Electronic Supplementary Material (ESI) for New Journal of Chemistry.

SUPPORTING INFORMATION

Synthesis, Characterization and Cytotoxic Activity Studies on Cancer Cell Lines of New Paraben Decorated *Monospiro*-Cyclotriphosphazenes

Elif Şenkuytu[1], Nadide Akbaş[1], Tuba Yıldırım[2] and Gönül Yenilmez Çiftçi[1]*

[1] Department of Chemistry, Faculty of Science, Atatürk University, 25100, Erzurum, Turkey

[2]Department of Chemistry, Gebze Technical University, 41400, Gebze/Kocaeli, Turkey

[3]Department of Biology, Faculty of Arts and Sciences, Amasya University, 05100 Amasya, Turkey

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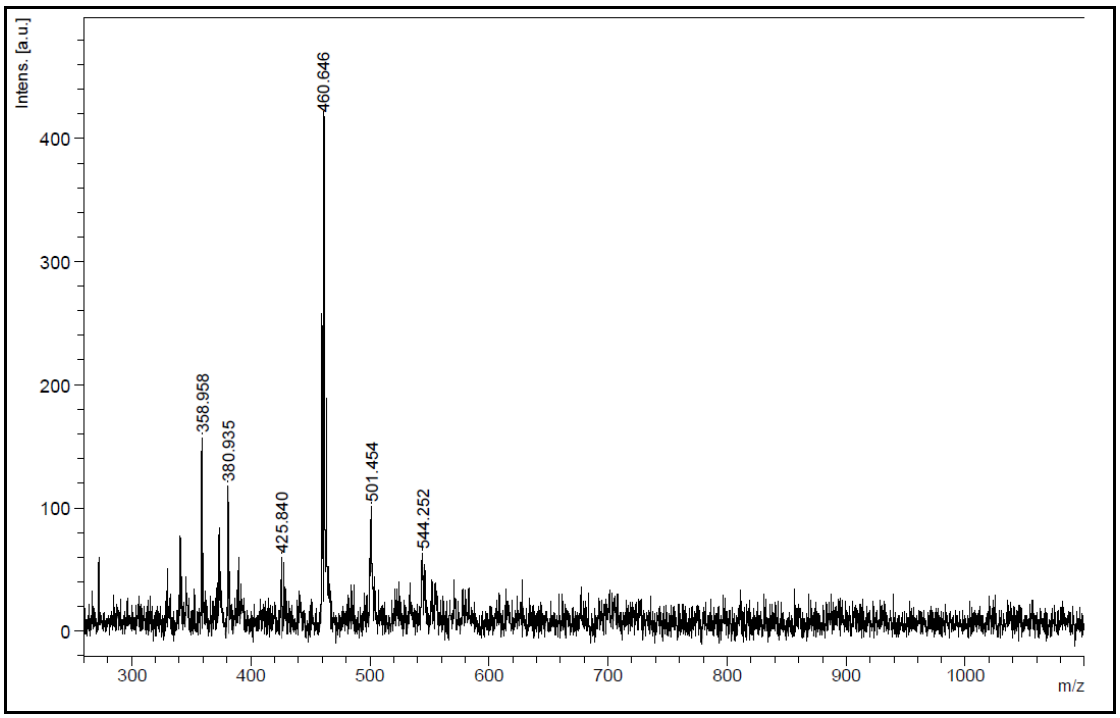

