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Supporting Information for:

The photomechanic effects of the molecular crystals based on 5-chloro-2-(naphthalenylvinyl)benzoxazols fueled by topo-photochemical reactions

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Measurement and characterization

^{1}H NMR and ^{13}C NMR spectra were recorded with a Bruker-Avance III 400 MHz and 101 MHz spectrometer with $CDCl_3$ and DMSO-d_6 as solvents and tetramethylsilane (TMS) as the internal standard. The samples for irradiation time-dependent ^{1}H NMR measurements were gained via the irradiation of the crystals of **BOV1N**, **BOV1NF**, **BOV1NM**, **BOV2N** and **BOV2NM** by 365 nm (3 W) light for different times, followed by dissolving in DMSO-d_6. FT-IR spectra were obtained with a Nicolet-360 FT-IR spectrometer by the incorporation of samples into KBr disks. Mass spectra were measured on an Agilent 1100MS series and an AXIMA CFR MAL DI-TOF (matrix-assisted laser desorption ionization/time-of-light) MS (COMPACT). UV-vis absorption spectra were measured by a Shimadzu UV-1601PC spectrophotometer. Fluorescence emission spectra were taken on a Shimadzu RF-5301 luminescence spectrometer. The solid samples of **BOV1N**, **BOV1NF**, **BOV1NM**, **BOV2N** and **BOV2NM** for electronic spectra measurements were gained by grinding the crystals into microcrystals, which were smeared onto the quartz substrates and irradiated by 365 nm (3 W) light for different times. Scanning electron microscopy (SEM) was performed on JEOL JSM-6700F (operating at 5 kV), and the sample was prepared by casting the xerogel and crystal onto conductive adhesive followed by drying in air. The dried sample was then annealed at 45 °C overnight in an oven, followed by coating with gold. X-ray diffraction patterns were obtained on Empyrean XRD equipped with graphite monochromatized Cu-Kα radiation (λ = 1.5418 Å) employing a scanning rate of 0.00267 °/s in the 2θ range of 5° to 40° and

the crystals and xerogel fibers were kept at room temperature during data collection. The crystals of **BOV1N**, **BOV1NF**, **BOV1NM**, **BOV2N** and **BOV2NM** were obtained by slow evaporation from the solution in DCM/petroleum ether (v/v = 1/4).

The preparation of single crystals of β-type and α-type **D-BOV1N**: The microcrystals of **BOV1N** were irradiated by pocket lamp (365 nm, 3 W) for 30 min. The β-type and α-type **D-BOV1N** were isolated by column chromatography (silica gel) using ethyl acetate/petroleum ether (v/v = 1/10) as the eluent. The single crystals of β-type and α-type **D-BOV1N** were obtained by slow evaporation from the solution in DCM/petroleum ether (v/v = 1/4).

The single crystals of **BOV1N**, β-type **D-BOV1N**, α-type **D-BOV1N** and **BOV1NM** were selected for X-ray diffraction analysis on a Rigaku RA XIS-RA PID diffractometer using graphite-monochromated MoK_α radiation (λ = 0.71073 Å), and it was kept at 149 K, 100.0 K, 100.0 K and 273 K during data collection, respectively.

Investigation of photomechanic behavior: The crystals were put on the glass substrate and irradiated by pocket lamp (365 nm, 3 W) for different times at 298 K under microscope.

Ring opening reaction: β-Type **D-BOV1N** was dissolved in DMSO-d_6, and was irradiated by 254 nm (6 W) light for 30 h at 293 K. After that, the ^{1}H NMR spectrum was measured.

Preparation of the fibers: A clear solution of **BOV1N** in *n*-hexane (7.0 mM) was obtained by heating. After the hot solution was subjected to sonication for 1 min, followed by aging for 5 min at room temperature, the organogel was formed. The

organogel was coated on the substrate, and dried at room temperature.

Synthetic procedures

The compound (*E*)-5-chloro-2-(2-(naphthalen-1-yl)vinyl)benzo[*d*]oxazole (**BOV1N**) was synthesized according to the reported procedures, and the synthetic route was shown followed. After *t*-BuOK (0.72 g, 6.4 mmol) was added into dry THF (10 mL) and stirred for 10 min at 0 ºC in ice-bath, 5-chloro-2-methylbenzo[*d*]oxazole (0.64 g, 3.8 mmol) was dropwise added into the above suspension and stirred for another 30 min at 0 ºC. Then, a dry THF solution containing 1-naphthaldehyde (0.5 g, 3.2 mmol) was added slowly at 0 ºC. After stirred for 3 h in ice-bath, the mixture was poured into water (200 mL) and light yellow solid was collected by filtration. The crude product was purified by column chromatography (silica gel) using ethyl acetate/petroleum ether (v/v = 1/10) as the eluent. Yellow solid of **BOV1N** (0.63 g) was obtained in a yield of 65 %. M.p.: 130.0-132.0 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.65 (d, *J* = 16.0 Hz, 1H), 8.36 (d, *J* = 8.0 Hz, 1H), 8.15 (d, *J* = 8.0 Hz, 1H), 8.04 (dd, *J* = 12.0, 8.0 Hz, 2H), 7.90 (d, *J* = 2.0 Hz, 1H), 7.82 (d, *J* = 8.0 Hz, 1H), 7.70-7.60 (m, 3H), 7.49 (dd, *J* = 8.0, 2.0 Hz, 1H), 7.43 (d, *J* = 16.0 Hz, 1H) (Fig. S23). ^{13}C NMR (101 MHz, DMSO-d_6) δ 164.31, 149.19, 143.49, 136.93, 133.83, 131.74, 131.17, 130.92, 129.45, 129.24, 127.68, 126.82, 126.26, 126.06, 125.51, 123.53, 119.82, 116.21, 112.55 (Fig. S24). FT- IR (KBr, cm^{-1}): 3057, 1640, 1541, 1500, 1451, 1337, 1258, 1175, 1061, 967, 923, 793, 766, 707. MS (MALDI-TOF): Calcd. for $C_{19}H_{12}NOCl$: 305.0, found: 305.0 [M^{+}] (Fig. S25).

(*E*)-5-Chloro-2-(2-(4-fluoronaphthalen-1-yl)vinyl)benzo[*d*]oxazole (**BOV1NF**)

The synthetic method for compound **BOV1NF** was similar to that of compound **BOV1N**. It was synthesized from compound 5-chloro-2-methylbenzo[*d*]oxazole (1.15 g, 6.9 mmol) and 4-fluoro-1-naphthaldehyde (1.0 g, 5.7 mmol). The crude product was purified by column chromatography (silica gel) using ethyl acetate/petroleum ether (v/v = 1/10) as the eluent. Yellow solid of **BOV1NF** (1.17 g) was obtained in a yield of 63 %. M.p.: 150.0-152.0 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.58 (d, *J* = 16.0 Hz, 1H), 8.43 (d, *J* = 8.0 Hz, 1H), 8.19-8.14 (m, 2H), 7.89 (d, *J* = 2.0 Hz, 1H), 7.83-7.74 (m, 3H), 7.50-7.45 (m, 2H), 7.41 (d, *J* = 16.0 Hz, 1H) (Fig. S26). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.80, 148.94, 142.77, 136.80, 132.72, 130.25, 128.38, 127.96, 126.68, 125.71, 125.00, 123.95, 123.38, 121.37, 119.76, 115.24, 111.19, 109.81, 109.60 (Fig. S27). FT- IR (KBr, cm^{-1}): 3045, 1641, 1603, 1537, 1509, 1451, 1347, 1250, 1055, 969, 928, 867, 811, 758, 707. MS (MALDI-TOF): Calcd. for $C_{19}H_{11}NOCl$: 323.0, found: 323.0 [M^+] (Fig. S28).

(*E*)-5-Chloro-2-(2-(4-methoxynaphthalen-1-yl)vinyl)benzo[*d*]oxazole (**BOV1NM**)

The synthetic method for compound **BOV1NM** was similar to that of compound **BOV1N**. It was synthesized from compound 5-chloro-2-methylbenzo[*d*]oxazole (0.8 g, 4.8 mmol) and 4-methoxy-1-naphthaldehyde (0.74 g, 4.0 mmol). The crude product was purified by column chromatography (silica gel) using ethyl acetate/petroleum ether (v/v = 1/10) as the eluent. Yellow solid of **BOV1NM** (0.82 g) was obtained in a yield of 61 %. M.p.: 156.0-158.0 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.55 (d, J = 16.0 Hz, 1H), 8.32 (d, J = 8.0 Hz, 1H), 8.25 (d, J = 8.0 Hz, 1H), 8.14 (d, J = 8.0 Hz, 1H), 7.85 (s, 1H), 7.78 (d, J = 8.0 Hz, 1H), 7.69 (t, J = 6.0 Hz, 1H), 7.62-7.58 (m, 1H),

7.45 (dd, J = 8.0, 4.0 Hz, 1H), 7.29 (d, J = 16.0 Hz, 1H), 7.11 (d, J = 8.0 Hz, 1H), 4.05 (s, 3H) (Fig. S29). ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.62, 157.40, 149.00, 143.35, 137.22, 132.30, 129.95, 127.50, 125.62, 125.53, 125.23, 124.53, 122.96, 122.76, 119.61, 113.18, 110.96, 103.95, 55.73 (Fig. S30). FT- IR (KBr, cm^{-1}): 3060, 2933, 2867, 1643, 1531, 1451, 1258, 960, 925, 812, 746, 704. MS (MALDI-TOF): Calcd. for $C_{20}H_{14}ClNO_2$ 335.0, found: 335.0 [M^+] (Fig. S31).

(*E*)-5-Chloro-2-(2-(naphthalen-2-yl)vinyl)benzo[*d*]oxazole (**BOV2N**)

The synthetic method for compound **BOV2N** was similar to that of compound **BOA1N**. It was synthesized from compound 5-chloro-2-methylbenzo[*d*]oxazole (0.64 g, 3.8 mmol) and 2-naphthaldehyde (0.5 g, 3.2 mmol). The crude product was purified by column chromatography (silica gel) using ethyl acetate/petroleum ether (v/v = 1/10) as the eluent. Yellow solid of **BOV2N** (0.57 g) was obtained in a yield of 58 %. M.p.: 174.0-176.0 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.30 (s, 1H), 8.06-7.95 (m, 5H), 7.88 (d, *J* = 2.0 Hz, 1H), 7.80 (d, *J* = 8.0 Hz, 1H), 7.60-7.56 (m, 2H), 7.50-7.45 (m, 2H) (Fig. S32). ^{13}C NMR (101 MHz, DMSO-d_6) δ 164.47, 149.15, 143.54, 140.94, 134.12, 133.41, 132.82, 129.99, 129.42, 129.06, 128.93, 128.21, 127.78, 127.31, 125.92, 124.27, 119.74, 114.21, 112.45 (Fig. S33). FT- IR (KBr, cm^{-1}): 3056, 1640, 1533, 1454, 1253, 1170, 1060, 957, 933, 811, 748, 708. MS (MALDI-TOF): Calcd. for $C_{19}H_{12}NOCl$ 305.0, found: 304.9 [M^+] (Fig. S34).

(*E*)-5-Chloro-2-(2-(6-methoxynaphthalen-2-yl)vinyl)benzo[*d*]oxazole (**BOV2NM**)

The synthetic method for compound **BOV2NM** was similar to that of compound **BOV1N**. It was synthesized from compound 5-chloro-2-methylbenzo[*d*]oxazole (0.8

g, 4.8 mmol) and 6-methoxy-2-naphthaldehyde (0.74 g, 4.0 mmol). The crude product was purified by column chromatography (silica gel) using ethyl acetate/petroleum ether (v/v = 1/10) as the eluent. Yellow solid of **BOV2NM** (0.85 g) was obtained in a yield of 63 %. M.p.: 163.0-165.0 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.22 (s, 1H), 8.00-7.96 (m, 2H), 7.89 (d, J = 12.0 Hz, 3H), 7.79 (d, J = 8.0 Hz, 1H), 7.46 (d, J = 8.0 Hz, 1H), 7.42-7.38 (m, 2H), 7.23 (d, J = 8.0 Hz, 1H), 3.91 (s, 3H) (Fig. S35). ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.42, 158.81, 149.01, 143.45, 140.61, 135.53, 130.30, 130.09, 129.90, 129.25, 128.74, 127.64, 125.22, 123.77, 119.66, 119.54, 112.39, 110.94, 106.02, 55.39 (Fig. S36). FT- IR (KBr, cm^{-1}): 3072, 2946, 2847, 1626, 1530, 1450, 1277, 1178, 977, 922, 845. MS (MALDI-TOF): Calcd. for $C_{20}H_{14}ClNO_2$ 335.0, found: 334.9 [M^+] (Fig. S37).

Table S1 Single crystal data of **BOV1N**, α-type **D-BOV1N**, β-type **D-BOV1N** and **BOV1NM**.

	BOV1N	**D-BOV1N** (α-type)	**D-BOV1N** (β-type)	**BOV1NM**
Formula	C19H12ClNO	$C_{38}H_{24}Cl_2N_2O_2$	$C_{38}H_{24}N_2O_2Cl_2$	$C_{20}H_{14}ClNO_2$
Formula weight	305.75	611.49	611.49	335.77
Space group	C2/c	P-1	P-1	P-1
Crystal system	Monoclinic	Triclinic	Triclinic	Triclinic
a (Å)	23.323(2)	9.8015(4)	10.2664(4)	3.9720(3)
b (Å)	3.8319(3)	12.0723(6)	11.4804(4)	12.2566(7)
c (Å)	31.479(3)	12.9926(6)	13.9234(6)	16.4309(11)
α (deg)	90.000	71.138(2)	106.434(2)	79.392(4)
β (deg)	90.288(4)	85.828(2)	108.935(2)	86.478(4)
γ (deg)	90.000	79.452(2)	99.360(2)	84.244(4)
V ($Å^3$)	2813.2(5)	1430.08(11)	1429.08(10)	781.52(9)
Z	8	2	2	2
D_{calc}(g/cm^3)	1.444	1.420	1.421	1.427
μ (mm^{-1})	0.272	0.267	0.268	0.26
Final R indices	R1 = 0.0604	0.0579	0.0378	0.0467
[I>2sigma(I)]	wR2 = 0.1146	0.1513	0.0919	0.1142
R indices(all data)	R1 = 0.0751	0.0707	0.0465	0.0804
	wR2 = 0.1195	0.1581	0.0973	0.1008
GoF	1.228	1.148	1.020	1.022
CCDC	1904295	1887614	1888929	1879572

Table S2 Photophysical data of **BOV1N**, **BOV1NF**, **BOV1NM**, **BOV2N** and **BOV2NM** in cyclohexane.

