

S1.







**S4**.

Figure S1. Proton NMR of ATNA (S1–S4).







Figure S2. Carbon NMR of ATNA (S5 and S6).



Figure S3. A unit cell diagram of ATNA showing Intramolecular hydrogen bonding using dashed lines.



**Figure S4.** A packing diagram where planes are parallel to each other and showing the possibility of  $\pi$ - $\pi$  interactions.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C1	C2	1.400(3)	C18	C19	1.392(3)
C1	C11	1.441(3)	C18	S2	1.787(2)
C1	C6	1.450(3)	C19	C20	1.384(3)
C2	01	1.342(3)	C19	N2	1.416(3)
C2	C3	1.397(4)	C20	C21	1.378(4)
C3	C4	1.351(4)	C21	C22	1.373(4)
C4	C5	1.409(4)	C22	C23	1.365(3)
C5	C6	1.409(4)	C24	N2	1.282(3)
C5	C10	1.425(4)	C24	C25	1.433(3)
C6	C7	1.402(3)	C25	C26	1.398(3)
C7	C8	1.366(4)	C25	C30	1.446(3)
C8	C9	1.393(4)	C26	O2	1.344(3)
C9	C10	1.346(4)	C26	C27	1.411(4)
C11	N1	1.286(3)	C27	C28	1.341(4)
C12	C13	1.397(3)	C28	C29	1.414(4)
C12	C17	1.402(3)	C29	C34	1.409(4)
C12	N1	1.407(3)	C29	C30	1.419(3)
C13	C14	1.385(3)	C30	C31	1.405(3)
C13	S1	1.780(3)	C31	C32	1.377(3)
C14	C15	1.386(4)	C32	C33	1.380(4)
C15	C16	1.377(4)	C33	C34	1.355(4)
C16	C17	1.362(4)	<b>S</b> 1	S2	2.0234(10)
<mark>C18</mark>	<mark>C23</mark>	1.384(3)			

Table S1. Bond Lengths for ATNA.

Atom	Ato m	Ato m	Angle/°	Ato m	Ato m	Ato m	Angle/°
C2	C1	C11	120.0(2)	C19	C18	S2	115.80(18)
C2	C1	C6	118.5(2)	C20	C19	C18	118.5(2)
C1 1	C1	C6	121.4(2)	C20	C19	N2	125.1(2)
01	C2	C3	116.5(2)	C18	C19	N2	116.4(2)
01	C2	C1	122.5(2)	C21	C20	C19	120.8(2)
C3	C2	C1	121.0(3)	C22	C21	C20	119.7(2)
C4	C3	C2	120.3(3)	C23	C22	C21	120.8(3)
C3	C4	C5	121.9(3)	C22	C23	C18	119.7(2)
C6	C5	C4	119.3(3)	N2	C24	C25	122.8(2)
C6	C5	C10	119.5(3)	C26	C25	C24	120.2(2)
C4	C5	C10	121.3(3)	C26	C25	C30	118.4(2)
C7	C6	C5	117.6(2)	C24	C25	C30	121.4(2)
C7	C6	C1	123.4(2)	O2	C26	C25	122.0(2)
C5	C6	C1	119.0(2)	O2	C26	C27	117.2(2)
C8	C7	C6	121.9(3)	C25	C26	C27	120.8(2)
C7	C8	C9	120.1(3)	C28	C27	C26	120.5(3)
C1 0	С9	C8	120.3(3)	C27	C28	C29	122.2(3)
C9	C10	C5	120.7(3)	C34	C29	C28	122.0(3)
N1	C11	C1	122.3(2)	C34	C29	C30	119.3(3)
C1 3	C12	C17	118.5(2)	C28	C29	C30	118.6(2)
C1 3	C12	N1	116.8(2)	C31	C30	C29	117.2(2)
C1 7	C12	N1	124.6(2)	C31	C30	C25	123.3(2)
C1	C13	C12	120.1(3)	C29	C30	C25	119.5(2)
C1	C13	<b>S</b> 1	124.5(2)	C32	C31	C30	121.3(3)
C1 2	C13	<b>S</b> 1	115.39(19 )	C31	C32	C33	121.2(3)
C1 3	C14	C15	120.2(3)	C34	C33	C32	119.1(3)
C1 6	C15	C14	119.6(3)	C33	C34	C29	121.9(3)
C1 7	C16	C15	120.9(3)	C11	N1	C12	122.0(2)
C1	C17	C12	120.6(3)	C24	N2	C19	122.80(19)
C2 3	C18	C19	120.4(2)	C13	<b>S</b> 1	S2	105.28(9)
C2 3	C18	S2	123.76(19)	C18	S2	<b>S</b> 1	104.91(9)