Electronic Supplementary Material (ESI) for Dalton Transactions.

Supplementary Information

Organophosphorus Decorated Lithium Borate and Phosphate Salts with Extended π-Conjugated Backbone

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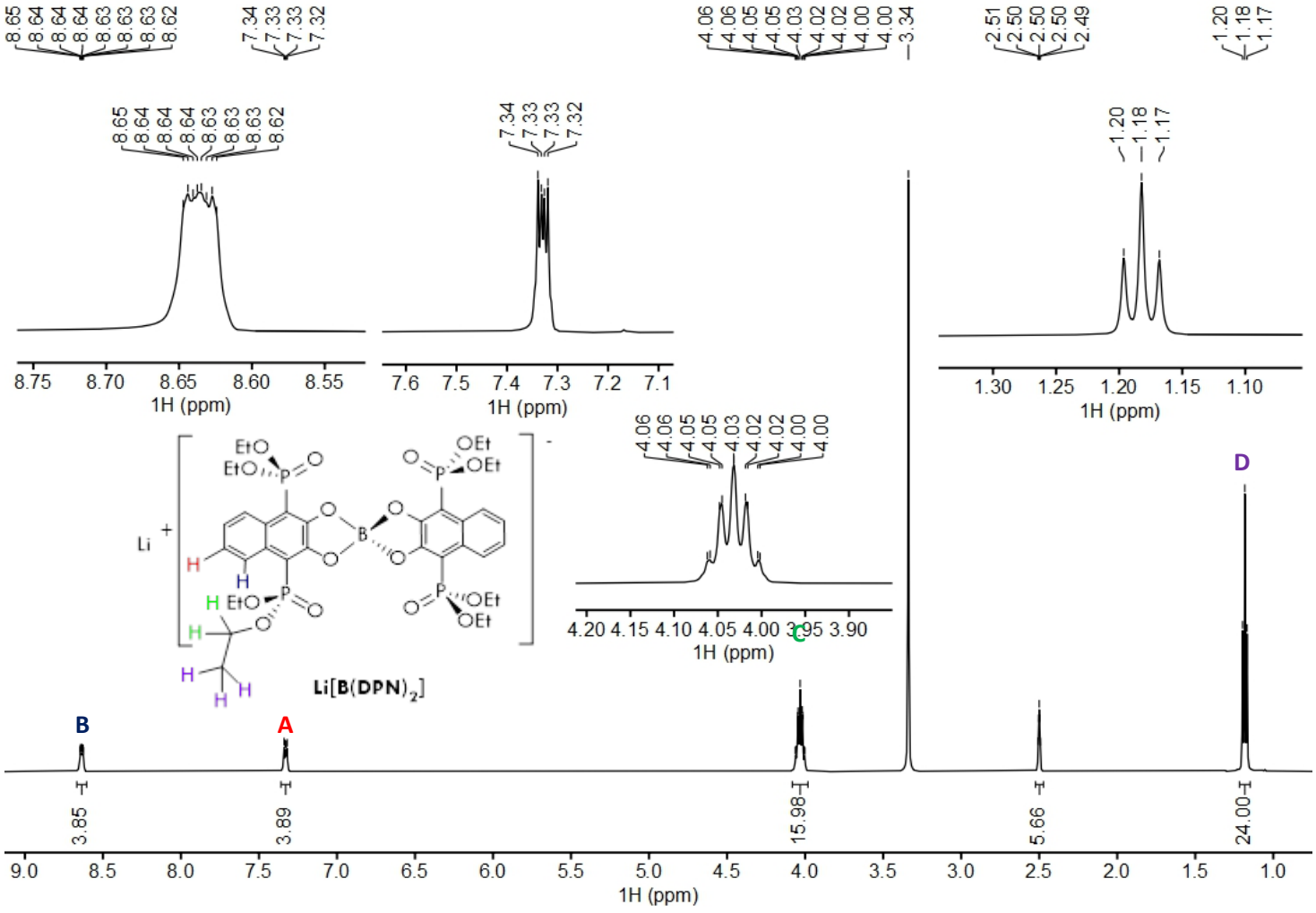

Figure S1. ^{1}H NMR (500 MHz, DMSO-d_6) spectrum of Li[B(DPN)$_2$].

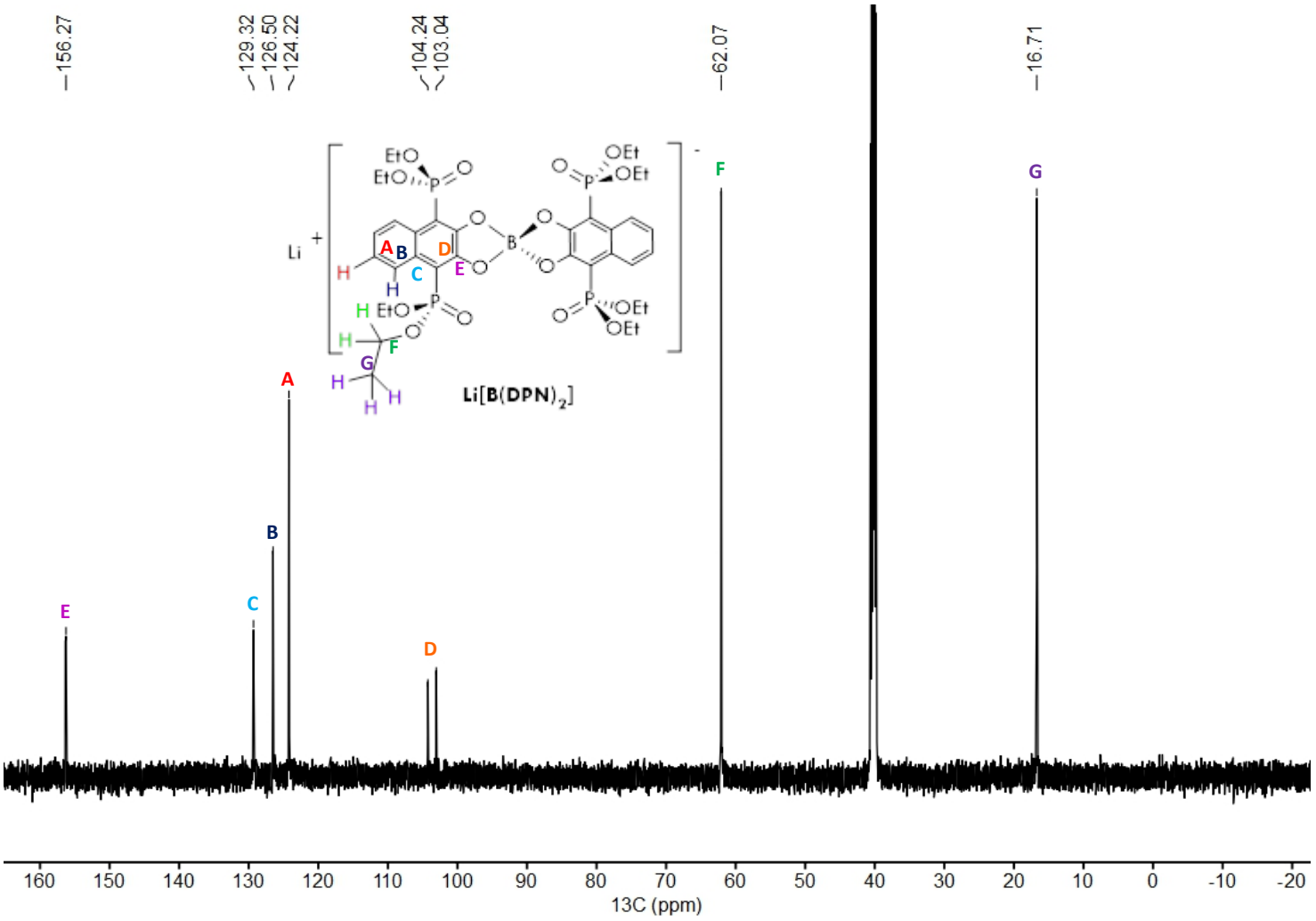

Figure S2. $^{13}C\{^{1}H\}$ NMR (126 MHz, DMSO-d_6) spectrum of Li[B(DPN)$_2$].

