Supporting Information

for

Visibly Emitting Thiazolyl-uridine Analogues as promising fluorescent probes

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Fluorescence date

Sensitivity to polarity

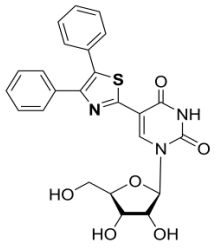
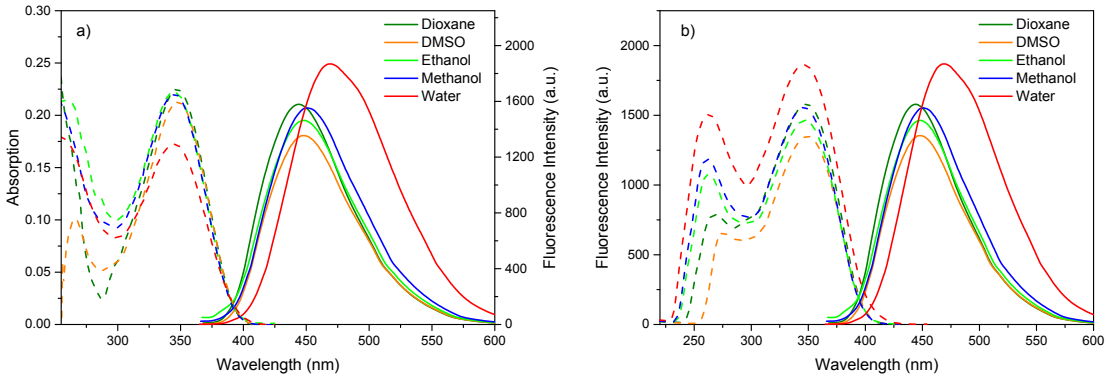
compound	solvent	λ_{abs}	λ_{em}	Stokes shift	ϕ
 **7a**	Dioxane	350	442	5946 (92)	0.026
	DMSO	348	446	6314 (98)	0.026
	Ethanol	345	447	6614 (102)	0.032
	Methanol	345	452	6862 (107)	0.031
	Water	345	472	7572 (127)	0.073

Table S1. Absorbance and emission maxima of **7a** in dioxane, DMSO, ethanol, methanol and water. λ_{abs}, λ_{em} and Stokes shift are reported in nm, nm and cm^{-1} (nm). Quantum yield values were measured at λ_{abs} = 360 nm using quinine sulfate in 0.5 M H_2SO_4 (Φ_{fl} = 0.55) as the standard.



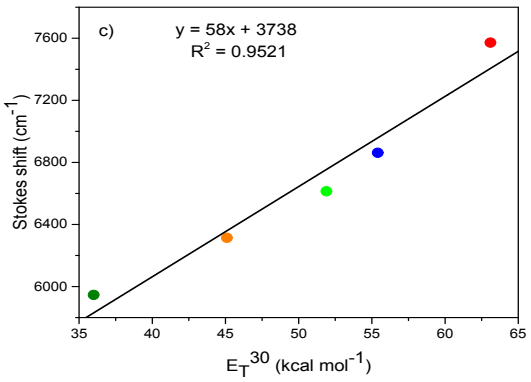


Figure S1. (a) Absorbance (10.0 μM, dash) and emission (5.0 μM, solid) spectra of **7a** in various solvents. (b) Excitation (dash line) and emission (solid line) spectra of **7a** in various solvents. (c) Linear relationship between stokes shift and solvent polarity of **7a** in various solvents.

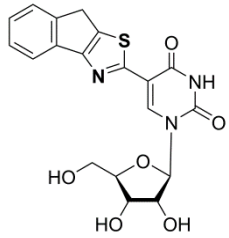
compound	solvent	λ_{abs}	λ_{em}	Stokes shift	ϕ
 **7b**	Dioxane	359	439	5076 (80)	0.165
	DMSO	359	449	5583 (90)	0.198
	Ethanol	356	451	5917 (95)	0.260
	Methanol	355	460	6430 (105)	0.317
	Water	355	484	7550 (129)	0.117

Table S2. Absorbance and emission maxima of **7b** in dioxane, DMSO, ethanol, methanol and water. λ_{abs}, λ_{em} and Stokes shift are reported in nm, nm and cm^{-1} (nm). Quantum yield values were measured at λ_{abs} = 360 nm using quinine sulfate in 0.5 M H_2SO_4 (Φ_{fl} = 0.55) as the standard.

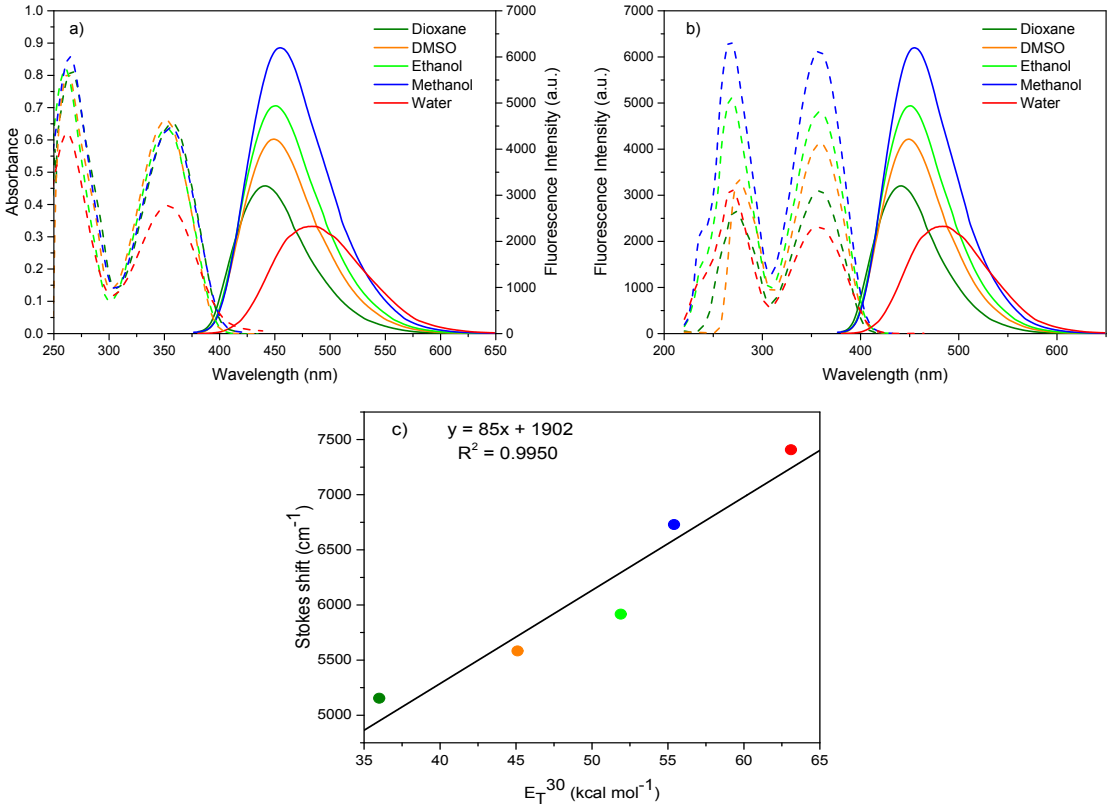


Figure S2. (a) Absorbance (30.0 μM, dash) and emission (5.0 μM, solid) spectra of **7b** in various solvents. (b) Excitation (dash line) and emission (solid line) spectra of **7b** in various solvents. (c) Linear relationship between stokes shift and solvent polarity of **7b** in various solvents.

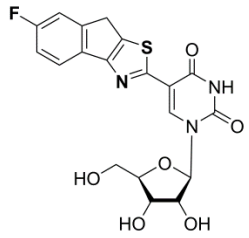
compound	solvent	λ_{abs}	λ_{em}	Stokes shift	ϕ
 **7c**	Dioxane	363	442	4924 (79)	0.123
	DMSO	359	449	5583 (90)	0.278
	Ethanol	358	452	5809 (94)	0.266
	Methanol	358	456	6003 (98)	0.294
	Water	359	489	7405 (130)	0.072

Table S3. Absorbance and emission maxima of **7c** in dioxane, DMSO, ethanol, methanol and water. λ_{abs}, λ_{em} and Stokes shift are reported in nm, nm and cm^{-1} (nm). Quantum yield values were measured at λ_{abs} = 360 nm using quinine sulfate in 0.5 M H_2SO_4 (Φ_{fl} = 0.55) as the standard.

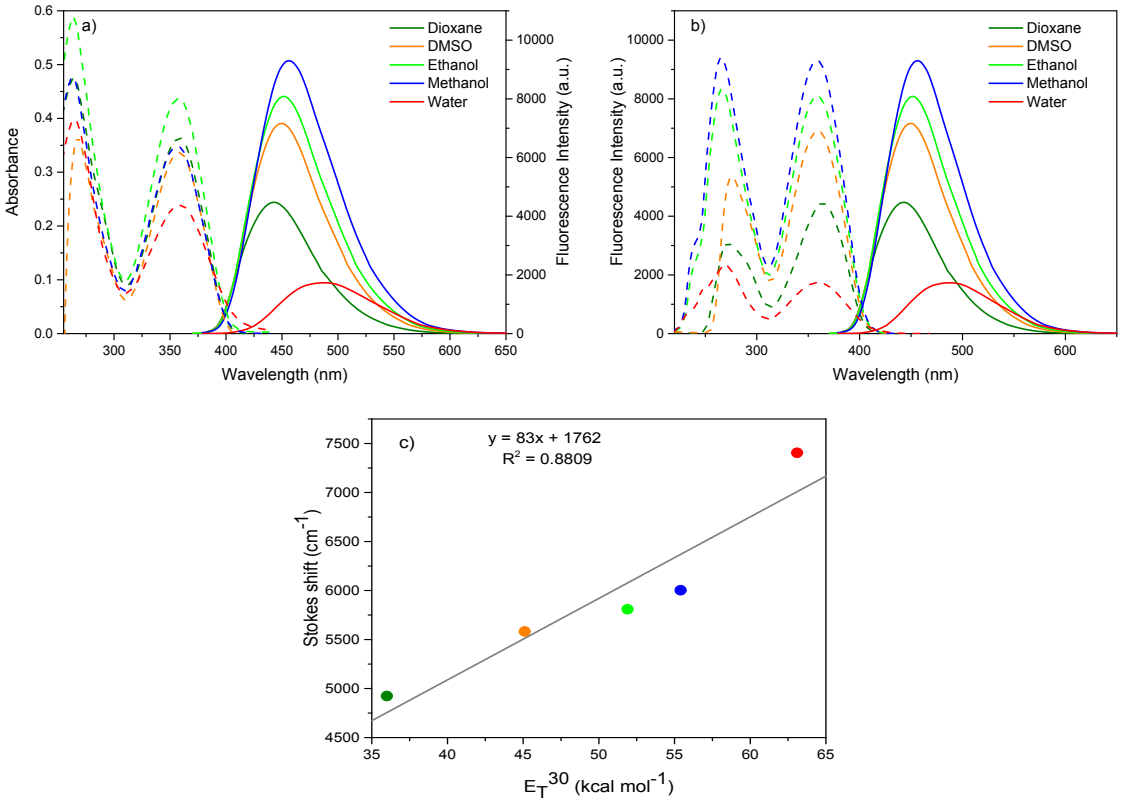


Figure S3. (a) Absorbance (30.0 μM, dash) and emission (10.0 μM, solid) spectra of **7c** in various solvents. (b) Excitation (dash line) and emission (solid line) spectra of **7c** in various solvents. (c) Linear relationship between stokes shift and solvent polarity of **7c** in various solvents.

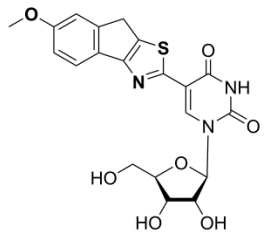
compound	solvent	λ_{abs}	λ_{em}	Stokes shift	ϕ
 **7d**	Dioxane	373	464	5257 (91)	0.331
	DMSO	373	490	6401 (117)	0.315
	Ethanol	372	495	6679 (123)	0.086
	Methanol	370	502	7107 (132)	0.044
	Water	371	507	7230 (136)	0.014

Table S4. Absorbance and emission maxima of **7d** in dioxane, DMSO, ethanol, methanol and water. λ_{abs}, λ_{em} and Stokes shift are reported in nm, nm and cm^{-1} (nm). Quantum yield values were measured at λ_{abs} = 360 nm using quinine sulfate in 0.5 M H_2SO_4 (Φ_{fl} = 0.55) as the standard.

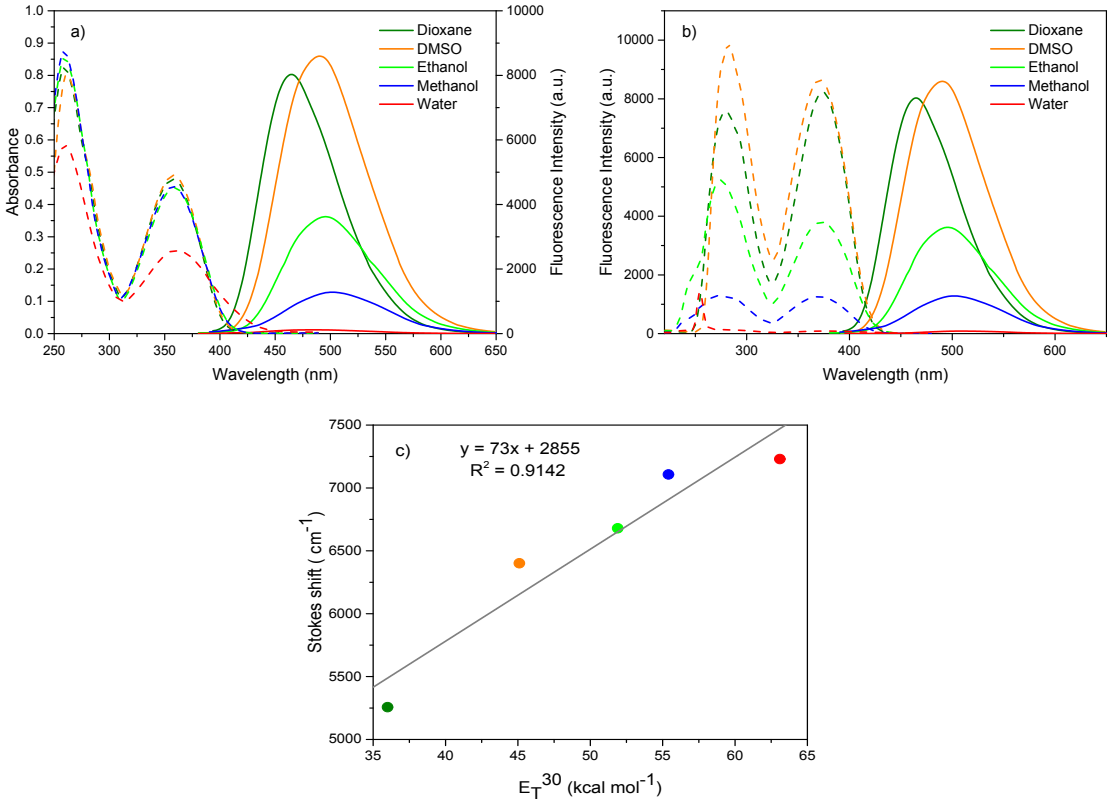


Figure S4. (a) Absorbance (30.0 μM, dash) and emission (10.0 μM, solid) spectra of **7d** in various solvents. (b) Excitation (dash line) and emission (solid line) spectra of **7d** in various solvents. (c) Linear relationship between stokes shift and solvent polarity of **7d** in various solvents.

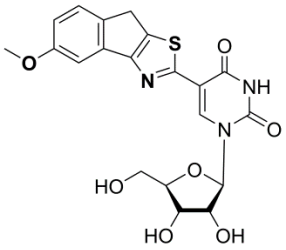
compound	solvent	λ_{abs}	λ_{em}	Stokes shift	ϕ
 **7e**	Dioxane	355	442	5544 (87)	0.082
	DMSO	360	455	5800 (95)	0.153
	Ethanol	360	461	6085 (101)	0.168
	Methanol	358	468	6565 (110)	0.153
	Water	360	499	7737(139)	0.014

Table S5. Absorbance and emission maxima of **7e** in dioxane, DMSO, ethanol, methanol and water. λ_{abs}, λ_{em} and Stokes shift are reported in nm, nm and cm^{-1}. Quantum yield values were measured at λ_{abs} = 360 nm using quinine sulfate in 0.5 M H_2SO_4 (Φ_{fl} = 0.55) as the standard.

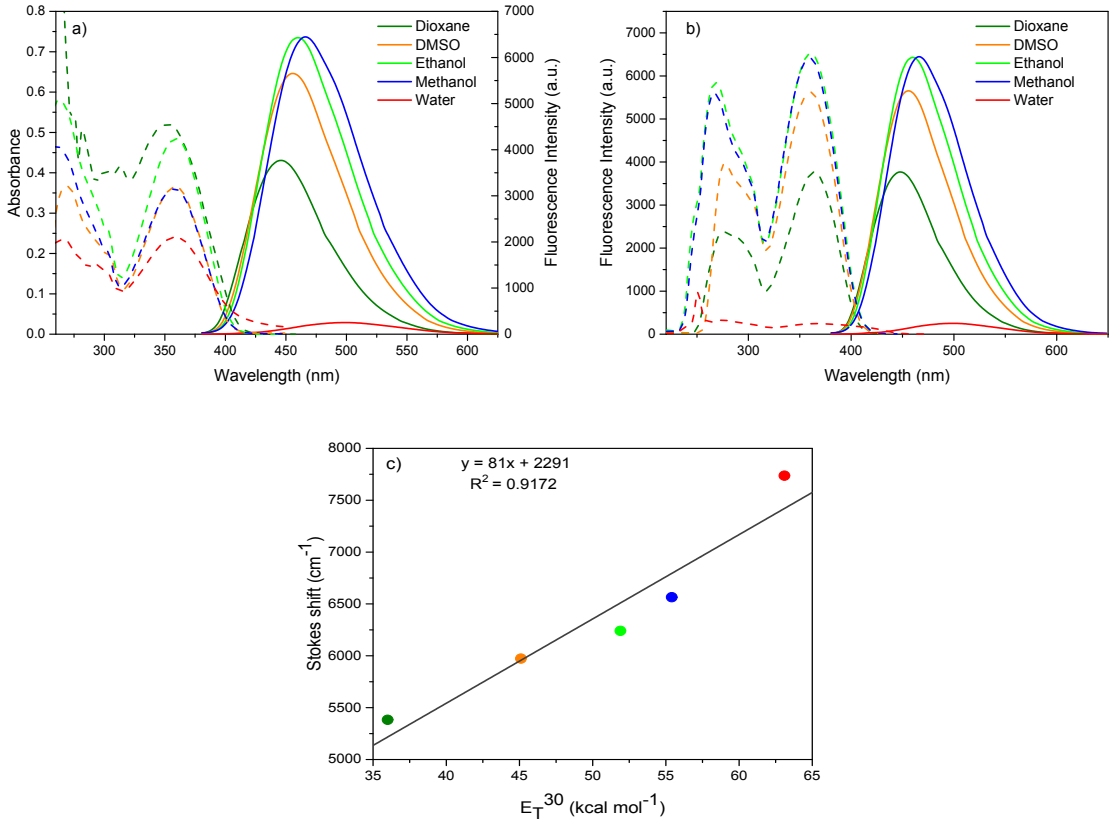


Figure S5. (a) Absorbance (30.0 μM, dash) and emission (10.0 μM, solid) spectra of **7e** in various solvents. (b) Excitation (dash line) and emission (solid line) spectra of **7e** in various solvents. (c) Linear relationship between stokes shift and solvent polarity of **7e** in various solvents.

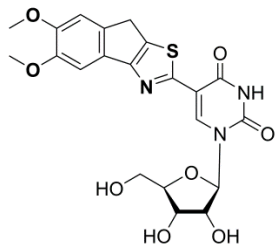
compound	solvent	λ_{abs}	λ_{em}	Stokes shift	ϕ
 **7f**	Dioxane	373	493	6526 (120)	0.267
	DMSO	373	518	7505 (145)	0.030
	Ethanol	373	520	7579 (147)	0.001
	Methanol	371	530	8080 (159)	0.001
	Water	370	539	8508 (169)	＜0.001

Table S6. Absorbance and emission maxima of **7f** in dioxane, DMSO, ethanol, methanol and water. λ_{abs}, λ_{em} and Stokes shift are reported in nm, nm and cm^{-1} (nm). Quantum yield values were measured at λ_{abs} = 360 nm using quinine sulfate in 0.5 M H_2SO_4 (Φ_{fl} = 0.55) as the standard.

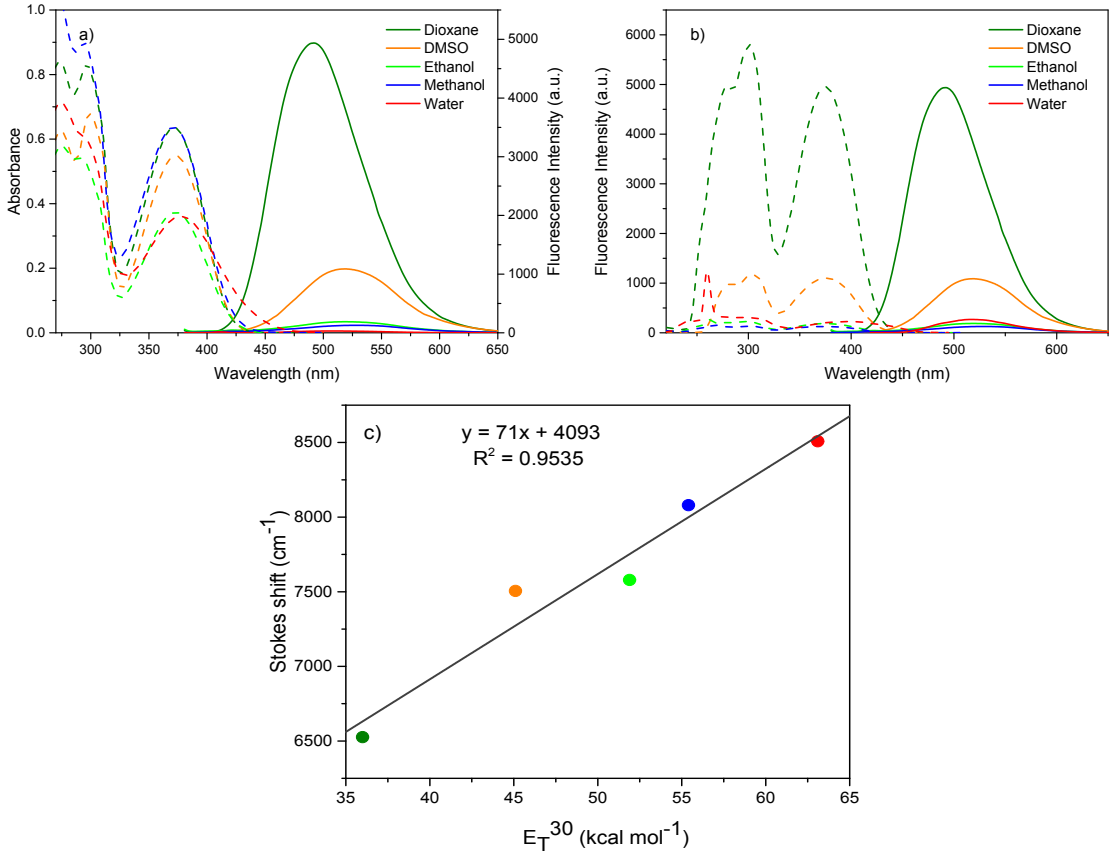


Figure S6. (a) Absorbance (50.0 μM, dash) and emission (10.0 μM, solid) spectra of **7f** in various solvents. (b) Excitation (dash line) and emission (solid line) spectra of **7f** in various solvents. (c) Linear relationship between stokes shift and solvent polarity of **7f** in various solvents.

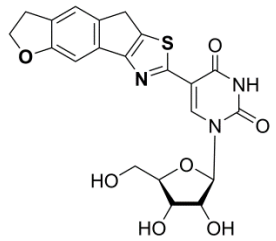
compound	solvent	λ_{abs}	λ_{em}	Stokes shift	ϕ
 **7g**	Dioxane	365	455	5419 (90)	0.097
	DMSO	363	473	6017 (110)	0.150
	Ethanol	365	486	6821 (121)	0.064
	Methanol	364	491	7106 (127)	0.019
	Water	374	508	7787 (134)	0.002

Table S7. Absorbance and emission maxima of **7g** in dioxane, DMSO, ethanol, methanol and water. λ_{abs}, λ_{em} and Stokes shift are reported in nm, nm and cm^{-1} (nm). Quantum yield values were measured at λ_{abs} = 360 nm using quinine sulfate in 0.5 M H_2SO_4 (Φ_{fl} = 0.55) as the standard.

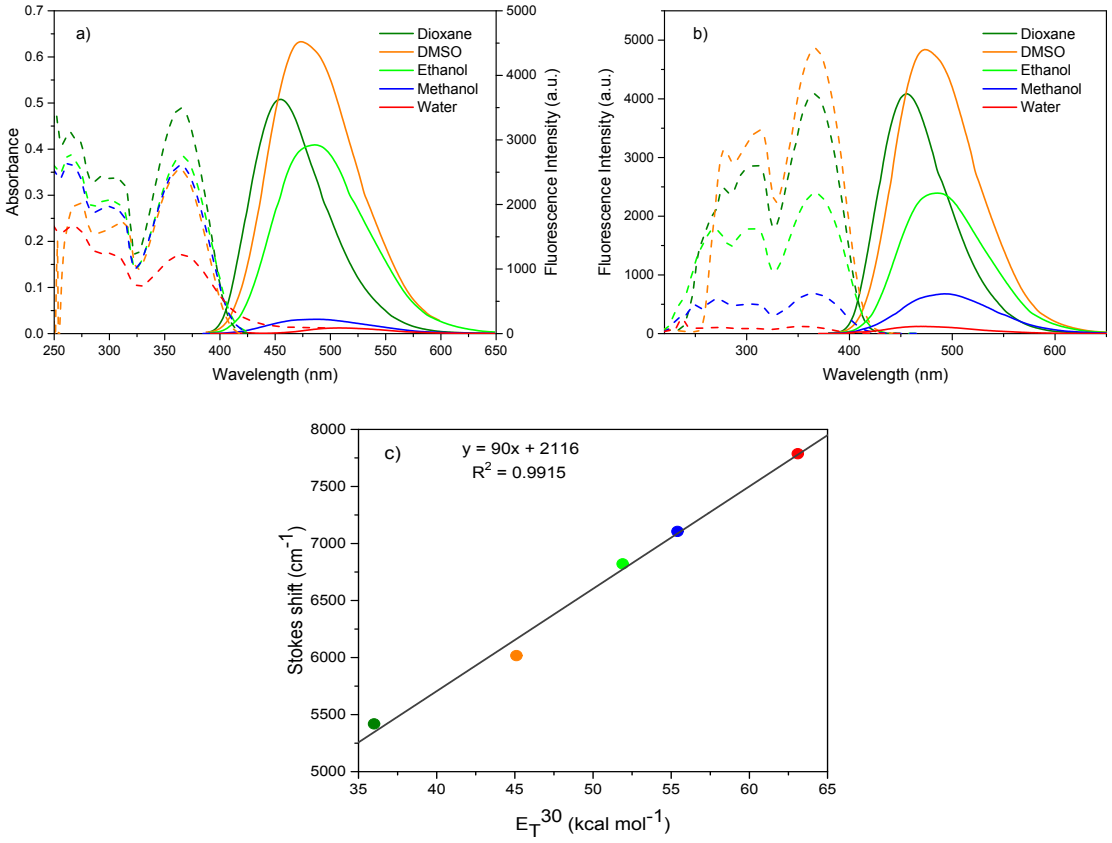


Figure S7. (a) Absorbance (30.0 μM, dash) and emission (10.0 μM, solid) spectra of **7g** in various solvents. (b) Excitation (dash line) and emission (solid line) spectra of **7g** in various solvents. (c) Linear relationship between stokes shift and solvent polarity of **7g** in various solvents.

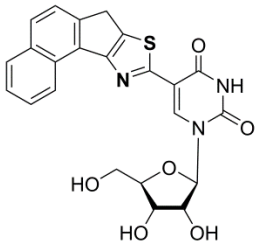
compound	solvent	λ_{abs}	λ_{em}	Stokes shift	ϕ
 **7h**	Dioxane	372	461	5190 (89)	0.071
	DMSO	375	472	5480 (97)	0.037
	Ethanol	370	484	6366 (114)	0.037
	Methanol	370	495	6825 (125)	0.033
	Water	412	522	5115 (110)	0.003

Table S8. Absorbance and emission maxima of **7h** in dioxane, DMSO, ethanol, methanol and water. λ_{abs}, λ_{em} and Stokes shift are reported in nm, nm and cm^{-1} (nm). Quantum yield values were measured at λ_{abs} = 360 nm using quinine sulfate in 0.5 M H_2SO_4 (Φ_{fl} = 0.55) as the standard.

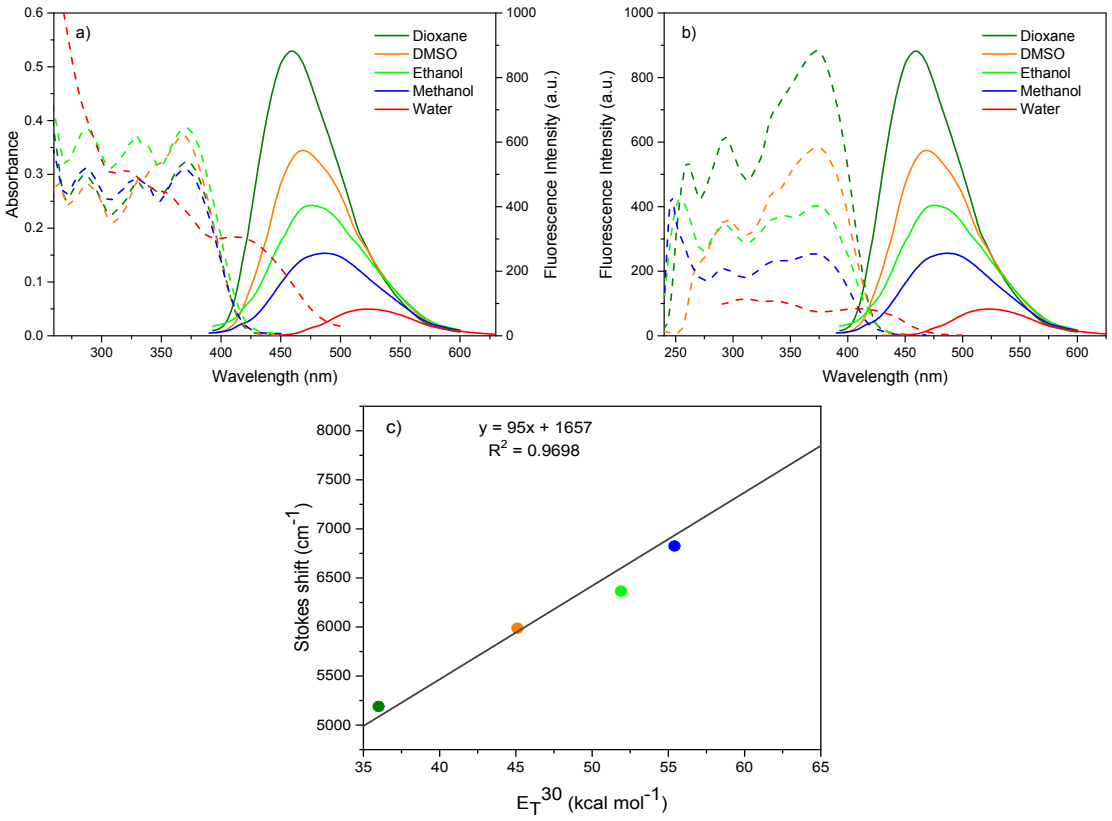


Figure S8. (a) Absorbance (30.0 μM, dash) and emission (10.0 μM, solid) spectra of **7h** in various solvents. (b) Excitation (dash line) and emission (solid line) spectra of **7h** in various solvents. (c) Linear relationship between stokes shift and solvent polarity of **7h** in various solvents.

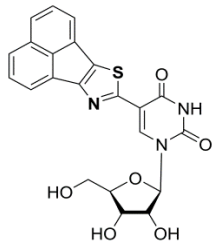
compound	solvent	λ_{abs}	λ_{em}	Stokes shift	ϕ
 **7i**	Dioxane	350	549	10356 (199)	0.004
	DMSO	351	552	10374 (201)	0.002
	Ethanol	348	547	10454 (199)	0.003
	Methanol	348	549	10521 (201)	0.004
	Water	350	557	10618 (207)	0.001

Table S9. Absorbance and emission maxima of **7i** in dioxane, DMSO, ethanol, methanol and water. λ_{abs}, λ_{em} and Stokes shift are reported in nm, nm and cm^{-1} (nm). Quantum yield values were measured at λ_{abs} = 360 nm using quinine sulfate in 0.5 M H_2SO_4 (Φ_{fl} = 0.55) as the standard.

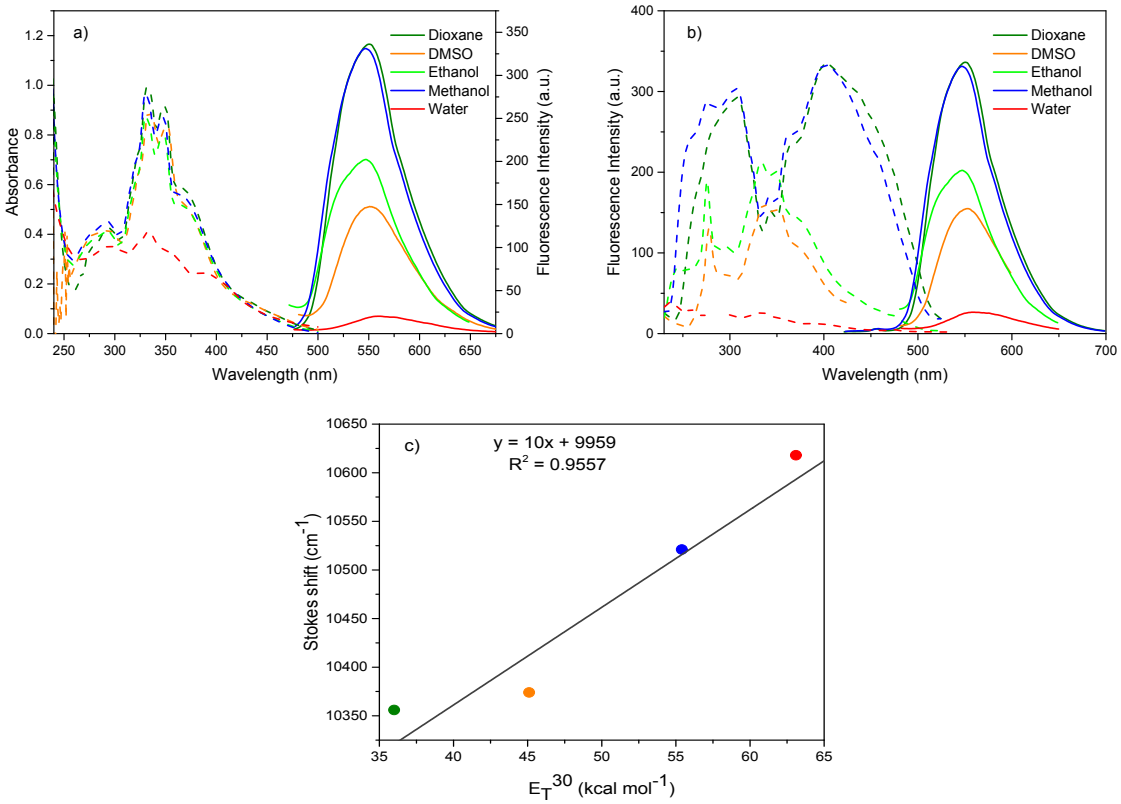


Figure S9. (a) Absorbance (30.0 μM, dash) and emission (10.0 μM, solid) spectra of **7i** in various solvents. (b) Excitation (dash line) and emission (solid line) spectra of **7i** in various solvents. (c) Linear relationship between stokes shift and solvent polarity of **7i** in various solvents.

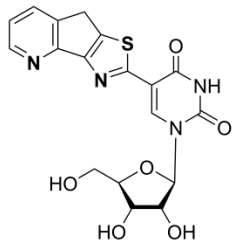
compound	solvent	λ_{abs}	λ_{em}	Stokes shift	ϕ
 **7j**	Dioxane	354	420	4439 (66)	0.082
	DMSO	354	435	5260 (81)	0.124
	Ethanol	347	425	5289 (78)	0.101
	Methanol	347	428	5454 (81)	0.112
	Water	347	447	6447 (100)	0.161

Table S10. Absorbance and emission maxima of **7j** in dioxane, DMSO, ethanol, methanol and water. λ_{abs}, λ_{em} and Stokes shift are reported in nm, nm and cm^{-1} (nm). Quantum yield values were measured at λ_{abs} = 360 nm using quinine sulfate in 0.5 M H_2SO_4 (Φ_{fl} = 0.55) as the standard.

