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Supporting Information

Modulating the Enantiodiscrimination Features of Inherently Chiral Selectors by Molecular Design: A HPLC and Voltammetry Study Case with Atropisomeric 2,2'-Biindole-Based Monomers and Oligomer Films

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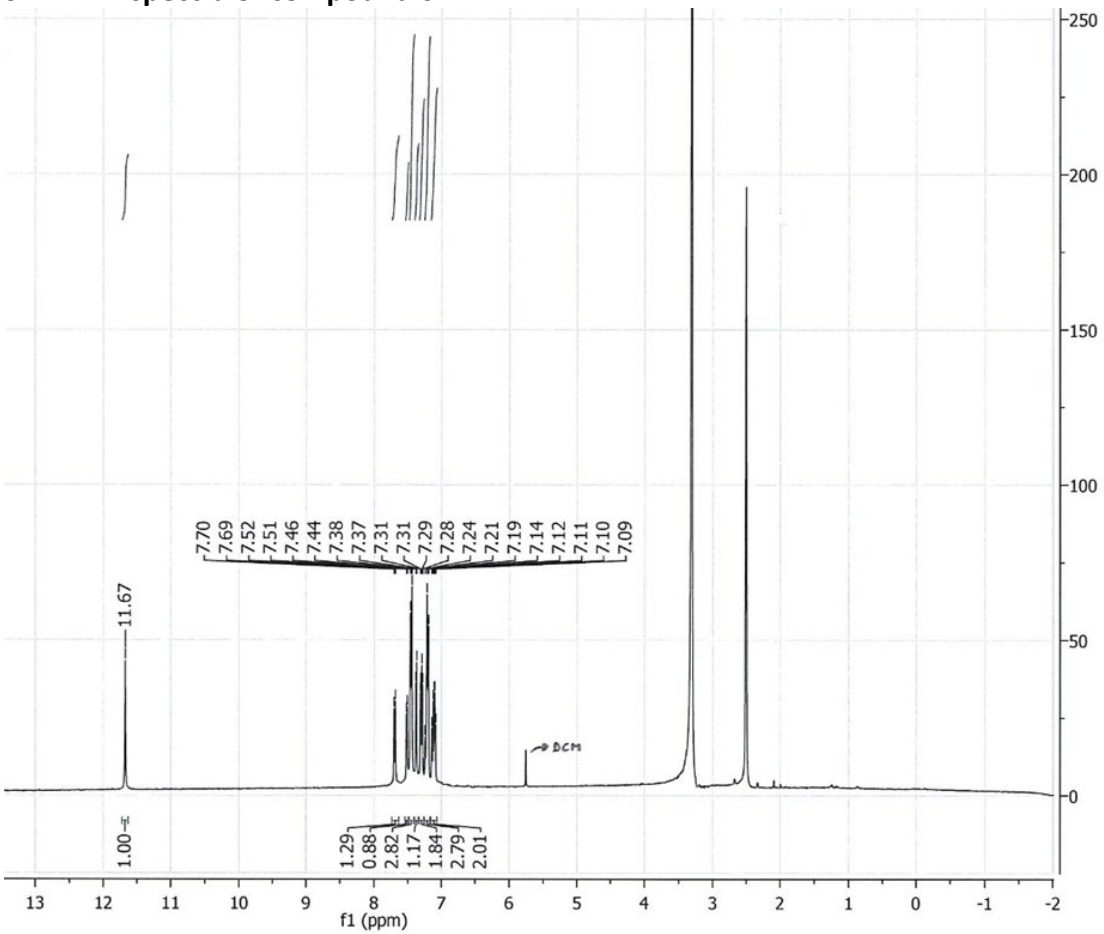
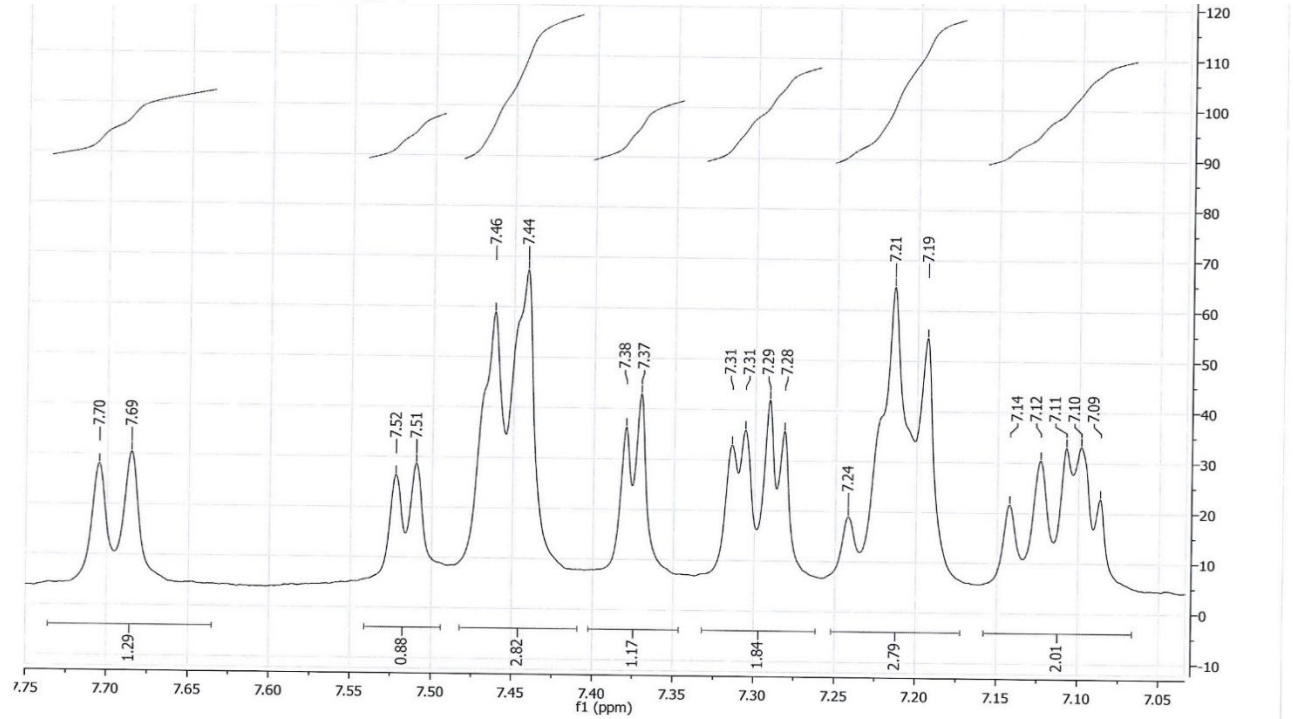
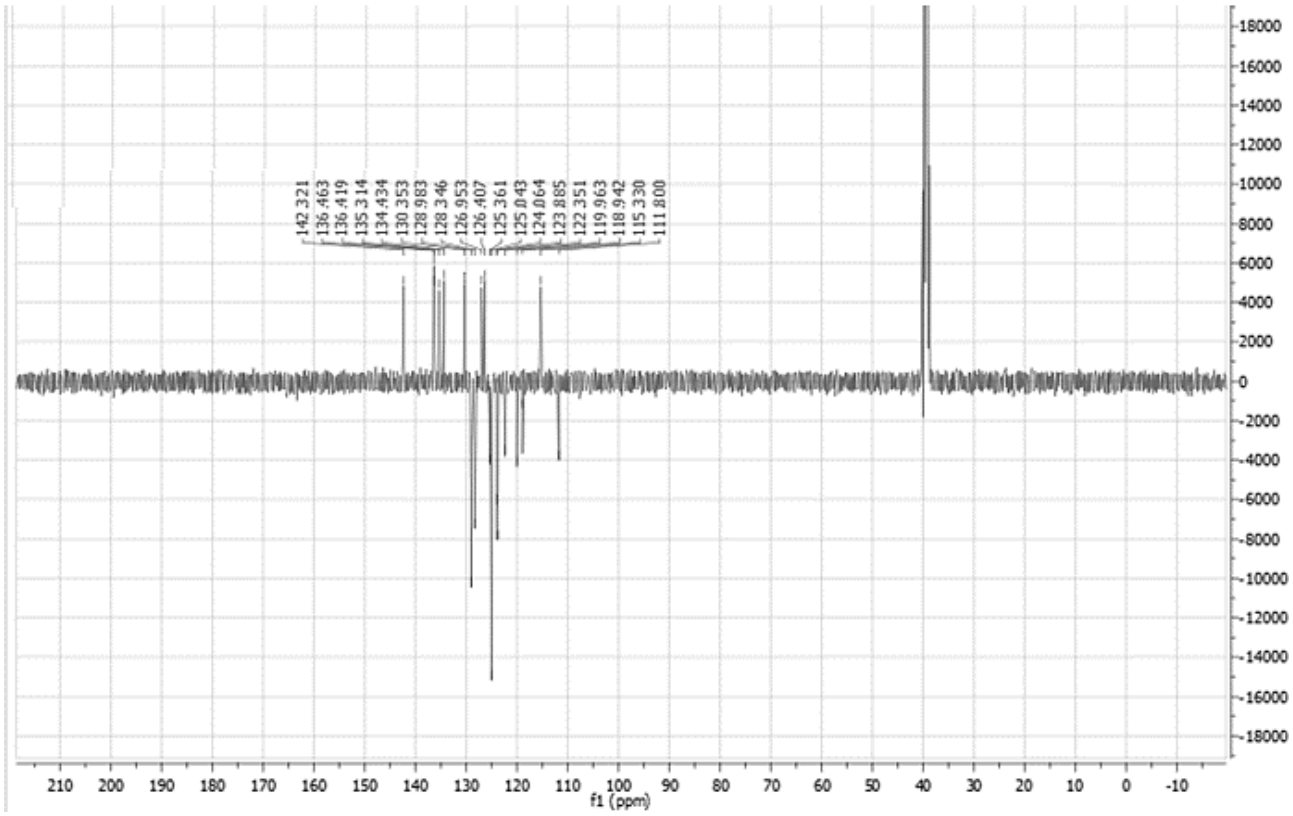
SUPPORTING INFORMATION