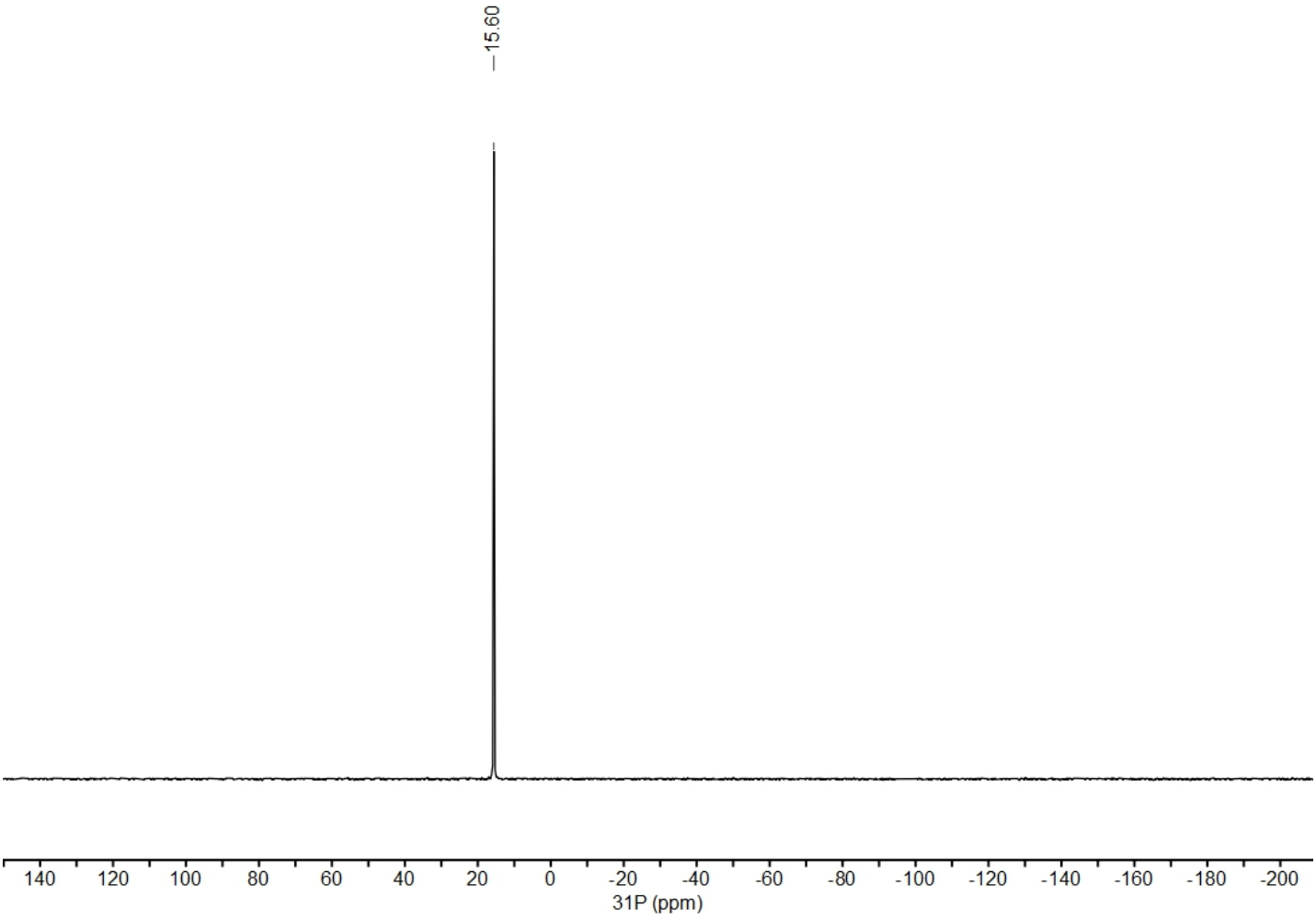

Figure S3. $^{31}P\{^{1}H\}$ NMR (202 MHz, DMSO-d_6) spectrum of $Li[B(DPN)_2]$.

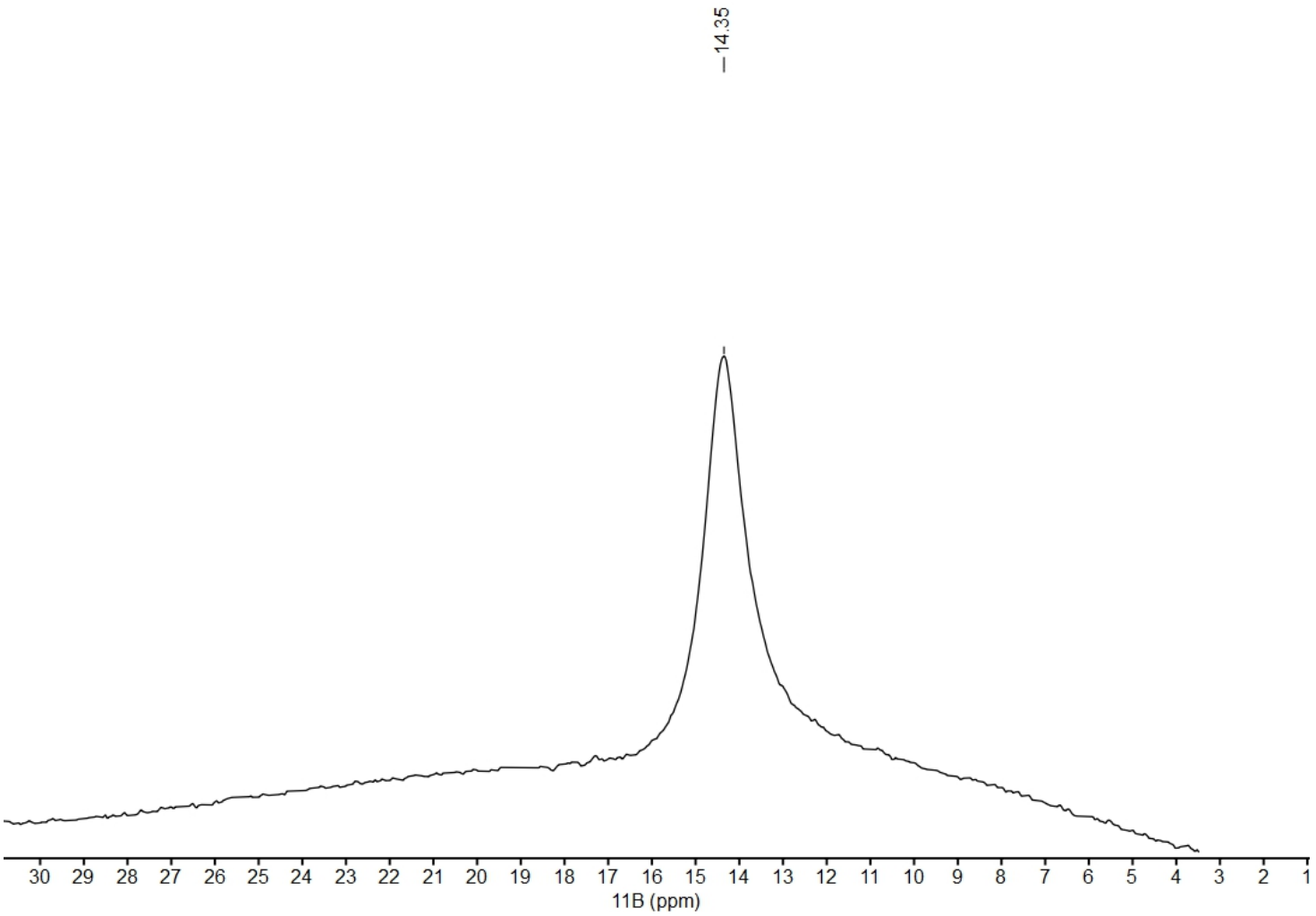

Figure S4. ^{11}B NMR (160 MHz, DMSO-d_6) spectrum of Li[B(DPN)$_2$].

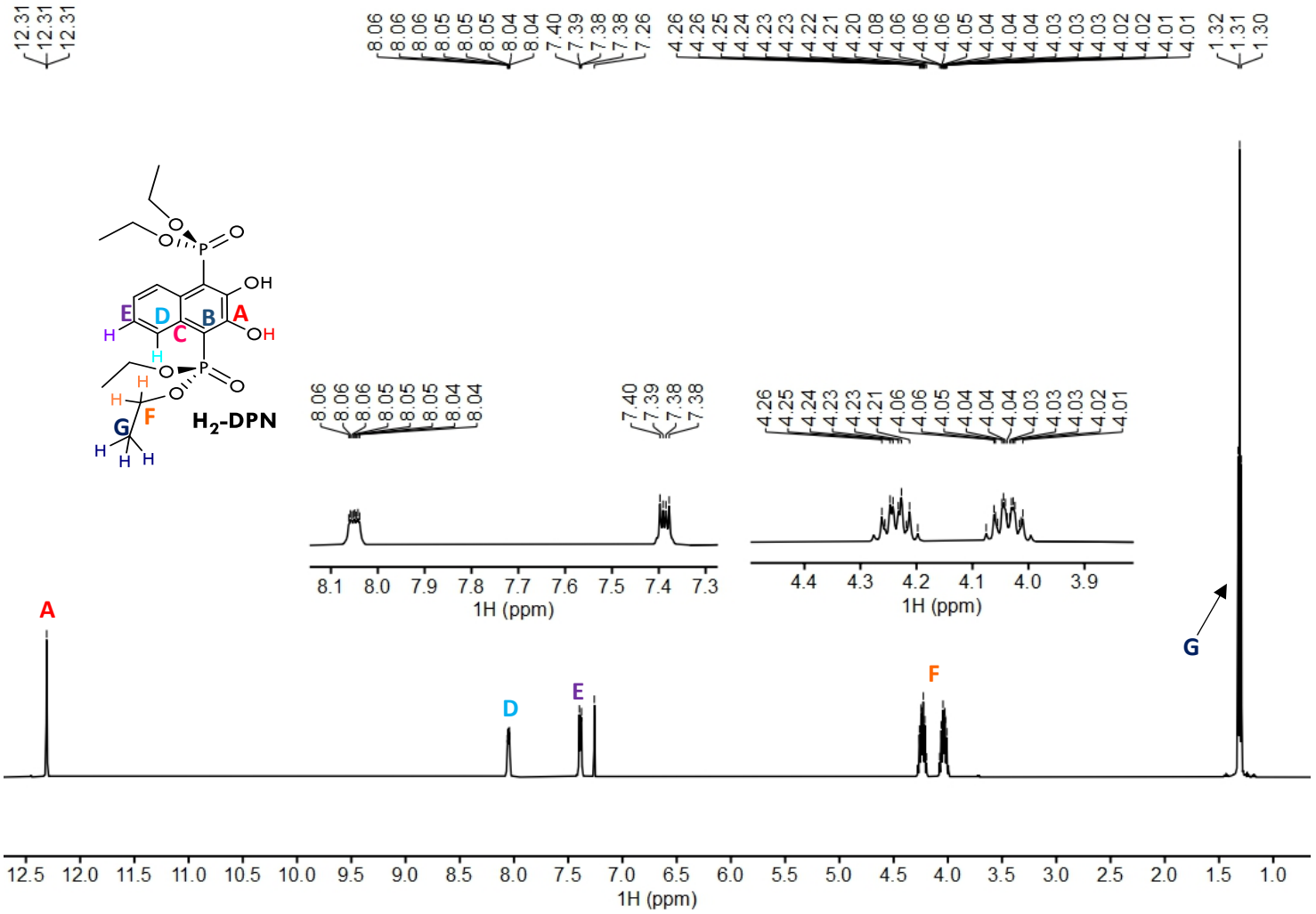

Figure S5. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of H_2-DPN.

