Electronic supplementary information:

Ru(0)-catalysed cross-dimerisation and -trimeisation of alkynyl- with butadienylheteroarenes

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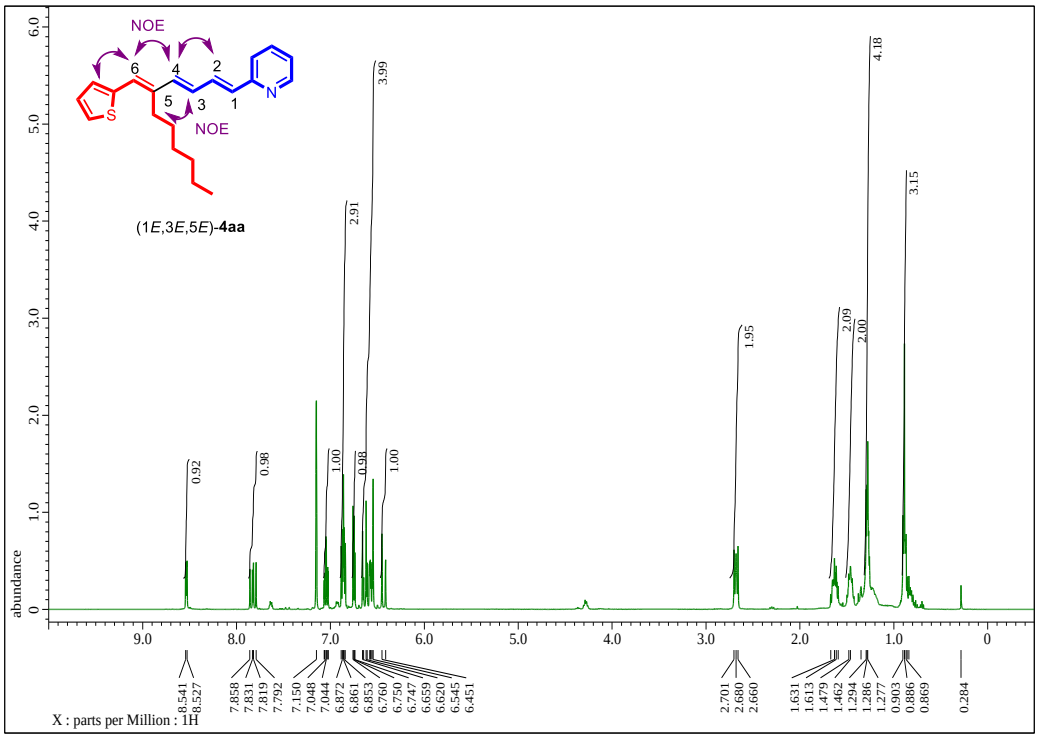


Figure S1. ^{1}H NMR Spectrum of (1*E*,3*E*,5*E*)-4aa in C_6D_6.

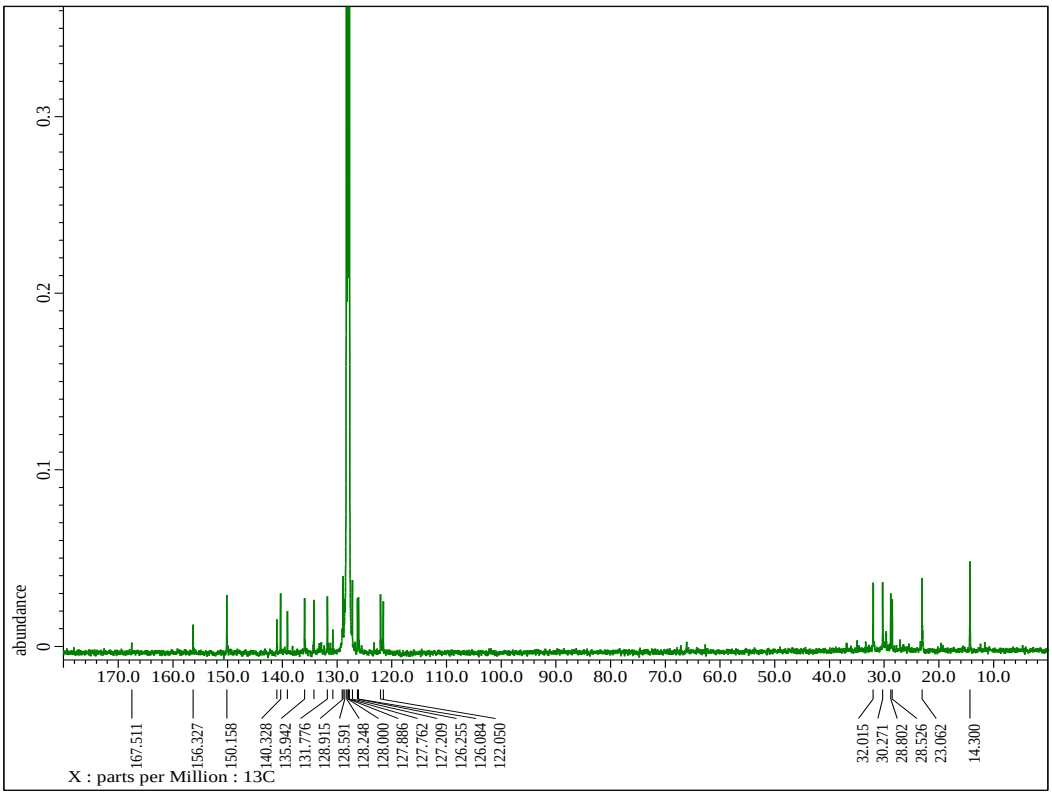


Figure S2. ^{13}C{^{1}H} NMR Spectrum of (1*E*,3*E*,5*E*)-4aa in C_6D_6.

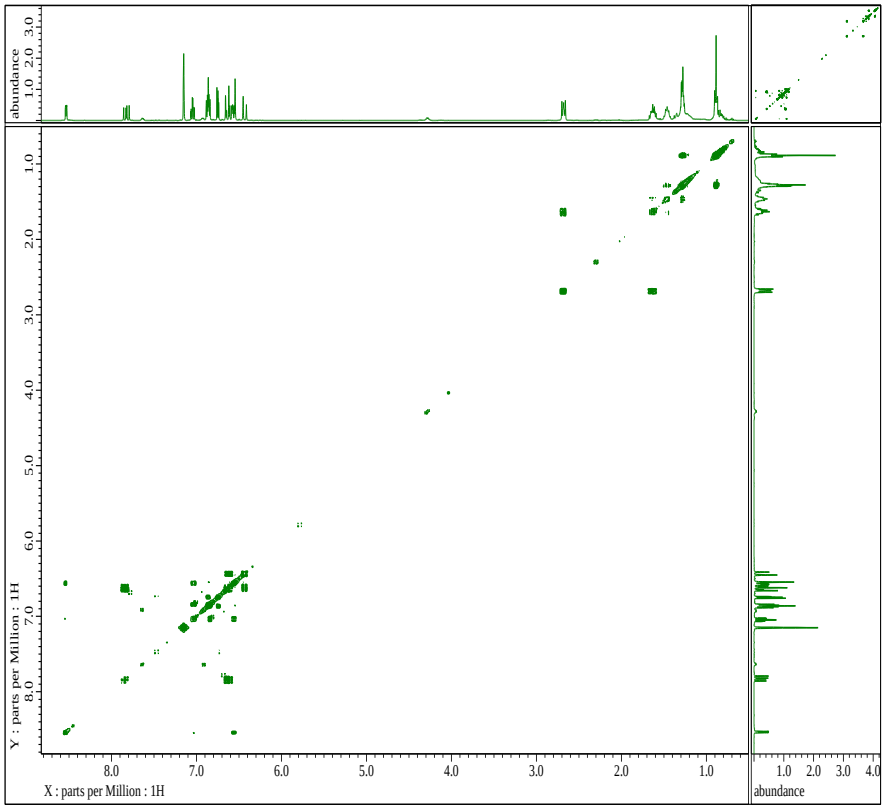


Figure S3. ^{1}H-^{1}H COSY NMR Spectrum of (1*E*,3*E*,5*E*)-4aa in C_6D_6.

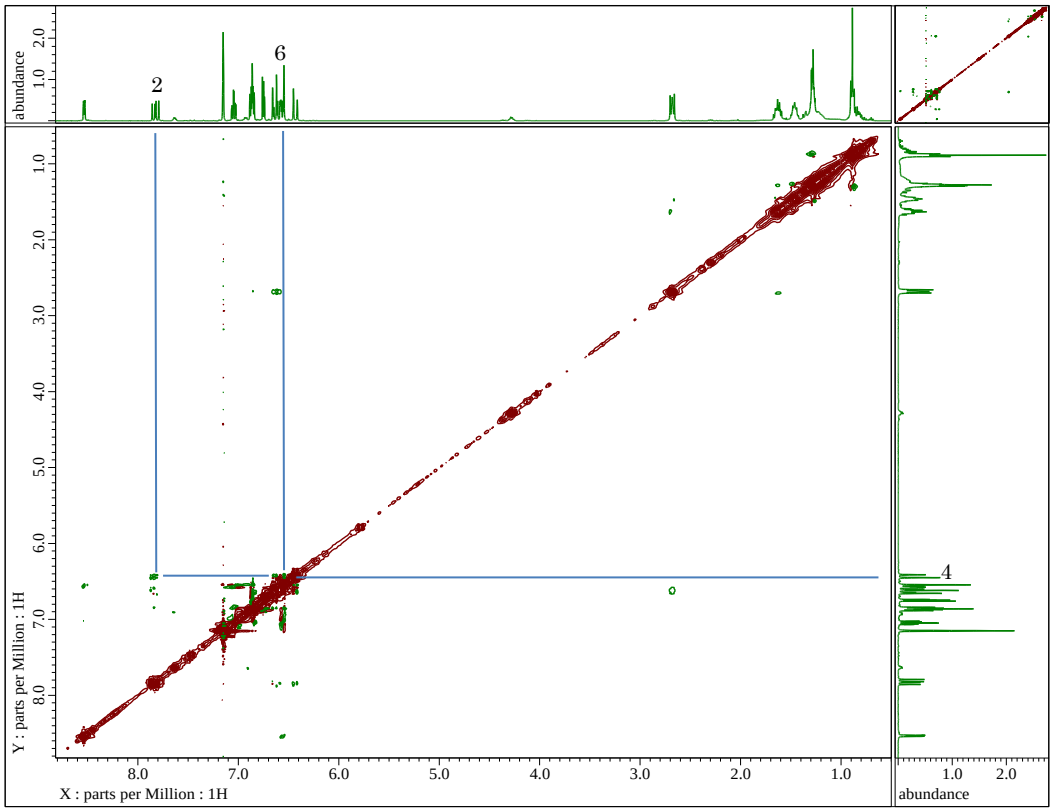


Figure S4. ^{1}H-^{1}H pNOESY NMR Spectrum of (1*E*,3*E*,5*E*)-4aa in C_6D_6.

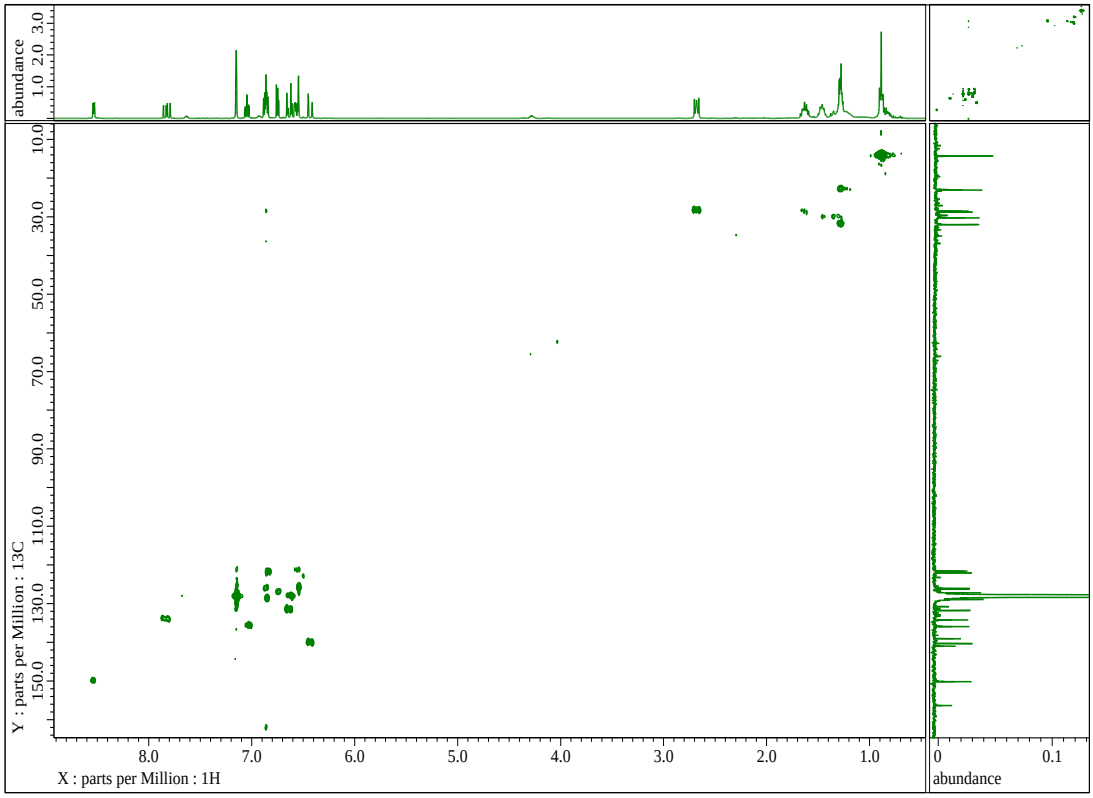


Figure S5. ^{13}C-^{1}H Correlation Spectrum of (1*E*,3*E*,5*E*)-4aa in C_6D_6.

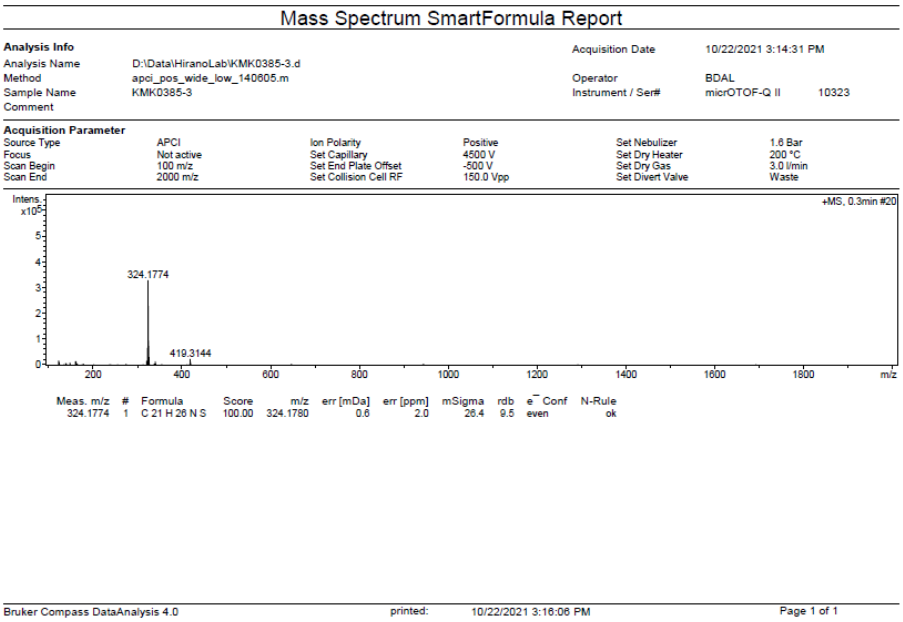


Figure S6. HRMS (APCI) data for (1*E*,3*E*,5*E*)-4aa.

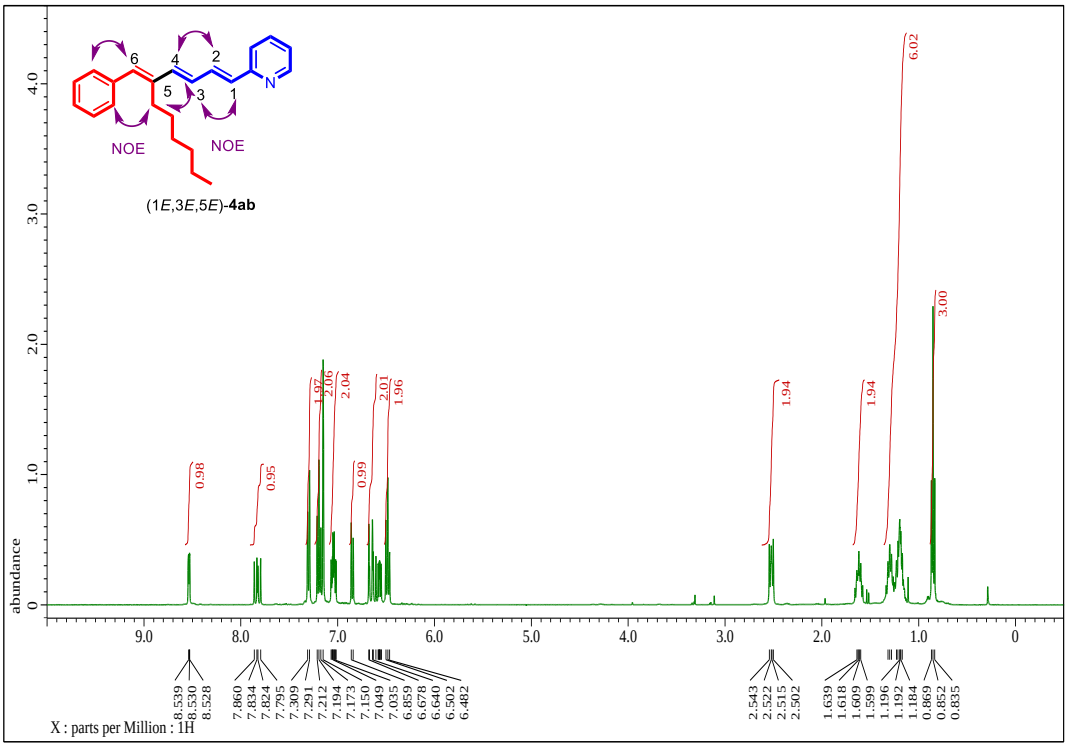


Figure S7. ^{1}H NMR Spectrum of (1*E*,3*E*,5*E*)-4ab in C_6D_6.

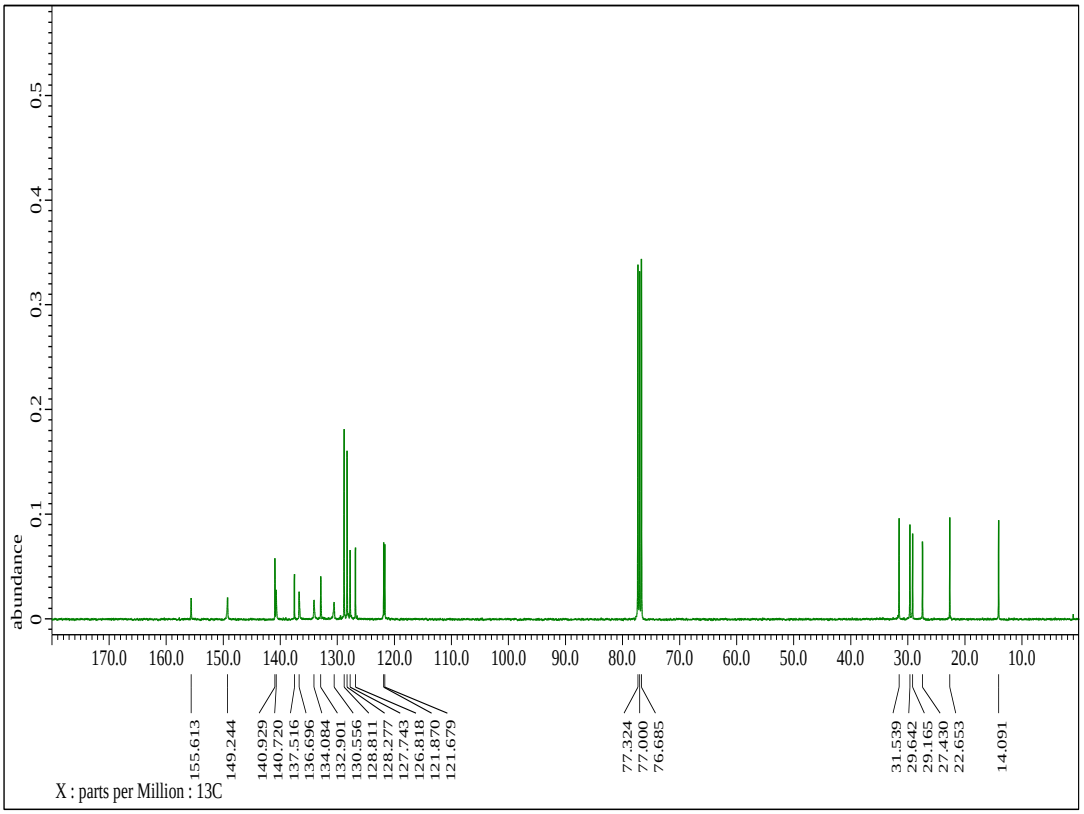


Figure S8. ^{13}C{^{1}H} NMR Spectrum of (1*E*,3*E*,5*E*)-4ab in $CDCl_3$.

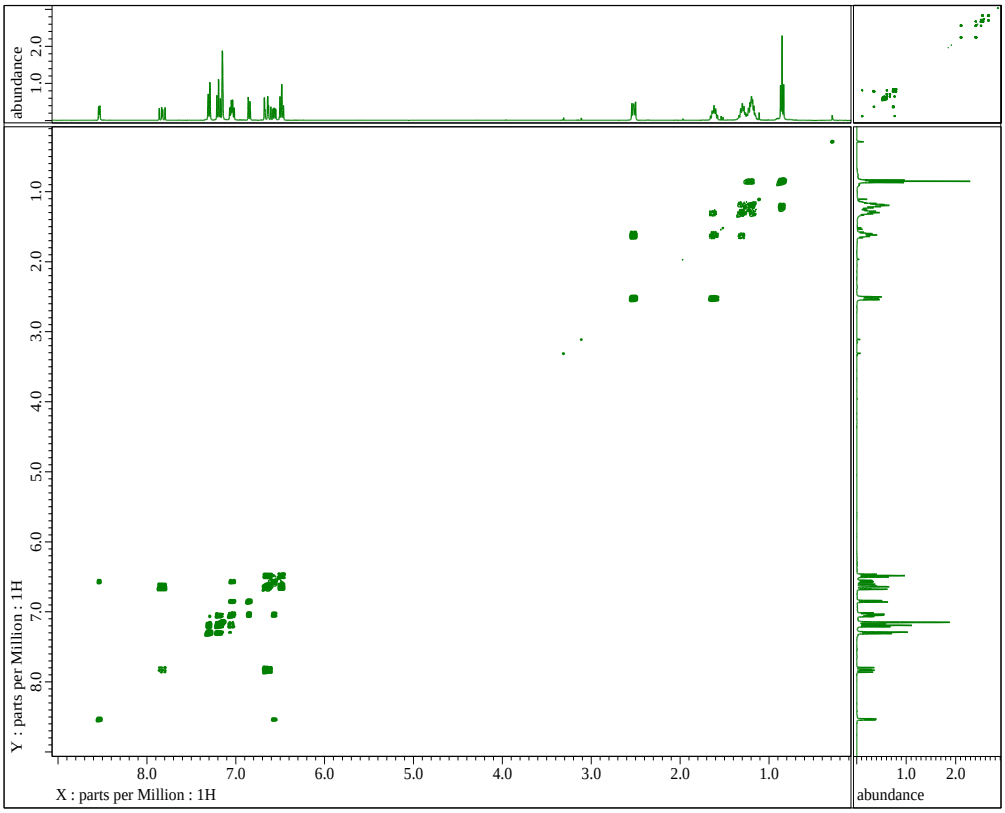


Figure S9. ^{1}H-^{1}H COSY NMR Spectrum of (1*E*,3*E*,5*E*)-4ab in C_6D_6.

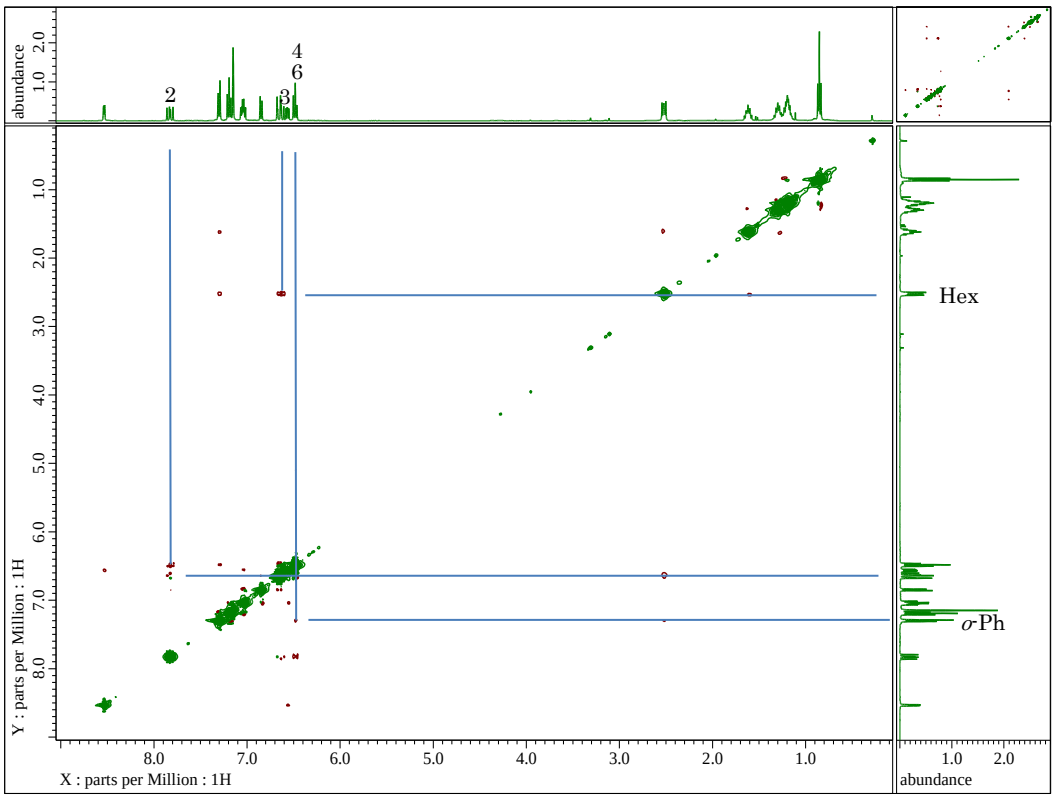


Figure S10. ^{1}H-^{1}H pNOESY NMR Spectrum of (1*E*,3*E*,5*E*)-4ab in C_6D_6.

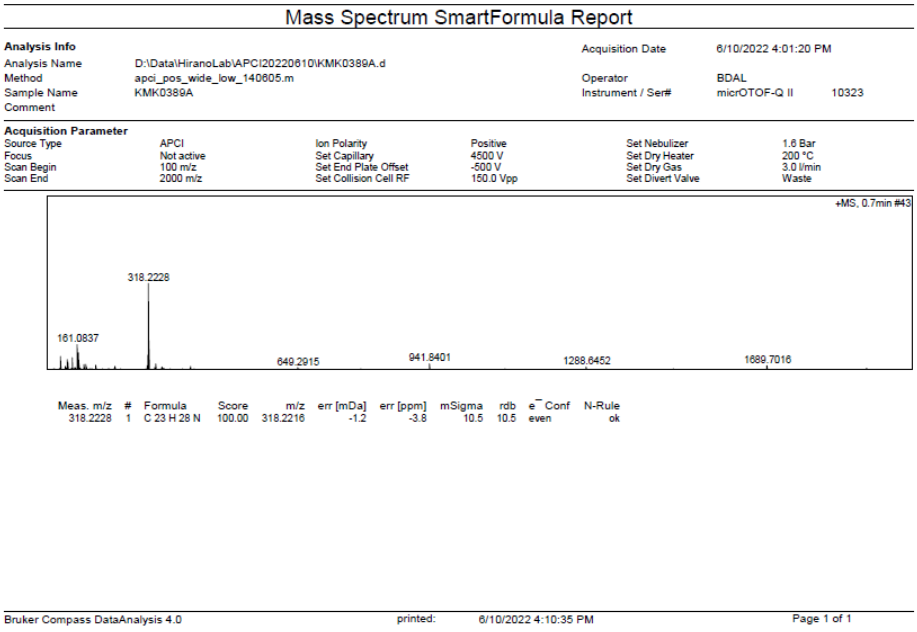


Figure S11. HRMS (APCI) data for (1*E*,3*E*,5*E*)-4ab.

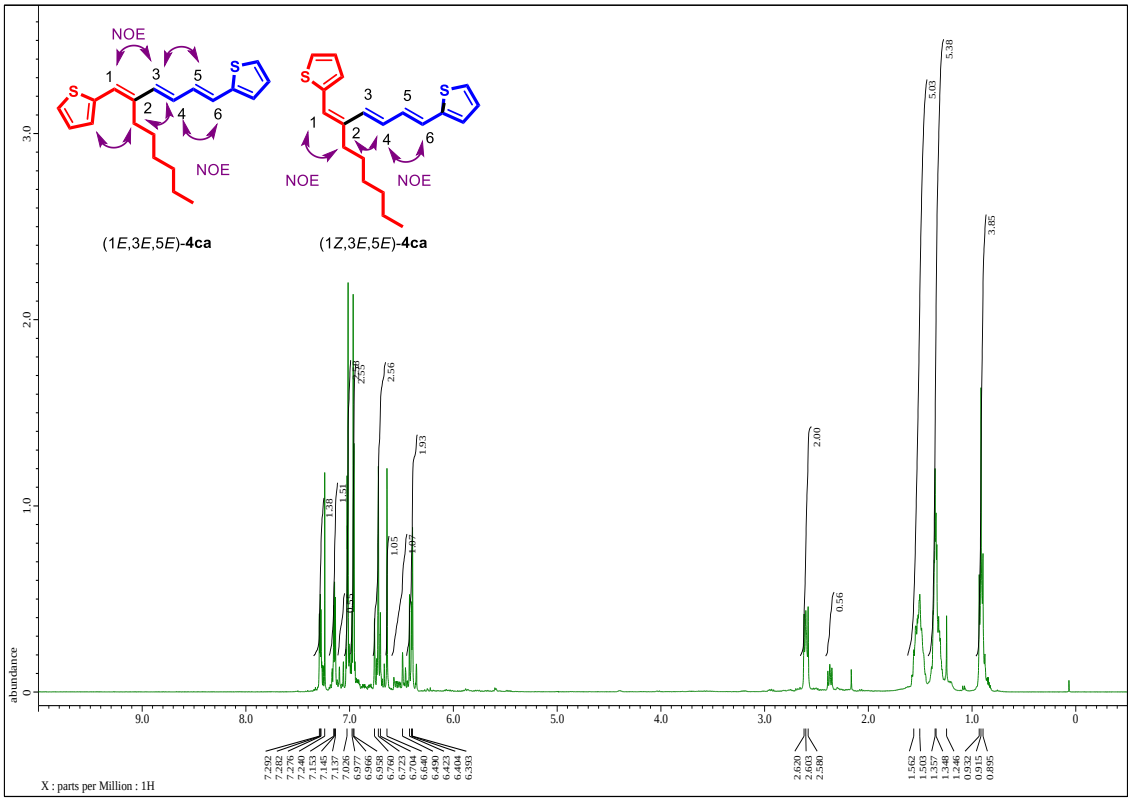


Figure S12. ^{1}H NMR Spectrum of 4ca in $CDCl_3$.

