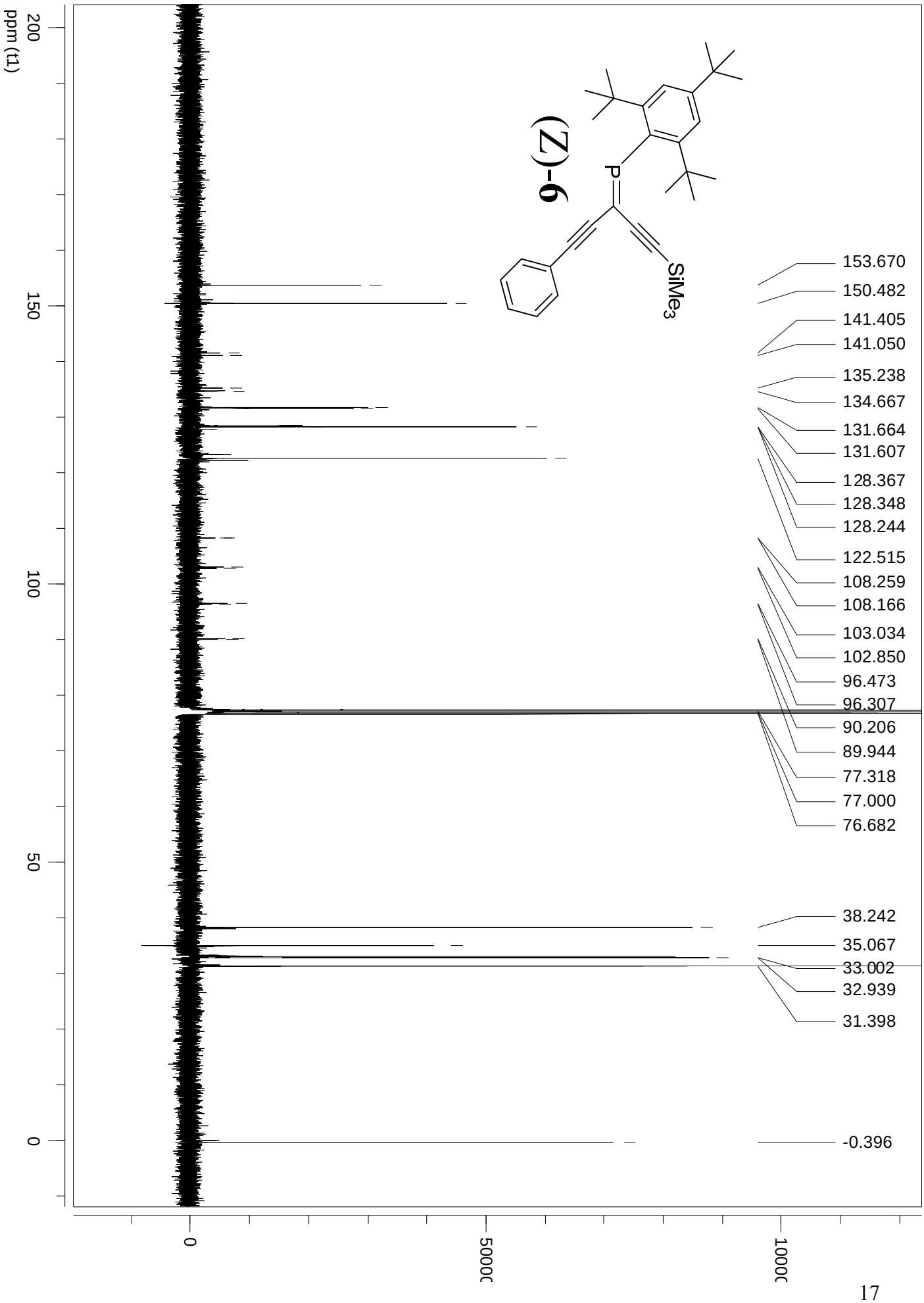

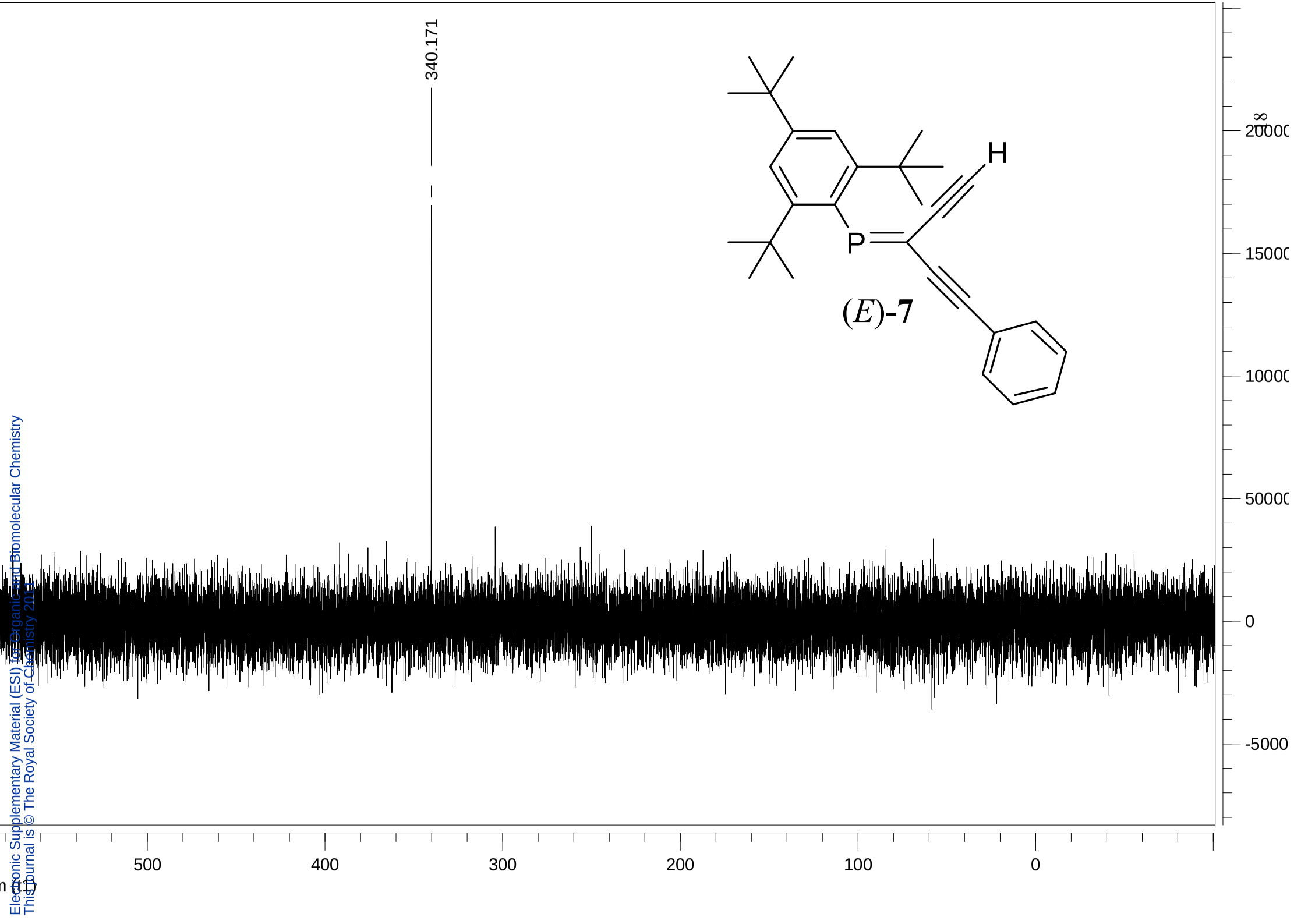

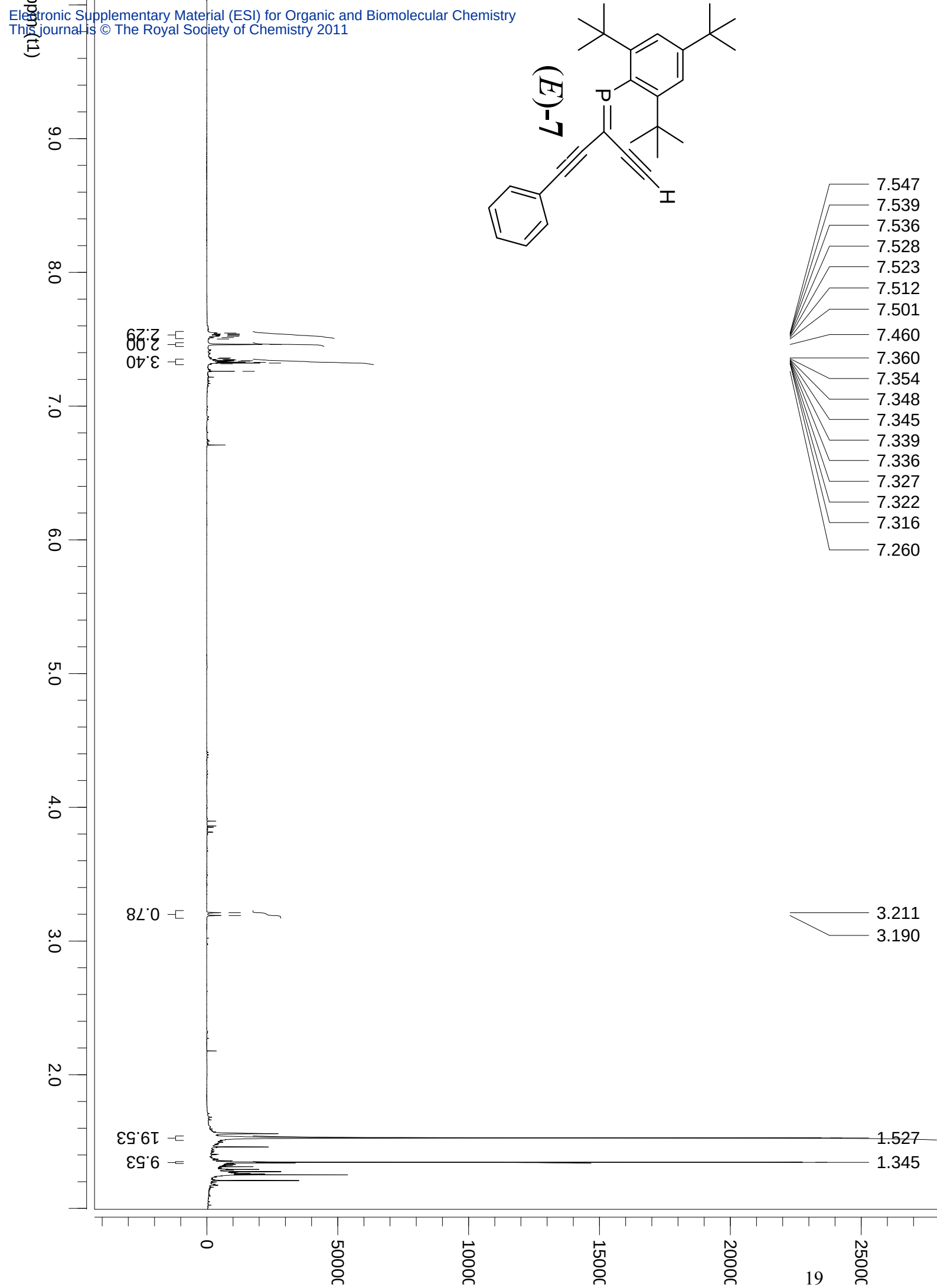

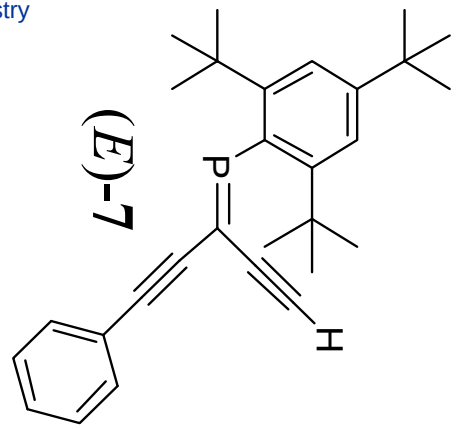

