SUPPORTING INFORMATION

Homoconjugation in Triptycenes: An Inquiry Through Photochromism

Kanyashree Jana and Jarugu Narasimha Moorthy[a,b,*]

[a] *Department of Chemistry, Indian Institute of Technology, Kanpur 208016, INDIA*

[b] *School of Chemistry, Indian Institute of Science Education and Research Thiruvananthapuram, Trivandrum 695551, INDIA*

[*]Corresponding Author; E-mail: moorthy@iitk.ac.in

TABLE OF CONTENTS

Single Crystal X-ray Structure Determinations. The single crystals of **Trip-chrom** were obtained by slow evaporation of chloroform/hexane mixture (9:1, v/v) at ambient temperature. Thus grown single crystals were subjected to intensity data collection in a CCD detector system equipped with Mo-sealed Siemens ceramic diffraction tube (λ = 0.7107 Å) and a highly oriented graphite monochromator operating at 50 kV and 30 mA. The structure was solved by direct methods using the SHELXL package and refined by the full matrix least-squares method based on F^2.

Table S1 X-Ray Crystallographic Data of **Trip-chrom**

Compound	**Trip-chrom**
molecular formula	$C_{35}H_{24}O$
formula weight	460.54
solvent for crystallization	Chloroform
crystal system	Monoclinic
space group	P 2_1/c
a (Å)	8.858(1)
b (Å)	14.662 (2)
c (Å)	18.902 (2)
α (deg)	90
β (deg)	102.09 (13)
γ (deg)	90
volume (Å^3)	2400.6 (17)
Z	4
calculated density (g/cm^3)	1.274
absorption coefficient (mm^{-1})	0.075
F (000)	968
goodness-of-fit on F^2	0.960
final *R* indices [$I>2\sigma(I)$]	R_1 = 0.0730, wR_2 = 0.1756
R indices (all data)	R_1 = 0.1746, wR_2 = 0.2308
CCDC deposition number	1979544

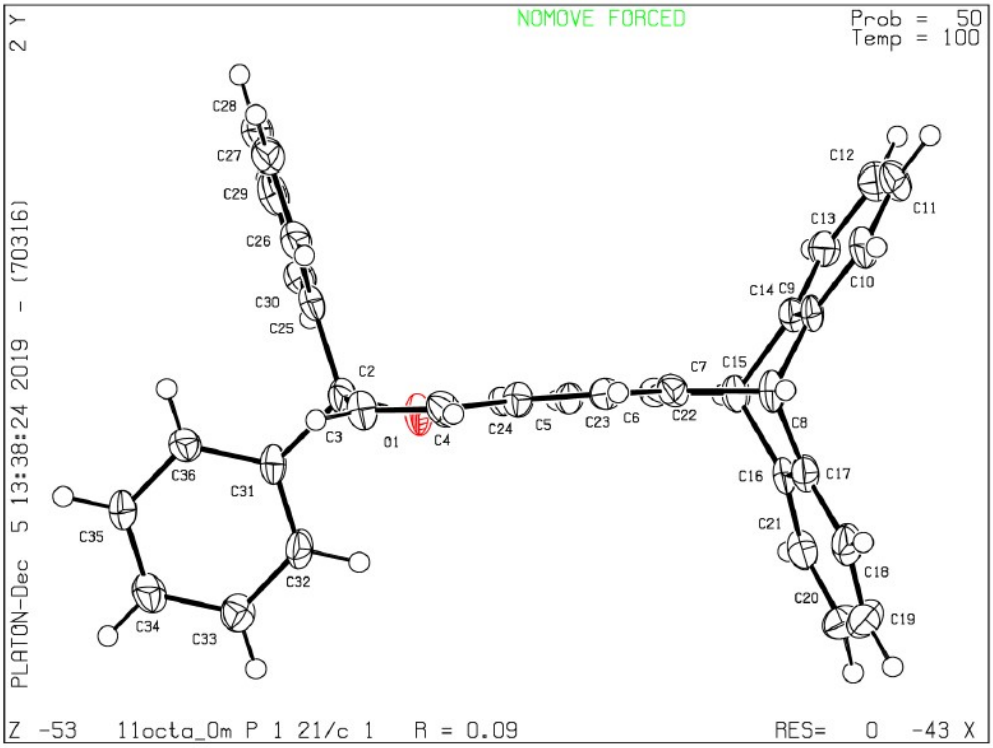

Fig. S1 Thermal ellipsoid plot for **Trip-chrom** drawn at the contour probability of 50%.

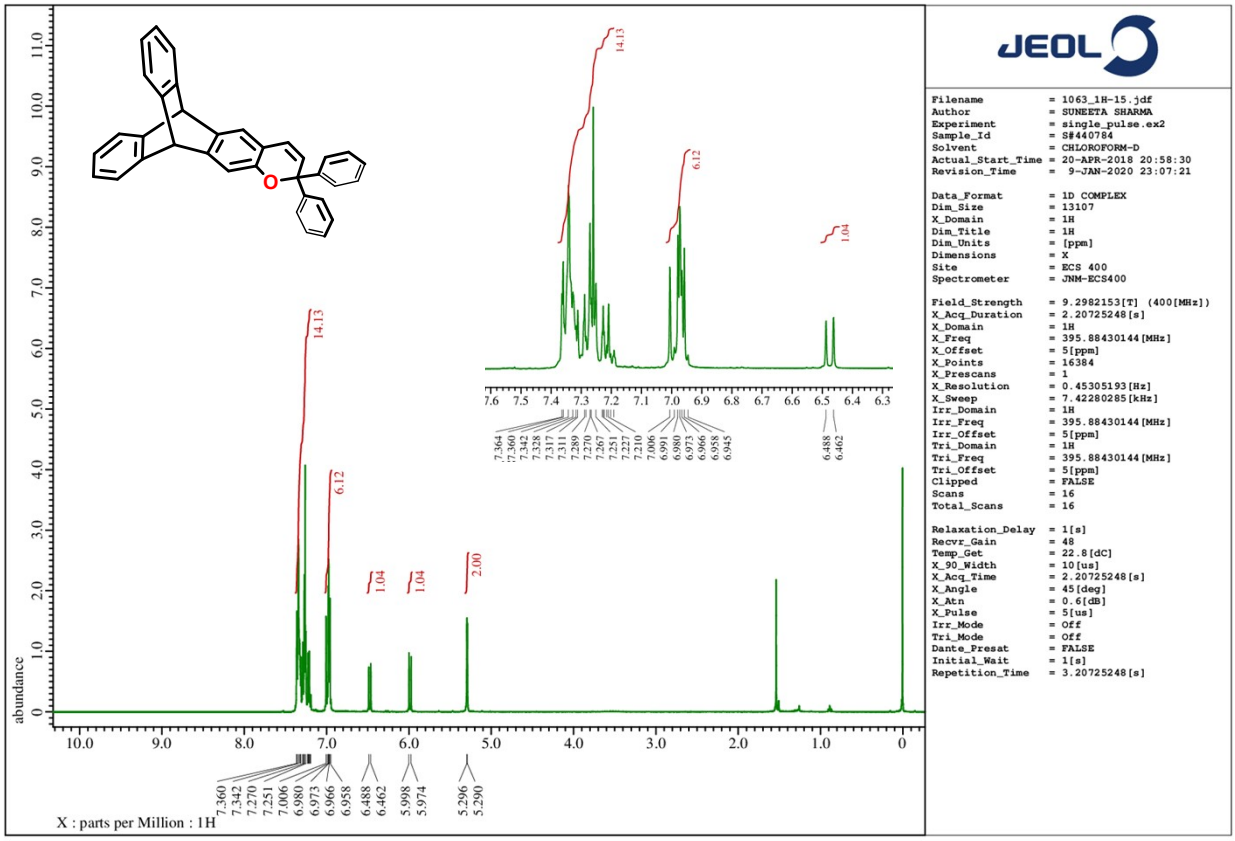

Fig. S2 ^{1}H NMR (400 MHz) spectrum of **4** in $CDCl_3$.

