Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

ON THE ORIGINS OF STEREOSELECTIVITY IN THE THE AMINOCATALYTIC REMOTE ALKYLATION OF 5-ALKYLFURFURALS

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Contents

Experimental section

Preparation of 5-benzylthiophene-2-carbaldehyde 7

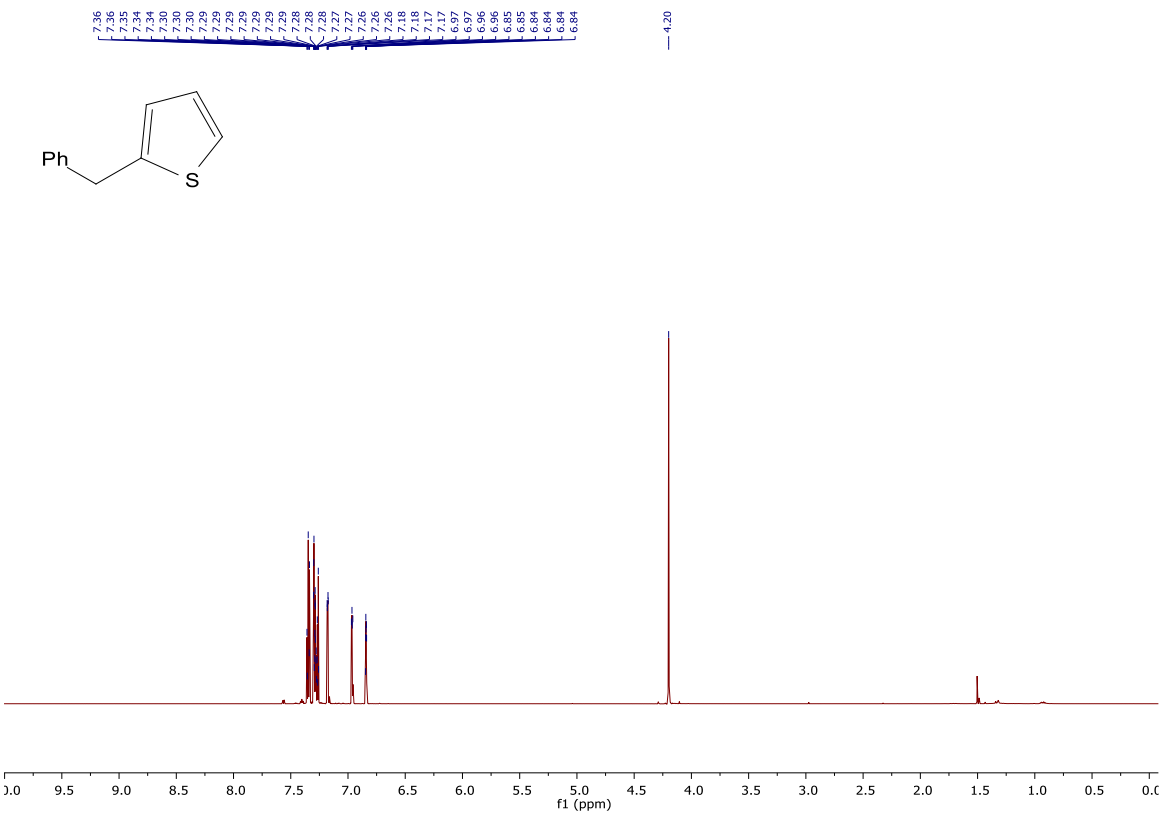
This compound was prepared based on previously reported procedures for furan analogue.[8d] *n*-BuLi solution (6.25 mL, 10 mmol; 1.6 M in hexane) was added dropwise to the solution of thiophene (800 μL, 10 mmol) in dry THF (10 mL) at 0°C and under an argon atmosphere and stirred for 30 min. at RT. The mixture was then cooled down to 0°C and the solution of benzyl bromide (9 mmol) in dry THF (10 mL) was added dropwise. After full addition, the reaction mixture was warmed up to RT and stirred overnight. The reaction was quenched with water (10 mL), resulting mixture was extracted with AcOEt (2 x 20 mL), the organic layers were combined, washed with brine (2 x 15 mL) and dried over Na_2SO_4. FC on silica (Hexanes) yielded 1.27 g (73%) of the pure 2-benzylthiophene. ^{1}H NMR (700 MHz, Chloroform-*d*) δ 7.35 (t, *J* = 7.6 Hz, 2H), 7.31 – 7.26 (m, 3H), 7.18 (dd, *J* = 5.2, 1.2 Hz, 1H), 6.96 (dd, *J* = 5.2, 3.4 Hz, 1H), 6.85 – 6.83 (m, 1H), 4.20 (s, 2H). ^{13}C NMR (176 MHz, Chloroform-*d*) δ 144.2, 140.5, 128.7 (2C), 128.7 (2C), 126.9, 126.6, 125.3, 124.0, 36.2. HRMS calculated for $[C_{11}H_{10}S+Na]^+$: 197.0396; found: 197.0388.

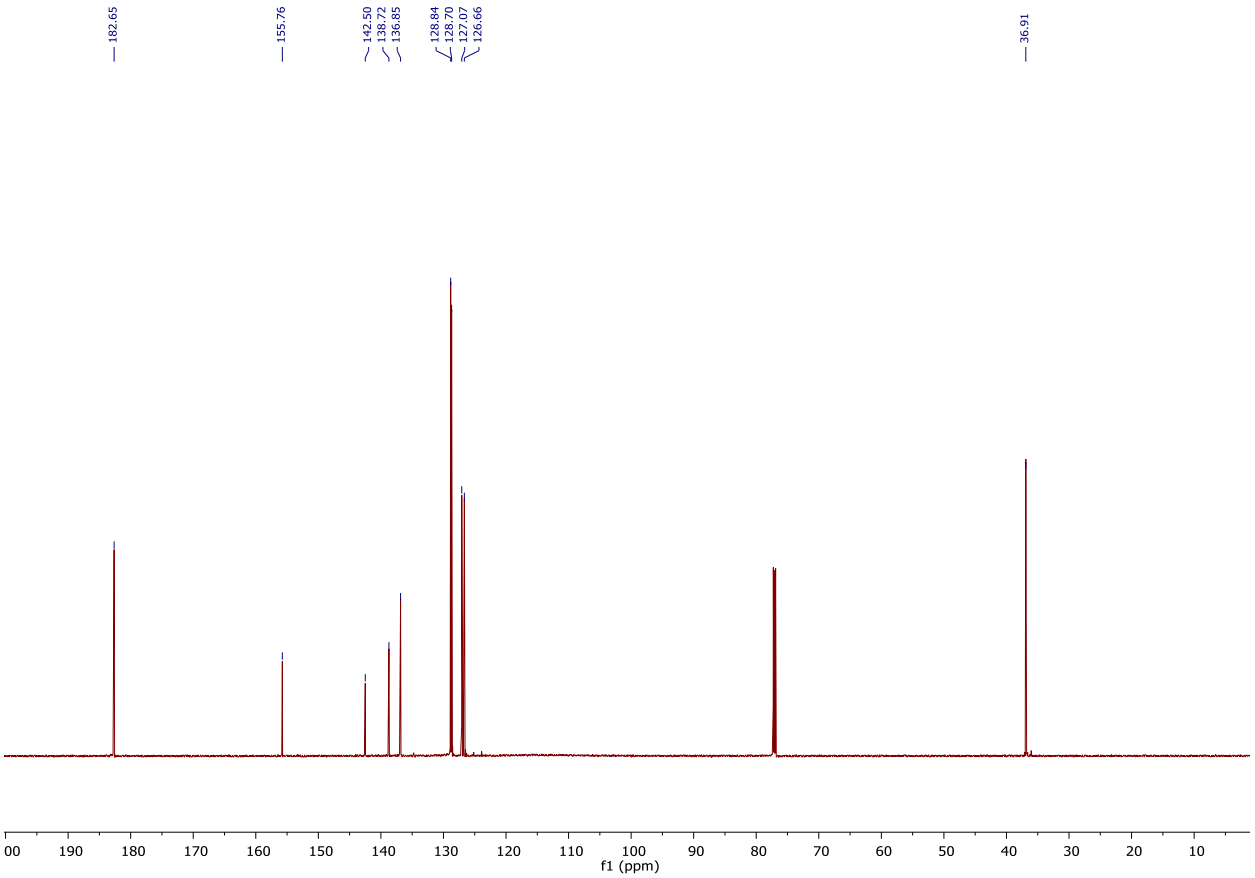
To a dry DMF (704 μL, 9.1 mmol) at 0°C under argon atmosphere, $POCl_3$ (718 μL, 7.7 mmol) was added dropwise and the mixture was stirred at 40°C for 1 h. Then a solution of 2-benzylthiophene (1.2 g, 7 mmol) in dry DMF (1 mL) was added dropwise and the reaction mixture was stirred at the same temperature overnight. The reaction was quenched with water (5 mL), CH_2Cl_2 (15 mL) was added and the resulting mixture was washed with 1M $NaOH_{(aq.)}$ until basic pH was reached. Phases were separated, the organic layer was washed with brine (10 mL) and dried over Na_2SO_4. FC on silica (Hexanes : AcOEt 4:1) yielded 0.92 g (65%) of pure 5-benzyl-2-formylthiophene as dark-orange oil. ^{1}H NMR (700 MHz, Chloroform-*d*) δ 9.81 (s, 1H), 7.60 (d, *J* = 3.8 Hz, 1H), 7.36 – 7.30 (m, 2H), 7.29 – 7.20 (m, 3H), 6.91 (d, *J* = 3.8 Hz, 1H), 4.19 (s, 2H). ^{13}C NMR (176 MHz, Chloroform-*d*) δ 182.6, 155.8, 142.5, 138.7, 136.8, 128.8 (2C), 128.7 (2C), 127.1, 126.7, 36.9. HRMS calculated for $[C_{12}H_{10}OS+Na]^+$: 225.0345; found: 225.0349.

(6*R*,7*S*)-5-(3-Nitro-1,2-diphenylpropyl)-thiophene-2-carbaldehyde 9 To the solution of aldehyde X (20 mg, 0.1 mmol) and β-nitrostyrene X (15 mg, 0.1 mmol) in CH_2Cl_2 (0.2 ml) in an ordinary vial catalyst X (3.7 mg, 0.02 mmol) was added and the reaction mixture was stirred at 40°C in vial heating block for 2 days. Afterwards reaction mixture was directly subjected to column chromatography (Hexanes : Ethyl Acetate 4:1) to provide 32.6 mg (93%) of a pure product as light yellow oil. ^{1}H NMR (700 MHz, Chloroform-*d*) δ 9.70 (s, 1H), 7.51 – 7.48 (m, 2H), 7.45 (dd, *J* = 8.5, 7.0 Hz, 2H), 7.39 – 7.35 (m, 2H), 7.31 – 7.27 (m, 2H), 7.26 – 7.23 (m, 2H), 6.73 (dd, *J* = 3.9, 0.6 Hz, 1H), 4.61 – 4.54 (m, 2H), 4.49 (dd, *J* = 12.8, 4.2 Hz, 1H), 4.28 (ddd, *J* = 11.8, 10.5, 4.2 Hz, 1H). ^{13}C NMR (176 MHz, Chloroform-*d*) δ 182.7, 156.3, 142.6, 139.8, 137.2, 136.1, 129.9 (2C), 129.1 (2C) , 128.56, 128.4, 128.2 (2C), 127.9 (2C), 126.9, 79.6, 51.7, 50.0. HRMS calculated for $[C_{20}H_{17}NO_3S+Na]^+$: 374.0822; found: 374.0829. The er was determined by UPC^2 using a chiral Chiralpack IA column, gradient from 100% CO_2 up to 40%; i-PrOH, 2.5 mL/min; detection wavelength = 280nm; ; τmajor= 3.49 min, τminor= 3.61min, (73.5: 26.5 er).

