Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

Identification and development of 1-((1-(substituted)-1*H*-1,2,3-triazol-4-pyrazolo[4,3-*c*]pyridine-5(4*H*)-carboxamides as *Mycobacterium tuberculosis* Pantothenate synthetase inhibitors

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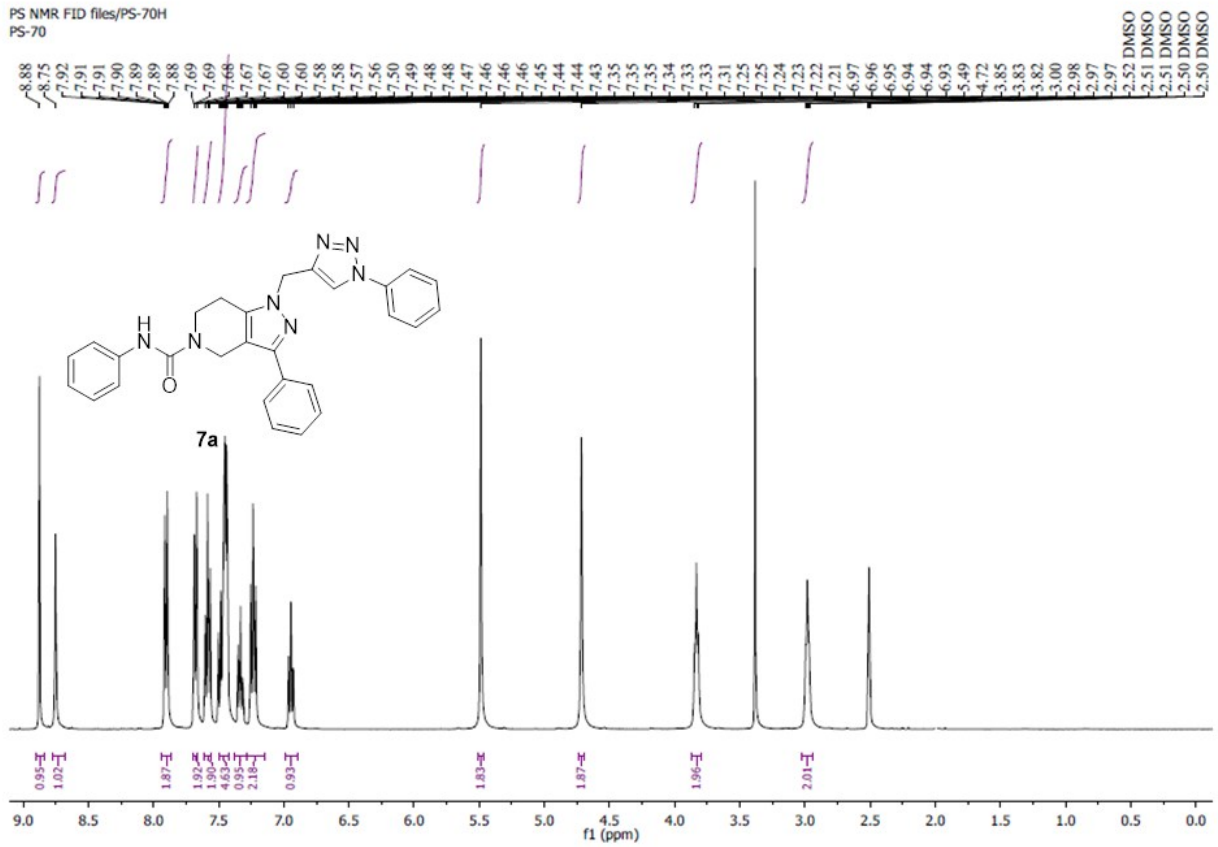

