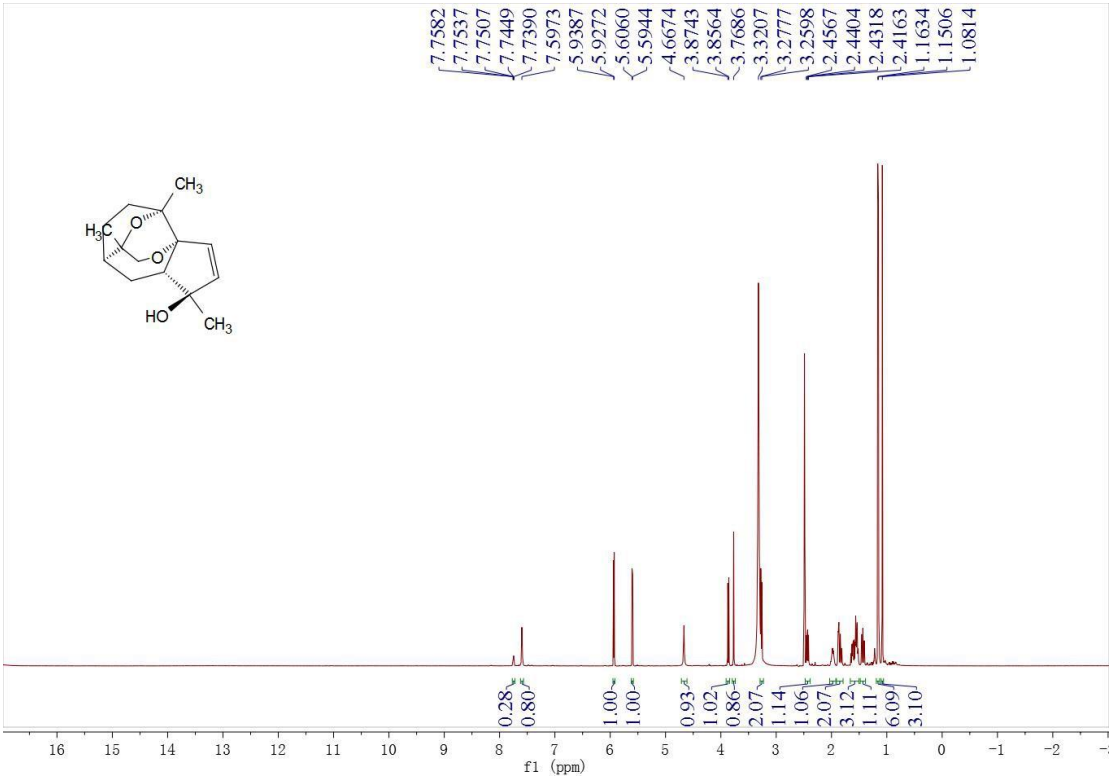



**Figure S1.** $^{1}$H NMR spectrum of compound **1** in DMSO-*d6*.

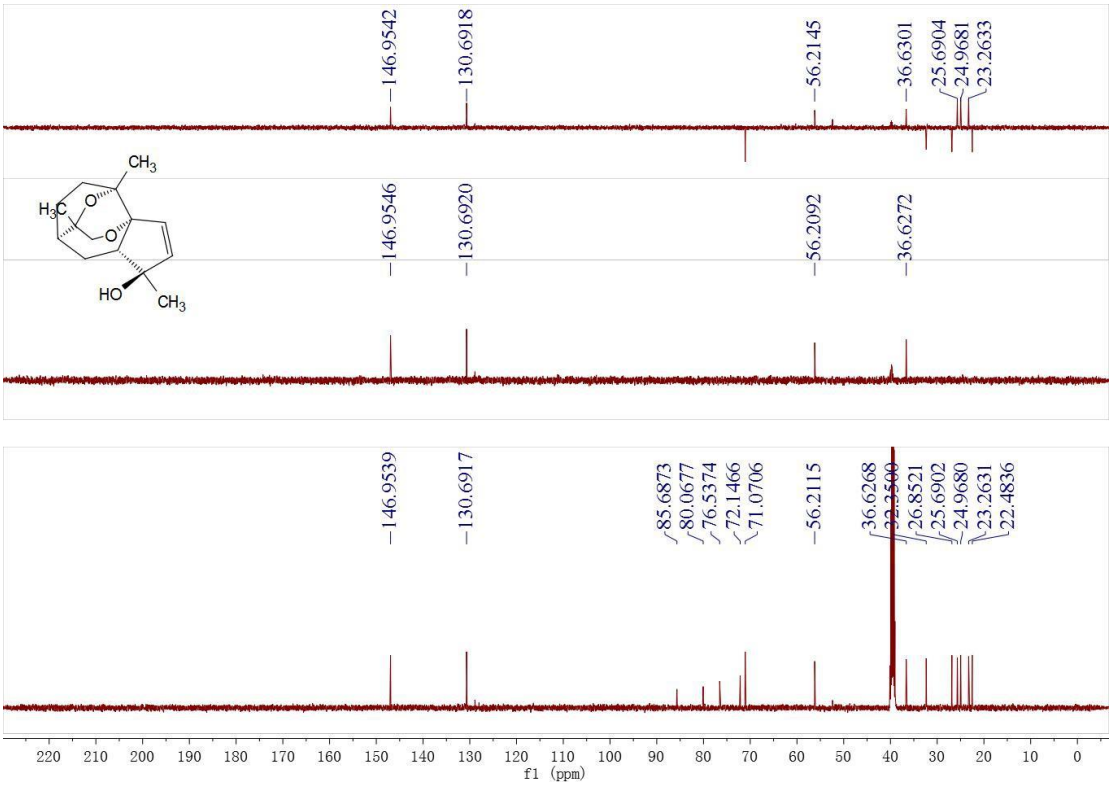



**Figure S2.** $^{13}$C NMR and DEPT spectrum of compound **1** in DMSO-*d6*.

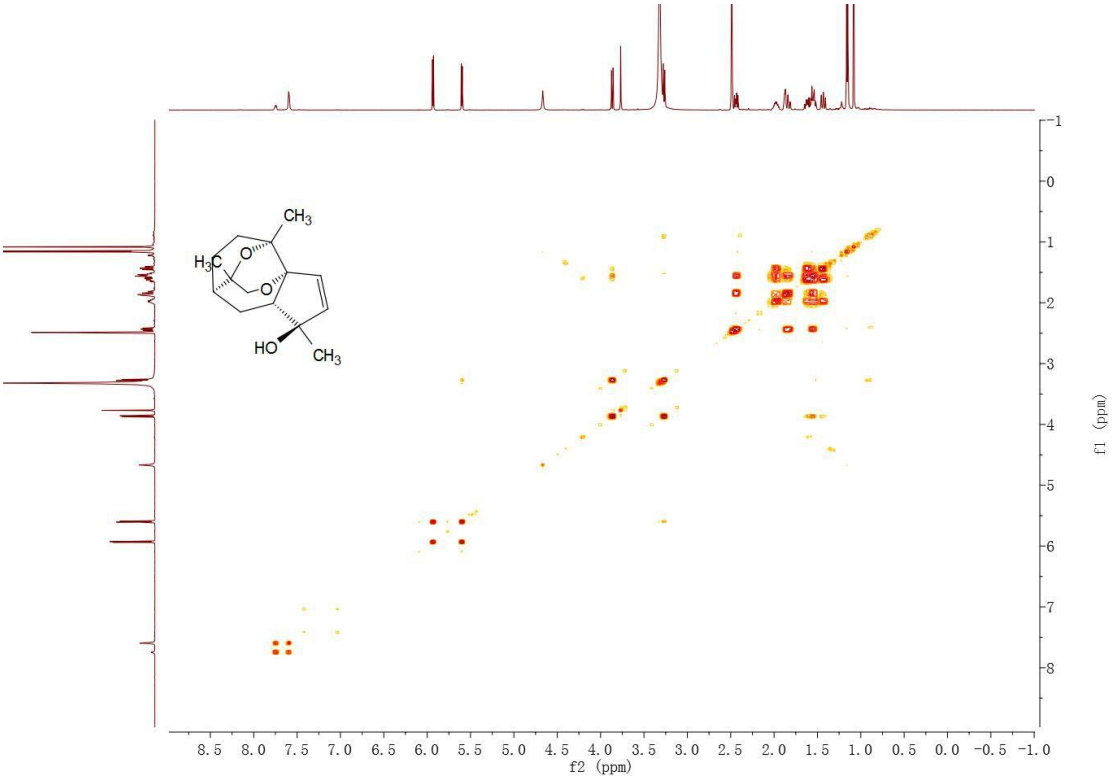



**Figure S3.** $^{1}$H-$^{1}$H COSY spectrum of compound **1** in DMSO-*d6*.

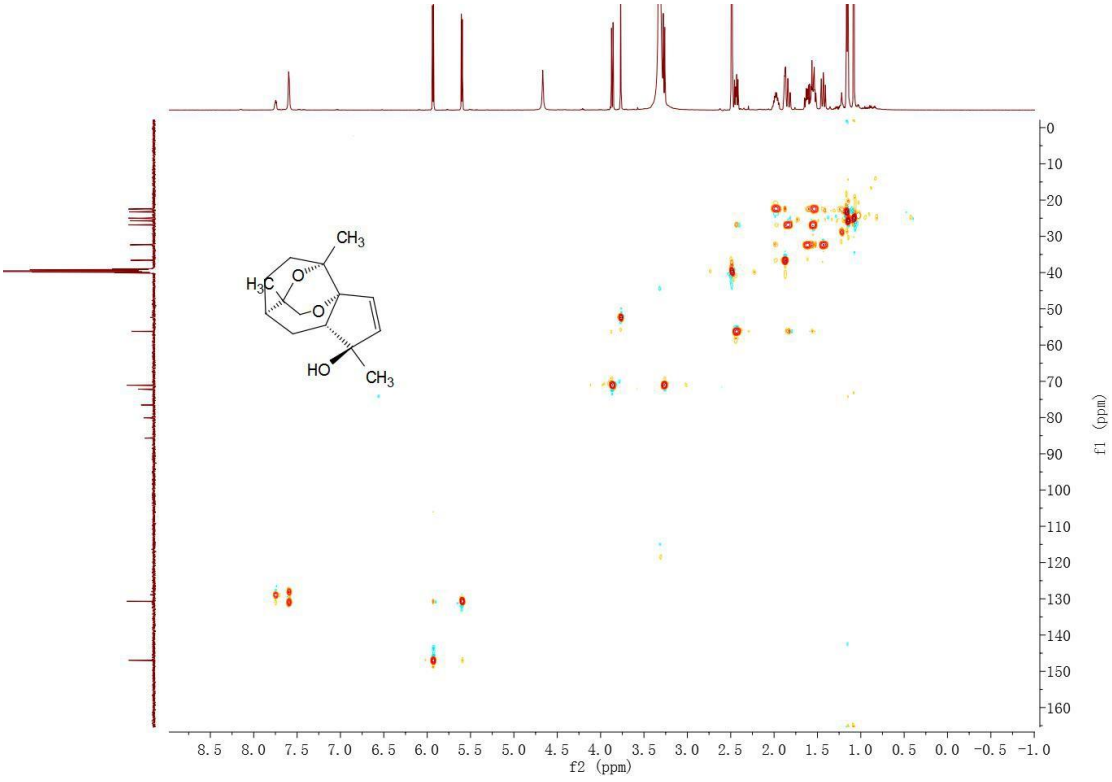



**Figure S4.** HSQC spectrum of compound **1** in DMSO-*d6*.

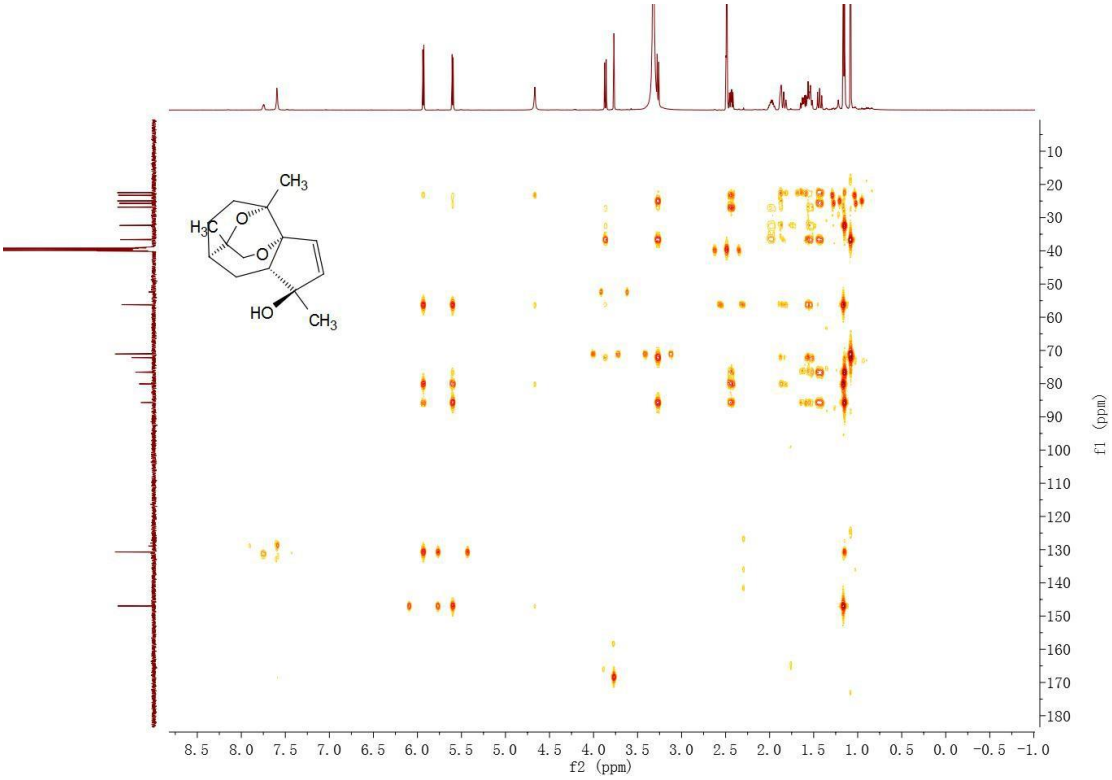



**Figure S5.** HMBC spectrum of compound **1** in DMSO-*d6*.

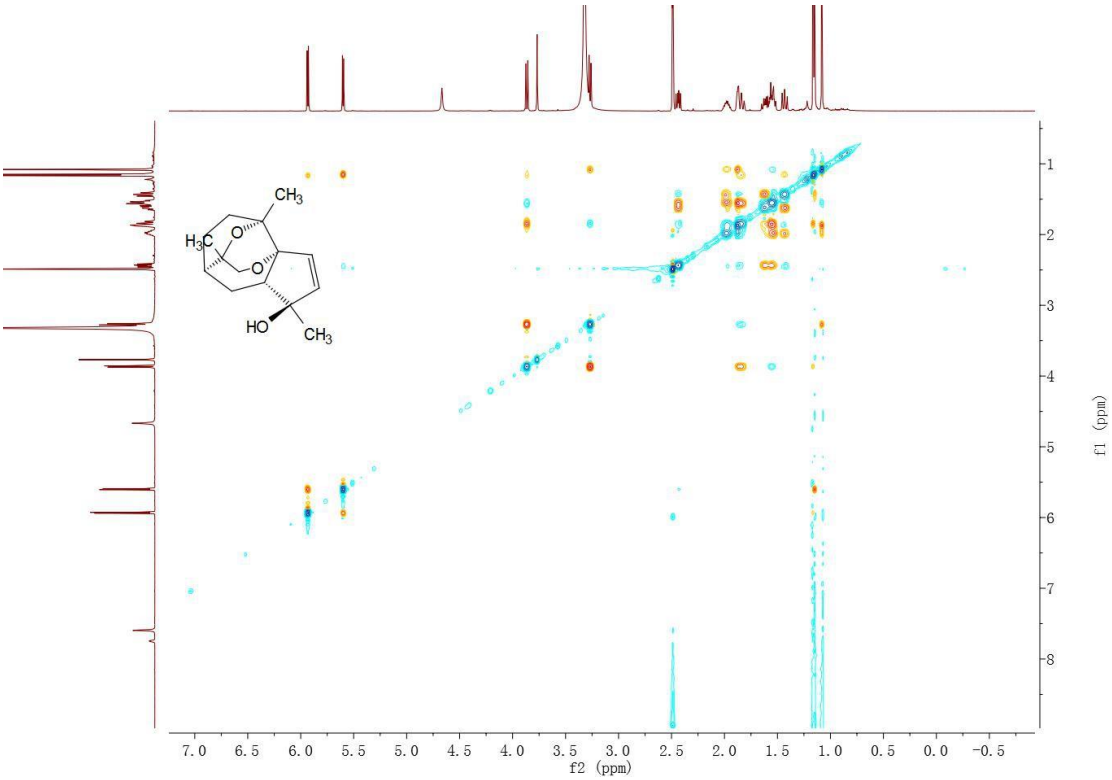



**Figure S6.** ROESY spectrum of compound **1** in DMSO-*d6*.

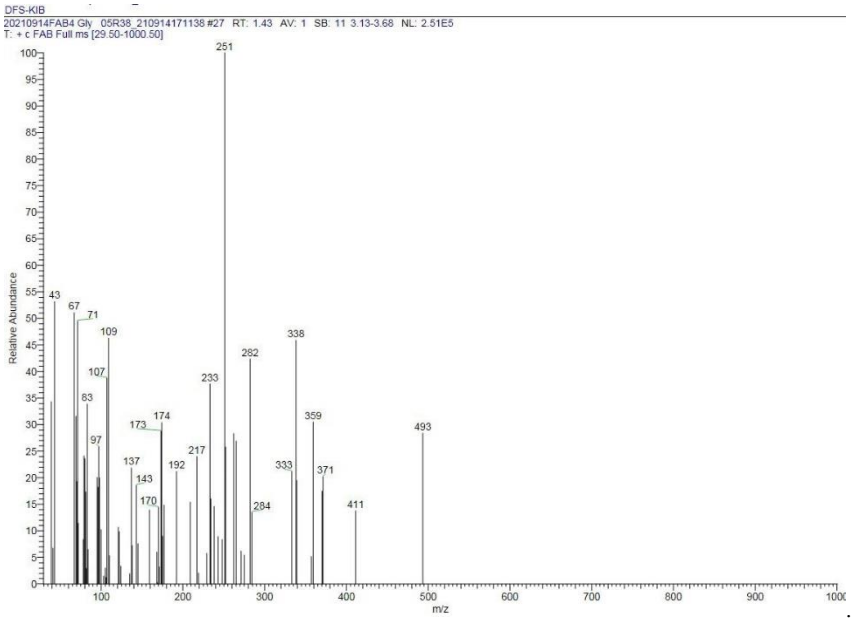



**Figure S7.** HRFABMS spectrum of compound **1.**

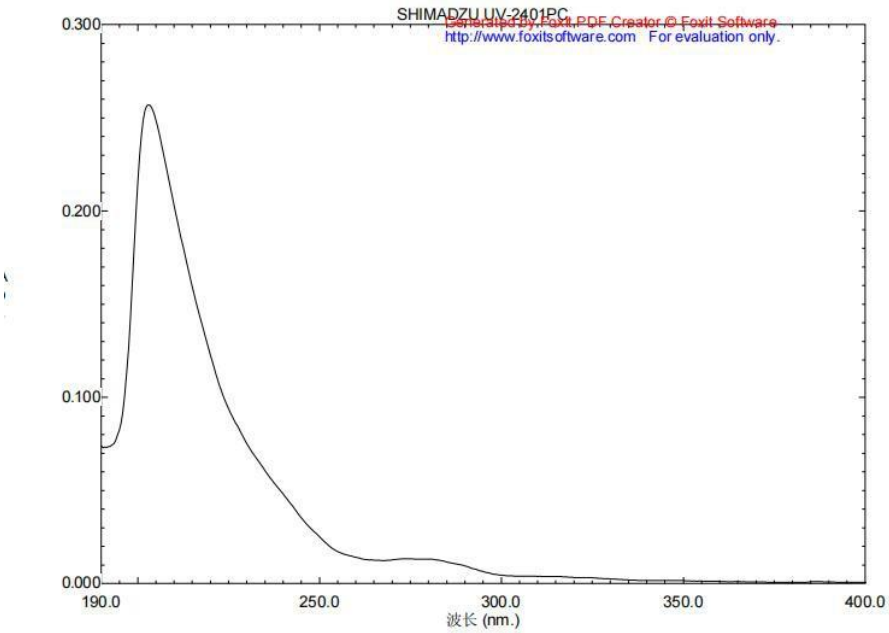



**Figure S8.** UV spectrum of **1** in methanol.

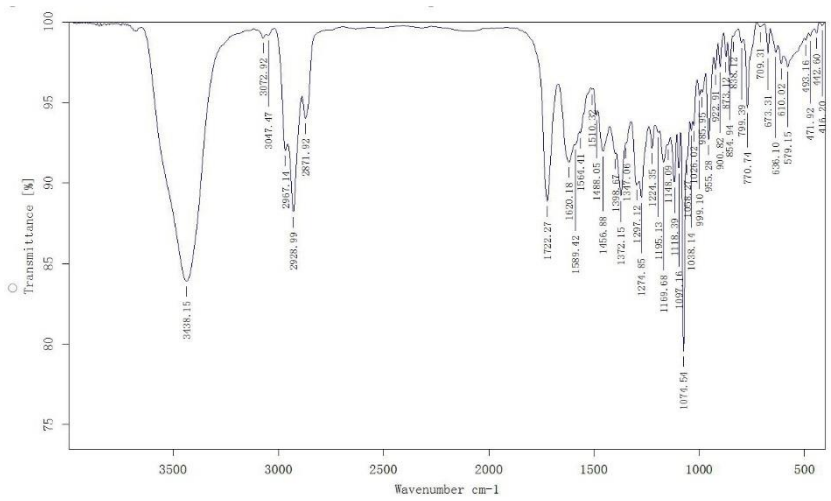
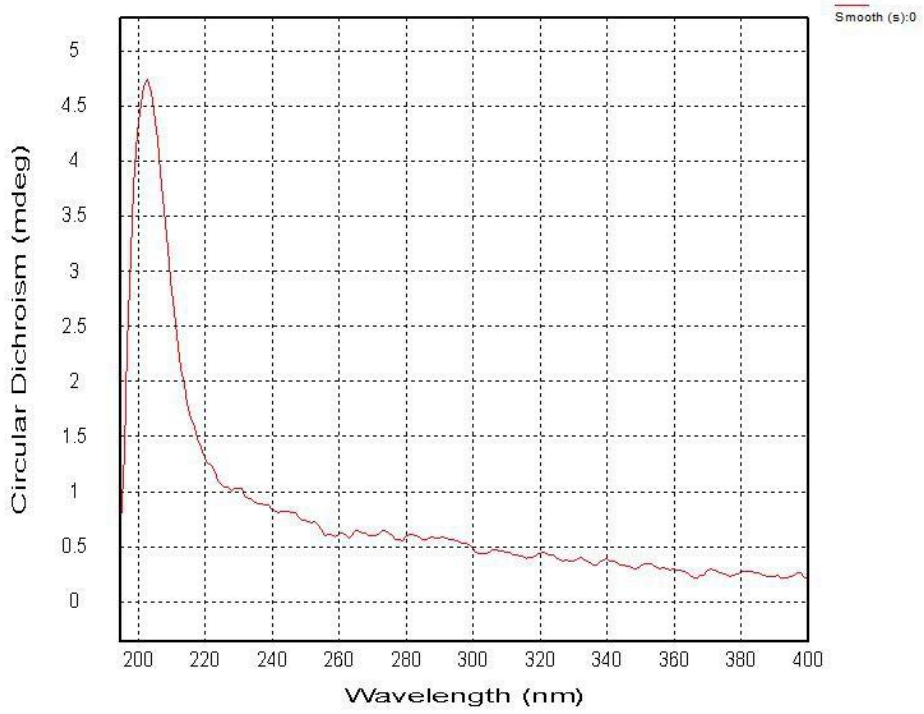



**Figure S9.** IR spectrum of **1** in methanol.



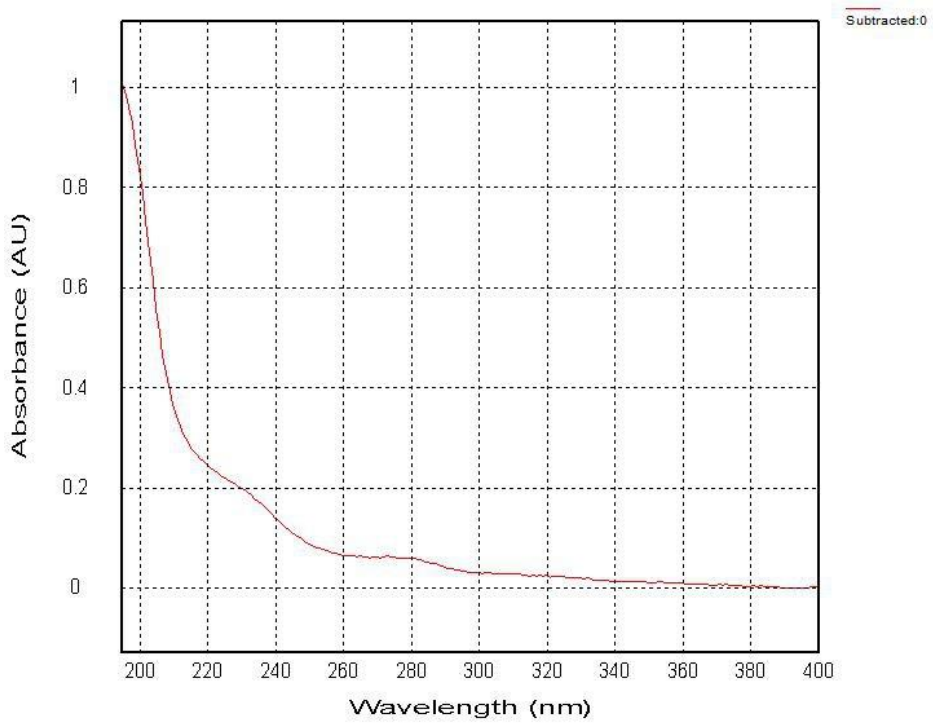



**Figure S10.** CD spectrum of **1** in methanol.

**Rudolph Research Analytical**

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Wednesday, 09-FEB-2022

Set Temperature : 20.0

Time Delay : Disabled

Delay between Measurement : Disabled

| n | Average | Std.Dev. | % RSD | Maximum | Minimum |
|---|---|---|---|---|---|
| 5 | 36.50 | 0.50 | 1.36 | 37.00 | 36.00 |

| S.No | Sample ID | Time | Result | Scale | OR °Arc | WLG.nm | Lg.mm | Conc.g/100ml | Temp. |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 05R38 | 05:37:12 PM | 36.00 | SR | 0.072 | 589 | 100.00 | 0.200 | 20.3 |
| 2 | 05R38 | 05:37:18 PM | 36.00 | SR | 0.072 | 589 | 100.00 | 0.200 | 20.2 |
| 3 | 05R38 | 05:37:25 PM | 36.50 | SR | 0.073 | 589 | 100.00 | 0.200 | 20.2 |
| 4 | 05R38 | 05:37:32 PM | 37.00 | SR | 0.074 | 589 | 100.00 | 0.200 | 20.1 |
| 5 | 05R38 | 05:37:39 PM | 37.00 | SR | 0.074 | 589 | 100.00 | 0.200 | 20.1 |

