SUPPORTING INFORMATION

Quantitative Analysis of Steric Effects on the Regioselectivity of the Larock Heteroannulation Reaction

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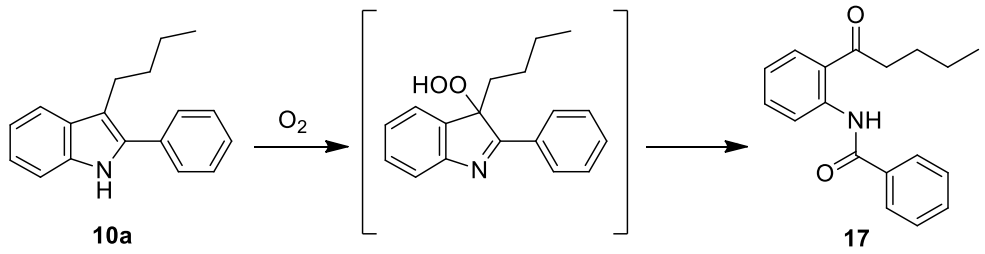
Proposed Auto-Oxidation of 9b to 17

It is worth noting that the regioisomeric product ratios obtained from the ^{1}H NMR analysis are not in accordance with those calculated from the isolated yields (See **Figure S1**) due to separation difficulties and compound stability issues. Indeed, aerobic oxidation of 3-alkyl-2-arylindoles was first reported in 1951 by Witkop and Patrick,[1] followed by several reports on similar observations,[2] including the oxidation/photorearrangement to afford *N*-(2-acylphenyl)benzamide.[3] We demonstrated the auto-oxidation of 3-alkyl-2-phenylindole using **10a** as a representative. After the ^{1}H NMR acquisition, the crude reaction mixtures containing **10a** were kept in $CDCl_3$ at room temperature for four weeks. Then, the mixtures were purified to afford **17**.[3b] The proposed auto-oxidation of **10a** to **17** was illustrated below.



References:

1. B. Witkop and J. B. Patrick, *J. Am. Chem. Soc.*, 1952, **74**, 3855.

2. (*a*) M. S. Masako Nakagawa, Yasuji Watanabe, Tohru Hino, Yasumaru Hatanaka, and Yuichi Kanaoka, *Heterocycles*, 1982, **19**, 503; (*b*) F. McCarpa and P. V. Long, *Tetrahedron Lett.*, 1981, **22**, 3009; (*c*) B. Robinson and M. U. Zubair, *Tetrahedron*, 1973, **29**, 1429; (*d*) B. Robinson and M. U. Zubair, *J. Chem. Soc. C*, 1971, 976.

3. (*a*) W. Ding, Q.-Q. Zhou, J. Xuan, T.-R. Li, L.-Q. Lu and W.-J. Xiao, *Tetrahedron Lett.*, 2014, **55**, 4648; (*b*) A. Alberti, P. Astolfi, P. Carloni, D. Döpp, L. Greci, C. Rizzoli and P. Stipa, *Tetrahedron*, 2011, **67**, 6889.

Regioisomeric ratios from ^{1}H-NMR of the crude reaction mixtures and the isolated yields.

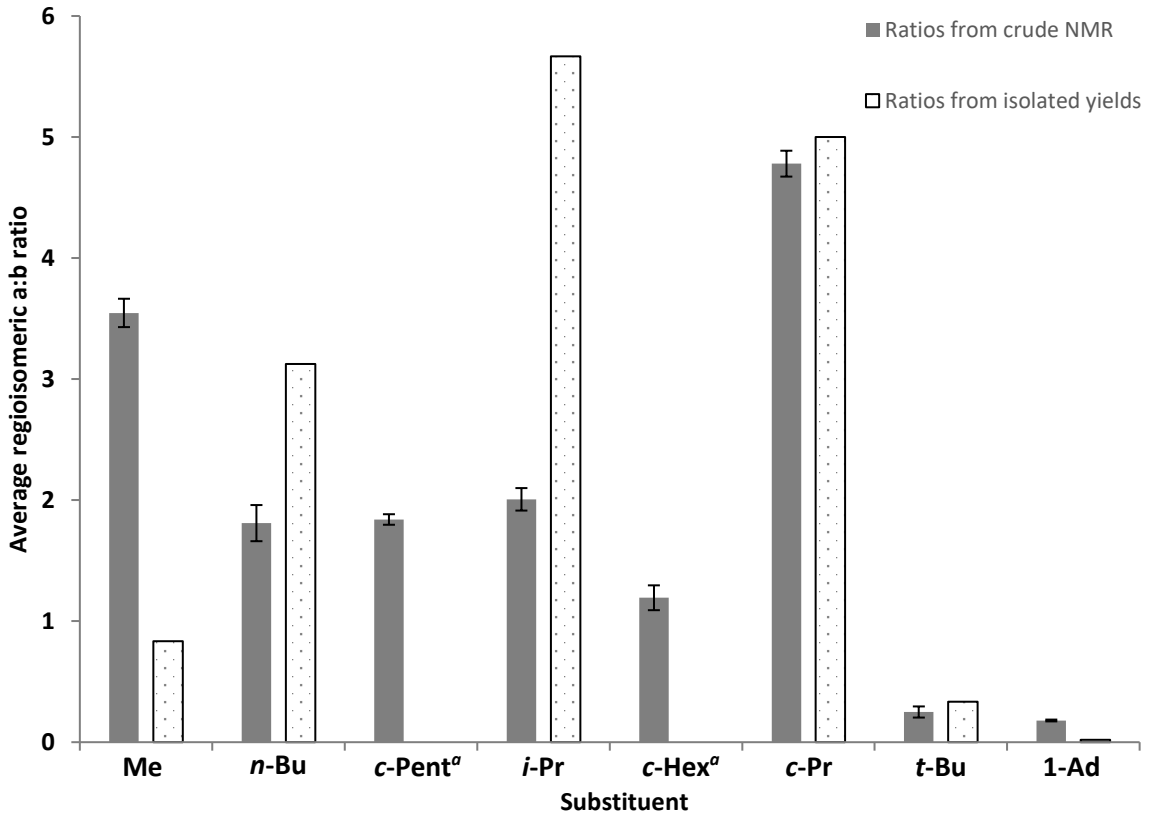


Figure S1. Correlation between substituent and average regioisomeric ratio determined by ^{1}H NMR of crude reaction mixture and isolated yields.

[a]Only one regioisomer was purified to homogeneity.

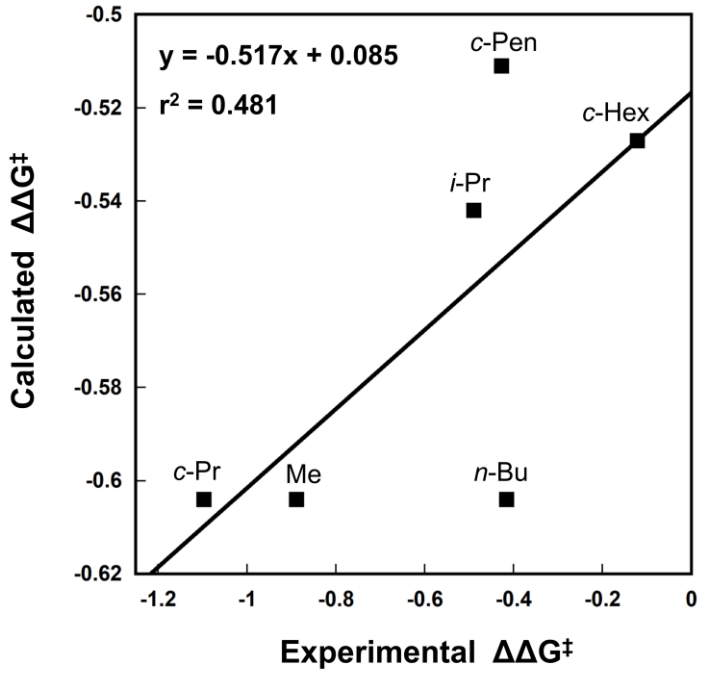


Figure S2. Correlation between predicted and experimental $\Delta\Delta G^{\ddagger}$ (kcal/mol) without the *t*-Bu and 1-Ad groups

Linear regression with wSterimol steric parameter

The Boltzmann-weighted Sterimol parameters (wSterimol) were obtained according to the protocol previously reported. (Brethomé, A. V.; Fletcher, S. P.; Paton, R. S. Conformational effects on physical-organic descriptors: The case of sterimol steric parameters. *ACS Catal.* **2019**, 2313-2323.) The calculated wB_1, wB_5, and wL are listed in **Table S1**.

Table S1. List of calculated wSterimol steric parameters utilized in the linear free energy relationship analysis.

entry	R	wSterimol		
		wB_1	wB_5	wL
1	Me	1.88	2.02	3.42
2	*n*-Bu	1.88	4.66	6.08
3	*c*-Pen	1.94	3.60	5.71
4	*i*-Pr	1.92	3.18	4.57
5	*c*-Hex	1.93	3.50	6.66
6	*c*-Pr	1.88	3.26	4.57
7	*t*-Bu	2.76	3.19	4.55
8	1-Ad	3.17	3.51	6.63

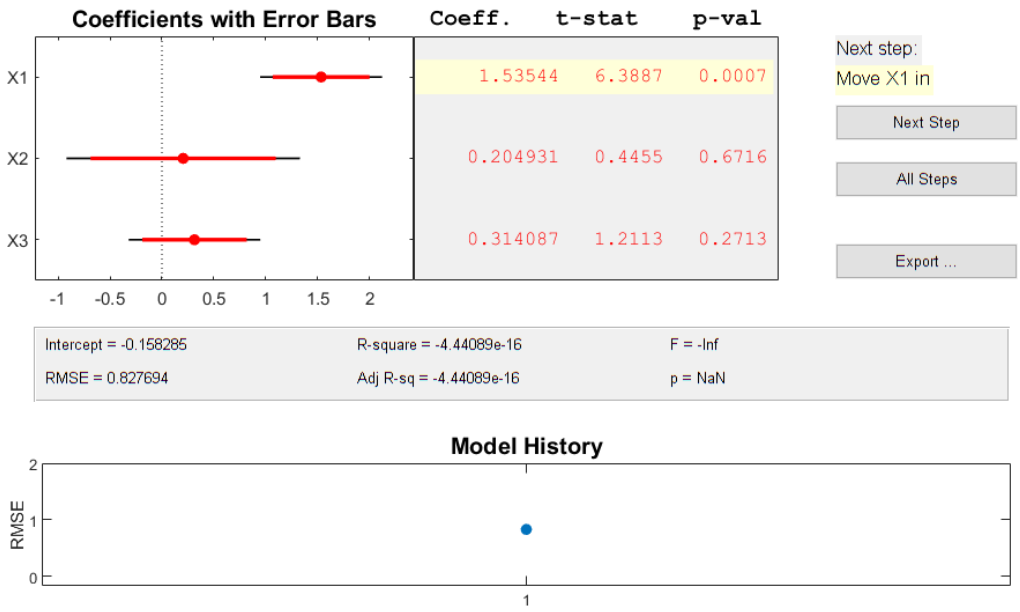
Subsequently, the model was constructed from the $\Delta\Delta G^{‡}$ (Estimated at 353.15 K (80 °C), $\Delta\Delta G^{‡} = -RT \ln(\mathbf{a}/\mathbf{b})$, R = 0.001986 kcal K^{-1} mol^{-1}) and the wSterimol parameters using Matlab™ software with statistics toolbox to perform the stepwise linear regression. Matrices **X** and **Y** (**Table S2**) were submitted to the Matlab™ software using **X** = [Matrix **X**] and **Y** = [Matrix **Y**] notations. (**Note:** X1 = wB_1, X2 = wB_5, and X3 = wL)

Table S2. Matrix formatting for the stepwise linear regression.

Y Group	**Matrix X**			**Matrix Y**
	X1	**X2**	**X3**	
Me	1.88	2.02	3.42	-0.889
n-Bu	1.88	4.66	6.08	-0.416
c-Pent	1.94	3.60	5.71	-0.428
i-Pr	1.92	3.18	4.57	-0.490
c-Hex	1.93	3.50	6.66	-0.122
c-Pr	1.88	3.26	4.57	-1.097
t-Bu	2.76	3.19	4.55	0.972
1-Ad	3.17	3.51	6.63	1.203

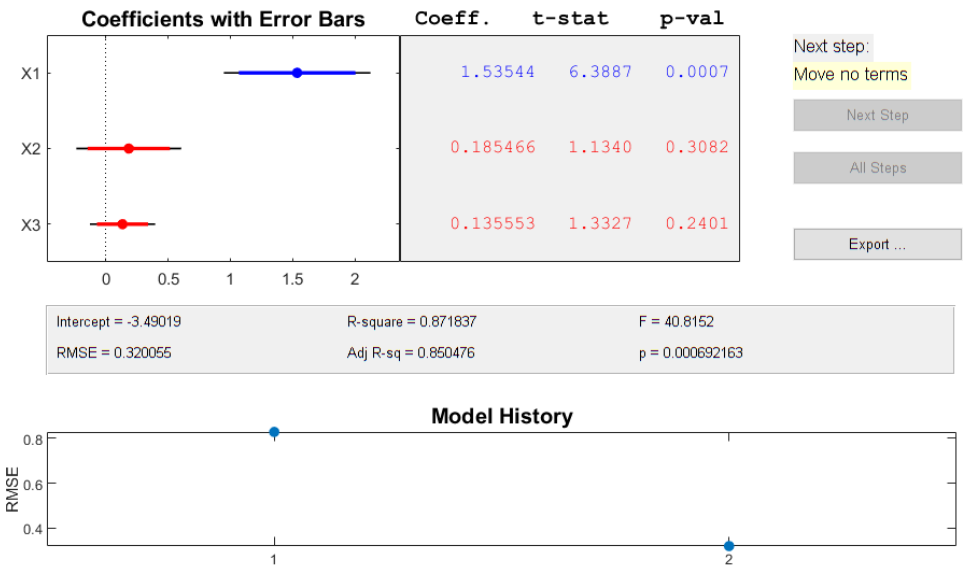
Next, the stepwise solver was initiated using the command "stepwise(**X**,**Y**)", this command produced the prompt window shown in **Figure S3a**.

Figure S3a. The stepwise regression prompt.



By clicking *All-Steps* button in the upper right box, the final iteration for regression is completed, as shown in **Figure S3b**.

Figure S3b. Final iteration in the stepwise regression.



Finally, the model was obtained together with its statistic parameters, as shown in equation 1.

$$\mathbf{\Delta\Delta G^{\ddagger}} = -3.49019 + 1.53544\mathbf{wB_1} \quad \textbf{(1)}$$

$$R^2 = 0.872,\ RMSE = 0.320,\ F = 40.82,\ p = 0.00069,\ q^2 = 0.748,$$

$$(R^2\text{-}R_0^2)/R^2 = -0.147,\ k = 1.000$$

The regioselectivity of the Larock heteroannulation reaction was then predicted, as demonstrated in **Table S3**.

Table S3. Experimental values compared to predicted values from equation **1** for the regioselectivity of the Larock reaction.

Entry	R	estimated ΔΔG‡	predicted ΔΔG‡
1	Me	-0.889	-0.604
2	*n*-Bu	-0.416	-0.604
3	*c*-Pent	-0.428	-0.511
4	*i*-Pr	-0.490	-0.542
5	*c*-Hex	-0.122	-0.527
6	*c*-Pr	-1.097	-0.604
7	*t*-Bu	0.972	0.748
8	1-Ad	1.203	1.377

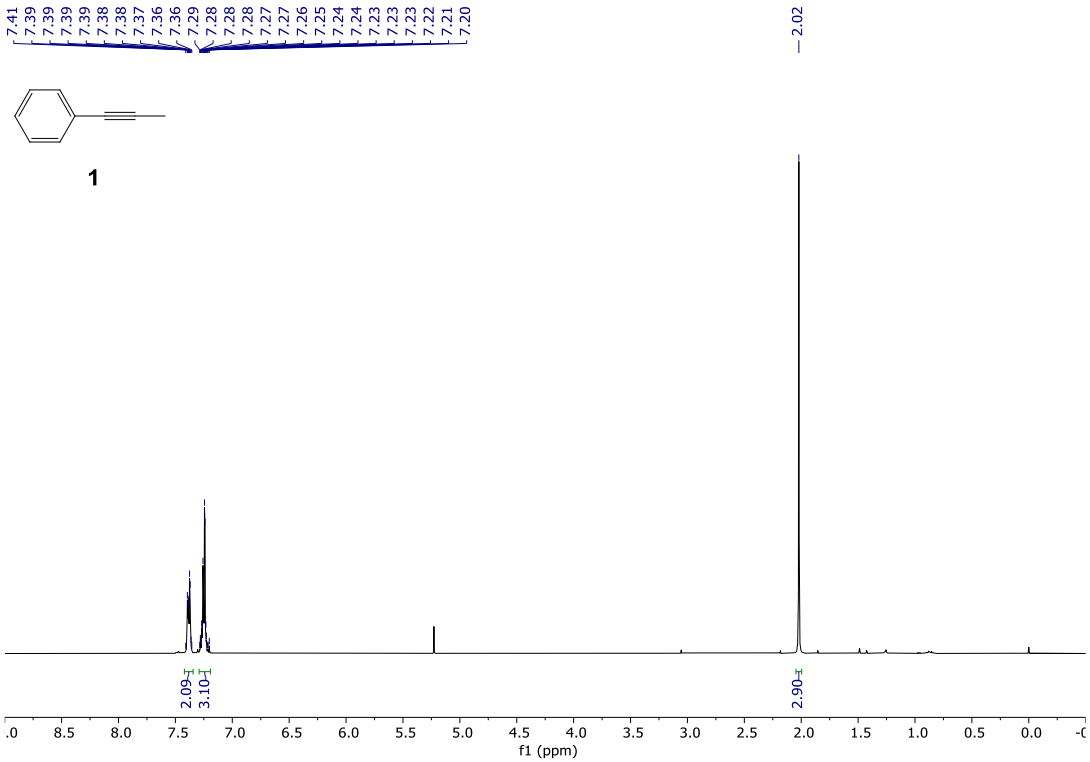


Figure S4. ^{1}H NMR spectrum (400 MHz) of prop-1-yn-1-ylbenzene (**1**) in $CDCl_3$

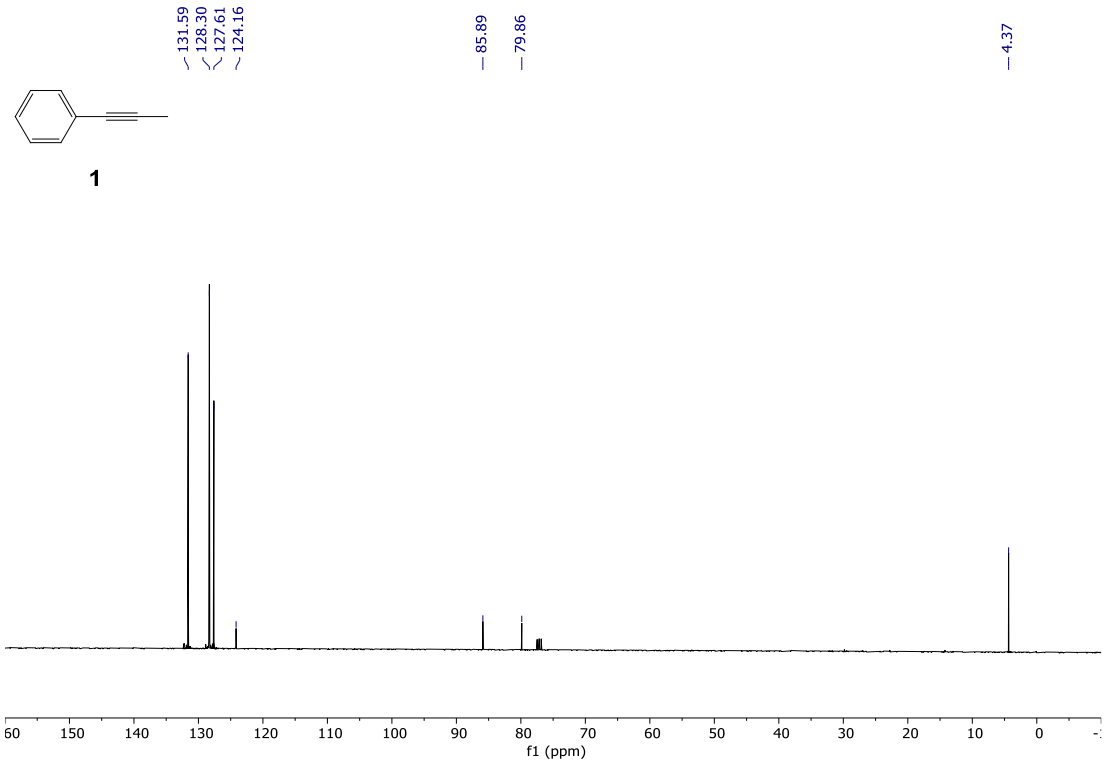


Figure S5. $^{13}C\{^{1}H\}$ NMR spectrum (100 MHz) of prop-1-yn-1-ylbenzene (**1**) in $CDCl_3$

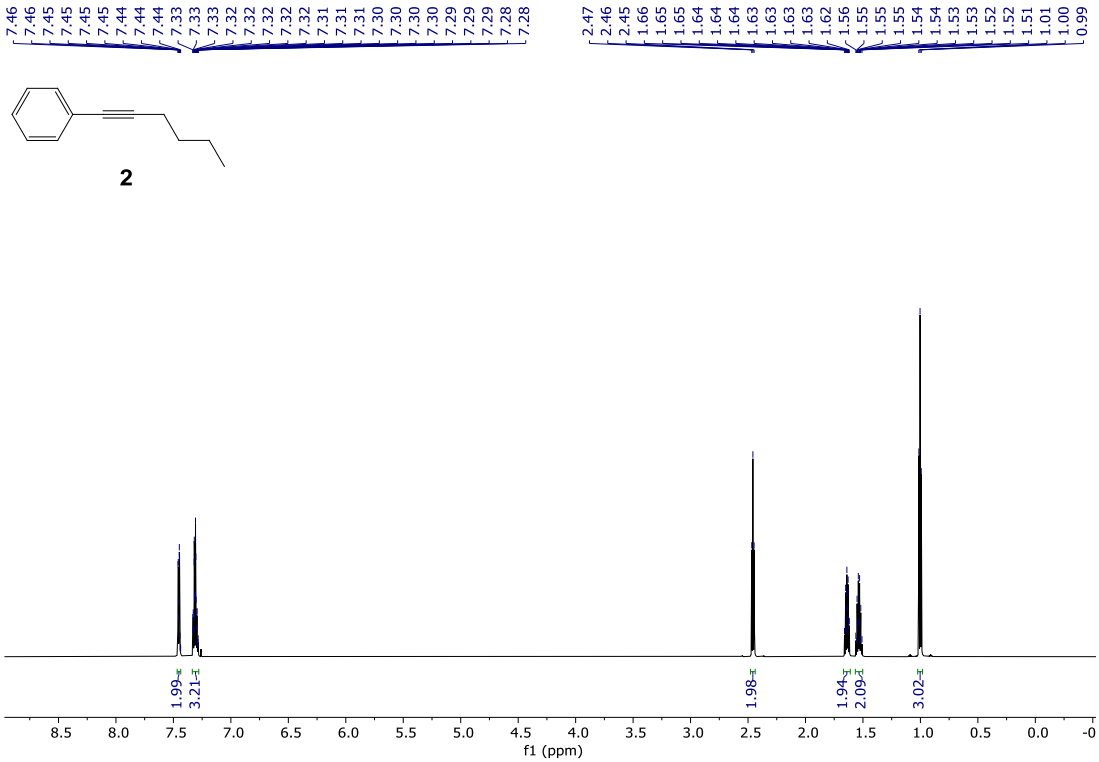


Figure S6. ^{1}H NMR spectrum (700 MHz) of hex-1-yn-1-ylbenzene (**2**) in $CDCl_3$

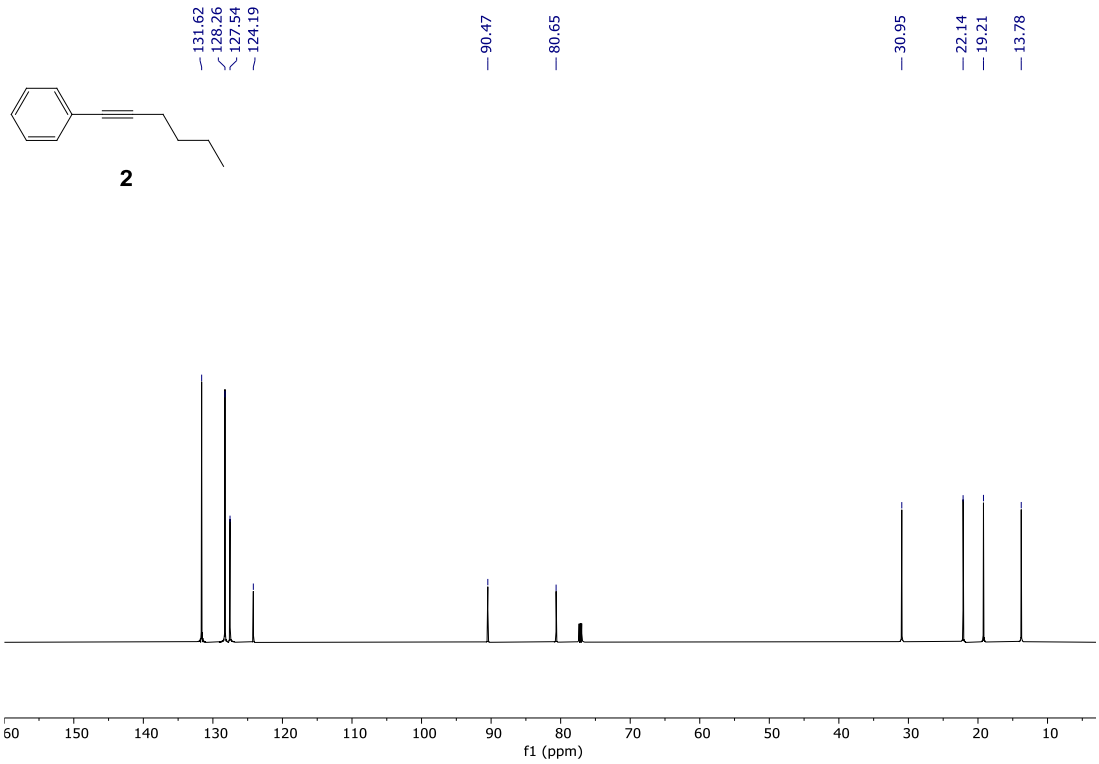


Figure S7. $^{13}C\{^{1}H\}$ NMR spectrum (175 MHz) of hex-1-yn-1-ylbenzene (**2**) in $CDCl_3$

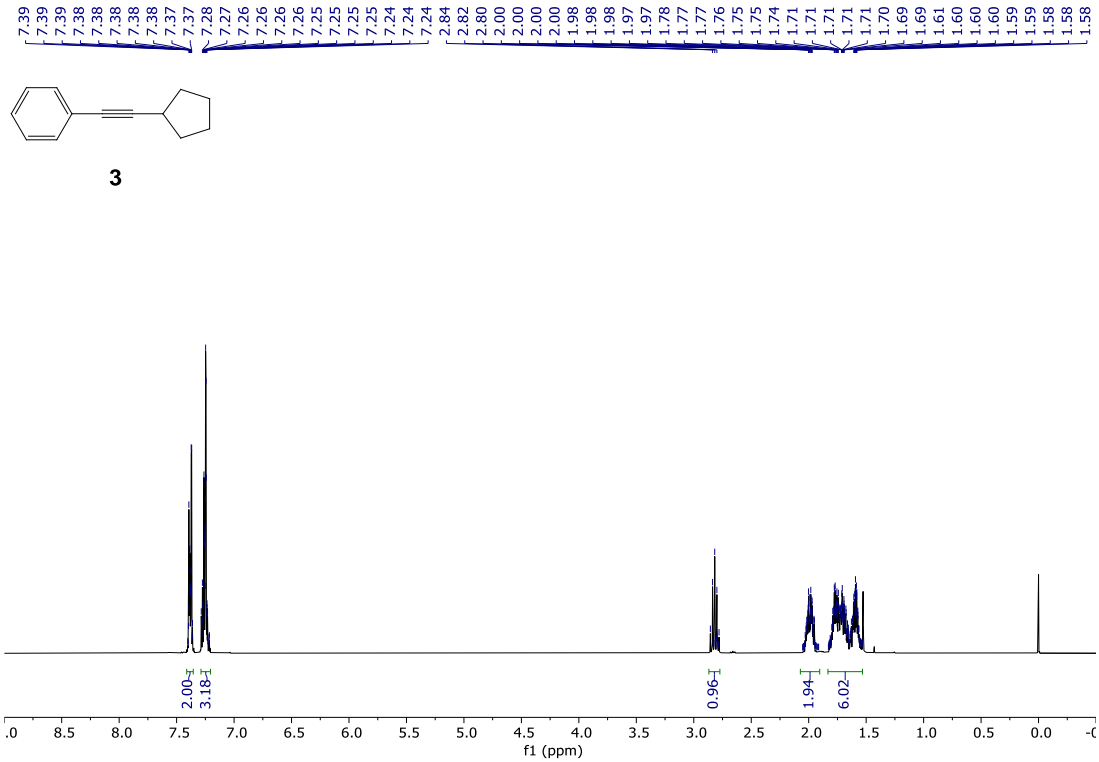


Figure S8. ^{1}H NMR spectrum (400 MHz) of (cyclopentylethynyl)benzene (**3**) in $CDCl_3$

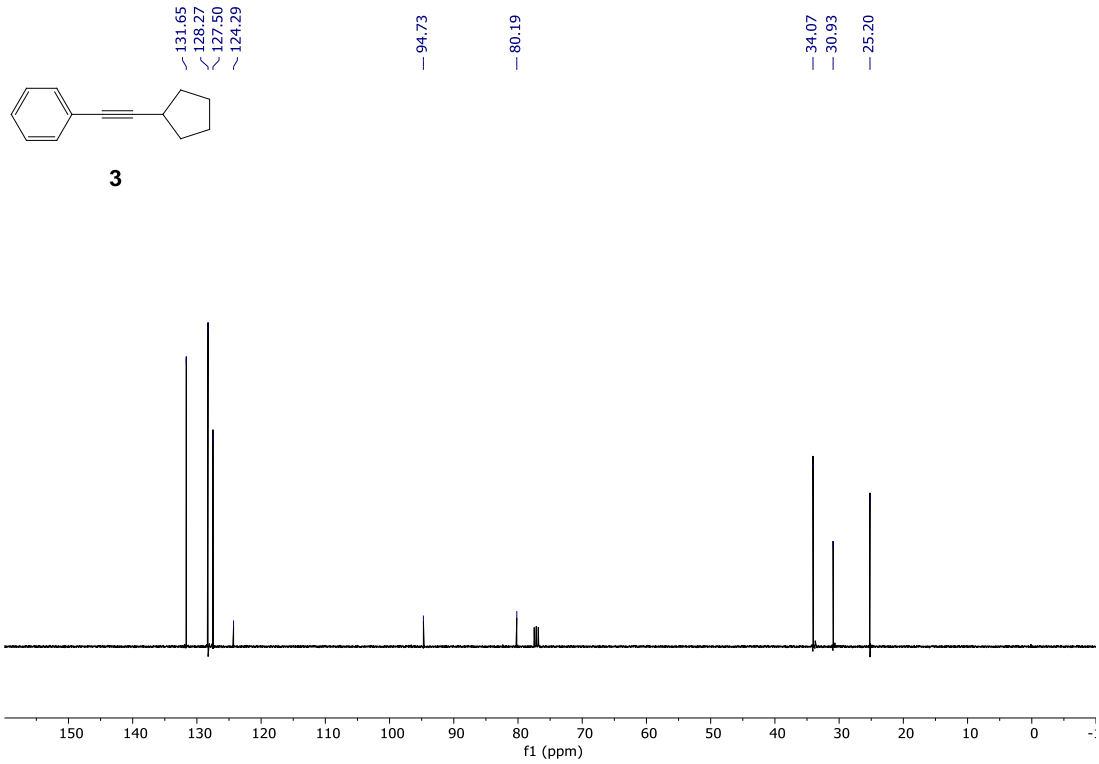


Figure S9. $^{13}C\{^{1}H\}$ NMR spectrum (100 MHz) of (cyclopentylethynyl)benzene (**3**) in $CDCl_3$

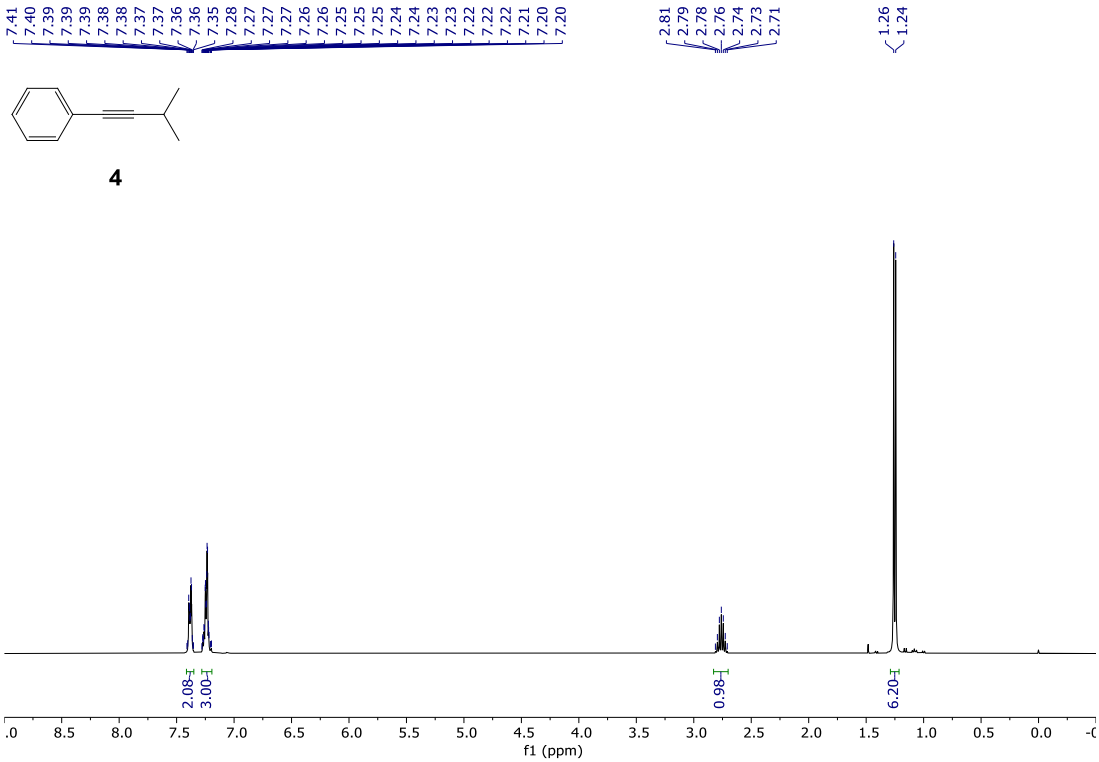


Figure S10. ^{1}H NMR spectrum (400 MHz) of (3-methylbut-1-yn-1-yl)benzene (**4**) in $CDCl_3$

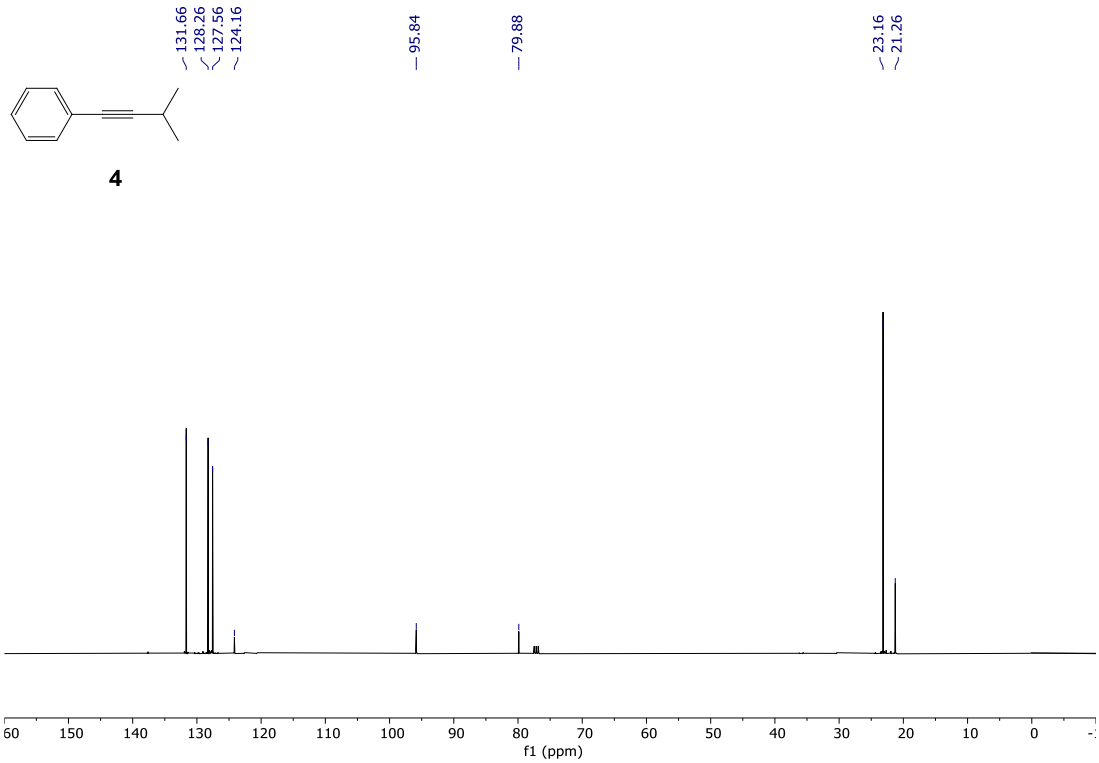


Figure S11. $^{13}C\{^{1}H\}$ NMR spectrum (100 MHz) of (3-methylbut-1-yn-1-yl)benzene (**4**) in $CDCl_3$

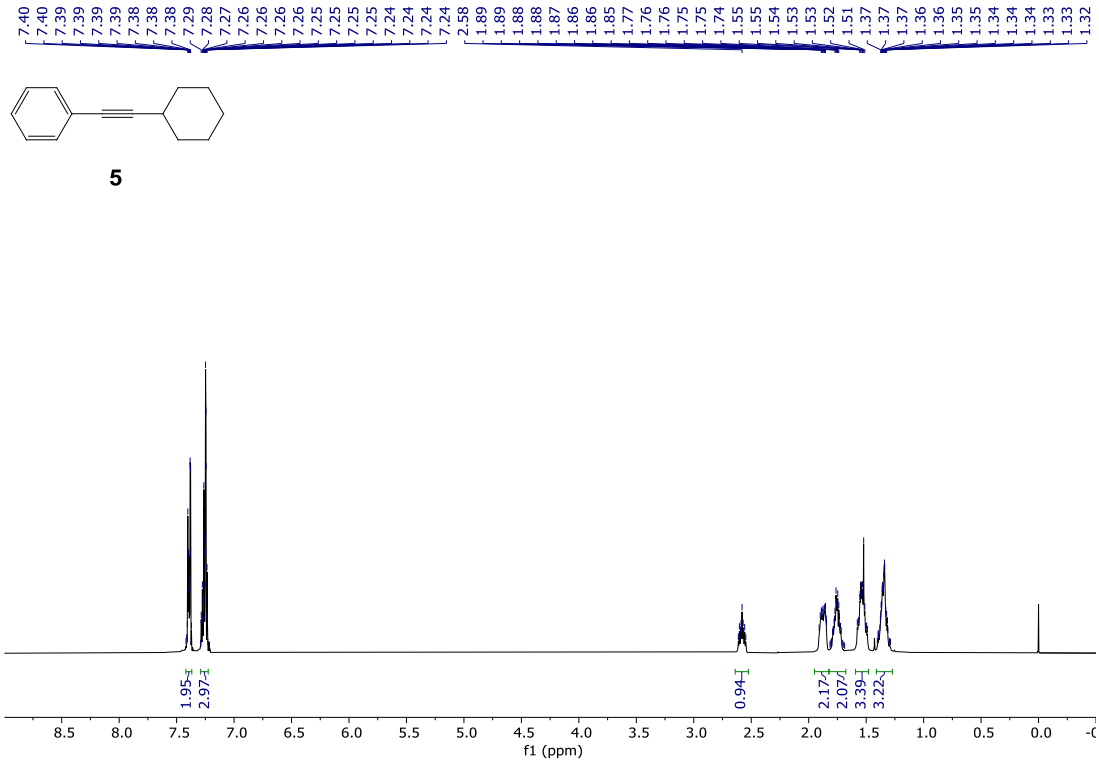


Figure S12. ^{1}H NMR spectrum (400 MHz) of (cyclohexylethynyl)benzene (**5**) in $CDCl_3$

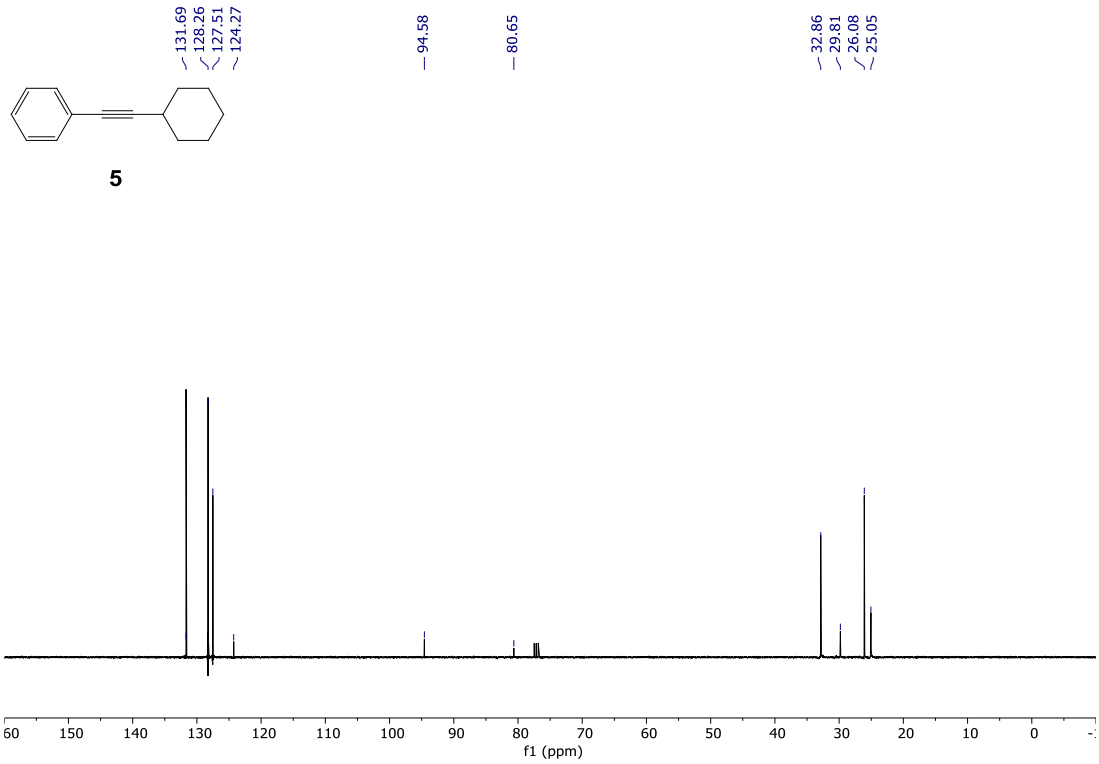


Figure S13. ^{13}C{^{1}H} NMR spectrum (100 MHz) of (cyclohexylethynyl)benzene (**5**) in $CDCl_3$

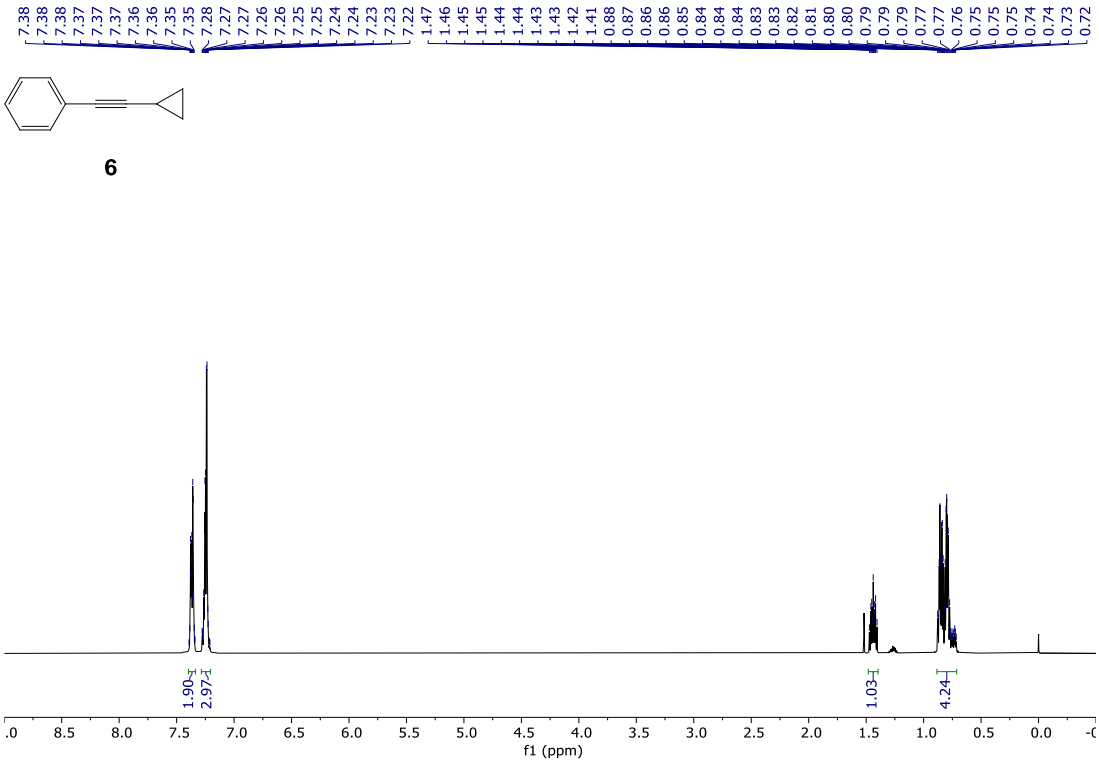


Figure S14. ^{1}H NMR spectrum (400 MHz) of (cyclopropylethynyl)benzene (**6**) in $CDCl_3$

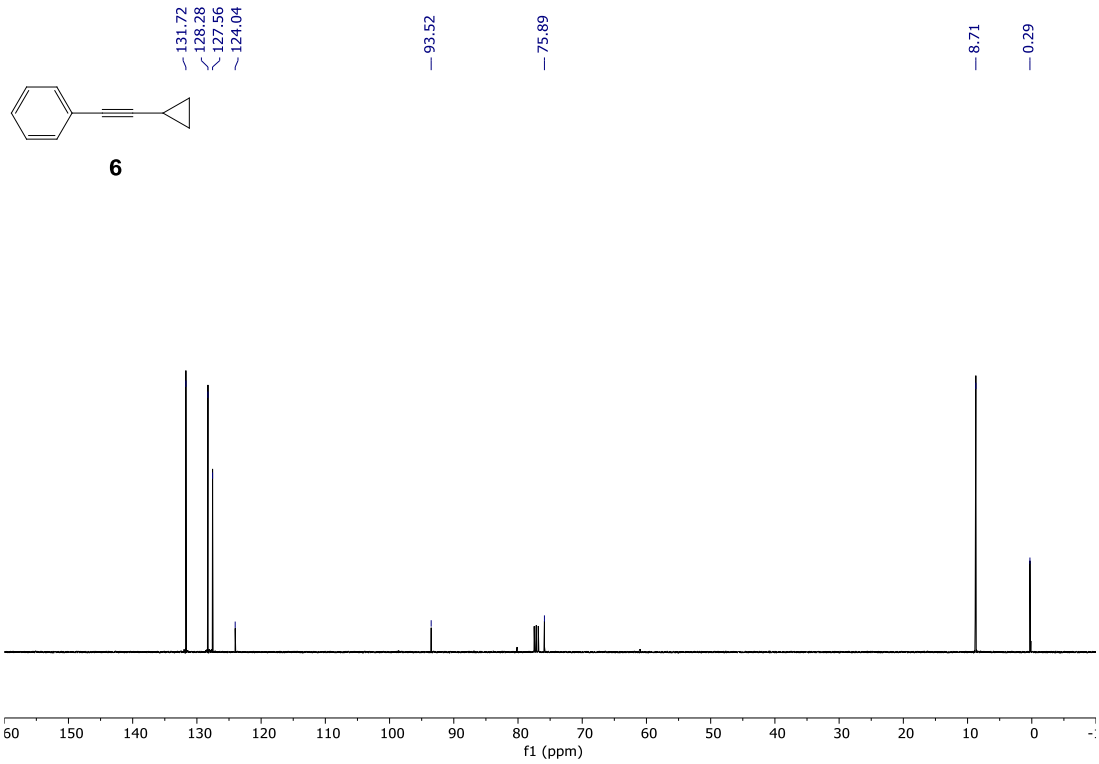


Figure S15. $^{13}C\{^{1}H\}$ NMR spectrum (100 MHz) of (cyclopropylethynyl)benzene (**6**) in $CDCl_3$

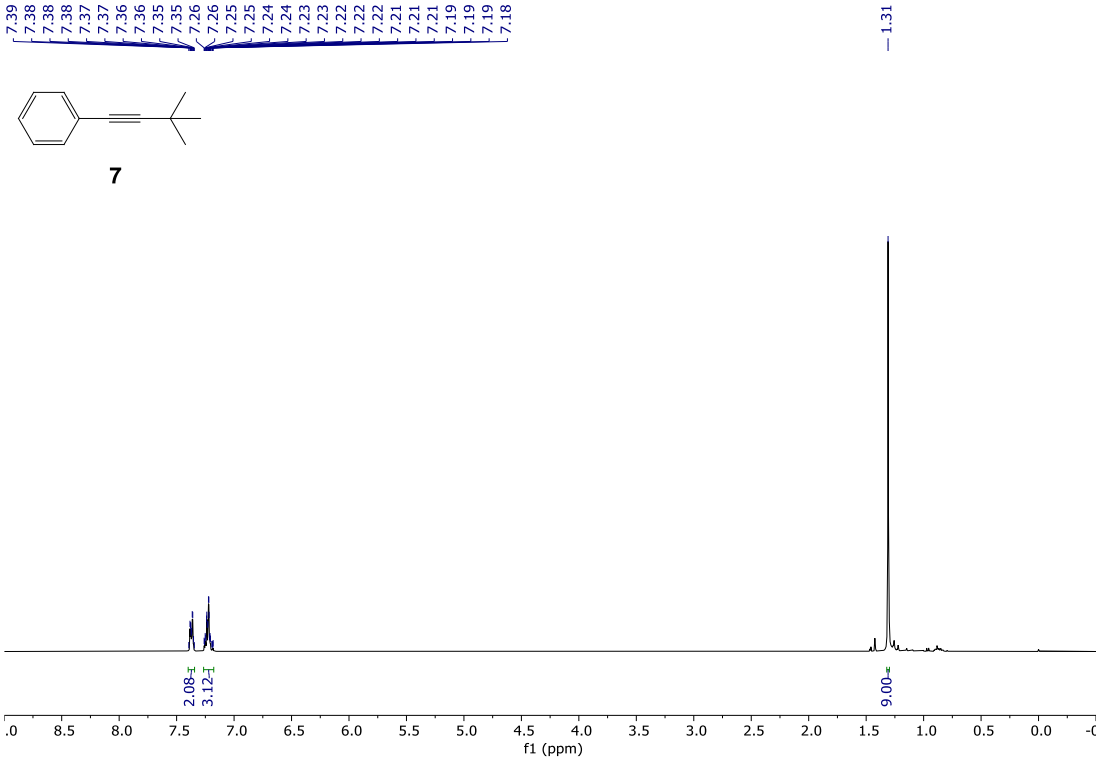


Figure S16. ^{1}H NMR spectrum (400 MHz) of (3,3-dimethylbut-1-yn-1-yl)benzene (**7**) in $CDCl_3$