Figure S1. ^{1}H NMR spectrum (400MHz, DMSO-d_6) of compound **7a.**

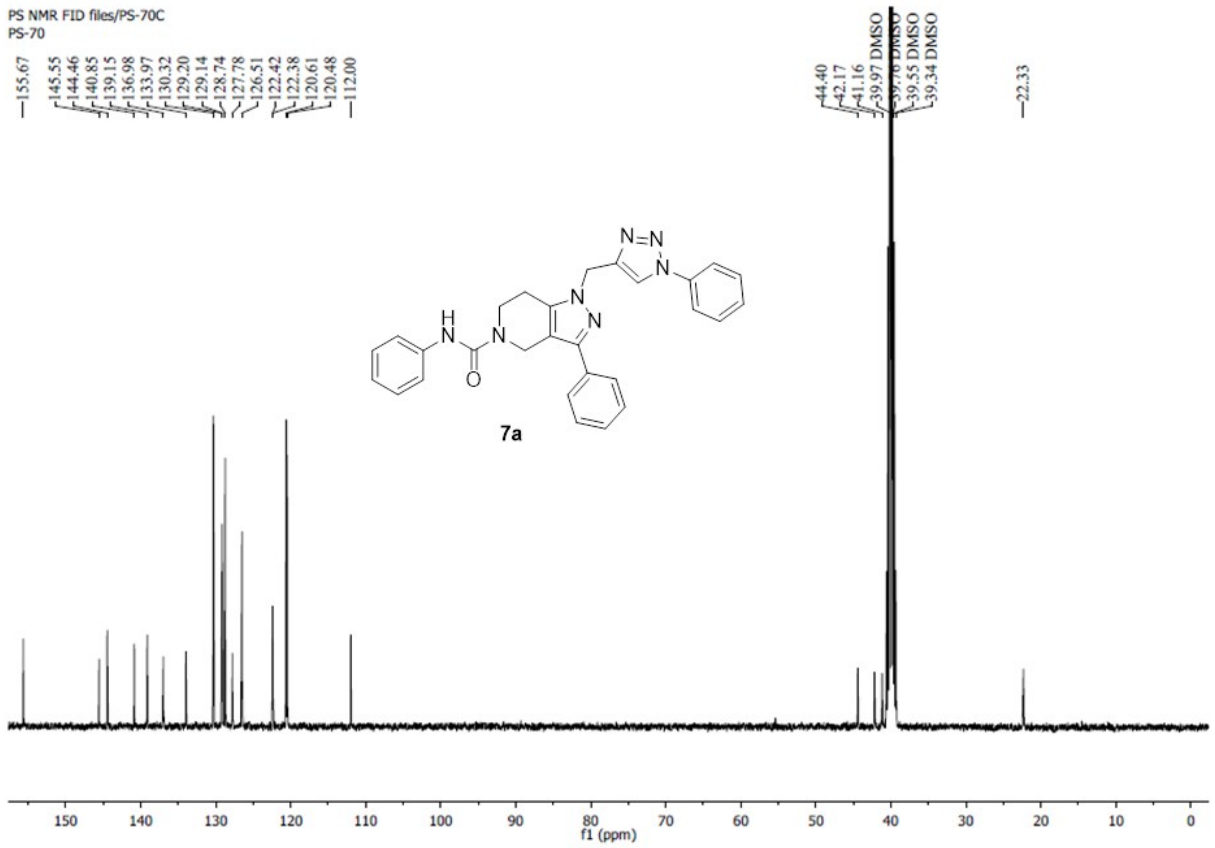

Figure S2. ^{13}C NMR spectrum (101MHz, DMSO-d_6) of compound **7a.**

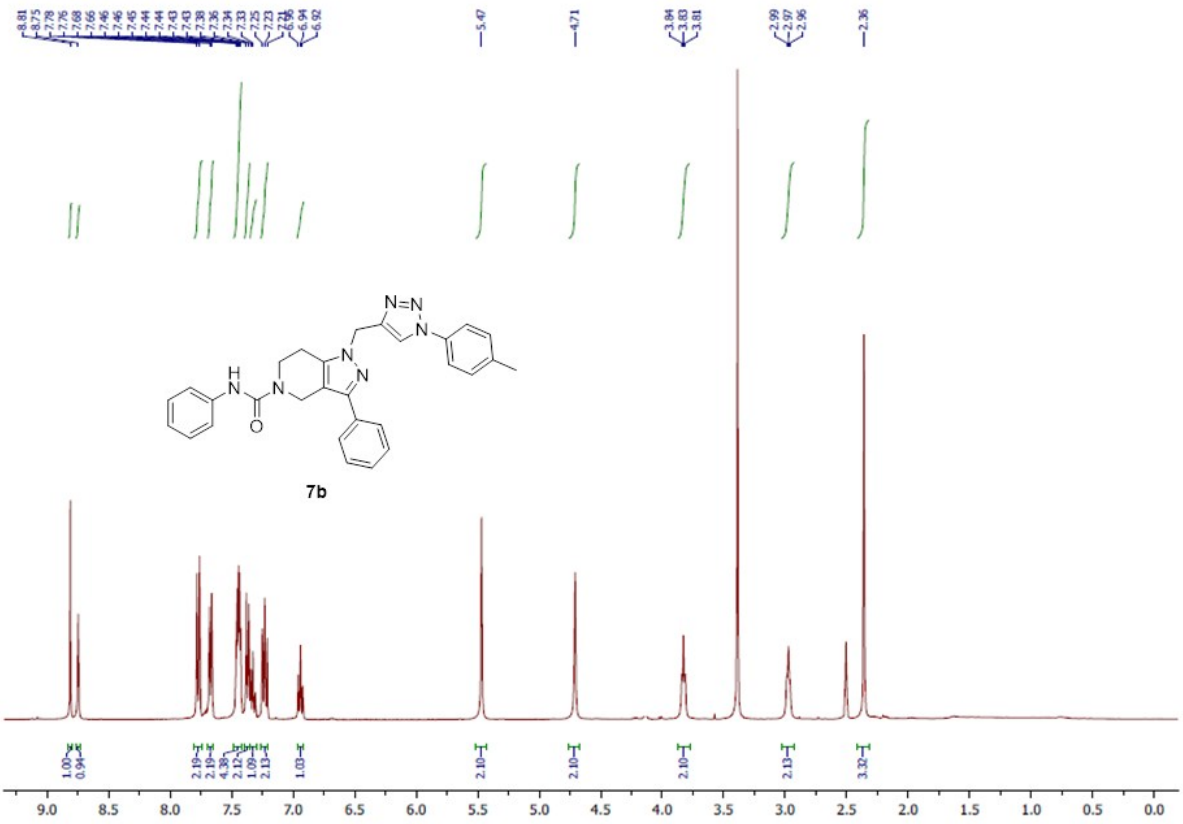

Figure S3. ^{1}H NMR spectrum (400 MHz, DMSO-d_6) of compound **7b.**

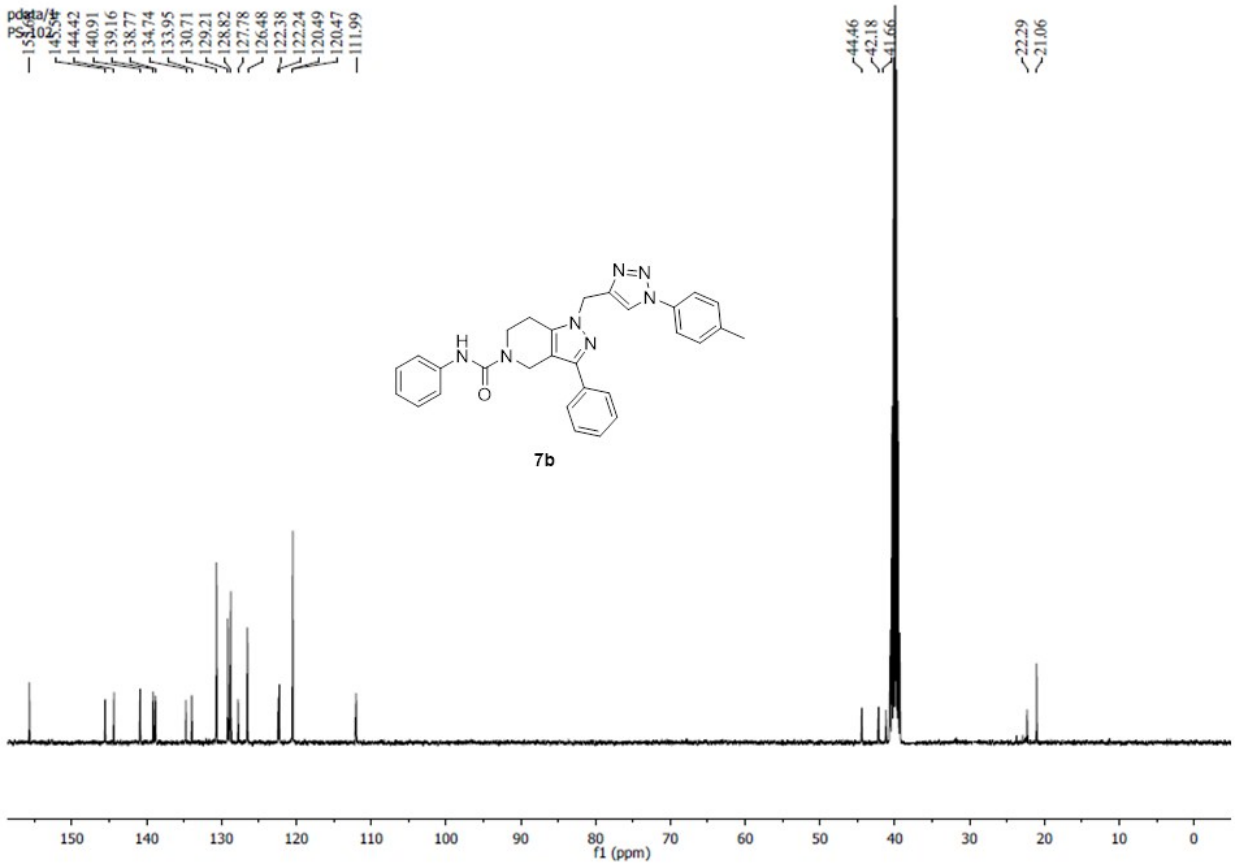

Figure S4. ^{13}C NMR spectrum (101MHz, DMSO-d_6) of compound **7b.**

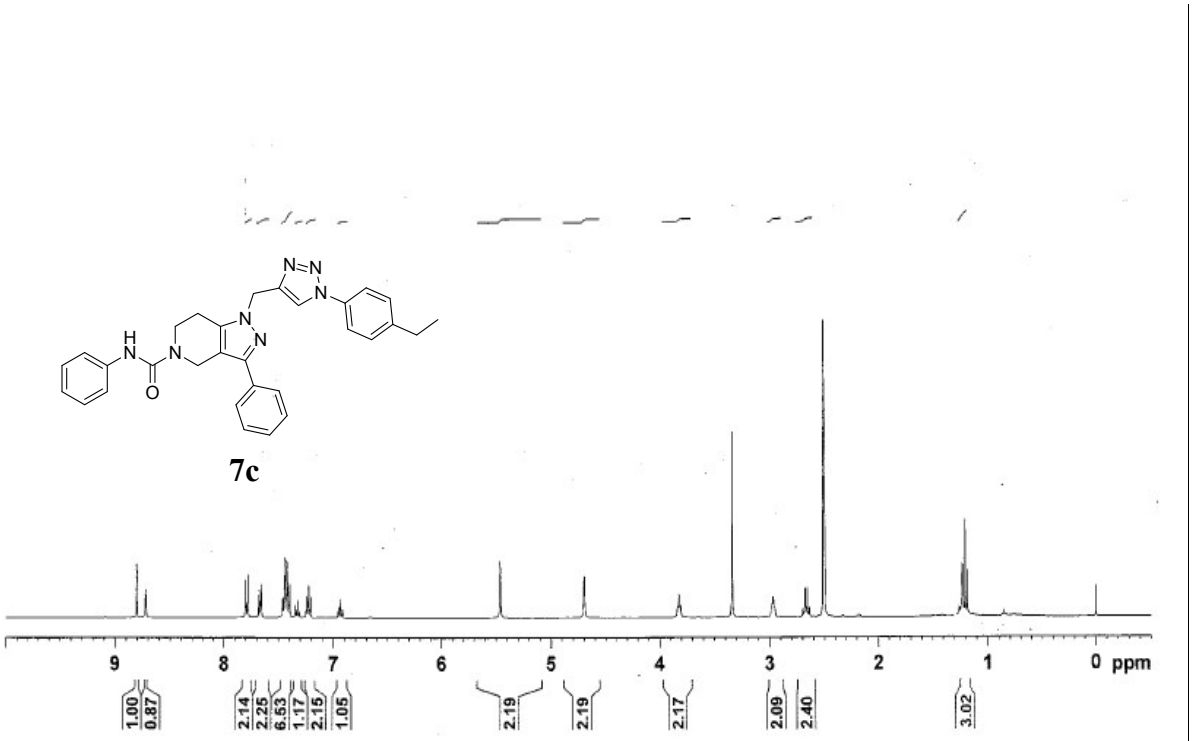

Figure S5. ^{1}H NMR spectrum (400 MHz, DMSO-d_6) of compound **7c.**

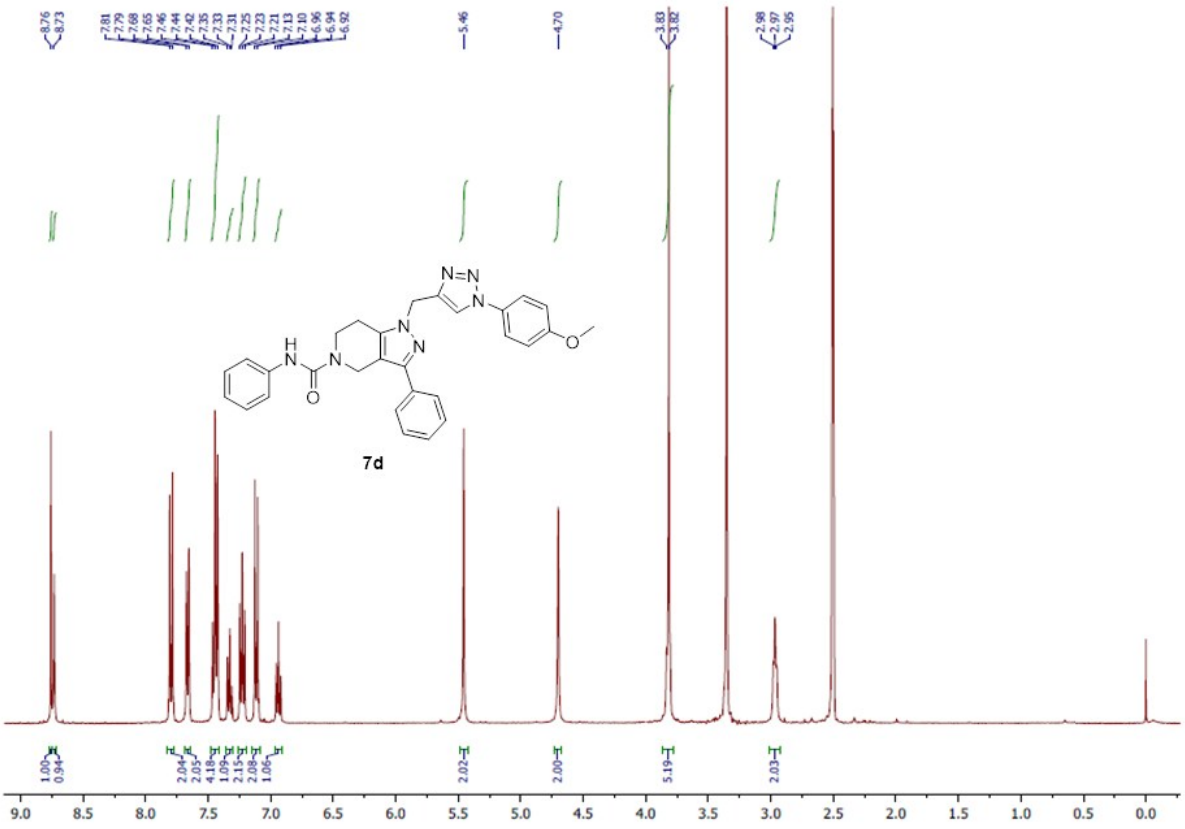

Figure S6. ^{1}H NMR spectrum (400 MHz, DMSO-d_6) of compound **7d.**

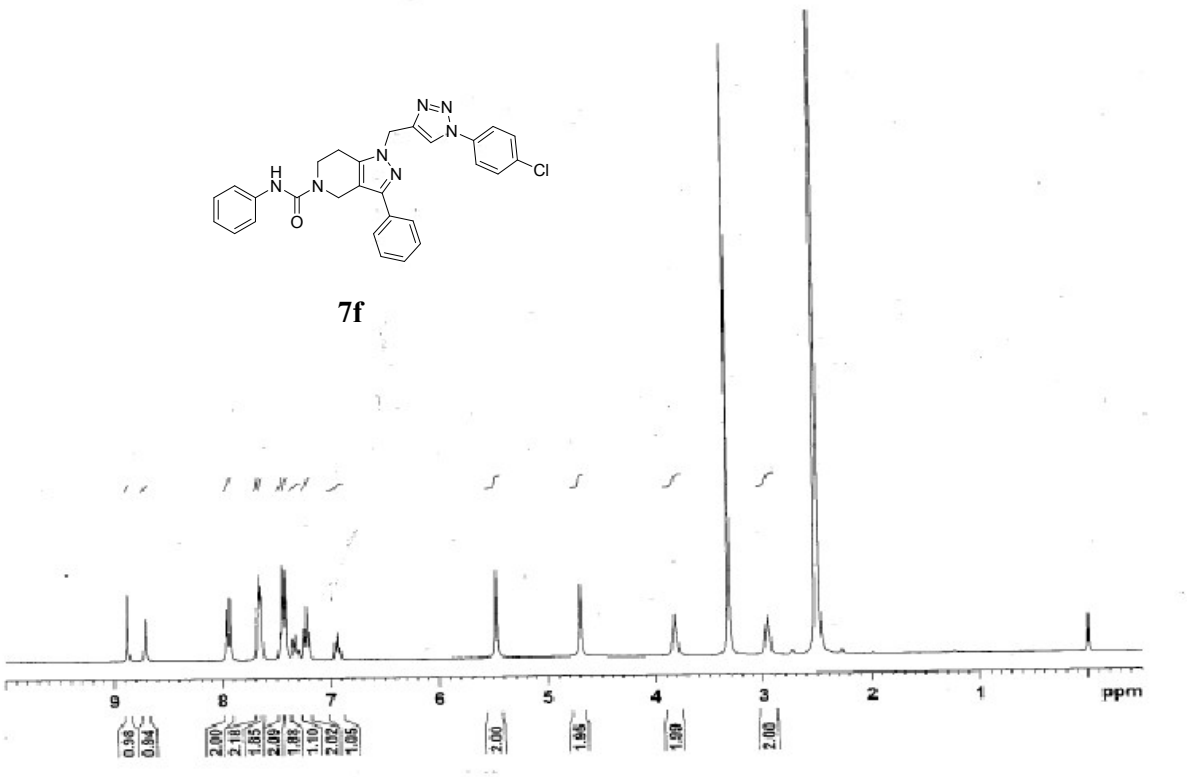

Figure S7. ^{1}H NMR spectrum (400 MHz, DMSO-d_6) of compound **7f.**

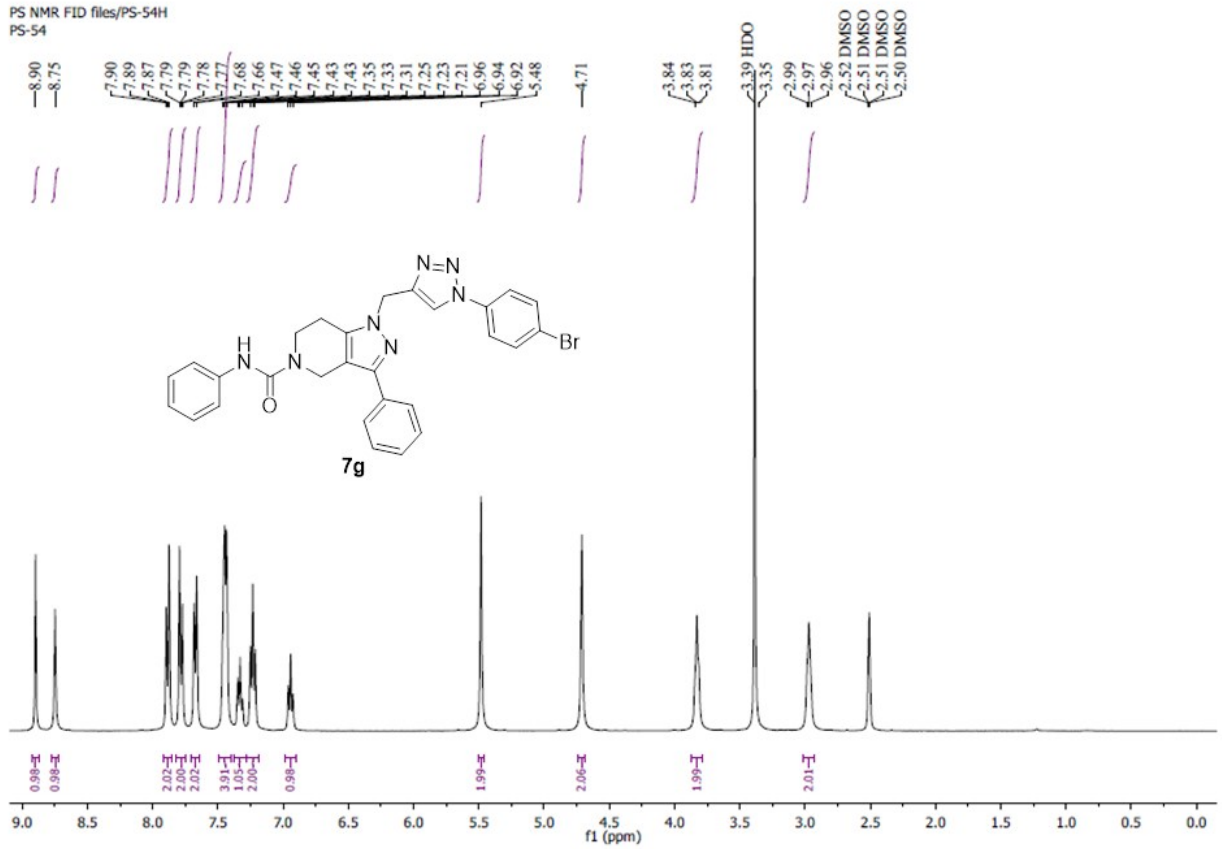

Figure S8. ^{1}H NMR spectrum (400 MHz, DMSO-d_6) of compound **7g.**

