2-Diphenylphosphinomethyl-3-methylpyrazine

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Figure S1.[1]H NMR spectrum of compound **2**.

^{1}H NMR (400 MHz, C_6D_6)

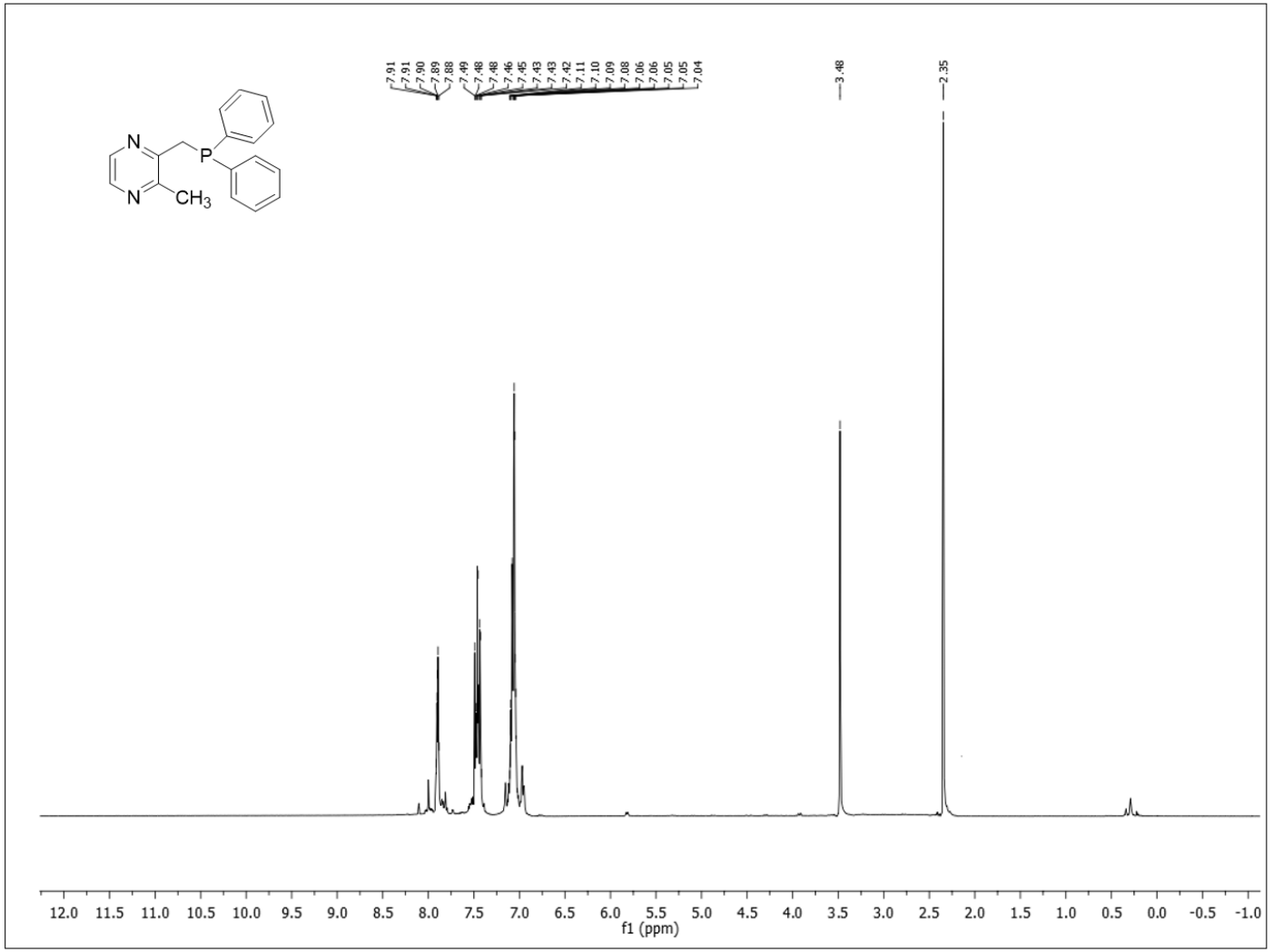

Figure S2. ^{13}C NMR spectrum of compound **2**

^{13}C NMR (100 MHz, C_6D_6)

