Electronic Supplementary Information (ESI) for *Dalton. Trans.*

A simple BODIPY-aniline-based fluorescent chemosensor as multiple logic operations for the detection of pH and CO_2 gas

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Electronic Supplementary Information (ESI)

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Table S1 Crystallographic data for **1•CH_2Cl_2**, **1** and **3**.

BODIPY	**1•CH_2Cl_2 (orange)**	**1 (deep red)**	**3 (orange red)**
formula	$C_{20}H_{22}BF_2Cl_2N_3$	$C_{19}H_{20}BF_2N_3$	$C_{19}H_{19}BF_2N_2$
formula weight	424.12	339.19	324.17
crystal system	triclinic	monoclinic	monoclinic
space group	$P\bar{1}$	$P2_1/n$	$P2_1/n$
a (Å)	6.9723(7)	10.8093(4)	11.9007(5)
b (Å)	11.1202(14)	11.5942(4)	7.0792(4)
c (Å)	14.3071(16)	14.0953(4)	19.4220(4)
α (deg)	96.362(4)	90.00	90.00
β (deg)	102.577(3)	104.6620(10)	99.6390(10)
γ (deg)	108.094(2)	90.00	90.00
Z, D_{calcd}(g m^{-3})	2, 1.395	4, 1.318	4, 1.335
V ($Å^3$)	1009.9(2)	1708.97(10)	1613.15(10)
μ (mm^{-1})	0.350	0.093	0.094
F (000)	440	712	680
T (K)	173(2)	173(2)	173(2)
no. of reflns collected	7977	13119	20783
no. of unique reflns.	3543 (R_{int} = 0.0693)	2993 (R_{int} = 0.0426)	3167 (R_{int} = 0.0479)
no. of observed reflns	1700	2064	2210
parameters	254	227	218
R indices	R_1 = 0.0725,	R_1 = 0.0653,	R_1 = 0.0705,
$[I > 2\sigma(I)]^{a,b}$	wR_2 = 0.1800	wR_2 = 0.1788	wR_2 = 0.2075
R indices	R_1 = 0.1357,	R_1 = 0.0974,	R_1 = 0.0932,
all data	wR_2 = 0.2375	wR_2 = 0.2401	wR_2 = 0.2590
GOF	1.134	1.186	1.195
Max., min electron Density (e $Å^{-3}$)	0.424, -0.437	0.454, -0.464	0.423, -0.405

$^a R_1 = \Sigma| |F_o|-|F_c| | / \Sigma|F_o|$, $^b wR_2 = [\Sigma w(F_o^2-F_c^2)^2] / \Sigma w(F_o^2)^2]^{1/2}$

Table S2 Selected bond lengths, bond angles and dihedral angles of **1•CH_2Cl_2**, **1** and **3**.

1•CH_2Cl_2		**1**		**3**	
Bond lengths		Bond lengths		Bond lengths	
B1-F1	1.390(5)	B1-F1	1.391(4)	B1-F1	1.393(4)
B1-F2	1.390(6)	B1-F2	1.418(4)	B1-F2	1.390(4)
B1-N1	1.540(6)	B1-N1	1.536(5)	B1-N1	1.536(4)
B1-N2	1.528(6)	B1-N2	1.520(5)	B1-N2	1.543(4)
N1-C12	1.345(5)	N1-C12	1.352(4)	N1-C12	1.346(4)
N1-C15	1.409(5)	N1-C15	1.406(4)	N1-C15	1.406(3)
N2-C11	1.355(5)	N2-C11	1.354(4)	N2-C11	1.354(3)
N2-C8	1.417(5)	N2-C8	1.411(4)	N2-C8	1.412(3)
N3-C1	1.394(4)	N3-C1	1.395(4)		
Bond angles		Bond angles		Bond angles	
F1-B1-F2	108.5(4)	F1-B1-F2	107.9(3)	F1-B1-F2	109.7(3)
F1-B1-N2	110.4(4)	F1-B1-N2	112.5(3)	F1-B1-N2	109.6(2)
F2-B1-N2	110.0(4)	F2-B1-N2	108.9(3)	F2-B1-N2	110.1(2)
F1-B1-N1	110.2(4)	F1-B1-N1	110.5(3)	F1-B1-N1	110.2(2)
F2-B1-N1	110.3(4)	F2-B1-N1	109.3(3)	F2-B1-N1	109.5(2)
N1-B1-N2	110.1(3)	N1-B1-N2	107.6(3)	N1-B1-N2	107.7(2)

Table S3 Percentage contribution from individual intermolecular interactions to the Hirshfeld surface of **1•CH_2Cl_2**, **1** and **3**.

