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**Supporting information for article:**

# Synthesis and properties of a novel decacyclic *S*,*N*-heteroacene

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| Supporting Figures | |
|---|---|
| Figure S1-S10 | $^{1}$H NMR, $^{13}$C NMR and MALDI-TOF mass spectrometry |
| Figure S11 | The disordered hydrocarbon chains |
| Supporting Tables | |
| Table S1 | Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters |
| Table S2 | Atomic displacement parameters |
| Table S3 | Atomic occupancy |

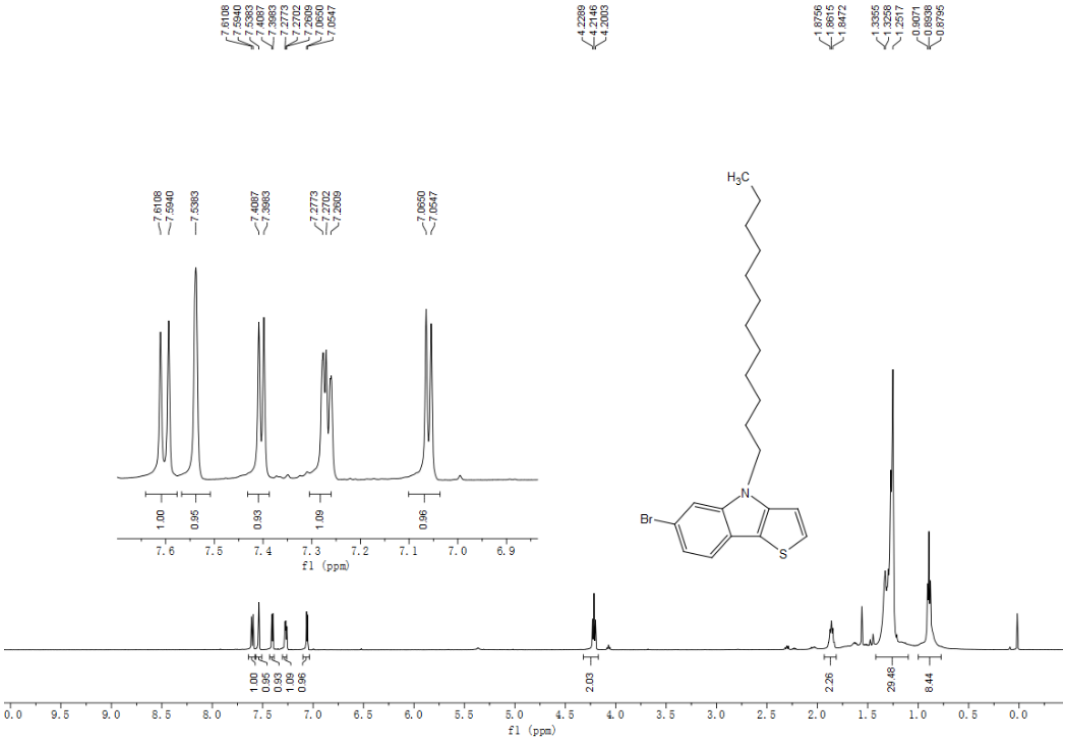


**Figure S1** $^{1}$H NMR of compound **1**.

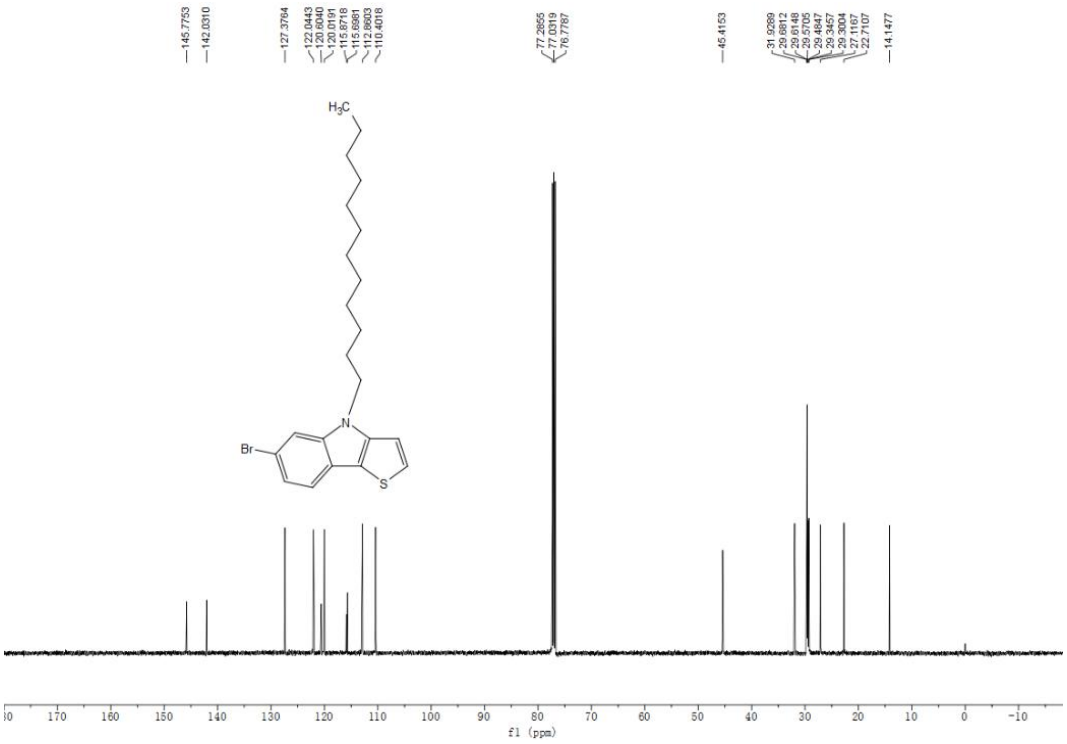


**Figure S2** $^{13}$C NMR of compound **1**.

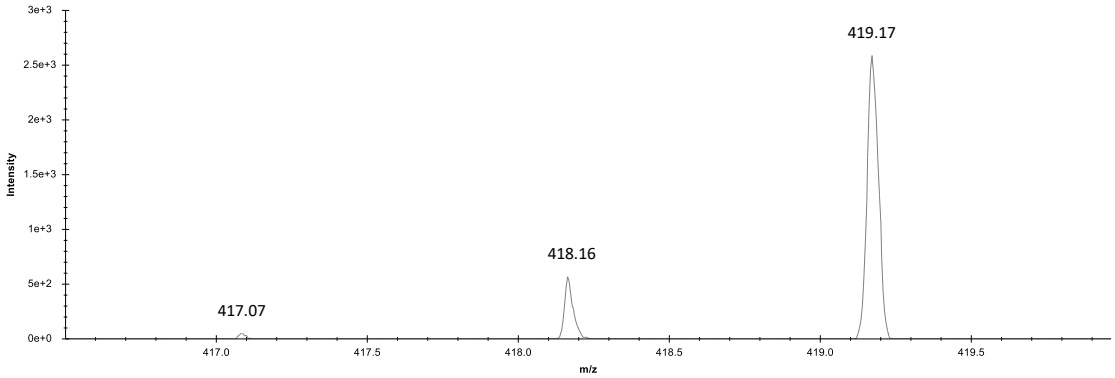


**Figure S3** MALDI-TOF mass spectrometry of compound **1**.

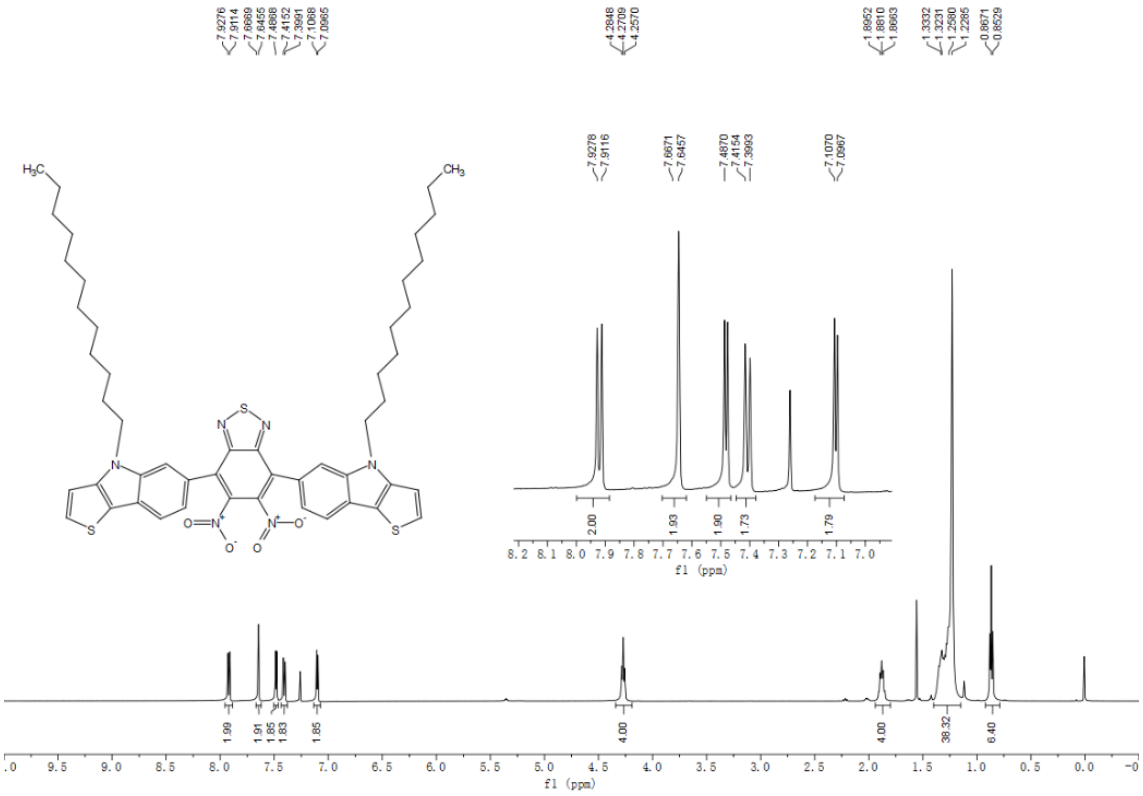

**Figure S4** $^{1}$H NMR of compound **3**.

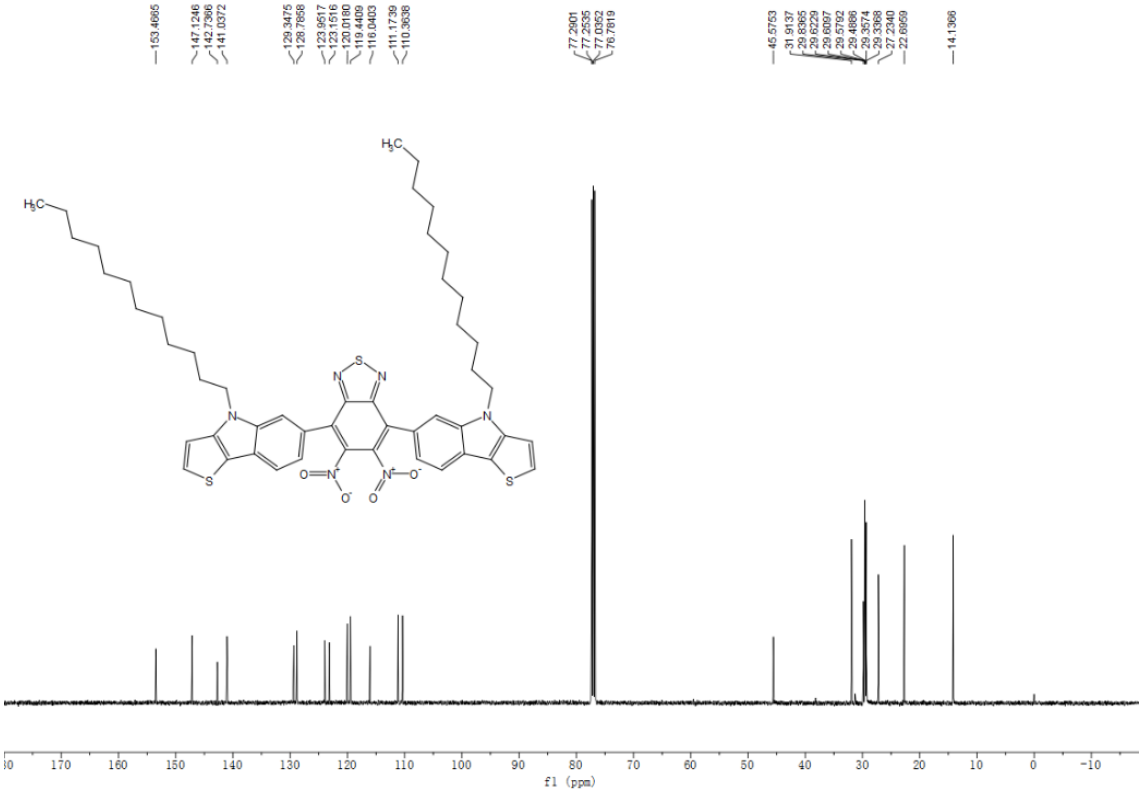

