Electronic Supplementary Material (ESI) for RSC Advances.

SUPPLEMENTARY DATA

Synthesis and photophysical properties of β-triazole bridged porphyrin-coumarin dyads

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1. ^{1}H and ^{13}C NMR spectra of newly synthesized free-base and zinc porphyrins
2. Single crystal X-ray analysis of porphyrin (**5f**)

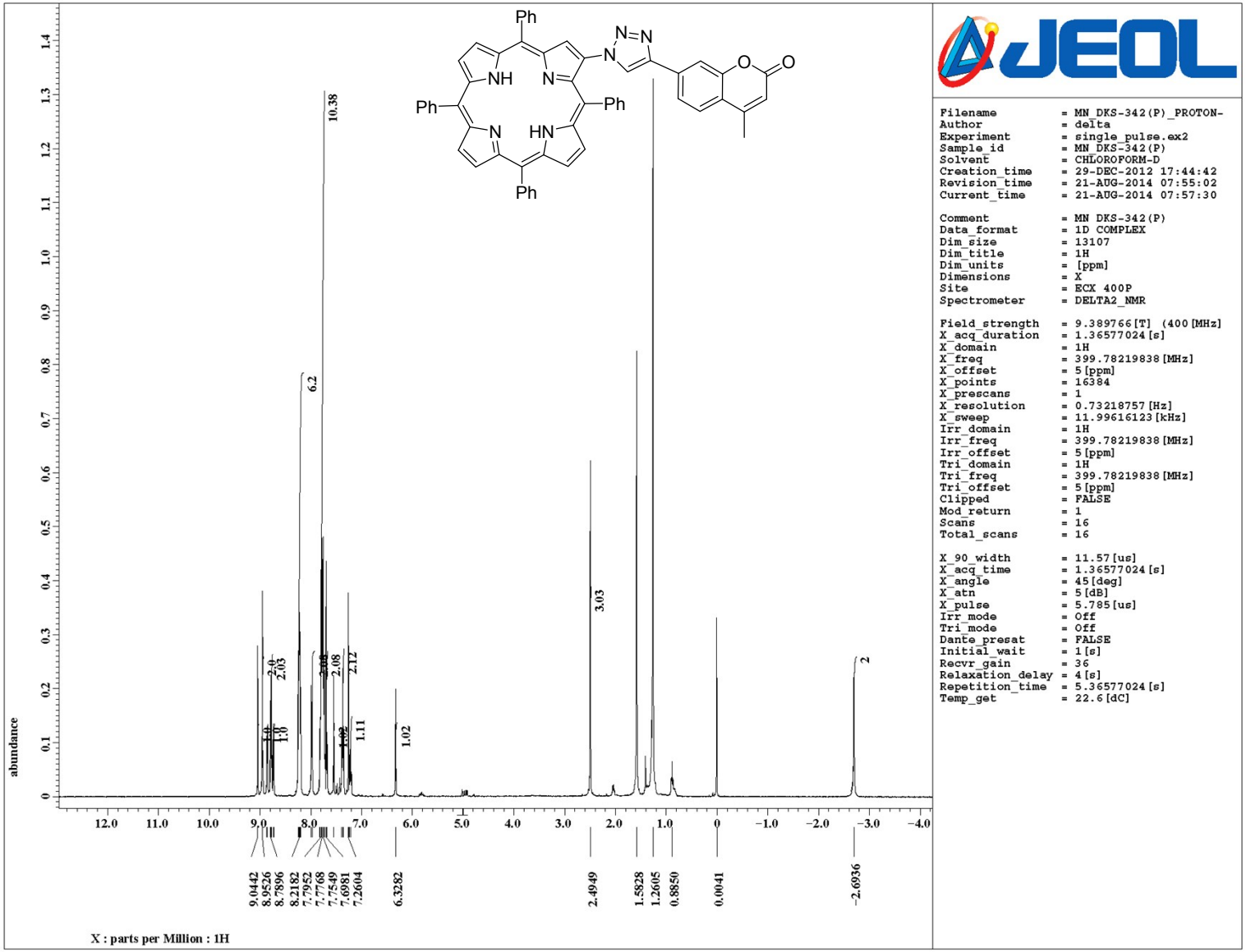

Figure 1. ^{1}H NMR spectrum of compound (**4b**) in $CDCl_3$.

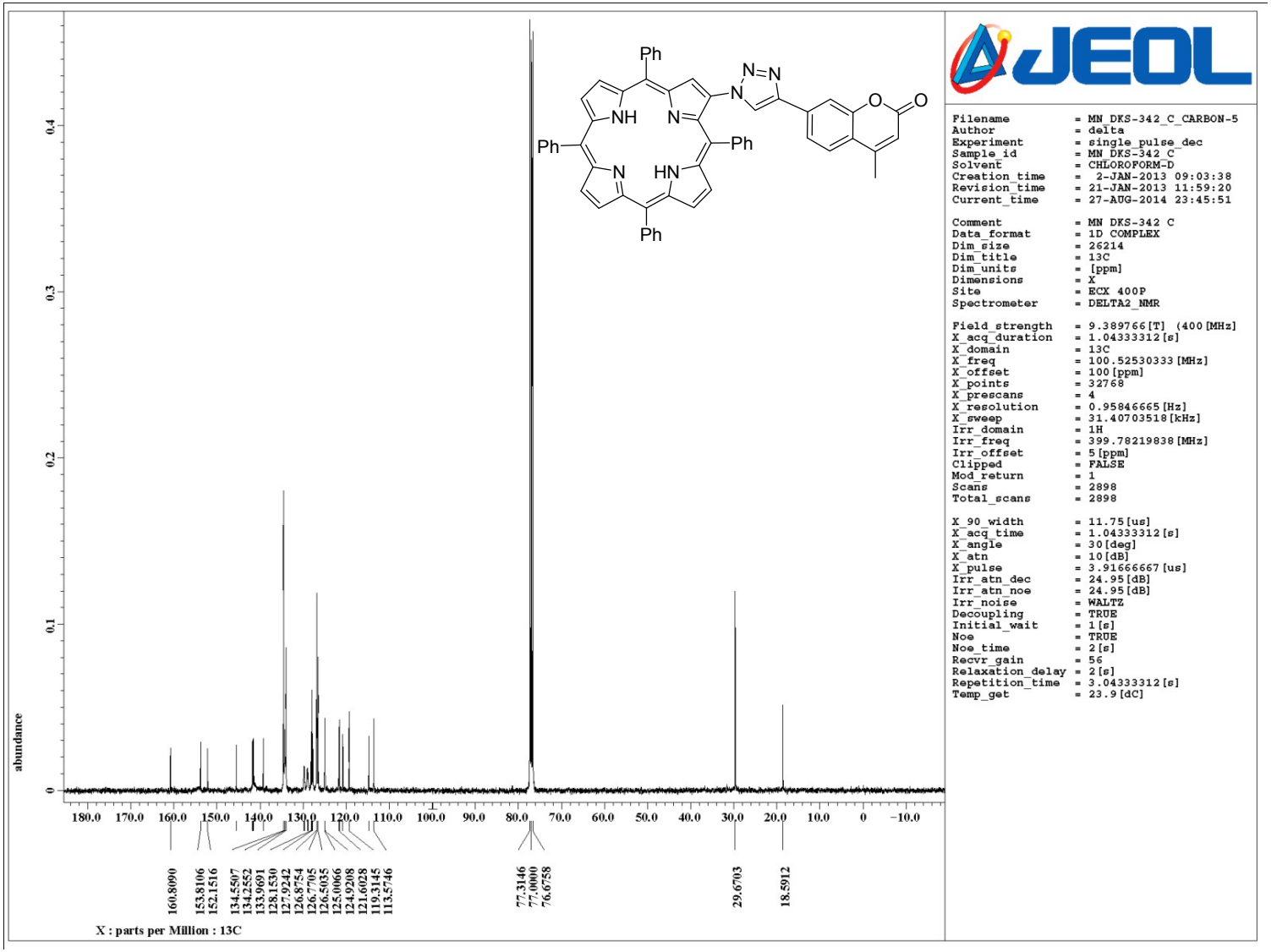

Figure 2. ^{13}C NMR spectrum of compound (**4b**) in $CDCl_3$.

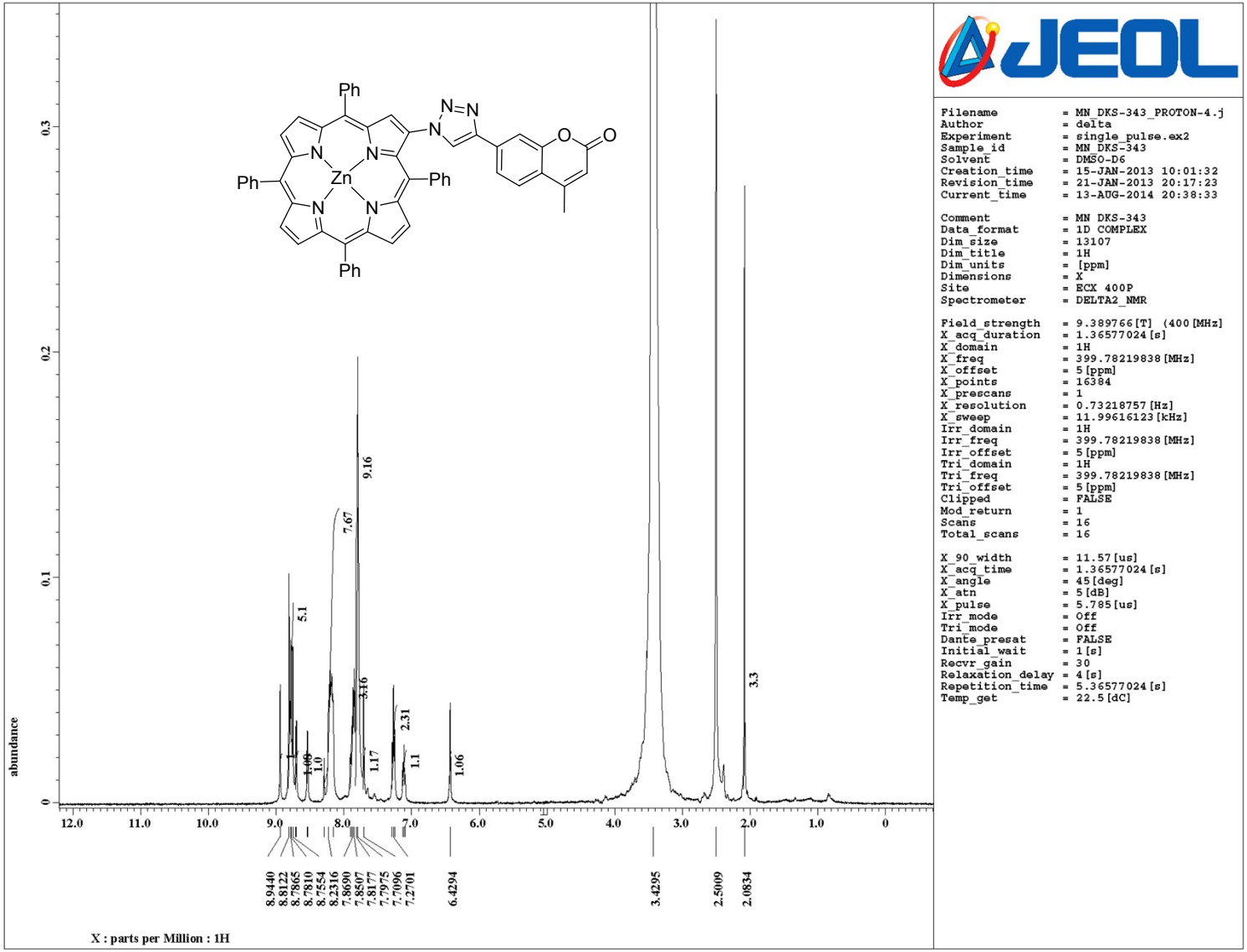

Figure 3. ^{1}H NMR spectrum of compound (**4c**) in DMSO-d_6.

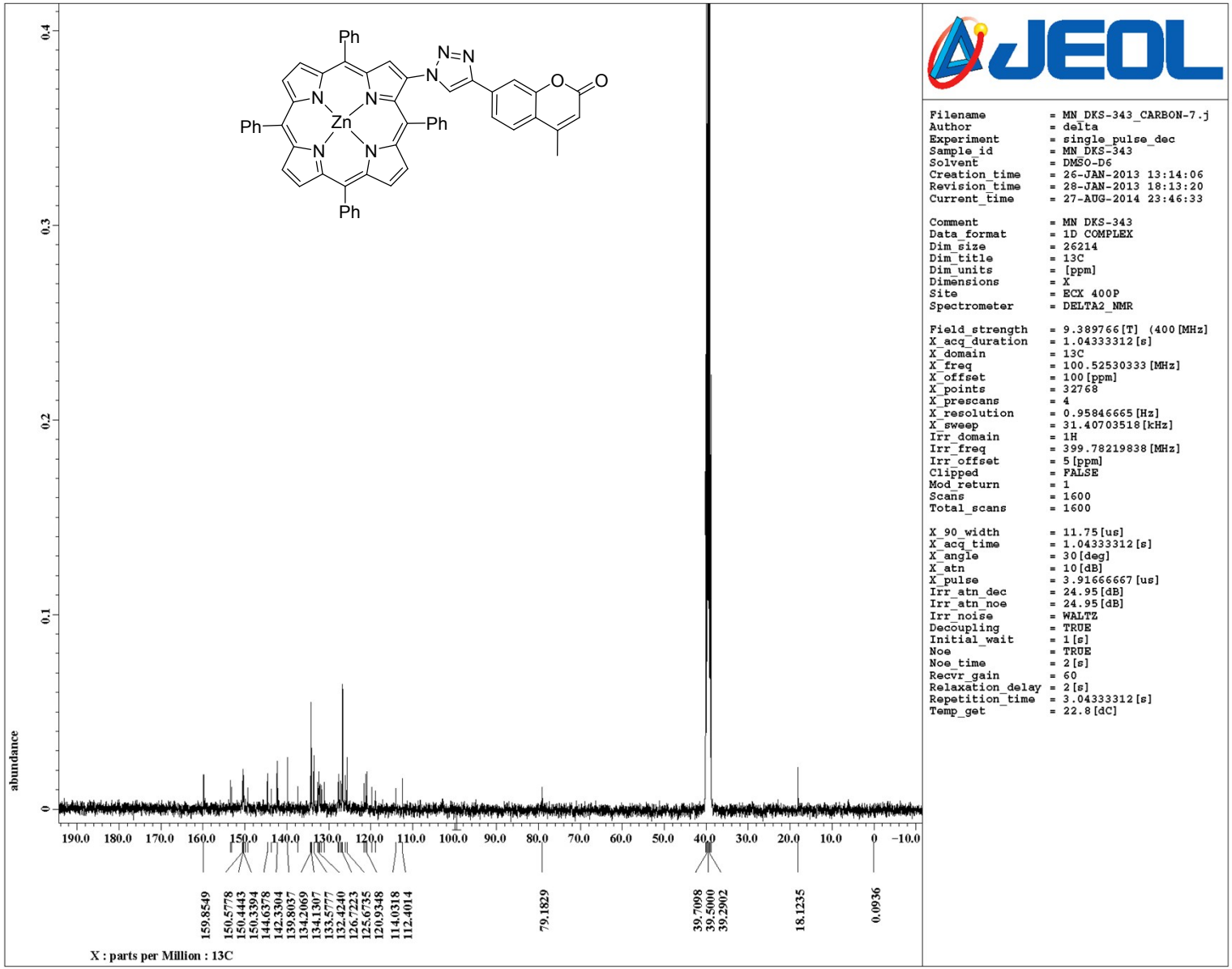

Figure 4. ^{13}C NMR spectrum of compound (**4c**) in DMSO-d_6.