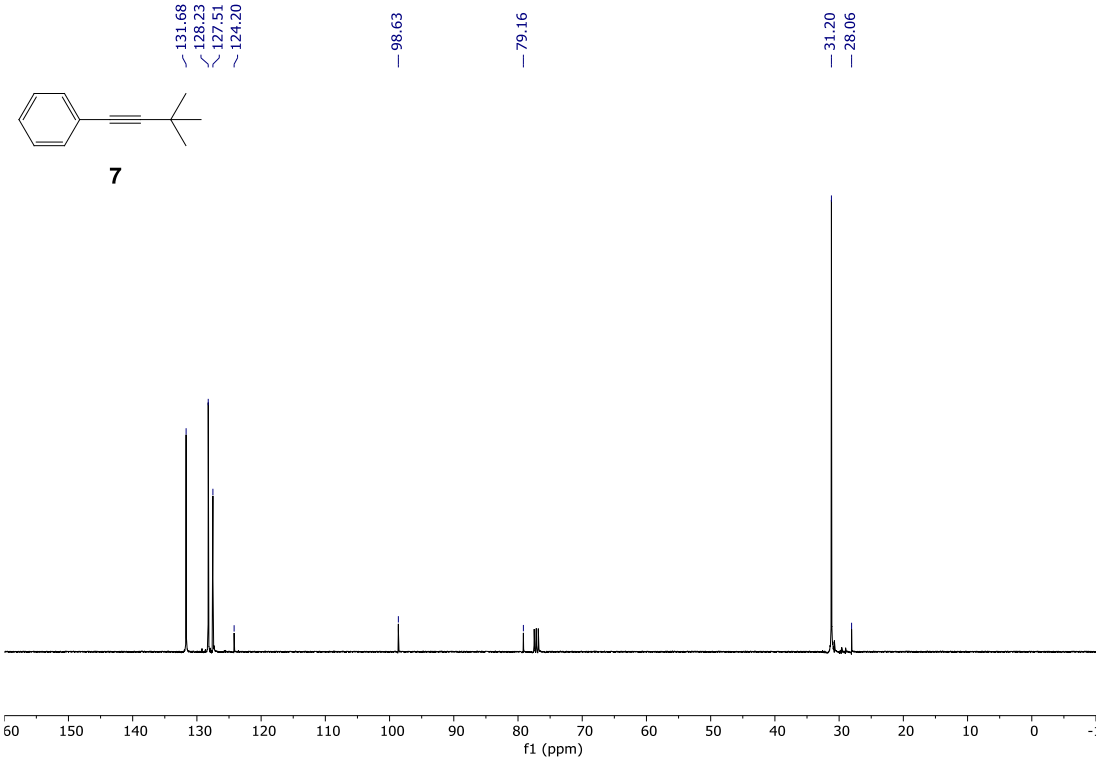


Figure S17. $^{13}C\{^{1}H\}$ NMR spectrum (100 MHz) of (3,3-dimethylbut-1-yn-1-yl)benzene (**7**) in $CDCl_3$

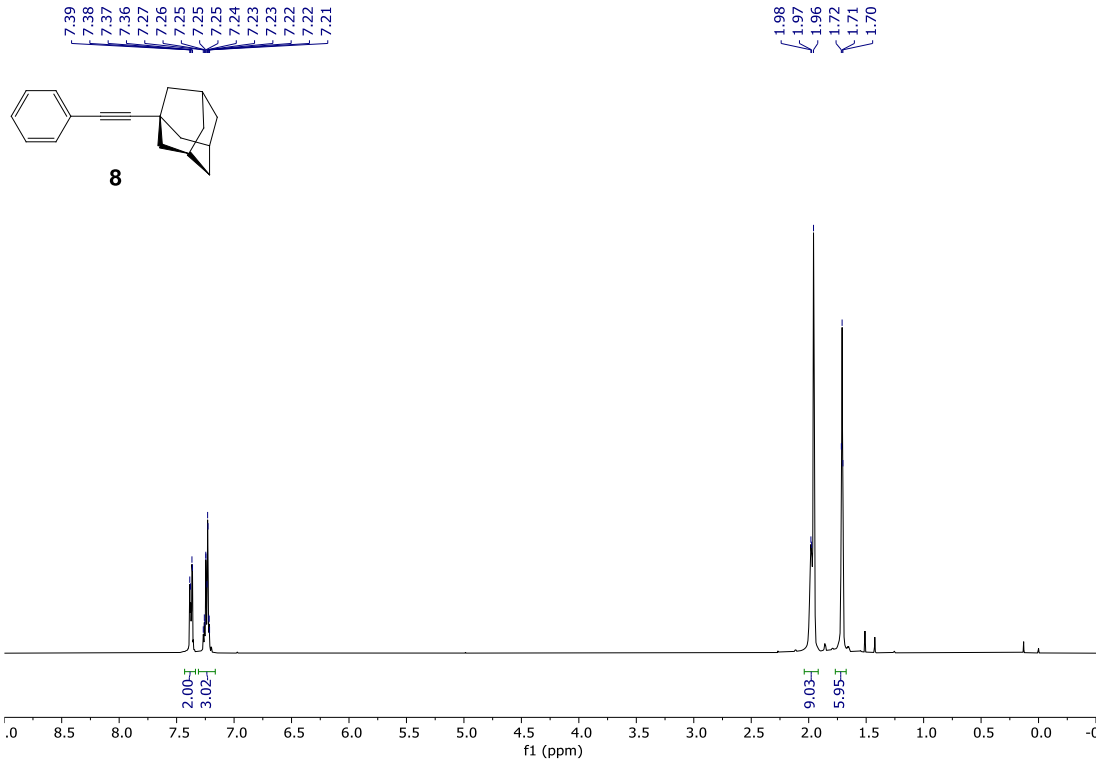


Figure S18. ^{1}H NMR spectrum (400 MHz) of 1-(phenylethynyl)adamantane (**8**) in $CDCl_3$

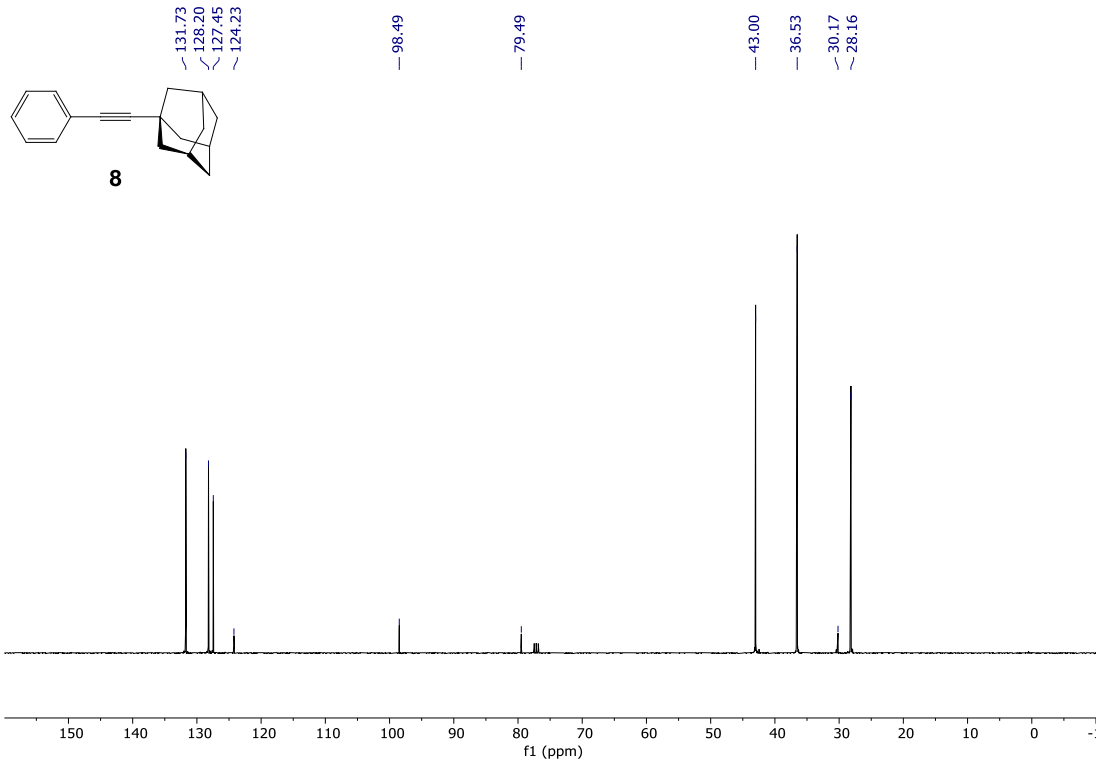


Figure S19. $^{13}C\{^{1}H\}$ NMR spectrum (100 MHz) of 1-(phenylethynyl)adamantane (**8**) in $CDCl_3$

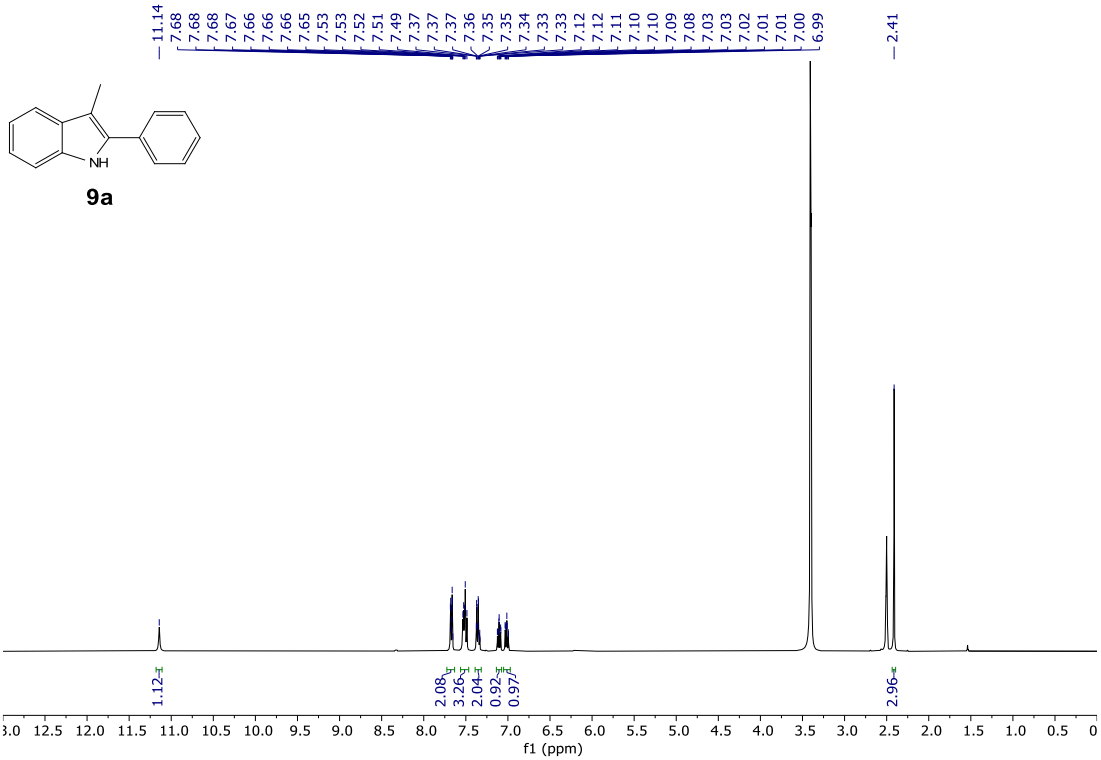


Figure S20. ^{1}H NMR spectrum (400 MHz) of 3-methyl-2-phenyl-1*H*-indole (**9a**) in DMSO-d_6

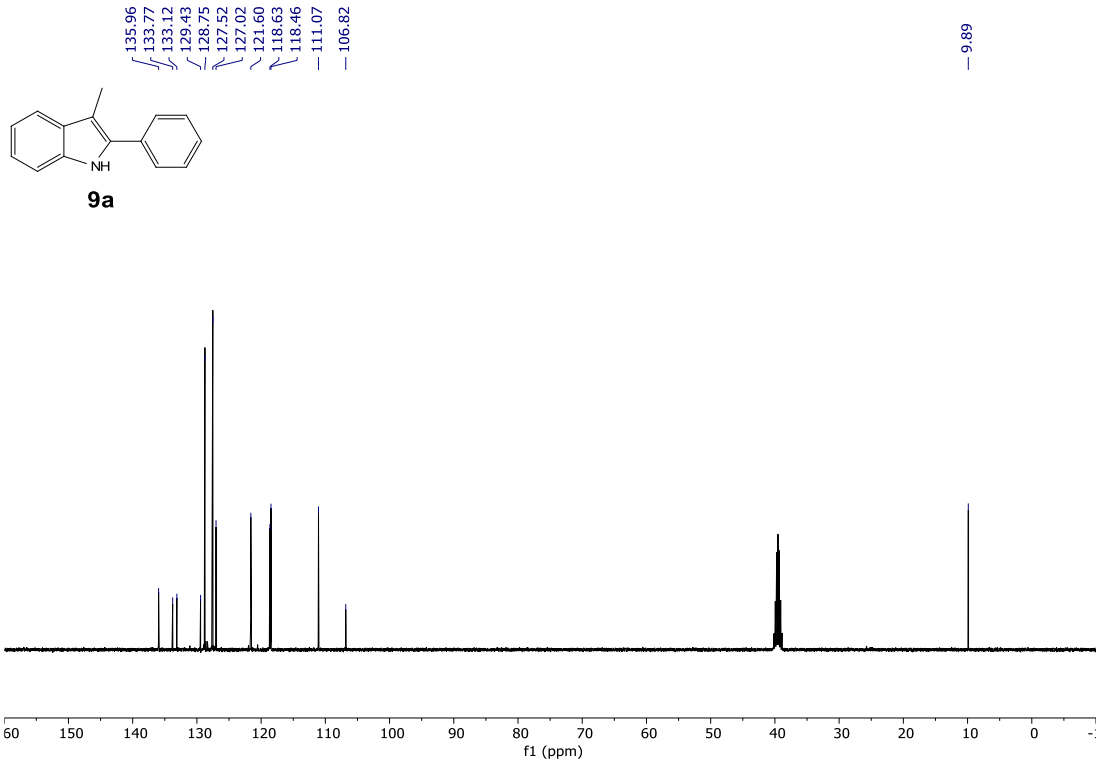


Figure S21. ^{13}C{^{1}H} NMR spectrum (100 MHz) of 3-methyl-2-phenyl-1*H*-indole (**9a**) in DMSO-d_6

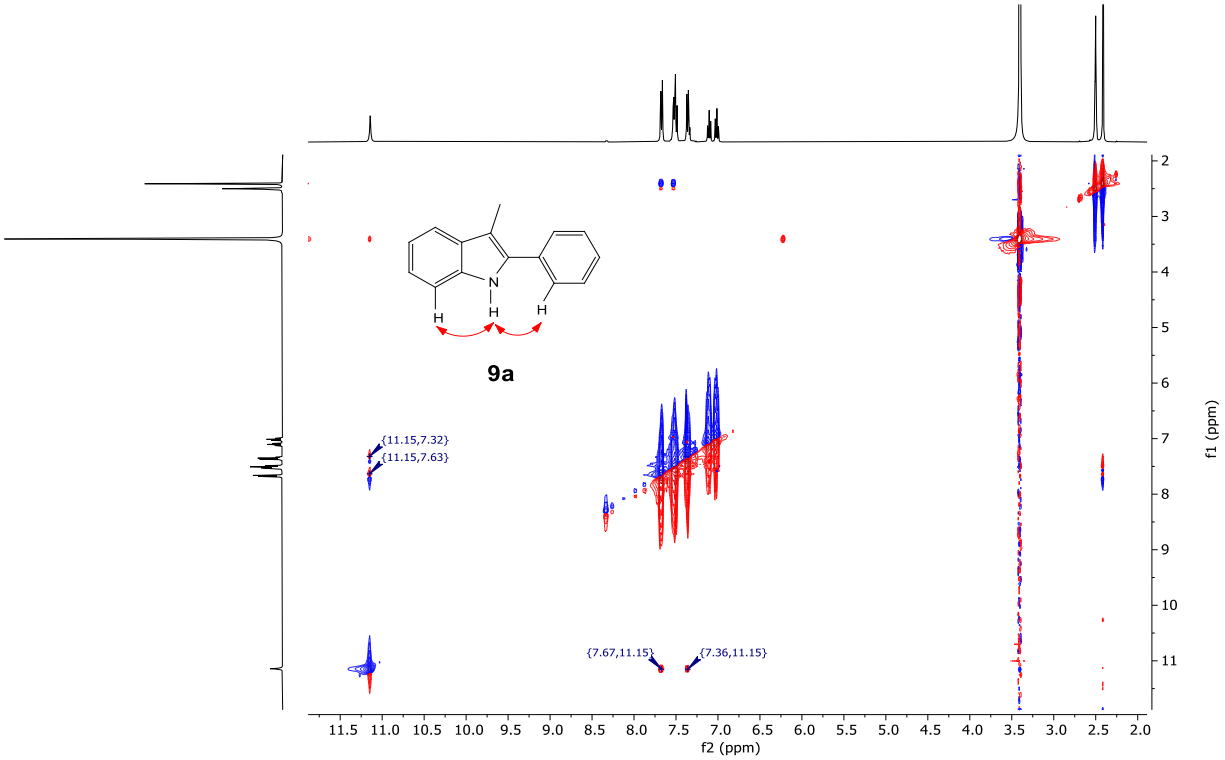


Figure S22. NOESY spectrum of 3-methyl-2-phenyl-1*H*-indole (**9a**) in DMSO-d_6

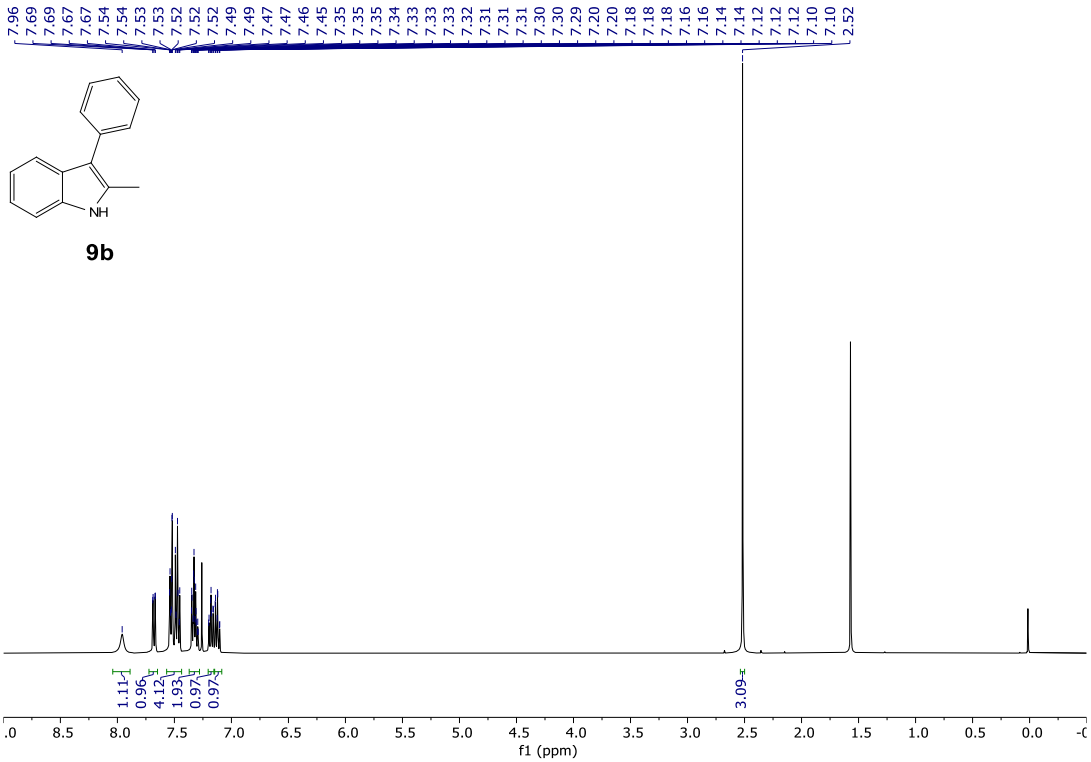


Figure S23. ^{1}H NMR spectrum (400 MHz) of 2-methyl-3-phenyl-1*H*-indole (**9b**) in $CDCl_3$

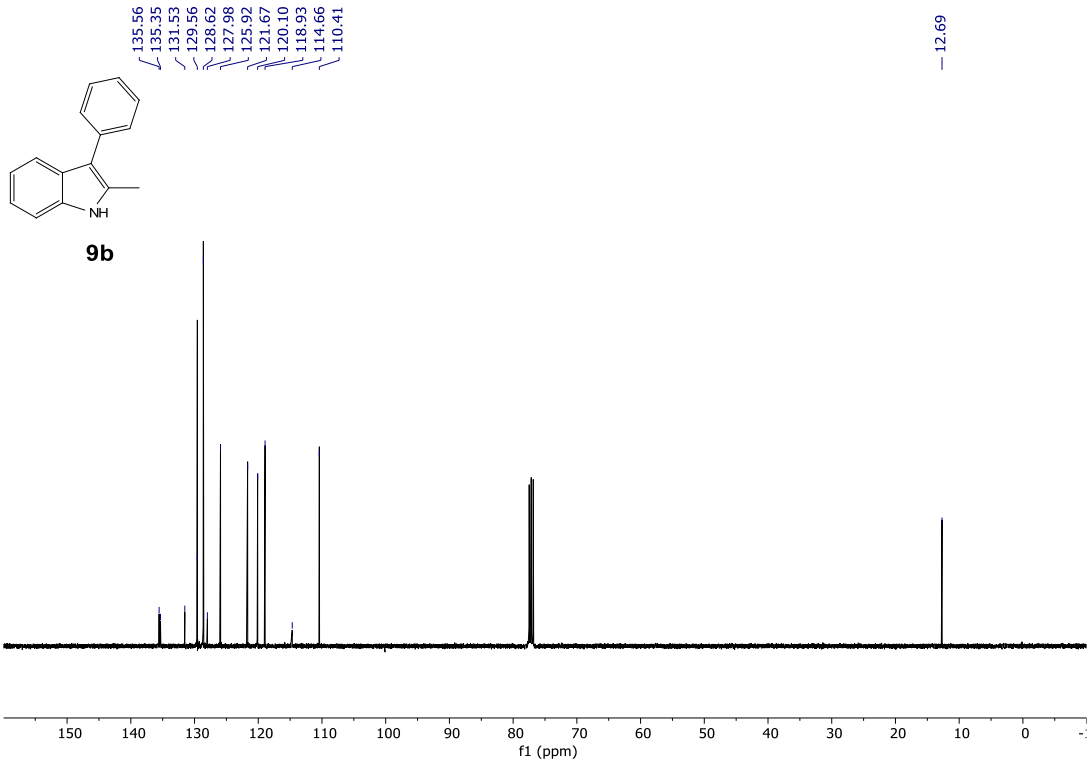


Figure S24. $^{13}C\{^{1}H\}$ NMR spectrum (100 MHz) of 2-methyl-3-phenyl-1*H*-indole (**9b**) in $CDCl_3$

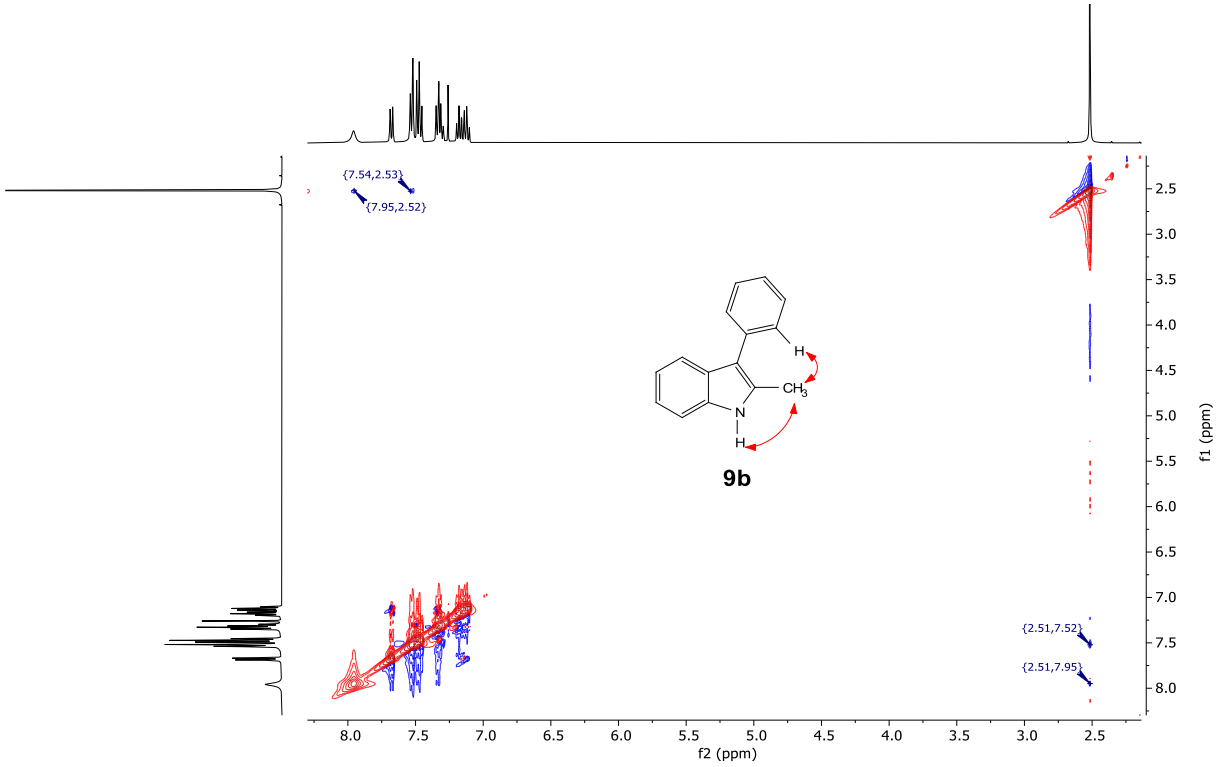


Figure S25. NOESY spectrum of 2-methyl-3-phenyl-1*H*-indole (**9b**) in $CDCl_3$

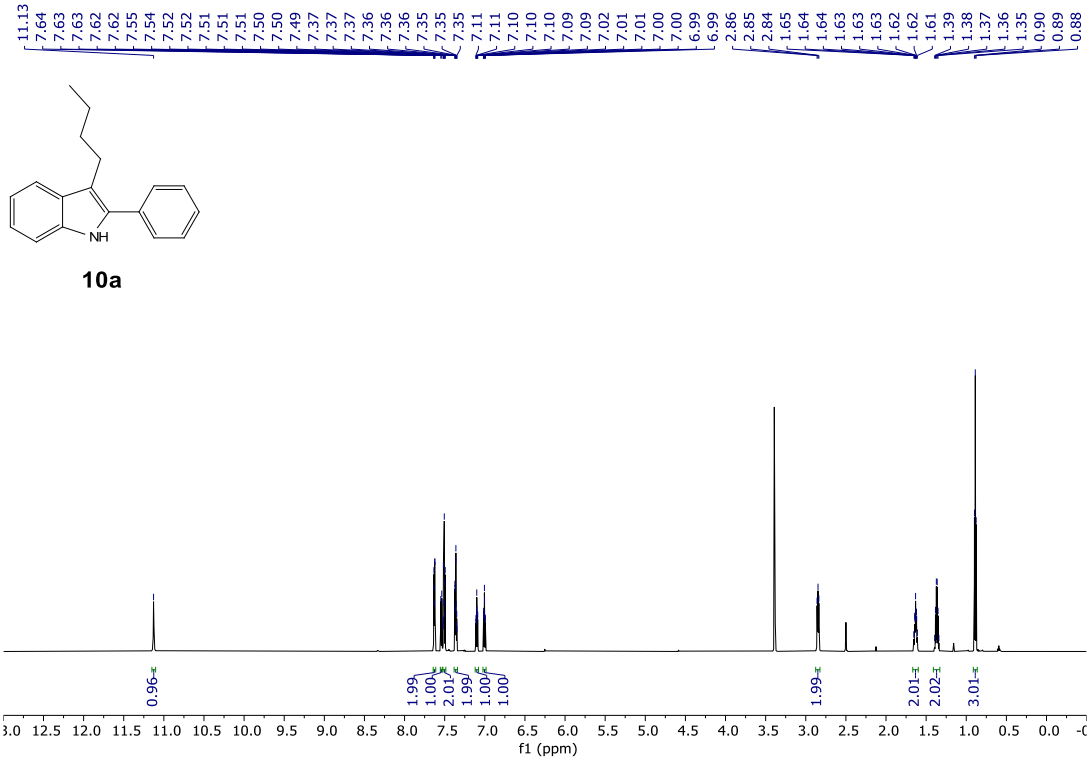


Figure S26. ^{1}H NMR spectrum (700 MHz) of 3-butyl-2-phenyl-1*H*-indole (**10a**) in DMSO-d_6

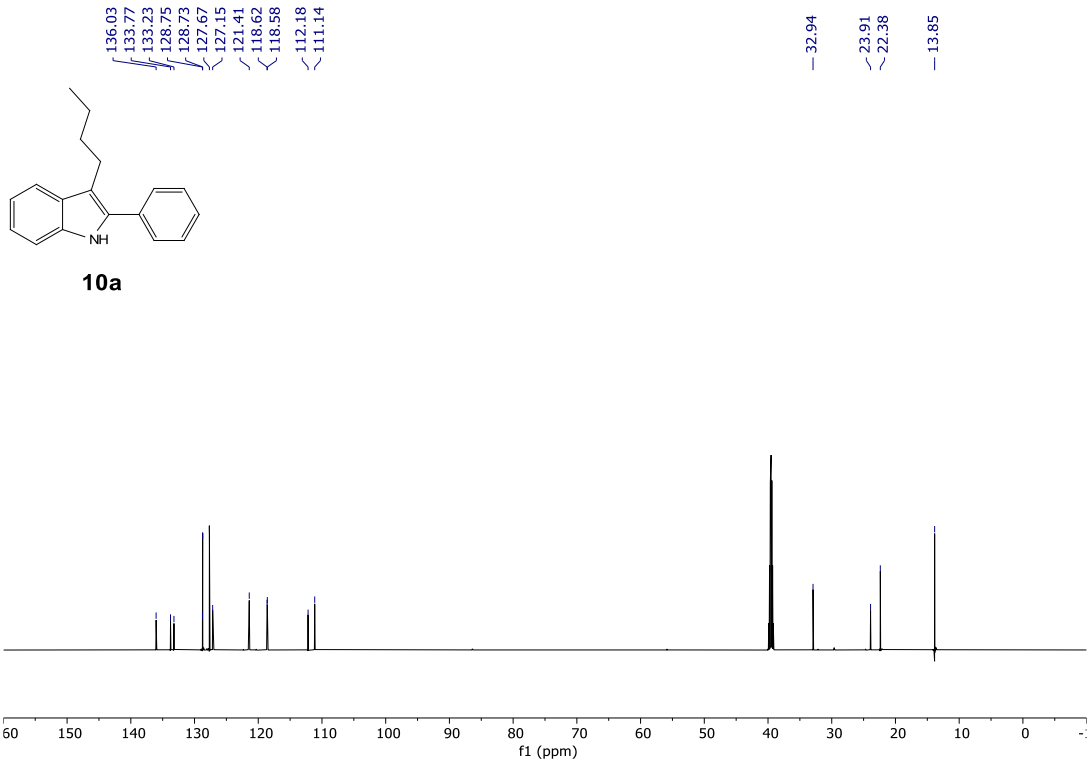


Figure S27. ^{13}C{^{1}H} NMR spectrum (175 MHz) of 3-butyl-2-phenyl-1*H*-indole (**10a**) in DMSO-d_6

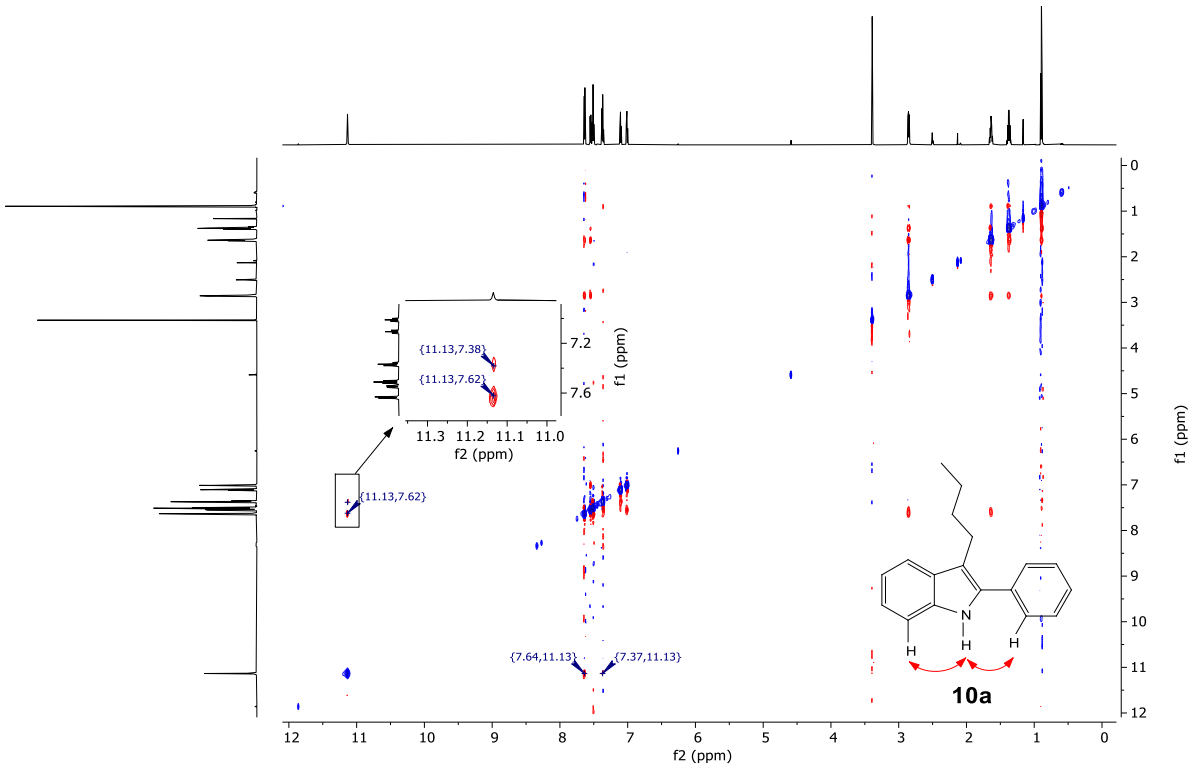


Figure S28. NOESY spectrum of 3-butyl-2-phenyl-1*H*-indole (**10a**) in DMSO-d_6

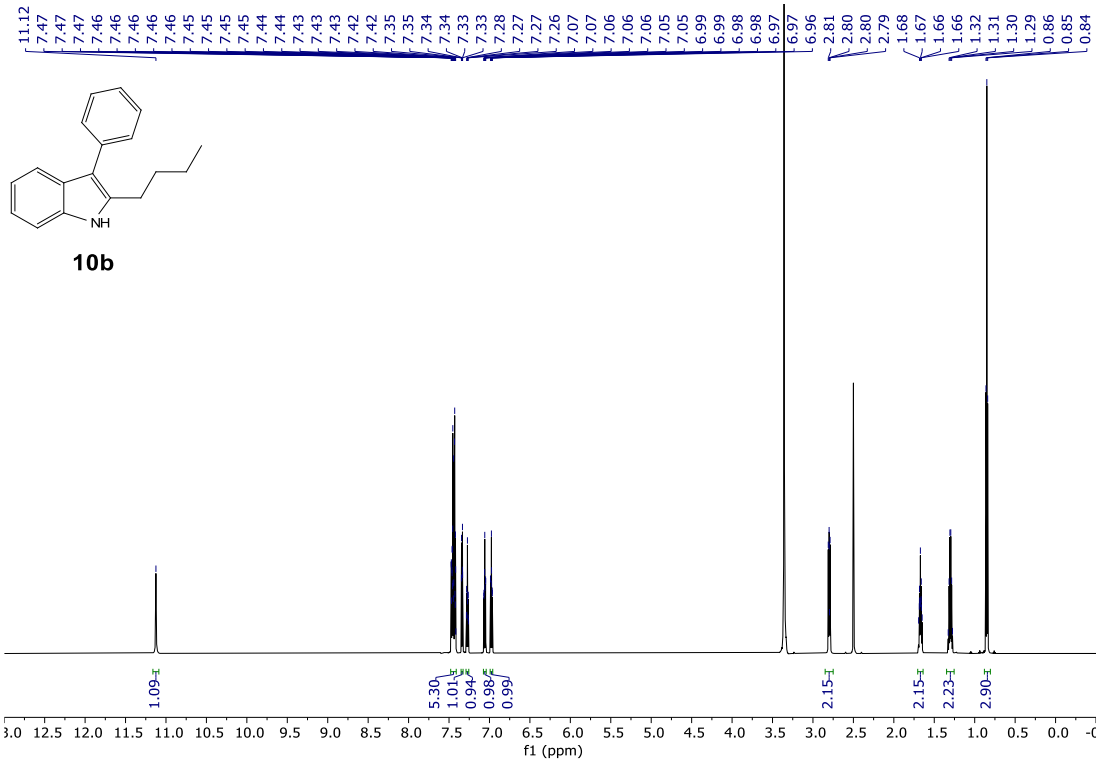


Figure S29. ^{1}H NMR spectrum (700 MHz) of 2-butyl-3-phenyl-1*H*-indole (**10b**) in DMSO-d_6

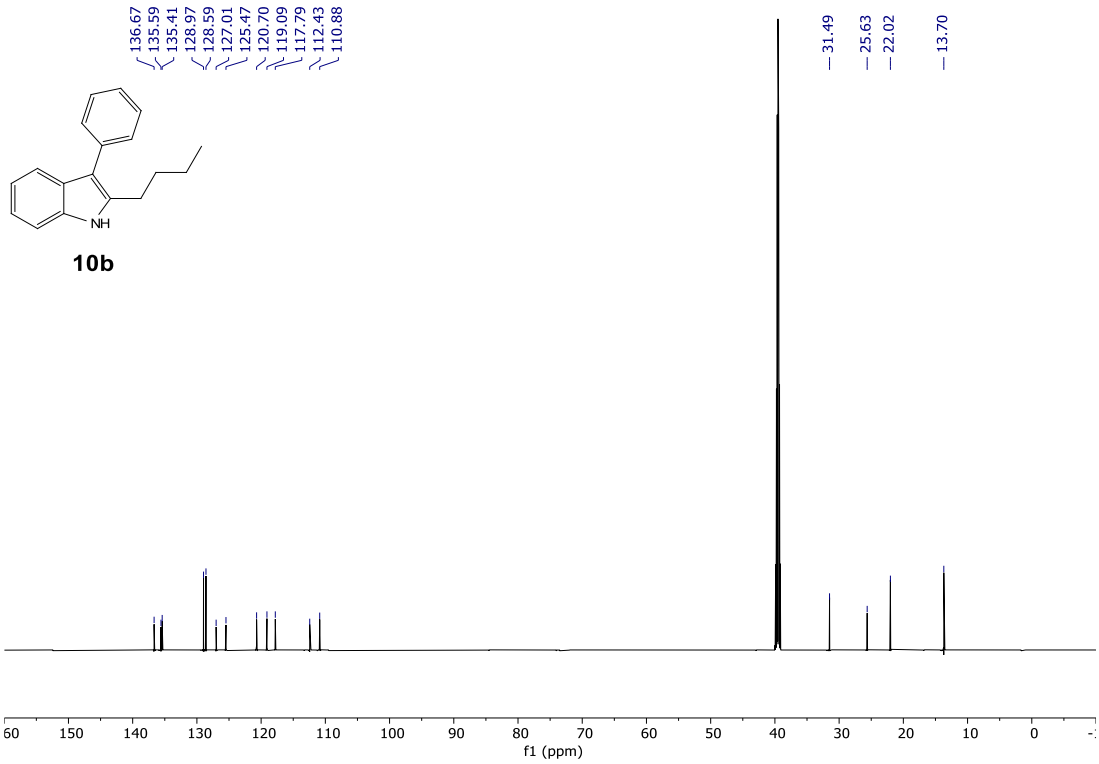


Figure S30. ^{13}C{^{1}H} NMR spectrum (175 MHz) of 2-butyl-3-phenyl-1*H*-indole (**10b**) in DMSO-d_6

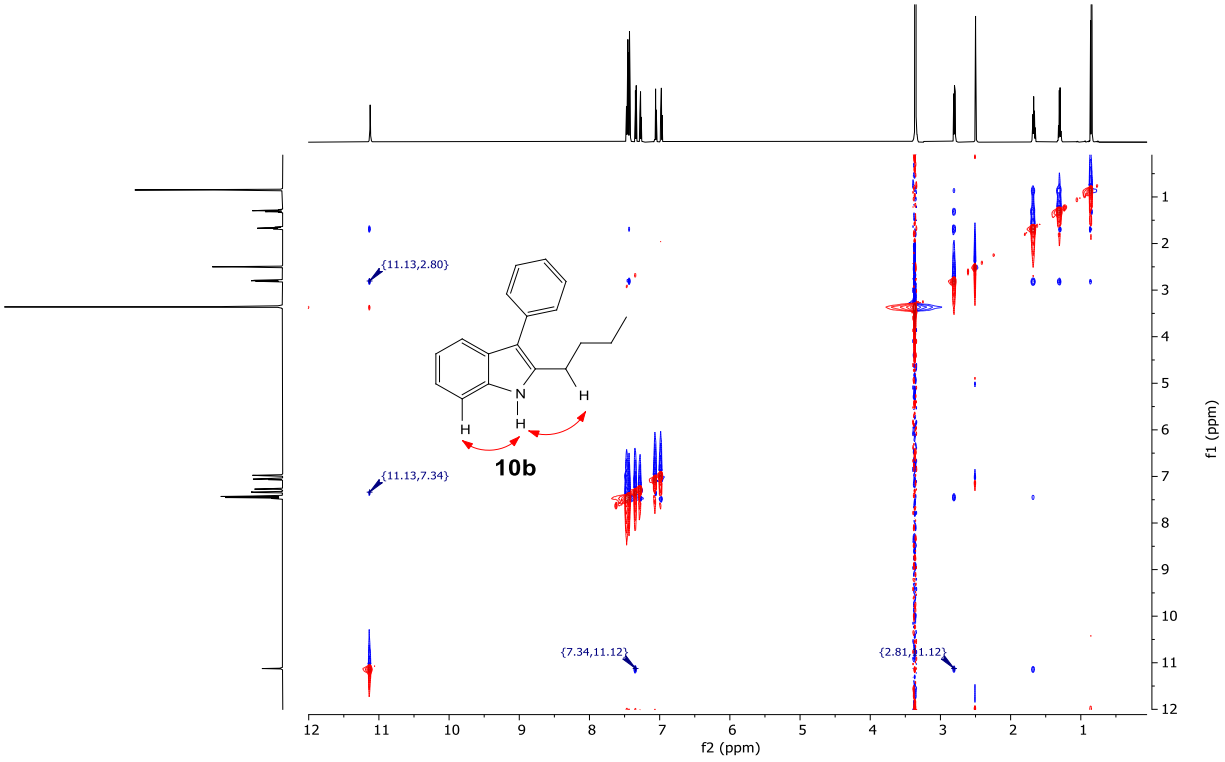


Figure S31. NOESY spectrum of 2-butyl-3-phenyl-1*H*-indole (**10b**) in DMSO-d_6

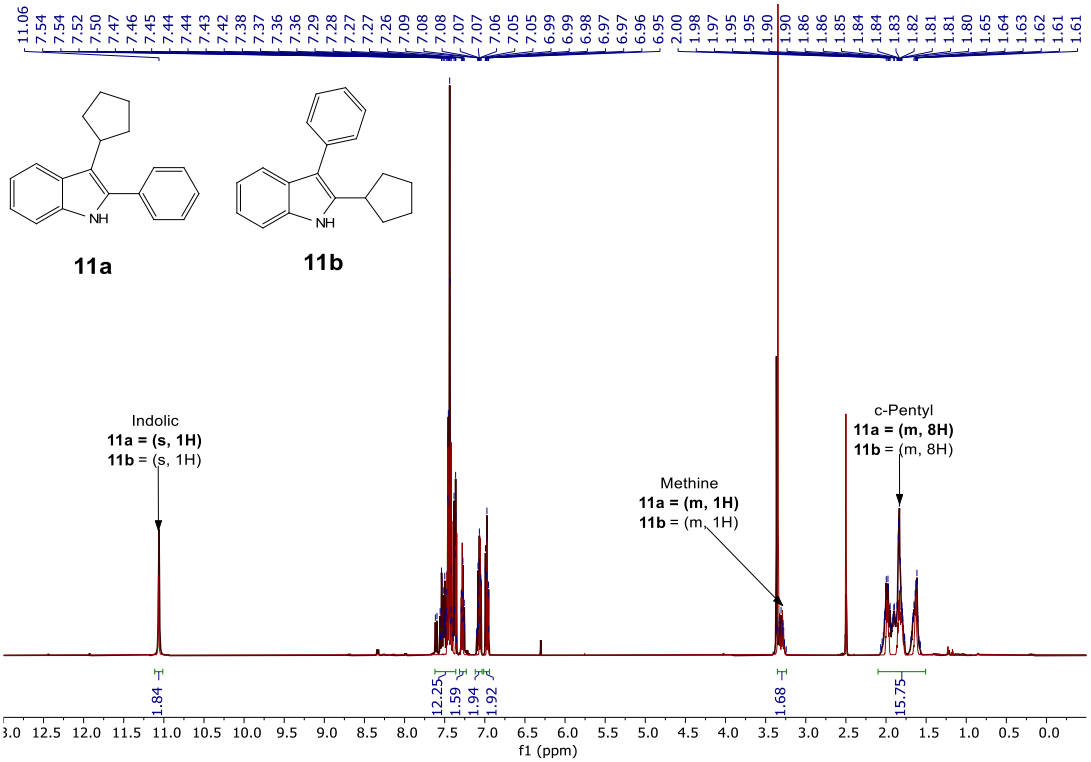


Figure S32. ^{1}H NMR spectrum (700 MHz) of the mixture between compound 3-cyclopentyl-2-phenyl-1*H*-indole (**11a**) and 2-cyclopentyl-3-phenyl-1*H*-indole (**11b**) in DMSO-d_6

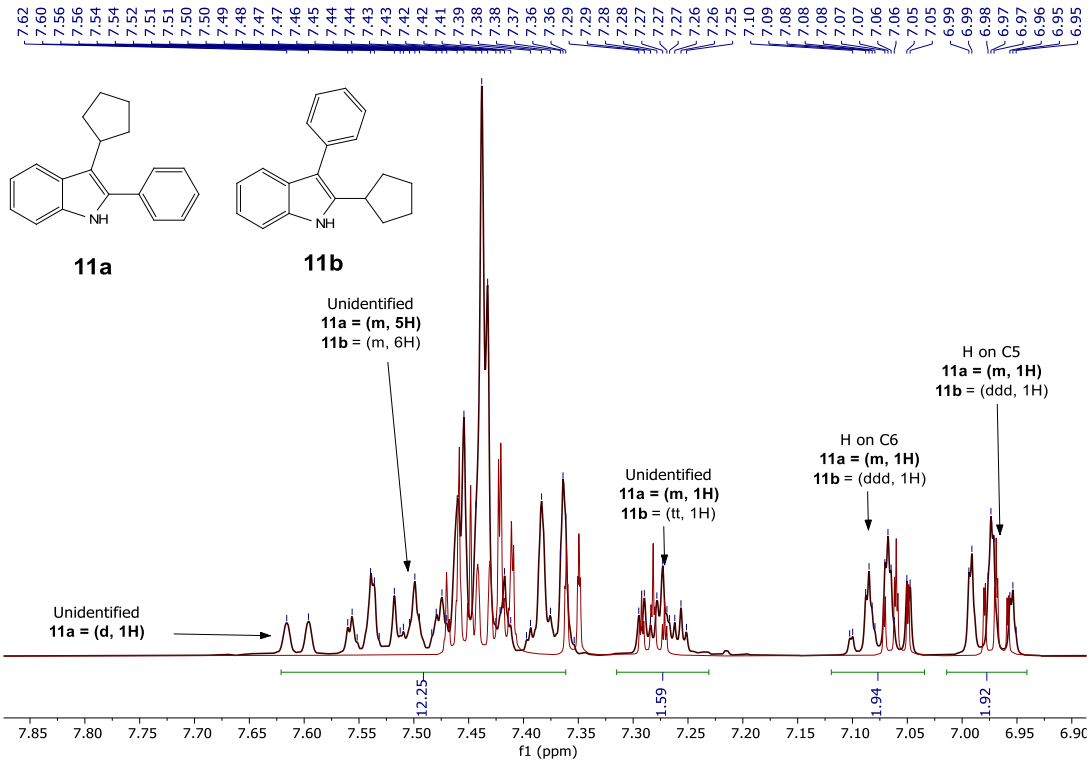


Figure S33. Expanded ^{1}H NMR spectrum (700 MHz) of the mixture between compound 3-cyclopentyl-2-phenyl-1*H*-indole (**11a**) and 2-cyclopentyl-3-phenyl-1*H*-indole (**11b**) in DMSO-d_6 (expanding aromatic region)

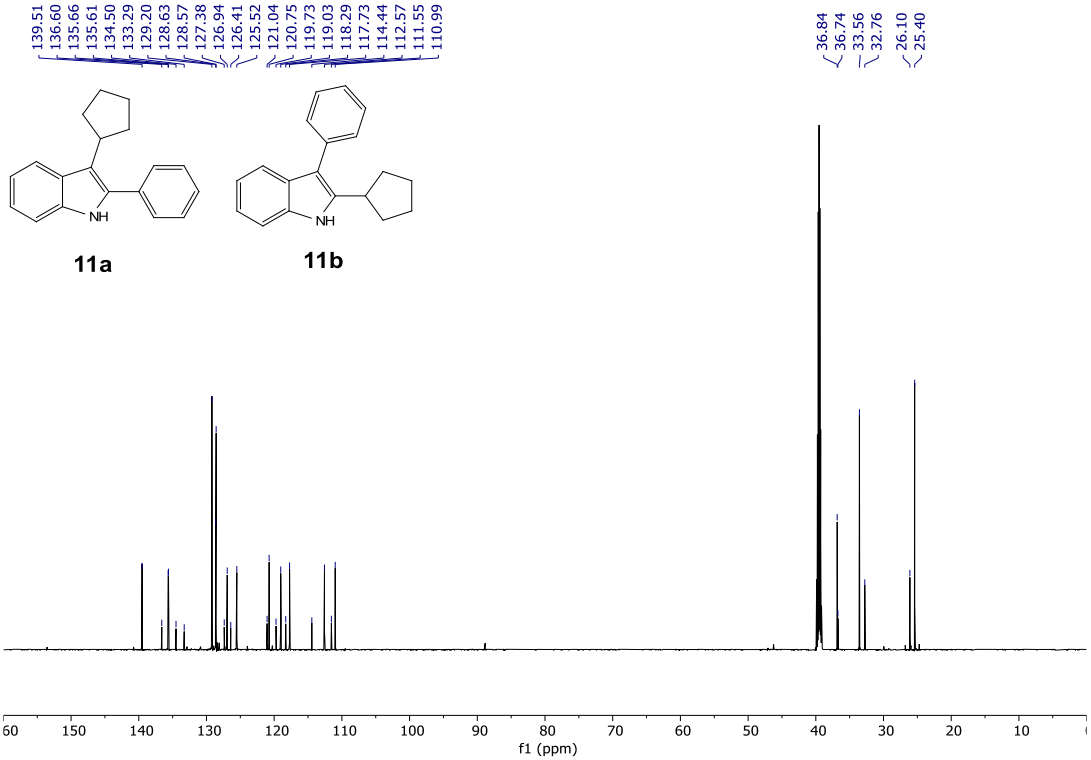


Figure S34. $^{13}C\{^{1}H\}$ NMR spectrum (175 MHz) of the mixture between compound 3-cyclopentyl-2-phenyl-1*H*-indole (**11a**) and 2-cyclopentyl-3-phenyl-1*H*-indole (**11b**) in DMSO-d_6

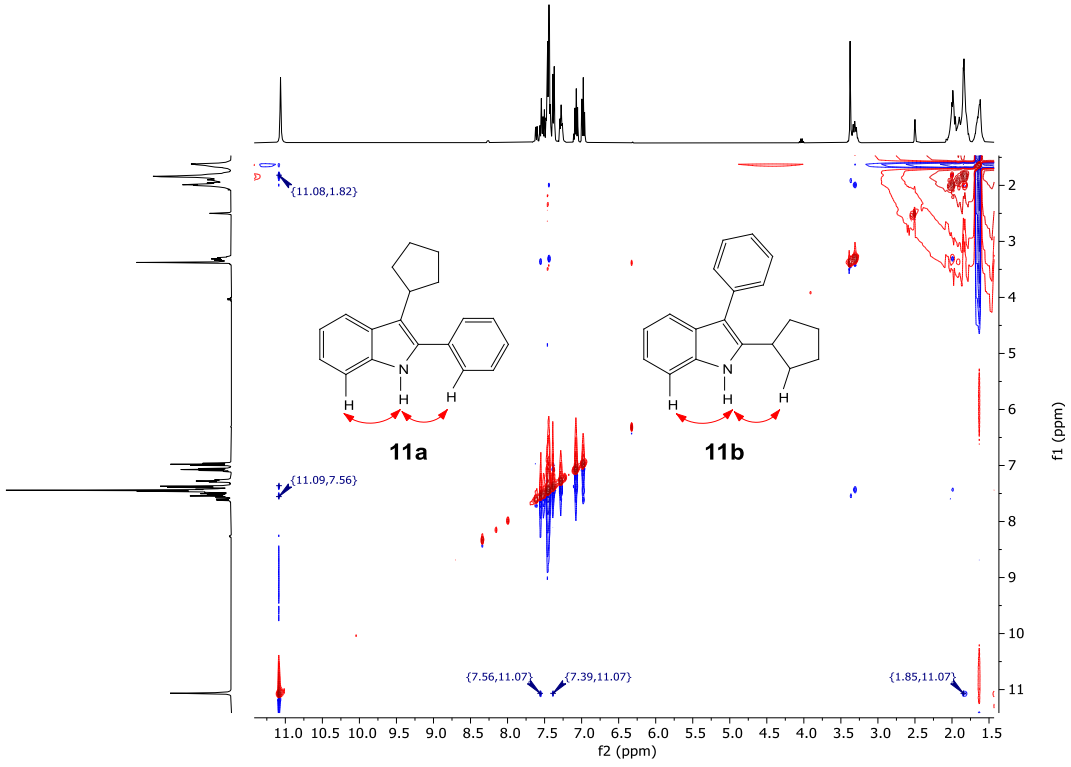


Figure S35. NOESY spectrum of the mixture between compound 3-cyclopentyl-2-phenyl-1*H*-indole (**11a**) and 2-cyclopentyl-3-phenyl-1*H*-indole (**11b**) in DMSO-*d*