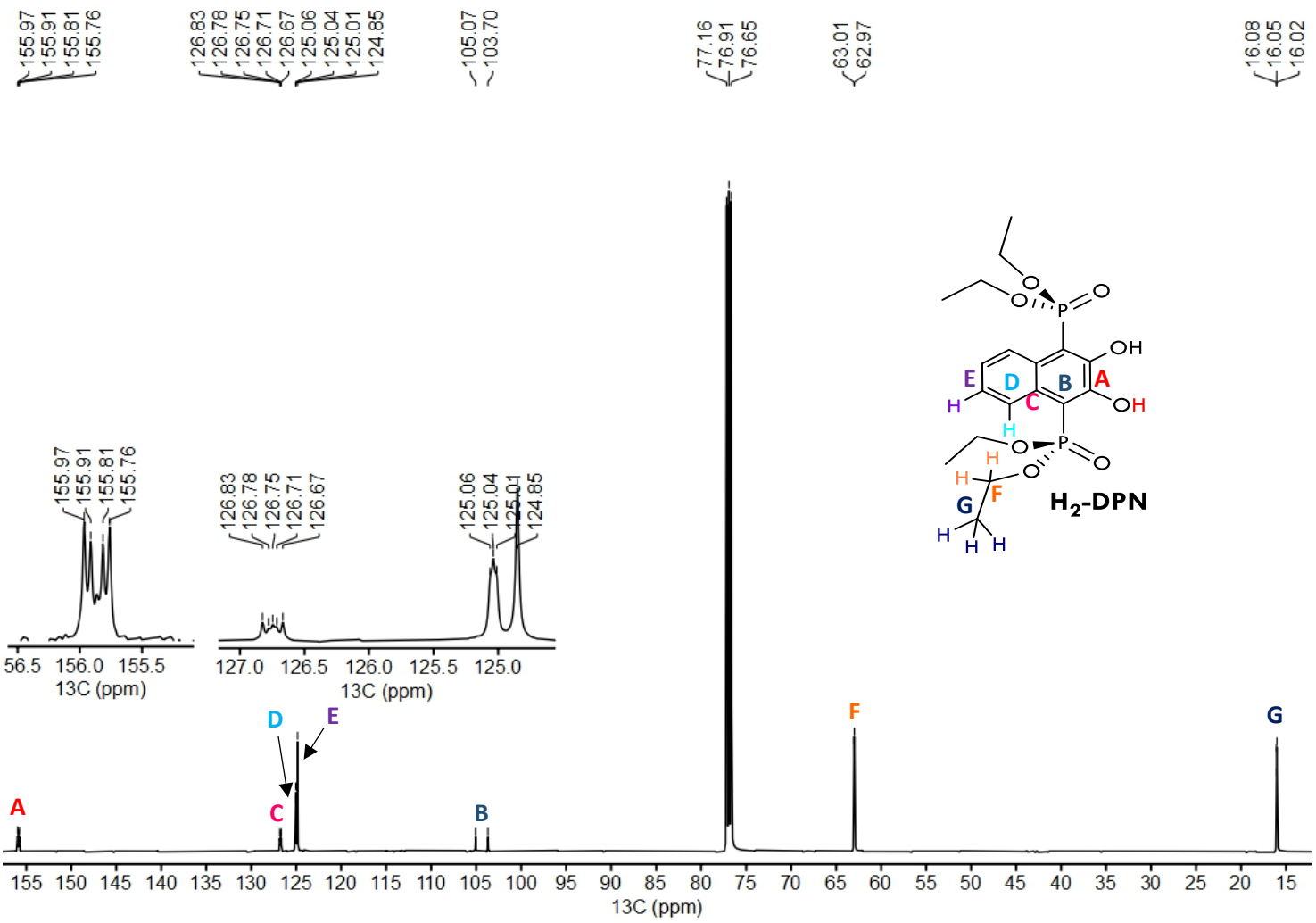

Figure S6. $^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$) spectrum of H_2-DPN.

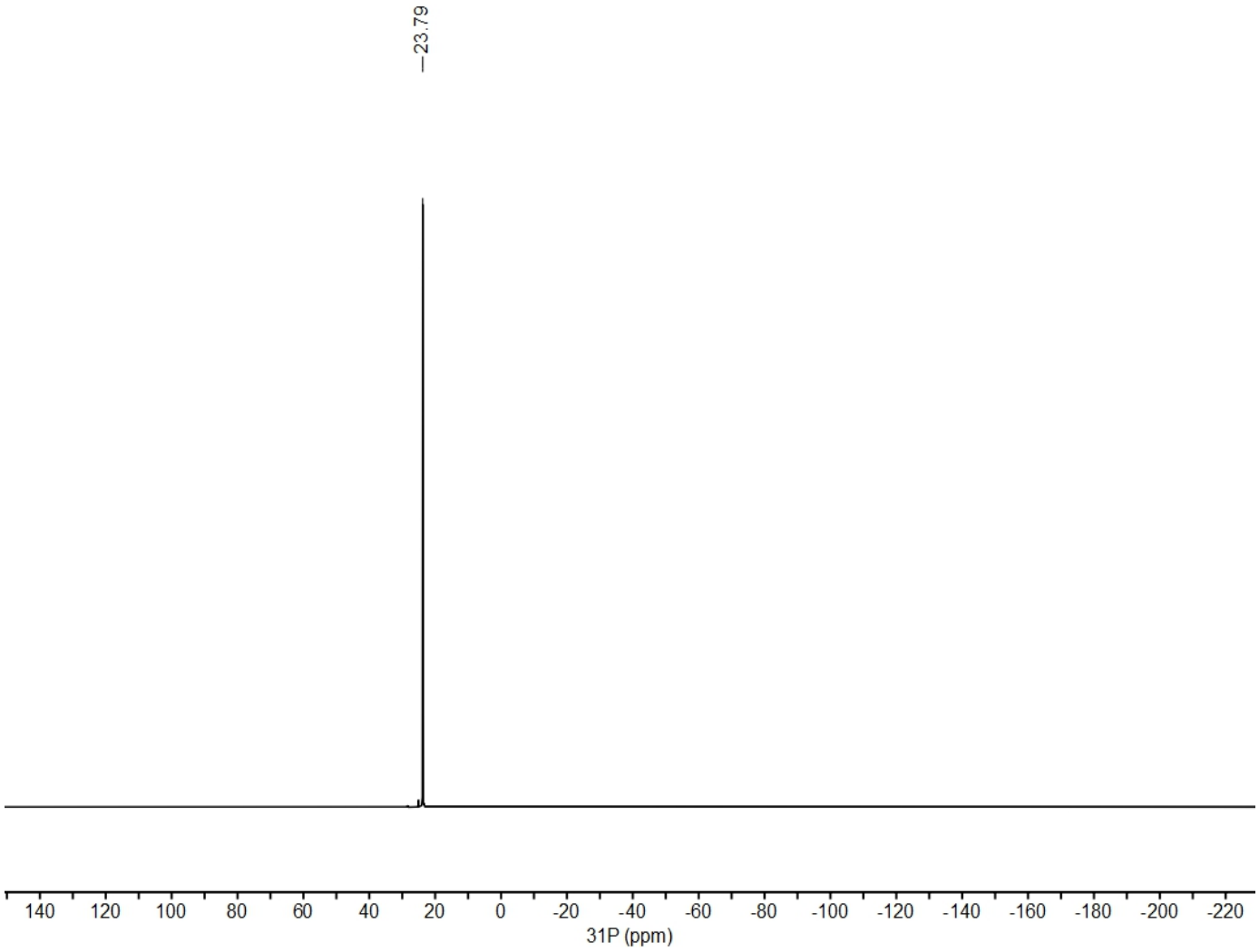

Figure S7. $^{31}P\{^{1}H\}$ NMR (202 MHz, $CDCl_3$) spectrum of H_2-DPN.

