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Supplementary Information

Synthesis and Properties of 2'-Deoxyuridine Analogues Bearing Various Azobenzene Derivatives at the C5 Position *Chemosensors* 2015, *3*, 36-54

Shohei Mori [1], Kunihiko Morihiro [1,2,*], Yuuya Kasahara [1,2], Shin-ichi Tsunoda [2] and Satoshi Obika [1,2,*]

[1] Graduate School of Pharmaceutical Sciences, Osaka University, 1-6 Yamadaoka, Suita, Osaka 565-0871, Japan; E-Mails: mori-s@phs.osaka-u.ac.jp (S.M.); y-kasahara@nibio.go.jp (Y.K.)

[2] National Institute of Biomedical Innovation (NIBIO), 7-6-8 Saito-Asagi, Osaka 567-0085, Japan; E-Mail: tsunoda@nibio.go.jp

***** Authors to whom correspondence should be addressed; E-Mails: k-morihiro@nibio.go.jp (K.M.); obika@phs.osaka-u.ac.jp (S.O.); Tel.: +81-72-641-9882 (K.M.); +81-6-6879-8200 (S.O.); Fax: +81-72-641-9884 (K.M.); +81-6-6879-8204 (S.O.).

1. ^{1}H, ^{13}C and ^{31}P Spectra of New Compounds

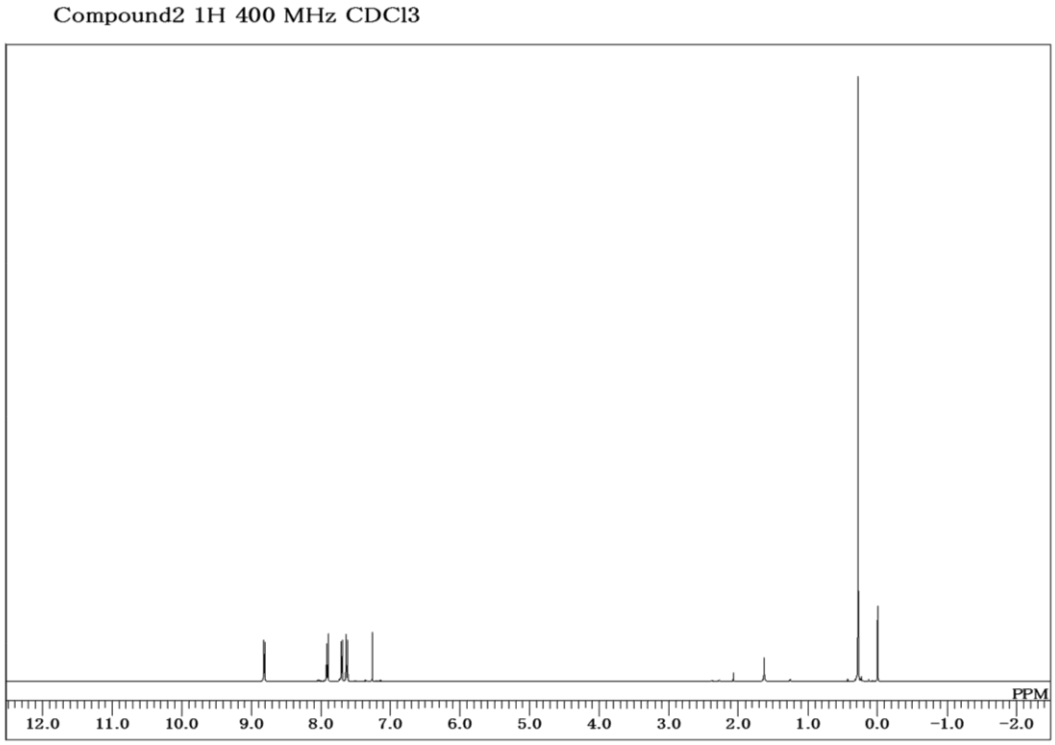

Figure S1. ^{1}H-NMR spectrum of compound 2.

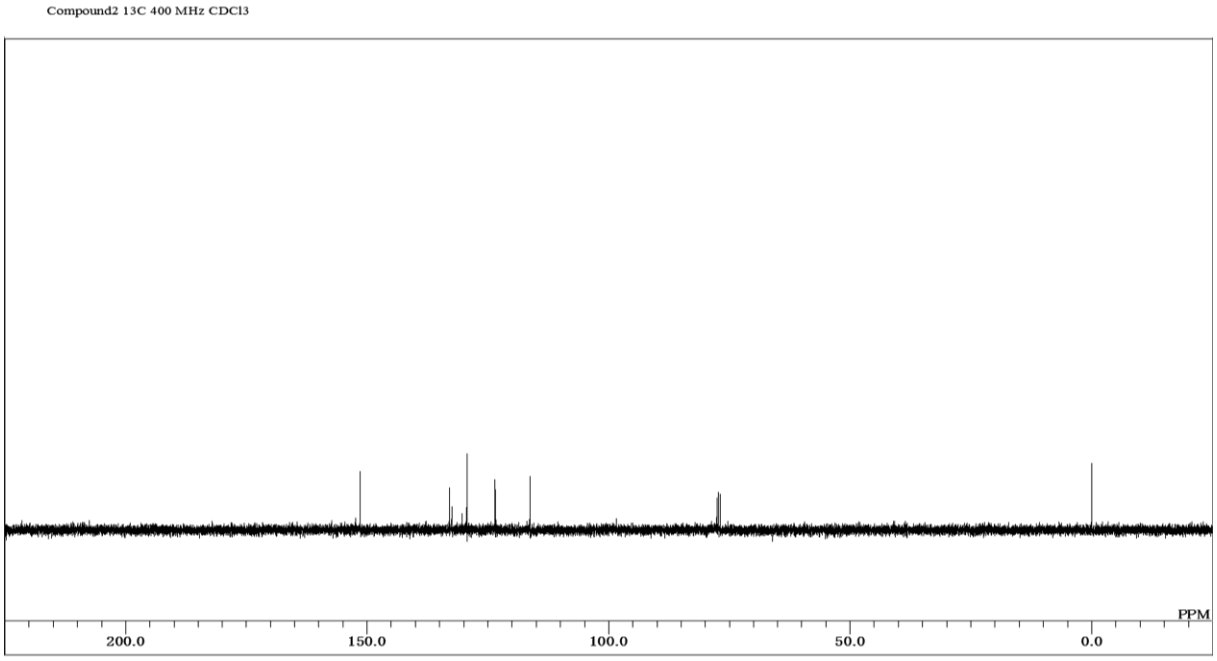

Figure S2. ^{13}C-NMR spectrum of compound 2.

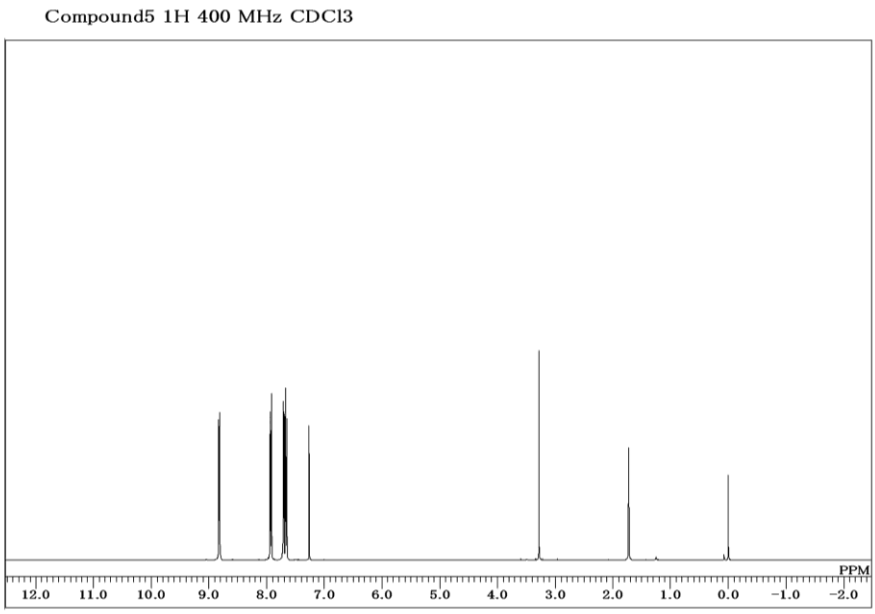

Figure S3. ^{1}H-NMR spectrum of compound 5.

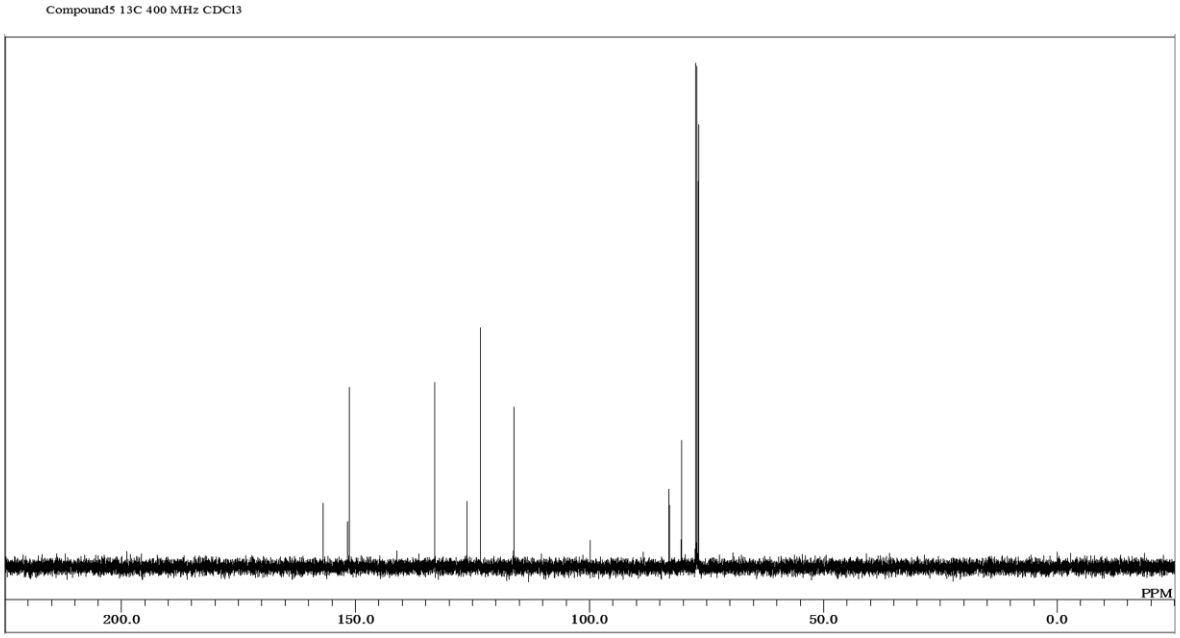

Figure S4. ^{13}C-NMR spectrum of compound 5.

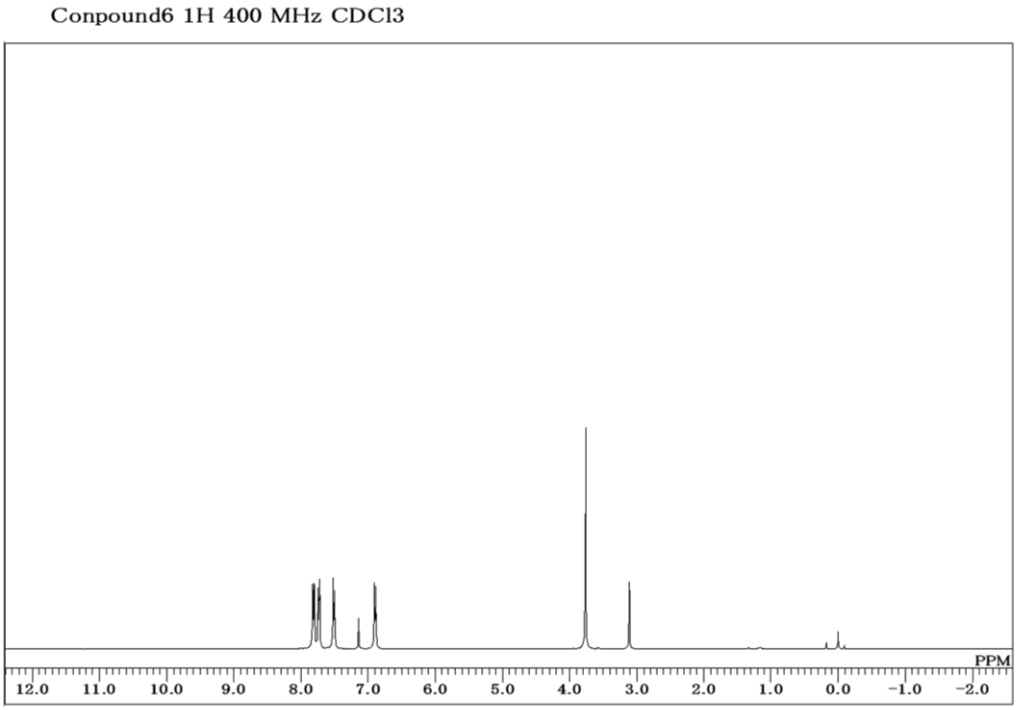

Figure S5. ^{1}H-NMR spectrum of compound 6.

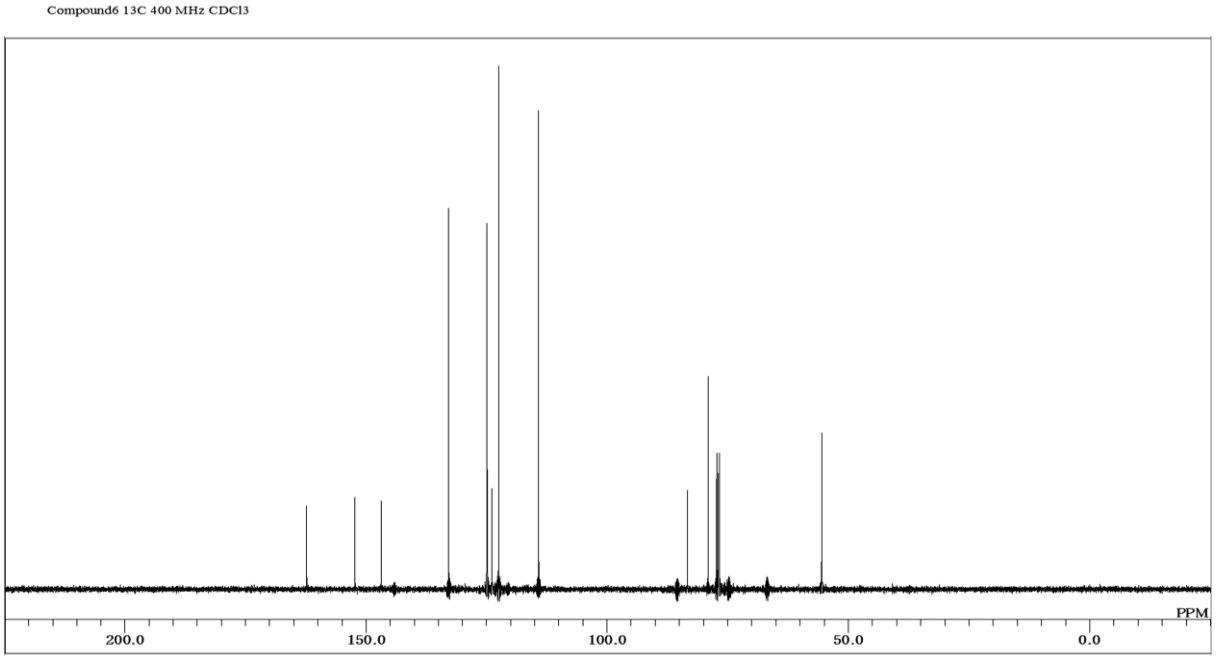

Figure S6. ^{13}C-NMR spectrum of compound 6.

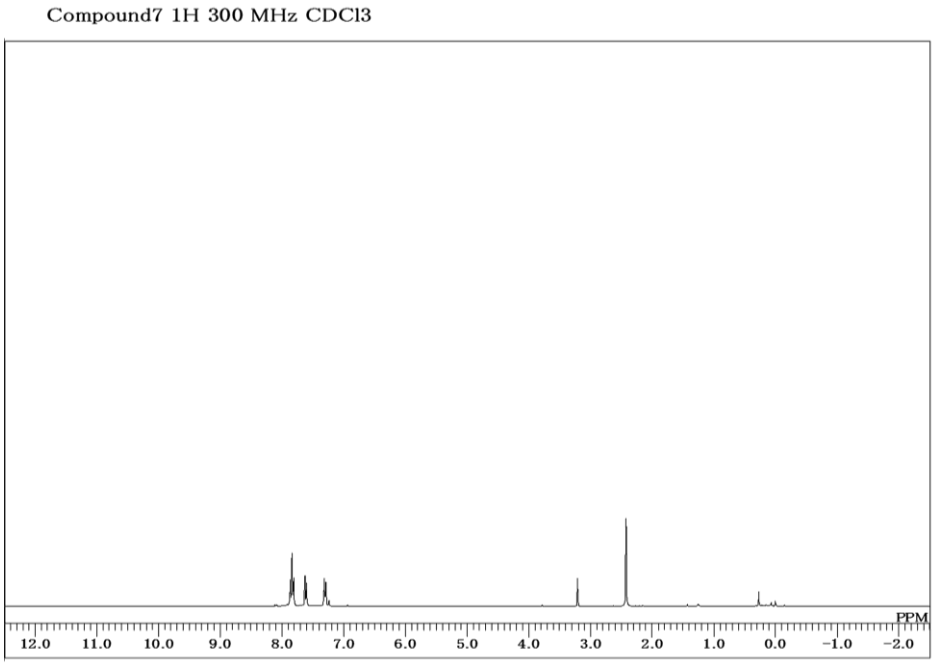

Figure S7. ^{1}H-NMR spectrum of compound 7.

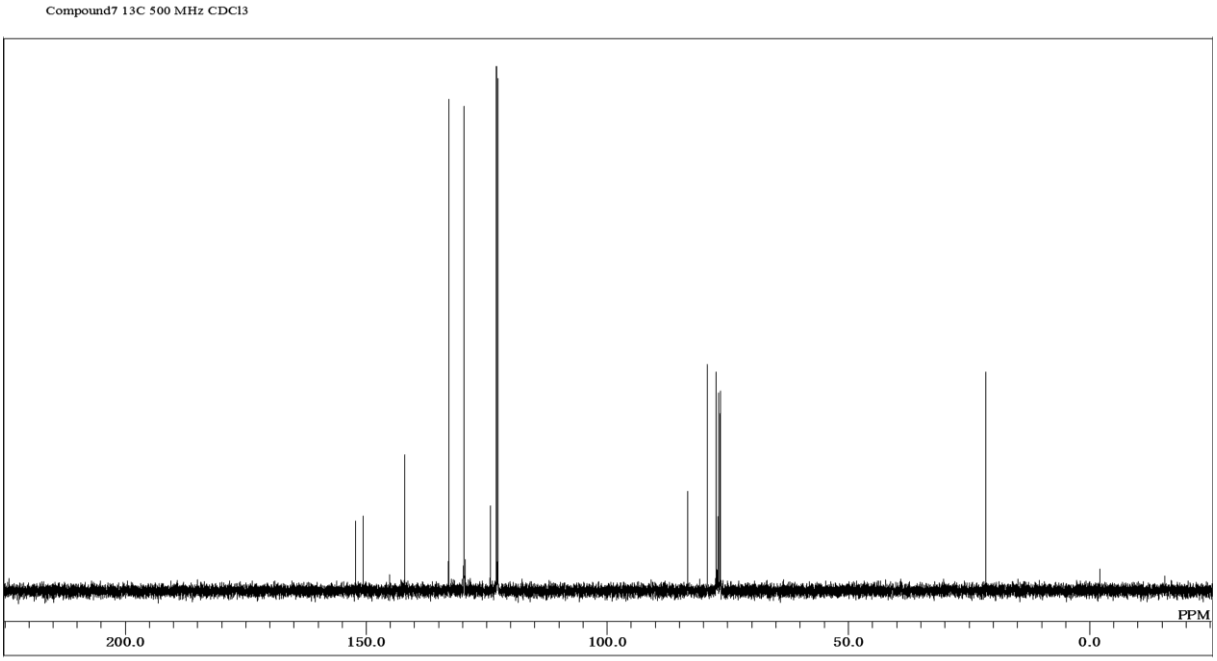

Figure S8. ^{13}C-NMR spectrum of compound 7.