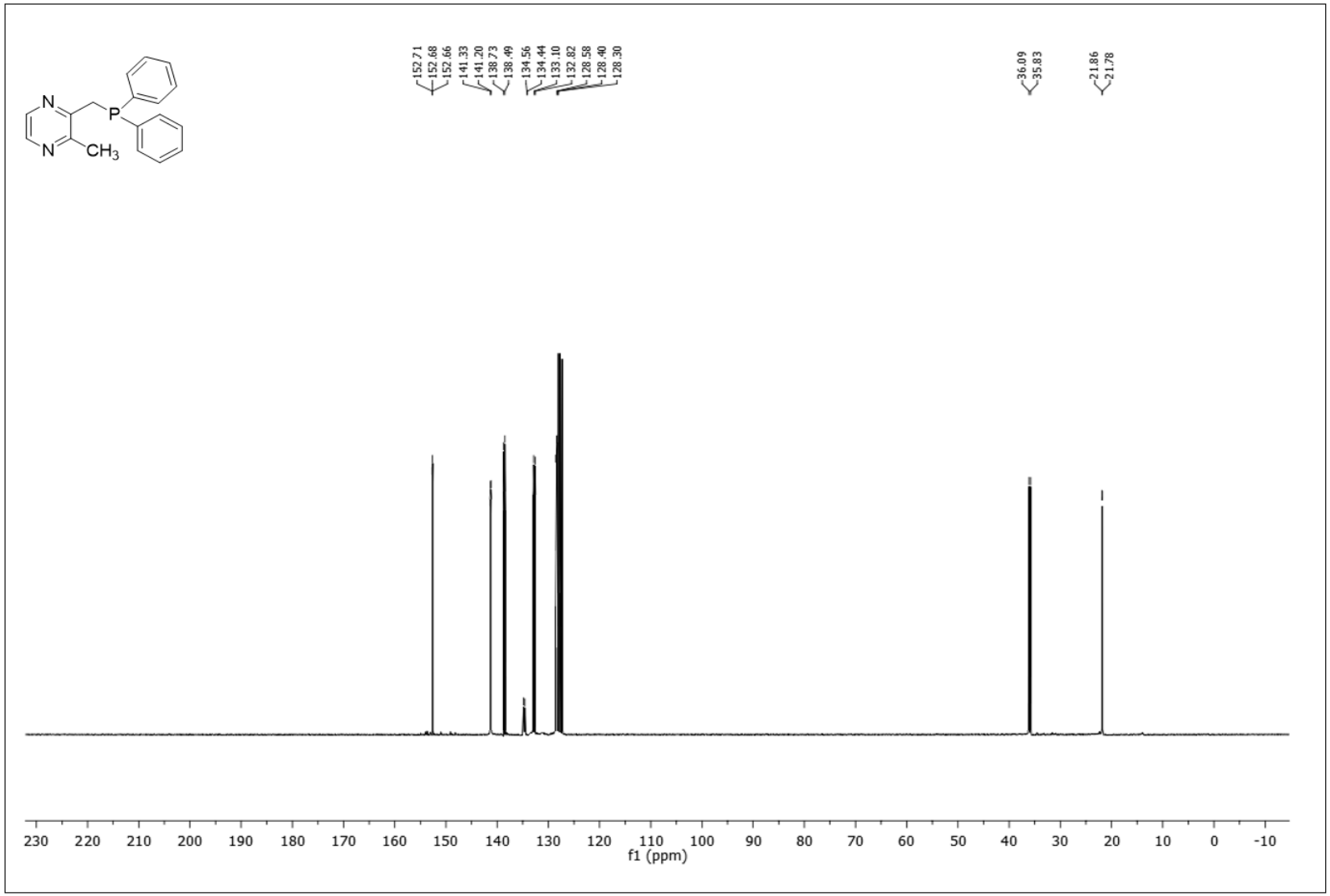

Figure S3. ^{31}P NMR spectrum of compound **2**

^{31}P (162.00 MHz, C_6D_6)

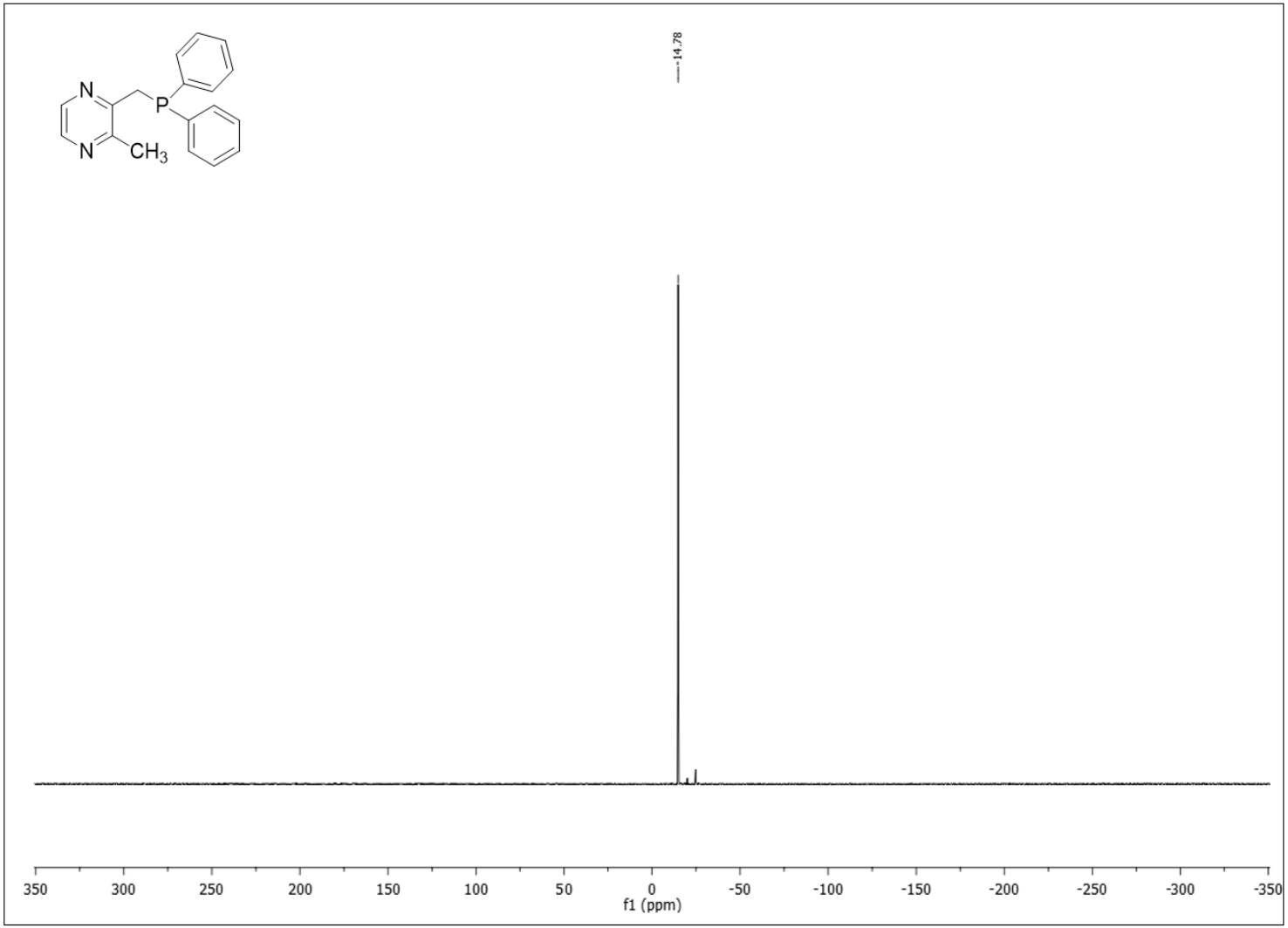

Figure S4. ^{1}H NMR spectrum of compound **3**

^{1}H NMR (400 MHz, C_6D_6)

