## Supplementary Information

## Polycyclic arene-fused selenophenes via site selective selenocyclization of arylethynyl substituted polycyclic arenes

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## Effect of additional water on product formation.

2-(4-(tert-butyl)phenyl)naphtho[1,2-b]selenophene (2c) and (E)-2-(4-(tert-butyl)styryl)naphthalene (2ca).





Four sets of reactions were put in four 15 ml volume capacity sealed tubes (pressure tube) containing $\mathbf{1 c}(95 \mathrm{mg}, 0.34 \mathrm{mmol})$ and selenium powder ( $221 \mathrm{mg}, 2.66 \mathrm{mmol}$ ) in dry NMP ( 1.2 ml ) in each with different percentage of additional water and simultaneously refluxed at 205 ${ }^{\circ} \mathrm{C}$ for 78 h using a single oil bath.

Set 1. -1.2 ml NMP $+1 \%$ distilled water
Set 2. -1.2 ml NMP $+2 \%$ distilled water
Set 3. -1.2 ml NMP $+3 \%$ distilled water
Set 4. -2 ml NMP $+15 \%$ distilled water
It was observed that with increase in water percentage in the reaction mixture fraction of $E$ alkene is increased with respect to the fused selenophene but total yield of the product was decreased gradually. But adding 2 ml of NMP with $15 \%(\mathrm{v} / \mathrm{v})$ water to the reaction mixture no product was formed, rather it gave the starting material back (Figure S44).

2-(4-(tert-butyl)phenyl)phenanthro[9,10-b]selenophene (2a) and (E)-9-(4-(tert-butyl)styryl)phenanthrene (2aa)


Reaction between 1a ( $100 \mathrm{mg}, 0.30 \mathrm{mmol}$ ) and selenium powder ( $190 \mathrm{mg}, 2.4 \mathrm{mmol}$ ) was carried out in dry NMP ( 2 ml ) in a sealed tube in presence of additional $2 \%$ of water ( 2.22 Tmmol). The trans-alkene 2aa corresponding to 1a was obtained in major quantity (87\%) in mixture with 2a (Figure S45). The mixture of 2a and 2aa is not separable using simple column chromatography. After fractional crystallization of 50 mg of product mixture from DCM/Hexane ( $1: 20$ ) solvent mixture ( 20 ml ) at room temperature white needle shaped crystals of 2aa ( 30 mg ) was obtained after $24 \mathrm{~h} .{ }^{1} \mathrm{H}$ NMR ( $\left.400 \mathrm{MHz}, \mathrm{CDCl}_{3}, \mathrm{ppm}\right) \delta=8.75(\mathrm{~d}, J=7.8$, $1 \mathrm{H}), 8.67(\mathrm{~d}, J=7.9,1 \mathrm{H}), 8.26(\mathrm{~d}, J=7.8,1 \mathrm{H}), 7.96(\mathrm{~s}, 1 \mathrm{H}), 7.92(\mathrm{~d}, J=7.3,1 \mathrm{H}), 7.84(\mathrm{~d}, J=$ $15.9,1 \mathrm{H}), 7.72-7.56(\mathrm{~m}, 6 \mathrm{H}), 7.45(\mathrm{~d}, J=8.4,2 \mathrm{H}), 7.26\left(\mathrm{~s}, \mathrm{CDCl}_{3}\right) 7.22(\mathrm{~d}, J=15.9,1 \mathrm{H}), 1.55$ (s, $\mathrm{H}_{2} \mathrm{O}$ ), $1.38(\mathrm{~s}, 9 \mathrm{H}) .{ }^{13} \mathrm{C}\left\{{ }^{1} \mathrm{H}\right\}$ NMR ( $100 \mathrm{MHz}, \mathrm{CDCl}_{3}$ ) $\delta=151.2,135.0,134.4,132.1$, 132.1, $131.0,130.6,130.3,128.8,128.3,127.5,127.0,126.8,126.7,126.2,125.9,125.8,124.9,124.6$,
123.7, 123.3, 122.7, 34.9, 31.5. HRMS (ESI-TOF) m/z $[\mathrm{M}+\mathrm{H}]^{+}$calcd for $\mathrm{C}_{26} \mathrm{H}_{25}$ 337.1950, found 337.1949 .

## Recycling of Selenium powder.

The selenium powder was used during the formation of fused selenophene is immiscible with NMP and can be reused after purification. Also, no significant change in powder XRD data of selenium powder was found after the reaction from its initial state (Figure S1). ${ }^{1}$ It signifies that there is no chemical change that occurred during the reaction in selenium powder. Only the crystallinity of selenium powder was improved during reaction, which was indicated by the sharpening of peaks of respective positions (Figure S1).


Figure S1. PXRD data of selenium powder (i) initially (ii) after first cycle and (iii) after Third cycle

## Experimental details

## First Cycle

To verify the reusability of selenium powder, $\mathbf{1 a}(112 \mathrm{mg}, 0.334 \mathrm{mmol})$ and $\mathrm{Se}(210 \mathrm{mg} ; 2.67$ $m \mathrm{~mol}$.) was taken in a 15 ml Schlenk tube containing a magnetic stirrer bar. The system was degassed and refilled with nitrogen, and dry NMP ( 1.2 ml ) was added. The temperature of the system was slowly raised to $205^{\circ} \mathrm{C}$ and kept constant for a further 48 h . After cooling to room temperature $\operatorname{DCM}(10 \mathrm{ml})$ was added to dilute the mixture and collected using a glass syringe after allowing to settled remaining selenium powder for 15 min . The process was repeated 2-3 times until the solution becomes clear, and the sealed tube containing unreacted selenium powder was dried in an oven. The liquid part was treated with $\mathrm{NH}_{4} \mathrm{Cl}$ and washed with $2 \times 100$ ml of water to remove NMP. The product mixture was collected in DCM and dried over $\mathrm{Na}_{2} \mathrm{SO}_{4}$ to concentrated under reduced pressure. Residual NMP was removed from the product mixture by performing flash column chromatography on silica gel (100-200) packed column
using Hexane/DCM solvent mixture (50:1) to obtain 118 mg crude solid. It was observed from ${ }^{1}$ H NMR analysis (Figure S47(a)) that $63 \%$ of the starting material was converted to product 2a, and the remaining $37 \%$ starting material remain as such.

