Supporting Information

A NIR fluorescent probe for the detection and visualization of hydrogen sulfide using aldehyde group assisted thiolysis of dinitrophenyl ether strategy

Ming Qian†‡, Liuwei Zhang‡, Zhongji Pu‡, Jing Xia‡, Lili Chen‡, Ying Xia‡, Hongyan Cui‡, Jingyun Wang†*, Xiaojun Peng†

†State Key Laboratory of Fine Chemicals, Dalian University of Technology, 116024, Dalian, Liaoning, P. R. China
‡School of Life Science and Biotechnology, Dalian University of Technology, 116024, Dalian, Liaoning, P.R. China
List of contents

Scheme S1 The synthesis procedure of intermediates.

Table S1 A comparison of NIR fluorescent probes for H₂S.

Table S2 The photophysical properties of NDCM-CHO-OH in different co-solvents.

Figure S1 The optical spectra of NDCM-OH and NDCM-CHO-OH.

Figure S2 The optical spectra of NDCM-CHO-OH and NDCM-OH in different solvents.

Figure S3 The fluorescence spectra for the verification of the reaction product.

Figure S4 The absorption response behavior of NDCM-2 toward H₂S.

Figure S5 The fluorescence response of probe NDCM-2 (10 μM) toward different concentrations of H₂S.

Figure S6 The HRMS for the verification of the sensing mechanism.

Figure S7 ¹H NMR for the verification of the sensing mechanism.

Figure S8 The selectivity of NDCM-2 toward H₂S over various biological related analytes.

Figure S9 The selectivity of NDCM-2 toward H₂S over biothiols.

Figure S10 Density functional theory (DFT) calculation of NDCM-1 and NDCM-OH.

Figure S11 Effect of pH on NDCM-2 and its sensing performance toward H₂S.

Figure S12 Photobleaching curves of NDCM-2.

Figure S13 Evaluating the preservation stability of probe NDCM-2.

Figure S14 Cytotoxicity of the probe NDCM-2 on HeLa cells.

Figure S15 The confocal fluorescence imaging of the basal H₂S in four different cells.

Figure S16 The co-staining experiment of NDCM-2 with Hoechst 33342.

Figure S17 The co-staining experiment of NDCM-2 with Lyso tracker red.

Figure S18 Fluorescence images of NDCM-2 against different concentration of exogenous H₂S

Figure S19 Evaluating the photostability of NDCM-2 in the sensing process against H₂S in living HeLa cells.

Figure S20- Figure S34 Structure verification of the synthesized compound by MS and NMR.
Scheme S1. The synthetic route of the probe. Reaction conditions: (a) malononitrile, piperidine, glacial acetic acid, EtOH, reflux, N\textsubscript{2} protection; (b) p-hydroxybenzaldehyde, piperidine, acetonitrile, reflux, N\textsubscript{2} protection; (c) Hexamethylenetetramine, trifluoroacetic acid, reflux; (d) DIEPA, 2,4-dinitrofluorobenzene, dry CH\textsubscript{2}Cl\textsubscript{2}, room temperature. (e) DIEPA, 2,4-dinitrofluorobenzene, dry CH\textsubscript{2}Cl\textsubscript{2}, room temperature.

The synthesis of NDCM

Isophorone (2.3 g, 16.7 mmol), malononitrile (1.32 g, 20.0 mmol), piperidine (0.2 mL, 2.0 mmol) and glacial acetic acid (0.10 g, 1.6 mmol) were dissolved in 100 mL EtOH. Then, the mixture was refluxed for 6 h under argon atmosphere. After the solvent was removed, the residue was dissolved with CH\textsubscript{2}Cl\textsubscript{2}, washed with water, and dried over Na\textsubscript{2}SO\textsubscript{4}. Finally, the solvent was evaporated under reduced pressure, and the crude product was purified by silica column chromatography (petroleum/dichloromethane = 1:2, v/v) to give a white solid (2.1 g, 67.7%). \textsuperscript{1}H NMR (400 MHz, DMSO): δ 6.56 (d, J = 1.2 Hz, 1H), 2.53 (s, 2H), 2.23 (s, 2H), 2.05 (s, 3H), 0.95 (s, 6H). \textsuperscript{13}C NMR (126 MHz, DMSO): 171.28, 162.37, 119.38, 113.42, 112.63, 76.08, 44.69, 41.71, 31.87, 27.04, 24.99. HRMS: calculated for [M-H]\textsuperscript{−} : 185.1079; found: 185.1089.

