SUPPORTING INFORMATION

Photophysical and Electrical Properties of Highly Luminescent 2/6-Triazolyl Substituted Push–Pull Purines

Armands Sebris,[1] Irina Novosjolova,[1,*] Kaspars Traskovskis,[1,*] Valdis Kokars,[1]

Natalija Tetervenoka,[2] Aivars Vembris,[2] Māris Turks[1,*]

[1] *Faculty of Materials Science and Applied Chemistry, Riga Technical University, P. Valdena Str. 3, LV-1048, Riga, Latvia, E-mails: irina.novosjolova@rtu.lv; kaspars.traskovskis@rtu.lv ; maris.turks@rtu.lv*
[2] *Institute of Solid State Physics, University of Latvia, 8 Kengaraga Street, LV-1063, Riga, Latvia*

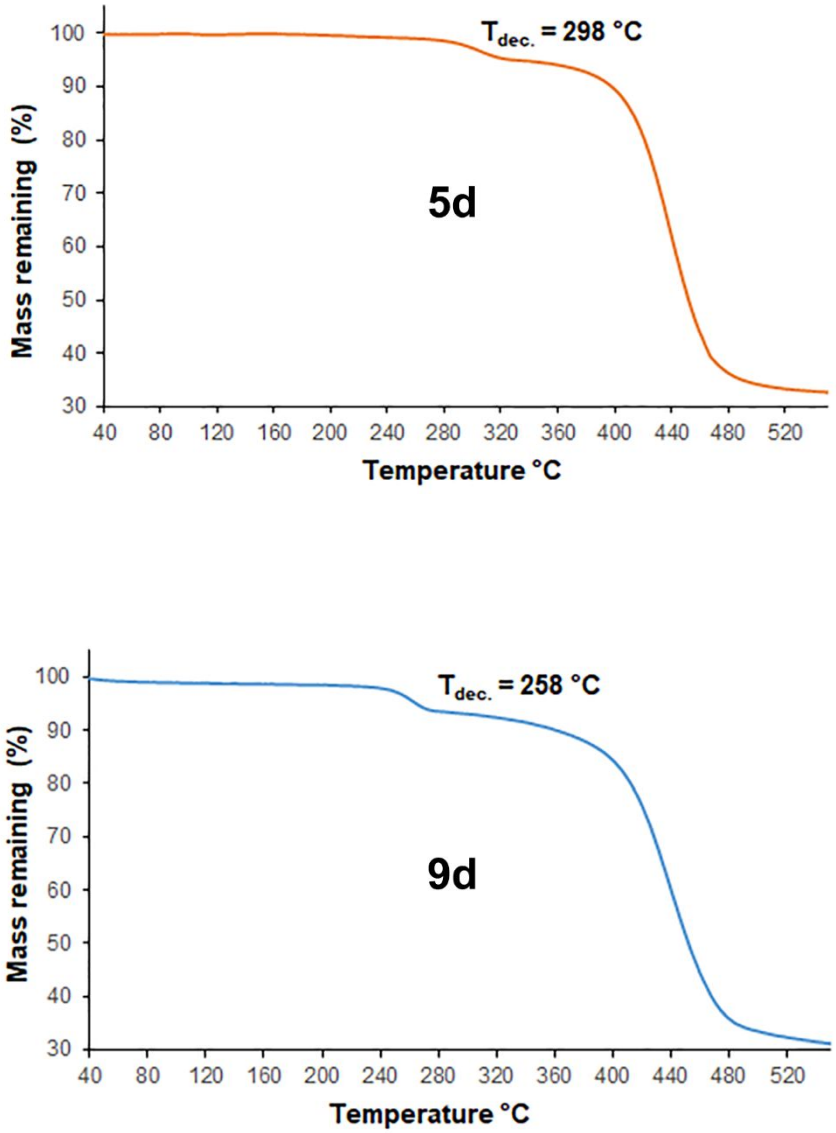

Figure S1. Thermogravimetric analysis of compounds **9a** and **9b**.

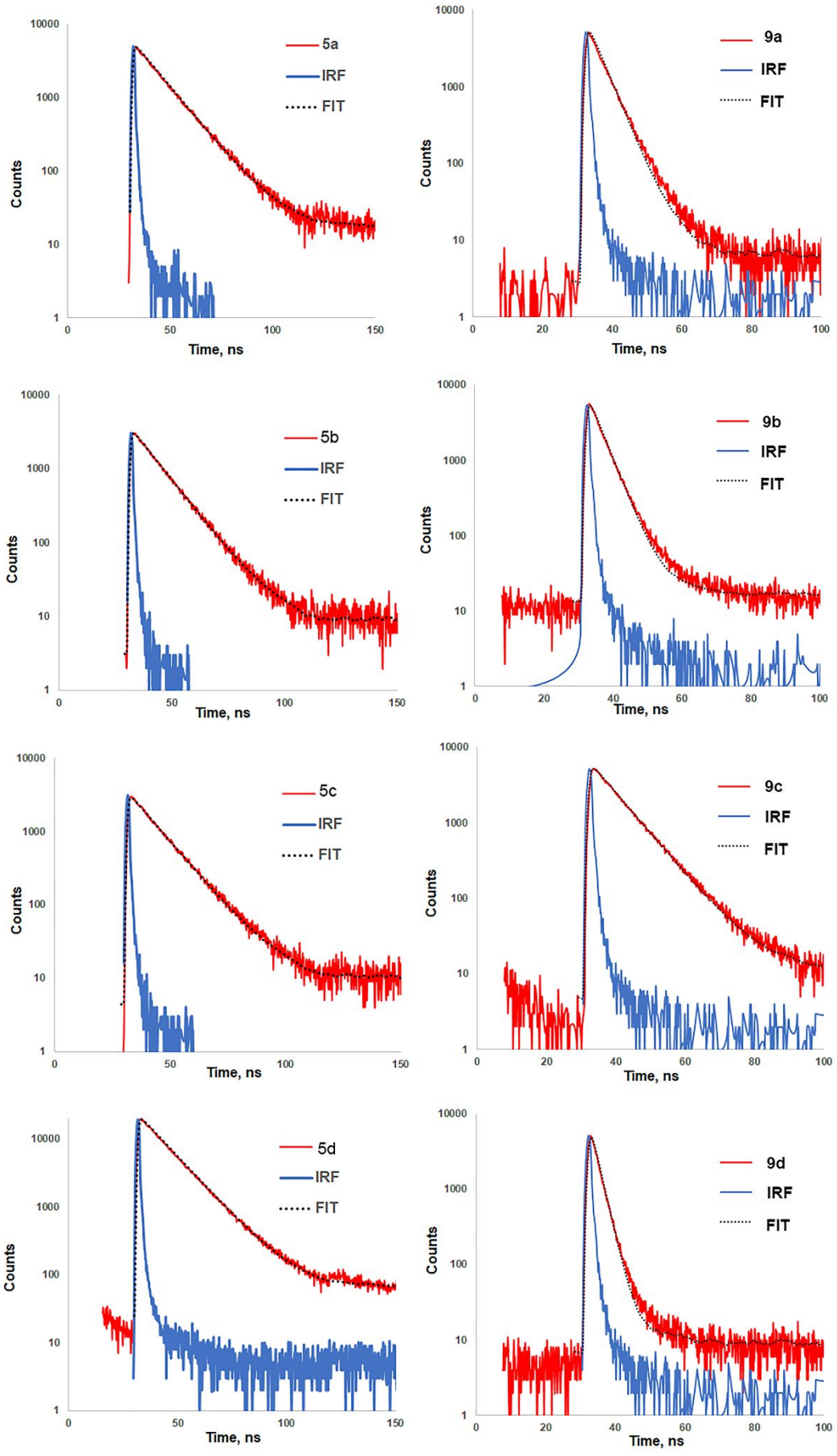

Figure S2. Emission lifetime measurements for compounds **5a-d** and **9a-d**.

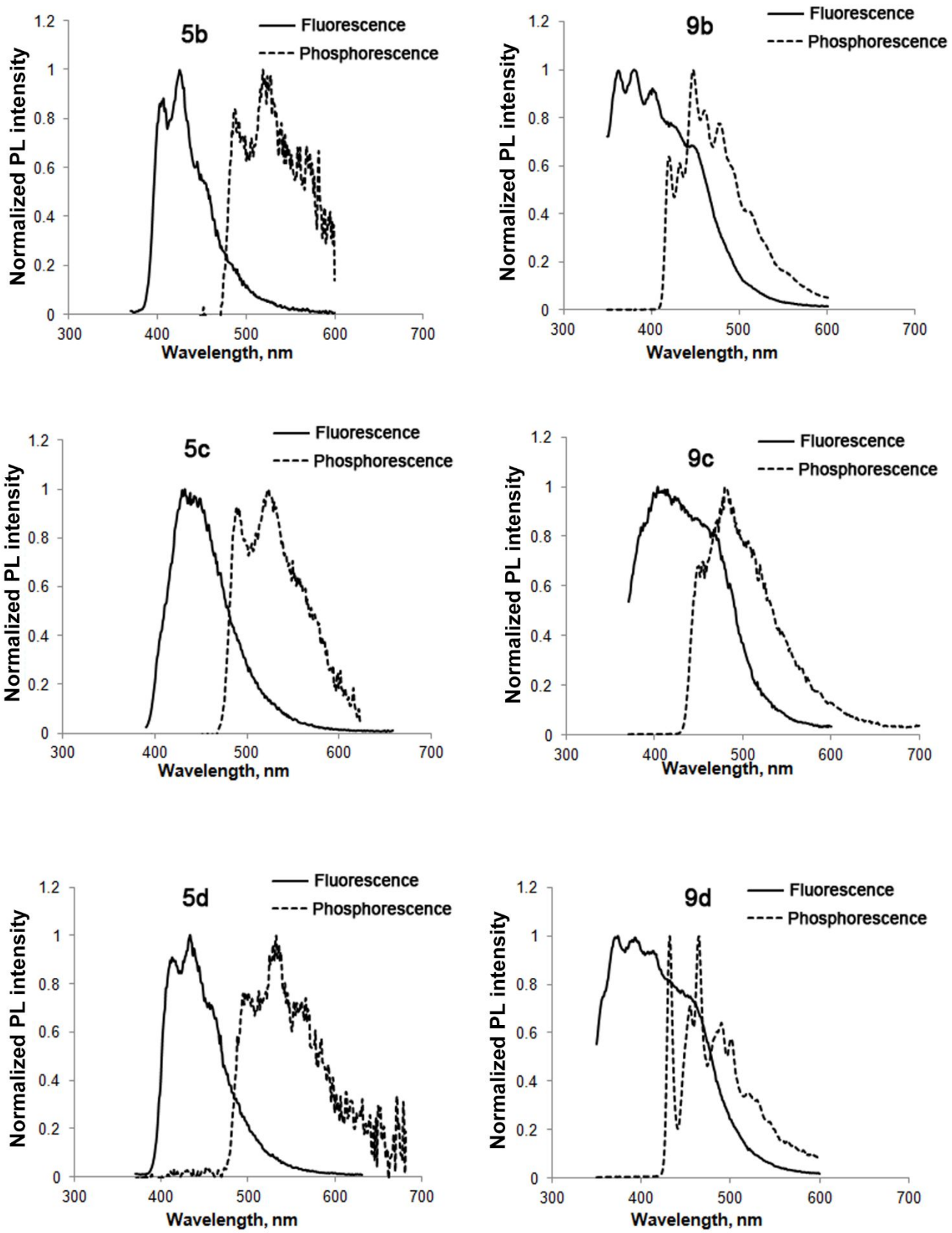

Figure S3. Fluorescence and phosphorescence spectra of **5b-c** and **9b-c** in 2-MeTHF matrix at 77K.