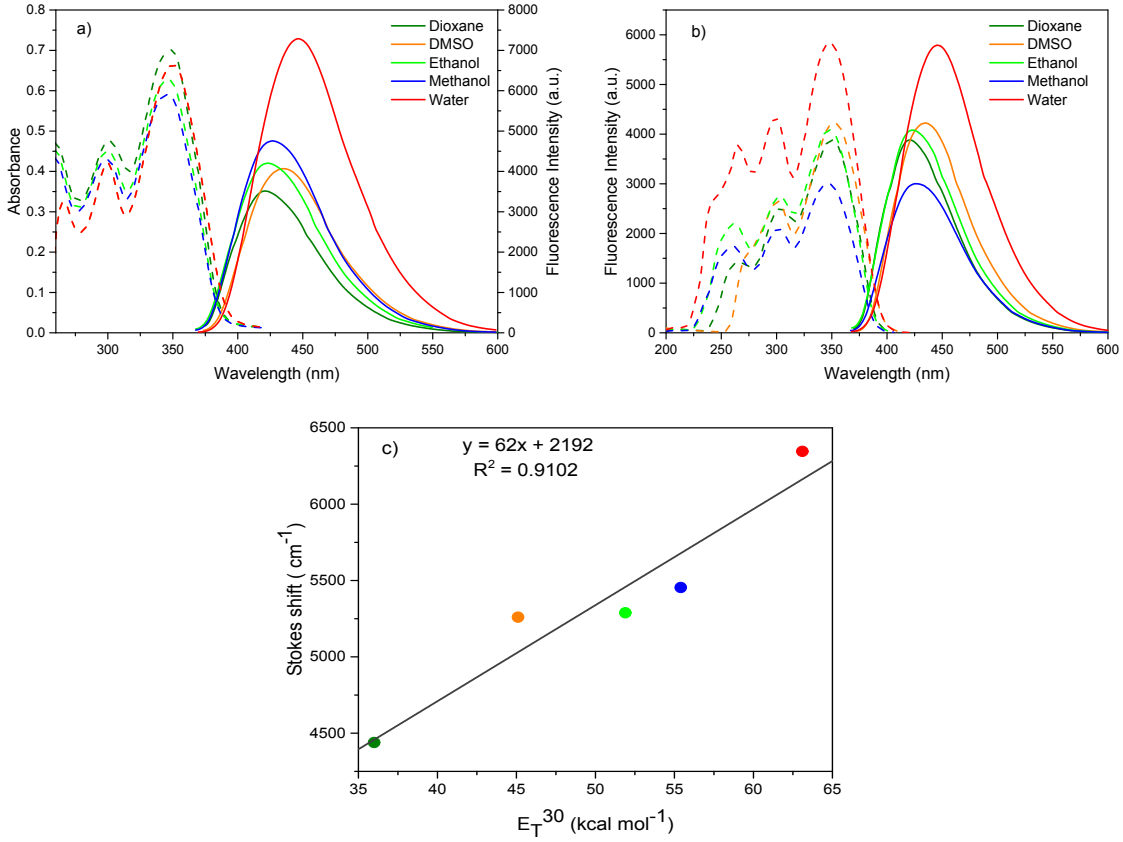


Figure S10. (a) Absorbance (30 μM, dash) and emission (10.0 μM, solid) spectra of **7j** in .and mixtures (grey). (b) Excitation (dash line) and emission (solid line) spectra of **7j** in various solvents. (c) Linear relationship between stokes shift and solvent polarity of **7j** in various solvents.

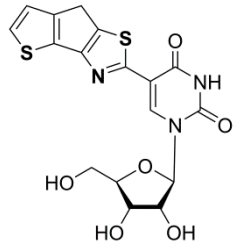
compound	solvent	λ_{abs}	λ_{em}	Stokes shift	ϕ
 **7k**	Dioxane	369	468	5733 (99)	0.039
	DMSO	371	493	6670 (122)	0.042
	Ethanol	372	496	6720 (124)	0.039
	Methanol	371	502	7034 (131)	0.040
	Water	372	535	8190 (163)	0.002

Table S11. Absorbance and emission maxima of **7k** in dioxane, DMSO, ethanol, methanol and water. λ_{abs}, λ_{em} and Stokes shift are reported in nm, nm and cm^{-1} (nm). Quantum yield values were measured at λ_{abs} = 365 nm using quinine sulfate in 0.5 M H_2SO_4 (Φ_{fl} = 0.55) as the standard.

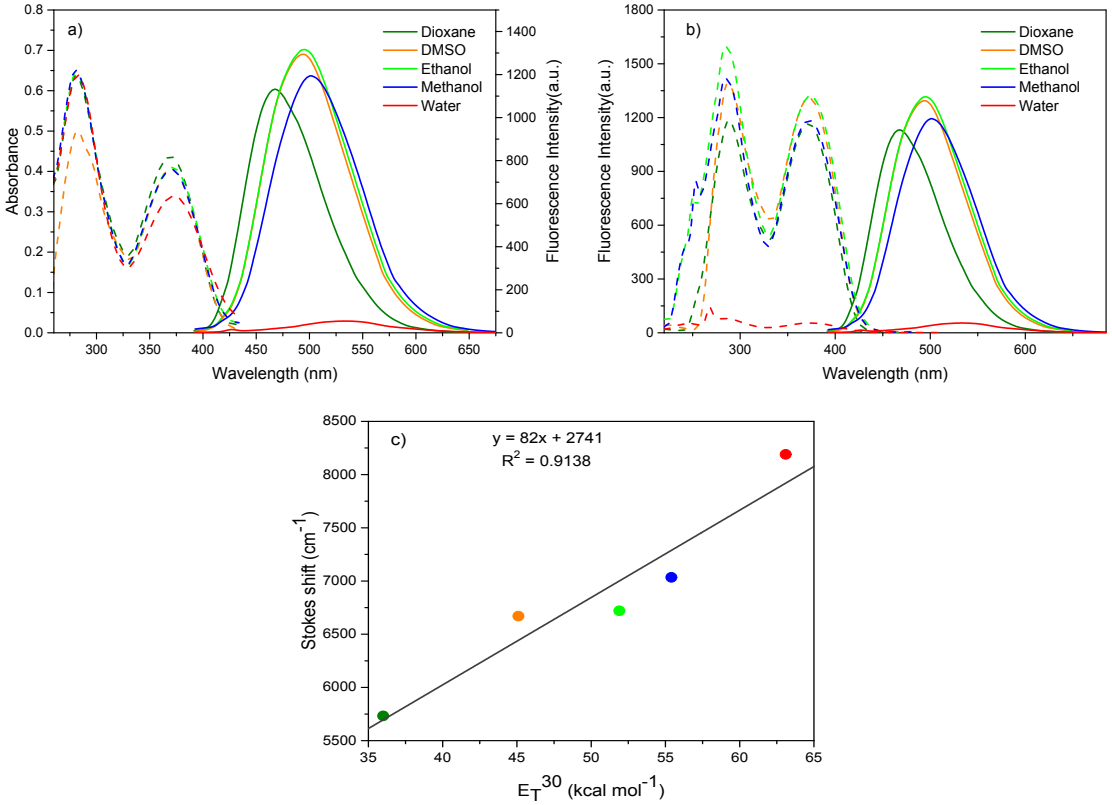


Figure S11. (a) Absorbance (30.0 μM, dash) and emission (10.0 μM, solid) spectra of **7k** in various solvents. (b) Excitation (dash line) and emission (solid line) spectra of **7k** in various solvents. (c) Linear relationship between stokes shift and solvent polarity of **7k** in various solvents.

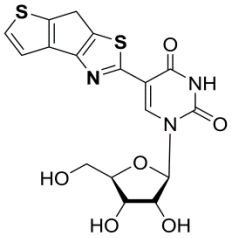
compound	solvent	λ_{abs}	λ_{em}	Stokes shift	ϕ
 **7l**	Dioxane	363	456	5666 (93)	0.091
	DMSO	364	473	6331 (109)	0.176
	Ethanol	360	474	6681 (116)	0.175
	Methanol	363	486	6972 (123)	0.157
	Water	364	513	7979 (149)	0.005

Table S12. Absorbance and emission maxima of **7l** in dioxane, DMSO, ethanol, methanol and water. λ_{abs}, λ_{em} and Stokes shift are reported in nm, nm and cm^{-1} (nm). Quantum yield values were measured at λ_{abs} = 360 nm using quinine sulfate in 0.5 M H_2SO_4 (Φ_{fl} = 0.55) as the standard.

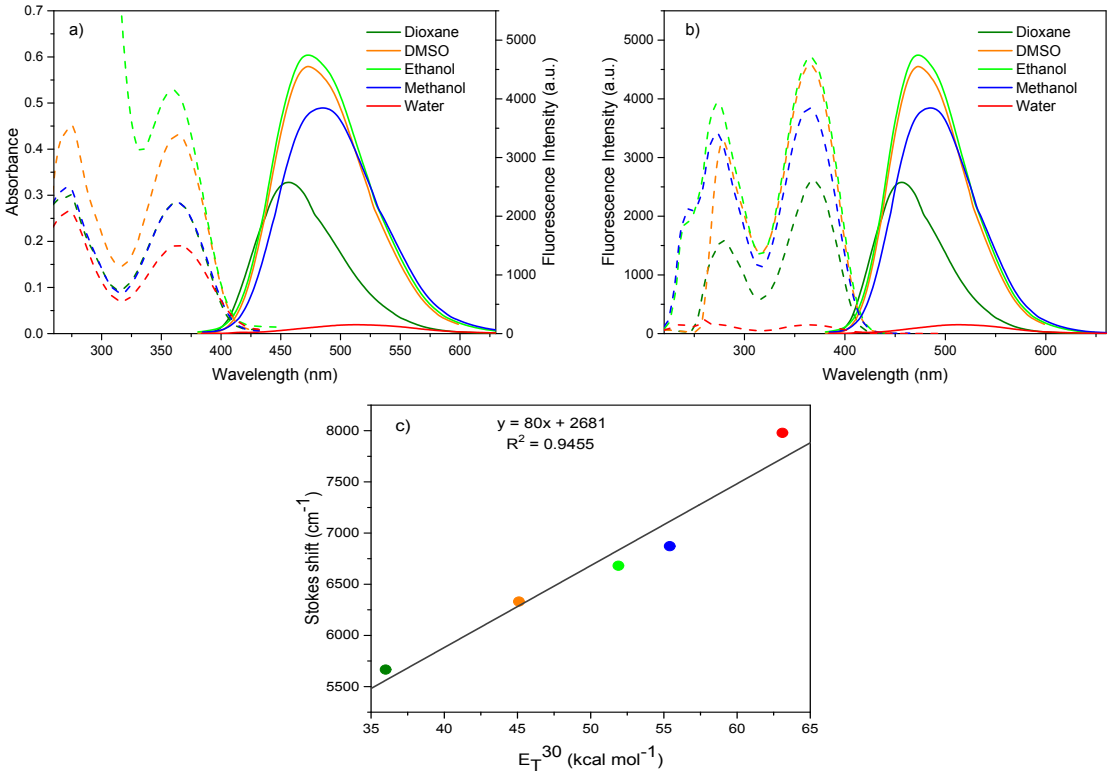


Figure S12. (a) Absorbance (30.0 μM, dash) and emission (10.0 μM, solid) spectra of **7l** in various solvents. (b) Excitation (dash line) and emission (solid line) spectra of **7l** in various solvents. (c) Linear relationship between stokes shift and solvent polarity of **7l** in various solvents.

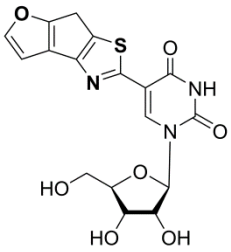
compound	solvent	λ_{abs}	λ_{em}	Stokes shift	ϕ
 **7m**	Dioxane	370	464	5475 (94)	0.126
	DMSO	368	488	6682 (120)	0.181
	Ethanol	368	492	6849 (124)	0.143
	Methanol	367	497	7127 (130)	0.069
	Water	356	485	7471 (129)	0.005

Table S13. Absorbance and emission maxima of **7m** in dioxane, DMSO, ethanol, methanol and water. λ_{abs}, λ_{em} and Stokes shift are reported in nm, nm and cm^{-1} (nm). Quantum yield values were measured at λ_{abs} = 360 nm using quinine sulfate in 0.5 M H_2SO_4 (Φ_{fl} = 0.55) as the standard.

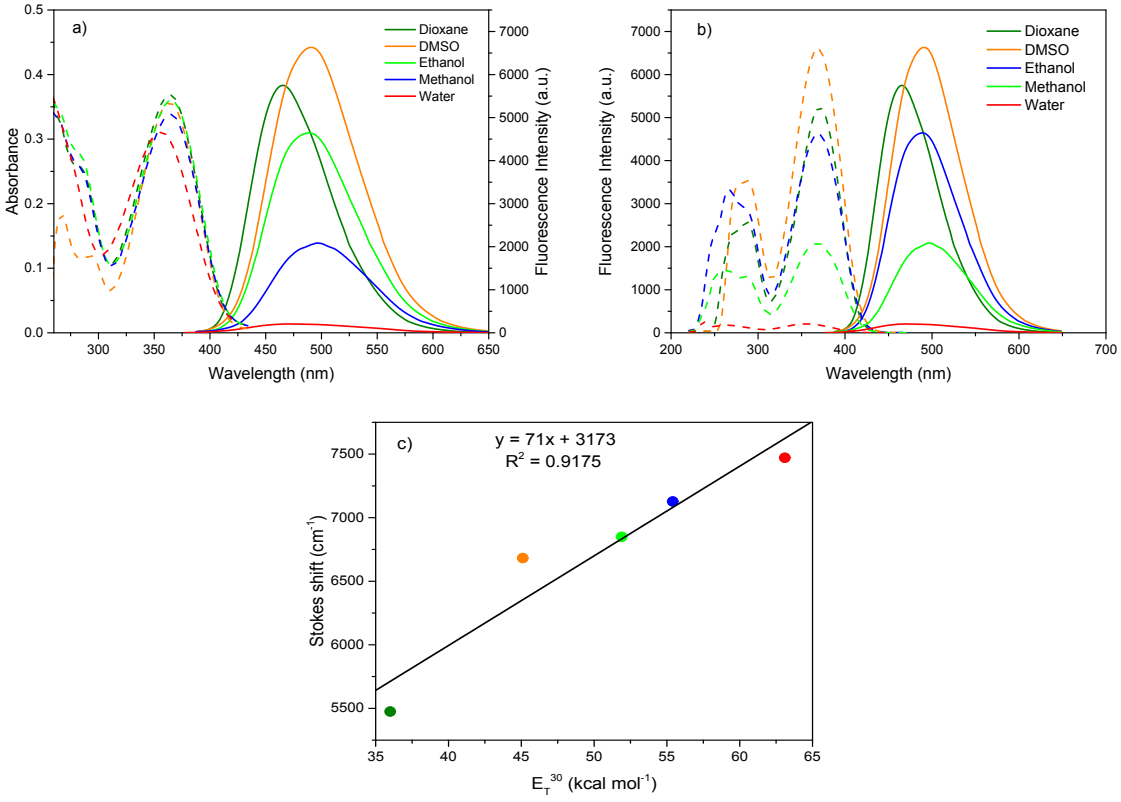
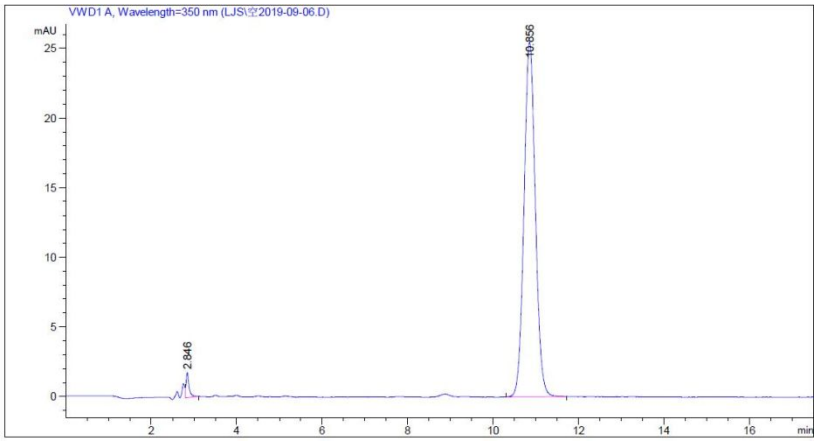


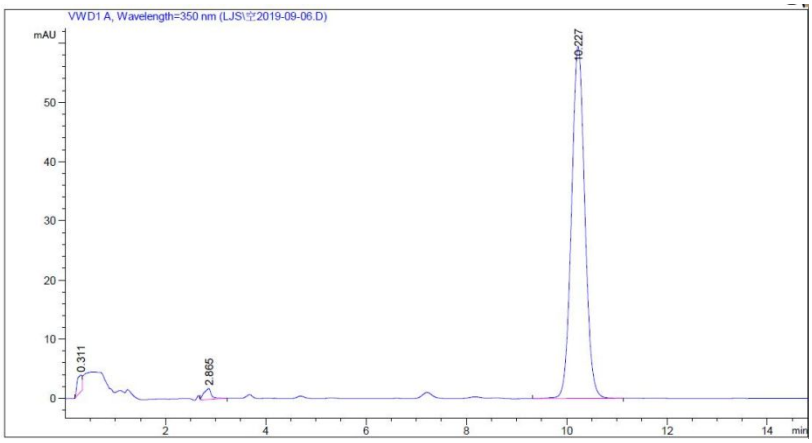
Figure S13. (a) Absorbance (30.0 μM, dash) and emission (10.0 μM, solid) spectra of **7m** in various solvents.(b) Excitation (dash line) and emission (solid line) spectra of **7m** in various solvents. (c) Linear relationship between stokes shift and solvent polarity of **7m** in various solvents.

LC chromatograms of compound 7b, 7c, 7e and 7l at pH 1, 7 and 13.

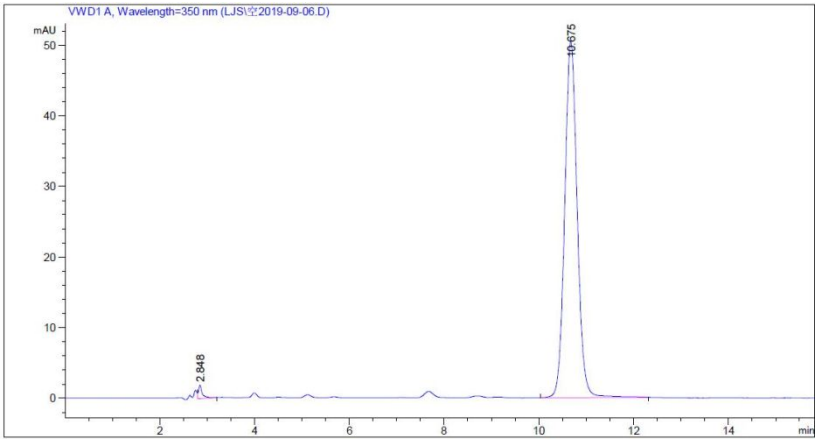
(a) pH = 7 time = 0 h



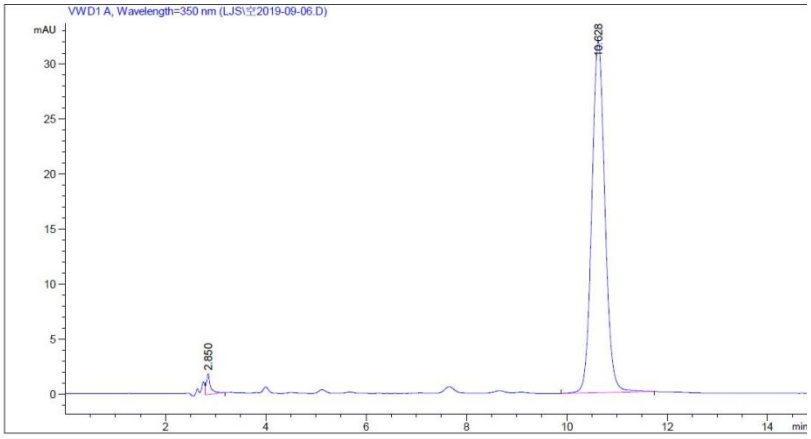
(b) pH = 1 time = 0 h



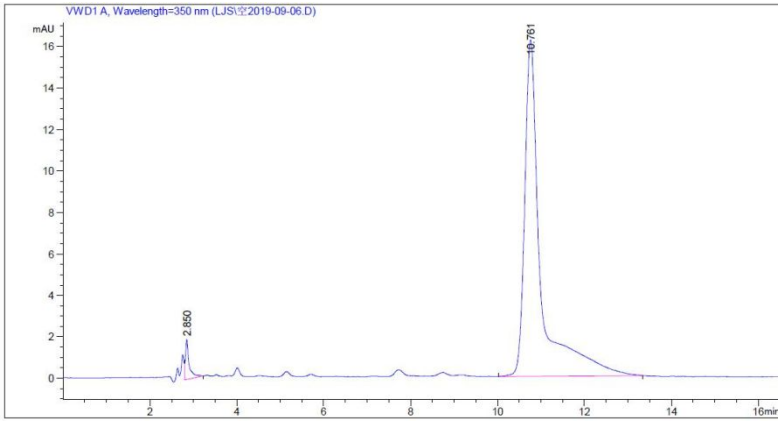
(c) pH = 1 time = 0 h



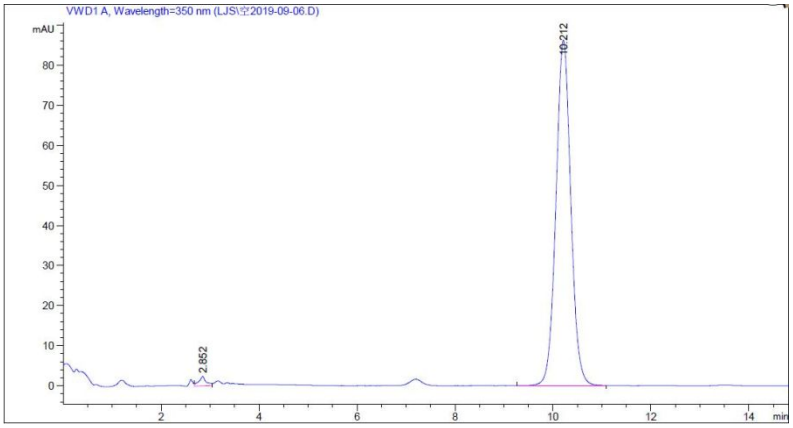
(d) pH = 1 time = 1 h



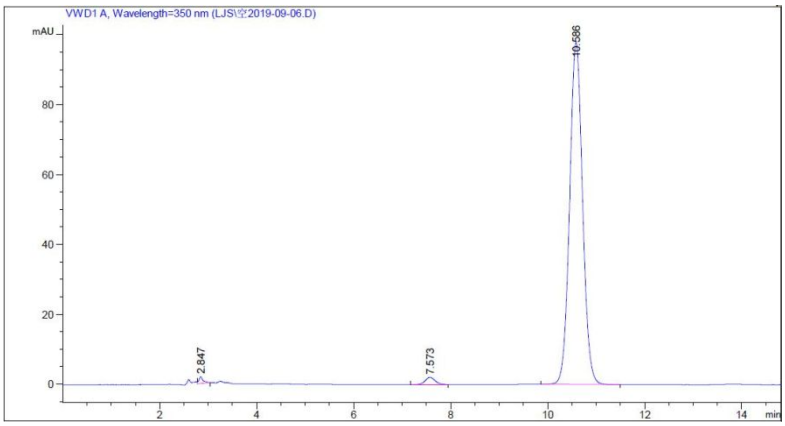
(e) pH = 1 time = 3 h



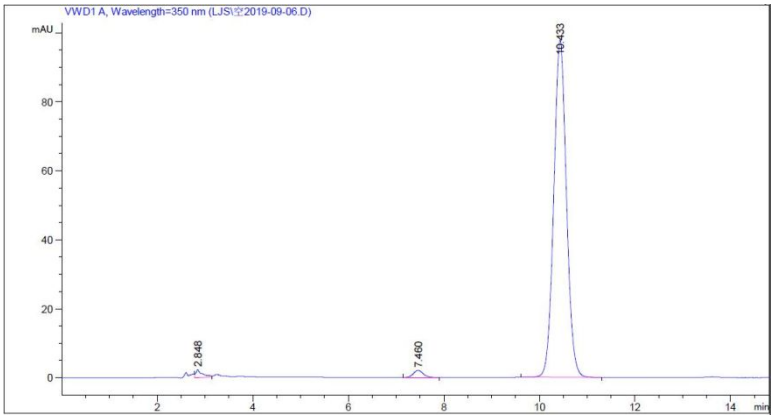
(f) pH = 13 time = 0 h



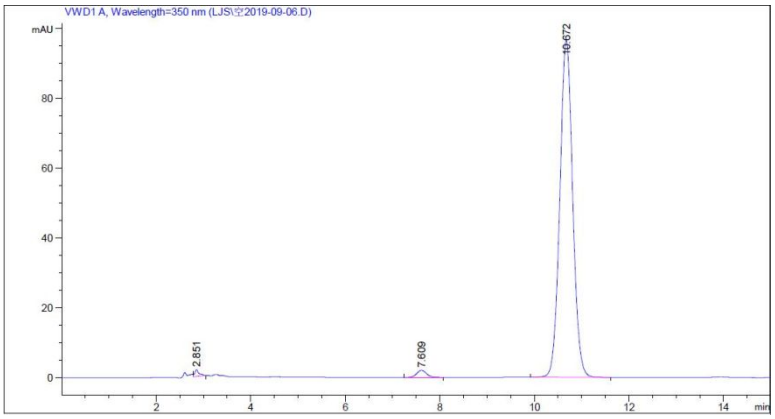
(g) pH = 13 time = 0.5 h



(h) pH = 13 time = 1 h

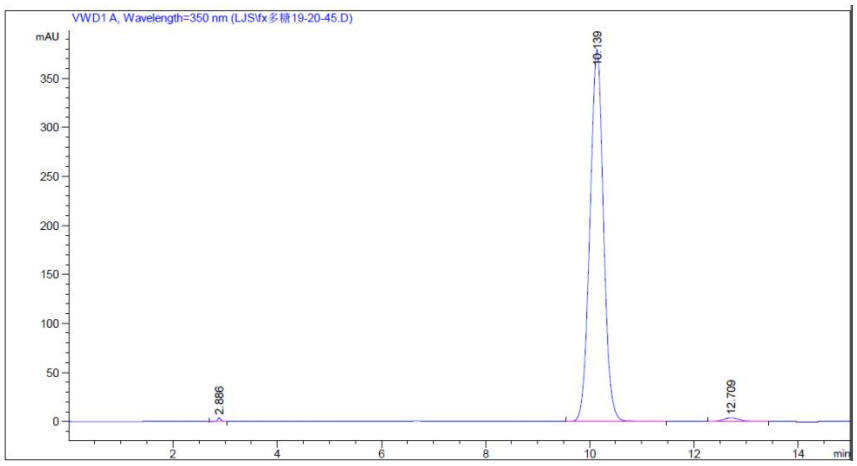


(i) pH = 13 time = 3 h

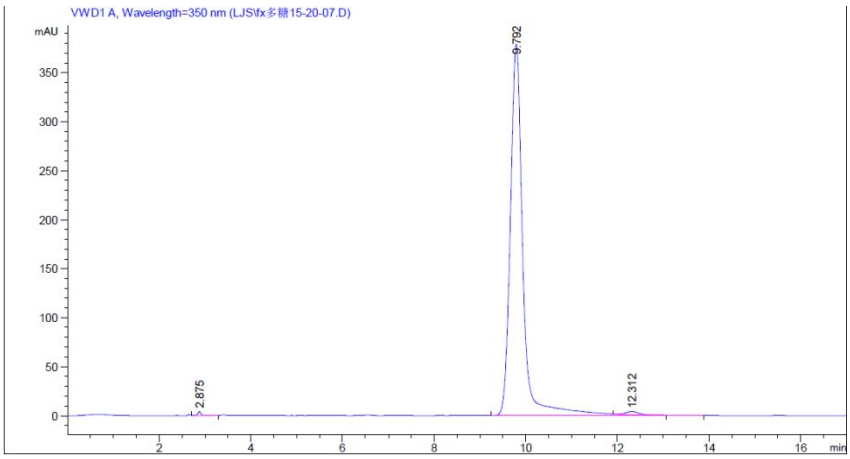


S14 HPLC profiles (column 250 × 10 mm, RP-18) of the **7b** at room temperature (a) in pH=7; (b) in pH=1, after 0 h; (c) in pH=1, after 0.5 h; (d) in pH=1, after 1 h; (e) in pH=1, after 3 h; (f) in pH=13, after 0 h; (g) in pH=13, after 0.5 h; (h) in pH=13, after 1 h; (i) in pH=3h, after 3 h. Buffer: 45% MeOH in aqueous 10 mM phosphate, pH = 7.0, 1.0 mL min^{-1}. The profile was measured at 350 nm.

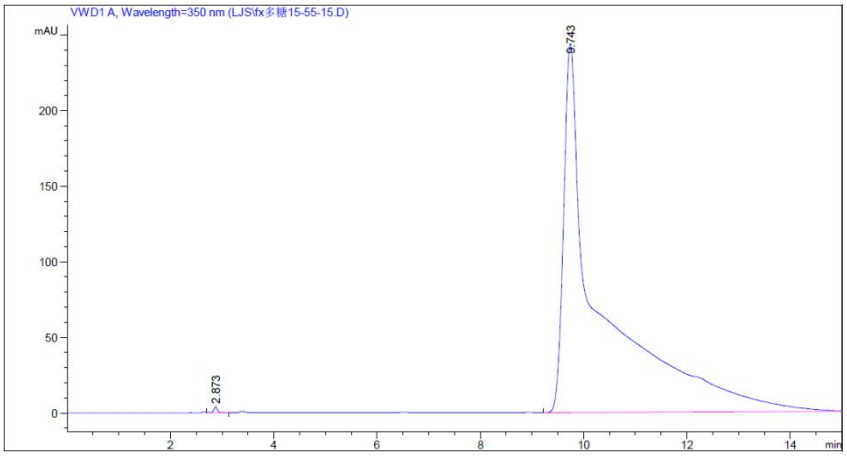
(a) pH = 7.0



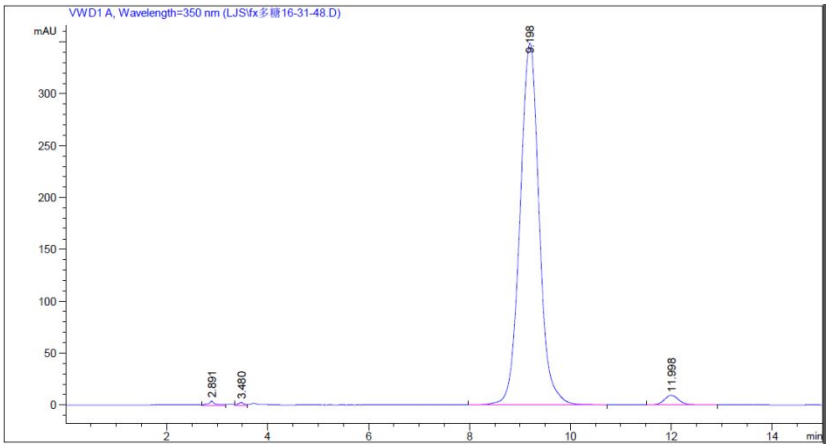
(b) pH = 1 time = 0 h



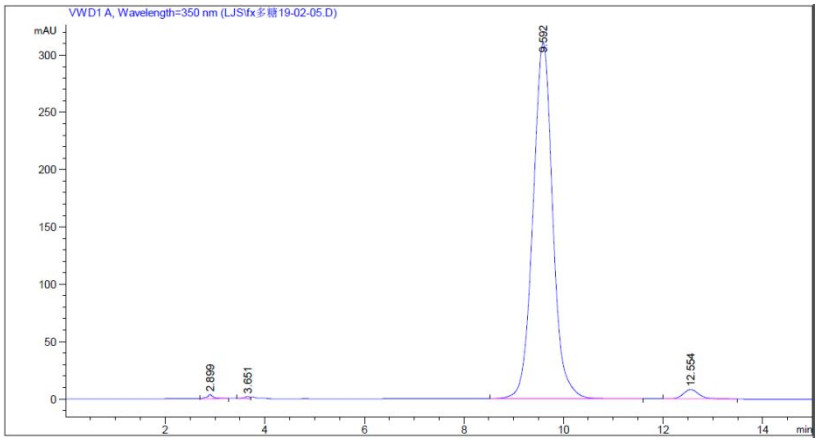
(c) pH = 1 time = 0.5 h



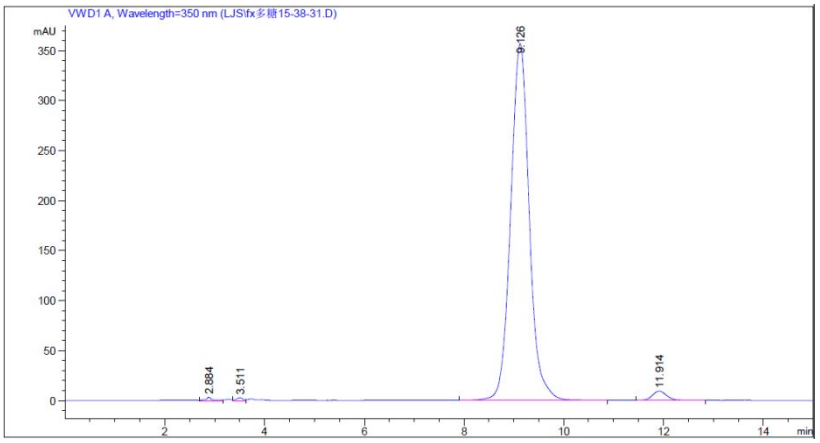
(d) pH = 1 time = 1 h



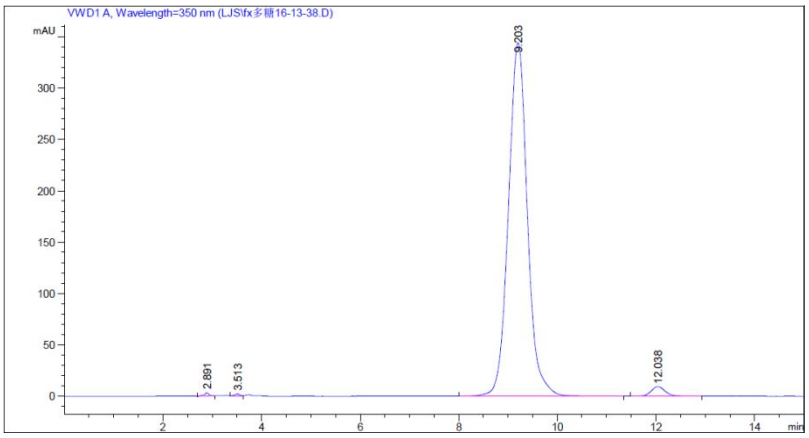
(e) pH = 1 time = 3 h



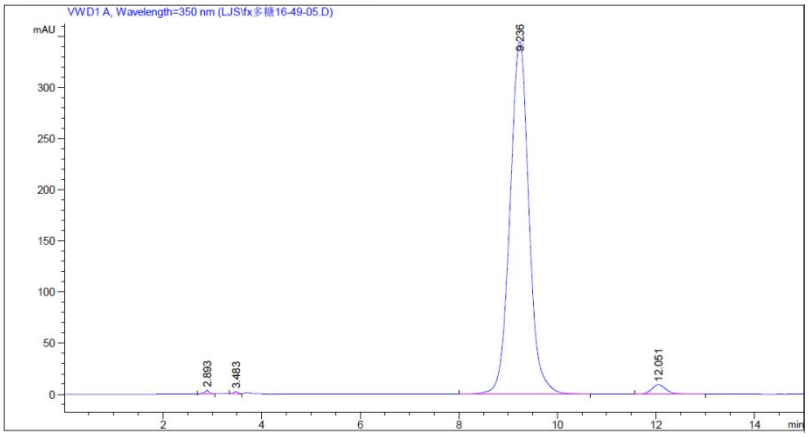
(f) pH = 13 time = 0 h



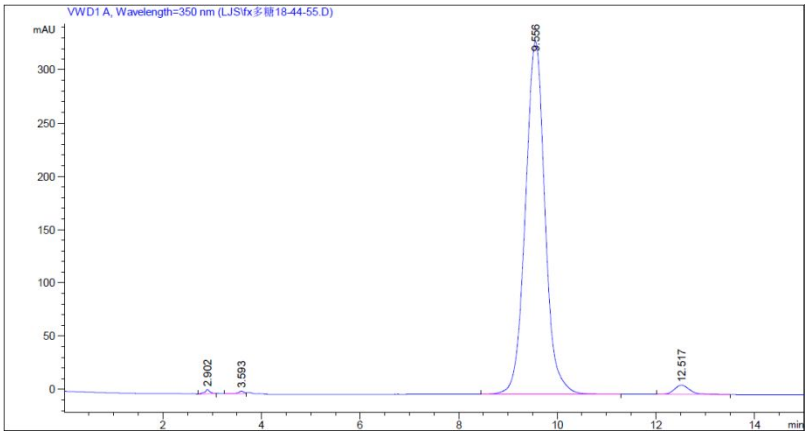
(g) pH = 13 time = 0.5 h



(h) pH = 13 time = 1 h

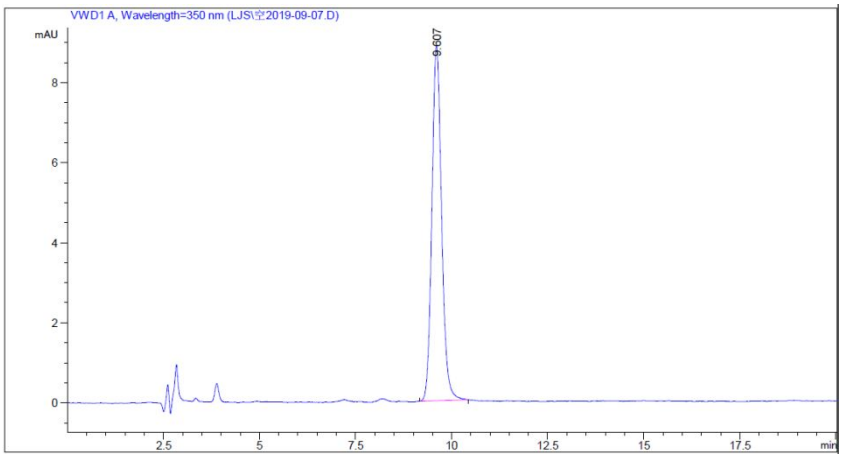


(i) pH = 13 time = 3 h

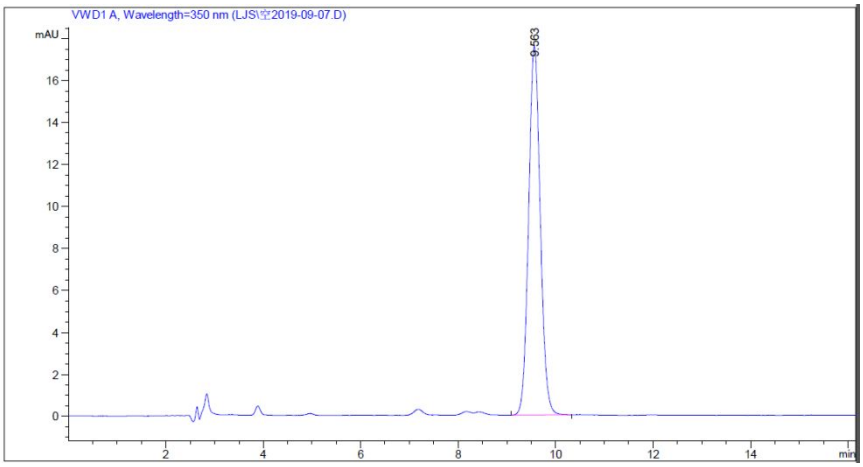


S15 HPLC profiles (column 250 × 10 mm, RP-18) of the **7c** at room temperature (a) in pH=7; (b) in pH=1, after 0 h; (c) in pH=1, after 0.5 h; (d) in pH=1, after 1 h; (e) in pH=1, after 3 h; (f) in pH=13, after 0 h; (g) in pH=13, after 0.5 h; (h) in pH=13, after 1 h; (i) in pH=3h, after 3 h. Buffer: 45% MeOH in aqueous 10 mM phosphate, pH = 7.0, 1.0 mL min^{-1}. The profile was measured at 350 nm.