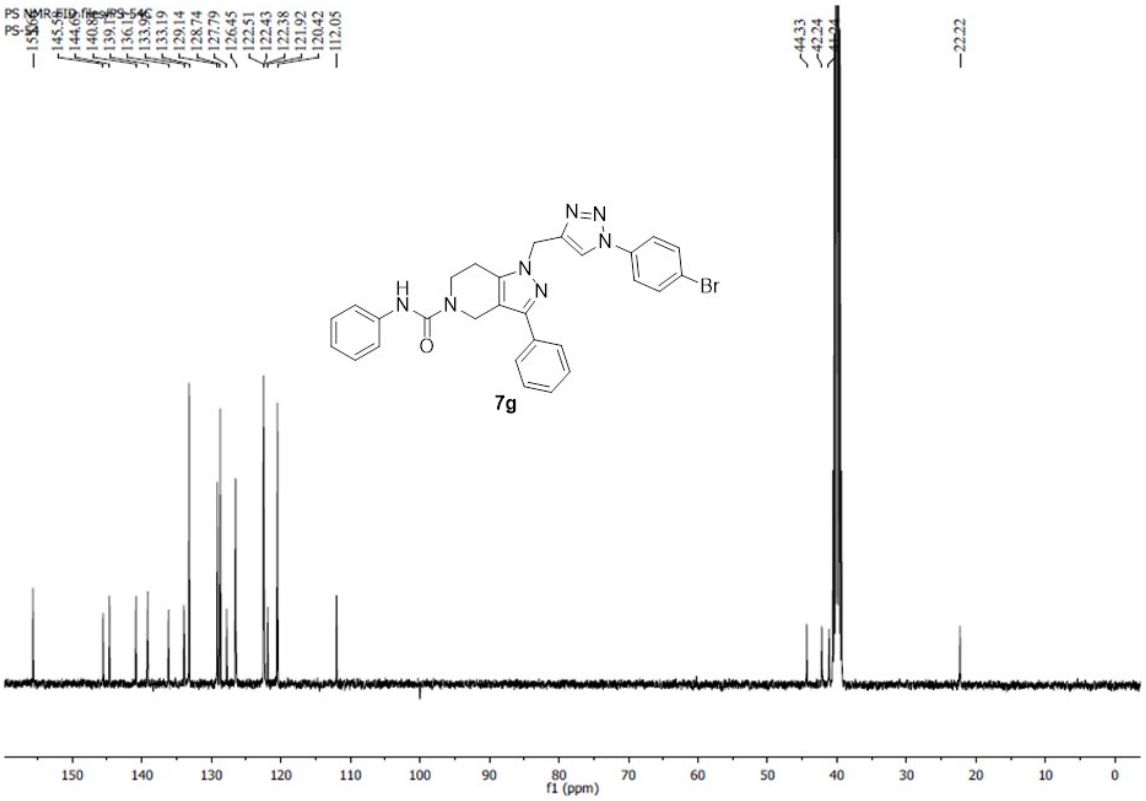

Figure S9. ^{13}C NMR spectrum (101 MHz, DMSO-d_6) of compound **7g.**

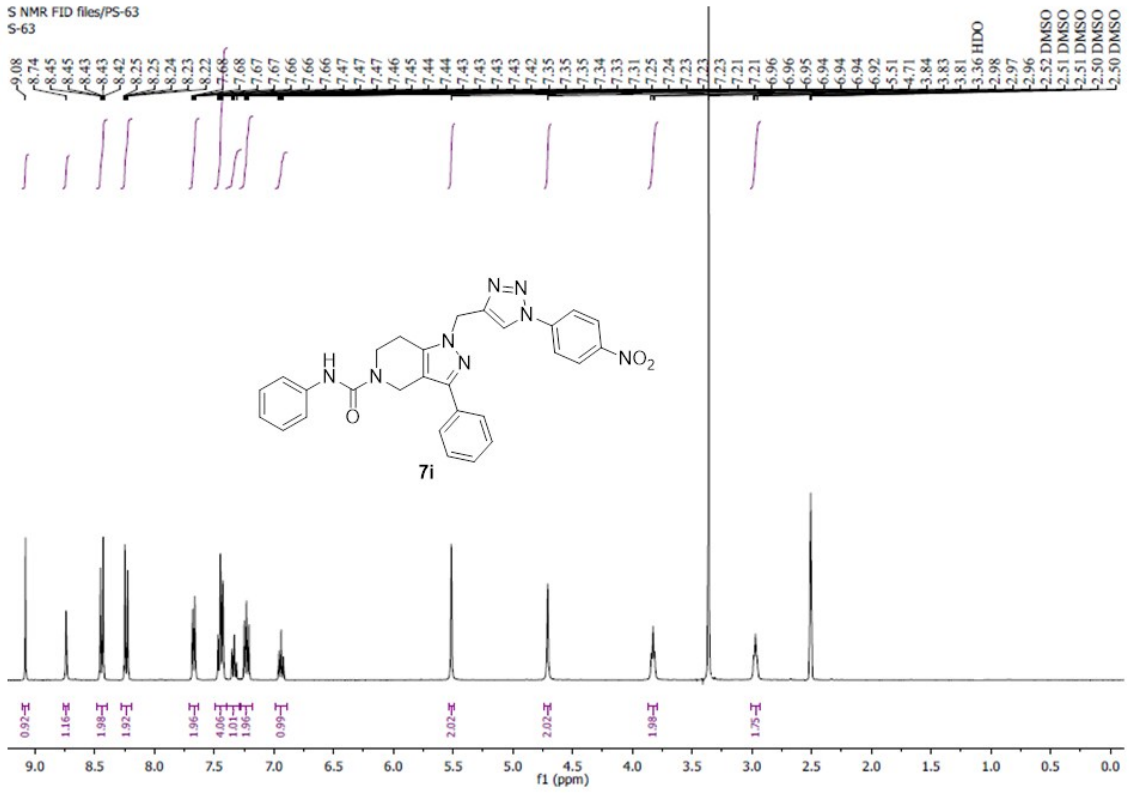

Figure S10. ^{1}H NMR spectrum (400 MHz, DMSO-d_6) of compound **7i.**

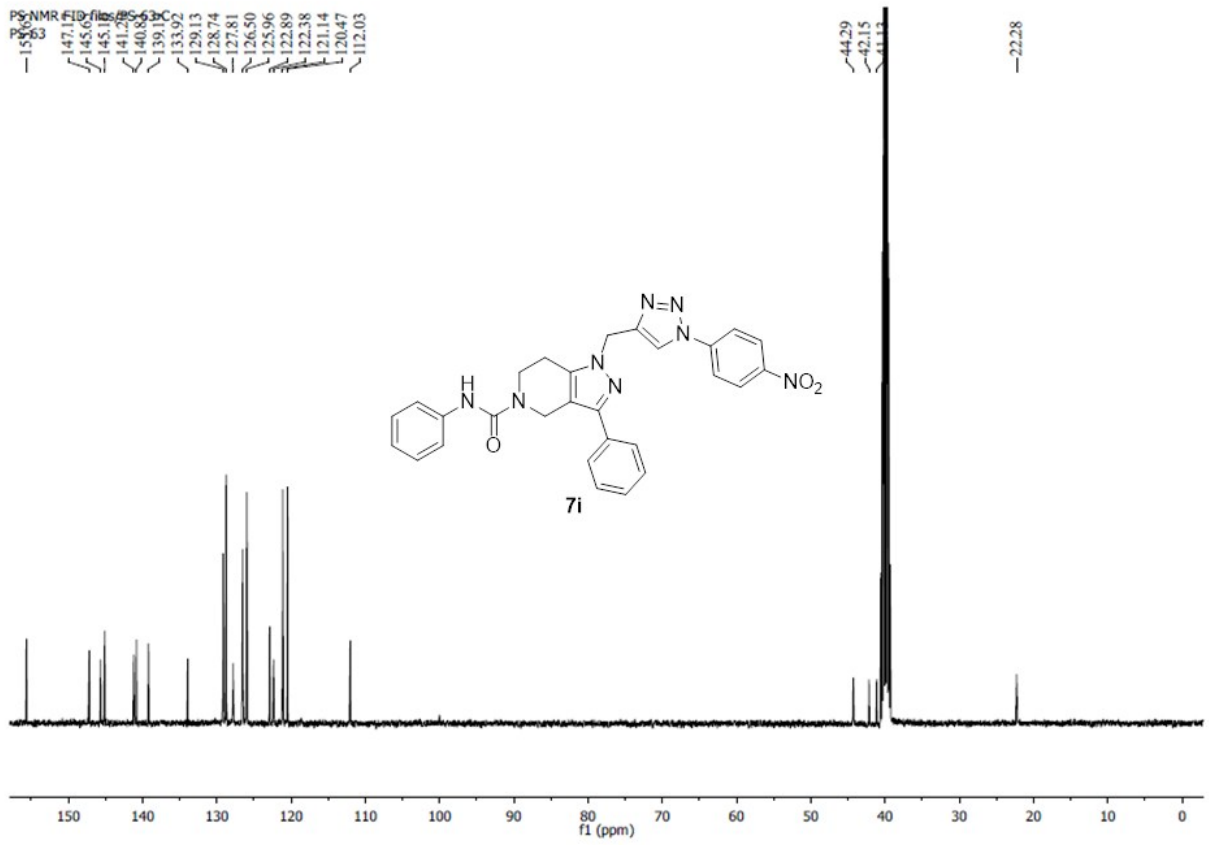

Figure S11. ^{13}C NMR spectrum (101 MHz, DMSO-d_6) of compound **7i.**

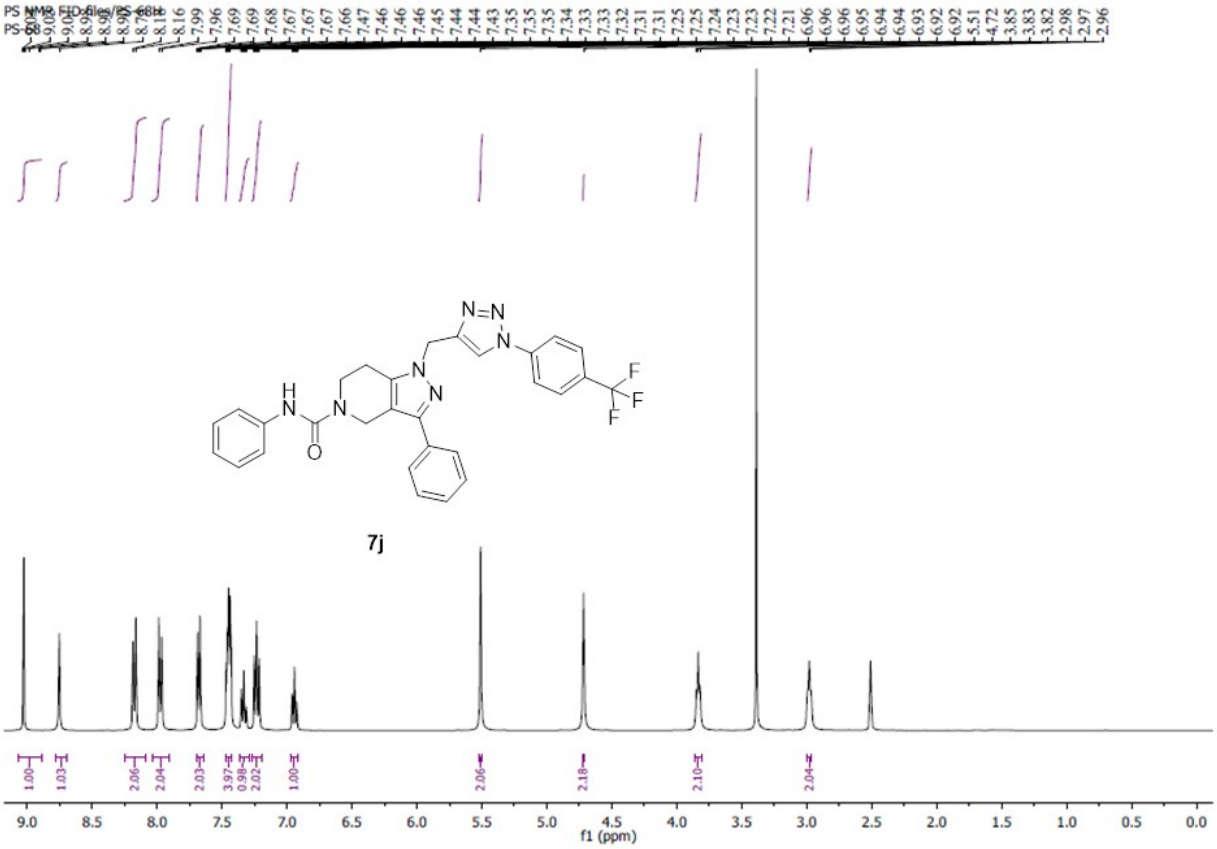

Figure S12. ^{1}H NMR spectrum (400 MHz, DMSO-d_6) of compound **7j.**

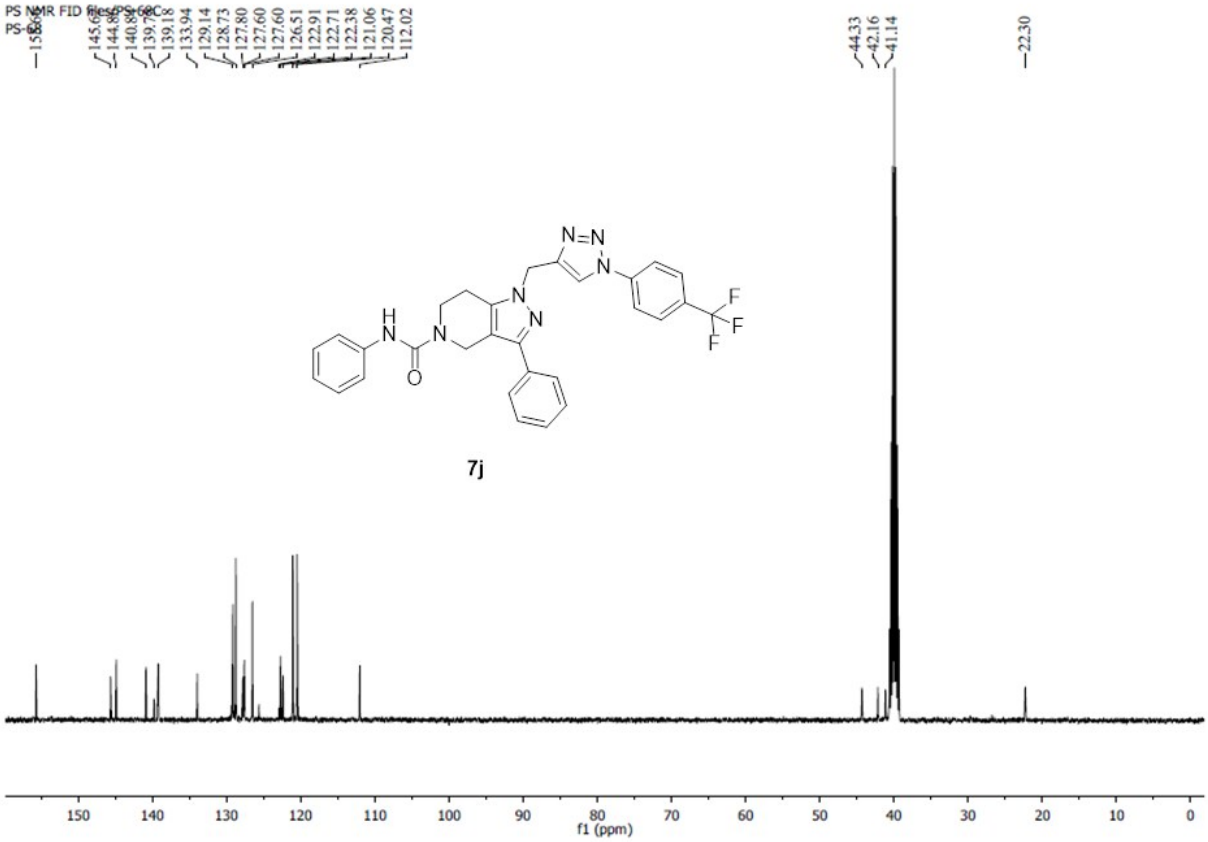

Figure S13. ^{13}C NMR spectrum (101 MHz, DMSO-d_6) of compound **7j.**

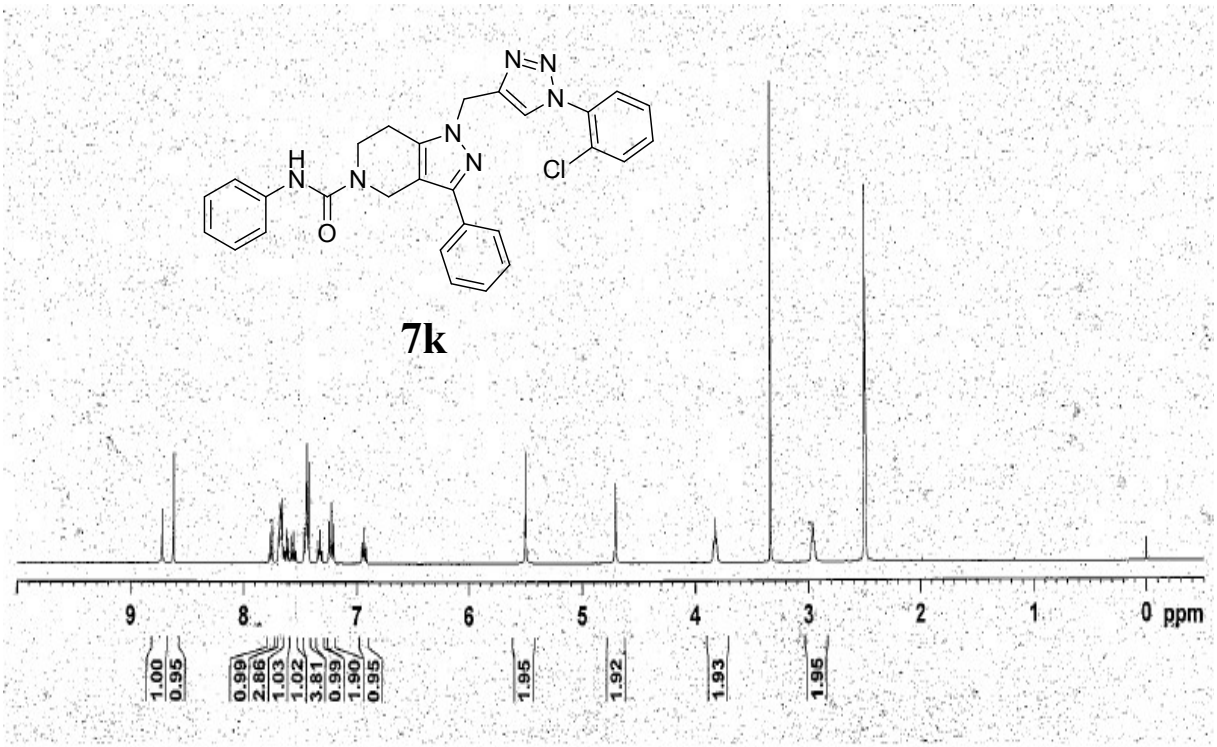

Figure S14. ^{1}H NMR spectrum (400 MHz, DMSO-d_6) of compound **7k.**

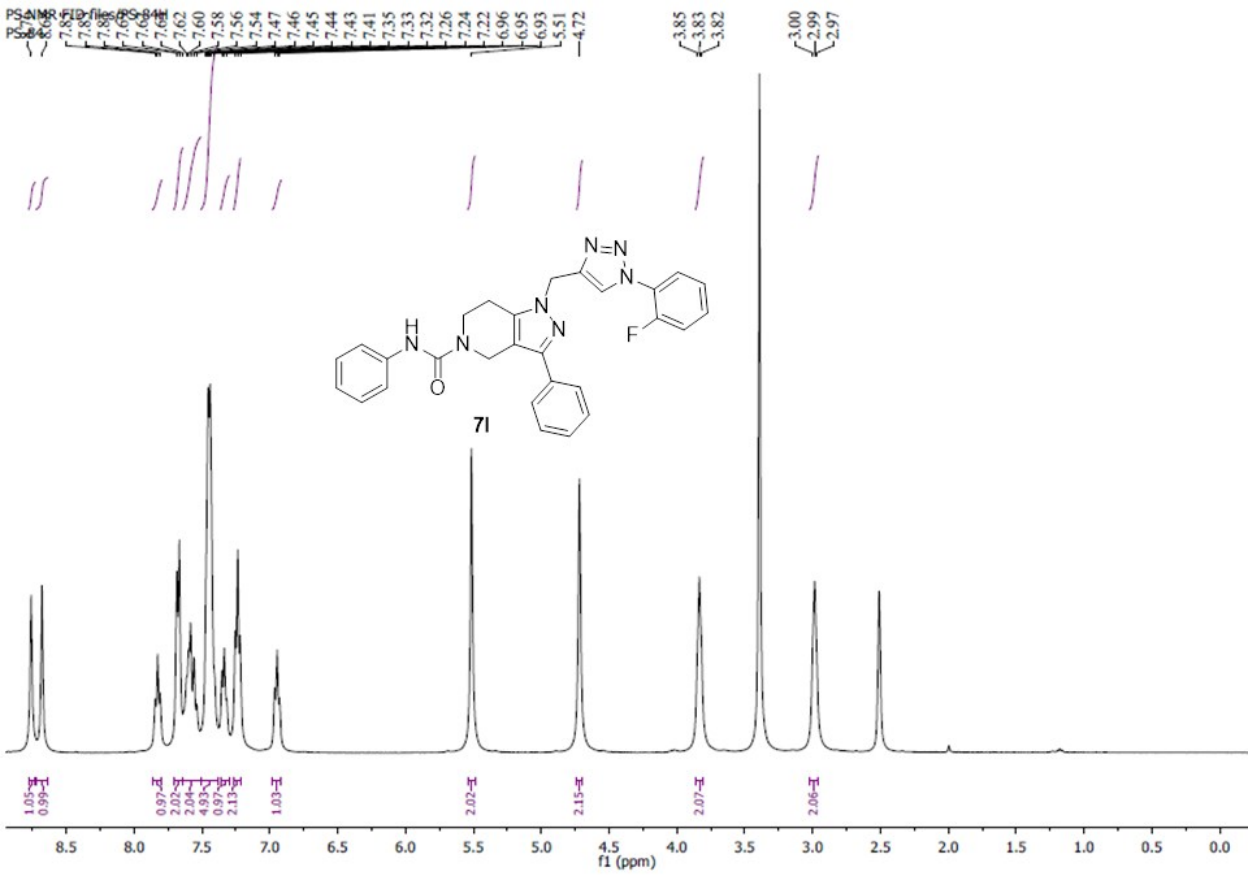

Figure S15. ^{1}H NMR spectrum (400 MHz, DMSO-d_6) of compound **7l.**