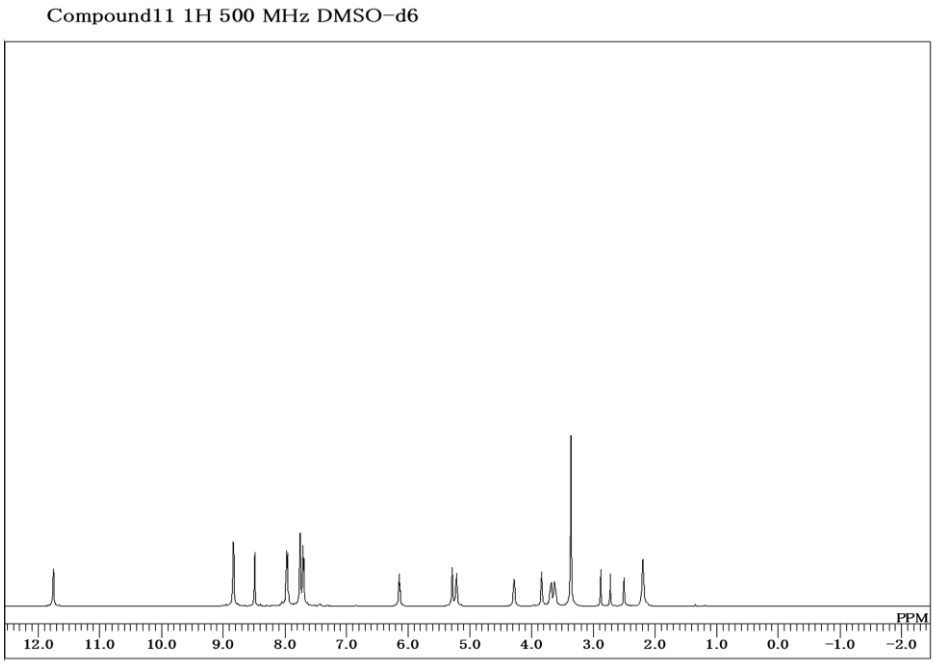

Figure S9. ^{1}H-NMR spectrum of compound 11.

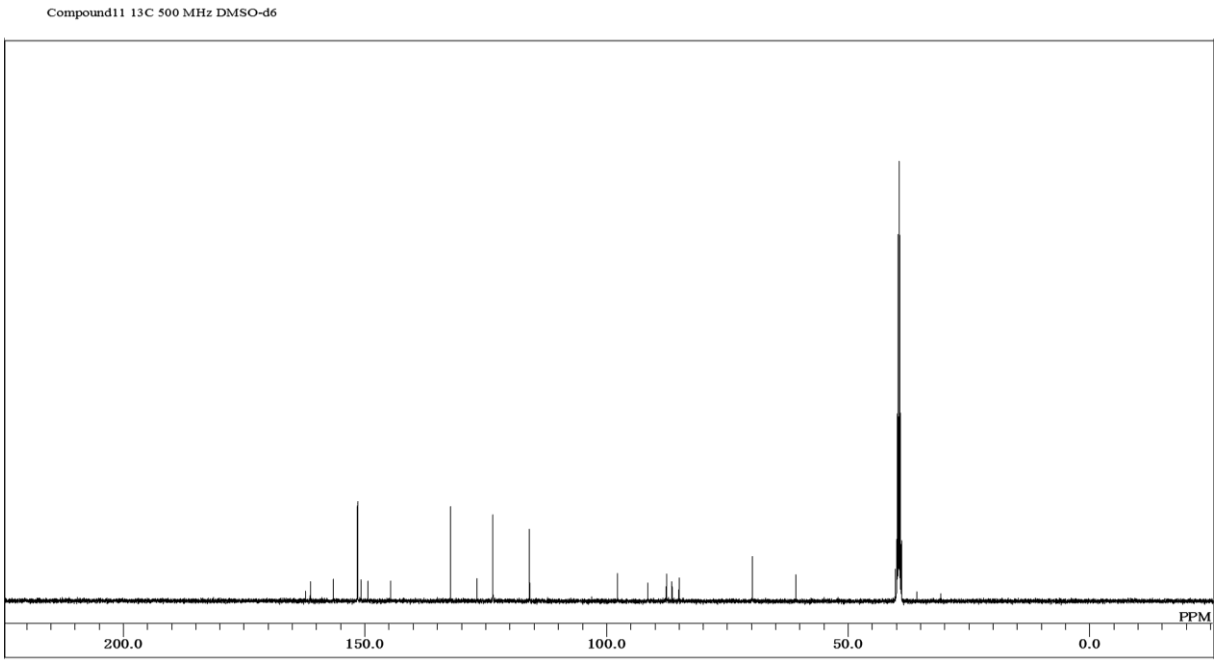

Figure S10. ^{13}C-NMR spectrum of compound 11.

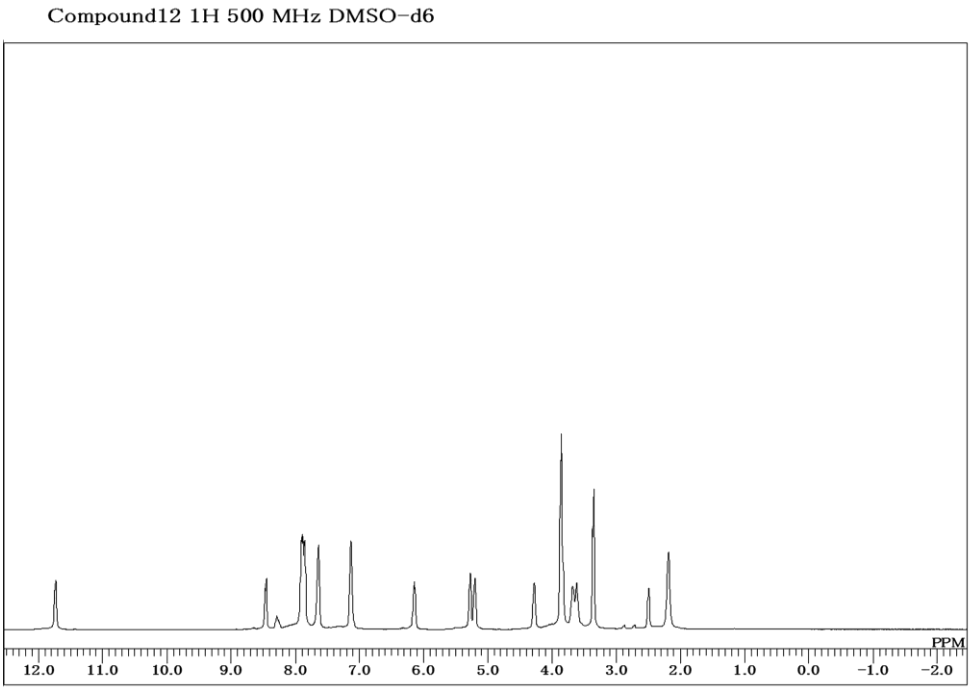

Figure S11. ^{1}H-NMR spectrum of compound 12.

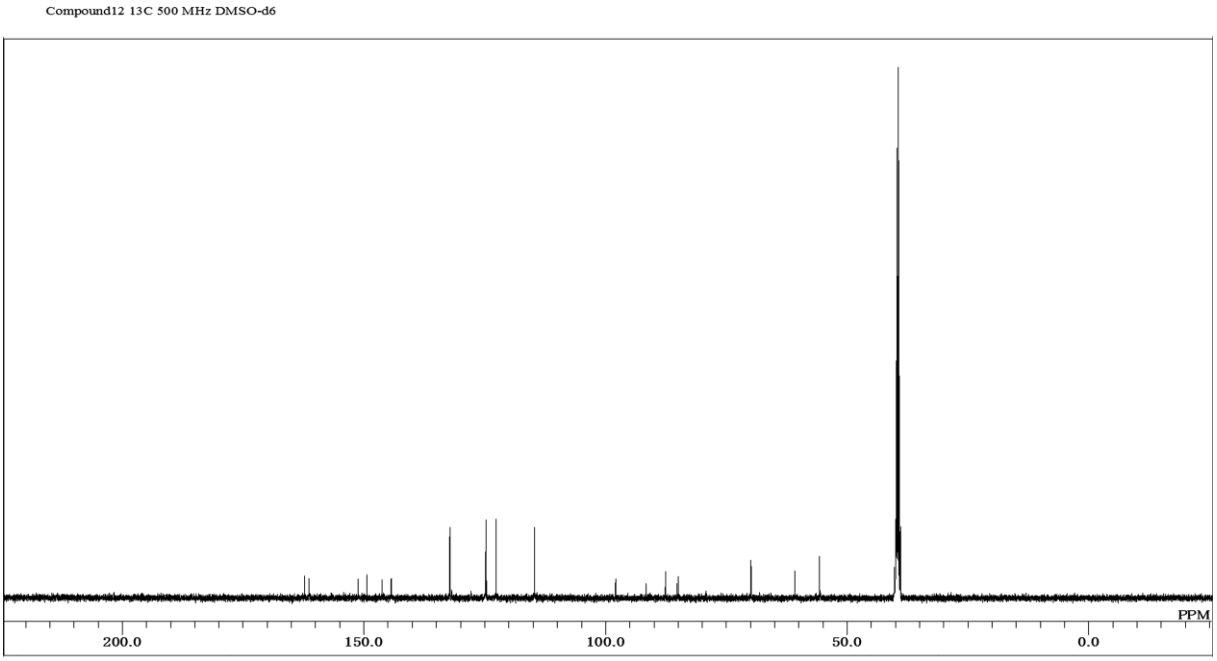

Figure S12. ^{13}C-NMR spectrum of compound 12.

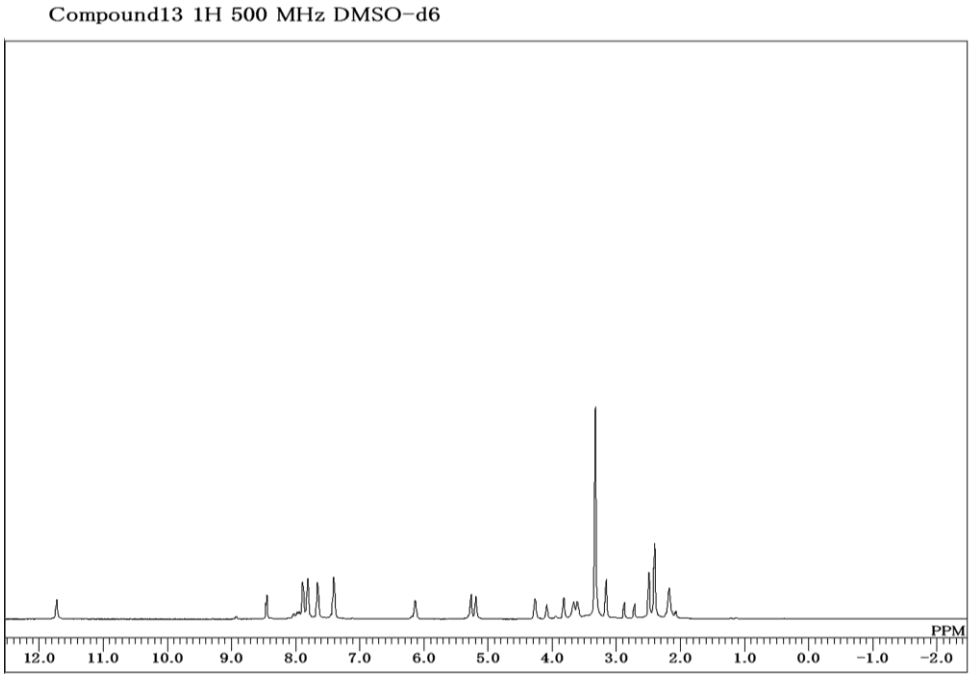

Figure S13. ^{1}H-NMR spectrum of compound 13.

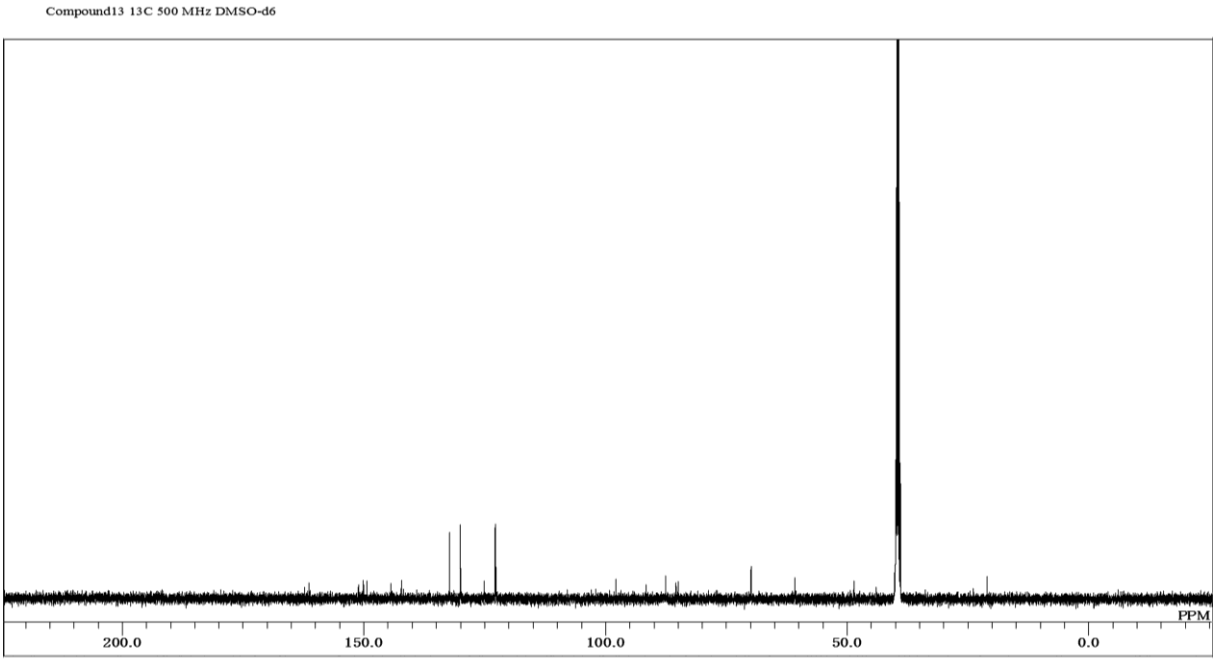

Figure S14. ^{13}C-NMR spectrum of compound 13.

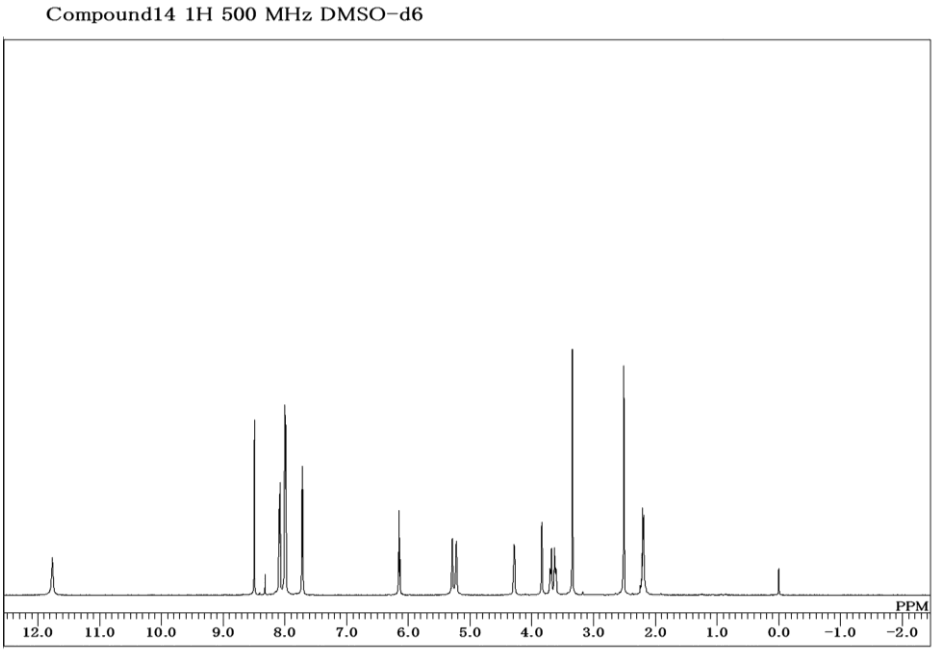

Figure S15. ^{1}H-NMR spectrum of compound 14.

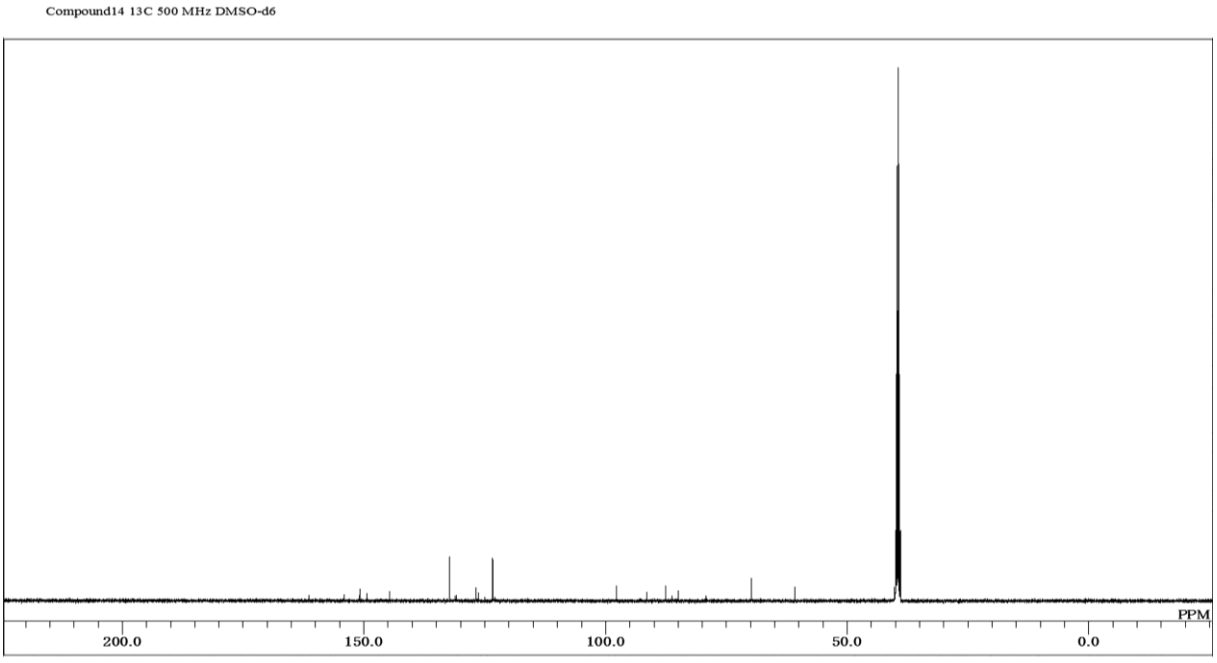

Figure S16. ^{13}C-NMR spectrum of compound 14.

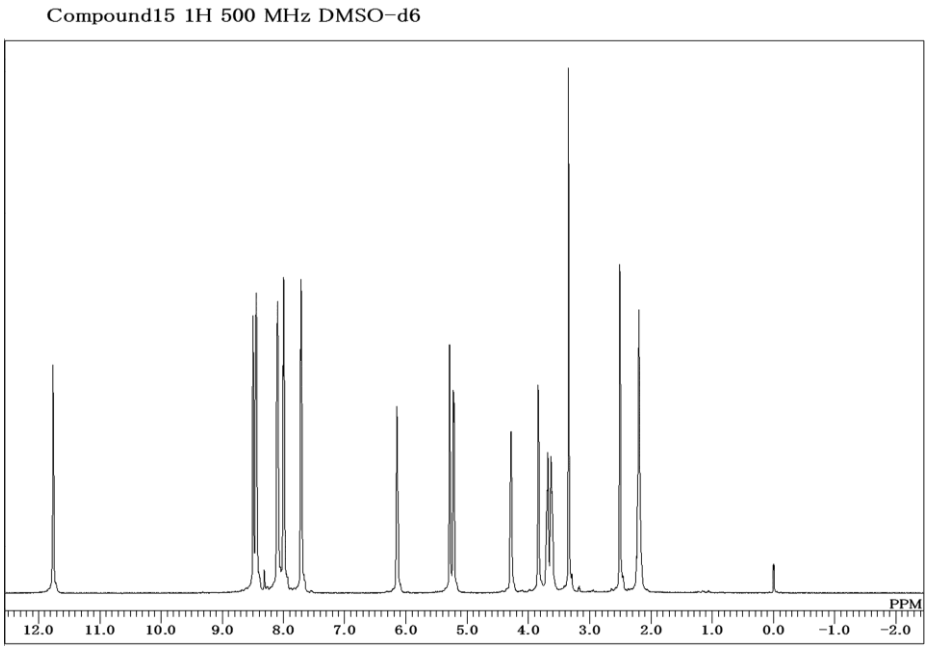

Figure S17. ^{1}H-NMR spectrum of compound 15.

