Electronic Supporting Information

Zn(II)-coordination-driven chiroptical and emissive sensing for chiral amines using a quaterphenyl-5'-carbaldehyde

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Table of contents

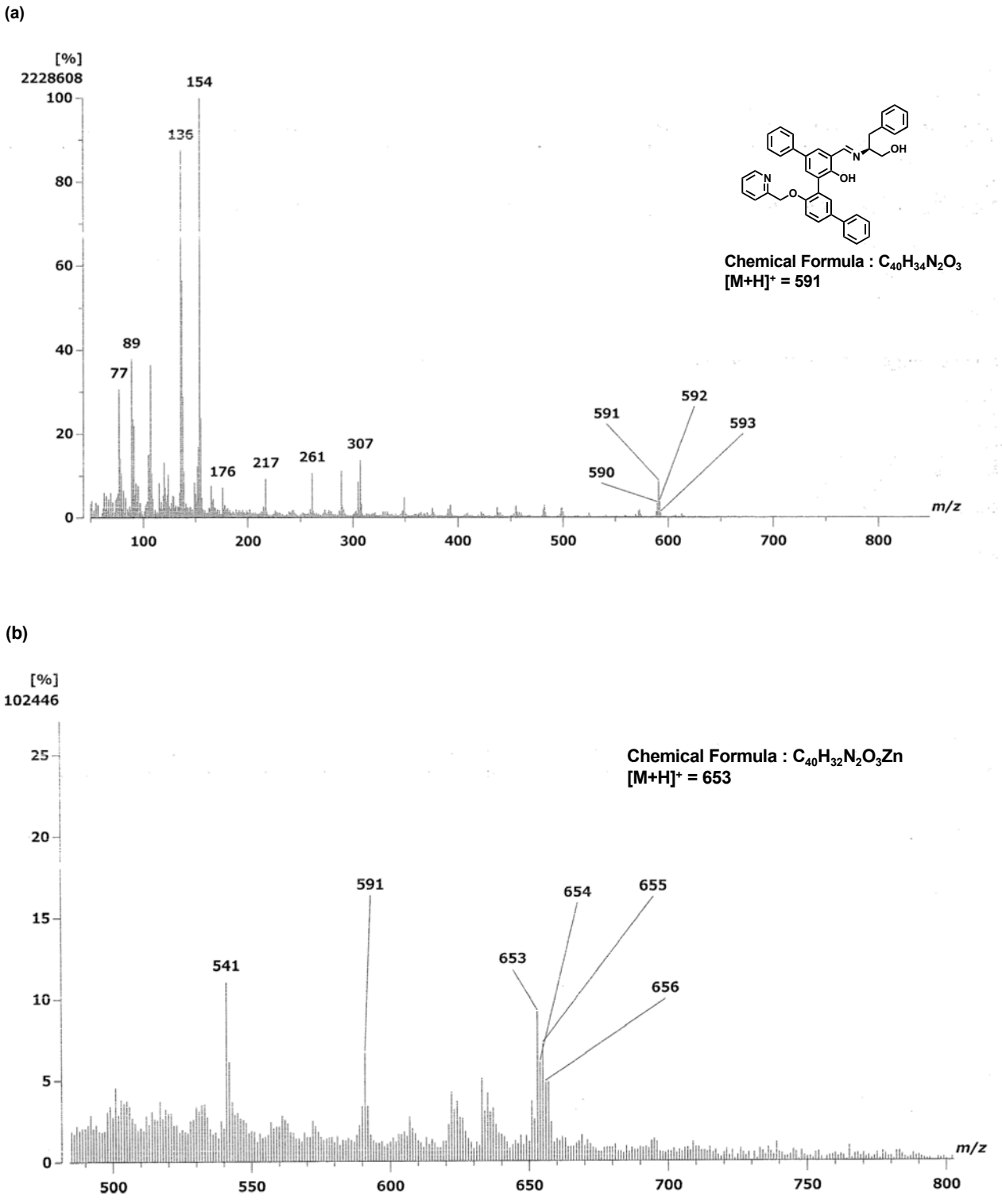
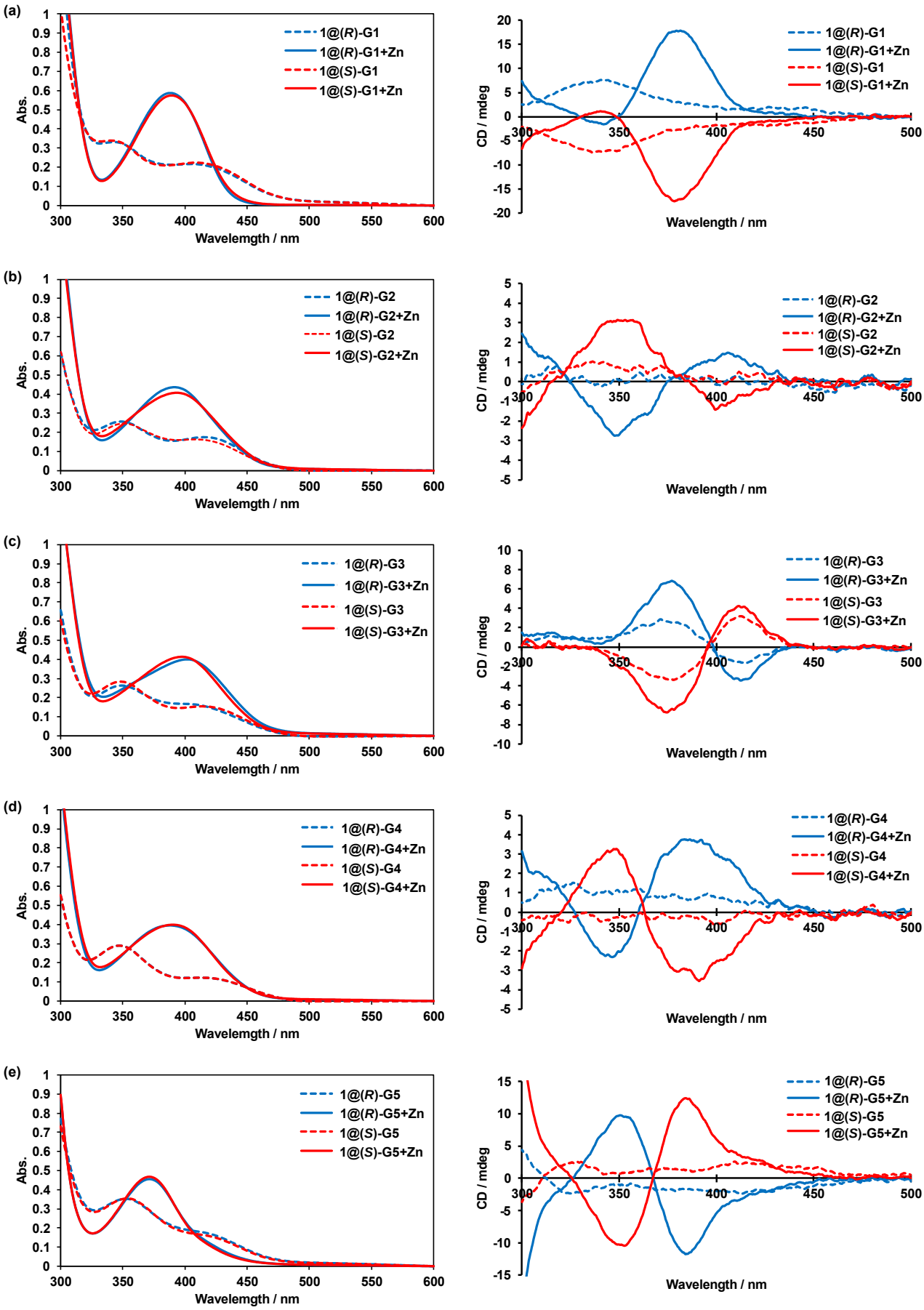


Fig. S1. FAB-MS spectra of **1@**(*S*)-**G1** (a) and Zn(II)-coordinated **1@**(*S*)-**G1**(b).


(a)
Abs.
Wavelemgth / nm
1@(R)-G1
1@(R)-G1+Zn
1@(S)-G1
1@(S)-G1+Zn
CD / mdeg
Wavelength / nm
(b)
1@(R)-G2
1@(R)-G2+Zn
1@(S)-G2
1@(S)-G2+Zn
(c)
1@(R)-G3
1@(R)-G3+Zn
1@(S)-G3
1@(S)-G3+Zn
(d)
1@(R)-G4
1@(R)-G4+Zn
1@(S)-G4
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(e)
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1@(R)-G5+Zn
1@(S)-G5
1@(S)-G5+Zn

