

*Supporting Information*

**Length Dependence of Electron Conduction for oligo(1,4-phenylene ethynylene)s:  
A Conductive Probe Atomic Force Microscopy Investigation**

Ke Liu<sup>1,2</sup>, Guorong Li<sup>1</sup>, Xianhong Wang<sup>1\*</sup> and Fosong Wang<sup>3</sup>

*1 State Key Laboratory of Polymer Physics and Chemistry, Changchun Institute of Applied Chemistry,  
Chinese Academy of Sciences, Changchun 130022, China*

*2 Graduate School of the Chinese Academy of Science, Beijing 100039, China*

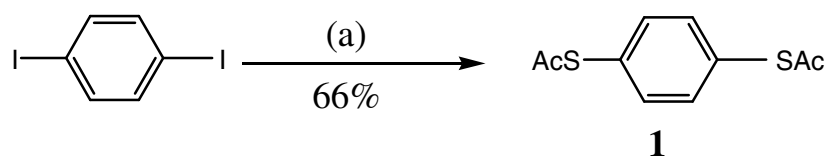
*3 Chinese Academy of Science, Beijing 100039, China*

*\* Corresponding author. Fax: 86-431-85689095. Tel: 86-431-85262250. E-mail: [xhwang@ciac.jl.cn](mailto:xhwang@ciac.jl.cn)*

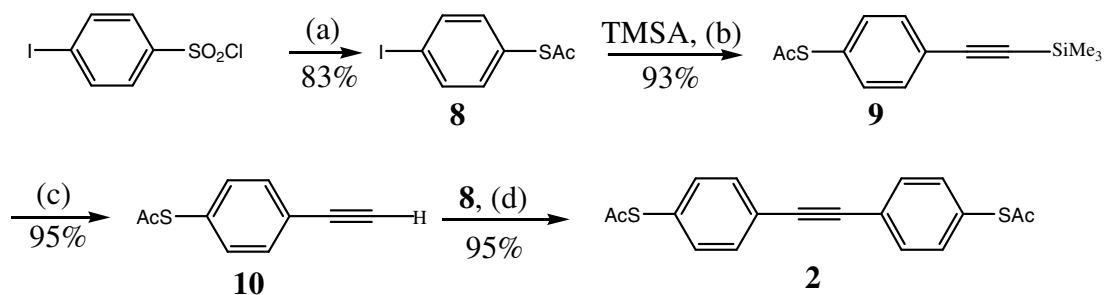
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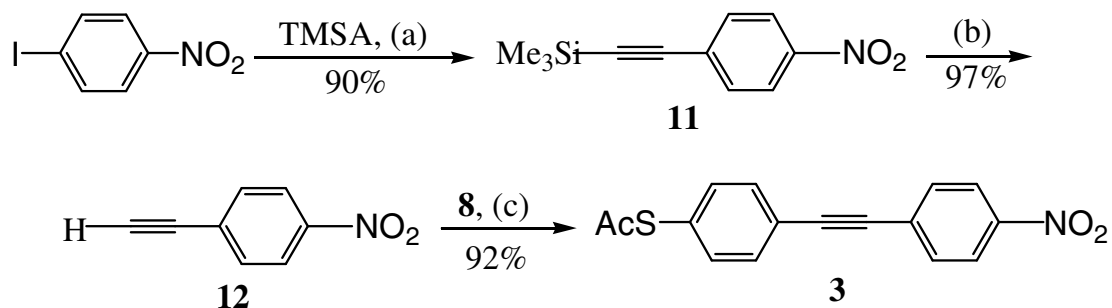
## 1. Synthetic scheme for OPE1-7



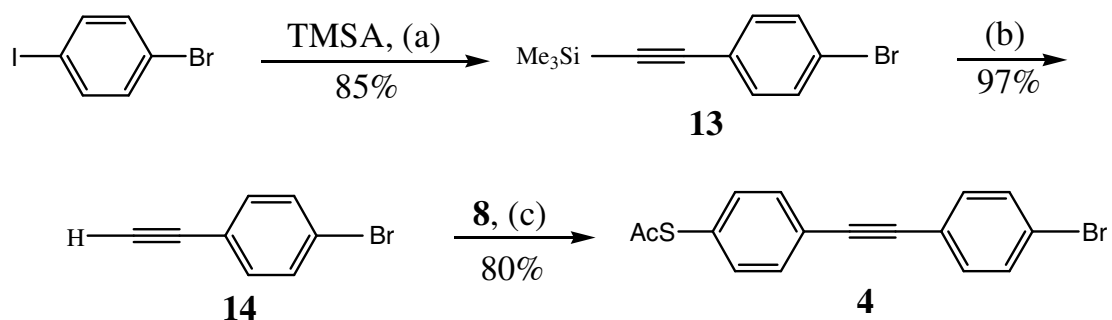
(a) *t*-BuLi, -78 °C; Sulfur powder, 0 °C; AcCl, r.t.



(a) Zn-Me<sub>2</sub>SiCl<sub>2</sub>-DMA, 75 °C; K<sub>2</sub>CO<sub>3</sub>, 75 °C; AcCl, r.t.; (b) 5mol% Pd(PPh<sub>3</sub>)<sub>2</sub>Cl<sub>2</sub>, 5mol% CuI, THF/*i*-Pr<sub>2</sub>NEt, 50 °C; (c) TBAF, AcOH/Ac<sub>2</sub>O; (d) 5mol% Pd(dba)<sub>2</sub>, 25mol% PPh<sub>3</sub>, 10mol% CuI, THF/*i*-Pr<sub>2</sub>NEt, 50 °C.

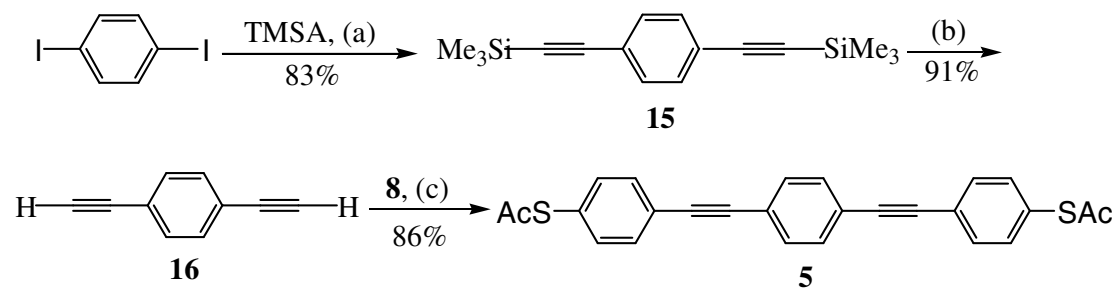


(a) 5mol% Pd(PPh<sub>3</sub>)<sub>2</sub>Cl<sub>2</sub>, 5mol% CuI, THF/*i*-Pr<sub>2</sub>NEt, 50 °C; (b) K<sub>2</sub>CO<sub>3</sub>/MeOH; (c) 5mol% Pd(dba)<sub>2</sub>, 25mol% PPh<sub>3</sub>, 10mol% CuI, THF/*i*-Pr<sub>2</sub>NEt, 50 °C.

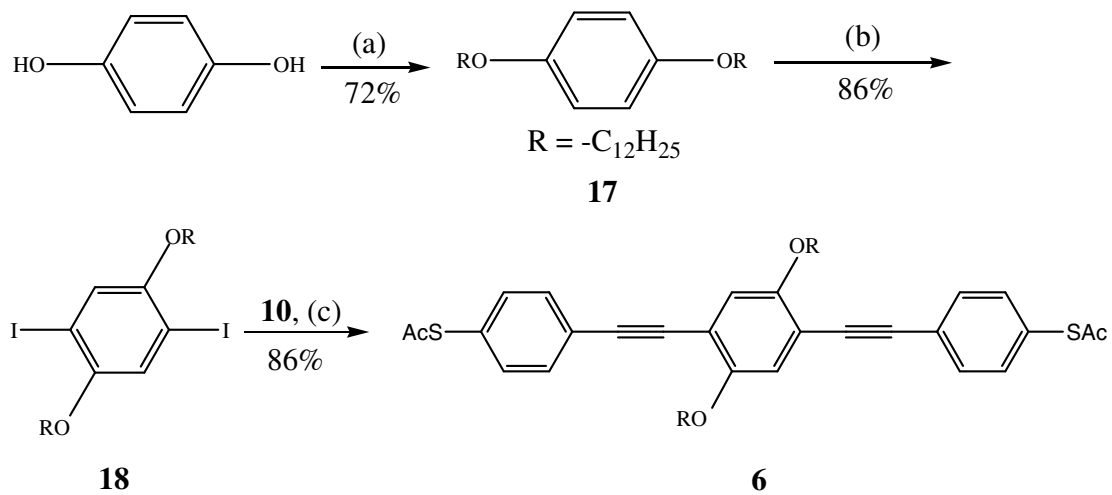


(a) 5mol% Pd(PPh<sub>3</sub>)<sub>2</sub>Cl<sub>2</sub>, 5mol% CuI, THF/*i*-Pr<sub>2</sub>NEt, r.t.; (b) K<sub>2</sub>CO<sub>3</sub>/MeOH; (c)

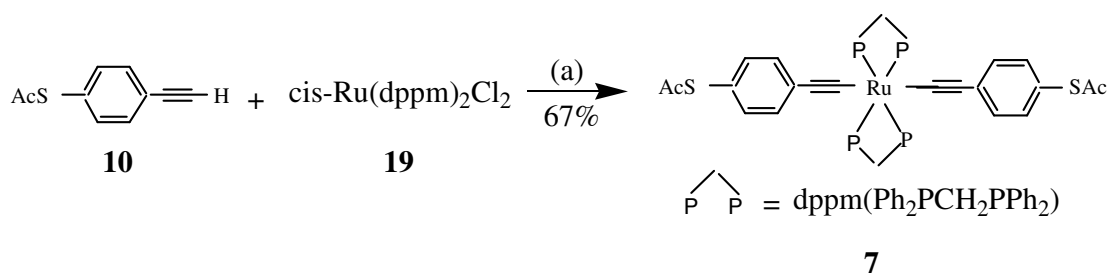
5mol% Pd(dba)<sub>2</sub>, 25mol% PPh<sub>3</sub>, 10mol% CuI, THF/*i*-Pr<sub>2</sub>NEt, r.t..