Compound	Absorption [a] (nm) (ε / × 10^4 $M^{-1}cm^{-1}$)	Emission [b] (nm)	Φ_F [c]
BOV1N	255 (1.7), 349 (2.0)	420, 443 (shoulder)	0.20
BOV1NF	265 (1.2), 338 (1.4)	424, 448 (shoulder)	0.12
BOV1NM	296 (0.9), 363 (2.1)	450, 473 (shoulder)	0.11
BOV2N	263 (1.7), 341 (3.0)	395, 413 (shoulder)	0.33
BOV2NM	284 (1.1), 354 (3.6)	410, 428 (shoulder)	0.31

[a] Measured in cyclohexane (1.0×10^{-5} M); [b] Excited at 350 nm; [c] The fluorescence quantum yields were determined against quinine sulfate in 0.1 M H_2SO_4 (Φ_F = 0.577) as a standard excited at 350 nm.

Table S3 Calculated attachment energies (E_{att}) for different crystalline planes in the single crystal of **BOV1N**.

hkl	Multiplicity	d_{hkl} / Å	Eatt (total) / kcal·mol^{-1}	Total facet area/ %
(0 0 2)	2	15.739	-60.740	50.072
(2 0 0)	2	11.661	-82.428	34.823
(2 0 2)	2	9.347	-96.614	3.617
(1 1 0)	4	3.781	-283.710	9.220
(1 1 -1)	4	3.755	-286.458	2.092
(1 1 1)	4	3.754	-288.640	0.176

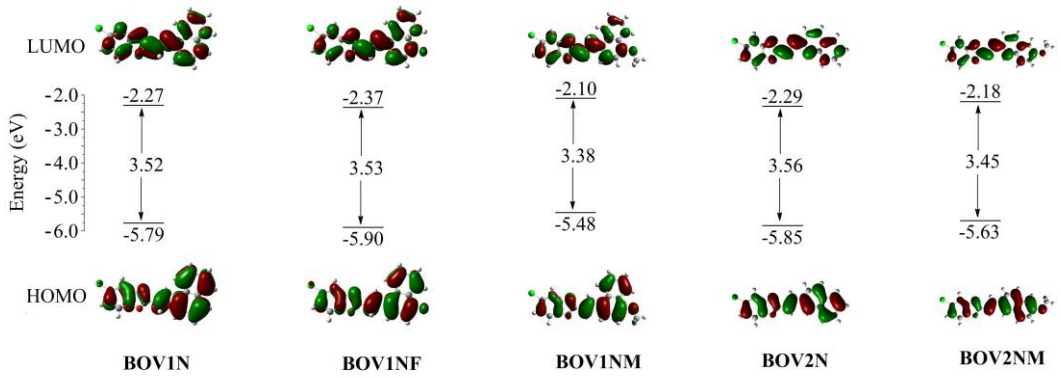

Figure S1 The frontier orbital plots and energy levels for the HOMOs and LUMOs of **BOV1N**, **BOV1NF**, **BOV1NM**, **BOV2N** and **BOV2NM**.

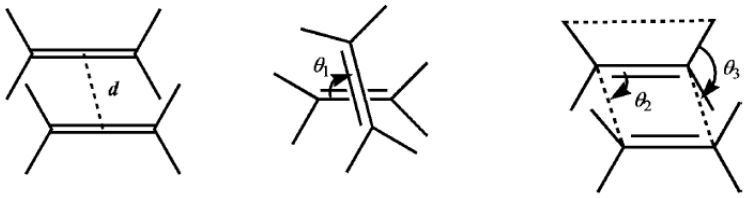

Figure S2 Definitions of the parameters usually considered to be geometric criteria for [2+2] photodimerization of double bonds; θ_1 corresponds to the rotational angle of one double bond with respect to the other; θ_2 corresponds to the obtuse angle of the parallelogram formed by double bond carbons; θ_3 is the angle between the alkene substituents and cyclobutane planes; *d* is the bond-center-to-bond-center distance of the potentially reactant double bonds and the line joining the nearest carbons in "olefin pair".

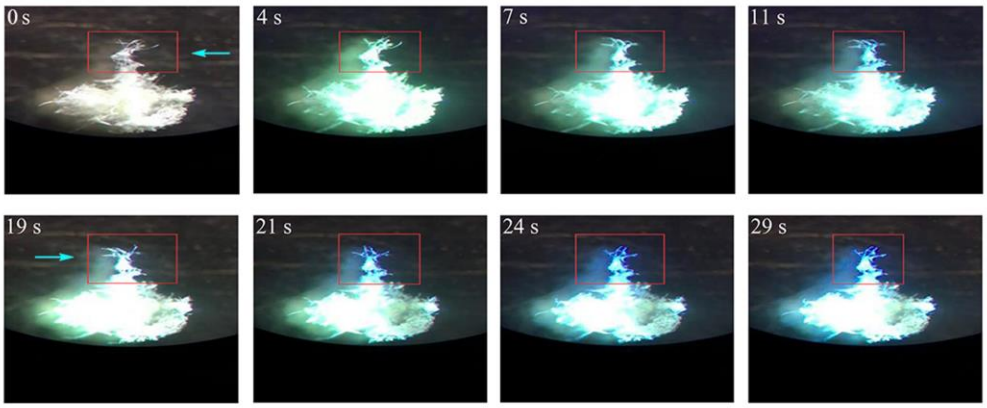

Figure S3 Optical microscope images of the organogel fibers of **BOV1N** before and after irradiation by 365 nm light (3 W) for different times (the arrows indicate the irradiation direction).

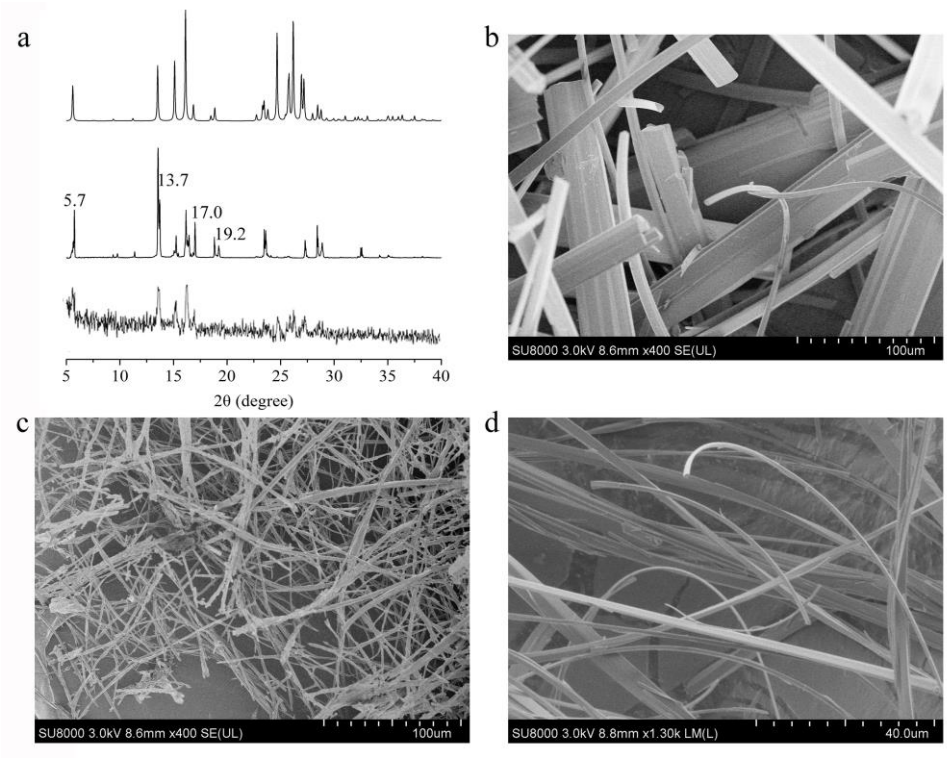

Figure S4 (a) PXRD patterns simulated from single crystal (upper), the crystal (middle) and the xerogel (lower) of **BOV1N**; SEM images of (b) needle-like crystals of **BOV1N**, (c) xerogel of **BOV1N** obtained from *n*-hexane and (d) fibrous-like crystals of **BOV1NF**.

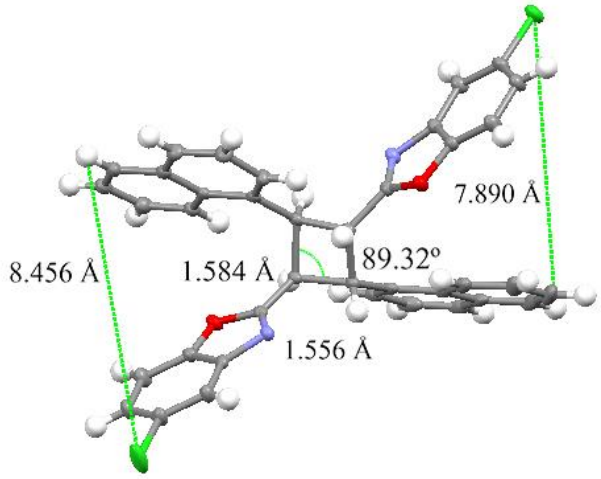

Figure S5 The molecular configuration of **D-BOV1N** (α-type, centrosymmetric manner) in single crystal.

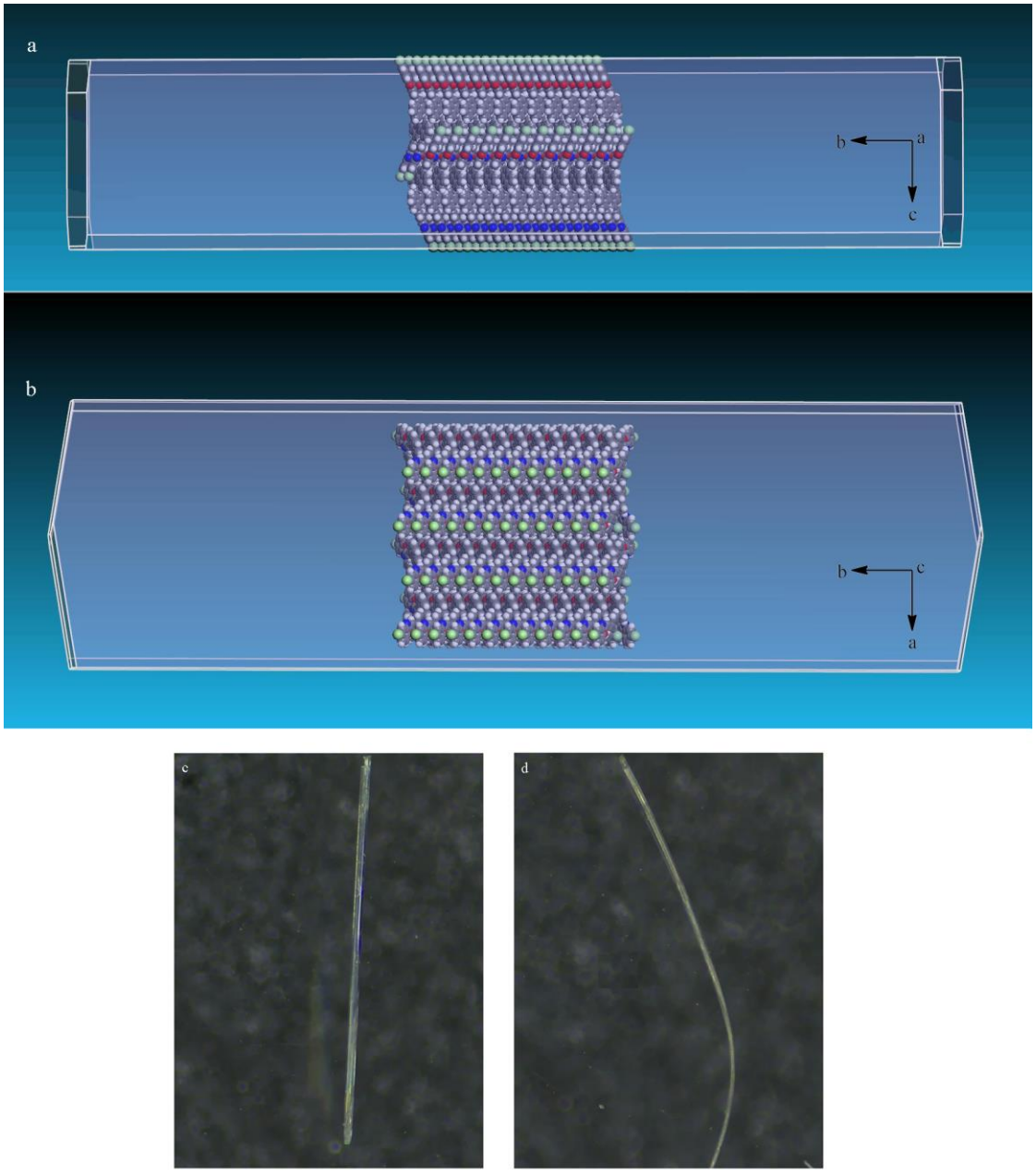

Figure S6 Calculated growth morphology of **BOV1N** in single crystal (a, b) and microscopic images showing the widest face (c) and the bending of the widest face (d) of **BOV1N** crystal.

