# Benzyl furanones and pyrones from the marine-derived fungus *Aspergillus terreus* induced by chemical epigenetic modification

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# List of supporting information

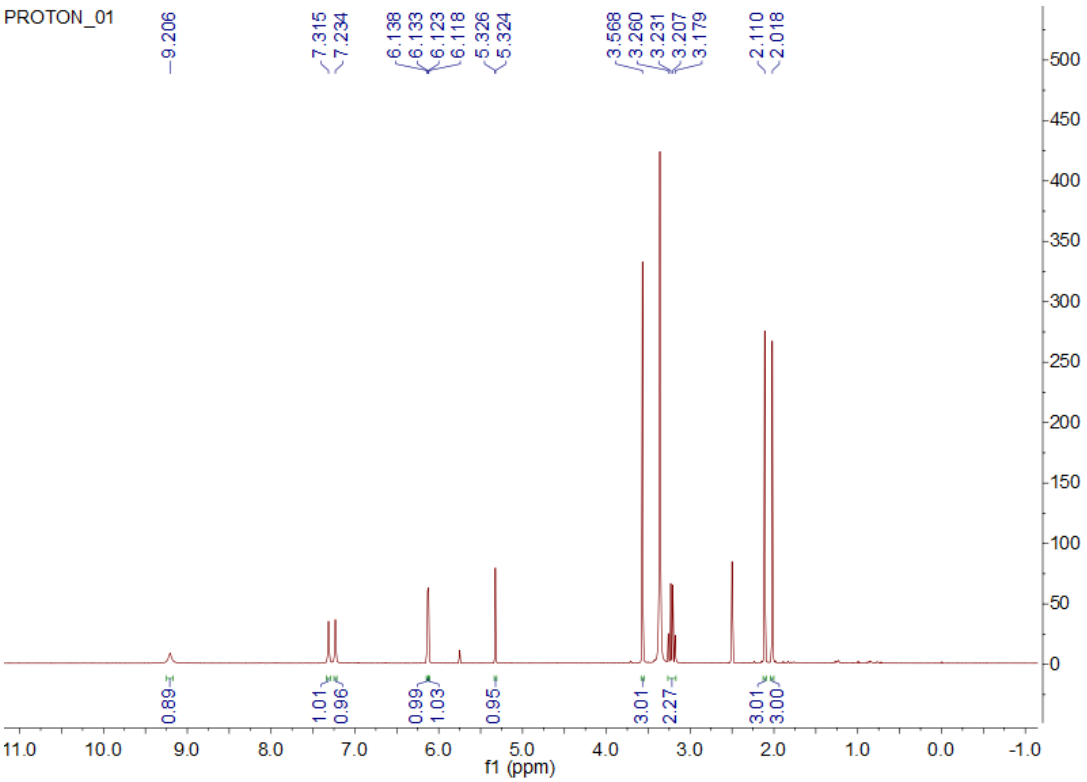


**Figure S1.** $^{1}$H NMR (500 MHz, DMSO-$d_6$) spectrum of (±)-**1**

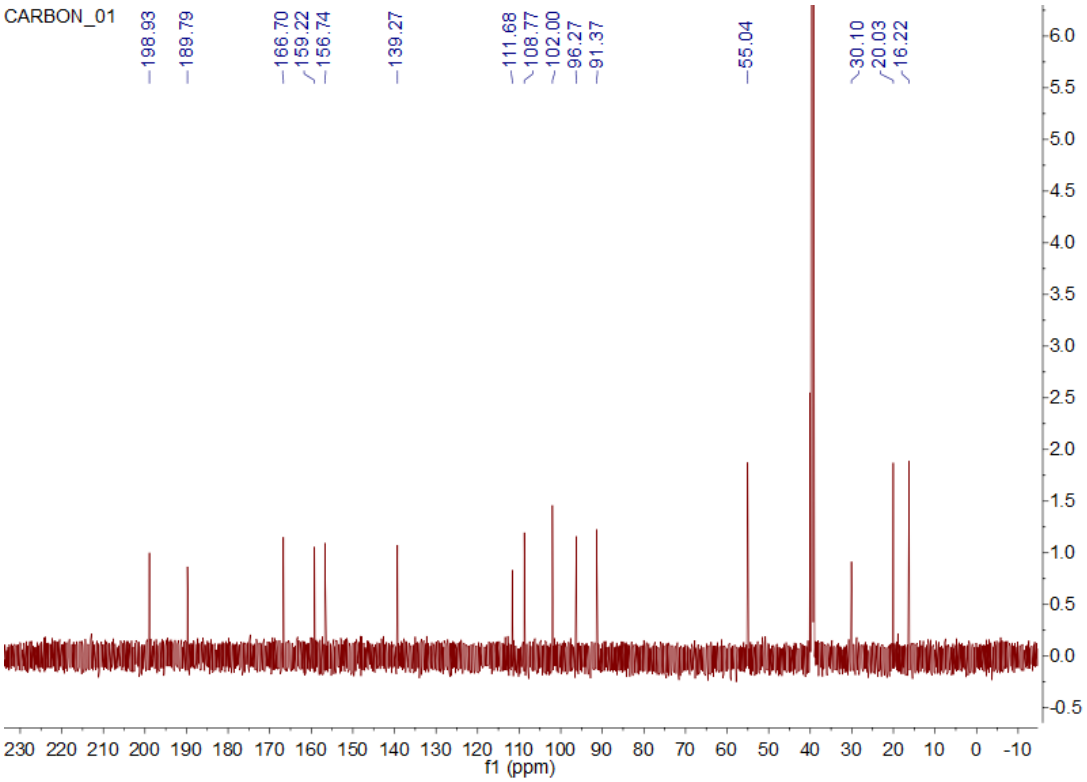


**Figure S2.** $^{13}$C NMR (125 MHz, DMSO-$d_6$) spectrum of (±)-**1**

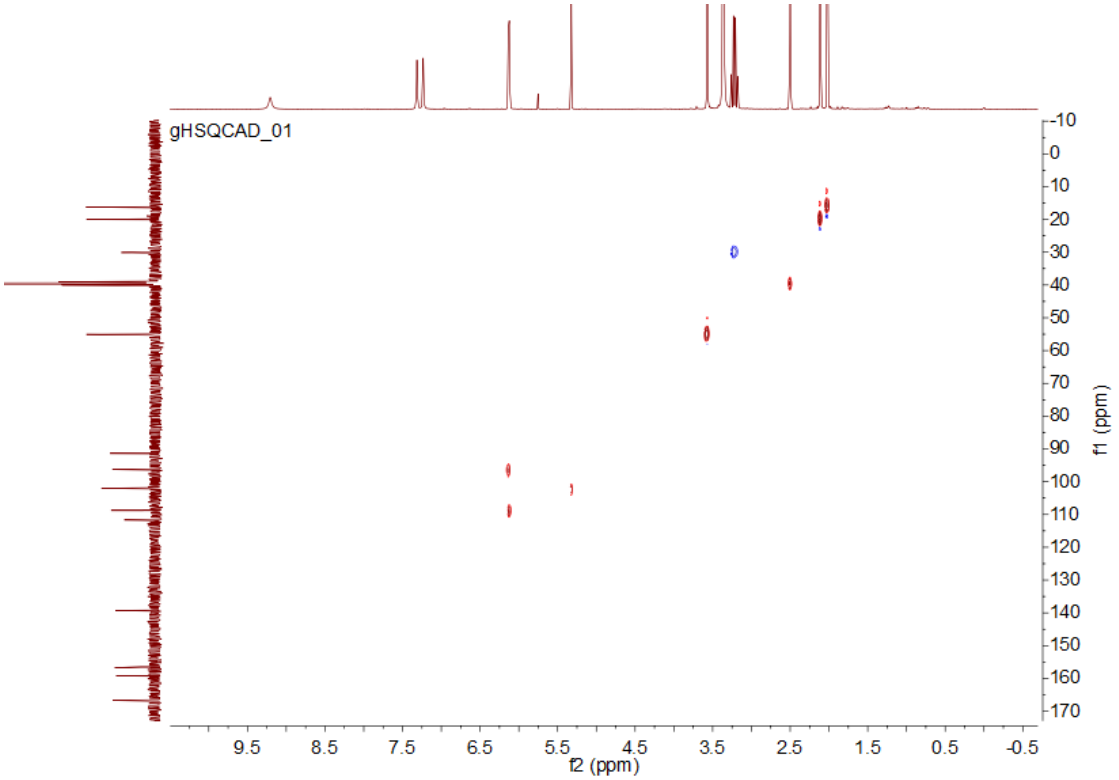


**Figure S3.** HSQC (DMSO-$d_6$) spectrum of (±)-**1**

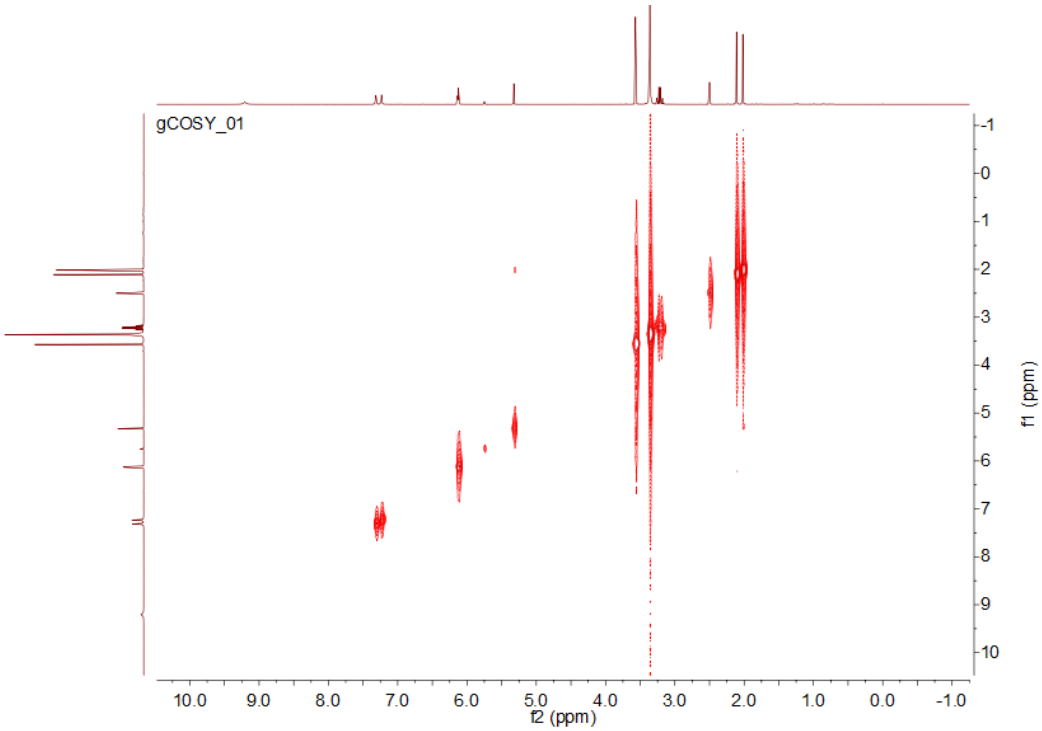


**Figure S4.** $^{1}$H–$^{1}$H COSY (DMSO-$d_6$) spectrum of (±)-**1**

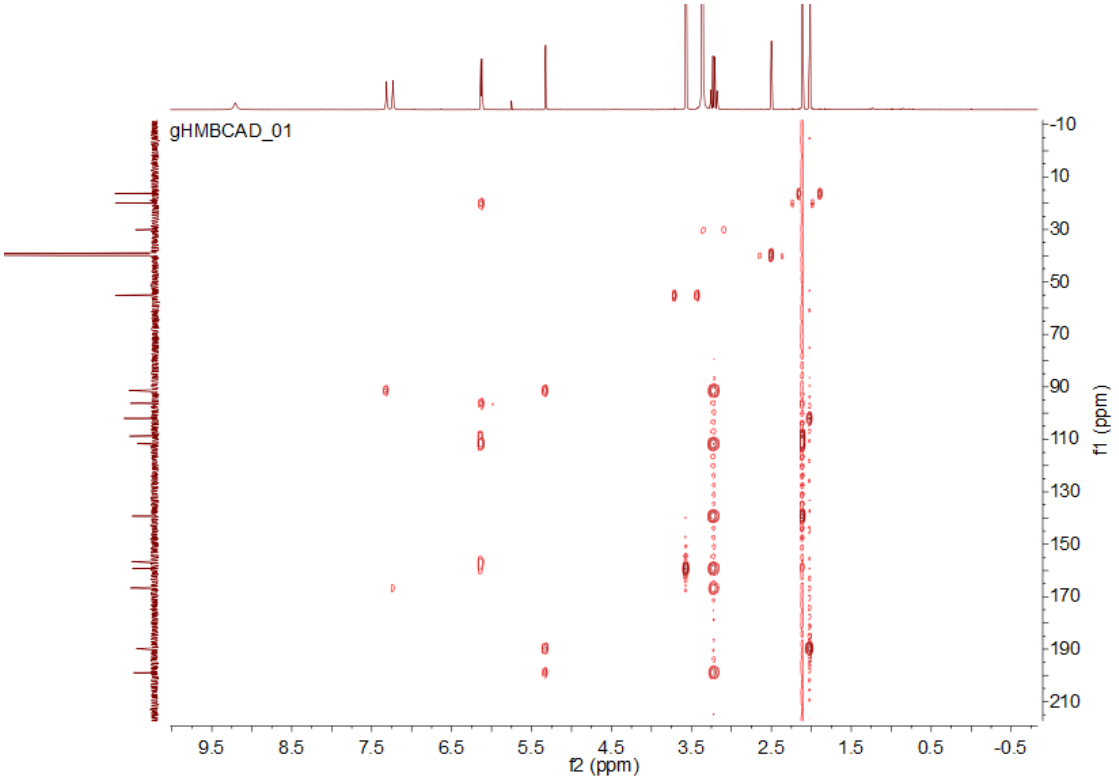


**Figure S5.** HMBC (DMSO-$d_6$) spectrum of (±)-**1**

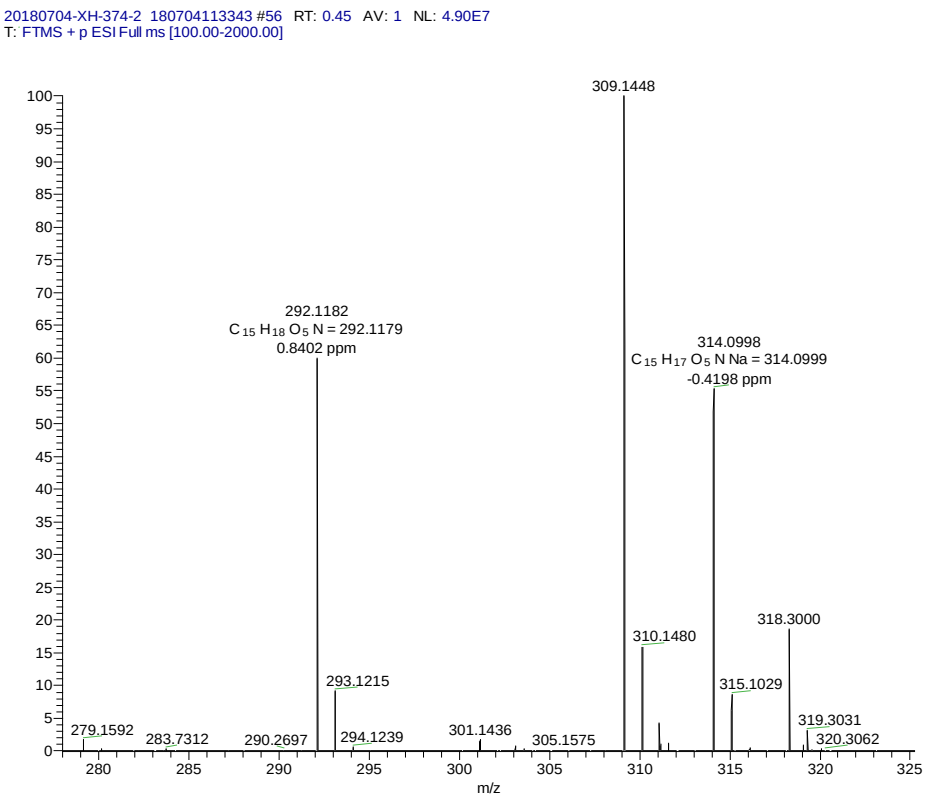


**Figure S6.** HRESIMS spectrum of (±)-**1**

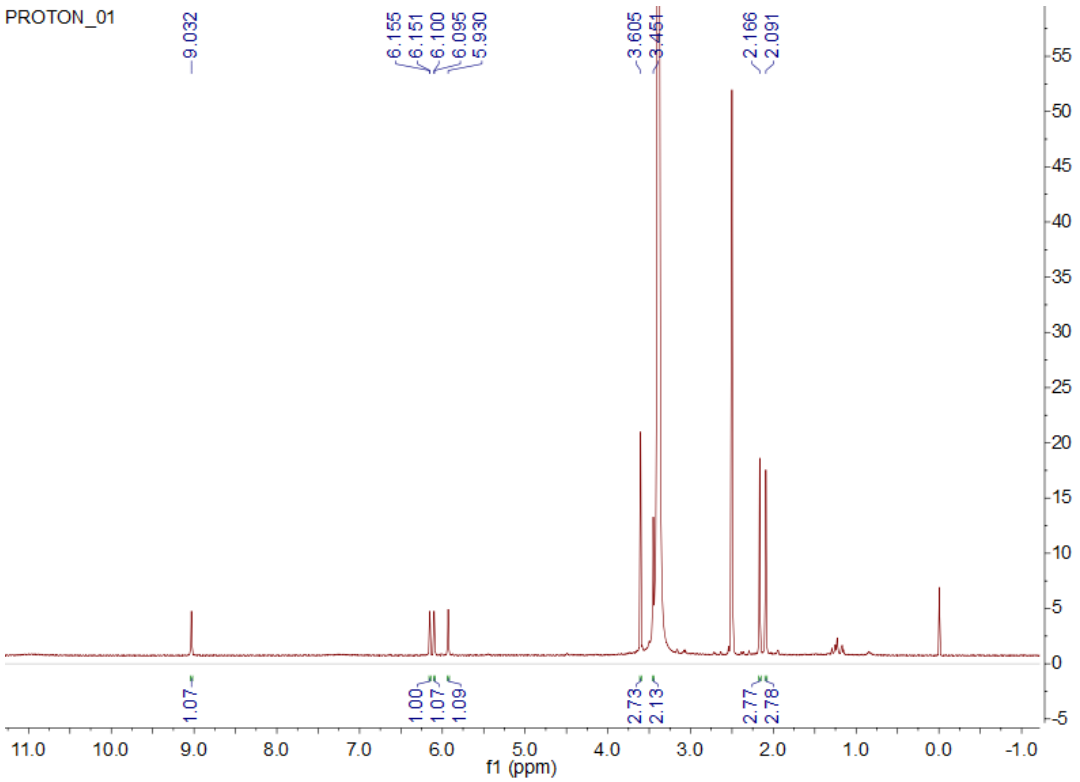


**Figure S7.** $^{1}$H NMR (500 MHz, DMSO-$d_6$) spectrum of compound **2**

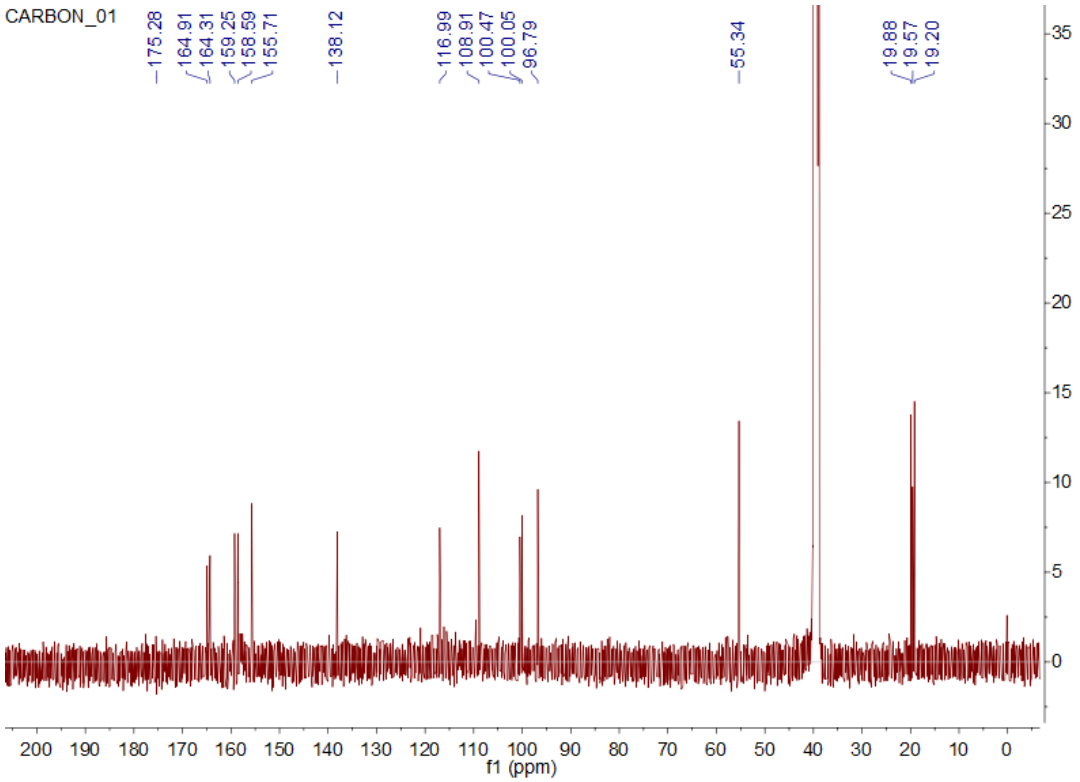


**Figure S8.** $^{13}$C NMR (125 MHz, DMSO-$d_6$) spectrum of compound **2**

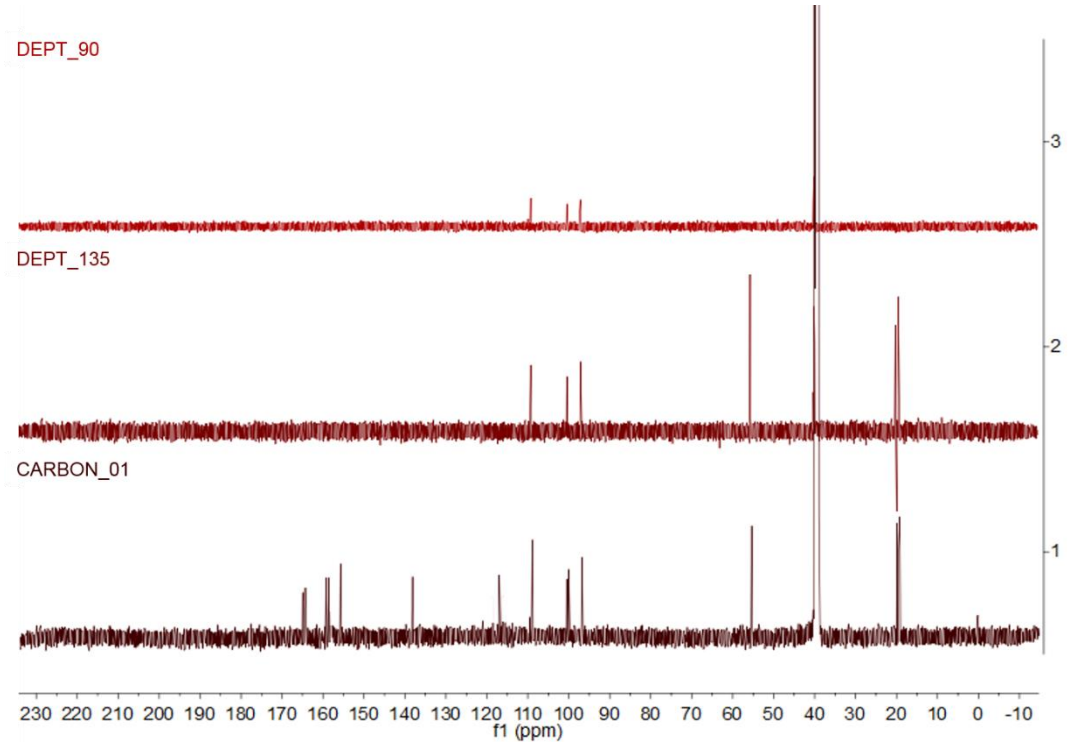


**Figure S9.** DEPT (125 MHz, DMSO-$d_6$) spectrum of compound **2**

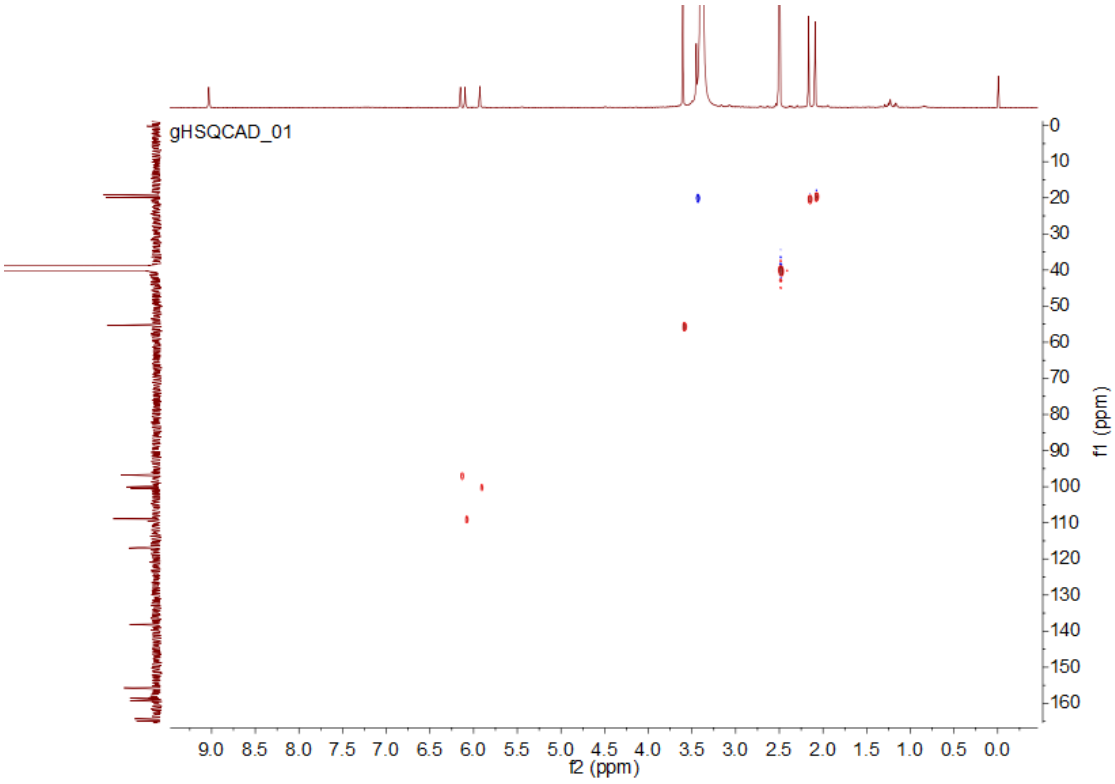


**Figure S10.** HSQC (DMSO-$d_6$) spectrum of compound **2**

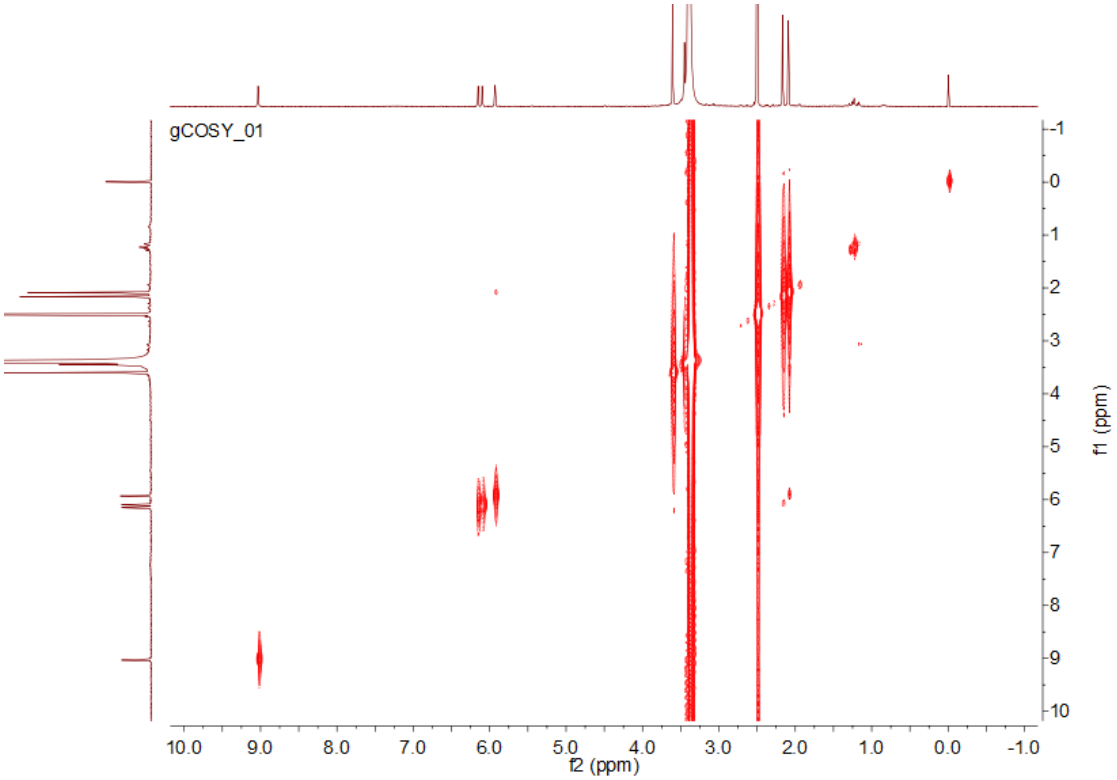


**Figure S11.** $^{1}H–^{1}H$ COSY (DMSO-$d_6$) spectrum of compound **2**

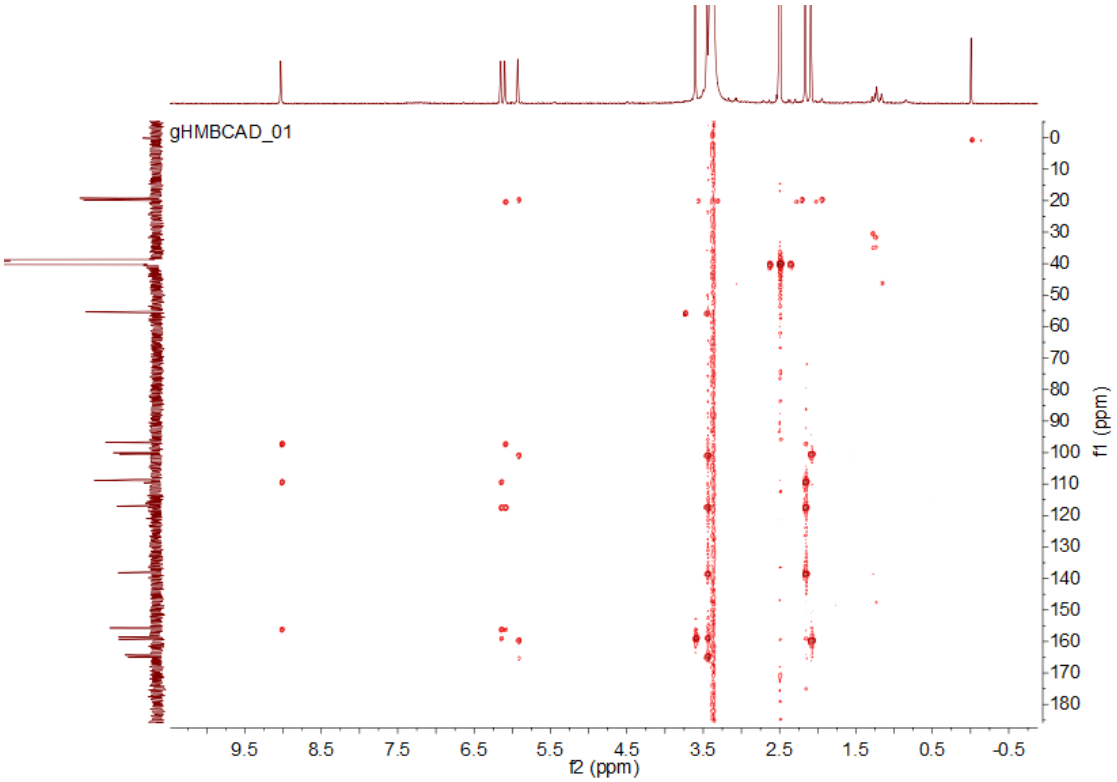


**Figure S12.** HMBC (DMSO-$d_6$) spectrum of compound **2**

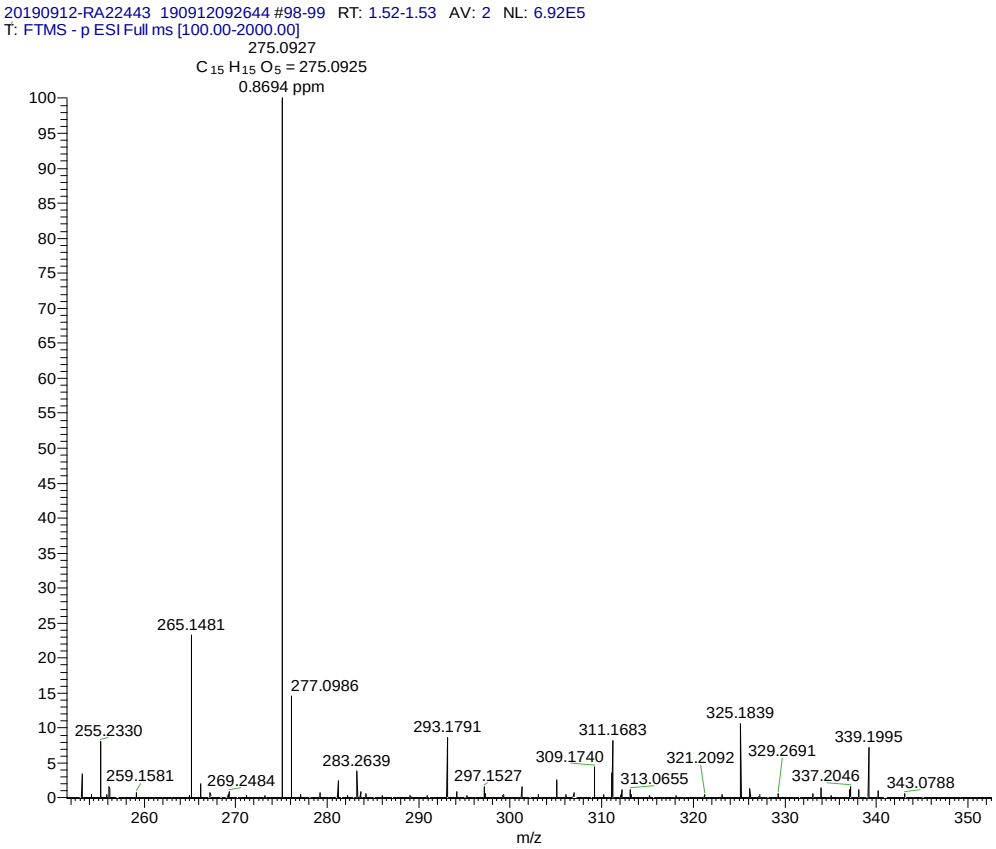


**Figure S13.** HRESIMS spectrum of compound **2**

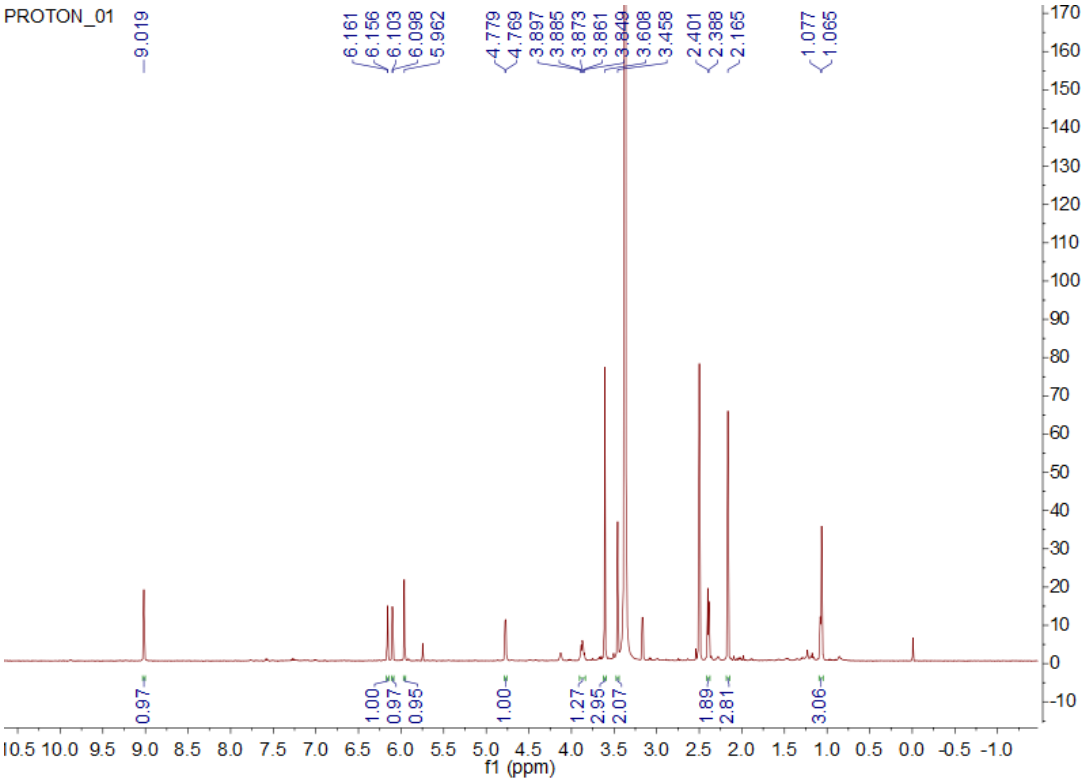


**Figure S14.** $^{1}$H NMR (500 MHz, DMSO-$d_6$) spectrum of compound **3**

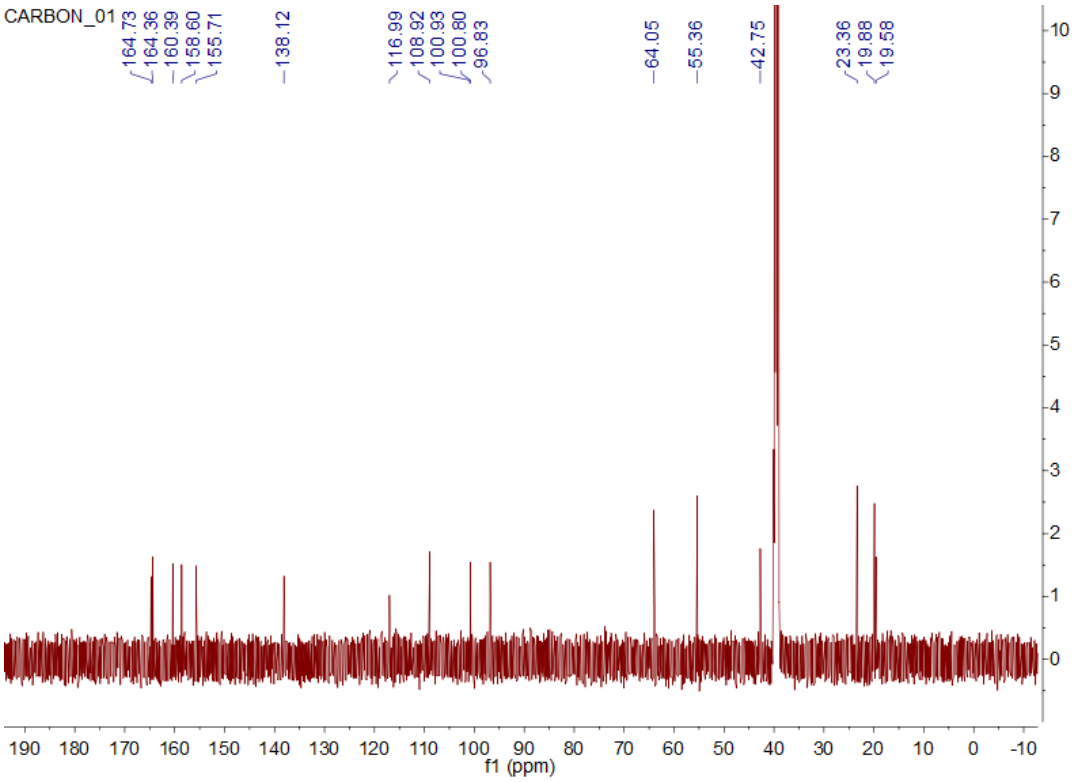