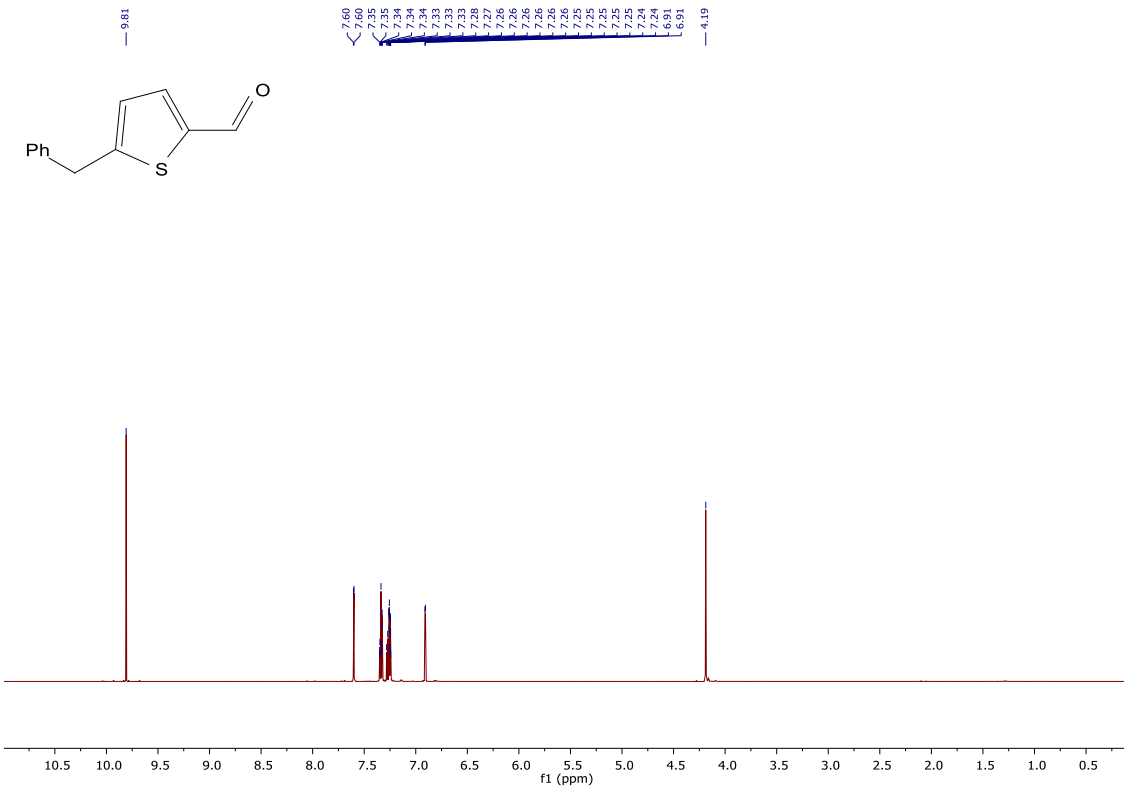
^{1}H and ^{13}C NMR Spectra

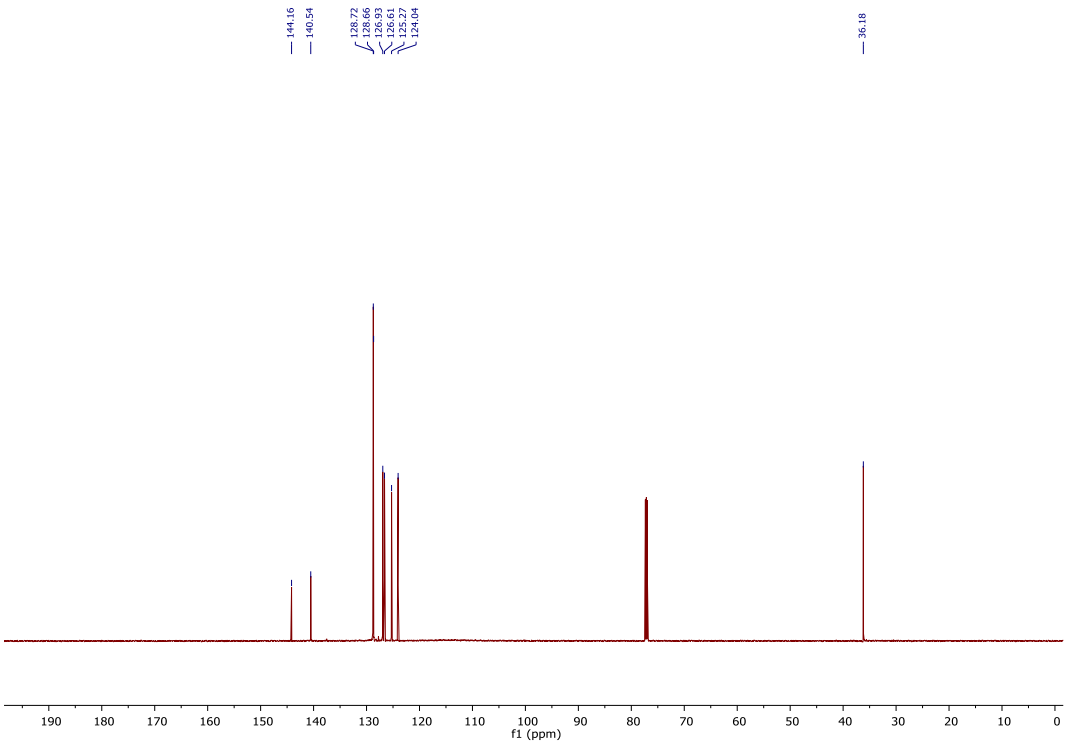
2-Benzylthiophene



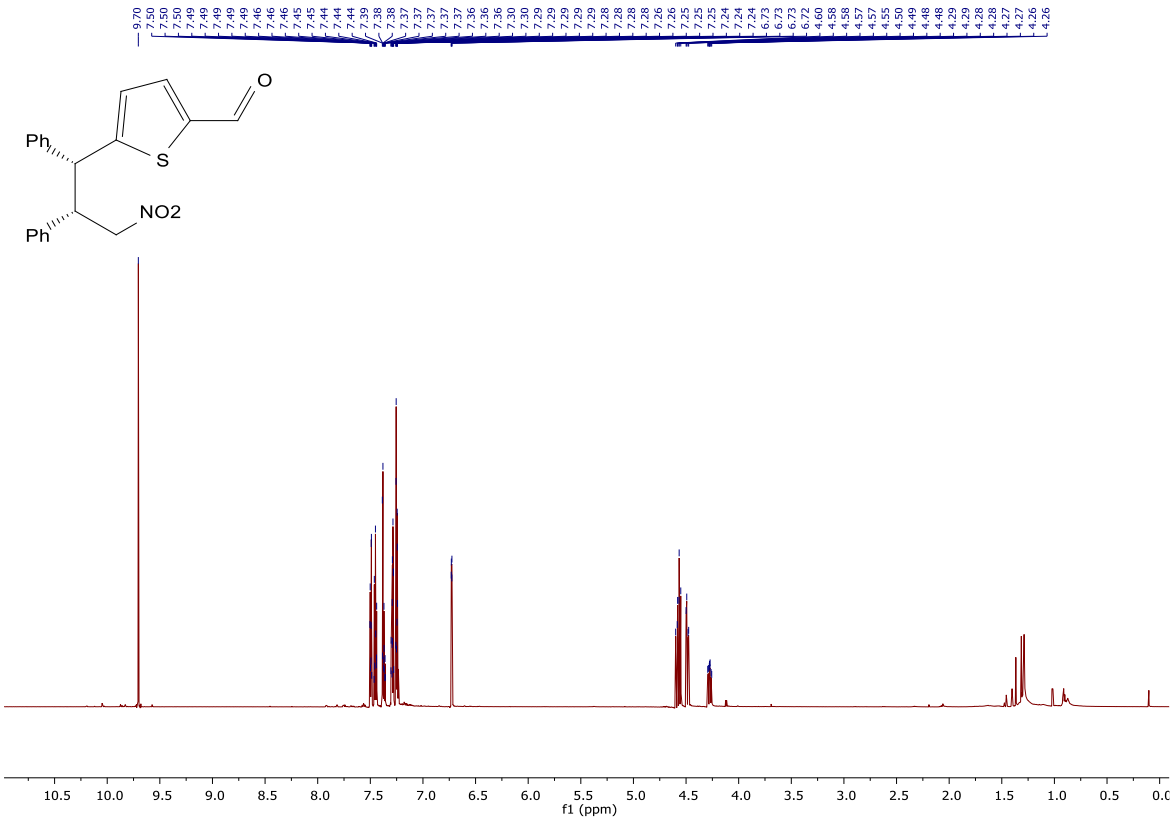


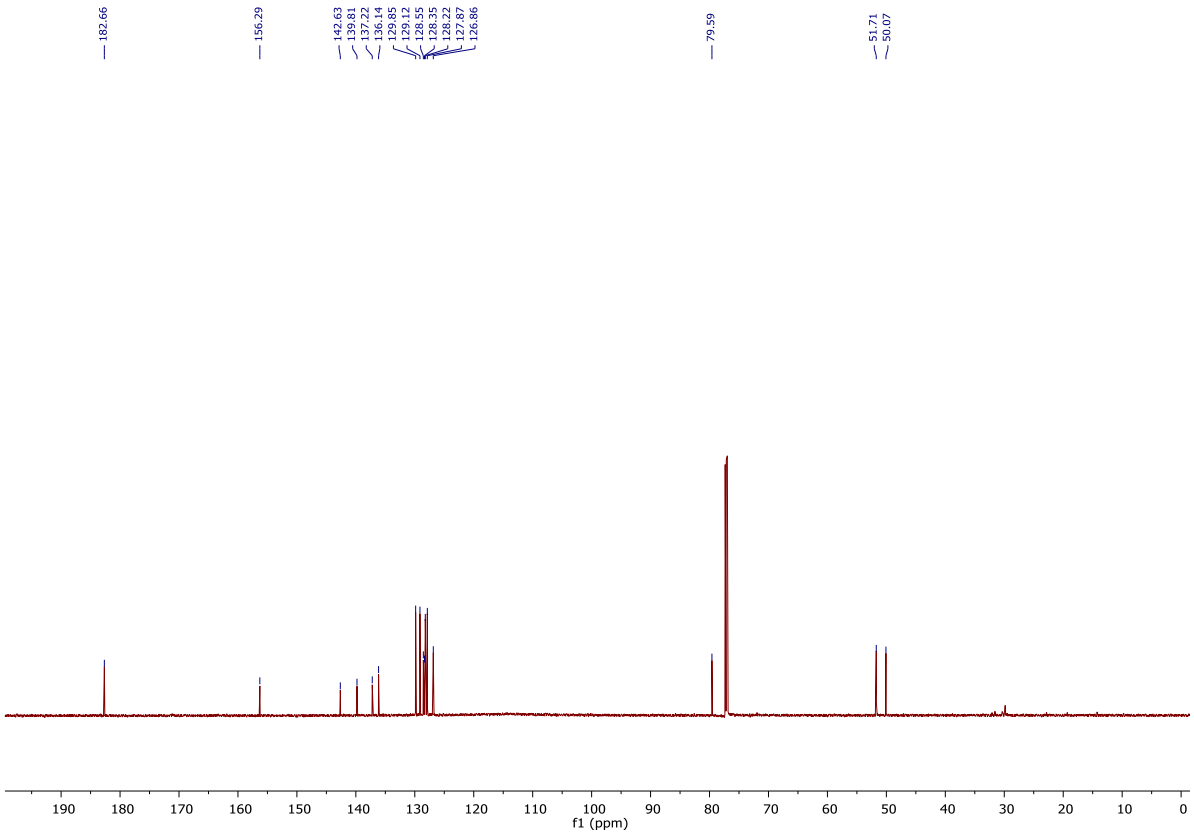
5-Benzyl-2-formylthiophene





(6*R*,7*S*)-5-(3-Nitro-1,2-diphenylpropyl)-thiophene-2-carbaldehyde




182.66
156.29
142.63
139.81
137.22
136.14
129.85
129.12
128.55
128.35
128.22
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126.86
79.59
51.71
50.07
190
180
170
160
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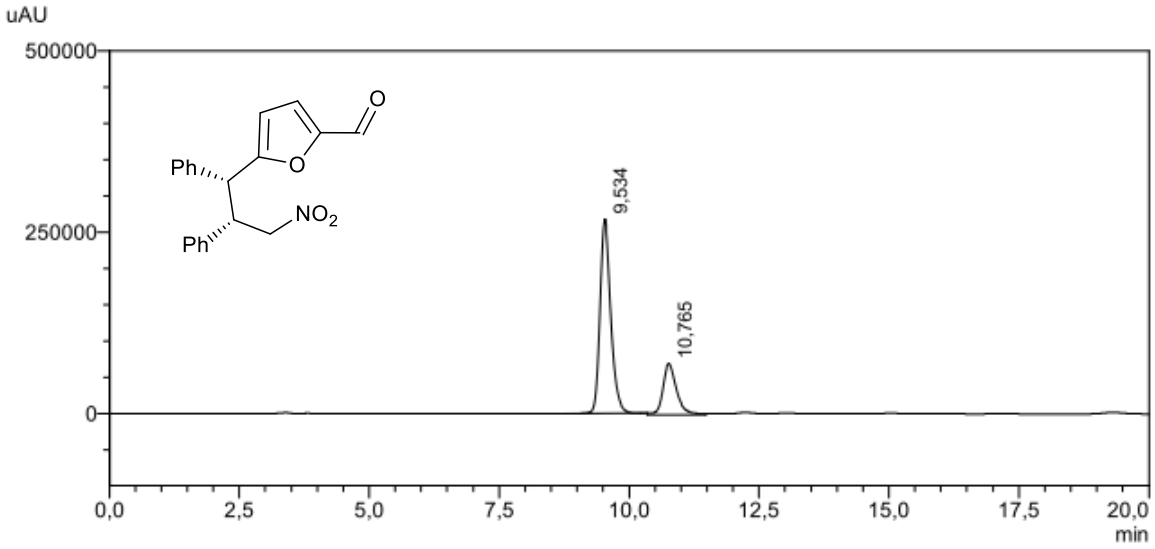
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

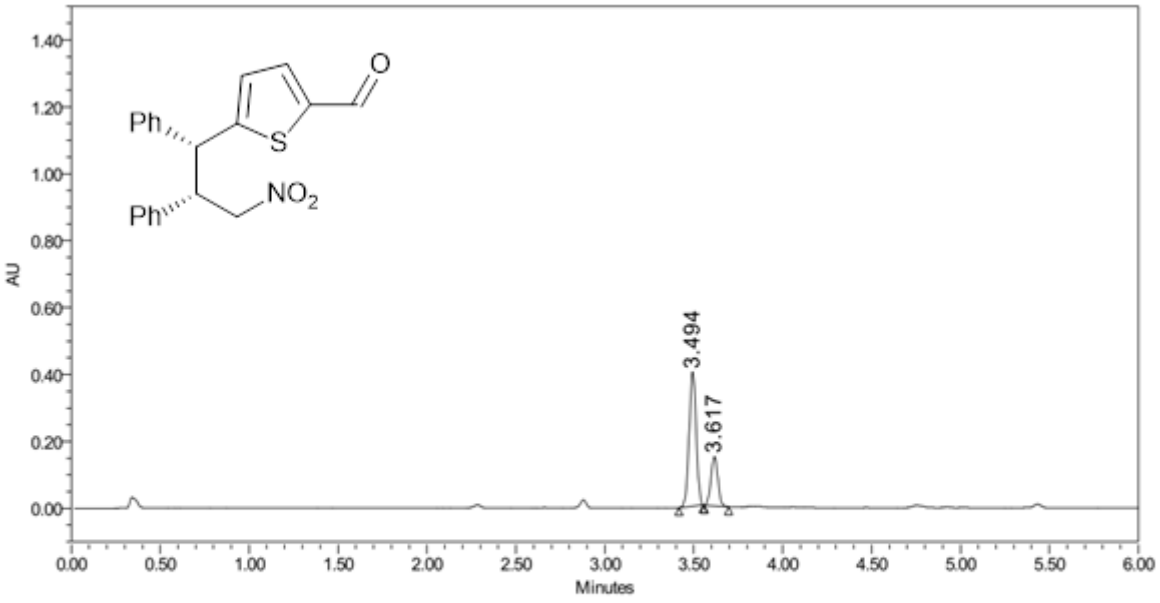
HPLC traces



PDA Ch2 284nm

Peak#	Ret. Time	Area%
1	9,534	75,103
2	10,765	24,897
Total		100,000

UPC^2 traces



	RT	% Area
1	3.494	73.57
2	3.617	26.43

Computational Data

Table S1. Comparison between different DFT functionals and CCSD(T) potential energies reported in kcal·mol^{-1} obtained for four possible reactant complex conformations, referred to ZZZ-isomer. The MUE is computed with respect to CCSD(T).

	Z,Z,Z	***Z,Z,E***	***E,Z,Z***	***E,Z,E***	***MUE***
M06-2X/6-31+G(d,p)	0	2.4	2.0	4.4	0.8
MPW1K/6-31+G(d,p)	0	1.5	1.3	3.5	1.6
B3LYP/6-31+G(d,p)	0	1.7	1.6	4.1	1.3
CCSD(T)/6-31+G(d,p)	0	2.7	2.1	6.4	-

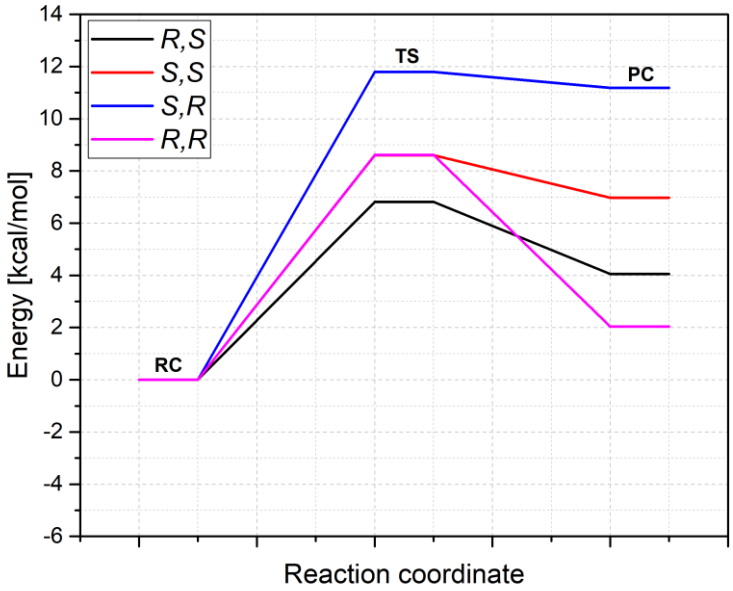


Fig. S.1. Obtained potential energy barriers computed for studied reactions for 5-alkylfurfural **1**. Values are given in kcal/mol.

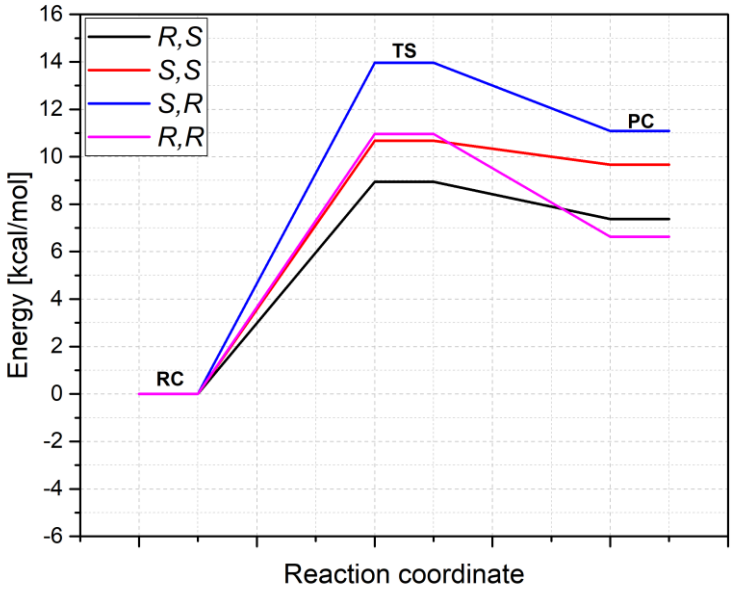


Fig. S.2. Obtained potential energy barriers computed for studied reactions for thiophene analogue **7**. Values are given in kcal/mol.

Table S2. Coordination for RC structure (Cartesian coordinates are written in Å) of pro-*R*,*S*-RC located at B97D/6-31+G(d,p) with the total energy and zero-point energy (ZPE) reported in Hartree per particle.

B97D	pro-*R*,*S*-RC with furan ring			B97D	pro-*R*,*S*-RC with thiophene ring		
total energy	-2243.2418225			-2566.2500239			
ZPE	0.478965			0.475524			
Atoms	x	y	z	Atoms	x	y	z
C	3.03104700	3.83330100	-0.22371200	C	3.56632700	3.80544300	-0.76764500
C	1.72541300	3.71294500	-1.04767900	C	2.24835400	3.87935900	-1.57416800
C	0.76421800	2.90516700	-0.14300400	C	1.19200800	3.24405700	-0.63992100
N	1.64547600	2.29379900	0.87572200	N	1.98445200	2.45671800	0.33053900
H	3.92081700	3.96943000	-0.85261400	H	4.45906500	3.81585900	-1.40699200
H	1.91392900	3.16572400	-1.98129500	H	2.33273300	3.29248200	-2.49933200
H	0.23136800	2.11664400	-0.69236500	H	0.49943100	2.58551600	-1.18204800
C	1.24139100	1.53265700	1.91332500	C	1.48236000	1.62349900	1.26674700
H	2.02752900	1.21302100	2.59466300	H	2.24141300	1.09883900	1.84645300
C	-0.04026500	1.10541000	2.21844400	C	0.16838900	1.31365600	1.58721100
C	-0.48774400	0.28688300	3.29014800	C	-0.16932800	0.26109200	2.49562600
O	-1.12555900	1.36581200	1.37841100	C	-1.50659400	-0.06426700	2.52848200

C	-1.83404300	0.04123200	3.09682900	H	0.60439400	-0.26706200	3.05205900
H	0.14873200	-0.07992000	4.09047900	C	-2.33825400	0.71420900	1.64607900
C	-2.23487100	0.71639100	1.89743700	H	-1.92984900	-0.87509800	3.11962100
H	-2.49803100	-0.55429100	3.71601800	C	-3.68257300	0.45955100	1.42576500
C	-3.46577900	0.73278900	1.27038100	H	-4.06768600	-0.36767800	2.02765600
H	-4.22566700	0.15749000	1.80101200	C	-4.65824700	1.06615900	0.54608000
C	-3.91219900	1.40729500	0.06883500	C	-5.97937400	0.52835300	0.56025700
C	-5.29604600	1.33263800	-0.26042500	C	-4.40590000	2.13608900	-0.36142400
C	-3.06080000	2.10655300	-0.83469500	C	-6.98631500	1.02575400	-0.27313900
C	-5.80596900	1.92791900	-1.42150300	H	-6.19714300	-0.30172400	1.23419100
H	-5.96593800	0.79081900	0.40925900	C	-5.41531400	2.62594300	-1.20106000
C	-3.57538700	2.69657400	-1.99517200	H	-3.41858900	2.58856300	-0.42385800
H	-1.99609500	2.16929600	-0.63007200	C	-6.71303000	2.07980200	-1.16543800
C	-4.94949200	2.61466200	-2.30132400	H	-7.98371900	0.58432900	-0.23513100
H	-6.87178200	1.84966900	-1.64355900	H	-5.18700200	3.44370600	-1.88701400
H	-2.89780800	3.22018500	-2.67245200	H	-7.49425100	2.46883300	-1.81983100
H	-5.34147500	3.07469700	-3.20941400	C	3.42558300	2.48793000	0.01489600
C	3.06956500	2.51287500	0.56818600	H	4.00530400	2.47356700	0.94756100
H	3.63756200	2.57684600	1.50638900	C	3.83774100	1.27014300	-0.85085700
C	3.64718200	1.36614800	-0.29508000	H	3.23481800	1.23324300	-1.76716200
H	3.10924000	1.30307900	-1.25176000	H	4.89278700	1.37706700	-1.13231800
H	4.70327000	1.58581300	-0.49273600	H	0.61000600	4.00434900	-0.09700000
H	0.02481600	3.53927100	0.36500100	H	1.97995800	4.90725800	-1.84785400
H	1.30598600	4.69266400	-1.30850300	H	3.63360200	4.64233700	-0.05832800
H	2.96844500	4.67261900	0.48306100	N	3.63822400	-0.00661900	-0.14852000
N	3.55009200	0.08040100	0.42560400	H	2.73273900	-0.51095100	-0.20298800
H	2.61288000	-0.37615700	0.43951400	O	5.90711100	0.15979400	0.98507200
O	6.06911400	-0.33341500	0.41962800	S	4.83412400	-0.79142000	0.63490100
S	4.76746800	-1.02523900	0.35868700	O	4.24763700	-1.72630800	1.61181300
O	4.42668300	-2.14471500	1.25368000	C	5.61680000	-1.92282600	-0.70848900
C	4.69993500	-1.76940700	-1.41848300	F	4.69351800	-2.78990100	-1.17563900
F	3.50300400	-2.35568500	-1.62741500	F	6.65314800	-2.61602800	-0.19232900
F	5.67681700	-2.68572000	-1.57926200	F	6.06260600	-1.16461800	-1.73751600
F	4.86647700	-0.78135200	-2.32886500	C	-5.97424100	-3.45418100	-0.38082400
C	-6.10076700	-3.24815200	-0.11904800	C	-4.86404800	-3.88430600	0.37791000
C	-5.05192800	-3.64551400	0.73796100	C	-3.63586800	-3.22771400	0.26763300
C	-3.78667300	-3.06271400	0.62349600	C	-3.49003700	-2.11203100	-0.60324900
C	-3.54160400	-2.05798500	-0.35201500	C	-4.62049500	-1.68065600	-1.34519900
C	-4.60596600	-1.66852500	-1.20680400	C	-5.84629800	-2.35058900	-1.24059200
C	-5.87102200	-2.26013600	-1.09222400	H	-6.92916800	-3.97380200	-0.29333100
H	-7.08559900	-3.70746200	-0.02523300	H	-4.96225400	-4.73595600	1.05224500
H	-5.22753400	-4.41150600	1.49439000	H	-2.78936400	-3.57293500	0.86061700
H	-2.98882300	-3.37588800	1.29676800	H	-4.52592000	-0.81181600	-1.99685700
H	-4.42966000	-0.89192500	-1.95055800	H	-6.70314100	-2.00044100	-1.81625000
H	-6.67744600	-1.94532500	-1.75563000	C	-2.23247800	-1.41027300	-0.79459000

C	-2.25369500	-1.40670000	-0.52115400	H	-2.24599600	-0.53985600	-1.45173100
H	-2.19999000	-0.61124600	-1.26505800	C	-1.02987200	-1.79030300	-0.27059900
C	-1.10032000	-1.73583400	0.13330400	H	-0.87608500	-2.62211400	0.40745700
H	-1.01692600	-2.47058100	0.92662600	N	0.18433900	-1.12682900	-0.59632600
N	0.12321400	-1.07735800	-0.13185400	O	0.22504600	-0.18587000	-1.41771200
O	0.25769000	-0.28304100	-1.09587700	O	1.22788200	-1.55246900	-0.01391300
O	1.08025500	-1.32977300	0.66747100	S	-1.33698800	1.95585700	0.85638900

Table S3. Coordination for RC structure (Cartesian coordinates are written in Å) of pro-*R,R*-RC located at B97D/6-31+G(d,p) with total energy and zero-point energy (ZPE) reported in Hartree per particle.

