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Synthesis, Photochemical Isomerization and Photophysical Properties of Hydrazide-Hydrazone Derivatives

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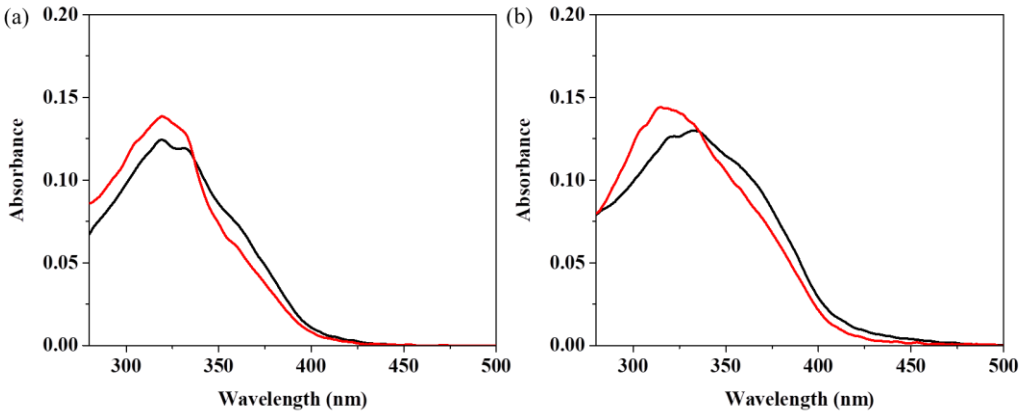


Fig. S1 UV-Vis absorption spectra of (a) **3b** and (b) **3c** before irradiation (black) and after irradiation (red) with 365 nm light (Molecule concentration: 50 μM).

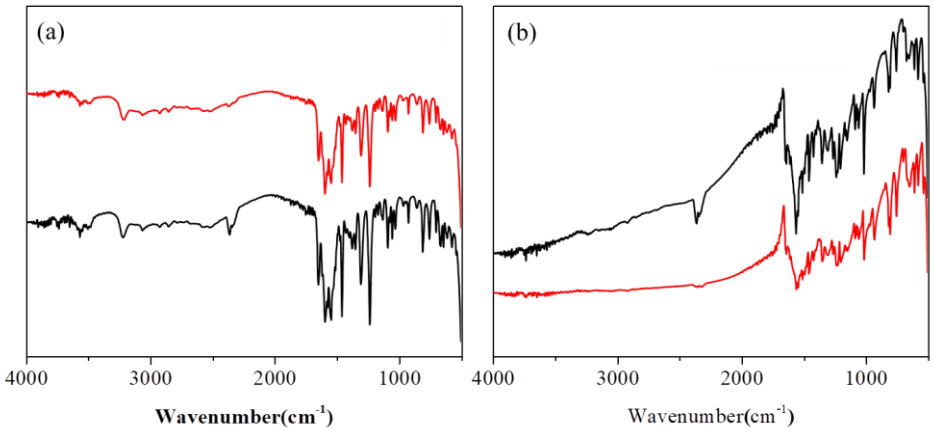


Fig. S2 FT-IR spectra of (a) **3b** and (b) **3c** before irradiation (black) and after irradiation (red) with 365 nm light.

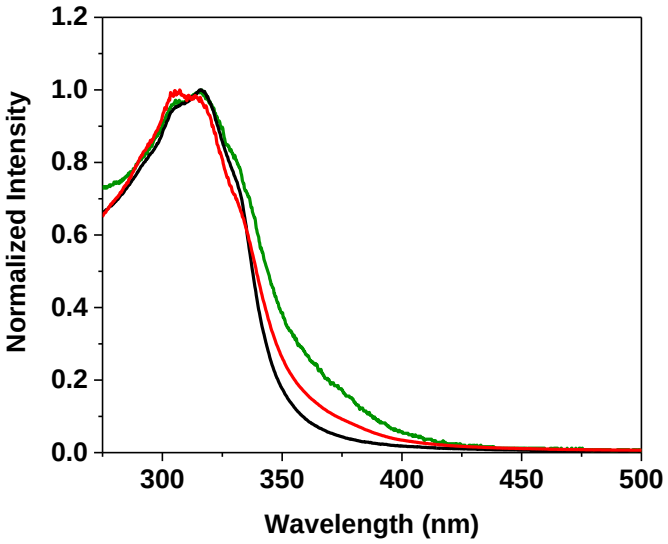


Fig. S3 Concentration dependence of UV-Vis absorption spectra of **3a** after irradiation with 365 nm light in DMSO (black for 50 μM, red for 500 μM and green for 5,000 μM).

