

Supplementary

A Facile One-Pot Synthesis of New Poly Functionalized Pyrrolotriazoles via a Regioselective Multicomponent Cyclisation and Suzuki–Miyaura Coupling Reactions

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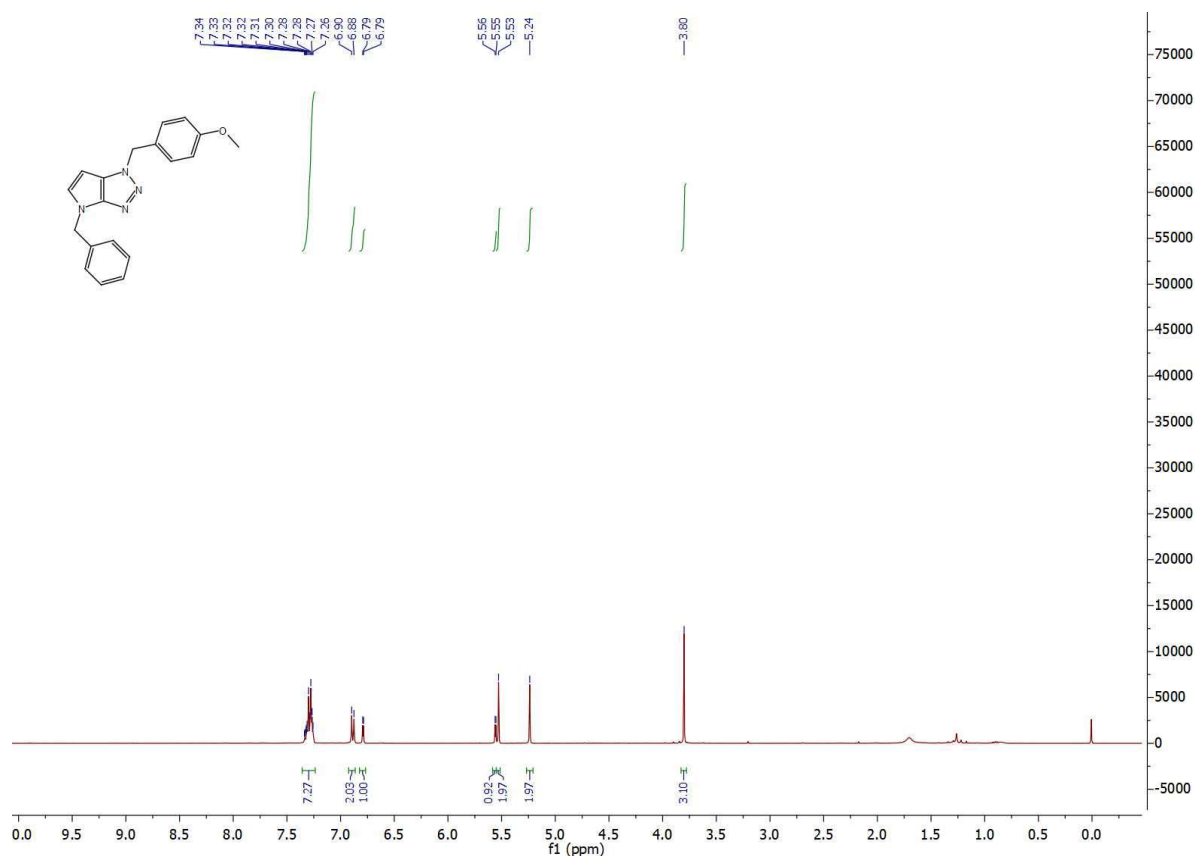
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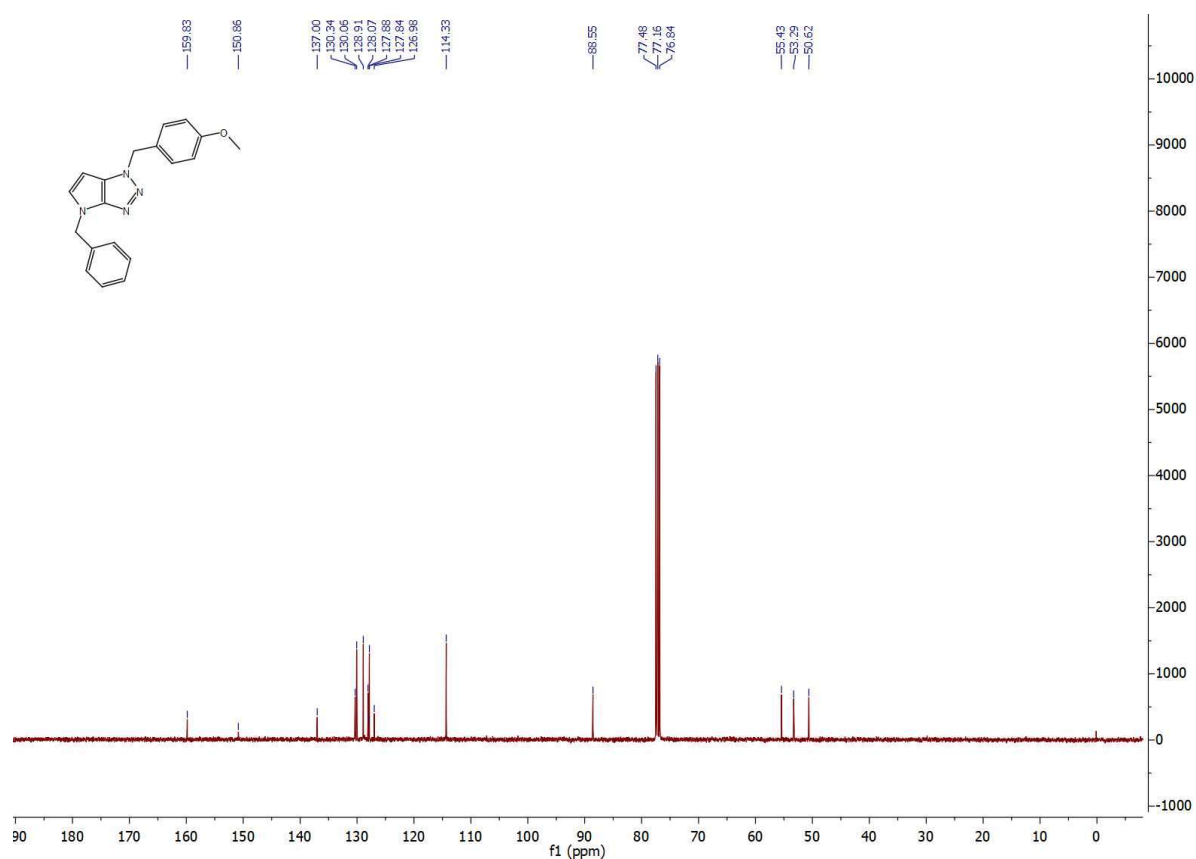
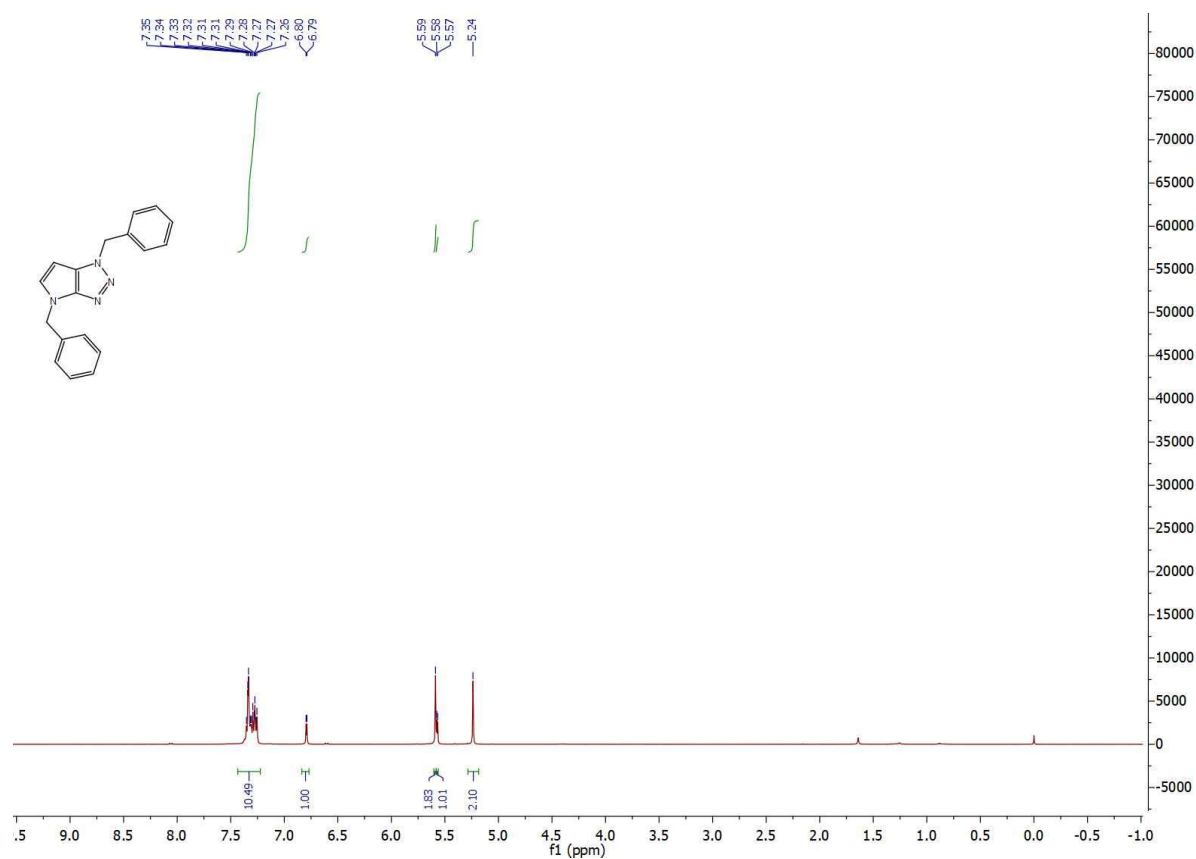


Figure S1. : 4-Benzyl-1-(4-methoxybenzyl)-1,4-dihydropyrrolo[2,3-*d*][1,2,3]triazole (4).



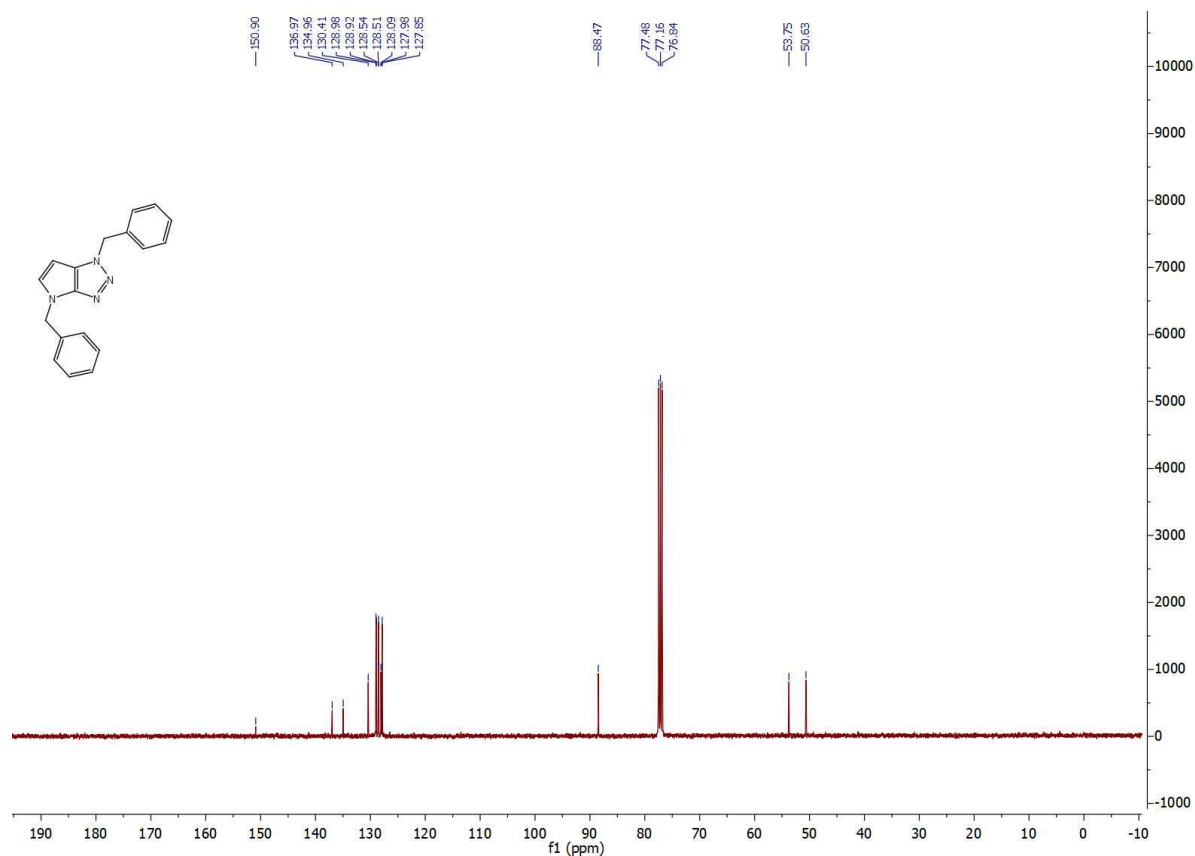
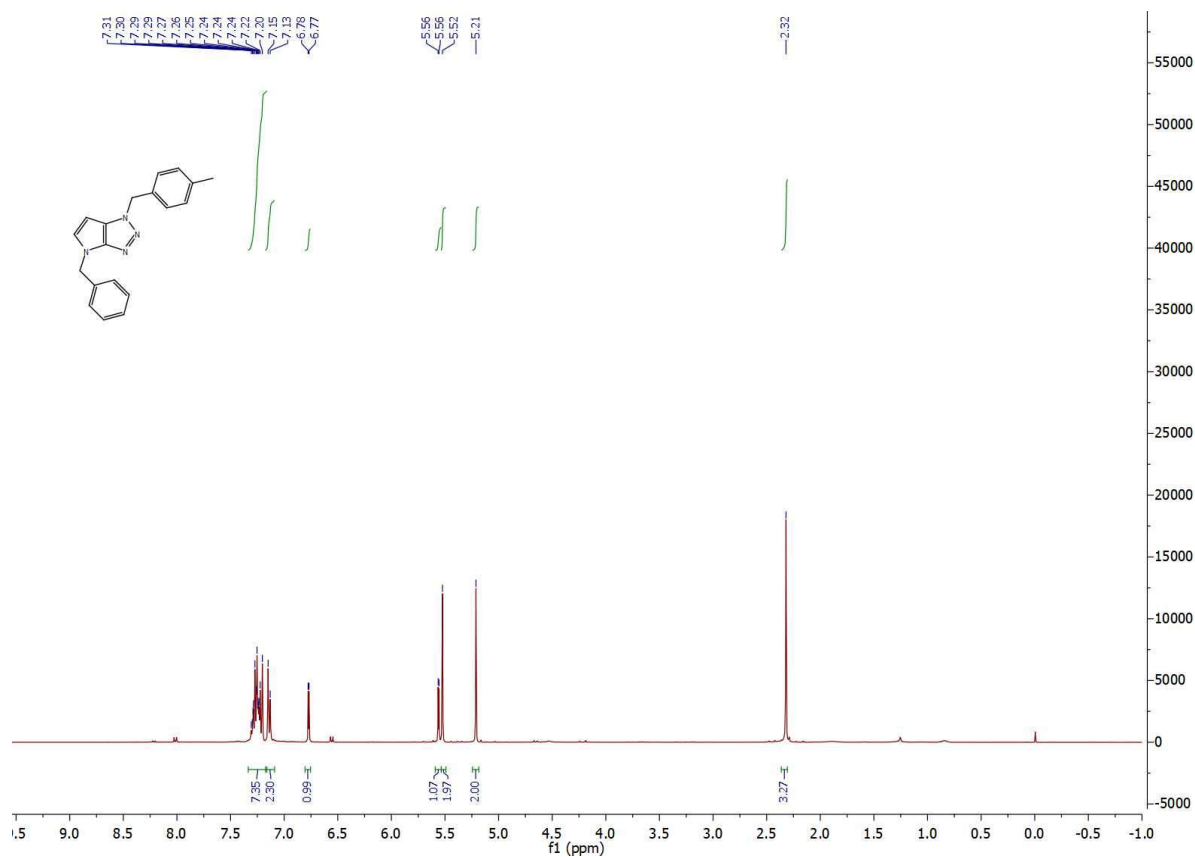


Figure S2. : 1,4-Dibenzyl-1,4-dihydropyrrolo[2,3-d][1,2,3]triazole (5).



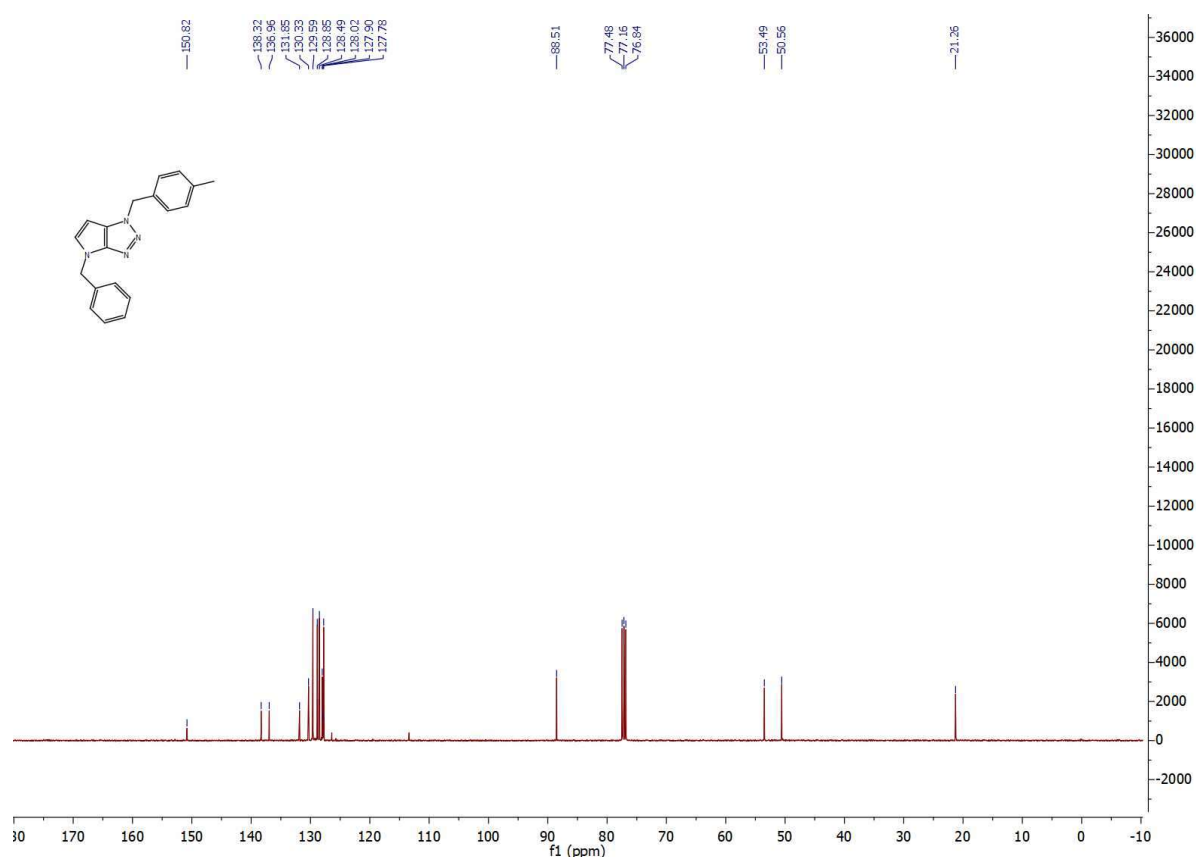
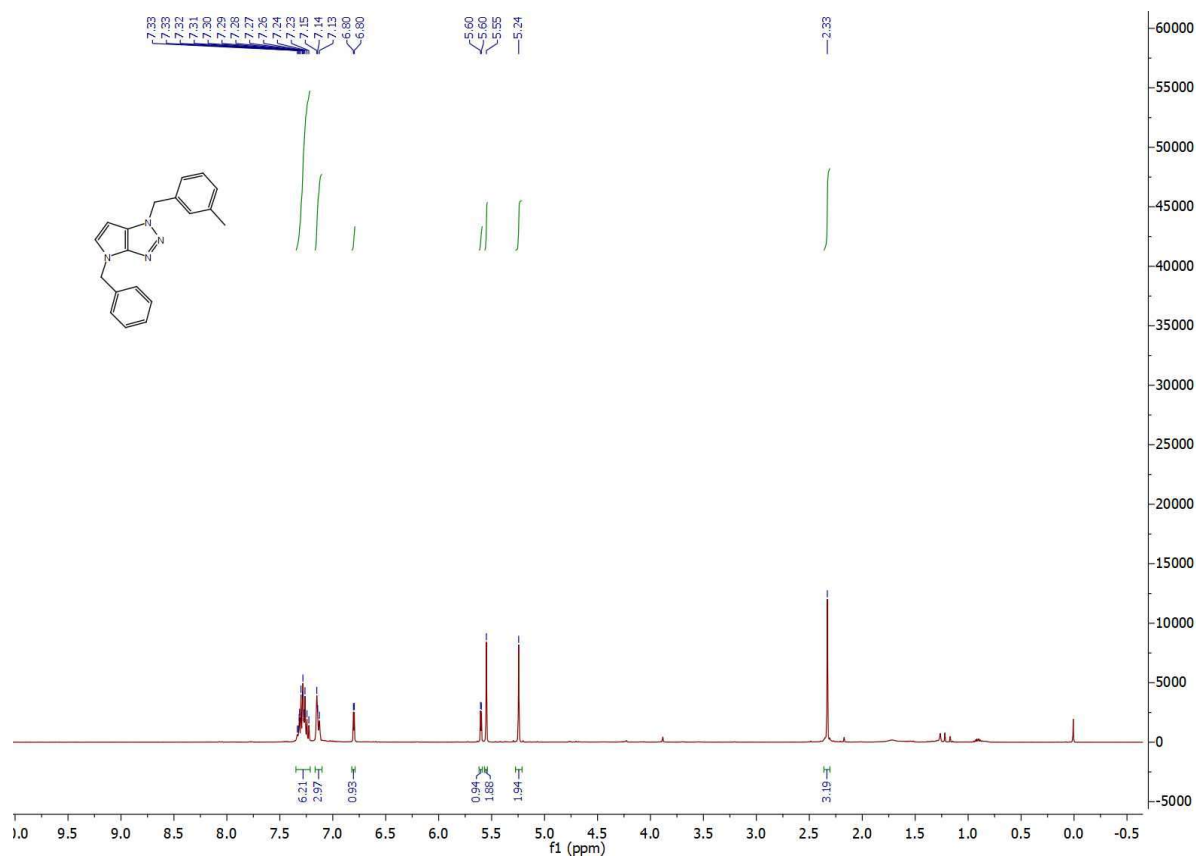


Figure S3. 4-Benzyl-1-(4-methylbenzyl)-1,4-dihydropyrrolo[2,3-d][1,2,3]triazole (6).



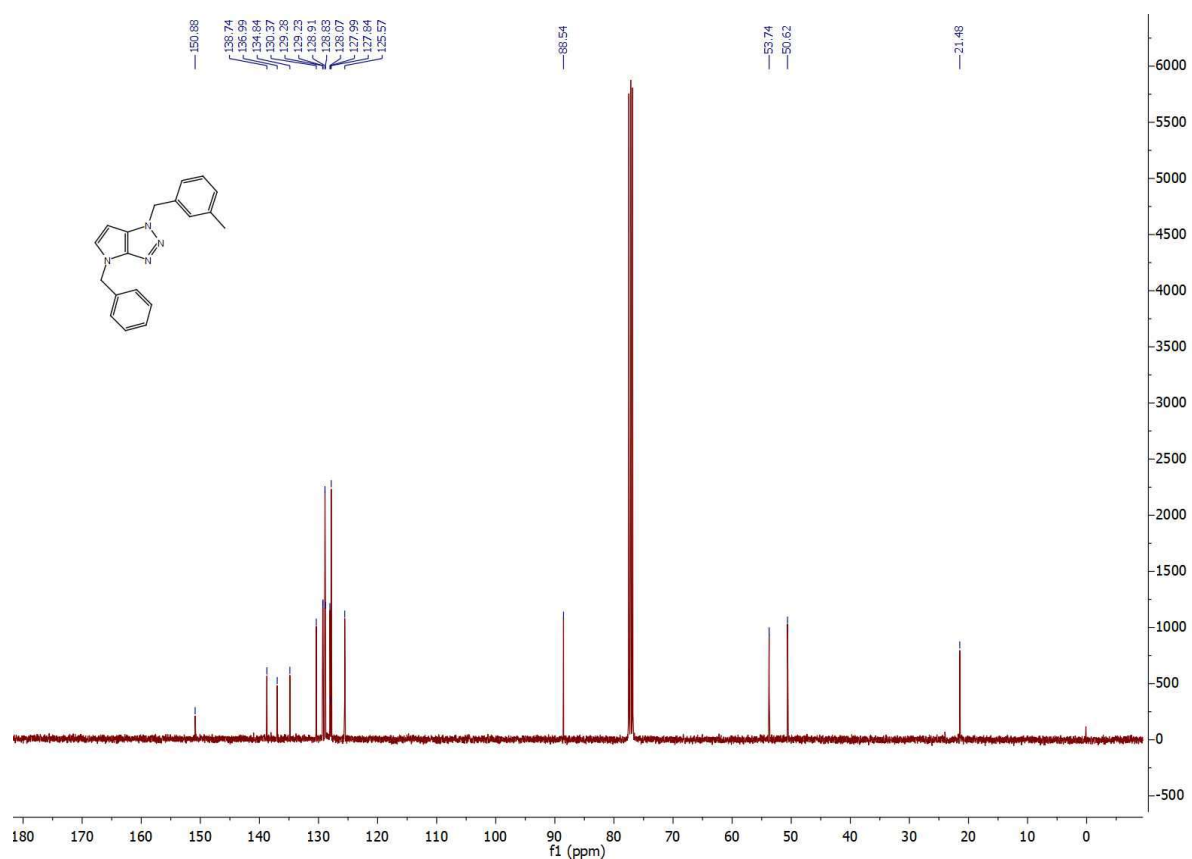
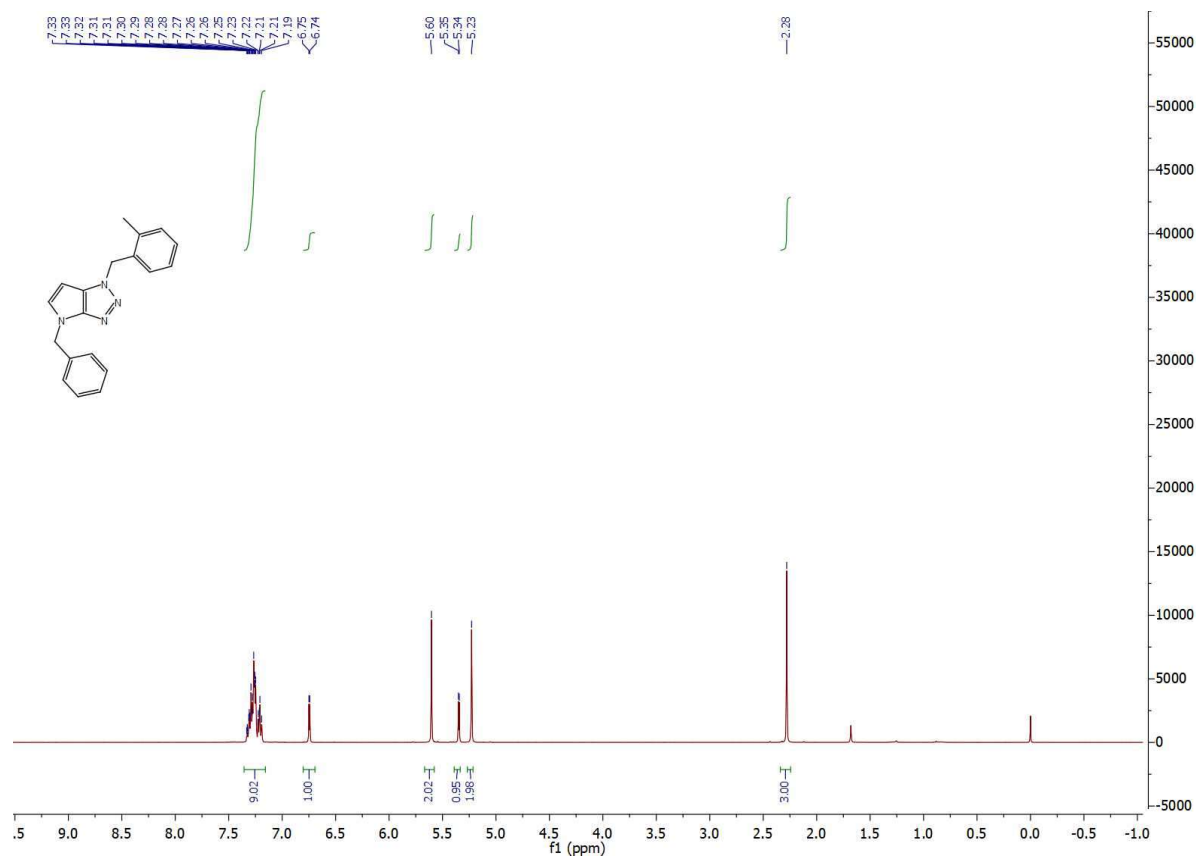


Figure S4. 4-Benzyl-1-(3-methylbenzyl)-1,4-dihydropyrrolo[2,3-*d*][1,2,3]triazole (7).