(a) 5mol% Pd(PPh<sub>3</sub>)<sub>2</sub>Cl<sub>2</sub>, 5mol% CuI, THF/*i*-Pr<sub>2</sub>NEt, 50 °C; (b) K<sub>2</sub>CO<sub>3</sub>/MeOH; (c) 5mol% Pd(dba)<sub>2</sub>, 25mol% PPh<sub>3</sub>, 10mol% CuI, THF/*i*-Pr<sub>2</sub>NEt, 50 °C.



(a) C<sub>12</sub>H<sub>25</sub>Br, K<sub>2</sub>CO<sub>3</sub>, acetone; (b) I<sub>2</sub>, H<sub>5</sub>IO<sub>6</sub>, AcOH/H<sub>2</sub>SO<sub>4</sub>/H<sub>2</sub>O/CCl<sub>4</sub>; (c) 5mol% Pd(dba)<sub>2</sub>, 25mol% PPh<sub>3</sub>, 10mol% CuI, THF/*i*-Pr<sub>2</sub>NEt, 50 °C.



(a) NaPF<sub>6</sub>, CH<sub>2</sub>Cl<sub>2</sub>, *i*-Pr<sub>2</sub>NEt, DBU, r.t..

## 2. Experimental detail

### General procedure for the coupling of terminal alkyne with an aryl halide (Castro-Stephens-Sonogashira coupling).

(Method A): All of the reagents were thoroughly dried and flushed with argon before use. To a flame-dried vessel were added the alkyne, the iodide (1.0 equiv based on per alkyne), bis(dibenzylideneacetone)-palladium(0) ( $\text{Pd}(\text{dba})_2$ ) (5 mol% per alkyne), triphenylphosphine ( $\text{PPh}_3$ ) (25 mol% per alkyne), copper(I) iodide ( $\text{CuI}$ ) (15 mol% per alkyne) and THF/*i*- $\text{Pr}_2\text{NEt}$  at room temperature under argon. The vessel was sealed and allowed to stir at room temperature for 1–3 days. The reaction mixture was then poured into water, and the aqueous layer was extracted three times with dichloromethane. After drying the combined organic layers over magnesium sulfate ( $\text{MgSO}_4$ ), the solvent was removed in vacuum to afford a crude product, which was then purified by column chromatography (silica gel, 200–300 mesh). Eluents and other slight modifications were described below for each reaction.

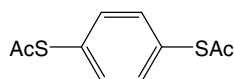
(Method B): All of the reagents were thoroughly dried and flushed with argon before use. To a flame-dried vessel were added the trimethylsilylacetylene (TMSA), the iodide (1.0 equiv based on per alkyne), bis(triphenylphosphine)-palladium(II) chloride ( $\text{Pd}(\text{PPh}_3)_2\text{Cl}_2$ ) (5 mol% per alkyne), copper(I) iodide ( $\text{CuI}$ ) (5 mol% per alkyne) and THF/*i*- $\text{Pr}_2\text{NEt}$  at room temperature under argon. The vessel was sealed and allowed to stir at room temperature for 1–3 days. The reaction mixture was then poured into water, and the aqueous layer was extracted three times with dichloromethane. After drying the combined organic layers over magnesium sulfate, the solvent was removed in vacuum to afford a crude product, which was then purified by column chromatography (silica gel, 200–300 mesh). Eluents and other slight modifications were described below for each reaction.

### General procedure for the deprotection of trimethylsilyl-protected alkynes

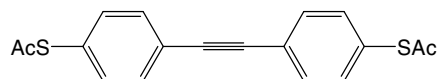
(Method A): The silylated alkyne was dissolved in methanol and often a cosolvent, and potassium carbonate ( $\text{K}_2\text{CO}_3$ ) was added. The mixture was stirred at room temperature before being poured into water. The solution was extracted with ether or

ethyl acetate and washed with brine. After drying over magnesium sulfate ( $\text{MgSO}_4$ ), the solvent was evaporated in vacuo to afford the products that generally required no purification.

(Method B): The silylated alkyne was dissolved in THF in a plastic vessel. A mixed solution of acetic anhydride/acetic acid 1:1 and 1.0M tetrabutylammonium fluoride (TBAF) in THF was added dropwise at  $-15\text{ }^\circ\text{C}$ . The solution was stirred for 15 min and quenched with silica gel. The mixture was poured into water and extracted with diethyl ether. The extract was washed with brine and dried over magnesium sulfate. After filtration the solvent was evaporated in vacuo. The crude product was purified by a flash chromatography on silica gel.

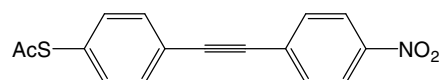


**Thioacetic acid S-(4-acetylsulfanylphenyl) ester (1).** An oven-dried flask equipped with a magnetic stir bar was charged with 1,4-diiodobenzene (1.32g, 4mmol) and dry THF (30mL) under inert atmosphere. The solution was cooled to  $-78\text{ }^\circ\text{C}$  and *tert*-butyl lithium (1mL, 21mmol) was added dropwise. The mixture was stirred at  $-78\text{ }^\circ\text{C}$  for 40min and powder sulfur (0.8g, 25mmol) was added. The mixture was stirred at  $-78\text{ }^\circ\text{C}$  for an additional 15min and warmed to  $0\text{ }^\circ\text{C}$  for 30min. The mixture was recooled to  $-78\text{ }^\circ\text{C}$  and acetyl chloride (3.20mL, 45mmol) was added immediately. The mixture was back to room temperature and stirred overnight. The resulting mixture was poured into brine and extracted twice with dichloromethane. The combined organic layers were washed with water and dried over  $\text{MgSO}_4$ , filtered and the solvent was removed under reduced pressure. The resulting solid was purified by column chromatography (silica gel, petroleum ester/dichloromethane from 2:1 to 1:1 as eluent) to provide 0.6g of white solid product (66%).  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 600 MHz):  $\delta$  7.46 (s, 4H), 2.44 (s, 6H). LDI-MS ( $m/z$ ): 226 ( $\text{M}^+$ ).

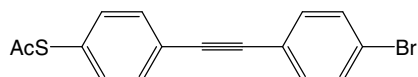


**Thioacetic acid S-[4-(4-acetylsulfanyl-phenylethynyl)-phenyl] ester (2).** See the

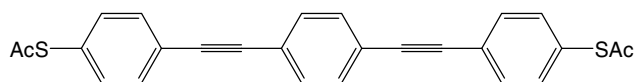
general procedure for Castro-Stephens-Sonogashira coupling method A. The compounds used were **8** (0.278g, 1.0mmol), **10** (0.176g, 1.0mmol), Pd(dba)<sub>2</sub> (0.0288g, 0.05mmol), PPh<sub>3</sub> (0.0655g, 0.25mmol), CuI (0.0286g, 0.15mmol), well-degassed *i*-Pr<sub>2</sub>NEt (1mL) and THF (4mL) at 50 °C for 1 day. The crude product was purified by column chromatography (silica gel, petroleum ester/dichloromethane from 2:1 to 1:1 as eluent) to provide 0.31g of white solid product (95%). <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz): δ 7.56 (d, 4H), 7.41 (d, 4H), 2.43 (s, 6H). EI-MS(m/z): 326 (M<sup>+</sup>).



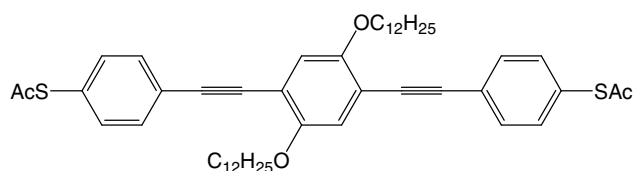
**Thioacetic acid S-[4-(4-nitro-phenylethynyl)-phenyl] ester (3).** See the general procedure for Castro-Stephens-Sonogashira coupling method A. The compounds used were **8** (0.278g, 1.0mmol), **12** (0.147g, 1.0mmol), Pd(dba)<sub>2</sub> (0.0288g, 0.05mmol), PPh<sub>3</sub> (0.0655g, 0.25mmol), CuI (0.0286g, 0.15mmol), well-degassed *i*-Pr<sub>2</sub>NEt (1mL) and THF (4mL) at 50 °C for 1 day. The crude product was purified by column chromatography (silica gel, petroleum ester/dichloromethane 1:1 as eluent) to provide 0.27g of yellow solid product (92%). <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): δ 8.23 (d, 2H), 7.68 (d, 2H), 7.59 (d, 2H), 7.44 (d, 2H), 2.45(s, 3H). EI-MS(m/z): 297 (M<sup>+</sup>).



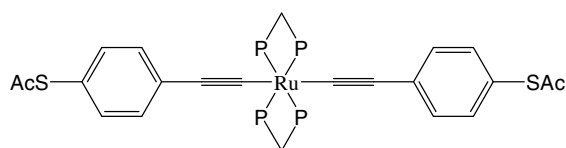
**Thioacetic acid S-[4-(4-bromo-phenylethynyl)-phenyl] ester (4).** See the general procedure for Castro-Stephens-Sonogashira coupling method A. The compounds used were **8** (0.278g, 1.0mmol), **14** (0.181g, 1.0mmol), Pd(dba)<sub>2</sub> (0.0288g, 0.05mmol), PPh<sub>3</sub> (0.0655g, 0.25mmol), CuI (0.0286g, 0.15mmol), well-degassed *i*-Pr<sub>2</sub>NEt (1mL) and THF (4mL) at 50 °C for 1 day. The crude product was purified by column chromatography (silica gel, petroleum ester/dichloromethane from 2:1 to 1:1 as eluent) to provide 0.26g of white solid product (80%). <sup>1</sup>H NMR (CDCl<sub>3</sub>, 600 MHz): δ 7.54 (d, 2H), 7.49 (d, 2H), 7.40 (d, 2H), 7.38 (d, 2H), 2.44(s, 3H). LDI-MS(m/z): 331 (M<sup>+</sup>).