	H···F	**H···H**	**C···C**	**H···C**	**H···Cl**
1•CH_2Cl_2	13.7	53.0	1.4	17.1	9.2
1	11.9	63.2	0.9	16.9	0
3	16.9	59.5	2.0	18	0

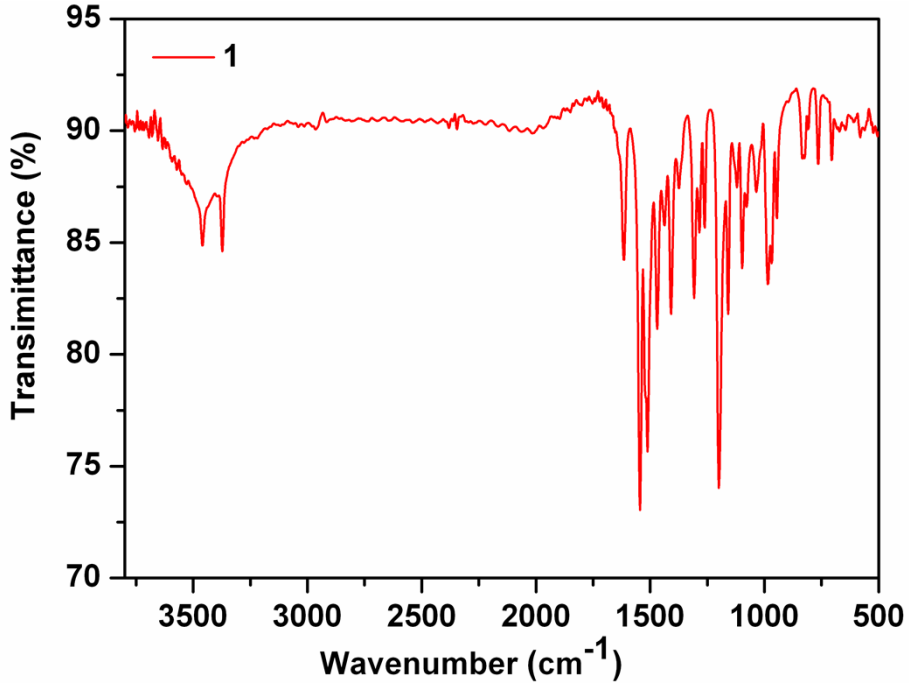


Fig. S1 Solid-state IR spectrum of **1**.