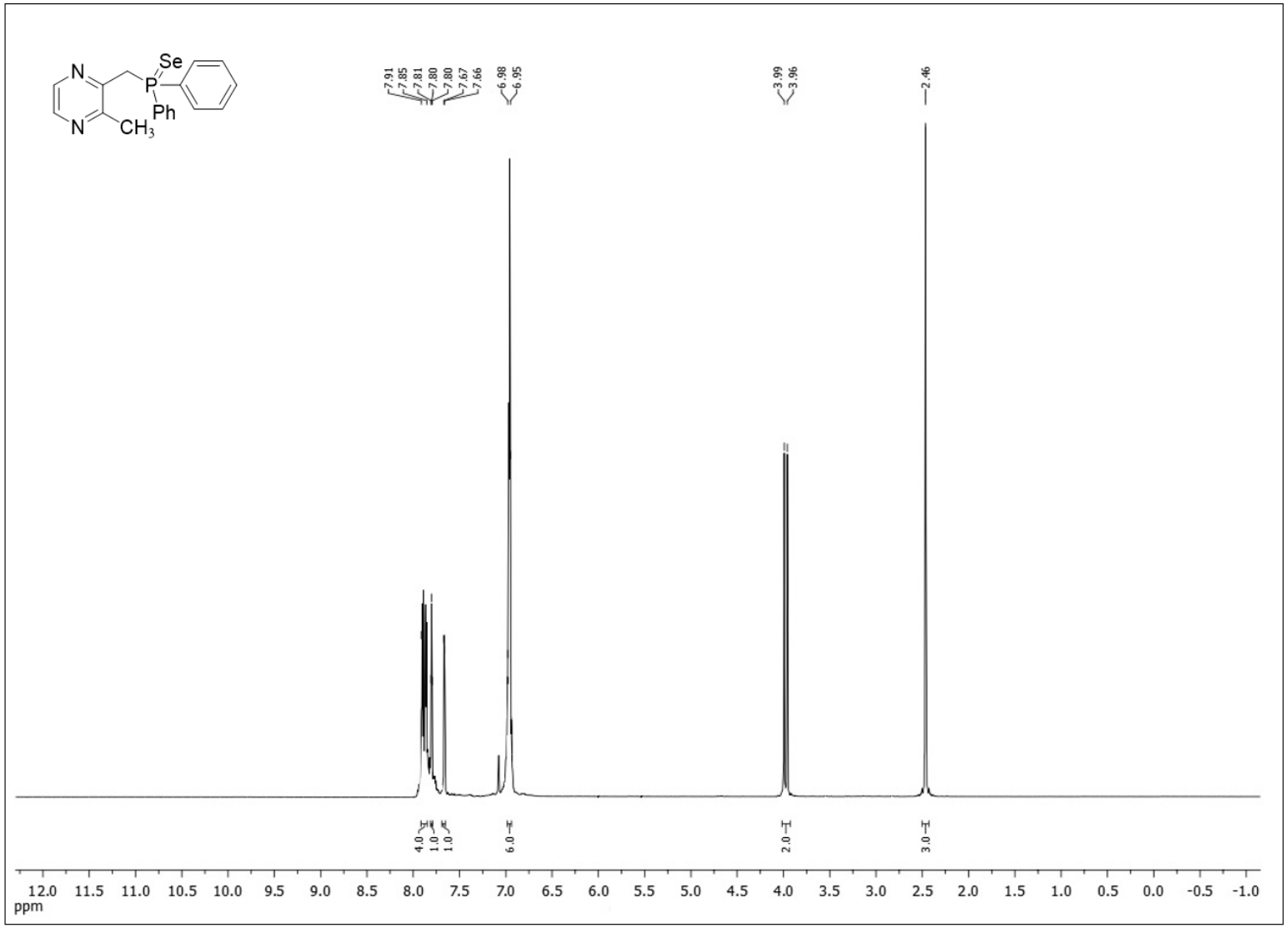

Figure S5. ^{13}C NMR spectrum of compound **3**

^{13}C NMR (100 MHz, C_6D_6)