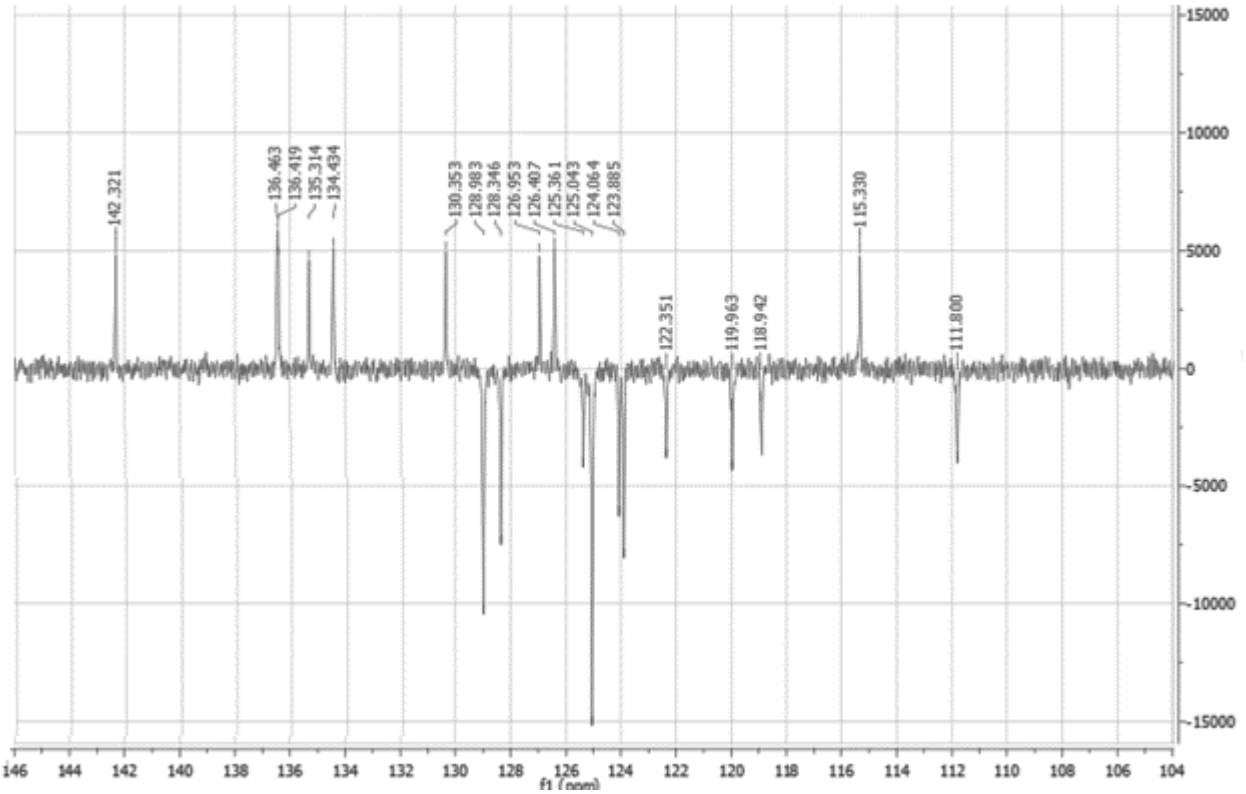
SI.1.1 ^{1}H spectra of compound 6



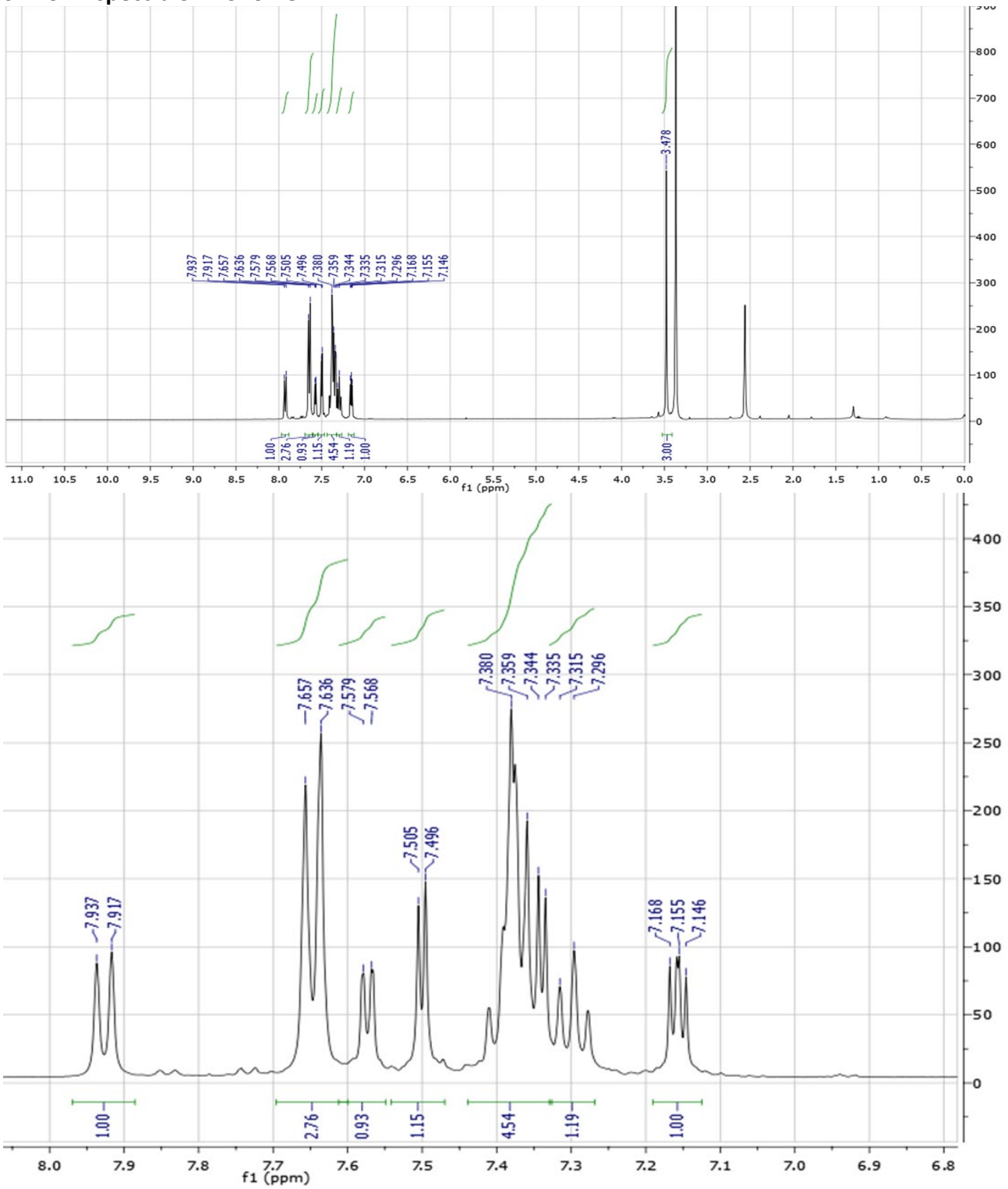


SI.1.2 ^{13}C NMR spectra of compound 6

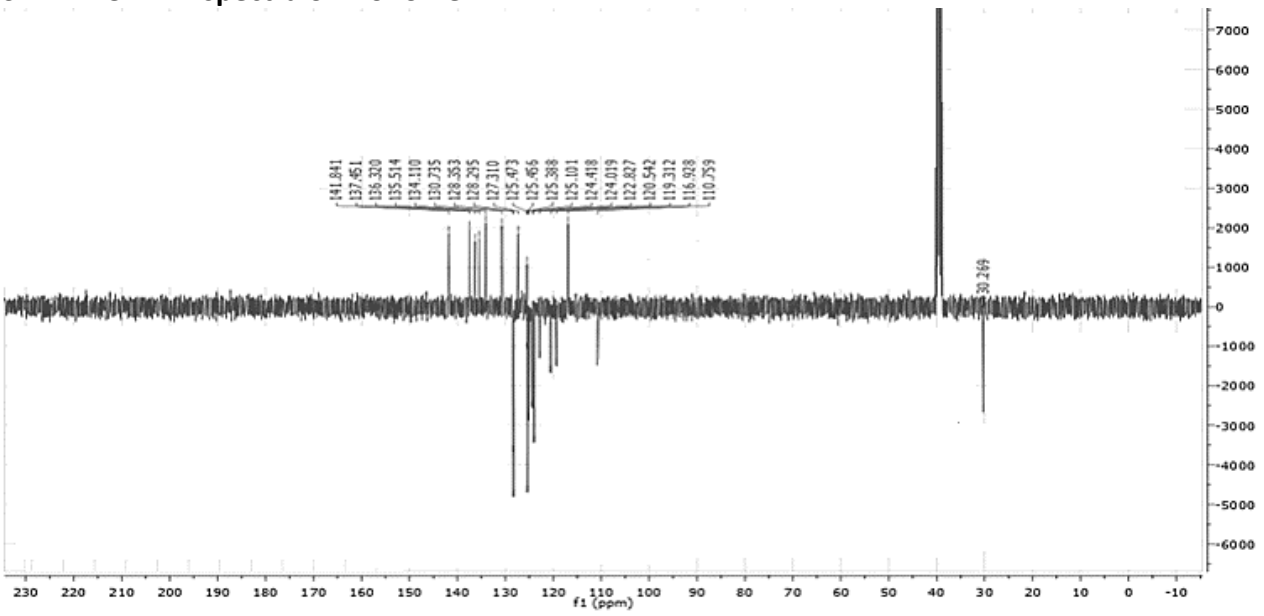




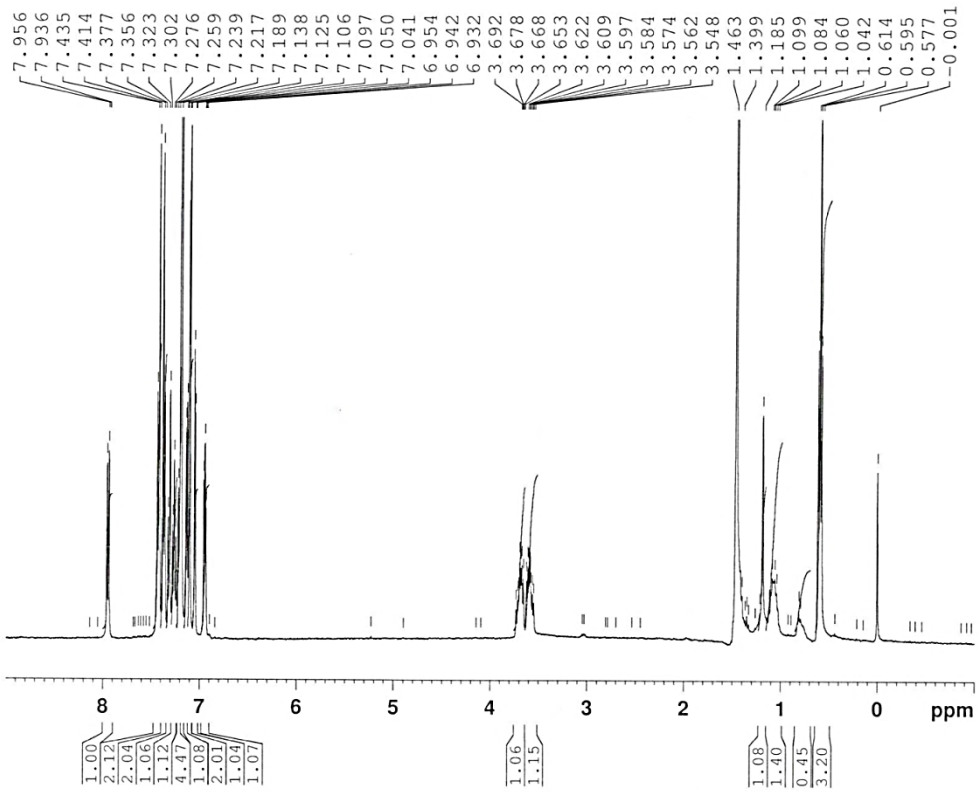
SI.1.3 ^{1}H spectra of monomer 1

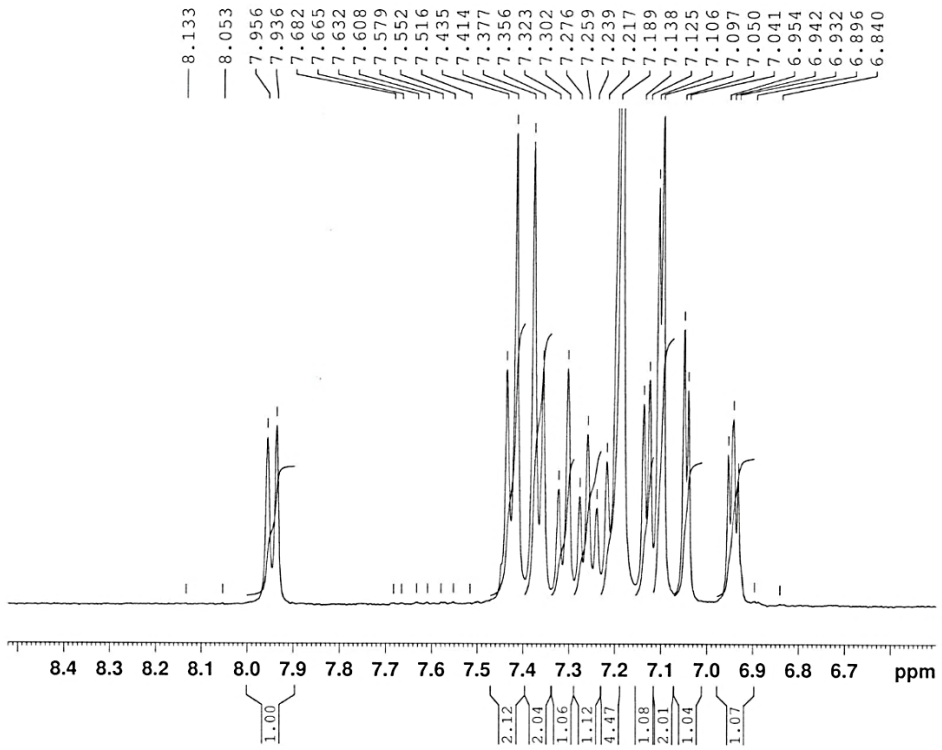


SI.1.4 ^{13}C NMR spectra of monomer 1

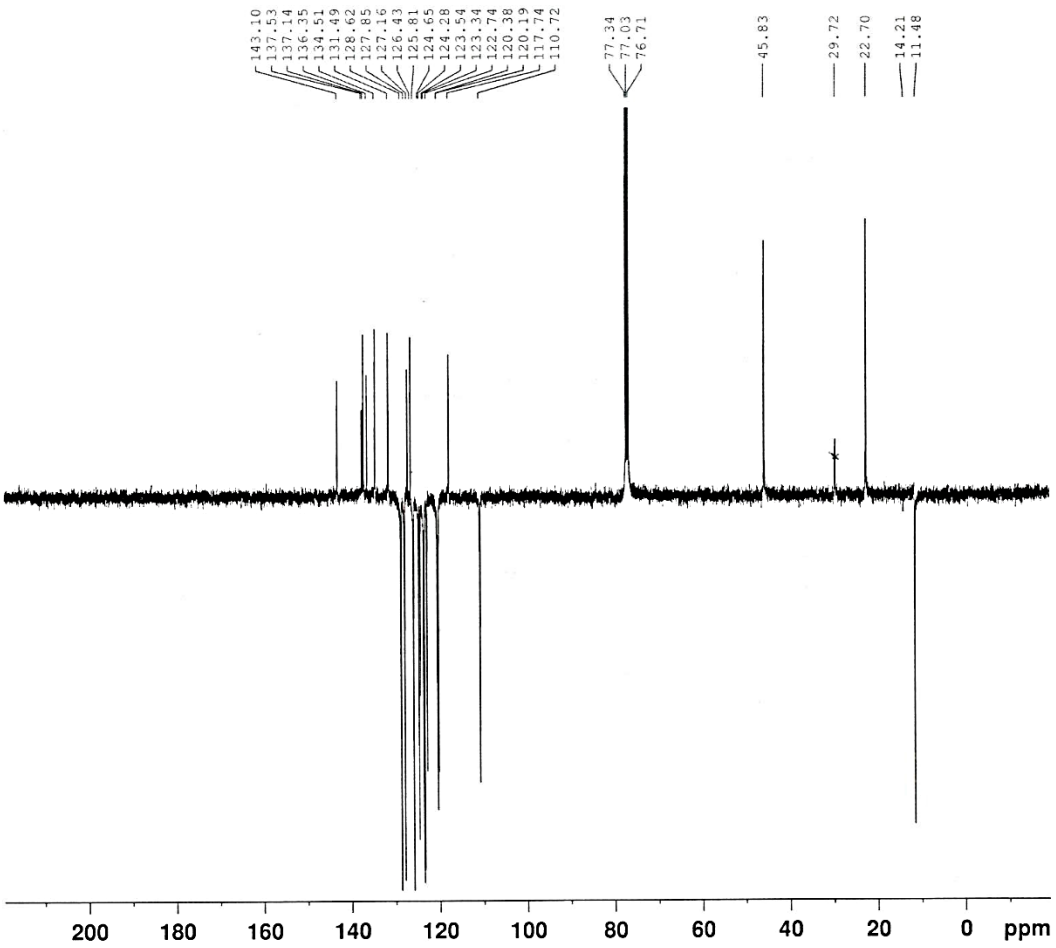


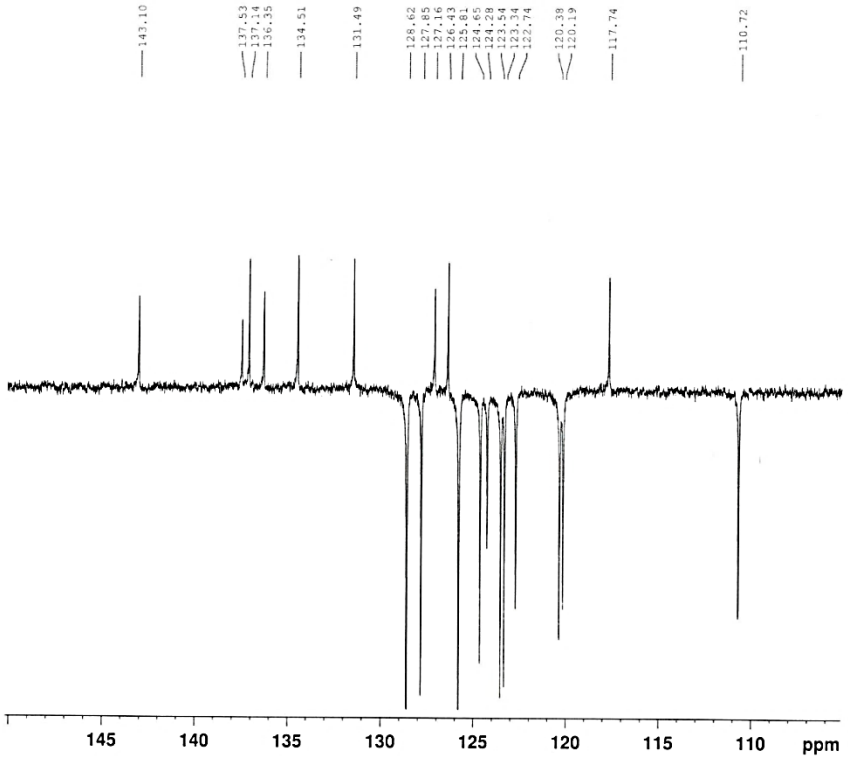
SI.1.5 ^{1}H and ^{13}C NMR spectra of monomer 2