(a) **(b)**

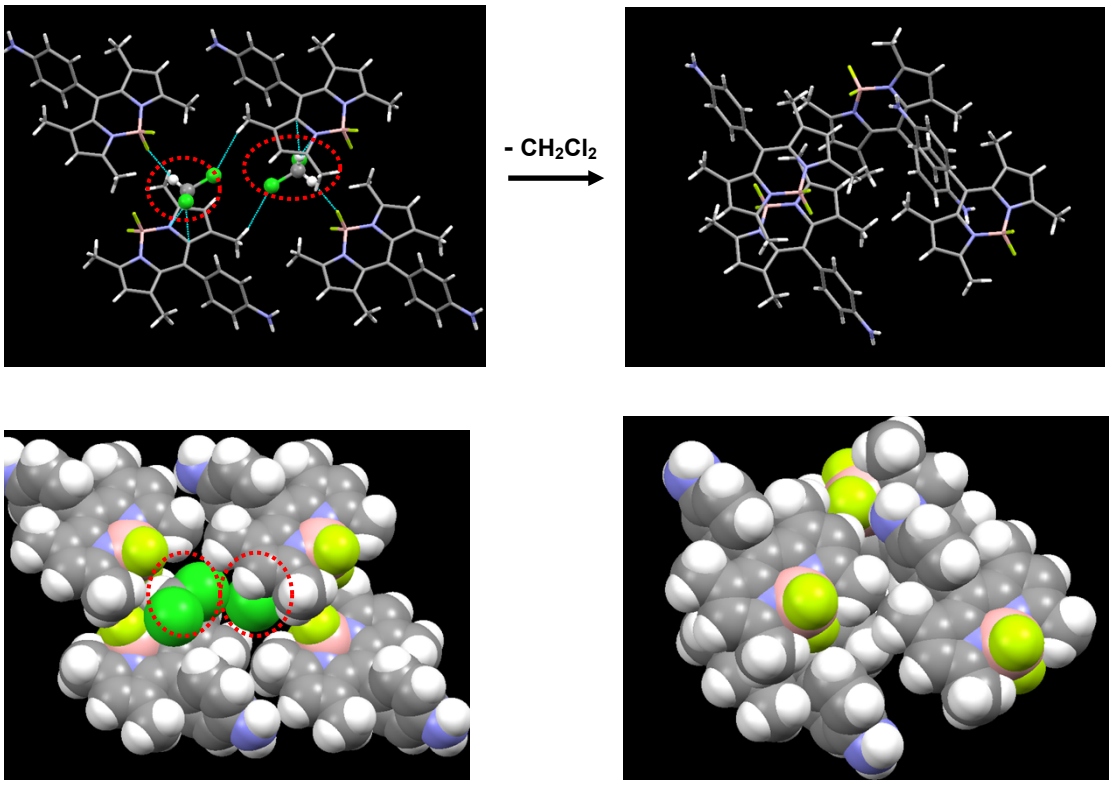


Fig. S2 Molecular structures (top) and space-filling projections (bottom) showing the packing arrangement of **1**•CH_2Cl_2 (a) and **1**(b). The CH_2Cl_2 molecule (green) in **1**•CH_2Cl_2 are found to reside within voids, which are marked as dotted red circles.

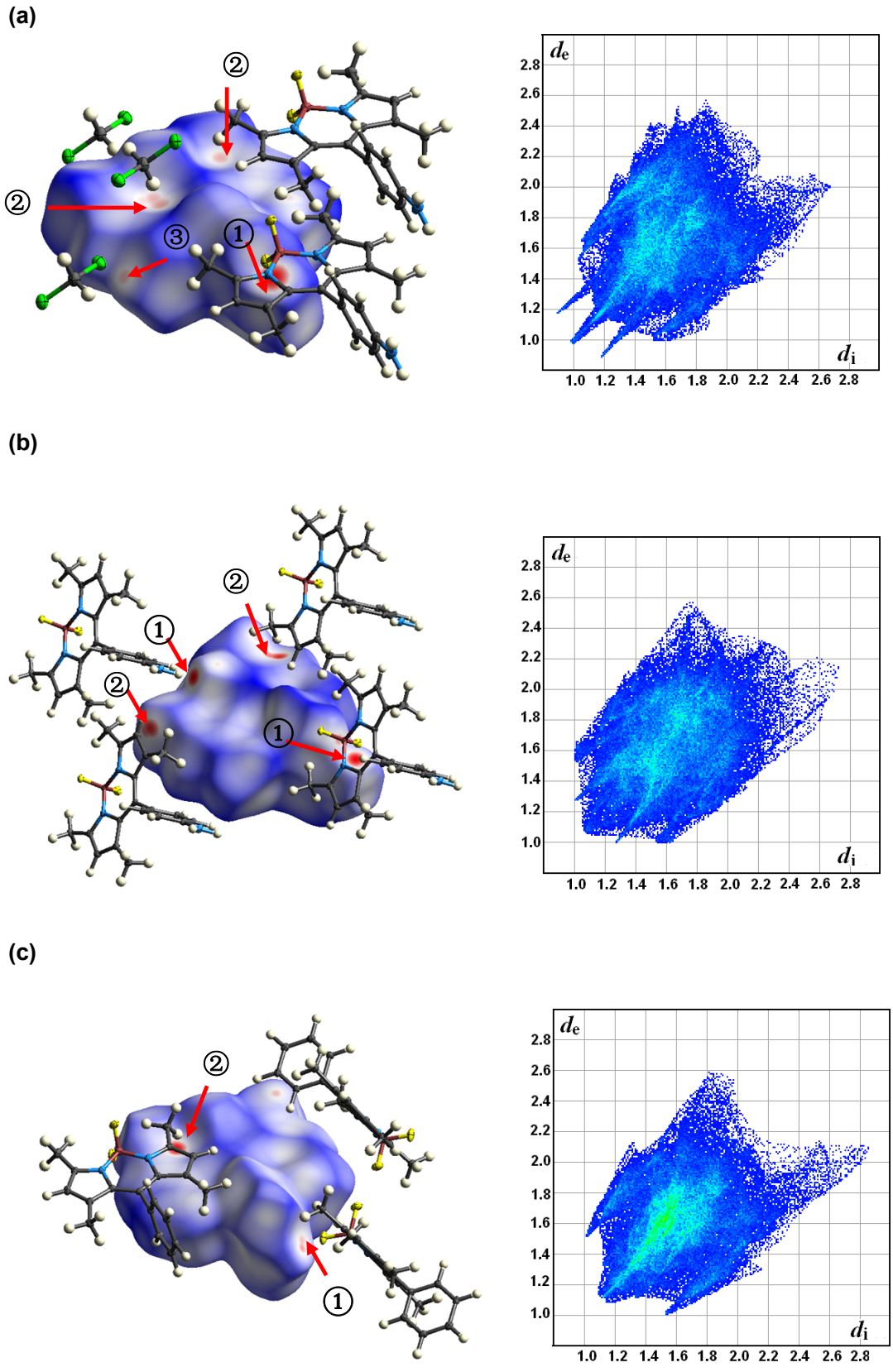
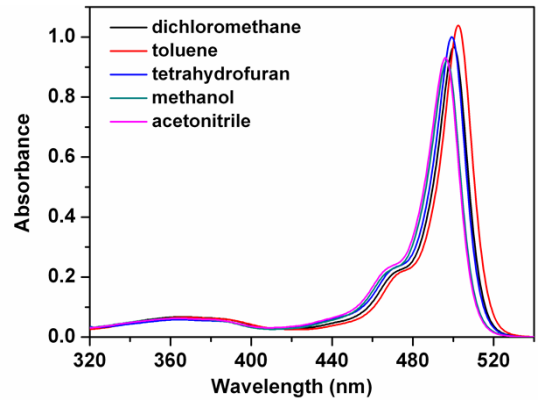