The synthesis of NDCM-OH

NDCM (1 g, 5.4 mmol), p-hydroxybenzaldehyde (732 mg, 6.0 mmol), five drops of piperidine were dissolved in 40 mL anhydrous acetonitrile. The mixture was refluxed for 5 h under argon atmosphere. Subsequently, the solvent was removed under reduced pressure. The resulting residue
was dissolved in 20 mL dichloromethane, washed with water for three times, and dried over anhydrous Na$_2$SO$_4$. After the removal of the solvent, the crude product was purified by silica column chromatography (dichloromethane: acetic ether = 100:1) to afford the NDCM-OH as a red solid (1.17 g, 75%). $^1$H NMR (400 MHz, DMSO): $\delta$ 9.98 (s, 1H), 7.55 (d, J = 8.7 Hz, 2H), 7.29 – 7.14 (m, 2H), 6.83 ~ 6.76 (m, 3H), 2.59 (s, 2H), 2.53 (s, 2H), 1.01 (s, 6H). $^{13}$C NMR (126 MHz, DMSO): $\delta$ 170.23, 159.31, 156.67, 138.25, 129.83, 127.10, 126.22, 121.34, 115.85, 114.09, 113.27, 74.79, 42.31, 38.19, 31.62, 27.41. HRMS: calculated for [M-H]$^-$: 289.1341; found: 289.1351.

The synthesis of NDCM-CHO-OH

Hexamethylenetetramine (168 mg, 1.2 mmol) was added to solution of NDCM-OH (290.0 mg, 1.0 mmol) in trifluoroacetic acid (10 mL). The mixture was refluxed for 5 h. After complete reaction, the solvent was evaporated under a rotary evaporator, diluted with water and then neutralized with NaOH until the pH reached 7.0. Subsequently, the solution was extracted with dichloromethane. The organic layer was washed with water for three times, dried over anhydrous sodium sulfate. The crude product was purified by silica gel column chromatography with dichloromethane as the eluent to afford NDCM-CHO-OH as a yellow solid (116.6 mg, 43%). $^1$H NMR (400 MHz, DMSO): $\delta$ 11.15 (s, 1H), 10.29 (s, 1H), 7.97 (d, J = 2.2 Hz, 1H), 7.89 (dd, J = 8.7, 2.2 Hz, 1H), 7.37 ~ 7.25 (m, 2H), 7.04 (d, J = 8.6 Hz, 1H), 6.88 (s, 1H), 2.61 (s, 2H), 2.53 (s, 2H), 1.01 (s, 6H). $^{13}$C NMR (126 MHz, DMSO): $\delta$ 190.63, 170.27, 161.87, 156.09, 136.69, 134.96, 128.75, 127.96, 127.64, 122.62, 122.19, 118.08, 113.92, 113.08, 75.75, 42.27, 38.14, 31.62, 27.41. HRMS: calculated for [M-H]$^-$: 317.1290; found: 317.1293.

The synthesis of NDCM-1

The control compound NDCM-1 was synthesized according to the similar synthesis procedure of NDCM-2 using NDCM-OH as the reactant. $^1$H NMR (500 MHz, DMSO-d$_6$): $\delta$ 10.18 (s, 1H), 8.93 (d, J = 2.7 Hz, 1H), 8.47 (dd, J = 9.2, 2.8 Hz, 1H), 8.30 (d, J = 1.9 Hz, 1H), 8.10 (dd, J = 8.6, 1.9 Hz, 1H), 7.57 (d, J = 16.2 Hz, 1H), 7.46~7.29 (m, 3H), 6.96 (s, 1H), 2.63 (s, 2H), 2.55 (s, 2H), 1.02 (s, 6H). $^{13}$C NMR (DMSO-d$_6$): $\delta$ 170.26, 155.57, 154.64, 154.33, 141.77, 139.68, 136.08, 133.91, 130.05, 129.97, 129.65, 123.03, 121.89, 120.40, 120.06, 113.76, 112.95, 76.54, 42.28, 38.17, 31.65, 27.41. HRMS: calculated for [M-H]$^-$: 455.1356; found: 455.1368.
Table S1. A comparison of NIR fluorescent probes for H$_2$S.