B97D	pro-*R,R*-RC with furan ring			B97D	pro-*R,R*-RC with thiophene ring		
total energy	-2243.2383154			-2566.2456303			
ZPE	0.4788882			0.4750789			
Atoms	x	y	z	Atoms	x	y	z
C	3.34893200	3.70169400	-0.56088800	C	3.95279900	3.57128400	-1.06201700
C	1.99158200	3.69740500	-1.30986400	C	2.61263400	3.71743200	-1.82933100
C	0.99027000	3.03439000	-0.32881500	C	1.52510000	3.18934900	-0.85420800
N	1.84257900	2.44408400	0.72290600	N	2.28406900	2.57814800	0.25469600
H	4.20894200	3.66618200	-1.24294900	H	4.80499900	3.39313800	-1.73129500
H	2.06387300	3.09915300	-2.22804900	H	2.62213900	3.10602600	-2.74141300
H	0.40246200	2.24926200	-0.82415100	H	0.88859000	2.43268000	-1.33937600
C	1.41413300	1.82576000	1.84098500	C	1.76315900	1.98460300	1.34980700
H	2.19393000	1.55965100	2.55309800	H	2.51294200	1.61744900	2.05129700
C	0.12326900	1.47893500	2.20085300	C	0.44312900	1.74674000	1.70309900
C	-0.34011900	0.89578800	3.41274400	C	0.07274800	1.02299200	2.88487400
O	-0.95925500	1.62114400	1.33118100	C	-1.25391100	0.67206800	2.94607100
C	-1.69338100	0.66388400	3.27405800	H	0.82011700	0.73904500	3.62515800
H	0.29115200	0.67444200	4.26872000	C	-2.03811100	1.08975800	1.80879300
C	-2.07496600	1.08902300	1.95939600	H	-1.70107800	0.07741800	3.74139000
H	-2.37177600	0.21452200	3.99290800	C	-3.35838700	0.72583200	1.59684500
C	-3.29761400	0.97157700	1.32095800	H	-3.77469400	0.12731400	2.41170900
H	-4.07147300	0.52700300	1.94786500	C	-4.29523000	1.02167200	0.53189600
C	-3.70447100	1.36251000	-0.00952300	C	-5.64351700	0.59743700	0.70854100
C	-5.06958600	1.17272300	-0.37243700	C	-3.97506800	1.67571700	-0.69151600
C	-2.82607000	1.87660100	-1.00758000	C	-6.62178000	0.83768900	-0.26055900
C	-5.53783500	1.49498400	-1.65123900	H	-5.90804800	0.06511500	1.62376500
H	-5.75607000	0.75940300	0.36830700	C	-4.95791200	1.91157400	-1.66279600
C	-3.29878500	2.18769700	-2.28868400	H	-2.95500000	1.99074200	-0.89977900
H	-1.77596900	2.02179700	-0.77650700	C	-6.28819000	1.50371800	-1.45505000
C	-4.65512200	2.00354000	-2.62248500	H	-7.64427200	0.49674400	-0.09053000

H	-6.58945400	1.33629600	-1.89591500	H	-4.68004500	2.41530900	-2.59035700
H	-2.60166500	2.57465000	-3.03427600	H	-7.04832600	1.69254600	-2.21428700
H	-5.01551700	2.24831100	-3.62262100	C	3.69657800	2.38640900	-0.11674500
C	3.26338000	2.45485900	0.33691800	H	4.31640500	2.40134100	0.78979800
H	3.88310300	2.51588900	1.24193100	C	3.88682200	1.02797200	-0.84137300
C	3.63187400	1.17111700	-0.44697100	H	3.29666500	1.00533400	-1.76683400
H	3.05269100	1.11958300	-1.37885200	H	4.94717400	0.90472700	-1.09332800
H	4.70200700	1.20442800	-0.68334600	H	0.88842500	3.98995500	-0.45189800
H	0.30101800	3.75089100	0.13798000	H	2.41879800	4.75643000	-2.12314700
H	1.67170500	4.70879900	-1.59011000	H	4.15922600	4.46973300	-0.46426200
H	3.44120100	4.59424500	0.07346900	N	3.43606300	-0.09330300	-0.00334600
N	3.34509300	-0.02462100	0.37003400	H	2.43898200	-0.38626900	-0.03392500
H	2.35330700	-0.34525600	0.37918900	O	5.75307400	-0.50459700	0.95854500
O	5.78616300	-0.72939900	0.57353900	S	4.44891800	-1.15035500	0.71156800
S	4.41255500	-1.26372600	0.50121200	O	3.71526400	-1.88656300	1.75686300
O	3.88686900	-2.22677800	1.48538500	C	4.81209400	-2.46520500	-0.64524800
C	4.34875600	-2.19632200	-1.18427300	F	3.66316600	-3.06759400	-1.02000400
F	3.11044900	-2.69015300	-1.39241400	F	5.66982500	-3.39874000	-0.18212400
F	5.23713400	-3.21190400	-1.19012800	F	5.35961500	-1.86167200	-1.72663600
F	4.65205100	-1.33900000	-2.18714300	C	-6.03727400	-3.02602700	-0.38211200
C	-6.11753300	-2.99635200	0.00544000	C	-5.51096900	-2.25798900	-1.43724300
C	-5.56161600	-2.30901600	-1.08905800	C	-4.21209400	-1.74449900	-1.36008300
C	-4.25311400	-1.81468200	-1.02615300	C	-3.40398400	-1.99382600	-0.22025300
C	-3.46385300	-2.01099100	0.13766300	C	-3.95334400	-2.75947200	0.84142400
C	-4.04092200	-2.70225600	1.23690700	C	-5.25414300	-3.26974500	0.76234100
C	-5.35112700	-3.18847100	1.17282600	H	-7.05117200	-3.42291500	-0.44681600
H	-7.13873300	-3.37588100	-0.04779800	H	-6.11903800	-2.05222500	-2.31850000
H	-6.15492300	-2.14539400	-1.98946200	H	-3.82725300	-1.14454300	-2.18289900
H	-3.84781500	-1.26731800	-1.87536100	H	-3.34391400	-2.94618300	1.72747200
H	-3.44406500	-2.85022300	2.13887800	H	-5.65741700	-3.85821300	1.58749600
H	-5.77651200	-3.71808200	2.02625900	C	-2.03462100	-1.52241200	-0.09442000
C	-2.09412300	-1.54235400	0.25985800	H	-1.49703300	-1.79770300	0.81290200
H	-1.59504100	-1.71826100	1.21257600	C	-1.34684000	-0.83384100	-1.05549000
C	-1.35905400	-0.97273900	-0.74477900	H	-1.76292500	-0.48639300	-1.99462100
H	-1.73694400	-0.72184600	-1.72898300	N	0.03479200	-0.53671300	-0.93814900
N	-0.00418100	-0.61542300	-0.57889300	O	0.68827500	-0.91359000	0.07780800
O	0.61847300	-0.91546600	0.48568600	O	0.59017200	0.08195800	-1.88846500
O	0.56663900	-0.00165400	-1.52685200	S	-1.01858000	2.06632300	0.72901000

Table S4. Coordination for RC structure (Cartesian coordinates are written in Å) of pro-*S*,*S*-RC located at B97D/6-31+G(d,p) with total energy and zero-point energy (ZPE) reported in Hartree per particle.

B97D	pro-*S*,*S*-RC with furan ring			B97D	pro-S,*S*-RC with thiophene ring		
total energy	-2243.2313375			-2566.2415099			
ZPE	0.4784586			0.4759352			
Atoms	x	y	z	Atoms	x	y	z
C	2.65522500	2.31865600	2.31085400	C	-3.25083100	3.11240000	1.28977700
C	1.82092500	2.88782600	1.14127700	C	-2.44610800	2.35180800	2.36725400
C	0.94333100	1.69623200	0.71590400	C	-1.46781700	1.48872700	1.54611800
N	1.74805100	0.51051300	1.09144100	N	-2.16570100	1.28226600	0.25577900
H	3.56918400	2.89412200	2.51070400	H	-4.21534000	3.48784100	1.65714400
H	2.47710000	3.19969200	0.31615500	H	-3.11178200	1.71298300	2.96506700
H	0.71720600	1.68020700	-0.35737100	H	-1.25095600	0.52632100	2.02990500
C	1.34209900	-0.77765800	0.99128500	C	-1.61436100	0.72647600	-0.85181000
H	2.00663400	-1.51123100	1.44545300	H	-2.20573900	0.86194200	-1.75876600
C	0.21688500	-1.29381600	0.37749200	C	-0.43349800	0.02017300	-1.00820500
C	-0.16376400	-2.65881400	0.22436500	C	0.03130000	-0.44594200	-2.28491800
O	-0.73758200	-0.49360600	-0.25379100	C	1.26082600	-1.05554000	-2.25925800
C	-1.34202900	-2.68756700	-0.49042100	H	-0.56036900	-0.28845900	-3.18652600
H	0.40117000	-3.50073100	0.61478200	C	1.87512200	-1.12150300	-0.95357800
C	-1.71469700	-1.33084100	-0.77305100	H	1.77741500	-1.44468600	-3.13563700
H	-1.92290900	-3.55575400	-0.78668300	C	3.13707600	-1.63507400	-0.71078300
C	-2.83933700	-0.84606800	-1.41375500	H	3.62118600	-2.03242700	-1.60696500
H	-3.50011800	-1.62902600	-1.78718900	C	3.91121100	-1.78145000	0.50604700
C	-3.25558200	0.51462600	-1.67082800	C	5.11994200	-2.53150600	0.43080500
C	-4.42559400	0.71819200	-2.45875900	C	3.58227000	-1.20636900	1.76636000
C	-2.61032300	1.67219600	-1.14498200	C	5.94025400	-2.71758900	1.54722700
C	-4.91671400	2.00176200	-2.72242600	H	5.40952500	-2.96079600	-0.53003100
H	-4.94776900	-0.15401100	-2.85555700	C	4.41073600	-1.38975600	2.88258700
C	-3.11342300	2.95390600	-1.40364700	H	2.69206200	-0.59173700	1.87947000
H	-1.72429400	1.56354000	-0.52760300	C	5.59070900	-2.14963800	2.78721200
C	-4.26550200	3.13274400	-2.19413300	H	6.85993000	-3.29674900	1.44965500
H	-5.81568300	2.12076000	-3.32979000	H	4.13258000	-0.93050800	3.83294900
H	-2.60296000	3.82130600	-0.98067600	H	6.22955500	-2.28949000	3.66031800
H	-4.64962100	4.13452800	-2.39171900	C	-3.41930800	2.06432200	0.17223400
C	2.96107000	0.87814000	1.85428300	H	-3.50468000	2.50957200	-0.82828600
H	3.09382800	0.17698500	2.68934900	C	-4.65682800	1.17751400	0.43091900
C	4.22326800	0.84570800	0.96327600	H	-4.64349600	0.79702400	1.46292100
H	4.15319600	1.61344800	0.17861800	H	-5.55945100	1.78138400	0.27933800
H	5.10042400	1.04742600	1.58948200	H	-0.52053100	2.01835100	1.35641300
H	-0.00019500	1.67811100	1.28168100	H	-1.91149700	3.02466800	3.04922000
H	1.20993900	3.74897600	1.43944700	H	-2.66703500	3.95889400	0.90230800
H	2.05252400	2.28409400	3.22894700	N	-4.68224200	0.06009300	-0.53912000
N	4.38267600	-0.50108500	0.36904700	H	-3.94885900	-0.63966200	-0.41601100
H	3.67102600	-0.75631500	-0.31767300	O	-7.07859300	0.42868500	-1.32153300

O	6.83445400	-0.78237300	1.00542400	S	-6.10837500	-0.63725000	-1.02416400
S	5.87412000	-1.08706600	-0.06712700	O	-5.77981000	-1.71273600	-1.97416400
O	5.67968500	-2.44124200	-0.61115500	C	-6.80680900	-1.53031700	0.53663500
C	6.42734800	-0.01217700	-1.57087000	F	-5.88749000	-2.40168200	1.00462700
F	5.47584700	-0.06628200	-2.52791200	F	-7.93387400	-2.19499200	0.22346500
F	7.58889700	-0.47220500	-2.06975600	F	-7.07619900	-0.61960800	1.49743300
F	6.58369300	1.27129200	-1.18017400	C	7.92527900	-0.25101700	-0.96604000
C	-7.73207700	-1.45839200	-0.57790800	C	7.37274700	0.20919800	0.24376000
C	-7.27272100	-0.13778600	-0.41847100	C	6.07565600	0.73159700	0.27595900
C	-6.04235400	0.11574800	0.19983200	C	5.30022800	0.80905900	-0.90946700
C	-5.24634500	-0.95506000	0.68390100	C	5.86649400	0.33289900	-2.11997300
C	-5.71943100	-2.28262100	0.51012200	C	7.16427200	-0.19165300	-2.14910700
C	-6.94740300	-2.53263000	-0.11309100	H	8.93651400	-0.65948900	-0.98541500
H	-8.69009400	-1.64966700	-1.06309100	H	7.95158800	0.14981700	1.16572600
H	-7.86951300	0.69623200	-0.78978200	H	5.65941000	1.06947200	1.22327000
H	-5.69071700	1.14173800	0.29213000	H	5.27339500	0.37965700	-3.03499200
H	-5.10866000	-3.11212300	0.87114000	H	7.58391300	-0.55123200	-3.08951700
H	-7.29544800	-3.55901200	-0.23644500	C	3.95833300	1.37214700	-0.94958700
C	-3.96730900	-0.75903500	1.34904600	H	3.45768600	1.38934200	-1.91819900
H	-3.40914700	-1.65516500	1.62080600	C	3.30862000	1.93911900	0.10559700
C	-3.44418300	0.44523800	1.72047700	H	3.68106300	1.98158700	1.12307400
H	-3.88425100	1.41283700	1.50895100	N	2.05424300	2.61150400	-0.04406800
N	-2.21872200	0.54422400	2.43733800	O	1.50681700	2.70881300	-1.16548900
O	-1.59953300	-0.48242300	2.80834000	O	1.56120500	3.12676200	0.99738400
O	-1.79888800	1.71217400	2.68707600	S	0.75699000	-0.42992600	0.24738500

Table S5. Coordination for RC structure (Cartesian coordinates are written in Å) of pro-*S*,*R*-RC located at B97D/6-31+G(d,p) with total energy and zero-point energy (ZPE) reported in Hartree per particle.