Figure S1. Mass spectrum of compound **1**

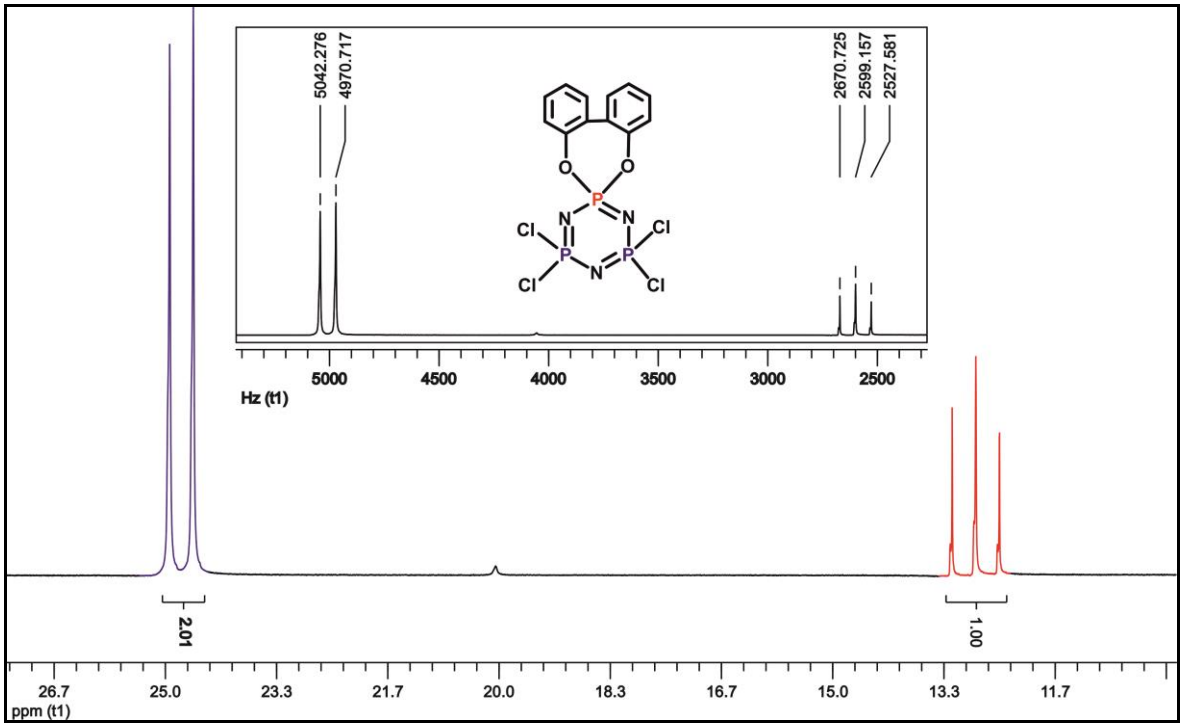

Figure S2. The proton decoupled ^{31}P NMR spectrum of compound **1**

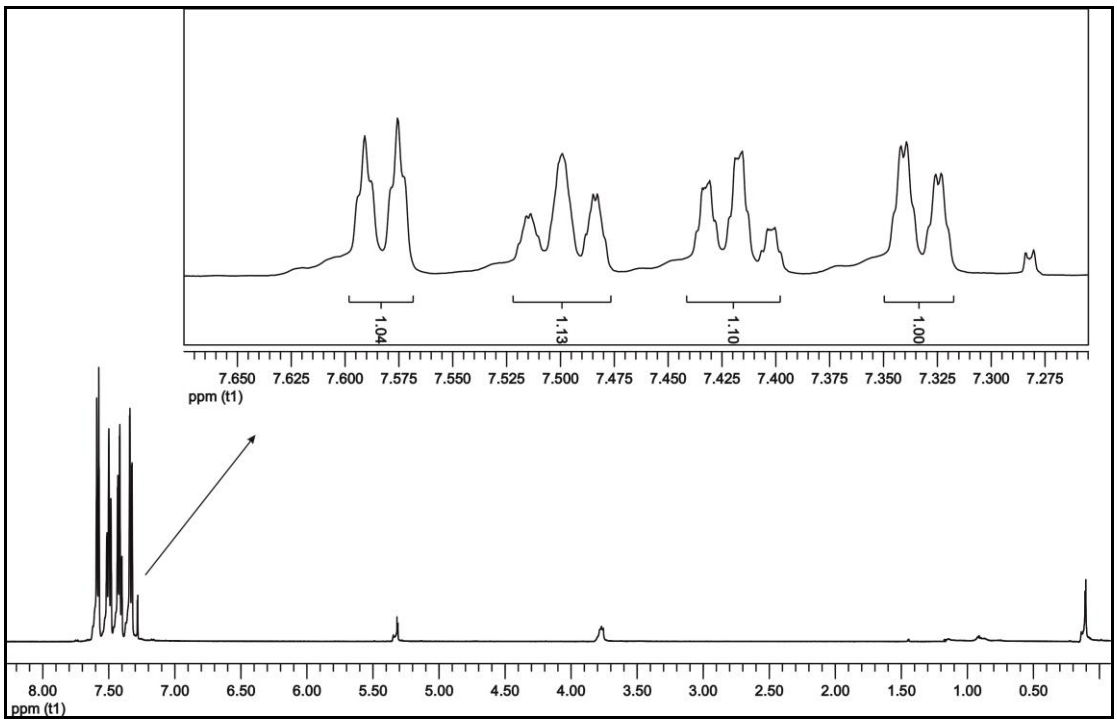

Figure S3. ^{1}H NMR spectrum of compound **1**

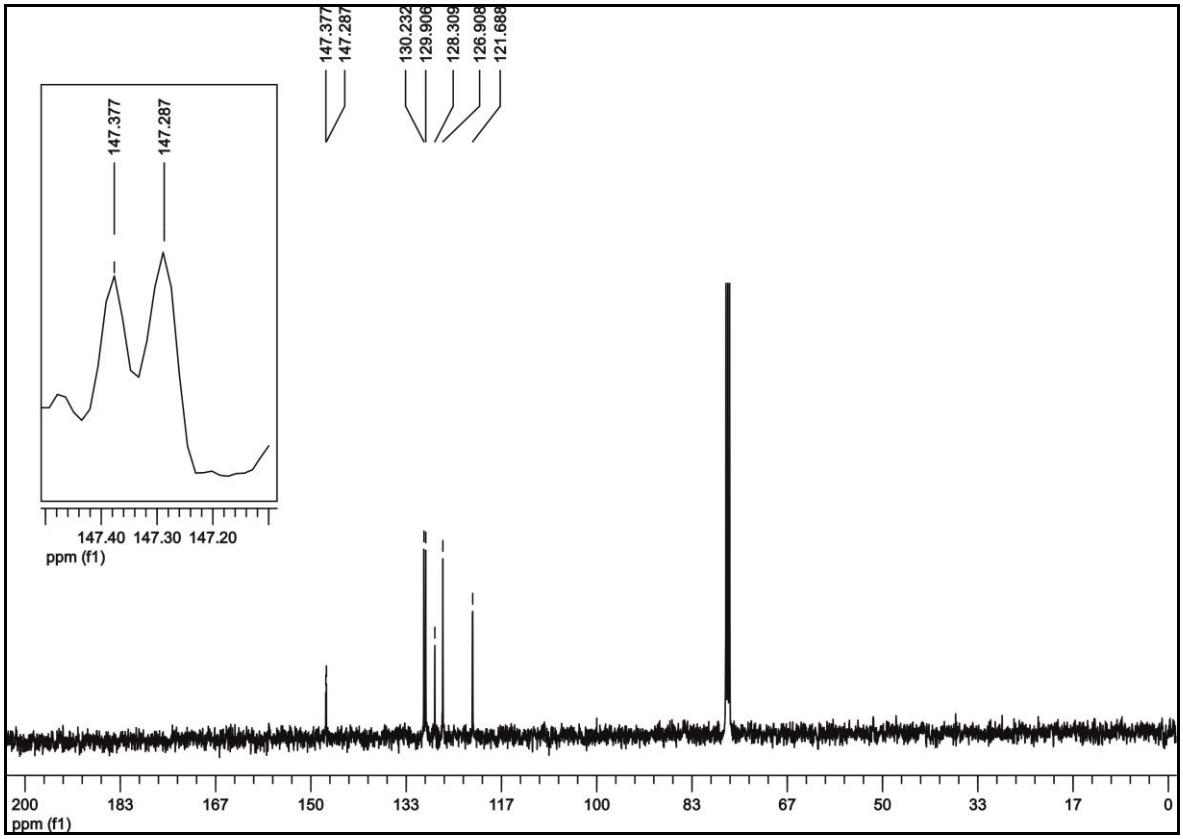

Figure S4. ^{13}C NMR spectrum of compound **1**

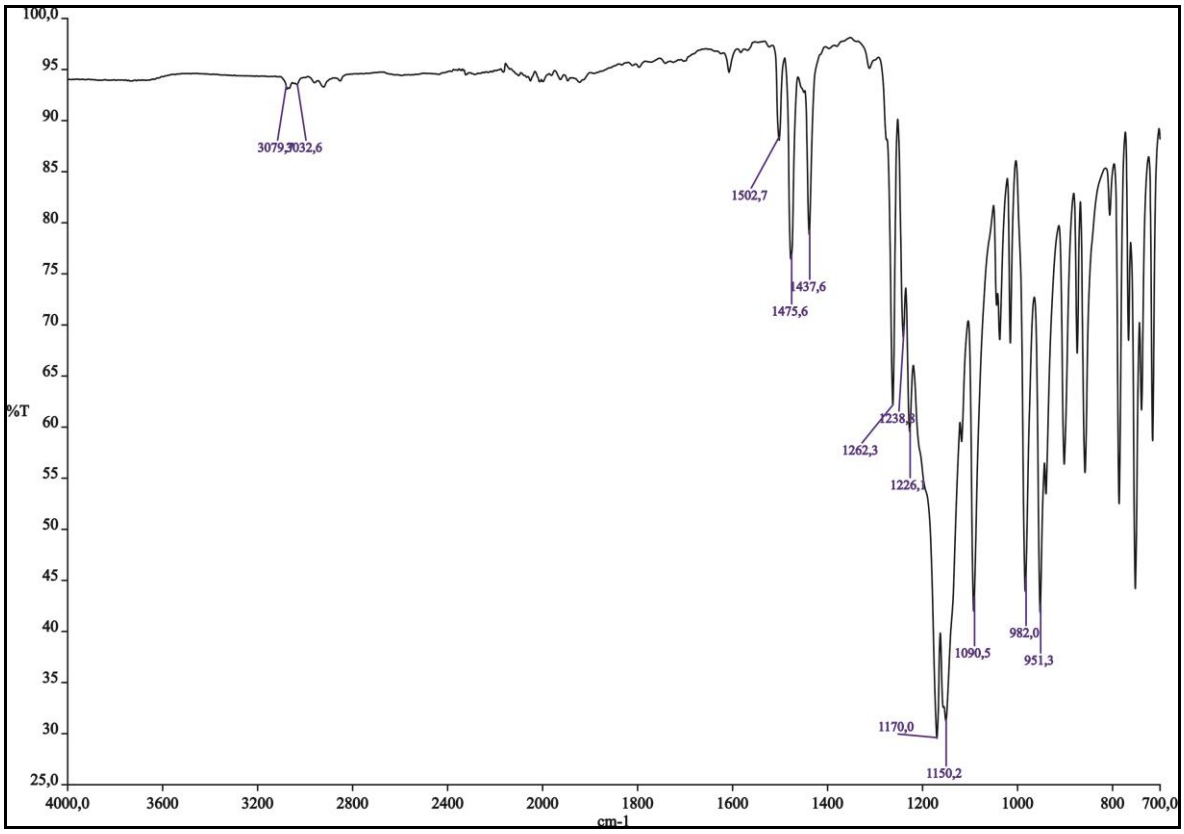

Figure S5. FT-IR spectrum of compound **1**

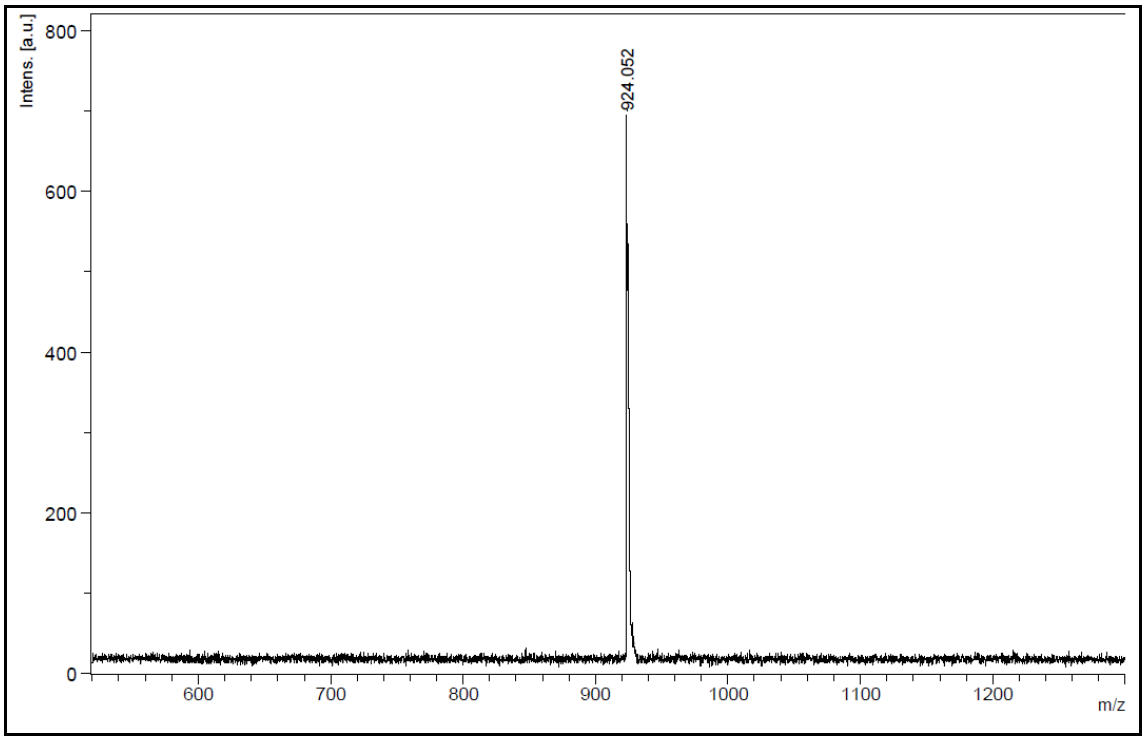

Figure S6. Mass spectrum of compound **2**.