**Figure S11.** Specific Rotation of **1** in methanol.

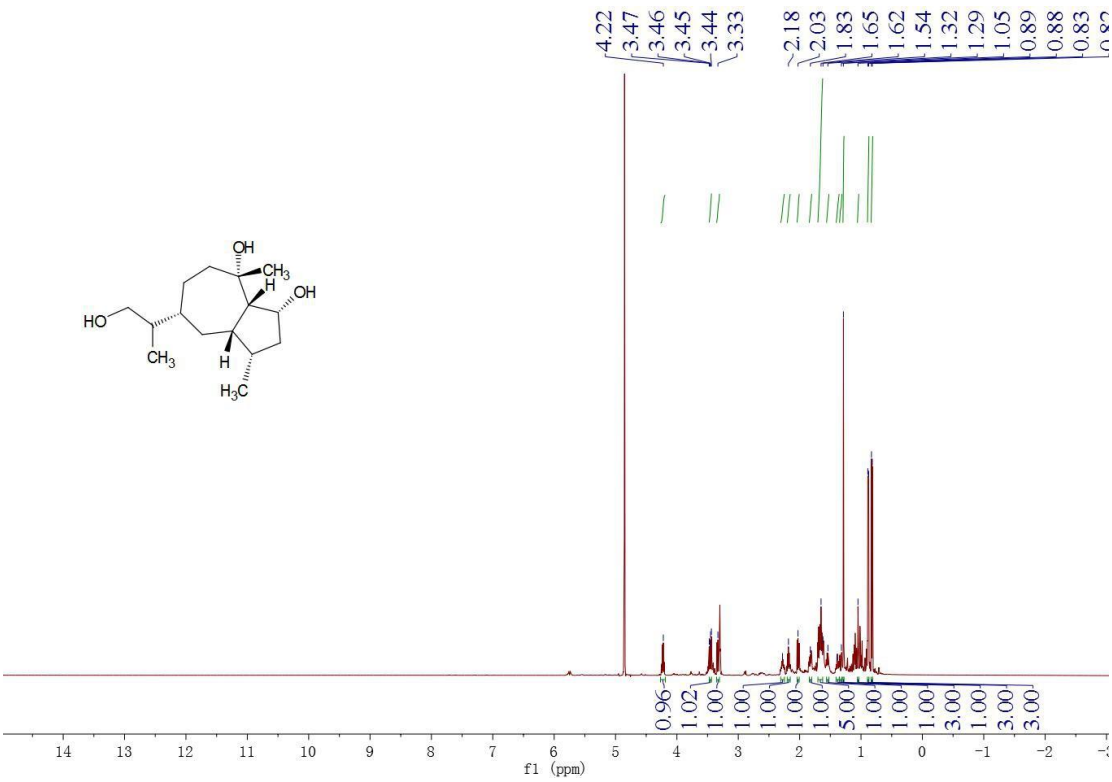



**Figure S12.** $^{1}$H NMR spectrum of compound **2** in CD3OD.

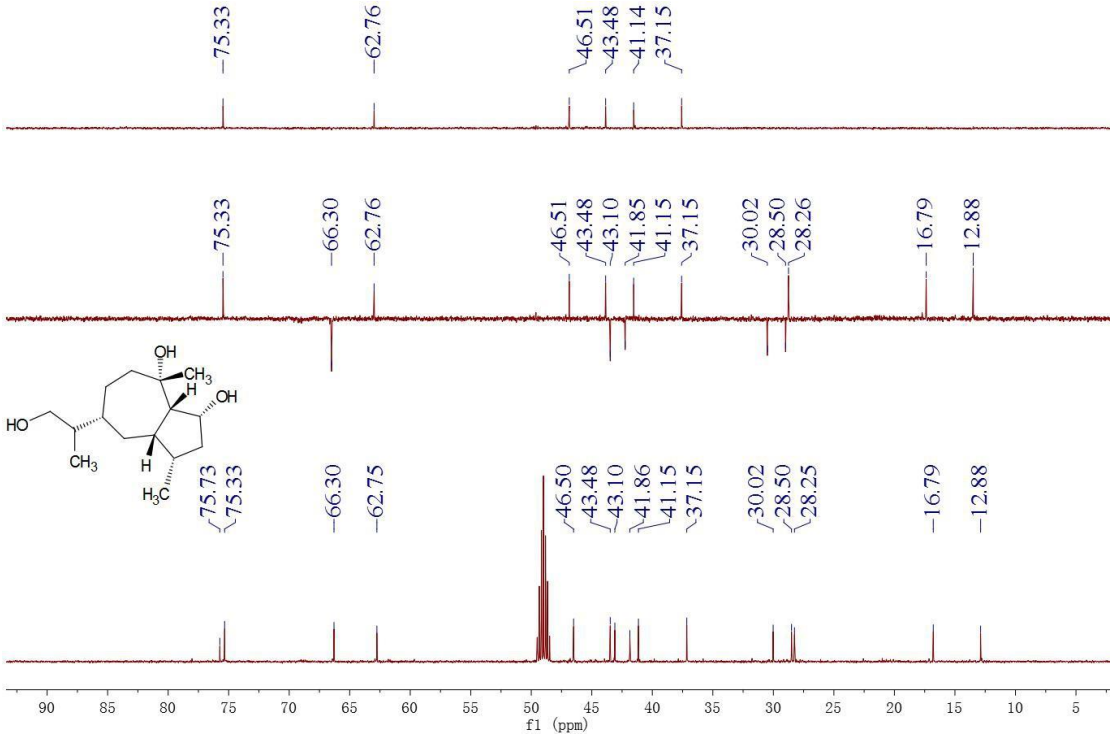



**Figure S13.** $^{13}$C NMR and DEPT spectrum of compound **2** in CD3OD.

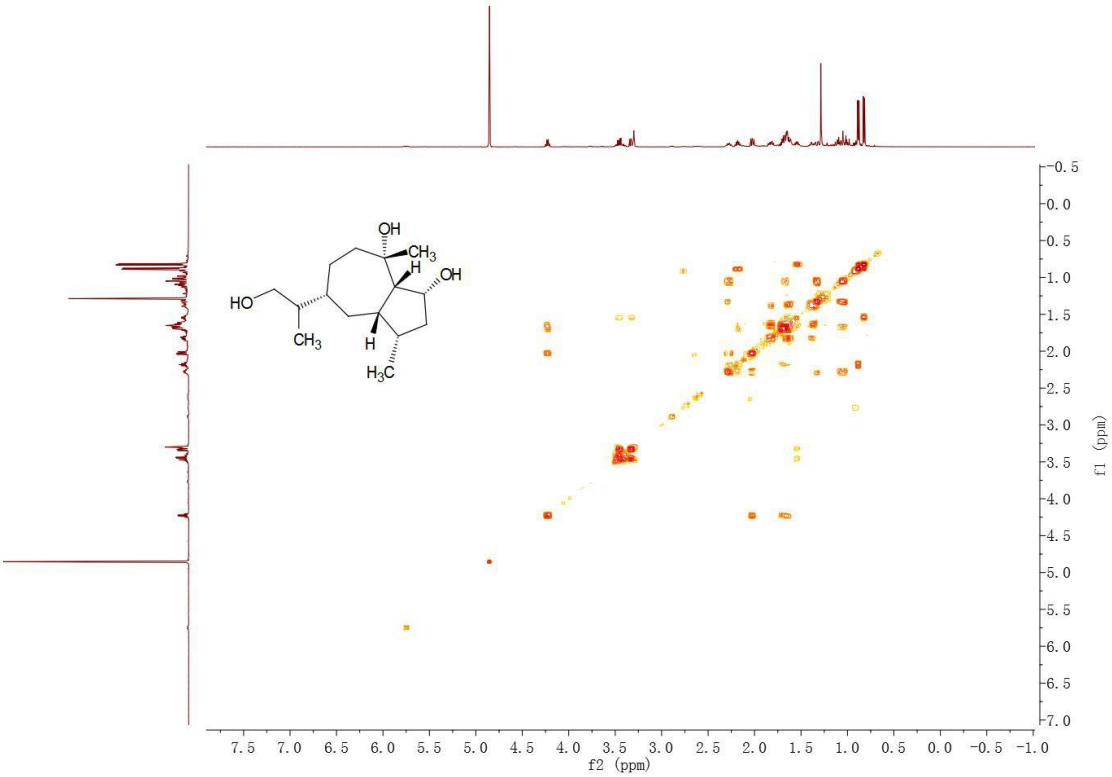



**Figure S14.** $^{1}$H-$^{1}$H COSY spectrum of compound **2** in CD3OD.

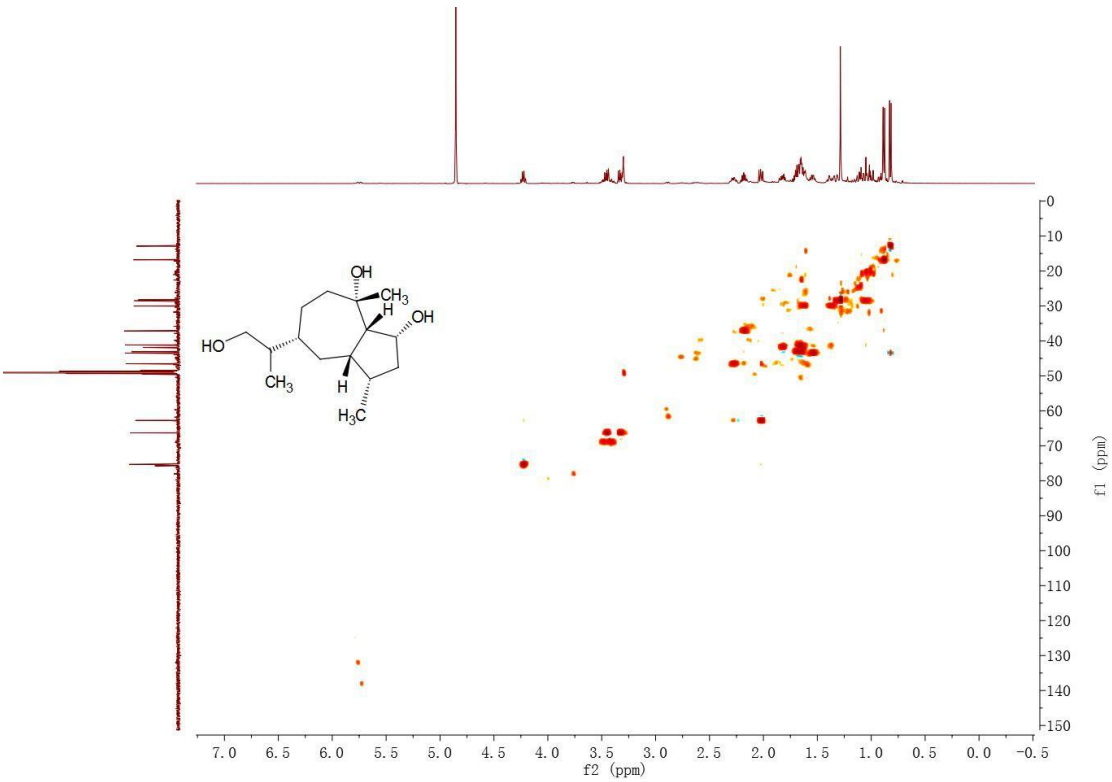



**Figure S15.** HSQC spectrum of compound **2** in CD3OD.

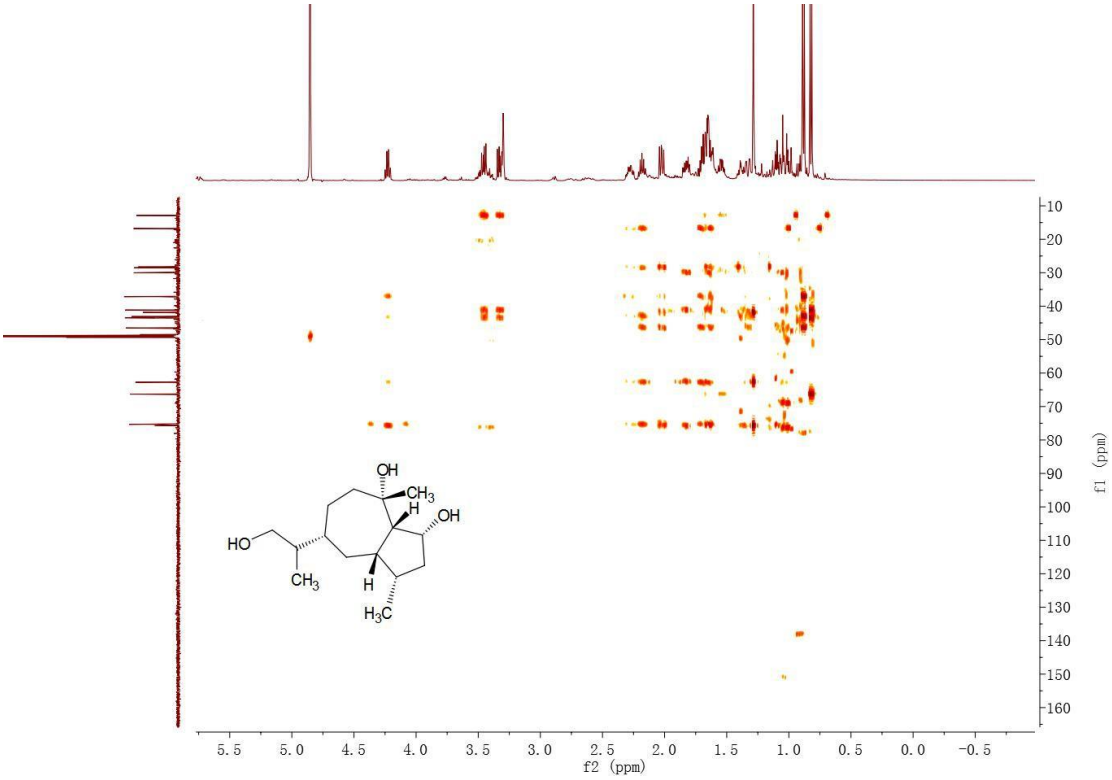



**Figure S16.** HMBC spectrum of compound **2** in CD3OD.

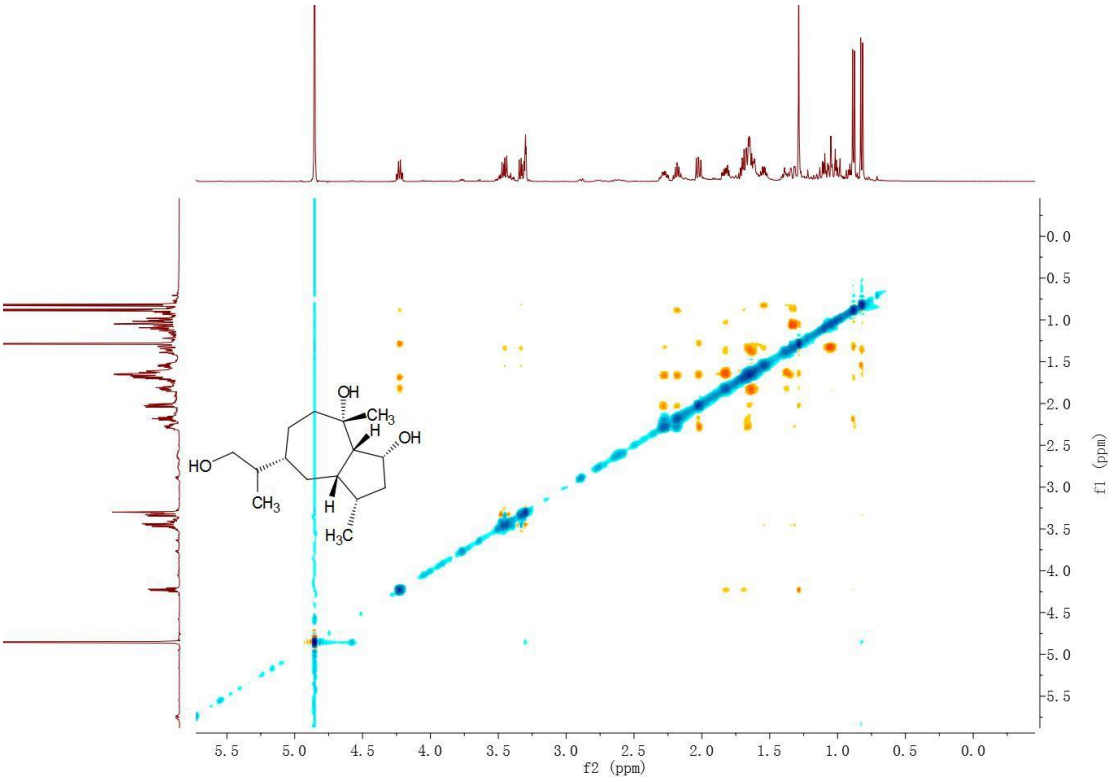



**Figure S17.** ROESY spectrum of compound **2** in CD3OD.

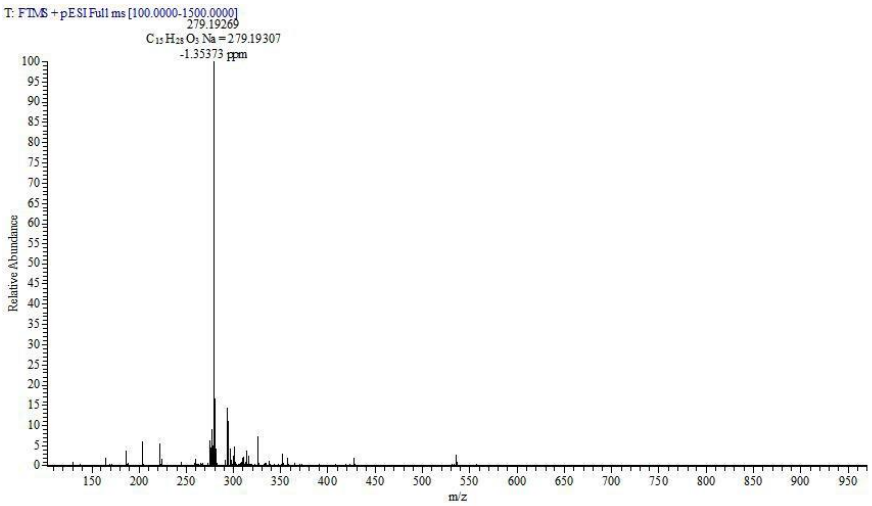



**Figure S18.** HRESIMS spectrum of compound **2.**

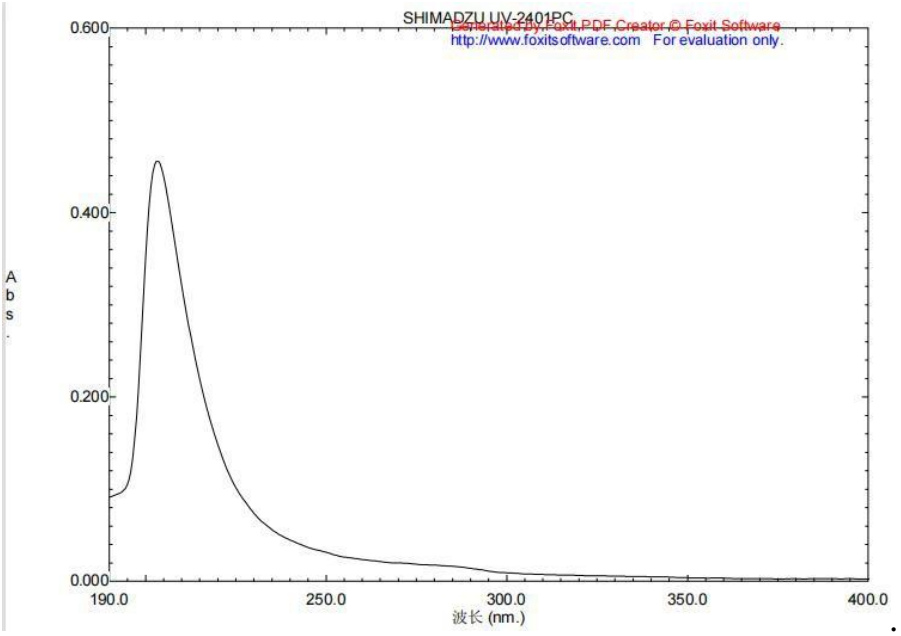



**Figure S19.** UV spectrum of **2** in methanol.

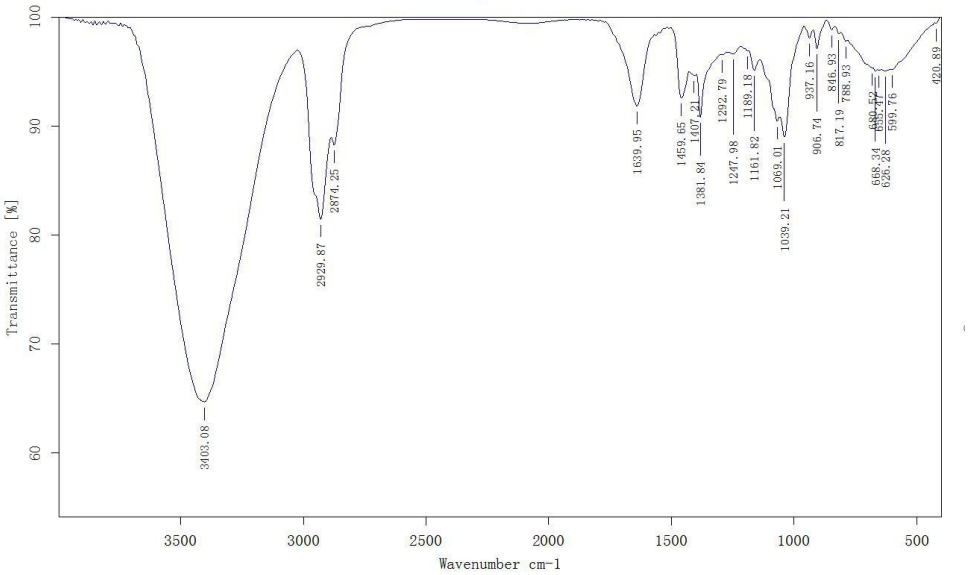
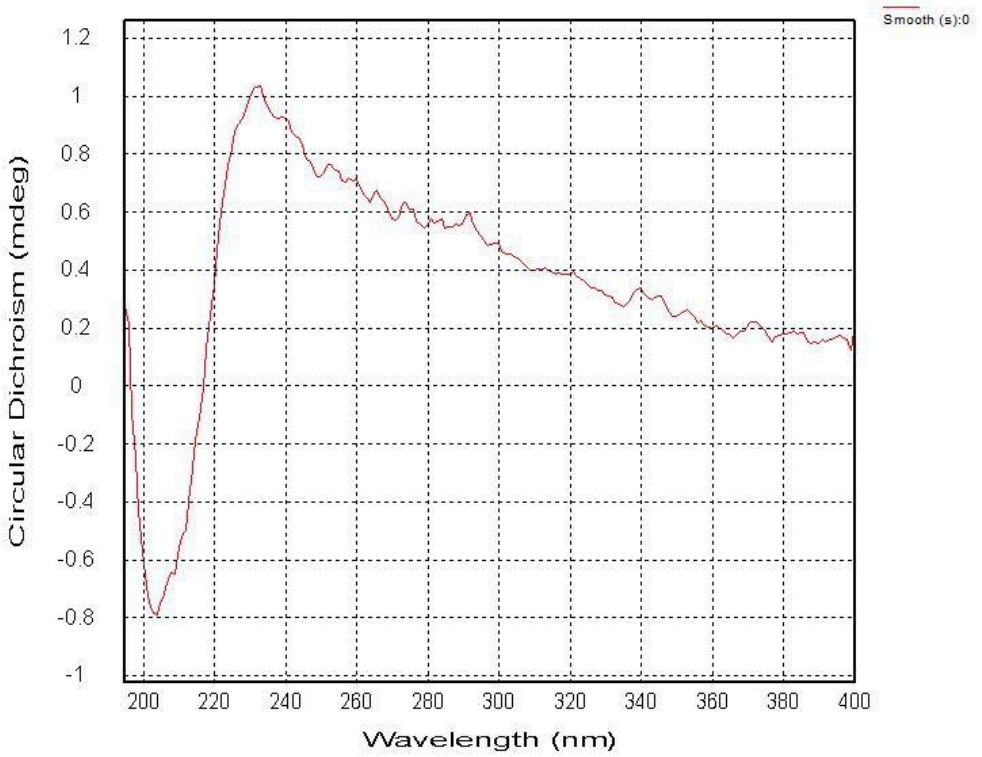



**Figure S20.** IR spectrum of **2** in methanol.



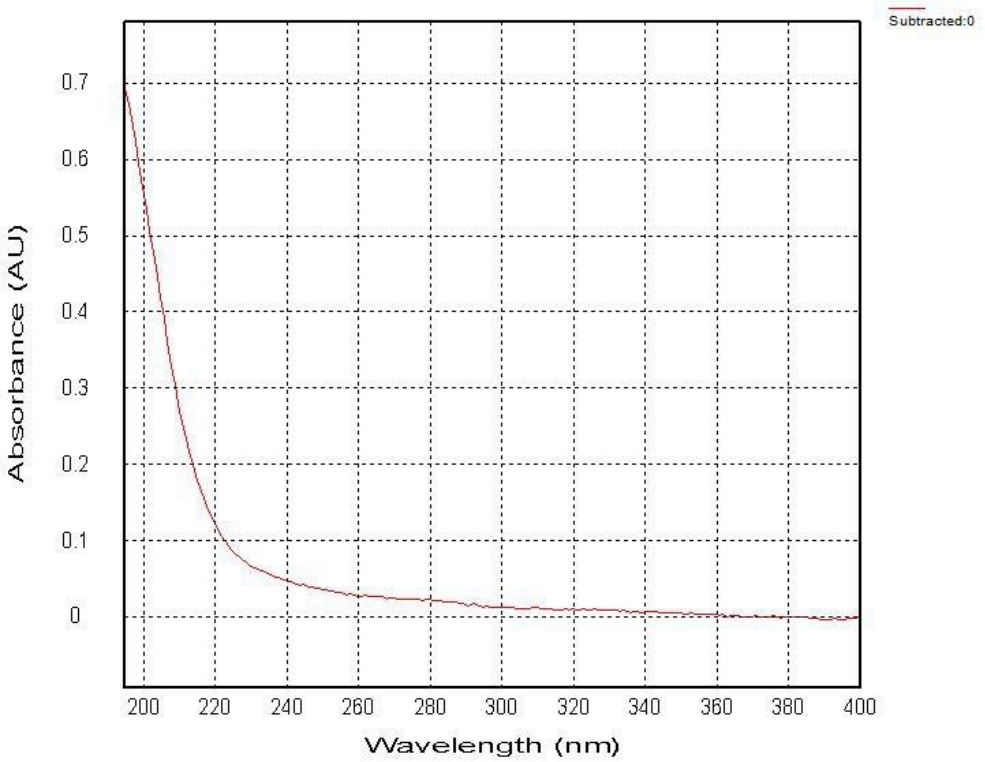



**Figure S21.** CD spectrum of **2** in methanol.

**Rudolph Research Analytical**

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Wednesday, 09-FEB-2022

Set Temperature : 20.0

Time Delay : Disabled

Delay between Measurement : Disabled

| n | Average | Std.Dev. | % RSD | Maximum | Minimum |
|---|---|---|---|---|---|
| 5 | -2.33 | 0.37 | -15.87 | -1.67 | -2.50 |

| S.No | Sample ID | Time | Result | Scale | OR °Arc | WLG.nm | Lg.mm | Conc.g/100ml | Temp. |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 05R47 | 05:53:55 PM | -1.67 | SR | -0.002 | 589 | 100.00 | 0.120 | 20.1 |
| 2 | 05R47 | 05:54:02 PM | -2.50 | SR | -0.003 | 589 | 100.00 | 0.120 | 20.1 |
| 3 | 05R47 | 05:54:08 PM | -2.50 | SR | -0.003 | 589 | 100.00 | 0.120 | 20.1 |
| 4 | 05R47 | 05:54:15 PM | -2.50 | SR | -0.003 | 589 | 100.00 | 0.120 | 20.0 |
| 5 | 05R47 | 05:54:22 PM | -2.50 | SR | -0.003 | 589 | 100.00 | 0.120 | 20.0 |

**Figure S22.** Specific Rotation of **2** in methanol.

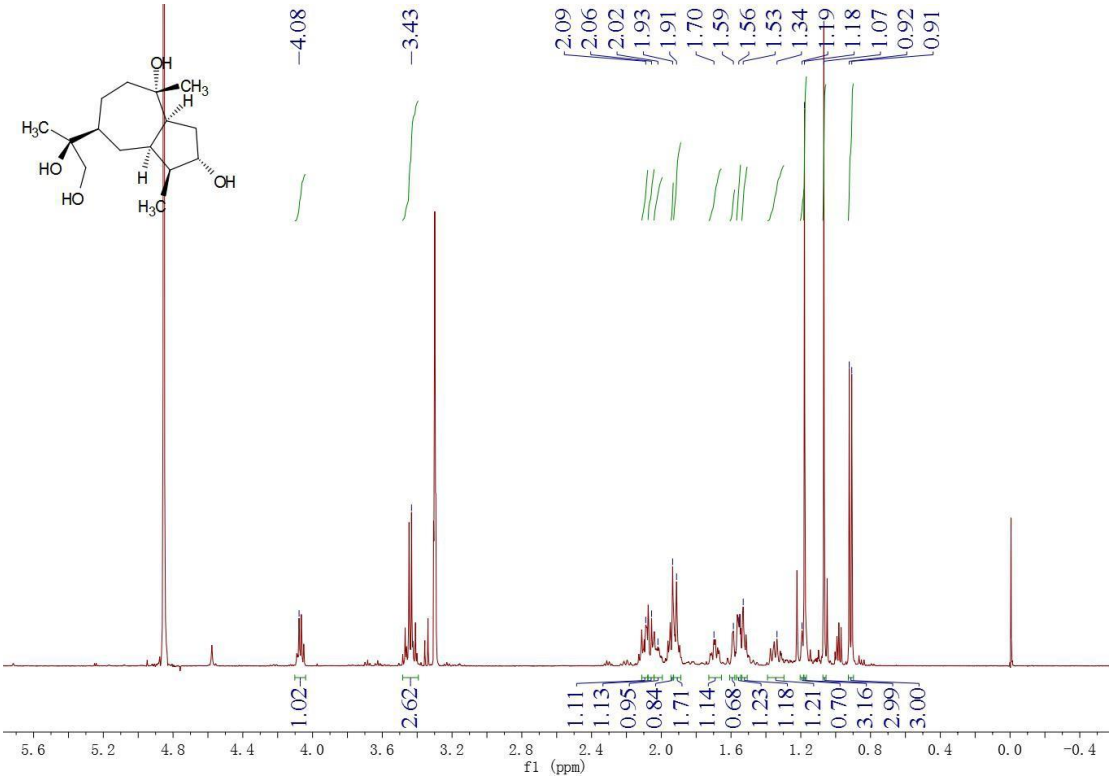



**Figure S23.** $^{1}$H NMR spectrum of compound **3** in CD3OD.

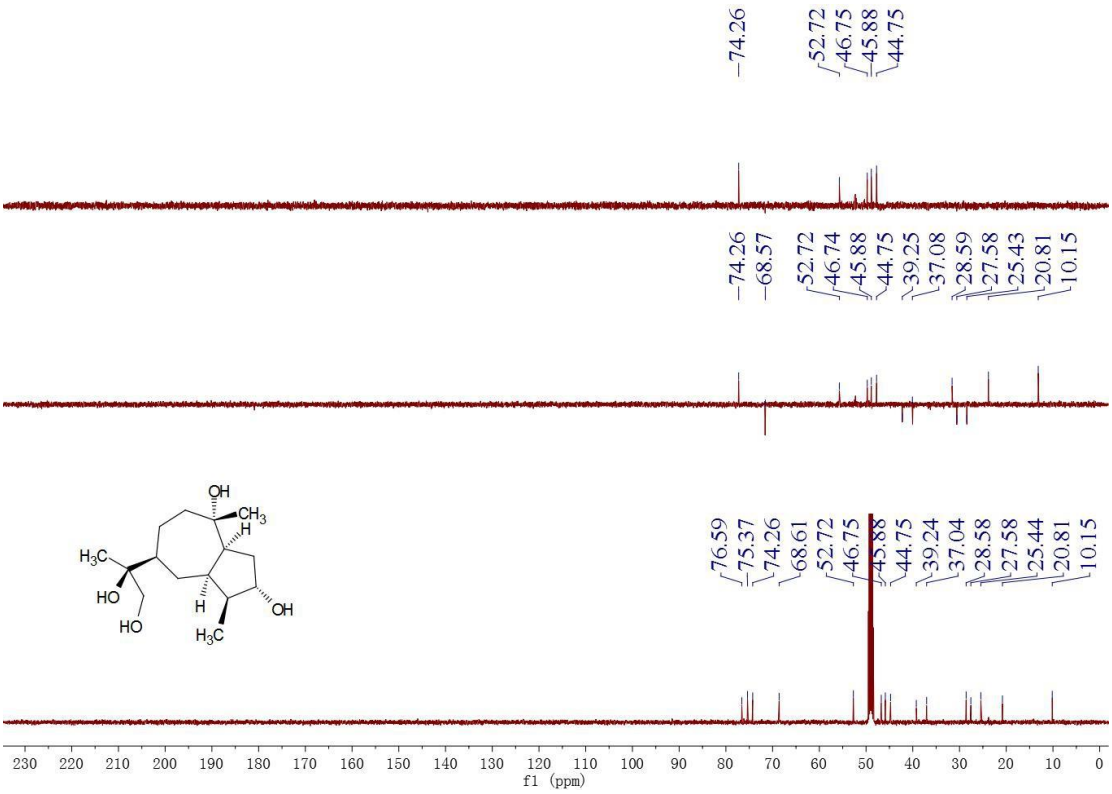



**Figure S24.** $^{13}$C NMR and DEPT spectrum of compound **3** in CD3OD.

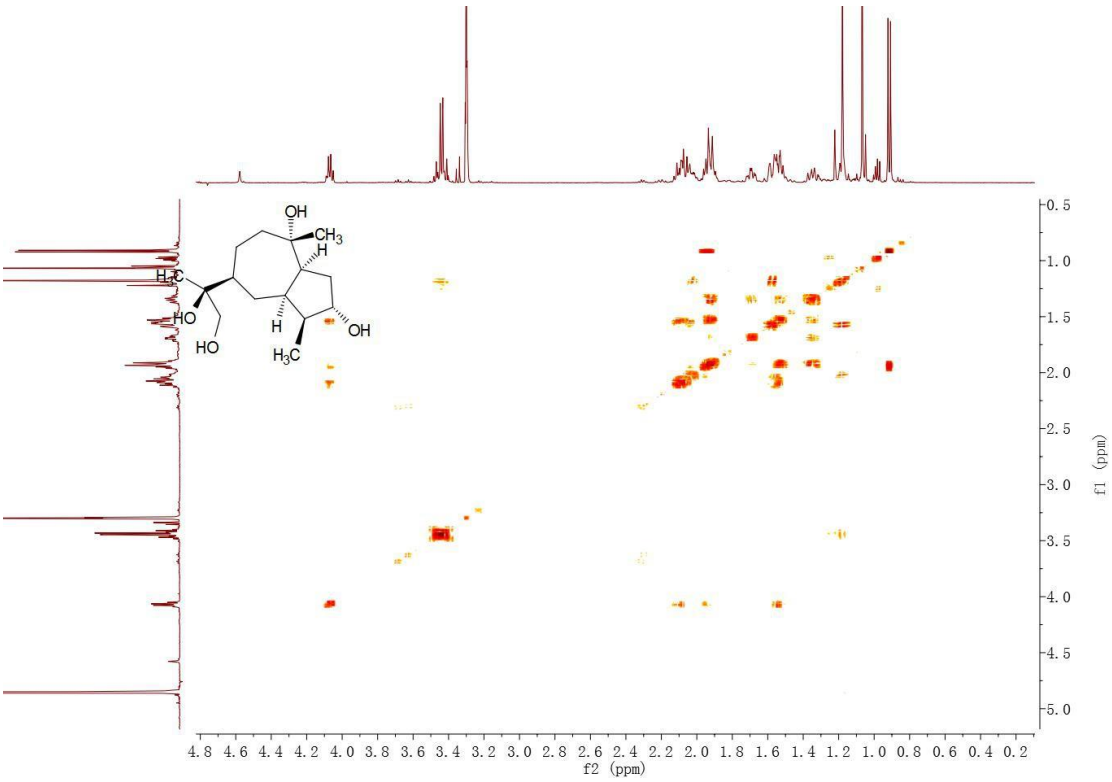



**Figure S25.** $^{1}$H-$^{1}$H COSY spectrum of compound **3** in CD3OD.

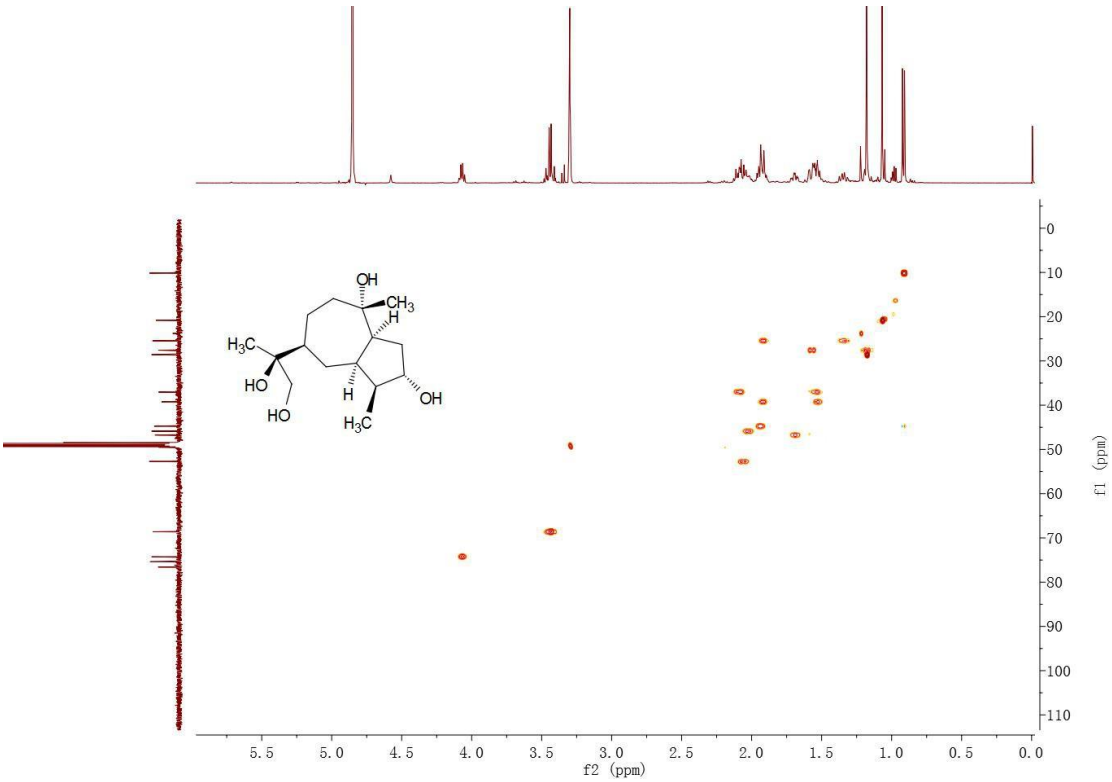



**Figure S26.** HSQC spectrum of compound **3** in CD3OD.

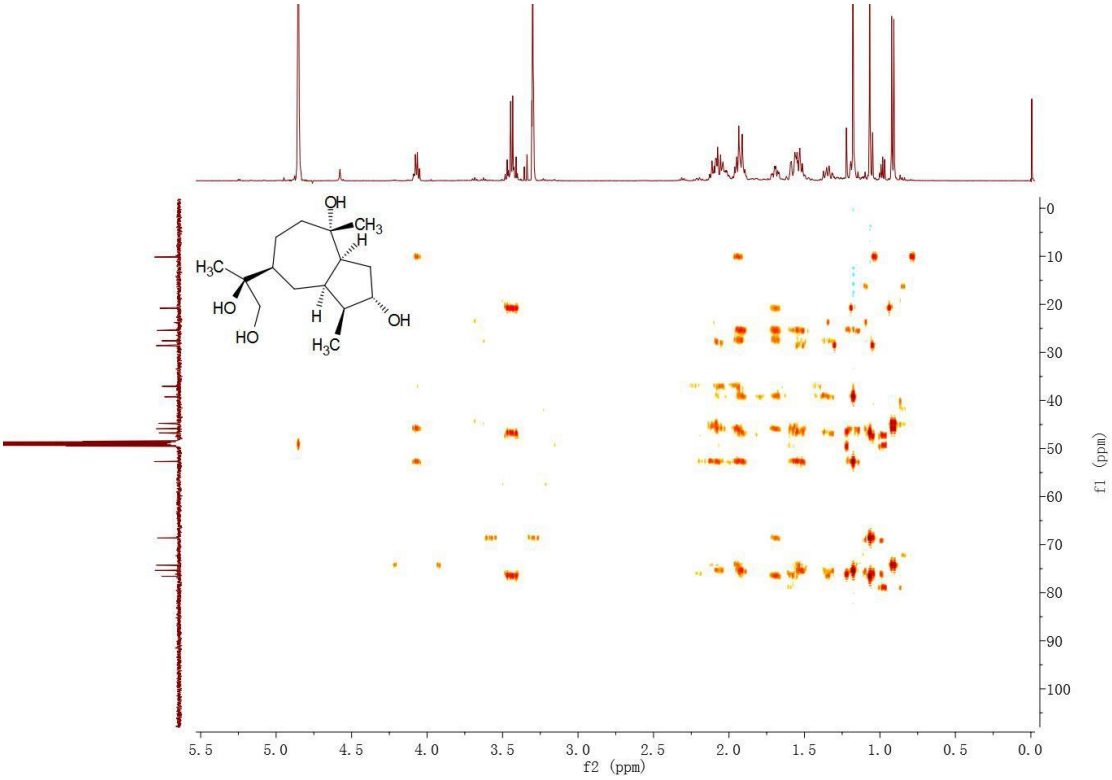



**Figure S27.** HMBC spectrum of compound **3** in CD3OD.

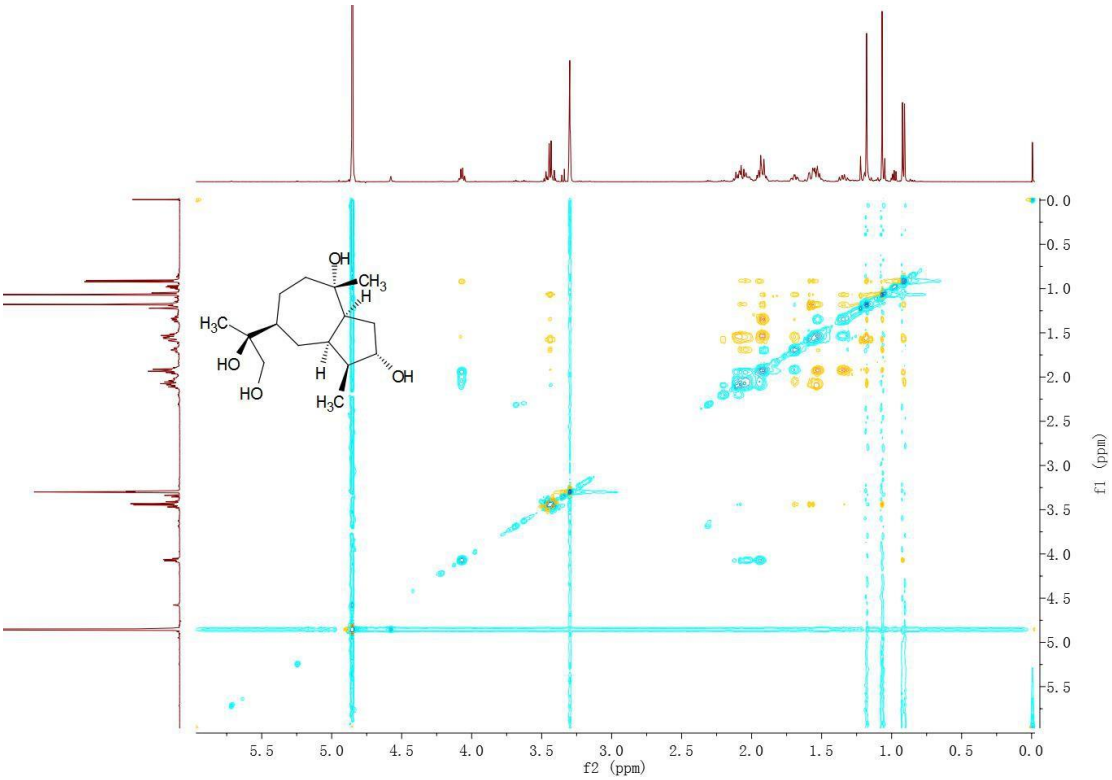



**Figure S28.** ROESY spectrum of compound **3** in CD3OD.

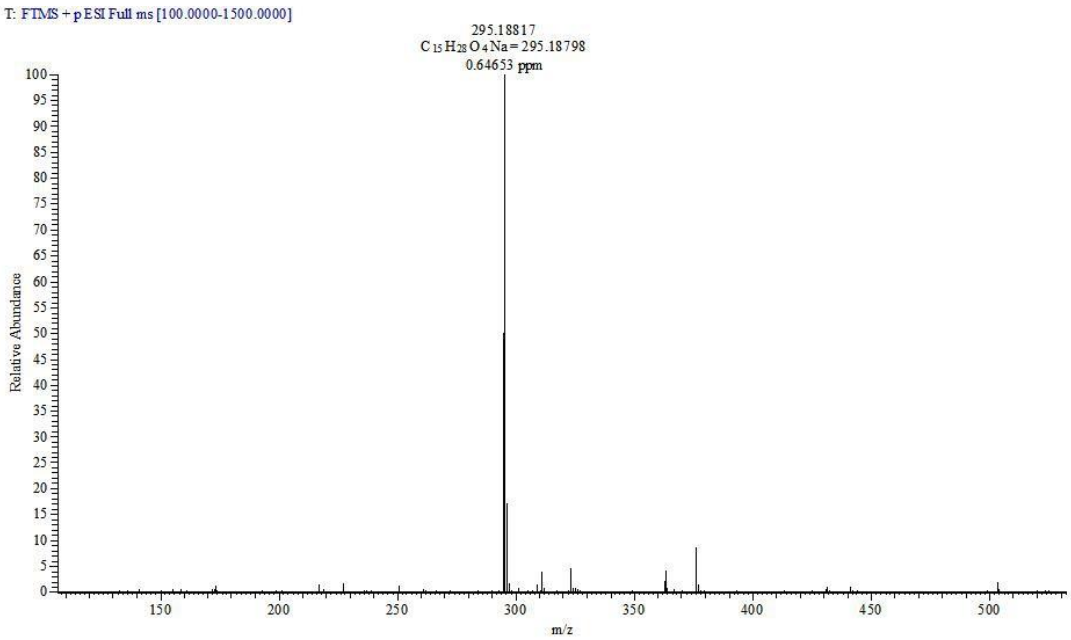



**Figure S29.** HRESIMS spectrum of compound **3.**

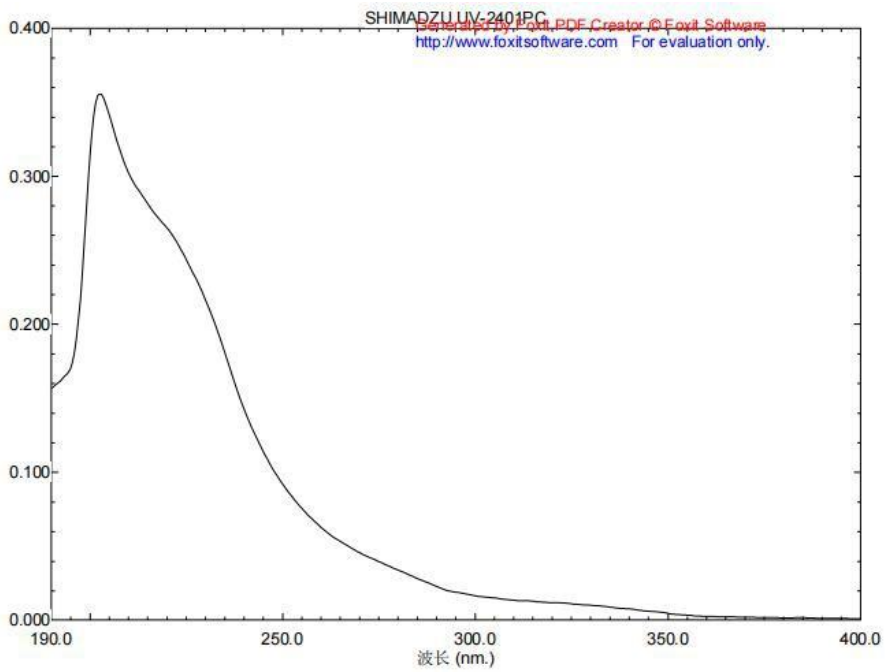



**Figure S30.** UV spectrum of **3** in methanol.

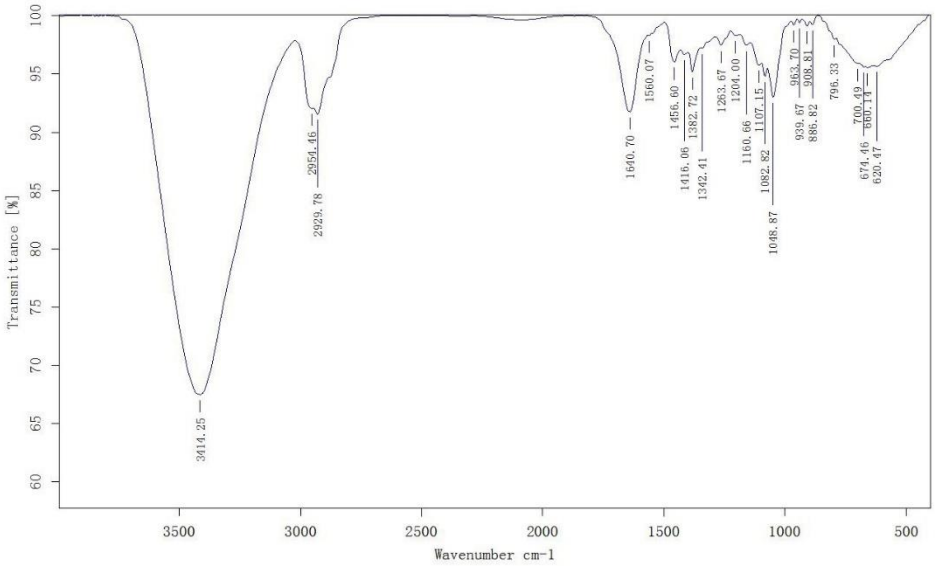



**Figure S31.** IR spectrum of **3** in methanol.

**Rudolph Research Analytical**

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Saturday, 28-MAY-2022

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled

| n | Average | Std.Dev. | % RSD | Maximum | Minimum |
|---|---|---|---|---|---|
| 5 | -10.78 | 0.26 | -2.41 | -10.40 | -11.10 |

| S.No | Sample ID | Time | Result | Scale | OR °Arc | WLG.nm | Lg.mm | Conc.g/100ml | Temp. |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 05R14 | 11:10:52 AM | -10.90 | SR | -0.0109 | 589 | 100.00 | 0.100 | 24.4 |
| 2 | 05R14 | 11:11:01 AM | -10.40 | SR | -0.0104 | 589 | 100.00 | 0.100 | 24.4 |
| 3 | 05R14 | 11:11:09 AM | -10.80 | SR | -0.0108 | 589 | 100.00 | 0.100 | 24.4 |
| 4 | 05R14 | 11:11:17 AM | -11.10 | SR | -0.0111 | 589 | 100.00 | 0.100 | 24.4 |
| 5 | 05R14 | 11:11:25 AM | -10.70 | SR | -0.0107 | 589 | 100.00 | 0.100 | 24.4 |

