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SUPPLEMENTARY MATERIAL TO  
**Sodium ion chemosensor of 3-oxo-3*H*-benzo[*f*]chromene-2-  
-carboxylic acid: An experimental and computational study**

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ANALYTICAL AND SPECTRAL DATA FOR 3-OXO-3*H*-BENZO[*f*]CHROMENE-2-  
-CARBOXYLIC ACID (1)

Yield: 83 mg, (60 %); m.p.: 235.6–236.7 °C; IR (KBr,  $\nu$  /  $\text{cm}^{-1}$ ): 3420 (–OH), 3058 (C–H *sp*<sup>2</sup>), 1750 (C=O carboxylate), 1683 (C=O lactone), 1571 (C=C aromatic), 1218 (C–O–C ester); <sup>1</sup>H-NMR (500 MHz, DMSO-*d*<sub>6</sub>,  $\delta$  / ppm): 9.34 (1H, *s*, H-14), 8.56 (1H, *d*, *J* = 8.4 Hz, H-8), 8.29 (1H, *d*, *J* = 9.0 Hz, H-7), 8.06 (1H, *d*, *J* = 8.0 Hz, H-3), 7.75 (1H, *t*, *J* = 7.7 Hz, H-2), 7.64 (1H, *t*, *J* = 7.5 Hz, H-1), 7.57 (1H, *d*, *J* = 9.0 Hz, H-6); <sup>13</sup>C-NMR (126 MHz, DMSO-*d*<sub>6</sub>,  $\delta$  / ppm): 164.76, 157.23, 155.48, 144.18, 136.30, 130.26, 129.48, 129.45, 126.88, 122.75, 117.66, 116.93, 112.53; (–)ESI-HRMS (*m/z*): calcd. for [C<sub>14</sub>H<sub>8</sub>O<sub>4</sub> –H]<sup>–</sup> 239.0344, observed 239.0293; (+)ESI-HRMS (*m/z*): calcd. for [C<sub>14</sub>H<sub>8</sub>O<sub>4</sub> +H]<sup>+</sup> 241.0342, observed 241.0549; UV/Vis. spectra in MeOH (8×10<sup>–6</sup> mol dm<sup>–3</sup>):  $\lambda_{\text{max}}$  / nm ( $\epsilon$  / mol<sup>–1</sup> dm<sup>3</sup> cm<sup>–1</sup>): 258 (6.5×10<sup>4</sup>) 374 (6.7×10<sup>4</sup>); Emission spectra in MeOH (8×10<sup>–6</sup> mol dm<sup>–3</sup>):  $\lambda_{\text{ex}}$  / nm: 361,  $\lambda_{\text{em}}$  / nm: 445. Stokes Shift: 71 nm.

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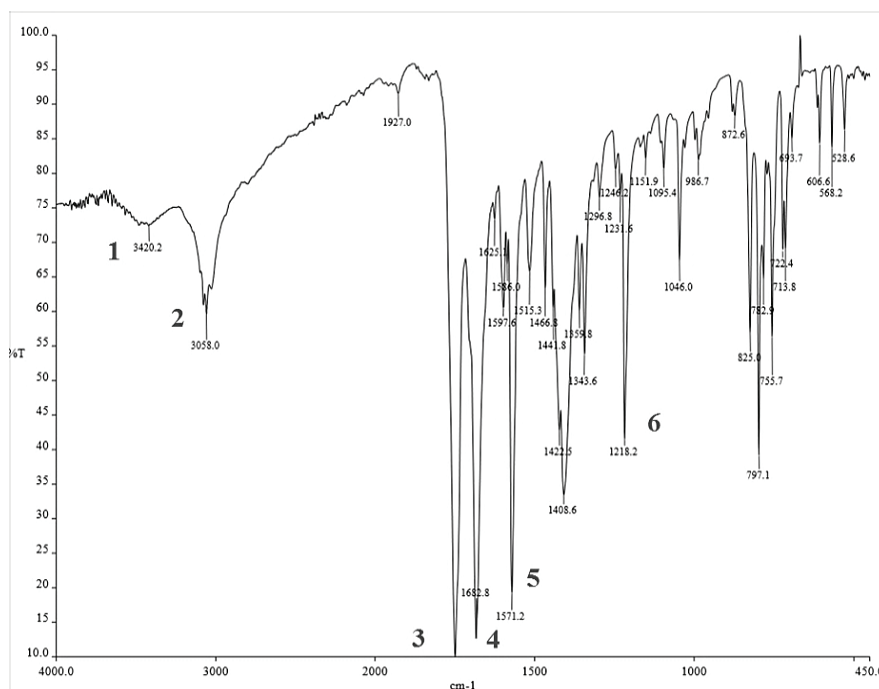


