

## Supporting information

**Figure S1.** Extract (A) and corresponding precipitate (B) from ‘Gonggan’.

**Figure S2.** Color changes of ABS under different pH values.

**Figure S3.** The  $^1\text{H}$  NMR (600 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of ABS.

**Figure S4.** The UV-Vis spectrum of ABS-D.

**Figure S5.** The MS (A) and  $\text{MS}^2$  (B) of ABS-D.

**Figure S6.** The MS (A) and  $\text{MS}^2$  (B) of ABS.

**Figure S7.** The  $^1\text{H}$  NMR (600 MHz,  $\text{CD}_3\text{OD}:\text{CF}_3\text{COOD}=20:1$ ) spectrum of ABS-D.

**Figure S8.** The  $^1\text{H}$  NMR (600 MHz,  $\text{DMSO}-d_6$ ) spectrum of ABS-D.

**Figure S9.** The  $^{13}\text{C}$  NMR (150 MHz,  $\text{CD}_3\text{OD}:\text{CF}_3\text{COOD}=20:1$ ) spectrum of ABS-D.

**Figure S10.** The  $^{13}\text{C}$  NMR (150 MHz,  $\text{DMSO}-d_6$ ) spectrum of ABS-D.

**Figure S11.** The  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of ABS-D in  $\text{CD}_3\text{OD}:\text{CF}_3\text{COOD}=20:1$ .

**Figure S12.** The HSQC spectrum of ABS-D in  $\text{DMSO}-d_6$ .

**Figure S13.** The ROESY spectrum of ABS-D in  $\text{DMSO}-d_6$ .

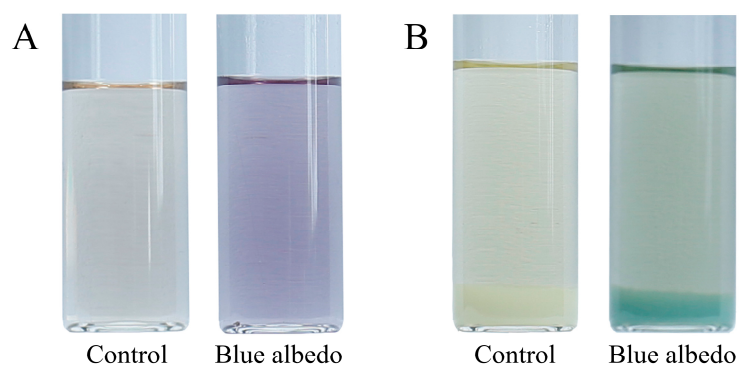
**Figure S14.** The HMBC spectrum of ABS-D in  $\text{DMSO}-d_6$ .

**Figure S15.** Experimental and calculated chemical shifts for DP4+ probability analysis for three possible isomers of ABS-D.

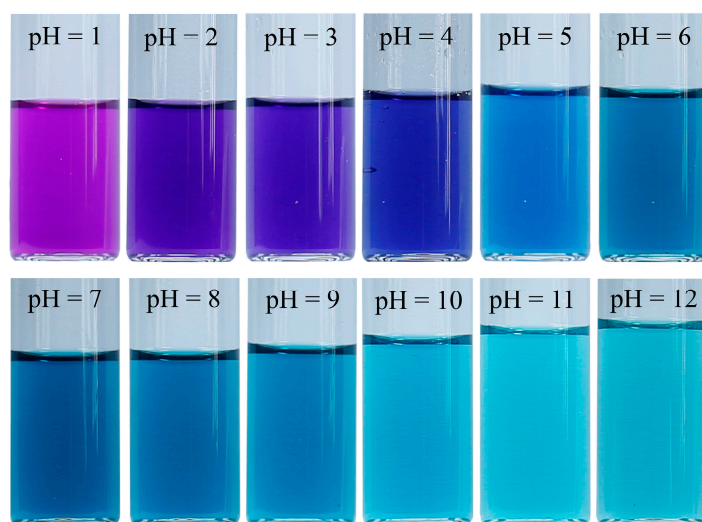
**Table S1.**  $^1\text{H}$  NMR (600 MHz) and  $^{13}\text{C}$  NMR (150 MHz) spectra of ABS-D in  $\text{CD}_3\text{OD}:\text{CF}_3\text{COOD}=20:1$ .

**Table S2.** Calculated and experimental values of ABS-D  $^{13}\text{C}$  NMR chemical shifts.

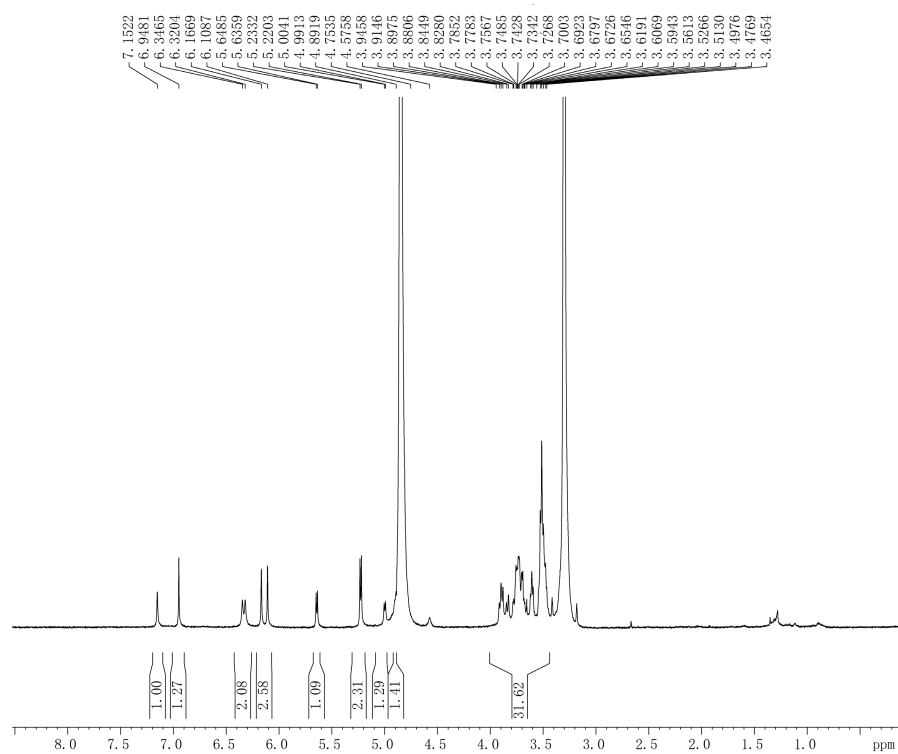
**Table S3.** B3-LYP geometries for all the optimized compounds.