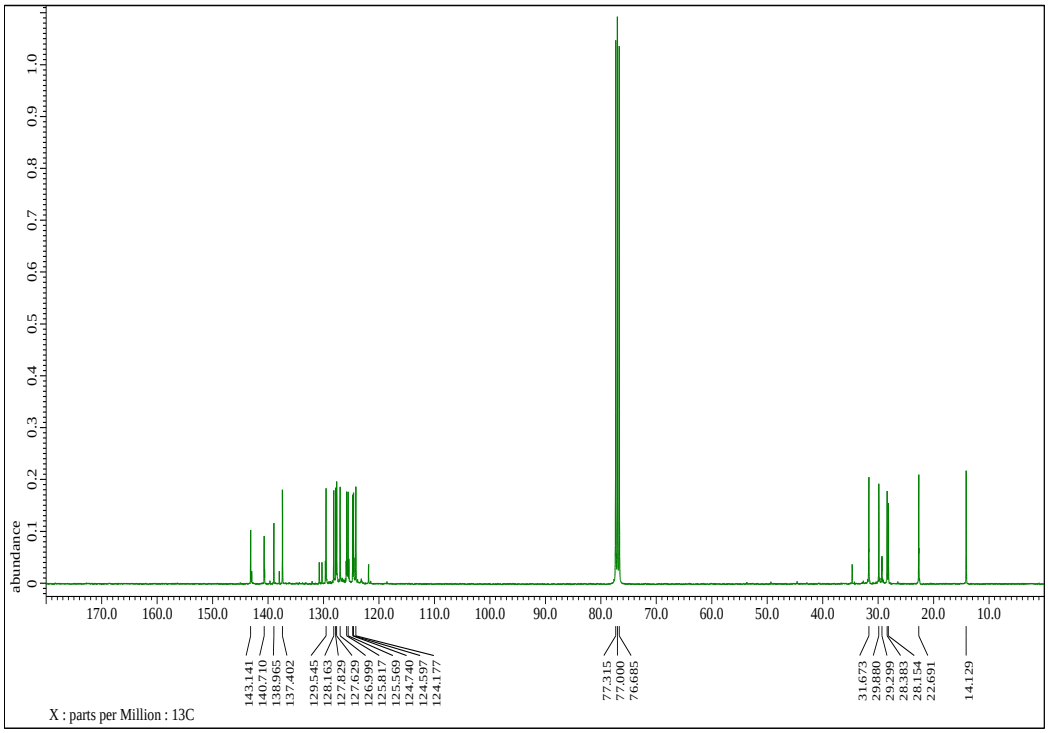


Figure S13. $^{13}C\{^{1}H\}$ NMR Spectrum of 4ca in $CDCl_3$.

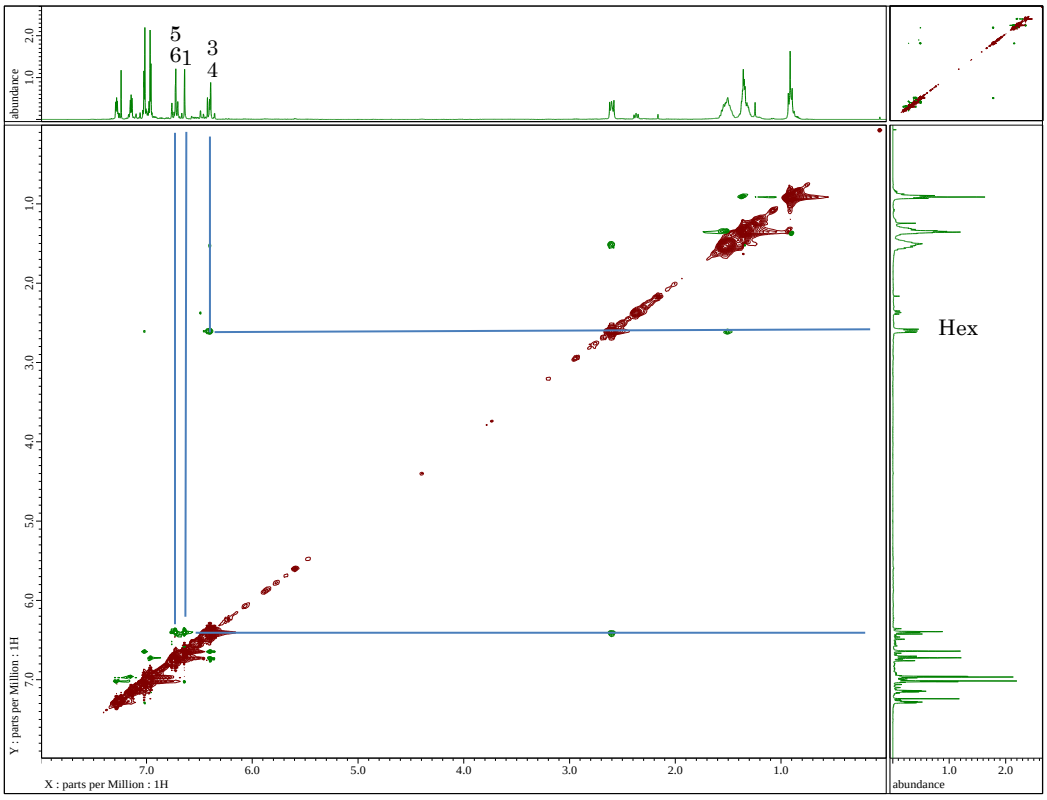


Figure S14. ^{1}H-^{1}H pNOESY NMR Spectrum of 4ca in $CDCl_3$.

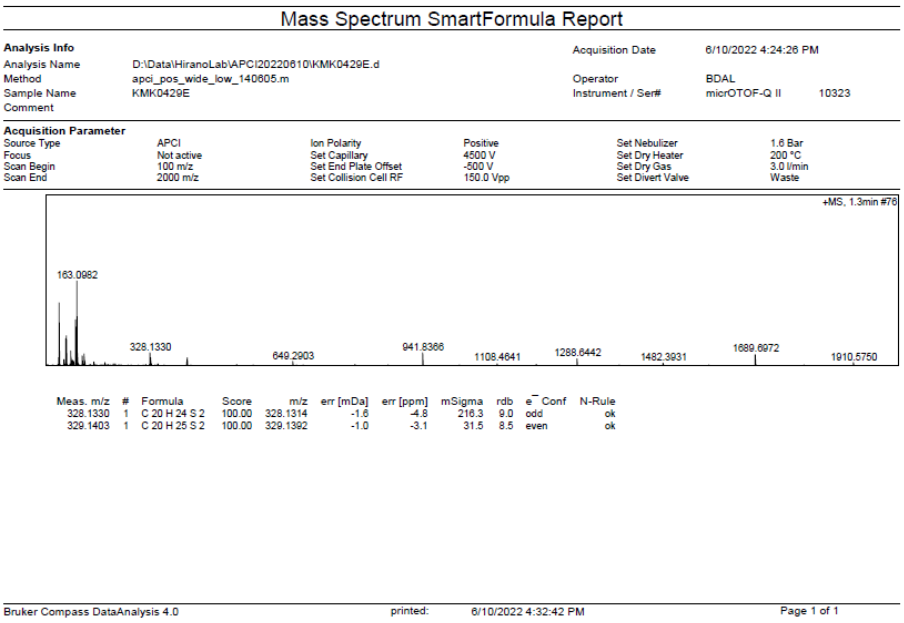


Figure S15-1. HRMS (APCI) data for 4ca.

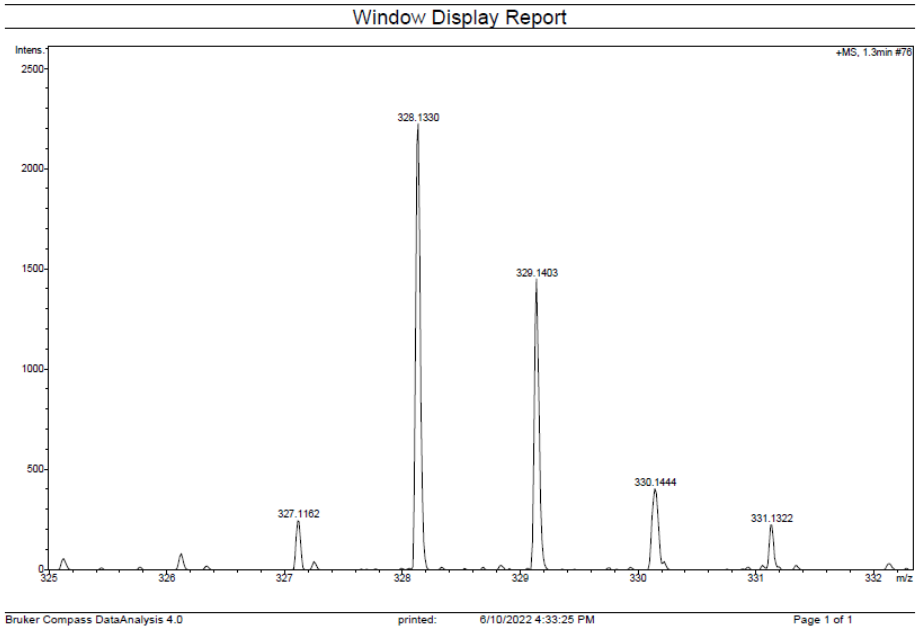


Figure S15-2. HRMS (APCI) data for 4ca.

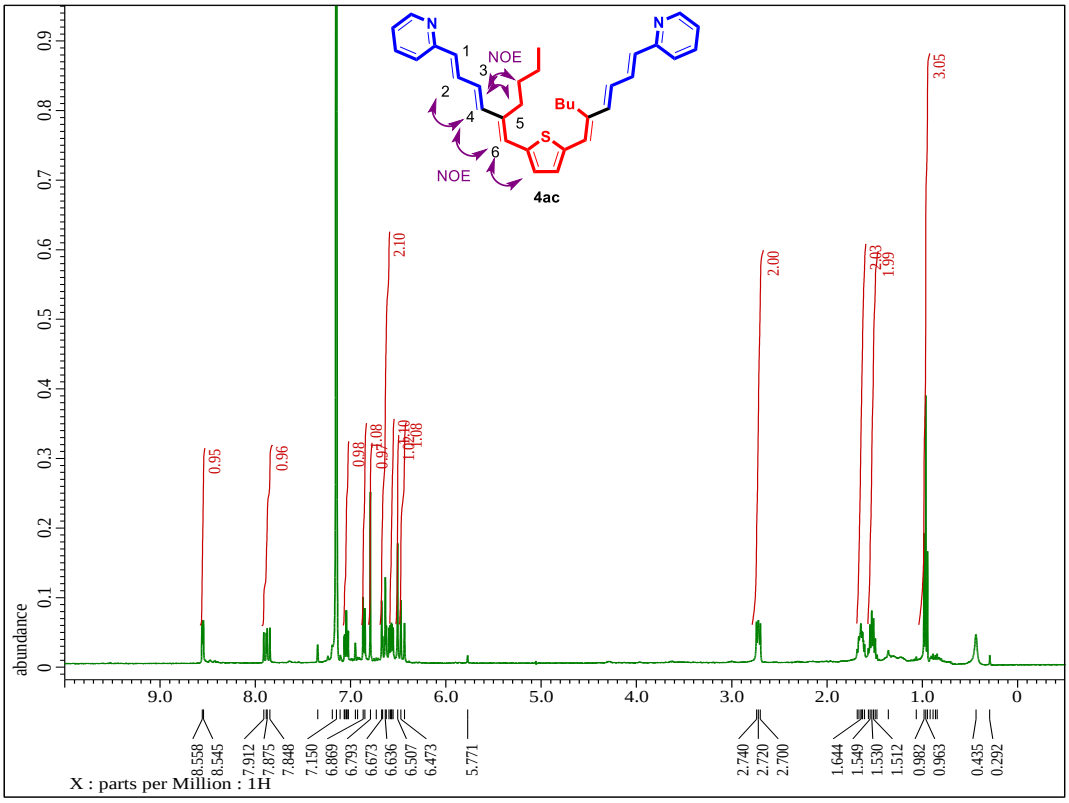


Figure S16. ^{1}H NMR Spectrum of 4ac in C_6D_6.

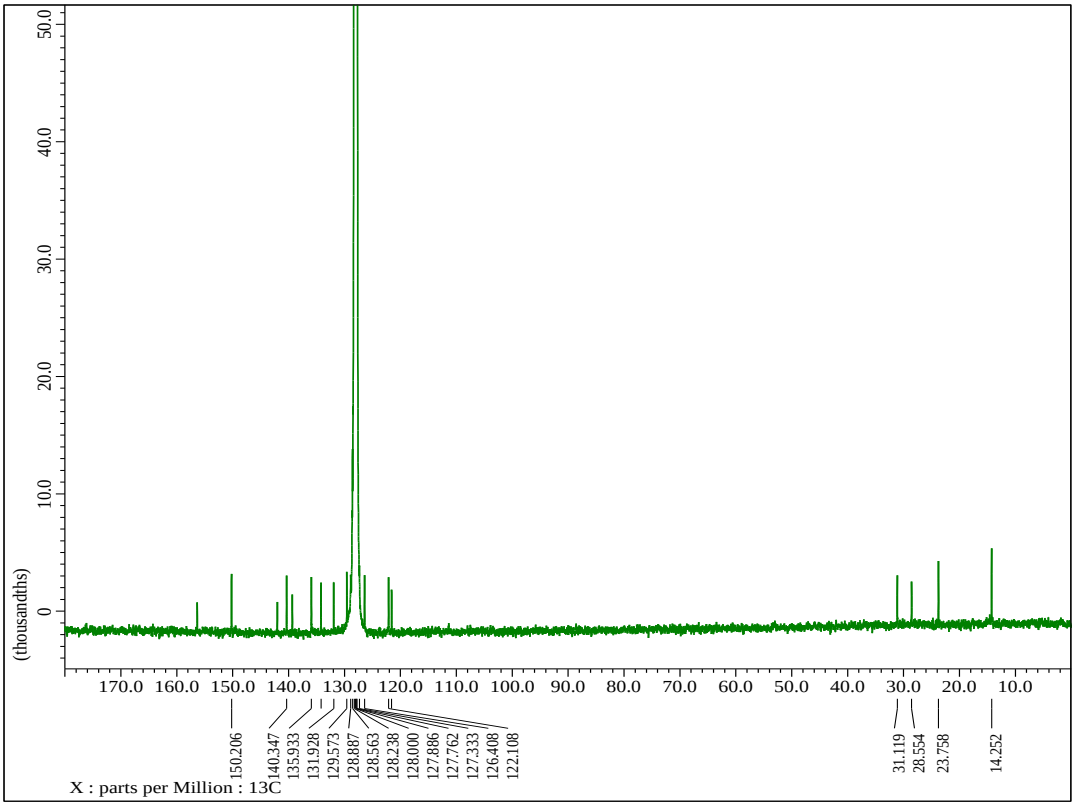


Figure S17. $^{13}C\{^{1}H\}$ NMR Spectrum of 4ac in C_6D_6.

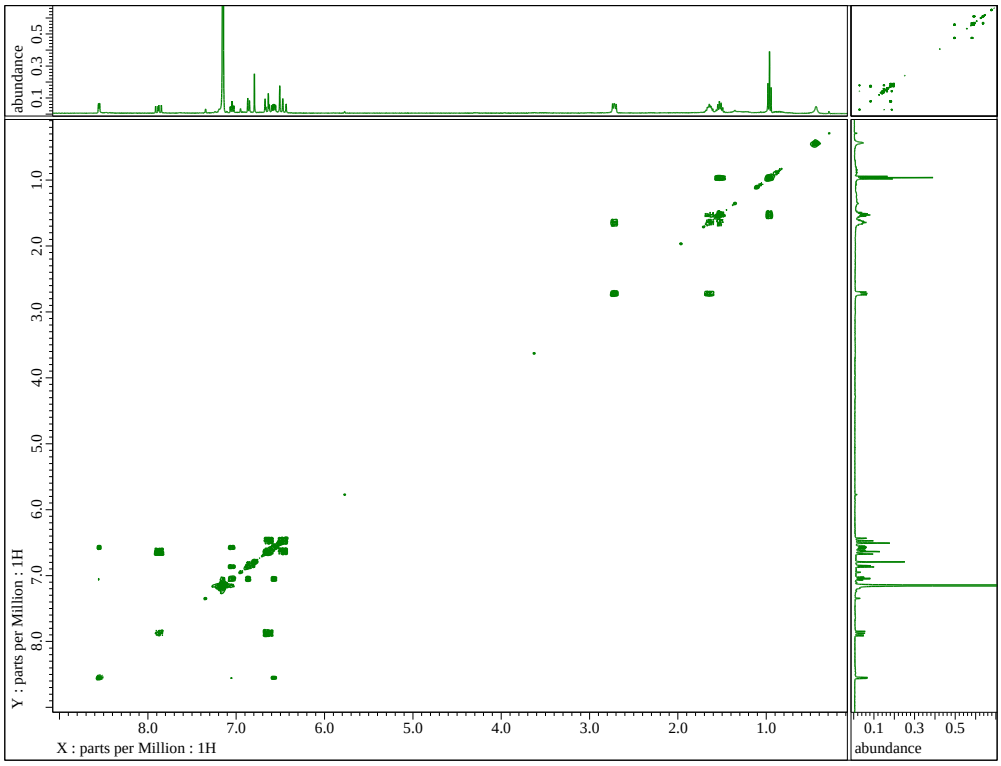


Figure S18. ^{1}H-^{1}H COSY NMR Spectrum of 4ac in C_6D_6.

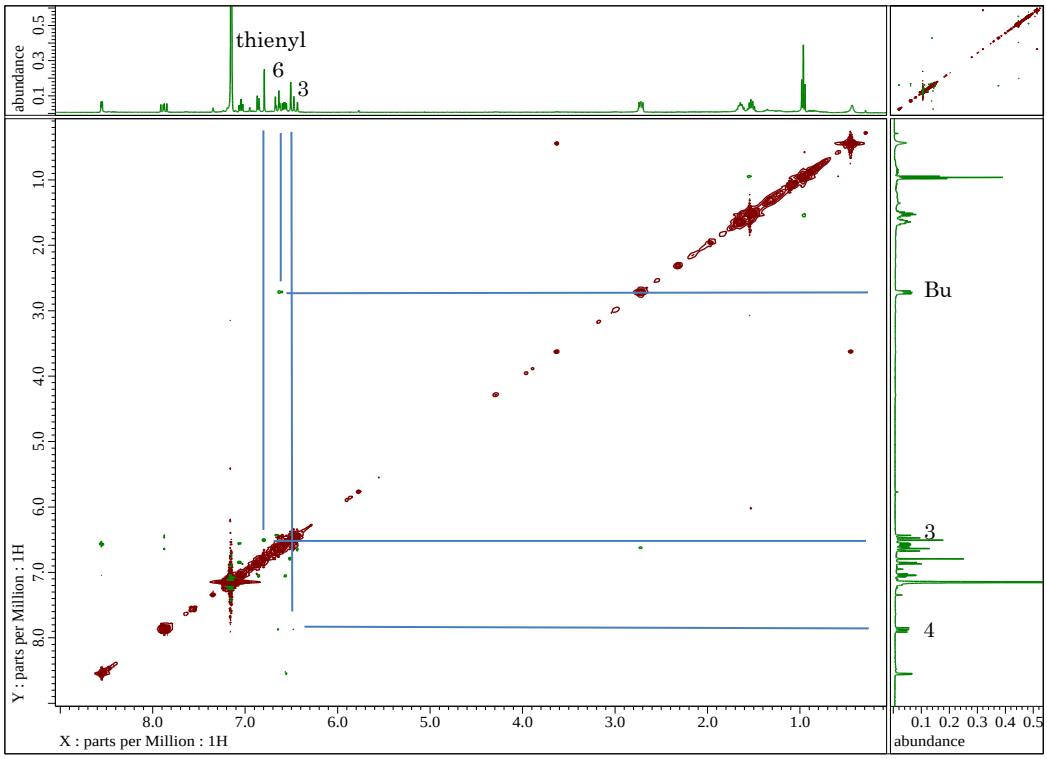


Figure S19. ^{1}H-^{1}H pNOESY NMR Spectrum of 4ac in C_6D_6.

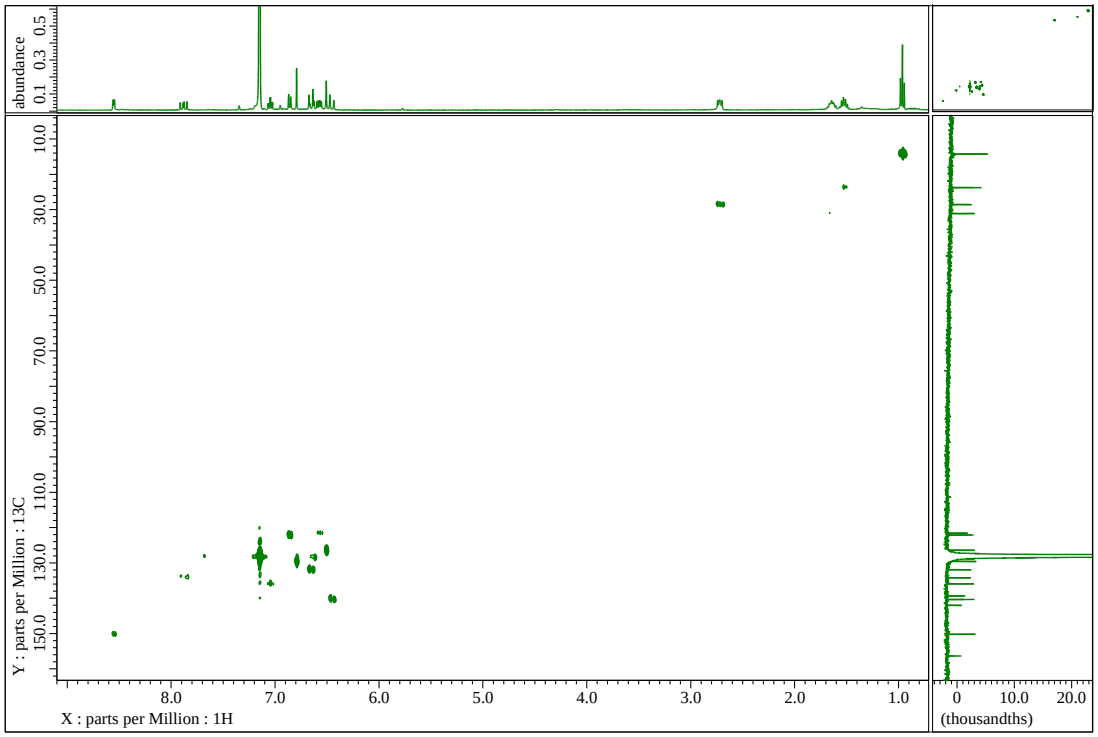
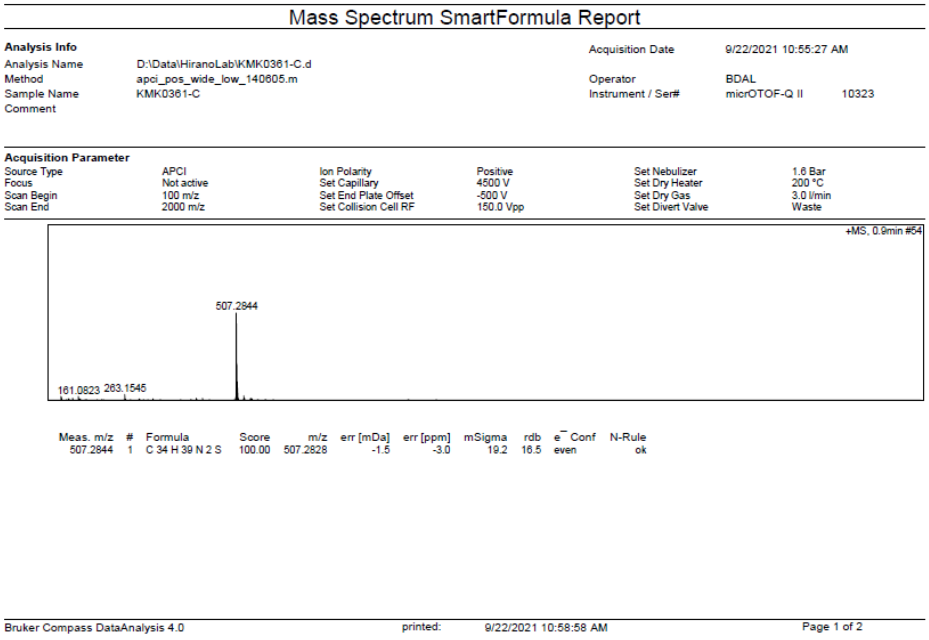


Figure S20. ^{13}C-^{1}H Correlation Spectrum of 4ac in C_6D_6.



Mass Spectrum SmartFormula Report

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Comment			

Acquisition Parameter

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Figure S21. HRMS (APCI) data for 4ac.

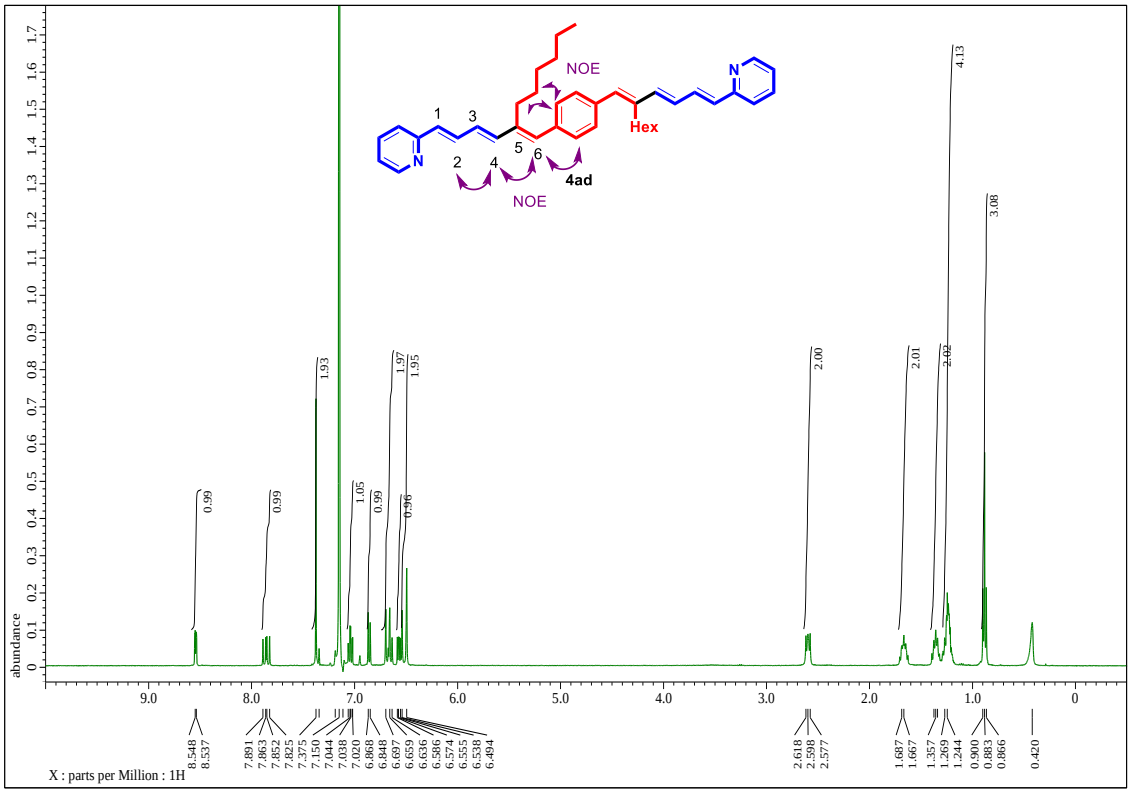


Figure S22. ^{1}H NMR Spectrum of 4ad in C_6D_6.

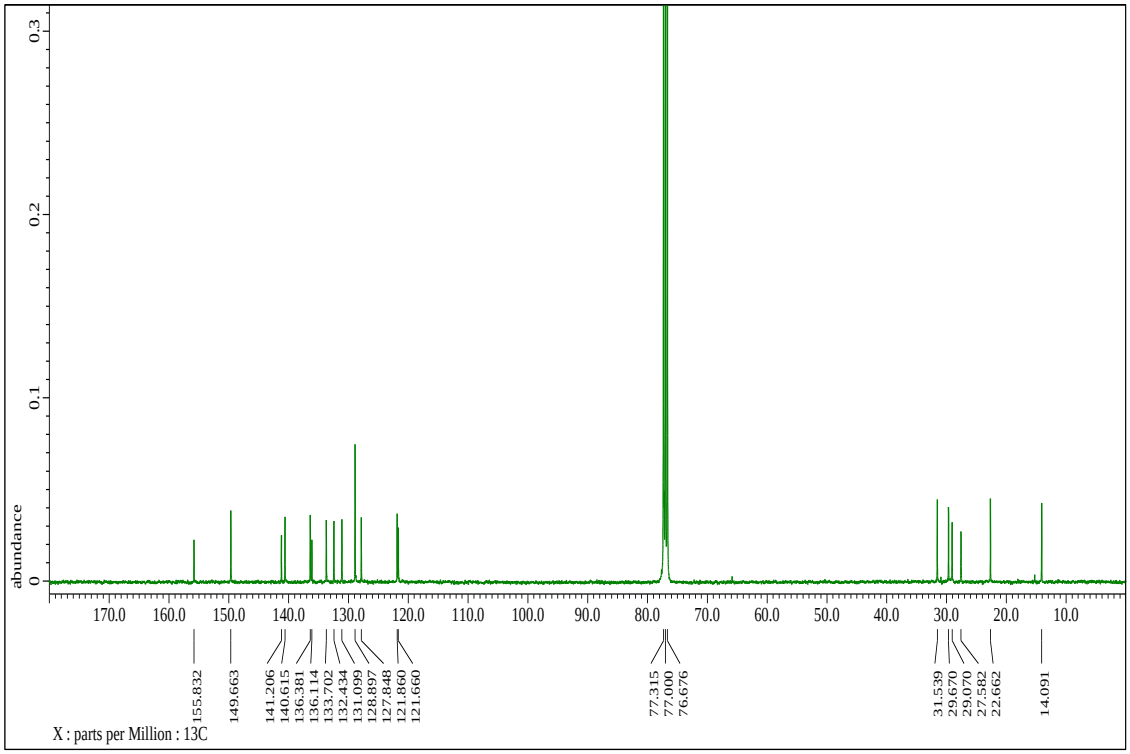


Figure S23. $^{13}C\{^{1}H\}$ NMR Spectrum of 4ad in $CDCl_3$.

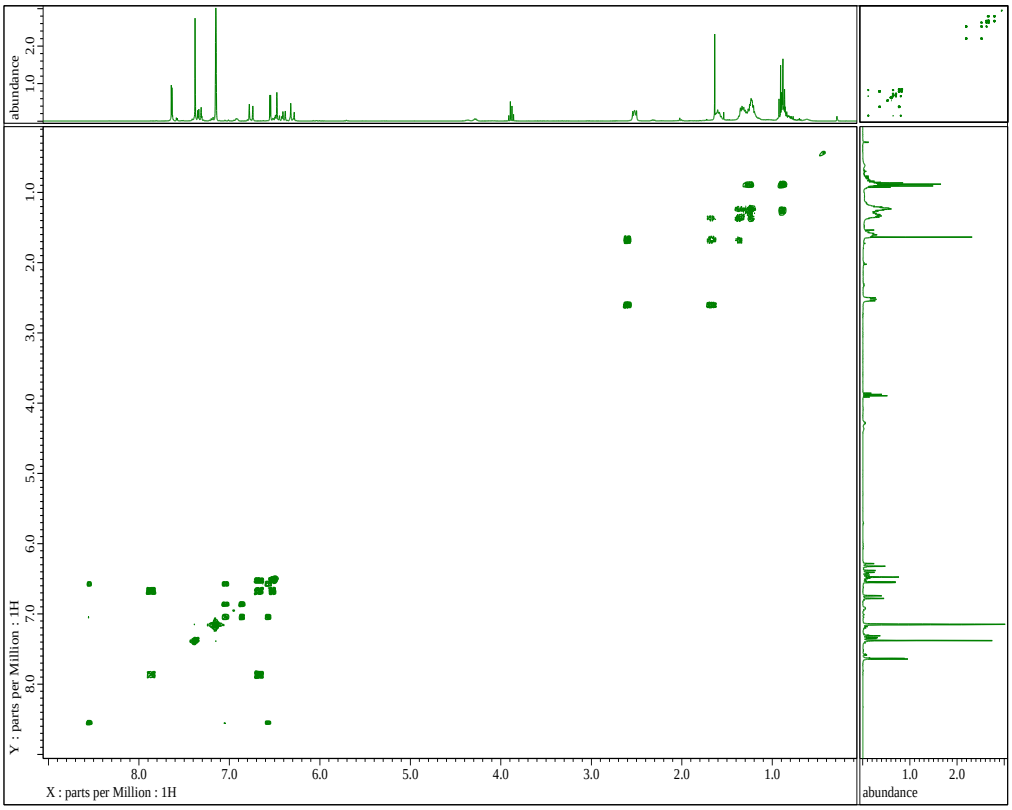


Figure S24. ^{1}H-^{1}H COSY NMR Spectrum of 4ad in C_6D_6.