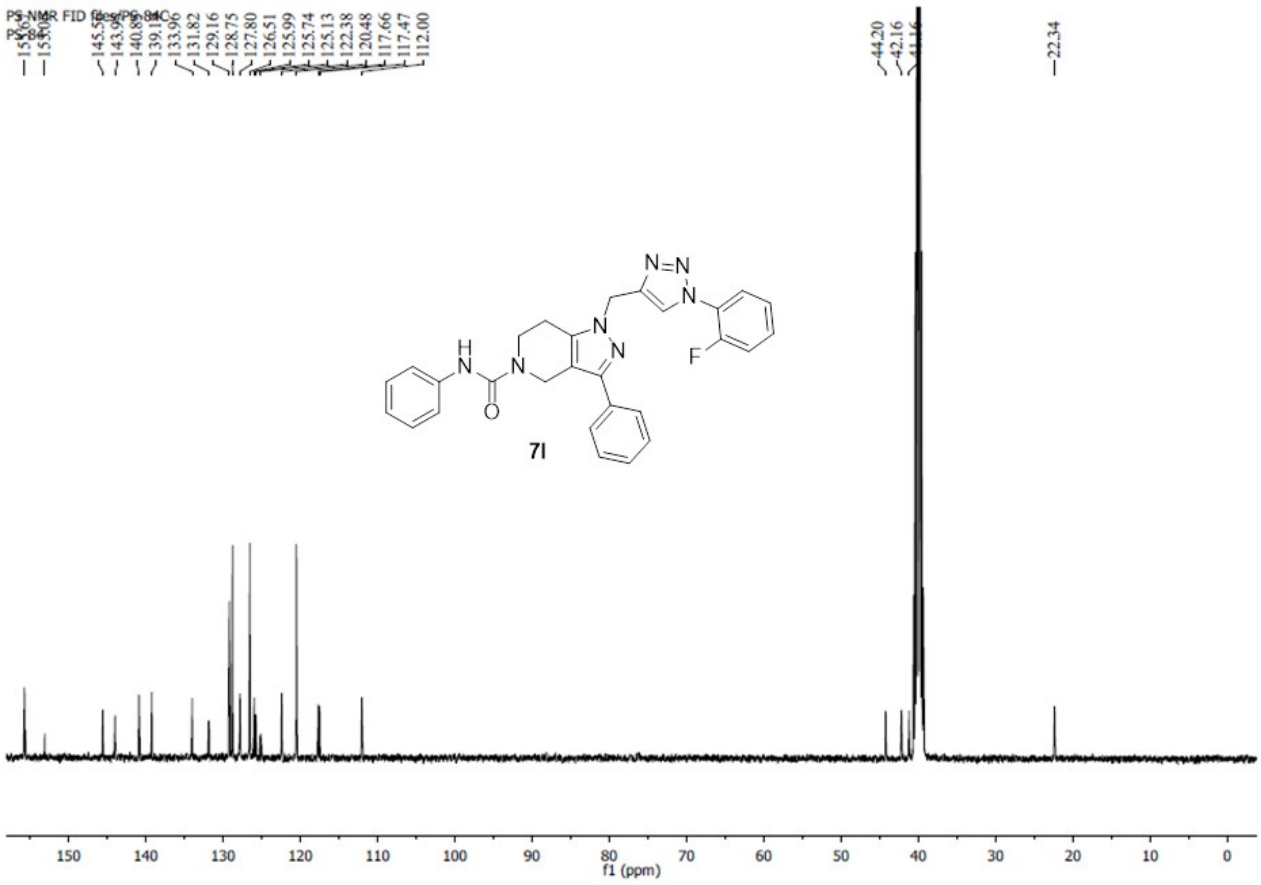

Figure S16. ^{13}CNMR spectrum (101 MHz, DMSO-d_6) of compound **7l.**

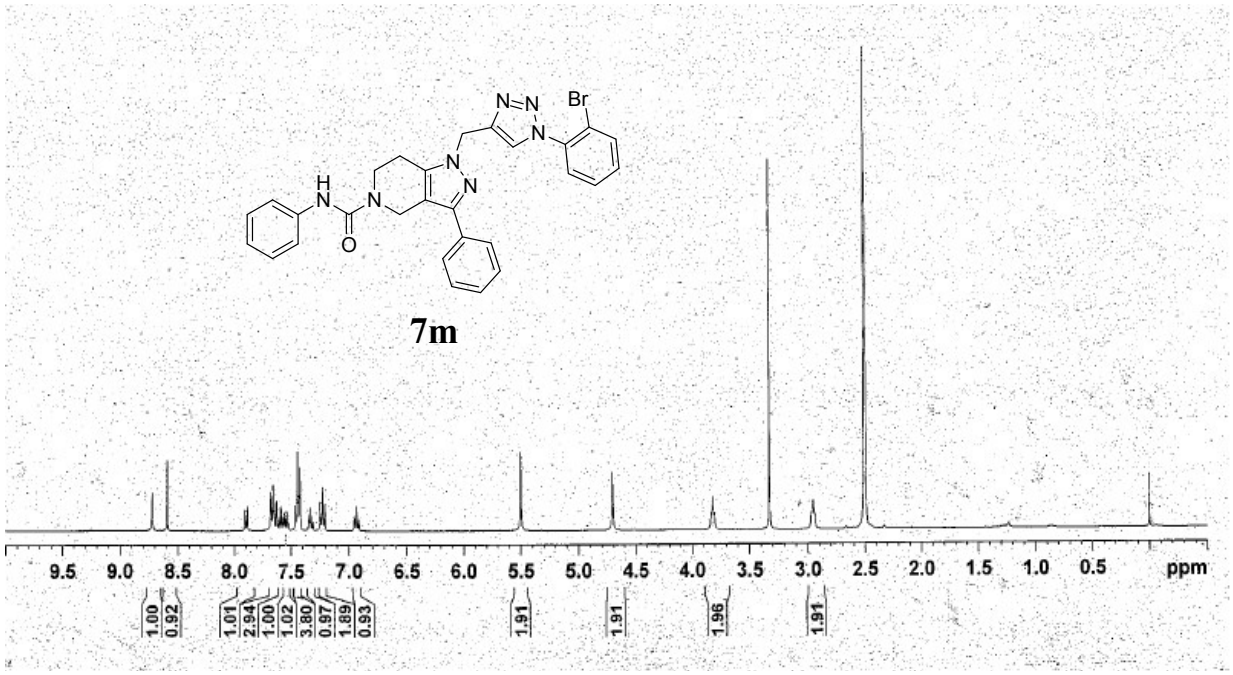

Figure S17. ^{1}H NMR spectrum (400 MHz, DMSO-d_6) of compound **7m.**

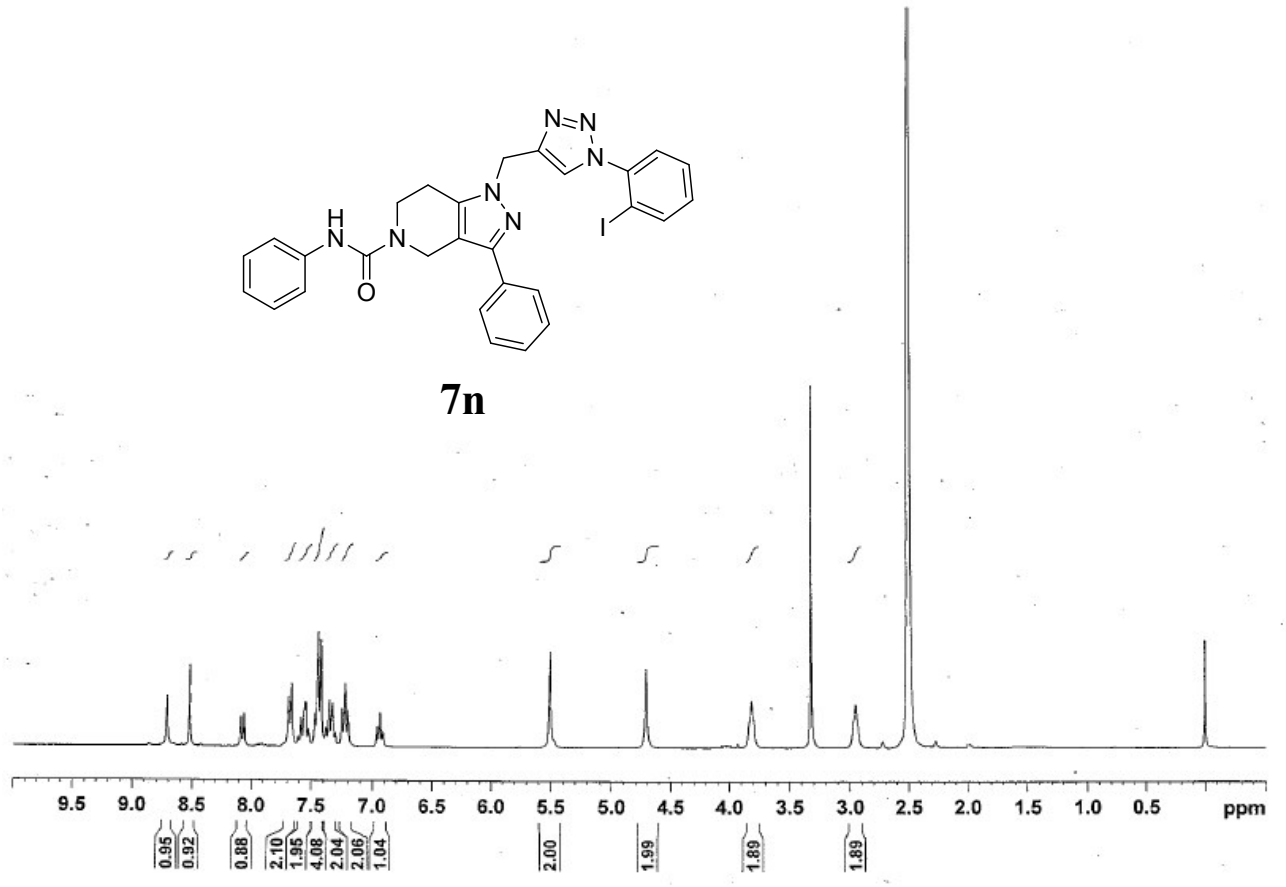

Figure S18. ^{1}H NMR spectrum (400 MHz, DMSO-d_6) of compound **7n.**

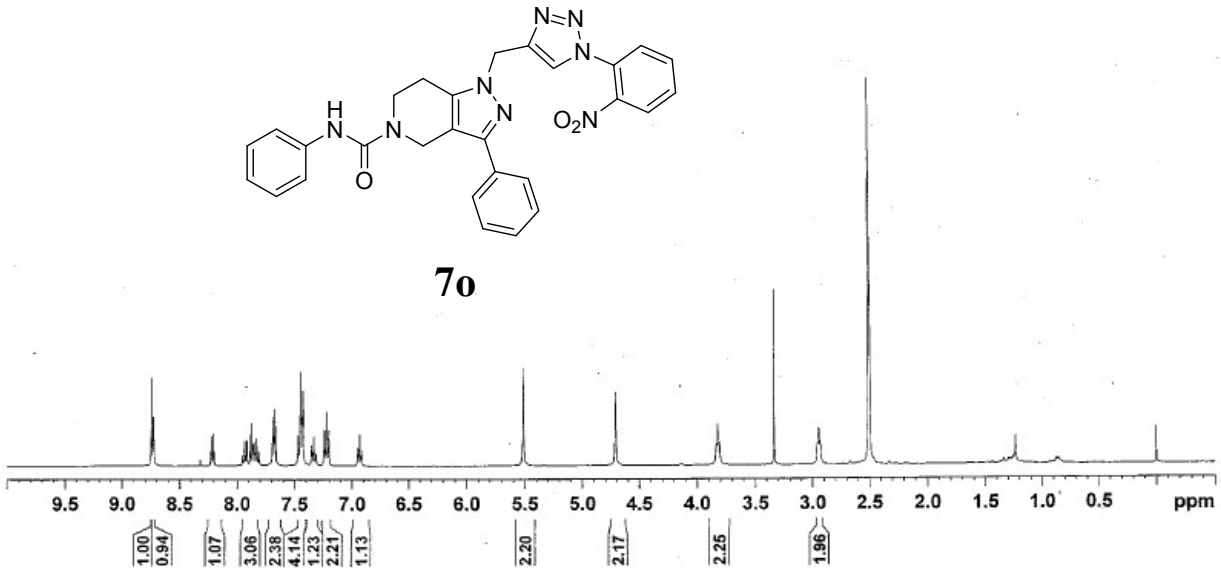

Figure S19. ^{1}H NMR spectrum (400 MHz, DMSO-d_6) of compound **7o.**

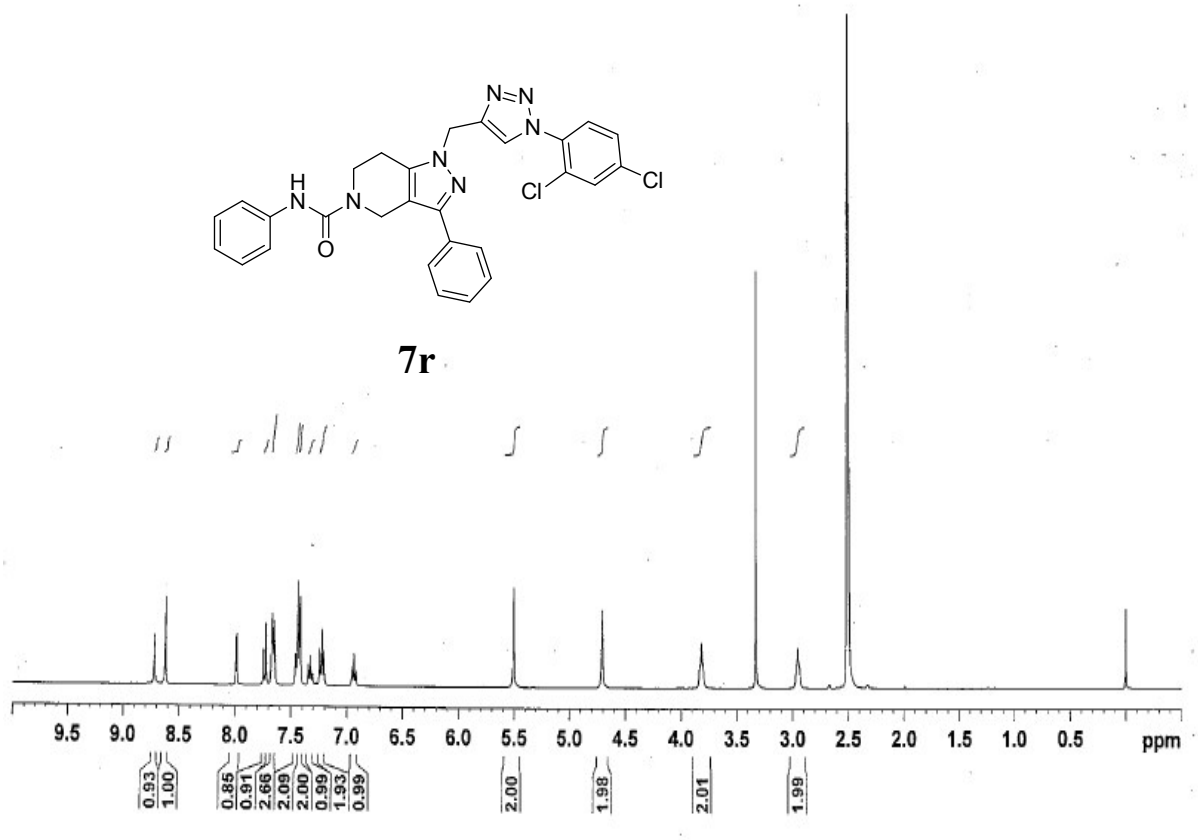

Figure S20. ^{1}H NMR spectrum (400 MHz, DMSO-d_6) of compound **7r.**

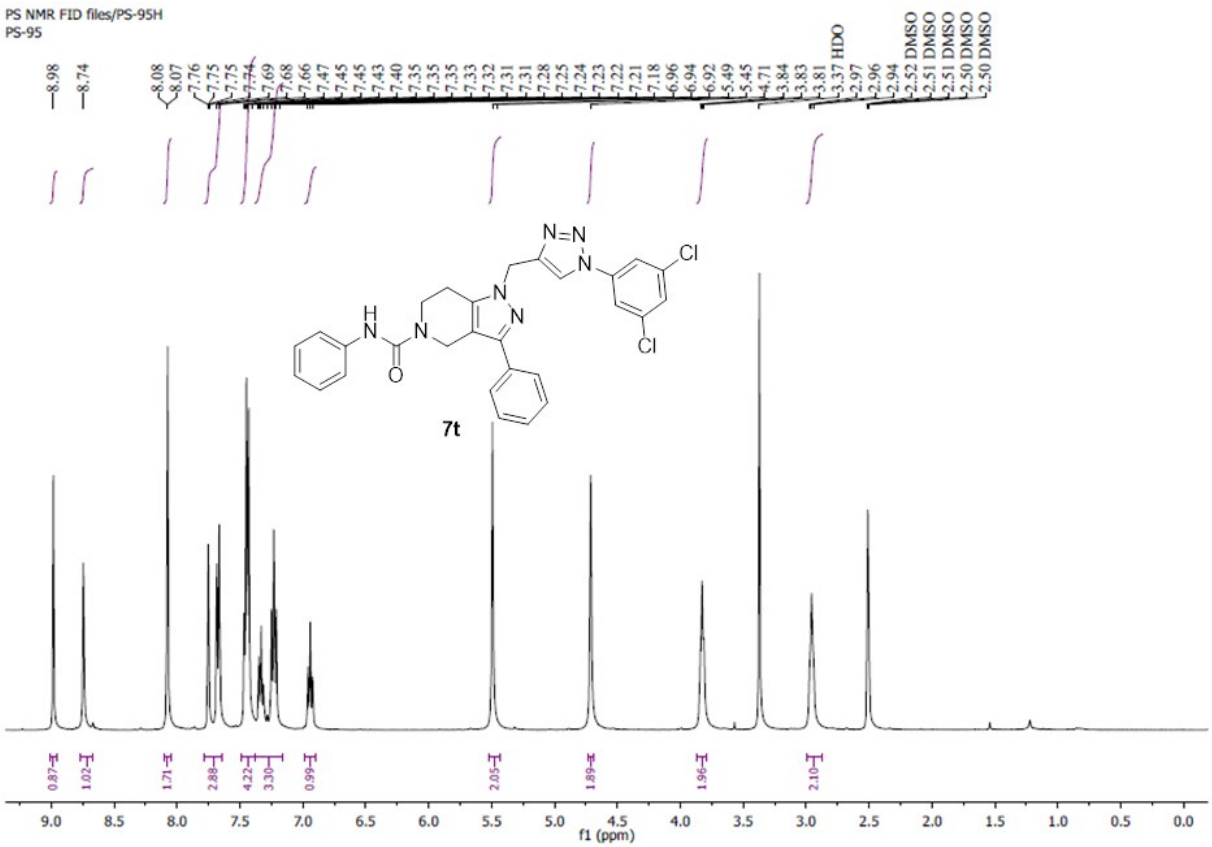

Figure S21. ^{1}H NMR spectrum (400 MHz, DMSO-d_6) of compound **7t.**

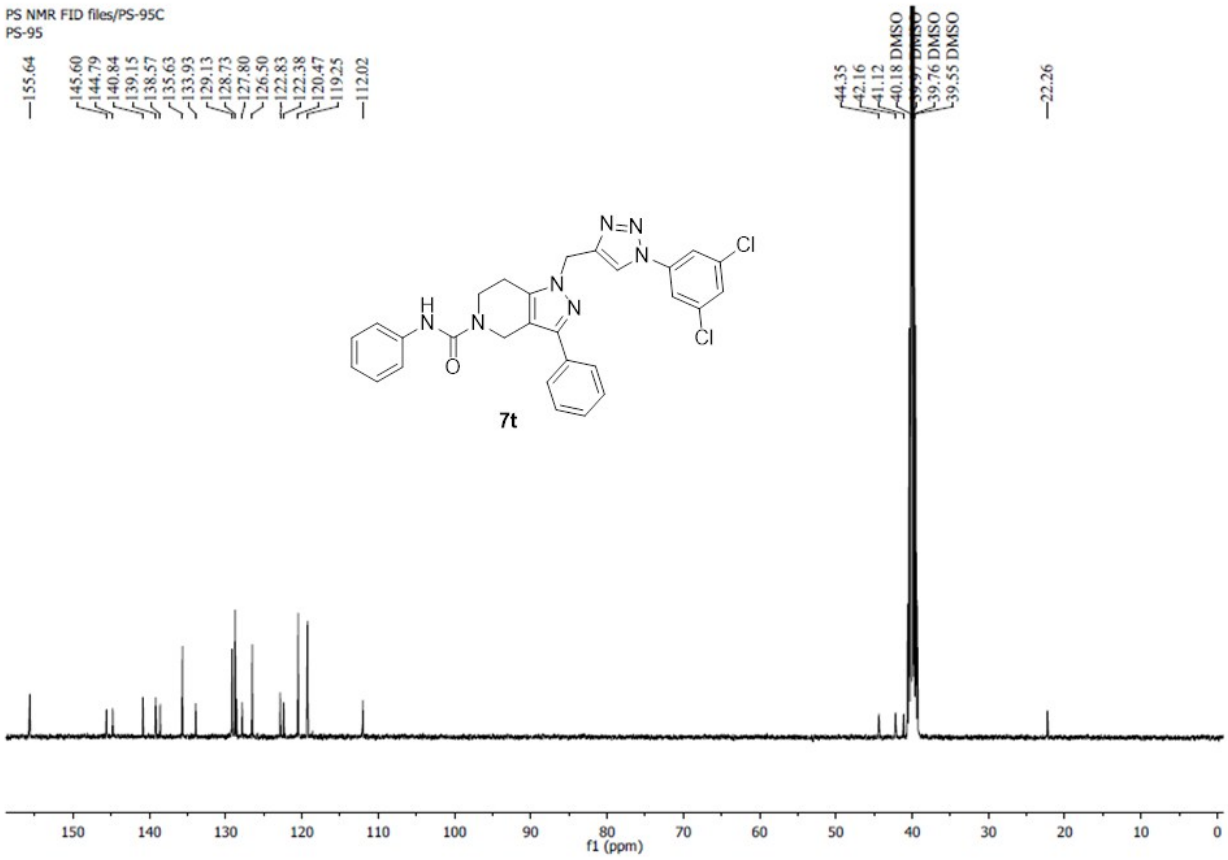

Figure S22. ^{13}C NMR spectrum (101 MHz, DMSO-d_6) of compound **7t.**

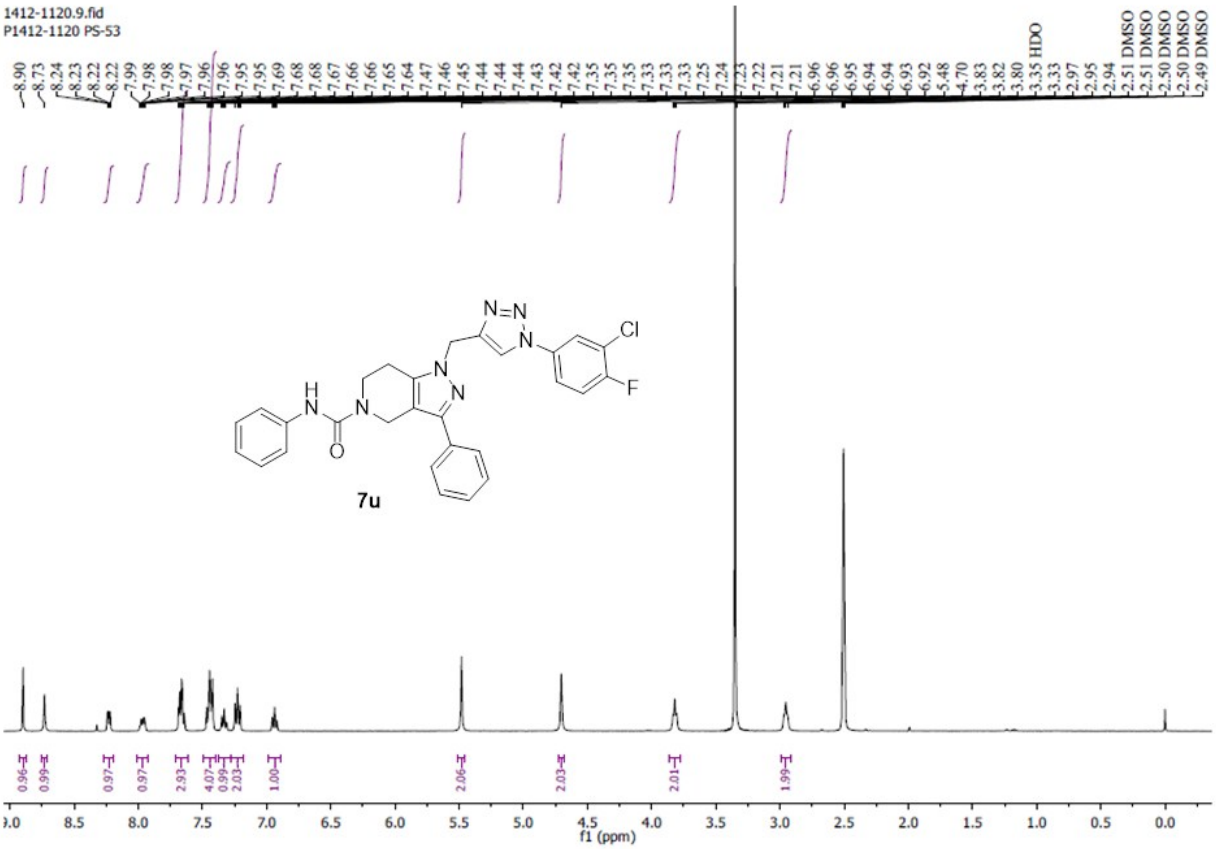

