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

Table 1: Crystal data and structure refinement details **3P**.

Empirical formula	$C_{35}H_{36}N_2O_6S_2$	
Formula weight	644.78	
Temperature	296(2) K	
Wavelength	1.54178 Å	
Reflns. for cell determination	4501	
θ range for above	2.62° to 64.92°	
Crystal system	Monoclinic	
Space group	$P21/c$	
Cell dimensions		
$a = 17.5740(17)$ Å	$b = 8.9640(9)$ Å	$c = 20.843(2)$ Å
$\alpha = 90.00°$	$\beta = 106.682(4)°$	$\gamma = 90.00°$
Volume	3145.3(5) Å^3	
Z	4	
Density(calculated)	1.362 Mg m^{-3}	
Absorption coefficient	1.943 mm^{-1}	
F_{000}	1360	
Crystal size	0.27 × 0.27 × 0.27 mm	
θ range for data collection	2.62° to 64.92°	
Index ranges	$-20 \leq h \leq 20$	
	$-10 \leq k \leq 10$	
	$-24 \leq l \leq 20$	
Reflections collected	14873	
Independent reflections	5126 [$R_{\text{int}} = 0.0399$]	
Absorption correction	multi-scan	
Refinement method	Full matrix least-squares on F^2	
Data / restraints / parameters	5126 / 0 / 410	
Goodness-of-fit on F^2	1.078	
Final [$I > 2\sigma(I)$]	$R1 = 0.0545$, $wR2 = 0.1671$	
R indices (all data)	$R1 = 0.0596$, $wR2 = 0.1727$	
Largest diff. peak and hole	0.752 and −0.630 e Å^{-3}	

Table 2: Bond lengths (Å).

Atoms	Length	Atoms	Length
S36-O38	1.427(2)	C9-C10	1.532(3)
S36-O37	1.428(3)	C4-C5	1.404(3)
S36-N14	1.670(2)	C4-C3	1.501(3)
S36-C39	1.757(3)	C7-C8	1.378(3)
S26-C25	1.690(3)	C7-C6	1.407(4)
S26-C22	1.704(2)	C21-C20	1.503(3)
O33-C31	1.337(3)	C21-C12	1.504(3)
O33-C34	1.453(3)	C20-C19	1.388(4)
O27-C7	1.374(3)	C20-C15	1.406(4)
O27-C28	1.413(4)	C15-C16	1.404(4)
O29-C6	1.374(3)	C12-C13	1.516(3)
O29-C30	1.421(4)	C3-C2	1.513(3)
O32-C31	1.199(3)	C5-C6	1.373(4)
N1-C2	1.470(3)	C19-C18	1.384(4)
N1-C21	1.481(3)	C16-C17	1.375(5)
N1-C10	1.495(3)	C39-C44	1.389(5)
N14-C15	1.441(4)	C39-C40	1.391(4)
N14-C13	1.488(3)	C18-C17	1.372(5)
C23-C24	1.468(4)	C24-C25	1.343(5)
C23-C22	1.489(4)	C40-C41	1.373(4)
C22-C10	1.520(3)	C41-C42	1.383(5)
C11-C31	1.516(3)	C42-C43	1.390(4)
C11-C12	1.525(3)	C42-C45	1.504(5)
C11-C10	1.631(3)	C44-C43	1.364(5)
C9-C4	1.378(4)	C34-C35	1.476(5)
C9-C8	1.405(3)		

Table 3: Bond angles (°).

Atoms	Angle	Atoms	Angle
O38-S36-O37	119.15(15)	O27-C7-C6	115.6(2)
O38-S36-N14	108.23(13)	C8-C7-C6	119.2(2)
O37-S36-N14	105.50(13)	C7-C8-C9	121.7(2)
O38-S36-C39	108.73(14)	N1-C21-C20	119.4(2)
O37-S36-C39	109.01(14)	N1-C21-C12	104.31(18)
N14-S36-C39	105.36(12)	C20-C21-C12	113.1(2)
C25-S26-C22	92.12(14)	C19-C20-C15	119.1(2)
C31-O33-C34	116.0(2)	C19-C20-C21	121.1(2)
C7-O27-C28	117.2(2)	C15-C20-C21	119.6(2)
C6-O29-C30	116.5(2)	C16-C15-C20	118.6(3)
C2-N1-C21	113.04(19)	C16-C15-N14	120.5(2)
C2-N1-C10	114.09(18)	C20-C15-N14	120.8(2)
C21-N1-C10	101.74(18)	C21-C12-C13	108.1(2)
C15-N14-C13	117.0(2)	C21-C12-C11	101.79(19)
C15-N14-S36	118.49(18)	C13-C12-C11	120.4(2)
C13-N14-S36	115.92(19)	N14-C13-C12	108.8(2)
C24-C23-C22	105.0(2)	C4-C3-C2	109.2(2)
C23-C22-C10	127.8(2)	N1-C2-C3	108.1(2)
C23-C22-S26	113.36(17)	C6-C5-C4	122.0(2)
C10-C22-S26	118.80(18)	C5-C6-O29	124.8(2)
C31-C11-C12	111.7(2)	C5-C6-C7	118.9(2)
C31-C11-C10	115.72(19)	O29-C6-C7	116.2(2)
C12-C11-C10	102.46(18)	C18-C19-C20	121.3(3)
C4-C9-C8	119.0(2)	C17-C16-C15	120.8(3)
C4-C9-C10	121.8(2)	C44-C39-C40	120.0(3)
C8-C9-C10	119.1(2)	C44-C39-S36	120.1(2)
O32-C31-O33	123.7(2)	C40-C39-S36	119.7(2)
O32-C31-C11	125.5(2)	C17-C18-C19	119.5(3)
O33-C31-C11	110.7(2)	C18-C17-C16	120.6(3)
C9-C4-C5	119.1(2)	C25-C24-C23	115.6(3)
C9-C4-C3	120.9(2)	C41-C40-C39	119.0(3)
C5-C4-C3	120.0(2)	C40-C41-C42	121.9(3)
N1-C10-C22	106.51(18)	C41-C42-C43	117.9(3)
N1-C10-C9	112.36(19)	C41-C42-C45	121.6(3)
C22-C10-C9	109.27(19)	C43-C42-C45	120.5(3)
N1-C10-C11	105.41(17)	C24-C25-S26	113.9(2)
C22-C10-C11	107.80(19)	C43-C44-C39	119.7(3)
C9-C10-C11	115.05(18)	C44-C43-C42	121.5(3)
O27-C7-C8	125.2(2)	O33-C34-C35	108.3(3)