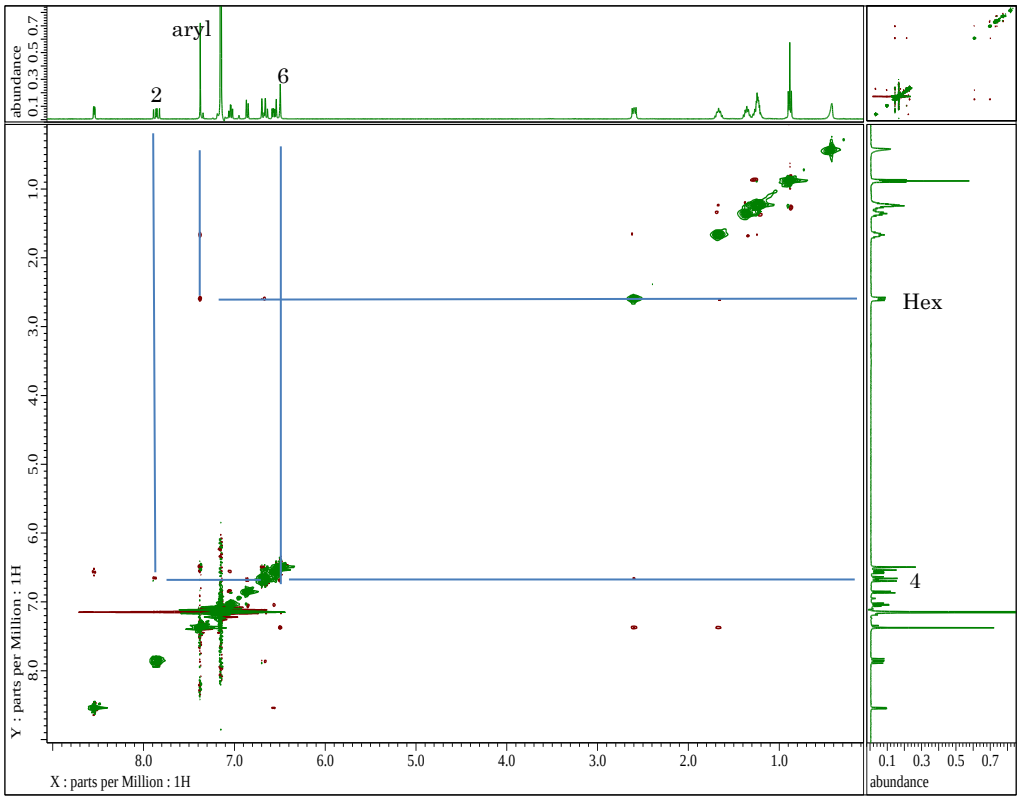


Figure S25. ^{1}H-^{1}H pNOESY NMR Spectrum of 4ad in C_6D_6.

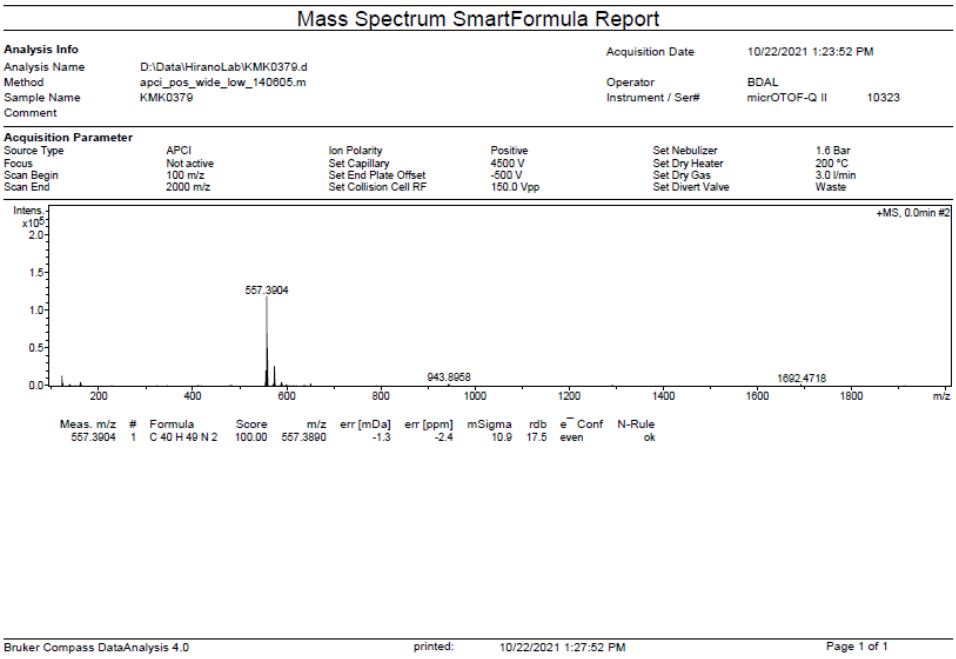


Figure S26. HRMS (APCI) data for 4ad.

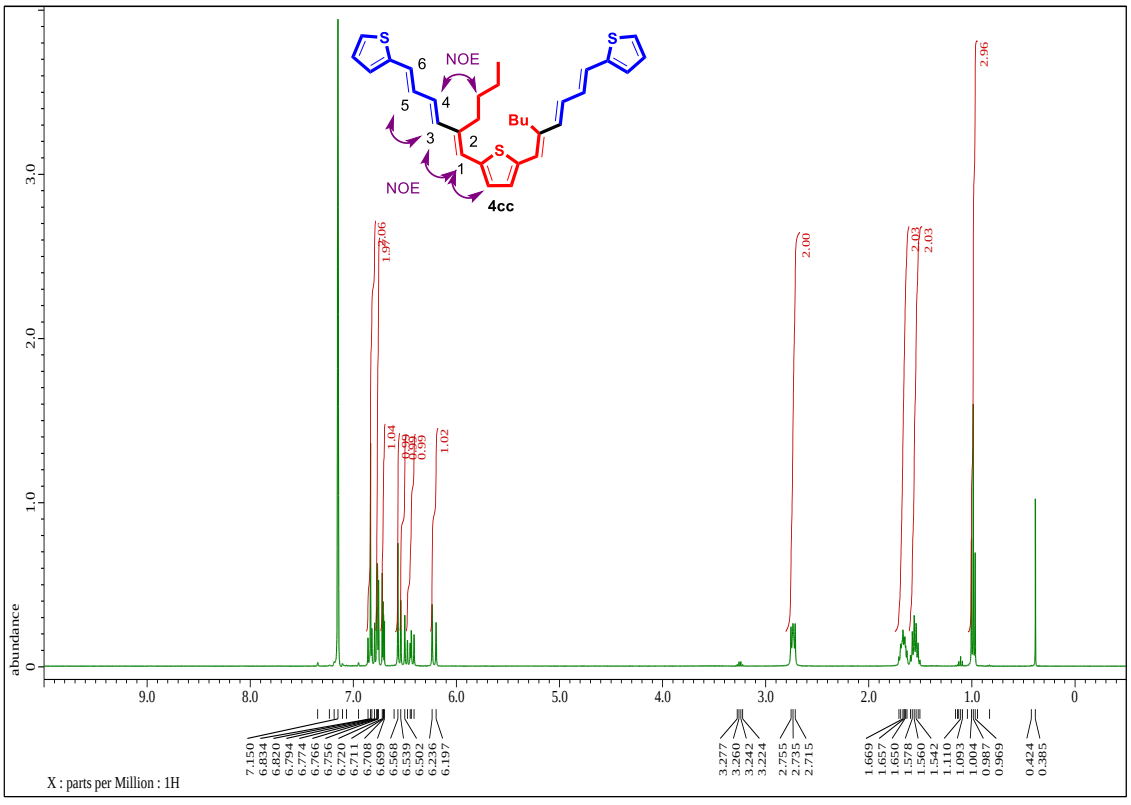


Figure S27. ^{1}H NMR Spectrum of 4cc in C_6D_6.

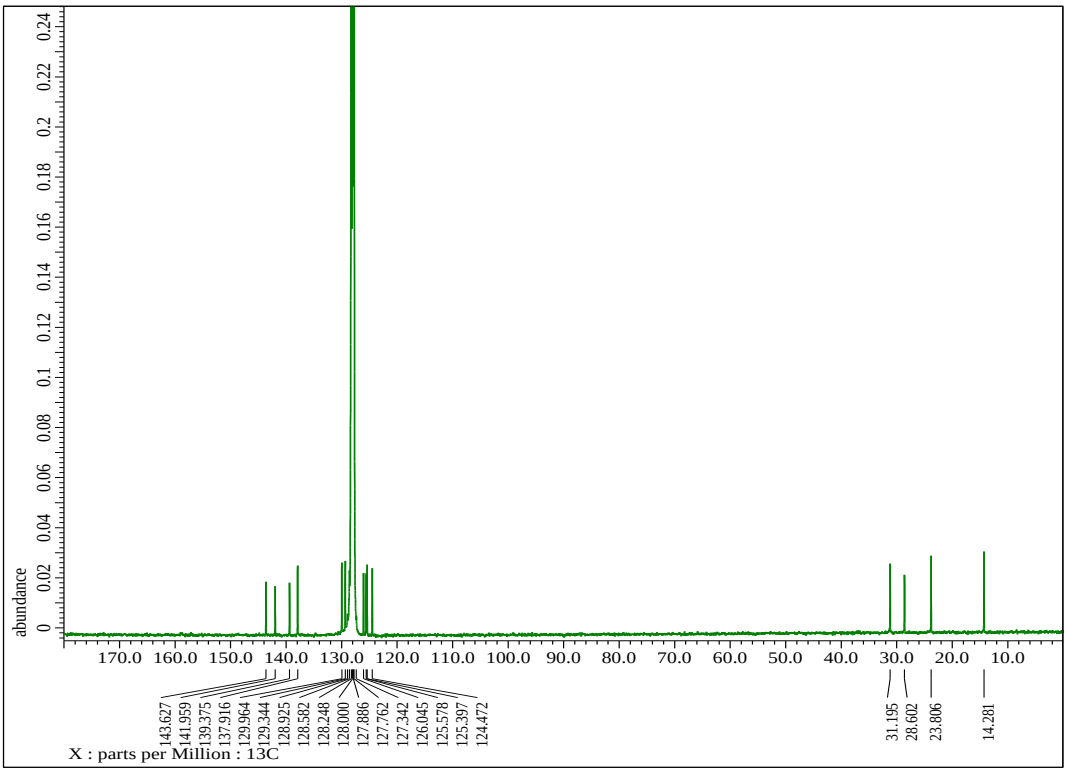


Figure S28. $^{13}C\{^{1}H\}$ NMR Spectrum of 4cc in C_6D_6.

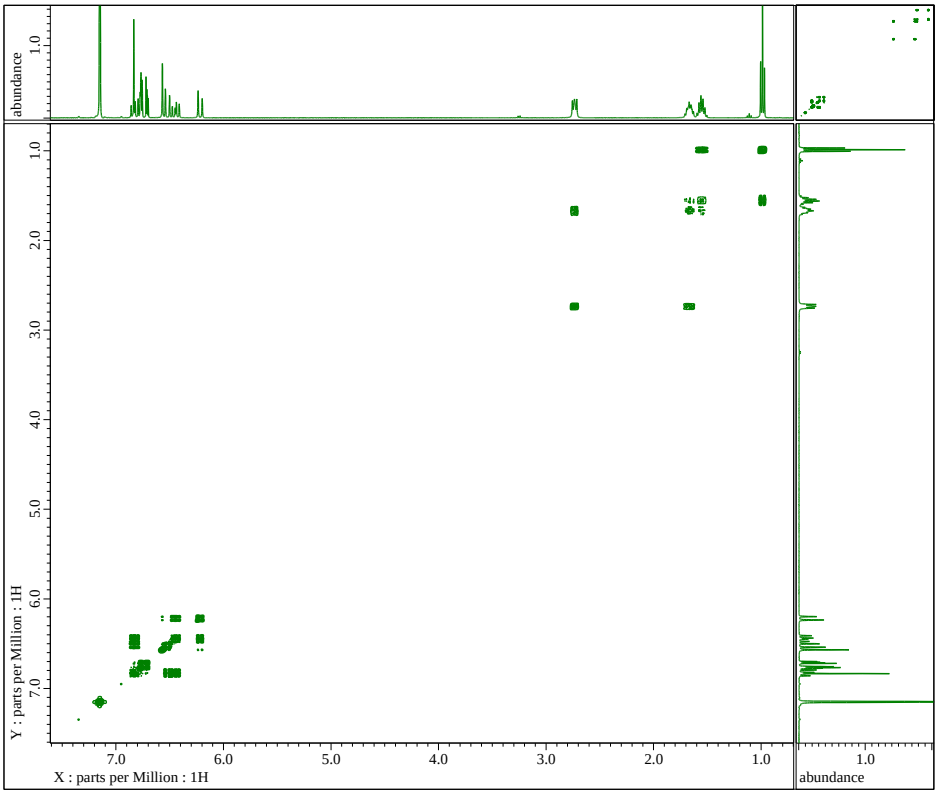


Figure S29. ^{1}H-^{1}H COSY NMR Spectrum of 4cc in C_6D_6.

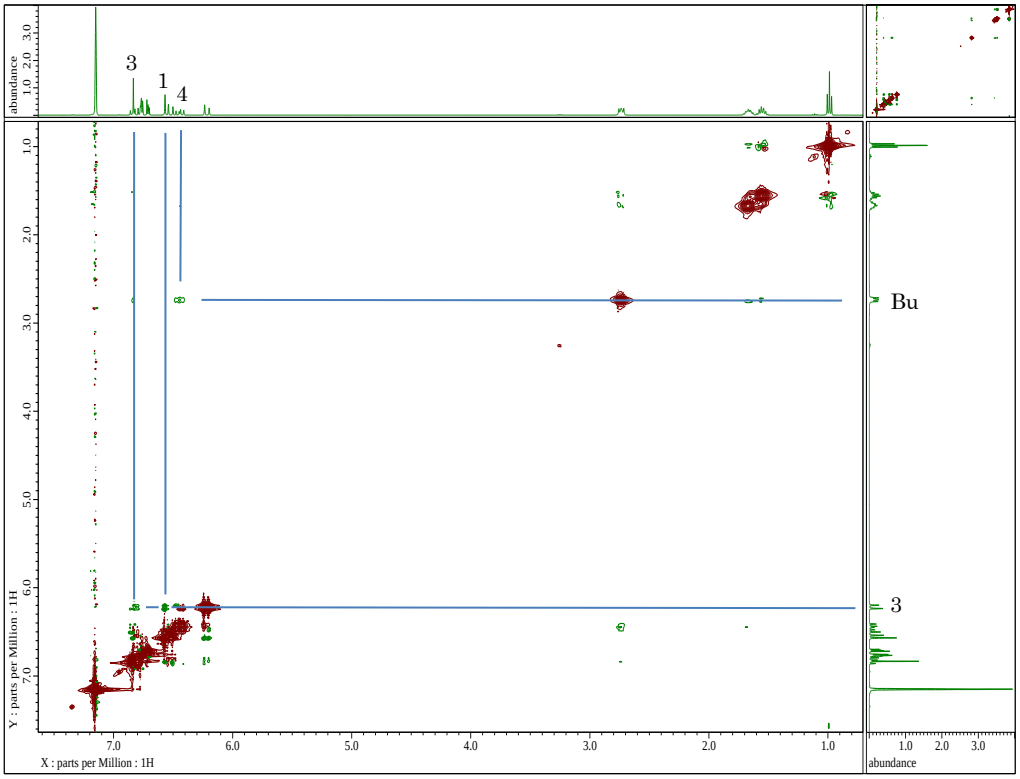


Figure S30. ^{1}H-^{1}H pNOESY NMR Spectrum of 4cc in C_6D_6.

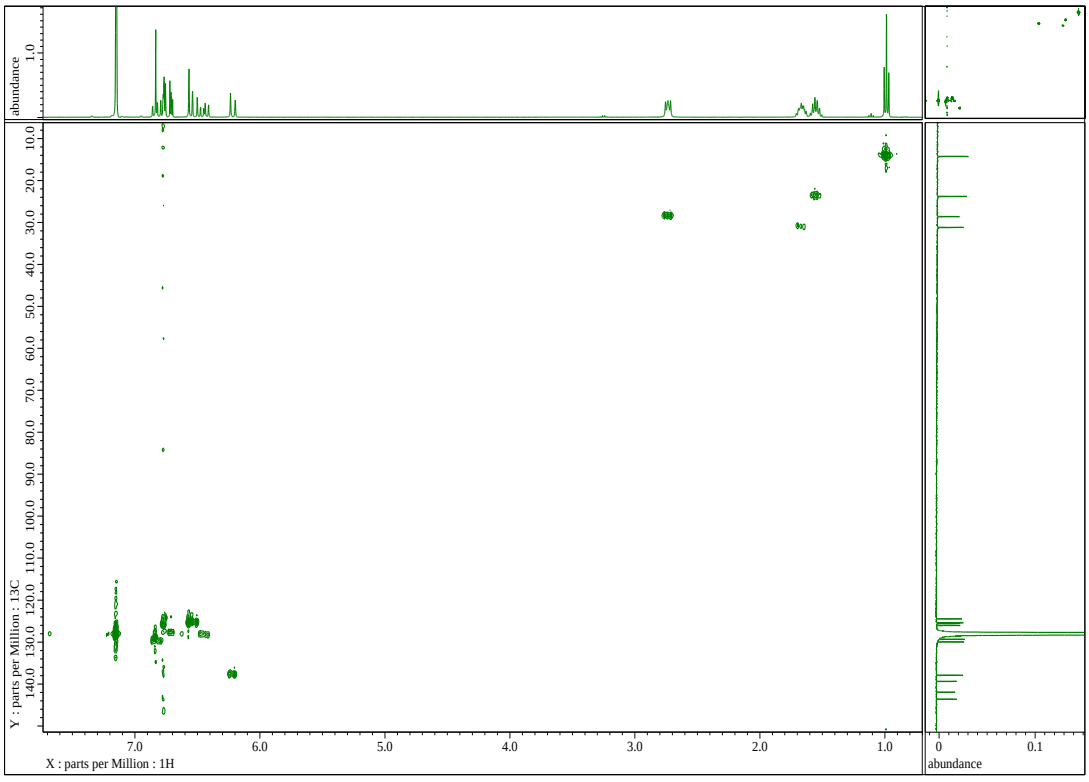


Figure S31. ^{13}C-^{1}H Correlation Spectrum of 4cc in C_6D_6.

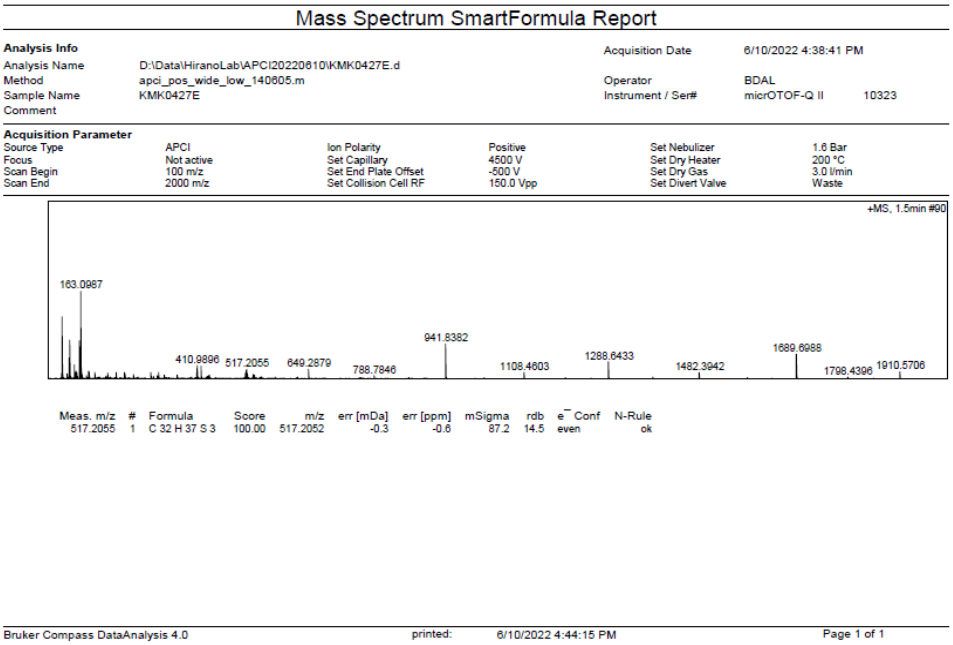


Figure S32. HRMS (APCI) data for 4cc.

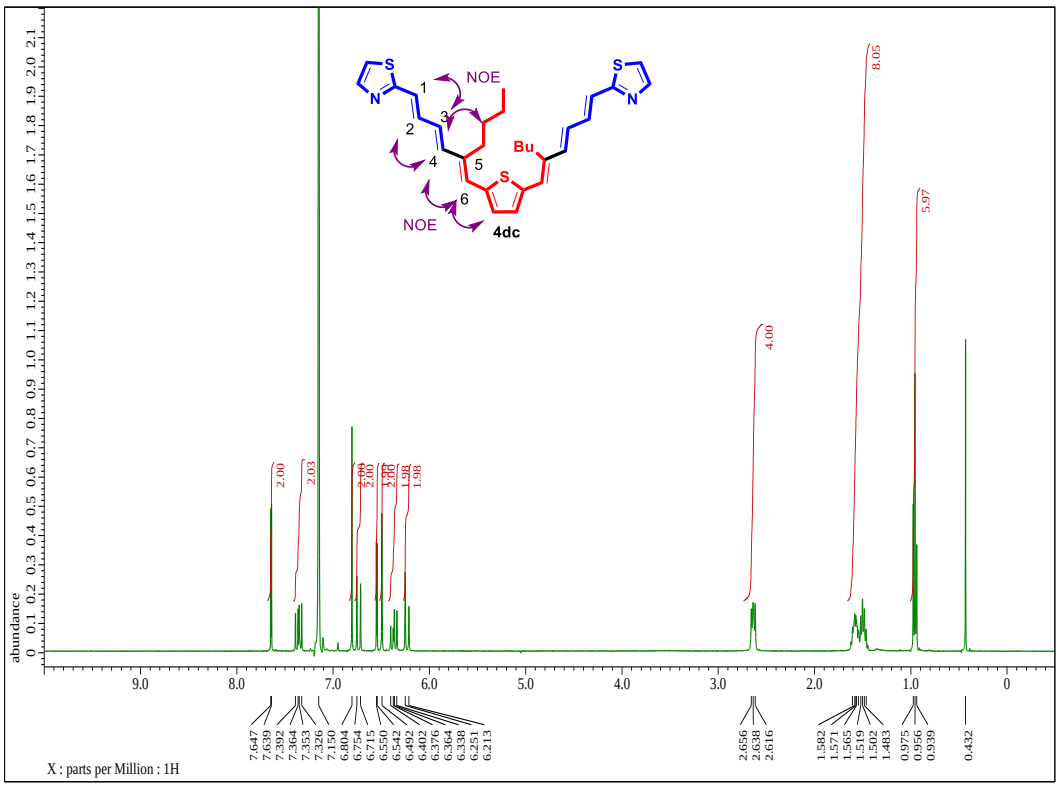


Figure S33. ^{1}H NMR Spectrum of 4dc in C_6D_6.

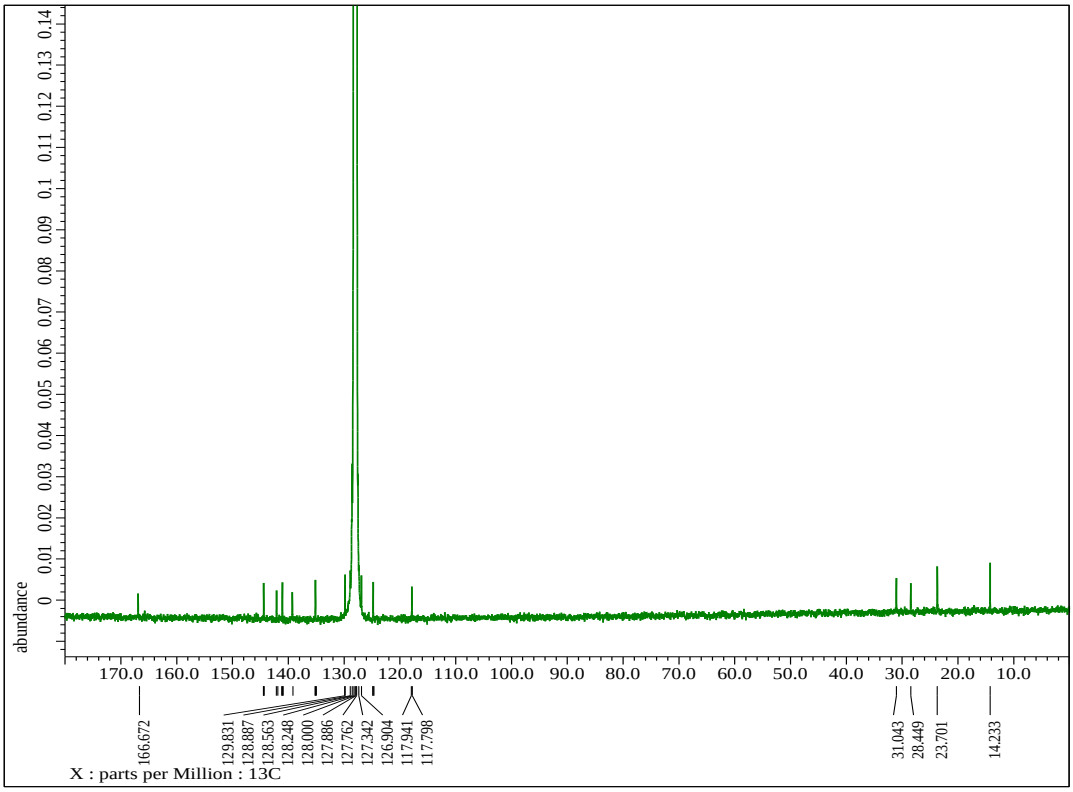


Figure S34. $^{13}C\{^{1}H\}$ NMR Spectrum of 4dc in C_6D_6.

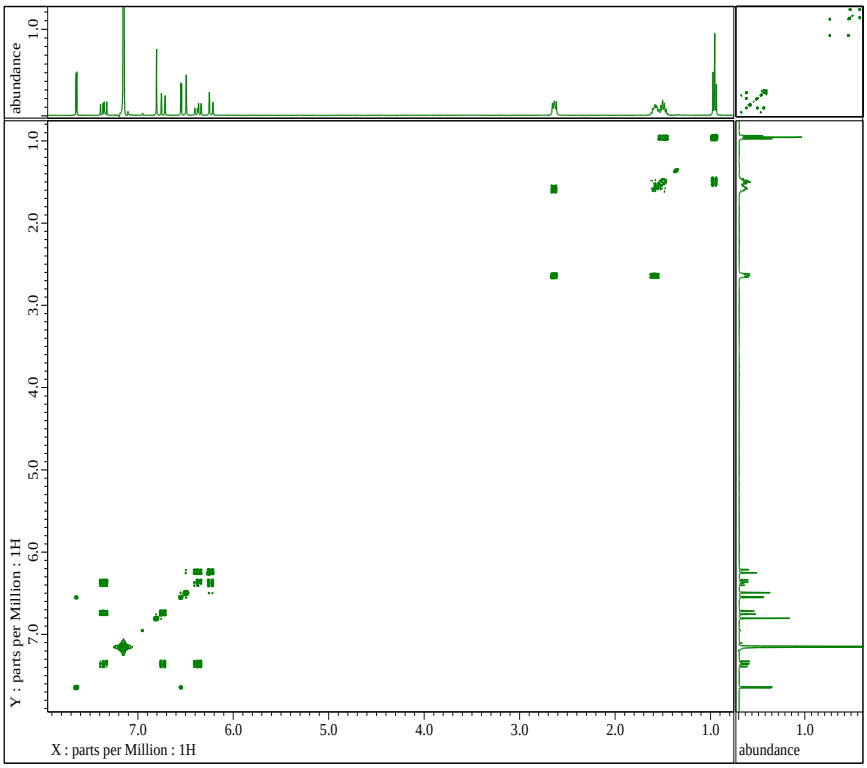


Figure S35. ^{1}H-^{1}H COSY NMR Spectrum of 4dc in C_6D_6.

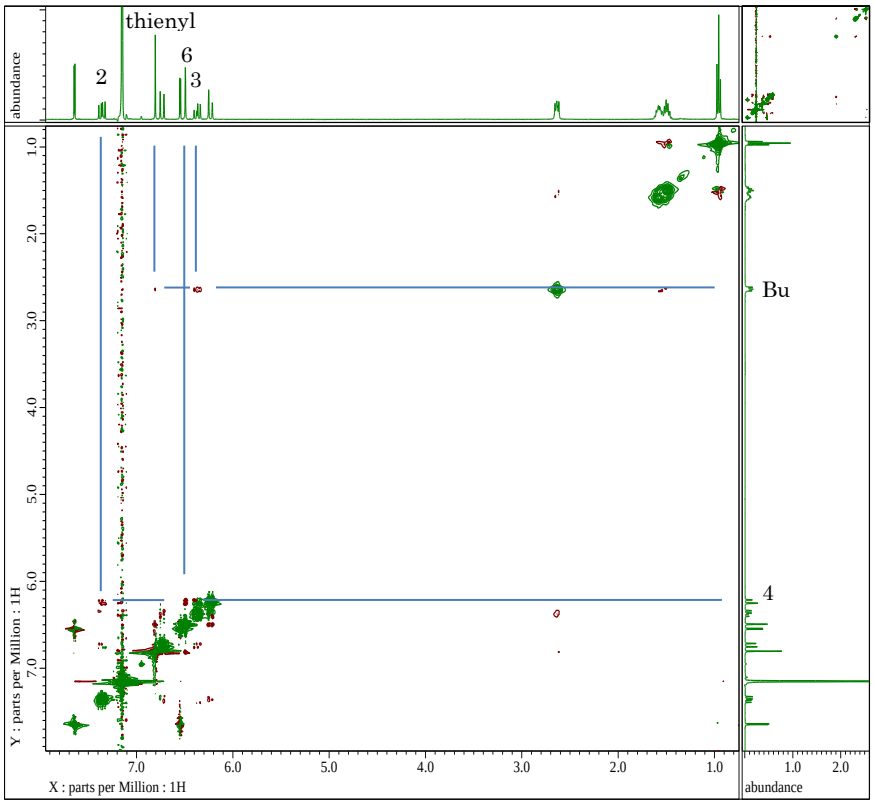


Figure S36. ^{1}H-^{1}H pNOESY NMR Spectrum of 4dc in C_6D_6.