<table>
<thead>
<tr>
<th>Probe</th>
<th>Properties</th>
<th>Stokes shift</th>
<th>Fluorescence enhancement</th>
<th>Response time</th>
<th>Detection limit</th>
<th>Applications</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image" alt="Analytica Chimica Acta 896 (2015) 128-136" /></td>
<td>Abs: 450 nm Em 490 nm Two-photon</td>
<td>40 nm</td>
<td>35-fold</td>
<td>2 min</td>
<td>120 nM</td>
<td>Cells and tissues</td>
</tr>
<tr>
<td><img src="image" alt="Sensors and Actuators B 221 (2015) 951–955" /></td>
<td>Abs: 450 nm Em: 612 nm</td>
<td>162 nm</td>
<td>112-fold</td>
<td>30 min</td>
<td>90 nM</td>
<td>Cells</td>
</tr>
<tr>
<td><img src="image" alt="Anal. Chem. 2016, 88, 5476–5481" /></td>
<td>Abs: 394/520 nm Em 532 nm Mitochondria-Targeted</td>
<td>138 nm</td>
<td>68-fold</td>
<td>40 min</td>
<td>2.46 μM</td>
<td>Cells</td>
</tr>
<tr>
<td><img src="image" alt="Chem. Commun. 2013, 49, 3890-3892." /></td>
<td>Abs:520 nm Em:670 nm NIR emission</td>
<td>150 nm</td>
<td>65-fold</td>
<td>60 min</td>
<td>3.05 μM</td>
<td>Cells</td>
</tr>
<tr>
<td><img src="image" alt="Sci. Rep. 2017, 7, 12944." /></td>
<td>Abs :440 nm Em :545 nm ER Targeted</td>
<td>105 nm</td>
<td>45-fold</td>
<td>30 min</td>
<td>7.77 μM</td>
<td>Cells, tissues and zebrafish</td>
</tr>
<tr>
<td><img src="image" alt="Sci. Rep. 2016, 6, 18868." /></td>
<td>Abs :670 nm Em :723 nm NIR excitation and emission</td>
<td>53 nm</td>
<td>50-fold</td>
<td>20 min</td>
<td>38 nM</td>
<td>Cells and mice</td>
</tr>
<tr>
<td>Compound</td>
<td>Absorption (nm)</td>
<td>Emission (nm)</td>
<td>Excitation and Emission</td>
<td>Fold Change</td>
<td>Time (min)</td>
<td>Concentration (nM)</td>
</tr>
<tr>
<td>----------</td>
<td>----------------</td>
<td>--------------</td>
<td>--------------------------</td>
<td>-------------</td>
<td>------------</td>
<td>-------------------</td>
</tr>
<tr>
<td><img src="image" alt="Chem. Sci. 2017, 8, 2776–2781." /></td>
<td>740 nm</td>
<td>796 nm</td>
<td>NIR excitation and emission</td>
<td>87-fold</td>
<td>30 min</td>
<td>39.6 nM</td>
</tr>
<tr>
<td><img src="image" alt="Sensors and Actuators B 232 (2016) 705–711" /></td>
<td>370 nm</td>
<td>424 nm</td>
<td></td>
<td>200-fold</td>
<td>180 min</td>
<td>90 nM</td>
</tr>
<tr>
<td><img src="image" alt="Sensors and Actuators B 255 (2018) 2347–2355" /></td>
<td>518 nm</td>
<td>655 nm</td>
<td>NIR emission</td>
<td>32-fold</td>
<td>8 min</td>
<td>83 nM</td>
</tr>
<tr>
<td><img src="image" alt="Biosens. Bioelectron.2017, 89, 919–926." /></td>
<td>680 nm</td>
<td>720 nm</td>
<td>NIR excitation and emission</td>
<td>20-fold</td>
<td>30 min</td>
<td>260 nM</td>
</tr>
<tr>
<td><img src="image" alt="Dyes Pigm. 2018, 153, 206–212." /></td>
<td>560 nm</td>
<td>680 nm</td>
<td>NIR emission</td>
<td>About 25-fold</td>
<td>30 min</td>
<td>1.1 nM</td>
</tr>
<tr>
<td><img src="image" alt="Sensors and Actuators B 261 (2018) 51–57" /></td>
<td>452 nm</td>
<td>552 nm</td>
<td>Two photon Ratio metric detection</td>
<td>Not mentioned</td>
<td>5 min</td>
<td>0.24 µM</td>
</tr>
<tr>
<td><img src="image" alt="This work" /></td>
<td>490 nm</td>
<td>660 nm</td>
<td>NIR emission</td>
<td>160-fold</td>
<td>15 min</td>
<td>58.797 nM</td>
</tr>
</tbody>
</table>