**Figure S15.** $^{13}$C NMR (125 MHz, DMSO-$d_6$) spectrum of compound **3**

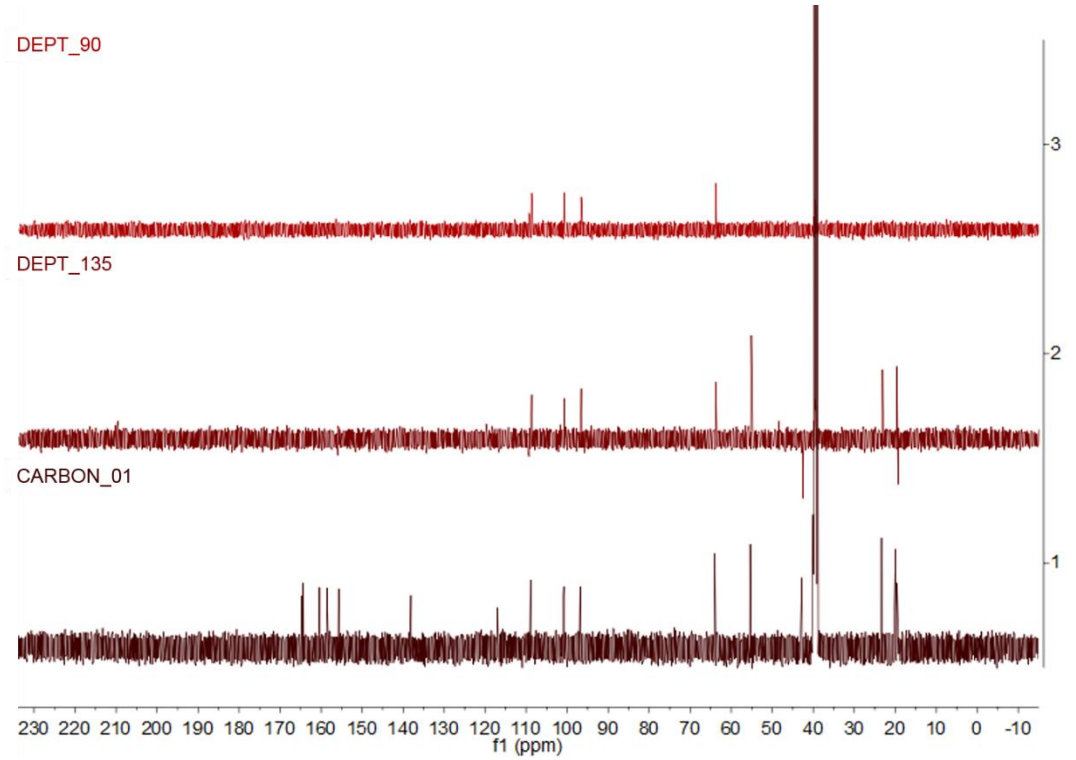


**Figure S16.** DEPT (125 MHz, DMSO-$d_6$) spectrum of compound **3**

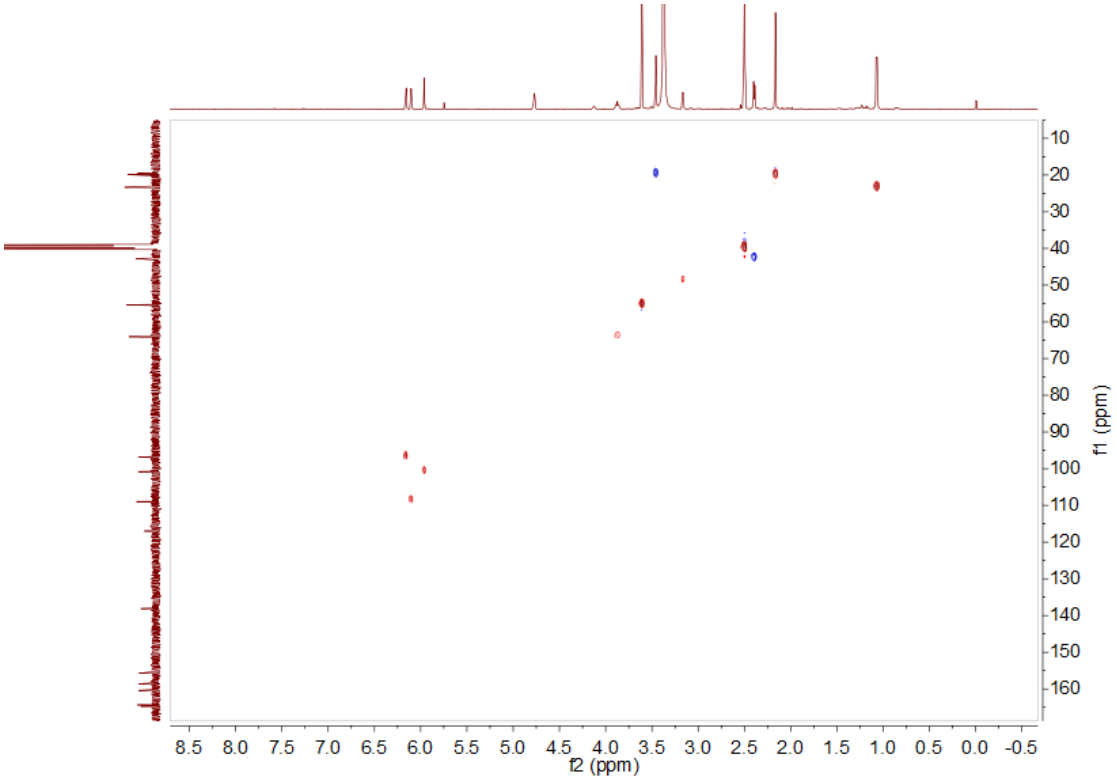


**Figure S17.** HSQC (DMSO-$d_6$) spectrum of compound **3**

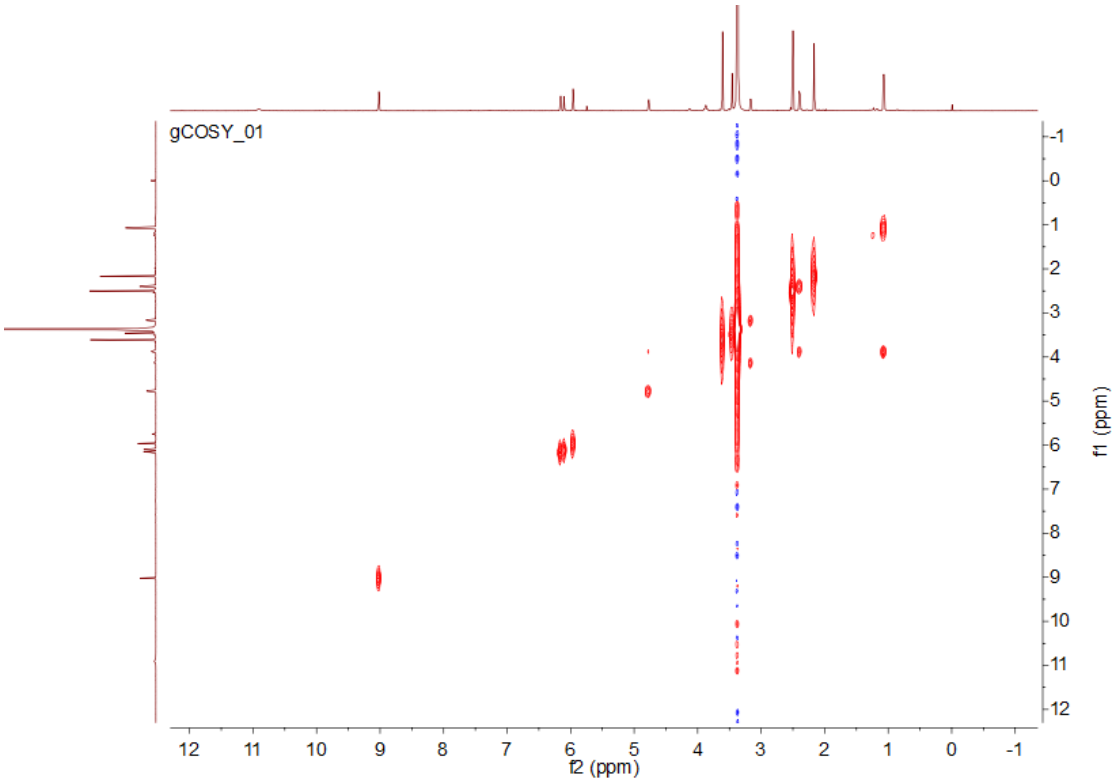


**Figure S18.** $^{1}$H–$^{1}$H COSY (DMSO-$d_6$) spectrum of compound **3**

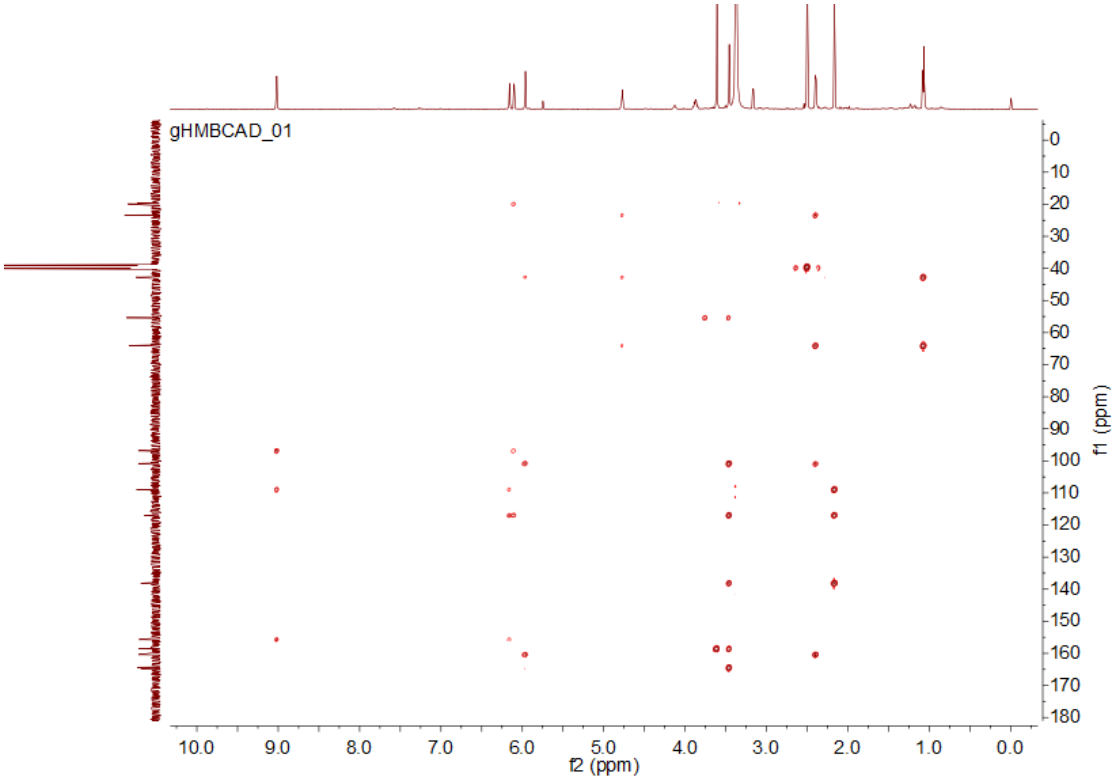


**Figure S19.** HMBC (DMSO-$d_6$) spectrum of compound **3**

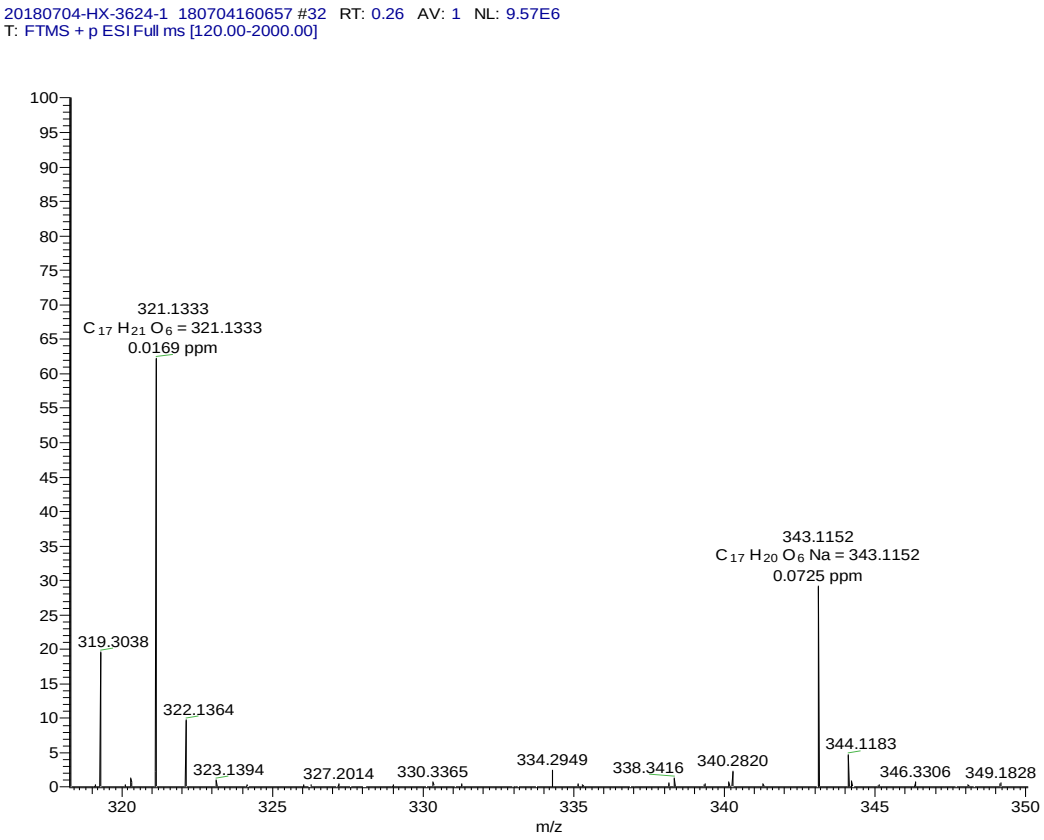


**Figure S20.** HRESIMS spectrum of compound **3**

**Table S1.** The ECD calculation results of **(+)-1**, **(−)-1** and **3**

1 For (+)-**1**

Gibbs free energies[a] and equilibrium populations[b] of low-energy conformers of (+)-**1**.

| Conformers | In MeOH | |
|---|---|---|
| | Δ*G* | *P* (%) |
| (+)-**1-1** | 0.00 | 49.8 |
| (+)-**1-2** | 0.85 | 11.9 |
| (+)-**1-3** | 0.96 | 9.8 |
| (+)-**1-4** | 1.36 | 5.0 |

[a]B3LYP/6-31+G(d,p), in kcal/mol. [b]From Δ*G* values at 298.15K.

Cartesian coordinates for the low-energy reoptimized MMFF conformers of (+)-**1** at B3LYP/6-311+G(d,p) level of theory in MeOH.

(+)-**1-1**

| (+)-**1-1** | | Standard Orientation (Ångstroms) | | | |
|---|---|---|---|---|---|
| No. | Atom | Type | X | Y | Z |
| 1. | 6. | 0. | -1.991691 | 2.269669 | 0.510516 |
| 2. | 6. | 0. | -1.346782 | 2.561846 | 1.711541 |
| 3. | 6. | 0. | -0.530331 | 1.611686 | 2.328147 |
| 4. | 6. | 0. | -0.371197 | 0.366865 | 1.718662 |
| 5. | 6. | 0. | -1.013429 | 0.045024 | 0.502222 |
| 6. | 6. | 0. | -1.834165 | 1.016559 | -0.097347 |
| 7. | 8. | 0. | -1.472713 | 3.769628 | 2.340665 |
| 8. | 8. | 0. | 0.402656 | -0.625970 | 2.243147 |
| 9. | 6. | 0. | 1.140441 | -0.378911 | 3.429483 |
| 10. | 6. | 0. | -2.573770 | 0.732213 | -1.386103 |