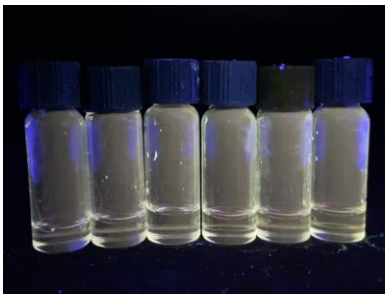


Fig. S4 Optical images of **3a** before irradiation with 365 nm light taken under UV illumination (Concentrations from left to right: 50, 100, 500, 1000, 5000 μM).

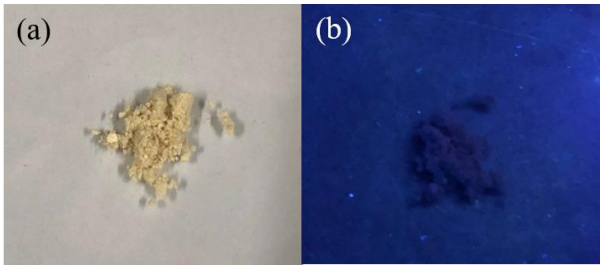


Fig. S5 Photographs of solid powders of **3a** taken under (a) ambient room lighting and (b) UV illumination.

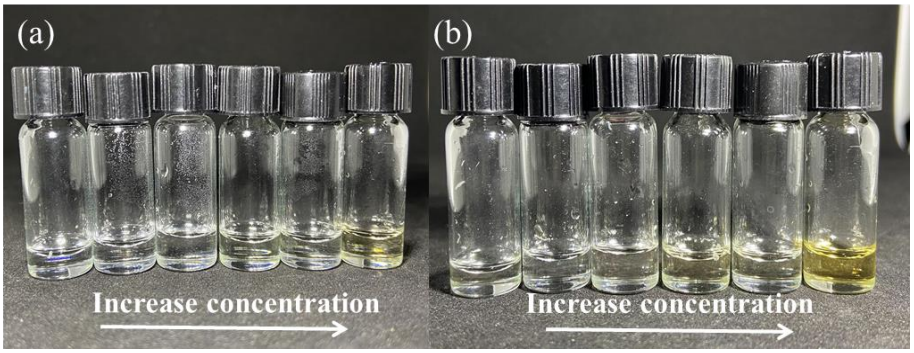


Fig. S6 Optical images of **3a** (a) before irradiation and (b) after irradiation with 365 nm light taken under ambient room lighting (Concentrations from left to right: 50, 100, 500, 1000, 5000 μM).