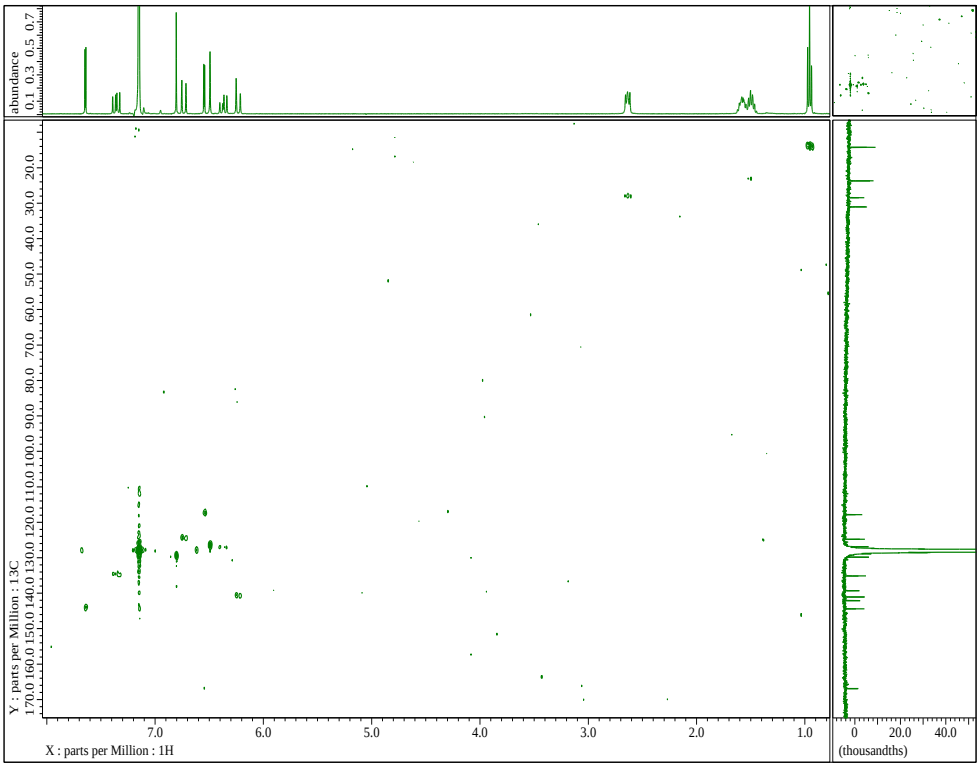


Figure S37. ^{13}C-^{1}H Correlation Spectrum of 4dc in C_6D_6.

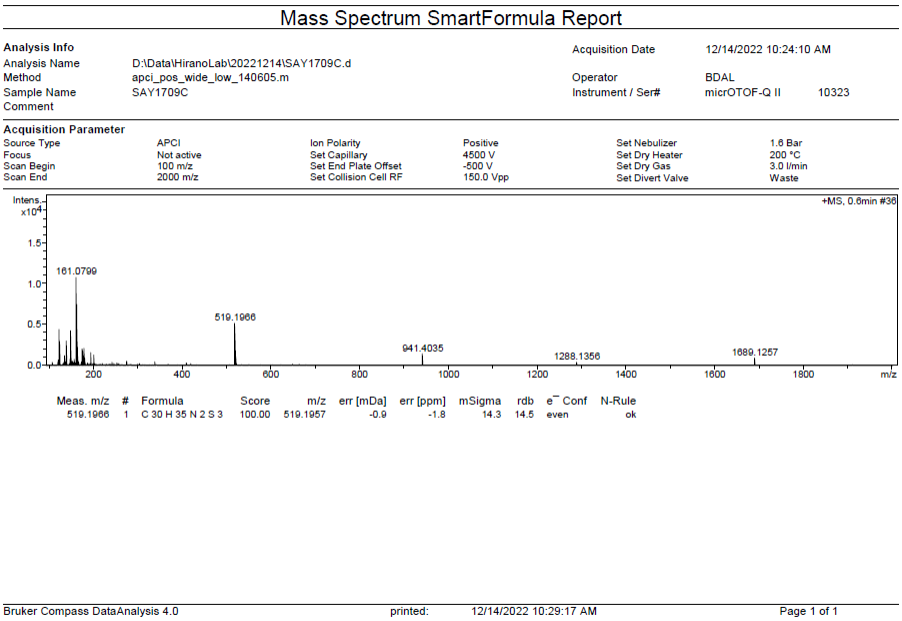


Figure S38. HRMS (APCI) data for 4dc.

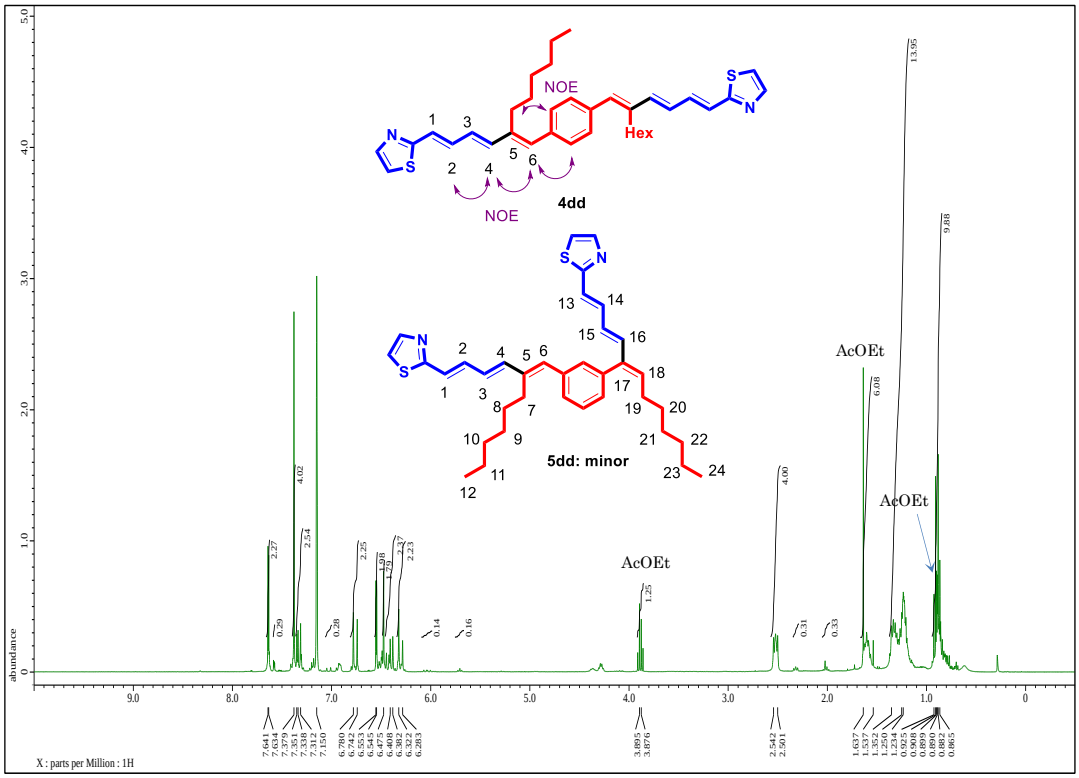


Figure S39. ^{1}H NMR Spectrum of 4dd and 5dd in C_6D_6.

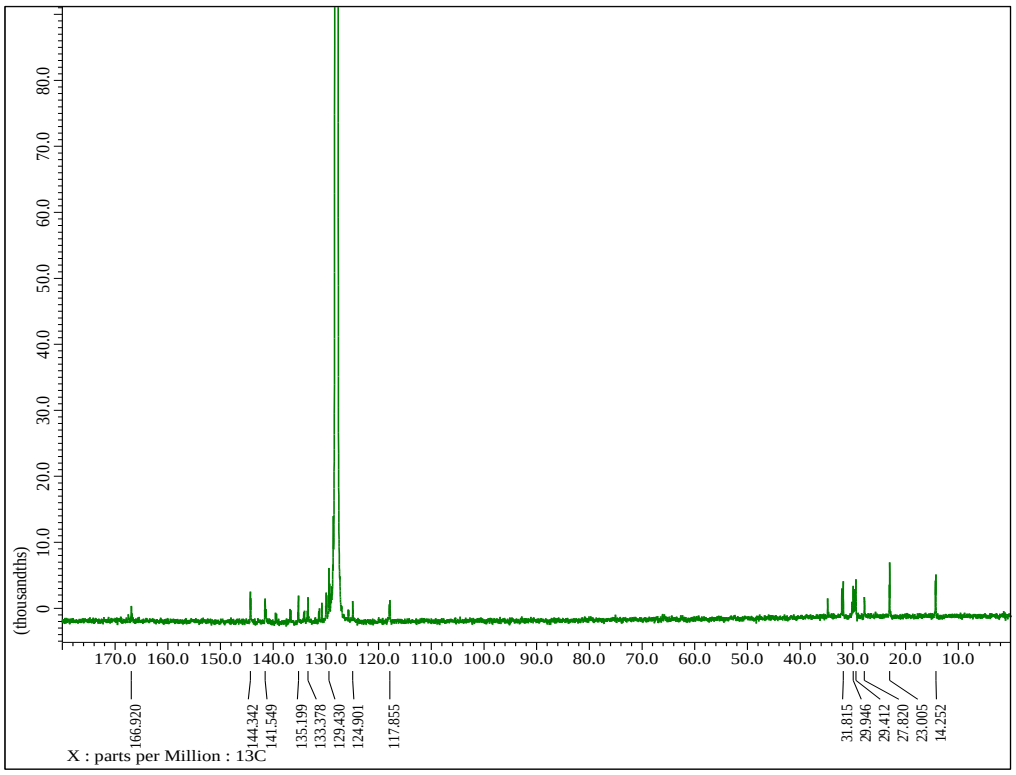


Figure S40. $^{13}C\{^{1}H\}$ NMR Spectrum of 4dd (included 5dd) in C_6D_6.

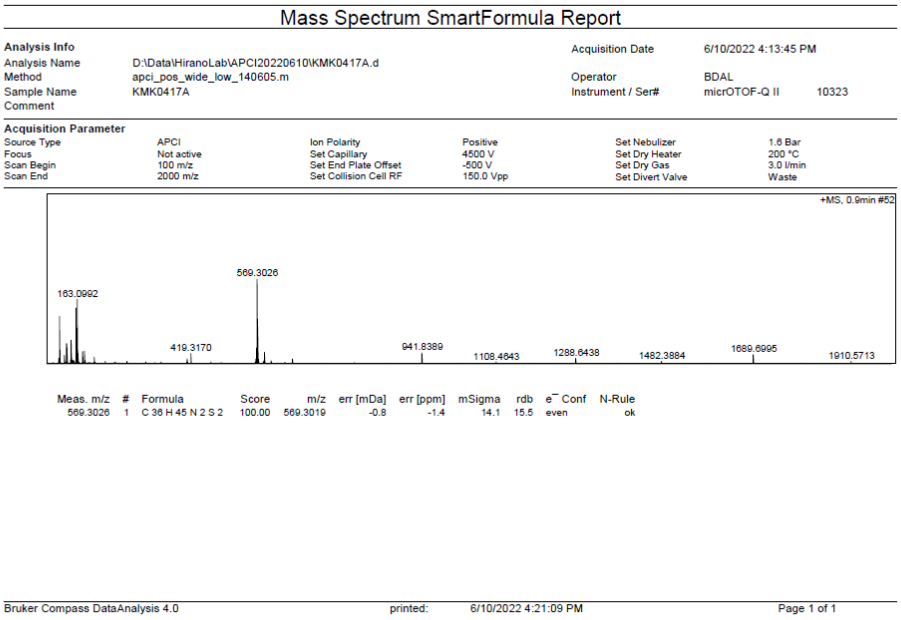


Figure S41. HRMS (APCI) data for 4dd (included 5dd).

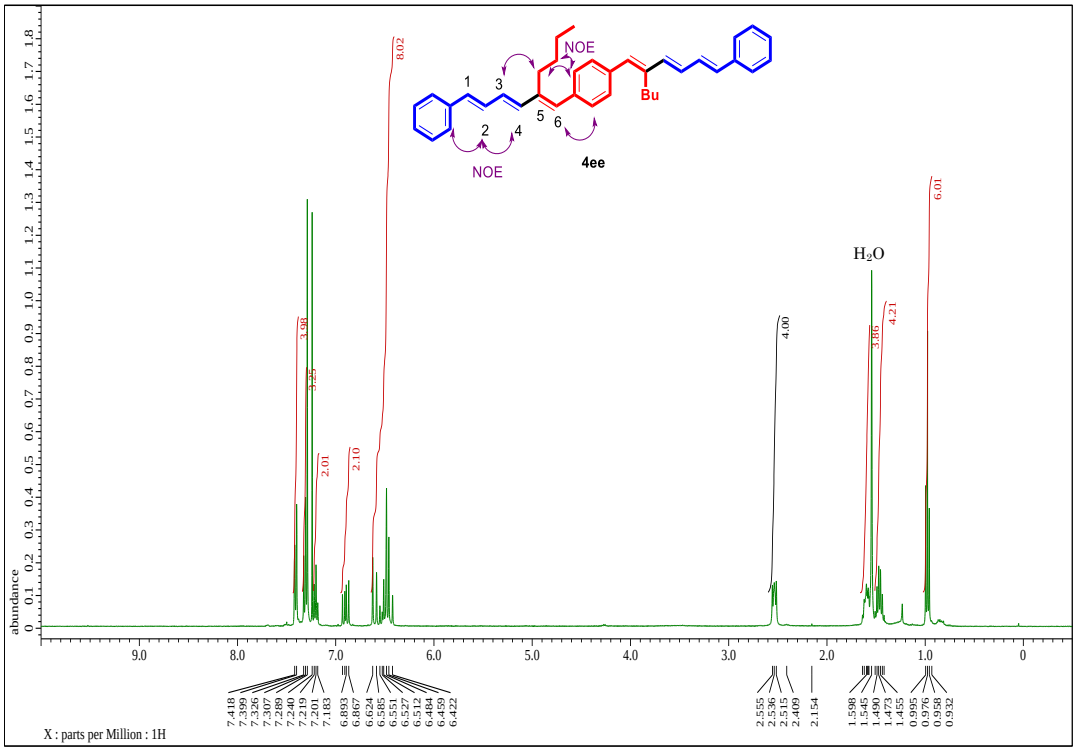


Figure S42. ^{1}H NMR Spectrum of 4ee in $CDCl_3$.

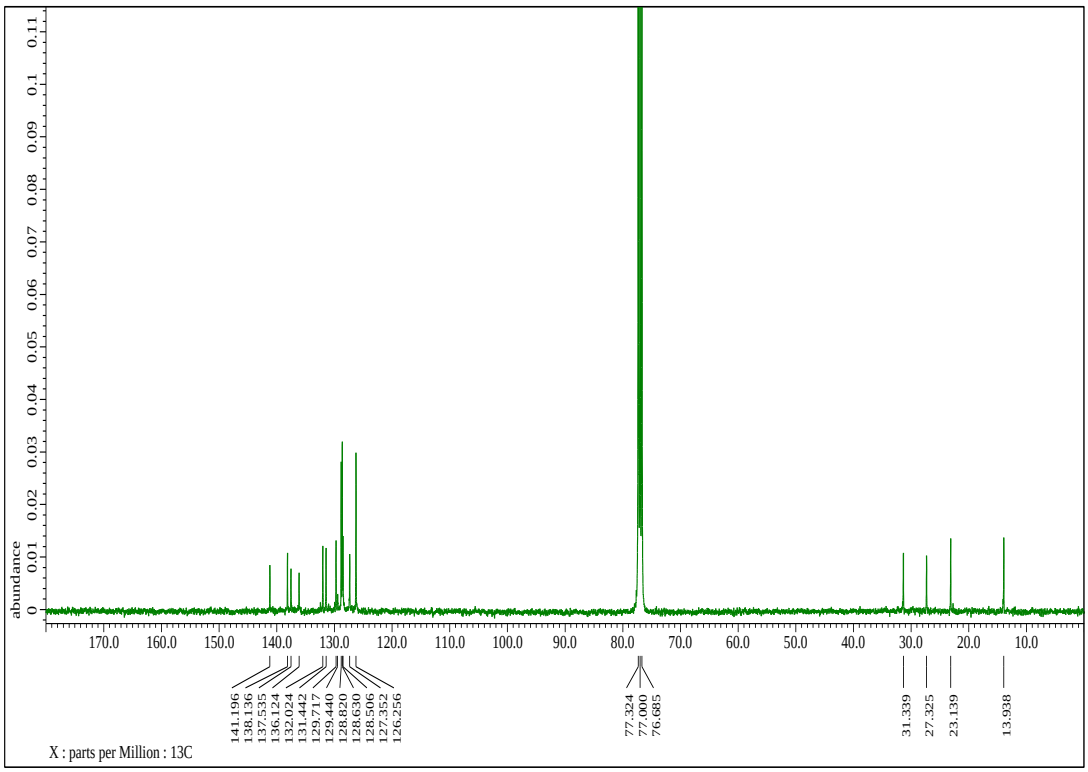


Figure S43. $^{13}C\{^{1}H\}$ NMR Spectrum of 4ee in $CDCl_3$.

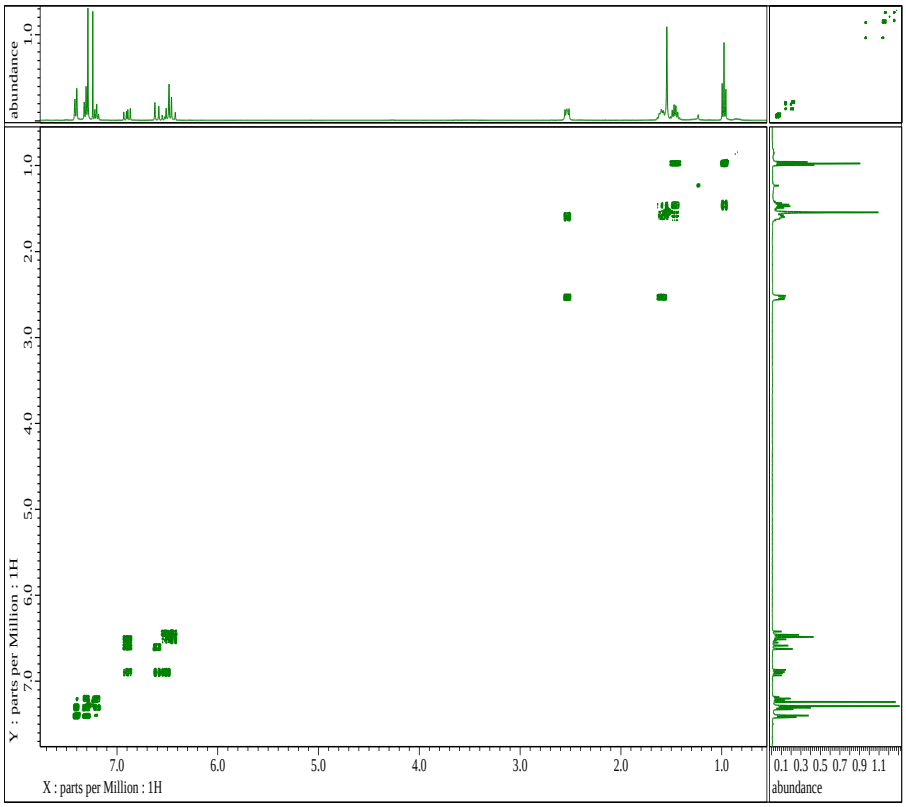


Figure S44. ^{1}H-^{1}H COSY NMR Spectrum of 4ee in $CDCl_3$.

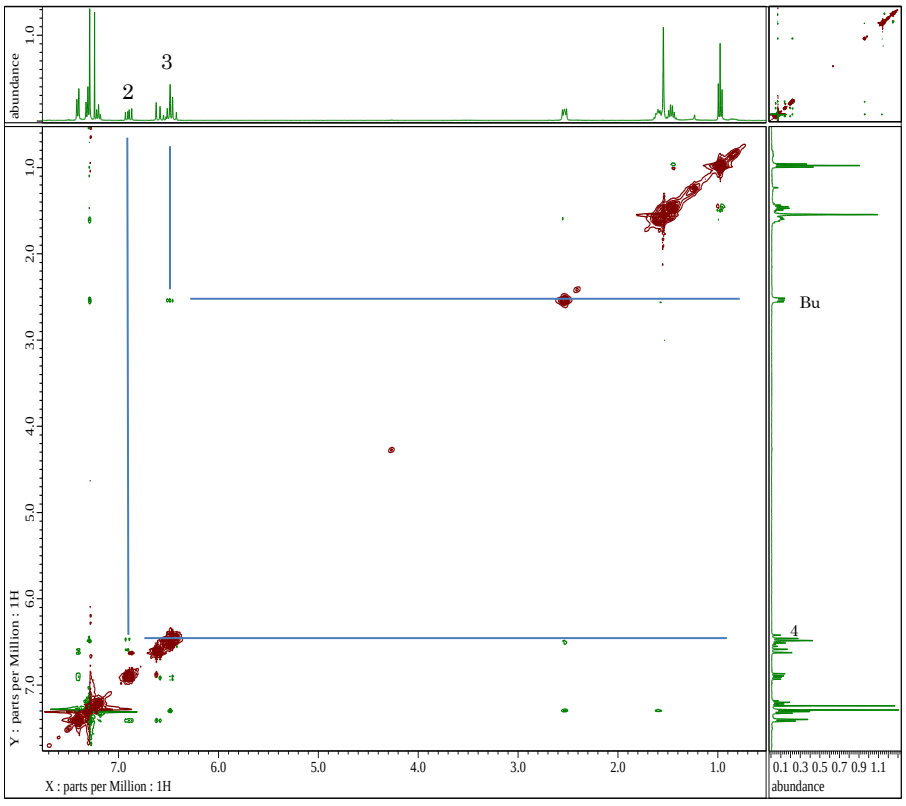
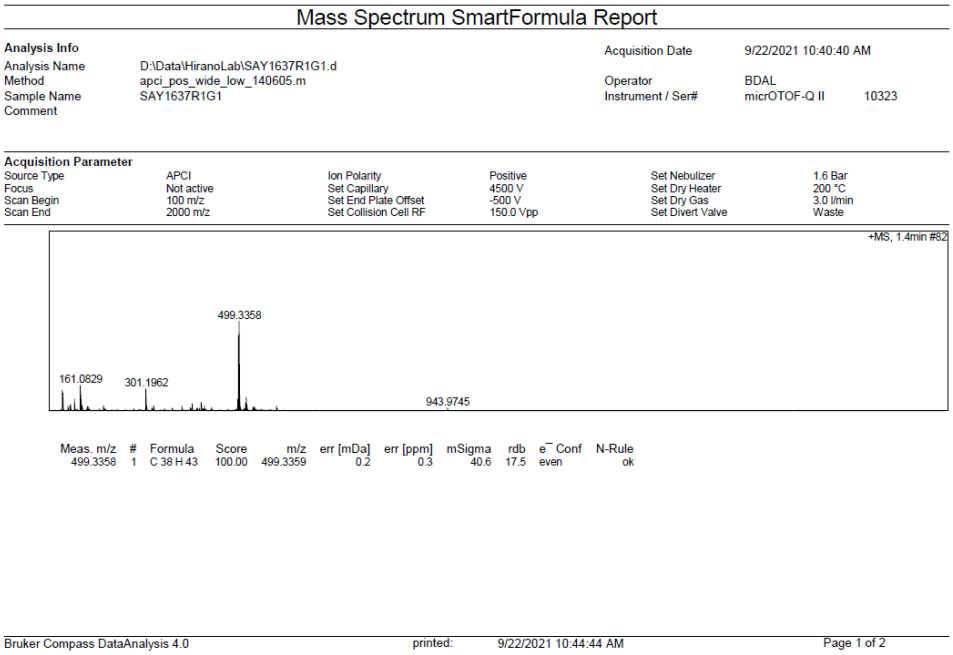


Figure S45. ^{1}H-^{1}H NOESY NMR Spectrum of 4ee in $CDCl_3$.



Mass Spectrum SmartFormula Report

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Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.6 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	3.0 l/min
Scan End	2000 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Waste

Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
499.3358	1	C 38 H 43	100.00	499.3359	0.2	0.3	40.6	17.5	even	ok

Figure S46. HRMS (APCI) data for 4ee.

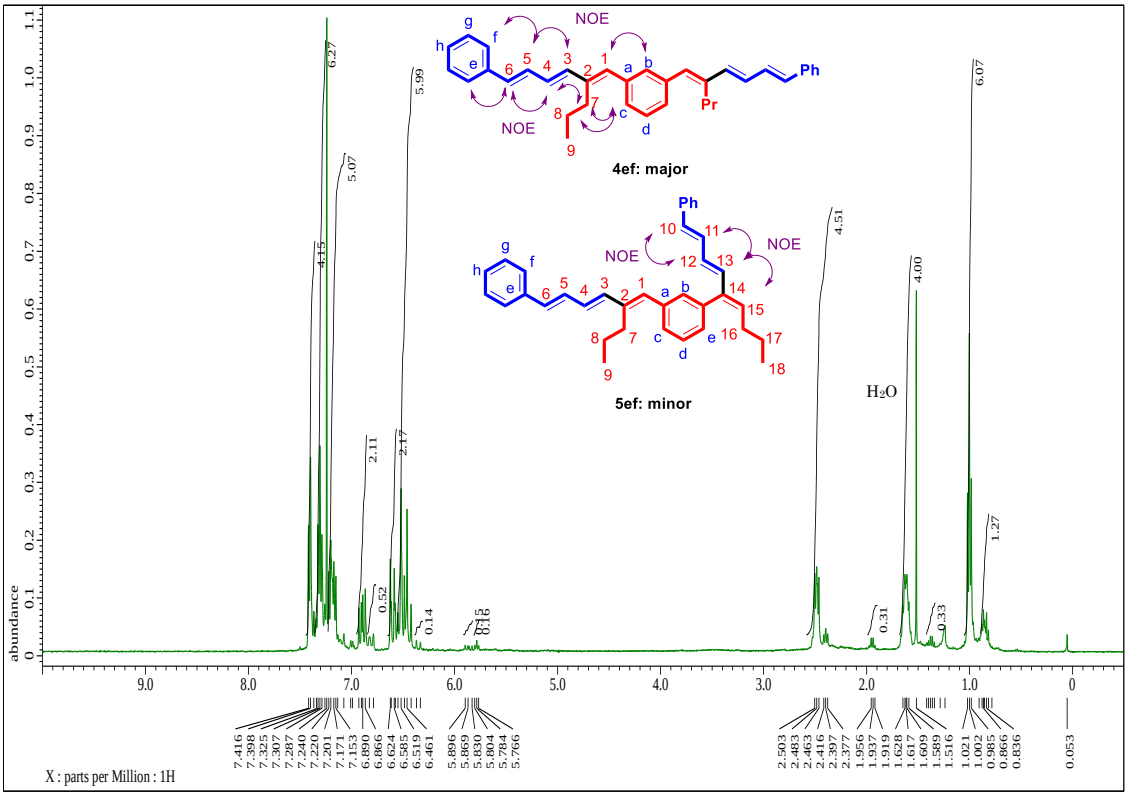


Figure S47. ^{1}H NMR Spectrum of 4ef and 5ef in $CDCl_3$.

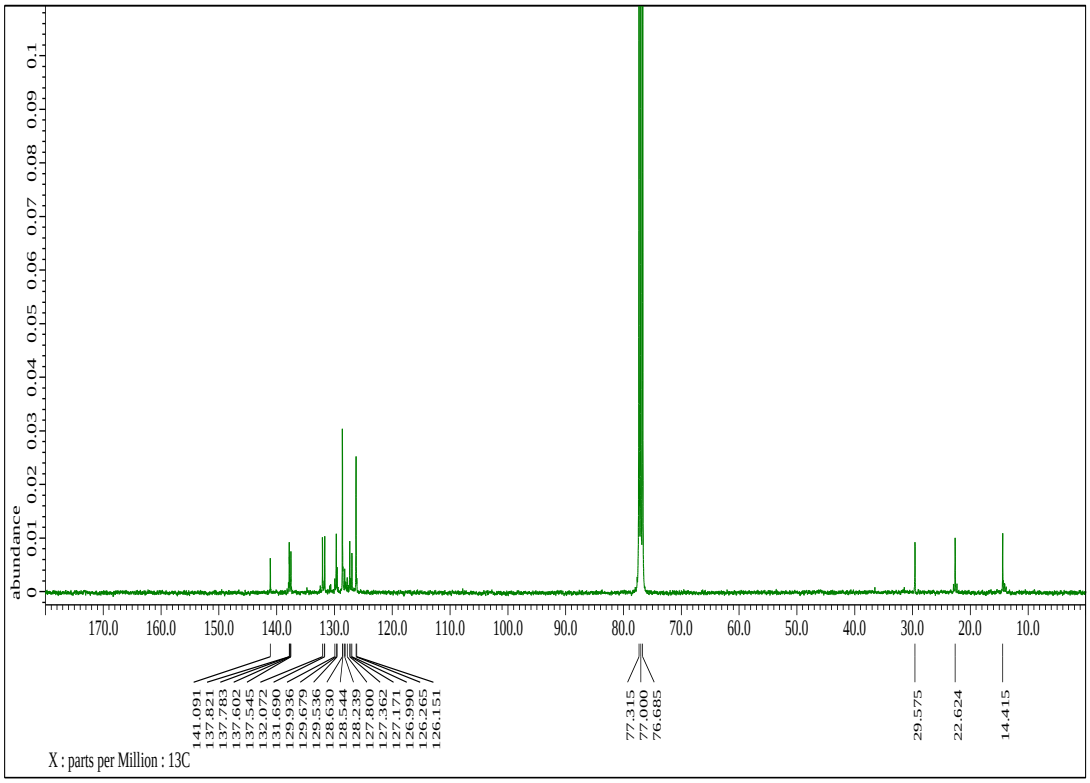


Figure S48. $^{13}C\{^{1}H\}$ NMR Spectrum of 4ef (included 5ef) in $CDCl_3$.

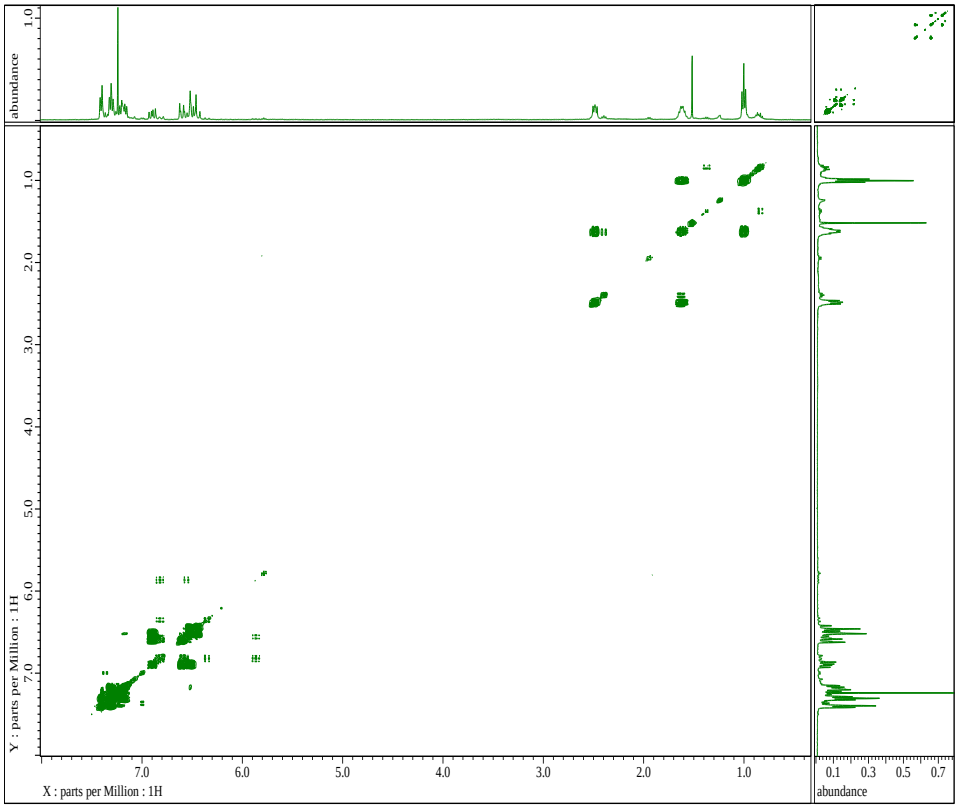


Figure S49. ^{1}H-^{1}H COSY NMR Spectrum of 4ef and 5ef in $CDCl_3$.