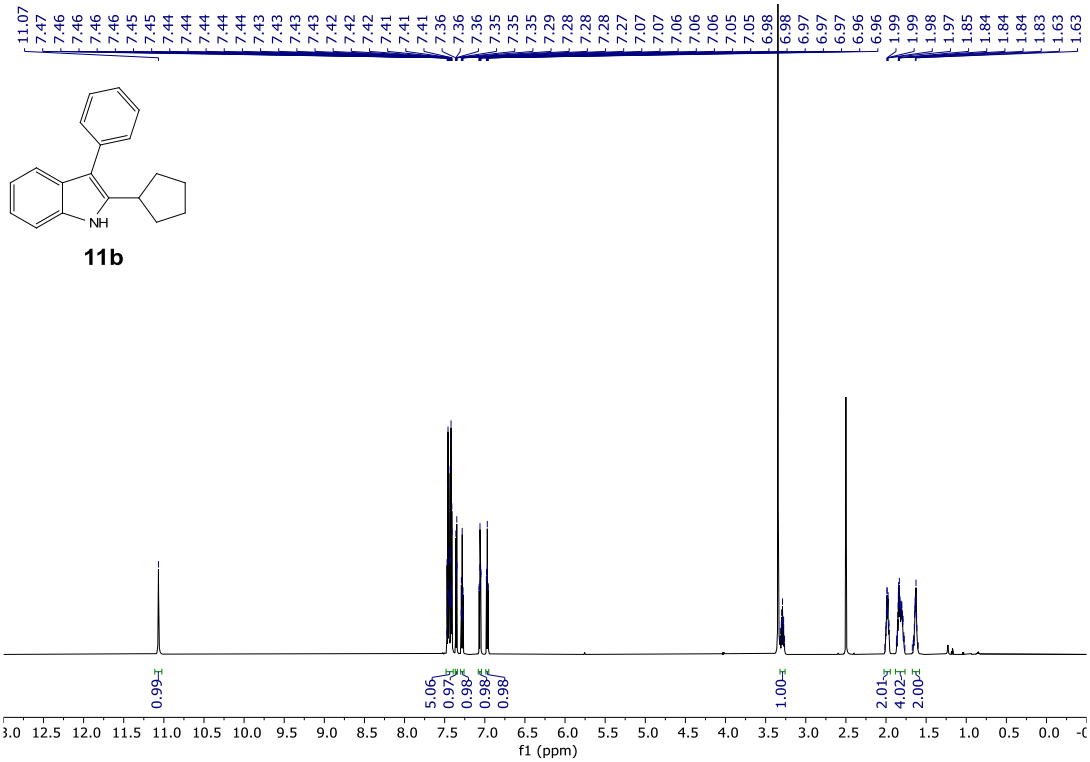


Figure S36. ^{1}H NMR spectrum (700 MHz) of 2-cyclopentyl-3-phenyl-1*H*-indole (**11b**) in DMSO-d_6

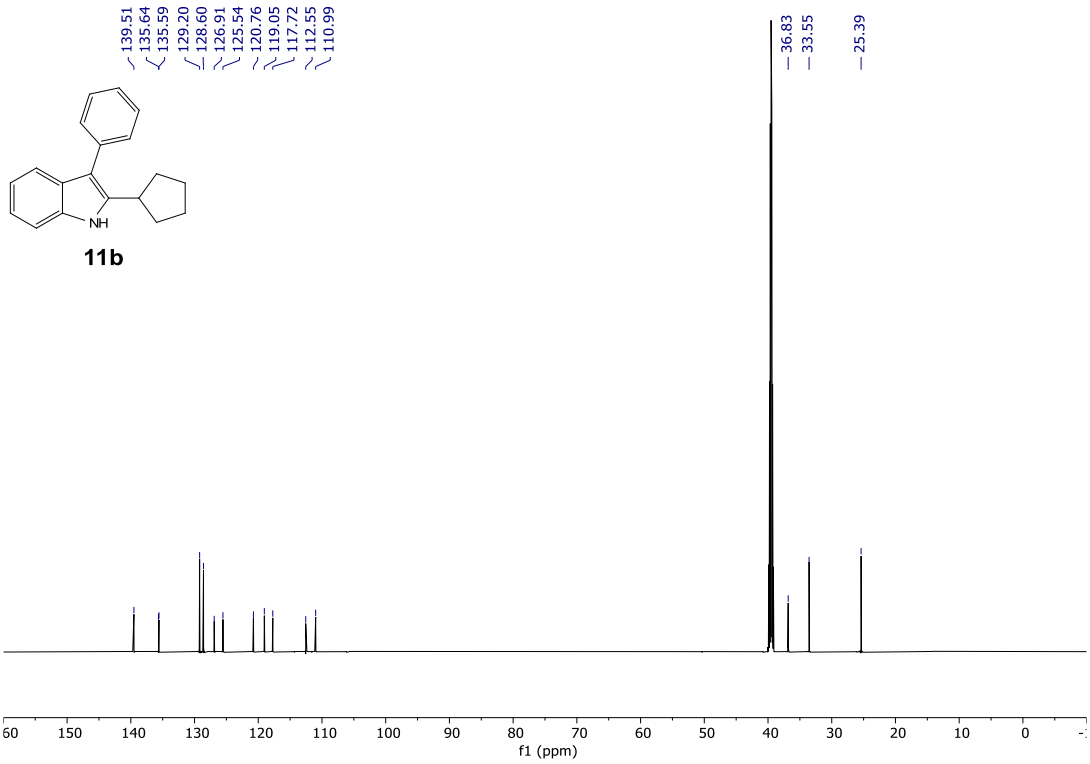


Figure S37. ^{13}C{^{1}H} NMR spectrum (175 MHz) of 2-cyclopentyl-3-phenyl-1*H*-indole (**11b**) in DMSO-d_6

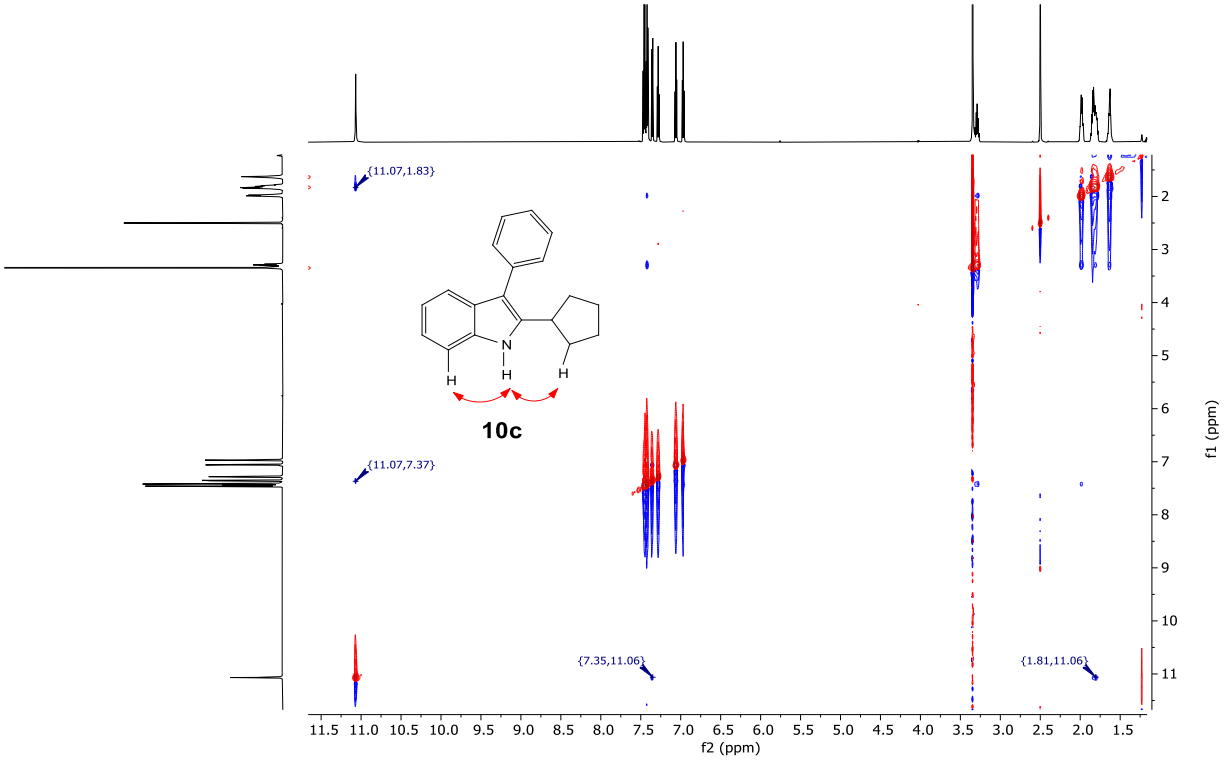


Figure S38. NOESY spectrum of 2-cyclopentyl-3-phenyl-1*H*-indole (**11b**) in DMSO-d_6

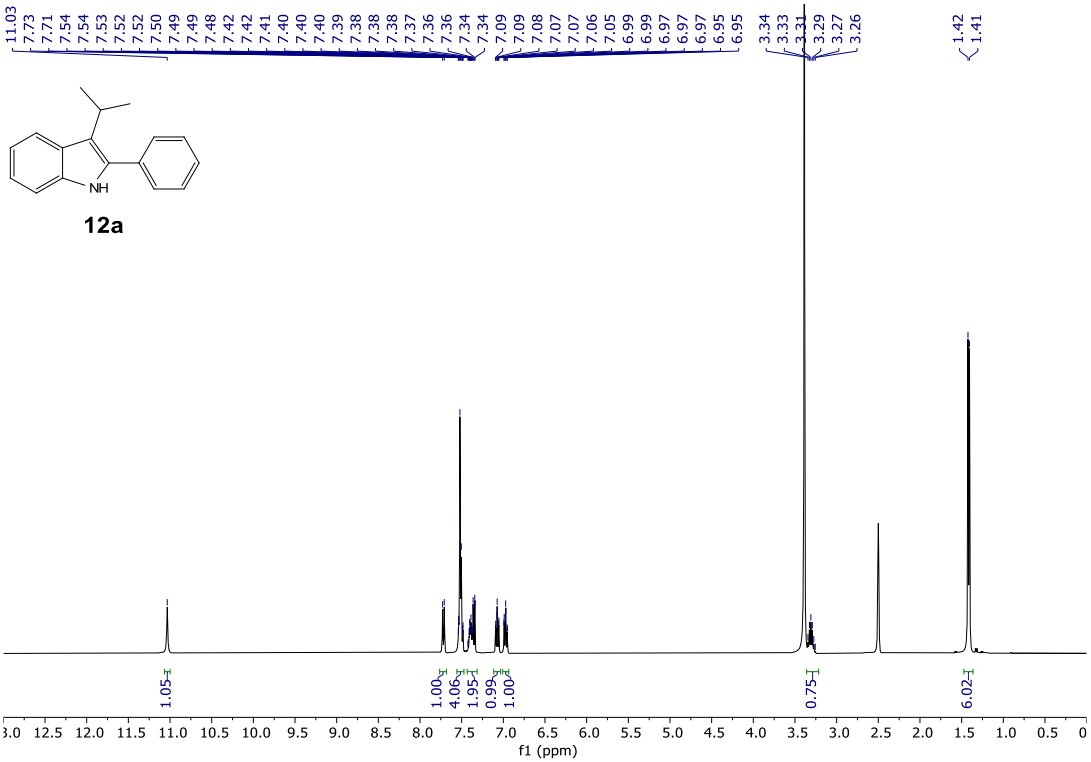


Figure S39. ^{1}H NMR spectrum (400 MHz) of 3-isopropyl-2-phenyl-1*H*-indole (**12a**) in DMSO-d_6

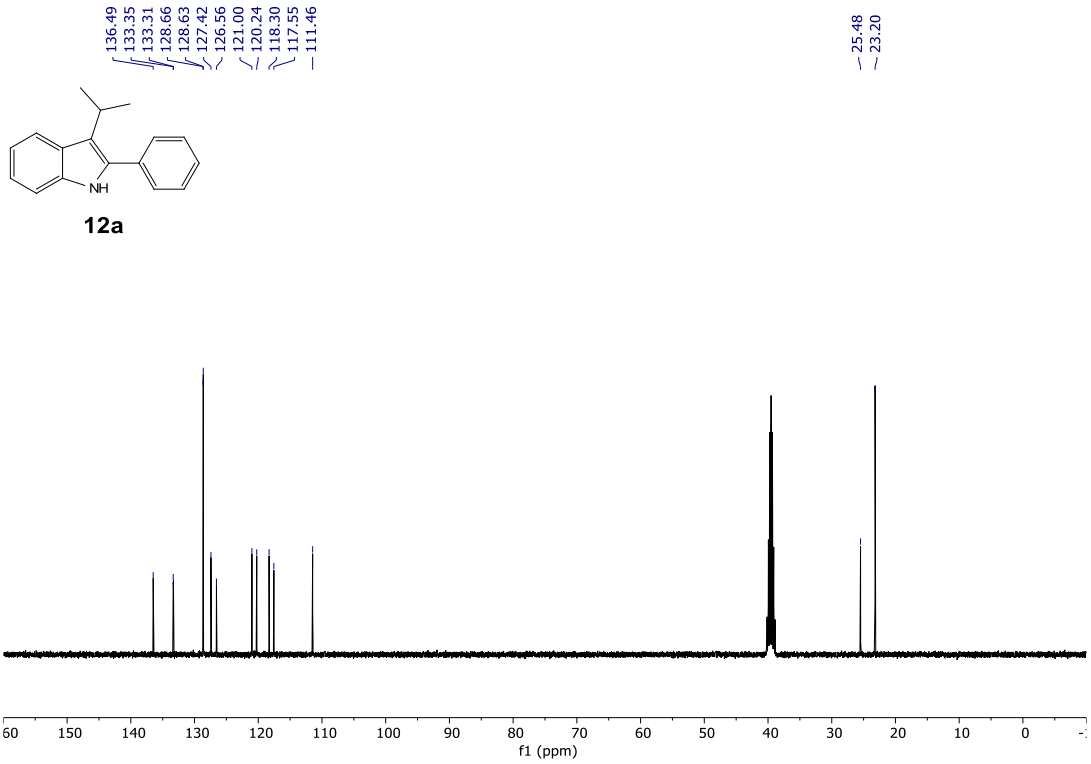


Figure S40. ^{13}C{^{1}H} NMR spectrum (100 MHz) of 3-isopropyl-2-phenyl-1*H*-indole (**12a**) in DMSO-d_6

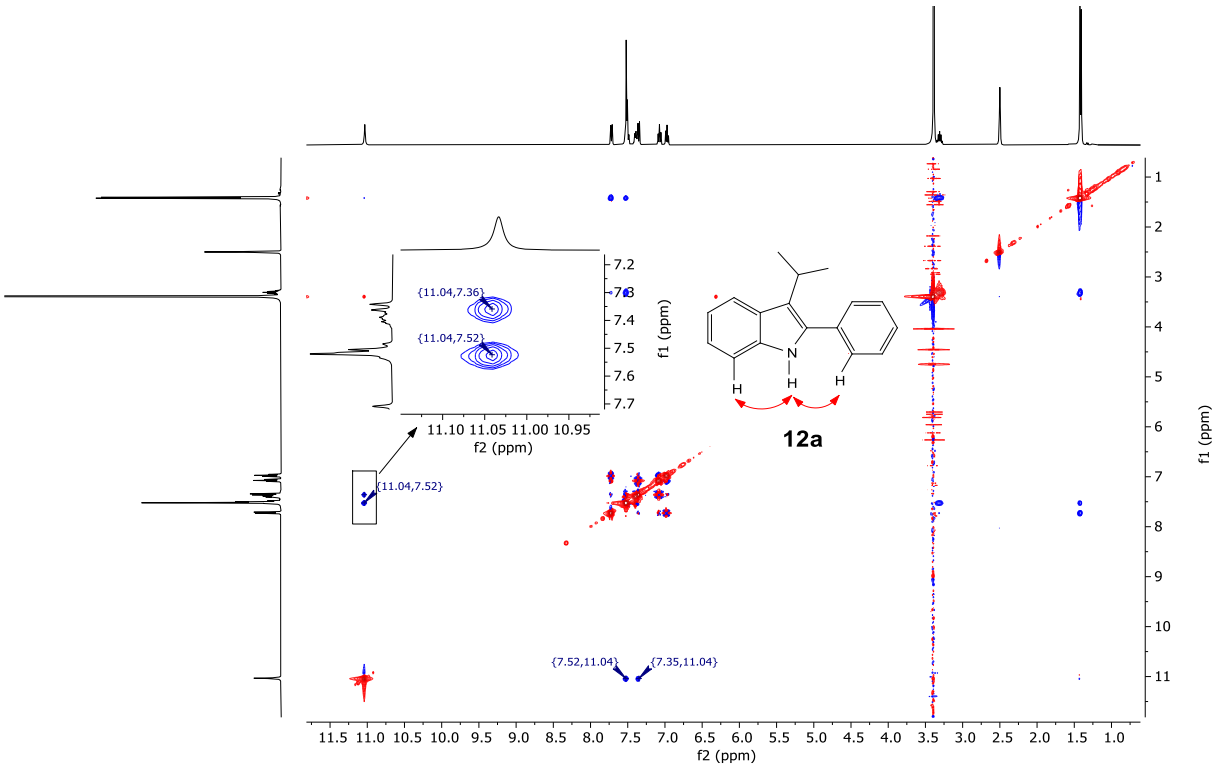


Figure S41. NOESY spectrum of 3-isopropyl-2-phenyl-1*H*-indole (**12a**) in DMSO-d_6

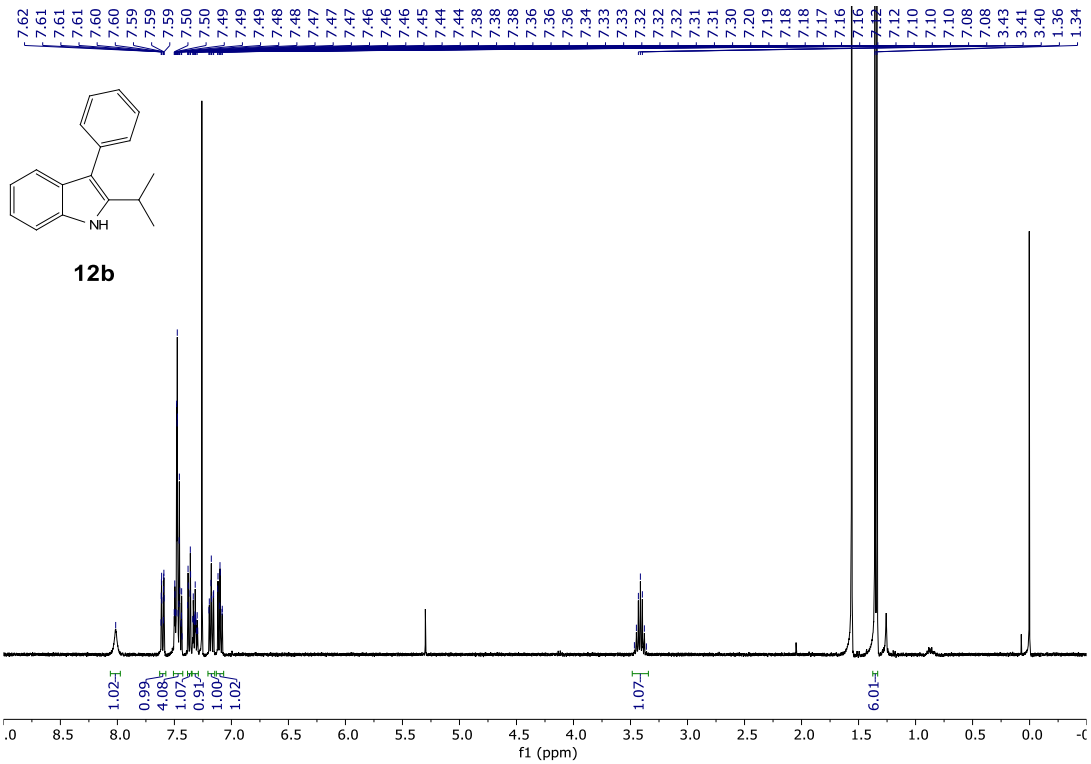


Figure S42. ^{1}H NMR spectrum (400 MHz) of 2-isopropyl-3-phenyl-1*H*-indole (**12b**) in $CDCl_3$

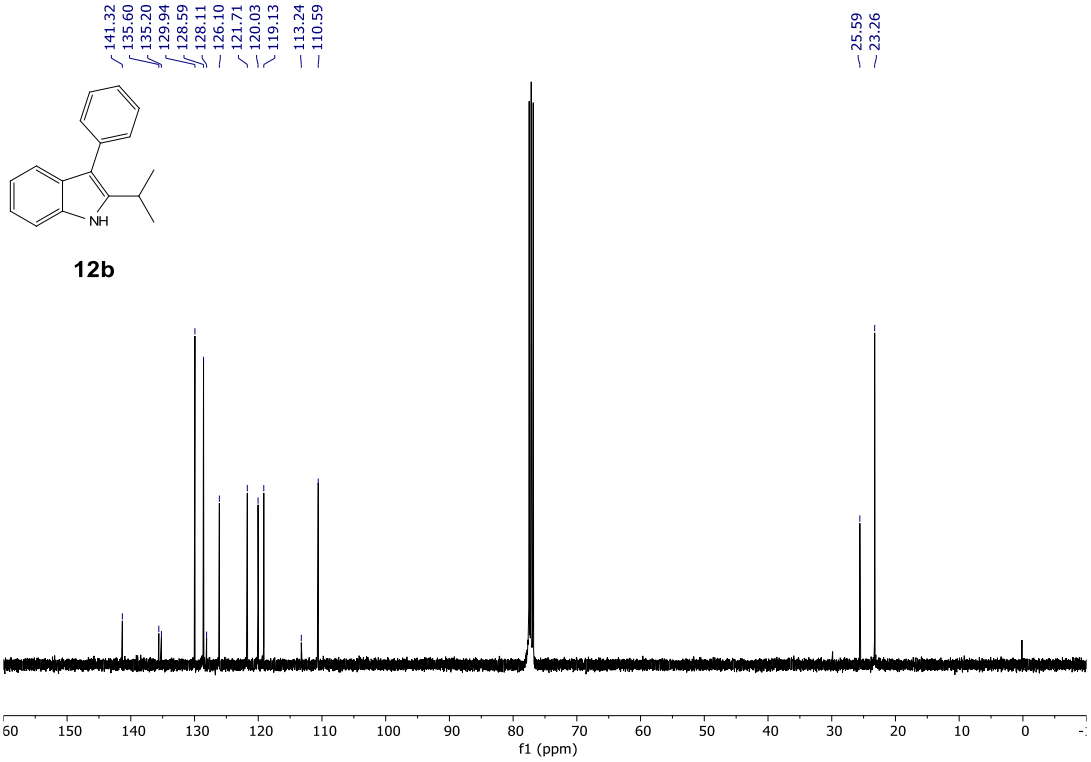


Figure S43. $^{13}C\{^{1}H\}$ NMR spectrum (100 MHz) of 2-isopropyl-3-phenyl-1*H*-indole (**12b**) in $CDCl_3$

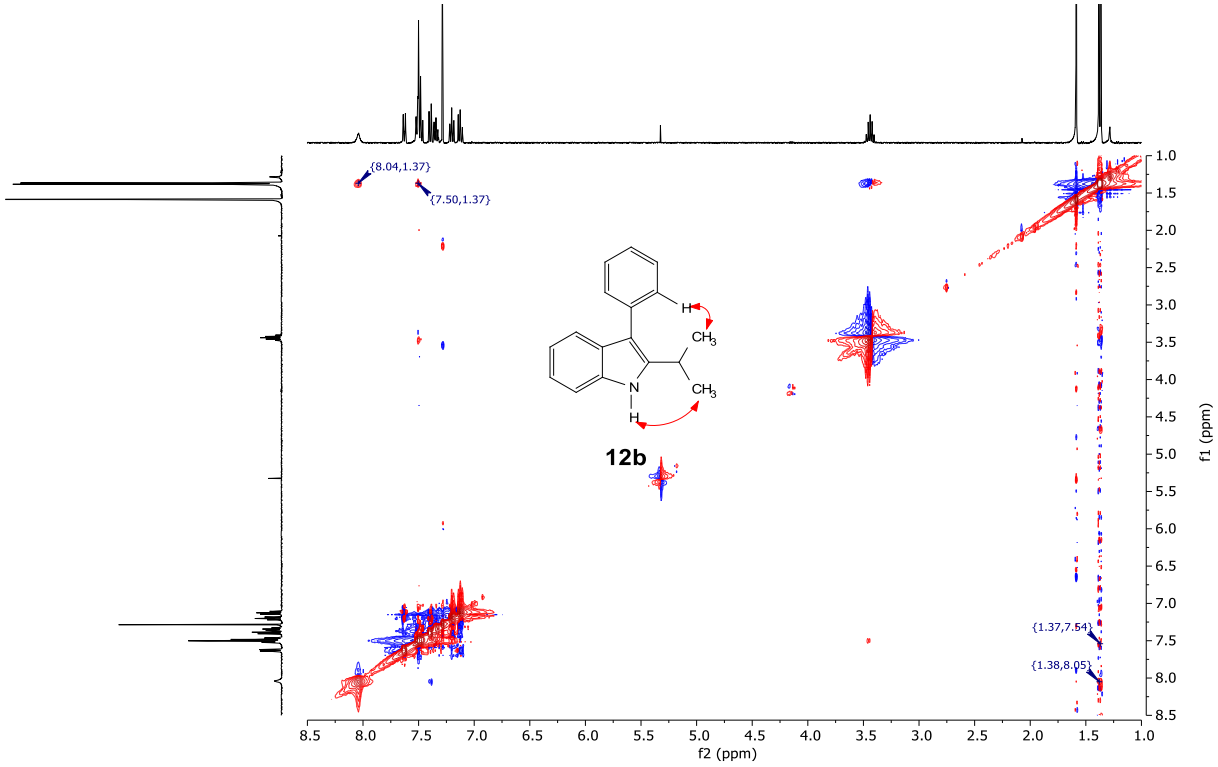


Figure S44. NOESY spectrum of 2-isopropyl-3-phenyl-1*H*-indole (**12b**) in $CDCl_3$

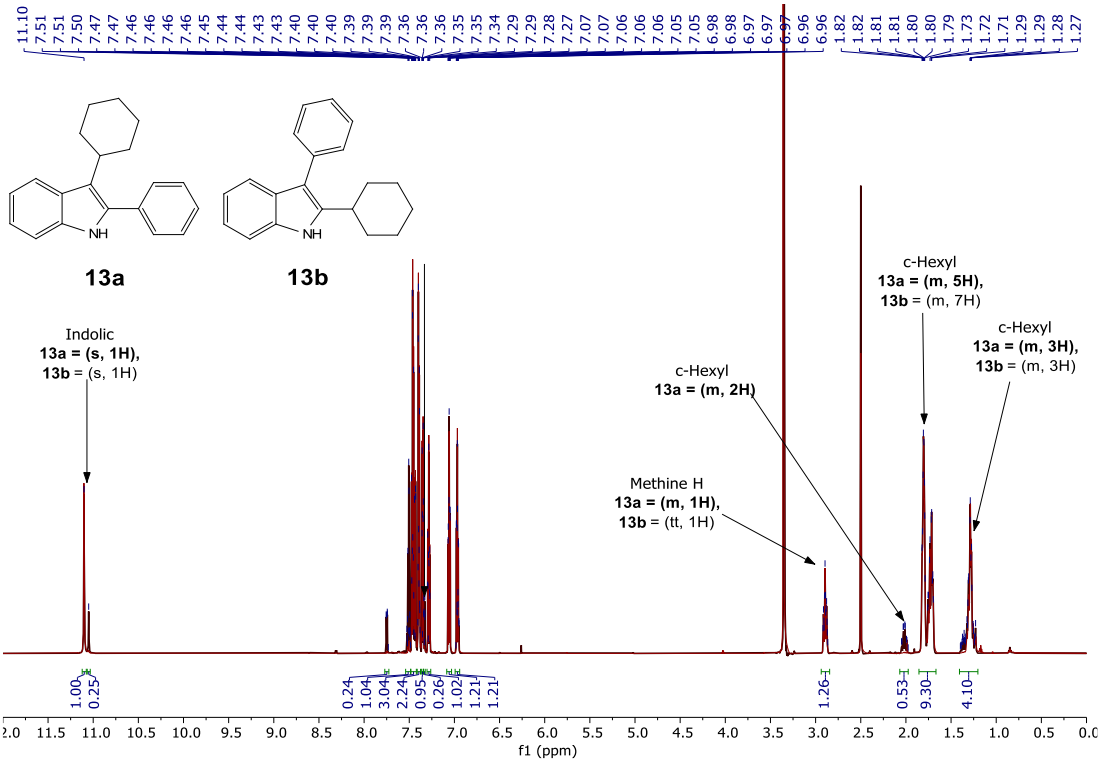


Figure S45. ^{1}H NMR spectrum (700 MHz) of the mixture between 3-cyclohexyl-2-phenyl-1*H*-indole (**13a**) and 2-cyclohexyl-3-phenyl-1*H*-indole (**13b**) in DMSO-d_6

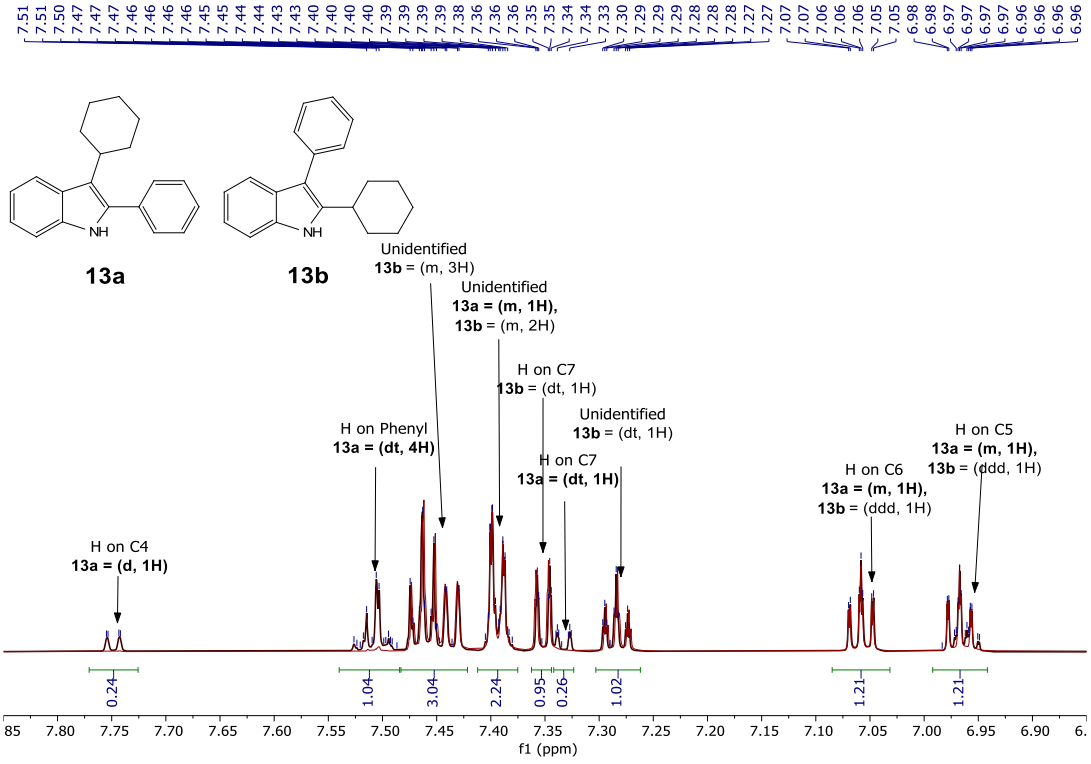


Figure S46. Expanded ^{1}H NMR spectrum (700 MHz) of the mixture between 3-cyclohexyl-2-phenyl-1*H*-indole (**13a**) and 2-cyclohexyl-3-phenyl-1*H*-indole (**13b**) in DMSO-d_6 (expanding aromatic region)

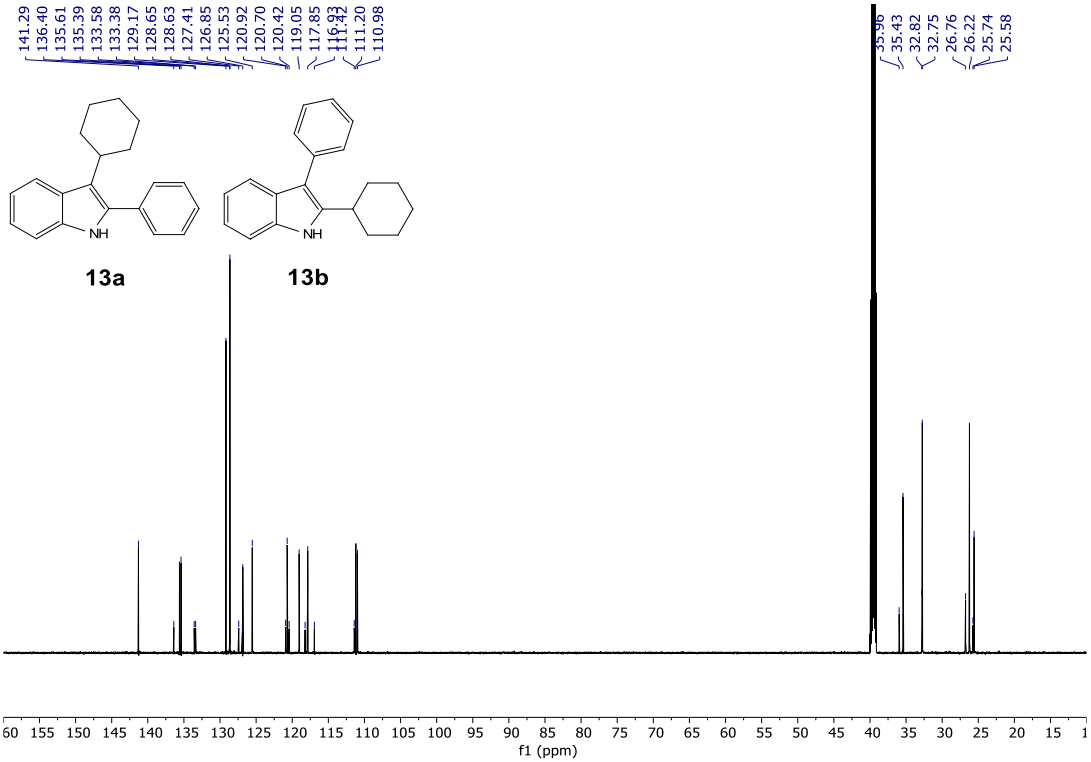


Figure S47. $^{13}C\{^{1}H\}$ NMR spectrum (175 MHz) of the mixture between 3-cyclohexyl-2-phenyl-1*H*-indole (**13a**) and 2-cyclohexyl-3-phenyl-1*H*-indole (**13b**) in DMSO-d_6

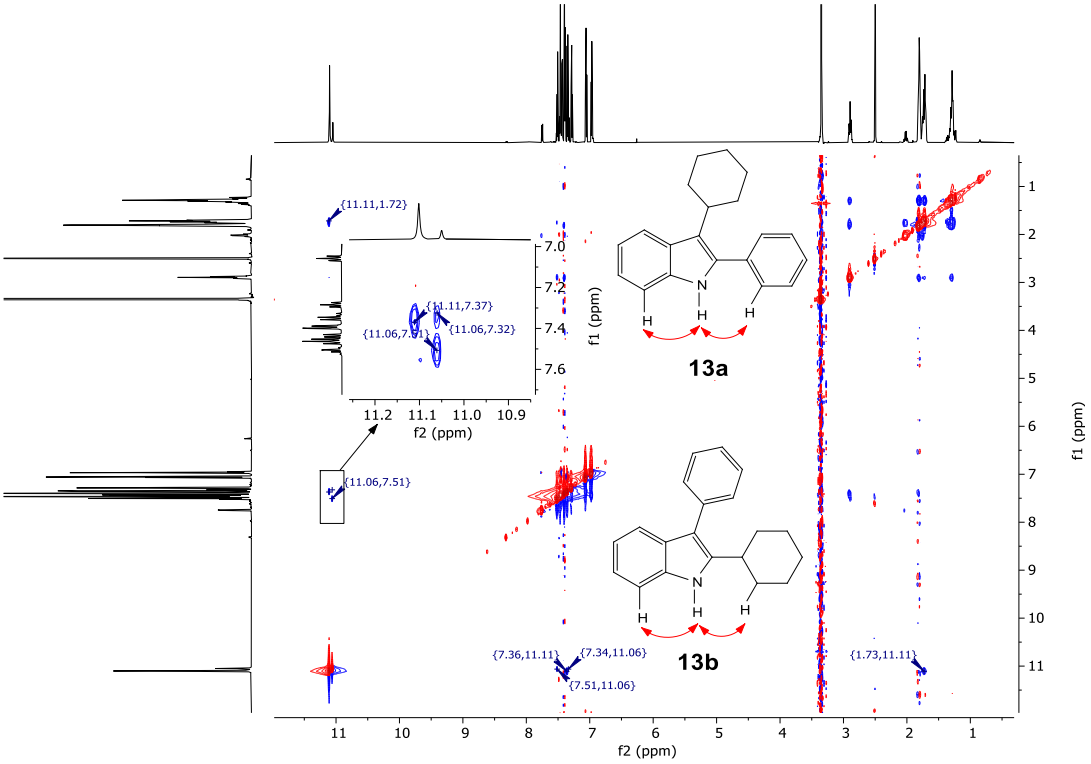


Figure S48. NOESY spectrum of the mixture between 3-cyclohexyl-2-phenyl-1*H*-indole (**13a**) and 2-cyclohexyl-3-phenyl-1*H*-indole (**13b**) in DMSO-d_6

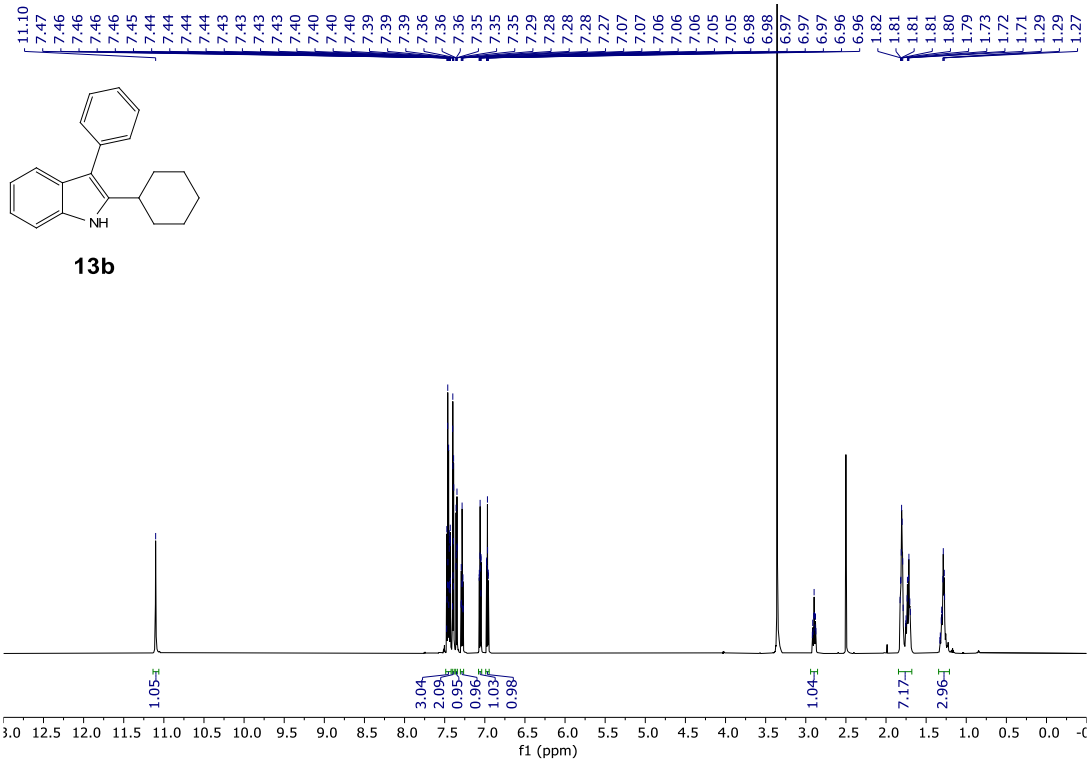


Figure S49. ^{1}H NMR spectrum (700 MHz) of 2-cyclohexyl-3-phenyl-1*H*-indole (**13b**) in DMSO-d_6

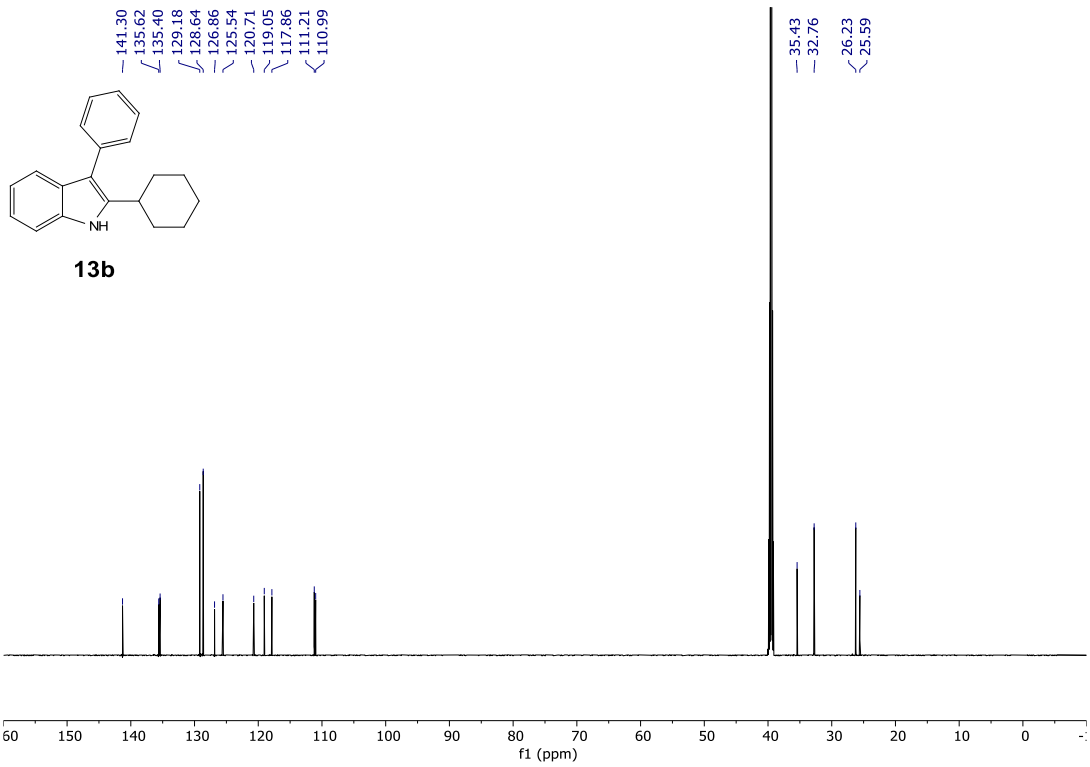


Figure S50. ^{13}C{^{1}H} NMR spectrum (175 MHz) of -cyclohexyl-3-phenyl-1*H*-indole (**13b**) in DMSO-d_6

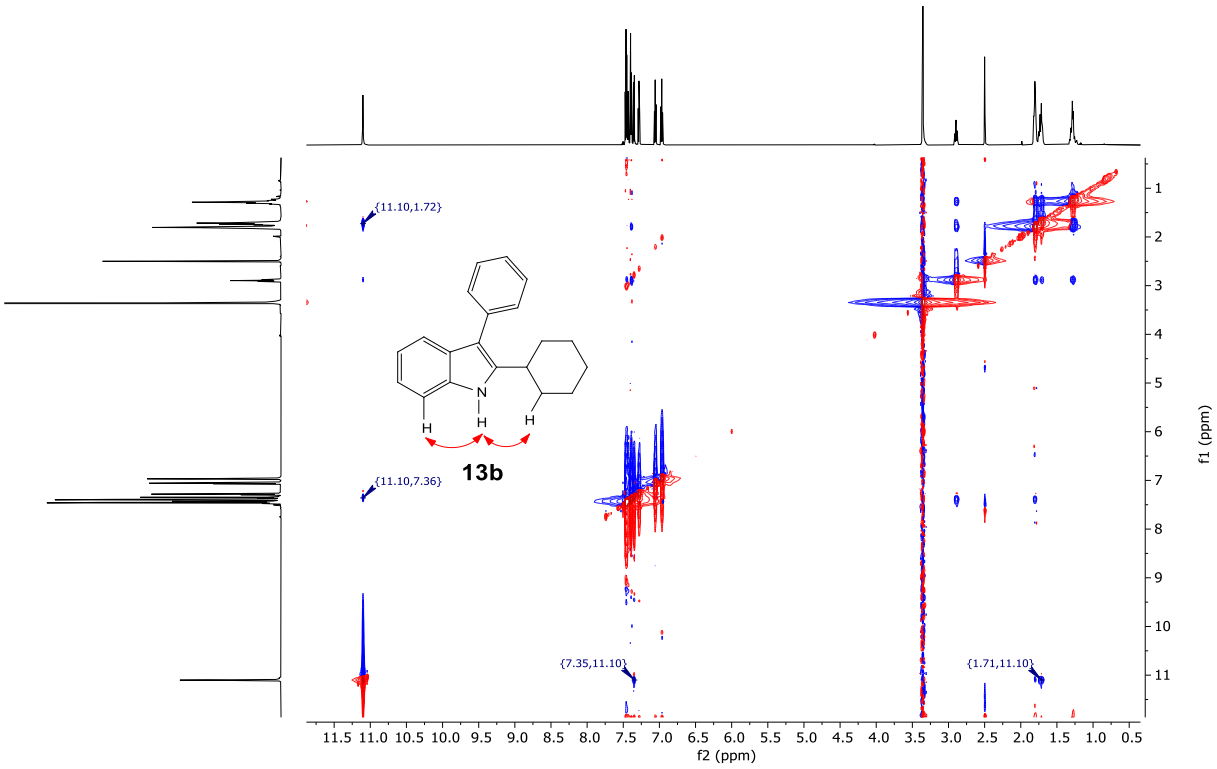


Figure S51. NOESY spectrum of cyclohexyl-3-phenyl-1*H*-indole (**13b**) in DMSO-d_6

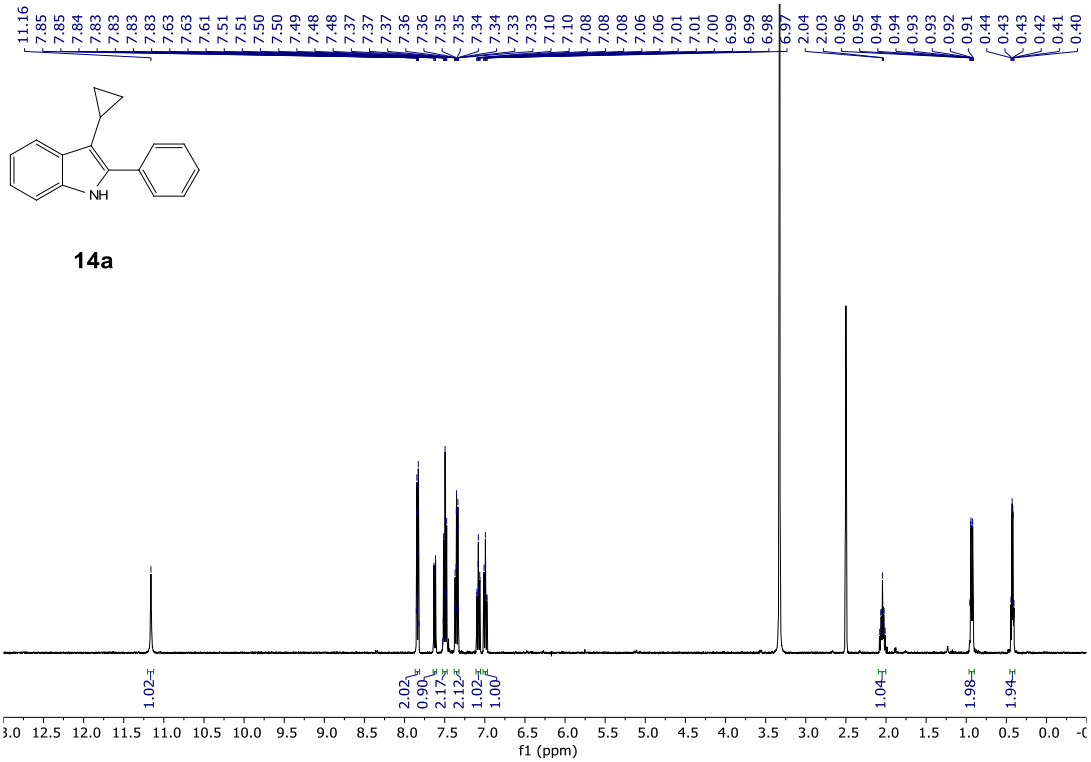


Figure S52. ^{1}H NMR spectrum (400 MHz) of 3-cyclopropyl-2-phenyl-1*H*-indole (**14a**) in DMSO-d_6

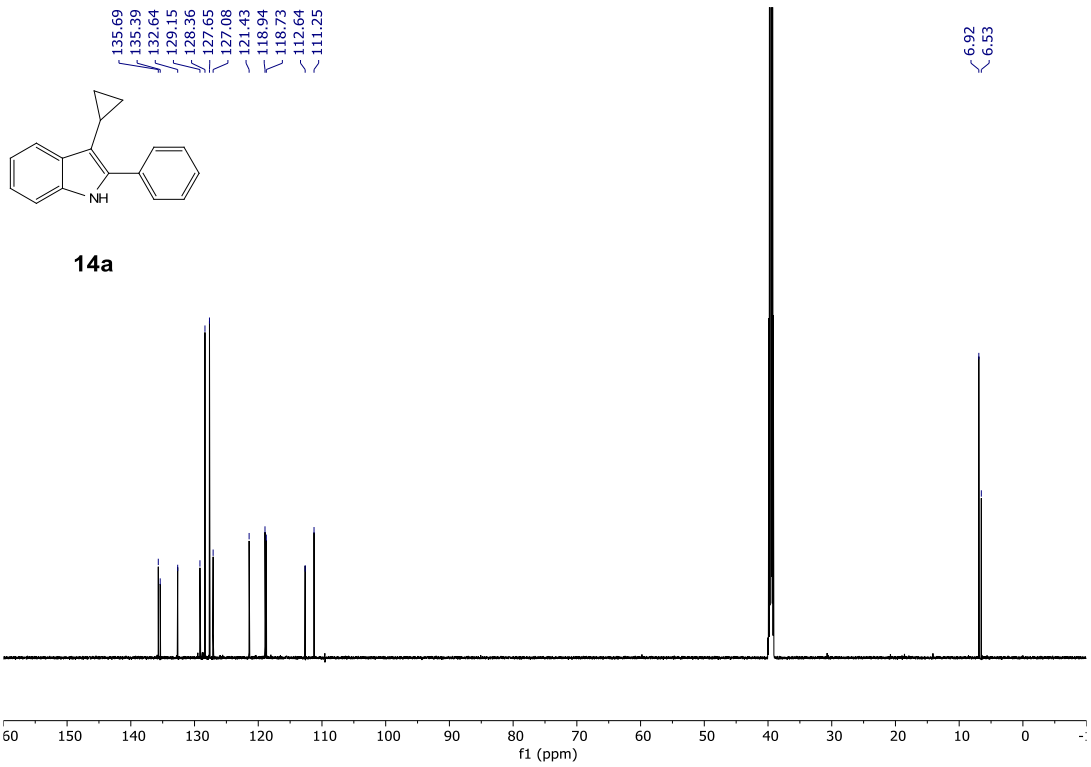


Figure S53. ^{13}C{^{1}H} NMR spectrum (100 MHz) of 3-cyclopropyl-2-phenyl-1*H*-indole (**14a**) in DMSO-d_6