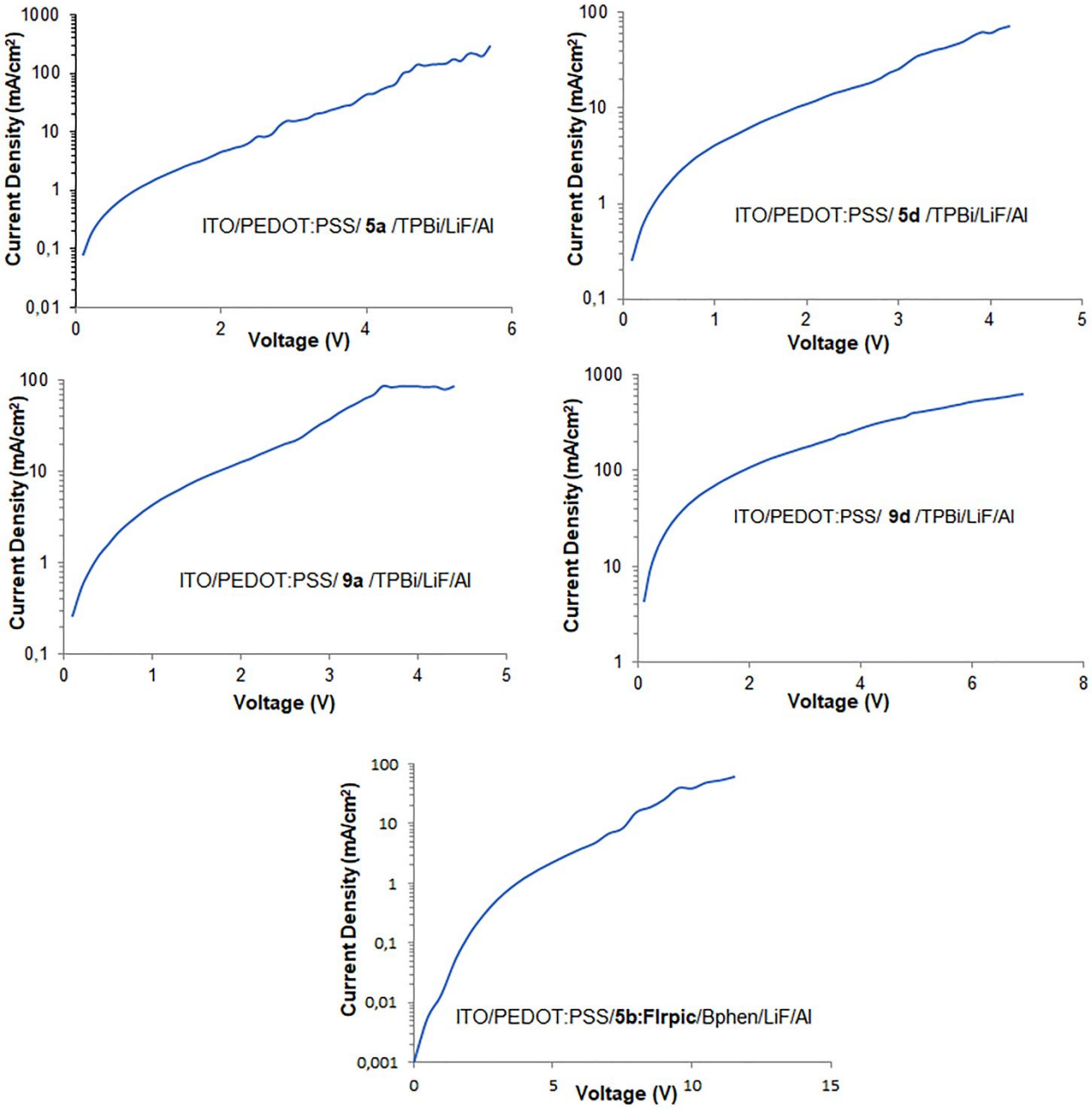

Figure S4. Current density-voltage dependencies for purine-only and purine host-FIrpic OLEDs.

Table S1. Calculated ground state dipole moment values of the compounds.

Compound	**5a**	**5b**	**5c**	**5d**	**9a**	**9b**	**9c**	**9d**
μ, D	6.99	7.36	5.39	11.86	5.54	5.88	3.93	10.49

Table S2. Radiative and nonradiative decay rates of the compounds.

Compound	**5a**	**5b**	**5c**	**5d**	**9a**	**9b**	**9c**	**9d**
$\mathbf{k_r}$, [a] $\mathbf{\times 10^7\ s^{-1}}$	7.00	7.09	6.17	7.50	8.61	8.50	3.80	11.28
$\mathbf{kn_r}$, [b] $\mathbf{\times 10^7\ s^{-1}}$	0.69	2.00	2.17	0.83	19.17	41.50	8.86	14.36

[a]Radiative decay rate $k_r = \Phi_{FL}/\tau$.

[b]Nonradiative decay rate $k_{nr} = (1- \Phi_{FL})/ \tau$.

NMR spectra of synthesized compounds

9-(5,5,5-Triphenylpentyl)-2,6-dichloro-9*H*-purine (2)

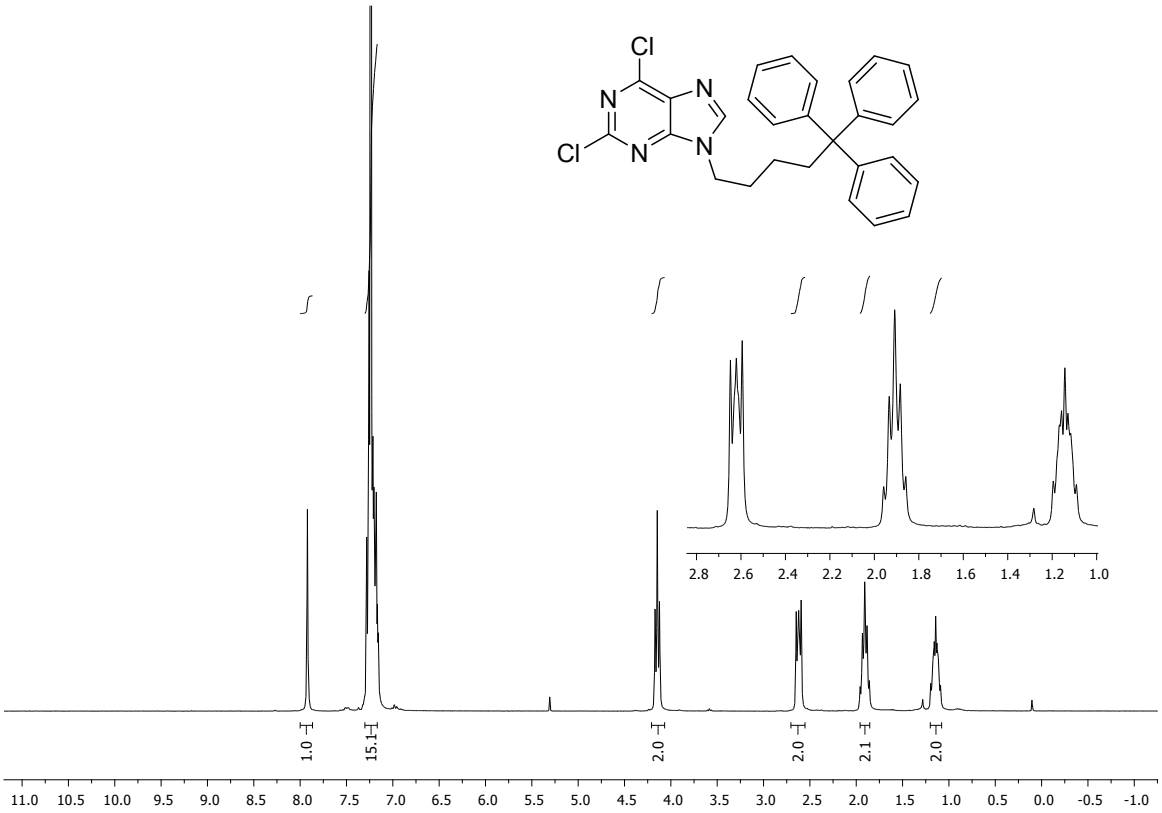

Figure S5. ^{1}H-NMR (300 MHz, $CDCl_3$) spectrum of compound 2

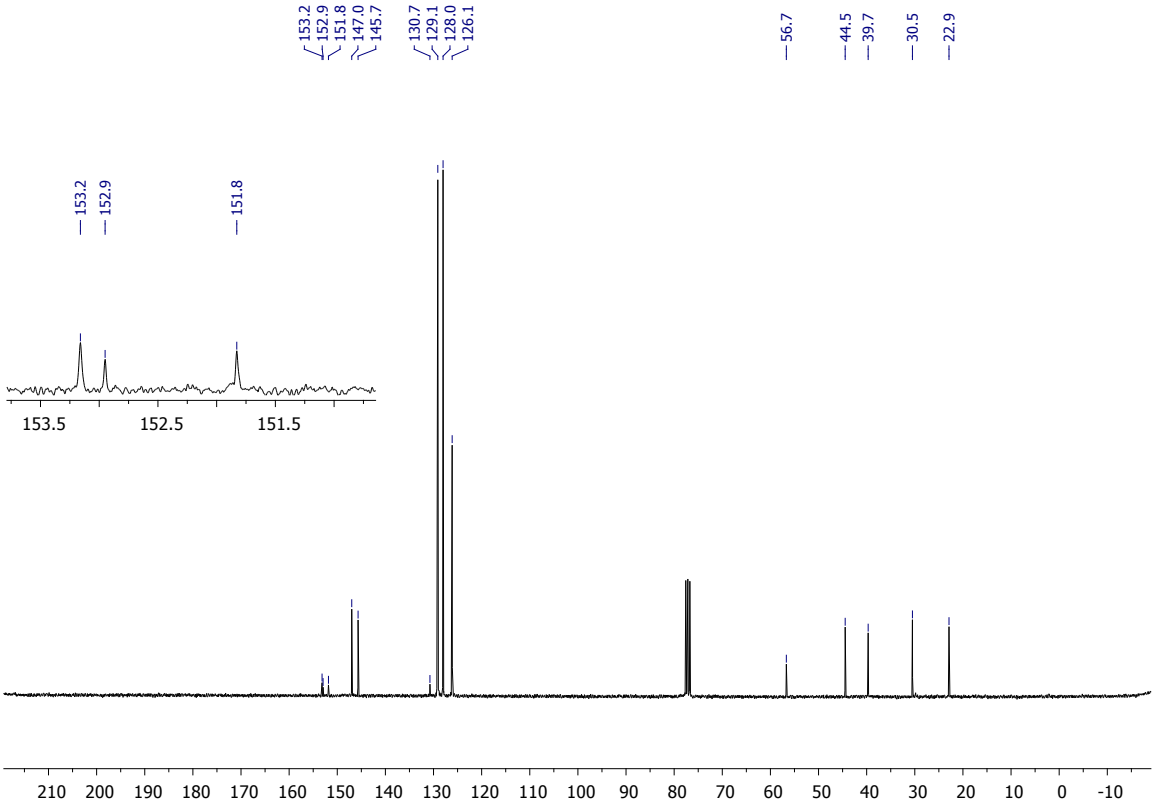

Figure S6. ^{13}C-NMR (75.5 MHz, $CDCl_3$) spectrum of compound 2

2,6-Diazido-9-(5,5,5-triphenylpentyl)-9*H*-purine (3)