## Second Cycle

Unreacted selenium powder obtained after the first cycle was weighed ( $183 \mathrm{mg}, 2.32 \mathrm{mmol}$ ) and reused for the second cycle. It was reacted with $\mathbf{1 a}(97 \mathrm{mg}, 0.290 \mathrm{mmol})$ in the presence of NMP ( 1 ml ) following the same procedure employed in the first cycle by maintaining exactly the same substrate to selenium ratio (1:8). After workup total of 96 mg of crude solid was obtained containing the majority of $\mathbf{2 a}(59 \%)$ and the rest is $\mathbf{1 a}(41 \%)$ as observed in their ${ }^{1} \mathrm{H}$ NMR data (Figure S47(b)).

## Third Cycle

After the second cycle remaining selenium powder ( $160 \mathrm{mg}, 2.02 \mathrm{mmol}$ ) was reacted with 1a ( $84 \mathrm{mg}, 0.253 \mathrm{mmol}$ ) in the presence of NMP ( 1 ml ), yielding 78 mg of crude solid. This time corresponding $E$-alkene 2aa ( $20 \%$ ) was obtained along with fused selenophene 2a ( $40 \%$ ) and unreacted starting material 1a (40\%) (Figure S47(c)).

Table S1 Recycling of selenium powder

| Cycles | Substrate <br> (1a) <br> mg (mmol) | selenium <br> mg (mmol) | NMP | Isolated Mixture after Reaction* |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | Substrate <br> (1a) $\%$ | Selenophene <br> (2a) $) \%$ | Alkene <br> $(\mathbf{2 a a}) \%$ |  |  |  |
| 1 | $112(0.334)$ | $210(2.67)$ | 1.2 ml | 63 | 37 | - |
| 2 | $97(0.290)$ | $183(2.32)$ | 1 ml | 59 | 41 | - |
| 3 | $84(0.253)$ | $160(2.02)$ | 1 ml | 40 | 40 | 20 |

* percentage yield determined using NMR spectra


Figure S2. Yield of product formation at different cycles.

## Single Crystal X-ray Diffraction Study.

All the crystals were obtained by the slow evaporation method from the mixture of solvents at room temperature. After the formation of good quality crystals, they are generally kept under ethanol as an anti-solvent. For diffraction, a suitable crystal was chosen from a glass slide covered with mineral oil. The crystals were diffracted on Super Nova, Dual, Cu/Mo at zero,

Eos diffractometer. The crystals were solved using Olex $2,{ }^{2}$ the structure was solved with the ShelXT ${ }^{3}$ structure solution program and refined with the ShelXL ${ }^{4}$ refinement package using Least Squares minimization. Details of crystal data were listed in Table S1.