**Thioacetic acid S-{4-[4-(4-acetylsulfanyl-phenylethynyl)-phenylethynyl]-phenyl} ester (5).** See the general procedure for Castro-Stephens-Sonogashira coupling method A. The compounds used were **8** (0.310g, 1.10mmol), **16** (0.070g, 0.55mmol), Pd(dba)<sub>2</sub> (0.0317g, 0.055mmol), PPh<sub>3</sub> (0.0721g, 0.28mmol), CuI (0.0209g, 0.055mmol), well-degassed *i*-Pr<sub>2</sub>NEt (1mL) and THF (4mL) at 50 °C for 1 day. The crude product was purified by column chromatography (silica gel, petroleum ester/THF 4:1 as eluent) to provide 0.20g of white solid product (86%). <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): δ 7.56 (d, 4H), 7.52 (s, 4H), 7.41 (d, 4H), 2.44(s, 6H). EI-MS(m/z): 426 (M<sup>+</sup>).

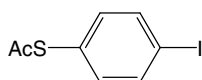


**Thioacetic acid S-{4-[4-(4-acetylsulfanyl-phenylethynyl)-2,5-bis-dodecyloxy-phenylethynyl]-phenyl} ester (6).** See the general procedure for Castro-Stephens-Sonogashira coupling method A. The compounds used were **10** (0.1938g, 1.10mmol), **18** (0.3842g, 0.55mmol), Pd(dba)<sub>2</sub> (0.0317g, 0.055mmol), PPh<sub>3</sub> (0.0721g, 0.28mmol), CuI (0.0209g, 0.055mmol), well-degassed *i*-Pr<sub>2</sub>NEt (1mL) and THF (4mL) at 50 °C for 1 day. The crude product was purified by column chromatography (silica gel, petroleum ester/dichloromethane from 2:1 to 1:1 as eluent) to provide 0.38g of white solid product (86%). <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): δ 7.55 (d, 4H), 7.39 (d, 4H), 7.01 (s, 2H), 4.03 (t, 4H), 2.44(s, 6H), 1.84 (p, 4H), 1.55-1.25 (m, 36H). 0.88 (t, 6H). LDI-MS(m/z): 796 (M+H).

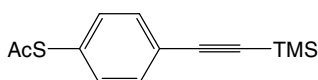


**Bis-alkynyl ruthenium(II) complex (7).** An oven-dried flask equipped with a magnetic stir bar was charged with **19** (0.470g, 0.5mmol), NaPF<sub>6</sub> (0.252g, 1.50mmol) and

dichloromethane (25mL). The mixture was stirred for 1 day in the absence of light with **10** (0.264g, 1.50mmol), *i*-Pr<sub>2</sub>NEt (0.70mL) and dichloromethane (25mL). 1,8-diazabicyclo[5.4.0]-undec-7-ene (0.15mL, 1.0mmol) was added and the mixture was stirred for an additional 2h, filtered through Al<sub>2</sub>O<sub>3</sub> and the solvent was removed under reduced pressure to afford crude product. The crude product was purified by column chromatography (neutral Al<sub>2</sub>O<sub>3</sub>, petroleum ester/dichloromethane from 6:1 to 3:2 as eluent) to provide 0.41g of green yellow solid product (67%). <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400MHz): δ 7.48(br s, 16H), 7.29-7.23(m, 8H), 7.17-7.08(m, 16H), 6.96(d, 4H), 6.23(d, 4H), 4.82(s, 4H), 2.43(s, 6H). ES-MS(m/z):1221[M]<sup>+</sup>.



**Thioacetic acid S-(4-iodo-phenyl) ester (8).** An oven-dried flask equipped with a magnetic stir bar was charged with Zn powder (4.55g, 70.0mmol) and dichlorodimethylsilane (8.49mL, 70.0mmol) in dry 1,2-dichloroethane (160mL). 4-Iodo-benzenesulfonyl chloride (6.05g, 20.0mmol) and N,N-Dimethyl-acetamide (5.60mL, 60.0mmol) in dry 1,2-dichloroethane (160mL) was added dropwise and the solution was stirred at 75 °C for 4h. The mixture was stirred at 75 °C for an additional 30min after the addition of K<sub>2</sub>CO<sub>3</sub> (1.52g, 11.0mmol). The mixture was cooled to room temperature and acetyl chloride (5.68mL, 80.0mmol) was added. The mixture was stirred overnight and filtered. The resulting solution was diluted with 80mL dichloromethane, washed with brine and dried over MgSO<sub>4</sub>. The solvent was removed under reduced pressure. The resulting solid was purified by column chromatography (silica gel, petroleum ester as eluent) to provide 4.62g of white solid product (83%). <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400MHz): δ 7.742(d, 2H), 7.128(d, 2H), 2.425(s, 3H).



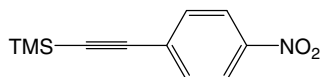
**Thioacetic acid S-(4-trimethylsilyl ethynyl-phenyl) ester (9).** See the general procedure for Castro-Stephens-Sonogashira coupling method B. The compounds used were **8** (4.17g, 15.0mmol), Pd(PPh<sub>3</sub>)Cl<sub>2</sub> (0.525g, 0.75mmol), CuI (0.143g, 0.75mmol),



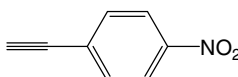
TMSA (2.8mL, 20.0mmol), well-degassed *i*-Pr<sub>2</sub>NEt (5.3mL) and THF (24mL) at 50 °C for 1 day. The crude product was purified by column chromatography (silica gel, petroleum ester and petroleum ester/dichloromethane 4:1 as eluent) to provide 3.46g of light yellow solid product (93%). <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400MHz): δ 7.48(d, 2H), 7.34 (d, 2H), 2.43 (s, 3H), 0.25(s, 9H).



**Thioacetic acid S-(4-ethynyl-phenyl) ester (10).** See the general procedure for the deprotection of trimethylsilyl-protected alkynes method B. The compounds used were **9** (1.87g, 7.53mmol), acetic anhydride (4.8mL), acetic acid (4.8mL), TBAF (2.59g, 8.21mmol) and THF (10mL). The crude product was purified by a flash chromatography (silica gel, petroleum ester/dichloromethane from 5:1 to 1:1 as eluent) to provide 1.30g of light yellow liquid product (95%). <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400MHz): δ 7.52(d, 2H), 7.37(d, 2H), 3.16(s, 1H), 2.43(s, 3H).

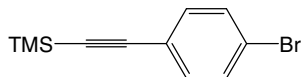


**Trimethyl-(4-nitro-phenylethynyl)-silane (11).** See the general procedure for Castro-Stephens-Sonogashira coupling method B. The compounds used were 1-iodo-4-nitro-benzene (0.93g, 3.75mmol), Pd(PPh<sub>3</sub>)Cl<sub>2</sub> (0.1313g, 0.188mmol), CuI (0.071g, 0.375mmol), TMSA (0.7mL, 5.0mmol), well-degassed *i*-Pr<sub>2</sub>NEt (1.3mL) and THF (5mL) at room temperature for 1 day. The crude product was purified by column chromatography (silica gel, petroleum ester/dichloromethane 4:1 as eluent) to provide 0.74g of orange yellow solid product (90%). <sup>1</sup>H NMR (CDCl<sub>3</sub>, 600 MHz): δ 8.16 (d, 2H), 7.59 (d, 2H), 0.27 (s, 9H).

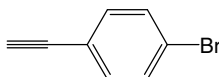


**1-Ethynyl-4-nitro-benzene (12).** See the general procedure for the deprotection of trimethylsilyl-protected alkynes method A. The compounds used were **11** (0.74g, 3.38mmol), methanol (10mL), dichloromethane (10mL) and K<sub>2</sub>CO<sub>3</sub> (1.40g,

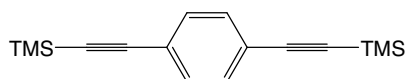
10.13mmol). The product was yellow solid of 0.48g (97%).  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 600 MHz):  $\delta$  8.20 (d, 2H), 7.64 (d, 2H), 3.36 (s, 9H).



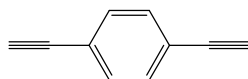
**(4-Nitro-phenylethynyl)-trimethyl-silane (13).** See the general procedure for Castro-Stephens-Sonogashira coupling method B. The compounds used were 1-bromo-4-iodo-benzene (2.83g, 10.0mmol),  $\text{Pd}(\text{PPh}_3)\text{Cl}_2$  (0.35g, 0.5mmol),  $\text{CuI}$  (0.095g, 0.5mmol), TMSA (1.48mL, 10.5mmol), well-degassed *i*- $\text{Pr}_2\text{NEt}$  (7.0mL) and THF (40mL) at room temperature for 2 day. The crude product was purified by column chromatography (silica gel, petroleum ester/dichloromethane 9:1 as eluent) to provide 2.15g of brown yellow solid product (85%).  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400MHz):  $\delta$  7.43 (d, 2H), 7.32 (d, 2H), 0.25(s, 9H).



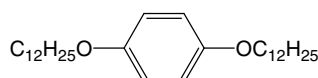
**1-Bromo-4-ethynyl-benzene (14).** See the general procedure for the deprotection of trimethylsilyl-protected alkynes method A. The compounds used were **13** (0.50g, 2.0mmol), methanol (20mL) and  $\text{K}_2\text{CO}_3$  (0.83g, 6.0mmol). The product was white solid of 0.35g (97%).  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400MHz):  $\delta$  7.46 (d, 2H), 7.34 (d, 2H), 3.12(s, 1H).



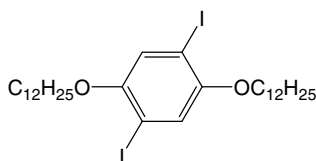
**1,4-Bis-trimethylsilanylethynyl-benzene (15).** See the general procedure for Castro-Stephens-Sonogashira coupling method B. The compounds used were 1,4-diiodobenzene (1.24g, 3.75mmol),  $\text{Pd}(\text{PPh}_3)\text{Cl}_2$  (0.263g, 0.375mmol),  $\text{CuI}$  (0.143g, 0.375mmol), TMSA (1.4mL, 9.90mmol), well-degassed *i*- $\text{Pr}_2\text{NEt}$  (2.5mL) and THF (5mL) at room temperature for 1 day. The crude product was purified by column chromatography (silica gel, petroleum ester as eluent) to provide 0.84g of white solid product (83%).  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400MHz):  $\delta$  7.39(s, 4H), 0.25(s, 18H).