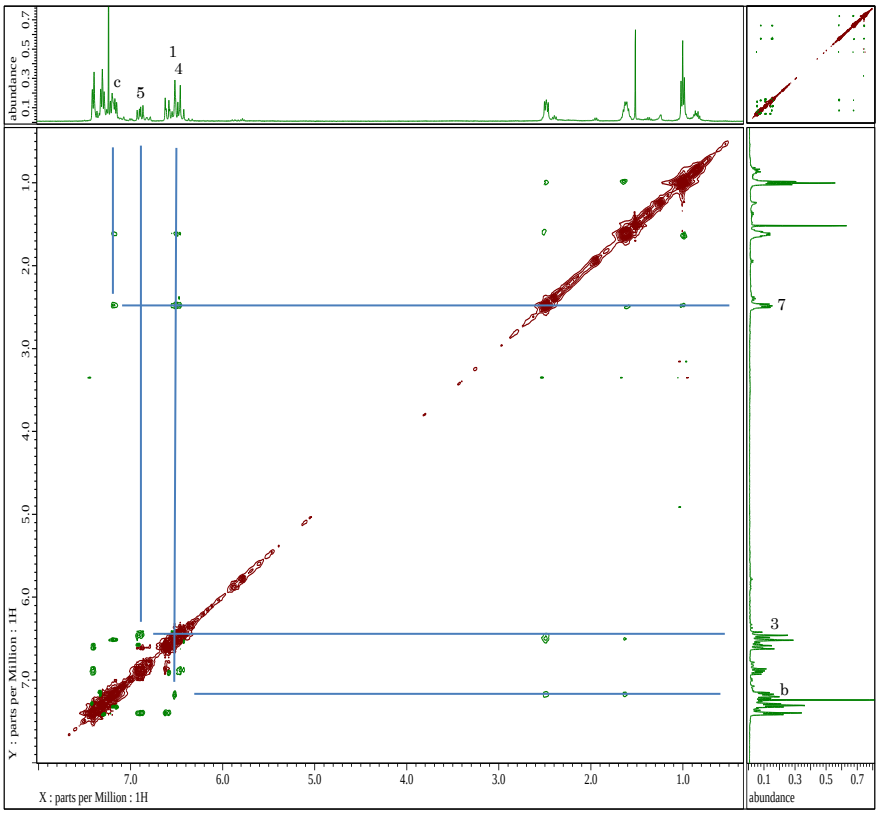


Figure S50. ^{1}H-^{1}H NOESY NMR Spectrum of 4ef and 5ef in $CDCl_3$.

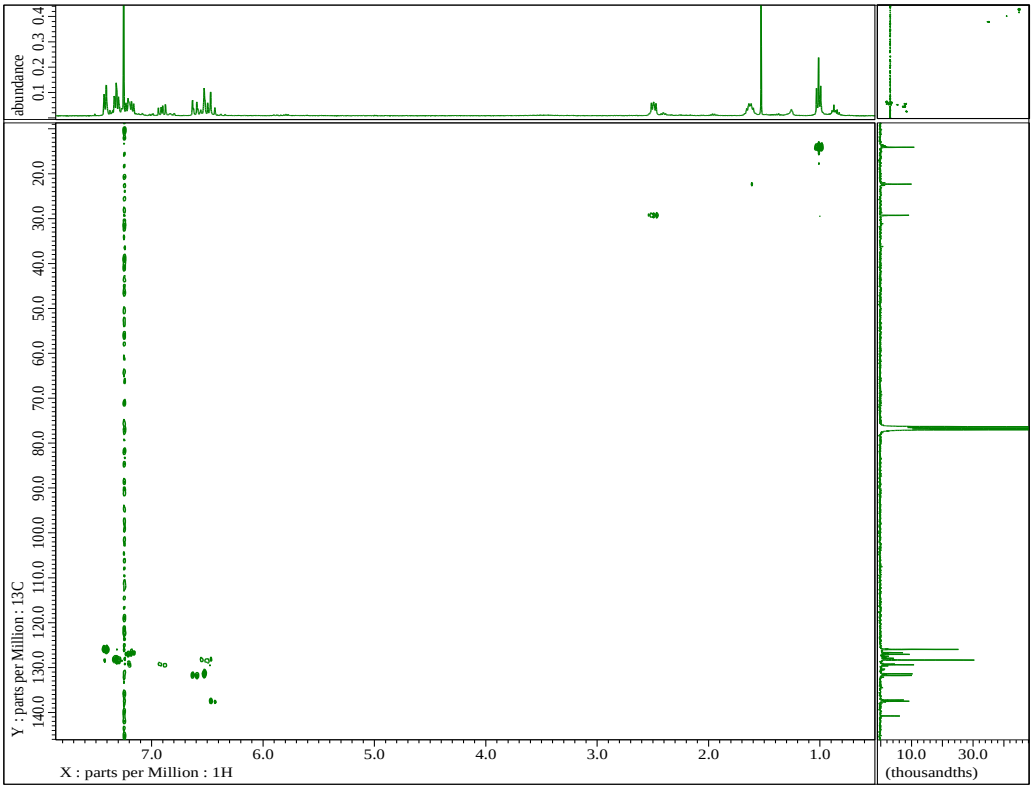


Figure S51. ^{13}C-^{1}H Correlation Spectrum of 4gf (included 5gf) in $CDCl_3$.

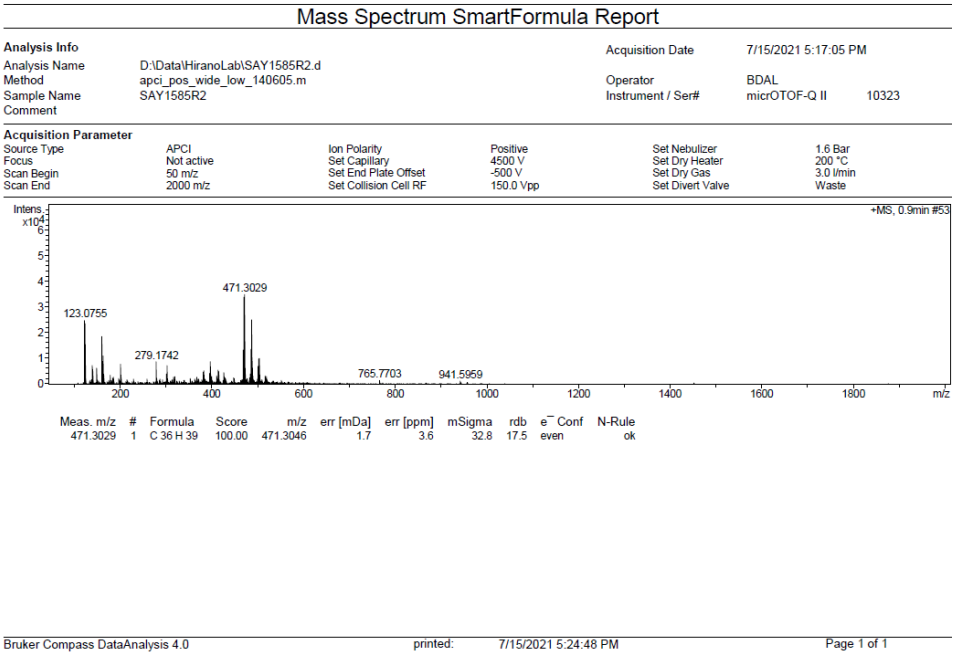


Figure S52. HRMS (APCI) data for 4ef and 5ef.

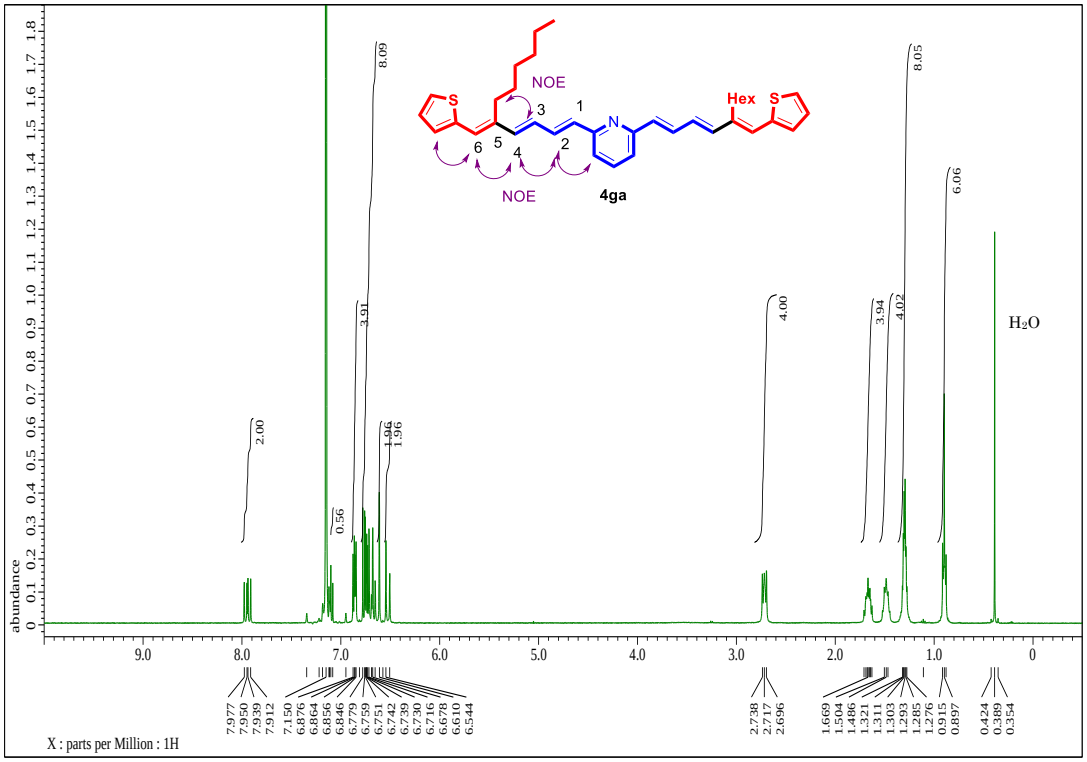


Figure S53. ^{1}H NMR Spectrum of 4ga in C_6D_6.

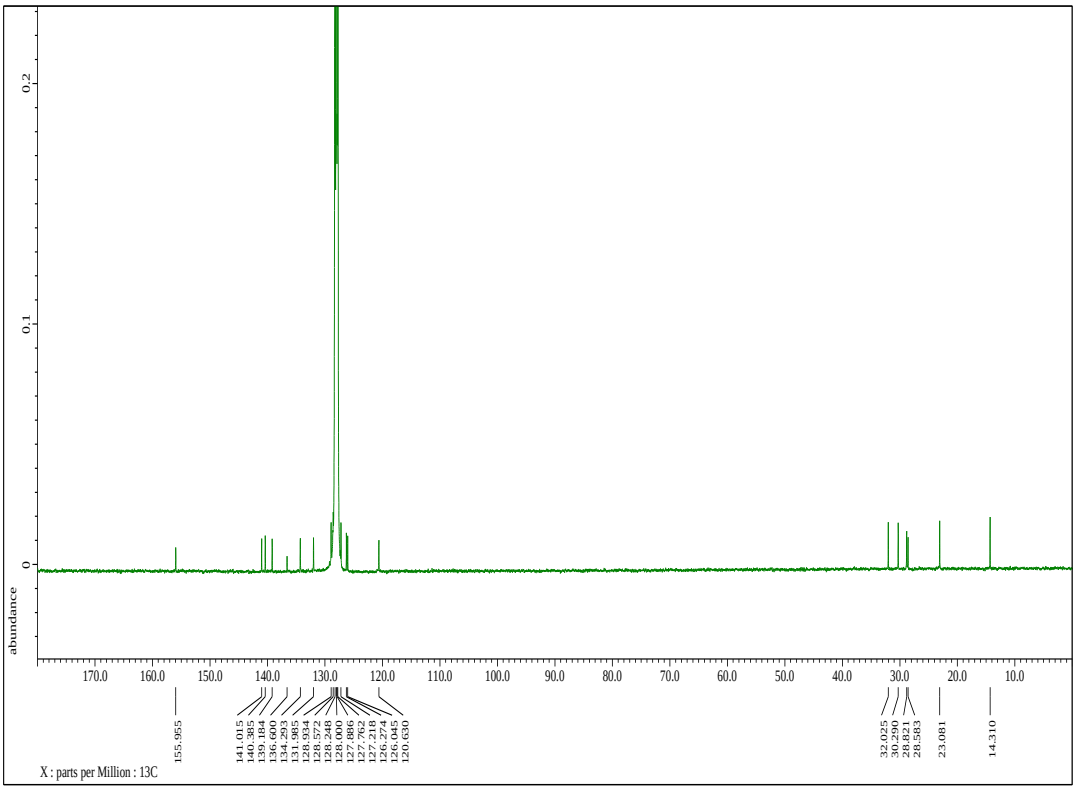


Figure S54. $^{13}C\{^{1}H\}$ NMR Spectrum of 4ga in C_6D_6.

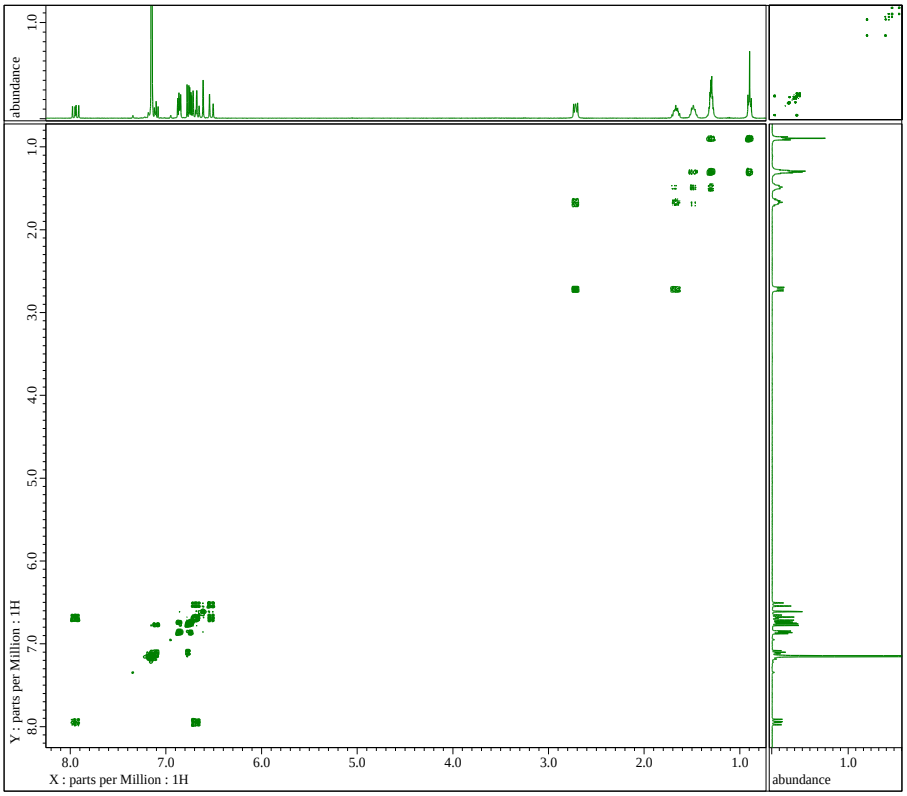


Figure S55. ^{1}H-^{1}H COSY NMR Spectrum of 4ga in C_6D_6.

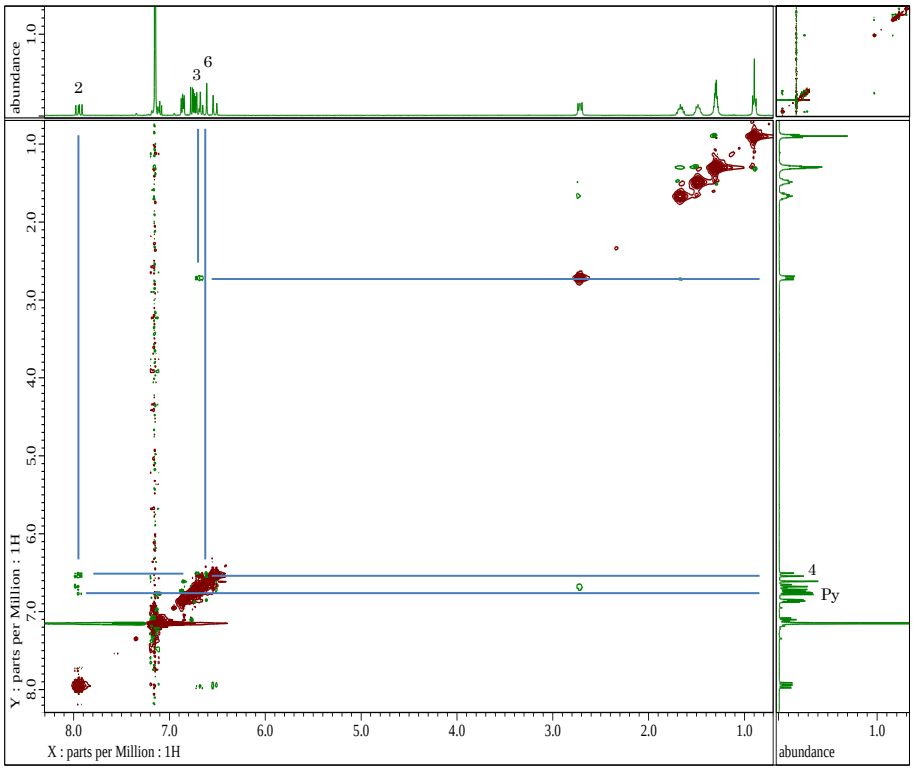


Figure S56. ^{1}H-^{1}H pNOESY NMR Spectrum of 4ga in C_6D_6.

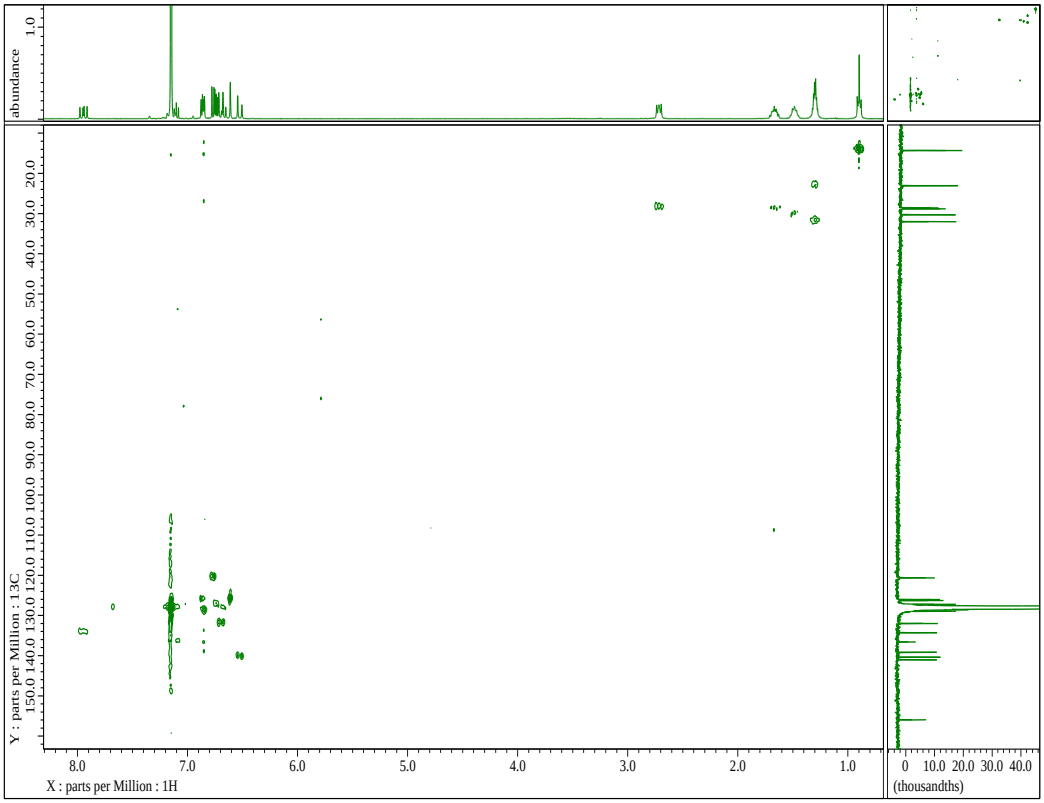


Figure S57. ^{13}C-^{1}H Correlation Spectrum of 4ga in C_6D_6.

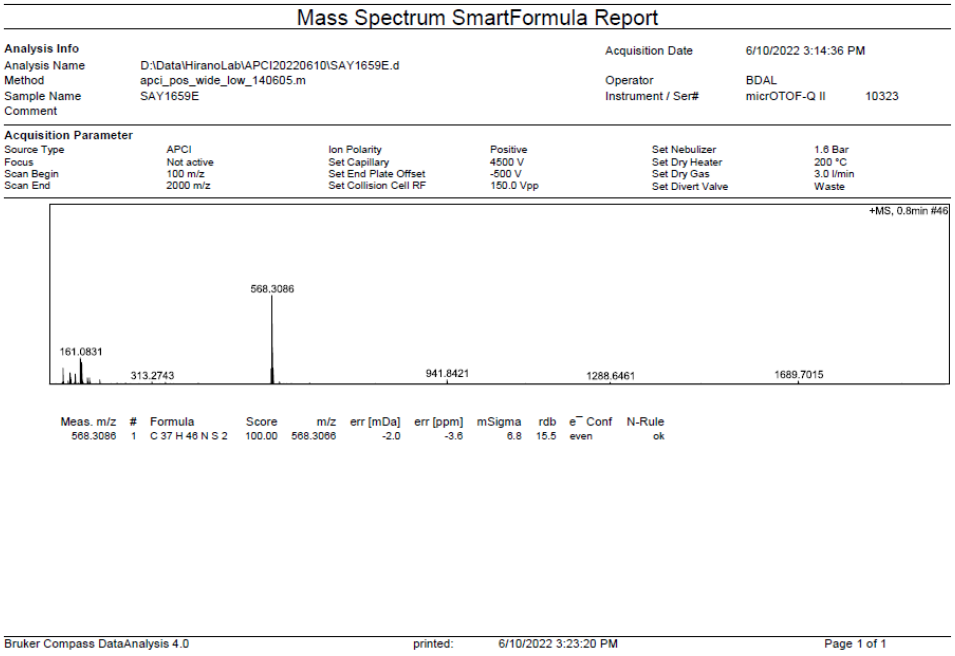


Figure S58. HRMS (APCI) data for 4ga.

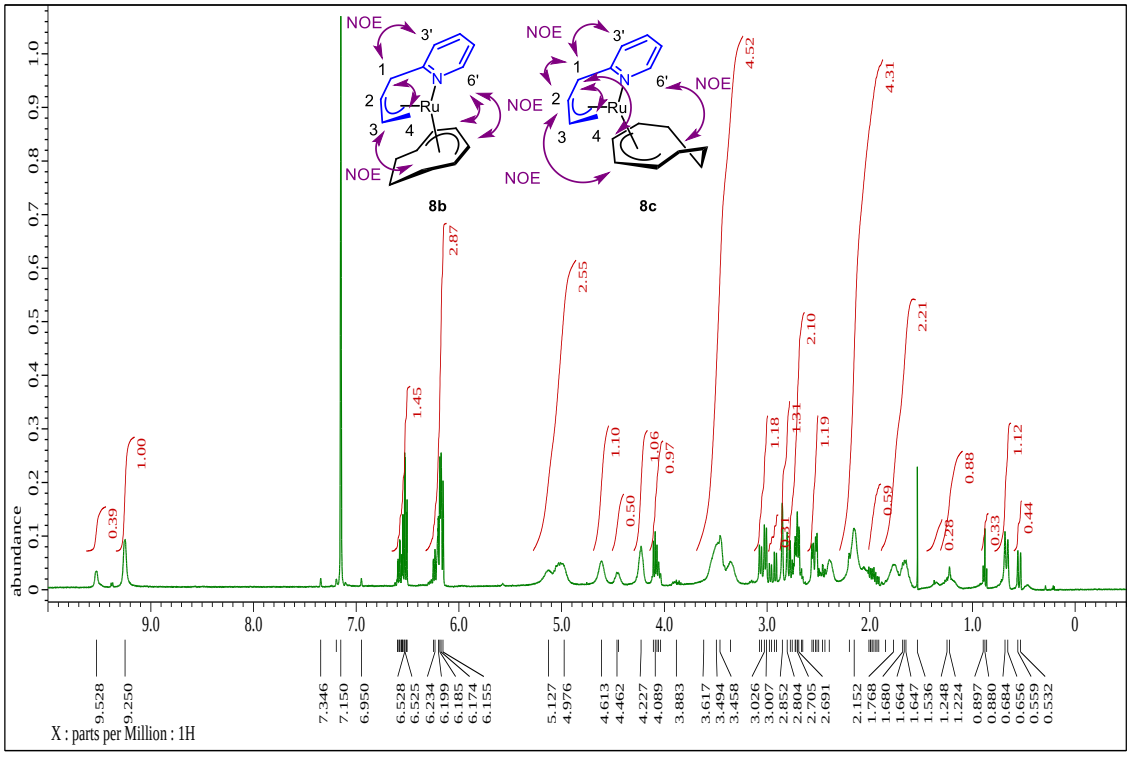


Figure S59. ^{1}H NMR Spectrum of 8b and 8c in C_6D_6.

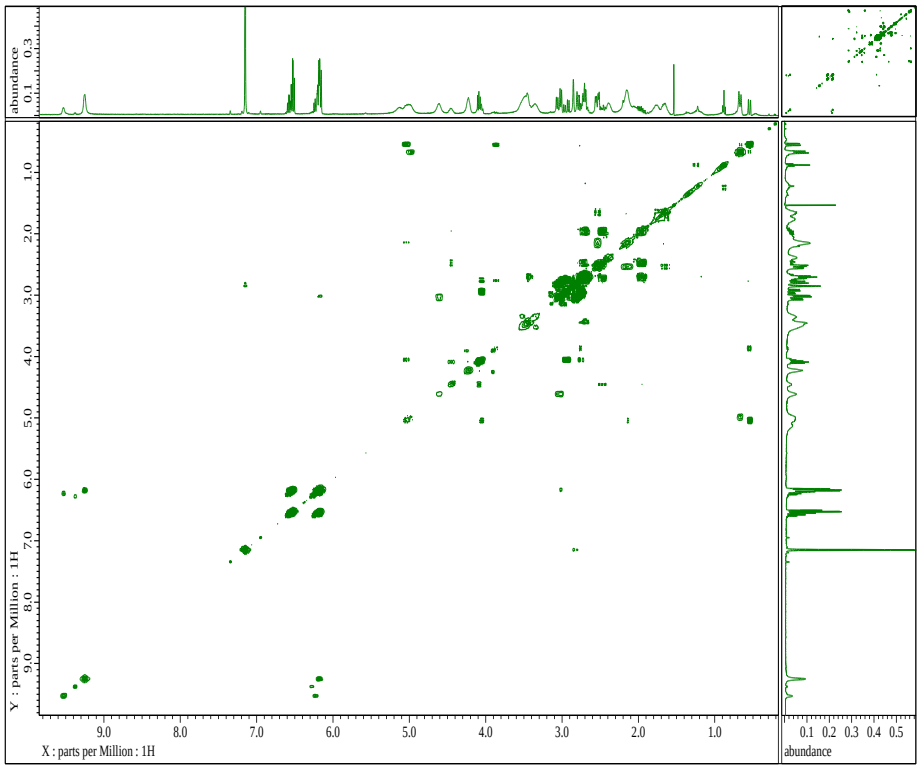


Figure S60. ^{1}H-^{1}H COSY NMR Spectrum of 8b and 8c in C_6D_6.

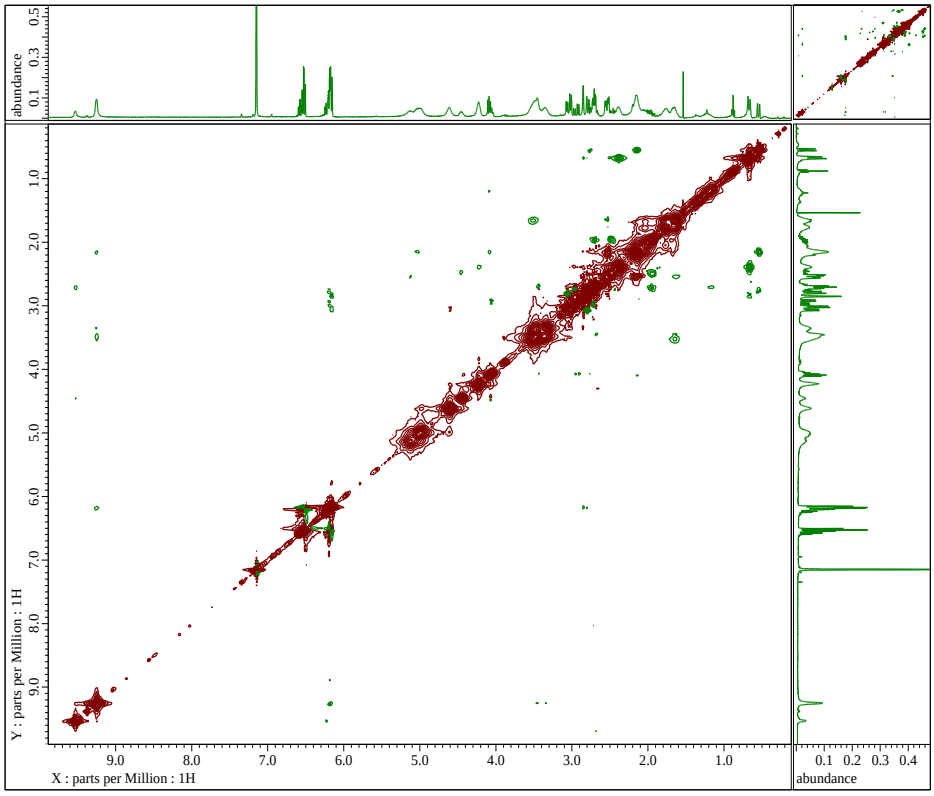


Figure S61. ^{1}H-^{1}H NOESY NMR Spectrum of 8b and 8c in C_6D_6.

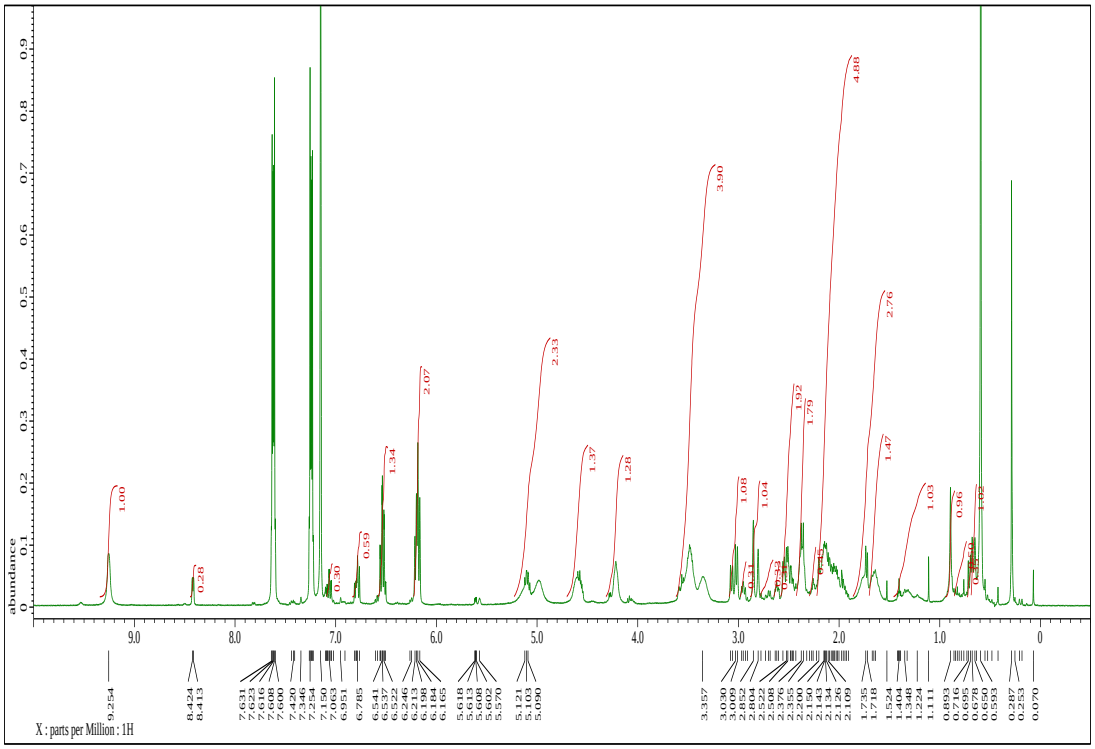


Figure S62. ^{1}H NMR Spectrum of Stoichiometric Reaction (7 and 8b in C_6D_6).