B97D	pro-*S*,*R*-RC with furan ring			B97D	pro-*S*,*R*-RC with thiophene ring		
total energy	-2243.2139268			-2566.2407987			
ZPE	0.4793382			0.4753218			
Atoms	x	y	z	Atoms	x	y	z
C	2.62714200	0.74356700	3.16545400	C	3.30870200	-2.95144700	-1.91943500
C	1.84845700	1.90117700	2.50072700	C	2.36495600	-3.69407900	-0.94633300
C	0.93766600	1.18840900	1.48281900	C	1.35995500	-2.60910000	-0.50673900
N	1.67326700	-0.05789400	1.15626200	N	2.09992700	-1.33780700	-0.68685300
H	3.56065600	1.07004300	3.64359600	H	4.28396800	-3.44417600	-2.03220900
H	2.53951300	2.58585900	1.98816400	H	2.92606700	-4.06822600	-0.07825000
H	0.76304500	1.77708300	0.57316000	H	1.04381000	-2.73458000	0.53806800
C	1.16263200	-1.09582700	0.45011600	C	1.56100600	-0.09736100	-0.59322300

H	1.75542200	-2.00893700	0.46633200	H	2.18538400	0.69644400	-1.00630100
C	0.00367600	-1.15006600	-0.29892000	C	0.35007900	0.31631300	-0.06285900
C	-0.53630200	-2.24698900	-1.02851800	C	-0.10411400	1.67609000	-0.12124800
O	-0.86312700	-0.06140700	-0.43032000	C	-1.35141100	1.88939300	0.41636500
C	-1.71939400	-1.82843200	-1.60274300	H	0.51238900	2.45301400	-0.57331800
H	-0.07254500	-3.22733400	-1.09452900	C	-1.99463000	0.70844500	0.94110500
C	-1.92845700	-0.45944300	-1.22891600	H	-1.85764000	2.85252000	0.44276900
H	-2.39918800	-2.40208600	-2.22503700	C	-3.28576100	0.69128900	1.43501800
C	-2.99936200	0.36277400	-1.51130100	H	-3.75971100	1.67575900	1.41931600
H	-3.75955700	-0.12099300	-2.12511900	C	-4.13644600	-0.37312700	1.93054700
C	-3.27389700	1.73416200	-1.13194700	C	-5.45767600	-0.01987800	2.33562400
C	-4.49578900	2.31507900	-1.57940300	C	-3.77701700	-1.74843100	2.01567300
C	-2.42360800	2.53868800	-0.31995200	C	-6.36740500	-0.98010500	2.79307700
C	-4.85370400	3.62407300	-1.23212400	H	-5.75959700	1.02715300	2.27546500
H	-5.16409500	1.71614400	-2.20043700	C	-4.69079100	-2.70673300	2.47446200
C	-2.78625100	3.84722300	0.02214000	H	-2.78744900	-2.08251900	1.71153900
H	-1.48732700	2.12945800	0.04844900	C	-5.99138900	-2.33528700	2.86615600
C	-4.00141000	4.40287600	-0.42678300	H	-7.37129100	-0.67311900	3.09201200
H	-5.79858500	4.03764900	-1.58956100	H	-4.38535100	-3.75341800	2.52220500
H	-2.11661500	4.43928800	0.64901300	H	-6.69705400	-3.08741400	3.22127600
H	-4.27677200	5.42259000	-0.15421300	C	3.43111300	-1.55147500	-1.28812300
C	2.87841500	-0.22905500	1.99589900	H	3.63112400	-0.76377600	-2.02723300
H	2.95377000	-1.27751000	2.31509200	C	4.53683400	-1.51484600	-0.20578700
C	4.16183400	0.15318200	1.22710600	H	4.40974200	-2.34650000	0.49992900
H	4.16664400	1.23011000	1.00340900	H	5.52019800	-1.61215300	-0.68101200
H	5.03220300	-0.09006800	1.84804900	H	0.46793700	-2.58759300	-1.15253900
H	-0.03428300	0.92040300	1.92270000	H	1.85598300	-4.54434300	-1.41682400
H	1.26274300	2.48338400	3.22312800	H	2.84450600	-2.86090700	-2.91139000
H	2.00103900	0.24485100	3.91813100	N	4.52697800	-0.28402100	0.60901200
N	4.24669600	-0.64073300	-0.01993700	H	3.67435400	-0.09755300	1.13668600
H	3.54361100	-0.41366600	-0.72483700	O	5.73830200	0.95403100	-1.30564600
O	6.62728400	-1.47453500	0.33472600	S	5.23222800	1.12171200	0.06925200
S	5.70356300	-1.01872600	-0.71640700	O	4.41042800	2.27110000	0.49053300
O	5.42795300	-1.79576700	-1.93618000	C	6.80528300	1.17861900	1.16758900
C	6.43214100	0.65792600	-1.33275900	F	6.46075700	1.28817500	2.46492400
F	5.54486900	1.25798600	-2.15563100	F	7.55641700	2.24022500	0.81458400
F	7.58394200	0.44691600	-1.99530500	F	7.52073000	0.04844400	0.99061100
F	6.66475300	1.46585900	-0.27527700	C	-5.88471500	3.75520900	-0.99604100
C	-7.34584700	-1.87304400	-1.44237800	C	-4.59146000	3.70490000	-1.55471500
C	-6.32911700	-2.80602400	-1.15293700	C	-3.94914900	2.47624800	-1.74253900
C	-5.26078300	-2.45315700	-0.32124800	C	-4.58919000	1.26595800	-1.36545400
C	-5.18313500	-1.14963000	0.23703400	C	-5.89406600	1.33102200	-0.81157300
C	-6.21529900	-0.22242800	-0.05963900	C	-6.53486400	2.56232400	-0.62846000
C	-7.28512600	-0.58048500	-0.88992700	H	-6.38007500	4.71614400	-0.85185900
H	-8.17620000	-2.15357400	-2.09152700	H	-4.08532800	4.62774700	-1.84097900

H	-6.37216900	-3.80878400	-1.58013100	H	-2.94479700	2.45389100	-2.16287000
H	-4.47729900	-3.18194800	-0.11611700	H	-6.38665100	0.40615400	-0.51008200
H	-6.15658200	0.78371900	0.35605800	H	-7.53566300	2.59434900	-0.19607400
H	-8.06771200	0.14680400	-1.10987200	C	-3.96537300	-0.04107900	-1.50205800
C	-4.08541700	-0.71000600	1.08623400	H	-4.51912400	-0.89490700	-1.10971800
H	-4.07830400	0.34069700	1.37690400	C	-2.76634200	-0.28849300	-2.09642700
C	-3.09221500	-1.50741500	1.57179000	H	-2.10245200	0.45902400	-2.51642400
H	-2.96543400	-2.56109500	1.34868000	N	-2.24648700	-1.61678900	-2.22654600
N	-2.05330800	-0.99532600	2.40235500	O	-2.88794400	-2.60245200	-1.79724600
O	-2.09443800	0.18614200	2.83086800	O	-1.13598100	-1.72948000	-2.80845900
O	-1.10551700	-1.77999100	2.67331400	S	-0.89488800	-0.68071800	0.74739700

Table S6. Coordination for TS structure (Cartesian coordinates are written in Å) of pro-*R*,*S*-TS located at B97D/6-31+G(d,p) with obtained imaginary frequencies $v^{\ddagger}$ with total energy and zero-point energy (ZPE) reported in Hartree per particle.

B97D	pro-*R*,*S*-TS with furan ring ($v^{\ddagger}$ = -309.65 cm^{-1})			B97D	pro-*R*,*S*-TS with thiophene ring($v^{\ddagger}$ = -307.42 cm^{-1})		
total energy	-2243.2318838			-2566.2500239			
ZPE	0.479886			0.475524			
Atoms	x	y	z	Atoms	x	y	z
C	2.82943400	3.73240400	-0.96758100	C	3.63407800	3.53604900	-1.34832200
C	1.37320100	3.65478700	-1.49037000	C	2.21480700	3.67882800	-1.95096500
C	0.58353700	2.93702000	-0.37164800	C	1.25436000	3.26910500	-0.80793500
N	1.62968300	2.32584300	0.48890200	N	2.12074900	2.58603700	0.18571400
H	3.56909800	3.76910200	-1.77790500	H	4.39840200	3.33164800	-2.10897400
H	1.32930700	3.06267700	-2.41409100	H	2.09053500	2.99840100	-2.80354200
H	-0.06597500	2.14183100	-0.75553100	H	0.47895100	2.56839100	-1.14551400
C	1.42363000	1.54780900	1.54374400	C	1.71681900	1.93838300	1.27111600
H	2.31390600	1.23267800	2.08422800	H	2.51987200	1.47055100	1.83961800
C	0.21059300	1.03403200	2.01934200	C	0.41676900	1.65104200	1.72626300
C	-0.00822500	0.10309700	3.04754000	C	0.22191100	0.53742200	2.57619300
O	-0.97023000	1.21174000	1.31571800	C	-1.06861600	0.01423200	2.51375200
C	-1.33977600	-0.31873500	2.93845200	H	1.04841200	0.07589000	3.11436600
H	0.74452200	-0.23626100	3.75287300	C	-1.92595000	0.71896700	1.64213300
C	-1.90404800	0.37130000	1.85196000	H	-1.38528900	-0.90109600	3.00885800
H	-1.85477500	-1.05697500	3.54420500	C	-3.14266900	0.14886300	1.11744000
C	-3.11927800	0.11309500	1.13420500	H	-3.52760200	-0.61683800	1.79891600
H	-3.74021900	-0.58342700	1.70293000	C	-4.23787700	0.93994200	0.49296700
C	-3.91786800	1.15499500	0.44409200	C	-5.56656600	0.71042300	0.91729900
C	-5.32894000	1.06377500	0.49940300	C	-4.02512500	1.84379400	-0.57448800

C	-3.34313200	2.18475600	-0.33995600	C	-6.64509200	1.37900000	0.31837200
C	-6.14162500	1.98151400	-0.18377100	H	-5.74895700	-0.00604000	1.72010700
H	-5.78510800	0.26277800	1.08300800	C	-5.10224400	2.51478100	-1.17379400
C	-4.15620700	3.10358600	-1.01962300	H	-3.02098200	2.00142200	-0.96695700
H	-2.26194700	2.25681800	-0.42705800	C	-6.41749300	2.28894100	-0.72925000
C	-5.55896100	3.00939100	-0.94577300	H	-7.66128500	1.18434700	0.66477200
H	-7.22731500	1.89055300	-0.12345900	H	-4.91384200	3.20459800	-1.99798100
H	-3.69281200	3.89059700	-1.61712100	H	-7.25370700	2.80791300	-1.19970800
H	-6.18732500	3.72325500	-1.48017500	C	3.48426900	2.37310100	-0.35723100
C	2.97073900	2.45998700	-0.11941800	H	4.21286100	2.39053700	0.46138700
H	3.72646300	2.53067200	0.67217300	C	3.53850200	0.99043600	-1.06843000
C	3.25808600	1.20513800	-0.99281200	H	2.74779300	0.92585400	-1.82544000
H	2.48805100	1.10107800	-1.76668800	H	4.51155100	0.90015200	-1.56857400
H	4.23384300	1.33951400	-1.47735200	H	0.77918600	4.13265500	-0.32257100
H	-0.00833300	3.62321900	0.24892900	H	2.01134300	4.69882400	-2.29841700
H	0.95593800	4.64654300	-1.70311300	H	3.91911100	4.44519400	-0.80091400
H	2.96831000	4.61422900	-0.32670700	N	3.30229200	-0.12608400	-0.14012400
N	3.21631800	-0.03373900	-0.20802700	H	2.41354800	-0.70763900	-0.21327500
H	2.36113900	-0.66883900	-0.25234200	O	5.61804800	0.14441800	0.88040900
O	5.51072700	0.43713300	0.78686600	S	4.53438100	-0.83687500	0.66192100
S	4.53727900	-0.64381500	0.52204800	O	3.99109200	-1.66297200	1.75507000
O	4.12397600	-1.60176200	1.56416700	C	5.28406100	-2.10622200	-0.57802700
C	5.38305700	-1.73113500	-0.82066100	F	4.35371300	-3.01834400	-0.92593700
F	4.54396900	-2.71043800	-1.21731100	F	6.33749600	-2.73852500	-0.01881900
F	6.51192900	-2.28770400	-0.33123000	F	5.70160300	-1.46133500	-1.69427500
F	5.69955100	-0.96732600	-1.89355200	C	-5.98006600	-3.52981000	-0.78978000
C	-6.06084800	-3.50304000	-0.74245300	C	-5.01721000	-3.84333600	0.18888800
C	-5.03846700	-3.90003300	0.14167700	C	-3.86917400	-3.05025800	0.32991100
C	-3.86827600	-3.13661100	0.25815100	C	-3.65734100	-1.93146600	-0.50833000
C	-3.69423200	-1.96152500	-0.51063500	C	-4.63687300	-1.61829900	-1.47622900
C	-4.73077900	-1.56826500	-1.38724000	C	-5.78458600	-2.41375800	-1.62169400
C	-5.90131300	-2.33446600	-1.50699400	H	-6.87332800	-4.14670000	-0.89788200
H	-6.96999300	-4.09919200	-0.83257800	H	-5.16320600	-4.70397800	0.84358500
H	-5.15483100	-4.80464400	0.74059800	H	-3.13713100	-3.29514500	1.10059800
H	-3.08899500	-3.44996400	0.95367700	H	-4.49399100	-0.74274600	-2.11039900
H	-4.61018300	-0.65733100	-1.97423300	H	-6.52745700	-2.15737100	-2.37865600
H	-6.68736900	-2.01702900	-2.19394400	C	-2.47132500	-1.04156100	-0.35471000
C	-2.49026300	-1.09931200	-0.38895300	H	-2.40651500	-0.25564100	-1.11082600
H	-2.43906800	-0.30007500	-1.13110400	C	-1.20353200	-1.66277600	-0.08199600
C	-1.21575400	-1.70663400	-0.13306900	H	-1.10341900	-2.60213800	0.45029700
H	-1.08734600	-2.60353800	0.46260300	N	-0.01633800	-1.11178900	-0.46312500

N	-0.04797400	-1.13936500	-0.54023900	O	0.06603300	-0.01709200	-1.11530200
O	0.00359900	-0.09183400	-1.27139400	O	1.08315900	-1.75288200	-0.17337900
O	1.06987800	-1.71387700	-0.18234200	S	-1.12480400	2.13805700	1.00107000

Table S7. Coordination for TS structure (Cartesian coordinates are written in Å) of pro-*R*,*R*-TS located at B97D/6-31+G(d,p) with obtained imaginary frequencies $v^{\ddagger}$ with total energy and zero-point energy (ZPE) reported in Hartree per particle.

B97D	pro-*R*,*R*-TS with furan ring ($v^{\ddagger}$ = -296.87 cm^{-1})			B97D	pro-*R*,*R*-TS with thiophene ring ($v^{\ddagger}$ = -304.32 cm^{-1})		
total energy	-2243.2253241			-2566.2292121			
ZPE	0.4796326			0.4761215			
Atoms	x	y	z	Atoms	x	y	z
C	3.07269700	3.73409500	-0.93017500	C	-3.98079700	-3.47765300	-1.22798100
C	1.61313900	3.71652300	-1.46034700	C	-2.59097700	-3.69993500	-1.88608500
C	0.79044400	2.94959600	-0.39172600	C	-1.55328800	-3.18676400	-0.84974400
N	1.80667000	2.41913800	0.54708500	N	-2.36676700	-2.60196800	0.23953800
H	3.81504400	3.72028800	-1.73896300	H	-4.75880800	-3.23194600	-1.96245800
H	1.55805400	3.18191100	-2.41742600	H	-2.50353300	-3.11926600	-2.81311100
H	0.24116700	2.11090600	-0.84033900	H	-0.91257400	-2.39924800	-1.28079900
C	1.57808800	1.72157400	1.65704300	C	-1.91618700	-2.04673100	1.36350500
H	2.45925800	1.46859600	2.24428900	H	-2.69725000	-1.66713700	2.02248000
C	0.36592700	1.23176400	2.14543300	C	-0.60059700	-1.79452000	1.77849100
C	0.13228800	0.44147300	3.28672900	C	-0.31857900	-0.93144500	2.86961800
O	-0.80158100	1.30485100	1.39776600	C	0.97396500	-0.42053700	2.85128800
C	-1.18396600	-0.01407600	3.20451600	H	-1.09088500	-0.63397600	3.57732300
H	0.87137400	0.21765300	4.05019300	C	1.74965500	-0.87505000	1.75710500
C	-1.72877400	0.50944700	2.01429200	H	1.35443500	0.32382500	3.54838800
H	-1.70741300	-0.67098700	3.89147500	C	2.95460000	-0.24433100	1.28273600
C	-2.94156300	0.17366100	1.33545500	H	3.35814400	0.42545900	2.04948700
H	-3.58981200	-0.41979800	1.98470500	C	4.03667800	-0.93428700	0.53063800
C	-3.68831700	1.09540100	0.45168300	C	5.37441200	-0.67497400	0.90959900
C	-5.10191700	1.02365800	0.45474900	C	3.81299100	-1.76048900	-0.59544200
C	-3.06417400	1.97832400	-0.46230900	C	6.45119100	-1.24041600	0.21161000
C	-5.87027000	1.82145500	-0.40588100	H	5.56493300	-0.01584900	1.75820600

H	-5.59436200	0.32959000	1.13774500	C	4.88989200	-2.32594500	-1.29657700
C	-3.83377500	2.77265200	-1.32627600	H	2.80248300	-1.93865000	-0.95802700
H	-1.98096500	2.03518100	-0.50649200	C	6.21371800	-2.07298300	-0.89641300
C	-5.23871200	2.70123700	-1.30282900	H	7.47296800	-1.02437400	0.52739500
H	-6.95867000	1.74877900	-0.38210900	H	4.69154800	-2.95655900	-2.16467700
H	-3.33258900	3.44577300	-2.02400400	H	7.04791500	-2.51252000	-1.44496500
H	-5.83232600	3.32037400	-1.97696500	C	-3.73544100	-2.32371600	-0.24601600
C	3.15272300	2.47467700	-0.05505600	H	-4.42766100	-2.29948900	0.60463800
H	3.90547100	2.52549000	0.74187300	C	-3.73809700	-0.94414700	-0.96613300
C	3.37681600	1.19035100	-0.90396700	H	-3.07324700	-0.97380300	-1.83881700
H	2.67219500	1.16515800	-1.74430200	H	-4.75975300	-0.73284600	-1.30505900
H	4.40197000	1.20509500	-1.29356400	H	-0.92550600	-3.98598800	-0.43476900
H	0.09384800	3.58352100	0.17065300	H	-2.42213600	-4.75536400	-2.13119000
H	1.22437800	4.73030800	-1.61548500	H	-4.29689500	-4.36894200	-0.66927600
H	3.25189900	4.62020600	-0.30596600	N	-3.23902300	0.12884400	-0.09847500
N	3.13199000	-0.02695000	-0.12226300	H	-2.21750100	0.40829000	-0.14252800
H	2.16102000	-0.44250700	-0.10785500	O	-5.53516200	0.50402100	0.93302200
O	5.51730100	-0.09074300	0.76115300	S	-4.22536400	1.14766000	0.70029200
S	4.32039200	-0.92530800	0.52758400	O	-3.47087300	1.81199200	1.77909900
O	3.75305100	-1.80269100	1.56847000	C	-4.59535700	2.54890200	-0.56507500
C	4.84006400	-2.12356800	-0.88356300	F	-3.44788500	3.16327100	-0.92107700
F	3.78098500	-2.86548900	-1.27017500	F	-5.43661900	3.45949600	-0.02958000
F	5.82684600	-2.94566700	-0.46612700	F	-5.16824000	2.01976000	-1.67252500
F	5.28278300	-1.40965900	-1.94576800	C	5.89513000	3.32550500	-0.69313700
C	-6.07312200	-3.25334800	-0.68011700	C	5.48877200	2.32467500	-1.59382300
C	-5.64527000	-2.20325700	-1.51155300	C	4.29384600	1.62142700	-1.38134000
C	-4.41539800	-1.56909200	-1.27843400	C	3.47554600	1.91197800	-0.26674800
C	-3.58249400	-1.98328700	-0.21384300	C	3.89891700	2.91311500	0.63647800
C	-4.02918800	-3.03253500	0.62279500	C	5.09375900	3.61786900	0.42579900
C	-5.25908300	-3.66566400	0.39179000	H	6.82563500	3.87003800	-0.85979000
H	-7.03000100	-3.74409400	-0.86348100	H	6.10713900	2.08479100	-2.46008700
H	-6.27346300	-1.86990800	-2.33894400	H	4.00875300	0.83402400	-2.07712000
H	-4.11052500	-0.74391900	-1.92008100	H	3.27972300	3.13548300	1.50789200
H	-3.39748800	-3.35309900	1.45372200	H	5.39799400	4.39246700	1.13147500
H	-5.58058300	-4.47991500	1.04296700	C	2.22225300	1.16429200	0.03517300
C	-2.28457600	-1.32799200	0.09188700	H	1.59127700	1.65479200	0.77932400
H	-1.68550900	-1.85409400	0.83715800	C	1.48019000	0.58154700	-1.04571700
C	-1.52792900	-0.74678500	-0.97115700	H	1.94032100	0.22075300	-1.95825800
H	-1.98560100	-0.34444900	-1.86703500	N	0.12292600	0.42088800	-1.02248300
N	-0.17932600	-0.55972000	-0.92213500	O	-0.57647600	0.83920500	-0.01736900
O	0.52904700	-1.00079300	0.06811100	O	-0.47394000	-0.13769300	-2.01180500

O	0.40524900	0.06202700	-1.88402100	S	0.86859500	-2.06163400	0.82836300

Table S8. Coordination for TS structure (Cartesian coordinates are written in Å) of pro-*S,S*-TS located at B97D/6-31+G(d,p) with obtained imaginary frequencies $v^{\ddagger}$ with total energy and zero-point energy (ZPE) reported in Hartree per particle.