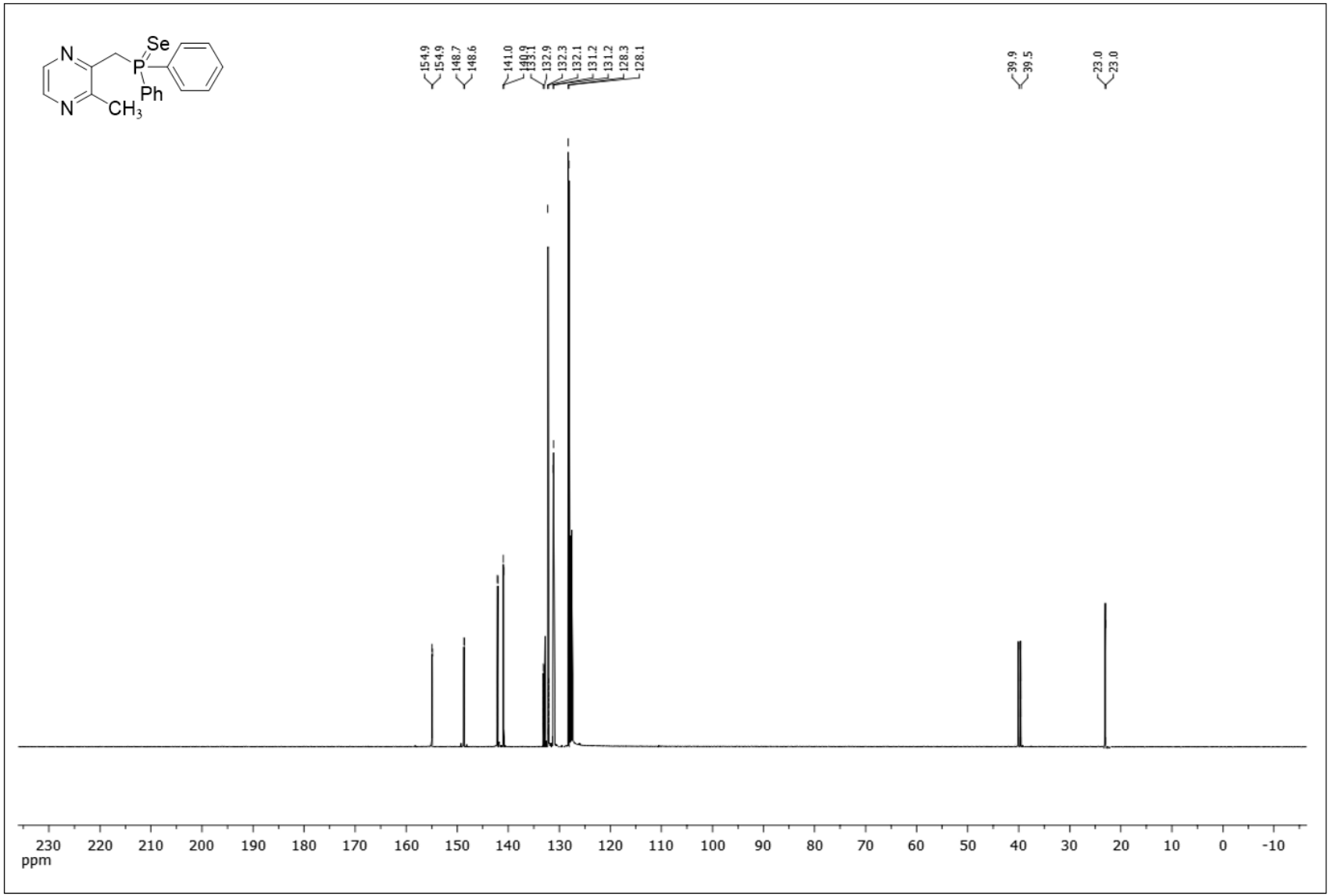

Figure S6. ^{31}P NMR spectrum of compound **3**

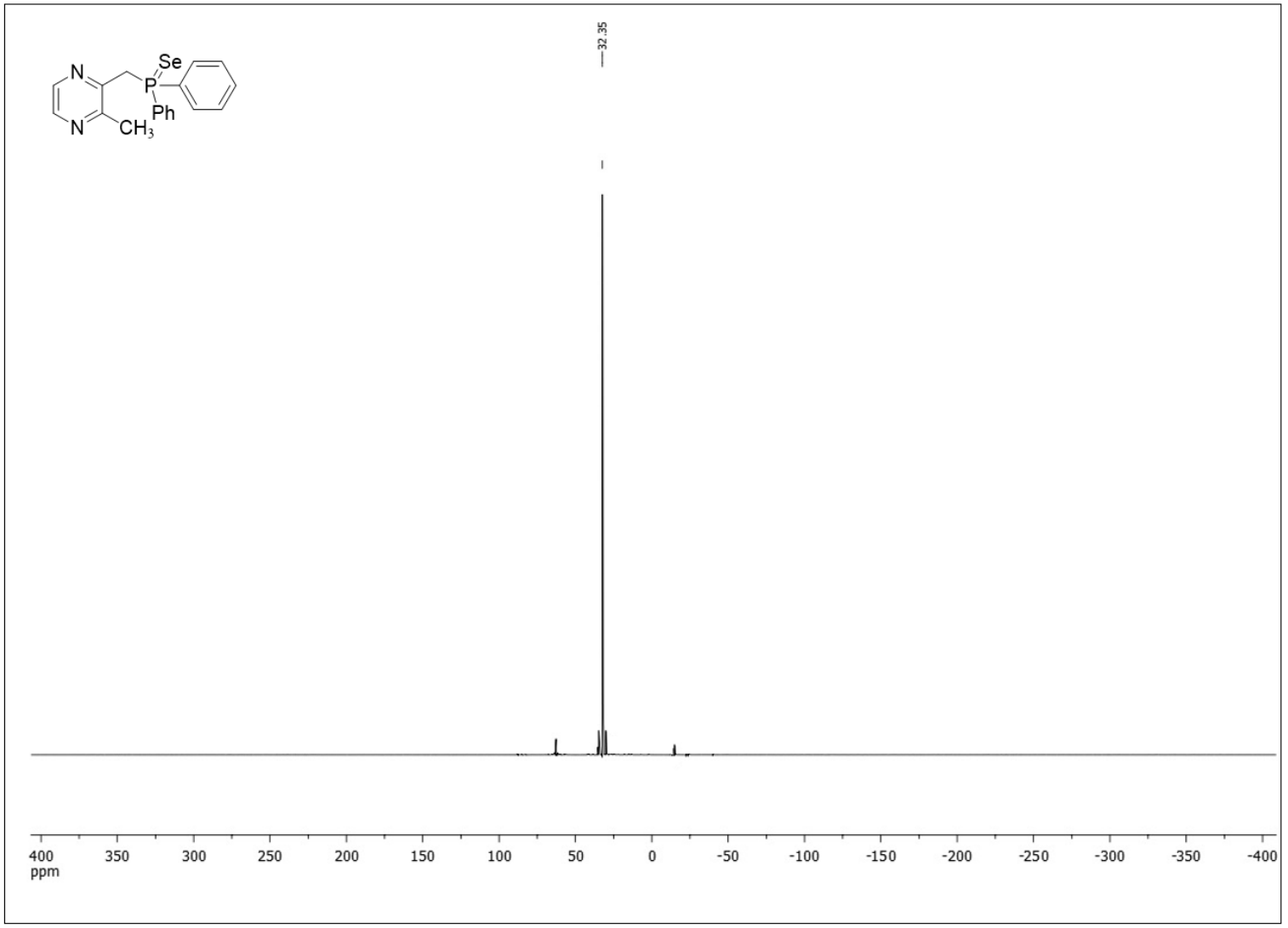

Figure S7. ^{31}P NMR (163 MHz) spectrum of compound **3** in C_6D_6. The $^{1}J_{SeP}$ coupling constant resulting from the ^{77}Se satellites has been marked.