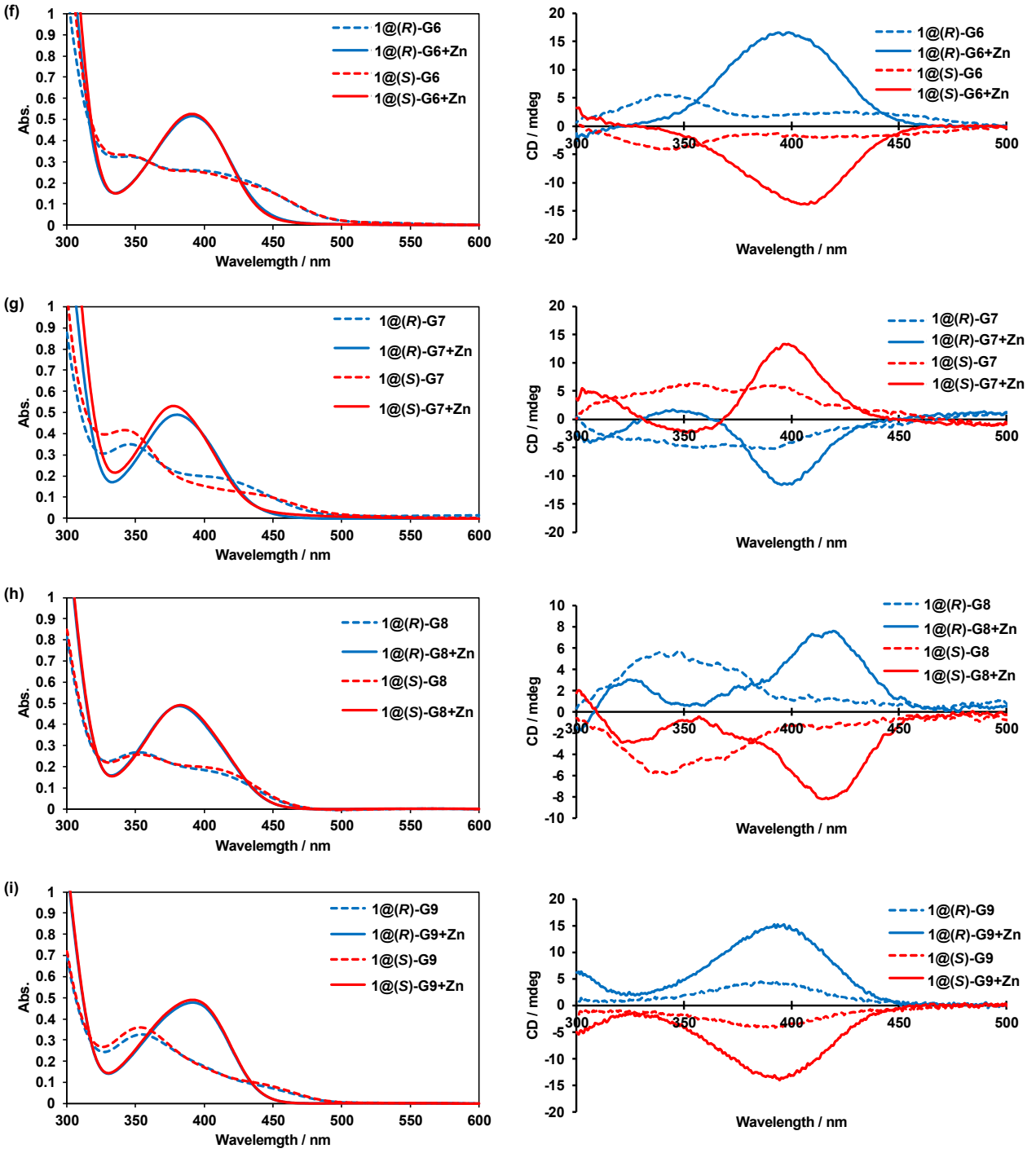

Fig. S2. UV/Vis absorption and CD spectra of imines **1**@(*S*)/(*R*)-**G**$_n$ (***n*** **= 1 ~ 9**) in the presence or absence of Zn(II) in MeOH.

Table S1. UV/Vis (ε, in $cm^{-1} M^{-1}$) and CD ($\Delta\varepsilon$, in $cm^{-1} M^{-1}$) data of **1**@(*S*)/(R)-$\mathbf{G}_{\boldsymbol{n}}$ ($\boldsymbol{n}$ **= 1 ~ 9**) in the presence or absence of Zn(II) in MeOH.

	UV-Vis [ε (nm)]	CD [$\Delta\varepsilon$ (nm)]	g_{abs} (= $\lvert A \rvert/\varepsilon$) ($\times 10^{-3}$)[a]
1	5700 (414)	-	-
1@(*R*)-**G1**	2240 (413), 3320 (344)	23.2 (341)	7.0
1@(*S*)-**G1**	2170 (413), 3400 (340)	-22.4 (341)	6.6
1@(*R*)-**G1**+ Zn(II)	5870 (388)	53.9 (380), -4.80 (342)	10
1@(*S*)-**G1**+ Zn(II)	5740 (389)	-53.1 (379), 3.48 (341)	9.8
1@(*R*)-**G2**	1750 (415), 2560 (348)	3.32 (359)	1.3
1@(*S*)-**G2**	1620 (409), 2450 (350)	-3.37 (355)	1.4
1@(*R*)-**G2**+ Zn(II)	4080 (393)	4.30 (400), -9.56 (349)	3.4
1@(*S*)-**G2**+ Zn(II)	4370 (392)	-4.30 (400), 9.56 (349)	3.2
1@(*R*)-**G3**	1580 (414), 2630 (350)	8.20 (417), -10.4 (378)	7.1
1@(*S*)-**G3**	1540 (413), 2830 (349)	-4.97 (415), 8.63 (371)	4.8
1@(*R*)-**G3**+ Zn(II)	4000 (402)	12.5 (414), -20.4 (374)	8.2
1@(*S*)-**G3**+ Zn(II)	4130 (398)	-10.2 (414), 20.8 (377)	7.5
1@(*R*)-**G4**	3300 (414), 2760 (348)	4.62 (326)	1.7
1@(*S*)-**G4**	3160 (410), 2770 (346)	-1.63 (324)	0.59
1@(*R*)-**G4**+ Zn(II)	3940 (388)	11.3 (392), -7.10 (346)	4.7
1@(*S*)-**G4**+ Zn(II)	3990 (390)	-10.8 (391), 9.87 (347)	5.2
1@(*R*)-**G5**	1760 (416), 3520 (352)	-7.32 (413), -7.06 (325)	4.2
1@(*S*)-**G5**	1620(416), 3530 (354)	7.69 (409), 7.30 (326)	4.7
1@(*R*)-**G5**+ Zn(II)	4560(372)	-35.5 (384), 29.8 (351)	14
1@(*S*)-**G5**+ Zn(II)	4670 (372)	37.6 (384), -31.4 (351)	15
1@(*R*)-**G6**	2600 (392), 3240 (342)	7.90 (430), 15.6 (335)	4.8
1@(*S*)-**G6**	2550 (389), 3320 (342)	-6.04 (433), -12.8 (339)	3.8
1@(*R*)-**G6**+ Zn(II)	5150 (392)	50.3 (399)	9.8
1@(*S*)-**G6**+ Zn(II)	5250 (391)	-41.8 (405)	8.0
1@(*R*)-**G7**	1920 (410), 3500 (346)	-16.1 (389), -15.3 (356)	4.4
1@(*S*)-**G7**	1340 (416), 4160 (342)	17.9 (388), 19.1 (355)	4.6
1@(R)-**G7**+ Zn(II)	4890 (381)	-35.0 (398), 5.14 (345)	8.2
1@(*S*)-**G7**+ Zn(II)	5290 (377)	40.3 (399), -7.25 (351)	9.0
1@(*R*)-**G8**	1610 (416), 2690 (352)	16.9 (339)	6.3
1@(*S*)-**G8**	1760 (415), 2570 (353)	-17.6 (342)	6.8
1@(*R*)-**G8**+ Zn(II)	4870 (382)	22.9 (418), 9.26 (325)	4.7
1@(S)-**G8**+ Zn(II)	4910 (382)	-24.9 (417), -8.81 (322)	5.1
1@(*R*)-**G9**	3260 (354)	13.1 (393)	4.0
1@(*S*)-**G9**	3600 (353)	-12.7 (393)	3.5
1@(*R*)-**G9**+ Zn(II)	4770 (393)	45.9 (392)	9.6
1@(*S*)-**G9**+ Zn(II)	4900 (393)	-42.8 (394)	8.7

[a] The amplitude (A) of exciton Cotton effects is defined as the difference between the first long-wavelength ($\Delta\varepsilon_1$) Cotton effect and the second short-wavelength ($\Delta\varepsilon_2$) Cotton effect ($A = \Delta\varepsilon_1 - \Delta\varepsilon_2$).

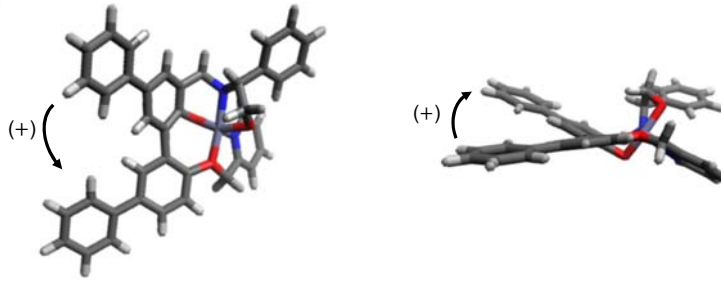

Fig. S3. Proposed Zn(II)-coordinated structure **1@**(*R*)**-G1.**

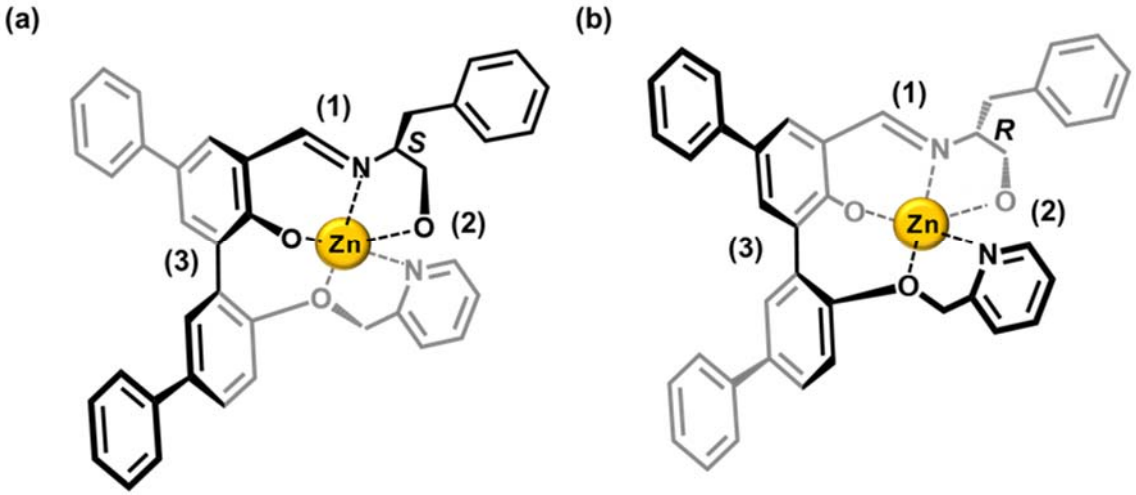

Fig. S4. A plausible mechanism of chiroptical sensing on Zn(II)-coordinated **1@**(*S*)**-G1** (a) and the corresponding complex with (*R*)**-G1** (b).