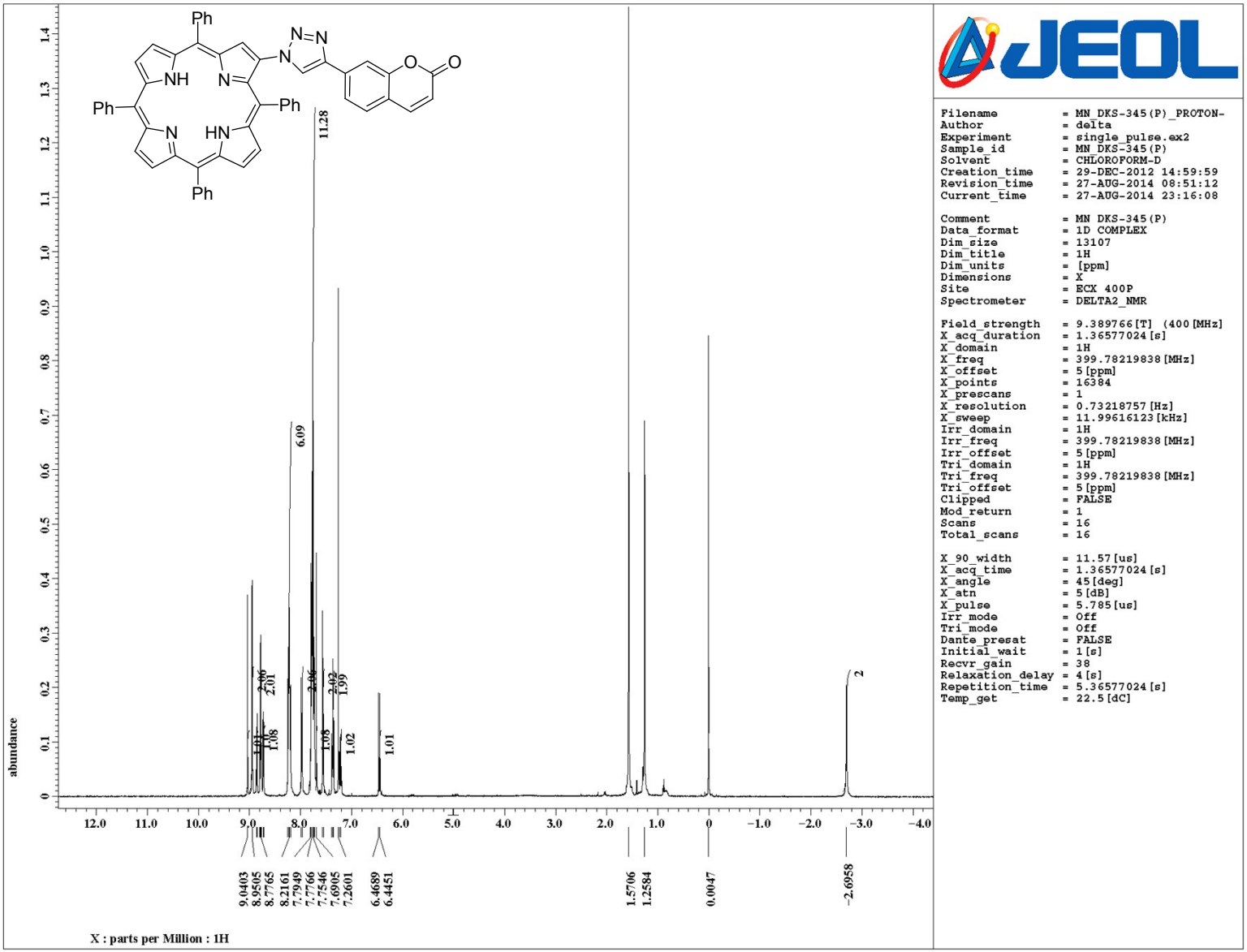

Figure 5. ^{1}H NMR spectrum of compound (**4e**) in $CDCl_3$.

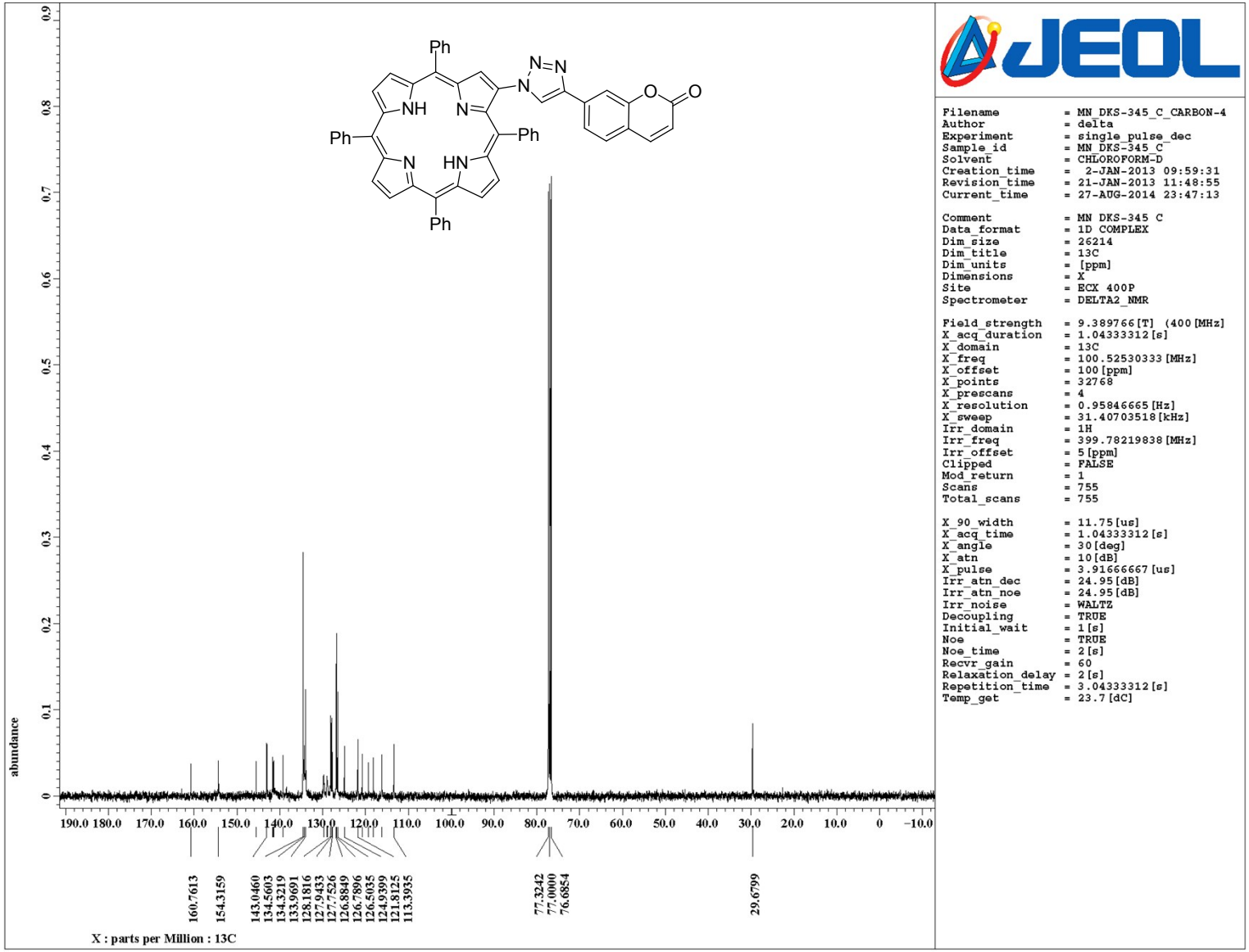

Figure 6. ^{13}C NMR spectrum of compound (**4e**) in $CDCl_3$.

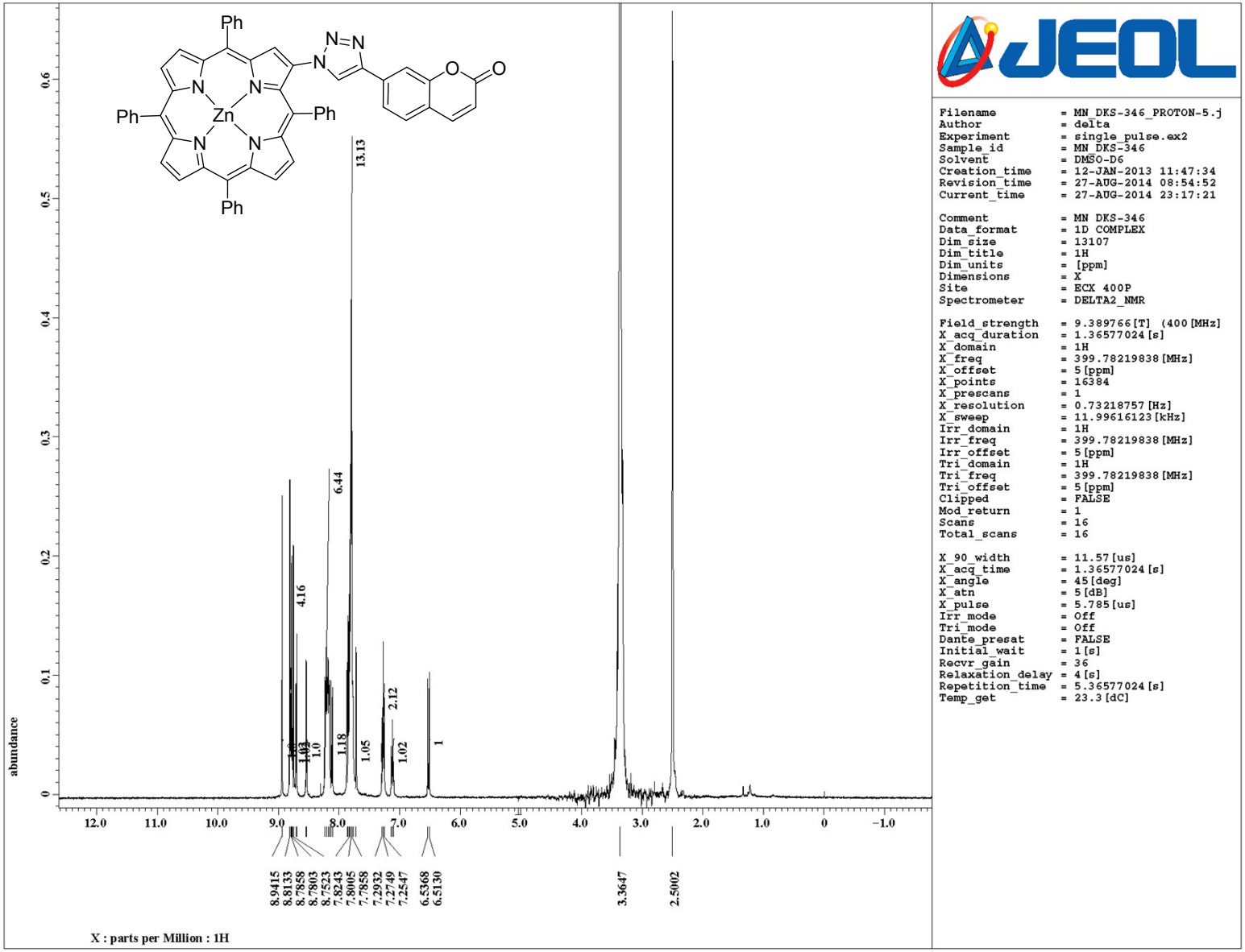

Figure 7. ^{1}H NMR spectrum of compound (**4f**) in DMSO-d_6.