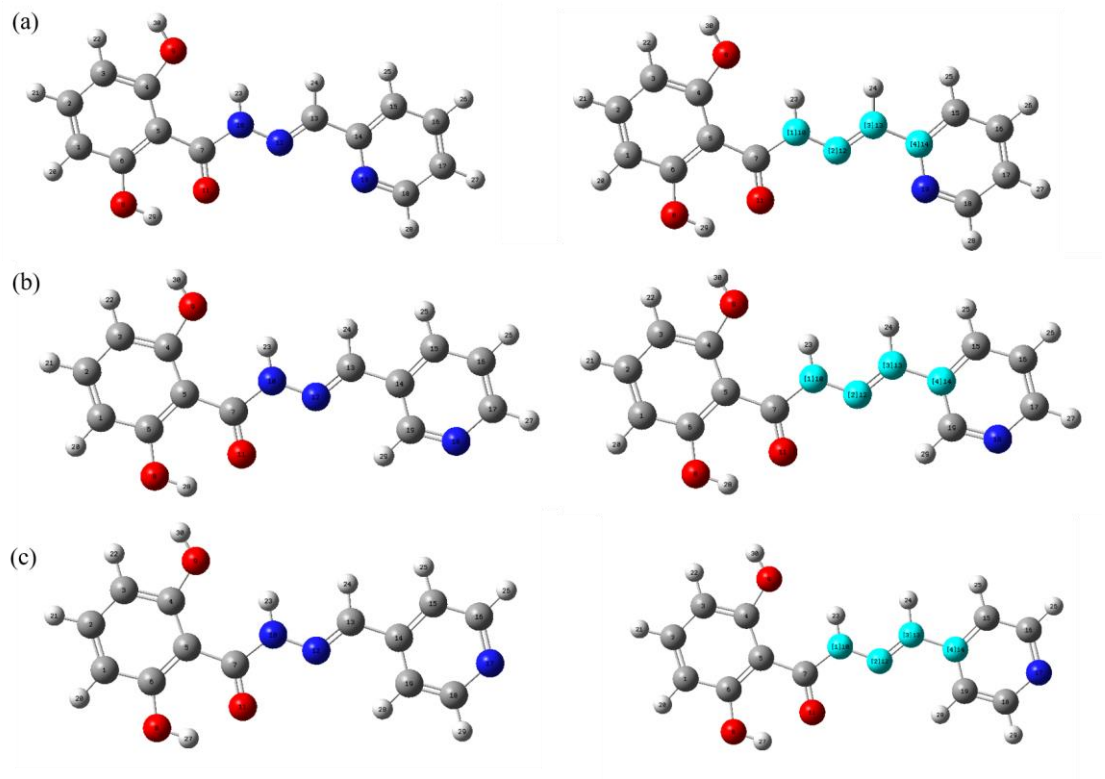


Fig. S7 The calculated isomerization of (a) **3a**, (b) **3b** and (c) **3c** along a reaction coordinate corresponding to the N_{10}–N_{12}=C_{13}–C_{14} dihedral angle.

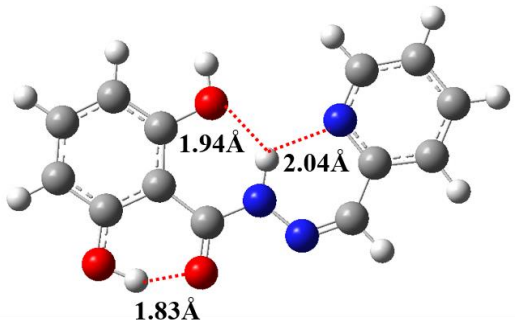


Fig. S8 The optimized structure of **3a-*Z***.

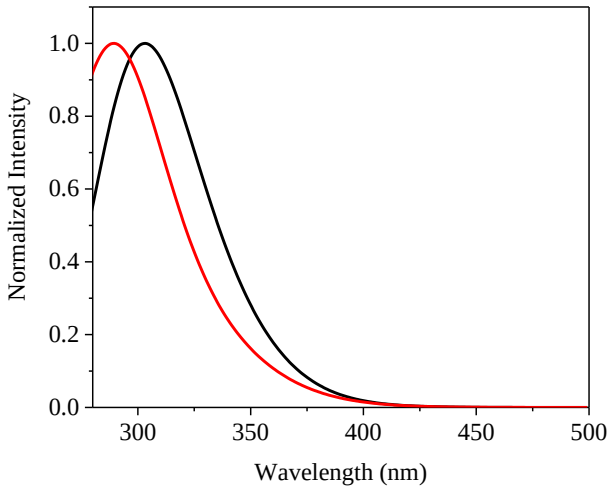


Fig. S9 The calculated absorption spectra of **3a**-***E*** (black) and **3a**-***Z*** (red).