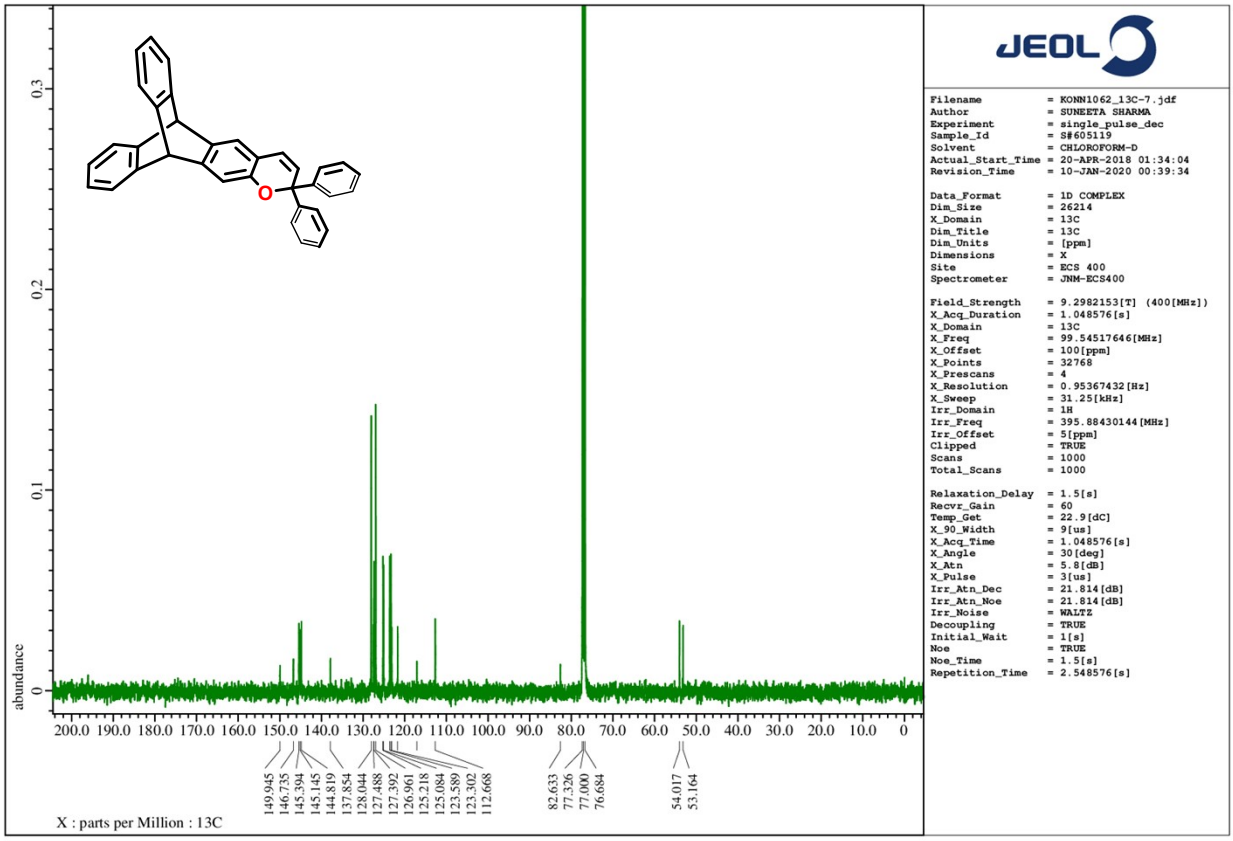

Fig. S3 ^{13}C NMR (100 MHz) spectrum of **4** in $CDCl_3$.

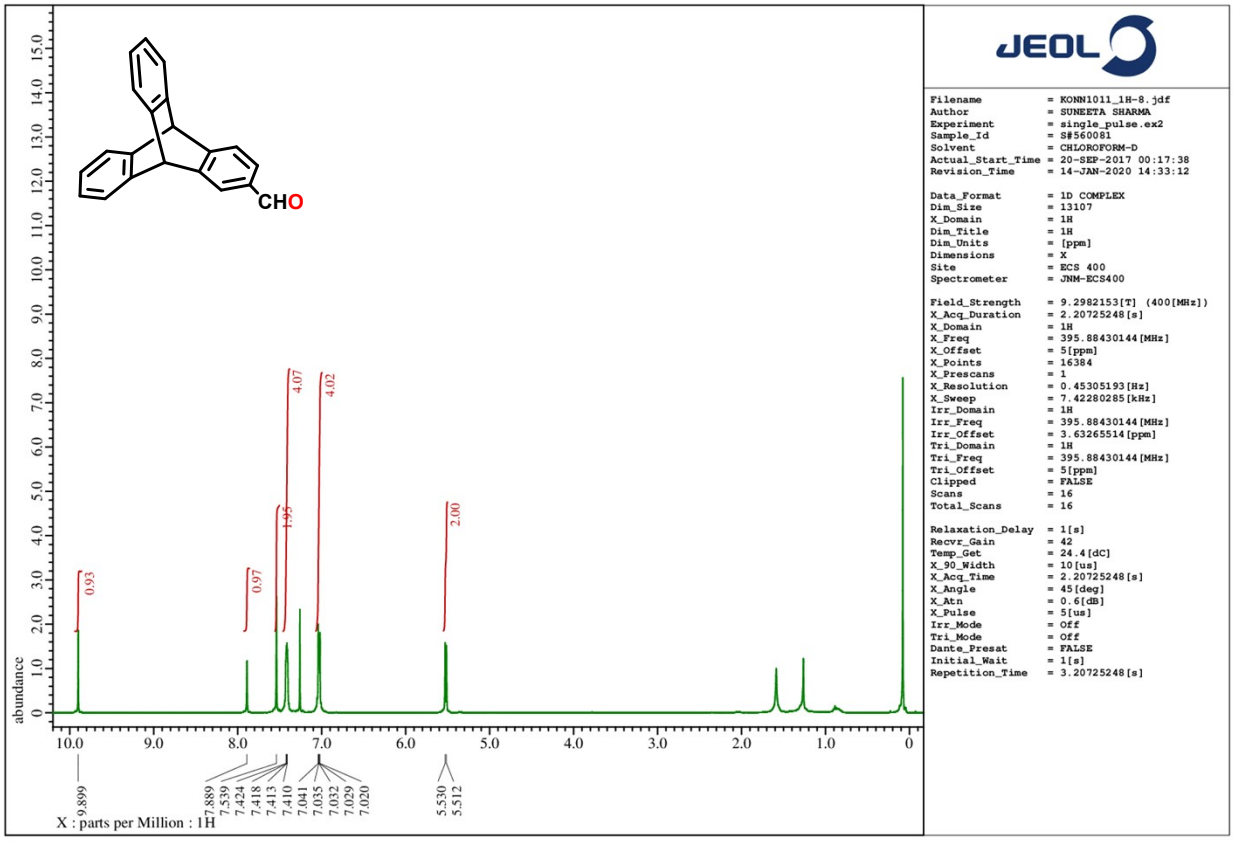

Fig. S4 ^{1}H NMR (400 MHz) spectrum of **2** in $CDCl_3$.

