# Supplementary material

## Synthesis and Biological Evaluation of New Ozonides with Improved Plant Growth Regulatory Activity

LUIZ C. A. BARBOSA[§*], CÉLIA R. A. MALTHA[§], RAPHAEL C. CUSATI[§], RÓBSON R. TEIXEIRA[§], FILIPE F. RODRIGUES[§] , ANTÔNIO A. SILVA[‡] , MICHAEL G. B. DREW[†], FYAZ M. D. ISMAIL[#]

*Author to whom correspondence should be addressed [fax: (55) 31 3899 3065; e-mail lcab@ufv.br].

[§] Department of Chemistry, Federal University of Viçosa, Avenida P.H. Rolfs, CEP 36570-000, Viçosa, MG, Brazil.

[‡] Department of Plant Science, Federal University of Viçosa.

[†] School of Chemistry, The University of Reading, P.O. Box 224, Whiteknights, Reading RG6 6AD, UK: m.g.b.drew@reading.ac.uk

[#]Medicinal Chemistry Research Group, School of Pharmacy & Biomolecular Sciences, Institute for Health Research, Liverpool John Moores University, Byrom Street, Liverpool L3 3AF, United Kingdom. f.m.ismail@ljmu.ac.uk

**Table 1: *Data for* 16-*exo* ozonide of 2-methyl-(1α,6α,2β,5β)-12-oxatricyclo-[4.4.1.1$^{2,5}$]-dodec-3-en-11-one**

SCF Done: E(RB+HF-LYP) = -842.935106886 A.U. after 8 cycles

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.612548 | 0.836143 | 0.969044 |
| 2 | 6 | 0 | -0.591056 | 1.094650 | 0.014024 |
| 3 | 6 | 0 | -0.504126 | -1.081984 | -0.921866 |
| 4 | 6 | 0 | 0.749022 | -1.523565 | -0.140069 |
| 5 | 6 | 0 | 0.911912 | -0.661480 | 1.114365 |
| 6 | 1 | 0 | 0.343790 | 1.190854 | 1.972869 |
| 7 | 1 | 0 | 0.621850 | -2.554469 | 0.210511 |
| 8 | 8 | 0 | -0.435456 | 0.319144 | -1.190172 |
| 9 | 6 | 0 | -1.803398 | -1.378441 | -0.151333 |
| 10 | 6 | 0 | -1.894516 | 0.604593 | 0.706880 |
| 11 | 1 | 0 | -2.013425 | -2.442799 | -0.018758 |
| 12 | 8 | 0 | 1.364893 | -1.117937 | 2.148886 |
| 13 | 6 | 0 | 2.029362 | -1.447332 | -1.043410 |
| 14 | 1 | 0 | 2.513425 | -2.430230 | -1.019975 |
| 15 | 1 | 0 | 1.710033 | -1.280644 | -2.079873 |
| 16 | 6 | 0 | 1.935047 | 1.550101 | 0.578880 |
| 17 | 1 | 0 | 1.746266 | 2.628291 | 0.515877 |
| 18 | 1 | 0 | 2.622902 | 1.410328 | 1.423078 |

| | | | | | |
|---|---|---|---|---|---|
| 19 | 6 | 0 | 3.100010 | -0.393140 | -0.695218 |
| 20 | 1 | 0 | 3.550000 | -0.628223 | 0.279368 |
| 21 | 1 | 0 | 3.903709 | -0.511861 | -1.433894 |
| 22 | 6 | 0 | 2.640161 | 1.079367 | -0.706786 |
| 23 | 1 | 0 | 2.004805 | 1.258979 | -1.582761 |
| 24 | 1 | 0 | 3.527907 | 1.714115 | -0.831249 |
| 25 | 1 | 0 | -0.548519 | -1.571672 | -1.900136 |
| 26 | 8 | 0 | -2.934382 | -0.788022 | -0.787337 |
| 27 | 8 | 0 | -1.746911 | -0.744262 | 1.115839 |
| 28 | 8 | 0 | -2.994056 | 0.572587 | -0.202104 |
| 29 | 1 | 0 | -2.192329 | 1.213673 | 1.564376 |
| 30 | 6 | 0 | -0.755633 | 2.545730 | -0.420841 |
| 31 | 1 | 0 | -0.791563 | 3.212993 | 0.448653 |
| 32 | 1 | 0 | 0.075277 | 2.854068 | -1.060490 |
| 33 | 1 | 0 | -1.682829 | 2.656672 | -0.990501 |

**Table 2: Data for 16-*endo* ozonide of 2-methyl-(1α,6α,2β,5β)-12-oxatricyclo-[4.4.1.1$^{2,5}$]-dodec-3-en-11-one**

SCF Done: E(RB+HF-LYP) = -842.927101578 A.U. after 10 cycles

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.483217 | 0.751392 | 1.009228 |
| 2 | 6 | 0 | -0.548546 | 1.226722 | -0.052089 |
| 3 | 6 | 0 | -0.502983 | -0.787082 | -1.261098 |
| 4 | 6 | 0 | 0.550448 | -1.468163 | -0.362906 |
| 5 | 6 | 0 | 0.641037 | -0.774869 | 0.999060 |
| 6 | 1 | 0 | 0.113959 | 1.015774 | 2.006932 |
| 7 | 1 | 0 | 0.256880 | -2.503775 | -0.165774 |
| 8 | 8 | 0 | -0.253097 | 0.614217 | -1.316139 |
| 9 | 6 | 0 | -1.991720 | -1.010869 | -0.822495 |
| 10 | 6 | 0 | -2.017469 | 0.788805 | 0.339984 |
| 11 | 1 | 0 | -2.539422 | -1.704267 | -1.463437 |
| 12 | 8 | 0 | 0.954012 | -1.385352 | 2.003859 |
| 13 | 6 | 0 | 1.958654 | -1.455165 | -1.059079 |
| 14 | 1 | 0 | 2.342477 | -2.481666 | -1.052953 |
| 15 | 1 | 0 | 1.820124 | -1.179005 | -2.112190 |
| 16 | 6 | 0 | 1.903261 | 1.365986 | 0.864357 |
| 17 | 1 | 0 | 1.819898 | 2.458804 | 0.900136 |

| | | | | | |
|---|---|---|---|---|---|
| 18 | 1 | 0 | 2.456660 | 1.073658 | 1.766291 |
| 19 | 6 | 0 | 3.057211 | -0.547952 | -0.465121 |
| 20 | 1 | 0 | 3.349280 | -0.921701 | 0.525752 |
| 21 | 1 | 0 | 3.940531 | -0.671941 | -1.105644 |
| 22 | 6 | 0 | 2.733158 | 0.957512 | -0.367605 |
| 23 | 1 | 0 | 2.242871 | 1.289536 | -1.290574 |
| 24 | 1 | 0 | 3.682765 | 1.506302 | -0.304593 |
| 25 | 1 | 0 | -2.616141 | 1.610770 | 0.738116 |
| 26 | 1 | 0 | -0.399423 | -1.139544 | -2.292320 |
| 27 | 8 | 0 | -2.654729 | 0.237170 | -0.788490 |
| 28 | 8 | 0 | -2.058776 | -0.262264 | 1.317920 |
| 29 | 8 | 0 | -2.124411 | -1.498371 | 0.509703 |
| 30 | 6 | 0 | -0.550767 | 2.732404 | -0.299604 |
| 31 | 1 | 0 | -1.373512 | 2.997475 | -0.972846 |
| 32 | 1 | 0 | -0.676652 | 3.281267 | 0.641149 |
| 33 | 1 | 0 | 0.382696 | 3.052780 | -0.768662 |