Figure S23. ^{1}H NMR spectrum (400 MHz, DMSO-d_6) of compound **7u.**

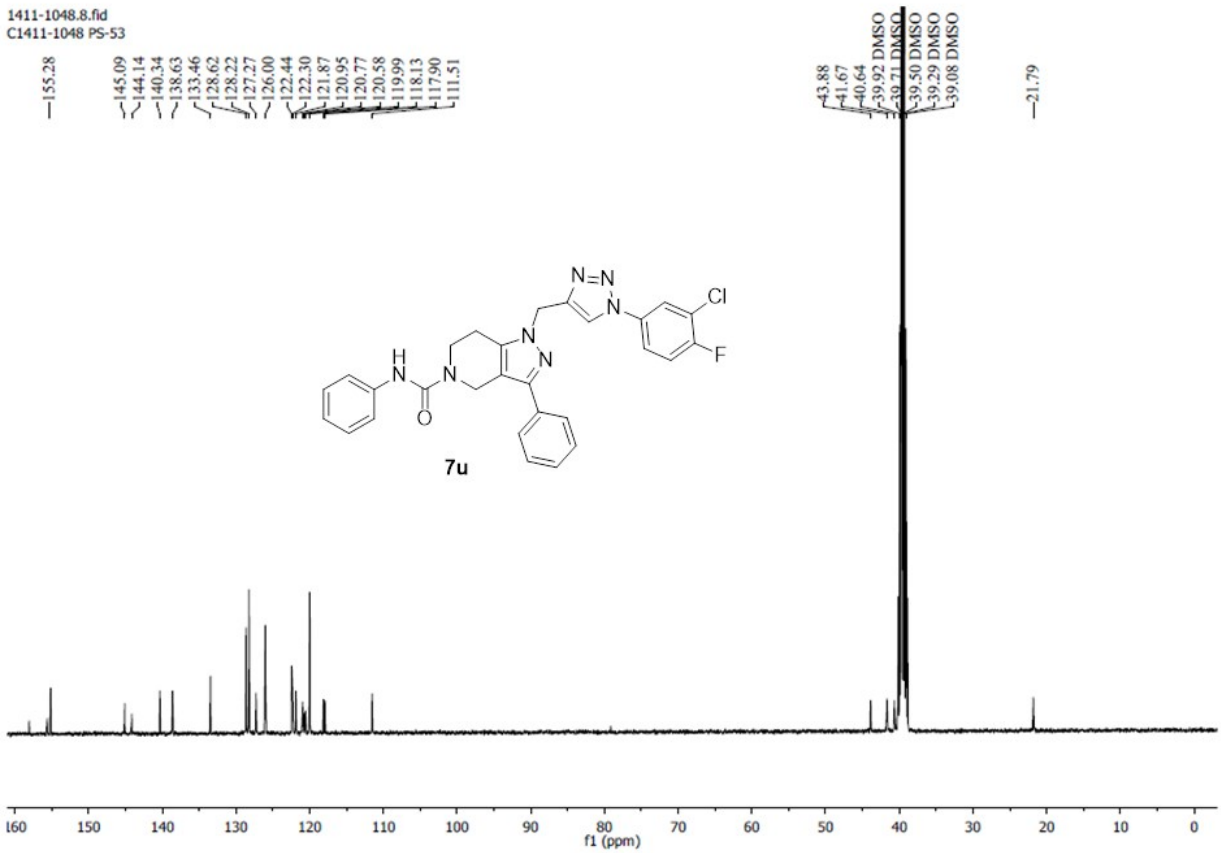

Figure S24. ^{13}C NMR spectrum (101 MHz, DMSO-d_6) of compound **7u.**

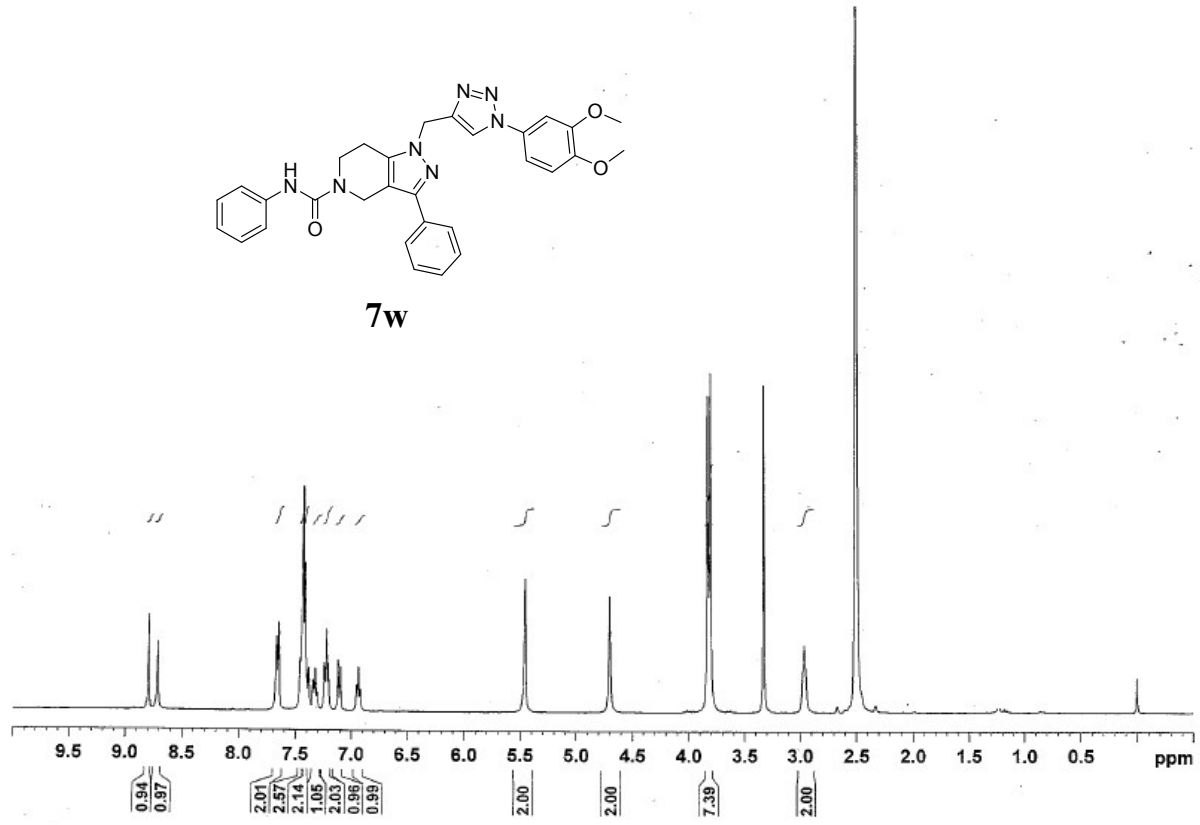

Figure S25. ^{1}H NMR spectrum (400 MHz, DMSO-d_6) of compound **7w.**

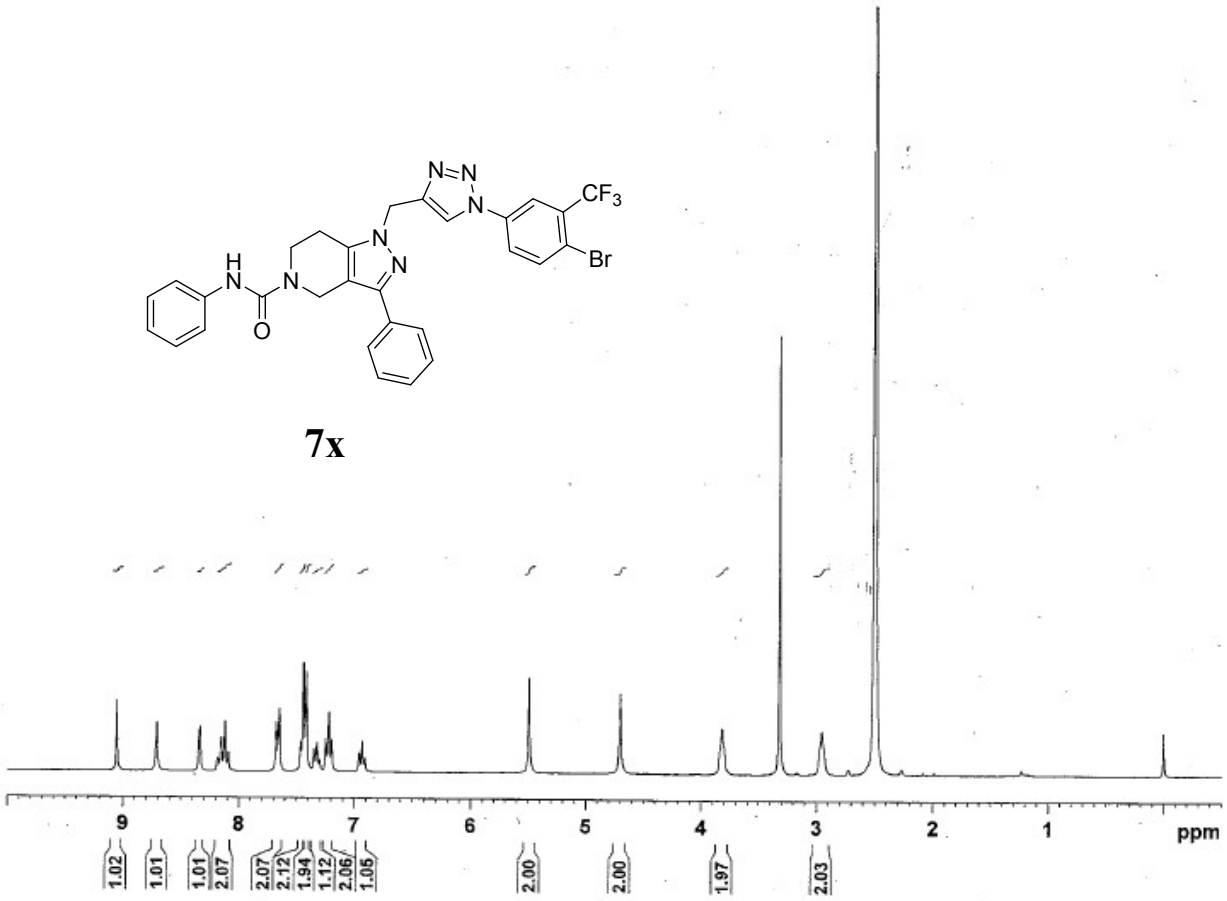

Figure S26. ^{1}H NMR spectrum (400 MHz, DMSO-d_6) of compound **7x.**

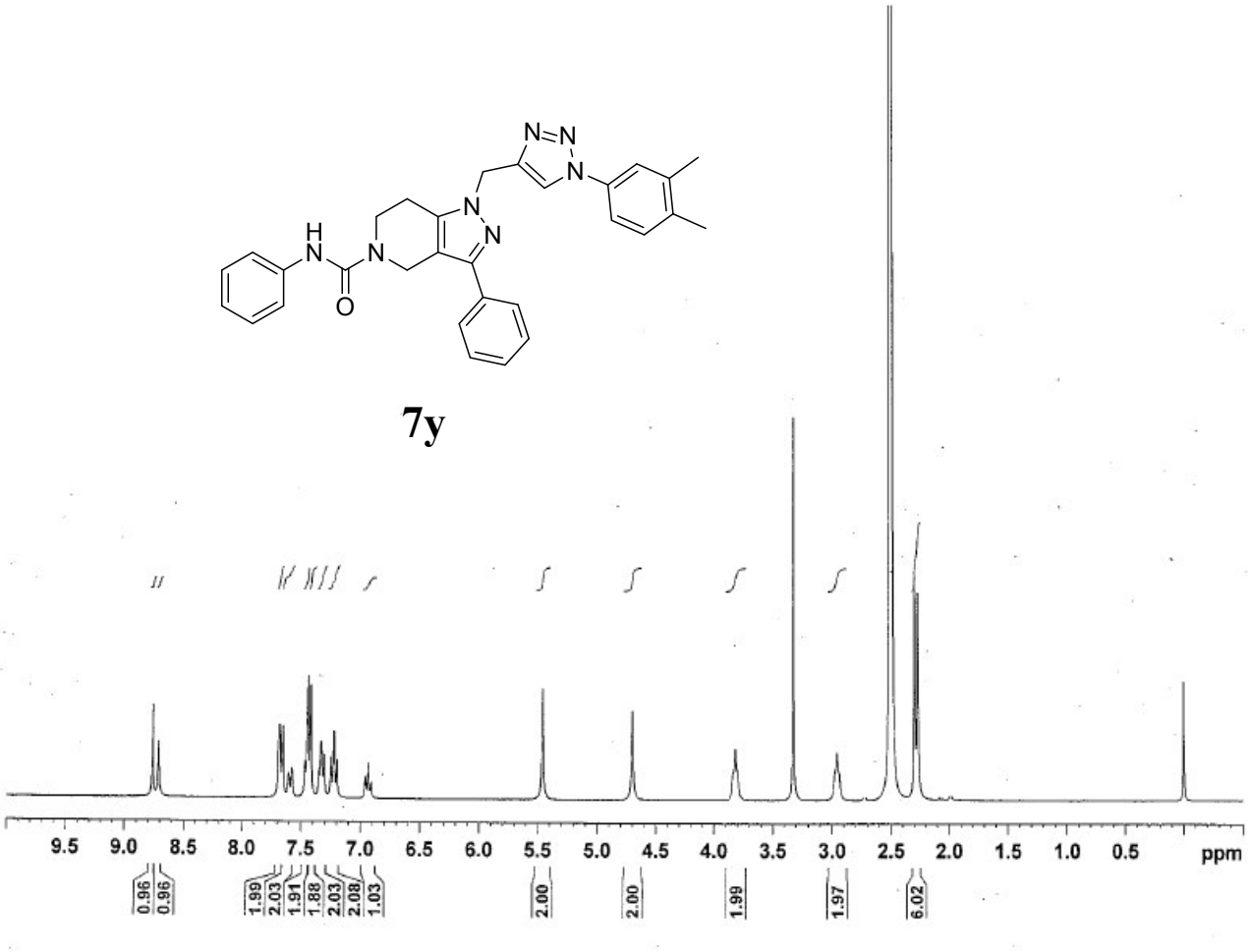

Figure S27. ^{1}H NMR spectrum (400 MHz, DMSO-d_6) of compound **7y.**

Single Crystal X-ray Crystallographic Structure of Compound 7g

Experimental

Data Collection

A nONE nONE crystal of $C_{28}H_{24}BrN_7O$was mounted on a glass fiber. All measurements were made on a Rigaku XtaLAB P200 diffractometer using graphite monochromated Mo-Kα radiation.