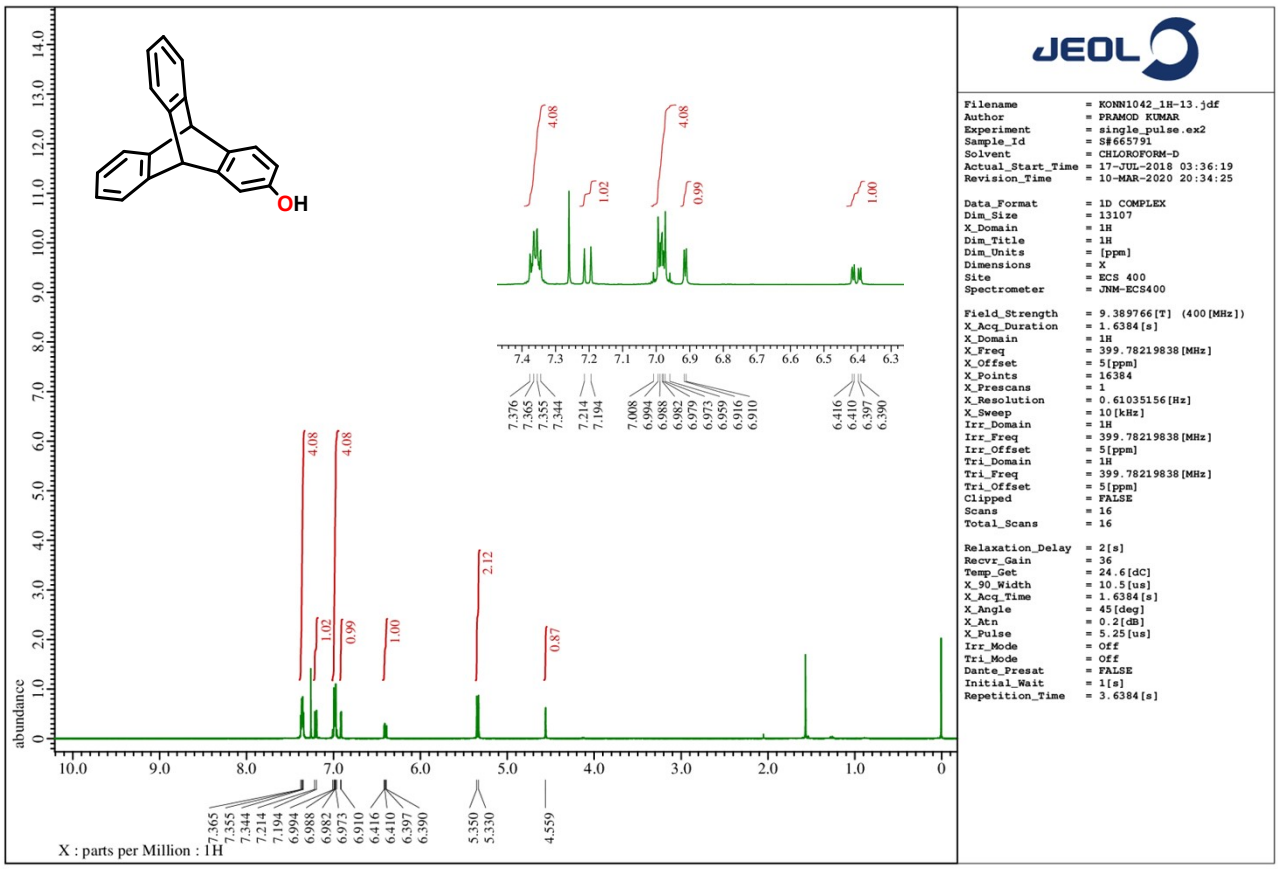

Fig. S5 ^{1}H NMR (400 MHz) spectrum of **3** in $CDCl_3$.

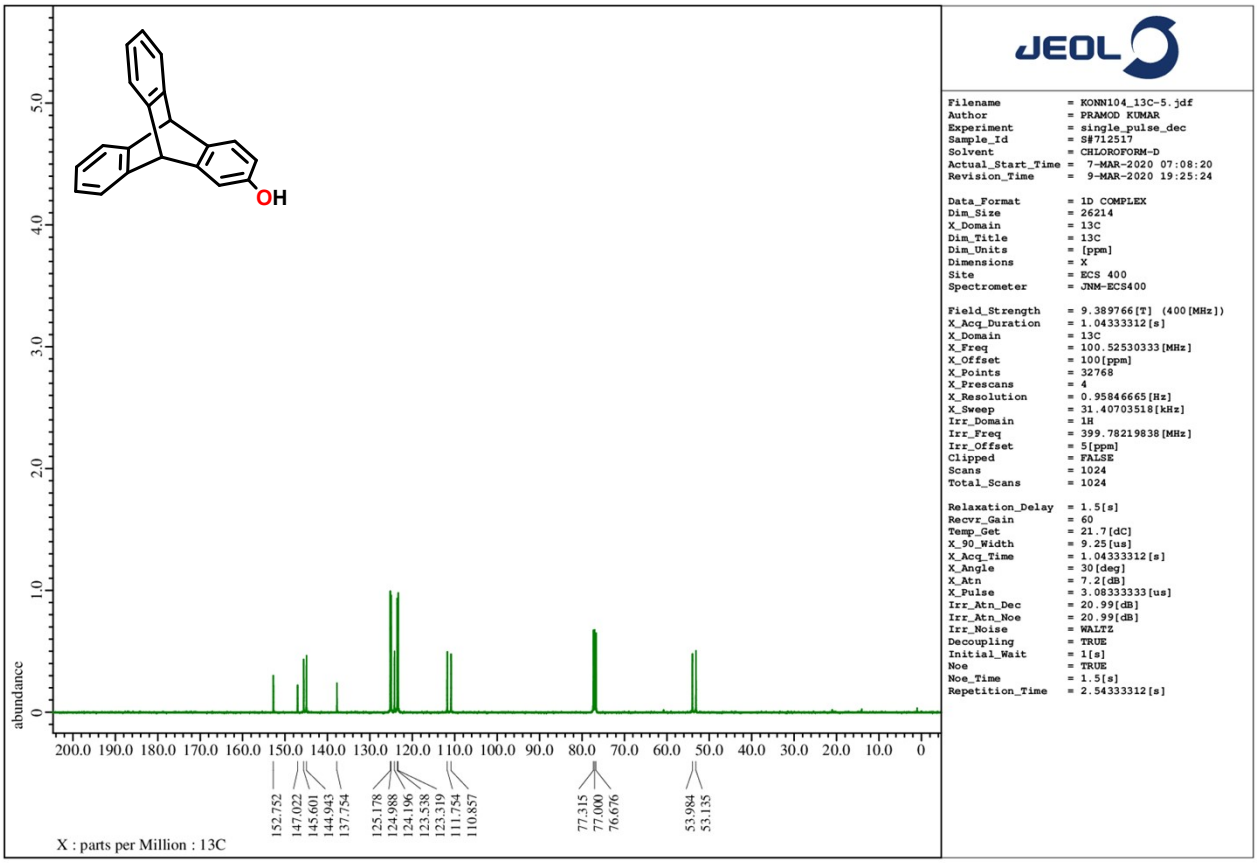

Fig. S6 ^{13}C NMR (100 MHz) spectrum of **3** in $CDCl_3$.