Table S2. Crystal data and structure refinement

| Identification code | 2 a | 2 c | 2 ea | 2 g |
| :---: | :---: | :---: | :---: | :---: |
| Empirical formula | $\mathrm{C}_{26} \mathrm{H}_{22} \mathrm{Se}$ | C22H20Se | C24H16 | $\mathrm{C}_{26} \mathrm{H}_{16} \mathrm{Se}$ |
| Formula weight | 413.40 | 363.34 | 304.37 | 407.35 |
| Temperature/K | 100.00 | 100.00(10) | 100 | 100.00 |
| Crystal system | monoclinic | monoclinic | monoclinic | orthorhombic |
| Space group | $\mathrm{I}_{2}$ | P2 ${ }_{1}$ | $\mathrm{P} 2_{1}$ | $\mathrm{P}_{\text {bca }}$ |
| a/Ă | 19.253(2) | 7.9313(3) | 12.7769(9) | 9.58910(10) |
| b/Ă | 6.0322(4) | 11.3299(4) | 4.0491(2) | 14.4311(2) |
| c/Ă | 18.774(2) | 18.9666(7) | 15.6492(10) | 25.6817(3) |
| $\alpha /{ }^{\circ}$ | 90.00 | 90.00 | 90.00 | 90.00 |
| $\beta /{ }^{\circ}$ | 118.999(15) | 91.108(3) | 107.939(7) | 90.00 |
| $\gamma^{\prime}$ | 90.00 | 90.00 | 90.00 | 90.00 |
| Volume/Å ${ }^{3}$ | 1907.0(4) | 1704.04(11) | 770.25(8) | 3553.87(7) |
| Z | 4 | 4 | 2 | 8 |
| $\rho_{\text {calcg }} / \mathrm{cm}^{3}$ | 1.440 | 1.416 | 1.312 | 1.523 |
| $\mu / \mathrm{mm}^{-1}$ | 2.696 | 2.201 | 0.074 | 2.892 |
| $\mathrm{F}(000)$ | 848.0 | 744.0 | 320.0 | 1648.0 |
| Crystal size/mm ${ }^{3}$ | $\begin{gathered} 0.08 \times 0.06 \times \\ 0.04 \end{gathered}$ | $\begin{gathered} 0.5 \times 0.2 \times \\ 0.1 \end{gathered}$ | $\begin{gathered} 0.09 \times 0.03 \times \\ 0.01 \end{gathered}$ | $\begin{gathered} 0.05 \times 0.05 \times \\ 0.01 \end{gathered}$ |
| Radiation | $\begin{gathered} \operatorname{CuK\alpha }(\lambda= \\ 1.54184) \end{gathered}$ | $\begin{gathered} \operatorname{MoK\alpha } \operatorname{Ko}(\lambda= \\ 0.71073) \end{gathered}$ | $\begin{gathered} \operatorname{MoK} \operatorname{Kog}(\lambda= \\ 0.71073) \end{gathered}$ | $\begin{gathered} \operatorname{CuK\alpha }(\lambda= \\ 1.54184) \end{gathered}$ |
| $2 \Theta$ range for data collection/ ${ }^{\circ}$ | 9.16 to 131.1 | 4.18 to 50.04 | 3.36 to 49.98 | 6.88 to 132.34 |
| Index ranges | $\begin{gathered} -22 \leq \mathrm{h} \leq 22, \\ 7 \leq \mathrm{k} \leq 5,-21 \\ \leq 1 \leq 22 \end{gathered}$ | $\begin{aligned} & -9 \leq \mathrm{h} \leq 9,-7 \\ & \leq \mathrm{k} \leq 13,-22 \\ & \leq 1 \leq 22 \end{aligned}$ | $\begin{gathered} -15 \leq \mathrm{h} \leq 15,- \\ 4 \leq \mathrm{k} \leq 4,-18 \\ \leq 1 \leq 18 \end{gathered}$ | $\begin{array}{r} -11 \leq \mathrm{h} \leq 11, \\ 17 \leq \mathrm{k} \leq 16, \\ 30 \leq 1 \leq 30 \end{array}$ |
| Reflections collected | 6302 | 7623 | 5353 | 32979 |
| Independent reflections | $\begin{gathered} 2571\left[\mathrm{R}_{\text {int }}=\right. \\ 0.0525, \\ \mathrm{R}_{\text {sigma }}= \\ 0.0537] \end{gathered}$ | $\begin{gathered} 4300[\text { Rint }= \\ 0.0308, \\ \text { Rsigma }= \\ 0.0514] \end{gathered}$ | $\begin{gathered} 2623[\text { Rint }= \\ 0.0212, \\ \text { Rsigma }= \\ 0.0300] \end{gathered}$ | $\begin{gathered} 3102\left[\mathrm{R}_{\text {int }}=\right. \\ 0.0510 \\ \mathrm{R}_{\text {sigma }}= \\ 0.0216] \end{gathered}$ |
| Data/restraints/parameters | 2571/1/248 | 4300/1/421 | 2623/1/217 | 3102/0/244 |
| Goodness-of-fit on $\mathrm{F}^{2}$ | 1.048 | 1.069 | 1.293 | 1.068 |
| Final R indexes $[\mathrm{I}>=2 \sigma$ (I)] | $\begin{gathered} \mathrm{R}_{1}=0.0603, \\ \mathrm{wR}_{2}=0.1521 \end{gathered}$ | $\begin{aligned} \mathrm{R} 1 & =0.0379 \\ \mathrm{wR} 2 & =0.0892 \end{aligned}$ | $\begin{aligned} \mathrm{R} 1 & =0.0519 \\ \mathrm{wR} 2 & =0.1594 \end{aligned}$ | $\begin{gathered} \mathrm{R}_{1}=0.0384, \\ \mathrm{wR}_{2}=0.0955 \end{gathered}$ |
| Final R indexes [all data] | $\begin{gathered} \mathrm{R}_{1}=0.0618 \\ \mathrm{wR}_{2}=0.1542 \end{gathered}$ | $\begin{gathered} \mathrm{R} 1=0.0430, \\ \mathrm{wR} 2=0.0920 \end{gathered}$ | $\begin{gathered} \mathrm{R} 1=0.0603, \\ \mathrm{wR} 2=0.1643 \end{gathered}$ | $\begin{aligned} \mathrm{R}_{1} & =0.0413, \\ \mathrm{wR}_{2} & =0.0977 \end{aligned}$ |
| $\underset{\AA^{-3}}{\text { Largest diff. peak/hole / e }}$ | 1.73/-1.21 | 0.74/-0.40 | 0.14/-0.22 | 1.62/-0.51 |
| Flack parameter | -0.03(4) | 0.044(12) | 3(10) |  |
| Identification code | 2041369 | 2041373 | 2042639 | 2042641 |