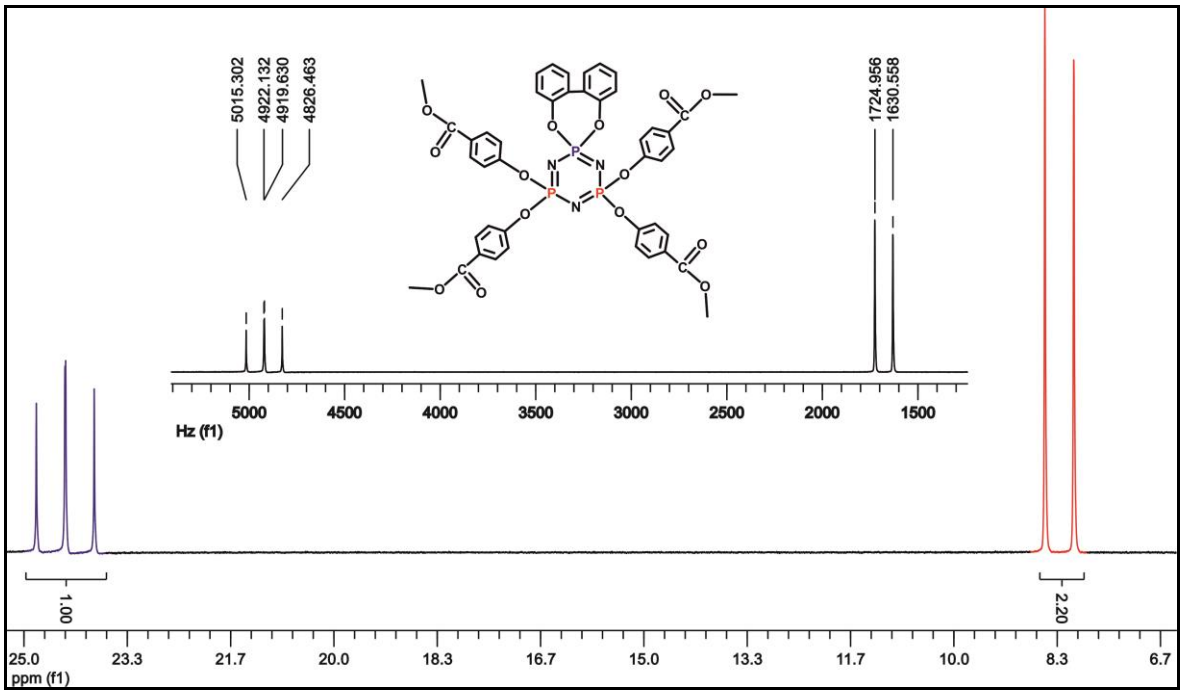

Figure S7. The proton decoupled ^{31}P NMR spectrum of compound **2**

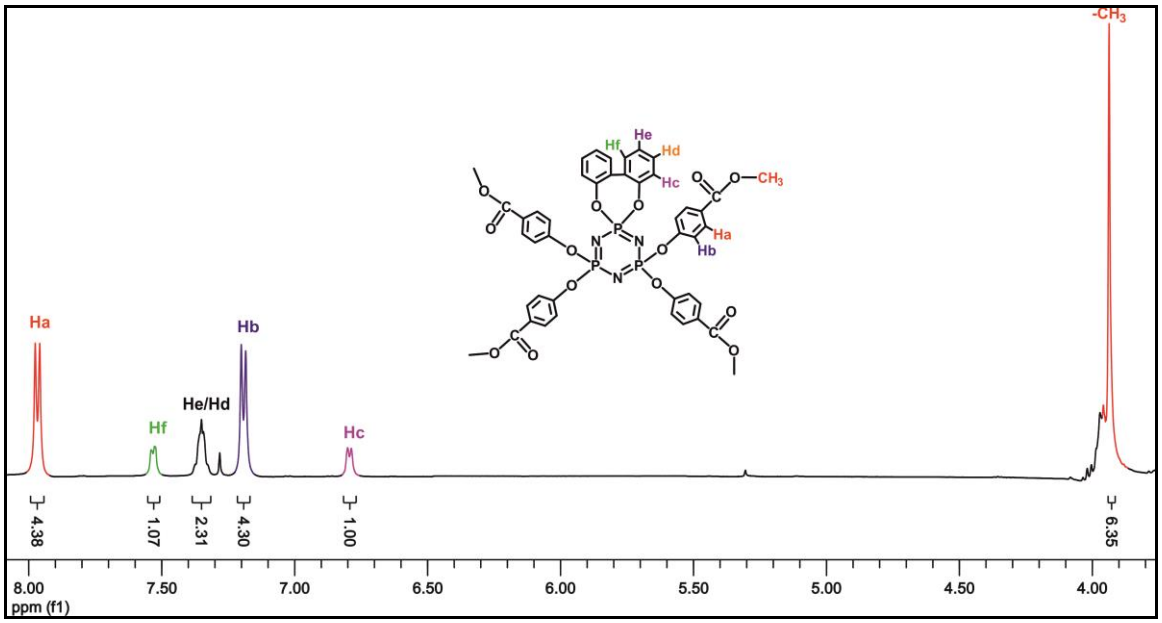

Figure S8. ^{1}H NMR spectrum of compound **2**

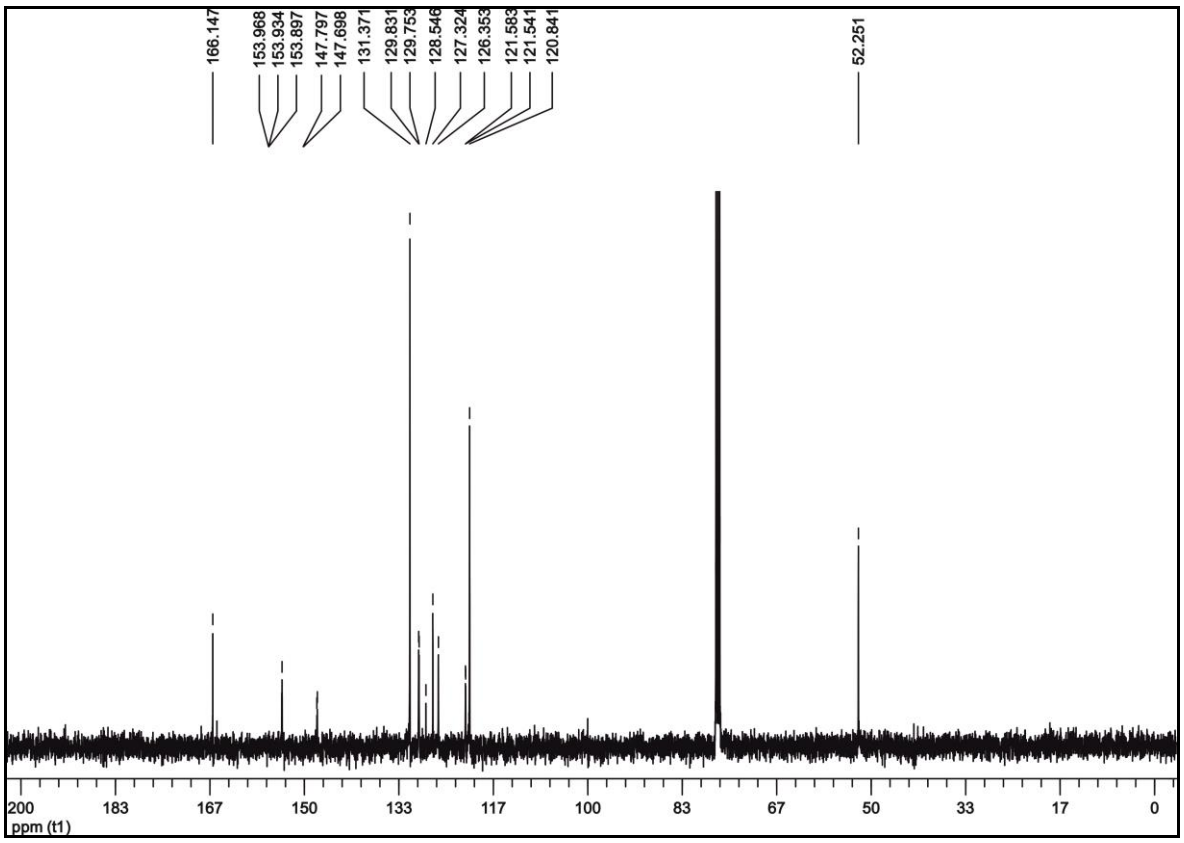

Figure S9. ^{13}C NMR spectrum of compound **2**

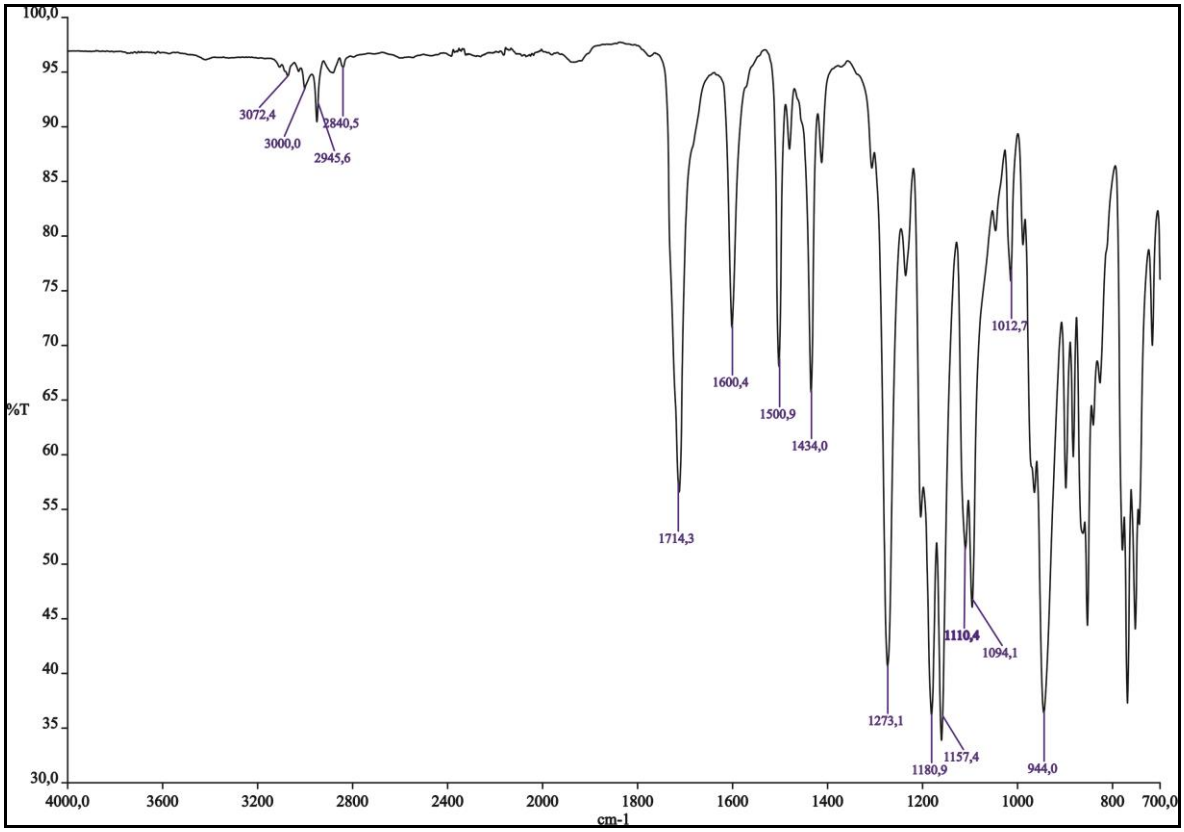

Figure S10. FT-IR spectrum of compound **2**

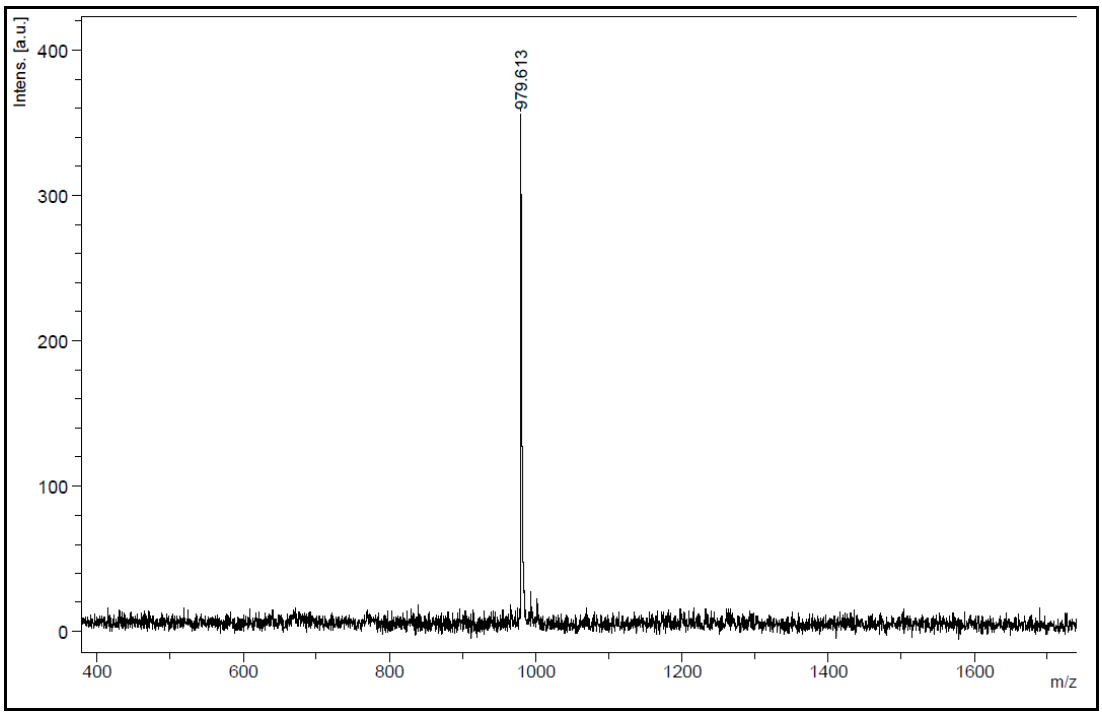

Figure S11. Mass spectrum of compound **3**.