**Figure S32.** Specific Rotation of **3** in methanol.

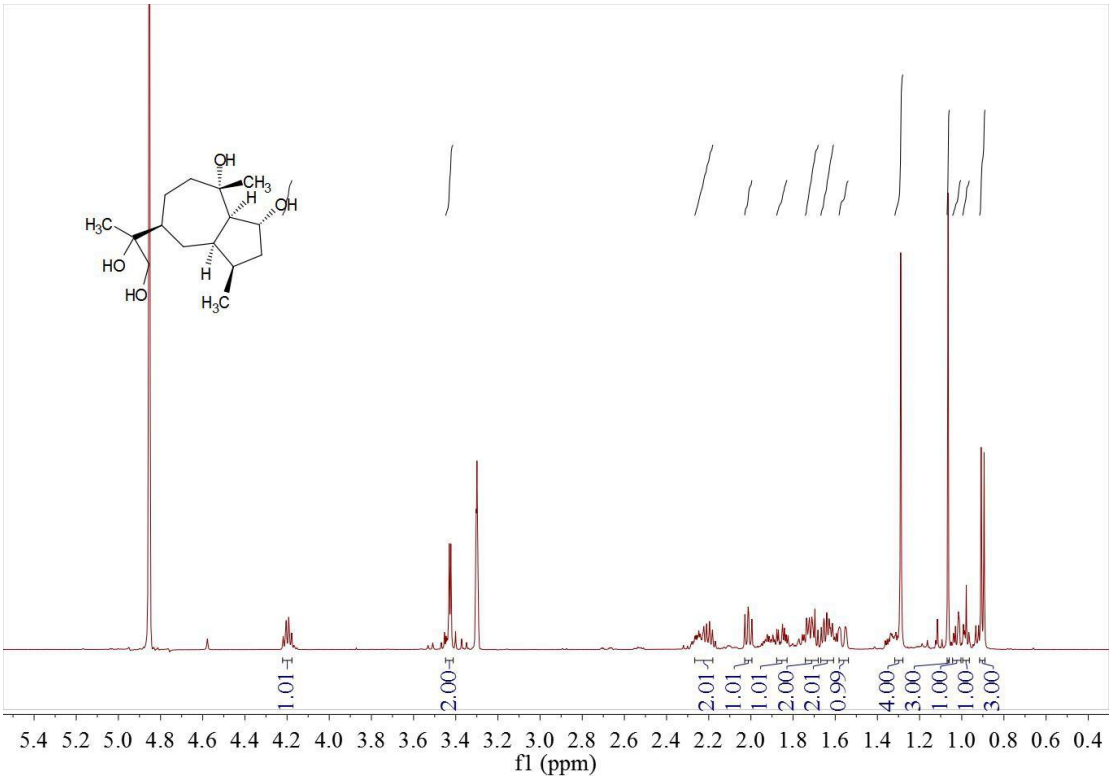



**Figure S33.** $^{1}$H NMR spectrum of compound **4** in CD3OD.

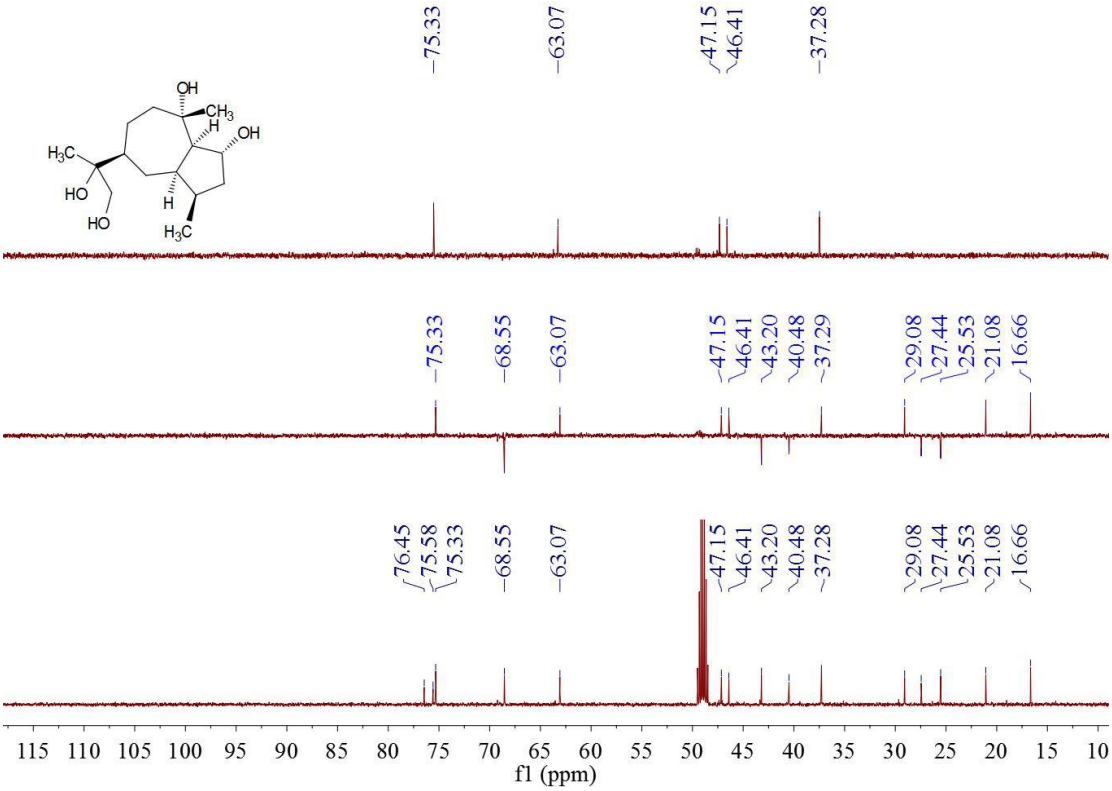



**Figure S34.** $^{13}$C NMR and DEPT spectrum of compound **4** in CD3OD.

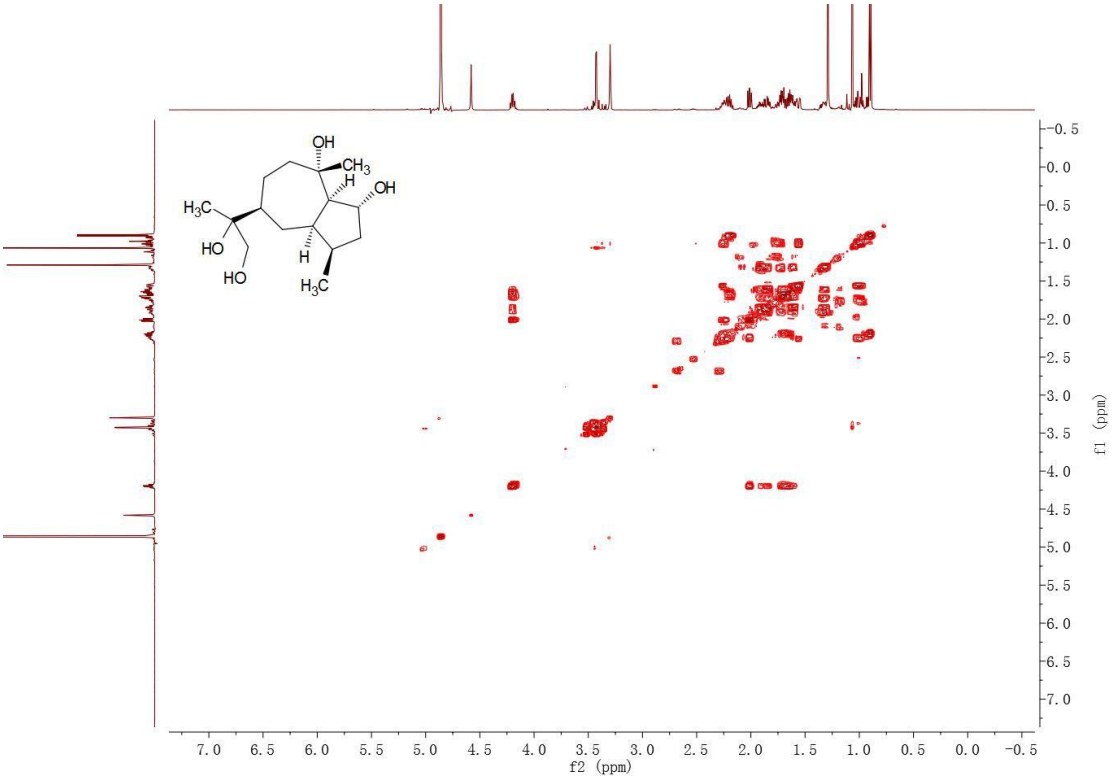



**Figure S35.** $^{1}$H-$^{1}$H COSY spectrum of compound **4** in CD3OD.

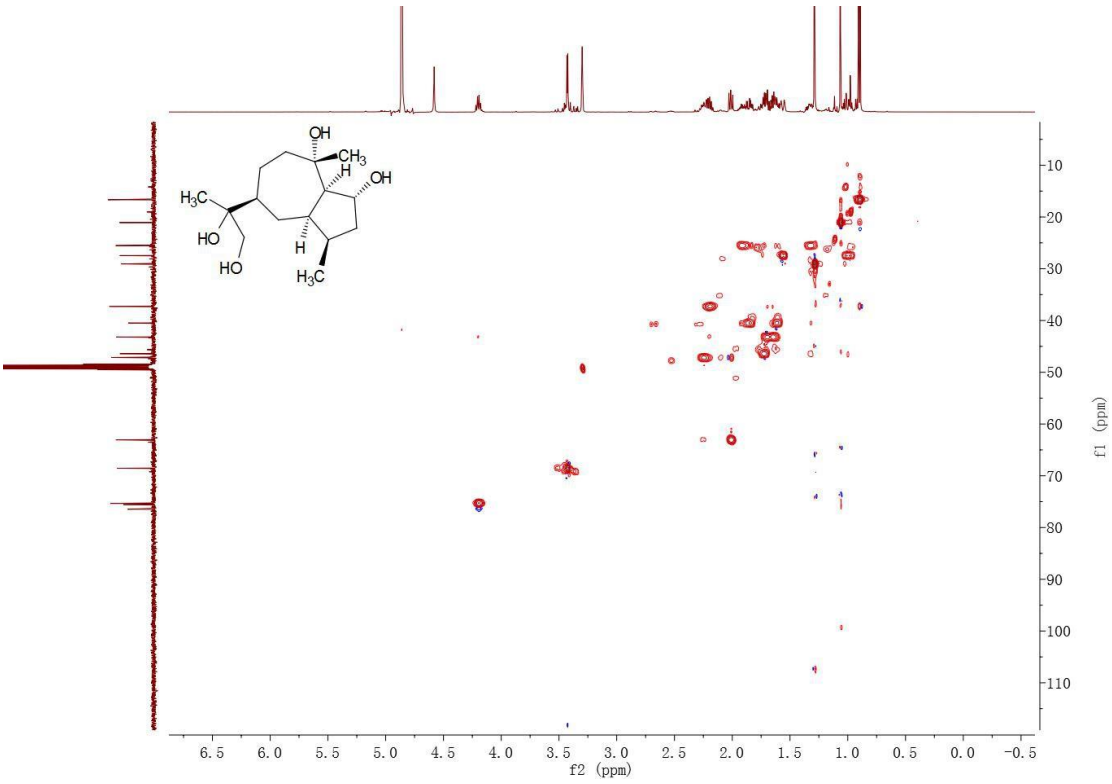



**Figure S36.** HSQC spectrum of compound **4** in CD3OD.

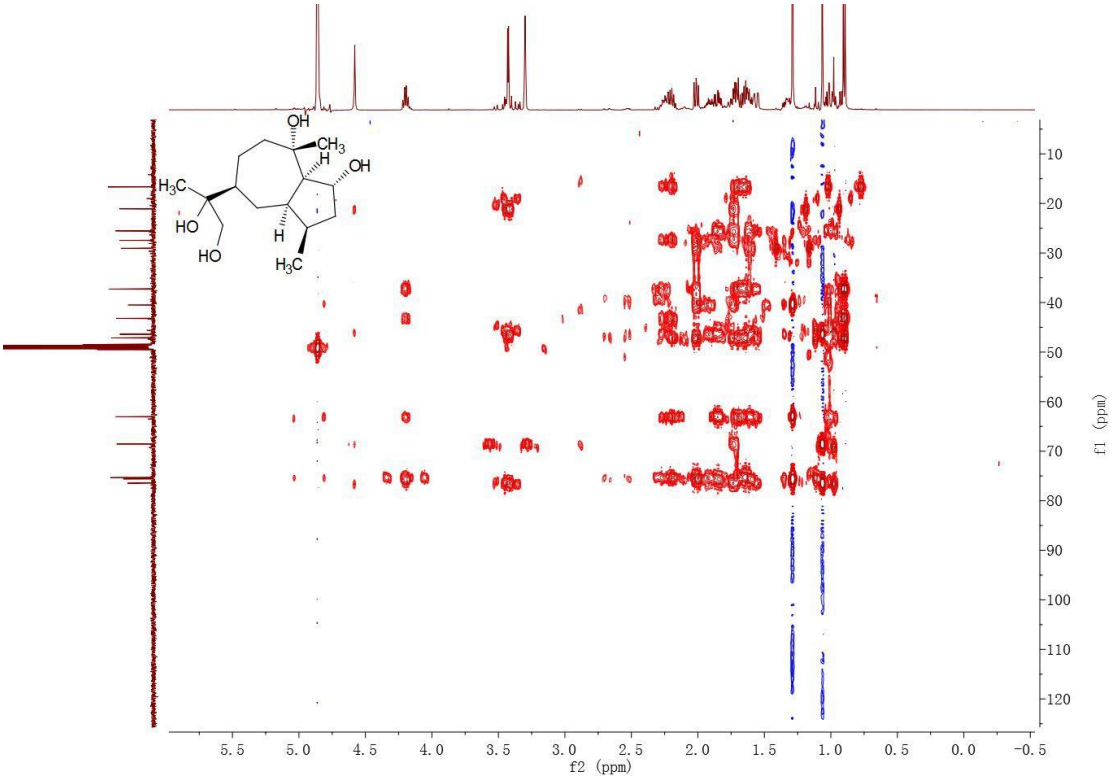



**Figure S37.** HMBC spectrum of compound **4** in $CD_3OD$.

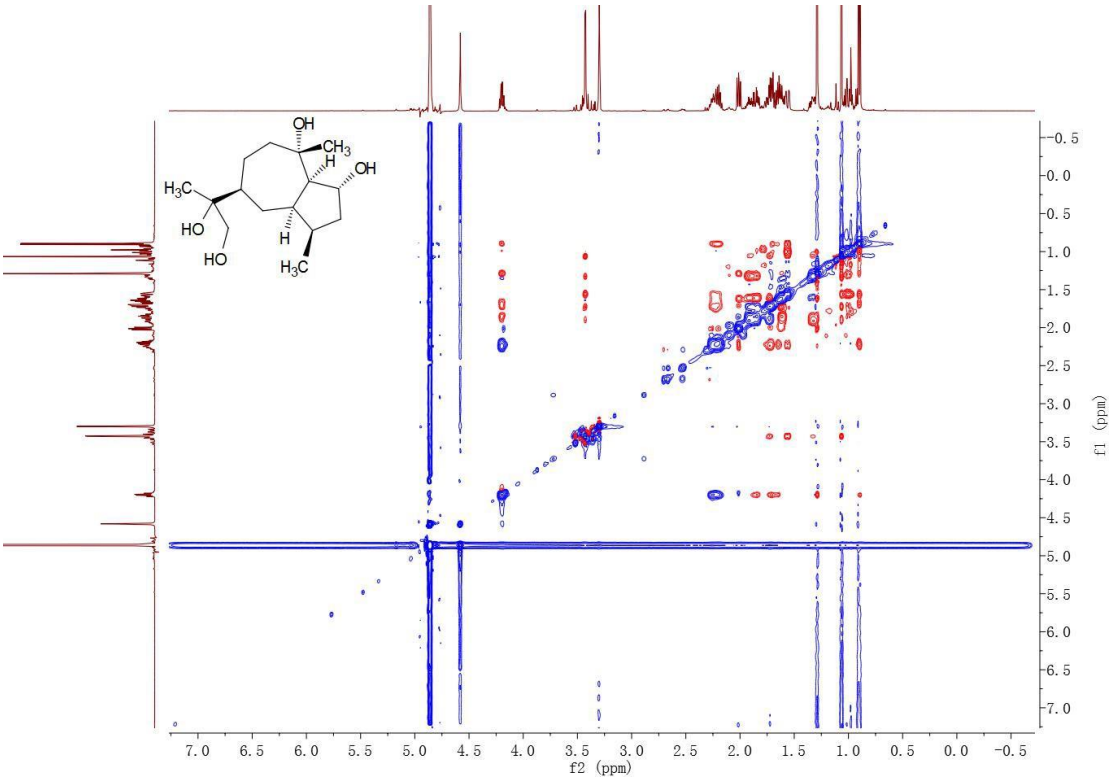



**Figure S38.** ROESY spectrum of compound **4** in $CD_3OD$.

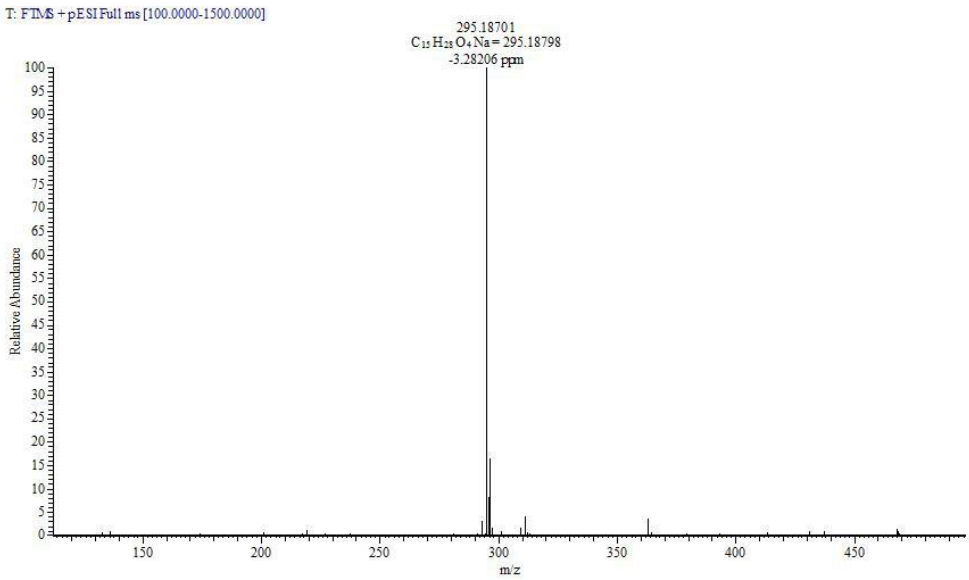



**Figure S39.** HRESIMS spectrum of compound **4.**

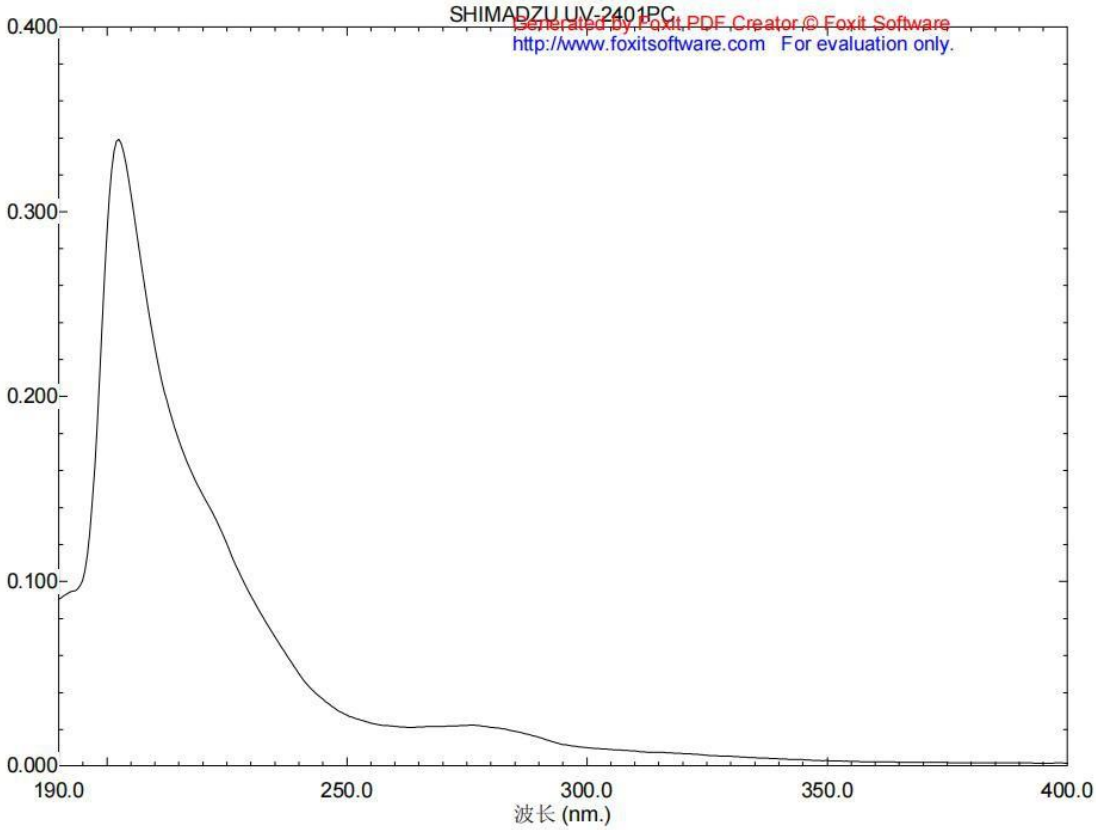



**Figure S40.** UV spectrum of **4** in methanol.

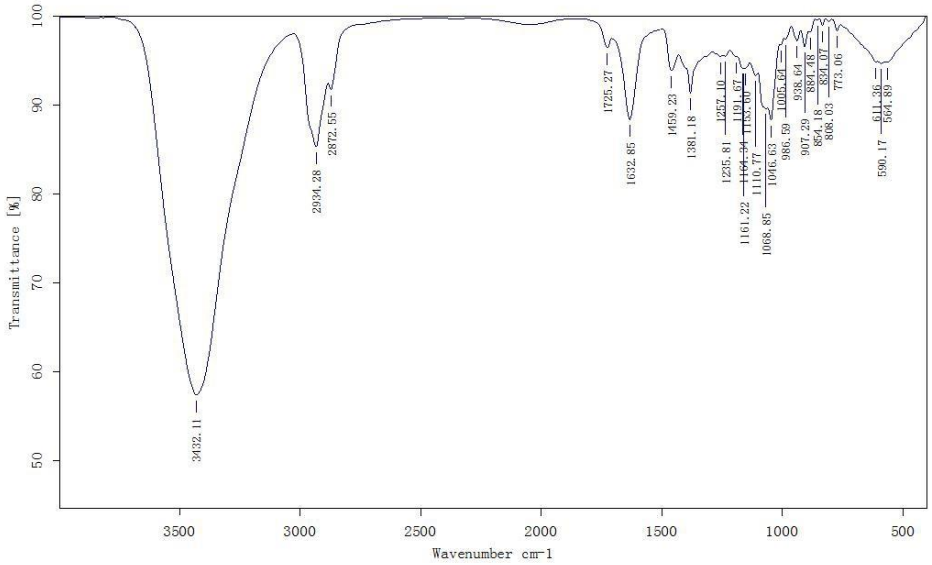



**Figure S41.** IR spectrum of **4** in methanol.

**Rudolph Research Analytical**

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Tuesday, 30-AUG-2022

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled

| n | Average | Std.Dev. | % RSD | Maximum | Minimum |
|---|---|---|---|---|---|
| 5 | -1.88 | 0.64 | -34.04 | -0.75 | -2.33 |

| S.No | Sample ID | Time | Result | Scale | OR °Arc | WLG.nm | Lg.mm | Conc.g/100ml | Temp. |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 05R49 | 10:50:31 AM | -0.75 | SR | -0.0009 | 589 | 100.00 | 0.120 | 24.7 |
| 2 | 05R49 | 10:50:40 AM | -2.08 | SR | -0.0025 | 589 | 100.00 | 0.120 | 24.7 |
| 3 | 05R49 | 10:50:52 AM | -2.17 | SR | -0.0026 | 589 | 100.00 | 0.120 | 24.6 |
| 4 | 05R49 | 10:51:00 AM | -2.33 | SR | -0.0028 | 589 | 100.00 | 0.120 | 24.6 |
| 5 | 05R49 | 10:51:09 AM | -2.08 | SR | -0.0025 | 589 | 100.00 | 0.120 | 24.6 |

**Figure S42.** Specific Rotation of **4** in methanol.

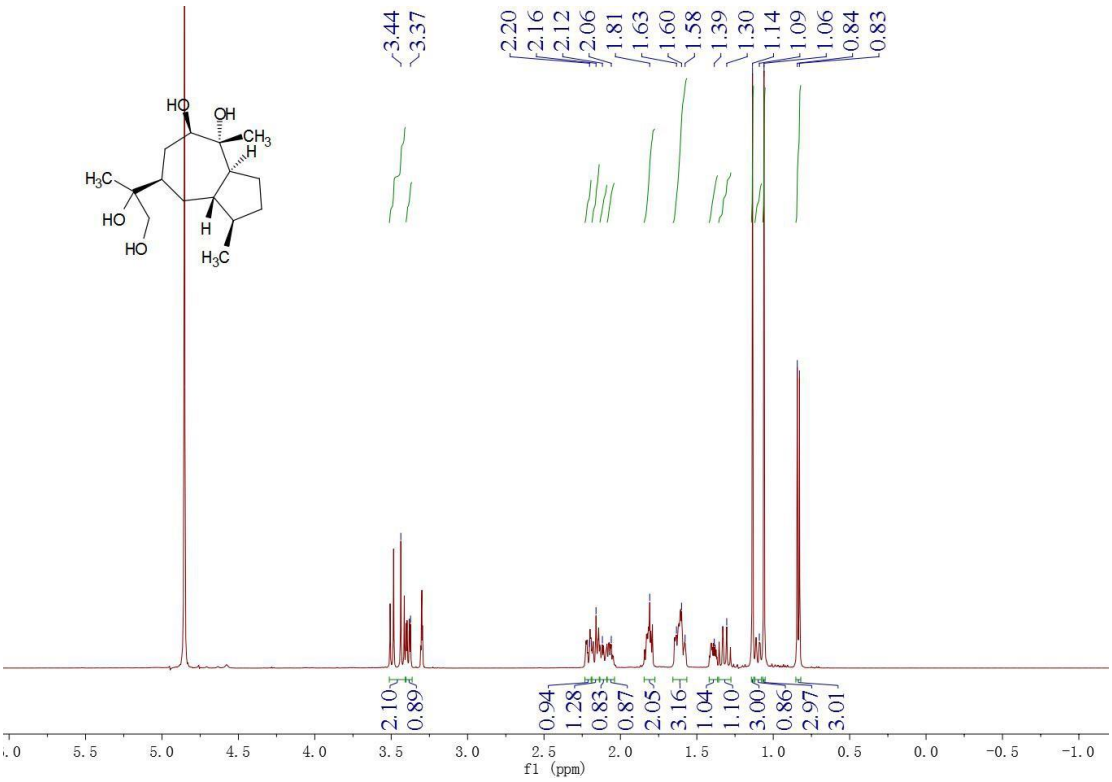



**Figure S43.** $^{1}$H NMR spectrum of compound **5** in CD3OD.

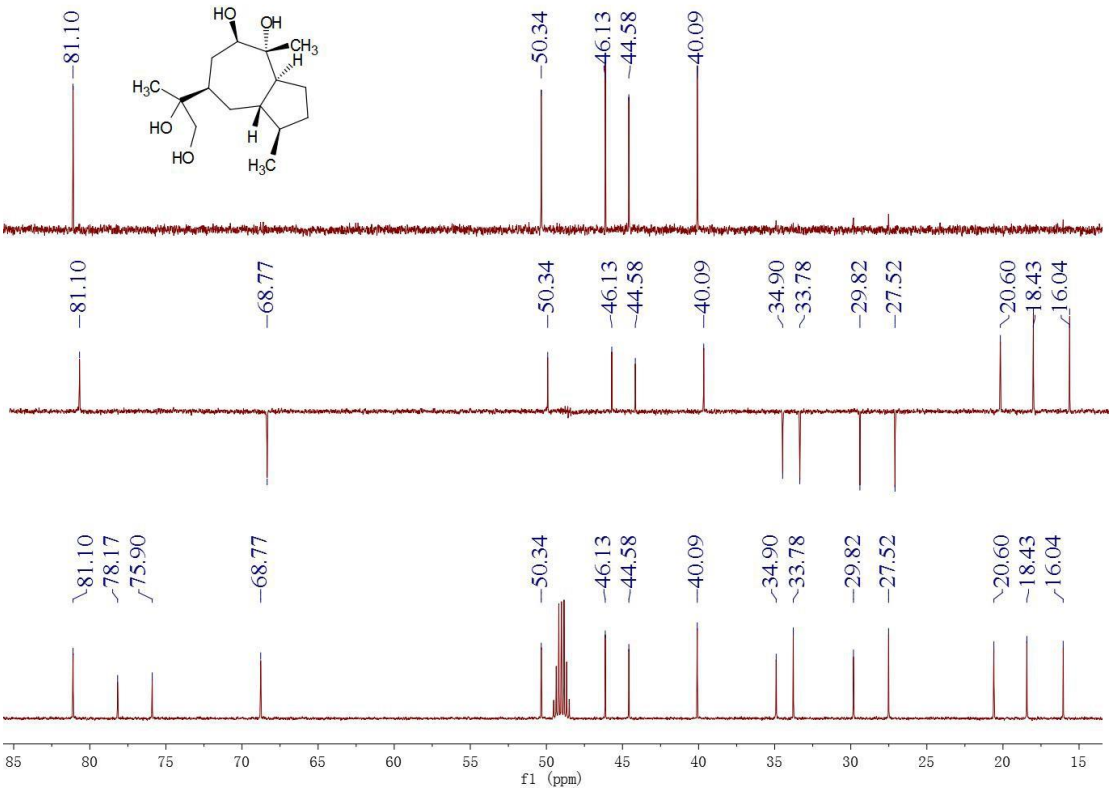



**Figure S44.** $^{13}$C NMR and DEPT spectrum of compound **5** in CD3OD.

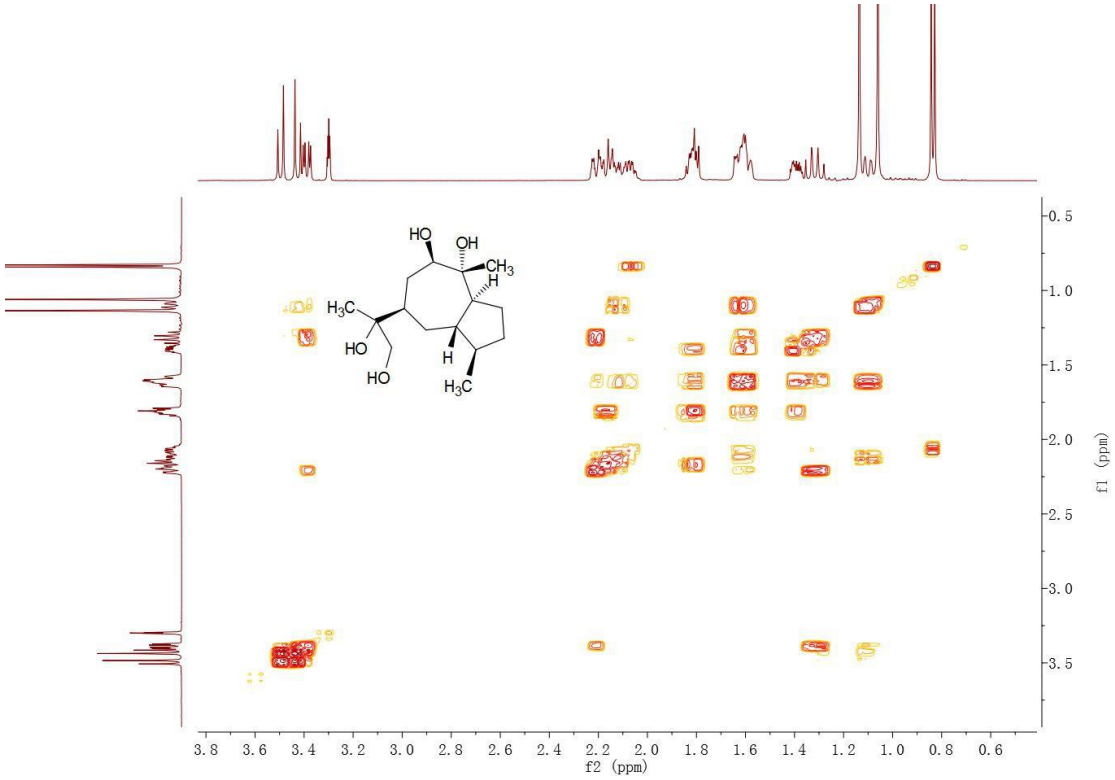



**Figure S45.** $^{1}$H-$^{1}$H COSY spectrum of compound **5** in CD3OD.

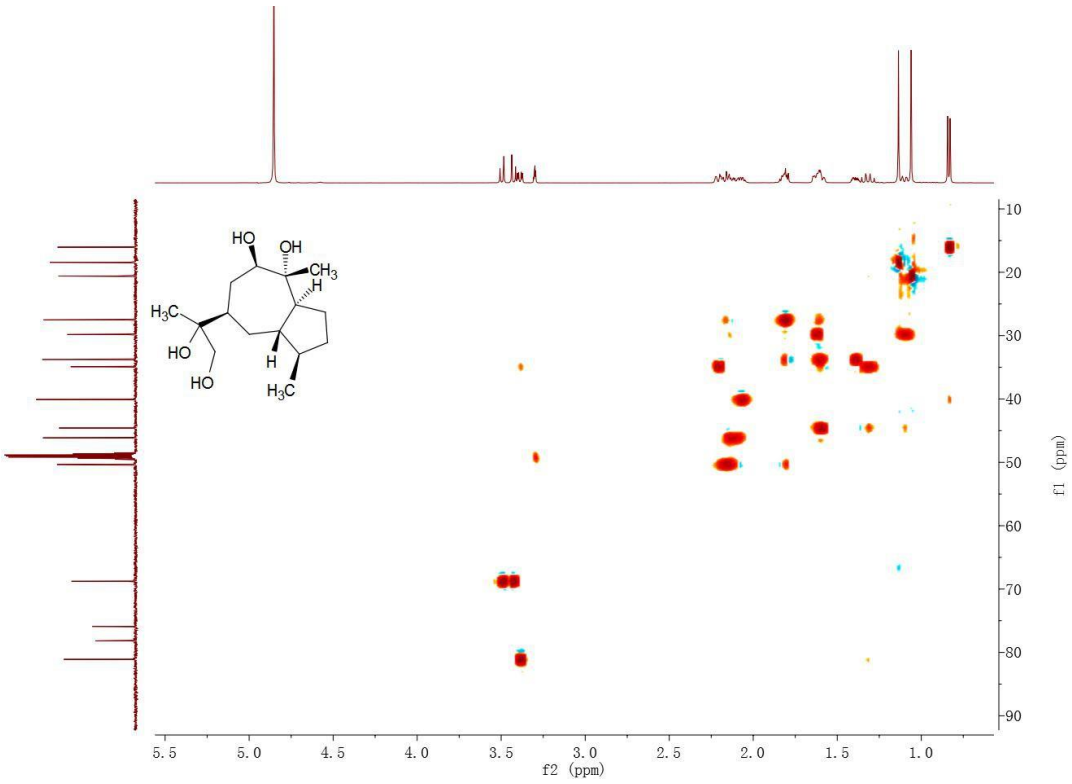



**Figure S46.** HSQC spectrum of compound **5** in CD3OD.

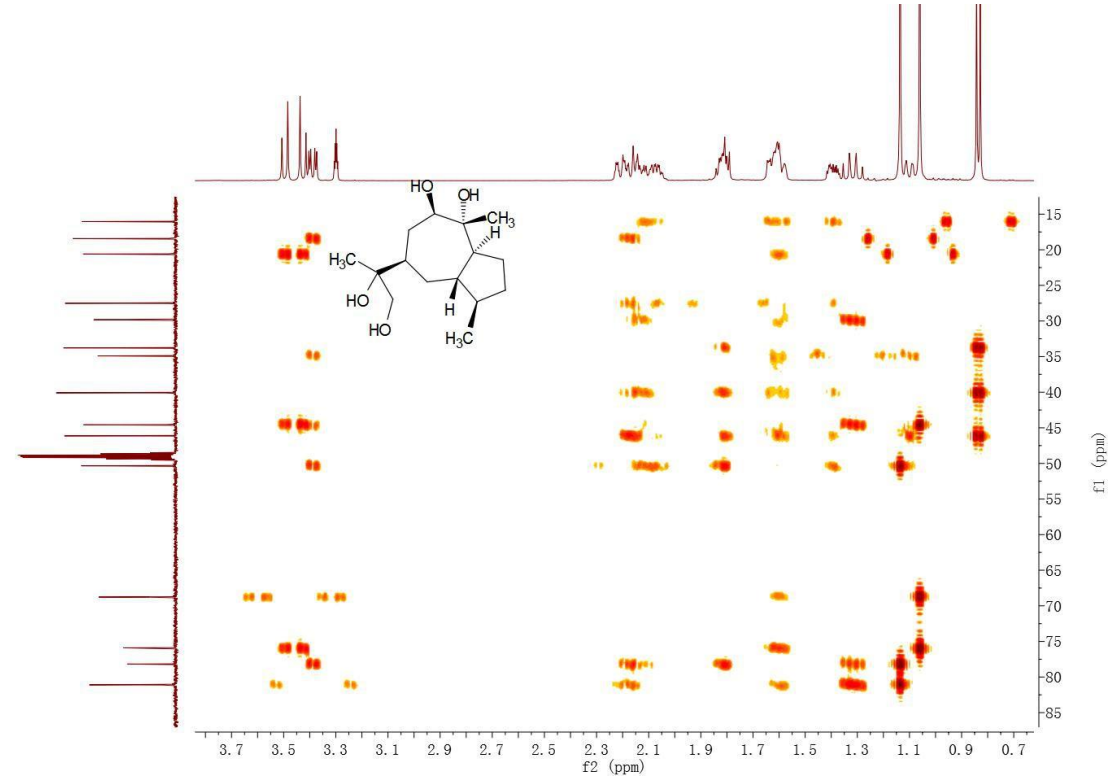



**Figure S47.** HMBC spectrum of compound **5** in CD3OD.

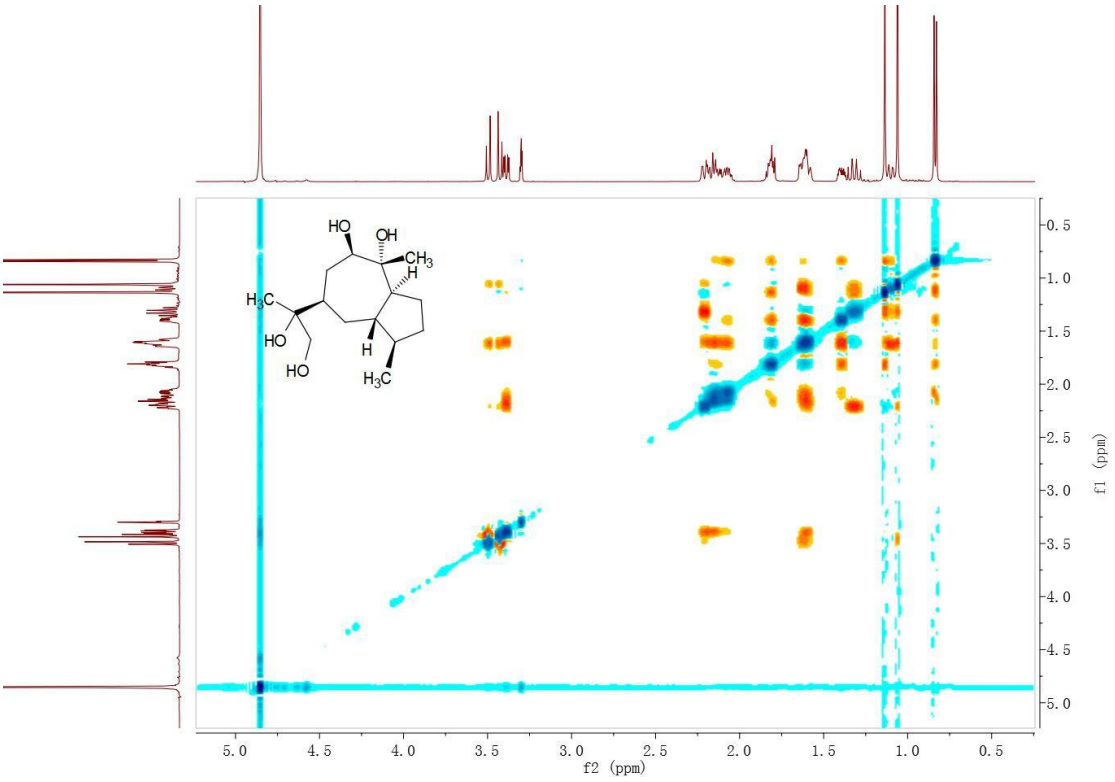



**Figure S48.** ROESY spectrum of compound **5** in CD3OD.

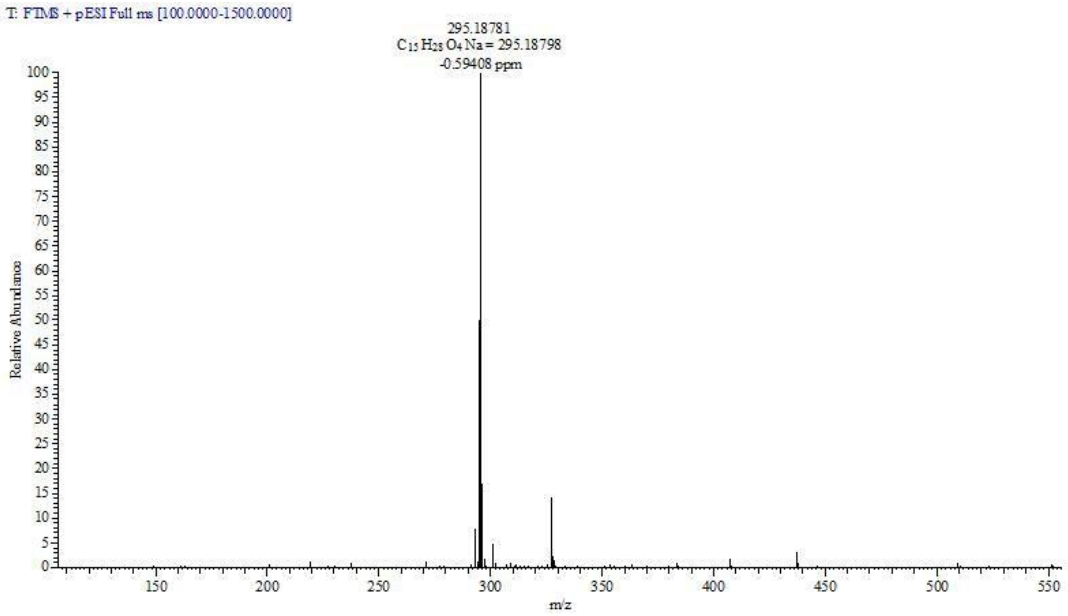



**Figure S49.** HRESIMS spectrum of compound **5.**

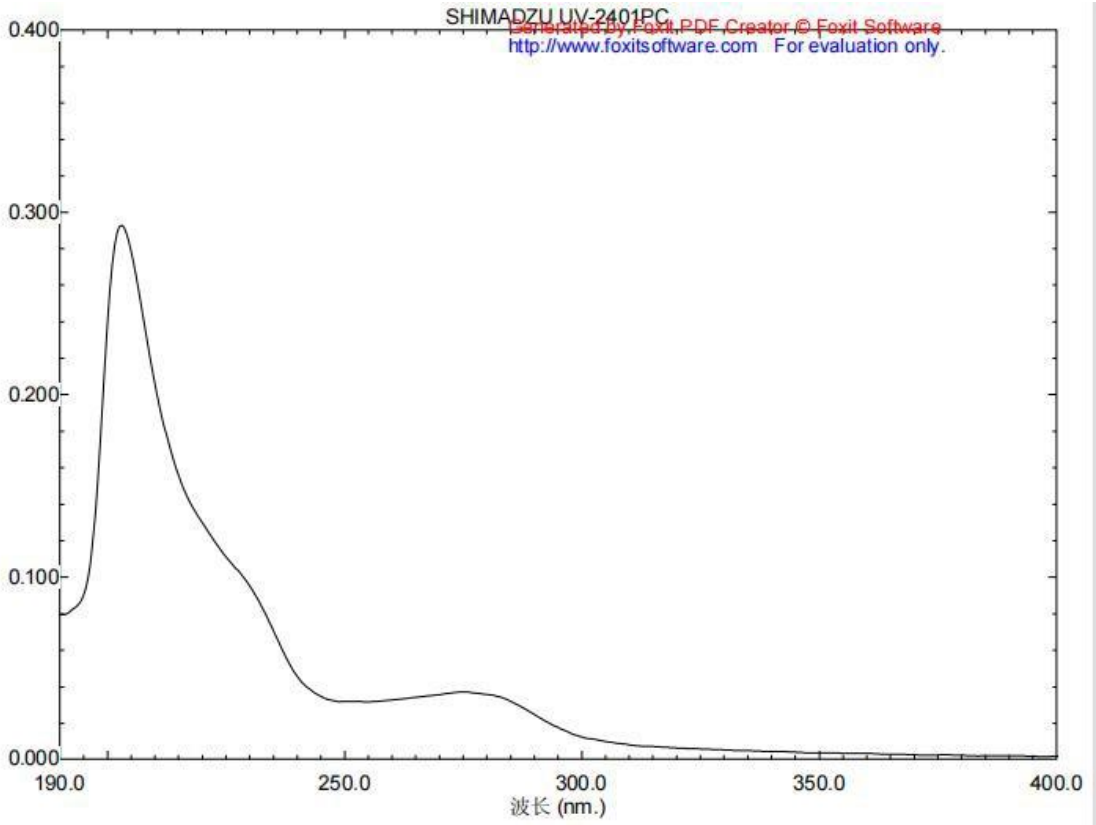



**Figure S50.** UV spectrum of **5** in methanol.

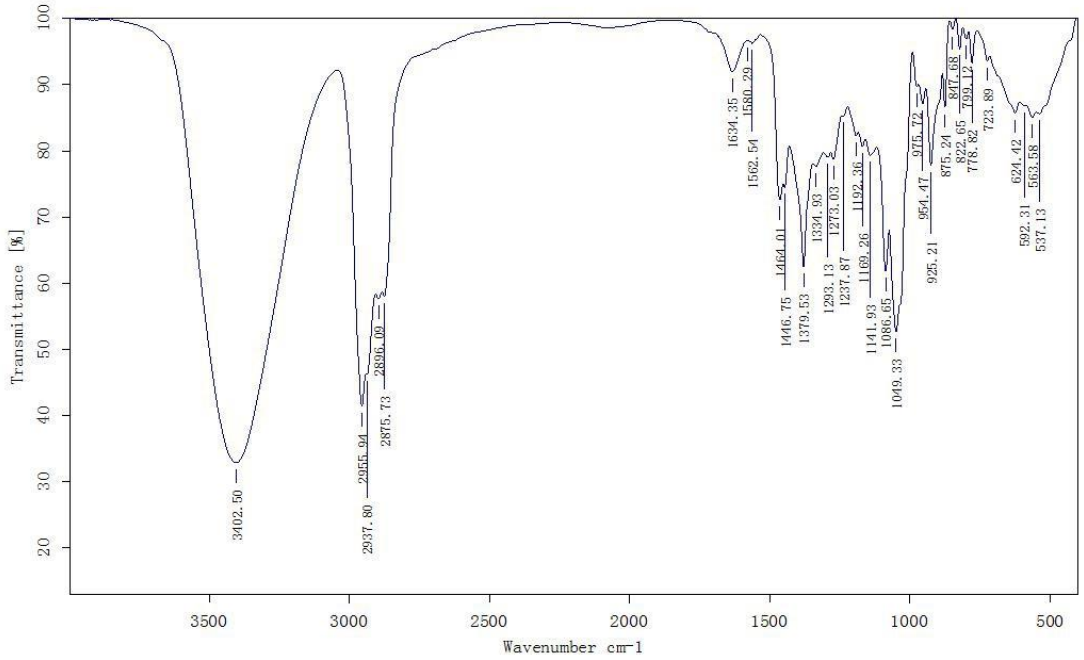
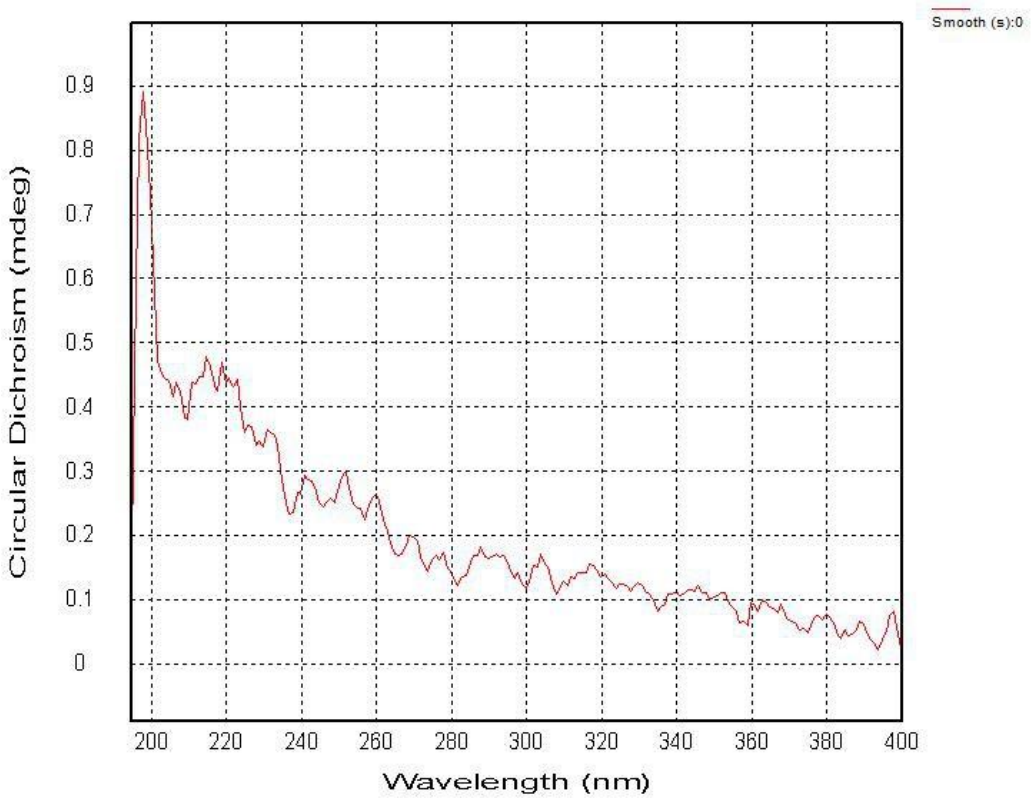