**1,4-Diethynylbenzene (16).** See the general procedure for the deprotection of trimethylsilyl-protected alkynes method A. The compounds used were **15** (0.54g, 2.0mmol), methanol (10mL), dichloromethane (10mL) and  $K_2CO_3$  (1.66g, 12.0mmol). The product was white solid of 0.23g (93%).  $^1H$  NMR ( $CDCl_3$ , 400MHz):  $\delta$  7.44 (s, 4H), 3.17 (s, 2H).



**1,4-Bis-dodecyloxybenzene (17).** An oven-dried 1L three-neck round bottom flask equipped with a magnetic stir bar was charged with hydroquinone (8.19g, 74.4mmol) and acetone (600mL). The mixture was refluxed with  $K_2CO_3$  (27.64g, 200mmol) and 1-bromododecane (39.54mL, 164mmol) for 3 day.  $K_2CO_3$  (13.82g, 100mmol) was added with an additional 2 day of reflux. The mixture was filtered and washed with hot toluene. The solvent was removed under reduced pressure to provide brown crude product. The crude product was purified by recrystallization in toluene/ acetone three times to provide 23.9g of white solid product (72%).  $^1H$  NMR ( $CDCl_3$ , 300 MHz):  $\delta$  6.85 (s, 4H), 3.92 (t, 4H), 1.78 (p, 4H), 1.47-1.29 (m, 36H), 0.91 (t, 6H).



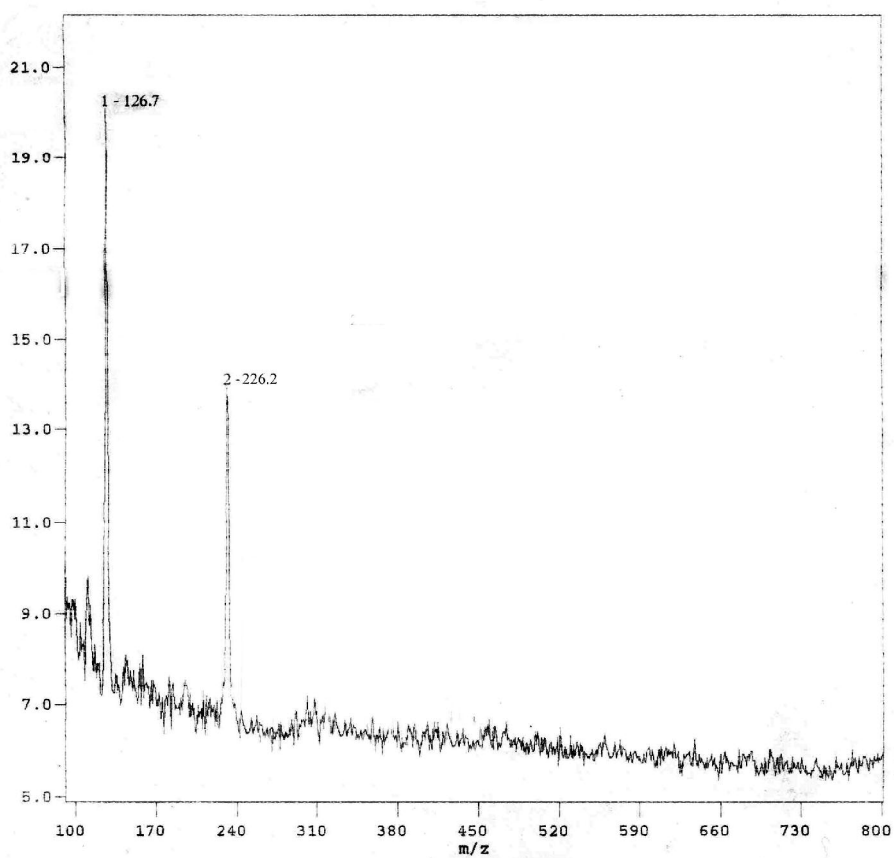
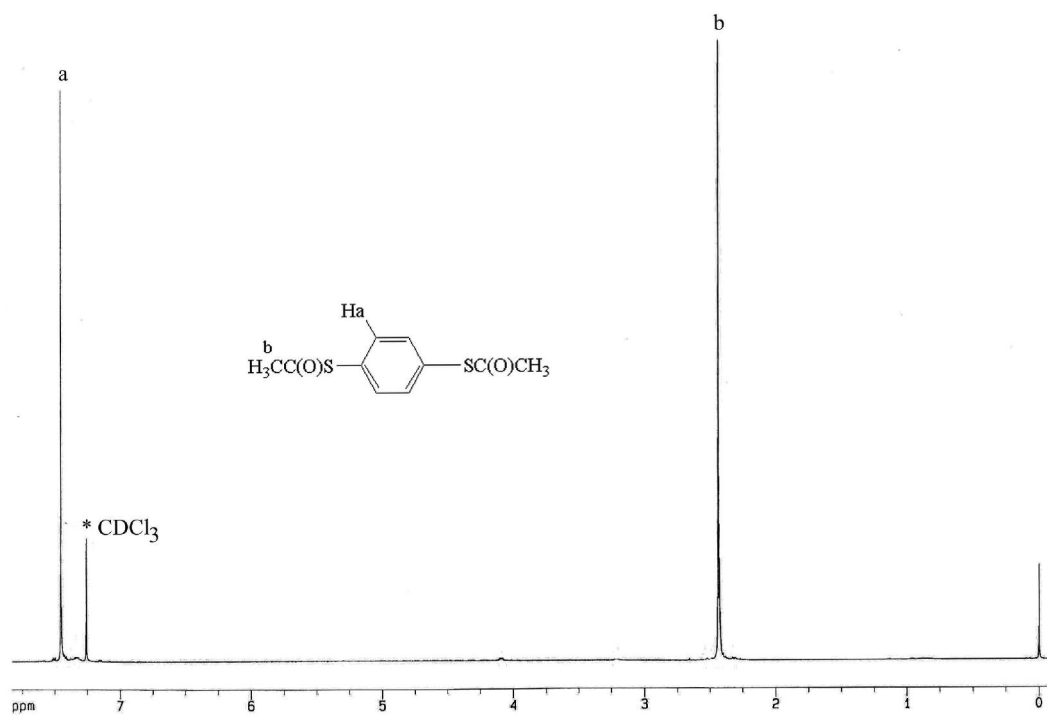
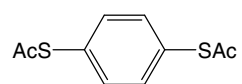
**1,4-Bis-dodecyloxy-2,5-diiodobenzene (18).** An oven-dried flask equipped with a magnetic stir bar was charged with acetic acid (30mL), sulfuric acid (0.9mL), water (3mL), perchloromethane (6mL), iodine (1.27g, 5mmol) and periodic acid (0.57g, 2.5mmol). The mixture was refluxed overnight, solution of 20% sodium sulfate in water was added until colour of iodine disappeared. The precipitation was washed with cold ethanol and recrystallized in ethanol/chloroform three times to provide 3.01g of white solid crude product (86%). The crude product was purified by column chromatography (silica gel, petroleum ester as eluent).  $^1H$  NMR ( $CDCl_3$ , 300 MHz):  $\delta$

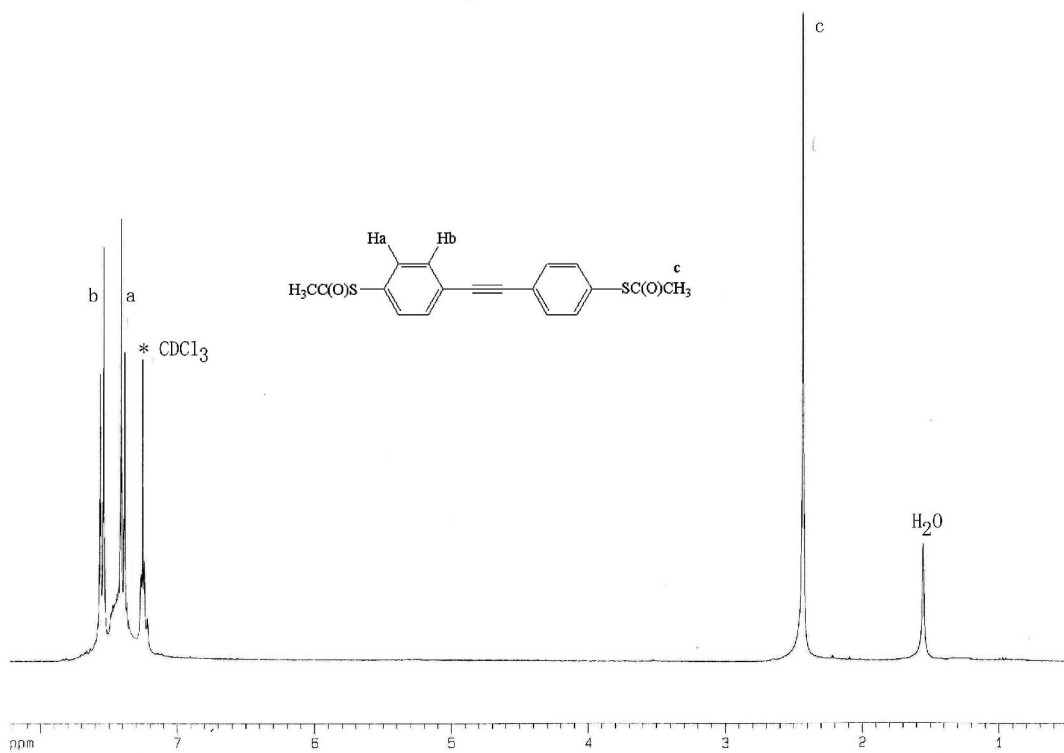
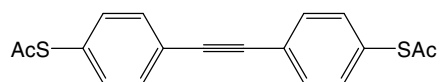
7.17 (s, 2H), 3.92 (t, 4H), 1.79 (p, 4H), 1.49-1.27 (m, 36H), 0.88 (t, 6H).