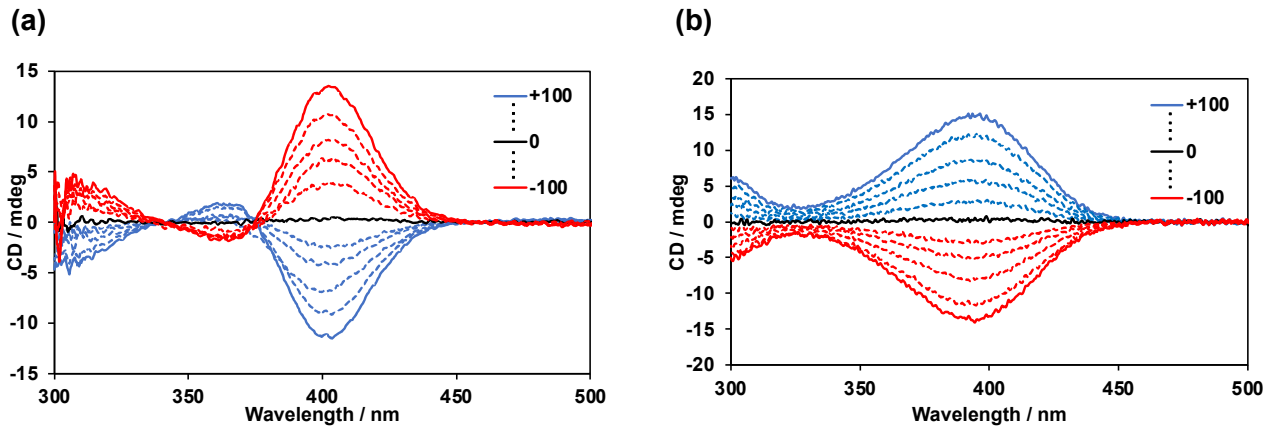

Fig. S5. CD spectra of Zn(II)-coordinated **1@**(*S*)**-G7** (a) and Zn(II)-coordinated **1@**(*S*)**-G9** (b) with variable *ee* values.

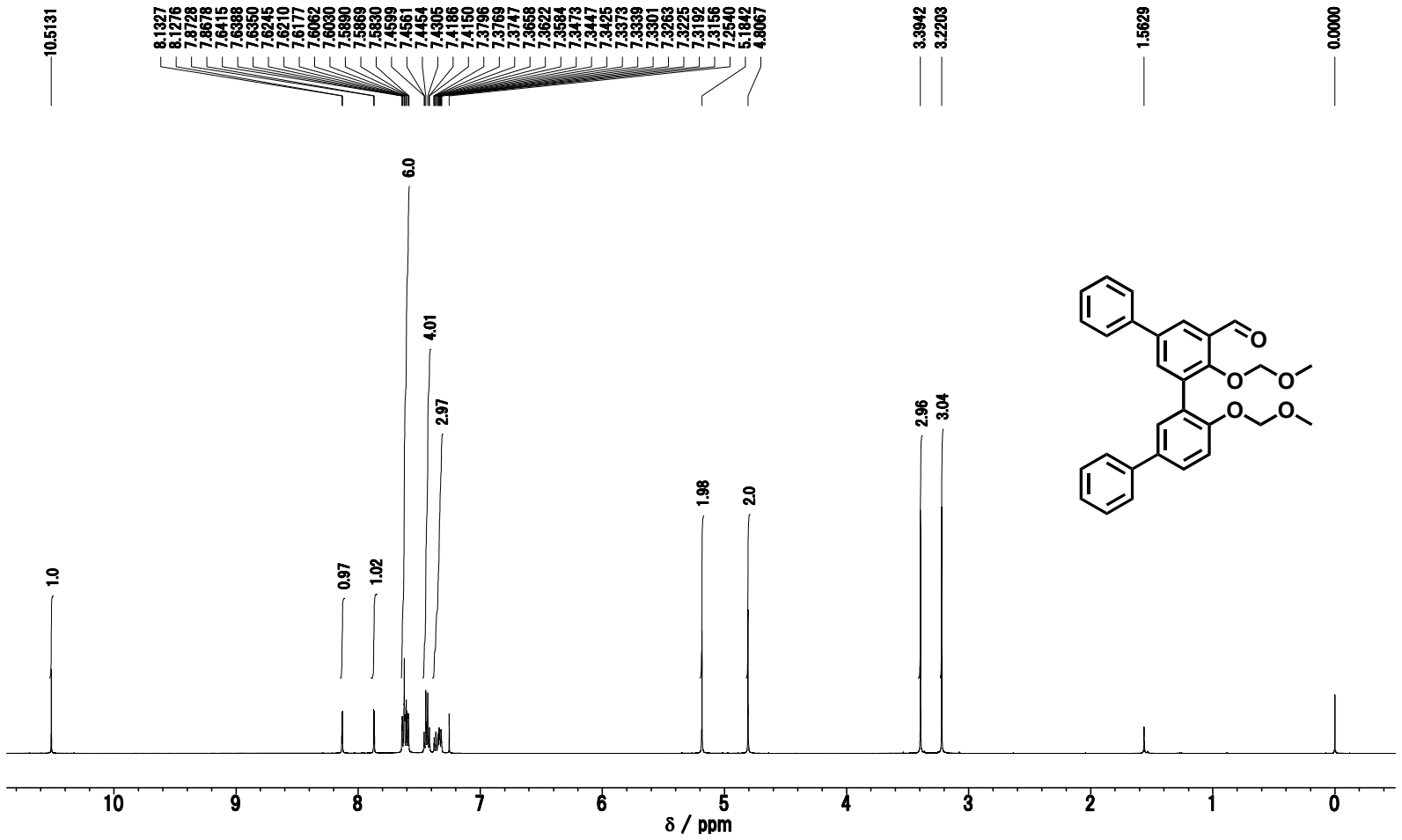

Fig. S6. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of **3**.