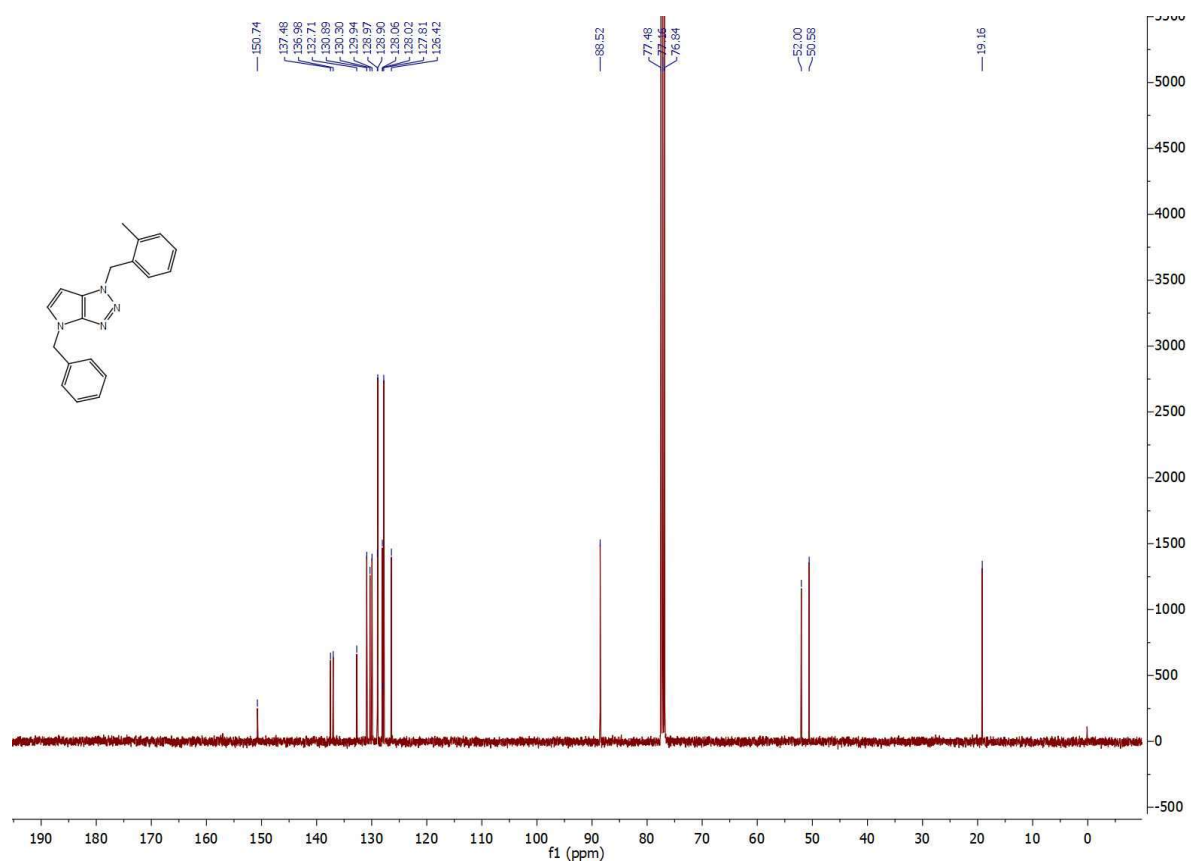
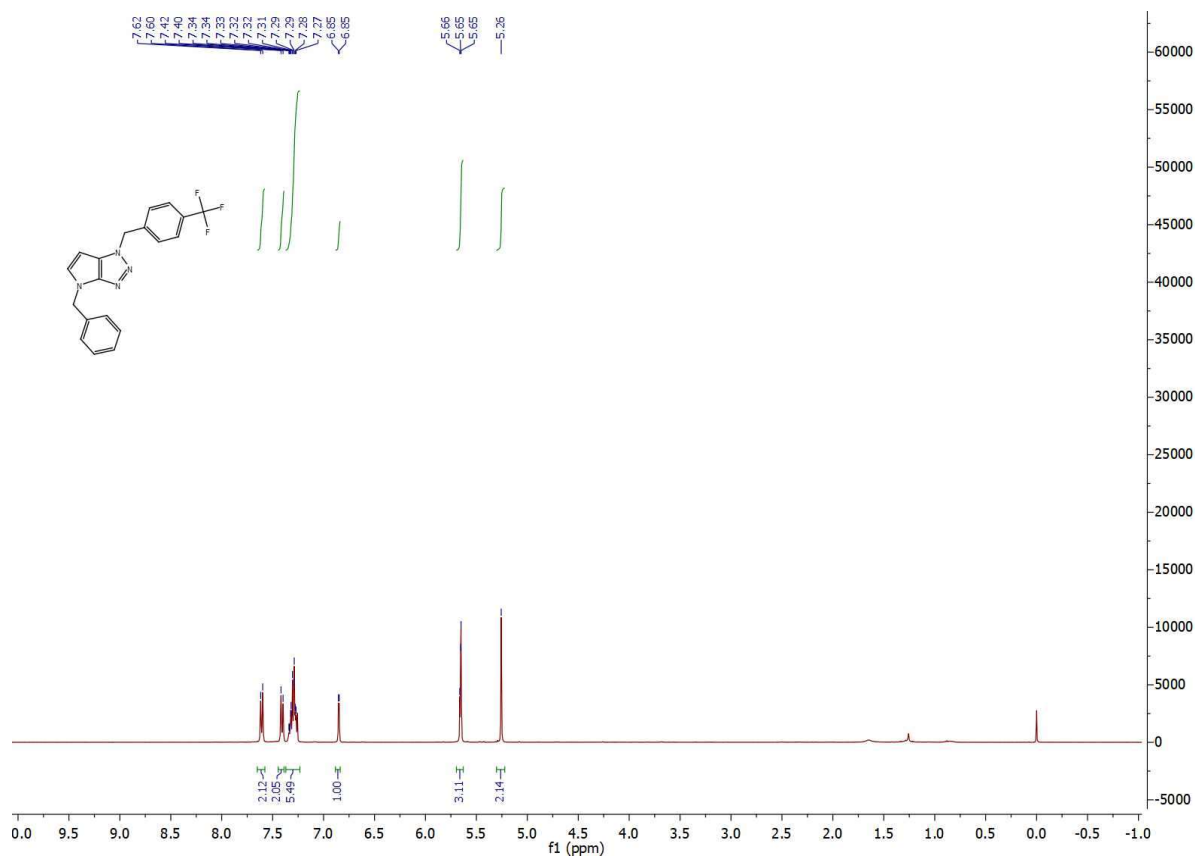


Figure S5. 4-Benzyl-1-(2-methylbenzyl)-1,4-dihydropyrrolo[2,3-d][1,2,3]triazole (8).



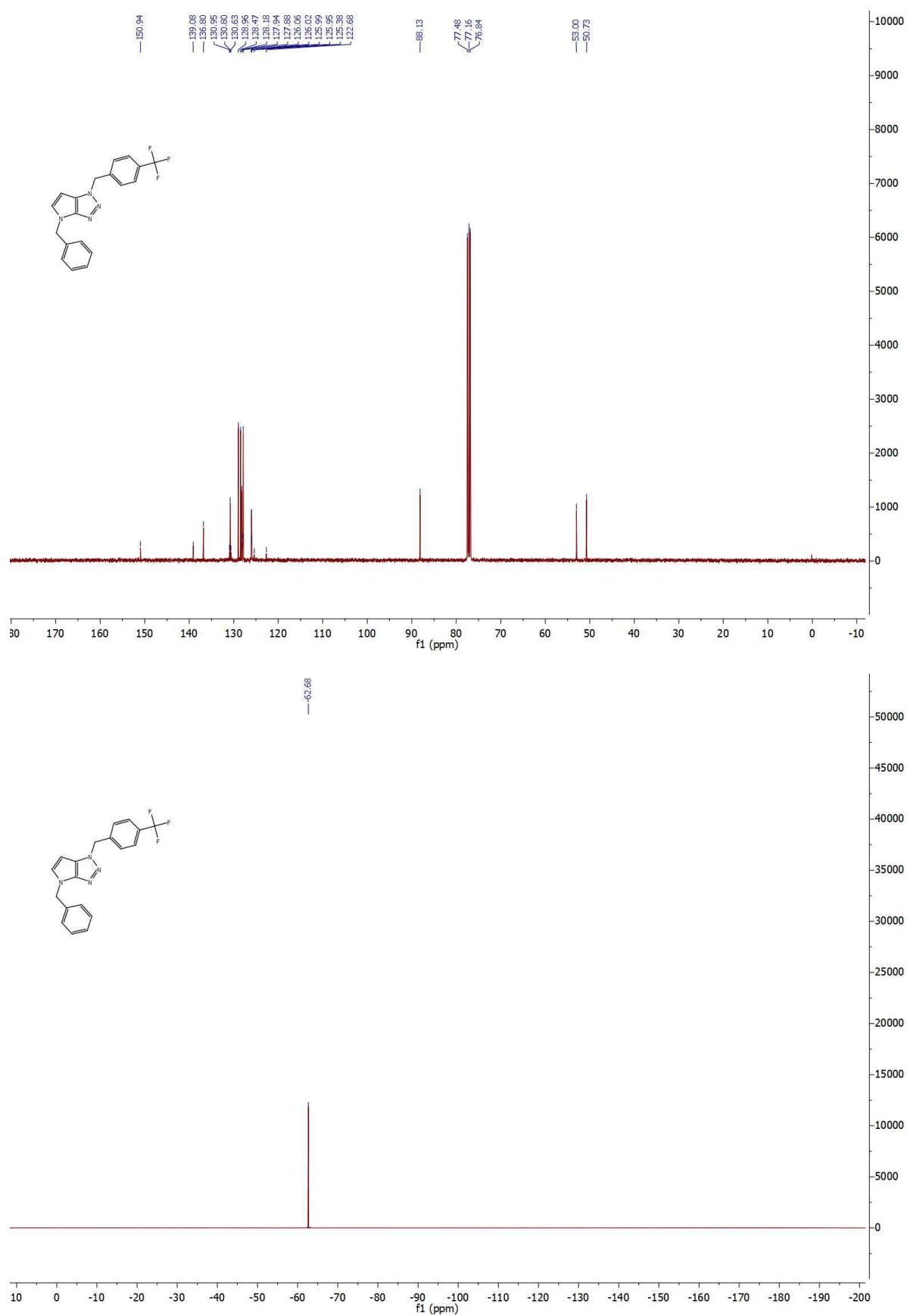


Figure S6. 4-Benzyl-1-(4-(trifluoromethyl)benzyl)-1,4-dihydropyrrolo[2,3-d][1,2,3]triazole (9).

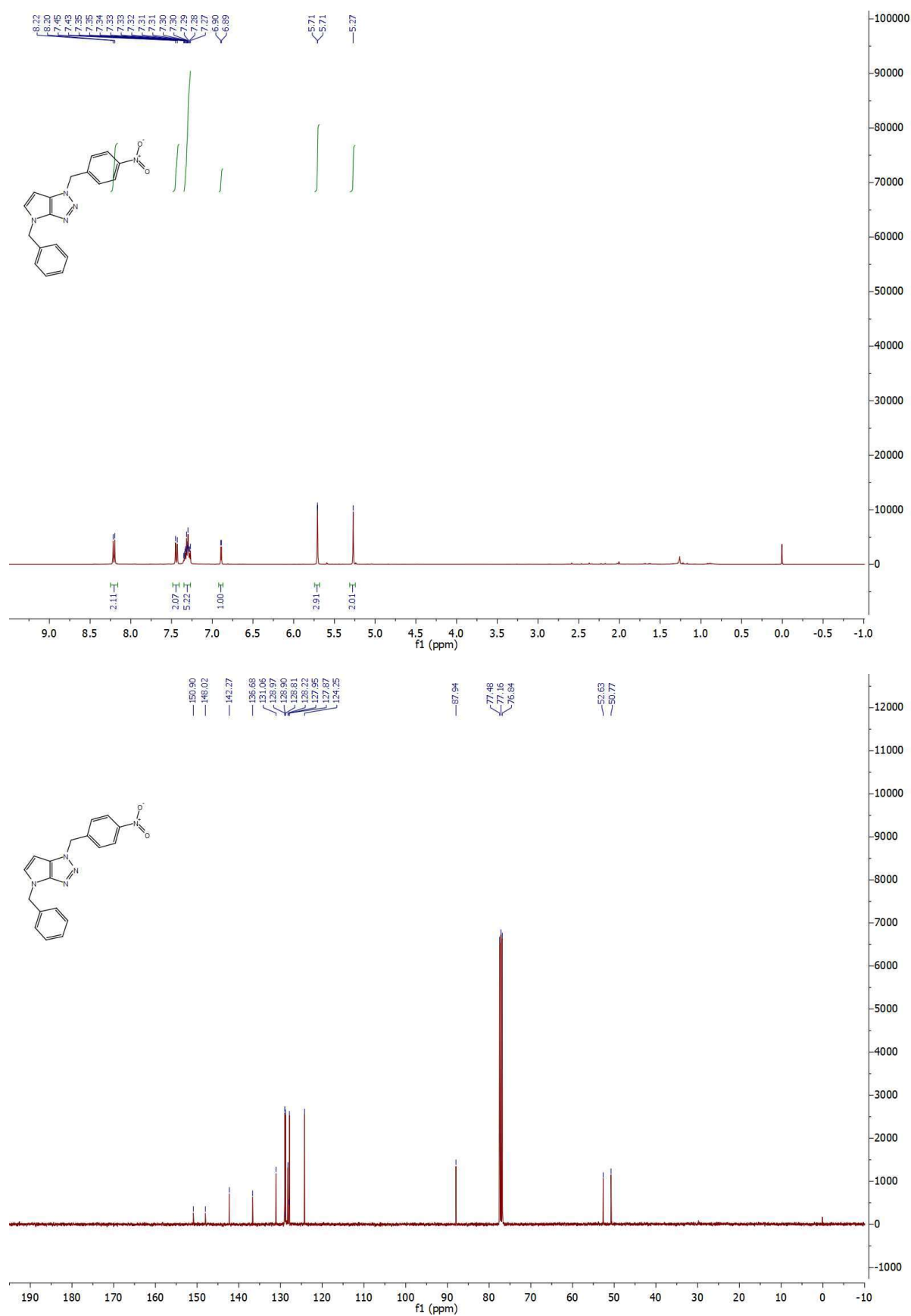


Figure S7. 4-Benzyl-1-(4-nitrobenzyl)-1,4-dihydropyrrolo[2,3-d][1,2,3]triazole (10).

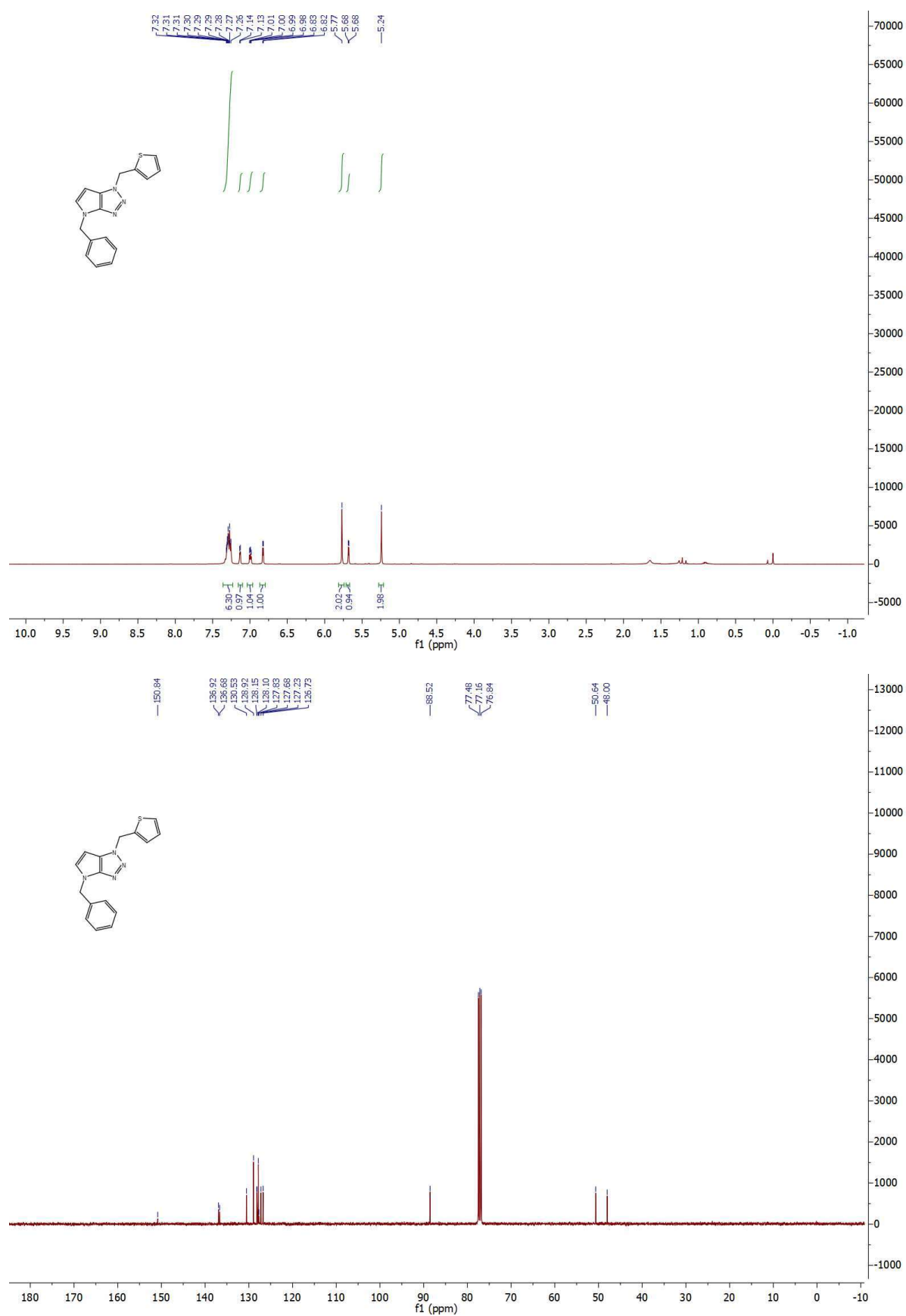


Figure S8. 4-Benzyl-1-(thiophen-2-ylmethyl)-1,4-dihydropyrrolo[2,3-*d*][1,2,3]triazole (11).

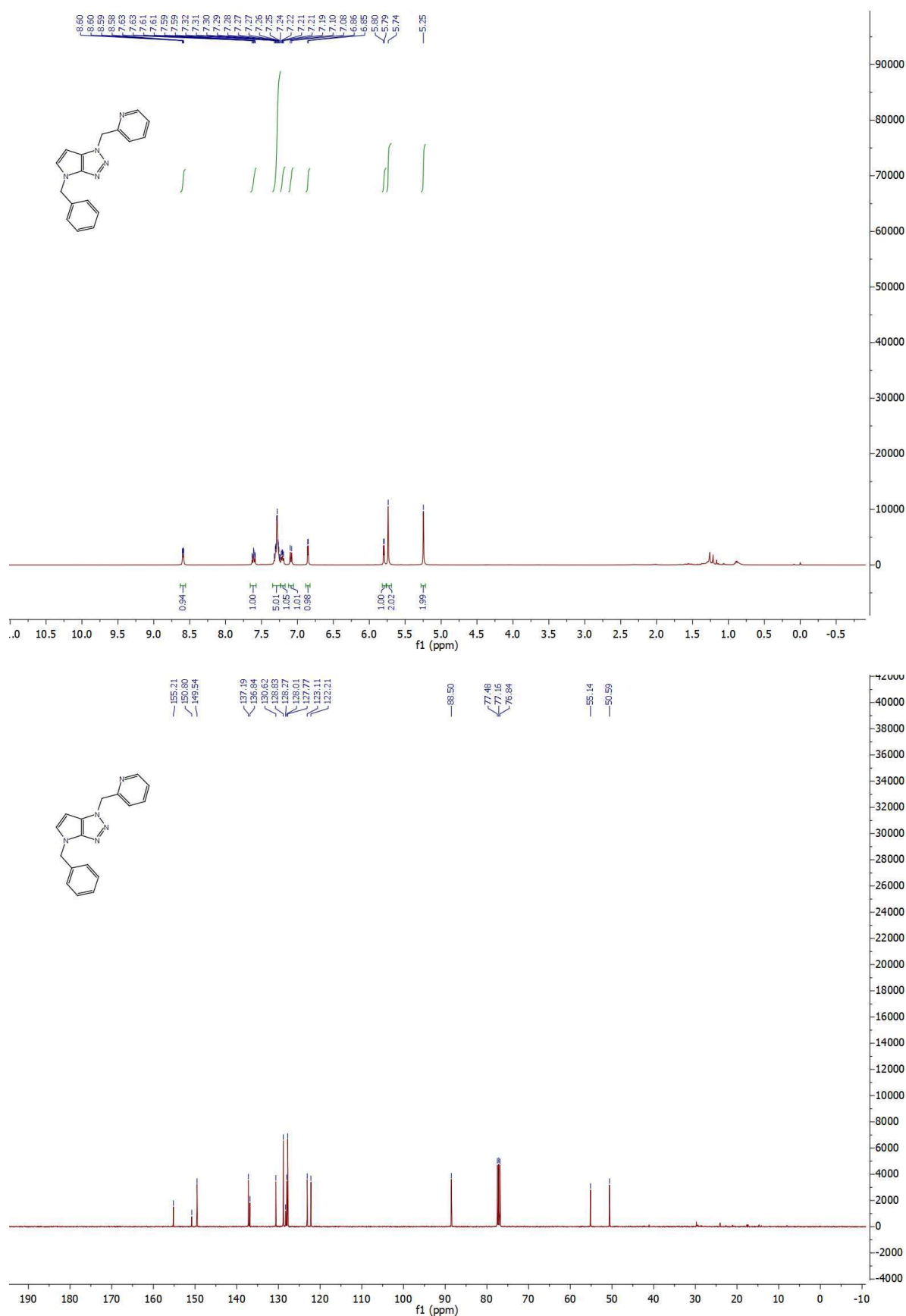


Figure S9. 4-Benzyl-1-(pyridin-2-ylmethyl)-1,4-dihydropyrrolo[2,3-*d*][1,2,3]triazole (12).

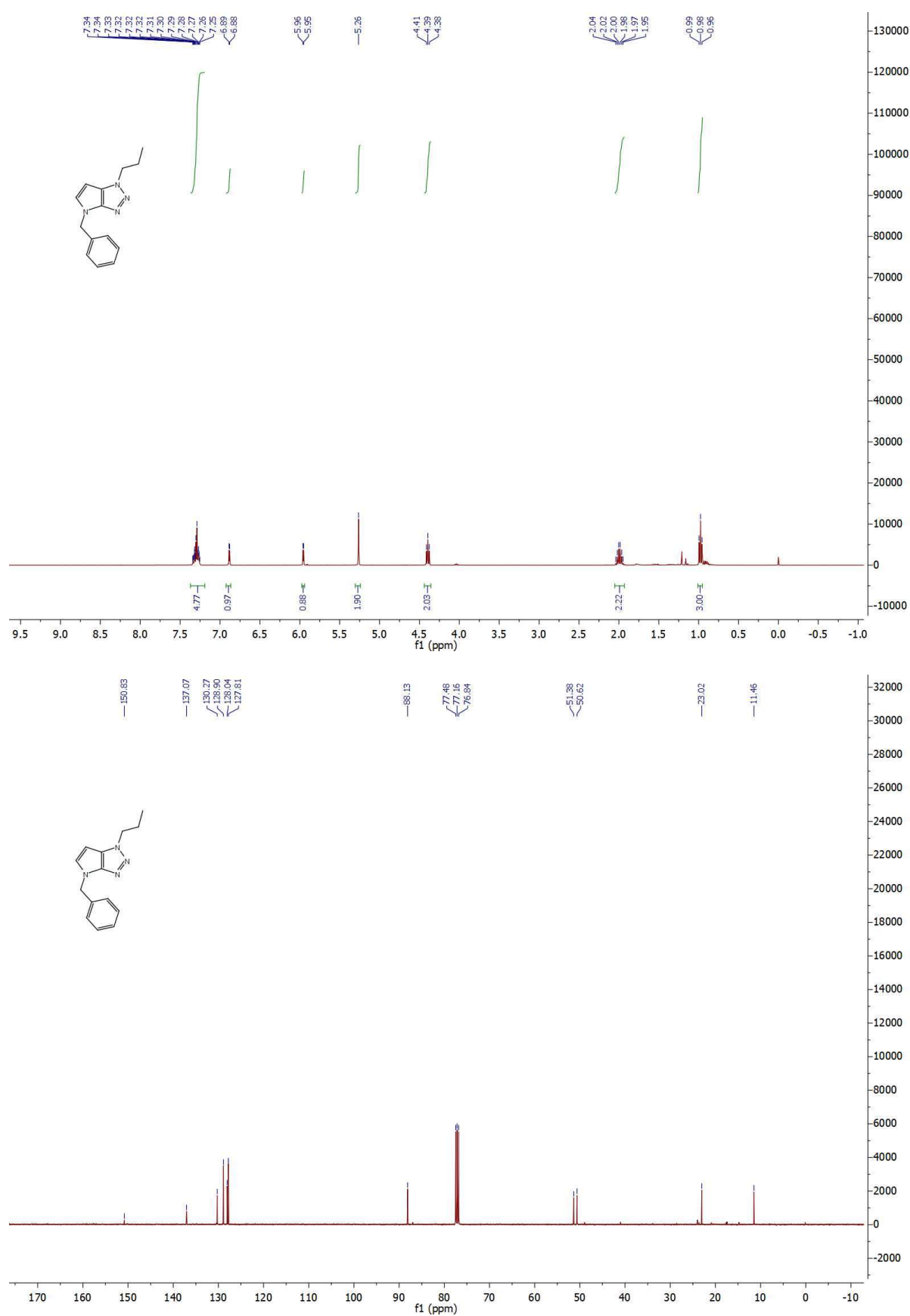


Figure S10. 4-Benzyl-1-propyl-1,4-dihydropyrrolo[2,3-d][1,2,3]triazole (14).

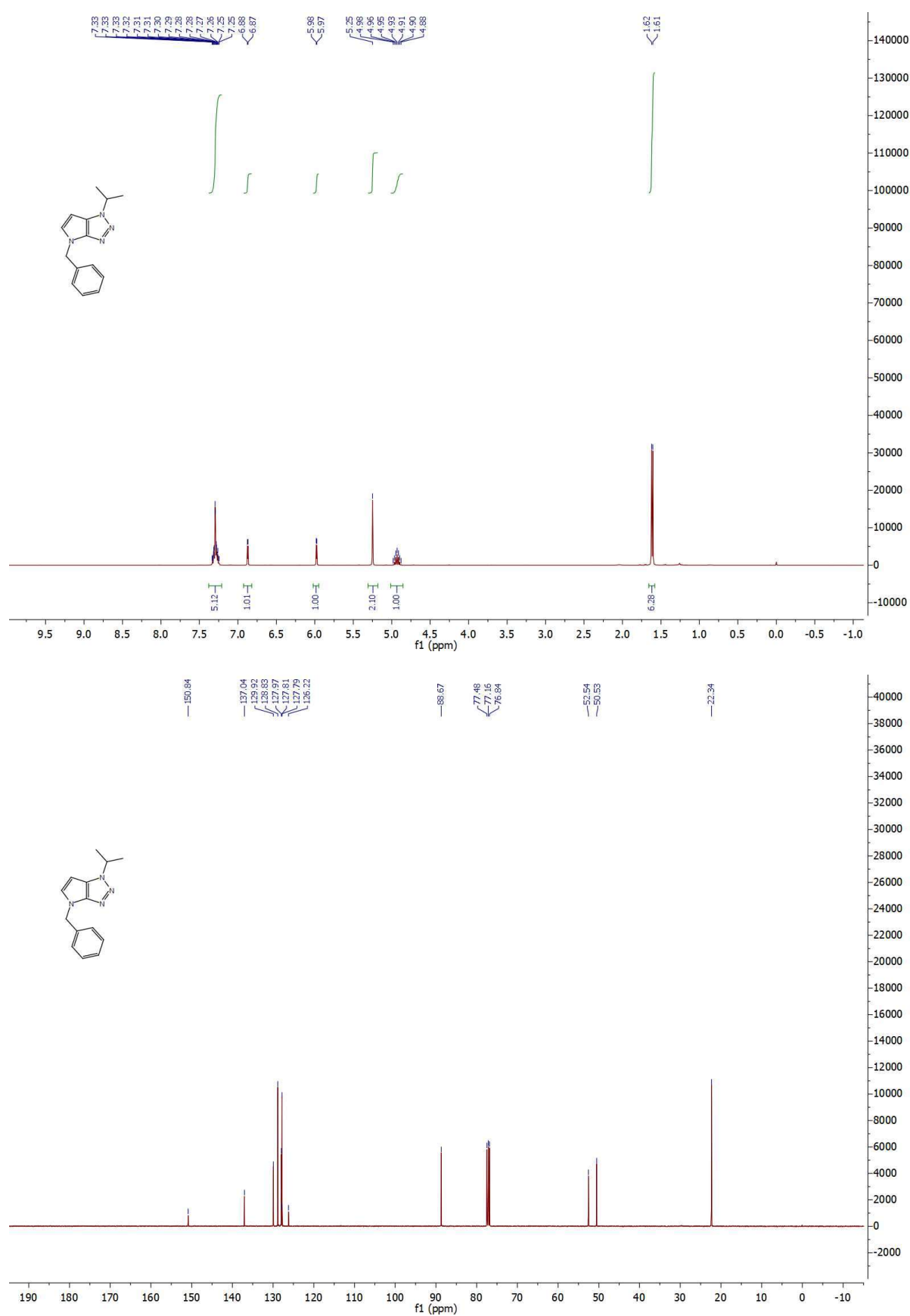


Figure S11. 4-Benzyl-1-isopropyl-1,4-dihydropyrrolo[2,3-d][1,2,3]triazole (15).

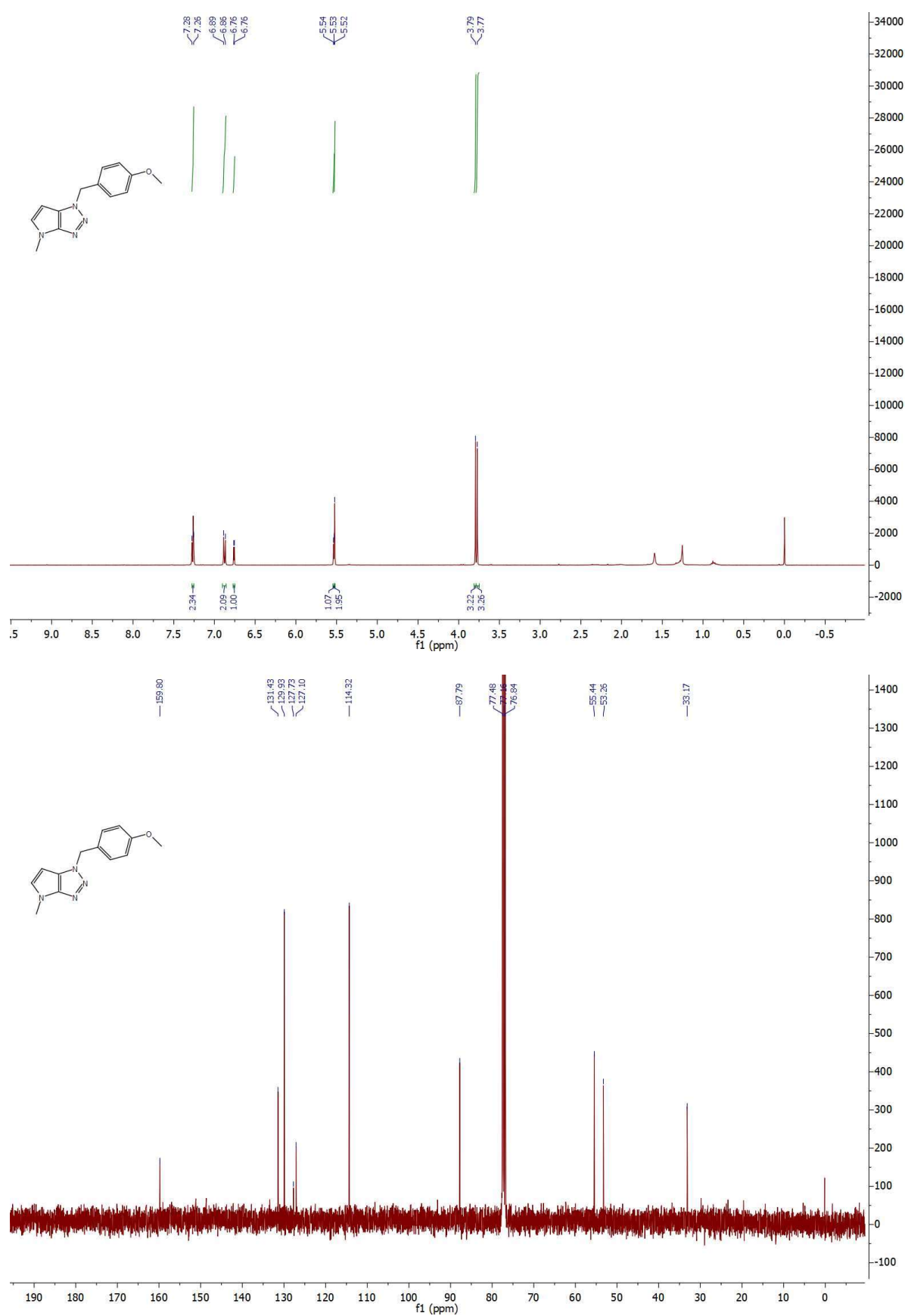


Figure S12. 1-(4-Methoxybenzyl)-4-methyl-1,4-dihydropyrrolo[2,3-*d*][1,2,3]triazole (16).