**Cis-Ru(dppm)<sub>2</sub>Cl<sub>2</sub> (19).** An oven-dried flask equipped with a magnetic stir bar was charged with bis(diphenylphosphino)methane (3.38g, 8.8mmol) and ethanol (240mL). The mixture was refluxed at 90 °C for 2h with solution of ruthenium(III) chloride (0.84g, 4.2mmol) in water (25mL). Water (200mL) was added and the mixture was extracted with chloroform, dried over MgSO<sub>4</sub> and recrystallized in dichloromethane/ethanol to provide 2.71g trans-Ru(dppm)<sub>2</sub>Cl<sub>2</sub> of orange yellow solid product (65%).

An oven-dried flask equipped with a magnetic stir bar was charged with trans-Ru(dppm)<sub>2</sub>Cl<sub>2</sub> (1.41g, 1.4mmol) and 1,2-dichloroethane (100mL). The mixture was refluxed for 1 day, cooled to room temperature, poured into pentane (400mL) and filtered to provide 1.13g of yellow solid product (80%).

### 3. $^1\text{H}$ NMR and MS spectra for OPE1-7

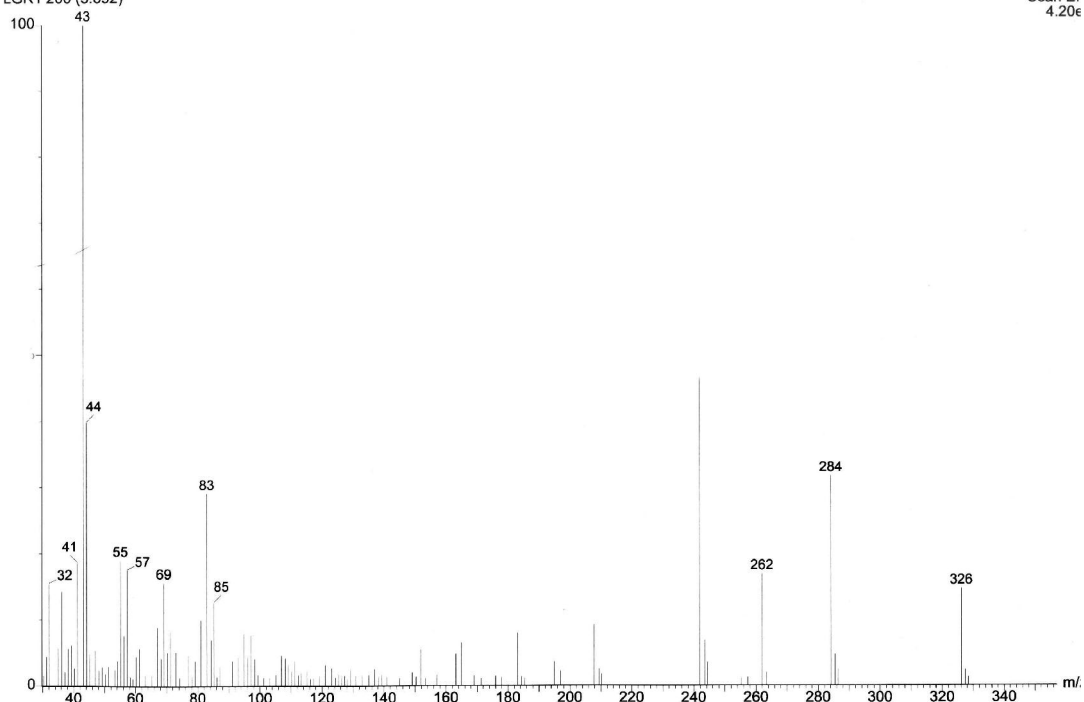


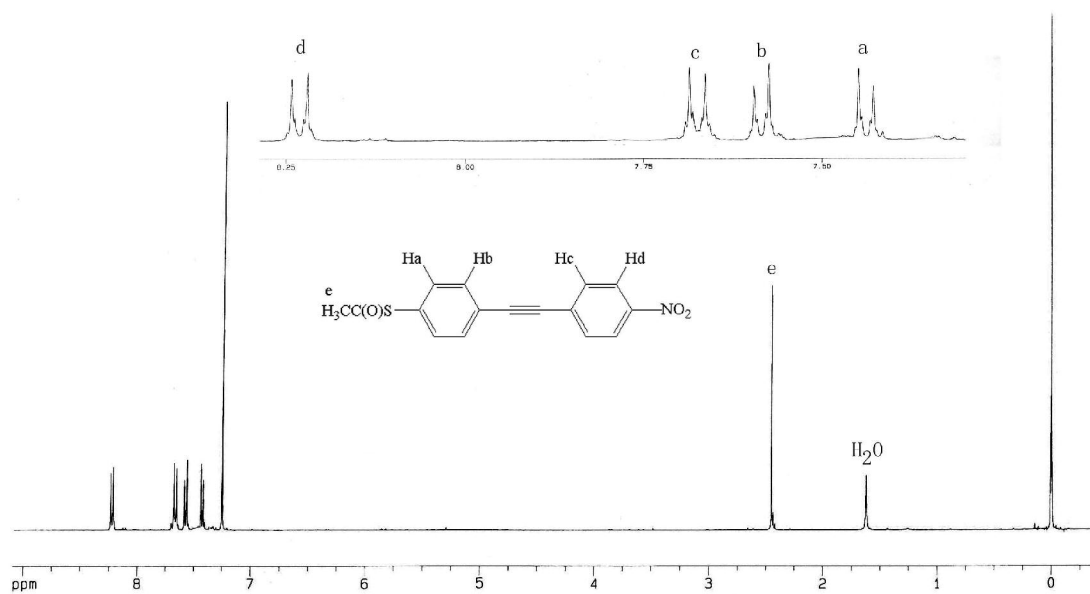
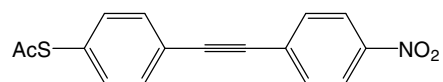


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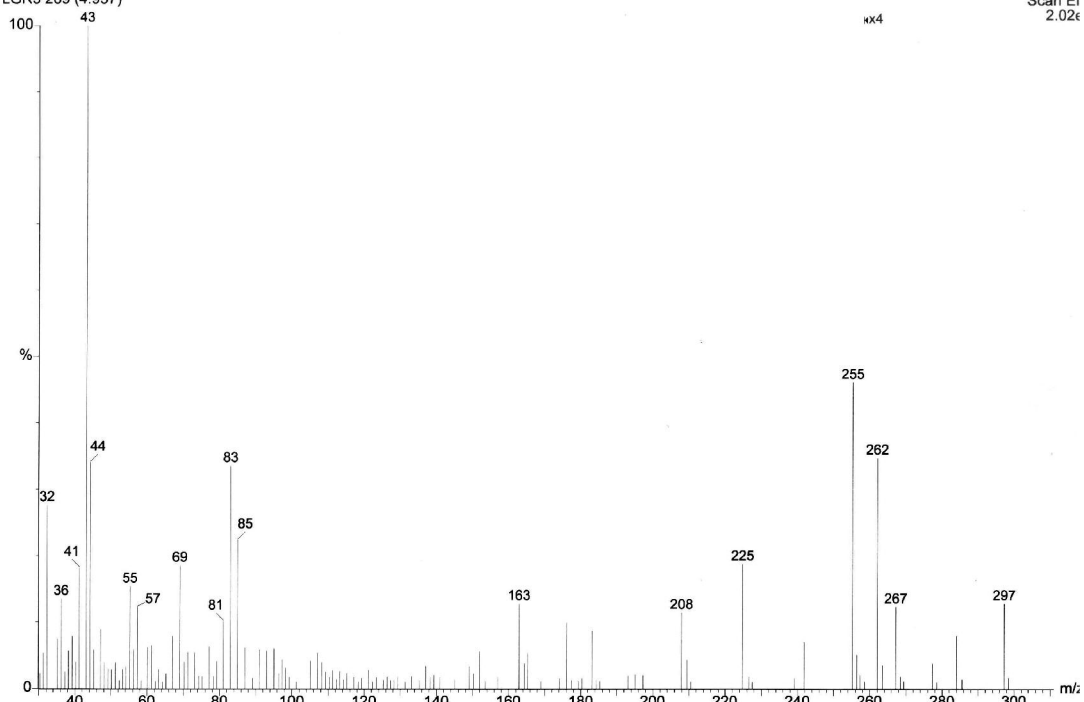
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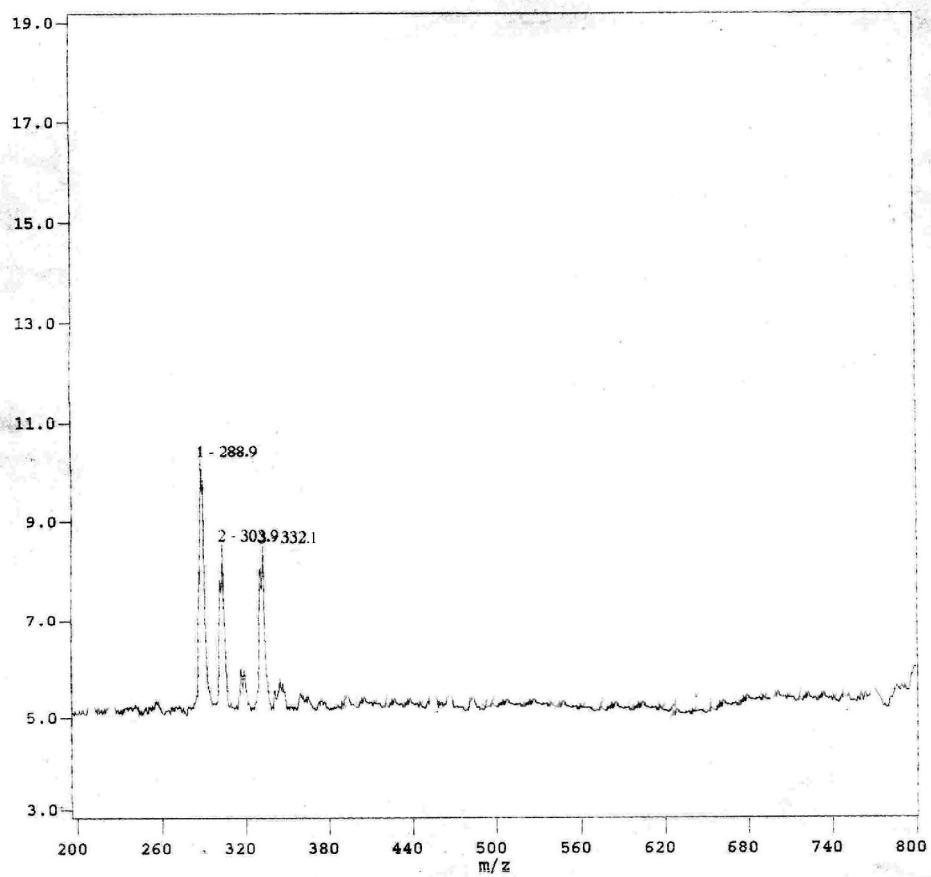
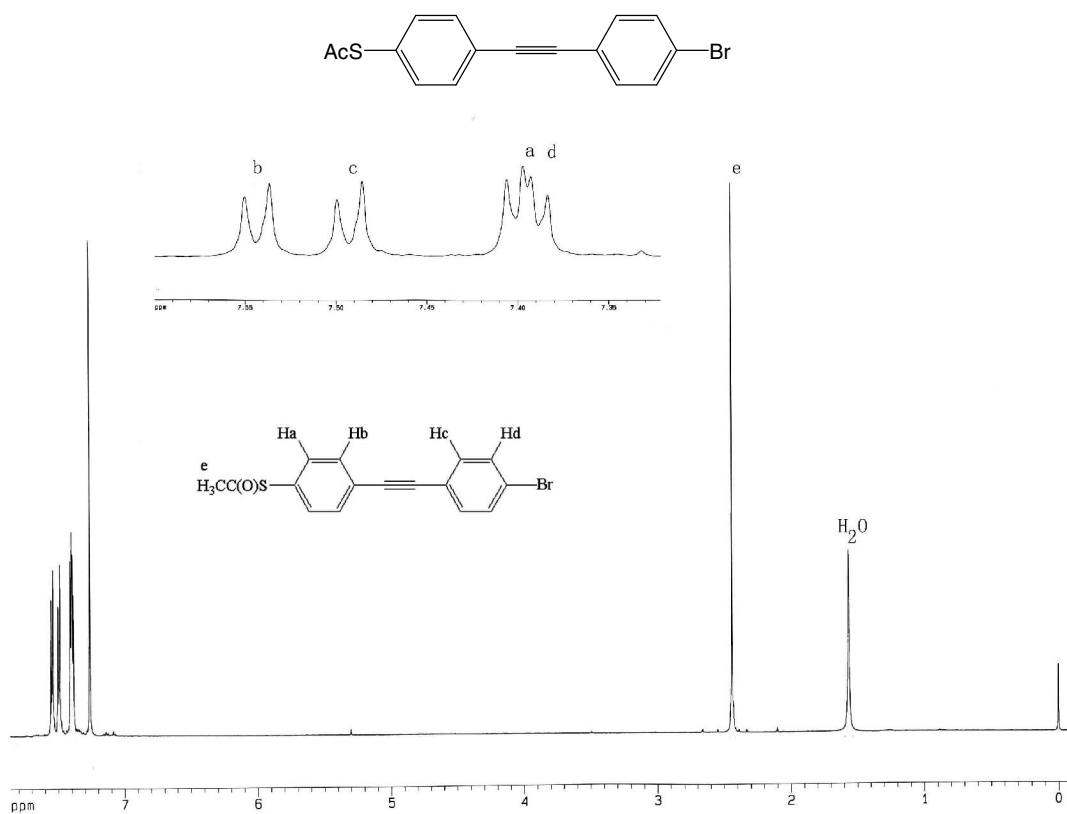