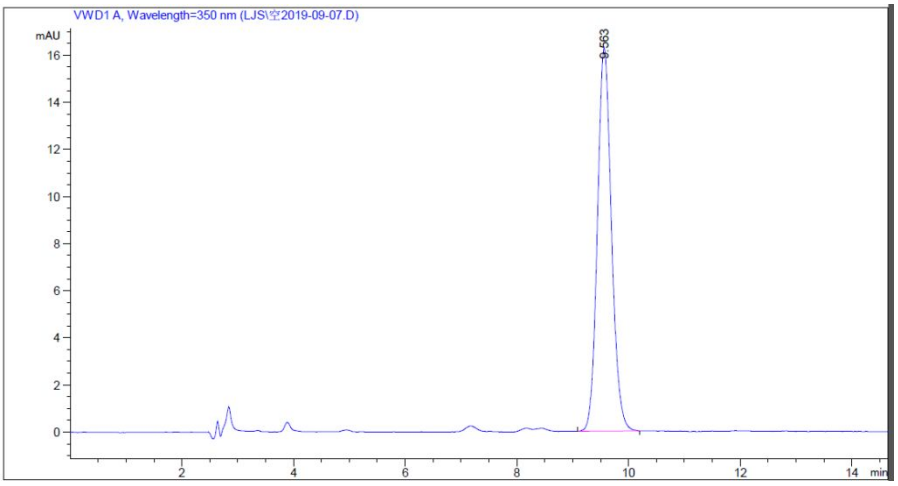
(a) pH = 7



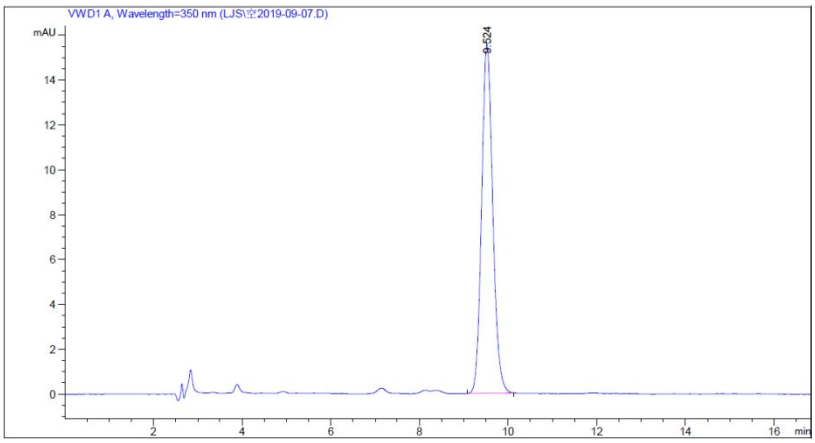
(b) pH = 1 time = 0 h



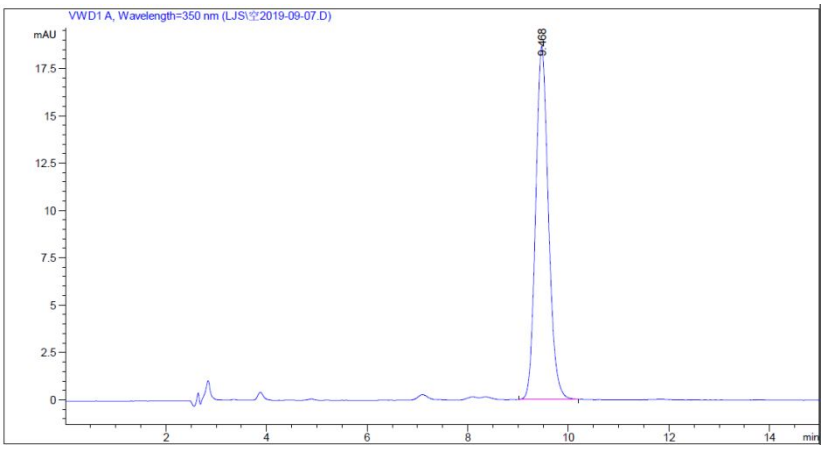
(c) pH = 1 time = 0.5 h



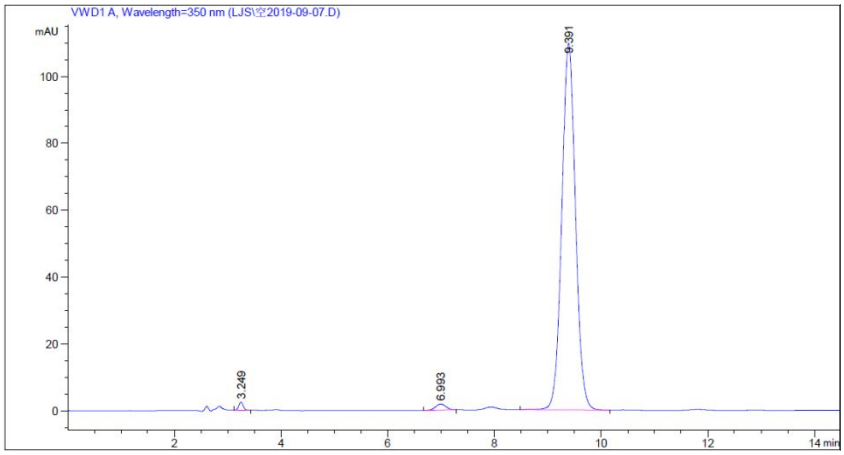
(d) pH = 1 time = 1 h



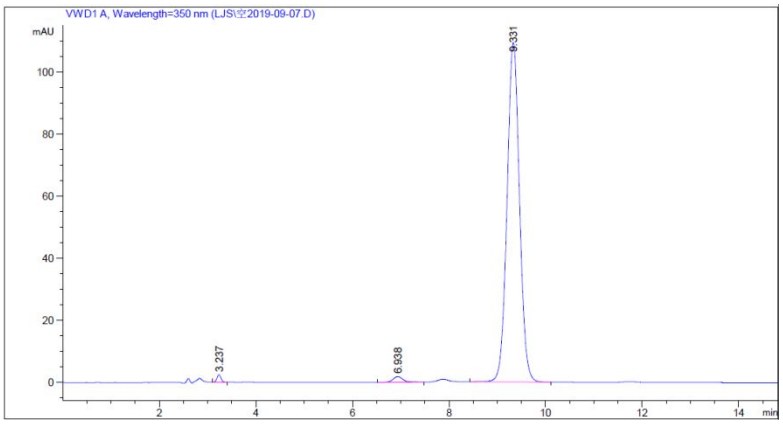
(e) pH = 1 time = 3 h



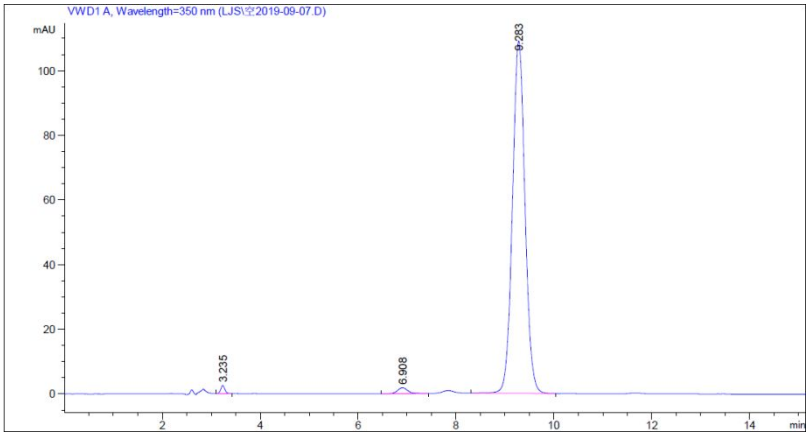
(f) pH = 13 time = 0 h



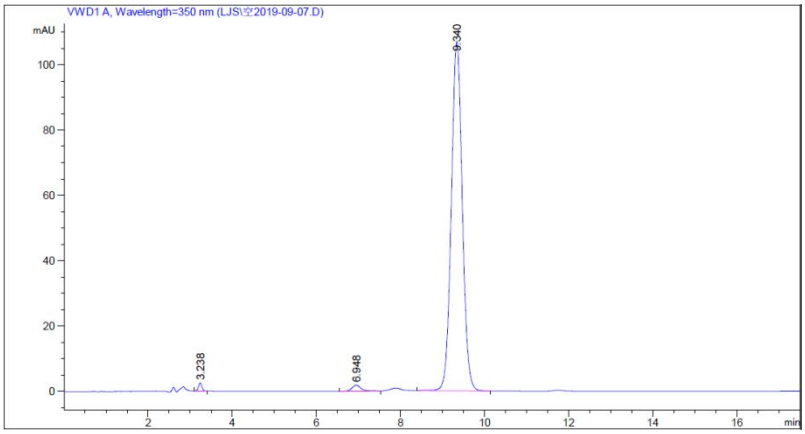
(g) pH = 13 time = 0.5 h



(h) pH = 13 time = 1 h

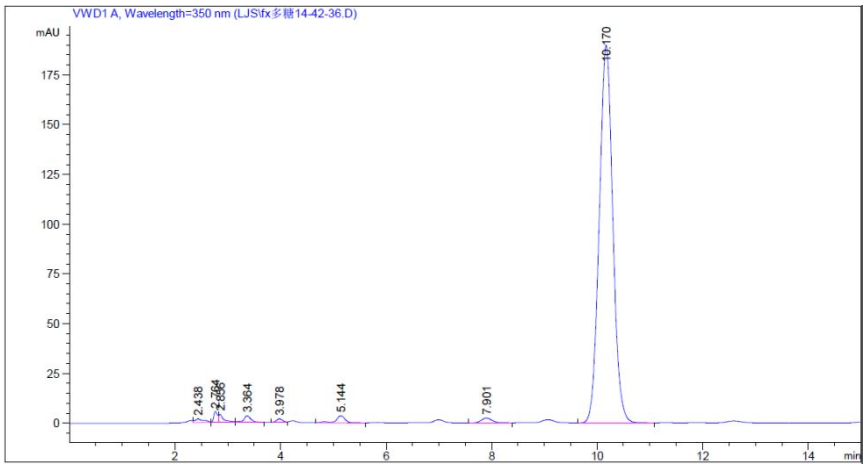


(i) pH = 13 time = 3 h

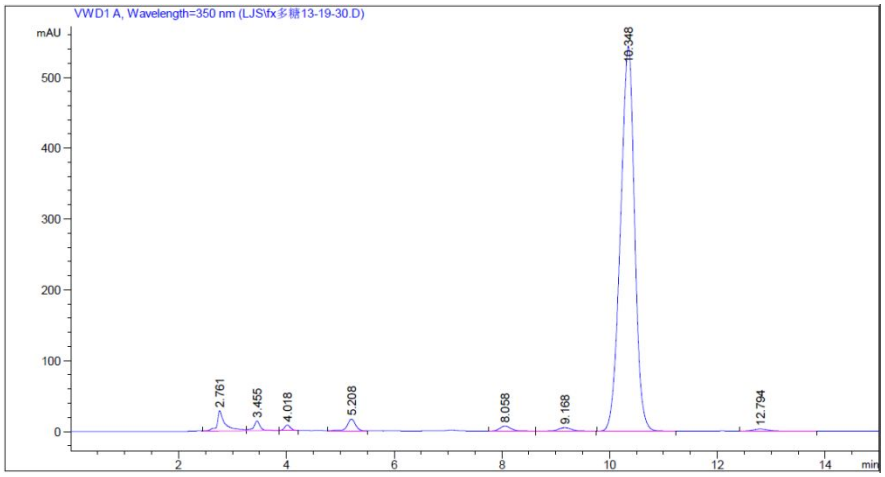


S16 HPLC profiles (column 250 × 10 mm, RP-18) of the **7e** at room temperature (a) in pH=7; (b) in pH=1, after 0 h; (c) in pH=1, after 0.5 h; (d) in pH=1, after 1 h; (e) in pH=1, after 3 h; (f) in pH=13, after 0 h; (g) in pH=13, after 0.5 h; (h) in pH=13, after 1 h; (i) in pH=3h, after 3 h. Buffer: 45% MeOH in aqueous 10 mM phosphate, pH = 7.0, 1.0 mL min^{-1}. The profile was measured at 350 nm.

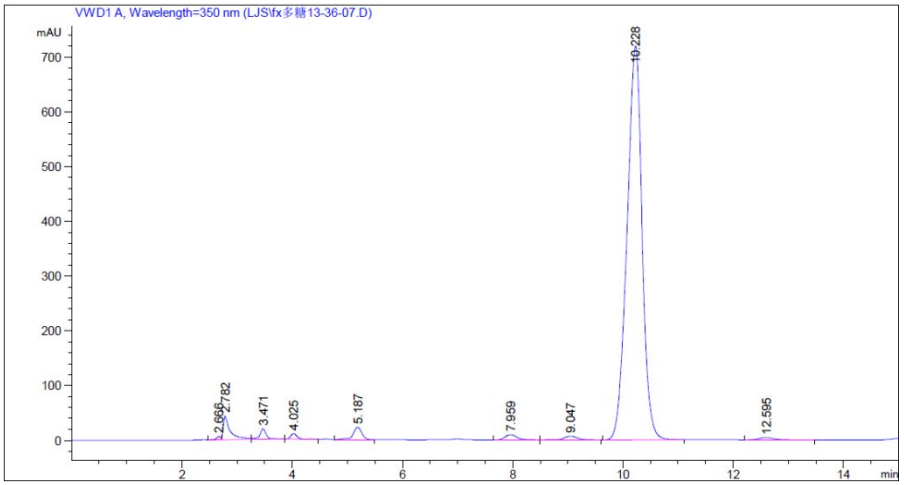
(a) pH = 7



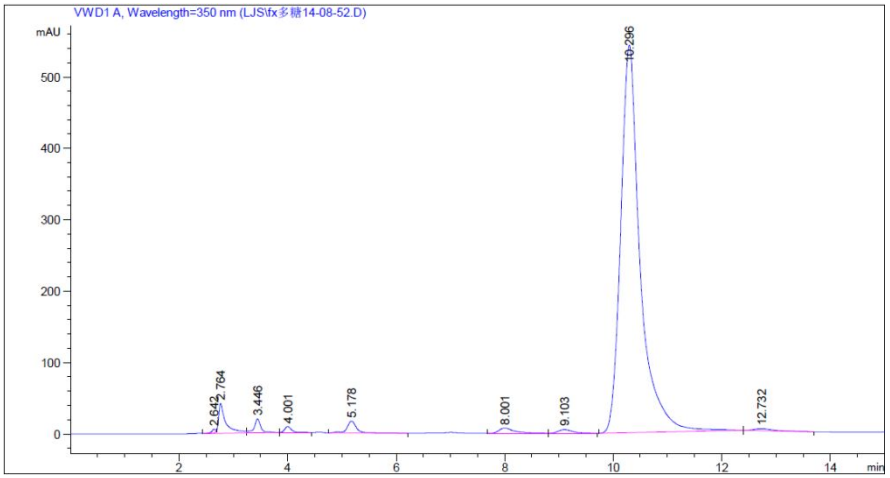
(b) pH = 1 time = 0 h



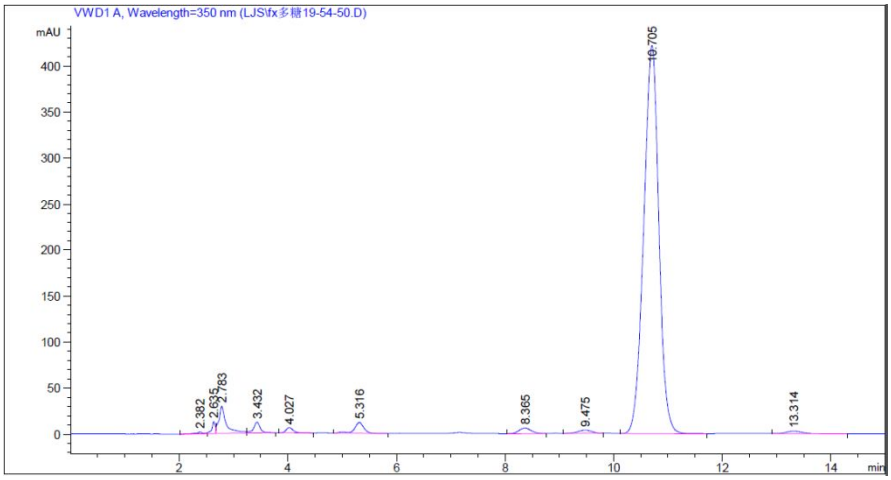
(c) pH = 1 time = 0.5 h



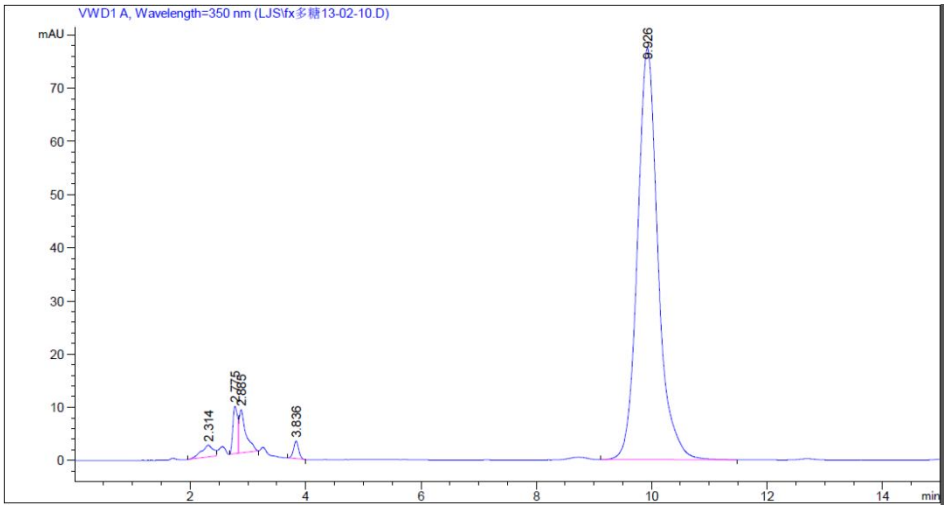
(d) pH = 1 time = 1 h



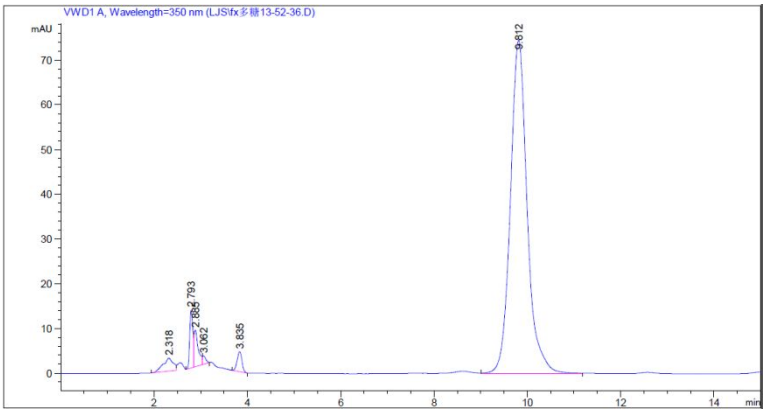
(e) pH = 1 time = 3 h



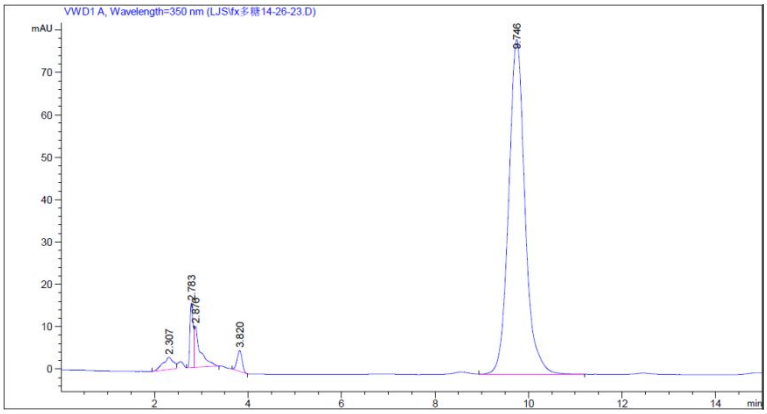
(f) pH = 13 time = 0 h



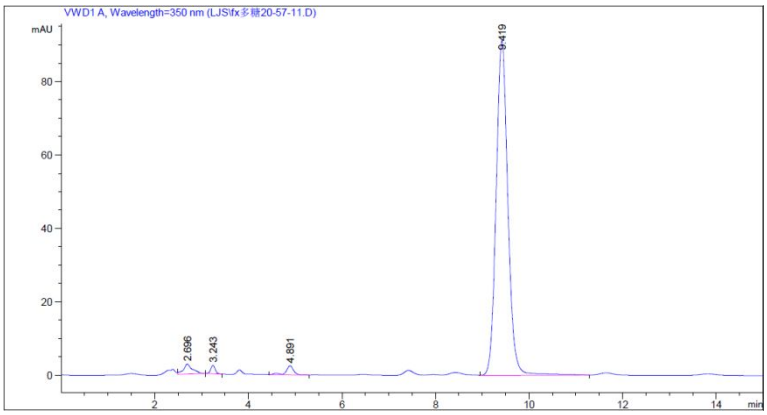
(g) pH = 13 time = 0.5 h



(h) pH = 13 time = 1 h



(i) pH = 13 time = 3 h



S17 HPLC profiles (column 250 × 10 mm, RP-18) of the **7l** at room temperature (a) in pH=7; (b) in pH=1, after 0 h; (c) in pH=1, after 0.5 h; (d) in pH=1, after 1 h; (e) in pH=1, after 3 h; (f) in pH=13, after 0 h; (g) in pH=13, after 0.5 h; (h) in pH=13, after 1 h; (i) in pH=3h, after 3 h. Buffer: 45% MeOH in aqueous 10 mM phosphate, pH = 7.0, 1.0 mL min^{-1}. The profile was measured at 350 nm.

Sensitivity to pH

Aqueous stock solutions (100 mL) were prepared by mixing aqueous sodium phosphate monobasic (0.5 M), aqueous sodium phosphate dibasic (0.5 M) and aqueous sodium chloride (2 M) to have a final concentration of 100 mM NaCl and 10 mM phosphate ions. The pH of each solution was adjusted to the desire value by adding aliquots of 2 M aqueous HCl or 2 M aqueous NaOH prior to spectral measurements.

The absorption and the emission were plotted versus the pH and fitted using a Boltzmann sigmoidal curve using OriginPro 2016.

Absorption and steady-state emission spectroscopy for **7a**

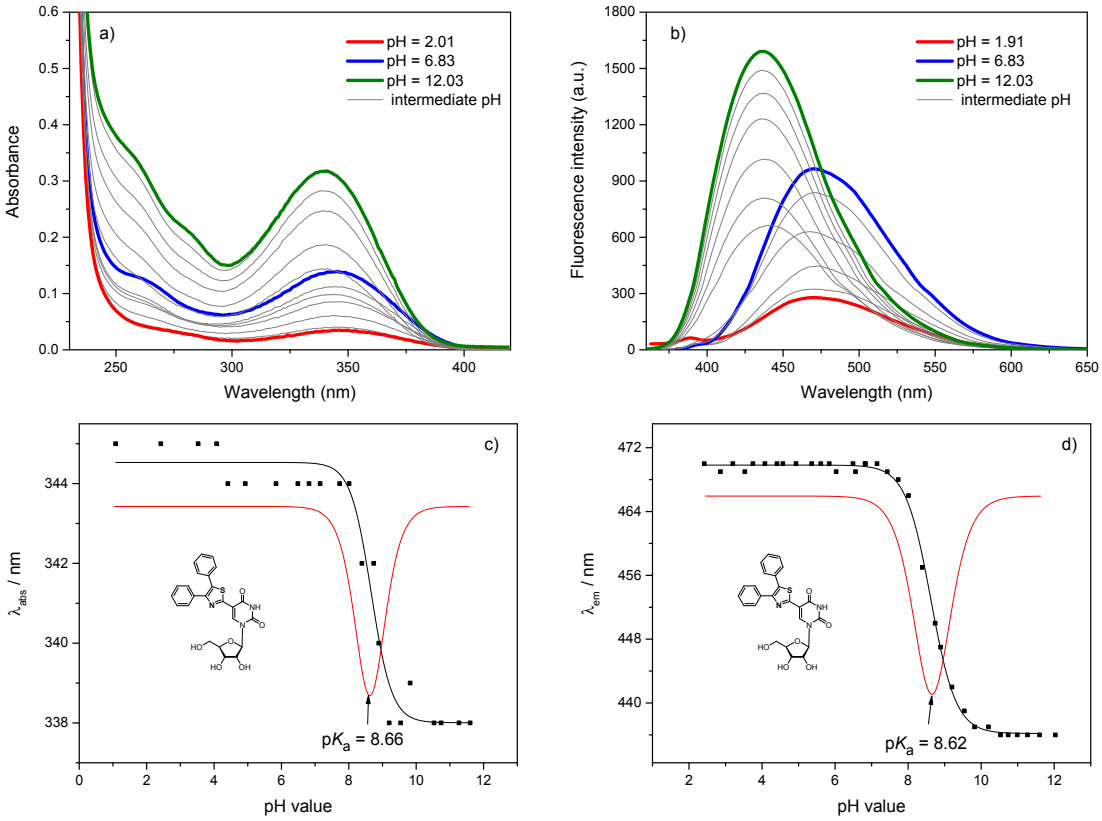


Figure S18. pH-Dependent UV spectra and fluorescence spectra of **7a** measured in 0.1 M sodium phosphate buffer with (a) UV-spectra at pH values from 2.01 to 12.03, (b) emission spectra at pH values from 1.91 to 12.03. (c) Graph of the absorption (abs) maxima against pH value (black line) and its first derivative (line marked in red) using data from (a). (d) Graph of the emission (em) maxima against pH value (black line) and its first derivative (line marked in red) using data from (b).

Absorption and steady-state emission spectroscopy for **7b**

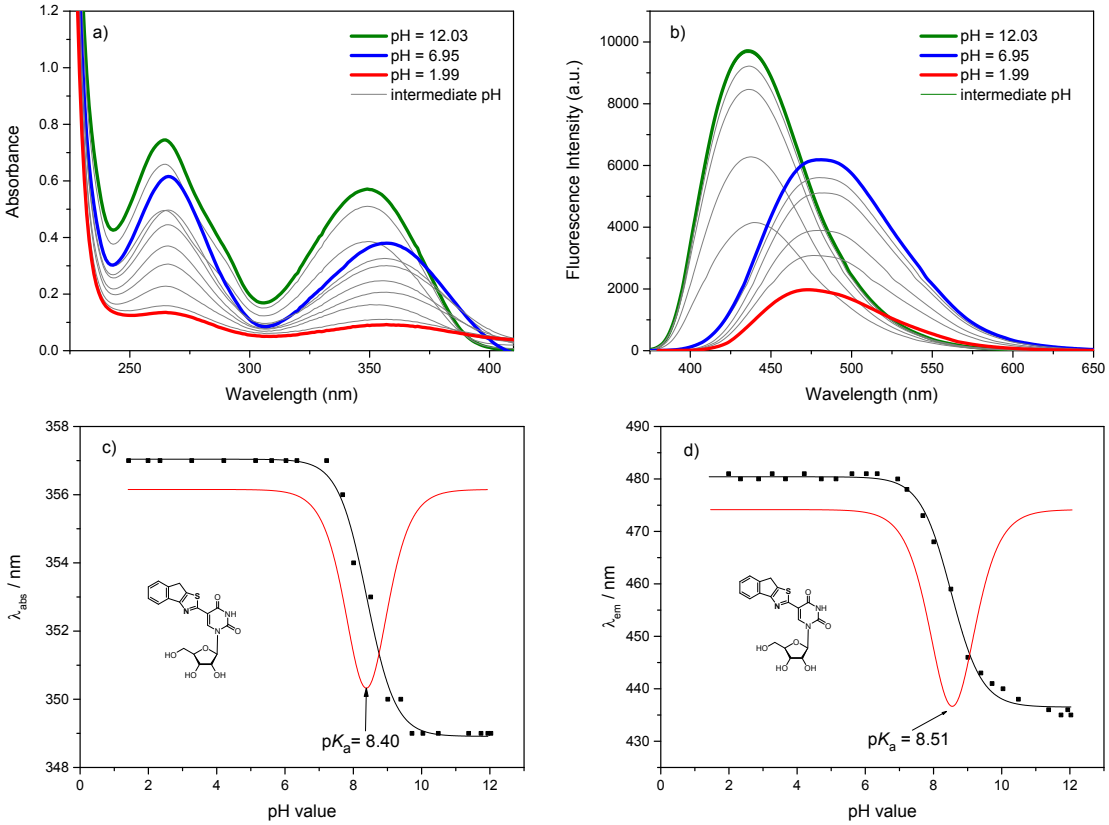


Figure S19. pH-Dependent UV spectra and fluorescence spectra of **7b** measured in 0.1 M sodium phosphate buffer with (a) UV-spectra at pH values from 1.99 to 12.03, (b) emission spectra at pH values from 1.99 to 12.03. (c) Graph of the absorption (abs) maxima against pH value (black line) and its first derivative (line marked in red) using data from (a). (d) Graph of the emission (em) maxima against pH value (black line) and its first derivative (lines marked in red) using data from (b).

Absorption and fluorescence emission spectroscopy for **7c**

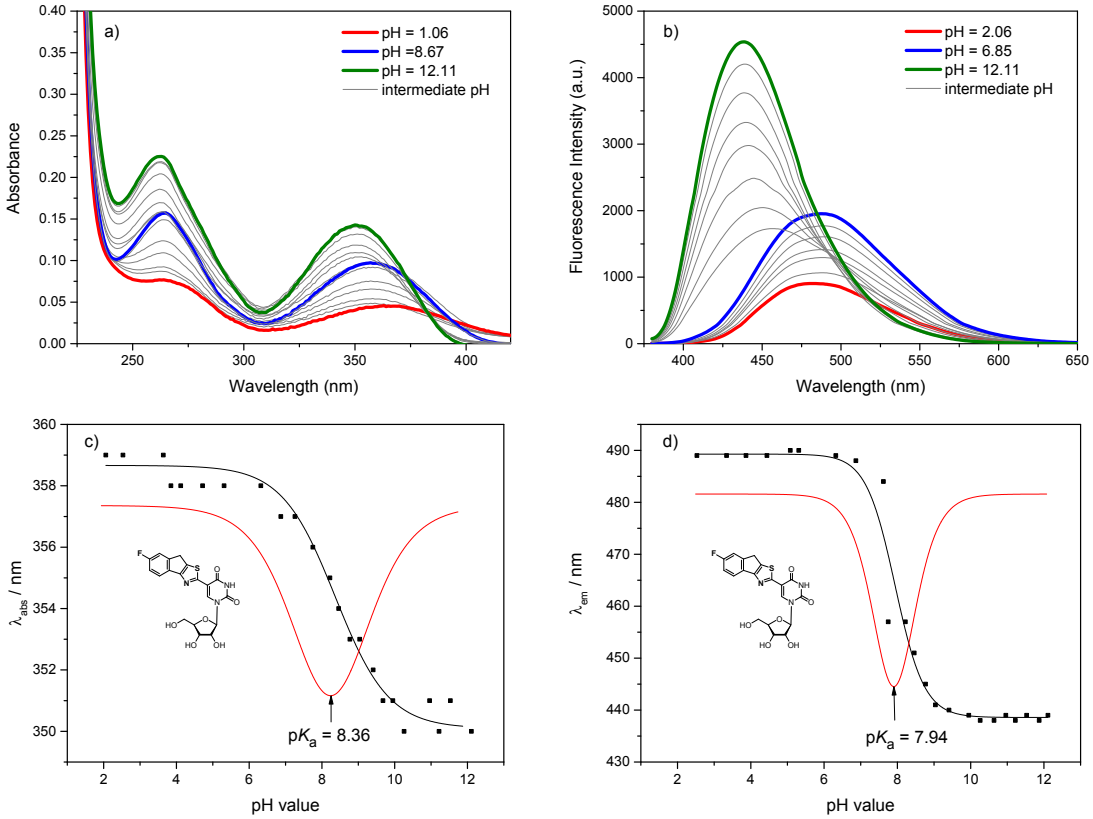


Figure S20. pH-Dependent UV spectra and fluorescence spectra of **7c** measured in 0.1 M sodium phosphate buffer with (a) UV-spectra at pH values from 1.06 to 12.11, (b) emission spectra at pH values from 2.06 to 12.11. (c) Graph of the absorption (abs) maxima against pH value (black line) and its first derivative (line marked in red) using data from (a). (d) Graph of the emission (em) maxima against pH value (black line) and its first derivative (line marked in red) using data from (b).