| 11. | 6. | 0. | -0.828621 | -1.327921 | -0.103446 |
| 12. | 6. | 0. | 0.398734 | -1.479300 | -1.059242 |
| 13. | 8. | 0. | 0.524896 | -0.297279 | -1.876408 |
| 14. | 6. | 0. | 1.705732 | 0.292131 | -1.591939 |
| 15. | 6. | 0. | 2.470309 | -0.377916 | -0.688788 |
| 16. | 6. | 0. | 1.749520 | -1.568917 | -0.309470 |
| 17. | 6. | 0. | 0.141764 | -2.688491 | -1.995948 |
| 18. | 8. | 0. | -0.340696 | -2.547972 | -3.107299 |
| 19. | 6. | 0. | 1.959752 | 1.562702 | -2.322105 |
| 20. | 8. | 0. | 2.077952 | -2.511649 | 0.406854 |
| 21. | 7. | 0. | 0.412052 | -3.880039 | -1.404594 |
| 22. | 1. | 0. | -2.628515 | 3.017216 | 0.042335 |
| 23. | 1. | 0. | -0.046513 | 1.866490 | 3.261731 |
| 24. | 1. | 0. | -2.073738 | 4.326345 | 1.828443 |
| 25. | 1. | 0. | 0.479081 | -0.182939 | 4.282764 |

| | | | | | |
|---|---|---|---|---|---|
| 26. | 1. | 0. | 1.714861 | -1.287287 | 3.613119 |
| 27. | 1. | 0. | 1.828184 | 0.466758 | 3.306319 |
| 28. | 1. | 0. | -1.902088 | 0.362996 | -2.165373 |
| 29. | 1. | 0. | -3.350495 | -0.028671 | -1.240691 |
| 30. | 1. | 0. | -3.067892 | 1.633795 | -1.757464 |
| 31. | 1. | 0. | -0.697934 | -2.079282 | 0.679438 |
| 32. | 1. | 0. | -1.717702 | -1.598517 | -0.677819 |
| 33. | 1. | 0. | 3.453418 | -0.093844 | -0.344108 |
| 34. | 1. | 0. | 1.895347 | 1.393443 | -3.401844 |
| 35. | 1. | 0. | 2.943118 | 1.965471 | -2.075975 |
| 36. | 1. | 0. | 1.192799 | 2.299096 | -2.059736 |
| 37. | 1. | 0. | 0.305478 | -4.710580 | -1.967746 |
| 38. | 1. | 0. | 0.995177 | -3.894452 | -0.571940 |

(+)-**1-2**

| (+)-**1-2** | | Standard Orientation (Ångstroms) | | | |
|---|---|---|---|---|---|
| No. | Atom | Type | X | Y | Z |
| 1. | 6. | 0. | -2.033861 | 2.290785 | 0.308437 |
| 2. | 6. | 0. | -1.306185 | 2.765224 | 1.398389 |
| 3. | 6. | 0. | -0.421191 | 1.925943 | 2.080184 |
| 4. | 6. | 0. | -0.275286 | 0.604594 | 1.647118 |