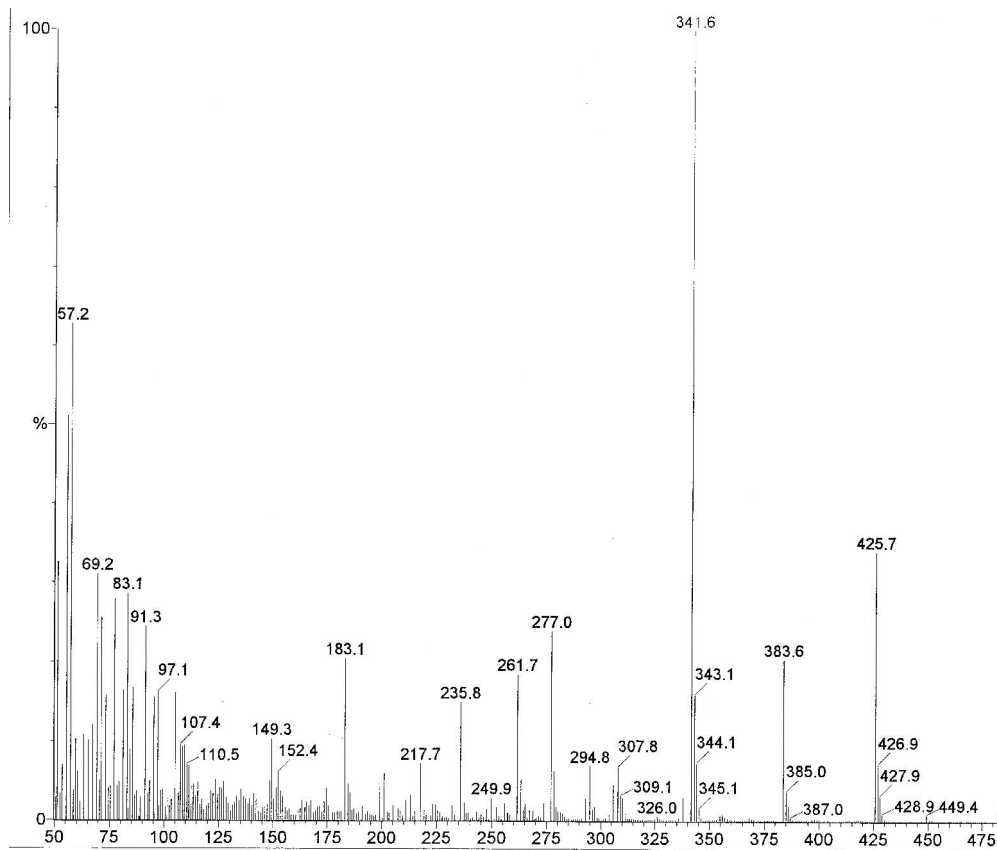
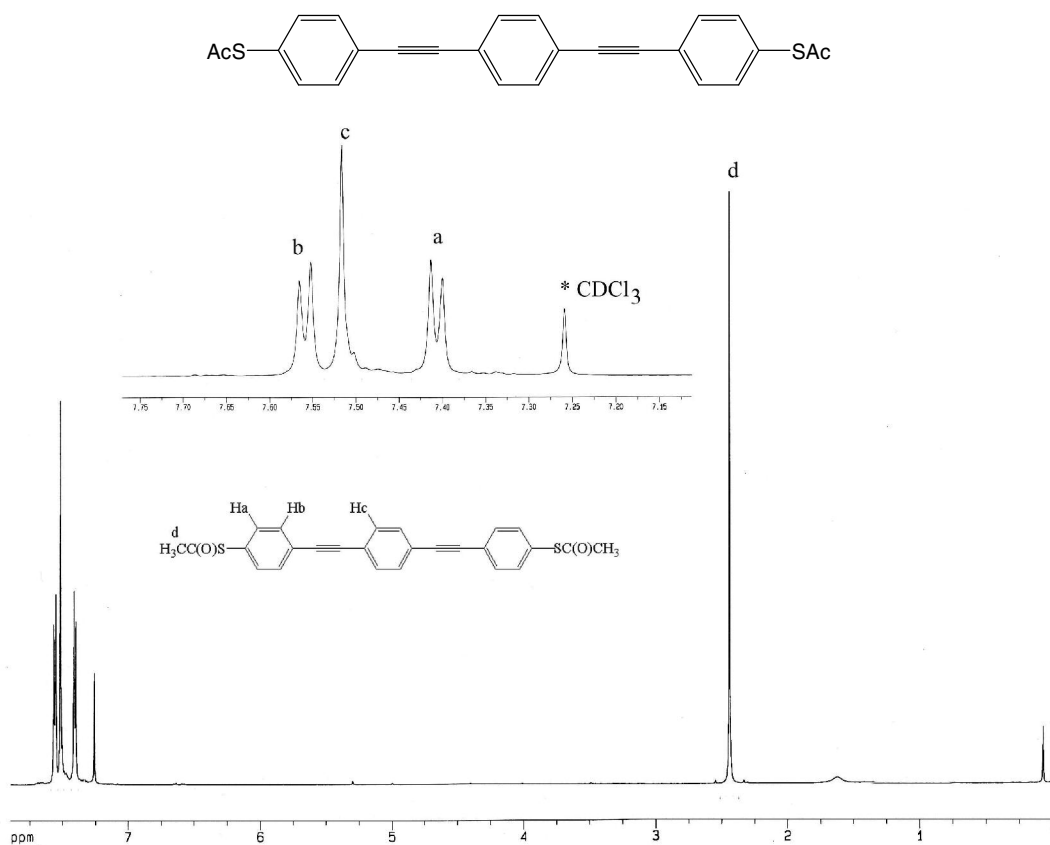
**Sample Description**  
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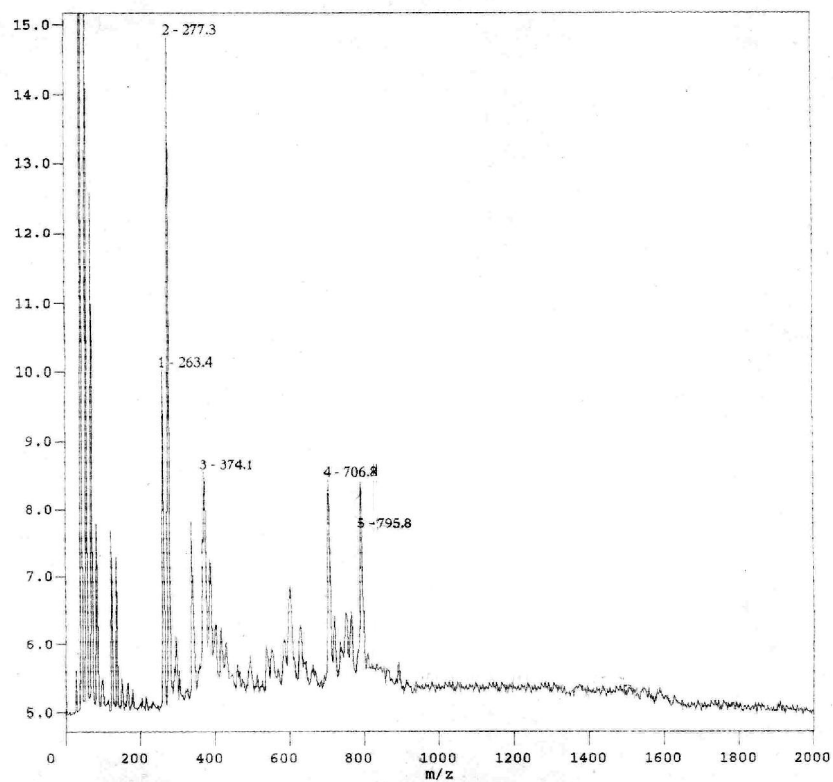
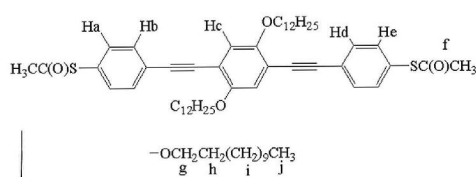
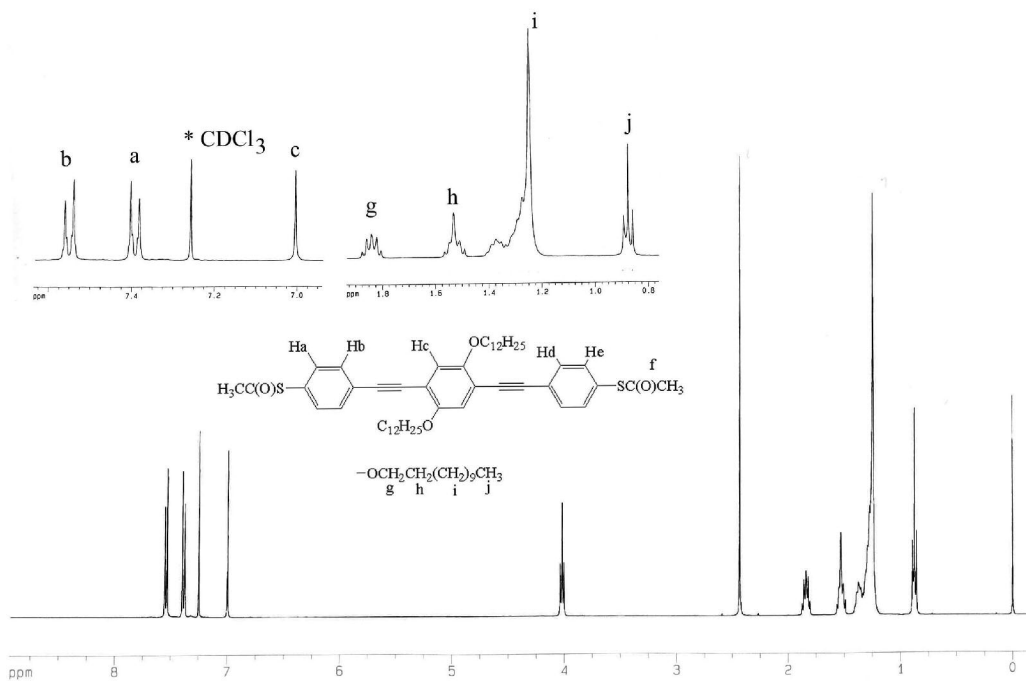