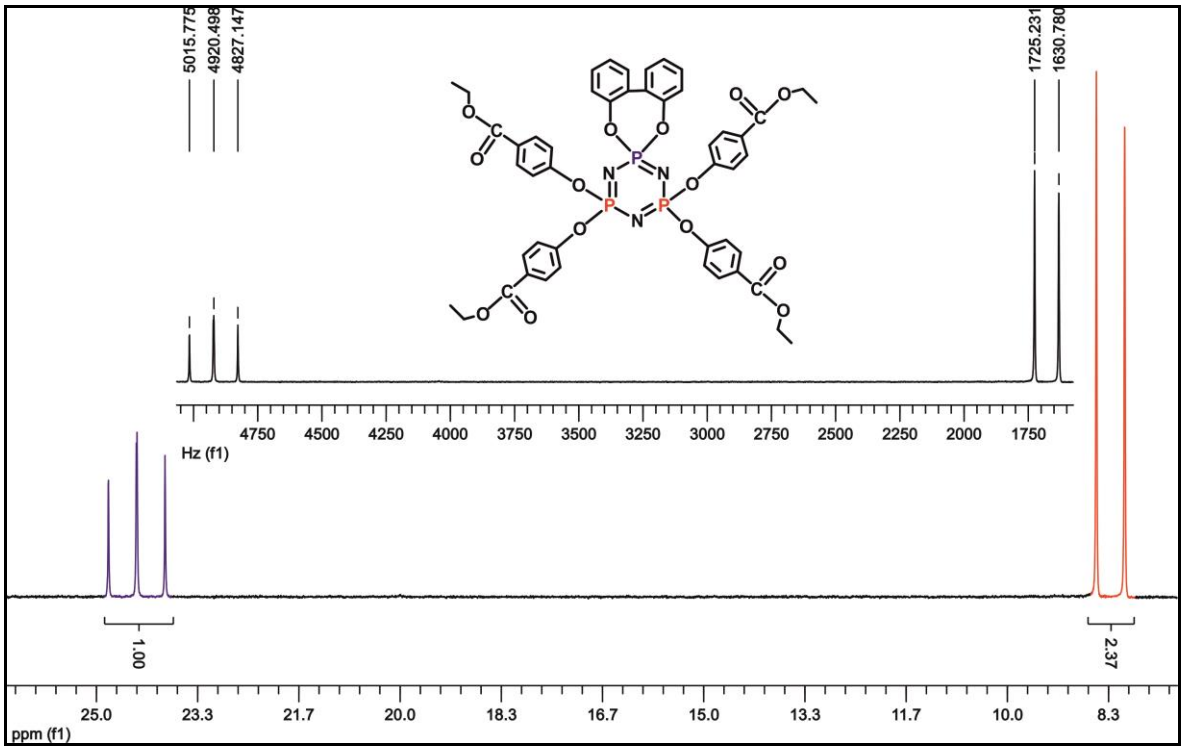

Figure S12. The proton decoupled ^{31}P NMR spectrum of compound **3**

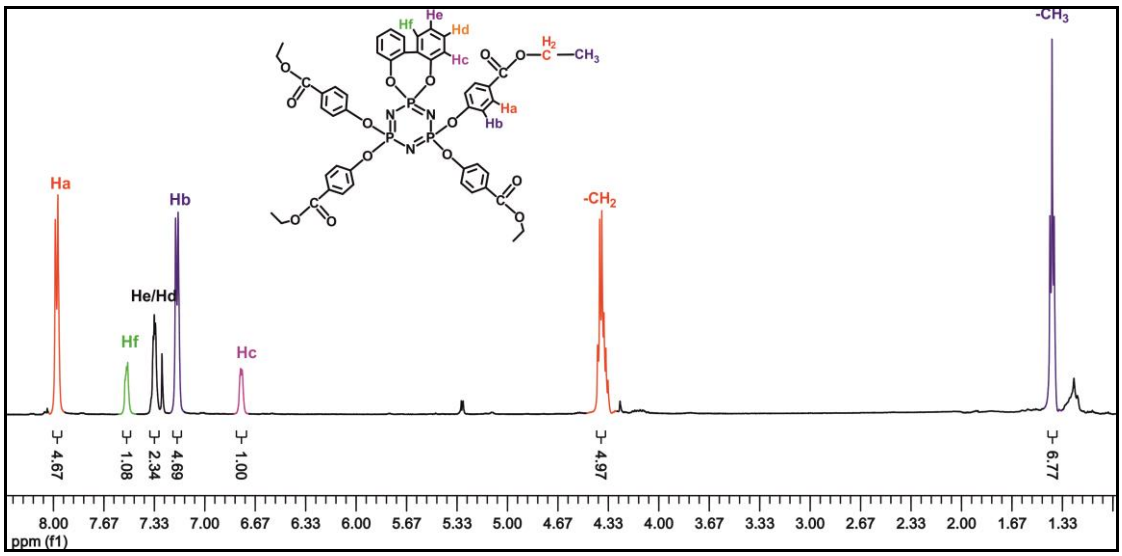

Figure S13. ^{1}H NMR spectrum of compound **3**

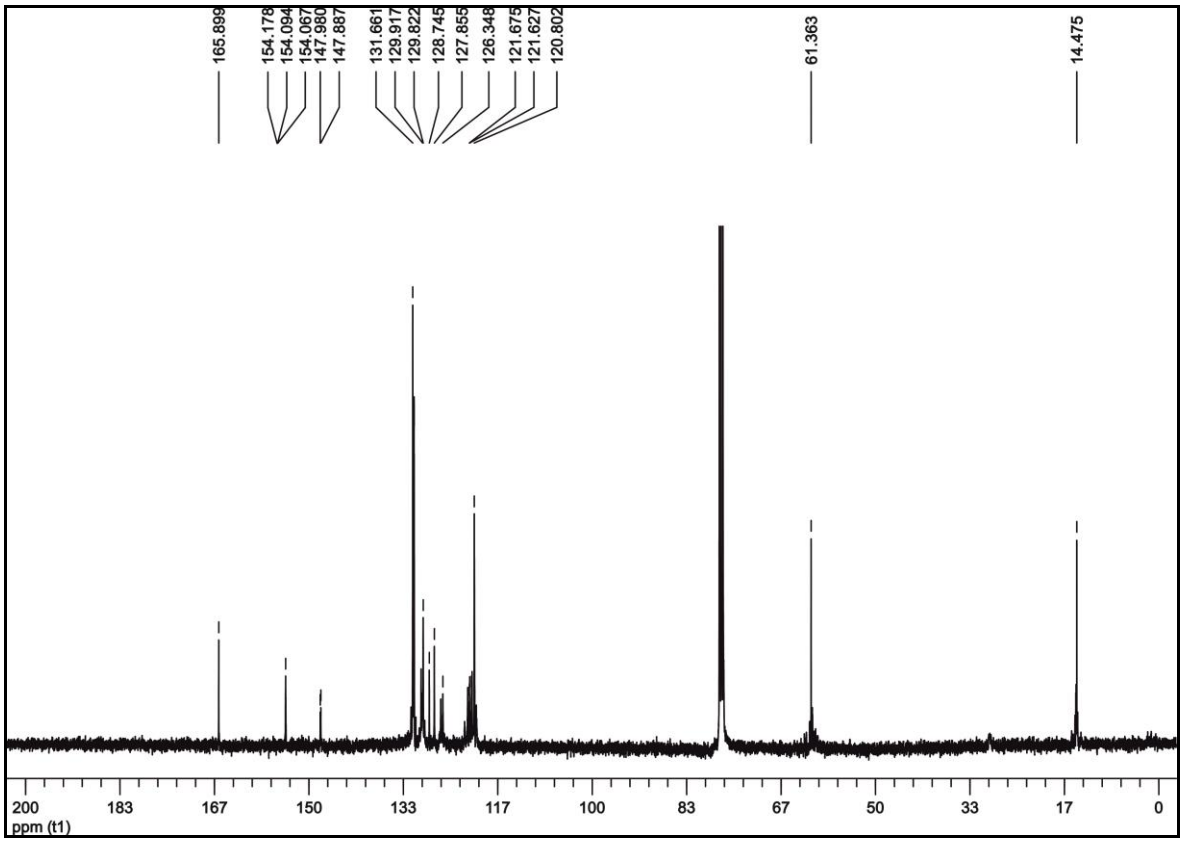

Figure S14. ^{13}C NMR spectrum of compound **3**

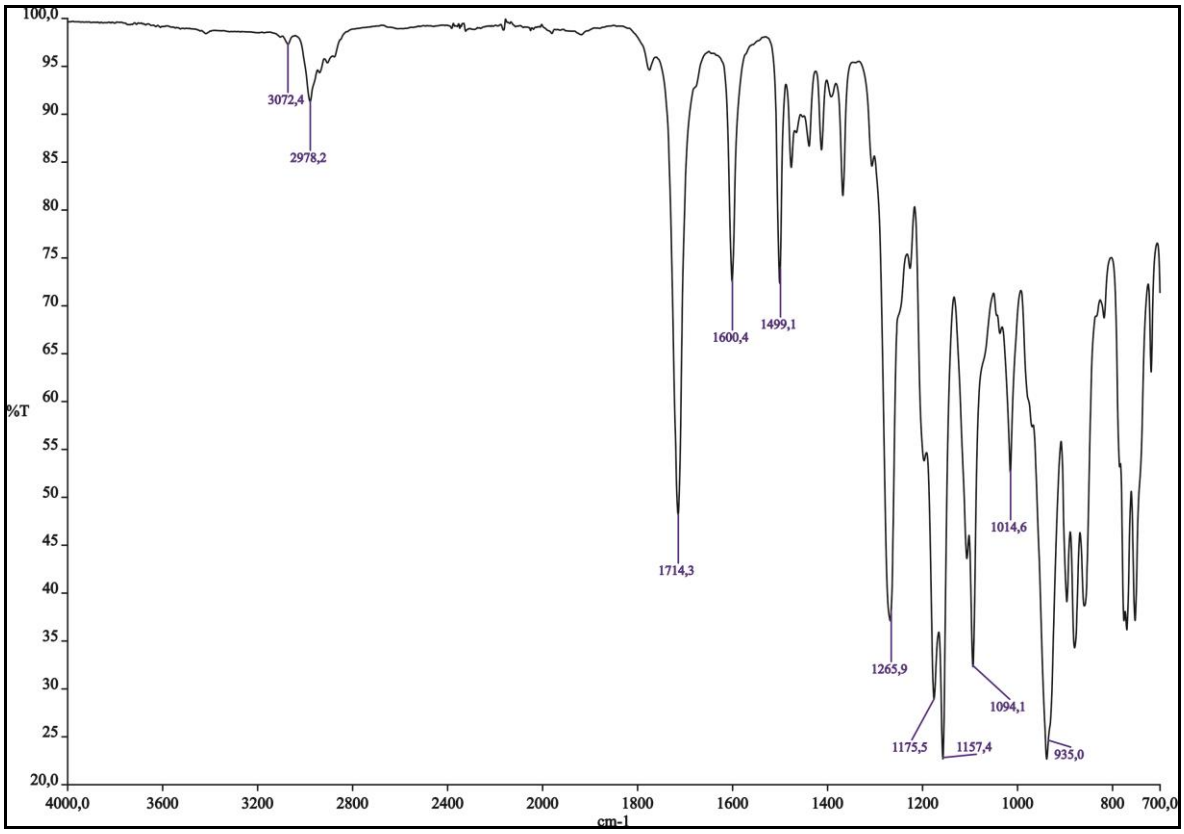

Figure S15. FT-IR spectrum of compound **3**

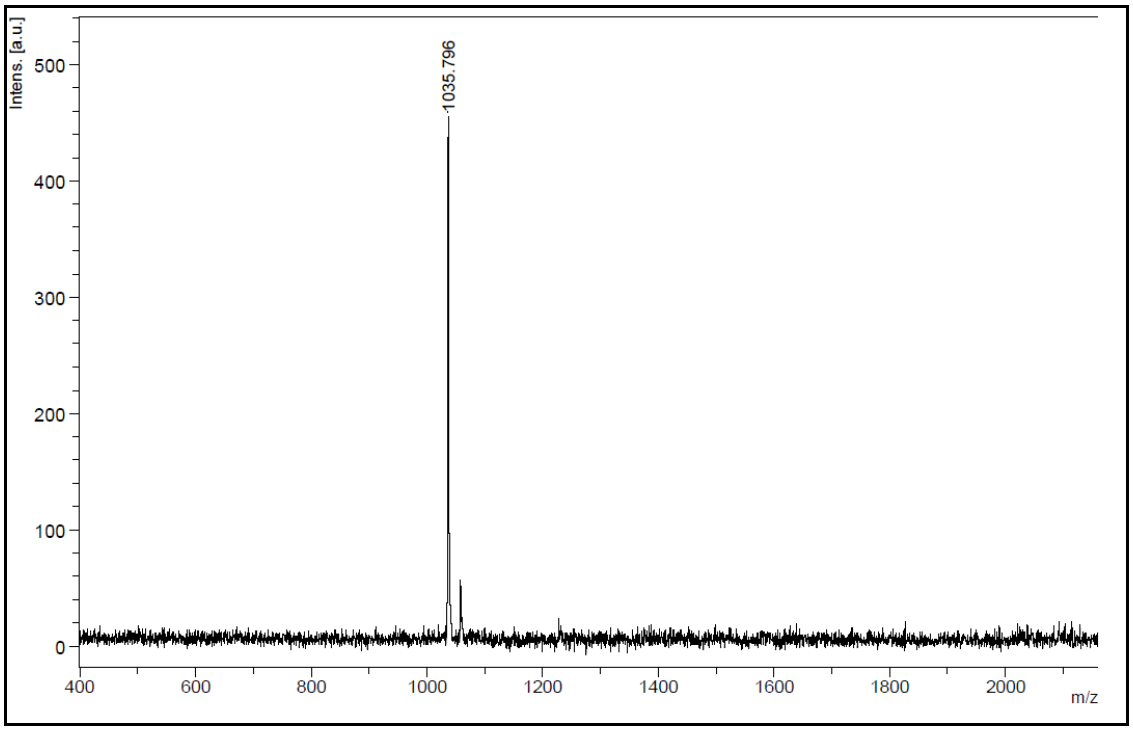

Figure S16. Mass spectrum of compound **4**.