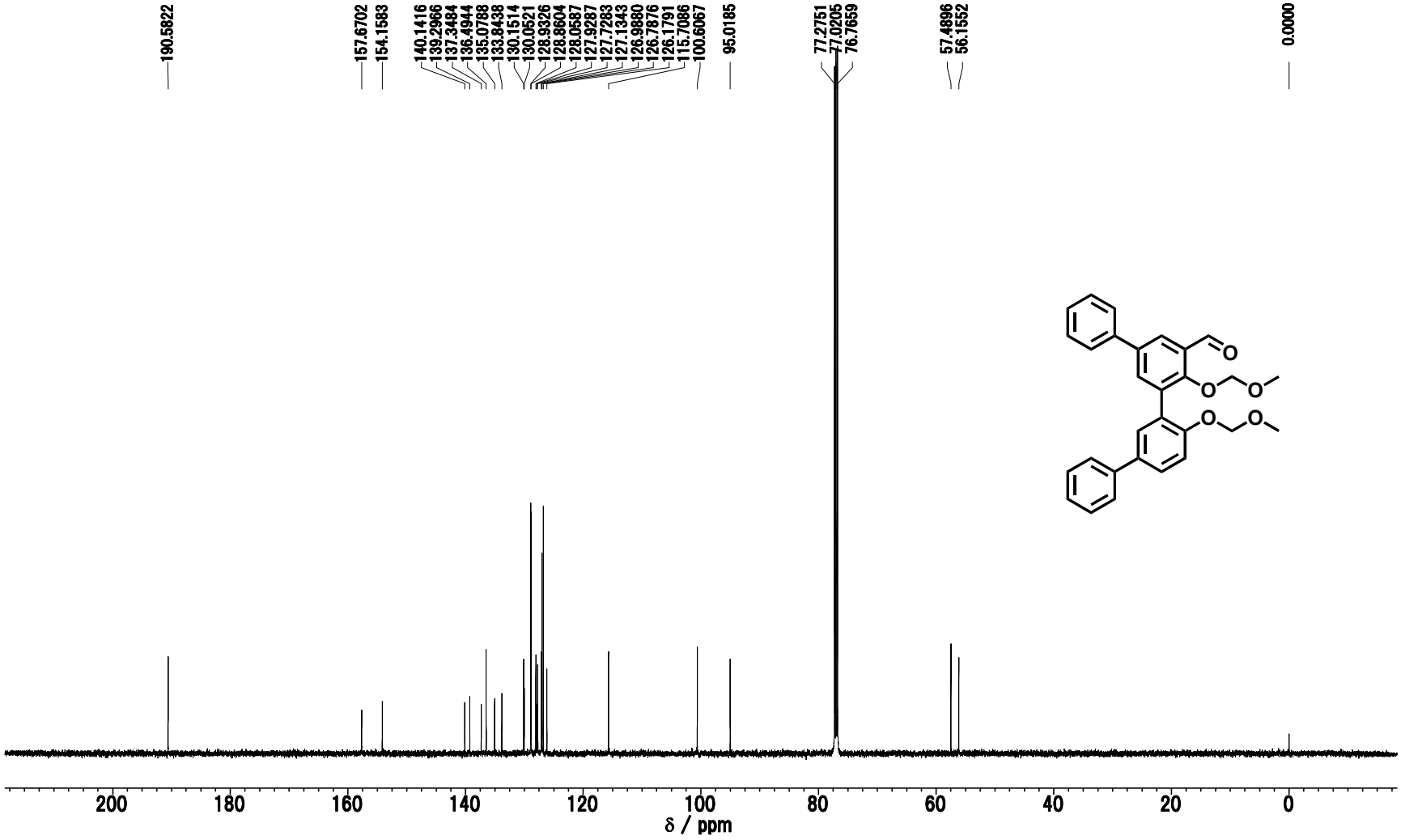

Fig. S7. ^{13}C NMR (126 MHz, $CDCl_3$) spectrum of **3**.

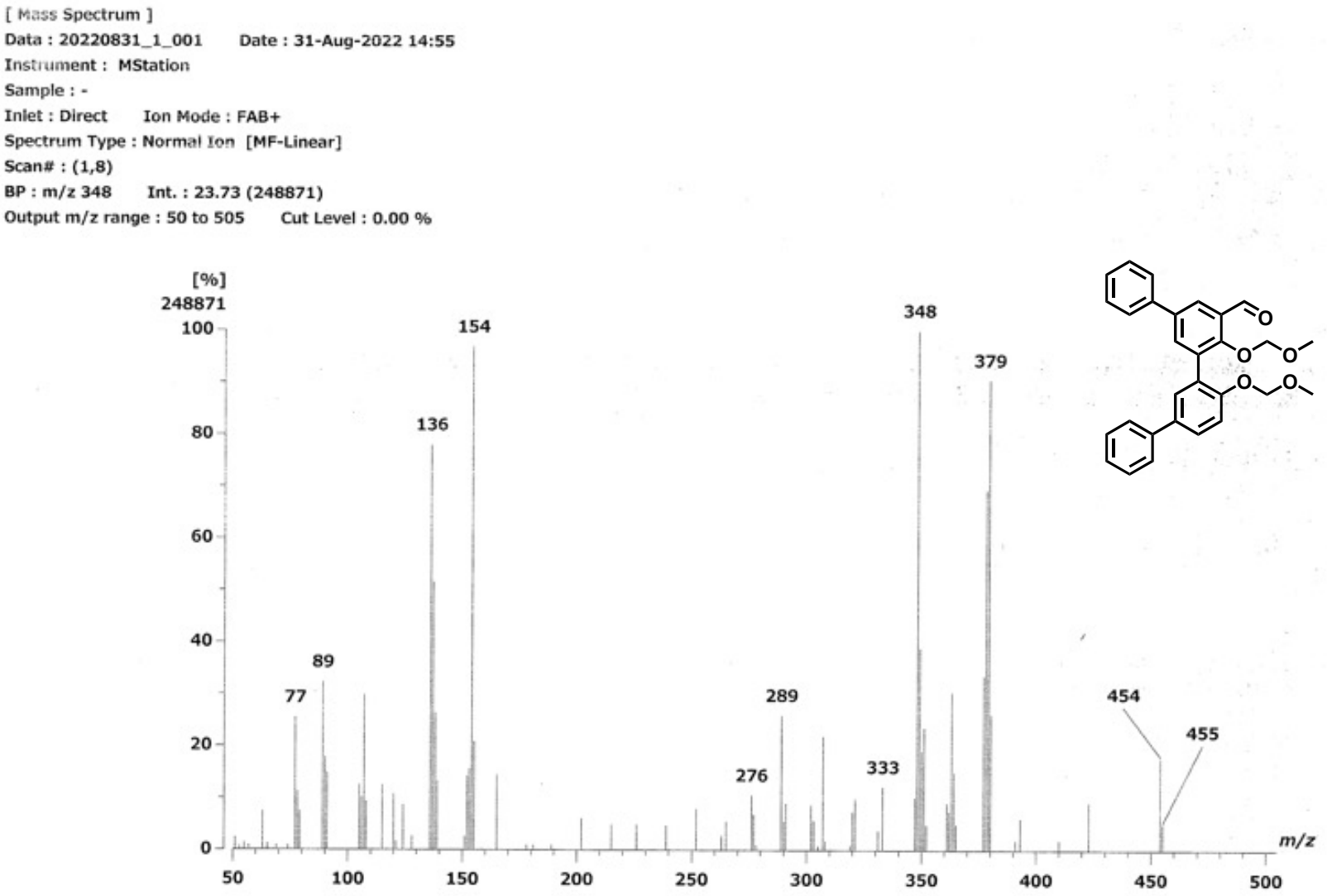

Fig. S8. FAB-MS (positive mode) spectrum of **3**.

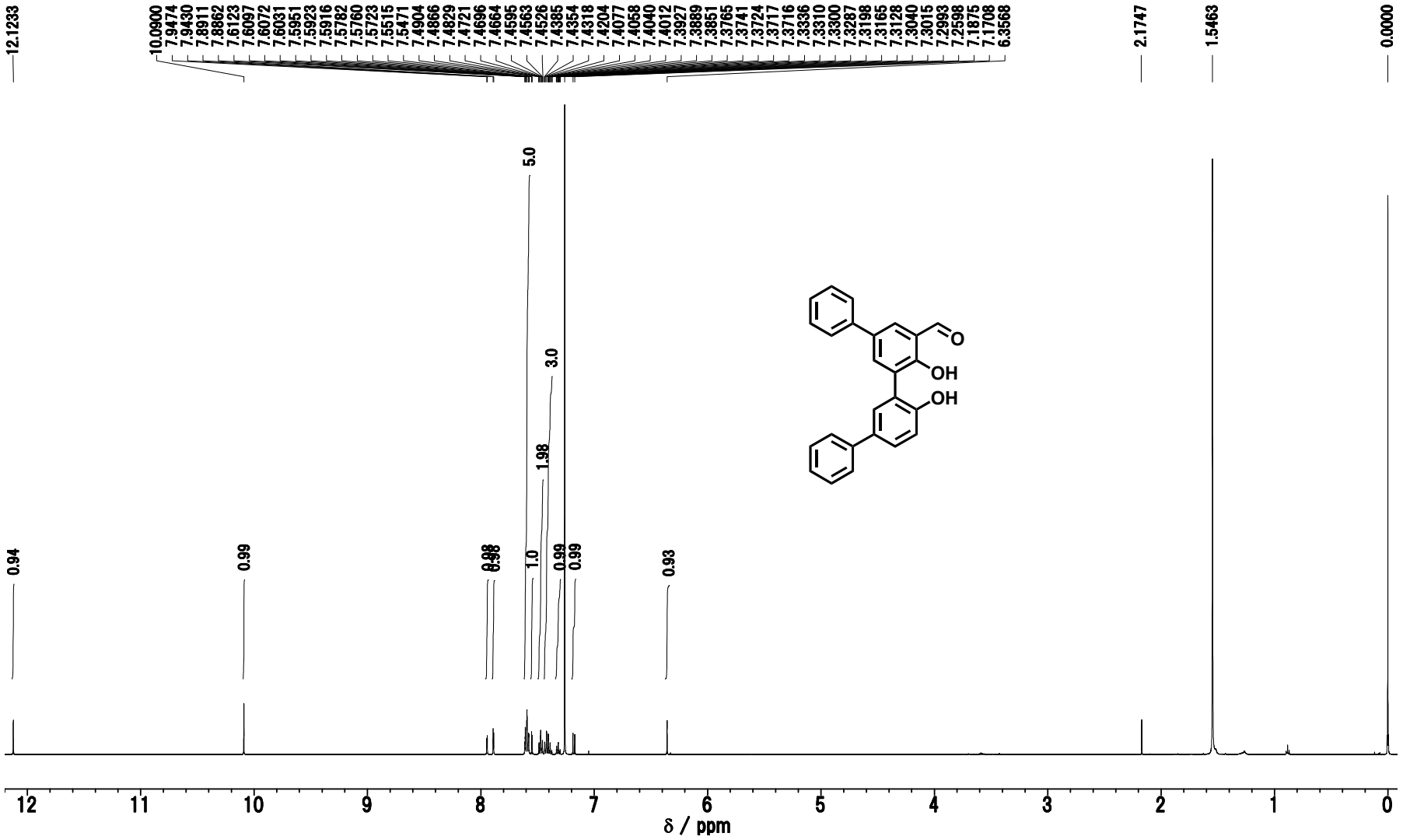

Fig. S9. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of **4**.