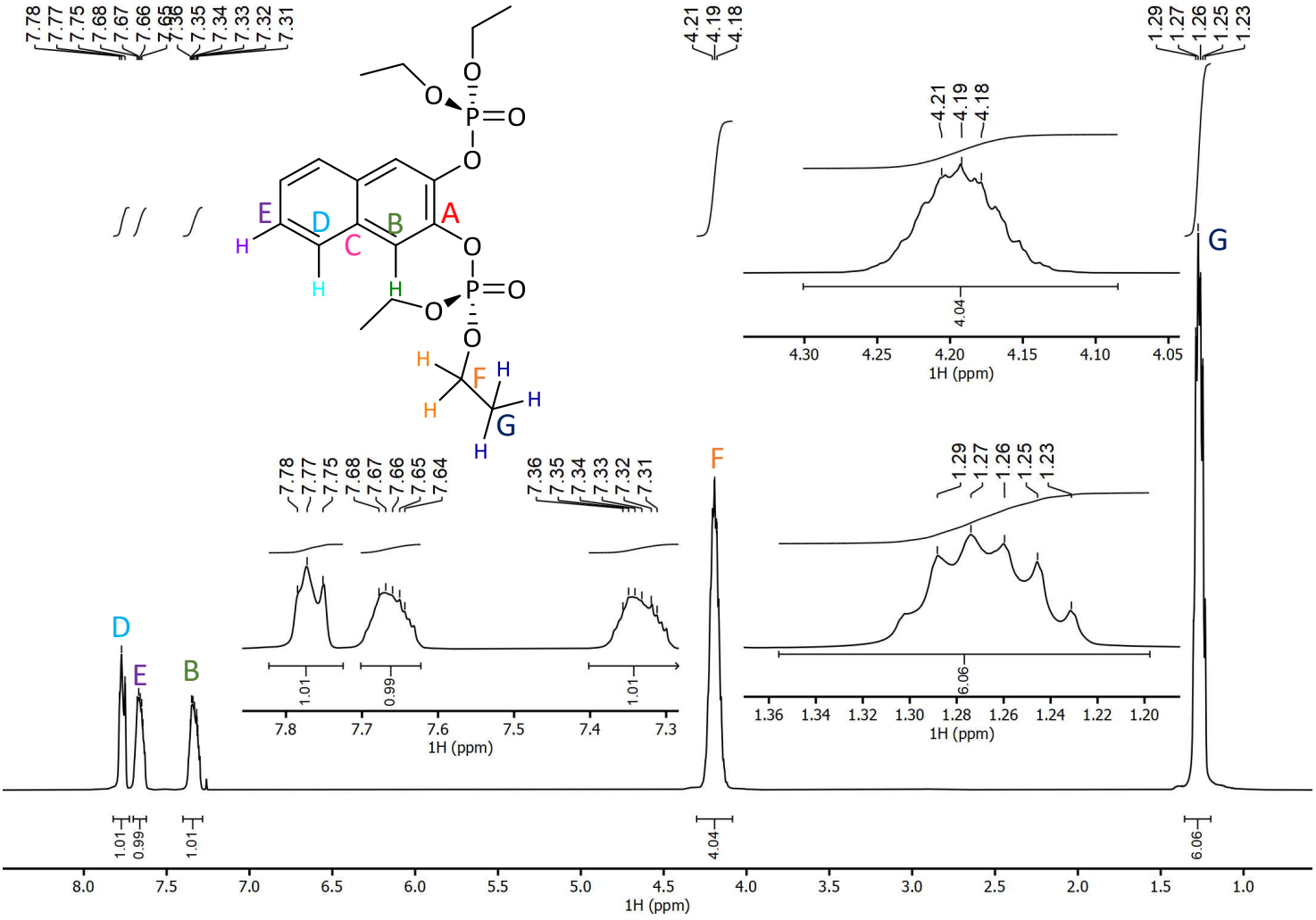

Figure S8. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of 2,3-dihydroxy-1,4-diphosphinatonaphthalene.

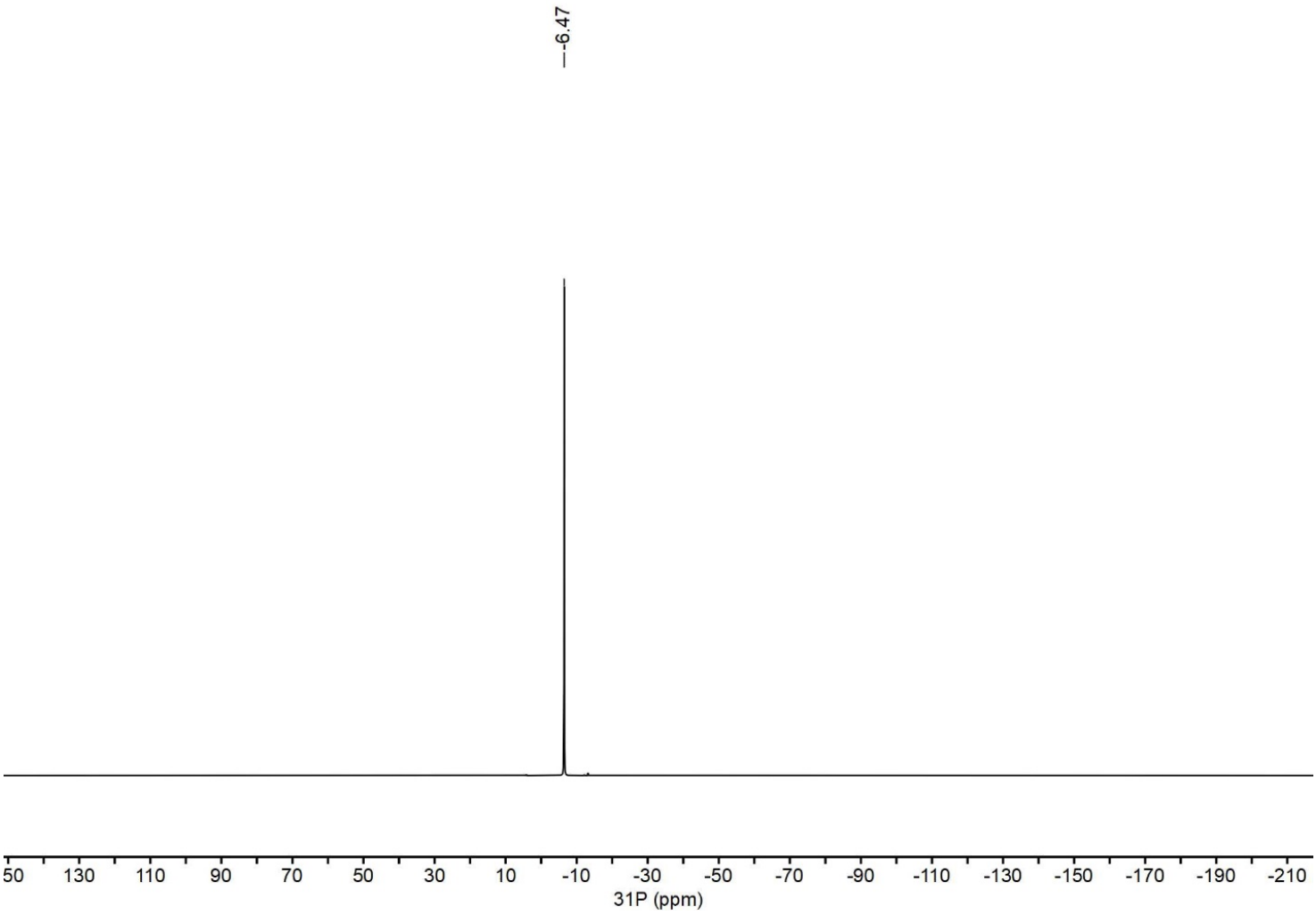

Figure S9. $^{31}P\{^{1}H\}$ NMR (202 MHz, $CDCl_3$) spectrum of 2,3-dihydroxy-1,4-diphosphinatonaphthalene.

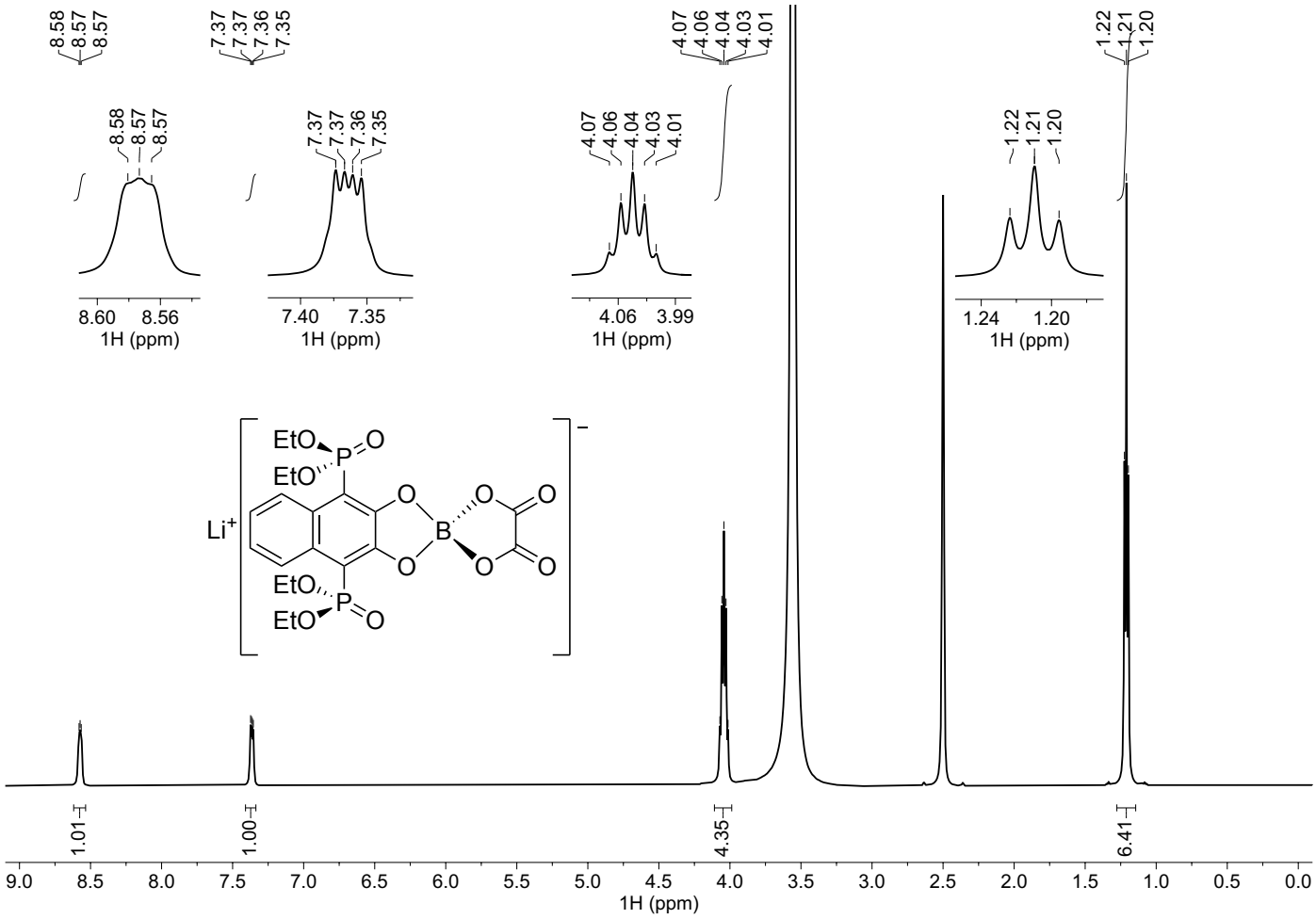

Figure S10. ^{1}H NMR (500 MHz, DMSO-d_6) spectrum of Li[B(DPN)(oxalato)].