B97D	pro-*S,S*-TS with furan ring ($v^{\ddagger}$ = -307.63 cm^{-1})			B97D	pro-*S,S*-TS with thiophene ring ($v^{\ddagger}$ = -313.41 cm^{-1})		
total energy	-2243.2188618			-2566.2250223			
ZPE	0.4796842			0.4764539			
Atoms	x	y	z	Atoms	x	y	z
C	2.63398700	1.50742300	2.83176500	C	-3.41509000	3.25415800	0.66248300
C	1.50765300	2.33730600	2.17471500	C	-2.33759600	3.08948400	1.75898500
C	0.71805400	1.29748300	1.35928300	C	-1.41165000	1.97977400	1.21629500
N	1.71805100	0.23880600	1.06275800	N	-2.25963500	1.24095100	0.24521300
H	3.49190100	2.11706000	3.14493600	H	-4.34661800	3.69526100	1.04086300
H	1.92959200	3.10943500	1.51522800	H	-2.79665300	2.77287700	2.70579700
H	0.30333000	1.69272900	0.42491500	H	-1.06100100	1.30502900	2.00845700
C	1.49054700	-0.88911000	0.39155900	C	-1.85754800	0.27695400	-0.58182400
H	2.31136800	-1.60327800	0.37308800	H	-2.59409000	-0.01448300	-1.33159200
C	0.33457800	-1.28501500	-0.28347400	C	-0.61586000	-0.36909800	-0.66148500
C	0.07051300	-2.50288900	-0.94148000	C	-0.23987000	-1.17616000	-1.76750700
O	-0.78549800	-0.46961600	-0.37654600	C	1.09472200	-1.56637200	-1.74093000
C	-1.24234100	-2.43872000	-1.40792700	H	-0.93825700	-1.40727200	-2.57065500
H	0.77640400	-3.32249600	-1.03837800	C	1.80205100	-1.10789500	-0.60274700
C	-1.75304000	-1.17844100	-1.03619200	H	1.58706000	-2.14369900	-2.52146400
H	-1.79622200	-3.19826000	-1.95016600	C	3.23184000	-1.16476400	-0.42732300
C	-3.07847200	-0.64647700	-1.14603800	H	3.67378900	-1.82226700	-1.18367000
H	-3.68033500	-1.27657100	-1.80664500	C	3.89576700	-1.33517300	0.89587200
C	-3.34929600	0.80138400	-1.32657400	C	4.92888800	-2.29481700	1.00262500
C	-4.35369400	1.19012200	-2.24318300	C	3.61256500	-0.53481500	2.02665300
C	-2.71768600	1.80805600	-0.55823700	C	5.63742400	-2.47124800	2.20000500
C	-4.70196200	2.53888100	-2.40882800	H	5.17811500	-2.90167400	0.13043100
H	-4.86721900	0.42115500	-2.82293300	C	4.32297600	-0.70760200	3.22563500
C	-3.07086800	3.15723100	-0.71935500	H	2.86727100	0.25601400	1.96833600

H	-1.96826900	1.53366900	0.17786200	C	5.33613000	-1.67755400	3.32128400
C	-4.06095200	3.53153600	-1.64586800	H	6.42861700	-3.22072600	2.25416500
H	-5.47936600	2.81239900	-3.12404500	H	4.08941500	-0.07361000	4.08255800
H	-2.57408600	3.91727600	-0.11354900	H	5.88675600	-1.80845200	4.25393000
H	-4.33246500	4.58120300	-1.76769400	C	-3.61893000	1.81707500	0.14876000
C	3.01416900	0.49822700	1.73205200	H	-3.95152400	1.77335600	-0.89410800
H	3.41458800	-0.44536600	2.12281400	C	-4.61868100	1.04208700	1.04135200
C	4.03412600	1.11168400	0.74383800	H	-4.34027900	1.14413000	2.09708700
H	3.66653900	2.07009700	0.35791000	H	-5.61615200	1.48371100	0.91030500
H	4.97093500	1.29547800	1.28433200	H	-0.53814900	2.38588900	0.67806900
H	-0.09341900	0.84556600	1.95387600	H	-1.78104800	4.01621300	1.94221200
H	0.86591700	2.83164200	2.91415500	H	-3.03849600	3.87909300	-0.15847800
H	2.25069800	0.96426400	3.70621800	N	-4.62059200	-0.41462900	0.77805300
N	4.27414200	0.24087000	-0.42367800	H	-4.56529300	-1.03181400	1.58592800
H	3.89741600	0.51533400	-1.32791000	O	-5.25365000	-0.26232000	-1.67577300
O	5.82060300	-1.30681400	0.84977700	S	-5.43665600	-1.10875800	-0.48443100
S	5.53456600	-0.82011900	-0.50973100	O	-5.14324800	-2.55034800	-0.46805100
O	5.31136800	-1.70893300	-1.66111200	C	-7.31191500	-0.97311800	-0.04650500
C	7.06099300	0.25312800	-0.99070400	F	-7.52437600	-1.49962100	1.17731700
F	6.83349200	0.86023100	-2.17382400	F	-8.03757700	-1.64631600	-0.95648300
F	8.15433000	-0.52446700	-1.08977500	F	-7.69098400	0.32314600	-0.04036400
F	7.26666600	1.19667600	-0.04550000	C	8.11952800	-0.19493600	-1.17233100
C	-8.09501400	-0.56573300	-0.40148300	C	7.54313100	0.45027100	-0.06334900
C	-7.34734400	0.51605400	0.09718000	C	6.16664500	0.72057900	-0.03608200
C	-5.99517000	0.34947600	0.43333300	C	5.33945600	0.35976300	-1.12284300
C	-5.36709900	-0.90833900	0.28909100	C	5.92859200	-0.29450600	-2.22787700
C	-6.12515300	-1.98461200	-0.22524200	C	7.30498700	-0.56734400	-2.25726900
C	-7.47688400	-1.81954500	-0.56388800	H	9.18984300	-0.40554200	-1.19080500
H	-9.14593100	-0.43314800	-0.66281800	H	8.16465000	0.73737900	0.78626700
H	-7.81465400	1.49475100	0.21665800	H	5.73413300	1.20124100	0.83988000
H	-5.42387700	1.20312100	0.79515700	H	5.29676400	-0.58704700	-3.06931800
H	-5.64611500	-2.95778700	-0.35153000	H	7.74046100	-1.06691800	-3.12418200
H	-8.04665000	-2.66624200	-0.95006500	C	3.86369400	0.58865400	-1.12989000
C	-3.92910400	-1.13002800	0.61004100	H	3.41790000	0.48856300	-2.12212900
H	-3.63666200	-2.18215700	0.60100500	C	3.32290000	1.68381000	-0.38154800
C	-3.33282000	-0.37304500	1.66477300	H	3.76059300	2.05701700	0.53651700
H	-3.67851200	0.61043800	1.95975700	N	2.19114300	2.36258800	-0.77618900
N	-2.20977900	-0.79478500	2.32804400	O	1.58640200	2.07038900	-1.86177400
O	-1.67652800	-1.93027600	2.08740300	O	1.76018600	3.32188300	-0.03547500
O	-1.69764500	-0.01571500	3.22055600	S	0.74351500	-0.21809200	0.46179100

Table S9. Coordination for TS structure (Cartesian coordinates are written in Å) of pro-*S*,*R*-TS located at B97D/6-31+G(d,p) with obtained imaginary frequencies $v^{\ddagger}$ with total energy and zero-point energy (ZPE) reported in Hartree per particle.

B97D	pro-*S*,*R*-TS with furan ring ($v^{\ddagger}$ = -289.13 cm^{-1})			B97D	pro-S,*R*-TS with thiophene ring ($v^{\ddagger}$ = -274.96 cm^{-1})		
total energy	-2243.2117989			-2566.2193846			
ZPE	0.479365			0.4761528			
Atoms	x	y	z	Atoms	x	y	z
C	2.64620400	1.55778400	2.78008900	C	3.29062900	0.60795000	3.29912400
C	1.64629500	2.51699800	2.09367600	C	2.33713300	1.80510700	3.08047700
C	0.77524700	1.58675300	1.22811700	C	1.33619500	1.30272000	2.01768800
N	1.64334500	0.40263000	0.98446100	N	2.05016200	0.18982200	1.33617300
H	3.55826600	2.06195700	3.12575200	H	4.26836600	0.90716500	3.69879100
H	2.17903300	3.24579800	1.46620700	H	2.88986400	2.67561600	2.70134700
H	0.47471000	2.02796300	0.27007600	H	1.07003600	2.08319600	1.29300100
C	1.30110200	-0.69122100	0.31515600	C	1.54093700	-0.62985200	0.42111100
H	2.03765900	-1.49199700	0.29698800	H	2.17666800	-1.47625800	0.15942900
C	0.10465600	-0.95110600	-0.36450100	C	0.28604100	-0.59063100	-0.21057300
C	-0.28815100	-2.10217300	-1.06730500	C	-0.22275000	-1.67107000	-0.97418500
O	-0.93336000	-0.03341900	-0.38917400	C	-1.53851400	-1.47995600	-1.39933200
C	-1.59271600	-1.87315500	-1.52697400	H	0.37156500	-2.56152400	-1.17540200
H	0.32760400	-2.98491900	-1.21309800	C	-2.08638500	-0.23734900	-1.01411600
C	-1.96399100	-0.59182500	-1.09145800	H	-2.11771500	-2.20652900	-1.96563300
H	-2.22432300	-2.54379600	-2.10000200	C	-3.49117800	0.11811200	-1.05881100
C	-3.26109100	0.03391600	-1.03986700	H	-4.01060700	-0.59141500	-1.71158100
H	-3.92924300	-0.48661500	-1.73197300	C	-3.92599300	1.52127500	-1.36414900
C	-3.39810300	1.51908000	-1.15687200	C	-4.67371000	1.75264500	-2.54105600
C	-4.23114900	2.05038000	-2.16684600	C	-3.63904100	2.61727000	-0.52000300
C	-2.75930800	2.41160000	-0.26543200	C	-5.09709200	3.04720100	-2.88468300
C	-4.40082400	3.43840400	-2.30464000	H	-4.91579500	0.91026300	-3.19224900
H	-4.74276400	1.36842000	-2.84908000	C	-4.05524600	3.91252000	-0.86821200
C	-2.92336600	3.79780400	-0.40918400	H	-3.13842800	2.44782300	0.43303000
H	-2.16805800	2.00854900	0.55457400	C	-4.78172700	4.13570200	-2.05209100
C	-3.74089000	4.31936000	-1.42980200	H	-5.67160200	3.20337000	-3.79925500
H	-5.04737400	3.82870300	-3.09239000	H	-3.82692800	4.74614100	-0.20188100
H	-2.42356800	4.47291500	0.28800000	H	-5.11042200	5.14237700	-2.31462500
H	-3.87186300	5.39760000	-1.53311700	C	3.40654200	-0.01415000	1.89653700
C	2.94419500	0.51591400	1.68567100	H	3.63309700	-1.08700800	1.91081200
H	3.22675200	-0.46696300	2.08153500	C	4.46378900	0.71350300	1.03310700
C	4.04652400	1.01255600	0.72072600	H	4.26159300	1.79086800	0.99964100

H	3.79567700	2.00470200	0.32730800	H	5.44783600	0.56304700	1.49349800
H	4.98484300	1.09225300	1.28331400	H	0.41359200	0.89674900	2.46646600
H	-0.12985500	1.24537900	1.75552600	H	1.82003100	2.10293400	4.00010900
H	1.03599500	3.07068600	2.81733500	H	2.84111500	-0.12499200	3.98285400
H	2.17350400	1.05742600	3.63594000	N	4.46166600	0.22711800	-0.36012300
N	4.21326800	0.11620000	-0.44057900	H	4.10477200	0.83565300	-1.09318000
H	3.88983700	0.43129100	-1.35228600	O	5.75928700	-1.87084600	0.20965500
O	5.58301900	-1.56773900	0.86077600	S	5.49543400	-0.94189400	-0.90137300
S	5.36378900	-1.06644700	-0.50564200	O	5.04358400	-1.37451600	-2.23311400
O	5.06236900	-1.93713900	-1.65316400	C	7.16521200	-0.02897900	-1.20779600
C	6.99671800	-0.15898500	-0.98093800	F	6.98269800	0.95279900	-2.11457900
F	6.84187000	0.45701200	-2.17111800	F	8.08378400	-0.89800400	-1.66606600
F	8.00413900	-1.04644600	-1.06433500	F	7.60216100	0.51636600	-0.05153300
F	7.29094400	0.76619900	-0.04171000	C	-6.75288100	-3.65435800	-0.50023900
C	-7.65419100	-2.37405900	-0.58117500	C	-5.40002500	-3.89573000	-0.19599200
C	-6.47287000	-3.13374000	-0.48576000	C	-4.56514100	-2.84236600	0.20822200
C	-5.27843000	-2.53510200	-0.05674400	C	-5.06816200	-1.52602400	0.31929800
C	-5.24272500	-1.16550000	0.29126200	C	-6.42451700	-1.29361300	0.00125600
C	-6.43132700	-0.41059100	0.18166100	C	-7.26215900	-2.34733600	-0.39958500
C	-7.62837600	-1.00879200	-0.24552700	H	-7.40074500	-4.47491400	-0.81178100
H	-8.58225300	-2.84136600	-0.91354100	H	-4.99446700	-4.90587800	-0.27382100
H	-6.48218700	-4.19313900	-0.74733500	H	-3.51729900	-3.04321500	0.43096500
H	-4.36848100	-3.13292400	0.00144100	H	-6.81924600	-0.27833100	0.07304000
H	-6.41036700	0.65051200	0.43650900	H	-8.30937100	-2.14773800	-0.63251600
H	-8.53785300	-0.40989300	-0.31578900	C	-4.19862800	-0.36438500	0.69180500
C	-3.97847200	-0.47789000	0.69961400	H	-4.76557400	0.55312100	0.87235500
H	-4.14365000	0.53543200	1.07412800	C	-3.21051900	-0.60293200	1.71640200
C	-3.06187000	-1.22232900	1.52827600	H	-2.72287500	-1.56326000	1.84598900
H	-2.95516800	-2.30032800	1.47130400	N	-2.74951600	0.36468500	2.56808400
N	-2.14308500	-0.61920700	2.33806500	O	-3.21210900	1.55969700	2.53888900
O	-2.14148800	0.65500500	2.51556200	O	-1.83892700	0.05065600	3.42458800
O	-1.27470600	-1.34886300	2.94930400	S	-0.92937000	0.68810300	-0.09825900

Table S10. Coordination for PC structure (Cartesian coordinates are written in Å) of *R,S*-PC located at B97D/6-31+G(d,p) with total energy and zero-point energy (ZPE) reported in Hartree per particle.

B97D	*R,S*-PC with furan ring	B97D	*R,S*-PC with thiophene ring
total energy	-2243.2381056	-2566.2409229	

ZPE	0.4816961			0.4781782			
Atoms	x	y	z	Atoms	x	y	z
C	-2.73104800	-3.00625500	-2.39835000	C	3.76079700	-3.25568900	1.93006700
C	-1.24585400	-2.74472900	-2.75569700	C	2.34738000	-3.31536500	2.56660400
C	-0.53474600	-2.54020200	-1.39946800	C	1.35969300	-3.00828400	1.41015100
N	-1.64522700	-2.27365000	-0.44080700	N	2.22438500	-2.56719900	0.28363800
H	-3.41581700	-2.70747000	-3.20279900	H	4.52796700	-2.92200000	2.64061400
H	-1.15344600	-1.83150400	-3.35728500	H	2.24470900	-2.55406300	3.35015300
H	0.15142100	-1.68907000	-1.41218800	H	0.67110700	-2.19092200	1.66697500
C	-1.54546500	-1.97233900	0.83711600	C	1.84017700	-2.16479900	-0.91385100
H	-2.47711400	-1.96104200	1.40099000	H	2.65492300	-1.90938600	-1.59104700
C	-0.38171400	-1.60907000	1.55359000	C	0.53861900	-1.89508800	-1.40103300
C	-0.24734100	-1.23114300	2.88879500	C	0.36446100	-1.07258300	-2.53246400
O	0.77152000	-1.27124800	0.86900900	C	-0.88887400	-0.43768300	-2.56093900
C	1.02064000	-0.61333000	3.01042200	H	1.17731000	-0.86496800	-3.22607600
H	-1.00708000	-1.34989300	3.65519600	C	-1.69505300	-0.76560900	-1.46848700
C	1.59296300	-0.63009600	1.74694500	H	-1.18142900	0.31389600	-3.29123600
H	1.45579300	-0.15994800	3.89472300	C	-2.90307500	0.00507000	-0.99265200
C	2.79788400	0.04643400	1.17009600	H	-3.10079100	0.75591600	-1.77146200
H	3.12976000	0.76734500	1.93047200	C	-4.16969300	-0.82069000	-0.79873800
C	3.95648600	-0.90007000	0.86644500	C	-5.25301100	-0.65004100	-1.68179700
C	5.23620900	-0.62403200	1.38169300	C	-4.29669600	-1.74148700	0.26105800
C	3.77894500	-2.01547300	0.02391500	C	-6.43838200	-1.38686600	-1.51732000
C	6.32699700	-1.45061500	1.06237300	H	-5.16729700	0.07025700	-2.49756600
H	5.37739000	0.24728700	2.02346100	C	-5.47657800	-2.48432000	0.42593100
C	4.86658900	-2.84424200	-0.29404700	H	-3.48276500	-1.87266000	0.97505500
H	2.79268300	-2.23423800	-0.38556400	C	-6.55227800	-2.30960900	-0.46338300
C	6.14440700	-2.56332000	0.22339000	H	-7.26931200	-1.23759700	-2.20832200
H	7.31511100	-1.22300800	1.46467300	H	-5.55834600	-3.19118500	1.25288700
H	4.71758200	-3.70574400	-0.94663100	H	-7.47111800	-2.88258800	-0.33163400
H	6.98966500	-3.20591100	-0.02647000	C	3.59048100	-2.26819800	0.76878000
C	-2.94500000	-2.16628600	-1.13250000	H	4.30671800	-2.40016300	-0.04941500
H	-3.73696500	-2.53046200	-0.46932800	C	3.61707500	-0.78454500	1.25659500
C	-3.20722000	-0.65258800	-1.46245400	H	2.93983000	-0.66466200	2.11169400
H	-2.48350000	-0.33232700	-2.22337700	H	4.64015900	-0.56486500	1.59082900
H	-4.21521200	-0.61133300	-1.90557700	H	0.78990500	-3.88775300	1.08276100
H	-0.00867500	-3.43840500	-1.04684200	H	2.14186400	-4.29409600	3.01575600
H	-0.80081300	-3.57371900	-3.31927100	H	4.05453400	-4.23692700	1.53300200
H	-2.89931400	-4.06852400	-2.17149300	N	3.14084500	0.16391300	0.24218000
N	-3.01883300	0.26231000	-0.33529700	H	2.23844000	0.77841700	0.44384800
H	-1.87354800	1.35701500	-0.37566400	O	5.19397700	-0.28044300	-1.21091600