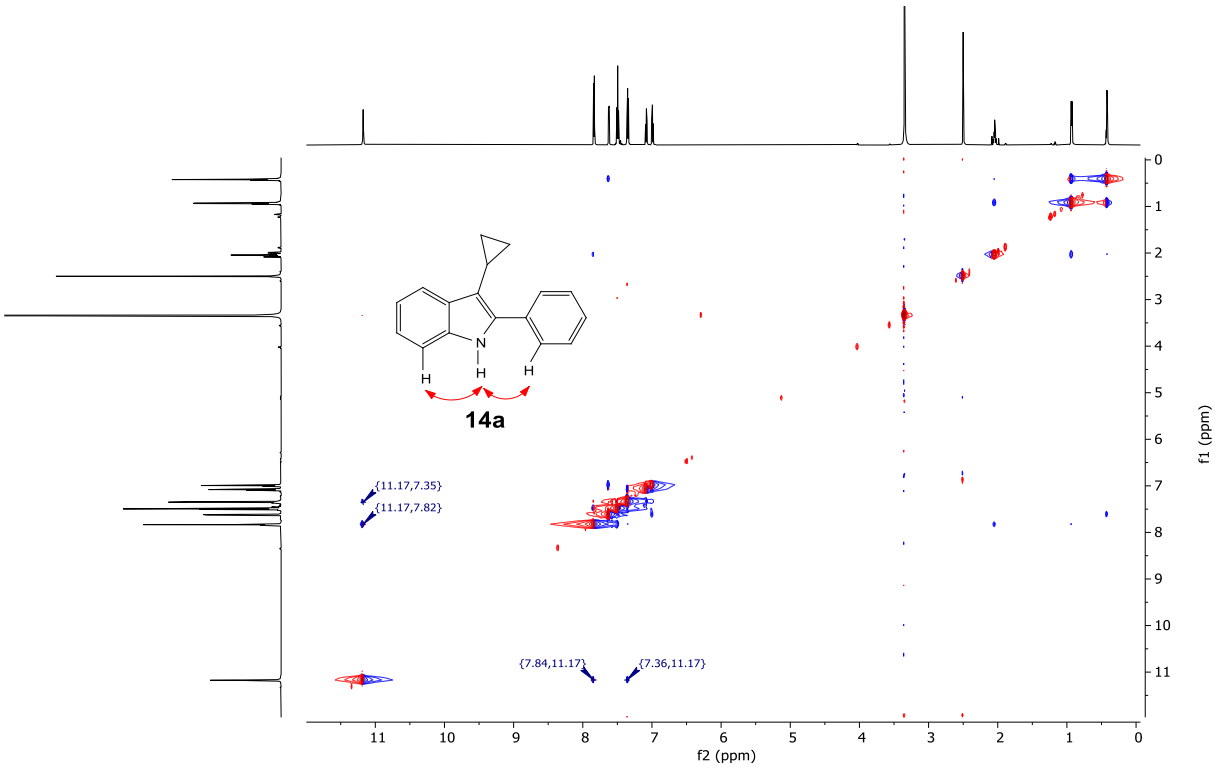


Figure S54. NOESY spectrum of 3-cyclopropyl-2-phenyl-1*H*-indole (**14a**) in DMSO-d_6

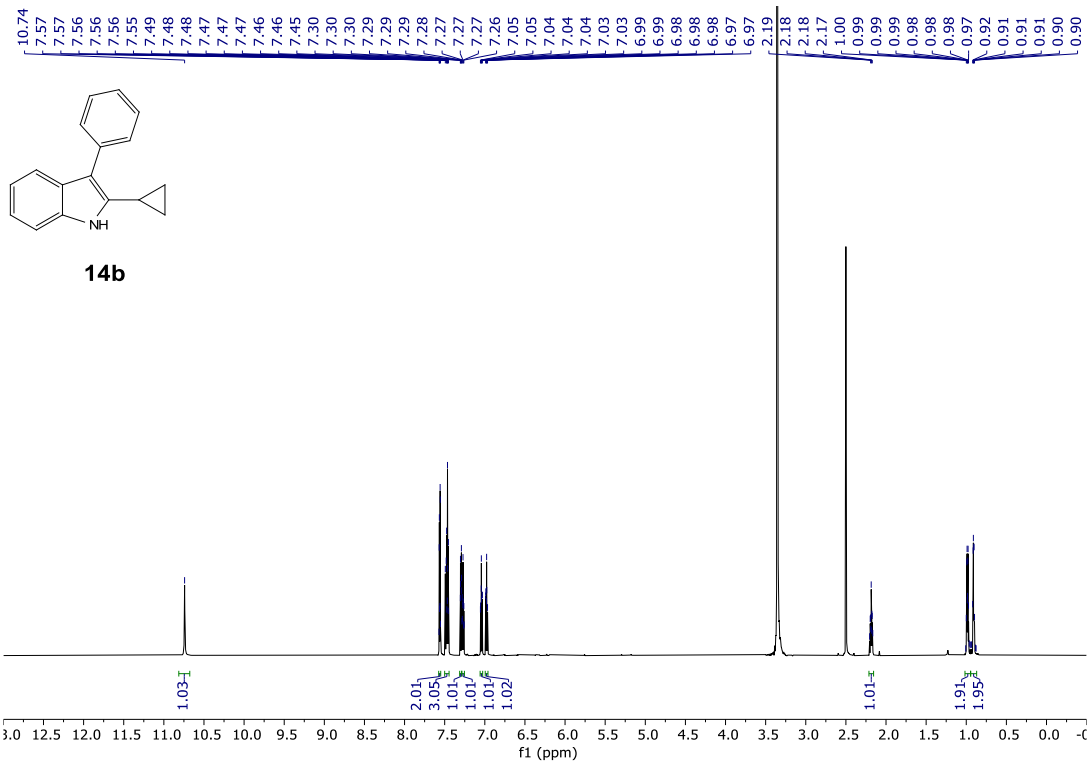


Figure S55. ^{1}H NMR spectrum (700 MHz) of 2-cyclopropyl-3-phenyl-1*H*-indole (**14b**) in DMSO-d_6

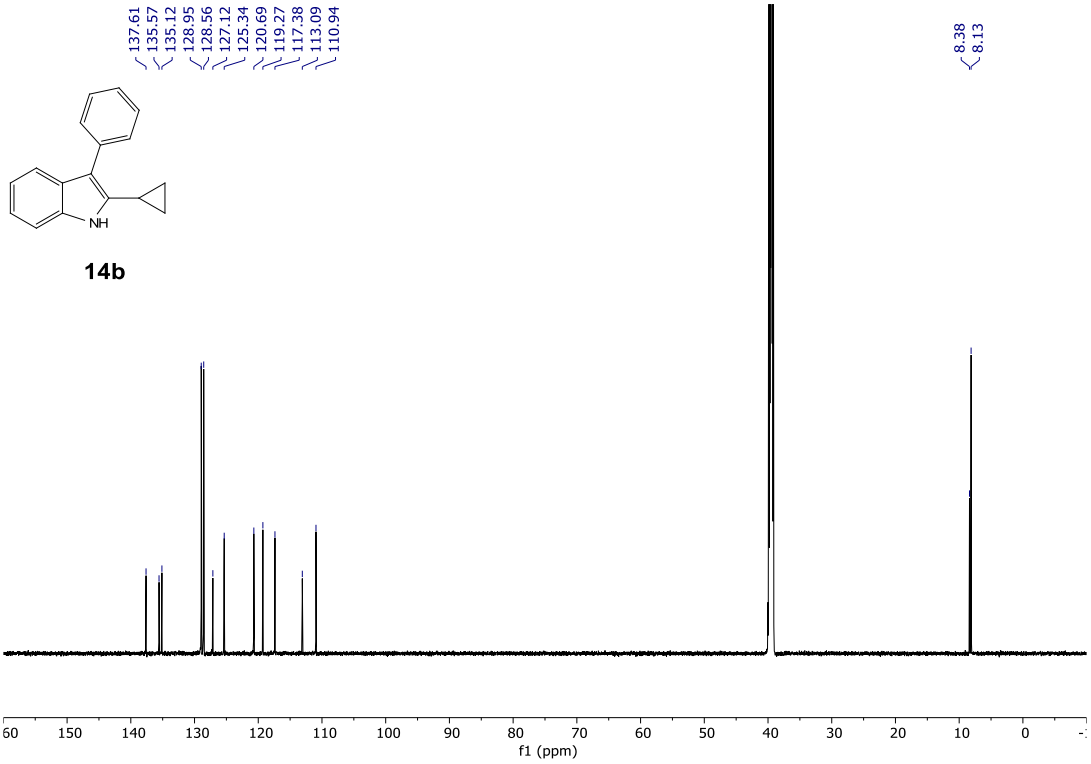


Figure S56. ^{13}C{^{1}H} NMR spectrum (175 MHz) of 2-cyclopropyl-3-phenyl-1*H*-indole (**14b**) in DMSO-d_6

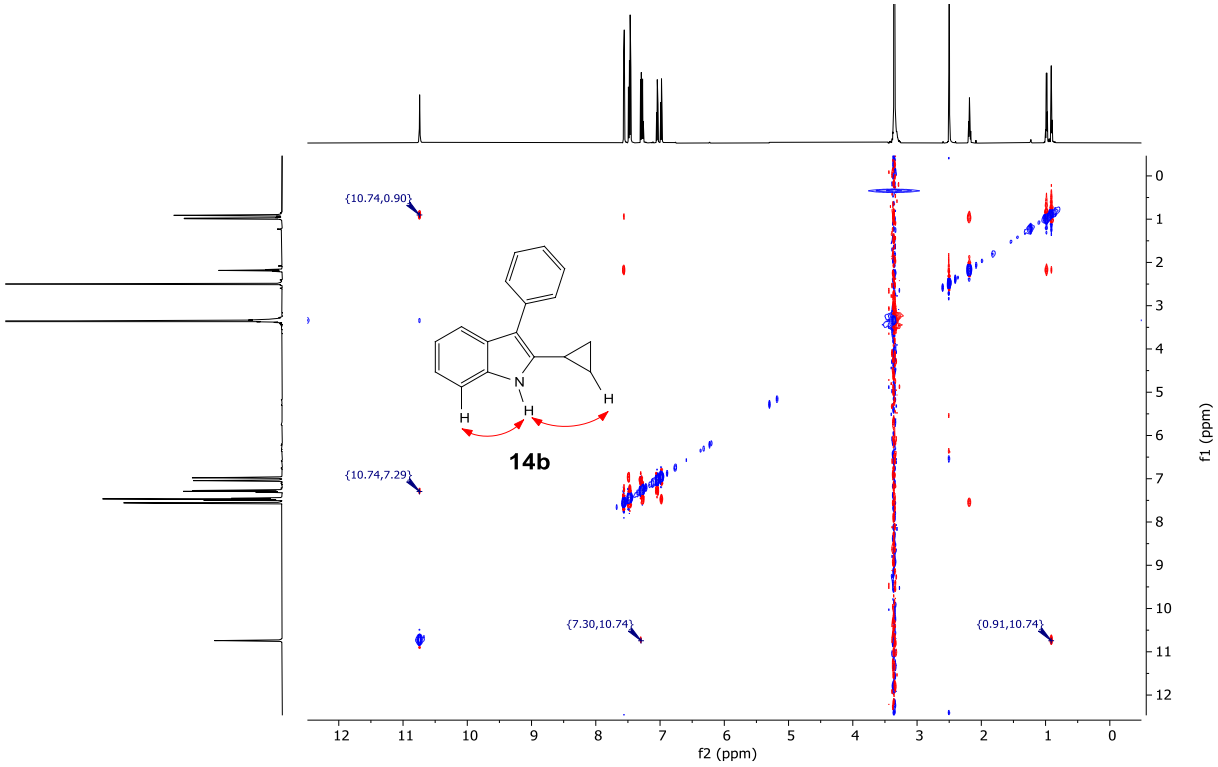


Figure S57. NOESY spectrum of 2-cyclopropyl-3-phenyl-1*H*-indole (**14b**) in DMSO-d_6

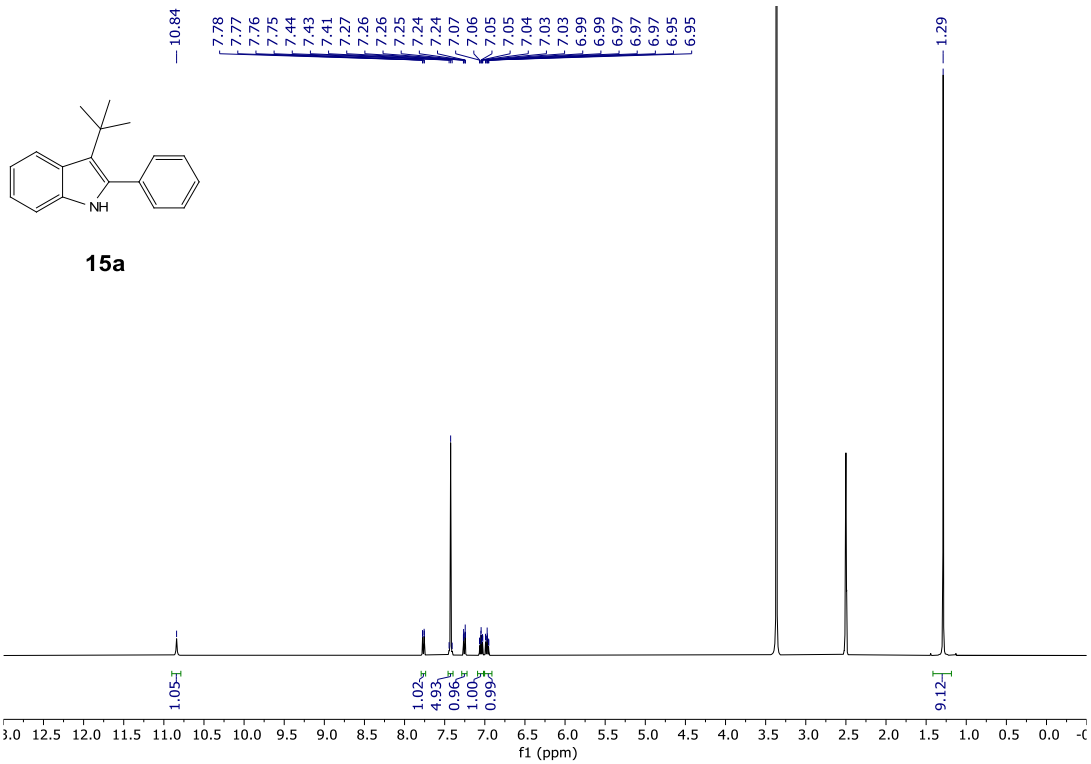


Figure S58. ^{1}H NMR spectrum (400 MHz) of 3-(*tert*-butyl)-2-phenyl-1*H*-indole (**15a**) in DMSO-d_6

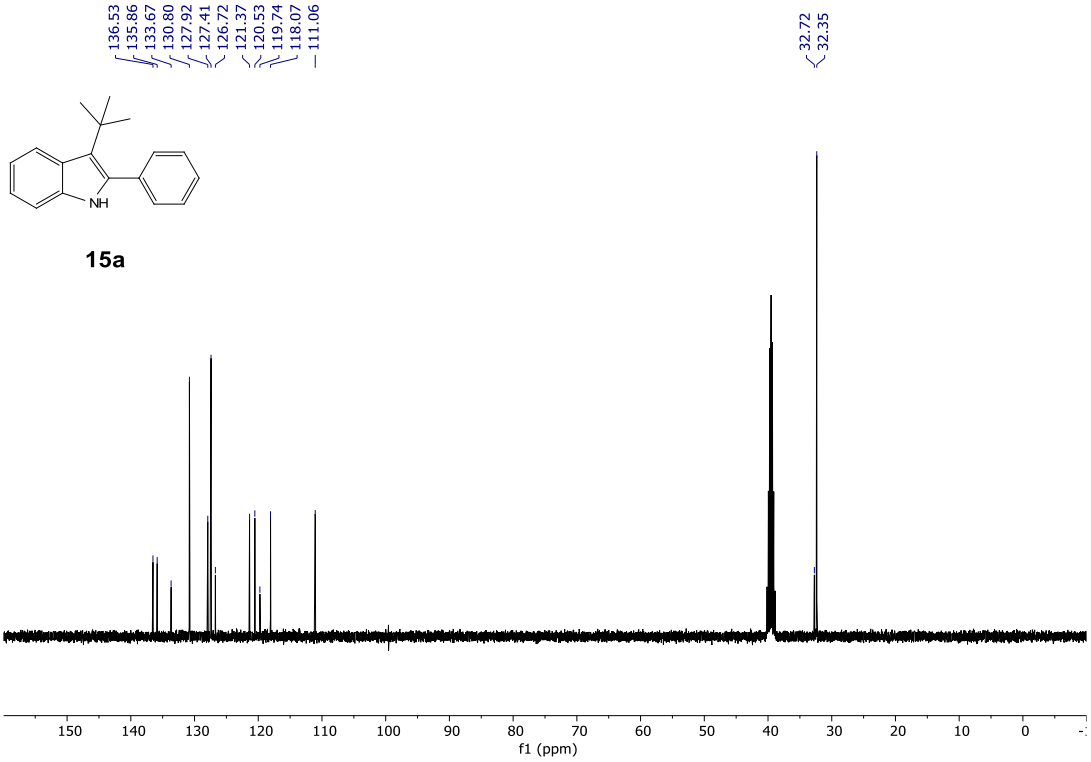


Figure S59. ^{13}C{^{1}H} NMR spectrum (100 MHz) of 3-(*tert*-butyl)-2-phenyl-1*H*-indole (**15a**) in DMSO-d_6

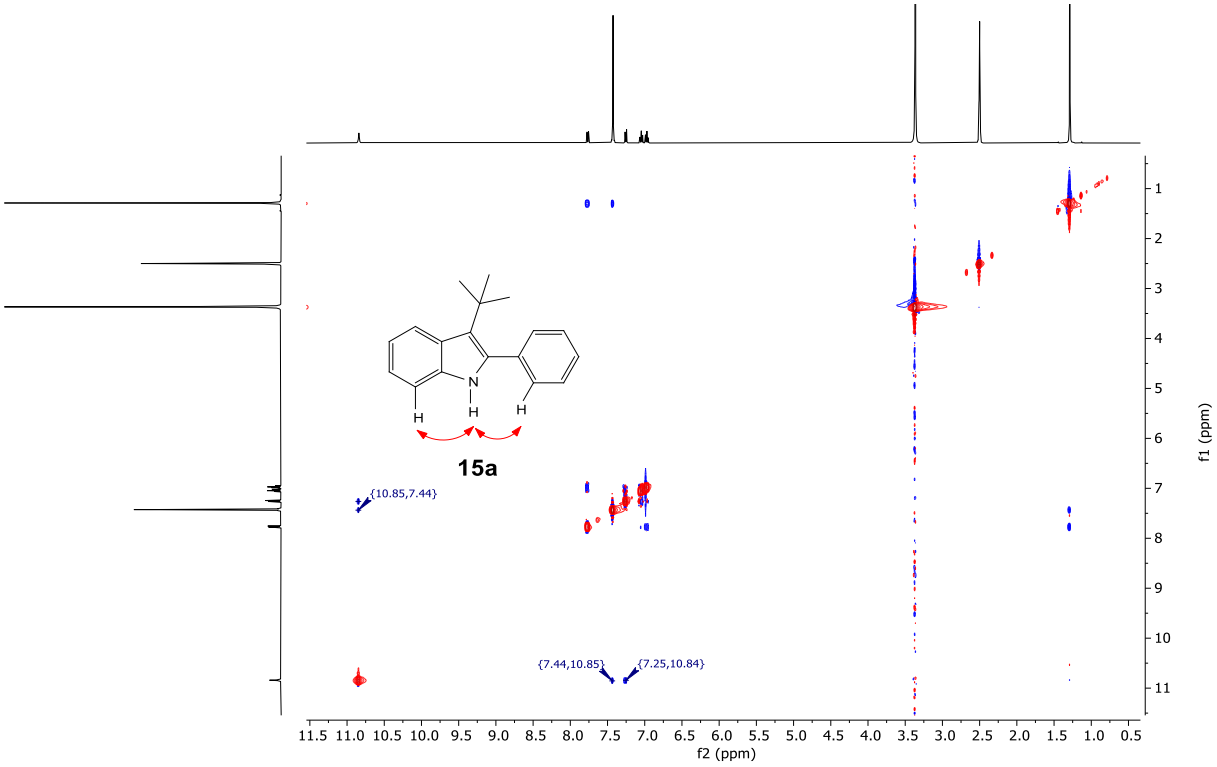


Figure S60. NOESY spectrum of 3-(*tert*-butyl)-2-phenyl-1*H*-indole (**15a**) in DMSO-d_6

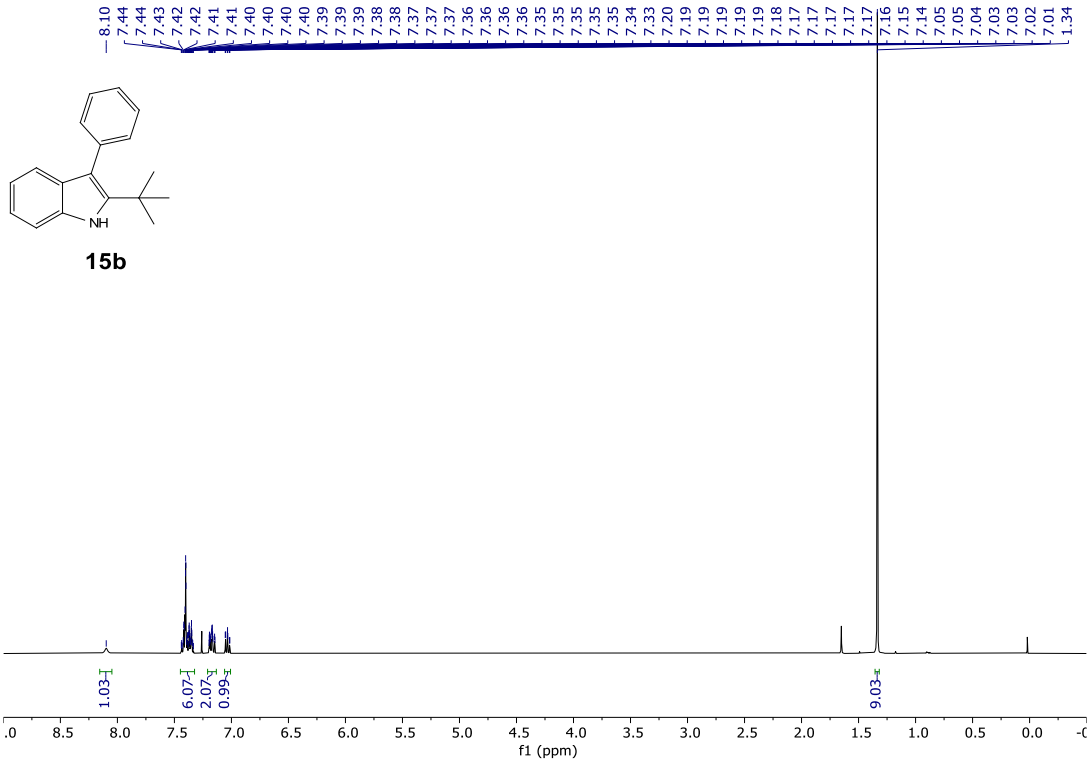


Figure S61. ^{1}H NMR spectrum (400 MHz) of 2-(*tert*-butyl)-3-phenyl-1*H*-indole (**15b**) in $CDCl_3$

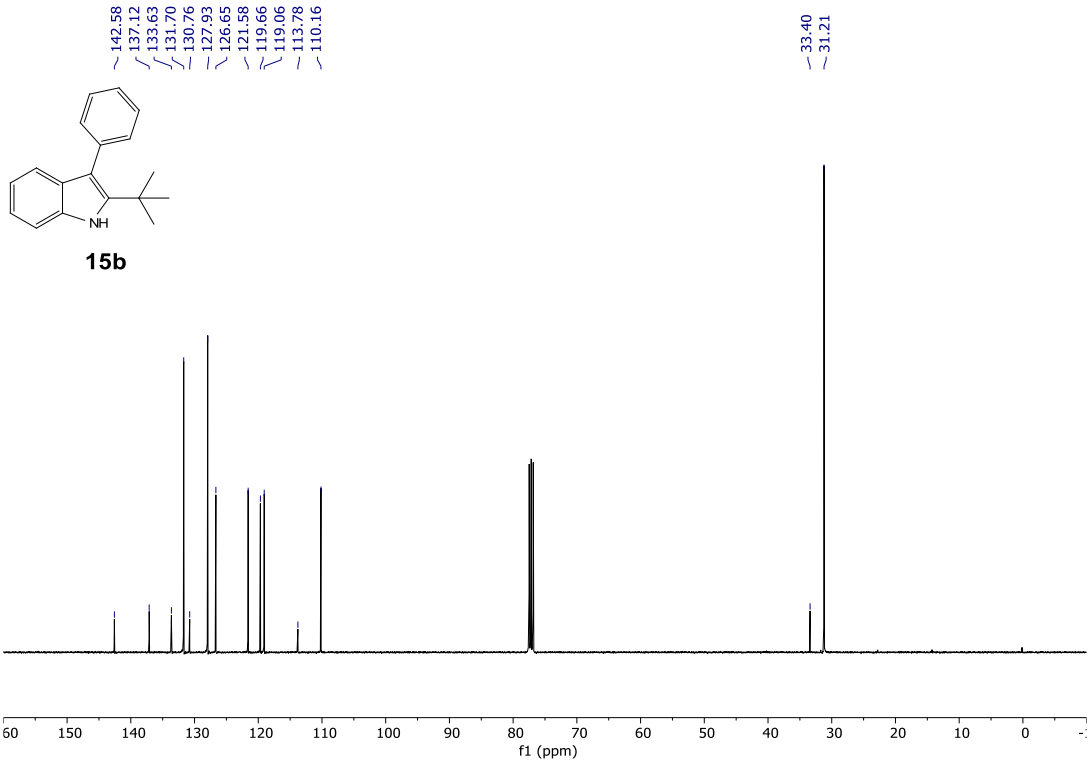


Figure S62. ^{13}C{^{1}H} NMR spectrum (100 MHz) of 2-(*tert*-butyl)-3-phenyl-1*H*-indole (**15b**) in $CDCl_3$

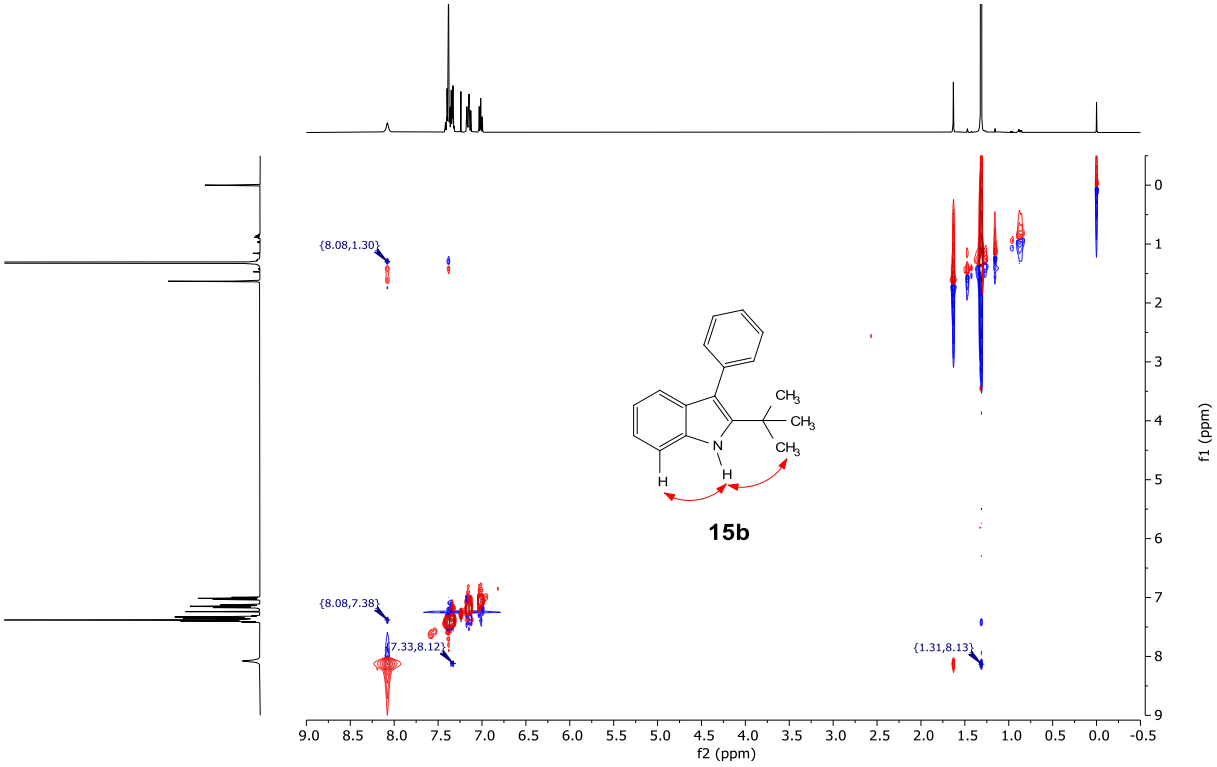


Figure S63. NOESY spectrum of 2-(*tert*-butyl)-3-phenyl-1*H*-indole (**15b**) in $CDCl_3$

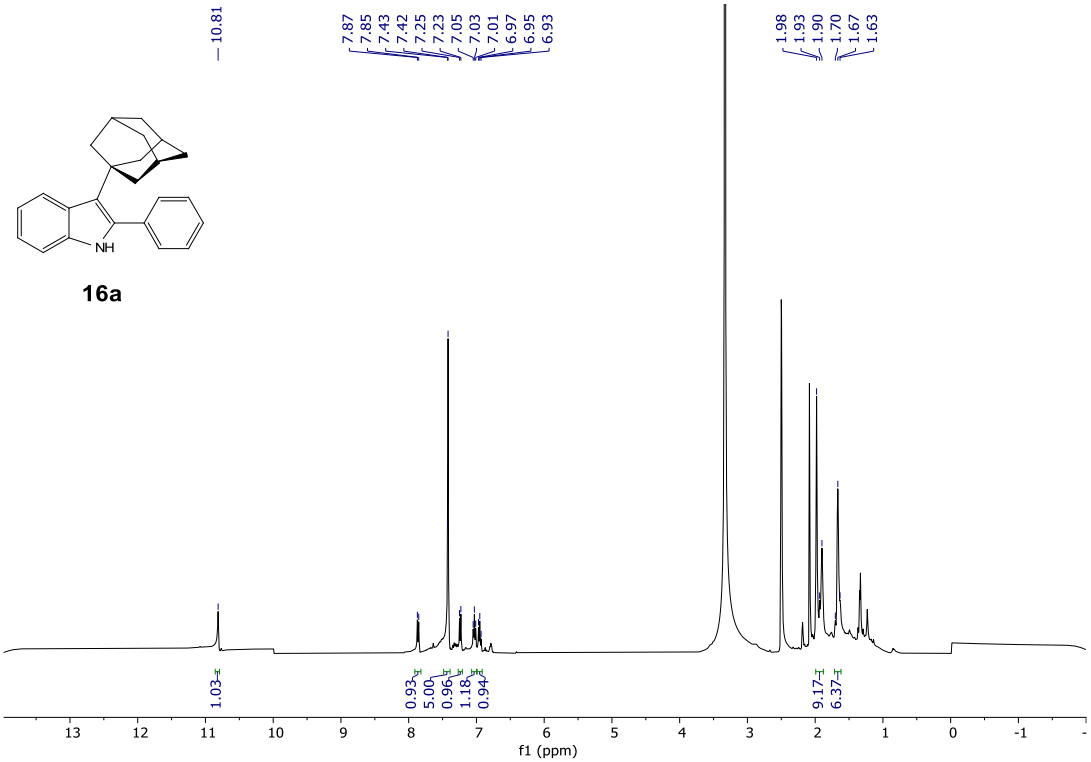


Figure S64. ^{1}H NMR spectrum (400 MHz) of 3-(adamantan-1-yl)-2-phenyl-1*H*-indole (**16a**) in DMSO-d_6

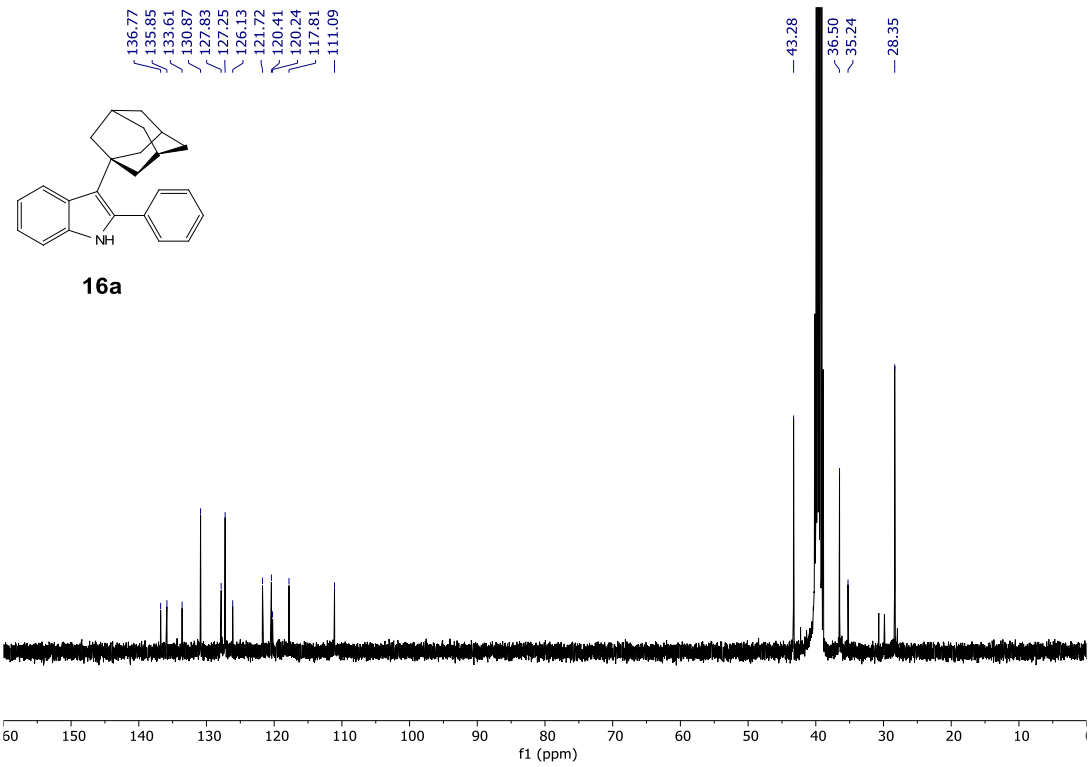


Figure S65. ^{13}C{^{1}H} NMR spectrum (100 MHz) of 3-(adamantan-1-yl)-2-phenyl-1*H*-indole (**16a**) in DMSO-d_6

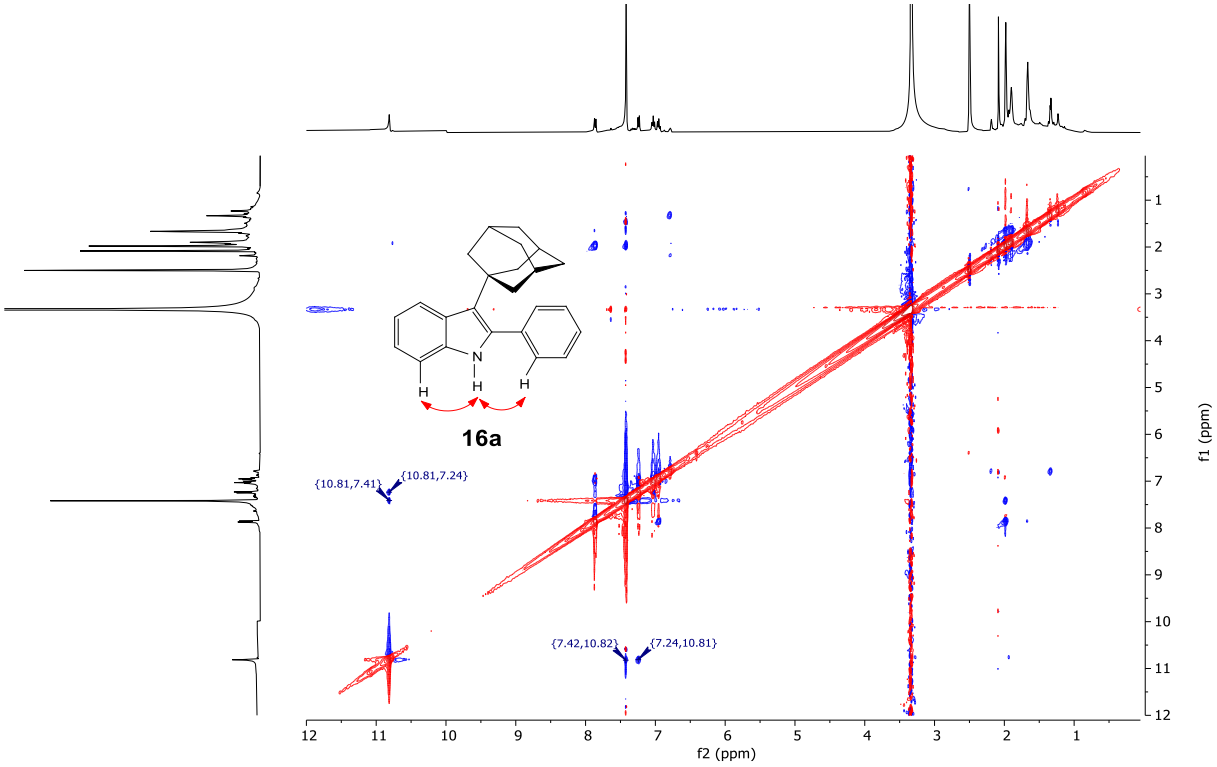


Figure S66. NOESY spectrum of 3-(adamantan-1-yl)-2-phenyl-1*H*-indole (**16a**) in DMSO-d_6

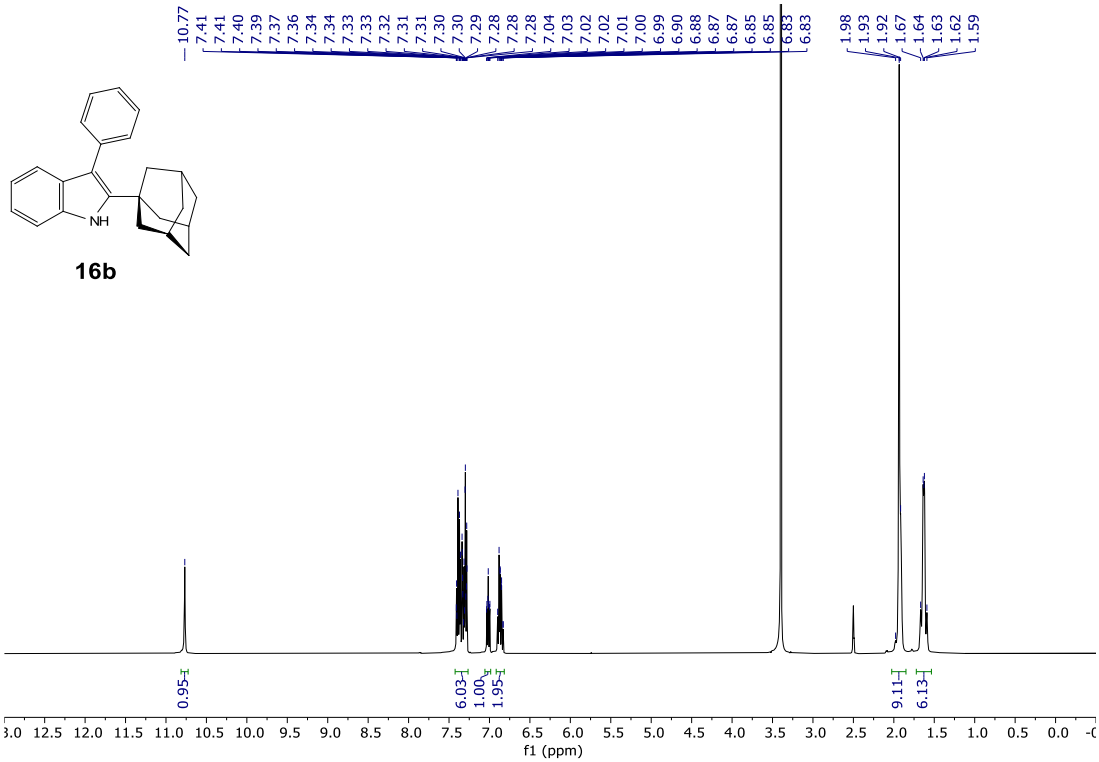


Figure S67. ^{1}H NMR spectrum (400 MHz) of 2-(adamantan-1-yl)-3-phenyl-1*H*-indole (**16b**) in DMSO-d_6

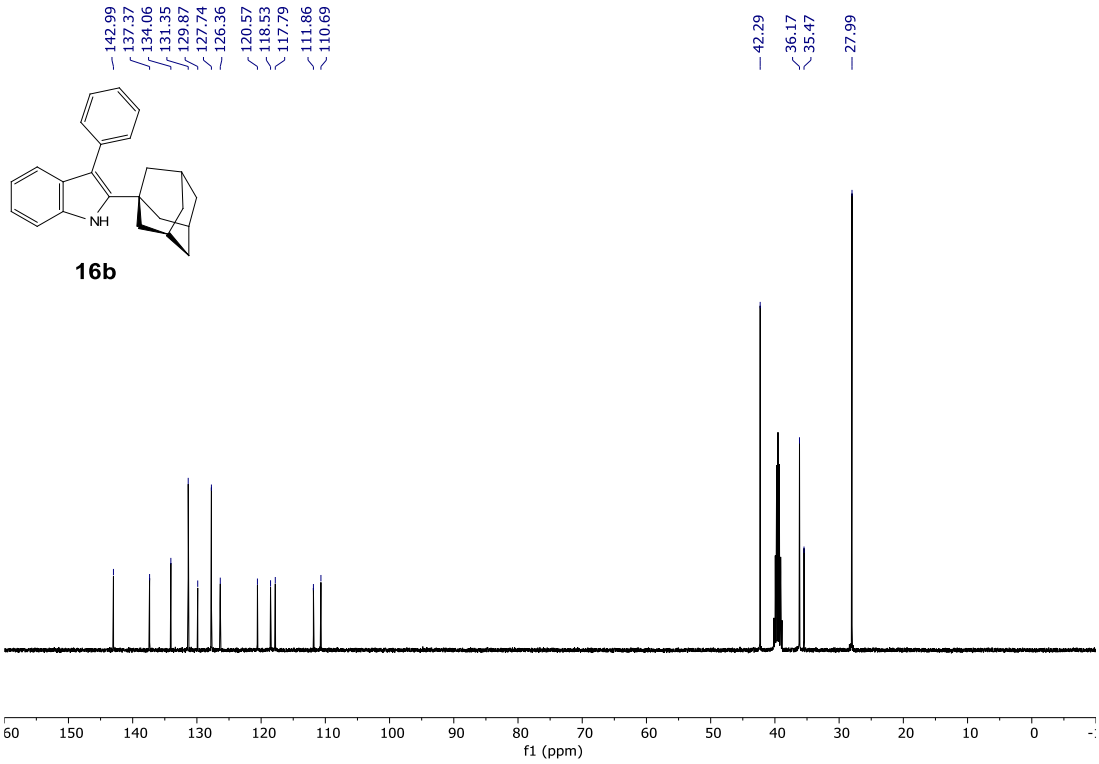


Figure S68. ^{13}C{^{1}H} NMR spectrum (100 MHz) of 2-(adamantan-1-yl)-3-phenyl-1*H*-indole (**16b**) in DMSO-d_6

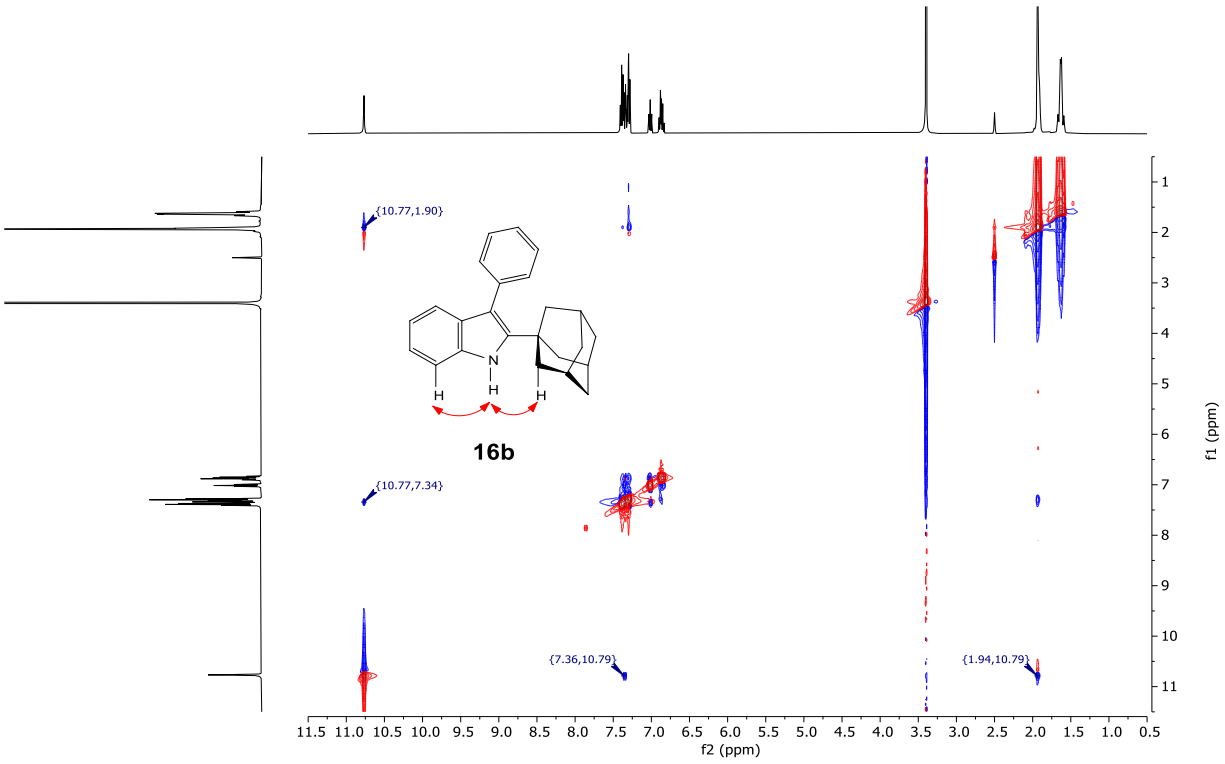


Figure S69. NOESY spectrum of 2-(adamantan-1-yl)-3-phenyl-1*H*-indole (**16b**) in DMSO-d_6

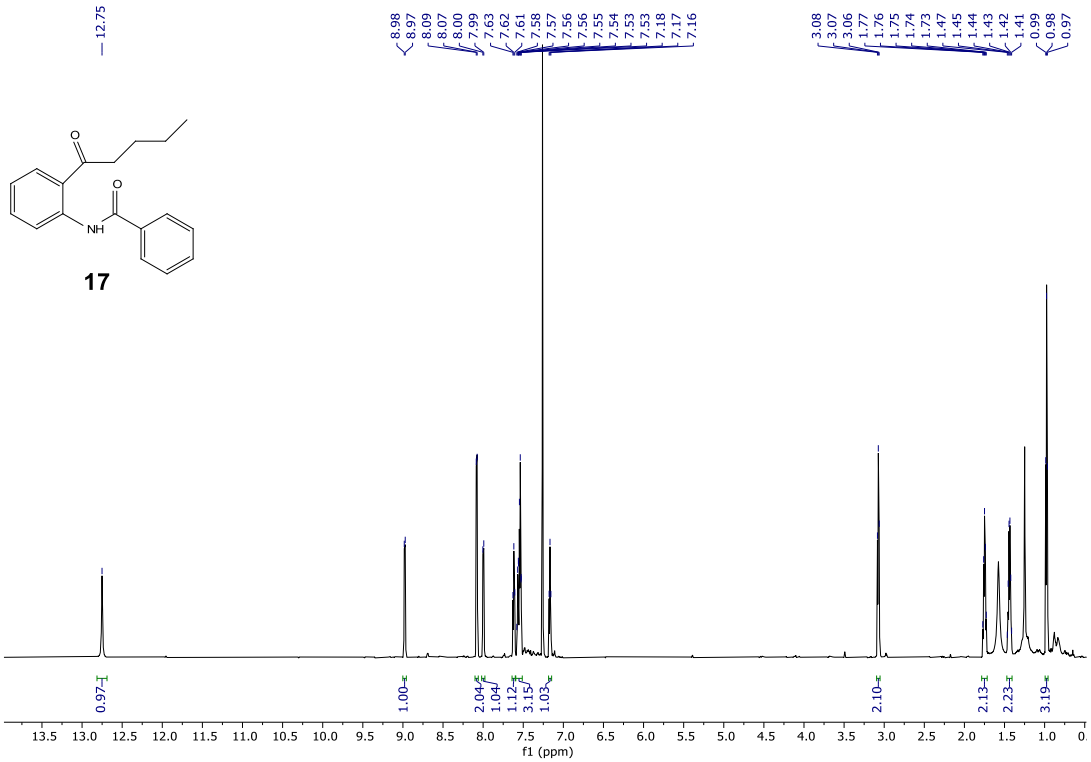


Figure S70. ^{1}H NMR spectrum (700 MHz) of *N*-(2-pentanoylphenyl)benzamide (**17**) in $CDCl_3$

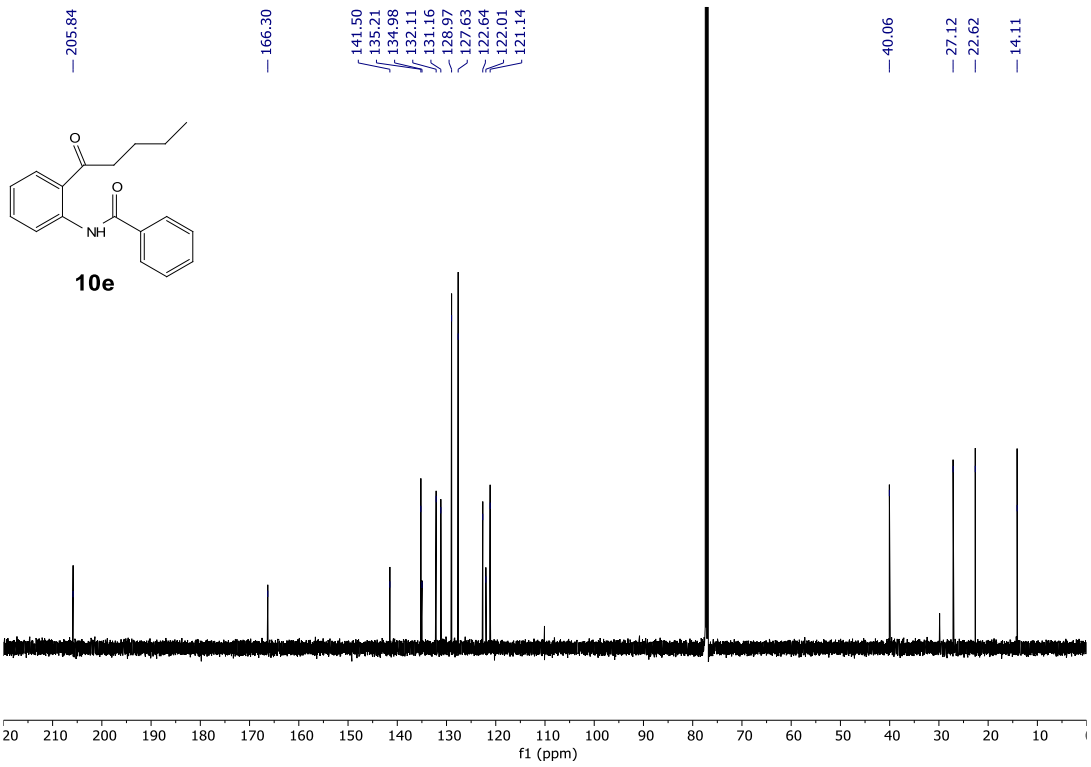


Figure S71. $^{13}C\{^{1}H\}$ NMR spectrum (175 MHz) of *N*-(2-pentanoylphenyl)benzamide (**17**) in $CDCl_3$

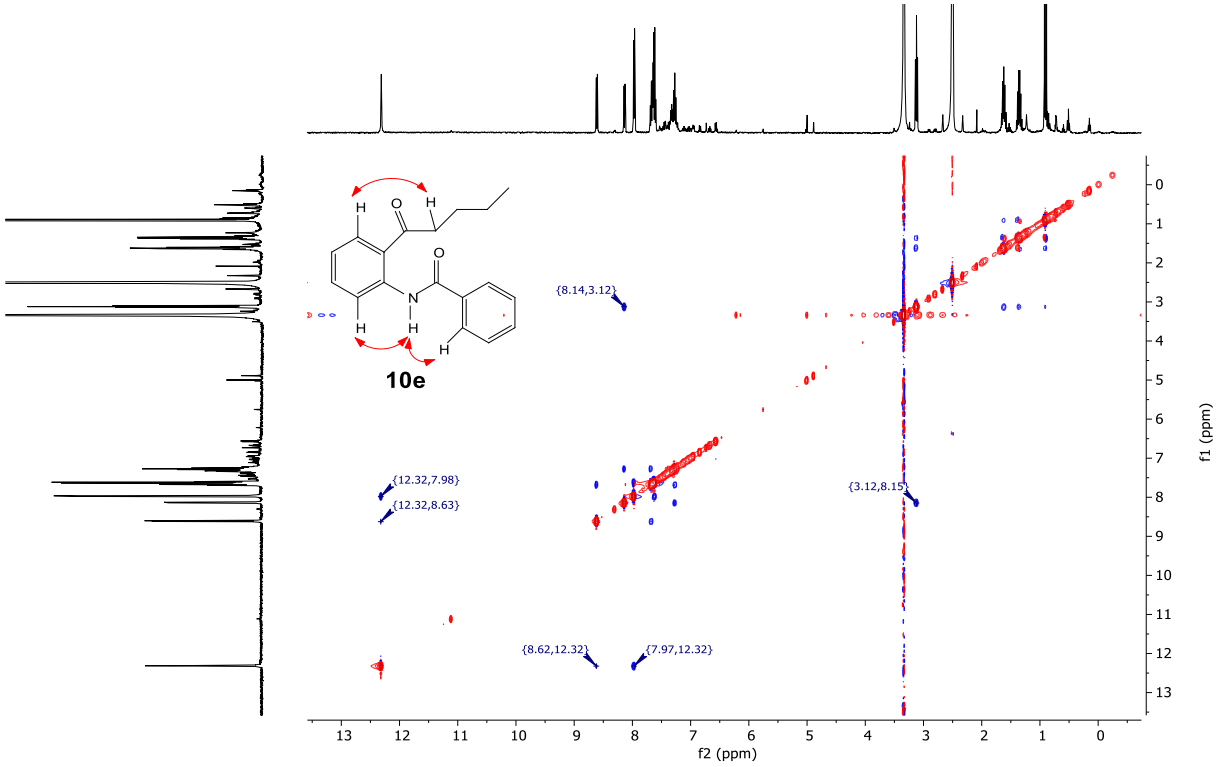


Figure S72. NOESY spectrum of *N*-(2-pentanoylphenyl)benzamide (**17**) in $CDCl_3$