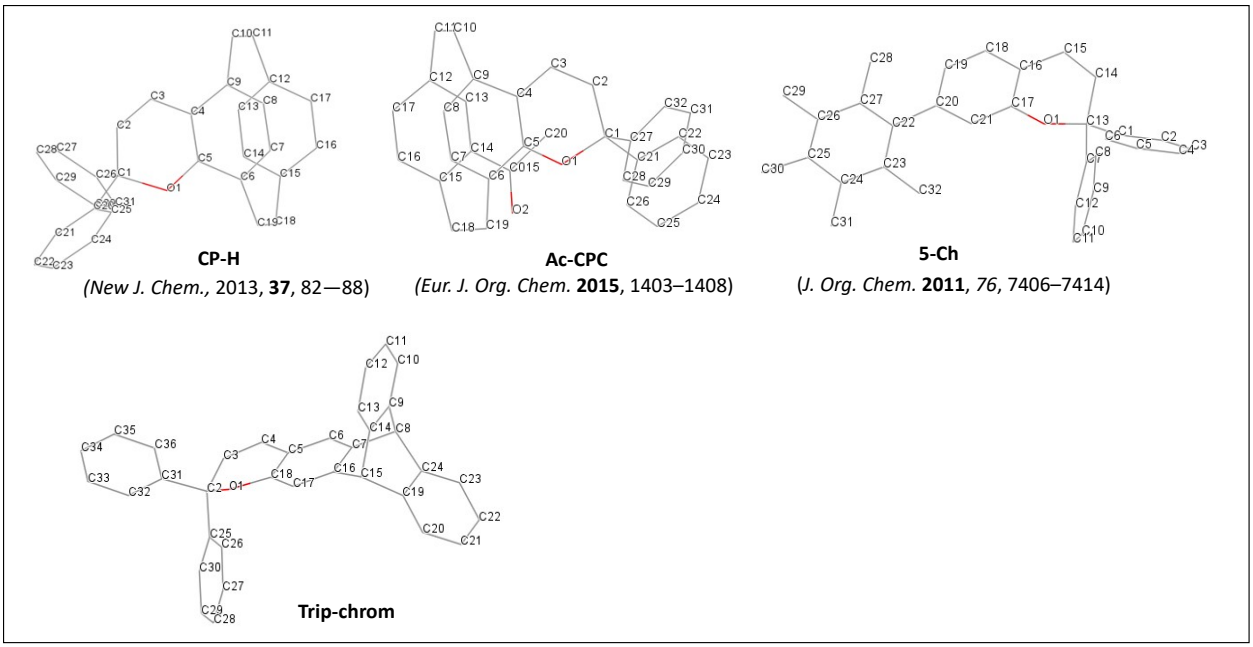

Fig. S7 Bond length comparison of **Trip-chrom** with other reported chromenes.

Table S2 Bond length comparison data

Compound	Bond	Bond length (Å)
CP-H	C9-C4	1.417
Ac-CPC	C9-C4	1.411
	C14-C15	1.420
5-Ch	C22-C23	1.409
	C22-C27	1.410
Trip-chrom	C7-C16	1.415

Theoretical Calculations

All the density functional theory calculations were performed using the Gaussian 09[1] program package. The geometry optimizations of all the molecules and their respective photogenerated intermediates namely, **Trip-chrom**, **Trip-chrom(TC)**, **Trip-chrom (TT)**, **BP**, **BP_TC**, **BP_TT**, **5-6Nap**, **5-6_TC**, **5-6_TT**, **7-8Nap**, **7-8_TC** and **7-8_TT**, were carried out using CAMB3LYP functional and 6-311G(d,p) basis set taking toluene as the solvent. Vibrational calculations of the optimized structures at the same level of theory were carried out to find their relative thermodynamic stabilities.

Table S3 Cartesian coordinates (in Angstroms) for the optimized structure of **Trip-chrom**

Atom type	X	Y	Z
O	-1.93446900	-0.71625700	-0.39600900
C	0.36122000	-0.44063600	-0.86084200
H	0.12501000	-0.48828700	-1.91676200
C	0.90950200	-0.33409300	1.87806000
H	1.11408900	-0.30277100	2.94326300
C	3.82805900	-1.31669000	-0.80449100
C	-0.66938900	-0.51531200	0.07087100
C	-3.22574500	1.24947700	0.10166900
C	-0.41198500	-0.47003100	1.44041300
C	1.65699000	-0.30477000	-0.40712900
C	3.58607100	1.10171600	-0.85471100
C	-5.54298300	-0.59127700	0.23231400
H	-5.67512200	0.36358800	0.72736500
C	3.86634900	1.15713100	0.51326100
C	3.92222300	2.15670900	-1.67975700
H	3.70341300	2.11417200	-2.74090300
C	2.90654100	-0.19663800	-1.27005900
H	2.69069800	-0.24049700	-2.33658900
C	4.37011700	-2.31696500	-1.58702000
H	4.15283300	-2.36139900	-2.64842800
C	-2.79011600	-0.52948800	1.86463600
H	-3.65546100	-0.65012600	2.50372300
C	-1.55056800	-0.61821800	2.33589800
H	-1.36541800	-0.81534000	3.38606100
C	-4.26034600	-1.04906500	-0.05908800
C	3.42068000	-0.09294900	1.26053900
H	3.63782600	-0.04914100	2.32699700
C	4.82464600	3.33311500	0.22166200

H	5.30928600	4.20770600	0.63898700
C	4.10777500	-1.25960200	0.56356900
C	1.93508300	-0.24721600	0.96284300
C	-4.11067800	-2.26874000	-0.70845700
H	-3.11700600	-2.62869800	-0.93480600
C	-5.22628900	-3.01417200	-1.06752300
H	-5.09453100	-3.96034700	-1.57913900
C	4.48417400	2.26744700	1.05388800
H	4.70218500	2.31106500	2.11518700
C	-3.35555500	1.64711900	-1.22908500
H	-3.32722900	0.89775300	-2.01074800
C	-6.50126500	-2.55529700	-0.77276200
H	-7.37036300	-3.13862300	-1.05250300
C	-3.04341600	-0.24411300	0.39909400
C	-3.42454700	3.55878800	0.77284900
H	-3.44705900	4.30173200	1.56127500
C	-6.65581700	-1.34046400	-0.11842200
H	-7.64713300	-0.96954300	0.11354300
C	-3.51398600	2.98270500	-1.55395000
H	-3.60996700	3.27698700	-2.59239900
C	4.93043200	-2.20296500	1.14691300
H	5.14817800	-2.15903600	2.20829500
C	-3.25702200	2.21592300	1.09699300
H	-3.14114300	1.92662600	2.13356700
C	-3.55224800	3.94532600	-0.55044200
H	-3.67822300	4.99121500	-0.80375300
C	4.54576300	3.27829100	-1.13450900
H	4.81245400	4.11003100	-1.77558600
C	5.47836100	-3.21349500	0.35775200
H	6.12433000	-3.95731200	0.80876800
C	5.20040900	-3.27016100	-0.99853900
H	5.62948000	-4.05805600	-1.60599500

Table S4 Cartesian coordinates (in Angstroms) for the optimized structure of **Trip-chrom (TC)**

Atom type	X	Y	Z
C	0.89294500	0.55312800	0.30005100
H	0.62504200	1.49486700	0.76843700
C	1.58783600	-1.91066300	-0.91990400