**Figure S5** $^{13}$C NMR of compound **3**.

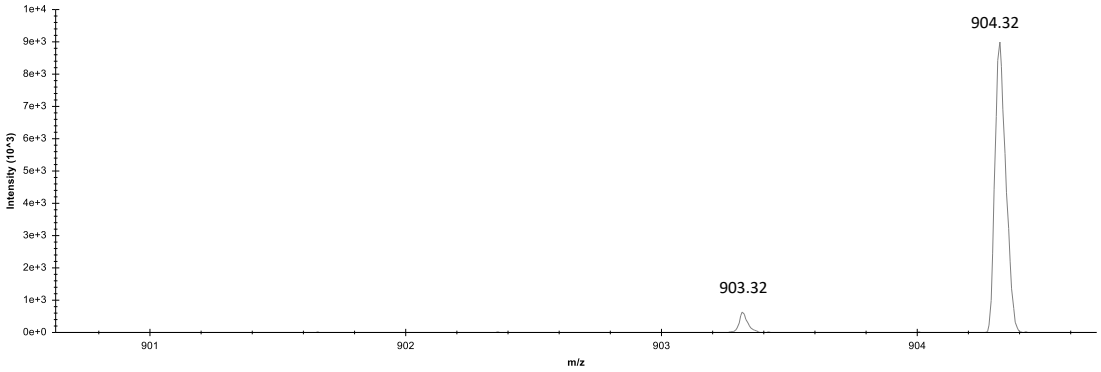


**Figure S6** MALDI-TOF mass spectrometry of compound **3**.

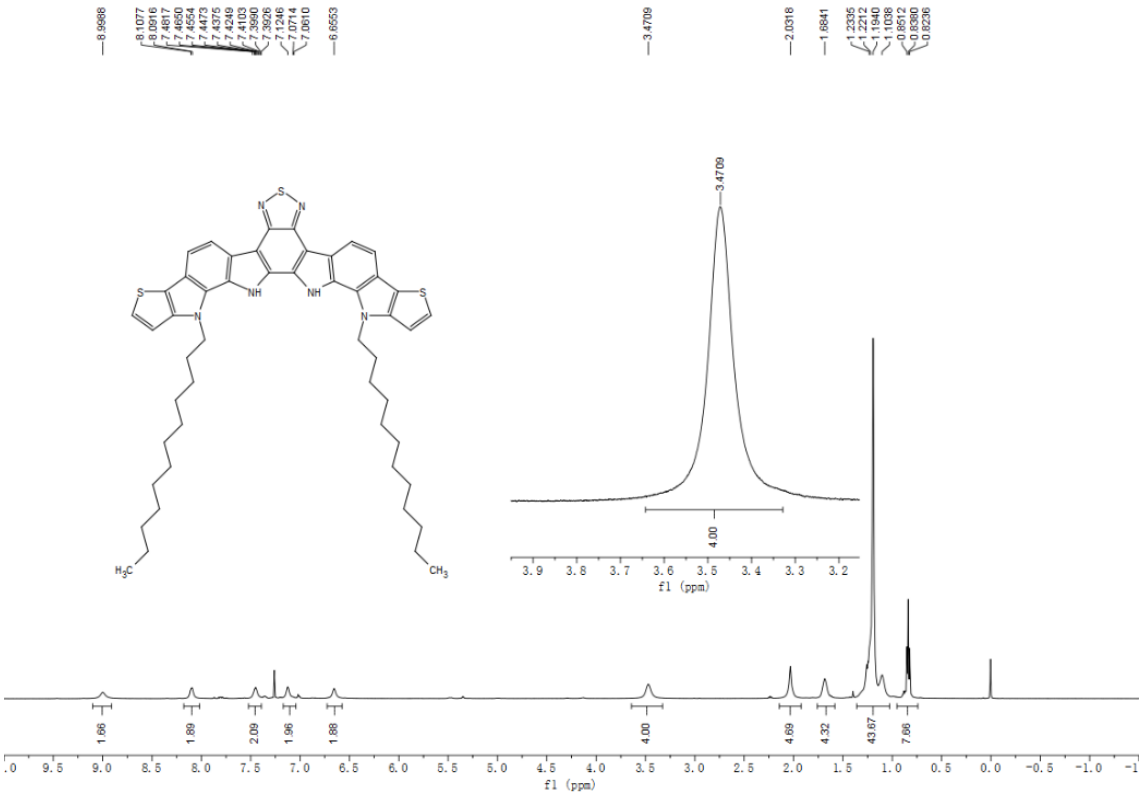


**Figure S7** $^{1}$H NMR of compound **4**.

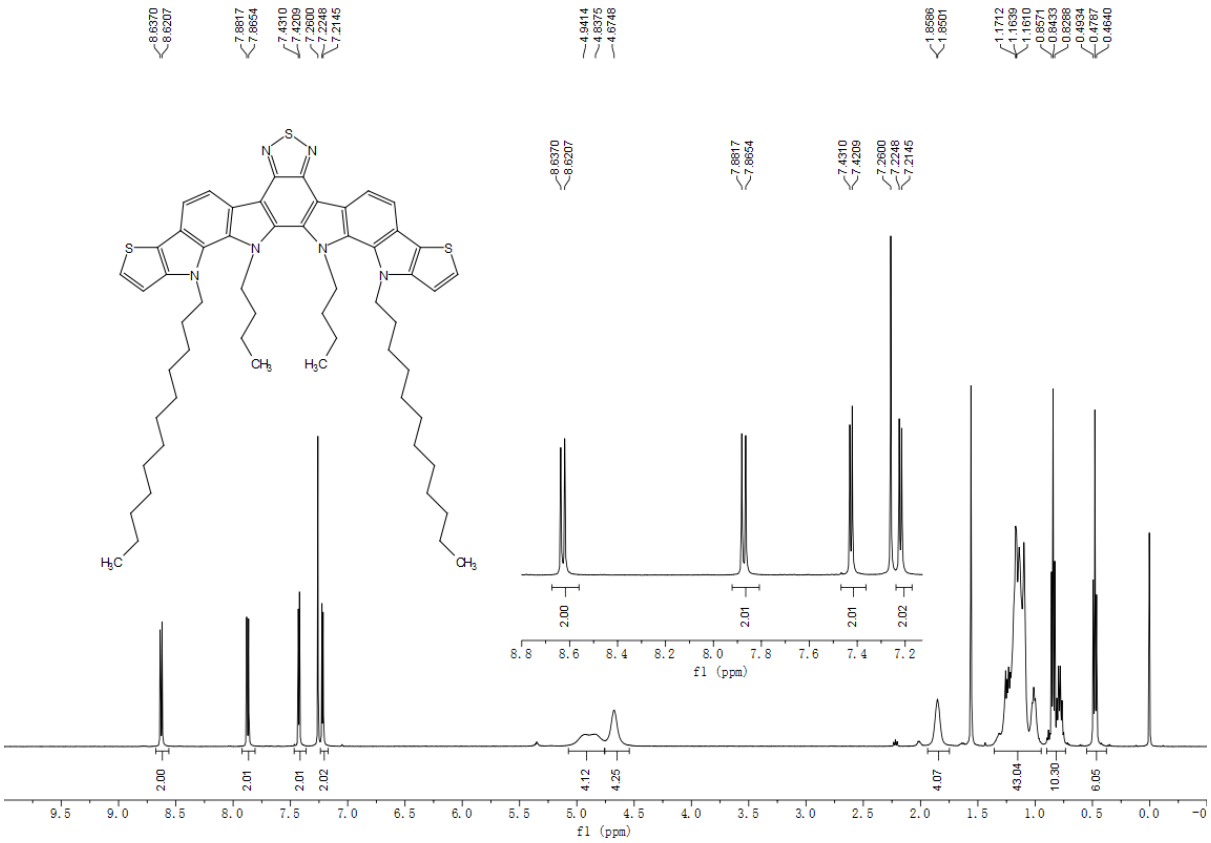

**Figure S8** $^{1}$H NMR of **TIP**.

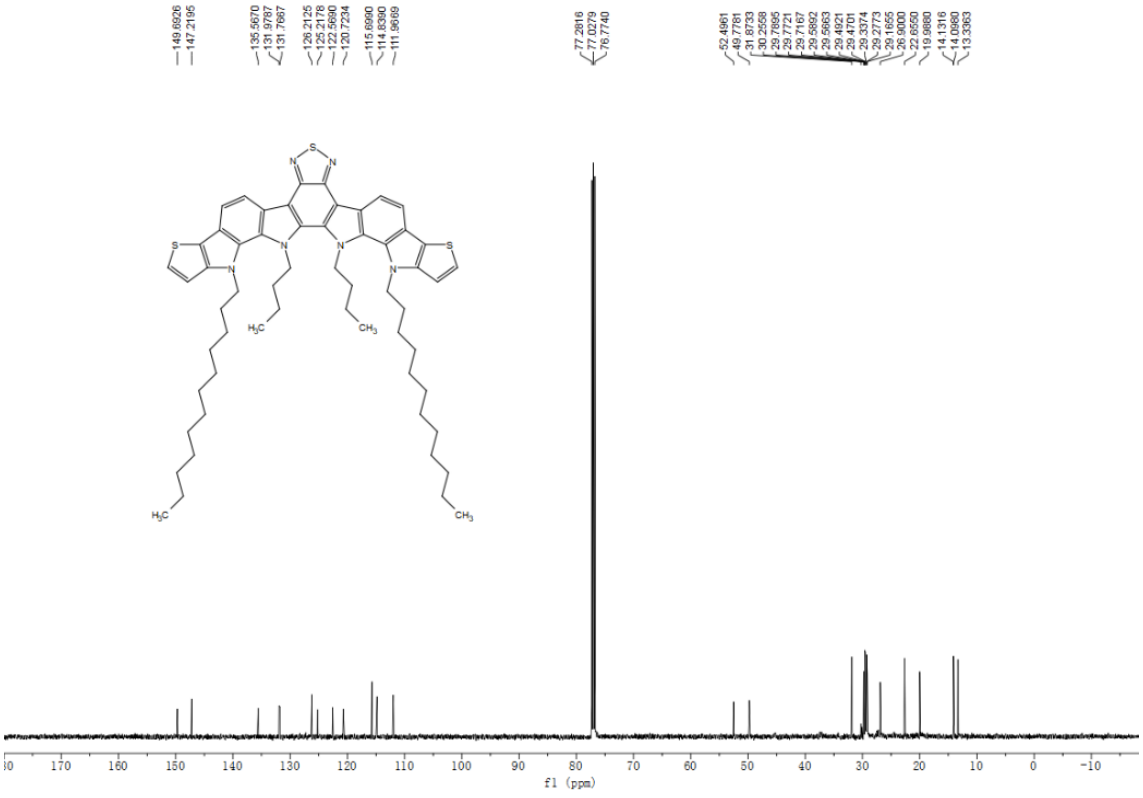

**Figure S9** $^{13}$C NMR of **TIP**.

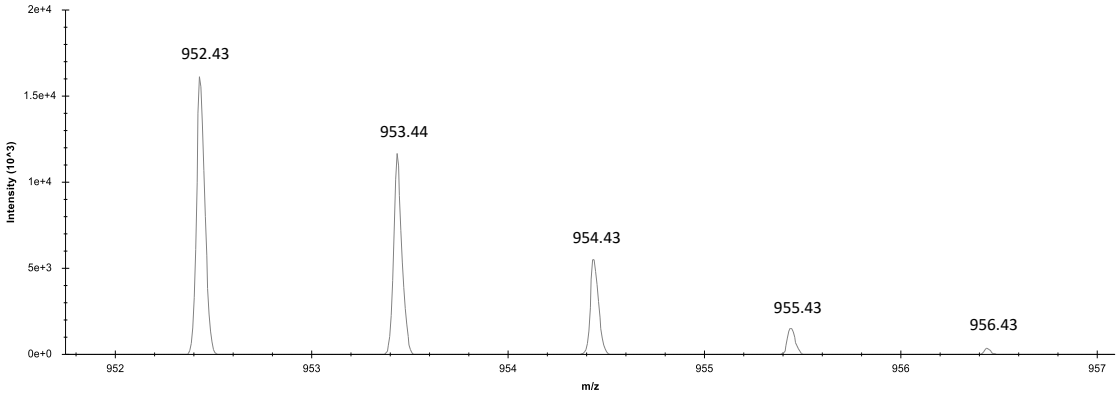