| 5. | 6. | 0. | -0.998064 | 0.102093 | 0.546379 |
| 6. | 6. | 0. | -1.890150 | 0.966570 | -0.119045 |
| 7. | 8. | 0. | -1.495315 | 4.069647 | 1.763230 |
| 8. | 8. | 0. | 0.562220 | -0.288593 | 2.249437 |
| 9. | 6. | 0. | 1.396764 | 0.141778 | 3.311012 |
| 10. | 6. | 0. | -2.722369 | 0.483944 | -1.286621 |
| 11. | 6. | 0. | -0.820560 | -1.340788 | 0.129626 |
| 12. | 6. | 0. | 0.332947 | -1.606120 | -0.890565 |
| 13. | 8. | 0. | 0.341930 | -0.564303 | -1.888294 |
| 14. | 6. | 0. | 1.513975 | 0.098978 | -1.800612 |
| 15. | 6. | 0. | 2.377335 | -0.397173 | -0.874046 |
| 16. | 6. | 0. | 1.742401 | -1.535221 | -0.255049 |
| 17. | 6. | 0. | 0.056487 | -2.956065 | -1.602853 |
| 18. | 8. | 0. | -0.511321 | -3.009147 | -2.680734 |
| 19. | 6. | 0. | 1.651258 | 1.247428 | -2.735479 |
| 20. | 8. | 0. | 2.168764 | -2.342400 | 0.567701 |
| 21. | 7. | 0. | 0.418301 | -4.029600 | -0.854386 |
| 22. | 1. | 0. | -2.717875 | 2.965195 | -0.195260 |
| 23. | 1. | 0. | 0.138106 | 2.301870 | 2.930246 |
| 24. | 1. | 0. | -0.949910 | 4.264120 | 2.536398 |

| | | | | | |
|---|---|---|---|---|---|
| 25. | 1. | 0. | 2.048724 | 0.968356 | 3.001309 |
| 26. | 1. | 0. | 0.811682 | 0.452582 | 4.186276 |
| 27. | 1. | 0. | 2.010636 | -0.720789 | 3.571683 |
| 28. | 1. | 0. | -2.105457 | 0.017856 | -2.059218 |
| 29. | 1. | 0. | -3.460733 | -0.262023 | -0.967543 |
| 30. | 1. | 0. | -3.272032 | 1.313525 | -1.738091 |
| 31. | 1. | 0. | -0.608578 | -1.969505 | 0.998066 |
| 32. | 1. | 0. | -1.742532 | -1.707233 | -0.327918 |
| 33. | 1. | 0. | 3.371997 | -0.032997 | -0.664047 |
| 34. | 1. | 0. | 1.502325 | 0.910904 | -3.766557 |
| 35. | 1. | 0. | 2.634060 | 1.711635 | -2.643613 |
| 36. | 1. | 0. | 0.878700 | 1.993115 | -2.519767 |
| 37. | 1. | 0. | 0.307606 | -4.941614 | -1.271985 |
| 38. | 1. | 0. | 1.066201 | -3.893568 | -0.082808 |