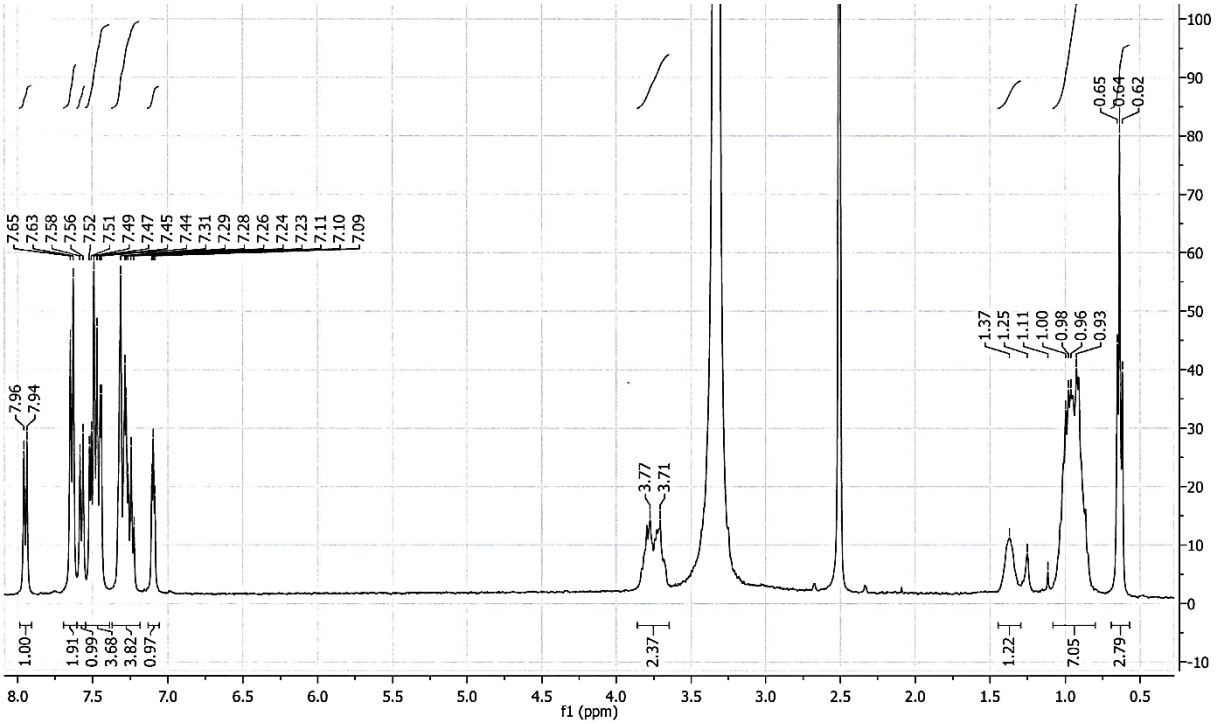


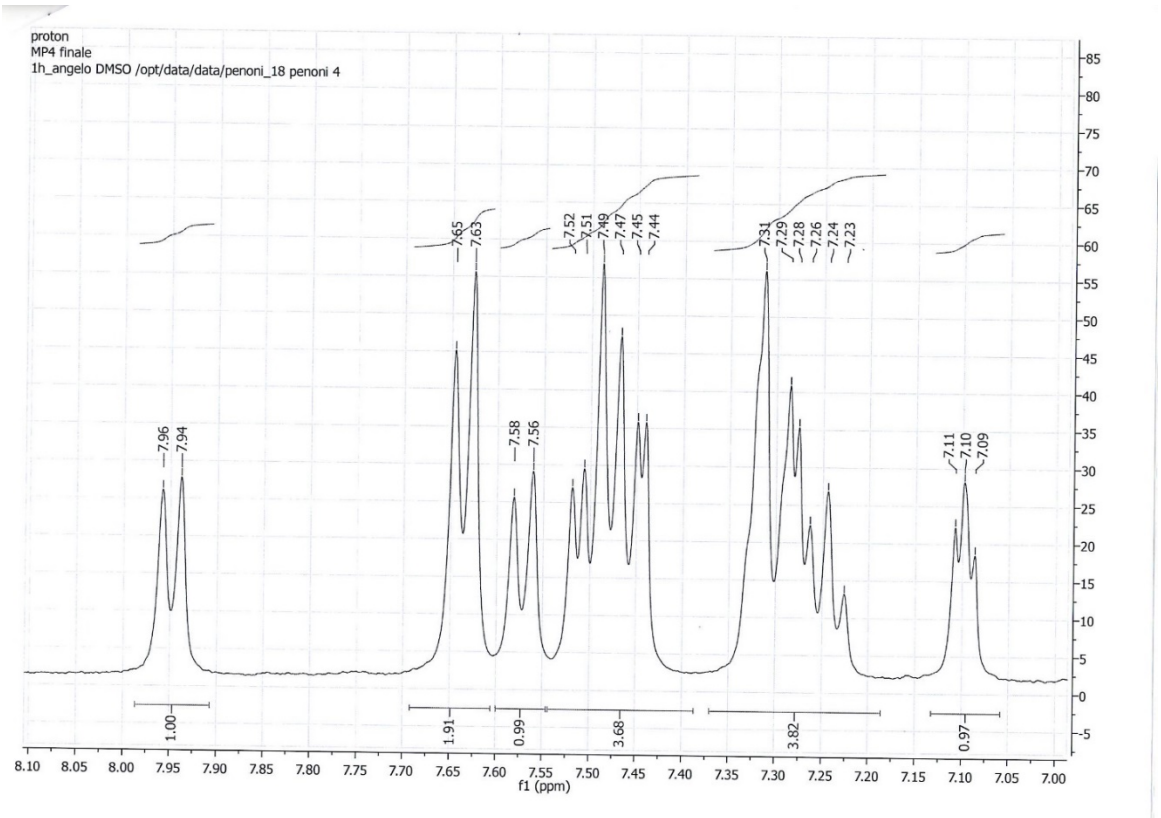
SI.1.6 ^{13}C NMR spectra of monomer 2



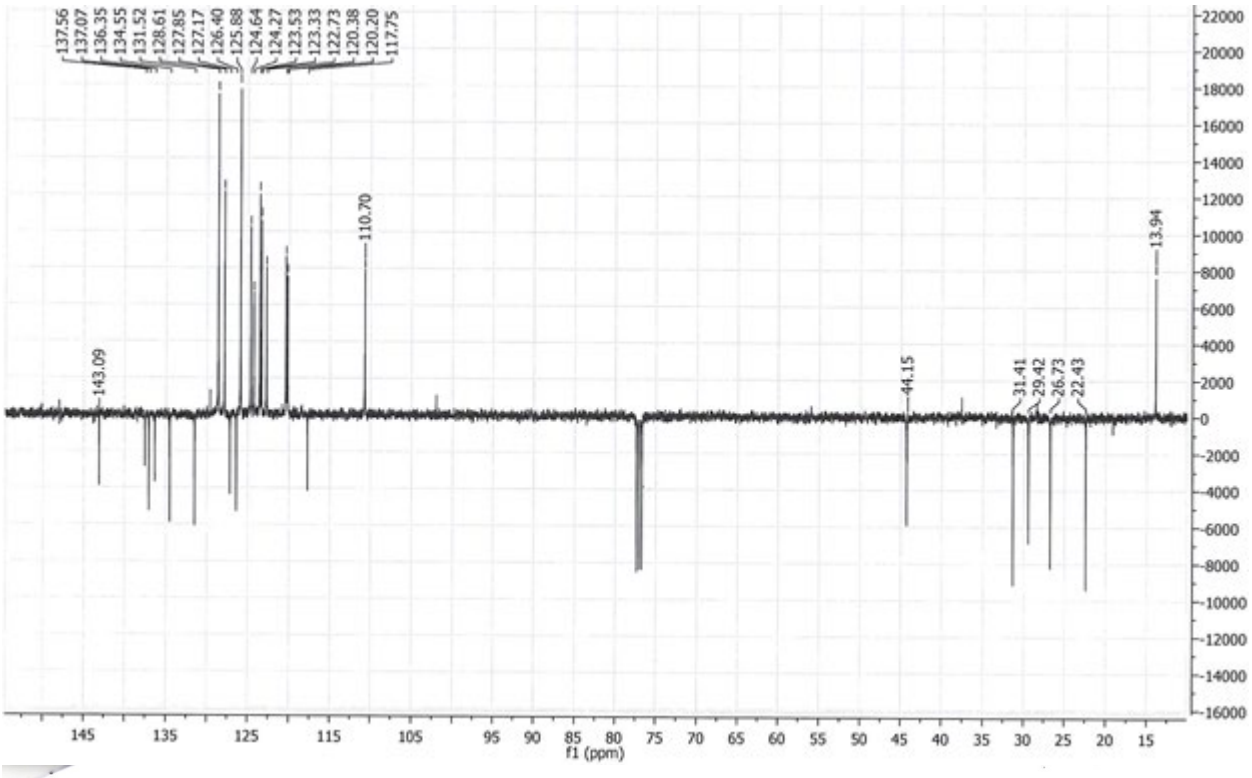


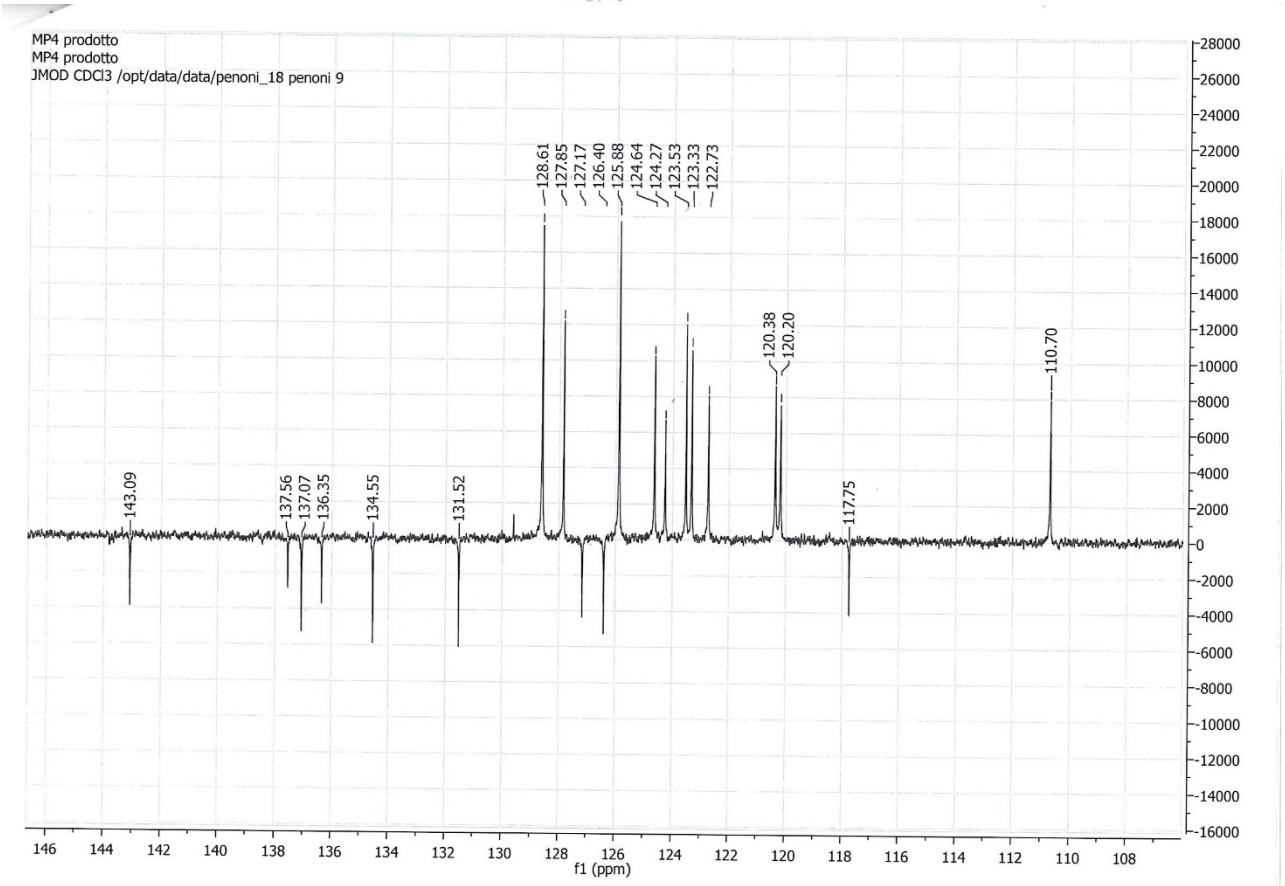
SI.1.7 ^{1}H NMR spectra of monomer 3



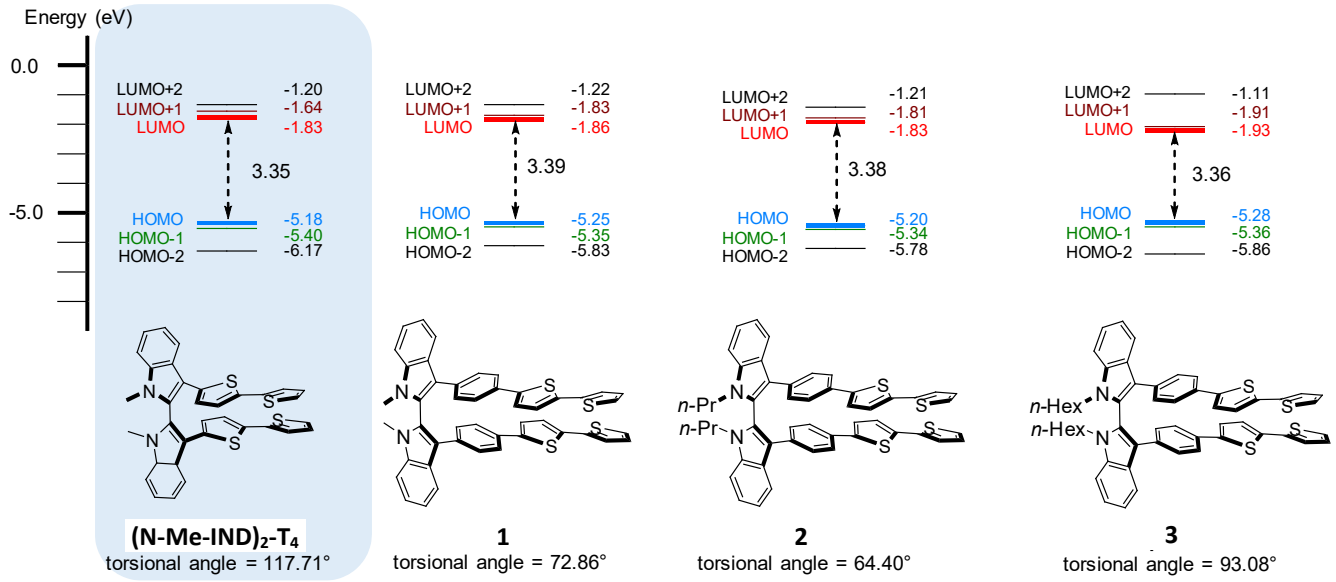


SI.1.8 ^{13}C NMR spectra of monomer 3





SI.2 Energy levels, torsional angles and racemization barriers and pathways from DFT calculations for 1,2,3 *vs* parent (N-Me-IND)$_2$-T$_4$.



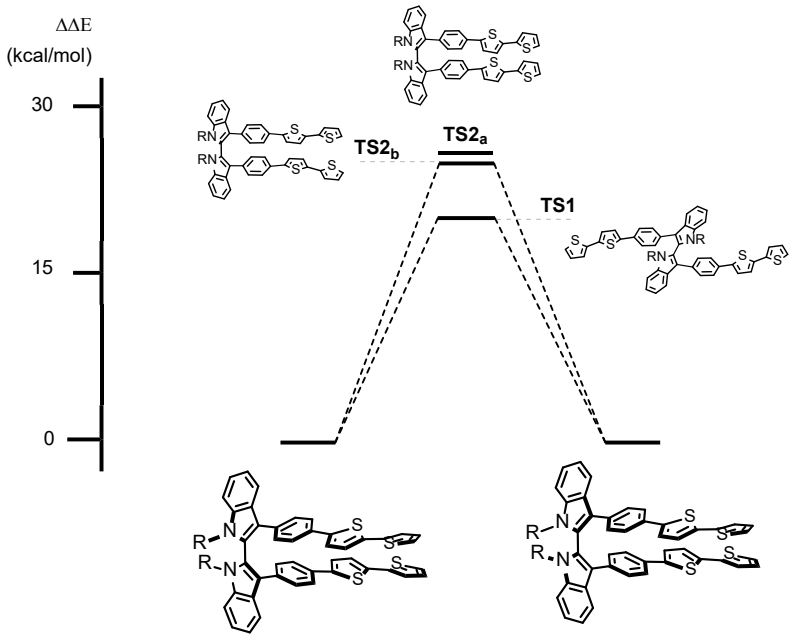


FIgure SI3. Top: Energy levels and torsional angles from DFT calculations for **1,2,3** *vs* parent (N-Me-IND)$_2$-T$_4$. B3LYP/6-311+g(3df,3pd) // B3LYP/6-31G(d,p) level of theory. Bottom: Schematic racemization pathway.

DFT computational studies performed on **1,2** and **3** also provide interesting clues concerning preferred monomer conformations, also in relationship to the racemization barrier. (Figure SI3 bottom)

- The thiophenyl pendant units connected to the 2,2'-biindole scaffold are oriented in a *s*-trans conformation, in an orthogonal arrangement respect to the bi-indole backbone.
- Two possible transition states for racemization were located for all of the three above compounds, *i.e.* **TS1**, related to a rotation process in which the two coplanar aromatic pendants face the 2,2'-biindole scaffold in a transoid arrangement (s-trans) and **TS2**, where the two bithiophenyl chains face the bisindole backbone in a cisoid arrangement (*s*-cis). As found, **TS1** is generally more accessible

than **TS2** and the torsional barrier around the bond interconnecting the NMe-indole rings, calculated by B3LYP/6-311G+(3df,3pd) // B3LYP/6-31G(d,p) level from such ground energy level, range between 24-26 Kcal mol^{-1} (Figure SI3 bottom).