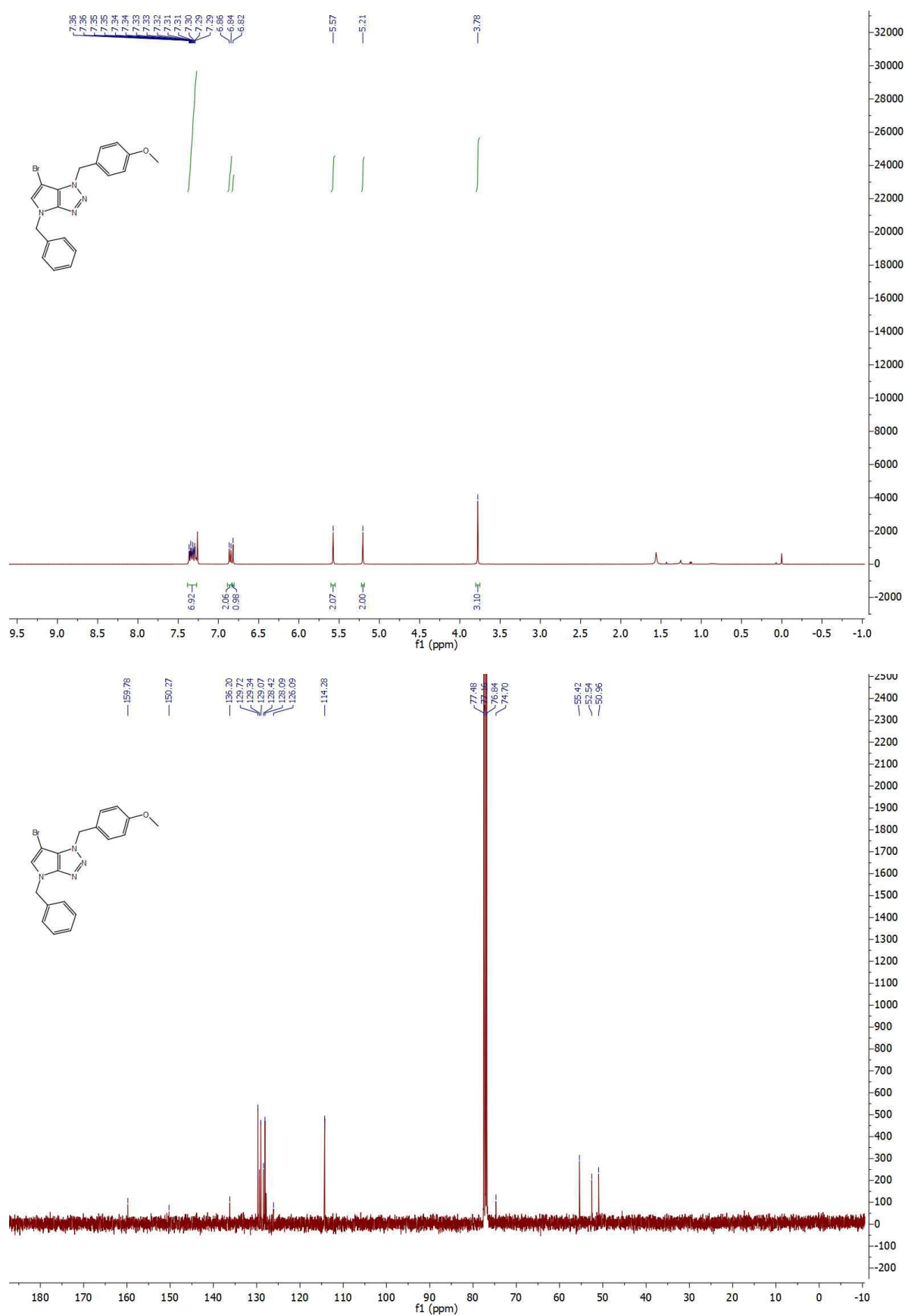
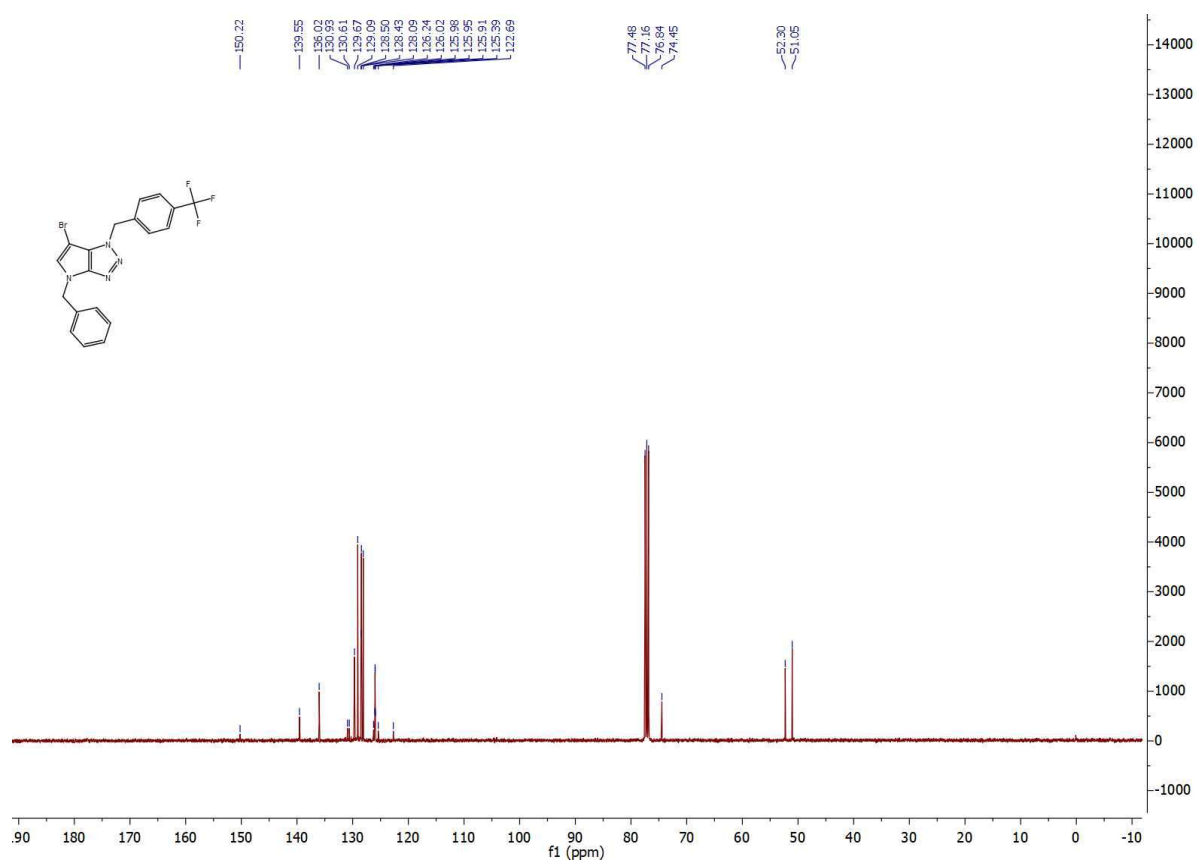
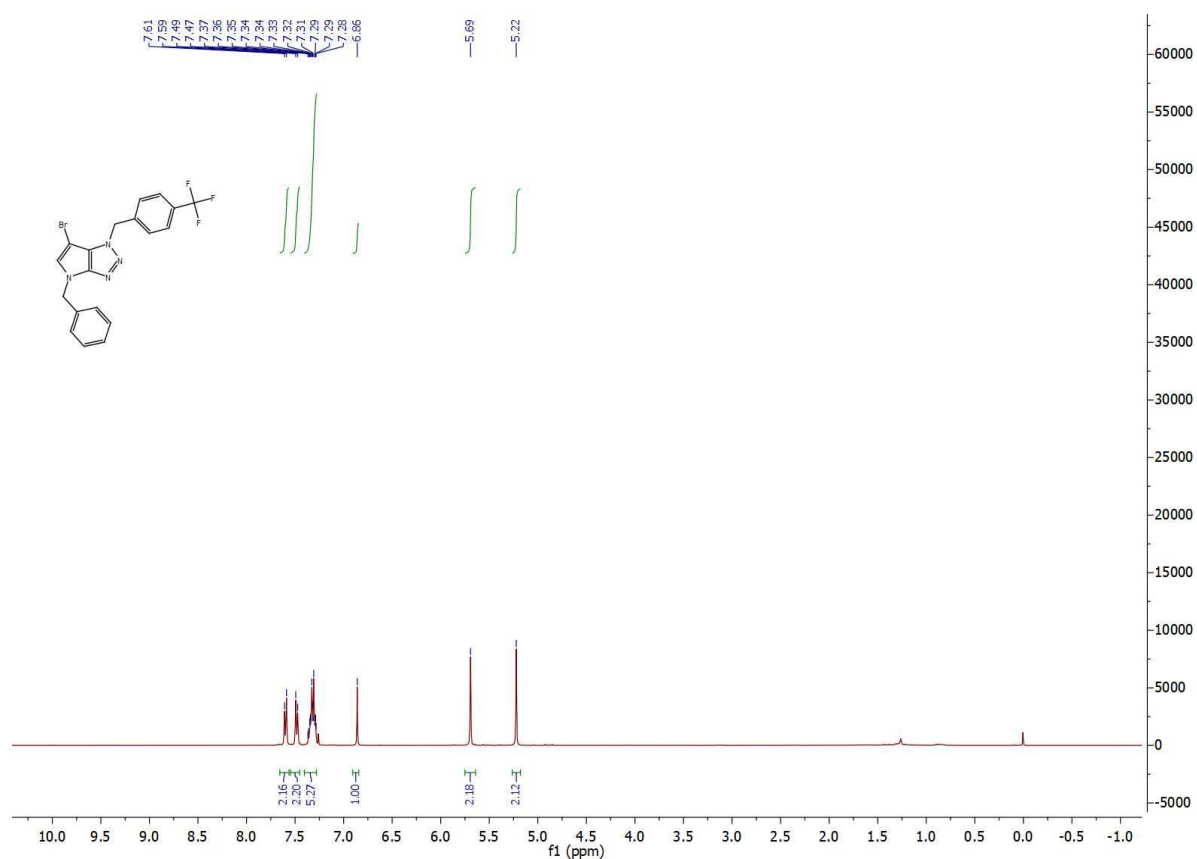


Figure S13. 4-Benzyl-6-bromo-1-(4-methoxybenzyl)-1,4-dihydropyrrolo[2,3-d][1,2,3]triazole (17).



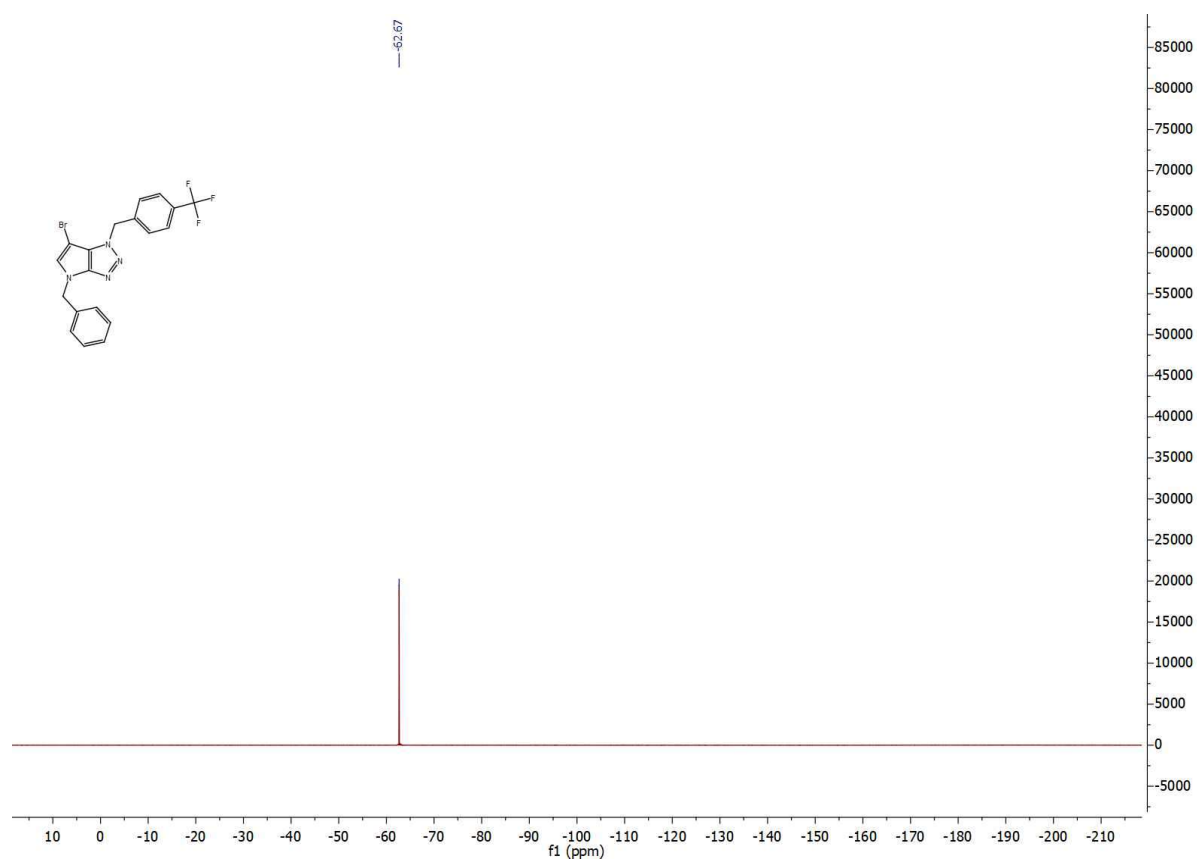


Figure S14. 4-Benzyl-6-bromo-1-(4-(trifluoromethyl)benzyl)-1,4-dihydropyrrolo[2,3-*d*][1,2,3]triazole (18).

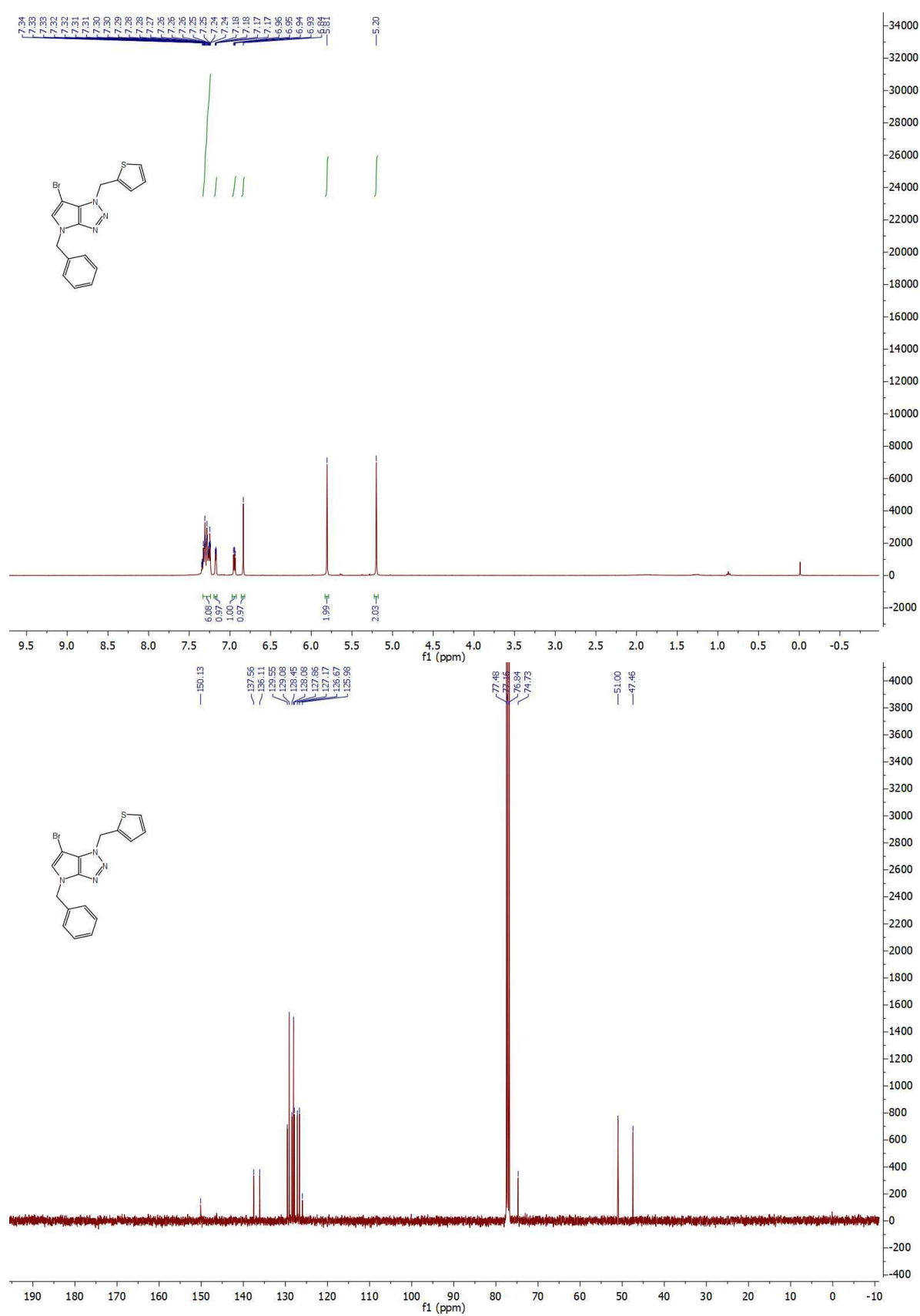


Figure S15. 4-Benzyl-6-bromo-1-(thiophen-2-ylmethyl)-1,4-dihydropyrrolo[2,3-d][1,2,3]triazole (19).

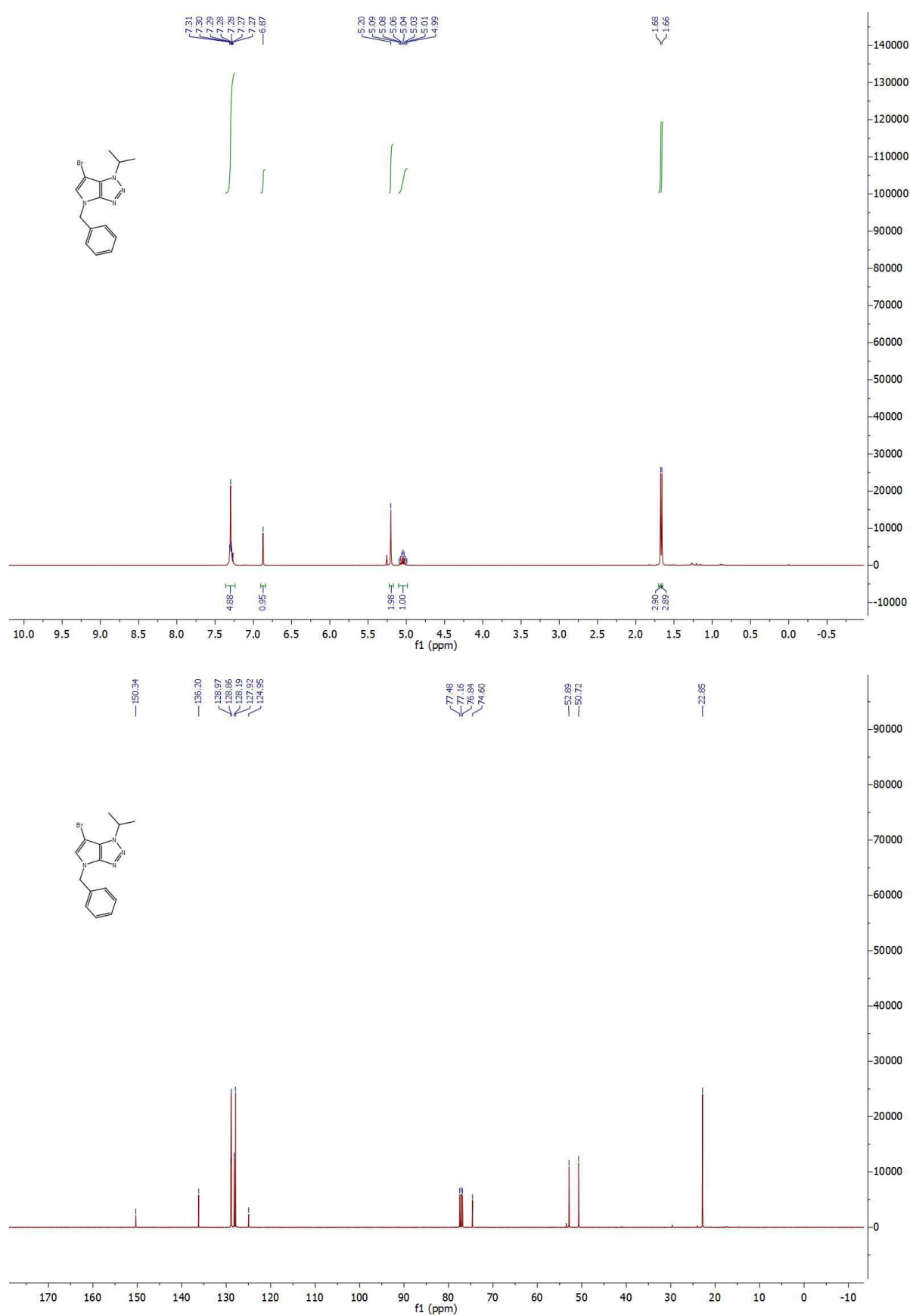


Figure S16. 4-Benzyl-6-bromo-1-isopropyl-1,4-dihydropyrrolo[2,3-d][1,2,3]triazole (20).

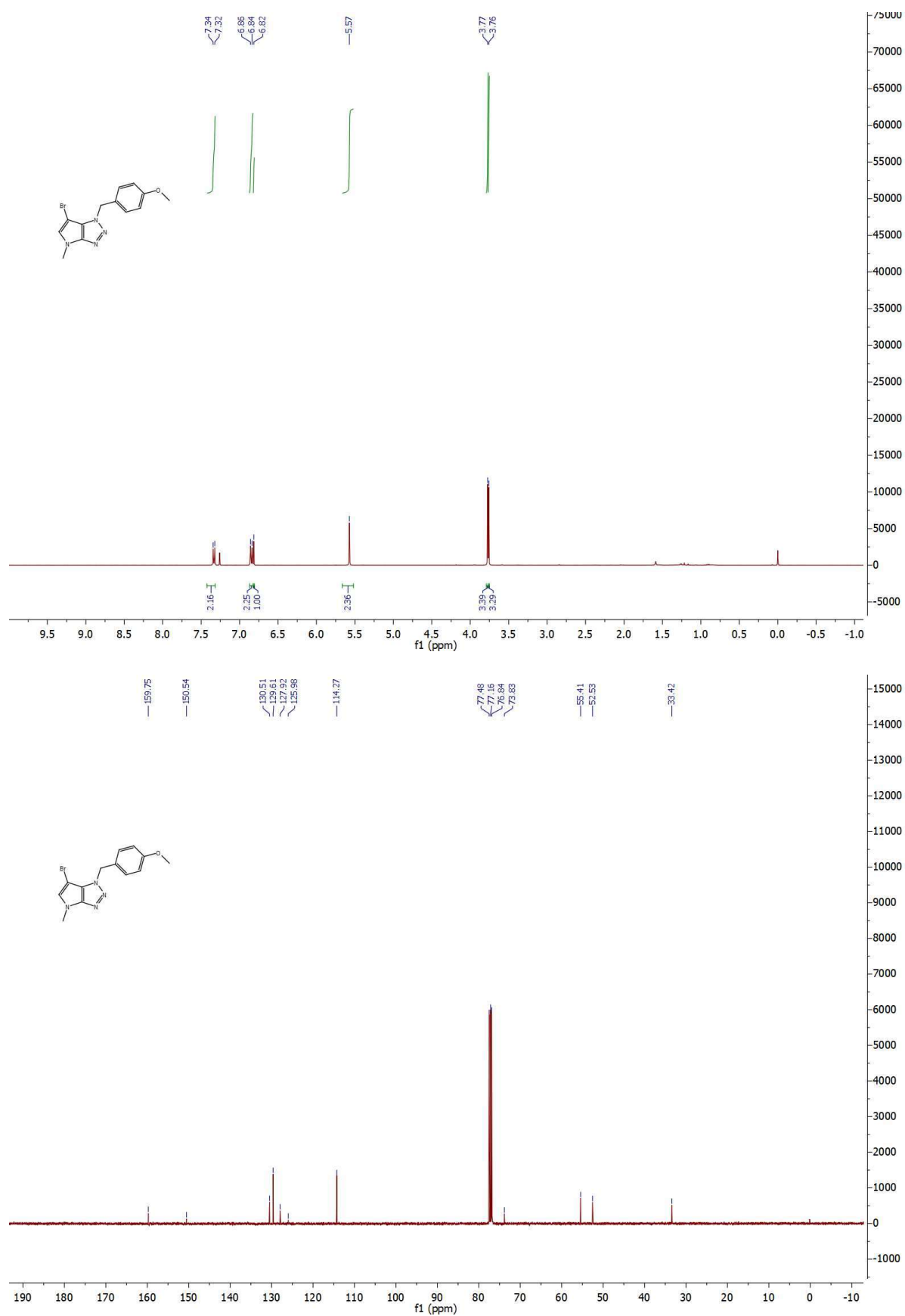


Figure S17. 6-Bromo-1-(4-methoxybenzyl)-4-methyl-1,4-dihydropyrrolo[2,3-d][1,2,3]triazole (21).

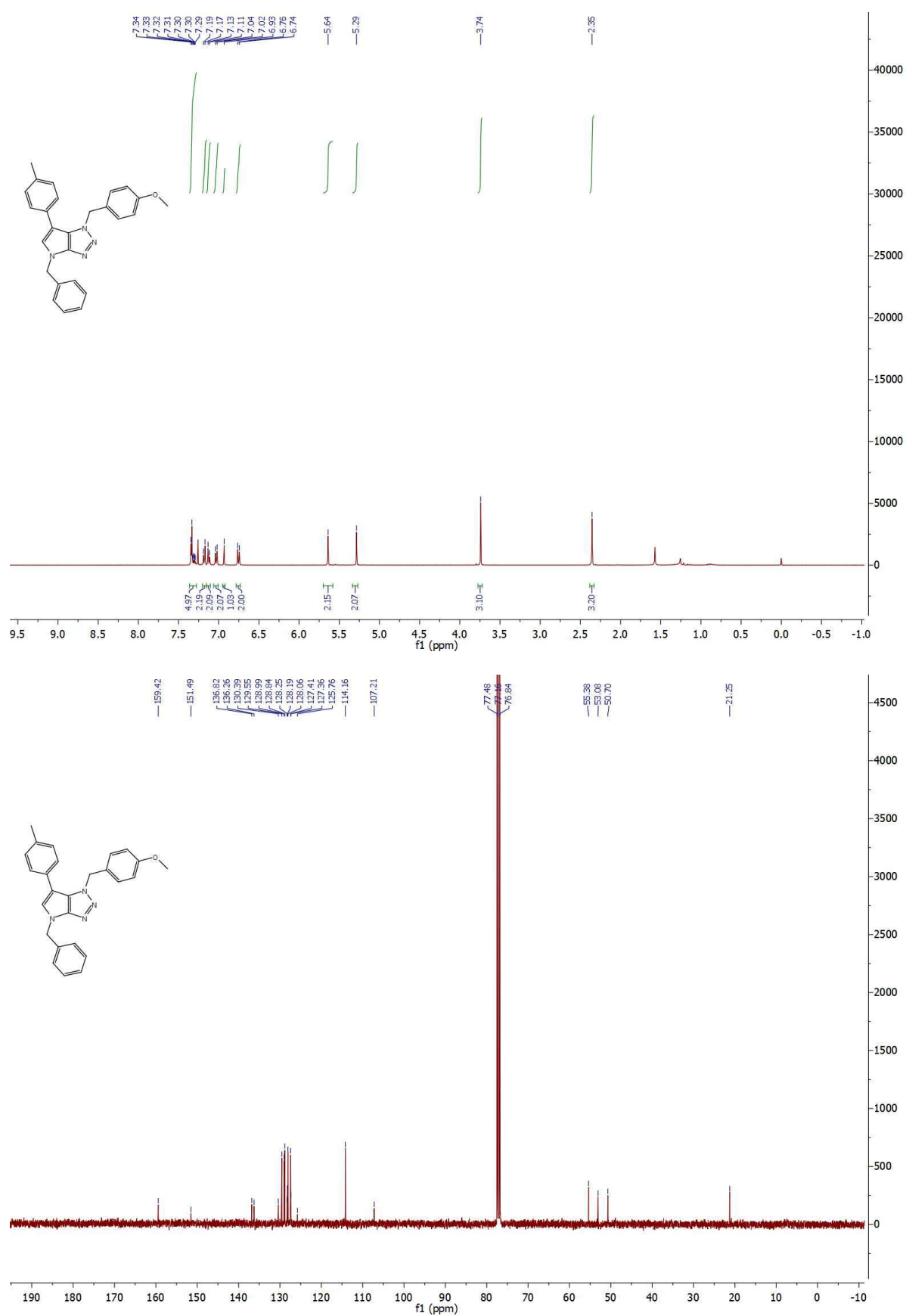


Figure S18. 4-Benzyl-1-(4-methoxybenzyl)-6-(*p*-tolyl)-1,4-dihydropyrrolo[2,3-*d*][1,2,3]triazole (22).

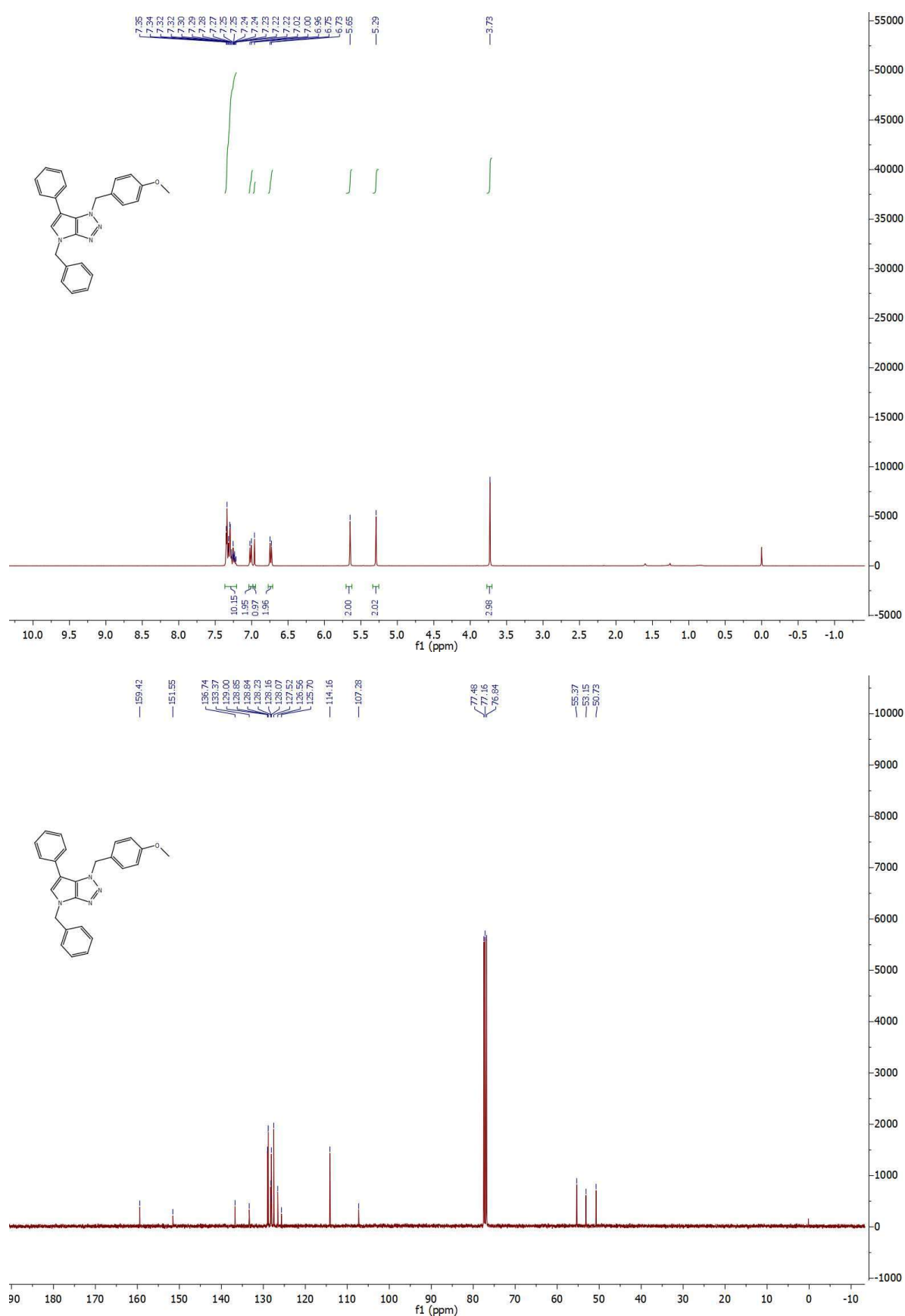


Figure S19. 4-Benzyl-1-(4-methoxybenzyl)-6-phenyl-1,4-dihydropyrrolo[2,3-d][1,2,3]triazole (23).