(+)-**1-3**

| (+)-**1-3** | | Standard Orientation (Ångstroms) | | | |
|---|---|---|---|---|---|
| No. | Atom | Type | X | Y | Z |
| 1. | 6. | 0. | -2.044562 | 2.703325 | 0.289526 |
| 2. | 6. | 0. | -1.238196 | 3.051972 | 1.369407 |
| 3. | 6. | 0. | -0.405645 | 2.102090 | 1.962866 |
| 4. | 6. | 0. | -0.373480 | 0.810183 | 1.437056 |
| 5. | 6. | 0. | -1.136295 | 0.445688 | 0.301413 |
| 6. | 6. | 0. | -2.012563 | 1.405850 | -0.241664 |
| 7. | 8. | 0. | -1.228987 | 4.307919 | 1.911386 |
| 8. | 8. | 0. | 0.372364 | -0.189358 | 2.004177 |
| 9. | 6. | 0. | 1.040335 | 0.076385 | 3.226311 |
| 10. | 6. | 0. | -2.987957 | 1.066816 | -1.348667 |
| 11. | 6. | 0. | -1.045930 | -0.973151 | -0.223313 |
| 12. | 6. | 0. | 0.133080 | -1.291228 | -1.177498 |
| 13. | 8. | 0. | 1.409028 | -0.973764 | -0.559910 |
| 14. | 6. | 0. | 2.121997 | -2.123254 | -0.417338 |
| 15. | 6. | 0. | 1.502339 | -3.229921 | -0.885842 |
| 16. | 6. | 0. | 0.200580 | -2.836641 | -1.405228 |
| 17. | 6. | 0. | 0.024312 | -0.558108 | -2.527003 |
| 18. | 8. | 0. | -0.983821 | -0.655716 | -3.210187 |
| 19. | 6. | 0. | 3.449713 | -1.951108 | 0.231489 |
| 20. | 8. | 0. | -0.699472 | -3.507179 | -1.870320 |
| 21. | 7. | 0. | 1.127079 | 0.141285 | -2.904265 |
| 22. | 1. | 0. | -2.722011 | 3.438881 | -0.138701 |
| 23. | 1. | 0. | 0.185110 | 2.395491 | 2.820091 |

| | | | | | |
|---|---|---|---|---|---|
| 24. | 1. | 0. | -1.852764 | 4.861006 | 1.422901 |
| 25. | 1. | 0. | 1.826497 | 0.832882 | 3.105573 |
| 26. | 1. | 0. | 0.343636 | 0.409343 | 4.005583 |
| 27. | 1. | 0. | 1.495184 | -0.867575 | 3.532136 |
| 28. | 1. | 0. | -3.727213 | 0.334888 | -1.000012 |
| 29. | 1. | 0. | -3.537102 | 1.958798 | -1.661297 |
| 30. | 1. | 0. | -2.501683 | 0.633206 | -2.224366 |
| 31. | 1. | 0. | -0.964397 | -1.665535 | 0.619361 |
| 32. | 1. | 0. | -1.938894 | -1.251189 | -0.786807 |
| 33. | 1. | 0. | 1.884688 | -4.239678 | -0.862948 |
| 34. | 1. | 0. | 4.076736 | -1.270418 | -0.355169 |
| 35. | 1. | 0. | 3.963032 | -2.908496 | 0.330790 |
| 36. | 1. | 0. | 3.323532 | -1.502689 | 1.222321 |
| 37. | 1. | 0. | 1.059803 | 0.688498 | -3.748822 |
| 38. | 1. | 0. | 1.860931 | 0.326500 | -2.240031 |

(+)-**1-4**

| (+)-**1-4** | | Standard Orientation (Ångstroms) | | | |
|---|---|---|---|---|---|
| No. | Atom | Type | X | Y | Z |
| 1. | 6. | 0. | -0.412104 | 3.014241 | -1.294474 |
| 2. | 6. | 0. | 0.104437 | 3.493630 | -0.093618 |
| 3. | 6. | 0. | 0.837101 | 2.652528 | 0.745177 |
| 4. | 6. | 0. | 1.018531 | 1.320167 | 0.372531 |
| 5. | 6. | 0. | 0.466124 | 0.795213 | -0.818880 |
| 6. | 6. | 0. | -0.227541 | 1.676993 | -1.671653 |
| 7. | 8. | 0. | -0.057641 | 4.788539 | 0.316608 |
| 8. | 8. | 0. | 1.756276 | 0.444363 | 1.125614 |
| 9. | 6. | 0. | 2.481027 | 0.948497 | 2.234859 |
| 10. | 6. | 0. | -0.737257 | 1.236974 | -3.026924 |
| 11. | 6. | 0. | 0.711077 | -0.651462 | -1.195867 |
| 12. | 6. | 0. | -0.227515 | -1.721501 | -0.583742 |
| 13. | 8. | 0. | 0.038205 | -1.878661 | 0.837691 |
| 14. | 6. | 0. | -1.107647 | -1.634904 | 1.527760 |
| 15. | 6. | 0. | -2.176582 | -1.346286 | 0.752129 |
| 16. | 6. | 0. | -1.747248 | -1.366643 | -0.635848 |
| 17. | 6. | 0. | 0.017300 | -3.066349 | -1.307479 |
| 18. | 8. | 0. | 0.009419 | -3.124233 | -2.525372 |
| 19. | 6. | 0. | -0.972179 | -1.727818 | 3.006355 |
| 20. | 8. | 0. | -2.387357 | -1.162582 | -1.651270 |
| 21. | 7. | 0. | 0.202108 | -4.142578 | -0.494465 |
| 22. | 1. | 0. | -0.952673 | 3.686436 | -1.957188 |

| | | | | | |
|---|---|---|---|---|---|
| 23. | 1. | 0. | 1.246296 | 3.061310 | 1.659409 |
| 24. | 1. | 0. | -0.576860 | 5.260753 | -0.347511 |
| 25. | 1. | 0. | 3.171052 | 1.748376 | 1.938658 |
| 26. | 1. | 0. | 1.815264 | 1.328978 | 3.020616 |
| 27. | 1. | 0. | 3.052386 | 0.105962 | 2.628301 |
| 28. | 1. | 0. | 0.097091 | 0.988879 | -3.695017 |
| 29. | 1. | 0. | -1.377019 | 0.354279 | -2.960558 |
| 30. | 1. | 0. | -1.306163 | 2.040457 | -3.501851 |
| 31. | 1. | 0. | 0.618523 | -0.786927 | -2.274157 |
| 32. | 1. | 0. | 1.729770 | -0.938927 | -0.916262 |
| 33. | 1. | 0. | -3.175832 | -1.116086 | 1.090516 |
| 34. | 1. | 0. | -0.649801 | -2.732942 | 3.300612 |
| 35. | 1. | 0. | -1.918076 | -1.500233 | 3.499599 |
| 36. | 1. | 0. | -0.205421 | -1.026593 | 3.351337 |
| 37. | 1. | 0. | 0.443366 | -5.016233 | -0.937195 |
| 38. | 1. | 0. | 0.399562 | -4.006616 | 0.483559 |

2 For (−)-**1**

Gibbs free energies[a] and equilibrium populations[b] of low-energy conformers of (−)-**1**.

| Conformers | In MeOH | |
|---|---|---|
| | Δ*G* | *P* (%) |
| **(−)-1-1** | 0 | 69.47 |
| **(−)-1-2** | 0.50 | 29.94 |
| **(−)-1-3** | 3.07 | 0.39 |
| **(−)-1-4** | 3.45 | 0.21 |

[a]B3LYP/6-31+G(d,p), in kcal/mol. [b]From Δ*G* values at 298.15K.

Cartesian coordinates for the low-energy reoptimized MMFF conformers of (−)-**1** at B3LYP/6-311+G(d,p) level of theory in MeOH.

**(−)-1-1**

| **(−)-1-1** | | Standard Orientation (Ångstroms) | | | |
|---|---|---|---|---|---|
| Center number | Atomic number | Atomic Type | X | Y | Z |
| 1. | 6. | 0. | 0.527477 | 3.013929 | 0.133792 |
| 2. | 6. | 0. | 0.091010 | 3.028713 | 1.457806 |
| 3. | 6. | 0. | 0.056075 | 1.850825 | 2.206769 |
| 4. | 6. | 0. | 0.463907 | 0.660340 | 1.604442 |
| 5. | 6. | 0. | 0.910859 | 0.617694 | 0.264963 |
| 6. | 6. | 0. | 0.941431 | 1.817442 | -0.467591 |
| 7. | 8. | 0. | -0.320155 | 4.172180 | 2.085339 |

| | | | | | |
|---|---|---|---|---|---|
| 8. | 8. | 0. | 0.467671 | -0.539455 | 2.252616 |
| 9. | 6. | 0. | -0.023693 | -0.613154 | 3.581485 |
| 10. | 6. | 0. | 1.433127 | 1.851288 | -1.897913 |
| 11. | 6. | 0. | 1.366842 | -0.694231 | -0.332373 |
| 12. | 6. | 0. | 0.243520 | -1.555444 | -0.995298 |
| 13. | 8. | 0. | -0.659674 | -0.696920 | -1.721993 |
| 14. | 6. | 0. | -1.883780 | -0.795666 | -1.161102 |
| 15. | 6. | 0. | -1.966536 | -1.683350 | -0.134310 |
| 16. | 6. | 0. | -0.661522 | -2.275673 | 0.032841 |
| 17. | 6. | 0. | 0.906154 | -2.526099 | -2.007401 |
| 18. | 8. | 0. | 0.997621 | -2.252988 | -3.192579 |
| 19. | 6. | 0. | -2.921006 | 0.078180 | -1.771515 |
| 20. | 8. | 0. | -0.279859 | -3.180816 | 0.770928 |
| 21. | 7. | 0. | 1.442227 | -3.622307 | -1.412807 |
| 22. | 1. | 0. | 0.553983 | 3.939270 | -0.437696 |
| 23. | 1. | 0. | -0.283634 | 1.894894 | 3.233043 |
| 24. | 1. | 0. | -0.230173 | 4.913451 | 1.472176 |
| 25. | 1. | 0. | 0.028060 | -1.667052 | 3.856150 |
| 26. | 1. | 0. | -1.064436 | -0.272297 | 3.644665 |
| 27. | 1. | 0. | 0.590565 | -0.022198 | 4.272391 |
| 28. | 1. | 0. | 0.917444 | 1.115776 | -2.520694 |
| 29. | 1. | 0. | 1.281313 | 2.840492 | -2.337602 |
| 30. | 1. | 0. | 2.505952 | 1.629869 | -1.956286 |
| 31. | 1. | 0. | 2.121260 | -0.505763 | -1.099780 |
| 32. | 1. | 0. | 1.822862 | -1.327422 | 0.432918 |
| 33. | 1. | 0. | -2.852994 | -1.930440 | 0.430608 |
| 34. | 1. | 0. | -3.891272 | -0.076549 | -1.297753 |
| 35. | 1. | 0. | -3.001907 | -0.129385 | -2.843438 |
| 36. | 1. | 0. | -2.630042 | 1.128293 | -1.662338 |
| 37. | 1. | 0. | 1.143657 | -3.866825 | -0.472241 |
| 38. | 1. | 0. | 1.856665 | -4.318603 | -2.014223 |

**(−)-1-2**

| **(−)-1-2** | | Standard Orientation (Ångstroms) | | | |
|---|---|---|---|---|---|
| Center number | Atom number | Type | X | Y | Z |
| 1. | 6. | 0. | 0.519048 | 3.033178 | 0.110080 |
| 2. | 6. | 0. | 0.096470 | 3.038329 | 1.438243 |
| 3. | 6. | 0. | 0.080814 | 1.855789 | 2.182415 |
| 4. | 6. | 0. | 0.491611 | 0.667815 | 1.570252 |
| 5. | 6. | 0. | 0.920981 | 0.636427 | 0.228173 |

| | | | | | |
|---|---|---|---|---|---|
| 6. | 6. | 0. | 0.935106 | 1.844049 | -0.498053 |
| 7. | 8. | 0. | -0.296203 | 4.235401 | 1.970412 |
| 8. | 8. | 0. | 0.512532 | -0.534311 | 2.215567 |
| 9. | 6. | 0. | 0.019291 | -0.624863 | 3.541134 |
| 10. | 6. | 0. | 1.415697 | 1.888887 | -1.931847 |
| 11. | 6. | 0. | 1.375407 | -0.670439 | -0.382258 |
| 12. | 6. | 0. | 0.247887 | -1.531878 | -1.036836 |
| 13. | 8. | 0. | -0.650612 | -0.672413 | -1.768257 |
| 14. | 6. | 0. | -1.874562 | -0.759108 | -1.206227 |
| 15. | 6. | 0. | -1.962421 | -1.640656 | -0.174169 |
| 16. | 6. | 0. | -0.661341 | -2.240467 | -0.003990 |
| 17. | 6. | 0. | 0.903492 | -2.514547 | -2.042127 |
| 18. | 8. | 0. | 0.990071 | -2.254928 | -3.230480 |
| 19. | 6. | 0. | -2.905490 | 0.119587 | -1.820134 |
| 20. | 8. | 0. | -0.285738 | -3.143640 | 0.739938 |
| 21. | 7. | 0. | 1.439706 | -3.605727 | -1.437632 |
| 22. | 1. | 0. | 0.526270 | 3.968850 | -0.438442 |
| 23. | 1. | 0. | -0.245285 | 1.869224 | 3.216930 |
| 24. | 1. | 0. | -0.545986 | 4.104179 | 2.894246 |
| 25. | 1. | 0. | 0.076906 | -1.681064 | 3.805578 |
| 26. | 1. | 0. | -1.024665 | -0.293011 | 3.606154 |
| 27. | 1. | 0. | 0.628296 | -0.038457 | 4.241311 |
| 28. | 1. | 0. | 0.897706 | 1.156403 | -2.556264 |
| 29. | 1. | 0. | 1.257730 | 2.881280 | -2.361209 |
| 30. | 1. | 0. | 2.488738 | 1.670879 | -1.998885 |
| 31. | 1. | 0. | 2.119003 | -0.474698 | -1.158395 |
| 32. | 1. | 0. | 1.843857 | -1.306410 | 0.373085 |
| 33. | 1. | 0. | -2.850514 | -1.879588 | 0.391753 |
| 34. | 1. | 0. | -3.877551 | -0.028344 | -1.347866 |
| 35. | 1. | 0. | -2.985701 | -0.089403 | -2.891800 |
| 36. | 1. | 0. | -2.608085 | 1.168095 | -1.712527 |
| 37. | 1. | 0. | 1.139319 | -3.841722 | -0.495453 |
| 38. | 1. | 0. | 1.846217 | -4.310699 | -2.034421 |

**(−)-1-3**

| **(−)-1-3** | | Standard Orientation (Ångstroms) | | | |
|---|---|---|---|---|---|
| Center number | Atom number | Type | X | Y | Z |
| 1. | 6. | 0. | 0.220555 | 3.391321 | 0.051091 |
| 2. | 6. | 0. | -0.260265 | 3.286662 | 1.353318 |
| 3. | 6. | 0. | -0.209062 | 2.065774 | 2.027424 |

| | | | | | |
|---|---|---|---|---|---|
| 4. | 6. | 0. | 0.302533 | 0.949798 | 1.364594 |
| 5. | 6. | 0. | 0.741062 | 1.014344 | 0.019994 |
| 6. | 6. | 0. | 0.733725 | 2.270528 | -0.617595 |
| 7. | 8. | 0. | -0.779516 | 4.350658 | 2.038532 |
| 8. | 8. | 0. | 0.439661 | -0.265501 | 1.982199 |
| 9. | 6. | 0. | 0.160052 | -0.353806 | 3.369496 |
| 10. | 6. | 0. | 1.332627 | 2.475978 | -1.992704 |
| 11. | 6. | 0. | 1.277047 | -0.239451 | -0.641269 |
| 12. | 6. | 0. | 0.231982 | -1.206961 | -1.252581 |
| 13. | 8. | 0. | -0.752348 | -1.610069 | -0.263423 |
| 14. | 6. | 0. | -0.648331 | -2.951971 | -0.066867 |
| 15. | 6. | 0. | 0.291716 | -3.559116 | -0.825689 |
| 16. | 6. | 0. | 0.942307 | -2.544282 | -1.641852 |
| 17. | 6. | 0. | -0.489402 | -0.611418 | -2.475460 |
| 18. | 8. | 0. | 0.146643 | -0.172114 | -3.421557 |
| 19. | 6. | 0. | -1.585039 | -3.502369 | 0.949475 |
| 20. | 8. | 0. | 1.867599 | -2.633948 | -2.424038 |
| 21. | 7. | 0. | -1.847133 | -0.661116 | -2.436183 |
| 22. | 1. | 0. | 0.216128 | 4.356529 | -0.450622 |
| 23. | 1. | 0. | -0.561596 | 2.023816 | 3.049128 |
| 24. | 1. | 0. | -0.745961 | 5.131542 | 1.470455 |
| 25. | 1. | 0. | 0.414080 | -1.373899 | 3.663344 |
| 26. | 1. | 0. | -0.900619 | -0.170320 | 3.584541 |
| 27. | 1. | 0. | 0.767440 | 0.350345 | 3.951504 |
| 28. | 1. | 0. | 0.915255 | 1.801613 | -2.742608 |
| 29. | 1. | 0. | 1.179758 | 3.505540 | -2.326714 |
| 30. | 1. | 0. | 2.415003 | 2.297645 | -1.972139 |
| 31. | 1. | 0. | 1.949838 | -0.002443 | -1.467936 |
| 32. | 1. | 0. | 1.850567 | -0.816050 | 0.089925 |
| 33. | 1. | 0. | 0.543185 | -4.609390 | -0.820051 |
| 34. | 1. | 0. | -1.441359 | -4.576746 | 1.072138 |
| 35. | 1. | 0. | -2.623367 | -3.313726 | 0.654578 |
| 36. | 1. | 0. | -1.425238 | -3.002888 | 1.910571 |
| 37. | 1. | 0. | -2.321136 | -0.877081 | -1.574362 |
| 38. | 1. | 0. | -2.347389 | -0.216430 | -3.190655 |