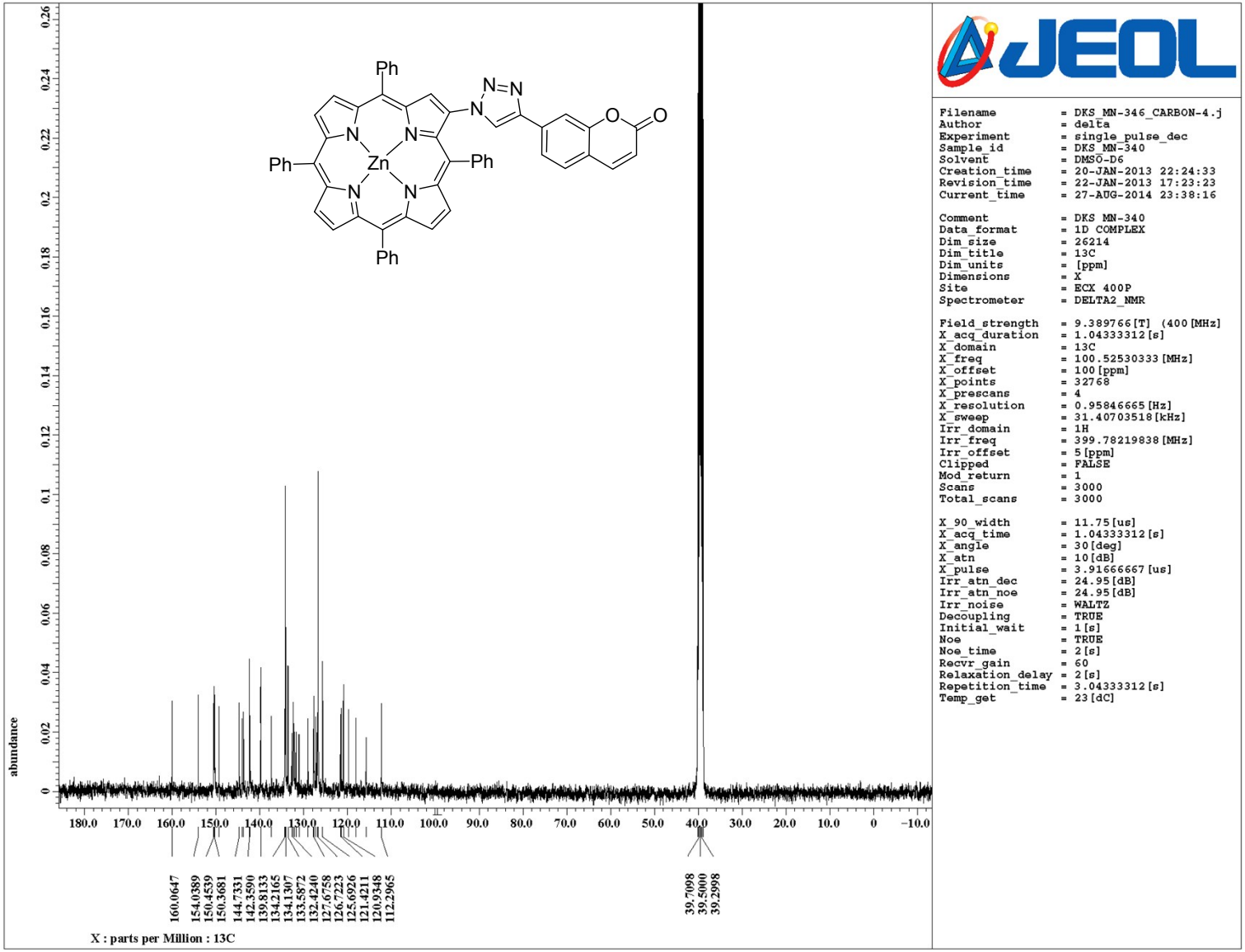

Figure 8. ^{13}C NMR spectrum of compound (**4f**) in DMSO-d_6.

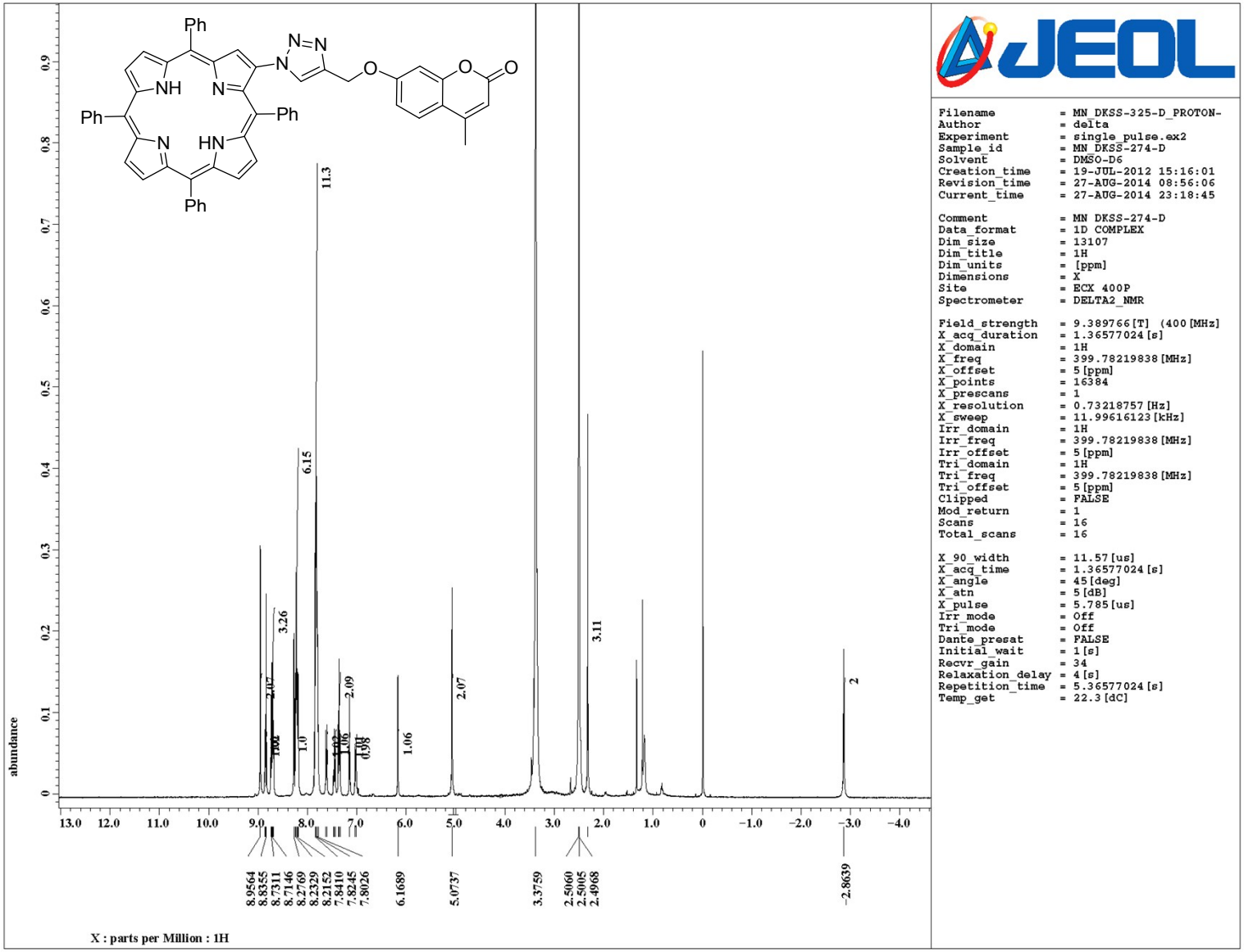

Figure 9. ^{1}H NMR spectrum of compound (**5b**) in DMSO-d_6.

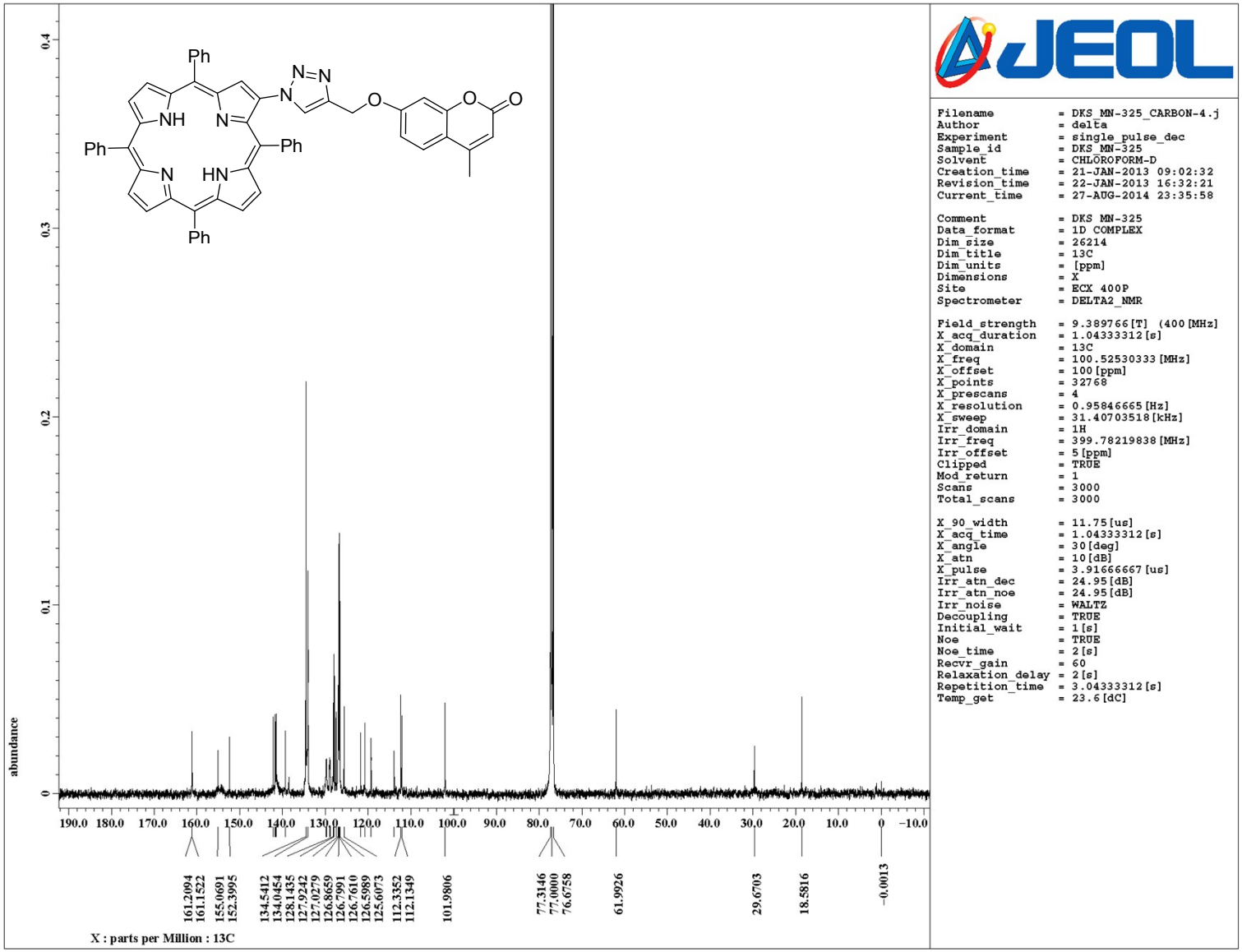

Figure 10. ^{13}C NMR spectrum of compound (**5b**) in $CDCl_3$.

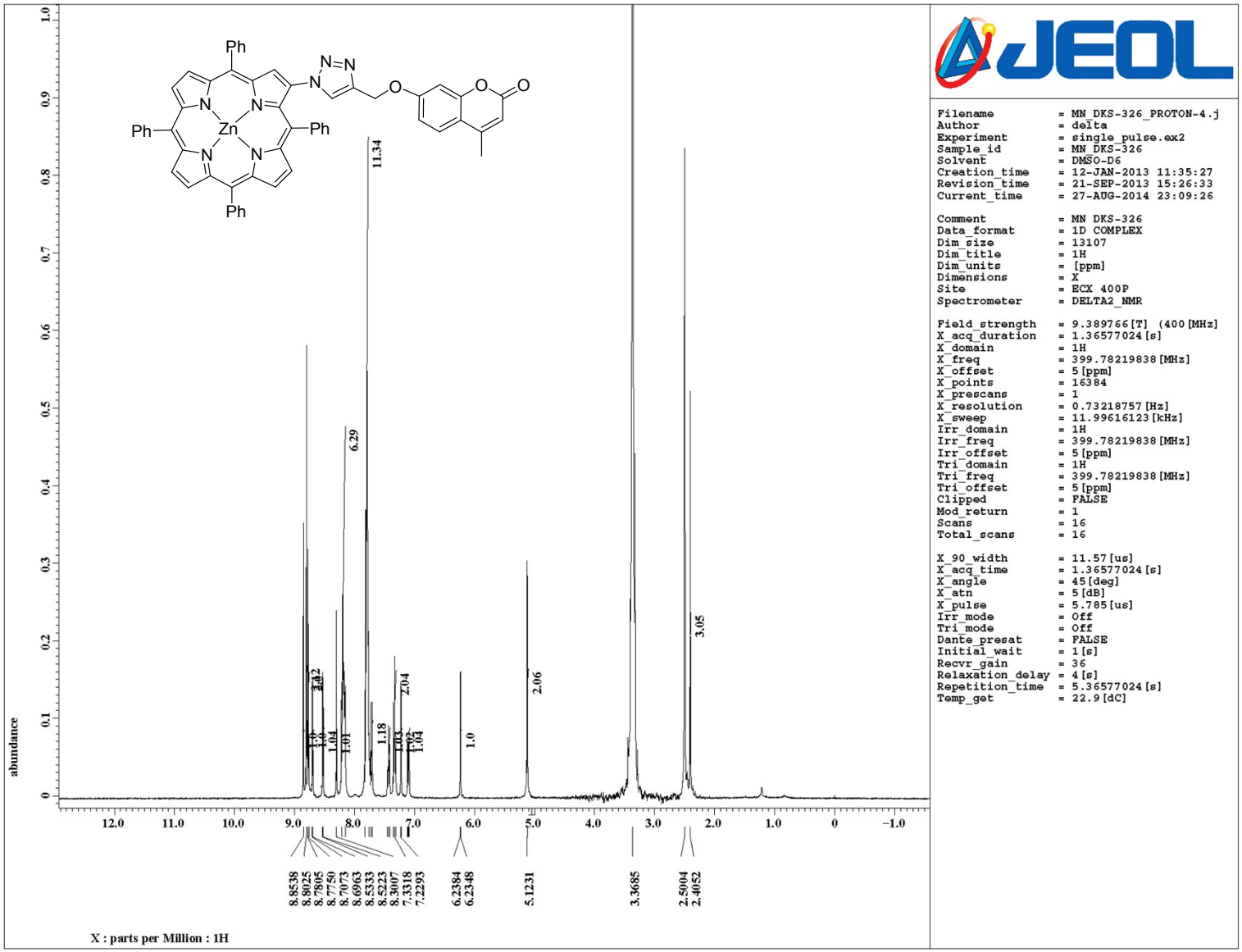

Figure 11. ^{1}H NMR spectrum of compound (**5c**) in DMSO-d_6.