This work
Figure S1. The spectra of NDCM-OH and NDCM-CHO-OH in PBS-DMSO solution (pH=7.4, 1:1). (a) The normalized spectra of NDCM-OH. (b) The normalized spectra of NDCM-CHO-OH. (c) Comparison of two fluorophores in absorbance. (d) Comparison of two fluorophores in fluorescence emission.

Table S2. The photophysical properties of fluorophore NDCM-CHO-OH in different co-solvents (PBS solution with addition of 50% organic solvents).

<table>
<thead>
<tr>
<th>solvents</th>
<th>$\lambda_{\text{max}}$ (nm)</th>
<th>$\varepsilon_{\text{max}}$ ($\times 10^4$)</th>
<th>$\lambda_{\text{em}}$ (nm)</th>
<th>$\Phi$</th>
<th>$\delta$ shift (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CH$_3$CN</td>
<td>490</td>
<td>4.01</td>
<td>660</td>
<td>0.233777</td>
<td>170</td>
</tr>
<tr>
<td>DMSO</td>
<td>505</td>
<td>4.53</td>
<td>664</td>
<td>0.381135</td>
<td>159</td>
</tr>
<tr>
<td>Acetone</td>
<td>505</td>
<td>4.38</td>
<td>664</td>
<td>0.157977</td>
<td>159</td>
</tr>
<tr>
<td>DMF</td>
<td>510</td>
<td>4.72</td>
<td>664</td>
<td>0.368865</td>
<td>154</td>
</tr>
<tr>
<td>CH$_3$OH</td>
<td>485</td>
<td>4.32</td>
<td>652</td>
<td>0.200058</td>
<td>167</td>
</tr>
<tr>
<td>THF</td>
<td>525</td>
<td>4.19</td>
<td>666</td>
<td>0.233269</td>
<td>141</td>
</tr>
<tr>
<td>1,4-Dioxane</td>
<td>505</td>
<td>4.45</td>
<td>662</td>
<td>0.279373</td>
<td>157</td>
</tr>
<tr>
<td>EtOH</td>
<td>500</td>
<td>4.74</td>
<td>658</td>
<td>0.215895</td>
<td>158</td>
</tr>
</tbody>
</table>
Figure S2. The optical spectra of fluorophore NDCM-CHO-OH and NDCM-OH in different co-solvents (PBS solution with addition of 50% organic solvents). (a) The absorption spectrum of NDCM-OH in different co-solvents. (b) The absorption spectrum of NDCM-CHO-OH in different co-solvents. (c) The fluorescence spectrum of NDCM-OH in different co-solvents. (b) The fluorescence spectrum of NDCM-CHO-OH in different co-solvents.

Figure S3. The spectra for the verification of the reaction product. (a) The fluorescence spectra of NDCM-2 (10 μM), NDCM-2 (10 μM) + 100 μM Na₂S and NDCM-CHO-OH (10 μM) in PBS-CH₃CN solution (pH 7.4, 1:1), excitation wavelength: 490 nm. (b) The fluorescence spectra of NDCM-1 (10 μM), NDCM-1(10
μM) + 100 μM Na₂S and NDCM-OH (10 μM) in PBS-DMSO solution (pH 7.4, 1:1), excitation wavelength: 560 nm.