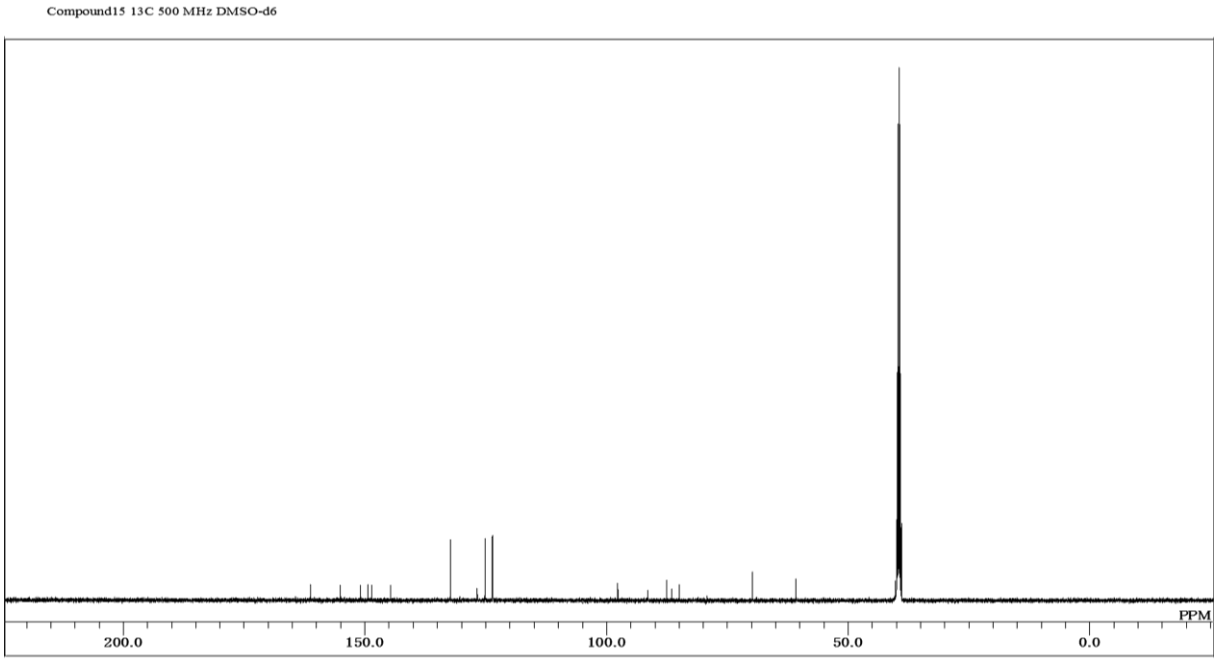

Figure S18. ^{13}C-NMR spectrum of compound 15.

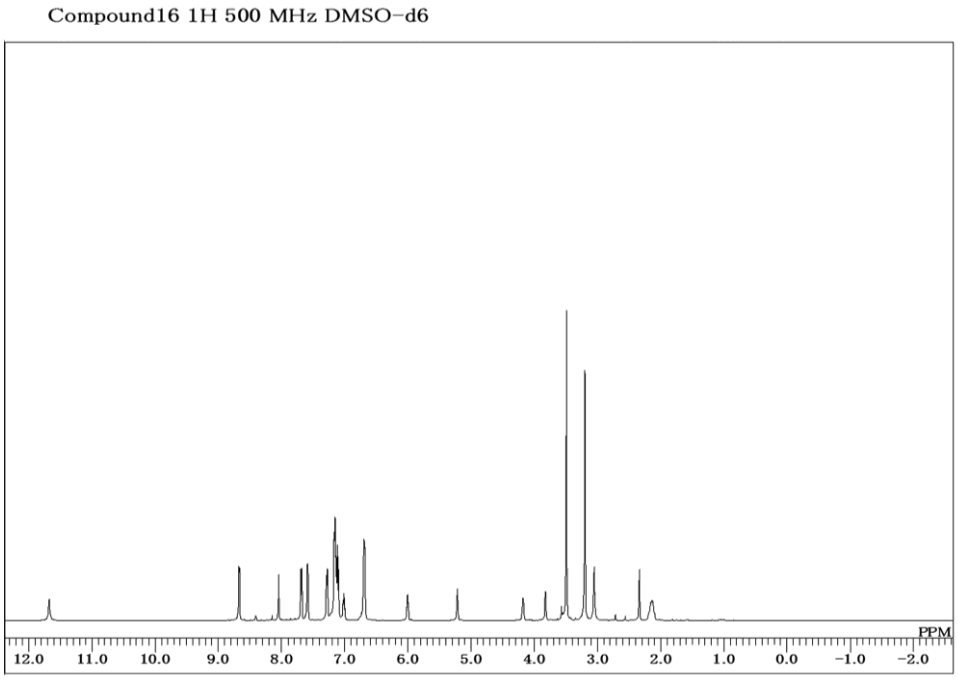

Figure S19. ^{1}H-NMR spectrum of compound 16.

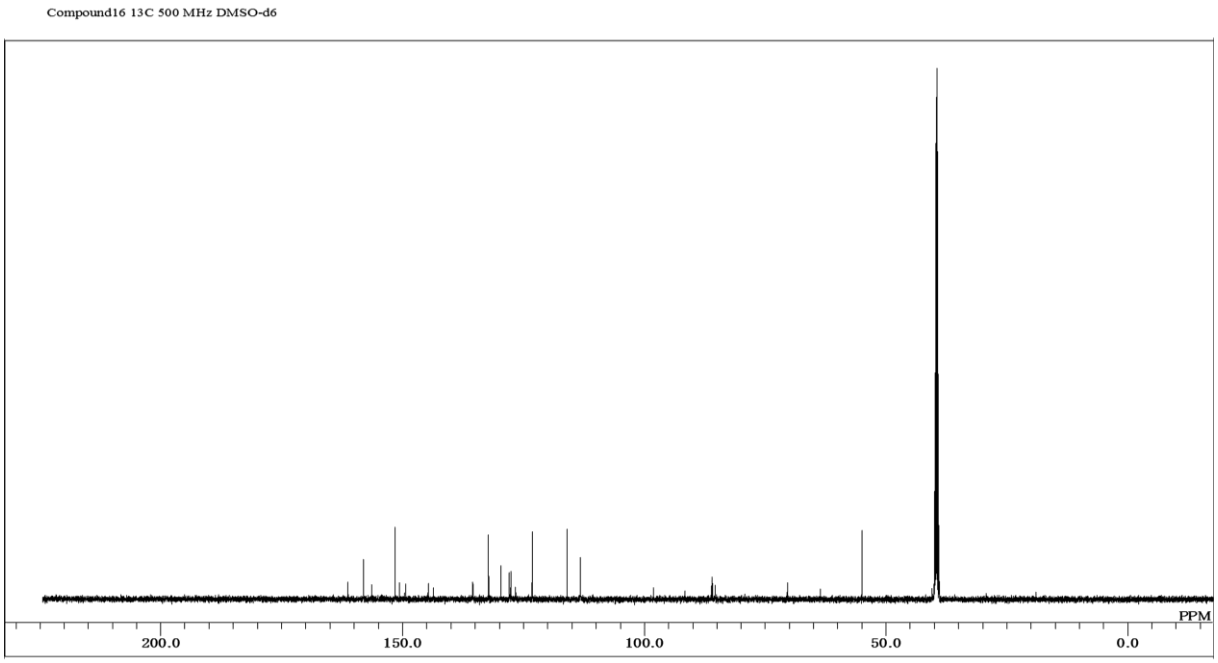

Figure S20. ^{13}C-NMR spectrum of compound 16.

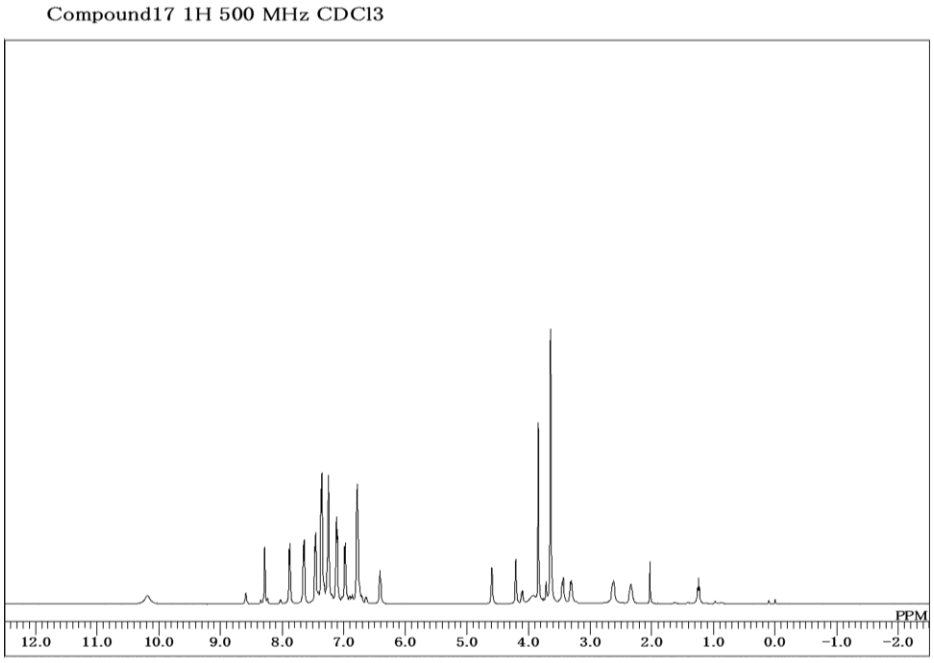

Figure S21. [1]H-NMR spectrum of compound 17.

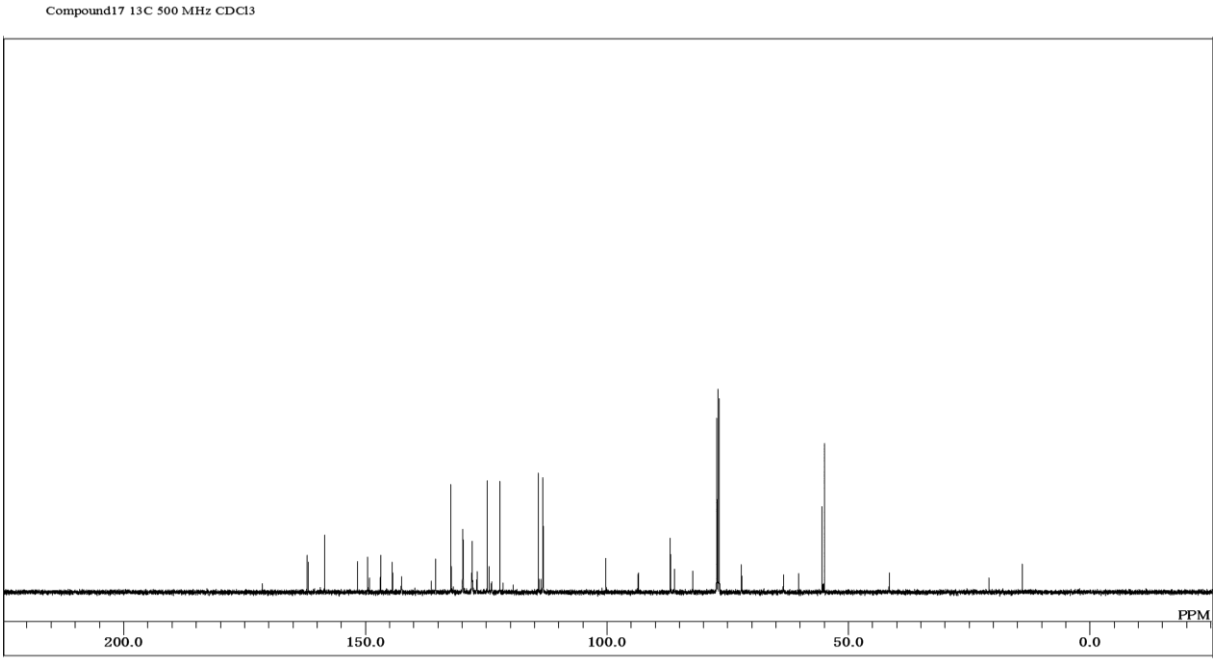

Figure S22. [13]C-NMR spectrum of compound 17.

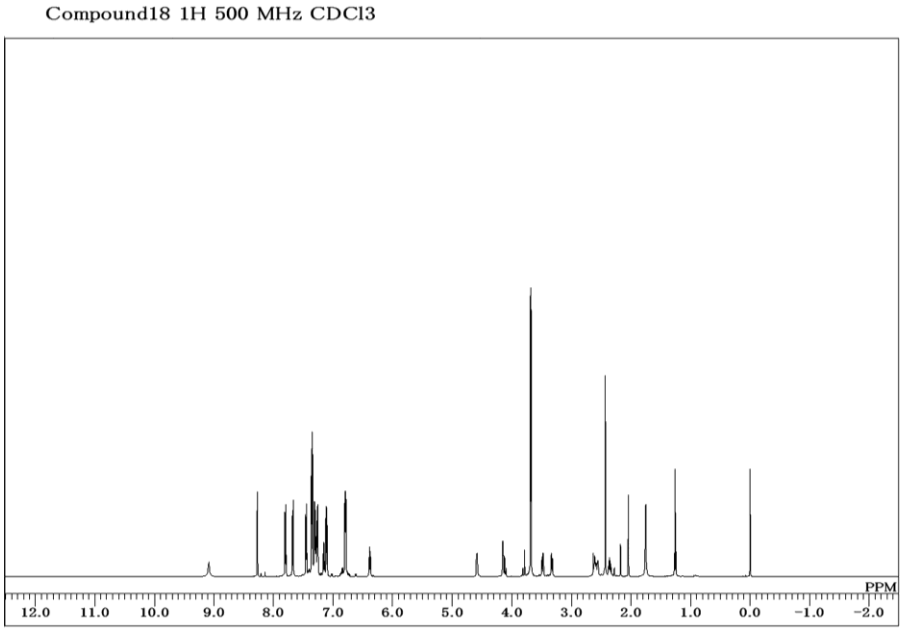

Figure S23. ^{1}H-NMR spectrum of compound 18.

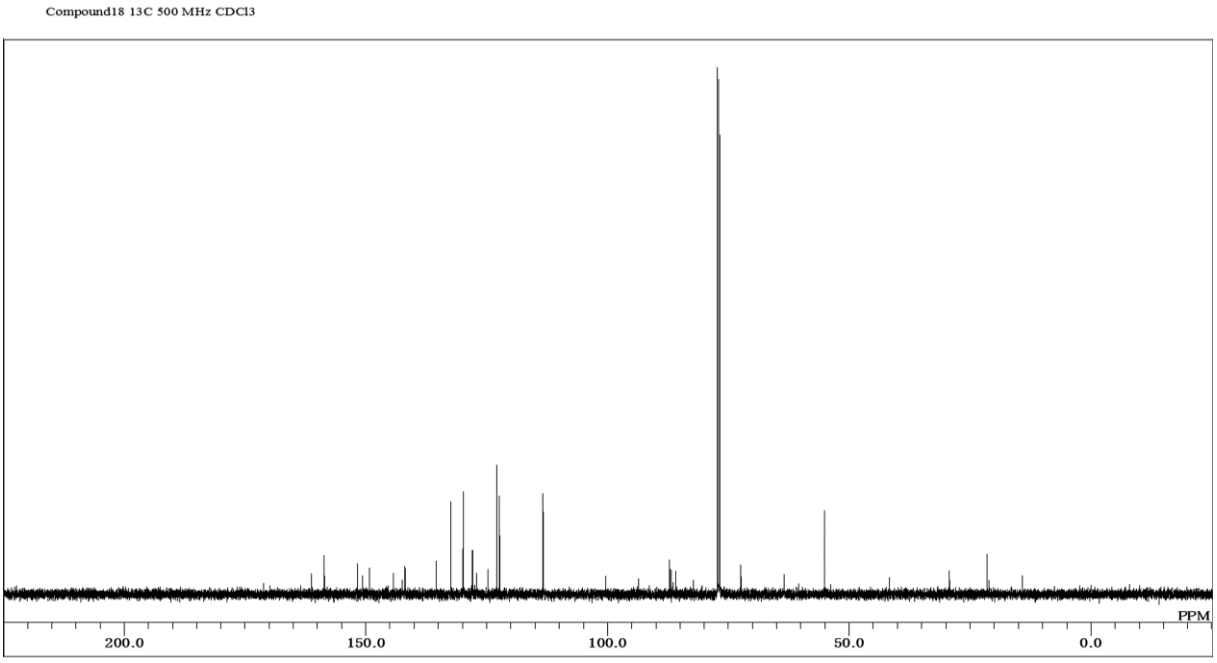

Figure S24. ^{13}C-NMR spectrum of compound 18.

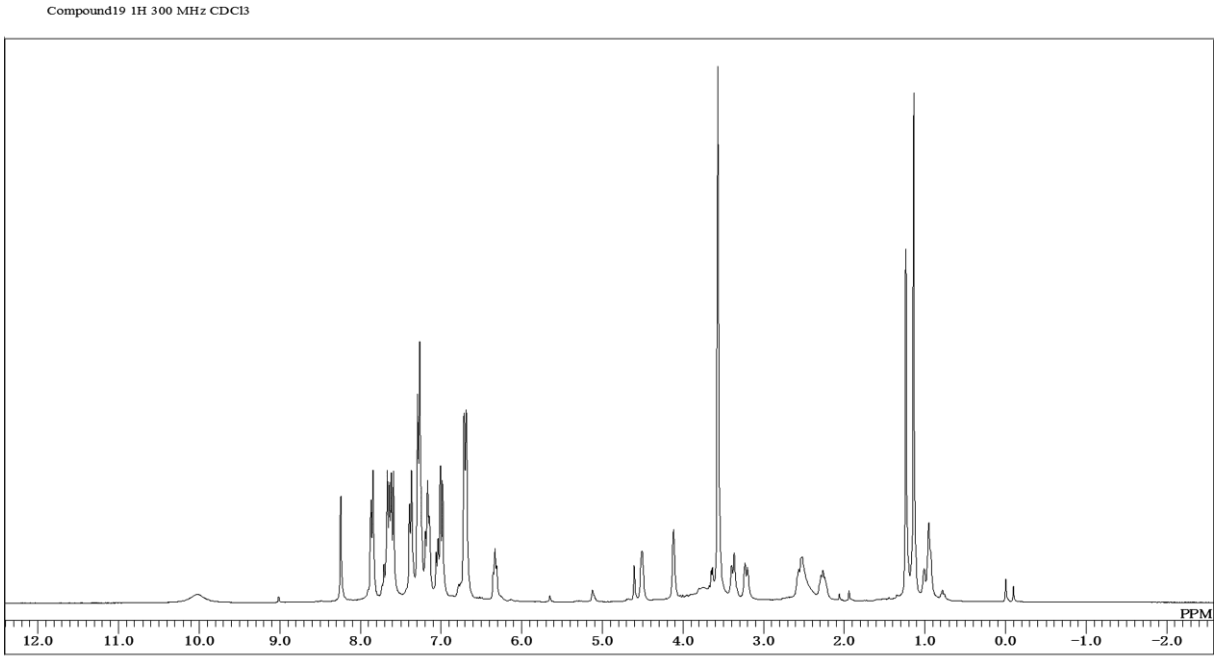

Figure S25. ^{1}H-NMR spectrum of compound 19.