Absorption and fluorescence emission spectroscopy for **7d**

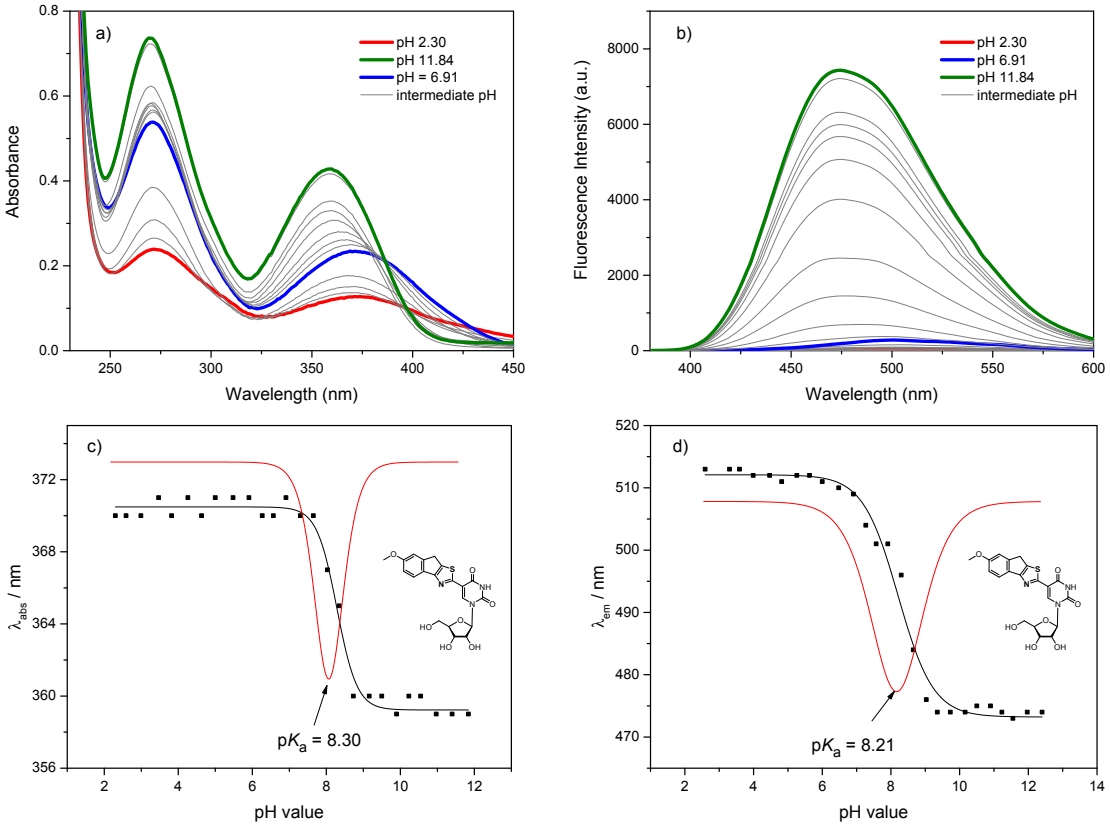


Figure S21. pH-Dependent UV spectra and fluorescence spectra of **7d** measured in 0.1 M sodium phosphate buffer with (a) UV-spectra at pH values from 1.06 to 12.11, (b) emission spectra at pH values from 2.06 to 12.11. (c) Graph of the absorbance against pH value (black line) and its first derivative (line marked in red) using data from (a). (d) Graph of the fluorescence emission against pH value (black line) and its first derivative (line marked in red) using data from (b).

Absorption and fluorescence emission spectroscopy for **7e**

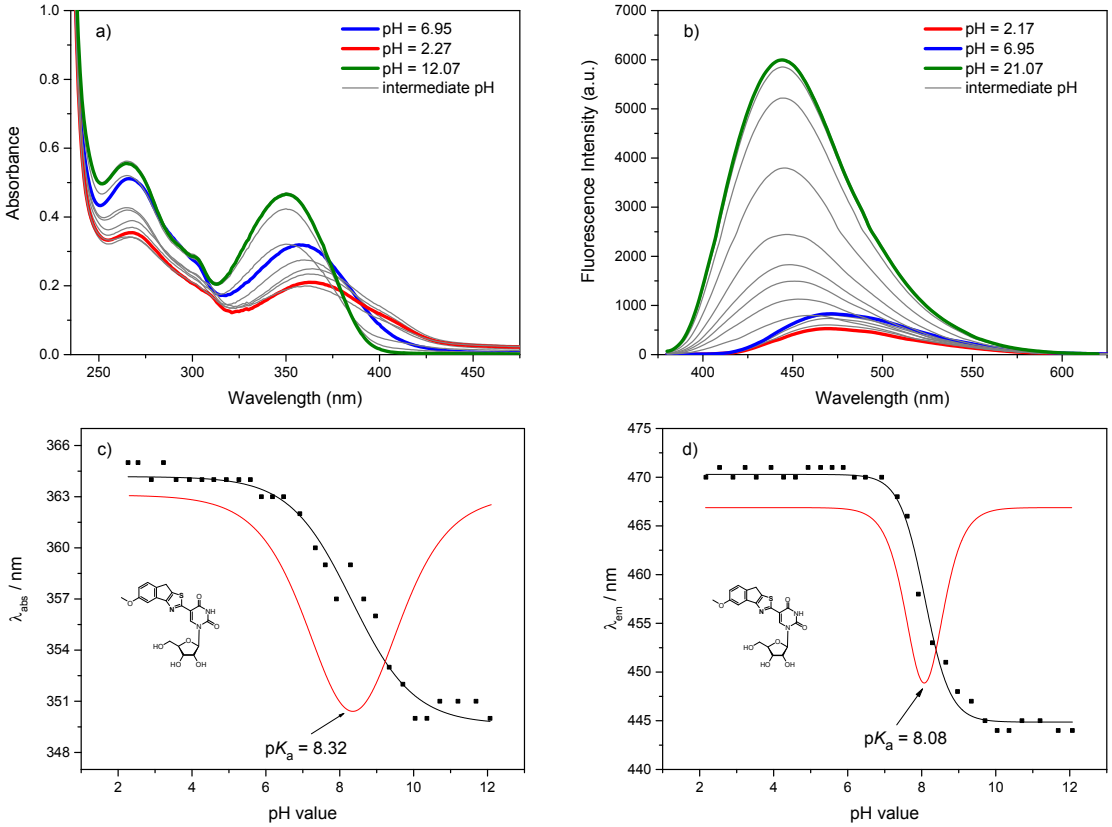


Figure S22. pH-Dependent UV spectra and fluorescence spectra of **7e** measured in 0.1 M sodium phosphate buffer with (a) UV-spectra at pH values from 2.27 to 12.07, (b) emission spectra at pH values from 2.17 to 12.07. (c) Graph of the absorbance against pH value (black line) and its first derivative (line marked in red) using data from (a). (d) Graph of the fluorescence emission against pH value (black line) and its first derivative (line marked in red) using data from (b).

Absorption and fluorescence emission spectroscopy for **7g**

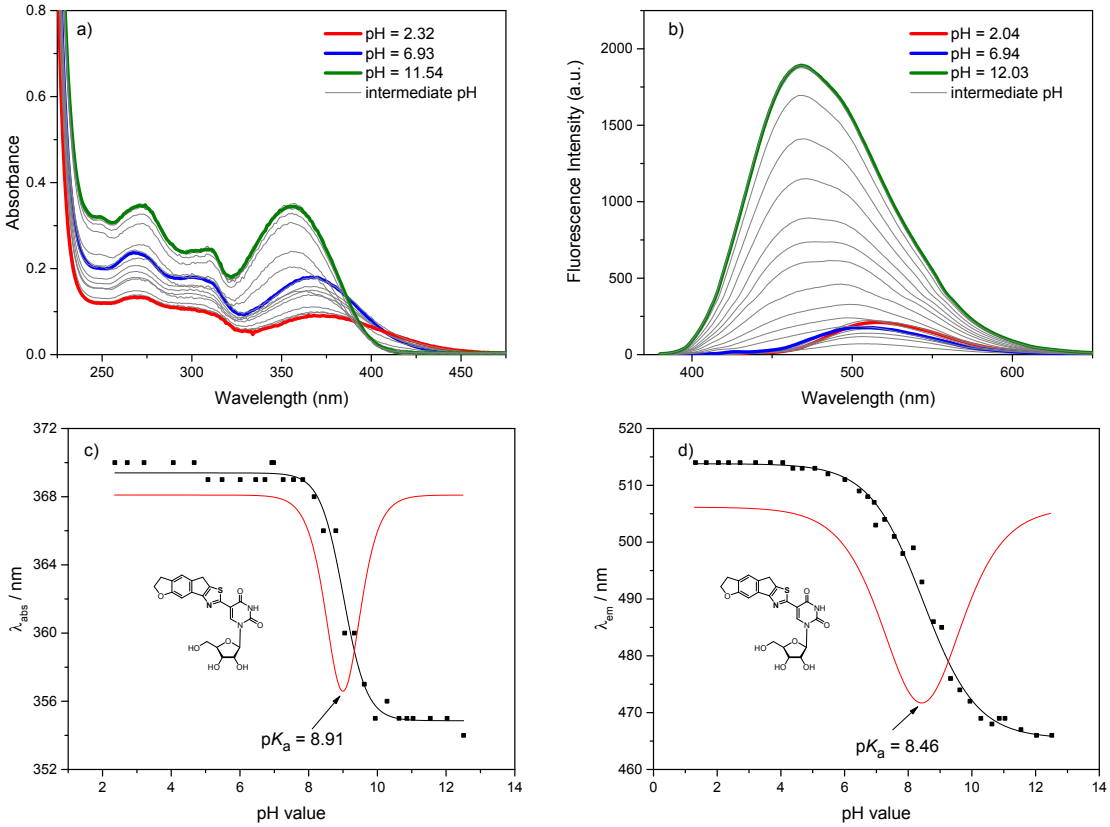


Figure S23. pH-dependent UV spectra and fluorescence spectra of **7g** measured in 0.1 M sodium phosphate buffer with (a) UV-spectra at pH values from 2.32 to 11.54, (b) emission spectra at pH values from 2.04 to 12.03. (c) Graph of the absorbance against pH value (black line) and its first derivative (line marked in red) using data from (a). (d) Graph of the fluorescence emission against pH value (black line) and its first derivative (line marked in red) using data from (b).

Absorption and fluorescence emission spectroscopy for **7h**

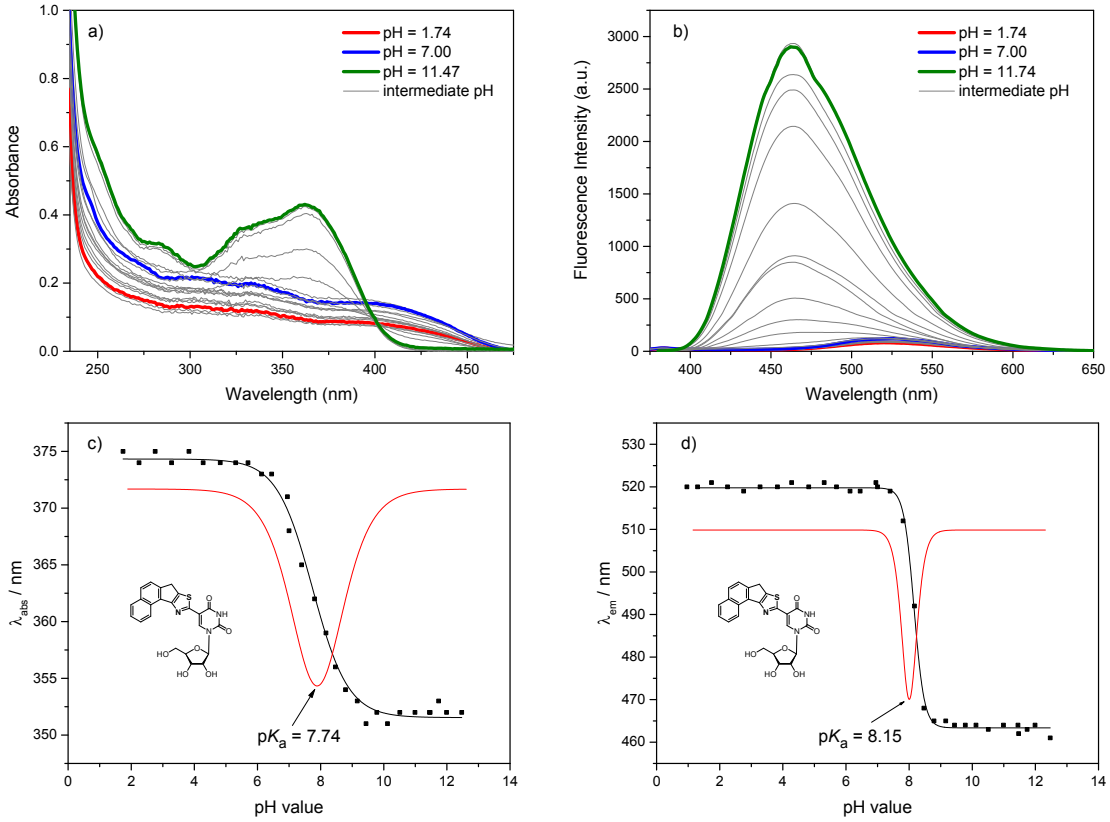


Figure S24. pH-Dependent UV spectra and fluorescence spectra of **7h** measured in 0.1 M sodium phosphate buffer with (a) UV-spectra at pH values from 1.71 to 11.47, (b) emission spectra at pH values from 1.71 to 11.47. (c) Graph of the absorbance against pH value (black line) and its first derivative (line marked in red) using data from (a). (d) Graph of the fluorescence emission against pH value (black line) and its first derivative (line marked in red) using data from (b).

Absorption and fluorescence emission spectroscopy for **7j**

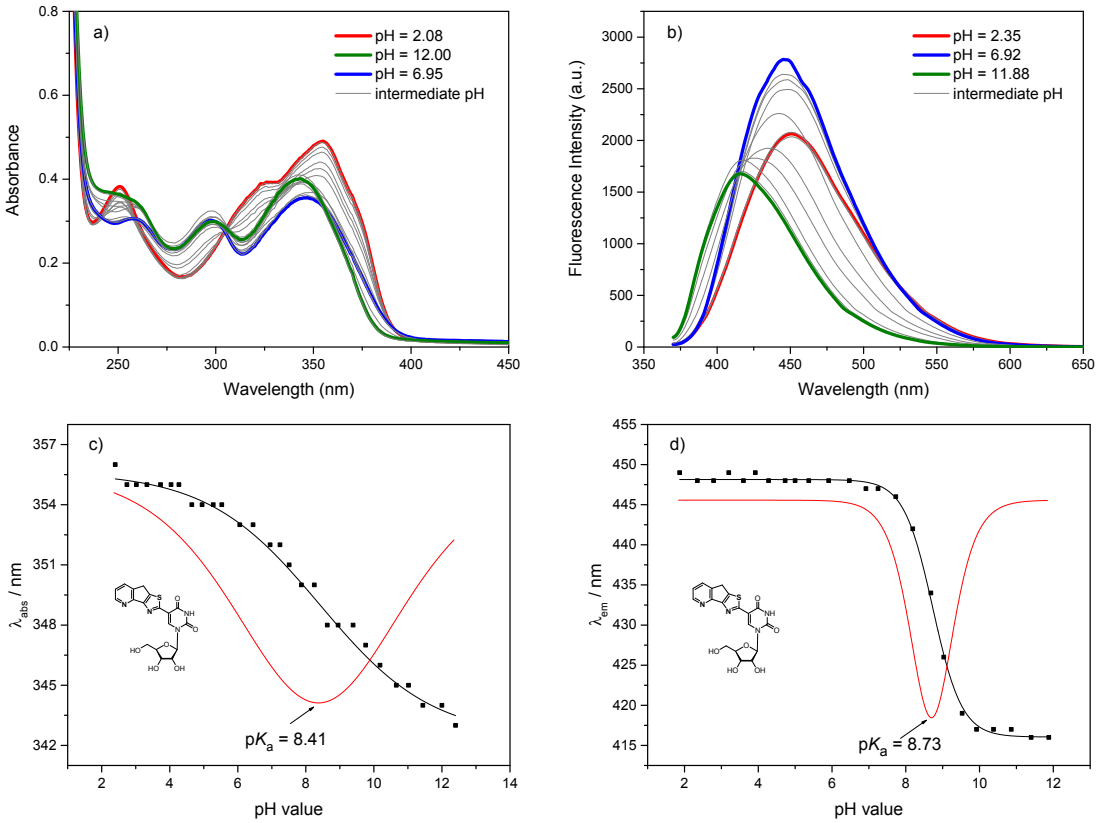


Figure S25. pH-Dependent UV spectra and fluorescence spectra of **7j** measured in 0.1 M sodium phosphate buffer with (a) UV-spectra at pH values from 2.08 to 12.00, (b) emission spectra at pH values from 2.35 to 11.88. (c) Graph of the absorbance against pH value (black line) and its first derivative (lines marked in red) using data from (a). (d) Graph of the fluorescence emission against pH value (black line) and its first derivative (lines marked in red) using data from (b).

Absorption and fluorescence emission spectroscopy for **7k**

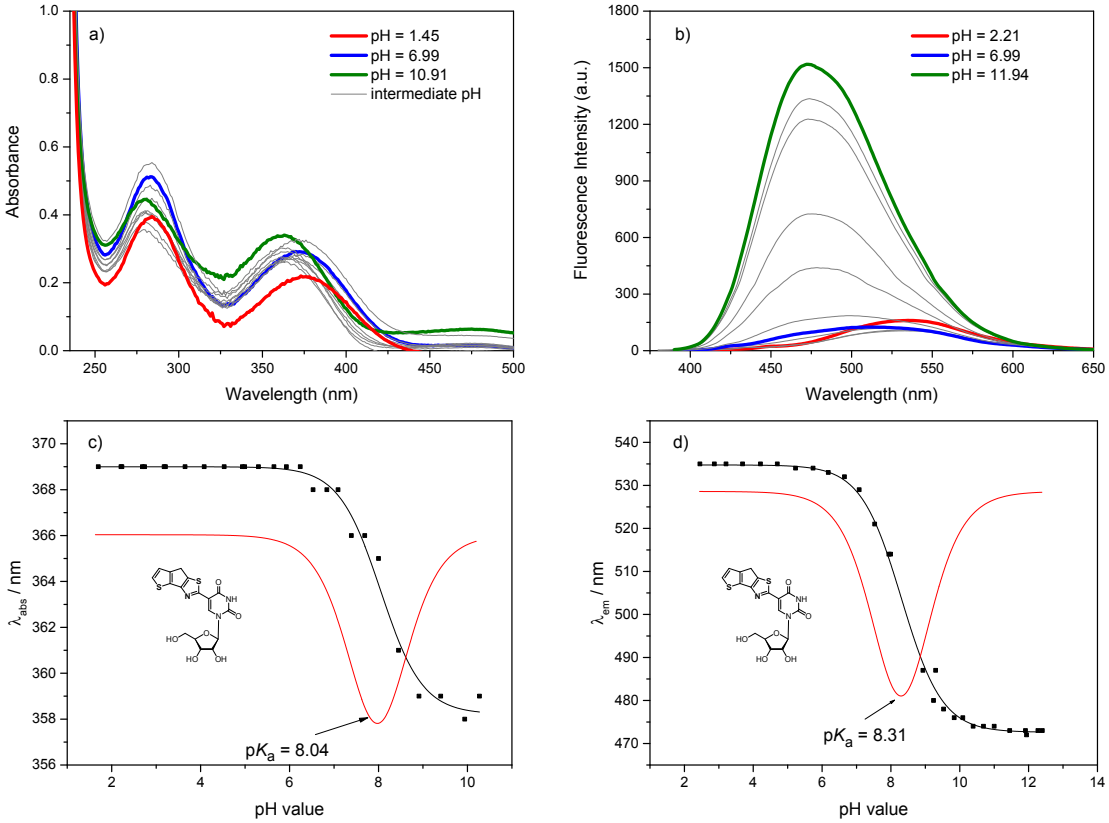


Figure S26. pH-Dependent UV spectra and fluorescence spectra of **7k** measured in 0.1 M sodium phosphate buffer with (a) UV-spectra at pH values from 1.45 to 10.91, (b) emission spectra at pH values from 2.21 to 11.94.(c) Graph of the absorbance against pH value (black line) and its first derivative (line marked in red) using data from (a). (d) Graph of the fluorescence emission against pH value (black line) and its first derivative (line marked in red) using data from (b).

Absorption and fluorescence emission spectroscopy for **7l**

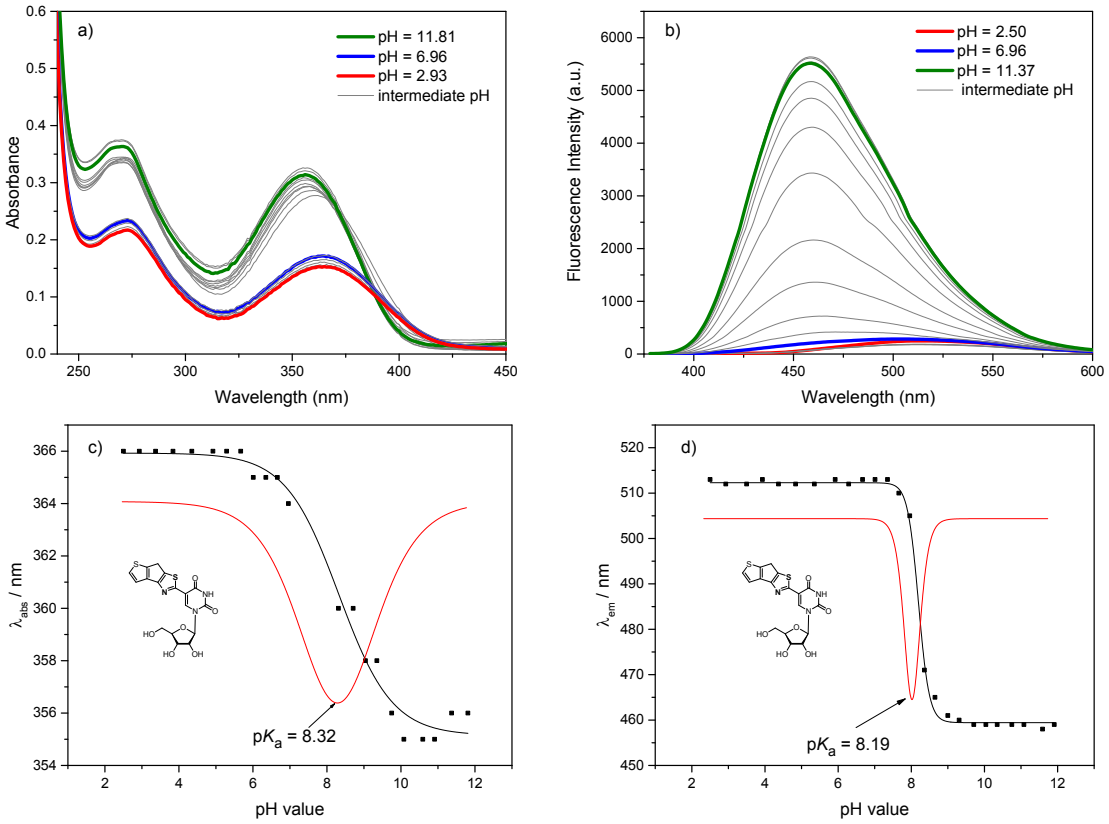


Figure S27. pH-Dependent UV spectra and fluorescence spectra of **7l** measured in 0.1 M sodium phosphate buffer with (a) UV-spectra at pH values from 2.93 to 11.81, (b) emission spectra at pH values from 2.50 to 11.37.(c) Graph of the absorbance against pH value (black line) and its first derivative (line marked in red) using data from (a). (d) Graph of the fluorescence emission against pH value (black line) and its first derivative (line marked in red) using data from (b).

Absorption and fluorescence emission spectroscopy for **7m**

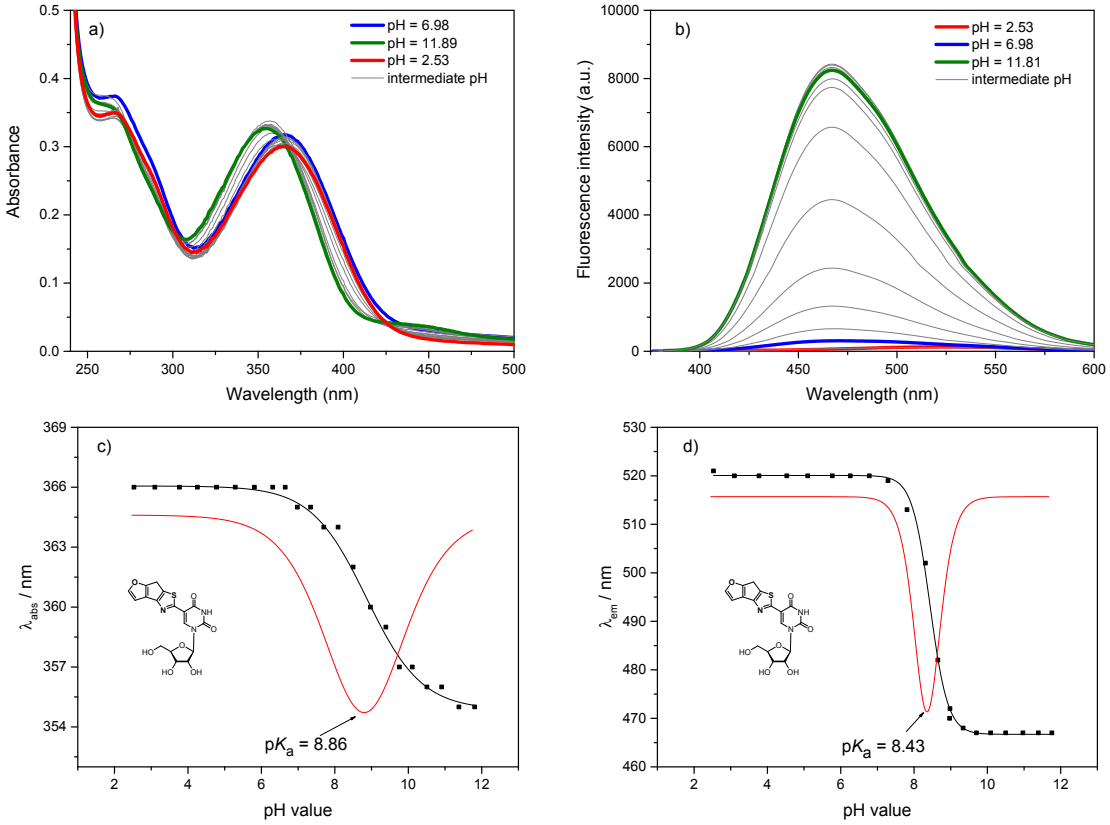
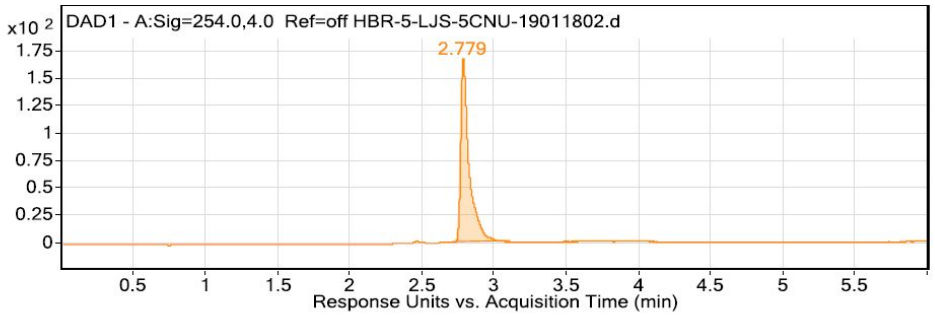


Figure S28. pH-Dependent UV spectra and fluorescence spectra of **7m** measured in 0.1 M sodium phosphate buffer with (a) UV-spectra at pH values from 2.53 to 11.89, (b) emission spectra at pH values from 2.53 to 11.81.(c) Graph of the absorbance against pH value (black line) and its first derivative (line marked in red) using data from (a). (d) Graph of the fluorescence emission against pH value (black line) and its first derivative (line marked in red) using data from (b).

LC-ESI-MS chromatograms and NMR spectra of new compounds

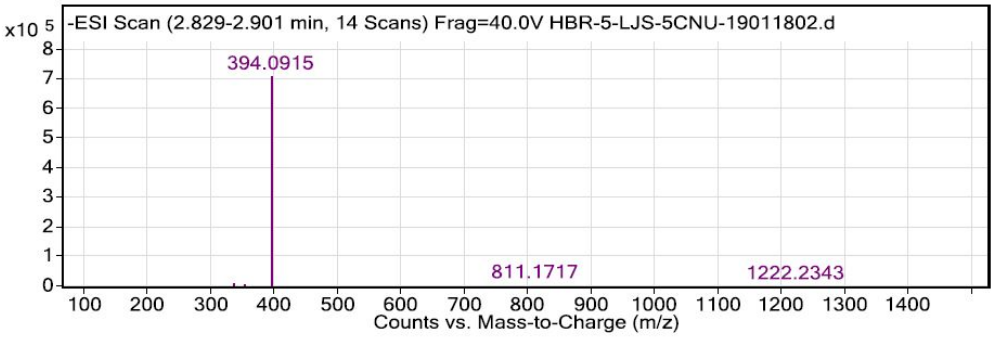
LC-ESI-MS chromatograms of compound **4**



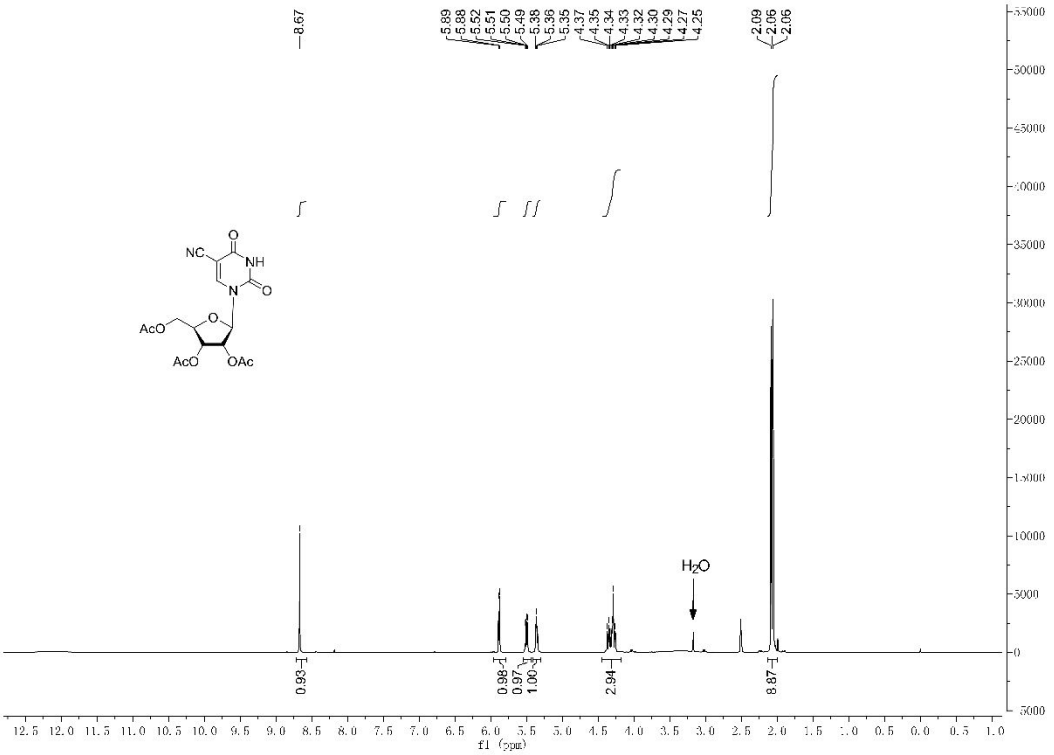
Integration Peak List

Peak	Start	RT	End	Height	Area	AreaSumPercent
1	2.716	2.779	3.111	167.15	681.84	100.00

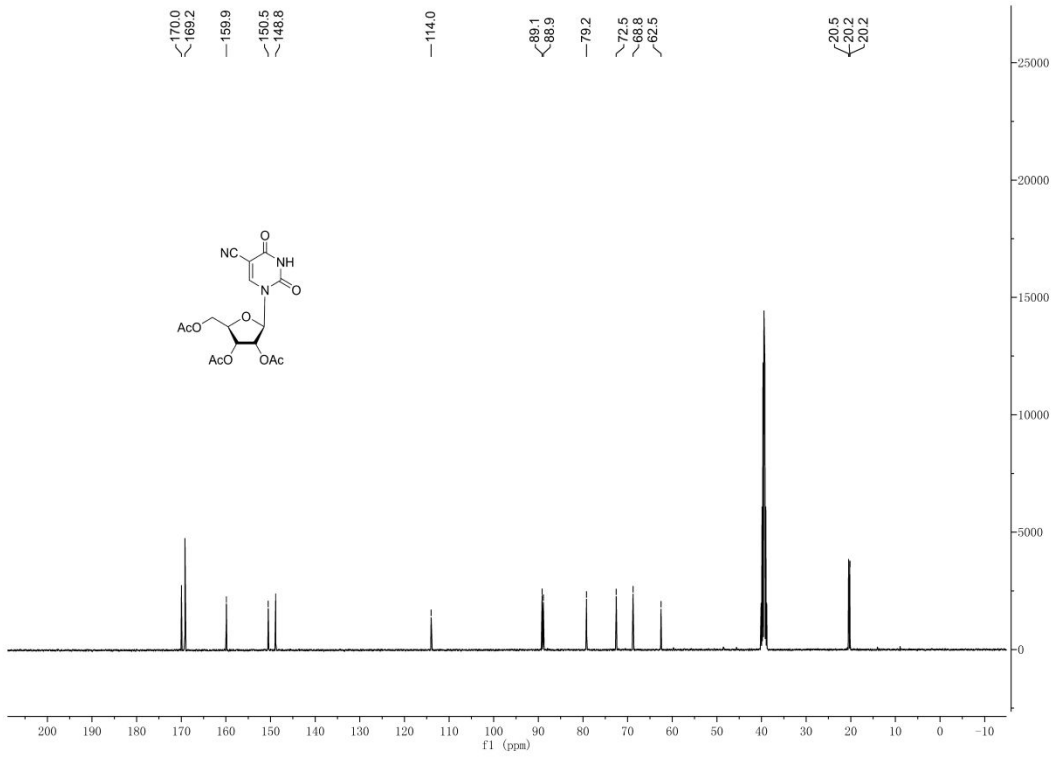
Fragmentor Voltage	Collision Energy	Ionization Mode
40	0	ESI



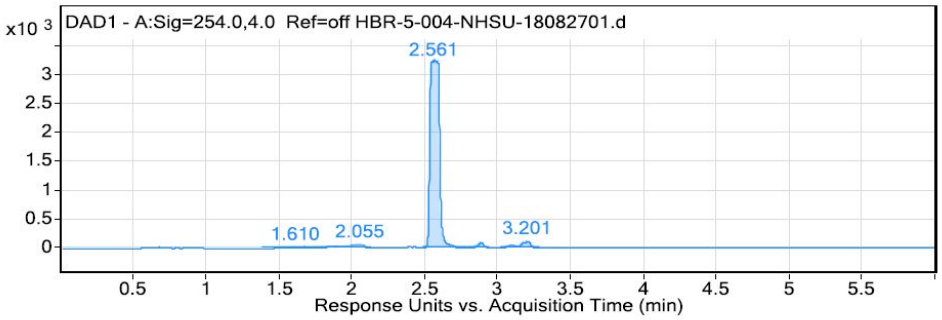
^{1}H-NMR spectra of compound **4**



^{13}C-NMR spectra of compound **4**



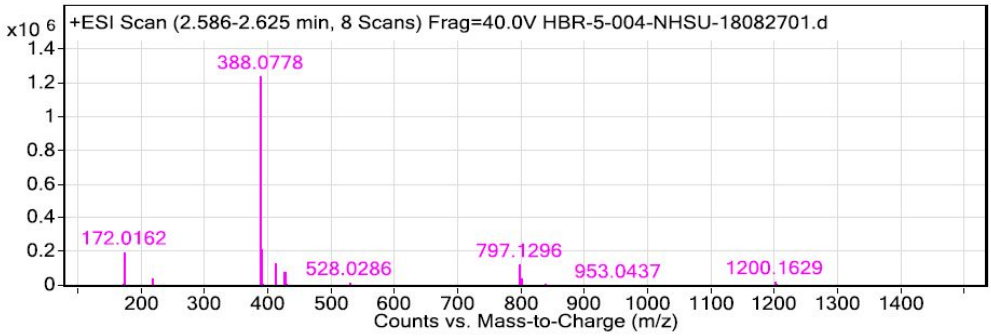
LC-ESI-MS chromatograms of compound **5**