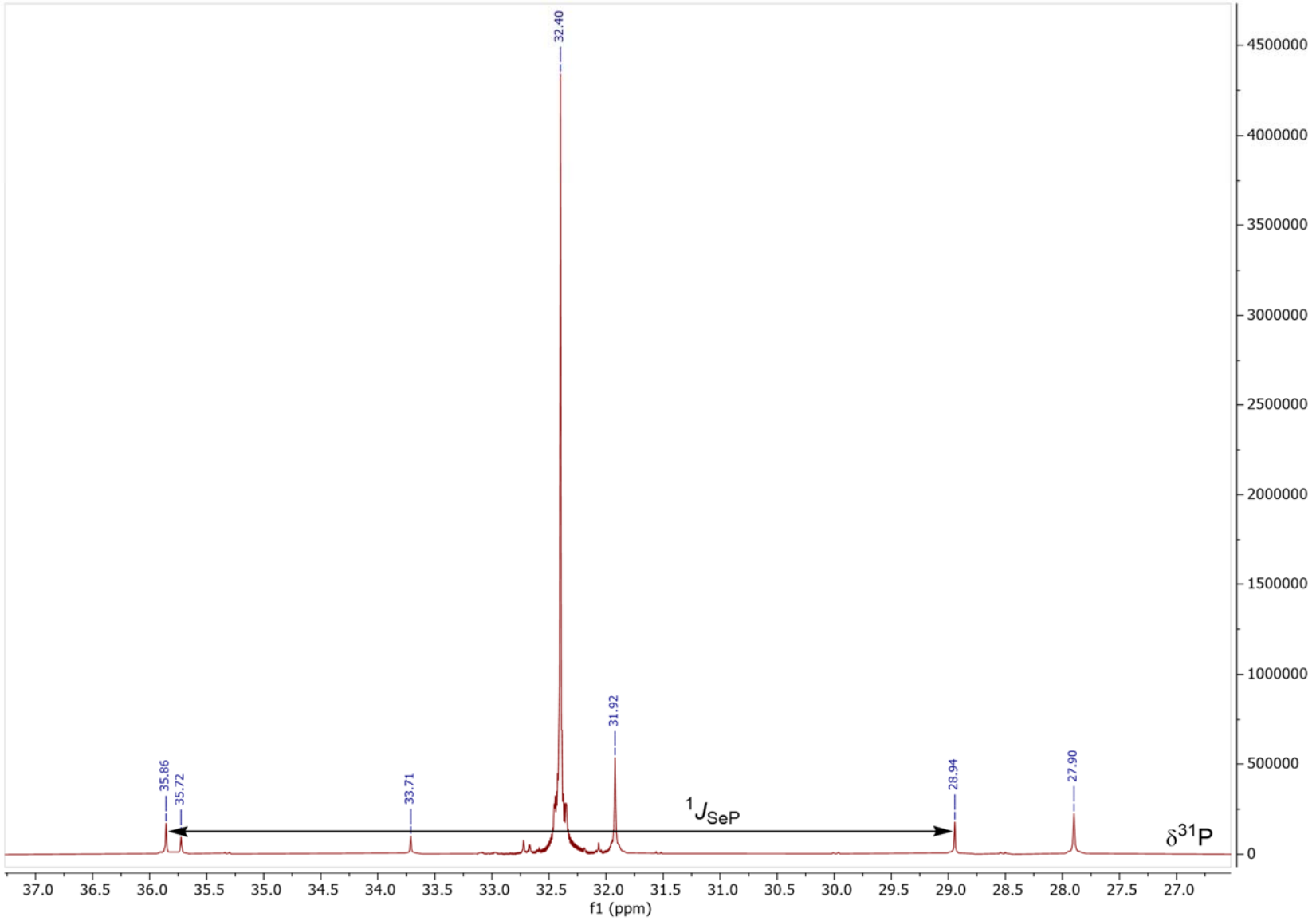

Figure S8. ^{77}Se NMR (76 MHz) spectrum of compound **3** in C_6D_6. The $^1J_{SeP}$ coupling constant has been marked.