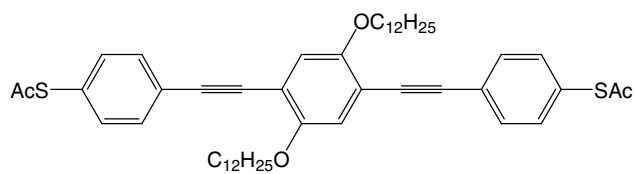
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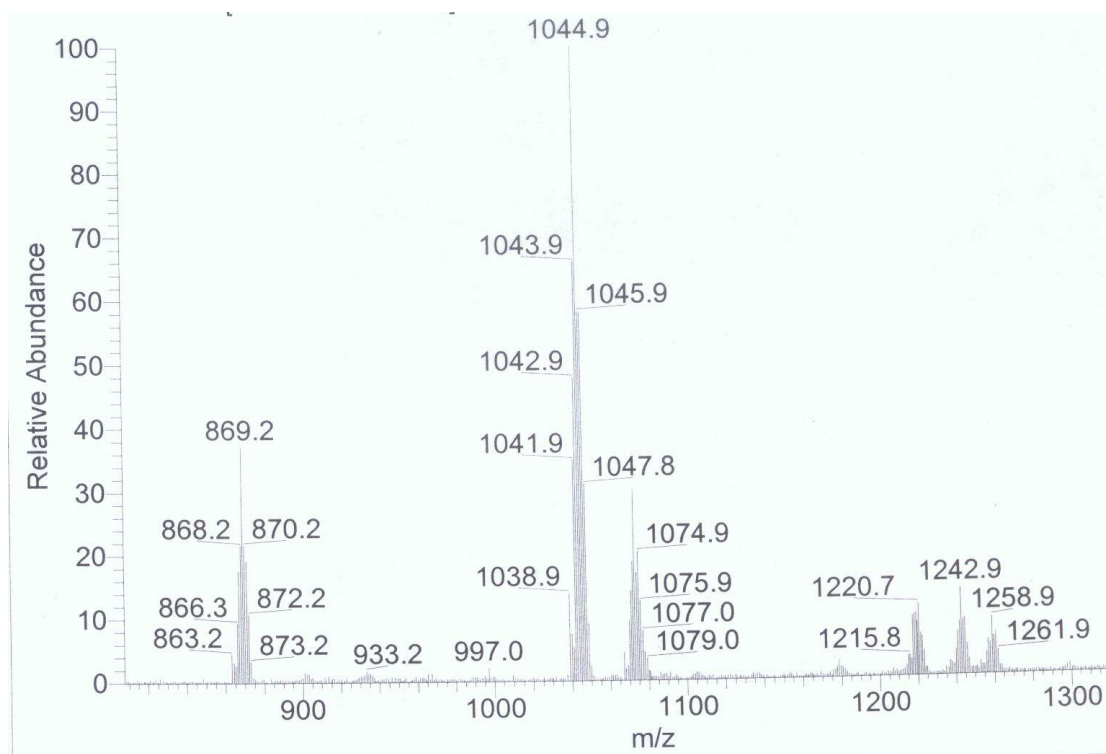
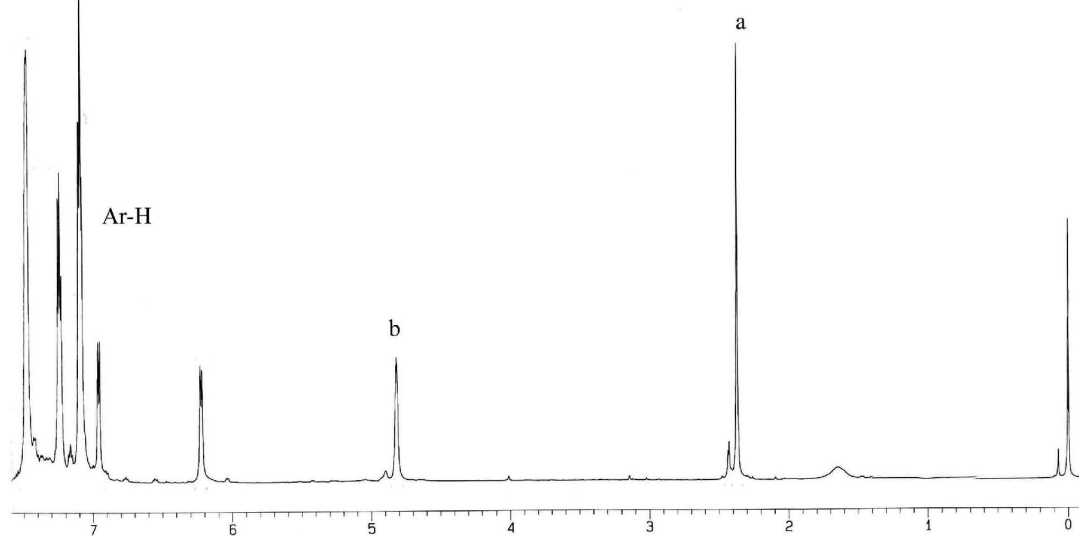
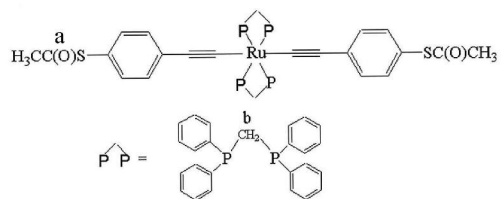
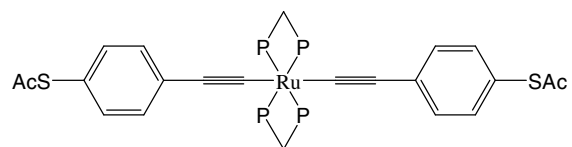