**Figure S10** MALDI-TOF mass spectrometry of **TIP**.

**Table S1** Fractional atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for **TIP**. U(eq) is defined as 1/3 of the trace of the orthogonalised $U^{ij}$ tensor.

| Atom | x | y | z | U(eq) |
|---|---|---|---|---|
| S1 | 212.4(2) | -5584.0(2) | 2834.3(5) | 35.72(11) |
| S2 | -2527.1(2) | -2886.1(2) | -1281.9(4) | 31.41(11) |
| S3 | -5495.9(2) | -2928.4(2) | 5462.3(5) | 29.91(10) |
| N1 | -1040.0(5) | -5289.3(6) | 4767.5(15) | 25.6(3) |
| N2 | -2034.1(5) | -4357.7(6) | 4077.9(14) | 22.5(3) |
| N3 | -2103.4(5) | -3318.7(7) | -471.3(15) | 28.3(3) |
| N4 | -2971.7(5) | -2882.3(6) | -69.0(15) | 27.9(3) |
| N5 | -3175.9(5) | -3882.1(6) | 4509.1(14) | 21.1(3) |
| N6 | -4206.9(5) | -3646.9(6) | 6327.0(14) | 24.2(3) |
| C1 | 198.6(7) | -6026.8(9) | 4410(2) | 37.8(4) |
| C2 | -233.2(7) | -5963.5(9) | 5182(2) | 34.5(4) |
| C3 | -565.3(6) | -5537.7(8) | 4471.9(19) | 28.2(3) |