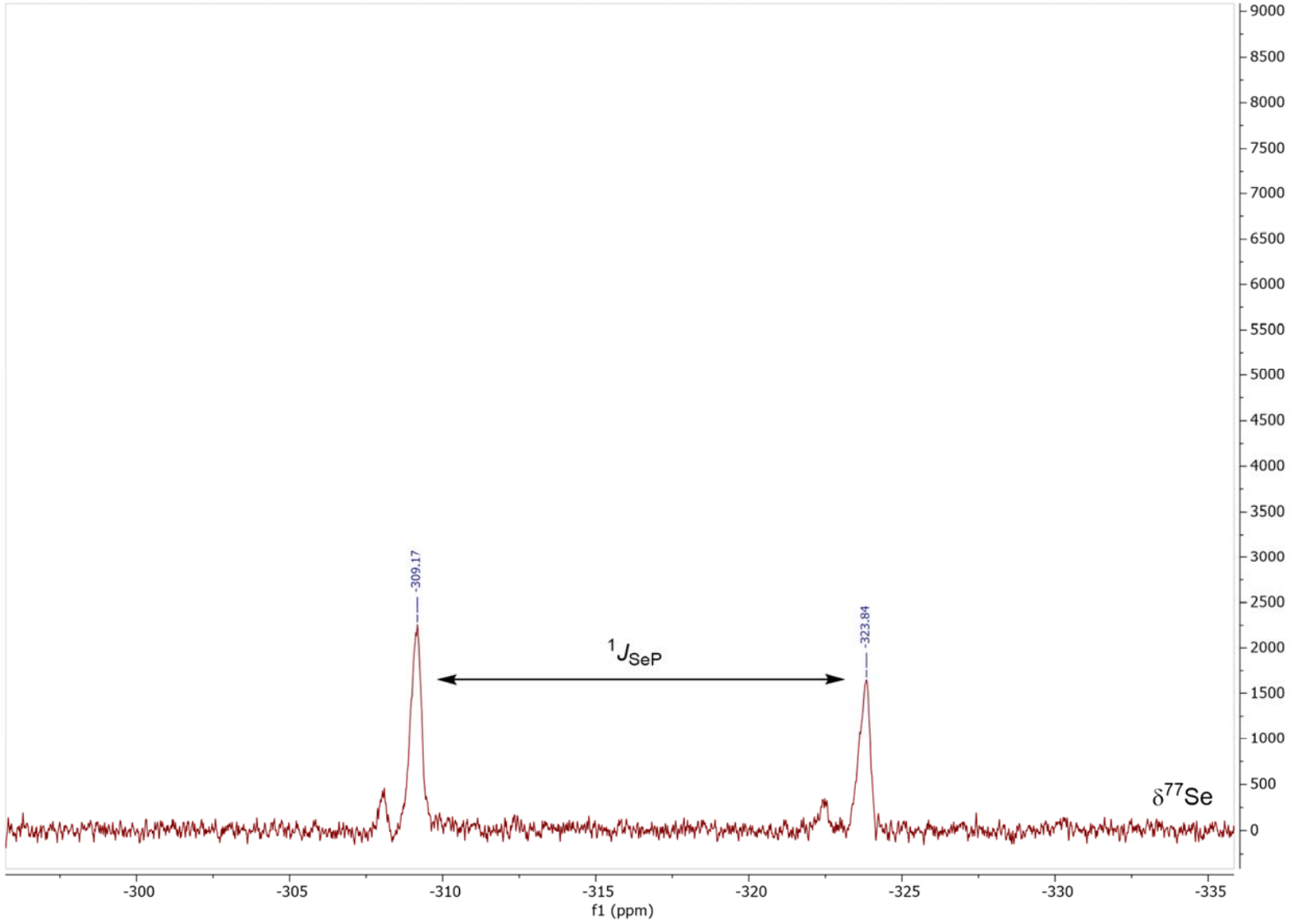

Figure S9. 2D ^{1}H-^{1}H COSY spectrum (C_6D_6) of compound **3**

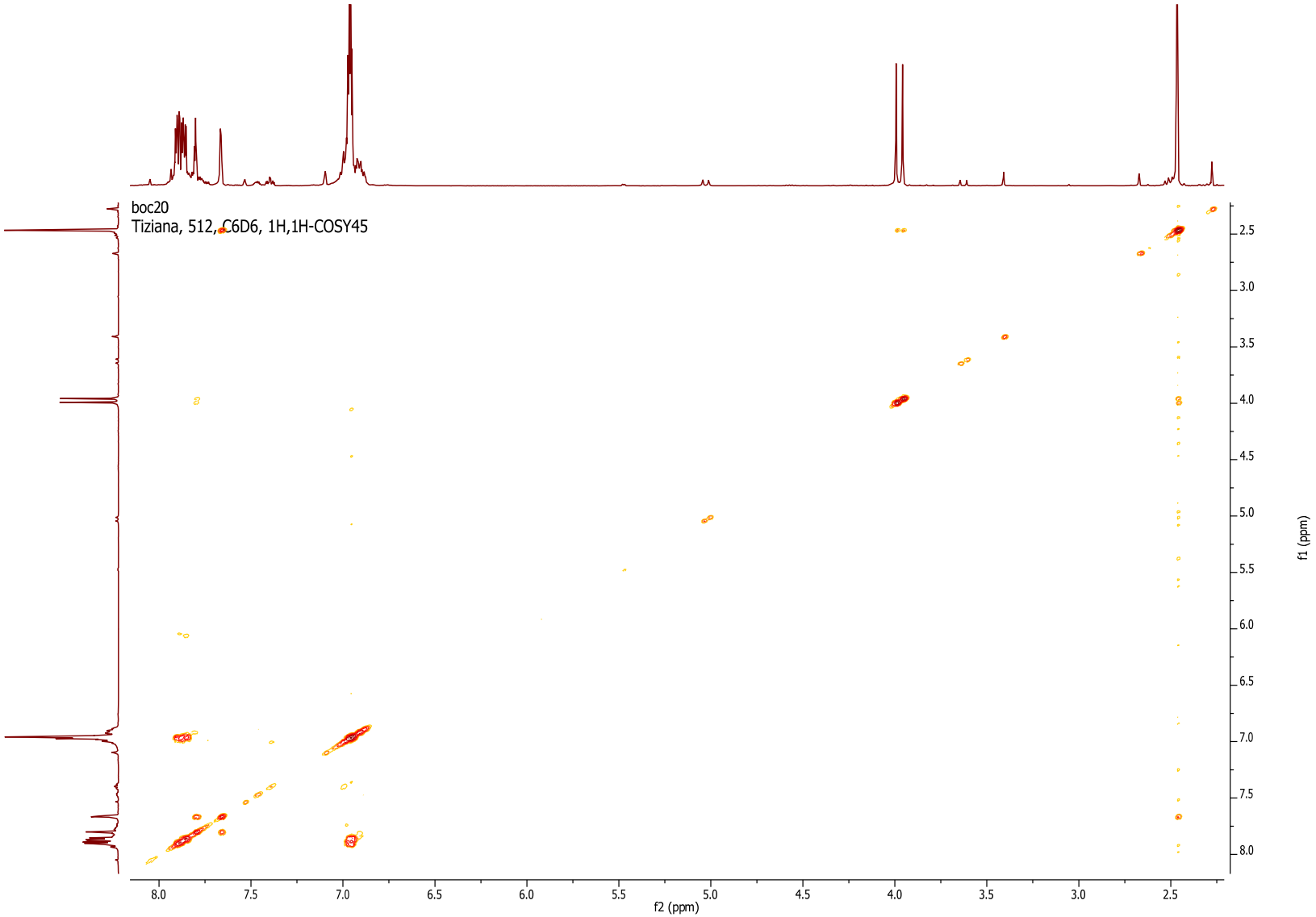

Figure S10. Enhancements of 2D ^{1}H-^{13}C HMQC spectrum (C_6D_6) of compound **3**

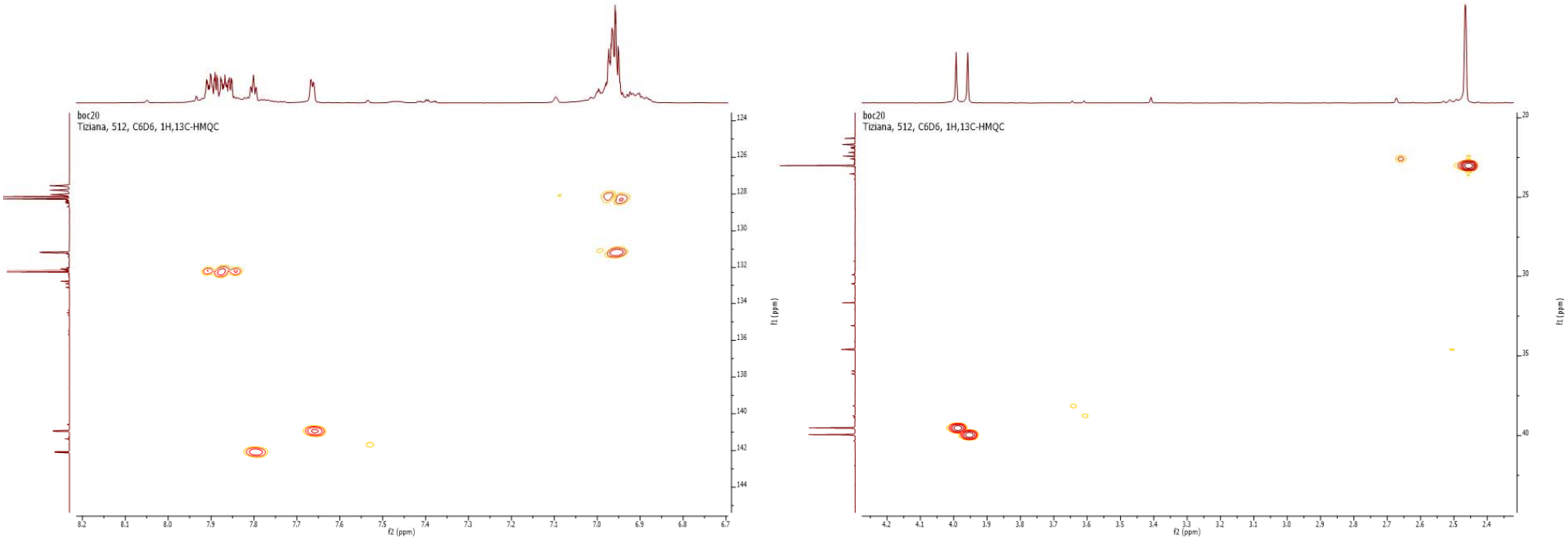

Figure S11. Enhancements of 2D ^{1}H-^{13}C HMBC spectrum (C_6D_6) of compound **3**