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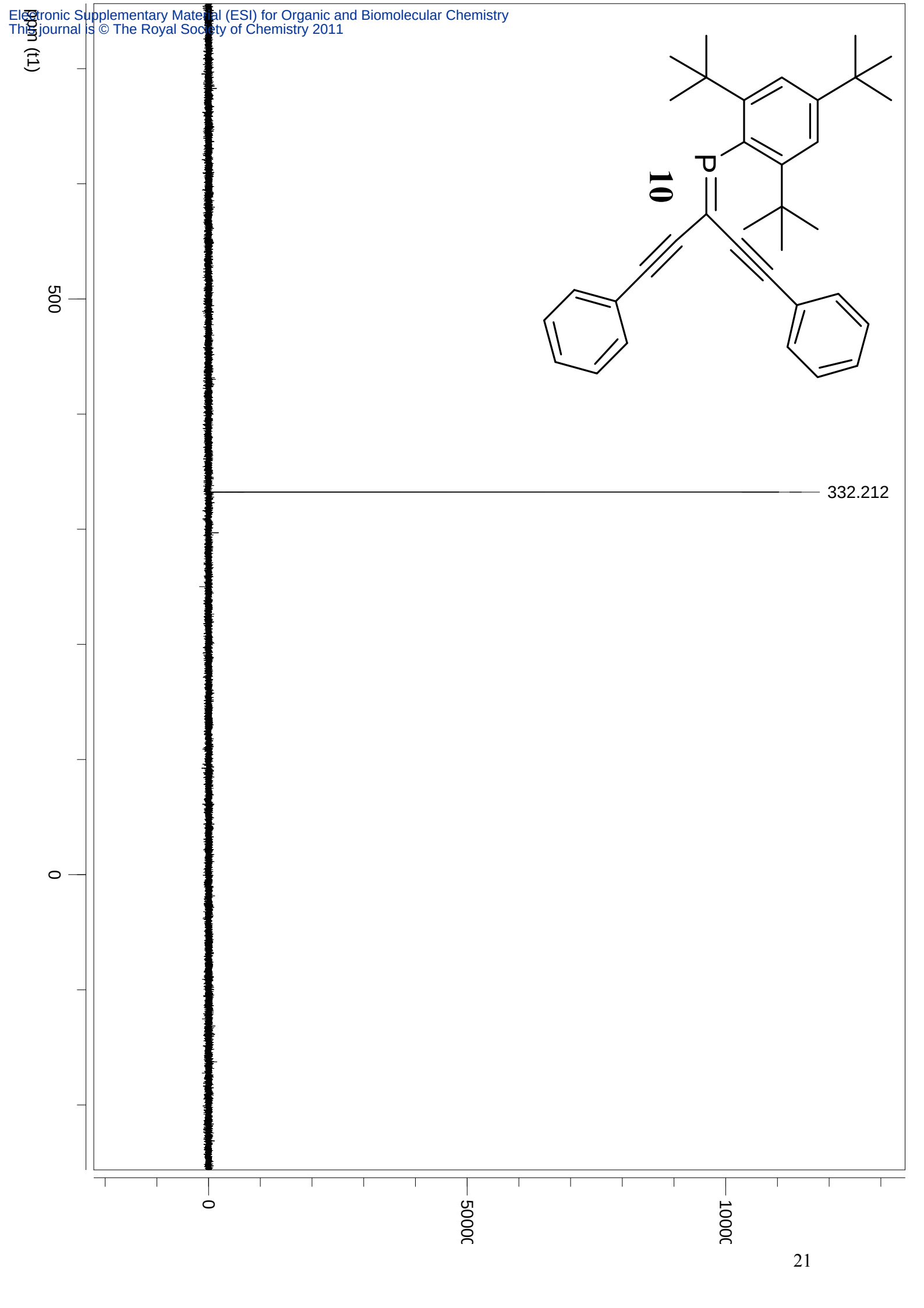
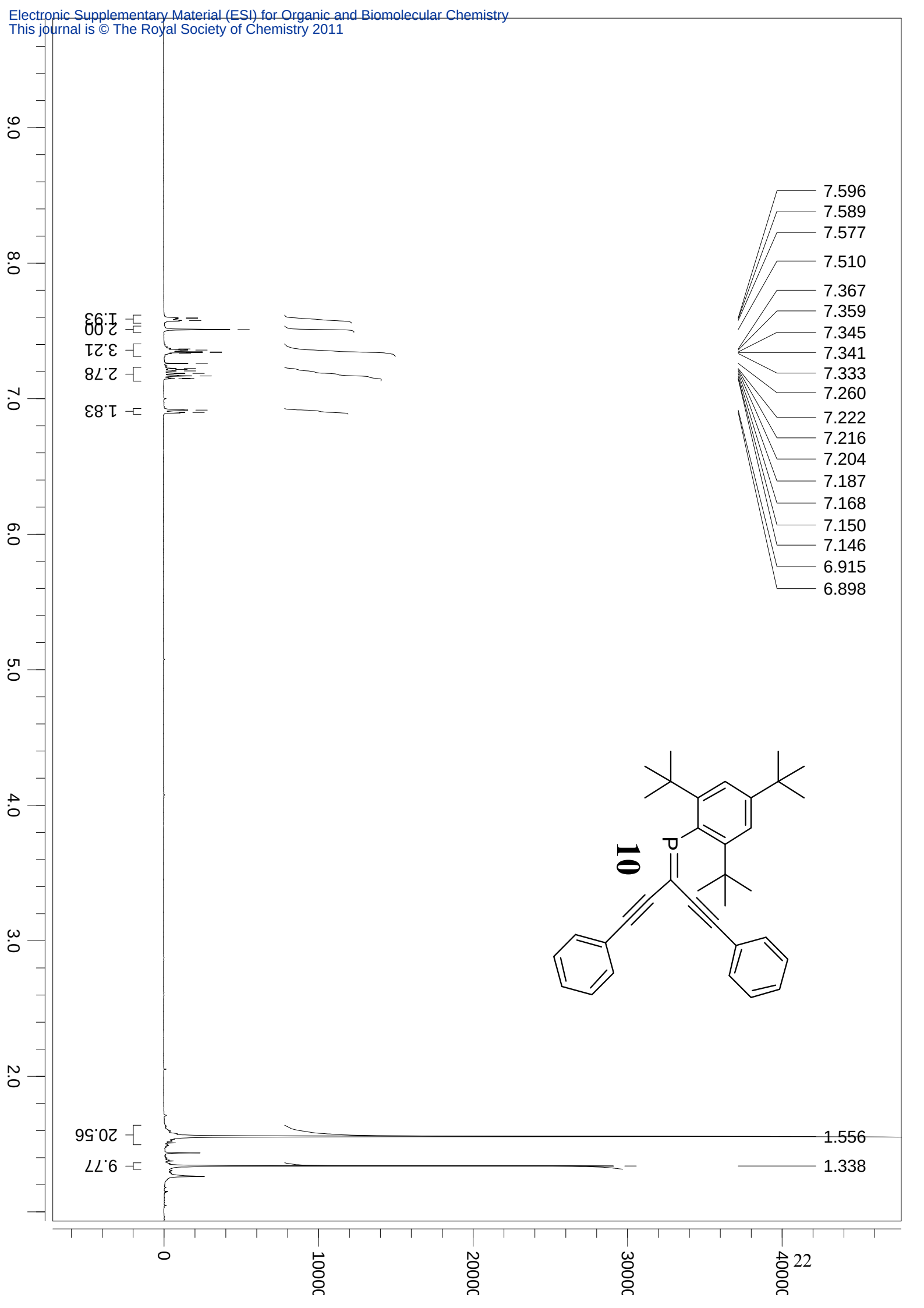