H	1.83514700	-2.85568400	-1.38849200
C	4.22298000	1.17717500	-0.73102200
C	2.17830400	0.21236300	0.13672400
C	4.20637700	0.09253200	1.45415800
C	4.53806100	-1.12498000	0.85374500
C	4.58852400	0.35434200	2.75655500
H	4.32874600	1.29749300	3.22408700
C	3.40797000	1.00995200	0.54160600
H	3.15392900	1.95938200	1.01081000
C	4.62004400	2.37045400	-1.30474100
H	4.36095400	3.31456300	-0.83867900
C	4.03150900	-1.24875200	-0.57484600
H	4.30230100	-2.19424800	-1.04156600
C	5.63869500	-1.81354800	2.86620900
H	6.20014700	-2.55511800	3.42168100
C	4.55411700	-0.03907800	-1.33420300
C	2.52631600	-1.05374600	-0.48866900
C	5.24883700	-2.08006200	1.55602700
H	5.50159000	-3.02628900	1.09099500
C	5.27871300	-0.06128000	-2.51113000
H	5.53103300	-1.00518800	-2.98105900
C	5.31079300	-0.60492100	3.46212700
H	5.61692400	-0.40516400	4.48202500
C	5.68332400	1.14102600	-3.08589700
H	6.25573300	1.13163200	-4.00566300
C	5.35642600	2.34831600	-2.48674500
H	5.67432100	3.27962500	-2.93998300
C	0.16238100	-1.61103900	-0.78911200
C	-0.18676100	-0.31481200	-0.13446000
C	-1.46905900	0.09399500	0.08547300
H	-1.57863600	1.06034000	0.56879700
C	-2.68611000	-0.60682300	-0.20337400
H	-2.58203800	-1.61706600	-0.56951100
C	-3.92553100	-0.08954700	-0.02024600
C	-5.12153900	-0.94296200	-0.20420400
C	-5.08327900	-2.31200900	0.08034300
C	-6.31717600	-0.39910900	-0.68353400
C	-6.19722600	-3.10997300	-0.12108900
H	-4.17772300	-2.74918100	0.48134400
C	-7.42874000	-1.20009800	-0.89228700

H	-6.36967900	0.65860700	-0.90833300
C	-7.37355400	-2.55819800	-0.61154300
H	-6.14869400	-4.16669300	0.11260700
H	-8.34167500	-0.76121800	-1.27662800
H	-8.24436700	-3.18322300	-0.76860900
C	-4.15450800	1.33246400	0.34542000
C	-4.91519200	1.65511700	1.47174200
C	-3.63278800	2.36916900	-0.42892800
C	-5.12405300	2.97748700	1.82785100
H	-5.33624600	0.85969900	2.07496600
C	-3.85483600	3.69438600	-0.07987800
H	-3.06494700	2.13160900	-1.32036100
C	-4.59563800	4.00175300	1.05167200
H	-5.70468100	3.21064800	2.71231800
H	-3.44992600	4.48719000	-0.69735500
H	-4.76702100	5.03571000	1.32593200
O	-0.67864900	-2.40183200	-1.20513700

Table S5 Cartesian coordinates (in Angstroms) for the optimized structure of **Trip_chrom (TT)**

Atom type	X	Y	Z
C	0.68227000	0.18990700	0.03881300
H	0.23546300	1.11120700	0.39288800
C	1.91287300	-2.22306800	-0.86064300
H	2.36591600	-3.14503200	-1.20483200
C	3.93447400	1.30240800	-0.78776100
C	2.01599500	0.06189700	0.01260500
C	3.90241300	0.42458200	1.48886600
C	4.49699800	-0.75845700	1.04248700
C	4.10844800	0.86317700	2.78354300
H	3.64465300	1.77945000	3.13121900
C	3.04643600	1.09961500	0.42923400
H	2.58815500	2.02361000	0.77901200
C	4.16766900	2.49438700	-1.44779600
H	3.70460300	3.41153400	-1.10134500
C	4.15642600	-1.09450800	-0.40085600
H	4.63014700	-2.01130800	-0.74750100
C	5.50819000	-1.05706400	3.19280400
H	6.13694100	-1.63197700	3.86200200

C	4.52842200	0.12006500	-1.23688000
C	2.63889000	-1.17249800	-0.45122300
C	5.29546800	-1.50269500	1.89069200
H	5.75310700	-2.42282200	1.54519100
C	5.35325000	0.12990700	-2.34613400
H	5.81022000	-0.78853900	-2.69694000
C	4.91873400	0.11753900	3.63608000
H	5.08835300	0.45736900	4.65072800
C	5.59309300	1.33201400	-3.00701800
H	6.24239200	1.34870300	-3.87408700
C	5.00450500	2.50595100	-2.56087400
H	5.19553400	3.43717800	-3.08059200
C	0.45077500	-2.17133900	-0.86290600
C	-0.17653600	-0.89471200	-0.39281400
C	-1.53377200	-0.84397600	-0.40206900
H	-2.02722700	-1.74991500	-0.73616000
C	-2.35383300	0.28009400	-0.05107400
H	-1.85552900	1.22192300	0.14494600
C	-3.70574200	0.27270800	0.01922900
C	-4.44055400	1.53959600	0.24928700
C	-4.00250600	2.74114900	-0.31481000
C	-5.58611300	1.56087200	1.04989000
C	-4.67742100	3.92712300	-0.07231200
H	-3.14137200	2.73943500	-0.97166000
C	-6.25492400	2.74859700	1.29943900
H	-5.94552500	0.63904800	1.48978700
C	-5.80343800	3.93616800	0.73957900
H	-4.32862800	4.84613700	-0.52791400
H	-7.13358700	2.74648400	1.93322300
H	-6.33160200	4.86298700	0.92827600
C	-4.51129000	-0.96705000	-0.10961300
C	-5.58312200	-1.01520100	-1.00472900
C	-4.23171600	-2.09643700	0.66060300
C	-6.33414400	-2.17021000	-1.14542800
H	-5.81814900	-0.14199900	-1.60134900
C	-4.99347000	-3.24886000	0.52892400
H	-3.42146400	-2.06455600	1.37844000
C	-6.04209400	-3.29082000	-0.37760700
H	-7.15172300	-2.19653100	-1.85575600
H	-4.76457100	-4.11528200	1.13738400

H	-6.63362300	-4.19209300	-0.48409600
O	-0.21880000	-3.12627200	-1.23350300

Table S6 Cartesian coordinates (in Angstroms) for the optimized structure of **7-8Nap**

Atom type	X	Y	Z
O	0.07252200	-0.67222000	-0.01552200
C	2.42263500	-0.54637000	-0.28584900
C	1.28109500	-0.40472300	0.54489700
C	-1.22385300	1.35169300	-0.04256700
C	1.39536100	-0.09046000	1.87971000
C	-3.57790800	-0.42623100	0.14845300
H	-3.74247000	0.61375300	0.40414100
C	-1.01407400	-0.05828000	2.06245300
H	-1.94262000	-0.05572600	2.61863100
C	0.17043100	-0.05524900	2.66562900
H	0.24593600	-0.04797200	3.74738400
C	-2.28302800	-0.93824600	0.12646300
C	-2.09044400	-2.27127100	-0.21774700
H	-1.08796500	-2.67541900	-0.23300300
C	-3.17453000	-3.07566600	-0.54400300
H	-3.00843800	-4.11110500	-0.81706000
C	-1.23450900	1.48653000	-1.43100700
H	-1.16893300	0.60063200	-2.05097700
C	-4.46222300	-2.56142600	-0.51893800
H	-5.30693400	-3.19066100	-0.77257400
C	-1.10806700	-0.05692300	0.55167900
C	-1.40887100	3.74948700	0.15495700
H	-1.47405200	4.63085900	0.78184700
C	-4.66055300	-1.23281600	-0.16845900
H	-5.66167800	-0.81883300	-0.14886100
C	-1.32678700	2.73611900	-2.01779400
H	-1.33004200	2.82557700	-3.09762700
C	-1.30713300	2.49244300	0.74307700
H	-1.28548600	2.40682100	1.82178700
C	-1.41778200	3.87468800	-1.22380400
H	-1.49267800	4.85344400	-1.68242900
C	3.70232100	-0.33756600	0.29071400
C	4.72143600	-0.81059700	-1.85407900
H	5.60534600	-0.91521500	-2.47190300

C	3.44592800	-1.01678700	-2.42107900
H	3.36159900	-1.27631500	-3.46948800
C	2.68237400	0.11550400	2.43113600
H	2.76071100	0.36186700	3.48420200
C	3.80325400	0.00199600	1.66474000
H	4.78484500	0.16163100	2.09483600
C	2.32095700	-0.88621800	-1.65581800
C	4.84416800	-0.47803900	-0.53389900
H	1.33827000	-1.03761600	-2.08129600
H	5.82321600	-0.31750800	-0.09662000