**(−)-1-4**

| **(−)-1-4** | | Standard Orientation (Ångstroms) | | | |
|---|---|---|---|---|---|
| Center number | Atom number | Type | X | Y | Z |
| 1. | 6. | 0. | -1.913611 | 2.637561 | -0.559618 |

| | | | | | |
|---|---|---|---|---|---|
| 2. | 6. | 0. | -1.981666 | 2.759826 | 0.825702 |
| 3. | 6. | 0. | -1.665050 | 1.676095 | 1.646130 |
| 4. | 6. | 0. | -1.254401 | 0.480543 | 1.055365 |
| 5. | 6. | 0. | -1.132309 | 0.342818 | -0.346875 |
| 6. | 6. | 0. | -1.504631 | 1.436091 | -1.154385 |
| 7. | 8. | 0. | -2.368733 | 3.914929 | 1.448005 |
| 8. | 8. | 0. | -0.962264 | -0.636925 | 1.793202 |
| 9. | 6. | 0. | -1.234292 | -0.620307 | 3.184460 |
| 10. | 6. | 0. | -1.533538 | 1.336717 | -2.664175 |
| 11. | 6. | 0. | -0.707735 | -0.982622 | -0.945157 |
| 12. | 6. | 0. | 0.810973 | -1.276265 | -1.034292 |
| 13. | 8. | 0. | 1.361879 | -1.515180 | 0.290571 |
| 14. | 6. | 0. | 2.362006 | -0.622464 | 0.517297 |
| 15. | 6. | 0. | 2.608069 | 0.215268 | -0.514779 |
| 16. | 6. | 0. | 1.674837 | -0.097284 | -1.583713 |
| 17. | 6. | 0. | 1.021520 | -2.529687 | -1.915737 |
| 18. | 8. | 0. | 0.496540 | -2.609786 | -3.013309 |
| 19. | 6. | 0. | 2.996933 | -0.730705 | 1.858329 |
| 20. | 8. | 0. | 1.551619 | 0.412296 | -2.682627 |
| 21. | 7. | 0. | 1.839706 | -3.482794 | -1.390808 |
| 22. | 1. | 0. | -2.194939 | 3.477496 | -1.190978 |
| 23. | 1. | 0. | -1.751421 | 1.795231 | 2.717909 |
| 24. | 1. | 0. | -2.559012 | 4.580636 | 0.774020 |
| 25. | 1. | 0. | -2.287003 | -0.388709 | 3.388983 |
| 26. | 1. | 0. | -0.603258 | 0.103499 | 3.716739 |
| 27. | 1. | 0. | -1.008516 | -1.624780 | 3.546640 |
| 28. | 1. | 0. | -2.300542 | 0.624235 | -2.992968 |
| 29. | 1. | 0. | -1.778282 | 2.305423 | -3.107466 |
| 30. | 1. | 0. | -0.578272 | 1.001543 | -3.074029 |
| 31. | 1. | 0. | -1.147376 | -1.804905 | -0.371477 |
| 32. | 1. | 0. | -1.067223 | -1.072095 | -1.971014 |
| 33. | 1. | 0. | 3.349446 | 0.999720 | -0.546325 |
| 34. | 1. | 0. | 3.774371 | 0.024066 | 1.983691 |
| 35. | 1. | 0. | 3.439160 | -1.723883 | 1.995443 |
| 36. | 1. | 0. | 2.238170 | -0.602480 | 2.637109 |
| 37. | 1. | 0. | 2.077988 | -3.458594 | -0.412725 |
| 38. | 1. | 0. | 1.930856 | -4.344529 | -1.907138 |

3 For 17*S*-**3**

Gibbs free energies[a] and equilibrium populations[b] of low-energy conformers of 17*S*-**3**.

| Conformers | In MeOH | |
|---|---|---|
| | $\Delta G$ | *P* (%) |
| 17*S*-**3**-1 | 0.19 | 29.48 |

| | | |
|---|---|---|
| 17*S*-**3**-2 | 0 | 40.44 |
| 17*S*-**3**-3 | 0.72 | 11.89 |
| 17*S*-**3**-4 | 0.83 | 10.00 |
| 17*S*-**3**-5 | 0.95 | 8.19 |

[a]B3LYP/6-31+G(d,p), in kcal/mol. [b]From Δ*G* values at 298.15K.

Cartesian coordinates for the low-energy reoptimized MMFF conformers of 17*S*-**3** at B3LYP/6-311+G(d,p) level of theory in MeOH.

17*S*-**3**-1

| 17*S*-**3**-1 | | Standard Orientation (Ångstroms) | | | |
|---|---|---|---|---|---|
| Center number | Atomic number | Atomic Type | X | Y | Z |
| 1. | 8. | 0. | -2.206597 | 1.269680 | 0.983157 |
| 2. | 6. | 0. | -1.425441 | 1.543059 | 2.058697 |
| 3. | 6. | 0. | -0.369781 | 0.754080 | 2.353670 |
| 4. | 6. | 0. | -0.084466 | -0.384730 | 1.526308 |
| 5. | 6. | 0. | -0.849247 | -0.671432 | 0.411638 |
| 6. | 6. | 0. | -1.973263 | 0.178806 | 0.106583 |
| 7. | 8. | 0. | -2.761274 | 0.078024 | -0.813783 |
| 8. | 6. | 0. | -0.633464 | -1.884353 | -0.489521 |
| 9. | 6. | 0. | 0.587612 | -1.859597 | -1.407118 |
| 10. | 6. | 0. | 0.556612 | -1.282011 | -2.691849 |
| 11. | 6. | 0. | 1.702135 | -1.304943 | -3.498466 |
| 12. | 6. | 0. | 2.878299 | -1.907741 | -3.059049 |
| 13. | 6. | 0. | 2.930319 | -2.506861 | -1.799570 |
| 14. | 6. | 0. | 1.789428 | -2.474283 | -1.002494 |
| 15. | 8. | 0. | 1.767244 | -3.054048 | 0.258695 |
| 16. | 6. | 0. | -0.706090 | -0.675276 | -3.258709 |
| 17. | 6. | 0. | 2.907996 | -3.784185 | 0.707908 |
| 18. | 8. | 0. | 4.017075 | -1.952038 | -3.812821 |
| 19. | 8. | 0. | 0.959306 | -1.112047 | 1.944096 |
| 20. | 6. | 0. | -1.868663 | 2.763332 | 2.805646 |
| 21. | 6. | 0. | -2.023977 | 4.022936 | 1.914577 |
| 22. | 8. | 0. | -3.172093 | 3.937092 | 1.085976 |
| 23. | 6. | 0. | -2.187894 | 5.279316 | 2.762080 |
| 24. | 1. | 0. | 0.263471 | 0.956849 | 3.207314 |
| 25. | 1. | 0. | -1.535798 | -1.977753 | -1.096572 |
| 26. | 1. | 0. | -0.582293 | -2.785604 | 0.130991 |
| 27. | 1. | 0. | 1.665321 | -0.854316 | -4.487965 |
| 28. | 1. | 0. | 3.853725 | -2.971581 | -1.481619 |

| | | | | | |
|---|---|---|---|---|---|
| 29. | 1. | 0. | -1.434635 | -1.457596 | -3.506039 |
| 30. | 1. | 0. | -0.490420 | -0.126838 | -4.179276 |
| 31. | 1. | 0. | -1.208956 | -0.004247 | -2.561166 |
| 32. | 1. | 0. | 3.787959 | -3.137877 | 0.798495 |
| 33. | 1. | 0. | 2.642006 | -4.177004 | 1.689875 |
| 34. | 1. | 0. | 3.128843 | -4.613353 | 0.028252 |
| 35. | 1. | 0. | 3.853716 | -1.503100 | -4.652725 |
| 36. | 1. | 0. | 1.160707 | -1.859957 | 1.337980 |
| 37. | 1. | 0. | -1.147601 | 2.953612 | 3.606606 |
| 38. | 1. | 0. | -2.844455 | 2.573723 | 3.272218 |
| 39. | 1. | 0. | -1.110685 | 4.123132 | 1.302678 |
| 40. | 1. | 0. | -3.126083 | 3.100625 | 0.599806 |
| 41. | 1. | 0. | -1.298880 | 5.464490 | 3.372829 |
| 42. | 1. | 0. | -3.056516 | 5.182937 | 3.421481 |
| 43. | 1. | 0. | -2.351203 | 6.142076 | 2.111186 |

17*S*-**3**-2

| 17*S*-**3**-2 | | Standard Orientation (Ångstroms) | | | |
|---|---|---|---|---|---|
| Center number | Atom number | Type | X | Y | Z |
| 1. | 8. | 0. | -1.137521 | 1.161110 | 1.973074 |
| 2. | 6. | 0. | -0.495048 | 2.279990 | 1.552106 |
| 3. | 6. | 0. | 0.021052 | 2.342455 | 0.305519 |
| 4. | 6. | 0. | -0.097161 | 1.207424 | -0.566506 |
| 5. | 6. | 0. | -0.737603 | 0.052694 | -0.158844 |
| 6. | 6. | 0. | -1.328188 | 0.017246 | 1.155909 |
| 7. | 8. | 0. | -1.980917 | -0.875543 | 1.660982 |
| 8. | 6. | 0. | -0.958983 | -1.164756 | -1.052192 |
| 9. | 6. | 0. | 0.250843 | -2.057445 | -1.322775 |
| 10. | 6. | 0. | 0.607302 | -3.125413 | -0.475732 |
| 11. | 6. | 0. | 1.718122 | -3.922537 | -0.782270 |
| 12. | 6. | 0. | 2.476306 | -3.688428 | -1.926841 |
| 13. | 6. | 0. | 2.131946 | -2.651632 | -2.795369 |
| 14. | 6. | 0. | 1.029507 | -1.861738 | -2.480912 |
| 15. | 8. | 0. | 0.624243 | -0.820379 | -3.304671 |
| 16. | 6. | 0. | -0.211519 | -3.477137 | 0.744818 |
| 17. | 6. | 0. | 1.302948 | -0.609778 | -4.542163 |
| 18. | 8. | 0. | 3.567202 | -4.439795 | -2.262151 |
| 19. | 8. | 0. | 0.446776 | 1.390983 | -1.776194 |
| 20. | 6. | 0. | -0.462876 | 3.358728 | 2.590628 |
| 21. | 6. | 0. | -1.857988 | 3.716637 | 3.165840 |

| | | | | | |
|---|---|---|---|---|---|
| 22. | 8. | 0. | -2.342464 | 2.700687 | 4.028884 |
| 23. | 6. | 0. | -1.801670 | 4.999757 | 3.986687 |
| 24. | 1. | 0. | 0.529712 | 3.229065 | -0.049420 |
| 25. | 1. | 0. | -1.365660 | -0.832005 | -2.013377 |
| 26. | 1. | 0. | -1.741158 | -1.756929 | -0.573636 |
| 27. | 1. | 0. | 1.983363 | -4.743326 | -0.119379 |
| 28. | 1. | 0. | 2.733010 | -2.492309 | -3.680176 |
| 29. | 1. | 0. | -0.440363 | -2.612650 | 1.369460 |
| 30. | 1. | 0. | 0.306003 | -4.222513 | 1.354115 |
| 31. | 1. | 0. | -1.178603 | -3.905539 | 0.453213 |
| 32. | 1. | 0. | 1.236288 | -1.499402 | -5.176505 |
| 33. | 1. | 0. | 0.790026 | 0.222857 | -5.024830 |
| 34. | 1. | 0. | 2.355037 | -0.348938 | -4.383099 |
| 35. | 1. | 0. | 3.701508 | -5.115668 | -1.584787 |
| 36. | 1. | 0. | 0.408057 | 0.578043 | -2.328714 |
| 37. | 1. | 0. | 0.002001 | 4.244933 | 2.147531 |
| 38. | 1. | 0. | 0.163536 | 3.038771 | 3.433871 |
| 39. | 1. | 0. | -2.548443 | 3.866836 | 2.317828 |
| 40. | 1. | 0. | -2.318128 | 1.862462 | 3.544078 |
| 41. | 1. | 0. | -1.516529 | 5.855021 | 3.366278 |
| 42. | 1. | 0. | -1.079069 | 4.898704 | 4.803000 |
| 43. | 1. | 0. | -2.782896 | 5.197454 | 4.425721 |

17*S*-**3**-3

| **17*S*-3**-3 | | Standard Orientation (Ångstroms) | | | |
|---|---|---|---|---|---|
| Center number | Atom number | Type | X | Y | Z |
| 1. | 8. | 0. | -0.853112 | 2.717816 | 0.221278 |
| 2. | 6. | 0. | -0.345587 | 2.594654 | 1.468453 |
| 3. | 6. | 0. | 0.627015 | 1.692856 | 1.737792 |
| 4. | 6. | 0. | 1.134963 | 0.867738 | 0.676492 |
| 5. | 6. | 0. | 0.628713 | 0.964172 | -0.604235 |
| 6. | 6. | 0. | -0.399437 | 1.944432 | -0.872503 |
| 7. | 8. | 0. | -0.924369 | 2.190691 | -1.941351 |
| 8. | 6. | 0. | 1.149677 | 0.162534 | -1.793724 |
| 9. | 6. | 0. | 0.778392 | -1.318256 | -1.848165 |
| 10. | 6. | 0. | -0.411574 | -1.777485 | -2.446850 |
| 11. | 6. | 0. | -0.694488 | -3.149438 | -2.482506 |
| 12. | 6. | 0. | 0.193515 | -4.080064 | -1.948824 |
| 13. | 6. | 0. | 1.390936 | -3.654679 | -1.371661 |
| 14. | 6. | 0. | 1.661601 | -2.289487 | -1.335163 |

| | | | | | |
|---|---|---|---|---|---|
| 15. | 8. | 0. | 2.836915 | -1.796934 | -0.784673 |
| 16. | 6. | 0. | -1.383545 | -0.829754 | -3.111596 |
| 17. | 6. | 0. | 3.827336 | -2.716090 | -0.326059 |
| 18. | 8. | 0. | -0.043277 | -5.425775 | -1.961945 |
| 19. | 8. | 0. | 2.117307 | 0.038250 | 1.052679 |
| 20. | 6. | 0. | -1.025732 | 3.483796 | 2.462575 |
| 21. | 6. | 0. | -2.364674 | 2.884626 | 2.961612 |
| 22. | 8. | 0. | -2.141281 | 1.676361 | 3.679864 |
| 23. | 6. | 0. | -3.084758 | 3.833780 | 3.909404 |
| 24. | 1. | 0. | 1.045640 | 1.597775 | 2.731313 |
| 25. | 1. | 0. | 0.768309 | 0.660101 | -2.687076 |
| 26. | 1. | 0. | 2.241073 | 0.248281 | -1.831608 |
| 27. | 1. | 0. | -1.617519 | -3.490455 | -2.946452 |
| 28. | 1. | 0. | 2.066703 | -4.396737 | -0.968612 |
| 29. | 1. | 0. | -1.610652 | 0.047908 | -2.505023 |
| 30. | 1. | 0. | -2.318494 | -1.342808 | -3.351393 |
| 31. | 1. | 0. | -0.968541 | -0.448369 | -4.053169 |
| 32. | 1. | 0. | 3.453668 | -3.327703 | 0.502512 |
| 33. | 1. | 0. | 4.159973 | -3.365455 | -1.142117 |
| 34. | 1. | 0. | 4.662456 | -2.105745 | 0.019437 |
| 35. | 1. | 0. | -0.898159 | -5.588533 | -2.381874 |
| 36. | 1. | 0. | 2.406707 | -0.550983 | 0.320337 |
| 37. | 1. | 0. | -1.213197 | 4.456432 | 1.995109 |
| 38. | 1. | 0. | -0.372126 | 3.632930 | 3.327626 |
| 39. | 1. | 0. | -3.001424 | 2.696850 | 2.082371 |
| 40. | 1. | 0. | -1.678961 | 1.062315 | 3.091902 |
| 41. | 1. | 0. | -3.331792 | 4.774047 | 3.407517 |
| 42. | 1. | 0. | -2.456980 | 4.052739 | 4.779237 |
| 43. | 1. | 0. | -4.010221 | 3.373665 | 4.265071 |