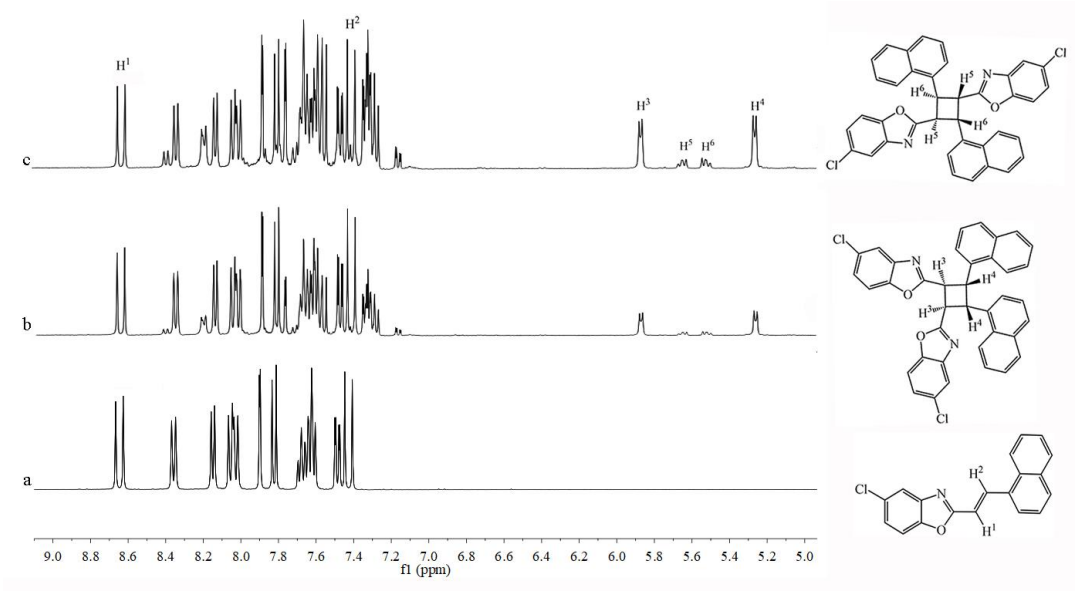

Figure S7 ^{1}H NMR (400 M) spectra of **BOV1N** before (a) irradiation and after irradiation of xerogels for 2 min (b, xerogel) and 5 min (c, xerogel) by 365 nm (3 W), followed by dissolving in DMSO-d_6.

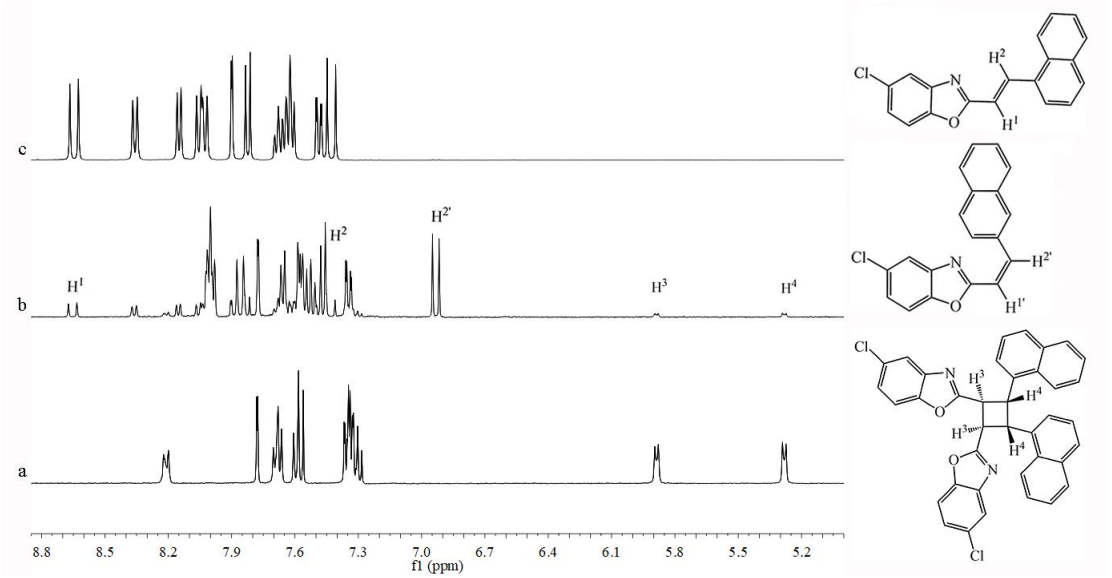

Figure S8 ^{1}H NMR (400 M) spectra of β-type **D-BOV1N** before (a) and after (b) irradiation for 30 h by 254 nm (6 W) in DMSO-d_6, and (c) ^{1}H NMR spectrum of **BOV1N** in DMSO-d_6.

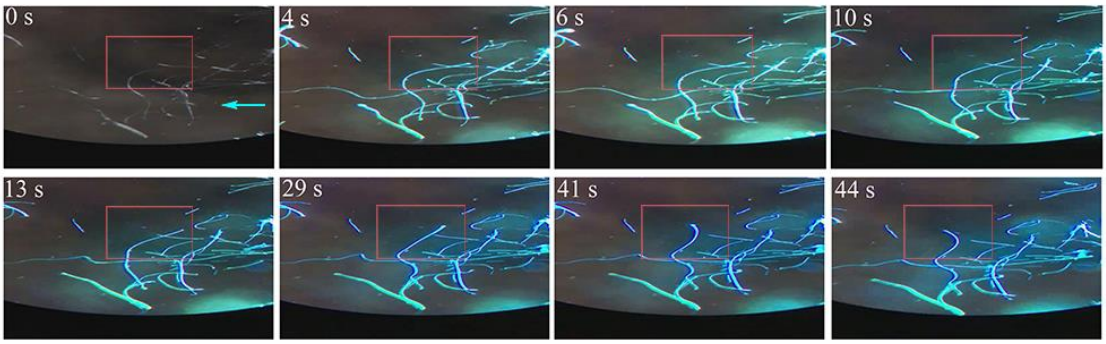

Figure S9 Optical microscope images of fibers of **BOV1NF** before and after irradiation by 365 nm light (3 W) for different times (the arrows indicate the irradiation direction).

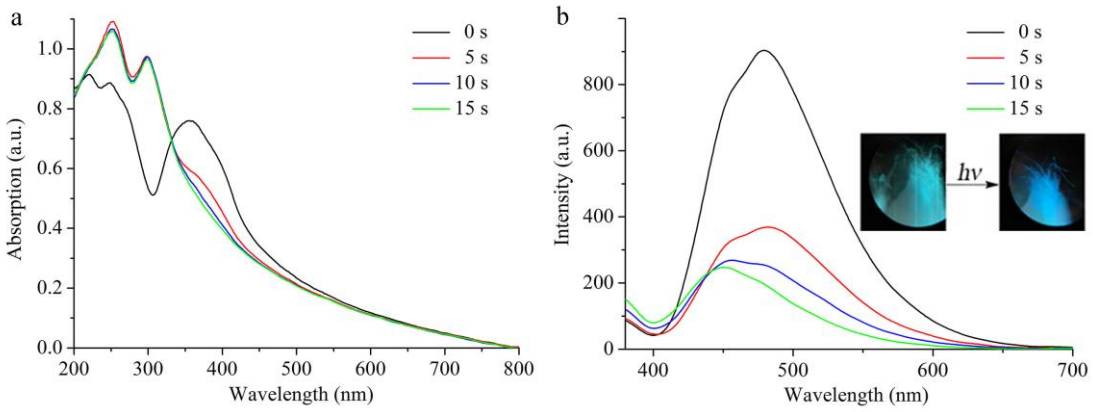

Figure S10 UV-vis absorption (a) and fluorescence emission (b, λ_{ex} = 350 nm) spectra of **BOV1NF** in fibers before and after irradiation by 365 nm light (3 W) for different times. Inset in Figure S8b: photos of fibers of **BOV1NF** before (left) and after irradiated by 365 nm light for 15 s (right).

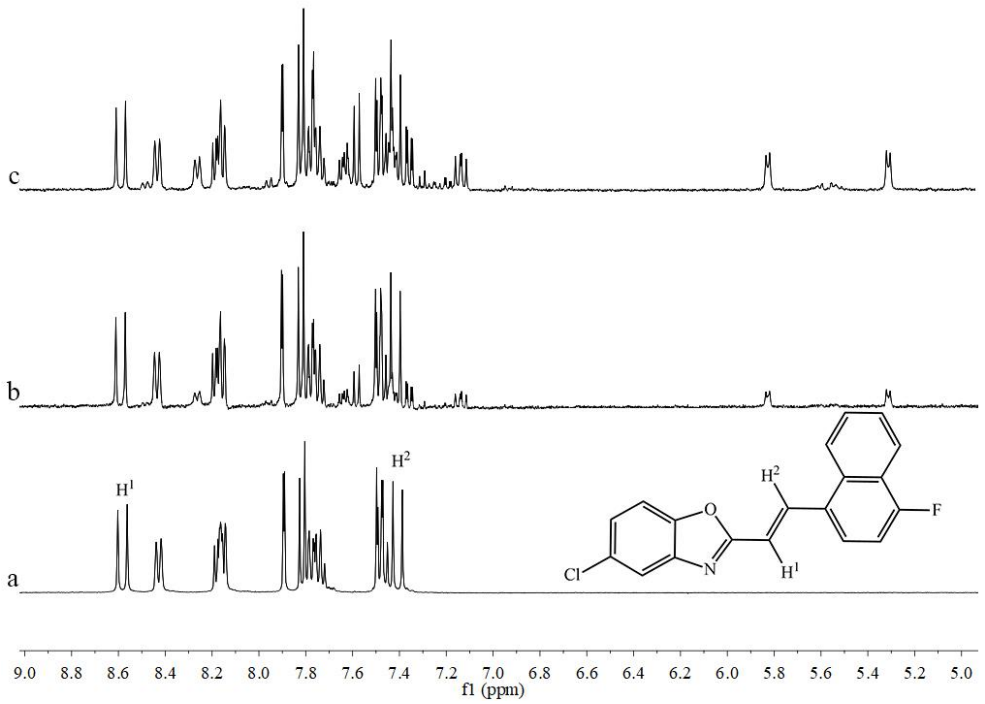

Figure S11 ^{1}H NMR (400 M) spectra of **BOV1NF** (a) before irradiation and after irradiation of crystals for (b) 2 min and (c) 5 min by 365 nm (3 W), followed by dissolving in DMSO-d_6.

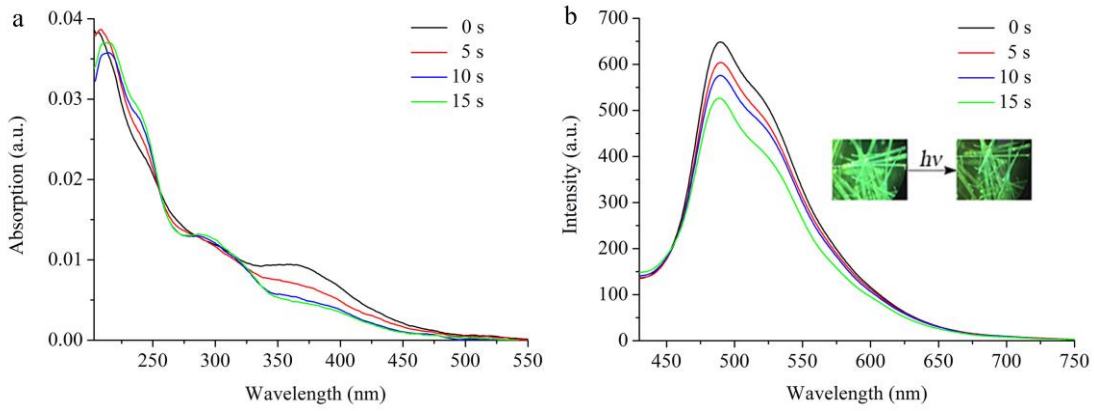

Figure S12 UV-vis absorption (a) and fluorescence emission (b, λ_{ex} = 350 nm) spectra of **BOV1NM** in microcrystals before and after irradiation by 365 nm light (3 W) for different times. Inset in Figure S10b: photos of xerogel of **BOV1NM** under UV light (left: before irradiation, right: after irradiation by 365 nm for 15 s).

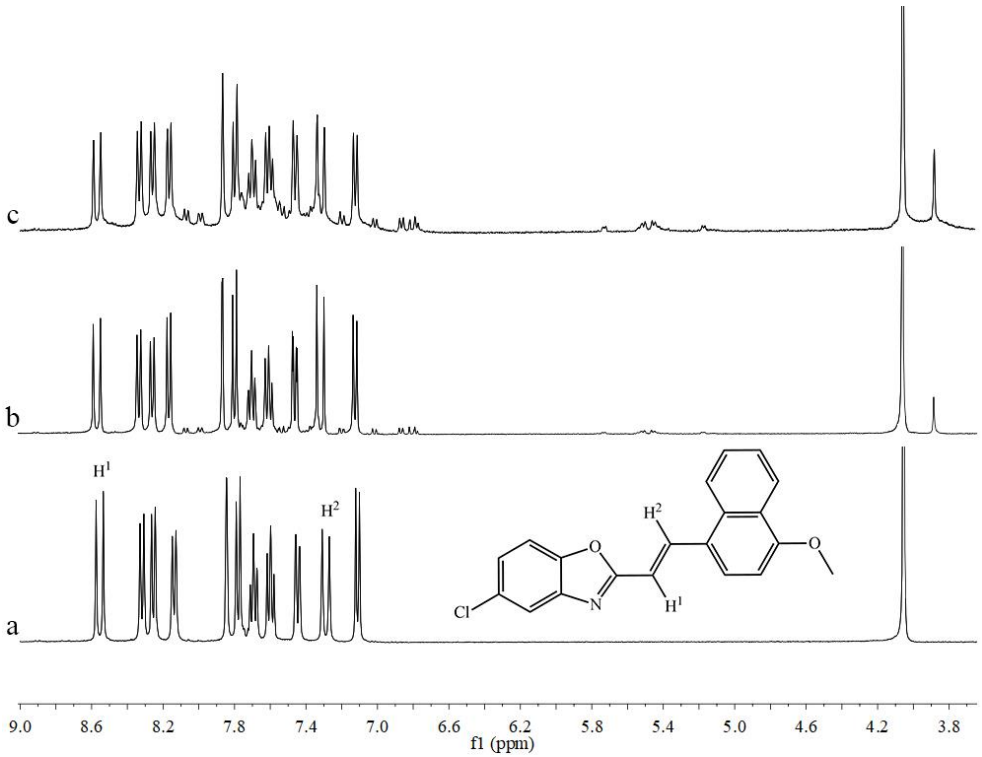

Figure S13 ^{1}H NMR (400 M) spectra of **BOV1NM** (a) before irradiation and after irradiation of crystals for (b) 2 min and (c) 5 min by 365 nm (3 W), followed by dissolving in DMSO-d_6.