| Identification code | 2ha | 2 i | 2kb |
| :---: | :---: | :---: | :---: |
| Empirical formula | C28H18 | C17H16Se | $\mathrm{C}_{34} \mathrm{H}_{32}$ |
| Formula weight | 354.42 | 299.26 | 440.60 |
| Temperature/K | 293(2) | 100.00(10) | 293(2) |
| Crystal system | monoclinic | triclinic | triclinic |
| Space group | $\mathrm{C}_{\mathrm{c}}$ | P-1 | P-1 |
| a/Ā | 32.303(5) | 6.1989(5) | 9.8772(5) |
| b/A | 6.2174(12) | 11.0621(10) | 13.1988(5) |
| c/Ā | 9.0416(19) | 20.7731(19) | 21.2332(9) |
| $\alpha{ }^{\circ}$ | 90.00 | 104.826(8) | 92.631(3) |
| $\beta /{ }^{\circ}$ | 97.505(16) | 98.430(7) | 98.313(4) |
| $\gamma{ }^{\circ}$ | 90.00 | 92.099(7) | 107.660(4) |
| Volume/A3 | 1800.4(6) | 1358.1(2) | 2598.1(2) |
| Z | 4 | 4 | 4 |
| ¢calcg/cm3 | 1.308 | 1.464 | 1.126 |
| $\mu / \mathrm{mm}$-1 | 0.562 | 2.744 | 0.063 |
| F(000) | 744.0 | 608.0 | 944.0 |
| Crystal size/mm3 | $\begin{gathered} 0.08 \times 0.03 \times \\ 0.01 \end{gathered}$ | $\begin{gathered} 0.56 \times 0.42 \times \\ 0.25 \end{gathered}$ | $\begin{gathered} 0.08 \times 0.03 \times \\ 0.01 \end{gathered}$ |
| Radiation | $\begin{gathered} \operatorname{CuK\alpha }(\lambda= \\ 1.54184) \end{gathered}$ | $\begin{gathered} \operatorname{MoK\alpha }(\lambda= \\ 0.71073) \end{gathered}$ | $\begin{gathered} \operatorname{MoK} \operatorname{Kog}(\lambda= \\ 0.71073) \end{gathered}$ |
| $2 \Theta$ range for data collection/ ${ }^{\circ}$ | 5.52 to 132.02 | 3.82 to 54.94 | 6.34 to 50.58 |
| Index ranges | $\begin{gathered} -38 \leq \mathrm{h} \leq 37,- \\ 7 \leq \mathrm{k} \leq 6,-10 \\ \leq 1 \leq 10 \end{gathered}$ | $\begin{aligned} & -8 \leq \mathrm{h} \leq 5,-9 \\ & \leq \mathrm{k} \leq 14,-25 \\ & \leq 1 \leq 23 \end{aligned}$ | $\begin{array}{r} -11 \leq \mathrm{h} \leq 11, \\ 15 \leq \mathrm{k} \leq 15, \\ 25 \leq 1 \leq 25 \end{array}$ |
| Reflections collected | 3316 | 3776 | 49023 |
| Independent reflections | $\begin{gathered} 2164[\text { Rint }= \\ 0.0334, \\ \text { Rsigma }= \\ 0.0487] \end{gathered}$ | $\begin{gathered} 3328 \text { [Rint }= \\ 0.0139, \\ \text { Rsigma }= \\ 0.0447] \end{gathered}$ | $\begin{aligned} & 9443\left[\mathrm{R}_{\text {int }}=\right. \\ & 0.0527, \\ & \mathrm{R}_{\text {sigma }}= \\ & 0.0423] \end{aligned}$ |
| Data/restraints/parameters | 2164/2/253 | 3328/0/181 | 9443/0/625 |
| Goodness-of-fit on F2 | 1.037 | 1.030 | 1.026 |
| Final R indexes $[\mathrm{I}>=2 \sigma$ (I)] | $\begin{gathered} \mathrm{R} 1=0.0802 \\ \mathrm{wR} 2=0.2116 \end{gathered}$ | $\begin{aligned} \mathrm{R} 1 & =0.0440, \\ \mathrm{wR} 2 & =0.1057 \end{aligned}$ | $\begin{gathered} \mathrm{R}_{1}=0.0631, \\ \mathrm{wR}_{2}=0.1656 \end{gathered}$ |
| Final R indexes [all data] | $\begin{aligned} & \mathrm{R} 1=0.0878 \\ & \mathrm{wR} 2=0.2256 \end{aligned}$ | $\begin{gathered} \mathrm{R} 1=0.0574, \\ \mathrm{wR} 2=0.1145 \end{gathered}$ | $\begin{gathered} \mathrm{R}_{1}=0.1220 \\ \mathrm{wR}_{2}=0.2009 \end{gathered}$ |
| Largest diff. peak/hole / e A-3 | 0.51/-0.25 | 0.77/-0.50 | 0.34/-0.23 |
| Flack parameter | -5(4) |  |  |
| Identification code | 2041466 | 2042640 | 2047804 |

We have found that the large flack parameter (3(10)) was associated with the crystal 2ea, which is most probably due to the presence of twinning nature in the crystal which was believed to cause the inversion of the structure (as observed during changing the thermal ellipsoids to anisotropy while solving the crystal in Olex2) via changing the coordinates.

The diffraction measured fraction theta full value for the crystal $\mathbf{2 i}$ was found as 0.622 , which is lower than the expected value. The reason for this error may be the crystals obtained for $\mathbf{2 i}$ were found to be twinned with a severe overlap of Bragg reflections from both domains. Data reduction was performed for both domains, while a significant number of reflections were rejected due to bad agreement between reflection profiles (mostly partially overlapped) in order to obtain a reasonable structural model.


Figure S3. ORTEP of 2a with 50\% probability (Hydrogens are omitted for clarity).


Figure S4. ORTEP of 2c with $50 \%$ probability (Hydrogens are omitted for clarity).


Figure S5. ORTEP of 2ea with 50\% probability (Hydrogens are omitted for clarity).


Figure S6. ORTEP of $\mathbf{2 g}$ with $50 \%$ probability (Hydrogens are omitted for clarity).


Figure S7. ORTEP of 2ha with 50\% probability (Hydrogens are omitted for clarity).


Figure S8. ORTEP of $\mathbf{2 i}$ with $50 \%$ probability (Hydrogens are omitted for clarity).


Figure S9. ORTEP of $\mathbf{2 k}$ with $50 \%$ probability (Hydrogens are omitted for clarity).

## Optical Study.

## Experimental details of $U V$-vis absorption and fluorescence spectroscopy.

The UV-vis absorption and fluorescence spectra of the compounds were recorded in solution state by dissolving them in chloroform at the concentration of $10^{-5} \mathrm{M}$ on Perkin Elemer Lamba 35 UV-Vis spectrometer. Fluorescence spectra of the same were recorded on Horiba JobinYvon, Fluoromax-3 (Xe-150 W, 250-900 nm). Most of the compounds absorbed light in UV region (340-390 nm) except for pyrene based compounds, which shows absorption maxima at the visible region (beyond 400 nm ). All of them emits mainly in the blue region. The only pyrene based trans-alkenes 2fa and 2ha emit in the green region, which is also observed under UV light ( 335 nm ). The relative fluorescence quantum yield ( $\Phi_{\mathrm{F}}$ ) of the fluorophores were calculated against the standard solution of Quinine sulfate in $0.1 \mathrm{M} \mathrm{H}_{2} \mathrm{SO}_{4}$, which give $\Phi_{\mathrm{F}}=$ 0.57 when excited at 350 nm . For this purpose, the solutions were diluted to $10^{-6} \mathrm{M}$ concentration range to restrict the absorbance of each compound under 0.1 , which maintain a proper balance between absorption and emission during the calculation of $\Phi_{\mathrm{F}}$. The emission spectra for all the fluorophores were recorded by exciting each of them at 350 nm . The $\Phi_{\mathrm{F}}$ values of the fluorophores were calculated from the following equation (eqn. 1).