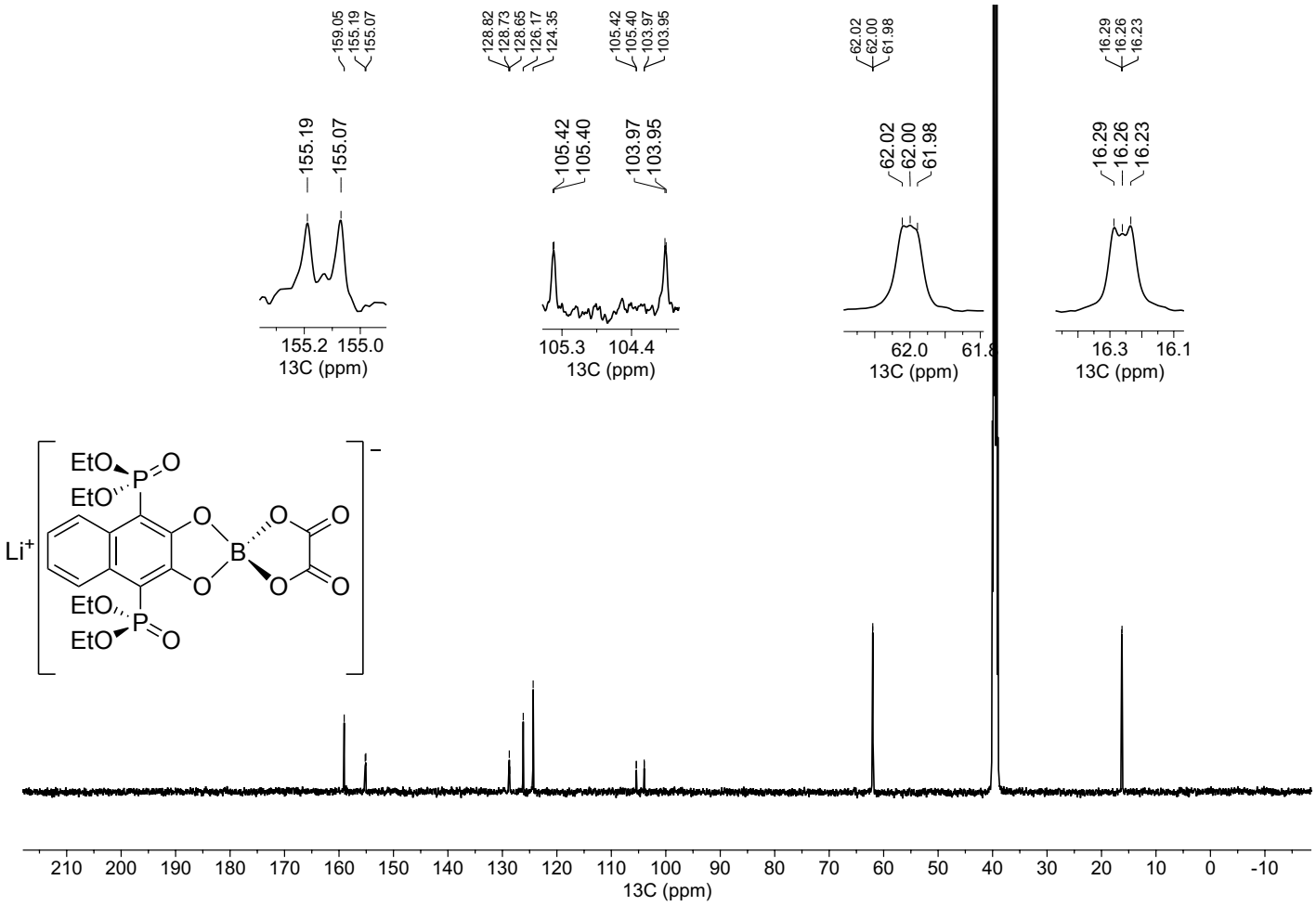

Figure S11. $^{13}C\{^{1}H\}$ NMR (500 MHz, $CDCl_3$) spectrum of Li[B(DPN)(oxalato)].

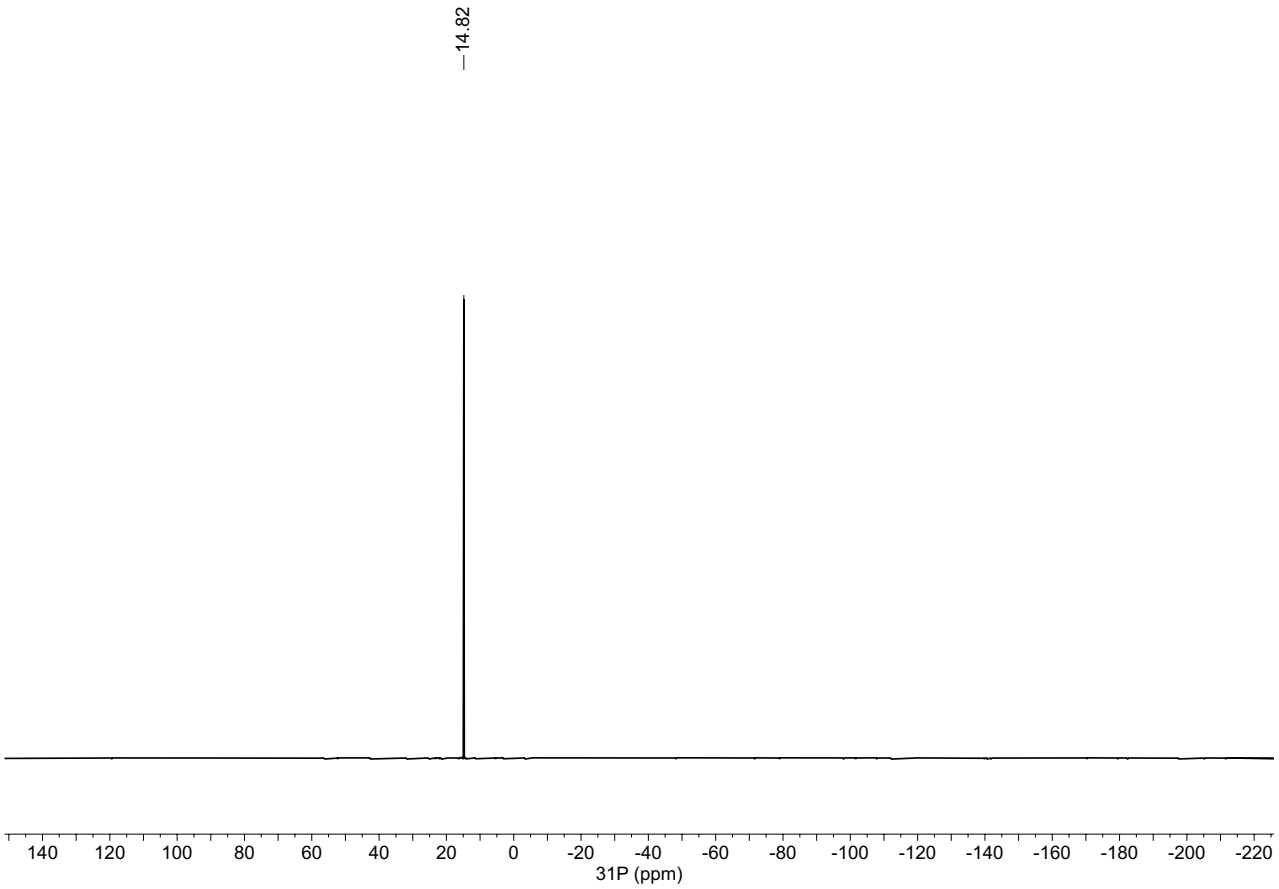

Figure S12. $^{31}P\{^{1}H\}$ NMR (500 MHz, DMSO-d_6) spectrum of Li[B(DPN)(oxalato)].