Fig. S-1. Infrared spectra of 3-oxo-3H-benzo[f]chromene-2-carboxylic acid **1** in KBr disk.

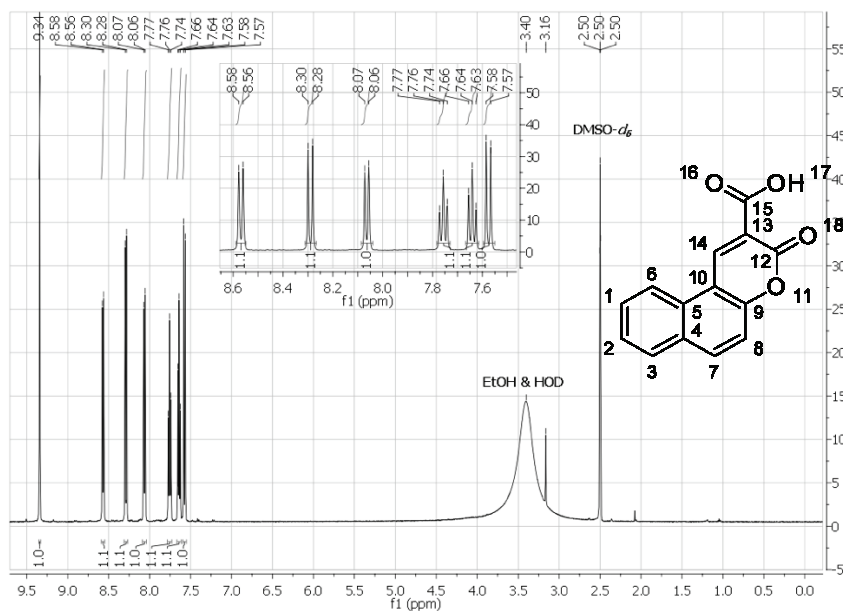


Fig. S-2.  $^1\text{H-NMR}$  spectra (500 MHz) of 3-oxo-3H-benzo[f]chromene-2-carboxylic acid (**1**) in  $\text{DMSO-}d_6$ .

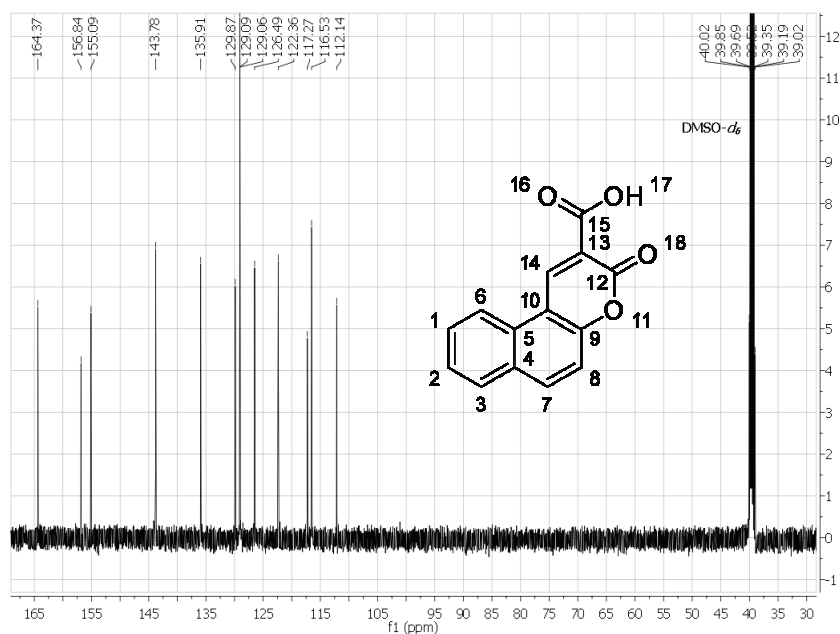


Fig. S-3.  $^{13}\text{C}$ -NMR spectra (126 MHz) of 3-oxo-3*H*-benzo[*f*]chromene-2-carboxylic acid **1** in  $\text{DMSO-}d_6$ .