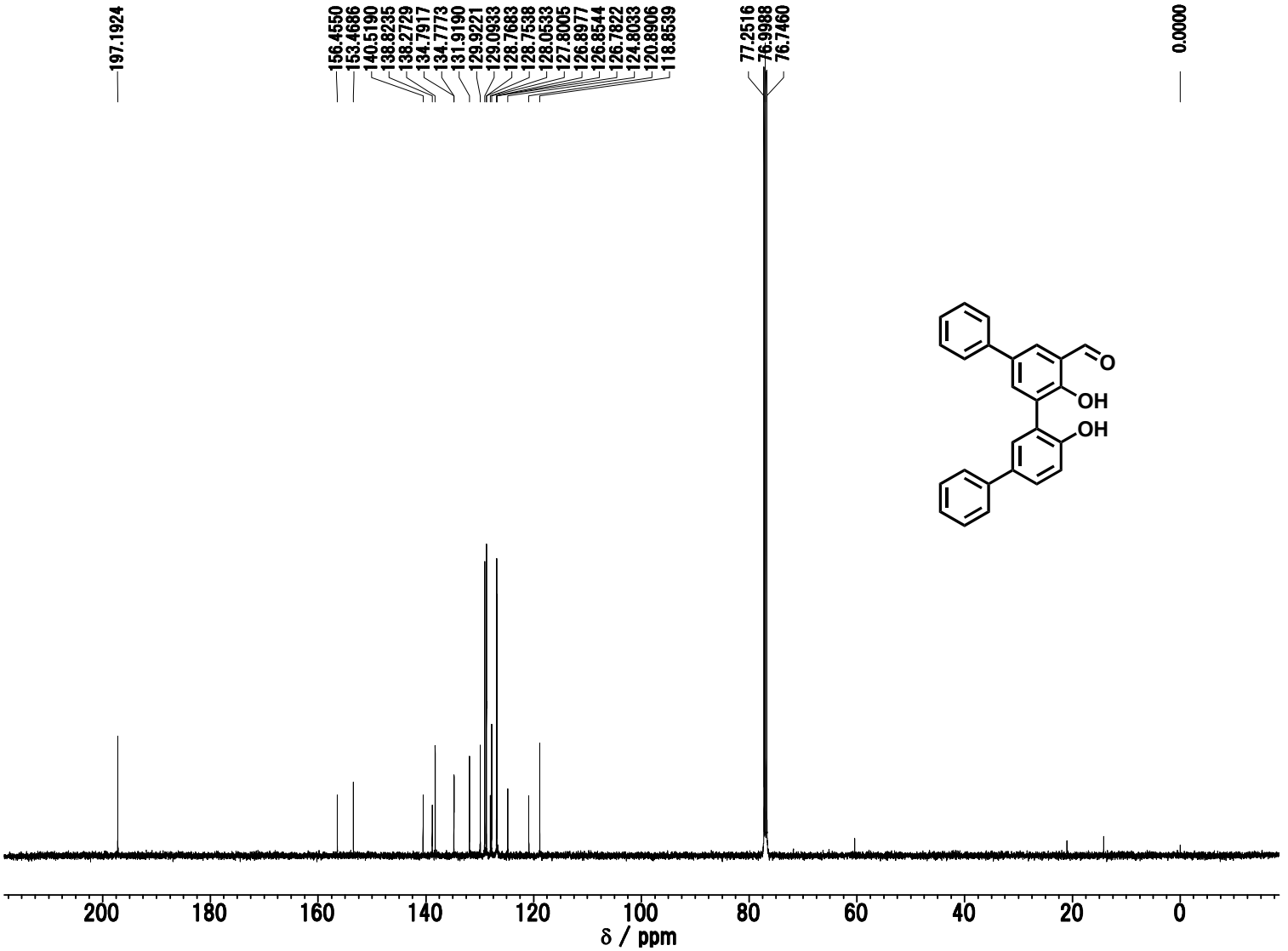

Fig. S10. ^{13}C NMR (126 MHz, $CDCl_3$) spectrum of **4**.

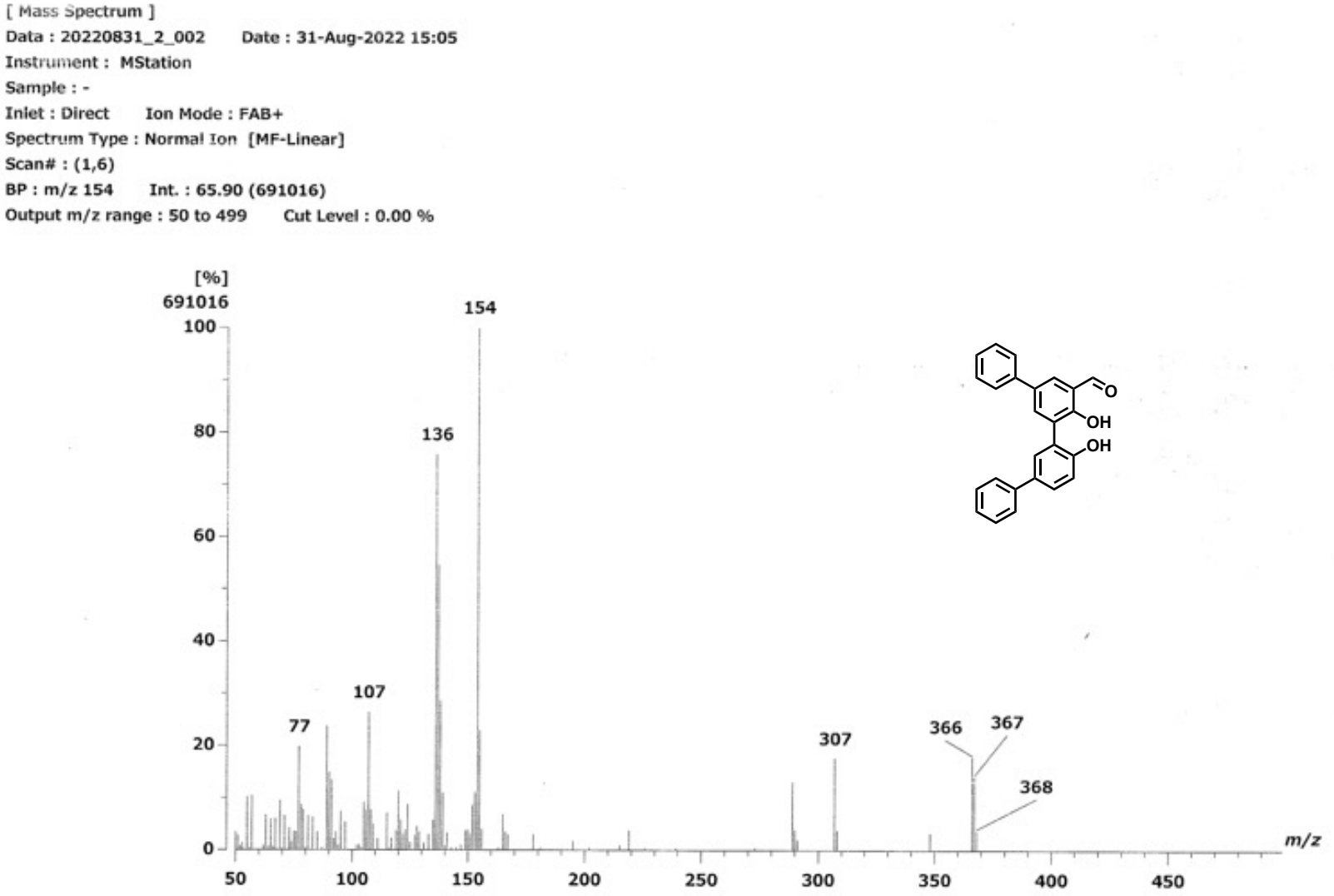

Fig. S11. FAB-MS (positive mode) spectrum of **4**.