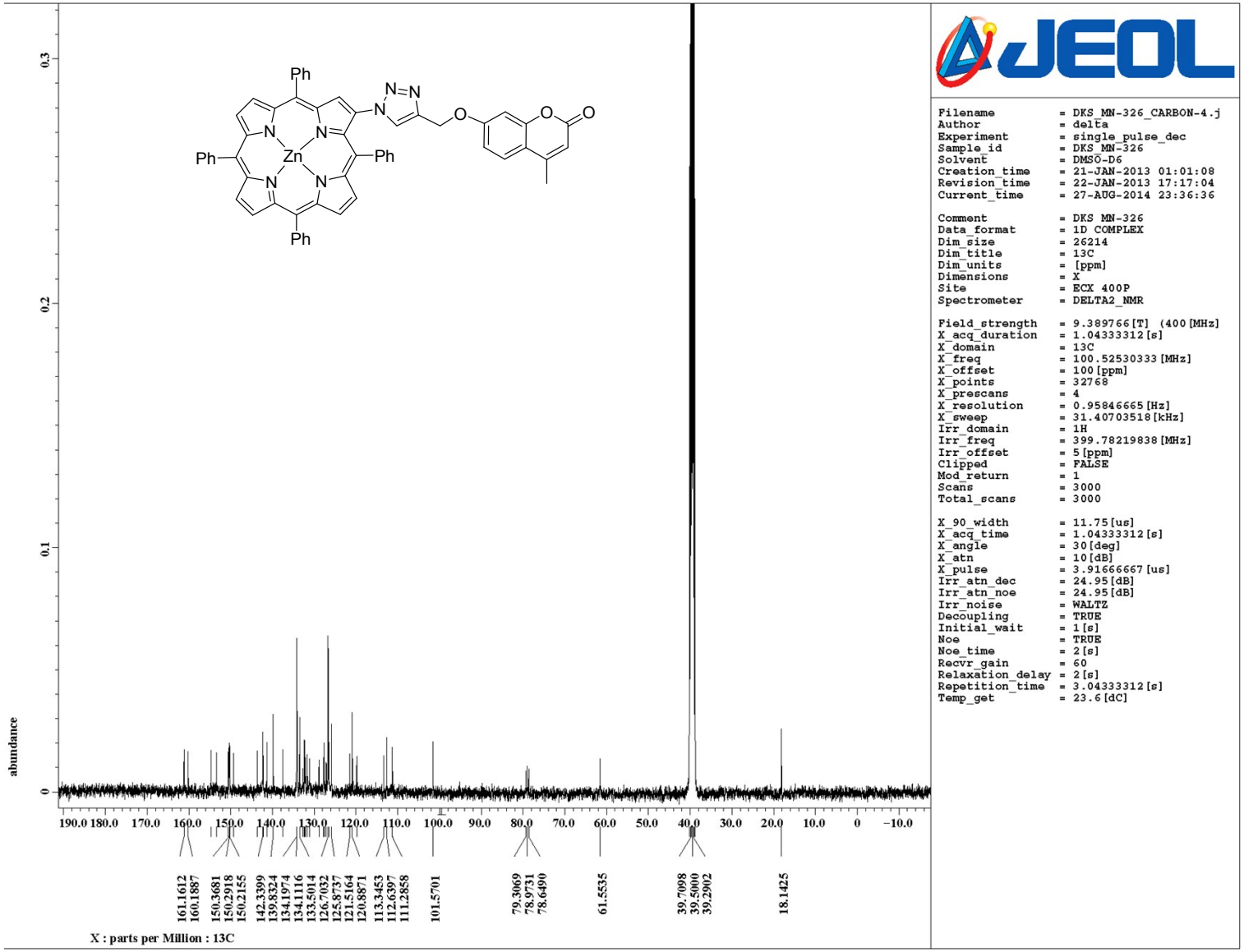

Figure 12. ^{13}C NMR spectrum of compound (**5c**) in DMSO-d_6.

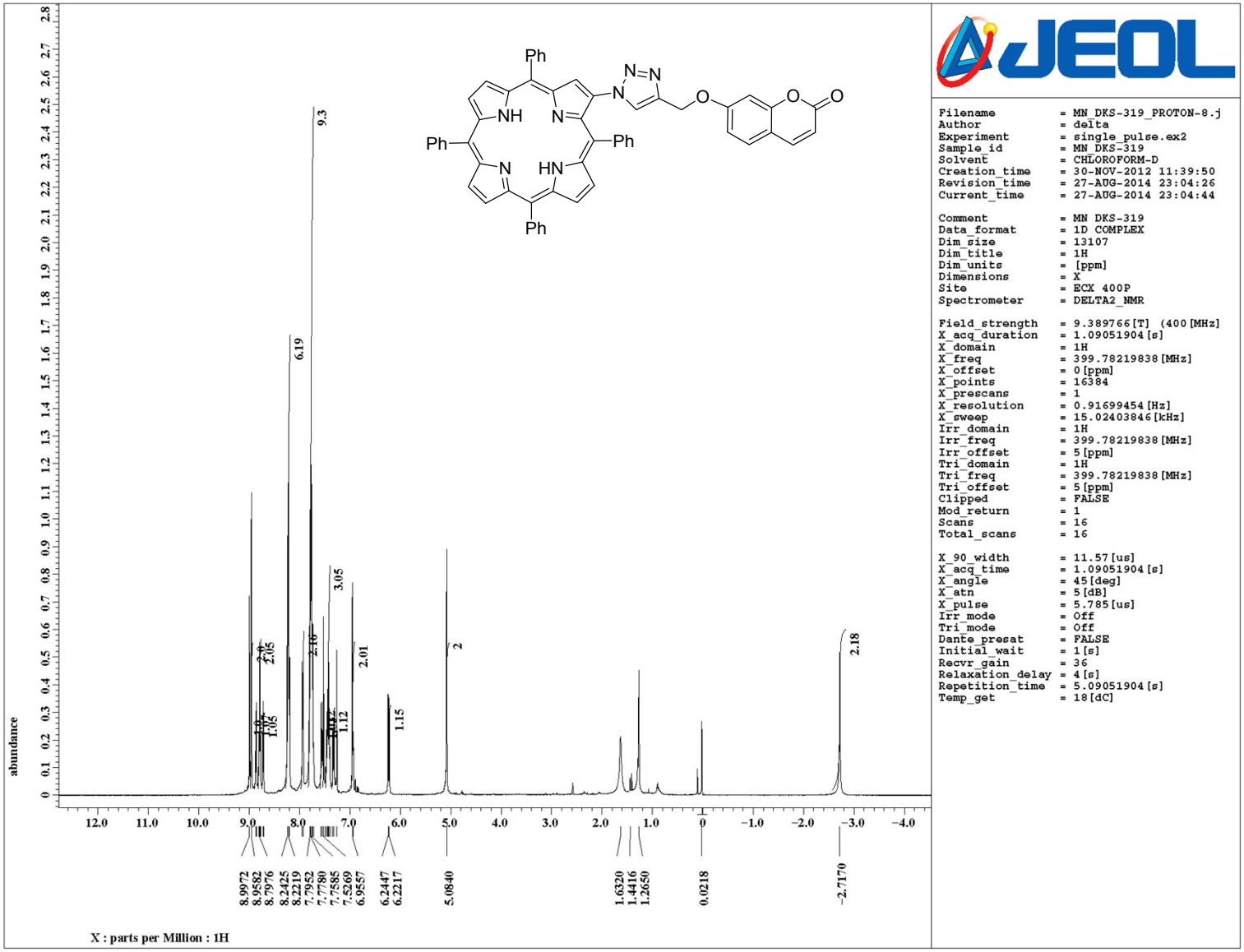

Figure 13. ^{1}H NMR spectrum of compound (**5e**) in $CDCl_3$.

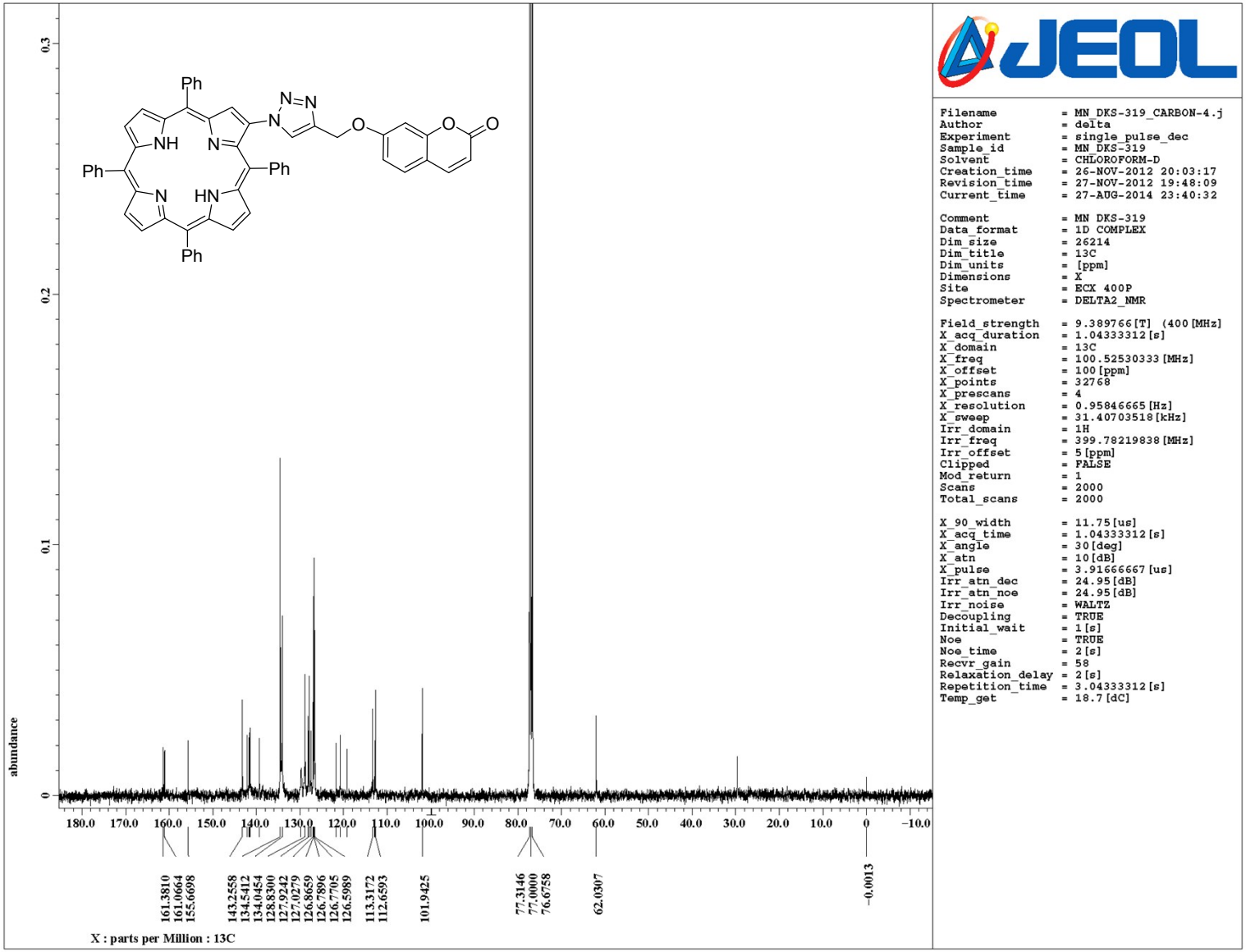

Figure 14. ^{13}C NMR spectrum of compound (**5e**) in $CDCl_3$.

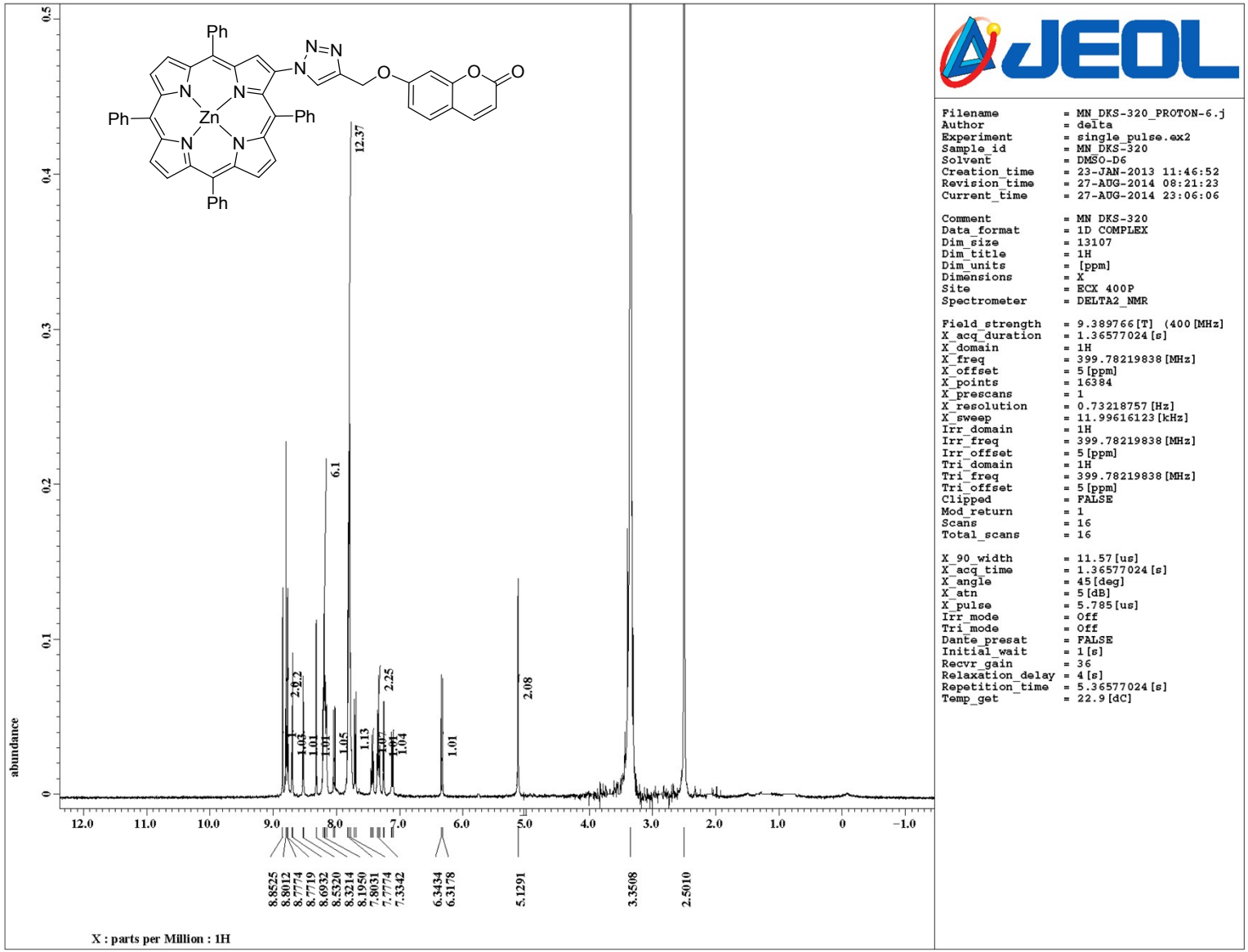

Figure 15. ^{1}H NMR spectrum of compound (**5f**) in DMSO-d_6.

