Electronic Supplementary Information (ESI)

A Photoswitchable Diarylethene Heterodimer for Use as a Multifunctional Logic Gate

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Supporting Information

Table of Contents:

1. BTF-BTH functions as OR gate

Table S1. Truth Tables for OR gate

inputs		output
a (312nm)	*b* (378nm)	OR gate (*A* 542nm)
0	0	0
1	0	1
0	1	1
1	1	1

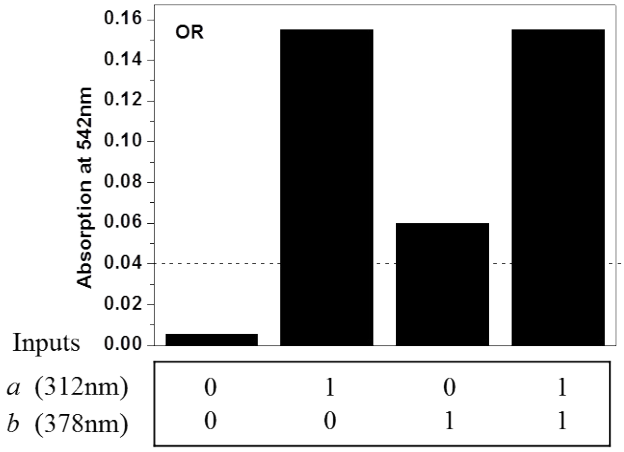


Figure S1. Performance of **BTF-BTH** as the OR gate. The input combinations (0 =off, 1 = on) for the gate are shown at the bottom of the figure. The each bar shows the output in response to Input. The threshold (dashed line) was set arbitrary to demonstrate the gate.

2. BTF-BTH functions as INHIBIT, and AND gate

Table S2. Truth Tables for INH and AND gate

inputs		outputs	
a (312nm)	*b* (Cu^{2+})	INH gate (*A* 542nm)	AND gate (Em 492nm)
0	0	0	0
1	0	1	0
0	1	0	0
1	1	0	1

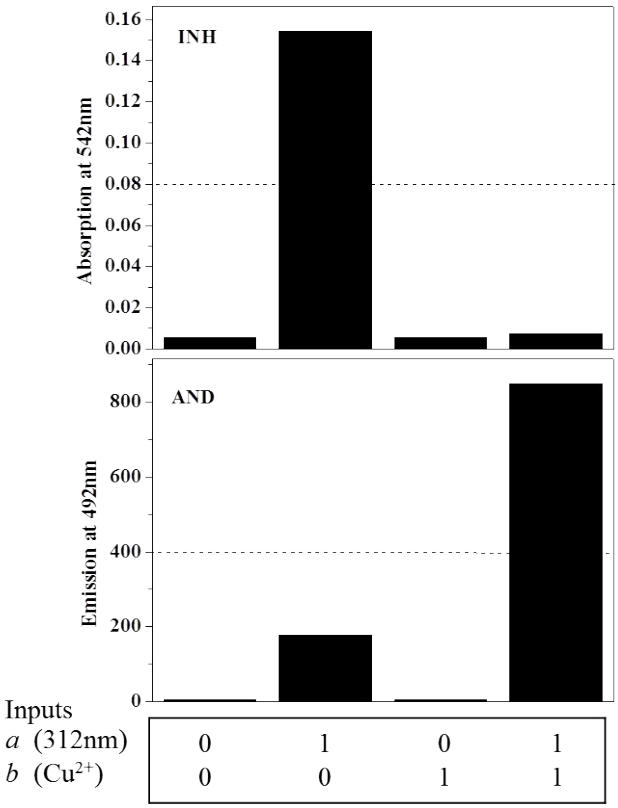


Figure S2. Performance of **BTF-BTH** as INH and AND gates. The input combinations (0 =off, 1 = on) for all gates are shown at the bottom of the figure. The each bar shows the output in response to Input. The threshold (dashed line) was assigned arbitrary to demonstrate the gate.

3. Detailed information on inputs

The conditions for applying inputs and measuring outputs for the various functions shown in the paper are given below.

Figure S1.