Fig. S3 Crystal packing for (a) **1**•CH_2Cl_2, (b) **1**, and (c) **3**, showing the Hirshfeld surfaces of the central molecules mapped with d_{norm} (left) and the 2D fingerprint plots showing the

distribution of the d_e distances as a function of d_i (right). The most significant intermolecular interactions are: (a) N-H•••F hydrogen bonds (①), C-H•••π interactions (②), and C-H•••Cl interactions (③); (b) N-H•••F hydrogen bonds (①), and C-H•••π interactions (②); (c) C-H•••F hydrogen bonds (①), C-H•••π interactions (②).

(a)



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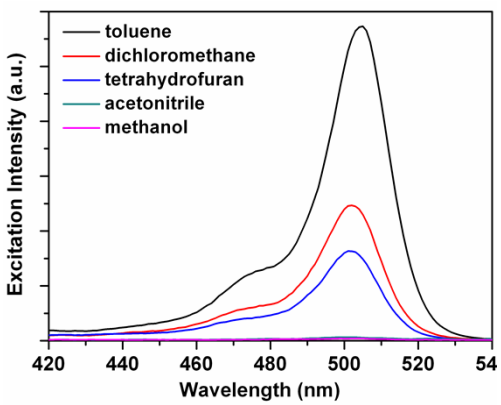


(c)

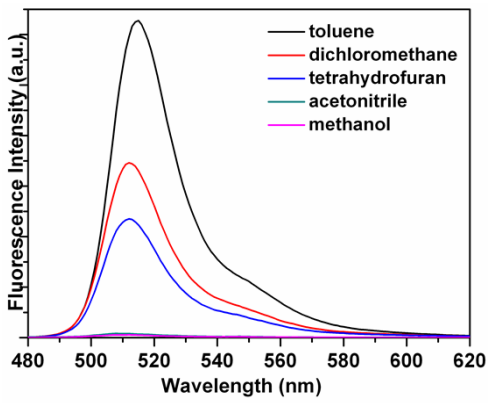


Fig. S4 (a) Absorption, (b) excitation and (c) emission spectra of **1** in several solvents.