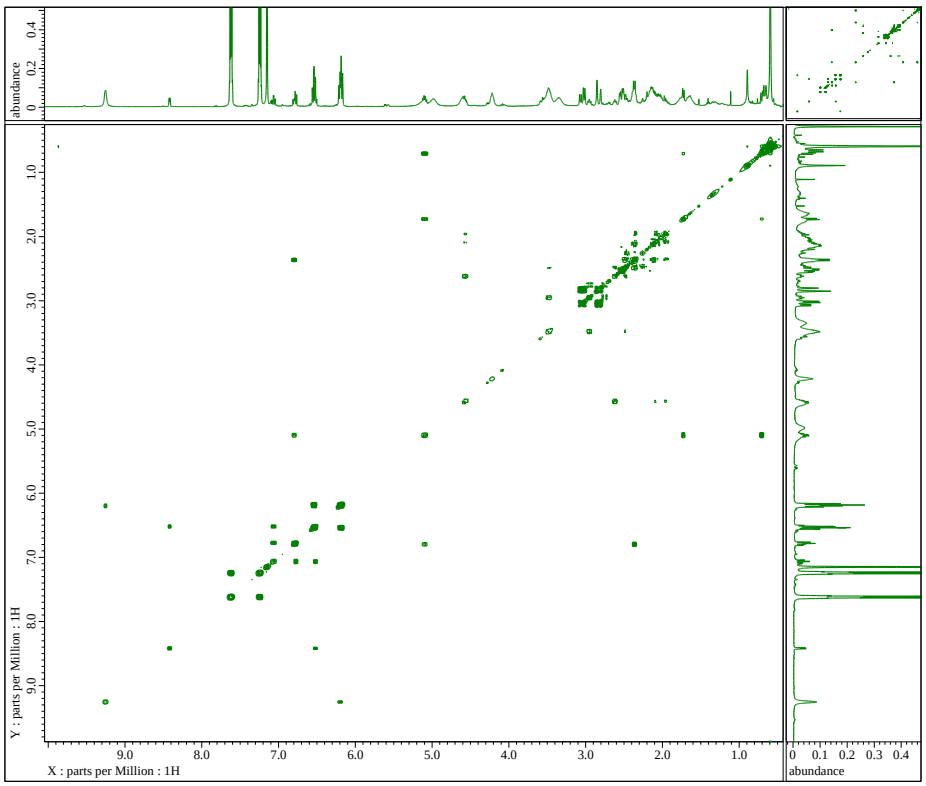


Figure S63. ^{1}H-^{1}H COSY NMR Spectrum of Stoichiometric Reaction (7 and 8b in C_6D_6).

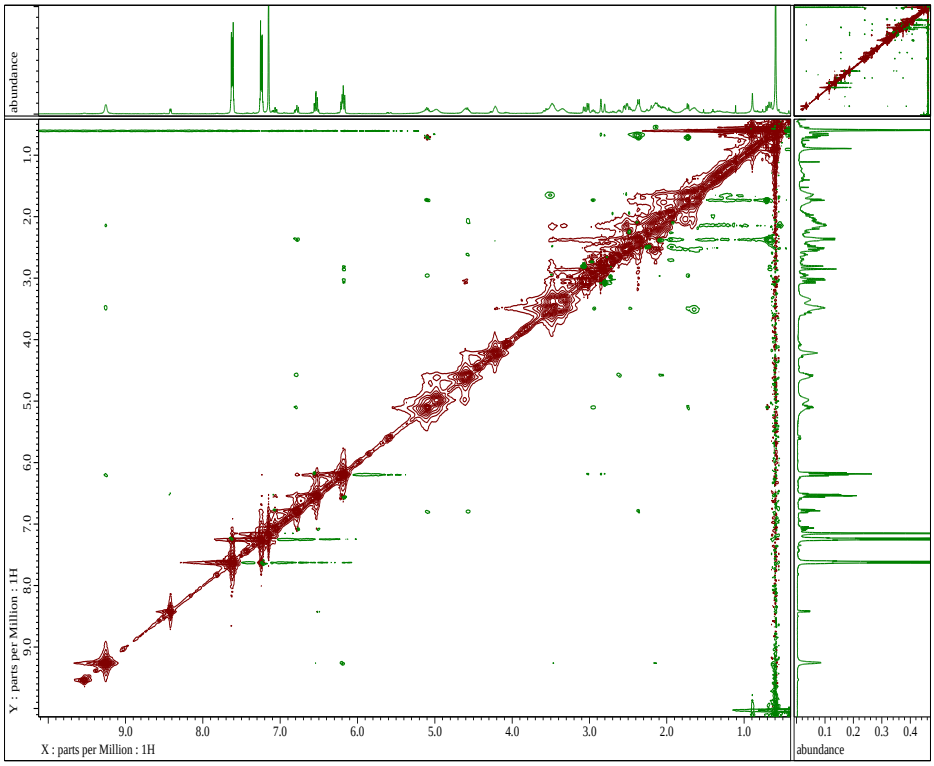


Figure S64. ^{1}H-^{1}H NOESY NMR Spectrum of Stoichiometric Reaction (7 and 8b in C_6D_6).

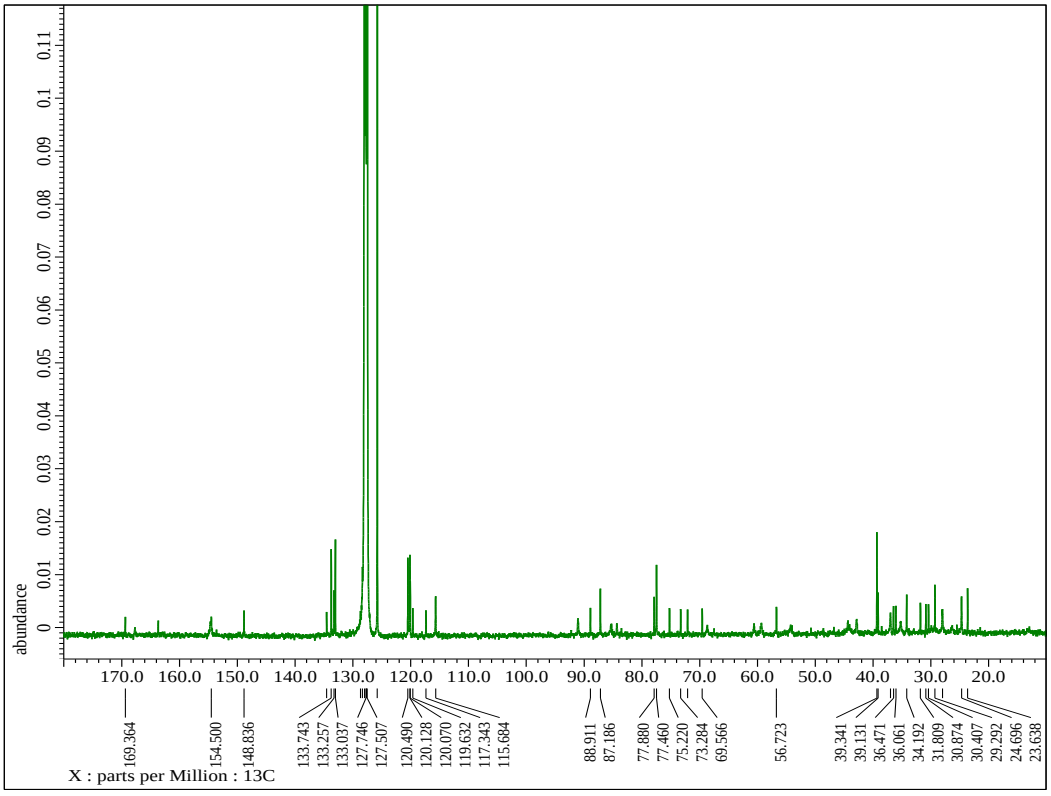


Figure S65. ^{13}C{^{1}H} NMR Spectrum of Stoichiometric Reaction (7, 8b and 8c in C_6D_6).

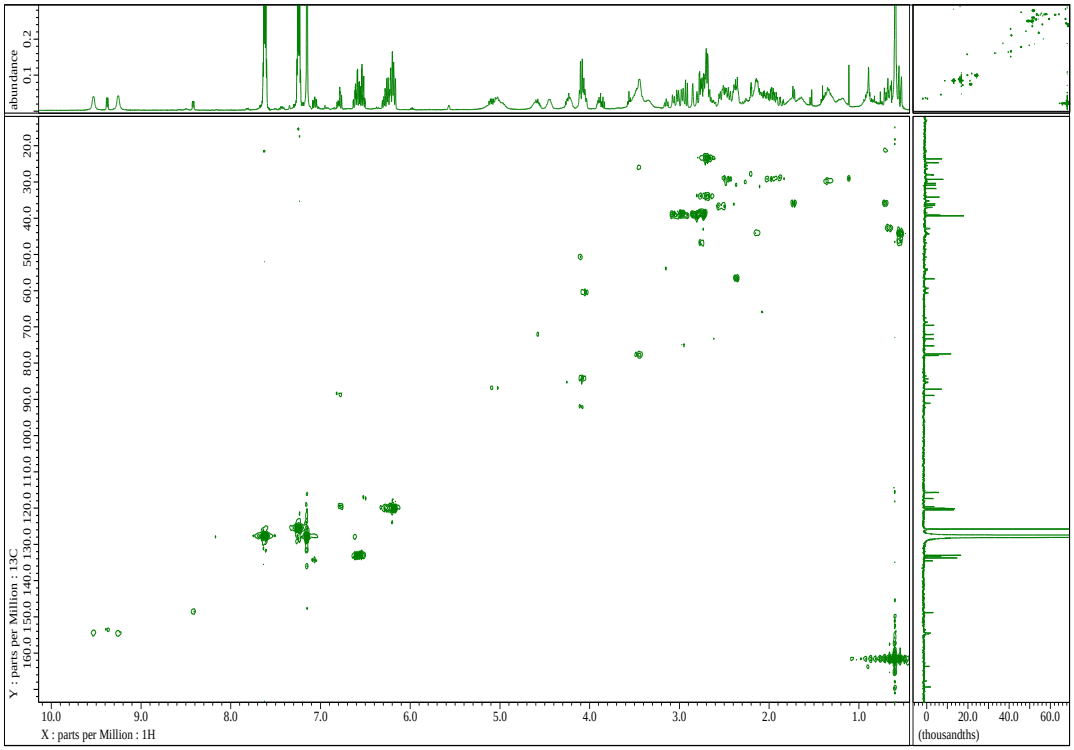


Figure S66. ^{13}C-^{1}H Correlation Spectrum of Stoichiometric Reaction (7, 8b and 8c in C_6D_6).

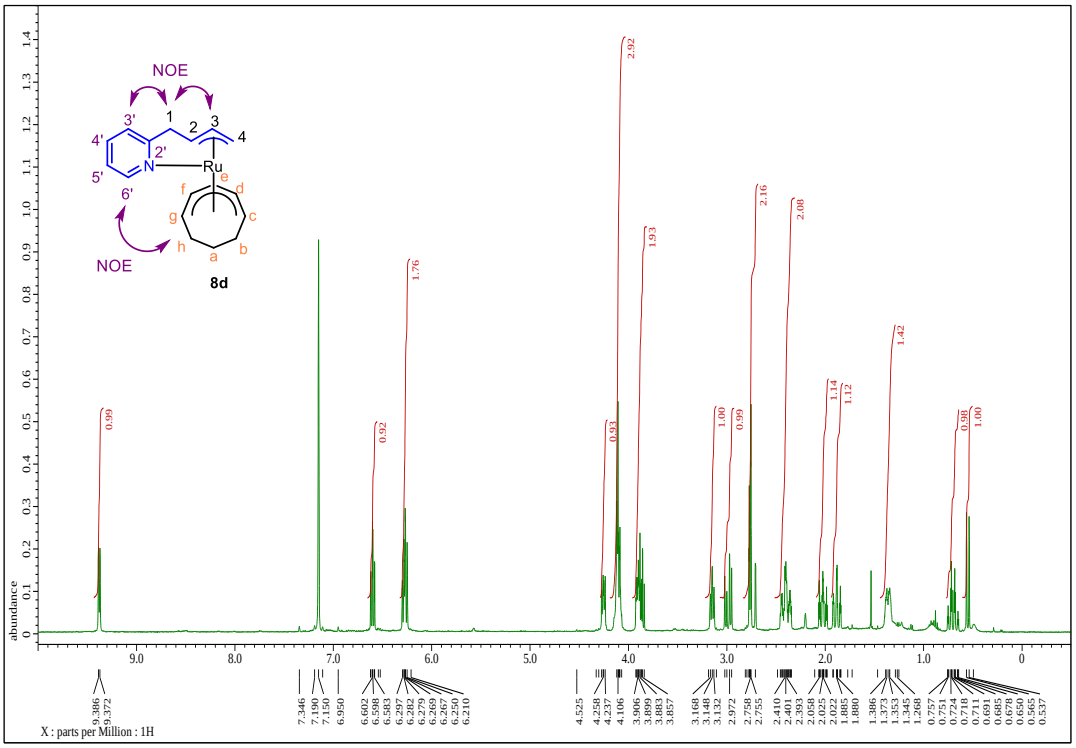


Figure S67. ^{1}H NMR Spectrum of 8d in C_6D_6.

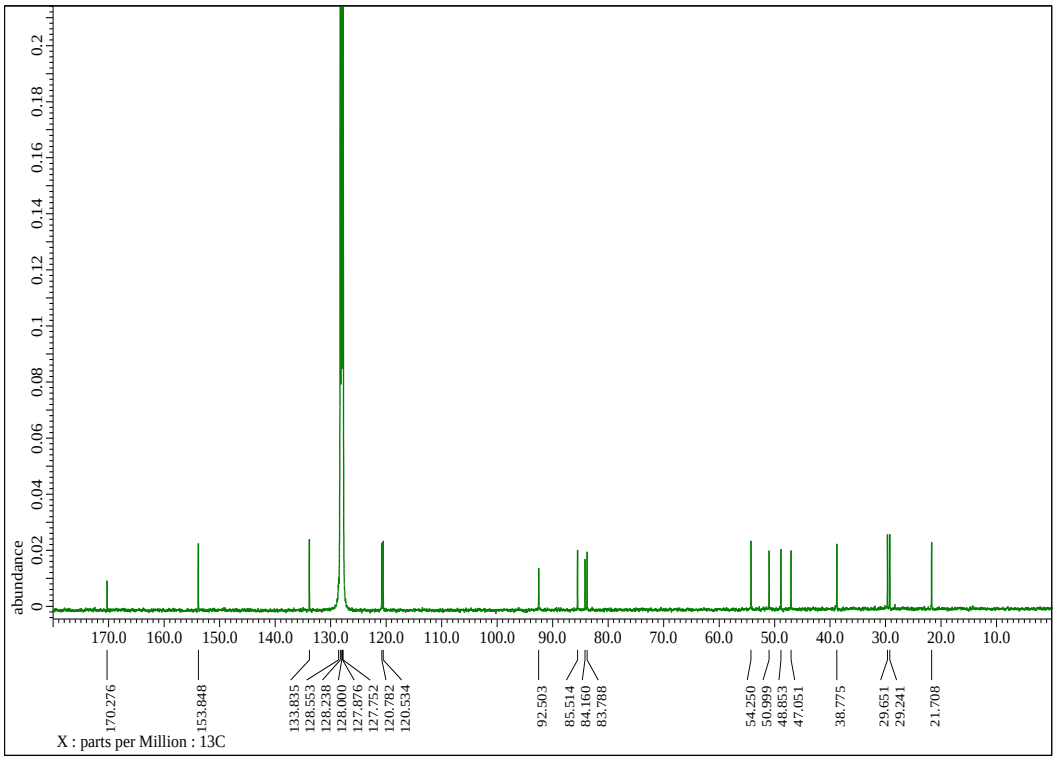


Figure S68. $^{13}C\{^{1}H\}$ NMR Spectrum of 8d in C_6D_6.

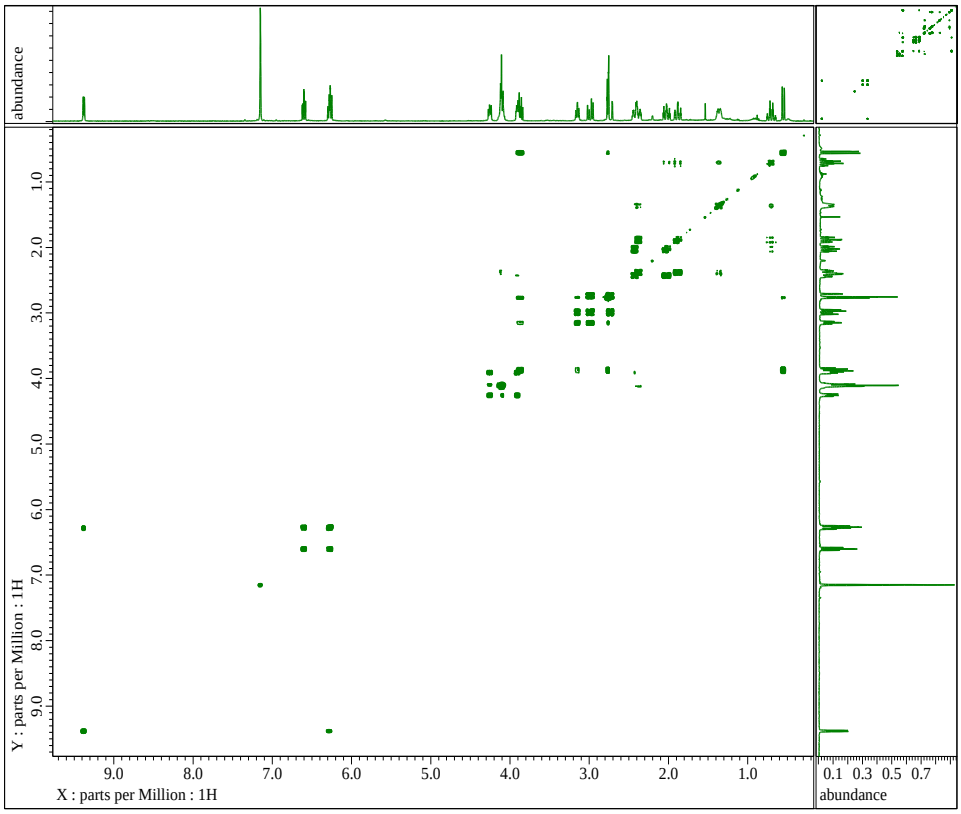


Figure S69. ^{1}H-^{1}H COSY NMR Spectrum of 8d in C_6D_6.

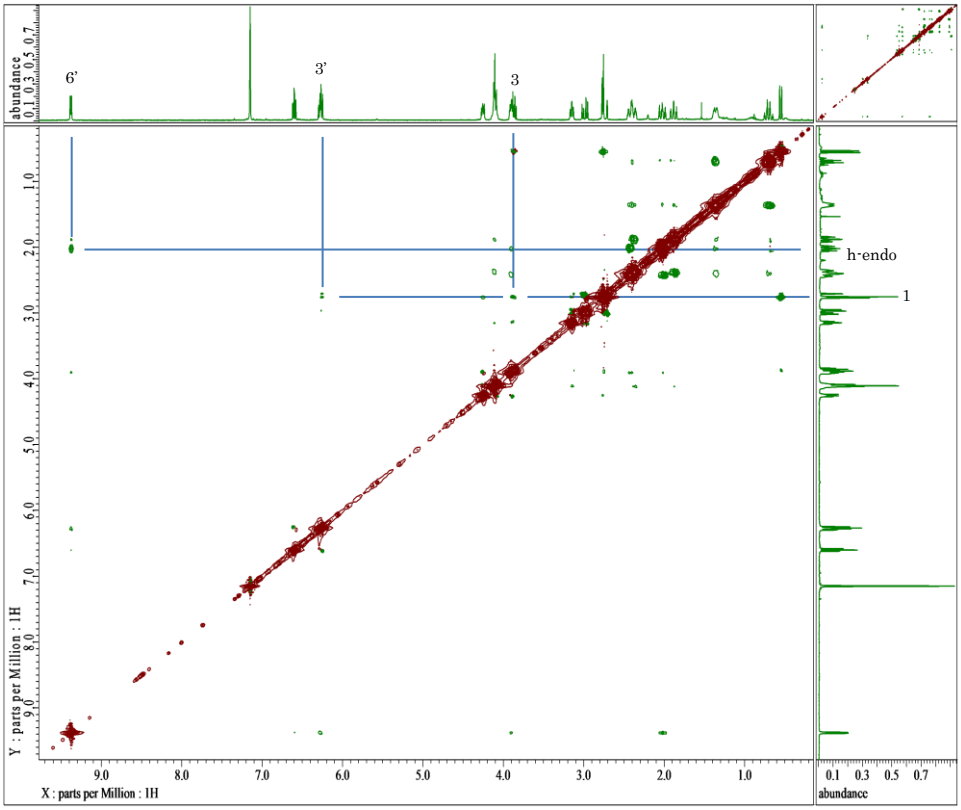


Figure S70. ^{1}H-^{1}H pNOESY NMR Spectrum of 8d in C_6D_6.

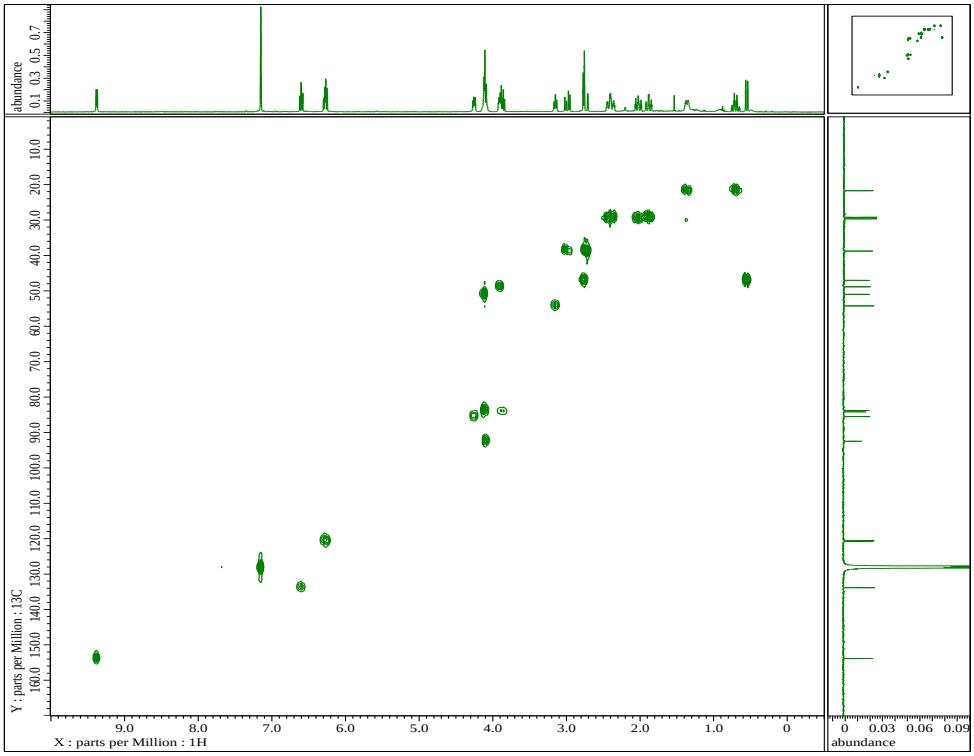


Figure S71. ^{13}C-^{1}H Correlation Spectrum of 8d in C_6D_6.

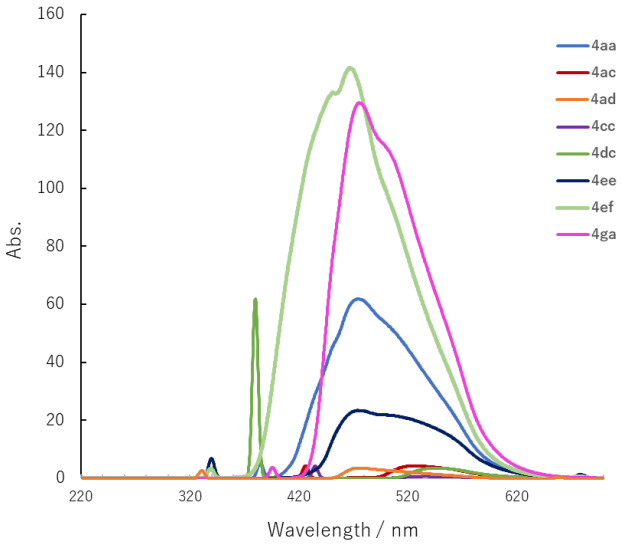


Figure S72. Fluorescence emission (0.1 mM) spectra of compounds 4 in MeCN at r.t.. Since excitation spectra were not observed, fluorescence emission spectra measured at the excitation wavelength that fluorescence intensity was maximized. Excitation wavelength: 4aa (384.5 nm), 4ac (426.5 nm), 4ad (330 nm), 4cc (435 nm), 4dc (380 nm), 4ee (340 nm), 4ef (339 nm), 4ga (395.5 nm).

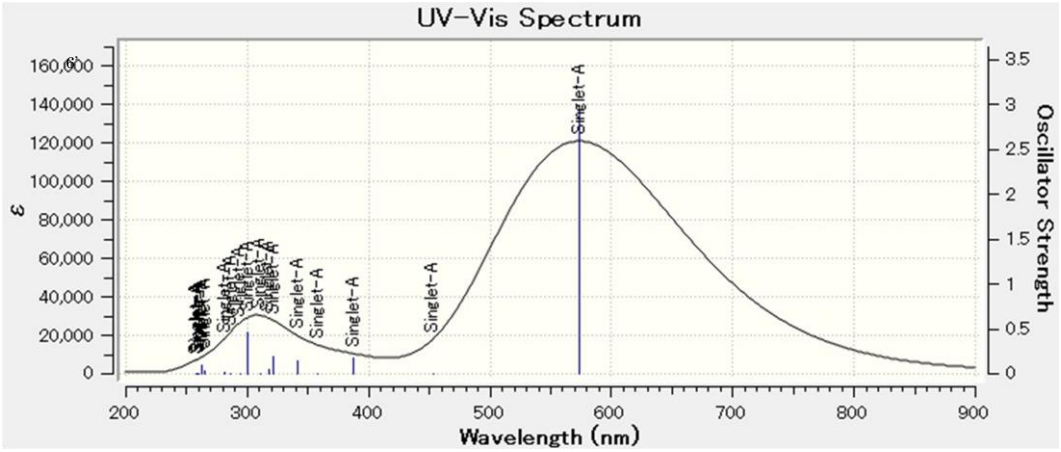


Figure S73. Calculated UV-Vis spectrum of isomer A of 4ac in acetonitrile by TD-DFT.

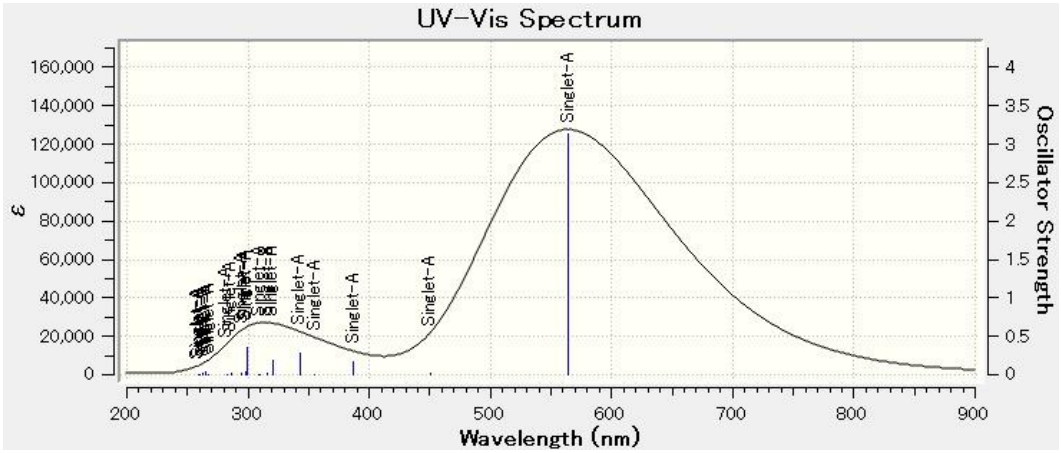


Figure S74. Calculated UV-Vis spectrum of isomer B of 4ac in acetonitrile by TD-DFT.

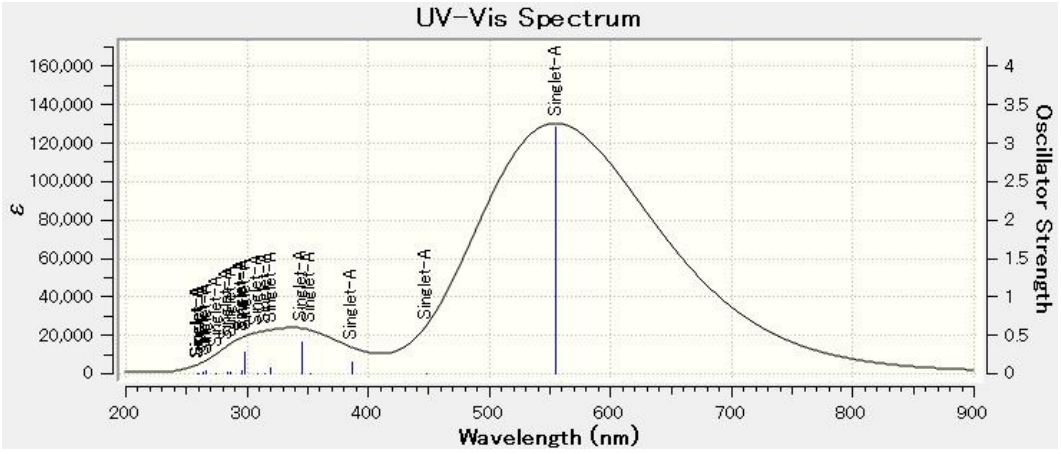


Figure S75. Calculated UV-Vis spectrum of isomer C of 4ac in acetonitrile by TD-DFT.

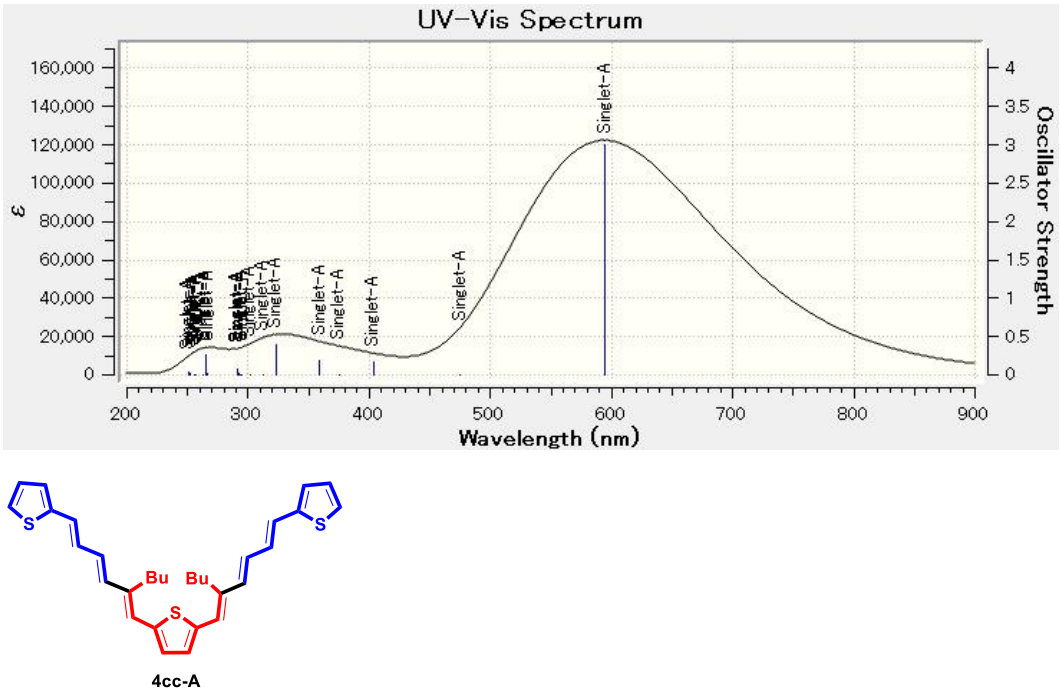


Figure S76. Calculated UV-Vis spectrum of 4cc-A in acetonitrile by TD-DFT.