Initial state: **BTFo-BTHo**

Inputs:

Input *a*: 312 nm for 115s

Input *b*: 378nm for 1h

Output: Absorbance at 542 nm

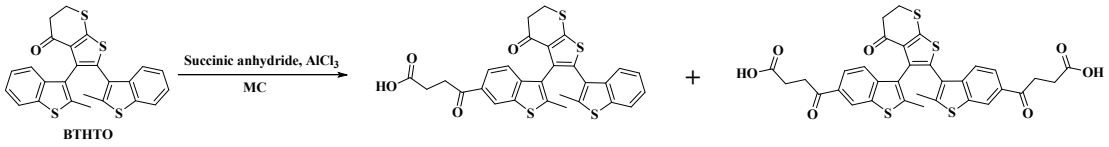
Reset: Visible light for 600s

Figure 5.
Initial state: **BTFo-BTHo**
Inputs:
First input: 312 nm for 115 s
Second input: 540nm for 2 h
Output: Emission at 492 nm after 400 nm excitation
Reset: Visible light for 600s

Figure S2.
Initial state: **BTFo-BTHo**
Inputs:
Input *a*: 312 nm for 115s
Input *b*: Cu^{2+} 1eq
Outputs:
INH2 gate: Absorbance at 542 nm
AND gate: Emission at 492 nm after excitation at 400 nm
Reset: Visible light for 600s

Figure 6.
Initial state: **BTFo-BTHo**
Inputs:
In: 312 nm for 115s
Ad: Cu^{2+} 1eq
Output: Emission at 605 and 492 nm after excitation at 400 nm
Reset: Visible light for 600s

4. Synthesis

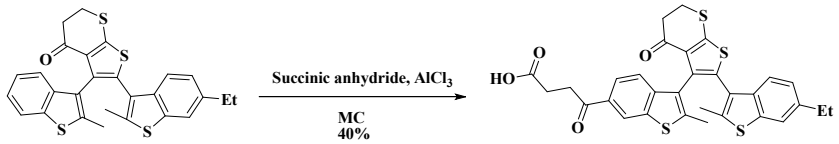


4,4'-(3,3'-(4-oxo-5,6-dihydro-4H-thieno[2,3-b]thiopyran-2,3-diyl)bis(2-methyl-benzo[b]thiophene-6,3-diyl))bis(4-oxobutanoic acid) (5)

$AlCl_3$ (0.18 g, 1.32 mmol) was added to a solution of **BTHTO** (0.10 g, 0.22 mmol) in CH_2Cl_2 (15 mL) at room temperature. After stirring for 5 min at room temperature, succinic anhydride (0.13 g, 1.32 mmol) was added to the reaction mixture. The solution was stirred for 4 h at room temperature, and then 1 M HCl (5 mL) was added to quench the reaction. The reaction mixture was extracted with CH_2Cl_2. The organic layer was washed with water followed by brine solution and dried over $MgSO_4$. The

organic layer was filtered and concentrated to give the crude product, which was purified by column chromatography (EA) to give **2** (0.03 g, 20%) as a reddish powder;

^{1}H NMR(CDCl3, 300MHz) δ (ppm): 8.32 (s, 1 H), 8.22 (s, 1H), 7.93 (d, J = 9Hz, 0.66H), 7.86 (d, J = 9 Hz, 0.66H), 7.70 (t, J = 15 Hz, 1.54H), 7.52 (d, J = 9 Hz, 0.71H), 7.37-7.26 (m, 0.43H), 3.48-3.21 (m, 6H), 2.83-2.76 (m, 6H), 2.48 (s,1.5H), 2.24 (s,1.5H), 1.90 (d, J = 6 Hz, 3H); HRMS (FAB+): *m/z* calcd for $C_{33}H_{26}O_7S_4$ $[M+H]^+$: 663.8361; found: 663.8382.