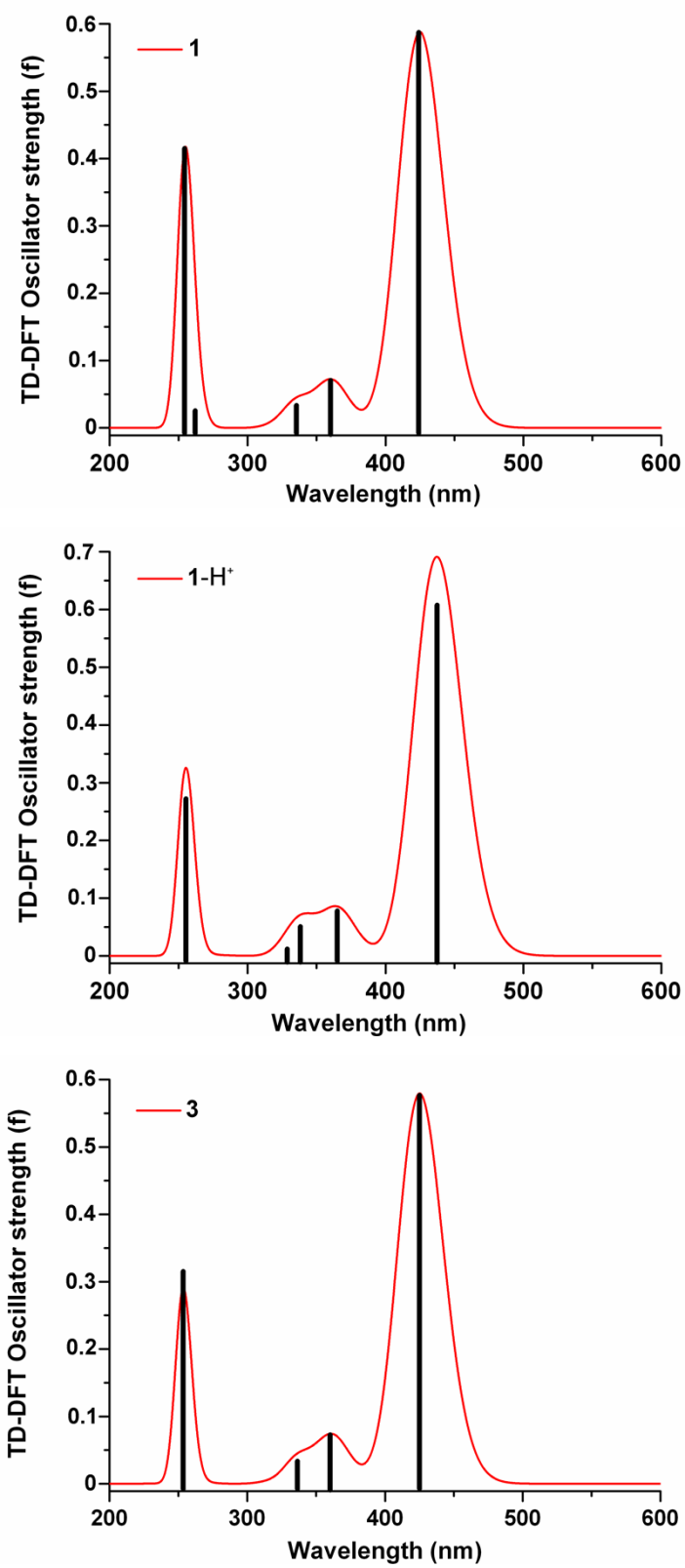
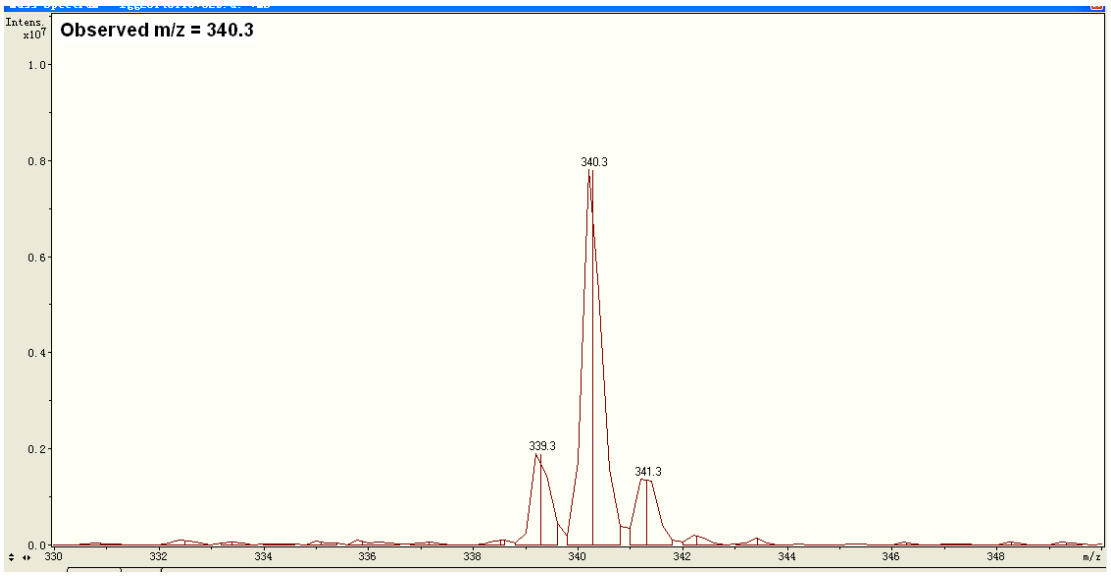