TABLE S-I. Data of  $^1\text{H}$ -NMR (500 MHz) of **1** in  $\text{DMSO-}d_6$  compared to literature data<sup>1</sup>

No	Compound <b>1</b> (500 MHz, $\text{DMSO-}d_6$ )			Literature (500 MHz, $\text{DMSO-}d_6$ )		Type of proton
	$\delta_{\text{H}}$ / ppm	$\Sigma_{\text{H}}$	Multiplicity	$\delta_{\text{H}}$ / ppm	Multiplicity	
1	7.57	1	Doublet ( $J = 9.0$ Hz)	7.57	Doublet ( $J = 9.0$ Hz)	H-6
2	7.64	1	Triplet ( $J = 7.5$ Hz)	7.64	Triplet ( $J = 7.2$ Hz)	H-1
3	7.75	1	Triplet ( $J = 7.7$ Hz)	7.75	Triplet ( $J = 7.7$ Hz)	H-2
4	8.06	1	Doublet ( $J = 8.0$ Hz)	8.06	Doublet ( $J = 8.0$ Hz)	H-3
5	8.29	1	Doublet ( $J = 9.0$ Hz)	8.29	Doublet ( $J = 9.0$ Hz)	H-7
6	8.56	1	Doublet ( $J = 8.4$ Hz)	8.57	Doublet ( $J = 8.4$ Hz)	H-8
7	9.34	1	Singlet	9.34	Singlet	H-14

TABLE S-II. Data of  $^{13}\text{C}$ -NMR (126 MHz) of **1** in  $\text{DMSO-}d_6$  compared to literature data<sup>1</sup>

$\delta_{\text{C}} / \text{ppm}$		
Literature (126 MHz, $\text{DMSO-}d_6$ )	Compound <b>1</b> (126 MHz, $\text{DMSO-}d_6$ )	Type of carbon
112.55	112.14	C14
116.94	116.53	C1
117.68	117.27	C2
122.77	122.36	C3
126.88	126.49	C6
129.45	129.06	C7
129.50	129.09	C8
130.27	129.87	C4
136.30	135.91	C5
144.18	143.78	C10
155.49	155.09	C9
157.24	156.84	C12
164.78	164.37	C15