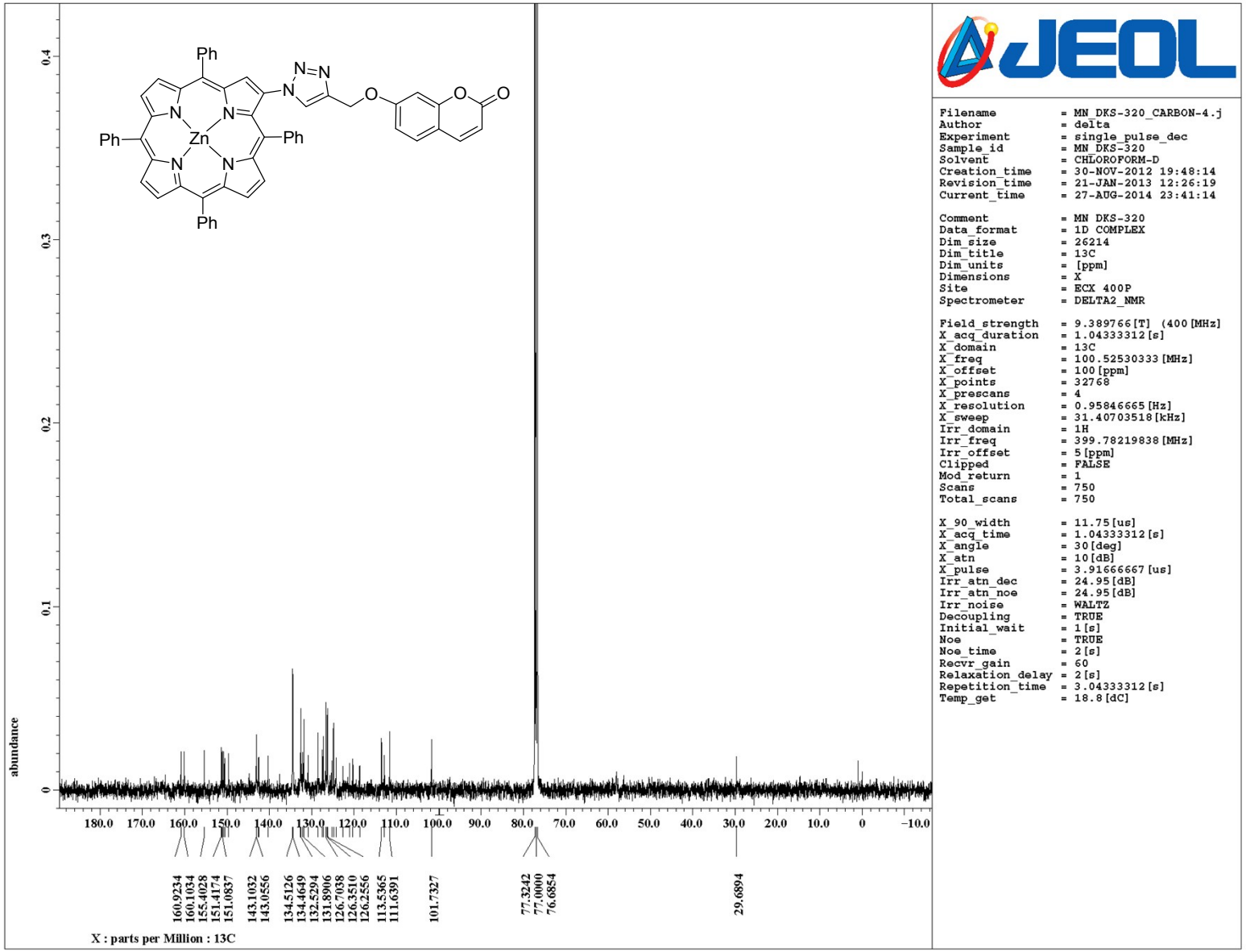

Figure 16. ^{13}C NMR spectrum of compound (**5f**) in $CDCl_3$.

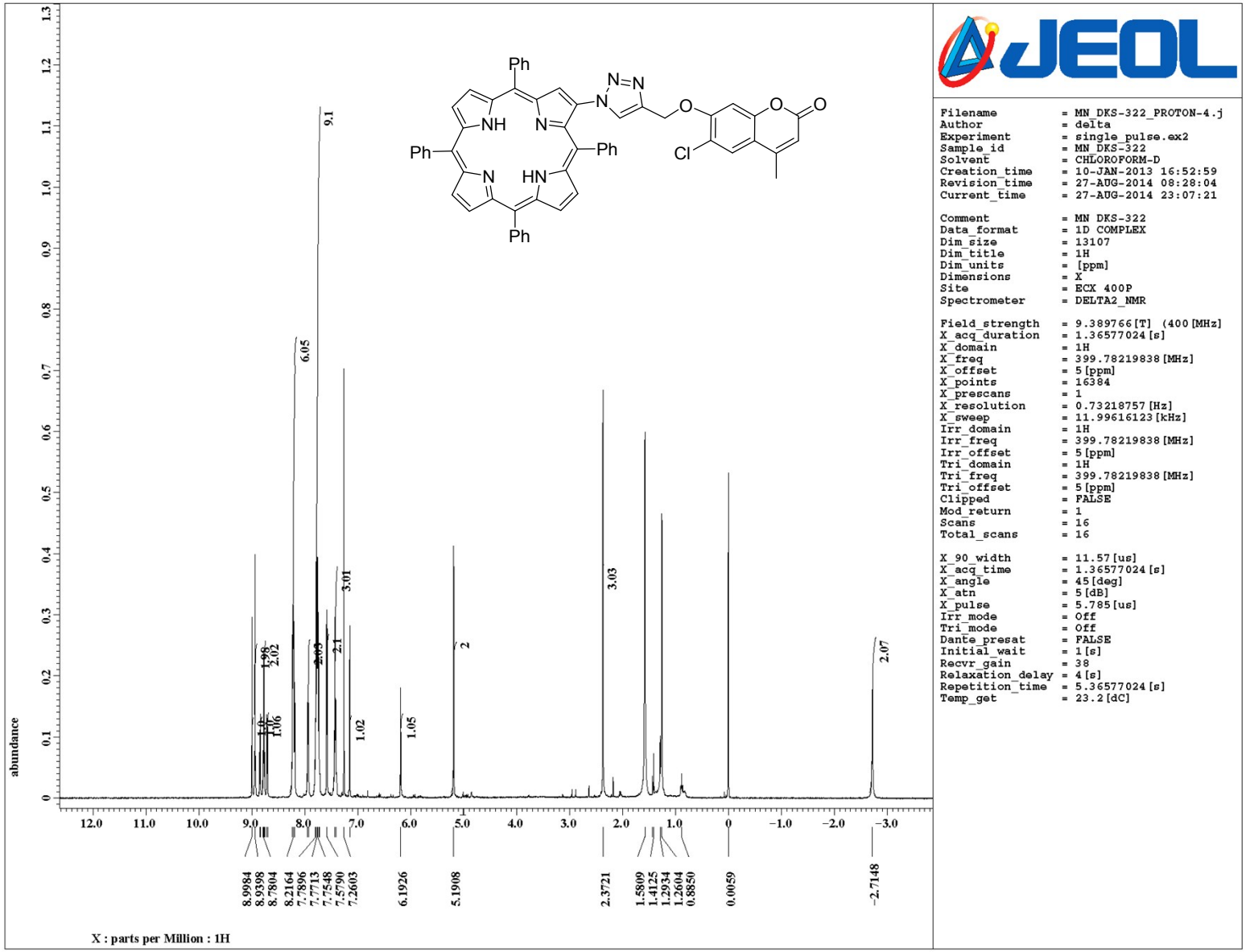

Figure 17. ^{1}H NMR spectrum of compound (**5h**) in $CDCl_3$.

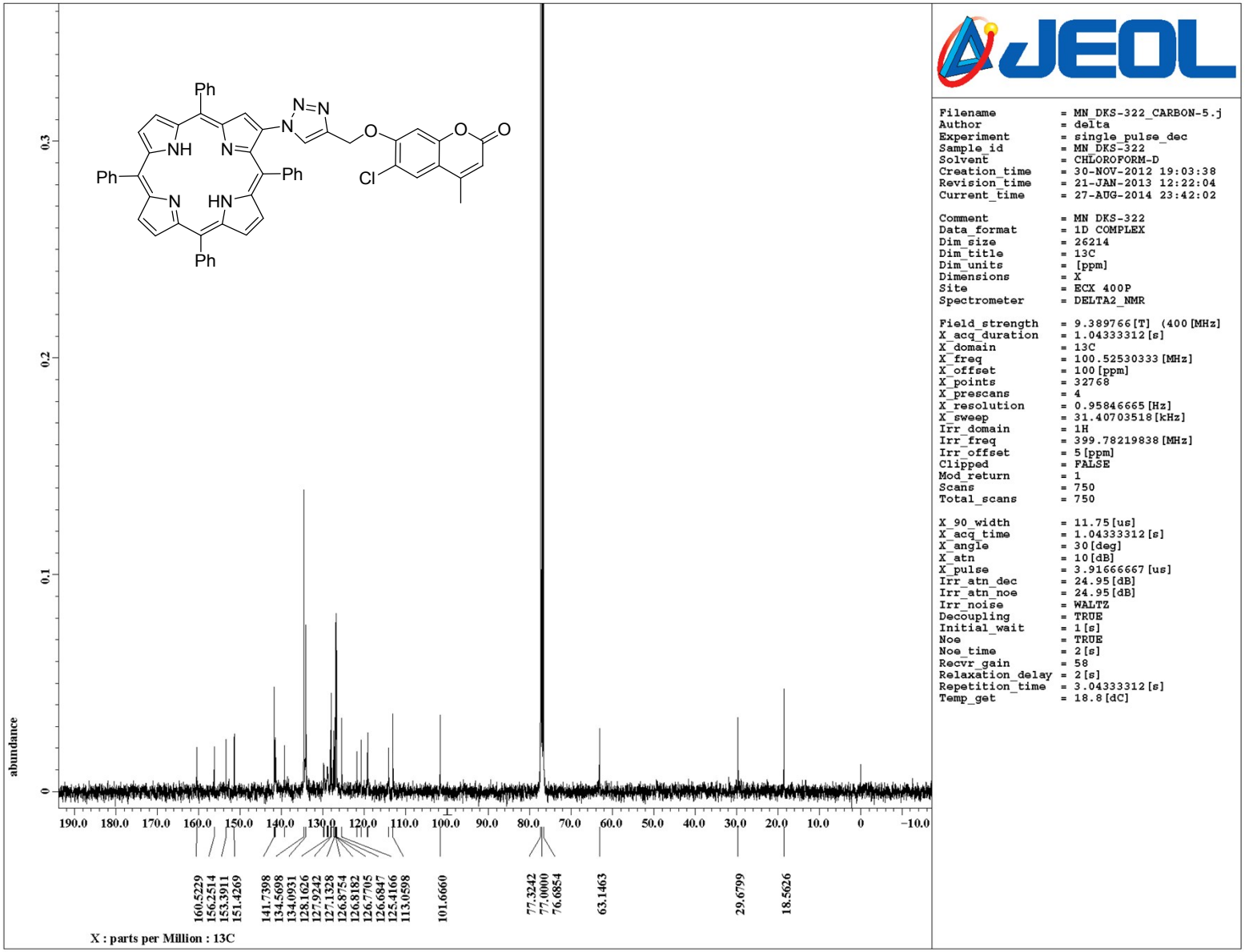

Figure 18. ^{13}C NMR spectrum of compound (**5h**) in $CDCl_3$.

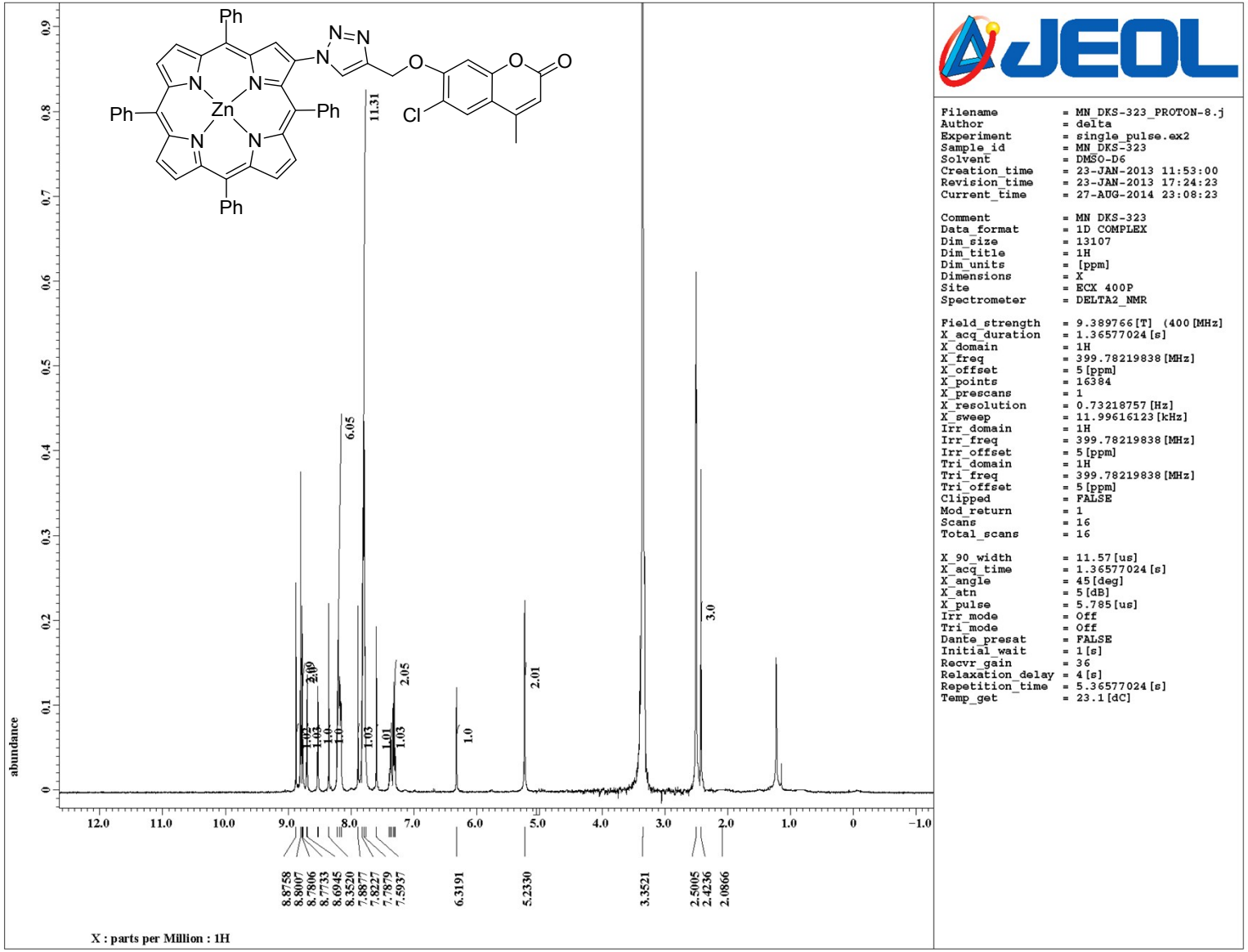

Figure 19. ^{1}H NMR spectrum of compound (**5i**) in DMSO-d_6.