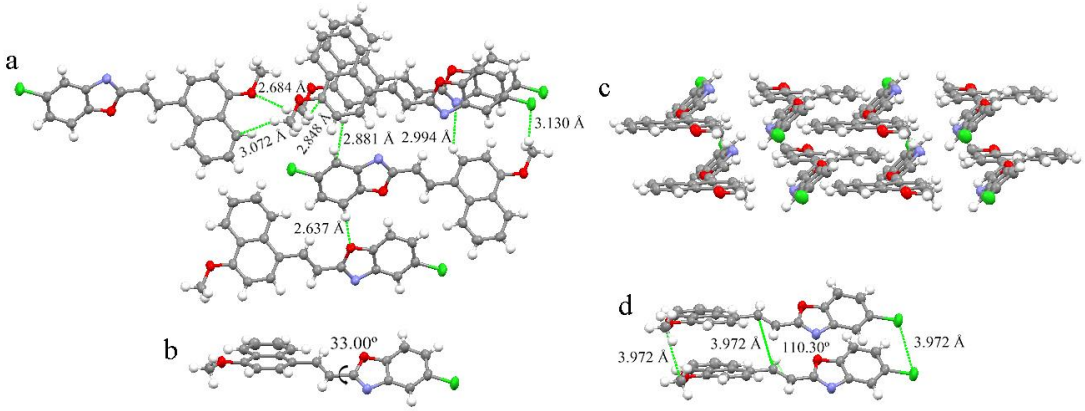

Figure S14 (a) The H-bondings and the C-H···π intermolecular interactions in singel crystal; (b) the single crystal structure of **BOV1NM** viewed along b-axis; (c) the dihedral angle between the naphthyl and benzoxazole planes and (d) the angle and distance between one of the potentially reactant double bonds and the line joining the nearest carbons in "olefin pairs".

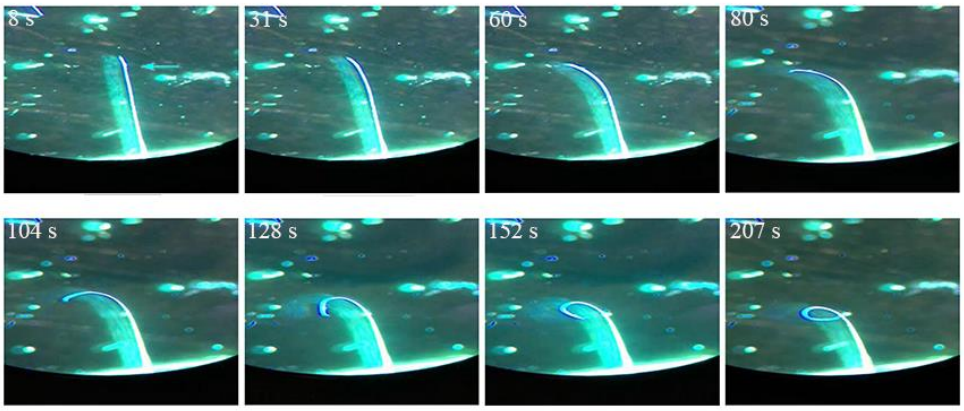

Figure S15 Optical microscope images of the nonuniform fiber of **BOV2N** before and after irradiation by 365 nm light (3 W) for different times (the arrows indicate the irradiation direction).

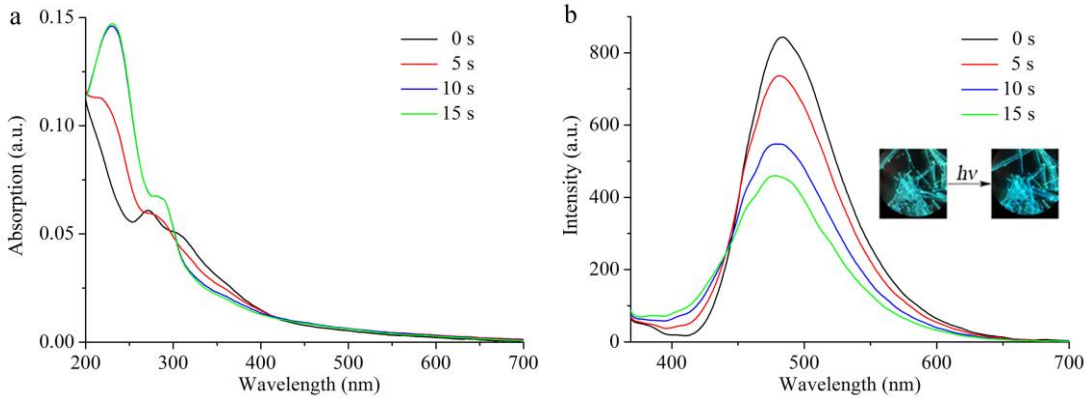

Figure S16 UV-vis absorption (a) and fluorescence emission (b, λ_{ex} = 350 nm) spectra of **BOV2N** in microcrystals before and after irradiation by 365 nm (3 W) light for different times. Inset in Figure S14b: photos of crystals of **BOV2N** under UV light (left: before irradiation, right: after irradiation by 365 nm for 15 s).

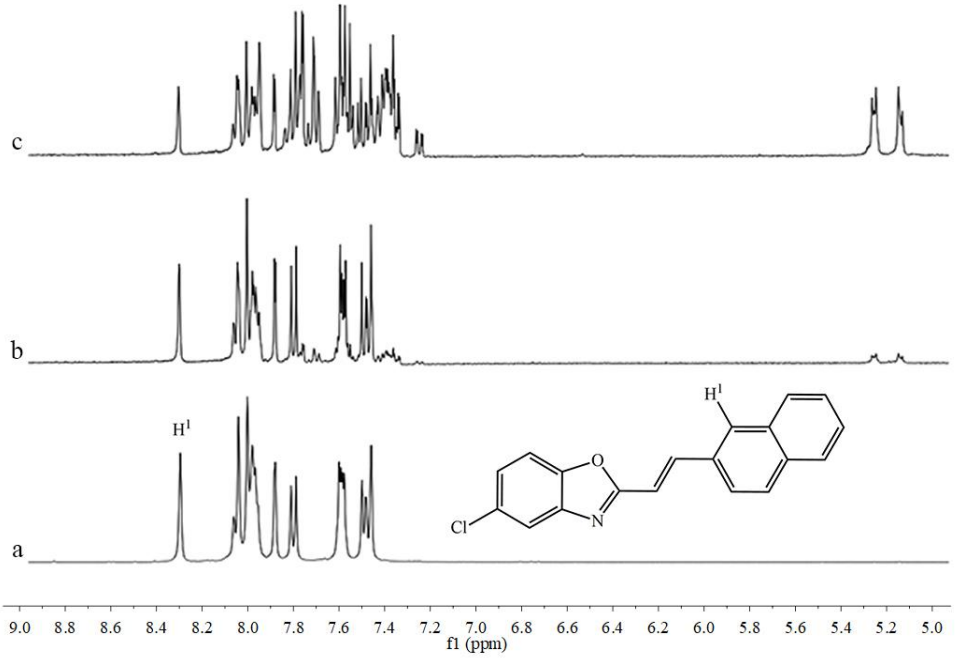

Figure S17 ^{1}H NMR (400 M) spectra of **BOV2N** (a) before irradiation and after irradiation of crystals for (b) 2 min and (c) 5 min by 365 nm (3 W), followed by dissolving in DMSO-d_6.

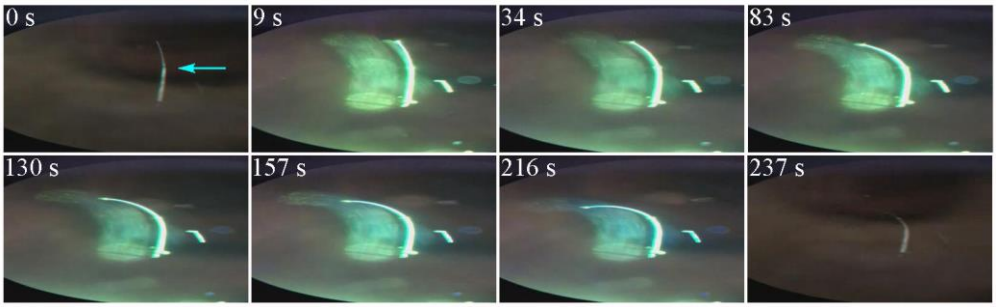

Figure S18 Optical microscope images of the nonuniform fiber of **BOV2NM** before and after irradiation by 365 nm light (3 W) for different times (the arrows indicate the irradiation direction).

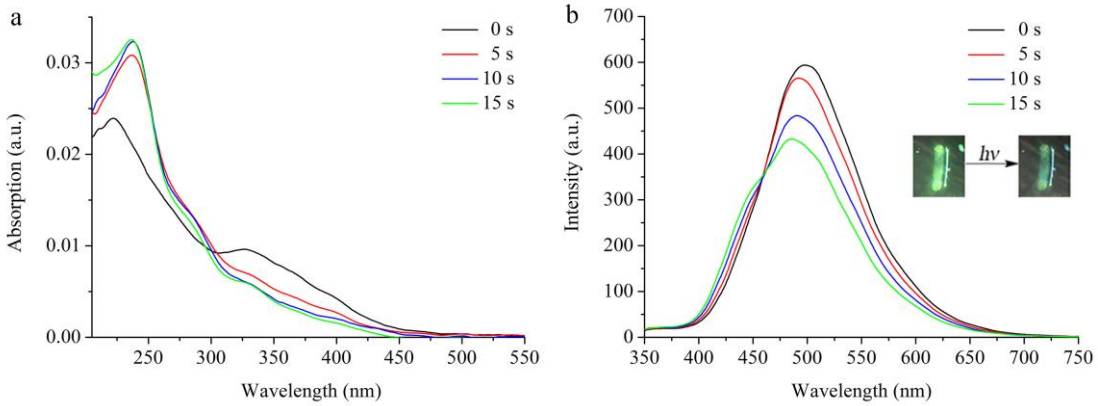

Figure S19 UV-vis absorption (a) and fluorescence emission (b, λ_{ex} = 350 nm) spectra of **BOV2NM** in crystals before and after irradiation by 365 nm light (3 W) for different times. Inset in Figure S17b: photos of crystals of **BOV2NM** under UV light (left: before irradiation, right: after irradiation by 365 nm for 15 s).

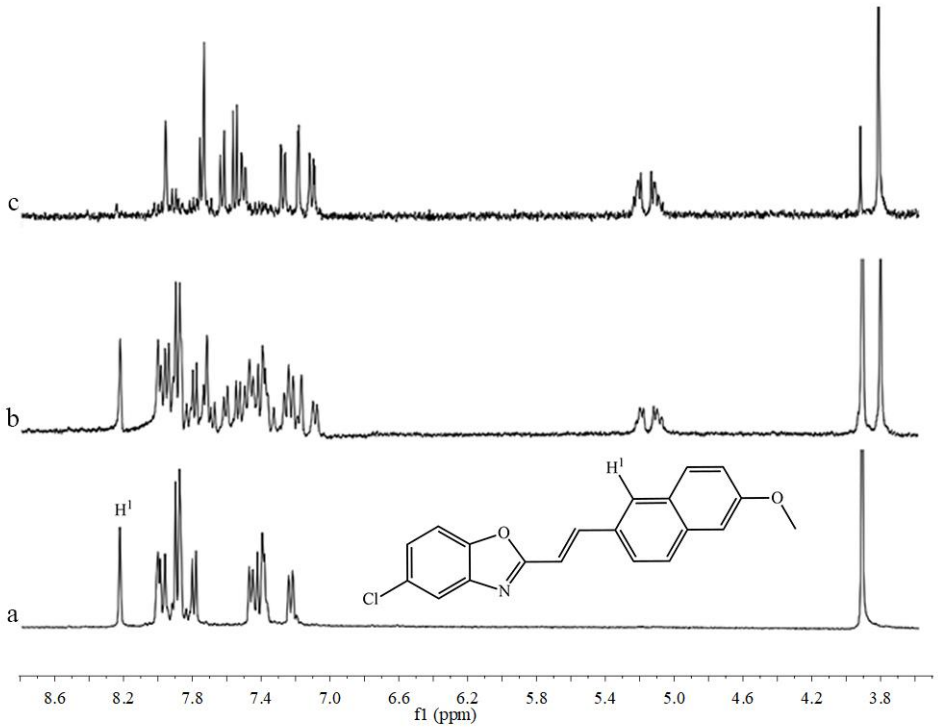

Figure S20 ^{1}H NMR (400 M) spectra of **BOV2NM** (a) before irradiation and after irradiation of crystals for (b) 2 min and (c) 5 min by 365 nm (3 W), followed by dissolving in DMSO-d_6.

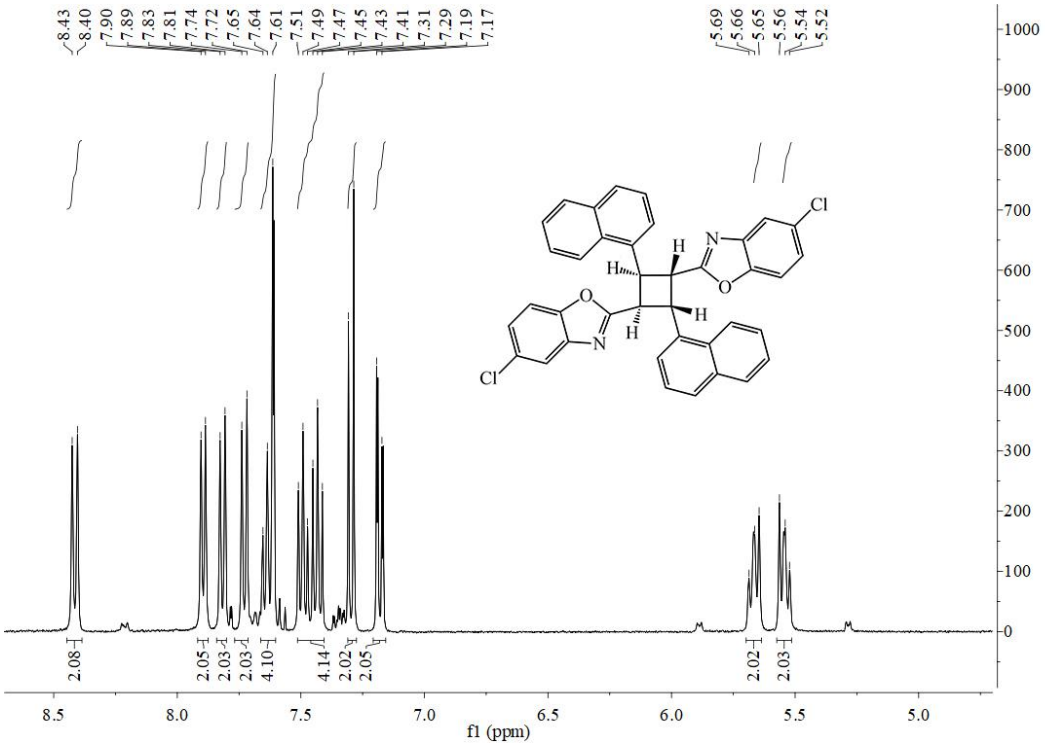

Figure S21 ^{1}H NMR (400 MHz) spectrum of α-type **D-BOV1N** in DMSO-d_6.