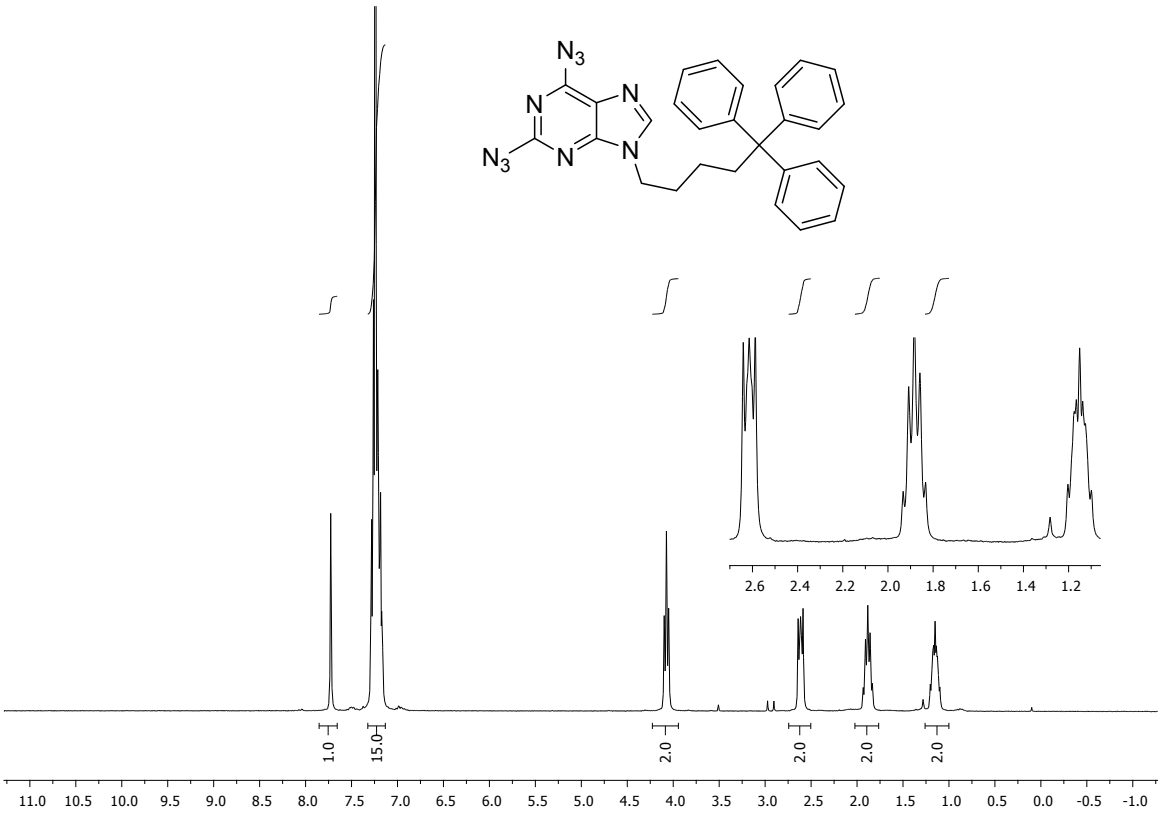

Figure S7. ^{1}H-NMR (300 MHz, $CDCl_3$) spectrum of compound 3

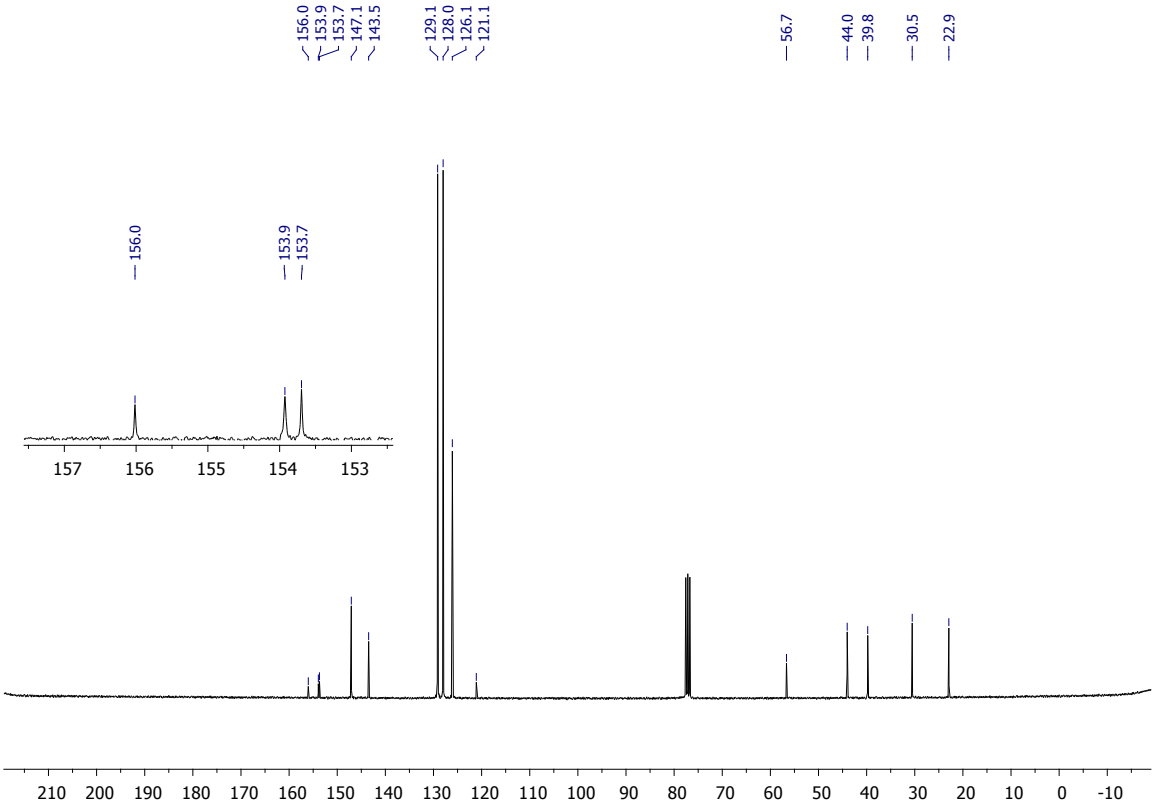

Figure S8. ^{13}C-NMR (75.5 MHz, $CDCl_3$) spectrum of compound 3

6-Azido-9-(5,5,5-triphenylpentyl)-2-(piperidin-1-yl)-9*H*-purine (4)

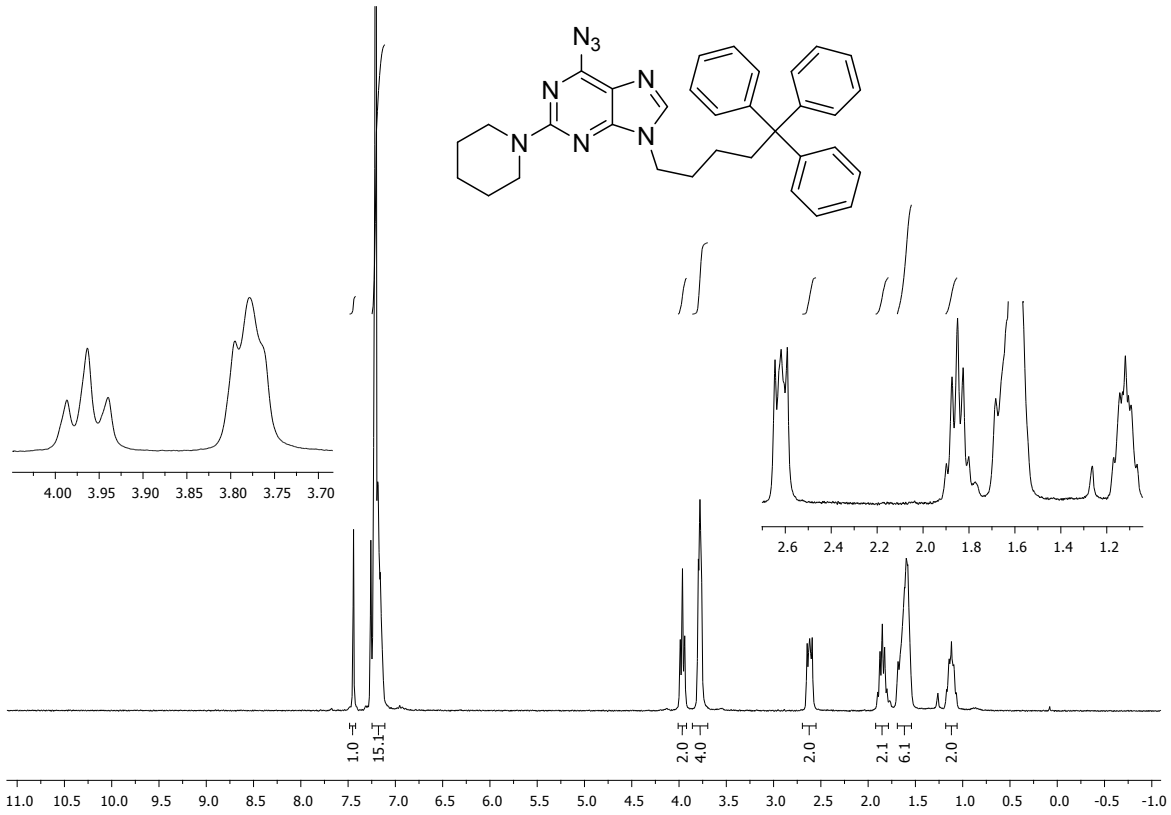

Figure S9. ^{1}H-NMR (300 MHz, $CDCl_3$) spectrum of compound 4

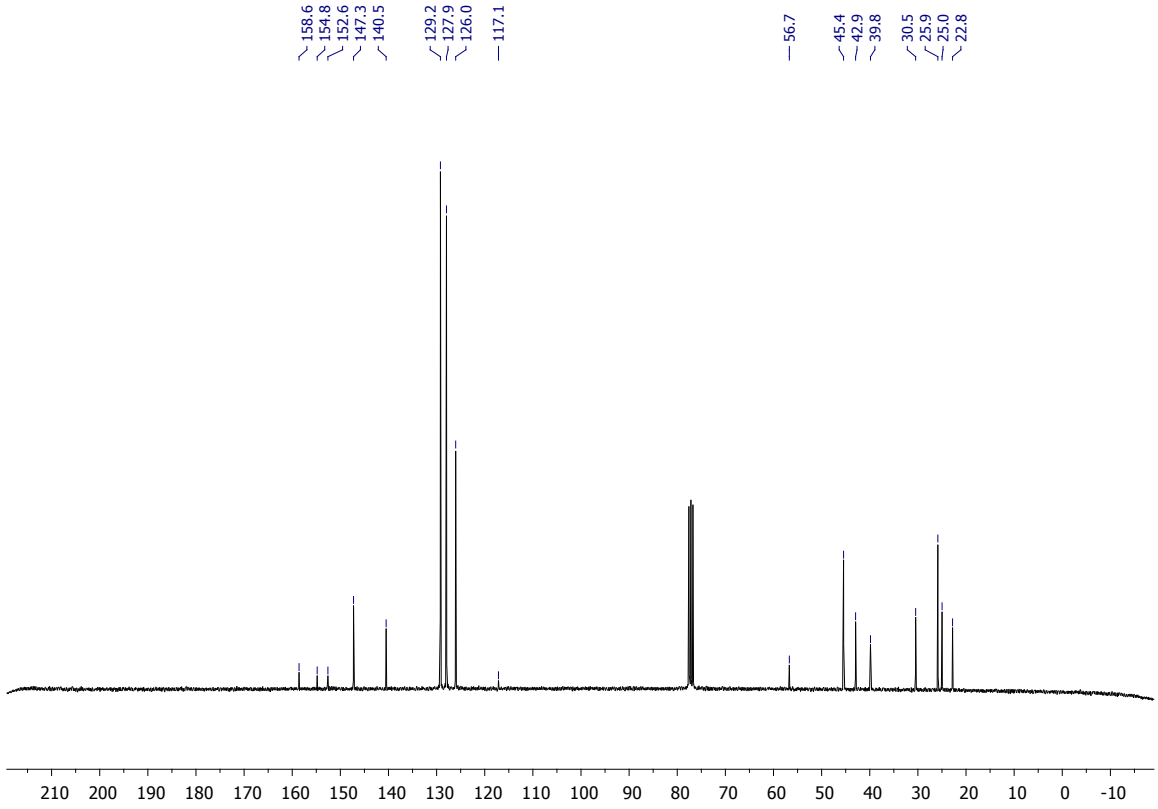

Figure S10. ^{13}C-NMR (75.5 MHz, $CDCl_3$) spectrum of compound 4

2-Azido-6-(piperidin-1-yl)-9*H*-purine (7)