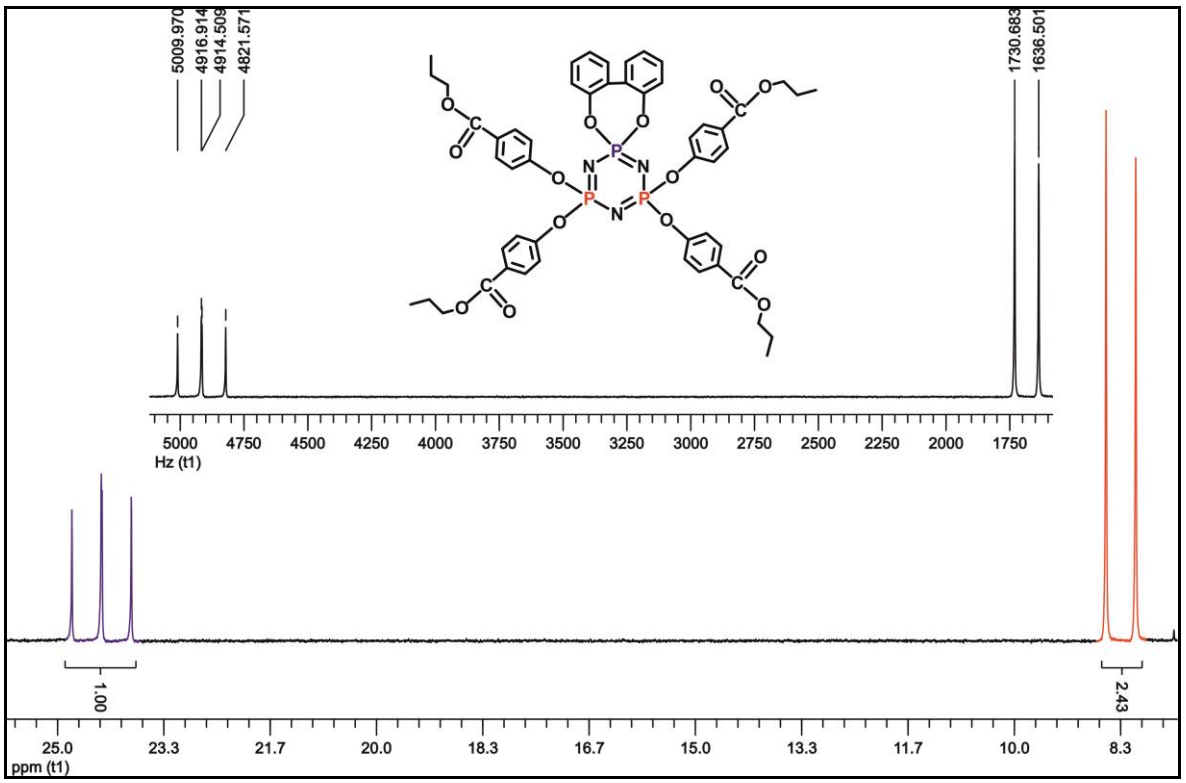

Figure S17. The proton decoupled ^{31}P NMR spectrum of compound **4**

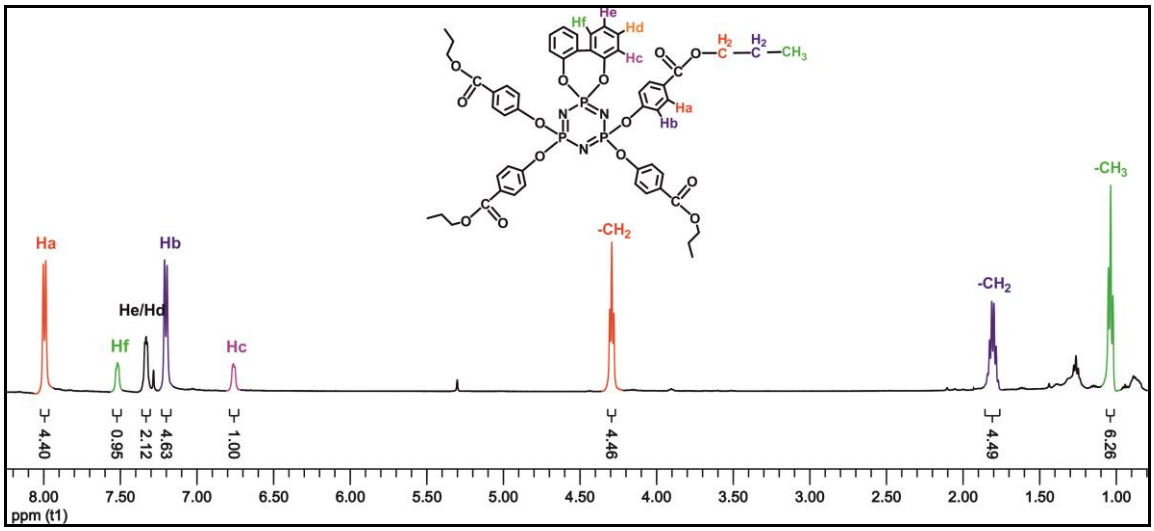

Figure S18. ^{1}H NMR spectrum of compound **4**

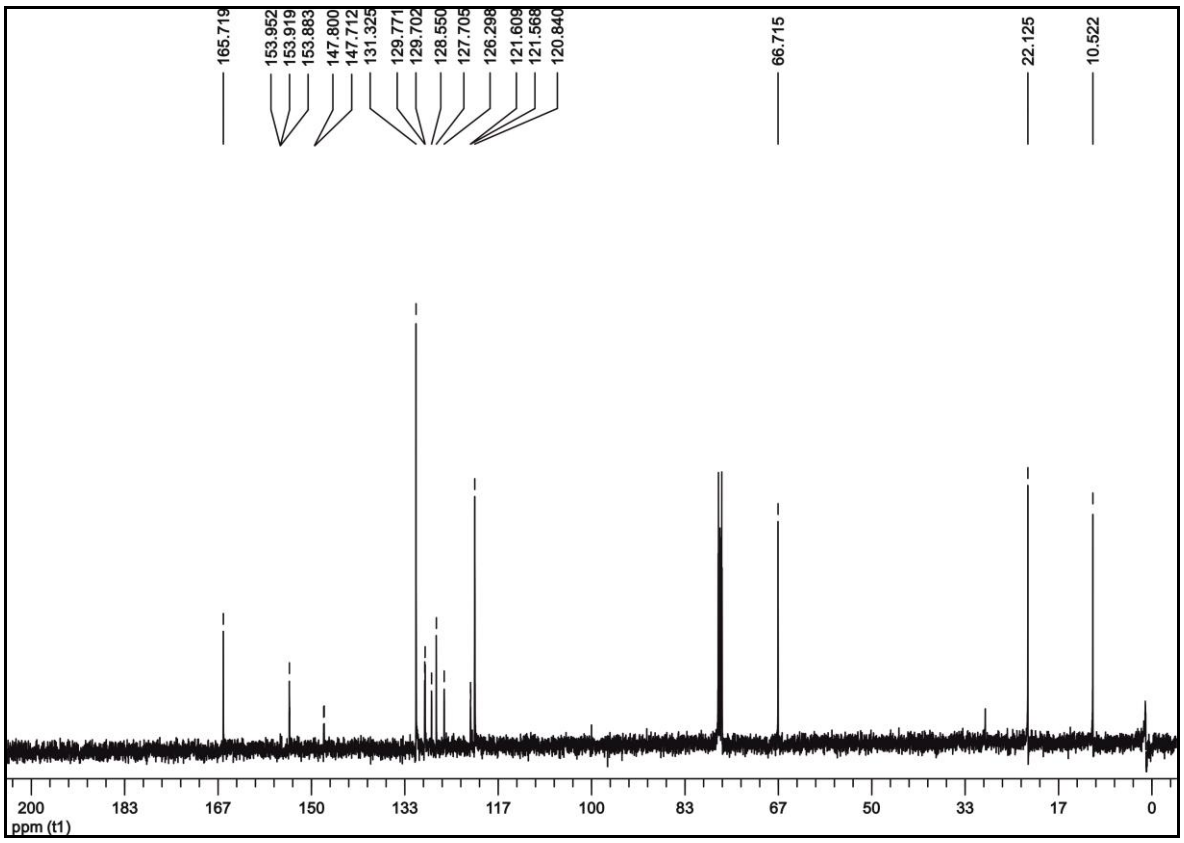

Figure S19. ^{13}C NMR spectrum of compound **4**

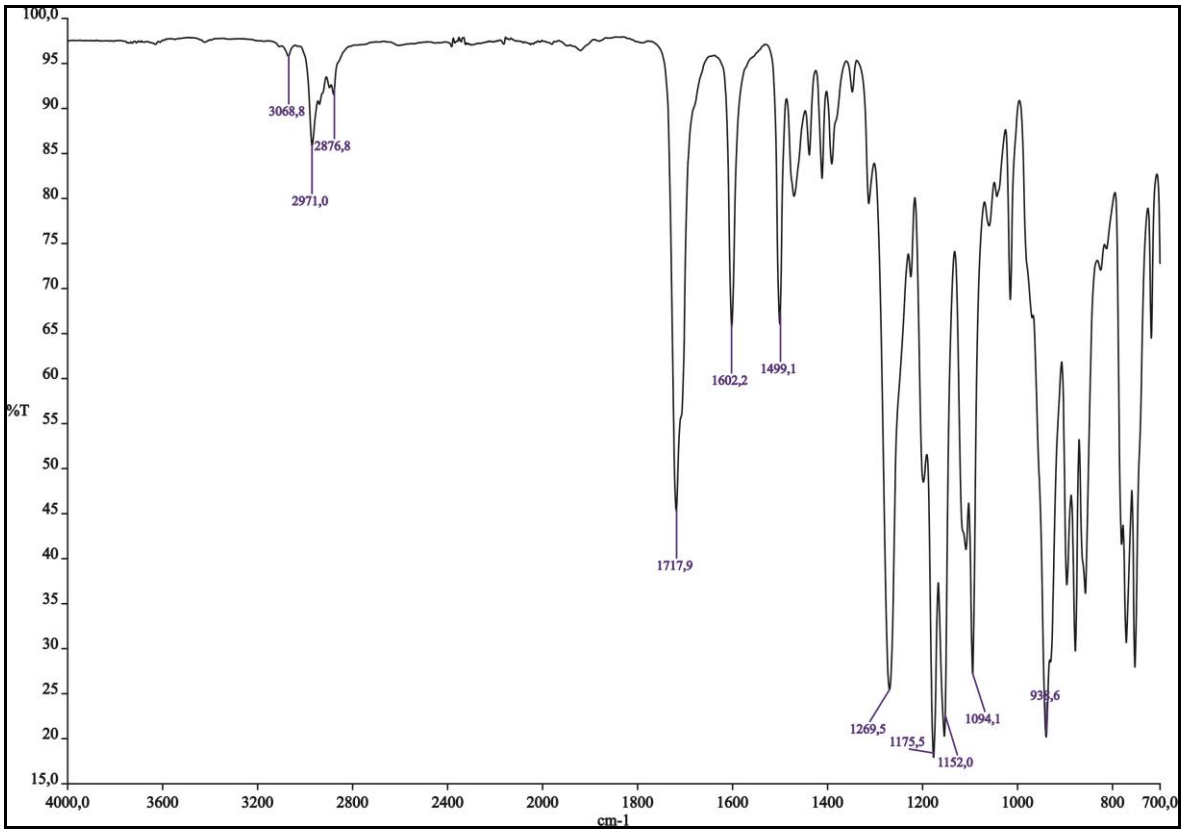

Figure S20. FT-IR spectrum of compound **4**

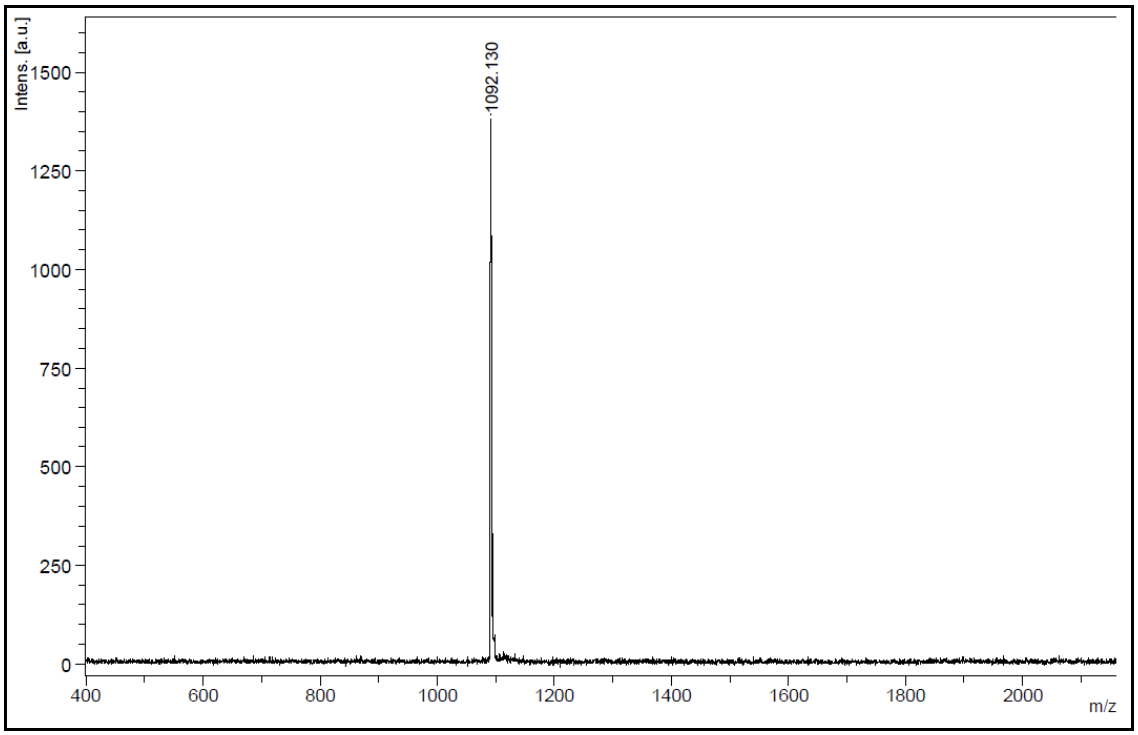

Figure S21. Mass spectrum of compound **5**.