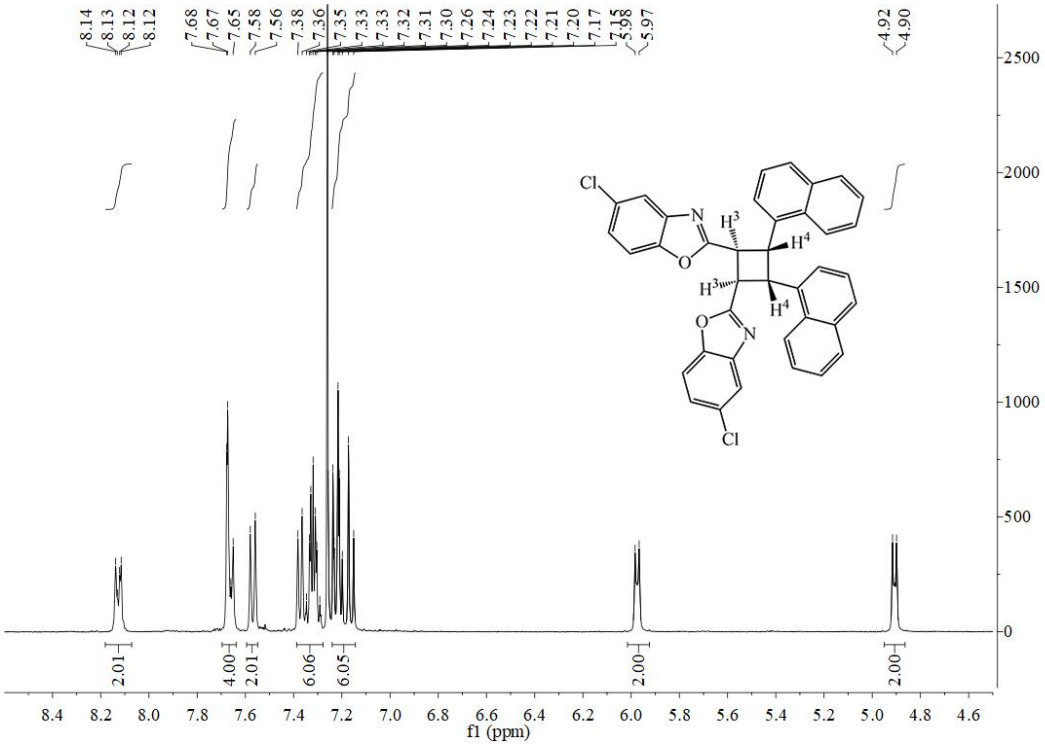

Figure S22 ^{1}H NMR (400 MHz) spectrum of β-type **D-BOV1N** in $CDCl_3$.

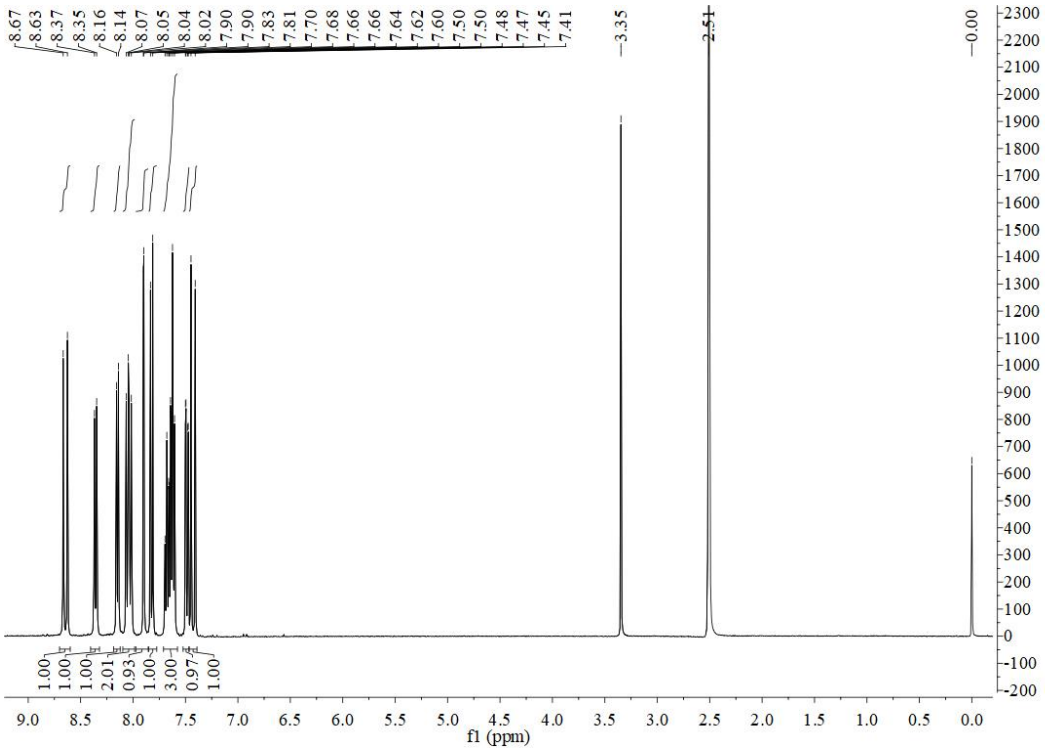

Figure S23 ^{1}H NMR (400 MHz) spectrum of **BOV1N** in DMSO-d_6.

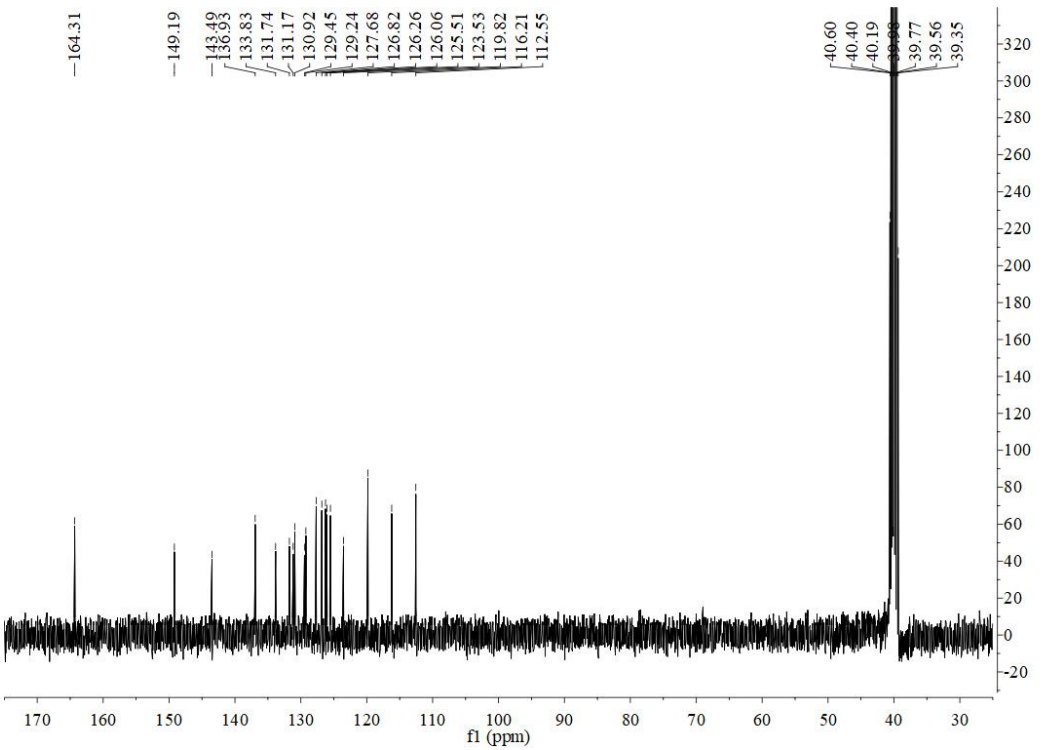

Figure S24 ^{13}C NMR (101 MHz) spectrum of **BOV1N** in DMSO-d_6.

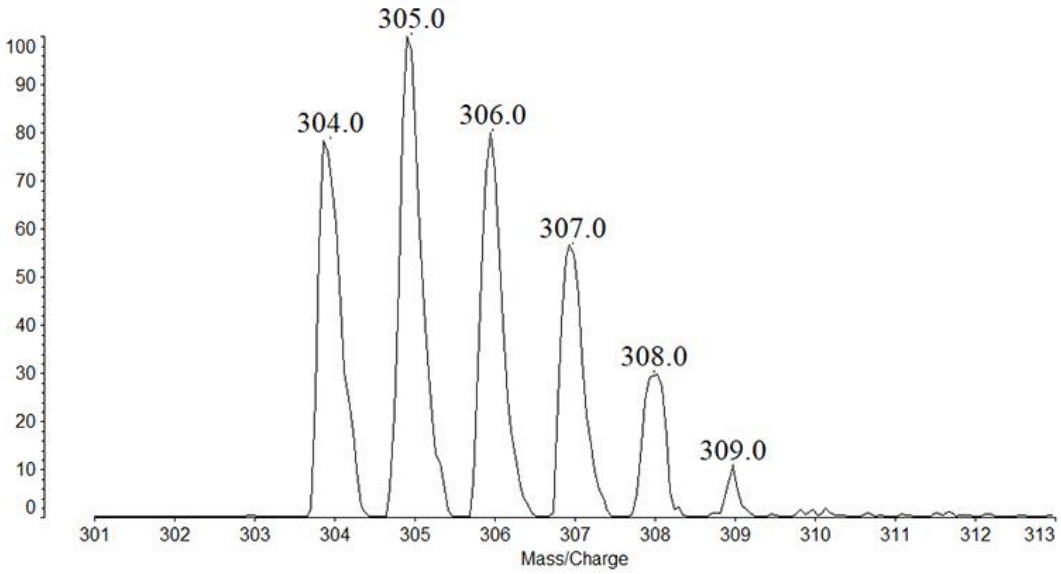

Figure S25 MALDI-TOF mass spectrum of **BOV1N**.

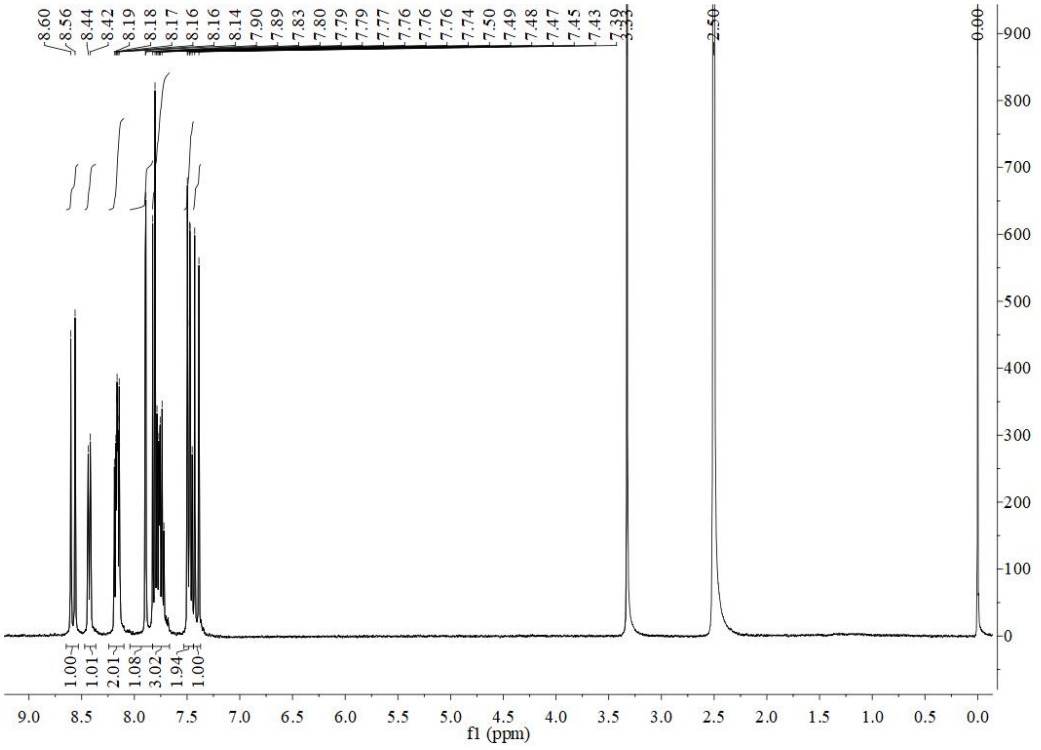

Figure S26 ^{1}H NMR (400 MHz) spectrum of **BOV1NF** in DMSO-d_6.