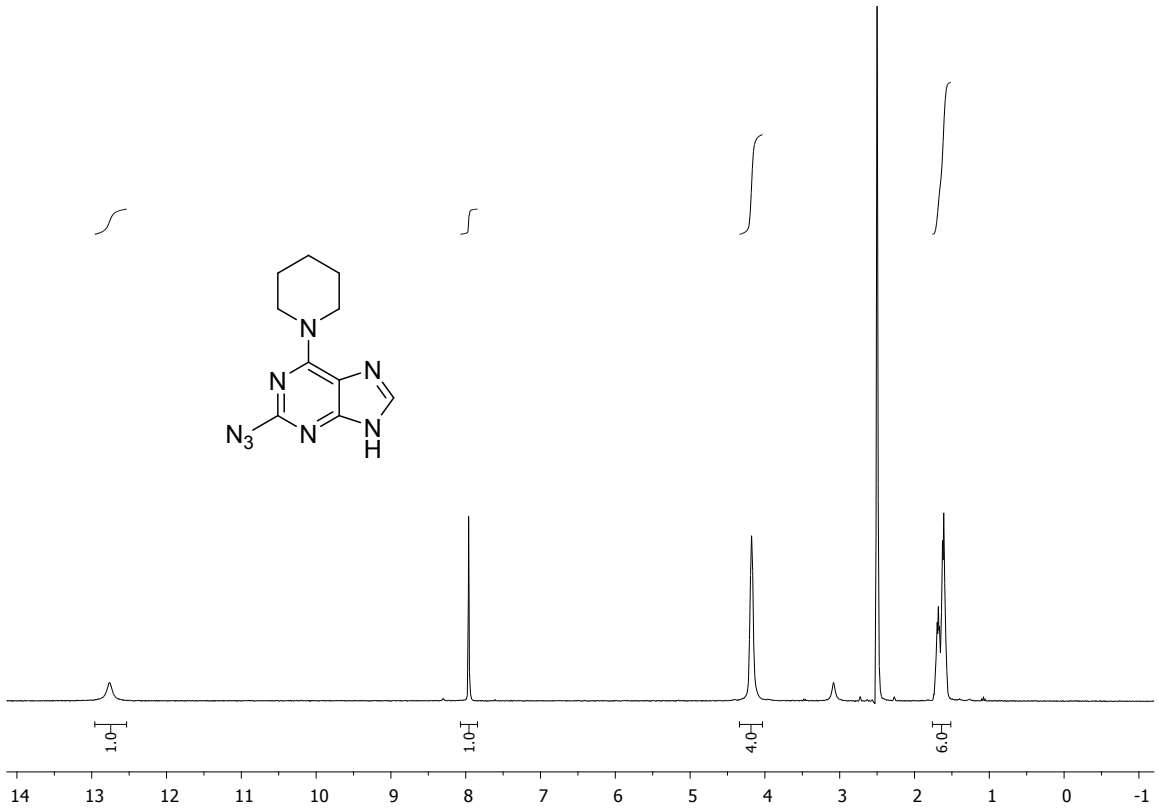

Figure S11. ^{1}H-NMR (300 MHz, DMSO-d$_6$) spectrum of compound 7

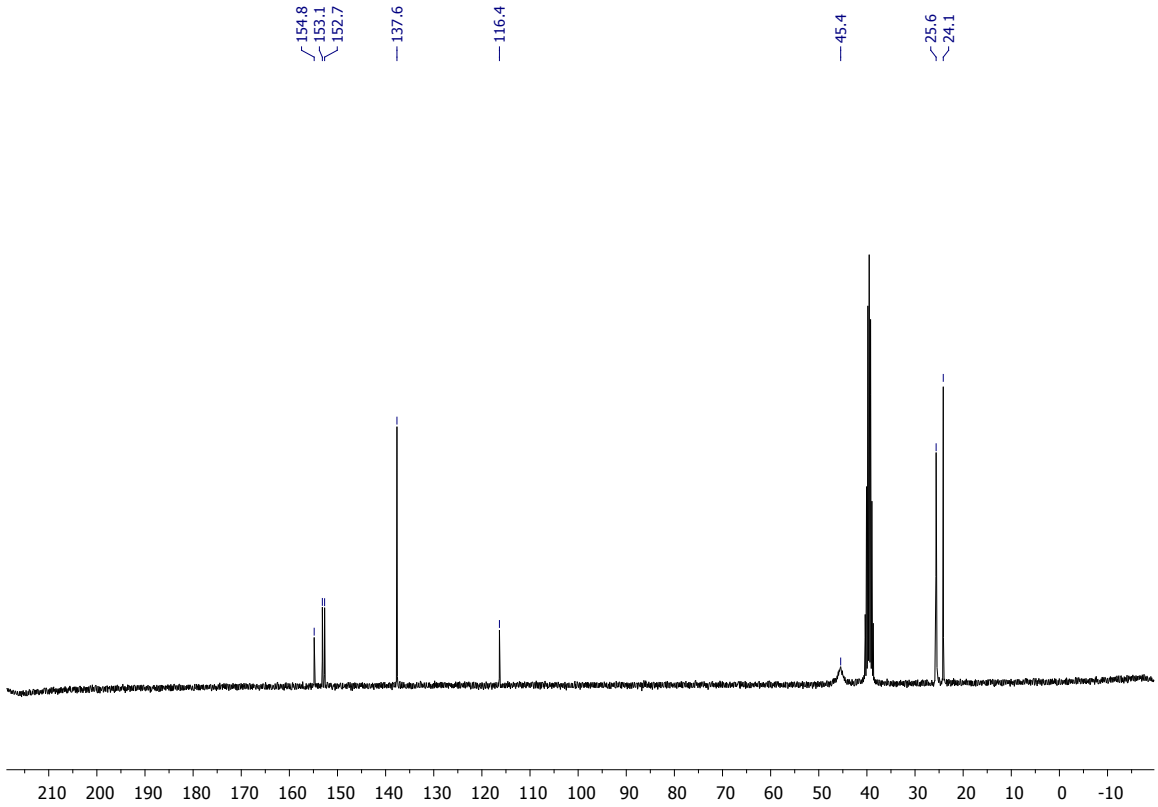

Figure S12. ^{13}C-NMR (75.5 MHz, DMSO-d$_6$) spectrum of compound 7

2-Azido-9-(5,5,5-triphenylpentyl)-6-(piperidin-1-yl)-9*H*-purine (8)

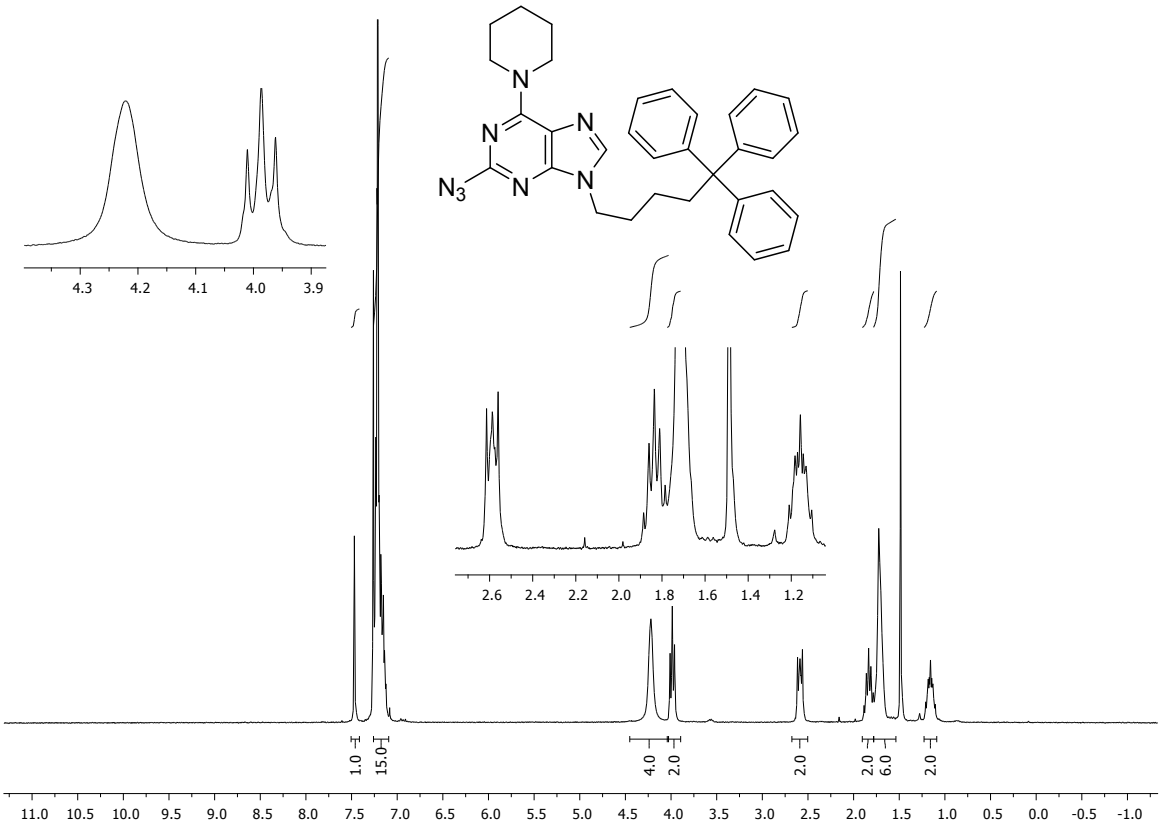

Figure S13. ^{1}H-NMR (300 MHz, $CDCl_3$) spectrum of compound 8

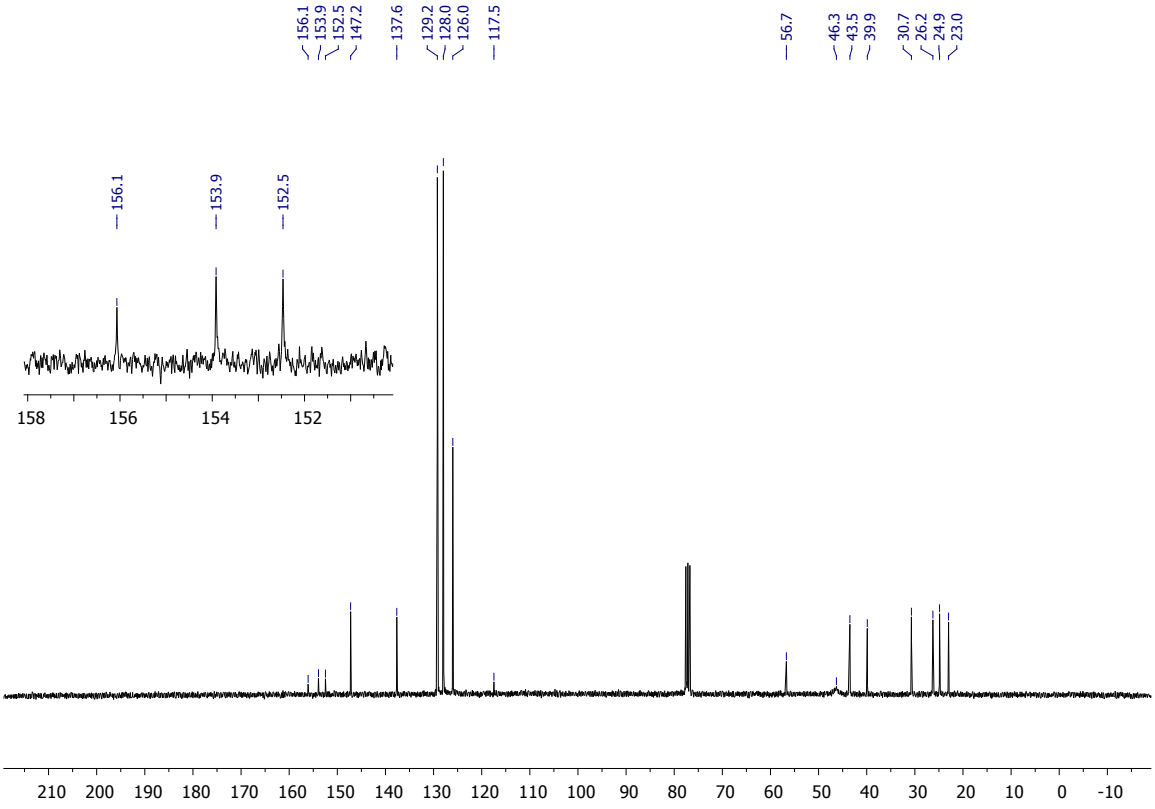

Figure S14. ^{13}C-NMR (75.5 MHz, $CDCl_3$) spectrum of compound 8

SYNTHESIS OF 2-(PIPERIDIN-1-YL)-6-TRIAZOLYL-9-ALKYLPURINES 5

6-(4-Phenyl-1*H*-1,2,3-triazol-1-yl)-9-(5,5,5-triphenylpentyl)-2-(piperidin-1-yl)-9*H*-purine (5a)