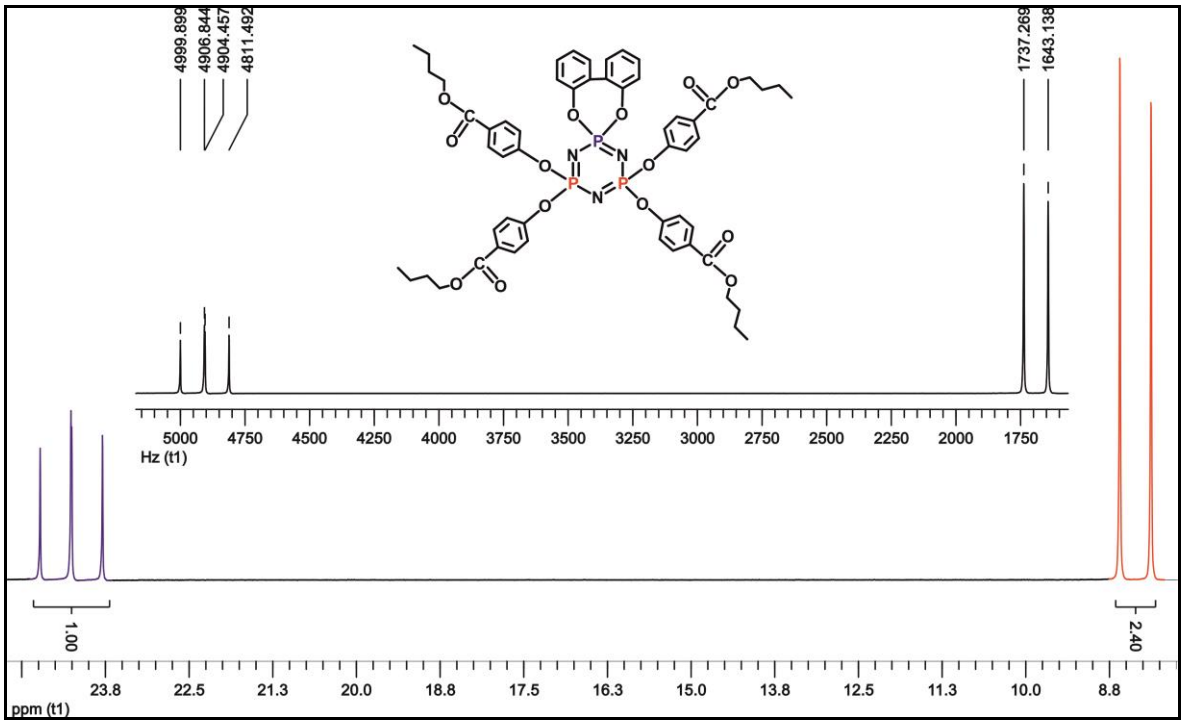

Figure S22. The proton decoupled ^{31}P NMR spectrum of compound **5**

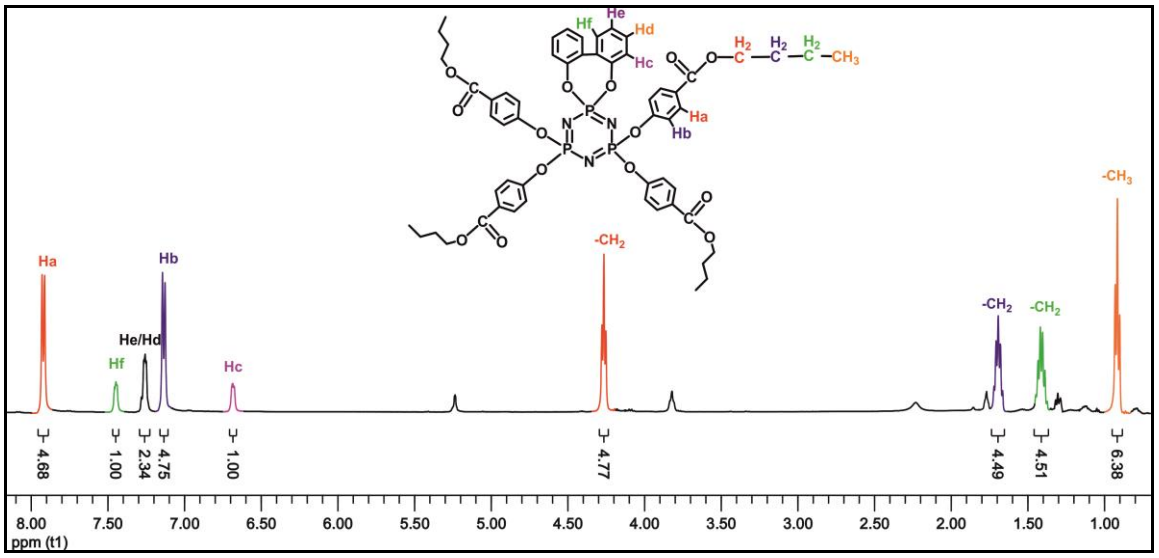

Figure S23. ^{1}H NMR spectrum of compound **5**

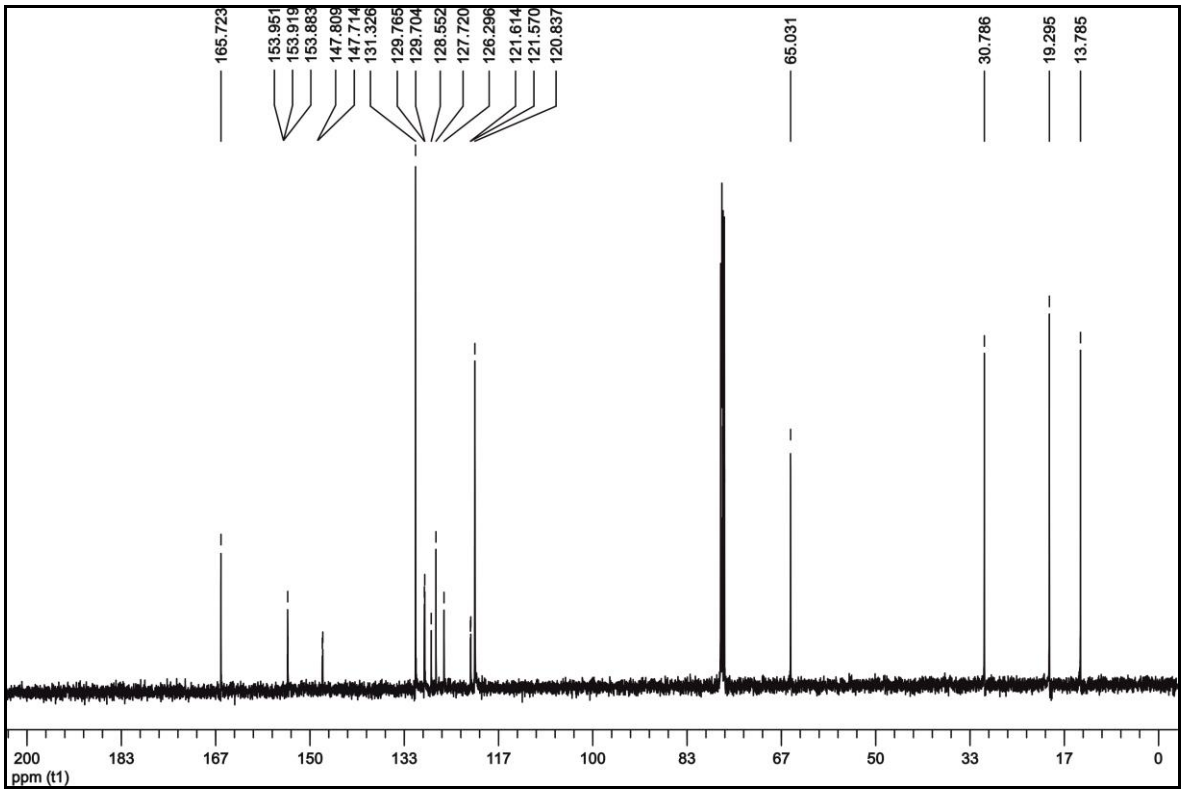

Figure S24. ^{13}C NMR spectrum of compound **5**

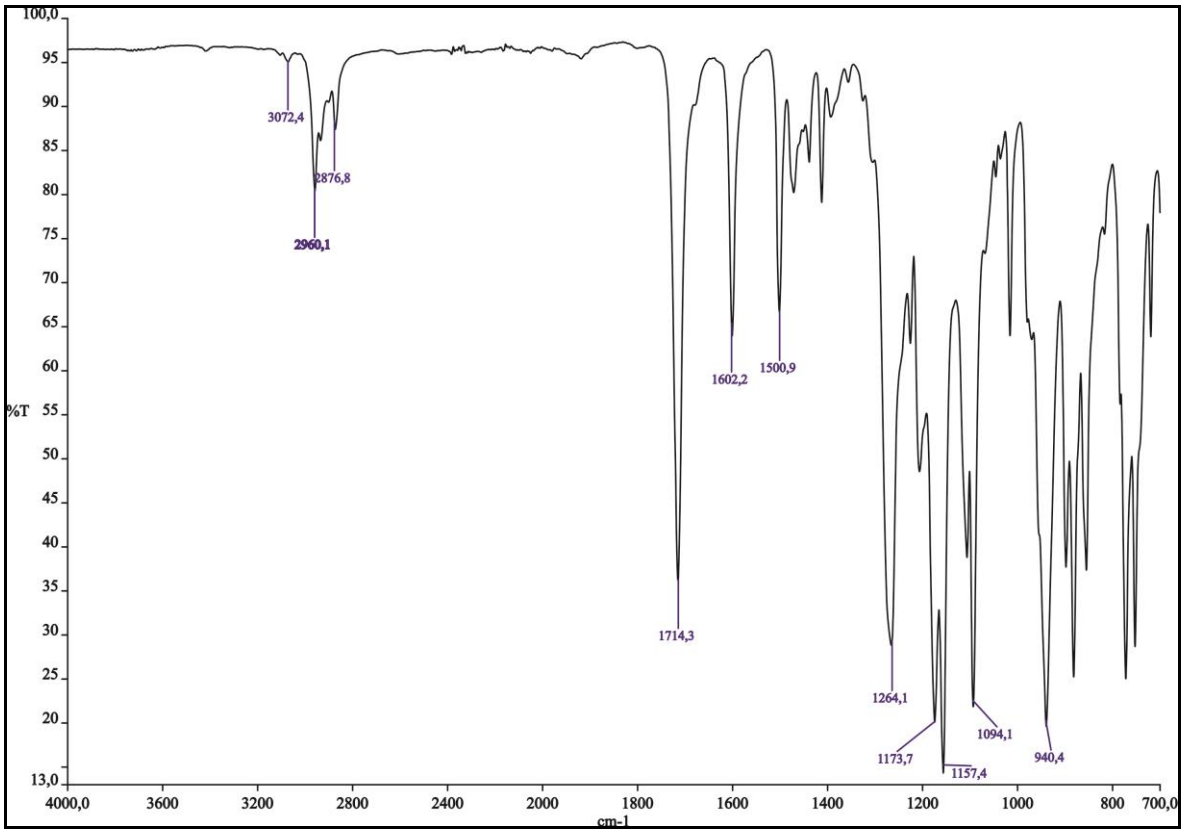

Figure S25. FT-IR spectrum of compound **5**

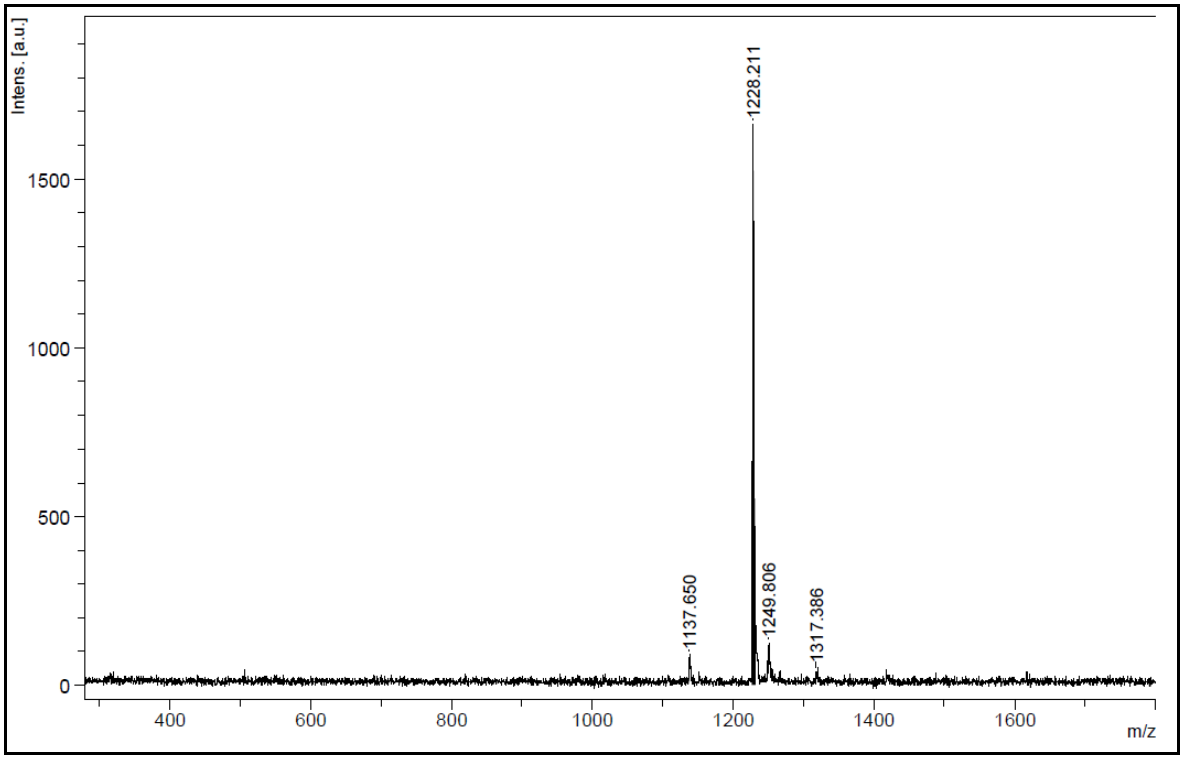

Figure S26. Mass spectrum of compound **6**.