- As expected, in each aromatic pendant, the two thiophene rings adopted a *head-to-tail* (HT) configuration, which is usually preferred to a *tail-to-tail* (TT) configuration. However, since in the case of **TS2** the two aromatic pendants are faced and closed together, two more transition states have been identified, where the two HT thiophene units can be oriented in a specular (**TS2a**) or in an opposite conformation (**TS2b**). Energies associate to those transition states are reported in Table SI1

	1 $\Delta\Delta G$ (kcal/mol)	**1** $\Delta\Delta G$ (kcal/mol)	**1** $\Delta\Delta G$ (kcal/mol)
TS1	24.74	26.60	25.23
TS2a	29.08	34.77	33.25
TS2b	29.19	33.52	32.04

Table SI1: A comparison of torsional energy barrier for compounds B,C, D calculated at B3LYP/6-311+g(3df,3pd) // B3LYP/6-31G(d,p) level of theory

XYZ geometries

Global minimum$_{(compoundB)}$

C	4.21200	-0.09300	-5.25800
C	5.24300	-1.03900	-5.08300
C	5.63200	-1.45000	-3.81400
C	4.95400	-0.90100	-2.71900
C	3.90000	0.03900	-2.87200
C	3.54400	0.45100	-4.16900
N	5.14400	-1.11600	-1.37000
C	4.23400	-0.32700	-0.65700
C	3.45300	0.39700	-1.54700
C	3.71500	-0.56500	5.38800
C	4.94000	0.12700	5.30800
C	5.51400	0.43200	4.08000
C	4.82300	0.03800	2.92800
C	3.57800	-0.64200	2.98300
C	3.03400	-0.95500	4.24200
N	5.16800	0.19400	1.60100
C	4.16700	-0.37800	0.80700
C	3.17400	-0.90300	1.62200
C	6.08300	-2.07000	-0.81300
C	6.33500	0.91700	1.13400
C	2.37500	1.34300	-1.21300
C	-0.43800	-2.93300	0.39300
C	0.79500	-3.20200	-0.23100
C	1.95600	-2.54600	0.15700
C	1.94700	-1.59200	1.19000
C	0.71600	-1.32700	1.81600
C	-0.44800	-1.97900	1.42700
C	-1.65400	-3.62700	-0.03500
C	-1.92600	-4.21400	-1.25200
C	-3.20800	-4.81200	-1.33000
C	-3.94800	-4.69300	-0.17200
S	-3.02800	-3.82000	1.04100
C	-5.28300	-5.17500	0.11100
C	-5.94400	-5.24700	1.31900
C	-7.25800	-5.78600	1.22000
C	-7.59900	-6.12700	-0.05900
S	-6.31500	-5.78200	-1.17600
H	2.76200	1.18900	-4.31500
H	3.94200	0.21800	-6.26300
H	5.74700	-1.44700	-5.95400
H	6.43800	-2.16600	-3.68100

H	6.46600	0.95200	4.02200
H	5.44800	0.42000	6.22200
H	3.30000	-0.80000	6.36400
H	2.09800	-1.49900	4.31500
H	7.11900	-1.73500	-0.94100
H	5.88100	-2.19400	0.25100
H	5.97100	-3.04200	-1.30400
H	7.26000	0.38000	1.37300
H	6.27000	1.04500	0.05300
H	6.38000	1.90800	1.59800
H	0.84700	-3.95900	-1.00800
H	2.89200	-2.79500	-0.33200
H	0.66700	-0.57100	2.59300
H	-1.38500	-1.72000	1.91100
H	-1.22800	-4.19500	-2.08100
H	-3.57800	-5.32000	-2.21400
H	-5.49400	-4.93300	2.25400
H	-7.91900	-5.92000	2.06900
H	-8.52200	-6.55800	-0.41900
C	2.50500	2.28200	-0.17400
C	1.48100	3.16900	0.13100
C	0.28100	3.17700	-0.60500
C	0.15000	2.24100	-1.64600
C	1.17000	1.34300	-1.93800
C	-0.77900	4.13700	-0.28600
H	3.42200	2.31400	0.40400
H	1.60600	3.85900	0.95900
H	-0.75800	2.22100	-2.24100
H	1.02700	0.61500	-2.73000
C	-0.67300	5.35700	0.34600
C	-1.90800	6.03300	0.50600
S	-2.45600	3.82200	-0.69900
H	0.27600	5.76900	0.67000
H	-2.00400	6.99800	0.99000
C	-2.98800	5.34300	-0.00400
C	-4.38700	5.71800	-0.02000
C	-5.49600	4.93100	-0.25100
C	-6.72500	5.64500	-0.18300
C	-6.55600	6.97200	0.10100
S	-4.87900	7.37900	0.27800
H	-5.42900	3.86700	-0.44600
H	-7.69600	5.18600	-0.33200
H	-7.31100	7.73700	0.21700

TS1 **(compoundB)**

C	1.16600	5.22600	0.19000
C	-0.21800	5.29600	0.44000
C	-0.99100	4.14300	0.52400
C	-0.35300	2.91600	0.31800
C	1.03400	2.82500	0.07400
C	1.80100	4.00200	0.01900
N	-0.88800	1.63700	0.39300
C	0.15300	0.70700	0.12000
C	1.36000	1.41900	0.00400
C	-1.16600	-5.22600	-0.19000
C	0.21800	-5.29600	-0.44100
C	0.99100	-4.14300	-0.52400
C	0.35300	-2.91600	-0.31800
C	-1.03400	-2.82500	-0.07400
C	-1.80100	-4.00200	-0.01900
N	0.88800	-1.63700	-0.39300
C	-0.15300	-0.70700	-0.12000
C	-1.36000	-1.41900	-0.00400
H	2.87200	3.95700	-0.14300
H	1.74600	6.14300	0.14000
H	-0.68900	6.26600	0.57300
H	-2.05600	4.19800	0.72500

H	2.05600	-4.19800	-0.72500
H	0.68900	-6.26500	-0.57300
H	-1.74600	-6.14300	-0.14100
H	-2.87200	-3.95700	0.14300
C	-1.92100	1.43000	1.42300
H	-1.74200	2.12800	2.24600
H	-2.92600	1.58900	1.02800
H	-1.85700	0.41800	1.81200
C	1.92100	-1.43000	-1.42300
H	1.74200	-2.12800	-2.24600
H	1.85700	-0.41800	-1.81200
H	2.92600	-1.58900	-1.02800
C	-2.76500	-0.96800	-0.03200
C	-3.71900	-1.46500	0.87400
C	-3.22100	-0.11000	-1.04900
C	-5.05800	-1.09800	0.78800
H	-3.39800	-2.12100	1.67700
C	-4.55900	0.25100	-1.14300
H	-2.51100	0.26600	-1.77900
C	-5.51100	-0.22900	-0.22100
H	-5.75800	-1.47200	1.53000
H	-4.88100	0.88800	-1.96100
C	2.76500	0.96800	0.03200
C	3.71900	1.46500	-0.87400
C	3.22100	0.11000	1.04900
C	5.05800	1.09800	-0.78800
H	3.39800	2.12100	-1.67700
C	4.55900	-0.25100	1.14300
H	2.51100	-0.26600	1.77900
C	5.51100	0.22900	0.22100
H	5.75800	1.47200	-1.53000
H	4.88100	-0.88800	1.96100
C	6.91500	-0.17300	0.32600
C	7.44600	-1.29500	0.92500
S	8.20400	0.81200	-0.34700
C	8.85700	-1.38400	0.83200
H	6.83300	-2.05900	1.38800
C	9.43700	-0.32800	0.16100
H	9.43200	-2.21700	1.22200
C	10.83500	-0.08600	-0.12800
C	11.39600	0.75100	-1.06900
S	12.09700	-0.90500	0.77900
C	12.81900	0.73200	-1.07300
H	10.80000	1.34700	-1.75200
C	13.34200	-0.11900	-0.13900
H	13.42700	1.32100	-1.75000
H	14.38100	-0.33300	0.07000
C	-6.91500	0.17300	-0.32600
C	-7.44600	1.29500	-0.92500
S	-8.20400	-0.81200	0.34700
C	-8.85700	1.38400	-0.83200
H	-6.83300	2.05900	-1.38800
C	-9.43700	0.32800	-0.16100
H	-9.43200	2.21700	-1.22200
C	-10.83500	0.08600	0.12800
C	-11.39500	-0.75100	1.07000
S	-12.09700	0.90500	-0.77900
C	-12.81900	-0.73200	1.07300
H	-10.80000	-1.34700	1.75200
C	-13.34200	0.11900	0.13900
H	-13.42700	-1.32100	1.75000
H	-14.38100	0.33300	-0.07000

TS2a **(compoundB)**

C	-4.23900	0.14600	-5.19900
C	-5.62200	-0.08700	-5.08000

C	-6.22800	-0.18300	-3.83000
C	-5.41200	-0.07300	-2.70000
C	-4.02500	0.16200	-2.79900
C	-3.43800	0.28300	-4.07200
N	-5.78400	-0.09000	-1.35800
C	-4.59300	0.06800	-0.58200
C	-3.52400	0.30300	-1.45200
C	-3.44100	-0.31900	5.37200
C	-4.80200	0.02700	5.46400
C	-5.58300	0.18000	4.32200
C	-4.96100	0.01000	3.08100
C	-3.59900	-0.33900	2.96800
C	-2.83700	-0.51400	4.13600
N	-5.53200	0.06400	1.81100
C	-4.49200	-0.18700	0.86300
C	-3.32500	-0.51500	1.56100
H	-2.37900	0.49100	-4.17300
H	-3.79500	0.22700	-6.18600
H	-6.22700	-0.19300	-5.97500
H	-7.29500	-0.35900	-3.74300
H	-6.63300	0.44300	4.39800
H	-5.25200	0.17700	6.44100
H	-2.85900	-0.44100	6.28000
H	-1.79500	-0.80900	4.07600
C	-7.06900	0.56000	-1.04700
H	-7.88100	-0.15900	-0.90700
H	-6.97200	1.17400	-0.15400
H	-7.33700	1.22300	-1.87400
C	-6.89800	-0.47900	1.70700
H	-7.08700	-1.12300	2.57000
H	-7.66100	0.30400	1.69000
H	-6.99000	-1.09300	0.81400
C	-2.08400	-1.14900	1.07900
C	-2.14400	-2.28100	0.24400
C	-0.82000	-0.75300	1.54500
C	-0.99700	-2.97600	-0.11300
H	-3.11100	-2.62900	-0.10400
C	0.33200	-1.44300	1.18300
H	-0.73400	0.13000	2.16800
C	0.27300	-2.57100	0.34600
H	-1.08600	-3.86700	-0.72700
H	1.29400	-1.08400	1.53600
C	1.47500	-3.30700	-0.04800
C	1.66500	-4.12700	-1.14000
S	2.94900	-3.23400	0.90500
C	2.96100	-4.69500	-1.21800
H	0.89500	-4.30400	-1.88200
C	3.79500	-4.31800	-0.18600
H	3.27200	-5.36900	-2.00800
C	5.17100	-4.69500	0.06100
C	5.91800	-4.55500	1.21100
S	6.14000	-5.44600	-1.19900
C	7.24800	-5.04900	1.09100
H	5.51800	-4.12500	2.12200
C	7.51500	-5.56600	-0.14600
H	7.97300	-5.02600	1.89600
H	8.43100	-6.01000	-0.50800
C	-2.17200	0.82300	-1.17100
C	-2.00200	1.95500	-0.35500
C	-1.03400	0.31000	-1.81600
C	-0.75200	2.53300	-0.17500
H	-2.86700	2.38600	0.13900
C	0.21600	0.89400	-1.64900
H	-1.12900	-0.56800	-2.44600
C	0.38900	2.01500	-0.81800
H	-0.65500	3.39400	0.47900
H	1.07000	0.48400	-2.17900
C	1.71700	2.60500	-0.63400
C	2.94900	2.00000	-0.75700
S	1.91900	4.29500	-0.20600
C	4.04200	2.86400	-0.49500
H	3.06500	0.94900	-0.99100
C	3.66700	4.15000	-0.16700

H	5.07800	2.54200	-0.51600
C	4.49900	5.28800	0.16600
C	4.15700	6.45500	0.81500
S	6.20000	5.31800	-0.27300
C	5.24500	7.36000	0.97000
H	3.15700	6.64600	1.18800
C	6.41300	6.88500	0.44200
H	5.16100	8.32200	1.46300
H	7.38600	7.35600	0.42700

TS2b (compoundB)

C	-3.64000	0.60000	5.27100
C	-5.01400	0.89900	5.21600
C	-5.71300	0.84000	4.01400
C	-4.99700	0.50600	2.86000
C	-3.62000	0.20300	2.89500
C	-2.94100	0.24200	4.12600
N	-5.47400	0.33900	1.56200
C	-4.36100	-0.01200	0.73600
C	-3.23800	-0.17400	1.55400
C	-3.64100	-0.60000	-5.27100
C	-5.01400	-0.89900	-5.21600
C	-5.71300	-0.84000	-4.01400
C	-4.99700	-0.50600	-2.86000
C	-3.62000	-0.20300	-2.89500
C	-2.94100	-0.24200	-4.12600
N	-5.47400	-0.33900	-1.56200
C	-4.36100	0.01200	-0.73600
C	-3.23800	0.17400	-1.55400
H	-1.88900	-0.01500	4.18300
H	-3.12300	0.64300	6.22500
H	-5.53900	1.17900	6.12500
H	-6.77300	1.06800	3.97600
H	-6.77300	-1.06800	-3.97600
H	-5.53900	-1.17900	-6.12400
H	-3.12300	-0.64300	-6.22500
H	-1.88900	0.01500	-4.18300
C	-6.81700	-0.25600	1.45200
H	-7.59100	0.48600	1.23300
H	-6.82500	-1.02400	0.68200
H	-7.06600	-0.73900	2.40000
C	-6.81700	0.25500	-1.45100
H	-7.06600	0.73800	-2.39900
H	-7.59100	-0.48600	-1.23200
H	-6.82500	1.02400	-0.68200
C	-1.93500	0.80200	-1.26400
C	-1.87200	2.04900	-0.61700
C	-0.73300	0.25900	-1.74600
C	-0.66200	2.70900	-0.44200
H	-2.78700	2.50200	-0.25100
C	0.47700	0.92400	-1.58700
H	-0.74500	-0.70800	-2.23900
C	0.54300	2.16300	-0.92300
H	-0.65100	3.66100	0.08100
H	1.38100	0.48200	-1.99200
C	1.82800	2.84000	-0.74300
C	3.09600	2.29900	-0.76300
S	1.92400	4.57000	-0.45900
C	4.13000	3.24100	-0.53500
H	3.28000	1.24000	-0.90600
C	3.67400	4.52700	-0.33700
H	5.18100	2.97800	-0.48900
C	4.42800	5.73500	-0.07300

C	3.99500	6.93200	0.45500
S	6.14400	5.82300	-0.44000
C	5.02500	7.90800	0.57400
H	2.97000	7.09800	0.76700
C	6.24000	7.45600	0.14100
H	4.86700	8.90300	0.97500
H	7.18600	7.97700	0.12500
C	-1.93500	-0.80200	1.26400
C	-1.87200	-2.04900	0.61700
C	-0.73300	-0.25900	1.74600
C	-0.66200	-2.70900	0.44200
H	-2.78700	-2.50300	0.25100
C	0.47700	-0.92400	1.58700
H	-0.74500	0.70800	2.23800
C	0.54300	-2.16300	0.92300
H	-0.65000	-3.66100	-0.08100
H	1.38100	-0.48200	1.99200
C	1.82800	-2.84000	0.74300
C	3.09600	-2.29800	0.76300
S	1.92400	-4.57000	0.45900
C	4.13000	-3.24100	0.53500
H	3.28000	-1.24000	0.90500
C	3.67400	-4.52700	0.33700
H	5.18100	-2.97800	0.48900
C	4.42800	-5.73500	0.07300
C	3.99500	-6.93200	-0.45500
S	6.14500	-5.82300	0.44000
C	5.02500	-7.90800	-0.57400
H	2.97000	-7.09800	-0.76600
C	6.24000	-7.45500	-0.14100
H	4.86800	-8.90300	-0.97500
H	7.18700	-7.97700	-0.12400

Global minimum(compoundC)

C	4.02300	0.15000	-5.24700
C	5.13000	-0.70300	-5.06900
C	5.52400	-1.11800	-3.80400
C	4.77900	-0.66500	-2.70600
C	3.64800	0.17900	-2.86600
C	3.28400	0.59600	-4.16000
N	4.96400	-0.88400	-1.35100
C	3.96900	-0.18600	-0.65000
C	3.14000	0.47200	-1.54800
C	3.45400	-0.50100	5.39500
C	4.69600	0.16200	5.32500
C	5.26900	0.48600	4.10100
C	4.56500	0.13800	2.94100
C	3.30200	-0.50800	2.99000
C	2.75800	-0.84100	4.24300
N	4.91400	0.30300	1.61200

C	3.89200	-0.22800	0.81500
C	2.88300	-0.73200	1.62500
C	5.92600	-1.82500	-0.77600
C	1.96300	1.30300	-1.24000
C	-0.85500	-2.55700	0.44300
C	0.34500	-2.87000	-0.22400
C	1.54800	-2.28300	0.14500
C	1.61900	-1.35900	1.20400
C	0.41800	-1.04900	1.87000
C	-0.78800	-1.63100	1.49800
C	-2.11600	-3.17800	0.03400
C	-2.45700	-3.70900	-1.19200
C	-3.77600	-4.22500	-1.25000
C	-4.47300	-4.10000	-0.06700
S	-3.46000	-3.34500	1.15100
C	-5.83000	-4.50000	0.24100
C	-6.64400	-4.08900	1.27500
C	-7.93100	-4.69800	1.26300
C	-8.09900	-5.57000	0.22300
S	-6.67200	-5.67500	-0.75900
H	2.44300	1.26600	-4.30300
H	3.74900	0.46600	-6.24900
H	5.69000	-1.04000	-5.93600
H	6.38300	-1.76800	-3.68000
H	6.23200	0.98500	4.05300
H	5.21800	0.41900	6.24200
H	3.04000	-0.75200	6.36700
H	1.81100	-1.36500	4.30800
H	6.76600	-1.89100	-1.47400
H	6.31800	-1.39700	0.14900
H	0.33700	-3.60700	-1.02100
H	2.45200	-2.55900	-0.38500
H	0.42800	-0.31200	2.66600
H	-1.69700	-1.33700	2.01500
H	-1.78700	-3.69400	-2.04300
H	-4.21400	-4.64900	-2.14700
H	-6.33300	-3.35400	2.00800
H	-8.70200	-4.48700	1.99500
H	-8.97000	-6.15800	-0.02800
C	1.95500	2.23800	-0.18900
C	0.83000	3.00500	0.08800
C	-0.34000	2.88900	-0.68600
C	-0.33300	1.95600	-1.73800
C	0.78900	1.18000	-2.00400
C	-1.51100	3.71800	-0.39100
H	2.83800	2.35700	0.42700
H	0.85100	3.69400	0.92500
H	-1.21500	1.84200	-2.36200
H	0.75100	0.45000	-2.80500
C	-1.56100	4.94400	0.23600
C	-2.87100	5.46800	0.37400
S	-3.13200	3.20300	-0.82600
H	-0.67300	5.46700	0.57200
H	-3.08900	6.41700	0.85100
C	-3.85200	4.65200	-0.14800
C	-5.28600	4.85600	-0.18500
C	-6.28800	3.94400	-0.44000
C	-7.59500	4.50300	-0.38600
C	-7.59200	5.83800	-0.09000
S	-5.97900	6.44300	0.11700
H	-6.09000	2.89700	-0.64200
H	-8.50100	3.93200	-0.55400
H	-8.43500	6.50600	0.01900
C	6.04100	1.11700	1.16100
H	6.92700	0.81200	1.73200
H	6.23600	0.87500	0.11400
C	5.82300	2.63100	1.30400
H	5.54500	2.86100	2.33800
H	4.97700	2.92700	0.67500
C	7.07100	3.42300	0.90300
H	6.89900	4.49900	1.00100
H	7.92800	3.16500	1.53500
H	7.35200	3.22600	-0.13700