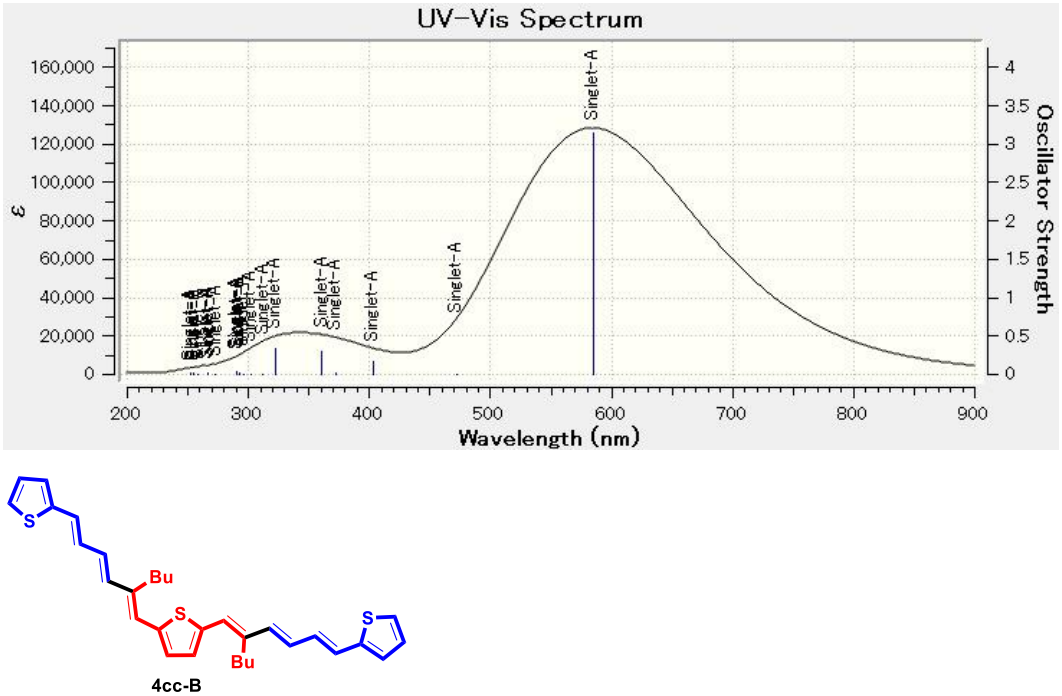


Figure S77. Calculated UV-Vis spectrum of 4cc-B in acetonitrile by TD-DFT.

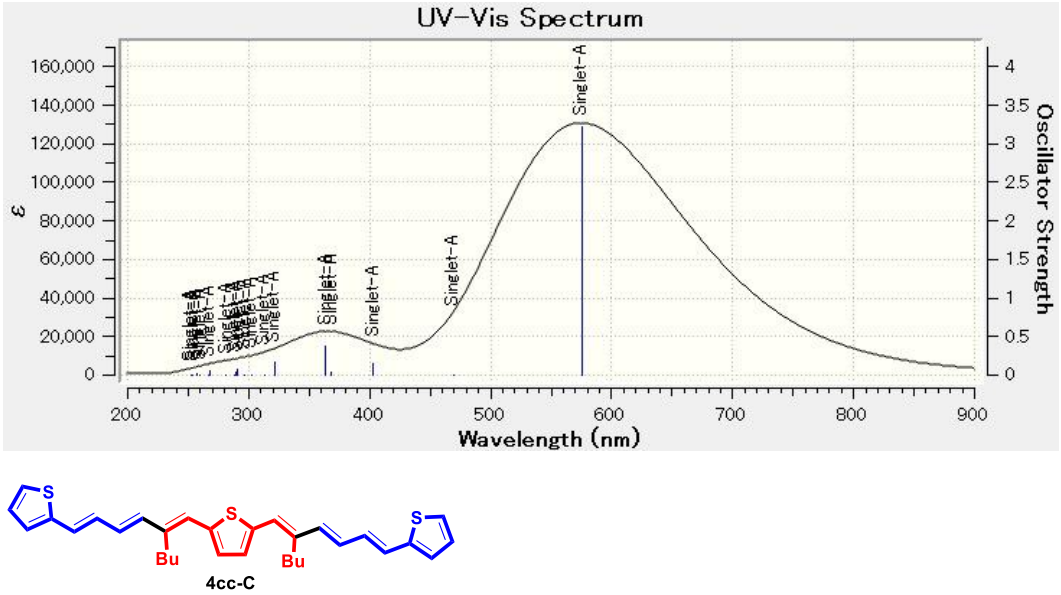


Figure S78. Calculated UV-Vis spectrum of 4cc-C in acetonitrile by TD-DFT.

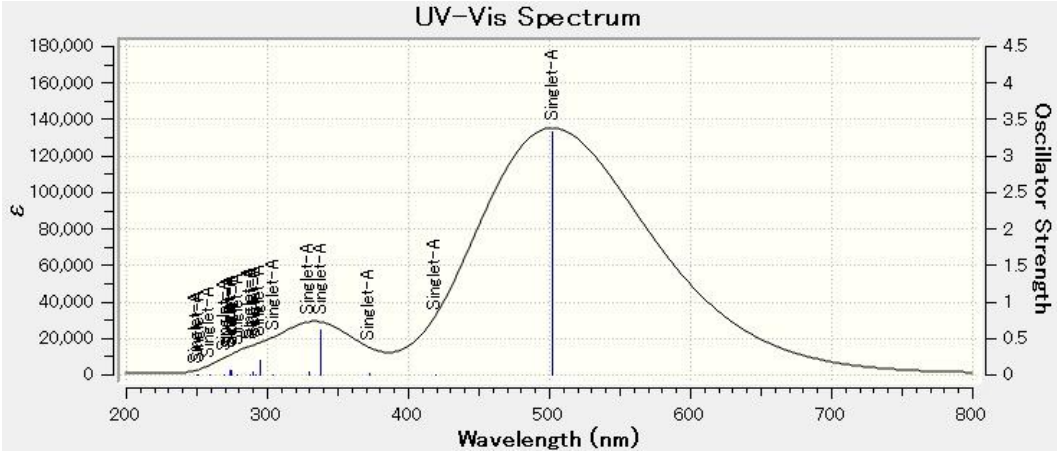


Figure S79. Calculated UV-Vis spectrum of 4ee in acetonitrile by TD-DFT.

Table S1. TD-DFT results for 4ac (isomer A) in acetonitrile

Excited State 1: Singlet-A 2.1607 eV 573.81 nm f=2.9724 <S**2>=0.000
136 ->137 0.70749
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -1826.05223894
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 2.7373 eV 452.94 nm f=0.0004 <S**2>=0.000
135 ->137 -0.47037
136 ->138 0.52008

Excited State 3: Singlet-A 3.1970 eV 387.82 nm f=0.1745 <S**2>=0.000
135 ->137 0.52151
136 ->138 0.47139

Excited State 4: Singlet-A 3.4585 eV 358.49 nm f=0.0002 <S**2>=0.000
134 ->137 -0.42764
136 ->139 0.55379

Excited State 5: Singlet-A 3.6297 eV 341.58 nm f=0.1510 <S**2>=0.000
134 ->137 0.31677
135 ->138 0.56943
136 ->139 0.26579

Excited State 6: Singlet-A 3.8568 eV 321.47 nm f=0.1887 <S**2>=0.000
134 ->137 -0.33867
135 ->138 0.31718
135 ->140 -0.11994
136 ->139 -0.27486
136 ->141 0.42827

Excited State 7: Singlet-A 3.9073 eV 317.31 nm f=0.0464 <S**2>=0.000
131 ->137 -0.13918
135 ->141 -0.10222
136 ->140 0.67143

Table S1. continued.

Excited State 8:	Singlet-A	3.9967 eV	310.22 nm	f=0.0001	<S**2>=0.000
132 ->137	0.13606				
132 ->138	0.26681				
133 ->137	0.61570				
133 ->139	-0.12385				
Excited State 9:	Singlet-A	3.9968 eV	310.21 nm	f=0.0012	<S**2>=0.000
132 ->137	0.62022				
132 ->139	-0.12500				
133 ->137	-0.13479				
133 ->138	0.26452				
Excited State 10:	Singlet-A	4.1245 eV	300.60 nm	f=0.4571	<S**2>=0.000
134 ->137	0.30784				
135 ->138	-0.25608				
136 ->139	0.19057				
136 ->141	0.54357				
Excited State 11:	Singlet-A	4.1289 eV	300.29 nm	f=0.0322	<S**2>=0.000
131 ->137	0.61550				
136 ->140	0.11831				
136 ->142	-0.28692				
Excited State 12:	Singlet-A	4.2209 eV	293.74 nm	f=0.0019	<S**2>=0.000
130 ->137	0.58107				
134 ->138	-0.16012				
135 ->139	0.27875				
136 ->142	0.19982				
Excited State 13:	Singlet-A	4.3293 eV	286.39 nm	f=0.0002	<S**2>=0.000
130 ->137	-0.24557				
134 ->138	-0.19135				
135 ->139	0.56932				

Table S1. continued.

136 ->142	-0.23125				
Excited State 14:	Singlet-A	4.4058 eV	281.41 nm	f=0.0151	<S**2>=0.000
130 ->137	0.19631				
131 ->137	-0.12558				
134 ->138	0.57951				
135 ->139	0.14953				
136 ->142	-0.25684				
Excited State 15:	Singlet-A	4.6792 eV	264.97 nm	f=0.0312	<S**2>=0.000
127 ->137	-0.13786				
128 ->138	-0.10369				
129 ->137	-0.22043				
134 ->141	0.11005				
135 ->140	0.59625				
136 ->141	0.11799				
Excited State 16:	Singlet-A	4.7147 eV	262.97 nm	f=0.0958	<S**2>=0.000
128 ->137	0.24415				
130 ->137	0.12588				
131 ->137	-0.16402				
134 ->138	-0.11935				
134 ->140	0.11734				
135 ->141	0.41971				
136 ->142	-0.39336				
Excited State 17:	Singlet-A	4.7625 eV	260.33 nm	f=0.0047	<S**2>=0.000
127 ->137	-0.12898				
129 ->137	0.58201				
135 ->140	0.23545				
135 ->142	0.13970				
136 ->143	0.15898				
136 ->144	-0.15049				
Excited State 18:	Singlet-A	4.7866 eV	259.02 nm	f=0.0015	<S**2>=0.000

Table S1. continued.

132 ->137 -0.29239
132 ->138 0.15202
132 ->139 -0.23710
133 ->138 0.54098
133 ->140 -0.11928

Excited State 19: Singlet-A 4.7866 eV 259.02 nm f=0.0002 <S**2>=0.000
132 ->138 0.54497
132 ->140 -0.12041
133 ->137 -0.28972
133 ->138 -0.15067
133 ->139 -0.23515

Excited State 20: Singlet-A 4.8062 eV 257.97 nm f=0.0004 <S**2>=0.000
136 ->143 0.41903
136 ->144 0.55535

SavETr: write IOETrn= 770 NScale= 10 NData= 16 NLR=1 NState= 20 LETran= 370.

Table S2. TD-DFT results for 4ac (isomer B) in acetonitrile

Excited State 1: Singlet-A 2.1967 eV 564.42 nm f=3.1338
<S**2>=0.000
136 ->137 0.70719
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -1826.04969518
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 2.7533 eV 450.31 nm f=0.0106
<S**2>=0.000
135 ->137 0.45769
136 ->138 0.53114

Excited State 3: Singlet-A 3.2023 eV 387.17 nm f=0.1657
<S**2>=0.000
135 ->137 0.53328
136 ->138 -0.45904

Excited State 4: Singlet-A 3.4889 eV 355.37 nm f=0.0063
<S**2>=0.000
134 ->137 0.43643
136 ->139 0.54581

Excited State 5: Singlet-A 3.6160 eV 342.88 nm f=0.2826
<S**2>=0.000
134 ->137 0.26028
135 ->138 0.60964
136 ->139 -0.23460

Excited State 6: Singlet-A 3.8679 eV 320.55 nm f=0.1778
<S**2>=0.000
134 ->137 0.37609
135 ->138 -0.26583
135 ->140 0.11825
136 ->139 -0.31419

Table S2. continued.

136 ->141 0.40400

Excited State 7: Singlet-A 3.9240 eV 315.96 nm f=0.0105 <S**2>=0.000

130 ->137 -0.12807

135 ->141 0.10409

136 ->140 0.67159

Excited State 8: Singlet-A 4.0045 eV 309.61 nm f=0.0007 <S**2>=0.000

131 ->137 0.16774

132 ->137 0.60740

132 ->138 0.27382

132 ->139 -0.12420

Excited State 9: Singlet-A 4.0122 eV 309.02 nm f=0.0007 <S**2>=0.000

133 ->137 0.61842

133 ->138 -0.28766

133 ->139 -0.12833

Excited State 10: Singlet-A 4.1435 eV 299.22 nm f=0.3618 <S**2>=0.000

131 ->137 -0.10097

134 ->137 -0.29989

135 ->138 0.21685

136 ->139 0.18960

136 ->141 0.55302

Excited State 11: Singlet-A 4.1600 eV 298.04 nm f=0.0318 <S**2>=0.000

130 ->137 -0.40050

131 ->137 0.44017

132 ->137 -0.13142

Table S2. continued.

136 ->142 -0.29862

Excited State 12: Singlet-A 4.2040 eV 294.92 nm f=0.0098 <S**2>=0.000

130 ->137 0.32283
131 ->137 0.42528
132 ->137 -0.10711
134 ->138 -0.19843
135 ->139 0.26903
136 ->142 0.25690

Excited State 13: Singlet-A 4.3310 eV 286.27 nm f=0.0099 <S**2>=0.000

130 ->137 -0.11457
131 ->137 -0.23037
134 ->138 -0.25084
135 ->139 0.54553
136 ->142 -0.21128

Excited State 14: Singlet-A 4.3877 eV 282.57 nm f=0.0085 <S**2>=0.000

130 ->137 0.26034
134 ->138 0.54508
135 ->139 0.22407
136 ->142 -0.24164

Excited State 15: Singlet-A 4.6297 eV 267.80 nm f=0.0026 <S**2>=0.000

136 ->142 -0.12779
136 ->143 0.65268

Excited State 16: Singlet-A 4.6710 eV 265.43 nm f=0.0423 <S**2>=0.000

127 ->137 -0.14100
129 ->137 0.14744

Table S2. continued.

134 ->141 0.10325
135 ->140 0.61200
136 ->141 -0.12335
136 ->143 0.10064

Excited State 17: Singlet-A 4.7099 eV 263.24 nm f=0.0126 <S**2>=0.000
128 ->137 0.20260
130 ->137 0.22403
134 ->138 -0.12465
134 ->140 0.10615
135 ->139 -0.10552
135 ->141 0.38320
136 ->142 -0.38138
136 ->143 -0.19972

Excited State 18: Singlet-A 4.7699 eV 259.93 nm f=0.0072 <S**2>=0.000
127 ->137 0.10326
129 ->137 0.58151
130 ->138 -0.10688
135 ->140 -0.18227
135 ->142 0.15936
136 ->144 0.22551

Excited State 19: Singlet-A 4.7779 eV 259.50 nm f=0.0007 <S**2>=0.000
133 ->137 0.31895
133 ->138 0.55634
133 ->139 0.23127
133 ->140 -0.11835

Excited State 20: Singlet-A 4.7913 eV 258.77 nm f=0.0007 <S**2>=0.000
131 ->138 0.14497

Table S2. continued.

```
      132 ->137          -0.30470
      132 ->138           0.54792
      132 ->139          -0.22860
      132 ->140          -0.11971
 SavETr:  write IOETrn=     770 NScale=  10 NData=   16 NLR=1 NState=     20
LETran=      370.
```

Table S3. TD-DFT results for 4ac (isomer C) in acetonitrile

Excited State 1: Singlet-A 2.2331 eV 555.20 nm f=3.2010
<S**2>=0.000
136 ->137 0.70702
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -1826.04683789
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 2.7676 eV 447.99 nm f=0.0052
<S**2>=0.000
135 ->137 -0.44287
136 ->138 0.54349

Excited State 3: Singlet-A 3.2077 eV 386.52 nm f=0.1407
<S**2>=0.000
135 ->137 0.54611
136 ->138 0.44466

Excited State 4: Singlet-A 3.5188 eV 352.35 nm f=0.0046
<S**2>=0.000
134 ->137 -0.43682
136 ->139 0.54433

Excited State 5: Singlet-A 3.5896 eV 345.40 nm f=0.4134
<S**2>=0.000
134 ->137 0.20884
135 ->138 0.64090
136 ->139 0.19684

Excited State 6: Singlet-A 3.8799 eV 319.56 nm f=0.0823
<S**2>=0.000
134 ->137 0.41120
135 ->138 -0.21497
135 ->140 0.11415
136 ->139 0.34430

Table S3. continued.

136 ->141 -0.37492

Excited State 7: Singlet-A 3.9387 eV 314.79 nm f=0.0013 <S**2>=0.000

130 ->137 -0.12912
135 ->141 -0.10516
136 ->140 0.67175

Excited State 8: Singlet-A 4.0215 eV 308.30 nm f=0.0001 <S**2>=0.000

131 ->138 -0.29962
132 ->137 0.61986
132 ->139 -0.13180

Excited State 9: Singlet-A 4.0216 eV 308.30 nm f=0.0013 <S**2>=0.000

131 ->137 0.62007
131 ->139 -0.13191
132 ->138 -0.29950

Excited State 10: Singlet-A 4.1557 eV 298.35 nm f=0.2855 <S**2>=0.000

134 ->137 0.29601
135 ->138 -0.18188
136 ->139 0.18467
136 ->141 0.57397

Excited State 11: Singlet-A 4.1849 eV 296.27 nm f=0.0299 <S**2>=0.000

133 ->137 0.59714
134 ->138 -0.20879
135 ->139 0.26015
136 ->142 -0.11947

Excited State 12: Singlet-A 4.1967 eV 295.43 nm f=0.0040

Table S3. continued.

<S**2>=0.000

130 ->137 0.50117

133 ->137 0.12647

134 ->138 0.13418

136 ->142 0.42886

Excited State 13: Singlet-A 4.3244 eV 286.71 nm f=0.0176

<S**2>=0.000

133 ->137 -0.30373

134 ->138 -0.33077

135 ->139 0.48803

136 ->142 0.18996

Excited State 14: Singlet-A 4.3752 eV 283.38 nm f=0.0096

<S**2>=0.000

130 ->137 -0.28510

134 ->138 0.48622

135 ->139 0.32764

136 ->140 -0.10344

136 ->142 0.20348

Excited State 15: Singlet-A 4.5087 eV 274.99 nm f=0.0000

<S**2>=0.000

134 ->143 0.10250

136 ->143 0.69188

Excited State 16: Singlet-A 4.6558 eV 266.30 nm f=0.0435

<S**2>=0.000

127 ->137 0.13469

129 ->137 -0.10731

135 ->140 0.63323

136 ->141 0.13701

Excited State 17: Singlet-A 4.6902 eV 264.35 nm f=0.0192

<S**2>=0.000

Table S3. continued.

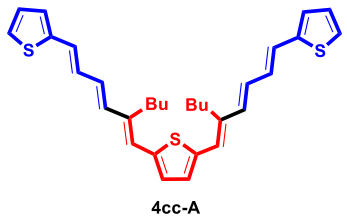
128 ->137 0.18402
130 ->137 -0.27792
134 ->138 -0.15323
134 ->140 0.10219
135 ->139 -0.13802
135 ->141 0.36823
136 ->142 0.41144

Excited State 18: Singlet-A 4.7697 eV 259.94 nm f=0.0021 <S**2>=0.000
129 ->137 0.53389
133 ->138 0.30167
135 ->140 0.14195
135 ->142 -0.17892
136 ->144 0.21227

Excited State 19: Singlet-A 4.7827 eV 259.23 nm f=0.0013 <S**2>=0.000
131 ->137 0.33475
131 ->139 0.22052
132 ->138 0.56403
132 ->140 -0.11933

Excited State 20: Singlet-A 4.7827 eV 259.23 nm f=0.0001 <S**2>=0.000
131 ->138 0.56512
131 ->140 -0.11968
132 ->137 0.33491
132 ->139 0.22080
SavETr: write IOETrn= 770 NScale= 10 NData= 16 NLR=1 NState= 20 LETran= 370.

Table S4. TD-DFT results for 4cc (isomer A) in acetonitrile



4cc-A

Excited State 1: Singlet-A 2.0771 eV 596.92 nm f=3.0210 <S**2>=0.000

138 ->139 0.70828

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-DFT) = -2435.48232688

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 2.5971 eV 477.39 nm f=0.0005 <S**2>=0.000

137 ->139 0.54059

138 ->140 0.44658

Excited State 3: Singlet-A 3.0747 eV 403.24 nm f=0.2202 <S**2>=0.000

137 ->139 -0.45372

138 ->140 0.54529

Excited State 4: Singlet-A 3.3007 eV 375.63 nm f=0.0143 <S**2>=0.000

136 ->139 0.56316

137 ->140 0.11010

138 ->141 0.40276

Excited State 5: Singlet-A 3.4503 eV 359.34 nm f=0.1898 <S**2>=0.000

136 ->139 0.13971

137 ->140 0.59171

138 ->141 -0.35413

Excited State 6: Singlet-A 3.8607 eV 321.14 nm f=0.4454 <S**2>=0.000

136 ->139 -0.39770

137 ->140 0.36401

138 ->141 0.45405

Excited State 7: Singlet-A 3.9746 eV 311.94 nm f=0.0072 <S**2>=0.000

Table S4. continued.

135 ->139	0.52850				
136 ->140	-0.11244				
137 ->141	0.20401				
138 ->142	0.38550				
Excited State 8:	Singlet-A	4.1063 eV	301.94 nm	f=0.0052	<S**2>=0.000
132 ->139	0.22360				
135 ->139	0.18152				
136 ->140	0.51728				
137 ->141	-0.36172				
Excited State 9:	Singlet-A	4.1966 eV	295.44 nm	f=0.0030	<S**2>=0.000
132 ->139	0.51019				
135 ->139	-0.24176				
136 ->140	-0.28963				
137 ->141	-0.19063				
138 ->142	0.22391				
Excited State 10:	Singlet-A	4.2391 eV	292.48 nm	f=0.0595	<S**2>=0.000
132 ->139	-0.30296				
134 ->139	0.51290				
137 ->141	-0.29367				
138 ->142	0.19674				
Excited State 11:	Singlet-A	4.2445 eV	292.11 nm	f=0.0013	<S**2>=0.000
133 ->139	0.69179				
134 ->140	-0.11264				
Excited State 12:	Singlet-A	4.2553 eV	291.37 nm	f=0.0024	<S**2>=0.000
132 ->139	0.27313				
134 ->139	0.46122				
136 ->140	0.15688				
137 ->141	0.34243				
138 ->142	-0.24763				

Table S4. continued.

Excited State 13:	Singlet-A	4.6307 eV	267.74 nm	f=0.0011	<S**2>=0.000
131 ->139	0.50047				
135 ->140	-0.16498				
137 ->142	0.22495				
138 ->143	-0.38545				
Excited State 14:	Singlet-A	4.6933 eV	264.17 nm	f=0.1351	<S**2>=0.000
135 ->139	-0.34285				
136 ->140	0.30655				
137 ->141	0.27486				
138 ->142	0.43238				
Excited State 15:	Singlet-A	4.7137 eV	263.03 nm	f=0.0023	<S**2>=0.000
136 ->146	-0.11588				
138 ->146	0.68550				
Excited State 16:	Singlet-A	4.7476 eV	261.15 nm	f=0.0001	<S**2>=0.000
136 ->144	0.10961				
137 ->145	0.26819				
138 ->144	0.64232				
Excited State 17:	Singlet-A	4.7479 eV	261.14 nm	f=0.0000	<S**2>=0.000
136 ->145	0.10965				
137 ->144	0.26810				
138 ->145	0.64126				
Excited State 18:	Singlet-A	4.8167 eV	257.41 nm	f=0.0040	<S**2>=0.000
131 ->139	0.31650				
135 ->140	0.55453				
137 ->142	-0.26738				
Excited State 19:	Singlet-A	4.9040 eV	252.82 nm	f=0.0308	<S**2>=0.000
131 ->139	0.19994				
132 ->140	-0.12015				
134 ->140	0.10140				

Table S4. continued.

136 ->141 0.26255

137 ->142 0.37702

138 ->143 0.45501

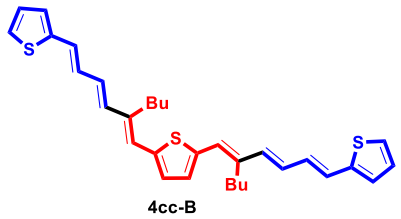
Excited State 20: Singlet-A 4.9550 eV 250.22 nm f=0.0220 <S**2>=0.000

132 ->140 0.62381

136 ->141 0.28539

SavETr: write IOETrn= 770 NScale= 10 NData= 16 NLR=1 NState= 20 LETran= 370.

Table S5. TD-DFT results for 4cc (isomer B) in acetonitrile



4cc-B

Excited State 1: Singlet-A 2.1206 eV 584.68 nm f=3.1542 <S**2>=0.000

138 ->139 0.70783

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-DFT) = -2435.48278464

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 2.6269 eV 471.99 nm f=0.0068 <S**2>=0.000

137 ->139 0.52091

138 ->140 0.46909

Excited State 3: Singlet-A 3.0758 eV 403.10 nm f=0.1641 <S**2>=0.000

137 ->139 -0.47533

138 ->140 0.52524

Excited State 4: Singlet-A 3.3348 eV 371.78 nm f=0.0119 <S**2>=0.000

136 ->139 0.54237

137 ->140 -0.10528

138 ->141 0.43049

Excited State 5: Singlet-A 3.4368 eV 360.75 nm f=0.2996 <S**2>=0.000

136 ->139 -0.13083

137 ->140 0.61602

138 ->141 0.31293

Excited State 6: Singlet-A 3.8516 eV 321.91 nm f=0.3347 <S**2>=0.000

136 ->139 -0.42486

137 ->140 -0.31777

138 ->141 0.45612

Table S5. continued.

Excited State 7:	Singlet-A	3.9735 eV	312.03 nm	f=0.0004	<S**2>=0.000
132 ->139	0.10598				
135 ->139	0.45322				
136 ->140	0.20066				
137 ->141	-0.22808				
138 ->142	-0.42514				
Excited State 8:	Singlet-A	4.1059 eV	301.96 nm	f=0.0005	<S**2>=0.000
132 ->139	-0.25701				
135 ->139	-0.18315				
136 ->140	0.46740				
137 ->141	-0.37188				
138 ->142	0.16072				
Excited State 9:	Singlet-A	4.1859 eV	296.19 nm	f=0.0010	<S**2>=0.000
132 ->139	0.32604				
135 ->139	-0.34390				
136 ->140	0.34833				
137 ->141	0.26495				
138 ->142	-0.26461				
Excited State 10:	Singlet-A	4.2372 eV	292.61 nm	f=0.0258	<S**2>=0.000
132 ->139	0.46500				
133 ->139	-0.31122				
135 ->139	-0.11306				
136 ->140	-0.11030				
137 ->141	-0.34692				
138 ->142	0.13738				
Excited State 11:	Singlet-A	4.2664 eV	290.61 nm	f=0.0337	<S**2>=0.000
133 ->139	-0.26994				
133 ->140	0.10529				
134 ->139	0.62855				
Excited State 12:	Singlet-A	4.2764 eV	289.93 nm	f=0.0228	<S**2>=0.000

Table S5. continued.

132 ->139	0.24778				
133 ->139	0.53921				
134 ->139	0.24857				
137 ->141	-0.17606				
138 ->142	0.18164				
Excited State 13:	Singlet-A	4.5409 eV	273.04 nm	f=0.0017	<S**2>=0.000
136 ->143	0.10563				
138 ->143	0.64939				
138 ->144	0.18600				
Excited State 14:	Singlet-A	4.6476 eV	266.77 nm	f=0.0152	<S**2>=0.000
131 ->139	0.42186				
135 ->139	-0.15683				
135 ->140	-0.21845				
136 ->140	-0.13237				
137 ->141	-0.12022				
137 ->142	-0.27977				
138 ->142	-0.17625				
138 ->144	0.27042				
Excited State 15:	Singlet-A	4.6580 eV	266.17 nm	f=0.0200	<S**2>=0.000
131 ->139	0.19511				
132 ->139	0.13738				
133 ->139	-0.10555				
135 ->139	0.29454				
135 ->140	-0.10798				
136 ->140	0.26452				
137 ->141	0.23824				
137 ->142	-0.15410				
138 ->142	0.35465				
138 ->143	0.10388				
138 ->144	0.17387				
Excited State 16:	Singlet-A	4.7984 eV	258.39 nm	f=0.0025	<S**2>=0.000

Table S5. continued.

131 ->139 0.37451
135 ->140 0.50306
137 ->142 0.27285
138 ->144 0.10718

Excited State 17: Singlet-A 4.8610 eV 255.06 nm f=0.0002 <S**2>=0.000
136 ->146 -0.11190
137 ->146 -0.26682
138 ->146 0.62755

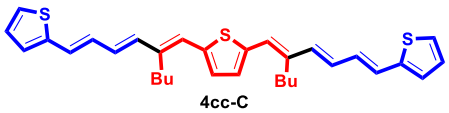
Excited State 18: Singlet-A 4.8712 eV 254.52 nm f=0.0007 <S**2>=0.000
136 ->145 -0.10827
137 ->145 0.27966
138 ->145 0.61843

Excited State 19: Singlet-A 4.8756 eV 254.30 nm f=0.0138 <S**2>=0.000
132 ->140 0.38212
135 ->140 -0.22420
137 ->142 0.40709
138 ->144 0.26473
138 ->145 -0.13636
138 ->146 -0.11001

Excited State 20: Singlet-A 4.9219 eV 251.90 nm f=0.0251 <S**2>=0.000
131 ->139 0.11889
132 ->140 0.51154
133 ->140 0.18546
134 ->140 0.13758
136 ->141 0.22590
137 ->142 -0.14433
138 ->144 -0.27023

SavETr: write IOETrn= 770 NScale= 10 NData= 16 NLR=1 NState= 20 LETran= 370.

Table S6. TD-DFT results for 4cc (isomer C) in acetonitrile



4cc-C

Excited State 1: Singlet-A 2.1544 eV 575.48 nm f=3.2120
<S**2>=0.000
138 ->139 0.70763
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -2435.48005761
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 2.6430 eV 469.11 nm f=0.0002
<S**2>=0.000
137 ->139 0.50940
138 ->140 -0.48147

Excited State 3: Singlet-A 3.0771 eV 402.92 nm f=0.1570
<S**2>=0.000
137 ->139 0.48770
138 ->140 0.51409

Excited State 4: Singlet-A 3.3626 eV 368.71 nm f=0.0397
<S**2>=0.000
136 ->139 0.54820
137 ->140 -0.18858
138 ->141 -0.39247

Excited State 5: Singlet-A 3.4116 eV 363.42 nm f=0.3786
<S**2>=0.000
137 ->140 0.61834
138 ->141 -0.33225

Excited State 6: Singlet-A 3.8551 eV 321.61 nm f=0.1602
<S**2>=0.000
136 ->139 0.43579
137 ->140 0.27153

Table S6. continued.