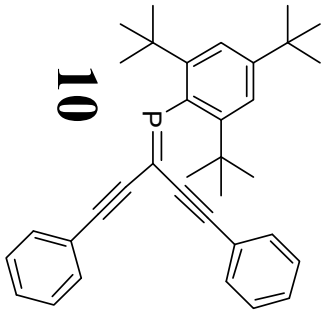
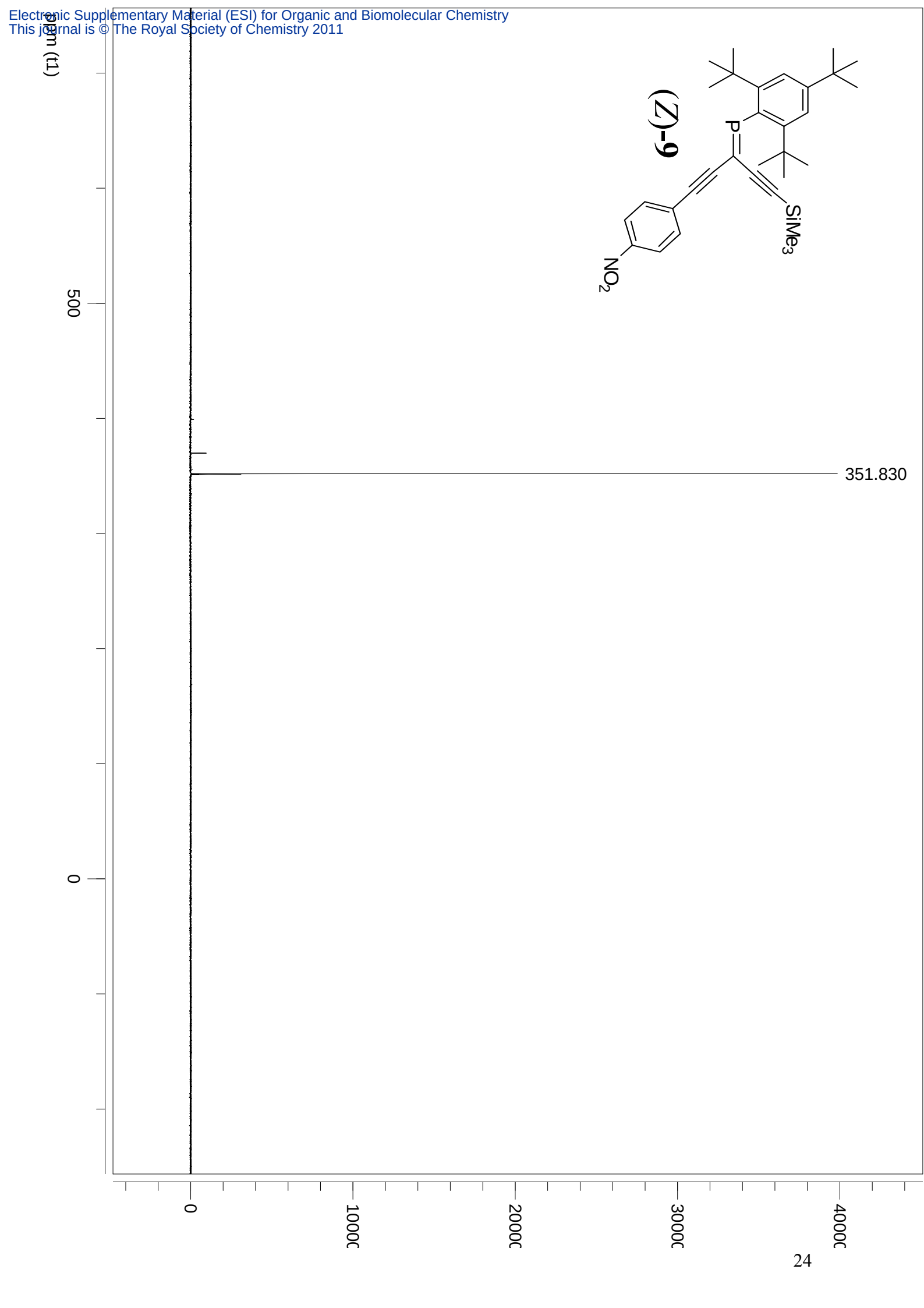
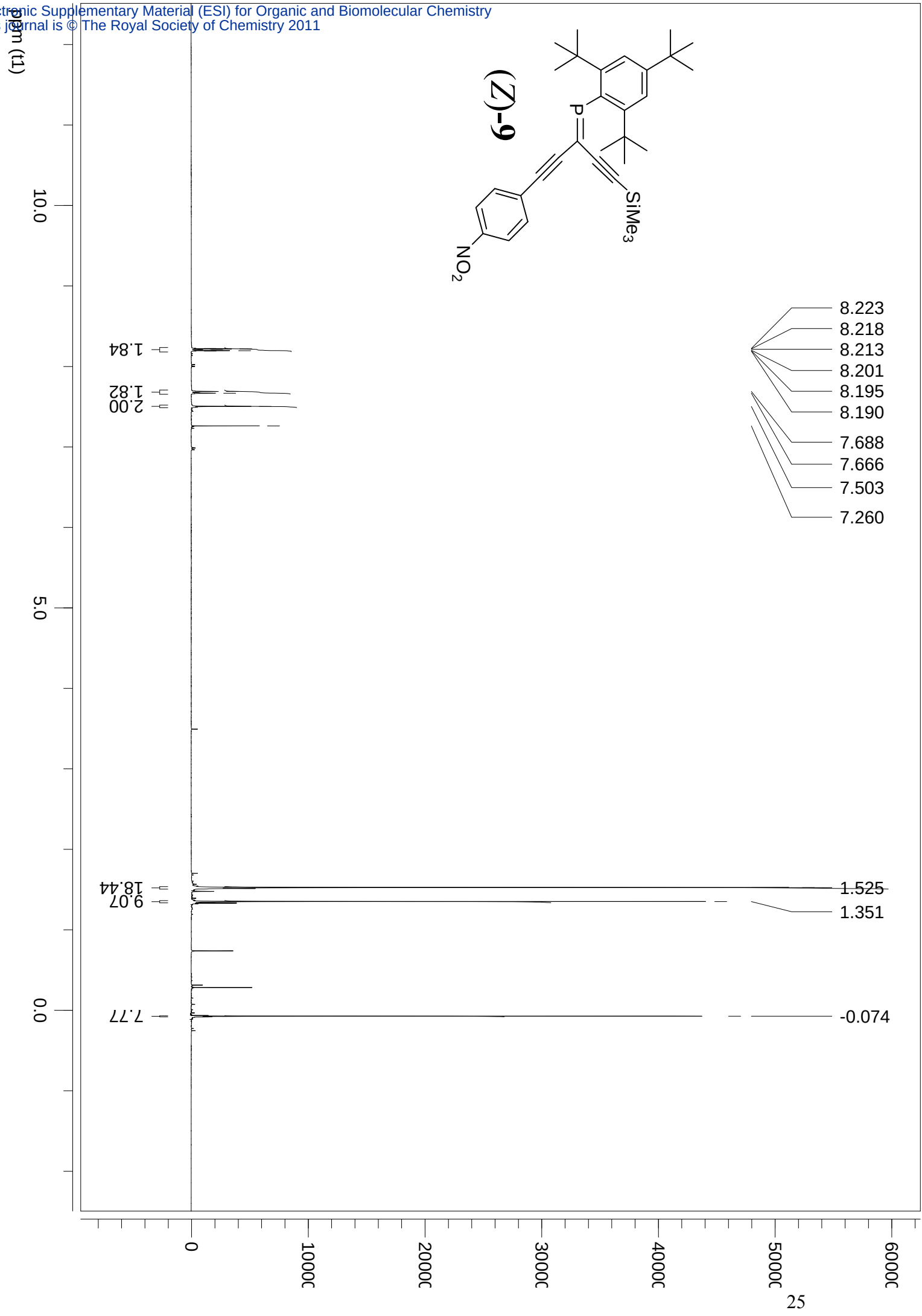
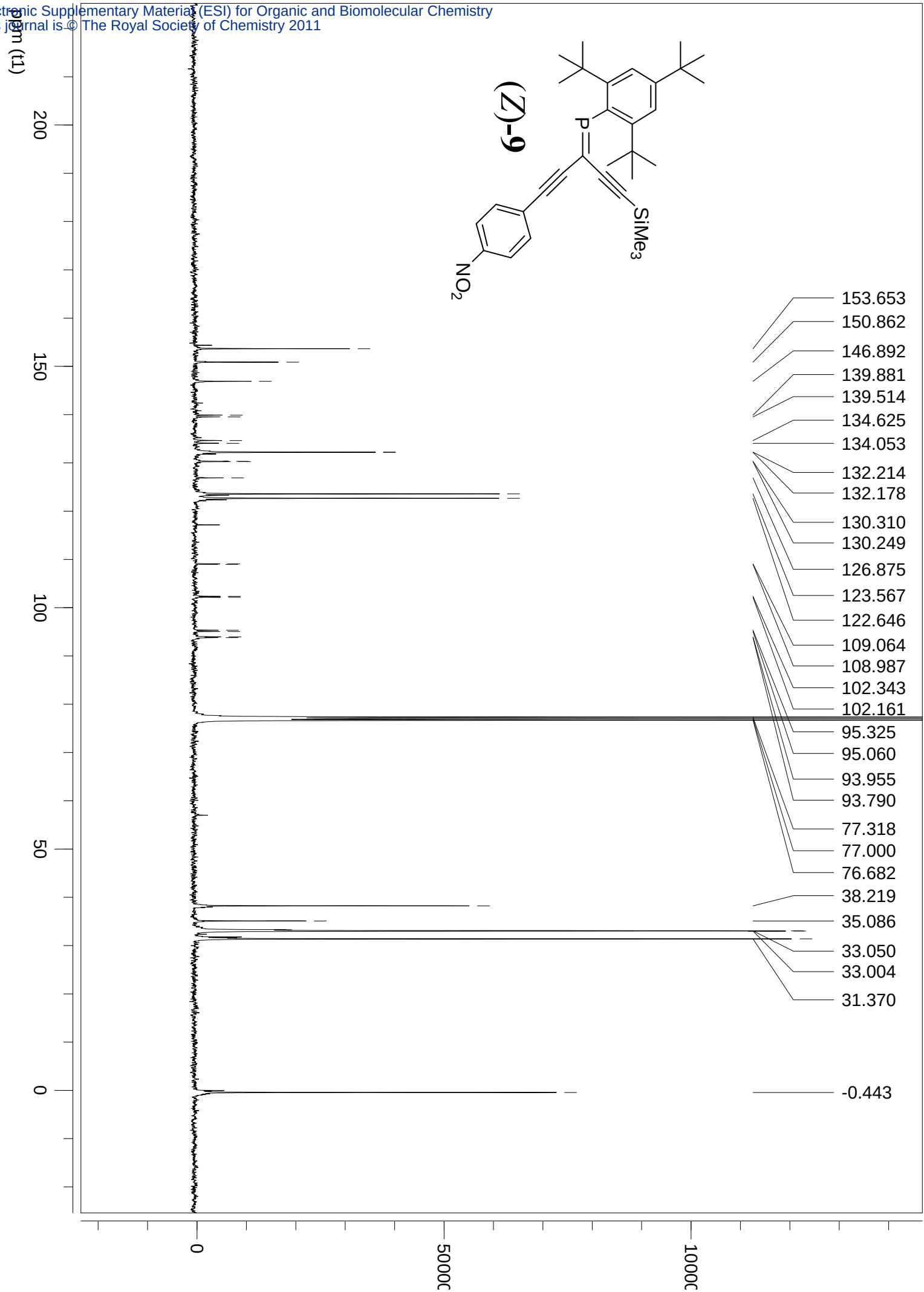