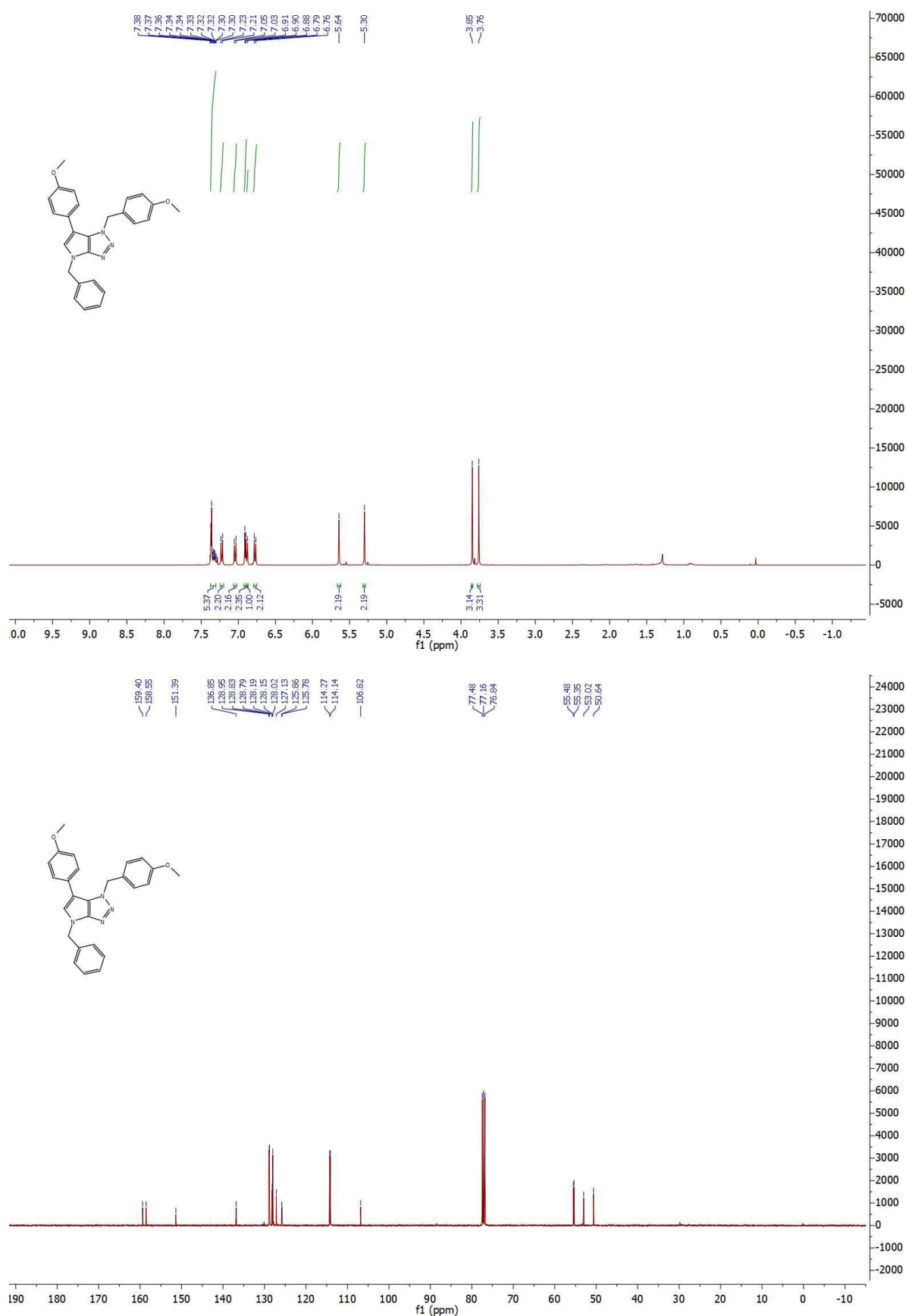


Figure S20. 4-Benzyl-1-(4-methoxybenzyl)-6-(4-methoxyphenyl)-1,4-dihydropyrrolo[2,3-d][1,2,3]triazole (24).

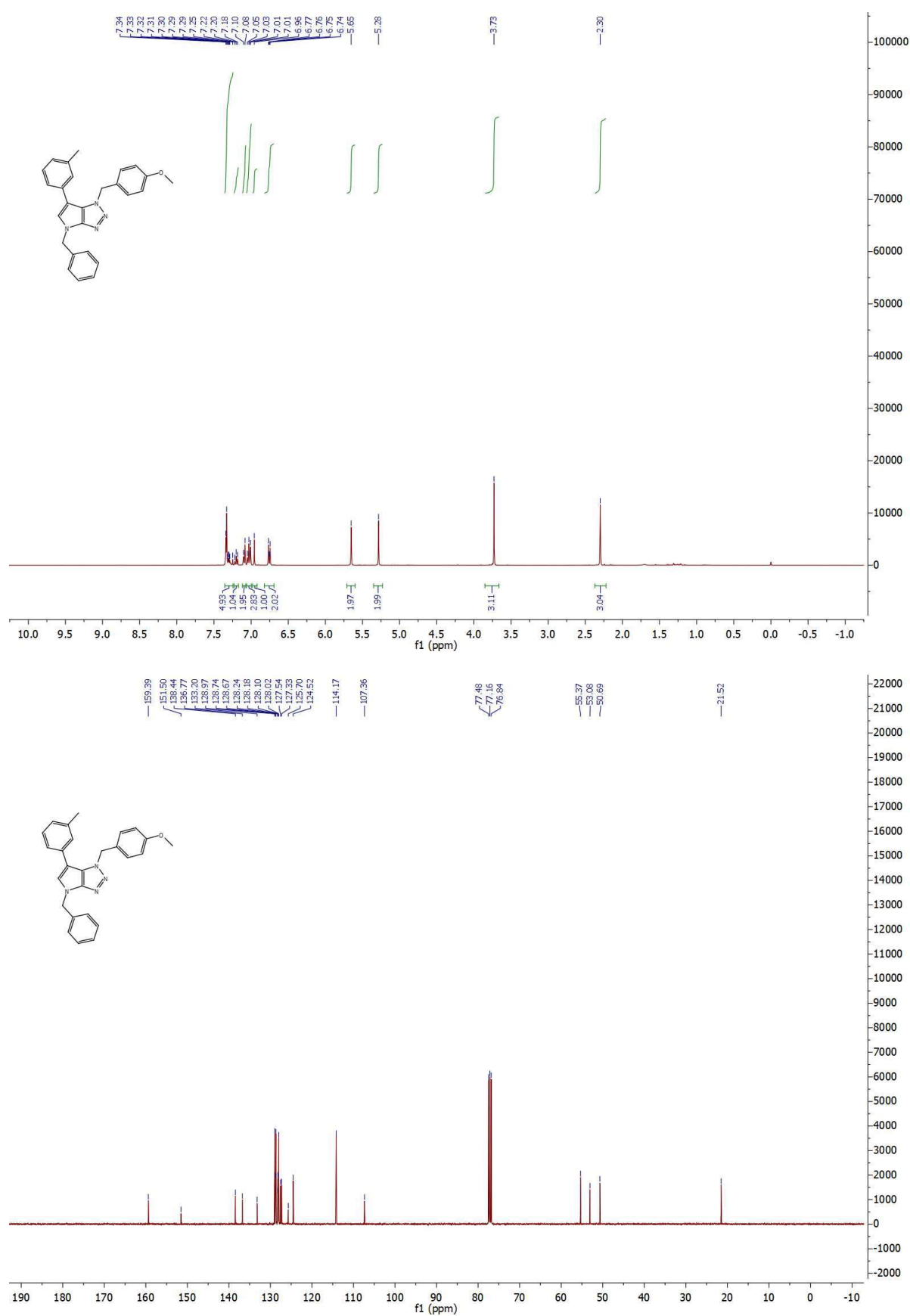


Figure S21. 4-Benzyl-1-(4-methoxybenzyl)-6-(*m*-tolyl)-1,4-dihydropyrrolo[2,3-*d*][1,2,3]triazole (25).

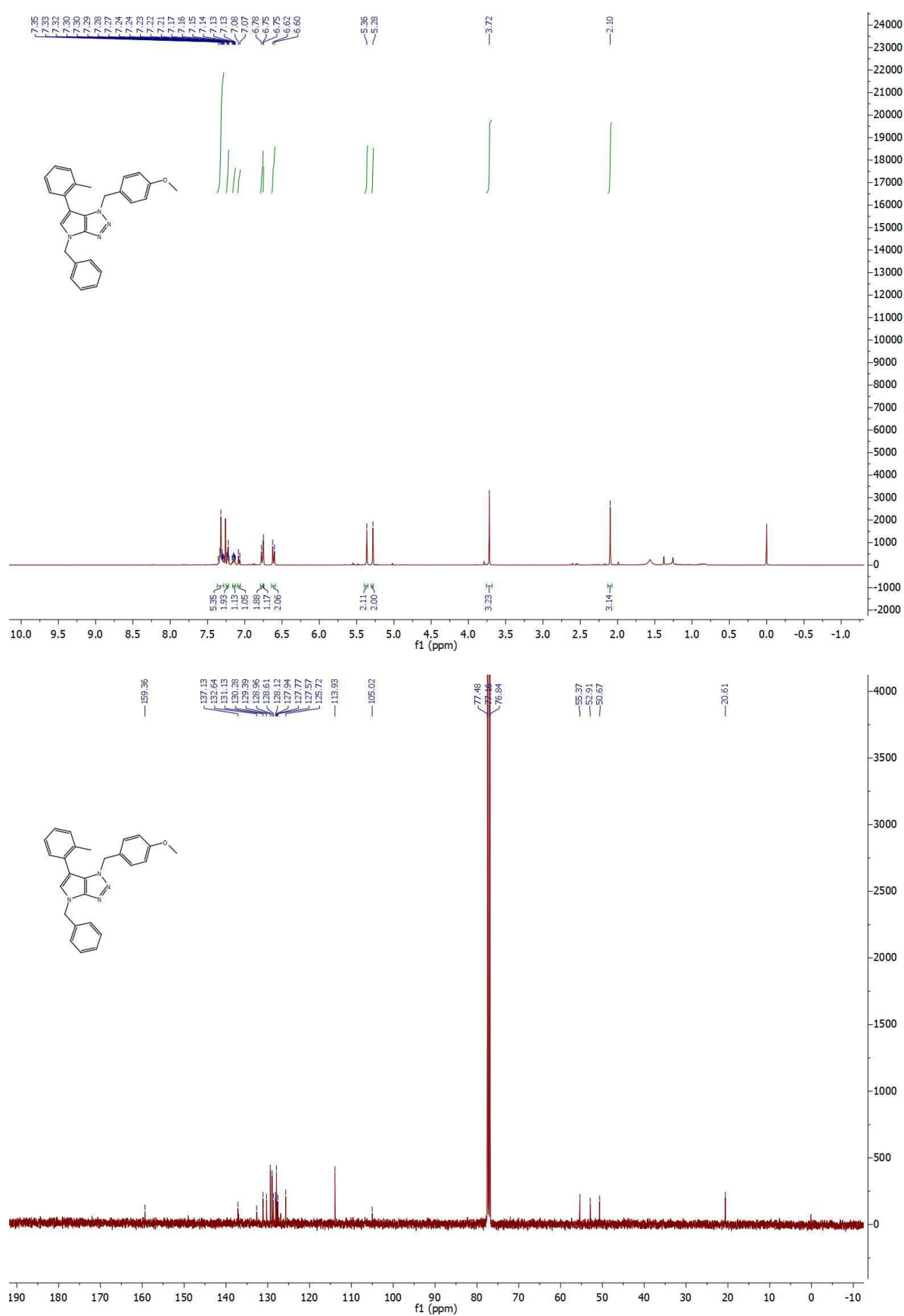
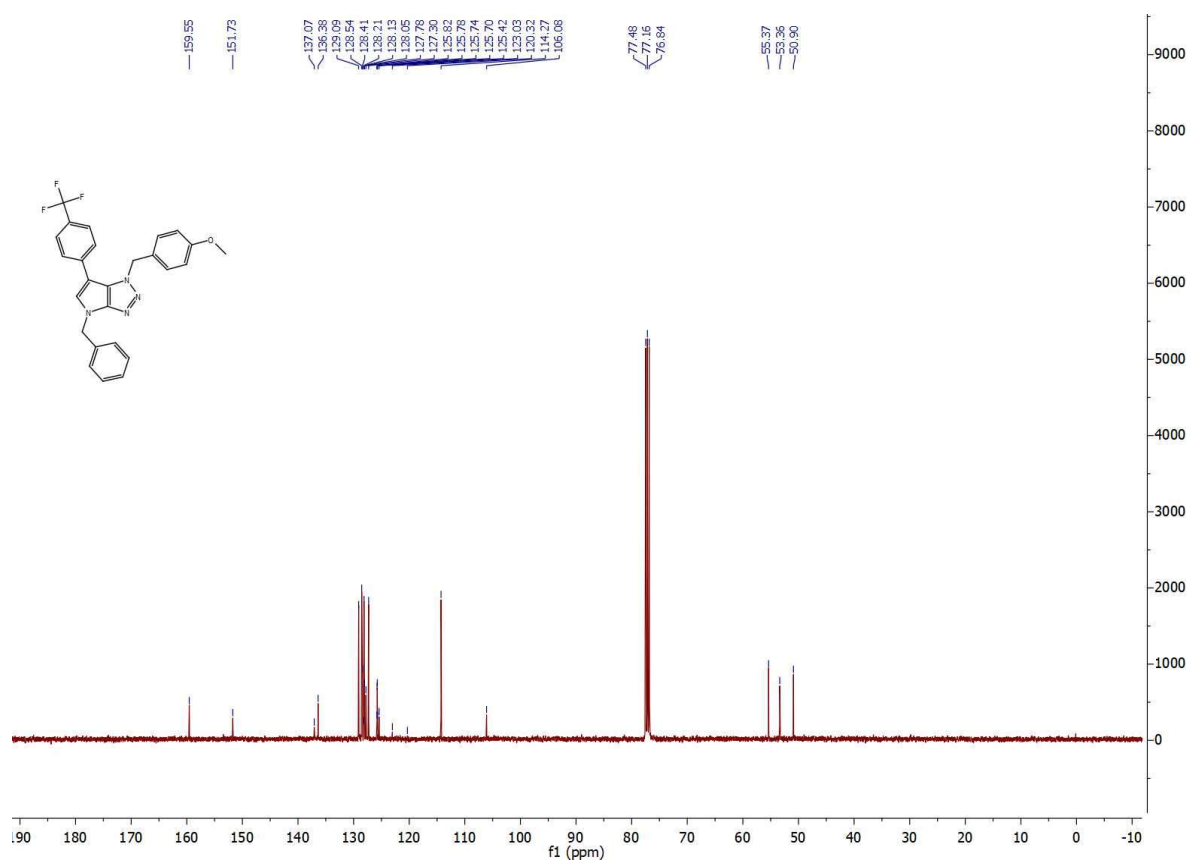
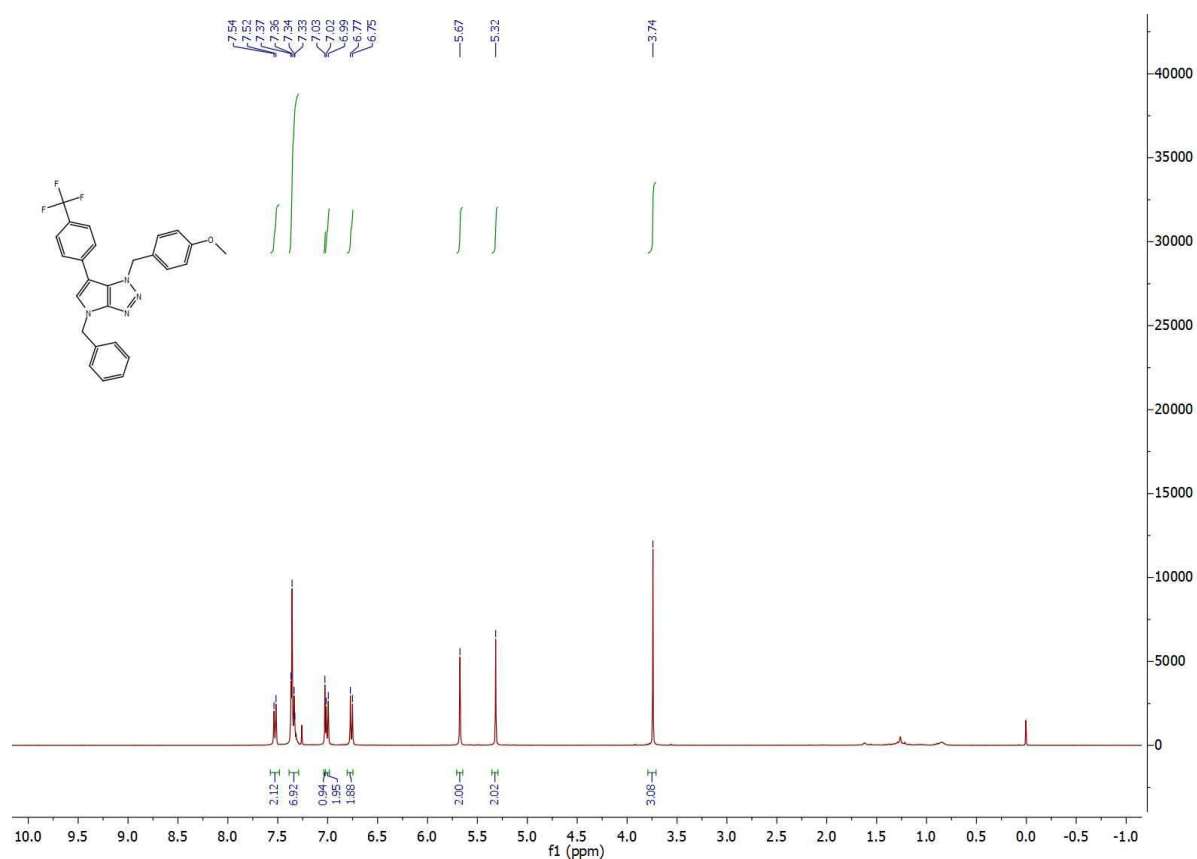


Figure S22. 4-Benzyl-1-(4-methoxybenzyl)-6-(*o*-tolyl)-1,4-dihydropyrrolo[2,3-*d*][1,2,3]triazole (26).



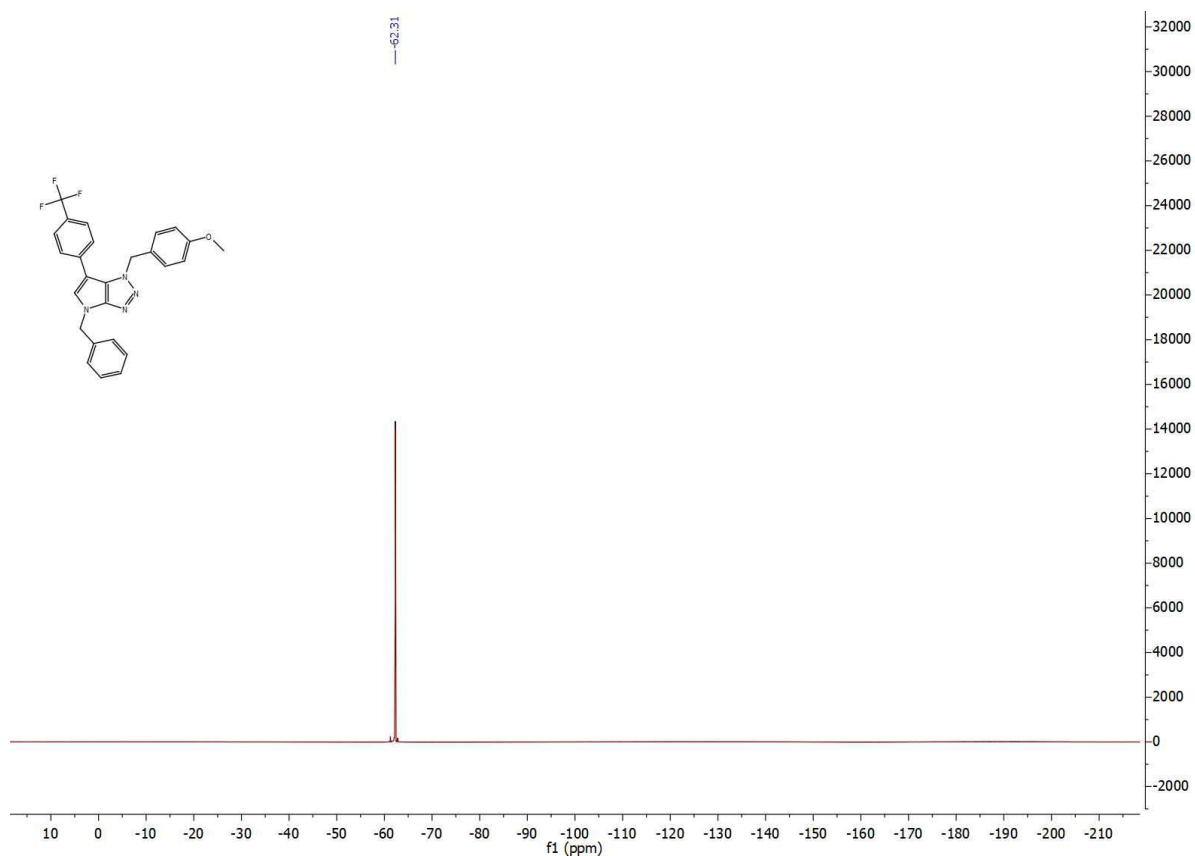
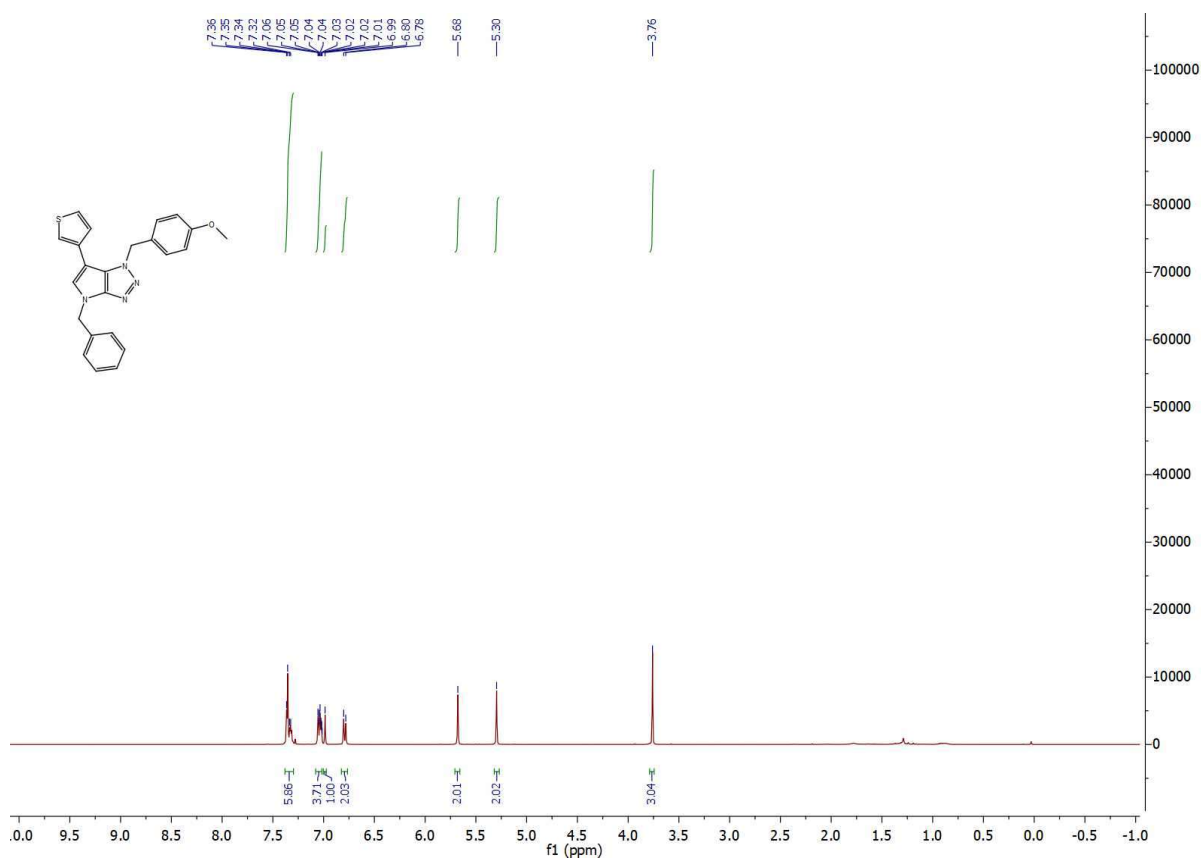


Figure S23. 4-Benzyl-1-(4-methoxybenzyl)-6-(4-(trifluoromethyl)phenyl)-1,4-dihydropyrrolo[2,3-d][1,2,3]triazole (28).



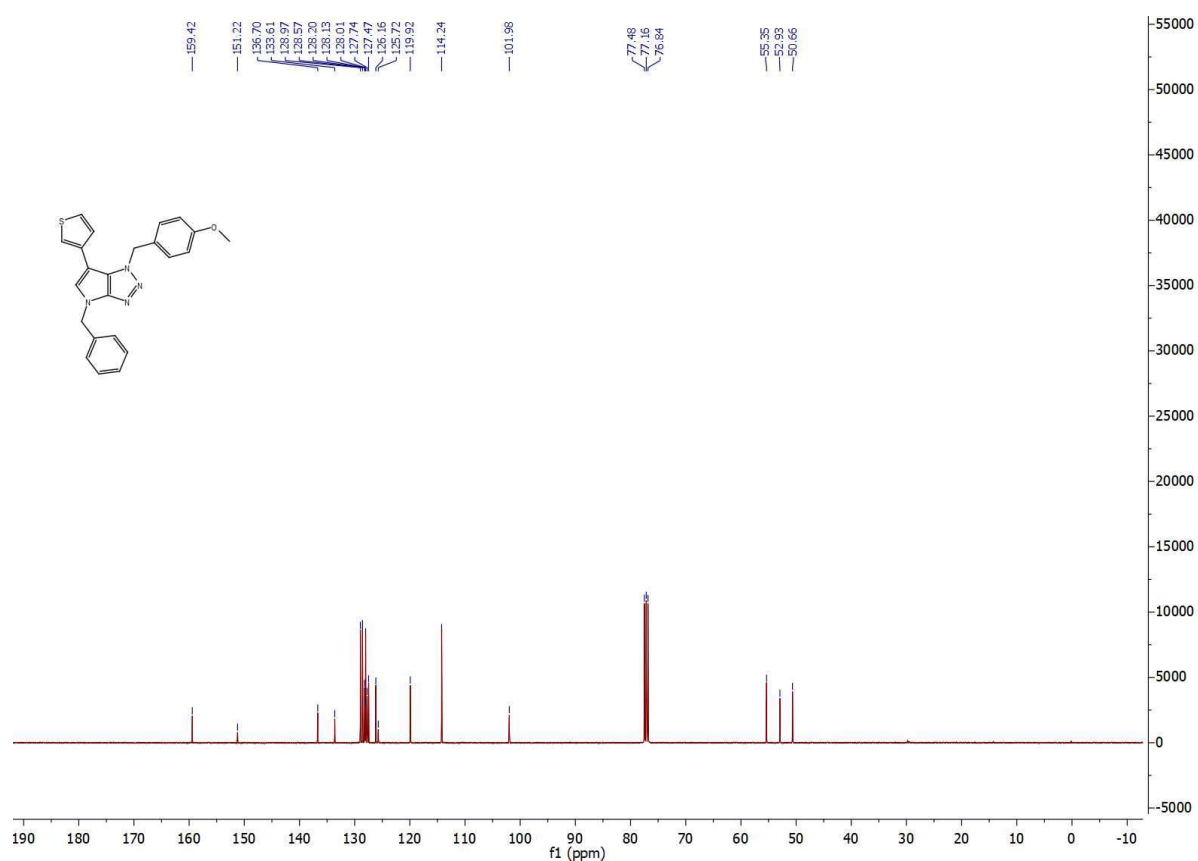
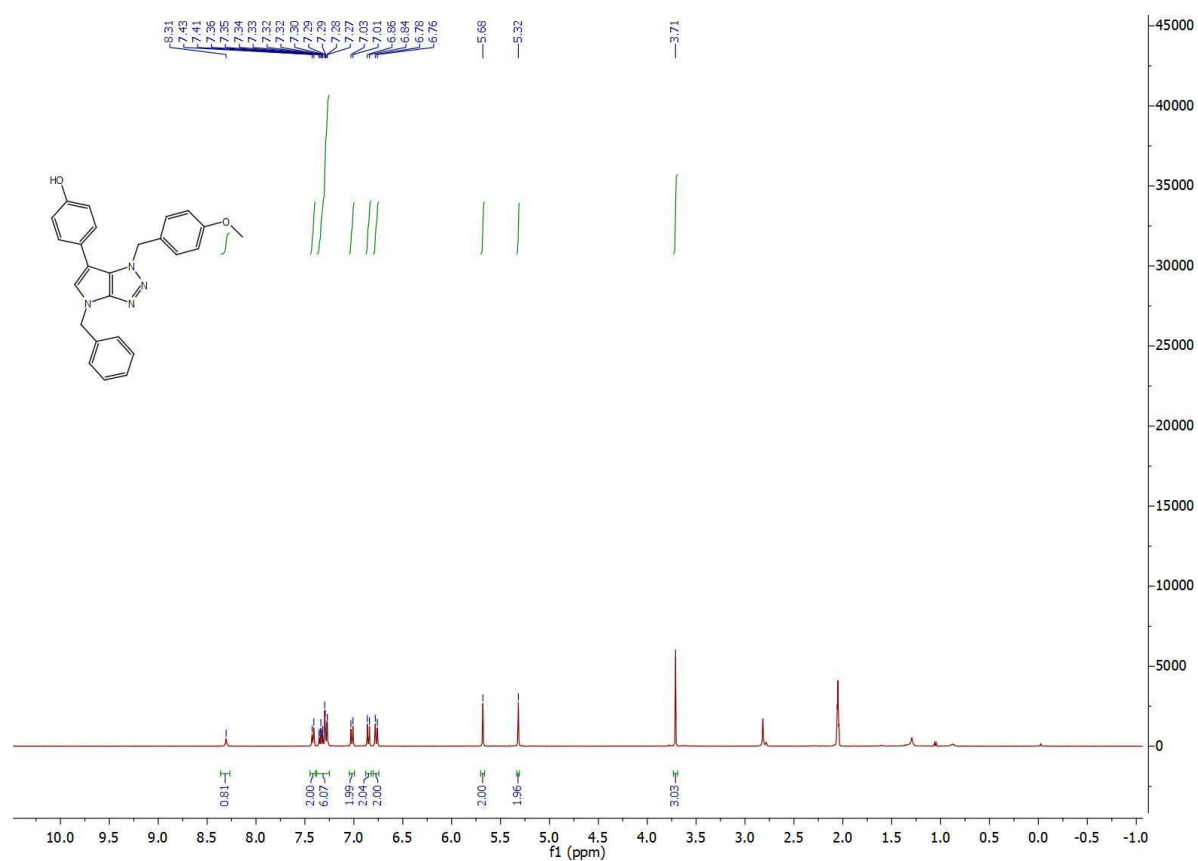


Figure S24. 4-Benzyl-1-(4-methoxybenzyl)-4-methyl-5,6-di-*p*-tolyl-1,4-dihydropyrrolo[2,3-*d*][1,2,3]triazole (29).