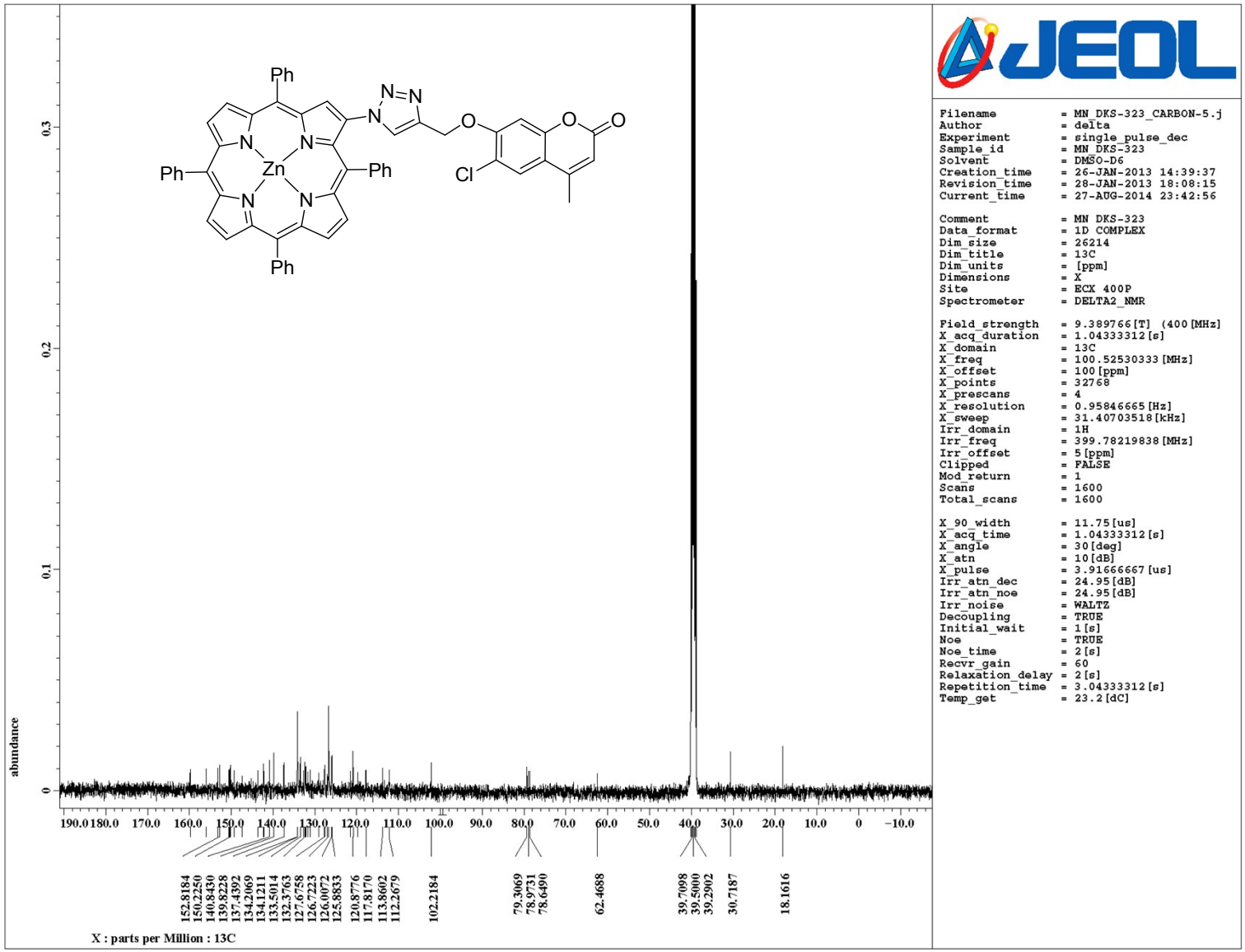

Figure 20. ^{13}C NMR spectrum of compound (**5i**) in DMSO-d_6.

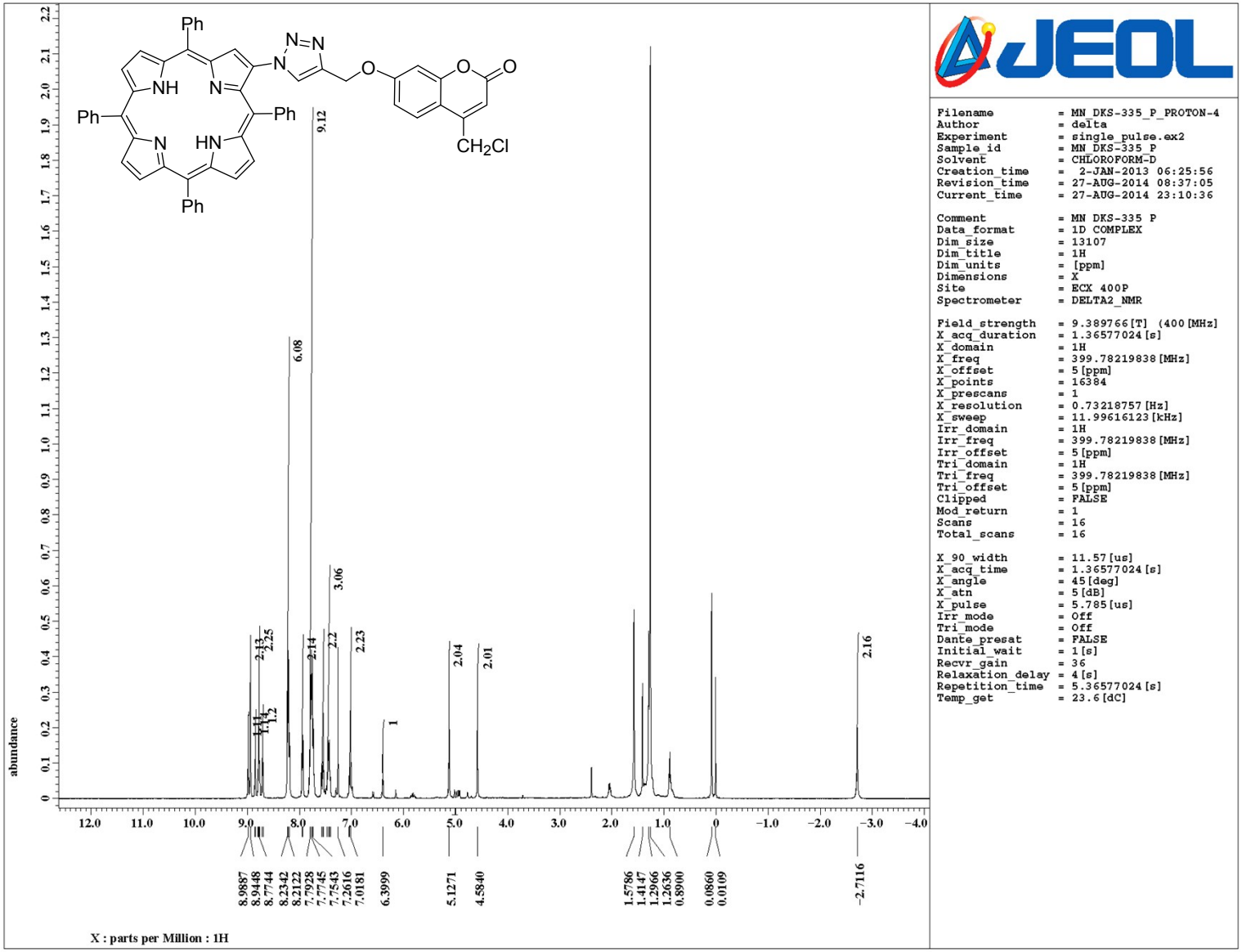

Figure 21. ^{1}H NMR spectrum of compound (**5k**) in $CDCl_3$.

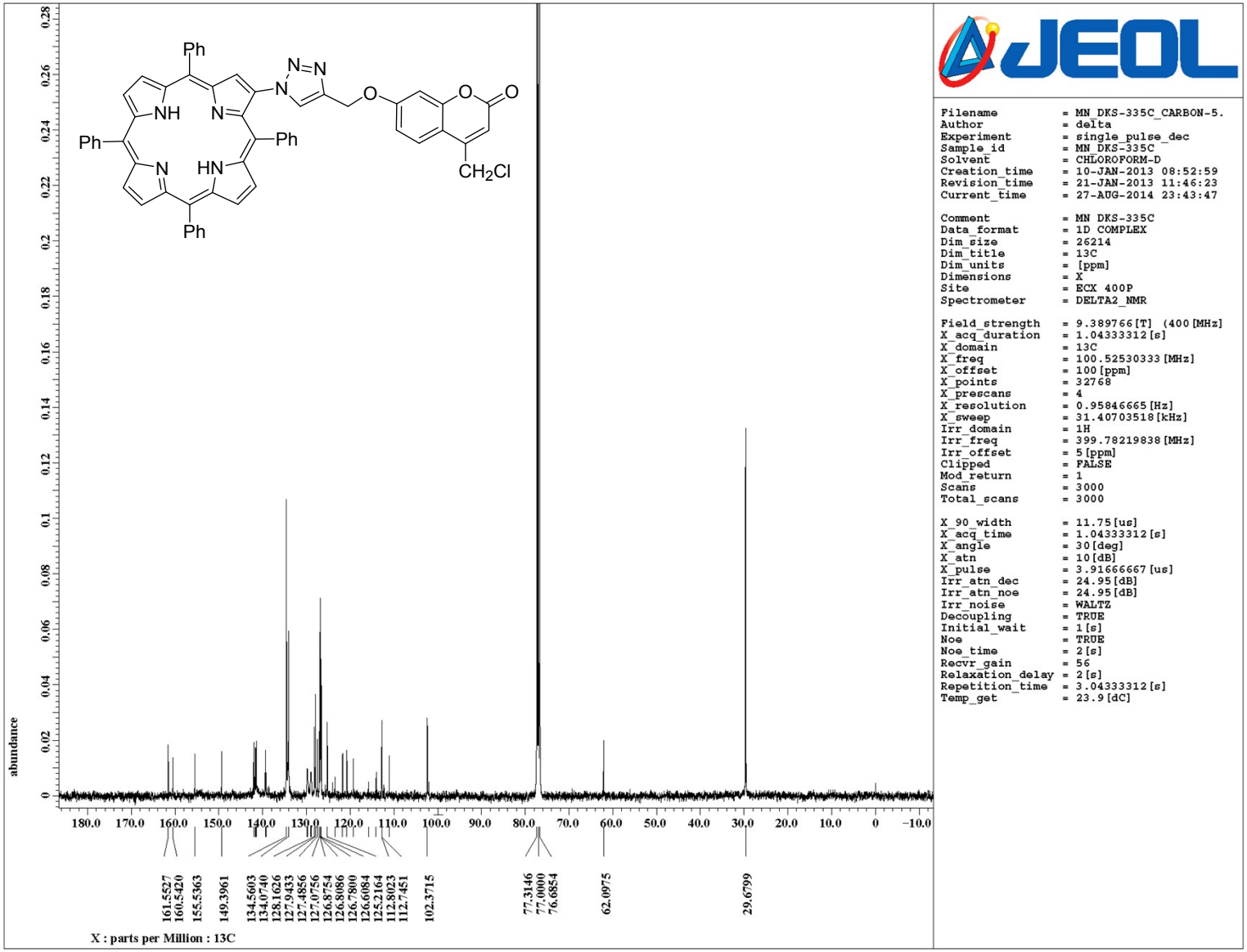

Figure 22. ^{13}C NMR spectrum of compound (**5k**) in $CDCl_3$.