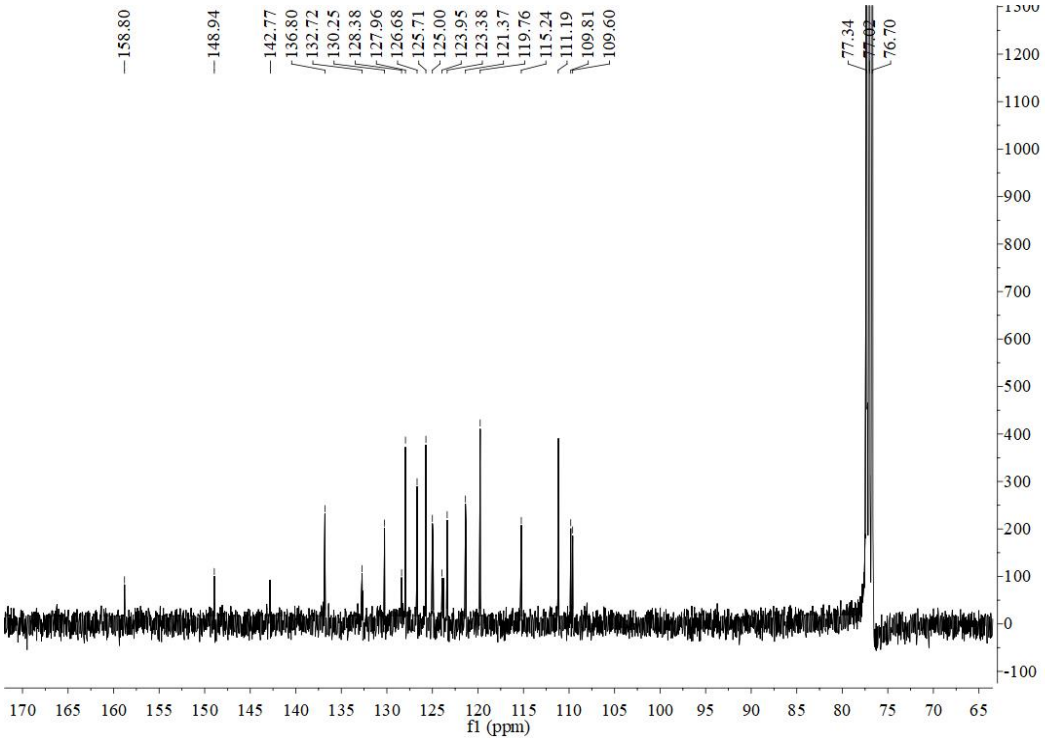

Figure S27 ^{13}C NMR (101 MHz) spectrum of **BOV1NF** in $CDCl_3$.

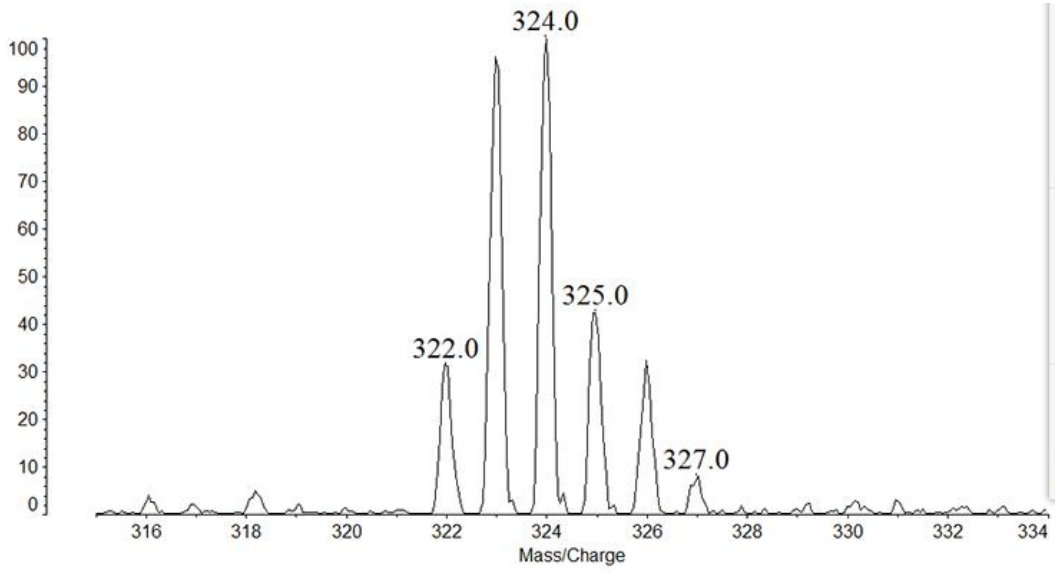

Figure S28 MALDI-TOF mass spectrum of **BOV1NF**.

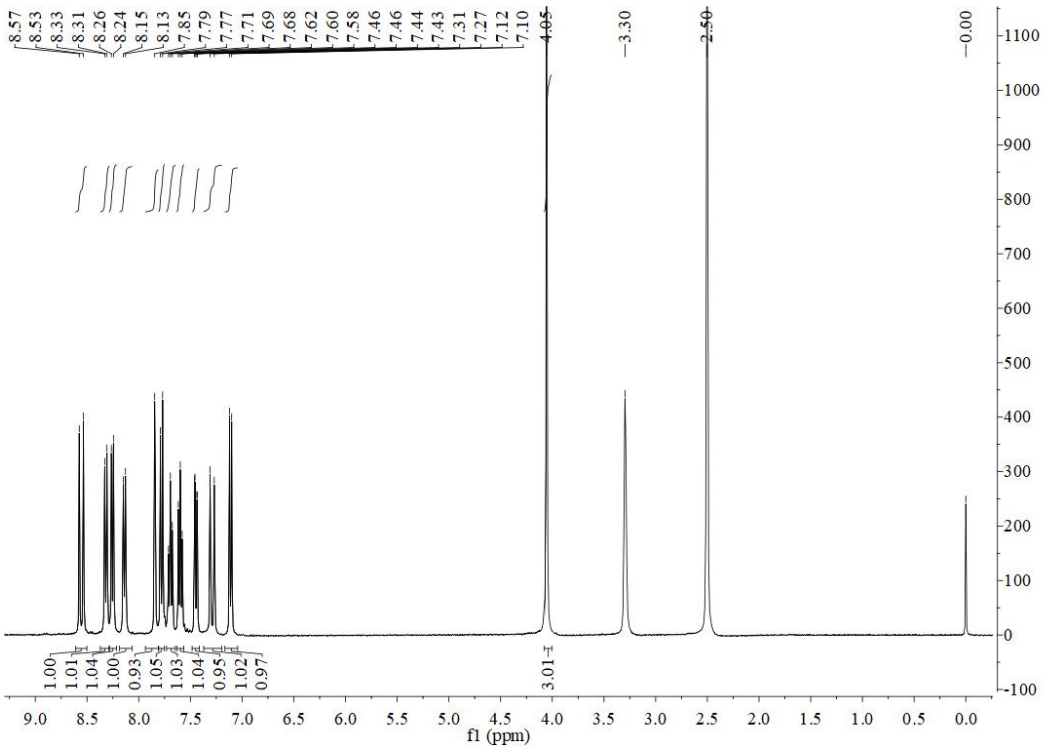

Figure S29 ^{1}H NMR (400 MHz) spectrum of **BOV1NM** in DMSO-d_6.

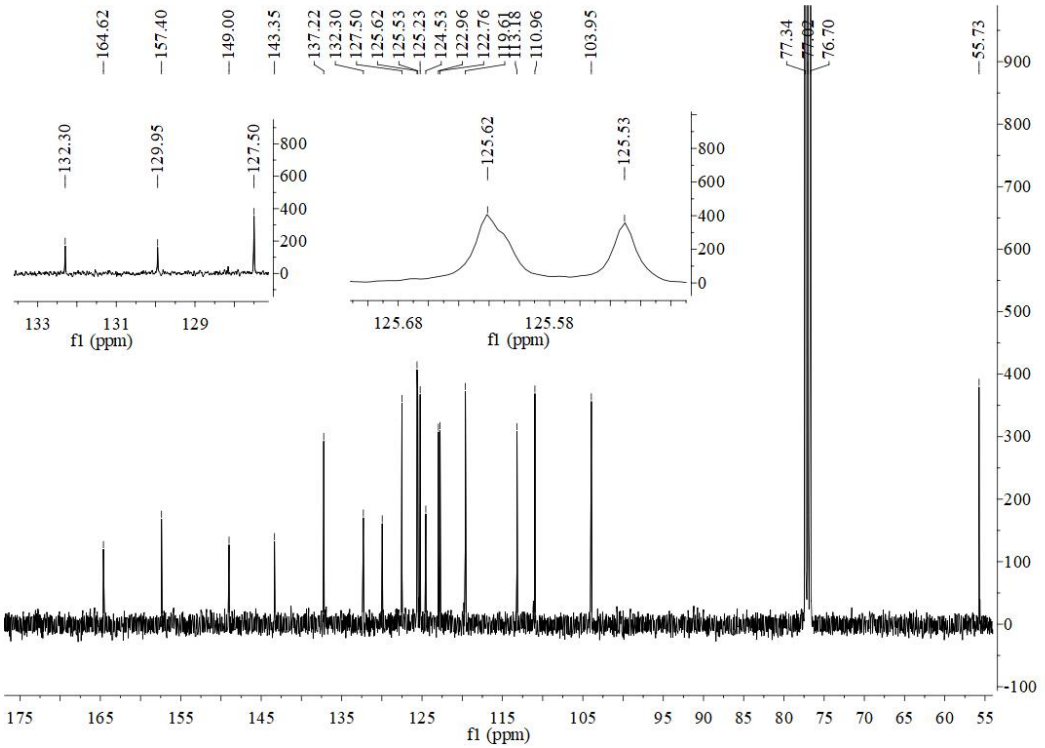

Figure S30 ^{13}C NMR (101 MHz) spectrum of **BOV1NM** in $CDCl_3$.

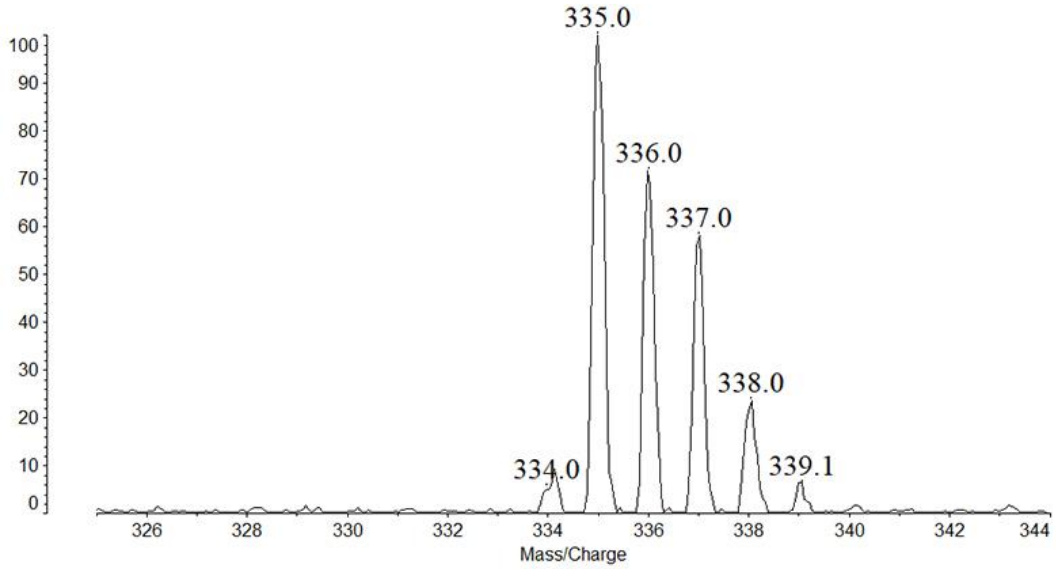

Figure S31 MALDI-TOF mass spectrum of **BOV1NM**.

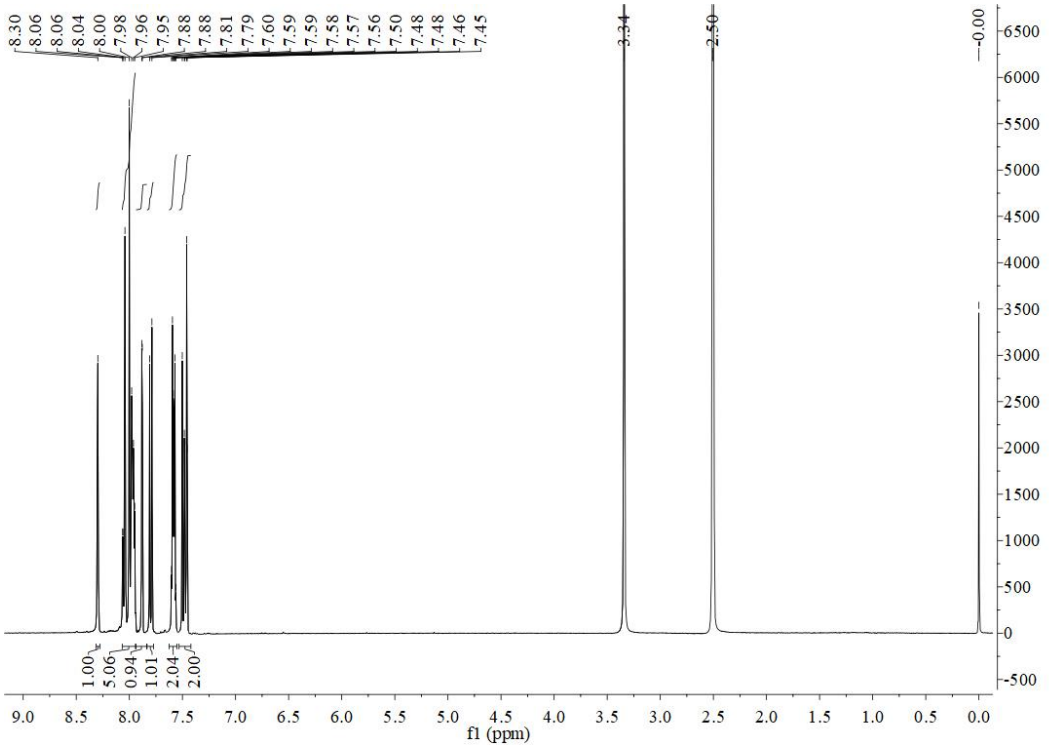

Figure S32 ^{1}H NMR (400 MHz) spectrum of **BOV2N** in DMSO-d_6.