NMR spectra of the crude reaction mixtures from the Larock heteroannulation reaction

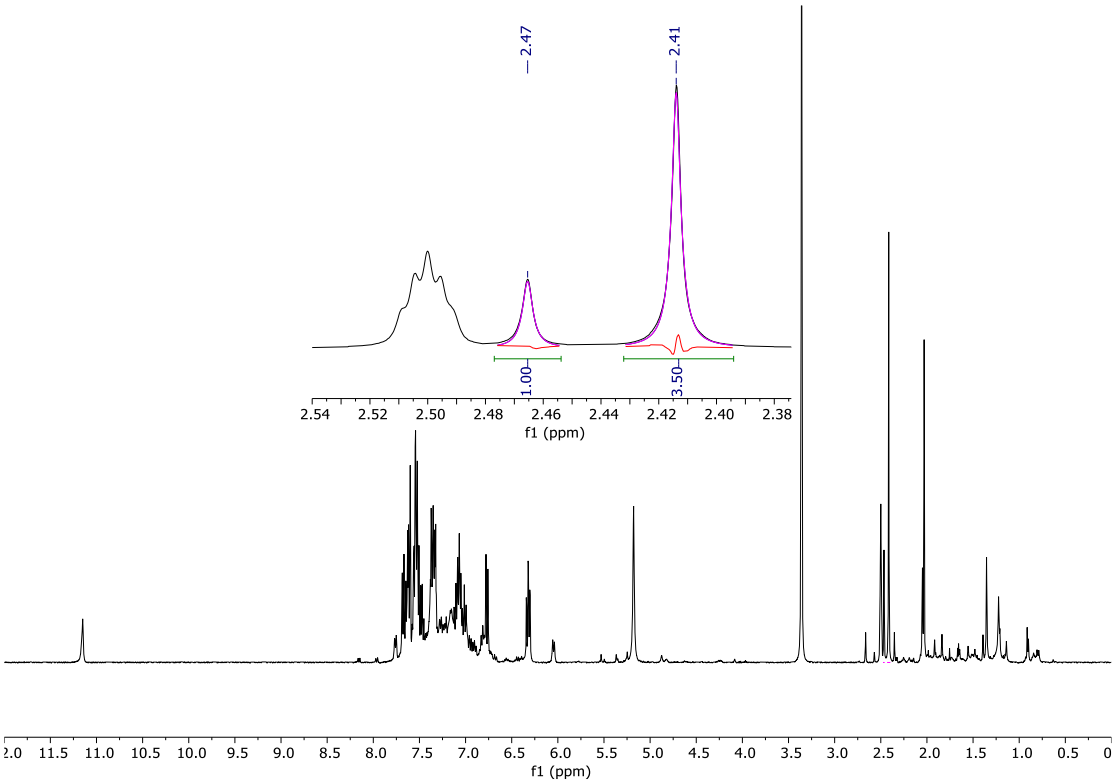


Figure S73. ^{1}H NMR spectrum (400 MHz) of the crude reaction mixtures of **9a** and **9b** in DMSO-d_6

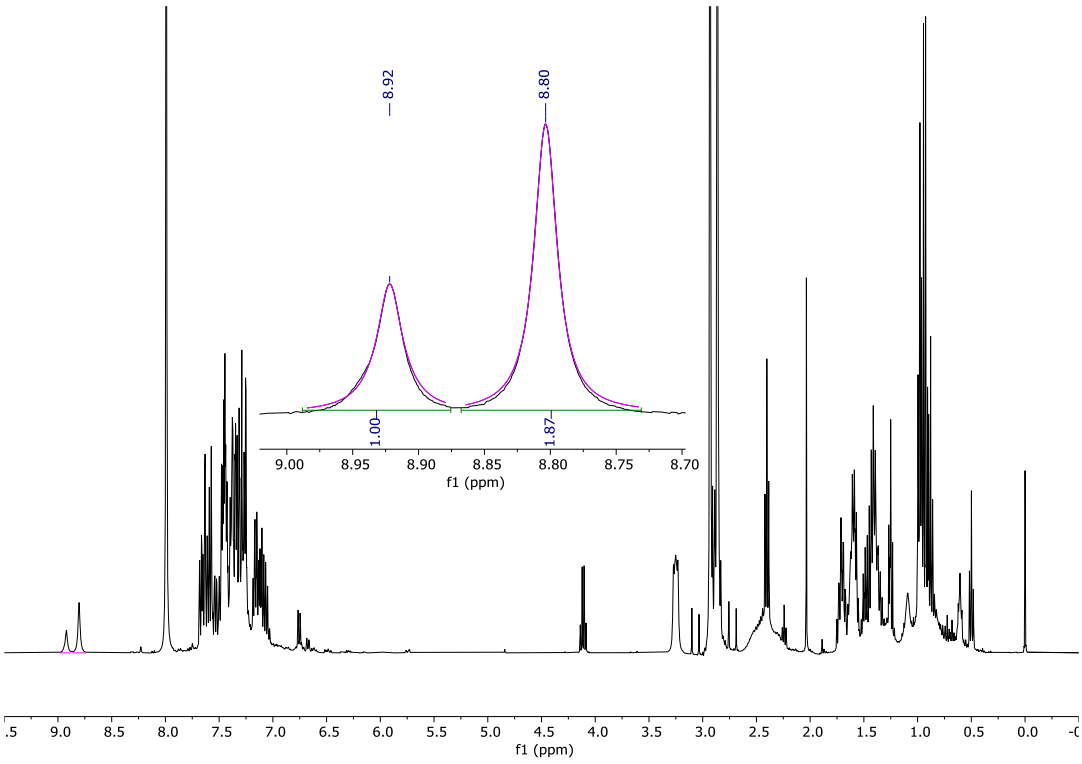


Figure S74. ^{1}H NMR spectrum (400 MHz) of the crude reaction mixtures of **10a** and **10b** in $CDCl_3$

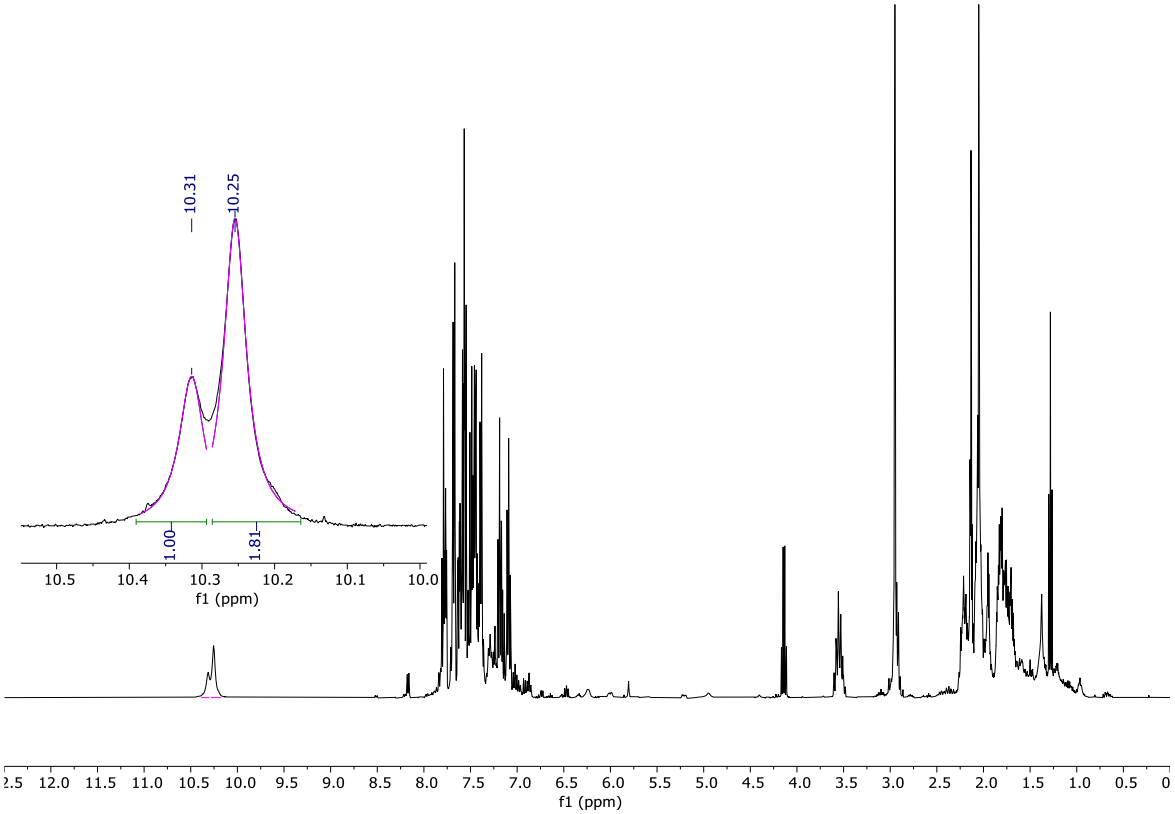


Figure S75. ^{1}H NMR spectrum (400 MHz) of the crude reaction mixtures of **11a** and **11b** in acetone-d_6

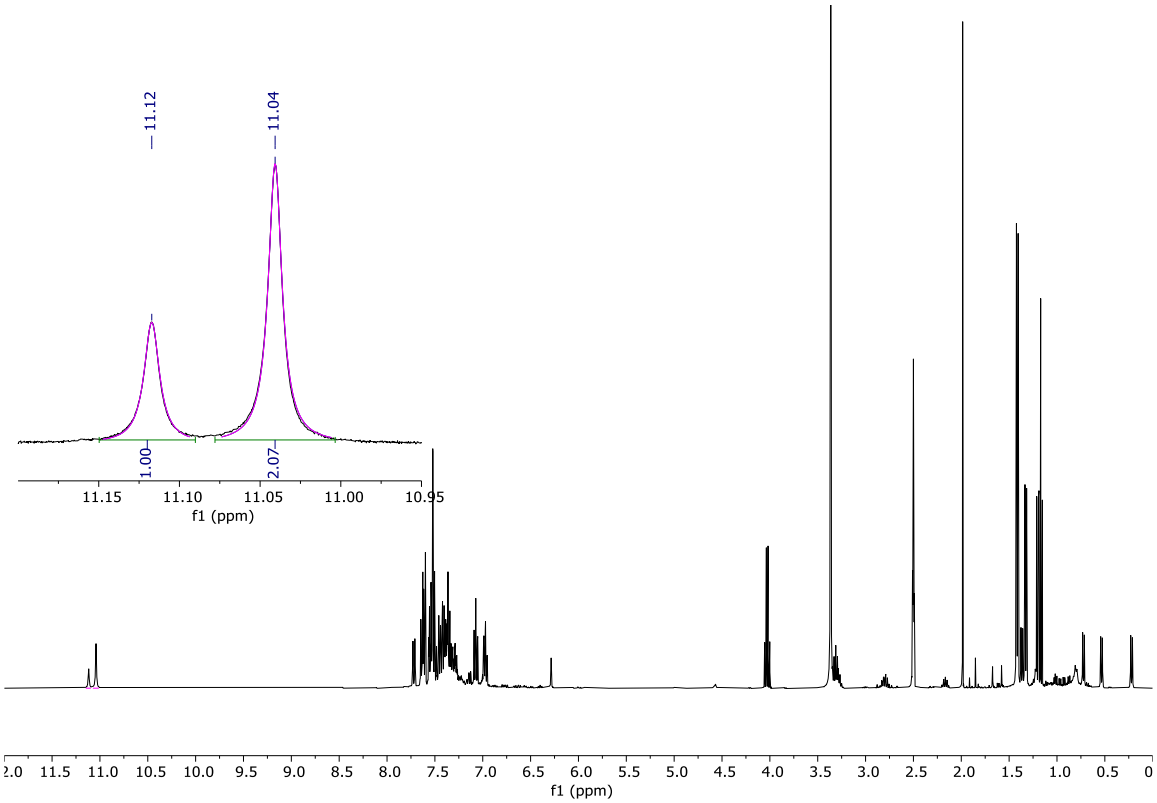


Figure S76. ^{1}H NMR spectrum (400 MHz) of the crude reaction mixtures of **12a** and **12b** in DMSO-d_6

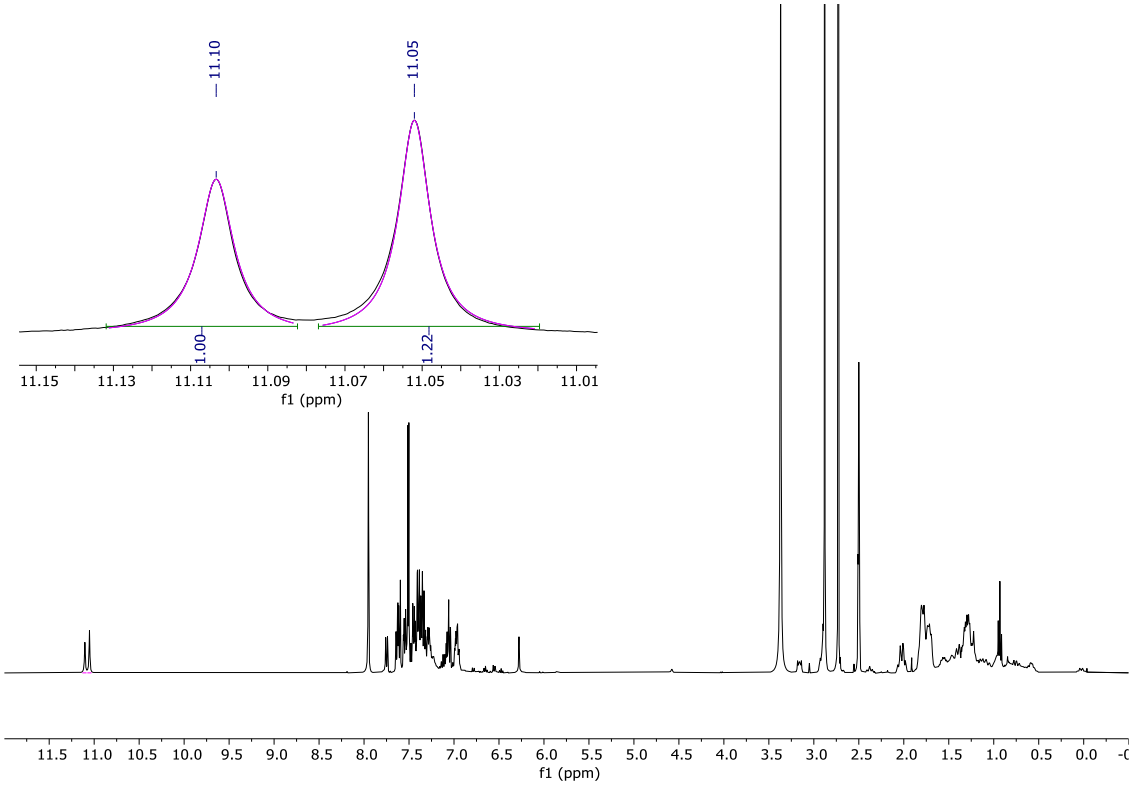


Figure S77. ^{1}H NMR spectrum (400 MHz) of the crude reaction mixtures of **13a** and **13b** in DMSO-d_6

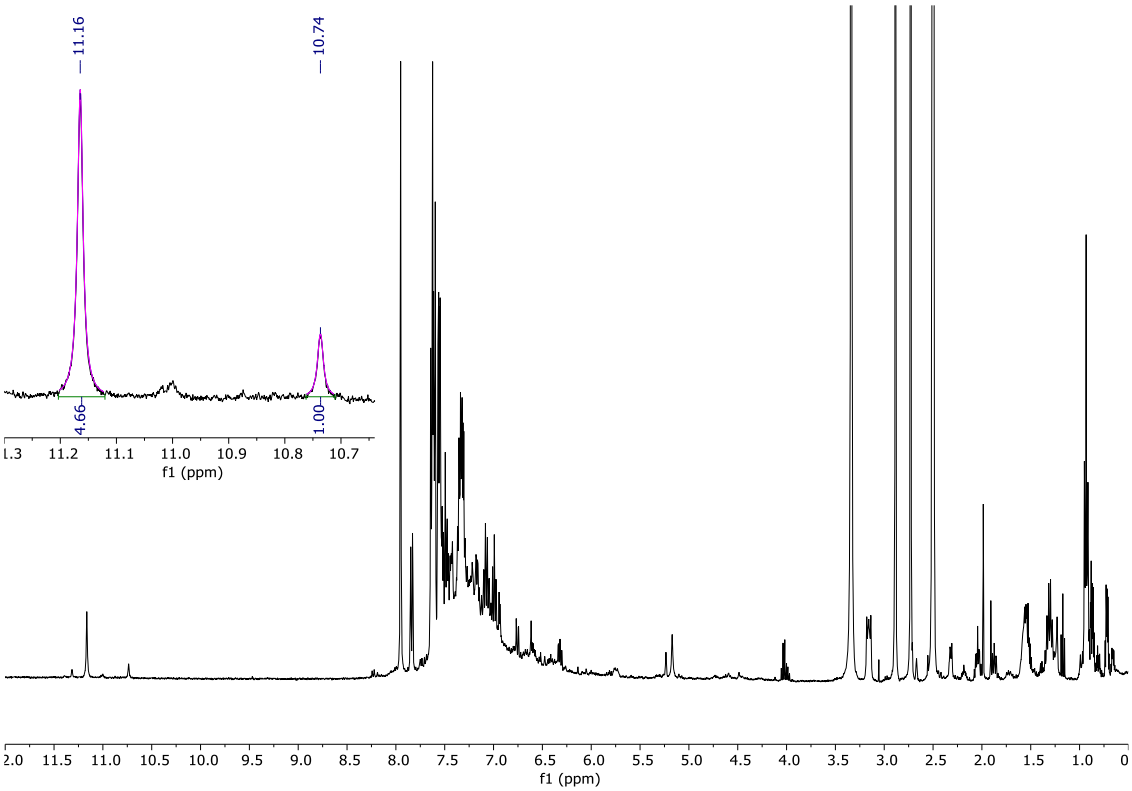


Figure S78. ^{1}H NMR spectrum (400 MHz) of the crude reaction mixtures of **14a** and **14b** in DMSO-d_6

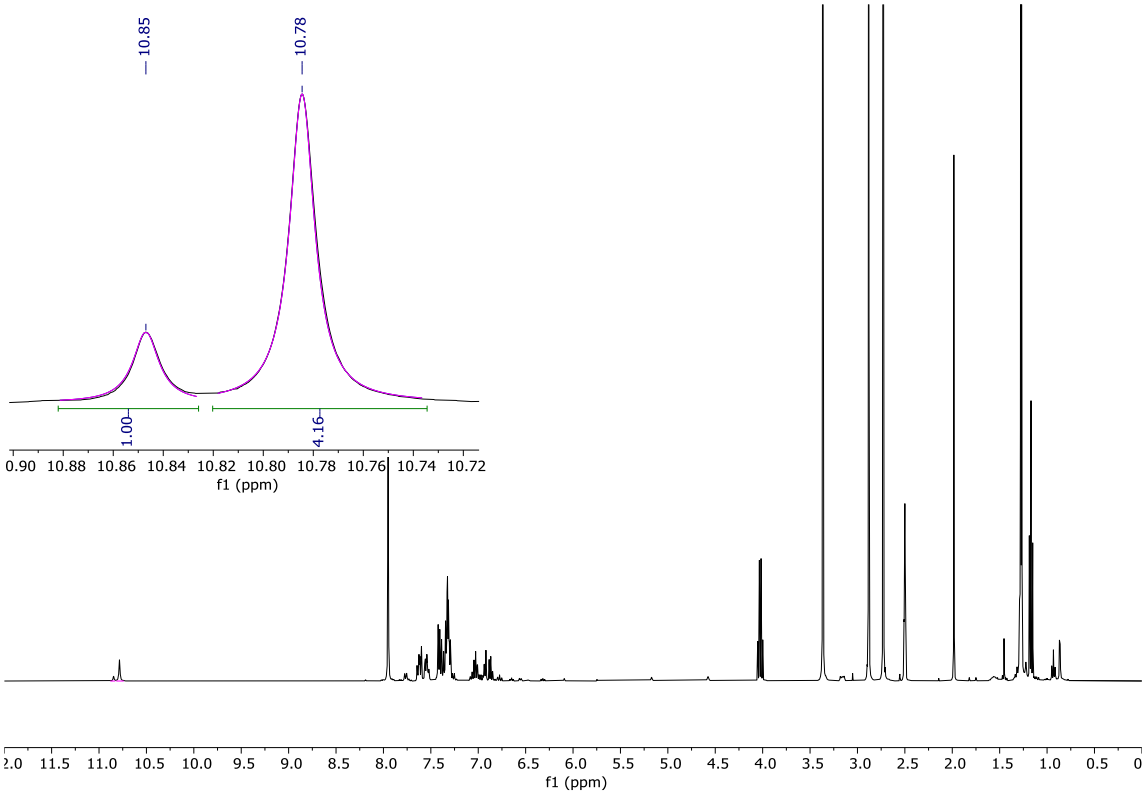


Figure S79. ^{1}H NMR spectrum (400 MHz) of the crude reaction mixtures of **15a** and **15b** in DMSO-d_6

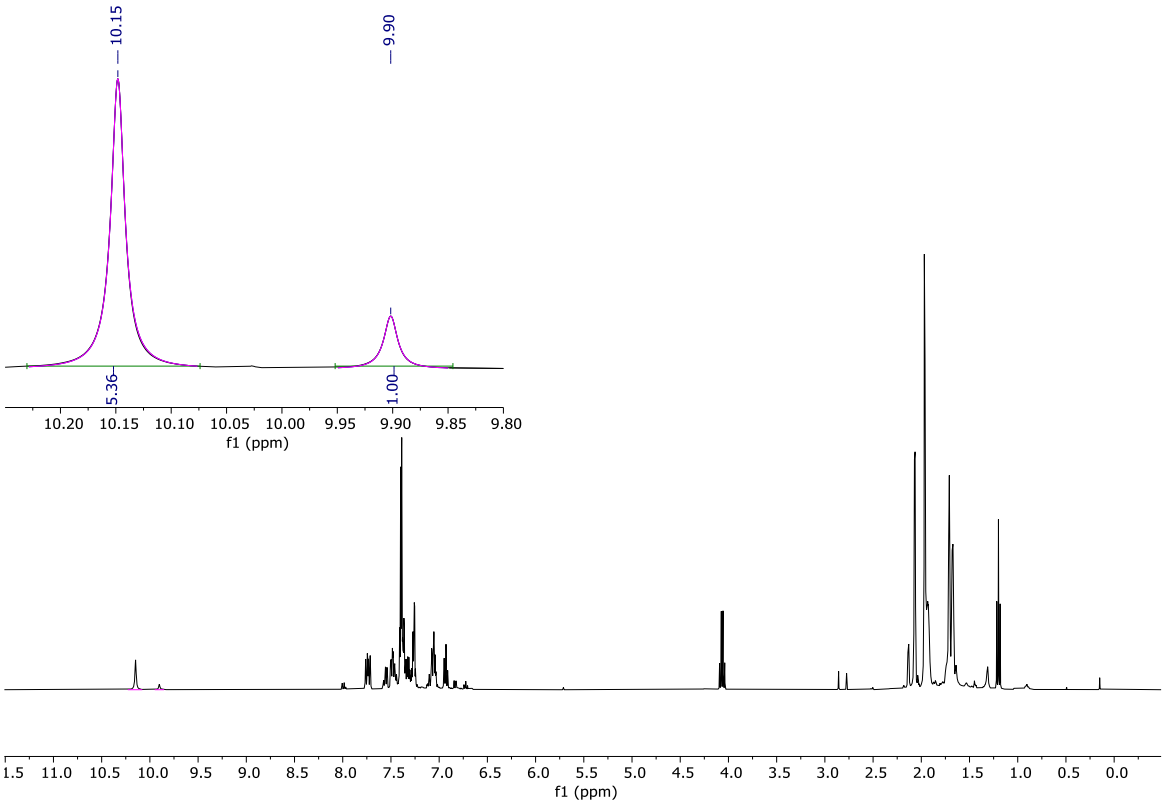
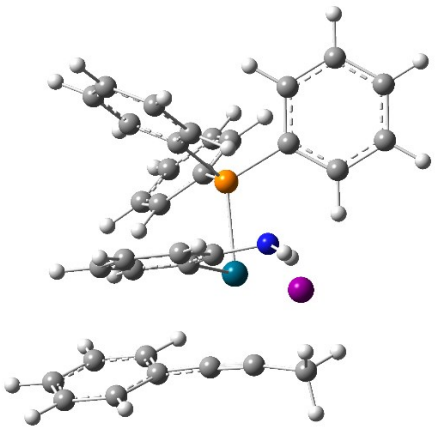


Figure S80. ^{1}H NMR spectrum (400 MHz) of the crude reaction mixtures of **16a** and **16b** in DMSO-d_6

Energy and coordinate for all calculated structures

M06

ADS complex of prop-1-yn-1-ylbenzene
Energy = -1134654.927677 kcal/mol
Electronic Energy + Thermal Free Energy Correction (353.150 K) = -1134385.531788 kcal/mol
Symmetry c1



Pd	0.53865200	-0.30121700	-0.79930600
P	-1.31687100	0.30834500	0.46957500
I	-0.09817800	-3.04311700	-0.85438800
C	1.00800100	1.68246700	-0.87112400
C	1.84931000	2.22425800	0.09291200
C	0.54632400	2.47857100	-1.93152100
C	2.27255600	3.55314300	0.01257200
H	2.19001000	1.60623900	0.92629100
C	0.98888200	3.80712800	-2.01377700
C	1.84178200	4.33734300	-1.05356900
H	2.93418600	3.96156200	0.77365800
H	0.63943500	4.42616300	-2.84076600
H	2.16609700	5.37250300	-1.13898500
N	-0.40329700	2.00947100	-2.84130200
H	-0.44670300	1.00099100	-2.92586200
H	-0.39442500	2.46627300	-3.74441300
C	2.84696000	-0.72885500	-1.30620900
C	2.28265000	-0.74004500	-2.39609500
C	3.61136800	-0.63099900	-0.09922600
C	4.63973000	0.31955100	-0.01757200
C	3.31640700	-1.43109700	1.01492700
C	5.35216300	0.47289200	1.16437300
H	4.85596500	0.94332800	-0.88196900
C	4.02963200	-1.26478000	2.19499700
H	2.51370300	-2.16417900	0.94530400
C	5.04440300	-0.31230900	2.27319900
H	6.14444500	1.21470500	1.22432400
H	3.79126600	-1.88103100	3.05860000
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C	-1.08214300	2.25030600	2.51015700
C	-1.66805700	3.06430900	0.31279000
C	-1.05493100	3.56022700	2.98328800
H	-0.86741700	1.43120700	3.19261600
C	-1.64592900	4.36731200	0.79141900
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H	-1.86047900	5.19137000	0.11492500
H	-1.30880500	5.64074800	2.49659900
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C	-2.47317100	-1.55428800	2.26388900
C	-0.15251200	-0.98839900	2.62181200
C	-2.40340800	-2.46761400	3.31357600
H	-3.40320800	-1.43818400	1.71114900
C	-0.08886700	-1.89204500	3.67377000
H	0.73820300	-0.42697400	2.33491000
C	-1.21466100	-2.63981600	4.01532600
H	-3.28249400	-3.04984500	3.57868500
H	0.84320900	-2.02237600	4.21870900
H	-1.16293200	-3.35853900	4.82946000
C	-2.91996000	0.13133200	-0.38052900
C	-2.99933900	-0.53514600	-1.60529700

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C	-4.22731800	-0.68459500	-2.24294700
H	-2.09335500	-0.94412500	-2.05140200
C	-5.30913400	0.49834100	-0.43931800
H	-4.02968100	1.18651200	1.14644800
C	-5.38099100	-0.17028300	-1.65963900
H	-4.28053100	-1.20169900	-3.19766900
H	-6.20963800	0.90334000	0.01543500
H	-6.34045200	-0.28678500	-2.15774100
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H	5.59664900	-0.18279500	3.20068900
H	0.98369800	-1.55958600	-3.84295200
H	2.60597600	-1.14076700	-4.43617100
H	1.42336800	0.14093100	-4.11322100

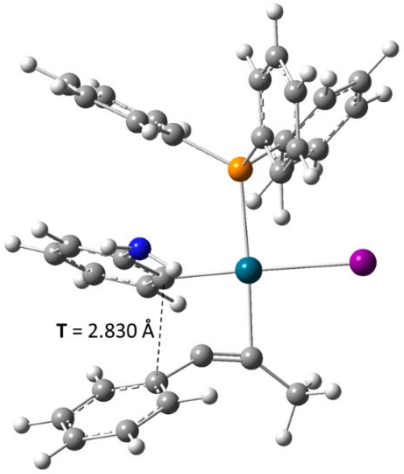
TS1 complex of prop-1-yn-1-ylbenzene

Energy = -1134639.150218 kcal/mol

Electronic Energy + Thermal Free Energy Correction (353.150 K) = -1134369.567959 kcal/mol

Imaginary frequency = -310.06 cm^{-1}

Symmetry c1



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C	-1.93787500	0.83664900	-2.16120100
C	-2.06311900	1.55944800	0.15925000
C	-2.43626700	2.06427100	-2.59124200
H	-1.72317700	0.05013300	-2.88420900
C	-2.57538600	2.78652700	-0.28505900
C	-2.75315800	3.03418500	-1.63934300
H	-2.58916700	2.25395300	-3.65074500
H	-2.81428100	3.55342500	0.45177400
H	-3.15127400	3.99627900	-1.95525300
N	-1.83944300	1.32682900	1.50048500
H	-1.77452100	0.35601600	1.77871700
H	-2.35420300	1.90343700	2.15181300
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C	-1.95453800	-2.25850200	-0.84154200
C	-3.95074000	-0.89113400	0.15023800
C	-4.80531000	0.02893600	-0.46965700
C	-4.33577700	-1.48421200	1.36007400
C	-6.02906200	0.33676500	0.10845800
H	-4.49895400	0.49602600	-1.40363300
C	-5.55995700	-1.16611800	1.93714800
H	-3.66323500	-2.19425100	1.83769100
C	-6.40782700	-0.25597700	1.31230400
H	-6.69258200	1.04560000	-0.38076400
H	-5.85022800	-1.62910300	2.87699400
C	1.05550200	2.49020600	-0.08605700
C	1.21766800	3.08029800	-1.34259400
C	0.62188300	3.28435300	0.98226900
C	0.94854000	4.43338100	-1.52798700
H	1.56646300	2.49016000	-2.18761500
C	0.36148200	4.63670400	0.79627100
H	0.47707100	2.84127300	1.96463400
C	0.52297200	5.21554600	-0.45979000
H	1.08362000	4.87724200	-2.51167800
H	0.03258600	5.24103500	1.63873700
H	0.32089700	6.27438500	-0.60398200
C	2.71755600	0.31869300	-0.99486200

C	4.05342000	0.19176200	-0.61167900
C	2.36967400	0.08053700	-2.33138700
C	5.02254900	-0.16538900	-1.54682100
H	4.34602800	0.34548800	0.42438700
C	3.33952200	-0.25948900	-3.26670500
H	1.32273300	0.13468600	-2.63508700
C	4.66983900	-0.38921000	-2.87336100
H	6.05793100	-0.27174400	-1.23194700
H	3.05411600	-0.43997700	-4.30027000
H	5.42841500	-0.66955400	-3.60008400
C	2.05235000	0.63771100	1.85364900
C	3.06530700	1.51842100	2.25681800
C	1.53571900	-0.27363100	2.77729400
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C	2.03704200	-0.32387400	4.07540600
H	0.73620700	-0.94694400	2.46958800
C	3.05749300	0.53989300	4.46021000
H	4.35885700	2.14702200	3.85245800
H	1.62677100	-1.03715400	4.78607500
H	3.45061200	0.50035300	5.47324600
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H	-7.36498300	-0.00610500	1.76360400
H	-1.27882100	-3.68064600	-2.27900800
H	-2.88988300	-4.00122200	-1.58976000
H	-1.41130200	-4.29843200	-0.63662300

INT1 complex of prop-1-yn-1-ylbenzene

Energy = -1134673.951240 kcal/mol

Electronic Energy + Thermal Free Energy Correction (353.150 K) = -1134403.256407 kcal/mol

Symmetry c1

Pd	-0.54885900	-0.63316100	-0.10582300
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C	-2.23504800	0.95092500	-0.32419900
C	-1.66418300	1.23009600	-1.59211900
C	-2.13441300	1.93924000	0.70543700
C	-1.00348400	2.42810300	-1.84550600
H	-1.81976200	0.50213400	-2.38703700
C	-1.49647200	3.14996200	0.41742800
C	-0.94407800	3.38379000	-0.83537900
H	-0.56459500	2.62160700	-2.82089700
H	-1.42281800	3.90765400	1.19639500
H	-0.44346400	4.33287300	-1.01808300
N	-2.63688500	1.68446300	1.95242000
H	-3.31201000	0.93932500	2.05073100
H	-2.77899600	2.47024800	2.56993400
C	-3.14225500	-0.23834000	-0.16108700
C	-2.45175700	-1.38521700	-0.19296400
C	-4.59821000	-0.01799200	-0.03748600
C	-5.19159200	1.07519600	-0.68461800
C	-5.41012200	-0.85313500	0.74248400
C	-6.55774800	1.30660000	-0.58297000
H	-4.57054700	1.74301700	-1.28158600
C	-6.77770900	-0.62037600	0.84316300
H	-4.95887000	-1.67598700	1.29376600
C	-7.35741800	0.45661000	0.17773200
H	-7.00172500	2.15455200	-1.09970600
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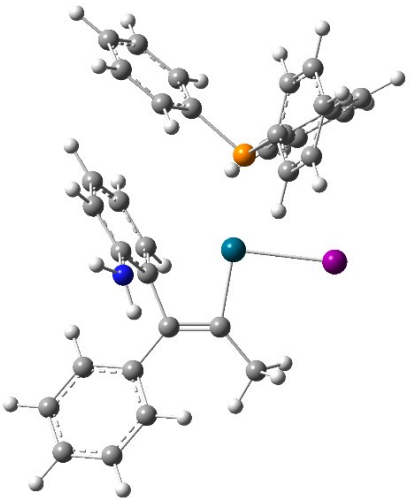
C	2.01759200	2.22763900	-0.06365600



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C	2.75818400	4.24569600	-1.17405300
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C	1.89035700	4.36593500	1.06914600
H	1.24598600	2.51073000	1.93623800
C	2.43059500	4.99689100	-0.04991900
H	3.18409200	4.73024300	-2.04965300
H	1.62742200	4.94577200	1.95106100
H	2.59666400	6.07146300	-0.04360500
C	2.64553500	-0.27263600	-1.38942200
C	3.80585200	-1.03802200	-1.26131200
C	2.07561800	-0.11157800	-2.65995400
C	4.39194900	-1.62006200	-2.38337700
H	4.24985800	-1.19985000	-0.28135400
C	2.66867500	-0.68171300	-3.77981900
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C	3.82820200	-1.44173700	-3.64229000
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C	4.00244700	0.44169500	1.68578400
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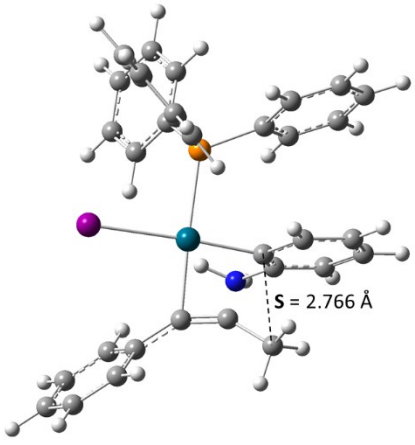
C	4.69087000	0.18861300	2.86612900
H	4.49899100	0.97377500	0.87451800
C	2.72504900	-0.85889500	3.79272700
H	1.00056200	-0.93031400	2.49581800
C	4.05214800	-0.46316100	3.92003500
H	5.72511400	0.50821600	2.96833100
H	2.22048900	-1.35634100	4.61748800
H	4.59051500	-0.65492300	4.84525000
C	-2.93731900	-2.78651300	-0.20987200
H	-8.42625200	0.63886300	0.25978100
H	-2.39126200	-3.39234600	-0.94147500
H	-4.00836500	-2.82358600	-0.45432700
H	-2.79154200	-3.27373100	0.76331500

TS2 complex of prop-1-yn-1-ylbenzene
Energy = -1134638.393442 kcal/mol
Electronic Energy + Thermal Free Energy Correction (353.150 K) = -1134368.498684 kcal/mol
Imaginary frequency = -333.74 cm^{-1}
Symmetry c1

Pd	-0.66098100	0.41239900	-0.28421000
P	1.49215000	-0.58407700	0.04662200
I	-1.84655600	-2.06898500	-0.24194800
C	0.14226200	2.34595900	-0.31916500
C	0.99949000	2.73726800	-1.35619700
C	0.10823900	3.09583900	0.87677200
C	1.76486900	3.88935800	-1.26509100
H	1.03276500	2.13400100	-2.26472800
C	0.88035800	4.26879300	0.95274300
C	1.68692100	4.66149100	-0.10301200
H	2.41698900	4.18308200	-2.08400600
H	0.84349000	4.86197000	1.86623400
H	2.27404300	5.57310400	-0.01425300
N	-0.69999400	2.73091900	1.93840700
H	-0.86818500	1.73890200	2.04207100
H	-0.50077500	3.18870200	2.81760600
C	-2.53370900	1.43881000	-0.46458200



C	-1.83385100	2.32618000	-1.03089900
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C	-4.17182700	0.87984500	1.29296800
C	-4.73366300	0.46886800	-1.02403400
C	-5.41214000	0.38835100	1.67843900
H	-3.45540700	1.22766700	2.03537400
C	-5.97100900	-0.02691700	-0.63076600
H	-4.45439800	0.49497000	-2.07541600
C	-6.31284200	-0.07073500	0.71912600
H	-5.67594500	0.35838300	2.73291300
H	-6.67177100	-0.38307700	-1.38220300
C	2.96333500	0.48971100	-0.13719500
C	3.80870400	0.42999900	-1.24667600
C	3.20660400	1.44301000	0.85866200
C	4.88276200	1.31015600	-1.35723700
H	3.63858600	-0.30888800	-2.02714600
C	4.27765900	2.31887100	0.74552700
H	2.54685500	1.50657600	1.72460300
C	5.11771200	2.25521700	-0.36470900
H	5.53842600	1.25212300	-2.22290200
H	4.45171200	3.06011100	1.52236900
H	5.95568100	2.94257400	-0.45343300
C	1.77022300	-1.96033800	-1.12378400
C	2.19020500	-3.23232900	-0.73433000
C	1.47380200	-1.71849800	-2.47101000
C	2.31494600	-4.24706800	-1.68067400
H	2.40720500	-3.44341700	0.31074900
C	1.61304800	-2.72754700	-3.41561300
H	1.11481800	-0.73430300	-2.77654900
C	2.02973600	-3.99696400	-3.01903300
H	2.63520800	-5.23773100	-1.36705200
H	1.38328400	-2.52750700	-4.45932100
H	2.12834700	-4.79123300	-3.75498700
C	1.73361100	-1.26082700	1.72909100
C	2.99258300	-1.71633900	2.14289800
C	0.66591800	-1.29570000	2.62929900
C	3.16907700	-2.22218300	3.42479200
H	3.83930300	-1.66991800	1.45888700
C	0.84667500	-1.79471600	3.91680700
H	-0.31385300	-0.93780100	2.31319600
C	2.09523800	-2.26237200	4.31263200
H	4.14780600	-2.57980000	3.73500800
H	0.00944200	-1.81588100	4.60996800
H	2.23603700	-2.65469000	5.31692600
C	-1.80251500	3.51053300	-1.90480300
H	-7.28024100	-0.46234900	1.02400600
H	-1.35903500	4.37612400	-1.40120800
H	-1.22799100	3.31858300	-2.81658600
H	-2.83493500	3.74556100	-2.19009900

INT2 complex of prop-1-yn-1-ylbenzene

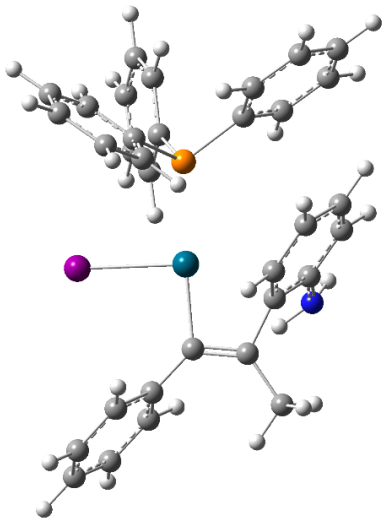
Energy = -1134673.309298 kcal/mol

Electronic Energy + Thermal Free Energy Correction (353.150 K) = -1134403.727039 kcal/mol

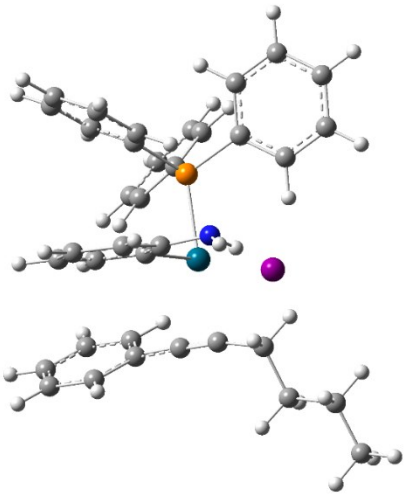
Symmetry c1

Pd	0.72515000	0.35091900	0.07106700
P	-1.61451000	-0.39468300	-0.11509600
I	1.57296200	-2.11344100	0.60673200
C	0.89747700	2.69440000	0.40872300
C	0.47317400	2.52680100	1.75025600
C	0.01617700	3.33755300	-0.50874400

C	-0.76928000	2.96723600	2.18213200
H	1.17674400	2.07744200	2.44943500
C	-1.22151200	3.80692900	-0.04519500
C	-1.60265300	3.62476400	1.27372200
H	-1.07127100	2.83371800	3.21762000
H	-1.88427100	4.31836000	-0.74052100
H	-2.57020500	3.99965900	1.60064900
N	0.40697100	3.55526500	-1.80807500
H	1.11755100	2.93634200	-2.17629100
H	-0.32835100	3.76293100	-2.46997900
C	2.61636900	1.12377900	-0.02478600
C	2.33689100	2.42486500	0.05521100
C	3.88840200	0.45550800	-0.26215900
C	4.14381000	-0.21131400	-1.46950300
C	4.88551200	0.47102800	0.72261800
C	5.36386100	-0.83775600	-1.68662900
H	3.36548400	-0.24036300	-2.23147700
C	6.10463300	-0.16355300	0.50556300
H	4.68964600	0.98427900	1.66311800
C	6.34763800	-0.82031400	-0.69808600
H	5.54950100	-1.34539800	-2.63063900
H	6.86857400	-0.14317600	1.27961600
C	-2.93236000	0.84038000	-0.44828900
C	-3.97067300	1.13014900	0.43651100
C	-2.86283200	1.52528000	-1.66789700
C	-4.92626800	2.09016800	0.10631000
H	-4.04274700	0.60303600	1.38619200
C	-3.82389100	2.47038000	-2.00204600
H	-2.05069700	1.31251300	-2.36534100
C	-4.85654700	2.75918600	-1.11062500
H	-5.73252300	2.30697100	0.80326200
H	-3.76354200	2.98916900	-2.95625000
H	-5.60679100	3.50298200	-1.36791800
C	-2.15437400	-1.26096800	1.40302700
C	-2.55726800	-2.59744100	1.42021000
C	-2.04089300	-0.56595600	2.61545600
C	-2.85844000	-3.22515400	2.62678900
H	-2.62599000	-3.15883000	0.49081600
C	-2.35542800	-1.19099600	3.81614900
H	-1.70220000	0.47258800	2.61773400
C	-2.76275700	-2.52383600	3.82387900
H	-3.16765700	-4.26764100	2.62776900
H	-2.27310200	-0.63981700	4.74990400
H	-2.99864100	-3.01556400	4.76458000
C	-1.91193900	-1.55404900	-1.50522600
C	-3.19779500	-2.03896100	-1.77935700
C	-0.85876000	-1.89967700	-2.35458700
C	-3.41612700	-2.87694200	-2.86603300
H	-4.03378300	-1.75537600	-1.14009900
C	-1.08036600	-2.73177500	-3.44994400
H	0.14009000	-1.51384200	-2.15222900
C	-2.35588000	-3.22498600	-3.70170100
H	-4.41609300	-3.25417400	-3.06605200
H	-0.25357700	-2.99256300	-4.10619900
H	-2.52909500	-3.87652900	-4.55487900
C	3.27012400	3.58298800	-0.12770700
H	7.30055300	-1.31633000	-0.86699200
H	2.89969100	4.27880200	-0.89098400
H	3.34842900	4.15220800	0.80888000
H	4.27106100	3.24572200	-0.41488600



ADS complex of hex-1-yn-1-ylbenzene
Energy = -1208604.808862 kcal/mol
Electronic Energy + Thermal Free Energy Correction (353.150 K) = -1208287.331979 kcal/mol
Symmetry c1

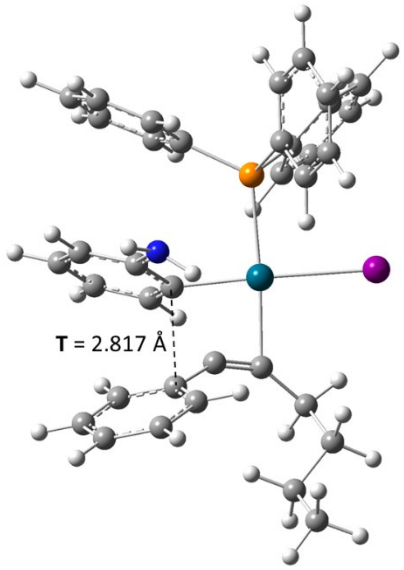


Pd	0.56691600	-0.00448400	-0.11455700
P	-1.72191400	-0.41181600	-0.03267600
I	1.22688200	-2.13050400	1.61400500
C	0.14284200	1.51719800	-1.40438400
C	-0.13722900	2.78170500	-0.89992600
C	0.19906300	1.30832100	-2.79149600
C	-0.34616000	3.86771100	-1.75344000
H	-0.19787100	2.93465100	0.17970500
C	0.00229100	2.40720800	-3.64154300
C	-0.26815500	3.67010800	-3.12862900
H	-0.56246600	4.85109500	-1.34148700
H	0.05143800	2.25175100	-4.71985000
H	-0.42113200	4.50270400	-3.81230800
N	0.35675300	0.03254600	-3.33684200
H	0.81706200	-0.63264600	-2.72720500
H	0.74693800	0.01640300	-4.27065600
C	2.66448300	1.11158600	0.28376100
C	2.88414400	0.23506400	-0.54924100
C	2.44890100	2.18965500	1.20004600
C	2.76644100	3.50032300	0.81598100
C	1.88245000	1.95433600	2.46271100
C	2.50984100	4.55763800	1.67886000
H	3.19898700	3.67626200	-0.16638900
C	1.62115900	3.01904900	3.31456000
H	1.63413300	0.93375800	2.75198400
C	1.93183200	4.32056200	2.92428700
H	2.75454700	5.57252400	1.37596600
H	1.17261400	2.83273000	4.28750900
C	-2.87484800	0.79981300	-0.76999300
C	-3.64409900	1.66723000	0.00701100
C	-2.93937700	0.88301700	-2.16606800
C	-4.46242100	2.61406600	-0.60568600
H	-3.61111800	1.60788800	1.09260700
C	-3.75764800	1.82659200	-2.77151100
H	-2.33689700	0.21387700	-2.78025600
C	-4.51800100	2.69733100	-1.99202300
H	-5.06049700	3.28384700	0.00751000
H	-3.79477000	1.88954300	-3.85653300
H	-5.15546400	3.43845000	-2.46816000
C	-2.17951700	-0.47429500	1.73299400
C	-2.90978400	-1.52180600	2.29434500
C	-1.71426800	0.56078500	2.55401600
C	-3.16640600	-1.53566800	3.66372800
H	-3.26627200	-2.34016000	1.67195900
C	-1.98017400	0.54876000	3.91671100
H	-1.12600500	1.37334000	2.12368300
C	-2.70237100	-0.50506300	4.47471600
H	-3.72832900	-2.35957200	4.09664100
H	-1.61744600	1.35748500	4.54652000
H	-2.90189400	-0.52181000	5.54327900
C	-2.23483000	-1.98408200	-0.79889500
C	-1.28072800	-2.89311200	-1.26137000
C	-3.59707300	-2.27678700	-0.94696800
C	-1.68227300	-4.08790900	-1.85230800
H	-0.22083000	-2.66340600	-1.15062500

C	-3.99386100	-3.47421200	-1.52945300
H	-4.34740100	-1.56275900	-0.60887000
C	-3.03641800	-4.37954800	-1.98272800
H	-0.93471500	-4.78950400	-2.21378100
H	-5.05219000	-3.69818400	-1.63649400
H	-3.34920000	-5.31292100	-2.44444100
C	3.44346500	-0.74974300	-1.47548200
H	1.72350100	5.15209500	3.59293600
H	2.86572900	-1.68455800	-1.40995500
H	3.32539500	-0.38203300	-2.50637300
C	4.91763200	-1.03908100	-1.18592700
H	5.48639700	-0.09822000	-1.21469100
H	5.01051900	-1.42708000	-0.16021300
C	5.50605500	-2.03310000	-2.17463900
H	4.91599200	-2.96143400	-2.14847400
H	5.39909100	-1.63374900	-3.19431900
C	6.96612200	-2.33583700	-1.88416500
H	7.38471400	-3.04724200	-2.60378000
H	7.57280600	-1.42258100	-1.92550100
H	7.08669700	-2.76502200	-0.88166600

TS1 complex of hex-1-yn-1-ylbenzene
Energy = -1208589.594907 kcal/mol
Electronic Energy + Thermal Free Energy Correction (353.150 K) = -1208270.323975 kcal/mol
Imaginary frequency = -302.86 cm^{-1}
Symmetry c1

Pd	-0.37219700	-0.48747000	-0.39842100
P	1.85559900	0.24374900	0.21039000
I	0.35311500	-3.11931900	-0.06412400
C	-0.95075400	1.45867000	-0.86811800
C	-1.00844600	1.76465200	-2.23029200
C	-0.82959000	2.48805200	0.08718700
C	-0.90433500	3.08098100	-2.67072800
H	-1.15421000	0.95833300	-2.94828400
C	-0.74189300	3.81081800	-0.36879700
C	-0.77047600	4.09899900	-1.72562700
H	-0.94371700	3.30978400	-3.73274500
H	-0.63912300	4.61185400	0.36283400
H	-0.69949700	5.13548200	-2.04911800
N	-0.74746400	2.19748600	1.43312800
H	-1.14759900	1.31445800	1.72371700
H	-0.94805900	2.95826600	2.06797000
C	-2.59832800	0.15541900	-0.52711100
C	-2.34599300	-0.99890000	-0.99244500
C	-3.53850400	1.02774200	0.15726800
C	-3.96612000	2.24062400	-0.39420500
C	-4.06825000	0.60102100	1.38331500
C	-4.91823100	3.00549200	0.26675300
H	-3.54665100	2.57386600	-1.34148100
C	-5.01687700	1.37424200	2.04288400
H	-3.72674100	-0.34386400	1.80573700
C	-5.44228200	2.57697500	1.48560300
H	-5.25409700	3.94295600	-0.16958400
H	-5.42149200	1.03655700	2.99381500
C	2.32027100	2.00970100	-0.01898700
C	2.54198900	2.51224500	-1.30441600
C	2.37855800	2.88911900	1.06779800
C	2.82203900	3.85996700	-1.50002300
H	2.50924500	1.85077300	-2.16789900
C	2.66277400	4.23611800	0.87105700



H	2.19219800	2.52459700	2.07502900
C	2.88444700	4.72581000	-0.41288000
H	2.99457900	4.23246800	-2.50720700
H	2.71106700	4.90492100	1.72744300
H	3.10578200	5.77966000	-0.56530700
C	3.00381500	-0.64574200	-0.91517900
C	4.15281500	-1.31341100	-0.48729800
C	2.64722300	-0.71256000	-2.26886600
C	4.93558900	-2.02146800	-1.39670000
H	4.43558800	-1.30712500	0.56267900
C	3.43845300	-1.40397900	-3.17825800
H	1.72267200	-0.24385300	-2.60900700
C	4.58497600	-2.06399900	-2.74206700
H	5.82300800	-2.54410700	-1.04752000
H	3.14972200	-1.44126400	-4.22588400
H	5.19824000	-2.61771200	-3.44881100
C	2.39981800	-0.12623000	1.91517100
C	3.67073600	0.22774300	2.38921800
C	1.50059600	-0.75112700	2.78287300
C	4.03750000	-0.06430200	3.69780500
H	4.37282100	0.74618100	1.73763700
C	1.86664900	-1.03752000	4.09523000
H	0.50863500	-1.01767400	2.41974000
C	3.13678800	-0.69943100	4.55054700
H	5.02693700	0.21055100	4.05484000
H	1.15726000	-1.52216900	4.76138400
H	3.42516800	-0.92369800	5.57473200
C	-2.87759200	-2.26909300	-1.53854100
H	-6.18343400	3.18266100	2.00131000
H	-2.05674000	-2.94254400	-1.80289700
H	-3.41297500	-2.03717900	-2.47209700
C	-3.83329700	-2.95199700	-0.55431400
H	-3.95449400	-4.00498500	-0.84788800
H	-3.36853800	-2.96370900	0.44449700
C	-5.19809200	-2.28211200	-0.48581000
H	-5.70836800	-2.41561900	-1.45146800
H	-5.06889000	-1.19697400	-0.36029000
C	-6.05491000	-2.82488900	0.64453500
H	-5.58827000	-2.62061200	1.61747000
H	-7.05341100	-2.37485200	0.65349500
H	-6.17876600	-3.91231700	0.56182700