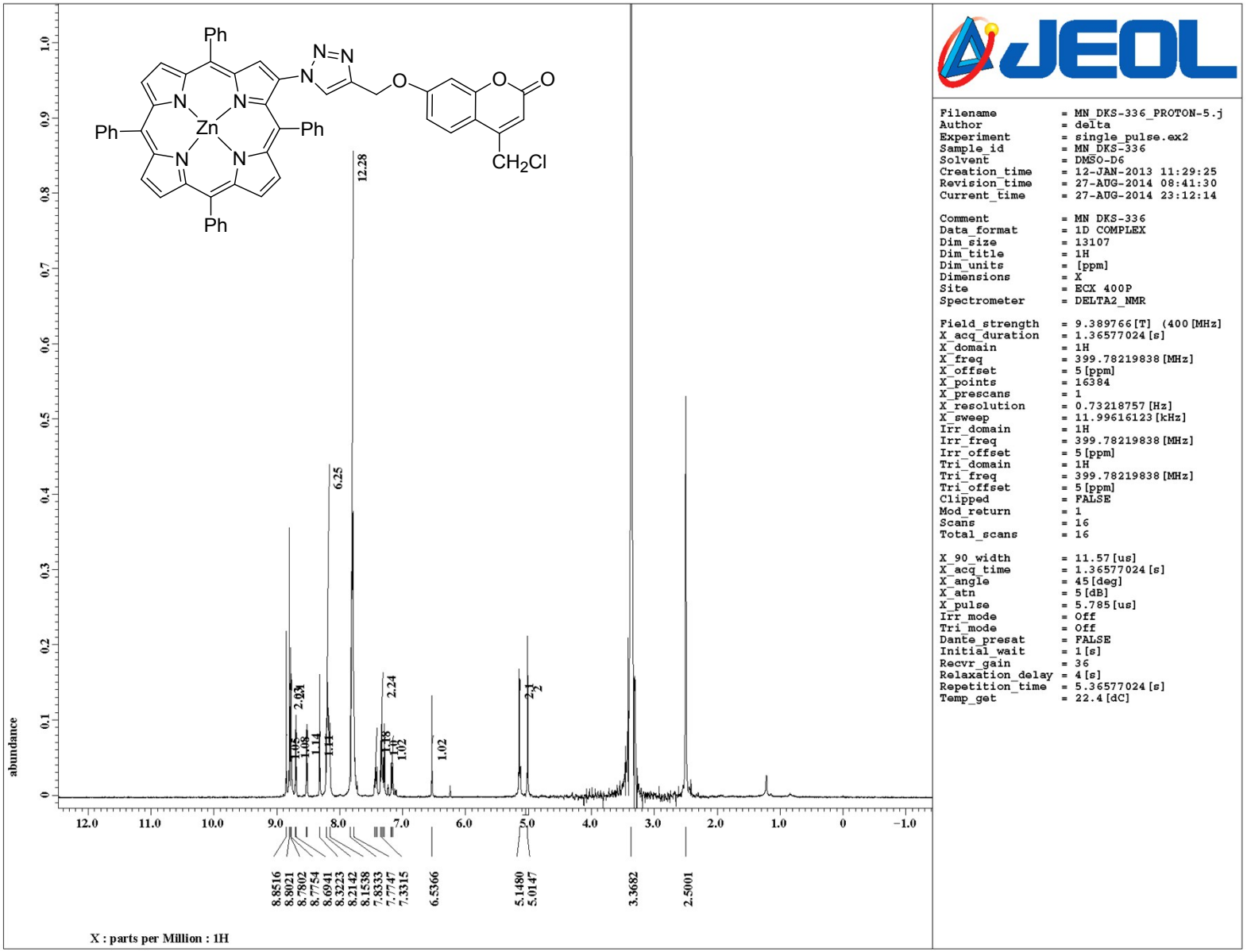

Figure 23. ^{1}H NMR spectrum of compound (**5l**) in DMSO-d_6.

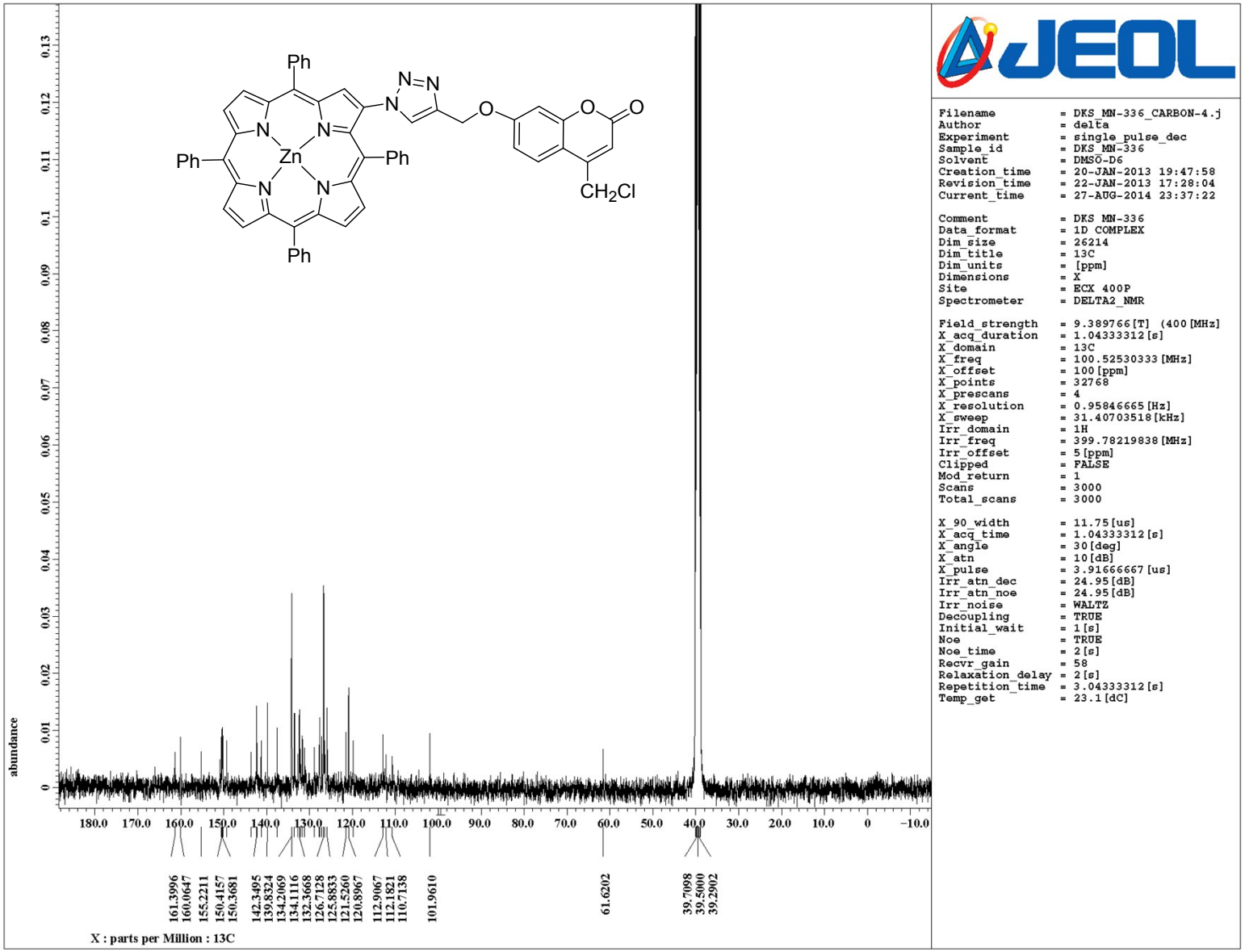

Figure 24. ^{13}C NMR spectrum of compound (**5l**) in DMSO-d_6.

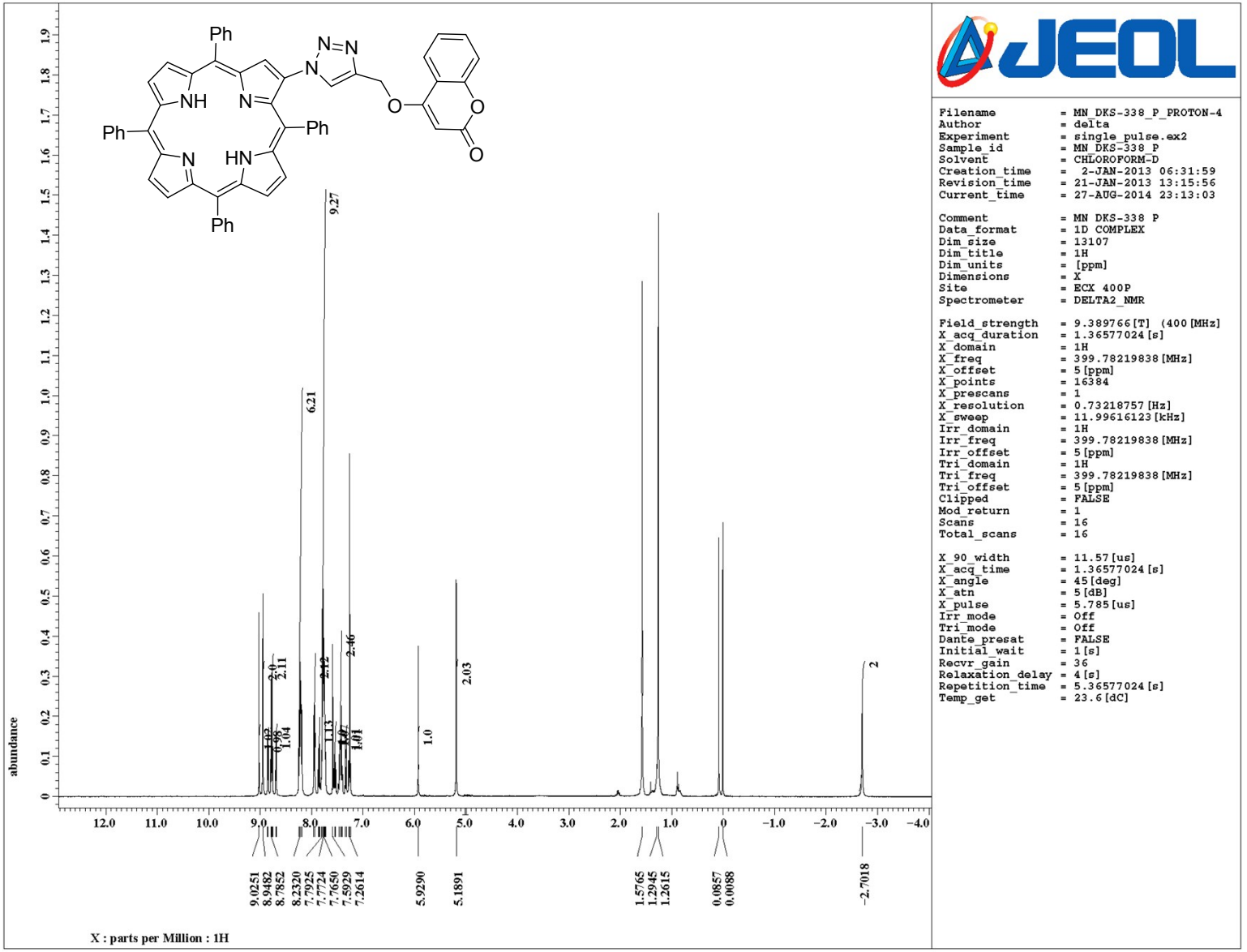

Figure 25. ^{1}H NMR spectrum of compound (**6b**) in $CDCl_3$.

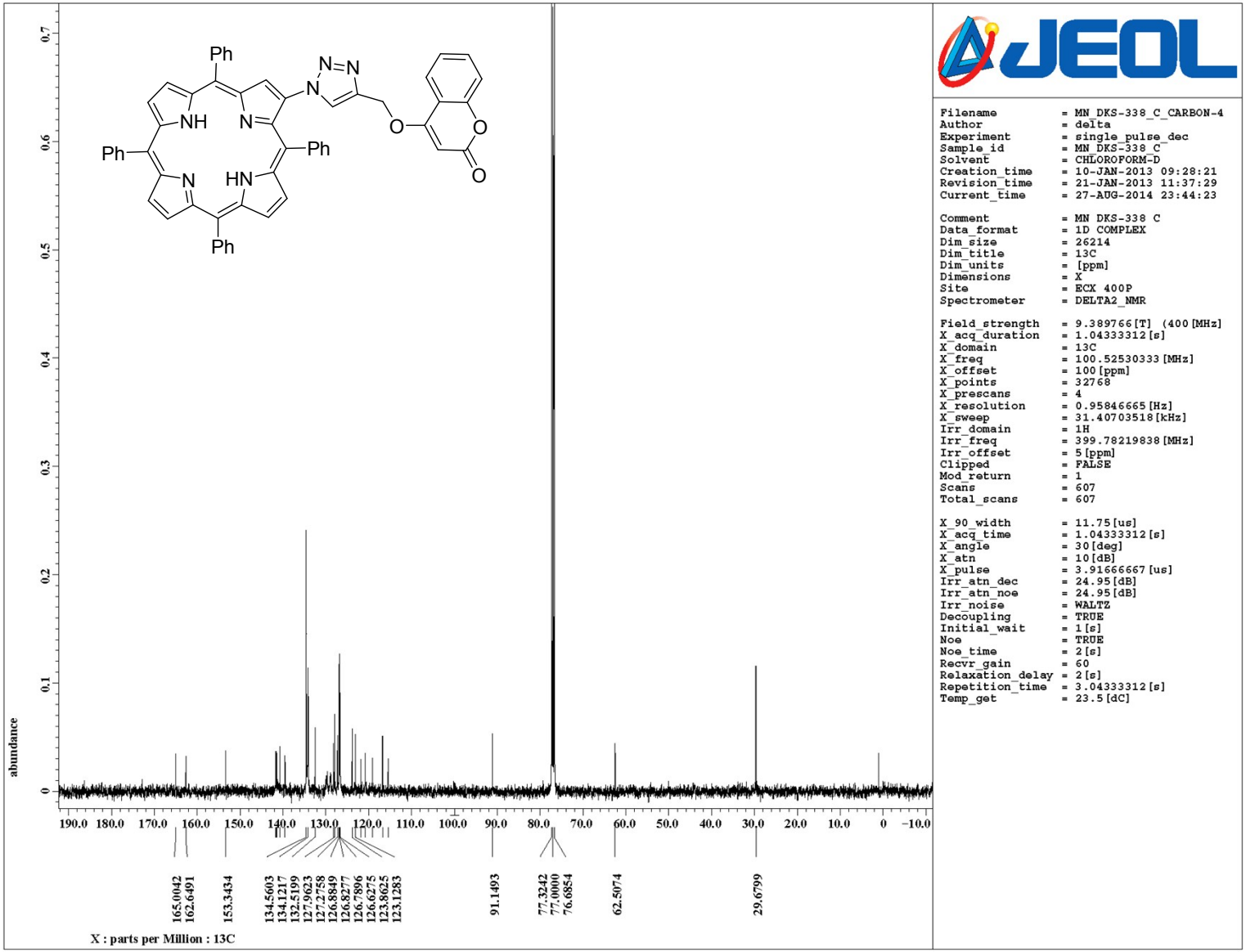

Figure 26. ^{13}C NMR spectrum of compound (**6b**) in $CDCl_3$.

