Supporting Information-3:

Antiviral New Limonoids Including Khayanolides from the Trang Mangrove Plant, *Xylocarpus moluccensis*

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Copies of CD spectra for compounds **2-12**, and quantum-chemical electronic circular dichroism (ECD) calculations for compounds **3**, **4**, **6**, **11**, and **12**.

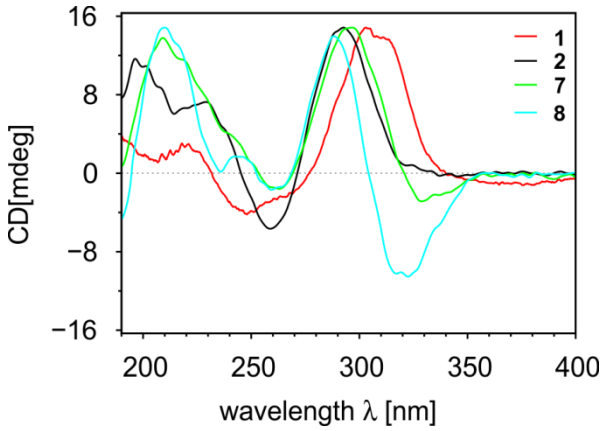

Figure S1. Comparison of the experimental CD spectra of **1**, **2**, **7**, and **8**, due to the similarity of these curves all compounds do have the *R*-configuration at the stereocenters C-13 and C-17.

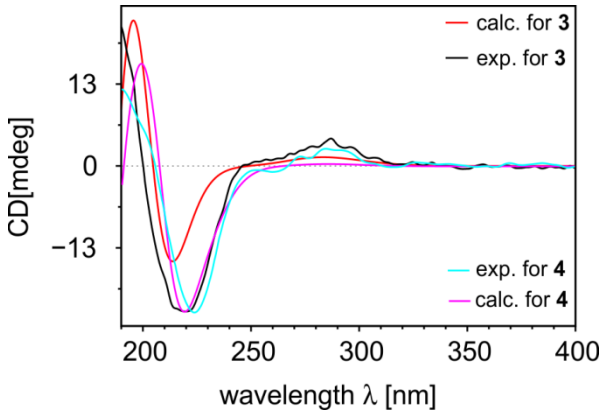

Figure S2. Comparison of the experimental and calculated (both of the 1*R*,2*R*,4*R*,5*R*,9*R*,10*R*,13*R*,17*R*,30*R* configuration) CD spectra of **3** and **4**.

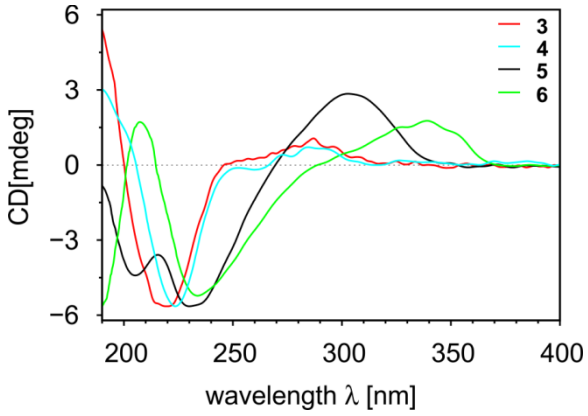

Figure S3. Comparison of the experimental CD spectra of **3**, **4**, **5**, and **6**, due to the similarity of these curves all compounds do have the same configuration at the stereocenters C-13 and C-17.

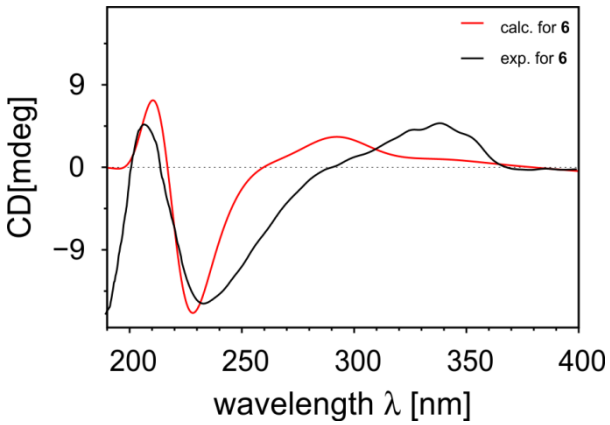

Figure S4. Comparison of the experimental CD spectra of **6** with that calculated for the 1*R*,3*S*,4*R*,5*S*,9*R*,10*S*,13*R*,17*R*,30*S*-configured **6**.