Table S7 Cartesian coordinates (in Angstroms) for the optimized structure of **7-8_TC**

Atom type	X	Y	Z
C	3.92412800	-0.50775000	0.08230100
C	1.69465300	0.66357400	-0.16875900
C	-0.62289200	-0.32233700	-0.05787900
H	-0.22799200	-1.32405300	0.01520900
C	0.33401100	0.73561000	-0.20756200
H	-0.07602400	1.72109100	-0.40715800
C	4.57714900	0.71199200	-0.15687700
C	6.70247200	-0.41294400	0.07707500
H	7.78544800	-0.37512900	0.07493900
C	6.04955000	-1.62139100	0.31362100
H	6.62221600	-2.52255000	0.49504200
C	2.45720700	1.87795500	-0.40313700
H	1.89265100	2.78538500	-0.58841900
C	3.79610300	1.91085000	-0.39909900
H	4.32610500	2.83876300	-0.57902800
C	4.66850100	-1.66314900	0.31591500
C	5.97513400	0.73936500	-0.15494500
H	4.13242600	-2.58559500	0.49798800
H	6.48564700	1.67801600	-0.33820500
C	2.44105000	-0.59474900	0.09650900
O	1.88913200	-1.66333300	0.31781600
C	-1.96538600	-0.13705200	-0.03097300
C	-2.87611900	-1.30486300	-0.02533800
C	-2.58791400	1.21132800	0.01567200
C	-2.53073700	-2.49414900	-0.67573100
C	-4.10149000	-1.24862100	0.64573500

C	-2.24599400	2.12866700	1.00995100
C	-3.54396400	1.57855400	-0.93433200
C	-3.37488400	-3.59169700	-0.64344700
H	-1.60156400	-2.55058300	-1.22843600
C	-4.94172000	-2.35007000	0.68407700
H	-4.39014900	-0.33720100	1.15369200
C	-2.83427100	3.38550900	1.04630700
H	-1.52719800	1.84496200	1.76906900
C	-4.12007000	2.83810400	-0.90610000
H	-3.82747600	0.87138400	-1.70462100
C	-4.58229800	-3.52552700	0.03953300
H	-3.09193100	-4.50080400	-1.16025800
H	-5.88112200	-2.28973300	1.22040300
C	-3.76779900	3.74530000	0.08574500
H	-2.56372700	4.08255800	1.83030500
H	-4.84947000	3.11254300	-1.65867100
H	-5.24215100	-4.38439200	0.06405200
H	-4.22525400	4.72696100	0.11200900

Table S8 Cartesian coordinates (in Angstroms) for the optimized structure of **7-8_TT**

Atom type	X	Y	Z
C	4.13150200	0.19357100	-0.11276300
C	1.65282800	-0.33153900	-0.00023700
C	-0.81906300	-0.67952700	0.01298400
H	-0.70227300	-1.75411600	0.08379900
C	0.37314800	0.11143500	-0.10230500
H	0.26213800	1.16827700	-0.31682000
C	4.40460200	-1.15128200	0.18298900
C	6.76775800	-0.66374700	0.07020100
H	7.79574400	-0.99897100	0.14139900
C	6.49060700	0.66974600	-0.22286300
H	7.30044900	1.37154500	-0.37964500
C	2.02877100	-1.69828400	0.30635500
H	1.24497600	-2.42491400	0.47814000
C	3.30938300	-2.08327000	0.39219100
H	3.55847900	-3.11205400	0.62534000
C	5.17722500	1.09183400	-0.31267600
C	5.73693400	-1.56368500	0.27100500
H	4.92899300	2.12085800	-0.53891500

H	5.95614700	-2.60062600	0.49904500
C	2.73173000	0.67541200	-0.21751900
O	2.48547400	1.84335300	-0.47175100
C	-2.08371600	-0.19683900	0.00342000
C	-3.23255200	-1.13357100	-0.01514200
C	-2.38947200	1.25532900	0.02905400
C	-3.17445700	-2.33449200	-0.72826200
C	-4.39887600	-0.84042900	0.69727800
C	-1.82911000	2.09657200	0.99085200
C	-3.26485600	1.80331900	-0.91207100
C	-4.23968700	-3.22086100	-0.71408800
H	-2.29646700	-2.56203600	-1.32014100
C	-5.46002600	-1.73141100	0.71826900
H	-4.46629000	0.08834600	1.24975300
C	-2.12370900	3.45263300	1.00283400
H	-1.17063200	1.68074800	1.74342800
C	-3.54747800	3.15911700	-0.90788800
H	-3.71599900	1.15993000	-1.65787600
C	-5.38461000	-2.92500200	0.01320800
H	-4.17922300	-4.14175800	-1.28160200
H	-6.35029800	-1.49209500	1.28734800
C	-2.97836200	3.98809500	0.05098900
H	-1.68279500	4.09043100	1.75922700
H	-4.21576200	3.57115700	-1.65442000
H	-6.21739300	-3.61776700	0.02365900
H	-3.20466400	5.04747400	0.05740200

Table S9 Cartesian coordinates (in Angstroms) for the optimized structure of **5-6Nap**

Atom type	X	Y	Z
O	0.42199000	-0.70259500	0.87676800
C	-1.61130600	-0.52594500	2.04592200
H	-1.02895300	-0.54617100	2.95806900
C	-0.93080000	-0.57826200	0.81399100
C	1.35536100	1.29674500	-0.08054400
C	-1.60251200	-0.58044600	-0.38878900
C	3.66019400	-0.40628500	-0.81253300
H	3.57005300	0.52581800	-1.35764000
C	0.52976600	-0.62264300	-1.53126700
H	1.15922800	-0.79245000	-2.39525100

C	-0.79148500	-0.76507200	-1.58564000
H	-1.26551300	-1.06273700	-2.51207700
C	2.55777200	-0.92392400	-0.13711300
C	2.69641900	-2.11341100	0.56853800
H	1.84311000	-2.52066800	1.09221200
C	3.92029300	-2.76878900	0.60620700
H	4.01526500	-3.69154300	1.16638300
C	1.82218000	1.79249200	1.13671100
H	2.06092600	1.09956800	1.93435500
C	5.01475300	-2.24996400	-0.06912200
H	5.96865200	-2.76279300	-0.03945500
C	1.20406000	-0.22098600	-0.23847400
C	1.21110700	3.55923300	-0.90633500
H	0.96703600	4.24488600	-1.70906300
C	4.87945400	-1.06624400	-0.78184400
H	5.72842100	-0.64932700	-1.31050800
C	1.97642700	3.15388100	1.33077500
H	2.33624100	3.52511300	2.28308000
C	1.04817700	2.19052800	-1.09659000
H	0.67020700	1.82323400	-2.04204800
C	1.67332300	4.04376100	0.30557300
H	1.79581400	5.10973000	0.45602400
C	-3.02760500	-0.47924300	-0.38741700
C	-3.79515700	-0.43876200	-1.57764500
H	-3.29709800	-0.47071800	-2.53768600
C	-5.15928200	-0.34511000	-1.53588900
H	-5.72428600	-0.31393900	-2.45995400
C	-3.71514200	-0.41200200	0.85376700
C	-5.12655700	-0.31433700	0.86335700
H	-5.63532800	-0.26331900	1.81964600
C	-5.83803200	-0.28304400	-0.30252100
H	-6.91839300	-0.20793800	-0.28397700
C	-2.97105100	-0.44664500	2.06029100
H	-3.50344200	-0.39914300	3.00330000

Table S10 Cartesian coordinates (in Angstroms) for the optimized structure of **5-6_TC**