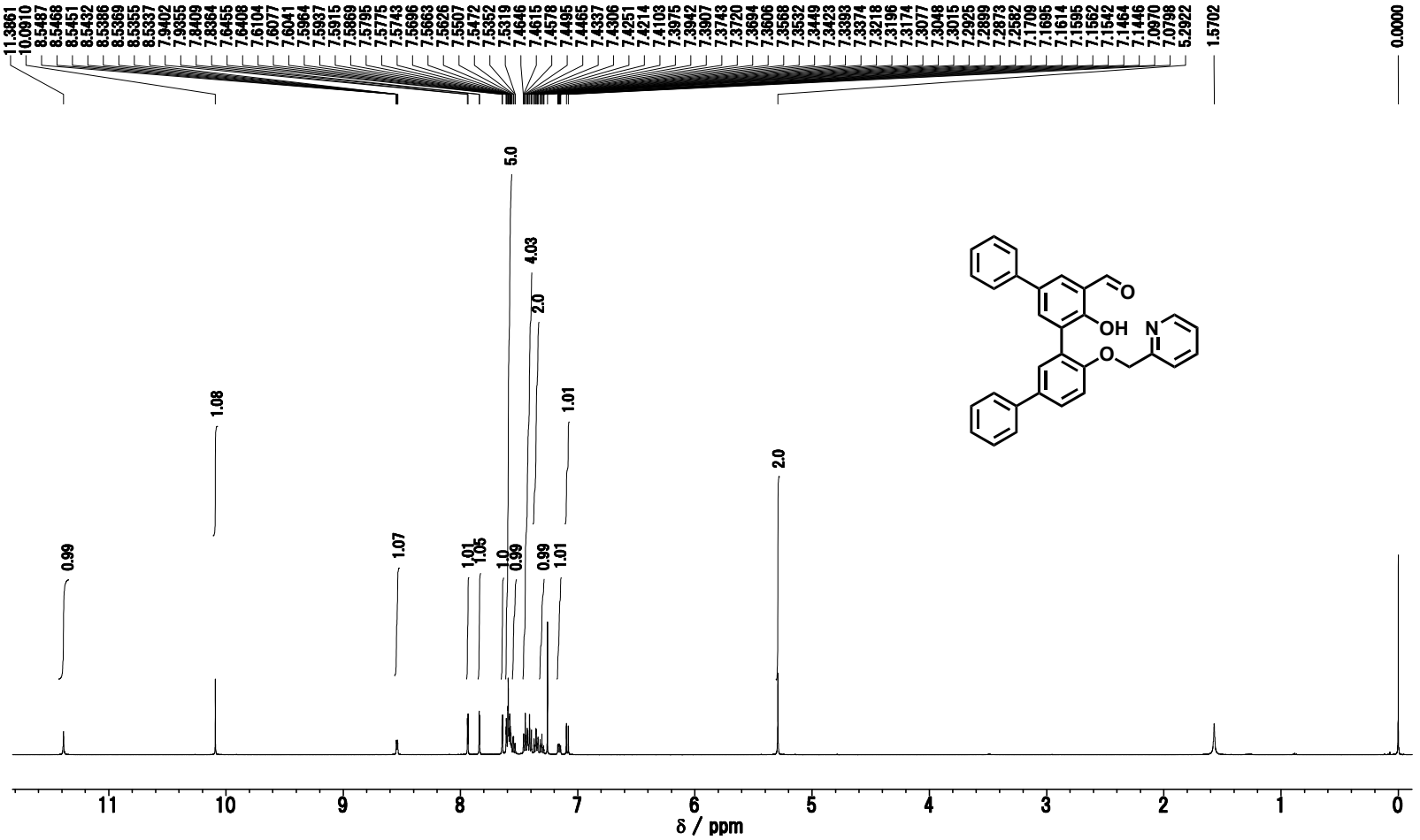

Fig. S12. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of **1**.

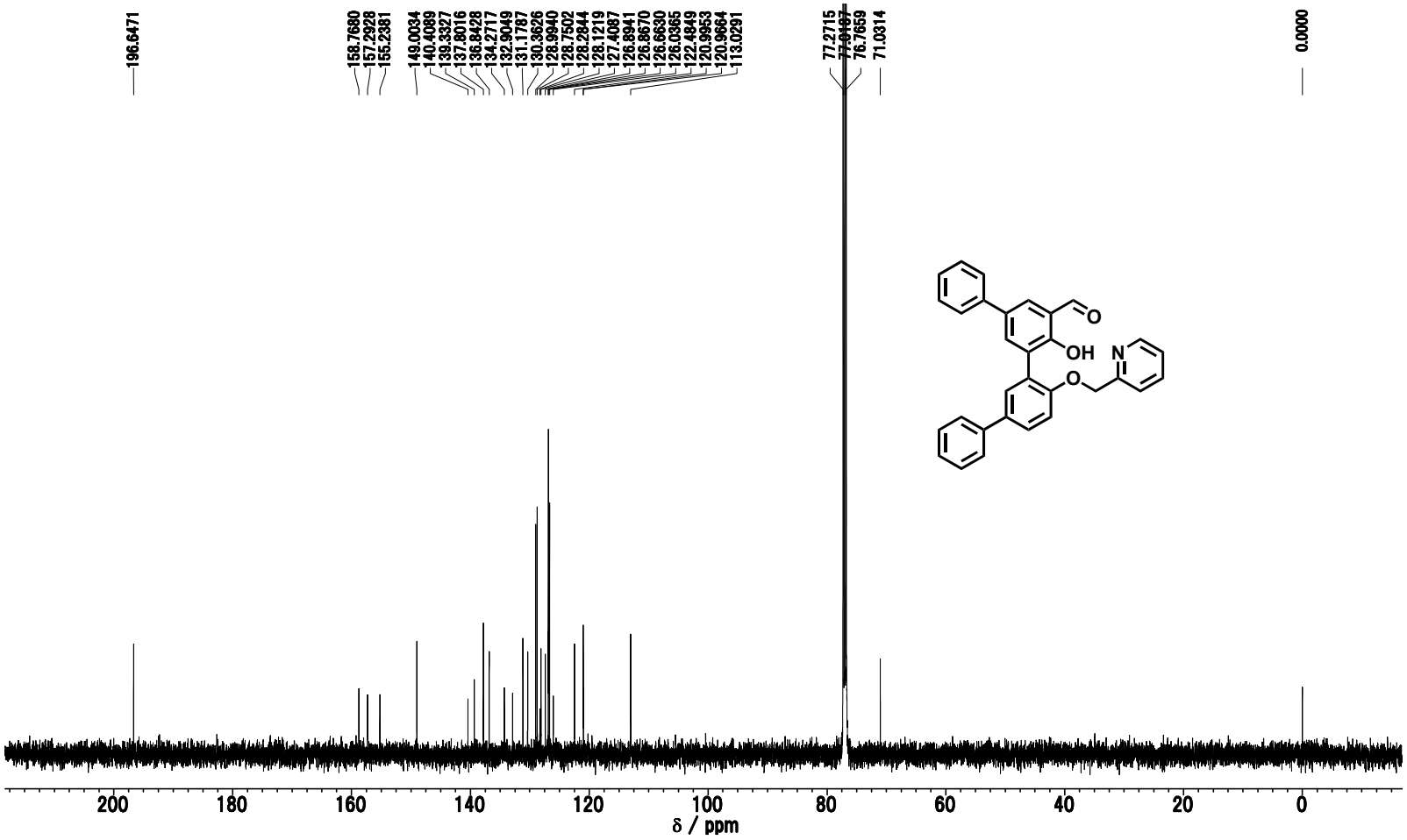

Fig. S13. ^{13}C NMR (126 MHz, $CDCl_3$) spectrum of **1**.

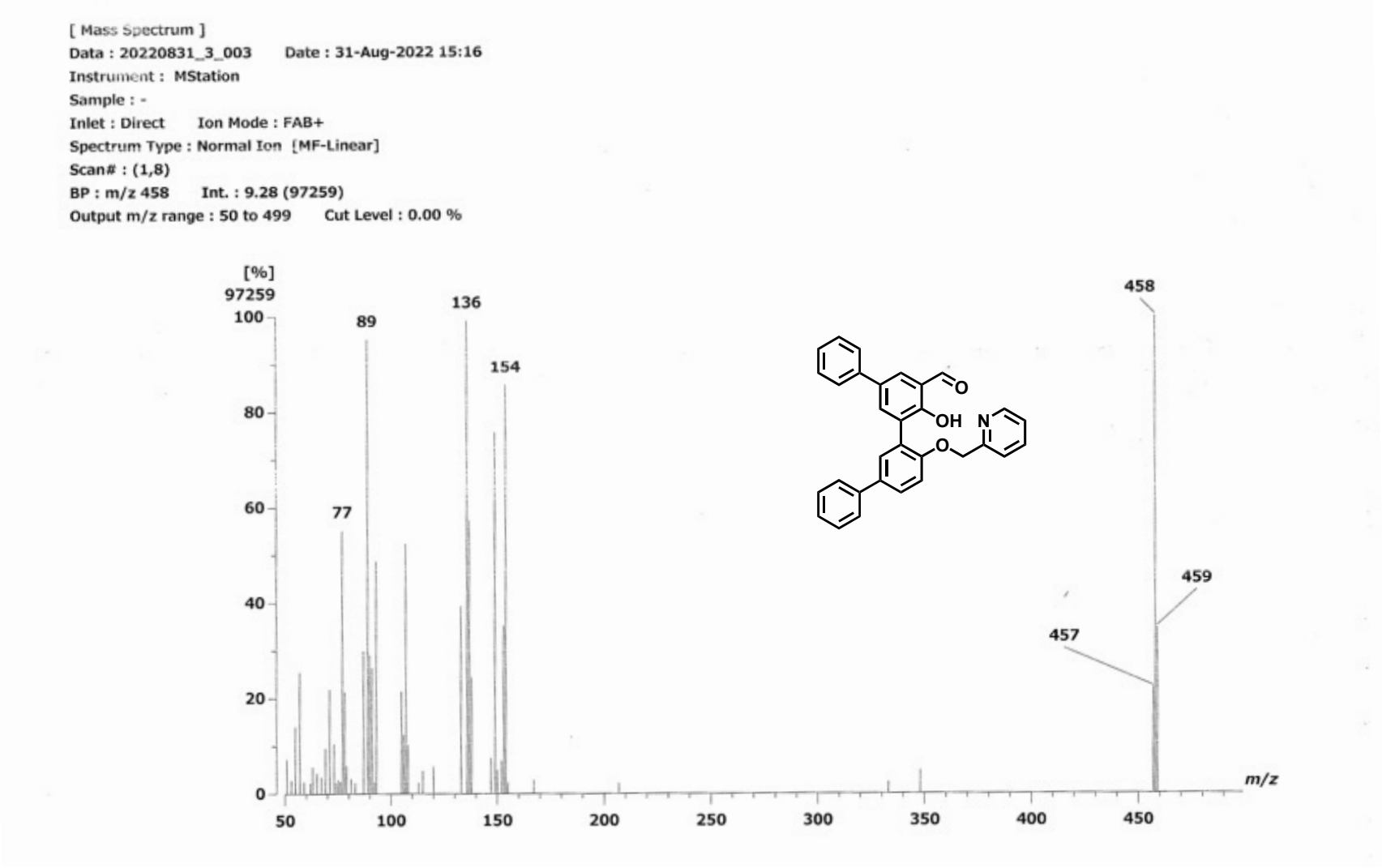

Fig. S14. FAB-MS (positive mode) spectrum of **1**.