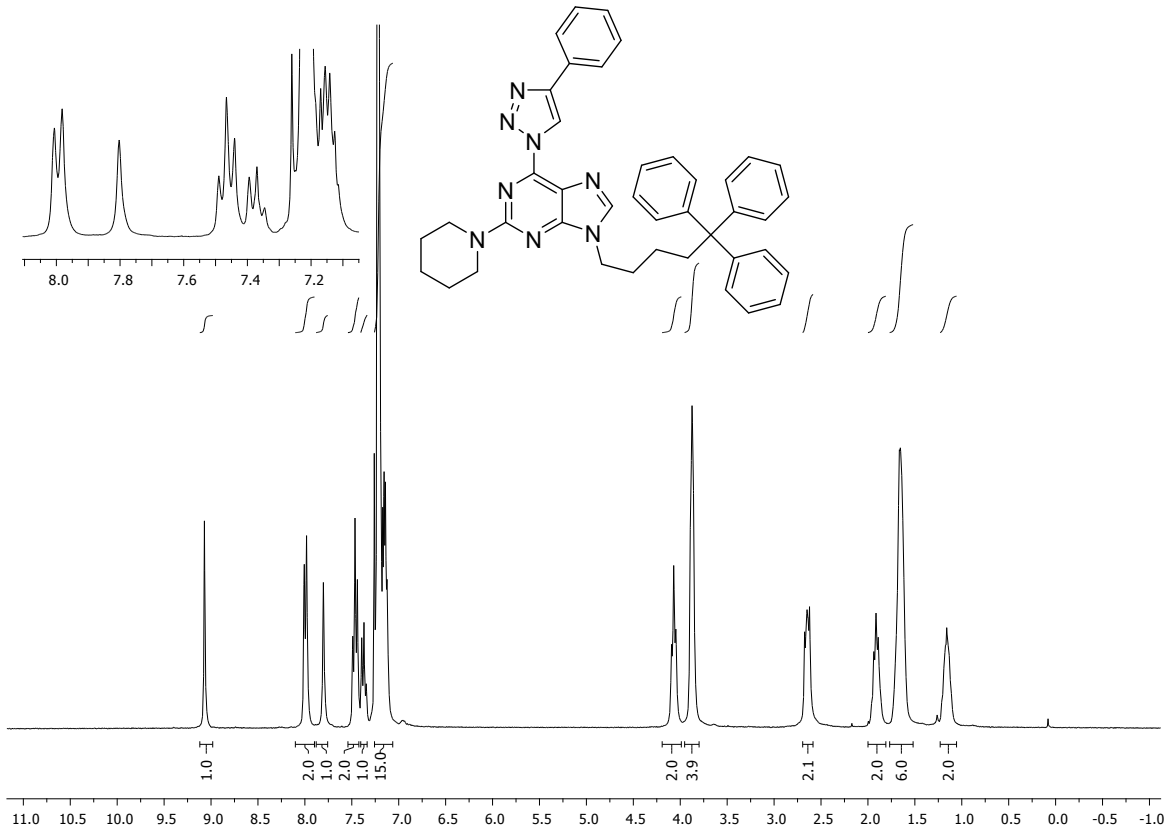

Figure S15. ^{1}H-NMR (300 MHz, $CDCl_3$) spectrum of compound 5a

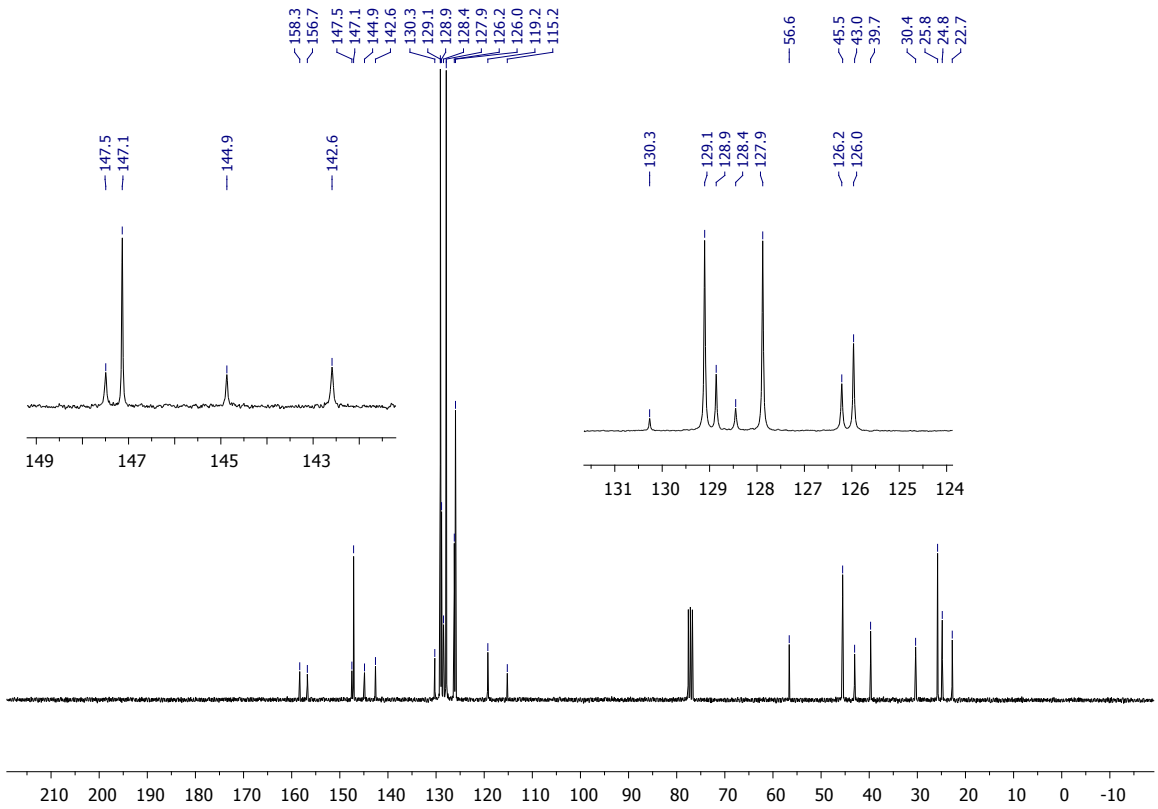

Figure S16. ^{13}C-NMR (75.5 MHz, $CDCl_3$) spectrum of compound 5a

6-(4-(4-Methoxyphenyl)-1*H*-1,2,3-triazol-1-yl)-9-(5,5,5-triphenylpentyl)-2-(piperidin-1-yl)-9*H*-purine (5b)

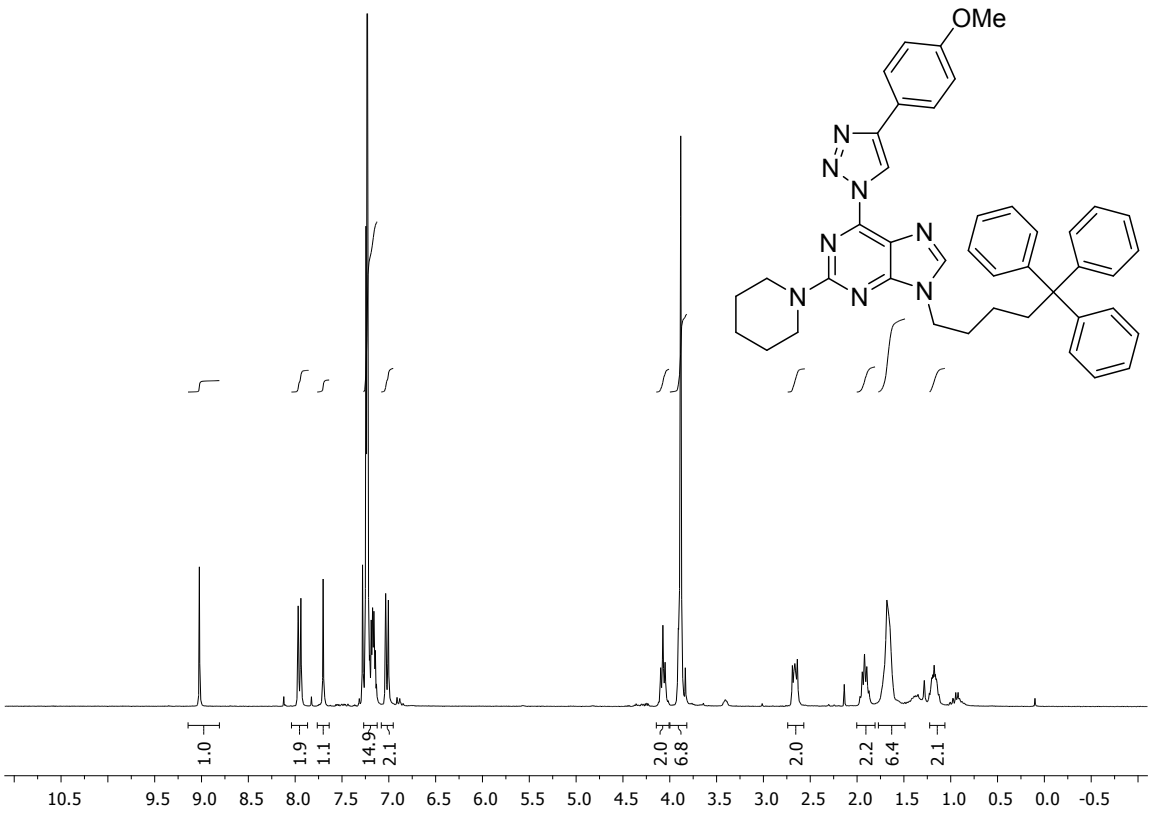

Figure S17. ^{1}H-NMR (300 MHz, $CDCl_3$) spectrum of compound 5b

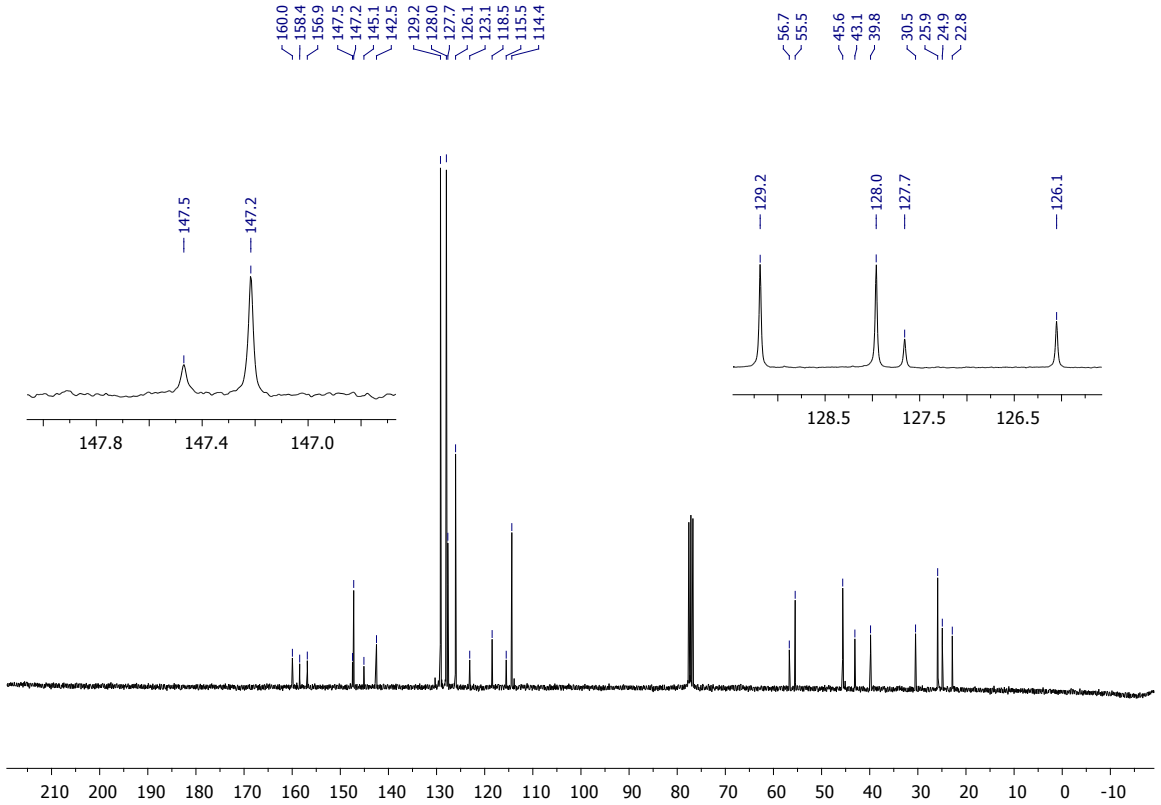

Figure S18. ^{13}C-NMR (75.5 MHz, $CDCl_3$) spectrum of compound 5b

9-(5,5,5-Triphenylpentyl)-6-(4-(4-(*N*,*N*-dimethylamino)phenyl)-1*H*-1,2,3-triazol-1-yl)-2-(piperidin-1-yl)-9*H*-purine (5c)