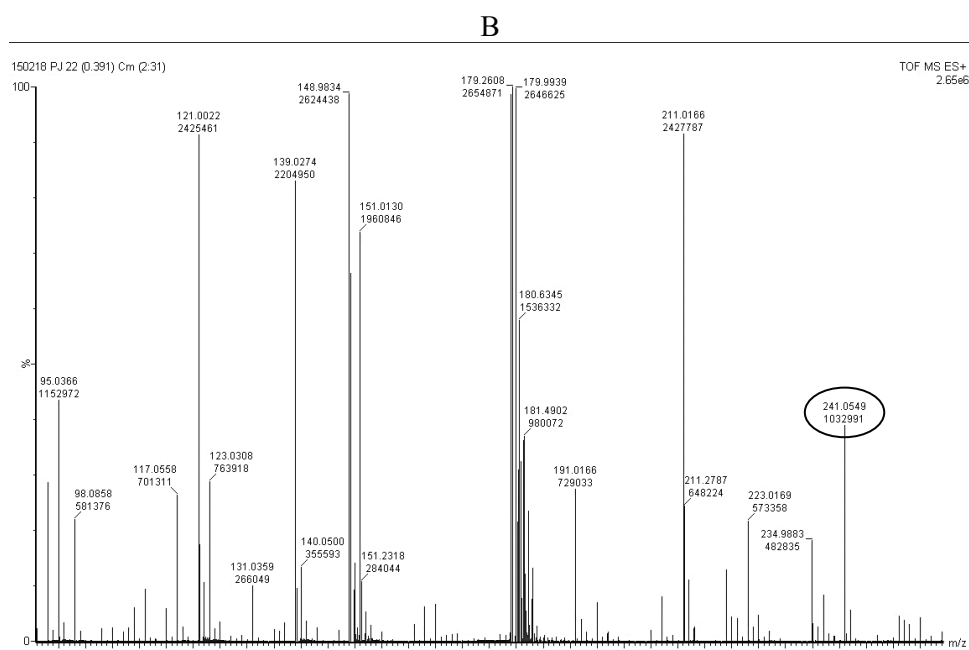
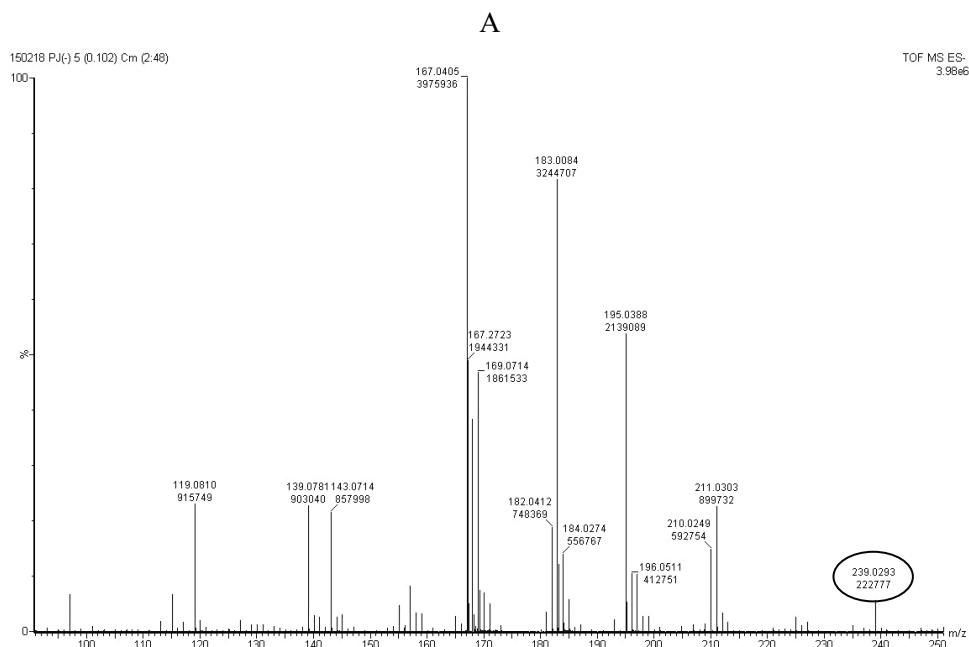


Fig. S-4. Mass spectra of 3-oxo-3*H*-benzo[*f*]chromene-2-carboxylic acid 1 (A) (-)ES and (B) (+)ES.

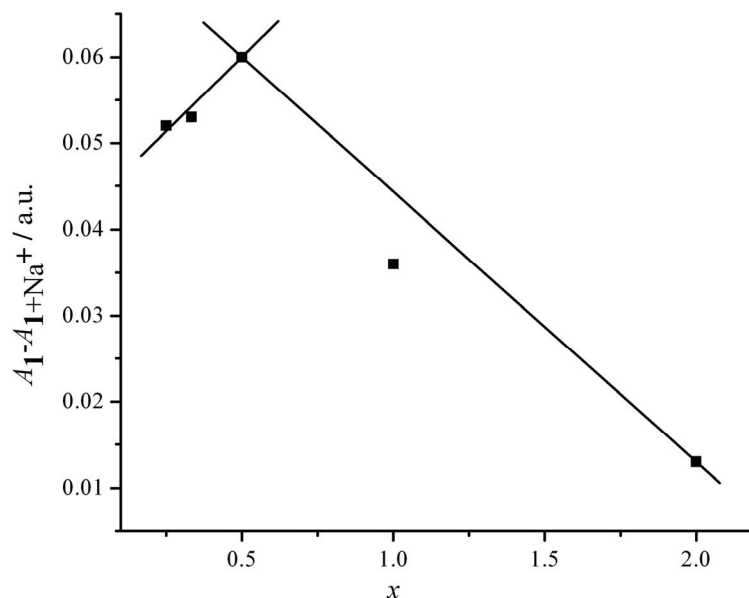


Fig. S-5. Job's Plot for the binding of **1** ( $1.5 \times 10^{-5}$  mol dm<sup>-3</sup>) with Na<sup>+</sup>.  $\Delta A$  at 360 nm was plotted as a function of mole fraction.