The crystal-to-detector distance was 40.00 mm.

Cell constants and an orientation matrix for data collection corresponded to a primitive triclinic cell with dimensions:

a = 7.8845(3) Å α = 102.268(2)^o
b = 11.9643(4) Å β = 101.916(2)^o
c = 14.9423(4) Å γ = 95.003(3)^o
V = 1334.95(8) Å^3

For Z = 2 and F.W. = 554.45, the calculated density is 1.379 g/cm^3. Based on a statistical analysis of intensity distribution, and the successful solution and refinement of the structure, the space group was determined to be:

P-1 (#2)

The data were collected at a temperature of -180 $\pm$ 1^{o}C to a maximum 2θ value of 58.2^o. A total of 1158 oscillation images were collected. A sweep of data was done using ω scans from -49.0 to 37.0^o in 0.50^o step, at χ=-77.0^o and ϕ = -90.0^o. The exposure rate was 30.0 [sec./^{o}]. The detector swing angle was -7.30^o. A second sweep was performed using ω scans from -42.0 to 3.0^o in 0.50^o step, at χ=-77.0^o and ϕ = -60.0^o. The exposure rate was 30.0 [sec./^{o}]. The detector swing angle was -7.30^o. Another sweep was performed using ω scans from -95.0 to 45.0^o in 0.50^o step, at χ=-37.0^o and ϕ = 90.0^o. The exposure rate was 30.0 [sec./^{o}]. The detector swing angle was -7.30^o. Another sweep was performed using ω scans from -26.0 to 30.0^o in 0.50^o step, at χ=-57.0^o and ϕ = 60.0^o. The exposure rate was 30.0 [sec./^{o}]. The detector swing angle was 7.30^o. Another sweep was performed using ω scans from -33.0 to 33.0^o in 0.50^o step, at χ=57.0^o and ϕ = 120.0^o. The exposure rate was 30.0 [sec./^{o}].

The detector swing angle was 7.30°. Another sweep was performed using ω scans from 35.0 to 97.0° in 0.50° step, at χ=37.0° and φ = -90.0°. The exposure rate was 30.0 [sec./°]. The detector swing angle was 7.30°. Another sweep was performed using ω scans from -36.0 to 88.0° in 0.50° step, at χ=77.0° and φ = -150.0°. The exposure rate was 30.0 [sec./°]. The detector swing angle was 7.30°. The crystal-to-detector distance was 40.00 mm. Readout was performed in the 0.172 mm pixel mode.

Data Reduction

Of the 19673 reflections were collected, where 6164 were unique (R_{int} = 0.0791); equivalent reflections were merged. Data were collected and processed using CrysAlisPro (Rigaku Oxford Diffraction). [1]

The linear absorption coefficient, μ, for Mo-Kα radiation is 15.786 cm^{-1}. An empirical absorption correction was applied which resulted in transmission factors ranging from 0.494 to 1.000. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by direct methods[2] and expanded using Fourier techniques. Some non-hydrogen atoms were refined anisotropically, while the rest were refined isotropically. Hydrogen atoms were refined using the riding model. The final cycle of full-matrix least-squares refinement[3] on F^2 was based on 6164 observed reflections and 370 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R1 = \Sigma \, ||Fo| - |Fc|| \, / \, \Sigma \, |Fo| = 0.0582$$

$$wR2 = [\Sigma \, (w \, (Fo^2 - Fc^2)^2) / \Sigma \, w(Fo^2)^2]^{1/2} = 0.2317$$

The goodness of fit[4] was 1.00. A Sheldrick weighting scheme was used. Plots of Σ w $(|Fo| - |Fc|)^2$ versus |Fo|, reflection order in data collection, sin θ/λ and various classes of indices showed no unusual trends. The maximum and minimum peaks on the final difference Fourier map corresponded to 2.87 and -1.01 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from International Tables for X-ray Crystallography (IT), Vol. IV, Table 2.2B [5]. Anomalous dispersion effects were included in Fcalc[6]; the values for Δf' and Δf'' were those of Creagh and McAuley[7]. The values for

the mass attenuation coefficients are those of Creagh and Hubbell[8]. All calculations were performed using the CrystalStructure[9,10] crystallographic software package.

References

(1) CrysAlisPro: Data Collection and Processing Software, Rigaku Corporation (2015). Tokyo 196-8666, Japan.

(2) SIR92: Altomare, A., Cascarano, G., Giacovazzo, C. and Guagliardi, A. (1993). J. Appl. Cryst. 26, 343-350.

(3) Least Squares function minimized:

$\Sigma w(F_o^2-F_c^2)^2$ where w = Least Squares weights.

(4) Goodness of fit is defined as:

$[\Sigma w(F_o^2-F_c^2)^2/(N_o-N_v)]^{1/2}$

where: N_o = number of observations
N_v = number of variables

(5) International Tables for X-ray Crystallography, Vol. IV (1974). Ed. J.A. Ibers and W.C. Hamilton, The Kynoch Press, Birmingham, England, Table 2.2B, pp. 99.

(6) Ibers, J. A. & Hamilton, W. C.; Acta Crystallogr., 17, 781 (1964).

(7) Creagh, D. C. & McAuley, W.J .; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.6.8, pages 219-222 (1992).

(8) Creagh, D. C. & Hubbell, J.H..; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.4.3, pages 200-206 (1992).

(9) CrystalStructure 4.2.2: Crystal Structure Analysis Package, Rigaku Corporation (2000-2016). Tokyo 196-8666, Japan.

(10) CRYSTALS Issue 11: Carruthers, J.R., Rollett,J.S., Betteridge, P.W., Kinna, D., Pearce, L., Larsen, A., and Gabe, E. Chemical Crystallography Laboratory, Oxford, UK. (1999)

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{28}H_{24}BrN_7O.\ CH_3OH$
Formula Weight	586.49
Crystal Color, Habit	Light yellow
Crystal Dimensions	0.1 mm x 0.1 mm x 0.1 mm
Crystal System	triclinic
Lattice Type	Primitive
Lattice Parameters	a = 7.8845(3) Å b = 11.9643(4) Å c = 14.9423(4) Å α = 102.268(2) ^{o} β = 101.916(2) ^{o} γ = 95.003(3) ^{o} V = 1334.95(8) Å^3
Space Group	P-1 (#2)
Z value	2
D_{calc}	1.379 g/cm^3
F_{000}	604.00
μ(MoKα)	15.855cm^{-1}

B. Intensity Measurements

Diffractometer	XtaLAB P200
Radiation	MoKα (λ = 0.71073 Å) graphite monochromated
Voltage, Current	50kV, 40mA
Temperature	-180.0^{o}C
Detector Aperture	83.8 x 70.0 mm
Data Images	1158 exposures
ω oscillation Range (χ=-77.0, ϕ=-90.0)	-49.0 - 37.0^{o}
Exposure Rate	30.0 sec./^{o}
Detector Swing Angle	-7.30^{o}
ω oscillation Range (χ=-77.0, ϕ=-60.0)	-42.0 - 3.0^{o}
Exposure Rate	30.0 sec./^{o}
Detector Swing Angle	-7.30^{o}
ω oscillation Range (χ=-37.0, ϕ=90.0)	-95.0 - 45.0^{o}
Exposure Rate	30.0 sec./^{o}
Detector Swing Angle	-7.30^{o}
ω oscillation Range (χ=-57.0, ϕ=60.0)	-26.0 - 30.0^{o}
Exposure Rate	30.0 sec./^{o}
Detector Swing Angle	7.30^{o}
ω oscillation Range (χ=57.0, ϕ=120.0)	-33.0 - 33.0^{o}

Exposure Rate	30.0 sec./^{o}
Detector Swing Angle	7.30^{o}
ω oscillation Range (χ=37.0, ϕ=-90.0)	35.0 - 97.0^{o}
Exposure Rate	30.0 sec./^{o}
Detector Swing Angle	7.30^{o}
ω oscillation Range (χ=77.0, ϕ=-150.0)	-36.0 - 88.0^{o}
Exposure Rate	30.0 sec./^{o}
Detector Swing Angle	7.30^{o}
Detector Position	40.00 mm
Pixel Size	0.172 mm
$2\theta_{max}$	58.2^{o}
No. of Reflections Measured	Total: 19673 Unique: 6164 (R_{int} = 0.0791)
Corrections	Lorentz-polarization Absorption (trans. factors: 0.494 - 1.000)

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SIR92)
Refinement	Full-matrix least-squares on F^2
Function Minimized	Σ w $(Fo^2 - Fc^2)^2$
Least Squares Weights	$1/[0.0111Fo^2+1.0000\sigma(Fo^2)]/(4Fo^2)$
$2\theta_{max}$ cutoff	58.2^o
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	6164
No. Variables	370
Reflection/Parameter Ratio	16.22
Residuals: R1 ($I>2.00\sigma(I)$)	0.0479
Residuals: R (All reflections)	0.0538
Residuals: wR2 (All reflections)	0.1931
Goodness of Fit Indicator	1.004
Max Shift/Error in Final Cycle	0.000
Maximum peak in Final Diff. Map	2.87 $e^-/Å^3$
Minimum peak in Final Diff. Map	-1.01 $e^-/Å^3$

Table 1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
Br1	-0.49284(4)	0.25297(2)	-0.12832(2)	1.680(10)
O1	0.0504(3)	0.75463(19)	0.76260(16)	1.51(4)
O2	0.7672(3)	0.5984(2)	0.75672(18)	2.11(4)
N1	-0.0194(3)	0.6463(2)	0.16695(18)	1.11(4)
N2	-0.0502(3)	0.7560(2)	0.16786(18)	1.24(5)
N3	0.0712(3)	0.8239(2)	0.23617(18)	1.17(5)
N4	0.2950(3)	0.8937(2)	0.43404(17)	1.14(5)
N5	0.2946(3)	1.0052(2)	0.43024(17)	1.07(4)
N6	0.1514(3)	0.8720(2)	0.67764(18)	1.16(5)
N7	-0.0283(4)	0.9353(2)	0.77787(18)	1.27(5)
C1	-0.3405(4)	0.3738(3)	-0.0360(2)	1.32(5)
C2	-0.2645(4)	0.3552(3)	0.0513(2)	1.47(6)
C3	-0.1577(4)	0.4460(3)	0.1188(2)	1.36(5)
C4	-0.1287(4)	0.5526(3)	0.0983(2)	1.17(5)
C5	-0.2043(4)	0.5698(3)	0.0103(2)	1.49(6)
C6	-0.3122(4)	0.4806(3)	-0.0566(2)	1.53(6)
C7	0.1230(4)	0.6445(2)	0.2358(2)	1.05(5)
C8	0.1791(4)	0.7584(3)	0.2790(2)	1.06(5)
C9	0.3365(4)	0.8115(3)	0.3563(2)	1.23(5)
C10	0.2517(4)	1.0569(3)	0.5100(2)	1.02(5)
C11	0.2409(3)	1.1827(3)	0.5286(2)	1.15(5)
C12	0.2190(4)	1.2443(3)	0.6151(2)	1.38(5)
C13	0.2129(4)	1.3628(3)	0.6309(2)	1.61(6)
C14	0.2265(5)	1.4215(3)	0.5609(3)	1.87(6)
C15	0.2461(5)	1.3601(3)	0.4757(3)	1.92(6)
C16	0.2552(4)	1.2424(3)	0.4584(2)	1.61(6)
C17	0.2262(3)	0.9759(2)	0.5641(2)	1.01(5)
C18	0.2527(4)	0.8722(3)	0.5129(2)	1.00(5)
C19	0.2427(4)	0.7599(3)	0.5412(2)	1.33(5)
C20	0.2677(4)	0.7896(3)	0.6482(2)	1.40(5)
C21	0.1734(4)	0.9865(3)	0.6563(2)	1.08(5)
C22	0.0572(4)	0.8494(3)	0.7413(2)	1.12(5)
C23	-0.1463(4)	0.9198(3)	0.8357(2)	1.37(5)
C24	-0.3122(4)	0.9523(3)	0.8113(2)	1.43(5)
C25	-0.4313(4)	0.9439(3)	0.8677(2)	1.70(6)
C26	-0.3831(5)	0.9009(3)	0.9485(2)	1.66(6)
C27	-0.2172(5)	0.8709(3)	0.9724(2)	1.65(6)

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
C28	-0.0980(4)	0.8798(3)	0.9168(2)	1.55(6)
C29	0.6004(5)	0.6334(3)	0.7458(3)	2.06(5)

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Table 2. Atomic coordinates and B_{iso} involving hydrogen atoms

atom	x	y	z	B_{iso}
H1	-0.28453	0.28289	0.06382	1.702
H2	-0.10756	0.43565	0.17801	1.548
H3	-0.18262	0.64142	-0.00315	1.774
H4	-0.36643	0.49139	-0.11504	1.756
H5	0.17045	0.58021	0.25025	1.272
H6	0.39006	0.75148	0.38159	1.442
H7	0.41975	0.85304	0.33124	1.445
H8	0.20741	1.20594	0.66197	1.716
H9	0.20046	1.40337	0.68911	1.891
H10	0.22149	1.50049	0.57176	2.217
H11	0.25447	1.39859	0.42853	2.336
H12	0.27183	1.20261	0.40088	1.822
H13	0.33504	0.71870	0.52232	1.577
H14	0.12999	0.71453	0.50976	1.576
H15	0.23926	0.72118	0.67011	1.675
H16	0.38655	0.82459	0.67983	1.682
H17	0.26440	1.03593	0.70636	1.364
H18	0.06434	1.01882	0.65391	1.356
H19	-0.34356	0.97985	0.75733	1.769
H20	-0.54153	0.96625	0.85192	2.063
H21	-0.46284	0.89314	0.98545	2.066
H22	-0.18567	0.84357	1.02643	2.026
H23	0.01360	0.85984	0.93346	1.841
H24	-0.00594	1.00781	0.76625	1.631
H25	0.75617	0.52780	0.73975	2.587
H26	0.53710	0.60915	0.68125	2.525
H27	0.61336	0.71605	0.76571	2.504
H28	0.53710	0.59993	0.78433	2.509