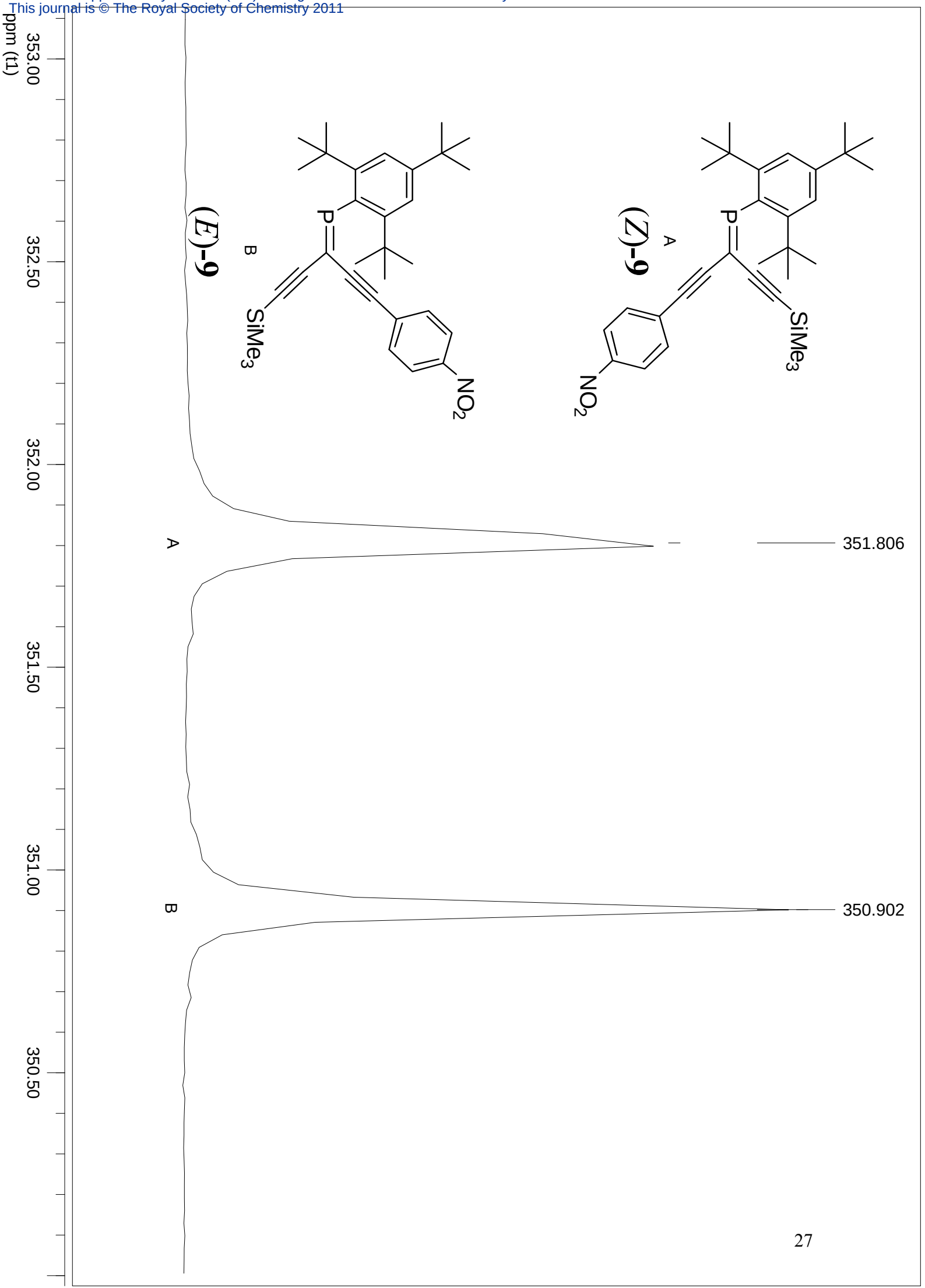


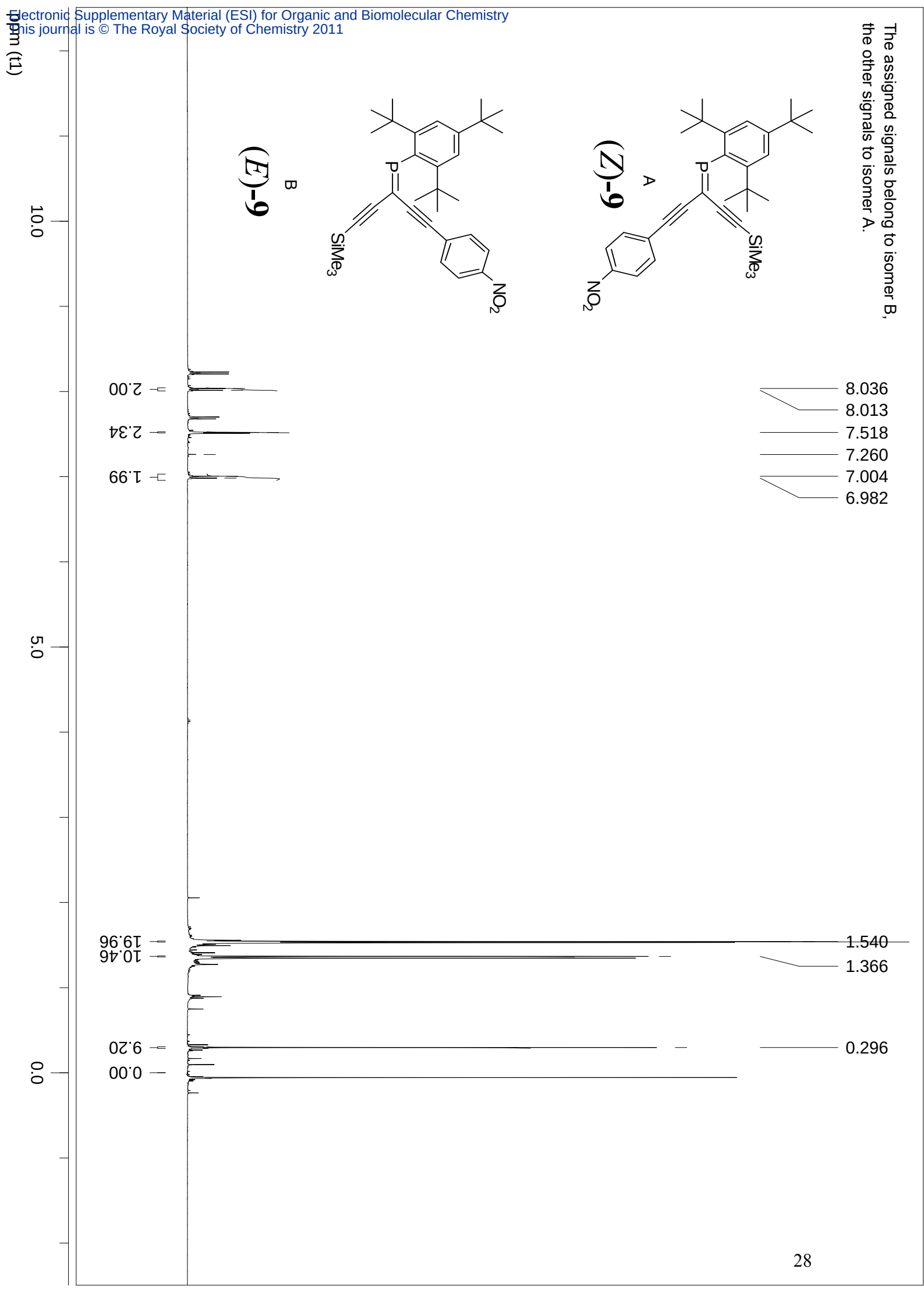




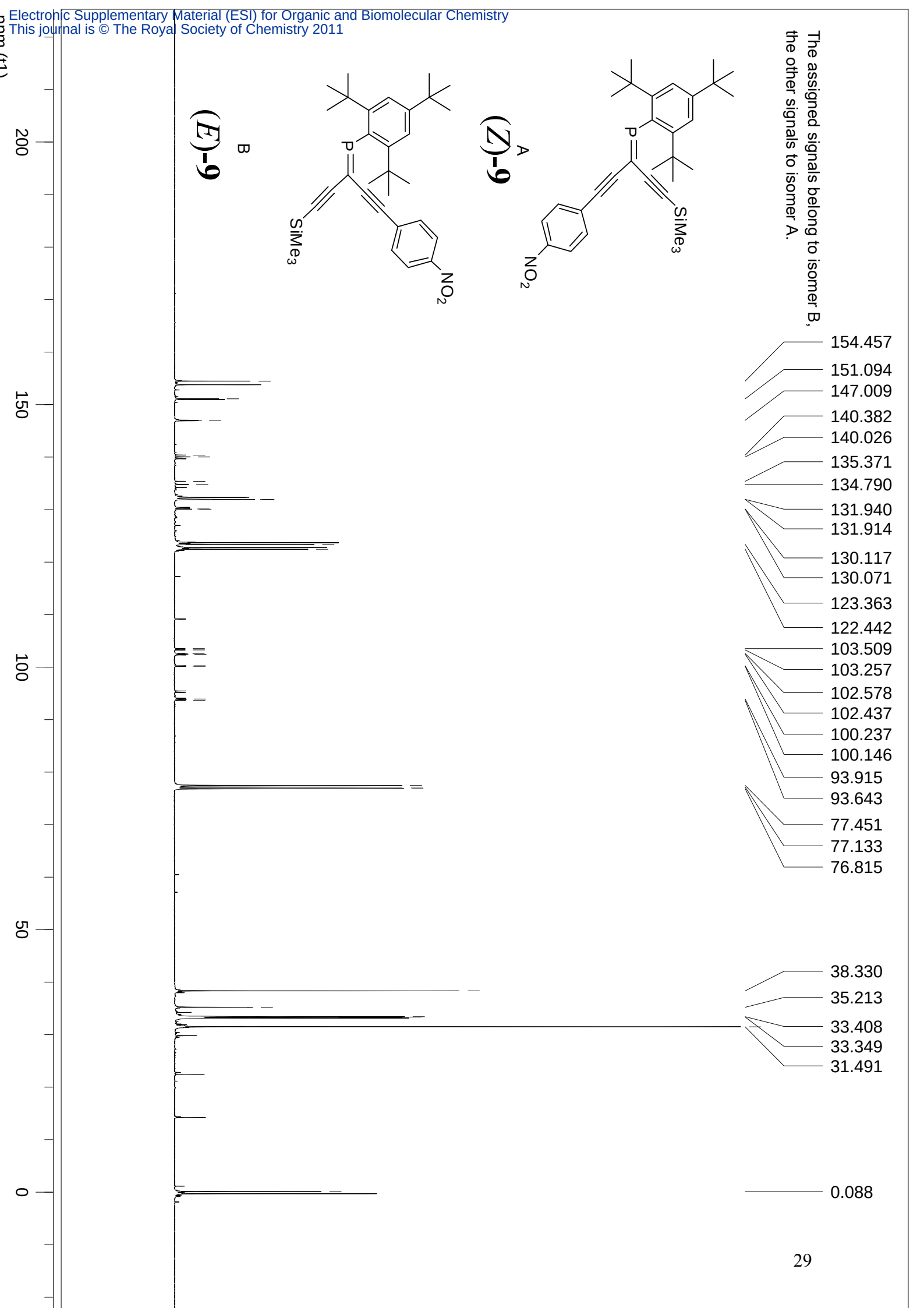


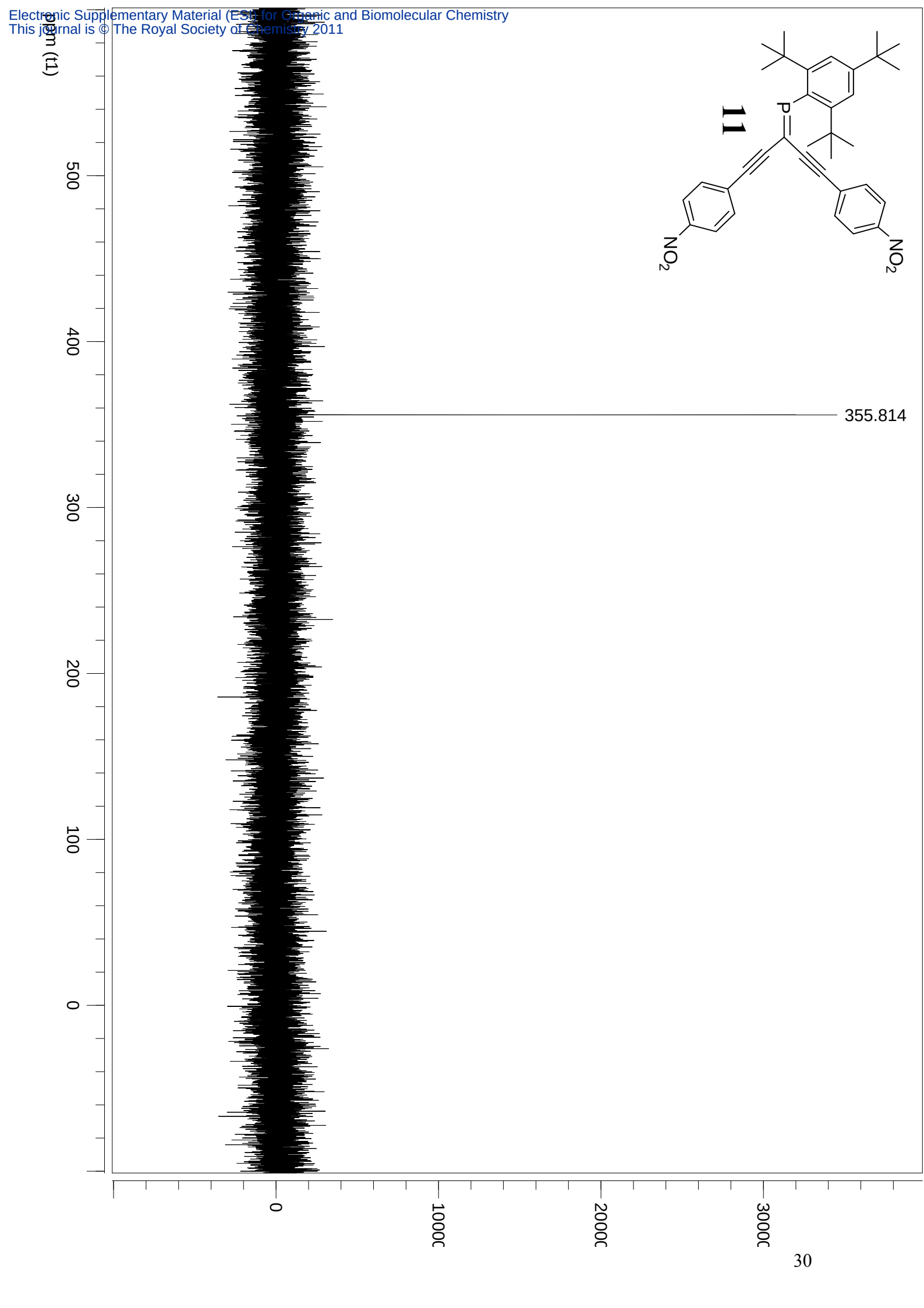