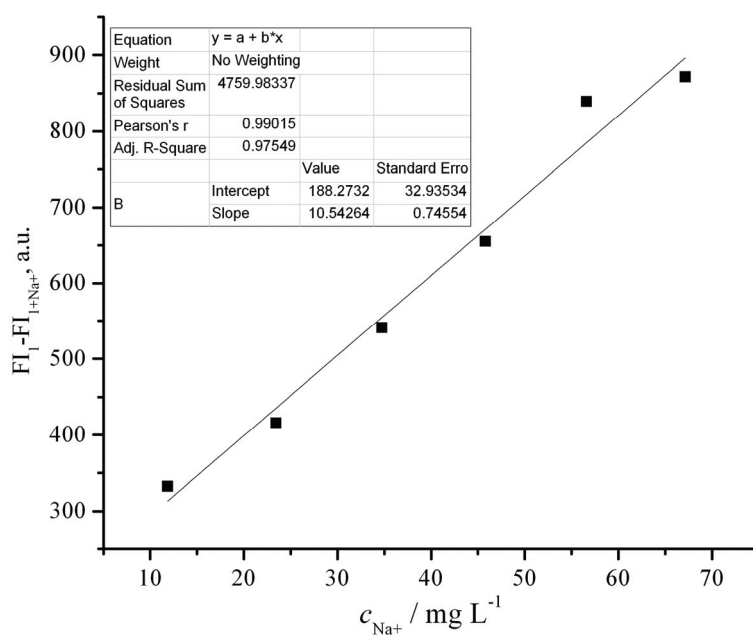


Fig. S-6. Calibration curve of **1** against various concentration of Na<sup>+</sup> in MeOH:H<sub>2</sub>O (2:8 v/v)

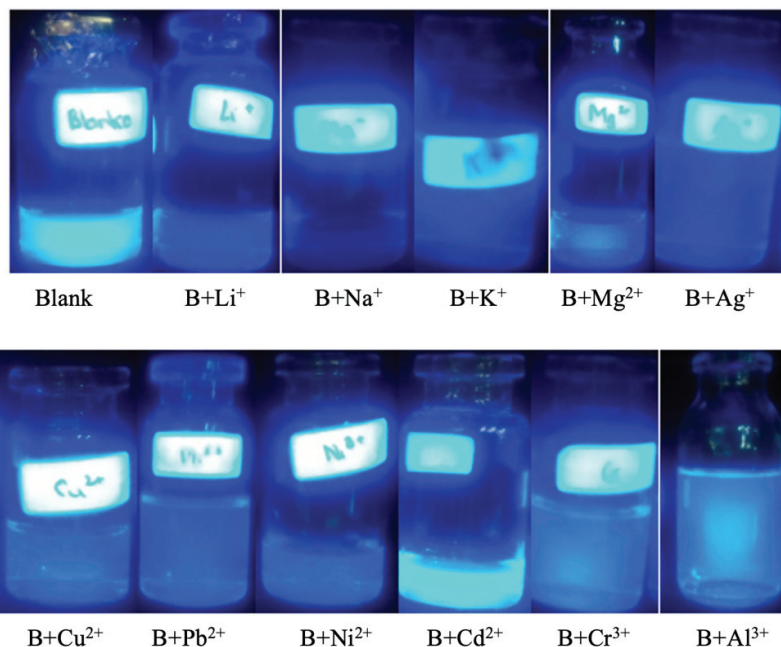


Fig. S-7. Fluorescent intensity quenching of **1** (B;  $8.32 \times 10^{-8} \text{ mol dm}^{-3}$ ) by addition of molar equivalents of various metal ions ( $\text{Li}^+$ : 100,  $\text{Na}^+$ : 6,  $\text{K}^+$ : 15,  $\text{Mg}^{2+}$ : 30,  $\text{Ag}^+$ : 500,  $\text{Cu}^{2+}$ : 15,  $\text{Pb}^{2+}$ : 170,  $\text{Ni}^{2+}$ : 60,  $\text{Cd}^{2+}$ : 500,  $\text{Cr}^{3+}$ : 400,  $\text{Al}^{3+}$ : 200), observed under UV light at 365 nm.