INT1 complex of hex-1-yn-1-ylbenzene

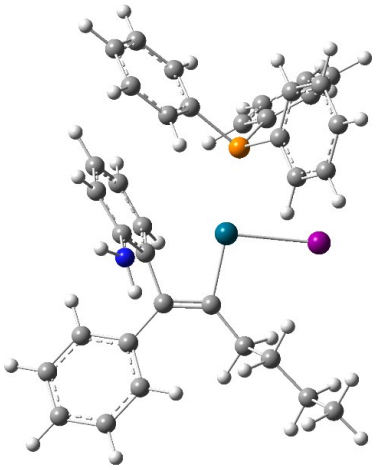
Energy = -1208624.419774 kcal/mol

Electronic Energy + Thermal Free Energy Correction (353.150 K) = -1208303.971008 kcal/mol

Symmetry c1

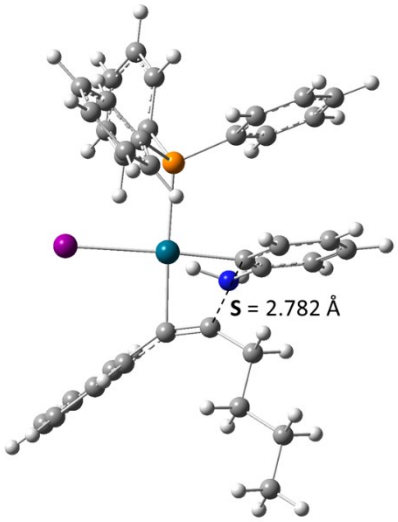
Pd	-0.40631700	-0.24629300	-0.31394700
P	1.98208800	0.26421000	0.15892800
I	0.23827000	-2.77869600	-0.84840900
C	-1.69282800	1.68584900	-0.39527400
C	-1.05681300	1.97899500	-1.62974200
C	-1.40800300	2.51614000	0.73363000
C	-0.15670400	3.02907800	-1.75575500
H	-1.34266000	1.38597800	-2.49708900
C	-0.53006700	3.59551800	0.57337800
C	0.08603100	3.83846300	-0.64503400
H	0.32376000	3.23267400	-2.70916900
H	-0.32149000	4.23642200	1.42820000
H	0.78227000	4.67152500	-0.72240700
N	-1.97316700	2.24471600	1.94914900

H	-2.78502400	1.64347700	1.97351800
H	-1.96099600	2.97360400	2.64730200
C	-2.84684300	0.71612600	-0.36174800
C	-2.42242600	-0.54713100	-0.49706000
C	-4.21802100	1.25634500	-0.24323700
C	-4.49279300	2.54413800	-0.72685700
C	-5.26114900	0.53724100	0.35798600
C	-5.77023500	3.08280300	-0.63803600
H	-3.69201900	3.12375600	-1.18605600
C	-6.53913400	1.07766600	0.44678200
H	-5.06533100	-0.44512100	0.78229500
C	-6.80068400	2.35046400	-0.05313100
H	-5.96216100	4.08040000	-1.02672400
H	-7.33239700	0.50487400	0.92175400
C	2.57407400	1.95621900	0.57024200
C	3.38277500	2.71852000	-0.27352000
C	2.17017000	2.49587500	1.79714900
C	3.78495200	3.99794200	0.10607100
H	3.70996100	2.31402500	-1.22964000
C	2.58511500	3.76409000	2.18164400
H	1.51564500	1.92059000	2.45440600
C	3.39167500	4.52100200	1.33335300
H	4.41691600	4.58219000	-0.55883300
H	2.26895500	4.16816900	3.14077700
H	3.71329800	5.51617000	1.63110000
C	2.98351000	-0.21366300	-1.29770900
C	4.03084700	-1.13495500	-1.25744600
C	2.59357000	0.32173100	-2.53272200
C	4.68509800	-1.50611600	-2.43009800
H	4.33122900	-1.58153900	-0.31200000
C	3.25654200	-0.03895300	-3.69967500
H	1.75659400	1.02095800	-2.57703100
C	4.30328700	-0.95767200	-3.65017100
H	5.49618700	-2.22913600	-2.38676500
H	2.94812100	0.38848700	-4.65078300
H	4.81634900	-1.24883600	-4.56357400
C	2.65843900	-0.65718900	1.59298300
C	3.99260300	-0.50733600	1.99418400
C	1.80541400	-1.46016500	2.35392400
C	4.46951000	-1.17865500	3.11341200
H	4.65969900	0.14427100	1.43018500
C	2.28088000	-2.12288500	3.48311900
H	0.76355200	-1.56783500	2.05248500
C	3.61353700	-1.98881900	3.85798400
H	5.50888700	-1.06356600	3.41119600
H	1.60769800	-2.74264000	4.07046100
H	3.98643100	-2.50859700	4.73735500
C	-3.18221100	-1.82083500	-0.58779000
H	-7.79945300	2.77382100	0.02166600
H	-2.72751200	-2.47161200	-1.34878800
H	-4.20877300	-1.60235100	-0.92993000
C	-3.24226700	-2.59160000	0.73110700
H	-2.22084100	-2.71724400	1.12248600
H	-3.78386300	-1.99930100	1.48688800
C	-3.89673500	-3.95466900	0.57472100
H	-4.90465600	-3.83003900	0.14969400
H	-3.32520600	-4.53736500	-0.16491600
C	-3.97409100	-4.71655300	1.88664400
H	-4.56204000	-4.16296900	2.62977500
H	-4.43732200	-5.70131500	1.76214600



H	-2.97283900	-4.86974800	2.30948400

TS2 complex of hex-1-yn-1-ylbenzene
Energy = -1208589.194556 kcal/mol
Electronic Energy + Thermal Free Energy Correction (353.150 K) = -1208272.148771 kcal/mol
Imaginary frequency = -294.86 cm^{-1}
Symmetry c1



Pd	0.42053500	-0.09616900	-0.02954500
P	-1.96572800	-0.00947400	0.15835700
I	0.36169900	-2.81233100	0.37657200
C	0.54774300	1.95269500	-0.45001400
C	0.15731100	2.91109600	0.49319900
C	0.69231600	2.32613400	-1.80365900
C	-0.03259700	4.23887100	0.14003900
H	0.03404900	2.60716000	1.53375600
C	0.50709700	3.67691300	-2.14775300
C	0.15615200	4.61639700	-1.19109400
H	-0.33207200	4.96898600	0.88800200
H	0.63305800	3.97380500	-3.18879800
H	0.01620800	5.65327000	-1.48936800
N	1.06117100	1.40995700	-2.77381600
H	0.76861500	0.45628700	-2.60476500
H	0.90673100	1.70165900	-3.72956300
C	2.56256100	-0.07110200	-0.24897600
C	2.39940900	1.12339900	0.13173100
C	3.41875100	-1.18193700	-0.59048600
C	3.58457800	-1.56037000	-1.92894300
C	4.09976000	-1.88451800	0.41284400
C	4.42082300	-2.62058800	-2.25582200
H	3.04960600	-1.01494100	-2.70427000
C	4.93274900	-2.94484000	0.07832300
H	3.95789600	-1.59731000	1.45291400
C	5.09412200	-3.31750900	-1.25430200
H	4.54614500	-2.90604600	-3.29757100
H	5.45787600	-3.48407100	0.86317700
C	-2.75655300	1.64152600	0.20067600
C	-3.26052900	2.20993400	1.37156900
C	-2.80219900	2.37380500	-0.99131400
C	-3.80615600	3.49176900	1.34843000
H	-3.23802300	1.65175100	2.30566200
C	-3.34789000	3.64968100	-1.01168700
H	-2.40048100	1.94334100	-1.90896800
C	-3.85175500	4.21201700	0.16004100
H	-4.20204100	3.92316300	2.26493400
H	-3.37452700	4.21027000	-1.94341900
H	-4.27938300	5.21171500	0.14424700
C	-2.50984400	-0.81991300	1.70288100
C	-3.51864500	-1.78238900	1.76062600
C	-1.81620600	-0.48317900	2.87184800
C	-3.83216400	-2.39411400	2.97225200
H	-4.05277200	-2.07334900	0.85855400
C	-2.14098300	-1.08284600	4.08205300
H	-1.00331000	0.24312800	2.82560900
C	-3.14910800	-2.04382600	4.13246800
H	-4.61395500	-3.14900300	3.00678200
H	-1.59837400	-0.81045200	4.98397000
H	-3.39657200	-2.52375300	5.07619900
C	-2.86876800	-0.80392300	-1.22006400
C	-4.26287400	-0.69434500	-1.31321900
C	-2.16832500	-1.47400200	-2.22591400

C	-4.94216100	-1.26879400	-2.38034000
H	-4.81760000	-0.14870800	-0.55053800
C	-2.85010700	-2.03925900	-3.30102100
H	-1.08402900	-1.55983900	-2.15923200
C	-4.23555700	-1.94094800	-3.37589700
H	-6.02430300	-1.18409500	-2.44089200
H	-2.29567700	-2.55510500	-4.08109700
H	-4.76751900	-2.38398100	-4.21436800
C	3.05651700	2.32316100	0.69421200
H	5.74353900	-4.15041900	-1.51242000
H	2.96400800	3.16179100	-0.01214000
H	2.53523600	2.63945500	1.60873500
C	4.52301100	2.03362700	0.99988300
H	4.58943400	1.21082000	1.72785900
H	5.02638000	1.67824300	0.08767000
C	5.24178600	3.25995000	1.54264800
H	5.16518300	4.07756200	0.81052500
H	4.72225400	3.61227300	2.44631400
C	6.70110000	2.97866400	1.85791500
H	7.24009000	2.64829800	0.96110100
H	7.21191700	3.86626900	2.24593900
H	6.79529600	2.18414800	2.60875900

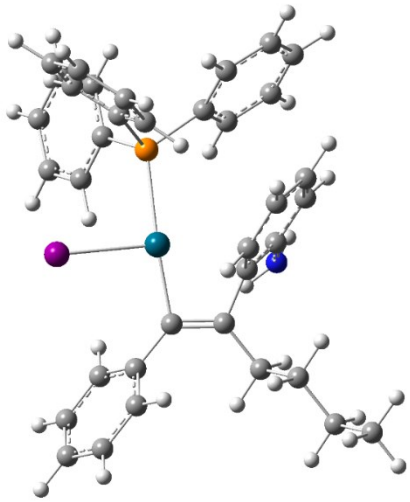
INT2 complex of hex-1-yn-1-ylbenzene

Energy = -1208623.924669 kcal/mol

Electronic Energy + Thermal Free Energy Correction (353.150 K) = -1208305.561115 kcal/mol

Symmetry c1

Pd	0.39776000	-0.22592600	0.01826000
P	-2.03669800	0.16400100	-0.05710900
I	0.06631600	-2.75936700	0.75585800
C	1.61745900	1.79667400	0.03370100
C	1.32761800	1.94669900	1.41338400
C	1.01566500	2.69986200	-0.89049900
C	0.47663400	2.93892600	1.87774400
H	1.84286500	1.28536100	2.10850300
C	0.18445400	3.71649000	-0.39979800
C	-0.07589200	3.83165300	0.95619900
H	0.27246400	3.03747900	2.94047000
H	-0.26876200	4.41157600	-1.10430100
H	-0.72663300	4.63251800	1.30101900
N	1.29757600	2.60849100	-2.23215500
H	1.60828300	1.70659000	-2.56915700
H	0.65769900	3.07601800	-2.85983600
C	2.41837900	-0.41362200	-0.25074300
C	2.73832300	0.87582200	-0.37490400
C	3.24908300	-1.59662500	-0.42578900
C	3.02679100	-2.50078600	-1.47493400
C	4.30645700	-1.84331000	0.46143400
C	3.84521300	-3.61043600	-1.63692500
H	2.19681300	-2.32335000	-2.15792500
C	5.11929100	-2.96121600	0.30289100
H	4.48058800	-1.14680300	1.28052400
C	4.89188300	-3.84812200	-0.74561900
H	3.66486700	-4.29877800	-2.45961300
H	5.93419800	-3.13846400	1.00123300
C	-2.68501000	1.84203600	-0.42598000
C	-3.35572700	2.63559800	0.50476700
C	-2.45285900	2.34630200	-1.71157600
C	-3.78775500	3.91366100	0.15352400
H	-3.54939700	2.25869200	1.50751300



C	-2.89374800	3.61524400	-2.06337400
H	-1.92902800	1.73353100	-2.44714700
C	-3.55983800	4.40529900	-1.12694300
H	-4.31220600	4.52284600	0.88612600
H	-2.71420200	3.99161200	-3.06806600
H	-3.90296200	5.40064200	-1.39874300
C	-2.83710600	-0.30292400	1.51955700
C	-3.86148900	-1.24527900	1.62684900
C	-2.30406100	0.26265800	2.68550200
C	-4.35242400	-1.60673400	2.87942700
H	-4.27319000	-1.71226700	0.73450100
C	-2.80618900	-0.08791400	3.93285300
H	-1.48181200	0.97675700	2.60894200
C	-3.83084200	-1.02757200	4.03144900
H	-5.14591400	-2.34666600	2.95263200
H	-2.38935000	0.36272800	4.83036900
H	-4.21655000	-1.31251200	5.00729700
C	-2.86721000	-0.79827000	-1.37829700
C	-4.24461900	-0.68080200	-1.60775900
C	-2.10250500	-1.60071800	-2.22780700
C	-4.84632000	-1.38151900	-2.64603600
H	-4.84823800	-0.03131600	-0.97391100
C	-2.70445400	-2.29406000	-3.27571600
H	-1.02793900	-1.68071700	-2.06340600
C	-4.07610500	-2.19075100	-3.47982600
H	-5.91715900	-1.29013000	-2.81078900
H	-2.09828200	-2.91371900	-3.93211400
H	-4.54807800	-2.73348900	-4.29540400
C	4.05692300	1.46499900	-0.79603900
H	5.52644400	-4.72242400	-0.86934600
H	3.91595000	2.10593800	-1.68098300
H	4.73316700	0.65124300	-1.09366100
C	4.69687600	2.29898100	0.31102200
H	4.01234000	3.11165500	0.60407400
H	4.82864200	1.67485700	1.21017300
C	6.03570200	2.89156900	-0.10261700
H	6.71289600	2.07765000	-0.40284900
H	5.89237400	3.51104900	-1.00088700
C	6.67365200	3.71623900	1.00227300
H	7.63683400	4.13701800	0.69405300
H	6.02397600	4.55041100	1.29617000
H	6.84758100	3.10577900	1.89744400

ADS complex of (cyclopentylethynyl)benzene

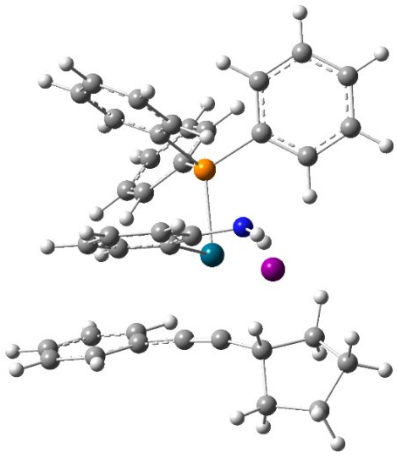
Energy = -1232498.711274 kcal/mol

Electronic Energy + Thermal Free Energy Correction (353.150 K) = -1232174.393287 kcal/mol

Symmetry c1

Pd	-0.60330100	-0.13807200	0.01604800
P	1.72884400	-0.17327000	0.02501900
I	-0.77735000	-1.39774600	-2.49926400
C	-0.48732900	0.72689800	1.85813000
C	-0.42709500	2.11220300	1.94213300
C	-0.51692600	-0.05010800	3.02629000
C	-0.41918100	2.75931200	3.17998000
H	-0.39059500	2.70867800	1.02846300
C	-0.52808000	0.60714100	4.26614100
C	-0.47479100	1.99388300	4.34071200
H	-0.37017300	3.84486800	3.22943400
H	-0.55907900	0.00903100	5.17742600
H	-0.47563300	2.47629300	5.31610700

N	-0.44552300	-1.44539500	2.97968300
H	-0.78246100	-1.85383100	2.11589900
H	-0.82903300	-1.91738900	3.78924000
C	-2.76040400	0.87868200	-0.24382500
C	-2.97437700	-0.18772300	0.32936000
C	-2.61318400	2.19506100	-0.78946400
C	-2.96046800	3.29811300	0.00638400
C	-2.11570700	2.40417400	-2.08450800
C	-2.80946800	4.58707800	-0.48713200
H	-3.34022000	3.12900500	1.01160700
C	-1.96492700	3.69767200	-2.56691900
H	-1.84105000	1.54340700	-2.69243000
C	-2.30892900	4.78903500	-1.77150400
H	-3.07994400	5.43755100	0.13344300
H	-1.57793900	3.85554900	-3.57073100
C	2.62025300	0.76042700	1.32154600
C	3.24101900	1.98400600	1.06497900
C	2.63226700	0.24067900	2.62190500
C	3.86418500	2.68150400	2.09769600
H	3.24474800	2.39840500	0.05912600
C	3.26066800	0.93637700	3.64561800
H	2.13388300	-0.70516400	2.83776800
C	3.87456700	2.16119600	3.38649500
H	4.34671100	3.63322300	1.88826500
H	3.25943900	0.52703200	4.65323000
H	4.36240500	2.70648100	4.19093000
C	2.24895400	0.59860400	-1.54658700
C	3.18314700	0.01349400	-2.40186100
C	1.63050100	1.79839800	-1.91965400
C	3.49334000	0.62134500	-3.61613100
H	3.65980900	-0.92731500	-2.13431000
C	1.94789700	2.40623300	-3.12705000
H	0.87733700	2.24691700	-1.26908100
C	2.87834600	1.81469800	-3.98013500
H	4.21628800	0.15531300	-4.28107200
H	1.46145700	3.33738400	-3.40744500
H	3.11983700	2.28416100	-4.93058400
C	2.51634800	-1.81673500	0.10453600
C	1.75145400	-2.98206400	0.02372300
C	3.90460700	-1.91214900	0.26972200
C	2.36666100	-4.22909300	0.09698500
H	0.67168300	-2.90821500	-0.09927600
C	4.51621100	-3.15802100	0.33255000
H	4.50744800	-1.00851400	0.35244900
C	3.74692800	-4.31672800	0.24809200
H	1.76408800	-5.13204200	0.03976600
H	5.59415300	-3.22528400	0.45536500
H	4.22595200	-5.29107900	0.30671700
H	-2.18745300	5.79923800	-2.15467700
C	-3.50622600	-1.35693600	1.02300500
C	-5.04214000	-1.34630900	1.12382600
C	-3.23161400	-2.71694900	0.37200200
H	-3.08429300	-1.37112900	2.04316600
C	-5.41222300	-2.79954700	1.46967600
H	-5.44939400	-1.06434600	0.14361000
H	-5.40560800	-0.61377200	1.85157300
C	-4.16028800	-3.64667300	1.14951300
H	-2.17444700	-3.00839500	0.40881900
H	-3.51323500	-2.66335200	-0.68957400
H	-5.68846000	-2.89634300	2.52533900



H	-6.28093500	-3.12463600	0.88734900
H	-3.66661400	-3.95488800	2.08059900
H	-4.39520700	-4.56123600	0.59584800

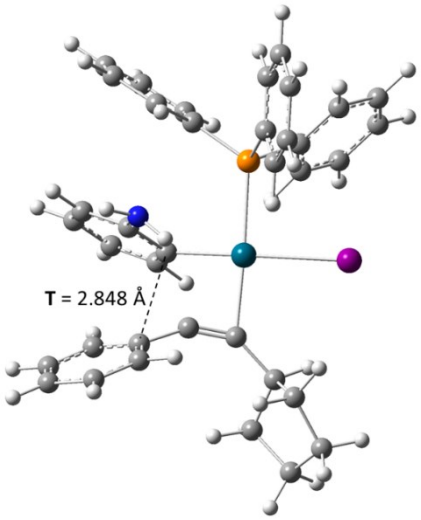
TS1 complex of (cyclopentylethynyl)benzene

Energy = -1232483.738282 kcal/mol

Electronic Energy + Thermal Free Energy Correction (353.150 K) = -1232157.759279 kcal/mol

Imaginary frequency = -272.78 cm^{-1}

Symmetry c1



Pd	-0.42187200	-0.39151100	-0.17360000
P	1.92394100	0.15643900	0.09691700
I	0.14493700	-3.05481000	0.19579700
C	-0.82515300	1.57280800	-0.74424100
C	-0.96125900	1.80048100	-2.11393400
C	-0.57467700	2.64177100	0.13588100
C	-0.81052700	3.08214300	-2.64093800
H	-1.20155700	0.96363500	-2.76964100
C	-0.44249800	3.92845000	-0.40387300
C	-0.55264600	4.14181500	-1.77149400
H	-0.90984100	3.25084400	-3.71036500
H	-0.23469200	4.76081400	0.26853000
H	-0.44242600	5.15138900	-2.16200400
N	-0.41255500	2.41913700	1.48902600
H	-0.82642900	1.56969500	1.85239400
H	-0.53559400	3.21944900	2.09422300
C	-2.62723500	0.45796600	-0.16534900
C	-2.48939100	-0.77276900	-0.43207700
C	-3.44712300	1.52811900	0.36613800
C	-3.75439200	2.67836300	-0.37157700
C	-4.01356200	1.35024500	1.63638600
C	-4.62392200	3.62500000	0.15186100
H	-3.30200200	2.81902200	-1.35150100
C	-4.87906200	2.30557700	2.15655000
H	-3.76297400	0.45652500	2.20598600
C	-5.18595300	3.44300200	1.41479800
H	-4.86594000	4.51234800	-0.42795800
H	-5.31275900	2.16150800	3.14302200
C	2.55604500	1.83607800	-0.30822000
C	2.92052700	2.17149300	-1.61549100
C	2.62993500	2.81848600	0.68652000
C	3.34562200	3.46061100	-1.92311200
H	2.88156400	1.42381000	-2.40497900
C	3.06362800	4.10236400	0.37844600
H	2.32973900	2.58707200	1.70568900
C	3.42039500	4.42829600	-0.92732100
H	3.62597300	3.70323700	-2.94550500
H	3.12143900	4.85279600	1.16370300
H	3.75824200	5.43392400	-1.16668400
C	2.86450100	-0.93007900	-1.04358700
C	3.99589000	-1.65414900	-0.66535200
C	2.37000200	-1.07194200	-2.34654000
C	4.62546400	-2.49923200	-1.57656800
H	4.38333300	-1.58005500	0.34845800
C	3.00703700	-1.90412900	-3.25872500
H	1.46308800	-0.54076500	-2.64012000
C	4.13635900	-2.62338800	-2.87283000
H	5.50130300	-3.06506400	-1.26784800
H	2.61293100	-2.00293600	-4.26728500
H	4.62915400	-3.28512900	-3.58094100
C	2.59607700	-0.13337000	1.77234000

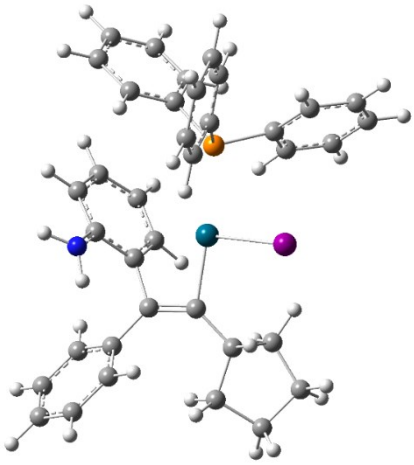
C	3.92199700	0.18067700	2.09997100
C	1.75238300	-0.63953800	2.76366800
C	4.39697400	-0.03559200	3.38815200
H	4.58313600	0.60899100	1.34747000
C	2.22728300	-0.84975500	4.05553800
H	0.71845800	-0.87586000	2.51292200
C	3.55028400	-0.55292100	4.36662100
H	5.42873000	0.20672400	3.63087300
H	1.56009300	-1.24302800	4.81859200
H	3.92291300	-0.71669800	5.37493600
H	-5.86316900	4.19046700	1.82091700
C	-3.24567100	-2.02124200	-0.66737700
C	-3.71464400	-2.69982100	0.62651500
C	-4.57678800	-1.78656600	-1.39664200
H	-2.63709300	-2.74251800	-1.23273000
C	-4.73151100	-3.72037000	0.11816000
H	-4.20196500	-1.94077100	1.25790700
H	-2.89007200	-3.13931500	1.19878000
C	-5.39046600	-3.06157800	-1.11696100
H	-4.44414100	-1.57500500	-2.46313000
H	-5.06600500	-0.91028500	-0.94617600
H	-4.20677600	-4.63814100	-0.17862100
H	-5.45760800	-4.00440100	0.88693100
H	-5.36485200	-3.74005900	-1.97721800
H	-6.44453300	-2.82214900	-0.93920800

INT1 complex of (cyclopentylethynyl)benzene

Energy = -1232514.365113 kcal/mol

Electronic Energy + Thermal Free Energy Correction (353.150 K) = -1232189.350592 kcal/mol

Symmetry c1



Pd	-0.34791700	-0.28541900	-0.11636700
P	2.10072200	0.22675000	-0.03755800
I	0.15681500	-2.68411400	0.95263600
C	-1.59876700	1.60238500	-0.53299300
C	-1.08757200	1.45880300	-1.85006800
C	-1.14441300	2.70304300	0.26178300
C	-0.15987400	2.35679200	-2.37590400
H	-1.51458700	0.67460300	-2.47391100
C	-0.25404700	3.61628500	-0.30564800
C	0.22756900	3.44154400	-1.60036000
H	0.22576100	2.22392200	-3.38316800
H	0.08223800	4.46502100	0.28872300
H	0.93435200	4.16755600	-1.99782400
N	-1.55493700	2.82541000	1.56529300
H	-2.40763500	2.35208300	1.83339200
H	-1.43122800	3.72829100	2.00113300
C	-2.75188600	0.72911300	-0.11620500
C	-2.38534800	-0.56058700	-0.11400100
C	-4.05111600	1.36847700	0.18897900
C	-4.52881200	2.41410200	-0.61135300
C	-4.78579500	1.00105600	1.32348100
C	-5.73059700	3.04402400	-0.30960200
H	-3.95197100	2.72340000	-1.48290300
C	-5.98656400	1.63346600	1.62680500
H	-4.39489200	0.22016500	1.97482500
C	-6.46524000	2.65301300	0.80806900
H	-6.09551000	3.84530600	-0.94821100
H	-6.54440700	1.33772100	2.51238300
C	2.88138400	1.76616400	-0.68207500
C	3.43806700	1.86719000	-1.95889900

C	2.87322200	2.89783300	0.14255300
C	3.98256800	3.07224100	-2.39716400
H	3.46164000	1.00154200	-2.61796000
C	3.42268700	4.09751200	-0.29230100
H	2.43315800	2.83985500	1.13851700
C	3.97944700	4.18839000	-1.56610000
H	4.41956000	3.13339400	-3.39122700
H	3.41313800	4.96452800	0.36440000
H	4.41092800	5.12583000	-1.90882200
C	2.87993200	-1.10790500	-1.01989800
C	3.83612100	-1.99326600	-0.52097200
C	2.37911500	-1.30635300	-2.31422300
C	4.28810100	-3.05340400	-1.30375800
H	4.21852100	-1.87662900	0.49066800
C	2.84130000	-2.35620700	-3.09925300
H	1.60473400	-0.64183200	-2.70259300
C	3.79496900	-3.23608000	-2.59150700
H	5.02705000	-3.74193400	-0.90059700
H	2.44606100	-2.49556500	-4.10261100
H	4.14757800	-4.06652400	-3.19835400
C	2.82759800	0.18019300	1.64218900
C	4.20786900	0.27131300	1.86364300
C	1.96320700	0.16470600	2.73936400
C	4.71062900	0.30464100	3.15897500
H	4.89217900	0.32941900	1.01778800
C	2.46618200	0.21124300	4.03707800
H	0.88788400	0.11518900	2.56912800
C	3.83980100	0.27174800	4.24700700
H	5.78407200	0.36631400	3.32055300
H	1.78317200	0.20207100	4.88292100
H	4.23508100	0.30432800	5.25948100
H	-7.40242400	3.15047600	1.04618900
C	-3.12664700	-1.84572600	-0.18539900
C	-4.66071600	-1.77749600	-0.28497000
C	-2.78184300	-2.62923200	-1.46435100
H	-2.84757200	-2.48177000	0.67082000
C	-5.08079300	-3.14187500	-0.86513000
H	-4.93375900	-0.96656300	-0.97522100
H	-5.14408300	-1.55510300	0.67189700
C	-3.79984100	-3.76293500	-1.46113600
H	-1.73924900	-2.96598900	-1.48404000
H	-2.93640300	-1.96134200	-2.32777400
H	-5.50434700	-3.78864700	-0.08807600
H	-5.86146400	-3.01666000	-1.62419300
H	-3.43291700	-4.57064400	-0.81221800
H	-3.95728600	-4.19885500	-2.45359900

TS2 complex of (cyclopentylethynyl)benzene

Energy = -1232484.797517 kcal/mol

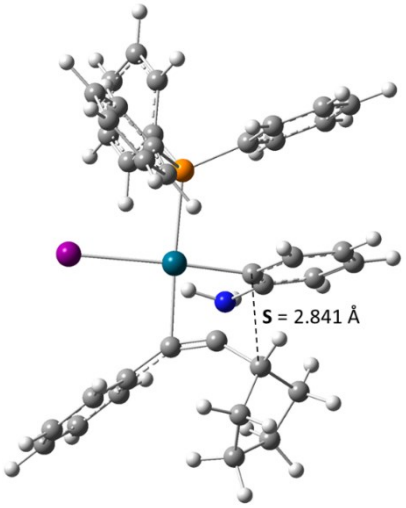
Electronic Energy + Thermal Free Energy Correction (353.150 K) = -1232159.014297 kcal/mol

Imaginary frequency = -290.25 cm^{-1}

Symmetry c1

Pd	-0.40649900	-0.08703700	-0.09042000
P	1.99153500	-0.14006600	-0.07945000
I	-0.46141500	-2.84166900	-0.08700300
C	-0.47513600	1.98776400	0.17555800
C	0.10733900	2.87049500	-0.74056700
C	-0.76894900	2.43184300	1.48322700
C	0.36462500	4.19295900	-0.40927300
H	0.34913000	2.50898600	-1.74108200

C	-0.48885700	3.77181500	1.81068500
C	0.06109200	4.63765900	0.87911100
H	0.81427900	4.86301100	-1.13802800
H	-0.71382100	4.12016000	2.81850100
H	0.26453000	5.66782100	1.16355000
N	-1.37280100	1.60907600	2.42049600
H	-1.17364500	0.62085000	2.33416300
H	-1.32071300	1.93198100	3.37754200
C	-2.55778900	0.05843500	-0.11452300
C	-2.24865000	1.16338700	-0.64832700
C	-3.52104900	-0.93004700	0.30071100
C	-3.97278500	-0.95210700	1.62730300
C	-4.03883800	-1.85294400	-0.61896900
C	-4.93162900	-1.87767700	2.02241400
H	-3.56701100	-0.23073000	2.33497600
C	-4.99815500	-2.77293100	-0.21602600
H	-3.67790600	-1.83966000	-1.64547000
C	-5.44478400	-2.79064000	1.10418000
H	-5.27984500	-1.88525300	3.05250200
H	-5.39935900	-3.48179500	-0.93651600
C	2.89276400	1.45142900	-0.21186100
C	3.44224000	1.91017000	-1.41038400
C	2.97442800	2.25618500	0.93061700
C	4.06688900	3.15405500	-1.46487700
H	3.39487300	1.29526100	-2.30681100
C	3.59745100	3.49546300	0.87334600
H	2.54458500	1.91015100	1.87083300
C	4.14540100	3.94753600	-0.32560200
H	4.49713000	3.49895500	-2.40221100
H	3.65020100	4.11371500	1.76663400
H	4.63365500	4.91821800	-0.36983800
C	2.57044100	-1.12173800	-1.50937600
C	3.50029800	-2.15838800	-1.41837200
C	1.97767200	-0.84146000	-2.74751200
C	3.83668300	-2.89797800	-2.54964800
H	3.95169600	-2.40908900	-0.46097400
C	2.32700100	-1.56960500	-3.87802800
H	1.22337800	-0.05605200	-2.82052600
C	3.25597900	-2.60344600	-3.77895200
H	4.55558500	-3.70942400	-2.46594300
H	1.86367900	-1.33971800	-4.83435600
H	3.52140400	-3.18317400	-4.65965400
C	2.75273700	-0.84402100	1.42738700
C	4.14581800	-0.87540500	1.57886900
C	1.94290600	-1.27155100	2.48156900
C	4.71330000	-1.35871200	2.75132900
H	4.79004300	-0.50902900	0.78034300
C	2.51295500	-1.74397800	3.66123200
H	0.85979900	-1.23795100	2.37215800
C	3.89658300	-1.79404900	3.79342500
H	5.79493700	-1.38621100	2.85668600
H	1.87316000	-2.07056800	4.47727700
H	4.34169600	-2.16479900	4.71363900
H	-6.19291200	-3.51520400	1.41630200
C	-2.74824200	2.27413700	-1.50514500
C	-3.99890100	1.79671800	-2.26051100
C	-3.31923500	3.42590800	-0.66666000
H	-1.95487600	2.60746700	-2.18310500
C	-5.13972600	1.88533200	-1.23249700
H	-3.87877900	0.79932300	-2.69870600



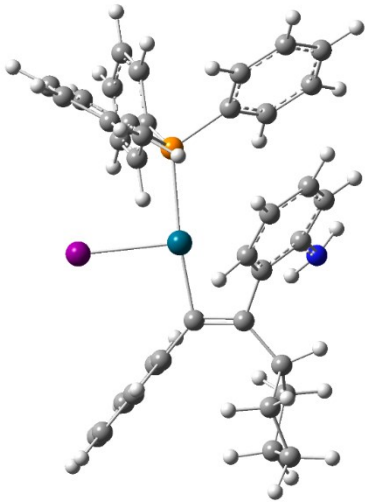
H	-4.17303500	2.49870800	-3.08662900
C	-4.64857700	2.87087600	-0.14713600
H	-3.49124200	4.27683300	-1.33997200
H	-2.64523400	3.76022500	0.12894400
H	-6.07037100	2.21949000	-1.70372600
H	-5.34387700	0.89979900	-0.79432200
H	-5.37241300	3.66519000	0.06301000
H	-4.47797700	2.33920400	0.79931400

INT2 complex of (cyclopentylethynyl)benzene

Energy = -1232517.164431 kcal/mol

Electronic Energy + Thermal Free Energy Correction (353.150 K) = -1232192.166225 kcal/mol

Symmetry c1



Pd	-0.33337600	-0.05165400	-0.16906000
P	2.11330200	-0.02538900	0.11133000
I	-0.32722900	-2.69103200	-0.52000800
C	-1.23330900	2.11083300	-0.50840100
C	-0.72973100	2.07588600	-1.83201200
C	-0.64780800	3.01838300	0.42251800
C	0.32016300	2.89335800	-2.23139700
H	-1.22902300	1.42113700	-2.54464900
C	0.38377200	3.86202300	-0.00960000
C	0.85603200	3.79621900	-1.31148200
H	0.68899100	2.85552900	-3.25305200
H	0.81420700	4.57189600	0.69408700
H	1.66201200	4.46179700	-1.61334000
N	-1.14647700	3.10418600	1.69976400
H	-1.63307200	2.28889200	2.05030500
H	-0.55610800	3.55206300	2.38731300
C	-2.37914500	0.08096700	-0.12091400
C	-2.51960900	1.40638000	-0.17496500
C	-3.34108700	-0.97944600	0.14846300
C	-3.53244500	-1.44827600	1.45713500
C	-4.07592700	-1.56815900	-0.88996200
C	-4.44935800	-2.45726400	1.72118600
H	-2.94492000	-1.01098000	2.26473800
C	-4.99253400	-2.57957700	-0.62382800
H	-3.90950200	-1.23089900	-1.91240800
C	-5.18392200	-3.02688700	0.68152900
H	-4.59129500	-2.80439200	2.74226200
H	-5.55723300	-3.02401900	-1.44031200
C	2.97743700	1.56744600	0.41505000
C	3.90616700	2.13842800	-0.45487000
C	2.65653300	2.23312300	1.60450100
C	4.50706400	3.35583000	-0.13744300
H	4.17041500	1.63318400	-1.38179300
C	3.26530900	3.43877300	1.92554800
H	1.92649700	1.79901500	2.29025200
C	4.18993100	4.00651200	1.04988400
H	5.23183700	3.79075800	-0.82187900
H	3.01241500	3.94214600	2.85608700
H	4.66460200	4.95331200	1.29624800
C	2.94414600	-0.75071400	-1.34785500
C	3.69661500	-1.92573800	-1.29702300
C	2.69876500	-0.15122700	-2.59074100
C	4.21457200	-2.47916700	-2.46554100
H	3.87179000	-2.42103900	-0.34422100
C	3.22966700	-0.69713100	-3.75343100
H	2.08420800	0.74962200	-2.64595200
C	3.98864600	-1.86446200	-3.69253200

H	4.79725800	-3.39584800	-2.41366700
H	3.04227200	-0.21673200	-4.71080500
H	4.39590600	-2.29707200	-4.60318300
C	2.71017500	-0.96924400	1.56625100
C	4.07838200	-1.05964600	1.85454700
C	1.78873500	-1.52356300	2.45711400
C	4.51321400	-1.72072200	2.99642500
H	4.80666700	-0.60641300	1.18199900
C	2.22492500	-2.17560400	3.60854000
H	0.72338900	-1.44436100	2.24136800
C	3.58585600	-2.27991600	3.87468900
H	5.57740500	-1.79259400	3.20766400
H	1.49863900	-2.60002800	4.29750000
H	3.92752800	-2.79105900	4.77162700
H	-5.90008700	-3.81853200	0.88834000
C	-3.77581500	2.23287500	-0.00445000
C	-4.75761600	2.06758600	-1.18851100
C	-4.62398200	1.93794300	1.26467100
H	-3.45604500	3.28465600	0.02826100
C	-6.13192000	2.29404000	-0.56854500
H	-4.70030300	1.03807400	-1.56852400
H	-4.52003400	2.73918500	-2.02184000
C	-6.01600400	1.54943600	0.75845400
H	-4.68138800	2.84640100	1.87858200
H	-4.17497900	1.15872700	1.89084200
H	-6.29081800	3.36685500	-0.38208100
H	-6.95484800	1.94274300	-1.20142500
H	-6.81352300	1.78957100	1.47035000
H	-6.05397600	0.46494300	0.57216100

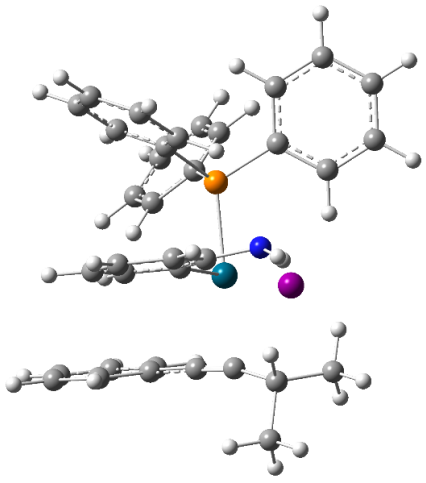
ADS complex of (3-methylbut-1-yn-1-yl)benzene

Energy = -1183955.445228 kcal/mol

Electronic Energy + Thermal Free Energy Correction (353.150 K) = -1183653.369298 kcal/mol

Symmetry c1

Pd	0.59668800	0.10898200	-0.44338400
P	-1.63480300	-0.13407000	0.30296200
I	0.84214300	-2.68110100	-1.13098400
C	0.47899100	2.10573600	-0.06795600
C	0.99045400	2.58649200	1.13777900
C	0.00126200	3.01494100	-1.03451200
C	1.07052300	3.96134400	1.39913500
H	1.34735500	1.88650600	1.88825600
C	0.09925000	4.39502800	-0.77135100
C	0.62742600	4.86322900	0.43032200
H	1.47560400	4.31367700	2.34354600
H	-0.25758700	5.09912200	-1.52040400
H	0.68745800	5.93364500	0.60730300
N	-0.63775700	2.58172500	-2.20715400
H	-0.39694200	1.64319100	-2.49833900
H	-0.59685500	3.23447300	-2.98031300
C	3.08433800	0.27435200	-0.37654100
C	2.70652000	0.62613900	-1.49393300
C	3.65971400	-0.04968400	0.89653500
C	4.12143200	0.98667900	1.73440000
C	3.81702800	-1.38940600	1.30455300
C	4.72255600	0.68389700	2.95444200
H	4.00500600	2.01777200	1.41913000
C	4.41739700	-1.67986600	2.52713200
H	3.45756500	-2.18398000	0.65989100
C	4.87019200	-0.64713100	3.35442700

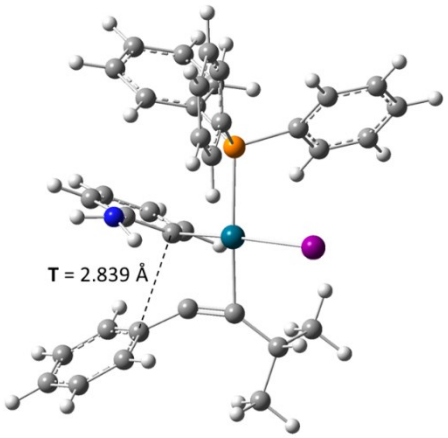


H	5.07698300	1.48763500	3.59247400
H	4.53479800	-2.71447800	2.83488600
C	-2.44507000	1.25167400	1.21681300
C	-2.64360400	1.20988200	2.60435600
C	-2.87208700	2.38244600	0.49890400
C	-3.25980500	2.27848000	3.26193300
H	-2.32932800	0.34602300	3.17863700
C	-3.49057000	3.44291700	1.15924000
H	-2.71771700	2.43666400	-0.57410700
C	-3.68582400	3.39503700	2.54277100
H	-3.41021300	2.22954800	4.33632900
H	-3.81864300	4.30898100	0.59195300
H	-4.16791300	4.22278800	3.05445100
C	-1.70108800	-1.54036100	1.49142000
C	-2.71861600	-2.50373100	1.46481600
C	-0.69654700	-1.63102000	2.46976300
C	-2.73246300	-3.53767800	2.40450900
H	-3.49746500	-2.45939900	0.71188400
C	-0.72103400	-2.65705700	3.41411300
H	0.11141900	-0.90503700	2.48790100
C	-1.73837900	-3.61510900	3.38130700
H	-3.52265300	-4.28170500	2.36959900
H	0.05858200	-2.71314700	4.16782900
H	-1.75284500	-4.41908200	4.11105600
C	-2.84595800	-0.49588600	-1.03613900
C	-2.40120000	-0.85354600	-2.31750000
C	-4.22864700	-0.40745800	-0.79311600
C	-3.31931700	-1.12572200	-3.33417500
H	-1.33782000	-0.92969800	-2.51644200
C	-5.14255900	-0.68660400	-1.80956800
H	-4.59474100	-0.11321700	0.18493300
C	-4.68989700	-1.04508700	-3.08196500
H	-2.96058700	-1.39765600	-4.32235400
H	-6.20715500	-0.61744900	-1.60764500
H	-5.40301200	-1.25537700	-3.87344300
C	2.71243800	1.12444500	-2.88923500
H	5.33848400	-0.87935800	4.30620100
H	1.88728200	1.83819200	-2.99374600
C	2.49963800	-0.00819900	-3.91129800
H	1.56107700	-0.53713400	-3.73047700
H	2.47830700	0.41140800	-4.92169200
H	3.31553000	-0.73591700	-3.85817600
C	4.03133400	1.88224400	-3.15290000
H	4.02345600	2.29009500	-4.16850900
H	4.16110300	2.70899500	-2.44925900
H	4.88961500	1.20960700	-3.05877200

TS1 complex of (3-methylbut-1-yn-1-yl)benzene
Energy = -1183941.747334 kcal/mol
Electronic Energy + Thermal Free Energy Correction (353.150 K) = -1183639.830164 kcal/mol
Imaginary frequency = -314.62 cm^{-1}
Symmetry c1

Pd	-0.42681400	-0.67119900	-0.06530100
P	1.64940400	0.56854500	0.07144000
I	0.88255900	-2.99704800	0.63464500
C	-1.51246800	1.02852900	-0.61722000
C	-1.68044600	1.24047300	-1.98774300
C	-1.66312700	2.09774500	0.28862200
C	-1.96734500	2.50977700	-2.48505100

H	-1.60342800	0.39141200	-2.66797100
C	-1.97793000	3.36510500	-0.22155900
C	-2.12100700	3.56731500	-1.58720900
H	-2.08817600	2.66610100	-3.55404200
H	-2.08783700	4.19779500	0.47335900
H	-2.36035900	4.56281200	-1.95502800
N	-1.45316400	1.91701400	1.64175100
H	-1.52722700	0.96410500	1.97604100
H	-1.88757600	2.59258200	2.25608700
C	-2.80365000	-0.61579500	-0.14702100
C	-2.22347000	-1.70116800	-0.45370000
C	-3.97324200	0.04316300	0.40020900
C	-4.64339600	1.05985000	-0.29181500
C	-4.48263900	-0.41402800	1.62353200
C	-5.81317700	1.59671500	0.22727600
H	-4.23692400	1.41787300	-1.23590000
C	-5.65076200	0.13404100	2.14120700
H	-3.95280400	-1.20233100	2.15538000
C	-6.31664600	1.13809100	1.44407600
H	-6.33572900	2.37910400	-0.31748100
H	-6.04046400	-0.22424300	3.09080400
C	1.73665300	2.30063300	-0.53849600
C	2.15114900	2.61313900	-1.83660100
C	1.33673600	3.33774200	0.31290700
C	2.16576600	3.93522200	-2.27314200
H	2.47811000	1.82731300	-2.51387600
C	1.35834200	4.65682400	-0.12385900
H	1.00301300	3.10923900	1.32416000
C	1.76958300	4.95944100	-1.41918700
H	2.49583500	4.16266100	-3.28407500
H	1.04547000	5.45121200	0.55013100
H	1.78455100	5.99188600	-1.76018000
C	2.80453200	-0.32440000	-1.03586300
C	4.10223200	-0.68659300	-0.67494900
C	2.31249200	-0.70844200	-2.29040200
C	4.89426500	-1.42358100	-1.55308800
H	4.49757700	-0.41228200	0.30106700
C	3.10838300	-1.42997600	-3.17112900
H	1.28878700	-0.45167800	-2.57023100
C	4.40108100	-1.79531000	-2.79936400
H	5.90108900	-1.70911000	-1.25763200
H	2.71567300	-1.71932600	-4.14289900
H	5.02145700	-2.37197700	-3.48113100
C	2.46645400	0.69561900	1.70156900
C	3.63836100	1.44463900	1.87106000
C	1.88870500	0.07084300	2.80931800
C	4.23058800	1.54677700	3.12420300
H	4.08426500	1.95819100	1.01982900
C	2.47998200	0.17955300	4.06550000
H	0.97289700	-0.50494300	2.68099400
C	3.65125600	0.91340900	4.22221300
H	5.14195700	2.12695400	3.24582000
H	2.02102500	-0.30781400	4.92228300
H	4.11185400	0.99968800	5.20348900
C	-2.41297500	-3.06839000	-0.99968700
H	-7.23072300	1.56570300	1.84911000
H	-1.83360300	-3.76609900	-0.37910900
C	-1.87167600	-3.13515900	-2.42755000
H	-0.80567000	-2.87910000	-2.46086500
H	-2.00050300	-4.14352500	-2.83746400



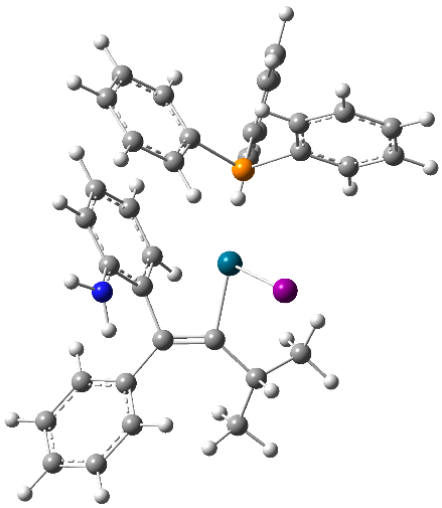
H	-2.41463800	-2.43226100	-3.07325200
C	-3.89270900	-3.44161300	-0.95044000
H	-4.28069200	-3.41577900	0.07379900
H	-4.48444400	-2.74283900	-1.55632400
H	-4.04321100	-4.45105600	-1.35084400

INT1 complex of (3-methylbut-1-yn-1-yl)benzene

Energy = -1183972.012093 kcal/mol

Electronic Energy + Thermal Free Energy Correction (353.150 K) = -1183668.642867 kcal/mol

Symmetry c1



Pd	0.41269000	-0.58706300	0.21520000
P	-1.87012200	0.44292300	0.06754300
I	-0.54145600	-2.95258800	-0.48606800
C	1.98651200	1.15196100	0.14364800
C	1.40094700	1.60663300	1.34923200
C	1.85035100	1.95460800	-1.03219500
C	0.69538100	2.80771100	1.41012600
H	1.60223900	1.03312700	2.25397700
C	1.17030000	3.17046200	-0.94222000
C	0.60802800	3.58549900	0.26085400
H	0.25409400	3.13983100	2.34569600
H	1.08123600	3.79471600	-1.82957500
H	0.09290100	4.54336200	0.29491800
N	2.36875900	1.51307400	-2.21987700
H	3.07509600	0.79069300	-2.18554700
H	2.49034700	2.19036800	-2.95861900
C	2.98228800	0.02853100	0.19788000
C	2.38830400	-1.16095900	0.38364500
C	4.41864100	0.38285500	0.16018200
C	4.83321500	1.63463000	0.63887100
C	5.39175300	-0.47862300	-0.36684800
C	6.17420500	1.99861400	0.62250800
H	4.09178100	2.32684800	1.03779600
C	6.73388100	-0.11424400	-0.38114500
H	5.09165600	-1.43309900	-0.79372800
C	7.13221200	1.12278100	0.11771500
H	6.47327200	2.97094900	1.00759300
H	7.47076900	-0.79826200	-0.79618300
C	-2.50898200	1.11003500	1.64944000
C	-3.78076700	1.68845600	1.75712000
C	-1.73632000	0.95386700	2.80281000
C	-4.24598700	2.13899800	2.98677800
H	-4.41631100	1.77478600	0.87659700
C	-2.20642800	1.39541800	4.03707100
H	-0.75977900	0.47622200	2.72825500
C	-3.45727100	1.99672800	4.12731300
H	-5.23129400	2.59318800	3.05841100
H	-1.59584400	1.26507100	4.92710500
H	-3.82614500	2.34555500	5.08889700
C	-3.28986400	-0.60621000	-0.45269300
C	-3.76157800	-0.64015900	-1.76607900
C	-3.85394100	-1.47038800	0.49309800
C	-4.77825100	-1.52165900	-2.12691800
H	-3.34212600	0.02589100	-2.51743100
C	-4.87330100	-2.34345400	0.13409300
H	-3.49212900	-1.46254800	1.52099000
C	-5.33573200	-2.37450100	-1.18006400
H	-5.13885000	-1.53386300	-3.15289400
H	-5.30572700	-3.00477300	0.88134300
H	-6.13247200	-3.05846500	-1.46260800

C	-1.88736600	1.80541600	-1.15361500
C	-2.43195200	3.07070000	-0.92763600
C	-1.28529000	1.53416400	-2.38890500
C	-2.39257900	4.04045500	-1.92616900
H	-2.87699500	3.31235400	0.03521700
C	-1.25884100	2.49778800	-3.39024200
H	-0.82627100	0.55873100	-2.56178100
C	-1.81315300	3.75492400	-3.15875900
H	-2.81681100	5.02394700	-1.73766400
H	-0.79270900	2.27180400	-4.34654300
H	-1.78646600	4.51365300	-3.93720600
C	3.05149800	-2.45368400	0.76133500
C	3.19673200	-3.45015700	-0.38702000
H	3.64540300	-2.98817300	-1.27532100
H	3.83735100	-4.28542700	-0.07751900
H	2.22348700	-3.85722700	-0.68043700
C	2.40324000	-3.10243500	1.98071500
H	2.33981500	-2.39618900	2.81769400
H	1.38797700	-3.44446200	1.74837400
H	2.99220300	-3.96851100	2.30727500
H	8.18165500	1.40697500	0.10397800
H	4.07330700	-2.15897800	1.06380400