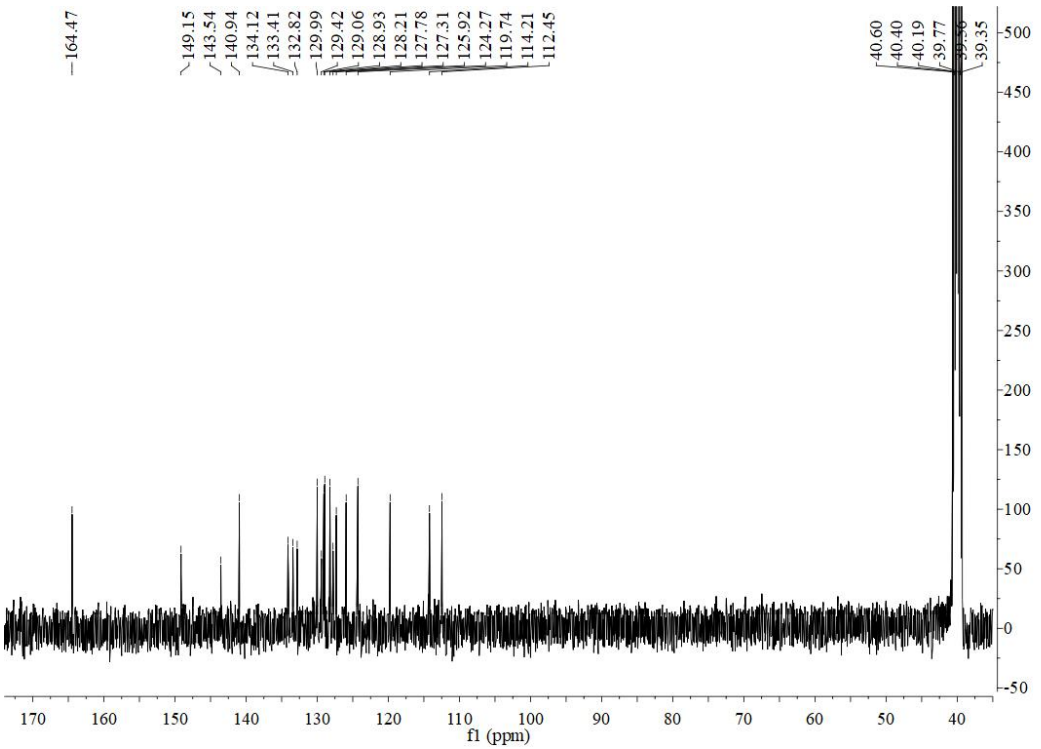

Figure S33 ^{13}C NMR (101 MHz) spectrum of **BOV2N** in DMSO-d_6.

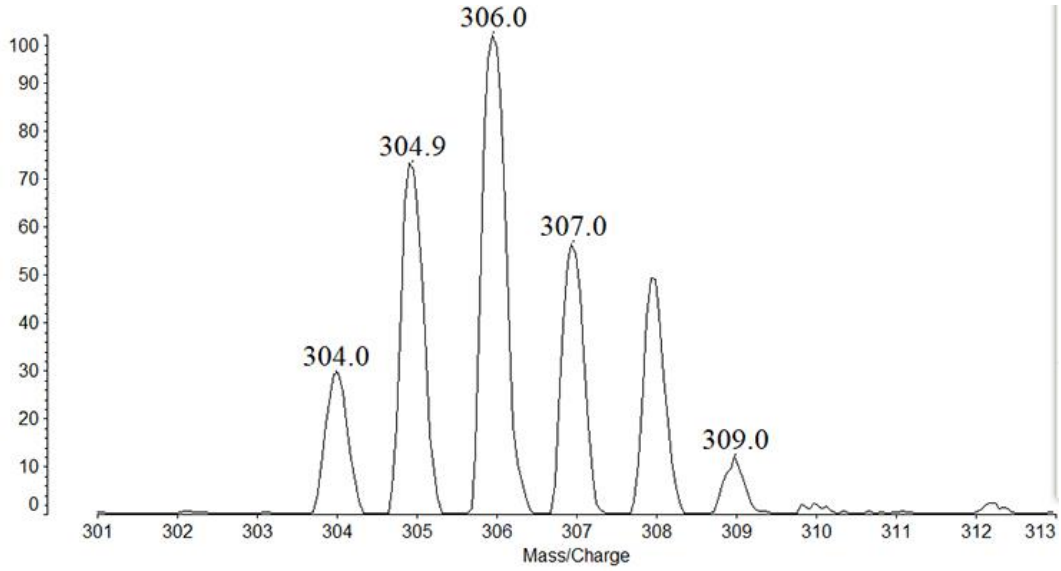

Figure S34 MALDI-TOF mass spectrum of **BOV2N**.

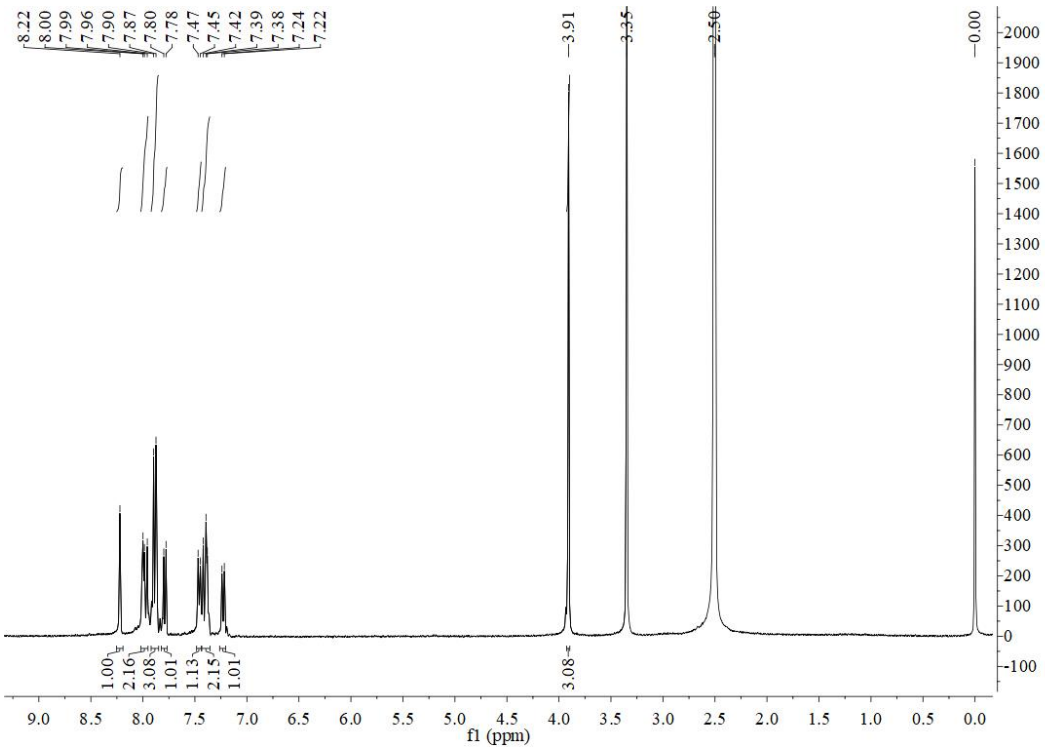

Figure S35 ^{1}H NMR (400 MHz) spectrum of **BOV2NM** in DMSO-d_6.

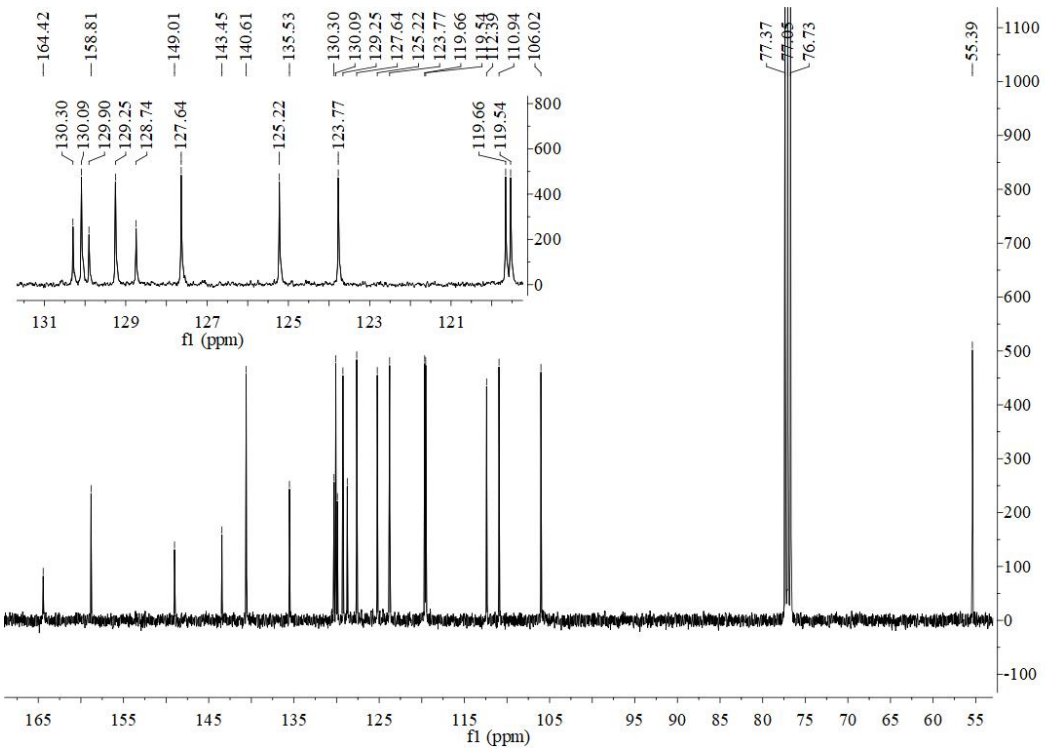

Figure S36 ^{13}C NMR (101 MHz) spectrum of **BOV2NM** in $CDCl_3$.

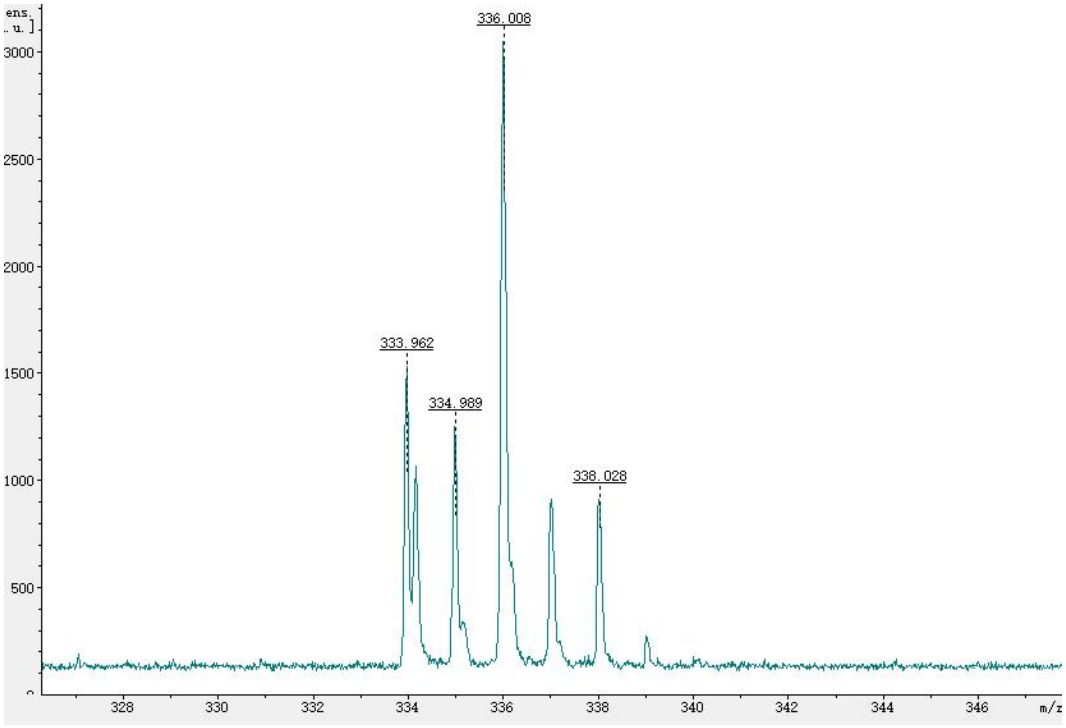

Figure S37 MALDI-TOF mass spectrum of **BOV2NM**.

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) BOV1N

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: BOV1N

```
Bond precision:  C-C = 0.0029 A          Wavelength=0.71073

Cell:            a=23.323(2)     b=3.8319(3)         c=31.479(3)
                 alpha=90        beta=90.288(4)      gamma=90
Temperature:     149 K
```

	Calculated	Reported
Volume	2813.3(4)	2813.2(5)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C19 H12 Cl N O	C19 H12 Cl N O
Sum formula	C19 H12 Cl N O	C19 H12 Cl N O
Mr	305.75	305.75
Dx,g cm-3	1.444	1.444
Z	8	8
Mu (mm-1)	0.272	0.272
F000	1264.0	1264.0
F000’	1265.65	
h,k,lmax	32,5,43	32,5,43
Nref	3986	3978
Tmin,Tmax	0.965,0.971	
Tmin’	0.965	

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Correction method= Not given

Data completeness= 0.998          Theta(max)= 29.653

R(reflections)= 0.0604( 3383)     wR2(reflections)= 0.1195( 3978)

S = 1.228                 Npar= 199
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The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

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PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......     10.648 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.292 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).          5 Note
```

Alert level G

```
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large       5.61 Why ?
PLAT398_ALERT_2_G Deviating  C-O-C    Angle From 120 for O1             103.8 Degree
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600          3 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         16 Info
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   3 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   4 ALERT level G = General information/check it is not something unexpected

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   3 ALERT type 2 Indicator that the structure model may be wrong or deficient
   3 ALERT type 3 Indicator that the structure quality may be low
   1 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