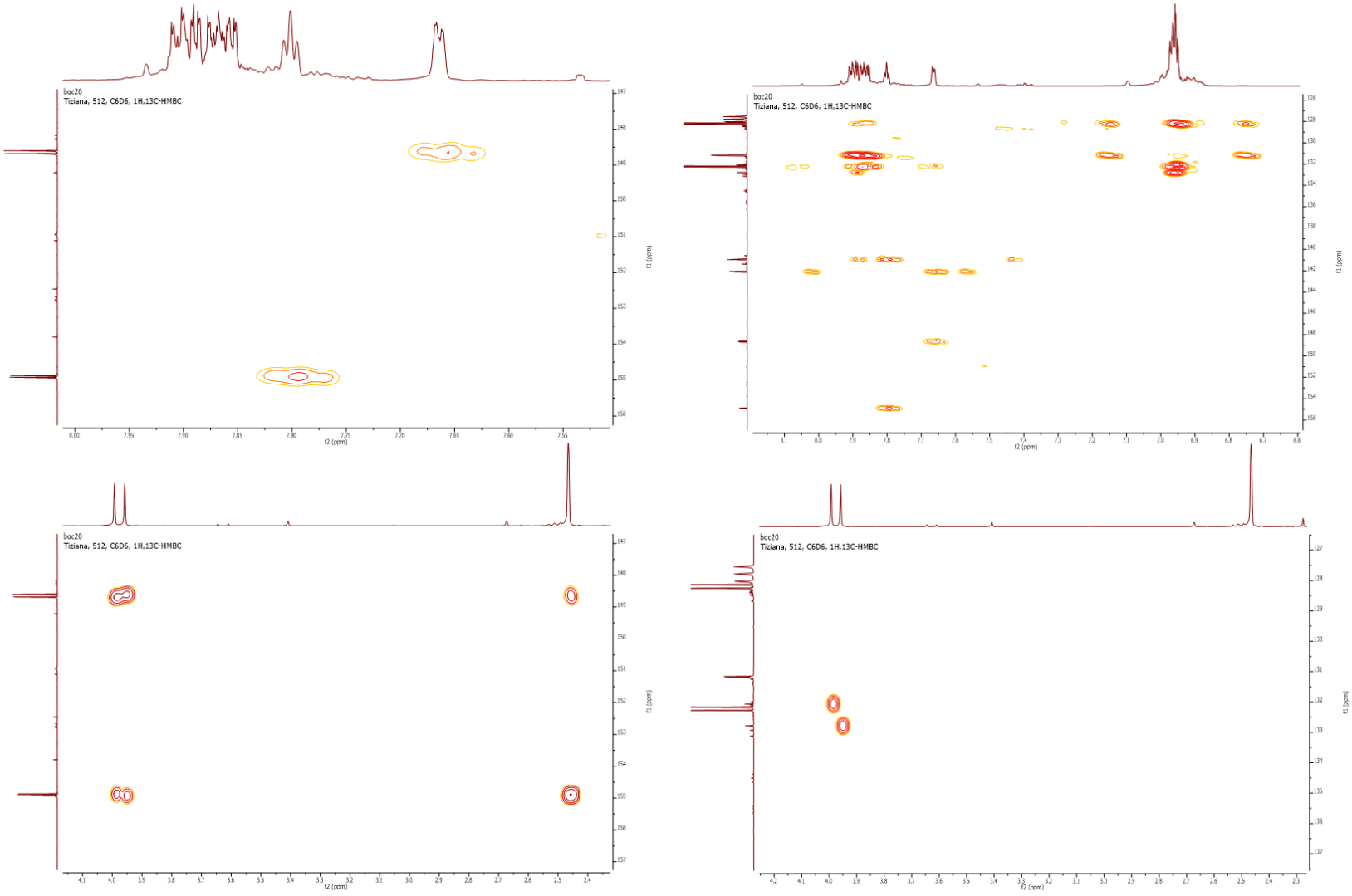

Table S1. Details for X-ray data collection and structure refinement of compound **3 · C_6H_6**.

Empirical formula	$C_{18}H_{17}N_2PSe \cdot C_6H_6$
Formula mass	449.37
T[K]	100(2)
Crystal size [mm]	0.32 × 0.24 × 0.24
Crystal description	colorless block
Crystal system	monoclinic
Space group	*P*21/*n*
a [Å]	8.8999(2)
b [Å]	14.6541(4)
c [Å]	16.1727(4)
α [°]	90.0
β [°]	96.439(2)
γ [°]	90.0
V [Å^3]	2095.94(9)
Z	4
$\rho_{calcd.}$ [g cm^{-3}]	1.424
μ [mm^{-1}]	1.880
F(000)	920
Θ range [°]	4.22 – 25.24
Index ranges	$-12 \leq h \leq 12$
	$-20 \leq k \leq 20$
	$-22 \leq l \leq 22$

Reflns. collected	41132
Reflns. obsd.	5268
Reflns. unique	6087 (R_{int} = 0.0375)
R_1, wR_2 (2σ data)	0.0283, 0.0661
R_1, wR_2 (all data)	0.0365, 0.0700
GOOF on F^2	1.055
Peak/hole [e Å^{-3}]	1.037 / -0.293

Table S2. Selected bond lengths (Å) of compound **3 · C_6H_6**.

Se1 – P1	2.109(1)	C23 – C22	1.384(3)
P1 – C13	1.815(2)	C23 – C24	1.385(3)
P1 – C7	1.820(1)	C8 – C9	1.395(2)
P1 – C1	1.837(1)	C3 – C4	1.503(2)
C13 – C14	1.393(2)	C20 – C21	1.378(3)
C13 – C18	1.394(2)	C18 – C17	1.391(2)
N1 – C2	1.338(2)	C21 – C22	1.383(3)
N1 – C6	1.339(2)	C17 – C16	1.383(2)
C11 – C10	1.388(3)	C15 – C16	1.385(2)
C11 – C12	1.389(2)	C7 – C8	1.396(2)
N2 – C5	1.336(2)	C7 – C12	1.400(2)
N2 – C3	1.343(2)	C10 – C9	1.384(3)
C14 – C15	1.392(2)	C5 – C6	1.382(2)
C2 – C3	1.412(2)	C19 – C24	1.383(3)

C2 – C1	1.501(2)	C19 – C20	1.386(3)

Table S3. Selected bond angles (°) of compound **3 · C_6H_6**.

C13 – P1 – C7	103.9(1)	N2 – C3 – C2	120.3(1)
C13 – P1 – C1	108.7(1)	N2 – C3 – C4	117.0(1)
C7 – P1 – C1	102.8(1)	C2 – C3 – C4	122.7(1)
C13 – P1 – Se1	113.4(1)	C19 – C24 – C23	120.0(2)
C7 – P1 – Se1	114.2(1)	C21 – C20 – C19	120.2(2)
C1 – P1 – Se1	113.0(1)	C17 – C18 – C13	120.1(2)
C14 – C13 – C18	119.2(1)	C20 – C21 – C22	120.0(2)
C14 – C13 – P1	117.6(1)	C16 – C17 – C18	120.4(2)
C18 – C13 – P1	123.1(1)	C10 – C9 – C8	120.1(2)
C2 – N1 – C6	116.7(1)	C16 – C15 – C14	120.3(2)
C10 – C11 – C12	120.0(2)	C2 – C1 – P1	113.3(1)
C5 – N2 – C3	117.0(1)	C17 – C16 – C15	119.7(2)
C15 – C14 – C13	120.2(2)	C21 – C22 – C23	120.0(2)
N1 – C2 – C3	122.0(1)	C12 – C7 – P1	119.8(1)
N1 – C2 – C1	116.0(1)	N1 – C6 – C5	121.5(2)
C3 – C2 – C1	122.0(1)	C9 – C10 – C11	120.4(2)
N2 – C5 – C6	122.5(2)	C22 – C23 – C24	119.9(2)
C24 – C19 – C20	119.8(2)	C9 – C8 – C7	119.7(2)
C8 – C7 – C12	119.9(1)	C11 – C12 – C7	119.9(2)
C8 – C7 – P1	120.3(1)		

Table S4. Selected torsion angles (°) of compound **3 · C_6H_6**.