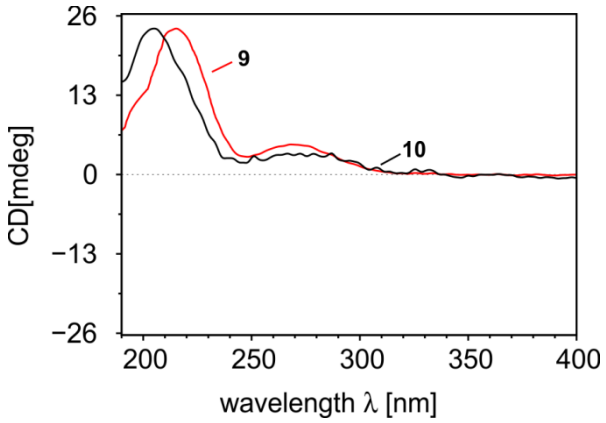

Figure S5. Comparison of the experimental CD spectra of **9** and **10**, due to the similarity of these curves the compounds do have the same configuration. In addition they are nearly identical with the CD curve of the known compound andirolide G.

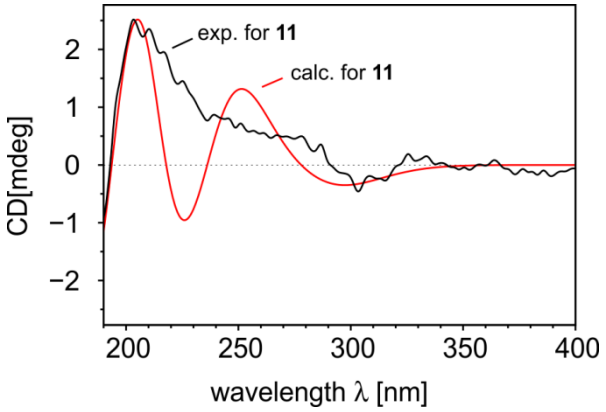

Figure S6. Comparison of the experimental CD spectra of **11** with the spectrum calculated of 2*R*,5*S*,9*S*,10*R*,13*R*,17*R*-**11**. The *R*-configuration at C-6 was arbitrarily chosen but has no influence to the CD and was thus not elucidated.

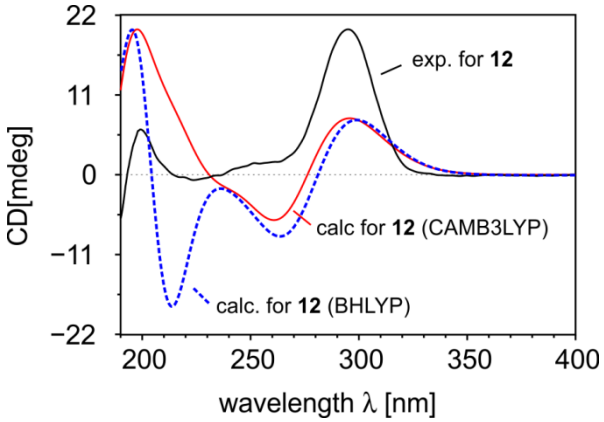

Figure S7. Comparison of the experimental CD spectra of **12** with the spectrum calculated for 2*R*,5*S*,9*S*,10*R*,13*R*,17*R*-**12**. The stereocenter at C-6 was arbitrarily set to an *R*-configuration it has no influence on the CD spectrum and was thus not elucidated. In this case two different methods were used: TDBHLYP/def2-SVP and TDCAM-B3LYP/def2-TZVP(-f).