17*S*-**3**-4

| 17*S*-**3**-4 | | Standard Orientation (Ångstroms) | | | |
|---|---|---|---|---|---|
| Center number | Atom number | Type | X | Y | Z |
| 1. | 8. | 0. | -0.043867 | 2.578582 | -0.579766 |
| 2. | 6. | 0. | -0.100782 | 2.685732 | 0.767017 |
| 3. | 6. | 0. | -0.400998 | 1.614631 | 1.538034 |
| 4. | 6. | 0. | -0.633072 | 0.341234 | 0.913659 |
| 5. | 6. | 0. | -0.556032 | 0.196438 | -0.456902 |
| 6. | 6. | 0. | -0.274612 | 1.362398 | -1.263821 |
| 7. | 8. | 0. | -0.216367 | 1.424511 | -2.476806 |

| | | | | | |
|---|---|---|---|---|---|
| 8. | 6. | 0. | -0.842241 | -1.106898 | -1.197254 |
| 9. | 6. | 0. | 0.216463 | -2.204281 | -1.108345 |
| 10. | 6. | 0. | 1.298830 | -2.285048 | -2.006731 |
| 11. | 6. | 0. | 2.231242 | -3.324463 | -1.889424 |
| 12. | 6. | 0. | 2.099736 | -4.299458 | -0.903749 |
| 13. | 6. | 0. | 1.024052 | -4.257106 | -0.015508 |
| 14. | 6. | 0. | 0.105739 | -3.217513 | -0.135034 |
| 15. | 8. | 0. | -0.991657 | -3.117262 | 0.709184 |
| 16. | 6. | 0. | 1.460582 | -1.304144 | -3.145267 |
| 17. | 6. | 0. | -1.228102 | -4.149188 | 1.665962 |
| 18. | 8. | 0. | 2.985934 | -5.328784 | -0.753623 |
| 19. | 8. | 0. | -0.931725 | -0.642055 | 1.773129 |
| 20. | 6. | 0. | 0.117895 | 4.086637 | 1.247701 |
| 21. | 6. | 0. | -1.162426 | 4.951391 | 1.127823 |
| 22. | 8. | 0. | -2.190118 | 4.453032 | 1.977150 |
| 23. | 6. | 0. | -0.906431 | 6.392736 | 1.545872 |
| 24. | 1. | 0. | -0.444150 | 1.693211 | 2.616595 |
| 25. | 1. | 0. | -0.990167 | -0.836195 | -2.244150 |
| 26. | 1. | 0. | -1.795076 | -1.515673 | -0.843649 |
| 27. | 1. | 0. | 3.063012 | -3.374602 | -2.588832 |
| 28. | 1. | 0. | 0.941144 | -5.028242 | 0.738352 |
| 29. | 1. | 0. | 0.699913 | -1.478298 | -3.916751 |
| 30. | 1. | 0. | 2.438738 | -1.421783 | -3.618758 |
| 31. | 1. | 0. | 1.343598 | -0.264681 | -2.836102 |
| 32. | 1. | 0. | -1.355565 | -5.116146 | 1.168934 |
| 33. | 1. | 0. | -0.412774 | -4.214284 | 2.394830 |
| 34. | 1. | 0. | -2.152194 | -3.875640 | 2.176409 |
| 35. | 1. | 0. | 3.680331 | -5.242864 | -1.420014 |
| 36. | 1. | 0. | -1.027578 | -1.511852 | 1.323862 |
| 37. | 1. | 0. | 0.920945 | 4.540836 | 0.657328 |
| 38. | 1. | 0. | 0.424529 | 4.069264 | 2.298102 |
| 39. | 1. | 0. | -1.489101 | 4.930372 | 0.075985 |
| 40. | 1. | 0. | -2.362641 | 3.534329 | 1.726947 |
| 41. | 1. | 0. | -0.154202 | 6.858637 | 0.902363 |
| 42. | 1. | 0. | -0.556968 | 6.432245 | 2.582623 |
| 43. | 1. | 0. | -1.831836 | 6.970242 | 1.476624 |

17*S*-**3**-5

| 17*S*-**3**-5 | | Standard Orientation (Ångstroms) | | | |
|---|---|---|---|---|---|
| Center number | Atom number | Type | X | Y | Z |

| | | | | | |
|---|---|---|---|---|---|
| 1. | 8. | 0. | -1.708292 | 1.525678 | 1.807572 |
| 2. | 6. | 0. | -1.047273 | 2.628742 | 1.372611 |
| 3. | 6. | 0. | -0.461677 | 2.638381 | 0.155751 |
| 4. | 6. | 0. | -0.551532 | 1.475413 | -0.682170 |
| 5. | 6. | 0. | -1.196300 | 0.330759 | -0.253748 |
| 6. | 6. | 0. | -1.818362 | 0.332963 | 1.047374 |
| 7. | 8. | 0. | -2.437338 | -0.566124 | 1.582936 |
| 8. | 6. | 0. | -1.366627 | -0.927000 | -1.101514 |
| 9. | 6. | 0. | -0.123001 | -1.784868 | -1.327620 |
| 10. | 6. | 0. | 0.269181 | -2.798819 | -0.431325 |
| 11. | 6. | 0. | 1.410012 | -3.567378 | -0.697812 |
| 12. | 6. | 0. | 2.163130 | -3.359120 | -1.850766 |
| 13. | 6. | 0. | 1.784640 | -2.376585 | -2.766890 |
| 14. | 6. | 0. | 0.653210 | -1.613705 | -2.491292 |
| 15. | 8. | 0. | 0.215254 | -0.623571 | -3.360096 |
| 16. | 6. | 0. | -0.542020 | -3.124624 | 0.801388 |
| 17. | 6. | 0. | 0.885311 | -0.448483 | -4.607855 |
| 18. | 8. | 0. | 3.281722 | -4.084944 | -2.148916 |
| 19. | 8. | 0. | 0.031069 | 1.621507 | -1.878994 |
| 20. | 6. | 0. | -1.068546 | 3.748882 | 2.367687 |
| 21. | 6. | 0. | -0.601503 | 3.357944 | 3.795504 |
| 22. | 8. | 0. | -1.576004 | 2.576534 | 4.469563 |
| 23. | 6. | 0. | 0.778307 | 2.694050 | 3.818997 |
| 24. | 1. | 0. | 0.068935 | 3.508918 | -0.206796 |
| 25. | 1. | 0. | -1.776737 | -0.647040 | -2.077851 |
| 26. | 1. | 0. | -2.131112 | -1.528252 | -0.606010 |
| 27. | 1. | 0. | 1.702672 | -4.346256 | 0.003035 |
| 28. | 1. | 0. | 2.383103 | -2.235857 | -3.656647 |
| 29. | 1. | 0. | -0.817281 | -2.240518 | 1.377888 |
| 30. | 1. | 0. | 0.004712 | -3.811868 | 1.452152 |
| 31. | 1. | 0. | -1.485403 | -3.613143 | 0.526877 |
| 32. | 1. | 0. | 0.849396 | -1.369159 | -5.198851 |
| 33. | 1. | 0. | 0.343060 | 0.341685 | -5.128338 |
| 34. | 1. | 0. | 1.927757 | -0.143520 | -4.464291 |
| 35. | 1. | 0. | 3.438164 | -4.723640 | -1.440916 |
| 36. | 1. | 0. | -0.004682 | 0.798065 | -2.415531 |
| 37. | 1. | 0. | -2.094585 | 4.127321 | 2.457663 |
| 38. | 1. | 0. | -0.447854 | 4.563311 | 1.980848 |
| 39. | 1. | 0. | -0.548337 | 4.292422 | 4.367002 |
| 40. | 1. | 0. | -1.763469 | 1.803462 | 3.916326 |
| 41. | 1. | 0. | 1.540972 | 3.336476 | 3.364751 |
| 42. | 1. | 0. | 0.769545 | 1.743296 | 3.275517 |
| 43. | 1. | 0. | 1.067784 | 2.488667 | 4.852784 |

4 For 17*R*-**3**

Gibbs free energies[a] and equilibrium populations[b] of low-energy conformers of 17*R*-**3**.

| Conformers | In MeOH | |
|---|---|---|
| | Δ*G* | *P* (%) |
| 17*R*-**3**-1 | 0.19 | 29.53 |
| 17*R*-**3**-2 | 0 | 40.46 |
| 17*R*-**3**-3 | 0.73 | 11.86 |
| 17*R*-**3**-4 | 0.83 | 9.97 |
| 17*R*-**3**-5 | 0.95 | 8.17 |

[a]B3LYP/6-31G(d,p), in kcal/mol. [b]From Δ*G* values at 298.15K.

Gibbs free energies[a] and equilibrium populations[b] of low-energy conformers of 17*R*-**3** in MeOH.

17*R*-**3**-1

| 17*R*-**3**-1 | | Standard Orientation (Ångstroms) | | | |
|---|---|---|---|---|---|
| Center number | Atomic number | Atomic Type | X | Y | Z |
| 1. | 8. | 0. | -1.247813 | 2.298546 | 0.779738 |
| 2. | 6. | 0. | -0.379228 | 2.916237 | -0.060351 |
| 3. | 6. | 0. | 0.167695 | 2.240758 | -1.094047 |
| 4. | 6. | 0. | -0.184308 | 0.864444 | -1.305419 |
| 5. | 6. | 0. | -1.047120 | 0.205119 | -0.450771 |
| 6. | 6. | 0. | -1.624113 | 0.936846 | 0.649693 |
| 7. | 8. | 0. | -2.406213 | 0.534597 | 1.489167 |
| 8. | 6. | 0. | -1.499735 | -1.240986 | -0.634296 |
| 9. | 6. | 0. | -0.471864 | -2.332879 | -0.342979 |
| 10. | 6. | 0. | -0.281472 | -2.867707 | 0.946509 |
| 11. | 6. | 0. | 0.662785 | -3.882364 | 1.152055 |
| 12. | 6. | 0. | 1.413309 | -4.390361 | 0.094482 |
| 13. | 6. | 0. | 1.229403 | -3.894173 | -1.196996 |
| 14. | 6. | 0. | 0.293380 | -2.882160 | -1.391134 |
| 15. | 8. | 0. | 0.054408 | -2.344803 | -2.648666 |
| 16. | 6. | 0. | -1.111890 | -2.413248 | 2.124538 |
| 17. | 6. | 0. | 0.712224 | -2.909613 | -3.781997 |
| 18. | 8. | 0. | 2.343890 | -5.378524 | 0.250992 |
| 19. | 8. | 0. | 0.388715 | 0.316560 | -2.384532 |
| 20. | 6. | 0. | -0.128711 | 4.346101 | 0.308689 |
| 21. | 6. | 0. | 0.308354 | 4.546600 | 1.783009 |
| 22. | 8. | 0. | -0.774805 | 4.355019 | 2.678586 |
| 23. | 6. | 0. | 0.824735 | 5.961779 | 2.015887 |
| 24. | 1. | 0. | 0.861592 | 2.717398 | -1.773863 |

| | | | | | |
|---|---|---|---|---|---|
| 25. | 1. | 0. | -1.865115 | -1.373520 | -1.658423 |
| 26. | 1. | 0. | -2.361785 | -1.376441 | 0.021430 |
| 27. | 1. | 0. | 0.800927 | -4.285917 | 2.152852 |
| 28. | 1. | 0. | 1.821395 | -4.306713 | -2.002659 |
| 29. | 1. | 0. | -1.184756 | -1.327798 | 2.203334 |
| 30. | 1. | 0. | -0.702549 | -2.806007 | 3.058845 |
| 31. | 1. | 0. | -2.141933 | -2.781187 | 2.037457 |
| 32. | 1. | 0. | 0.338508 | -2.360666 | -4.647053 |
| 33. | 1. | 0. | 1.799323 | -2.791198 | -3.715294 |
| 34. | 1. | 0. | 0.463259 | -3.970586 | -3.884845 |
| 35. | 1. | 0. | 2.378673 | -5.630421 | 1.183197 |
| 36. | 1. | 0. | 0.166691 | -0.636536 | -2.482774 |
| 37. | 1. | 0. | -1.046976 | 4.929702 | 0.160364 |
| 38. | 1. | 0. | 0.632715 | 4.744826 | -0.368740 |
| 39. | 1. | 0. | 1.121049 | 3.831316 | 1.998566 |
| 40. | 1. | 0. | -1.169509 | 3.491416 | 2.487420 |
| 41. | 1. | 0. | 0.055321 | 6.695507 | 1.754636 |
| 42. | 1. | 0. | 1.720221 | 6.160384 | 1.418973 |
| 43. | 1. | 0. | 1.072322 | 6.092654 | 3.072422 |