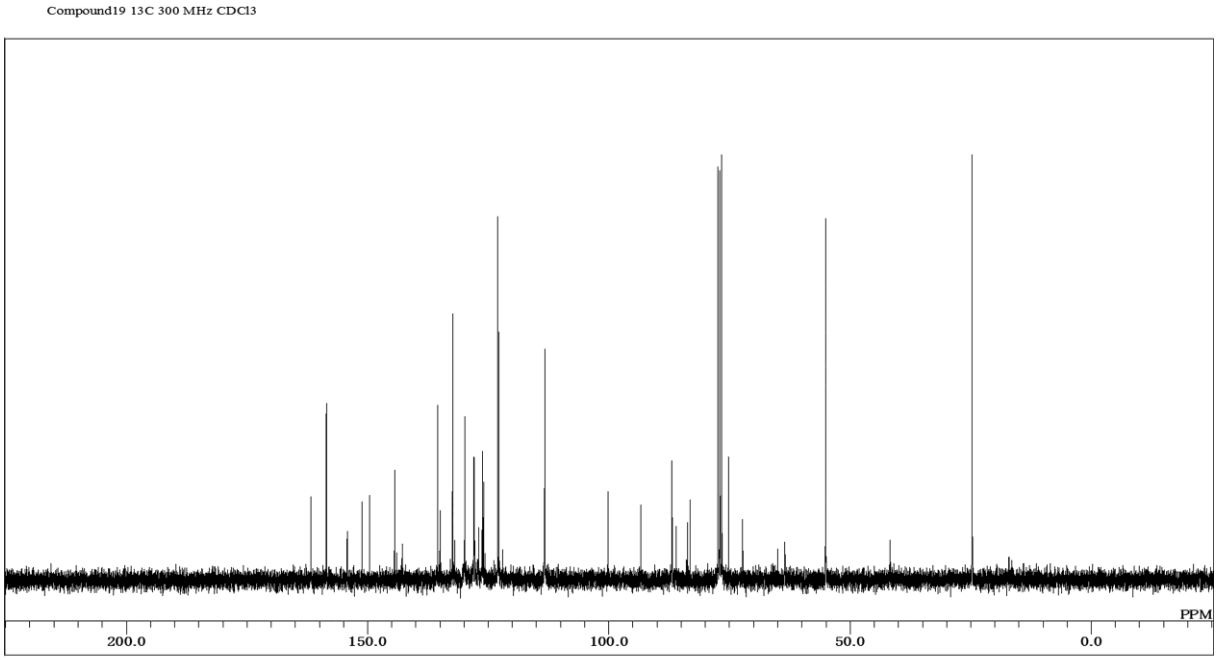

Figure S26. ^{13}C-NMR spectrum of compound 19.

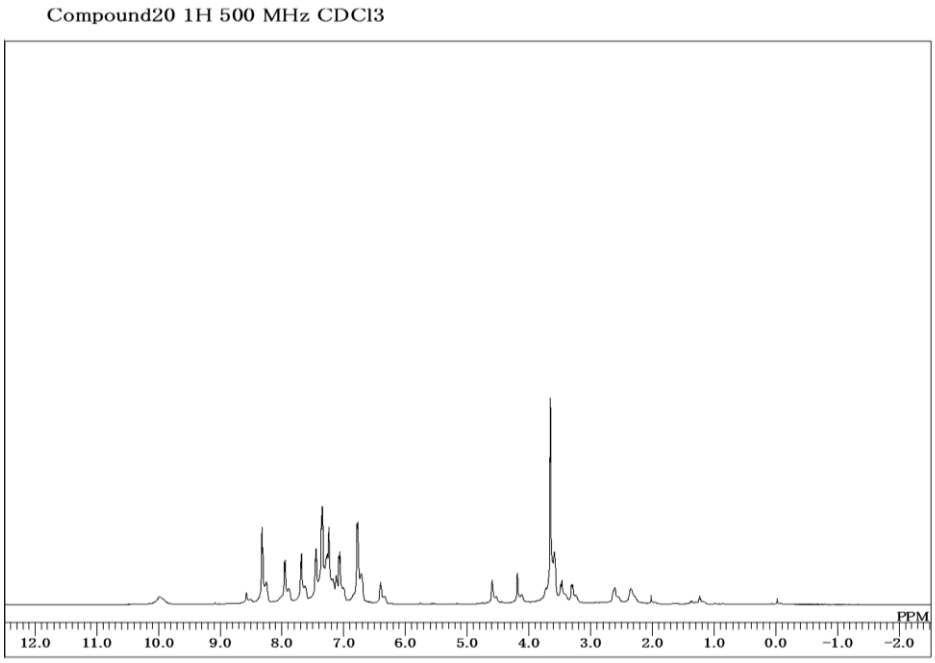

Figure S27. ^{1}H-NMR spectrum of compound 20.

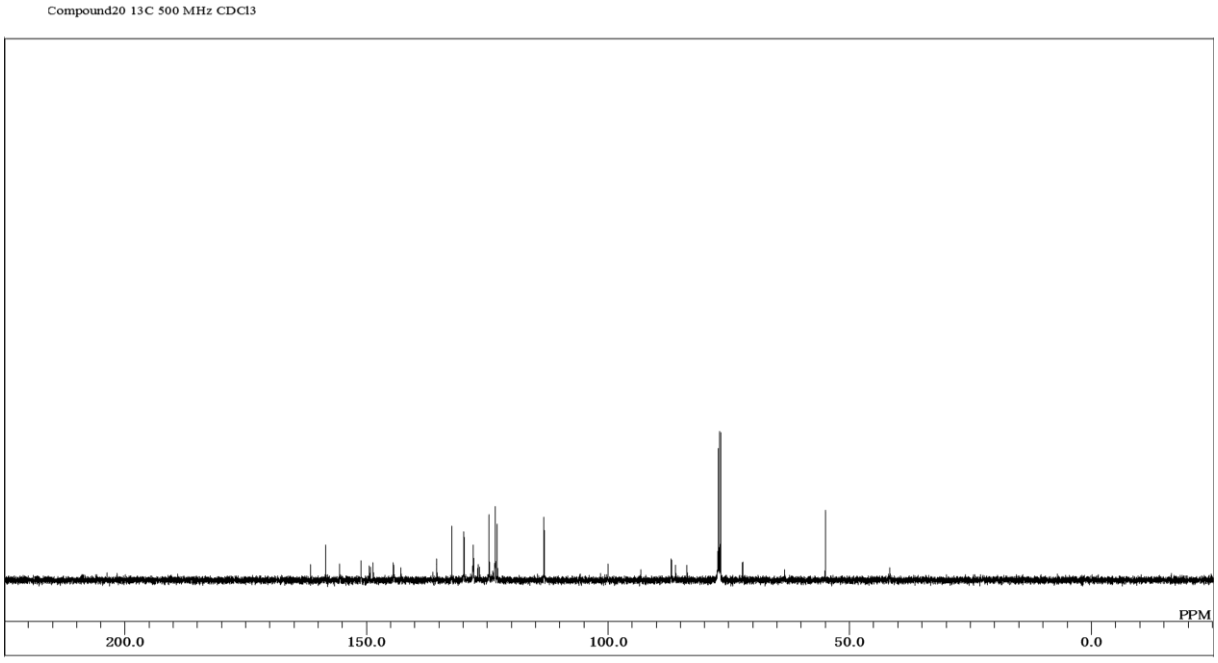

Figure S28. ^{13}C-NMR spectrum of compound 20.

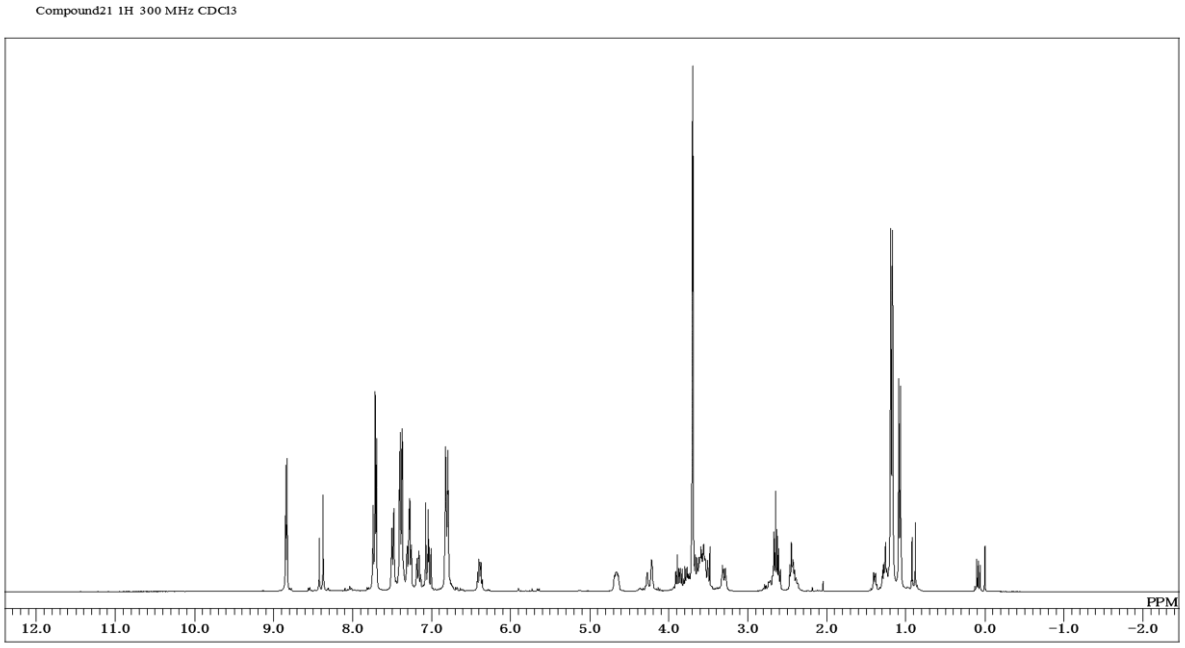

Figure S29. ^{1}H-NMR spectrum of compound 21.

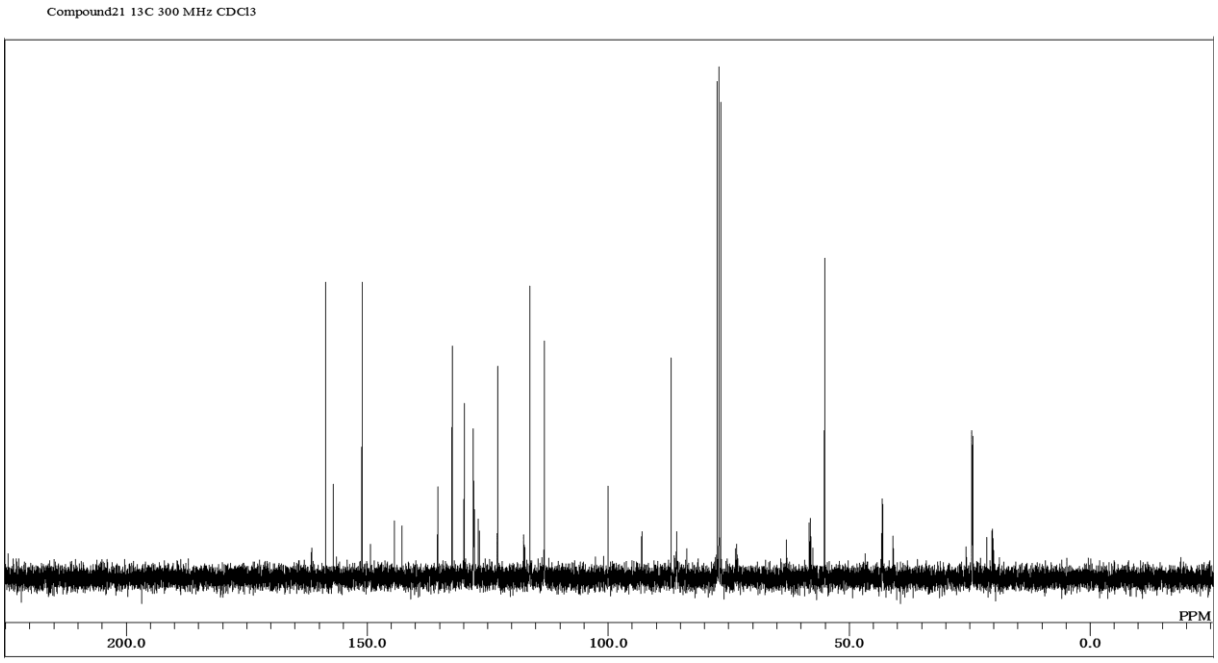

Figure S30. ^{13}C-NMR spectrum of compound 21.

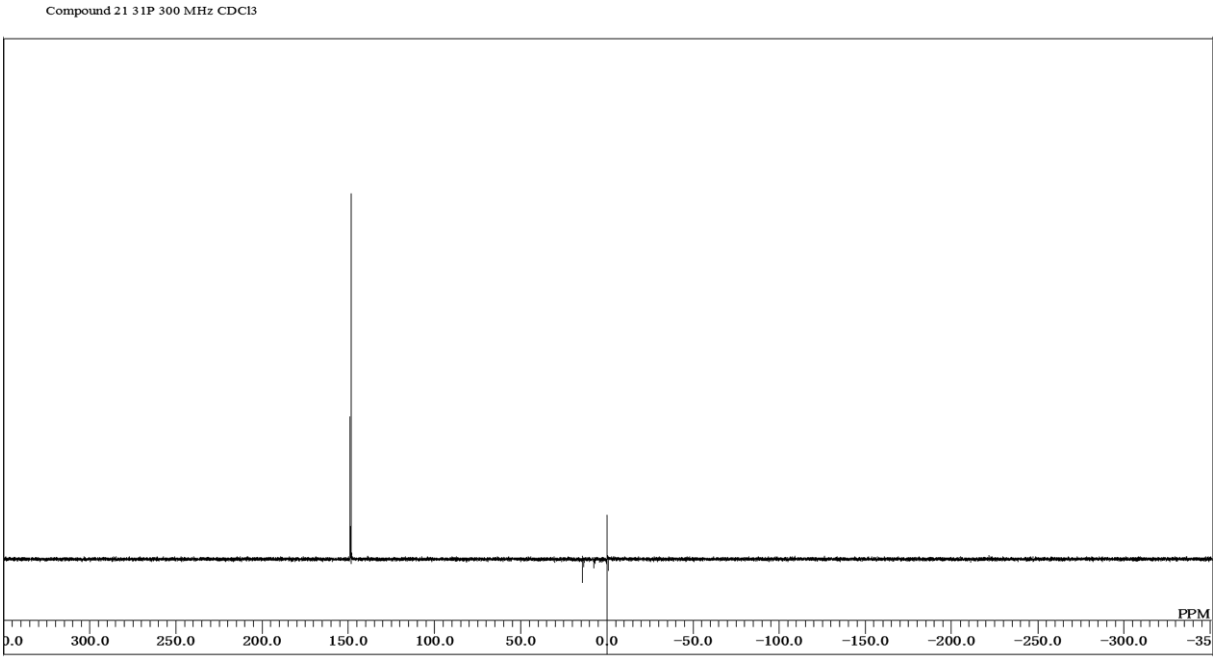

Figure S31. ^{31}P-NMR spectrum of compound 21.

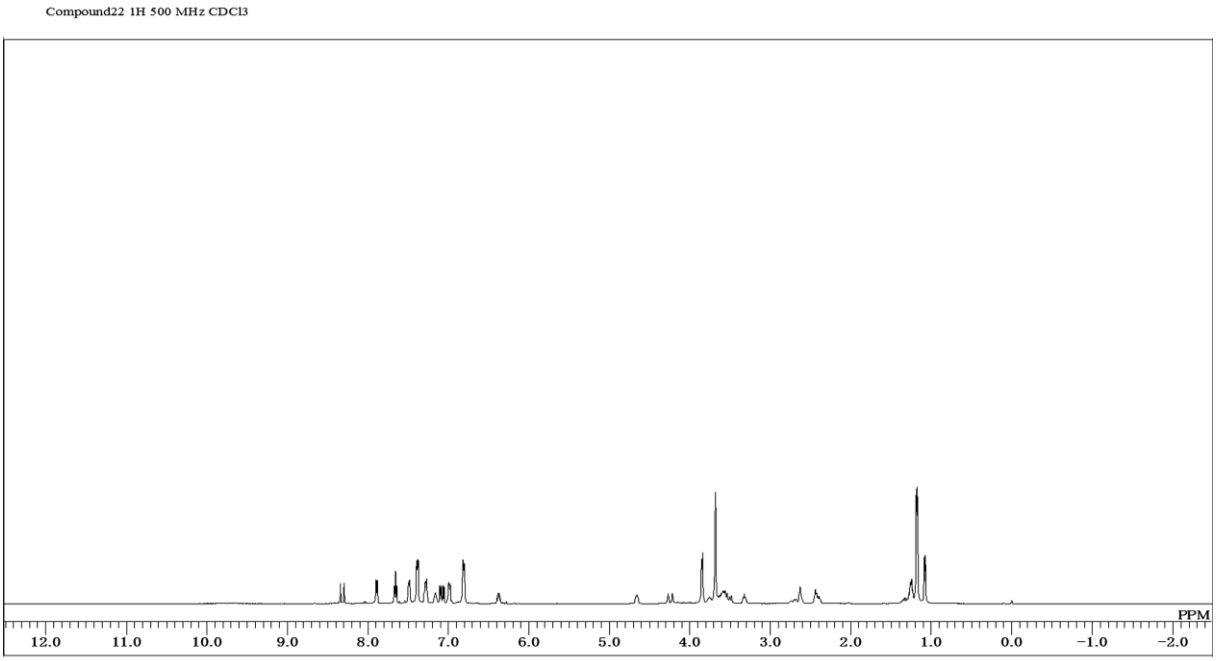

Figure S32. ^{1}H-NMR spectrum of compound 22.

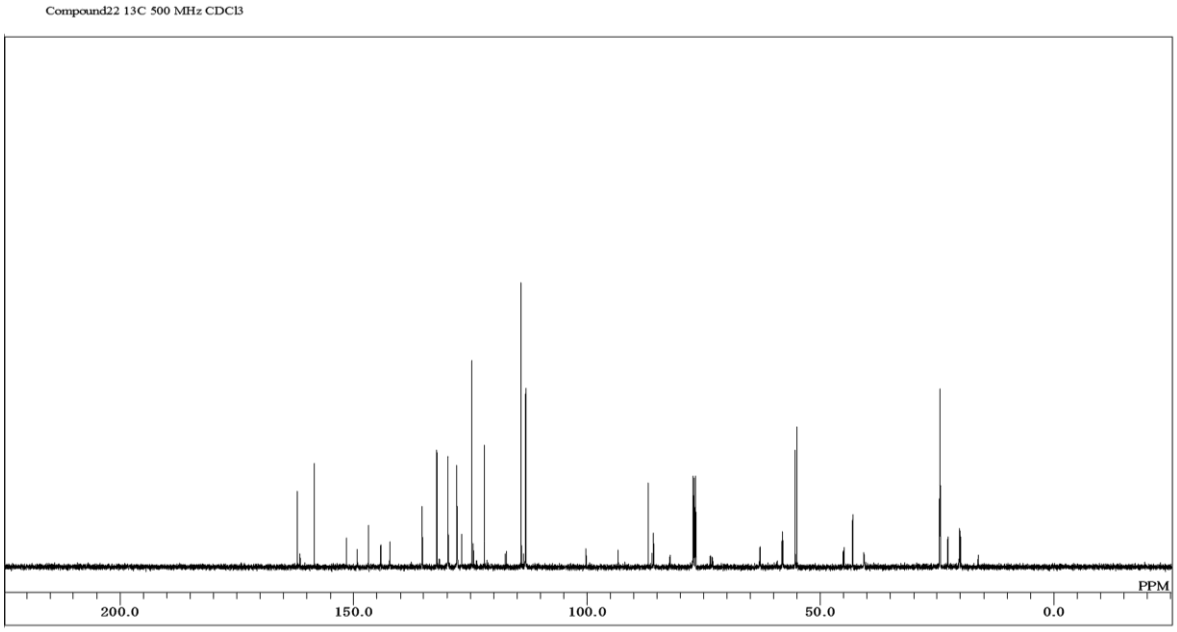

Figure S33. ^{13}C-NMR spectrum of compound 22.