#### 4. Symmetrical *I-V* curves of OPE5 using Au tip

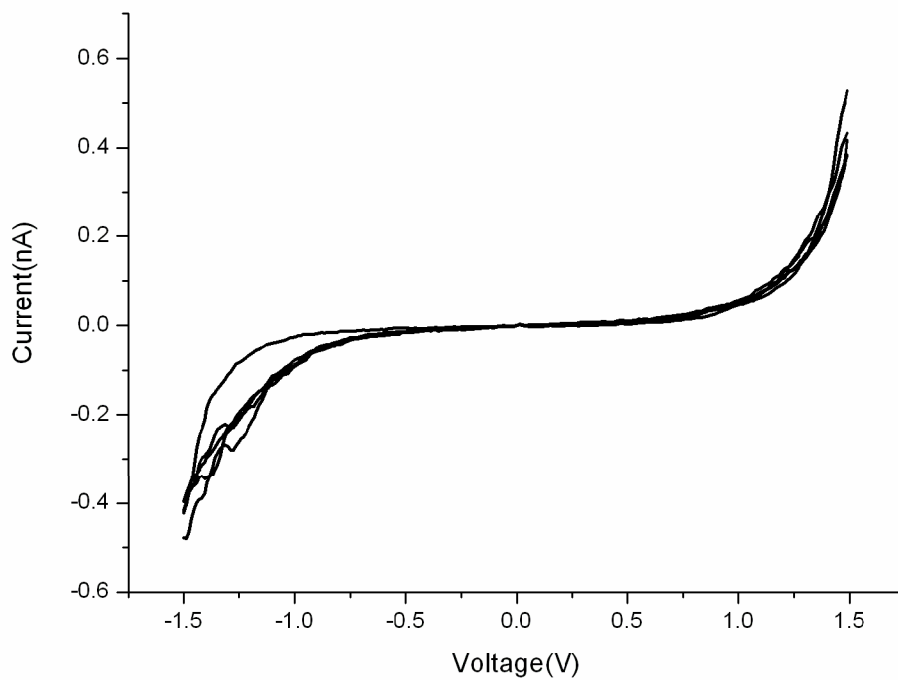


Figure S1

#### 5. Simulation curves for OPE2,3,4 and 7

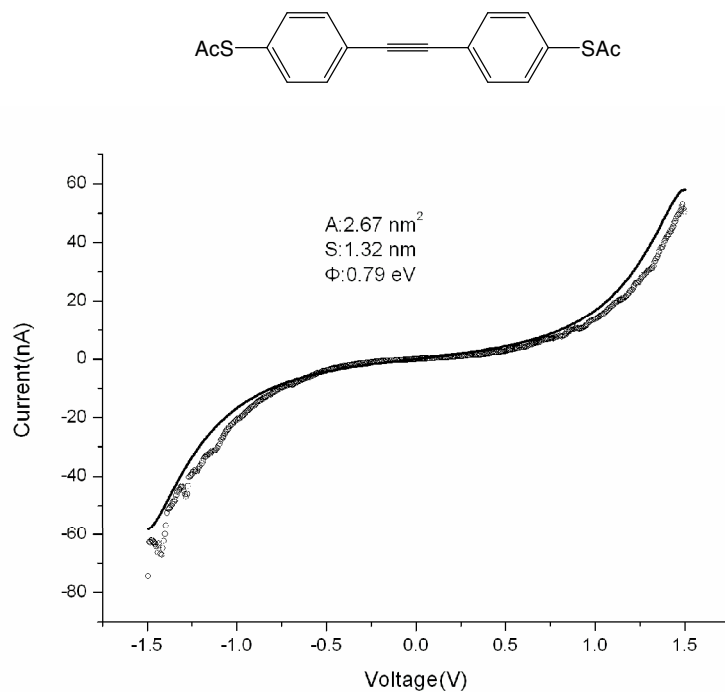
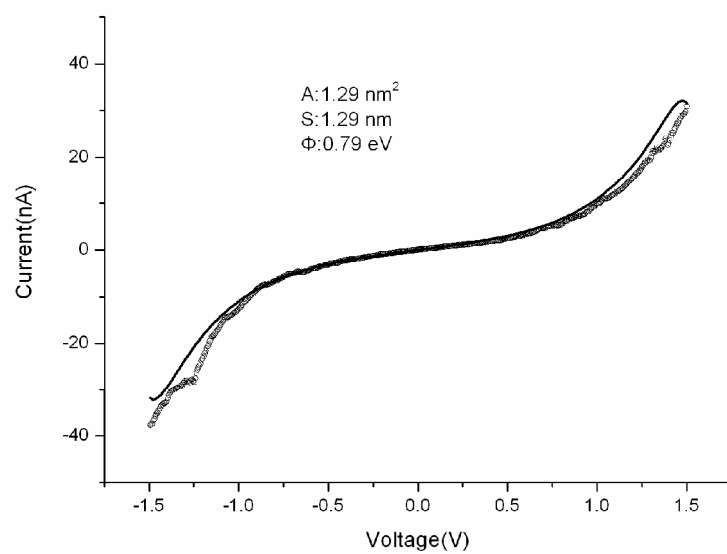
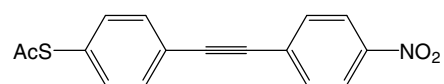
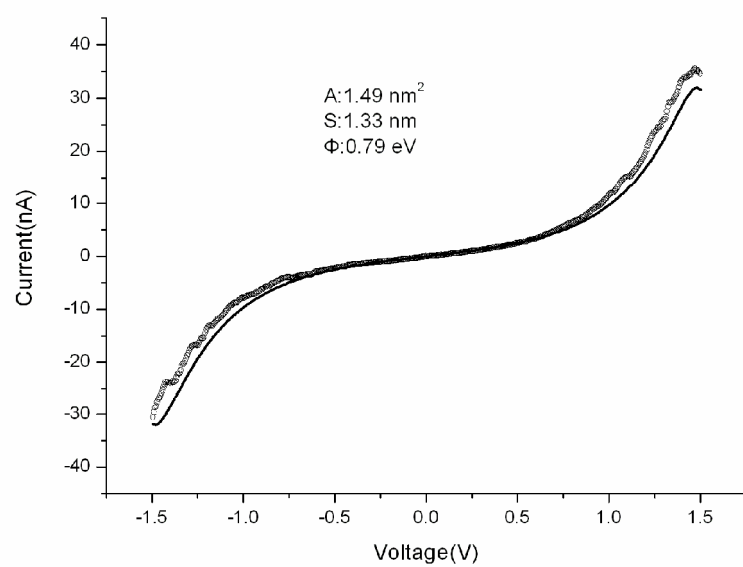
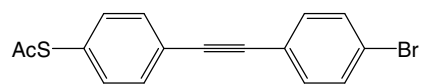


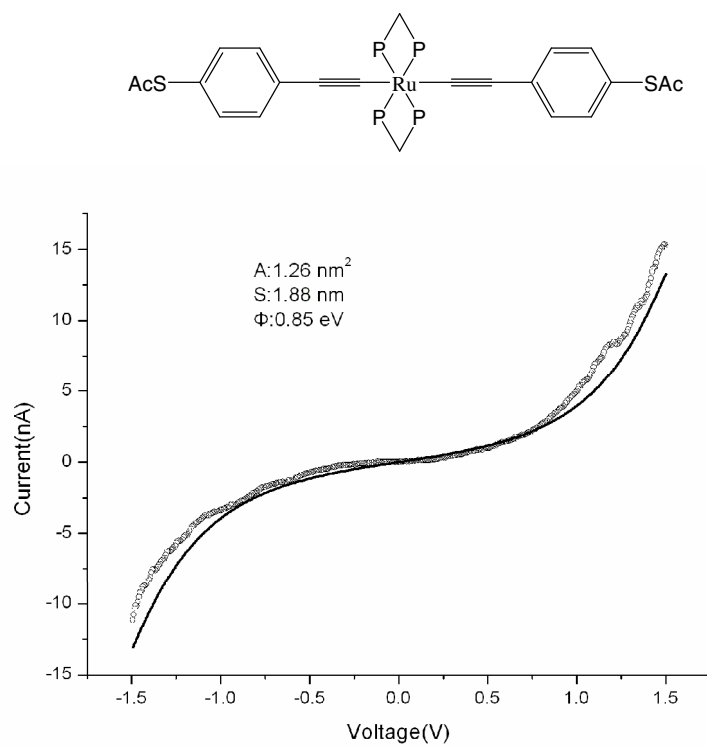
Figure S2



**Figure S3**

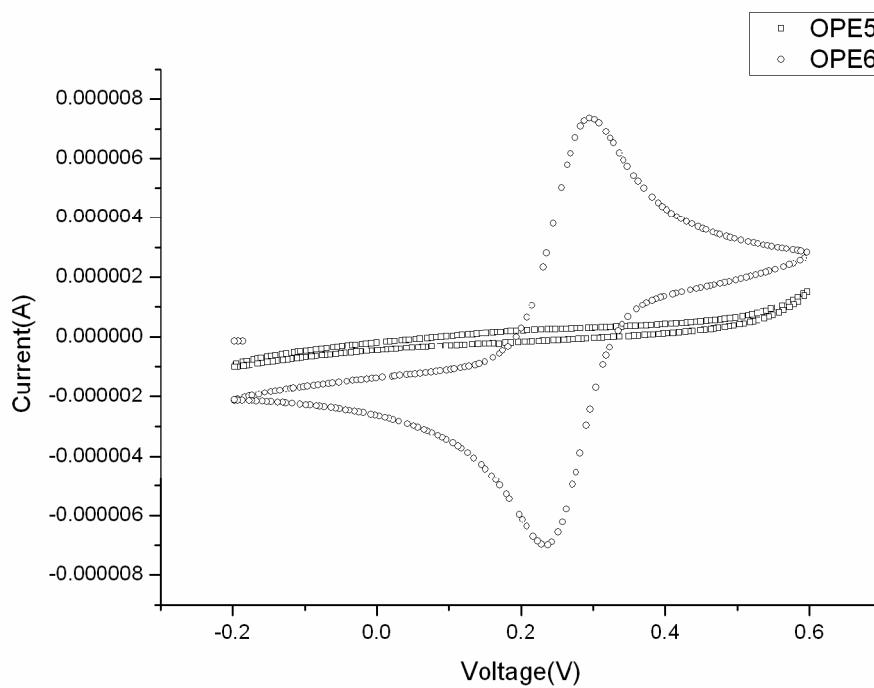


**Figure S4**



**Figure S5**

## 6. CV results of OPE5 vs OPE6



**Figure S6**

## 7. Reference

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