TS2 complex of (3-methylbut-1-yn-1-yl)benzene

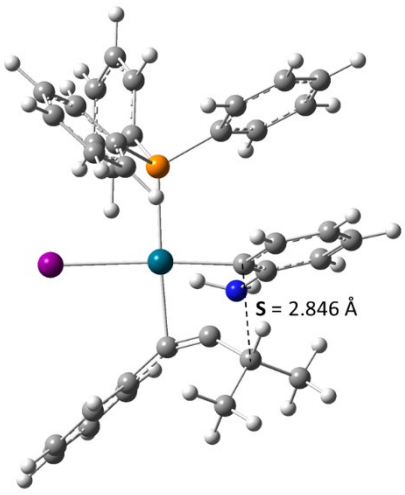
Energy = -1183940.224370 kcal/mol

Electronic Energy + Thermal Free Energy Correction (353.150 K) = -1183639.776198 kcal/mol

Imaginary frequency = -297.97 cm^{-1}

Symmetry c1

Pd	-0.60172600	0.14582900	-0.14921600
P	1.72319400	-0.42121200	-0.02056200
I	-1.24897500	-2.53307600	-0.27182800
C	-0.23383200	2.19918500	0.04271600
C	0.51931700	2.89812700	-0.90926400
C	-0.38101600	2.73638100	1.34044500
C	1.06595900	4.14190000	-0.63103700
H	0.65669000	2.45867900	-1.89829800
C	0.18238900	3.99688100	1.61210500
C	0.88661800	4.69000300	0.64137200
H	1.63852900	4.67110100	-1.38878500
H	0.06224900	4.41845300	2.60994600
H	1.31209200	5.66180500	0.88232200
N	-1.09926400	2.07725100	2.32390100
H	-1.06478500	1.06681400	2.28651000
H	-0.97301200	2.43252300	3.26246400
C	-2.66948100	0.76193100	-0.16938600
C	-2.13412800	1.76404200	-0.72843500
C	-3.79456300	-0.02071200	0.27728600
C	-4.10964100	-0.08217100	1.64133000
C	-4.58642600	-0.72054200	-0.64447500
C	-5.19982200	-0.82712100	2.07324900
H	-3.49051300	0.46446000	2.35030100
C	-5.67381100	-1.46459000	-0.20443100
H	-4.33196300	-0.68176800	-1.70202100
C	-5.98192700	-1.52260200	1.15336100
H	-5.43989700	-0.86606600	3.13306500
H	-6.28398400	-2.00341900	-0.92533200
C	2.94083200	0.94538400	-0.08913400
C	3.72140400	1.20921800	-1.21595400
C	3.05535600	1.77383500	1.03343400
C	4.60543400	2.28598200	-1.21850300

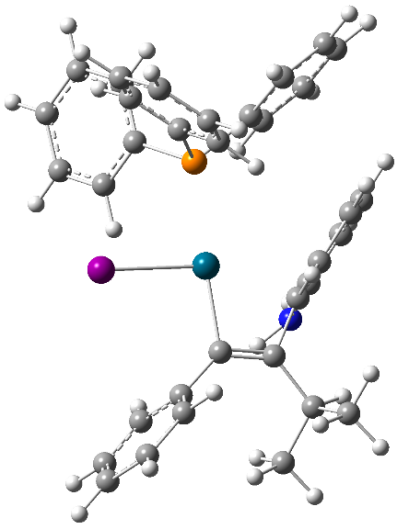


H	3.65021600	0.56982600	-2.09387300
C	3.93703000	2.84563800	1.02772100
H	2.44153500	1.58464600	1.91500400
C	4.71501200	3.10424400	-0.09968100
H	5.21375400	2.48009900	-2.09877500
H	4.01180700	3.48616900	1.90363400
H	5.40574600	3.94408900	-0.10366200
C	2.18020500	-1.51442300	-1.41287900
C	2.87329600	-2.71604100	-1.26232300
C	1.74379800	-1.13016600	-2.68696700
C	3.13031400	-3.51872000	-2.37147100
H	3.20109600	-3.04112200	-0.27698000
C	2.01483700	-1.92431900	-3.79411300
H	1.17207000	-0.20872800	-2.80724700
C	2.70569600	-3.12439000	-3.63605900
H	3.66272500	-4.45807500	-2.24307100
H	1.67476300	-1.61368100	-4.77899200
H	2.90864200	-3.75313900	-4.49952400
C	2.22873500	-1.26932800	1.51985700
C	3.58190800	-1.52661800	1.77782900
C	1.27391400	-1.61286700	2.47959500
C	3.96561000	-2.14291700	2.96240200
H	4.33907700	-1.23452000	1.05090000
C	1.66122400	-2.22126100	3.67119500
H	0.22144700	-1.40987800	2.28487000
C	3.00454600	-2.49111100	3.91014100
H	5.01715400	-2.34482500	3.15097200
H	0.91029300	-2.48190900	4.41288800
H	3.30688900	-2.96759300	4.83961100
C	-2.42021500	2.92000600	-1.63090400
H	-6.83229800	-2.10857500	1.49343900
C	-2.67855100	4.19400800	-0.83071600
H	-3.53428300	4.04814800	-0.15881300
H	-1.81218400	4.48395900	-0.22872000
H	-2.91886600	5.01873000	-1.51133600
C	-3.63274100	2.56195100	-2.48751500
H	-3.45416600	1.65694200	-3.07815400
H	-4.51349300	2.38953400	-1.85556600
H	-3.86451000	3.38507300	-3.17302500
H	-1.55445100	3.08165200	-2.28656000

INT2 complex of (3-methylbut-1-yn-1-yl)benzene
Energy = -1183974.474439 kcal/mol
Electronic Energy + Thermal Free Energy Correction (353.150 K) = -1183670.635836 kcal/mol
Symmetry c1

Pd	0.58011400	0.07185300	0.12983700
P	-1.85289500	-0.23257300	-0.11649000
I	0.95138100	-2.51735500	0.63317700
C	1.14846900	2.33785400	0.41621900
C	0.79498100	2.27012400	1.78730200
C	0.32016000	3.09296200	-0.46541200
C	-0.32974000	2.91282300	2.28226700
H	1.46820800	1.73145900	2.45261500
C	-0.80496800	3.74786700	0.05566600
C	-1.11718500	3.66012400	1.40250400
H	-0.57776800	2.85521200	3.33872500
H	-1.44791400	4.31258800	-0.61768300
H	-1.99975100	4.17816400	1.77226400
N	0.65828600	3.22425200	-1.79017800
H	1.26840500	2.51536300	-2.17676600

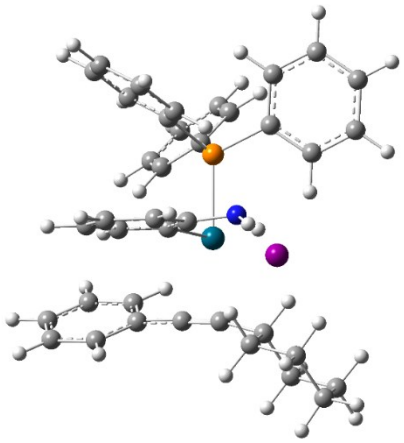
H	-0.07963200	3.51357000	-2.41779600
C	2.58043100	0.50609100	-0.00212700
C	2.50366600	1.83747300	-0.01483700
C	3.69397300	-0.40563300	-0.21345500
C	3.86289300	-1.07409800	-1.43491900
C	4.62753800	-0.62013000	0.80989400
C	4.95231000	-1.91063700	-1.63555300
H	3.12835400	-0.92095700	-2.22538500
C	5.71474600	-1.46371600	0.60777900
H	4.49018500	-0.11448100	1.76498700
C	5.88269700	-2.10843900	-0.61513100
H	5.08000200	-2.41097400	-2.59296300
H	6.43632200	-1.61577000	1.40735400
C	-2.88587700	1.22643700	-0.54560400
C	-3.84111500	1.79107000	0.29855500
C	-2.65976700	1.80115200	-1.80251700
C	-4.55596800	2.91769300	-0.10682000
H	-4.03126000	1.35502100	1.27756400
C	-3.37878600	2.91734300	-2.20920800
H	-1.91629000	1.36498400	-2.47193500
C	-4.32760200	3.48220700	-1.35691100
H	-5.29892300	3.34972600	0.55967700
H	-3.19896300	3.35001400	-3.19101800
H	-4.89016800	4.35821300	-1.67059300
C	-2.59541500	-0.91688700	1.40862800
C	-3.25912100	-2.14433400	1.46599800
C	-2.37695300	-0.20311700	2.59481600
C	-3.71707600	-2.63759300	2.68561300
H	-3.41357900	-2.72527000	0.55915800
C	-2.84881500	-0.69039600	3.80770600
H	-1.82543400	0.73882800	2.56604300
C	-3.51952100	-1.91117900	3.85520500
H	-4.22994800	-3.59594400	2.71855100
H	-2.68159700	-0.12267900	4.71992300
H	-3.88044700	-2.29836100	4.80500800
C	-2.34139800	-1.35352800	-1.48398800
C	-3.69144800	-1.61256400	-1.75526200
C	-1.36416600	-1.87631600	-2.33353900
C	-4.05065100	-2.40703100	-2.83688300
H	-4.46585100	-1.18228100	-1.12038800
C	-1.72567900	-2.66228400	-3.42557600
H	-0.31413200	-1.66475200	-2.13256800
C	-3.06700100	-2.93340700	-3.67300100
H	-5.10060800	-2.60863800	-3.03515000
H	-0.95695200	-3.06037800	-4.08349800
H	-3.35007500	-3.54840900	-4.52397400
C	3.57183600	2.87531600	-0.30998600
H	6.73469400	-2.76512800	-0.77383400
H	3.03960800	3.75537600	-0.70628000
C	4.24820000	3.29492800	0.99552700
H	4.94429100	4.12497200	0.82325300
H	3.51583100	3.62001200	1.74450900
H	4.81760900	2.45693800	1.41895300
C	4.59450900	2.44112800	-1.35021500
H	5.21297700	1.61044300	-0.98795800
H	4.10740300	2.11320900	-2.27733800
H	5.26346600	3.27548400	-1.59213700



ADS complex of (cyclohexylethynyl)benzene
Energy = -1257156.182952 kcal/mol
Electronic Energy + Thermal Free Energy Correction (353.150 K) = -1256815.197071 kcal/mol

Symmetry c1

Pd	-0.45435100	0.03561400	-0.11884600
P	1.81148200	-0.40876400	0.15669600
I	-0.65064500	-1.37574400	-2.54902900
C	-0.37574500	1.02047100	1.66581500
C	-0.12763600	2.38818400	1.67793100
C	-0.63413700	0.34241500	2.86779300
C	-0.15616200	3.11481500	2.87096300
H	0.08961200	2.90759100	0.74232600
C	-0.68387200	1.08218900	4.05814500
C	-0.44313300	2.45078800	4.05970100
H	0.03784800	4.18524200	2.86289600
H	-0.89551200	0.56054100	4.99213700
H	-0.47982300	2.99906600	4.99889900
N	-0.75216900	-1.04944400	2.91507100
H	-1.04672300	-1.47507100	2.04426500
H	-1.28031800	-1.40437600	3.70295300
C	-2.45752900	1.32812700	-0.60301100
C	-2.81434400	0.24413900	-0.14711200
C	-2.08749100	2.62155700	-1.08929300
C	-2.53710700	3.76940100	-0.42007300
C	-1.24672900	2.75387700	-2.20539500
C	-2.14203800	5.02695700	-0.85727100
H	-3.18346300	3.66071600	0.44795000
C	-0.84854000	4.01484000	-2.62784800
H	-0.89984400	1.85686400	-2.71695200
C	-1.29350200	5.15189600	-1.95523600
H	-2.49057700	5.91350700	-0.33371500
H	-0.18746500	4.11019300	-3.48603200
C	2.75074400	0.49163700	1.44277300
C	3.63763500	1.52285500	1.12786600
C	2.53105000	0.15883100	2.78562900
C	4.29307500	2.21722600	2.14285200
H	3.82841500	1.78807900	0.09039300
C	3.18672900	0.85422400	3.79252900
H	1.83664300	-0.64005100	3.04668300
C	4.06577600	1.88816100	3.47383600
H	4.98382000	3.01677900	1.88635700
H	3.00197100	0.59424900	4.83235700
H	4.57494000	2.43318800	4.26511100
C	2.62884400	0.03844800	-1.41254900
C	3.49309100	-0.82252800	-2.08893100
C	2.32186000	1.28643900	-1.96769300
C	4.04004400	-0.43763800	-3.31126200
H	3.73009400	-1.80032200	-1.67412200
C	2.87728100	1.67173700	-3.18026700
H	1.63025300	1.95420700	-1.45135000
C	3.73402000	0.80470300	-3.85730500
H	4.70640400	-1.11567200	-3.83875100
H	2.63458600	2.64392400	-3.60283000
H	4.16122600	1.09908000	-4.81275300
C	2.20579300	-2.15698300	0.49663600
C	1.22146200	-3.14193600	0.38378000
C	3.50210300	-2.51857300	0.88568400
C	1.52974400	-4.47265800	0.65112200
H	0.21238100	-2.86344600	0.07880200
C	3.80752500	-3.84934300	1.14532200
H	4.27213300	-1.75519400	0.99174400
C	2.82098600	-4.82622700	1.03019600



H	0.75760600	-5.23293000	0.56424400
H	4.81635800	-4.12309800	1.44373500
H	3.05994400	-5.86569800	1.24151700
H	-0.97794200	6.13762300	-2.28807700
C	-3.53005900	-0.93798700	0.34590100
C	-4.13027900	-0.66992100	1.73395200
C	-4.62145700	-1.37532500	-0.64077400
H	-2.81565500	-1.77562700	0.43233400
C	-4.85040700	-1.90930800	2.25016300
H	-4.83964500	0.16822200	1.64666700
H	-3.34145400	-0.34958500	2.42772700
C	-5.34540900	-2.61028600	-0.11702300
H	-5.33286000	-0.54370800	-0.76568900
H	-4.17212900	-1.56620400	-1.62400500
C	-5.92625500	-2.36830500	1.27199900
H	-5.28579300	-1.70642400	3.23642000
H	-4.11263400	-2.71640200	2.39345600
H	-6.13371800	-2.90774000	-0.81944300
H	-4.63276100	-3.44961500	-0.07193200
H	-6.42019700	-3.27484400	1.64346600
H	-6.70401800	-1.59069300	1.20548200

TS1 complex of (cyclohexylethynyl)benzene

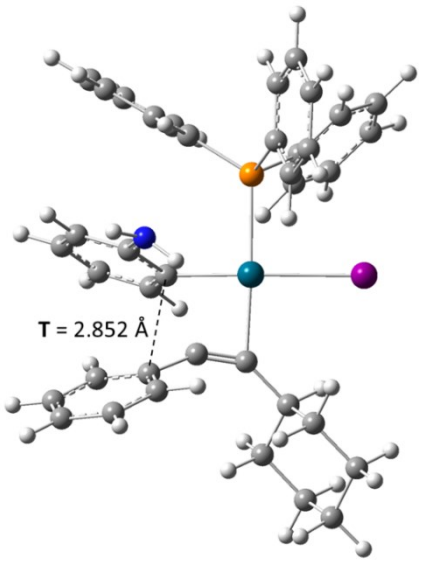
Energy = -1257141.144699 kcal/mol

Electronic Energy + Thermal Free Energy Correction (353.150 K) = -1256798.788338 kcal/mol

Imaginary frequency = -277.11 cm^{-1}

Symmetry c1

Pd	-0.35941000	-0.26241300	-0.12936300
P	2.04746100	-0.07412900	0.07695200
I	-0.19255100	-2.97028100	0.31859600
C	-0.49103800	1.72474100	-0.74864400
C	-0.64803800	1.94264000	-2.11787900
C	-0.04679800	2.76190000	0.09286800
C	-0.32579000	3.17508200	-2.68347800
H	-1.04419800	1.14087500	-2.74097200
C	0.26102900	4.00130200	-0.48486900
C	0.12936700	4.19948200	-1.85294200
H	-0.44372000	3.33617200	-3.75216900
H	0.62051500	4.80596600	0.15643200
H	0.37674000	5.17161700	-2.27450100
N	0.12453700	2.54354700	1.44563200
H	-0.41148500	1.77896800	1.83661600
H	0.14039900	3.36577500	2.03377000
C	-2.41415600	0.90561600	-0.09617200
C	-2.46069500	-0.33382400	-0.35571400
C	-3.04992300	2.08398300	0.45781100
C	-3.19987500	3.27072000	-0.27054000
C	-3.59815300	1.98728800	1.74463700
C	-3.90077200	4.33545100	0.27896100
H	-2.76014000	3.34502100	-1.26326600
C	-4.29330400	3.05997500	2.29085200
H	-3.46836200	1.06296700	2.30555800
C	-4.44665900	4.23354800	1.55810300
H	-4.02171200	5.25276800	-0.29193000
H	-4.71423100	2.97835000	3.28985500
C	2.91389000	1.48447100	-0.38008800
C	3.27241800	1.74831100	-1.70519100
C	3.17876300	2.45115900	0.59721400
C	3.87764200	2.95367600	-2.04777700
H	3.08827200	1.00902700	-2.48201000



C	3.78985000	3.65110500	0.25386000
H	2.89226800	2.27075800	1.63055100
C	4.13816000	3.90769000	-1.06966500
H	4.15173200	3.14175300	-3.08328200
H	3.99248600	4.39077600	1.02522400
H	4.61630300	4.84741600	-1.33627200
C	2.76651800	-1.30395000	-1.07975200
C	3.77688400	-2.20225500	-0.73388800
C	2.21322300	-1.36490300	-2.36550000
C	4.22838900	-3.14115500	-1.65886300
H	4.20279400	-2.19211100	0.26680000
C	2.67592800	-2.29057200	-3.29257500
H	1.39491100	-0.69465000	-2.63371900
C	3.68325600	-3.18534900	-2.93791800
H	5.00933000	-3.84222700	-1.37404100
H	2.23936100	-2.32396300	-4.28782600
H	4.03905800	-3.91909800	-3.65714300
C	2.72768800	-0.43851900	1.73422000
C	4.10040600	-0.35558600	2.00368800
C	1.84906300	-0.75988600	2.77178400
C	4.58223400	-0.61605000	3.28121000
H	4.79718300	-0.07556700	1.21481100
C	2.33213800	-1.01311200	4.05303000
H	0.78009400	-0.81312900	2.56644800
C	3.69827900	-0.94620400	4.30655400
H	5.64952700	-0.55414800	3.47873200
H	1.63841800	-1.25936000	4.85312100
H	4.07678100	-1.14363500	5.30662900
H	-4.98971700	5.07328500	1.98493400
C	-3.39902800	-1.45987900	-0.58123100
C	-3.94103500	-1.97295300	0.76015400
C	-4.56047300	-1.01470000	-1.47962500
H	-2.87318600	-2.29261900	-1.07384800
C	-4.91098700	-3.12640900	0.53804300
H	-4.45799600	-1.13944200	1.26455500
H	-3.10558700	-2.27512700	1.40516400
C	-5.54107700	-2.16147500	-1.69756500
H	-5.07370000	-0.16933200	-0.99109300
H	-4.17273800	-0.64094300	-2.43654400
C	-6.06099000	-2.70810000	-0.37223600
H	-5.29167700	-3.49089500	1.50051200
H	-4.36598700	-3.96688900	0.07684900
H	-6.37254700	-1.82933600	-2.33203700
H	-5.03091600	-2.96903700	-2.24663300
H	-6.74201700	-3.55081500	-0.54621100
H	-6.64985700	-1.92573800	0.13307700

INT1 complex of (cyclohexylethynyl)benzene

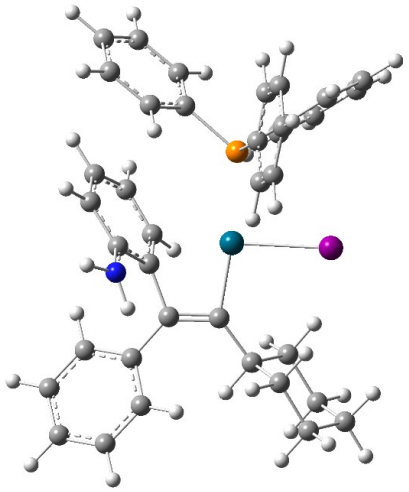
Energy = -1257172.050144 kcal/mol

Electronic Energy + Thermal Free Energy Correction (353.150 K)= -1256829.396345 kcal/mol

Symmetry c1

Pd	-0.33377300	-0.16266000	-0.13740200
P	2.15603100	0.13147000	0.02255200
I	0.06878800	-2.76544300	0.31029700
C	-1.31519300	1.89525500	-0.40234800
C	-0.76863800	1.90455600	-1.71246800
C	-0.81009500	2.82835200	0.55898000
C	0.24258600	2.78789900	-2.07241200
H	-1.22059300	1.24360000	-2.45068200
C	0.17036700	3.74156800	0.15920700

C	0.68168300	3.71613000	-1.13210800
H	0.65885800	2.77342300	-3.07606900
H	0.54444400	4.46737000	0.87992500
H	1.45585500	4.43182200	-1.40261500
N	-1.27794900	2.80799100	1.84362900
H	-2.15061100	2.33155000	2.02506600
H	-1.10522100	3.61756000	2.42140000
C	-2.59481500	1.14435200	-0.15433100
C	-2.40105900	-0.18268500	-0.18642200
C	-3.84149100	1.92642400	-0.00304000
C	-3.95885200	3.16725800	-0.64598100
C	-4.90642200	1.49209900	0.79977100
C	-5.11189500	3.93196000	-0.51924900
H	-3.13308300	3.52953200	-1.25875100
C	-6.06009800	2.25810100	0.92590800
H	-4.81955900	0.55715000	1.35055200
C	-6.17019900	3.47846400	0.26492600
H	-5.18469700	4.88737500	-1.03402500
H	-6.87305700	1.90444500	1.55604900
C	3.07615200	1.69657200	-0.29834500
C	3.69323100	1.97891400	-1.51905400
C	3.13404700	2.65115100	0.72403300
C	4.36269300	3.18586000	-1.70866700
H	3.66630500	1.25156300	-2.32791900
C	3.80755200	3.85209400	0.53696200
H	2.64988100	2.45193500	1.68050500
C	4.42527400	4.12282700	-0.68238200
H	4.84521200	3.38682000	-2.66245900
H	3.84894200	4.57890900	1.34503100
H	4.95471900	5.06108400	-0.83008200
C	2.87875400	-1.02730500	-1.19872300
C	3.82745500	-2.00391800	-0.89378100
C	2.36537800	-0.95955500	-2.50057600
C	4.25833100	-2.89505500	-1.87400200
H	4.21715500	-2.09284400	0.11797700
C	2.80761300	-1.83926600	-3.48164200
H	1.59973500	-0.21977800	-2.74139800
C	3.75237700	-2.81400300	-3.16736400
H	4.99098500	-3.65812200	-1.62201400
H	2.40380800	-1.77277700	-4.48908300
H	4.09011700	-3.51182700	-3.92974700
C	2.84198300	-0.29619300	1.66705100
C	4.22053600	-0.29660600	1.91650900
C	1.96002300	-0.52710100	2.72569800
C	4.70425000	-0.56254400	3.19201900
H	4.92093800	-0.07274300	1.11263700
C	2.44475900	-0.77895000	4.00716200
H	0.88635400	-0.51093200	2.53789300
C	3.81601800	-0.80536000	4.23837900
H	5.77632400	-0.56903500	3.37310600
H	1.74808200	-0.95234500	4.82366900
H	4.19616700	-1.00459100	5.23751600
H	-7.07178700	4.07747000	0.36764800
C	-3.44759700	-1.24876900	-0.22788300
C	-3.29107100	-2.19689200	-1.42113100
C	-3.61326500	-2.02023000	1.08554500
H	-4.40173000	-0.70964100	-0.39607100
C	-4.44670500	-3.18914300	-1.48957000
H	-2.33980400	-2.73916000	-1.32851800
H	-3.22887600	-1.60578900	-2.34630900



C	-4.77392900	-3.00422300	0.99506700
H	-2.68229500	-2.56222300	1.30384100
H	-3.76382400	-1.31290600	1.91487800
C	-4.58984400	-3.95791800	-0.18032100
H	-4.30204400	-3.88071500	-2.32968400
H	-5.38493100	-2.64590100	-1.68963400
H	-4.87161500	-3.56226100	1.93527800
H	-5.71570700	-2.44518000	0.86298100
H	-5.42886400	-4.66350600	-0.23830400
H	-3.68195900	-4.56122200	-0.01403400

TS2 complex of (cyclohexylethynyl)benzene

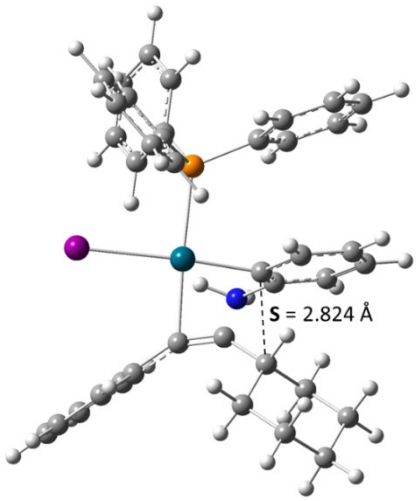
Energy = -1257140.600021 kcal/mol

Electronic Energy + Thermal Free Energy Correction (353.150 K) = -1256797.451117 kcal/mol

Imaginary frequency = -289.66 cm^{-1}

Symmetry c1

Pd	0.27961800	-0.30169000	-0.01787500
P	-2.04880100	0.25450900	0.14185900
I	-0.31457000	-2.94286000	0.48407800
C	0.83105300	1.64654100	-0.55535100
C	0.59598900	2.73662600	0.29300400
C	1.03411200	1.87417200	-1.93477900
C	0.63641800	4.04131100	-0.17491700
H	0.40270300	2.54826900	1.35026100
C	1.06572900	3.20260400	-2.39928200
C	0.87931500	4.26676800	-1.53268100
H	0.45794300	4.87240200	0.50313700
H	1.23586600	3.38049900	-3.46083500
H	0.90956200	5.28262300	-1.92062700
N	1.25669700	0.83183100	-2.81746300
H	0.79330400	-0.03860000	-2.59219000
H	1.18169500	1.06888800	-3.79775000
C	2.39225700	-0.68935400	-0.23926400
C	2.42571900	0.51157400	0.16362100
C	3.00128600	-1.94418900	-0.60415800
C	3.08713100	-2.31721800	-1.95252100
C	3.51358800	-2.80164400	0.37972700
C	3.67891100	-3.52278800	-2.30796300
H	2.68648000	-1.64695800	-2.71093500
C	4.10196900	-4.00664100	0.01643200
H	3.43760900	-2.51515100	1.42701900
C	4.18364000	-4.37236300	-1.32573800
H	3.74339900	-3.80224300	-3.35683500
H	4.49793100	-4.66532800	0.78573400
C	-2.51434400	2.02688500	0.09615900
C	-2.85004600	2.74834500	1.24325500
C	-2.47481500	2.68529800	-1.13883000
C	-3.14262700	4.10721100	1.15663800
H	-2.89570300	2.25148100	2.21025900
C	-2.76682200	4.03983200	-1.22217400
H	-2.21765600	2.13119200	-2.04185600
C	-3.10077800	4.75469400	-0.07338000
H	-3.41062400	4.65798800	2.05525000
H	-2.73110200	4.54052100	-2.18714000
H	-3.33022900	5.81555500	-0.13945600
C	-2.73083400	-0.35947000	1.72294600
C	-3.89057100	-1.12852100	1.82185100
C	-1.99196000	-0.08113600	2.87980700
C	-4.31042500	-1.60377200	3.06209500
H	-4.46299900	-1.37503200	0.93016100



C	-2.42079100	-0.54243000	4.11797300
H	-1.06492500	0.48979300	2.80403300
C	-3.58089100	-1.30919600	4.20944800
H	-5.21126200	-2.20907300	3.12822400
H	-1.84308000	-0.31448100	5.01035100
H	-3.91271900	-1.68136000	5.17568800
C	-3.09094900	-0.42457700	-1.19925200
C	-4.44638800	-0.08189200	-1.29760300
C	-2.52487100	-1.25294000	-2.17058600
C	-5.22379000	-0.58539700	-2.33344800
H	-4.89266600	0.58823000	-0.56350200
C	-3.30286500	-1.74820200	-3.21438100
H	-1.47070800	-1.51821600	-2.09997100
C	-4.65216500	-1.42040100	-3.29198400
H	-6.27611800	-0.32004300	-2.39720100
H	-2.85177600	-2.39080600	-3.96640100
H	-5.26058500	-1.80886800	-4.10511000
H	4.64132700	-5.31807500	-1.60558100
C	3.30052000	1.52793400	0.81005900
C	4.33621400	0.82729400	1.69698300
C	4.00441300	2.40220700	-0.23387200
H	2.68589400	2.18145300	1.44783100
C	5.24468400	1.85094500	2.37085900
H	4.93873100	0.14928800	1.07029200
H	3.82702400	0.20255500	2.44268800
C	4.90606700	3.42709600	0.44247600
H	4.60617000	1.74250900	-0.88120100
H	3.26650500	2.89560500	-0.87612100
C	5.92885300	2.75006500	1.34723200
H	5.98761100	1.33796100	2.99442900
H	4.64029700	2.47243900	3.05110500
H	5.40677100	4.04499800	-0.31343400
H	4.27907400	4.10957100	1.04052000
H	6.55393400	3.49762600	1.85189300
H	6.60560100	2.14003600	0.72736600

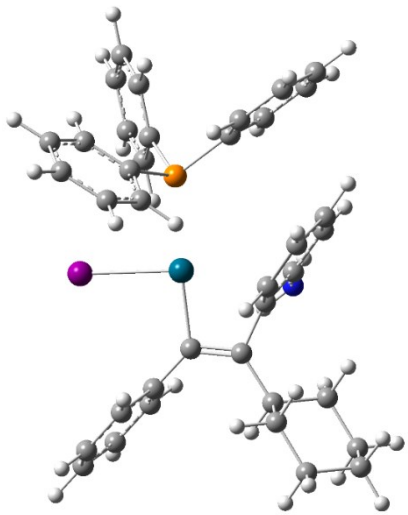
INT2 complex of (cyclohexylethynyl)benzene

Energy = -1257174.147907 kcal/mol

Electronic Energy + Thermal Free Energy Correction (353.150 K) = -1256831.280754 kcal/mol

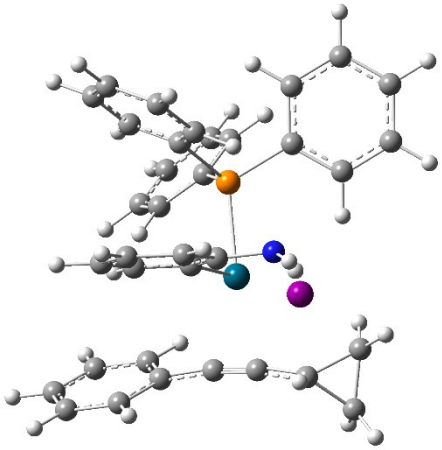
Symmetry c1

Pd	0.23601200	-0.25965200	-0.06972500
P	-2.19490600	0.25657600	0.07299100
I	-0.31052500	-2.86096600	-0.05554700
C	1.54319500	1.66689200	-0.09943800
C	1.06342300	2.10235700	1.16197400
C	1.06499600	2.32439500	-1.27699300
C	0.17489800	3.15856100	1.28059100
H	1.44447600	1.59331100	2.04683200
C	0.17933500	3.40372100	-1.13279000
C	-0.24316500	3.81440500	0.12063400
H	-0.18908800	3.47092600	2.25579200
H	-0.18318400	3.91186700	-2.02526900
H	-0.94244000	4.64544200	0.19289300
N	1.52060000	1.95385900	-2.51466900
H	1.93010500	1.03245000	-2.59432300
H	0.97538700	2.24223000	-3.31449000
C	2.27039400	-0.56225800	-0.14934100
C	2.69876000	0.69854400	-0.16601400
C	3.05149600	-1.79315000	-0.20773600
C	3.52860300	-2.25857600	-1.44075000



C	3.34779900	-2.52535400	0.94973900
C	4.28091400	-3.42564000	-1.51397700
H	3.29638400	-1.69216300	-2.34249200
C	4.10285900	-3.68955200	0.87487700
H	2.96727200	-2.17423700	1.90842000
C	4.56904800	-4.14614500	-0.35690100
H	4.64601300	-3.77391800	-2.47776000
H	4.32907900	-4.24545100	1.78219600
C	-2.90671300	1.95339600	0.15067000
C	-3.31698100	2.56155500	1.33850900
C	-3.01622000	2.66710700	-1.04897800
C	-3.83311900	3.85569400	1.32462000
H	-3.24592700	2.02501700	2.28276800
C	-3.53940900	3.95372700	-1.06369000
H	-2.69122100	2.20806700	-1.98323000
C	-3.94884700	4.55285200	0.12627700
H	-4.15539600	4.31446500	2.25653400
H	-3.62501300	4.49098000	-2.00547700
H	-4.35948000	5.55965000	0.11746800
C	-2.75557800	-0.52155700	1.63332500
C	-3.76906200	-1.47773700	1.71279700
C	-2.03713700	-0.19367700	2.79153300
C	-4.06823900	-2.08503100	2.93034400
H	-4.31724900	-1.76973000	0.81971100
C	-2.34725600	-0.78928000	4.00843500
H	-1.21885900	0.52658100	2.73555700
C	-3.36360200	-1.73984000	4.07896200
H	-4.85573000	-2.83339700	2.97826000
H	-1.78627400	-0.52029300	4.90023300
H	-3.59965600	-2.21570100	5.02767700
C	-3.21308000	-0.43762900	-1.28321300
C	-4.61128900	-0.34858500	-1.27545900
C	-2.57257100	-0.97614100	-2.40175200
C	-5.35163600	-0.82651700	-2.35016700
H	-5.12357800	0.10928600	-0.42967900
C	-3.31444600	-1.44408400	-3.48395900
H	-1.48456200	-1.02809500	-2.41997800
C	-4.70323600	-1.37742400	-3.45437200
H	-6.43665700	-0.76029100	-2.33110100
H	-2.80476500	-1.85885900	-4.35023300
H	-5.28399400	-1.74436500	-4.29728600
H	5.15647200	-5.05952700	-0.41362100
C	4.13052800	1.17742700	-0.08824100
C	4.41184400	2.41419700	-0.94362400
C	4.51001300	1.45713900	1.37444500
H	4.76976400	0.35149400	-0.44652800
C	5.85899100	2.87521400	-0.80799100
H	3.74025800	3.22844400	-0.61996700
H	4.16778000	2.21088000	-1.99370900
C	5.95764700	1.91545500	1.50566900
H	3.84399300	2.24447700	1.76687700
H	4.32535000	0.55779900	1.97922100
C	6.22236200	3.14593400	0.64671900
H	6.02826200	3.76899000	-1.42221800
H	6.52504600	2.09215600	-1.20541300
H	6.19642500	2.11722700	2.55794100
H	6.62384200	1.09906700	1.18305300
H	7.27145800	3.45752900	0.73113600
H	5.61328300	3.98483600	1.02093900

ADS complex of (cyclopropylethynyl)benzene
Energy = -1183181.552184 kcal/mol
Electronic Energy + Thermal Free Energy Correction (353.150 K) = -1182892.480123 kcal/mol
Symmetry c1

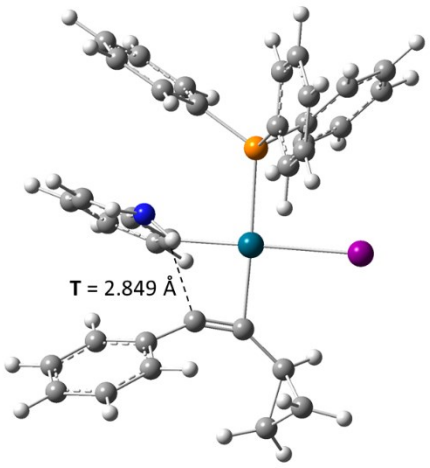


Pd	0.62600100	-0.03177500	-0.38726500
P	-1.63818700	0.00591400	0.30618000
I	0.83152400	-2.90443600	-0.24208100
C	0.60290300	1.99905300	-0.51477300
C	1.08404100	2.73551500	0.56804500
C	0.22693300	2.66287900	-1.70063500
C	1.21741400	4.12938700	0.49716200
H	1.37222900	2.22415500	1.48262500
C	0.37752800	4.06124300	-1.76885100
C	0.86509700	4.78623400	-0.68270900
H	1.59449300	4.68440600	1.35152000
H	0.09683700	4.57635700	-2.68541000
H	0.96794400	5.86504000	-0.76265100
N	-0.36169900	1.97623200	-2.77458200
H	-0.11926200	0.99485300	-2.82456200
H	-0.25449600	2.42962800	-3.67390900
C	2.99468000	0.09010400	-0.49424300
C	2.73346500	0.05932800	-1.69914500
C	3.69955400	0.25492700	0.75195400
C	4.80161400	1.13354000	0.79361100
C	3.33108300	-0.43973200	1.91909800
C	5.51480600	1.30810400	1.97740400
H	5.08799800	1.67112400	-0.10450400
C	4.05224500	-0.25882500	3.09850400
H	2.48879100	-1.12188800	1.88625300
C	5.14262300	0.61439100	3.13279100
H	6.36166300	1.98736600	1.99785200
H	3.76166200	-0.80226400	3.99255800
C	-2.42910100	1.61265400	0.75846700
C	-2.70759600	1.95593500	2.08912600
C	-2.76168500	2.51726000	-0.26511000
C	-3.30983600	3.18078200	2.39105600
H	-2.46642700	1.27225100	2.89491200
C	-3.36635800	3.73523500	0.04158400
H	-2.54257800	2.27367300	-1.30007900
C	-3.64211600	4.07133000	1.37034500
H	-3.52286700	3.43074800	3.42618800
H	-3.62068500	4.42367400	-0.75898000
H	-4.11345500	5.02089100	1.60611700
C	-1.81004000	-1.01368400	1.83083100
C	-2.86265800	-1.91967200	2.01996900
C	-0.85139300	-0.85569800	2.84606000
C	-2.95575400	-2.65162200	3.20650100
H	-3.60779000	-2.06520000	1.24594700
C	-0.95484800	-1.57858900	4.03427600
H	-0.01731100	-0.17420000	2.70506400
C	-2.00674400	-2.48097900	4.21583500
H	-3.77247100	-3.35499100	3.33854100
H	-0.21004500	-1.44357400	4.81278800
H	-2.08289700	-3.05008300	5.13747000
C	-2.80688100	-0.67986700	-0.94098700
C	-2.32265800	-1.39000200	-2.04950100
C	-4.19386000	-0.48959800	-0.80403500
C	-3.20696000	-1.90892700	-2.99789500
H	-1.25539200	-1.54302500	-2.16560000

C	-5.07417900	-1.01486900	-1.75032600
H	-4.58871100	0.07498000	0.03420300
C	-4.58264000	-1.72468800	-2.84903900
H	-2.81793500	-2.45367700	-3.85288700
H	-6.14273100	-0.86327600	-1.63139200
H	-5.26939700	-2.12704100	-3.58774400
H	5.69985500	0.75388000	4.05423100
C	2.59465900	0.01824600	-3.12918100
C	3.60474400	-0.79144800	-3.94493200
C	2.18970800	-1.26425000	-3.84687000
H	2.25611900	0.94768500	-3.57905700
H	4.36429500	-1.33278000	-3.39108100
H	3.94510900	-0.33713200	-4.86973000
H	1.54121800	-1.14409000	-4.70882700
H	1.97741200	-2.12520500	-3.22231800

TS1 complex of (cyclopropylethynyl)benzene
Energy = -1183166.107932 kcal/mol
Electronic Energy + Thermal Free Energy Correction (353.150 K) = -1182876.525079 kcal/mol
Imaginary frequency = -283.83 cm^{-1}
Symmetry c1

Pd	-0.43086800	-0.67746500	-0.26743000
P	1.62234300	0.53053200	0.14818500
I	0.87617300	-3.06994500	0.06354100
C	-1.41284900	1.08964900	-0.77632000
C	-1.59243100	1.32588300	-2.13979600
C	-1.51551300	2.14528400	0.15001100
C	-1.83424800	2.61393200	-2.61359400
H	-1.55666800	0.48625300	-2.83345400
C	-1.77225100	3.43474500	-0.33770100
C	-1.92266700	3.66332300	-1.69865800
H	-1.96705100	2.79105600	-3.67798200
H	-1.83820400	4.25986100	0.37130500
H	-2.12046800	4.67451700	-2.04824400
N	-1.31861900	1.92371200	1.49769700
H	-1.47134800	0.97628400	1.81994600
H	-1.68324500	2.62687400	2.12581400
C	-2.76931400	-0.55577500	-0.32117800
C	-2.25976200	-1.65674700	-0.69266400
C	-3.89830900	0.15092600	0.25245700
C	-4.52894000	1.21701400	-0.40128900
C	-4.41730100	-0.31743100	1.46819400
C	-5.66464000	1.79408100	0.14947800
H	-4.11731200	1.58332900	-1.33991100
C	-5.55403200	0.26733500	2.01512100
H	-3.91708500	-1.14103700	1.97558300
C	-6.17815000	1.32319200	1.35724200
H	-6.15476600	2.61655600	-0.36576200
H	-5.94968500	-0.10133600	2.95829500
C	1.72879300	2.34221700	-0.15494100
C	1.96923100	2.84512400	-1.43709300
C	1.51796000	3.24329900	0.89511100
C	1.99470000	4.21753300	-1.66521200
H	2.14868000	2.16694400	-2.26883600
C	1.55104500	4.61365700	0.66640700
H	1.31963500	2.87170800	1.89733200
C	1.78760900	5.10530100	-0.61469400
H	2.18666400	4.59159900	-2.66820000



H	1.39219200	5.30092100	1.49430100
H	1.81395300	6.17788700	-0.79214600
C	2.87260200	-0.15372500	-1.00816700
C	4.16781900	-0.51086700	-0.63162800
C	2.46809300	-0.36191600	-2.33350900
C	5.04548500	-1.05589800	-1.56619800
H	4.49765600	-0.38351300	0.39705100
C	3.34909300	-0.89175800	-3.26808100
H	1.44561500	-0.12216100	-2.63046800
C	4.64159000	-1.24284600	-2.88428500
H	6.05010600	-1.33661100	-1.25876200
H	3.02218600	-1.04297700	-4.29401100
H	5.33027200	-1.66737400	-3.61072000
C	2.30291700	0.35827300	1.83566600
C	3.47748700	1.01023600	2.23500400
C	1.60140100	-0.41101900	2.76687800
C	3.95069000	0.86936200	3.53435700
H	4.02001000	1.64056400	1.53159500
C	2.07319000	-0.54719400	4.06959600
H	0.68305200	-0.90909500	2.45679100
C	3.24971400	0.08880400	4.45181800
H	4.86499500	1.37582700	3.83357500
H	1.51814700	-1.14818800	4.78562200
H	3.62012100	-0.01660200	5.46870500
H	-7.06589400	1.78198400	1.78594600
C	-2.52568500	-3.03731800	-1.06080000
C	-3.10031500	-3.94663200	-0.00316100
C	-3.96809800	-3.48046300	-1.12273400
H	-1.82873100	-3.49805300	-1.75661900
H	-3.25907200	-3.51172600	0.98167100
H	-2.75520900	-4.97738600	0.00040700
H	-4.23630500	-4.18775400	-1.90263600
H	-4.72382900	-2.72933200	-0.90252700

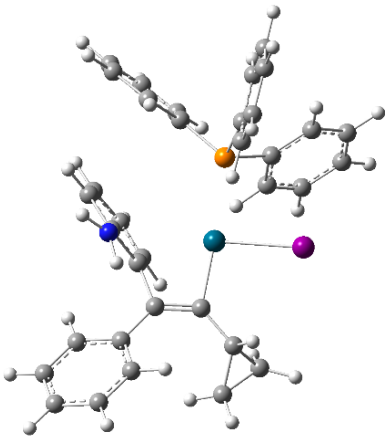
INT1 complex of (cyclopropylethynyl)benzene

Energy = -1183199.731747 kcal/mol

Electronic Energy + Thermal Free Energy Correction (353.150 K) = -1182909.564055 kcal/mol

Symmetry c1

Pd	-0.46179200	-0.48554900	-0.11438200
P	1.88429700	0.37091600	0.00458600
I	0.41230000	-2.93858100	0.42839100
C	-1.97790800	1.23104700	-0.40286400
C	-1.45056600	1.33627400	-1.71539800
C	-1.70407800	2.27724500	0.53346400
C	-0.68052400	2.42782500	-2.10500900
H	-1.73290300	0.56936800	-2.43530100
C	-0.96024500	3.38181200	0.10811600
C	-0.46548700	3.45250600	-1.18894900
H	-0.27909300	2.48887500	-3.11300200
H	-0.75909400	4.18773200	0.81259900
H	0.11350300	4.32628200	-1.48200800
N	-2.14802600	2.17566700	1.82578800
H	-2.89909900	1.52688000	2.01681900
H	-2.17421300	3.02139100	2.37668100
C	-3.00070500	0.16632900	-0.11081700
C	-2.43506500	-1.04843600	-0.10894400
C	-4.40979700	0.56300900	0.08099700
C	-4.89344400	1.72244300	-0.54044400
C	-5.27915600	-0.16788600	0.90304500
C	-6.21323400	2.12369900	-0.37070900

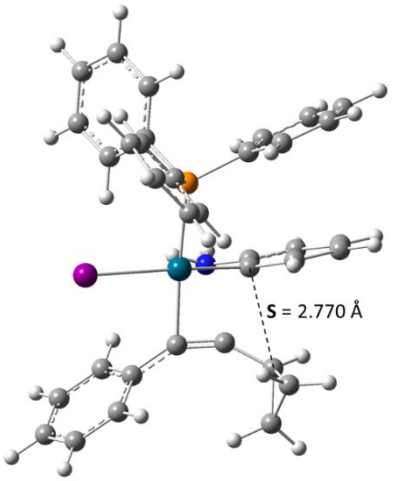


H	-4.22529200	2.30989600	-1.17033700
C	-6.59848600	0.23567800	1.07293100
H	-4.90927500	-1.05108800	1.41961300
C	-7.07192300	1.37989600	0.43498800
H	-6.57251700	3.02163800	-0.86837900
H	-7.25841600	-0.34198800	1.71626900
C	2.40385000	2.09204000	-0.39896900
C	2.89162100	2.46481800	-1.65341600
C	2.25093500	3.07535000	0.58573000
C	3.22767200	3.79132600	-1.91385500
H	3.02273600	1.71860200	-2.43462700
C	2.59390200	4.39712100	0.32820600
H	1.86402700	2.80249100	1.56773800
C	3.08301800	4.75958800	-0.92492000
H	3.61303600	4.06471100	-2.89345000
H	2.47564600	5.14667500	1.10750000
H	3.35256100	5.79319300	-1.12856500
C	2.86347200	-0.65536800	-1.15510700
C	3.99137200	-1.39348300	-0.79402600
C	2.37046500	-0.76296000	-2.46246800
C	4.62117300	-2.21511300	-1.72625400
H	4.37367000	-1.34967300	0.22350800
C	3.00724600	-1.57262800	-3.39529200
H	1.46771000	-0.21822200	-2.74589000
C	4.13465800	-2.30395200	-3.02641900
H	5.49515200	-2.79099200	-1.43093300
H	2.61537300	-1.64371600	-4.40709000
H	4.62768200	-2.94761500	-3.75084200
C	2.63428600	0.19116500	1.66596900
C	3.97706000	0.50499700	1.91492100
C	1.81150800	-0.16817900	2.73617200
C	4.49143700	0.42127900	3.20307100
H	4.62066900	0.83035300	1.09812700
C	2.32382300	-0.23903600	4.02945200
H	0.76079200	-0.39076300	2.54928000
C	3.66501800	0.04698700	4.26148500
H	5.53695300	0.65844800	3.38459100
H	1.67277500	-0.51580800	4.85508700
H	4.06778000	-0.01154800	5.26985900
H	-8.10355200	1.69513500	0.57214400
C	-3.02433800	-2.39230100	-0.10108300
C	-4.29253100	-2.66061900	-0.87510900
C	-2.99101400	-3.20758100	-1.36463500
H	-2.88341100	-2.96261000	0.81810600
H	-4.73287000	-1.82774400	-1.41843000
H	-5.01411400	-3.34548400	-0.43544200
H	-2.79967300	-4.27415600	-1.27467600
H	-2.53835500	-2.73297600	-2.23457900

TS2 complex of (cyclopropylethynyl)benzene
Energy = -1183165.754645 kcal/mol
Electronic Energy + Thermal Free Energy Correction (353.150 K) = -1182876.941117 kcal/mol
Imaginary frequency = -327.77 cm^{-1}
Symmetry c1

Pd	-0.60671000	0.19748500	-0.02697900
P	1.68623400	-0.47665900	-0.04383400
I	-1.39113400	-2.43075700	-0.27192200
C	-0.10897000	2.21584900	0.21944100
C	0.59398200	2.90983600	-0.77469400

C	-0.19513400	2.76141900	1.51914300
C	1.14803600	4.15707000	-0.53193500
H	0.66935400	2.47020900	-1.77007200
C	0.35557500	4.03570100	1.74953900
C	1.00874900	4.72222900	0.73907400
H	1.68119200	4.68498000	-1.31893400
H	0.27018200	4.47224700	2.74446700
H	1.42770500	5.70455000	0.94712600
N	-0.85356100	2.09742100	2.53704800
H	-0.84158000	1.08760000	2.48447200
H	-0.69020900	2.44713400	3.47137800
C	-2.61644000	0.93102500	0.02996100
C	-2.12304600	2.01248900	-0.40468800
C	-3.80255100	0.17648300	0.36756100
C	-4.12900400	-0.07726800	1.70498300
C	-4.62940300	-0.31636300	-0.65034300
C	-5.27011500	-0.80610100	2.01707000
H	-3.47433200	0.29952300	2.48919700
C	-5.76817100	-1.04576900	-0.33043500
H	-4.35652100	-0.13810200	-1.68967600
C	-6.09084800	-1.29423600	1.00188400
H	-5.51864100	-0.99781300	3.05826600
H	-6.40509200	-1.42536200	-1.12590600
C	2.95471000	0.84021900	-0.14540000
C	3.67786900	1.10984300	-1.30847900
C	3.15659900	1.63793900	0.98718500
C	4.59200600	2.16073600	-1.33632600
H	3.53701600	0.49619400	-2.19628100
C	4.06730800	2.68438500	0.95641900
H	2.59354500	1.43799500	1.89933400
C	4.78782600	2.94853700	-0.20726300
H	5.15607000	2.35860900	-2.24483700
H	4.21395200	3.29839400	1.84206700
H	5.50210400	3.76812100	-0.23148700
C	2.02703900	-1.55919200	-1.47521700
C	2.66515000	-2.79599400	-1.37366700
C	1.55461300	-1.13184400	-2.72244400
C	2.83192900	-3.59152800	-2.50495100
H	3.01725600	-3.15373000	-0.40828400
C	1.73684600	-1.91921500	-3.85244300
H	1.02345100	-0.18200800	-2.80416800
C	2.37264300	-3.15471000	-3.74321700
H	3.32110100	-4.55844200	-2.41423400
H	1.36957600	-1.57535900	-4.81627600
H	2.50422300	-3.77851900	-4.62387500
C	2.21730900	-1.37634900	1.45733100
C	3.56498100	-1.70462000	1.65741900
C	1.28507200	-1.68620200	2.45027900
C	3.96318700	-2.35425700	2.81926900
H	4.30734600	-1.44391500	0.90372900
C	1.68746200	-2.32844000	3.61877800
H	0.23697200	-1.42935300	2.29846600
C	3.02437100	-2.66578400	3.80138200
H	5.00992300	-2.61017500	2.96372100
H	0.95395900	-2.56167200	4.38656300
H	3.33916100	-3.16774700	4.71312800
H	-6.97991600	-1.86914900	1.24926100
C	-2.28109600	3.23479200	-1.16556100
C	-2.27839400	3.13071900	-2.67074200
C	-3.56163900	3.37601200	-1.95420400



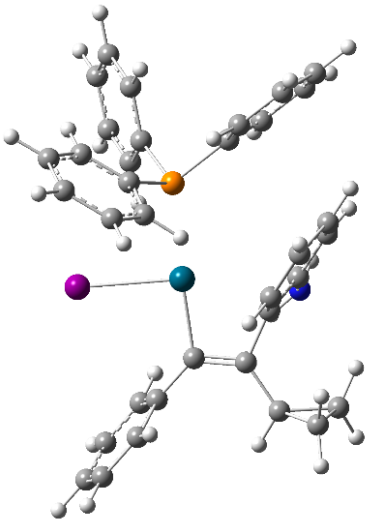
H	-1.84868500	4.13499200	-0.73319100
H	-2.11228600	2.13831600	-3.08665400
H	-1.81870800	3.94790900	-3.21984100
H	-3.99750500	4.37028500	-1.99167600
H	-4.28114400	2.56353200	-1.89298100

INT2 complex of (cyclopropylethynyl)benzene

Energy = -1183200.598964 kcal/mol

Electronic Energy + Thermal Free Energy Correction (353.150 K) = -1182910.096810 kcal/mol