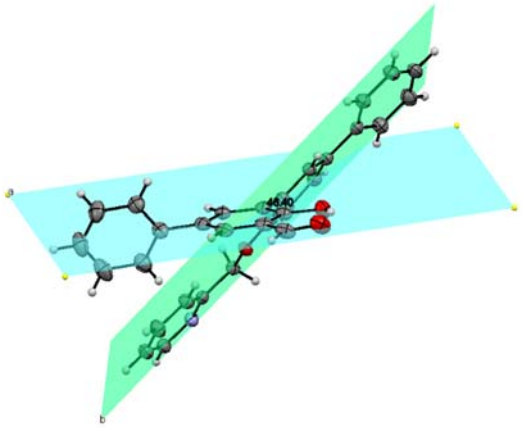

Fig. S15. The B-ring, denoted in Scheme 1, is tilted by 46.4° with respect to the C-ring.

Single Crystal Structure Report for compound **1** (CCDC No. 2207715)

A specimen of $C_{31}H_{23}NO_3$ was used for the X-ray crystallographic analysis. The X-ray intensity data were measured on a Bruker D8 goniometer system equipped with a sealed tube (CuKα, λ = 1.54178 Å) and a multilayered conforcal mirror monochromator.

Table S2. Data collection details for compound **1**.

Axis	dx/mm	2θ/°	ω/°	φ/°	χ/°	Width/°	Frames	Time/s	Wavelength/Å	Voltage/kV	Current/mA	Temperature/K
Phi	50.017	55.00	0.00	0.00	54.78	2.00	90.00	1.00	1.54184	50	1.1	120
Phi	34.017	-30.00	-45.00	0.00	54.78	0.40	500.00	1.00	1.54184	50	1.1	120
Omega	34.017	100.00	-64.00	0.00	54.74	0.40	375.00	1.00	1.54184	50	1.1	120
Omega	34.017	100.00	-64.00	72.00	54.74	0.40	375.00	1.00	1.54184	50	1.1	120
Omega	34.017	100.00	-64.00	144.00	54.74	0.40	375.00	1.00	1.54184	50	1.1	120
Omega	34.017	100.00	-64.00	216.00	54.74	0.40	375.00	1.00	1.54184	50	1.1	120
Omega	34.017	100.00	-64.00	288.00	54.74	0.40	375.00	1.00	1.54184	50	1.1	120

A total of 2465 frames were collected. The total exposure time was 0.68 hours. The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. The integration of the data using a monoclinic unit cell yielded a total of 18073 reflections to a maximum θ angle of 72.36° (0.81 Å resolution), of which 4399 were independent (average redundancy 4.108, completeness = 98.2%, R_{int} = 4.06%, R_{sig} = 4.90%) and 4005 (91.04%) were greater than 2σ(F^2). The final cell constants of a = 10.7112(4) Å, b = 7.8141(3) Å, c = 27.003(3) Å, β = 91.978(5)°, volume = 2258.8(3) Å^3, are based upon the refinement of the XYZ-centroids of 8664 reflections above 20 σ(I) with 11.78° < 2θ < 144.7°. Data were corrected for absorption effects using the Multi-Scan method (SADABS). The ratio of minimum to maximum apparent transmission was 0.880.

The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group P 2$_1$/n, with Z = 4 for the formula unit, $C_{31}H_{23}NO_3$. The final anisotropic full-matrix least-squares refinement on F^2 with 319 variables converged at R_1 = 5.94%, for the observed data and wR_2 = 16.74% for all data. The goodness-of-fit was 1.032. The largest peak in the final difference electron density synthesis was 0.410 e$^-$/Å^{3}and the largest hole was -0.353 e$^-$/Å^3 with an RMS deviation of 0.074 e$^-$/Å^3. On the basis of the final model, the calculated density was 1.345 g/cm^3 and F(000), 960 e$^-$.

Table S3. Sample and crystal data for compound **1.**

Identification code	Compound **1**	
Chemical formula	$C_{31}H_{23}NO_3$	
Formula weight	457.50 g/mol	
Temperature	120(0) K	
Wavelength	1.54178 Å	
Crystal system	monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 10.7112(4) Å	α = 90°
	b = 7.8141(3) Å	β = 91.978(5)°
	c = 27.003(3) Å	γ = 90°
Volume	2258.8(3) $Å^3$	
Z	4	
Density (calculated)	1.345 g/cm^3	
Absorption coefficient	0.688 mm^{-1}	
F(000)	960	

Table S4. Data collection and structure refinement for compound **1.**

Diffractometer	Bruker D8 goniometer	
Radiation source	sealed tube (CuKα, λ = 1.54178 Å)	
Theta range for data collection	4.39 to 72.36°	
Index ranges	-13<=*h*<=13, -9<=*k*<=9, -33<=*l*<=30	
Reflections collected	18073	
Independent reflections	4399 [*R*(int) = 0.0406]	
Coverage of independent reflections	98.20%	
Absorption correction	Multi-Scan	
Structure solution technique	direct methods	
Structure solution program	XT, VERSION 2018/2	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL-2019/1 (Sheldrick, 2019)	
Function minimized	$\Sigma\ w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	4399 / 0 / 319	
Goodness-of-fit on F^2	1.032	
Δ/σ_{max}	0.001	
Final R indices	4005 data; $I>2\sigma(I)$	R_1 = 0.0594, wR_2 = 0.1603
	all data	R_1 = 0.0630, wR_2 = 0.1674
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.1207P)^2+0.4417P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	0.410 and -0.353 eÅ^{-3}	
R.M.S. deviation from mean	0.074 eÅ^{-3}	

Table S5. Atomic coordinates and equivalent isotropic atomic displacement parameters ($Å^2$) for compound **1.**

	x/a	**y/b**	**z/c**	**U(eq)**
O001	0.92238(9)	0.23656(12)	0.49556(3)	0.0258(3)
O002	0.56319(10)	0.22164(15)	0.58498(4)	0.0339(3)
O003	0.33766(11)	0.10790(16)	0.56231(5)	0.0435(3)
N004	0.14852(11)	0.05660(15)	0.41482(4)	0.0284(3)
C005	0.77771(12)	0.45876(17)	0.59739(5)	0.0249(3)
C006	0.91280(12)	0.32736(16)	0.53854(5)	0.0233(3)
C007	0.04534(12)	0.19885(17)	0.47999(5)	0.0242(3)
C008	0.87982(12)	0.50494(16)	0.62831(5)	0.0246(3)
C009	0.79121(12)	0.37293(17)	0.55248(5)	0.0240(3)
C00A	0.99857(13)	0.46259(18)	0.61225(5)	0.0264(3)
C00B	0.68177(12)	0.33183(17)	0.51907(5)	0.0257(3)
C00C	0.03729(13)	0.11112(16)	0.43025(5)	0.0248(3)
C00D	0.01526(12)	0.37336(17)	0.56872(5)	0.0255(3)
C00E	0.68651(12)	0.36624(17)	0.46850(5)	0.0264(3)
C00F	0.57242(13)	0.25650(18)	0.53623(5)	0.0275(3)
C00G	0.86512(13)	0.59291(17)	0.67683(5)	0.0266(3)
C00H	0.47422(13)	0.21371(19)	0.50192(6)	0.0304(3)
C00I	0.14981(15)	0.98035(19)	0.37053(5)	0.0317(3)
C00J	0.59101(13)	0.32365(18)	0.43376(5)	0.0292(3)
C00K	0.92638(14)	0.09071(19)	0.40299(5)	0.0303(3)
C00L	0.75442(14)	0.67566(19)	0.68874(5)	0.0322(3)
C00M	0.48494(13)	0.24537(19)	0.45127(6)	0.0310(3)
C00N	0.61008(13)	0.3565(2)	0.38017(5)	0.0328(3)
C00O	0.04433(16)	0.9561(2)	0.34013(5)	0.0352(4)
C00P	0.93087(16)	0.0119(2)	0.35704(6)	0.0368(4)
C00Q	0.95051(16)	0.6756(2)	0.75798(6)	0.0384(4)
C00R	0.96298(14)	0.5954(2)	0.71251(5)	0.0329(3)
C00S	0.74195(16)	0.7565(2)	0.73410(6)	0.0377(4)
C00T	0.36071(14)	0.1320(2)	0.51854(6)	0.0362(4)
C00U	0.83979(17)	0.7566(2)	0.76919(6)	0.0383(4)
C00V	0.66310(15)	0.5097(2)	0.36475(6)	0.0363(4)
C00W	0.58051(16)	0.2321(2)	0.34455(6)	0.0425(4)
C00X	0.68751(16)	0.5372(3)	0.31504(6)	0.0453(4)
C00Y	0.60531(19)	0.2608(3)	0.29486(7)	0.0536(5)
C00Z	0.65892(18)	0.4114(3)	0.28025(6)	0.0534(5)