$$
\Phi_{F}=\Phi_{Q s} X \frac{(\text { Intigrated FL Intensity)Fluorophore }}{(\text { Intigrated FL Intensity)Qs }} X \frac{\text { (o.D.)Qs }}{(\text { (o.D.)Fluorophores }} X\left(\frac{\eta_{C H C l_{3}}}{\eta_{H_{2}} \mathrm{O}}\right)^{2} .
$$

$\qquad$
Where $\Phi_{\mathrm{Qs}}$ is the fluorescence quantum yield of quinine sulfate; $\eta_{\mathrm{CHCl}_{3}}$ and $\eta_{\mathrm{H}_{2} \mathrm{O}}$ are the refractive indices of $\mathrm{CHCl}_{3}$ and $\mathrm{H}_{2} \mathrm{O}$, respectively (refractive index of $0.1 \mathrm{M} \mathrm{H}_{2} \mathrm{SO}_{4}$ is similar to water).


Figure S10. UV absorption spectra of 2c

## Quantitative analysis of HOMO coefficient.

The HOMO coefficients of $\mathbf{1 b}, \mathbf{1 g}, \mathbf{1 n}$ and $\mathbf{1 0}$ was calculated from their optimized structure via DFT calculation at B3LYP/6-31G(d) using multiwfn program. ${ }^{6}$ Individual HOMO coefficient of each atom is given in Table S3.

Table S3. HOMO coefficient of different atoms for $\mathbf{1 b}, 1 \mathrm{~g}, 1 \mathrm{n}$ and 10.

| 1b, Orbital 76 |  |  |  | 1n, Orbital68 |  | 10, Orbital64 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Atom | HOMO coefficient | Atom | HOMO coefficient | Atom | HOMO coefficient | Atom | HOMO coefficient |
| 1 | 8.027 | 1 | 0.965 | 1 | 7.346 | 1 | 8.087 |
| 2 | 1.67 | 2 | 3.415 | 2 | 1.431 | 2 | 1.732 |
| 3 | 2.14 | 3 | 2.92 | 3 | 1.999 | 3 | 2.153 |
| 4 | 8.622 | 4 | 3.515 | 4 | 7.114 | 4 | 9.03 |
| 5 | 4.618 | 5 | 1.543 | 5 | 3.35 | 5 | 5.081 |
| 6 | 0.412 | 6 | 4.755 | 6 | 0.315 | 6 | 0.446 |
| 7 | 3.906 | 7 | 9.524 | 7 | 3.117 | 7 | 4.145 |
| 8 | 2.432 | 8 | 0.946 | 8 | 1.766 | 8 | 2.675 |
| 9 | 4.947 | 9 | 0.874 | 9 | 3.689 | 9 | 5.394 |
| 10 | 0.577 | 10 | 6.842 | 10 | 0.533 | 10 | 0.579 |
| 11 | 0.301 | 11 | 2.12 | 11 | 0.243 | 11 | 0.317 |


| 12 | 0.169 | 12 | 0.224 | 12 | 0.122 | 12 | 0.186 |
| :--- | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 13 | 0.369 | 13 | 0.79 | 13 | 0.275 | 13 | 0.401 |
| 14 | 9.933 | 14 | 1.69 | 14 | 10.705 | 14 | 9.425 |
| 15 | 11.65 | 15 | 1.543 | 15 | 10.711 | 15 | 11.508 |
| 16 | 4.709 | 16 | 0.68 | 16 | 6.432 | 16 | 4.33 |
| 17 | 3.511 | 17 | 0.044 | 17 | 3.378 | 17 | 3.531 |
| 18 | 1.659 | 18 | 0.247 | 18 | 2.848 | 18 | 1.586 |
| 19 | 0.241 | 19 | 0.096 | 19 | 0.217 | 19 | 0.247 |
| 20 | 5.632 | 20 | 0.396 | 20 | 6.163 | 20 | 4.828 |
| 21 | 0.083 | 21 | 0.05 | 21 | 0.183 | 21 | 0.092 |
| 22 | 10.784 | 22 | 0.135 | 22 | 9.371 | 22 | 11.109 |
| 23 | 0.845 | 23 | 0.117 | 23 | 0.743 | 23 | 0.867 |
| 24 | 4.414 | 24 | 8.965 | 24 | 3.59 | 24 | 4.678 |
| 25 | 0.288 | 25 | 9.156 | 25 | 0.228 | 25 | 0.308 |
| 26 | 4.072 | 26 | 6.039 | 26 | 4.576 | 26 | 3.535 |
| 27 | 0.287 | 27 | 1.7 | 27 | 0.315 | 27 | 0.248 |
| 28 | 1.672 | 28 | 6.229 | 28 | 2.893 | 28 | 1.575 |
| 29 | 0.092 | 29 | 2.857 | 29 | 0.211 | 29 | 0.091 |
| 30 | 0.627 | 30 | 1.214 | 30 | 5.054 | 30 | 1.816 |
| 31 | 0.415 | 31 | 3.065 | 31 | 0.501 |  |  |
| 32 | 0.031 | 32 | 0.451 | 32 | 0.275 |  |  |
| 33 | 0.106 | 33 | 2.653 | 33 | 0.032 |  |  |
| 34 | 0.055 | 34 | 0.268 | 34 | 0.275 |  |  |
| 35 | 0.415 | 35 | 3.147 |  |  |  |  |
| 36 | 0.055 | 36 | 7.958 |  |  |  |  |
| 37 | 0.106 | 37 | 0.195 |  |  |  |  |
| 38 | 0.031 | 38 | 1.498 |  |  |  |  |
| 39 | 0.057 | 39 | 0.207 |  |  |  |  |
| 40 | 0.019 | 40 | 0.234 |  |  |  |  |
| 41 | 0.019 | 41 | 0.63 |  |  |  |  |
| 42 | 0.003 | 42 | 0.103 |  |  |  |  |

The electronic states involved during the desired electronic transition of 2aS, 2aSe, 2dS and 2dSe were determined via TD-DFT calculation at B3LYP/6-31G. The HOMO coefficients of different atoms of those compounds were calculated using multiwfn program ${ }^{6}$ at the ground states of those particular transitions. The individual HOMO coefficient of each atom is given in Table S4.