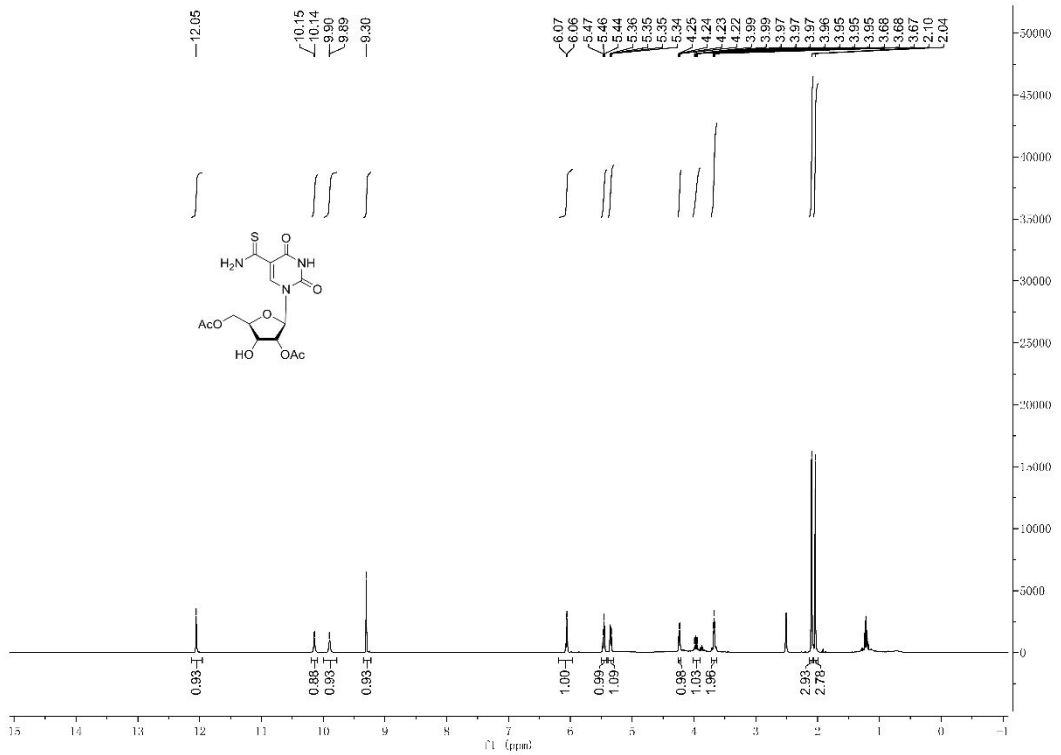
Integration Peak List

Peak	Start	RT	End	Height	Area	AreaSumPercent
1	1.382	1.61	1.675	16.2	155.83	0.93
2	1.675	1.859	1.892	22.71	251.75	1.51
3	1.892	2.055	2.128	62.49	480.72	2.88
4	2.493	2.561	2.813	3277.27	14859.71	88.90
5	2.813	2.881	2.94	93.26	293.78	1.76
6	3.024	3.091	3.124	46.42	172.17	1.03
7	3.124	3.201	3.286	120.47	502.04	3.00

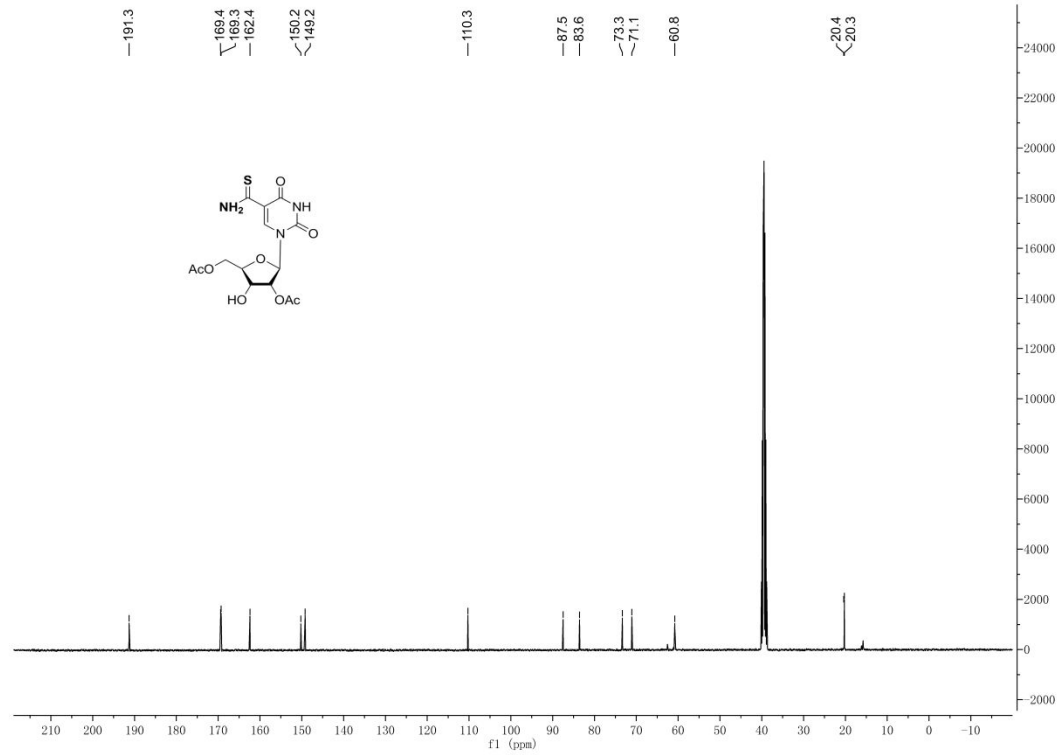
Fragmentor Voltage 40 **Collision Energy** 0 **Ionization Mode** ESI