| | | | | |
|---|---|---|---|---|
| C4 | -384.3(6) | -5297.0(8) | 3202.0(19) | 29.3(3) |
| C5 | -753.2(6) | -4880.6(8) | 2615.9(18) | 27.2(3) |
| C6 | -768.5(6) | -4533.9(9) | 1322.1(19) | 31.3(4) |
| C7 | -1188.5(6) | -4187.8(8) | 985.5(18) | 29.3(3) |
| C8 | -1591.2(6) | -4166.1(8) | 1985.7(17) | 24.6(3) |
| C9 | -2067.7(6) | -3852.4(7) | 1903.9(16) | 23.3(3) |
| C10 | -2329.8(5) | -3981.1(7) | 3172.2(16) | 21.7(3) |
| C11 | -1580.2(6) | -4486.7(7) | 3326.1(16) | 22.9(3) |
| C12 | -1161.2(6) | -4879.3(7) | 3632.3(17) | 24.2(3) |
| C13 | -2298.9(6) | -3477.4(7) | 807.2(16) | 23.2(3) |
| C14 | -2798.9(6) | -3227.7(7) | 1037.2(16) | 23.1(3) |
| C15 | -3065.8(6) | -3385.0(7) | 2325.3(16) | 22.2(3) |
| C16 | -2835.3(5) | -3760.7(7) | 3369.1(16) | 21.4(3) |
| C17 | -3620.7(5) | -3543.7(7) | 4151.0(16) | 21.2(3) |
| C18 | -3574.3(6) | -3257.4(7) | 2793.9(16) | 21.9(3) |
| C19 | -3985.8(6) | -2961.6(7) | 2101.0(17) | 24.7(3) |
| C20 | -4445.4(6) | -2949.3(7) | 2793.8(17) | 25.3(3) |
| C21 | -4485.8(6) | -3184.5(7) | 4211.6(17) | 23.2(3) |
| C22 | -4071.9(6) | -3473.3(7) | 4929.6(16) | 22.0(3) |
| C23 | -4886.7(6) | -3197.5(7) | 5247.1(17) | 24.8(3) |
| C24 | -4708.1(6) | -3464.9(7) | 6507.5(17) | 24.8(3) |

| | | | | |
|---|---|---|---|---|
| C25 | -5060.1(6) | -3454.5(8) | 7666.3(19) | 29.6(3) |
| C26 | -5500.1(6) | -3178.6(8) | 7238.9(19) | 31.4(4) |
| C27 | -1363.8(6) | -5560.7(8) | 5879.8(18) | 28.7(3) |
| C28 | -1770.7(6) | -6001.1(8) | 5282.8(19) | 31.7(4) |
| C29 | -1554.8(7) | -6628.7(9) | 4773(2) | 36.4(4) |
| C30 | -1920.0(8) | -7039.9(9) | 3913(2) | 38.9(4) |
| C31 | -2359.8(7) | -7325.8(9) | 4754(2) | 34.7(4) |
| C32 | -2704.6(7) | -7715.4(9) | 3783(2) | 37.3(4) |
| C33 | -3163.8(7) | -8011.9(9) | 4507(2) | 36.0(4) |
| C34 | -3502.7(7) | -8354.3(9) | 3431(2) | 38.8(4) |
| C35 | -3961.6(7) | -8682.3(8) | 4073(2) | 35.0(4) |
| C36 | -4302.4(7) | -8981.0(9) | 2939(2) | 38.1(4) |
| C37 | -4768.5(8) | -9309.4(10) | 3540(2) | 42.9(4) |
| C38 | -5070.8(8) | -9665.5(11) | 2408(3) | 53.4(6) |
| C39 | -2068.1(6) | -4272.5(8) | 5659.1(17) | 25.1(3) |
| C40 | -1631.9(6) | -3893.8(8) | 6294.8(17) | 27.9(3) |
| C41 | -1617.3(7) | -3217.9(9) | 5738(2) | 37.0(4) |
| C42 | -1269.0(8) | -2791.4(10) | 6615(2) | 45.7(5) |
| C47 | -3857.9(6) | -3726.8(7) | 7551.3(17) | 24.7(3) |

| | | | | |
|---|---|---|---|---|
| C48 | -3983.6(6) | -4316.1(8) | 8419.9(18) | 28.0(3) |
| C49 | -3587.6(6) | -4499.5(8) | 9537.4(18) | 28.3(3) |
| C50 | -3091.4(6) | -4735.0(8) | 8890.0(18) | 30.6(3) |
| C51 | -2757.3(6) | -5083.3(8) | 9965.1(18) | 29.4(3) |
| C52 | -2266.1(7) | -5323.7(9) | 9315.1(19) | 34.5(4) |
| C53 | -1960.2(7) | -5733.0(9) | 10348.1(19) | 32.8(4) |
| C54 | -1475.0(7) | -5990.5(9) | 9690(2) | 35.4(4) |
| C55 | -1172.4(7) | -6404.5(9) | 10719(2) | 35.4(4) |
| C56 | -672.4(7) | -6634.9(10) | 10110(2) | 43.1(4) |
| C57 | -384.6(8) | -7066.8(10) | 11124(3) | 49.7(5) |
| C58 | 126.5(9) | -7262.7(13) | 10537(4) | 68.4(8) |
| C44B | -3508.7(14) | -4905.7(16) | 3552(4) | 34.3(8) |
| C45B | -3679.2(14) | -5570.6(16) | 3899(4) | 36.8(6) |
| C46A | -3290(3) | -6186(3) | 3230(11) | 60.3(10) |
| C46B | -3255.6(14) | -6022.0(16) | 4286(5) | 60.3(10) |
| C44A | -3275(3) | -5011(3) | 3809(6) | 34.1(13) |

| | | | | |
|---|---|---|---|---|
| C45A | -3372.6(17) | -5689(2) | 4387(5) | 36.8(6) |
| C43 | -3263.2(6) | -4554.5(7) | 4892.8(18) | 26.7(3) |