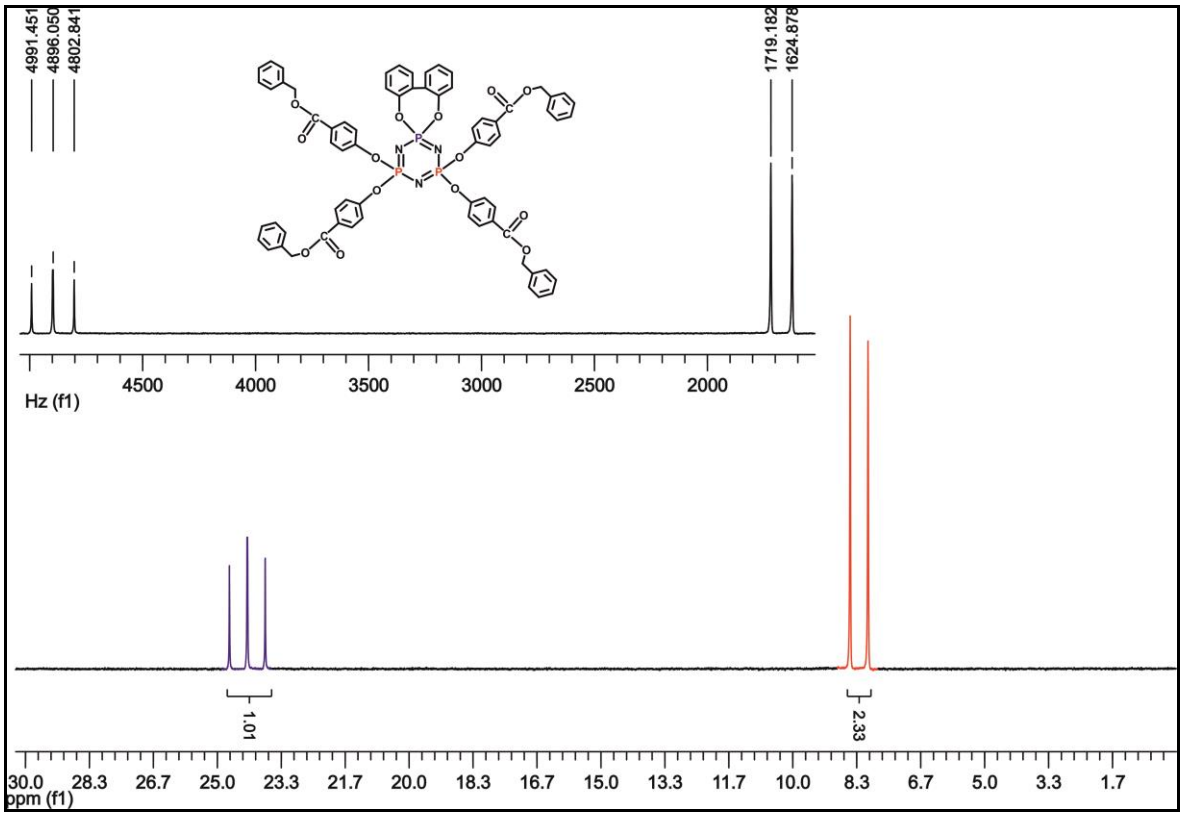

Figure S27. The proton decoupled ^{31}P NMR spectrum of compound **6**

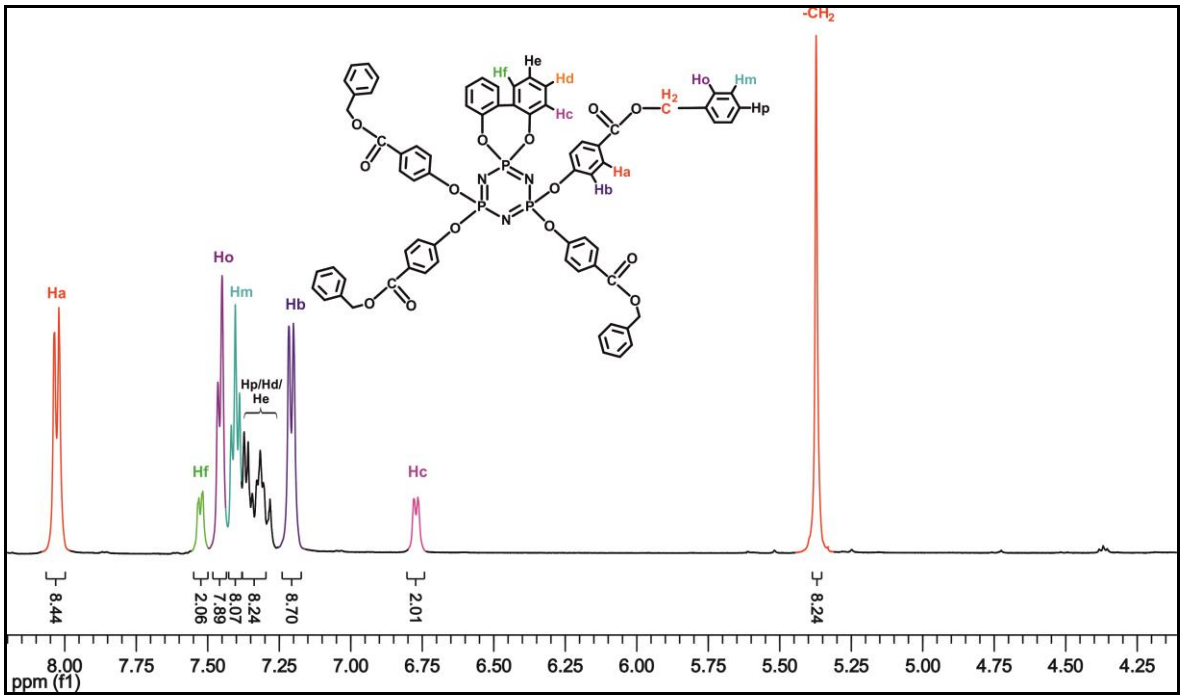

Figure S28. ^{1}H NMR spectrum of compound **6**

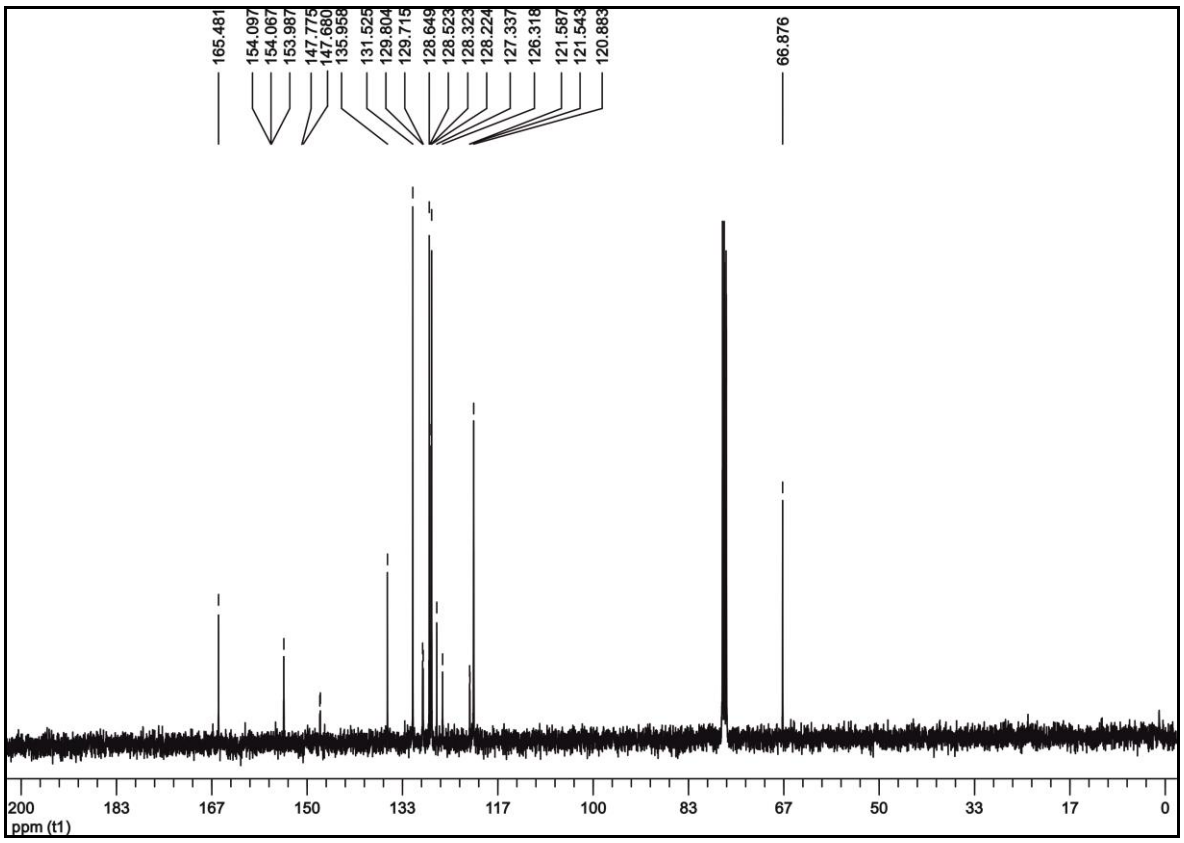

Figure S29. ^{13}C NMR spectrum of compound **6**

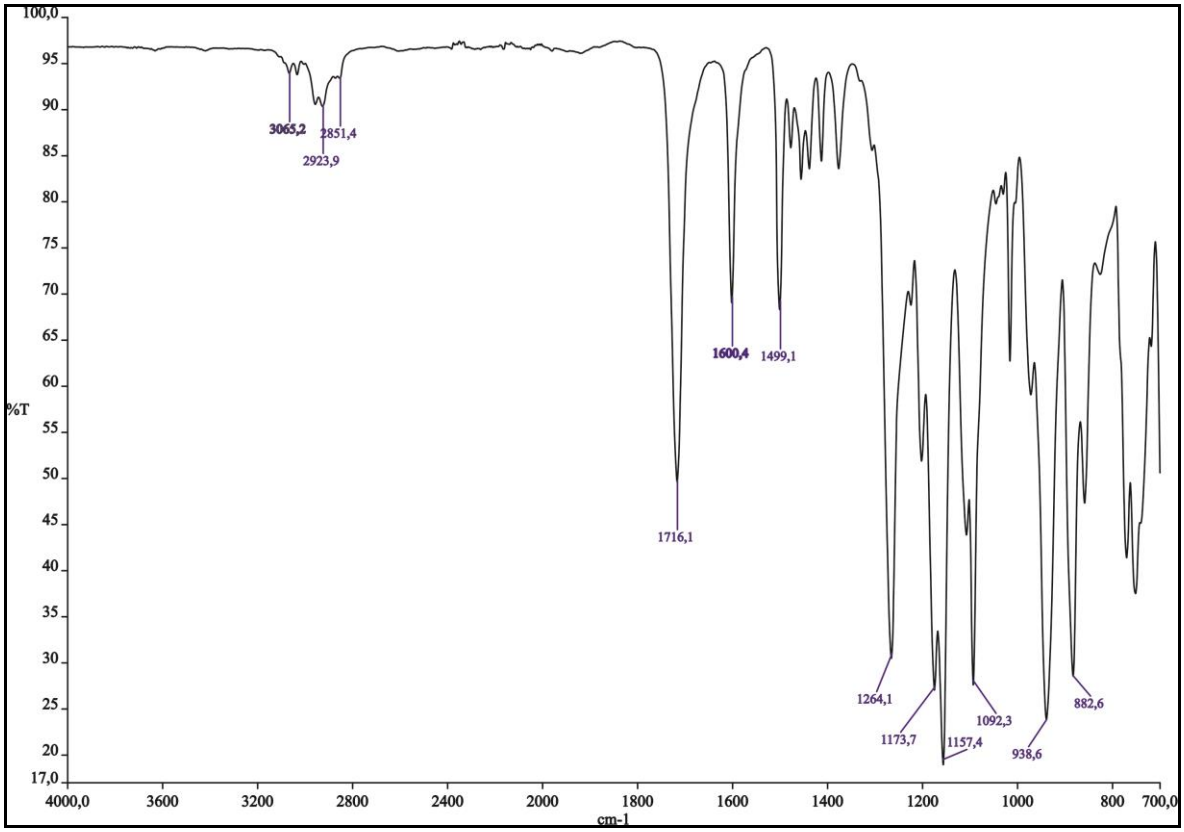

Figure S30. FT-IR spectrum of compound **6**

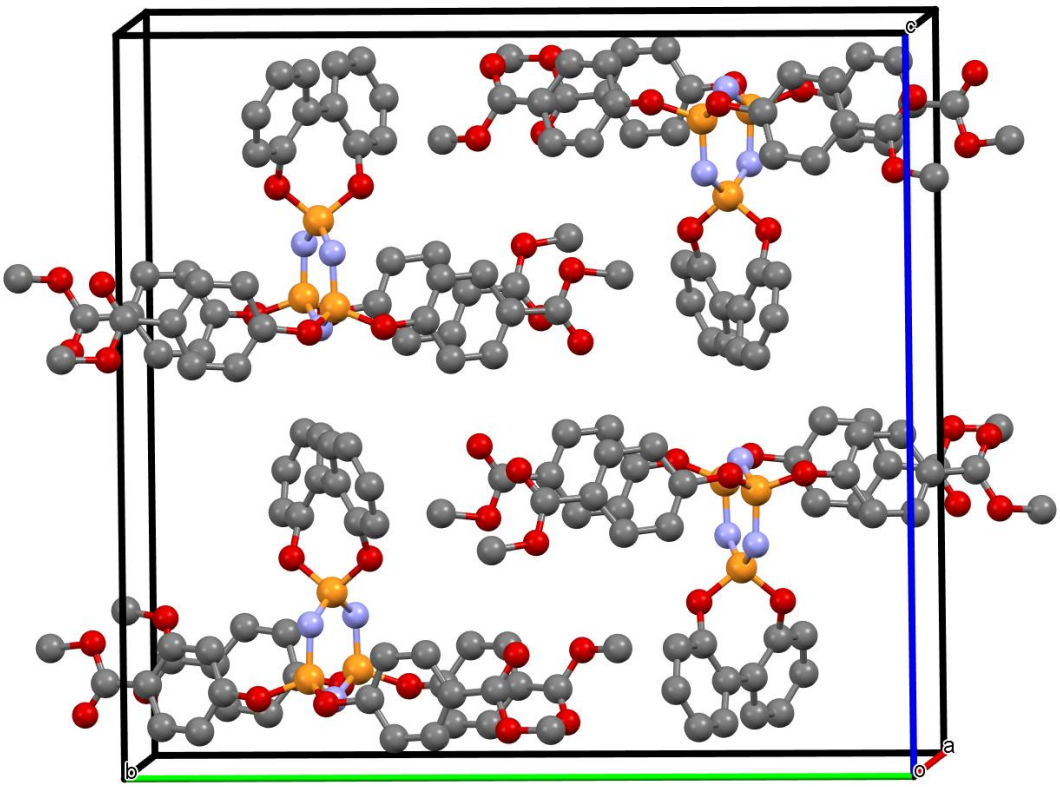

Figure S31. Perspective view of crystal packing of compound **2**

Table S1. The bond and conformational parameters for compounds **2.**

2			
Bond Lengths (Å)			
P2—O3	1.574 (2)	C24—C23	1.392 (5)
P2—O4	1.579 (3)	C24—C25	1.381 (5)
P2—N2	1.577 (3)	C21—C26	1.366 (5)
P2—N1	1.572 (3)	C21—C22	1.373 (5)
P1—O2	1.583 (2)	C29—C30	1.347 (6)
P1—O1	1.578 (2)	C29—C34	1.360 (6)
P1—N3	1.577 (3)	C11—C10	1.375 (6)
P1—N1	1.571 (3)	C2—C3	1.381 (5)
P3—O5	1.580 (2)	C18—C17	1.372 (5)
P3—O6	1.576 (2)	C16—C19	1.478 (5)
P3—N3	1.576 (3)	C16—C17	1.383 (5)
P3—N2	1.576 (3)	C16—C15	1.390 (6)
O2—C1	1.404 (4)	C40—C39	1.374 (6)
O5—C13	1.396 (4)	C40—C43	1.480 (6)
O1—C12	1.412 (4)	C40—C41	1.385 (6)
O3—C21	1.402 (4)	O12—C43	1.307 (6)
O4—C37	1.402 (4)	O12—C44	1.430 (6)
O6—C29	1.397 (4)	C23—C22	1.380 (5)
O9—C27	1.324 (5)	C5—C4	1.366 (6)

O9—C28	1.441 (5)	C25—C26	1.371 (5)
O8—C19	1.323 (5)	C8—C9	1.366 (6)
O8—C20	1.438 (5)	C38—C39	1.376 (6)
O10—C27	1.194 (5)	C4—C3	1.362 (6)
O7—C19	1.198 (5)	C9—C10	1.385 (6)
C37—C38	1.370 (5)	C15—C14	1.369 (6)
C37—C42	1.362 (5)	C42—C41	1.369 (6)
C7—C6	1.476 (5)	O11—C43	1.175 (6)
C7—C12	1.386 (5)	C30—C31	1.371 (6)
C7—C8	1.404 (5)	C34—C33	1.378 (7)
C1—C6	1.388 (5)	C32—C31	1.358 (7)
C1—C2	1.380 (5)	C32—C33	1.368 (8)
C13—C18	1.364 (5)	C32—C35	1.472 (8)
C13—C14	1.377 (5)	O13—C35	1.173 (9)
C6—C5	1.399 (5)	O14—C35	1.248 (9)
C12—C11	1.378 (5)	O14—C36	1.464 (7)
C24—C27	1.483 (5)		
Bond Angles (°)			
O3—P2—O4	92.77 (13)	C22—C21—O3	119.3 (3)
O3—P2—N2	111.11 (15)	C30—C29—O6	123.1 (3)
N2—P2—O4	111.11 (15)	C30—C29—C34	120.6 (4)
N1—P2—O3	111.46 (14)	C34—C29—O6	116.1 (4)
N1—P2—O4	112.01 (15)	C10—C11—C12	119.2 (4)
N1—P2—N2	116.05 (15)	C1—C2—C3	119.3 (4)
O1—P1—O2	102.91 (12)	C13—C18—C17	120.1 (4)
N3—P1—O2	104.88 (13)	O9—C27—C24	112.9 (3)
N3—P1—O1	111.76 (15)	O10—C27—O9	122.5 (4)
N1—P1—O2	112.13 (15)	O10—C27—C24	124.6 (4)
N1—P1—O1	105.75 (14)	C17—C16—C19	122.0 (4)
N1—P1—N3	118.42 (15)	C17—C16—C15	118.4 (4)
O6—P3—O5	93.05 (13)	C15—C16—C19	119.5 (4)
O6—P3—N2	110.88 (15)	C39—C40—C43	122.2 (4)
N3—P3—O5	111.38 (15)	C39—C40—C41	118.6 (4)