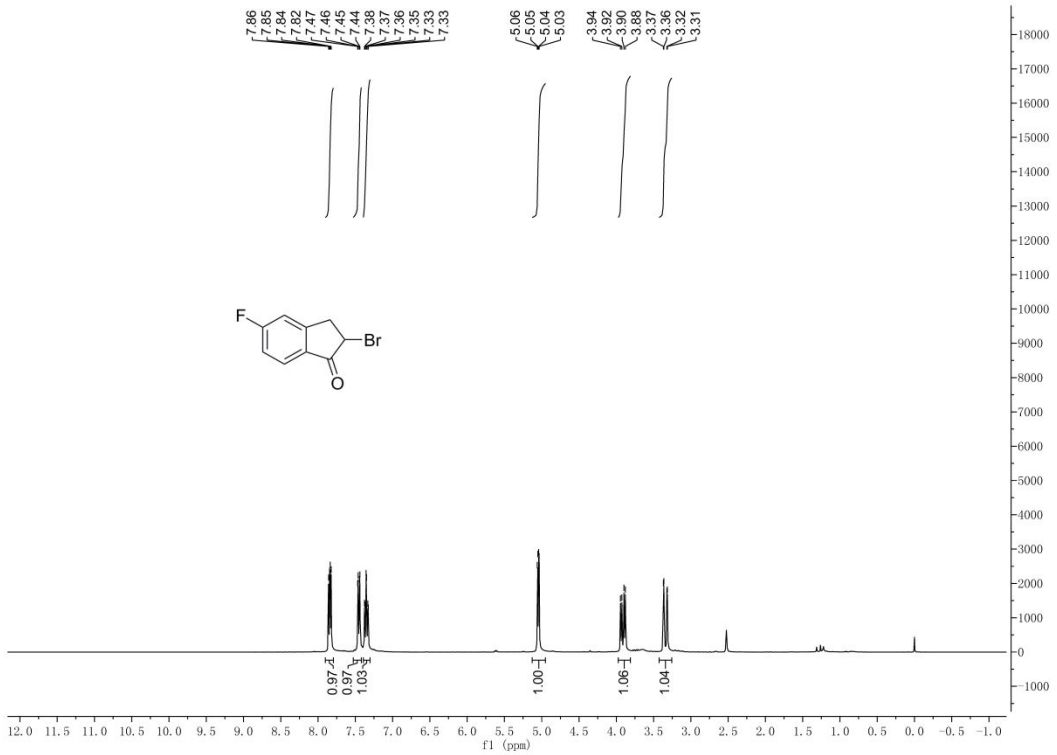
^{1}H-NMR spectra of compound **5**



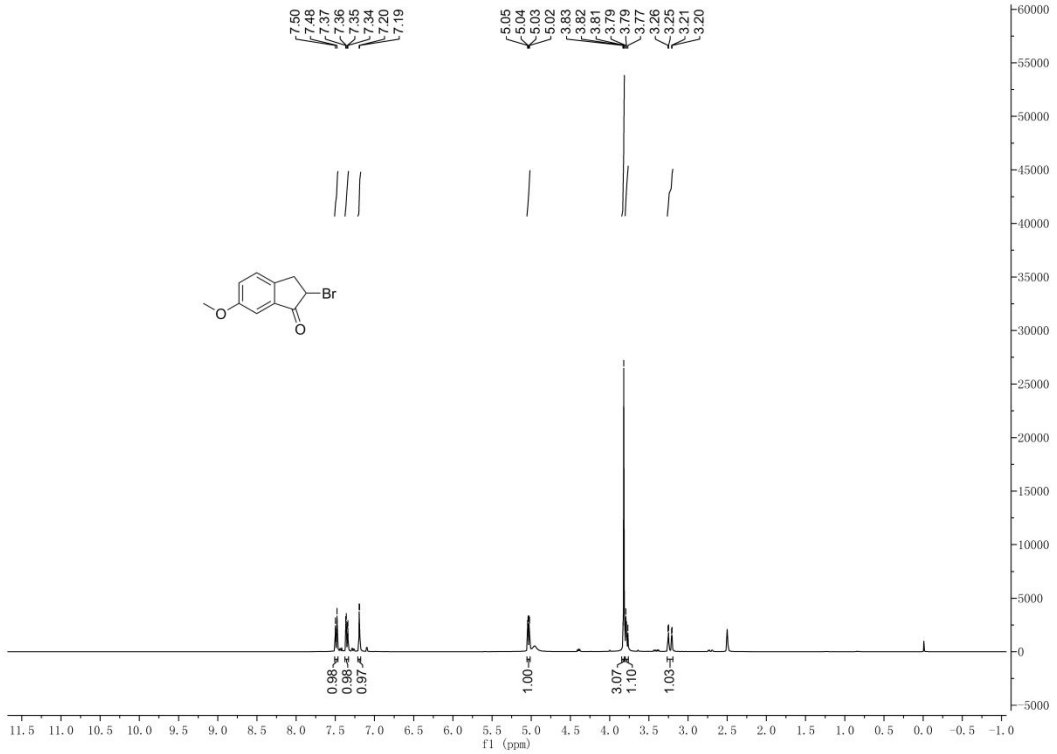
^{13}C-NMR spectra of compound **5**



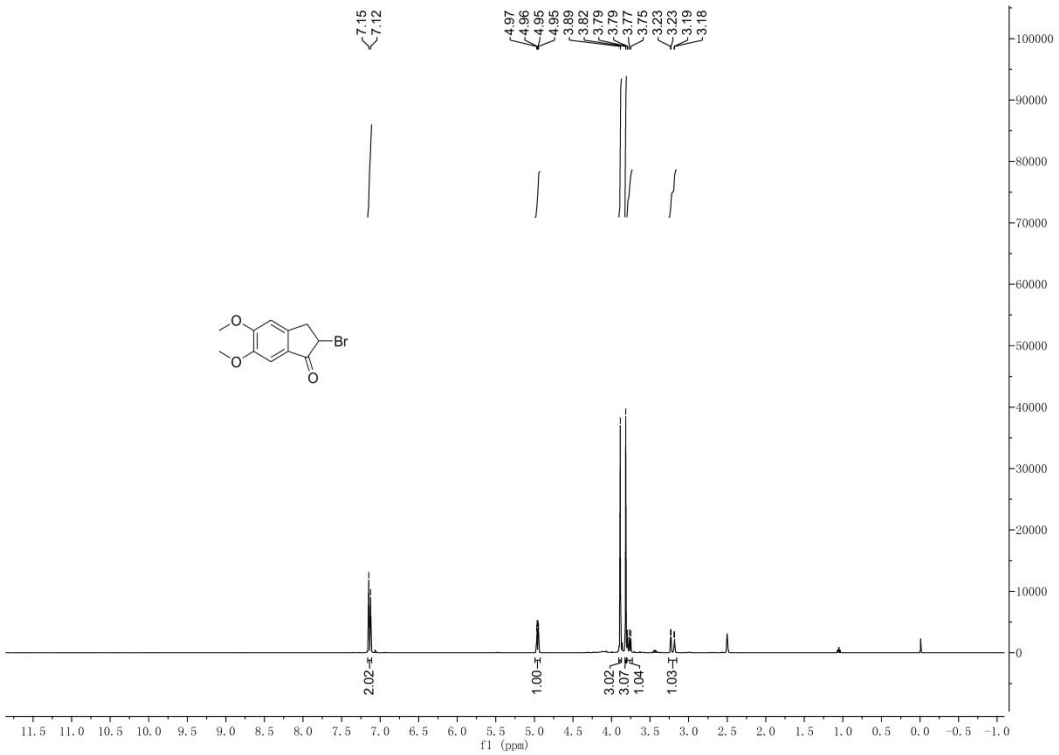
^{1}H-NMR spectra of compound **6c**



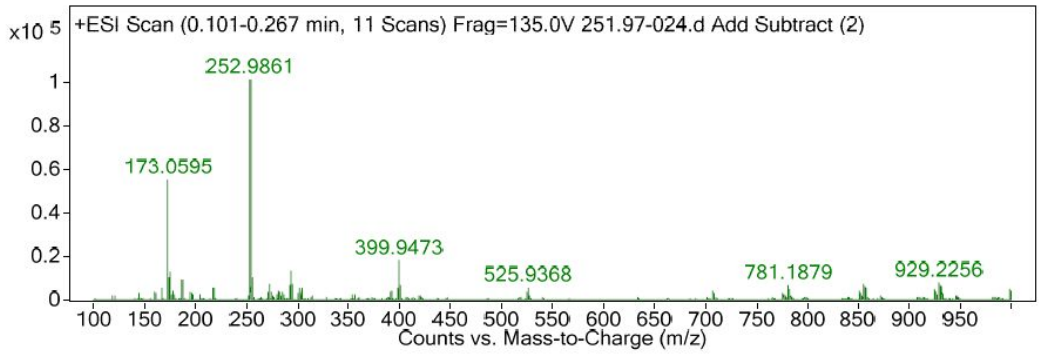
^{1}H-NMR spectra of compound **6e**



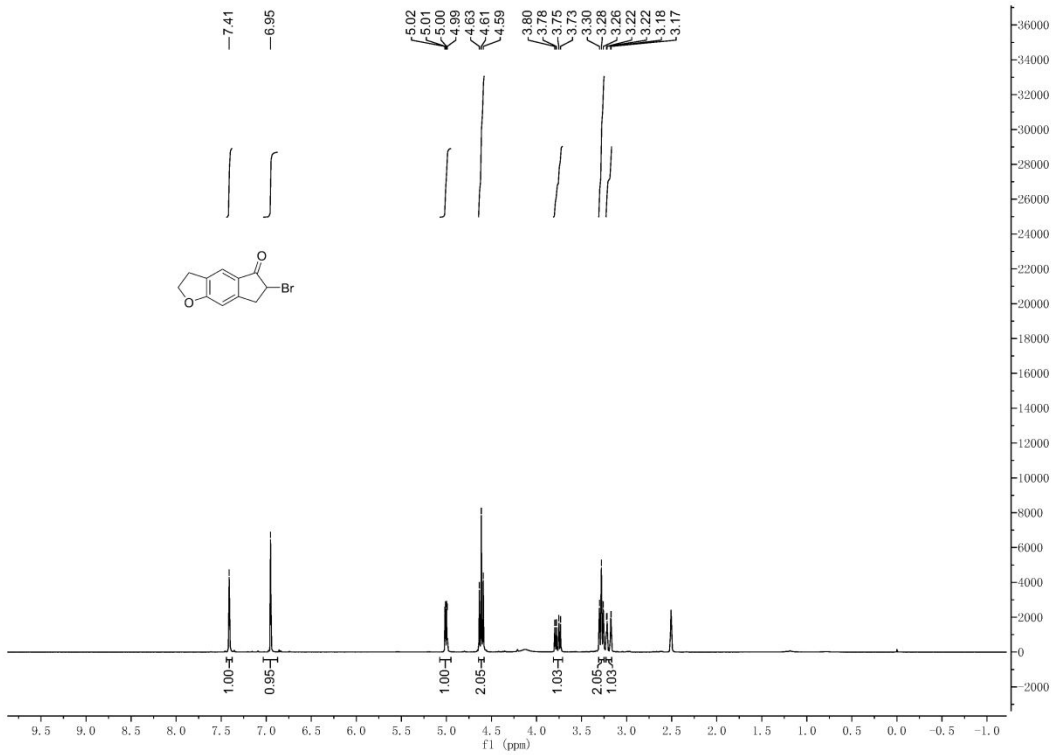
^{1}H-NMR spectra of compound **6f**



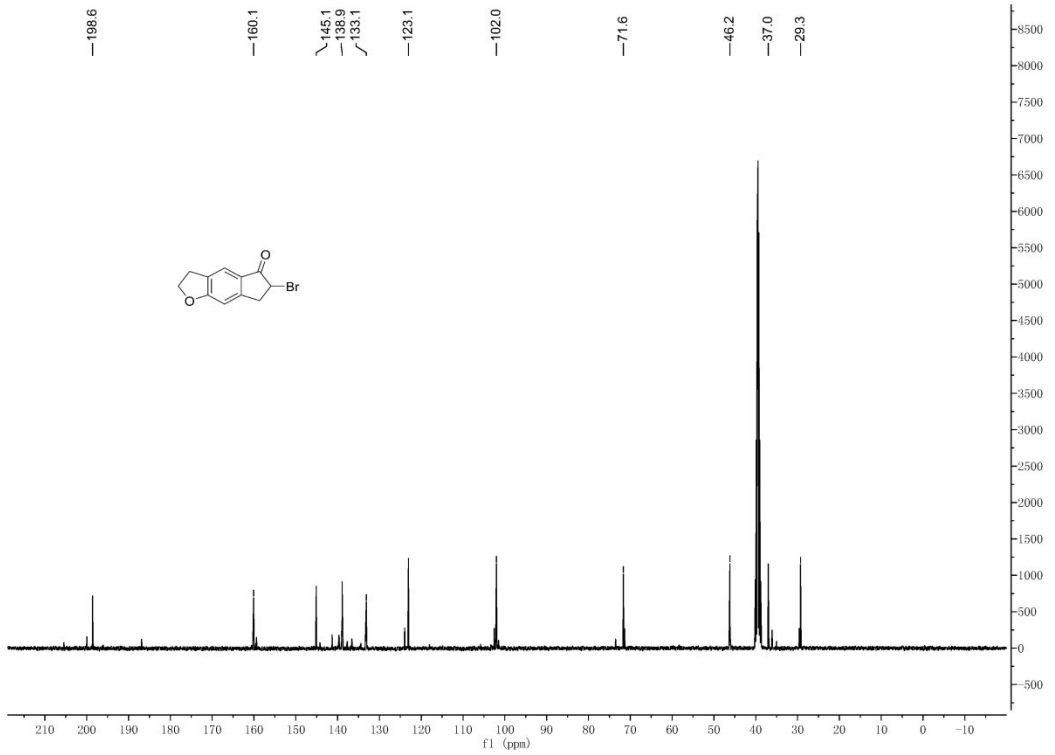
ESI-MS chromatograms of compound **6g**



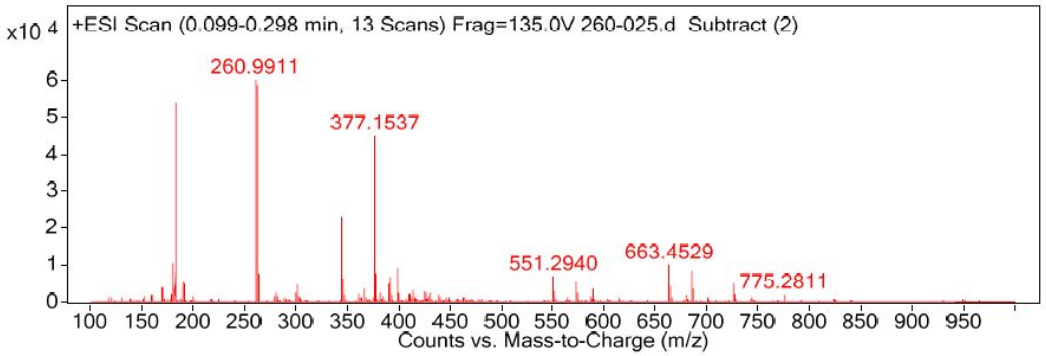
^{1}H-NMR spectra of compound **6g**



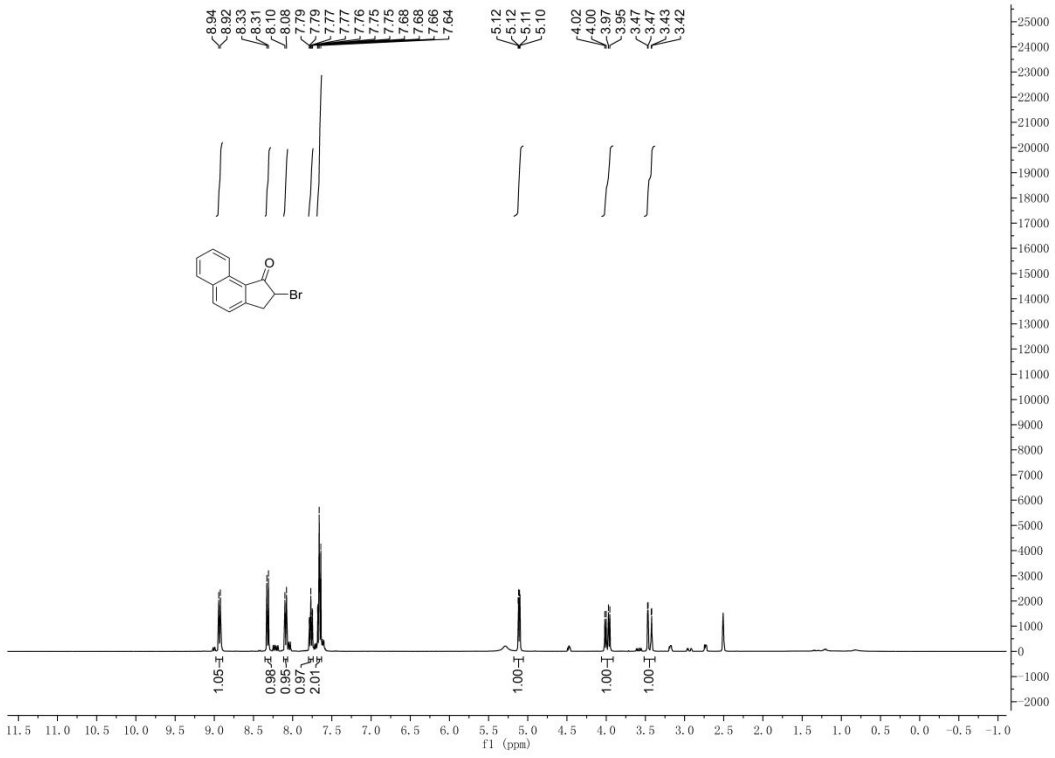
^{13}C-NMR spectra of compound **6g**



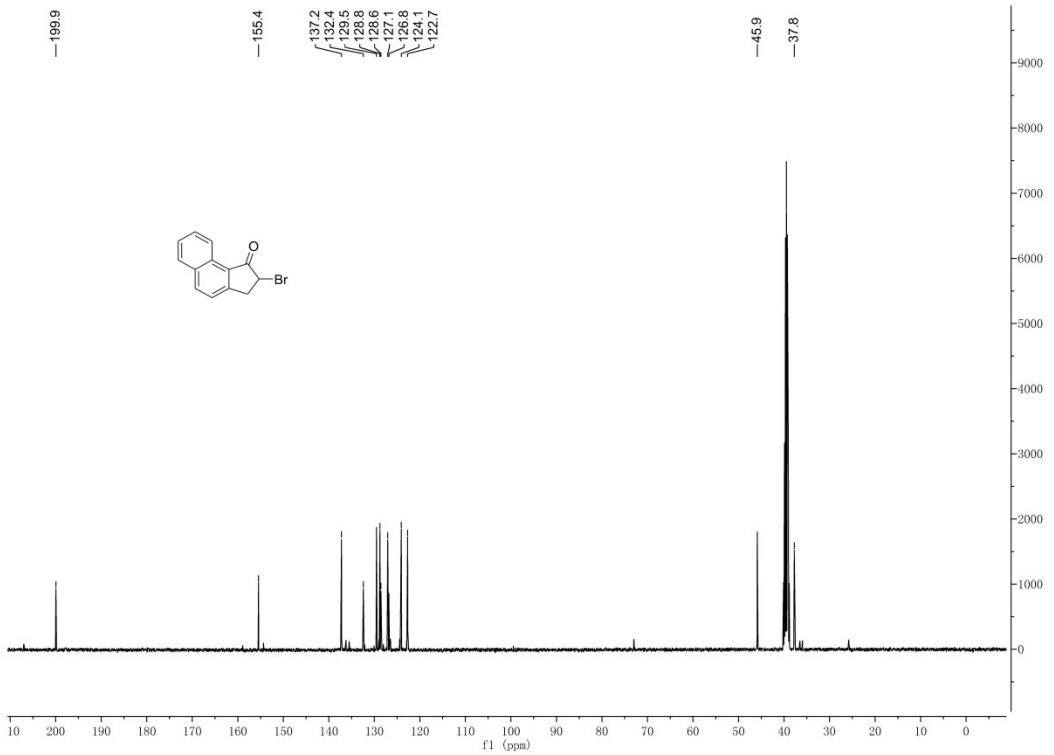
ESI-MS chromatograms of compound **6h**



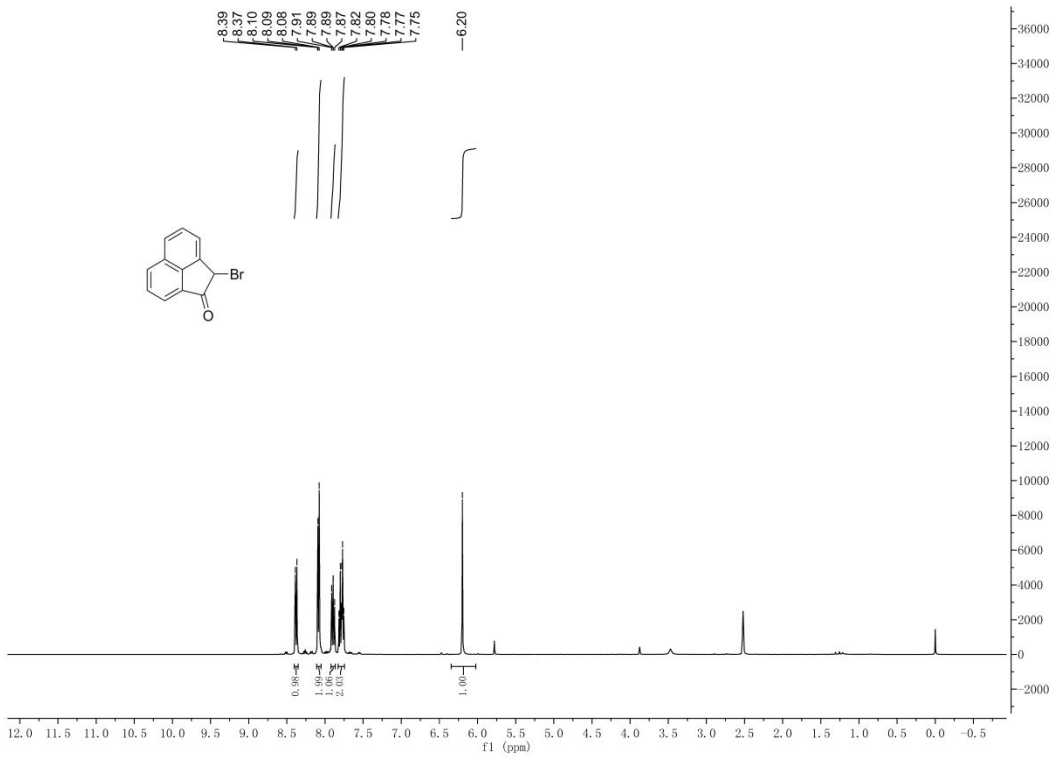
^{1}H-NMR spectra of compound **6h**



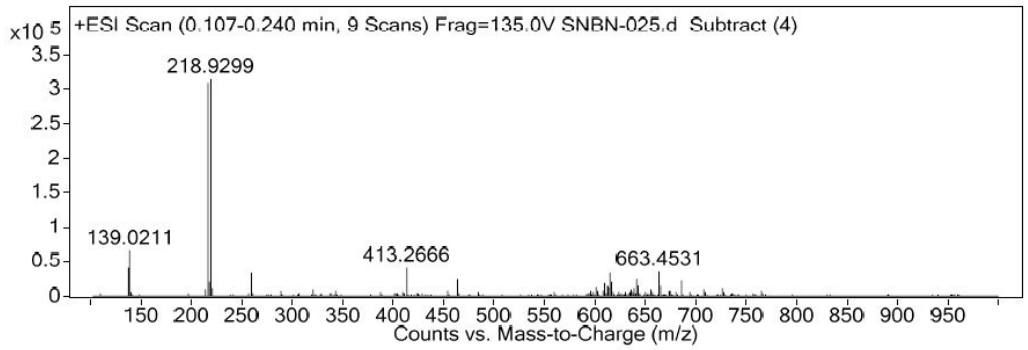
^{13}C-NMR spectra of compound **6h**



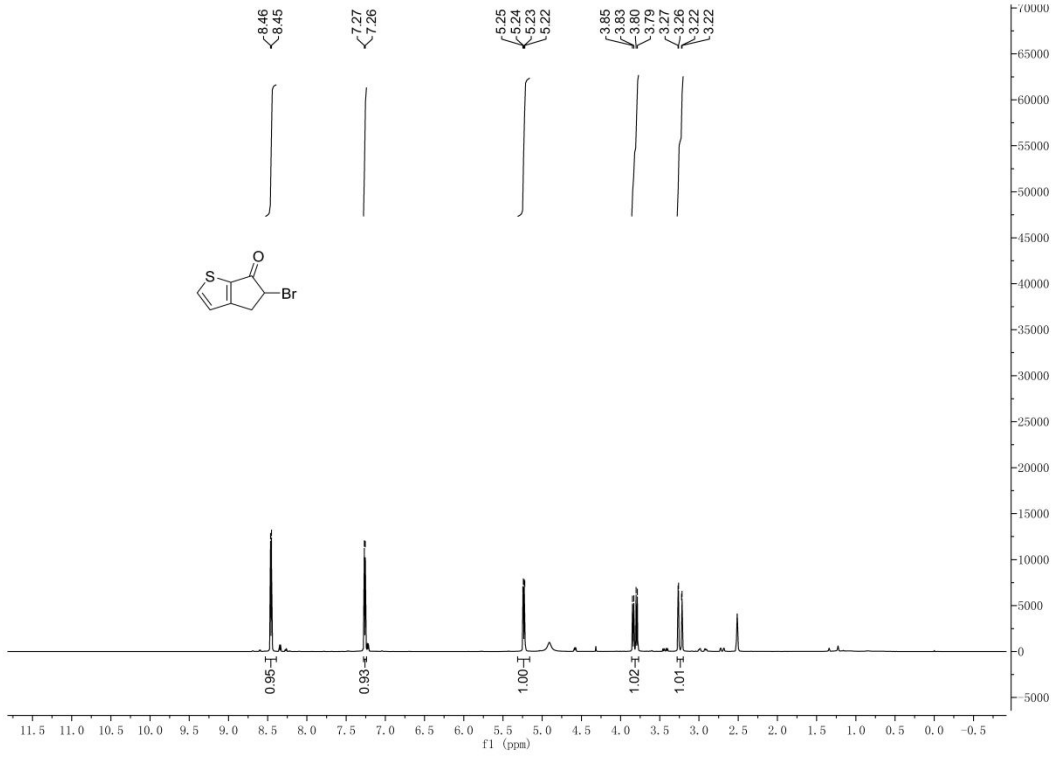
^{1}H-NMR spectra of compound **6i**



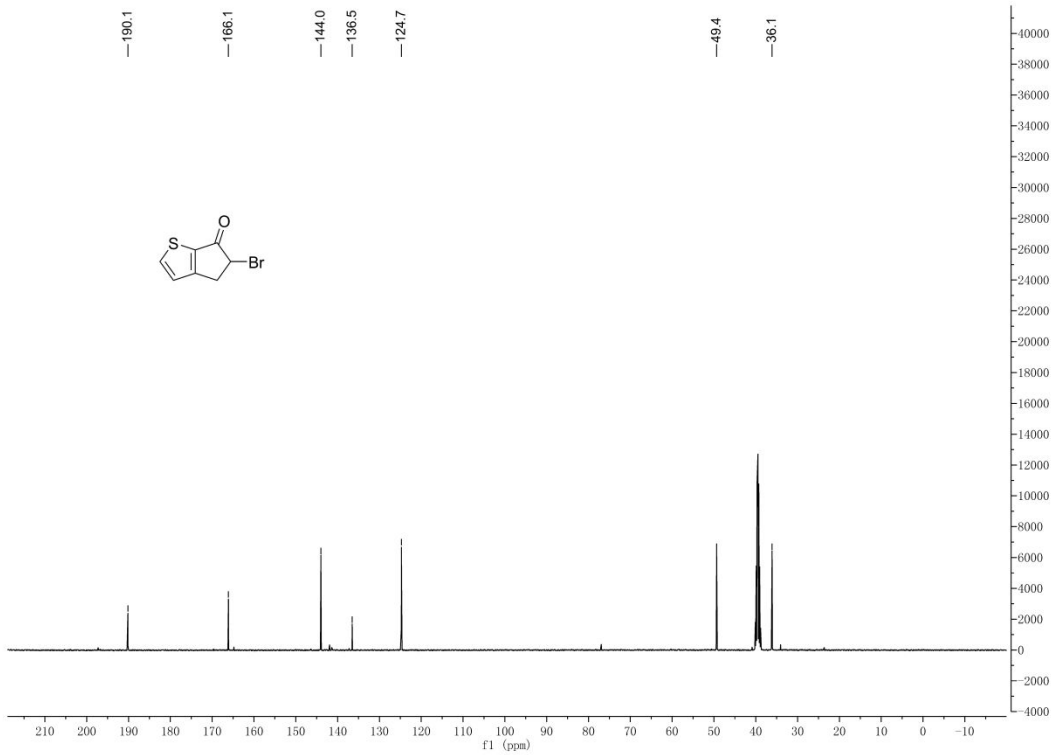
ESI-MS chromatograms of compound **6k**



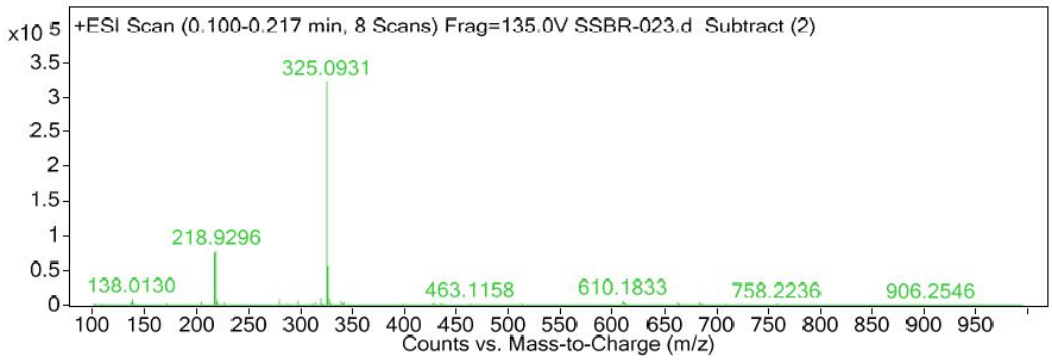
^{1}H-NMR spectra of compound **6k**



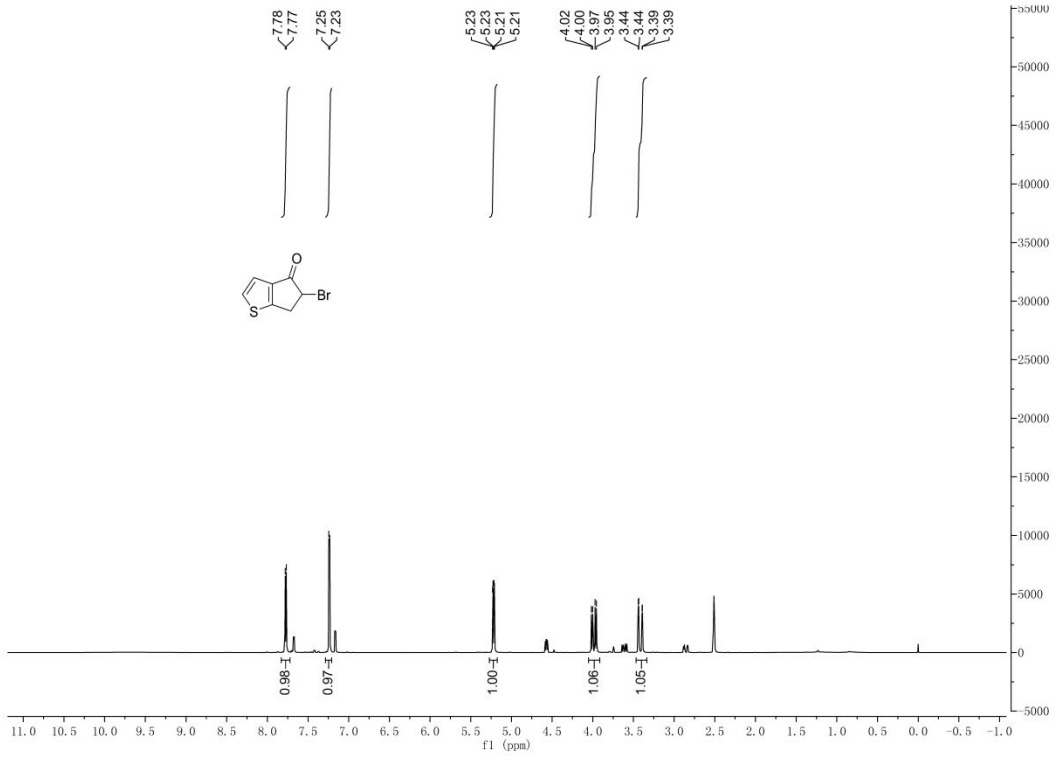
^{13}C-NMR spectra of compound **6k**



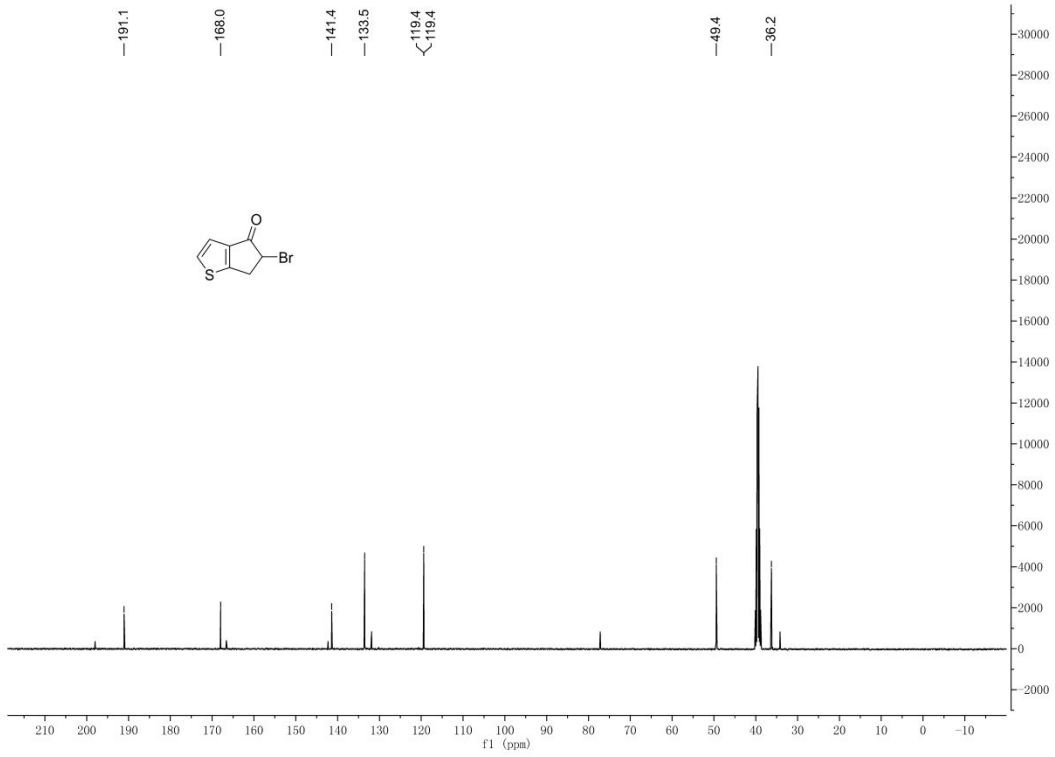
ESI-MS chromatograms of compound **6l**



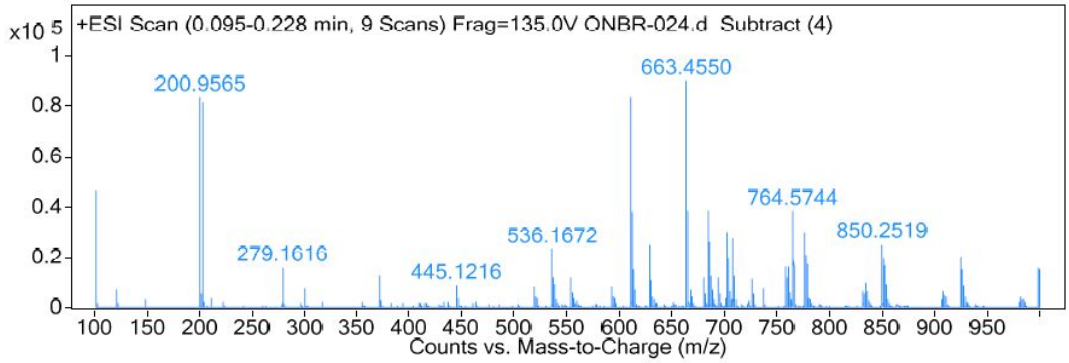
^{1}H-NMR spectra of compound **6l**



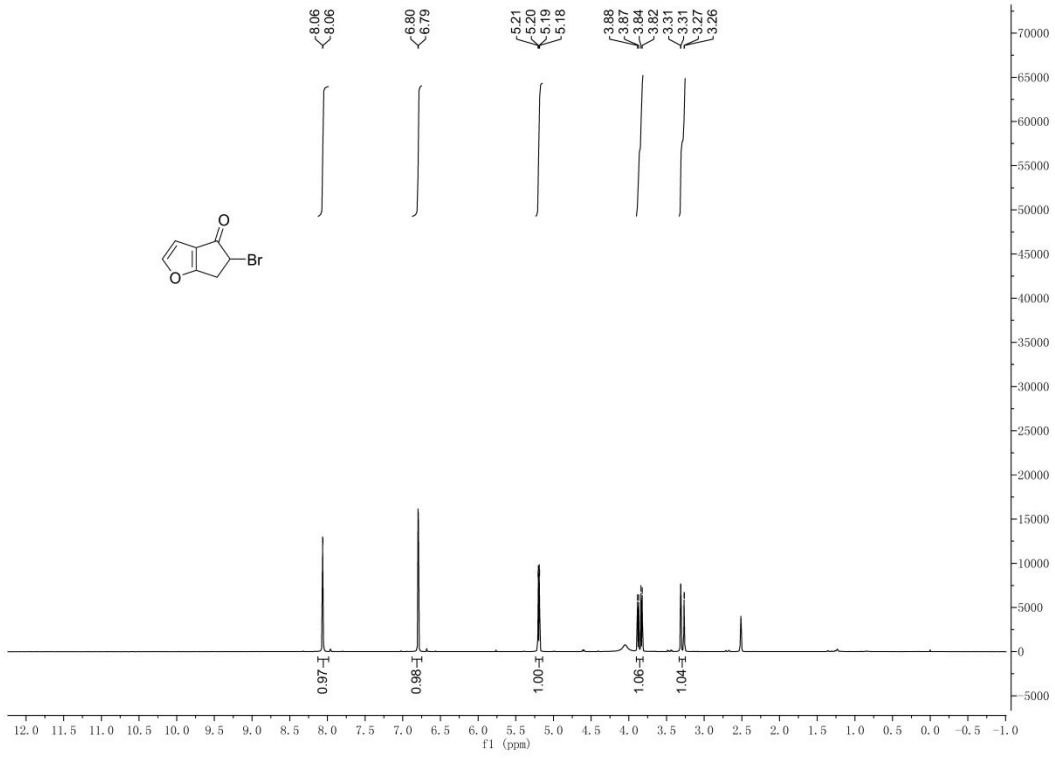
^{13}C-NMR spectra of compound **6l**



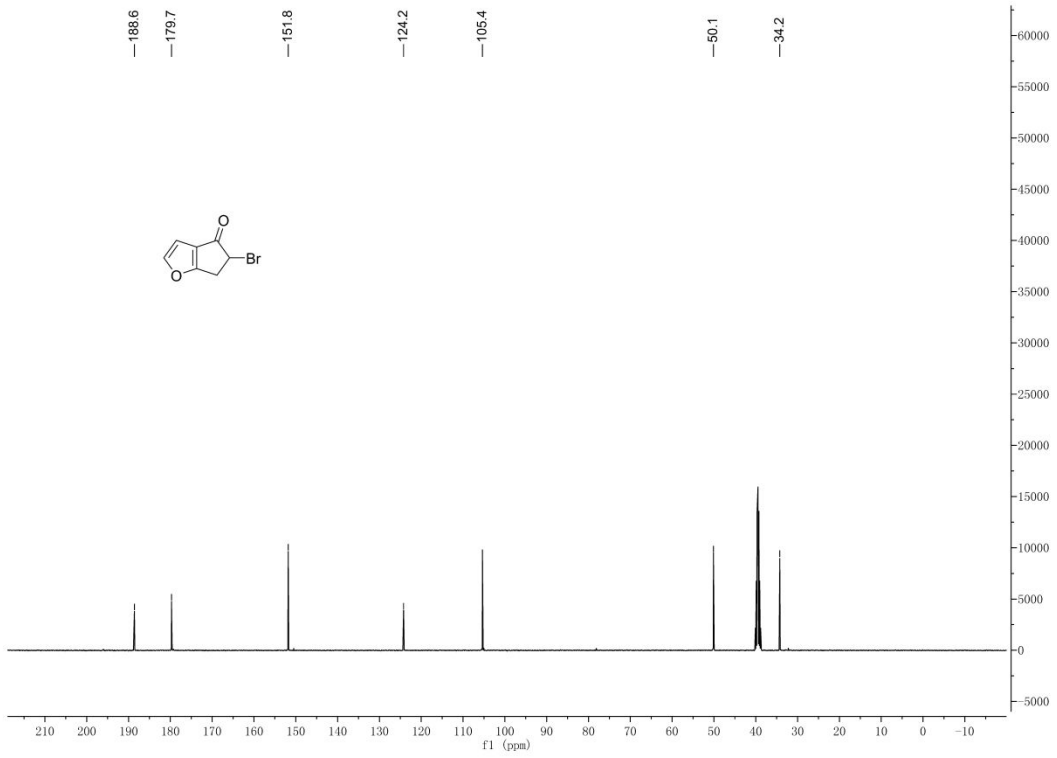
ESI-MS chromatograms of compound **6m**



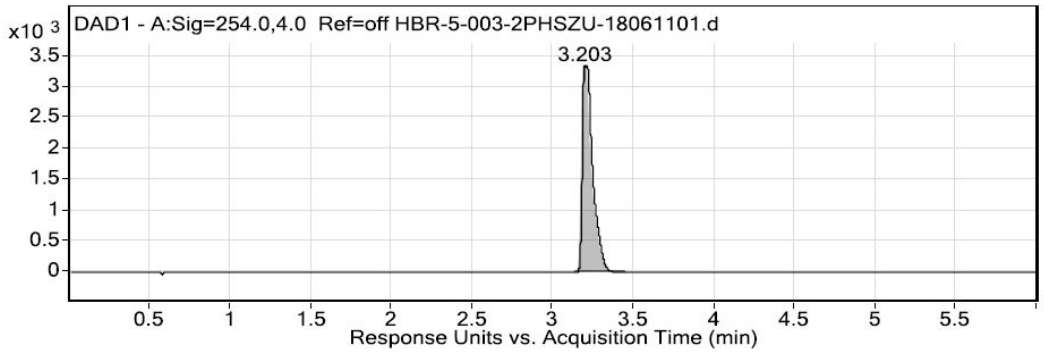
^{1}H-NMR spectra of compound **6m**



^{13}C-NMR spectra of compound **6m**



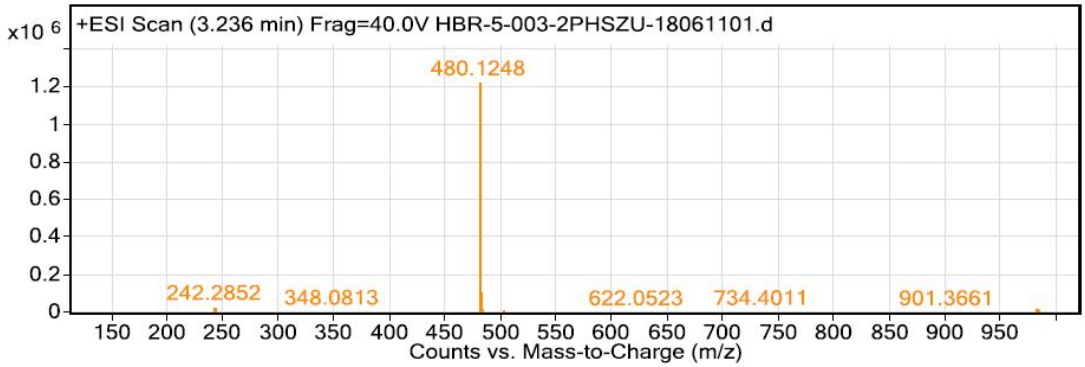
LC-ESI-MS chromatograms of compound **7a**



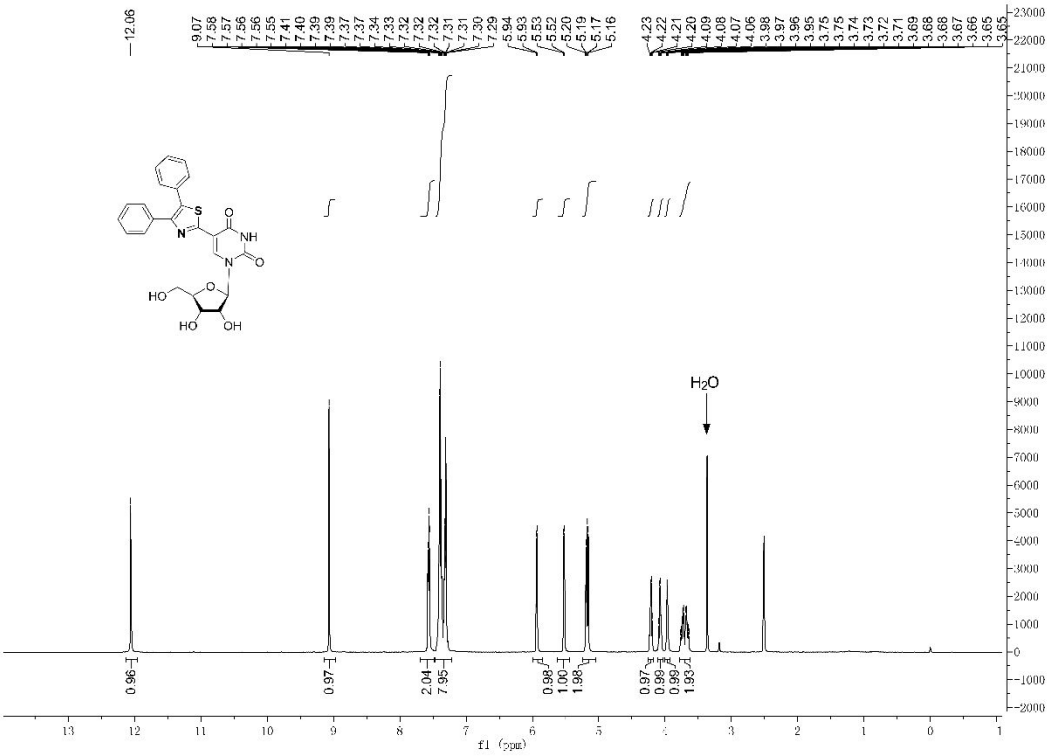
Integration Peak List

Peak	Start	RT	End	Height	Area	AreaSumPercent
1	3.141	3.203	3.451	3339.96	14858.05	100.00

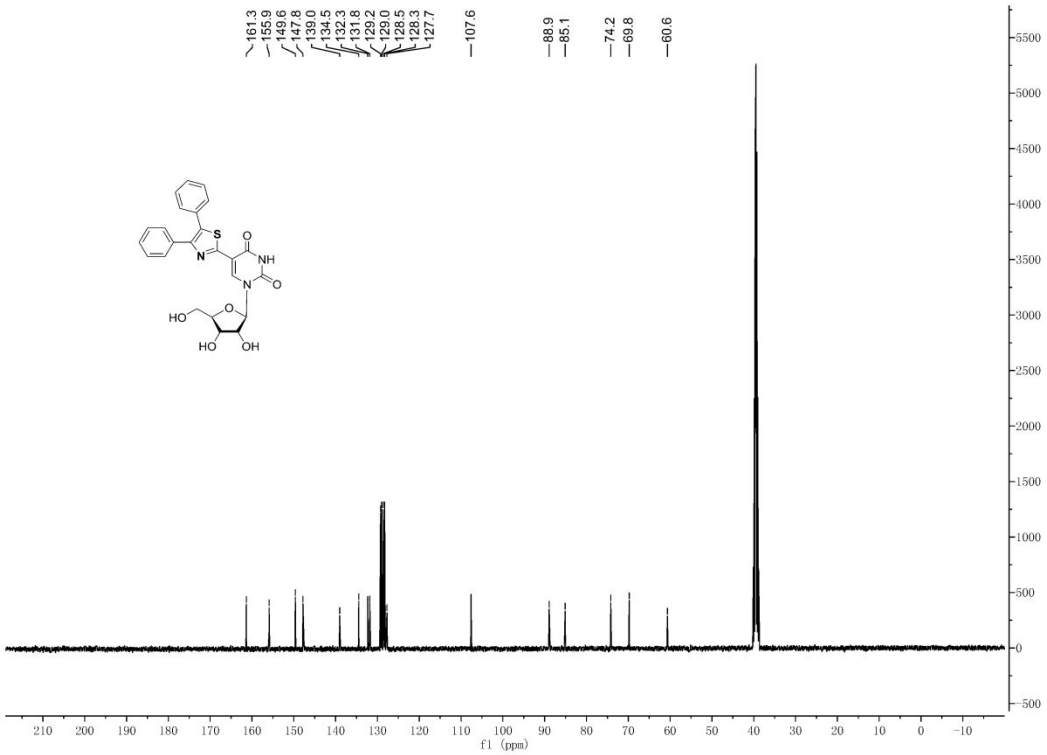
Fragmentor Voltage	Collision Energy	Ionization Mode
40	0	ESI



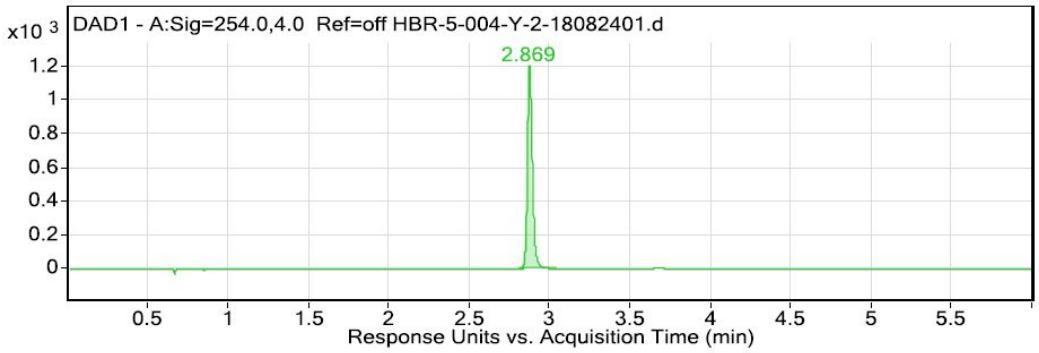
^{1}H-NMR spectra of compound **7a**



^{13}C-NMR spectra of compound **7a**

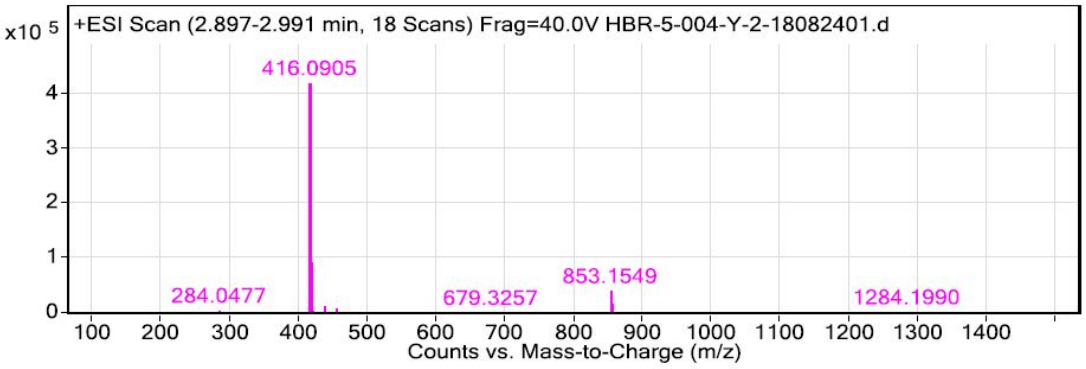


LC-ESI-MS chromatograms of compound **7b**

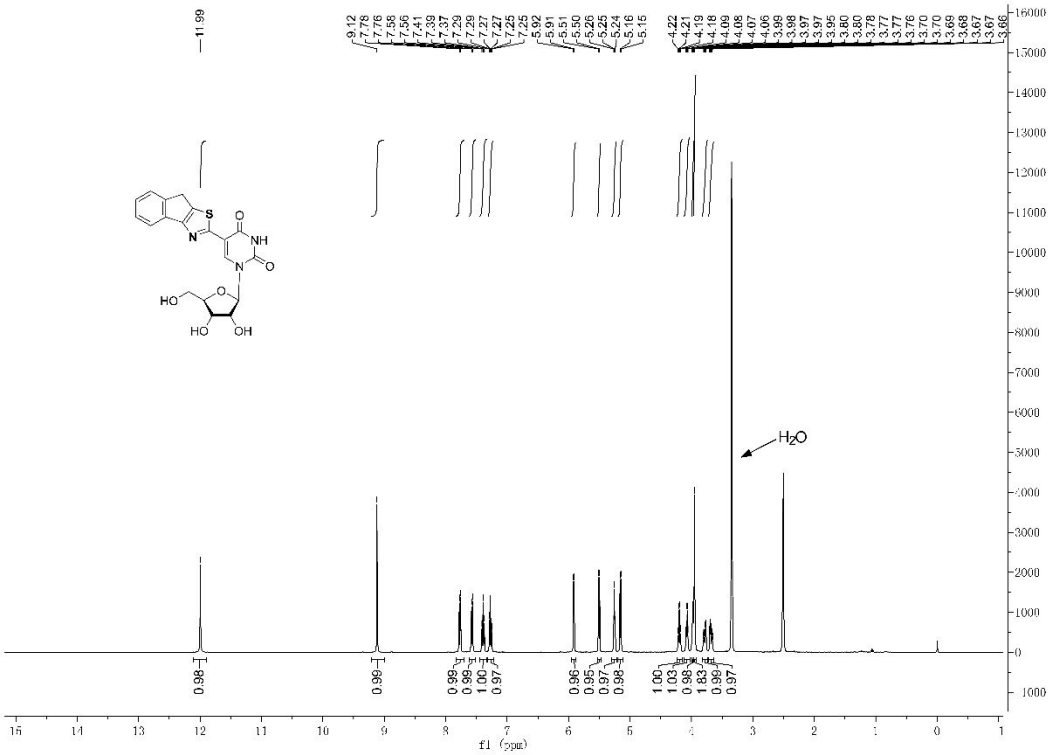


Integration Peak List

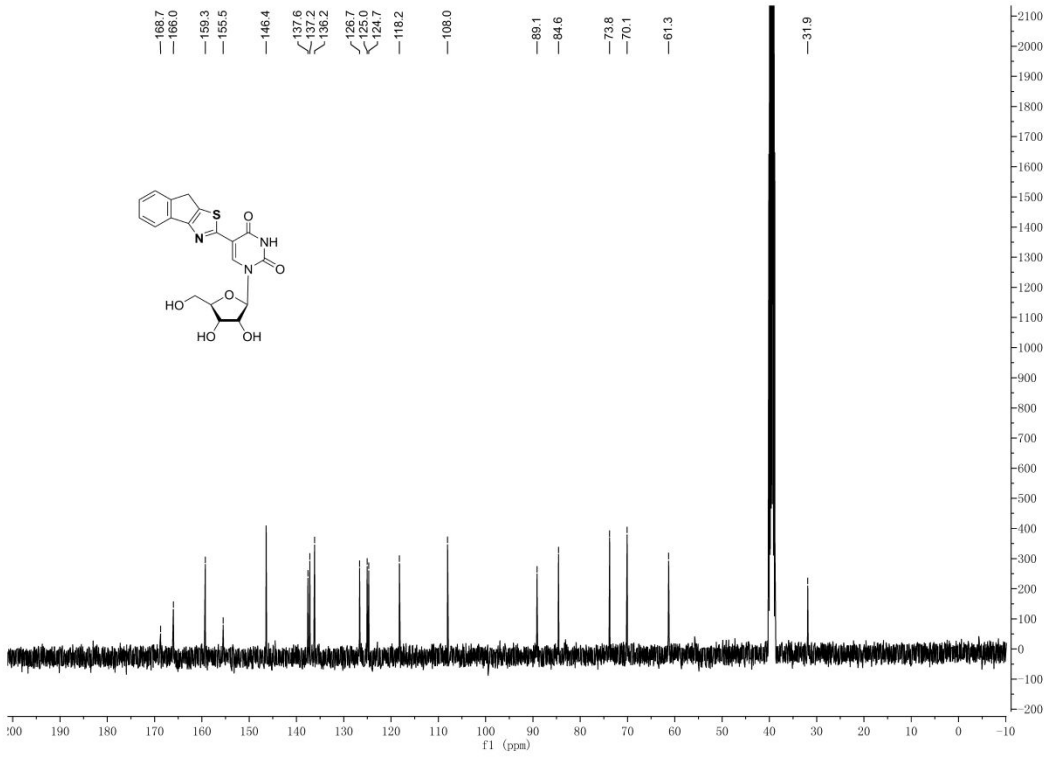
Peak	Start	RT	End	Height	Area	AreaSumPercent
1	2.814	2.869	3.041	1204.78	2567.83	100.00



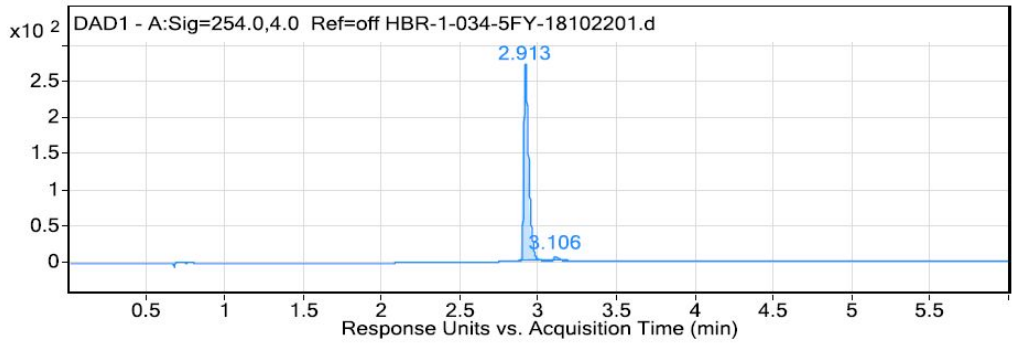
^{1}H-NMR spectra of compound **7b**



^{13}C-NMR spectra of compound **7b**



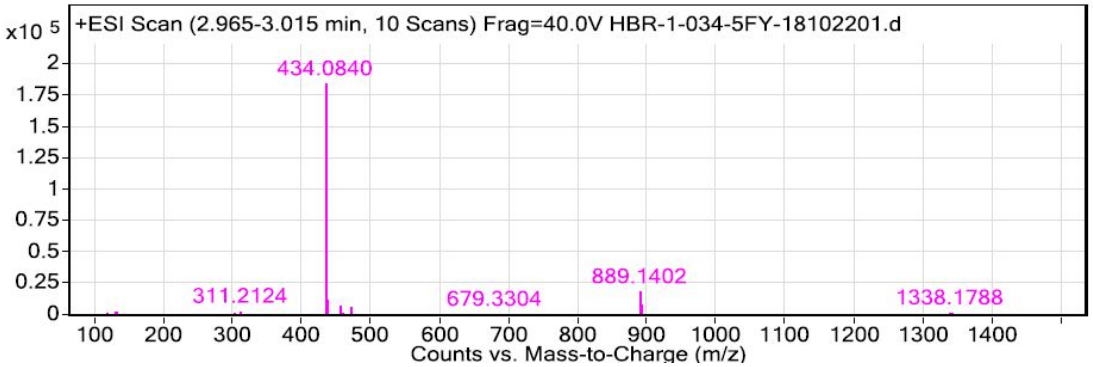
LC-ESI-MS chromatograms of compound **7c**



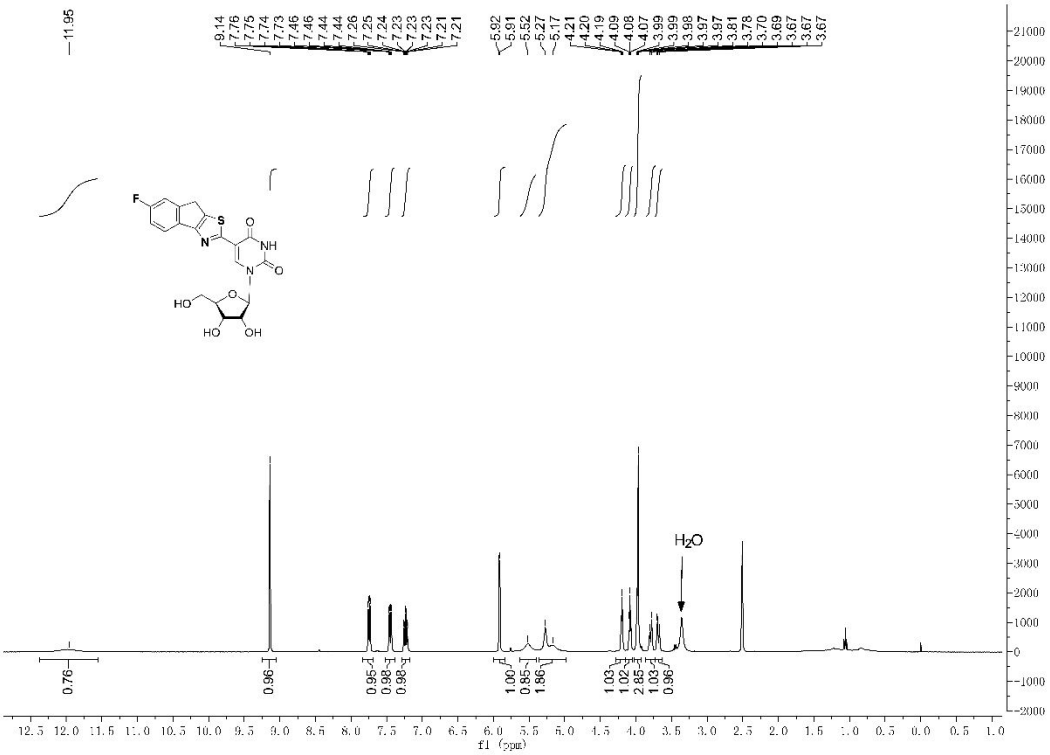
Integration Peak List

Peak	Start	RT	End	Height	Area	AreaSumPercent
1	2.875	2.913	3.072	273.79	581.41	97.43
2	3.072	3.106	3.188	6.21	15.35	2.57

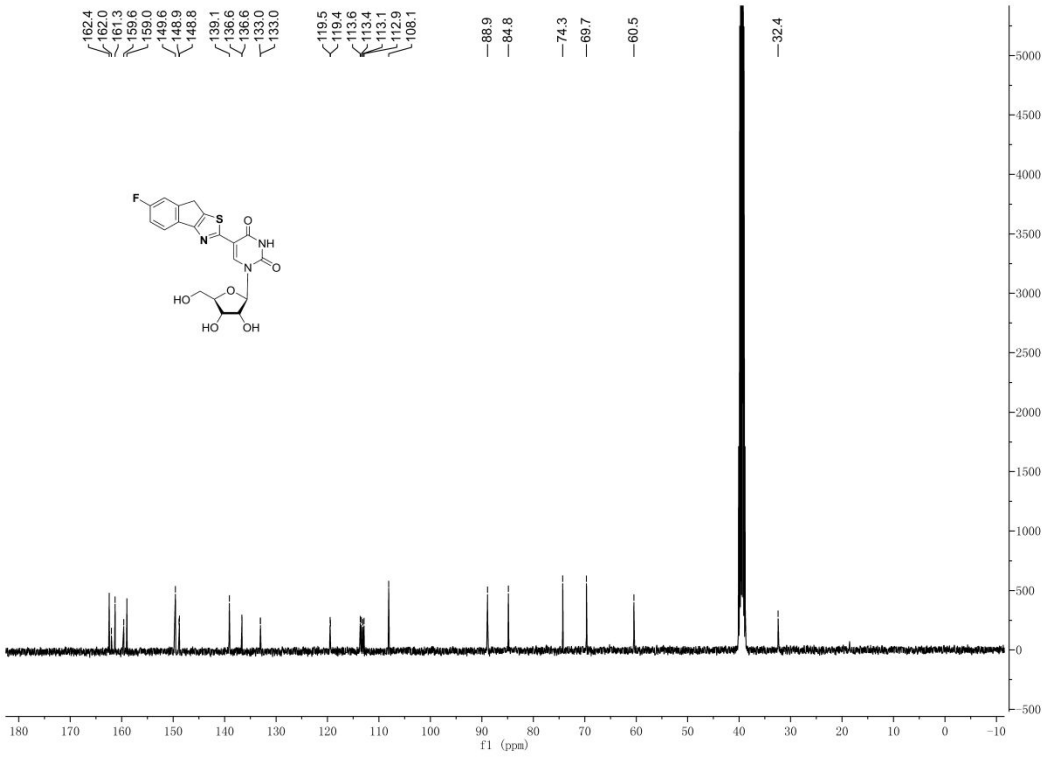
Fragmentor Voltage	Collision Energy	Ionization Mode
40	0	ESI



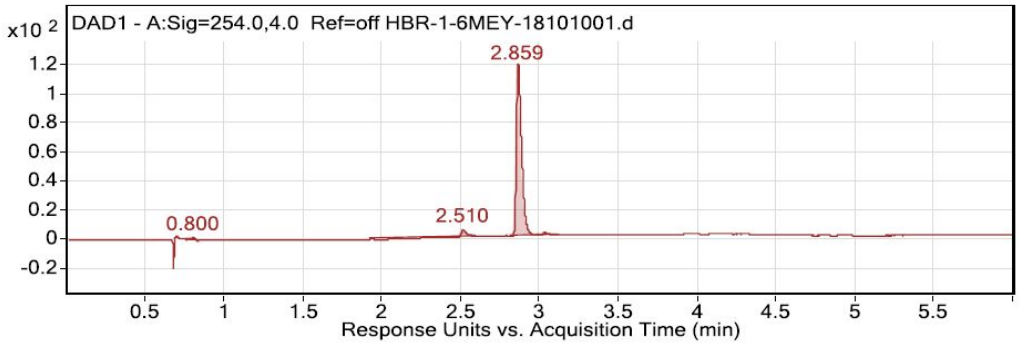
^{1}H-NMR spectra of compound **7c**



^{13}C-NMR spectra of compound **7c**



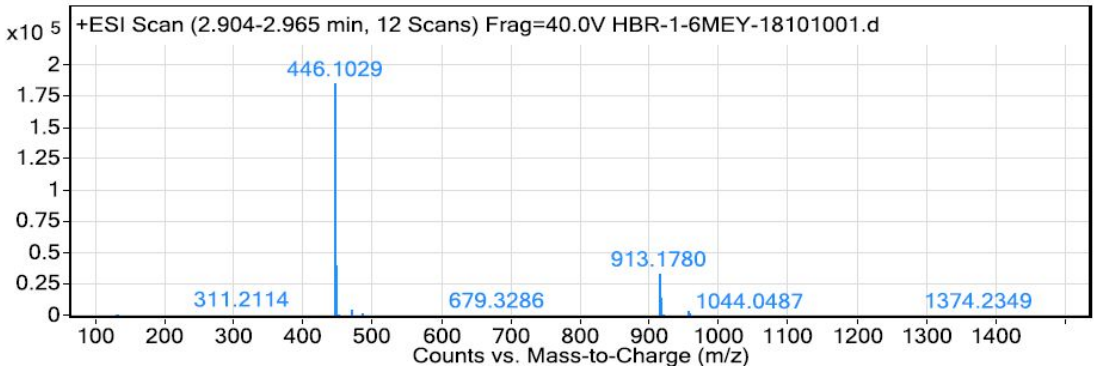
LC-ESI-MS chromatograms of compound **7d**