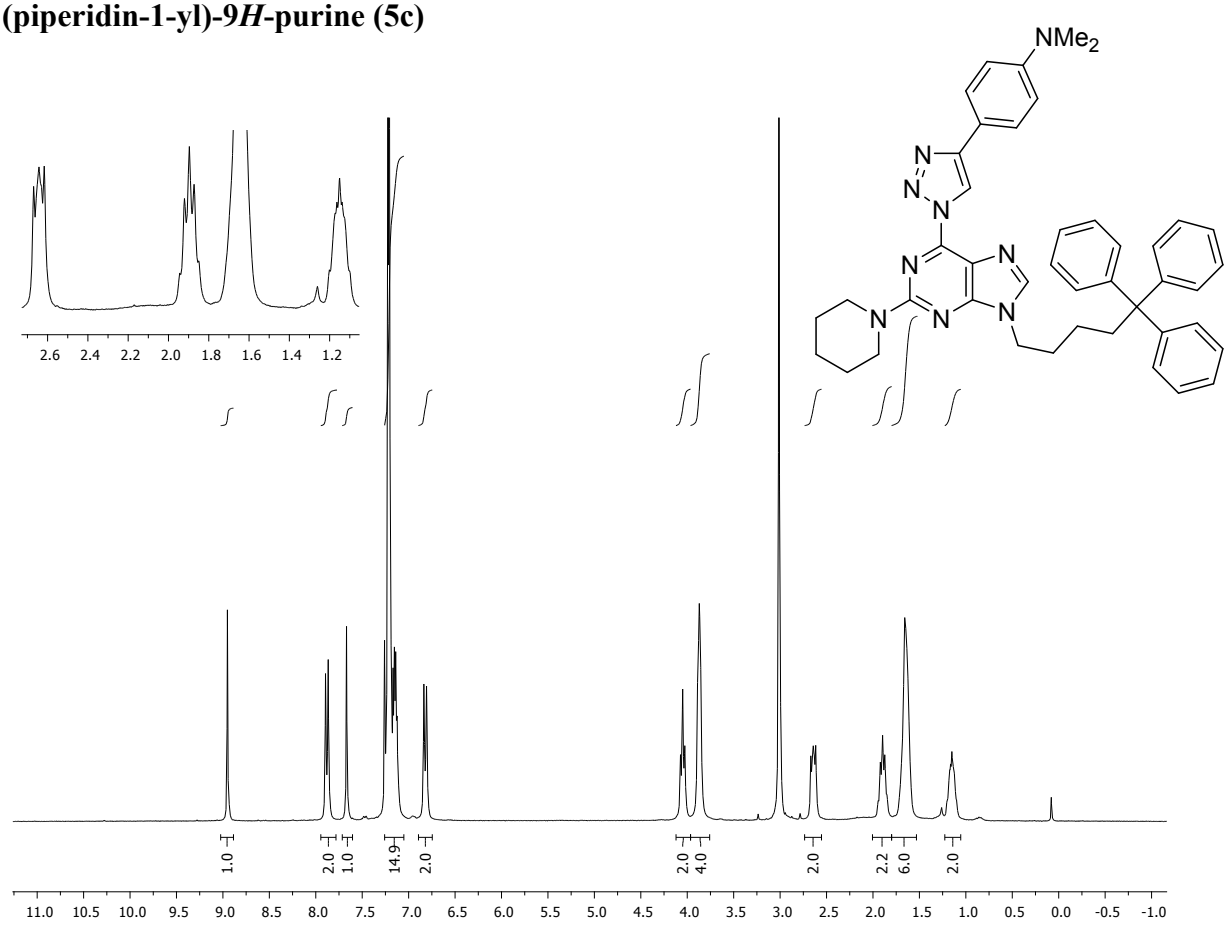

Figure S19. ^{1}H-NMR (300 MHz, $CDCl_3$) spectrum of compound 5c

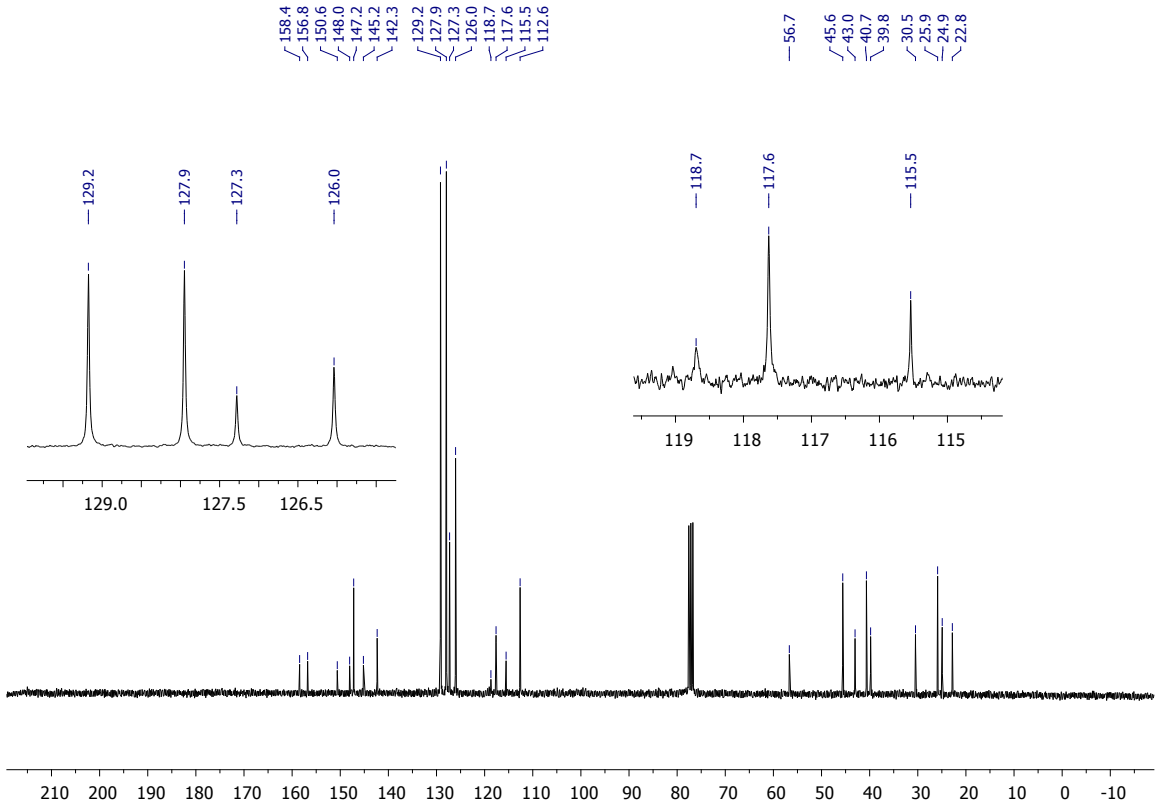

Figure S20. ^{13}C-NMR (75.5 MHz, $CDCl_3$) spectrum of compound 5c

6-(4-(4-Cyanophenyl)-1*H*-1,2,3-triazol-1-yl)-9-(5,5,5-triphenylpentyl)-2-(piperidin-1-yl)-9*H*-purine (5d)

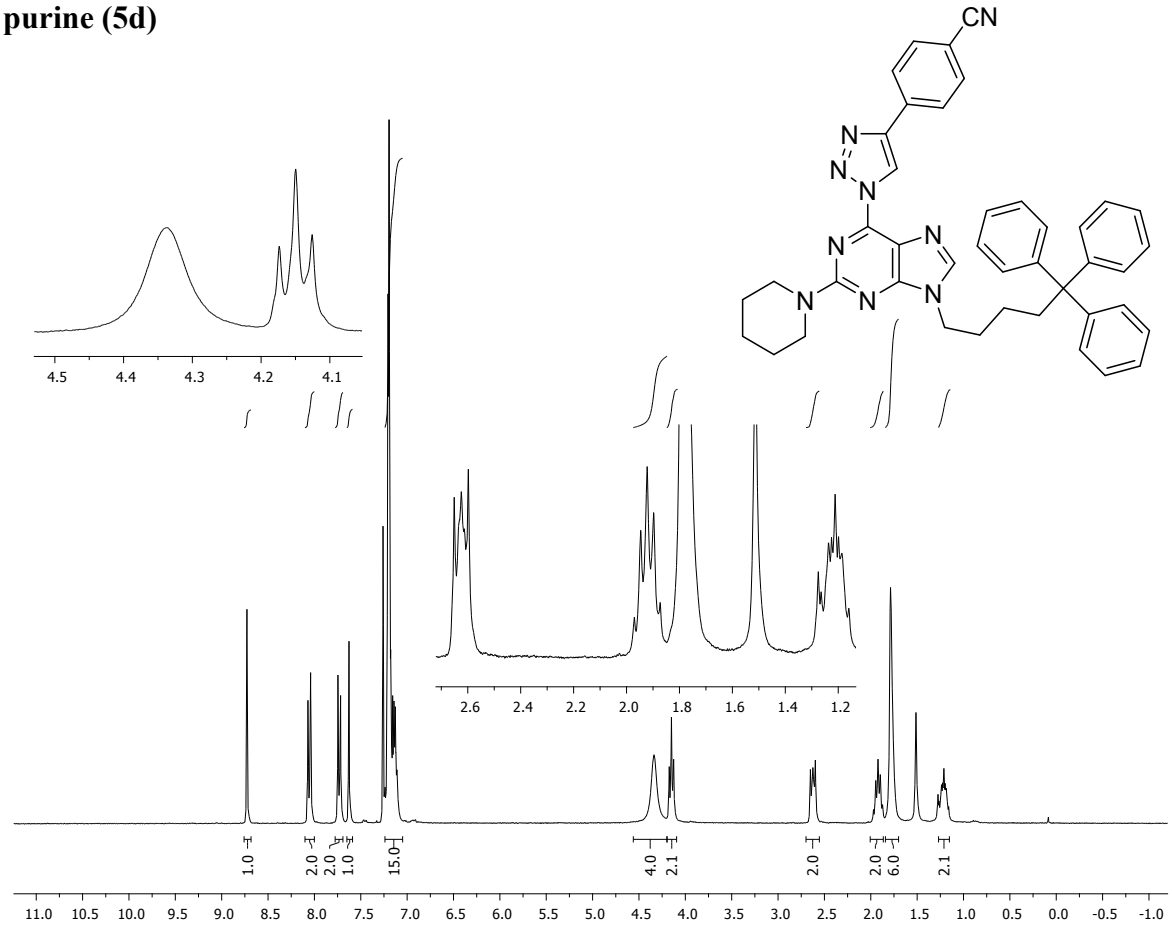

Figure S21. ^{1}H-NMR (300 MHz, $CDCl_3$) spectrum of compound 5d

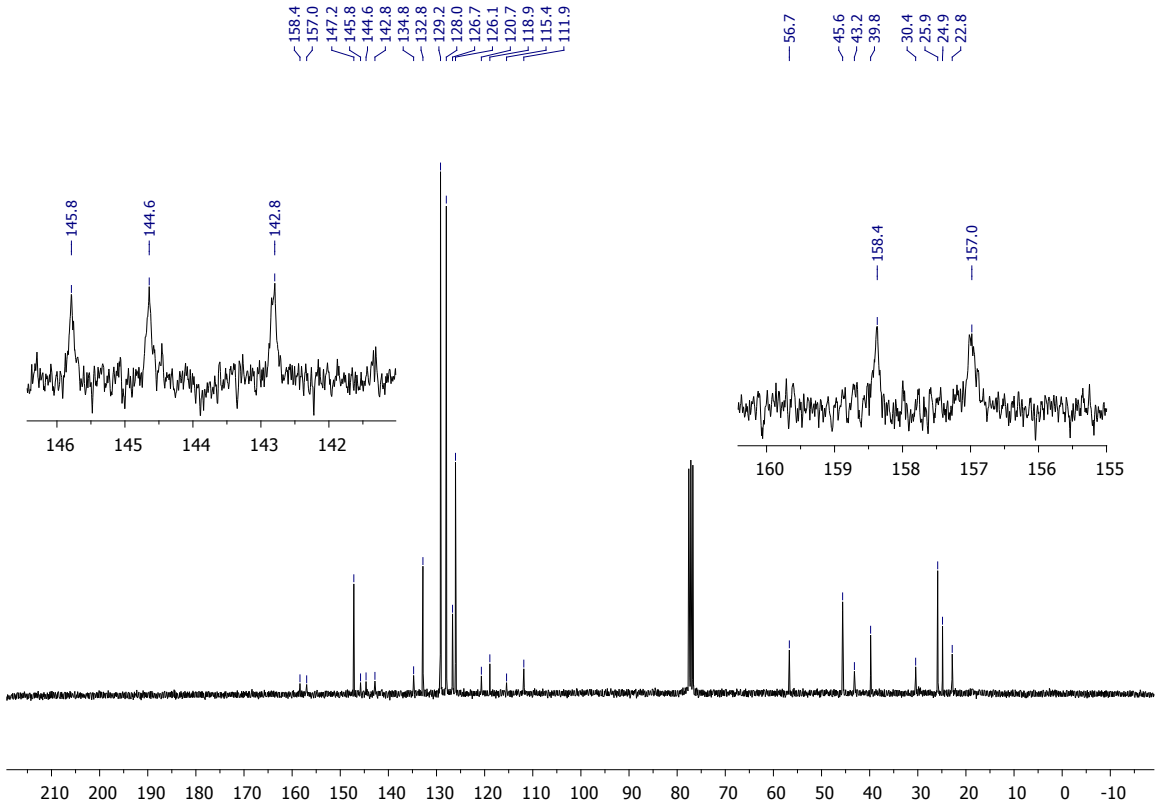

Figure S22. ^{13}C-NMR (75.5 MHz, $CDCl_3$) spectrum of compound 5d

SYNTHESIS OF 6-(PIPERIDIN-1-YL)-2-TRIAZOLYL-9-ALKYLPURINES 9

2-(4-Phenyl-1*H*-1,2,3-triazol-1-yl)-6-(piperidin-1-yl)-9-(5,5,5-triphenylpentyl)-9*H*-purine (9a)