O	-4.92063800	-0.89580100	1.02556600	S	4.14257200	0.72045700	-0.91467800
S	-4.15810200	0.36706700	0.77527600	O	3.34940900	1.34358100	-1.99088900
O	-3.65164500	1.13218600	1.94387300	C	5.09902600	2.18547200	-0.10867700
C	-5.51788700	1.53833100	0.05964900	F	4.23760600	3.15083300	0.27148200
F	-4.98271200	2.73630400	-0.28334800	F	5.98572600	2.70464500	-0.98582100
F	-6.50631500	1.75746100	0.96374600	F	5.77130900	1.74673500	0.98382200
F	-6.07970600	0.99484400	-1.05597100	C	-5.66211900	3.60217400	1.33447600
C	5.73729000	3.38429300	-1.29407500	C	-4.88272400	3.80050200	0.17935500
C	4.98208400	3.70033500	-0.14961700	C	-3.85454800	2.89927800	-0.13928300
C	3.89221800	2.89585400	0.21923400	C	-3.58756300	1.78933800	0.68879200
C	3.54189200	1.76849500	-0.55077600	C	-4.37442800	1.59782500	1.84064300
C	4.30153200	1.45920700	-1.69437500	C	-5.40386600	2.49827100	2.16545400
C	5.39361000	2.26153300	-2.06662000	H	-6.46159200	4.30170500	1.58312500
H	6.58482500	4.00854900	-1.58035900	H	-5.07543600	4.65546300	-0.47077100
H	5.24133600	4.57124500	0.45415300	H	-3.25422700	3.05965100	-1.03661000
H	3.31447800	3.14716500	1.11043000	H	-4.17859800	0.73710900	2.48231600
H	4.03819900	0.58213900	-2.28777700	H	-6.00332400	2.33567300	3.06272100
H	5.97426800	2.00852200	-2.95493300	C	-2.48965300	0.79519900	0.33341300
C	2.39230900	0.85871400	-0.13522900	H	-2.41045600	0.05520500	1.13911000
H	2.22729500	0.12111900	-0.92949900	C	-1.13830200	1.44420300	0.18402900
C	1.09503200	1.59193700	0.08020000	H	-0.95989800	2.21926500	-0.55443900
H	0.93216200	2.27208300	0.90946400	N	-0.07164600	1.08136800	0.89656600
N	0.05246200	1.36312700	-0.69213200	O	-0.08060000	0.16555400	1.80307700
O	-0.01936800	0.59837100	-1.69549500	O	1.08356000	1.71222500	0.66331800
O	-1.11061100	2.08136500	-0.36033500	S	-0.94855400	-1.96054400	-0.46040600

Table S11. Coordination for PC structure (Cartesian coordinates are written in Å) of *R,R*-PC located at B97D/6-31+G(d,p) with total energy and zero-point energy (ZPE) reported in Hartree per particle.

B97D	*R,R*-PC with furan ring			B97D	*R,R*-PC with thiophene ring		
total energy	-2243.237095			-2566.2374084			
ZPE	0.4809117			0.4774194			
Atoms	x	y	z	Atoms	x	y	z
C	-2.96013600	-3.63505400	-1.38703300	C	-3.93166400	-3.42543000	-1.42027300
C	-1.48341600	-3.54647900	-1.86305400	C	-2.52465600	-3.65007400	-2.04302000
C	-0.70850000	-2.85743800	-0.70964600	C	-1.50946300	-3.15052000	-0.97790500
N	-1.76444900	-2.44559900	0.25050300	N	-2.34842000	-2.61464000	0.11994700
H	-3.67380400	-3.54577500	-2.21621200	H	-4.68185500	-3.14223700	-2.16991200

H	-1.40608000	-2.93308700	-2.76948900	H	-2.40773200	-3.06431400	-2.96323800
H	-0.18088700	-1.96344000	-1.06418500	H	-0.88476900	-2.33220800	-1.37449100
C	-1.59329100	-1.87989400	1.43162800	C	-1.93509100	-2.11147200	1.27379800
H	-2.49417700	-1.73366100	2.02582900	H	-2.73461100	-1.77549200	1.93429900
C	-0.40502700	-1.38728200	1.99589700	C	-0.62366400	-1.83951800	1.71741600
C	-0.22428300	-0.71801500	3.21141700	C	-0.39013000	-0.97450100	2.81033700
O	0.74200000	-1.26443500	1.23203700	C	0.87811300	-0.38034200	2.77758300
C	1.05787800	-0.13973700	3.16458500	H	-1.17383500	-0.71917900	3.52154000
H	-0.96686800	-0.63767900	3.99934100	C	1.64703500	-0.77483500	1.67419000
C	1.60094200	-0.46892800	1.92349900	H	1.21698300	0.38602700	3.47218900
H	1.53553800	0.48307000	3.91353900	C	2.82861200	-0.04647600	1.12959500
C	2.79318200	0.05638000	1.21760500	H	3.22153900	0.57046100	1.95027100
H	3.36565600	0.61133000	1.97355300	C	3.97276900	-0.88760900	0.58607500
C	3.70609500	-0.98077400	0.58546500	C	5.22727800	-0.81334900	1.22430900
C	5.07833800	-0.96241100	0.90558900	C	3.84811200	-1.70415100	-0.55742900
C	3.24269700	-1.91797800	-0.36154300	C	6.32913000	-1.53887700	0.74246400
C	5.97336200	-1.85620100	0.29544900	H	5.34129800	-0.17267400	2.10081300
H	5.44717400	-0.23151400	1.62726100	C	4.94690400	-2.43258100	-1.04207600
C	4.13630600	-2.81130300	-0.97545200	H	2.90249100	-1.75299400	-1.09476500
H	2.18921000	-1.94138600	-0.62859600	C	6.19216100	-2.35378600	-0.39457000
C	5.50436700	-2.78343900	-0.65138700	H	7.29145700	-1.46239600	1.25073700
H	7.03280000	-1.82264900	0.55370800	H	4.82984900	-3.05349200	-1.93158100
H	3.76233800	-3.52702800	-1.70934000	H	7.04580900	-2.91690900	-0.77430500
H	6.19645300	-3.47706500	-1.13105600	C	-3.70142700	-2.30769100	-0.39523800
C	-3.09167400	-2.47120900	-0.39528500	H	-4.41733000	-2.29510100	0.43520300
H	-3.86644100	-2.60664700	0.36916300	C	-3.64799800	-0.90288800	-1.07097300
C	-3.29958700	-1.10600400	-1.12161800	H	-2.96243800	-0.92581400	-1.92781500
H	-2.57991000	-1.00868100	-1.94316700	H	-4.65632700	-0.65807600	-1.42796500
H	-4.31912400	-1.08751500	-1.52627000	H	-0.86915600	-3.94708400	-0.57900600
H	-0.00823900	-3.51847700	-0.18452200	H	-2.35611700	-4.70518100	-2.28905600
H	-1.07033600	-4.53750000	-2.08639200	H	-4.28004500	-4.32885200	-0.90189600
H	-3.14861200	-4.58228300	-0.86376000	N	-3.12799200	0.12868800	-0.16929400
N	-3.05126400	0.03718000	-0.24036300	H	-2.09590500	0.42922300	-0.23607100
H	-2.07468200	0.48532600	-0.22069800	O	-5.38156600	0.34375000	0.99719200
O	-5.35428300	-0.17547200	0.82994700	S	-4.09923800	1.04226200	0.76065000
S	-4.22236500	0.75503500	0.62554400	O	-3.31475100	1.63337900	1.86110900
O	-3.61831500	1.51145200	1.73915000	C	-4.56964100	2.54273000	-0.34664800
C	-4.92579900	2.10827700	-0.54504200	F	-3.46027700	3.22712500	-0.69454600
F	-3.95379000	2.98191200	-0.88047200	F	-5.40883500	3.36904300	0.31541800
F	-5.93068400	2.77780400	0.06134000	F	-5.18320500	2.10477000	-1.47179400
F	-5.40256000	1.53135200	-1.67365800	C	5.71328300	3.55605000	-0.92157100

C	5.83391800	3.48759400	-0.95139200	C	5.45412800	2.40101700	-1.68116800
C	5.57024000	2.26080900	-1.58679300	C	4.33759300	1.59958900	-1.39321200
C	4.42663900	1.51947200	-1.24831700	C	3.45748900	1.94161600	-0.34599700
C	3.52498000	1.99495400	-0.27323900	C	3.72824700	3.09902700	0.41175600
C	3.80060800	3.22296900	0.36119800	C	4.84469100	3.90393500	0.12786400
C	4.94415500	3.96791700	0.02558500	H	6.58119600	4.17798000	-1.14574400
H	6.72221900	4.06316400	-1.21593600	H	6.12350400	2.12000500	-2.49586400
H	6.25667300	1.87781800	-2.34363200	H	4.16081500	0.69934900	-1.97986300
H	4.24245900	0.56316000	-1.73660400	H	3.05435300	3.36998500	1.22751300
H	3.10925000	3.59670800	1.11948800	H	5.03239200	4.79981800	0.72195200
H	5.13645300	4.92008600	0.52270700	C	2.26909200	1.07244100	0.04106100
C	2.29799800	1.19877300	0.14933600	H	1.57413700	1.67203900	0.64170700
H	1.63691900	1.85010100	0.73534800	C	1.52247300	0.51985800	-1.12372200
C	1.53315800	0.65928200	-1.00885800	H	2.01374000	0.16753800	-2.02320400
H	2.02737600	0.26844300	-1.89050400	N	0.18047300	0.43738400	-1.15951500
N	0.19806100	0.60274600	-1.05329300	O	-0.53899000	0.86631600	-0.15176300
O	-0.53941900	1.04546600	-0.05960900	O	-0.43223800	-0.08306700	-2.17169800
O	-0.40567900	0.08911800	-2.08061000	S	0.83880700	-1.99506700	0.74461800

Table S12. Coordination for PC structure (Cartesian coordinates are written in Å) of *S,S*-PC located at B97D/6-31+G(d,p) with total energy and zero-point energy (ZPE) reported in Hartree per particle.

B97D	*S,S*-PC with furan ring			B97D	*S,S*-PC with thiophene ring		
total energy	-2243.2145017			-2566.2290946			
ZPE	0.4810881			0.4789274			
Atoms	x	y	z	Atoms	x	y	z
C	2.60957800	-2.00021200	2.55348200	C	-3.68795900	3.22749900	1.07457500
C	1.44613000	-1.08764400	3.00498400	C	-2.56031100	2.99598700	2.10812900
C	0.66615700	-0.82082400	1.70479300	C	-1.56913400	2.05644700	1.38667700
N	1.68536100	-0.98465400	0.63193500	N	-2.37740900	1.42201900	0.31167800
H	3.45804700	-1.99486800	3.25025500	H	-4.63933300	3.51701800	1.53939600
H	1.83119000	-0.15003500	3.43044400	H	-2.95506500	2.50944200	3.01042500
H	0.22813300	0.18231000	1.64740200	H	-1.15545100	1.28568400	2.05019500
C	1.48514100	-0.85311300	-0.66972300	C	-1.93695500	0.60417300	-0.63172000
H	2.32773500	-1.10612600	-1.31021400	H	-2.68120600	0.33247400	-1.38125000
C	0.32066700	-0.44625600	-1.33979900	C	-0.64818000	0.06578900	-0.82535200
C	0.08079200	-0.37782500	-2.71962500	C	-0.30140900	-0.66423000	-1.98415900
O	-0.82383900	-0.06898500	-0.65928900	C	1.04350300	-1.05567300	-2.00577400

C	-1.25703900	0.02367300	-2.87537900	H	-1.01947300	-0.86473400	-2.77784600
H	0.80483100	-0.61274500	-3.49403700	C	1.76352000	-0.64851400	-0.87365600
C	-1.78136600	0.18832800	-1.59272000	H	1.51354100	-1.60729800	-2.81775000
H	-1.80633800	0.16898900	-3.79965200	C	3.23289800	-0.80831900	-0.66491900
C	-3.15622900	0.47931900	-1.13486500	H	3.58812400	-1.41288600	-1.51211700
H	-3.71479100	0.77529200	-2.03359900	C	3.64145700	-1.53158300	0.61316700
C	-3.27755700	1.58854400	-0.10348400	C	4.35917600	-2.73964300	0.50473300
C	-4.11440500	2.68781600	-0.38042500	C	3.38289700	-1.01774000	1.90058500
C	-2.63587000	1.52431000	1.15102700	C	4.81001600	-3.42034000	1.64775200
C	-4.30926500	3.70377200	0.56938700	H	4.57658700	-3.14175200	-0.48663400
H	-4.62834900	2.73621300	-1.34218700	C	3.83412900	-1.69298100	3.04656300
C	-2.83111300	2.53756900	2.10441600	H	2.85605400	-0.07216200	2.01701100
H	-2.00421700	0.67240700	1.38811300	C	4.54976900	-2.89724700	2.92609800
C	-3.66791600	3.63087300	1.81850900	H	5.36792900	-4.35155400	1.53806100
H	-4.96572000	4.54376900	0.33724500	H	3.63089400	-1.27262200	4.03277100
H	-2.33272100	2.46864400	3.07287100	H	4.90077000	-3.41986300	3.81707000
H	-3.82011000	4.41552100	2.56112600	C	-3.78889900	1.87411400	0.34904600
C	2.99319400	-1.42760800	1.17743800	H	-4.16343500	1.95380900	-0.67655000
H	3.43358000	-2.16776500	0.49909900	C	-4.66364900	0.87799200	1.14855700
C	3.95962000	-0.22749000	1.31935500	H	-4.33886900	0.85196700	2.19509900
H	3.54808500	0.51891600	2.00882300	H	-5.70176300	1.23647400	1.12413400
H	4.90320400	-0.59762900	1.73860900	H	-0.74023800	2.60353900	0.91334400
H	-0.12503200	-1.57454000	1.54570300	H	-2.07192200	3.92957300	2.41007400
H	0.80654300	-1.56806300	3.75508500	H	-3.39920700	4.00307000	0.35264700
H	2.26129800	-3.03467900	2.43165700	N	-4.54367100	-0.51695800	0.66946300
N	4.19116600	0.45686800	0.03214500	H	-4.44811300	-1.23674900	1.38419000
H	3.82193400	1.39694400	-0.09120300	O	-5.22557200	-0.07126600	-1.73633600
O	5.78595300	-1.31723700	-0.81794800	S	-5.34410400	-1.08206500	-0.67105300
S	5.48591700	0.11853600	-0.93922000	O	-4.96399100	-2.49088300	-0.85396300
O	5.28060600	0.80112900	-2.22628000	C	-7.21749900	-1.11611400	-0.19707200
C	6.98032300	1.02002800	-0.11944400	F	-7.36743600	-1.77277500	0.97152500
F	6.72766400	2.34309000	-0.05184300	F	-7.91450900	-1.74425500	-1.15867200
F	8.09342300	0.81247400	-0.84496800	F	-7.67894100	0.14484300	-0.05811100
F	7.16520000	0.54264400	1.13091700	C	8.25995500	-0.23999700	-0.98953800
C	-8.11852100	0.01823000	-0.22086000	C	7.62577900	-0.05786200	0.25307000
C	-7.23716500	0.28374800	0.84276500	C	6.25336700	0.23323200	0.31231400
C	-5.87188100	-0.02286000	0.72485600	C	5.49088300	0.35274800	-0.86823600
C	-5.36463500	-0.60721400	-0.45459700	C	6.13487100	0.16329200	-2.10753600
C	-6.25536400	-0.86383200	-1.51647200	C	7.50880100	-0.12767700	-2.17256200
C	-7.62257900	-0.55769000	-1.40378500	H	9.32664700	-0.46516400	-1.03453600
H	-9.17921500	0.25674000	-0.12823800	H	8.19861500	-0.14572800	1.17783800

H	-7.61105700	0.73426500	1.76373800	H	5.77242000	0.35924000	1.28133200
H	-5.19718000	0.20322800	1.54963700	H	5.55253500	0.24968600	-3.02758700
H	-5.87142200	-1.31169600	-2.43568600	H	7.98947600	-0.26265100	-3.14302600
H	-8.29675700	-0.77123700	-2.23494800	C	3.99146800	0.62935200	-0.84660400
C	-3.88565300	-0.91451000	-0.63707200	H	3.68466200	0.96020900	-1.84673400
H	-3.76408900	-1.58861900	-1.49487000	C	3.58656800	1.68128900	0.12338800
C	-3.25651700	-1.54045600	0.55087400	H	3.99146400	1.74247100	1.12663400
H	-3.53063100	-1.27782600	1.56557100	N	2.78509500	2.71749300	-0.22709100
N	-2.27880500	-2.46159500	0.44009600	O	2.27676200	2.80850400	-1.40956500
O	-1.84968900	-2.86245800	-0.70869200	O	2.51436100	3.63223300	0.65025400
O	-1.74345700	-2.95298200	1.52330700	S	0.75543900	0.22066800	0.23946000

Table S13. Coordination for PC structure (Cartesian coordinates are written in Å) of *S,R*-PC located at B97D/6-31+G(d,p) with total energy and zero-point energy (ZPE) reported in Hartree per particle.