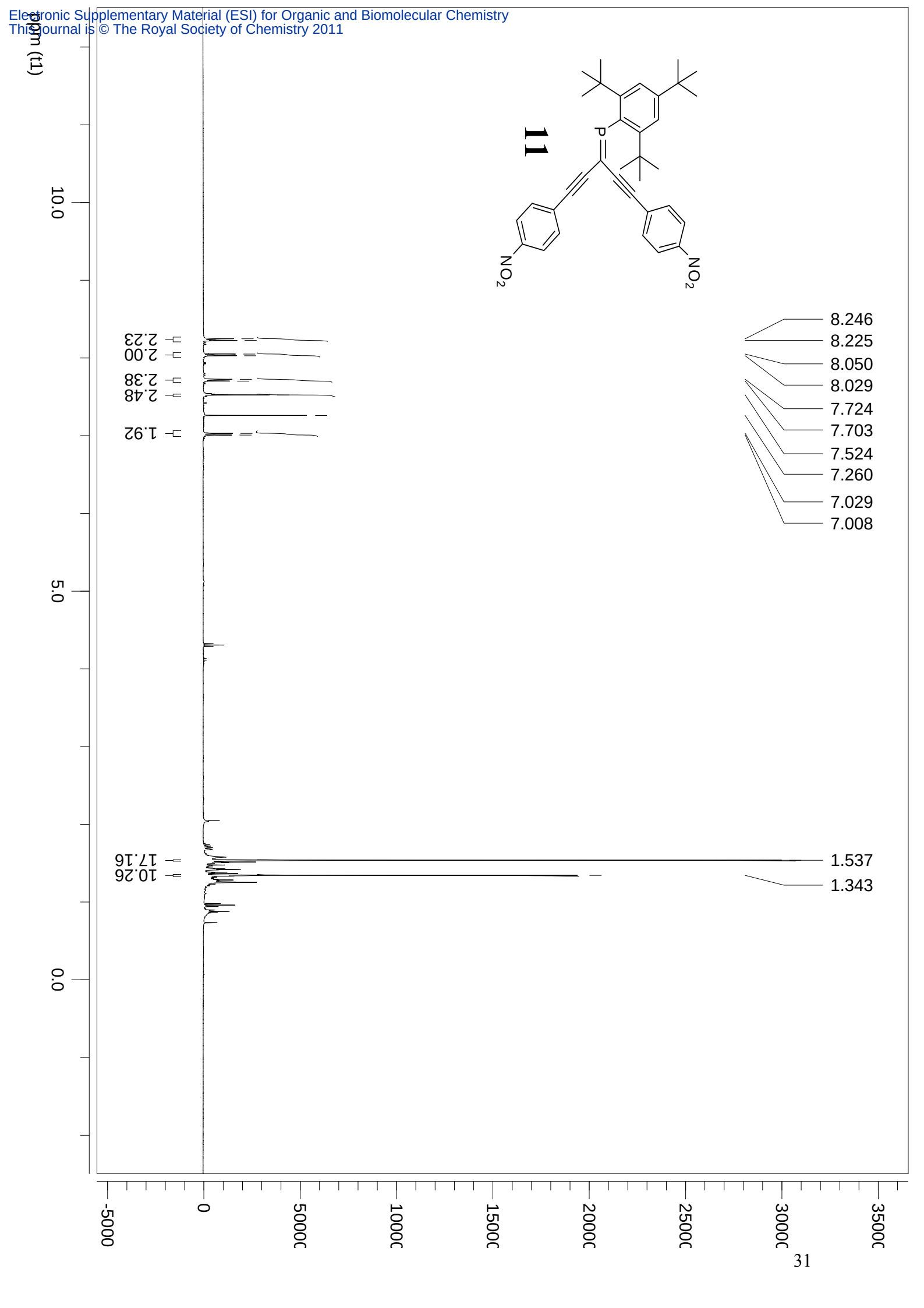


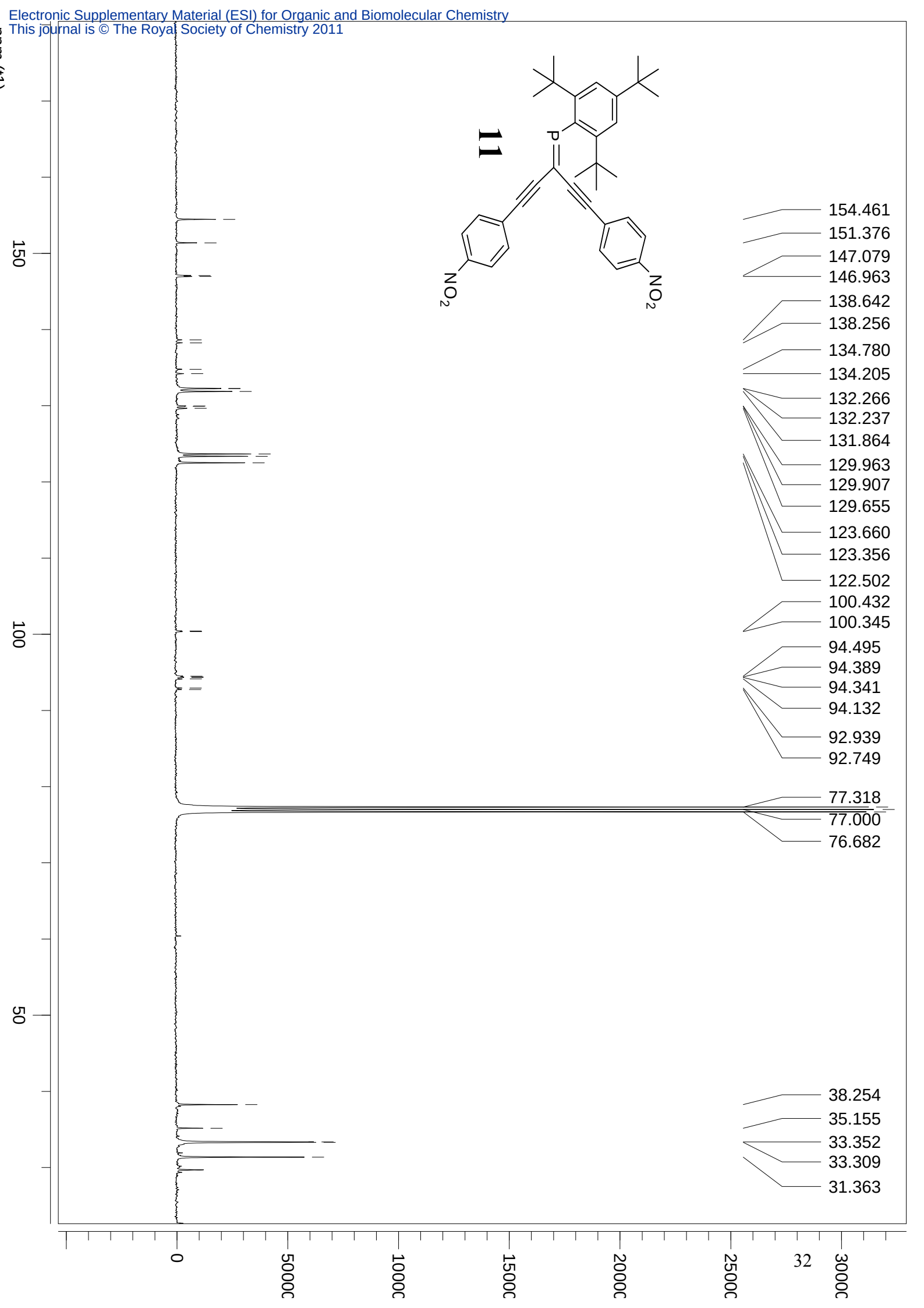


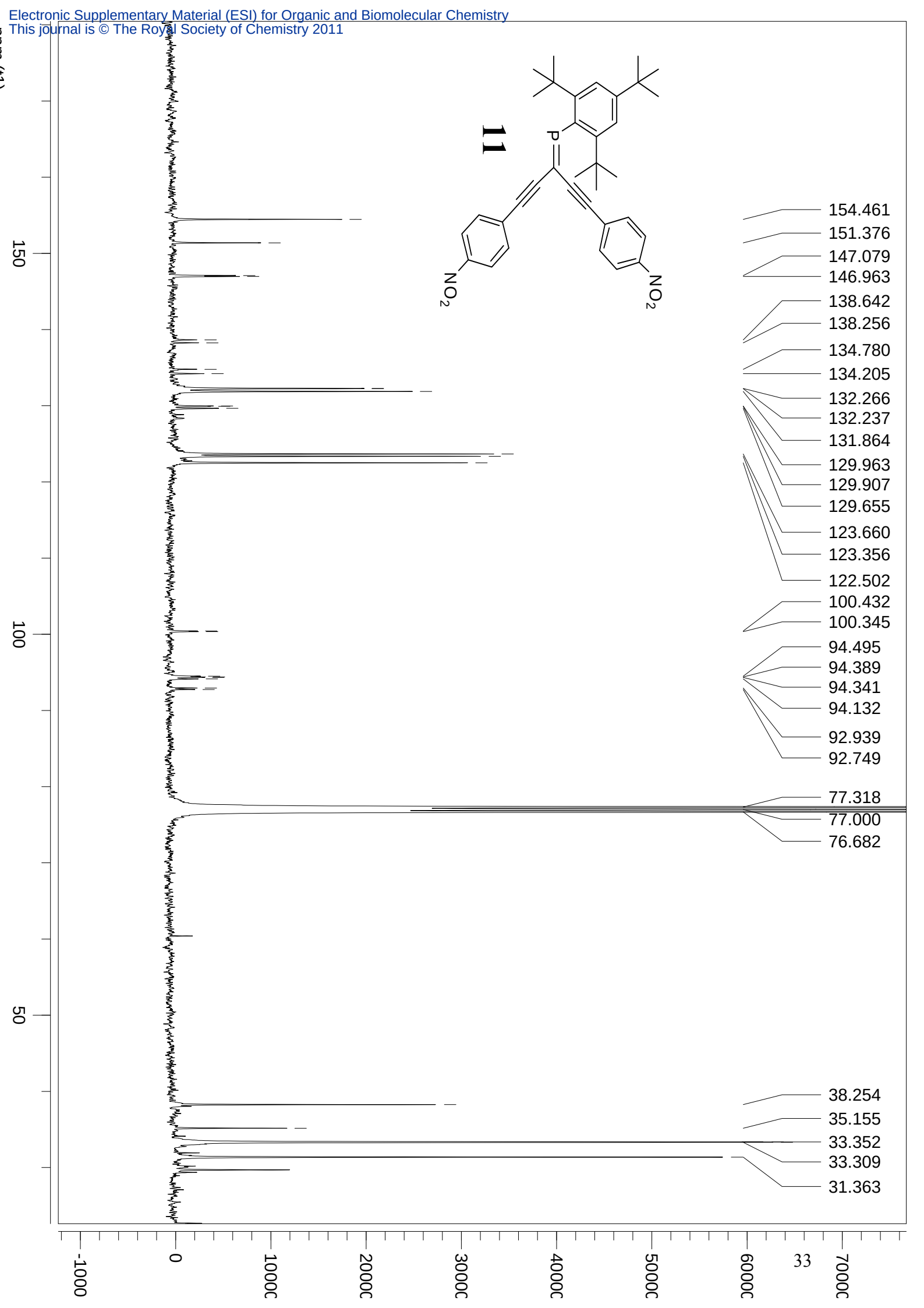
The assigned signals belong to isomer B, the other signals to isomer A.