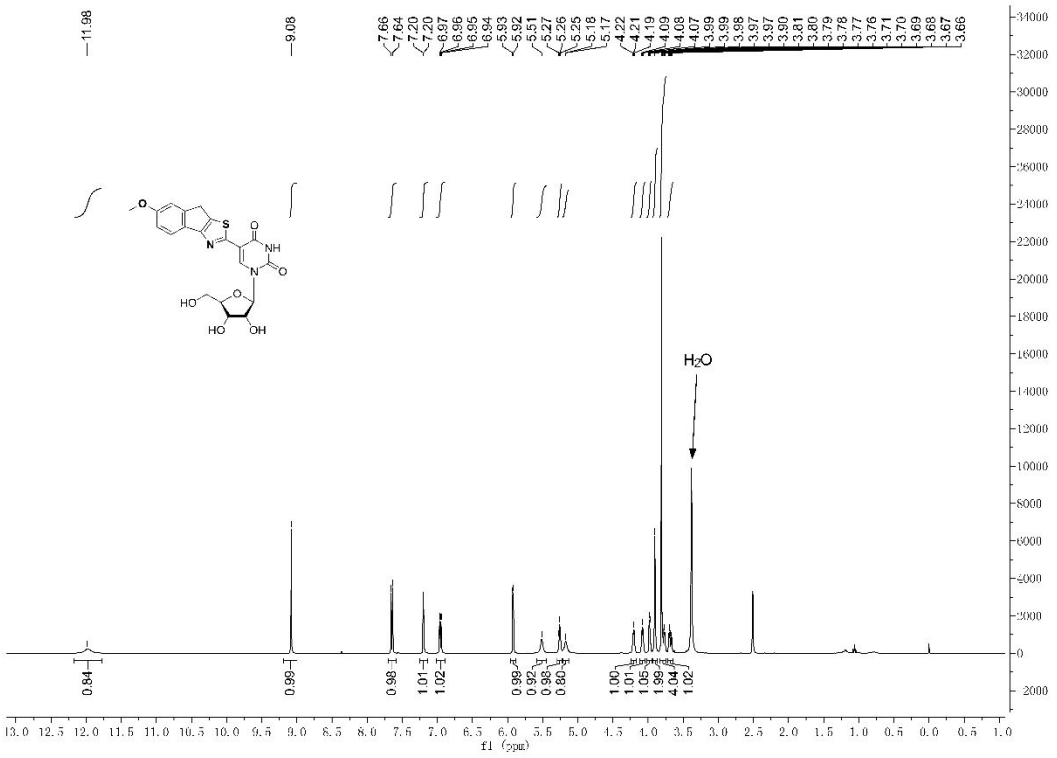
Integration Peak List

Peak	Start	RT	End	Height	Area	AreaSumPercent
1	0.76	0.8	0.828	2.07	5.72	1.86
2	1.921	2.51	2.593	5.18	18.61	6.04
3	2.818	2.859	2.991	118.52	275.94	89.58
4	2.991	3.029	3.121	2.14	7.77	2.52

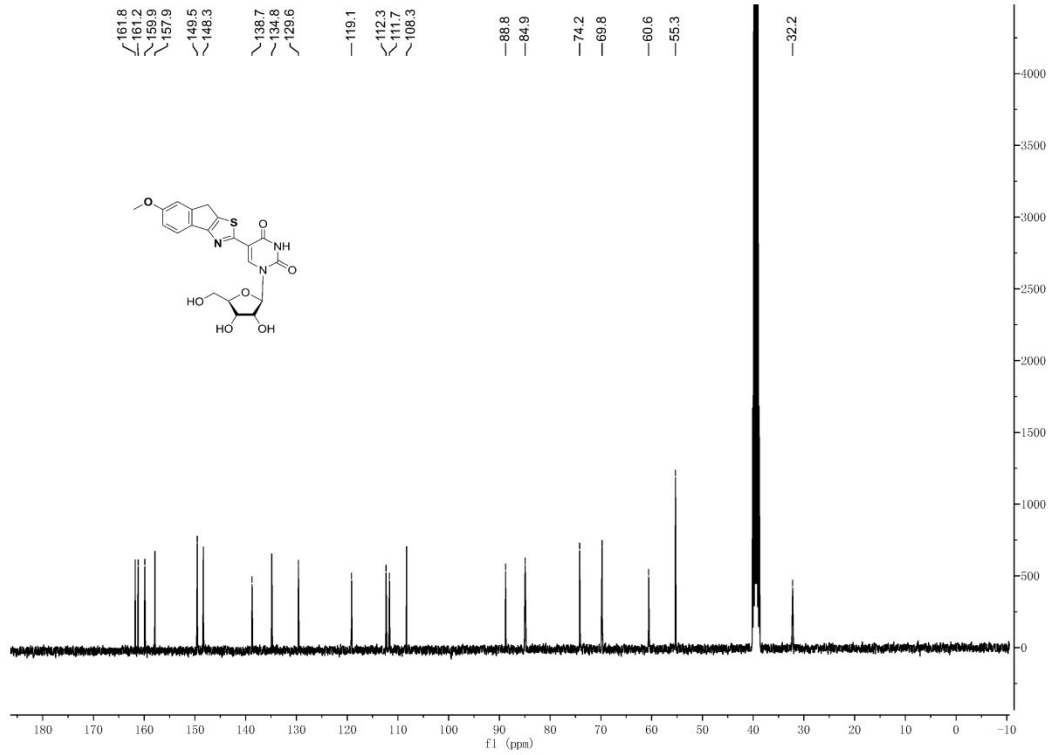
Fragmentor Voltage	Collision Energy	Ionization Mode
40	0	ESI



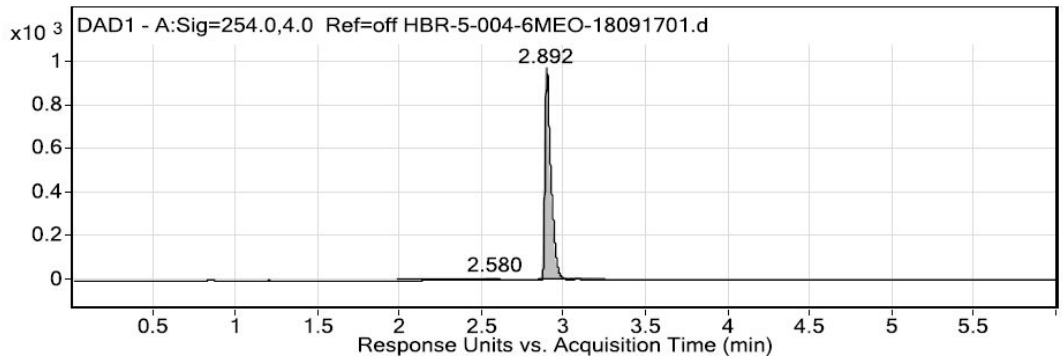
^{1}H-NMR spectra of compound **7d**



^{13}C-NMR spectra of compound **7d**

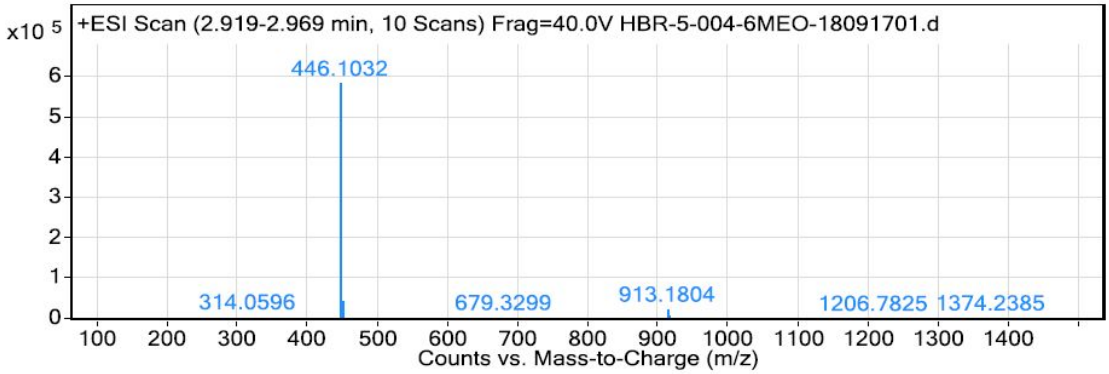


LC-ESI-MS chromatograms of compound **7e**

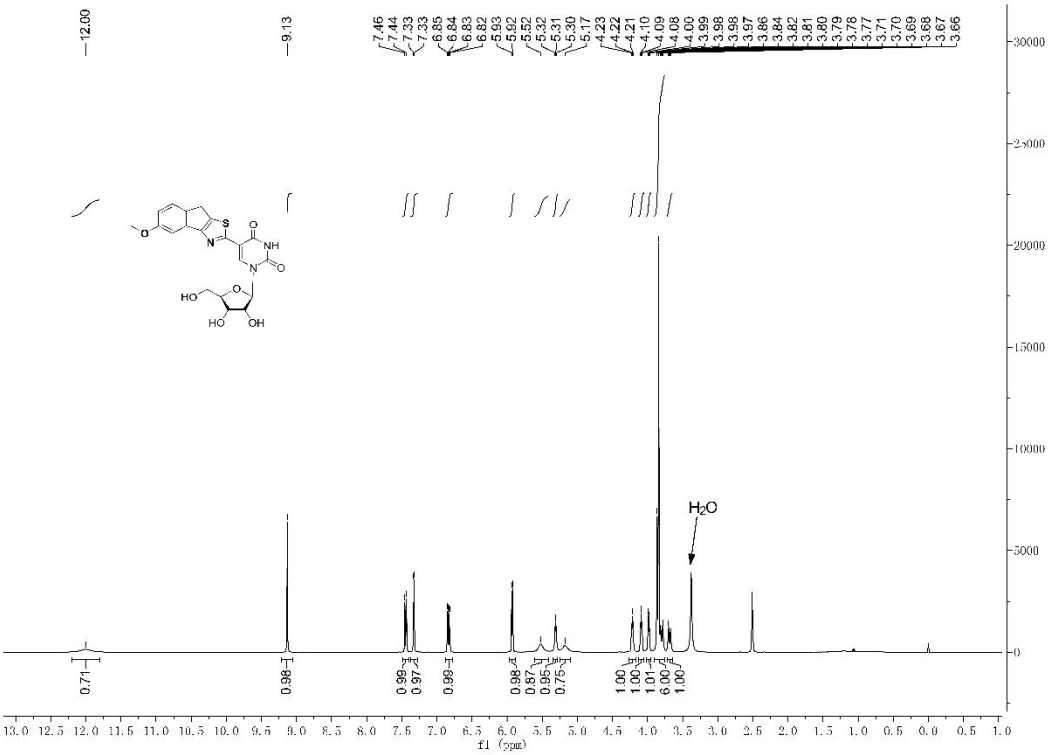


2	2.848	2.892	3.045	970.54	2433.24	97.23
3	3.045	3.075	3.251	7.13	40.22	1.61

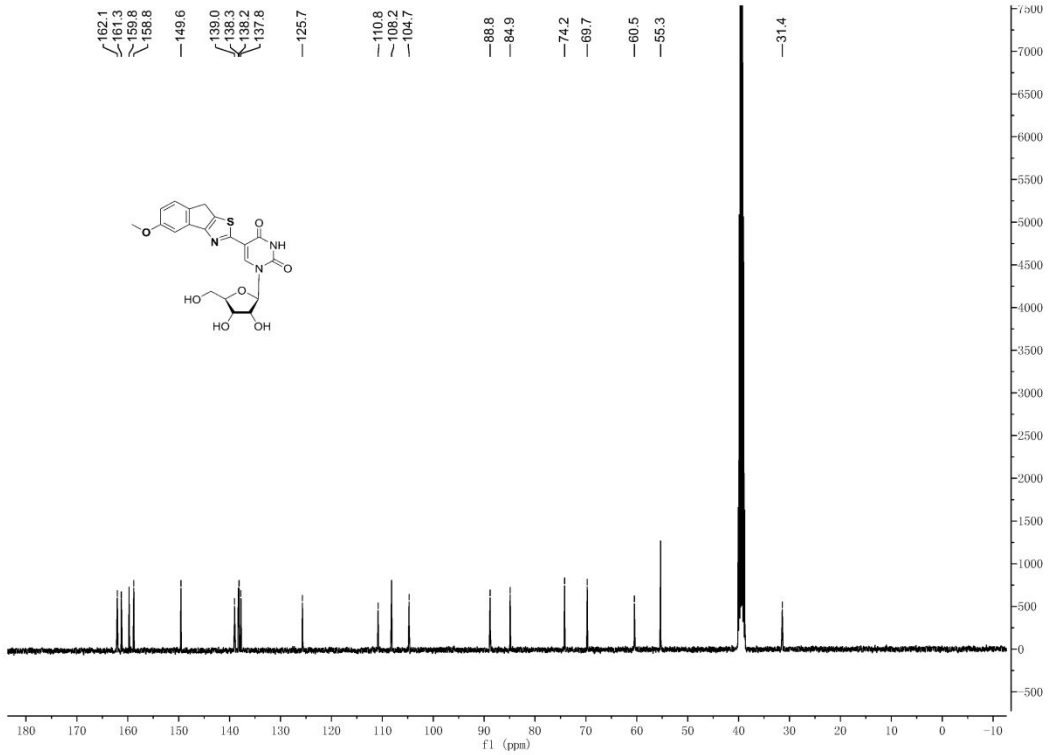
Fragmentor Voltage	Collision Energy	Ionization Mode
40	0	ESI



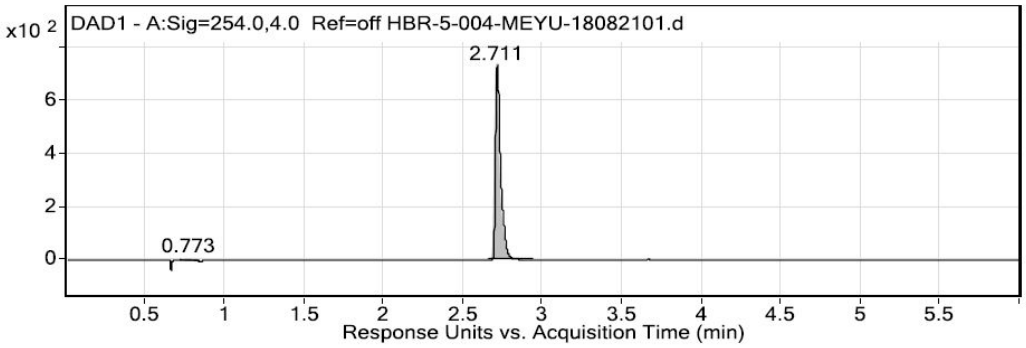
^{1}H-NMR spectra of compound **7e**



^{13}C-NMR spectra of compound **7e**



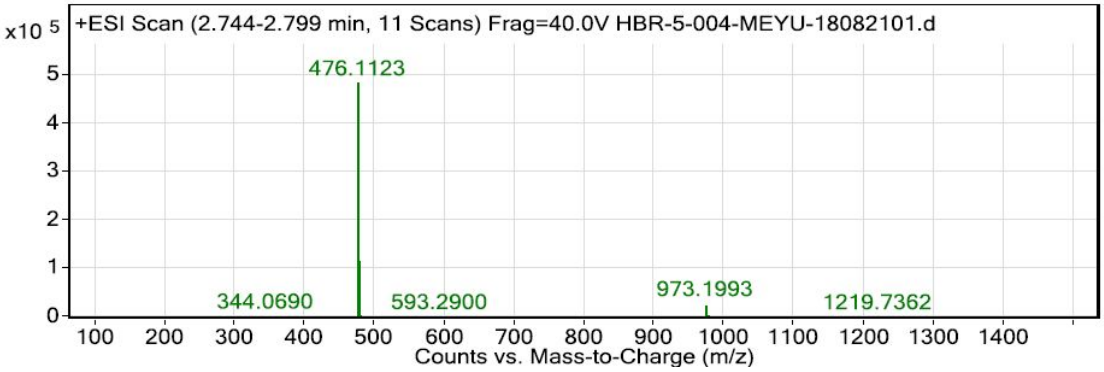
LC-ESI-MS chromatograms of compound **7f**



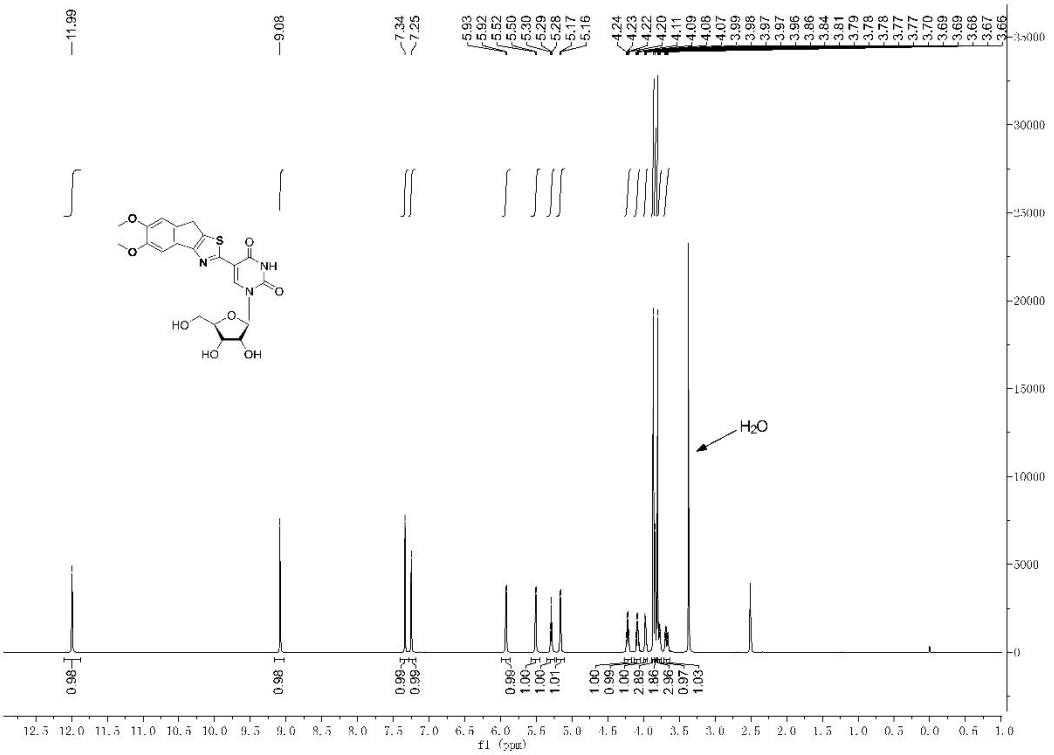
Integration Peak List

Peak	Start	RT	End	Height	Area	AreaSumPercent
1	0.725	0.773	0.844	5.66	35.5	2.08
2	2.663	2.711	2.941	734.73	1673.32	97.92

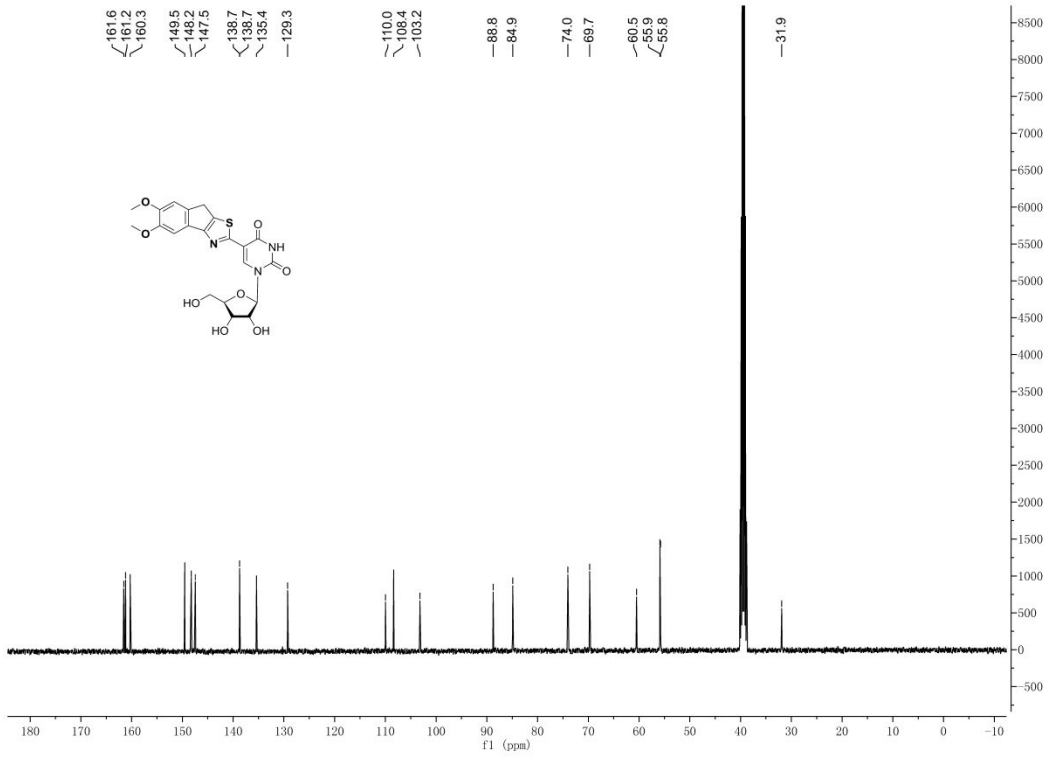
Fragmentor Voltage	Collision Energy	Ionization Mode
40	0	ESI



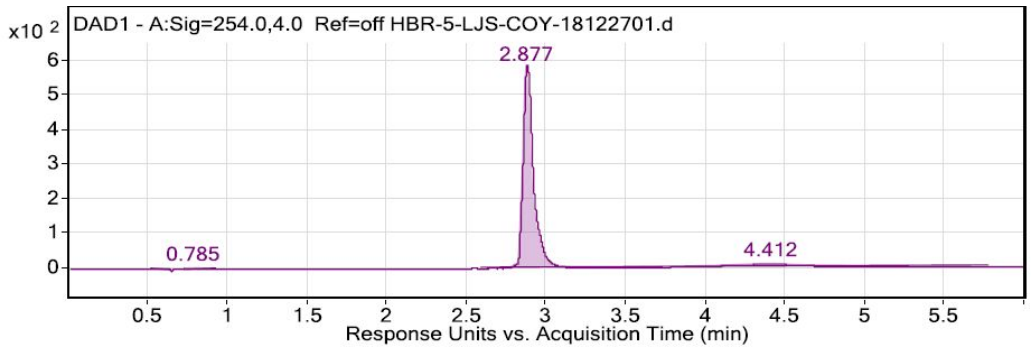
^{1}H-NMR spectra of compound **7f**



^{13}C-NMR spectra of compound **7f**



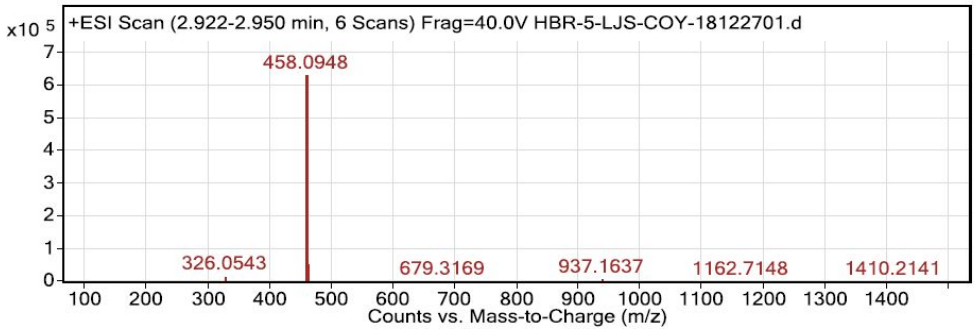
LC-ESI-MS chromatograms of compound **7g**



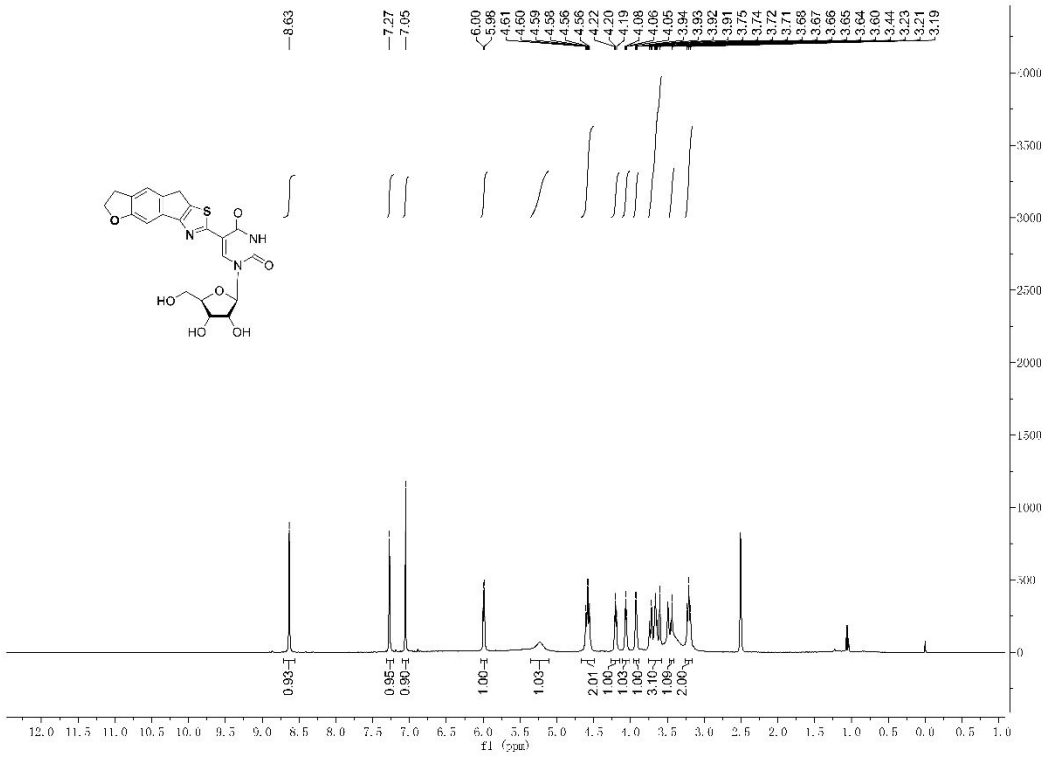
Integration Peak List

Peak	Start	RT	End	Height	Area	AreaSumPercent
1	0.522	0.589	0.647	4.59	30.14	0.93
2	0.732	0.785	0.925	5.16	42.43	1.31
3	2.593	2.877	3.288	586.48	2726.87	84.46
4	3.288	4.412	5.778	9.42	429.32	13.30

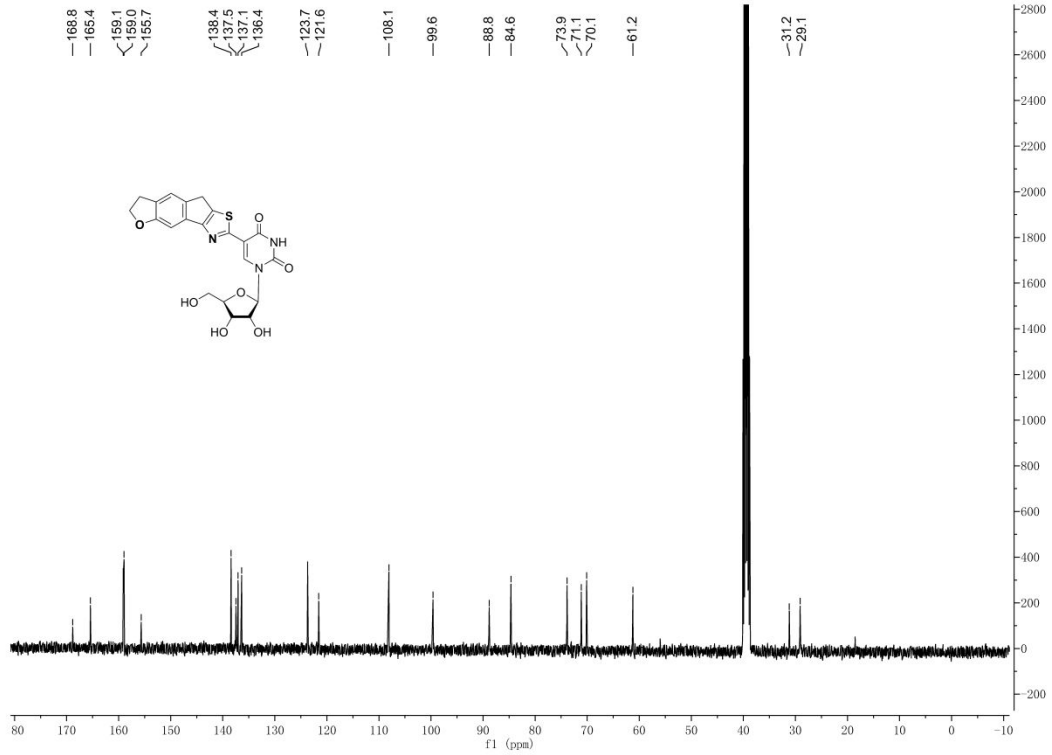
Fragmentor Voltage 40 **Collision Energy** 0 **Ionization Mode** ESI



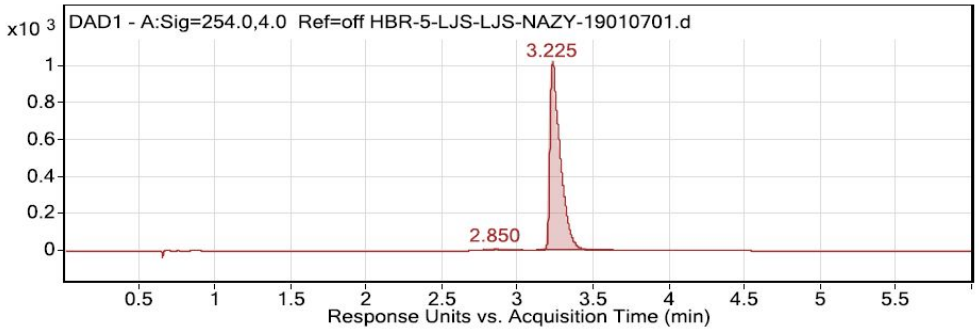
^{1}H-NMR spectra of compound **7g**



^{13}C-NMR spectra of compound **7g**



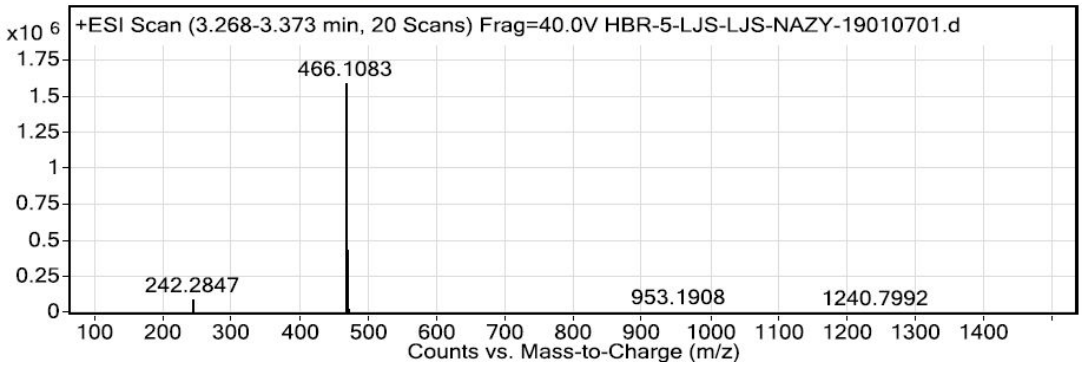
LC-ESI-MS chromatograms of compound **7h**



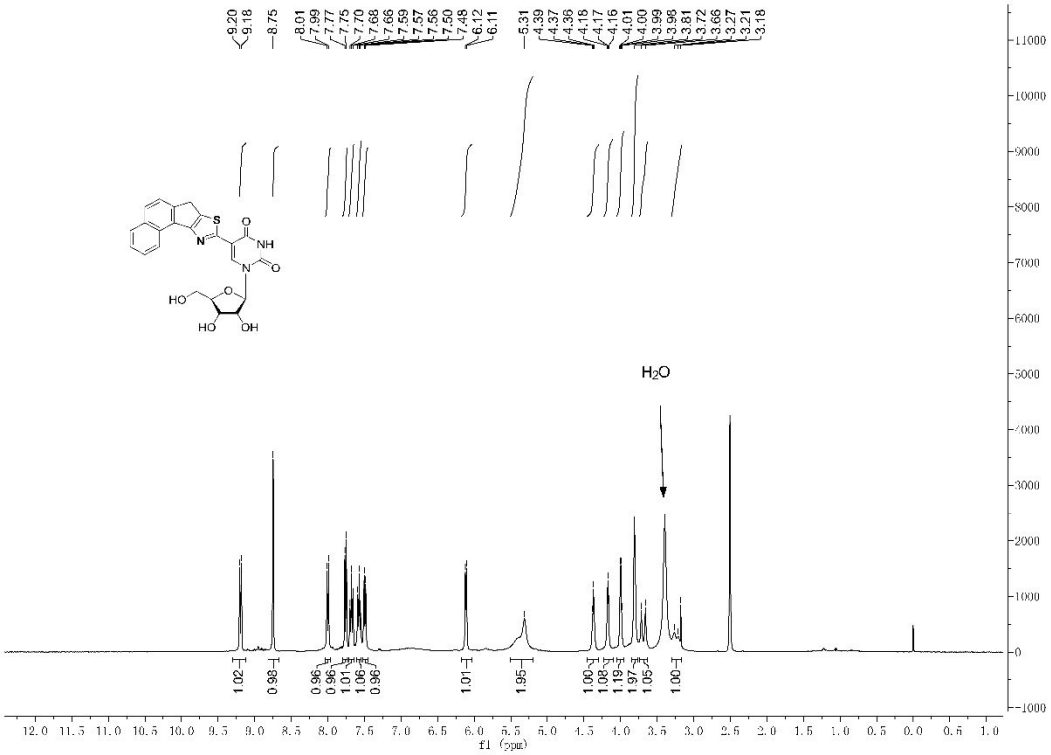
Integration Peak List

Peak	Start	RT	End	Height	Area	AreaSumPercent
1	2.775	2.85	3.033	9.42	99.67	1.98
2	3.129	3.225	3.631	1028.02	4940.93	98.02

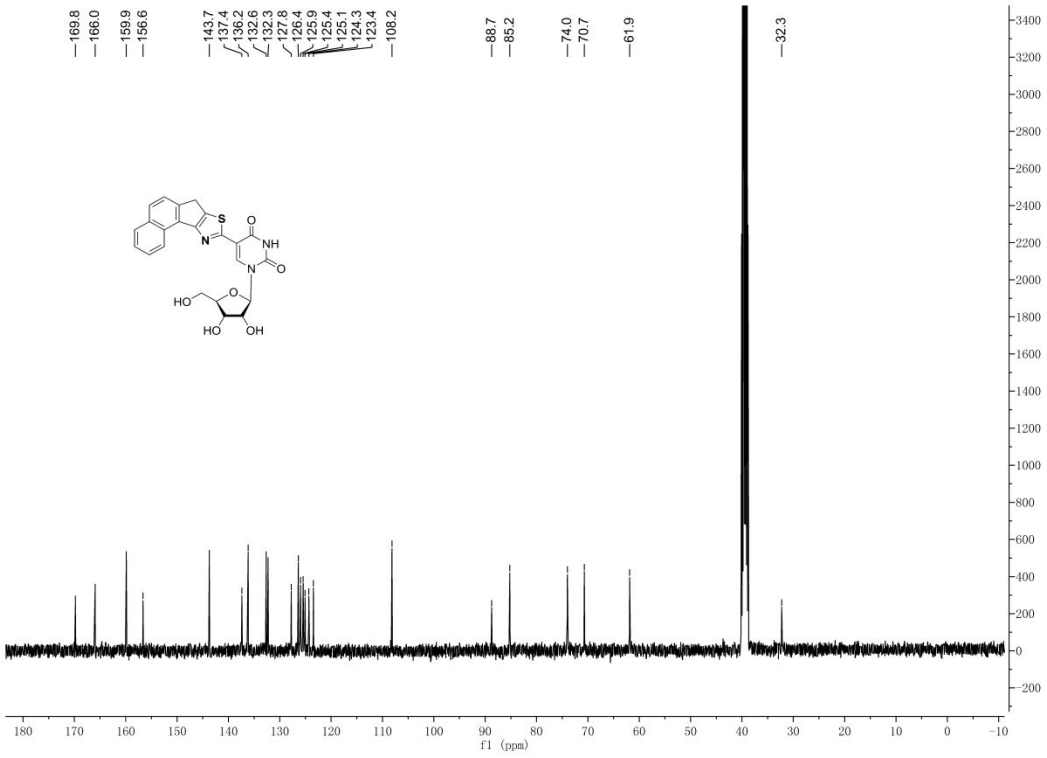
Fragmentor Voltage	Collision Energy	Ionization Mode
40	0	ESI