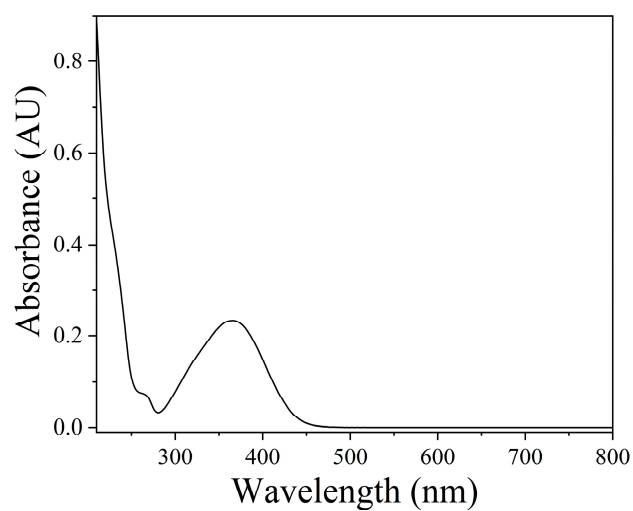
**Figure S1.** Extract (A) and corresponding precipitate (B) from 'Gonggan'



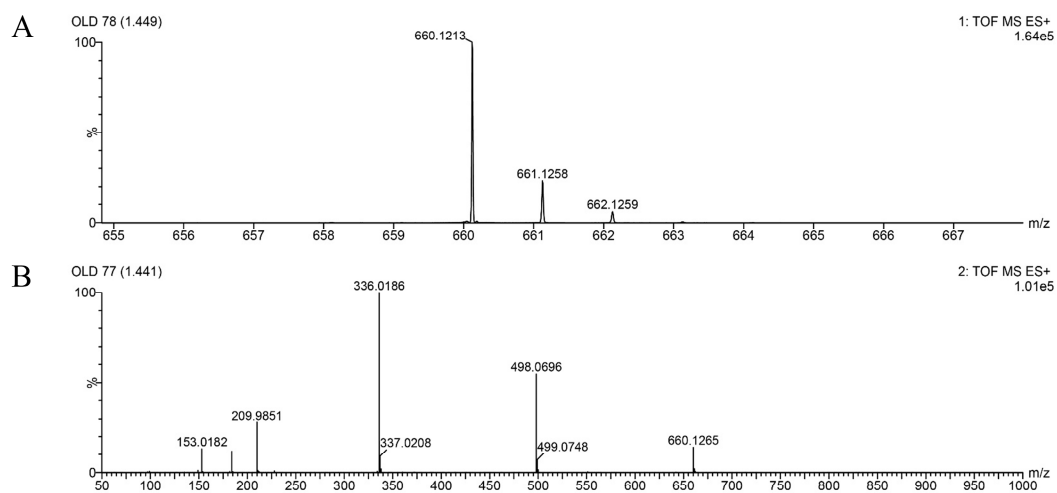
**Figure S2.** Color changes of ABS under different pH values



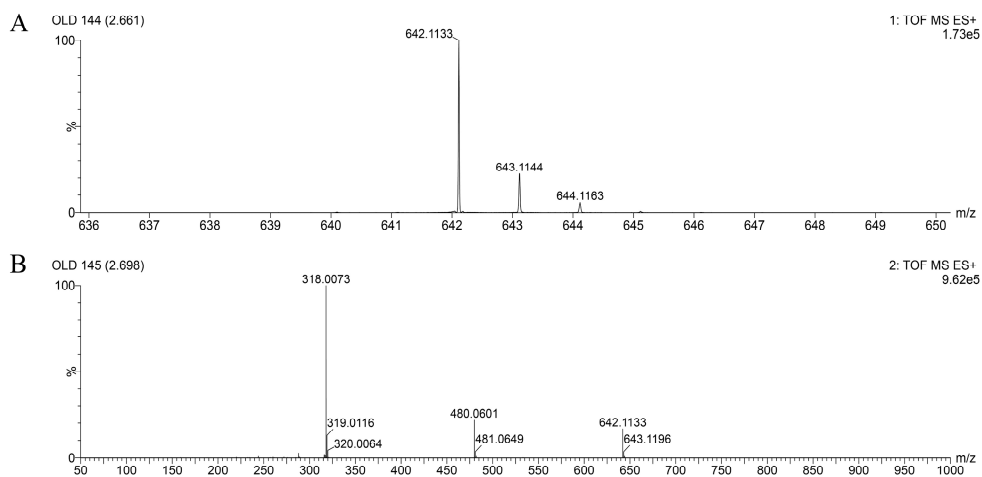
**Figure S3** The  $^1\text{H}$  NMR (600 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of ABS