C7 – P1 – C13 – C14	-87.6(1)	C5 – N2 – C3 – C2	-0.9(2)
C1 – P1 – C13 – C14	163.4(1)	C5 – N2 – C3 – C4	178.8(2)
Se1 – P1 – C13 – C14	36.9(1)	N1 – C2 – C3 – N2	0.2(2)
C7 – P1 – C13 – C18	88.1(1)	C1 – C2 – C3 – N2	-179.7(1)
C1 – P1 – C13 – C18	-20.9(2)	N1 – C2 – C3 – C4	-179.4(1)
Se1 – P1 – C13 – C18	-147.4(1)	C1 – C2 – C3 – C4	0.7(2)
C18 – C13 – C14 – C15	0.6(2)	C20 – C19 – C24 – C23	-0.5(3)
P1 – C13 – C14 – C15	176.5(1)	C22 – C23 – C24 – C19	0.0(3)
C6 – N1 – C2 – C3	0.9(2)	C24 – C19 – C20 – C21	0.2(3)
C6 – N1 – C2 – C1	-179.2(1)	C14 – C13 – C18 – C17	-0.3(2)
C3 – N2 – C5 – C6	0.4(2)	P1 – C13 – C18 – C17	-175.9(1)
C13 – P1 – C7 – C8	119.0(1)	C19 – C20 – C21 – C22	0.5(3)
C1 – P1 – C7 – C8	-127.8(1)	C13 – C18 – C17 – C16	-0.4(3)
Se1 – P1 – C7 – C8	-5.0(1)	C11 – C10 – C9 – C8	0.6(3)
C13 – P1 – C7 – C12	-60.5(1)	C7 – C8 – C9 – C10	-1.1(2)
C1 – P1 – C7 – C12	52.7(1)	C13 – C14 – C15 – C16	-0.2(3)
Se1 – P1 – C7 – C12	175.5(1)	N1 – C2 – C1 – P1	78.4(2)
C2 – N1 – C6 – C5	-1.3(2)	C3 – C2 – C1 – P1	-101.7(2)
N2 – C5 – C6 – N1	0.7(3)	C13 – P1 – C1 – C2	-79.9(1)
C12 – C11 – C10 – C9	0.4(3)	C7 – P1 – C1 – C2	170.4(1)
C12 – C7 – C8 – C9	0.6(2)	Se1 – P1 – C1 – C2	46.8(1)
P1 – C7 – C8 – C9	-179.0(1)	C18 – C17 – C16 – C15	0.8(3)
C10 – C11 – C12 – C7	-1.0(2)	C14 – C15 – C16 – C17	-0.5(3)

C8 – C7 – C12 – C11	0.5(2)	C20 – C21 – C22 – C23	-1.0(3)
P1 – C7 – C12 – C11	-180.0(1)	C24 – C23 – C22 – C21	0.7(3)

Figure S12. Molecular structure of compound **3 · C_6H_6** in the crystal. DIAMOND representation; thermal ellipsoids are drawn at 50 % probability level.

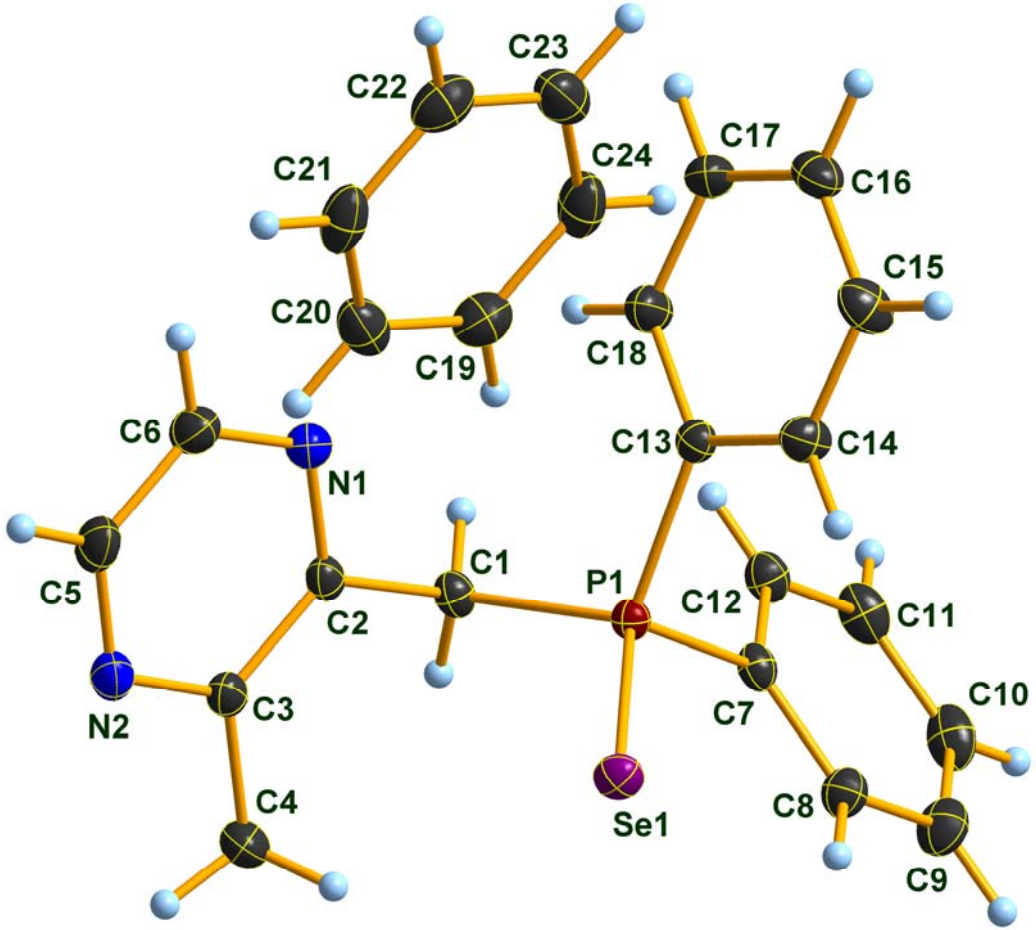

Figure S13. Crystal structure of compound **3 · C_6D_6** showing the interactions between selenium and the neighbouring protons; DIAMOND representation, thermal ellipsoids are drawn at 50 % probability level.