UPLC-MS analysis of thaixylomolin I (3) maintained in EtOH

In the experiment, 1.0 mg of compound **3** was dissolved and maintained in 1.0 mL EtOH at room temperature for a week. Then, UPLC-MS analysis was performed on an RP-18 column (ACQUITY UPLC BEH, 100 × 2.1 mm i.d., 1.7 μm, Waters) and eluted with 40% MeCN in water. In **Figure S10**, except for the peak of compound **3** (t_R = 3.6 min with a molecular weight of 542), the only new produced small peak at t_R = 5.5 min can be found. Its molecular weight is 568. At the moment, we do not know the genuine structure of this peak. But, undoubtedly, it was not compound **4**, which should appear at t_R = 7.4 min and have a molecular weight of 570 (Please see **Figure S9**).

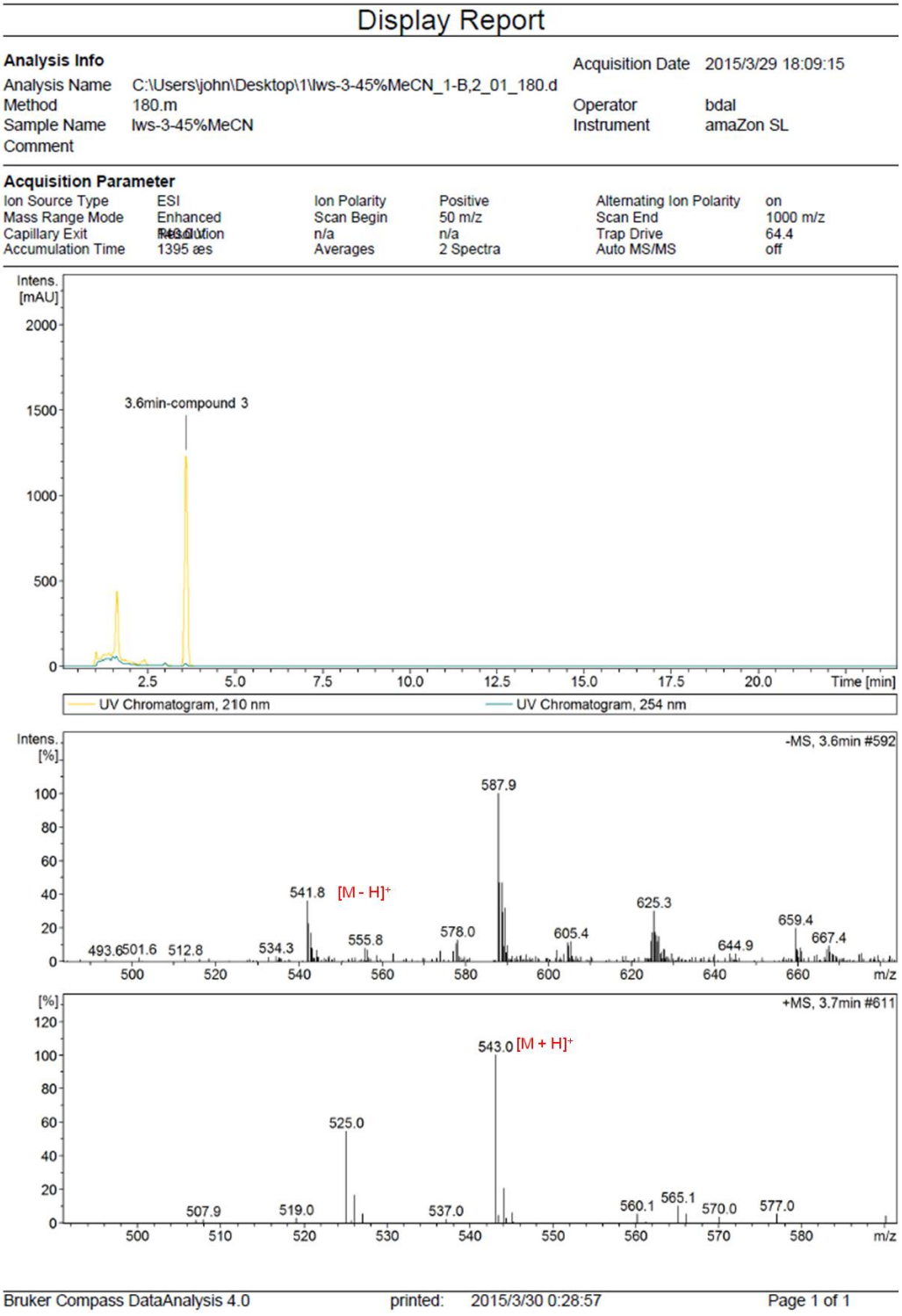

Figure S8. UPLC-MS analysis of thaixylomolin I (**3**)