C	5.37300	-3.22800	-0.47600
H	6.17700	-3.78600	0.02100
H	4.56700	-3.13700	0.26000
C	4.88800	-4.00700	-1.70100
H	5.69800	-4.16700	-2.42100
H	4.50800	-4.99100	-1.40600
H	4.08300	-3.48100	-2.22300

TS1 **(compoundC)**

C	-1.09100	5.21100	0.61200
C	0.30000	5.29500	0.42000
C	1.05700	4.15700	0.15700
C	0.39500	2.92600	0.12200
C	-0.99800	2.82300	0.31400
C	-1.74800	3.98900	0.55100
N	0.92000	1.66200	-0.15500
C	-0.14500	0.72000	-0.02900
C	-1.34500	1.42600	0.16000
C	1.09100	-5.21100	-0.61200
C	-0.30000	-5.29500	-0.42000
C	-1.05700	-4.15700	-0.15600
C	-0.39500	-2.92600	-0.12200
C	0.99800	-2.82300	-0.31400
C	1.74800	-3.98900	-0.55100
N	-0.92000	-1.66200	0.15500
C	0.14500	-0.72000	0.02900
C	1.34500	-1.42600	-0.16000
H	-2.82500	3.94000	0.67300
H	-1.65900	6.11700	0.80300
H	0.79200	6.26100	0.47600
H	2.12700	4.22600	-0.00400
H	-2.12700	-4.22600	0.00400
H	-0.79200	-6.26100	-0.47500
H	1.65900	-6.11700	-0.80300
H	2.82500	-3.94000	-0.67300
C	2.75500	-1.00000	-0.05500
C	3.72800	-1.43000	-0.97600
C	3.19300	-0.23000	1.03900
C	5.06800	-1.08800	-0.82600
H	3.42200	-2.00800	-1.84200
C	4.53200	0.10400	1.19600
H	2.46900	0.09600	1.77800
C	5.50400	-0.31300	0.26400
H	5.78200	-1.40900	-1.57800
H	4.83700	0.66900	2.07000
C	-2.75500	1.00000	0.05500
C	-3.72800	1.43000	0.97600
C	-3.19300	0.23000	-1.03900
C	-5.06800	1.08800	0.82600
H	-3.42200	2.00800	1.84200
C	-4.53200	-0.10400	-1.19600
H	-2.46900	-0.09600	-1.77800
C	-5.50400	0.31300	-0.26400
H	-5.78200	1.40900	1.57800
H	-4.83700	-0.66900	-2.07000
C	-6.90800	-0.06100	-0.43600
C	-7.43700	-1.11100	-1.15700
S	-8.20200	0.86000	0.31400
C	-8.85200	-1.18200	-1.11700
H	-6.82200	-1.82800	-1.68600
C	-9.43700	-0.18800	-0.36200
H	-9.42700	-1.94200	-1.63500
C	-10.84100	0.05200	-0.09800
C	-11.44700	1.17300	0.43000
S	-12.04700	-1.17600	-0.45000
C	-12.86000	1.05500	0.54500
H	-10.89300	2.06200	0.71100
C	-13.33200	-0.15100	0.10500
H	-13.50000	1.84000	0.93300

H	-14.35300	-0.50300	0.07300
C	6.90800	0.06100	0.43600
C	7.43700	1.11100	1.15700
S	8.20200	-0.86000	-0.31400
C	8.85200	1.18200	1.11700
H	6.82200	1.82800	1.68600
C	9.43700	0.18800	0.36200
H	9.42700	1.94200	1.63500
C	10.84100	-0.05200	0.09800
C	11.44700	-1.17300	-0.43000
S	12.04700	1.17600	0.45000
C	12.86000	-1.05500	-0.54500
H	10.89300	-2.06200	-0.71200
C	13.33200	0.15100	-0.10600
H	13.50000	-1.84000	-0.93300
H	14.35300	0.50300	-0.07300
C	1.24600	2.12900	-2.62600
H	0.35100	1.53800	-2.85300
H	0.91700	3.16800	-2.51700
C	2.24900	2.02000	-3.77900
H	1.80800	2.37300	-4.71700
H	3.14500	2.62200	-3.58800
H	2.57400	0.98500	-3.93300
C	-1.24600	-2.12900	2.62600
H	-0.91700	-3.16800	2.51700
H	-0.35100	-1.53800	2.85300
C	-2.24900	-2.02000	3.77900
H	-3.14500	-2.62200	3.58800
H	-1.80800	-2.37300	4.71700
H	-2.57400	-0.98500	3.93300
C	1.85300	1.62200	-1.30900
H	2.19100	0.60300	-1.45100
H	2.74000	2.20500	-1.03900
C	-1.85300	-1.62200	1.30900
H	-2.74000	-2.20500	1.03900
H	-2.19100	-0.60300	1.45100

TS2a **(compoundC)**

C	-3.12500	-1.12200	-5.05500
C	-4.46500	-1.53700	-4.95700
C	-5.17700	-1.38300	-3.77200
C	-4.50900	-0.83600	-2.67100
C	-3.15700	-0.43500	-2.74500
C	-2.46800	-0.56600	-3.96400
N	-5.01100	-0.55900	-1.39900
C	-3.91100	-0.09600	-0.60400
C	-2.80300	0.08100	-1.44100
C	-2.39300	0.56300	5.23300
C	-3.71200	1.04100	5.34100
C	-4.57800	1.00700	4.25400
C	-4.08600	0.51900	3.03800
C	-2.76200	0.04800	2.90800
C	-1.91500	0.05900	4.03100
N	-4.76200	0.35800	1.82700
C	-3.81200	-0.13100	0.87300
C	-2.61300	-0.40600	1.54500
H	-1.44100	-0.23400	-4.05800
H	-2.59700	-1.23900	-5.99700
H	-4.95300	-1.98400	-5.81900
H	-6.21400	-1.69800	-3.70100
H	-5.59800	1.36400	4.34900
H	-4.06200	1.43900	6.28900
H	-1.74300	0.58600	6.10200
H	-0.90400	-0.32700	3.96400
C	-6.36500	0.05400	-1.36000
H	-7.11600	-0.74200	-1.43200
H	-6.48000	0.53300	-0.39600
C	-6.16600	-0.09900	1.96800
H	-6.74000	0.72600	2.40400

H	-6.58100	-0.28600	0.98700
C	-1.44300	-1.17600	1.08700
C	-1.61100	-2.38200	0.37900
C	-0.13300	-0.81400	1.44400
C	-0.52700	-3.18200	0.04700
H	-2.61200	-2.70200	0.11100
C	0.95500	-1.61400	1.11300
H	0.04000	0.13000	1.94800
C	0.78700	-2.81700	0.40800
H	-0.70000	-4.12300	-0.46400
H	1.95400	-1.28300	1.38100
C	1.92000	-3.67200	0.05000
C	2.01200	-4.60200	-0.96300
S	3.42700	-3.61900	0.95000
C	3.27100	-5.25000	-1.03800
H	1.20600	-4.79000	-1.66300
C	4.16900	-4.83100	-0.07900
H	3.52100	-5.98700	-1.79300
C	5.53400	-5.25900	0.14400
C	6.53200	-4.64100	0.86800
S	6.12900	-6.76400	-0.54000
C	7.76200	-5.35700	0.86900
H	6.38900	-3.69100	1.36900
C	7.70400	-6.51700	0.14600
H	8.65500	-5.01800	1.38000
H	8.48600	-7.24300	-0.02600
C	-1.54500	0.80000	-1.17300
C	-1.55800	2.02800	-0.48500
C	-0.31300	0.36200	-1.69000
C	-0.39800	2.77100	-0.31200
H	-2.49600	2.40100	-0.08700
C	0.84600	1.11400	-1.53800
H	-0.25700	-0.59500	-2.19600
C	0.83400	2.33500	-0.84000
H	-0.44500	3.70400	0.24200
H	1.77200	0.75400	-1.97300
C	2.06500	3.11000	-0.67500
C	3.37100	2.67100	-0.71400
S	2.02600	4.84300	-0.39400
C	4.32900	3.69300	-0.50300
H	3.63500	1.62900	-0.85400
C	3.77600	4.94000	-0.30000
H	5.39800	3.51400	-0.47300
C	4.43700	6.20400	-0.05100
C	3.91900	7.36600	0.47900
S	6.13600	6.42300	-0.44100
C	4.87100	8.42000	0.58100
H	2.88800	7.45400	0.80400
C	6.11200	8.06100	0.13200
H	4.64200	9.40100	0.98000
H	7.01500	8.65500	0.10100
C	-6.65000	1.14500	-2.40800
H	-6.58700	0.73800	-3.42100
H	-7.69900	1.43700	-2.25900
C	-6.37000	-1.37900	2.79900
H	-6.02900	-1.22300	3.82600
H	-7.45600	-1.53700	2.85400
C	-5.75000	2.37700	-2.28600
H	-5.80300	2.81200	-1.28100
H	-4.70400	2.13200	-2.48800
H	-6.05500	3.14900	-2.99900
C	-5.69700	-2.62200	2.21000
H	-5.99900	-2.78700	1.17000
H	-4.60700	-2.53400	2.23000
H	-5.96800	-3.51500	2.78200

C	2.94400	0.72600	-5.12400
C	4.32900	0.97100	-5.08400
C	5.05800	0.77100	-3.91600
C	4.36400	0.35000	-2.77600
C	2.97200	0.11600	-2.79300
C	2.26200	0.29300	-3.99400
N	4.86700	0.05900	-1.50900
C	3.75400	-0.25400	-0.66900
C	2.60300	-0.32300	-1.46500
C	2.87100	-0.82900	5.31500
C	4.20600	-1.27000	5.28900
C	4.94600	-1.24800	4.11200
C	4.31700	-0.80000	2.94400
C	2.97400	-0.37600	2.95100
C	2.25200	-0.37500	4.15700
N	4.85800	-0.66000	1.65600
C	3.77500	-0.23100	0.80500
C	2.65700	0.03300	1.60300
H	1.19800	0.09100	-4.04200
H	2.40200	0.87800	-6.05300
H	4.83800	1.32100	-5.97700
H	6.12700	0.95600	-3.88800
H	5.97300	-1.59900	4.10400
H	4.66700	-1.63700	6.20100
H	2.31900	-0.84300	6.25000
H	1.22800	-0.01800	4.18600
C	6.14600	-0.68700	-1.44800
H	6.97600	0.01800	-1.57700
H	6.21700	-1.10900	-0.45400
C	6.21300	-0.03300	1.66000
H	6.60900	-0.18200	2.66500
H	6.90500	-0.55200	0.99700
C	1.41600	0.76600	1.28600
C	1.46900	2.00500	0.62300
C	0.16400	0.33700	1.75900
C	0.32500	2.76600	0.42500
H	2.42500	2.37200	0.26300
C	-0.98000	1.10500	1.57900
H	0.08400	-0.62200	2.26000
C	-0.93000	2.33600	0.90000
H	0.40300	3.70800	-0.11000
H	-1.92400	0.75000	1.98000
C	-2.14700	3.12300	0.69700
C	-3.45900	2.69900	0.71000
S	-2.08300	4.85100	0.38700
C	-4.40100	3.72700	0.45700
H	-3.73900	1.66300	0.86400
C	-3.82800	4.96400	0.24600
H	-5.47100	3.55900	0.40300
C	-4.46800	6.22900	-0.04700
C	-3.92300	7.37600	-0.58500
S	-6.17600	6.47400	0.28800
C	-4.86100	8.43500	-0.73800
H	-2.88200	7.44600	-0.88100
C	-6.11800	8.09800	-0.31900
H	-4.61000	9.40500	-1.15100
H	-7.01500	8.70200	-0.32700
C	1.28700	-0.91700	-1.16600
C	1.20300	-2.16500	-0.52200
C	0.09000	-0.34400	-1.62700
C	-0.01800	-2.80000	-0.33600
H	2.11200	-2.64000	-0.16900
C	-1.13100	-0.98600	-1.45900
H	0.11400	0.62900	-2.10500
C	-1.21600	-2.22900	-0.80500
H	-0.04400	-3.75400	0.18300
H	-2.03100	-0.52300	-1.85200
C	-2.51100	-2.88800	-0.62500
C	-3.77200	-2.33000	-0.63400
S	-2.62900	-4.62100	-0.36100
C	-4.81700	-3.26200	-0.41300

H	-3.94200	-1.26800	-0.76300
C	-4.37700	-4.55600	-0.23200
H	-5.86400	-2.98500	-0.36000
C	-5.14600	-5.75700	0.02000
C	-4.72600	-6.96600	0.53300
S	-6.86400	-5.82000	-0.34500
C	-5.76800	-7.93000	0.64300
H	-3.70300	-7.14800	0.84000
C	-6.97800	-7.45800	0.21700
H	-5.62200	-8.93100	1.03200
H	-7.93100	-7.96800	0.19600
C	6.21000	1.47000	1.35600
H	5.51400	1.96500	2.04400
H	5.83100	1.64300	0.34400
C	7.61000	2.07700	1.50100
H	7.59800	3.14600	1.27200
H	7.99400	1.96100	2.52100
H	8.32600	1.60100	0.82100
C	6.28900	-1.85900	-2.43600
H	6.25300	-1.50100	-3.46900
H	7.30000	-2.26000	-2.28400
C	5.25700	-2.97200	-2.23500
H	5.27600	-3.35000	-1.20700
H	4.24300	-2.62200	-2.44500
H	5.46300	-3.81400	-2.90400

Global minimum(compoundD)

C	-0.94200	-2.44500	-5.26300
C	-1.87700	-3.43200	-4.89400
C	-2.02500	-3.82100	-3.56900
C	-1.19900	-3.21200	-2.61300
C	-0.22000	-2.24700	-2.96900
C	-0.12000	-1.85100	-4.31600
N	-1.14800	-3.39400	-1.24300
C	-0.15000	-2.56800	-0.72200
C	0.45600	-1.85500	-1.75200
C	0.94200	-2.44500	5.26300
C	1.87700	-3.43200	4.89400
C	2.02500	-3.82100	3.56900
C	1.19900	-3.21200	2.61300
C	0.22000	-2.24700	2.96900
C	0.12000	-1.85000	4.31600
N	1.14800	-3.39400	1.24300
C	0.15000	-2.56800	0.72200
C	-0.45600	-1.85500	1.75200
H	0.58200	-1.07900	-4.61200
H	-0.86700	-2.14300	-6.30300
H	-2.50400	-3.88700	-5.65500
H	-2.76600	-4.56100	-3.29000
H	2.76600	-4.56100	3.29000
H	2.50400	-3.88700	5.65500
H	0.86800	-2.14300	6.30300
H	-0.58200	-1.07800	4.61200
C	-1.93200	-4.37600	-0.48900
C	-3.24600	-3.85900	0.11700
H	-2.12800	-5.21500	-1.16500
H	-1.29500	-4.75700	0.31400
C	1.93200	-4.37600	0.48900