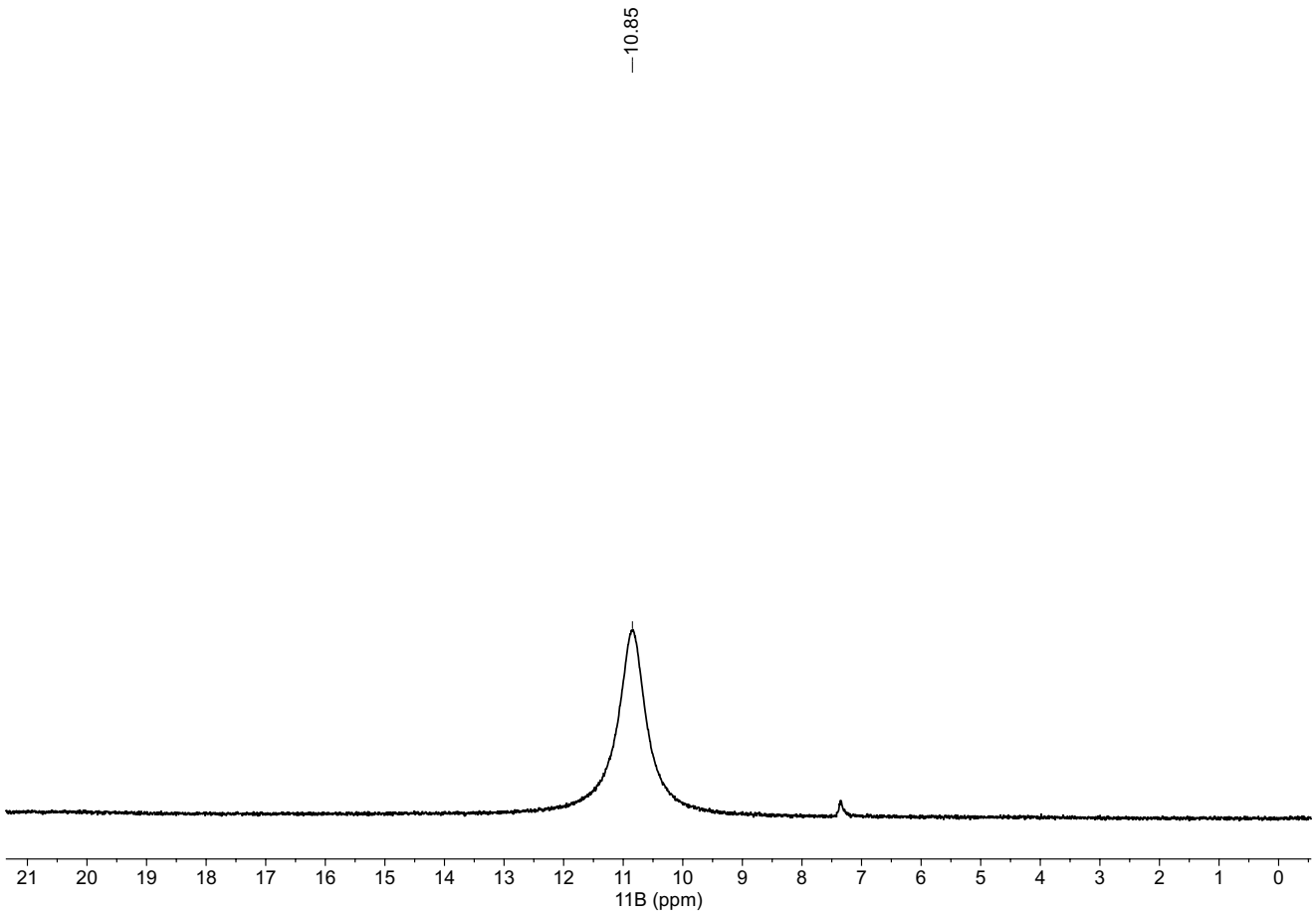

Figure S13. ^{11}B NMR (500 MHz, DMSO-d_6) spectrum of Li[B(DPN)(oxalato)].

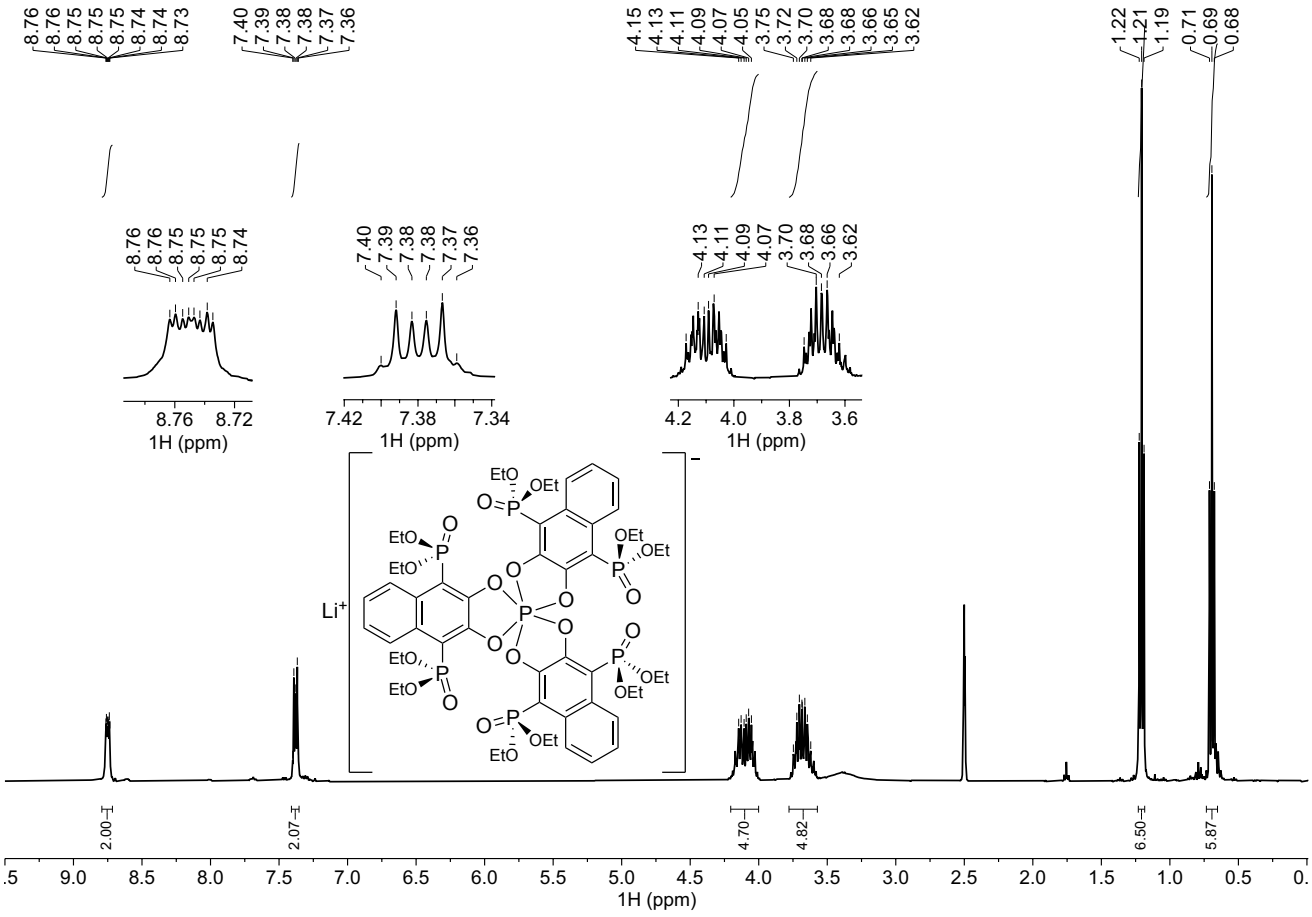

Figure S14. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of Li[P(DPN)$_3$].