Atom type	X	Y	Z
O	-1.08372500	-3.07946600	0.20790200
C	-3.35920400	-2.79131000	0.60437600
H	-3.41042600	-3.83269800	0.89636300
C	-2.02883300	-2.30177100	0.23437000
C	-1.90329900	-0.84557000	-0.06271400
C	-0.68792100	-0.23727200	-0.12420600
H	-0.69019500	0.83784500	-0.24926300
C	-3.14173800	-0.04942600	-0.21043400
C	-3.14682000	1.26559900	-0.69023200
H	-2.22629700	1.73327800	-1.01192800
C	-4.31872500	1.99297800	-0.79201900
H	-4.28388000	3.00799700	-1.16918400
C	-4.38238300	-0.62295200	0.12990300
C	-5.55886700	0.12319700	0.02644300
H	-6.49861100	-0.34255100	0.30136400
C	-5.53532100	1.42726400	-0.42534100
H	-6.45262200	1.99713900	-0.50540000
C	-4.44024500	-2.00598300	0.56316100
H	-5.41299200	-2.40323300	0.83493400
C	0.62129000	-0.82522800	-0.04484900
H	0.67445100	-1.90212300	-0.04242900
C	1.76885600	-0.10540500	-0.01069700
C	3.07896200	-0.79391300	-0.07503900
C	3.23547600	-1.98454100	-0.79212500
C	4.19001000	-0.27334800	0.59522900
C	4.45637700	-2.63776900	-0.82523200
H	2.39726900	-2.38948800	-1.34478200
C	5.40911800	-0.93210700	0.56801500
H	4.09201100	0.64878900	1.15399000
C	5.54746700	-2.11631900	-0.14241500
H	4.55817600	-3.55479600	-1.39299200
H	6.25446300	-0.51843000	1.10472600
H	6.50210200	-2.62778700	-0.16911200
C	1.78643600	1.37620600	0.10624700
C	1.13661400	2.02426900	1.15730100
C	2.47251300	2.14819500	-0.83436600
C	1.16039200	3.40875400	1.25869900
H	0.62469000	1.43537000	1.90871800

C	2.48402000	3.53031000	-0.74067300
H	2.99158100	1.65711800	-1.64883200
C	1.82885800	4.16507200	0.30766000
H	0.65709500	3.89496200	2.08573300
H	3.00917600	4.11521800	-1.48623800
H	1.84562300	5.24554300	0.38474000

Table S11 Cartesian coordinates (in Angstroms) for the optimized structure of **5-6_TT**

Atom type	X	Y	Z
O	-2.15663000	3.11475400	-0.65295400
C	-4.14965800	1.92545100	-0.96033400
H	-4.60573600	2.81122700	-1.38417200
C	-2.74158700	2.04692900	-0.56940300
C	-2.05695400	0.78473500	-0.14352700
C	-0.70520700	0.81742100	-0.24292500
H	-0.30035300	1.79553500	-0.48248800
C	-2.88561200	-0.37011200	0.23059100
C	-2.40809600	-1.44201100	0.99100500
H	-1.40147100	-1.41741600	1.38239200
C	-3.21868800	-2.52339600	1.29747800
H	-2.81931700	-3.33806400	1.88941900
C	-4.24536200	-0.38201500	-0.14384500
C	-5.04647800	-1.48221000	0.16008500
H	-6.08556000	-1.47592400	-0.14960900
C	-4.53788900	-2.55852900	0.86440000
H	-5.16974300	-3.40634100	1.09825600
C	-4.82714600	0.78585300	-0.78509800
H	-5.86965700	0.72181300	-1.08006100
C	0.23483100	-0.27156300	-0.18261100
H	-0.16095000	-1.27481800	-0.27600600
C	1.57797100	-0.13720300	-0.09698800
C	2.44916800	-1.33131500	-0.22236700
C	2.14064700	-2.35937300	-1.11729100
C	3.59327700	-1.46156500	0.56953900
C	2.94117400	-3.48750100	-1.20591300
H	1.27904700	-2.26077500	-1.76612500
C	4.38863600	-2.59342100	0.48638000
H	3.85252800	-0.67275800	1.26465400
C	4.06573800	-3.61080500	-0.40138900

H	2.69047600	-4.26911500	-1.91303600
H	5.26485000	-2.68109000	1.11753000
H	4.69169300	-4.49220600	-0.47146100
C	2.23573900	1.16982000	0.14408400
C	1.79724800	2.02947600	1.15216300
C	3.32045400	1.56387100	-0.64512800
C	2.41476900	3.25527600	1.35682300
H	0.97655700	1.72723000	1.79075200
C	3.92805400	2.79237900	-0.44850300
H	3.67839800	0.90384000	-1.42596200
C	3.47755500	3.64201800	0.55469100
H	2.06243800	3.90793800	2.14623000
H	4.75711700	3.08902400	-1.07967000
H	3.95721500	4.60061700	0.71149300

Table S12 Cartesian coordinates (in Angstroms) for the optimized structure of **BP**

Atom type	X	Y	Z
C	4.04099100	-0.94048600	-1.35940800
C	2.67139600	-0.85004700	-1.56034800
C	1.82306600	-0.81930700	-0.46475300
C	2.32755500	-0.89308700	0.83594600
C	3.70530000	-0.98565000	1.01557000
C	4.56320000	-1.00377400	-0.07263300
H	4.70481400	-0.95740100	-2.21541500
H	2.24589900	-0.80130900	-2.55454300
H	4.09985100	-1.04772200	2.02385000
H	5.63309300	-1.07203700	0.07900600
C	1.36072400	-0.91064200	1.92552600
H	1.69870400	-1.18759300	2.91792500
C	0.08857900	-0.60402400	1.69551800
H	-0.65432200	-0.61774100	2.48286400
C	-0.37935700	-0.20869100	0.31052000
C	-0.38079100	1.30862500	0.08983600
C	-0.07193100	2.21499400	1.09426100
C	-0.69671900	1.79082000	-1.18053400
C	-0.08670200	3.58313200	0.84025900
H	0.19117900	1.85797400	2.08162400
C	-0.70413300	3.15037100	-1.43700100
H	-0.93360400	1.08787400	-1.96987700

C	-0.40142500	4.05361100	-0.42321900
H	0.15595900	4.27849800	1.63502800
H	-0.94829200	3.51016900	-2.42951300
H	-0.40948200	5.11854900	-0.62265100
C	-1.76778800	-0.80401900	0.07128700
C	-1.92350700	-2.00631500	-0.60845400
C	-2.89309300	-0.17320600	0.59592300
C	-3.18536600	-2.56421700	-0.76768900
H	-1.05274300	-2.49985800	-1.01641500
C	-4.15154700	-0.73550700	0.44401700
H	-2.78834100	0.77073600	1.11770200
C	-4.30259700	-1.93345900	-0.24135500
H	-3.29238200	-3.49876000	-1.30572900
H	-5.01767300	-0.23139000	0.85602000
H	-5.28617500	-2.37046100	-0.36558500
O	0.47979900	-0.79428400	-0.69173800

Table S13 Cartesian coordinates (in Angstroms) for the optimized structure of **BP_TC**

Atom type	X	Y	Z
C	5.57447200	-0.42921500	-0.03101600
C	4.74873200	-1.46382700	0.21153500
C	3.29483500	-1.31217800	0.21019400
C	2.78285100	0.05322600	-0.09464600
C	3.74353800	1.10814500	-0.34228200
C	5.07093900	0.89158600	-0.31420100
H	6.64812000	-0.58258700	-0.01512000
H	5.11875700	-2.45845300	0.42678500
H	3.35343400	2.09734600	-0.55690300
H	5.76927100	1.69668700	-0.50322700
C	1.45386200	0.36371300	-0.16087200
H	1.22297000	1.40009900	-0.38898100
C	0.33434500	-0.51447300	-0.00719400
H	0.56054100	-1.56479500	0.09848000
C	-0.96006700	-0.10708100	-0.01480300
C	-2.05185900	-1.10594700	-0.00740000
C	-1.89278900	-2.35414800	-0.61880200
C	-3.26624200	-0.82803900	0.62781100
C	-2.90852100	-3.29474700	-0.58459600
H	-0.97231600	-2.57964500	-1.14198800