Fig. S5 TDDFT stick spectra of **1** (top), **1**-H^+ (middle) and **3** (bottom) calculated at the B3LYP/6-31+G(d) level. Also shown are the UV-visible absorption spectra of **1**, **1**-H^+ and

3 recorded in CH_3OH.

(a)



(b)

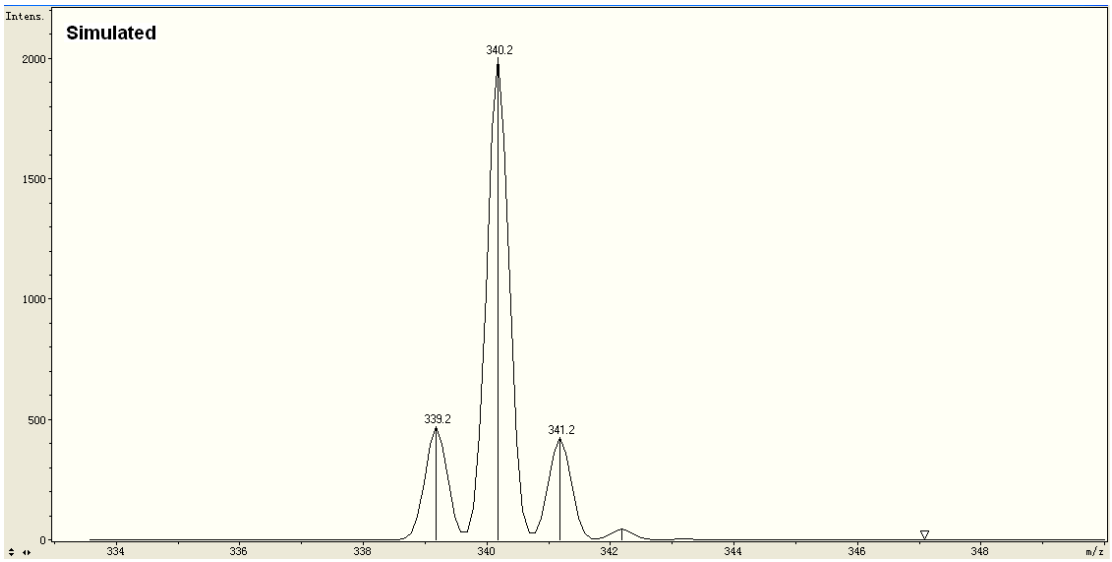


Fig. S6 The experimental ESI-MS (a) and its simulated isotope pattern (b) showing the presence of the protonated species of **1**.