**Figure S51.** IR spectrum of **5** in methanol.



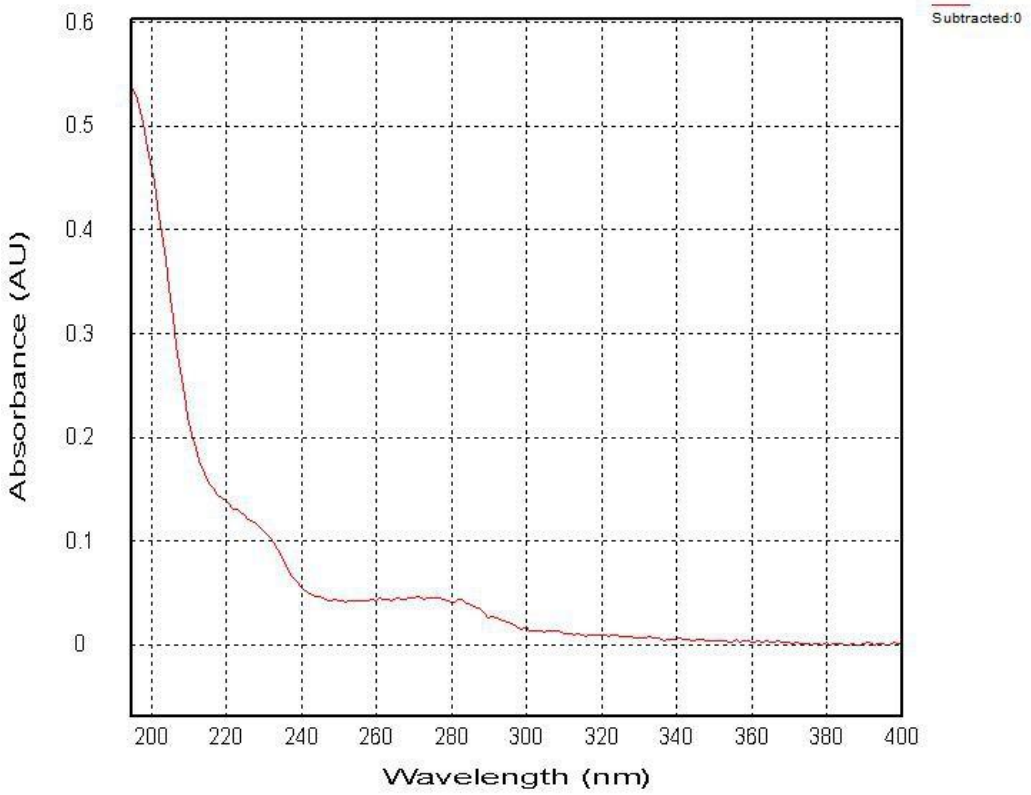



**Figure S52.** CD spectrum of **5** in methanol.

**Rudolph Research Analytical**

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Thursday, 07-APR-2022

Set Temperature : 20.0

Time Delay : Disabled

Delay between Measurement : Disabled

| n | Average | Std.Dev. | % RSD | Maximum | Minimum |
|---|---|---|---|---|---|
| 5 | -4.50 | 0.45 | -10.00 | -4.17 | -5.00 |

| S.No | Sample ID | Time | Result | Scale | OR °Arc | WLG.nm | Lg.mm | Conc.g/100ml | Temp. |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 05R53 | 11:31:06 AM | -4.17 | SR | -0.005 | 589 | 100.00 | 0.120 | 20.7 |
| 2 | 05R53 | 11:31:13 AM | -5.00 | SR | -0.006 | 589 | 100.00 | 0.120 | 20.6 |
| 3 | 05R53 | 11:31:20 AM | -5.00 | SR | -0.006 | 589 | 100.00 | 0.120 | 20.5 |
| 4 | 05R53 | 11:31:26 AM | -4.17 | SR | -0.005 | 589 | 100.00 | 0.120 | 20.4 |
| 5 | 05R53 | 11:31:33 AM | -4.17 | SR | -0.005 | 589 | 100.00 | 0.120 | 20.3 |



**Figure S53.** Specific Rotation of **5** in methanol.

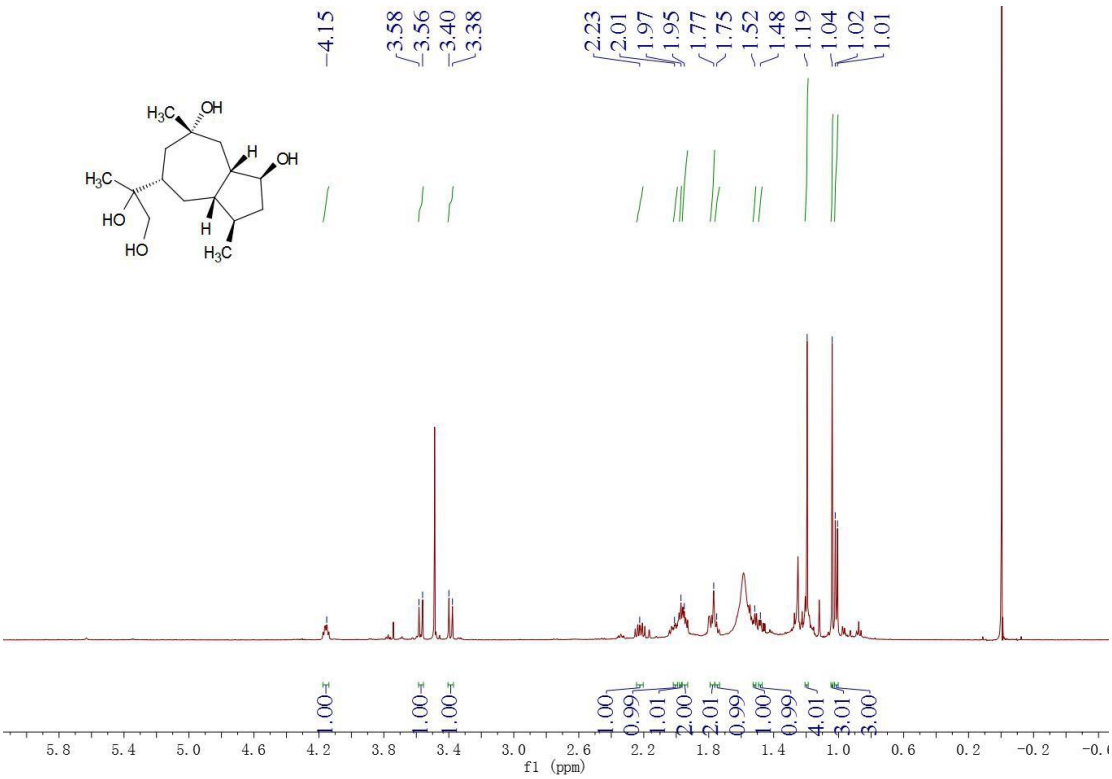



**Figure S54.** $^{1}$H NMR spectrum of compound **6** in CDCl3.

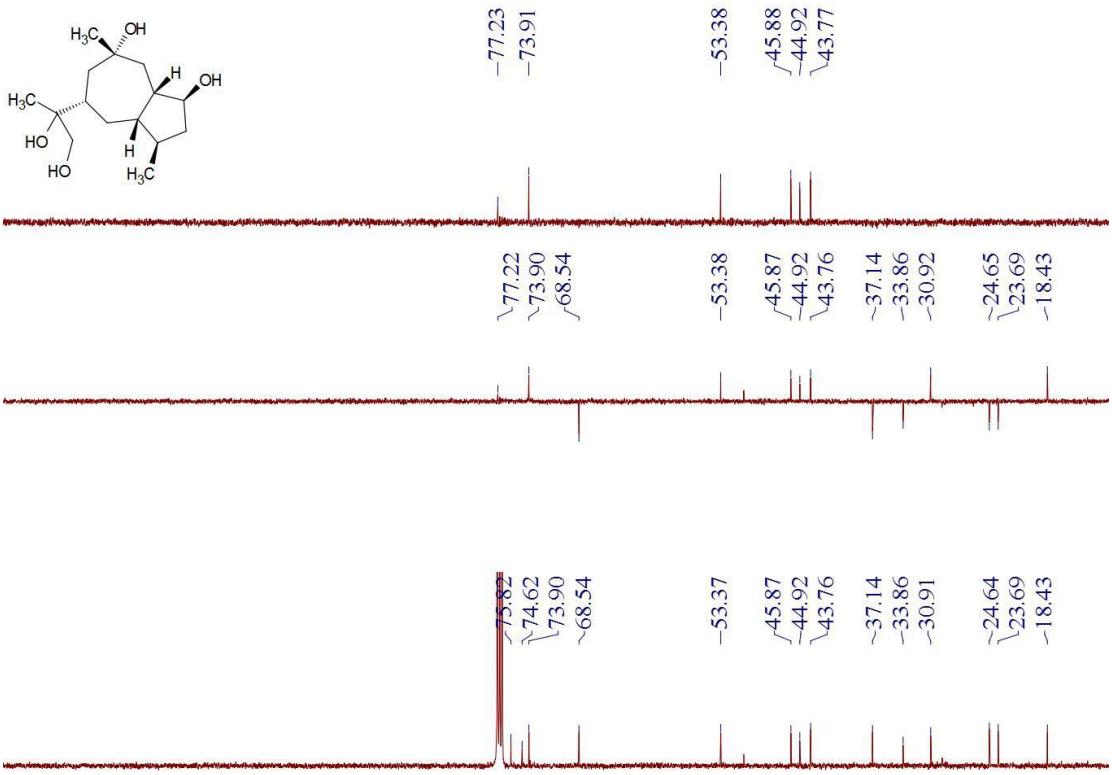



**Figure S55.** $^{13}$C NMR and DEPT spectrum of compound **6** in CDCl3.

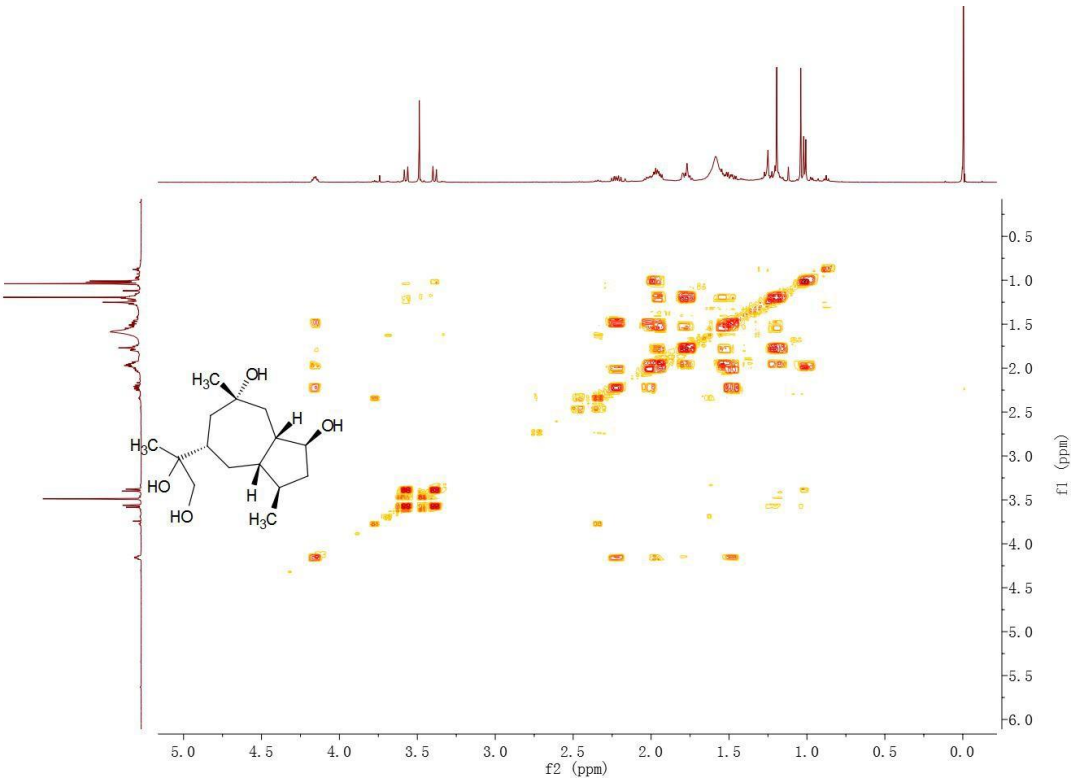



**Figure S56.** $^{1}$H-$^{1}$H COSY spectrum of compound **6** in CDCl3.

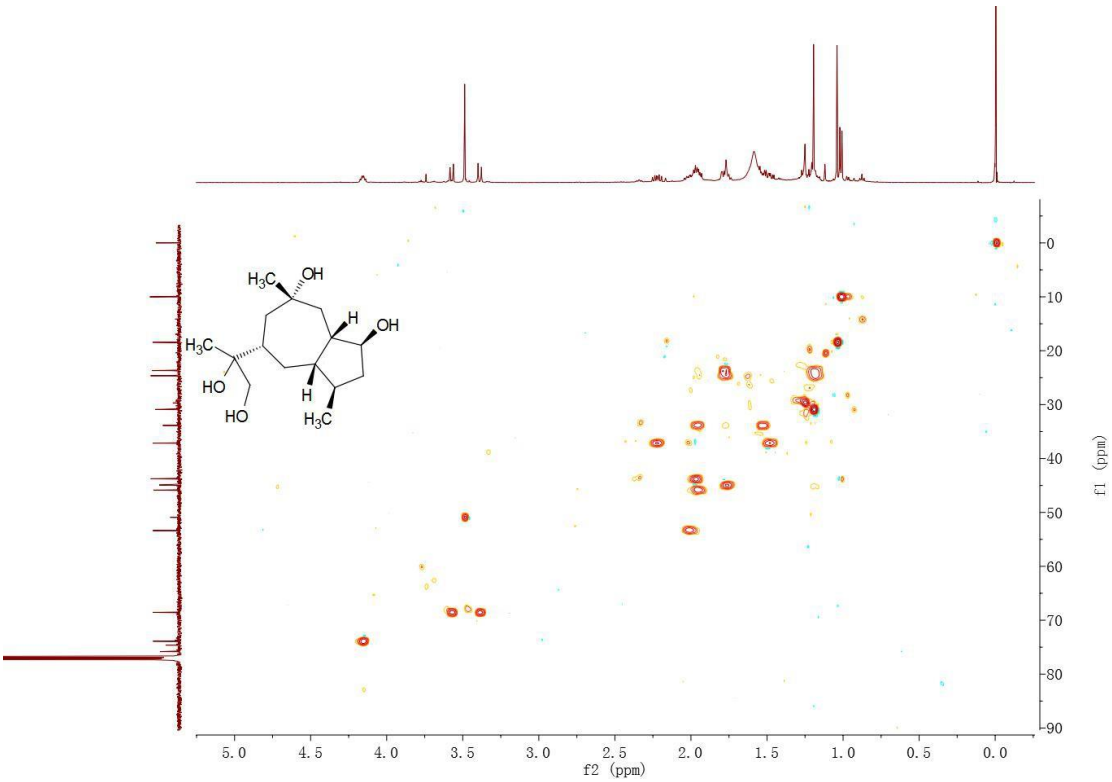



**Figure S57.** HSQC spectrum of compound **6** in CDCl3.

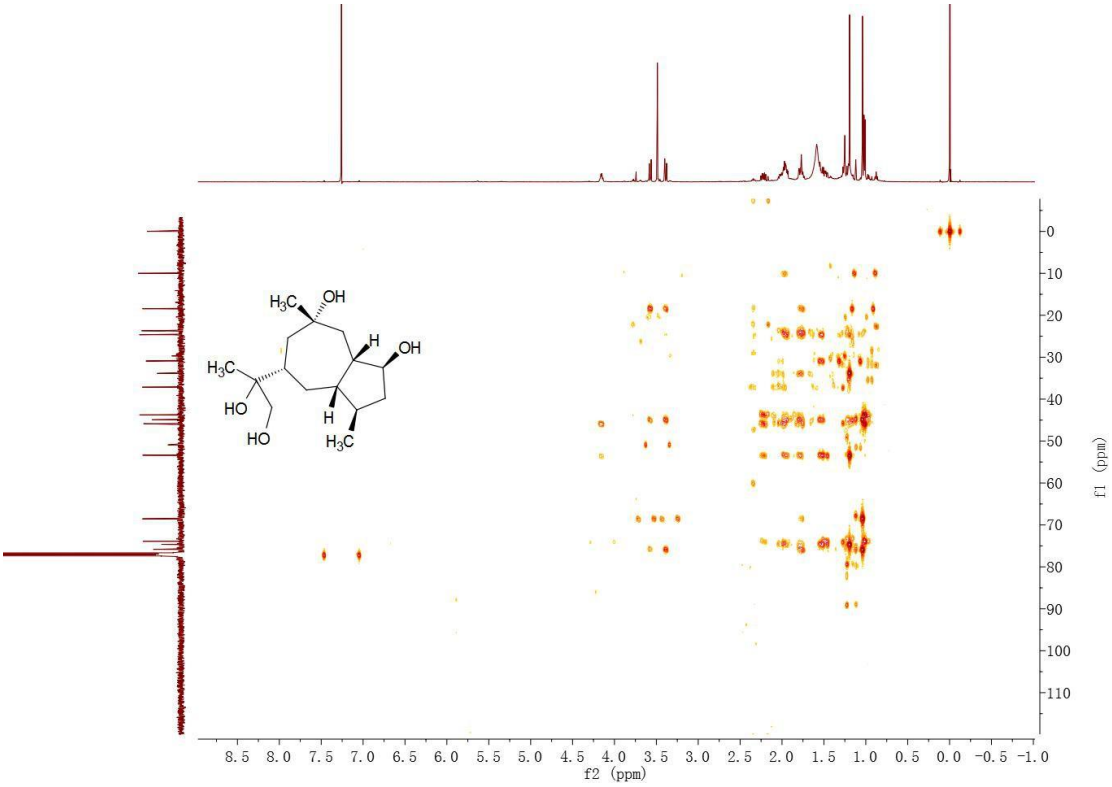



**Figure S58.** HMBC spectrum of compound **6** in CDCl3.

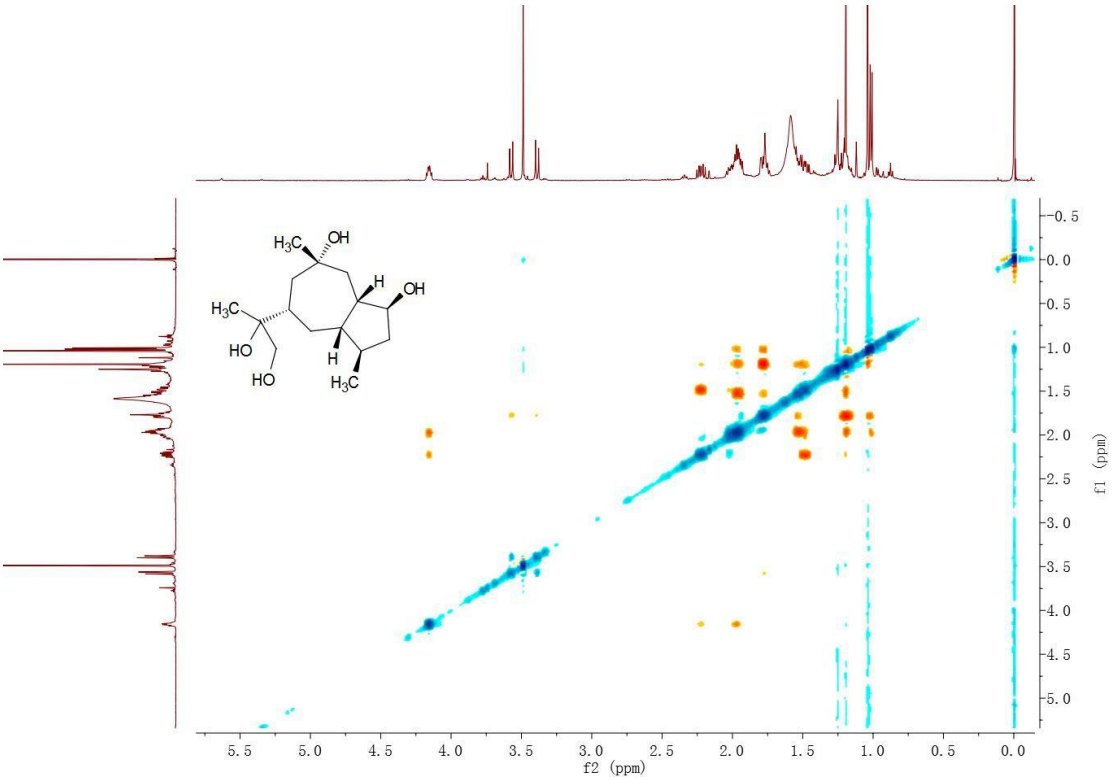



**Figure S59.** ROESY spectrum of compound **6** in CDCl3.

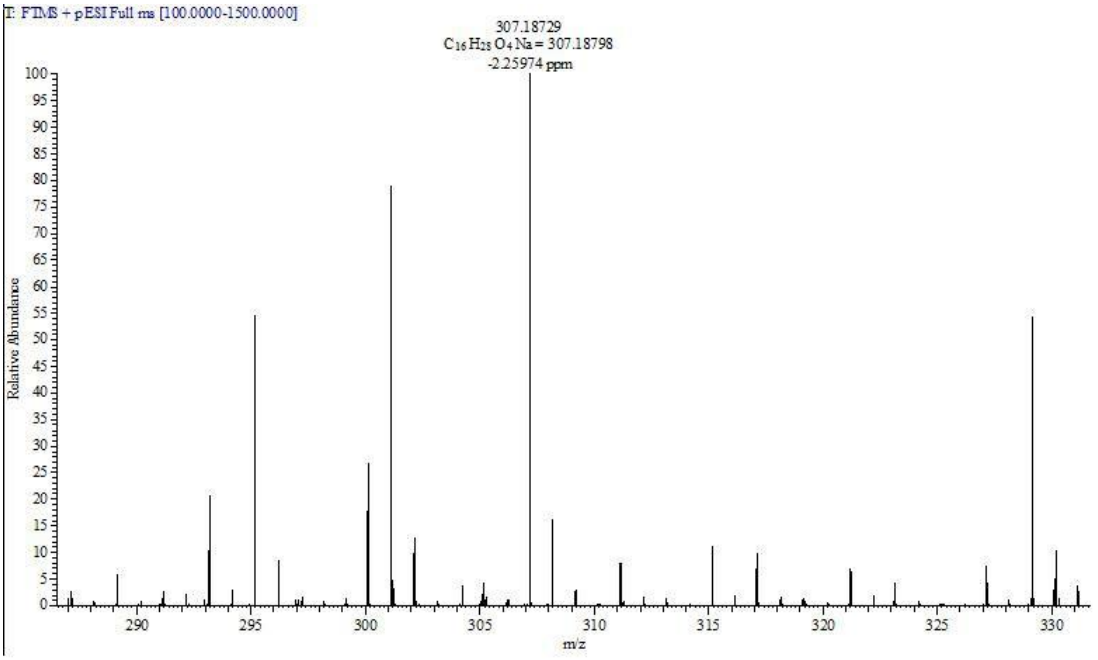



**Figure S60.** HRESIMS spectrum of compound **6.**

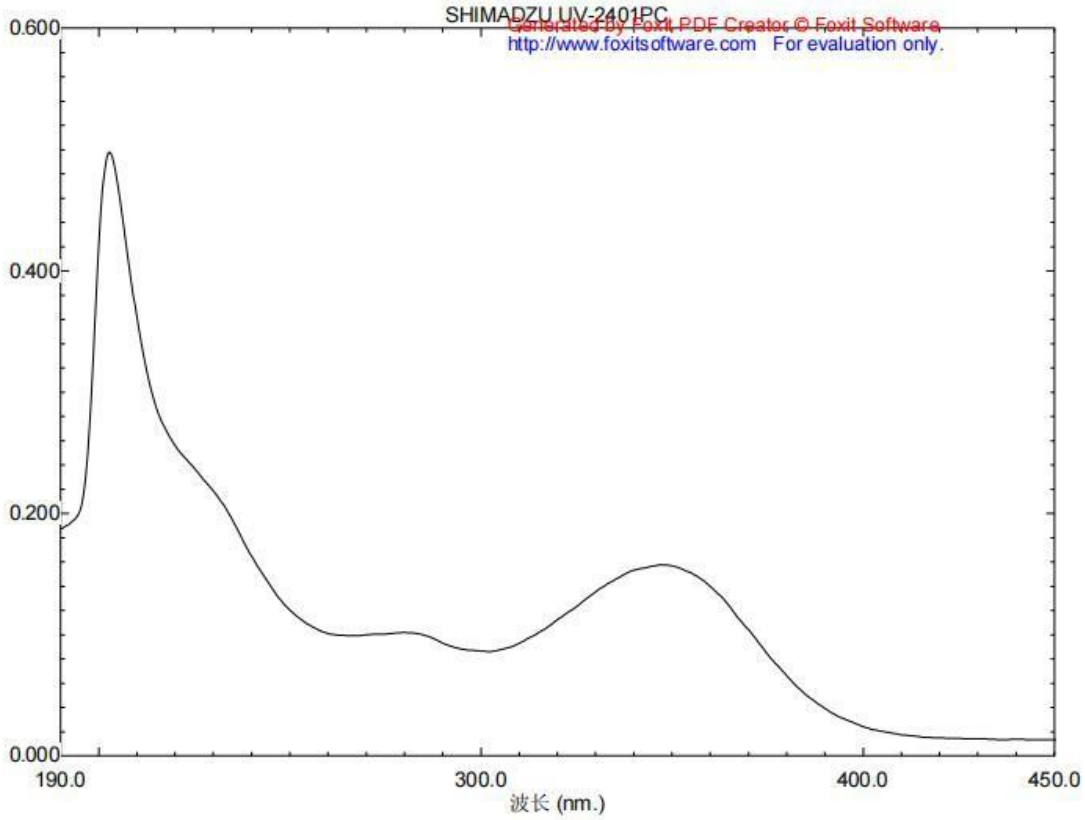



**Figure S61.** UV spectrum of **6** in methanol.

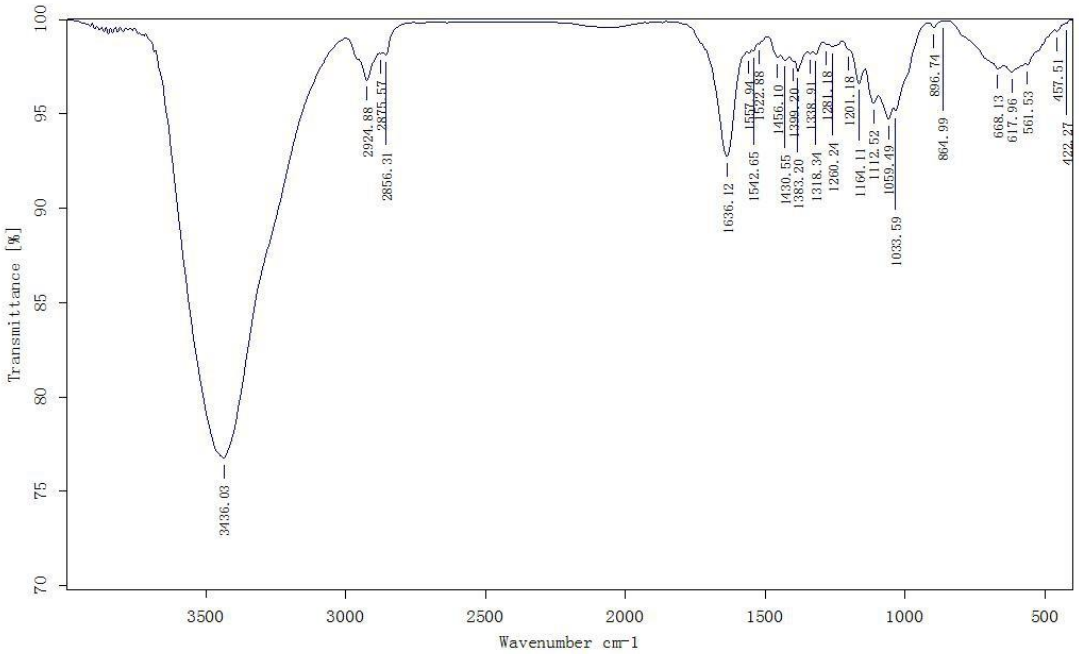



**Figure S62.** IR spectrum of **6** in methanol.

**Rudolph Research Analytical**

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Saturday, 18-JUN-2022

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled

| n | Average | Std.Dev. | % RSD | Maximum | Minimum |
|---|---|---|---|---|---|
| 5 | -11.30 | 0.86 | -7.61 | -10.50 | -12.70 |

| S.No | Sample ID | Time | Result | Scale | OR °Arc | WLG.nm | Lg.mm | Conc.g/100ml | Temp. |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 05R55 | 04:44:29 PM | -10.80 | SR | -0.0108 | 589 | 100.00 | 0.100 | 23.8 |
| 2 | 05R55 | 04:44:37 PM | -10.50 | SR | -0.0105 | 589 | 100.00 | 0.100 | 23.8 |
| 3 | 05R55 | 04:44:45 PM | -12.70 | SR | -0.0127 | 589 | 100.00 | 0.100 | 23.8 |
| 4 | 05R55 | 04:44:53 PM | -11.00 | SR | -0.0110 | 589 | 100.00 | 0.100 | 23.8 |
| 5 | 05R55 | 04:45:01 PM | -11.50 | SR | -0.0115 | 589 | 100.00 | 0.100 | 23.8 |