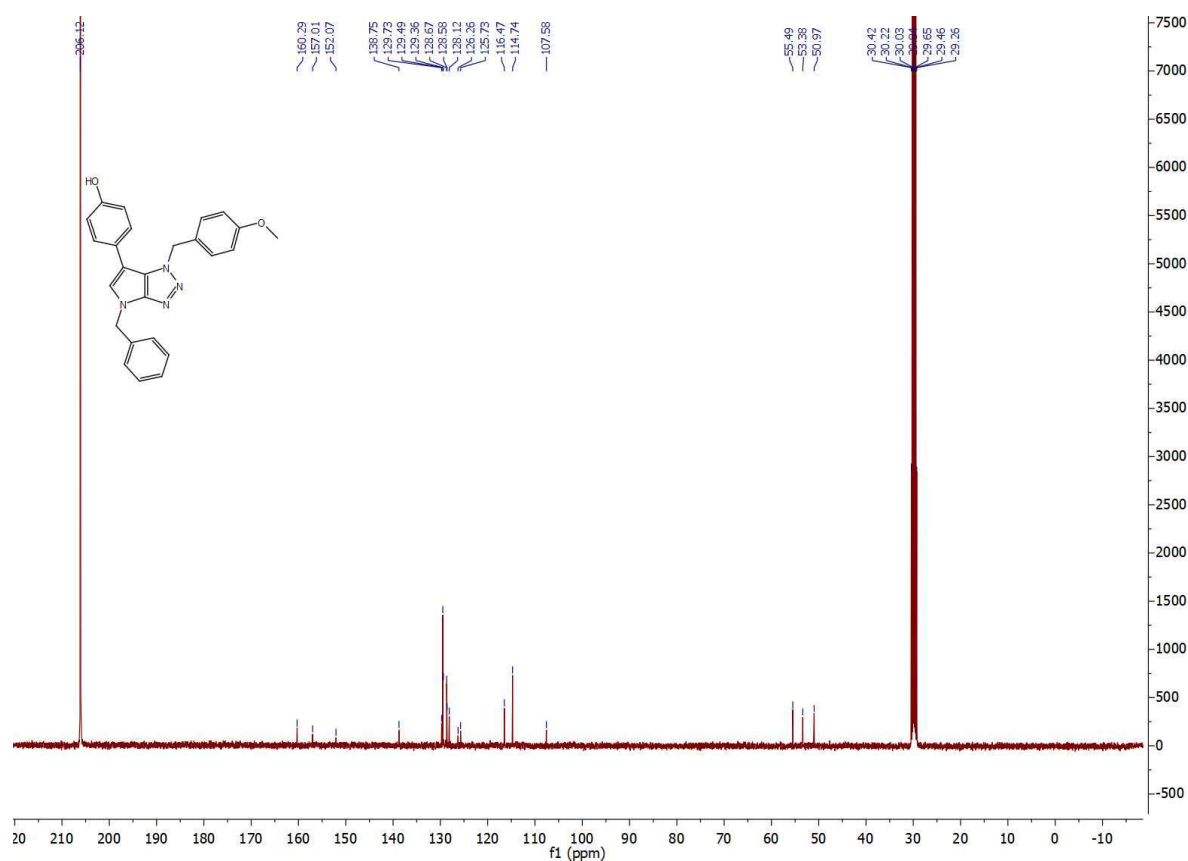
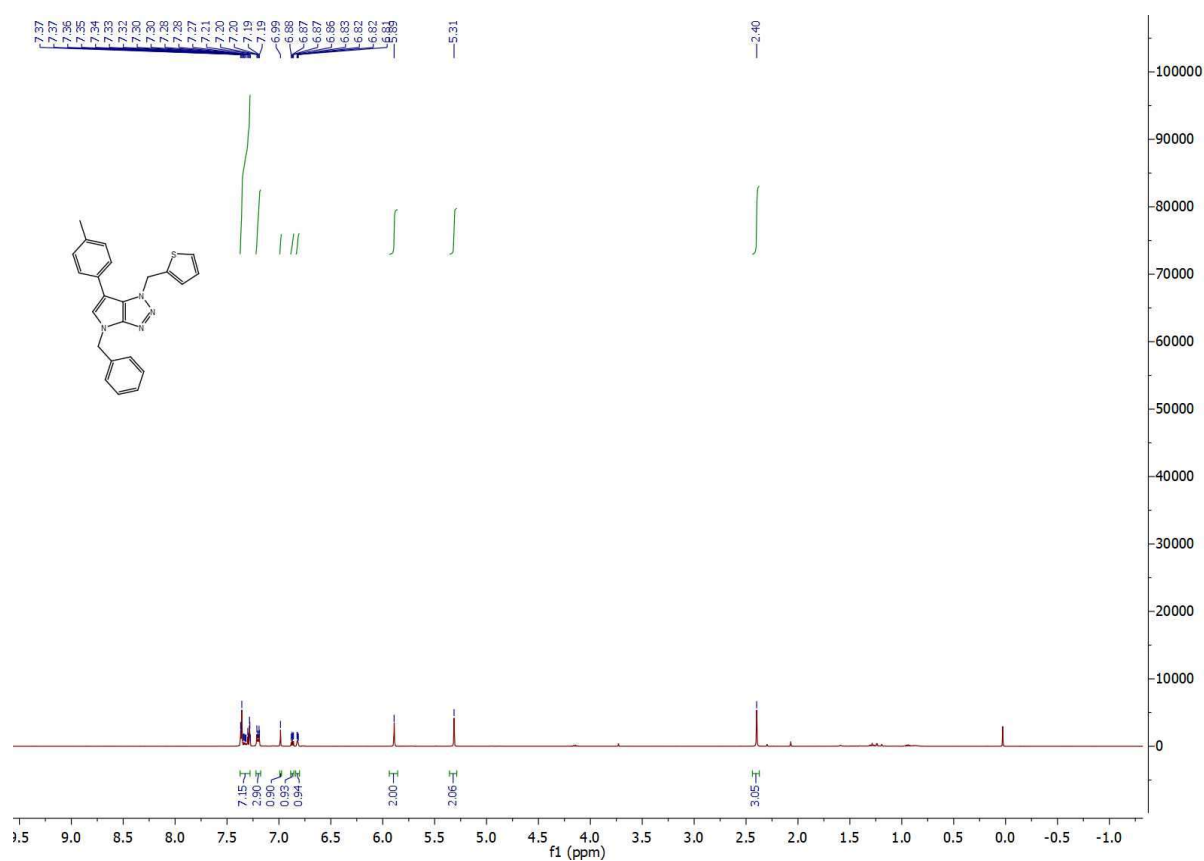


Figure S25. 4-(4-Benzyl-1-(4-methoxybenzyl)-1,4-dihydropyrrolo[2,3-*d*][1,2,3]triazol-6-yl)phenol (30).



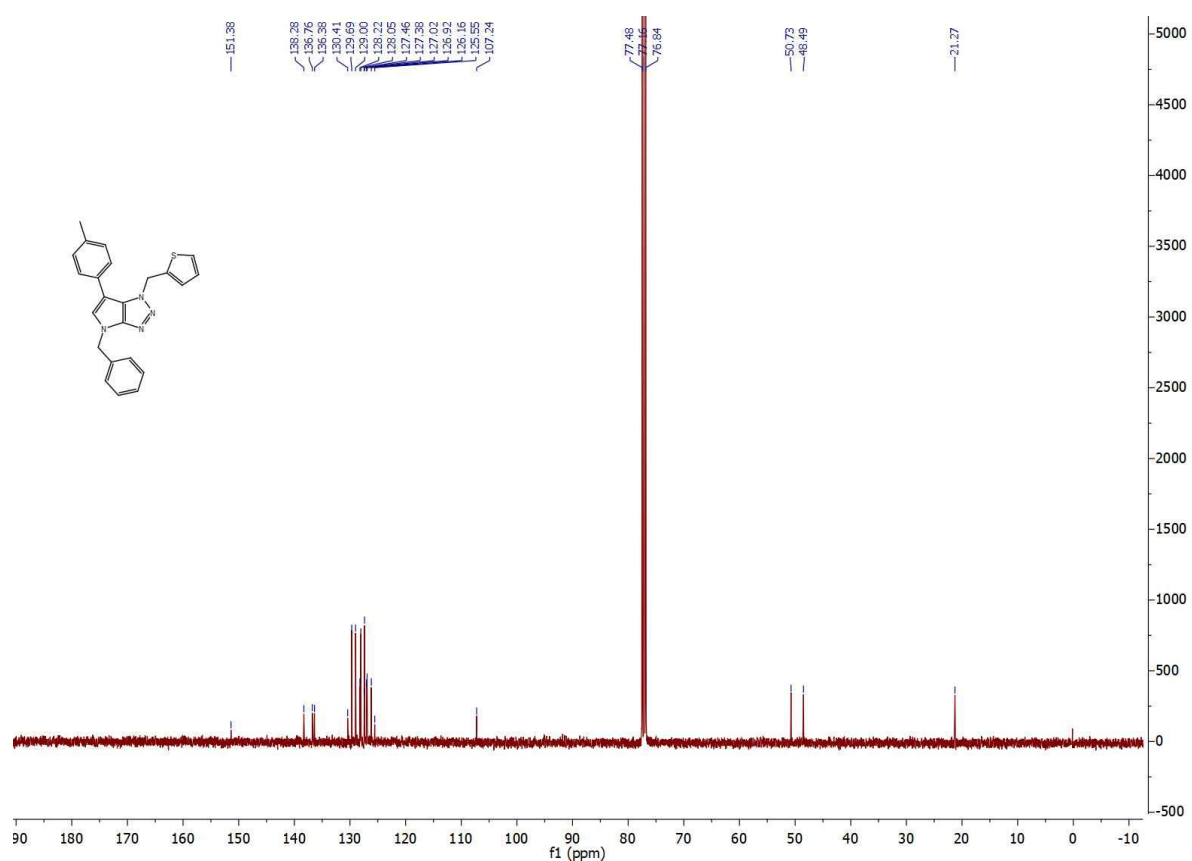
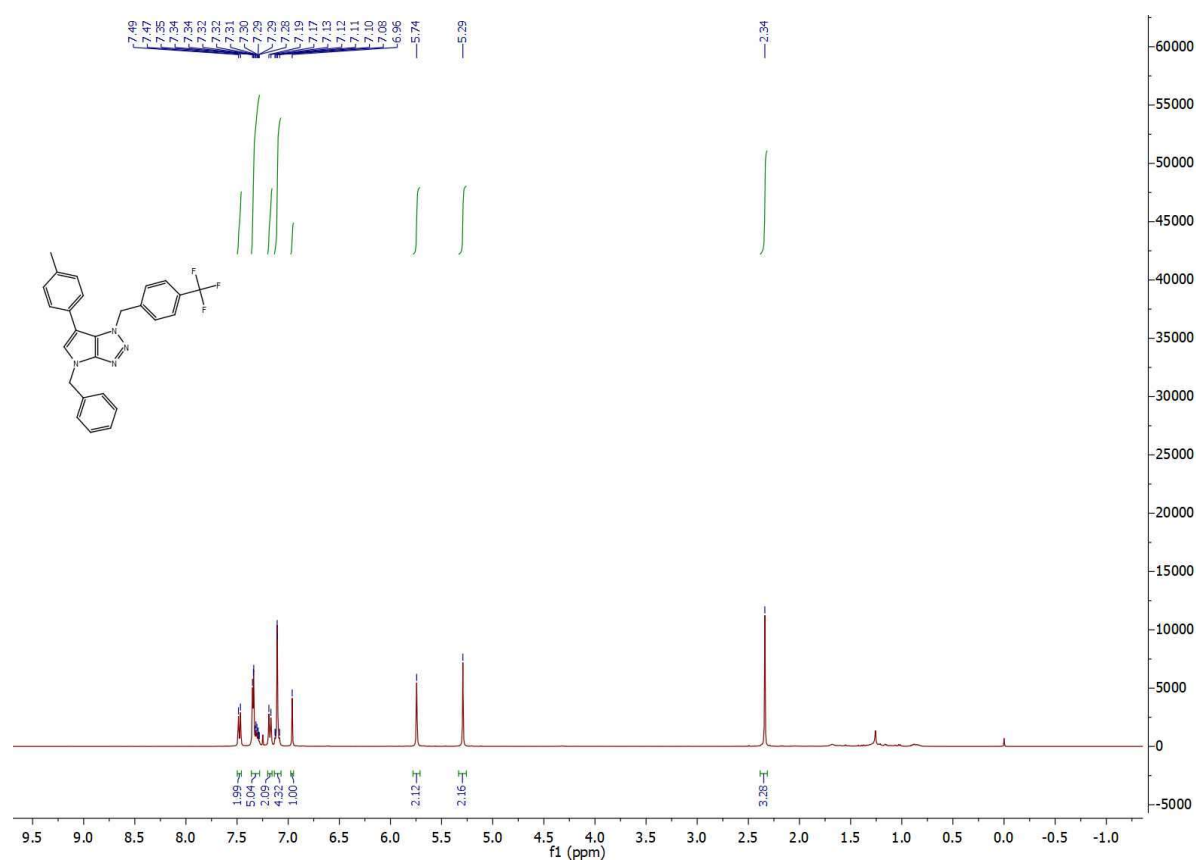


Figure S26. 4-Benzyl-1-(thiophen-2-ylmethyl)-6-(*p*-tolyl)-1,4-dihydropyrrolo[2,3-*d*][1,2,3]triazole (31).



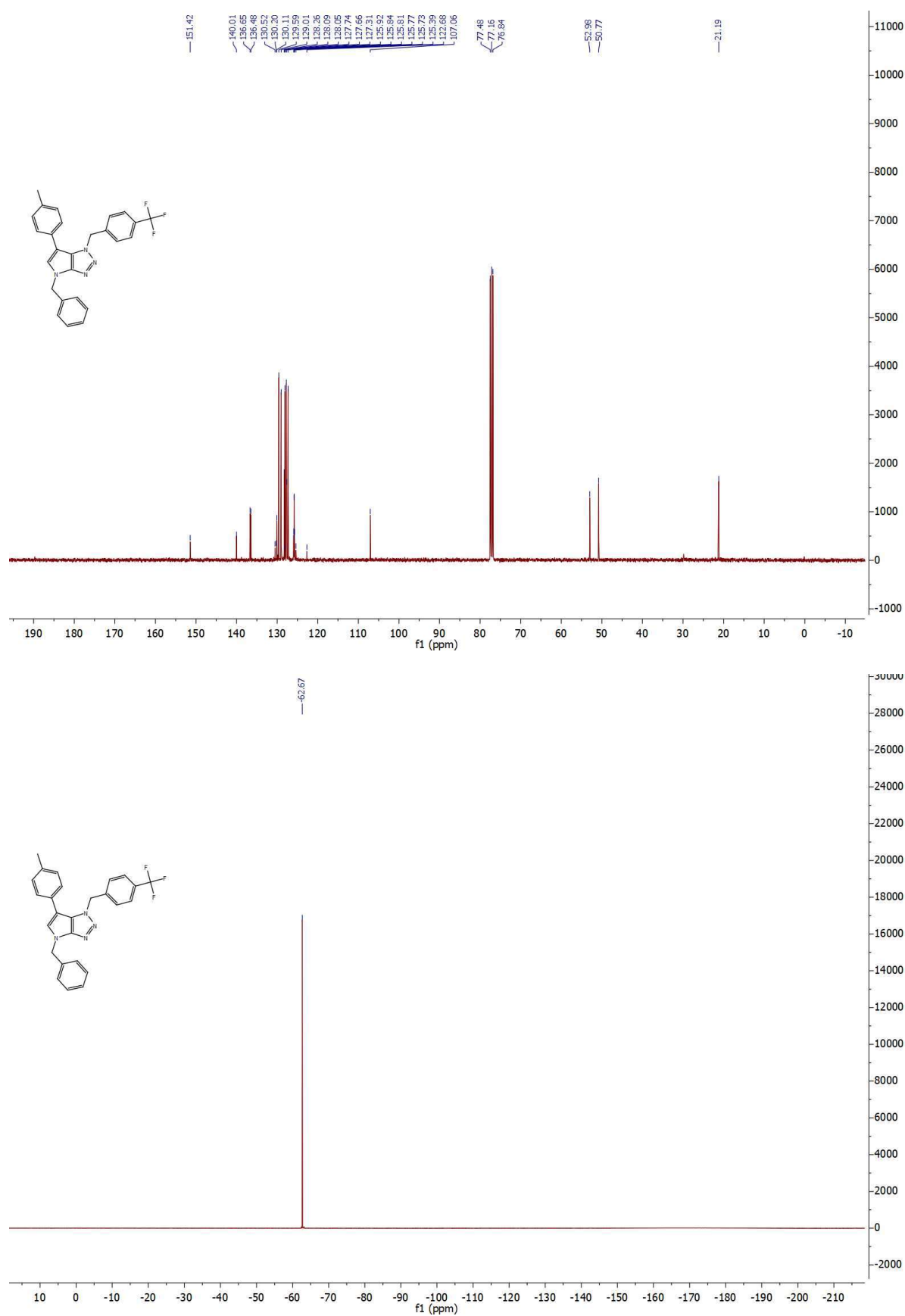


Figure S27. 4-Benzyl-6-(*p*-tolyl)-1-(4-(trifluoromethyl)benzyl)-1,4-dihydropyrrolo[2,3-*d*][1,2,3]triazole (32).

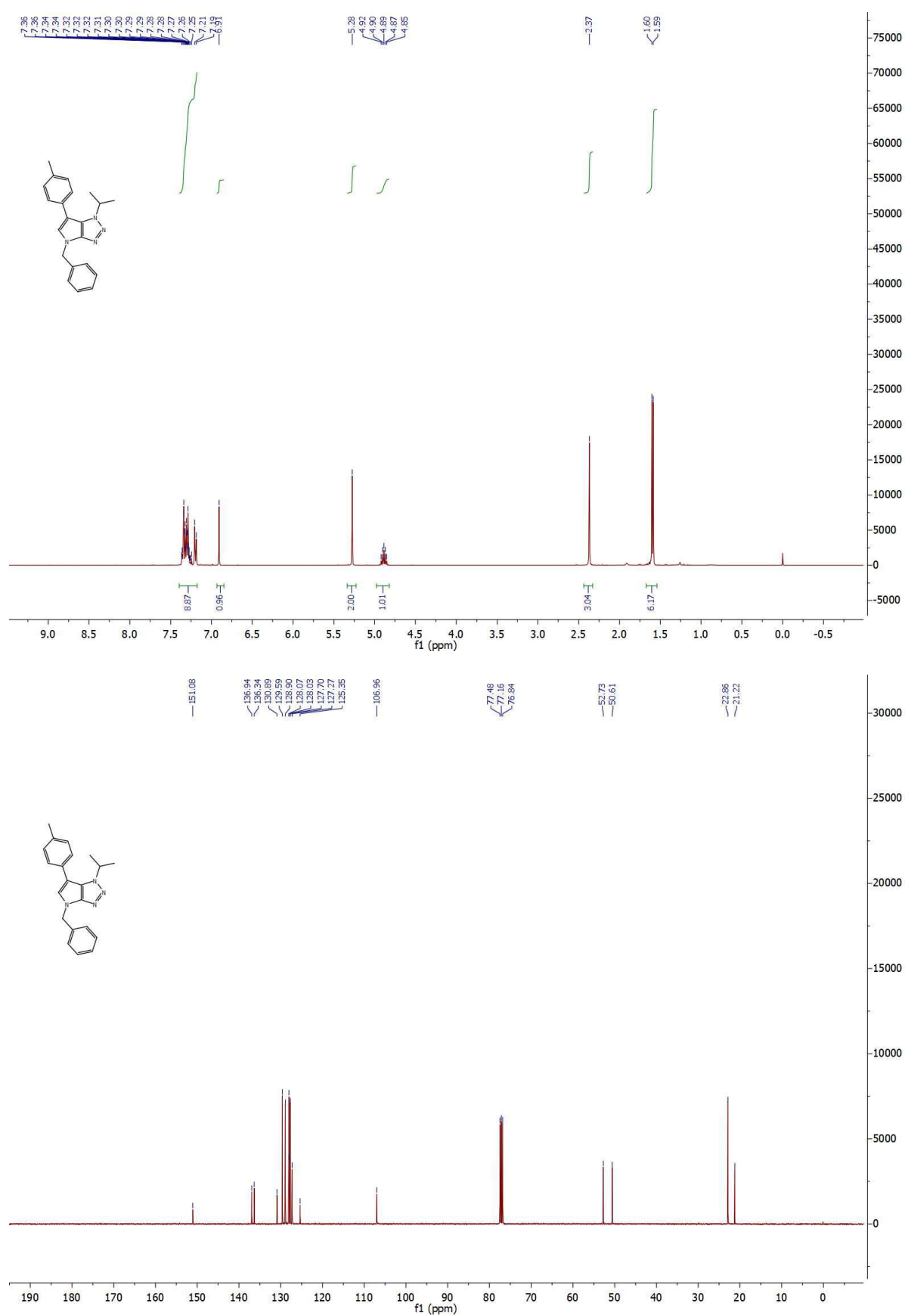


Figure S28. 4-Benzyl-1-isopropyl-6-(*p*-tolyl)-1,4-dihydropyrrolo[2,3-*d*][1,2,3]triazole (33).

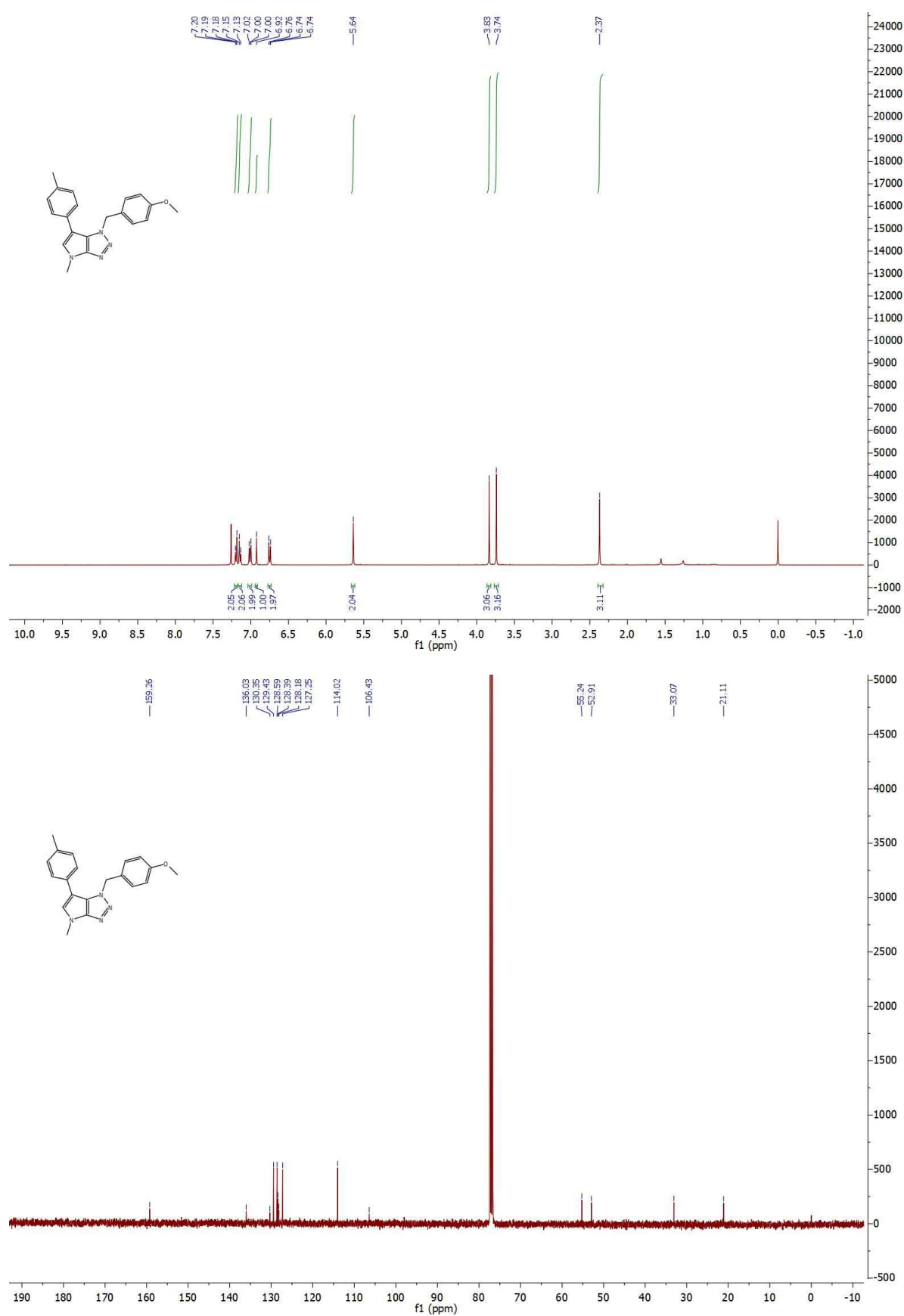


Figure S29. 1-(4-Methoxybenzyl)-4-methyl-6-(*p*-tolyl)-1,4-dihydropyrrolo[2,3-*d*][1,2,3]triazole (34).

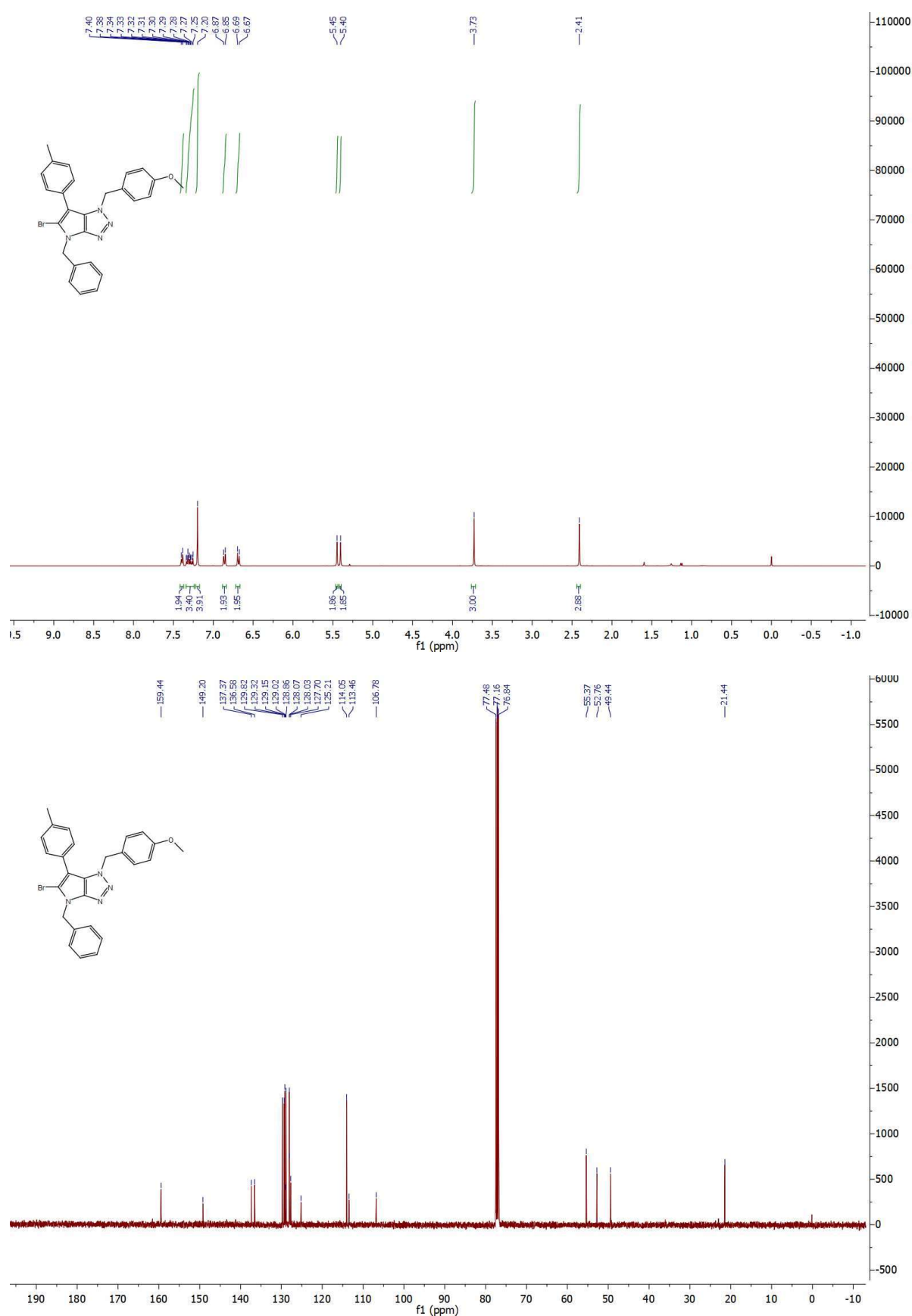
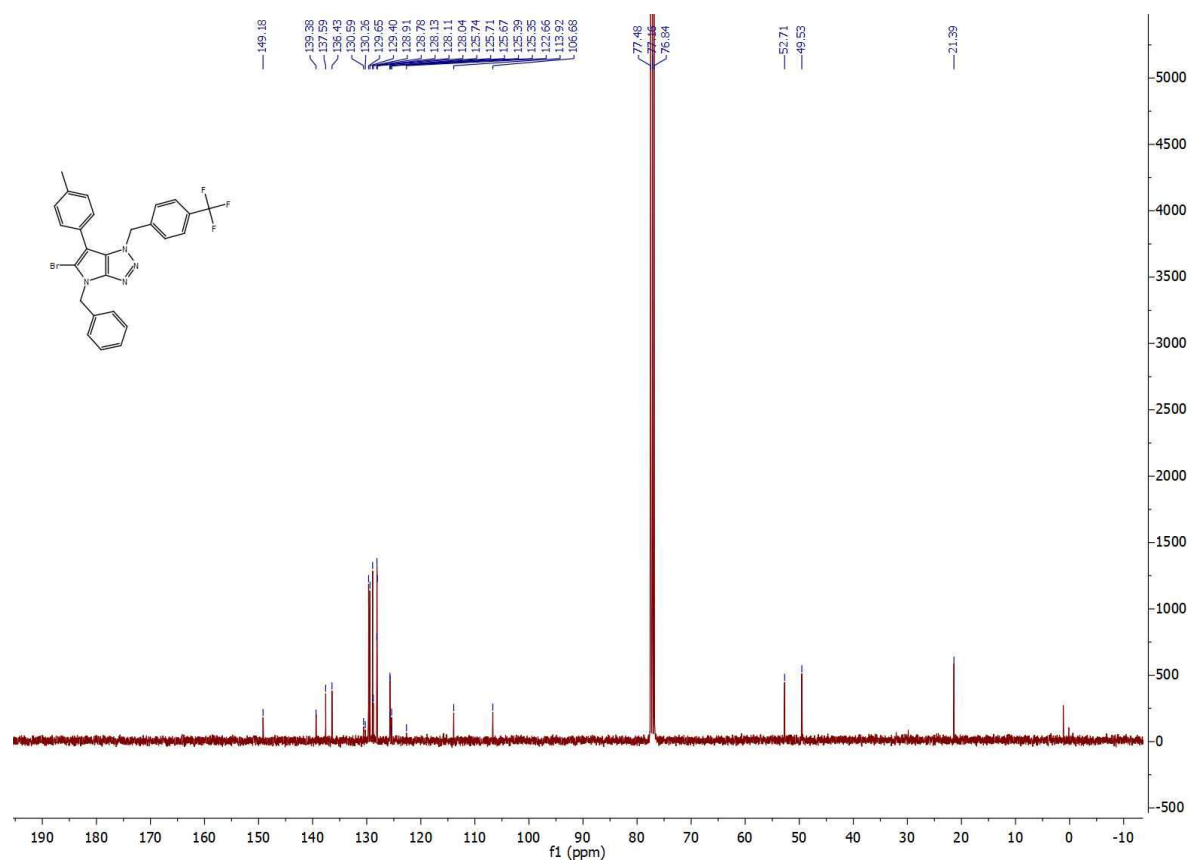
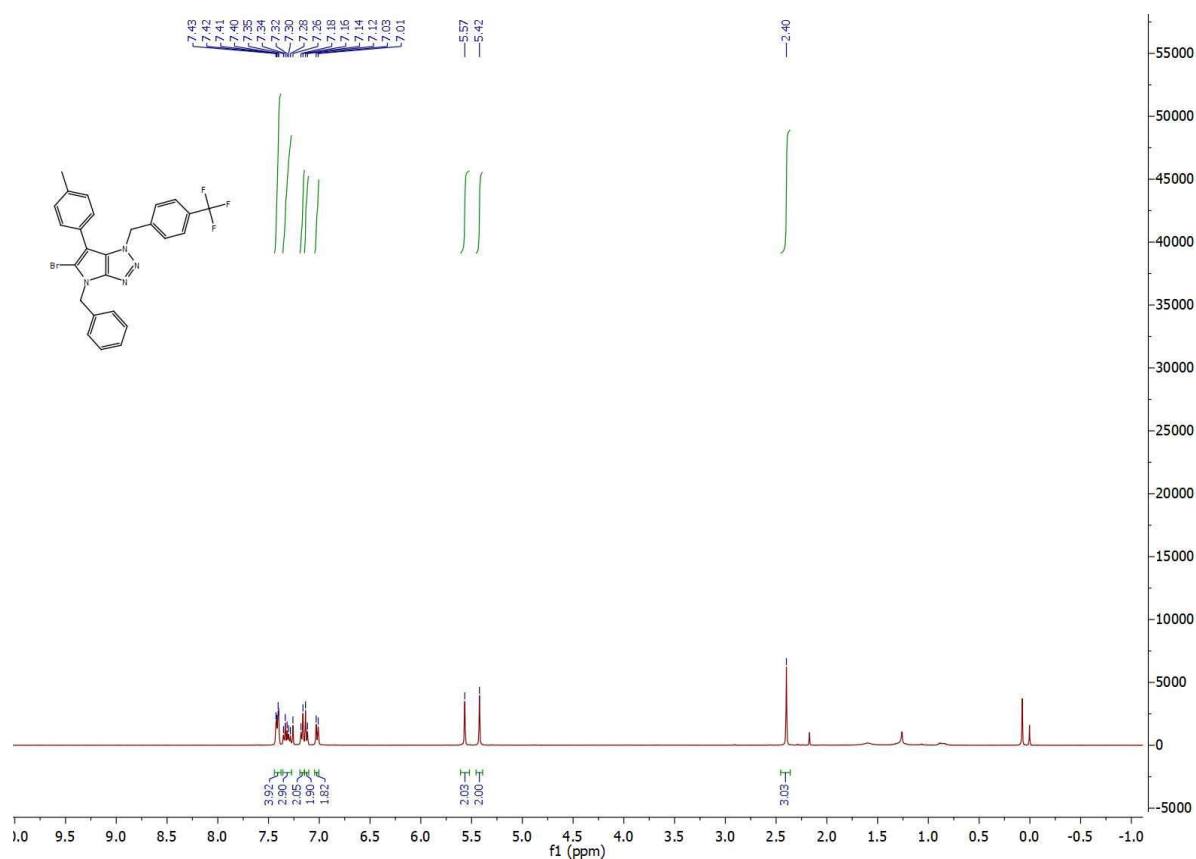


Figure S30. 4-Benzyl-5-bromo-1-(4-methoxybenzyl)-6-(*p*-tolyl)-1,4-dihydropyrrolo[2,3-*d*][1,2,3]triazole (35).