C	-4.27835800	-1.77368900	0.66908400
H	-3.41080000	0.13224500	1.10623400
C	-4.10391100	-3.00981900	0.06254300
H	-2.76861100	-4.25258600	-1.07086500
H	-5.20689400	-1.54400300	1.17771600
H	-4.89761500	-3.74665400	0.08906900
C	-1.34769900	1.32651000	-0.00868100
C	-0.87198200	2.19701900	0.97258400
C	-2.21185700	1.82593400	-0.98620800
C	-1.23948900	3.53562800	0.96946300
H	-0.22549900	1.81487800	1.75324400
C	-2.56553500	3.16517000	-0.99765500
H	-2.59813500	1.15826100	-1.74696200
C	-2.08154900	4.02407800	-0.01834700
H	-0.86843300	4.19590600	1.74404100
H	-3.22447900	3.54026300	-1.77144400
H	-2.36620500	5.06930800	-0.02310700
O	2.56545100	-2.27041800	0.45049700

Table S14 Cartesian coordinates (in Angstroms) for the optimized structure of **BP_TT**

Atom type	X	Y	Z
C	5.40850100	-1.28564100	0.14765700
C	5.18011100	0.00481800	-0.15303300
C	3.82034900	0.53392800	-0.26097100
C	2.71356300	-0.44085600	-0.02056700
C	3.04952400	-1.80992700	0.30179600
C	4.32901200	-2.21703000	0.38277200
H	6.42763200	-1.64979700	0.22000400
H	5.98444600	0.70813300	-0.32903700
H	2.24999000	-2.51584600	0.48824900
H	4.56677600	-3.24458800	0.62713700
C	1.44300100	0.03673100	-0.11793400
H	1.36465200	1.09405200	-0.34687100
C	0.22964100	-0.71289200	0.01803700
H	0.31123300	-1.78929100	0.10766700
C	-1.01881800	-0.18632500	0.00634000
C	-2.19863100	-1.08269500	0.00574100
C	-2.18371900	-2.29579000	-0.68899200
C	-3.35168400	-0.73805700	0.71683900

C	-3.27934700	-3.14366400	-0.65930700
H	-1.31605800	-2.56299400	-1.27949900
C	-4.44286200	-1.59137100	0.75424000
H	-3.38474700	0.20060000	1.25548300
C	-4.41095000	-2.79697900	0.06655100
H	-3.25309700	-4.07437000	-1.21318400
H	-5.32242800	-1.31298200	1.32211000
H	-5.26731300	-3.46005700	0.08948300
C	-1.27366300	1.27508000	0.01334000
C	-0.67490000	2.11016800	0.95744800
C	-2.13829400	1.83890500	-0.92859300
C	-0.92193600	3.47564200	0.95125600
H	-0.02515100	1.68282300	1.71110300
C	-2.37242800	3.20371800	-0.94298900
H	-2.61812200	1.20074500	-1.66079800
C	-1.76572600	4.02622900	-0.00164600
H	-0.45212100	4.10887900	1.69387100
H	-3.03209100	3.62803500	-1.69024700
H	-1.95436900	5.09292400	-0.00975500
O	3.60953900	1.70872400	-0.53420400

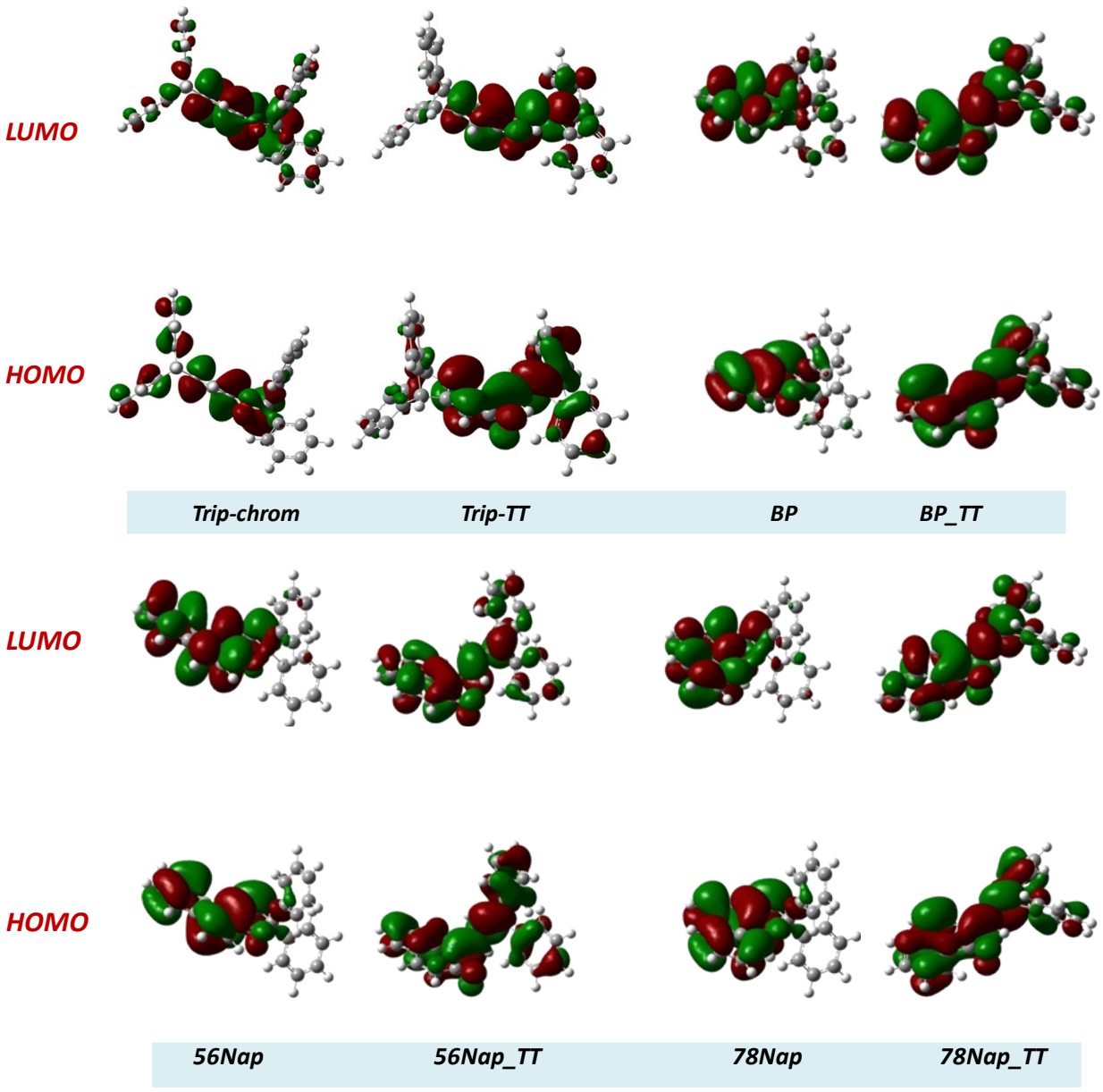

Fig. S8 Frontier orbital plots for **Trip-chrom** (top left), **BP** (top right), **56Nap** (down left) and **78Nap** (down right).

Reference

1. M. J Frisch, et. al. *Gaussian 09*, Revision E.01, Gaussian, Inc., Wallingford CT, 2009.