TABLE S-III. Calculated imaginary frequency values of vibrated atoms of compound **1**

Mode	Frequency, $\text{cm}^{-1}$	IR intensity, $\text{km mol}^{-1}$
1	55.44	0.5561
2	68.60	0.0011
3	105.12	2.6084
4	140.69	4.5864
5	159.17	0.5869
6	174.04	1.2744
7	251.91	11.1475
8	270.10	5.9061
9	323.47	1.3467
10	328.06	5.1032
11	375.91	13.8163
12	380.17	0.4003
13	431.69	2.3291
14	434.01	7.7653
15	443.01	12.0847
16	520.79	0.4615
17	534.95	2.8835
18	540.64	0.0489
19	571.60	6.6310
20	618.64	11.7080

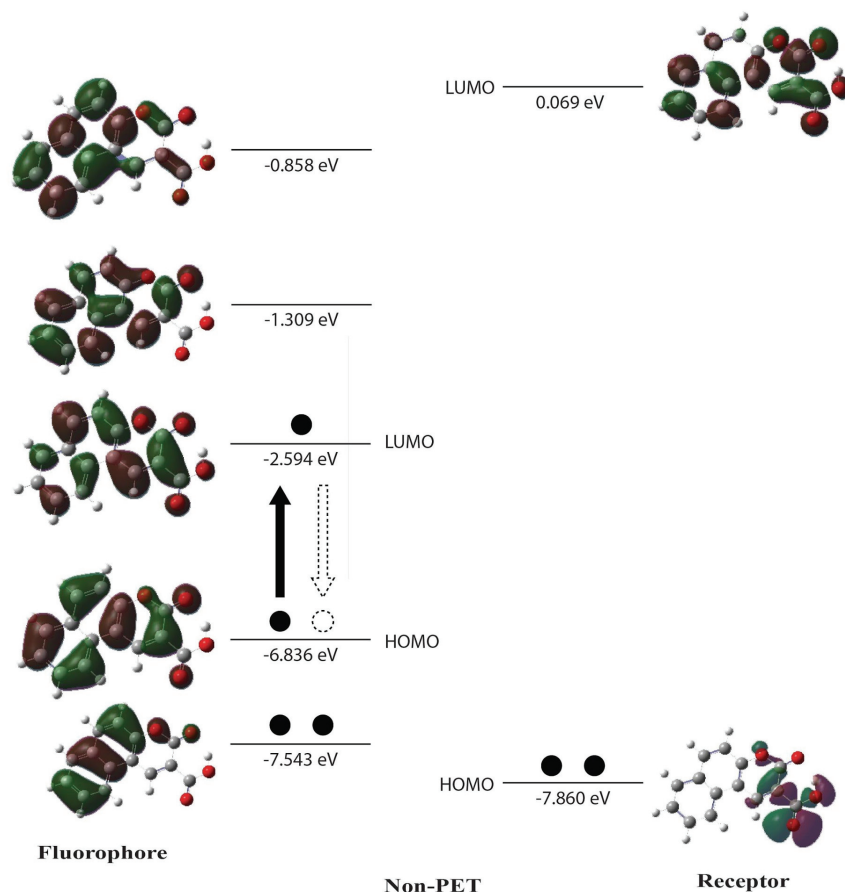


Fig. S-8. Calculated frontier molecular orbitals of compound **1** and the corresponding HOMO and LUMO orbitals.

#### REFERENCES

1. X. B. Fu, X. F. Wang, J. N. Chen, D. W. Wu, T. Li, X. C. Shen, J. K. Qin, *Molecules* **20** (2015) 18565 (<https://doi.org/10.3390/molecules201018565>).