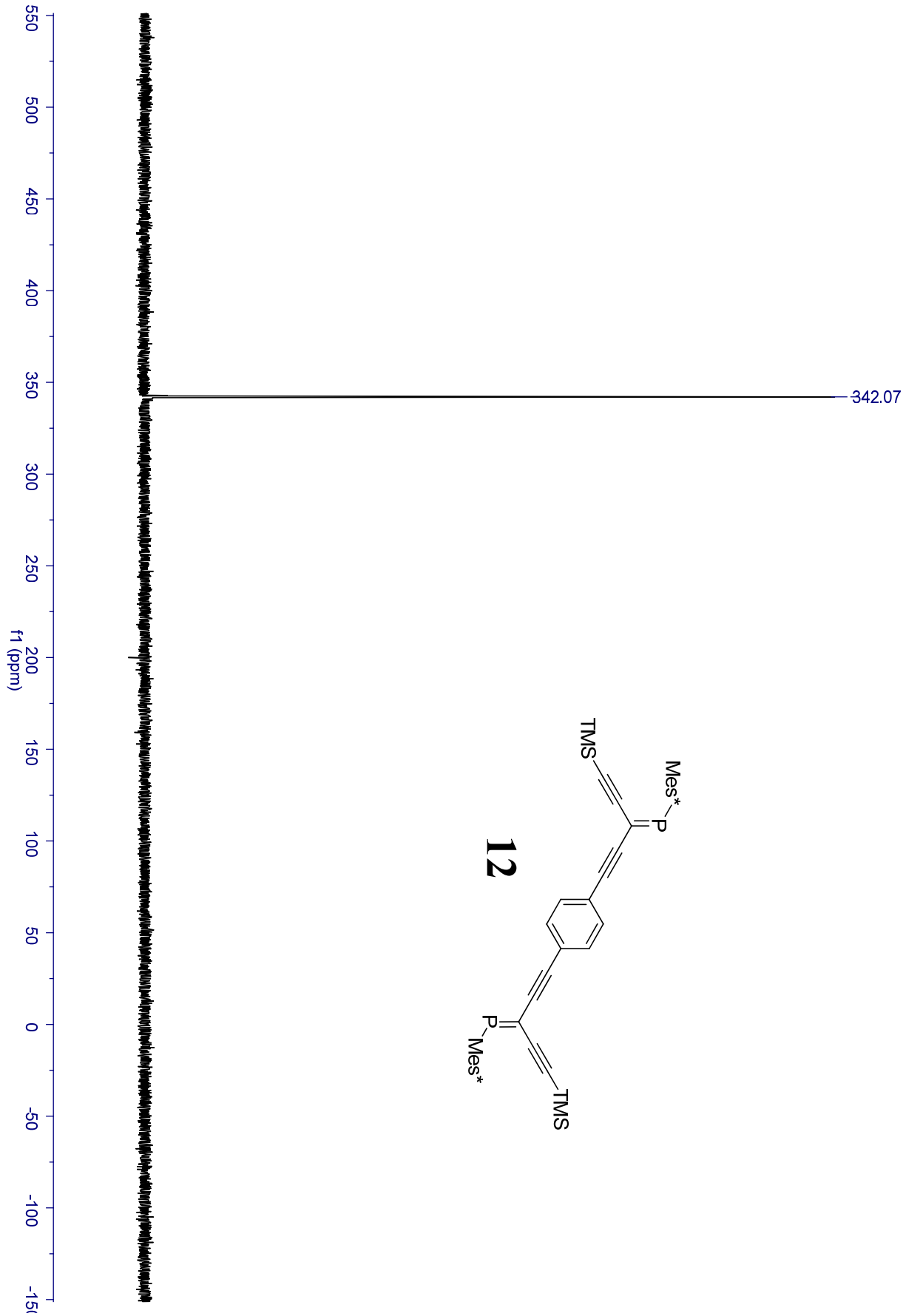


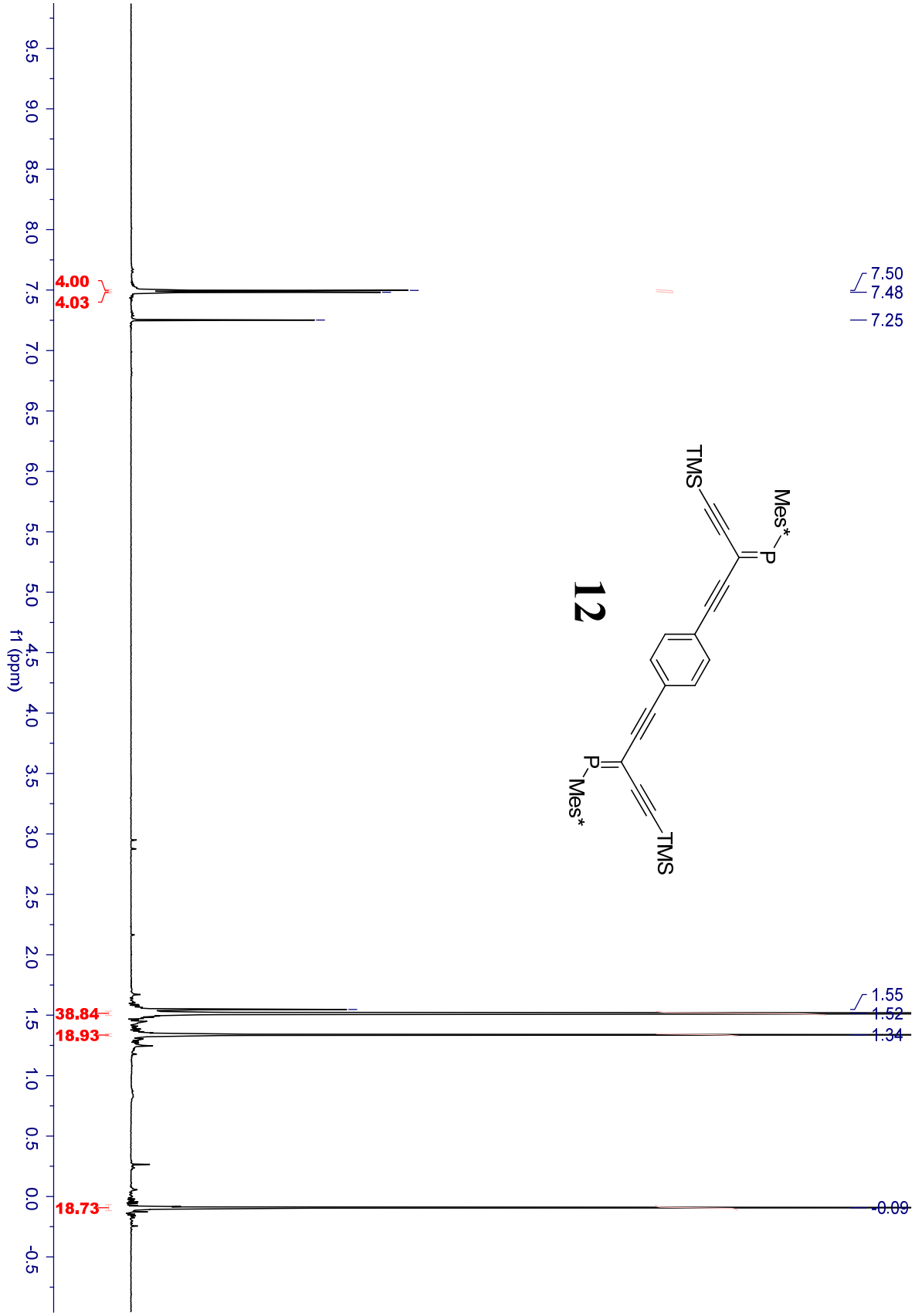


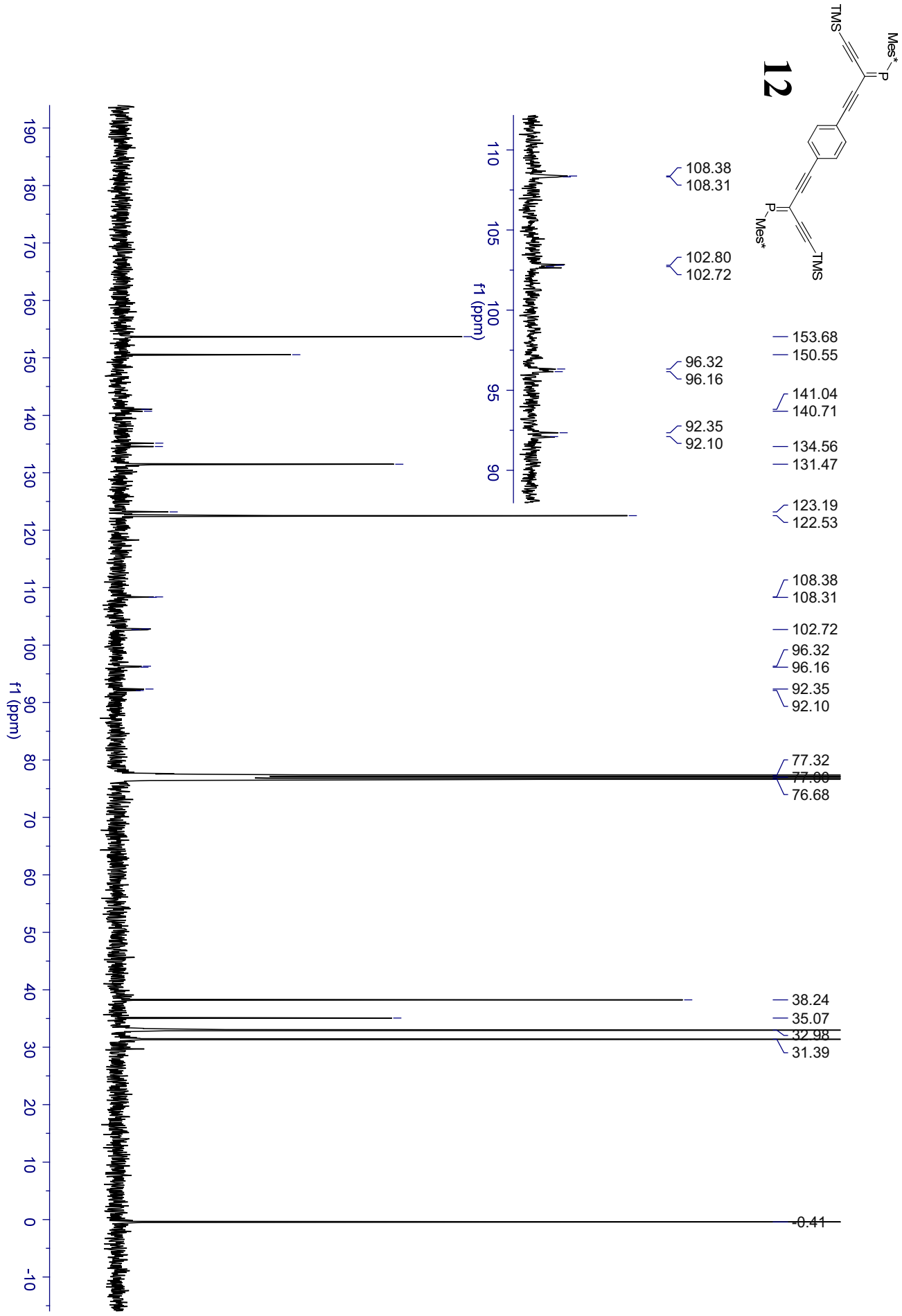


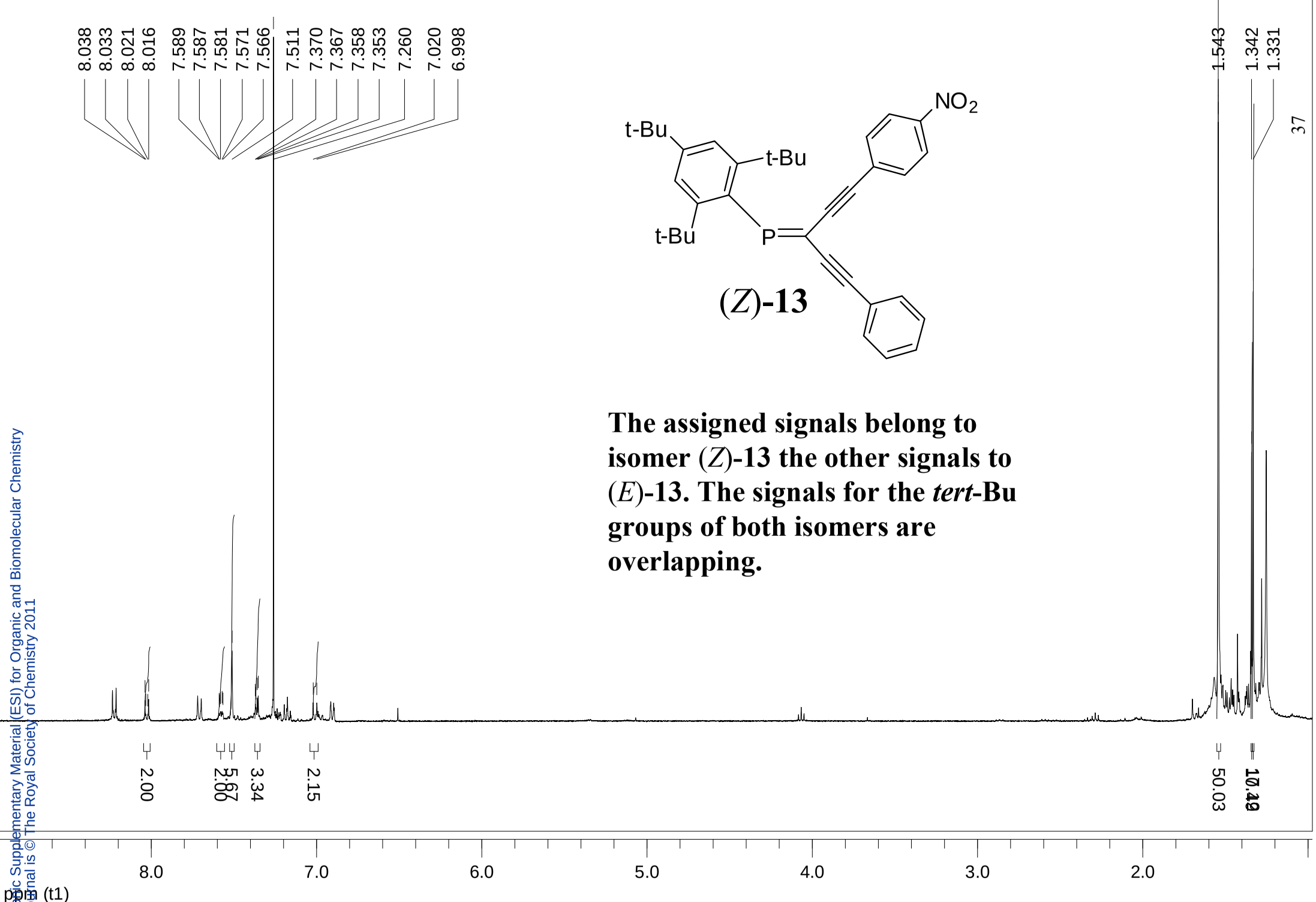


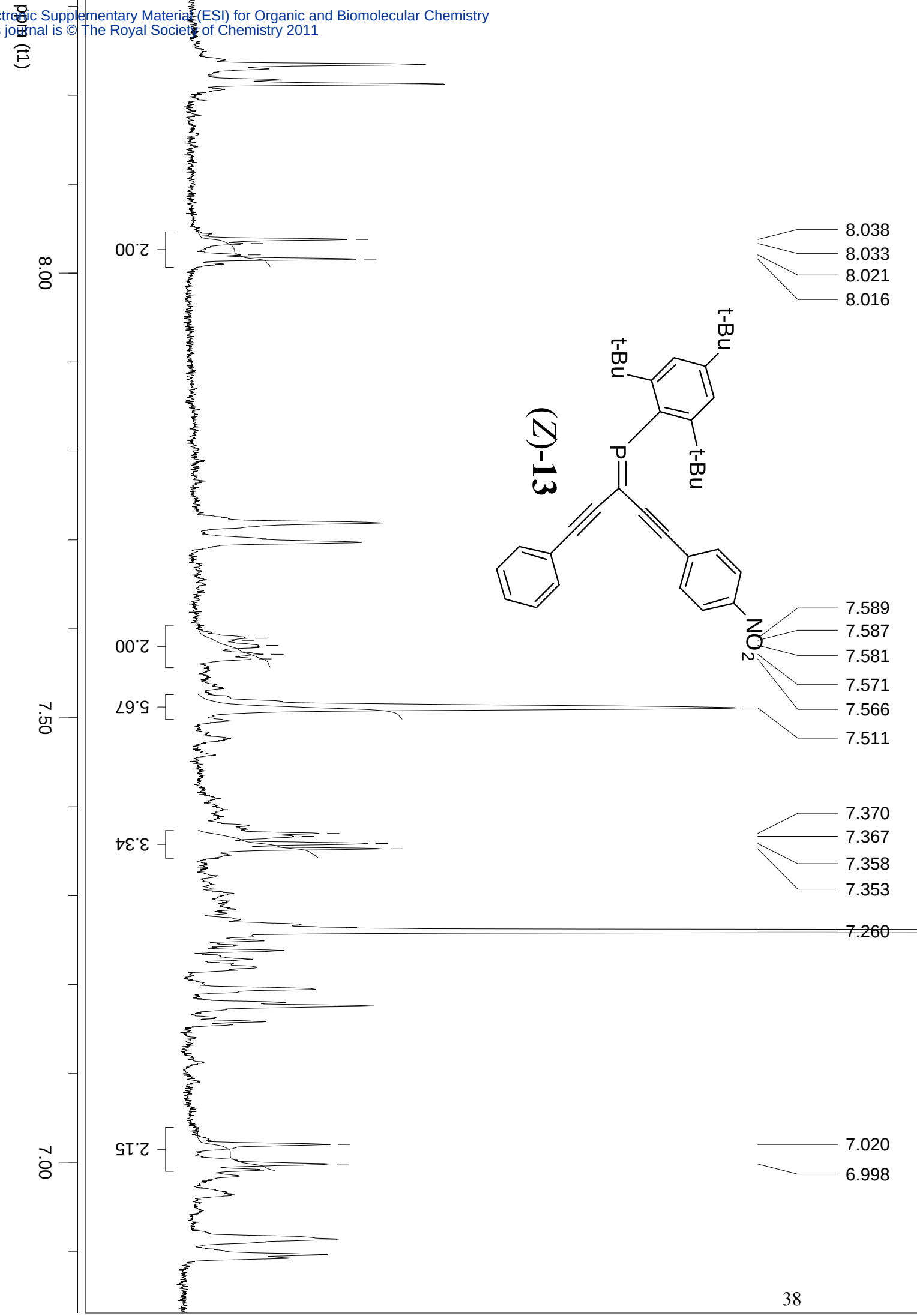