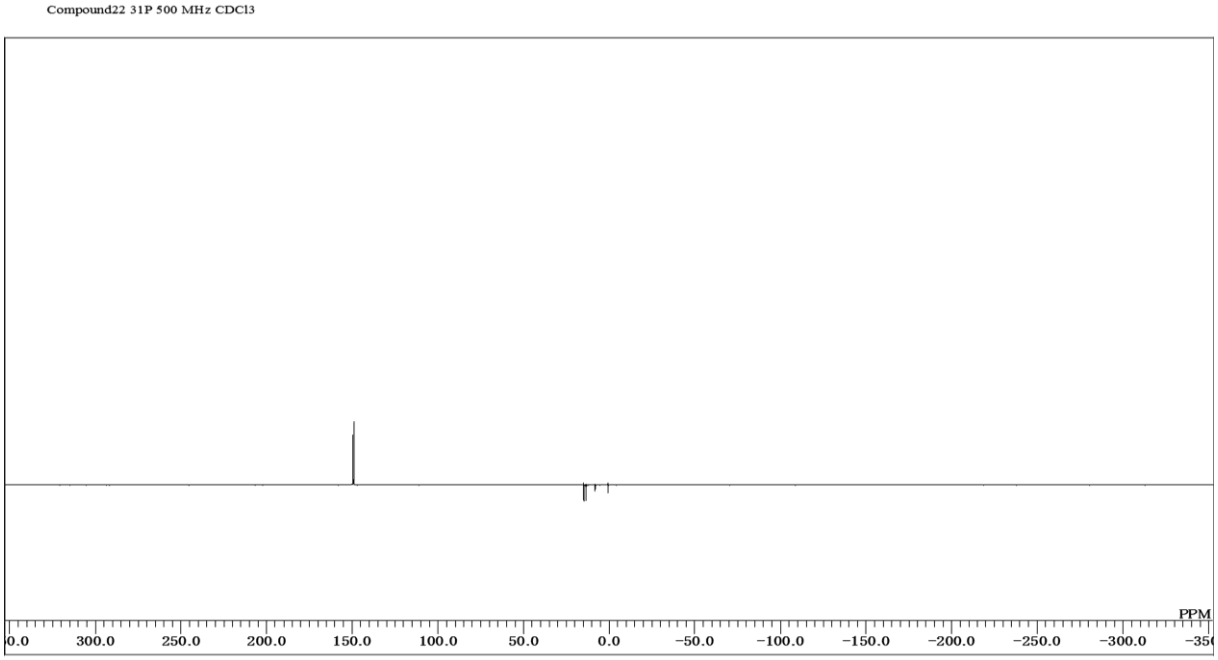

Figure S34. ^{31}P-NMR spectrum of compound 22.

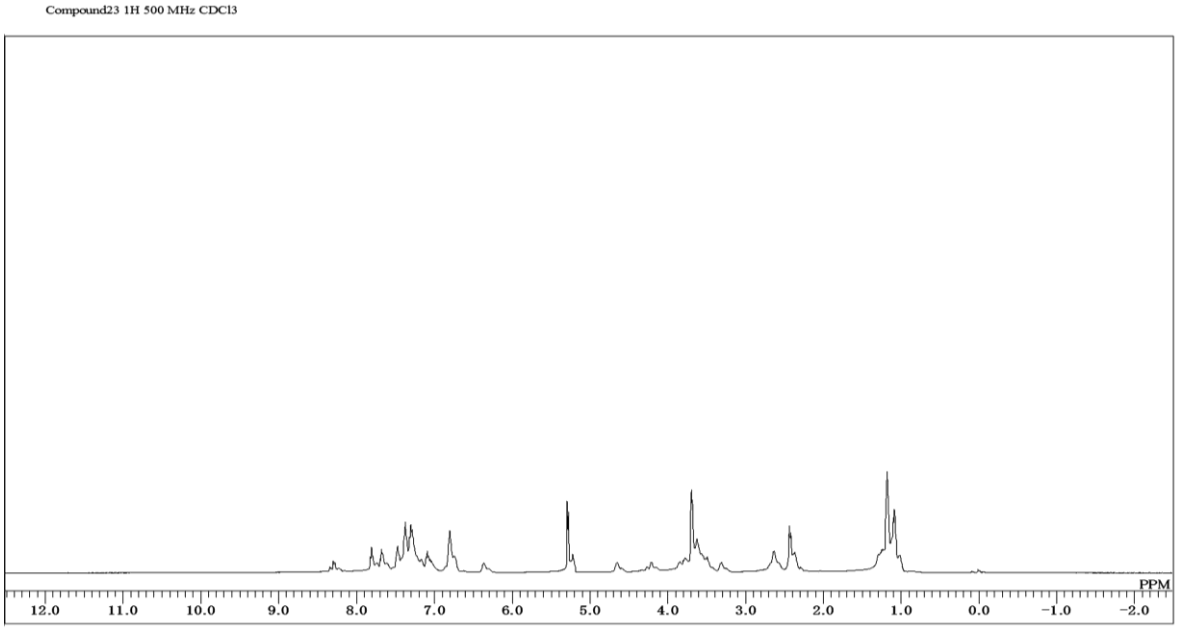

Figure S35. ^{1}H-NMR spectrum of compound 23.

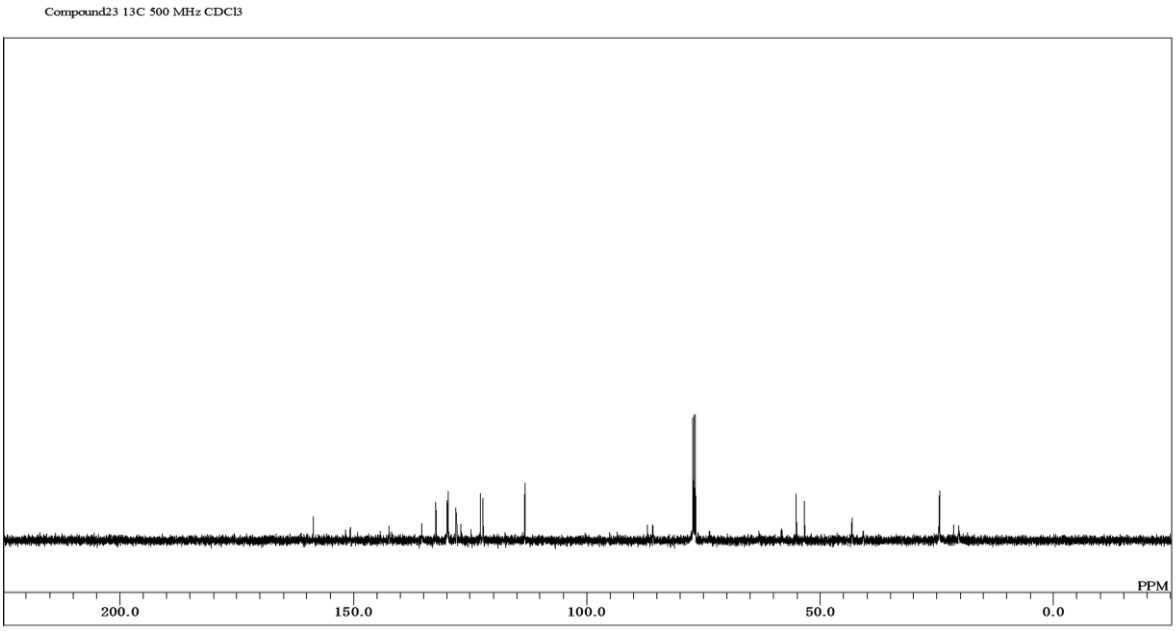

Figure S36. ^{13}C-NMR spectrum of compound 23.

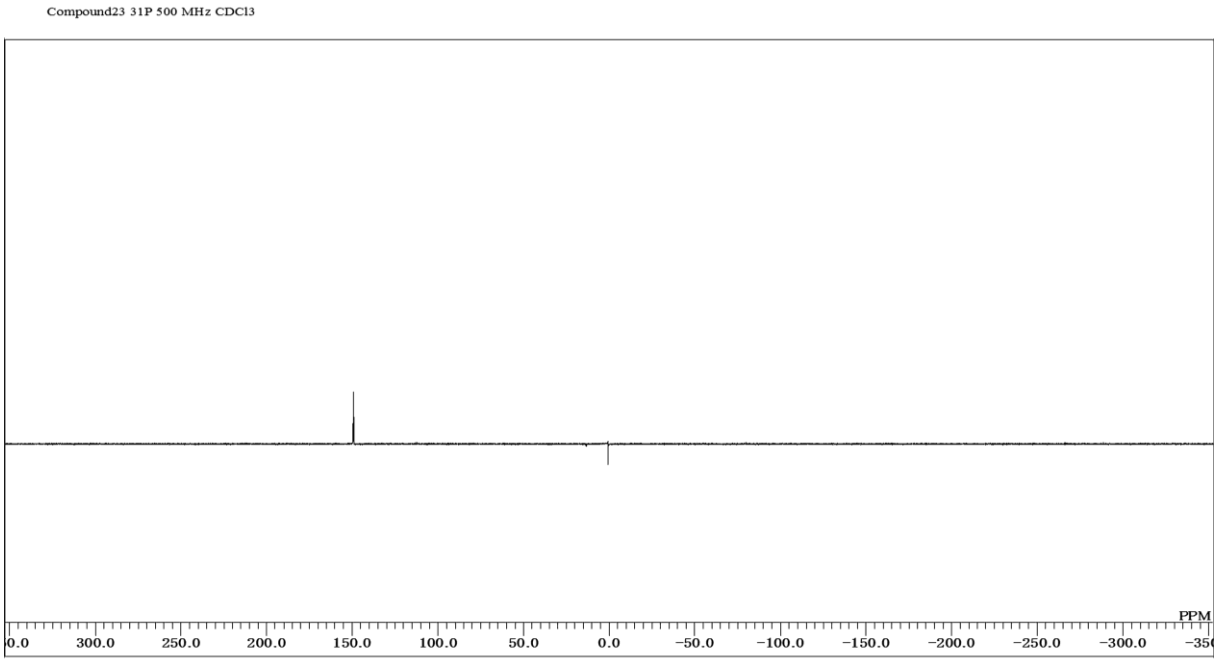

Figure S37. ^{31}P-NMR spectrum of compound 23.

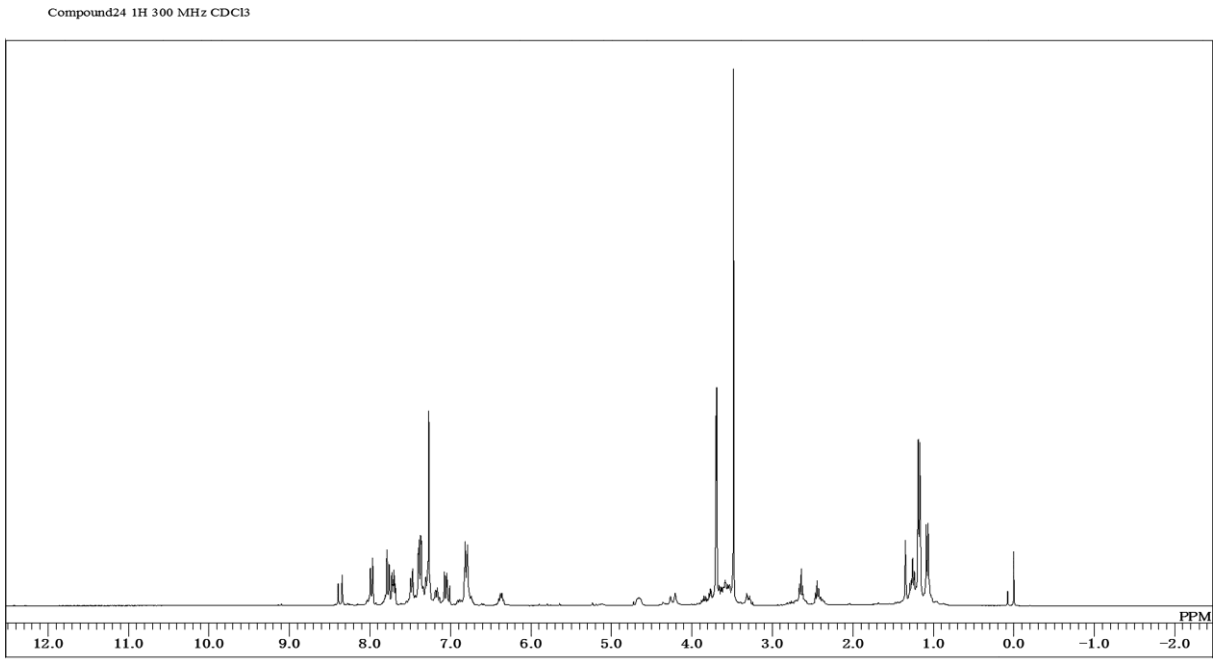

Figure S38. ^{1}H-NMR spectrum of compound 24.

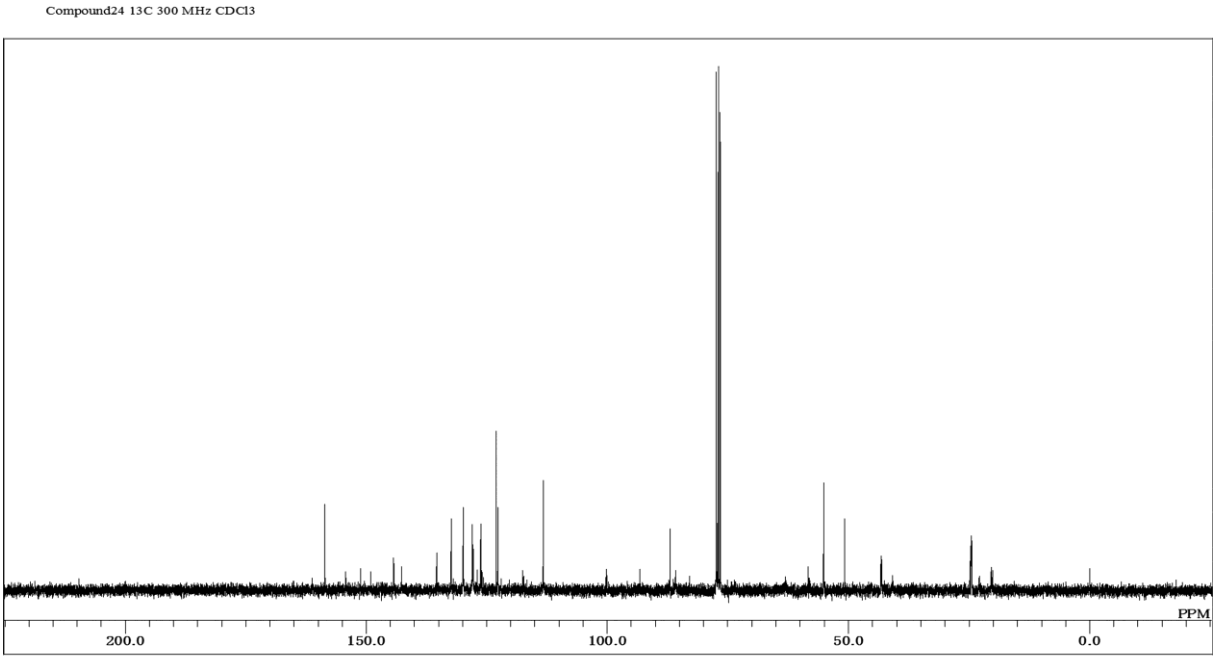

Figure S39. ^{13}C-NMR spectrum of compound 24.

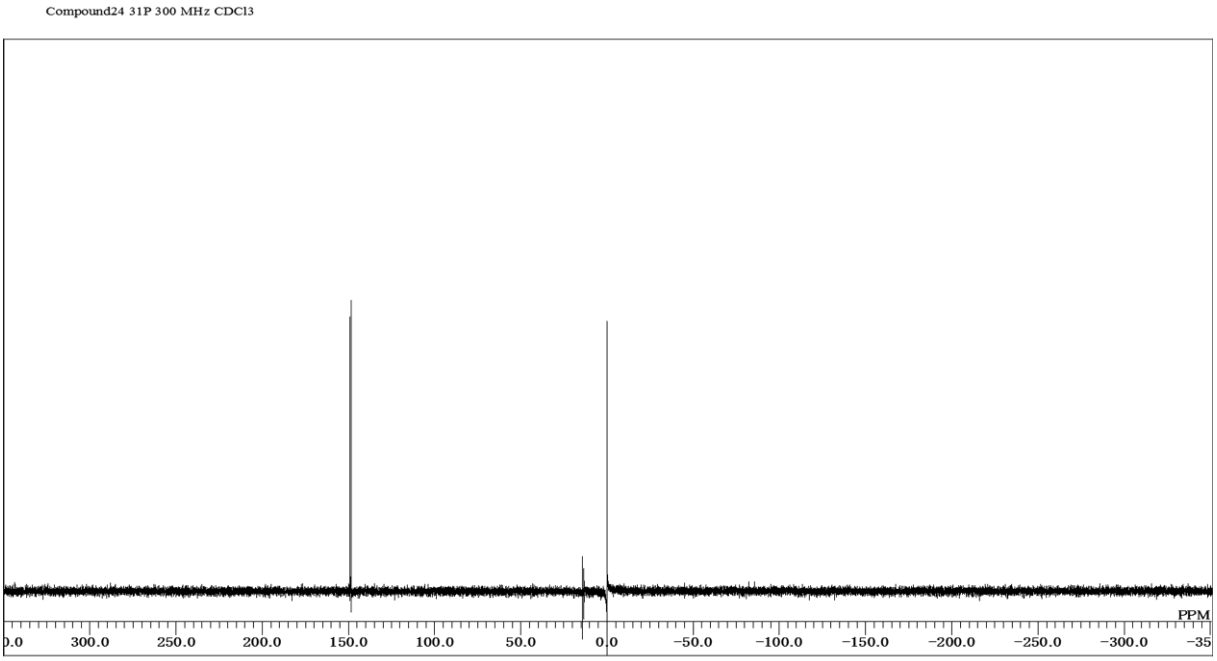

Figure S40. ^{31}P-NMR spectrum of compound 24.

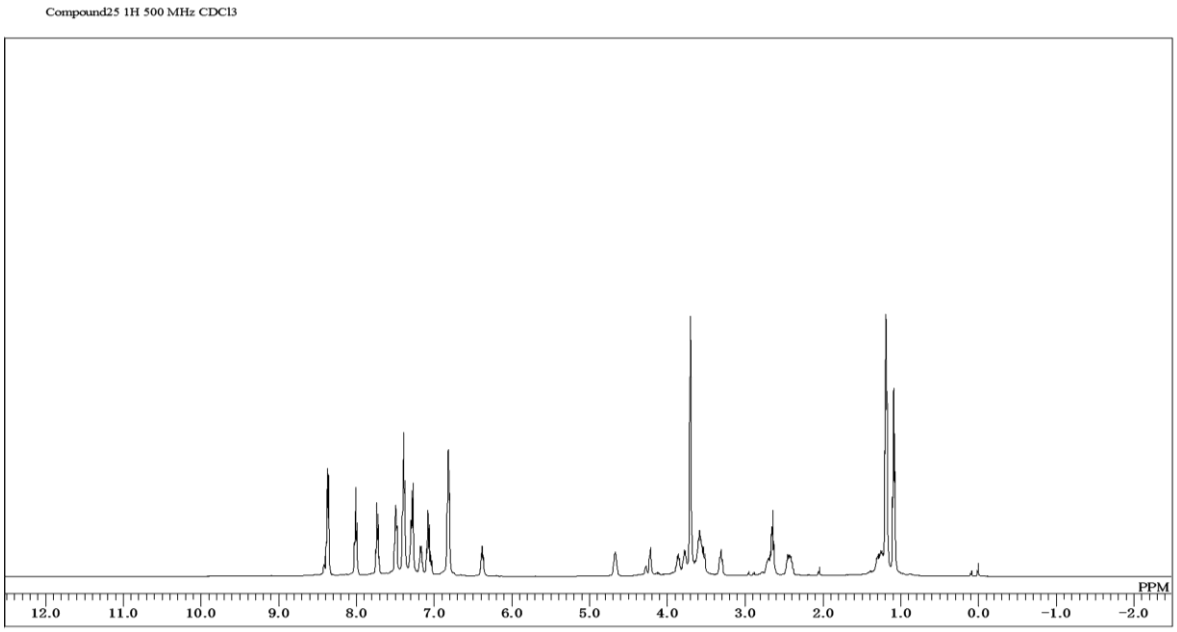

Figure S41. ^{1}H-NMR spectrum of compound 25.