N3—P3—O6	112.07 (14)	C41—C40—C43	119.2 (4)
N3—P3—N2	116.01 (15)	C43—O12—C44	117.9 (5)
N2—P3—O5	111.19 (15)	C22—C23—C24	120.5 (4)
C1—O2—P1	122.8 (2)	C4—C5—C6	122.1 (4)
C13—O5—P3	126.5 (2)	C26—C25—C24	120.6 (3)
C12—O1—P1	123.1 (2)	C21—C26—C25	119.5 (3)
C21—O3—P2	123.4 (2)	C9—C8—C7	121.7 (4)
C37—O4—P2	125.5 (2)	C37—C38—C39	118.5 (4)
C29—O6—P3	125.3 (2)	O8—C19—C16	112.2 (4)
P3—N3—P1	122.23 (18)	O7—C19—O8	123.7 (4)
P3—N2—P2	124.66 (18)	O7—C19—C16	124.0 (4)
C27—O9—C28	115.7 (3)	C21—C22—C23	118.7 (3)
P1—N1—P2	122.49 (17)	C18—C17—C16	120.4 (4)
C19—O8—C20	116.2 (4)	C3—C4—C5	120.3 (3)
C38—C37—O4	120.0 (3)	C4—C3—C2	120.0 (4)
C42—C37—O4	117.8 (3)	C8—C9—C10	120.1 (4)

C42—C37—C38	121.7 (3)	C14—C15—C16	121.3 (4)
C12—C7—C6	123.5 (3)	C37—C42—C41	119.1 (4)
C12—C7—C8	116.3 (3)	C15—C14—C13	118.9 (4)
C8—C7—C6	120.2 (3)	C40—C39—C38	121.2 (4)
C6—C1—O2	119.4 (3)	C11—C10—C9	119.9 (4)
C2—C1—O2	118.1 (3)	O12—C43—C40	113.2 (4)
C2—C1—C6	122.2 (3)	O11—C43—C40	123.3 (5)
C18—C13—O5	117.6 (3)	O11—C43—O12	123.1 (5)
C18—C13—C14	120.9 (3)	C42—C41—C40	120.8 (4)
C14—C13—O5	121.1 (3)	C29—C30—C31	119.8 (4)
C1—C6—C7	122.7 (3)	C29—C34—C33	119.0 (5)
C1—C6—C5	116.1 (3)	C31—C32—C33	118.2 (4)
C5—C6—C7	121.2 (3)	C31—C32—C35	124.3 (6)
C7—C12—O1	119.7 (3)	C33—C32—C35	117.5 (6)
C11—C12—O1	117.4 (3)	C35—O14—C36	106.9 (7)
C11—C12—C7	122.7 (3)	C32—C31—C30	121.2 (5)
C23—C24—C27	122.9 (3)	C32—C33—C34	121.1 (5)
C25—C24—C27	118.1 (3)	O13—C35—C32	126.6 (8)
C25—C24—C23	119.0 (3)	O13—C35—O14	119.2 (6)
C26—C21—O3	118.8 (3)	O14—C35—C32	114.2 (8)
C26—C21—C22	121.7 (3)		

Table S2. Predicted Log IC_{50} (μM) and calculated Log IC_{50} (μM) value of Compounds **1-6** for MCF-7 and DLD-1 cell lines

MCF-7 cell line	Experimental Doses	Predicted Log IC_{50} (μM)	Calculated IC_{50} value	Observed Log IC_{50} (μM)	Residual Error
Compound **1**	50	4.301	173.660	3.760	-0.678
Compound **2**	12.5	4.903	79.692	4.099	-1.016
Compound **3**	25	4.602	93.469	4.029	-0.769
Compound **4**	200	3.699	173.062	3.762	-0.075
Compound **5**	50	4.301	76.137	4.118	-0.399
Compound **6**	25	4.602	72.238	4.141	-0.682

DLD-1 cell line	Experimental Doses	Predicted Log IC_{50} (μM)	Calculated IC_{50} value	Observed Log IC_{50} (μM)	Residual Error
Compound **1**	25	4.602	14.712	4.832	-0.143
Compound **2**	25	4.602	107.328	3.969	-0.816
Compound **3**	25	4.602	54.320	4.265	-0.585
Compound **4**	200	3.699	157.244	3.803	-0.042
Compound **5**	25	4.602	67.192	4.173	-0.657
Compound **6**	12.5	4.903	36.087	4.443	-0.748