H	2.12800	-5.21500	1.16500
H	1.29500	-4.75700	-0.31400
C	3.24600	-3.85900	-0.11700
C	1.59500	-0.92400	-1.65600
C	1.79800	-0.07300	-0.55300
C	2.88900	0.78700	-0.49100
C	3.84100	0.84300	-1.52500
C	3.65100	-0.01800	-2.62200
C	2.55800	-0.87300	-2.68600
H	1.08900	-0.07200	0.26600
H	2.98700	1.44700	0.36600
H	4.38600	-0.03800	-3.42100
H	2.46900	-1.54800	-3.53000
C	4.98600	1.75300	-1.47900
C	5.72700	2.25900	-2.52500
C	6.78200	3.11500	-2.12300
C	6.87000	3.28500	-0.75800
S	5.61400	2.35900	0.04500
H	5.50300	2.03800	-3.56200
H	7.46400	3.59100	-2.82000
C	7.81100	4.07900	0.00600
C	8.06700	4.05800	1.36000
C	9.07000	4.98400	1.76500
C	9.57800	5.70800	0.72200
S	8.82700	5.27700	-0.78200
H	7.56000	3.38600	2.04300
H	9.40300	5.10100	2.79000
H	10.34600	6.46800	0.74000
C	-3.84100	0.84300	1.52500
C	-2.88900	0.78700	0.49100
C	-1.79800	-0.07300	0.55300
C	-1.59500	-0.92300	1.65600
C	-2.55800	-0.87300	2.68600
C	-3.65100	-0.01800	2.62200
H	-2.98700	1.44700	-0.36600
H	-1.08900	-0.07200	-0.26600
H	-2.46900	-1.54800	3.53000
H	-4.38600	-0.03800	3.42100
C	-4.98600	1.75300	1.47900
C	-5.72700	2.25900	2.52500
C	-6.78200	3.11500	2.12300
C	-6.87000	3.28500	0.75800
S	-5.61400	2.35900	-0.04500
H	-5.50300	2.03800	3.56200
H	-7.46400	3.59100	2.82000
C	-7.81100	4.07900	-0.00600
C	-8.06700	4.05800	-1.36000
C	-9.07000	4.98400	-1.76500
C	-9.57900	5.70800	-0.72200
S	-8.82700	5.27600	0.78200
H	-7.56100	3.38600	-2.04300
H	-9.40300	5.10000	-2.79000
H	-10.34600	6.46800	-0.74100
C	-4.29700	-3.37500	-0.88800
H	-3.66200	-4.68400	0.71200
H	-3.01700	-3.05500	0.82300
C	-5.57400	-2.86500	-0.20700
H	-3.87300	-2.57300	-1.50500
H	-4.55500	-4.19200	-1.57700
C	-6.64200	-2.38400	-1.19700
H	-5.99600	-3.66200	0.42200
H	-5.31400	-2.04400	0.47400
C	-7.90500	-1.85500	-0.51100
H	-6.21500	-1.59600	-1.83200
H	-6.90800	-3.20800	-1.87300
H	-8.65100	-1.52900	-1.24300
H	-8.36900	-2.62600	0.11500
H	-7.67600	-0.99900	0.13200
H	3.66200	-4.68400	-0.71200
H	3.01700	-3.05500	-0.82300
C	4.29700	-3.37500	0.88800
C	5.57400	-2.86500	0.20700
H	3.87300	-2.57300	1.50500

H	4.55500	-4.19200	1.57700
C	6.64200	-2.38400	1.19700
H	5.99600	-3.66200	-0.42200
H	5.31400	-2.04400	-0.47400
H	6.90800	-3.20800	1.87300
C	7.90500	-1.85500	0.51100
H	6.21500	-1.59600	1.83200
H	8.65100	-1.52900	1.24300
H	8.36900	-2.62600	-0.11500
H	7.67600	-0.99900	-0.13300

TS1 **(compoundD)**

C	1.03500	2.82400	-4.43600
C	-0.36300	2.97500	-4.39600
C	-1.11200	2.44100	-3.35100
C	-0.43500	1.72200	-2.36200
C	0.96600	1.55800	-2.38800
C	1.70700	2.13000	-3.43700
N	-0.95000	1.12600	-1.21000
C	0.13200	0.47800	-0.54200
C	1.32800	0.81700	-1.19900
C	-1.03600	-2.82300	4.43700
C	0.36300	-2.97400	4.39700
C	1.11100	-2.44100	3.35300
C	0.43400	-1.72100	2.36300
C	-0.96600	-1.55800	2.38900
C	-1.70800	-2.13000	3.43800
N	0.95000	-1.12600	1.21100
C	-0.13200	-0.47800	0.54300
C	-1.32800	-0.81700	1.19900
H	2.78800	2.04400	-3.46400
H	1.59600	3.26200	-5.25600
H	-0.86700	3.51900	-5.19000
H	-2.18900	2.57100	-3.31700
H	2.18800	-2.57100	3.31800
H	0.86600	-3.51800	5.19100
H	-1.59700	-3.26100	5.25700
H	-2.78800	-2.04300	3.46500
C	-2.73900	-0.68600	0.78500
C	-3.73900	-0.27100	1.68400
C	-3.14800	-1.07800	-0.50300
C	-5.07700	-0.22700	1.30800
H	-3.45800	0.05700	2.67900
C	-4.48500	-1.04500	-0.87700
H	-2.40300	-1.42700	-1.20900
C	-5.48400	-0.61200	0.01800
H	-5.81400	0.13400	2.01900
H	-4.76600	-1.38800	-1.86700
C	2.73900	0.68600	-0.78500
C	3.73900	0.27100	-1.68400
C	3.14900	1.07900	0.50300
C	5.07700	0.22700	-1.30800
H	3.45700	-0.05800	-2.67900
C	4.48500	1.04500	0.87700
H	2.40300	1.42700	1.21000
C	5.48400	0.61200	-0.01800
H	5.81400	-0.13500	-2.02000
H	4.76600	1.38800	1.86700
C	6.88700	0.56900	0.39800
C	7.40500	0.50100	1.67300
S	8.19400	0.60300	-0.77600
C	8.82100	0.48100	1.72000
H	6.78200	0.44700	2.55800
C	9.41900	0.53100	0.47900

H	9.38800	0.43900	2.64400
C	10.82700	0.52800	0.14200
C	11.43700	0.84100	-1.05400
S	12.03700	0.07900	1.33500
C	12.85500	0.73200	-1.01700
H	10.88100	1.15800	-1.93000
C	13.32700	0.33800	0.20400
H	13.49700	0.94500	-1.86400
H	14.35100	0.18100	0.51200
C	-6.88700	-0.56900	-0.39800
C	-7.40500	-0.50200	-1.67400
S	-8.19400	-0.60300	0.77500
C	-8.82100	-0.48200	-1.72200
H	-6.78100	-0.44700	-2.55900
C	-9.41900	-0.53100	-0.48000
H	-9.38700	-0.43900	-2.64500
C	-10.82700	-0.52900	-0.14400
C	-11.43700	-0.84200	1.05300
S	-12.03700	-0.08000	-1.33700
C	-12.85500	-0.73300	1.01500
H	-10.88200	-1.15800	1.92900
C	-13.32700	-0.33900	-0.20600
H	-13.49700	-0.94600	1.86200
H	-14.35100	-0.18200	-0.51400
C	-1.34800	3.31700	0.00100
H	-0.46600	3.13200	0.62700
H	-1.00400	3.90100	-0.86100
C	-2.38100	4.12900	0.79400
H	-3.27000	4.29900	0.17000
H	-2.72600	3.54100	1.65700
C	1.34800	-3.31700	0.00100
H	1.00400	-3.90100	0.86200
H	0.46600	-3.13200	-0.62600
C	2.38100	-4.12800	-0.79300
H	3.27000	-4.29900	-0.16800
H	2.72600	-3.54100	-1.65500
C	-1.92000	1.97000	-0.46400
H	-2.27200	1.41900	0.39800
H	-2.79000	2.12000	-1.11000
C	1.92000	-1.96900	0.46500
H	2.79000	-2.11900	1.11200
H	2.27200	-1.41900	-0.39700
C	1.84200	-5.47800	-1.28300
H	1.50100	-6.06800	-0.42000
H	0.95100	-5.30800	-1.90400
C	2.86700	-6.29400	-2.08100
H	3.75700	-6.46300	-1.46000
H	3.20700	-5.70300	-2.94300
C	2.32000	-7.63900	-2.56800
H	3.07300	-8.19700	-3.13400
H	2.00500	-8.26600	-1.72600
H	1.45000	-7.50000	-3.21900
C	-1.84200	5.47800	1.28400
H	-1.50100	6.06800	0.42200
H	-0.95100	5.30900	1.90500
C	-2.86600	6.29400	2.08300
H	-3.75700	6.46300	1.46200
H	-3.20600	5.70400	2.94400
C	-2.31900	7.63900	2.56900
H	-2.00400	8.26700	1.72800
H	-3.07200	8.19700	3.13600
H	-1.44900	7.50100	3.22000

TS2a **(compoundD)**

C	-2.56300	-0.26100	-5.20000
C	-3.90000	-0.69900	-5.17100
C	-4.60500	-0.76600	-3.97400
C	-3.93200	-0.42200	-2.79600
C	-2.58600	0.00200	-2.80500
C	-1.90400	0.09900	-4.03200
N	-4.42900	-0.38200	-1.49200
C	-3.33200	-0.04200	-0.63500
C	-2.23100	0.29000	-1.43300
C	-1.76900	-0.14000	5.21900
C	-3.09300	0.30100	5.39900
C	-3.97100	0.38800	4.32400
C	-3.48600	0.06200	3.05200
C	-2.15700	-0.36900	2.85200
C	-1.29700	-0.48500	3.96000
N	-4.17500	0.04300	1.83700
C	-3.22400	-0.29800	0.82000
C	-2.01600	-0.64200	1.44000
H	-0.88100	0.45400	-4.06900
H	-2.04200	-0.20200	-6.15100
H	-4.39200	-0.98600	-6.09600
H	-5.64000	-1.09400	-3.95700
H	-4.99500	0.71600	4.47100
H	-3.43700	0.57400	6.39200
H	-1.10900	-0.21500	6.07900
H	-0.28200	-0.84500	3.83600
C	-5.79900	0.17600	-1.35600
H	-6.51700	-0.59700	-1.65200
H	-5.97000	0.39800	-0.31200
C	-5.55900	-0.48800	1.92600
H	-6.17500	0.26800	2.42600
H	-5.95300	-0.61000	0.92600
C	-0.84100	-1.32700	0.87300
C	-1.00400	-2.42500	0.00700
C	0.46900	-1.00100	1.26400
C	0.08500	-3.15500	-0.44700
H	-2.00600	-2.71900	-0.29000
C	1.56200	-1.73200	0.81200
H	0.63700	-0.13400	1.89300
C	1.39800	-2.82600	-0.05500
H	-0.08200	-4.01800	-1.08400
H	2.56100	-1.42800	1.11200
C	2.53600	-3.60400	-0.54600
C	2.63300	-4.35600	-1.69700
S	4.04200	-3.69200	0.35300
C	3.89400	-4.97800	-1.87500
H	1.82700	-4.42900	-2.41800
C	4.79000	-4.71700	-0.86000
H	4.14800	-5.57900	-2.74100
C	6.15700	-5.17100	-0.70700
C	7.15100	-4.67600	0.10900
S	6.75900	-6.54100	-1.62800
C	8.38500	-5.37700	-0.00600
H	7.00500	-3.82000	0.75800
C	8.33200	-6.40300	-0.90800
H	9.27600	-5.12200	0.55500
H	9.11700	-7.08900	-1.19600
C	-0.98100	0.97400	-1.05500
C	-1.00800	2.07500	-0.18000
C	0.25500	0.63900	-1.63600
C	0.14200	2.79600	0.11000
H	-1.95000	2.36700	0.27200
C	1.40500	1.37200	-1.36400
H	0.32200	-0.22400	-2.28800
C	1.37900	2.46500	-0.47900
H	0.08500	3.62700	0.80700
H	2.33500	1.09800	-1.85100
C	2.60100	3.21600	-0.18700
C	3.91200	2.80100	-0.29000
S	2.54400	4.88000	0.37100
C	4.85900	3.78500	0.08900
H	4.18700	1.79800	-0.59500
C	4.29200	4.97600	0.48800

H	5.93000	3.61300	0.09700
C	4.93800	6.18900	0.94400
C	4.40600	7.24400	1.65500
S	6.63600	6.48700	0.60400
C	5.34600	8.27600	1.93300
H	3.37300	7.26600	1.98400
C	6.59200	8.00900	1.43800
H	5.10500	9.17600	2.48700
H	7.48800	8.60900	1.51000
C	-6.08000	1.47900	-2.12600
H	-5.96300	1.32500	-3.20300
H	-7.14300	1.70600	-1.96200
C	-5.71500	-1.84500	2.63600
H	-5.37500	-1.77400	3.67400
H	-6.79600	-2.04500	2.67900
C	-5.01000	-3.01500	1.94000
H	-5.32300	-3.05700	0.88600
H	-3.92800	-2.83600	1.92900
C	-5.23000	2.67500	-1.67900
H	-5.32500	2.80400	-0.59100
H	-4.17200	2.46600	-1.87000
C	-5.62100	3.98100	-2.38100
H	-6.68200	4.19800	-2.19100
H	-5.53000	3.84900	-3.46900
C	-4.77300	5.18400	-1.94800
H	-4.86600	5.31900	-0.86100
H	-3.71400	4.96400	-2.13600
C	-5.16000	6.48400	-2.65800
H	-4.53700	7.32100	-2.32800
H	-5.04300	6.39200	-3.74400
H	-6.20500	6.74900	-2.46100
C	-5.28900	-4.36600	2.60900
H	-6.37300	-4.55400	2.62000
H	-4.98000	-4.31900	3.66300
C	-4.57900	-5.54200	1.92800
H	-4.89000	-5.59200	0.87500
H	-3.49700	-5.35200	1.91500
C	-4.85300	-6.88900	2.60500
H	-4.33100	-7.70600	2.09600
H	-4.52000	-6.88100	3.64900
H	-5.92300	-7.12400	2.60100

TS2b **(compoundD)**

C	2.35800	-0.08900	-4.99900
C	3.76300	-0.01200	-4.95200
C	4.44800	-0.17900	-3.75400
C	3.69700	-0.39400	-2.59300
C	2.28600	-0.45300	-2.61800
C	1.61600	-0.31600	-3.84700
N	4.14600	-0.61300	-1.29200
C	2.99400	-0.69000	-0.45000
C	1.85100	-0.69800	-1.26000
C	1.98100	-0.44700	5.53600
C	3.23800	-1.07400	5.59500
C	3.98500	-1.29400	4.44200
C	3.43800	-0.89800	3.21600
C	2.17000	-0.28900	3.14000
C	1.44400	-0.04500	4.32000
N	4.00500	-0.98500	1.93400
C	3.00400	-0.50500	1.01300
C	1.92800	0.00400	1.74700
H	0.53600	-0.39000	-3.89900

H	1.84900	0.03000	-5.95000
H	4.32000	0.18000	-5.86400
H	5.53200	-0.12400	-3.72000
H	4.95000	-1.78600	4.50100
H	3.63300	-1.39600	6.55400
H	1.42500	-0.27400	6.45300
H	0.48300	0.45400	4.28200
C	5.31400	-1.51100	-1.12000
H	6.23400	-0.93400	-1.26800
H	5.29500	-1.85500	-0.09400
C	5.43600	-0.55700	1.90200
H	5.80400	-0.67000	2.92300
H	6.04700	-1.22700	1.30000
C	0.80500	0.85900	1.31600
C	1.03700	1.99200	0.51700
C	-0.50000	0.66100	1.80000
C	0.01100	2.87300	0.20100
H	2.03800	2.18100	0.14400
C	-1.52500	1.55100	1.50000
H	-0.71800	-0.21300	2.40300
C	-1.29600	2.67600	0.68700
H	0.22500	3.72600	-0.43700
H	-2.51400	1.37700	1.91100
C	-2.39000	3.59400	0.36300
C	-3.74800	3.35800	0.38700
S	-2.08200	5.25100	-0.13000
C	-4.53400	4.47200	-0.00200
H	-4.17100	2.39500	0.64500
C	-3.79200	5.58700	-0.33000
H	-5.61600	4.44700	-0.06700
C	-4.24600	6.88800	-0.77400
C	-3.54100	7.88000	-1.42300
S	-5.90300	7.40500	-0.50300
C	-4.31900	9.03700	-1.71000
H	-2.49900	7.77000	-1.70300
C	-5.61300	8.92800	-1.28300
H	-3.93200	9.91000	-2.22200
H	-6.41600	9.64600	-1.37600
C	0.46700	-1.07600	-0.92500
C	0.21200	-2.21500	-0.13900
C	-0.64100	-0.41100	-1.47800
C	-1.08300	-2.65600	0.09500
H	1.04800	-2.75900	0.28900
C	-1.93800	-0.86100	-1.26100
H	-0.48500	0.48600	-2.06700
C	-2.19200	-1.99300	-0.46500
H	-1.23900	-3.52800	0.72300
H	-2.76500	-0.33500	-1.72600
C	-3.56500	-2.44700	-0.23400
C	-4.73900	-1.73100	-0.33500
S	-3.91700	-4.10500	0.22700
C	-5.90100	-2.48200	-0.02900
H	-4.76300	-0.67800	-0.59000
C	-5.64100	-3.79300	0.31000
H	-6.90200	-2.06400	-0.03100
C	-6.56800	-4.84100	0.68400
C	-6.31900	-6.02900	1.33900
S	-8.27800	-4.71000	0.30200
C	-7.48300	-6.82200	1.54200
H	-5.33000	-6.31300	1.68200
C	-8.61700	-6.24100	1.04600
H	-7.47700	-7.78200	2.04600
H	-9.63100	-6.61500	1.06900
C	5.64300	0.89800	1.46500
H	5.01800	1.54500	2.09300
H	5.29600	1.02800	0.43400
C	7.11200	1.32600	1.57600
H	7.45400	1.20100	2.61300
H	7.73700	0.65500	0.96800
C	5.33300	-2.77000	-2.00500
H	5.36500	-2.49900	-3.06500
H	6.28500	-3.27700	-1.79000
C	4.17200	-3.73900	-1.75400

H	4.14500	-4.00700	-0.68800
H	3.22100	-3.23600	-1.96700
C	4.26700	-5.01500	-2.59900
H	5.22100	-5.52200	-2.39300
H	4.29200	-4.74200	-3.66300
C	3.11200	-5.99500	-2.35600
H	3.09200	-6.27300	-1.29400
H	2.16000	-5.48500	-2.55400
C	3.20300	-7.26000	-3.21500
H	2.36500	-7.93700	-3.01900
H	3.19000	-7.01500	-4.28300
H	4.12900	-7.81100	-3.01500
C	7.35400	2.77500	1.13600
H	6.73100	3.44700	1.74300
H	7.01300	2.90200	0.09900
C	8.82100	3.21100	1.24300
H	9.16000	3.08400	2.28000
H	9.44300	2.53800	0.63700
C	9.05500	4.65900	0.80200
H	8.47400	5.35800	1.41500
H	10.11000	4.93800	0.88900
H	8.75500	4.80800	-0.24100

SI.3 Van t'Hoff analysis of the enantiomer retention factors

The experimental k values determined for the two enantiomers of each compound as a function of temperature were submitted to van t'Hoff analysis according to the relationship

$$\ln k = -\Delta H°/RT + \Delta S°/R + \ln \phi \quad (1)$$

where $\Delta H°$ and $\Delta S°$ are the variations in enthalpy and entropy of adsorption, respectively, ϕ is the phase ratio, R is the gas constant and T the absolute temperature.