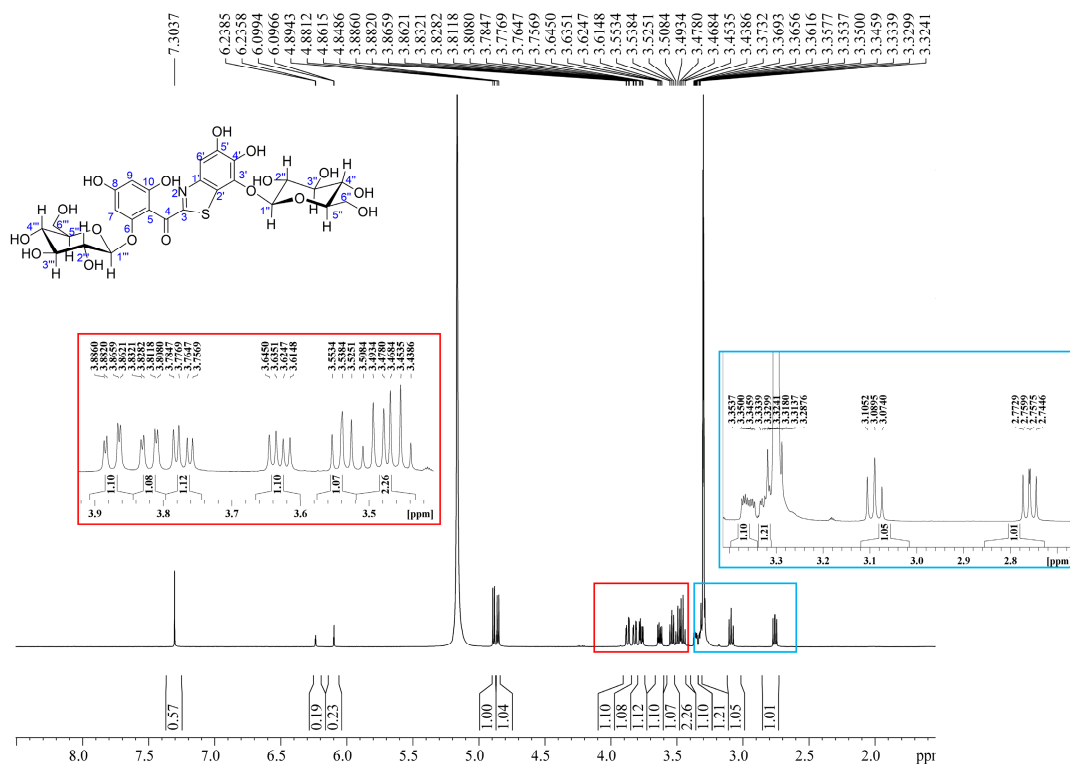
**Figure S4** The UV-Vis spectrum of ABS-D.



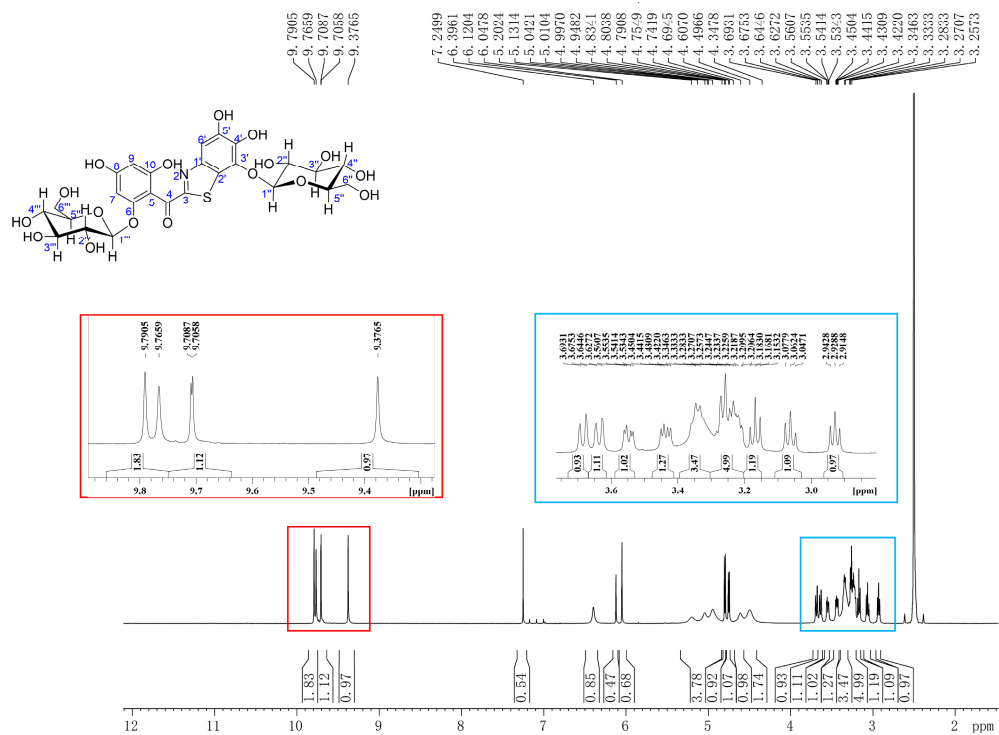
**Figure S5** The MS (A) and MS<sup>2</sup> (B) of ABS-D