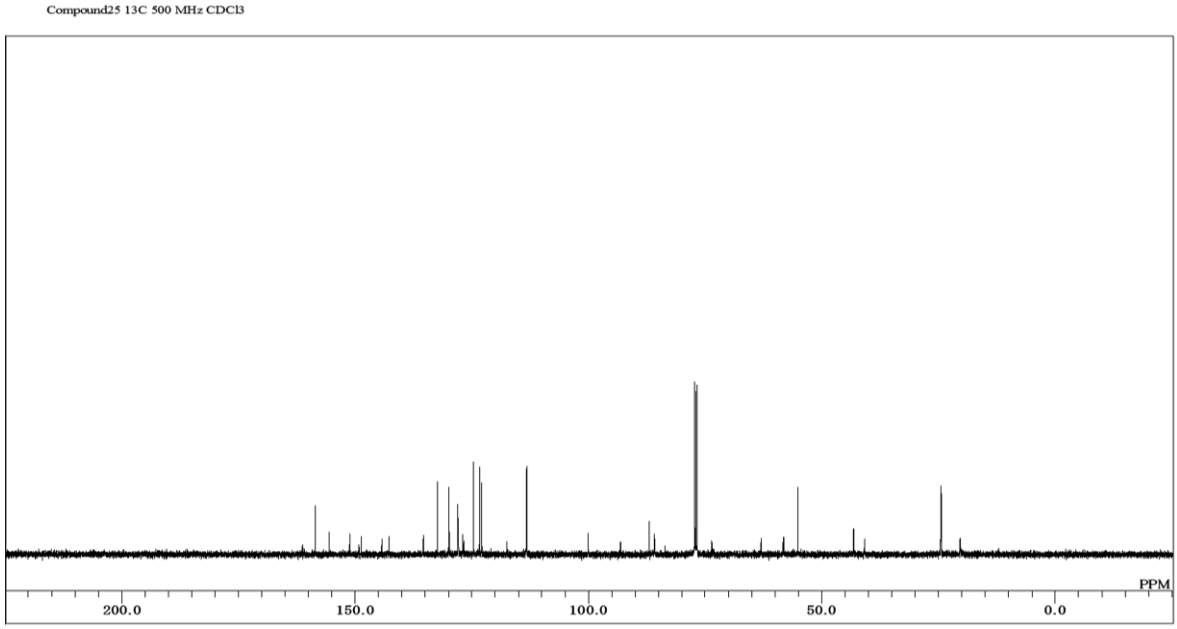

Figure S42. ^{13}C-NMR spectrum of compound 25.

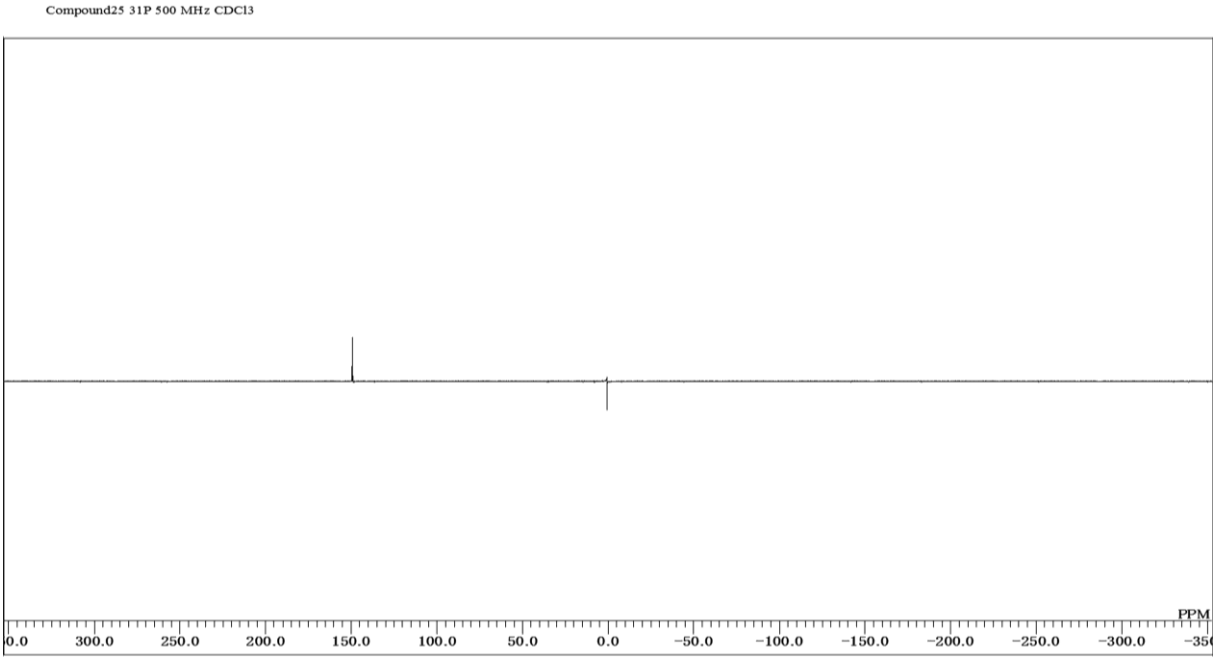

Figure S43. ^{31}P-NMR spectrum of compound 25.

2. UV-vis Spectra of dU^{Az} Analogue Modified ONs

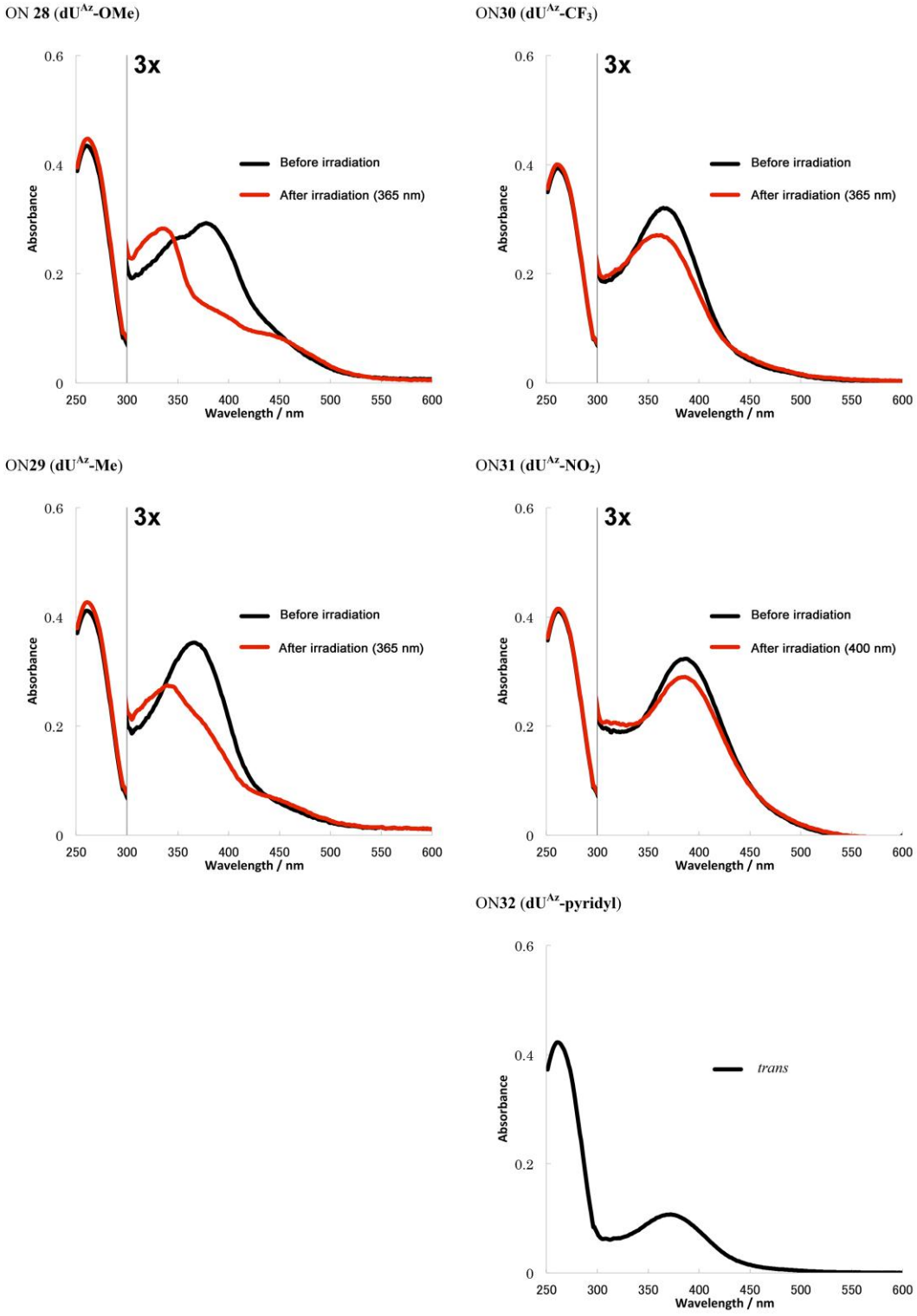

Figure S44. Absorbance spectra of dU^{Az} analogue-modified ONs before irradiation (black line) and after irradiation for 10 s (red line).

3. HPLC and MALDI-TOF MS Analysis of dU^{Az}-Analogue Modified ONs

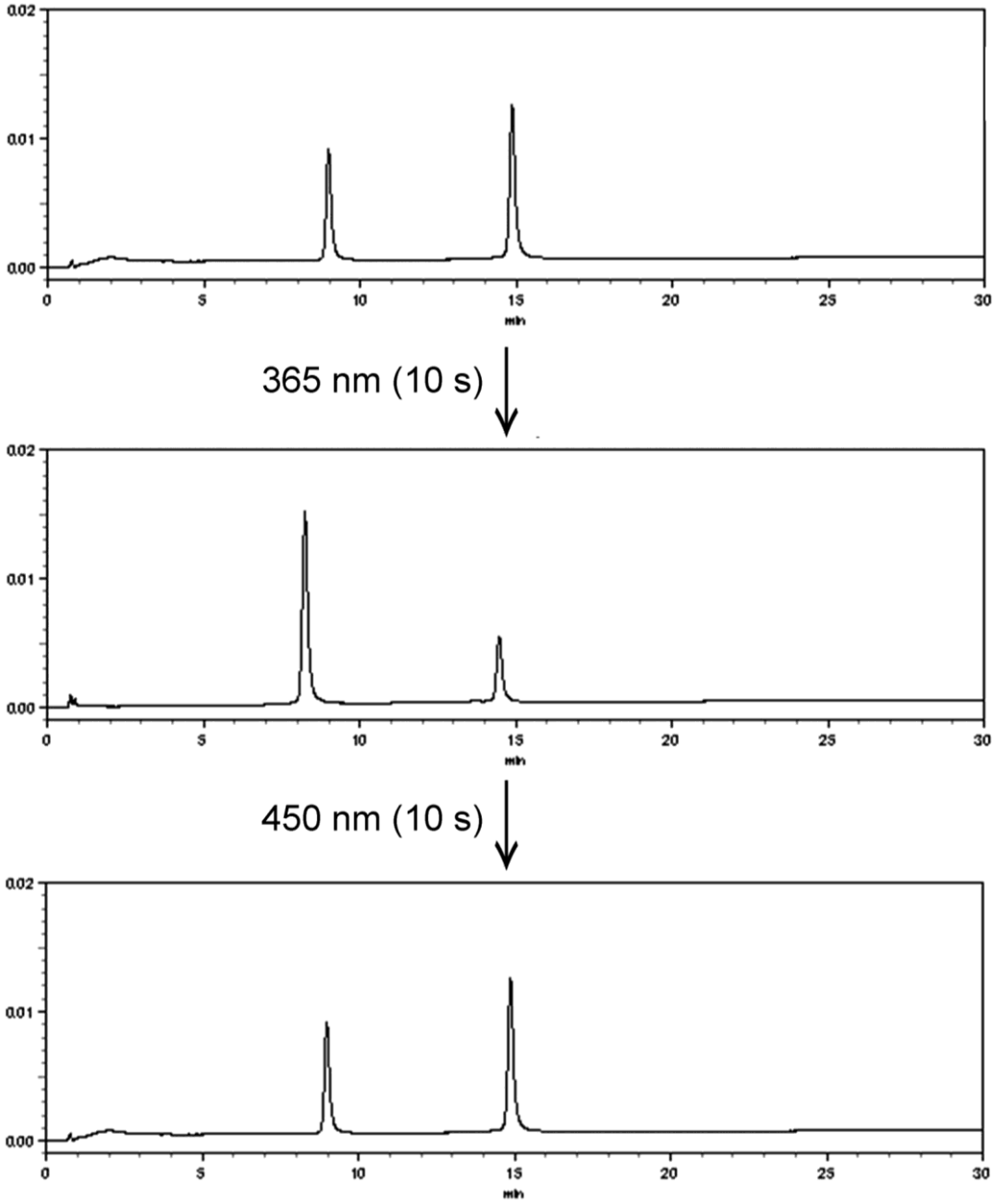

Figure S45. ON **28** HPLC: Column: Waters XBridge^{TM} OST C18 2.5 μm, 4.6 × 50 mm; Gradient: 10%–20% MeCN (over 30 min) in triethylammonium acetate buffer (pH 7.0, 0.1 M); Flow rate: 1.0 mL/min; Column temperature: 37 ℃.

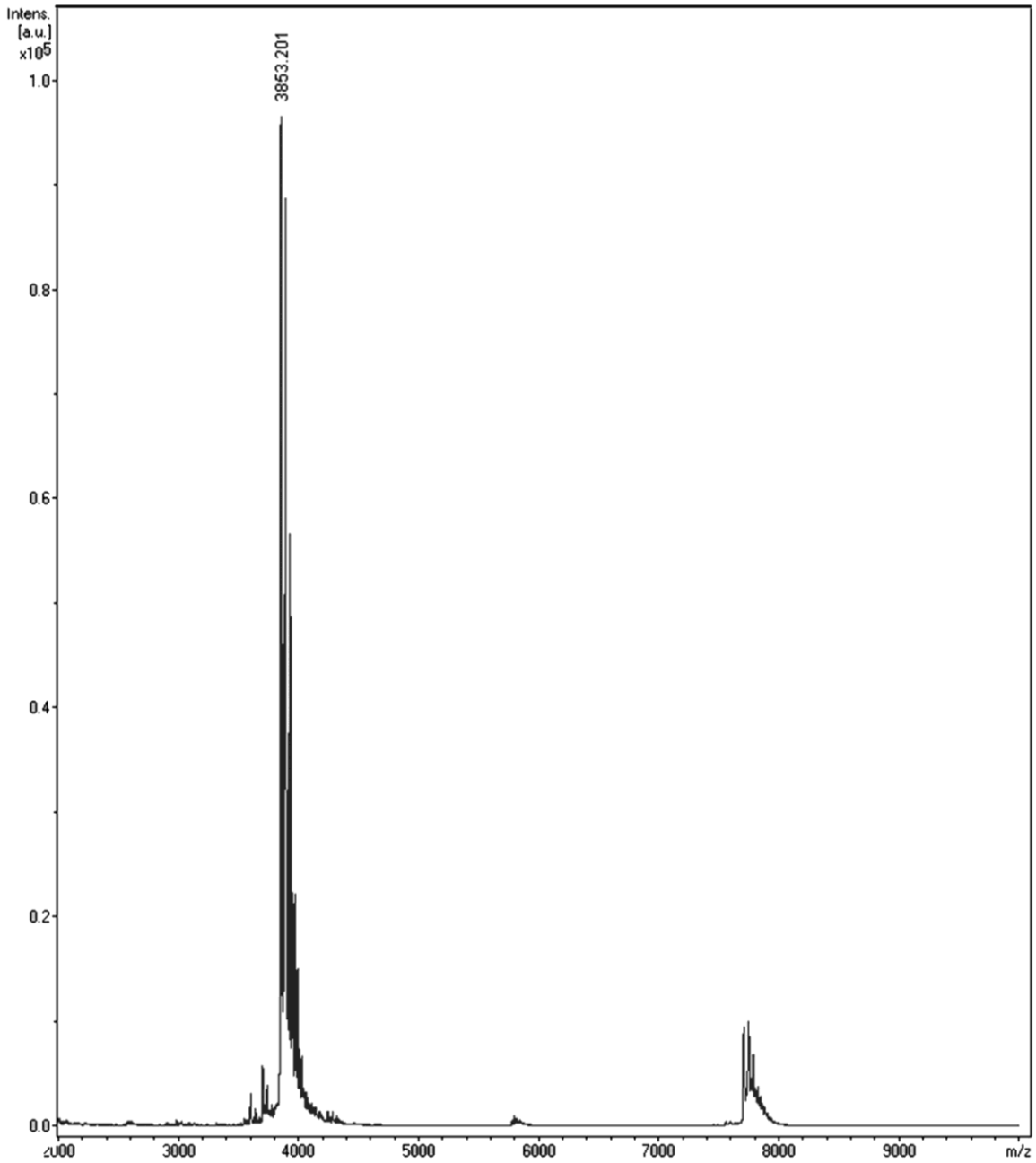

Figure S46. MALDI-TOF MS; Calcd. 3852.6 $[M-H]^-$.

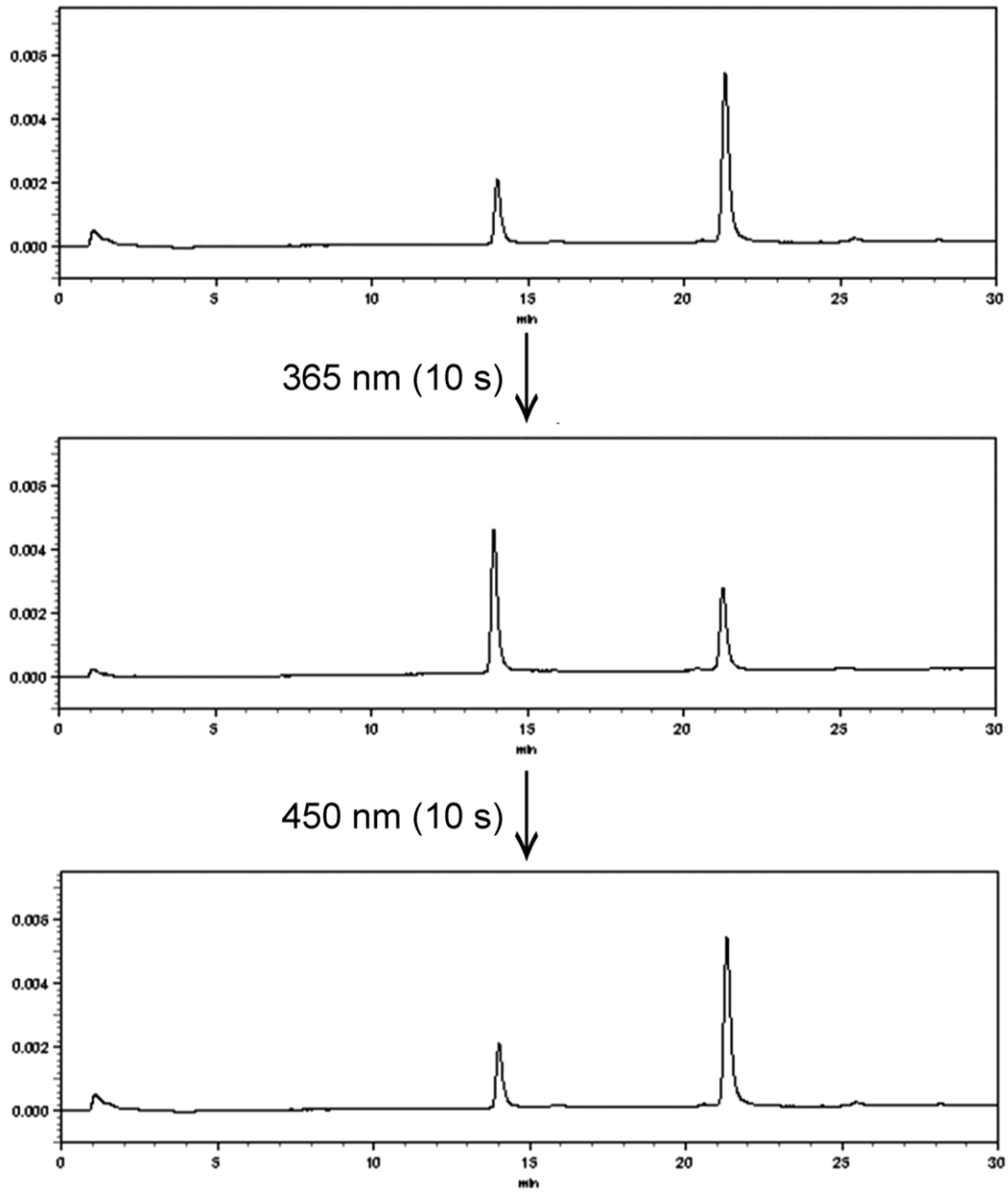

Figure S47. ON **29** HPLC: Column: Waters XBridge™ OST C18 2.5 μm, 4.6 × 50 mm; Gradient: 10%–20% MeCN (over 30 min) in triethylammonium acetate buffer (pH 7.0, 0.1 M); Flow rate: 1.0 mL/min; Column temperature: 37 ℃.