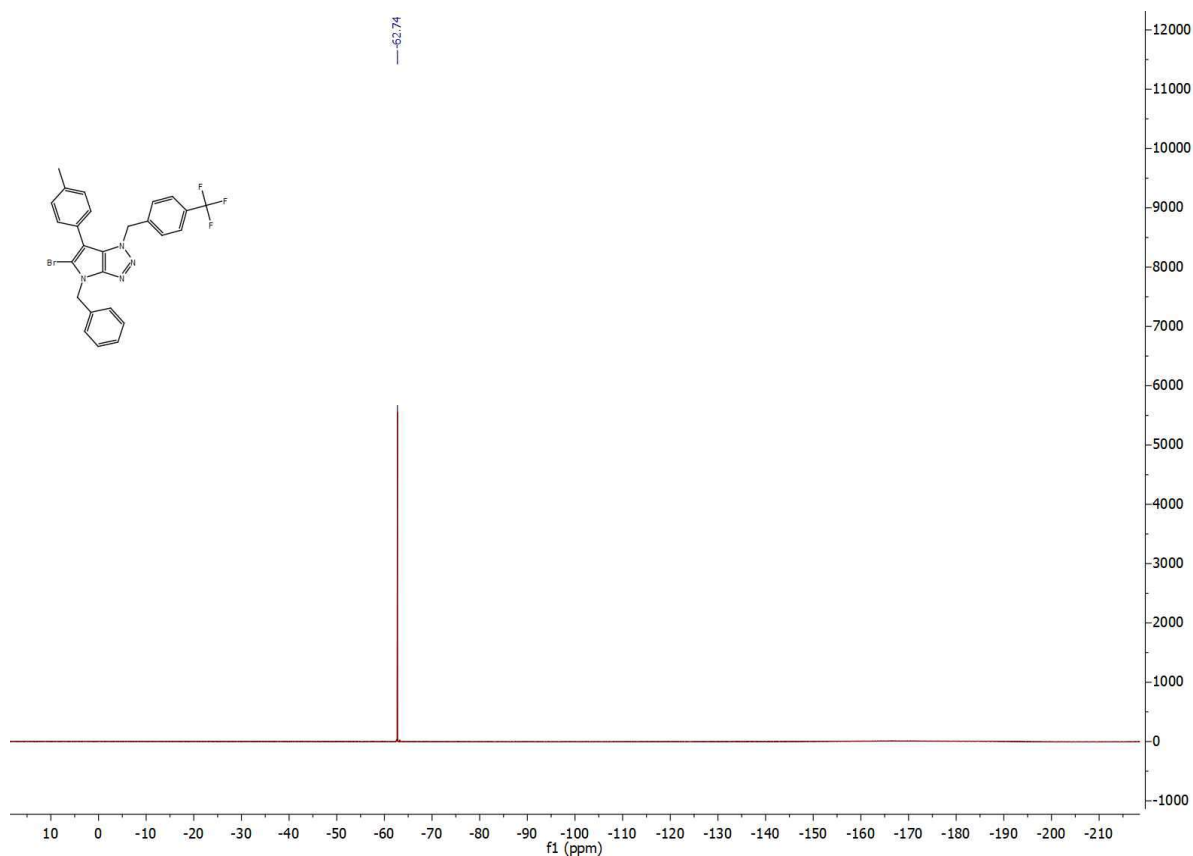
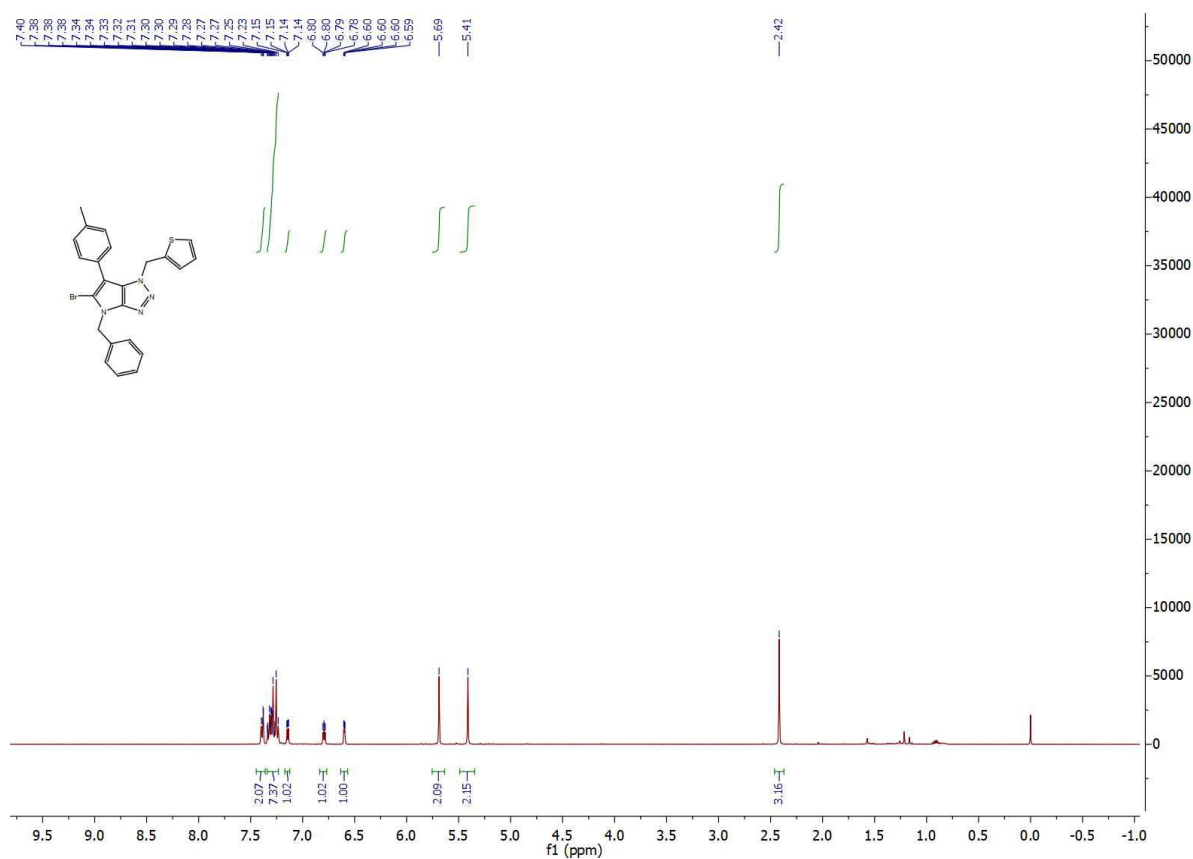


Figure S31. 4-Benzyl-5-bromo-6-(*p*-tolyl)-1-(4-(trifluoromethyl)benzyl)-1,4-dihydropyrrolo[2,3-*d*][1,2,3]triazole (36).



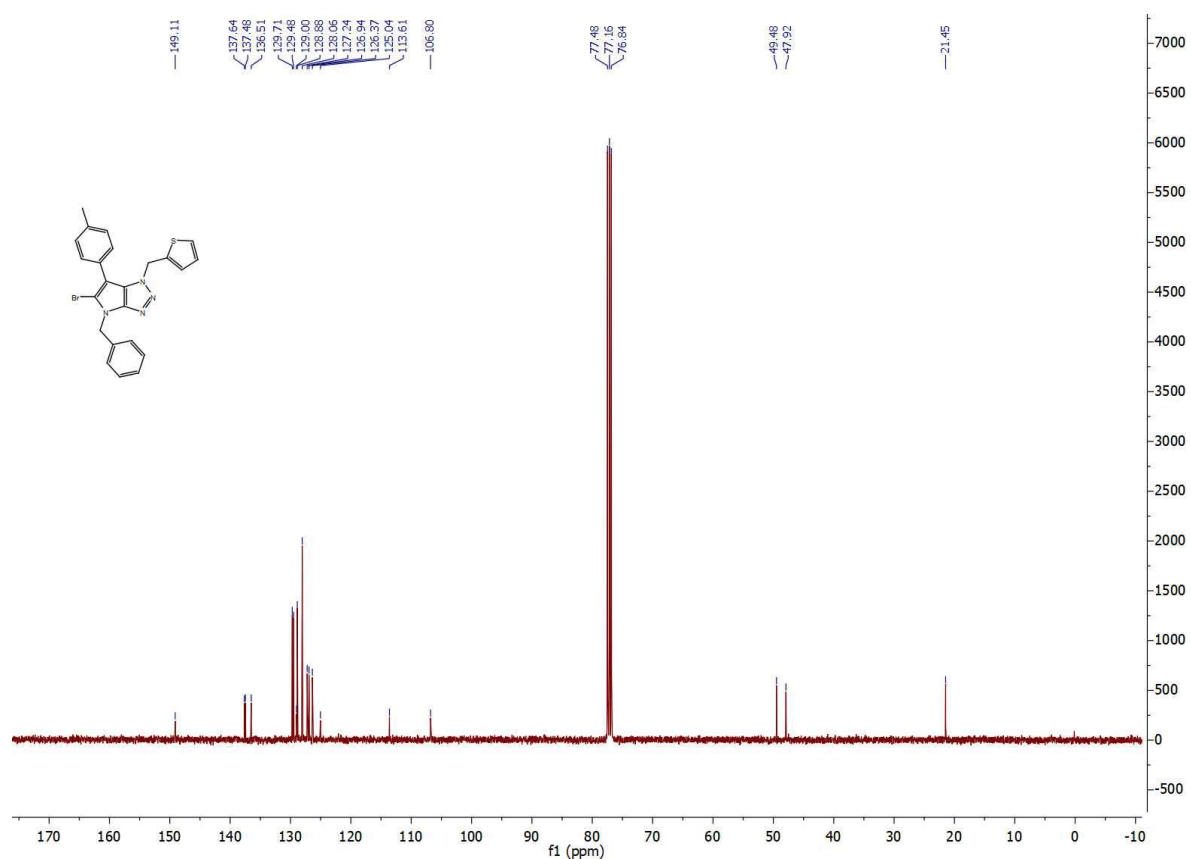
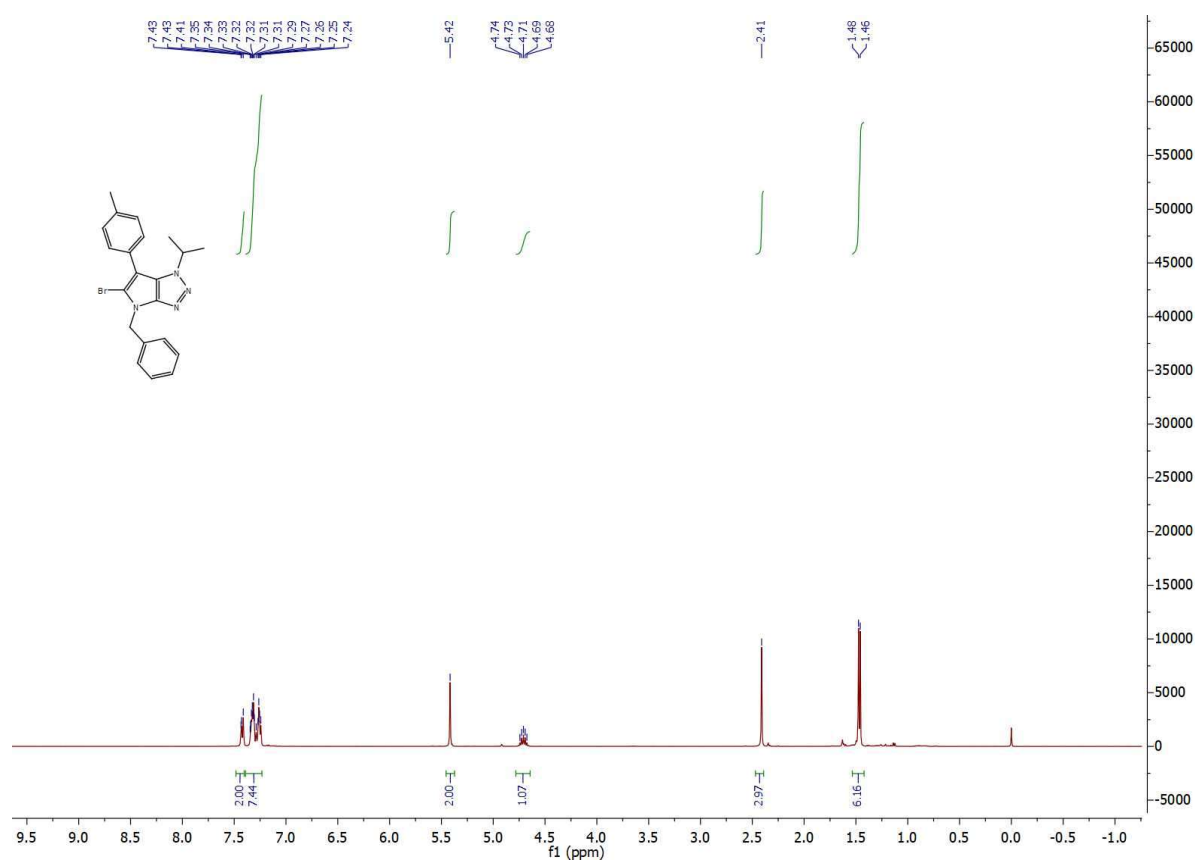


Figure S32. 4-Benzyl-5-bromo-1-(thiophen-2-ylmethyl)-6-(*p*-tolyl)-1,4-dihydropyrrolo[2,3-*d*][1,2,3]triazole (37).



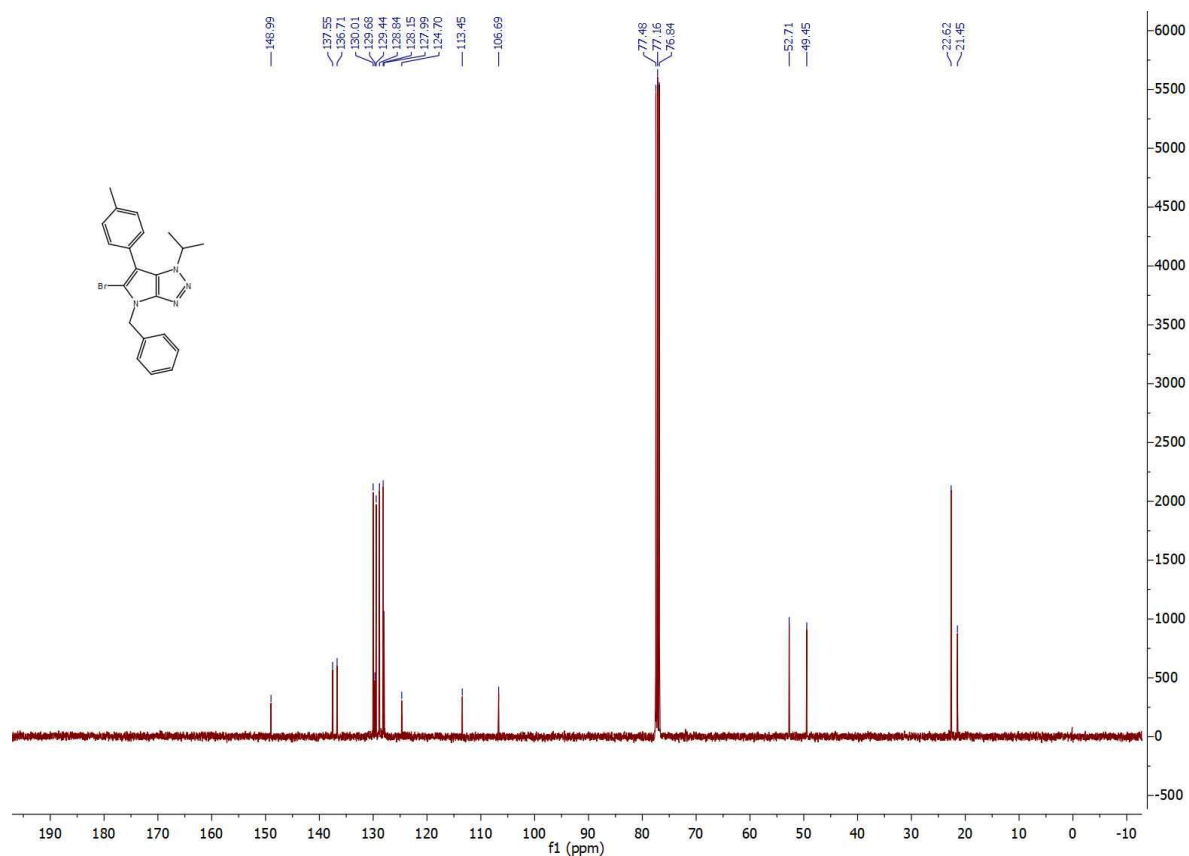
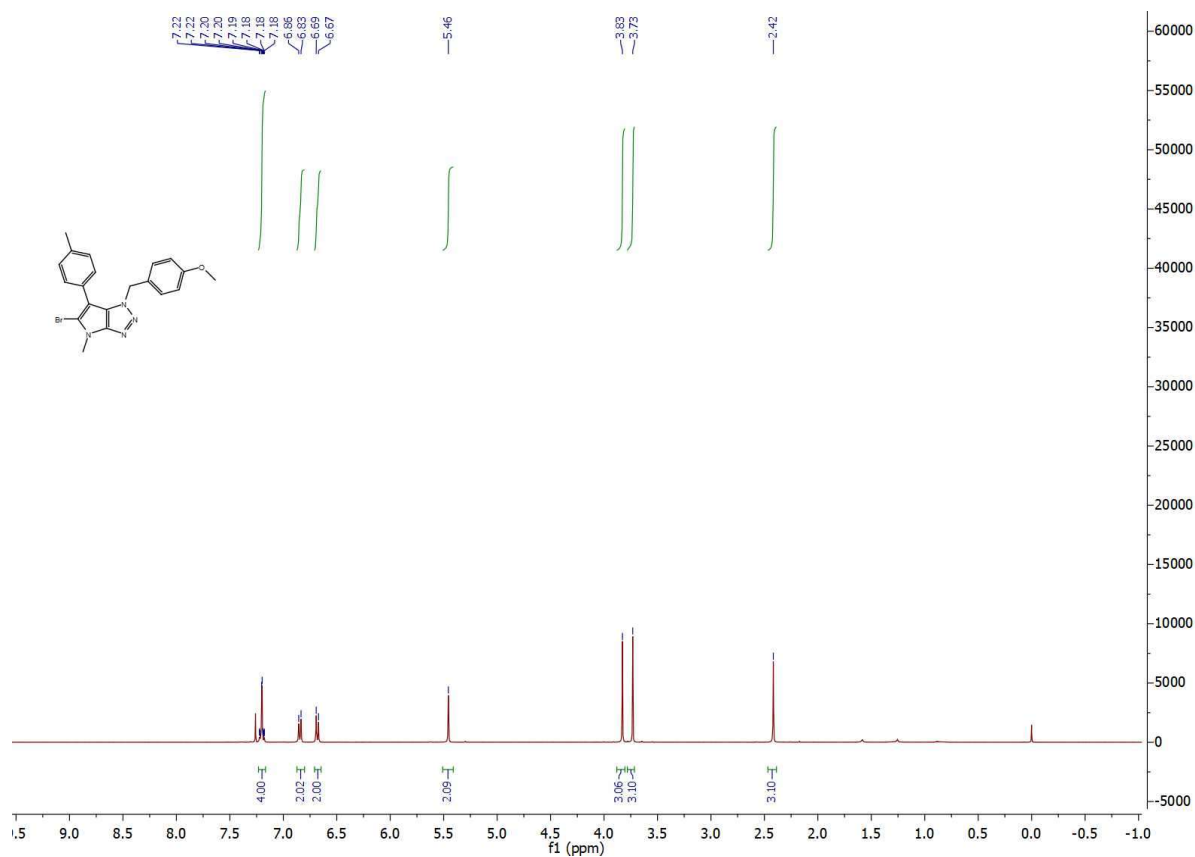
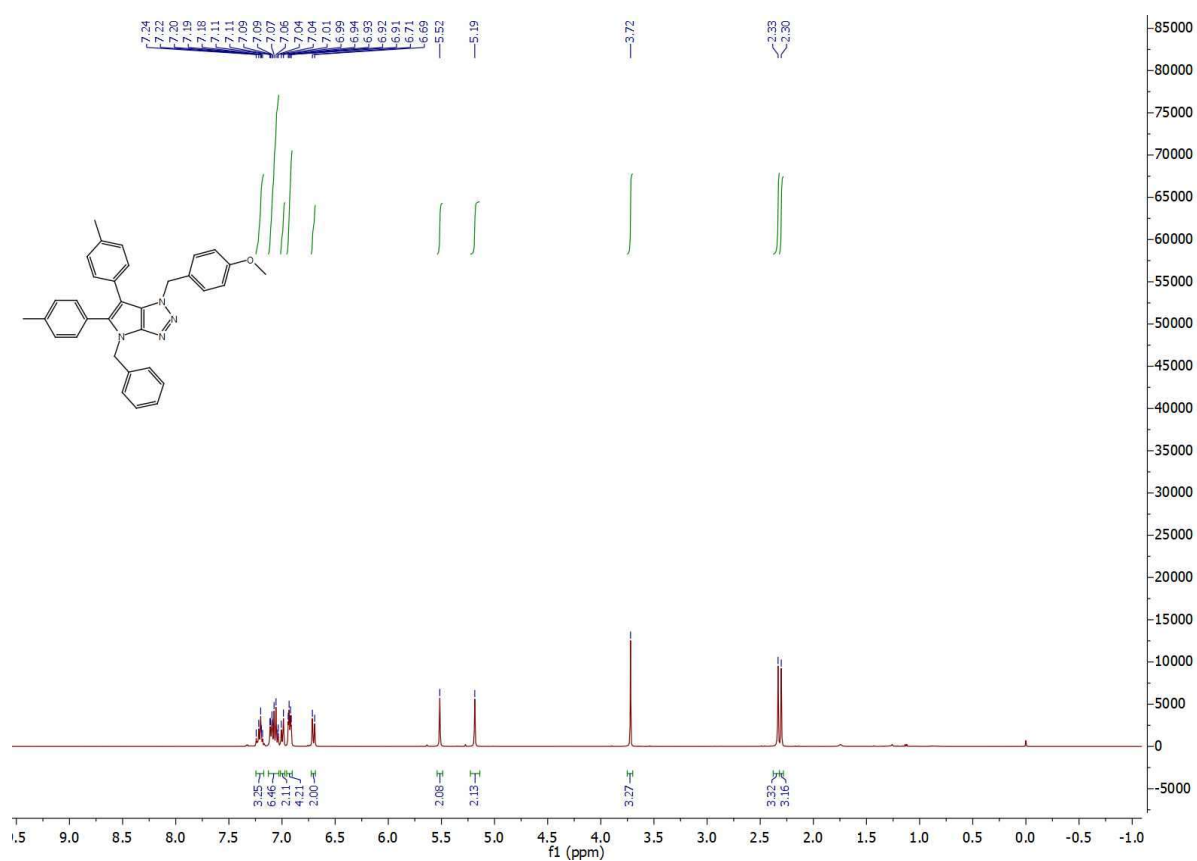
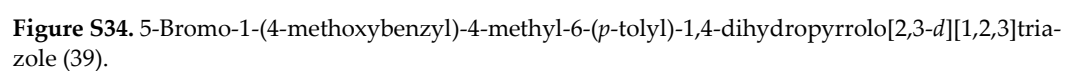


Figure S33. 4-Benzyl-5-bromo-1-isopropyl-6-(*p*-tolyl)-1,4-dihydropyrrolo[2,3-*d*][1,2,3]triazole (38).





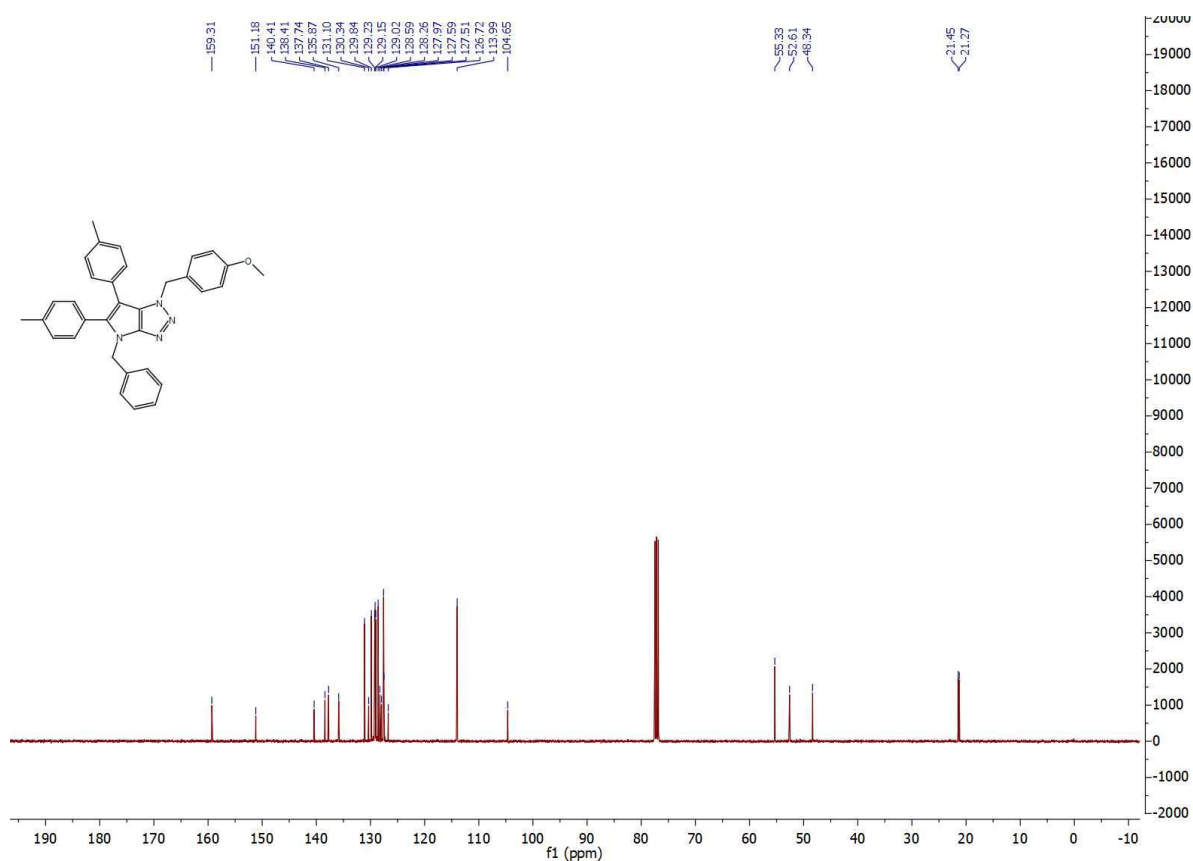
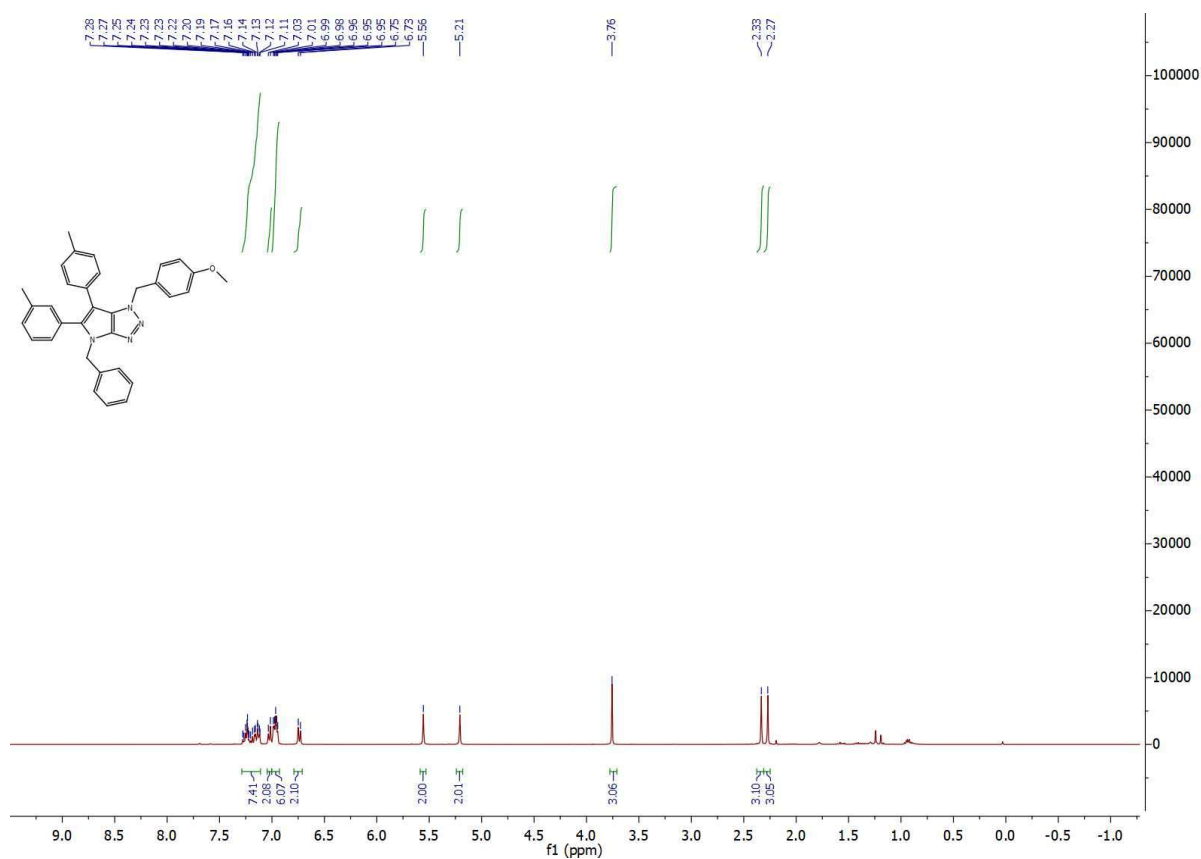


Figure S35. 4-Benzyl-1-(4-methoxybenzyl)-5,6-di-*p*-tolyl-1,4-dihydropyrrolo[2,3-*d*][1,2,3]triazole (40).



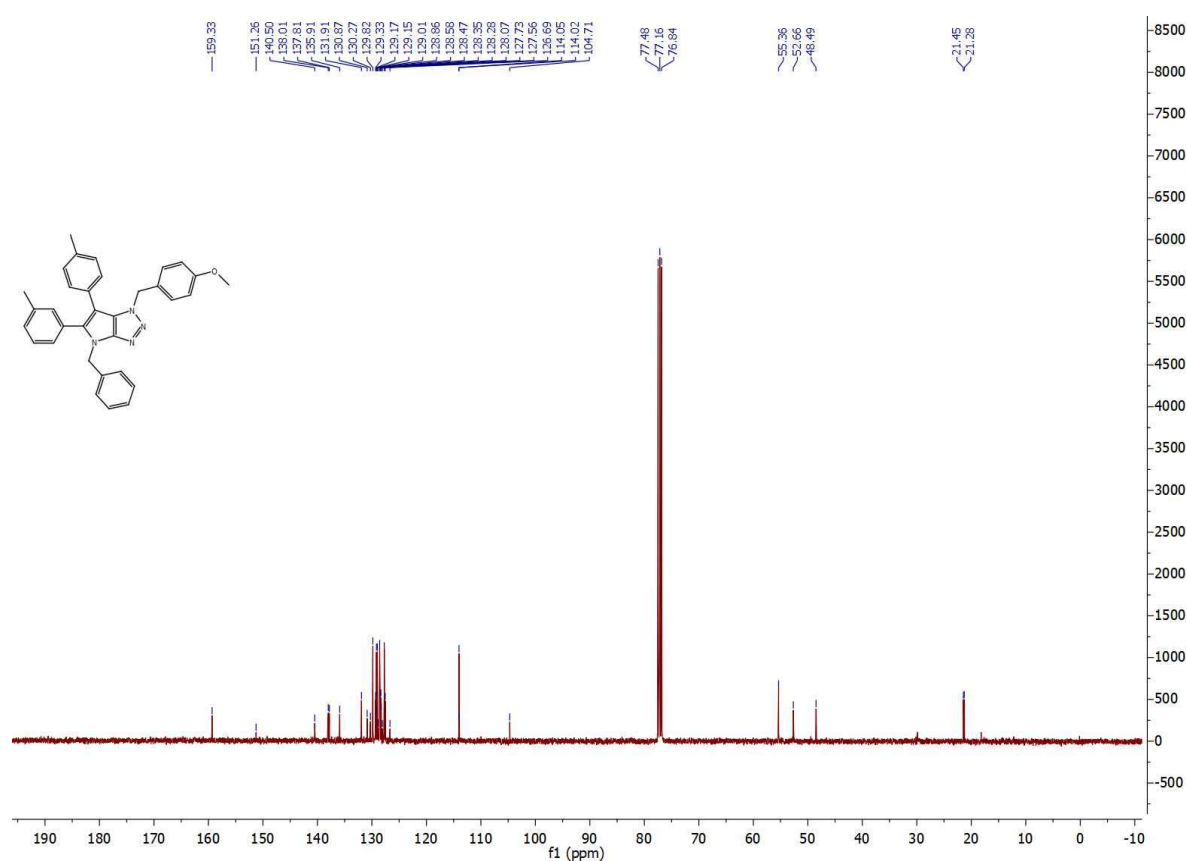
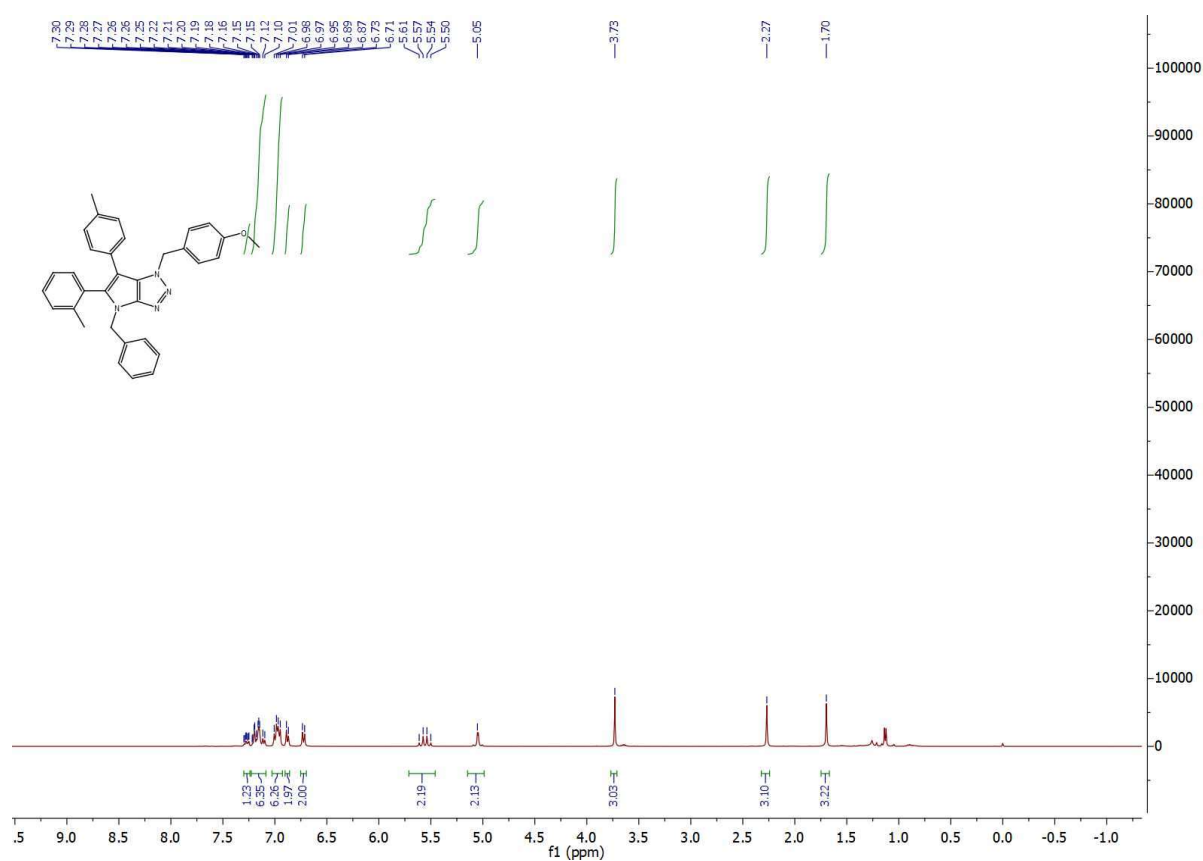


Figure S36. 4-Benzyl-1-(4-methoxybenzyl)-5-(*m*-tolyl)-6-(*p*-tolyl)-1,4-dihydropyrrolo[2,3-*d*][1,2,3]triazole (41).