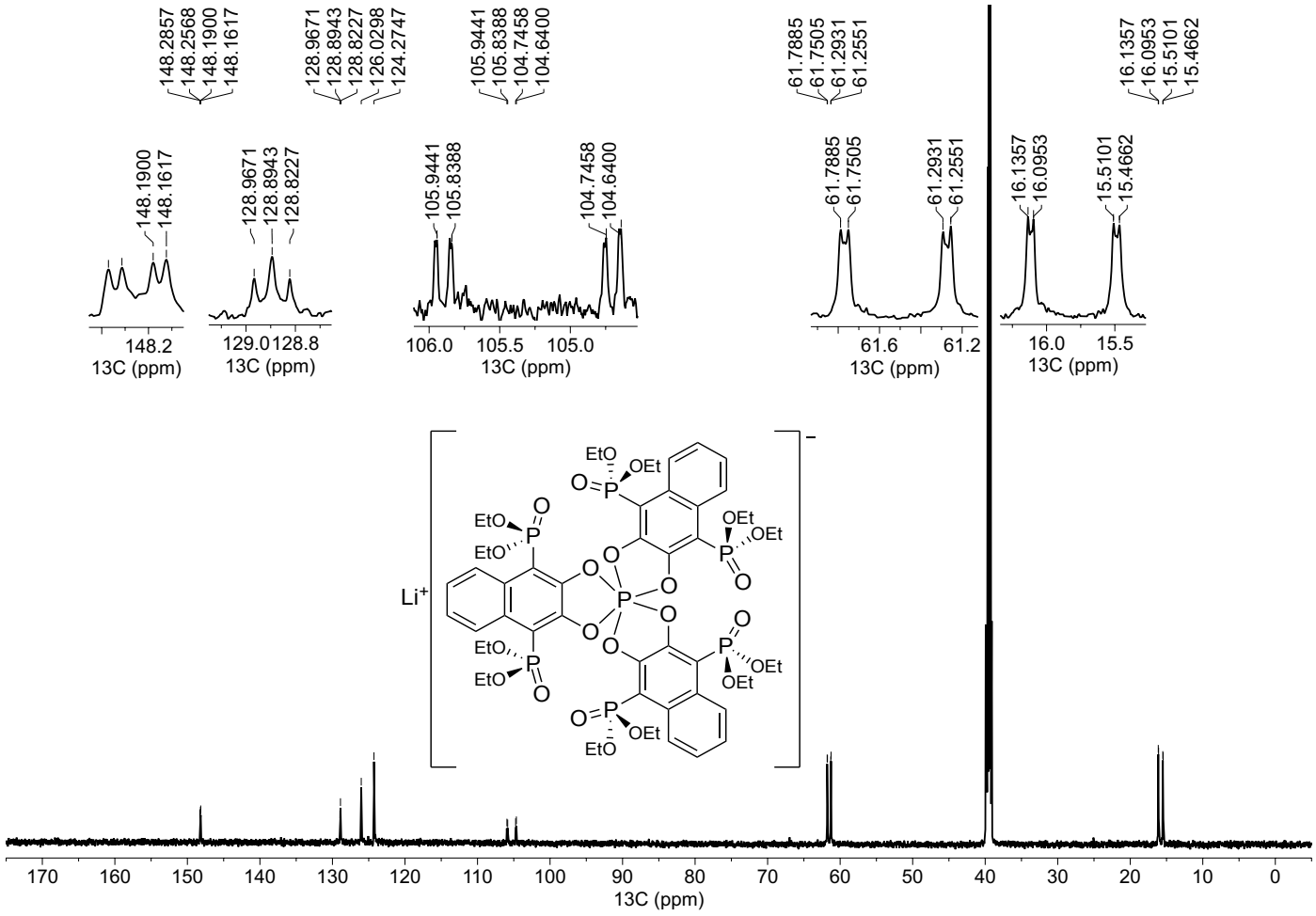

Figure S15. $^{13}C\{^{1}H\}$ NMR (400 MHz, DMSO-d_6) spectrum of Li[P(DPN)$_3$].

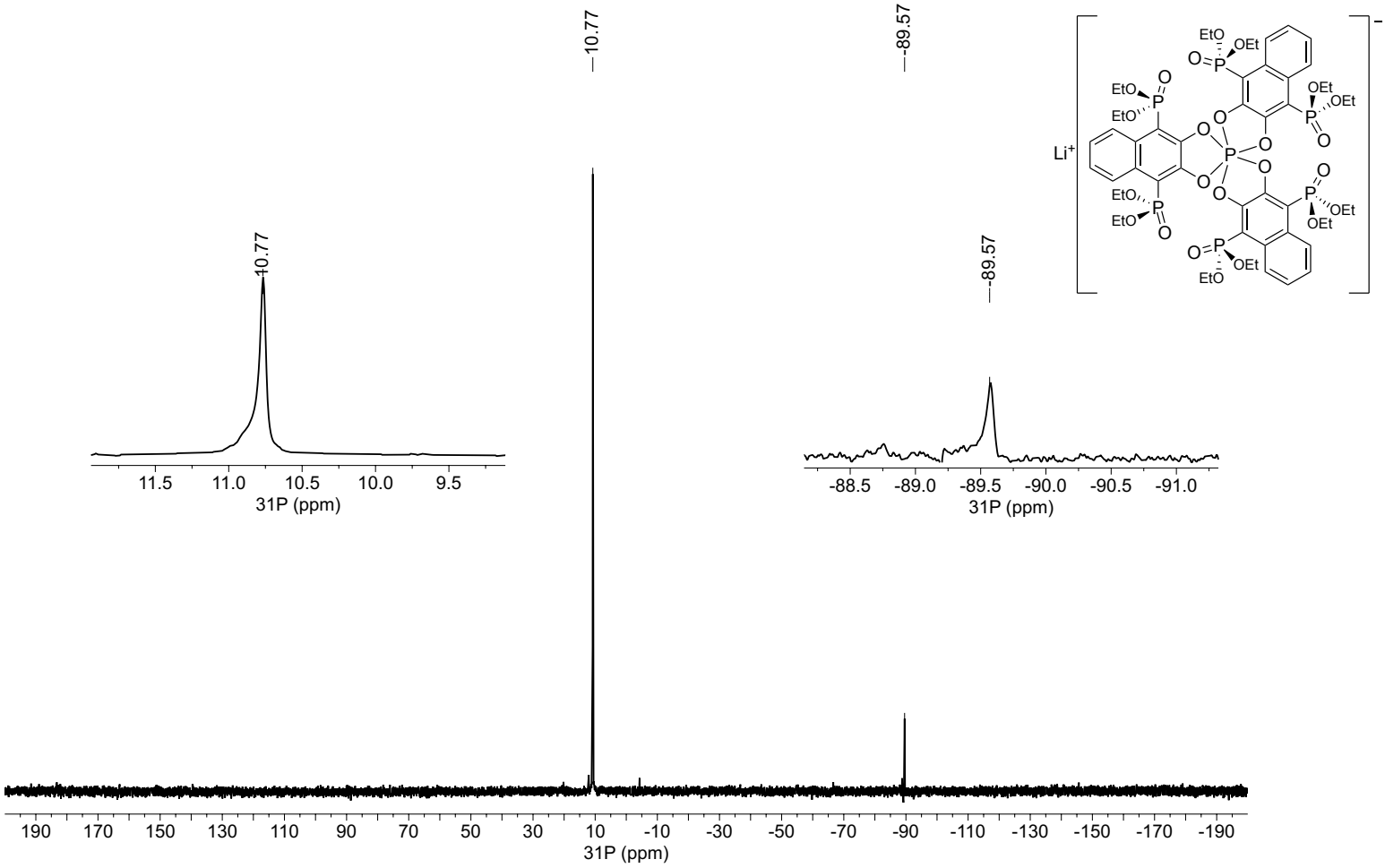

Figure S16. $^{31}P\{^{1}H\}$ NMR (400 MHz, DMSO-d_6) spectrum of Li[P(DPN)$_3$].

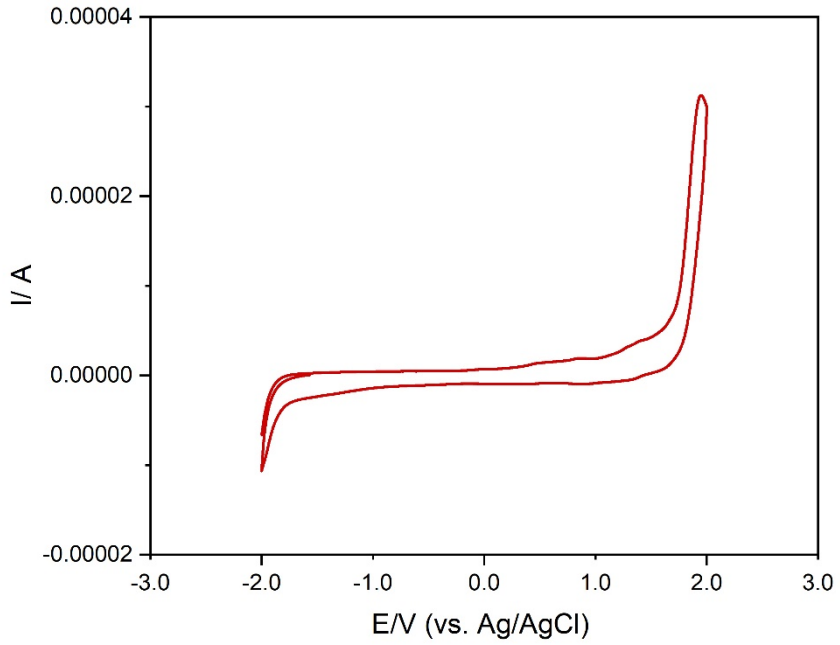

Figure S17. Cyclic Voltammogram of $Li[B(DPN)_2]$ (0.1 mM); $[Bu_4]NPF_6$ (Tetrabutylammonium hexafluorophosphate) 0.1 M in DCM, working electrode: glassy carbon (3 mm), reference electrode: non-aqueous Ag/Ag^+, counter electrode: Pt (2 mm), potential window: -2.0 V – 2.0 V) with a scan rate of 0.08 V s^{-1}.

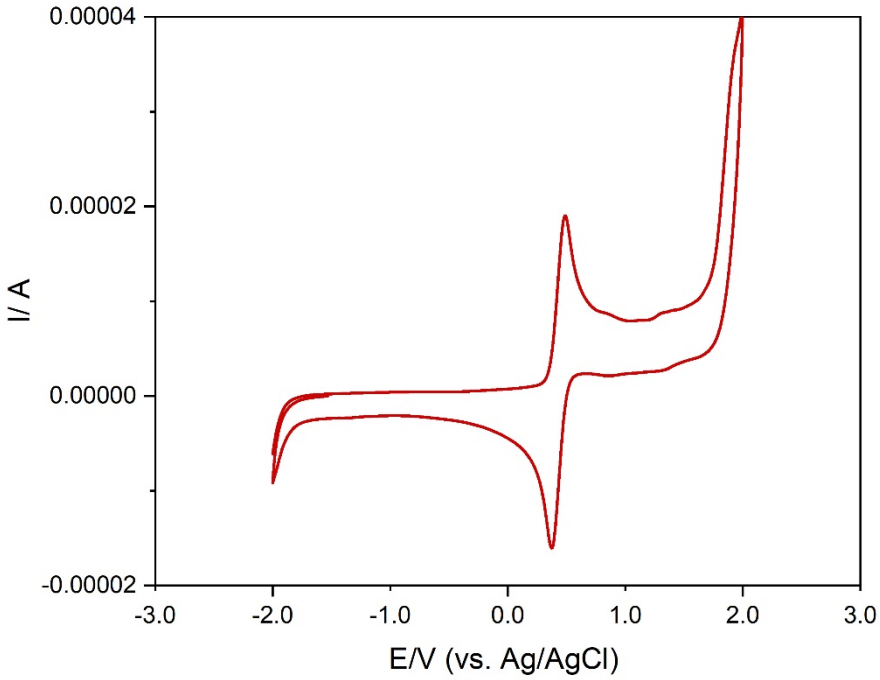

Figure S18. Cyclic Voltammogram of $Li[B(DPN)_2]$ (0.1 mM) with ferrocene (0.1 mM) as a standard; $[Bu_4]NPF_6$ (Tetrabutylammonium hexafluorophosphate) 0.1 M in DCM, working electrode: glassy carbon (3 mm), reference electrode: non-aqueous Ag/Ag^+, counter electrode: Pt (2 mm), potential window: -2.0 V – 2.0 V) with a scan rate of 0.08 V s^{-1}.