Combining eq. (1) for enantiomers (*S*) and (*R*) one gets

$$\ln \frac{k_R}{k_S} = \ln \alpha = -\frac{\Delta\Delta H^0_{R-S}}{RT} + \frac{\Delta\Delta S^0_{R-S}}{R} \quad (2)$$

where $\Delta\Delta H°$ and $\Delta\Delta S°$ are the differences between two enantiomers in enthalpy and entropy of adsorption, respectively, onto the working column.

$\Delta\Delta H°$ and $\Delta\Delta S°$ can be calculated from the slope and intercept of equation (2), or from the differences in the slopes and intercepts of equation (1) applied to each enantiomer; it is worthwhile noticing that knowledge of $\ln \phi$, necessary to obtain $\Delta S°$, is not required for $\Delta\Delta S°$, since it simplifies in the above differences.

SI.4 Detailed CV features of inherently chiral monomers (N-Me-IND)$_2$-T$_4$ and 1,2,3 in CH_3CN and in CH_2Cl_2

a) Comparison between the oxidative CV features of inherently chiral monomers (N-Me-IND)$_2$-T$_4$ and 1, in CH_3CN and in CH_2Cl_2

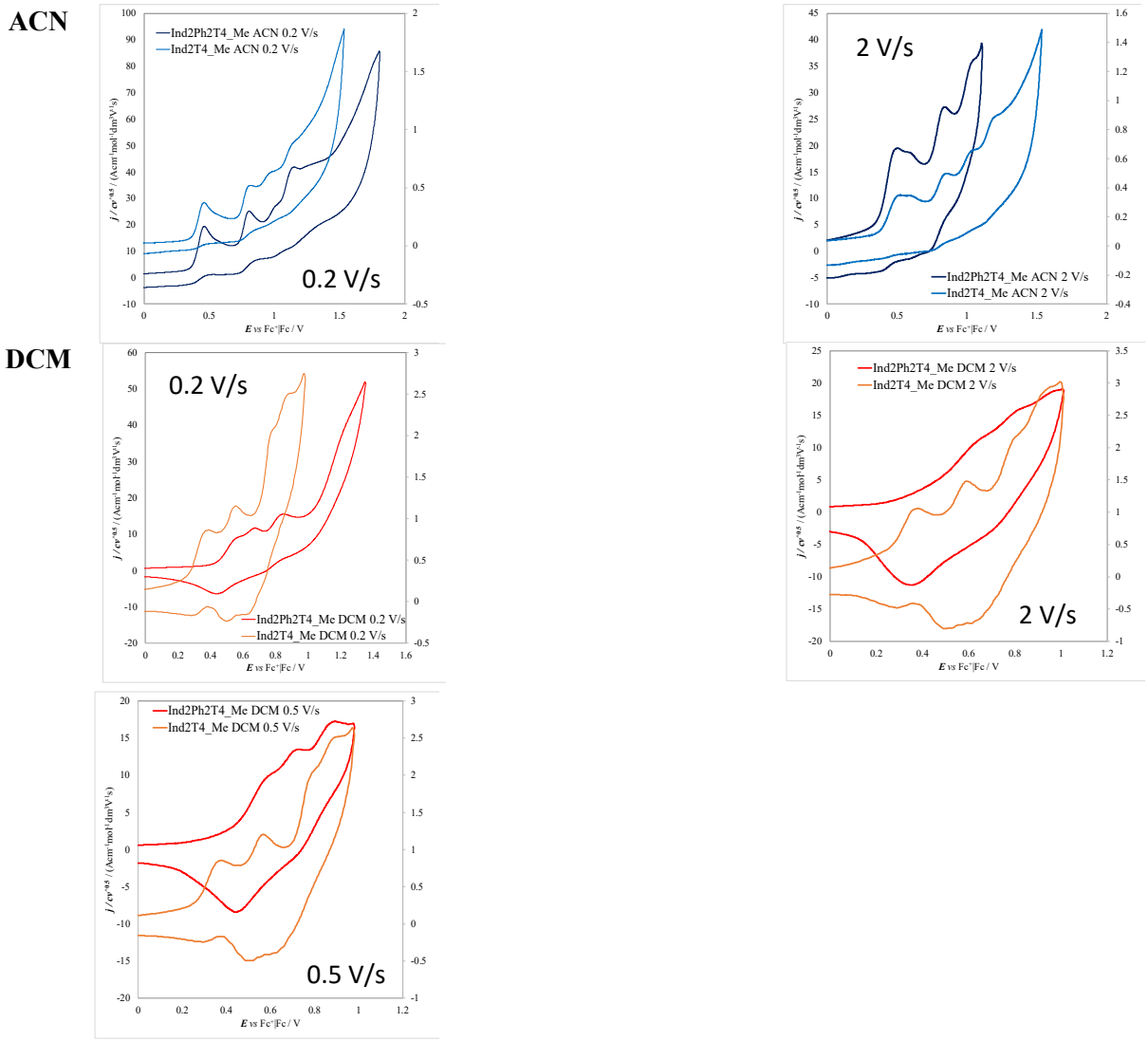
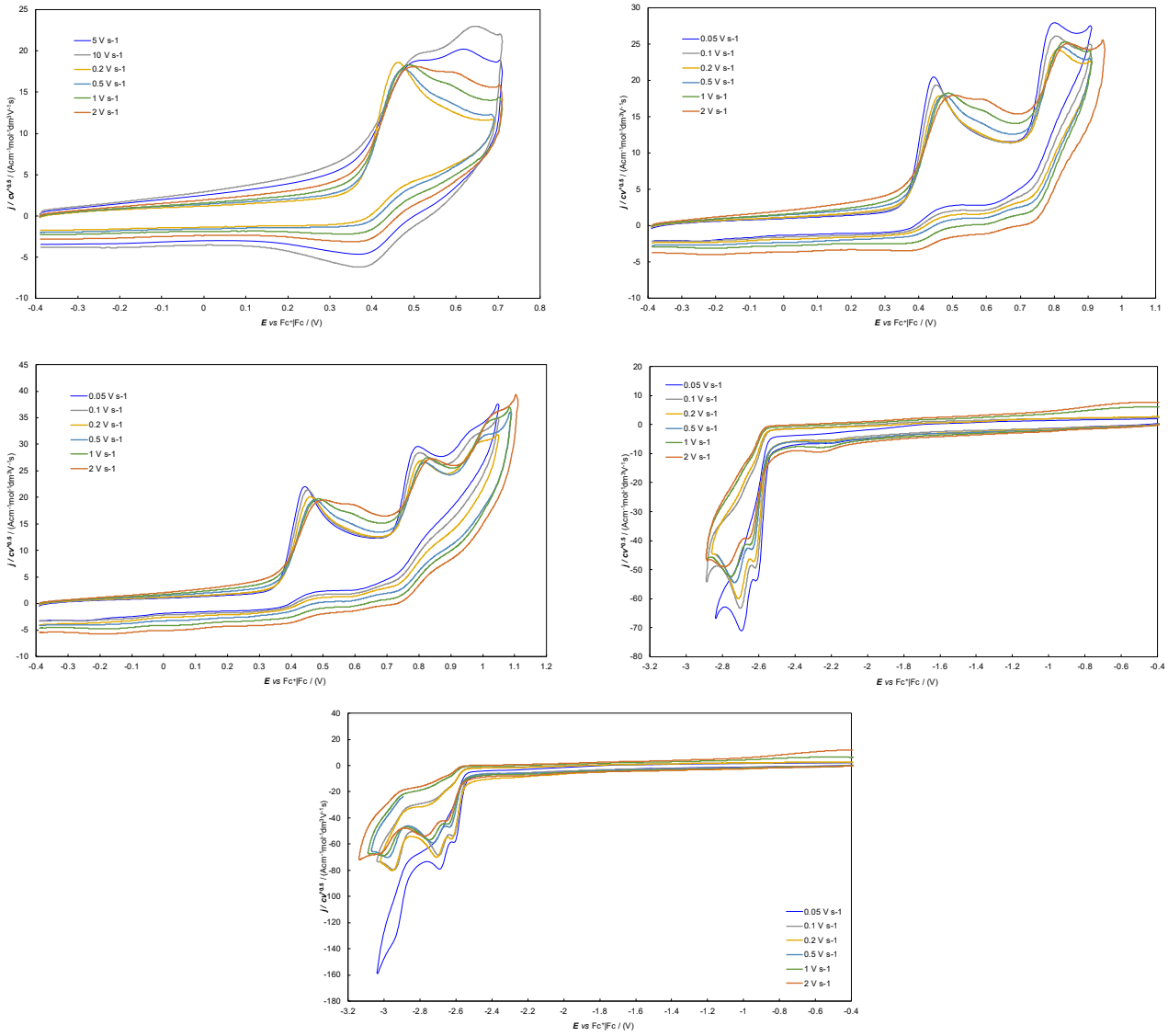


Figure SI 3.1. Comparison between the oxidative CV features of inherently chiral monomers (N-Me-IND)$_2$-T$_4$ and 1, in CH_3CN (top) and in CH_2Cl_2 (bottom), at different scan rates.

b) *Detailed CV features of 1 as a function of scan rate,* in CH_3CN and in CH_2Cl_2

CH_3CN



CH_2Cl_2

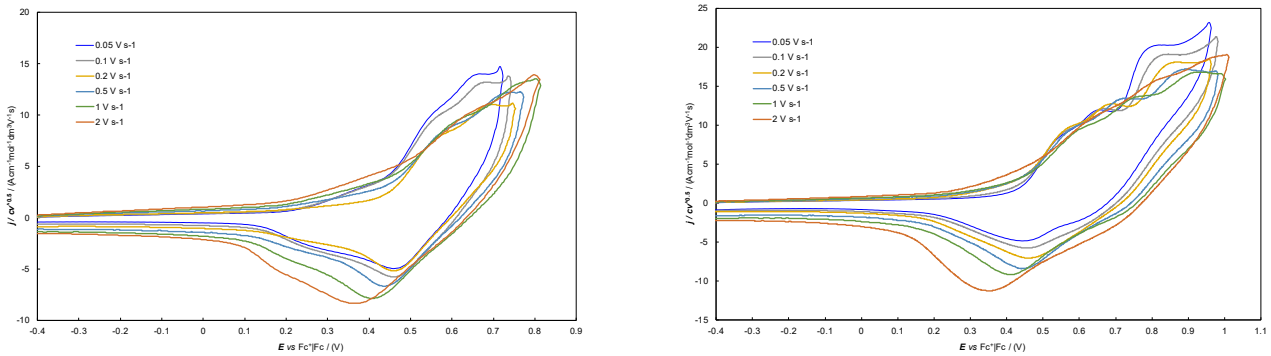
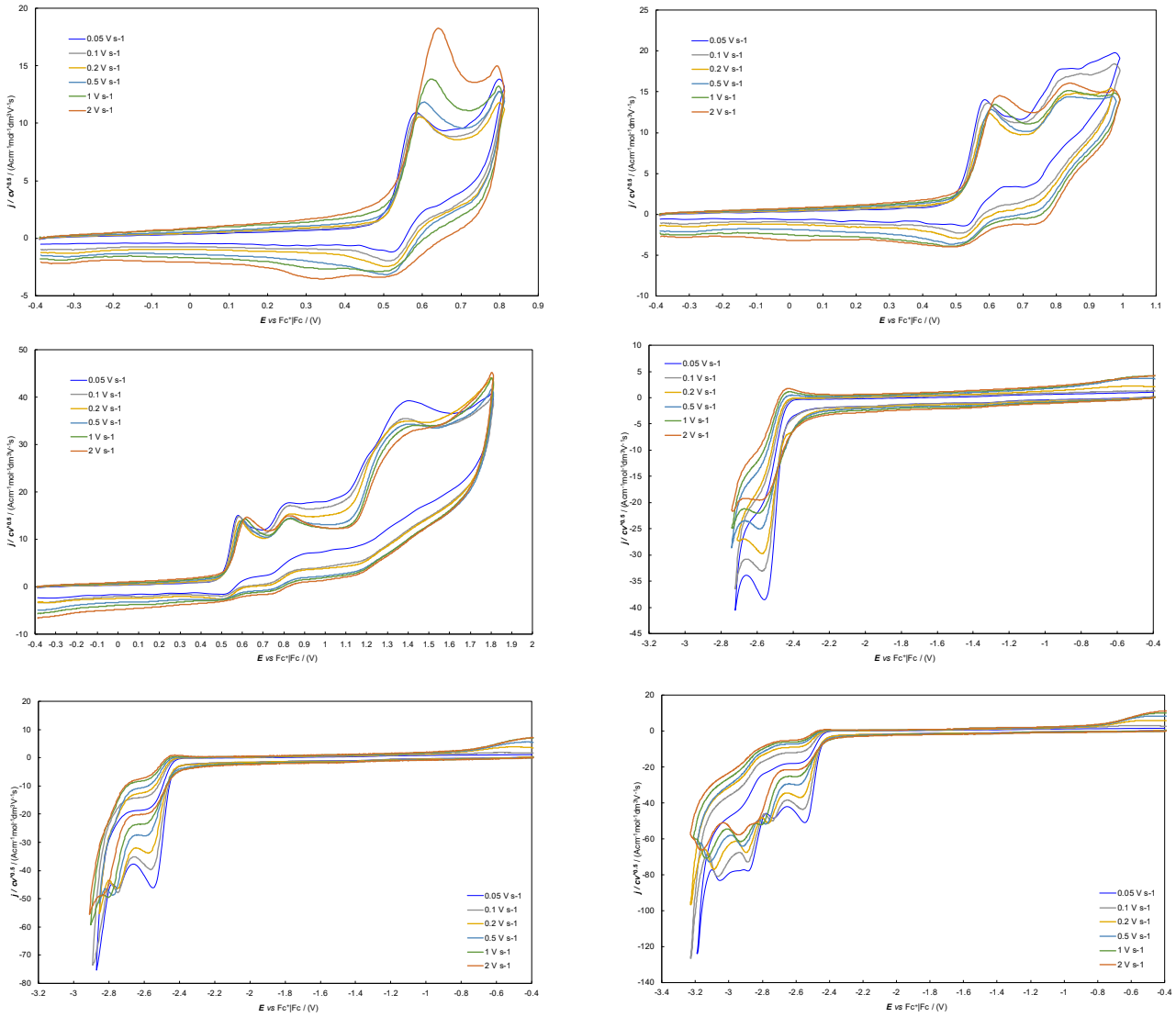