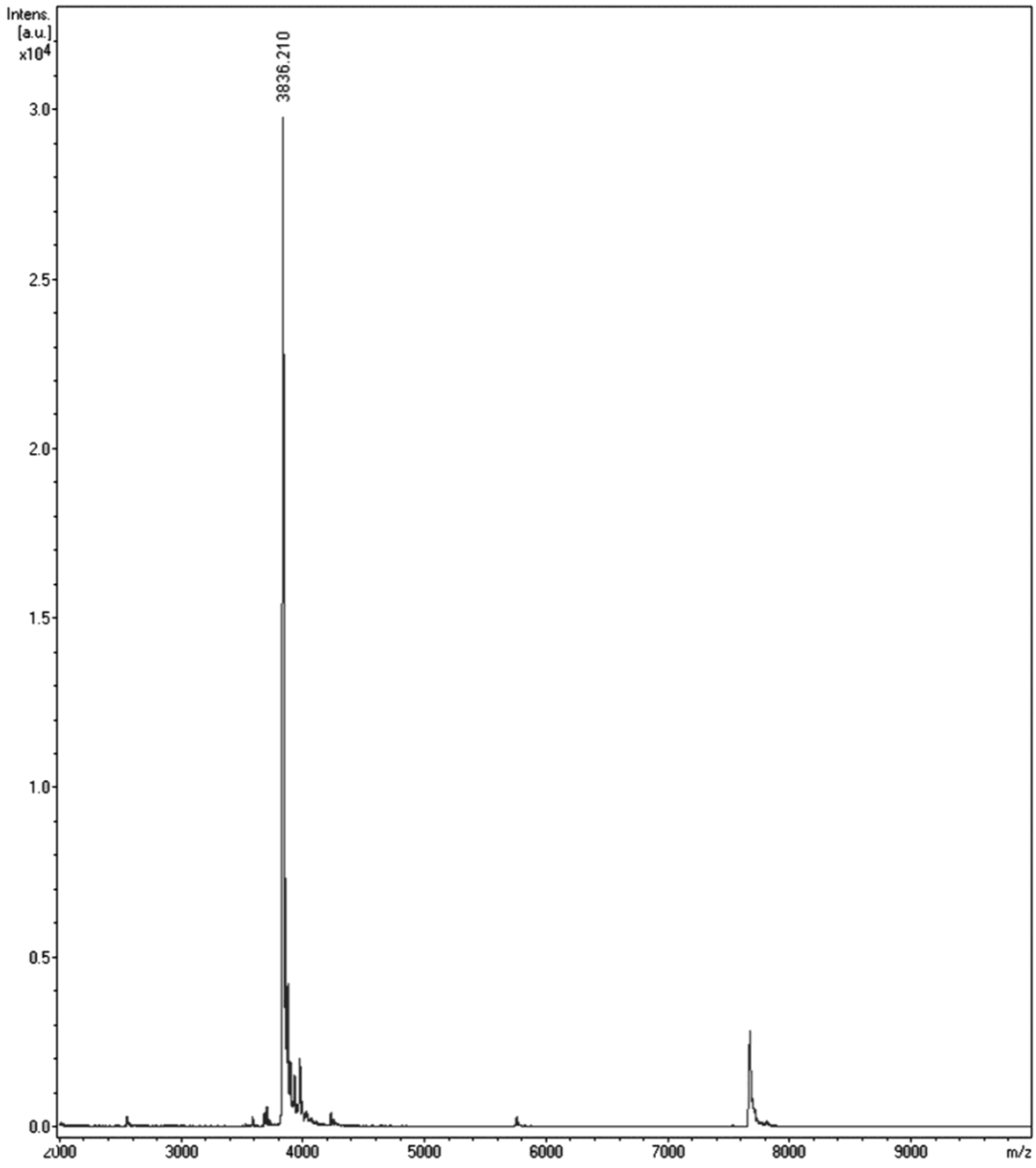

Figure S48. MALDI-TOF MS; Calcd. 3836.6 $[M-H]^-$.

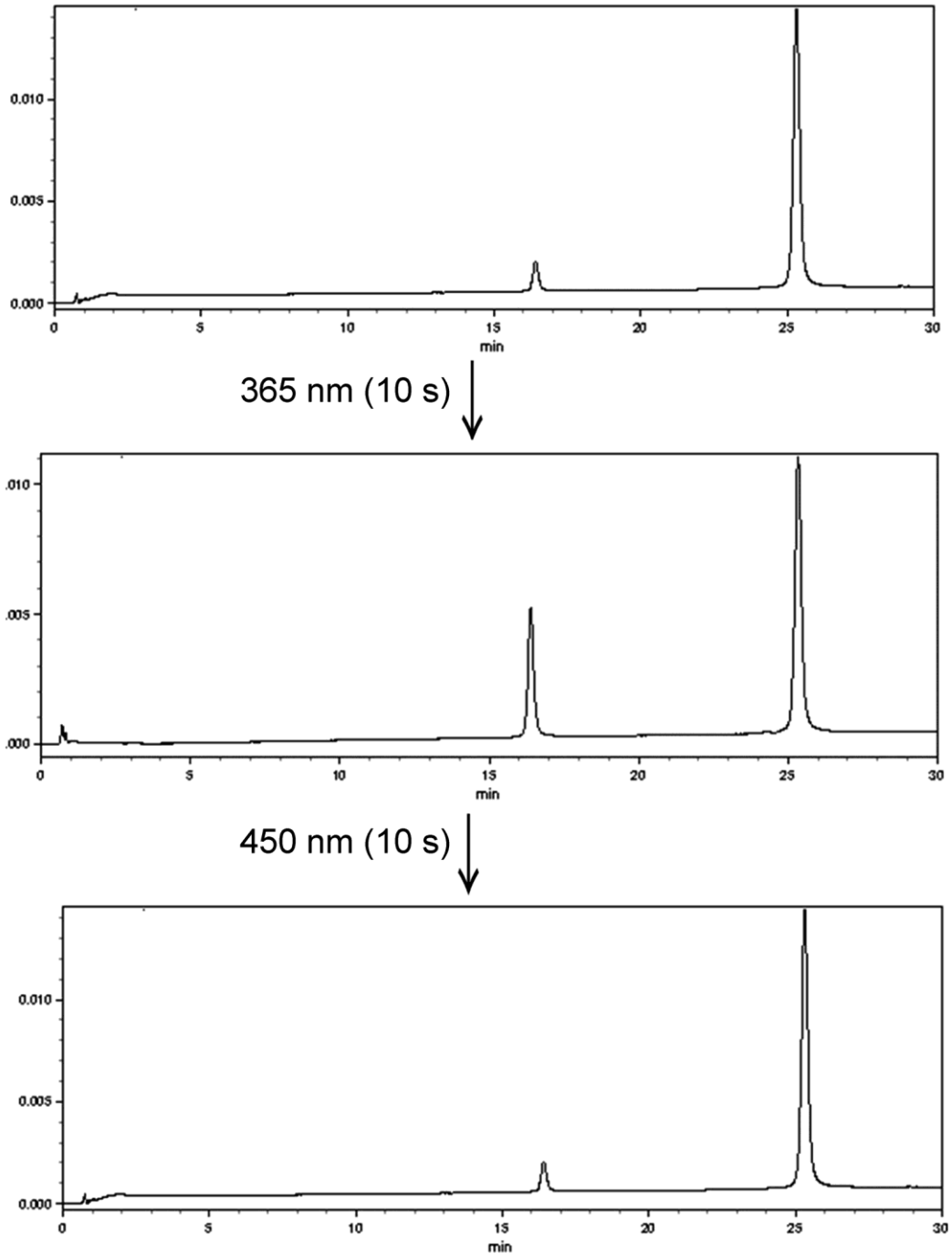

Figure S49. ON **30** HPLC: Column: Waters XBridge^{TM} OST C18 2.5 μm, 4.6 × 50 mm; Gradient: 10%–20% MeCN (over 30 min) in triethylammonium acetate buffer (pH 7.0, 0.1 M); Flow rate: 1.0 mL/min; Column temperature: 37 ℃.

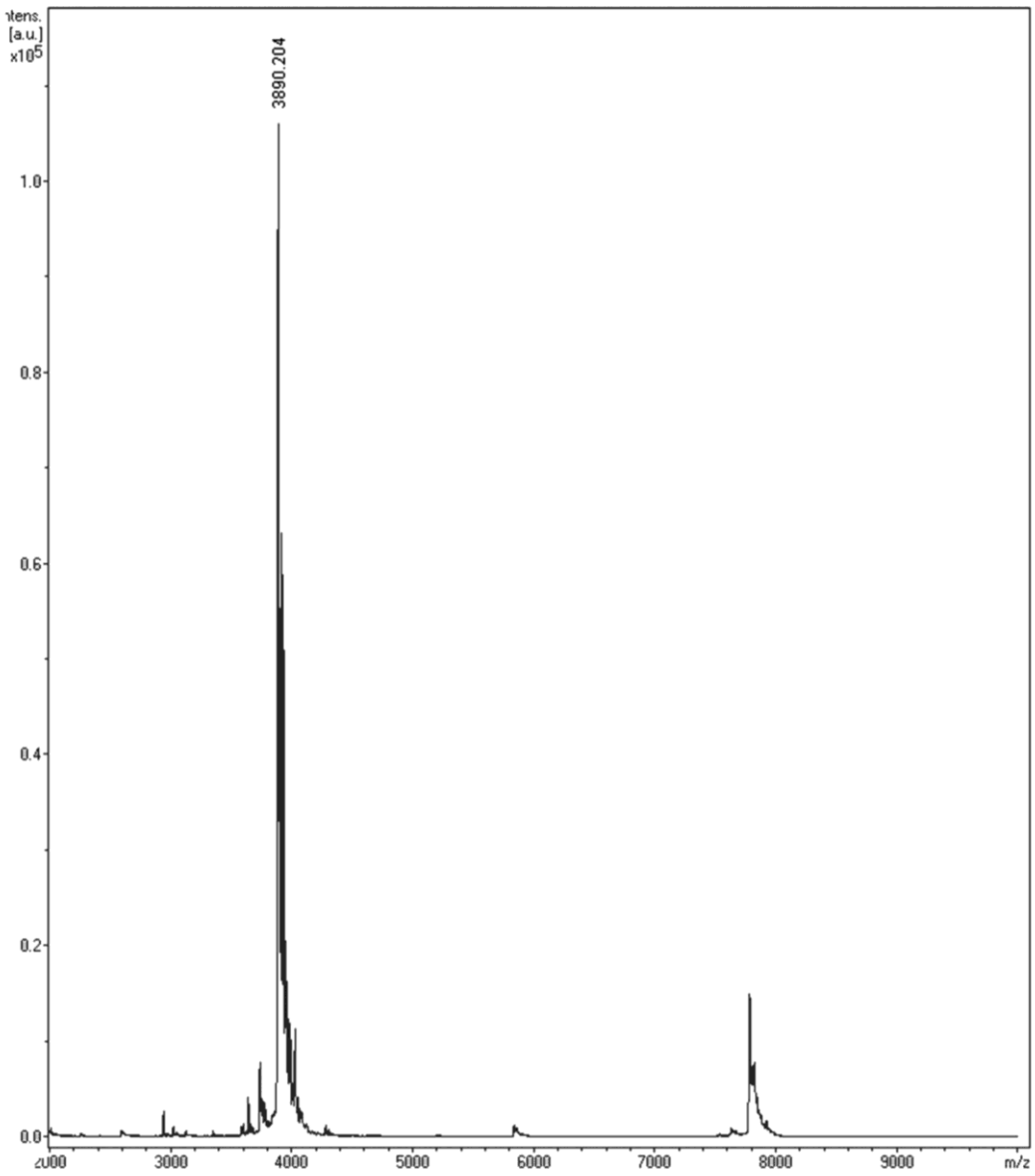

Figure S50. MALDI-TOF MS; Calcd. 3890.6 $[M-H]^-$.

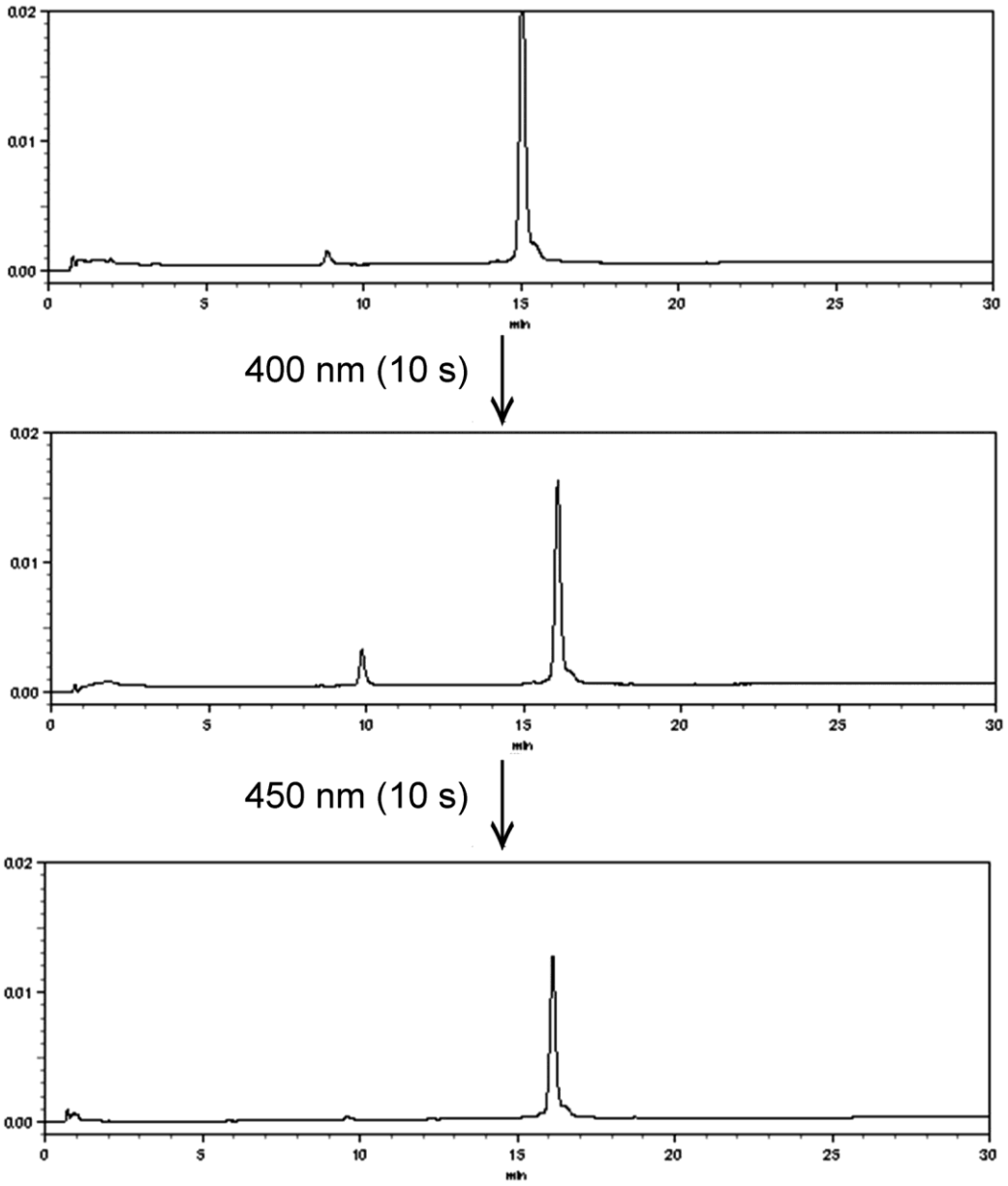

Figure S51. ON **31** HPLC: Column: Waters XBridge™ OST C18 2.5 μm, 4.6 × 50 mm; Gradient: 20%–30% MeCN (over 30 min) in triethylammonium acetate buffer (pH 7.0, 0.1 M); Flow rate: 1.0 mL/min; Column temperature: 37 ℃.

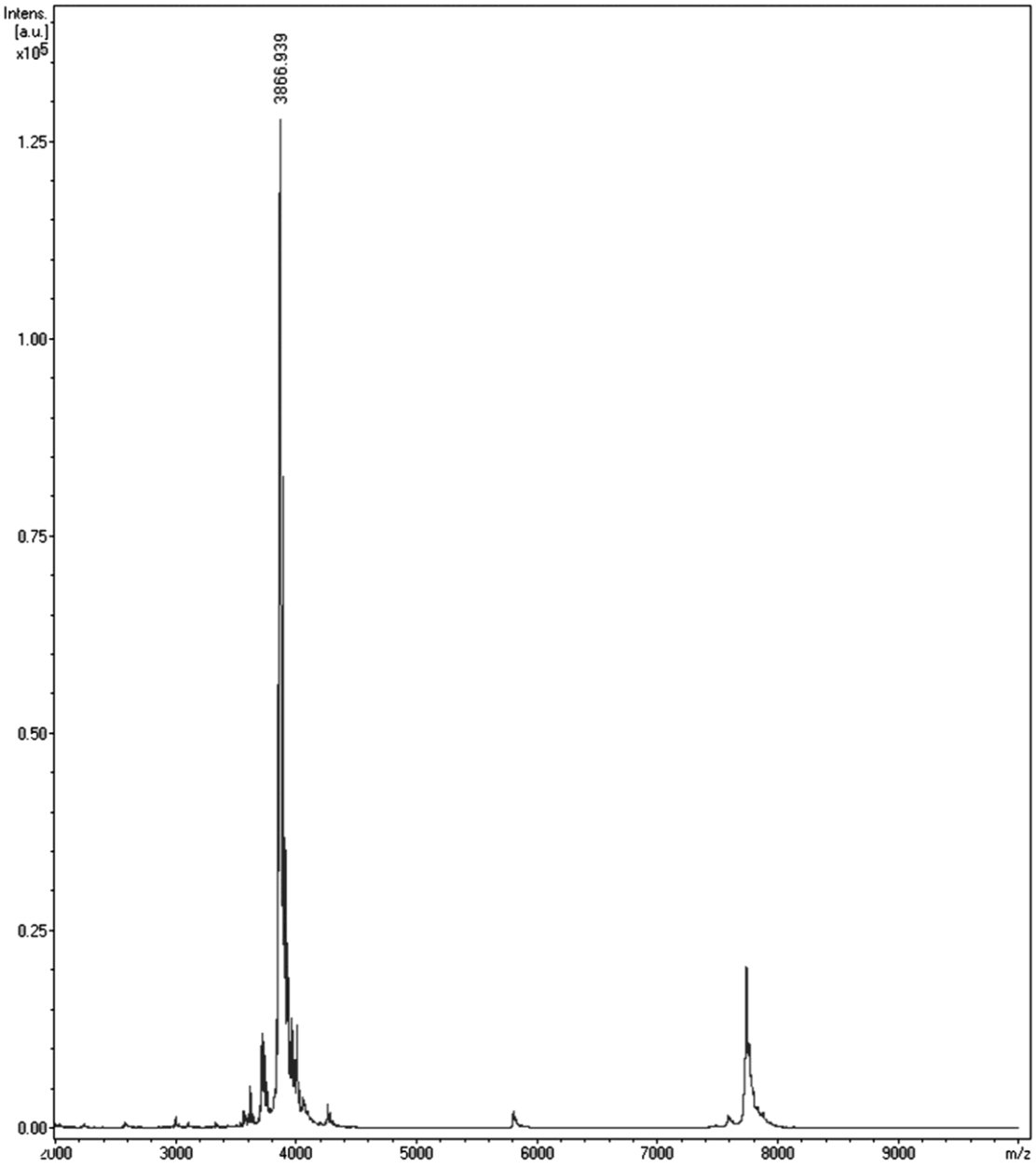

Figure S52. MALDI-TOF MS; Calcd. 3866.6 $[M-H]^-$.