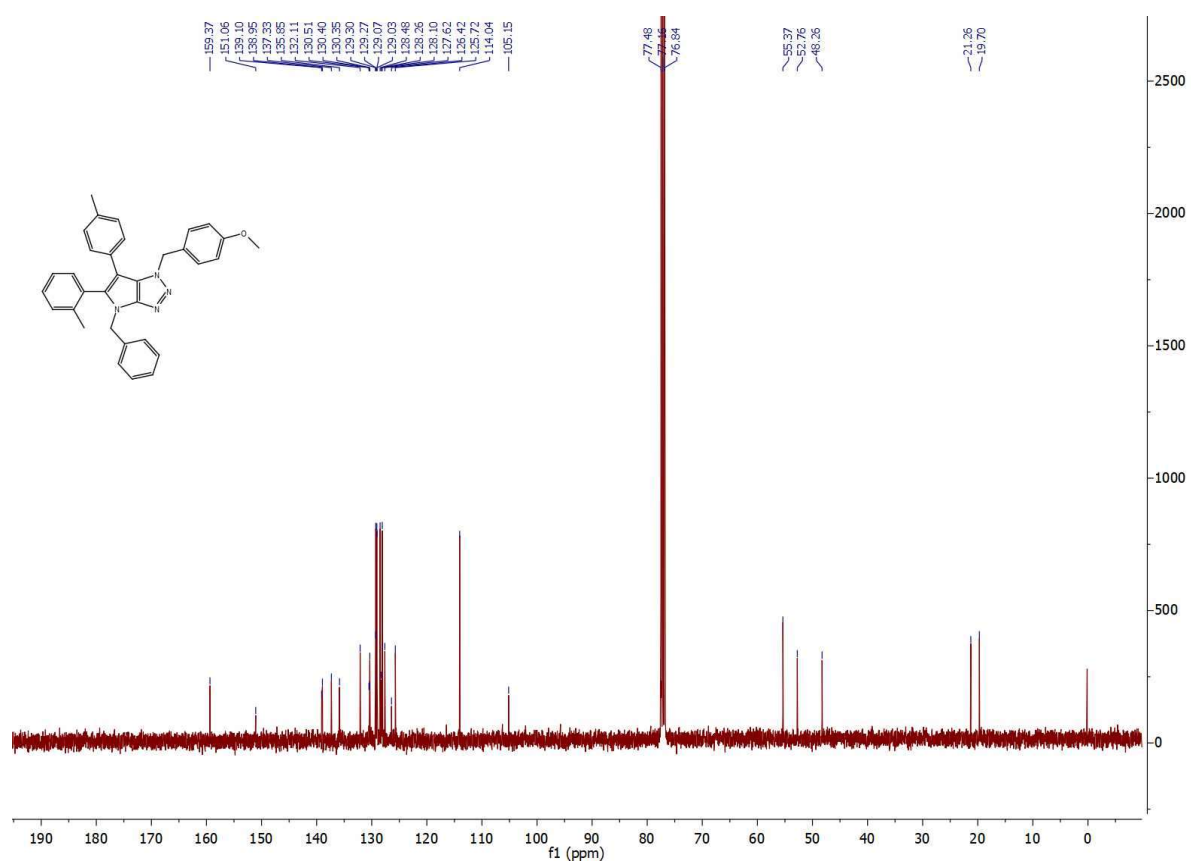
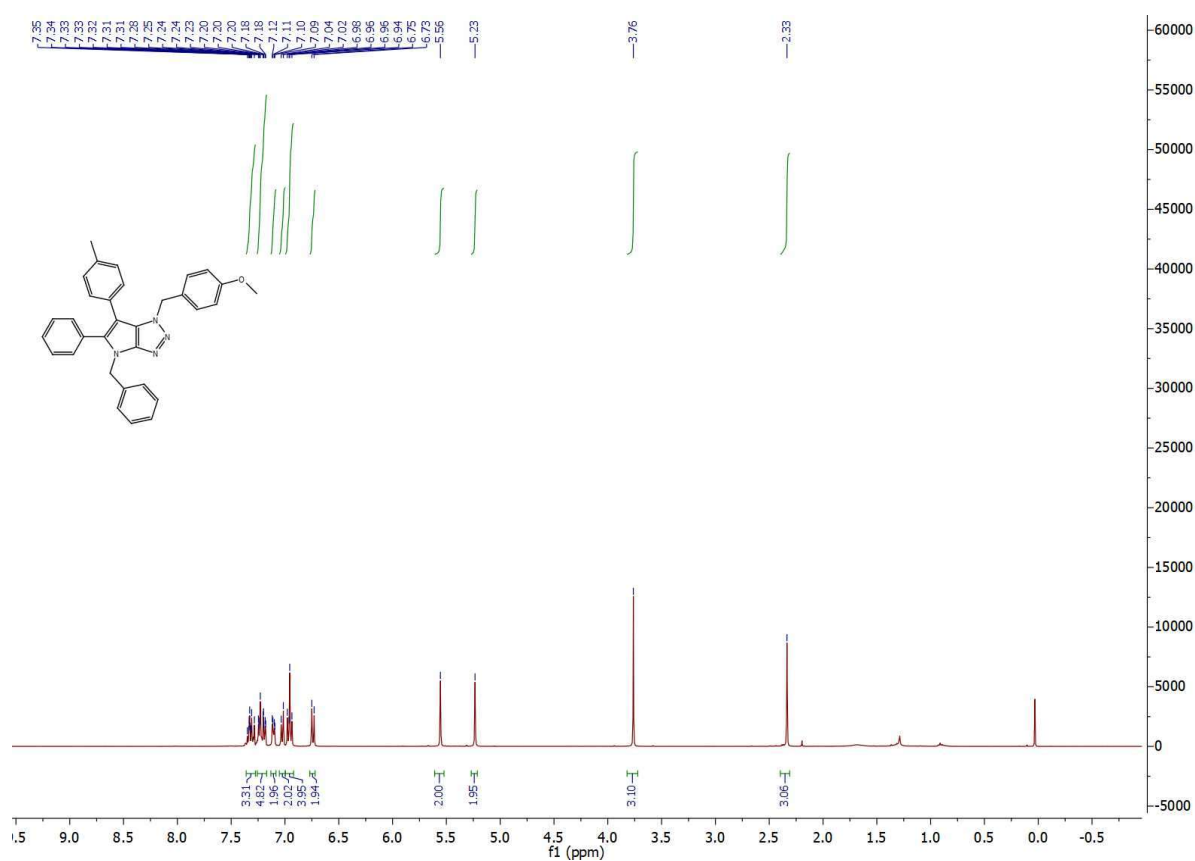


Figure S37. 4-Benzyl-1-(4-methoxybenzyl)-5-(*o*-tolyl)-6-(*p*-tolyl)-1,4-dihydropyrrolo[2,3-*d*][1,2,3]triazole (42).



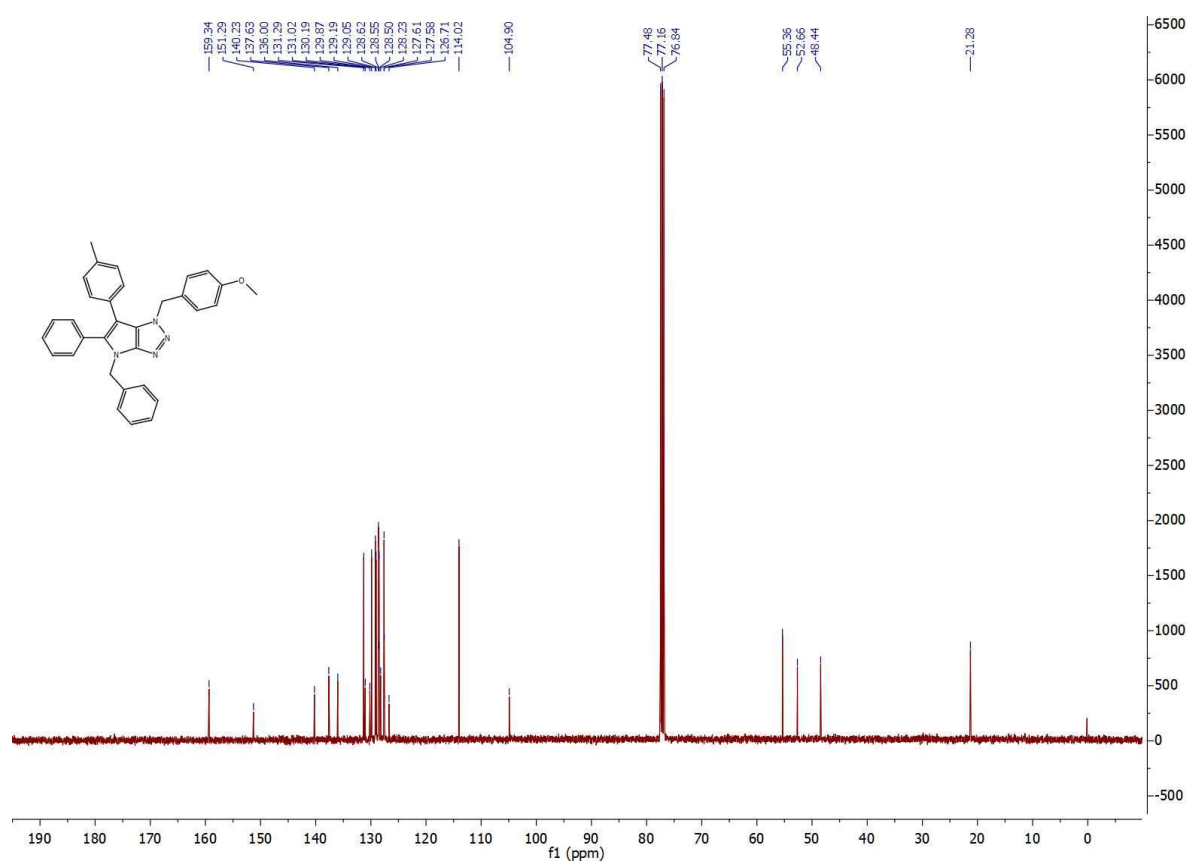
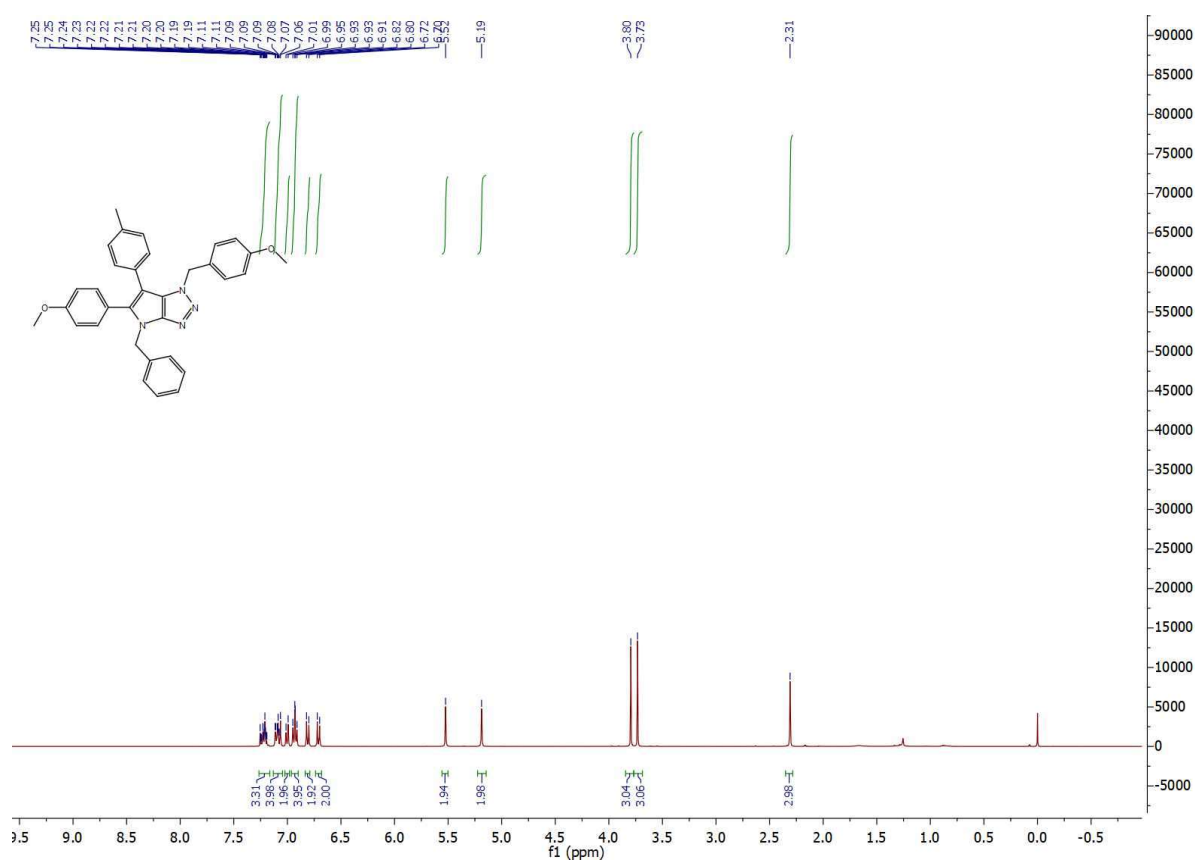


Figure S38. 4-(Benzyl-1-(4-methoxybenzyl)-5-phenyl-6-(*p*-tolyl)-1,4-dihydropyrrolo[2,3-*d*][1,2,3]triazole (43).



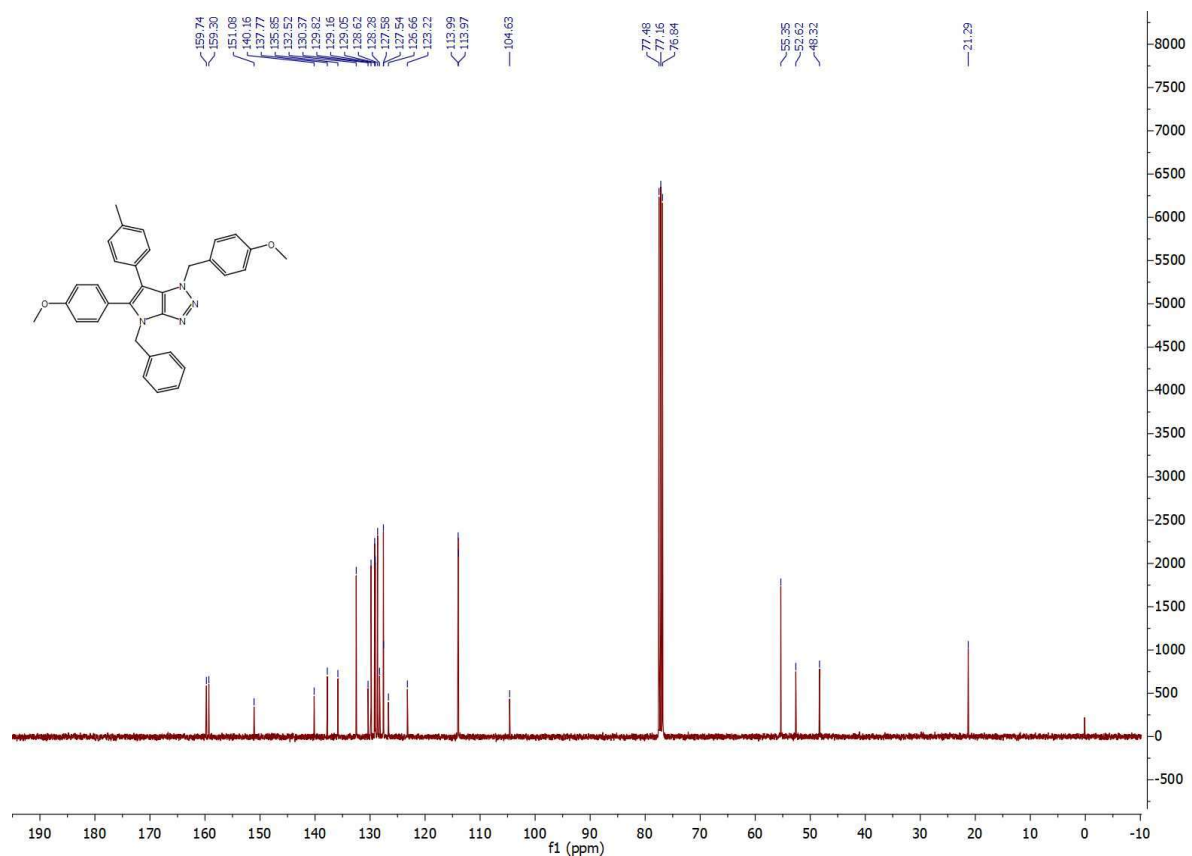
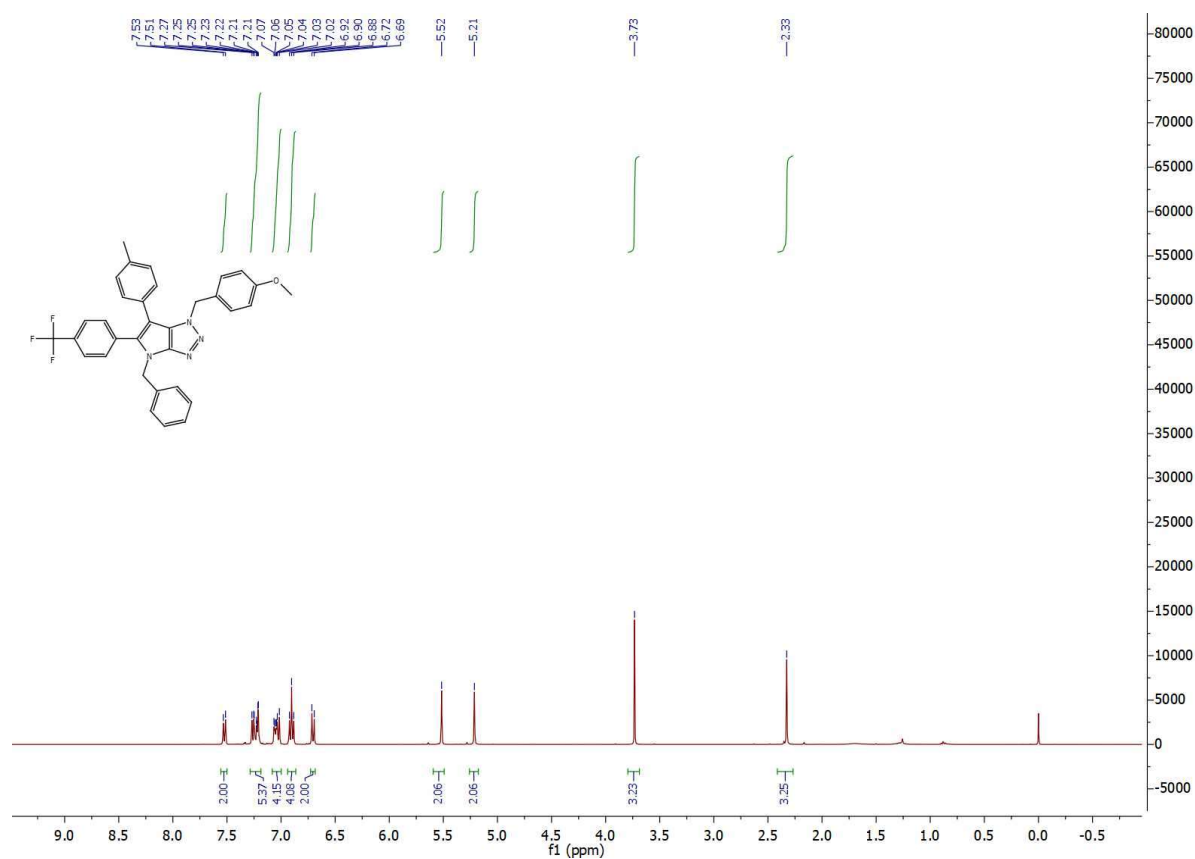
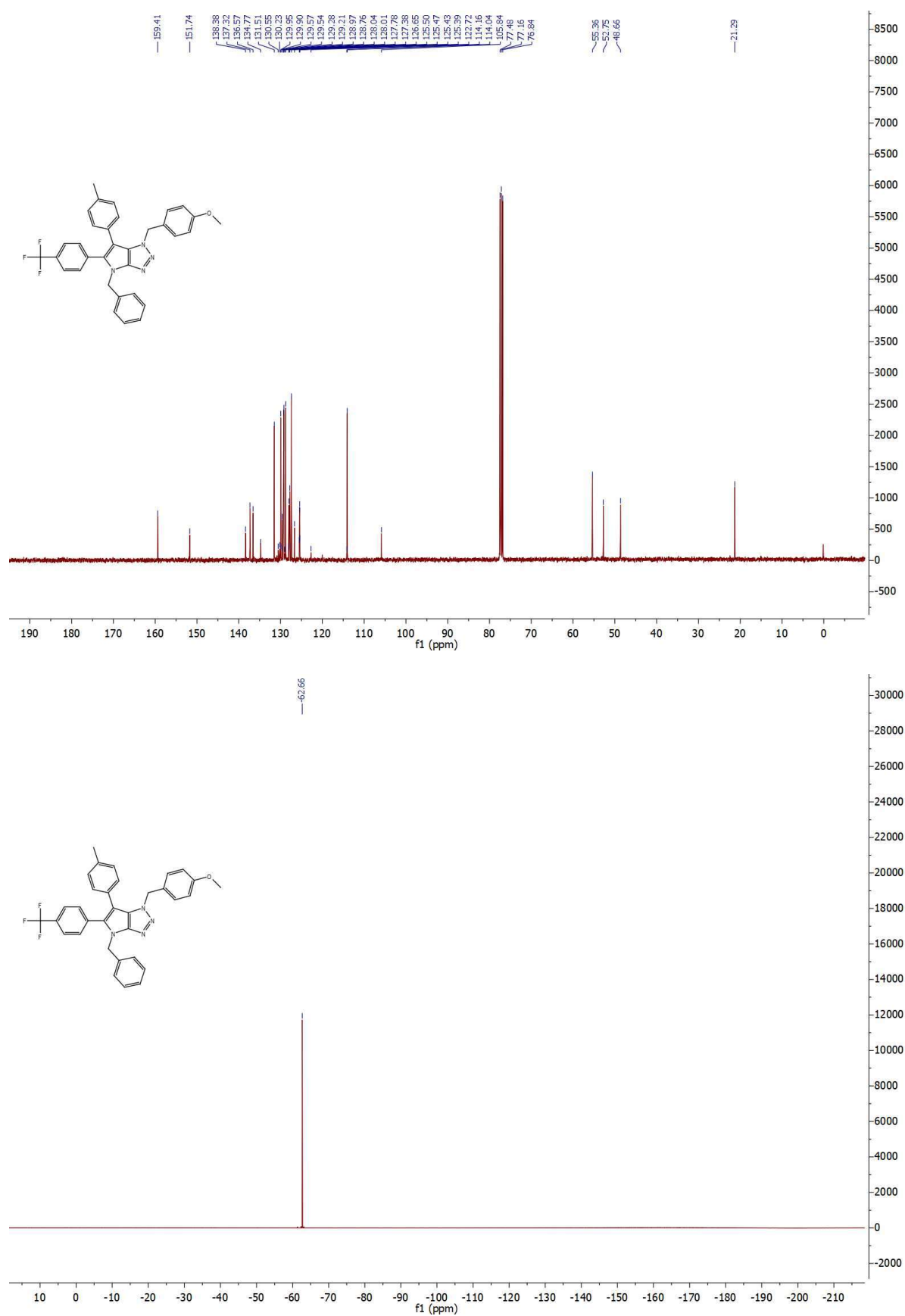


Figure S39. 4-(Benzyl-1-(4-methoxybenzyl)-5-(4-methoxyphenyl)-6-(*p*-tolyl)-1,4-dihydro-pyrrolo[2,3-*d*][1,2,3]triazole (44).





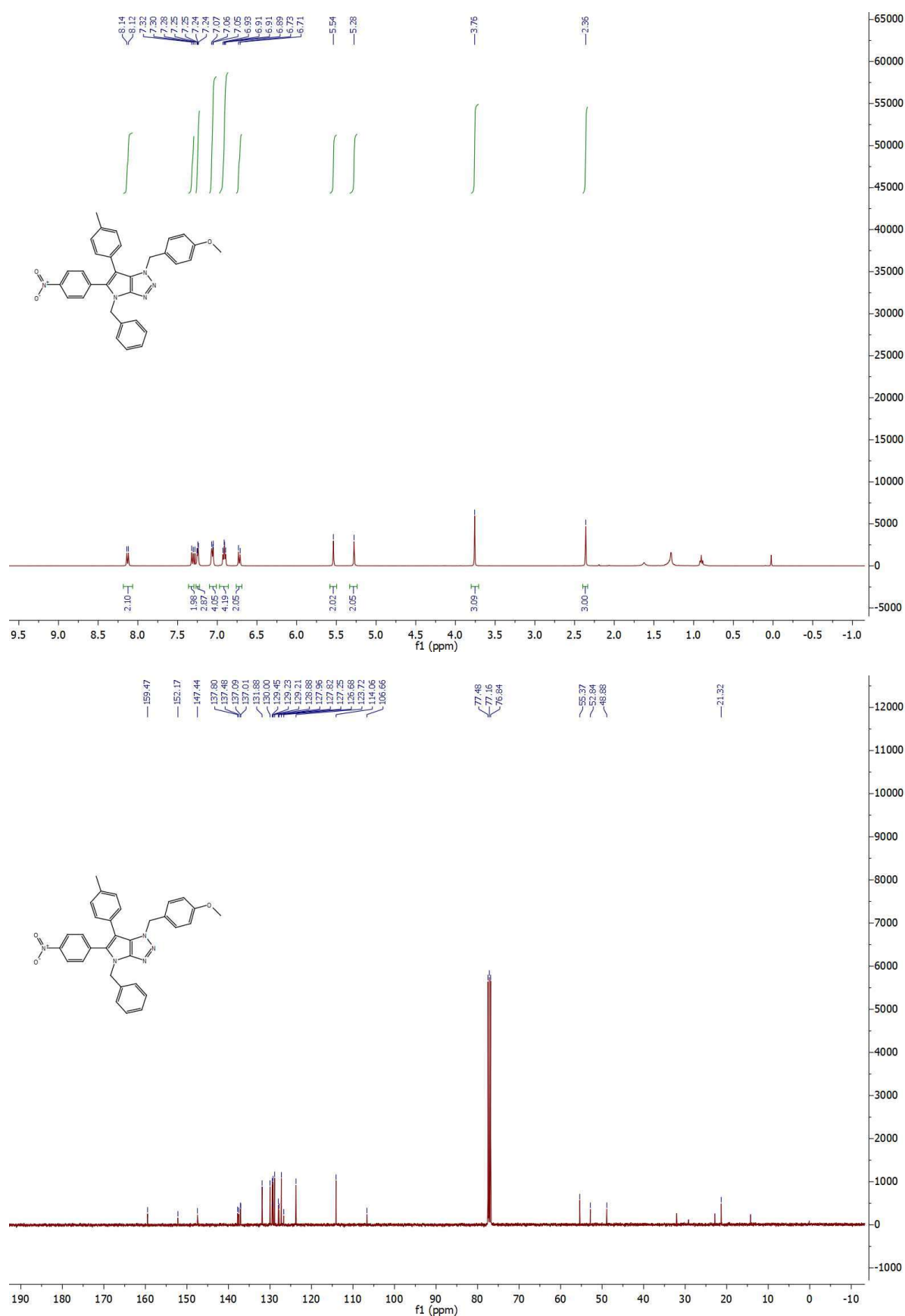


Figure S41. 4-(Benzyl-1-(4-methoxybenzyl)-5-(4-nitrophenyl)-6-(*p*-tolyl)-1,4-dihydropyrrolo[2,3-*d*][1,2,3]triazole (46).

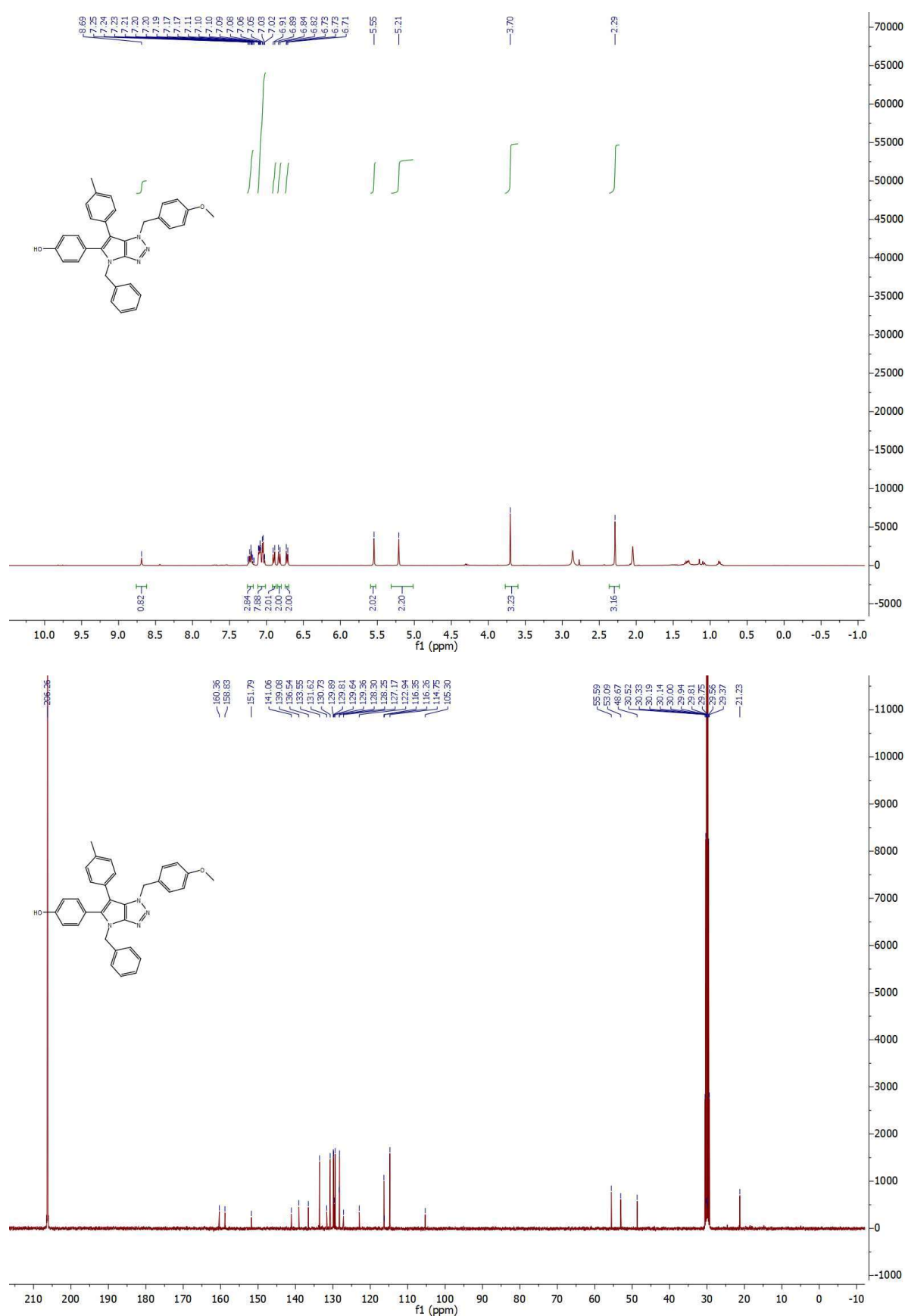


Figure S42. 4-(Benzyl-1-(4-methoxybenzyl)-6-(*p*-tolyl)-1,4-dihydropyrrolo[2,3-*d*][1,2,3]triazol-5-yl)phenol (47).