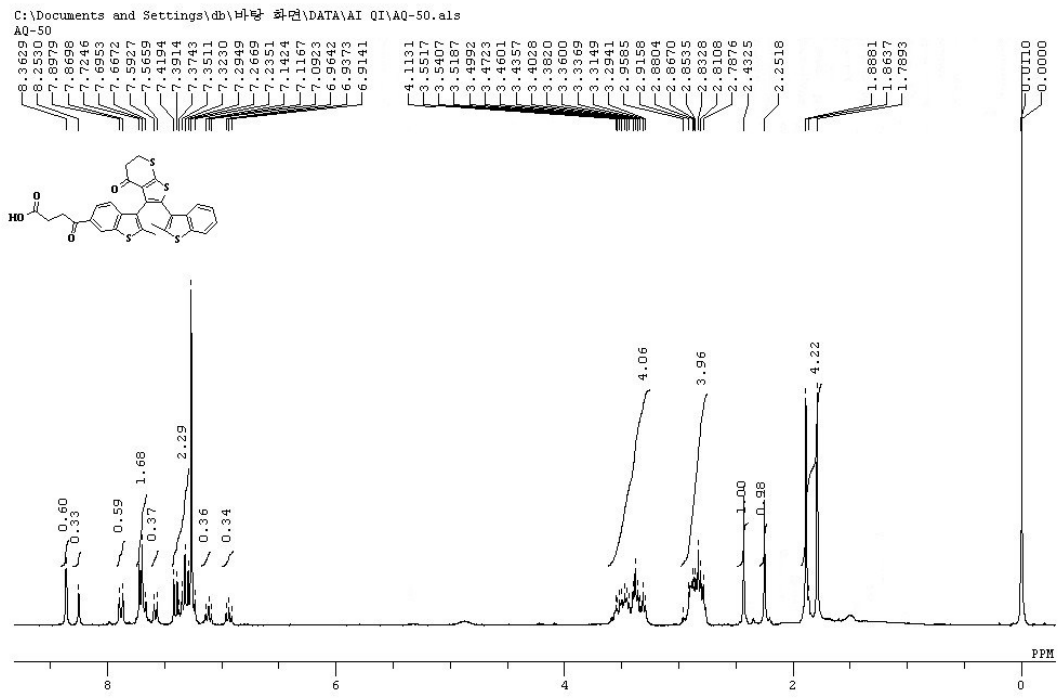


6 **7**

4-(3-(2-(6-ethyl-2-methylbenzo[b]thiophen-3-yl)-4-oxo-5,6-dihydro-4H-thieno[2,3-b]thiopyran-3-yl)-2-methylbenzo[b]thiophen-6-yl)-4-oxobutanoic acid (7)

$AlCl_3$ (0.11 g, 0.80 mmol) was added to a solution of **6**[1] (0.10 g, 0.20 mmol) in CH_2Cl_2 (15 mL) at room temperature. After stirring for 5 min at room temperature, succinic anhydride (0.08 g, 0.80 mmol) was added to the reaction mixture. The solution was stirred for 4 h at room temperature, and then 1 M HCl (5 mL) was added to quench the reaction. The reaction mixture was extracted with CH_2Cl_2. The organic layer was washed with water followed by brine solution and dried over $MgSO_4$. The organic layer was filtered and concentrated to give the crude product, which was purified by column chromatography (Hex/EA=4:1) to give **5** (0.047 g, 40%) as a reddish powder;