Table S6. Bond lengths (Å) for compound **1.**

O001-C006	1.3672(16)	O001-C007	1.4270(16)
O002-C00F	1.3512(18)	O003-C00T	1.230(2)
N004-C00I	1.3366(19)	N004-C00C	1.3449(18)
C005-C009	1.3976(19)	C005-C008	1.4001(19)
C006-C00D	1.3914(19)	C006-C009	1.4137(18)
C007-C00C	1.5079(18)	C008-C00A	1.3977(19)
C008-C00G	1.4927(19)	C009-C00B	1.4894(18)
C00A-C00D	1.3834(19)	C00B-C00E	1.395(2)
C00B-C00F	1.404(2)	C00C-C00K	1.385(2)
C00E-C00J	1.4038(19)	C00F-C00H	1.418(2)
C00G-C00L	1.398(2)	C00G-C00R	1.399(2)
C00H-C00M	1.398(2)	C00H-C00T	1.458(2)
C00I-C00O	1.386(2)	C00J-C00M	1.388(2)
C00J-C00N	1.491(2)	C00K-C00P	1.388(2)
C00L-C00S	1.389(2)	C00N-C00V	1.395(2)
C00N-C00W	1.396(2)	C00O-C00P	1.383(2)
C00Q-C00U	1.387(3)	C00Q-C00R	1.389(2)
C00S-C00U	1.388(3)	C00V-C00X	1.393(2)
C00W-C00Y	1.395(3)	C00X-C00Z	1.387(3)
C00Y-C00Z	1.373(3)		

Table S7. Bond angles (°) for compound **1.**

C006-O001-C007	117.02(10)	C00I-N004-C00C	117.06(12)
C009-C005-C008	122.61(12)	O001-C006-C00D	123.40(12)
O001-C006-C009	116.98(11)	C00D-C006-C009	119.61(12)
O001-C007-C00C	109.35(11)	C00A-C008-C005	117.03(12)
C00A-C008-C00G	120.40(12)	C005-C008-C00G	122.56(12)
C005-C009-C006	118.41(12)	C005-C009-C00B	121.75(12)
C006-C009-C00B	119.83(12)	C00D-C00A-C008	121.91(12)
C00E-C00B-C00F	117.59(12)	C00E-C00B-C009	119.81(12)
C00F-C00B-C009	122.59(12)	N004-C00C-C00K	123.48(12)
N004-C00C-C007	113.32(12)	C00K-C00C-C007	123.19(12)
C00A-C00D-C006	120.35(12)	C00B-C00E-C00J	123.94(13)
O002-C00F-C00B	119.74(12)	O002-C00F-C00H	120.77(13)
C00B-C00F-C00H	119.46(13)	C00L-C00G-C00R	117.16(13)
C00L-C00G-C008	122.07(13)	C00R-C00G-C008	120.77(13)
C00M-C00H-C00F	120.89(13)	C00M-C00H-C00T	118.43(13)
C00F-C00H-C00T	120.66(14)	N004-C00I-C00O	123.87(14)
C00M-C00J-C00E	117.59(13)	C00M-C00J-C00N	123.22(13)
C00E-C00J-C00N	119.12(13)	C00C-C00K-C00P	118.09(13)
C00S-C00L-C00G	121.44(14)	C00J-C00M-C00H	120.46(13)
C00V-C00N-C00W	118.50(15)	C00V-C00N-C00J	120.57(14)
C00W-C00N-C00J	120.87(15)	C00P-C00O-C00I	117.95(13)
C00O-C00P-C00K	119.53(14)	C00U-C00Q-C00R	120.52(15)
C00Q-C00R-C00G	121.48(14)	C00U-C00S-C00L	120.59(14)
O003-C00T-C00H	124.07(14)	C00Q-C00U-C00S	118.80(13)
C00X-C00V-C00N	120.80(16)	C00Y-C00W-C00N	120.29(18)
C00Z-C00X-C00V	119.93(19)	C00Z-C00Y-C00W	120.62(18)
C00Y-C00Z-C00X	119.85(16)		

Table S8. Anisotropic atomic displacement parameters ($Å^2$) compound **1.**

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O001	0.0218(5)	0.0299(5)	0.0258(5)	-0.0042(4)	0.0019(4)	0.0004(4)
O002	0.0254(5)	0.0431(6)	0.0336(6)	-0.0011(4)	0.0059(4)	-0.0049(4)
O003	0.0287(6)	0.0497(7)	0.0529(7)	-0.0099(5)	0.0120(5)	-0.0086(5)
N004	0.0300(6)	0.0270(6)	0.0285(6)	0.0004(4)	0.0062(5)	0.0016(4)
C005	0.0234(6)	0.0234(6)	0.0280(6)	0.0011(5)	0.0041(5)	0.0009(5)
C006	0.0253(6)	0.0216(6)	0.0229(6)	0.0008(5)	0.0023(5)	-0.0010(5)
C007	0.0212(6)	0.0253(6)	0.0263(6)	-0.0006(5)	0.0026(5)	-0.0002(5)
C008	0.0273(7)	0.0210(6)	0.0255(6)	0.0025(5)	0.0017(5)	-0.0013(5)
C009	0.0227(6)	0.0231(6)	0.0263(6)	0.0017(5)	0.0012(5)	-0.0011(5)
C00A	0.0243(6)	0.0275(7)	0.0271(6)	-0.0001(5)	-0.0013(5)	-0.0025(5)
C00B	0.0223(6)	0.0243(6)	0.0306(7)	-0.0033(5)	0.0006(5)	0.0022(5)
C00C	0.0284(7)	0.0215(6)	0.0248(6)	0.0027(5)	0.0037(5)	-0.0005(5)
C00D	0.0225(6)	0.0259(6)	0.0284(7)	0.0011(5)	0.0034(5)	-0.0002(5)
C00E	0.0230(6)	0.0257(6)	0.0305(7)	-0.0018(5)	0.0001(5)	0.0022(5)
C00F	0.0232(6)	0.0278(7)	0.0317(7)	-0.0041(5)	0.0027(5)	0.0022(5)
C00G	0.0314(7)	0.0218(6)	0.0267(7)	0.0015(5)	0.0039(5)	-0.0033(5)
C00H	0.0207(6)	0.0303(7)	0.0402(8)	-0.0072(6)	0.0013(5)	0.0030(5)
C00I	0.0371(8)	0.0281(7)	0.0305(7)	0.0001(5)	0.0098(6)	0.0027(5)
C00J	0.0265(7)	0.0291(7)	0.0317(7)	-0.0041(5)	-0.0021(5)	0.0056(5)
C00K	0.0280(7)	0.0313(7)	0.0316(7)	-0.0018(5)	0.0024(5)	-0.0002(5)
C00L	0.0350(8)	0.0316(7)	0.0302(7)	-0.0010(6)	0.0028(6)	0.0030(6)
C00M	0.0237(7)	0.0320(7)	0.0370(8)	-0.0082(6)	-0.0047(5)	0.0044(5)
C00N	0.0245(7)	0.0413(8)	0.0321(8)	-0.0026(6)	-0.0047(5)	0.0084(6)
C00O	0.0462(9)	0.0329(7)	0.0270(7)	-0.0046(6)	0.0068(6)	-0.0014(6)
C00P	0.0382(8)	0.0415(8)	0.0305(7)	-0.0050(6)	-0.0025(6)	-0.0035(6)
C00Q	0.0433(9)	0.0411(9)	0.0308(7)	-0.0060(6)	-0.0017(6)	-0.0056(7)
C00R	0.0330(7)	0.0354(7)	0.0305(7)	-0.0031(6)	0.0028(6)	-0.0011(6)
C00S	0.0432(9)	0.0336(8)	0.0370(8)	-0.0034(6)	0.0116(7)	0.0060(6)
C00T	0.0229(7)	0.0386(8)	0.0474(9)	-0.0110(6)	0.0047(6)	-0.0006(6)
C00U	0.0547(10)	0.0322(8)	0.0284(7)	-0.0070(6)	0.0081(7)	-0.0038(6)
C00V	0.0313(8)	0.0425(8)	0.0347(8)	0.0012(6)	-0.0035(6)	0.0077(6)
C00W	0.0378(8)	0.0531(10)	0.0361(8)	-0.0077(7)	-0.0048(6)	0.0012(7)
C00X	0.0371(9)	0.0592(11)	0.0393(9)	0.0118(8)	-0.0029(7)	0.0077(7)
C00Y	0.0489(10)	0.0773(14)	0.0340(9)	-0.0145(8)	-0.0059(7)	0.0009(9)
C00Z	0.0441(9)	0.0878(15)	0.0280(8)	0.0033(8)	-0.0037(7)	0.0084(9)

Table S9. Hydrogen atomic coordinates and isotropic atomic displacement parameters ($Å^2$) for compound **1.**

	x/a	**y/b**	**z/c**	**U(eq)**
H1	0.489(3)	0.182(3)	0.5888(8)	0.051
H005	0.696	0.4869	0.6073	0.03
H00A	1.0885	0.1236	0.5046	0.029
H00B	1.094	0.306	0.4775	0.029
H00C	1.0699	0.4961	0.6318	0.032
H00D	1.0971	0.3433	0.5594	0.031
H00E	0.7587	0.4218	0.4569	0.032
H00I	1.2276	-0.0596	0.3592	0.038
H00K	0.8495	0.1296	0.4154	0.036
H00L	0.6862	0.6766	0.6653	0.039
H00M	0.4191	0.213	0.4287	0.037
H00O	1.0498	-0.0971	0.3087	0.042
H00P	0.8565	-0.0037	0.3373	0.044
H00Q	1.0184	0.675	0.7816	0.046
H00R	1.0397	0.5409	0.7055	0.039
H00S	0.6658	0.8122	0.7412	0.045
H00T	0.3008	0.0951	0.4941	0.043
H00U	0.8311	0.8112	0.8003	0.046
H00V	0.6828	0.5963	0.3884	0.044
H00W	0.5434	0.1274	0.3542	0.051
H00X	0.7237	0.642	0.305	0.054
H00Y	0.5849	0.1753	0.2709	0.064
H00Z	0.6764	0.4293	0.2464	0.064