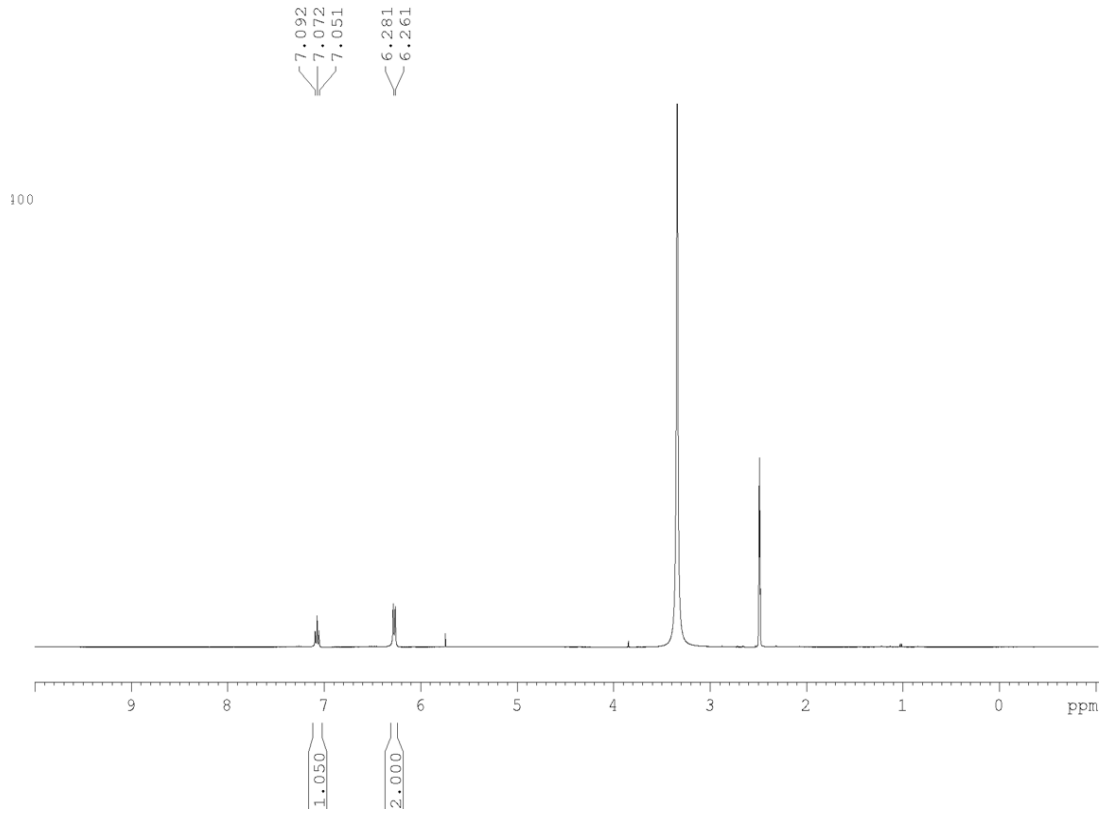


Fig. S10 ^{1}H NMR spectrum for **2** in DMSO-d_6.

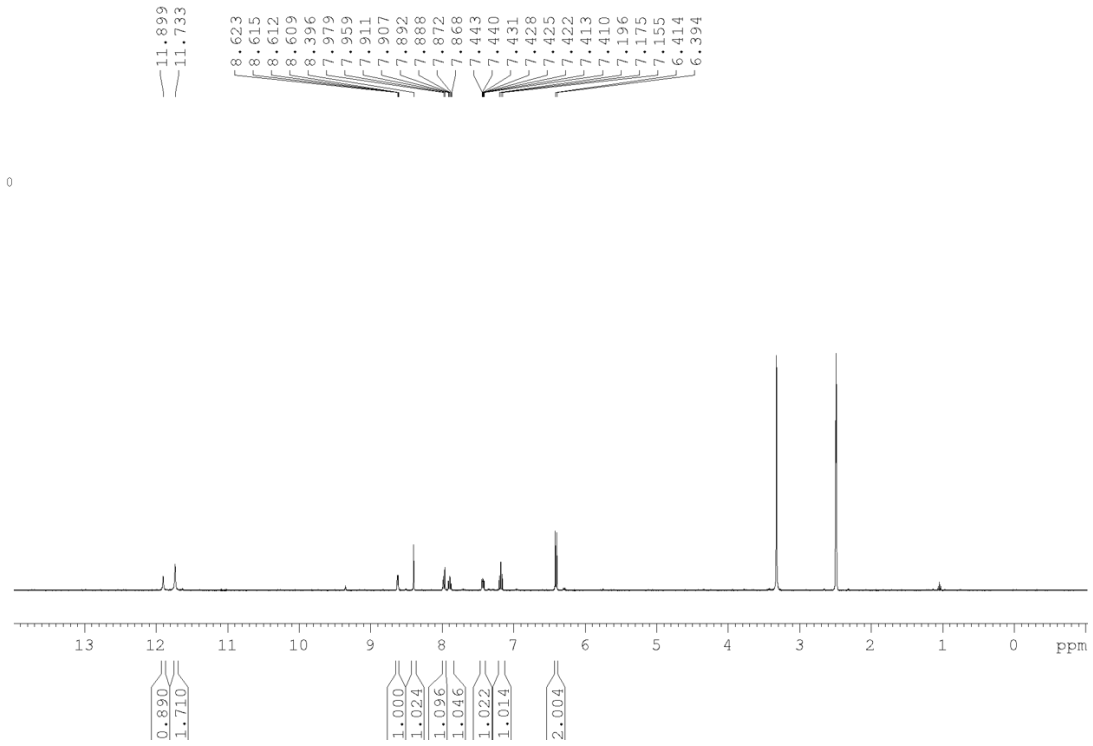


Fig. S11 ^{1}H NMR spectrum for **3a** in DMSO-d_6.