Table 3. Anisotropic displacement parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Br1	0.0224(3)	0.0181(3)	0.0185(2)	-0.00619(15)	0.00238(15)	-0.00034(15)
O1	0.0271(12)	0.0109(10)	0.0228(11)	0.0041(9)	0.0067(9)	0.0096(8)
N1	0.0128(11)	0.0086(11)	0.0195(12)	0.0030(9)	0.0006(9)	0.0033(9)
N2	0.0165(12)	0.0084(11)	0.0211(12)	0.0012(9)	0.0002(10)	0.0053(9)
N3	0.0144(11)	0.0118(12)	0.0180(12)	0.0025(9)	0.0004(9)	0.0056(9)
N4	0.0138(11)	0.0134(12)	0.0145(11)	0.0007(9)	0.0011(9)	0.0020(9)
N5	0.0115(11)	0.0109(11)	0.0180(12)	0.0021(9)	0.0014(9)	0.0045(9)
N6	0.0175(12)	0.0118(12)	0.0178(12)	0.0030(9)	0.0054(10)	0.0088(9)
N7	0.0220(12)	0.0102(11)	0.0188(12)	0.0016(10)	0.0065(10)	0.0076(9)
C1	0.0141(13)	0.0139(14)	0.0192(13)	-0.0003(11)	0.0041(11)	-0.0017(11)
C2	0.0185(14)	0.0103(13)	0.0246(15)	-0.0014(11)	0.0021(12)	0.0027(11)
C3	0.0169(14)	0.0145(14)	0.0173(14)	0.0002(11)	-0.0010(11)	0.0029(11)
C4	0.0103(12)	0.0119(14)	0.0200(14)	0.0021(11)	0.0016(10)	0.0003(11)
C5	0.0241(15)	0.0096(13)	0.0223(15)	0.0014(11)	0.0034(12)	0.0050(11)
C6	0.0209(14)	0.0188(15)	0.0160(13)	0.0007(12)	0.0011(11)	0.0028(11)
C7	0.0128(12)	0.0121(13)	0.0153(12)	0.0047(10)	0.0011(10)	0.0048(10)
C8	0.0122(12)	0.0123(13)	0.0168(12)	0.0022(10)	0.0022(10)	0.0064(10)
C9	0.0100(12)	0.0180(14)	0.0178(13)	0.0046(11)	0.0024(10)	0.0021(11)
C10	0.0086(12)	0.0134(13)	0.0146(13)	-0.0028(10)	-0.0011(9)	0.0043(10)
C11	0.0057(11)	0.0122(13)	0.0231(14)	-0.0005(10)	-0.0014(10)	0.0037(11)
C12	0.0182(14)	0.0167(14)	0.0191(14)	-0.0000(11)	0.0029(11)	0.0095(11)
C13	0.0219(15)	0.0142(14)	0.0238(15)	0.0023(12)	0.0070(12)	0.0003(12)
C14	0.0270(16)	0.0127(14)	0.0302(17)	0.0001(12)	0.0048(13)	0.0050(12)
C15	0.0305(17)	0.0171(15)	0.0267(16)	0.0006(13)	0.0051(13)	0.0106(13)
C16	0.0199(14)	0.0167(14)	0.0214(14)	-0.0007(12)	0.0016(12)	0.0019(12)
C17	0.0072(11)	0.0111(13)	0.0186(13)	-0.0013(10)	-0.0002(10)	0.0041(10)
C18	0.0090(12)	0.0140(13)	0.0145(12)	0.0014(10)	0.0014(10)	0.0031(10)
C19	0.0165(13)	0.0117(13)	0.0216(14)	0.0016(11)	0.0039(11)	0.0030(11)
C20	0.0178(14)	0.0147(14)	0.0209(14)	0.0049(11)	0.0017(11)	0.0066(11)
C21	0.0143(13)	0.0097(13)	0.0187(13)	0.0022(10)	0.0038(11)	0.0067(10)
C22	0.0127(12)	0.0144(13)	0.0162(13)	0.0015(10)	0.0009(10)	0.0078(10)
C23	0.0189(14)	0.0120(13)	0.0208(14)	-0.0006(11)	0.0069(12)	0.0022(11)
C24	0.0225(15)	0.0141(13)	0.0191(14)	0.0042(12)	0.0040(12)	0.0076(11)
C25	0.0230(15)	0.0191(15)	0.0231(15)	0.0043(12)	0.0065(12)	0.0044(12)
C26	0.0314(17)	0.0137(14)	0.0205(14)	0.0015(12)	0.0119(13)	0.0047(11)
C27	0.0358(18)	0.0118(14)	0.0170(14)	0.0030(13)	0.0080(13)	0.0059(11)
C28	0.0233(15)	0.0138(14)	0.0217(14)	0.0045(12)	0.0046(12)	0.0038(11)

Table 3. Anisotropic displacement parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}

The general temperature factor expression: $\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Table 4. Fragment Analysis

fragment: 1

Br(1)	O(1)	N(1)	N(2)	N(3)
N(4)	N(5)	N(6)	N(7)	C(1)
C(2)	C(3)	C(4)	C(5)	C(6)
C(7)	C(8)	C(9)	C(10)	C(11)
C(12)	C(13)	C(14)	C(15)	C(16)
C(17)	C(18)	C(19)	C(20)	C(21)
C(22)	C(23)	C(24)	C(25)	C(26)
C(27)	C(28)			

fragment: 2

O(2)	C(29)

Table 5. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
Br1	C1	1.897(3)	O1	C22	1.241(4)
O2	C29	1.403(5)	N1	N2	1.352(4)
N1	C4	1.424(3)	N1	C7	1.362(4)
N2	N3	1.314(3)	N3	C8	1.361(4)
N4	N5	1.347(4)	N4	C9	1.467(4)
N4	C18	1.356(4)	N5	C10	1.344(4)
N6	C20	1.465(4)	N6	C21	1.475(4)
N6	C22	1.376(4)	N7	C22	1.358(4)
N7	C23	1.420(5)	C1	C2	1.391(5)
C1	C6	1.387(5)	C2	C3	1.390(4)
C3	C4	1.384(5)	C4	C5	1.393(5)
C5	C6	1.379(4)	C7	C8	1.369(4)
C8	C9	1.495(3)	C10	C11	1.484(4)
C10	C17	1.415(5)	C11	C12	1.397(4)
C11	C16	1.406(5)	C12	C13	1.394(5)
C13	C14	1.394(5)	C14	C15	1.375(5)
C15	C16	1.388(5)	C17	C18	1.370(4)
C17	C21	1.502(5)	C18	C19	1.493(5)
C19	C20	1.528(5)	C23	C24	1.395(5)
C23	C28	1.389(5)	C24	C25	1.396(5)
C25	C26	1.406(5)	C26	C27	1.382(5)
C27	C28	1.388(5)			

Table 6. Bond lengths involving hydrogens (Å)

atom	atom	distance	atom	atom	distance
O2	H25	0.820	N7	H24	0.930
C2	H1	0.930	C3	H2	0.930
C5	H3	0.930	C6	H4	0.930
C7	H5	0.930	C9	H6	0.970
C9	H7	0.970	C12	H8	0.930
C13	H9	0.930	C14	H10	0.930
C15	H11	0.930	C16	H12	0.930
C19	H13	0.970	C19	H14	0.970
C20	H15	0.970	C20	H16	0.970
C21	H17	0.970	C21	H18	0.970
C24	H19	0.930	C25	H20	0.930
C26	H21	0.930	C27	H22	0.930
C28	H23	0.930	C29	H26	0.960
C29	H27	0.960	C29	H28	0.960

Table 7. Bond angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
N2	N1	C4	119.9(2)	N2	N1	C7	110.8(2)
C4	N1	C7	129.3(3)	N1	N2	N3	106.9(2)
N2	N3	C8	109.2(2)	N5	N4	C9	119.2(3)
N5	N4	C18	112.8(2)	C9	N4	C18	128.0(3)
N4	N5	C10	104.9(3)	C20	N6	C21	117.8(3)
C20	N6	C22	118.1(3)	C21	N6	C22	122.4(3)
C22	N7	C23	122.7(3)	Br1	C1	C2	119.9(2)
Br1	C1	C6	118.6(2)	C2	C1	C6	121.4(2)
C1	C2	C3	118.9(3)	C2	C3	C4	119.8(3)
N1	C4	C3	120.3(3)	N1	C4	C5	118.9(3)
C3	C4	C5	120.7(2)	C4	C5	C6	119.8(3)
C1	C6	C5	119.4(3)	N1	C7	C8	104.2(3)
N3	C8	C7	108.8(2)	N3	C8	C9	121.8(2)
C7	C8	C9	129.3(3)	N4	C9	C8	112.9(2)
N5	C10	C11	118.9(3)	N5	C10	C17	110.3(3)
C11	C10	C17	130.8(3)	C10	C11	C12	121.7(3)
C10	C11	C16	119.6(3)	C12	C11	C16	118.8(3)
C11	C12	C13	120.2(3)	C12	C13	C14	120.9(3)
C13	C14	C15	118.6(3)	C14	C15	C16	121.8(4)
C11	C16	C15	119.8(3)	C10	C17	C18	105.7(3)
C10	C17	C21	132.3(3)	C18	C17	C21	121.9(3)
N4	C18	C17	106.3(3)	N4	C18	C19	127.7(3)
C17	C18	C19	126.1(3)	C18	C19	C20	106.4(2)
N6	C20	C19	111.0(3)	N6	C21	C17	110.0(2)
O1	C22	N6	121.1(3)	O1	C22	N7	122.4(3)
N6	C22	N7	116.5(3)	N7	C23	C24	117.6(3)
N7	C23	C28	122.1(3)	C24	C23	C28	120.2(3)
C23	C24	C25	120.3(3)	C24	C25	C26	119.2(3)
C25	C26	C27	119.6(3)	C26	C27	C28	121.2(3)
C23	C28	C27	119.4(3)				

Table 8. Bond angles involving hydrogens (°)

atom	atom	atom	angle	atom	atom	atom	angle
C29	O2	H25	108.7	C22	N7	H24	118.7
C23	N7	H24	118.6	C1	C2	H1	120.3
C3	C2	H1	120.9	C2	C3	H2	120.1
C4	C3	H2	120.1	C4	C5	H3	120.1
C6	C5	H3	120.1	C1	C6	H4	119.9
C5	C6	H4	120.8	N1	C7	H5	127.7
C8	C7	H5	128.0	N4	C9	H6	107.9
N4	C9	H7	107.6	C8	C9	H6	109.6
C8	C9	H7	109.2	H6	C9	H7	109.5
C11	C12	H8	119.9	C13	C12	H8	120.0
C12	C13	H9	119.6	C14	C13	H9	119.6
C13	C14	H10	120.5	C15	C14	H10	120.9
C14	C15	H11	119.1	C16	C15	H11	119.1
C11	C16	H12	119.6	C15	C16	H12	120.6
C18	C19	H13	108.6	C18	C19	H14	109.2
C20	C19	H13	111.3	C20	C19	H14	111.8
H13	C19	H14	109.4	N6	C20	H15	106.9
N6	C20	H16	107.2	C19	C20	H15	110.7
C19	C20	H16	111.6	H15	C20	H16	109.3
N6	C21	H17	108.1	N6	C21	H18	109.2
C17	C21	H17	109.5	C17	C21	H18	110.5
H17	C21	H18	109.5	C23	C24	H19	120.0
C25	C24	H19	119.7	C24	C25	H20	120.5
C26	C25	H20	120.3	C25	C26	H21	119.7
C27	C26	H21	120.6	C26	C27	H22	119.1
C28	C27	H22	119.6	C23	C28	H23	119.9
C27	C28	H23	120.7	O2	C29	H26	110.6
O2	C29	H27	108.7	O2	C29	H28	109.2
H26	C29	H27	109.4	H26	C29	H28	109.4
H27	C29	H28	109.4				

Table 9. Torsion Angles(O)

(Those having bond angles > 160 or < 20 degrees are excluded.)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
N2	N1	C4	C3	-149.6(3)	N2	N1	C4	C5	30.9(4)
C4	N1	N2	N3	-178.6(3)	N2	N1	C7	C8	-0.3(3)
C7	N1	N2	N3	0.3(3)	C4	N1	C7	C8	178.5(3)
C7	N1	C4	C3	31.7(5)	C7	N1	C4	C5	-147.7(3)
N1	N2	N3	C8	-0.1(3)	N2	N3	C8	C7	-0.0(4)
N2	N3	C8	C9	176.5(2)	N5	N4	C9	C8	-88.1(3)
C9	N4	N5	C10	179.65(19)	N5	N4	C18	C17	-1.1(3)
N5	N4	C18	C19	-179.0(2)	C18	N4	N5	C10	0.4(3)
C9	N4	C18	C17	179.8(2)	C9	N4	C18	C19	1.8(4)
C18	N4	C9	C8	90.9(3)	N4	N5	C10	C11	179.48(19)
N4	N5	C10	C17	0.4(3)	C20	N6	C21	C17	34.4(3)
C21	N6	C20	C19	-61.8(3)	C20	N6	C22	O1	-10.5(3)
C20	N6	C22	N7	170.31(19)	C22	N6	C20	C19	132.8(2)
C21	N6	C22	O1	-175.2(2)	C21	N6	C22	N7	5.6(3)
C22	N6	C21	C17	-160.8(2)	C22	N7	C23	C24	-128.5(3)
C22	N7	C23	C28	54.9(3)	C23	N7	C22	O1	-6.6(4)
C23	N7	C22	N6	172.6(2)	Br1	C1	C2	C3	-178.0(2)
Br1	C1	C6	C5	178.9(2)	C2	C1	C6	C5	1.0(5)
C6	C1	C2	C3	-0.1(5)	C1	C2	C3	C4	-0.1(5)
C2	C3	C4	N1	-179.9(3)	C2	C3	C4	C5	-0.5(5)
N1	C4	C5	C6	-179.2(3)	C3	C4	C5	C6	1.3(5)
C4	C5	C6	C1	-1.6(5)	N1	C7	C8	N3	0.2(3)
N1	C7	C8	C9	-176.0(3)	N3	C8	C9	N4	54.4(4)
C7	C8	C9	N4	-129.9(3)	N5	C10	C11	C12	-171.7(2)
N5	C10	C11	C16	7.4(3)	N5	C10	C17	C18	-1.0(3)
N5	C10	C17	C21	-178.3(2)	C11	C10	C17	C18	-180.0(2)
C11	C10	C17	C21	2.7(5)	C17	C10	C11	C12	7.2(4)
C17	C10	C11	C16	-173.7(2)	C10	C11	C12	C13	178.7(2)
C10	C11	C16	C15	-179.7(2)	C12	C11	C16	C15	-0.5(4)
C16	C11	C12	C13	-0.5(4)	C11	C12	C13	C14	0.7(4)
C12	C13	C14	C15	-0.0(5)	C13	C14	C15	C16	-1.0(5)
C14	C15	C16	C11	1.2(5)	C10	C17	C18	N4	1.2(3)
C10	C17	C18	C19	179.2(2)	C10	C17	C21	N6	175.1(2)
C18	C17	C21	N6	-1.8(3)	C21	C17	C18	N4	178.9(2)
C21	C17	C18	C19	-3.1(4)	N4	C18	C19	C20	156.5(2)
C17	C18	C19	C20	-21.1(4)	C18	C19	C20	N6	49.9(3)
N7	C23	C24	C25	-177.2(2)	N7	C23	C28	C27	177.5(2)

Table 9. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C24	C23	C28	C27	1.0(4)	C28	C23	C24	C25	-0.5(4)
C23	C24	C25	C26	-0.9(4)	C24	C25	C26	C27	1.9(4)
C25	C26	C27	C28	-1.5(4)	C26	C27	C28	C23	0.1(4)

Table 10. Possible hydrogen bonds

Donor	H	Acceptor	D...A	D-H	H...A	D-H...A
N7	H24	N3[1]	2.976(4)	0.93	2.13	151.33

Symmetry Operators:

(1) -X,-Y+2,-Z+1

Table 11. Intramolecular contacts less than 3.60 Å

atom	atom	distance	atom	atom	distance
O1	C20	2.725(4)	O1	C23	2.796(4)
O1	C28	2.978(4)	N2	C5	2.845(3)
N3	N4	3.015(3)	N3	N5	3.281(3)
N3	C4	3.491(3)	N4	C11	3.545(4)
N5	C8	3.240(3)	N5	C16	2.833(4)
N6	C18	2.741(4)	N7	C21	2.775(5)
C1	C4	2.751(4)	C2	C5	2.788(5)
C3	C6	2.785(5)	C3	C7	3.051(4)
C4	C8	3.559(3)	C8	C18	3.377(4)
C9	C10	3.529(4)	C9	C19	3.171(5)
C11	C14	2.811(4)	C11	C21	3.396(5)
C12	C15	2.768(5)	C12	C17	3.147(4)
C12	C21	3.275(5)	C13	C16	2.774(5)
C17	C20	2.793(5)	C19	C21	3.045(4)
C19	C22	3.597(5)	C22	C24	3.525(5)
C22	C28	3.083(5)	C23	C26	2.786(5)
C24	C27	2.771(5)	C25	C28	2.798(5)

Table 12. Intramolecular contacts less than 3.60 Å involving hydrogens

atom	atom	distance	atom	atom	distance
Br1	H1	2.929	Br1	H4	2.890
O1	H15	2.237	O1	H16	3.265
O1	H23	2.682	O1	H24	3.090
N1	H2	2.604	N1	H3	2.587
N2	H3	2.580	N2	H5	3.133
N3	H5	3.123	N3	H6	3.274
N3	H7	2.775	N4	H13	2.709
N4	H14	2.953	N5	H6	3.161
N5	H7	2.499	N5	H12	2.507
N6	H13	3.300	N6	H14	2.763
N6	H24	2.459	N7	H17	3.000
N7	H18	2.486	N7	H19	2.558
N7	H23	2.637	C1	H2	3.237
C1	H3	3.230	C2	H4	3.256
C3	H3	3.251	C3	H5	2.994
C4	H1	3.245	C4	H4	3.243
C4	H5	2.856	C5	H2	3.252
C6	H1	3.259	C7	H2	2.817
C7	H6	2.696	C7	H7	3.135
C9	H5	2.921	C9	H13	2.928
C9	H14	3.406	C10	H8	2.679
C10	H12	2.643	C10	H17	2.980
C10	H18	2.937	C11	H9	3.255
C11	H11	3.253	C11	H17	3.465
C11	H18	3.383	C12	H10	3.264
C12	H12	3.252	C12	H17	3.098
C12	H18	3.079	C13	H11	3.221
C14	H8	3.261	C14	H12	3.250
C15	H9	3.221	C16	H8	3.255
C16	H10	3.254	C17	H8	2.861
C17	H13	3.235	C17	H14	3.044
C17	H16	2.948	C18	H6	2.656
C18	H7	3.227	C18	H15	3.267
C18	H16	2.699	C18	H17	3.107
C18	H18	3.147	C19	H6	2.848
C20	H17	2.894	C20	H18	3.290
C21	H8	2.597	C21	H14	3.459