^{1}H NMR ($CDCl_3$, 300MHz) δ (ppm): 8.35 and 8.25 (s×2, 1H), 7.86 (d, J = 9 Hz, 0.58 H), 7.64-7.51 (m, 1.59H) , 7.39 (d, J = 9Hz, 0.67H), 7.26-7.18(m, 2.16H), 3.55-3.29 (m, 4H), 2.91-2.78 (m, 6H), 2.45 (s, 1H), 2.38 (s, 1H), 1.90 and 1.77 (s×2, 4H), 1.28-1.18 (m, 3H); HRMS (FAB+): *m/z* calcd for $C_{31}H_{26}O_4S_4$ $[M+H]^+$: 591.8159; found: 591.8171.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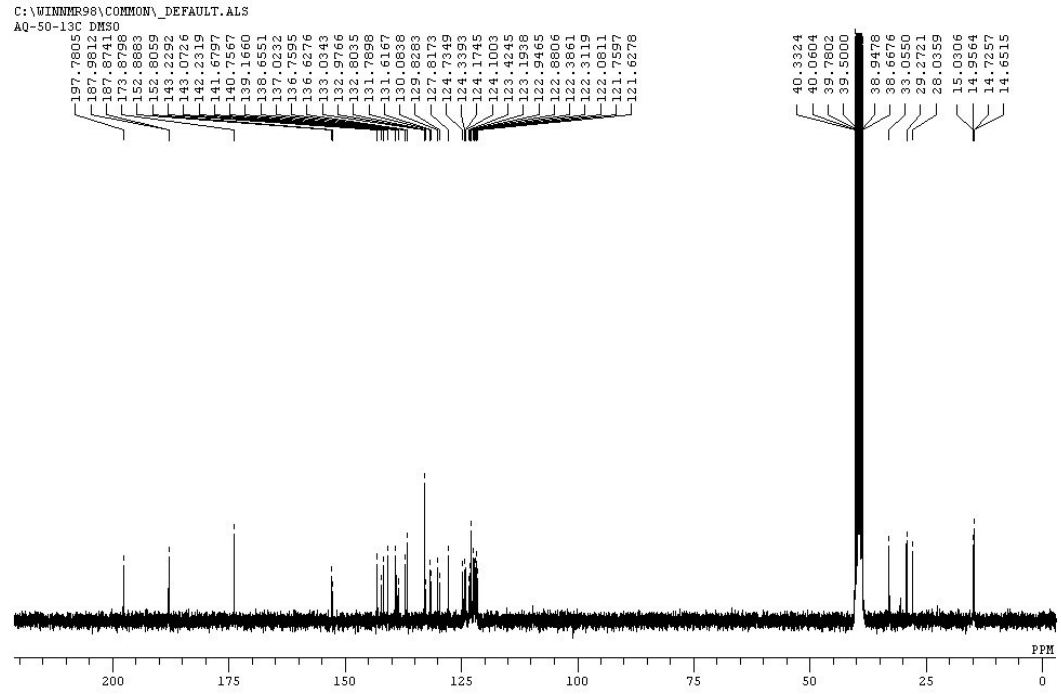
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Note : -
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Spectrum Type : Normal Ion (MT-Linear)
RT : 3.30 min Scans : 100
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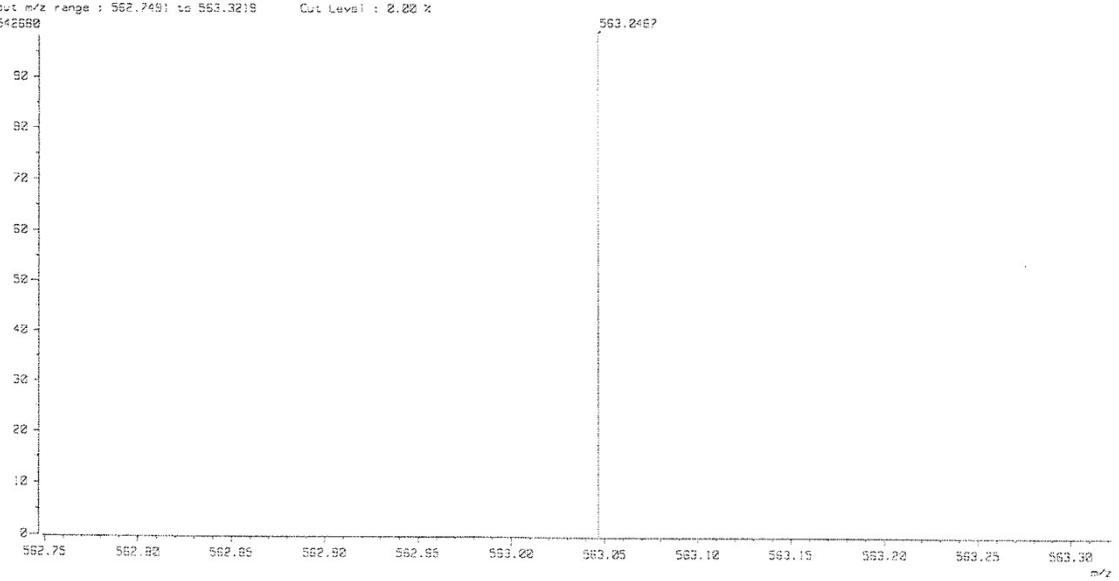