Figure S4. The absorption response behavior toward H₂S in PBS-CH₃CN solution (pH=7.4, 1:1). (a) The time-dependent normalized absorption spectra change in 15 min upon the addition of 100 μM Na₂S. (b) The normalized absorption spectra change of NDCM-2 toward different Na₂S concentration (0, 10, 20, 30, 40, 50, 60, 70, 80, 90, 100 μM) for 15 min. Excitation wavelength: 490 nm.
Figure S5. Fluorescence response of probe NDCM-2 (10 μM) toward different concentrations of Na₂S. (a) The time-dependent fluorescence intensity (660 nm) change of NDCM-2 without the addition of Na₂S. (b) The linear relationship between the fluorescence intensity (660 nm) and extremely low Na₂S concentration (0, 0.06, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1 μM). (c) The linear relationship between the fluorescence intensity (660 nm) and low Na₂S concentration (0, 0.06, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1, 2, 3, 4, 5, 6, 7 μM). (d) The fluorescence intensity (660 nm) change of NDCM-2 toward various Na₂S concentration (0, 0.06, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1, 2, 3, 4, 5, 6, 7, 10, 30, 60, 100 μM). Excitation wavelength: 490 nm.

Figure S6. Verifying the sensing mechanism of NDCM-2 toward H₂S by HRMS.
Figure S7. $^1$H NMR for the verification of the sensing mechanism. (a) $^1$H NMR spectra ($\delta$ 6.5–11.5) of NDCM-2. (b) The fluorophore NDCM-CHO-OH. (c) The isolated product of NDCM-2 + Na$_2$S.
Figure S8. The selectivity of NDCM-2 toward H₂S over various biological related analytes. (a) Absorption spectra change of NDCM-2 (10 μM) toward various analytes (Na₂S: 100μM, other analytes: 1 mM) in PBS-CH₃CN solution (pH 7.4, 1:1). (b) Fluorescence spectra change of probe NDCM-2 (10 μM) toward various analytes (Na₂S: 100μM, other analytes: 1 mM) in PBS-CH₃CN solution (pH 7.4, 1:1). (c) Color changes of probe NDCM-2 (10 μM) upon the addition of various analytes (100 μM for Na₂S and 1 mM for other analytes) under bright field. (d) Fluorescence color changes of probe NDCM-2 (10 μM) upon the addition of various analytes (100 μM for Na₂S and 1 mM for other analytes) under a 365 nm UV-lamp.

**Figure S9.** The selectivity of NDCM-2 toward H$_2$S over biothiols (GSH, Hcy, Cys) in PBS-CH$_3$CN solution (pH=7.4, 1:1). (a) The normalized fluorescence spectra change of NDCM-2 upon addition of Na$_2$S (100 μM) and three biothiols (100 μM), inset: the color change of NDCM-2 toward Na$_2$S and three biothiols under UV Lamp (365 nm). (b) The normalized fluorescence intensity at 660 nm changed with time upon addition of 100 μM Na$_2$S and 100 μM GSH, Hcy, Cys. The excitation wavelength: 490 nm.

**Figure S10.** Density functional theory (DFT) optimized structures and frontier molecular orbitals (MOs) of NDCM-1 and NDCM-OH. The calculations were obtained by DFT at the B3LYP/6-311G (d, p)/level using Gaussian 16 program.
Figure S11. Fluorescence intensity of probe NDCM-2 (10 μM) at 660 nm under different pH values (from 3.0 to 9.0) in the absence and presence of Na₂S (100 μM). Excitation wavelength: 490 nm.

Figure S12. Photobleaching curves for the final reaction solution of NDCM-2 and 100 μM H₂S exposed to the light irradiation under the high voltage mode (800 V) of fluorescence spectrophotometer.
Figure S13. Evaluating the preservation stability of probe NDCM-2. (a) Fluorescence spectra change of the stock solution of probe NDCM-2 (10 μM) in the preservation time period of 0-7 days. Excitation wavelength: 490 nm. (b-c) The NMR spectra comparison of NDCM-2 before and after preservation for four months. The spectrum of (c) was measured after the preservation of pure NDCM-2 solid in refrigerator for four months.

Figure S14. Cytotoxicity of the probe NDCM-2 against HeLa cells evaluated by a standard MTT assay, the data are presented as mean ± S.D.
**Figure S15.** The confocal fluorescence imaging of the basal H$_2$S in four different cells using probe NDCM-2 (10 μM). (2A) COS-7 cells. (2B) MCF-7 cells. (2C) HepG-2 cells. (2D) HeLa cells. 1A, 1B, 1C, and 1D are the corresponding bright-field image of 2A, 2B, 2C, and 2D. The fluorescence images were obtained by collecting the emissions ranging from 620 to 720 nm upon excitation at 488 nm. Scar bar=20 μm.