**Table S2** Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **TIP**.

| Atom | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|---|---|---|---|---|---|---|
| S1 | 21.74(19) | 37.7(2) | 47.7(3) | -5.49(19) | 3.93(17) | 6.09(16) |
| S2 | 34.6(2) | 34.4(2) | 25.2(2) | 7.87(16) | 3.98(15) | 5.67(17) |
| S3 | 19.69(18) | 34.7(2) | 35.4(2) | -2.88(16) | 0.16(15) | 5.08(15) |
| N1 | 19.4(6) | 28.6(7) | 28.9(7) | 0.9(5) | -1.5(5) | 3.8(5) |
| N2 | 18.6(6) | 26.5(7) | 22.5(6) | 0.9(5) | 0.7(5) | 1.7(5) |
| N3 | 30.5(7) | 29.5(7) | 24.9(7) | 4.0(5) | 3.4(5) | 1.9(6) |
| N4 | 29.7(7) | 28.1(7) | 26.1(7) | 3.7(5) | -0.1(5) | 2.2(5) |
| N5 | 17.3(6) | 22.4(6) | 23.7(6) | 1.5(5) | 0.9(5) | 0.8(5) |
| N6 | 19.6(6) | 28.5(7) | 24.5(6) | 0.7(5) | 1.1(5) | 2.4(5) |
| C1 | 25.9(8) | 34.3(9) | 53.3(11) | -2.7(8) | -4.0(8) | 7.4(7) |
| C2 | 27.2(8) | 32.4(9) | 43.8(10) | 0.0(7) | -4.7(7) | 4.8(7) |
| C3 | 19.8(7) | 29.0(8) | 35.8(9) | -4.0(7) | -2.9(6) | 2.9(6) |
| C4 | 21.3(7) | 31.4(9) | 35.2(9) | -4.6(7) | 1.2(6) | 1.6(6) |
| C5 | 21.3(7) | 30.2(8) | 30.3(8) | -3.8(6) | 1.9(6) | 2.3(6) |
| C6 | 24.0(8) | 37.5(9) | 32.4(8) | -1.0(7) | 7.9(6) | 1.4(7) |
| C7 | 26.7(8) | 34.5(9) | 26.7(8) | 2.0(7) | 4.6(6) | 0.9(7) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C8 | 22.1(7) | 27.2(8) | 24.7(7) | -0.5(6) | 0.8(6) | 0.2(6) |
| C9 | 21.6(7) | 24.6(7) | 23.9(7) | -0.6(6) | 0.6(6) | -1.2(6) |
| C10 | 19.8(7) | 21.9(7) | 23.3(7) | -0.2(6) | -1.3(5) | -0.5(6) |
| C11 | 18.6(7) | 25.8(8) | 24.4(7) | -2.2(6) | 1.7(6) | -0.2(6) |
| C12 | 20.5(7) | 26.7(8) | 25.3(7) | -1.8(6) | -0.9(6) | 0.8(6) |
| C13 | 23.8(7) | 22.6(7) | 23.1(7) | -0.5(6) | 1.3(6) | -1.7(6) |
| C14 | 23.6(7) | 20.7(7) | 24.9(7) | 0.1(6) | -1.8(6) | -0.9(6) |
| C15 | 21.2(7) | 21.4(7) | 24.0(7) | -0.7(6) | -0.8(5) | -0.3(6) |
| C16 | 20.2(7) | 22.0(7) | 22.0(7) | -1.0(6) | -0.1(5) | -1.6(6) |
| C17 | 18.3(7) | 20.4(7) | 24.7(7) | -2.2(6) | -1.6(5) | 1.4(5) |
| C18 | 21.5(7) | 19.0(7) | 25.2(7) | -1.6(6) | -0.9(6) | -0.4(6) |
| C19 | 25.7(8) | 22.9(7) | 25.4(7) | 1.7(6) | -2.1(6) | 2.0(6) |
| C20 | 23.0(7) | 23.4(8) | 29.5(8) | 0.2(6) | -4.3(6) | 4.2(6) |
| C21 | 19.9(7) | 21.4(7) | 28.4(8) | -3.3(6) | -0.6(6) | 1.6(6) |
| C22 | 21.5(7) | 20.4(7) | 24.2(7) | -1.7(6) | 0.2(6) | 0.0(6) |
| C23 | 21.6(7) | 23.5(7) | 29.3(8) | -3.6(6) | -0.8(6) | 1.5(6) |
| C24 | 20.5(7) | 24.0(8) | 30.0(8) | -2.6(6) | 1.6(6) | 0.4(6) |
| C25 | 25.2(8) | 32.4(9) | 31.2(8) | -0.9(7) | 4.4(6) | -1.0(6) |
| C26 | 23.2(8) | 34.2(9) | 36.8(9) | -3.9(7) | 6.0(6) | -0.2(7) |
| C27 | 26.9(8) | 31.1(9) | 28.2(8) | 2.1(7) | 1.6(6) | 5.0(7) |
| C28 | 26.8(8) | 34.1(9) | 34.2(9) | 4.1(7) | 2.1(7) | 1.2(7) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C29 | 32.7(9) | 36.7(10) | 40.0(10) | -0.9(8) | 3.9(7) | -0.1(7) |
| C30 | 43.2(10) | 38.6(10) | 34.9(9) | -2.5(8) | 6.1(8) | -4.6(8) |
| C31 | 38.5(9) | 33.1(9) | 32.5(9) | 1.6(7) | 1.0(7) | 0.3(7) |
| C32 | 42.4(10) | 35.2(9) | 34.2(9) | -0.9(7) | 3.0(8) | -3.3(8) |
| C33 | 40.3(10) | 32.0(9) | 35.6(9) | 2.4(7) | 0.9(7) | -0.3(7) |
| C34 | 41.8(10) | 35.0(10) | 39.6(10) | 0.1(8) | 2.7(8) | -2.3(8) |
| C35 | 38.8(9) | 29.5(9) | 36.6(9) | 2.8(7) | 0.1(7) | 3.2(7) |
| C36 | 42.4(10) | 32.6(9) | 39.3(10) | 4.5(8) | -1.1(8) | 1.1(8) |
| C37 | 37.5(10) | 39.0(10) | 52.1(12) | 4.4(9) | -2.0(9) | 2.2(8) |
| C38 | 42.9(11) | 42.6(12) | 74.8(16) | 10.7(11) | -16.6(11) | 0.3(9) |
| C39 | 21.0(7) | 32.1(8) | 22.4(7) | 3.2(6) | 1.6(6) | 3.5(6) |
| C40 | 24.3(8) | 34.5(9) | 24.9(8) | -2.6(6) | -0.1(6) | 3.8(6) |
| C41 | 38.0(10) | 35.0(9) | 38.1(10) | -1.5(8) | 0.7(8) | 0.8(8) |
| C42 | 37.1(10) | 42.9(11) | 57.3(13) | -12.2(9) | 7.7(9) | -4.8(8) |
| C47 | 22.8(7) | 25.3(8) | 26.0(7) | -0.6(6) | -1.7(6) | 0.5(6) |
| C48 | 26.0(8) | 28.0(8) | 29.9(8) | 2.5(6) | -0.6(6) | -1.4(6) |
| C49 | 31.0(8) | 27.7(8) | 26.2(8) | 2.8(6) | -0.8(6) | -0.1(6) |
| C50 | 30.8(8) | 33.8(9) | 27.1(8) | 3.0(7) | -2.8(6) | 2.8(7) |
| C51 | 29.9(8) | 30.4(8) | 27.9(8) | 2.4(6) | -3.6(6) | 0.6(7) |
| C52 | 33.3(9) | 40.3(10) | 30.0(8) | 3.6(7) | -1.6(7) | 5.7(8) |
| C53 | 32.0(9) | 35.8(9) | 30.6(8) | 2.9(7) | -2.3(7) | 3.7(7) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C54 | 32.7(9) | 40.6(10) | 33.1(9) | 3.2(7) | -0.7(7) | 3.8(7) |
| C55 | 33.0(9) | 37.7(10) | 35.5(9) | 2.4(7) | -1.8(7) | 3.4(7) |
| C56 | 32.2(9) | 47.8(11) | 49.4(11) | -0.5(9) | -1.2(8) | 5.1(8) |
| C57 | 36.5(10) | 42.9(11) | 69.5(15) | -4.8(10) | -13.8(10) | 4.8(9) |
| C58 | 39.6(12) | 60.6(15) | 105(2) | -18.6(15) | -14.8(13) | 14.6(11) |
| C44B | 36.9(18) | 29.3(16) | 36.8(16) | -0.9(12) | -16.1(15) | 0.1(14) |
| C45B | 35.9(15) | 27.9(13) | 46.7(16) | -2.0(12) | -1.3(11) | -4.8(13) |
| C46A | 54.2(18) | 21.9(15) | 105(3) | -2.4(17) | -10(2) | 4.3(13) |
| C46B | 54.2(18) | 21.9(15) | 105(3) | -2.4(17) | -10(2) | 4.3(13) |
| C44A | 46(4) | 31(3) | 26(3) | -1(2) | 10(3) | -8(3) |
| C45A | 35.9(15) | 27.9(13) | 46.7(16) | -2.0(12) | -1.3(11) | -4.8(13) |
| C43 | 24.5(8) | 22.3(8) | 33.2(8) | 4.6(6) | 4.5(6) | 2.1(6) |