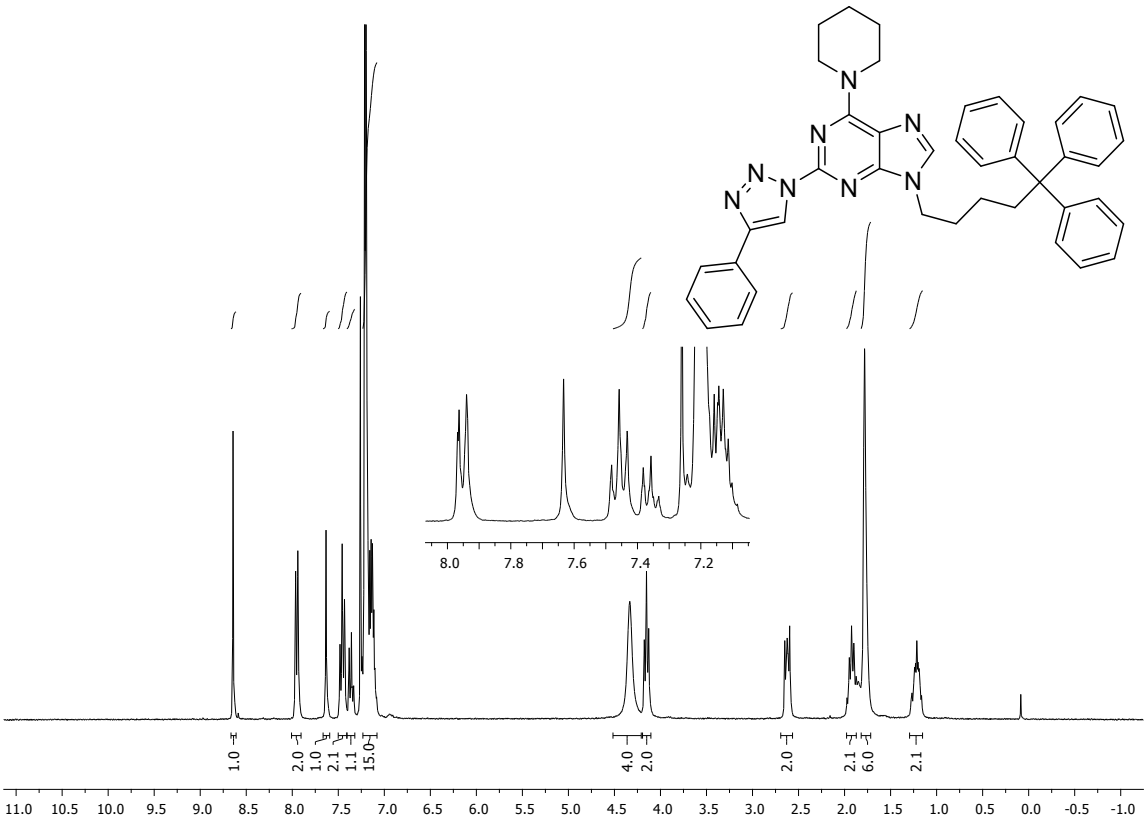

Figure S23. ^{1}H-NMR (300 MHz, $CDCl_3$) spectrum of compound 9a

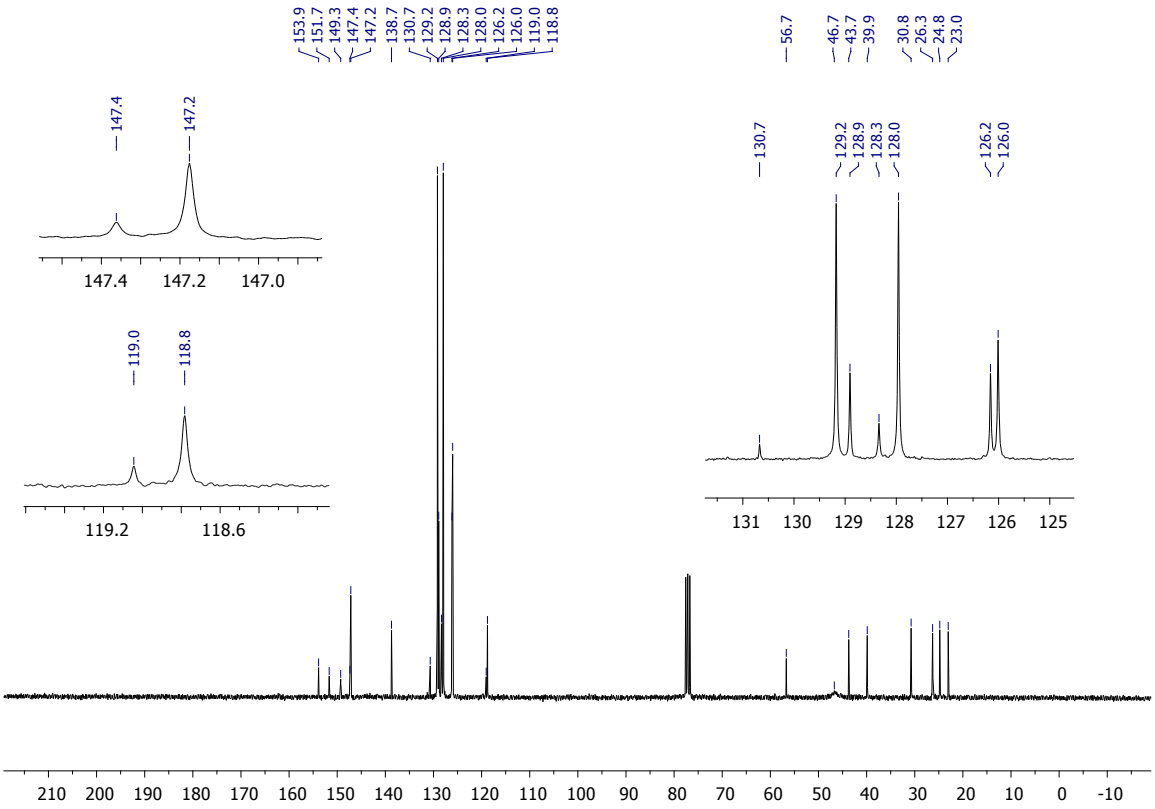

Figure S24. ^{13}C-NMR (75.5 MHz, $CDCl_3$) spectrum of compound 9a

2-(4-(4-Methoxyphenyl)-1*H*-1,2,3-triazol-1-yl)-6-(piperidin-1-yl)-9-(5,5,5-triphenylpentyl)-9*H*-purine (9b)

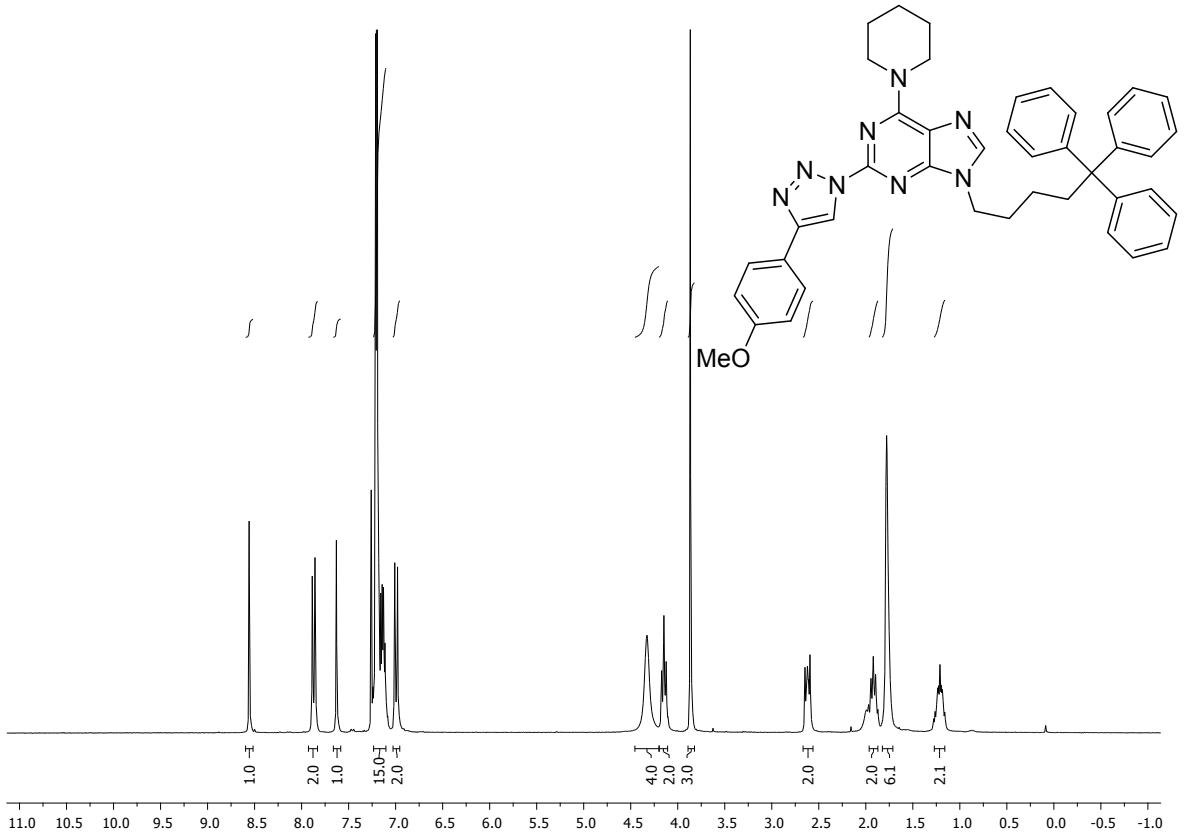

Figure S25. ^{1}H-NMR (300 MHz, $CDCl_3$) spectrum of compound 9b

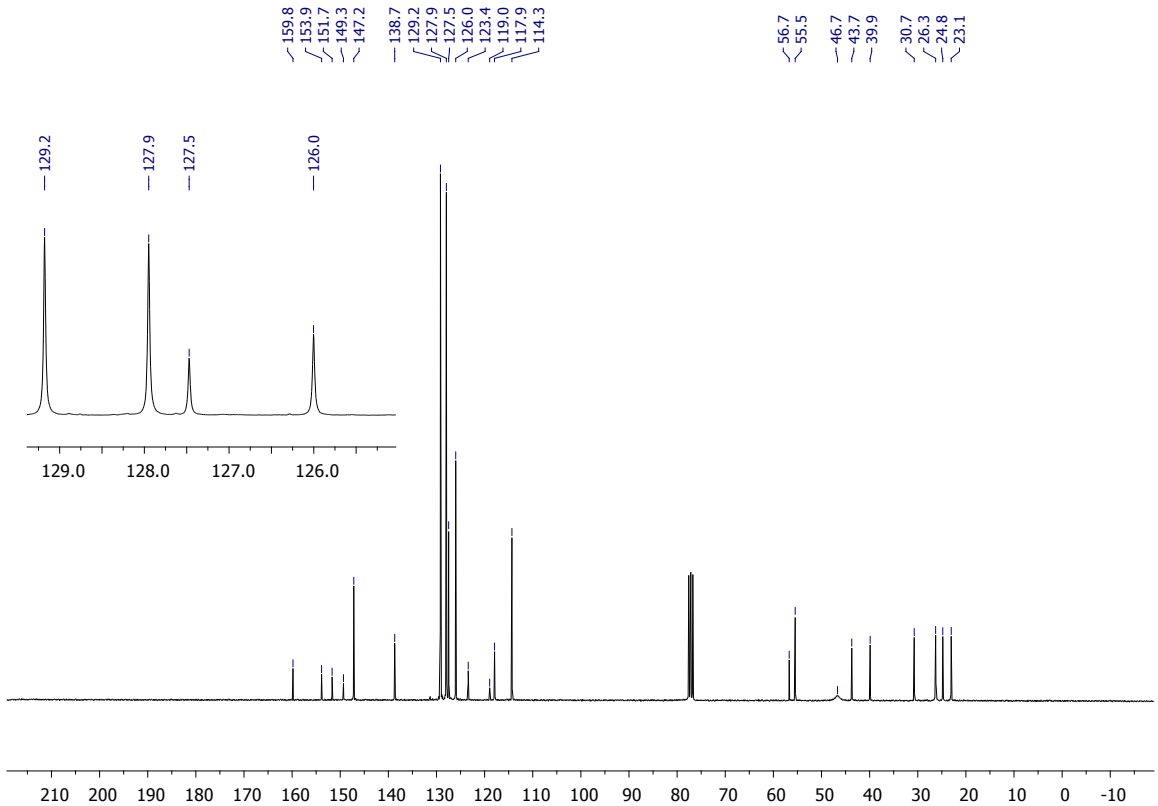

Figure S26. ^{13}C-NMR (75.5 MHz, $CDCl_3$) spectrum of compound 9b

9-(5,5,5-Triphenylpentyl)-2-(4-(4-(*N*,*N*-dimethylamino)phenyl)-1*H*-1,2,3-triazol-1-yl)-6-(piperidin-1-yl)-9*H*-purine (9c)