Table S4. Molecular Orbital diagram at ground states of 2aS, 2aSe, 2dS and 2dSe for different electronic transitions.


| Atom | HOMO coefficient | Atom | HOMO coefficient | Atom | HOMO coefficient | Atom | HOMO coefficient |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 2.456 | 1 | 12.562 | 1 | 24.315 | 1 | 2.764 |
| 2 | 12.887 | 2 | 2.703 | 2 | 0.274 | 2 | 4.208 |
| 3 | 1.565 | 3 | 11.006 | 3 | 2.177 | 3 | 10.913 |
| 4 | 6.164 | 4 | 6.268 | 4 | 4.071 | 4 | 3.78 |
| 5 | 0.46 | 5 | 0.432 | 5 | 9.041 | 5 | 1.498 |
| 6 | 2.726 | 6 | 8.528 | 6 | 8.193 | 6 | 6.209 |
| 7 | 10.164 | 7 | 1.23 | 7 | 0.615 | 7 | 0.433 |
| 8 | 1.893 | 8 | 3.298 | 8 | 9.117 | 8 | 1.284 |
| 9 | 0.072 | 9 | 0.273 | 9 | 2.45 | 9 | 4.658 |
| 10 | 8.534 | 10 | 1.088 | 10 | 0.256 | 10 | 0.343 |
| 11 | 0.662 | 11 | 0.065 | 11 | 0.172 | 11 | 4.842 |
| 12 | 5.974 | 12 | 2.826 | 12 | 6.426 | 12 | 1.089 |
| 13 | 0.437 | 13 | 0.227 | 13 | 0.493 | 13 | 0.065 |
| 14 | 2.706 | 14 | 2.362 | 14 | 4.342 | 14 | 4.467 |
| 15 | 0.124 | 15 | 0.179 | 15 | 0.174 | 15 | 3.638 |
| 16 | 10.85 | 16 | 1.441 | 16 | 0.159 | 16 | 0.269 |
| 17 | 5.509 | 17 | 4.541 | 17 | 0.181 | 17 | 3.204 |
| 18 | 6.194 | 18 | 2.163 | 18 | 0.044 | 18 | 0.257 |
| 19 | 0.428 | 19 | 0.138 | 19 | 1.957 | 19 | 2.391 |
| 20 | 1.543 | 20 | 6.437 | 20 | 0.08 | 20 | 0.18 |
| 21 | 0.065 | 21 | 0.534 | 21 | 3.261 | 21 | 8.872 |
| 22 | 8.121 | 22 | 1.312 | 22 | 1.193 | 22 | 6.346 |
| 23 | 0.643 | 23 | 0.059 | 23 | 0.055 | 23 | 0.526 |
| 24 | 4.128 | 24 | 4.697 | 24 | 3.956 | 24 | 2.164 |
| 25 | 0.346 | 25 | 0.342 | 25 | 0.268 | 25 | 0.139 |
| 26 | 4.212 | 26 | 3.909 | 26 | 5.676 | 26 | 2.938 |
| 27 | 0.247 | 27 | 4.272 | 27 | 0.427 | 27 | 0.236 |
| 28 | 0.19 | 28 | 3.724 | 28 | 0.036 | 28 | 1.405 |
| 29 | 0.036 | 29 | 0.297 | 29 | 0.002 | 29 | 0.075 |
| 30 | 0.039 | 30 | 1.444 | 30 | 2.241 | 30 | 12.571 |
| 31 | 0.002 | 31 | 0.084 | 31 | 5.86 | 31 | 1.283 |
| 32 | 0.18 | 32 | 4.893 | 32 | 0.467 | 32 | 0.058 |
| 33 | 0.152 | 33 | 1.49 | 33 | 1.727 | 33 | 3.384 |
| 34 | 0.011 | 34 | 0.082 | 34 | 0.07 | 34 | 0.281 |
| 35 | 0.118 | 35 | 3.186 | 35 | 0.15 | 35 | 1.486 |
| 36 | 0.085 | 36 | 0.228 | 36 | 0.012 | 36 | 0.089 |
| 37 | 0.023 | 37 | 0.543 | 37 | 0.023 | 37 | 0.537 |
| 38 | 0.013 | 38 | 0.351 | 38 | 0.017 | 38 | 0.35 |
| 39 | 0.002 | 39 | 0.048 | 39 | 0.002 | 39 | 0.047 |
| 40 | 0.003 | 40 | 0.087 | 40 | 0.001 | 40 | 0.025 |
| 41 | 0.001 | 41 | 0.026 | 41 | 0.005 | 41 | 0.088 |
| 42 | 0.018 | 42 | 0.368 | 42 | 0.008 | 42 | 0.356 |
| 43 | 0.002 | 43 | 0.048 | 43 | 0.001 | 43 | 0.093 |
| 44 | 0.002 | 44 | 0.029 | 44 | 0 | 44 | 0.028 |


| 45 | 0.006 | 45 | 0.097 | 45 | 0.002 | 45 | 0.047 |
| :--- | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 46 | 0.002 | 46 | 0.05 | 46 | 0.003 | 46 | 0.051 |
| 47 | 0.001 | 47 | 0.017 | 47 | 0 | 47 | 0.003 |
| 48 | 0 | 48 | 0.015 | 48 | 0.001 | 48 | 0.016 |
| 49 | 0 | 49 | 0.003 | 49 | 0.001 | 49 | 0.018 |


|  |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 2dS, Orbital102 |  |  |  |  |  |  |  |
| HOMO-1 |  |  |  |  |  |  |  |