Figure SI 3.2 Detailed CV features of **1** as a function of scan rate, in CH_3CN and in CH_2Cl_2

c) *Detailed CV features of 2 as a function of scan rate,* in CH_3CN and in CH_2Cl_2

CH_3CN



CH_2Cl_2

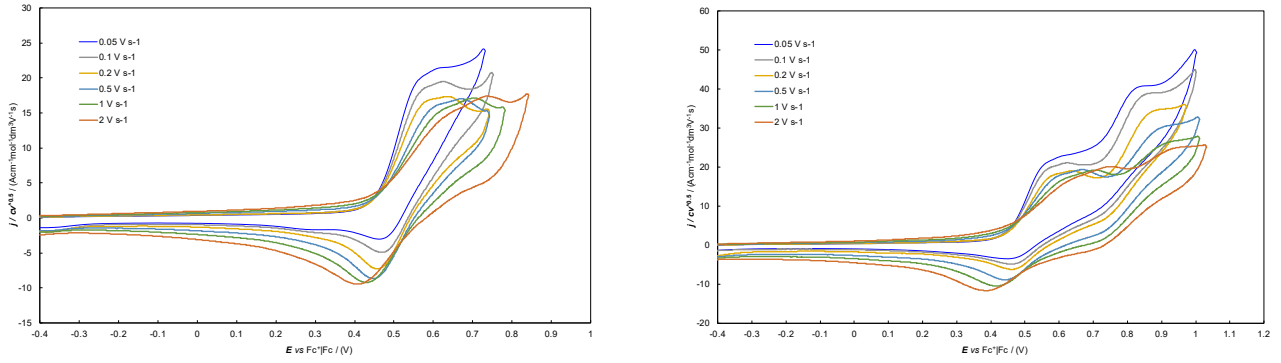
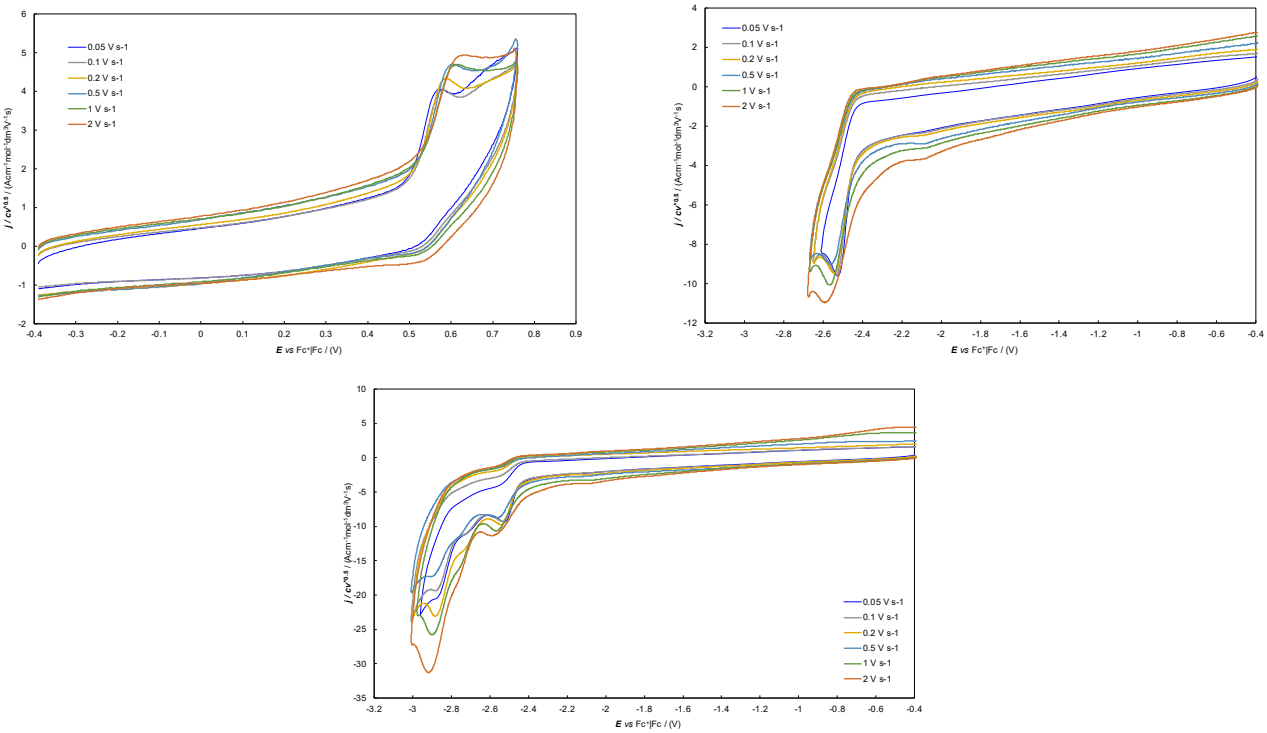


Figure SI 3.3. Detailed CV features of **2** as a function of scan rate, in CH_3CN and in CH_2Cl_2

d) *Detailed CV features of 3.as a function of scan rate,* in CH_3CN and in CH_2Cl_2

CH_3CN



CH_2Cl_2

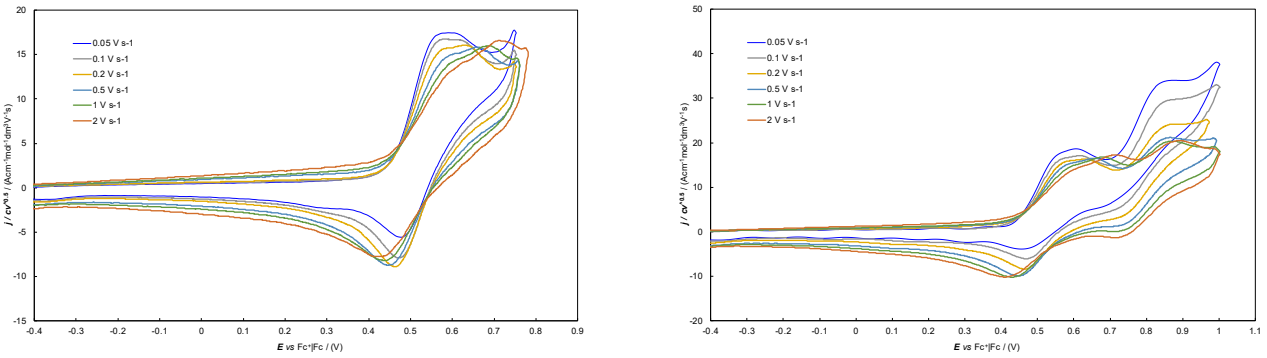


Figure SI 3.4. Detailed CV features of **3** as a function of scan rate, in CH_3CN and in CH_2Cl_2

e) Estimation of HOMO and LUMO levels from first oxidation and first reduction potentials.

There are different alternative conventions for the calculations of HOMO and LUMO values from CV first oxidation and first reduction potentials, differing in the estimation of the absolute potential of the reference couple $Fc|Fc^+$. A detailed 2011 survey is proposed in [SI 1]. Here, as in former papers (like e.g. [SI 2, SI 3]) we have employed the relationships

E_{HOMO} / eV = -1 e × [$E_{p,I\,a}$ *vs* $Fc^+|Fc$ /V + 4.8 V ($Fc^+|Fc$ *vs* zero)]

E_{LUMO} / eV = -1 e × [$E_{p,I\,c}$ *vs* $Fc^+|Fc$ /V + 4.8 V ($Fc^+|Fc$ *vs* zero)]

using first oxidation and reduction peak potentials (considerations about using onset, peak or formal potentials are provided in [SI 3]). The above relationships are adopted in many literature papers starting from [SI 4] (see [SI 1] and literature cited), and look consistent with calculation of $Fc^+|Fc$ absolute potentials either in water from absolute SHE potential in water [SI 5] combined with aqueous SCE and $Fc^+|Fc$ data, the latter redox couple assumed to have negligible solvent effects [SI 6, SI 7], or absolute SHE potential in acetonitrile [SI 4] combined with $Fc^+|Fc$ vs NHE data in the same solvent [SI 7].

In any case, alternative conventions would lead to small differences of a few tens of eV (constant for all values and therefore resulting in the same trends).

[SI 1] C. M. Cardona, W. Li, A.E. Kaifer, D. Stockdale, G. C. Bazan, *Adv. Mater*. **2011**, *23*, 2367-2371.

[SI 2] T. Benincori, M Capaccio, F. De Angelis, L. Falciola, M. Muccini, P. Mussini, A. Ponti, S. Toffanin, P. Traldi, F. Sannicolò, *Chem. Eur. J*. **2008**, *14*, 459 – 471.

[SI 3] A. Tacca, R. Po, M. Caldararo, S. Chiaberge, L. Gila, L. Longo, P.R. Mussini, A.Pellegrino, N.Perin, M. Salvalaggio, A. Savoini, S. Spera, *Electrochim. Acta* **2011**, 56, 6638– 6653.

[SI 4] J. Pommerehnem H. Vestweber, W. Guss, R. Mahrt, H. Bässler, M. Porsch, J. Daub, *Adv. Mater*. **1995**, *7*, 551-554.

[SI 5] S. Trasatti, *Pure & Appl. Chem*. **1986**, *58*, 955-966.

[SI 6] G. Gritzner, J. Kuta, *Pure & Appl. Chem.* **1984**, *56*, 461-466.

[SI 7] H.-M. Koepp, H. Wendt, H. Strehlow, *Phys. Chem*. **1960**, *64*, 483-491.

SI.5 Comparison between electrooligomerization and stability cycles for 1,2 and 3 in CH_2Cl_2

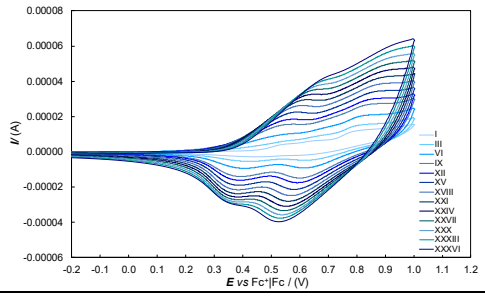
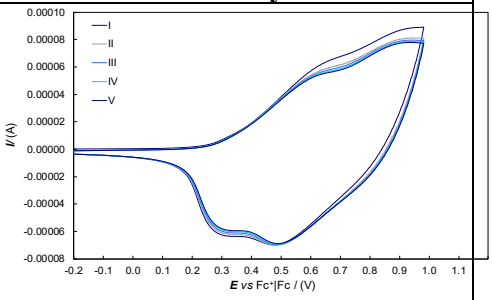
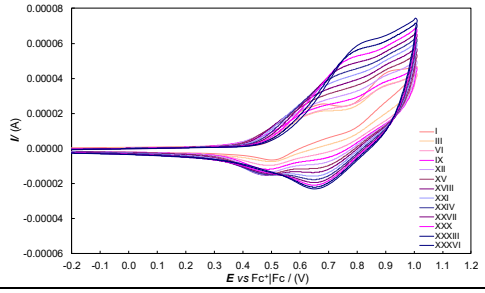
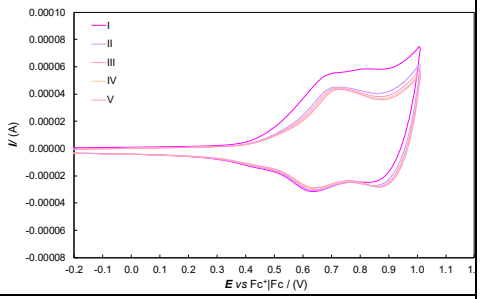
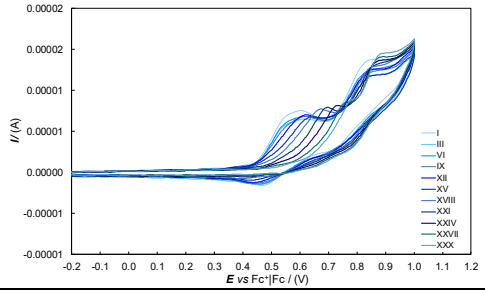
Monomer	Electrooligomerization	Stability
1		
2		
3		*(not available; film deposition neglible)*

Figure SI 4. Electrooligomerization of monomers 1, 2 and 3(0.00075 M in CH_2Cl_2 + 0.1 M $TBAPF_6$) on GC electrode by oxidative potential cycling at 0.05 V s^{-1} (left side) and stability cycles in monomer-free solution (right side). Electrodeposition and stability cycles are reported with the same scale to allow comparison of the electrooligomerization efficiency at first glance.

SI 6. Terazosin CV features

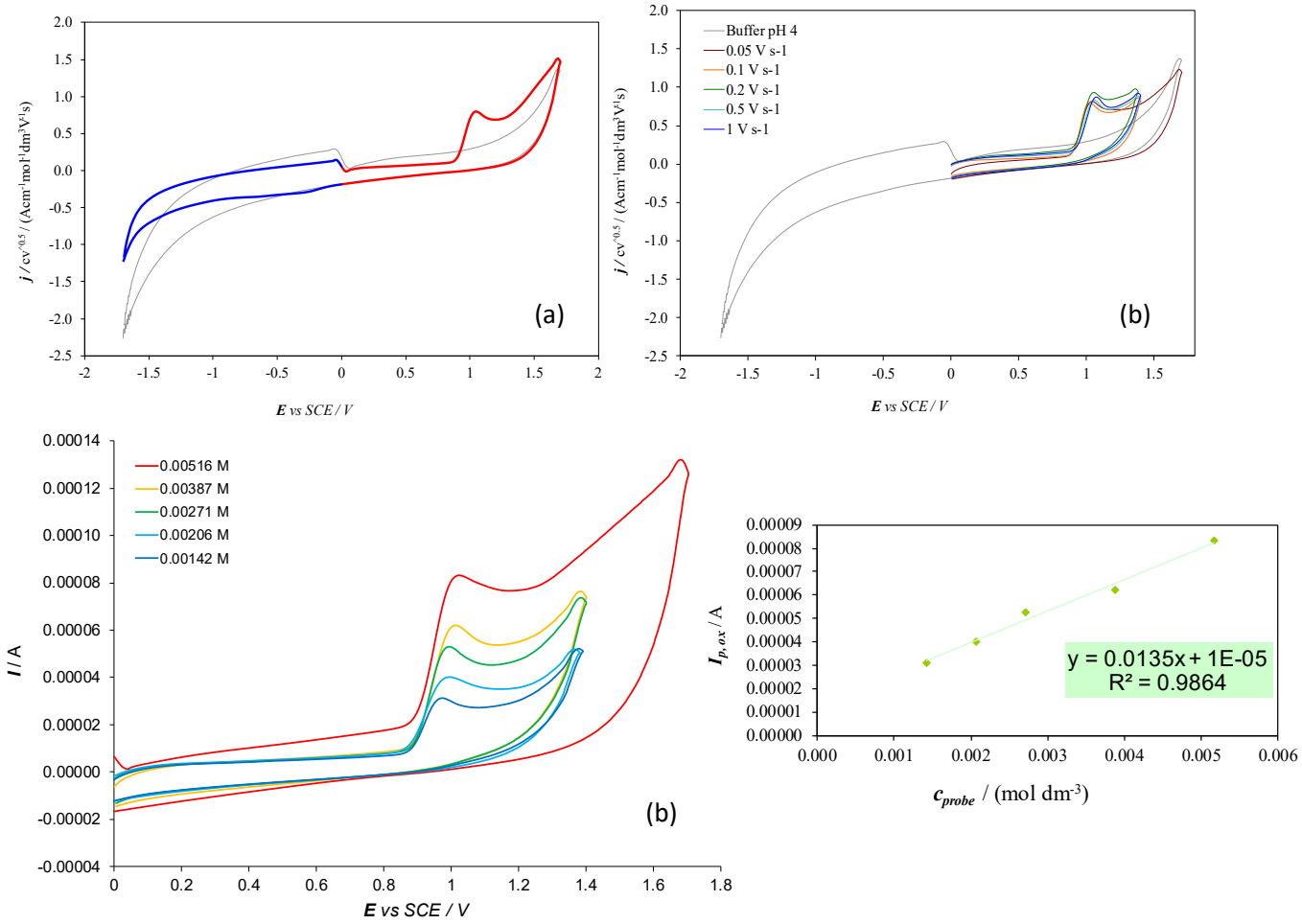


Figure SI 5. (a) Electrochemical characterization of terazosin, obtained at 0.2 V/s in pH 4 buffer, as combined pattern from oxidative and reductive half cycles (red and blue respectively; the background is also reported in grey); (b) focusing on the normalized CV patterns of the first oxidation peak in the 0.05-2 V/s range; (c) linear dynamic range tests on bare GC electrode for racemic terazosin.