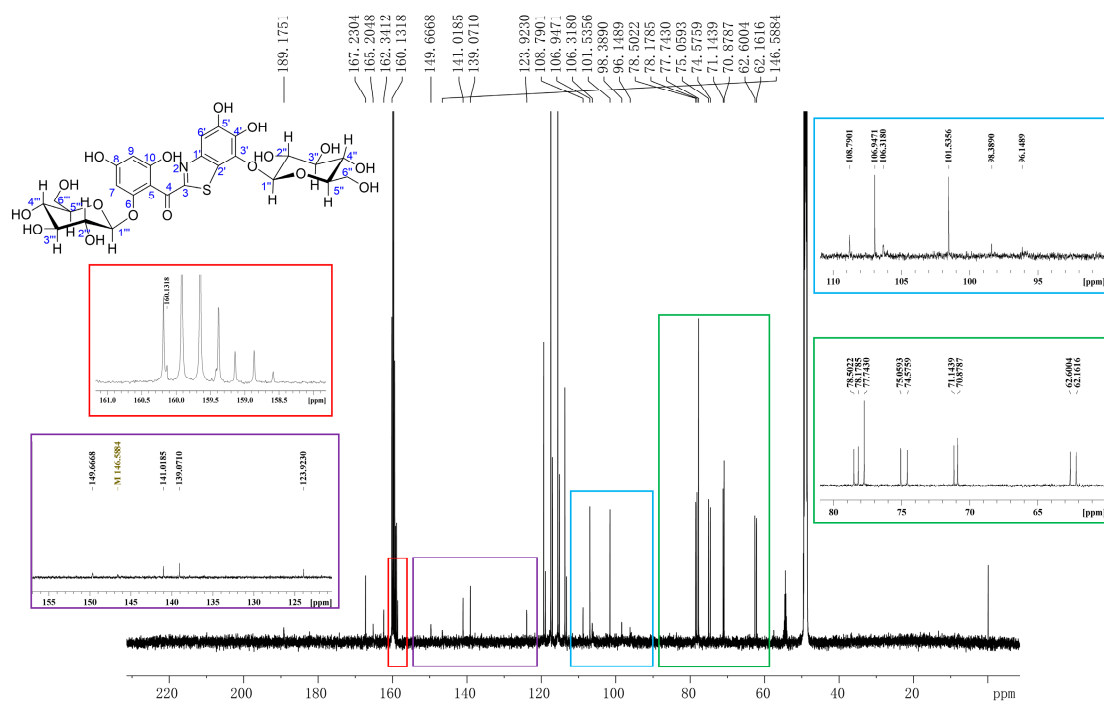
**Figure S6** The MS (A) and MS<sup>2</sup> (B) of ABS



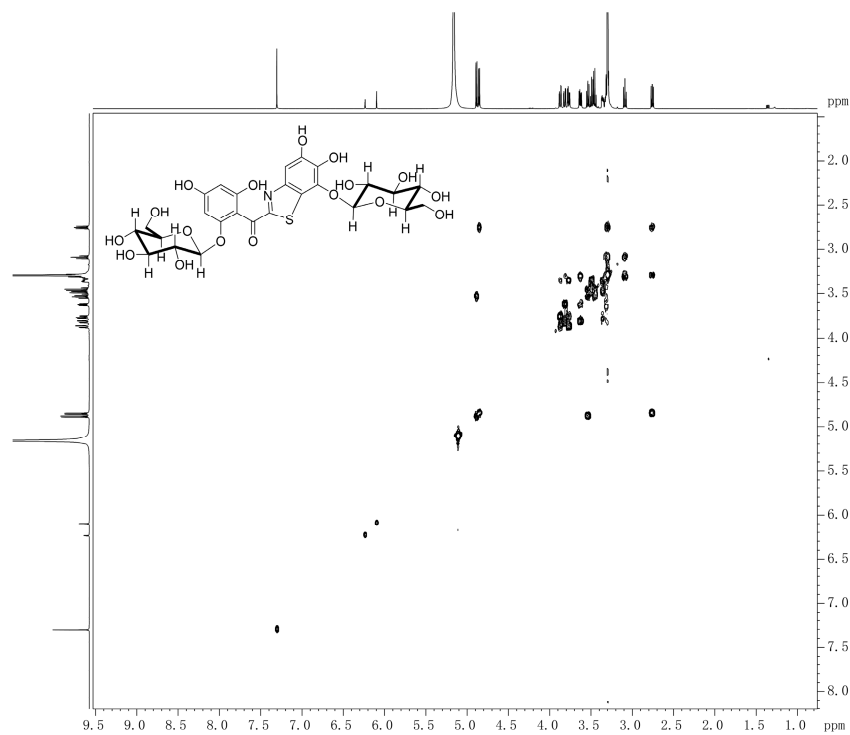
**Figure S7.** The <sup>1</sup>H NMR (600 MHz, CD<sub>3</sub>OD:CF<sub>3</sub>COOD=20:1) spectrum of ABS-D.