| 32 | 4.643 | 32 | 3.534 | 32 | 9.395 |
| :---: | :---: | :---: | :---: | :---: | :---: |
| 33 | 0.414 | 33 | 0.284 | 33 | 0.095 |
| 34 | 0.093 | 34 | 0.067 | 34 | 3.882 |
| 35 | 0.092 | 35 | 0.078 | 35 | 0.503 |
| 36 | 0.714 | 36 | 9.46 | 36 | 0.262 |
| 37 | 0.272 | 37 | 0.096 | 37 | 0.753 |
| 38 | 2.37 | 38 | 3.847 | 38 | 0.287 |
| 39 | 0.582 | 39 | 0.489 | 39 | 0.185 |
| 40 | 0.339 | 40 | 0.259 | 40 | 0.025 |
| 41 | 0.099 | 41 | 0.061 | 41 | 0.013 |
| 42 | 0.034 | 42 | 0.026 | 42 | 0.046 |
| 43 | 0.038 | 43 | 0.028 | 43 | 0.191 |
| 44 | 0.027 | 44 | 0.759 | 44 | 0.05 |
| 45 | 0.16 | 45 | 0.283 | 45 | 0.015 |
| 46 | 0.043 | 46 | 0.024 | 46 | 0.026 |
| 47 | 0.006 | 47 | 0.004 | 47 | 0.027 |
| 48 | 0.006 | 48 | 0.004 | 48 | 0.008 |
| 49 | 0.003 | 49 | 0.002 | 49 | 0.009 |
| 50 | 0.021 | 50 | 0.012 | 50 | 0.002 |
| 51 | 0.003 | 51 | 0.002 | $\mathbf{5 1}$ | $\mathbf{2 . 2 1 6}$ |

NMR spectra of Products (2a-n):


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Figure S11. (i) ${ }^{1} \mathrm{H}\left(400 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ and (ii) ${ }^{13} \mathrm{C}\left\{{ }^{1} \mathrm{H}\right\}\left(125 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ NMR Spectra of 2a

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Figure S12. (i) ${ }^{1} \mathrm{H}\left(400 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ and (ii) ${ }^{2} \mathrm{H}\left(77 \mathrm{MHz}, \mathrm{CHCl}_{3}\right)$ NMR Spectra of deuterated product 2a-1D and (iii) Comparison of ${ }^{1} \mathrm{H}\left(400 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ spectra of $\mathbf{2 a}$ and 2a-1D


(iii)

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Figure S13. (i) ${ }^{1} \mathrm{H}\left(500 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$, (ii) ${ }^{13} \mathrm{C}\left\{{ }^{1} \mathrm{H}\right\}\left(125 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ and (iii) ${ }^{77} \mathrm{Se}\left\{{ }^{1} \mathrm{H}\right\}(95$ $\mathrm{MHz}, \mathrm{CDCl}_{3}$ ) NMR Spectra of $\mathbf{2 b}$


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Figure S14. (i) ${ }^{1} \mathrm{H}\left(400 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ and (ii) ${ }^{13} \mathrm{C}\left\{{ }^{1} \mathrm{H}\right\}\left(100 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ NMR Spectra of 2c

(ii)
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Figure S15. (i) ${ }^{1} \mathrm{H}\left(400 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ and (ii) ${ }^{77} \mathrm{Se}\left\{{ }^{1} \mathrm{H}\right\}\left(95 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ NMR Spectra of mixture of 2c and 2ca

(iii)

Figure S16. (i) ${ }^{1} \mathrm{H}\left(400 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$, (ii) ${ }^{13} \mathrm{C}\left\{{ }^{1} \mathrm{H}\right\}\left(125 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ and (iii) ${ }^{77} \mathrm{Se}\left\{{ }^{1} \mathrm{H}\right\}(95$ $\mathrm{MHz}, \mathrm{CDCl}_{3}$ ) NMR Spectra of $\mathbf{2 d}$



Figure S17. (i) ${ }^{1} \mathrm{H}\left(400 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ and (ii) ${ }^{13} \mathrm{C}\left\{{ }^{1} \mathrm{H}\right\}\left(100 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ NMR Spectra of 2ea

(ii)





Figure S18. (i) ${ }^{1} \mathrm{H}\left(400 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ and (ii) ${ }^{13} \mathrm{C}\left\{{ }^{1} \mathrm{H}\right\}\left(100 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ NMR Spectra of $2 f a$



2fa-2D




(iii)


Figure S19. (i) ${ }^{1} \mathrm{H}\left(400 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ and (ii) ${ }^{2} \mathrm{H}\left(77 \mathrm{MHz}, \mathrm{CHCl}_{3}\right)$ NMR Spectra of 2fa-2D and (iii) Comparison of ${ }^{1} \mathrm{H}\left(400 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ of $\mathbf{2 f}$ and $\mathbf{2 f a}$


Figure S20. ${ }^{1} \mathrm{H}\left(400 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ NMR Spectra of (i) product mixture $(\mathbf{1 g + 2 g})(1: 2)$ and (ii) pure $\mathbf{2 g}$.


(i)





(ii)





Figure S21. ${ }^{1} \mathrm{H}\left(400 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ and ${ }^{13} \mathrm{C}\left\{{ }^{1} \mathrm{H}\right\}\left(100 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ NMR Spectra of 2ha


Figure S22. (i) ${ }^{1} \mathrm{H}\left(400 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ and (ii) ${ }^{13} \mathrm{C}\left\{{ }^{1} \mathrm{H}\right\}\left(125 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ NMR Spectra of 2i

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(ii)



Figure S23. (i) ${ }^{1} \mathrm{H}\left(400 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ and (ii) ${ }^{13} \mathrm{C}\left\{{ }^{1} \mathrm{H}\right\}\left(100 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ NMR Spectra of 2ja
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(ii)

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Figure S24. (i) ${ }^{1} \mathrm{H}\left(400 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ and (ii) ${ }^{13} \mathrm{C}\left\{{ }^{1} \mathrm{H}\right\}\left(100 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ NMR Spectra of