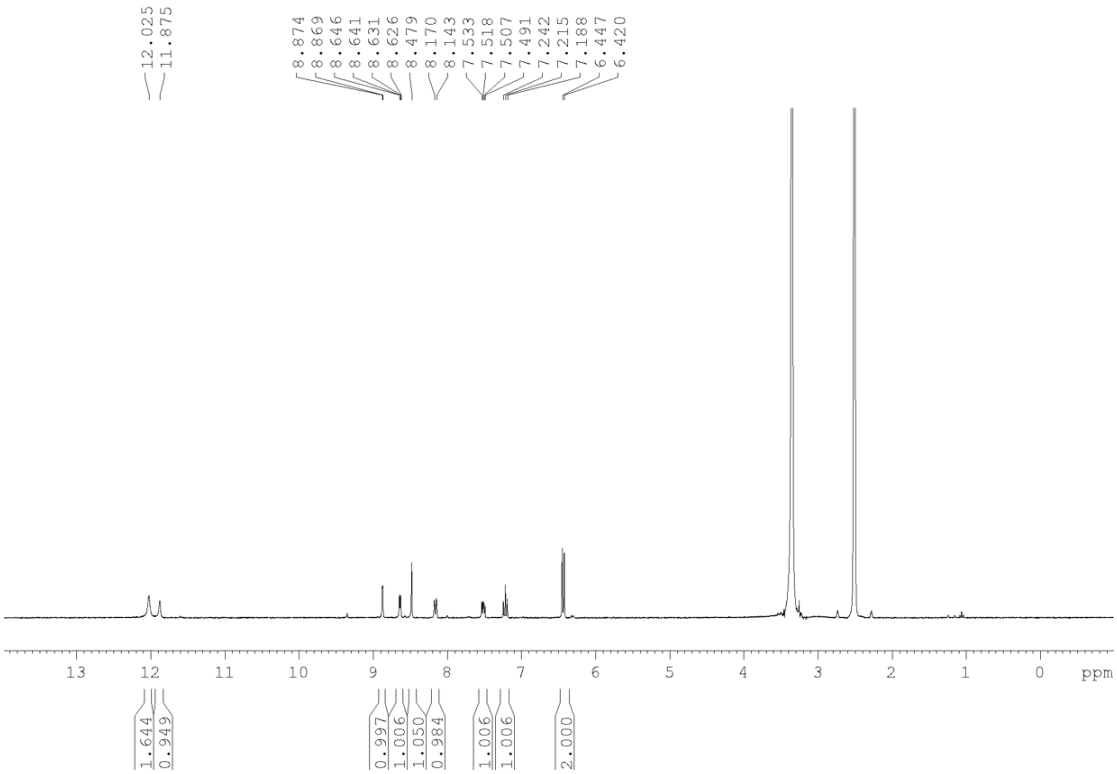


Fig. S12 ^{1}H NMR spectrum for **3b** in DMSO-d_6.