B97D	pro-*S,R*-PC with furan ring			B97D	pro-*S,R*-PC with thiophene ring		
total energy	-2243.2145017			-2566.2261921			
ZPE	0.4810881			0.4783901			
Atoms	x	y	z	Atoms	x	y	z
C	2.60995500	0.07532400	3.19240400	C	-3.29064300	-1.30227800	3.25789400
C	1.56869900	1.19995700	2.98753700	C	-2.27235300	-2.41032900	2.90637000
C	0.71767000	0.71057400	1.80074200	C	-1.25205100	-1.70128200	1.99273600
N	1.61483900	-0.23630900	1.07626400	N	-2.00539800	-0.55198800	1.42403000
H	3.51022400	0.41338200	3.72173700	H	-4.26524300	-1.70017600	3.56811900
H	2.06763800	2.14855800	2.74398900	H	-2.76327100	-3.22910800	2.36315200
H	0.40669300	1.51053500	1.11790800	H	-0.88117700	-2.34354900	1.18331600
C	1.31364900	-0.92485300	-0.00828700	C	-1.53707100	0.35676600	0.58024600
H	2.07653900	-1.60812500	-0.37586800	H	-2.24373900	1.14512300	0.32276800
C	0.11290600	-0.89758800	-0.74244600	C	-0.26695000	0.46625600	-0.02140500
C	-0.25037000	-1.62249700	-1.88247600	C	0.06485300	1.53312900	-0.88753600
O	-0.94630800	-0.09785300	-0.35663400	C	1.37564400	1.46533500	-1.37258100
C	-1.57437900	-1.24663500	-2.19220600	H	-0.64608900	2.32181700	-1.12909000
H	0.38475100	-2.33090800	-2.40572400	C	2.09511200	0.35751000	-0.90234400
C	-1.96419600	-0.31805500	-1.23051900	H	1.82759100	2.19870000	-2.03674500
H	-2.19572700	-1.60846900	-3.00457700	C	3.54357300	0.09997000	-1.13808900
C	-3.27391100	0.30620100	-0.93019100	H	3.83147900	0.77773600	-1.95472700
H	-3.89885900	0.10699900	-1.81046700	C	3.89956600	-1.31721700	-1.56832800
C	-3.17245800	1.81608700	-0.74505100	C	4.41970800	-1.51652200	-2.86371700

C	-3.63237000	2.67658200	-1.76109300	C	3.74630000	-2.43530400	-0.72366700
C	-2.61386500	2.36996500	0.42633700	C	4.77649200	-2.80019400	-3.31008100
C	-3.53197600	4.07171400	-1.61658200	H	4.54727100	-0.65721000	-3.52568200
H	-4.07219100	2.25157900	-2.66576400	C	4.10290800	-3.71948100	-1.16578300
C	-2.50866500	3.76319200	0.56765500	H	3.38359200	-2.30351200	0.29480000
H	-2.28434300	1.70077500	1.22259800	C	4.61703800	-3.90870200	-2.46073500
C	-2.96517800	4.61903500	-0.45228000	H	5.17831600	-2.93134300	-4.31603300
H	-3.89802600	4.72642700	-2.40908900	H	3.98820400	-4.56991700	-0.49207200
H	-2.07745800	4.18139600	1.47904800	H	4.89489400	-4.90723800	-2.80136200
H	-2.88794400	5.70126500	-0.33668700	C	-3.39122900	-0.48591300	1.95734100
C	2.92771700	-0.37818800	1.75664200	H	-3.66191400	0.56362500	2.11907600
H	3.25915900	-1.42026800	1.68437200	C	-4.39267400	-1.11972400	0.96359800
C	3.98216400	0.54226300	1.09652200	H	-4.12933900	-2.16432900	0.76092700
H	3.67110600	1.59113800	1.16251700	H	-5.38796200	-1.10300700	1.42550400
H	4.92390100	0.42903500	1.64801400	H	-0.39659800	-1.30492600	2.55895700
H	-0.18330700	0.16545500	2.12343900	H	-1.78554700	-2.83219200	3.79322000
H	0.94747500	1.35842100	3.87692600	H	-2.90261900	-0.66000700	4.06014600
H	2.16880700	-0.76320200	3.74774500	N	-4.39471100	-0.42141800	-0.33908400
N	4.16467900	0.23964500	-0.33785700	H	-4.13120100	-0.95296000	-1.16649800
H	3.92042200	0.96075300	-1.01374900	O	-5.61340200	1.61046000	0.56216200
O	5.49916900	-1.86796300	0.10838400	S	-5.43684700	0.82518200	-0.67028900
S	5.34404700	-0.78982500	-0.88121800	O	-5.04146700	1.41400800	-1.95882300
O	5.11185900	-1.02848600	-2.31417400	C	-7.14712500	-0.00667000	-0.99801100
C	6.97979000	0.22875200	-0.79822500	F	-7.01414300	-0.93763000	-1.96499400
F	6.83705800	1.36212400	-1.51603300	F	-8.03563500	0.92306200	-1.38859500
F	7.99447800	-0.49630200	-1.29986000	F	-7.58757800	-0.60241700	0.13068000
F	7.24958300	0.55127400	0.48483800	C	3.98547100	4.93646900	0.30256800
C	-7.95159100	-1.71810600	-0.96345200	C	3.10956500	4.10979700	1.02854000
C	-6.79934100	-2.38749300	-1.41824800	C	3.26230200	2.71385200	0.99405600
C	-5.52863700	-1.97511900	-0.98792900	C	4.29299800	2.11914900	0.23792600
C	-5.38510300	-0.89244700	-0.09292600	C	5.16319100	2.95725500	-0.48843900
C	-6.54360000	-0.22572700	0.35146200	C	5.01608700	4.35455000	-0.45725800
C	-7.81929100	-0.63541300	-0.07724300	H	3.86901100	6.02089800	0.33193500
H	-8.93978300	-2.03761300	-1.29769900	H	2.30640900	4.55083300	1.62148700
H	-6.89180700	-3.22949700	-2.10642700	H	2.57442800	2.08611500	1.55994800
H	-4.64015300	-2.49818400	-1.34667000	H	5.96340000	2.50637000	-1.07959200
H	-6.44183800	0.61769400	1.03711300	H	5.70583400	4.98568400	-1.02021600
H	-8.70558200	-0.10805600	0.27970000	C	4.45585500	0.60714200	0.13223900
C	-4.01163900	-0.42821300	0.36537900	H	5.47742900	0.38071200	-0.19976300
H	-4.13239200	0.37187300	1.10460400	C	4.21469400	-0.11735500	1.40241900
C	-3.25201900	-1.53579600	1.01257800	H	3.35047100	0.06870300	2.02927700

H	-3.26321400	-2.54708500	0.61807800	N	5.08892400	-1.02116000	1.90992800
N	-2.43107500	-1.34033900	2.05996200	O	6.19519800	-1.30384800	1.31560500
O	-2.31643200	-0.17415900	2.62318700	O	4.79775200	-1.61317900	3.02617100
O	-1.73600800	-2.33186500	2.53257500	S	1.12176300	-0.61948300	0.15919800

Table S14. Coordination for trienamine reactants (Cartesian coordinates are written in Å) located at M06-2X/6-31+G(d,p) with total energy and zero-point energy (ZPE) reported in Hartree per particle.

M06-2X	*Z,Z,Z*-trienamine reactant complex			M06-2X	*Z,Z,E*-trienamine reactant complex		
total energy	-749.5824124			-749.5788189			
ZPE	0.296446			0.2966828			
Atoms	x	y	z	Atoms	x	y	z
C	-1.05197700	3.16521200	0.02075100	C	1.18935600	1.93097200	-0.10055000
C	0.29579300	3.28083200	0.02106100	C	-0.05686000	2.45677500	-0.07979100
H	-1.78491700	3.96117700	0.03173700	H	2.11880100	2.47931500	-0.14127300
H	0.88742200	4.18518500	0.03106000	H	-0.33437400	3.50162700	-0.09256600
C	2.16139900	1.57109600	-0.00136800	C	-2.36194900	1.42416900	-0.01606600
H	2.86545100	2.39815000	0.01417400	H	-2.76840600	2.43153900	-0.01649500
C	0.85996600	1.94432900	0.00300700	C	-1.00935400	1.36464700	-0.04522900
C	2.73947500	0.23352800	-0.01814100	C	-3.33216900	0.33772400	0.01273500
C	4.14165900	0.11251600	0.02141800	C	-4.70075700	0.66946400	0.02414300
C	1.98482700	-0.95433400	-0.07309000	C	-2.99154800	-1.02892100	0.02925900
C	4.76421700	-1.12965700	0.01008100	C	-5.68547900	-0.30995200	0.05051900
H	4.74531700	1.01582800	0.06201500	H	-4.98660600	1.71847600	0.01179400
C	2.61188700	-2.19629100	-0.08411500	C	-3.98185800	-2.00654300	0.05564200
H	0.90473500	-0.89745300	-0.11067400	H	-1.94915100	-1.32064700	0.02245000
C	4.00197200	-2.29701200	-0.04221800	C	-5.33218800	-1.65959900	0.06638100
H	5.84825900	-1.18768300	0.04214900	H	-6.73215100	-0.01999600	0.05857700
H	2.00603500	-3.09730700	-0.12662100	H	-3.69318800	-3.05378200	0.06818200
H	4.48443300	-3.26926700	-0.05170500	H	-6.09805800	-2.42861300	0.08771500
O	-0.18679400	1.05170200	-0.00808900	O	-0.29623200	0.19536600	-0.05052600
C	-2.60014100	1.17490200	-0.01347500	C	1.06769600	0.49285200	-0.08158900
H	-3.45352100	1.84700300	-0.02821600	C	1.92389500	-0.55816900	-0.11820800
C	-1.37923800	1.76587400	0.00362500	H	1.47620100	-1.54791800	-0.14984700
C	-4.28747700	-0.61767500	-0.06722600	C	4.06914200	-1.76341700	-0.04908800
C	-1.94349900	-1.23649800	0.14238100	C	4.07928000	0.64989700	0.14729800
C	-4.13126900	-2.11454100	-0.33547900	C	5.49688400	-1.26285400	-0.25158400
H	-4.84981200	-0.10096600	-0.85224900	H	3.75066800	-2.48023600	-0.81239000
H	-4.79421500	-0.44053600	0.89446900	H	3.95465100	-2.23593500	0.93993200
C	-2.83549700	-2.45292700	0.41125000	C	5.47507200	0.09401400	0.46442200

H	-1.34485400	-1.36356500	-0.76964300	H	4.09285300	1.32539000	-0.72020300
H	-1.25930400	-1.02199300	0.96846500	H	3.64806700	1.19843200	0.99649100
H	-4.99183300	-2.69396600	0.00556900	H	6.24459300	-1.94861800	0.15223100
H	-4.00214600	-2.28572600	-1.40951400	H	5.69138900	-1.12582700	-1.32037600
H	-3.03650600	-2.53590000	1.48479600	H	5.57533600	-0.05697000	1.54428400
H	-2.37700800	-3.38642700	0.07814200	H	6.27436300	0.76459200	0.14225800
N	-2.90653700	-0.14804300	-0.02714700	N	3.28712500	-0.53573000	-0.14519000
M06-2X	*E,Z,Z*-trienamine reactant complex			M06-2X	*E,Z,E*-trienamine reactant complex		
total energy	-749.5790809			-749.5754584			
ZPE	0.2963462			0.296457			
Atoms	x	y	z	Atoms	x	y	z
C	-0.40941800	2.28245900	-0.32806200	C	0.76848500	0.98763300	0.11318500
C	0.84122500	1.76585700	-0.27229300	C	-0.58335800	0.92011400	0.11078400
H	-0.68775400	3.31229700	-0.51073900	H	1.36243100	1.87756000	0.26082000
H	1.77481300	2.28602900	-0.42334800	H	-1.27798800	1.72867700	0.28237500
C	1.62158000	-0.66759800	0.05840000	C	-2.15985700	-1.09585500	-0.13815900
H	1.22286900	-1.67685900	0.11077000	H	-2.13945800	-2.18086400	-0.18737200
C	0.72120000	0.33678500	-0.03800900	C	-0.96396200	-0.46530200	-0.10447200
C	3.07688300	-0.51510600	0.05833700	C	-3.46829900	-0.44297200	-0.06836900
C	3.87735900	-1.54417600	-0.46751700	C	-4.53970800	-1.10753800	0.55374100
C	3.72905000	0.60570800	0.60081200	C	-3.72296600	0.81838400	-0.63375600
C	5.26420900	-1.44360600	-0.48426400	C	-5.79863200	-0.52327200	0.64044200
H	3.39448500	-2.42724500	-0.87813300	H	-4.36919100	-2.09107500	0.98394900
C	5.11696500	0.70967200	0.57698800	C	-4.98133400	1.40653200	-0.54047800
H	3.14343800	1.38137900	1.08462400	H	-2.93713800	1.32134000	-1.18913500
C	5.89425900	-0.31006700	0.02974200	C	-6.02605200	0.74364400	0.10229000
H	5.85623200	-2.25231700	-0.90283000	H	-6.60576500	-1.05696000	1.13367100
H	5.59473600	1.58486900	1.00782100	H	-5.15110700	2.38052400	-0.99042000
H	6.97650700	-0.22935700	0.01724500	H	-7.00792500	1.20114300	0.17068200
O	-0.62563700	0.04475600	0.04254900	O	0.19490600	-1.19100900	-0.23761200
C	-1.34731900	1.21447200	-0.13073600	C	1.28832300	-0.33934600	-0.10681700
C	-2.70378200	1.26505000	-0.11678700	C	2.52014700	-0.89464900	-0.23063100
H	-3.14588700	2.24779700	-0.25335900	H	2.55045600	-1.96126900	-0.43603600
C	-5.03245200	0.46310000	-0.02332000	C	4.97833700	-1.04433000	-0.18251500
C	-3.23307200	-1.16204500	0.18979700	C	3.92719900	1.07451900	0.33354400
C	-5.58152700	-0.94411000	-0.26337100	C	6.03751300	0.05339500	-0.24326200
H	-5.28251800	1.15981500	-0.83115000	H	4.99824100	-1.71164600	-1.04969000
H	-5.41419600	0.88060500	0.92040800	H	5.09550100	-1.65444400	0.72788200
C	-4.57875300	-1.82878500	0.48613600	C	5.42957900	1.14667000	0.64488100
H	-2.78791700	-1.53905700	-0.74145000	H	3.62839300	1.80426400	-0.43338600
H	-2.50010300	-1.30001000	0.98810400	H	3.31119700	1.25208300	1.22637200

H	-6.60872700	-1.05846800	0.08967300	H	7.01570500	-0.28554700	0.10421100
H	-5.55661400	-1.17372300	-1.33401900	H	6.13860300	0.41190300	-1.27293800
H	-4.78252900	-1.79429100	1.56193400	H	5.59919200	0.90185900	1.69849100
H	-4.60351600	-2.87326900	0.16836400	H	5.84796700	2.13769000	0.45760100
N	-3.58952300	0.24972800	0.04722500	N	3.73559100	-0.28184800	-0.15551900

Table S15. Coordination for trienamine reactants (Cartesian coordinates are written in Å) located at MPW1K/6-31+G(d,p) with total energy and zero-point energy (ZPE) reported in Hartree per particle.

MPW1K	*Z,Z,Z*-trienamine reactant complex			MPW1K	*Z,Z,E*-trienamine reactant complex		
total energy	-749.8189739			-749.8165582			
ZPE	0.2863329			0.2863388			
Atoms	x	y	z	Atoms	x	y	z
C	-1.04188600	3.15583800	0.00606100	C	1.18992900	1.95305500	-0.06403500
C	0.32791500	3.26163800	0.00484000	C	-0.08313400	2.47316300	-0.06674400
H	-1.76908800	3.96564900	0.00851400	H	2.11682100	2.51912100	-0.09165100
H	0.92316600	4.17179300	0.00438300	H	-0.36532900	3.52351400	-0.08995800
C	2.20228700	1.54370000	-0.00170000	C	-2.39601800	1.41587500	-0.02762800
H	2.89913800	2.38679400	0.00739900	H	-2.80758800	2.42912100	-0.03956900
C	0.88186300	1.93186300	0.00094400	C	-1.01946500	1.38067400	-0.03908500
C	2.81015600	0.22713000	-0.01214400	C	-3.36573900	0.33852200	-0.00189900
C	4.23027900	0.13706800	0.02060900	C	-4.74925800	0.67368100	0.00660800
C	2.08620300	-0.99678500	-0.05612200	C	-3.03405300	-1.04573900	0.01527700
C	4.88850700	-1.09577600	0.01251200	C	-5.74257700	-0.30874200	0.03082000
H	4.81563700	1.06099200	0.05398600	H	-5.03509300	1.72998100	-0.00605200
C	2.75022500	-2.22812500	-0.06508600	C	-4.03397400	-2.02433200	0.03903300
H	0.99789400	-0.96888600	-0.08816600	H	-1.98620000	-1.34427700	0.00997000
C	4.15366600	-2.29318000	-0.02993100	C	-5.39381800	-1.67043000	0.04707900
H	5.98122800	-1.12415400	0.03928300	H	-6.79505200	-0.01220800	0.03690700
H	2.16467500	-3.15143200	-0.10089500	H	-3.74722400	-3.07975500	0.05156500
H	4.66529200	-3.25848900	-0.03687700	H	-6.16802500	-2.44113800	0.06579900
O	-0.18355200	1.02769700	0.00109000	O	-0.28813800	0.19940800	-0.02406600
C	-2.62625700	1.18412500	0.00472400	C	1.08358600	0.52348700	-0.03681900
H	-3.46451600	1.88410000	-0.00396800	C	1.95167400	-0.54743300	-0.03357100
C	-1.37676100	1.76497100	0.00501200	H	1.49894900	-1.54119100	-0.04542700
C	-4.39622000	-0.54759400	-0.01357600	C	4.10581700	-1.77956100	-0.00130100
C	-2.06512800	-1.28092700	0.06745200	C	4.15430600	0.65606600	0.09885500
C	-4.32259100	-2.05219600	-0.31703600	C	5.53152700	-1.29585300	-0.30602200
H	-4.95686900	0.01698500	-0.77776000	H	3.72392300	-2.49582400	-0.74724900
H	-4.87681100	-0.36031400	0.96800200	H	4.05194500	-2.26396600	0.99530400