**Figure S63.** Specific Rotation of **6** in methanol.

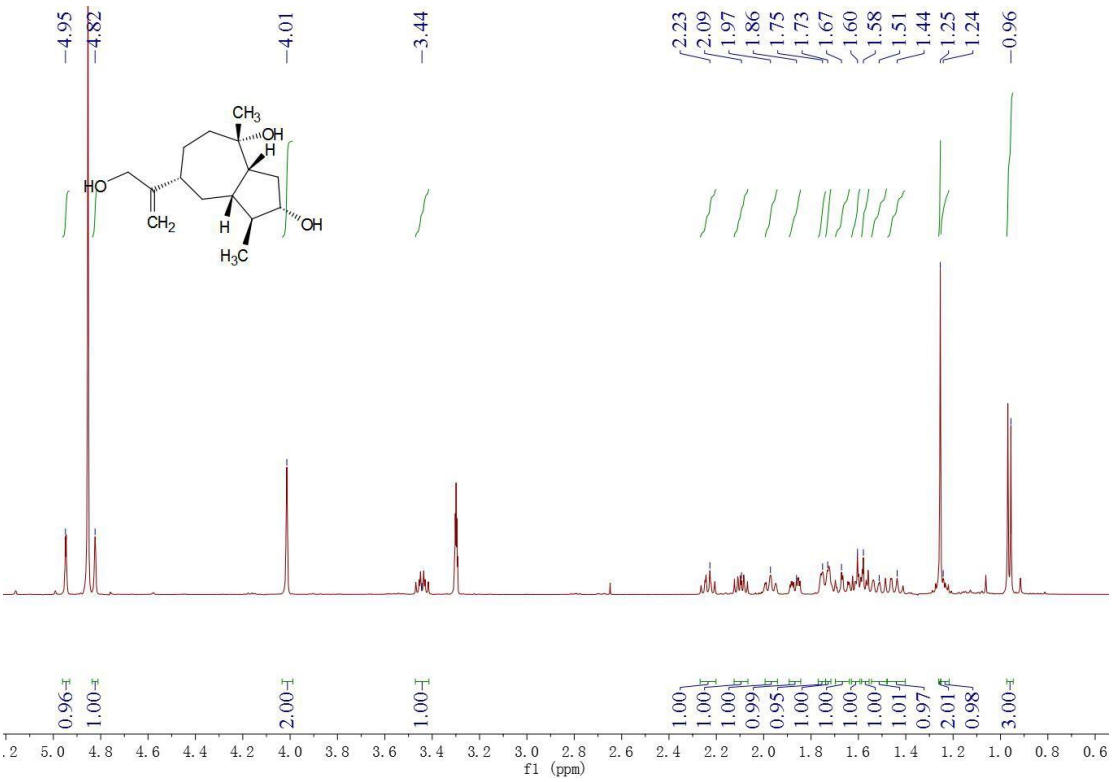



**Figure S64.** $^{1}$H NMR spectrum of compound **7** in CD3OD.

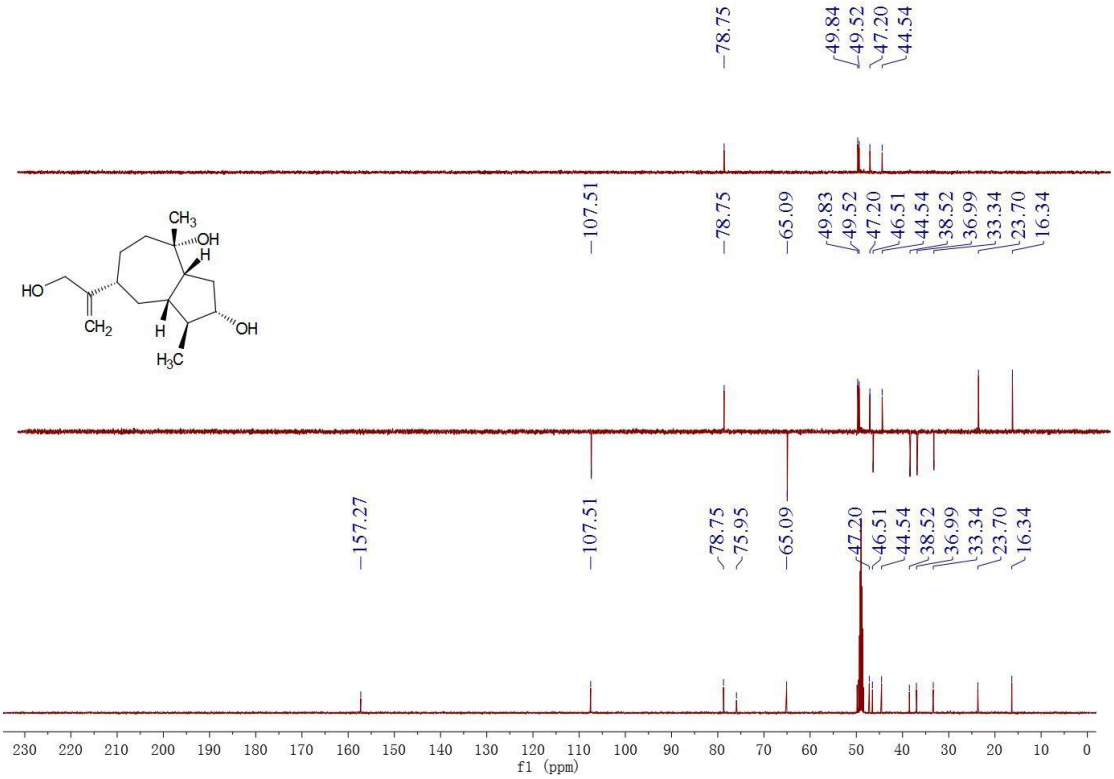



**Figure S65.** $^{13}$C NMR and DEPT spectrum of compound **7** in CD3OD.

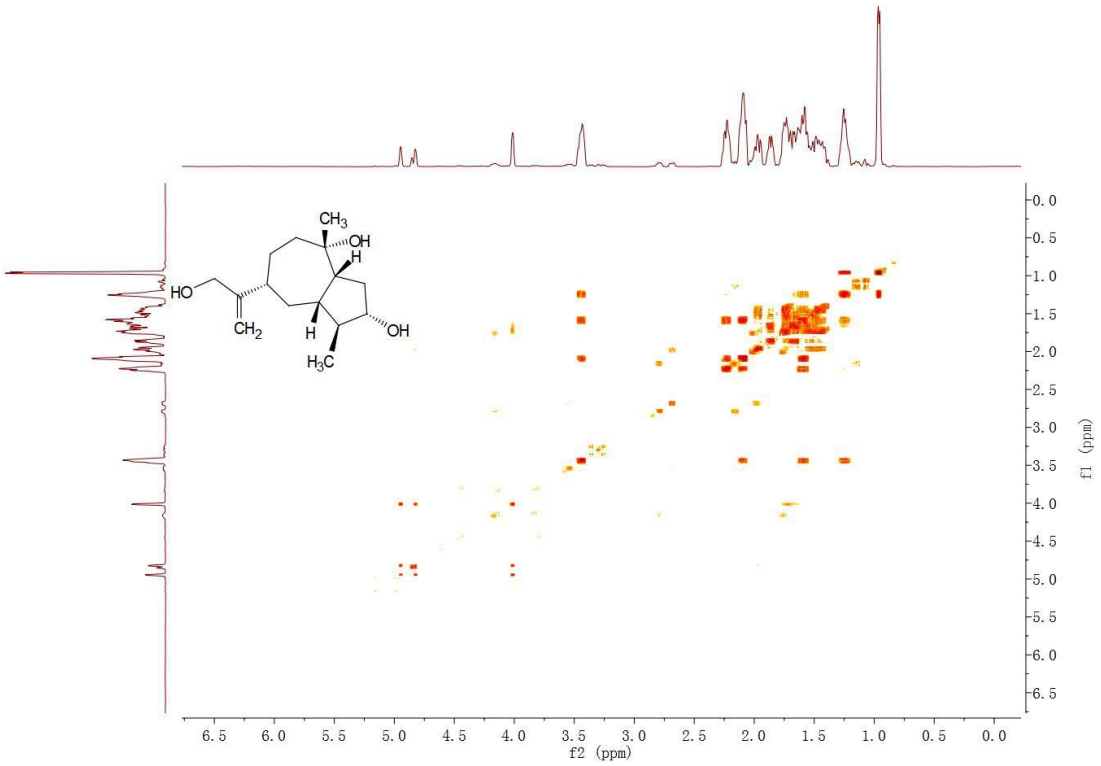



**Figure S66.** $^{1}$H-$^{1}$H COSY spectrum of compound **7** in CD3OD.

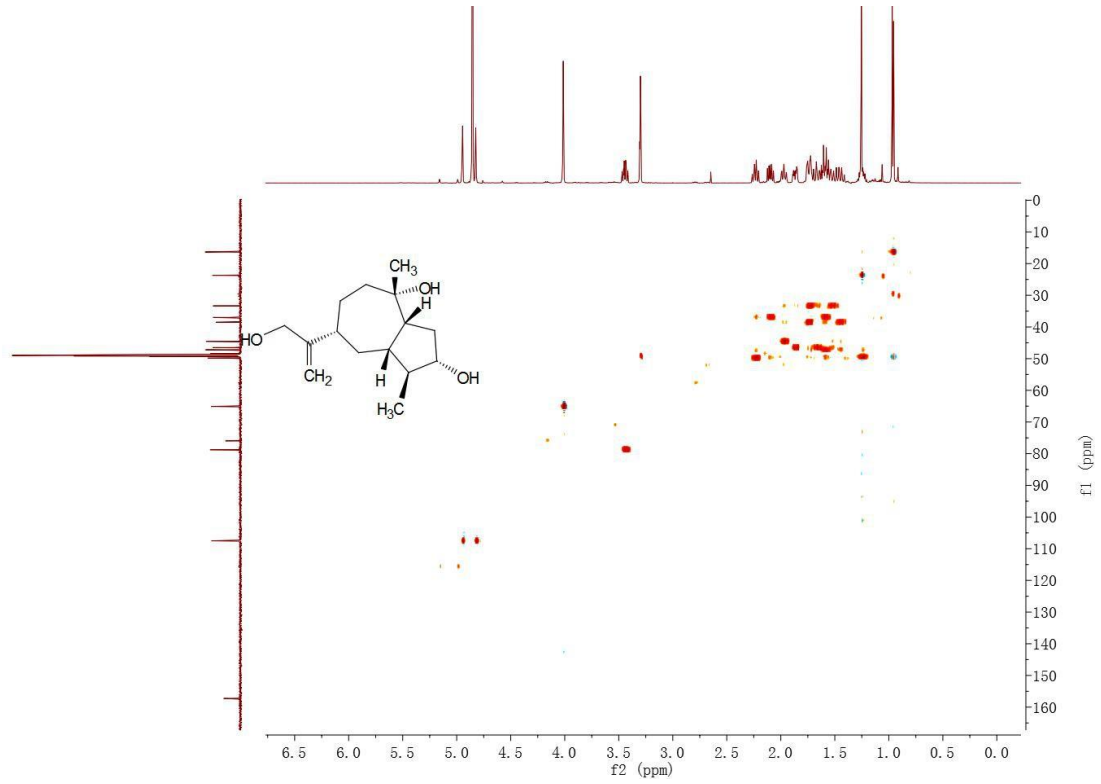



**Figure S67.** HSQC spectrum of compound **7** in CD3OD.

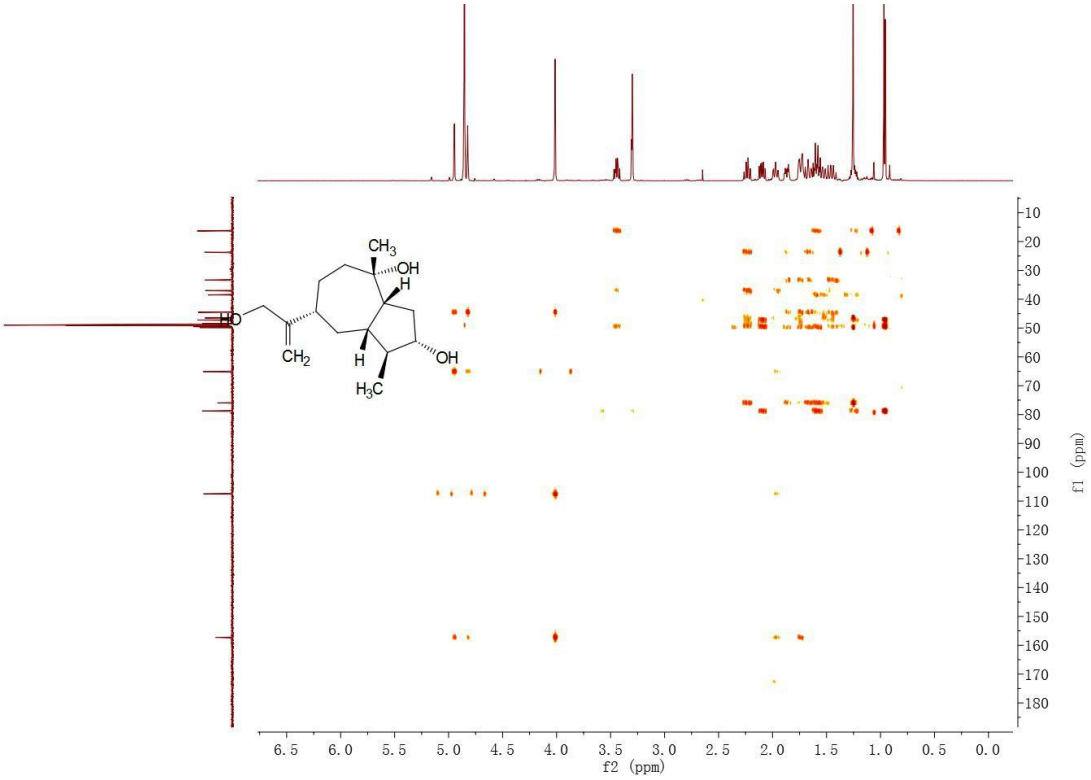



**Figure S68.** HMBC spectrum of compound **7** in CD3OD.

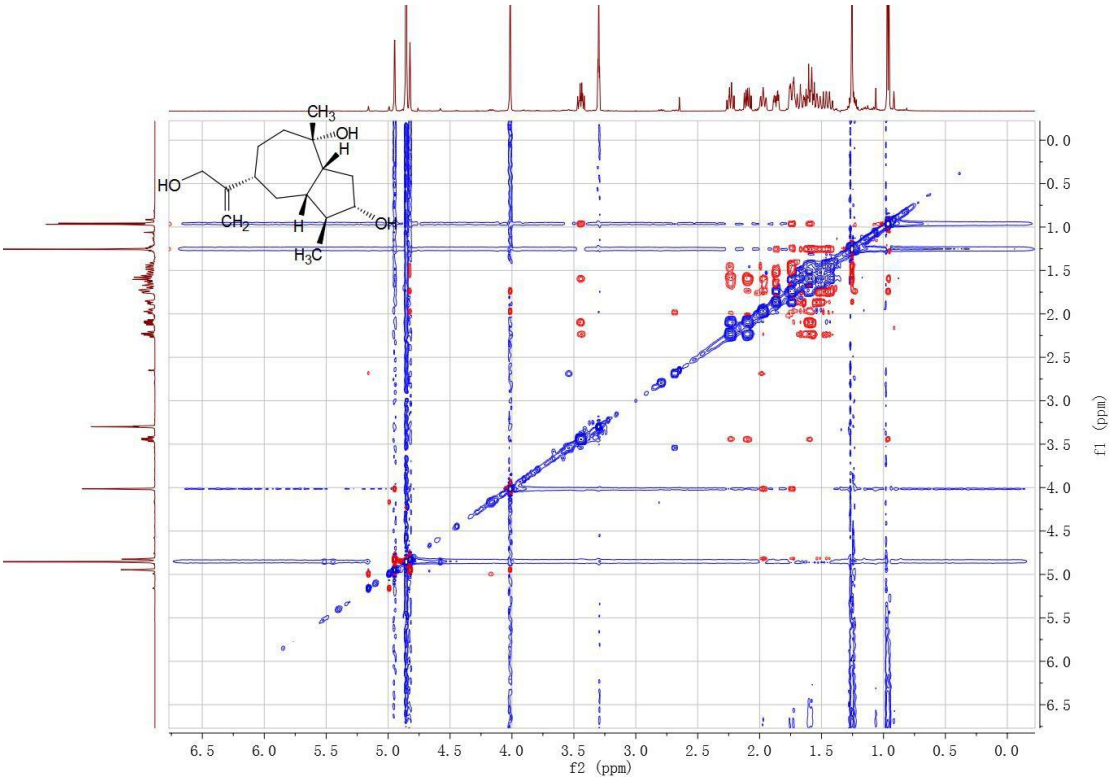



**Figure S69.** ROESY spectrum of compound **7** in CD3OD.

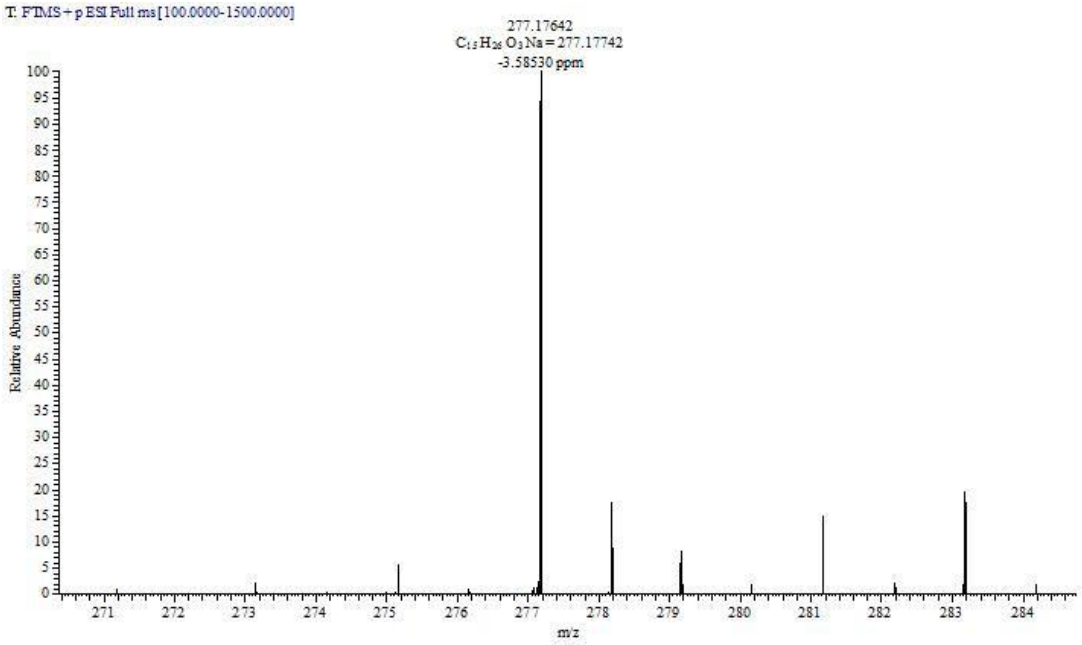



**Figure S70.** HRESIMS spectrum of compound **7.**

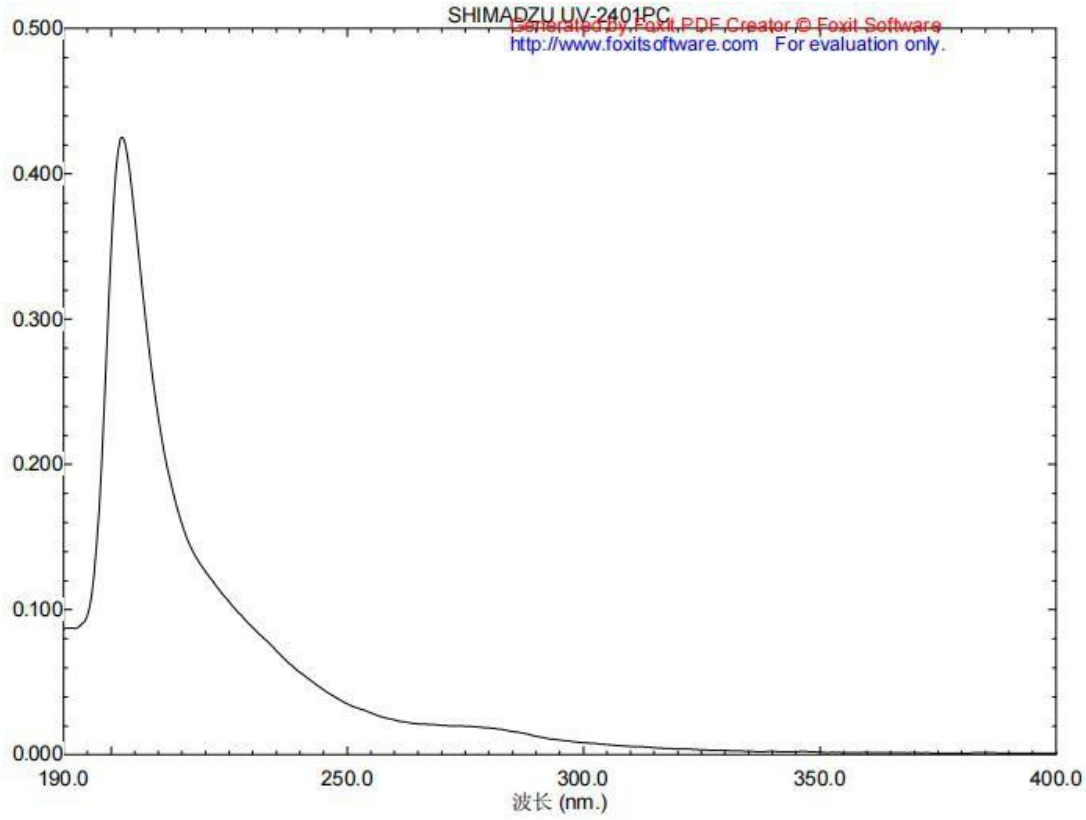



**Figure S71.** UV spectrum of **7** in methanol.

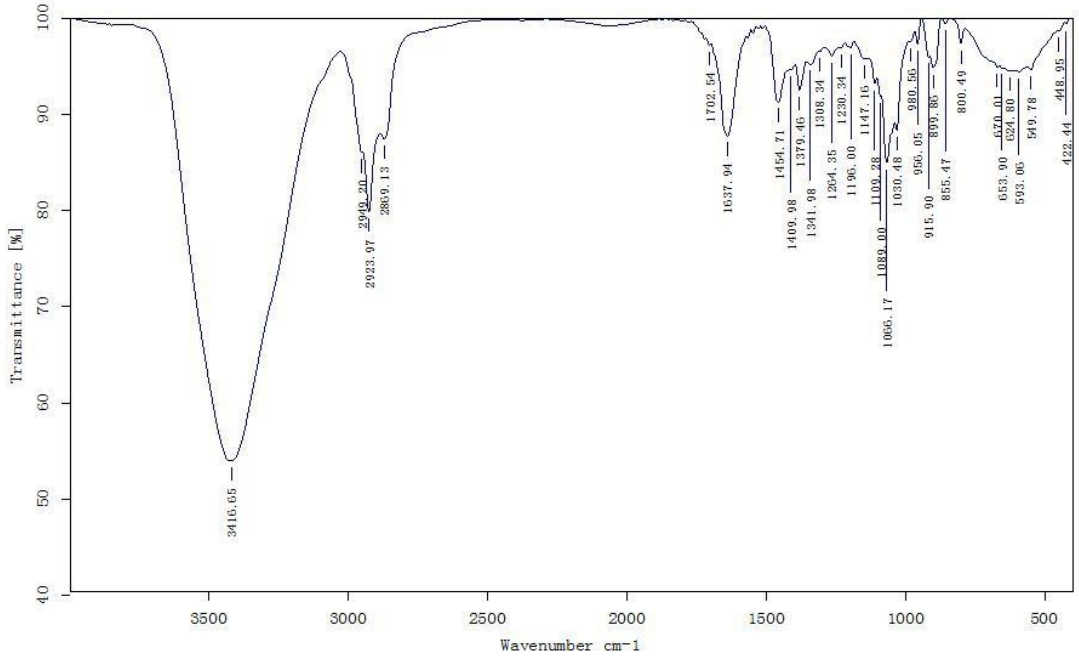
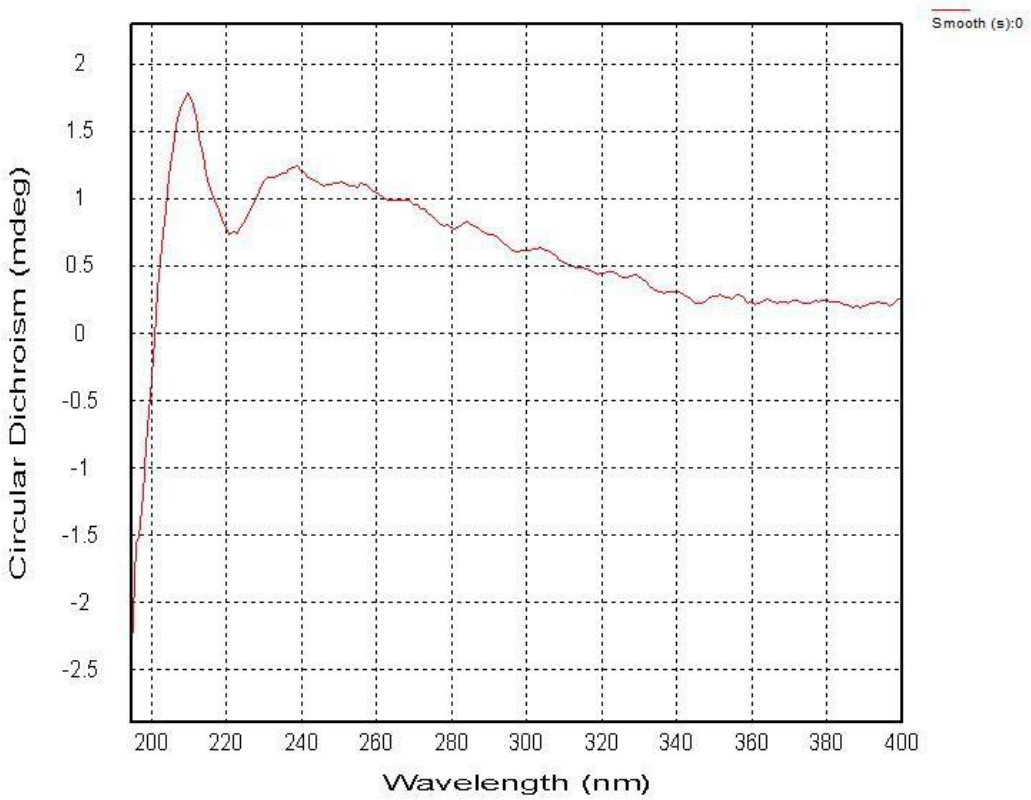



**Figure S72.** IR spectrum of **7** in methanol.



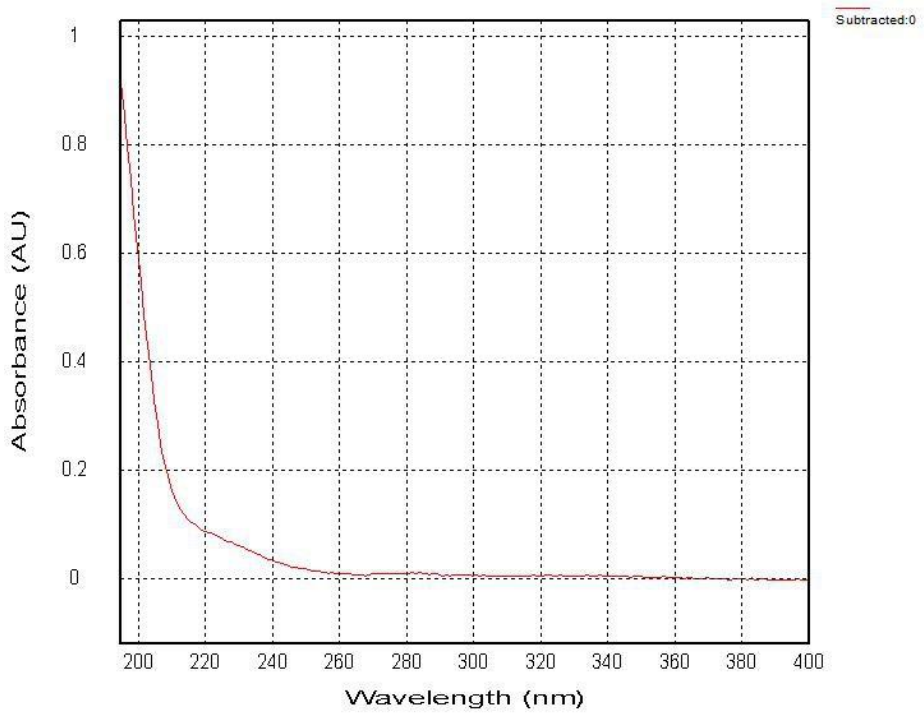



**Figure S73.** a CD spectrum of **7** in methanol.

**Rudolph Research Analytical**

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Saturday, 28-MAY-2022

Set Temperature : OFF

Time Delay : Disabled

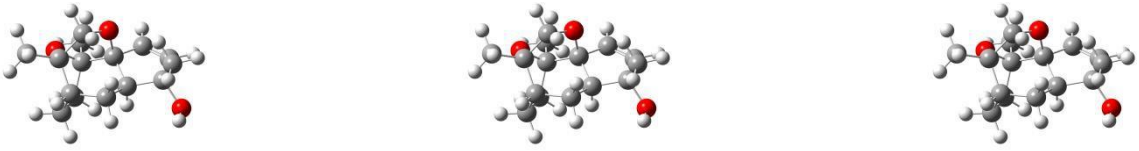
Delay between Measurement : Disabled

| n | Average | Std.Dev. | % RSD | Maximum | Minimum |
|---|---|---|---|---|---|
| 5 | -15.25 | 0.21 | -1.37 | -15.05 | -15.50 |

| S.No | Sample ID | Time | Result | Scale | OR °Arc | WLG.nm | Lg.mm | Conc.g/100ml | Temp. |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 05R58 | 11:17:06 AM | -15.45 | SR | -0.0309 | 589 | 100.00 | 0.200 | 24.6 |
| 2 | 05R58 | 11:17:14 AM | -15.05 | SR | -0.0301 | 589 | 100.00 | 0.200 | 24.6 |
| 3 | 05R58 | 11:17:23 AM | -15.50 | SR | -0.0310 | 589 | 100.00 | 0.200 | 24.6 |
| 4 | 05R58 | 11:17:30 AM | -15.10 | SR | -0.0302 | 589 | 100.00 | 0.200 | 24.6 |
| 5 | 05R58 | 11:17:39 AM | -15.15 | SR | -0.0303 | 589 | 100.00 | 0.200 | 24.6 |

**Figure S73.** b Specific Rotation of **7** in methanol.

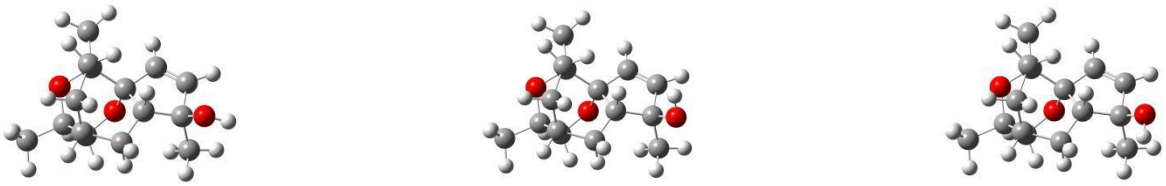
Three conformers for **1a**



**1a_1** **1a_2** **1a_3**

**Figure S74.** Optimized geometries of predominant conformers for compound 1a at the B3LYP/6-31G(d) level.

Three conformers for **1b**



**1b_1** **1b_2** **1b_3**

**Figure S75.** Optimized geometries of predominant conformers for compound **1b** at the B3LYP/6-31G(d) level.

**Table S1.** Boltzmann distribution of conformers **1a_1–1a_3.**

| | Conformer | E(Hartree) | ΔG(kcal/mol) | Proportion(%) |
|---|---|---|---|---|
| | **1a_1** | -810.157367 | 0.336345038 | 28.52 |
| | **1a_2** | -810.157903 | 0 | 50.34 |
| **1a** | **1a_3** | -810.157084 | 0.513930198 | 21.13 |

**Table S2.** Cartesian coordinates of conformers **1a_1–1a_2.**

| Atomic Type | 1a_1 | | | 1a_2 | | |
|---|---|---|---|---|---|---|
| | X | Y | Z | X | Y | Z |
| C | -0.329781 | 0.702491 | -0.39409 | -0.332725 | 0.693737 | -0.40107 |
| C | -1.056445 | -0.279275 | 0.568202 | -1.056214 | -0.280924 | 0.571146 |
| C | 1.022015 | 1.310801 | 0.189614 | 1.016941 | 1.315123 | 0.173949 |
| C | -0.305577 | -1.594106 | 0.771802 | -0.299376 | -1.589374 | 0.791231 |
| H | -1.108574 | 0.225346 | 1.536037 | -1.097055 | 0.236327 | 1.534684 |
| O | -0.041135 | 0.081734 | -1.674432 | -0.042716 | 0.059556 | -1.674044 |
| C | 1.175389 | 1.12046 | 1.710982 | 1.172872 | 1.143992 | 1.697354 |
| O | 2.143794 | 0.59761 | -0.374959 | 2.140788 | 0.599051 | -0.38241 |
| C | 1.215054 | -1.338618 | 0.877691 | 1.220168 | -1.325839 | 0.894306 |
| H | -0.509422 | -2.304978 | -0.035015 | -0.500644 | -2.309895 | -0.007497 |
| H | -0.64901 | -2.07635 | 1.695237 | -0.641863 | -2.062495 | 1.719776 |
| C | 0.978216 | -0.927217 | -1.690121 | 0.980494 | -0.94594 | -1.678294 |
| C | 1.556932 | -0.355673 | 2.024533 | 1.55802 | -0.327431 | 2.029085 |
| H | 1.984909 | 1.779158 | 2.0455 | 1.981555 | 1.808506 | 2.022094 |
| H | 0.278422 | 1.442418 | 2.249658 | 0.276393 | 1.471493 | 2.233786 |
| C | 1.876343 | -0.816136 | -0.456807 | 1.87871 | -0.816706 | -0.446844 |
| H | 1.685183 | -2.301077 | 1.113138 | 1.694761 | -2.283164 | 1.141417 |
| H | 1.584808 | -0.73852 | -2.583619 | 1.585698 | -0.765108 | -2.574252 |
| H | 0.525547 | -1.922193 | -1.794391 | 0.531294 | -1.943564 | -1.770787 |
| H | 2.635367 | -0.407413 | 2.208993 | 2.636386 | -0.373801 | 2.215112 |
| H | 1.071053 | -0.694012 | 2.94708 | 1.072482 | -0.655825 | 2.955414 |
| C | 3.221744 | -1.496362 | -0.694793 | 3.226597 | -1.494508 | -0.677397 |
| H | 3.850906 | -1.427951 | 0.199076 | 3.85586 | -1.412994 | 0.215294 |
| H | 3.750307 | -1.018555 | -1.526107 | 3.752886 | -1.024599 | -1.51461 |
| H | 3.080157 | -2.556168 | -0.933891 | 3.088949 | -2.557612 | -0.903752 |
| C | -1.453912 | 1.676557 | -0.709045 | -1.462009 | 1.658625 | -0.729433 |
| H | -1.286691 | 2.644419 | -1.16857 | -1.298165 | 2.620697 | -1.202009 |
| C | -2.646579 | 1.132318 | -0.459861 | -2.653834 | 1.111308 | -0.480048 |
| H | -3.610125 | 1.594557 | -0.662589 | -3.619942 | 1.562158 | -0.6938 |
| C | -2.538499 | -0.271664 | 0.114074 | -2.544908 | -0.283116 | 0.112605 |
| C | -2.923418 | -1.335825 | -0.920229 | -2.916349 | -1.361798 | -0.907215 |
| H | -2.852638 | -2.337598 | -0.482556 | -2.861964 | -2.354623 | -0.447135 |
| H | -3.95724 | -1.184463 | -1.256638 | -3.941702 | -1.207281 | -1.260214 |
| H | -2.269382 | -1.280183 | -1.79447 | -2.237652 | -1.325697 | -1.762286 |
| O | -3.338093 | -0.436342 | 1.301467 | -3.446849 | -0.485048 | 1.214329 |
| H | -4.264487 | -0.515869 | 1.019928 | -3.30467 | 0.242225 | 1.842776 |
| C | 1.223642 | 2.764167 | -0.230622 | 1.21215 | 2.763946 | -0.264454 |
| H | 0.509887 | 3.425525 | 0.270895 | 0.495662 | 3.42853 | 0.228913 |
| H | 2.235394 | 3.081613 | 0.041375 | 2.222522 | 3.089189 | 0.003327 |
| H | 1.10836 | 2.876772 | -1.313663 | 1.096207 | 2.862491 | -1.348784 |

**Table S3.** Cartesian coordinates of conformers **1a_3.**

| Atomic Type | (+)-1c | | |
|---|---|---|---|
| | X | Y | Z |
| C | -0.329135 | 0.702433 | -0.389408 |
| C | -1.05673 | -0.283601 | 0.568713 |
| C | 1.022177 | 1.31006 | 0.196861 |
| C | -0.303644 | -1.599116 | 0.76435 |
| H | -1.108923 | 0.216746 | 1.538429 |
| O | -0.039285 | 0.090623 | -1.673525 |
| C | 1.175569 | 1.112619 | 1.717228 |
| O | 2.1444 | 0.600355 | -0.371032 |
| C | 1.217017 | -1.342594 | 0.871932 |
| H | -0.506475 | -2.305874 | -0.04653 |
| H | -0.642819 | -2.089527 | 1.685939 |
| C | 0.979559 | -0.918585 | -1.693959 |
| C | 1.557464 | -0.364949 | 2.023698 |
| H | 1.984942 | 1.769908 | 2.054907 |
| H | 0.278275 | 1.431447 | 2.257145 |
| C | 1.877846 | -0.812831 | -0.460087 |
| H | 1.688174 | -2.305706 | 1.102663 |
| H | 1.585868 | -0.726031 | -2.586825 |
| H | 0.526972 | -1.913169 | -1.80248 |
| H | 2.635816 | -0.417322 | 2.208525 |
| H | 1.071221 | -0.708038 | 2.944345 |
| C | 3.223444 | -1.491454 | -0.701509 |
| H | 3.852697 | -1.427126 | 0.192626 |
| H | 3.751702 | -1.009372 | -1.53056 |
| H | 3.082174 | -2.550136 | -0.945762 |
| C | -1.454276 | 1.676791 | -0.699234 |
| H | -1.288814 | 2.64229 | -1.164013 |
| C | -2.647856 | 1.138482 | -0.442463 |
| H | -3.611708 | 1.601684 | -0.637071 |
| C | -2.546155 | -0.267588 | 0.113649 |
| C | -2.922831 | -1.315662 | -0.942344 |
| H | -2.861958 | -2.328846 | -0.524106 |
| H | -3.950972 | -1.152068 | -1.283002 |
| H | -2.250197 | -1.257373 | -1.80202 |
| O | -3.444761 | -0.368686 | 1.233453 |
| H | -3.448652 | -1.297572 | 1.517243 |
| C | 1.221589 | 2.765623 | -0.216739 |
| H | 0.506014 | 3.423333 | 0.287053 |
| H | 2.232469 | 3.083922 | 0.057613 |
| H | 1.107138 | 2.882726 | -1.299415 |

**Table S4.** Boltzmann distribution of conformers **1b_1–1b_3.**

| | Conformer | E(Hartree) | ΔG(kcal/mol) | Proportion(%) |
|---|---|---|---|---|
| **1b** | **1b_1** | -810.157367 | 0.336345038 | 28.52 |
| | **1b_2** | -810.157903 | 0 | 50.34 |
| | **1b_3** | -810.157084 | 0.513930198 | 21.13 |

**Table S5.** Cartesian coordinates of conformers **1b_1–1b_2.**

| Atomic Type | 1b_1 | | | 1b_2 | | |
|---|---|---|---|---|---|---|
| | X | Y | Z | X | Y | Z |
| C | 0.329781 | 0.702491 | -0.39409 | 0.332725 | 0.693737 | -0.40107 |
| C | 1.056445 | -0.279275 | 0.568202 | 1.056214 | -0.280924 | 0.571146 |
| C | -1.022015 | 1.310801 | 0.189614 | -1.016941 | 1.315123 | 0.173949 |
| C | 0.305577 | -1.594106 | 0.771802 | 0.299376 | -1.589374 | 0.791231 |
| H | 1.108574 | 0.225346 | 1.536037 | 1.097055 | 0.236327 | 1.534684 |
| O | 0.041135 | 0.081734 | -1.674432 | 0.042716 | 0.059556 | -1.674044 |
| C | -1.175389 | 1.12046 | 1.710982 | -1.172872 | 1.143992 | 1.697354 |
| O | -2.143794 | 0.59761 | -0.374959 | -2.140788 | 0.599051 | -0.38241 |
| C | -1.215054 | -1.338618 | 0.877691 | -1.220168 | -1.325839 | 0.894306 |
| H | 0.509422 | -2.304978 | -0.035015 | 0.500644 | -2.309895 | -0.007497 |
| H | 0.64901 | -2.07635 | 1.695237 | 0.641863 | -2.062495 | 1.719776 |
| C | -0.978216 | -0.927217 | -1.690121 | -0.980494 | -0.94594 | -1.678294 |
| C | -1.556932 | -0.355673 | 2.024533 | -1.55802 | -0.327431 | 2.029085 |

| | | | | | | |
|---|---|---|---|---|---|---|
| H | -1.984909 | 1.779158 | 2.0455 | -1.981555 | 1.808506 | 2.022094 |
| H | -0.278422 | 1.442418 | 2.249658 | -0.276393 | 1.471493 | 2.233786 |
| C | -1.876343 | -0.816136 | -0.456807 | -1.87871 | -0.816706 | -0.446844 |
| H | -1.685183 | -2.301077 | 1.113138 | -1.694761 | -2.283164 | 1.141417 |
| H | -1.584808 | -0.73852 | -2.583619 | -1.585698 | -0.765108 | -2.574252 |
| H | -0.525547 | -1.922193 | -1.79439 | -0.531294 | -1.943564 | -1.770787 |
| H | -2.635367 | -0.407413 | 2.208993 | -2.636386 | -0.373801 | 2.215112 |
| H | -1.071053 | -0.694012 | 2.94708 | -1.072482 | -0.655825 | 2.955414 |
| C | -3.221744 | -1.496362 | -0.694793 | -3.226597 | -1.494508 | -0.677397 |
| H | -3.850906 | -1.427951 | 0.199076 | -3.85586 | -1.412994 | 0.215294 |
| H | -3.750307 | -1.018555 | -1.526107 | -3.752886 | -1.024599 | -1.51461 |
| H | -3.080157 | -2.556168 | -0.933891 | -3.088949 | -2.557612 | -0.903752 |
| C | 1.453912 | 1.676557 | -0.709045 | 1.462009 | 1.658625 | -0.729433 |
| H | 1.286691 | 2.644419 | -1.16857 | 1.298165 | 2.620697 | -1.202009 |
| C | 2.646579 | 1.132318 | -0.459861 | 2.653834 | 1.111308 | -0.480048 |
| H | 3.610125 | 1.594557 | -0.662589 | 3.619942 | 1.562158 | -0.6938 |
| C | 2.538499 | -0.271664 | 0.114074 | 2.544908 | -0.283116 | 0.112605 |
| C | 2.923418 | -1.335825 | -0.920229 | 2.916349 | -1.361798 | -0.907215 |
| H | 2.852638 | -2.337598 | -0.482556 | 2.861964 | -2.354623 | -0.447135 |
| H | 3.95724 | -1.184463 | -1.256638 | 3.941702 | -1.207281 | -1.260214 |
| H | 2.269382 | -1.280183 | -1.79447 | 2.237652 | -1.325697 | -1.762286 |
| O | 3.338093 | -0.436342 | 1.301467 | 3.446849 | -0.485048 | 1.214329 |
| H | 4.264487 | -0.515869 | 1.019928 | 3.30467 | 0.242225 | 1.842776 |
| C | -1.223642 | 2.764167 | -0.230622 | -1.21215 | 2.763946 | -0.264454 |
| H | -0.509887 | 3.425525 | 0.270895 | -0.495662 | 3.428529 | 0.228913 |
| H | -2.235394 | 3.081613 | 0.041375 | -2.222522 | 3.089189 | 0.003327 |
| H | -1.10836 | 2.876772 | -1.313663 | -1.096207 | 2.862491 | -1.348784 |

**Table S6.** Cartesian coordinates of conformers **1b_3.**

| **Atomic** | **1b_3** | | |
|---|---|---|---|
| **Type** | **X** | **Y** | **Z** |
| C | 0.329135 | 0.702433 | -0.38941 |
| C | 1.05673 | -0.2836 | 0.568713 |
| C | -1.02218 | 1.31006 | 0.196861 |
| C | 0.303644 | -1.59912 | 0.76435 |
| H | 1.108923 | 0.216746 | 1.538429 |
| O | 0.039285 | 0.090623 | -1.67353 |
| C | -1.17557 | 1.112619 | 1.717228 |
| O | -2.1444 | 0.600355 | -0.37103 |
| C | -1.21702 | -1.34259 | 0.871932 |
| H | 0.506475 | -2.30587 | -0.04653 |
| H | 0.642819 | -2.08953 | 1.685939 |
| C | -0.97956 | -0.91859 | -1.69396 |
| C | -1.55746 | -0.36495 | 2.023698 |
| H | -1.98494 | 1.769908 | 2.054907 |
| H | -0.27828 | 1.431447 | 2.257145 |
| C | -1.87785 | -0.81283 | -0.46009 |
| H | -1.68817 | -2.30571 | 1.102663 |
| H | -1.58587 | -0.72603 | -2.58683 |
| H | -0.52697 | -1.91317 | -1.80248 |
| H | -2.63582 | -0.41732 | 2.208525 |
| H | -1.07122 | -0.70804 | 2.944345 |
| C | -3.22344 | -1.49145 | -0.70151 |
| H | -3.8527 | -1.42713 | 0.192626 |
| H | -3.7517 | -1.00937 | -1.53056 |
| H | -3.08217 | -2.55014 | -0.94576 |
| C | 1.454275 | 1.676791 | -0.69923 |
| H | 1.288814 | 2.64229 | -1.16401 |
| C | 2.647856 | 1.138482 | -0.44246 |
| H | 3.611708 | 1.601684 | -0.63707 |
| C | 2.546155 | -0.26759 | 0.113649 |
| C | 2.922831 | -1.31566 | -0.94234 |
| H | 2.861958 | -2.32885 | -0.52411 |
| H | 3.950972 | -1.15207 | -1.283 |
| H | 2.250197 | -1.25737 | -1.80202 |
| O | 3.444761 | -0.36869 | 1.233453 |
| H | 3.448652 | -1.29757 | 1.517243 |
| C | -1.22159 | 2.765623 | -0.21674 |
| H | -0.50601 | 3.423333 | 0.287053 |
| H | -2.23247 | 3.083922 | 0.057613 |

| | | | |
|---|---|---|---|
| H | -1.10714 | 2.882726 | -1.29942 |

**Table S7.** Gibbs free energies[a] and equilibrium populations[b] of low-energy conformers of compound **2**.

| Conformers | ΔG(a.u.) | P(%)/100 | G(a.u.) |
|---|---|---|---|
| **2_a** | 0.0058 | 0.12 | -813.72172 |
| **2_b** | 0.0 | 55.84 | -813.727517 |
| **2_c** | 0.01318 | 0.0 | -813.714337 |
| **2_d** | 0.0014 | 12.71 | -813.726119 |
| **2-e** | 0.00714 | 0.03 | -813.720374 |
| **2_f** | 0.0037 | 1.1 | -813.723813 |
| **2_g** | 0.00058 | 30.2 | -813.726936 |

[a]wB97M-V/def2-TZVP, in a.u.m[b]From ΔG values at 298.15K.