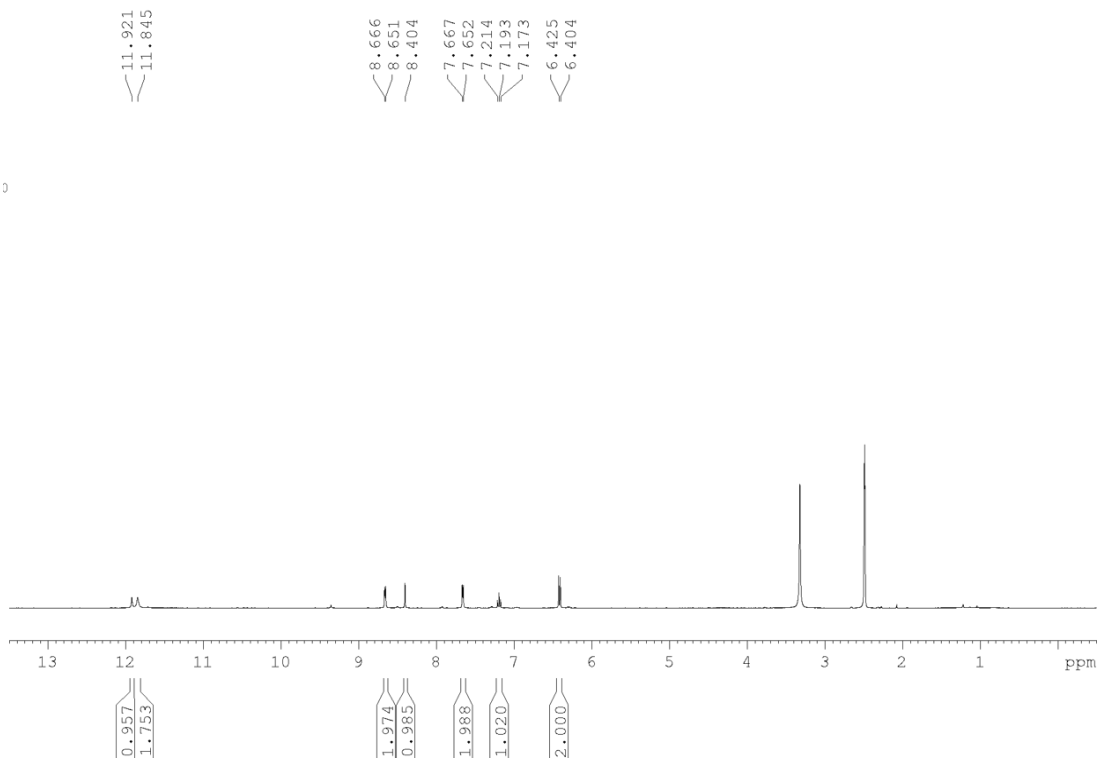
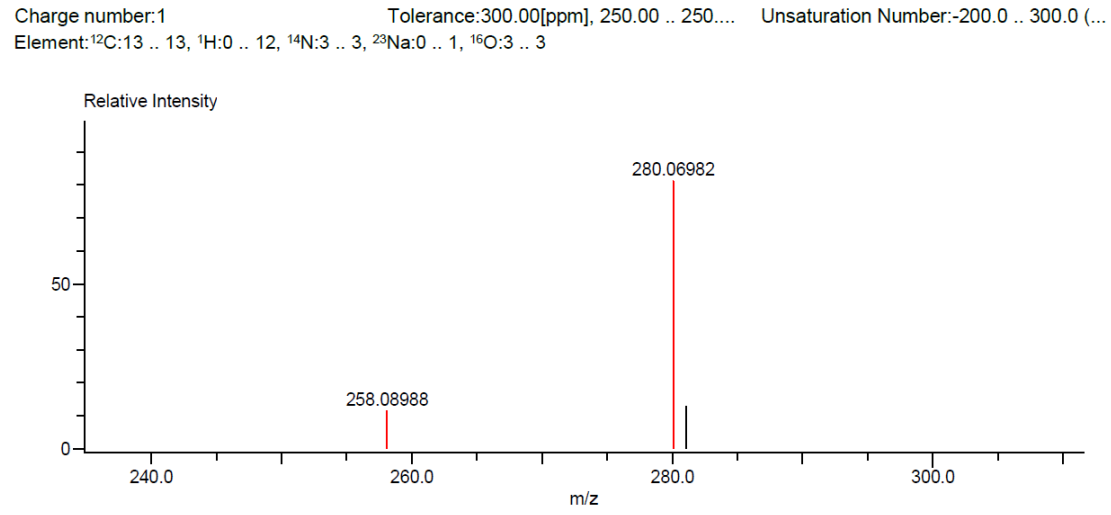


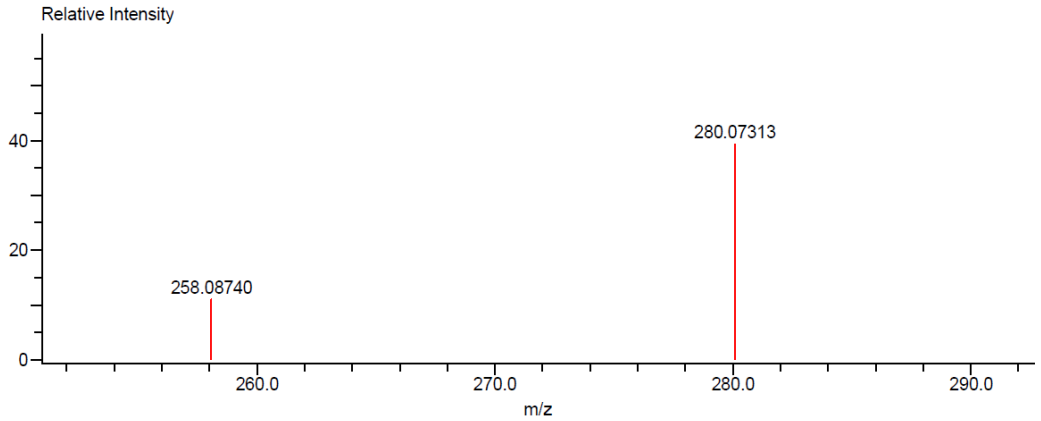
Fig. S13 ^{1}H NMR spectrum for **3c** in DMSO-d_6.