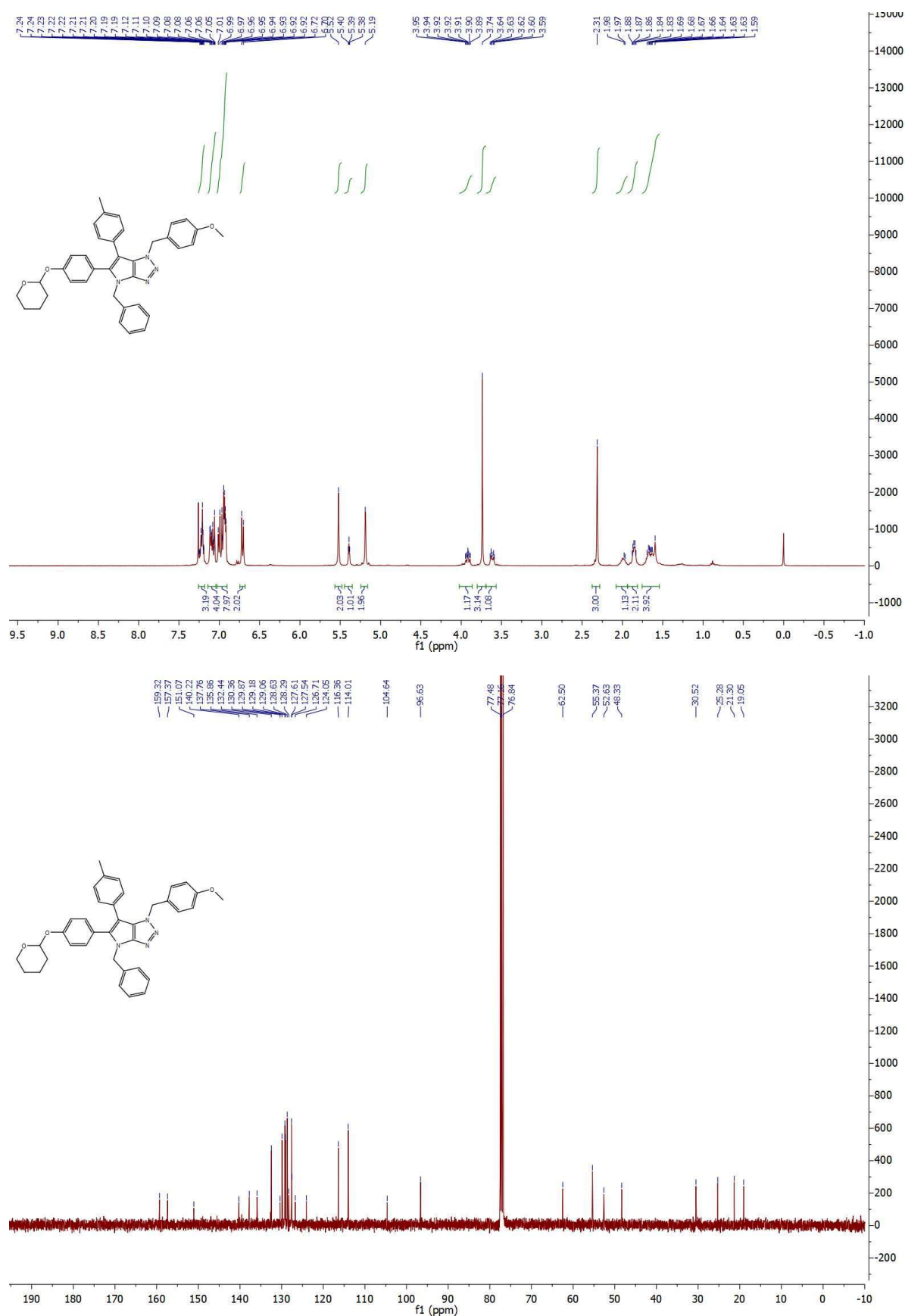
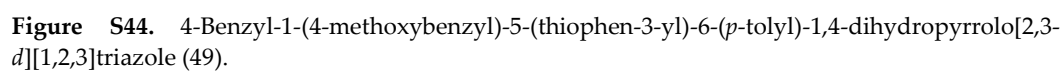


Figure S43. 4-Benzyl-1-(4-methoxybenzyl)-5-(4-((tetrahydro-2H-pyran-2-yl)oxy)phenyl)-6-(p-tolyl)-1,4-dihydropyrrolo[2,3-d][1,2,3]triazol-5-yl) (48).



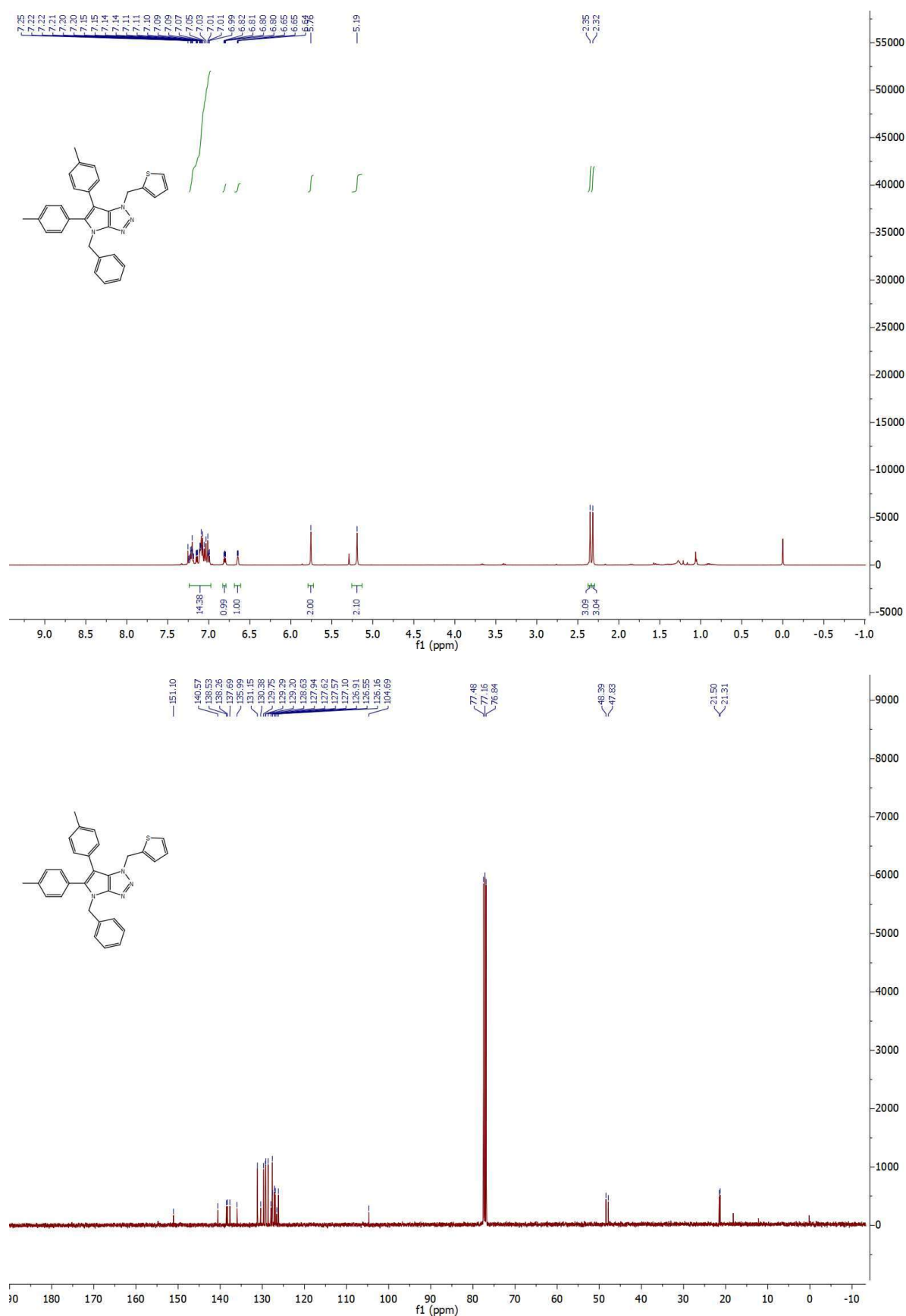
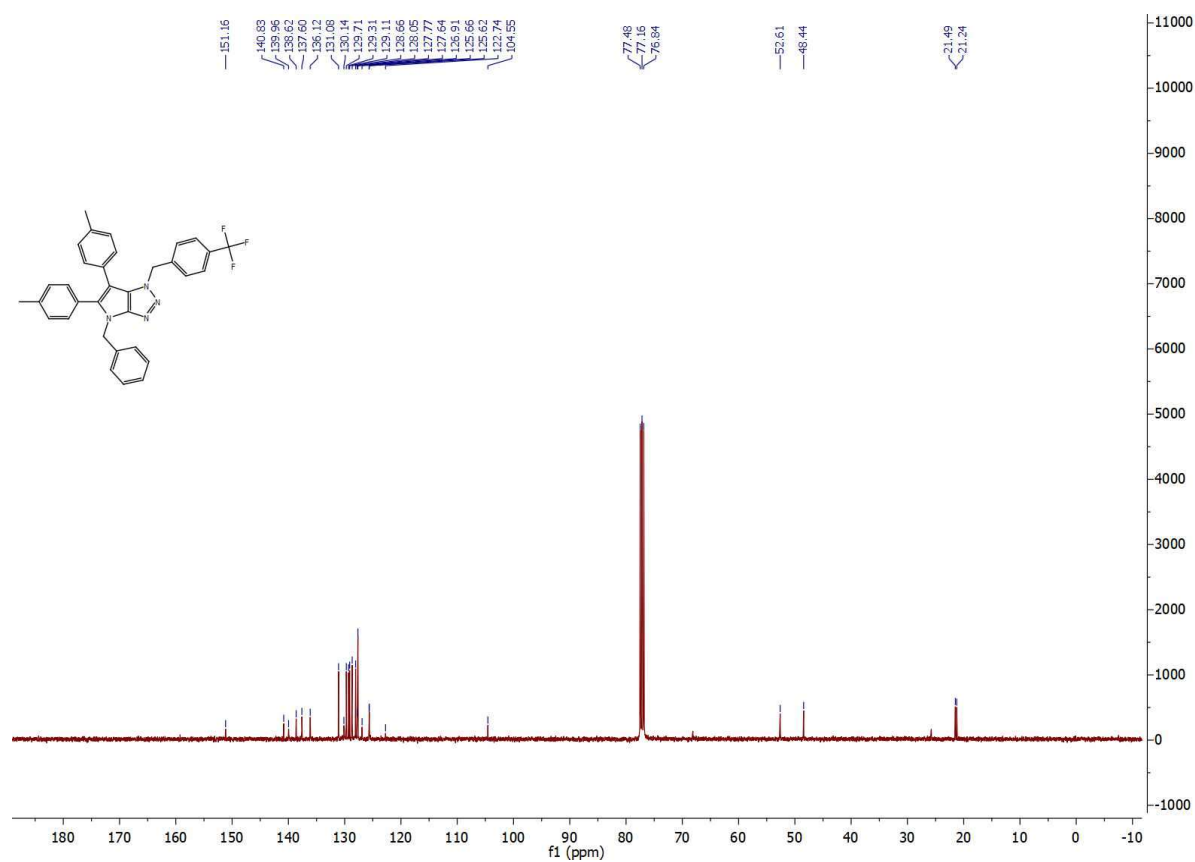
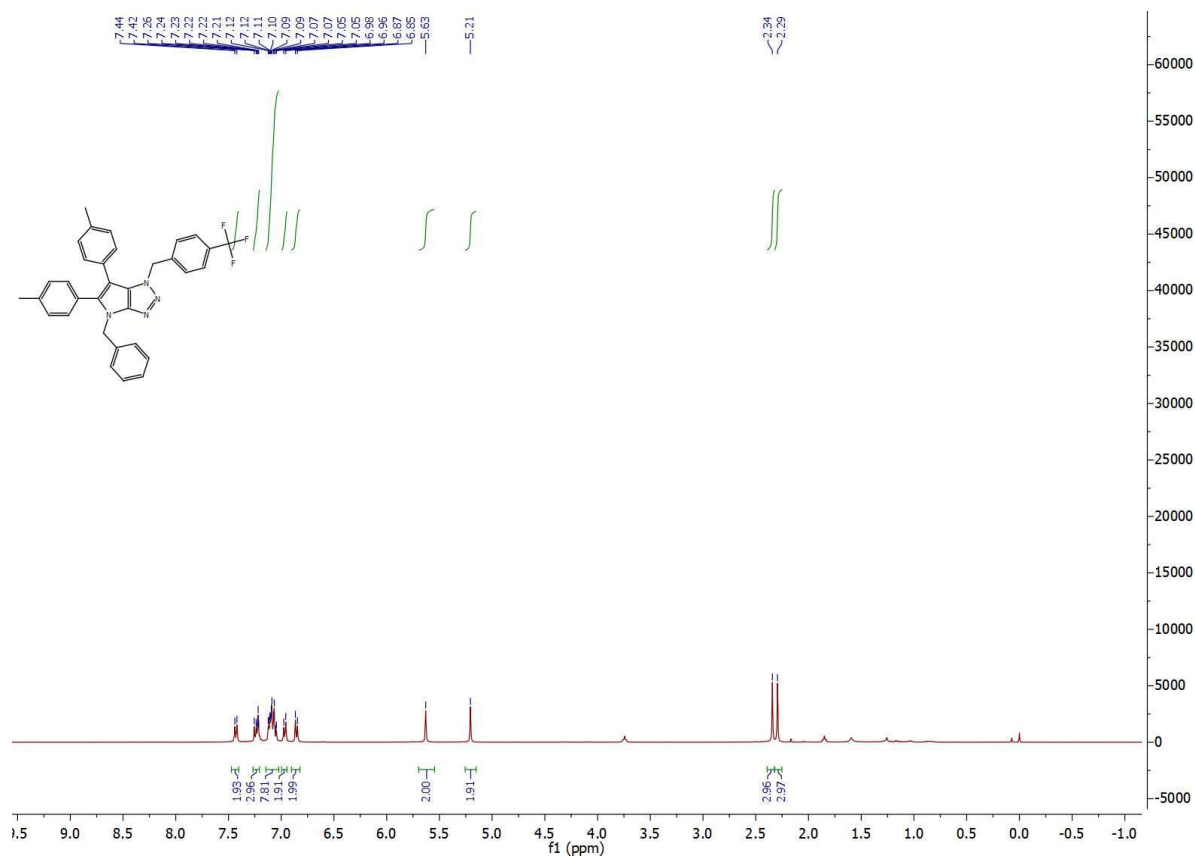


Figure S45. 4-Benzyl-1-(thiophen-2-ylmethyl)-5,6-di-*p*-tolyl-1,4-dihydropyrrolo[2,3-*d*][1,2,3]triazole (50).



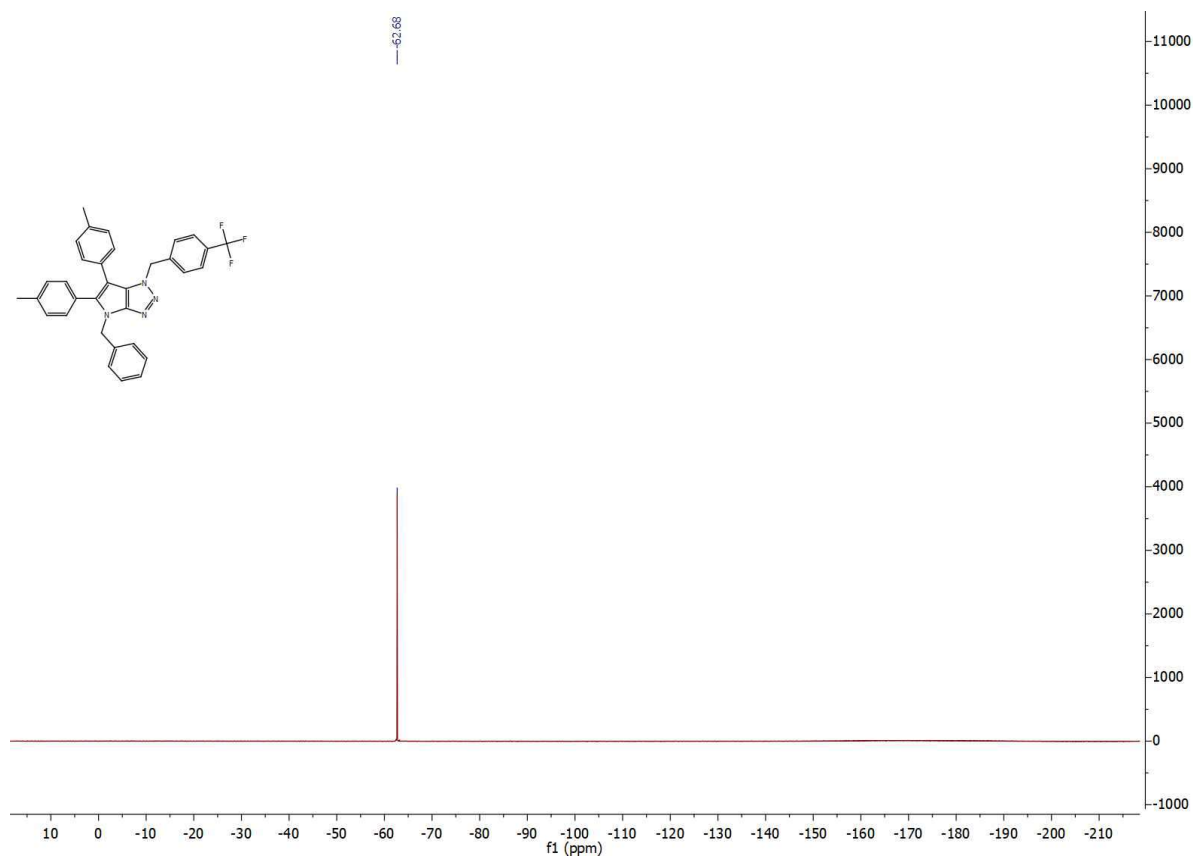
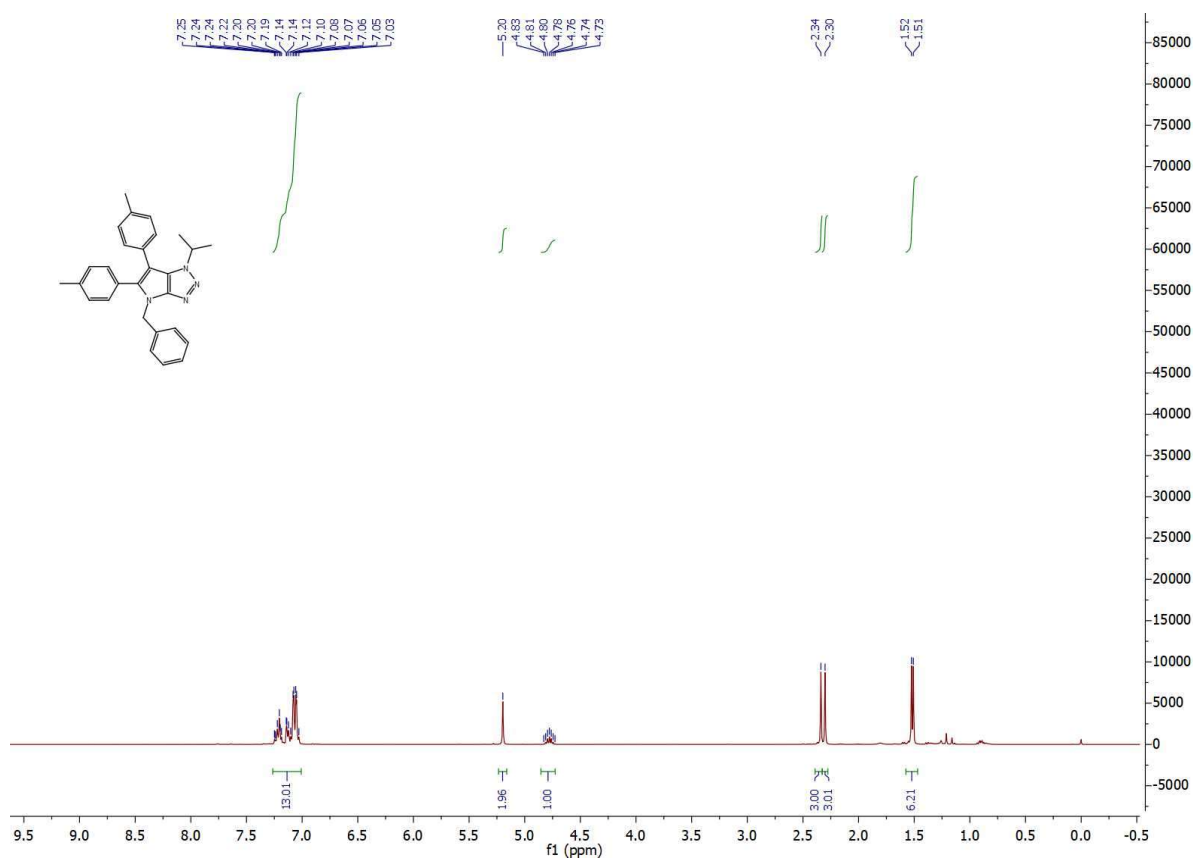


Figure S46. 4-Benzyl-5,6-di-*p*-tolyl-1-(4-(trifluoromethyl)benzyl)-1,4-dihydropyrrolo[2,3-*d*][1,2,3]triazole (51).



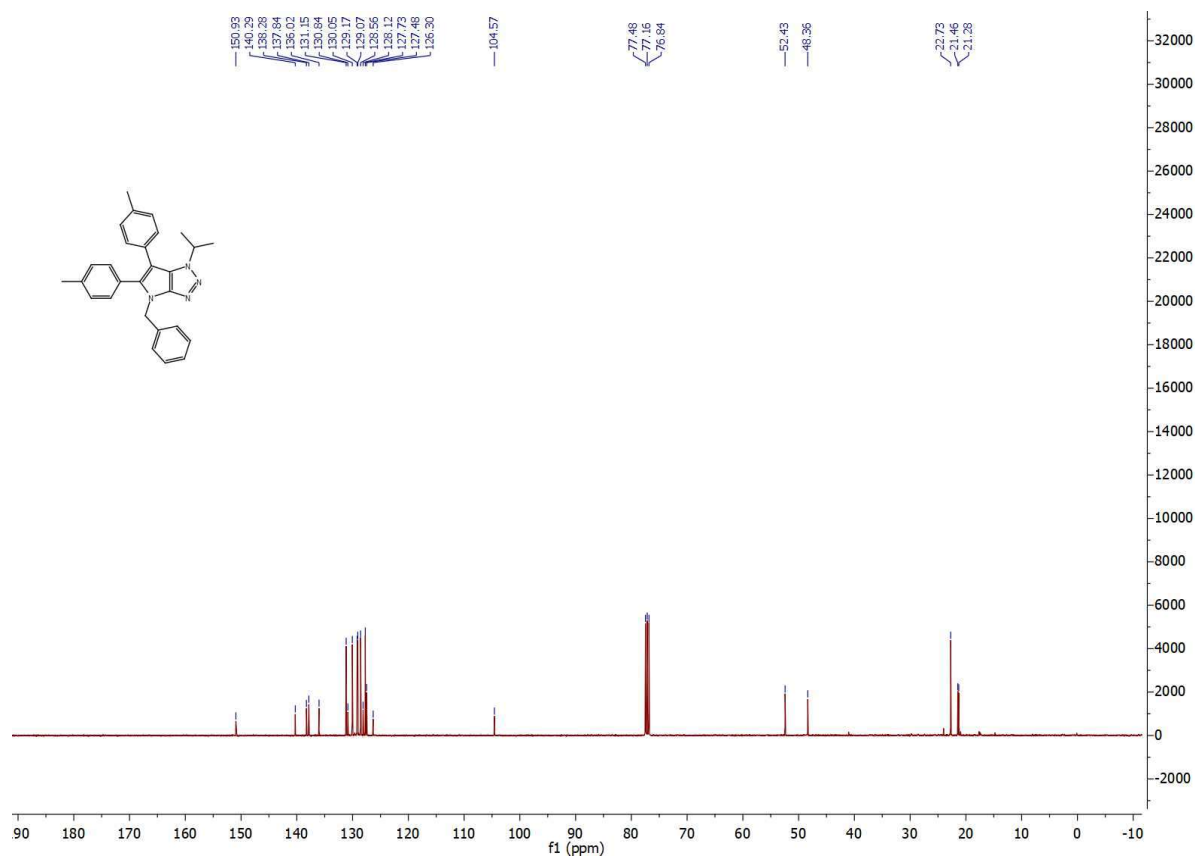
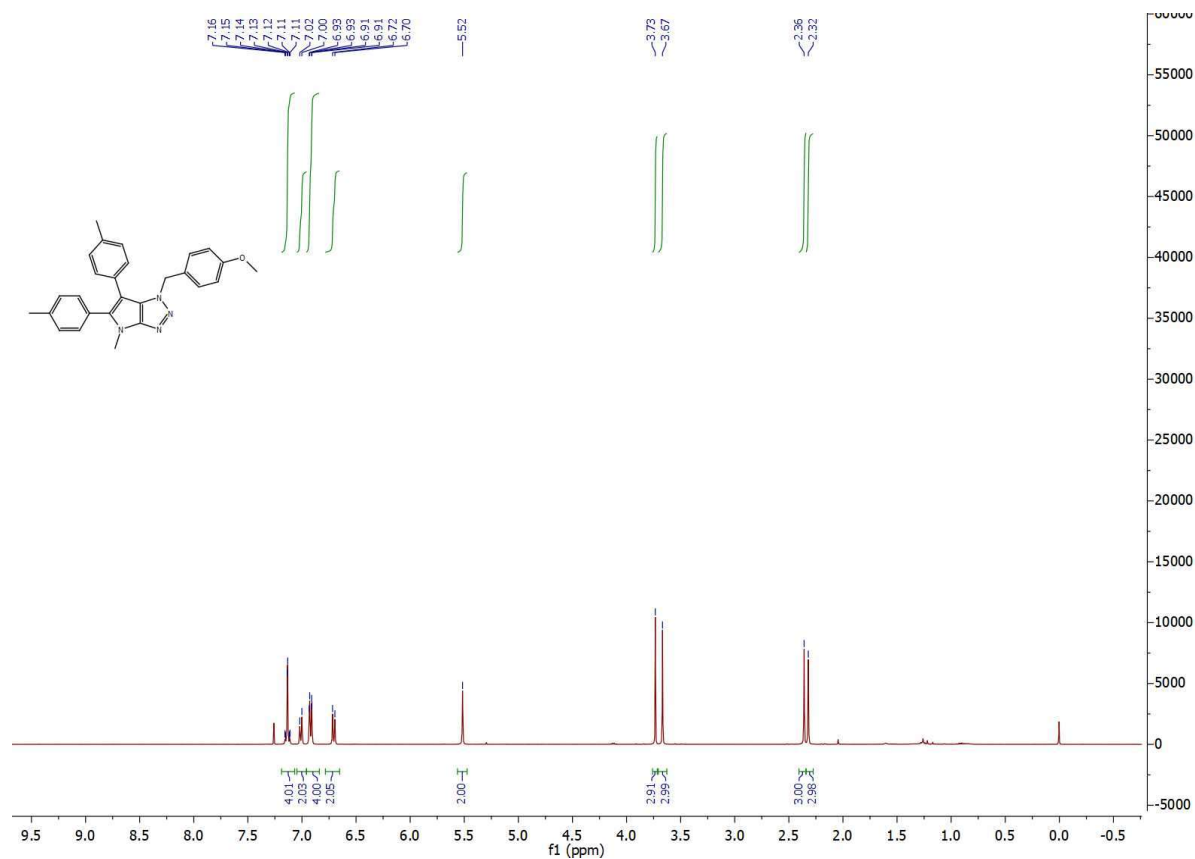


Figure S47. 4-Benzyl-1-isopropyl-5,6-di-*p*-tolyl-1,4-dihydropyrrolo[2,3-*d*][1,2,3]triazole (52).



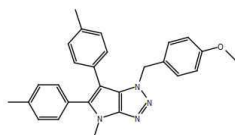


Figure S48. 1-(4-Methoxybenzyl)-4-methyl-5,6-di-*p*-tolyl-1,4-dihydropyrrolo[2,3-*d*][1,2,3]triazole (53).

Table S1. Crystal data and structure refinement for 41.

Identification code	SG450
Empirical formula	C ₃₃ H ₃₀ N ₄ O
Formula weight	498.61
Temperature/K	296.15
Crystal system	monoclinic
Space group	P2 ₁ /c
a/Å	17.973(4)
b/Å	6.0142(9)
c/Å	24.901(5)
α/°	90
β/°	96.422(16)
γ/°	90
Volume/Å ³	2674.8(9)
Z	4
ρ _{calc} /cm ³	1.238
μ/mm ⁻¹	0.076
F(000)	1056.0
Crystal size/mm ³	0.32 × 0.12 × 0.12
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	2.28 to 52.744
Index ranges	-22 ≤ h ≤ 22, -7 ≤ k ≤ 7, -31 ≤ l ≤ 31
Reflections collected	64723

Independent reflections	5440 [$R_{\text{int}} = 0.0526$, $R_{\text{sigma}} = 0.0219$]
Data/restraints/parameters	5440/0/357
Goodness-of-fit on F^2	1.025
Final R indexes [$I \geq 2\sigma(I)$]	$R_1 = 0.0463$, $wR_2 = 0.1163$
Final R indexes [all data]	$R_1 = 0.0642$, $wR_2 = 0.1280$
Largest diff. peak/hole / $e \text{ \AA}^{-3}$	0.17/−0.15

Table S2. Bond Lengths for 41.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	C1	1.371(2)	C28	C29	1.375(2)
O1	C7	1.415(3)	C5	C6	1.384(2)
N4	C12	1.3906(19)	C14	C15	1.385(2)
N4	C9	1.3738(19)	C10	C9	1.366(2)
N4	C27	1.4497(19)	C3	C2	1.375(2)
N1	N2	1.3712(19)	C20	C25	1.390(2)
N1	C10	1.3665(18)	C20	C21	1.378(2)
N1	C8	1.451(2)	C15	C16	1.383(2)
N3	N2	1.326(2)	C16	C17	1.388(2)
N3	C9	1.350(2)	C16	C19	1.504(2)
C4	C5	1.383(2)	C2	C1	1.382(2)
C4	C3	1.382(2)	C33	C32	1.389(2)
C4	C8	1.509(2)	C1	C6	1.379(2)
C13	C11	1.473(2)	C25	C24	1.379(3)
C13	C18	1.397(2)	C32	C31	1.357(3)
C13	C14	1.392(2)	C29	C30	1.380(3)
C11	C12	1.3932(19)	C21	C22	1.380(3)
C11	C10	1.433(2)	C31	C30	1.360(3)
C12	C20	1.484(2)	C24	C23	1.387(4)
C18	C17	1.377(2)	C24	C26B	1.622(5)
C28	C33	1.376(2)	C23	C22	1.385(4)
C28	C27	1.510(2)	C22	C26A	1.620(7)