Figure S25. (i) ${ }^{1} \mathrm{H}\left(400 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ and (ii) ${ }^{13} \mathrm{C}\left\{{ }^{1} \mathrm{H}\right\}\left(100 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ NMR Spectra of $2 \mathbf{l}$

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Figure S26. (i) ${ }^{1} \mathrm{H}\left(400 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ and (ii) ${ }^{13} \mathrm{C}\left\{{ }^{1} \mathrm{H}\right\}\left(100 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ NMR Spectra of $\mathbf{2 m}$
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Figure S27. (i) ${ }^{1} \mathrm{H}\left(400 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ and (ii) ${ }^{13} \mathrm{C}\left\{{ }^{1} \mathrm{H}\right\}\left(100 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ NMR Spectra of 2n



(ii)商楞



Figure S28. (i) ${ }^{1} \mathrm{H}\left(400 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$, (ii) ${ }^{13} \mathrm{C}\left\{{ }^{1} \mathrm{H}\right\}\left(100 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ and (iii) ${ }^{19} \mathrm{~F}\left\{{ }^{1} \mathrm{H}\right\}(375$ $\mathrm{MHz}, \mathrm{CDCl}_{3}$ ) NMR Spectra of $\mathbf{2 0}$

## NMR spectra of arylethynyl substituted polyarenes (1a-n).



Figure S29. ${ }^{1} \mathrm{H}\left(400 \mathrm{MHz}, \mathrm{CDCl}_{3}\right) \mathrm{NMR}$ Spectra of $\mathbf{1 a}$


Figure S30. ${ }^{1} \mathrm{H}$ NMR ( $400 \mathrm{MHz}, \mathrm{CDCl}_{3}$ ) Spectra of $\mathbf{1 b}$


Figure S31. ${ }^{1} \mathrm{H}$ NMR ( $400 \mathrm{MHz}, \mathrm{CDCl}_{3}$ ) Spectra of $\mathbf{1 c}$

(ii)


Figure S32. (i) ${ }^{1} \mathrm{H}\left(400 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ and (ii) ${ }^{13} \mathrm{C}\left\{{ }^{1} \mathrm{H}\right\}\left(100 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ NMR Spectra of 1d



Figure S33. (i) ${ }^{1} \mathrm{H}\left(400 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ and (ii) ${ }^{13} \mathrm{C}\left\{{ }^{1} \mathrm{H}\right\}\left(100 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ NMR Spectra of $\mathbf{1 f}$

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Figure S34. (i) ${ }^{1} \mathrm{H}\left(400 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ and (ii) ${ }^{13} \mathrm{C}\left\{{ }^{1} \mathrm{H}\right\}\left(100 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ NMR Spectra of $\mathbf{1 g}$

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Figure S35. (i) ${ }^{1} \mathrm{H}\left(400 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ and (ii) ${ }^{13} \mathrm{C}\left\{{ }^{1} \mathrm{H}\right\}\left(100 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ NMR Spectra of $\mathbf{1 h}$
(i)


(ii)



Figure S36. (i) ${ }^{1} \mathrm{H}\left(400 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ and (ii) ${ }^{13} \mathrm{C}\left\{{ }^{1} \mathrm{H}\right\}\left(100 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ NMR Spectra of $\mathbf{1 i}$



Figure S37. (i) ${ }^{1} \mathrm{H}\left(400 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ and (ii) ${ }^{13} \mathrm{C}\left\{{ }^{1} \mathrm{H}\right\}\left(100 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ NMR Spectra of $\mathbf{1} \mathbf{j}$


Figure S38. ${ }^{1} \mathrm{H}$ NMR ( $400 \mathrm{MHz}, \mathrm{CDCl}_{3}$ ) Spectra of $\mathbf{1 k}$





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Figure S39. ${ }^{1} \mathrm{H}\left(400 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ and ${ }^{13} \mathrm{C}\left\{{ }^{1} \mathrm{H}\right\}\left(100 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ NMR Spectra of $\mathbf{1 1}$


Figure S40. (i) ${ }^{1} \mathrm{H}\left(400 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ and (ii) ${ }^{13} \mathrm{C}\left\{{ }^{1} \mathrm{H}\right\}\left(100 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ NMR Spectra of $\mathbf{1 m}$

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Figure S41. ${ }^{1} \mathrm{H}$ NMR ( $400 \mathrm{MHz}, \mathrm{CDCl}_{3}$ ) Spectra of $\mathbf{1 n}$


Figure S42. ${ }^{1} \mathrm{H}$ NMR Spectra ( $400 \mathrm{MHz}, \mathrm{CDCl}_{3}$ ) of $\mathbf{1 0}$

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Figure S 43 . ${ }^{1} \mathrm{H}\left(400 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ NMR Spectra obtained during selenocyclization of $\mathbf{1 c}$ in 1.2 ml of (a) $1 \%$ (b) $2 \%$ (c) $3 \% ~(\mathrm{v} / \mathrm{v}$ ) water in NMP and (d) 2 ml of $15 \% ~(\mathrm{v} / \mathrm{v})$ water in NMP


Figure $\mathrm{S} 44 .{ }^{1} \mathrm{H}\left(400 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ NMR Spectra for products formed during selenocyclization of 1a in 2 ml of $2 \%(\mathrm{v} / \mathrm{v})$ water in NMP





Figure S45. (i) ${ }^{1} \mathrm{H}\left(400 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ and (ii) ${ }^{13} \mathrm{C}\left\{{ }^{1} \mathrm{H}\right\}\left(100 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ NMR Spectra of 2aa
(i)


(iii) $\underbrace{\text { orongion }}$


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Figure S46. ${ }^{1} \mathrm{H}\left(400 \mathrm{MHz}, \mathrm{CDCl}_{3}\right)$ NMR Spectra of products obtained during selenocyclization of $\mathbf{1 a}$ at different cycles (i) first cycle (ii) second cycle and (iii) third cycle

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