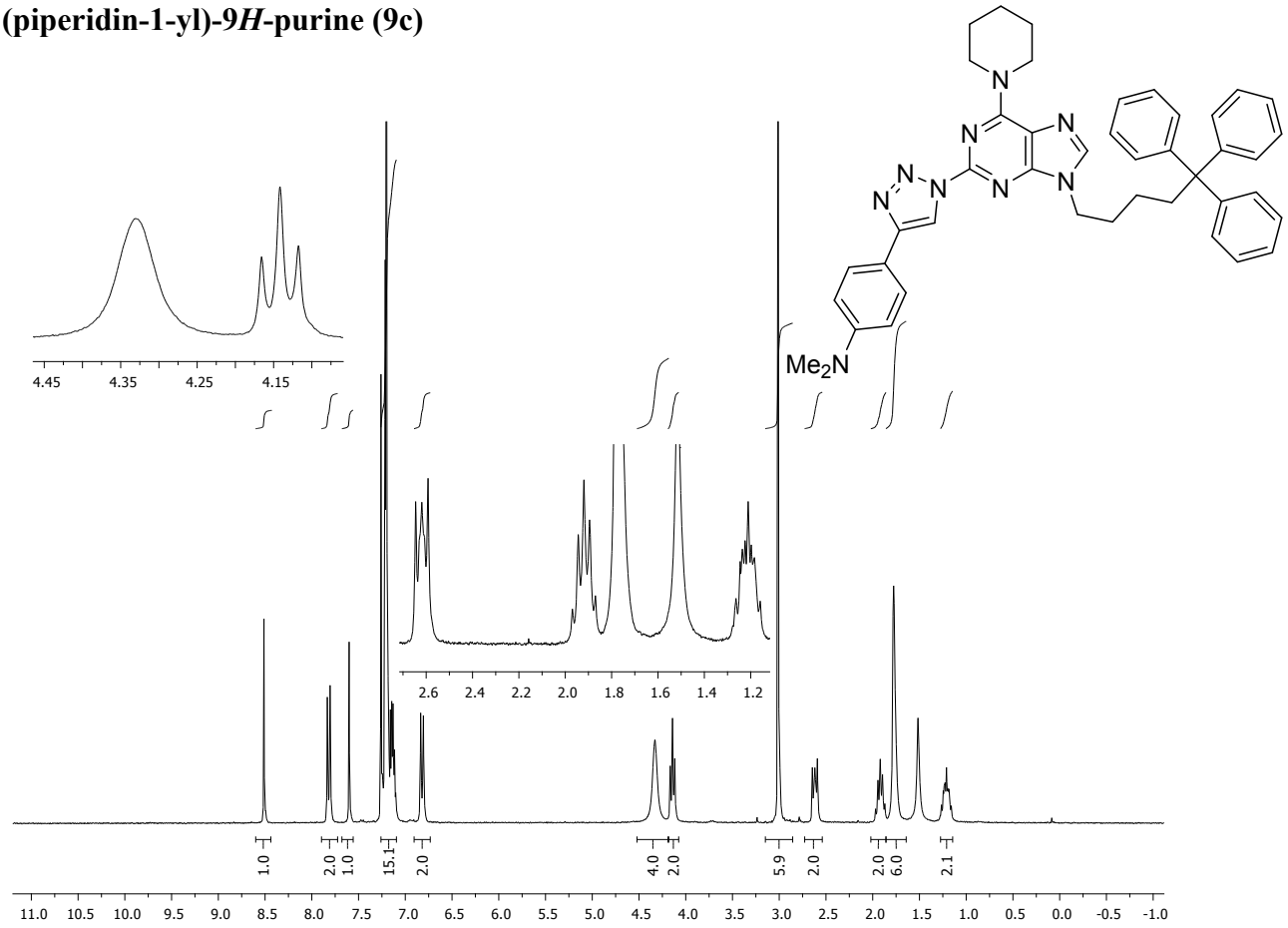

Figure S27. ^{1}H-NMR (300 MHz, $CDCl_3$) spectrum of compound 9c

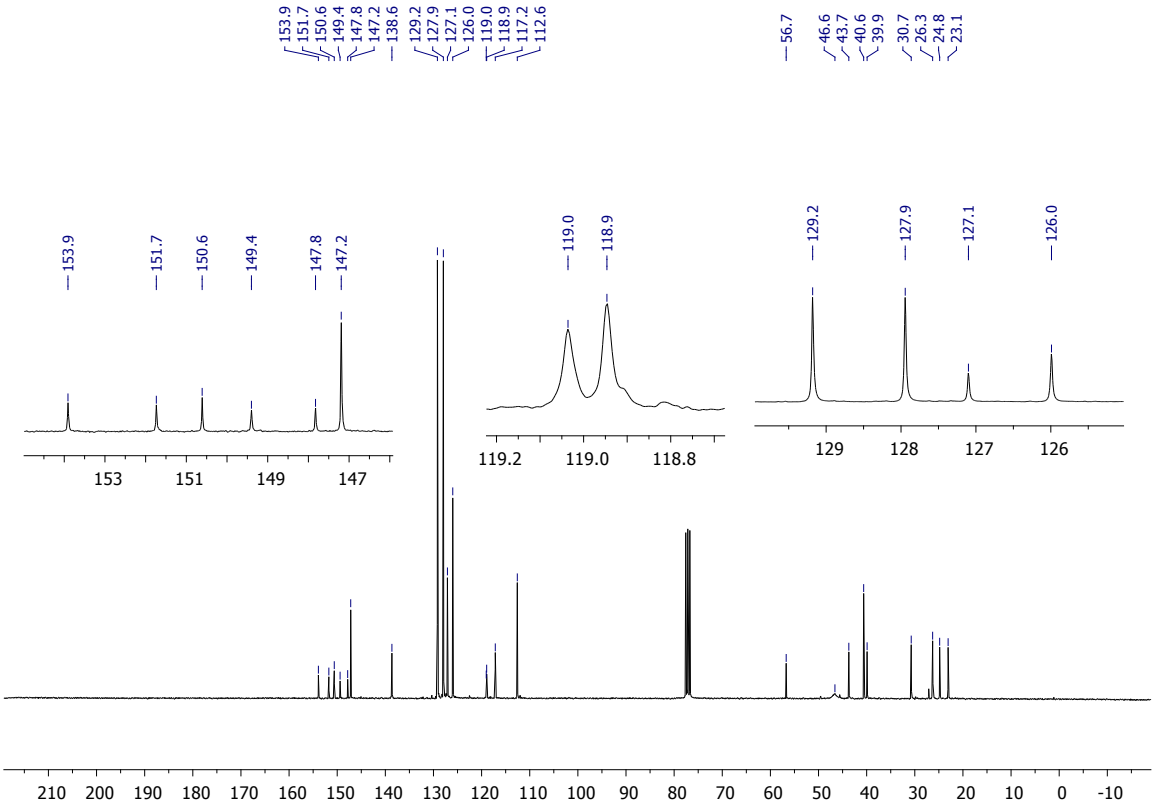

Figure S28. ^{13}C-NMR (75.5 MHz, $CDCl_3$) spectrum of compound 9c

2-(4-(4-Cyanophenyl)-1*H*-1,2,3-triazol-1-yl)-9-(5,5,5-triphenylpentyl)-6-(piperidin-1-yl)-9*H*-purine (9d)

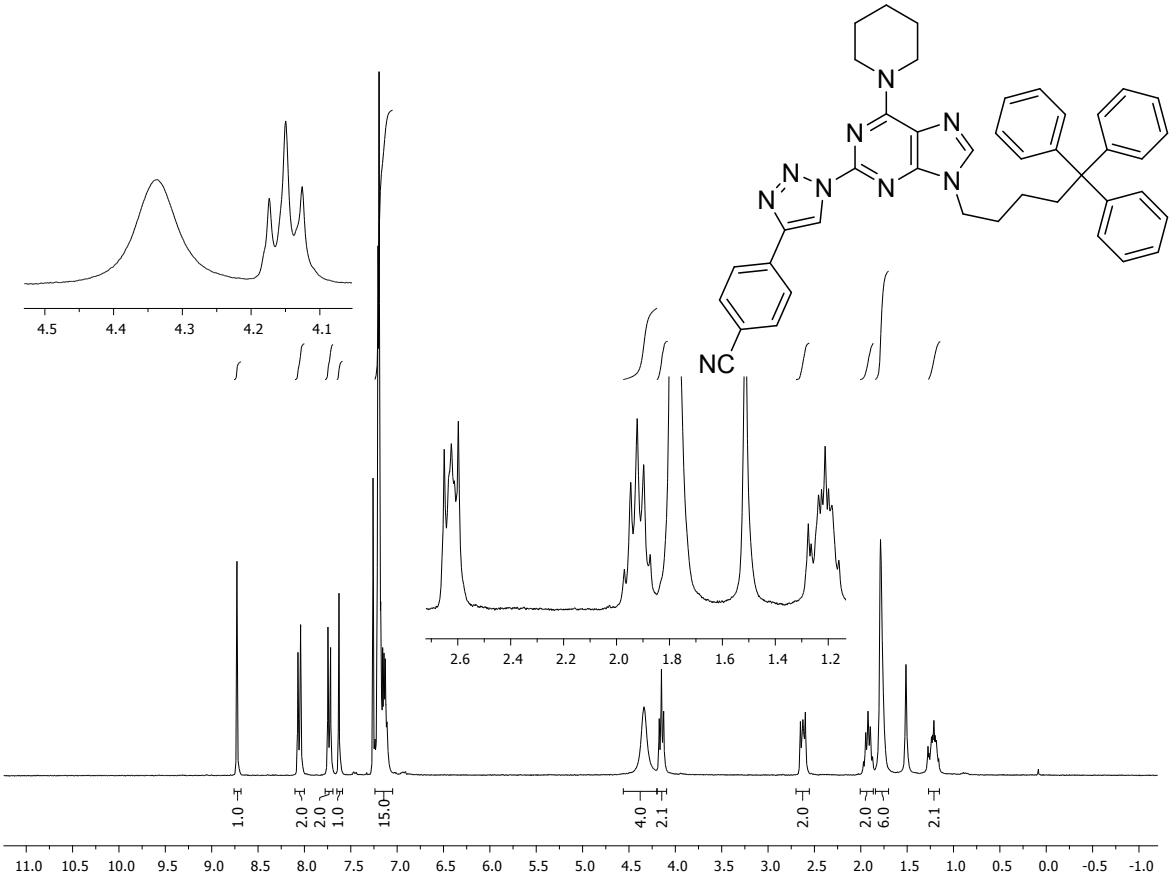

Figure S29.[1]H-NMR (300 MHz, $CDCl_3$) spectrum of compound 9d

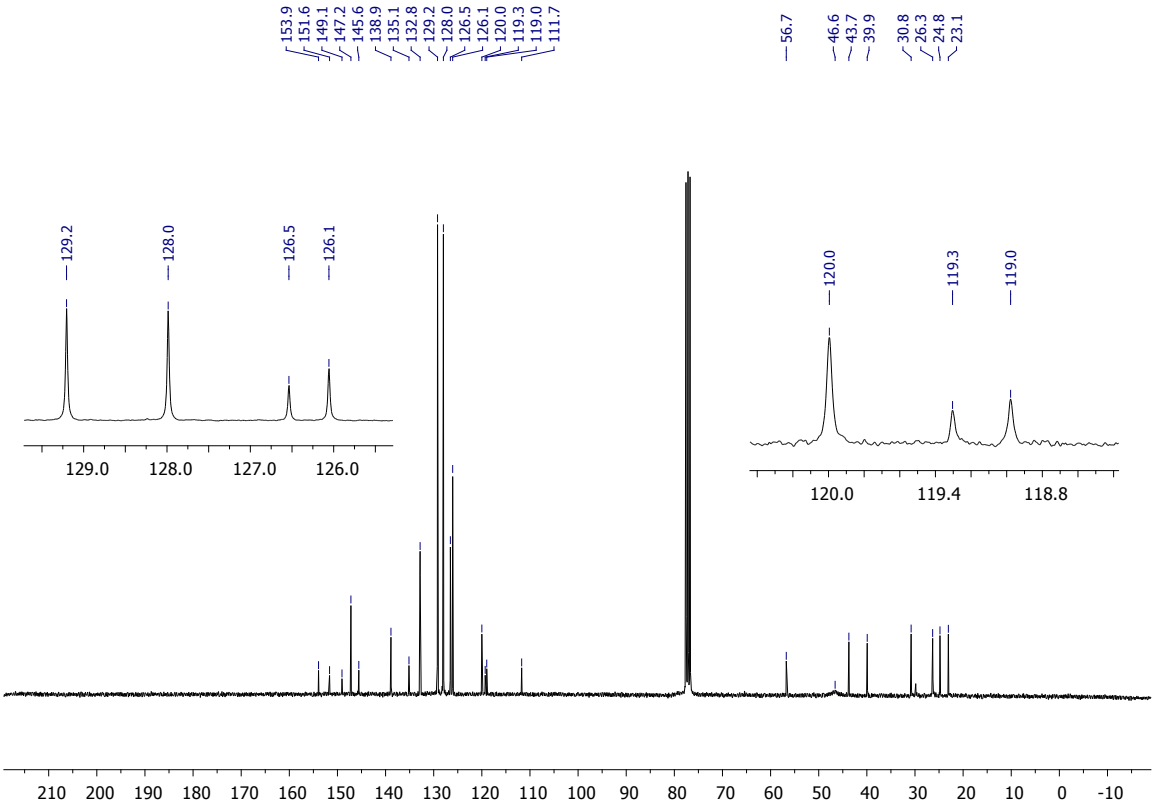

Figure S30. [13]C-NMR (75.5 MHz, $CDCl_3$) spectrum of compound 9d