**Figure S8.** The <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) spectrum of ABS-D.

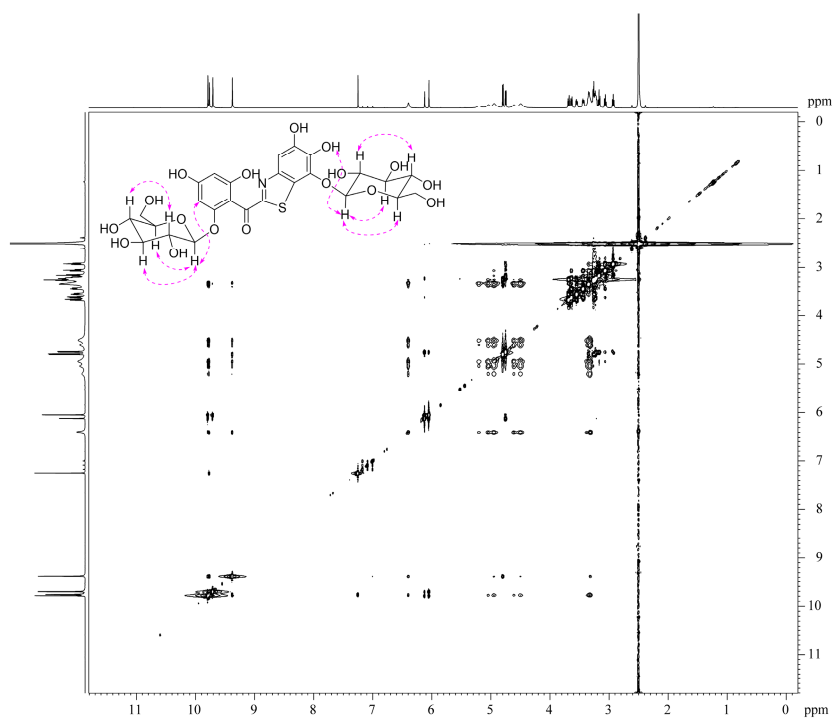


**Figure S9.** The <sup>13</sup>C NMR (150 MHz, CD<sub>3</sub>OD:CF<sub>3</sub>COOD=20:1) spectrum of ABS-D.

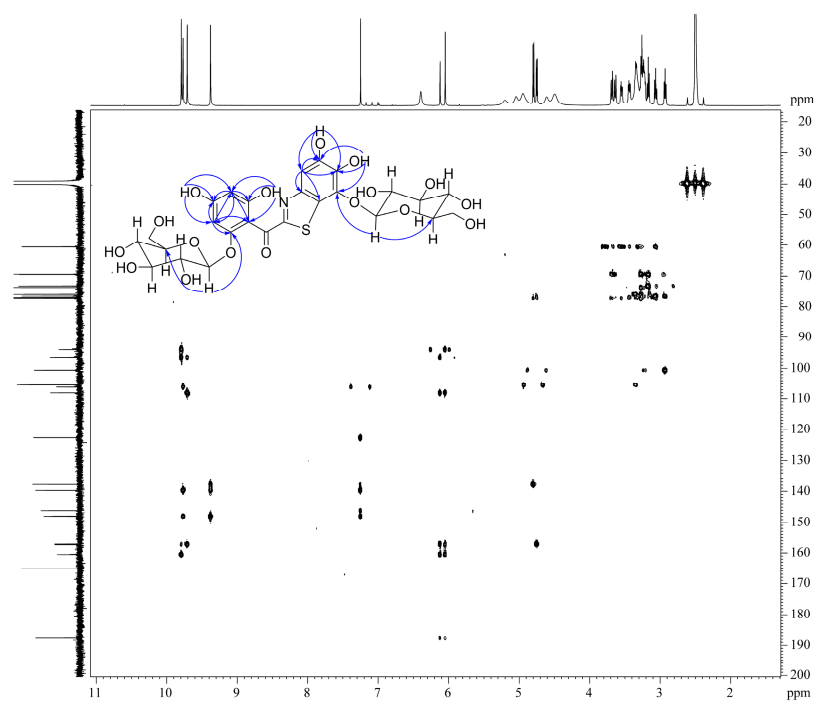








**Figure S13.** The ROESY spectrum of ABS-D in DMSO- $d_6$ .





respectively)

**Table S1.**  $^1\text{H}$  NMR (600 MHz) and  $^{13}\text{C}$  NMR (150 MHz) data of ABS-D in  $\text{CD}_3\text{OD}:\text{CF}_3\text{COOD}=20:1$

| position | $\delta_{\text{H}}$ ( $J$ in Hz) <sup>a</sup> | $\delta_{\text{C}}$ |
|----------|---|---------------------|
| 2        |   |                     |
| 3        |   | 167.2               |
| 4        |   | 189.2               |
| 5        |   | 108.8               |
| 6        |   | 160.1               |
| 7        | 6.24, br s                                    | 96.1                |
| 8        |   | 165.2               |
| 9        | 6.10, br s                                    | 98.4                |
| 10       |   | 162.3               |
| 1'       |   | 146.6               |
| 2'       |   | 123.9               |
| 3'       |   | 139.1               |
| 4'       |   | 141.0               |
| 5'       |   | 149.7               |
| 6'       | 7.30, s                                       | 106.3               |
| 1''      | 4.89, d (7.9)                                 | 107.0               |
| 2''      | 3.54, dd (9.0, 7.9)                           | 75.1                |
| 3''      | 3.45, t (9.0)                                 | 77.7                |
| 4''      | 3.49 t (9.1)                                  | 70.9                |
| 5''      | 3.36, ddd (9.3, 4.6, 2.4)                     | 78.5                |
| 6''      | 3.88, dd (12.1, 2.4)                          | 62.2                |
|          | 3.77, dd (12.0, 4.7)                          |                     |
| 1'''     | 4.85, d (7.8)                                 | 101.5               |
| 2'''     | 2.76, dd (9.2, 7.8)                           | 74.6                |
| 3'''     | 3.30, t (9.2)                                 | 77.7                |
| 4'''     | 3.09, t (9.3)                                 | 71.1                |
| 5'''     | 3.32, ddd (9.5, 5.9, 2.3)                     | 78.2                |
| 6'''     | 3.82, dd (12.2, 2.3)                          | 62.6                |
|          | 3.63, dd (12.2, 5.9)                          |                     |

<sup>a</sup> The indiscernible signals due to overlap or complex multiplicity are reported without designating multiplicity.

**Table S2.** Calculated and experimental values of ABS-D  $^{13}\text{C}$  NMR chemical shifts.

| position | $\delta_{\text{exp}}$ | $\delta_{\text{cal}}$ |          |          |
|----------|-----------------------|-----------------------|----------|----------|
|          |                       | <b>a</b>              | <b>b</b> | <b>c</b> |
| 3        | 165.1                 | 174.5968              | 175.5468 | 170.4983 |

|      |       |          |          |          |
|------|-------|----------|----------|----------|
| 4    | 187.6 | 197.0714 | 195.7996 | 199.3725 |
| 5    | 108   | 112.0692 | 114.3085 | 113.2979 |
| 6    | 157.1 | 165.5861 | 166.5191 | 165.6023 |
| 7    | 94    | 101.5868 | 105.5239 | 103.4206 |
| 8    | 160.5 | 171.357  | 171.6536 | 172.451  |
| 9    | 96.5  | 101.1236 | 102.3467 | 103.1789 |
| 10   | 157.3 | 174.5486 | 173.5212 | 177.0954 |
| 1'   | 146.1 | 150.295  | 139.2849 | 156.2652 |
| 2'   | 122.7 | 135.5817 | 145.6144 | 127.2674 |
| 3'   | 137.7 | 144.4289 | 145.9652 | 144.4458 |
| 4'   | 139.7 | 148.1582 | 145.3112 | 146.4393 |
| 5'   | 147.9 | 151.3315 | 152.8004 | 154.3323 |
| 6'   | 106.1 | 110.6924 | 106.9259 | 105.011  |
| 1''  | 105.4 | 109.7015 | 111.1838 | 107.135  |
| 2''  | 73.6  | 80.1778  | 79.7563  | 78.2528  |
| 3''  | 75.9  | 84.0411  | 82.6088  | 82.7629  |
| 4''  | 69.3  | 73.8024  | 72.8469  | 72.8003  |
| 5''  | 77.3  | 80.7574  | 81.8894  | 81.4101  |
| 6''  | 60.5  | 63.9476  | 63.9996  | 63.5556  |
| 1''' | 100.5 | 106.7628 | 107.7408 | 108.3932 |
| 2''' | 73.1  | 74.005   | 73.6071  | 72.9418  |
| 3''' | 76.5  | 83.6299  | 83.2633  | 82.1063  |
| 4''' | 69.4  | 73.3175  | 73.7202  | 72.768   |
| 5''' | 77    | 82.0405  | 80.7707  | 81.5574  |
| 6''' | 60.6  | 63.8077  | 61.9255  | 63.8311  |