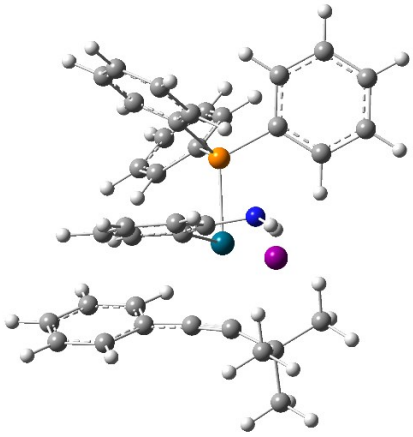
Symmetry c1



Pd	0.62594400	0.10608800	0.01516500
P	-1.83981600	-0.20337400	0.00628100
I	0.96237000	-2.52549900	-0.03392300
C	1.24625000	2.35777900	0.15873000
C	0.60578000	2.48258600	1.41715800
C	0.63355300	2.95610800	-0.98693700
C	-0.58411600	3.17922200	1.56261700
H	1.10428400	2.04212400	2.28027900
C	-0.56250300	3.66816900	-0.81464500
C	-1.14762400	3.78208500	0.43645800
H	-1.06472400	3.25879400	2.53404800
H	-1.03404400	4.12792900	-1.68203400
H	-2.08363900	4.32974700	0.53004100
N	1.24756400	2.89181700	-2.20773600
H	1.96024400	2.18542900	-2.33196900
H	0.68977000	3.08603600	-3.02644600
C	2.64900800	0.47537900	0.02989700
C	2.64564100	1.80815100	0.07902600
C	3.79503800	-0.42156700	-0.07755800
C	4.41467400	-0.61995600	-1.31924800
C	4.31412600	-1.07867400	1.04625400
C	5.52215900	-1.45315300	-1.43361900
H	4.01500000	-0.10986300	-2.19561900
C	5.42468200	-1.90633800	0.93095400
H	3.83133000	-0.93553200	2.01211500
C	6.03048000	-2.09981700	-0.30931800
H	5.99299200	-1.59489900	-2.40408300
H	5.82033800	-2.40414200	1.81362400
C	-3.06102300	1.17119200	0.10359000
C	-3.73066800	1.52588000	1.27591800
C	-3.30773100	1.90059400	-1.06573200
C	-4.63633900	2.58468800	1.27562200
H	-3.55710200	0.97190000	2.19632400
C	-4.21651400	2.95089600	-1.06770800
H	-2.78576900	1.63593500	-1.98592600
C	-4.88429000	3.29631900	0.10608800
H	-5.15724800	2.84554500	2.19398700
H	-4.40357300	3.50200400	-1.98651900
H	-5.59757400	4.11701700	0.10699500
C	-2.20767600	-1.22297600	1.48305600
C	-2.85180200	-2.46023100	1.43449300
C	-1.71506100	-0.75880800	2.71016000
C	-3.01029300	-3.21503200	2.59449000
H	-3.21468000	-2.85140900	0.48645200
C	-1.88742700	-1.50635700	3.86918600
H	-1.17831300	0.19047500	2.75434600
C	-2.53366200	-2.73982700	3.81176300
H	-3.50667500	-4.18124300	2.54268200
H	-1.50568200	-1.13182600	4.81599100
H	-2.65855100	-3.33164800	4.71525700

C	-2.50451800	-1.10426700	-1.44382300
C	-3.86236500	-1.43729400	-1.53874300
C	-1.65746800	-1.39099700	-2.51655400
C	-4.35155600	-2.07559400	-2.67209000
H	-4.54295200	-1.18754000	-0.72520700
C	-2.15126300	-2.01886800	-3.65815600
H	-0.60329500	-1.12312000	-2.45113400
C	-3.49550400	-2.36782100	-3.73258900
H	-5.40497900	-2.33799500	-2.73219000
H	-1.48337200	-2.23366900	-4.48876400
H	-3.88157200	-2.86079100	-4.62164800
H	6.89680700	-2.75105300	-0.39810400
C	3.82919200	2.69943700	0.12863300
C	3.74765500	4.15152700	-0.25503400
C	3.89858800	3.78207900	1.18111000
H	4.76670700	2.19079800	-0.09319800
H	2.78399400	4.53916100	-0.57873900
H	4.60119400	4.57646900	-0.77664100
H	4.85418800	3.94475100	1.67219200
H	3.02764200	3.90283000	1.82346600

ADS complex of (3,3-dimethylbut-1-yn-1-yl)benzene
Energy = -1208607.084210 kcal/mol
Electronic Energy + Thermal Free Energy Correction (353.150 K) = -1208289.080219 kcal/mol
Symmetry c1



Pd	0.60257600	-0.14996800	-0.41943700
P	-1.64331300	0.06693600	0.19727100
I	0.56500400	-2.97543800	-0.21526600
C	0.63351400	1.88447200	-0.59473000
C	1.02583800	2.64761000	0.49868600
C	0.30894300	2.51293900	-1.80717600
C	1.14154800	4.03663700	0.40504900
H	1.24610200	2.16013900	1.45004700
C	0.45414500	3.90514400	-1.90237700
C	0.86149000	4.65769200	-0.80821900
H	1.44882500	4.61793200	1.27178500
H	0.21611700	4.39347800	-2.84788300
H	0.95498500	5.73729000	-0.90662300
N	-0.23419600	1.80392100	-2.87987000
H	-0.04634400	0.80905700	-2.86932500
H	-0.08217100	2.21325800	-3.79309600
C	2.95717900	-0.09393100	-0.02175200
C	2.84049400	-0.24864500	-1.23793400
C	3.20761000	0.16215700	1.36403800
C	3.91835200	1.31782800	1.72410800
C	2.75192300	-0.71053100	2.36419200
C	4.16388700	1.59478900	3.06229900
H	4.26270400	1.99316500	0.94395400
C	2.99637800	-0.42023500	3.70007300
H	2.19781900	-1.60346900	2.07758200
C	3.70028400	0.73018200	4.05152200
H	4.71533700	2.49094900	3.33492200
H	2.63791500	-1.09774100	4.47150000
C	-2.28549300	1.72523800	0.62599200
C	-2.46883700	2.13125700	1.94929900
C	-2.53432400	2.63112900	-0.41237900
C	-2.88501700	3.43081500	2.23072100
H	-2.29093900	1.43702700	2.76762700
C	-2.95308000	3.92358700	-0.12646900
H	-2.38435600	2.32727700	-1.44841100

C	-3.12272700	4.32848700	1.19627100
H	-3.02551600	3.73709400	3.26451700
H	-3.13615500	4.62193000	-0.93980000
H	-3.44403600	5.34331500	1.41837100
C	-1.86696200	-0.91745000	1.71905300
C	-2.90199200	-1.83998400	1.87285500
C	-0.92200800	-0.76405800	2.74048700
C	-2.98548900	-2.60513000	3.03389800
H	-3.63626600	-1.97977900	1.08204900
C	-1.01280800	-1.52185100	3.90054400
H	-0.09540800	-0.06265400	2.61439700
C	-2.04269900	-2.45027500	4.04507700
H	-3.78888400	-3.32936200	3.14386400
H	-0.27262300	-1.39610900	4.68748600
H	-2.10744400	-3.05389700	4.94702800
C	-2.84992000	-0.55407100	-1.02099800
C	-2.42606700	-1.31398100	-2.11372900
C	-4.21445000	-0.28079900	-0.85874200
C	-3.35402700	-1.80123300	-3.02963400
H	-1.36561000	-1.53150400	-2.23947100
C	-5.13867200	-0.77562900	-1.77084500
H	-4.55283900	0.32231500	-0.01702700
C	-4.70873600	-1.53482300	-2.85712300
H	-3.01639300	-2.38899100	-3.87950900
H	-6.19640200	-0.56393600	-1.63606800
H	-5.43295300	-1.91652800	-3.57267900
C	3.19879100	-0.43178600	-2.66447100
H	3.88909500	0.95273000	5.09884800
C	2.17118200	-1.25102500	-3.44393700
H	2.51925300	-1.37050300	-4.47729300
H	2.03163500	-2.24437600	-3.00326700
H	1.19387400	-0.75389400	-3.47358000
C	3.35645000	0.95049300	-3.30884300
H	4.08796800	1.55821000	-2.76356100
H	3.70650900	0.83235400	-4.34204200
H	2.40112000	1.48906800	-3.32827400
C	4.54419200	-1.17220600	-2.68130800
H	5.31423200	-0.60360600	-2.14751700
H	4.44902400	-2.15711000	-2.20833100
H	4.87380600	-1.31475200	-3.71798500

TS1 complex of (3,3-dimethylbut-1-yn-1-yl)benzene

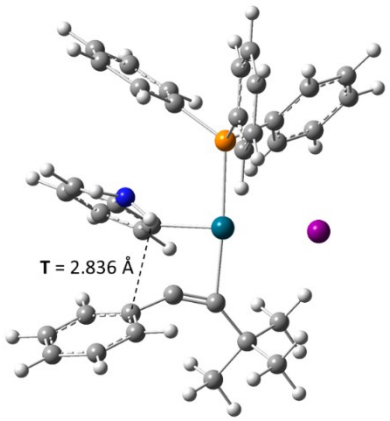
Energy = -1208591.483709 kcal/mol

Electronic Energy + Thermal Free Energy Correction (353.150 K) = -1208271.724575 kcal/mol

Imaginary frequency = -291.63 cm^{-1}

Symmetry c1

Pd	-0.44000400	-0.62457100	-0.10887900
P	1.68890300	0.53422000	0.09410900
I	0.84620400	-2.98006200	0.56786000
C	-1.35954100	1.13100100	-0.75173700
C	-1.61753600	1.23237300	-2.12076700
C	-1.31569200	2.28638000	0.05235200
C	-1.78188000	2.47649300	-2.72391400
H	-1.70714600	0.32027000	-2.71194800
C	-1.50022900	3.53160300	-0.56424000
C	-1.71765700	3.62306400	-1.93156800
H	-1.97188700	2.54810600	-3.79189600
H	-1.45330100	4.43221900	0.04751000
H	-1.85144200	4.60418900	-2.38278000



N	-1.04227400	2.19613300	1.40261700
H	-1.27244200	1.31356800	1.84175600
H	-1.29570000	2.99867200	1.96302900
C	-2.73489300	-0.35381300	-0.05842800
C	-2.34697300	-1.49733800	-0.45001900
C	-3.75955200	0.44118300	0.59193200
C	-4.41650500	1.48428200	-0.07255700
C	-4.14496300	0.09684800	1.89424600
C	-5.44907100	2.16412400	0.55874200
H	-4.10730800	1.75008800	-1.08209900
C	-5.17279200	0.78968000	2.52430400
H	-3.62656900	-0.71592800	2.40087600
C	-5.82519000	1.82272300	1.85725900
H	-5.96350300	2.96775800	0.03747200
H	-5.46331100	0.52194600	3.53712000
C	1.82634700	2.29345800	-0.42792900
C	1.81482100	2.62335100	-1.78606500
C	1.86702500	3.32451900	0.51742400
C	1.85261300	3.95294100	-2.19176400
H	1.78115400	1.84047900	-2.54107100
C	1.90468600	4.65339600	0.11000000
H	1.86549500	3.08833600	1.57896600
C	1.89832600	4.97140100	-1.24533300
H	1.84743800	4.19153100	-3.25291600
H	1.94342200	5.44319500	0.85684600
H	1.92956500	6.01123500	-1.56228300
C	2.81405600	-0.32613900	-1.07651000
C	4.13195700	-0.67709900	-0.77993500
C	2.28067900	-0.68404300	-2.32202400
C	4.90496100	-1.36126800	-1.71540500
H	4.55946100	-0.43963500	0.19137400
C	3.05686300	-1.35383300	-3.25987200
H	1.23657100	-0.45868200	-2.54776200
C	4.37282300	-1.69601600	-2.95604500
H	5.92791000	-1.63543100	-1.46842100
H	2.62941200	-1.62187800	-4.22304600
H	4.97900500	-2.23022300	-3.68361900
C	2.49583900	0.51875700	1.73456400
C	3.74207500	1.11880800	1.96220700
C	1.82076100	-0.06991300	2.80701700
C	4.30978700	1.09962100	3.23105900
H	4.26695400	1.61727900	1.14851900
C	2.38687500	-0.08289800	4.07865200
H	0.84634500	-0.52640300	2.63752500
C	3.63443400	0.49553300	4.28931000
H	5.27961600	1.56303700	3.39474100
H	1.85128000	-0.54539700	4.90402500
H	4.07949600	0.48414400	5.28134900
C	-2.85261600	-2.80078200	-0.98457100
H	-6.62935900	2.36429400	2.34953900
C	-1.97548000	-3.30861900	-2.12861000
H	-0.96220700	-3.53373300	-1.77750400
H	-2.41159600	-4.22141800	-2.55454600
H	-1.90427200	-2.55794600	-2.92705200
C	-4.26550200	-2.52332800	-1.51691100
H	-4.92096100	-2.15602200	-0.71712700
H	-4.24118800	-1.76943300	-2.31439300
H	-4.69925300	-3.44602400	-1.92320600
C	-2.93134000	-3.83411800	0.14094600
H	-3.33647400	-4.77550700	-0.25276600

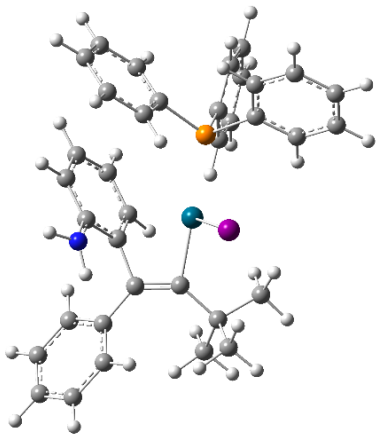
H	-1.94235600	-4.03097700	0.56902100
H	-3.59421500	-3.48239400	0.94184300

INT1 complex of (3,3-dimethylbut-1-yn-1-yl)benzene

Energy = -1208620.076784 kcal/mol

Electronic Energy + Thermal Free Energy Correction (353.150 K) = -1208299.914789 kcal/mol

Symmetry c1

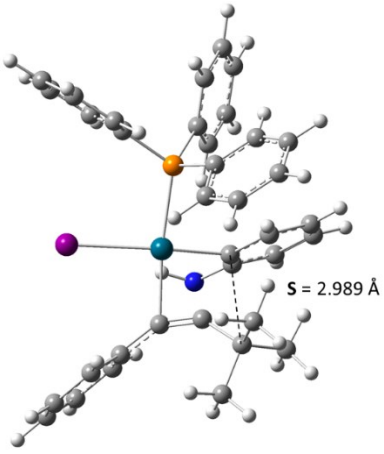


Pd	0.30899000	-0.40208100	0.37443000
P	-2.06282500	0.29091200	0.18178900
I	0.04376000	-2.52422900	-1.26397900
C	1.87659200	1.37707000	-0.02429700
C	1.18221400	1.93125600	1.07773800
C	1.69868300	1.95860100	-1.31404500
C	0.34756400	3.04550000	0.92778000
H	1.41530200	1.53855500	2.06898900
C	0.87282200	3.07538700	-1.43749500
C	0.21186800	3.60986700	-0.33137500
H	-0.16395500	3.46728300	1.78885200
H	0.74267900	3.52955000	-2.41875400
H	-0.41880800	4.48520600	-0.46980500
N	2.29448600	1.38224300	-2.41328000
H	3.11125900	0.81088100	-2.24139900
H	2.37520000	1.96211100	-3.23689000
C	2.88417000	0.29749200	0.23775200
C	2.28868000	-0.82799600	0.65963000
C	4.32061800	0.64596800	0.13563400
C	4.79910700	1.80798500	0.75340200
C	5.21398000	-0.13831000	-0.60427900
C	6.14218900	2.15501000	0.66613100
H	4.10821300	2.43002700	1.32184300
C	6.55742900	0.21232400	-0.69677800
H	4.83989500	-1.02138400	-1.12133300
C	7.02626300	1.35609900	-0.05660500
H	6.50223200	3.05211500	1.16476800
H	7.23733900	-0.40610800	-1.27817600
C	-2.79195800	1.07734200	1.66931300
C	-4.15312300	1.40219800	1.73121900
C	-1.98826100	1.29580900	2.79051800
C	-4.68942400	1.96216200	2.88441600
H	-4.79653600	1.21215400	0.87227300
C	-2.52781100	1.84880100	3.94968200
H	-0.93252700	1.02714600	2.75348900
C	-3.87606200	2.18748700	3.99386400
H	-5.74565300	2.21753500	2.92118300
H	-1.89370800	2.01262300	4.81752200
H	-4.29841900	2.62062500	4.89746800
C	-3.25443700	-1.07732300	-0.08716400
C	-4.14079600	-1.14083200	-1.16158600
C	-3.23226900	-2.11971100	0.84723300
C	-4.99116000	-2.23651800	-1.30264800
H	-4.17000100	-0.33600200	-1.89385400
C	-4.08709400	-3.20526200	0.71140300
H	-2.52947200	-2.08229500	1.68190000
C	-4.96603500	-3.26733700	-0.36975600
H	-5.67779900	-2.27944000	-2.14493600
H	-4.06327200	-4.00912100	1.44335900
H	-5.63116800	-4.12018500	-0.48199200
C	-2.35613800	1.44693600	-1.20393100
C	-2.92396600	2.71323800	-1.05556100
C	-1.89117400	1.05142200	-2.46587700

C	-3.03691200	3.56526500	-2.15260000
H	-3.27226700	3.04541800	-0.07938600
C	-2.01562400	1.89767100	-3.56041100
H	-1.42970600	0.06992000	-2.58800700
C	-2.58687300	3.15952000	-3.40422000
H	-3.47832100	4.55096600	-2.02402300
H	-1.65870000	1.57494200	-4.53566200
H	-2.67736700	3.82620100	-4.25849600
C	2.79016300	-2.03301400	1.43147100
C	1.64824600	-2.65213900	2.24839800
H	0.87786200	-3.08642100	1.60128500
H	2.04613100	-3.44654600	2.89377800
H	1.17020900	-1.89982100	2.89274400
C	3.85333200	-1.54898500	2.43144300
H	4.73991300	-1.15148800	1.92635400
H	3.44812200	-0.76313400	3.08304100
H	4.16865600	-2.38990100	3.06296100
C	3.40248100	-3.11018400	0.53156300
H	3.69762200	-3.97389900	1.14302400
H	2.68684600	-3.45320700	-0.22325400
H	4.29818900	-2.73983800	0.02046000
H	8.07646500	1.62917000	-0.12590800

TS2 complex of (3,3-dimethylbut-1-yn-1-yl)benzene
Energy = -1208589.440539 kcal/mol
Electronic Energy + Thermal Free Energy Correction (353.150 K) = -1208272.383460 kcal/mol
Imaginary frequency = -300.22 cm^{-1}
Symmetry c1

Pd	-0.55666900	0.05568400	-0.11921500
P	1.80998100	-0.35253000	-0.01932600
I	-0.99170200	-2.65044900	-0.43675600
C	-0.34708900	2.11724000	0.17882600
C	0.41101600	2.87675300	-0.72241500
C	-0.55800700	2.61077900	1.48636700
C	0.88374800	4.13965800	-0.39264100
H	0.63730200	2.46164300	-1.70389100
C	-0.07577400	3.89219600	1.80826600
C	0.62626300	4.64677100	0.88244500
H	1.46538400	4.71106200	-1.11196500
H	-0.24690000	4.27680900	2.81349400
H	0.99405500	5.63106900	1.16424300
N	-1.25272100	1.88202100	2.43828000
H	-1.14388100	0.87781000	2.37904400
H	-1.15911900	2.22016000	3.38709900
C	-2.65126000	0.48349800	-0.04463600
C	-2.29606800	1.58281500	-0.56198700
C	-3.69290300	-0.40973900	0.40767700
C	-4.00803400	-0.48895100	1.77029600
C	-4.41245100	-1.18695500	-0.51071500
C	-5.03186600	-1.32371400	2.20294900
H	-3.44950500	0.11929000	2.47912300
C	-5.43465900	-2.01773700	-0.07051700
H	-4.15630800	-1.13484900	-1.56715300
C	-5.74613300	-2.09094400	1.28596100
H	-5.27378800	-1.37310000	3.26197700
H	-5.99180100	-2.61245900	-0.79045200
C	2.94188500	1.08879800	-0.00495700
C	3.67745700	1.48830200	-1.12209600
C	3.02113100	1.84170900	1.17215500
C	4.48350800	2.62300800	-1.06075200



H	3.63273500	0.91033200	-2.04305300
C	3.82326900	2.97297800	1.22997200
H	2.44611900	1.54057800	2.04820700
C	4.55803000	3.36546600	0.11260900
H	5.05933100	2.92074000	-1.93397400
H	3.87165500	3.55355400	2.14848000
H	5.18810700	4.25061500	0.15791100
C	2.36688800	-1.36459700	-1.43788700
C	3.13296800	-2.52361100	-1.30657900
C	1.92826800	-0.97503300	-2.70977800
C	3.45758700	-3.27941500	-2.43080900
H	3.46608600	-2.85446400	-0.32507400
C	2.26568200	-1.72211800	-3.83164800
H	1.29921000	-0.08998100	-2.81813500
C	3.02776400	-2.88044000	-3.69209100
H	4.04683700	-4.18608200	-2.31681900
H	1.92104500	-1.40822500	-4.81389400
H	3.28150400	-3.47370700	-4.56722300
C	2.33306200	-1.22506900	1.50173400
C	3.69285600	-1.40777400	1.78765200
C	1.37825900	-1.66539000	2.42111300
C	4.08459600	-2.04350600	2.95933100
H	4.44767100	-1.04094700	1.09275200
C	1.77288500	-2.29281700	3.60049100
H	0.31984800	-1.52380000	2.20407000
C	3.12412900	-2.48688600	3.86683400
H	5.14176300	-2.18693700	3.16887600
H	1.02153800	-2.62986500	4.31034200
H	3.43243600	-2.97875600	4.78626400
C	-2.82240700	2.73235500	-1.37957100
H	-6.54546100	-2.74429000	1.62707100
C	-2.74901800	4.06521800	-0.63723500
H	-3.22340800	3.98808500	0.34928900
H	-1.71984700	4.40852600	-0.50367600
H	-3.28913900	4.82455500	-1.21661500
C	-2.14559800	2.82668600	-2.74678200
H	-2.70929400	3.52667100	-3.37602500
H	-1.12030800	3.19831400	-2.67548500
H	-2.13329900	1.85009300	-3.24693500
C	-4.30314100	2.37932100	-1.60028500
H	-4.41017200	1.44498100	-2.16358700
H	-4.83297800	2.27190900	-0.64632000
H	-4.78214800	3.18369700	-2.17186000

INT2 complex of (3,3-dimethylbut-1-yn-1-yl)benzene

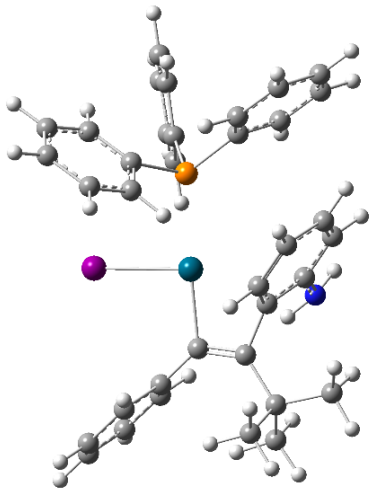
Energy = -1208625.714325 kcal/mol

Electronic Energy + Thermal Free Energy Correction (353.150 K) = -1208305.613199 kcal/mol

Symmetry c1

Pd	-0.52491800	0.05817800	-0.05449300
P	1.96358000	-0.13552800	-0.01478200
I	-0.70726200	-2.60189300	0.05889600
C	-1.21747500	2.23650300	-0.19563800
C	-0.60244100	2.39989700	-1.46340600
C	-0.60836500	2.84410600	0.94690100
C	0.54965900	3.15426500	-1.61927200
H	-1.09547600	1.94834800	-2.32359200
C	0.54969600	3.61298400	0.76547900
C	1.10239100	3.77243300	-0.49578600
H	1.01195300	3.26619300	-2.59625000
H	1.01518500	4.08449200	1.62975200

H	2.00783200	4.36744600	-0.59959200
N	-1.21075400	2.74583100	2.17399600
H	-1.85352100	1.97519300	2.30527100
H	-0.65166500	2.96924000	2.98522100
C	-2.57238600	0.35565000	-0.05012300
C	-2.61828800	1.68582600	-0.10766200
C	-3.61251000	-0.66282700	0.03591500
C	-4.08542500	-1.09315100	1.28397800
C	-4.13204900	-1.25679800	-1.12197700
C	-5.05800400	-2.08170600	1.36972900
H	-3.67601200	-0.63894400	2.18671300
C	-5.10754200	-2.24371000	-1.03416600
H	-3.75145800	-0.94128500	-2.09303800
C	-5.57167900	-2.66235800	0.21103400
H	-5.41792100	-2.40224700	2.34496500
H	-5.50486900	-2.69112500	-1.94262700
C	3.14642100	1.25827100	-0.24761500
C	3.69820800	1.57658500	-1.49128200
C	3.46426300	2.05964700	0.85545500
C	4.55415100	2.66651800	-1.62667200
H	3.47022800	0.96835600	-2.36452600
C	4.32541900	3.14228800	0.72190500
H	3.03789100	1.83246400	1.83212000
C	4.87242100	3.45020600	-0.52191400
H	4.98054500	2.89571900	-2.60054100
H	4.56863400	3.74812100	1.59180700
H	5.54746400	4.29602100	-0.62770900
C	2.41872100	-1.29529200	-1.35845500
C	3.16907700	-2.45664800	-1.17256700
C	1.89838900	-1.01655000	-2.62890400
C	3.40601300	-3.31810200	-2.24124800
H	3.55533300	-2.70718900	-0.18687600
C	2.14915800	-1.86805100	-3.69821300
H	1.27898200	-0.13006100	-2.77712900
C	2.90171400	-3.02484100	-3.50420400
H	3.98570900	-4.22430300	-2.08219700
H	1.74471800	-1.63684700	-4.68074900
H	3.08859400	-3.69935800	-4.33625400
C	2.59733700	-0.84569500	1.55123400
C	3.96119100	-1.09664500	1.75315500
C	1.70438700	-1.06370200	2.60347200
C	4.41290000	-1.58656700	2.97253300
H	4.67651600	-0.89570400	0.95644600
C	2.15877800	-1.54469400	3.82913000
H	0.64425200	-0.85839400	2.45359800
C	3.51138300	-1.81222100	4.01155700
H	5.47236700	-1.78428800	3.11647000
H	1.45382500	-1.70682700	4.64083100
H	3.86838900	-2.18925000	4.96705000
C	-3.83058500	2.62257800	-0.19197200
H	-6.33129900	-3.43742700	0.27961000
C	-3.39503300	4.08747500	-0.12503600
H	-2.92279100	4.32769200	0.83544700
H	-2.69189200	4.34419200	-0.92844100
H	-4.27539900	4.73240400	-0.23859400
C	-4.53015500	2.38401000	-1.53556900
H	-5.39106100	3.05837700	-1.63990400
H	-3.84831800	2.57430200	-2.37491700
H	-4.89288600	1.35237000	-1.61637500
C	-4.81573000	2.34962400	0.94694000



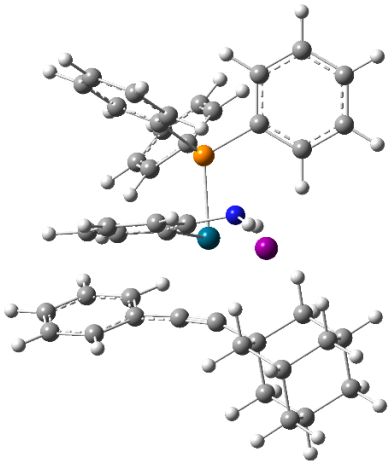
H	-5.20893500	1.32792400	0.90583900
H	-4.34031800	2.49314700	1.92613600
H	-5.66595000	3.04162900	0.88052700

ADS complex of 1-(phenylethynyl)adamantane

Energy = -1354257.372398 kcal/mol

Electronic Energy + Thermal Free Energy Correction (353.150 K) = -1353871.153159 kcal/mol

Symmetry c1



Pd	-0.12045300	0.17401200	-0.12973100
P	2.03415700	-0.68126100	0.15240900
I	-0.23073000	-0.58960500	-2.84967600
C	-0.03748000	0.72119500	1.83754500
C	0.43923300	1.98738100	2.15775400
C	-0.48130300	-0.13587300	2.85763600
C	0.43770800	2.44927700	3.47574600
H	0.82228000	2.63809600	1.36962000
C	-0.50501000	0.34408100	4.17597400
C	-0.04963200	1.62013400	4.48164700
H	0.81215500	3.44471300	3.70485800
H	-0.86553300	-0.31529600	4.96620900
H	-0.06965500	1.96245300	5.51430300
N	-0.81300100	-1.46944000	2.60963600
H	-1.05713600	-1.67440000	1.64824400
H	-1.46630100	-1.88156000	3.26424700
C	-1.72716000	1.91326900	-0.48932700
C	-2.41148500	0.91704200	-0.25555000
C	-1.02211500	3.14396700	-0.68553500
C	-1.23902900	4.20438300	0.20813600
C	-0.10246600	3.29945700	-1.73400600
C	-0.54104600	5.39529000	0.05697200
H	-1.94785400	4.07450100	1.02301000
C	0.59679800	4.49141300	-1.87106800
H	0.06293200	2.47097600	-2.42153500
C	0.38189000	5.53870900	-0.97691500
H	-0.71172100	6.21167000	0.75403800
H	1.31334000	4.60421700	-2.68139100
C	2.97530500	-0.23452300	1.65657200
C	3.98187600	0.73286600	1.63950800
C	2.62611100	-0.84210500	2.86896100
C	4.62580100	1.09368900	2.82108700
H	4.27333300	1.20805300	0.70548100
C	3.27553600	-0.48393200	4.04269300
H	1.83472900	-1.59068500	2.89493700
C	4.27318200	0.48937300	4.02232600
H	5.40969300	1.84676000	2.79636700
H	2.99192200	-0.95796200	4.97958100
H	4.77670900	0.77260200	4.94357900
C	3.04952500	-0.04848900	-1.22791600
C	3.84240600	-0.88176300	-2.01741000
C	2.98142300	1.31898100	-1.52073100
C	4.54995200	-0.35374000	-3.09496400
H	3.89483300	-1.94839100	-1.80846500
C	3.69691300	1.84410400	-2.58851600
H	2.34384200	1.97375900	-0.92421500
C	4.47792300	1.00552400	-3.38223600
H	5.15823100	-1.01019100	-3.71233300
H	3.63786900	2.90768300	-2.80825300
H	5.02934000	1.41360100	-4.22571200
C	2.14110400	-2.50175500	0.10841500
C	1.04389400	-3.26341200	-0.30139900

C	3.32620200	-3.14773700	0.48391700
C	1.13074700	-4.65204200	-0.34064400
H	0.12306200	-2.76376100	-0.60087100
C	3.41153100	-4.53409900	0.43634900
H	4.18436500	-2.56462600	0.81530100
C	2.31312900	-5.28673300	0.02634000
H	0.27090300	-5.23741800	-0.65652000
H	4.33572800	-5.02813200	0.72535200
H	2.37992300	-6.37144700	-0.00354200
H	0.93307100	6.46932300	-1.08720800
C	-3.95939700	0.07624100	1.45918600
H	-4.14427600	1.12226500	1.74642700
H	-3.12238900	-0.28827000	2.07240500
C	-3.56118300	0.02612700	-0.03222900
C	-5.20925000	-0.77518400	1.69295300
H	-5.47511800	-0.73048600	2.75822200
C	-6.36512700	-0.23070500	0.84866600
H	-6.59098100	0.80550500	1.14145300
H	-7.27362800	-0.82388600	1.02895600
C	-4.74026900	0.56145800	-0.87845900
H	-4.45518000	0.54132500	-1.94137900
H	-4.92913900	1.61150200	-0.61054100
C	-5.98954700	-0.28863800	-0.63484600
H	-6.81337300	0.10964600	-1.24318700
C	-5.70555500	-1.73919700	-1.03214300
H	-6.60395700	-2.35416700	-0.87546100
H	-5.45542600	-1.79707900	-2.10186100
C	-3.29711300	-1.43423500	-0.43914500
H	-2.45049000	-1.83414300	0.13961700
H	-2.99990500	-1.47194500	-1.49702100
C	-4.91785900	-2.22423000	1.29326700
H	-4.09427400	-2.62459400	1.90484300
H	-5.79924800	-2.85330600	1.48597800
C	-4.54647000	-2.28179600	-0.19130100
H	-4.33264300	-3.32001700	-0.48054500

TS1 complex of 1-(phenylethynyl)adamantane

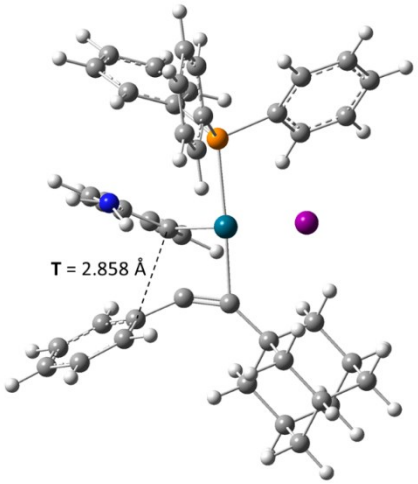
Energy = -1354241.313815 kcal/mol

Electronic Energy + Thermal Free Energy Correction (353.150 K) = -1353855.257101 kcal/mol

Imaginary frequency = -284.60 cm^{-1}

Symmetry c1

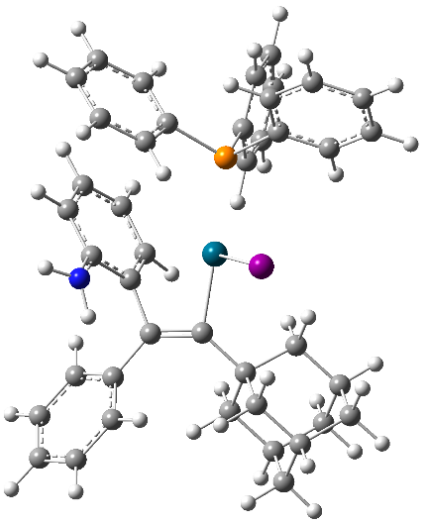
Pd	-0.10338000	-0.06353700	0.04399500
P	2.31078500	-0.38057500	-0.01825200
I	-0.35570200	-2.64420000	1.01928600
C	0.08794000	1.81465700	-0.83583900
C	-0.26531100	1.90388300	-2.18416600
C	0.89808900	2.80344600	-0.24579300
C	0.21534700	2.94109500	-2.97985900
H	-0.94415500	1.16075500	-2.60442400
C	1.36342200	3.85082800	-1.05412900
C	1.03346100	3.91175200	-2.40072700
H	-0.05902600	2.99859000	-4.03020600
H	2.00489000	4.61133200	-0.60892800
H	1.41064800	4.73546000	-3.00316200
N	1.26508600	2.71670500	1.08225500
H	0.63883000	2.19346200	1.68084500
H	1.60184800	3.57059000	1.50671700
C	-1.77510200	1.51706900	0.19580000
C	-2.19410600	0.33820000	-0.01937000
C	-2.03620000	2.81195700	0.79518400



C	-2.03438400	3.99684700	0.04946900
C	-2.38871300	2.84583800	2.15130000
C	-2.38614100	5.19532100	0.65626400
H	-1.76230500	3.96413600	-1.00389000
C	-2.73130800	4.05078100	2.75400800
H	-2.38972600	1.91611200	2.71867100
C	-2.72959100	5.22563600	2.00735900
H	-2.39315600	6.11256100	0.07256300
H	-3.00105700	4.07131100	3.80687500
C	3.39799400	0.84195700	-0.86313900
C	3.55516500	0.81996500	-2.25231900
C	4.04251400	1.84370500	-0.12824800
C	4.33565500	1.77856800	-2.89191500
H	3.07490000	0.04612800	-2.84778300
C	4.82746600	2.79592600	-0.76838700
H	3.92297000	1.88846800	0.95134000
C	4.97478500	2.76785400	-2.15245300
H	4.44961000	1.74285100	-3.97286500
H	5.32607900	3.56389200	-0.18132100
H	5.58927900	3.51289500	-2.65236300
C	2.59408800	-1.91144300	-0.99033800
C	3.46642300	-2.92956900	-0.60390200
C	1.83881500	-2.07108900	-2.15954600
C	3.58350300	-4.08390500	-1.37503000
H	4.04444600	-2.84128500	0.31323300
C	1.96903100	-3.21517600	-2.93720400
H	1.12088700	-1.29996700	-2.44692100
C	2.84032600	-4.22814300	-2.54194600
H	4.25837800	-4.87507100	-1.05687700
H	1.37828900	-3.32310400	-3.84358100
H	2.93369500	-5.13124900	-3.14012400
C	3.13671000	-0.61786500	1.59608100
C	4.52424200	-0.78527000	1.70079300
C	2.36629700	-0.58108800	2.76109900
C	5.12108500	-0.93655900	2.94701700
H	5.14499400	-0.78261200	0.80590600
C	2.96573500	-0.72739800	4.00909800
H	1.28836400	-0.44282200	2.68084300
C	4.34211000	-0.90967200	4.10167900
H	6.19792900	-1.06835500	3.01758900
H	2.35610900	-0.69595700	4.90880300
H	4.81137800	-1.02367500	5.07603300
H	-2.99767400	6.16874300	2.47749700
C	-3.27321300	-1.48040300	-1.38118300
H	-2.49718400	-2.20215800	-1.09066500
H	-2.92287900	-0.97509800	-2.29610100
C	-3.44081300	-0.43582500	-0.26533100
C	-4.60337100	-2.19352600	-1.63477000
H	-4.46296500	-2.94497600	-2.42457400
C	-5.05893400	-2.88275700	-0.34422500
H	-4.31015700	-3.62564900	-0.02872700
H	-6.00006600	-3.42488800	-0.51990500
C	-3.93238000	-1.11910200	1.02523100
H	-4.05759800	-0.35228900	1.80658000
H	-3.17271900	-1.82757300	1.38050900
C	-5.25791100	-1.83838100	0.75877200
H	-5.58652100	-2.33442500	1.68293900
C	-6.31318600	-0.82200600	0.31480100
H	-7.27526100	-1.32698700	0.14117400
H	-6.47812300	-0.07687300	1.10765500

C	-4.51775500	0.58181200	-0.70997700
H	-4.16967500	1.09867000	-1.61838600
H	-4.63738600	1.34655500	0.07334500
C	-5.65954600	-1.17406800	-2.07197700
H	-5.34701700	-0.68470200	-3.00673900
H	-6.61421300	-1.68167500	-2.27535500
C	-5.84726800	-0.13001300	-0.96899300
H	-6.59416500	0.61285400	-1.28327000

INT1 complex of 1-(phenylethynyl)adamantane
Energy = -1354269.736835 kcal/mol
Electronic Energy + Thermal Free Energy Correction (353.150 K) = -1353881.542198 kcal/mol
Symmetry c1



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P	-2.49233200	-0.10474900	0.28043700
I	0.01951500	-1.48058300	-2.22252900
C	0.91009800	2.13410800	0.28965700
C	0.30267400	2.03690900	1.56511400
C	0.35634100	3.03111000	-0.67169800
C	-0.80642600	2.82026100	1.90490400
H	0.80231300	1.42176600	2.31545900
C	-0.73673600	3.81514300	-0.30516700
C	-1.30305100	3.71171300	0.96576800
H	-1.25344000	2.73782600	2.89221000
H	-1.15673600	4.50966200	-1.03159900
H	-2.15312000	4.34366800	1.21360100
N	0.87405100	3.06749500	-1.94559000
H	1.82170900	2.73411500	-2.06478600
H	0.65749100	3.88343100	-2.50065300
C	2.20755000	1.41563000	0.06390600
C	2.01909500	0.08652600	0.07732900
C	3.44283200	2.22617800	-0.01977500
C	3.63419200	3.30282800	0.85602700
C	4.40869000	1.98454400	-1.00510100
C	4.77653900	4.09043600	0.77240500
H	2.88166400	3.50995300	1.61635100
C	5.55084000	2.77356400	-1.08979500
H	4.24109100	1.18307300	-1.72296300
C	5.74081900	3.82585800	-0.19790700
H	4.91611300	4.91419700	1.46876600
H	6.28902500	2.57386600	-1.86309800
C	-3.13734300	-0.15362400	1.99624300
C	-4.50604300	-0.29489700	2.25810700
C	-2.23952900	-0.12350300	3.06596000
C	-4.96652400	-0.37441700	3.56665300
H	-5.21462100	-0.34630000	1.43161100
C	-2.70048800	-0.21110800	4.37754200
H	-1.17105600	-0.03536000	2.86823100
C	-4.06336300	-0.33041900	4.62772400
H	-6.03145400	-0.47809500	3.76019500
H	-1.99263800	-0.18899000	5.20255700
H	-4.42483600	-0.39731100	5.65105900
C	-3.30526300	-1.59147300	-0.42390100
C	-4.31866500	-1.54411100	-1.38077100
C	-2.84781600	-2.83488100	0.02884900
C	-4.86275400	-2.72463700	-1.88415100
H	-4.68599500	-0.58398100	-1.73916000
C	-3.39709700	-4.01015100	-0.46624900
H	-2.04275800	-2.88032600	0.76477100
C	-4.40410700	-3.95641900	-1.42983000

H	-5.65068600	-2.67749100	-2.63227200
H	-3.03503900	-4.97055400	-0.10677800
H	-4.82914100	-4.87639800	-1.82419000
C	-3.31239600	1.30854800	-0.54031800
C	-4.14428700	2.21612600	0.11761800
C	-2.98945400	1.53111300	-1.88637400
C	-4.65966500	3.31755800	-0.56269200
H	-4.38383200	2.07292200	1.16966900
C	-3.51211600	2.62400600	-2.56514200
H	-2.32067700	0.83986500	-2.40208100
C	-4.34851700	3.52166900	-1.90251400
H	-5.30538900	4.01851100	-0.03881300
H	-3.26179700	2.78082500	-3.61175600
H	-4.75367900	4.38093500	-2.43164000
H	6.63280000	4.44417800	-0.26374100
C	3.98591700	-0.65773000	1.39599400
H	4.59646500	0.15914100	0.98759400
H	3.47439800	-0.26316000	2.28910200
C	4.88976900	-1.83560200	1.77035300
H	5.63652500	-1.48770600	2.49886900
C	2.91952800	-1.08992000	0.35726200
C	3.65030100	-1.63678000	-0.88596300
H	4.25818300	-0.83809300	-1.33373200
H	2.91470500	-1.94719900	-1.63977600
C	5.59649400	-2.35152300	0.51425500
H	6.26604000	-3.18502600	0.77467800
H	6.22110200	-1.55686500	0.07826000
C	4.55119800	-2.81473600	-0.50367100
H	5.05420000	-3.18421400	-1.40878500
C	3.70347000	-3.93362200	0.10662600
H	2.95428300	-4.27973400	-0.62230500
H	4.33904900	-4.79702900	0.35444100
C	4.05405100	-2.96031300	2.38359700
H	3.56132800	-2.60761100	3.30235600
H	4.70270200	-3.80304600	2.66647200
C	2.10416100	-2.23923600	0.99602100
H	1.58582700	-1.85522300	1.89251200
H	1.32626200	-2.57017700	0.29355000
C	3.00592500	-3.41691400	1.36785600
H	2.38833000	-4.21546500	1.80325200

TS2 complex of 1-(phenylethynyl)adamantane

Energy = -1354239.052273 kcal/mol

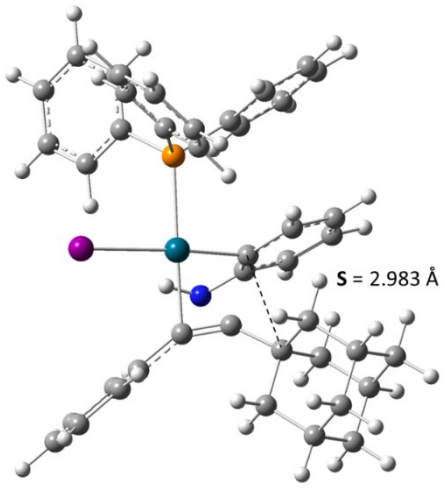
Electronic Energy + Thermal Free Energy Correction (353.150 K) = -1353853.576004 kcal/mol

Imaginary frequency = -312.58 cm^{-1}

Symmetry c1

Pd	0.11598700	0.42954500	-0.04516800
P	2.29290900	-0.56779500	0.15269300
I	1.18311900	2.82433000	0.81138500
C	-0.78210300	-1.34435000	-0.70936300
C	-0.76448400	-2.46887900	0.12850500
C	-0.93021100	-1.52933700	-2.10332900
C	-0.97368700	-3.74981000	-0.36428800
H	-0.57138600	-2.33055400	1.19196500
C	-1.14475300	-2.83142000	-2.59112400
C	-1.17240000	-3.92098000	-1.73588500
H	-0.94893800	-4.60553800	0.30629400
H	-1.27018100	-2.97246100	-3.66449700
H	-1.32936600	-4.91648000	-2.14579400
N	-0.90482900	-0.46336800	-2.98559900

H	-0.33582100	0.32305200	-2.70117900
H	-0.77380500	-0.70675200	-3.95823700
C	-1.79605000	1.28086300	-0.43186500
C	-2.25560100	0.13024500	-0.16590800
C	-2.03777900	2.66612100	-0.77140200
C	-1.83022400	3.11221100	-2.08308200
C	-2.48661700	3.57188100	0.19931600
C	-2.07347500	4.43911400	-2.41688700
H	-1.47965900	2.40708400	-2.83478700
C	-2.72738900	4.89698600	-0.14158700
H	-2.63150600	3.22713100	1.22160100
C	-2.51901100	5.33534500	-1.44787900
H	-1.91322100	4.77520800	-3.43856700
H	-3.07870500	5.59216800	0.61721700
C	2.44715500	-2.38187100	-0.04738900
C	2.68099400	-3.24684000	1.02356300
C	2.28154300	-2.91126800	-1.33213300
C	2.75068200	-4.62169400	0.80944400
H	2.81859300	-2.84904000	2.02738700
C	2.35250900	-4.28137400	-1.54240800
H	2.08477800	-2.24497800	-2.17264700
C	2.58700700	-5.14039700	-0.47049100
H	2.94004800	-5.28732900	1.64833900
H	2.21636100	-4.68145500	-2.54470700
H	2.64314600	-6.21389600	-0.63462600
C	3.05060900	-0.22318500	1.78077200
C	4.34089600	0.28208600	1.94480800
C	2.24662900	-0.42799200	2.90889400
C	4.81989500	0.57516800	3.21944900
H	4.97307400	0.46677200	1.07868000
C	2.73231100	-0.15162500	4.18085700
H	1.22464200	-0.78971800	2.78509100
C	4.02052800	0.35645300	4.33691900
H	5.82287800	0.97853300	3.33694600
H	2.10071300	-0.31923700	5.04973800
H	4.39832700	0.58632700	5.33021900
C	3.46519700	0.02836500	-1.12153000
C	4.72760000	-0.56447100	-1.25748000
C	3.09166400	1.04558900	-2.00367700
C	5.60869700	-0.12593000	-2.23811500
H	5.01949700	-1.37971400	-0.59627300
C	3.97202600	1.47657100	-2.99353000
H	2.11022000	1.50922500	-1.90345500
C	5.23102400	0.89632000	-3.10692600
H	6.58875600	-0.58745000	-2.33055300
H	3.67072700	2.26758800	-3.67587100
H	5.91887000	1.23568800	-3.87769800
H	-2.70570800	6.37387600	-1.71007700
C	-5.13377200	-2.86030200	1.13181800
H	-4.37491900	-3.65773300	1.10935200
H	-6.07841600	-3.31979100	1.45841700
C	-5.29864300	-2.25719600	-0.26649800
H	-5.59849300	-3.04269200	-0.97424900
C	-4.71657200	-1.76612300	2.11953200
H	-4.60070700	-2.19747000	3.12361000
C	-3.37448800	-1.17289500	1.68004600
H	-2.60439200	-1.95245400	1.69484000
H	-3.05311800	-0.37919500	2.37241400
C	-3.96016600	-1.66872000	-0.72262800
H	-4.05783200	-1.22250500	-1.72474700



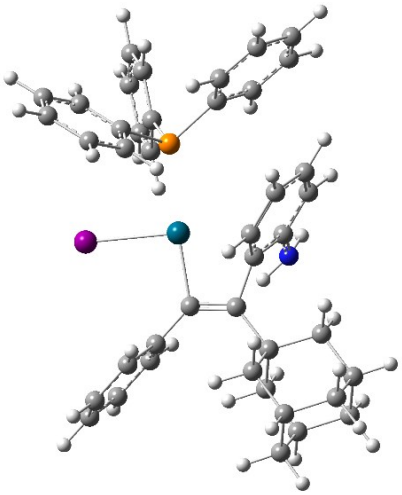
H	-3.21263500	-2.46540600	-0.78823200
C	-3.49791100	-0.58525100	0.26373200
C	-4.58413000	0.52013900	0.30248000
H	-4.27147200	1.31426400	0.99640400
H	-4.67503000	0.97582400	-0.69511900
C	-6.36150700	-1.15839900	-0.23289100
H	-7.33113600	-1.57589200	0.07667300
H	-6.49710800	-0.73297300	-1.23847300
C	-5.78036300	-0.66665200	2.14710700
H	-6.74303200	-1.08048600	2.48180300
H	-5.49573600	0.11574500	2.86640500
C	-5.92668500	-0.06735400	0.74708000
H	-6.67254200	0.73979400	0.76337300

INT2 complex of 1-(phenylethynyl)adamantane

Energy = -1354274.856681 kcal/mol

Electronic Energy + Thermal Free Energy Correction (353.150 K) = -1353887.654135 kcal/mol

Symmetry c1



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P	-2.57522500	0.39806300	0.03818200
I	-0.98205900	-2.86502400	-0.06482800
C	1.25316000	1.46271900	0.09484100
C	0.76218000	1.83085800	1.37329400
C	0.88168300	2.25421600	-1.03707900
C	-0.03815800	2.94953700	1.54934500
H	1.07720000	1.22957100	2.22543000
C	0.09158200	3.39353800	-0.83369100
C	-0.34576200	3.73444900	0.43719300
H	-0.41242400	3.21398200	2.53478700
H	-0.18376400	4.00718000	-1.69023400
H	-0.97227700	4.61643400	0.55703500
N	1.37182600	1.94178600	-2.27855000
H	1.67811600	0.98757000	-2.41909700
H	0.90947500	2.35500900	-3.07614900
C	1.83250000	-0.78167300	-0.03561300
C	2.35868200	0.44277400	-0.01408900
C	2.43043200	-2.11017400	-0.10196000
C	2.68906100	-2.71641100	-1.33983900
C	2.73000600	-2.81893400	1.06913400
C	3.24279000	-3.98935000	-1.40357500
H	2.44782800	-2.17119600	-2.25269200
C	3.28622200	-4.09136500	1.00344000
H	2.51364400	-2.36107000	2.03399800
C	3.54183500	-4.68308700	-0.23203000
H	3.44155000	-4.44339400	-2.37193700
H	3.51925800	-4.62600400	1.92171400
C	-3.14953200	2.14371700	0.17883500
C	-3.58392400	2.71801700	1.37535800
C	-3.12104100	2.93205600	-0.97772800
C	-3.98767000	4.05124100	1.41123400
H	-3.61921200	2.12459400	2.28697800
C	-3.52962800	4.25925500	-0.94327200
H	-2.77535900	2.50355600	-1.91880400
C	-3.96453100	4.82362100	0.25458300
H	-4.33103400	4.48209700	2.34896500
H	-3.50710500	4.85500900	-1.85295100
H	-4.28670100	5.86170300	0.28409900
C	-3.32996200	-0.42096800	1.49309400
C	-4.42844800	-1.27913700	1.42658400
C	-2.68832000	-0.23097700	2.72423300

C	-4.88521200	-1.92507500	2.57297600
H	-4.92168600	-1.46556100	0.47488200
C	-3.15358900	-0.86539500	3.87002800
H	-1.80741700	0.41099900	2.77996100
C	-4.25366700	-1.71752800	3.79492400
H	-5.73853200	-2.59599200	2.50743600
H	-2.65062300	-0.70393800	4.82047000
H	-4.61286400	-2.22350200	4.68780100
C	-3.54471200	-0.11808000	-1.42943200
C	-4.92444100	0.11274500	-1.51186200
C	-2.88133100	-0.66484000	-2.53008700
C	-5.62899300	-0.23723700	-2.65723800
H	-5.44817900	0.58136100	-0.67907200
C	-3.58532400	-1.00223000	-3.68398300
H	-1.80550600	-0.82780800	-2.47750200
C	-4.95962000	-0.79794000	-3.74388100
H	-6.70105300	-0.06305900	-2.70717400
H	-3.05717700	-1.42457000	-4.53540000
H	-5.51148900	-1.06534400	-4.64192100
H	3.97312100	-5.68003400	-0.28240900
C	3.95340200	2.41335800	-0.07918900
H	3.51303600	2.76524400	-1.02424800
H	3.39080100	2.89221100	0.73863500
C	5.42265200	2.83823600	-0.00512900
H	5.48085600	3.93365500	-0.07896200
C	3.82219100	0.88118200	0.01748100
C	4.62725000	0.25294900	-1.13598900
H	4.18674000	0.56029900	-2.09798100
H	4.55528100	-0.84212300	-1.08435400
C	6.19571100	2.20270600	-1.16326900
H	7.25027700	2.51564700	-1.13012800
H	5.78557100	2.54716300	-2.12471000
C	6.09611300	0.67920600	-1.06505300
H	6.64501800	0.21601600	-1.89756500
C	6.69301800	0.21415800	0.26665200
H	6.63936000	-0.88265700	0.34074400
H	7.75651100	0.49127400	0.32057400
C	6.02503900	2.37898500	1.32449000
H	5.49141800	2.84988000	2.16405500
H	7.07717700	2.69424400	1.39162500
C	4.45497700	0.43315800	1.35406400
H	3.88810700	0.87408400	2.19014600
H	4.37203700	-0.65973200	1.44797800
C	5.92483000	0.85567000	1.42605800
H	6.34924700	0.51760300	2.38248400