17*R*-**3**-2

| 17*R*-**3**-2 | | Standard Orientation (Ångstroms) | | | |
|---|---|---|---|---|---|
| Center number | Atom number | Type | X | Y | Z |
| 1. | 8. | 0. | 0.502403 | 2.505475 | -0.075758 |
| 2. | 6. | 0. | 0.883874 | 2.363426 | 1.218900 |
| 3. | 6. | 0. | 0.515022 | 1.271597 | 1.923244 |
| 4. | 6. | 0. | -0.268242 | 0.250300 | 1.285958 |
| 5. | 6. | 0. | -0.661239 | 0.365867 | -0.033868 |
| 6. | 6. | 0. | -0.303986 | 1.559448 | -0.759394 |
| 7. | 8. | 0. | -0.611456 | 1.867188 | -1.894711 |
| 8. | 6. | 0. | -1.548361 | -0.645256 | -0.754927 |
| 9. | 6. | 0. | -0.900615 | -1.963886 | -1.173788 |
| 10. | 6. | 0. | -0.239627 | -2.123418 | -2.407790 |
| 11. | 6. | 0. | 0.322242 | -3.361341 | -2.747122 |
| 12. | 6. | 0. | 0.226699 | -4.453242 | -1.887869 |
| 13. | 6. | 0. | -0.442583 | -4.329453 | -0.669426 |
| 14. | 6. | 0. | -0.993940 | -3.094763 | -0.338147 |
| 15. | 8. | 0. | -1.681890 | -2.903102 | 0.852333 |
| 16. | 6. | 0. | -0.159276 | -1.000143 | -3.415607 |
| 17. | 6. | 0. | -1.899563 | -4.018406 | 1.715516 |

| | | | | | |
|---|---|---|---|---|---|
| 18. | 8. | 0. | 0.761340 | -5.676641 | -2.178547 |
| 19. | 8. | 0. | -0.576643 | -0.778242 | 2.085913 |
| 20. | 6. | 0. | 1.696913 | 3.518616 | 1.716630 |
| 21. | 6. | 0. | 1.025029 | 4.898940 | 1.496387 |
| 22. | 8. | 0. | 1.053438 | 5.280853 | 0.130754 |
| 23. | 6. | 0. | 1.748512 | 5.992806 | 2.273210 |
| 24. | 1. | 0. | 0.803648 | 1.145486 | 2.958415 |
| 25. | 1. | 0. | -1.932582 | -0.137400 | -1.641458 |
| 26. | 1. | 0. | -2.416181 | -0.870333 | -0.125463 |
| 27. | 1. | 0. | 0.830966 | -3.470957 | -3.702452 |
| 28. | 1. | 0. | -0.507843 | -5.192631 | -0.021192 |
| 29. | 1. | 0. | -1.143882 | -0.804893 | -3.858581 |
| 30. | 1. | 0. | 0.520044 | -1.261968 | -4.230848 |
| 31. | 1. | 0. | 0.167305 | -0.055897 | -2.977849 |
| 32. | 1. | 0. | -2.485828 | -3.637023 | 2.552285 |
| 33. | 1. | 0. | -2.462792 | -4.802787 | 1.199972 |
| 34. | 1. | 0. | -0.954027 | -4.427999 | 2.087570 |
| 35. | 1. | 0. | 1.196900 | -5.630855 | -3.039856 |
| 36. | 1. | 0. | -1.057398 | -1.490538 | 1.607262 |
| 37. | 1. | 0. | 2.662667 | 3.540616 | 1.194454 |
| 38. | 1. | 0. | 1.897082 | 3.361270 | 2.781045 |
| 39. | 1. | 0. | -0.015416 | 4.833750 | 1.859244 |
| 40. | 1. | 0. | 0.660717 | 4.562520 | -0.386951 |
| 41. | 1. | 0. | 2.800701 | 6.040520 | 1.974286 |
| 42. | 1. | 0. | 1.695335 | 5.814430 | 3.351656 |
| 43. | 1. | 0. | 1.290533 | 6.961068 | 2.055569 |

17*R*-**3**-3

| 17*R*-**3**-3 | | Standard Orientation (Ångstroms) | | | |
|---|---|---|---|---|---|
| Center number | Atom number | Type | X | Y | Z |
| 1. | 8. | 0. | 0.022365 | 2.857073 | 0.010002 |
| 2. | 6. | 0. | 0.296917 | 2.678278 | 1.321815 |
| 3. | 6. | 0. | -0.087482 | 1.551625 | 1.965730 |
| 4. | 6. | 0. | -0.810963 | 0.540972 | 1.244380 |
| 5. | 6. | 0. | -1.096305 | 0.691554 | -0.097915 |
| 6. | 6. | 0. | -0.689134 | 1.909408 | -0.762005 |
| 7. | 8. | 0. | -0.892354 | 2.223220 | -1.919095 |
| 8. | 6. | 0. | -1.903586 | -0.309572 | -0.919470 |
| 9. | 6. | 0. | -1.208317 | -1.615642 | -1.299390 |
| 10. | 6. | 0. | -0.429697 | -1.745541 | -2.466528 |

| | | | | | |
|---|---|---|---|---|---|
| 11. | 6. | 0. | 0.172984 | -2.972539 | -2.774461 |
| 12. | 6. | 0. | 0.002265 | -4.083164 | -1.951785 |
| 13. | 6. | 0. | -0.783831 | -3.989233 | -0.802386 |
| 14. | 6. | 0. | -1.374272 | -2.765018 | -0.500697 |
| 15. | 8. | 0. | -2.175696 | -2.602442 | 0.621043 |
| 16. | 6. | 0. | -0.264373 | -0.603149 | -3.442445 |
| 17. | 6. | 0. | -2.471123 | -3.737543 | 1.433675 |
| 18. | 8. | 0. | 0.571997 | -5.297127 | -2.214239 |
| 19. | 8. | 0. | -1.168445 | -0.512095 | 1.991255 |
| 20. | 6. | 0. | 1.105756 | 3.795873 | 1.903374 |
| 21. | 6. | 0. | 2.614602 | 3.653738 | 1.580902 |
| 22. | 8. | 0. | 3.154350 | 2.486974 | 2.191660 |
| 23. | 6. | 0. | 3.414315 | 4.837025 | 2.108177 |
| 24. | 1. | 0. | 0.118830 | 1.407871 | 3.018413 |
| 25. | 1. | 0. | -2.203297 | 0.213922 | -1.828986 |
| 26. | 1. | 0. | -2.826395 | -0.551520 | -0.381122 |
| 27. | 1. | 0. | 0.772813 | -3.058783 | -3.677948 |
| 28. | 1. | 0. | -0.905641 | -4.866904 | -0.182211 |
| 29. | 1. | 0. | -1.196880 | -0.428025 | -3.993812 |
| 30. | 1. | 0. | 0.510803 | -0.834077 | -4.177722 |
| 31. | 1. | 0. | -0.018198 | 0.342943 | -2.958600 |
| 32. | 1. | 0. | -1.564557 | -4.152221 | 1.887999 |
| 33. | 1. | 0. | -3.138948 | -3.377074 | 2.216864 |
| 34. | 1. | 0. | -2.976519 | -4.511840 | 0.847746 |
| 35. | 1. | 0. | 1.088709 | -5.230405 | -3.028001 |
| 36. | 1. | 0. | -1.612790 | -1.210452 | 1.460097 |
| 37. | 1. | 0. | 0.986145 | 3.806739 | 2.991184 |
| 38. | 1. | 0. | 0.734923 | 4.745154 | 1.502083 |
| 39. | 1. | 0. | 2.724355 | 3.600076 | 0.485982 |
| 40. | 1. | 0. | 2.652908 | 1.724273 | 1.870201 |
| 41. | 1. | 0. | 3.297956 | 4.922384 | 3.193456 |
| 42. | 1. | 0. | 3.082832 | 5.770544 | 1.643765 |
| 43. | 1. | 0. | 4.475976 | 4.695721 | 1.890015 |

17*R*-**3**-4

| 17*R*-**3**-4 | | Standard Orientation (Ångstroms) | | | |
|---|---|---|---|---|---|
| Center number | Atom number | Type | X | Y | Z |
| 1. | 8. | 0. | -1.596949 | 1.915330 | 0.876462 |
| 2. | 6. | 0. | -0.787570 | 2.679418 | 0.108594 |
| 3. | 6. | 0. | 0.038889 | 2.117740 | -0.804277 |

| | | | | | |
|---|---|---|---|---|---|
| 4. | 6. | 0. | 0.074175 | 0.687050 | -0.935142 |
| 5. | 6. | 0. | -0.721748 | -0.119218 | -0.146613 |
| 6. | 6. | 0. | -1.626742 | 0.503805 | 0.792854 |
| 7. | 8. | 0. | -2.424600 | -0.047596 | 1.526314 |
| 8. | 6. | 0. | -0.781539 | -1.639587 | -0.263349 |
| 9. | 6. | 0. | 0.407977 | -2.426480 | 0.283332 |
| 10. | 6. | 0. | 0.489298 | -2.836047 | 1.628984 |
| 11. | 6. | 0. | 1.596367 | -3.571945 | 2.072145 |
| 12. | 6. | 0. | 2.620639 | -3.925515 | 1.197317 |
| 13. | 6. | 0. | 2.554211 | -3.553338 | -0.146159 |
| 14. | 6. | 0. | 1.453922 | -2.816942 | -0.576765 |
| 15. | 8. | 0. | 1.318830 | -2.419541 | -1.899965 |
| 16. | 6. | 0. | -0.621128 | -2.551292 | 2.614115 |
| 17. | 6. | 0. | 2.288197 | -2.847317 | -2.855756 |
| 18. | 8. | 0. | 3.717512 | -4.641012 | 1.587618 |
| 19. | 8. | 0. | 0.919745 | 0.245401 | -1.875726 |
| 20. | 6. | 0. | -0.984665 | 4.145748 | 0.337596 |
| 21. | 6. | 0. | -2.218629 | 4.694509 | -0.422393 |
| 22. | 8. | 0. | -2.033695 | 4.588245 | -1.829653 |
| 23. | 6. | 0. | -2.453852 | 6.167835 | -0.119485 |
| 24. | 1. | 0. | 0.691822 | 2.723714 | -1.418933 |
| 25. | 1. | 0. | -0.922046 | -1.910879 | -1.315343 |
| 26. | 1. | 0. | -1.687240 | -1.949793 | 0.260700 |
| 27. | 1. | 0. | 1.647398 | -3.880992 | 3.113976 |
| 28. | 1. | 0. | 3.359730 | -3.843764 | -0.806931 |
| 29. | 1. | 0. | -0.964063 | -1.516208 | 2.586870 |
| 30. | 1. | 0. | -0.302764 | -2.789125 | 3.632399 |
| 31. | 1. | 0. | -1.501433 | -3.168140 | 2.393442 |
| 32. | 1. | 0. | 2.328713 | -3.940189 | -2.903505 |
| 33. | 1. | 0. | 1.954579 | -2.451353 | -3.815570 |
| 34. | 1. | 0. | 3.282786 | -2.451656 | -2.622327 |
| 35. | 1. | 0. | 3.646624 | -4.830969 | 2.532360 |
| 36. | 1. | 0. | 0.965871 | -0.736821 | -1.902273 |
| 37. | 1. | 0. | -0.099513 | 4.691460 | -0.003538 |
| 38. | 1. | 0. | -1.110367 | 4.321315 | 1.411422 |
| 39. | 1. | 0. | -3.098897 | 4.113015 | -0.105351 |
| 40. | 1. | 0. | -1.878639 | 3.656360 | -2.039239 |
| 41. | 1. | 0. | -1.578638 | 6.759960 | -0.405717 |
| 42. | 1. | 0. | -2.650209 | 6.321358 | 0.945827 |
| 43. | 1. | 0. | -3.312355 | 6.532457 | -0.689316 |

17*R*-**3**-5

| 17*R*-**3**-5 | | Standard Orientation (Ångstroms) | | | |
|---|---|---|---|---|---|
| Center number | Atom number | Type | X | Y | Z |
| 1. | 8. | 0. | 1.019812 | 2.728440 | 0.170614 |
| 2. | 6. | 0. | 0.637138 | 2.704792 | 1.472877 |
| 3. | 6. | 0. | -0.354545 | 1.882664 | 1.878383 |
| 4. | 6. | 0. | -1.010967 | 1.038834 | 0.919351 |
| 5. | 6. | 0. | -0.624062 | 1.024649 | -0.407151 |
| 6. | 6. | 0. | 0.435661 | 1.907597 | -0.828188 |
| 7. | 8. | 0. | 0.896848 | 2.044682 | -1.944801 |
| 8. | 6. | 0. | -1.299088 | 0.186339 | -1.489395 |
| 9. | 6. | 0. | -1.042809 | -1.319384 | -1.461307 |
| 10. | 6. | 0. | 0.061388 | -1.910481 | -2.106750 |
| 11. | 6. | 0. | 0.237843 | -3.299780 | -2.063058 |
| 12. | 6. | 0. | -0.674089 | -4.119185 | -1.402142 |
| 13. | 6. | 0. | -1.788830 | -3.562381 | -0.773462 |
| 14. | 6. | 0. | -1.953183 | -2.180647 | -0.816806 |
| 15. | 8. | 0. | -3.040807 | -1.559233 | -0.218549 |
| 16. | 6. | 0. | 1.049274 | -1.087635 | -2.900967 |
| 17. | 6. | 0. | -4.061454 | -2.362954 | 0.372094 |
| 18. | 8. | 0. | -0.539982 | -5.477289 | -1.334831 |
| 19. | 8. | 0. | -2.003736 | 0.301771 | 1.433447 |
| 20. | 6. | 0. | 1.417513 | 3.658718 | 2.325160 |
| 21. | 6. | 0. | 2.959340 | 3.524752 | 2.204956 |
| 22. | 8. | 0. | 3.435510 | 4.043571 | 0.972596 |
| 23. | 6. | 0. | 3.463388 | 2.100918 | 2.457570 |
| 24. | 1. | 0. | -0.672351 | 1.851165 | 2.912226 |
| 25. | 1. | 0. | -0.958892 | 0.589670 | -2.444935 |
| 26. | 1. | 0. | -2.380691 | 0.354608 | -1.449100 |
| 27. | 1. | 0. | 1.095361 | -3.743395 | -2.564412 |
| 28. | 1. | 0. | -2.484900 | -4.219199 | -0.269772 |
| 29. | 1. | 0. | 0.592297 | -0.723067 | -3.829538 |
| 30. | 1. | 0. | 1.917762 | -1.690371 | -3.178727 |
| 31. | 1. | 0. | 1.394255 | -0.201346 | -2.366885 |
| 32. | 1. | 0. | -3.675064 | -2.947166 | 1.214532 |
| 33. | 1. | 0. | -4.819552 | -1.665405 | 0.729888 |
| 34. | 1. | 0. | -4.502542 | -3.035491 | -0.370432 |
| 35. | 1. | 0. | 0.266219 | -5.735537 | -1.800685 |
| 36. | 1. | 0. | -2.406798 | -0.299441 | 0.767646 |
| 37. | 1. | 0. | 1.109842 | 3.519137 | 3.366339 |
| 38. | 1. | 0. | 1.160969 | 4.686244 | 2.038029 |
| 39. | 1. | 0. | 3.384788 | 4.185794 | 2.969613 |

| | | | | | |
|---|---|---|---|---|---|
| 40. | 1. | 0. | 2.966805 | 3.581833 | 0.261282 |
| 41. | 1. | 0. | 3.079341 | 1.405389 | 1.703828 |
| 42. | 1. | 0. | 3.155922 | 1.734963 | 3.443598 |
| 43. | 1. | 0. | 4.555067 | 2.084856 | 2.405864 |

**Table S2.** The bioactivity assays of isolated compounds[a]

| Compds | (±)-**1** | (+)-**1** | (−)-**1** | **2** | **3** | vancomycin | amphotericin B | oleanolic acid | adriamycin |
|---|---|---|---|---|---|---|---|---|---|
| *Staphylococcus epidermidis* ATCC 12228 | >128 | >128 | >128 | >128 | >128 | 1 | | | |
| *Staphylococcus aureus* ATCC 25923 | >128 | >128 | >128 | >128 | >128 | 1 | | | |
| *Pseudomonas aeruginosa* ATCC 27853 | >128 | >128 | >128 | 32 | 128 | 1 | | | |
| *Bacillus cereus* ATCC 14579 | >128 | >128 | >128 | 128 | >128 | 1 | | | |
| *Escherichia coli* ATCC 25922 | >128 | >128 | >128 | 128 | >128 | 1 | | | |
| *Sarcina lutea* ATCC 9341 | >128 | >128 | >128 | >128 | >128 | 1 | | | |
| *Candida albicans ATCC 10231* | 32 | 16 | 64 | 64 | >128 | | 0.5 | | |
| *Candida tropicalis ATCC 20962* | >128 | 128 | >128 | >128 | >128 | | 0.5 | | |
| *Candida parapsilosis ATCC 22019* | >128 | >128 | >128 | >128 | >128 | | 0.5 | | |
| PTP1B | 45.8 | 17.3 | 35.5 | 42.3 | >50 | | | 4 | |
| A549 | >50 | >50 | >50 | >50 | >50 | | | | 0.3 |
| HCT116 | >50 | >50 | >50 | >50 | >50 | | | | 0.8 |
| MCF-7 | >50 | >50 | >50 | >50 | >50 | | | | 0.2 |
| Hela | >50 | >50 | >50 | >50 | >50 | | | | 0.9 |

| | | | | | | |
|---|---|---|---|---|---|---|
| Hep G2 | >50 | >50 | >50 | >50 | >50 | 0.4 |

[a] μg/mL for MIC value of antibacterial or antifungal activity, and μM for $IC_{50}$ value of cytotoxic or PTP1B inhibitory activity.