Table 12. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C21	H15	3.303	C21	H16	2.705
C21	H24	2.368	C22	H15	2.422
C22	H16	2.945	C22	H17	2.852
C22	H18	2.637	C22	H23	2.940
C23	H20	3.261	C23	H22	3.236
C24	H21	3.255	C24	H23	3.251
C24	H24	2.703	C25	H22	3.246
C26	H19	3.257	C26	H23	3.253
C27	H20	3.250	C28	H19	3.251
C28	H21	3.253	C28	H24	3.142
H1	H2	2.334	H2	H5	2.555
H3	H4	2.321	H5	H6	2.705
H5	H7	3.493	H6	H13	2.337
H6	H14	3.145	H8	H9	2.318
H8	H17	2.321	H8	H18	2.385
H8	H24	3.582	H9	H10	2.325
H10	H11	2.304	H11	H12	2.314
H13	H15	2.472	H13	H16	2.357
H14	H15	2.355	H14	H16	2.877
H16	H17	2.763	H17	H24	2.500
H18	H24	1.899	H19	H20	2.329
H19	H24	2.626	H20	H21	2.336
H21	H22	2.309	H22	H23	2.324
H23	H24	3.342	H25	H26	2.174
H25	H27	2.597	H25	H28	2.159

Table 13. Intermolecular contacts less than 3.60 Å

atom	atom	distance	atom	atom	distance
Br1	N2[1]	3.517(3)	O1	O2[2]	2.758(4)
O1	C2[3]	3.508(4)	O1	C3[3]	3.341(4)
O2	O1[4]	2.758(4)	O2	C3[5]	3.400(4)
O2	C6[6]	3.521(5)	O2	C7[5]	3.121(4)
O2	C15[7]	3.593(5)	N2	Br1[1]	3.517(3)
N2	N7[8]	3.579(3)	N2	C27[9]	3.549(4)
N3	N7[8]	2.976(4)	N3	C21[8]	3.455(4)
N3	C23[8]	3.500(4)	N3	C24[8]	3.429(4)
N4	N5[7]	3.408(3)	N4	C10[7]	3.466(4)
N5	N4[7]	3.408(3)	N5	N5[7]	3.499(3)
N5	C18[7]	3.594(4)	N6	C16[8]	3.412(4)
N7	N2[8]	3.579(3)	N7	N3[8]	2.976(4)
C2	O1[3]	3.508(4)	C3	O1[3]	3.341(4)
C3	O2[5]	3.400(4)	C6	O2[10]	3.521(5)
C6	C7[11]	3.460(5)	C7	O2[5]	3.121(4)
C7	C6[11]	3.460(5)	C9	C10[7]	3.480(3)
C9	C11[7]	3.408(4)	C9	C12[7]	3.581(4)
C10	N4[7]	3.466(4)	C10	C9[7]	3.480(3)
C11	C9[7]	3.408(4)	C12	C9[7]	3.581(4)
C15	O2[7]	3.593(5)	C16	N6[8]	3.412(4)
C16	C22[8]	3.358(4)	C18	N5[7]	3.594(4)
C20	C29	3.597(5)	C21	N3[8]	3.455(4)
C22	C16[8]	3.358(4)	C23	N3[8]	3.500(4)
C24	N3[8]	3.429(4)	C26	C26[12]	3.432(5)
C27	N2[13]	3.549(4)	C27	C28[14]	3.567(4)
C28	C27[14]	3.567(4)	C28	C28[14]	3.383(4)
C29	C20	3.597(5)			

Symmetry Operators:

(1) -X-1,-Y+1,-Z
(2) X-1,Y,Z
(3) -X,-Y+1,-Z+1
(4) X+1,Y,Z
(5) -X+1,-Y+1,-Z+1
(6) X+1,Y,Z+1
(7) -X+1,-Y+2,-Z+1
(8) -X,-Y+2,-Z+1
(9) X,Y,Z-1
(10) X-1,Y,Z-1
(11) -X,-Y+1,-Z
(12) -X-1,-Y+2,-Z+2
(13) X,Y,Z+1
(14) -X,-Y+2,-Z+2

Table 14. Intermolecular contacts less than 3.60 Å involving hydrogens

atom	atom	distance	atom	atom	distance
Br1	H7[1]	3.217	Br1	H8[2]	3.418
Br1	H17[2]	3.311	Br1	H20[3]	3.361
Br1	H21[4]	3.086	Br1	H22[4]	3.451
O1	H1[5]	3.000	O1	H2[5]	2.654
O1	H11[6]	3.386	O1	H12[6]	3.298
O1	H25[7]	3.323	O1	H27[7]	3.448
O2	H2[8]	2.756	O2	H3[9]	3.448
O2	H4[9]	2.840	O2	H5[8]	2.220
O2	H11[10]	2.746	N1	H8[6]	3.458
N1	H9[6]	2.946	N1	H25[8]	3.374
N2	H8[6]	3.020	N2	H9[6]	3.463
N2	H17[6]	3.555	N2	H18[6]	3.390
N2	H22[11]	2.629	N2	H24[6]	2.752
N3	H8[6]	2.958	N3	H17[6]	3.413
N3	H18[6]	2.672	N3	H19[6]	3.011
N3	H22[11]	3.428	N3	H24[6]	2.127
N4	H18[6]	3.227	N4	H19[6]	3.578
N5	H18[6]	2.812	N5	H19[6]	2.947
N5	H24[6]	3.288	N6	H12[6]	3.275
N6	H20[12]	3.096	N7	H12[6]	3.000
N7	H22[13]	3.506	C2	H21[4]	3.384
C2	H23[5]	3.396	C2	H28[5]	3.573
C3	H3[1]	3.594	C3	H9[6]	3.147
C3	H25[8]	3.372	C4	H9[6]	3.282
C5	H22[11]	3.220	C6	H5[1]	3.276
C6	H25[14]	3.350	C6	H28[14]	3.110
C7	H4[1]	3.211	C7	H9[6]	3.048
C7	H25[8]	2.410	C8	H8[6]	3.379
C8	H9[6]	3.591	C8	H18[6]	3.513
C8	H19[6]	3.477	C8	H24[6]	3.351
C8	H25[8]	3.467	C9	H19[6]	3.306
C10	H6[10]	3.356	C10	H7[10]	3.064
C10	H18[6]	3.028	C11	H6[10]	2.903
C11	H7[10]	3.161	C11	H14[6]	3.260
C11	H18[6]	3.539	C12	H6[10]	3.068
C12	H7[10]	3.185	C12	H14[6]	3.131
C13	H6[10]	3.547	C13	H14[6]	2.996

Table 14. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C13	H26[15]	3.569	C14	H14[6]	2.985
C14	H15[15]	3.593	C14	H26[15]	3.127
C15	H13[10]	3.509	C15	H14[6]	3.086
C15	H26[10]	3.236	C16	H6[10]	3.267
C16	H13[10]	3.167	C16	H14[6]	3.238
C16	H26[10]	3.559	C17	H7[10]	3.204
C17	H18[6]	3.591	C19	H10[16]	3.227
C20	H10[16]	3.367	C20	H19[12]	3.518
C20	H20[12]	3.289	C20	H26	3.200
C20	H27	3.223	C21	H7[10]	3.541
C21	H20[12]	3.367	C22	H12[6]	2.917
C22	H20[12]	3.284	C23	H12[6]	3.424
C23	H27[7]	2.814	C24	H7[6]	3.520
C24	H12[6]	3.407	C24	H16[7]	2.828
C24	H27[7]	2.743	C25	H16[7]	2.873
C25	H17[7]	3.461	C25	H21[17]	2.922
C25	H27[7]	2.916	C26	H1[4]	3.219
C26	H20[17]	3.265	C26	H21[17]	2.917
C26	H27[7]	3.121	C27	H3[18]	2.874
C27	H23[13]	3.343	C27	H27[7]	3.191
C28	H3[18]	3.386	C28	H23[13]	3.349
C28	H27[7]	3.055	C29	H4[9]	2.938
C29	H5[8]	3.260	C29	H10[16]	3.525
C29	H11[10]	3.021	C29	H12[10]	3.474
C29	H15	3.192	C29	H16	3.161
H1	O1[5]	3.000	H1	C26[4]	3.219
H1	H21[4]	2.636	H1	H23[5]	2.848
H1	H28[5]	3.476	H2	O1[5]	2.654
H2	O2[8]	2.756	H2	H9[6]	2.722
H2	H15[5]	3.492	H2	H25[8]	2.744
H2	H28[5]	3.550	H3	O2[14]	3.448
H3	C3[1]	3.594	H3	C27[11]	2.874
H3	C28[11]	3.386	H3	H22[11]	2.368
H3	H23[11]	3.327	H3	H28[14]	3.384
H4	O2[14]	2.840	H4	C7[1]	3.211
H4	C29[14]	2.938	H4	H5[1]	2.826
H4	H25[14]	2.651	H4	H26[14]	3.589

Table 14. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H4	$H27^{14}$	3.524	H4	$H28^{14}$	2.248
H5	$O2^{8}$	2.220	H5	$C6^{1}$	3.276
H5	$C29^{8}$	3.260	H5	$H4^{1}$	2.826
H5	$H9^{6}$	3.245	H5	$H25^{8}$	1.485
H5	$H26^{8}$	3.524	H5	$H28^{8}$	3.334
H6	$C10^{10}$	3.356	H6	$C11^{10}$	2.903
H6	$C12^{10}$	3.068	H6	$C13^{10}$	3.547
H6	$C16^{10}$	3.267	H6	$H8^{10}$	3.386
H6	$H25^{8}$	3.416	H7	$Br1^{1}$	3.217
H7	$C10^{10}$	3.064	H7	$C11^{10}$	3.161
H7	$C12^{10}$	3.185	H7	$C17^{10}$	3.204
H7	$C21^{10}$	3.541	H7	$C24^{6}$	3.520
H7	$H8^{10}$	3.069	H7	$H17^{10}$	2.933
H7	$H19^{6}$	2.667	H8	$Br1^{19}$	3.418
H8	$N1^{6}$	3.458	H8	$N2^{6}$	3.020
H8	$N3^{6}$	2.958	H8	$C8^{6}$	3.379
H8	$H6^{10}$	3.386	H8	$H7^{10}$	3.069
H9	$N1^{6}$	2.946	H9	$N2^{6}$	3.463
H9	$C3^{6}$	3.147	H9	$C4^{6}$	3.282
H9	$C7^{6}$	3.048	H9	$C8^{6}$	3.591
H9	$H2^{6}$	2.722	H9	$H5^{6}$	3.245
H9	$H14^{6}$	3.462	H9	$H26^{15}$	3.497
H9	$H28^{15}$	3.245	H10	$C19^{15}$	3.227
H10	$C20^{15}$	3.367	H10	$C29^{15}$	3.525
H10	$H13^{15}$	2.975	H10	$H14^{15}$	2.999
H10	$H14^{6}$	3.437	H10	$H15^{15}$	2.712
H10	$H26^{15}$	2.722	H10	$H28^{15}$	3.509
H11	$O1^{6}$	3.386	H11	$O2^{10}$	2.746
H11	$C29^{10}$	3.021	H11	$H14^{6}$	3.583
H11	$H25^{10}$	2.824	H11	$H26^{10}$	2.545
H11	$H27^{10}$	3.346	H12	$O1^{6}$	3.298
H12	$N6^{6}$	3.275	H12	$N7^{6}$	3.000
H12	$C22^{6}$	2.917	H12	$C23^{6}$	3.424
H12	$C24^{6}$	3.407	H12	$C29^{10}$	3.474
H12	$H13^{10}$	3.062	H12	$H16^{10}$	3.185
H12	$H18^{6}$	3.416	H12	$H19^{6}$	3.041
H12	$H24^{6}$	3.349	H12	$H26^{10}$	3.193

Table 14. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H12	H27[10]	3.126	H13	C15[10]	3.509
H13	C16[10]	3.167	H13	H10[16]	2.975
H13	H12[10]	3.062	H13	H26	3.165
H14	C11[6]	3.260	H14	C12[6]	3.131
H14	C13[6]	2.996	H14	C14[6]	2.985
H14	C15[6]	3.086	H14	C16[6]	3.238
H14	H9[6]	3.462	H14	H10[16]	2.999
H14	H10[6]	3.437	H14	H11[6]	3.583
H15	C14[16]	3.593	H15	C29	3.192
H15	H2[5]	3.492	H15	H10[16]	2.712
H15	H20[12]	3.572	H15	H26	2.797
H15	H27	3.012	H15	H28	3.244
H16	C24[12]	2.828	H16	C25[12]	2.873
H16	C29	3.161	H16	H12[10]	3.185
H16	H19[12]	2.588	H16	H20[12]	2.680
H16	H26	2.933	H16	H27	2.588
H16	H28	3.556	H17	Br1[19]	3.311
H17	N2[6]	3.555	H17	N3[6]	3.413
H17	C25[12]	3.461	H17	H7[10]	2.933
H17	H19[12]	3.192	H17	H20[12]	2.718
H18	N2[6]	3.390	H18	N3[6]	2.672
H18	N4[6]	3.227	H18	N5[6]	2.812
H18	C8[6]	3.513	H18	C10[6]	3.028
H18	C11[6]	3.539	H18	C17[6]	3.591
H18	H12[6]	3.416	H19	N3[6]	3.011
H19	N4[6]	3.578	H19	N5[6]	2.947
H19	C8[6]	3.477	H19	C9[6]	3.306
H19	C20[7]	3.518	H19	H7[6]	2.667
H19	H12[6]	3.041	H19	H16[7]	2.588
H19	H17[7]	3.192	H19	H27[7]	3.177
H20	Br1[20]	3.361	H20	N6[7]	3.096
H20	C20[7]	3.289	H20	C21[7]	3.367
H20	C22[7]	3.284	H20	C26[17]	3.265
H20	H15[7]	3.572	H20	H16[7]	2.680
H20	H17[7]	2.718	H20	H21[17]	2.637
H20	H27[7]	3.429	H21	Br1[4]	3.086
H21	C2[4]	3.384	H21	C25[17]	2.922

Table 14. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H21	C26[17]	2.917	H21	H1[4]	2.636
H21	H20[17]	2.637	H21	H21[17]	2.639
H22	Br1[4]	3.451	H22	N2[18]	2.629
H22	N3[18]	3.428	H22	N7[13]	3.506
H22	C5[18]	3.220	H22	H3[18]	2.368
H22	H23[13]	3.565	H22	H24[13]	3.209
H23	C2[5]	3.396	H23	C27[13]	3.343
H23	C28[13]	3.349	H23	H1[5]	2.848
H23	H3[18]	3.327	H23	H22[13]	3.565
H23	H23[13]	3.566	H24	N2[6]	2.752
H24	N3[6]	2.127	H24	N5[6]	3.288
H24	C8[6]	3.351	H24	H12[6]	3.349
H24	H22[13]	3.209	H25	O1[12]	3.323
H25	N1[8]	3.374	H25	C3[8]	3.372
H25	C6[9]	3.350	H25	C7[8]	2.410
H25	C8[8]	3.467	H25	H2[8]	2.744
H25	H4[9]	2.651	H25	H5[8]	1.485
H25	H6[8]	3.416	H25	H11[10]	2.824
H26	C13[16]	3.569	H26	C14[16]	3.127
H26	C15[10]	3.236	H26	C16[10]	3.559
H26	C20	3.200	H26	H4[9]	3.589
H26	H5[8]	3.524	H26	H9[16]	3.497
H26	H10[16]	2.722	H26	H11[10]	2.545
H26	H12[10]	3.193	H26	H13	3.165
H26	H15	2.797	H26	H16	2.933
H27	O1[12]	3.448	H27	C20	3.223
H27	C23[12]	2.814	H27	C24[12]	2.743
H27	C25[12]	2.916	H27	C26[12]	3.121
H27	C27[12]	3.191	H27	C28[12]	3.055
H27	H4[9]	3.524	H27	H11[10]	3.346
H27	H12[10]	3.126	H27	H15	3.012
H27	H16	2.588	H27	H19[12]	3.177
H27	H20[12]	3.429	H28	C2[5]	3.573
H28	C6[9]	3.110	H28	H1[5]	3.476
H28	H2[5]	3.550	H28	H3[9]	3.384
H28	H4[9]	2.248	H28	H5[8]	3.334
H28	H9[16]	3.245	H28	H10[16]	3.509

Table 14. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H28	H15	3.244	H28	H16	3.556

Symmetry Operators:

(1) -X,-Y+1,-Z
(2) X-1,Y-1,Z-1
(3) X,Y-1,Z-1
(4) -X-1,-Y+1,-Z+1
(5) -X,-Y+1,-Z+1
(6) -X,-Y+2,-Z+1
(7) X-1,Y,Z
(8) -X+1,-Y+1,-Z+1
(9) X+1,Y,Z+1
(10) -X+1,-Y+2,-Z+1
(11) X,Y,Z-1
(12) X+1,Y,Z
(13) -X,-Y+2,-Z+2
(14) X-1,Y,Z-1
(15) X,Y+1,Z
(16) X,Y-1,Z
(17) -X-1,-Y+2,-Z+2
(18) X,Y,Z+1
(19) X+1,Y+1,Z+1
(20) X,Y+1,Z+1