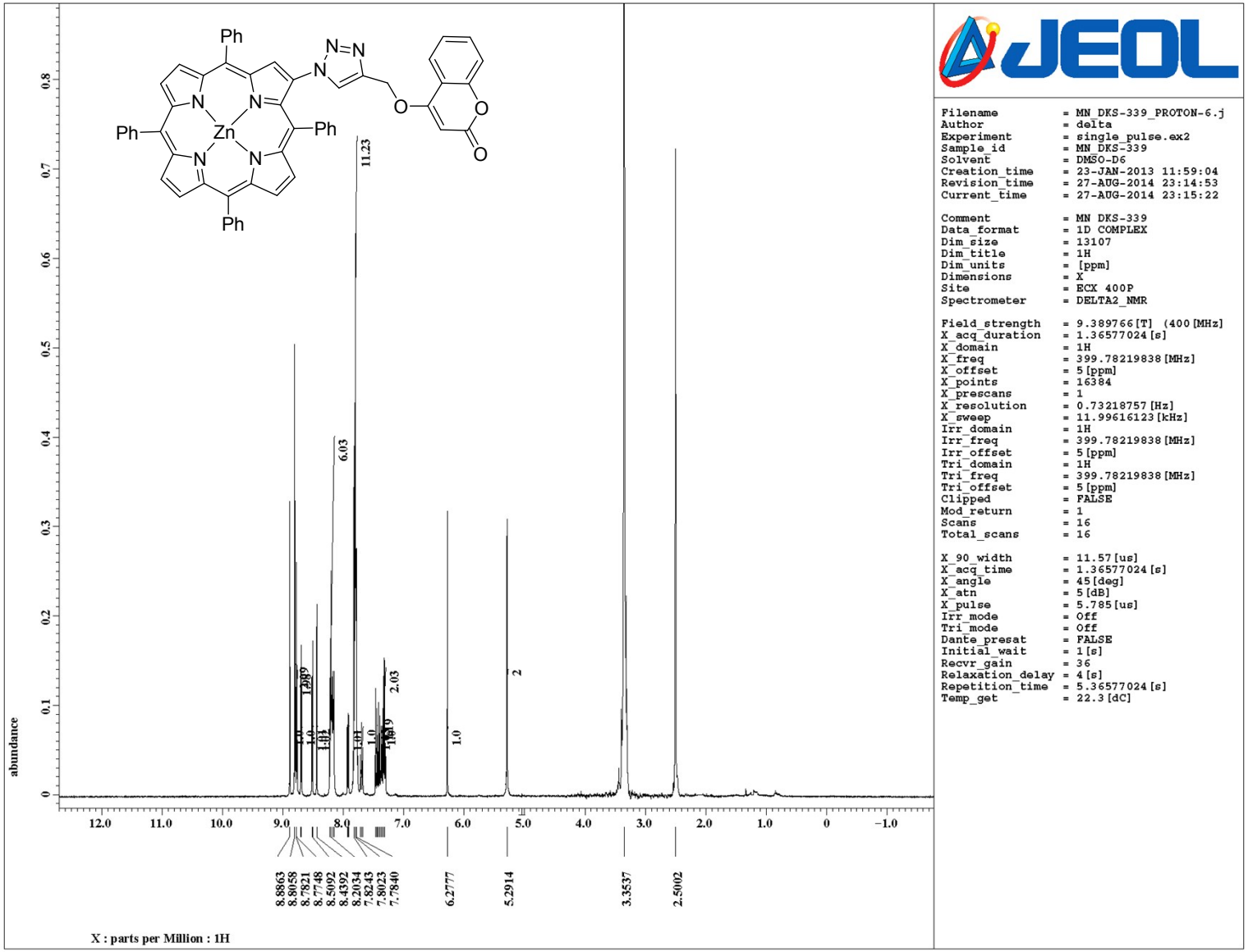

Figure 27. ^{1}H NMR spectrum of compound (**6c**) in DMSO-d_6.

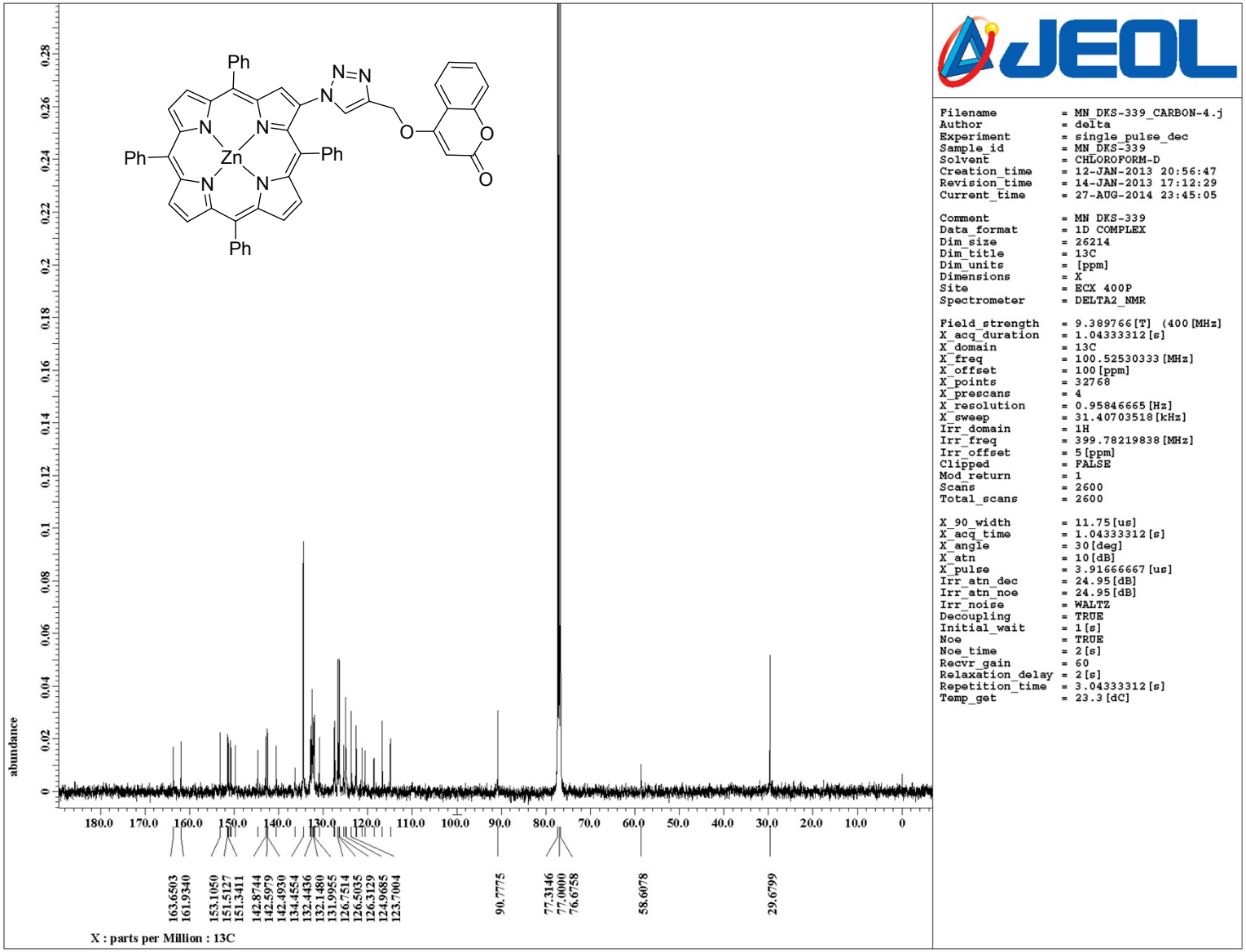

Figure 28. ^{13}C NMR spectrum of compound (**6c**) in $CDCl_3$.

2. Single crystal X-ray analysis of porphyrins 5f:

The intensity data of suitably sized crystal of zinc (II) 7-[1-(5,10,15,20-tetraphenyl-porphyrin-2-yl)-1*H*-[1,2,3]triazol-4-yl]-chromen-2-one (**5f**) was collected on an Oxford Xcalibur S diffractometer (Sapphire-3 CCD detector, 4-circle κ goniometer, graphite monochromator, a single wavelength enhanced X-ray source with MoKα radiation (λ = 0.71073 Å), and ω scans) at 298(2) K.[1] Data collection, Pre-experiment, absorption corrections and data reduction were performed with the CrysAlisPro software suite.[2] The structure was solved by direct method using SIR-92[3] and refined by full-matrix least-squares refinement techniques on F^2 using SHELXL97[4] program package. The hydrogen atoms were placed into the calculated positions and included in the last cycles of the refinement. Non-hydrogen atoms were refined anisotropically. All calculations were done using Wingx software package.[5] In the crystal structure of this compound, the **A level** and **B level** alerts are appearing due to the presence of disorder in solvent molecules (three chloroform, three methanol and one water).

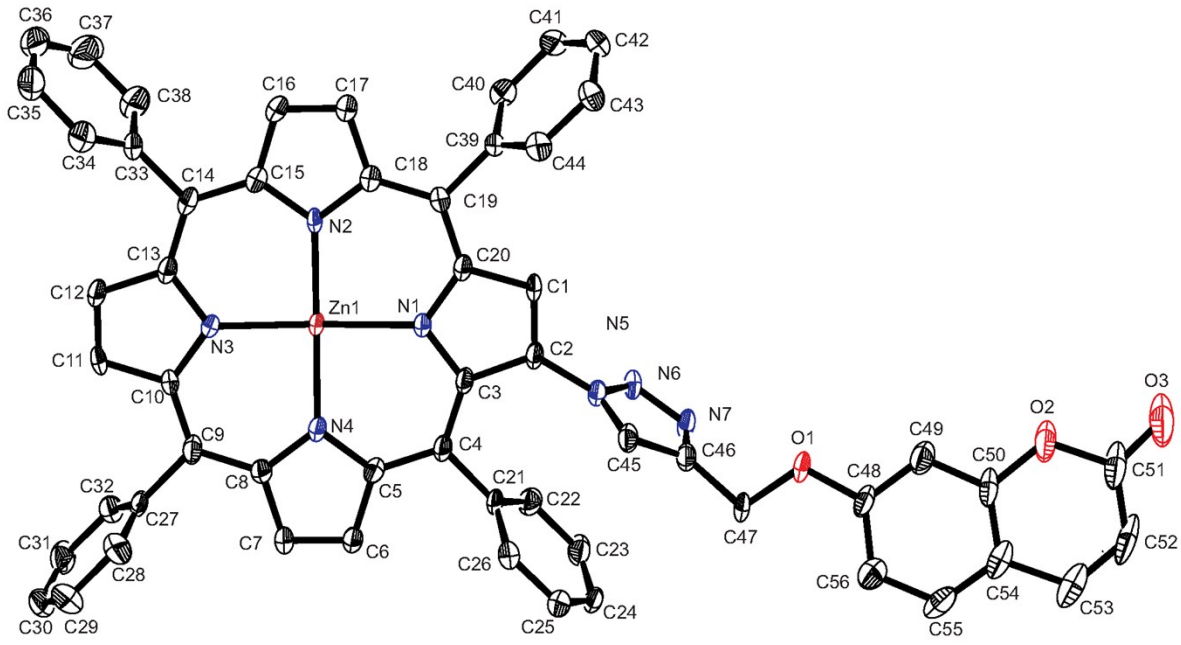

Figure 29. X-Ray crystal structure of compound **5f**. Thermal ellipsoids are shown at the 50% probability level and solvent molecules and all hydrogen atoms are omitted for clarity.

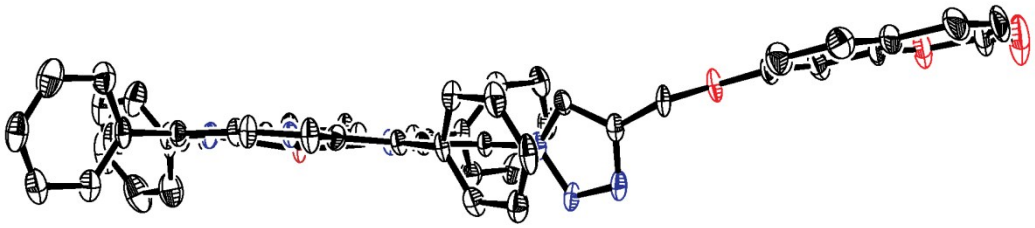

Figure 30. The side view of X-ray crystal structure of **5f**. Thermal ellipsoids are shown at the 50% probability level and solvent molecules and all hydrogen atoms are omitted for clarity.

Table 1. Crystallographic data and structure refinements for porphyrin **5f.**

Compound	**5f.**$3CHCl_3.3CH_3OH.H_2O$
Formula	$C_{62}H_{52}Cl_9N_7O_7Zn$
Fw	1391.53
Crystal system	Monoclinic
Temperature (K)	150(2)
Wavelength (Å)	0.71073
Space group	$P\,2_1/n$
a (Å)	16.046(5)
b (Å)	23.614(5)
c (Å)	16.271(5)
α (deg)	90.000(5)
β (deg)	102.957(5)
γ (deg)	90.000(5)
Volume ($Å^3$)	6008(3)
Z	4
μ(Mo Kα) (mm^{-1})	0.870
θ range (deg)	2.89-26.37
F(000)	2848
$\rho_{calcd.}$(g cm^{-3})	1.538
Completeness	0.999
Reflections collected	87671
Independent reflections	12264
R(int.)	0.0830

Max. and min. transmission	0.8805 and 0.8118
R_1 [I>2σ (I)][a]	0.1020
wR_2 [I>2σ (I)]	0.2525
R_1 (all data)	0.1311
wR_2 (all data)[b]	0.2711
GooF on F^2 [c]	1.105
Largest diff. peak and hole (e.Å^{-3})	1.311 and -1.153
Solvent System	$CHCl_3$/MeOH
CCDC No.	1406270

[a]$R_1 = \sum(\|Fo| - |Fc|)/\sum|Fo|$

[b]$_wR_2 = \{\sum[w(F_o^2 - F_c^2)^2]/\sum[w(F_o^2)^2]\}^{1/2}$; [c]$S = \{\sum[w(F_o^2 - F_c^2)^2]/[(n - p)\}^{1/2}$

References

1. ENHANCE, Oxford Xcalibur Single Crystal Diffractometer, version 1.171.34.40; Oxford Diffraction Ltd: Oxford, U.K. 2006.
2. CrysAlisPro, version 1.171.34.40; Oxford Diffraction Ltd: Oxford, U.K. 2006.
3. A. Altomare, G. Cascarano, C. Giacovazzo, A. Guagliardi, M. C. Burla, G. olidori, M. J. Camalli, *Appl. Crystallogr.* 1994, **27**, 435.
4. SHELXL-97 and SHELXS-97, program for refinement of crystal structures from diffraction data, University of Goettingen, Goettingen (Germany); G. Sheldrick, T. Schneider, *Methods Enzymol.* 1997, **277**, 319.
5. L. J. Farrugia, WinGX Version 1.80.05, An integrated system of Windows Programs for the Solution, Refinement and Analysis of Single Crystal X-Ray Diffraction Data; Department of Chemistry, University of Glasgow, 1997-2009.