Mass	Intensity	Calc. Mass	Mass Difference [mDa]	Mass Difference [ppm]	Possible Formula
258.08988	1032.87	258.08787	2.01	7.81	$^{12}C_{13}{}^{1}H_{12}{}^{14}N_3{}^{16}O_3$
280.06982	7432.50	280.06981	0.01	0.03	$^{12}C_{13}{}^{1}H_{11}{}^{14}N_3{}^{23}Na_1{}^{16}O_3$

Fig. S14 HRMS spectrum for **3a**.

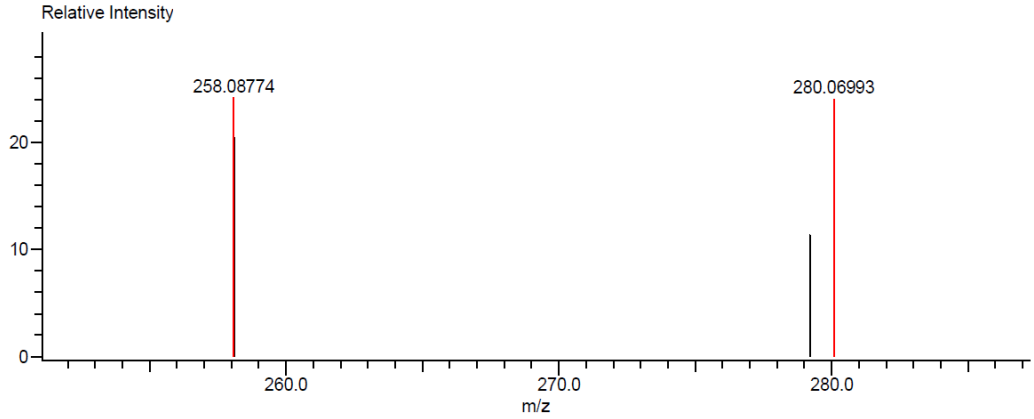
Charge number:1 Tolerance:300.00[ppm], 250.00 .. 250.... Unsaturation Number:-200.0 .. 300.0 (...
Element:^{12}C:13 .. 13, ^{1}H:0 .. 12, ^{14}N:3 .. 3, ^{23}Na:0 .. 1, ^{16}O:3 .. 3



Mass	Intensity	Calc. Mass	Mass Difference [mDa]	Mass Difference [ppm]	Possible Formula
258.08740	137.51	258.08787	-0.46	-1.80	$^{12}C_{13}{}^{1}H_{12}{}^{14}N_{3}{}^{16}O_{3}$
280.07313	491.43	280.06981	3.32	11.85	$^{12}C_{13}{}^{1}H_{11}{}^{14}N_{3}{}^{23}Na_{1}{}^{16}O_{3}$

Fig. S15 HRMS spectrum for **3b**.

Charge number:1 Tolerance:300.00[ppm], 250.00 .. 250.... Unsaturation Number:-200.0 .. 300.0 (...
Element:^{12}C:13 .. 13, ^{1}H:0 .. 12, ^{14}N:3 .. 3, ^{23}Na:0 .. 1, ^{16}O:3 .. 3



Mass	Intensity	Calc. Mass	Mass Difference [mDa]	Mass Difference [ppm]	Possible Formula
258.08774	476.08	258.08787	-0.13	-0.50	$^{12}C_{13}{}^{1}H_{12}{}^{14}N_{3}{}^{16}O_{3}$
280.06993	473.36	280.06981	0.12	0.44	$^{12}C_{13}{}^{1}H_{11}{}^{14}N_{3}{}^{23}Na_{1}{}^{16}O_{3}$

Fig. S16 HRMS spectrum for **3c**.