**Table S3** Atomic occupancy for **TIP**.

| Atom | Occupancy | Atom | Occupancy | Atom | Occupancy |
|---|---|---|---|---|---|
| C44B | 0.65 | H44A | 0.65 | H44B | 0.65 |
| C45B | 0.52 | H45A | 0.52 | H45B | 0.52 |
| C46A | 0.3 | H46A | 0.3 | H46B | 0.3 |
| H46C | 0.3 | C46B | 0.7 | H46D | 0.7 |
| H46E | 0.7 | H46F | 0.7 | C44A | 0.35 |
| H44C | 0.35 | H44D | 0.35 | C45A | 0.48 |
| H45C | 0.48 | H45D | 0.48 | | |

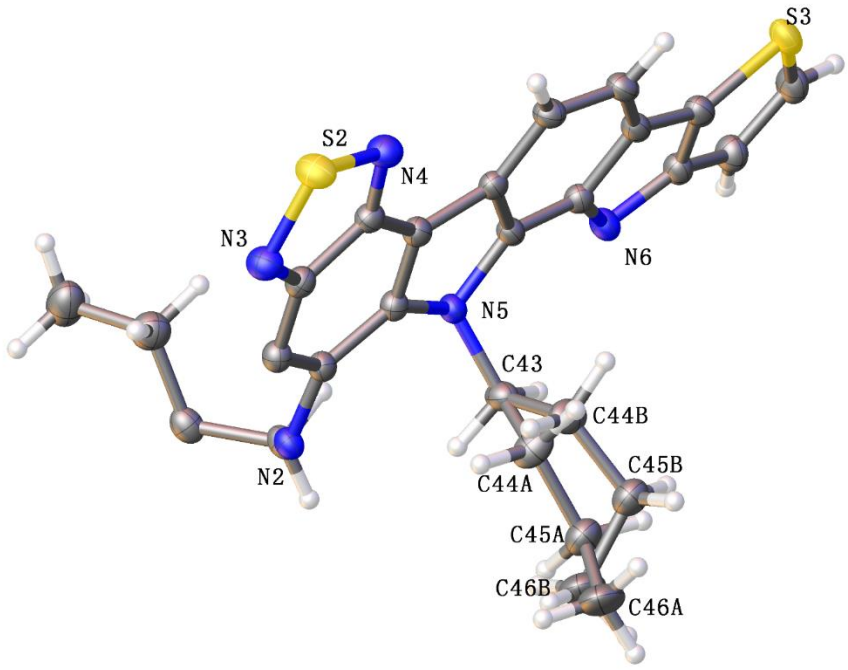


**Figure S11** The disordered hydrocarbon chains in **TIP**.