**Figure S16.** The co-staining experiments of NDCM-2 (10 μM) in HepG-2 cells using Hoechst 33342 as the nucleus staining dyes. (1A): Bright field. (1B): Fluorescence imaging of basal H$_2$S using NDCM-2. (2A): Fluorescence imaging of Hoechst 33342. (2B): Merge of (1B) and (2A). Excitation wavelength: 405 nm for Hoechst 33342 and 488 nm for NDCM-2. The fluorescence images of NDCM-2 were obtained by collecting the emissions at 620-720 nm upon excitation at 488 nm and the fluorescence images of Hoechst 33342 were obtained by collecting the emissions at 420-520 nm. Scar bar=20 μm.
**Figure S17** The co-staining experiments of NDCM-2 (10 μM) in HeLa cells using Lyso-tracker red as the specific lysosome staining dyes. (A): Bright field. (B): Fluorescence images of NDCM-2 against 100μM exogenous H₂S. (C): Fluorescence images of Lyso-tracker red. (D): Merge of (B) and (C). Excitation wavelength: 559 nm for Lyso-tracker red and 488 nm for NDCM-2. The fluorescence images of NDCM-2 and Lyso tracker red were obtained by collecting the emissions at 620-720 nm and 560-600 nm with confocal laser scanning microscopy (Olympus, FV1000-IX81), respectively. Scar bar=20 μm.

**Figure S18.** Fluorescence images of NDCM-2 against different concentration of exogenous H₂S (0, 2 μM, 20 μM, 50 μM, 100 μM) in living HeLa cells. (2A): PPG (1 mM) pre-treated cells were incubated with 10 μM NDCM-2 for 30 min only. (2B-2E): PPG (1 mM) pre-treated cells were incubated with 5 μM, 20 μM,
50 μM, 100 μM Na₂S for 30 min respectively, then incubated with 10 μM NDCM-2 for 30 min. (1A-1E) and (3A-3E) are the corresponding bright filed and merge field of (2A-2E), respectively. The fluorescence images were obtained by collecting the emissions at 620-720 nm under the excitation wavelength of 488 nm with confocal laser scanning microscopy (Olympus, FV1000-IX81). Scar bar=20 μm.

Figure S19. Evaluating the photostability of probe NDCM-2 in the sensing process against H₂S in living HeLa cells. The cells were incubated with 100 μM H₂S at 37 °C for 30 min, followed by the incubation of 10 μM NDCM-2 for 30 min at 37 °C. Images were taken by confocal fluorescent microscopy (Olympus, FV1000-IX81) for different times (0, 120s, 240s, 360s, 480s, 600s, 720s, 840s, 960s, 1080s, 1200s, 1320s) with the excitation at 488 nm and the emission collection range from 620 to 700 nm. Scale bar=20 μm.
**Figure S20.** $^1$H NMR spectra of NDCM in DMSO-$d_6$

**Figure S21.** $^{13}$C NMR spectra of NDCM in DMSO-$d_6$
Figure S22. HRMS spectra of NDCM

Figure S23. 1H NMR spectra of NDCM-OH in DMSO-d$_6$
Figure S24. $^{13}$C NMR spectra of NDCM-OH in DMSO-$d_6$.

Figure S25. HRMS spectra of NDCM-OH.
Figure S26. $^1$H NMR spectra of NDCM-OH in DMSO-$d_6$

Figure S27. $^{13}$C NMR spectra of NDCM-CHO-OH in DMSO-$d_6$
Figure S28. HRMS spectra of NDCM-CHO-OH

Figure S29. $^1$H NMR spectra of NDCM-1 in DMSO-d$_6$
Figure S30. $^{13}$C NMR spectra of NDCM-1 in DMSO-d$_6$

Figure S31. HRMS spectra of NDCM-1
Figure S32. $^1$H NMR spectra of NDCM-2 in DMSO-d$_6$

Figure S33. $^{13}$C NMR spectra of NDCM-2 in DMSO-d$_6$
Figure S34. HRMS spectra of NDCM-2