138 ->141 0.47580

Excited State 7: Singlet-A 3.9623 eV 312.91 nm f=0.0010
<S**2>=0.000

132 ->139 -0.10266
135 ->139 0.39305
136 ->140 -0.27402
137 ->141 0.24468
138 ->142 0.43617

Excited State 8: Singlet-A 4.1013 eV 302.30 nm f=0.0006
<S**2>=0.000

132 ->139 -0.23453
135 ->139 0.21677
136 ->140 0.46410
137 ->141 -0.33382
138 ->142 0.23123

Excited State 9: Singlet-A 4.1752 eV 296.96 nm f=0.0044
<S**2>=0.000

132 ->139 0.23239
135 ->139 0.39144
136 ->140 0.31331
137 ->141 0.31927
138 ->142 -0.27885

Excited State 10: Singlet-A 4.2588 eV 291.12 nm f=0.0661
<S**2>=0.000

132 ->139 0.52129
133 ->139 -0.21926
135 ->139 0.17165
136 ->140 -0.11602
137 ->141 -0.34237

Excited State 11: Singlet-A 4.2874 eV 289.18 nm f=0.0355

Table S6. continued.

<S**2>=0.000

133 ->140 0.13017

134 ->139 0.68284

Excited State 12: Singlet-A 4.2933 eV 288.78 nm f=0.0000

<S**2>=0.000

132 ->139 0.17407

133 ->139 0.63894

134 ->140 0.11737

137 ->141 -0.14065

138 ->142 0.14088

Excited State 13: Singlet-A 4.4091 eV 281.20 nm f=0.0034

<S**2>=0.000

136 ->143 -0.11470

138 ->143 0.68636

Excited State 14: Singlet-A 4.6304 eV 267.76 nm f=0.0487

<S**2>=0.000

132 ->139 0.26209

135 ->139 -0.32312

136 ->140 0.29026

137 ->141 0.27694

138 ->142 0.37814

Excited State 15: Singlet-A 4.6372 eV 267.37 nm f=0.0047

<S**2>=0.000

131 ->139 -0.38264

135 ->140 0.32959

137 ->142 0.39758

138 ->144 0.25986

Excited State 16: Singlet-A 4.7705 eV 259.90 nm f=0.0083

<S**2>=0.000

131 ->139 0.43148

Table S6. continued.

132 ->140 0.12711
135 ->140 0.49297
137 ->142 0.10990
138 ->144 -0.15600

Excited State 17: Singlet-A 4.8260 eV 256.91 nm f=0.0167 <S**2>=0.000
131 ->139 0.12038
132 ->140 -0.35560
135 ->140 -0.21658
137 ->142 0.47533
138 ->144 -0.26096

Excited State 18: Singlet-A 4.8838 eV 253.87 nm f=0.0000 <S**2>=0.000
136 ->145 0.11527
137 ->146 0.28858
138 ->145 0.62969

Excited State 19: Singlet-A 4.8840 eV 253.86 nm f=0.0001 <S**2>=0.000
136 ->146 0.11506
137 ->145 0.28837
138 ->146 0.62784

Excited State 20: Singlet-A 4.9121 eV 252.40 nm f=0.0054 <S**2>=0.000
131 ->139 -0.14580
132 ->140 0.44066
133 ->140 0.37148
135 ->140 -0.12282
136 ->141 0.12183
137 ->142 0.15382
138 ->144 -0.26485
SavETr: write IOETrn= 770 NScale= 10 NData= 16 NLR=1 NState= 20

Table S6. continued.

LETran= 370.

Table S7. TD-DFT results for 4ee in acetonitrile

Excited State 1: Singlet-A 2.4678 eV 502.40 nm f=3.3248
<S**2>=0.000
135 ->136 0.70589
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -1473.19491733
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 2.9587 eV 419.05 nm f=0.0003
<S**2>=0.000
134 ->136 0.56007
135 ->137 -0.42251

Excited State 3: Singlet-A 3.3317 eV 372.14 nm f=0.0124
<S**2>=0.000
134 ->136 0.42805
135 ->137 0.56383

Excited State 4: Singlet-A 3.6688 eV 337.94 nm f=0.6069
<S**2>=0.000
133 ->136 -0.28588
134 ->137 0.64087

Excited State 5: Singlet-A 3.7674 eV 329.09 nm f=0.0490
<S**2>=0.000
133 ->136 0.46175
134 ->137 0.20088
135 ->138 0.48381

Excited State 6: Singlet-A 4.0707 eV 304.57 nm f=0.0096
<S**2>=0.000
129 ->136 0.46219
135 ->139 0.50989

Excited State 7: Singlet-A 4.2062 eV 294.77 nm f=0.1898

Table S7. continued.

<S**2>=0.000

131 ->136	0.13980
133 ->136	-0.40886
134 ->137	-0.18209
134 ->140	0.10343
135 ->138	0.46407
135 ->141	0.18476

Excited State 8: Singlet-A 4.2503 eV 291.70 nm f=0.0001

<S**2>=0.000

131 ->137	0.16508
132 ->136	0.48907
133 ->137	0.11080
134 ->138	0.21451
134 ->141	0.15566
135 ->140	0.36552

Excited State 9: Singlet-A 4.2808 eV 289.63 nm f=0.0454

<S**2>=0.000

130 ->137	0.11036
131 ->136	0.50875
132 ->137	0.15570
133 ->136	0.15366
134 ->140	0.16002
135 ->138	-0.18047
135 ->141	0.31688

Excited State 10: Singlet-A 4.3090 eV 287.74 nm f=0.0000

<S**2>=0.000

130 ->136	0.49814
131 ->137	0.11341
133 ->137	-0.21326
134 ->138	-0.30904
134 ->141	0.11503
135 ->140	0.11492

Table S7. continued.

135 ->142 -0.24086

Excited State 11: Singlet-A 4.4505 eV 278.59 nm f=0.0004 <S**2>=0.000

130 ->136 0.35206
132 ->136 -0.20131
133 ->137 0.46220
134 ->138 0.30033
135 ->142 -0.12316

Excited State 12: Singlet-A 4.5105 eV 274.88 nm f=0.0571 <S**2>=0.000

129 ->136 0.51126
135 ->139 -0.47395

Excited State 13: Singlet-A 4.5248 eV 274.01 nm f=0.0076 <S**2>=0.000

130 ->136 -0.16730
132 ->136 -0.40823
135 ->140 0.53272

Excited State 14: Singlet-A 4.5419 eV 272.98 nm f=0.0498 <S**2>=0.000

131 ->136 -0.42151
134 ->140 0.10186
135 ->141 0.54170

Excited State 15: Singlet-A 4.5995 eV 269.56 nm f=0.0000 <S**2>=0.000

133 ->137 -0.38578
134 ->138 0.45812
135 ->142 -0.35479

Excited State 16: Singlet-A 4.7837 eV 259.18 nm f=0.0000 <S**2>=0.000

Table S7. continued.

129 ->137 0.10496
134 ->139 0.69268

Excited State 17: Singlet-A 4.9322 eV 251.38 nm f=0.0016 <S**2>=0.000
128 ->136 0.37992
130 ->137 0.10871
131 ->136 0.10400
132 ->137 -0.33094
134 ->140 -0.33135
134 ->142 -0.20852
135 ->141 0.14684
135 ->143 0.17515

Excited State 18: Singlet-A 4.9615 eV 249.89 nm f=0.0003 <S**2>=0.000
130 ->136 -0.12135
131 ->137 0.45663
132 ->136 -0.14870
133 ->140 0.10254
134 ->141 0.39785
135 ->140 -0.22818

Excited State 19: Singlet-A 4.9616 eV 249.89 nm f=0.0006 <S**2>=0.000
128 ->136 0.33443
130 ->137 0.30165
131 ->136 -0.15602
132 ->137 0.24871
134 ->140 0.28308
134 ->142 -0.19736
135 ->141 -0.19803
135 ->143 0.15863

Excited State 20: Singlet-A 4.9619 eV 249.87 nm f=0.0002

Table S7. continued.

<S**2>=0.000

129 ->137 0.68701

134 ->139 -0.10250

SavETr: write IOETrn= 770 NScale= 10 NData= 16 NLR=1 NState= 20 LETran= 370.

Table S8. Cartesian coordinates of isomer A of 4ac by TD-DFT calculations

Energy: -1145911.8049426

C	-1.27531	-2.27601	0.03629
C	-2.69343	-2.04307	0.05852
S	0.00000	-1.06183	-0.00000
C	-0.70209	-3.54486	0.01623
C	1.27531	-2.27601	-0.03629
C	0.70209	-3.54486	-0.01623
H	-1.30529	-4.44672	0.02821
C	2.69343	-2.04307	-0.05853
H	1.30529	-4.44672	-0.02821
C	-3.45016	-0.90048	0.13027
H	-3.24982	-2.97933	0.01016
C	-2.87533	0.49851	0.19823
C	-4.88941	-1.07248	0.10821
C	3.45016	-0.90047	-0.13028
H	3.24982	-2.97933	-0.01016
C	2.87533	0.49851	-0.19823
C	4.88941	-1.07248	-0.10821
C	5.84023	-0.09731	-0.15197
H	5.23846	-2.10392	-0.04477
H	5.55231	0.95059	-0.20974
C	7.25240	-0.37588	-0.12352
C	-5.84023	-0.09731	0.15197
H	-5.23846	-2.10392	0.04477
H	-5.55231	0.95059	0.20974
C	-7.25240	-0.37588	0.12352
C	-8.21132	0.58348	0.16633
H	-7.53478	-1.42660	0.06398
H	-7.91043	1.62816	0.22525
C	-9.66037	0.38869	0.14215
C	8.21132	0.58348	-0.16633
H	7.53478	-1.42660	-0.06398
H	7.91043	1.62816	-0.22525
C	9.66037	0.38869	-0.14215

Table S8. continued.

C	−10.27775	−0.87719	0.06966
N	−10.39243	1.52851	0.19504
C	−11.72577	1.42801	0.17680
C	−11.66496	−0.95961	0.05176
C	−12.41633	0.21731	0.10633
H	−12.27447	2.36800	0.22096
H	−9.67885	−1.78089	0.02817
H	−12.15440	−1.92794	−0.00392
H	−13.50138	0.20002	0.09486
C	10.27775	−0.87719	−0.06966
N	10.39243	1.52851	−0.19505
C	11.72578	1.42802	−0.17681
C	11.66496	−0.95960	−0.05176
C	12.41633	0.21731	−0.10634
H	12.27447	2.36800	−0.22098
H	9.67885	−1.78089	−0.02815
H	12.15441	−1.92793	0.00393
H	13.50138	0.20003	−0.09487
C	2.71607	1.16426	1.18618
H	3.52340	1.12658	−0.82129
H	1.90586	0.48676	−0.70793
H	−3.52340	1.12657	0.82129
H	−1.90586	0.48676	0.70793
C	−2.71608	1.16426	−1.18618
H	−2.05058	0.55103	−1.80872
H	−3.68979	1.17573	−1.69411
C	−2.16535	2.59320	−1.10052
H	2.05058	0.55102	1.80872
H	3.68978	1.17572	1.69412
C	2.16535	2.59319	1.10053
H	−2.82979	3.20011	−0.46933
H	−1.19111	2.57607	−0.59103
C	−2.01313	3.25844	−2.47262
H	−1.32742	2.69073	−3.11373
H	−2.97790	3.31998	−2.99125

Table S8. continued.

H	−1.61803	4.27667	−2.38013
H	2.82979	3.20011	0.46935
H	1.19111	2.57607	0.59104
C	2.01311	3.25842	2.47263
H	1.32740	2.69071	3.11374
H	2.97788	3.31996	2.99126
H	1.61802	4.27665	2.38015

Table S9. Cartesian coordinates of isomer B of 4ac by TD-DFT calculations

Energy: -1145904.3798678

C	1.12420	1.00426	-0.11116
C	2.42212	0.37850	-0.11431
S	-0.28073	-0.05980	-0.18386
C	0.69705	2.32630	-0.03718
C	-1.41549	1.28032	-0.13220
C	-0.70297	2.47355	-0.04858
H	1.36958	3.16772	0.06038
C	-2.85161	1.21035	-0.14616
H	-1.20280	3.43500	0.01162
C	3.66783	0.91852	-0.31399
H	2.39540	-0.69742	0.05570
C	3.91404	2.38083	-0.61466
C	4.79538	0.01159	-0.22148
C	-3.72960	0.16412	-0.27427
H	-3.29944	2.19797	-0.03432
C	-3.31029	-1.28133	-0.43837
C	-5.14161	0.48910	-0.21949
C	-6.19270	-0.37355	-0.30576
H	-5.37573	1.54643	-0.08930
H	-6.02017	-1.44092	-0.42982
C	-7.56654	0.05237	-0.23896
C	6.11476	0.31790	-0.36735
H	4.54641	-1.02791	-0.00434
H	6.42264	1.34071	-0.57604
C	7.16568	-0.66025	-0.25572
C	8.48325	-0.36858	-0.39746
H	6.85243	-1.68231	-0.04466
H	8.77617	0.65885	-0.60686
C	9.61118	-1.29445	-0.30067
C	-8.62283	-0.79536	-0.32371
H	-7.73382	1.12177	-0.11330
H	-8.43529	-1.86035	-0.44977
C	-10.04288	-0.45107	-0.26606

Table S9. continued.

C	9.47002	−2.67347	−0.04213
N	10.83123	−0.73124	−0.47963
C	11.91030	−1.51744	−0.40474
C	10.60438	−3.47310	0.03185
C	11.86037	−2.88920	−0.15271
H	12.86986	−1.02413	−0.55458
H	8.48675	−3.11010	0.09789
H	10.51129	−4.53715	0.23036
H	12.77235	−3.47541	−0.10361
C	−10.52232	0.86513	−0.10322
N	−10.89179	−1.50183	−0.38139
C	−12.20685	−1.26320	−0.33761
C	−11.89288	1.09147	−0.06036
C	−12.76493	0.00616	−0.17976
H	−12.85211	−2.13551	−0.43401
H	−9.83093	1.69617	−0.01154
H	−12.27682	2.10008	0.06460
H	−13.84193	0.13661	−0.15164
C	−3.20744	−2.04813	0.89818
H	−4.02888	−1.79556	−1.08792
H	−2.35063	−1.34026	−0.96354
H	4.76252	2.47024	−1.30376
H	3.05261	2.79777	−1.14749
C	4.20621	3.23139	0.64084
H	3.36262	3.15458	1.34064
H	5.07513	2.81175	1.16523
C	4.46873	4.70683	0.31277
H	−2.47529	−1.54872	1.54709
H	−4.17172	−1.99200	1.42097
C	−2.80856	−3.51741	0.71156
H	5.31162	4.77605	−0.38929
H	3.59795	5.12259	−0.21414
C	4.76613	5.55225	1.55582
H	3.92610	5.52838	2.26104
H	5.65315	5.18077	2.08374

Table S9. continued.

H	4.94965	6.59977	1.29041
H	−3.54017	−4.01046	0.05585
H	−1.84442	−3.56677	0.18593
C	−2.70966	−4.28291	2.03548
H	−1.96113	−3.83162	2.69850
H	−3.66921	−4.27909	2.56729
H	−2.42319	−5.32807	1.87097

Table S10. Cartesian coordinates of isomer C of 4ac by TD-DFT calculations

Energy: -1145898.9577530

C	-1.27925	-0.08216	0.00523
C	-2.64181	-0.55447	-0.00862
S	-0.00000	-1.29009	-0.00001
C	-0.70545	1.18524	-0.00073
C	1.27925	-0.08216	-0.00523
C	0.70545	1.18524	0.00073
H	-1.28044	2.10094	-0.03025
C	2.64181	-0.55447	0.00862
H	1.28044	2.10094	0.03026
C	-3.81648	0.11392	0.22649
H	-2.73931	-1.61711	-0.22848
C	-3.89425	1.57973	0.59422
C	-5.04082	-0.65397	0.10312
C	3.81648	0.11392	-0.22649
H	2.73931	-1.61711	0.22848
C	3.89425	1.57973	-0.59422
C	5.04082	-0.65397	-0.10312
C	6.31595	-0.20565	-0.27142
H	4.91247	-1.70436	0.16129
H	6.50394	0.83534	-0.52711
C	7.47318	-1.05004	-0.12324
C	-6.31595	-0.20565	0.27141
H	-4.91247	-1.70436	-0.16130
H	-6.50394	0.83534	0.52711
C	-7.47318	-1.05004	0.12324
C	-8.74778	-0.61390	0.28510
H	-7.28097	-2.09119	-0.13441
H	-8.91930	0.43021	0.54134
C	-9.97609	-1.39666	0.15352
C	8.74778	-0.61390	-0.28509
H	7.28097	-2.09120	0.13441
H	8.91930	0.43021	-0.54133
C	9.97609	-1.39666	-0.15352

Table S10. continued.

C	−9.99710	−2.76952	−0.16765
N	−11.12185	−0.70354	0.36463
C	−12.28542	−1.35434	0.26079
C	−11.21709	−3.42724	−0.27066
C	−12.39619	−2.70977	−0.05272
H	−13.18071	−0.75972	0.43812
H	−9.07158	−3.31085	−0.33322
H	−11.24898	−4.48480	−0.51728
H	−13.37045	−3.18274	−0.12267
C	9.99710	−2.76952	0.16765
N	11.12185	−0.70354	−0.36462
C	12.28542	−1.35434	−0.26077
C	11.21709	−3.42724	0.27066
C	12.39619	−2.70977	0.05273
H	13.18071	−0.75972	−0.43810
H	9.07158	−3.31085	0.33321
H	11.24898	−4.48481	0.51727
H	13.37044	−3.18274	0.12268
C	4.08306	2.51388	0.62104
H	4.72879	1.73460	−1.28860
H	2.99268	1.87050	−1.14408
H	−4.72879	1.73460	1.28860
H	−2.99268	1.87050	1.14409
C	−4.08305	2.51388	−0.62104
H	−3.25149	2.37245	−1.32509
H	−4.99264	2.22030	−1.16198
C	−4.17620	3.99356	−0.22700
H	3.25150	2.37245	1.32509
H	4.99264	2.22030	1.16197
C	4.17620	3.99356	0.22700
H	−5.00656	4.12720	0.48065
H	−3.26432	4.28391	0.31421
C	−4.37407	4.92145	−1.43048
H	−3.54160	4.83316	−2.13953
H	−5.29718	4.67703	−1.97052

Table S10. continued.

H	−4.43722	5.97032	−1.11857
H	5.00656	4.12720	−0.48066
H	3.26432	4.28391	−0.31420
C	4.37408	4.92145	1.43048
H	3.54161	4.83315	2.13953
H	5.29718	4.67703	1.97052
H	4.43723	5.97032	1.11857

Table S11. Cartesian coordinates of isomer A of 4cc by TD-DFT calculations

Energy: -1528336.6082266

C	1.27676	-2.19734	-0.03650
C	2.69442	-1.96357	-0.05879
S	-0.00000	-0.98314	0.00000
C	0.70219	-3.46569	-0.01649
C	-1.27676	-2.19734	0.03650
C	-0.70219	-3.46569	0.01650
H	1.30503	-4.36790	-0.02872
C	-2.69442	-1.96357	0.05879
H	-1.30503	-4.36790	0.02873
C	3.45161	-0.82039	-0.12848
H	3.25144	-2.89971	-0.01231
C	2.87333	0.57773	-0.19277
C	4.89065	-0.98804	-0.10820
C	-3.45162	-0.82039	0.12848
H	-3.25144	-2.89971	0.01231
C	-2.87333	0.57773	0.19277
C	-4.89065	-0.98804	0.10820
C	-5.83837	-0.00835	0.15015
H	-5.24347	-2.01848	0.04809
H	-5.54221	1.03778	0.20415
C	-7.25103	-0.27186	0.12550
C	5.83837	-0.00835	-0.15015
H	5.24347	-2.01848	-0.04809
H	5.54221	1.03778	-0.20415
C	7.25103	-0.27186	-0.12550
C	8.20308	0.69875	-0.16712
H	7.55350	-1.31841	-0.07053
H	7.88166	1.73903	-0.22123
C	9.63386	0.51971	-0.14834
C	-8.20308	0.69875	0.16712
H	-7.55350	-1.31841	0.07052
H	-7.88166	1.73903	0.22123
C	-9.63386	0.51971	0.14834

Table S11. continued.

C	−2.71203	1.23960	−1.19313
H	−3.51971	1.20933	0.81407
H	−1.90390	0.56514	0.70253
H	3.51971	1.20933	−0.81407
H	1.90390	0.56514	−0.70252
C	2.71204	1.23960	1.19313
H	2.04736	0.62342	1.81364
H	3.68549	1.25140	1.70161
C	2.15865	2.66775	1.11149
H	−2.04736	0.62341	−1.81363
H	−3.68549	1.25140	−1.70161
C	−2.15865	2.66775	−1.11149
H	2.82225	3.27786	0.48244
H	1.18476	2.65032	0.60132
C	2.00422	3.32882	2.48537
H	1.31913	2.75797	3.12436
H	2.96850	3.39055	3.00493
H	1.60733	4.34662	2.39570
H	−2.82225	3.27786	−0.48244
H	−1.18476	2.65032	−0.60132
C	−2.00421	3.32882	−2.48537
H	−1.31912	2.75796	−3.12436
H	−2.96849	3.39055	−3.00493
H	−1.60732	4.34662	−2.39570
C	10.59080	1.51776	−0.19041
S	10.41852	−1.05550	−0.06701
C	11.99884	−0.33171	−0.09145
C	11.92923	1.03422	−0.15803
H	12.87839	−0.96057	−0.05513
H	10.32814	2.56936	−0.24301
H	12.80390	1.67506	−0.18318
C	−10.59080	1.51776	0.19040
S	−10.41853	−1.05549	0.06701
C	−11.99884	−0.33171	0.09145
C	−11.92923	1.03422	0.15803

Table S11. continued.

H	−12.87839	−0.96057	0.05512
H	−10.32814	2.56936	0.24301
H	−12.80390	1.67506	0.18317

Table S12. Cartesian coordinates of isomer B of 4cc by TD-DFT calculations

Energy: -1528335.8603734

C	1.12953	1.00968	-0.11282
C	2.43651	0.40387	-0.12004
S	-0.26056	-0.07537	-0.18972
C	0.68105	2.32431	-0.03233
C	-1.41684	1.24747	-0.13052
C	-0.72130	2.45033	-0.04199
H	1.34045	3.17568	0.06910
C	-2.85143	1.15574	-0.14314
H	-1.23529	3.40405	0.02340
C	3.67417	0.96356	-0.32024
H	2.42689	-0.67293	0.04680
C	3.89338	2.43110	-0.61796
C	4.81765	0.07777	-0.23221
C	-3.71533	0.09776	-0.27656
H	-3.31382	2.13607	-0.02538
C	-3.27302	-1.34005	-0.44961
C	-5.13163	0.39942	-0.21931
C	-6.16990	-0.47938	-0.31310
H	-5.38266	1.45186	-0.08052
H	-5.97738	-1.54258	-0.44623
C	-7.54986	-0.08270	-0.24425
C	6.13172	0.40946	-0.38056
H	4.58868	-0.96665	-0.01621
H	6.41593	1.43964	-0.58821
C	7.20511	-0.54072	-0.27395
C	8.51830	-0.21780	-0.41901
H	6.92608	-1.57400	-0.06369
H	8.77720	0.82010	-0.62900
C	9.65094	-1.10567	-0.32688
C	-8.59362	-0.94964	-0.33833
H	-7.74714	0.98153	-0.10852
H	-8.37771	-2.00948	-0.47444
C	-9.99928	-0.63238	-0.27931

Table S12. continued.

C	−3.15778	−2.11353	0.88195
H	−3.98328	−1.86194	−1.10230
H	−2.31245	−1.38052	−0.97492
H	4.73851	2.53791	−1.30878
H	3.02319	2.83362	−1.14774
C	4.17269	3.28426	0.63857
H	3.33292	3.18928	1.34074
H	5.05120	2.88032	1.15935
C	4.40525	4.76545	0.31383
H	−2.43274	−1.60716	1.53347
H	−4.12248	−2.07490	1.40558
C	−2.73712	−3.57558	0.68660
H	5.24436	4.85316	−0.39074
H	3.52483	5.16547	−0.20927
C	4.68991	5.61346	1.55813
H	3.85271	5.57127	2.26587
H	5.58565	5.25809	2.08244
H	4.85203	6.66509	1.29501
H	−3.46150	−4.07560	0.02807
H	−1.77254	−3.60754	0.16042
C	−2.62637	−4.34755	2.00584
H	−1.88439	−3.88915	2.67134
H	−3.58566	−4.36109	2.53800
H	−2.32448	−5.38737	1.83509
C	−11.05186	−1.52427	−0.37988
S	−10.62116	1.00146	−0.06161
C	−12.26629	0.44209	−0.11200
C	−12.33467	−0.91448	−0.28512
H	−13.07776	1.15039	−0.01062
H	−10.89684	−2.58932	−0.51850
H	−13.26939	−1.46157	−0.34317
C	10.98256	−0.76281	−0.47792
S	9.51302	−2.83019	0.00487
C	11.23706	−3.03881	−0.06866
C	11.87944	−1.85837	−0.33143

Table S12. continued.

H	11.66665	−4.01950	0.08673
H	11.29830	0.25384	−0.68857
H	12.95718	−1.77266	−0.41777

Table S13. Cartesian coordinates of isomer C of 4cc by TD-DFT calculations

Energy: -1528334.3297083

C	-1.28068	0.01248	0.00769
C	-2.64238	-0.46132	-0.00209
S	0.00000	-1.19559	-0.00001
C	-0.70564	1.27938	0.00045
C	1.28068	0.01248	-0.00770
C	0.70564	1.27938	-0.00046
H	-1.28017	2.19548	-0.02787
C	2.64238	-0.46132	0.00208
H	1.28017	2.19548	0.02786
C	-3.81879	0.20580	0.23174
H	-2.73878	-1.52514	-0.21715
C	-3.89559	1.67380	0.59195
C	-5.04276	-0.56213	0.11550
C	3.81879	0.20580	-0.23175
H	2.73878	-1.52514	0.21713
C	3.89559	1.67380	-0.59196
C	5.04276	-0.56213	-0.11550
C	6.31857	-0.11322	-0.28579
H	4.91522	-1.61389	0.14416
H	6.50290	0.92989	-0.53686
C	7.47787	-0.95235	-0.14842
C	-6.31857	-0.11322	0.28579
H	-4.91522	-1.61389	-0.14417
H	-6.50290	0.92989	0.53686
C	-7.47786	-0.95235	0.14842
C	-8.75417	-0.51320	0.31476
H	-7.29873	-1.99817	-0.10435
H	-8.91399	0.53538	0.56639
C	-9.96563	-1.28672	0.19646
C	8.75417	-0.51320	-0.31476
H	7.29873	-1.99817	0.10434
H	8.91399	0.53538	-0.56638
C	9.96563	-1.28672	-0.19645

Table S13. continued.

C	4.08230	2.60172	0.62823
H	4.73044	1.83360	−1.28489
H	2.99404	1.96668	−1.14086
H	−4.73043	1.83360	1.28489
H	−2.99404	1.96668	1.14085
C	−4.08230	2.60172	−0.62823
H	−3.25038	2.45538	−1.33086
H	−4.99189	2.30614	−1.16814
C	−4.17388	4.08376	−0.24279
H	3.25038	2.45537	1.33086
H	4.99189	2.30614	1.16815
C	4.17388	4.08376	0.24279
H	−5.00461	4.22259	0.46349
H	−3.26209	4.37604	0.29757
C	−4.36953	5.00523	−1.45157
H	−3.53655	4.91186	−2.15939
H	−5.29244	4.75895	−1.99112
H	−4.43161	6.05597	−1.14571
H	5.00461	4.22259	−0.46349
H	3.26209	4.37604	−0.29757
C	4.36952	5.00523	1.45157
H	3.53654	4.91186	2.15939
H	5.29243	4.75894	1.99113
H	4.43160	6.05597	1.14572
C	11.25856	−0.82576	−0.36740
S	9.99172	−3.00332	0.19808
C	11.72765	−3.05119	0.12245
C	12.25519	−1.82589	−0.18642
H	12.24811	−3.98075	0.31085
H	11.47624	0.20775	−0.61656
H	13.31985	−1.64219	−0.28187
C	−11.25856	−0.82576	0.36742
S	−9.99172	−3.00332	−0.19808
C	−11.72765	−3.05119	−0.12245
C	−12.25519	−1.82589	0.18644

Table S13. continued.

H	−12.24811	−3.98075	−0.31085
H	−11.47624	0.20775	0.61658
H	−13.31985	−1.64219	0.28189

Table S14. Cartesian coordinates of 4ee by TD-DFT calculations

Energy: -949157.0798626

C	-1.30502	-0.36690	-0.34699
C	-2.73743	-0.65181	-0.34384
C	-0.71315	0.91663	-0.37250
C	-0.41954	-1.46906	-0.37889
C	0.95986	-1.31445	-0.37363
C	0.66625	1.07124	-0.37786
C	1.55173	-0.03094	-0.34708
H	-0.83549	-2.47338	-0.40866
H	1.57787	-2.20163	-0.43144
H	-1.33116	1.80387	-0.42939
C	2.98414	0.25395	-0.34388
C	-3.81751	0.08793	0.05371
H	-2.96590	-1.66189	-0.68561
C	-3.73797	1.48018	0.64717
C	-5.12500	-0.53613	-0.08693
C	4.06424	-0.48601	0.05317
H	3.21261	1.26423	-0.68505
C	3.98474	-1.87850	0.64604
C	5.37172	0.13813	-0.08712
C	6.57919	-0.38636	0.25628
H	5.36808	1.13939	-0.52011
H	6.64128	-1.38407	0.68742
C	7.82696	0.31470	0.08103
C	-6.33247	-0.01179	0.25670
H	-5.12138	-1.53716	-0.52046
H	-6.39453	0.98569	0.68839
C	-7.58025	-0.71270	0.08096
C	-8.78796	-0.19513	0.41891
H	-7.51588	-1.71145	-0.35000
H	-8.80516	0.80880	0.84442
C	-10.09922	-0.82811	0.28064
C	9.03465	-0.20302	0.41881
H	7.76260	1.31369	-0.34938

Table S14. continued.

H	9.05185	−1.20719	0.84374
C	10.34590	0.43011	0.28107
C	−10.28610	−2.12888	−0.23520
C	−11.24498	−0.11052	0.68182
C	−12.52079	−0.66249	0.57361
C	−11.56021	−2.67952	−0.34286
C	−12.68591	−1.95123	0.06023
H	−11.12467	0.89330	1.08265
H	−13.38584	−0.08602	0.89055
H	−9.42897	−2.71489	−0.55360
H	−11.67790	−3.68315	−0.74302
H	−13.67818	−2.38518	−0.02549
C	10.53277	1.73121	−0.23393
C	11.49165	−0.28769	0.68193
C	12.76745	0.26441	0.57421
C	11.80688	2.28197	−0.34111
C	12.93256	1.55348	0.06166
H	11.37134	−1.29176	1.08211
H	13.63248	−0.31222	0.89088
H	9.67566	2.31738	−0.55205
H	11.92456	3.28586	−0.74061
H	13.92482	1.98753	−0.02367
H	3.00198	−2.03337	1.10278
C	4.26635	−3.01091	−0.36518
H	4.71028	−1.95638	1.46588
H	−2.75533	1.63470	1.10420
C	−4.01915	2.61286	−0.36416
H	−4.46368	1.55793	1.46682
H	1.08220	2.07559	−0.40680
H	3.54496	−2.95347	−1.19228
H	5.25503	−2.85623	−0.81706
C	4.20621	−4.40564	0.27091
H	4.92913	−4.45694	1.09737
H	3.21523	−4.55630	0.72237
C	4.48986	−5.53241	−0.72833

Table S14. continued.

H	3.76154	−5.52659	−1.54877
H	5.48830	−5.42685	−1.17057
H	4.44072	−6.51515	−0.24533
H	−3.29822	2.55355	−1.19140
H	−5.00809	2.45799	−0.81518
C	−3.95720	4.00739	0.27181
H	−4.67960	4.06122	1.09988
H	−2.96498	4.15921	0.72258
C	−4.24035	5.14227	−0.72150
H	−3.51880	5.08709	−1.54900
H	−5.23217	4.99041	−1.17052
C	−4.17717	6.53312	−0.08092
H	−4.91158	6.62958	0.72851
H	−3.18560	6.72698	0.34690
H	−4.38386	7.32092	−0.81463