**Table S8.** Cartesian coordinates for the low-energy reoptimized random reseach conformers of compound **2** at B3LYP-D3(BJ)/6-31G* level of theory in methanol.

| **2_a** | | | **Standard Orientation (A.U.)** | | |
|---|---|---|---|---|---|
| **Center number** | **Atomic number** | **Atomic Type** | **X** | Y | Z |
| 0 | 6 | 0 | 0.783819 | -0.605193 | 3.423168 |
| 1 | 6 | 0 | -0.877688 | -2.145008 | 1.598982 |
| 2 | 6 | 0 | -1.715782 | -0.478772 | -0.630255 |
| 3 | 6 | 0 | 0.274598 | 0.163238 | -2.642882 |
| 4 | 6 | 0 | 2.866612 | 1.249449 | -1.818345 |
| 5 | 6 | 0 | 4.594293 | -0.134303 | 0.096514 |
| 6 | 6 | 0 | 3.622086 | -0.478661 | 2.850835 |
| 7 | 6 | 0 | -0.651123 | 2.345135 | -4.379528 |
| 8 | 6 | 0 | -0.002107 | 4.732711 | -2.832737 |
| 9 | 6 | 0 | 2.472811 | 4.119149 | -1.405103 |
| 10 | 8 | 0 | 6.916375 | 1.268129 | 0.198901 |
| 11 | 6 | 0 | 5.355782 | -2.70157 | -1.012161 |
| 12 | 8 | 0 | 2.37878 | 4.694623 | 1.227486 |
| 13 | 6 | 0 | -3.38489 | 2.236634 | -5.296052 |
| 14 | 6 | 0 | -3.167898 | -3.3918 | 2.954516 |
| 15 | 6 | 0 | -4.755459 | -1.590374 | 4.584725 |
| 16 | 8 | 0 | -5.754795 | 0.525914 | 3.286709 |
| 17 | 1 | 0 | 4.001666 | 1.178141 | -3.567079 |
| 18 | 1 | 0 | 0.238348 | -3.739629 | 0.835322 |
| 19 | 1 | 0 | 0.605445 | -1.558235 | -3.776992 |
| 20 | 6 | 0 | -2.352007 | -5.67545 | 4.546806 |
| 21 | 1 | 0 | -4.434697 | -4.121634 | 1.449225 |
| 22 | 1 | 0 | 0.030383 | 1.333145 | 3.501663 |
| 23 | 1 | 0 | 0.615736 | -1.368878 | 5.358717 |
| 24 | 1 | 0 | -3.275948 | -1.446935 | -1.632296 |
| 25 | 1 | 0 | -2.543864 | 1.255841 | 0.164396 |
| 26 | 1 | 0 | 4.387057 | 1.098291 | 3.973175 |
| 27 | 1 | 0 | 4.546104 | -2.199594 | 3.592946 |
| 28 | 1 | 0 | 0.580969 | 2.331515 | -6.069204 |
| 29 | 1 | 0 | 0.145626 | 6.435773 | -4.02871 |
| 30 | 1 | 0 | -1.499321 | 5.082697 | -1.42059 |
| 31 | 1 | 0 | 4.08501 | 5.152567 | -2.243022 |
| 32 | 1 | 0 | 6.523088 | 2.846106 | 1.05767 |
| 33 | 1 | 0 | 3.738574 | -4.011252 | -1.094683 |
| 34 | 1 | 0 | 6.126626 | -2.469842 | -2.936685 |
| 35 | 1 | 0 | 6.83905 | -3.551731 | 0.180812 |
| 36 | 1 | 0 | 2.001495 | 6.480996 | 1.421624 |
| 37 | 1 | 0 | -3.774232 | 0.451724 | -6.309571 |
| 38 | 1 | 0 | -4.739286 | 2.385987 | -3.716097 |
| 39 | 1 | 0 | -3.783488 | 3.810033 | -6.611066 |
| 40 | 1 | 0 | -3.597463 | -0.801852 | 6.127308 |
| 41 | 1 | 0 | -6.294995 | -2.696508 | 5.49072 |
| 42 | 1 | 0 | -6.652676 | -0.077558 | 1.802927 |
| 43 | 1 | 0 | -3.994586 | -6.613071 | 5.432775 |
| 44 | 1 | 0 | -1.368029 | -7.089827 | 3.369533 |
| 45 | 1 | 0 | -1.048356 | -5.11572 | 6.079714 |
| **2_b** | | | Standard Orientation (A.U.) | | |
| Center number | Atomic number | Atomic Type | X | Y | Z |

| | | | | | |
|---|---|---|---|---|---|
| 0 | 6 | 0 | 0.9965 | -3.384837 | 1.400963 |
| 1 | 6 | 0 | -1.677936 | -2.591786 | 0.536248 |
| 2 | 6 | 0 | -1.755781 | 0.02062 | -0.735075 |
| 3 | 6 | 0 | 0.245041 | 0.485187 | -2.796167 |
| 4 | 6 | 0 | 2.809922 | 1.506477 | -1.806855 |
| 5 | 6 | 0 | 4.315851 | 0.058701 | 0.25671 |
| 6 | 6 | 0 | 2.716118 | -1.232141 | 2.310733 |
| 7 | 6 | 0 | -0.493224 | 2.700776 | -4.578764 |
| 8 | 6 | 0 | 0.079092 | 5.068963 | -2.971998 |
| 9 | 6 | 0 | 2.26297 | 4.335111 | -1.184736 |
| 10 | 8 | 0 | 5.832791 | 1.842086 | 1.681973 |
| 11 | 6 | 0 | 6.118548 | -1.833585 | -0.998634 |
| 12 | 8 | 0 | 1.53037 | 4.75027 | 1.356569 |
| 13 | 6 | 0 | -3.129647 | 2.656782 | -5.75071 |
| 14 | 6 | 0 | -3.696259 | -2.775055 | 2.659707 |
| 15 | 6 | 0 | -3.022527 | -1.28206 | 5.061179 |
| 16 | 8 | 0 | -4.991551 | -1.296464 | 6.877245 |
| 17 | 1 | 0 | 4.05903 | 1.566935 | -3.483749 |
| 18 | 1 | 0 | -2.273082 | -3.977599 | -0.912 |
| 19 | 1 | 0 | 0.503731 | -1.267644 | -3.905937 |
| 20 | 6 | 0 | -4.362533 | -5.515874 | 3.321824 |
| 21 | 1 | 0 | -5.431842 | -1.882343 | 1.887323 |
| 22 | 1 | 0 | 0.830256 | -4.796328 | 2.925633 |
| 23 | 1 | 0 | 1.938259 | -4.400534 | -0.155093 |
| 24 | 1 | 0 | -3.650552 | 0.20688 | -1.583766 |
| 25 | 1 | 0 | -1.608977 | 1.52815 | 0.689751 |
| 26 | 1 | 0 | 1.609551 | 0.230978 | 3.286315 |
| 27 | 1 | 0 | 4.079813 | -1.962769 | 3.709899 |
| 28 | 1 | 0 | 0.87838 | 2.649002 | -6.157167 |
| 29 | 1 | 0 | 0.530707 | 6.729016 | -4.148196 |
| 30 | 1 | 0 | -1.564722 | 5.576443 | -1.794044 |
| 31 | 1 | 0 | 3.97157 | 5.475511 | -1.596911 |
| 32 | 1 | 0 | 7.054437 | 2.605169 | 0.54058 |
| 33 | 1 | 0 | 5.105679 | -3.137844 | -2.27071 |
| 34 | 1 | 0 | 7.524944 | -0.815493 | -2.163949 |
| 35 | 1 | 0 | 7.140349 | -2.952028 | 0.43568 |
| 36 | 1 | 0 | 2.973458 | 4.189852 | 2.366636 |
| 37 | 1 | 0 | -4.630058 | 2.934884 | -4.327982 |
| 38 | 1 | 0 | -3.325793 | 4.189139 | -7.156825 |
| 39 | 1 | 0 | -3.497212 | 0.8481 | -6.730873 |
| 40 | 1 | 0 | -2.485399 | 0.683366 | 4.576453 |
| 41 | 1 | 0 | -1.387066 | -2.152944 | 6.017056 |
| 42 | 1 | 0 | -6.4635 | -0.492235 | 6.128811 |
| 43 | 1 | 0 | -5.089316 | -6.540692 | 1.65366 |
| 44 | 1 | 0 | -2.695056 | -6.555118 | 4.033396 |
| 45 | 1 | 0 | -5.808692 | -5.568106 | 4.820443 |

| **2_c** | | | Standard Orientation (A.U.) | | |
|---|---|---|---|---|---|
| Center number | Atomic number | Atomic Type | X | Y | Z |
| 0 | 6 | 0 | 1.818025 | -3.670372 | 1.559486 |
| 1 | 6 | 0 | -0.841921 | -3.050792 | 0.54816 |
| 2 | 6 | 0 | -0.731796 | -2.196132 | -2.245676 |
| 3 | 6 | 0 | 0.589467 | 0.265905 | -3.187224 |
| 4 | 6 | 0 | 2.594124 | 1.681472 | -1.561094 |
| 5 | 6 | 0 | 4.547211 | 0.242473 | 0.081957 |
| 6 | 6 | 0 | 3.50413 | -1.423247 | 2.23718 |
| 7 | 6 | 0 | -1.162975 | 2.518122 | -3.929577 |
| 8 | 6 | 0 | -1.40714 | 4.078715 | -1.494866 |
| 9 | 6 | 0 | 1.23506 | 3.972627 | -0.280456 |
| 10 | 8 | 0 | 6.141578 | 2.114555 | 1.215041 |
| 11 | 6 | 0 | 6.279919 | -1.300855 | -1.645325 |
| 12 | 8 | 0 | 1.195251 | 3.74807 | 2.411834 |
| 13 | 6 | 0 | -3.650875 | 1.928337 | -5.263237 |
| 14 | 6 | 0 | -2.455221 | -1.405306 | 2.350191 |
| 15 | 6 | 0 | -2.374377 | -2.413785 | 5.079956 |
| 16 | 8 | 0 | -3.88608 | -1.001653 | 6.779633 |
| 17 | 1 | 0 | 3.805738 | 2.608228 | -2.979666 |
| 18 | 1 | 0 | -1.833088 | -4.895635 | 0.451805 |
| 19 | 1 | 0 | 1.546708 | -0.324881 | -4.940593 |
| 20 | 6 | 0 | -5.212889 | -1.239463 | 1.472568 |
| 21 | 1 | 0 | -1.661877 | 0.514582 | 2.430606 |

| | | | | | |
|---|---|---|---|---|---|
| 22 | 1 | 0 | 1.631998 | -4.854689 | 3.266986 |
| 23 | 1 | 0 | 2.77974 | -4.889104 | 0.161359 |
| 24 | 1 | 0 | 0.22402 | -3.772522 | -3.223546 |
| 25 | 1 | 0 | -2.66349 | -2.218657 | -3.022794 |
| 26 | 1 | 0 | 2.50757 | -0.188168 | 3.579261 |
| 27 | 1 | 0 | 5.190518 | -2.138123 | 3.240639 |
| 28 | 1 | 0 | -0.028871 | 3.664196 | -5.2642 |
| 29 | 1 | 0 | -2.054785 | 6.029943 | -1.856297 |
| 30 | 1 | 0 | -2.787886 | 3.186922 | -0.215015 |
| 31 | 1 | 0 | 2.308232 | 5.702581 | -0.747474 |
| 32 | 1 | 0 | 5.070795 | 3.018101 | 2.412839 |
| 33 | 1 | 0 | 7.716475 | -2.300588 | -0.510861 |
| 34 | 1 | 0 | 5.213726 | -2.70594 | -2.756134 |
| 35 | 1 | 0 | 7.27251 | -0.028697 | -2.966618 |
| 36 | 1 | 0 | 0.25545 | 5.162342 | 3.111823 |
| 37 | 1 | 0 | -4.549093 | 3.689262 | -5.93737 |
| 38 | 1 | 0 | -3.346943 | 0.697375 | -6.922709 |
| 39 | 1 | 0 | -5.023027 | 0.981455 | -4.011258 |
| 40 | 1 | 0 | -0.446637 | -2.283734 | 5.846774 |
| 41 | 1 | 0 | -2.91583 | -4.446944 | 5.096019 |
| 42 | 1 | 0 | -5.650725 | -1.322055 | 6.401317 |
| 43 | 1 | 0 | -6.314669 | 0.032165 | 2.706706 |
| 44 | 1 | 0 | -5.387905 | -0.489397 | -0.458801 |
| 45 | 1 | 0 | -6.120193 | -3.126573 | 1.491836 |

| **2_d** | | | Standard Orientation (A.U.) | | |
|---|---|---|---|---|---|
| Center number | Atomic number | Atomic Type | X | Y | Z |
| 0 | 6 | 0 | 1.181423 | -2.566571 | 2.898415 |
| 1 | 6 | 0 | -1.144046 | -2.456787 | 1.13134 |
| 2 | 6 | 0 | -1.627322 | 0.155465 | -0.064658 |
| 3 | 6 | 0 | -0.014957 | 0.659255 | -2.428336 |
| 4 | 6 | 0 | 2.799492 | 1.333695 | -1.990723 |
| 5 | 6 | 0 | 4.431954 | -0.185835 | -0.084783 |
| 6 | 6 | 0 | 3.215336 | -0.537026 | 2.550296 |
| 7 | 6 | 0 | -0.905675 | 2.988263 | -3.981476 |
| 8 | 6 | 0 | 0.295927 | 5.232253 | -2.584964 |
| 9 | 6 | 0 | 2.875254 | 4.278486 | -1.628393 |
| 10 | 8 | 0 | 6.759634 | 1.148071 | 0.238582 |
| 11 | 6 | 0 | 5.170467 | -2.744043 | -1.208611 |
| 12 | 8 | 0 | 3.467526 | 5.156821 | 0.858885 |
| 13 | 6 | 0 | -3.738248 | 3.2612 | -4.453582 |
| 14 | 6 | 0 | -3.540913 | -3.607343 | 2.380225 |
| 15 | 6 | 0 | -4.526535 | -2.219316 | 4.716237 |
| 16 | 8 | 0 | -5.145968 | 0.316692 | 4.120506 |
| 17 | 1 | 0 | 3.731714 | 1.040203 | -3.83462 |
| 18 | 1 | 0 | -0.750633 | -3.729672 | -0.479729 |
| 19 | 1 | 0 | -0.156118 | -1.043575 | -3.630242 |
| 20 | 6 | 0 | -3.157935 | -6.408822 | 3.034248 |
| 21 | 1 | 0 | -5.063823 | -3.494444 | 0.951367 |
| 22 | 1 | 0 | 0.554095 | -2.416851 | 4.884085 |
| 23 | 1 | 0 | 2.062571 | -4.450191 | 2.743058 |
| 24 | 1 | 0 | -3.628861 | 0.222668 | -0.625357 |
| 25 | 1 | 0 | -1.431384 | 1.66661 | 1.355137 |
| 26 | 1 | 0 | 2.479743 | 1.296277 | 3.202432 |
| 27 | 1 | 0 | 4.798957 | -0.990819 | 3.831711 |
| 28 | 1 | 0 | 0.031513 | 2.832437 | -5.845702 |
| 29 | 1 | 0 | 0.455644 | 6.943286 | -3.764858 |
| 30 | 1 | 0 | -0.891082 | 5.74901 | -0.940876 |
| 31 | 1 | 0 | 4.431293 | 5.044355 | -2.771194 |
| 32 | 1 | 0 | 6.305062 | 2.771687 | 0.994662 |
| 33 | 1 | 0 | 6.35849 | -2.436477 | -2.893787 |
| 34 | 1 | 0 | 6.282174 | -3.847488 | 0.169845 |
| 35 | 1 | 0 | 3.499904 | -3.857927 | -1.765728 |
| 36 | 1 | 0 | 2.018369 | 4.882039 | 1.952505 |
| 37 | 1 | 0 | -4.791064 | 3.625177 | -2.688909 |
| 38 | 1 | 0 | -4.115528 | 4.857012 | -5.747465 |
| 39 | 1 | 0 | -4.532598 | 1.537748 | -5.32696 |
| 40 | 1 | 0 | -3.097397 | -2.300234 | 6.251728 |
| 41 | 1 | 0 | -6.217624 | -3.248373 | 5.415178 |
| 42 | 1 | 0 | -5.813969 | 1.120153 | 5.627355 |
| 43 | 1 | 0 | -2.476736 | -7.47095 | 1.371757 |

| | | | | | |
|---|---|---|---|---|---|
| 44 | 1 | 0 | -1.756955 | -6.664948 | 4.561635 |
| 45 | 1 | 0 | -4.942932 | -7.29098 | 3.664298 |
| **2_e** | | | Standard Orientation (A.U.) | | |
| Center number | Atomic number | Atomic Type | X | Y | Z |
| 0 | 6 | 0 | 0.888031 | -1.976937 | 3.39925 |
| 1 | 6 | 0 | -1.368567 | -1.948302 | 1.560776 |
| 2 | 6 | 0 | -1.258381 | 0.205073 | -0.401671 |
| 3 | 6 | 0 | 0.823883 | -0.100267 | -2.41724 |
| 4 | 6 | 0 | 3.472604 | 0.93884 | -1.667692 |
| 5 | 6 | 0 | 4.283429 | 0.803532 | 1.144399 |
| 6 | 6 | 0 | 3.564738 | -1.776815 | 2.307483 |
| 7 | 6 | 0 | 0.264414 | 1.169296 | -5.071836 |
| 8 | 6 | 0 | 2.436633 | 3.106251 | -5.50638 |
| 9 | 6 | 0 | 3.609569 | 3.569423 | -2.914252 |
| 10 | 8 | 0 | 3.094281 | 2.705416 | 2.634949 |
| 11 | 6 | 0 | 7.167469 | 1.155926 | 1.322654 |
| 12 | 8 | 0 | 2.280562 | 5.492138 | -1.525456 |
| 13 | 6 | 0 | -2.350469 | 2.372565 | -5.411399 |
| 14 | 6 | 0 | -3.926722 | -1.882095 | 3.010693 |
| 15 | 6 | 0 | -4.110328 | -3.945665 | 5.058591 |
| 16 | 8 | 0 | -6.456083 | -3.9497 | 6.353272 |
| 17 | 1 | 0 | 4.867732 | -0.213783 | -2.712024 |
| 18 | 1 | 0 | -1.338684 | -3.74673 | 0.479572 |
| 19 | 1 | 0 | 0.999558 | -2.149298 | -2.743496 |
| 20 | 6 | 0 | -6.236691 | -2.083507 | 1.260205 |
| 21 | 1 | 0 | -4.018091 | -0.036409 | 4.00886 |
| 22 | 1 | 0 | 0.654737 | -0.42556 | 4.772511 |
| 23 | 1 | 0 | 0.833434 | -3.756488 | 4.483721 |
| 24 | 1 | 0 | -3.08558 | 0.23539 | -1.3777 |
| 25 | 1 | 0 | -1.076531 | 2.017552 | 0.610813 |
| 26 | 1 | 0 | 4.880062 | -2.149644 | 3.88538 |
| 27 | 1 | 0 | 3.914809 | -3.279941 | 0.897799 |
| 28 | 1 | 0 | 0.417946 | -0.319084 | -6.521422 |
| 29 | 1 | 0 | 3.88955 | 2.300261 | -6.765817 |
| 30 | 1 | 0 | 1.790574 | 4.889659 | -6.373781 |
| 31 | 1 | 0 | 5.554964 | 4.291476 | -3.040408 |
| 32 | 1 | 0 | 3.005033 | 4.242286 | 1.607435 |
| 33 | 1 | 0 | 8.197652 | -0.408303 | 0.397077 |
| 34 | 1 | 0 | 7.766154 | 2.948107 | 0.435657 |
| 35 | 1 | 0 | 7.723004 | 1.226187 | 3.330605 |
| 36 | 1 | 0 | 0.476487 | 5.153387 | -1.614213 |
| 37 | 1 | 0 | -2.494097 | 3.227076 | -7.310582 |
| 38 | 1 | 0 | -3.890867 | 0.977872 | -5.235647 |
| 39 | 1 | 0 | -2.722576 | 3.890645 | -4.02366 |
| 40 | 1 | 0 | -2.542617 | -3.767252 | 6.427558 |
| 41 | 1 | 0 | -3.952723 | -5.829523 | 4.169981 |
| 42 | 1 | 0 | -6.632262 | -2.338042 | 7.217137 |
| 43 | 1 | 0 | -6.018423 | -3.683409 | -0.069637 |
| 44 | 1 | 0 | -7.948255 | -2.433151 | 2.392853 |
| 45 | 1 | 0 | -6.553887 | -0.356444 | 0.139492 |
| **2_f** | | | Standard Orientation (A.U.) | | |
| Center number | Atomic number | Atomic Type | X | Y | Z |
| 0 | 6 | 0 | 0.980897 | -1.068625 | 4.260427 |
| 1 | 6 | 0 | -1.297157 | -1.700282 | 2.585461 |
| 2 | 6 | 0 | -1.587934 | 0.035065 | 0.268804 |
| 3 | 6 | 0 | 0.320718 | -0.474305 | -1.870022 |
| 4 | 6 | 0 | 3.035416 | 0.669516 | -1.590109 |
| 5 | 6 | 0 | 4.073377 | 1.196718 | 1.100227 |
| 6 | 6 | 0 | 3.566505 | -1.007736 | 2.957357 |
| 7 | 6 | 0 | -0.553051 | 0.576955 | -4.476191 |
| 8 | 6 | 0 | 0.413934 | 3.296387 | -4.427703 |
| 9 | 6 | 0 | 3.12818 | 3.037533 | -3.438486 |
| 10 | 8 | 0 | 3.043906 | 3.523249 | 2.118039 |
| 11 | 6 | 0 | 6.933467 | 1.645547 | 0.966191 |
| 12 | 8 | 0 | 4.150016 | 5.294541 | -2.472319 |
| 13 | 6 | 0 | -3.336918 | 0.26043 | -5.168763 |
| 14 | 6 | 0 | -3.751479 | -1.868406 | 4.178566 |
| 15 | 6 | 0 | -5.829976 | -3.386464 | 2.830441 |
| 16 | 8 | 0 | -5.035459 | -5.796276 | 1.992717 |

| | | | | | |
|---|---|---|---|---|---|
| 17 | 1 | 0 | 4.33493 | -0.756465 | -2.376816 |
| 18 | 1 | 0 | -0.98986 | -3.623316 | 1.83383 |
| 19 | 1 | 0 | 0.466893 | -2.550628 | -2.007985 |
| 20 | 6 | 0 | -4.798108 | 0.695416 | 5.03326 |
| 21 | 1 | 0 | -3.262741 | -2.954781 | 5.905512 |
| 22 | 1 | 0 | 0.681732 | 0.751886 | 5.245619 |
| 23 | 1 | 0 | 1.081234 | -2.494628 | 5.784522 |
| 24 | 1 | 0 | -3.48701 | -0.29195 | -0.512523 |
| 25 | 1 | 0 | -1.595402 | 2.04935 | 0.83385 |
| 26 | 1 | 0 | 5.011936 | -0.899603 | 4.45833 |
| 27 | 1 | 0 | 3.891857 | -2.807435 | 1.946894 |
| 28 | 1 | 0 | 0.564699 | -0.453069 | -5.91669 |
| 29 | 1 | 0 | 0.332446 | 4.262281 | -6.274055 |
| 30 | 1 | 0 | -0.700591 | 4.440009 | -3.074786 |
| 31 | 1 | 0 | 4.352672 | 2.531639 | -5.04915 |
| 32 | 1 | 0 | 1.247073 | 3.297842 | 2.402983 |
| 33 | 1 | 0 | 7.378844 | 3.129293 | -0.420397 |
| 34 | 1 | 0 | 7.631752 | 2.24276 | 2.838527 |
| 35 | 1 | 0 | 7.908495 | -0.116485 | 0.422349 |
| 36 | 1 | 0 | 3.640142 | 5.408619 | -0.695532 |
| 37 | 1 | 0 | -3.968315 | -1.717133 | -4.927777 |
| 38 | 1 | 0 | -4.577338 | 1.477381 | -4.012113 |
| 39 | 1 | 0 | -3.649583 | 0.787781 | -7.1646 |
| 40 | 1 | 0 | -6.472692 | -2.383646 | 1.118945 |
| 41 | 1 | 0 | -7.494294 | -3.535518 | 4.102589 |
| 42 | 1 | 0 | -4.485217 | -6.766125 | 3.452736 |
| 43 | 1 | 0 | -5.449387 | 1.834802 | 3.408795 |
| 44 | 1 | 0 | -6.430069 | 0.445922 | 6.312178 |
| 45 | 1 | 0 | -3.369608 | 1.812367 | 6.064257 |

**Table S9.** Gibbs free energies[a] and equilibrium populations[b] of low-energy conformers of compound **5**.

| Conformers | ΔG(a.u.) | P(%)/100 | G(a.u.) |
|---|---|---|---|
| **5_a** | 0.00348 | 1.29 | -888.977565 |
| **5_b** | 0.00949 | 0.0 | -888.971558 |
| **5_c** | 0.01665 | 0.0 | -888.964394 |
| **5_d** | 0.0 | 51.35 | -888.981043 |
| **5_e** | 0.00354 | 1.21 | -888.977502 |
| **5_f** | 0.004 | 0.74 | -888.977044 |
| **5_g** | 0.00018 | 42.27 | -888.980859 |
| **5_h** | 0.00264 | 3.14 | -888.978405 |

[a]wB97M-V/def2-TZVP, in a.u. [b]From ΔG values at 298.15K.

**Table S10.** Cartesian coordinates for the low-energy reoptimized random reseach conformers of compound **5** at B3LYP-D3(BJ)/6-31G* level of theory in methanol.

| **5_a** | | | **Standard Orientation (A.U.)** | | |
|---|---|---|---|---|---|
| **Center number** | **Atomic number** | **Atomic Type** | **X** | Y | Z |
| 0 | 6 | 0 | 3.699469 | 0.641288 | -0.746003 |
| 1 | 6 | 0 | 1.768089 | 2.454823 | -1.966636 |
| 2 | 6 | 0 | -0.943302 | 1.397064 | -2.279731 |
| 3 | 6 | 0 | -1.955092 | -0.418293 | -0.26766 |
| 4 | 6 | 0 | -1.088262 | -3.183682 | -0.639001 |
| 5 | 6 | 0 | 1.645903 | -3.79879 | 0.097068 |
| 6 | 6 | 0 | 3.536922 | -2.162656 | -1.451177 |
| 7 | 6 | 0 | -4.865208 | -0.663891 | -0.274873 |
| 8 | 6 | 0 | -5.295831 | -3.021901 | 1.364356 |
| 9 | 6 | 0 | -3.134867 | -4.850354 | 0.66112 |
| 10 | 1 | 0 | -1.182159 | -3.575632 | -2.687197 |
| 11 | 1 | 0 | -1.411399 | 0.270973 | 1.622853 |
| 12 | 6 | 0 | -6.337484 | 1.656869 | 0.59901 |
| 13 | 6 | 0 | 2.138385 | -3.573278 | 2.955625 |
| 14 | 8 | 0 | 2.062013 | -6.34876 | -0.659493 |
| 15 | 8 | 0 | 5.992326 | -3.301519 | -1.273811 |
| 16 | 6 | 0 | 1.90386 | 5.136652 | -0.731963 |
| 17 | 6 | 0 | 4.580262 | 6.235096 | -0.948932 |
| 18 | 6 | 0 | 1.051808 | 5.291951 | 2.048626 |
| 19 | 8 | 0 | 0.167522 | 6.799777 | -1.990585 |

| | | | | | |
|---|---|---|---|---|---|
| 20 | 8 | 0 | -1.556512 | 4.922214 | 2.361318 |
| 21 | 1 | 0 | 2.454133 | 2.787412 | -3.918845 |
| 22 | 1 | 0 | 3.623876 | 0.810618 | 1.329899 |
| 23 | 1 | 0 | 5.606409 | 1.256596 | -1.314449 |
| 24 | 1 | 0 | -2.221987 | 3.026188 | -2.465673 |
| 25 | 1 | 0 | -1.039253 | 0.400307 | -4.113644 |
| 26 | 1 | 0 | 3.035547 | -2.376105 | -3.461135 |
| 27 | 1 | 0 | -5.445327 | -1.118442 | -2.238888 |
| 28 | 1 | 0 | -7.191558 | -3.850615 | 1.097374 |
| 29 | 1 | 0 | -5.150632 | -2.464834 | 3.374384 |
| 30 | 1 | 0 | -2.401041 | -5.848856 | 2.330553 |
| 31 | 1 | 0 | -3.779894 | -6.328571 | -0.65516 |
| 32 | 1 | 0 | -8.388101 | 1.257785 | 0.633058 |
| 33 | 1 | 0 | -6.046946 | 3.285414 | -0.67621 |
| 34 | 1 | 0 | -5.74616 | 2.240815 | 2.512291 |
| 35 | 1 | 0 | 1.13777 | -5.100407 | 3.951247 |
| 36 | 1 | 0 | 4.170306 | -3.814645 | 3.379923 |
| 37 | 1 | 0 | 1.517064 | -1.753247 | 3.75823 |
| 38 | 1 | 0 | 3.890072 | -6.507096 | -0.859103 |
| 39 | 1 | 0 | 6.73296 | -2.830435 | 0.34084 |
| 40 | 1 | 0 | 4.53376 | 8.261296 | -0.464863 |
| 41 | 1 | 0 | 5.309011 | 6.045068 | -2.897923 |
| 42 | 1 | 0 | 5.9249 | 5.287337 | 0.33316 |
| 43 | 1 | 0 | 2.02861 | 3.854365 | 3.195951 |
| 44 | 1 | 0 | 1.630603 | 7.172151 | 2.7802 |
| 45 | 1 | 0 | 0.384037 | 6.629889 | -3.806237 |
| 46 | 1 | 0 | -2.379291 | 5.881796 | 1.02139 |
| **5_b** | | | Standard Orientation (A.U.) | | |
| Center number | Atomic number | Atomic Type | X | Y | Z |
| 0 | 6 | 0 | 3.131929 | 0.864815 | -1.553838 |
| 1 | 6 | 0 | 0.552609 | 2.188494 | -1.000073 |
| 2 | 6 | 0 | -0.88175 | 1.135844 | 1.304431 |
| 3 | 6 | 0 | -1.998958 | -1.512508 | 0.863139 |
| 4 | 6 | 0 | -0.566698 | -3.207296 | -1.013526 |
| 5 | 6 | 0 | 2.200464 | -3.861703 | -0.412441 |
| 6 | 6 | 0 | 3.88123 | -1.468347 | -0.016207 |
| 7 | 6 | 0 | -4.716812 | -1.508056 | -0.223274 |
| 8 | 6 | 0 | -5.032282 | -4.12709 | -1.532303 |
| 9 | 6 | 0 | -2.415707 | -5.420855 | -1.388392 |
| 10 | 1 | 0 | -0.493922 | -2.19444 | -2.835648 |
| 11 | 1 | 0 | -2.065232 | -2.511249 | 2.701735 |
| 12 | 6 | 0 | -6.748572 | -0.935457 | 1.743931 |
| 13 | 6 | 0 | 2.49262 | -5.672849 | 1.830159 |
| 14 | 8 | 0 | 3.303958 | -5.002738 | -2.615 |
| 15 | 8 | 0 | 4.13016 | -0.721606 | 2.559012 |
| 16 | 6 | 0 | 0.820938 | 5.10355 | -0.88323 |
| 17 | 6 | 0 | 1.985454 | 6.168882 | -3.322575 |
| 18 | 6 | 0 | 2.321938 | 5.98263 | 1.441722 |
| 19 | 8 | 0 | -1.679144 | 6.086933 | -0.64152 |
| 20 | 8 | 0 | 2.075894 | 8.664291 | 1.549909 |
| 21 | 1 | 0 | -0.683769 | 1.893159 | -2.655464 |
| 22 | 1 | 0 | 4.693223 | 2.209336 | -1.259215 |
| 23 | 1 | 0 | 3.228139 | 0.321189 | -3.562664 |
| 24 | 1 | 0 | 0.389009 | 1.068732 | 2.939354 |
| 25 | 1 | 0 | -2.422887 | 2.460035 | 1.75079 |
| 26 | 1 | 0 | 5.752772 | -2.066752 | -0.733866 |
| 27 | 1 | 0 | -4.792954 | -0.015782 | -1.684319 |
| 28 | 1 | 0 | -5.636564 | -3.891221 | -3.513766 |
| 29 | 1 | 0 | -6.496775 | -5.280541 | -0.596914 |
| 30 | 1 | 0 | -2.348658 | -6.701742 | 0.25649 |
| 31 | 1 | 0 | -2.005141 | -6.570034 | -3.083871 |
| 32 | 1 | 0 | -8.650795 | -0.887033 | 0.882033 |
| 33 | 1 | 0 | -6.423574 | 0.914102 | 2.656796 |
| 34 | 1 | 0 | -6.762755 | -2.396114 | 3.241087 |
| 35 | 1 | 0 | 1.614371 | -7.514454 | 1.400975 |
| 36 | 1 | 0 | 4.516468 | -6.043315 | 2.195341 |
| 37 | 1 | 0 | 1.6097 | -4.924539 | 3.563403 |
| 38 | 1 | 0 | 2.179293 | -6.336868 | -3.183763 |
| 39 | 1 | 0 | 5.061004 | -2.020124 | 3.45648 |
| 40 | 1 | 0 | 3.923727 | 5.477851 | -3.656831 |
| 41 | 1 | 0 | 2.059112 | 8.248977 | -3.216366 |

| | | | | | |
|---|---|---|---|---|---|
| 42 | 1 | 0 | 0.792945 | 5.630632 | -4.946784 |
| 43 | 1 | 0 | 1.512809 | 5.105283 | 3.154333 |
| 44 | 1 | 0 | 4.330315 | 5.416344 | 1.304588 |
| 45 | 1 | 0 | -1.467549 | 7.82574 | -0.067313 |
| 46 | 1 | 0 | 2.631344 | 9.250815 | 3.193663 |
| **5_c** | | | Standard Orientation (A.U.) | | |
| Center number | Atomic number | Atomic Type | X | Y | Z |
| 0 | 6 | 0 | 3.066514 | 0.984322 | -2.068045 |
| 1 | 6 | 0 | 0.654612 | 2.672417 | -2.091579 |
| 2 | 6 | 0 | -1.932444 | 1.333732 | -1.634926 |
| 3 | 6 | 0 | -1.970845 | -1.157174 | -0.170817 |
| 4 | 6 | 0 | -0.456512 | -3.26491 | -1.541485 |
| 5 | 6 | 0 | 2.250477 | -3.603967 | -0.496751 |
| 6 | 6 | 0 | 3.553163 | -1.021745 | -0.000915 |
| 7 | 6 | 0 | -4.659947 | -2.231523 | 0.210252 |
| 8 | 6 | 0 | -4.181421 | -5.076445 | 0.53455 |
| 9 | 6 | 0 | -2.18339 | -5.644988 | -1.48847 |
| 10 | 1 | 0 | -0.188107 | -2.701036 | -3.528096 |
| 11 | 1 | 0 | -1.144146 | -0.855223 | 1.713243 |
| 12 | 6 | 0 | -6.133195 | -0.994697 | 2.358962 |
| 13 | 6 | 0 | 2.388472 | -5.221082 | 1.903593 |
| 14 | 8 | 0 | 3.784757 | -4.742484 | -2.423609 |
| 15 | 8 | 0 | 2.956569 | -0.243187 | 2.473669 |
| 16 | 6 | 0 | 0.834976 | 5.258407 | -0.652997 |
| 17 | 6 | 0 | 3.082451 | 6.851236 | -1.575947 |
| 18 | 6 | 0 | 0.842021 | 5.118588 | 2.257593 |
| 19 | 8 | 0 | -1.424746 | 6.665863 | -1.155781 |
| 20 | 8 | 0 | 3.260622 | 4.638627 | 3.330504 |
| 21 | 1 | 0 | 0.583487 | 3.331797 | -4.078372 |
| 22 | 1 | 0 | 4.719019 | 2.25212 | -2.108436 |
| 23 | 1 | 0 | 3.164838 | -0.049757 | -3.875266 |
| 24 | 1 | 0 | -3.209319 | 2.702535 | -0.720746 |
| 25 | 1 | 0 | -2.789037 | 0.937336 | -3.500972 |
| 26 | 1 | 0 | 5.595568 | -1.478378 | -0.134228 |
| 27 | 1 | 0 | -5.728732 | -1.966202 | -1.573706 |
| 28 | 1 | 0 | -5.909996 | -6.2293 | 0.335012 |
| 29 | 1 | 0 | -3.403887 | -5.434666 | 2.442215 |
| 30 | 1 | 0 | -1.160141 | -7.428422 | -1.144751 |
| 31 | 1 | 0 | -3.127593 | -5.851911 | -3.33786 |
| 32 | 1 | 0 | -6.379535 | 1.054111 | 2.035321 |
| 33 | 1 | 0 | -5.12842 | -1.234551 | 4.176723 |
| 34 | 1 | 0 | -8.035429 | -1.833487 | 2.564759 |
| 35 | 1 | 0 | 1.150108 | -4.4926 | 3.406937 |
| 36 | 1 | 0 | 1.851335 | -7.193455 | 1.485597 |
| 37 | 1 | 0 | 4.340909 | -5.230894 | 2.630666 |
| 38 | 1 | 0 | 2.94753 | -6.286676 | -2.957179 |
| 39 | 1 | 0 | 3.623991 | 1.453997 | 2.805072 |
| 40 | 1 | 0 | 2.996609 | 7.083075 | -3.649258 |
| 41 | 1 | 0 | 4.934088 | 6.011077 | -1.124057 |
| 42 | 1 | 0 | 2.975663 | 8.755939 | -0.726465 |
| 43 | 1 | 0 | 0.082203 | 6.931712 | 2.963678 |
| 44 | 1 | 0 | -0.399415 | 3.593878 | 2.927064 |
| 45 | 1 | 0 | -1.771579 | 6.573404 | -2.957766 |
| 46 | 1 | 0 | 4.370802 | 6.066318 | 3.028382 |
| **5_d** | | | Standard Orientation (A.U.) | | |
| Center number | Atomic number | Atomic Type | X | Y | Z |
| 0 | 6 | 0 | 3.102627 | 0.955056 | 0.590152 |
| 1 | 6 | 0 | 1.129208 | 2.458071 | -0.943328 |
| 2 | 6 | 0 | -1.644799 | 1.699074 | -0.42049 |
| 3 | 6 | 0 | -2.11676 | -1.066623 | 0.29323 |
| 4 | 6 | 0 | -0.693741 | -3.088292 | -1.29423 |
| 5 | 6 | 0 | 1.948072 | -3.782446 | -0.265903 |
| 6 | 6 | 0 | 3.823468 | -1.57252 | -0.607729 |
| 7 | 6 | 0 | -4.92677 | -1.840377 | 0.137662 |
| 8 | 6 | 0 | -4.793485 | -4.733975 | 0.23136 |
| 9 | 6 | 0 | -2.541688 | -5.380217 | -1.48411 |
| 10 | 1 | 0 | -0.377711 | -2.347333 | -3.217052 |
| 11 | 1 | 0 | -1.571423 | -1.320334 | 2.290189 |
| 12 | 6 | 0 | -6.624159 | -0.648314 | 2.140876 |
| 13 | 6 | 0 | 1.920782 | -4.759553 | 2.462155 |
| 14 | 8 | 0 | 3.062304 | -5.698025 | -1.852573 |

| | | | | | |
|---|---|---|---|---|---|
| 15 | 8 | 0 | 6.232252 | -2.278732 | 0.32071 |
| 16 | 6 | 0 | 1.506849 | 5.358197 | -0.705556 |
| 17 | 6 | 0 | 3.89628 | 6.241475 | -2.102964 |
| 18 | 6 | 0 | 1.603403 | 6.213923 | 2.072811 |
| 19 | 8 | 0 | -0.633826 | 6.525963 | -1.844068 |
| 20 | 8 | 0 | 1.422733 | 8.897595 | 2.058699 |
| 21 | 1 | 0 | 1.499383 | 2.042007 | -2.954544 |
| 22 | 1 | 0 | 2.495869 | 0.69248 | 2.569473 |
| 23 | 1 | 0 | 4.894166 | 2.010389 | 0.675203 |
| 24 | 1 | 0 | -2.419698 | 2.89271 | 1.102781 |
| 25 | 1 | 0 | -2.76533 | 2.18325 | -2.109233 |
| 26 | 1 | 0 | 3.945869 | -1.275093 | -2.680115 |
| 27 | 1 | 0 | -5.633764 | -1.2849 | -1.755083 |
| 28 | 1 | 0 | -6.56687 | -5.657325 | -0.365638 |
| 29 | 1 | 0 | -4.40829 | -5.337864 | 2.19721 |
| 30 | 1 | 0 | -1.662719 | -7.19795 | -0.957529 |
| 31 | 1 | 0 | -3.182864 | -5.601819 | -3.454613 |
| 32 | 1 | 0 | -6.678209 | 1.431021 | 1.965969 |
| 33 | 1 | 0 | -5.939285 | -1.113425 | 4.062296 |
| 34 | 1 | 0 | -8.586464 | -1.346316 | 1.9794 |
| 35 | 1 | 0 | 1.30577 | -3.312979 | 3.826155 |
| 36 | 1 | 0 | 0.635324 | -6.395284 | 2.654917 |
| 37 | 1 | 0 | 3.840834 | -5.349318 | 3.000322 |
| 38 | 1 | 0 | 2.215227 | -7.292519 | -1.529278 |
| 39 | 1 | 0 | 6.570119 | -3.935331 | -0.411113 |
| 40 | 1 | 0 | 4.121657 | 8.302002 | -1.878124 |
| 41 | 1 | 0 | 3.701828 | 5.814283 | -4.134164 |
| 42 | 1 | 0 | 5.628176 | 5.325663 | -1.387238 |
| 43 | 1 | 0 | -0.001116 | 5.376552 | 3.121664 |
| 44 | 1 | 0 | 3.382985 | 5.584778 | 2.973283 |
| 45 | 1 | 0 | -0.630162 | 8.265199 | -1.234008 |
| 46 | 1 | 0 | 1.153831 | 9.498628 | 3.767997 |
| **5_e** | | | Standard Orientation (A.U.) | | |
| Center number | Atomic number | Atomic Type | X | Y | Z |
| 0 | 6 | 0 | 2.869227 | 1.123008 | 0.290773 |
| 1 | 6 | 0 | 0.956568 | 2.363618 | -1.533701 |
| 2 | 6 | 0 | -1.85609 | 1.767177 | -0.966131 |
| 3 | 6 | 0 | -2.410231 | -0.726433 | 0.399014 |
| 4 | 6 | 0 | -1.058054 | -3.068297 | -0.742831 |
| 5 | 6 | 0 | 1.526377 | -3.673562 | 0.429261 |
| 6 | 6 | 0 | 3.483481 | -1.63966 | -0.33285 |
| 7 | 6 | 0 | -5.295695 | -1.374665 | 0.405402 |
| 8 | 6 | 0 | -5.499662 | -3.834748 | -1.15564 |
| 9 | 6 | 0 | -3.012782 | -5.216924 | -0.621958 |
| 10 | 1 | 0 | -0.707991 | -2.704194 | -2.771785 |
| 11 | 1 | 0 | -1.810315 | -0.504348 | 2.378212 |
| 12 | 6 | 0 | -6.330576 | -1.686478 | 3.092053 |
| 13 | 6 | 0 | 1.447094 | -4.033032 | 3.315613 |
| 14 | 8 | 0 | 2.340026 | -5.987763 | -0.691863 |
| 15 | 8 | 0 | 5.912954 | -2.3476 | 0.619491 |
| 16 | 6 | 0 | 1.365859 | 5.267506 | -1.847612 |
| 17 | 6 | 0 | 3.849726 | 5.851381 | -3.231146 |
| 18 | 6 | 0 | 1.237819 | 6.748128 | 0.663825 |
| 19 | 8 | 0 | -0.67056 | 6.321717 | -3.277374 |
| 20 | 8 | 0 | 3.354908 | 6.425181 | 2.255569 |
| 21 | 1 | 0 | 1.378871 | 1.56158 | -3.420927 |
| 22 | 1 | 0 | 2.255713 | 1.343746 | 2.271735 |
| 23 | 1 | 0 | 4.684503 | 2.124229 | 0.161574 |
| 24 | 1 | 0 | -2.692532 | 3.310119 | 0.159257 |
| 25 | 1 | 0 | -2.905231 | 1.783523 | -2.77031 |
| 26 | 1 | 0 | 3.696385 | -1.80827 | -2.399413 |
| 27 | 1 | 0 | -6.369201 | 0.158346 | -0.517804 |
| 28 | 1 | 0 | -5.610705 | -3.374653 | -3.191245 |
| 29 | 1 | 0 | -7.196874 | -4.953052 | -0.681443 |
| 30 | 1 | 0 | -3.060363 | -6.071786 | 1.280966 |
| 31 | 1 | 0 | -2.582208 | -6.74569 | -1.965669 |
| 32 | 1 | 0 | -6.056036 | 0.059841 | 4.206071 |
| 33 | 1 | 0 | -5.362222 | -3.235669 | 4.106953 |
| 34 | 1 | 0 | -8.374402 | -2.118114 | 3.071868 |
| 35 | 1 | 0 | 3.271156 | -4.803185 | 3.970185 |
| 36 | 1 | 0 | 1.076374 | -2.268888 | 4.363111 |