**Table S3.** B3-LYP geometries for all the optimized compounds

**a**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 4.83099200  | -0.93752500 | -0.40032500 |
| C | 3.47580100  | -1.24048100 | -0.35000900 |
| C | 3.02625100  | -2.59728000 | -0.29242700 |
| C | 4.02306300  | -3.62418900 | -0.39210000 |
| C | 5.38170500  | -3.31748900 | -0.37763000 |
| C | 5.77298100  | -1.98118100 | -0.37960700 |
| H | 5.16185700  | 0.08015800  | -0.55564500 |
| C | 1.63171900  | -3.01503400 | -0.19097000 |
| H | 6.11766700  | -4.11181600 | -0.41671200 |
| C | 0.59896000  | -2.19210100 | 0.49653900  |
| C | -0.38464300 | -0.96626100 | 2.04547300  |
| C | -0.50594900 | -0.17286800 | 3.20301700  |
| C | -1.53161600 | -1.28672800 | 1.27877500  |
| C | -1.76488500 | 0.27070100  | 3.56413400  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.80063100 | -0.81246600 | 1.63668500  |
| C | -2.91976400 | -0.04032800 | 2.79272000  |
| O | 3.69100600  | -4.92490800 | -0.46814800 |
| O | 1.24920600  | -4.13457100 | -0.59973700 |
| O | 7.10318800  | -1.72846300 | -0.41074000 |
| H | 7.25740700  | -0.76872300 | -0.41767800 |
| O | 2.48908200  | -0.30578800 | -0.45931900 |
| O | -4.13554900 | 0.40311700  | 3.19648700  |
| H | -4.00310800 | 0.89290700  | 4.02918000  |
| O | -3.92120200 | -1.17153100 | 0.91516700  |
| C | 2.70094300  | 1.09165100  | -0.39366300 |
| C | 3.21572100  | 1.61819400  | 0.96482900  |
| H | 1.69196700  | 1.49596000  | -0.57001200 |
| C | 3.39174300  | 3.15161400  | 0.87182400  |
| H | 4.18590500  | 1.16361800  | 1.18672700  |
| C | 3.67345200  | 2.88618300  | -1.63031400 |
| C | 4.23094400  | 3.54883500  | -0.35430500 |
| H | 2.67544100  | 3.30401500  | -1.84638900 |
| O | 3.55974600  | 1.46879400  | -1.44672000 |
| O | 2.37583600  | 1.24592600  | 2.03955500  |
| H | 1.46963000  | 1.54290900  | 1.85209400  |
| C | 4.54953100  | 3.11672400  | -2.85136700 |
| H | 4.10050400  | 2.59535200  | -3.70880100 |
| H | 4.55364400  | 4.19381500  | -3.06342500 |
| O | 5.85864200  | 2.63125000  | -2.57804600 |
| H | 6.41951500  | 2.85541000  | -3.33648200 |
| C | -4.18134800 | -0.42620800 | -0.25545700 |
| C | -5.00912900 | -1.31206600 | -1.19930600 |
| H | -3.23236700 | -0.13179100 | -0.73375100 |
| C | -5.49782100 | -0.49198600 | -2.40908200 |
| H | -5.87488000 | -1.66480900 | -0.62545300 |
| C | -5.22782100 | 1.57869800  | -0.98227400 |
| C | -6.14936700 | 0.83115900  | -1.96784000 |
| H | -4.29988400 | 1.86801900  | -1.50643100 |
| O | -4.90778400 | 0.72460300  | 0.12112100  |
| O | -4.29984200 | -2.47792100 | -1.58659200 |
| H | -3.66357700 | -2.23716200 | -2.28061800 |
| C | -5.85017100 | 2.84982800  | -0.42607200 |
| H | -5.14191000 | 3.30347500  | 0.28249300  |
| H | -5.99667400 | 3.54623200  | -1.26197000 |
| O | -7.08196300 | 2.52881300  | 0.20890200  |
| H | -7.51212200 | 3.36303100  | 0.45163100  |
| O | -2.04112400 | 1.03976300  | 4.66196100  |
| H | -1.23764400 | 1.19124500  | 5.18551200  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 2.70859400  | -4.96187300 | -0.60419200 |
| H | 2.39249800  | 3.59961500  | 0.76419400  |
| O | 3.89884900  | 3.69971400  | 2.07706900  |
| H | 4.80685700  | 3.37434500  | 2.19890100  |
| H | 5.26022800  | 3.20051800  | -0.21719400 |
| O | 4.33039900  | 4.95778400  | -0.50753400 |
| H | 3.43209400  | 5.32957600  | -0.51567400 |
| H | 0.37326100  | 0.06983400  | 3.79139800  |
| H | -7.09012900 | 0.61861000  | -1.44963400 |
| O | -6.50588000 | 1.64725700  | -3.07522400 |
| H | -5.71301600 | 1.78738500  | -3.62007200 |
| H | -4.62071500 | -0.24483100 | -3.02726200 |
| O | -6.33033700 | -1.25507600 | -3.26748900 |
| H | -7.13027900 | -1.49961000 | -2.77201700 |
| S | -1.08840700 | -2.32976400 | -0.04838500 |
| N | 0.79736800  | -1.49223800 | 1.56974900  |