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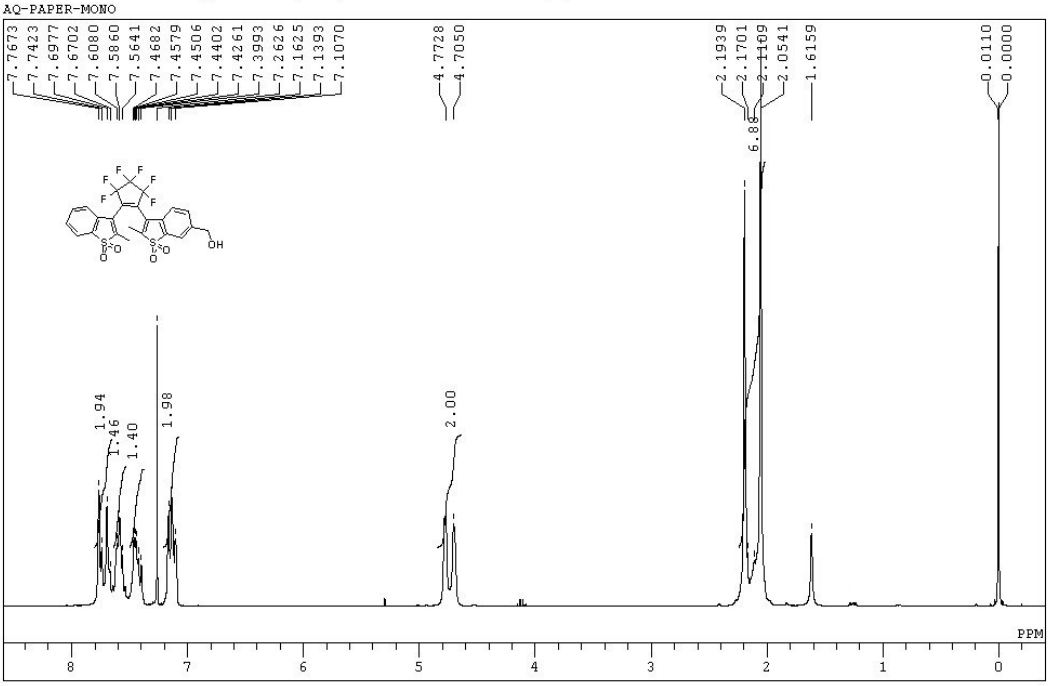

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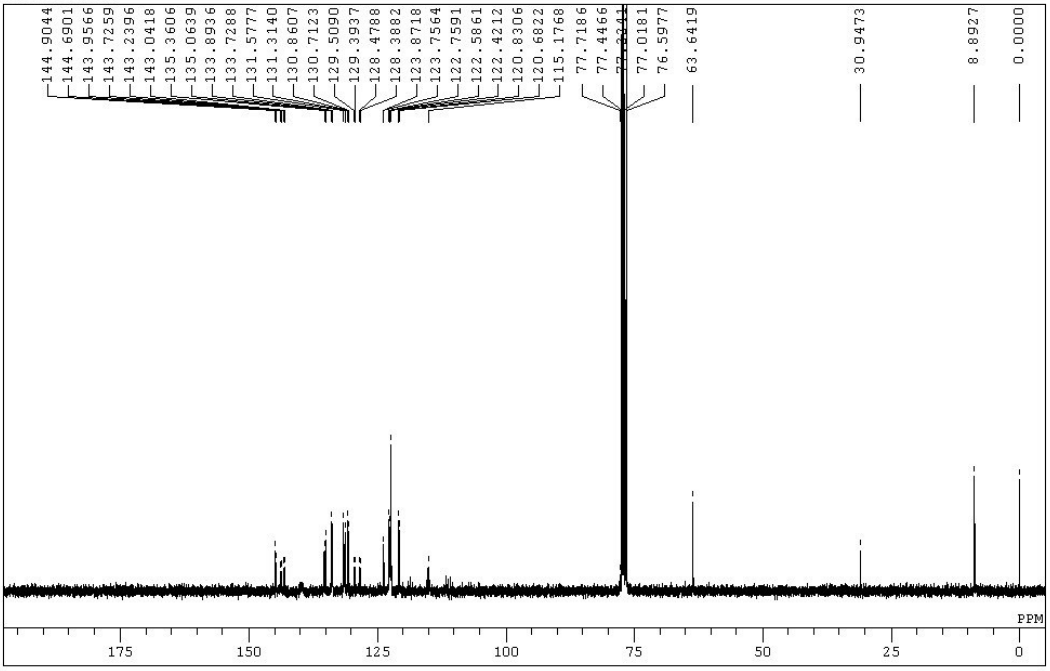