| | | | | | |
|---|---|---|---|---|---|
| 37 | 1 | 0 | -0.017675 | -5.417907 | 3.834625 |
| 38 | 1 | 0 | 4.14799 | -6.097343 | -0.350388 |
| 39 | 1 | 0 | 5.984092 | -1.90986 | 2.40256 |
| 40 | 1 | 0 | 5.534314 | 5.143134 | -2.228922 |
| 41 | 1 | 0 | 4.040242 | 7.91342 | -3.498543 |
| 42 | 1 | 0 | 3.841184 | 4.963995 | -5.122425 |
| 43 | 1 | 0 | 0.933401 | 8.759989 | 0.165997 |
| 44 | 1 | 0 | -0.41838 | 6.135399 | 1.76554 |
| 45 | 1 | 0 | -0.816151 | 5.387603 | -4.851716 |
| 46 | 1 | 0 | 4.800503 | 7.261349 | 1.497103 |
| **5_f** | | | Standard Orientation (A.U.) | | |
| Center number | Atomic number | Atomic Type | X | Y | Z |
| 0 | 6 | 0 | 3.535278 | 0.859307 | -1.066386 |
| 1 | 6 | 0 | 1.382529 | 2.44449 | -2.240873 |
| 2 | 6 | 0 | -1.207603 | 1.100887 | -2.331028 |
| 3 | 6 | 0 | -2.020241 | -0.515142 | -0.064005 |
| 4 | 6 | 0 | -0.957433 | -3.226292 | -0.064857 |
| 5 | 6 | 0 | 1.889597 | -3.578929 | 0.36615 |
| 6 | 6 | 0 | 3.468676 | -1.995279 | -1.546049 |
| 7 | 6 | 0 | -4.9238 | -0.943088 | -0.020213 |
| 8 | 6 | 0 | -5.336606 | -3.535509 | 1.309918 |
| 9 | 6 | 0 | -2.675136 | -4.601747 | 1.829638 |
| 10 | 1 | 0 | -1.323074 | -4.037669 | -1.957722 |
| 11 | 1 | 0 | -1.453655 | 0.416029 | 1.714615 |
| 12 | 6 | 0 | -6.401434 | 1.230138 | 1.175938 |
| 13 | 6 | 0 | 2.706854 | -3.034804 | 3.104215 |
| 14 | 8 | 0 | 2.389979 | -6.166113 | -0.194932 |
| 15 | 8 | 0 | 5.989608 | -2.998561 | -1.583517 |
| 16 | 6 | 0 | 1.241861 | 5.16996 | -1.111264 |
| 17 | 6 | 0 | 3.850062 | 6.403371 | -0.98525 |
| 18 | 6 | 0 | -0.073059 | 5.348809 | 1.477984 |
| 19 | 8 | 0 | -0.18972 | 6.747187 | -2.775233 |
| 20 | 8 | 0 | 1.20743 | 3.89991 | 3.33476 |
| 21 | 1 | 0 | 1.900136 | 2.79781 | -4.232095 |
| 22 | 1 | 0 | 3.617041 | 1.209212 | 0.979077 |
| 23 | 1 | 0 | 5.330239 | 1.542228 | -1.873566 |
| 24 | 1 | 0 | -2.685609 | 2.536032 | -2.697365 |
| 25 | 1 | 0 | -1.263593 | -0.124707 | -4.020484 |
| 26 | 1 | 0 | 2.743051 | -2.412286 | -3.453286 |
| 27 | 1 | 0 | -5.540288 | -1.123385 | -2.009691 |
| 28 | 1 | 0 | -6.43124 | -4.814562 | 0.080126 |
| 29 | 1 | 0 | -6.434027 | -3.323816 | 3.072013 |
| 30 | 1 | 0 | -2.099927 | -4.114046 | 3.773468 |
| 31 | 1 | 0 | -2.545739 | -6.670711 | 1.648035 |
| 32 | 1 | 0 | -6.066426 | 3.037053 | 0.180775 |
| 33 | 1 | 0 | -5.848992 | 1.491384 | 3.175746 |
| 34 | 1 | 0 | -8.458166 | 0.869081 | 1.128753 |
| 35 | 1 | 0 | 2.004471 | -4.549965 | 4.344242 |
| 36 | 1 | 0 | 4.790313 | -3.049247 | 3.261132 |
| 37 | 1 | 0 | 2.021152 | -1.199433 | 3.815161 |
| 38 | 1 | 0 | 4.185185 | -6.226622 | -0.621817 |
| 39 | 1 | 0 | 6.912179 | -2.286135 | -0.162879 |
| 40 | 1 | 0 | 5.016879 | 5.560595 | 0.515835 |
| 41 | 1 | 0 | 3.617882 | 8.436785 | -0.586331 |
| 42 | 1 | 0 | 4.836159 | 6.212014 | -2.813029 |
| 43 | 1 | 0 | -0.11499 | 7.375123 | 2.001598 |
| 44 | 1 | 0 | -2.058836 | 4.713162 | 1.279993 |
| 45 | 1 | 0 | -1.831805 | 5.971458 | -3.04678 |
| 46 | 1 | 0 | 0.366341 | 4.126507 | 4.948708 |
| **5_G** | | | Standard Orientation (A.U.) | | |
| Center number | Atomic number | Atomic Type | X | Y | Z |
| 0 | 6 | 0 | 3.117522 | 1.087177 | 0.25631 |
| 1 | 6 | 0 | 1.064396 | 2.352071 | -1.39171 |
| 2 | 6 | 0 | -1.681144 | 1.666959 | -0.650143 |
| 3 | 6 | 0 | -2.067343 | -0.93715 | 0.545109 |
| 4 | 6 | 0 | -0.754124 | -3.184278 | -0.813516 |
| 5 | 6 | 0 | 1.920674 | -3.75838 | 0.17507 |
| 6 | 6 | 0 | 3.778846 | -1.617977 | -0.546793 |
| 7 | 6 | 0 | -4.869994 | -1.723803 | 0.76655 |
| 8 | 6 | 0 | -4.687615 | -4.576207 | 1.256189 |
| 9 | 6 | 0 | -2.607361 | -5.459531 | -0.563943 |

| | | | | | |
|---|---|---|---|---|---|
| 10 | 1 | 0 | -0.527638 | -2.734889 | -2.837621 |
| 11 | 1 | 0 | -1.350095 | -0.850842 | 2.50081 |
| 12 | 6 | 0 | -6.383678 | -0.251105 | 2.729819 |
| 13 | 6 | 0 | 1.995033 | -4.322184 | 3.030036 |
| 14 | 8 | 0 | 2.75519 | -5.959534 | -1.141431 |
| 15 | 8 | 0 | 6.268384 | -2.302804 | 0.249761 |
| 16 | 6 | 0 | 1.435078 | 5.265799 | -1.562887 |
| 17 | 6 | 0 | 3.707753 | 5.974827 | -3.21027 |
| 18 | 6 | 0 | 1.654458 | 6.518518 | 1.057638 |
| 19 | 8 | 0 | -0.784683 | 6.427759 | -2.617277 |
| 20 | 8 | 0 | 1.540763 | 9.166094 | 0.865244 |
| 21 | 1 | 0 | 1.372466 | 1.641287 | -3.333949 |
| 22 | 1 | 0 | 2.597337 | 1.163846 | 2.277379 |
| 23 | 1 | 0 | 4.900745 | 2.146467 | 0.067014 |
| 24 | 1 | 0 | -2.426519 | 3.102782 | 0.662136 |
| 25 | 1 | 0 | -2.874348 | 1.816189 | -2.355167 |
| 26 | 1 | 0 | 3.899649 | -1.656098 | -2.626384 |
| 27 | 1 | 0 | -5.759164 | -1.449258 | -1.111531 |
| 28 | 1 | 0 | -6.50188 | -5.568505 | 0.976962 |
| 29 | 1 | 0 | -4.111165 | -4.890557 | 3.243111 |
| 30 | 1 | 0 | -1.640314 | -7.194594 | 0.050926 |
| 31 | 1 | 0 | -3.436987 | -5.882136 | -2.428938 |
| 32 | 1 | 0 | -6.472036 | 1.784563 | 2.274069 |
| 33 | 1 | 0 | -5.520255 | -0.444244 | 4.625249 |
| 34 | 1 | 0 | -8.346423 | -0.954583 | 2.85259 |
| 35 | 1 | 0 | 3.85947 | -5.10204 | 3.545285 |
| 36 | 1 | 0 | 1.641925 | -2.645613 | 4.218626 |
| 37 | 1 | 0 | 0.576059 | -5.767359 | 3.513907 |
| 38 | 1 | 0 | 4.580319 | -6.027164 | -0.892933 |
| 39 | 1 | 0 | 6.393667 | -2.038593 | 2.0637 |
| 40 | 1 | 0 | 5.472125 | 5.091862 | -2.53904 |
| 41 | 1 | 0 | 3.96453 | 8.04137 | -3.184496 |
| 42 | 1 | 0 | 3.402239 | 5.350898 | -5.183288 |
| 43 | 1 | 0 | 0.137383 | 5.782955 | 2.305983 |
| 44 | 1 | 0 | 3.482393 | 6.035198 | 1.929658 |
| 45 | 1 | 0 | -0.837482 | 6.084204 | -4.419434 |
| 46 | 1 | 0 | 0.157538 | 9.509786 | -0.304884 |
| **5_h** | | | Standard Orientation (A.U.) | | |
| Center number | Atomic number | Atomic Type | X | Y | Z |
| 0 | 6 | 0 | 3.457619 | 0.971606 | -0.106925 |
| 1 | 6 | 0 | 0.861474 | 2.04747 | -0.897477 |
| 2 | 6 | 0 | -1.203043 | 1.401563 | 1.051564 |
| 3 | 6 | 0 | -2.218614 | -1.331934 | 0.993668 |
| 4 | 6 | 0 | -0.615668 | -3.376284 | -0.318162 |
| 5 | 6 | 0 | 2.091082 | -3.771406 | 0.646175 |
| 6 | 6 | 0 | 3.883459 | -1.83692 | -0.629373 |
| 7 | 6 | 0 | -4.803505 | -1.669652 | -0.323974 |
| 8 | 6 | 0 | -5.033249 | -4.577154 | -0.717565 |
| 9 | 6 | 0 | -2.370407 | -5.687443 | -0.205162 |
| 10 | 1 | 0 | -0.454963 | -2.867098 | -2.339375 |
| 11 | 1 | 0 | -2.490275 | -1.94828 | 2.972714 |
| 12 | 6 | 0 | -7.030722 | -0.506105 | 1.094246 |
| 13 | 6 | 0 | 2.291066 | -3.70763 | 3.541193 |
| 14 | 8 | 0 | 2.885479 | -6.191562 | -0.2317 |
| 15 | 8 | 0 | 6.446438 | -2.514459 | -0.103185 |
| 16 | 6 | 0 | 0.987414 | 4.935844 | -1.462259 |
| 17 | 6 | 0 | 2.557107 | 5.508314 | -3.82803 |
| 18 | 6 | 0 | 1.949868 | 6.483429 | 0.80526 |
| 19 | 8 | 0 | -1.518465 | 5.914059 | -1.860531 |
| 20 | 8 | 0 | 1.706192 | 9.093141 | 0.361425 |
| 21 | 1 | 0 | 0.332819 | 1.176223 | -2.724856 |
| 22 | 1 | 0 | 3.761514 | 1.351805 | 1.928635 |
| 23 | 1 | 0 | 4.993416 | 1.950513 | -1.117049 |
| 24 | 1 | 0 | -0.450368 | 1.815191 | 2.952836 |
| 25 | 1 | 0 | -2.789121 | 2.717528 | 0.773799 |
| 26 | 1 | 0 | 3.689045 | -2.165259 | -2.678471 |
| 27 | 1 | 0 | -4.667512 | -0.743015 | -2.197624 |
| 28 | 1 | 0 | -5.683204 | -5.012704 | -2.650404 |
| 29 | 1 | 0 | -6.45158 | -5.386715 | 0.580997 |
| 30 | 1 | 0 | -2.286724 | -6.544416 | 1.695268 |
| 31 | 1 | 0 | -1.804029 | -7.158678 | -1.558615 |

| | | | | | |
|---|---|---|---|---|---|
| 32 | 1 | 0 | -6.79584 | 1.552858 | 1.356519 |
| 33 | 1 | 0 | -7.235494 | -1.371982 | 2.986932 |
| 34 | 1 | 0 | -8.821824 | -0.808126 | 0.062379 |
| 35 | 1 | 0 | 4.238319 | -4.172359 | 4.134447 |
| 36 | 1 | 0 | 1.782497 | -1.85449 | 4.347997 |
| 37 | 1 | 0 | 1.03893 | -5.152232 | 4.369108 |
| 38 | 1 | 0 | 4.729222 | -6.151324 | -0.183013 |
| 39 | 1 | 0 | 6.874029 | -1.913641 | 1.580209 |
| 40 | 1 | 0 | 4.517853 | 4.824603 | -3.665082 |
| 41 | 1 | 0 | 2.61781 | 7.566941 | -4.131953 |
| 42 | 1 | 0 | 1.705972 | 4.594872 | -5.506941 |
| 43 | 1 | 0 | 0.896816 | 5.907835 | 2.524545 |
| 44 | 1 | 0 | 3.969891 | 6.092841 | 1.130179 |
| 45 | 1 | 0 | -2.117659 | 5.361128 | -3.505982 |
| 46 | 1 | 0 | 0.006977 | 9.31646 | -0.317875 |

**Table S11.** Gibbs free energies[a] and equilibrium populations[b] of low-energy conformers of compound **7**.

| Conformers | ΔG(a.u.) | P(%)/100 | G(a.u.) |
|---|---|---|---|
| **7_a** | 0.00726 | 0.02 | -812.530382 |
| **7_b** | 0.0 | 52.84 | -812.537641 |
| **7_c** | 0.0042 | 0.62 | -812.533444 |
| **7_d** | 0.0032 | 1.78 | -812.534442 |
| **7_e** | 0.00381 | 0.94 | -812.533832 |
| **7_f** | 0.00725 | 0.02 | -812.53039 |
| **7_g** | 0.00757 | 0.02 | -812.530067 |
| **7_h** | 0.0003 | 38.58 | -812.537344 |
| **7_i** | 0.00468 | 0.37 | -812.532966 |
| **7_j** | 0.00333 | 1.56 | -812.534316 |
| **7_k** | 0.00494 | 0.28 | -812.532705 |
| **7_l** | 0.006 | 0.09 | -812.531639 |
| **7_m** | 0.00724 | 0.03 | -812.530398 |
| **7_n** | 0.00324 | 1.72 | -812.534405 |
| **7_o** | 0.00448 | 0.46 | -812.533162 |
| **7_p** | 0.00528 | 0.2 | -812.532358 |
| **7_q** | 0.00459 | 0.41 | -812.533056 |
| **7_r** | 0.00646 | 0.06 | -812.531183 |

[a]wB97M-V/def2-TZVP, in a.u. [b]From ΔG values at 298.15K.

**Table S12.** Cartesian coordinates for the low-energy reoptimized random reseach conformers of compound **7** at B3LYP-D3(BJ)/6-31G* level of theory in methanol.

| **7_a** | | | **Standard Orientation (A.U.)** | | |
|---|---|---|---|---|---|
| **Center number** | **Atomic number** | **Atomic Type** | **X** | **Y** | Z |
| 0 | 6 | 0 | 1.136158 | 0.534212 | 2.967955 |
| 1 | 6 | 0 | 3.58578 | 1.652329 | 1.90576 |
| 2 | 6 | 0 | 4.05392 | 1.559806 | -0.977049 |
| 3 | 6 | 0 | 1.666924 | 1.398074 | -2.648644 |
| 4 | 6 | 0 | -0.130501 | -0.967768 | -2.333009 |
| 5 | 6 | 0 | 0.619817 | -3.001278 | -0.403628 |
| 6 | 6 | 0 | 0.640192 | -2.272517 | 2.452027 |
| 7 | 6 | 0 | -0.091077 | 3.726914 | -2.546431 |
| 8 | 6 | 0 | -2.677266 | 2.698803 | -3.363123 |
| 9 | 6 | 0 | -2.832253 | 0.111634 | -2.057451 |
| 10 | 6 | 0 | -4.925545 | -1.593774 | -3.059179 |
| 11 | 8 | 0 | -4.755256 | 4.327802 | -2.881984 |
| 12 | 6 | 0 | 5.643227 | 3.865357 | -1.749165 |
| 13 | 8 | 0 | 5.586369 | -0.663734 | -1.383295 |
| 14 | 6 | 0 | -1.717376 | -3.245151 | 3.783368 |
| 15 | 6 | 0 | -1.786477 | -6.072951 | 4.209977 |
| 16 | 6 | 0 | -3.603216 | -1.815054 | 4.670146 |
| 17 | 8 | 0 | 0.217719 | -6.890739 | 5.825107 |
| 18 | 1 | 0 | -0.090958 | -1.947845 | -4.163656 |
| 19 | 1 | 0 | 2.409516 | 1.306266 | -4.589162 |
| 20 | 1 | 0 | 2.209073 | -3.334078 | 3.297869 |
| 21 | 1 | 0 | -0.454695 | 1.667026 | 2.295403 |
| 22 | 1 | 0 | 1.170111 | 0.806635 | 5.023748 |
| 23 | 1 | 0 | 5.221873 | 0.727134 | 2.775809 |

| | | | | | |
|---|---|---|---|---|---|
| 24 | 1 | 0 | 3.654511 | 3.63342 | 2.509598 |
| 25 | 1 | 0 | 2.504518 | -3.664124 | -0.905447 |
| 26 | 1 | 0 | -0.659892 | -4.607485 | -0.679812 |
| 27 | 1 | 0 | 0.551335 | 5.288085 | -3.738292 |
| 28 | 1 | 0 | -0.243661 | 4.463412 | -0.61126 |
| 29 | 1 | 0 | -2.693508 | 2.428676 | -5.42039 |
| 30 | 1 | 0 | -3.223712 | 0.477437 | -0.053736 |
| 31 | 1 | 0 | -4.581361 | -2.104739 | -5.039631 |
| 32 | 1 | 0 | -5.063323 | -3.342704 | -1.959997 |
| 33 | 1 | 0 | -6.751559 | -0.624464 | -2.959576 |
| 34 | 1 | 0 | -4.848652 | 4.552484 | -1.063205 |
| 35 | 1 | 0 | 4.631675 | 5.642688 | -1.437114 |
| 36 | 1 | 0 | 6.150613 | 3.766855 | -3.757898 |
| 37 | 1 | 0 | 7.392799 | 3.901931 | -0.645876 |
| 38 | 1 | 0 | 5.886263 | -0.788619 | -3.189355 |
| 39 | 1 | 0 | -3.639325 | -6.634553 | 4.967487 |
| 40 | 1 | 0 | -1.492878 | -7.107585 | 2.442639 |
| 41 | 1 | 0 | -5.223575 | -2.661912 | 5.608548 |
| 42 | 1 | 0 | -3.628628 | 0.229201 | 4.502932 |
| 43 | 1 | 0 | 0.050673 | -5.943533 | 7.386885 |

| **7_b** | | | Standard Orientation (A.U.) | | |
|---|---|---|---|---|---|
| Center number | Atomic number | Atomic Type | X | Y | Z |
| 0 | 6 | 0 | 0.901526 | 0.684223 | 4.710762 |
| 1 | 6 | 0 | 2.980503 | 2.112956 | 3.298678 |
| 2 | 6 | 0 | 2.407808 | 3.112088 | 0.629844 |
| 3 | 6 | 0 | 2.387537 | 0.956846 | -1.357383 |
| 4 | 6 | 0 | 0.18847 | -1.03739 | -1.343121 |
| 5 | 6 | 0 | -1.429306 | -1.421526 | 1.022514 |
| 6 | 6 | 0 | 0.053835 | -1.822346 | 3.51384 |
| 7 | 6 | 0 | 2.435524 | 1.970272 | -4.118798 |
| 8 | 6 | 0 | 0.643499 | 0.269379 | -5.640296 |
| 9 | 6 | 0 | -1.384381 | -0.462208 | -3.723838 |
| 10 | 6 | 0 | -3.117222 | -2.585198 | -4.613392 |
| 11 | 8 | 0 | -0.487445 | 1.472822 | -7.76175 |
| 12 | 6 | 0 | 0.067909 | 4.823885 | 0.60342 |
| 13 | 8 | 0 | 4.597859 | 4.655818 | 0.108285 |
| 14 | 6 | 0 | -1.51992 | -3.434154 | 5.297995 |
| 15 | 6 | 0 | -1.120506 | -6.258325 | 5.090251 |
| 16 | 6 | 0 | -3.177091 | -2.494408 | 6.952474 |
| 17 | 8 | 0 | -1.391243 | -7.232012 | 2.583412 |
| 18 | 1 | 0 | 1.114269 | -2.871388 | -1.695419 |
| 19 | 1 | 0 | 4.161657 | -0.04846 | -1.006512 |
| 20 | 1 | 0 | 1.779434 | -2.903345 | 3.058977 |
| 21 | 1 | 0 | -0.750773 | 1.913057 | 4.951345 |
| 22 | 1 | 0 | 1.60032 | 0.293527 | 6.621782 |
| 23 | 1 | 0 | 4.675986 | 0.92357 | 3.16815 |
| 24 | 1 | 0 | 3.523816 | 3.761974 | 4.428972 |
| 25 | 1 | 0 | -2.607098 | -3.087009 | 0.690045 |
| 26 | 1 | 0 | -2.752524 | 0.148767 | 1.294256 |
| 27 | 1 | 0 | 4.35015 | 2.035913 | -4.902069 |
| 28 | 1 | 0 | 1.649039 | 3.884901 | -4.241878 |
| 29 | 1 | 0 | 1.639031 | -1.459995 | -6.246996 |
| 30 | 1 | 0 | -2.519496 | 1.246237 | -3.377043 |
| 31 | 1 | 0 | -4.63969 | -2.955817 | -3.262465 |
| 32 | 1 | 0 | -3.972737 | -2.092853 | -6.430919 |
| 33 | 1 | 0 | -2.049869 | -4.347281 | -4.861744 |
| 34 | 1 | 0 | 0.821747 | 1.756119 | -9.010655 |
| 35 | 1 | 0 | -0.189447 | 5.715053 | -1.247015 |
| 36 | 1 | 0 | 0.317674 | 6.332425 | 1.996968 |
| 37 | 1 | 0 | -1.674547 | 3.812179 | 1.045287 |
| 38 | 1 | 0 | 4.343519 | 5.418752 | -1.538634 |
| 39 | 1 | 0 | 0.768036 | -6.736333 | 5.834828 |
| 40 | 1 | 0 | -2.511505 | -7.267601 | 6.23699 |
| 41 | 1 | 0 | -4.325723 | -3.729322 | 8.125684 |
| 42 | 1 | 0 | -3.45341 | -0.478475 | 7.217053 |
| 43 | 1 | 0 | 0.052532 | -6.665741 | 1.608873 |

| **7_C** | | | Standard Orientation (A.U.) | | |
|---|---|---|---|---|---|
| Center number | Atomic number | Atomic Type | X | Y | Z |
| 0 | 6 | 0 | 1.188632 | 0.466549 | 4.032789 |

| | | | | | |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 2.110019 | 2.48218 | 2.164602 |
| 2 | 6 | 0 | 3.508282 | 1.510683 | -0.206475 |
| 3 | 6 | 0 | 1.708811 | 0.77492 | -2.387599 |
| 4 | 6 | 0 | -0.355318 | -1.257707 | -1.907106 |
| 5 | 6 | 0 | -1.901573 | -1.053258 | 0.553769 |
| 6 | 6 | 0 | -0.38941 | -1.75191 | 2.927061 |
| 7 | 6 | 0 | 0.272589 | 3.013062 | -3.620959 |
| 8 | 6 | 0 | -2.243564 | 1.950156 | -4.634531 |
| 9 | 6 | 0 | -2.070601 | -0.943742 | -4.258511 |
| 10 | 6 | 0 | -1.00682 | -2.254224 | -6.614703 |
| 11 | 8 | 0 | -4.220715 | 3.074161 | -3.163933 |
| 12 | 6 | 0 | 5.356119 | 3.535489 | -1.133679 |
| 13 | 8 | 0 | 5.108837 | -0.597598 | 0.414477 |
| 14 | 6 | 0 | -1.947796 | -2.906227 | 5.041542 |
| 15 | 6 | 0 | -0.436194 | -4.131217 | 7.131123 |
| 16 | 6 | 0 | -4.46204 | -2.781036 | 5.213686 |
| 17 | 8 | 0 | 1.438871 | -5.74235 | 6.044625 |
| 18 | 1 | 0 | 0.507987 | -3.147074 | -1.922539 |
| 19 | 1 | 0 | 2.970324 | -0.025209 | -3.824031 |
| 20 | 1 | 0 | 0.931684 | -3.258699 | 2.380788 |
| 21 | 1 | 0 | 0.040094 | 1.436742 | 5.460596 |
| 22 | 1 | 0 | 2.822213 | -0.324655 | 5.027441 |
| 23 | 1 | 0 | 3.387287 | 3.73757 | 3.208551 |
| 24 | 1 | 0 | 0.515963 | 3.660299 | 1.56745 |
| 25 | 1 | 0 | -3.467411 | -2.396158 | 0.362586 |
| 26 | 1 | 0 | -2.76792 | 0.817029 | 0.720776 |
| 27 | 1 | 0 | 1.397226 | 3.890479 | -5.116152 |
| 28 | 1 | 0 | -0.184553 | 4.49892 | -2.258761 |
| 29 | 1 | 0 | -2.530219 | 2.420178 | -6.640088 |
| 30 | 1 | 0 | -3.960838 | -1.721329 | -3.889323 |
| 31 | 1 | 0 | -0.780612 | -4.286298 | -6.290741 |
| 32 | 1 | 0 | -2.272241 | -2.003321 | -8.235714 |
| 33 | 1 | 0 | 0.843914 | -1.496561 | -7.151181 |
| 34 | 1 | 0 | -5.795594 | 2.279369 | -3.662497 |
| 35 | 1 | 0 | 6.829782 | 3.816009 | 0.289858 |
| 36 | 1 | 0 | 4.396223 | 5.339467 | -1.450474 |
| 37 | 1 | 0 | 6.263919 | 2.9458 | -2.897474 |
| 38 | 1 | 0 | 4.033911 | -2.003168 | 0.88662 |
| 39 | 1 | 0 | 0.474089 | -2.648546 | 8.27663 |
| 40 | 1 | 0 | -1.70726 | -5.194353 | 8.385584 |
| 41 | 1 | 0 | -5.465167 | -3.637167 | 6.789098 |
| 42 | 1 | 0 | -5.614626 | -1.809893 | 3.823294 |
| 43 | 1 | 0 | 2.603633 | -6.216426 | 7.374293 |

| **7_d** | | | Standard Orientation (A.U.) | | |
|---|---|---|---|---|---|
| Center number | Atomic number | Atomic Type | X | Y | Z |
| 0 | 6 | 0 | 3.032459 | -0.451013 | 3.169789 |
| 1 | 6 | 0 | 3.425818 | 1.96585 | 1.614134 |
| 2 | 6 | 0 | 3.649107 | 1.672321 | -1.282495 |
| 3 | 6 | 0 | 1.074462 | 1.548024 | -2.655986 |
| 4 | 6 | 0 | -0.7922 | -0.598178 | -1.942145 |
| 5 | 6 | 0 | -1.307966 | -0.952685 | 0.899251 |
| 6 | 6 | 0 | 0.867065 | -2.248048 | 2.361751 |
| 7 | 6 | 0 | -0.570873 | 3.947965 | -2.518406 |
| 8 | 6 | 0 | -3.288847 | 3.122725 | -3.239973 |
| 9 | 6 | 0 | -3.217756 | 0.185596 | -3.386792 |
| 10 | 6 | 0 | -3.222442 | -0.756497 | -6.126709 |
| 11 | 8 | 0 | -5.160903 | 4.069491 | -1.547761 |
| 12 | 6 | 0 | 5.200358 | 3.870395 | -2.345521 |
| 13 | 8 | 0 | 5.110755 | -0.536854 | -1.902198 |
| 14 | 6 | 0 | -0.202016 | -3.740675 | 4.577315 |
| 15 | 6 | 0 | -0.461363 | -6.548171 | 4.097253 |
| 16 | 6 | 0 | -0.976845 | -2.697166 | 6.737883 |
| 17 | 8 | 0 | -1.375921 | -7.983566 | 6.156911 |
| 18 | 1 | 0 | -0.109527 | -2.422907 | -2.665258 |
| 19 | 1 | 0 | 1.571179 | 1.241091 | -4.646408 |
| 20 | 1 | 0 | 1.666686 | -3.653185 | 1.048048 |
| 21 | 1 | 0 | 2.715228 | 0.140042 | 5.125206 |
| 22 | 1 | 0 | 4.797297 | -1.532808 | 3.186471 |
| 23 | 1 | 0 | 5.173282 | 2.838635 | 2.306687 |
| 24 | 1 | 0 | 1.919886 | 3.323057 | 2.036783 |

| | | | | | |
|---|---|---|---|---|---|
| 25 | 1 | 0 | -3.001853 | -2.132271 | 1.081915 |
| 26 | 1 | 0 | -1.774857 | 0.845857 | 1.824929 |
| 27 | 1 | 0 | 0.138912 | 5.458965 | -3.736185 |
| 28 | 1 | 0 | -0.623853 | 4.722826 | -0.597703 |
| 29 | 1 | 0 | -3.839238 | 3.91138 | -5.06981 |
| 30 | 1 | 0 | -4.910625 | -0.558214 | -2.45079 |
| 31 | 1 | 0 | -3.155633 | -2.824838 | -6.204736 |
| 32 | 1 | 0 | -4.93457 | -0.135123 | -7.111478 |
| 33 | 1 | 0 | -1.595326 | -0.035162 | -7.187012 |
| 34 | 1 | 0 | -4.821799 | 3.347741 | 0.103289 |
| 35 | 1 | 0 | 4.41496 | 5.691041 | -1.757957 |
| 36 | 1 | 0 | 5.247492 | 3.802811 | -4.412877 |
| 37 | 1 | 0 | 7.142539 | 3.736792 | -1.647862 |
| 38 | 1 | 0 | 4.078953 | -2.005606 | -1.541907 |
| 39 | 1 | 0 | -1.803662 | -6.869686 | 2.54682 |
| 40 | 1 | 0 | 1.376739 | -7.276462 | 3.424596 |
| 41 | 1 | 0 | -1.872932 | -3.829978 | 8.193709 |
| 42 | 1 | 0 | -0.795261 | -0.686844 | 7.110147 |
| 43 | 1 | 0 | -0.184031 | -7.765809 | 7.533478 |

| **7_e** | | | Standard Orientation (A.U.) | | |
|---|---|---|---|---|---|
| Center number | Atomic number | Atomic Type | X | Y | Z |
| 0 | 6 | 0 | 0.411193 | 0.450463 | 4.289338 |
| 1 | 6 | 0 | 1.067646 | 2.831003 | 2.768396 |
| 2 | 6 | 0 | 3.033755 | 2.528229 | 0.631463 |
| 3 | 6 | 0 | 1.893124 | 1.58212 | -1.885892 |
| 4 | 6 | 0 | 0.484887 | -0.98756 | -1.916137 |
| 5 | 6 | 0 | -1.515392 | -1.389158 | 0.16301 |
| 6 | 6 | 0 | -0.376757 | -1.947986 | 2.775683 |
| 7 | 6 | 0 | 0.039403 | 3.406205 | -3.21015 |
| 8 | 6 | 0 | -1.564096 | 1.778051 | -5.049652 |
| 9 | 6 | 0 | -0.719615 | -0.998129 | -4.585498 |
| 10 | 6 | 0 | 1.121328 | -1.918337 | -6.625253 |
| 11 | 8 | 0 | -4.217816 | 2.152793 | -4.741882 |
| 12 | 6 | 0 | 4.36104 | 5.060753 | 0.191631 |
| 13 | 8 | 0 | 5.032048 | 0.857739 | 1.40799 |
| 14 | 6 | 0 | -2.027563 | -3.58481 | 4.458934 |
| 15 | 6 | 0 | -0.644901 | -4.939549 | 6.562554 |
| 16 | 6 | 0 | -4.526663 | -3.840271 | 4.204964 |
| 17 | 8 | 0 | 1.340902 | -6.515968 | 5.632559 |
| 18 | 1 | 0 | 1.840839 | -2.552797 | -1.75391 |
| 19 | 1 | 0 | 3.535834 | 1.349523 | -3.129494 |
| 20 | 1 | 0 | 1.334542 | -3.07981 | 2.444869 |
| 21 | 1 | 0 | -1.142264 | 0.953219 | 5.565801 |
| 22 | 1 | 0 | 2.02378 | -0.029236 | 5.49336 |
| 23 | 1 | 0 | 1.795238 | 4.219541 | 4.124184 |
| 24 | 1 | 0 | -0.657725 | 3.666862 | 1.985441 |
| 25 | 1 | 0 | -2.670419 | -3.010251 | -0.407858 |
| 26 | 1 | 0 | -2.811854 | 0.229271 | 0.280299 |
| 27 | 1 | 0 | 1.025464 | 4.941381 | -4.180157 |
| 28 | 1 | 0 | -1.248941 | 4.304382 | -1.859651 |
| 29 | 1 | 0 | -1.220686 | 2.313597 | -7.016226 |
| 30 | 1 | 0 | -2.397853 | -2.212841 | -4.639334 |
| 31 | 1 | 0 | 2.815562 | -0.730867 | -6.726308 |
| 32 | 1 | 0 | 1.738758 | -3.859046 | -6.24987 |
| 33 | 1 | 0 | 0.223288 | -1.882938 | -8.490677 |
| 34 | 1 | 0 | -4.647908 | 1.643149 | -3.034258 |
| 35 | 1 | 0 | 2.99322 | 6.569682 | -0.168053 |
| 36 | 1 | 0 | 5.655741 | 4.939306 | -1.417667 |
| 37 | 1 | 0 | 5.460594 | 5.555933 | 1.871521 |
| 38 | 1 | 0 | 4.341933 | -0.834975 | 1.518306 |
| 39 | 1 | 0 | 0.298316 | -3.584814 | 7.811667 |
| 40 | 1 | 0 | -1.990089 | -6.023716 | 7.717774 |
| 41 | 1 | 0 | -5.61246 | -5.00966 | 5.499477 |
| 42 | 1 | 0 | -5.593077 | -2.886708 | 2.733946 |
| 43 | 1 | 0 | 0.560837 | -7.744064 | 4.51554 |

| **7_f** | | | Standard Orientation (A.U.) | | |
|---|---|---|---|---|---|
| Center number | Atomic number | Atomic Type | X | Y | Z |
| 0 | 6 | 0 | -0.053564 | 0.844798 | 2.994473 |
| 1 | 6 | 0 | 2.288205 | 2.494633 | 2.578635 |

| | | | | | |
|---|---|---|---|---|---|
| 2 | 6 | 0 | 3.678671 | 2.363855 | 0.01148 |
| 3 | 6 | 0 | 2.076433 | 1.478926 | -2.262252 |
| 4 | 6 | 0 | 0.869886 | -1.249944 | -2.173501 |
| 5 | 6 | 0 | 1.395833 | -2.895212 | 0.158631 |
| 6 | 6 | 0 | 0.301723 | -2.020074 | 2.750876 |
| 7 | 6 | 0 | -0.103903 | 3.270411 | -3.01423 |
| 8 | 6 | 0 | -1.974433 | 1.568807 | -4.402306 |
| 9 | 6 | 0 | -1.948905 | -0.88863 | -2.858555 |
| 10 | 6 | 0 | -3.144676 | -3.152658 | -4.182079 |
| 11 | 8 | 0 | -4.373418 | 2.772512 | -4.542522 |
| 12 | 6 | 0 | 4.848202 | 4.960306 | -0.561143 |
| 13 | 8 | 0 | 5.734962 | 0.607286 | 0.396574 |
| 14 | 6 | 0 | -2.077164 | -3.494353 | 3.418018 |
| 15 | 6 | 0 | -1.634485 | -6.202607 | 4.224403 |
| 16 | 6 | 0 | -4.426787 | -2.563215 | 3.446551 |
| 17 | 8 | 0 | -0.169822 | -6.348299 | 6.489204 |
| 18 | 1 | 0 | 1.725311 | -2.293481 | -3.753064 |
| 19 | 1 | 0 | 3.415245 | 1.469566 | -3.854189 |
| 20 | 1 | 0 | 1.699527 | -2.584883 | 4.176034 |
| 21 | 1 | 0 | -1.549526 | 1.486141 | 1.724294 |
| 22 | 1 | 0 | -0.755819 | 1.23623 | 4.906362 |
| 23 | 1 | 0 | 3.716751 | 2.075271 | 4.018703 |
| 24 | 1 | 0 | 1.704206 | 4.456743 | 2.898129 |
| 25 | 1 | 0 | 3.440587 | -3.057528 | 0.349902 |
| 26 | 1 | 0 | 0.6938 | -4.800054 | -0.259641 |
| 27 | 1 | 0 | 0.520795 | 4.866704 | -4.168288 |
| 28 | 1 | 0 | -1.060085 | 4.051448 | -1.35147 |
| 29 | 1 | 0 | -1.25498 | 1.173781 | -6.322971 |
| 30 | 1 | 0 | -3.043587 | -0.50235 | -1.148672 |
| 31 | 1 | 0 | -3.12868 | -4.825737 | -2.963812 |
| 32 | 1 | 0 | -5.126903 | -2.781006 | -4.670513 |
| 33 | 1 | 0 | -2.131624 | -3.621751 | -5.930531 |
| 34 | 1 | 0 | -5.498445 | 1.651836 | -5.456626 |
| 35 | 1 | 0 | 5.990849 | 4.885192 | -2.290786 |
| 36 | 1 | 0 | 6.082815 | 5.523543 | 1.000317 |
| 37 | 1 | 0 | 3.404071 | 6.419031 | -0.817042 |
| 38 | 1 | 0 | 6.627818 | 0.466757 | -1.200471 |
| 39 | 1 | 0 | -3.452437 | -7.188233 | 4.441174 |
| 40 | 1 | 0 | -0.526043 | -7.235603 | 2.815083 |
| 41 | 1 | 0 | -6.026953 | -3.748757 | 3.955072 |
| 42 | 1 | 0 | -4.864786 | -0.617776 | 2.967031 |
| 43 | 1 | 0 | -1.063419 | -5.363819 | 7.752824 |

| **7_g** | | | Standard Orientation (A.U.) | | |
|---|---|---|---|---|---|
| Center number | Atomic number | Atomic Type | X | Y | Z |
| 0 | 6 | 0 | -0.188022 | 1.121713 | 2.975795 |
| 1 | 6 | 0 | 2.238167 | 2.657747 | 2.608672 |
| 2 | 6 | 0 | 3.76109 | 2.338251 | 0.135021 |
| 3 | 6 | 0 | 2.246659 | 1.403689 | -2.178531 |
| 4 | 6 | 0 | 0.916668 | -1.264429 | -2.02517 |
| 5 | 6 | 0 | 1.24717 | -2.811217 | 0.407867 |
| 6 | 6 | 0 | 0.069542 | -1.762423 | 2.897683 |
| 7 | 6 | 0 | 0.182024 | 3.237107 | -3.130995 |
| 8 | 6 | 0 | -1.693799 | 1.530342 | -4.535817 |
| 9 | 6 | 0 | -1.844764 | -0.8351 | -2.884204 |
| 10 | 6 | 0 | -3.065304 | -3.105071 | -4.171835 |
| 11 | 8 | 0 | -4.15283 | 2.575674 | -4.837863 |
| 12 | 6 | 0 | 5.074765 | 4.851171 | -0.496915 |
| 13 | 8 | 0 | 5.715683 | 0.521272 | 0.718856 |
| 14 | 6 | 0 | -2.394727 | -3.105045 | 3.536715 |
| 15 | 6 | 0 | -2.109293 | -5.800437 | 4.43048 |
| 16 | 6 | 0 | -4.700066 | -2.087201 | 3.384233 |
| 17 | 8 | 0 | -0.582455 | -5.81457 | 6.659935 |
| 18 | 1 | 0 | 1.808623 | -2.419023 | -3.504282 |
| 19 | 1 | 0 | 3.665194 | 1.261131 | -3.69347 |
| 20 | 1 | 0 | 1.377278 | -2.292618 | 4.415865 |
| 21 | 1 | 0 | -1.588863 | 1.751349 | 1.595757 |
| 22 | 1 | 0 | -0.971816 | 1.633761 | 4.825399 |
| 23 | 1 | 0 | 3.567045 | 2.261212 | 4.147276 |
| 24 | 1 | 0 | 1.720014 | 4.655563 | 2.794493 |
| 25 | 1 | 0 | 3.270305 | -3.058741 | 0.710376 |

| | | | | | |
|---|---|---|---|---|---|
| 26 | 1 | 0 | 0.474699 | -4.698615 | 0.037987 |
| 27 | 1 | 0 | 0.945317 | 4.75045 | -4.320676 |
| 28 | 1 | 0 | -0.820999 | 4.133986 | -1.557197 |
| 29 | 1 | 0 | -0.899982 | 1.012188 | -6.396096 |
| 30 | 1 | 0 | -3.016721 | -0.325194 | -1.259491 |
| 31 | 1 | 0 | -3.227478 | -4.703568 | -2.865962 |
| 32 | 1 | 0 | -4.965879 | -2.623926 | -4.832393 |
| 33 | 1 | 0 | -1.949203 | -3.723934 | -5.807945 |
| 34 | 1 | 0 | -4.016997 | 4.006786 | -5.972714 |
| 35 | 1 | 0 | 6.30465 | 4.641137 | -2.154435 |
| 36 | 1 | 0 | 6.24755 | 5.440353 | 1.102134 |
| 37 | 1 | 0 | 3.713548 | 6.355499 | -0.901995 |
| 38 | 1 | 0 | 6.677032 | 0.255026 | -0.821392 |
| 39 | 1 | 0 | -3.982813 | -6.620563 | 4.802038 |
| 40 | 1 | 0 | -1.211382 | -6.947984 | 2.942523 |
| 41 | 1 | 0 | -6.370745 | -3.164441 | 3.9014 |
| 42 | 1 | 0 | -5.029483 | -0.165253 | 2.750287 |
| 43 | 1 | 0 | -0.023595 | -7.535264 | 6.938829 |