## b

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.56540300 | -0.70490900 | 1.35552400  |
| C | -1.63621000 | -1.49049200 | 0.68889200  |
| C | -1.26481600 | -2.77531700 | 1.18246400  |
| C | -1.99838300 | -3.28897500 | 2.29955300  |
| C | -2.92656100 | -2.49889500 | 2.97469500  |
| C | -3.18986200 | -1.21141700 | 2.51041500  |
| H | -2.80526500 | 0.28486900  | 0.98669100  |
| C | -0.18712100 | -3.59112700 | 0.63640800  |
| H | -3.44983300 | -2.89395900 | 3.83745700  |
| C | 1.01874600  | -2.95751000 | 0.03234200  |
| C | 3.10909900  | -2.52970500 | -1.18501400 |
| C | 4.28001600  | -2.38239400 | -1.93623400 |
| C | 2.72929000  | -1.57548400 | -0.21365700 |
| C | 5.06242100  | -1.26208400 | -1.68784500 |
| C | 3.53876100  | -0.43946400 | 0.02254000  |
| C | 4.70438900  | -0.28504100 | -0.71626500 |
| O | -1.80071000 | -4.53911500 | 2.75474800  |
| O | -0.16662400 | -4.83427500 | 0.75206000  |
| O | -4.09623800 | -0.48042500 | 3.20051400  |
| H | -4.20722200 | 0.39018500  | 2.78234400  |
| O | -1.04288900 | -1.09925200 | -0.48302000 |
| O | 5.51005600  | 0.78971900  | -0.50971700 |
| H | 6.26858900  | 0.70688700  | -1.11582400 |
| O | 3.22742800  | 0.45168300  | 1.02053500  |
| C | -1.73175500 | -0.35061900 | -1.46633100 |
| C | -3.12601500 | -0.91619900 | -1.81896100 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -1.07653300 | -0.42759500 | -2.34594100 |
| C | -3.86352100 | 0.02204000  | -2.79579800 |
| H | -3.72037000 | -0.98755100 | -0.90358100 |
| C | -2.36785700 | 1.88169100  | -2.00737100 |
| C | -3.82676400 | 1.47601800  | -2.29134600 |
| H | -1.79642200 | 1.81700600  | -2.94969200 |
| O | -1.79512900 | 0.99623100  | -1.03795200 |
| O | -3.02268700 | -2.24454500 | -2.29904500 |
| H | -2.59820300 | -2.22639600 | -3.17354900 |
| C | -2.20911000 | 3.30276800  | -1.48087600 |
| H | -1.14857500 | 3.57093000  | -1.48940900 |
| H | -2.74120400 | 3.98373400  | -2.15003100 |
| O | -2.67596400 | 3.41977600  | -0.13107100 |
| H | -3.45583300 | 3.99469200  | -0.11184700 |
| C | 2.07817800  | 1.26492000  | 0.84660000  |
| C | 1.31402100  | 1.32058700  | 2.17400300  |
| H | 1.43754200  | 0.84405200  | 0.05639500  |
| C | 0.13836700  | 2.30850400  | 2.03636200  |
| H | 2.01602900  | 1.70908000  | 2.92969000  |
| C | 1.46038200  | 3.46093500  | 0.21467700  |
| C | 0.60930600  | 3.66632500  | 1.48821500  |
| H | 0.81761800  | 3.04463800  | -0.57904400 |
| O | 2.53348700  | 2.54539500  | 0.47359400  |
| O | 0.85300000  | 0.04832200  | 2.58858300  |
| H | 1.04617400  | -0.61269100 | 1.88939900  |
| C | 2.06636700  | 4.74959400  | -0.31745600 |
| H | 2.65947900  | 4.51545300  | -1.21380000 |
| H | 1.24005600  | 5.40952600  | -0.61155600 |
| O | 2.87479400  | 5.34377400  | 0.69254100  |
| H | 3.14094300  | 6.21996900  | 0.37434500  |
| O | 6.23026200  | -0.97740600 | -2.33311700 |
| H | 6.43257200  | -1.65241200 | -3.00160400 |
| H | -1.21590100 | -4.99798000 | 2.10036100  |
| H | -3.34710000 | -0.01113000 | -3.76740800 |
| O | -5.17556900 | -0.43402000 | -3.07593300 |
| H | -5.68952700 | -0.40500100 | -2.25111400 |
| H | -4.39419300 | 1.55592700  | -1.35621600 |
| O | -4.45398200 | 2.37749000  | -3.19088100 |
| H | -4.08721800 | 2.23147400  | -4.07929800 |
| H | 4.58080900  | -3.11417800 | -2.67885600 |
| H | 1.25394800  | 4.14890700  | 2.23304900  |
| O | -0.46290800 | 4.56430900  | 1.25192000  |
| H | -1.22496300 | 4.08245200  | 0.86294900  |
| H | -0.58042500 | 1.87416900  | 1.33044100  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -0.58643800 | 2.44589600  | 3.25283200  |
| H | 0.00865900  | 2.84677800  | 3.90885300  |
| S | 1.92836400  | -3.82007400 | -1.20983900 |
| N | 1.55537900  | -1.84737000 | 0.45118400  |