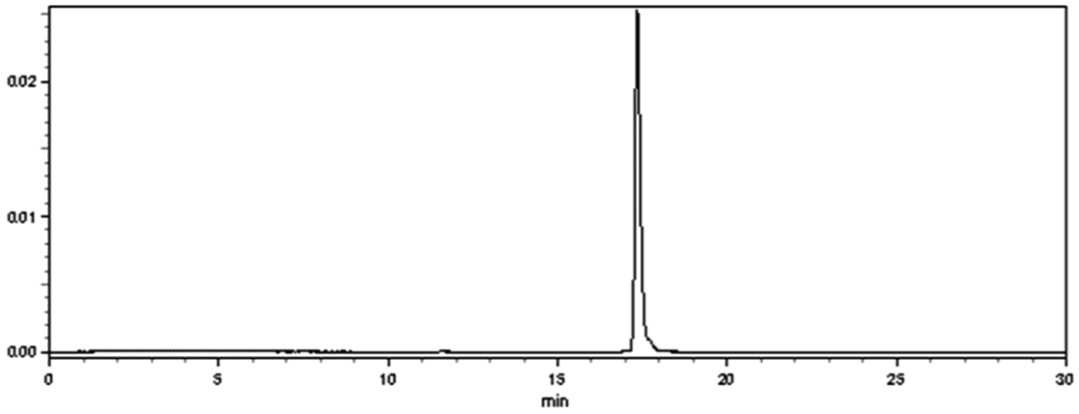

Figure S53. ON **32** HPLC: Column: Waters XBridge^{TM} OST C18 2.5 μm, 4.6 × 50 mm; Gradient: 5%–20% MeCN (over 30 min) in triethylammonium acetate buffer (pH 7.0, 0.1 M); Flow rate: 1.0 mL/min; Column temperature: 37 ℃.

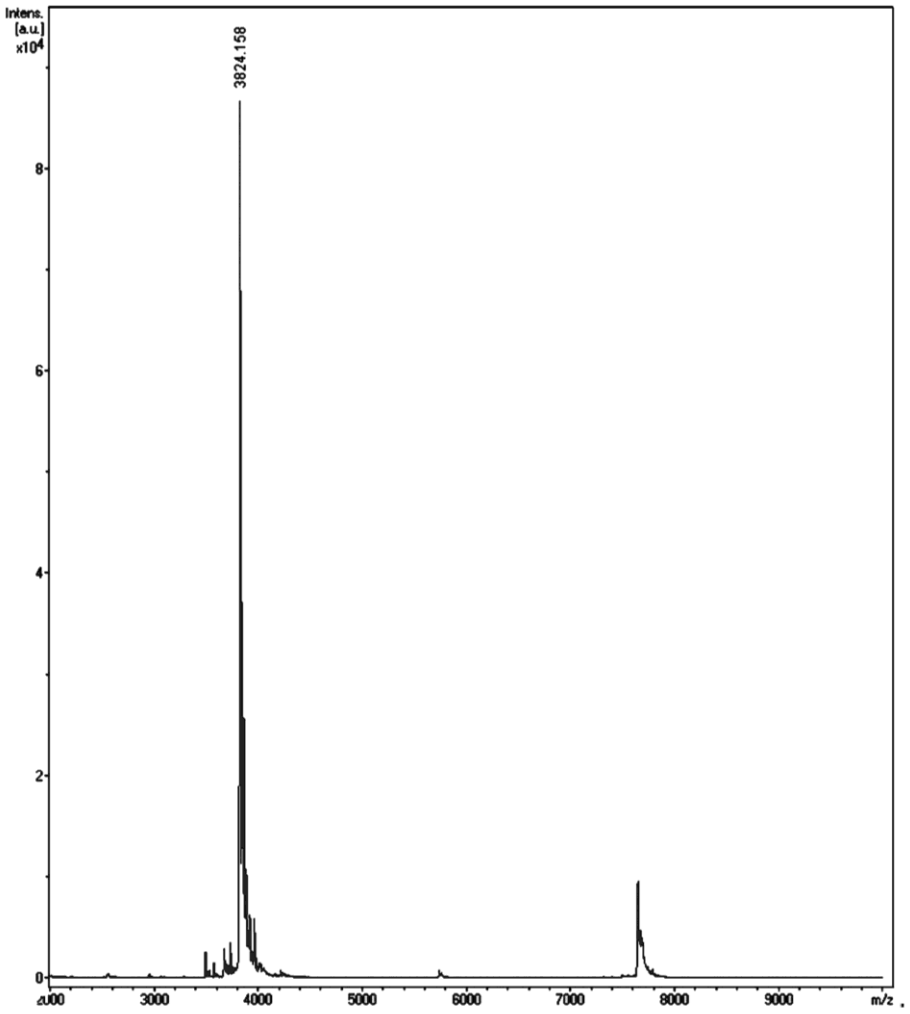

Figure S54. MALDI-TOF MS; Calcd. 3823.6 $[M-H]^-$.

4. Half-Life Time of *cis*-dU^{Az} Analogue Modified of ONs

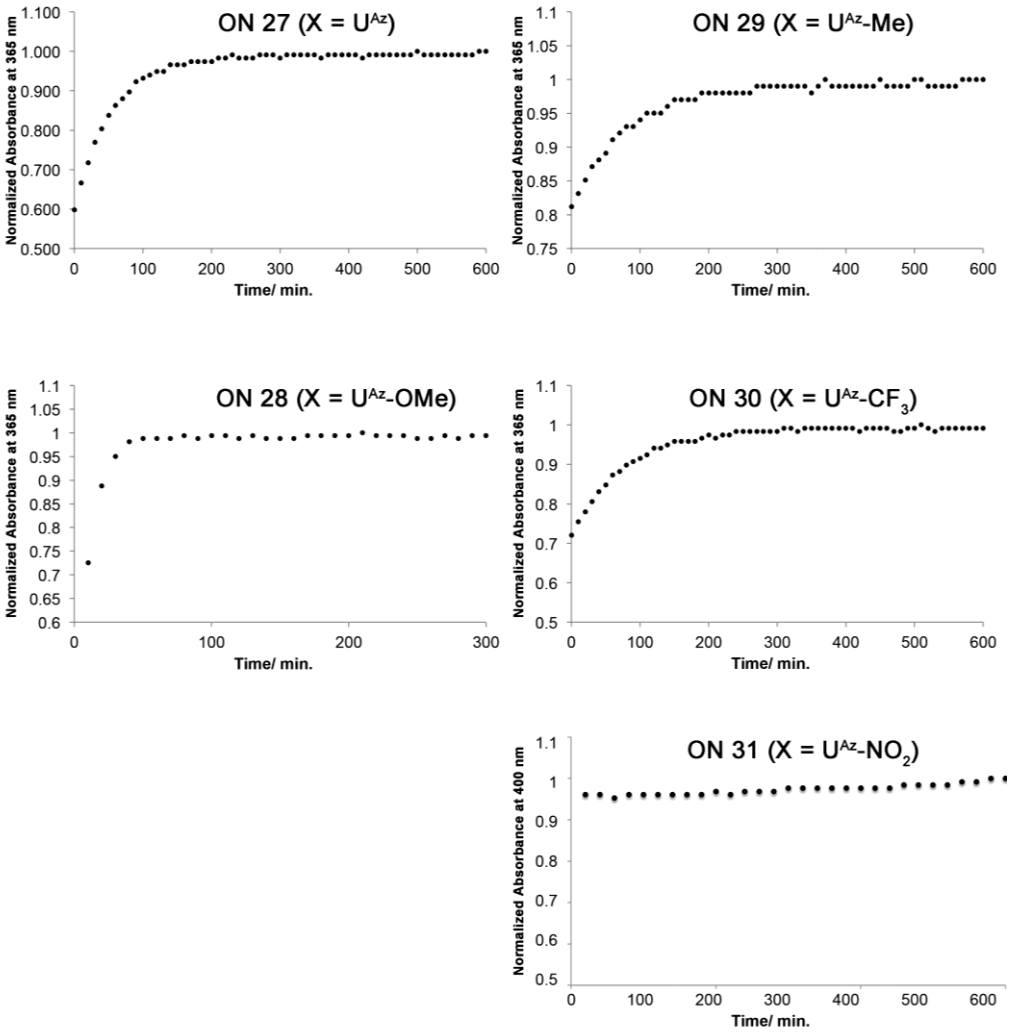

Figure S55. UV absorbance curves for *cis*-**dU^{AZ}** analogue containing ON **27-31** at 60 ℃.

5. UV Melting Curves of dU^{Az}-Modified Duplexes

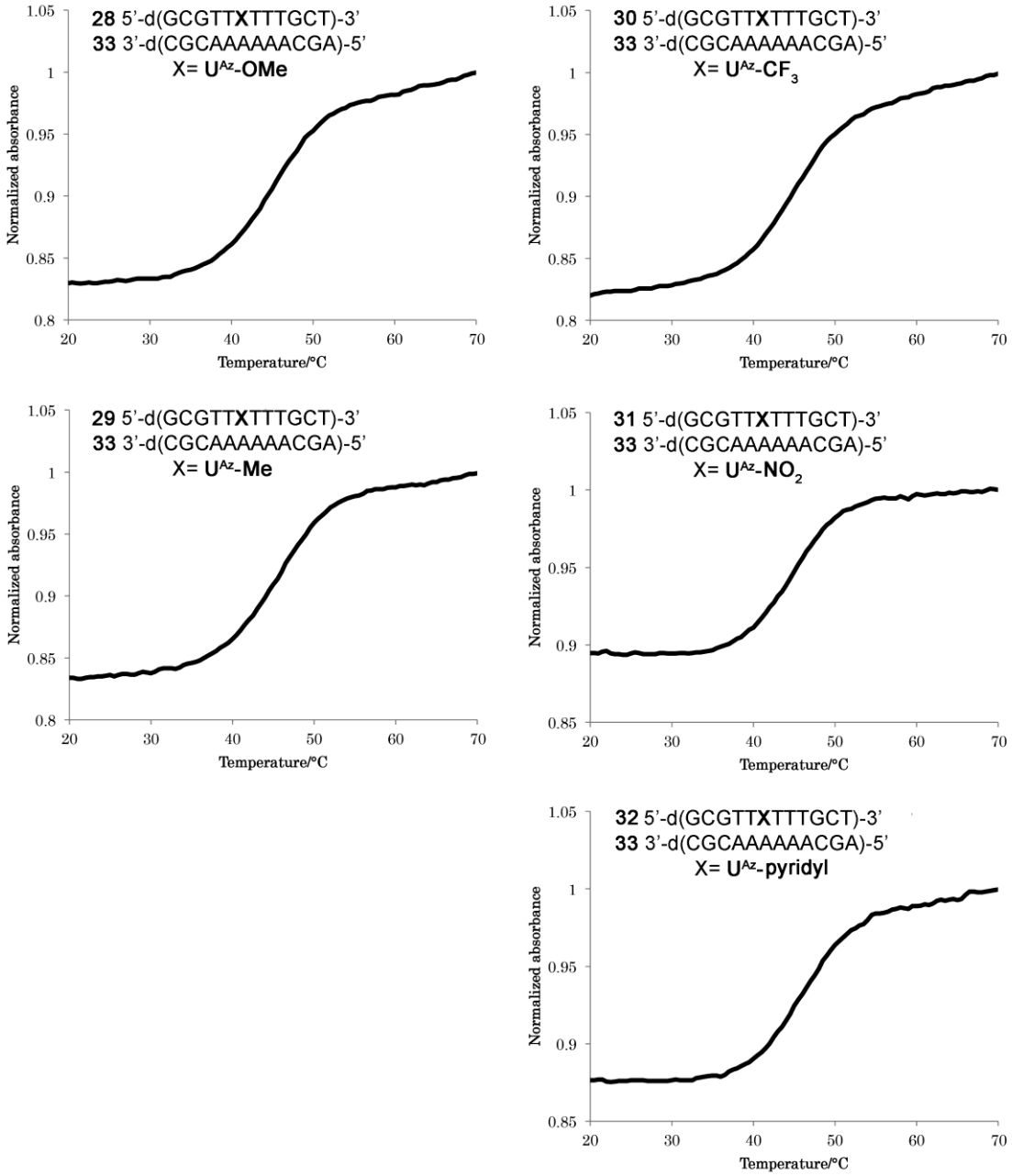

Figure S56. UV melting curves for the DNA/DNA duplexes formed between *trans*-**dU^{AZ}** analogue containing ON **28-32** and ON **33**.

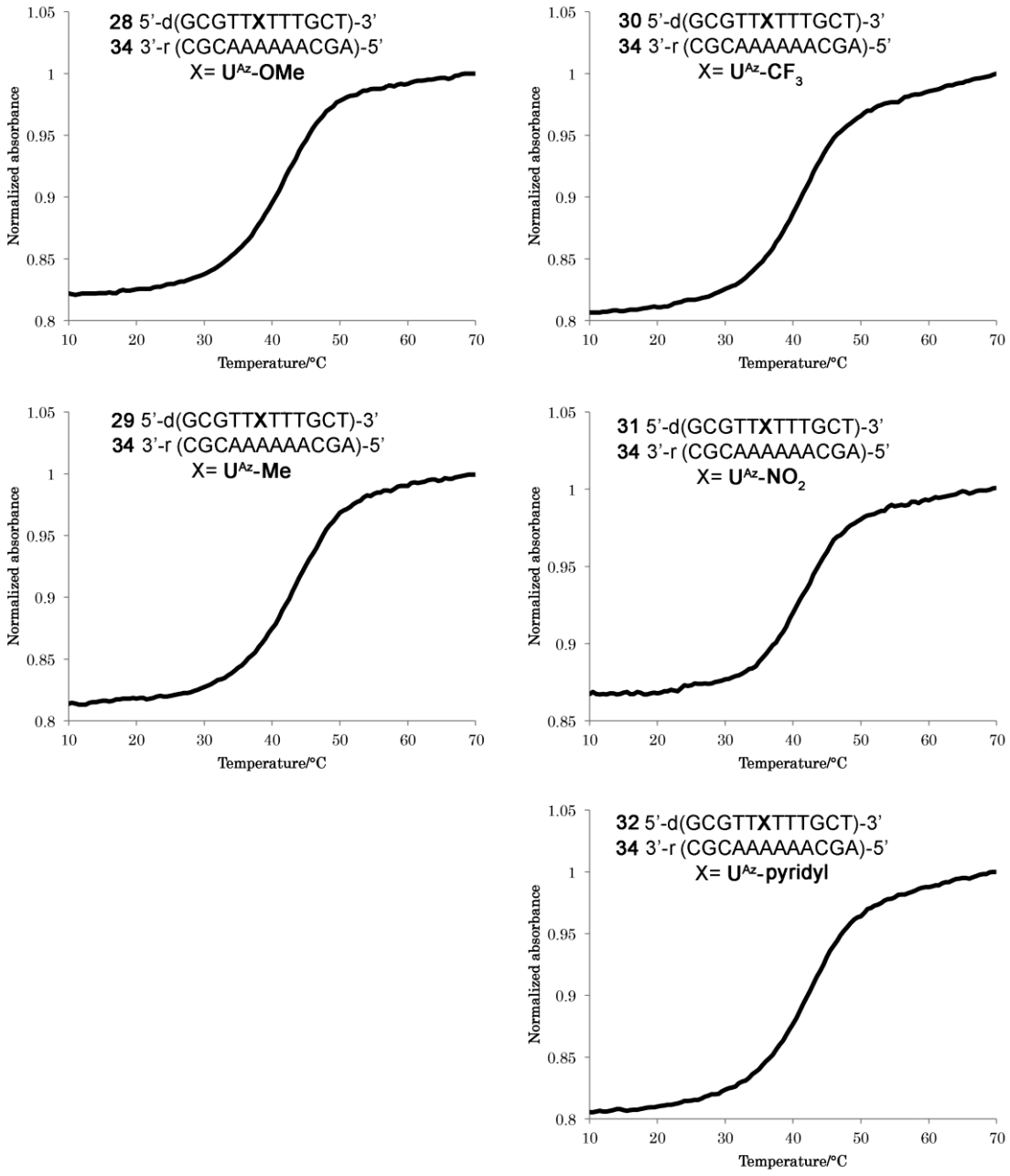

Figure S57. UV melting curves for the DNA/RNA duplexes formed between *trans*-**dU^{AZ}** analogue containing ON **28-32** and ON **34**.

6. ITC Measurements of dUAz Analogue Modified ONs/Complementary RNA

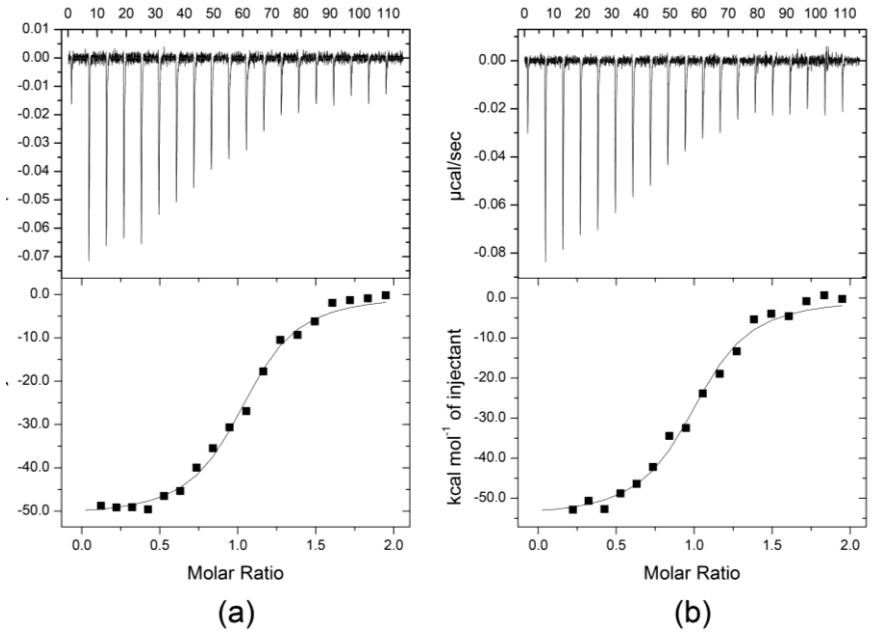

Figure S58. Representative ITC measurements on duplex formation between **dU^{Az}-MeO** modified ON (**28**) and complementary RNA strand (**34**). (**a**) before irradiation, (**b**) after 365 nm irradiation for 10 s.

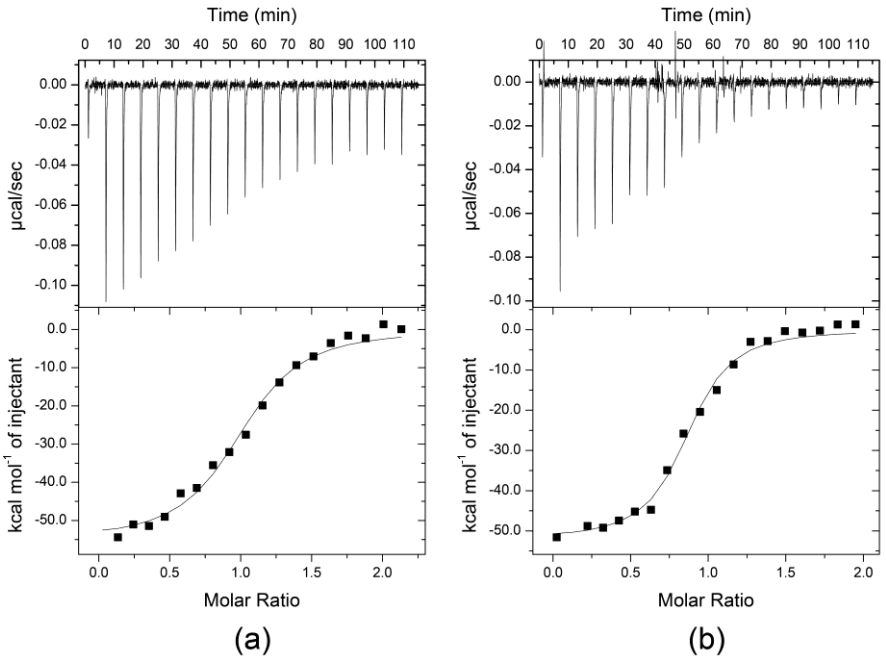

Figure S59. Representative ITC measurements on duplex formation between **dU^{Az}-Me** modified ON (**29**) and complementary RNA strand (**34**). (**a**) before irradiation, (**b**) after 365 nm irradiation for 10 s.