| **7_h** | | | Standard Orientation (A.U.) | | |
|---|---|---|---|---|---|
| Center number | Atomic number | Atomic Type | X | Y | Z |
| 0 | 6 | 0 | 0.710083 | 0.499388 | 4.78846 |
| 1 | 6 | 0 | 2.681608 | 2.157548 | 3.477417 |
| 2 | 6 | 0 | 2.030259 | 3.289339 | 0.880748 |
| 3 | 6 | 0 | 2.210322 | 1.290479 | -1.255638 |
| 4 | 6 | 0 | 0.255287 | -0.950997 | -1.356256 |
| 5 | 6 | 0 | -1.375331 | -1.591837 | 0.944787 |
| 6 | 6 | 0 | 0.073593 | -1.999124 | 3.454053 |
| 7 | 6 | 0 | 2.11659 | 2.480141 | -3.939792 |
| 8 | 6 | 0 | 0.641587 | 0.608858 | -5.592512 |
| 9 | 6 | 0 | -1.31524 | -0.497266 | -3.764956 |
| 10 | 6 | 0 | -2.70639 | -2.794778 | -4.804933 |
| 11 | 8 | 0 | -0.363617 | 1.647255 | -7.852003 |
| 12 | 6 | 0 | -0.454188 | 4.783876 | 0.956307 |
| 13 | 8 | 0 | 4.070746 | 5.058799 | 0.491797 |
| 14 | 6 | 0 | -1.421012 | -3.802197 | 5.120187 |
| 15 | 6 | 0 | -0.810804 | -6.577814 | 4.801016 |
| 16 | 6 | 0 | -3.185434 | -3.062328 | 6.765412 |
| 17 | 8 | 0 | -0.951723 | -7.452881 | 2.247493 |
| 18 | 1 | 0 | 1.394123 | -2.654876 | -1.729859 |
| 19 | 1 | 0 | 4.090877 | 0.468465 | -0.992331 |
| 20 | 1 | 0 | 1.883035 | -2.931082 | 2.995155 |
| 21 | 1 | 0 | -1.03474 | 1.582498 | 5.071503 |
| 22 | 1 | 0 | 1.420044 | 0.063731 | 6.685552 |
| 23 | 1 | 0 | 4.456857 | 1.102778 | 3.27389 |
| 24 | 1 | 0 | 3.108875 | 3.764539 | 4.713002 |
| 25 | 1 | 0 | -2.393933 | -3.333724 | 0.496469 |
| 26 | 1 | 0 | -2.837673 | -0.158234 | 1.257237 |
| 27 | 1 | 0 | 3.988945 | 2.906206 | -4.703927 |
| 28 | 1 | 0 | 1.043722 | 4.259923 | -3.930664 |
| 29 | 1 | 0 | 1.894112 | -0.913923 | -6.23503 |
| 30 | 1 | 0 | -2.700048 | 1.01158 | -3.361774 |
| 31 | 1 | 0 | -1.398233 | -4.383632 | -5.063648 |
| 32 | 1 | 0 | -4.223479 | -3.423141 | -3.546702 |
| 33 | 1 | 0 | -3.533164 | -2.351333 | -6.649336 |
| 34 | 1 | 0 | -1.536786 | 2.971362 | -7.363524 |
| 35 | 1 | 0 | -0.37244 | 6.161182 | 2.497821 |
| 36 | 1 | 0 | -2.109843 | 3.586107 | 1.240569 |
| 37 | 1 | 0 | -0.745896 | 5.840114 | -0.800361 |
| 38 | 1 | 0 | 3.798452 | 5.858433 | -1.134862 |
| 39 | 1 | 0 | 1.089246 | -6.952703 | 5.574006 |
| 40 | 1 | 0 | -2.1514 | -7.734352 | 5.865784 |
| 41 | 1 | 0 | -4.268502 | -4.430259 | 7.850085 |
| 42 | 1 | 0 | -3.617864 | -1.086466 | 7.110276 |
| 43 | 1 | 0 | 0.486268 | -6.766533 | 1.344474 |

| **7_i** | | | Standard Orientation (A.U.) | | |
|---|---|---|---|---|---|
| Center number | Atomic number | Atomic Type | X | Y | Z |
| 0 | 6 | 0 | -0.026912 | 0.111227 | 4.281932 |
| 1 | 6 | 0 | 2.20936 | 1.677209 | 3.323078 |
| 2 | 6 | 0 | 2.127352 | 2.69206 | 0.598924 |

| | | | | | |
|---|---|---|---|---|---|
| 3 | 6 | 0 | 2.362553 | 0.4705 | -1.316778 |
| 4 | 6 | 0 | -0.013712 | -1.15289 | -1.89258 |
| 5 | 6 | 0 | -1.867452 | -1.79068 | 0.245141 |
| 6 | 6 | 0 | -0.650024 | -2.349659 | 2.824564 |
| 7 | 6 | 0 | 3.210407 | 1.202856 | -4.015043 |
| 8 | 6 | 0 | 0.830557 | 1.49874 | -5.646817 |
| 9 | 6 | 0 | -1.312776 | 0.128105 | -4.182941 |
| 10 | 6 | 0 | -2.854103 | -1.696305 | -5.809644 |
| 11 | 8 | 0 | 0.362283 | 4.14691 | -5.984141 |
| 12 | 6 | 0 | -0.120929 | 4.470089 | 0.18834 |
| 13 | 8 | 0 | 4.416148 | 4.166083 | 0.458325 |
| 14 | 6 | 0 | -2.270483 | -4.030903 | 4.497688 |
| 15 | 6 | 0 | -0.874875 | -5.570864 | 6.467888 |
| 16 | 6 | 0 | -4.789828 | -4.114435 | 4.37774 |
| 17 | 8 | 0 | 1.007468 | -7.198613 | 5.419302 |
| 18 | 1 | 0 | 0.744531 | -2.965547 | -2.578106 |
| 19 | 1 | 0 | 3.826951 | -0.743178 | -0.498134 |
| 20 | 1 | 0 | 1.12632 | -3.372532 | 2.476764 |
| 21 | 1 | 0 | -1.751173 | 1.262789 | 4.333486 |
| 22 | 1 | 0 | 0.379994 | -0.360204 | 6.259616 |
| 23 | 1 | 0 | 3.956792 | 0.573388 | 3.511115 |
| 24 | 1 | 0 | 2.434742 | 3.32078 | 4.564399 |
| 25 | 1 | 0 | -2.965698 | -3.442516 | -0.345553 |
| 26 | 1 | 0 | -3.241069 | -0.253798 | 0.473477 |
| 27 | 1 | 0 | 4.349103 | -0.350701 | -4.775761 |
| 28 | 1 | 0 | 4.394775 | 2.890631 | -4.117708 |
| 29 | 1 | 0 | 1.109768 | 0.631155 | -7.515738 |
| 30 | 1 | 0 | -2.580839 | 1.602535 | -3.462574 |
| 31 | 1 | 0 | -1.646928 | -3.193913 | -6.58336 |
| 32 | 1 | 0 | -4.359857 | -2.603852 | -4.716509 |
| 33 | 1 | 0 | -3.74532 | -0.721365 | -7.407827 |
| 34 | 1 | 0 | -1.245396 | 4.318994 | -6.848264 |
| 35 | 1 | 0 | -1.935248 | 3.524318 | 0.468614 |
| 36 | 1 | 0 | -0.104525 | 5.24228 | -1.730078 |
| 37 | 1 | 0 | 0.003738 | 6.029853 | 1.543232 |
| 38 | 1 | 0 | 4.294442 | 5.204039 | -1.046699 |
| 39 | 1 | 0 | -0.022739 | -4.314407 | 7.893847 |
| 40 | 1 | 0 | -2.206537 | -6.801495 | 7.459221 |
| 41 | 1 | 0 | -5.878656 | -5.313341 | 5.641874 |
| 42 | 1 | 0 | -5.868278 | -2.998544 | 3.035059 |
| 43 | 1 | 0 | 2.503798 | -6.194199 | 5.104963 |

| **7_j** | | | Standard Orientation (A.U.) | | |
|---|---|---|---|---|---|
| Center number | Atomic number | Atomic Type | X | Y | Z |
| 0 | 6 | 0 | 3.056426 | -0.283504 | 3.33907 |
| 1 | 6 | 0 | 3.34018 | 2.132184 | 1.756221 |
| 2 | 6 | 0 | 3.619245 | 1.819279 | -1.132774 |
| 3 | 6 | 0 | 1.074185 | 1.530903 | -2.535521 |
| 4 | 6 | 0 | -0.66651 | -0.719453 | -1.828928 |
| 5 | 6 | 0 | -1.209353 | -1.077467 | 1.006521 |
| 6 | 6 | 0 | 1.013982 | -2.215071 | 2.526677 |
| 7 | 6 | 0 | -0.7196 | 3.820017 | -2.434525 |
| 8 | 6 | 0 | -3.33662 | 2.829266 | -3.292878 |
| 9 | 6 | 0 | -3.1138 | -0.106896 | -3.320973 |
| 10 | 6 | 0 | -3.052087 | -1.160726 | -6.01846 |
| 11 | 8 | 0 | -5.364859 | 3.744262 | -1.773718 |
| 12 | 6 | 0 | 5.055579 | 4.089904 | -2.204555 |
| 13 | 8 | 0 | 5.212229 | -0.30928 | -1.709255 |
| 14 | 6 | 0 | -0.009216 | -3.744122 | 4.74131 |
| 15 | 6 | 0 | -0.253622 | -6.52629 | 4.188935 |
| 16 | 6 | 0 | -0.761824 | -2.756698 | 6.932933 |
| 17 | 8 | 0 | -1.469631 | -7.80712 | 6.198336 |
| 18 | 1 | 0 | 0.143933 | -2.50377 | -2.520452 |
| 19 | 1 | 0 | 1.609119 | 1.243194 | -4.519756 |
| 20 | 1 | 0 | 1.918694 | -3.587951 | 1.245505 |
| 21 | 1 | 0 | 2.679069 | 0.317808 | 5.279889 |
| 22 | 1 | 0 | 4.87942 | -1.262507 | 3.401469 |
| 23 | 1 | 0 | 5.028506 | 3.10608 | 2.460599 |
| 24 | 1 | 0 | 1.758029 | 3.411655 | 2.141489 |
| 25 | 1 | 0 | -2.825479 | -2.364497 | 1.170137 |
| 26 | 1 | 0 | -1.814906 | 0.694771 | 1.90166 |

| | | | | | |
|---|---|---|---|---|---|
| 27 | 1 | 0 | -0.060946 | 5.400552 | -3.591026 |
| 28 | 1 | 0 | -0.905213 | 4.54604 | -0.502316 |
| 29 | 1 | 0 | -3.794366 | 3.517527 | -5.187992 |
| 30 | 1 | 0 | -4.775701 | -0.893963 | -2.364567 |
| 31 | 1 | 0 | -2.91804 | -3.227444 | -6.009847 |
| 32 | 1 | 0 | -4.768338 | -0.636222 | -7.051611 |
| 33 | 1 | 0 | -1.431791 | -0.431421 | -7.084644 |
| 34 | 1 | 0 | -5.084125 | 3.136637 | -0.066337 |
| 35 | 1 | 0 | 4.158904 | 5.868983 | -1.650082 |
| 36 | 1 | 0 | 5.133435 | 4.000594 | -4.270261 |
| 37 | 1 | 0 | 6.992813 | 4.077118 | -1.481203 |
| 38 | 1 | 0 | 4.283771 | -1.827966 | -1.281263 |
| 39 | 1 | 0 | -1.303826 | -6.761644 | 2.397348 |
| 40 | 1 | 0 | 1.657477 | -7.296626 | 3.844457 |
| 41 | 1 | 0 | -1.569297 | -3.943112 | 8.393927 |
| 42 | 1 | 0 | -0.606141 | -0.748949 | 7.330612 |
| 43 | 1 | 0 | -1.467325 | -9.593765 | 5.805641 |

**7_k** Standard Orientation (A.U.)

| Center number | Atomic number | Atomic Type | X | Y | Z |
|---|---|---|---|---|---|
| 0 | 6 | 0 | 2.223233 | -0.982448 | 3.604622 |
| 1 | 6 | 0 | 1.979974 | 1.84758 | 2.992572 |
| 2 | 6 | 0 | 3.15061 | 2.574691 | 0.420719 |
| 3 | 6 | 0 | 1.796275 | 1.472346 | -1.910458 |
| 4 | 6 | 0 | 0.834856 | -1.30328 | -1.879457 |
| 5 | 6 | 0 | -1.114396 | -1.899054 | 0.204999 |
| 6 | 6 | 0 | -0.046242 | -2.610823 | 2.831894 |
| 7 | 6 | 0 | -0.50434 | 2.943203 | -2.918519 |
| 8 | 6 | 0 | -1.789784 | 1.139747 | -4.843548 |
| 9 | 6 | 0 | -0.459837 | -1.469946 | -4.505066 |
| 10 | 6 | 0 | 1.396544 | -2.036586 | -6.655617 |
| 11 | 8 | 0 | -4.468543 | 1.030093 | -4.56531 |
| 12 | 6 | 0 | 3.34539 | 5.461029 | 0.214981 |
| 13 | 8 | 0 | 5.668385 | 1.53705 | 0.248465 |
| 14 | 6 | 0 | -2.191765 | -2.642846 | 4.74415 |
| 15 | 6 | 0 | -4.311352 | -4.493204 | 4.211155 |
| 16 | 6 | 0 | -2.329144 | -1.162104 | 6.786545 |
| 17 | 8 | 0 | -3.429675 | -6.977825 | 3.643621 |
| 18 | 1 | 0 | 2.412748 | -2.637882 | -1.73995 |
| 19 | 1 | 0 | 3.25628 | 1.556866 | -3.378702 |
| 20 | 1 | 0 | 0.617927 | -4.571062 | 2.675225 |
| 21 | 1 | 0 | 2.582076 | -1.25201 | 5.625301 |
| 22 | 1 | 0 | 3.906922 | -1.679829 | 2.630225 |
| 23 | 1 | 0 | 2.963701 | 2.95713 | 4.448317 |
| 24 | 1 | 0 | 0.00491 | 2.471873 | 3.059236 |
| 25 | 1 | 0 | -2.285541 | -3.479804 | -0.438067 |
| 26 | 1 | 0 | -2.400674 | -0.287015 | 0.440559 |
| 27 | 1 | 0 | 0.019402 | 4.747533 | -3.777107 |
| 28 | 1 | 0 | -1.854116 | 3.383305 | -1.407755 |
| 29 | 1 | 0 | -1.522505 | 1.825929 | -6.775345 |
| 30 | 1 | 0 | -1.913816 | -2.945696 | -4.520497 |
| 31 | 1 | 0 | 0.404845 | -2.111 | -8.472457 |
| 32 | 1 | 0 | 2.870738 | -0.590303 | -6.80939 |
| 33 | 1 | 0 | 2.335596 | -3.858898 | -6.363437 |
| 34 | 1 | 0 | -4.812069 | 0.32384 | -2.909112 |
| 35 | 1 | 0 | 4.578865 | 6.194755 | 1.712048 |
| 36 | 1 | 0 | 1.500059 | 6.373391 | 0.420727 |
| 37 | 1 | 0 | 4.156339 | 6.008936 | -1.60731 |
| 38 | 1 | 0 | 6.610655 | 2.155932 | 1.696832 |
| 39 | 1 | 0 | -5.646454 | -4.511604 | 5.804483 |
| 40 | 1 | 0 | -5.375806 | -3.919626 | 2.530869 |
| 41 | 1 | 0 | -3.918447 | -1.293005 | 8.082988 |
| 42 | 1 | 0 | -0.904863 | 0.239013 | 7.246193 |
| 43 | 1 | 0 | -2.456965 | -7.54359 | 5.09154 |

**7_l** Standard Orientation (A.U.)

| Center number | Atomic number | Atomic Type | X | Y | Z |
|---|---|---|---|---|---|
| 0 | 6 | 0 | 3.14743 | -2.759871 | 1.477411 |
| 1 | 6 | 0 | 2.141485 | -1.035948 | 3.579406 |
| 2 | 6 | 0 | 1.682416 | 1.787377 | 2.852203 |
| 3 | 6 | 0 | 1.480502 | 2.220921 | -0.033977 |

| | | | | | |
|---|---|---|---|---|---|
| 4 | 6 | 0 | -0.600071 | 0.771827 | -1.495219 |
| 5 | 6 | 0 | -1.194861 | -1.916505 | -0.623377 |
| 6 | 6 | 0 | 1.116666 | -3.698988 | -0.425517 |
| 7 | 6 | 0 | 0.99286 | 5.00449 | -0.777615 |
| 8 | 6 | 0 | -1.830657 | 5.238257 | -1.515332 |
| 9 | 6 | 0 | -2.921528 | 2.53797 | -1.473108 |
| 10 | 6 | 0 | -4.844026 | 2.035987 | -3.566386 |
| 11 | 8 | 0 | -3.298441 | 6.743758 | 0.188413 |
| 12 | 6 | 0 | -0.544935 | 2.810439 | 4.39878 |
| 13 | 8 | 0 | 3.920696 | 3.226371 | 3.469108 |
| 14 | 6 | 0 | 0.153826 | -6.35219 | 0.122851 |
| 15 | 6 | 0 | -0.681108 | -7.849543 | -2.162996 |
| 16 | 6 | 0 | 0.00131 | -7.375486 | 2.427355 |
| 17 | 8 | 0 | 1.339816 | -8.239287 | -3.911841 |
| 18 | 1 | 0 | 0.069164 | 0.65547 | -3.463337 |
| 19 | 1 | 0 | 3.333783 | 1.66499 | -0.755155 |
| 20 | 1 | 0 | 1.991928 | -3.786265 | -2.302835 |
| 21 | 1 | 0 | 4.057221 | -4.408438 | 2.334622 |
| 22 | 1 | 0 | 4.649686 | -1.766166 | 0.461392 |
| 23 | 1 | 0 | 3.501912 | -1.021442 | 5.144127 |
| 24 | 1 | 0 | 0.401898 | -1.845951 | 4.356488 |
| 25 | 1 | 0 | -2.560581 | -2.743028 | -1.944579 |
| 26 | 1 | 0 | -2.160832 | -1.863164 | 1.208453 |
| 27 | 1 | 0 | 2.175579 | 5.484841 | -2.408222 |
| 28 | 1 | 0 | 1.508351 | 6.311903 | 0.735912 |
| 29 | 1 | 0 | -1.997801 | 6.035661 | -3.429951 |
| 30 | 1 | 0 | -3.881422 | 2.343591 | 0.353211 |
| 31 | 1 | 0 | -5.673283 | 0.145114 | -3.407942 |
| 32 | 1 | 0 | -6.388601 | 3.4117 | -3.479182 |
| 33 | 1 | 0 | -3.958326 | 2.182554 | -5.436406 |
| 34 | 1 | 0 | -2.668562 | 8.461043 | 0.081608 |
| 35 | 1 | 0 | -0.966996 | 4.779355 | 3.94965 |
| 36 | 1 | 0 | -0.1023 | 2.667371 | 6.42285 |
| 37 | 1 | 0 | -2.262836 | 1.707179 | 4.077075 |
| 38 | 1 | 0 | 4.061621 | 3.243059 | 5.297341 |
| 39 | 1 | 0 | -1.520523 | -9.656633 | -1.568492 |
| 40 | 1 | 0 | -2.117865 | -6.819999 | -3.241646 |
| 41 | 1 | 0 | -0.750291 | -9.267706 | 2.705804 |
| 42 | 1 | 0 | 0.599969 | -6.381834 | 4.120459 |
| 43 | 1 | 0 | 2.6857 | -9.06808 | -2.981045 |

| **7_m** | | | Standard Orientation (A.U.) | | |
|---|---|---|---|---|---|
| Center number | Atomic number | Atomic Type | X | Y | Z |
| 0 | 6 | 0 | 0.012381 | 1.086088 | 2.900747 |
| 1 | 6 | 0 | 2.448947 | 2.598039 | 2.503555 |
| 2 | 6 | 0 | 3.938327 | 2.257616 | 0.013117 |
| 3 | 6 | 0 | 2.382089 | 1.34906 | -2.282819 |
| 4 | 6 | 0 | 1.02014 | -1.302292 | -2.119776 |
| 5 | 6 | 0 | 1.361234 | -2.861805 | 0.303664 |
| 6 | 6 | 0 | 0.233128 | -1.801056 | 2.811538 |
| 7 | 6 | 0 | 0.328729 | 3.212028 | -3.202404 |
| 8 | 6 | 0 | -1.588415 | 1.53445 | -4.58662 |
| 9 | 6 | 0 | -1.746424 | -0.836066 | -2.942799 |
| 10 | 6 | 0 | -3.009625 | -3.08597 | -4.224638 |
| 11 | 8 | 0 | -4.03818 | 2.612526 | -4.847571 |
| 12 | 6 | 0 | 5.282206 | 4.751338 | -0.631063 |
| 13 | 8 | 0 | 5.869871 | 0.411333 | 0.576319 |
| 14 | 6 | 0 | -2.236899 | -3.122451 | 3.466833 |
| 15 | 6 | 0 | -1.953629 | -5.798816 | 4.433685 |
| 16 | 6 | 0 | -4.53809 | -2.084315 | 3.3496 |
| 17 | 8 | 0 | -0.582096 | -5.885531 | 6.759811 |
| 18 | 1 | 0 | 1.878654 | -2.46456 | -3.612172 |
| 19 | 1 | 0 | 3.778819 | 1.19288 | -3.816383 |
| 20 | 1 | 0 | 1.554972 | -2.357613 | 4.310401 |
| 21 | 1 | 0 | -1.399697 | 1.731439 | 1.539679 |
| 22 | 1 | 0 | -0.743405 | 1.607416 | 4.760471 |
| 23 | 1 | 0 | 3.792529 | 2.191249 | 4.02667 |
| 24 | 1 | 0 | 1.951928 | 4.600997 | 2.691518 |
| 25 | 1 | 0 | 3.383358 | -3.142033 | 0.580244 |
| 26 | 1 | 0 | 0.553705 | -4.73612 | -0.056837 |
| 27 | 1 | 0 | 1.095514 | 4.719149 | -4.397542 |

| | | | | | |
|---|---|---|---|---|---|
| 28 | 1 | 0 | -0.642325 | 4.117439 | -1.613078 |
| 29 | 1 | 0 | -0.829095 | 1.014033 | -6.460257 |
| 30 | 1 | 0 | -2.892118 | -0.318387 | -1.301649 |
| 31 | 1 | 0 | -1.922815 | -3.707646 | -5.879097 |
| 32 | 1 | 0 | -3.170694 | -4.69 | -2.925636 |
| 33 | 1 | 0 | -4.913662 | -2.580619 | -4.856424 |
| 34 | 1 | 0 | -3.904133 | 4.037417 | -5.990421 |
| 35 | 1 | 0 | 6.490839 | 4.523575 | -2.301552 |
| 36 | 1 | 0 | 6.481054 | 5.321682 | 0.955419 |
| 37 | 1 | 0 | 3.939565 | 6.27626 | -1.020917 |
| 38 | 1 | 0 | 6.808252 | 0.123781 | -0.974201 |
| 39 | 1 | 0 | -3.822729 | -6.687854 | 4.63091 |
| 40 | 1 | 0 | -0.843846 | -6.956628 | 3.12604 |
| 41 | 1 | 0 | -6.211679 | -3.165374 | 3.854147 |
| 42 | 1 | 0 | -4.86497 | -0.152847 | 2.742365 |
| 43 | 1 | 0 | -1.474415 | -4.792141 | 7.931411 |

| **7_n** | | | Standard Orientation (A.U.) | | |
|---|---|---|---|---|---|
| Center number | Atomic number | Atomic Type | X | Y | Z |
| 0 | 6 | 0 | 2.38974 | 0.739344 | 3.62502 |
| 1 | 6 | 0 | 2.188702 | 3.0775 | 1.917853 |
| 2 | 6 | 0 | 3.013157 | 2.781131 | -0.866761 |
| 3 | 6 | 0 | 0.932451 | 1.684311 | -2.597192 |
| 4 | 6 | 0 | -0.146956 | -0.970397 | -1.981098 |
| 5 | 6 | 0 | -1.006404 | -1.3987 | 0.76508 |
| 6 | 6 | 0 | 1.180017 | -1.749459 | 2.675397 |
| 7 | 6 | 0 | -1.454088 | 3.314217 | -2.934471 |
| 8 | 6 | 0 | -3.473209 | 1.546665 | -4.100653 |
| 9 | 6 | 0 | -2.393397 | -1.182266 | -3.852105 |
| 10 | 6 | 0 | -1.591699 | -2.266167 | -6.415775 |
| 11 | 8 | 0 | -5.911636 | 1.849634 | -2.995586 |
| 12 | 6 | 0 | 3.857844 | 5.351686 | -1.890066 |
| 13 | 8 | 0 | 5.241293 | 1.231191 | -1.039391 |
| 14 | 6 | 0 | 0.31826 | -3.466597 | 4.818059 |
| 15 | 6 | 0 | 0.926884 | -6.230871 | 4.401631 |
| 16 | 6 | 0 | -0.976321 | -2.699508 | 6.840691 |
| 17 | 8 | 0 | -0.227568 | -7.930119 | 6.111097 |
| 18 | 1 | 0 | 1.259021 | -2.439049 | -2.410081 |
| 19 | 1 | 0 | 1.841289 | 1.516758 | -4.455218 |
| 20 | 1 | 0 | 2.647826 | -2.813866 | 1.648011 |
| 21 | 1 | 0 | 1.544001 | 1.254984 | 5.438832 |
| 22 | 1 | 0 | 4.387096 | 0.370931 | 4.02414 |
| 23 | 1 | 0 | 3.370909 | 4.543435 | 2.78268 |
| 24 | 1 | 0 | 0.255705 | 3.819325 | 1.969189 |
| 25 | 1 | 0 | -2.163922 | -3.118407 | 0.784919 |
| 26 | 1 | 0 | -2.25576 | 0.121936 | 1.425332 |
| 27 | 1 | 0 | -1.117552 | 4.99287 | -4.091027 |
| 28 | 1 | 0 | -2.164145 | 3.993946 | -1.109539 |
| 29 | 1 | 0 | -3.779025 | 2.000617 | -6.094346 |
| 30 | 1 | 0 | -3.881798 | -2.400608 | -3.079464 |
| 31 | 1 | 0 | -0.862456 | -4.194272 | -6.2169 |
| 32 | 1 | 0 | -3.195795 | -2.321392 | -7.72408 |
| 33 | 1 | 0 | -0.105424 | -1.12074 | -7.295078 |
| 34 | 1 | 0 | -5.756873 | 1.440833 | -1.21458 |
| 35 | 1 | 0 | 2.394453 | 6.785273 | -1.607462 |
| 36 | 1 | 0 | 4.289412 | 5.231367 | -3.909981 |
| 37 | 1 | 0 | 5.568188 | 5.954155 | -0.896214 |
| 38 | 1 | 0 | 4.754791 | -0.490082 | -0.649348 |
| 39 | 1 | 0 | 0.475744 | -6.726257 | 2.423028 |
| 40 | 1 | 0 | 2.970578 | -6.521462 | 4.611911 |
| 41 | 1 | 0 | -1.564036 | -4.038749 | 8.278739 |
| 42 | 1 | 0 | -1.459186 | -0.73094 | 7.157787 |
| 43 | 1 | 0 | -2.039897 | -7.695736 | 5.957575 |

| **7_o** | | | Standard Orientation (A.U.) | | |
|---|---|---|---|---|---|
| Center number | Atomic number | Atomic Type | X | Y | Z |
| 0 | 6 | 0 | 3.999454 | -1.786776 | -0.127874 |
| 1 | 6 | 0 | 3.648602 | -0.530686 | 2.463226 |
| 2 | 6 | 0 | 2.124995 | 1.988035 | 2.551289 |
| 3 | 6 | 0 | 0.805216 | 2.645123 | 0.013234 |
| 4 | 6 | 0 | -1.134344 | 0.693732 | -1.073557 |

| | | | | | |
|---|---|---|---|---|---|
| 5 | 6 | 0 | -0.84778 | -2.066648 | -0.276004 |
| 6 | 6 | 0 | 1.68276 | -3.296584 | -1.071641 |
| 7 | 6 | 0 | -0.662459 | 5.194923 | 0.080646 |
| 8 | 6 | 0 | -3.290935 | 4.660461 | -1.057281 |
| 9 | 6 | 0 | -3.744196 | 1.847606 | -0.514091 |
| 10 | 6 | 0 | -5.956753 | 0.73931 | -1.987727 |
| 11 | 8 | 0 | -5.234638 | 6.30914 | -0.218364 |
| 12 | 6 | 0 | 0.36744 | 1.941104 | 4.861978 |
| 13 | 8 | 0 | 4.028072 | 3.90095 | 2.967218 |
| 14 | 6 | 0 | 1.676023 | -6.062515 | -0.284052 |
| 15 | 6 | 0 | 0.033267 | -7.791107 | -1.865853 |
| 16 | 6 | 0 | 3.004389 | -7.026629 | 1.636858 |
| 17 | 8 | 0 | 0.706329 | -7.736204 | -4.479881 |
| 18 | 1 | 0 | -0.910406 | 0.739988 | -3.142358 |
| 19 | 1 | 0 | 2.363445 | 2.837394 | -1.326015 |
| 20 | 1 | 0 | 1.721316 | -3.301985 | -3.14568 |
| 21 | 1 | 0 | 5.630343 | -3.058518 | -0.042228 |
| 22 | 1 | 0 | 4.50064 | -0.350962 | -1.528872 |
| 23 | 1 | 0 | 5.500125 | -0.07726 | 3.26498 |
| 24 | 1 | 0 | 2.776306 | -1.891155 | 3.755298 |
| 25 | 1 | 0 | -2.403117 | -3.137546 | -1.12403 |
| 26 | 1 | 0 | -1.080081 | -2.258455 | 1.772304 |
| 27 | 1 | 0 | 0.318432 | 6.708422 | -0.92939 |
| 28 | 1 | 0 | -0.948108 | 5.872375 | 2.020285 |
| 29 | 1 | 0 | -3.238424 | 4.932633 | -3.111415 |
| 30 | 1 | 0 | -4.125365 | 1.661818 | 1.527477 |
| 31 | 1 | 0 | -6.364569 | -1.211757 | -1.430245 |
| 32 | 1 | 0 | -7.660814 | 1.8705 | -1.672676 |
| 33 | 1 | 0 | -5.555698 | 0.748343 | -4.022609 |
| 34 | 1 | 0 | -5.393454 | 6.075647 | 1.594887 |
| 35 | 1 | 0 | -0.561938 | 3.762594 | 5.181576 |
| 36 | 1 | 0 | 1.492026 | 1.519232 | 6.545968 |
| 37 | 1 | 0 | -1.106219 | 0.500936 | 4.68787 |
| 38 | 1 | 0 | 3.173595 | 5.524034 | 2.994961 |
| 39 | 1 | 0 | 0.112074 | -9.726093 | -1.109608 |
| 40 | 1 | 0 | -1.94724 | -7.191634 | -1.82156 |
| 41 | 1 | 0 | 2.900414 | -9.02671 | 2.097987 |
| 42 | 1 | 0 | 4.227913 | -5.890575 | 2.827582 |
| 43 | 1 | 0 | 2.475558 | -8.210388 | -4.577693 |

| **7_p** | | | Standard Orientation (A.U.) | | |
|---|---|---|---|---|---|
| Center number | Atomic number | Atomic Type | X | Y | Z |
| 0 | 6 | 0 | 0.207292 | 0.997055 | 4.381056 |
| 1 | 6 | 0 | -0.337201 | 3.269506 | 2.657743 |
| 2 | 6 | 0 | 1.426802 | 3.661165 | 0.364037 |
| 3 | 6 | 0 | 0.695066 | 2.071278 | -1.975361 |
| 4 | 6 | 0 | 0.613029 | -0.84716 | -1.731023 |
| 5 | 6 | 0 | -0.829047 | -1.910417 | 0.558635 |
| 6 | 6 | 0 | 0.604522 | -1.593207 | 3.089736 |
| 7 | 6 | 0 | -1.862935 | 2.74039 | -3.214649 |
| 8 | 6 | 0 | -2.686958 | 0.388713 | -4.765241 |
| 9 | 6 | 0 | -0.630154 | -1.644942 | -4.258974 |
| 10 | 6 | 0 | 1.282115 | -1.806864 | -6.430035 |
| 11 | 8 | 0 | -5.180503 | -0.444526 | -4.157239 |
| 12 | 6 | 0 | 1.441033 | 6.464783 | -0.352638 |
| 13 | 8 | 0 | 4.006792 | 3.133701 | 1.049558 |
| 14 | 6 | 0 | 0.024158 | -3.815981 | 4.821417 |
| 15 | 6 | 0 | 1.939426 | -5.9222 | 4.767378 |
| 16 | 6 | 0 | -2.035968 | -3.999596 | 6.265506 |
| 17 | 8 | 0 | 2.38457 | -6.635104 | 2.198679 |
| 18 | 1 | 0 | 2.534142 | -1.629243 | -1.626595 |
| 19 | 1 | 0 | 2.184174 | 2.490468 | -3.356346 |
| 20 | 1 | 0 | 2.617031 | -1.774183 | 2.609496 |
| 21 | 1 | 0 | -1.370397 | 0.86616 | 5.712697 |
| 22 | 1 | 0 | 1.881564 | 1.408216 | 5.527349 |
| 23 | 1 | 0 | -0.228897 | 4.962198 | 3.848584 |
| 24 | 1 | 0 | -2.294239 | 3.185872 | 1.985301 |
| 25 | 1 | 0 | -1.114559 | -3.929264 | 0.226491 |
| 26 | 1 | 0 | -2.718783 | -1.066301 | 0.7428 |
| 27 | 1 | 0 | -1.731409 | 4.440341 | -4.383006 |
| 28 | 1 | 0 | -3.328333 | 3.117385 | -1.801259 |

| | | | | | |
|---|---|---|---|---|---|
| 29 | 1 | 0 | -2.793433 | 0.82308 | -6.783357 |
| 30 | 1 | 0 | -1.553884 | -3.49108 | -4.079631 |
| 31 | 1 | 0 | 2.225275 | 0.006937 | -6.765316 |
| 32 | 1 | 0 | 2.748735 | -3.210577 | -6.021898 |
| 33 | 1 | 0 | 0.344091 | -2.35606 | -8.192711 |
| 34 | 1 | 0 | -5.155122 | -1.014598 | -2.415072 |
| 35 | 1 | 0 | 2.296609 | 7.559619 | 1.179285 |
| 36 | 1 | 0 | -0.480092 | 7.163266 | -0.666848 |
| 37 | 1 | 0 | 2.550592 | 6.776424 | -2.071043 |
| 38 | 1 | 0 | 4.18035 | 1.316311 | 1.18778 |
| 39 | 1 | 0 | 3.710415 | -5.236979 | 5.631705 |
| 40 | 1 | 0 | 1.271984 | -7.535791 | 5.894152 |
| 41 | 1 | 0 | -2.414949 | -5.685292 | 7.375569 |
| 42 | 1 | 0 | -3.421818 | -2.492324 | 6.407086 |
| 43 | 1 | 0 | 3.84897 | -7.733438 | 2.169205 |

**7_q** Standard Orientation (A.U.)

| Center number | Atomic number | Atomic Type | X | Y | Z |
|---|---|---|---|---|---|
| 0 | 6 | 0 | 1.230214 | 0.408472 | 3.80283 |
| 1 | 6 | 0 | 2.598082 | 2.113901 | 1.895084 |
| 2 | 6 | 0 | 3.794782 | 0.792101 | -0.417046 |
| 3 | 6 | 0 | 1.936949 | 0.414487 | -2.625262 |
| 4 | 6 | 0 | -0.516929 | -1.127532 | -2.157226 |
| 5 | 6 | 0 | -1.979592 | -0.642584 | 0.312667 |
| 6 | 6 | 0 | -0.591968 | -1.59593 | 2.688079 |
| 7 | 6 | 0 | 1.063666 | 2.890638 | -3.930568 |
| 8 | 6 | 0 | -1.660559 | 2.440326 | -4.852467 |
| 9 | 6 | 0 | -2.131675 | -0.419245 | -4.497448 |
| 10 | 6 | 0 | -1.386241 | -1.90954 | -6.869251 |
| 11 | 8 | 0 | -3.274264 | 3.963292 | -3.298404 |
| 12 | 6 | 0 | 6.082528 | 2.326962 | -1.33612 |
| 13 | 8 | 0 | 4.6415 | -1.719233 | 0.204106 |
| 14 | 6 | 0 | -2.363634 | -2.536005 | 4.746773 |
| 15 | 6 | 0 | -1.423538 | -4.712924 | 6.336681 |
| 16 | 6 | 0 | -4.616901 | -1.500172 | 5.234619 |
| 17 | 8 | 0 | 0.867192 | -4.145048 | 7.658588 |
| 18 | 1 | 0 | -0.05621 | -3.147955 | -2.195947 |
| 19 | 1 | 0 | 3.025304 | -0.672778 | -4.013703 |
| 20 | 1 | 0 | 0.582852 | -3.199371 | 2.11113 |
| 21 | 1 | 0 | 0.154255 | 1.64858 | 5.071156 |
| 22 | 1 | 0 | 2.602149 | -0.582861 | 4.990958 |
| 23 | 1 | 0 | 4.08439 | 3.134096 | 2.926109 |
| 24 | 1 | 0 | 1.304089 | 3.577269 | 1.211452 |
| 25 | 1 | 0 | -3.773817 | -1.666723 | 0.143729 |
| 26 | 1 | 0 | -2.480577 | 1.358222 | 0.478282 |
| 27 | 1 | 0 | 2.322583 | 3.397104 | -5.489847 |
| 28 | 1 | 0 | 1.029156 | 4.502779 | -2.637576 |
| 29 | 1 | 0 | -1.906165 | 2.996127 | -6.841668 |
| 30 | 1 | 0 | -4.147068 | -0.764481 | -4.129214 |
| 31 | 1 | 0 | -1.633253 | -3.942704 | -6.569769 |
| 32 | 1 | 0 | -2.54976 | -1.355748 | -8.4917 |
| 33 | 1 | 0 | 0.593106 | -1.5922 | -7.388497 |
| 34 | 1 | 0 | -5.00532 | 3.509305 | -3.695788 |
| 35 | 1 | 0 | 5.57102 | 4.285893 | -1.764917 |
| 36 | 1 | 0 | 6.900652 | 1.468134 | -3.031633 |
| 37 | 1 | 0 | 7.543515 | 2.371043 | 0.134807 |
| 38 | 1 | 0 | 5.744 | -1.586089 | 1.663348 |
| 39 | 1 | 0 | -2.908222 | -5.329203 | 7.656753 |
| 40 | 1 | 0 | -0.944275 | -6.326435 | 5.129372 |
| 41 | 1 | 0 | -5.811061 | -2.19682 | 6.755459 |
| 42 | 1 | 0 | -5.36439 | 0.063861 | 4.133509 |
| 43 | 1 | 0 | 0.524737 | -2.658446 | 8.676409 |

**7_r** Standard Orientation (A.U.)

| Center number | Atomic number | Atomic Type | X | Y | Z |
|---|---|---|---|---|---|
| 0 | 6 | 0 | 3.508137 | -0.18559 | 2.815325 |
| 1 | 6 | 0 | 1.245874 | 1.513295 | 3.477621 |
| 2 | 6 | 0 | 0.674385 | 3.546001 | 1.460779 |
| 3 | 6 | 0 | -0.379168 | 2.537194 | -1.058917 |
| 4 | 6 | 0 | 0.801637 | 0.142359 | -2.278456 |
| 5 | 6 | 0 | 0.697111 | -2.235716 | -0.598333 |

| | | | | | |
|---|---|---|---|---|---|
| 6 | 6 | 0 | 2.907701 | -2.5889 | 1.269801 |
| 7 | 6 | 0 | -3.235285 | 1.972961 | -1.149273 |
| 8 | 6 | 0 | -3.644463 | 0.40548 | -3.596323 |
| 9 | 6 | 0 | -0.946146 | -0.220775 | -4.602177 |
| 10 | 6 | 0 | -0.207568 | 1.442105 | -6.855951 |
| 11 | 8 | 0 | -5.178874 | -1.777864 | -3.207224 |
| 12 | 6 | 0 | -1.118552 | 5.535027 | 2.575721 |
| 13 | 8 | 0 | 2.989575 | 4.79617 | 0.736814 |
| 14 | 6 | 0 | 2.456674 | -4.889534 | 2.935058 |
| 15 | 6 | 0 | 0.685067 | -4.677169 | 5.1688 |
| 16 | 6 | 0 | 3.585239 | -7.099998 | 2.457285 |
| 17 | 8 | 0 | -1.884246 | -4.165227 | 4.474295 |
| 18 | 1 | 0 | 2.759983 | 0.491682 | -2.859938 |
| 19 | 1 | 0 | -0.022163 | 4.09488 | -2.378018 |
| 20 | 1 | 0 | 4.589204 | -3.011938 | 0.130484 |
| 21 | 1 | 0 | 4.498811 | -0.741803 | 4.548473 |
| 22 | 1 | 0 | 4.844806 | 0.967691 | 1.740697 |
| 23 | 1 | 0 | 1.668585 | 2.519578 | 5.246161 |
| 24 | 1 | 0 | -0.462565 | 0.407338 | 3.853734 |
| 25 | 1 | 0 | 0.665046 | -3.916106 | -1.813597 |
| 26 | 1 | 0 | -1.068022 | -2.265938 | 0.477008 |
| 27 | 1 | 0 | -4.381893 | 3.691306 | -1.129242 |
| 28 | 1 | 0 | -3.839905 | 0.845053 | 0.481075 |
| 29 | 1 | 0 | -4.691177 | 1.499048 | -5.004401 |
| 30 | 1 | 0 | -0.932911 | -2.192056 | -5.239226 |
| 31 | 1 | 0 | -1.499192 | 1.129695 | -8.444767 |
| 32 | 1 | 0 | -0.271962 | 3.459051 | -6.390562 |
| 33 | 1 | 0 | 1.713473 | 1.010866 | -7.498031 |
| 34 | 1 | 0 | -4.321772 | -2.820775 | -1.967641 |
| 35 | 1 | 0 | -0.218566 | 6.474113 | 4.190968 |
| 36 | 1 | 0 | -2.881316 | 4.686967 | 3.247991 |
| 37 | 1 | 0 | -1.571434 | 6.979705 | 1.166033 |
| 38 | 1 | 0 | 3.736812 | 5.479006 | 2.267896 |
| 39 | 1 | 0 | 0.796697 | -6.40753 | 6.312785 |
| 40 | 1 | 0 | 1.219913 | -3.094085 | 6.386396 |
| 41 | 1 | 0 | 3.259851 | -8.757889 | 3.628303 |
| 42 | 1 | 0 | 4.89094 | -7.33106 | 0.887075 |
| 43 | 1 | 0 | -2.414492 | -5.540401 | 3.382676 |