## C

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.39081600  | -1.31159300 | 1.41282900  |
| C | 1.38538500  | -0.35773300 | 1.35119200  |
| C | 0.46317300  | -0.17021700 | 2.42681600  |
| C | 0.59639600  | -1.04682500 | 3.55899800  |
| C | 1.63093400  | -1.97721100 | 3.63723600  |
| C | 2.51796200  | -2.10014600 | 2.57182800  |
| H | 3.03551100  | -1.48080500 | 0.56004900  |
| C | -0.60342100 | 0.81342200  | 2.44122100  |
| H | 1.72198600  | -2.61122100 | 4.51133400  |
| C | -1.79427600 | 3.45258900  | 0.00780900  |
| C | -2.78624800 | 3.96743400  | -0.83529800 |
| C | -1.87707400 | 2.16057200  | 0.57776000  |
| C | -3.87765500 | 3.15773500  | -1.10403900 |
| C | -2.97941600 | 1.33392200  | 0.23890900  |
| C | -3.98135500 | 1.83941000  | -0.57833900 |
| O | -0.25415600 | -0.98945500 | 4.59109600  |
| O | -1.46286900 | 0.85580200  | 3.34627400  |
| O | 3.49340300  | -3.03122300 | 2.68330300  |
| H | 4.05152300  | -3.02329200 | 1.88715000  |
| O | 1.15446800  | 0.40225800  | 0.23365200  |
| O | -5.06566000 | 1.07963300  | -0.88304600 |
| H | -5.64186000 | 1.61093100  | -1.46188500 |
| O | -3.12190000 | 0.05403600  | 0.73640500  |
| C | 2.18638600  | 0.78347800  | -0.66865700 |
| C | 3.32218500  | 1.56638900  | 0.01846700  |
| H | 1.67042000  | 1.45079900  | -1.37258700 |
| C | 4.42772100  | 1.86995800  | -1.00573100 |
| H | 3.74795000  | 0.94083000  | 0.81834000  |
| C | 3.61740400  | -0.11981600 | -2.35269000 |
| C | 4.84830200  | 0.60217000  | -1.76656500 |
| H | 3.16698400  | 0.51645400  | -3.13308800 |
| O | 2.64539000  | -0.37214300 | -1.32927400 |
| O | 2.85509800  | 2.79928400  | 0.52610900  |
| H | 2.06104800  | 2.64997300  | 1.08137300  |
| C | 3.95949100  | -1.46150200 | -2.98100200 |
| H | 3.03400700  | -1.91781300 | -3.36013900 |
| H | 4.62952300  | -1.27685800 | -3.83054500 |
| O | 4.57585100  | -2.28427100 | -1.99668000 |



|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 4.83451500  | -3.11428400 | -2.42594000 |
| C | -2.34947400 | -0.94835100 | 0.10784100  |
| C | -2.61870400 | -2.27455300 | 0.81375200  |
| H | -1.28185500 | -0.68564200 | 0.14837000  |
| C | -1.83397200 | -3.38380400 | 0.09476000  |
| H | -3.69956100 | -2.47243500 | 0.71859500  |
| C | -1.97616400 | -1.99558300 | -1.99177400 |
| C | -2.15229900 | -3.41547500 | -1.40437200 |
| H | -0.90942800 | -1.71687000 | -1.93203400 |
| O | -2.75655500 | -1.05522400 | -1.24229200 |
| O | -2.23587100 | -2.20758500 | 2.17391400  |
| H | -2.13132600 | -3.13454300 | 2.45607400  |
| C | -2.39353000 | -1.89747300 | -3.45030300 |
| H | -2.26139000 | -0.85740600 | -3.78215300 |
| H | -1.71782600 | -2.53509800 | -4.03527600 |
| O | -3.74765800 | -2.31355900 | -3.57994300 |
| H | -3.95223900 | -2.35296400 | -4.52680300 |
| O | -4.93029300 | 3.51215900  | -1.89309700 |
| H | -4.81453700 | 4.41059800  | -2.24392800 |
| H | -0.94743600 | -0.31273500 | 4.34883900  |
| H | 4.02032700  | 2.59480200  | -1.72423900 |
| O | 5.53379500  | 2.53325700  | -0.41363300 |
| H | 5.95226200  | 1.91839700  | 0.21254800  |
| H | 5.34643200  | -0.08707000 | -1.07663300 |
| O | 5.80708100  | 0.87791200  | -2.77855800 |
| H | 5.45920000  | 1.58902800  | -3.34285000 |
| H | -2.71547900 | 4.96408700  | -1.25956000 |
| H | -3.19467000 | -3.71456200 | -1.55530400 |
| O | -1.37844400 | -4.37650400 | -2.10836900 |
| H | -0.43901100 | -4.20828800 | -1.92327700 |
| H | -0.76379700 | -3.17169200 | 0.22596900  |
| O | -2.03025900 | -4.62807400 | 0.76128600  |
| H | -2.93930500 | -4.92720500 | 0.58518000  |
| S | -0.32954600 | 4.22624100  | 0.55447700  |
| N | 0.14199300  | 2.90650400  | 1.51497500  |
| C | -0.73833100 | 1.93638500  | 1.43581600  |

## TMS

|    |             |             |             |
|----|-------------|-------------|-------------|
| Si | 0.00017900  | -0.00011900 | -0.00004300 |
| C  | -0.94550700 | -1.43927300 | -0.78963900 |
| H  | -1.96310600 | -1.14165200 | -1.07558800 |
| H  | -0.44202900 | -1.80203200 | -1.69558600 |
| H  | -1.03295300 | -2.28868800 | -0.09921000 |
| C  | -0.91820600 | 0.58306600  | 1.55087500  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -1.00686300 | -0.22220900 | 2.29218200  |
| H | -0.39709500 | 1.41976100  | 2.03493600  |
| H | -1.93456900 | 0.92294200  | 1.31143900  |
| C | 0.12167300  | 1.42999500  | -1.23647200 |
| H | 0.66349300  | 2.28457800  | -0.80994600 |
| H | 0.65090600  | 1.12730100  | -2.14980000 |
| H | -0.87277100 | 1.78701100  | -1.53565700 |
| C | 1.74198300  | -0.57374000 | 0.47530600  |
| H | 1.70931200  | -1.40291500 | 1.19447900  |
| H | 2.30311300  | -0.92121300 | -0.40232700 |
| H | 2.32038800  | 0.23848300  | 0.93526700  |