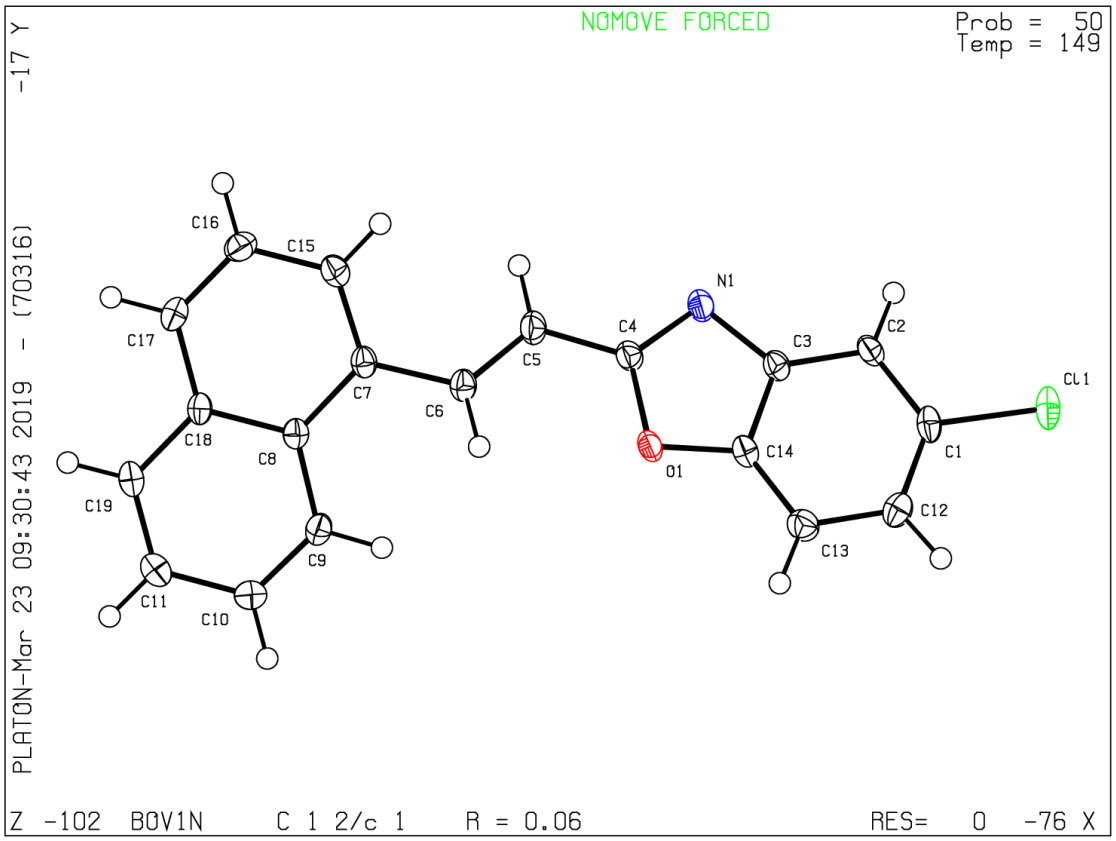
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 17/03/2019; check.def file version of 04/03/2019

Datablock BOV1N - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) D-BOV1N

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: D-BOV1N

```
Bond precision:  C-C = 0.0050 A          Wavelength=0.71073

Cell:          a=9.8015(4)       b=12.0723(6)     c=12.9926(6)
               alpha=71.138(2)   beta=85.828(2)   gamma=79.452(2)
Temperature:   100 K
```

	Calculated	Reported
Volume	1430.08(11)	1430.08(11)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C38 H24 Cl2 N2 O2	C38 H24 Cl2 N2 O2
Sum formula	C38 H24 Cl2 N2 O2	C38 H24 Cl2 N2 O2
Mr	611.49	611.49
Dx,g cm-3	1.420	1.420
Z	2	2
Mu (mm-1)	0.267	0.267
F000	632.0	632.0
F000’	632.83	
h,k,lmax	12,15,16	12,15,16
Nref	6562	6516
Tmin,Tmax	0.963,0.968	
Tmin’	0.963	

```
Correction method= Not given

Data completeness= 0.993          Theta(max)= 27.486

R(reflections)= 0.0579( 5450)     wR2(reflections)= 0.1581( 6516)

S = 1.148                 Npar= 398
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The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

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PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ..............      0.005 Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact  H5       ..H34      .       1.92 Ang.
                                                    x,y,z  =      1_555 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).          8 Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         25 Report
```

Alert level G

```
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)      0.002 Degree
PLAT398_ALERT_2_G Deviating  C-O-C    Angle From 120 for O1             103.5 Degree
PLAT398_ALERT_2_G Deviating  C-O-C    Angle From 120 for O2             103.7 Degree
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............          5 Note
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed ..          ! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         15 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....          2 Note
PLAT931_ALERT_5_G CIFcalcFCF  Twin Law ( 0 0 1)         Est.d BASF       0.09 Check
```

---

0 **ALERT level A** = Most likely a serious problem - resolve or explain
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A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica, Journal of Applied Crystallography, Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

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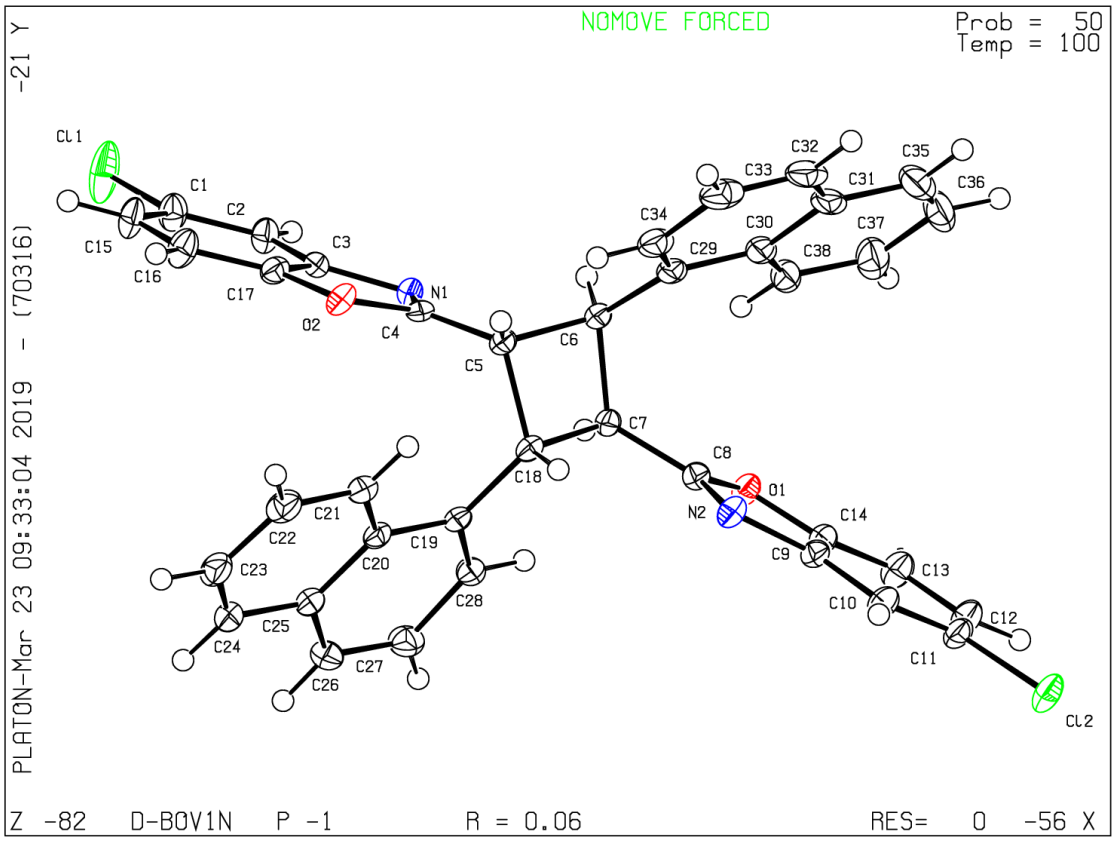
PLATON version of 17/03/2019; check.def file version of 04/03/2019

Datablock D-BOV1N - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) D-BOV1N

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: D-BOV1N

Bond precision: C-C = 0.0018 A Wavelength=0.71073

Cell: a=10.2664(4) b=11.4804(4) c=13.9234(6)
alpha=106.434(2) beta=108.935(2) gamma=99.360(2)
Temperature: 100 K

	Calculated	Reported
Volume	1429.08(10)	1429.08(10)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C38 H24 Cl2 N2 O2	C38 H24 Cl2 N2 O2
Sum formula	C38 H24 Cl2 N2 O2	C38 H24 Cl2 N2 O2
Mr	611.49	611.49
Dx,g cm-3	1.421	1.421
Z	2	2
Mu (mm-1)	0.268	0.268
F000	632.0	632.0
F000’	632.83	
h,k,lmax	14,16,19	14,16,19
Nref	8732	8704
Tmin,Tmax	0.966,0.971	
Tmin’	0.966	

Correction method= Not given

Data completeness= 0.997 Theta(max)= 30.514

R(reflections)= 0.0378(7428) wR2(reflections)= 0.0973(8704)

S = 1.020 Npar= 397

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

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PLAT410_ALERT_2_C Short Intra H...H Contact  H7       ..H29      .       1.98 Ang.
                                                    x,y,z  =      1_555 Check
PLAT480_ALERT_4_C Long H...A H-Bond Reported H14      ..CL2      .       2.96 Ang.
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).          7 Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600          3 Report
```

Alert level G

```
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)      0.002 Degree
PLAT398_ALERT_2_G Deviating  C-O-C    Angle From 120 for O1             103.2 Degree
PLAT398_ALERT_2_G Deviating  C-O-C    Angle From 120 for O2             103.6 Degree
PLAT793_ALERT_4_G Model has Chirality at C6          (Centro SPGR)          R Verify
PLAT793_ALERT_4_G Model has Chirality at C7          (Centro SPGR)          S Verify
PLAT793_ALERT_4_G Model has Chirality at C8          (Centro SPGR)          R Verify
PLAT793_ALERT_4_G Model has Chirality at C20         (Centro SPGR)          S Verify
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         18 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....          3 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         22 Info
```

```
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   0 ALERT level B = A potentially serious problem, consider carefully
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  10 ALERT level G = General information/check it is not something unexpected

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   4 ALERT type 2 Indicator that the structure model may be wrong or deficient
   3 ALERT type 3 Indicator that the structure quality may be low
   6 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

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Publication of your CIF in other journals

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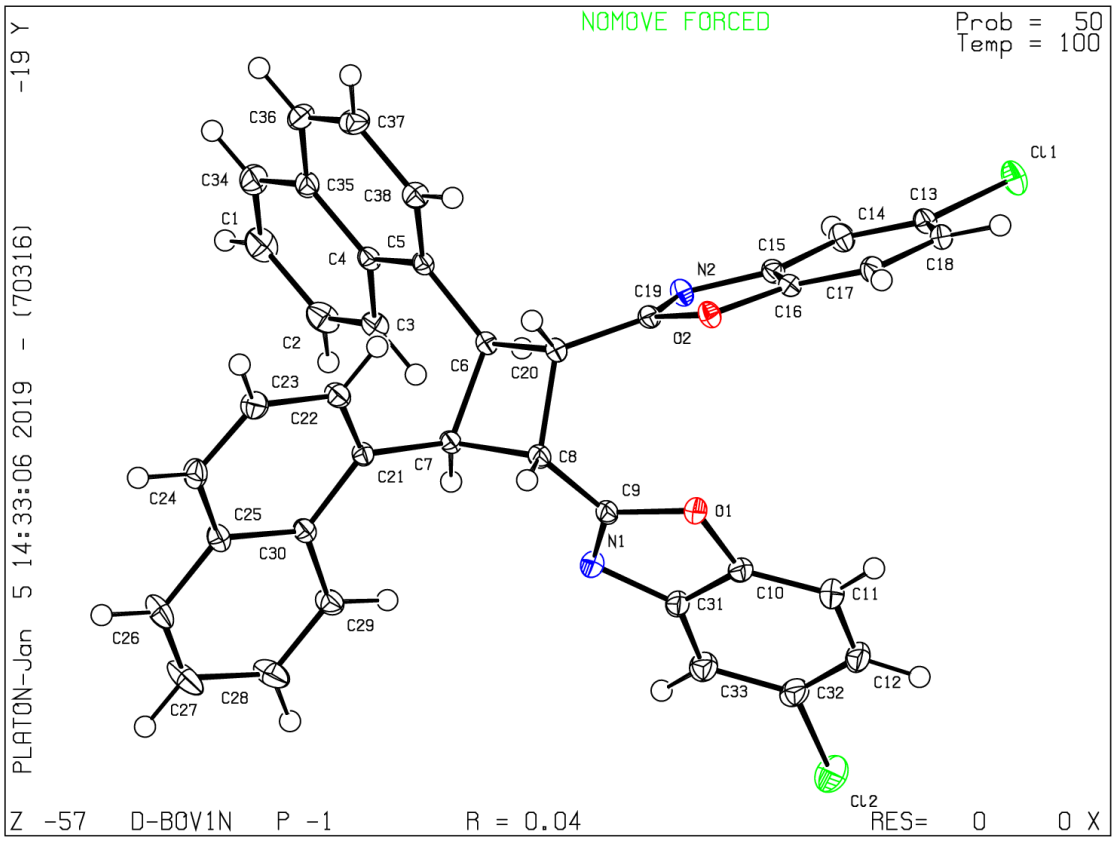
PLATON version of 13/12/2018; check.def file version of 11/12/2018

Datablock D-BOV1N - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) BOV1NM

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: BOV1NM

Bond precision: C-C = 0.0030 A Wavelength=0.71073

Cell: a=3.9720(3) b=12.2566(7) c=16.4309(11)
alpha=79.392(4) beta=86.478(4) gamma=84.244(4)
Temperature: 273 K

	Calculated	Reported
Volume	781.52(9)	781.52(9)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C20 H14 Cl N O2	?
Sum formula	C20 H14 Cl N O2	C20 H14 Cl N O2
Mr	335.77	335.77
Dx,g cm-3	1.427	1.427
Z	2	2
Mu (mm-1)	0.256	0.256
F000	348.0	348.0
F000’	348.44	
h,k,lmax	5,15,21	5,15,21
Nref	3672	3637
Tmin,Tmax	0.999,0.999	
Tmin’	0.887	

Correction method= Not given

Data completeness= 0.990 Theta(max)= 27.764

R(reflections)= 0.0467(2484) wR2(reflections)= 0.1142(3637)

S = 1.022 Npar= 218

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

```
PLAT480_ALERT_4_C Long H...A H-Bond Reported H2       ..O1       .       2.64 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      4.055 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).         5 Note
```

Alert level G

```
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)      0.004 Degree
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        273 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        273 Check
PLAT398_ALERT_2_G Deviating  C-O-C    Angle From 120 for O1             103.9 Degree
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         30 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         6 Info
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   3 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   6 ALERT level G = General information/check it is not something unexpected

   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
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PLATON version of 19/10/2018; check.def file version of 15/10/2018

Datablock BOV1NM - ellipsoid plot