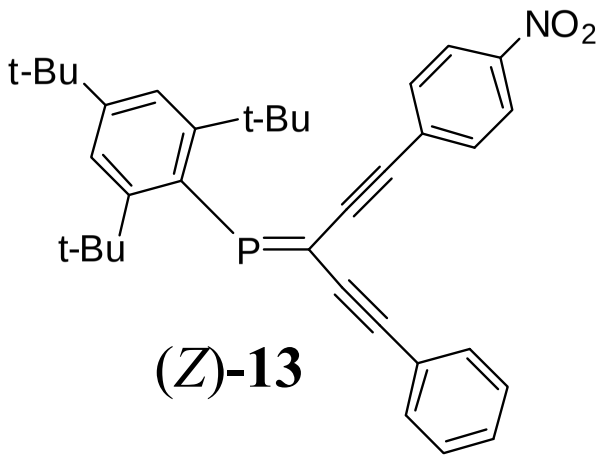




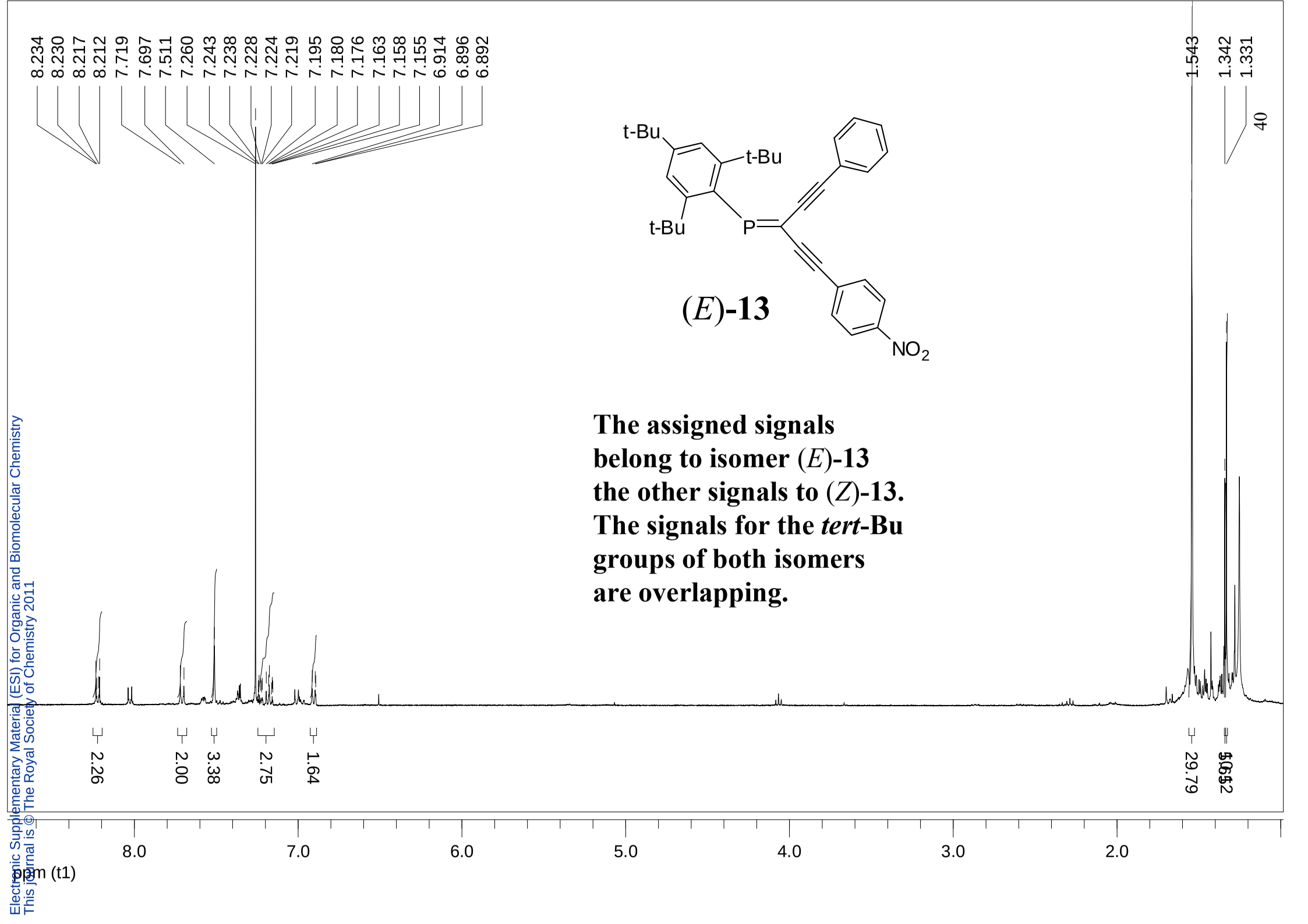


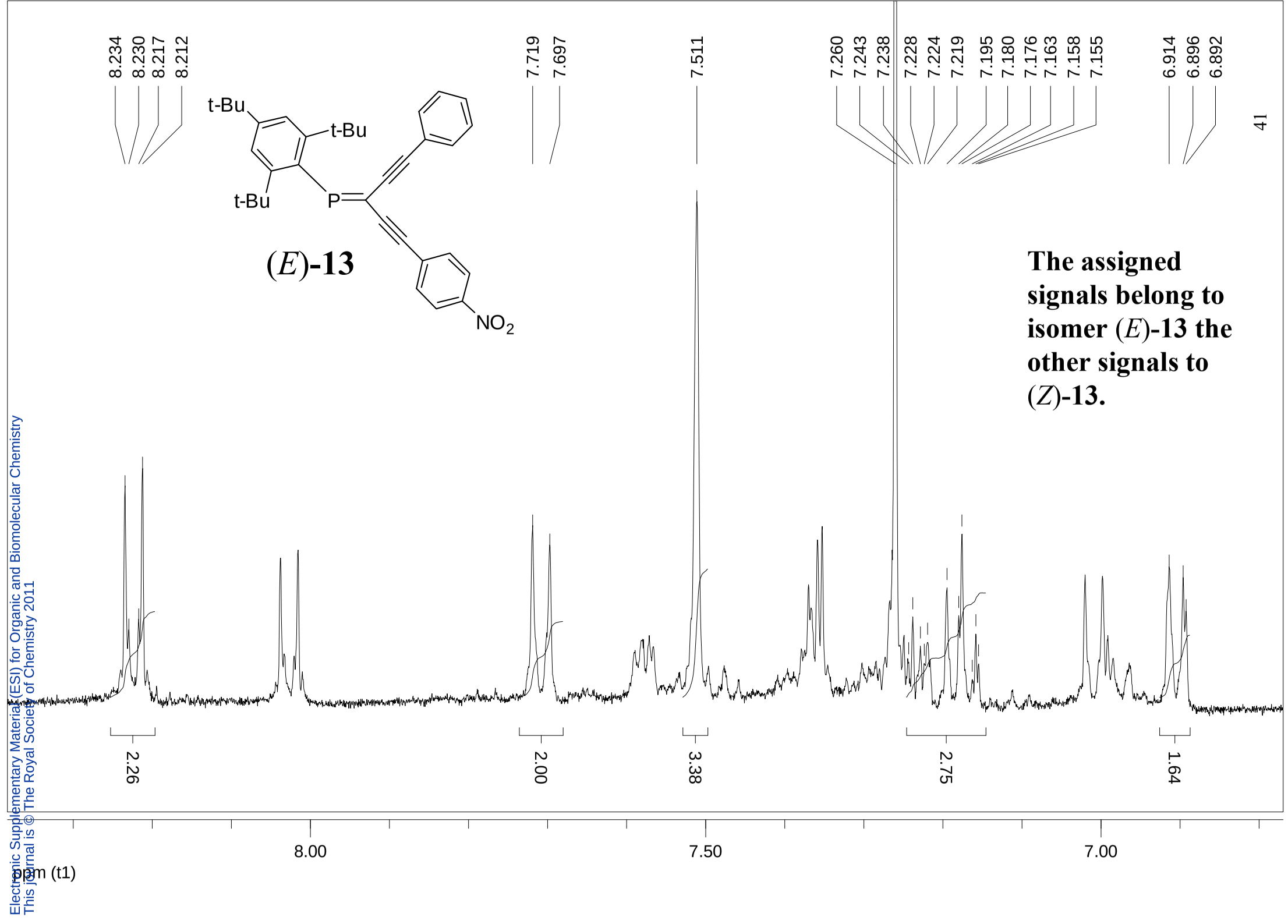
(Z)-13

The assigned signals belong to isomer (*Z*)-13 the other signals to (*E*)-13. The signals for the *tert*-Bu groups of both isomers are overlapping.

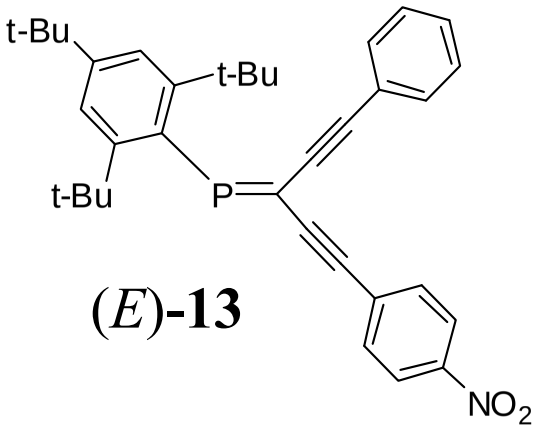


(*Z*)-13





The assigned signals belong to isomer (*E*)-13 the other signals to (*Z*)-13. The signals for the *tert*-Bu groups of both isomers are overlapping.



(*E*)-13