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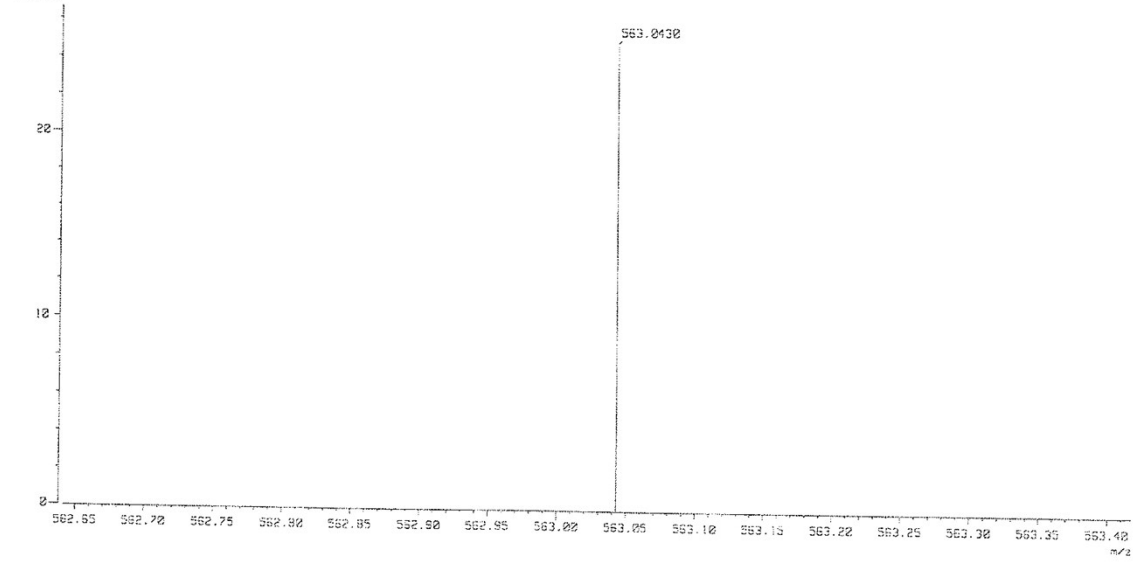

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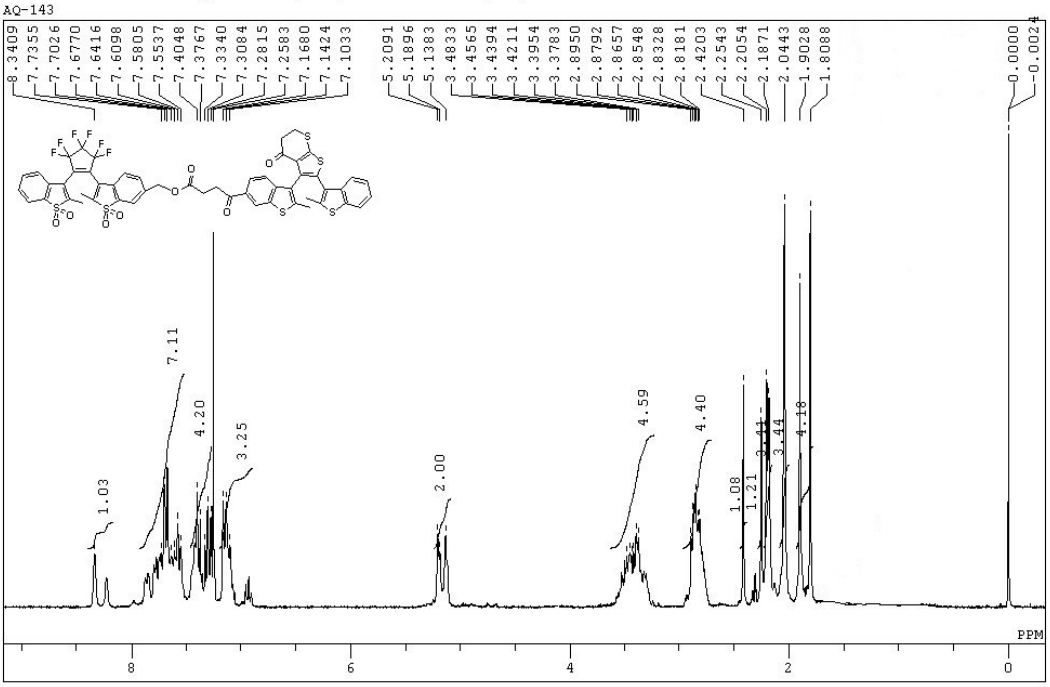
AQ-143