C	-2.99706800	-2.47232700	0.34767700	C	5.56822000	0.09821300	0.35206600
H	-1.53529500	-1.39582000	-0.89615100	H	4.10808600	1.25893200	-0.82968800
H	-1.30860300	-1.13252000	0.85148100	H	3.79887300	1.29257000	0.92926700
H	-5.19477300	-2.59998600	0.06813700	H	6.29932700	-1.97824700	0.08626400
H	-4.27144600	-2.21508800	-1.40614800	H	5.67504300	-1.21017500	-1.39560800
H	-3.13917800	-2.59346100	1.43431300	H	5.74463900	0.00010000	1.43566000
H	-2.59510600	-3.41681500	-0.04658700	H	6.35365400	0.74966500	-0.05735800
N	-2.98543900	-0.13249300	0.00956000	N	3.31946100	-0.53933900	-0.02735000
MPW1K	*E,Z,Z*-trienamine reactant complex			MPW1K	*E,Z,E*-trienamine reactant complex		
total energy	-749.8166568			-749.8129414			
ZPE	0.286041			0.2859401			
Atoms	x	y	z	Atoms	x	y	z
C	-0.49773400	2.38391900	-0.21312900	C	0.83719100	1.07395600	0.18269100
C	0.79245400	1.90441400	-0.18692900	C	-0.53922900	1.04614300	0.17215800
H	-0.81243500	3.41969600	-0.32853400	H	1.45705500	1.95586300	0.31873800
H	1.70195100	2.48556500	-0.30341000	H	-1.20140000	1.89284800	0.32566000
C	1.66108600	-0.54647800	-0.00521000	C	-2.17949400	-0.96087900	-0.05935800
H	1.23991900	-1.55611100	-0.02037100	H	-2.12435200	-2.05320900	-0.08262700
C	0.73658400	0.47162500	-0.04610800	C	-0.96341800	-0.31722700	-0.01407300
C	3.11157900	-0.46040400	0.02291700	C	-3.51425700	-0.38689800	-0.04937100
C	3.86627800	-1.61923200	-0.31196200	C	-4.61197000	-1.22787500	0.28654200
C	3.84667700	0.69834200	0.39551500	C	-3.81885300	0.96030000	-0.38811200
C	5.26416000	-1.61237000	-0.31026100	C	-5.92420300	-0.74697100	0.31762600
H	3.33082400	-2.53253600	-0.58808300	H	-4.41369200	-2.27427400	0.53682000
C	5.24606200	0.70280000	0.39360600	C	-5.13322500	1.43937200	-0.35308100
H	3.31737400	1.59132200	0.73120900	H	-3.02428500	1.62725200	-0.72624000
C	5.96963400	-0.44684100	0.03475900	C	-6.19788700	0.59595500	0.00638700
H	5.80766900	-2.52192800	-0.58034100	H	-6.73959100	-1.42378400	0.58722800
H	5.77813900	1.61063300	0.69147600	H	-5.33061000	2.47978400	-0.62632800
H	7.06203900	-0.43847700	0.03708300	H	-7.22246500	0.97429300	0.02940400
O	-0.61955600	0.11221500	0.01416500	O	0.18966700	-1.09827100	-0.11886300
C	-1.38596700	1.27297200	-0.08718800	C	1.31135600	-0.26453200	0.00058600
C	-2.76512800	1.26499700	-0.07207300	C	2.53874700	-0.89009300	-0.08539800
H	-3.24548200	2.24278200	-0.14565500	H	2.52222400	-1.97199100	-0.23309000
C	-5.08290200	0.39851700	0.02454400	C	5.00753500	-1.14808800	-0.11561200
C	-3.24437200	-1.21197000	0.10583000	C	4.07235900	1.07683300	0.22221100
C	-5.62990300	-1.01293000	-0.23821700	C	6.09902200	-0.10551100	-0.39686500
H	-5.38440600	1.12732800	-0.74674200	H	4.91220300	-1.90282000	-0.91320600
H	-5.42341400	0.78345500	1.00694200	H	5.19998600	-1.68209500	0.83766200
C	-4.57319800	-1.91942900	0.42323600	C	5.60486000	1.12667100	0.38772600
H	-2.81796200	-1.55219000	-0.85611000	H	3.72424100	1.69353700	-0.62986700

H	-2.47679500	-1.36364800	0.87853000	H	3.54359100	1.42768200	1.12704900
H	-6.64062400	-1.15355100	0.17157800	H	7.09636400	-0.44494800	-0.08178700
H	-5.67239000	-1.20471000	-1.32301100	H	6.13803500	0.11565800	-1.47602000
H	-4.73258200	-1.95396300	1.51370800	H	5.87102700	1.02832100	1.45279600
H	-4.59397100	-2.95267300	0.04774900	H	6.03267400	2.07146600	0.02285200
N	-3.62475500	0.20909900	0.01781100	N	3.78720600	-0.33633700	-0.02892500

Table S16. Coordination for trienamine reactants (Cartesian coordinates are written in Å) located at B3LYP/6-31+G(d,p) with total energy and zero-point energy (ZPE) reported in Hartree per particle.

B3LYP	*Z,Z,Z*-trienamine reactant complex			B3LYP	*Z,Z,E*-trienamine reactant complex		
total energy	-749,9234964			-749.9207706			
ZPE			0,2936217	0.2936522			
Atoms	x	y	z	Atoms	x	y	z
C	-1.03181000	3.14745200	0.00649900	C	1.18124100	1.94692400	-0.06631800
C	0.32572300	3.25342000	0.00458100	C	-0.07961800	2.46365500	-0.06562700
H	-1.75512000	3.95251100	0.00852300	H	2.10376800	2.50760400	-0.09280300
H	0.91855000	4.15763200	0.00350400	H	-0.36117100	3.50770800	-0.08551800
C	2.19213800	1.54231400	-0.00249600	C	-2.38363000	1.41328100	-0.02548600
H	2.88682600	2.37823200	0.00362000	H	-2.79313700	2.41993000	-0.03566400
C	0.88224300	1.92142100	0.00129900	C	-1.02007600	1.37057700	-0.03858200
C	2.79951800	0.22228200	-0.01176800	C	-3.35634700	0.33466200	-0.00003100
C	4.21173400	0.13354500	0.01620900	C	-4.73130100	0.67091600	0.00868700
C	2.07637800	-0.99318200	-0.05015400	C	-3.02569800	-1.04169300	0.01645400
C	4.86710100	-1.09505800	0.00830100	C	-5.72225500	-0.30668100	0.03278800
H	4.79481700	1.05096500	0.04529000	H	-5.01506000	1.72069400	-0.00360300
C	2.73691700	-2.22096500	-0.05867400	C	-4.02261700	-2.01639400	0.04025200
H	0.99509100	-0.96537000	-0.07719300	H	-1.98504400	-1.33937100	0.01078200
C	4.13395300	-2.28620500	-0.02894600	C	-5.37576700	-1.66239900	0.04864000
H	5.95329300	-1.12416400	0.03095800	H	-6.76813000	-0.01110600	0.03905000
H	2.15411200	-3.13825900	-0.08982400	H	-3.73852700	-3.06566400	0.05244300
H	4.64167600	-3.24625300	-0.03571200	H	-6.14602100	-2.42788400	0.06731400
O	-0.17853100	1.02598200	0.00265400	O	-0.29105200	0.19825900	-0.02751100
C	-2.61007500	1.18190900	0.00517200	C	1.07819600	0.51468900	-0.04165700
H	-3.44238500	1.87923700	-0.00338100	C	1.94398300	-0.54136900	-0.04443600
C	-1.37120700	1.75590900	0.00599700	H	1.49539600	-1.53006100	-0.05652400
C	-4.38036200	-0.53969000	-0.01536600	C	4.08922200	-1.77302200	-0.00135300
C	-2.05423800	-1.27735600	0.06979400	C	4.14151200	0.65789200	0.10137200
C	-4.31247200	-2.04270800	-0.31621900	C	5.51767900	-1.29744200	-0.29112300
H	-4.93586200	0.02013300	-0.77738500	H	3.71877700	-2.49067900	-0.74190600

H	-4.86052900	-0.35113600	0.95844600	H	4.02318300	-2.24695100	0.99212600
C	-2.98718800	-2.46759200	0.34033900	C	5.55319400	0.09907000	0.35630300
H	-1.51932700	-1.39111500	-0.88321600	H	4.10324800	1.27273700	-0.81099800
H	-1.30826900	-1.13542900	0.85583700	H	3.78553600	1.27808100	0.93510600
H	-5.17960700	-2.58460200	0.07143200	H	6.27427800	-1.97587000	0.11261700
H	-4.26781500	-2.20583900	-1.39926300	H	5.67317000	-1.22049900	-1.37334800
H	-3.12667000	-2.59687200	1.42004700	H	5.72884800	0.00792100	1.43422800
H	-2.58994500	-3.40444800	-0.05997200	H	6.33516400	0.74355900	-0.05442700
N	-2.97152800	-0.13086300	0.00852100	N	3.30969100	-0.53317500	-0.04972700
B3LYP	*E,Z,Z*-trienamine reactant complex			B3LYP	*E,Z,E*-trienamine reactant complex		
total energy	-749.9207185			-749.9167163			
ZPE	0.2933946			0.2933285			
Atoms	x	y	z	Atoms	x	y	z
C	-0.47908800	2.35738800	-0.23136700	C	0.81966500	1.05664400	0.17188300
C	0.79750700	1.87719100	-0.19570600	C	-0.54401500	1.02332400	0.16090700
H	-0.78674900	3.38753800	-0.35776000	H	1.43269200	1.93461300	0.31224000
H	1.70585000	2.44787200	-0.31096800	H	-1.20793200	1.86008100	0.31474000
C	1.65324700	-0.56219800	0.01862800	C	-2.17054600	-0.97662800	-0.08507100
H	1.24170600	-1.56836300	0.02537800	H	-2.12469600	-2.06193600	-0.12566900
C	0.73421500	0.44274200	-0.03810900	C	-0.96361900	-0.34414800	-0.03513400
C	3.10704900	-0.46508600	0.03426300	C	-3.50414700	-0.39032700	-0.05637700
C	3.86309800	-1.60102600	-0.33871700	C	-4.59237500	-1.20597000	0.33307100
C	3.82857300	0.68361600	0.43257500	C	-3.80129400	0.94035900	-0.43056900
C	5.25589200	-1.58186900	-0.34701200	C	-5.89486300	-0.71413400	0.37926800
H	3.33737300	-2.50525900	-0.63548900	H	-4.39859800	-2.23879300	0.61182300
C	5.22296000	0.70195200	0.42039500	C	-5.10542100	1.43195400	-0.38025400
H	3.29674100	1.55641000	0.79411600	H	-3.01363300	1.58398800	-0.80601400
C	5.94992700	-0.42552300	0.02529100	C	-6.16284300	0.61401100	0.03045200
H	5.80239300	-2.47246500	-0.64602000	H	-6.70448100	-1.36951600	0.68944800
H	5.74606900	1.60038000	0.73776400	H	-5.29928500	2.45843100	-0.68089400
H	7.03572500	-0.40759800	0.02010700	H	-7.17736800	0.99987600	0.06457000
O	-0.61556600	0.09733000	0.02080900	O	0.18780700	-1.11027400	-0.14376400
C	-1.37805500	1.25456000	-0.09521000	C	1.30576100	-0.27844200	-0.02038500
C	-2.74474900	1.25738000	-0.08560500	C	2.52849200	-0.88314800	-0.11210000
H	-3.21331500	2.23265500	-0.17472200	H	2.51951700	-1.95696600	-0.27247900
C	-5.06545600	0.41800500	0.00693200	C	4.99082800	-1.13336700	-0.12802500
C	-3.24486500	-1.20586800	0.12169500	C	4.04882600	1.07906500	0.24286600
C	-5.62490100	-0.98971400	-0.23672900	C	6.08698700	-0.08763600	-0.36193300
H	-5.35346900	1.13072600	-0.77519500	H	4.91554400	-1.86455000	-0.94044900
H	-5.41028500	0.82042700	0.97290300	H	5.16381500	-1.68627200	0.81014400
C	-4.57998700	-1.89842000	0.43469500	C	5.57659900	1.12892500	0.43192500

H	-2.81546800	-1.55987300	-0.82601800	H	3.71546600	1.71634100	-0.59068300
H	-2.49159200	-1.35664300	0.89895200	H	3.51207400	1.40387900	1.14453900
H	-6.63174500	-1.11448100	0.17145400	H	7.07108400	-0.43159700	-0.03178300
H	-5.66848500	-1.19370000	-1.31290100	H	6.15142800	0.15265200	-1.42933100
H	-4.74488800	-1.92427500	1.51828800	H	5.82478400	1.01512700	1.49329200
H	-4.60752600	-2.92825400	0.06809800	H	6.00558500	2.07496700	0.09075800
N	-3.61285700	0.21392800	0.01563400	N	3.77190700	-0.32443300	-0.04961300

Table S17. Coordination for trienamine reactants (Cartesian coordinates are written in Å) located at CCSD(T)/6-31+G(d,p) with total energy reported in Hartree per particle.

CCSD(T)	*Z,Z,Z*-trienamine reactant complex			CCSD(T)	*Z,Z,E*-trienamine reactant complex		
total energy	-747.9255952			-747.9212651			
Atoms	x	y	z	Atoms	x	y	z
C	-1.03180900	3.14745100	0.00695900	C	1.18124100	1.94692400	-0.06631800
C	0.32572300	3.25341900	0.00493900	C	-0.07961800	2.46365500	-0.06562700
H	-1.75511900	3.95251000	0.00914000	H	2.10376800	2.50760400	-0.09280300
H	0.91855000	4.15763100	0.00392000	H	-0.36117100	3.50770800	-0.08551800
C	2.19213800	1.54231400	-0.00250200	C	-2.38363000	1.41328100	-0.02548600
H	2.88682600	2.37823100	0.00365600	H	-2.79313700	2.41993000	-0.03566400
C	0.88224300	1.92142100	0.00145000	C	-1.02007600	1.37057700	-0.03858200
C	2.79951700	0.22228300	-0.01198300	C	-3.35634700	0.33466200	-0.00003100
C	4.21173500	0.13354300	0.01586400	C	-4.73130100	0.67091600	0.00868700
C	2.07637400	-0.99317600	-0.05045400	C	-3.02569800	-1.04169300	0.01645400
C	4.86710200	-1.09505900	0.00775300	C	-5.72225500	-0.30668100	0.03278800
H	4.79482100	1.05095900	0.04500500	H	-5.01506000	1.72069400	-0.00360300
C	2.73691200	-2.22095800	-0.05917700	C	-4.02261700	-2.01639400	0.04025200
H	0.99508400	-0.96536100	-0.07739800	H	-1.98504400	-1.33937100	0.01078200
C	4.13395000	-2.28620200	-0.02957500	C	-5.37576700	-1.66239900	0.04864000
H	5.95329500	-1.12416800	0.03031400	H	-6.76813000	-0.01110600	0.03905000
H	2.15410400	-3.13824800	-0.09038700	H	-3.73852700	-3.06566400	0.05244300
H	4.64167300	-3.24624900	-0.03649900	H	-6.14602100	-2.42788400	0.06731400
O	-0.17853100	1.02598200	0.00279100	O	-0.29105200	0.19825900	-0.02751100
C	-2.61007500	1.18190800	0.00553500	C	1.07819600	0.51468900	-0.04165700
H	-3.44238500	1.87923700	-0.00286500	C	1.94398300	-0.54136900	-0.04443600
C	-1.37120700	1.75590800	0.00632100	H	1.49539600	-1.53006100	-0.05652400
C	-4.38036300	-0.53968800	-0.01505200	C	4.08922200	-1.77302200	-0.00135300
C	-2.05423200	-1.27736400	0.06982200	C	4.14151200	0.65789200	0.10137200
C	-4.31249900	-2.04267100	-0.31608700	C	5.51767900	-1.29744200	-0.29112300
H	-4.93592900	0.02022400	-0.77695900	H	3.71877700	-2.49067900	-0.74190600
H	-4.86044700	-0.35124800	0.95882300	H	4.02318300	-2.24695100	0.99212600

C	-2.98715900	-2.46763200	0.34030800	C	5.55319400	0.09907000	0.35630300
H	-1.51940300	-1.39101200	-0.88324700	H	4.10324800	1.27273700	-0.81099800
H	-1.30819600	-1.13552900	0.85581800	H	3.78553600	1.27808100	0.93510600
H	-5.17960100	-2.58461000	0.07157500	H	6.27427800	-1.97587000	0.11261700
H	-4.26793500	-2.20567600	-1.39915400	H	5.67317000	-1.22049900	-1.37334800
H	-3.12654900	-2.59703800	1.42001300	H	5.72884800	0.00792100	1.43422800
H	-2.58995000	-3.40444100	-0.06014600	H	6.33516400	0.74355900	-0.05442700
N	-2.97152700	-0.13086400	0.00876200	N	3.30969100	-0.53317500	-0.04972700
CCSD(T)	*E,Z,Z*-trienamine reactant complex			CCSD(T)	*E,Z,E*-trienamine reactant complex		
total energy	-747.9222268			-747.9154154			
Atoms	x	y	z	Atoms	x	y	z
C	-0.47908800	2.35738800	-0.23136700	C	0.83719100	1.07395600	0.18269100
C	0.79750700	1.87719100	-0.19570600	C	-0.53922900	1.04614300	0.17215800
H	-0.78674900	3.38753800	-0.35776000	H	1.45705500	1.95586300	0.31873800
H	1.70585000	2.44787200	-0.31096800	H	-1.20140000	1.89284800	0.32566000
C	1.65324700	-0.56219800	0.01862800	C	-2.17949400	-0.96087900	-0.05935800
H	1.24170600	-1.56836300	0.02537800	H	-2.12435200	-2.05320900	-0.08262700
C	0.73421500	0.44274200	-0.03810900	C	-0.96341800	-0.31722700	-0.01407300
C	3.10704900	-0.46508600	0.03426300	C	-3.51425700	-0.38689800	-0.04937100
C	3.86309800	-1.60102600	-0.33871700	C	-4.61197000	-1.22787500	0.28654200
C	3.82857300	0.68361600	0.43257500	C	-3.81885300	0.96030000	-0.38811200
C	5.25589200	-1.58186900	-0.34701200	C	-5.92420300	-0.74697100	0.31762600
H	3.33737300	-2.50525900	-0.63548900	H	-4.41369200	-2.27427400	0.53682000
C	5.22296000	0.70195200	0.42039500	C	-5.13322500	1.43937200	-0.35308100
H	3.29674100	1.55641000	0.79411600	H	-3.02428500	1.62725200	-0.72624000
C	5.94992700	-0.42552300	0.02529100	C	-6.19788700	0.59595500	0.00638700
H	5.80239300	-2.47246500	-0.64602000	H	-6.73959100	-1.42378400	0.58722800
H	5.74606900	1.60038000	0.73776400	H	-5.33061000	2.47978400	-0.62632800
H	7.03572500	-0.40759800	0.02010700	H	-7.22246500	0.97429300	0.02940400
O	-0.61556600	0.09733000	0.02080900	O	0.18966700	-1.09827100	-0.11886300
C	-1.37805500	1.25456000	-0.09521000	C	1.31135600	-0.26453200	0.00058600
C	-2.74474900	1.25738000	-0.08560500	C	2.53874700	-0.89009300	-0.08539800
H	-3.21331500	2.23265500	-0.17472200	H	2.52222400	-1.97199100	-0.23309000
C	-5.06545600	0.41800500	0.00693200	C	5.00753500	-1.14808800	-0.11561200
C	-3.24486500	-1.20586800	0.12169500	C	4.07235900	1.07683300	0.22221100
C	-5.62490100	-0.98971400	-0.23672900	C	6.09902200	-0.10551100	-0.39686500
H	-5.35346900	1.13072600	-0.77519500	H	4.91220300	-1.90282000	-0.91320600
H	-5.41028500	0.82042700	0.97290300	H	5.19998600	-1.68209500	0.83766200
C	-4.57998700	-1.89842000	0.43469500	C	5.60486000	1.12667100	0.38772600
H	-2.81546800	-1.55987300	-0.82601800	H	3.72424100	1.69353700	-0.62986700
H	-2.49159200	-1.35664300	0.89895200	H	3.54359100	1.42768200	1.12704900

H	-6.63174500	-1.11448100	0.17145400	H	7.09636400	-0.44494800	-0.08178700
H	-5.66848500	-1.19370000	-1.31290100	H	6.13803500	0.11565800	-1.47602000
H	-4.74488800	-1.92427500	1.51828800	H	5.87102700	1.02832100	1.45279600
H	-4.60752600	-2.92825400	0.06809800	H	6.03267400	2.07146600	0.02285200
N	-3.61285700	0.21392800	0.01563400	N	3.78720600	-0.33633700	-0.02892500