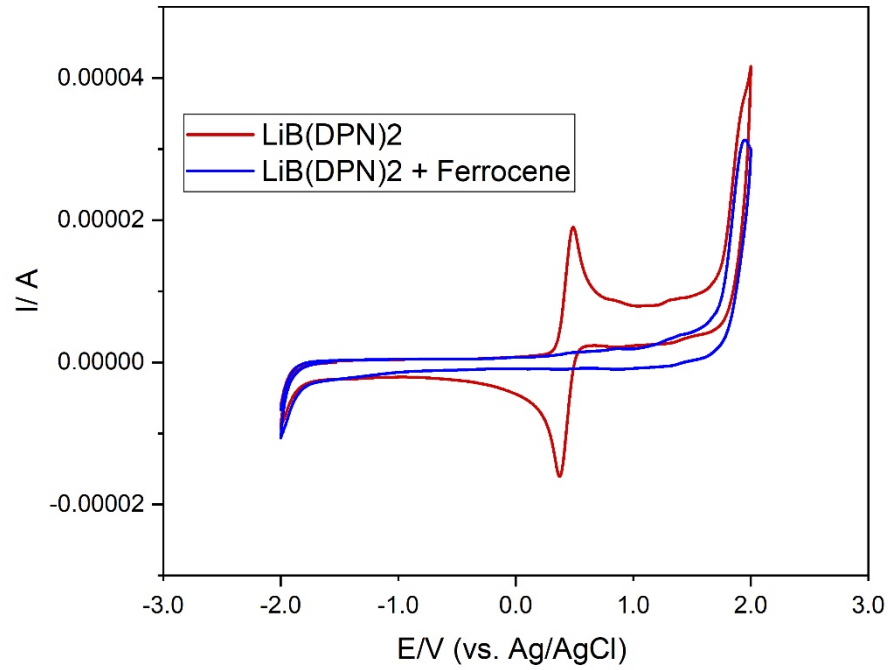

Figure S19. Cyclic Voltammograms of $Li[B(DPN)_2]$ (0.1 mM) with ferrocene (0.1 mM) as a standard and $Li[B(DPN)_2]$ (0.1 mM); $[Bu_4]NPF_6$ (Tetrabutylammonium hexafluorophosphate) 0.1 M in DCM, working electrode: glassy carbon (3 mm), reference electrode: non-aqueous Ag/Ag^+, counter electrode: Pt (2 mm), potential window: -2.0 V – 2.0 V) with a scan rate of 0.08 V s^{-1}.

Empirical formula	C_{18} H_{26} O_8 P_2
Formula weight	432.33
Temperature	100.0 K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P 21/c
	a = 9.8921(8) Å α= 90°
Unit cell dimensions	b = 24.310(2) Å β= 90.344(2)°
	c = 8.3864(8) Å γ = 90°
Volume	2016.7(3) Å3
Z	4
Density (calculated)	1.424 Mg/m3
Absorption coefficient	0.258 mm-1
F(000)	912
Crystal size	0.31 x 0.29 x 0.27 mm3
Theta range for data collection	1.675 to 28.356°.
Index ranges	-13<=h<=10, -29<=k<=32, -11<=l<=10
Reflections collected	12760
Independent reflections	5018 [R(int) = 0.0431]
Completeness to theta = 25.242°	100.00%
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7457 and 0.6973
Refinement method	Full-matrix least-squares on F2
Data / restraints / parameters	5018 / 0 / 276
Goodness-of-fit on F2	1.022
Final R indices [I>2sigma(I)]	R1 = 0.0383, wR2 = 0.0958
R indices (all data)	R1 = 0.0462, wR2 = 0.1020
Extinction coefficient	n/a
Largest diff. peak and hole	0.419 and -0.367 e.Å-3

Table S1. Crystallographic data for H_2-DPN

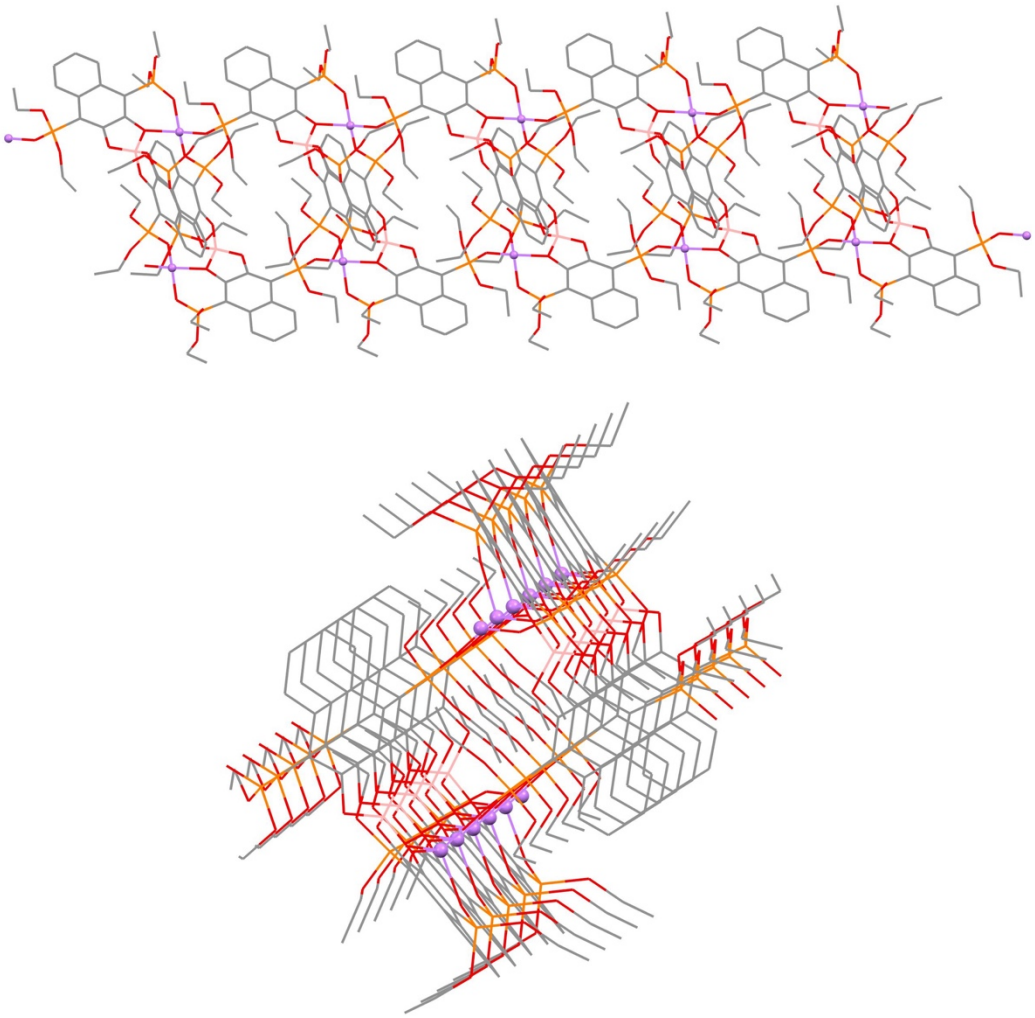

Figure S20. Packing diagram of $Li[B(DPN)_2]$ illustrating lithium ions (lavender color) bridging pairs of independent molecules to one another (along a-axis).

Empirical formula	C_{72} H_{96} B_2 Li_2 O_{32} P_8
Formula weight	1756.74
Temperature	100.0 K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P-1
	a = 9.3498(18) Å α= 73.891(5)°
Unit cell dimensions	b = 19.335(3) Å β= 83.711(4)°
	c = 23.900(4) Å γ = 78.620(4)°
Volume	4062.5(13) $Å^3$
Z	2
Density (calculated)	1.436 Mg/m^3
Absorption coefficient	0.257 mm^{-1}
F(000)	1840
Crystal size	0.26 x 0.26 x 0.12 mm^3
Theta range for data collection	0.888 to 26.376°.
Index ranges	-11<=h<=7, -24<=k<=23, -29<=l<=29
Reflections collected	41961
Independent reflections	16584 [R(int) = 0.0908]
Completeness to theta = 25.242°	100.00%
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.4908 and 0.4272
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	16584 / 0 / 1061
Goodness-of-fit on F^2	1.016
Final R indices [I>2sigma(I)]	R1 = 0.0665, wR2 = 0.1308
R indices (all data)	R1 = 0.1532, wR2 = 0.1597
Extinction coefficient	n/a
Largest diff. peak and hole	0.469 and -0.463 $e.Å^{-3}$

Table S2. Crystallographic data for $Li[B(DPN)_2]$