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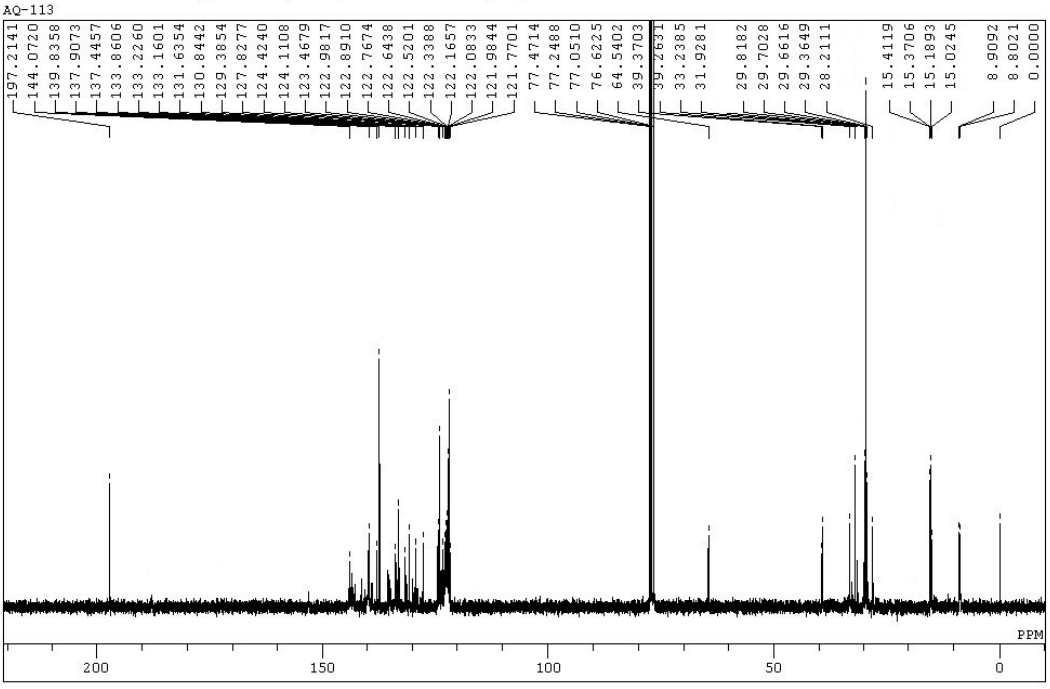
AQ-113



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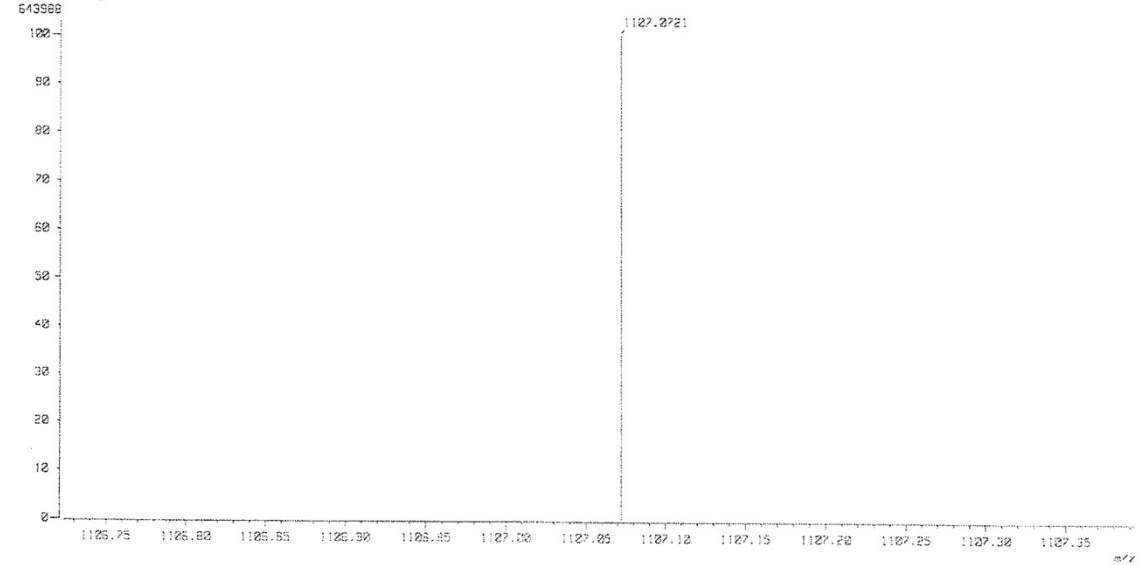

References

1. Q. Ai, S. Pang and K.-H. Ahn, *Chem. –Eur. J.*, 2015, DOI: 10.1002/chem.201504131, n/a-n/a.