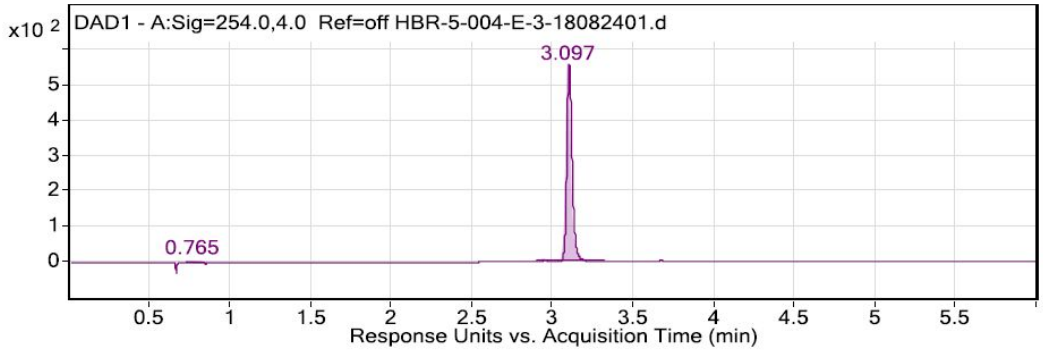
^{1}H-NMR spectra of compound **7h**



^{13}C-NMR spectra of compound **7h**



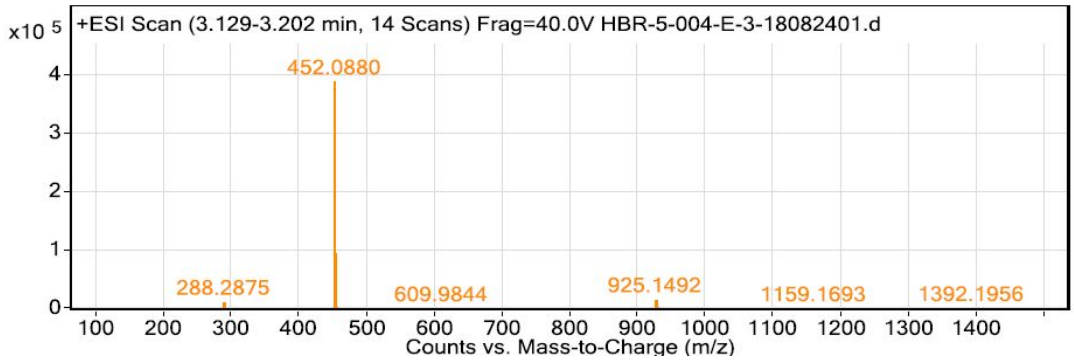
LC-ESI-MS chromatograms of compound **7i**



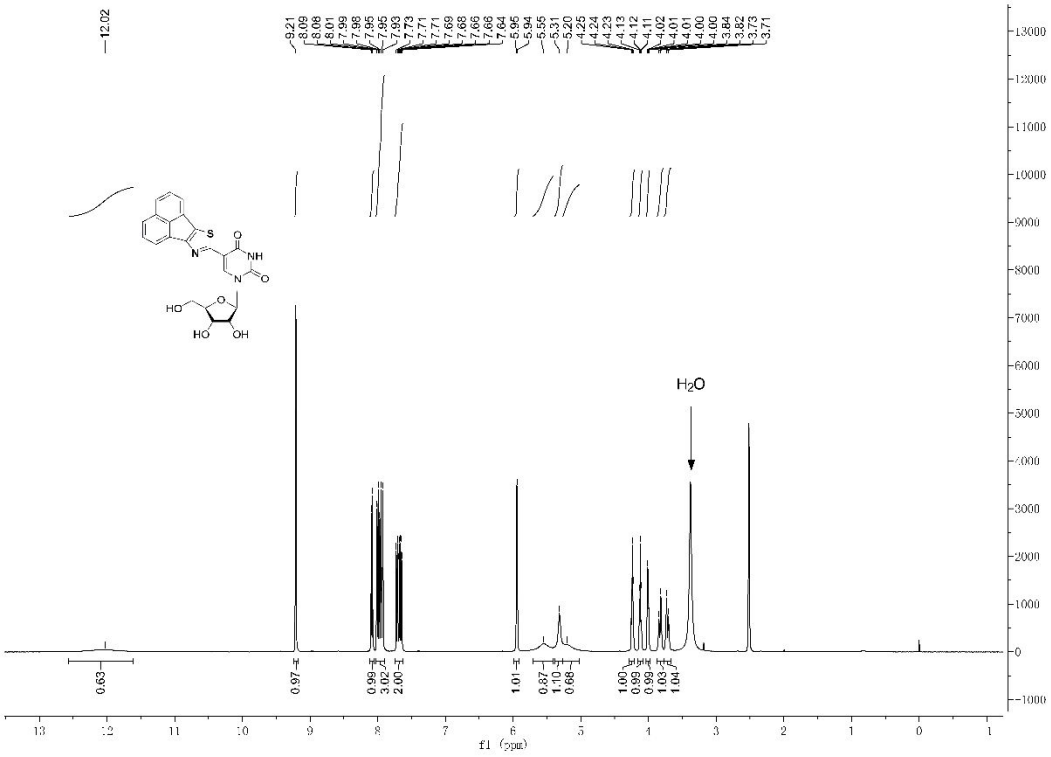
Integration Peak List

Peak	Start	RT	End	Height	Area	AreaSumPercent
1	0.732	0.765	0.844	4.07	20.66	1.55
2	2.901	2.946	3.038	4.73	13.06	0.98
3	3.038	3.097	3.325	554.47	1295.39	97.46

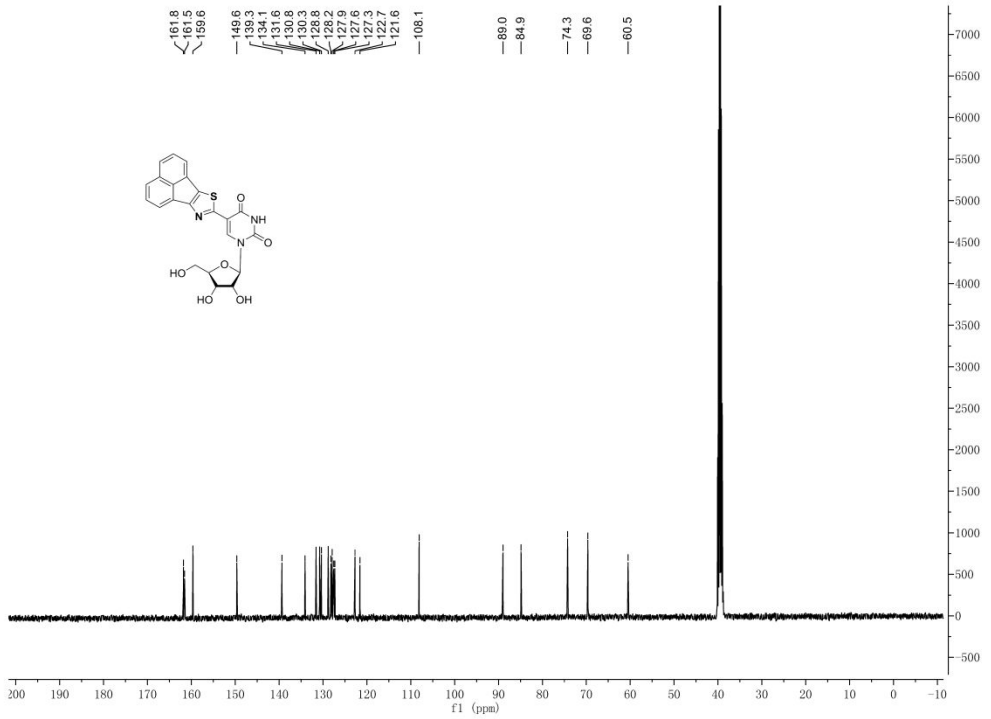
Fragmentor Voltage 40 **Collision Energy** 0 **Ionization Mode** ESI



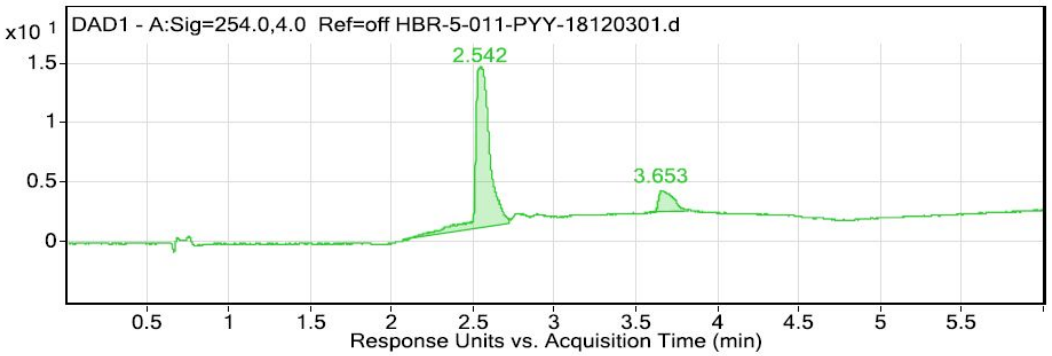
^{1}H-NMR spectra of compound **7i**



^{13}C-NMR spectra of compound **7i**



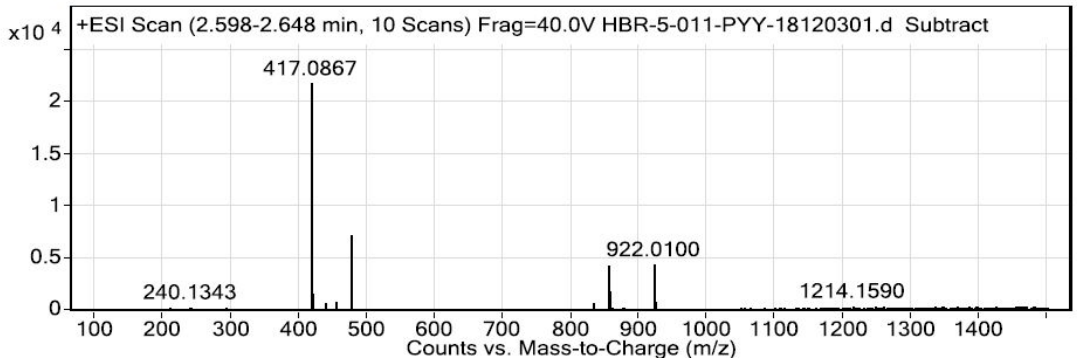
LC-ESI-MS chromatograms of compound **7j**



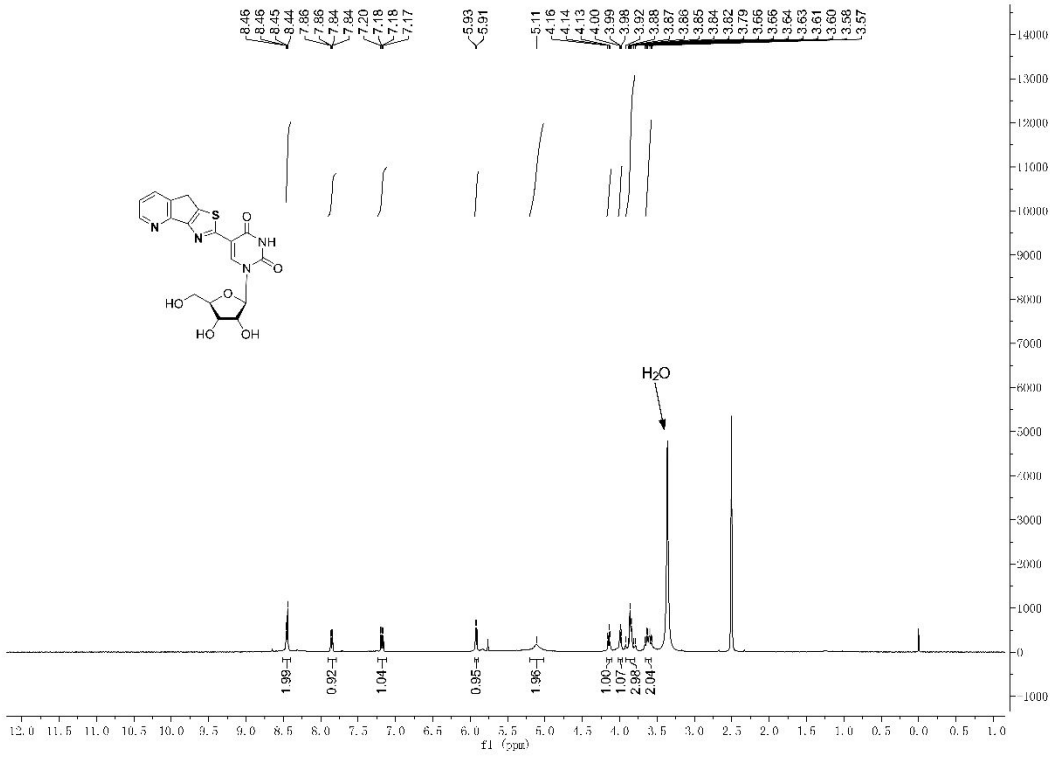
Integration Peak List

Peak	Start	RT	End	Height	Area	AreaSumPercent
1	2.071	2.542	2.721	13.67	89.95	88.00
2	3.586	3.653	3.821	1.87	12.26	12.00

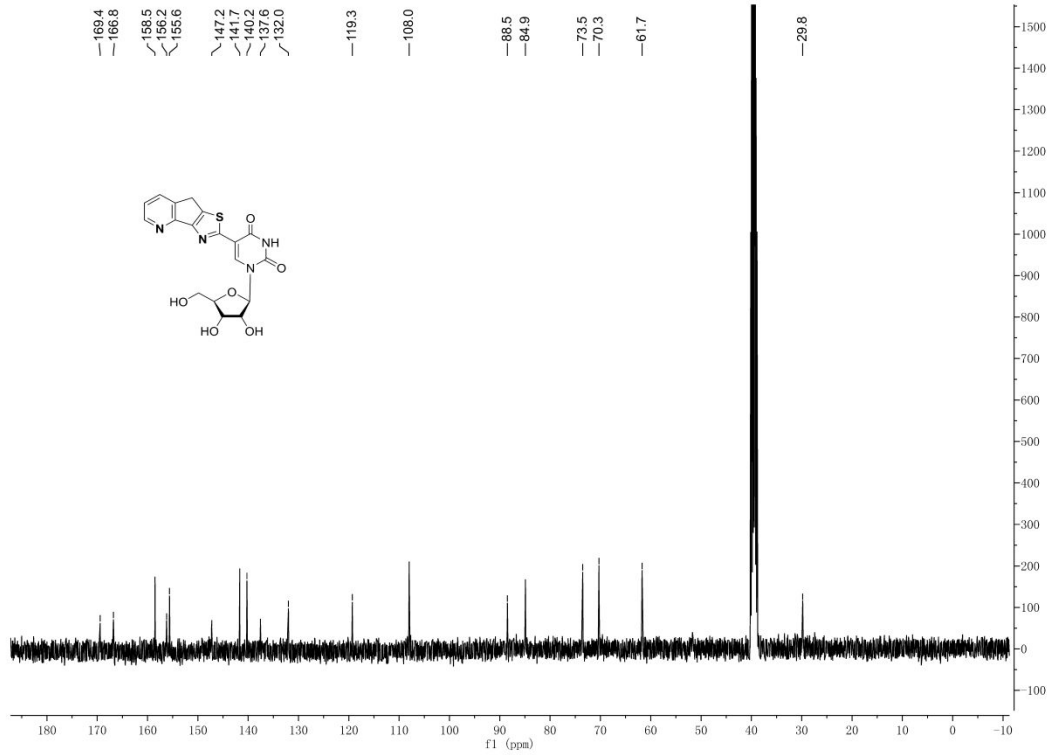
Spectrum Source	Fragmentor Voltage	Collision Energy	Ionization Mode
Peak (11) in "+ TIC Scan"	40	0	ESI



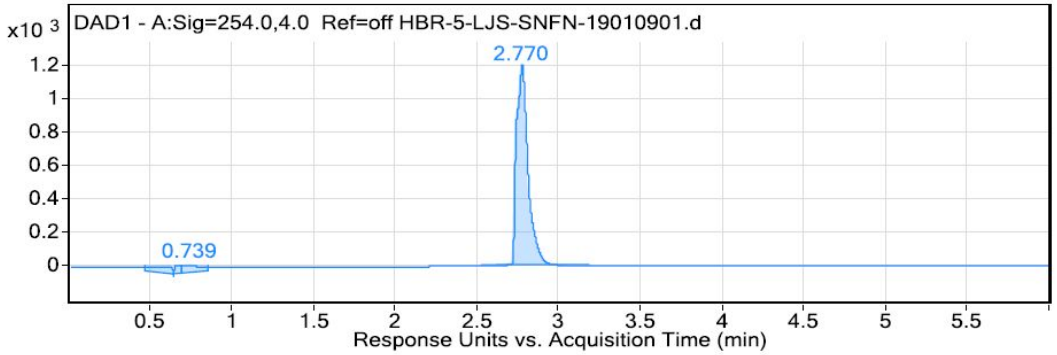
H-NMR spectra of compound **7j**



^{13}C-NMR spectra of compound **7j**



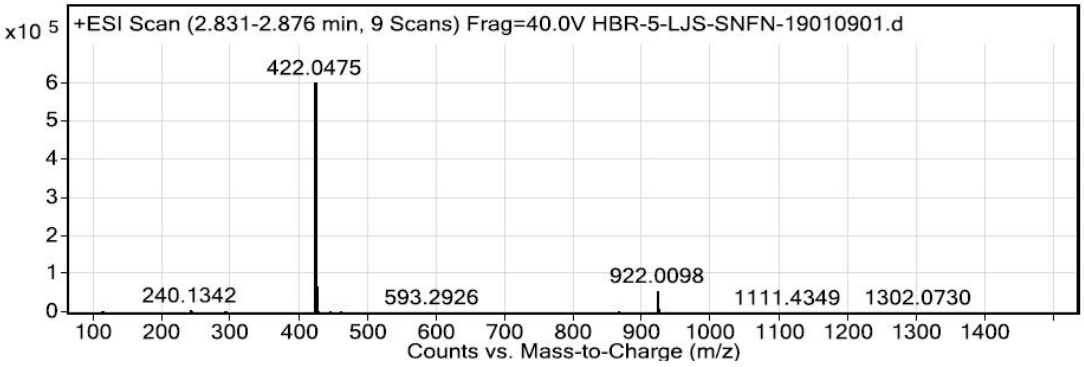
LC-ESI-MS chromatograms of compound **7k**



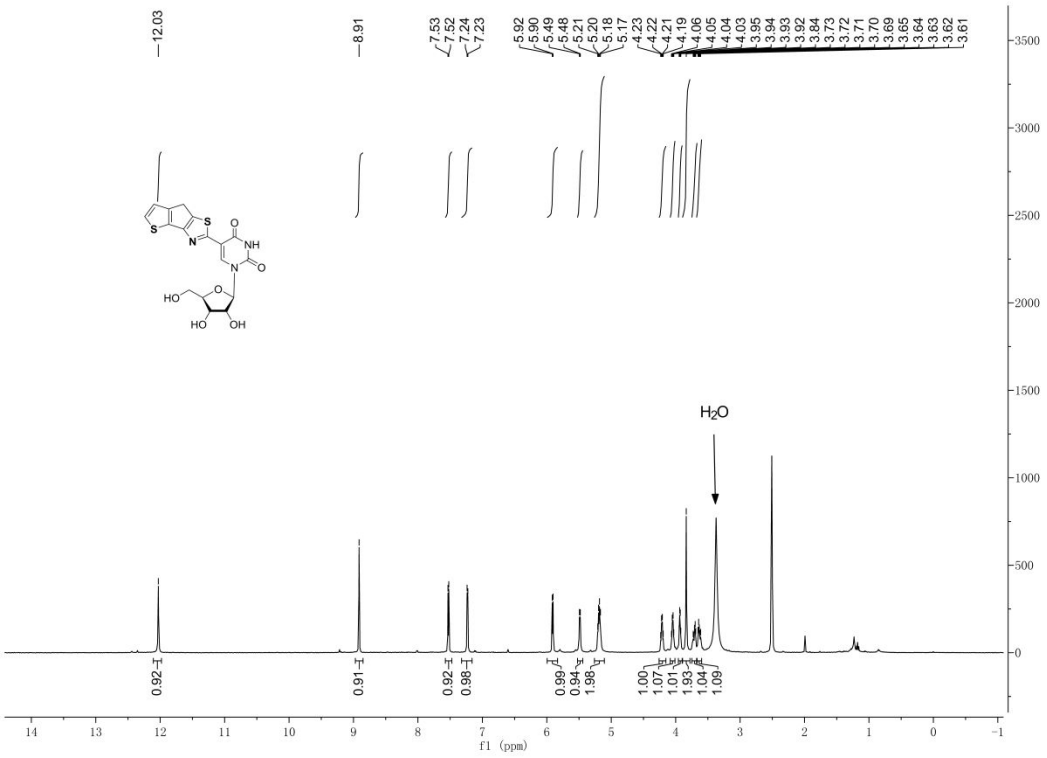
Integration Peak List

Peak	Start	RT	End	Height	Area	AreaSumPercent
1	0.468	0.579	0.638	47.7	441.07	6.27
2	0.638	0.658	0.693	53.91	160.85	2.29
3	0.693	0.739	0.855	49.36	421.19	5.99
4	2.529	2.77	3.188	1204.1	6010.14	85.45

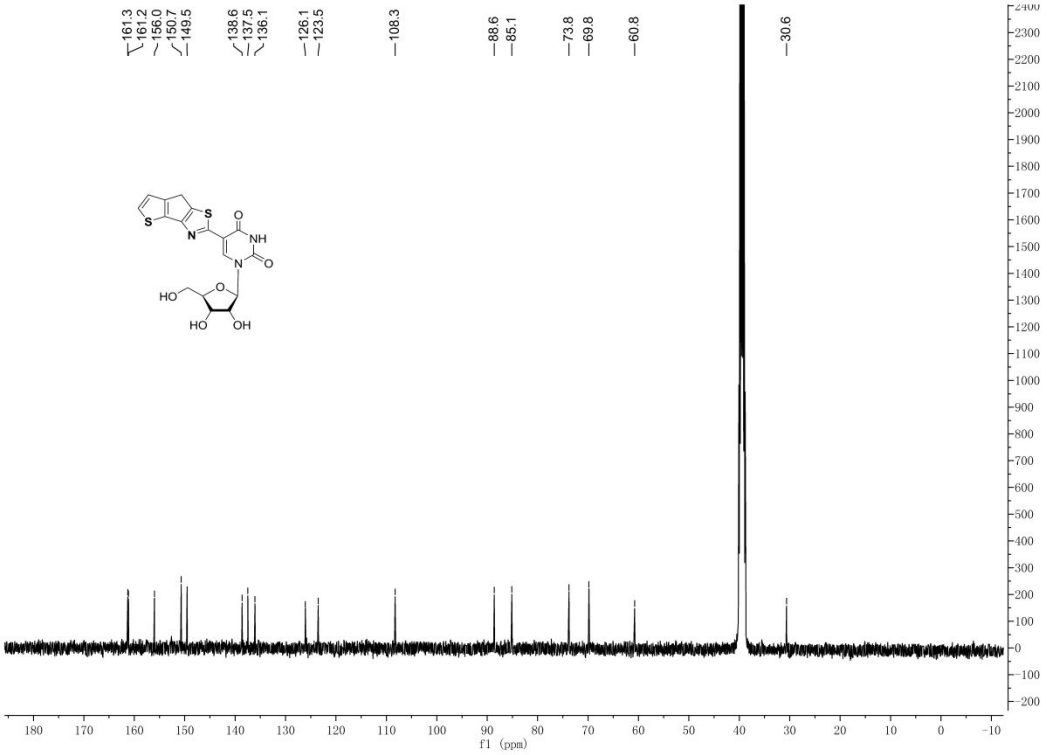
Fragmentor Voltage 40 **Collision Energy** 0 **Ionization Mode** ESI



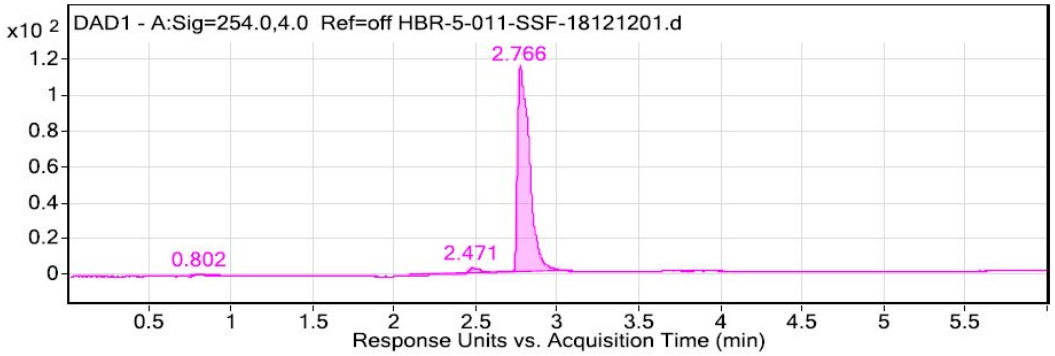
^{1}H-NMR spectra of compound **7k**



^{13}C-NMR spectra of compound **7k**



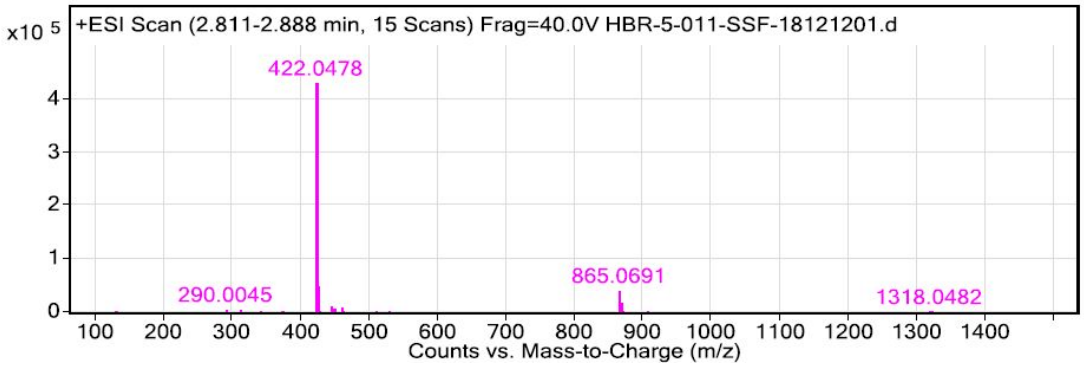
LC-ESI-MS chromatograms of compound **7l**



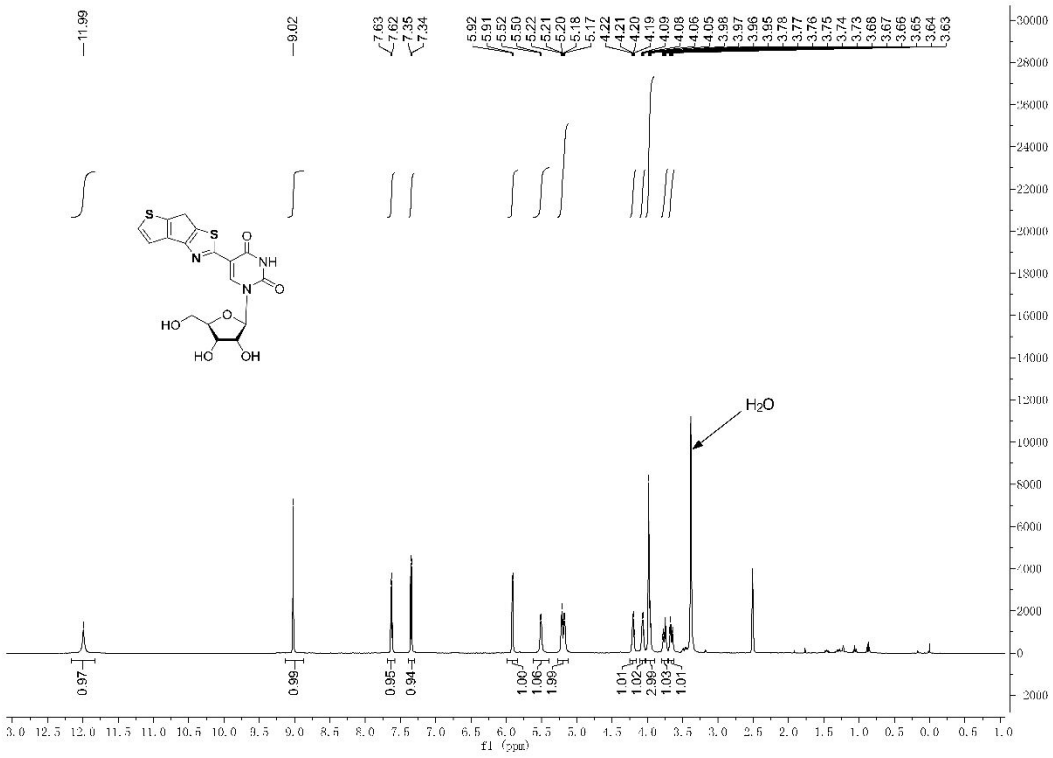
Integration Peak List

Peak	Start	RT	End	Height	Area	AreaSumPercent
1	0.745	0.802	0.931	1.07	6.43	1.03
2	2.091	2.471	2.582	3.44	21.83	3.49
3	2.582	2.766	3.091	115.31	596.73	95.48

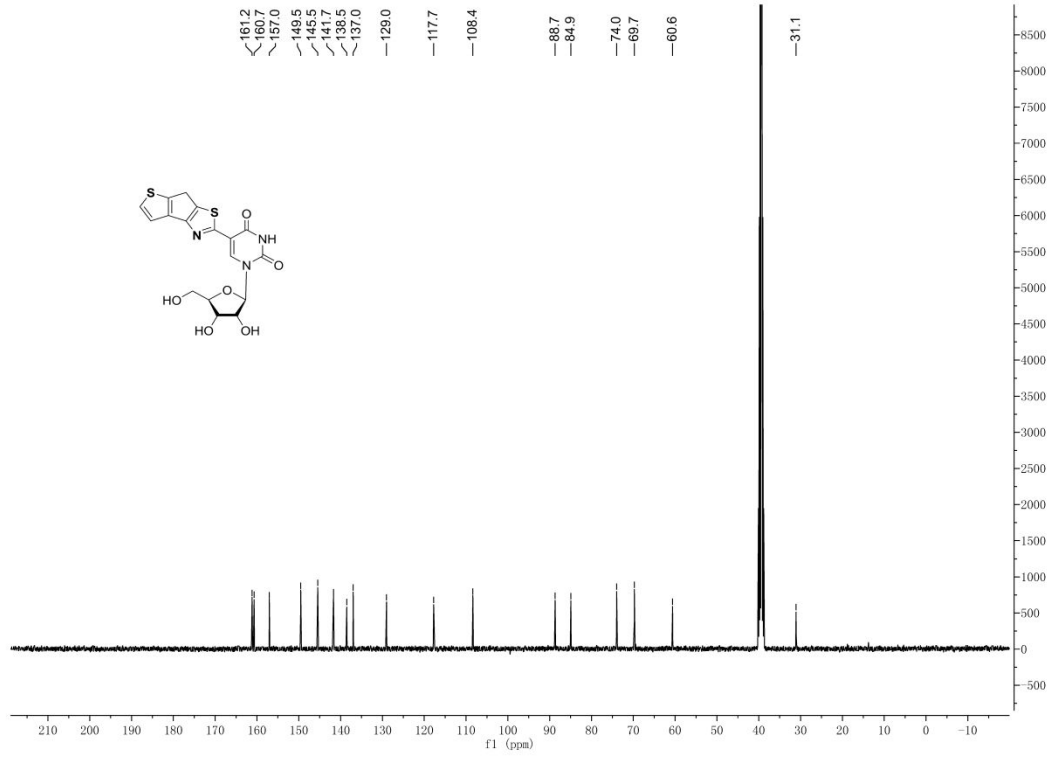
Fragmentor Voltage	Collision Energy	Ionization Mode
40	0	ESI



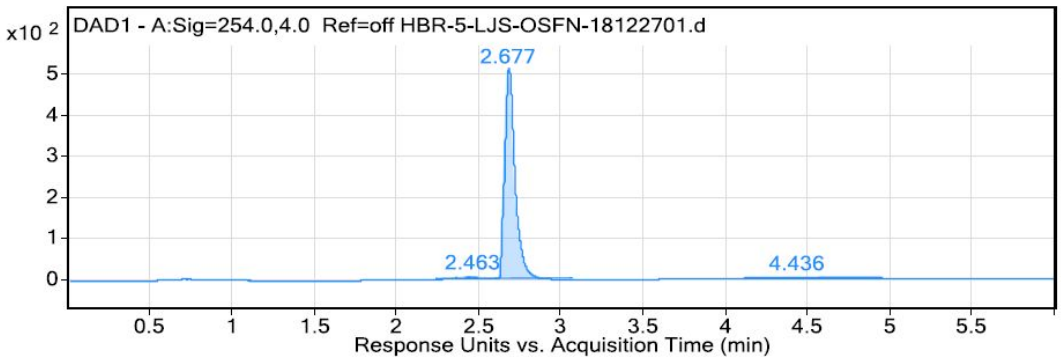
^{1}H-NMR spectra of compound **7l**



^{13}C-NMR spectra of compound **7l**



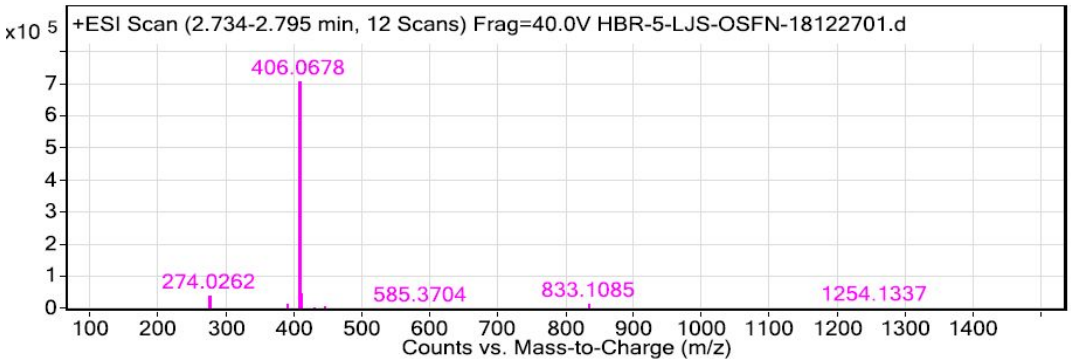
LC-ESI-MS chromatograms of compound **7m**



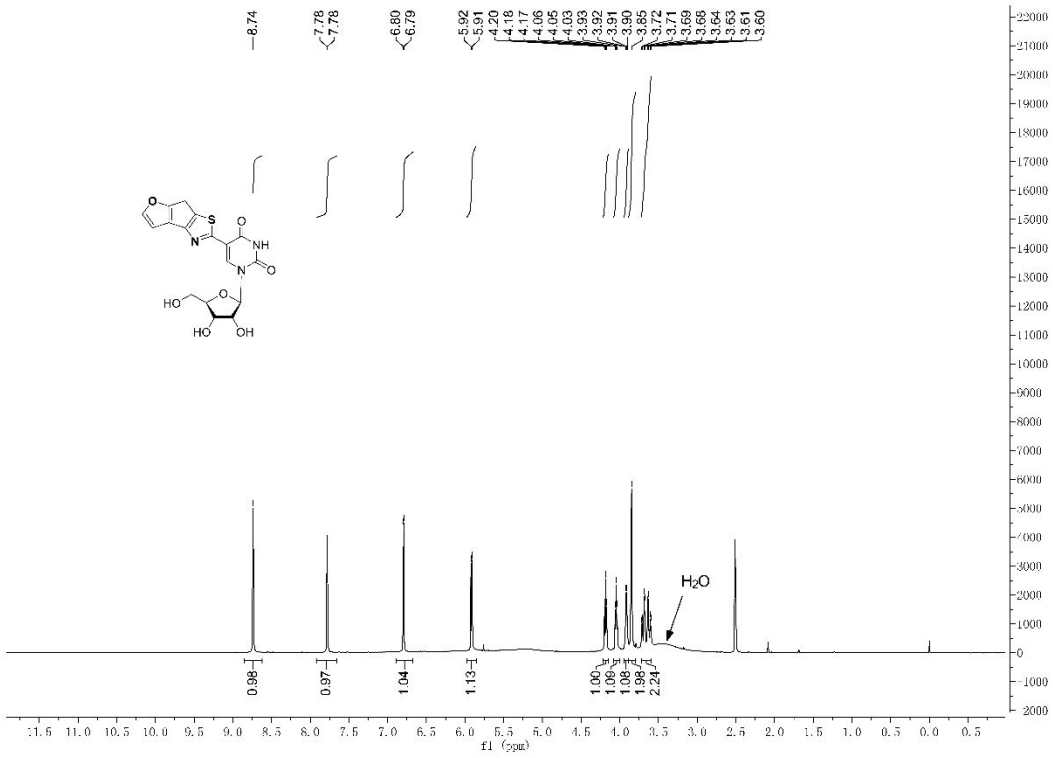
Integration Peak List

Peak	Start	RT	End	Height	Area	AreaSumPercent
1	2.242	2.354	2.366	3.91	22.81	0.96
2	2.366	2.426	2.442	5.86	22.75	0.95
3	2.442	2.463	2.607	5.87	39.97	1.68
4	2.607	2.677	3.071	515.86	2262.35	94.89

Fragmentor Voltage 40 | Collision Energy 0 | Ionization Mode ESI



^{1}H-NMR spectra of compound **7m**



^{13}C-NMR spectra of compound **7m**