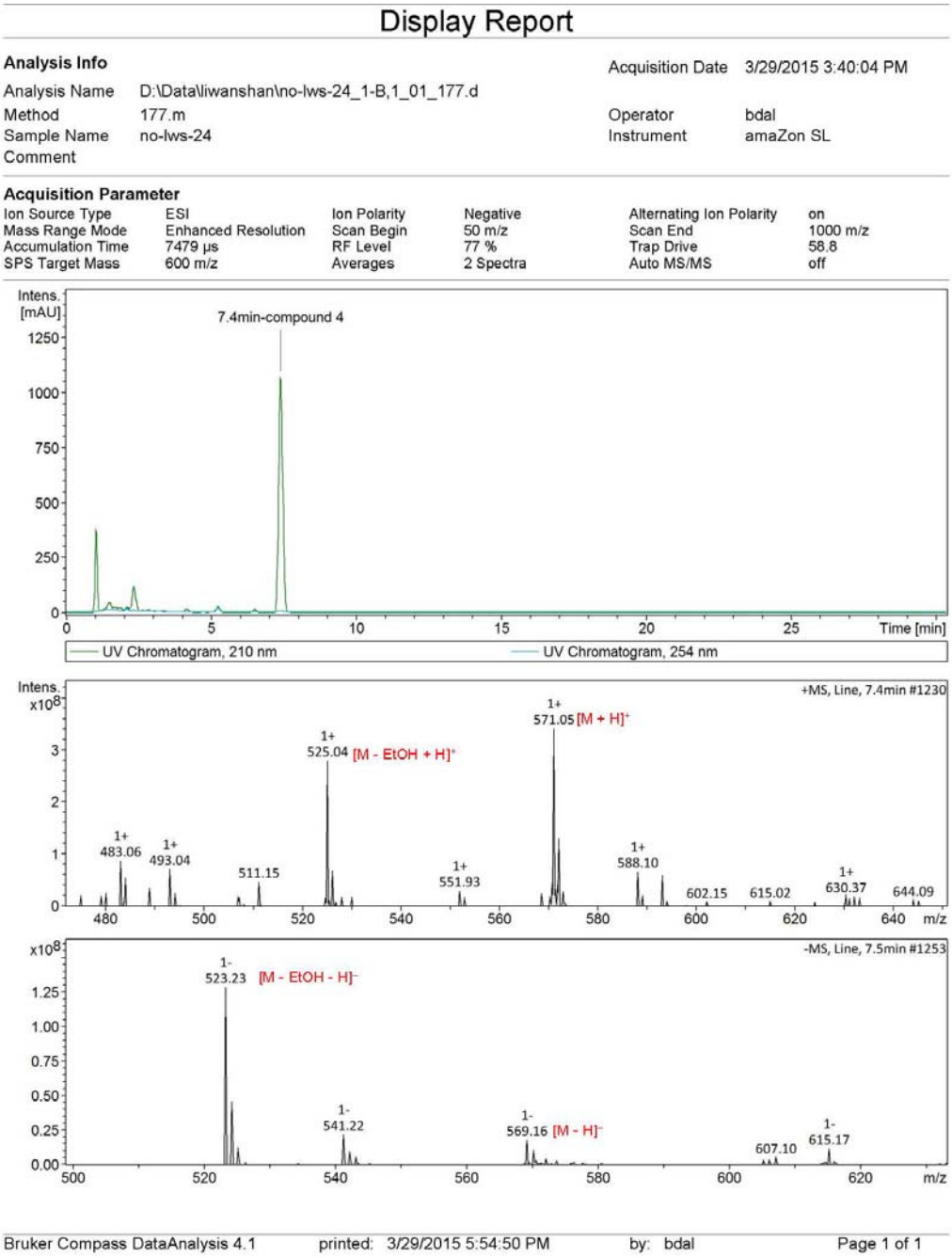

Figure S9. UPLC-MS analysis of thaixylomolin J (**4**)

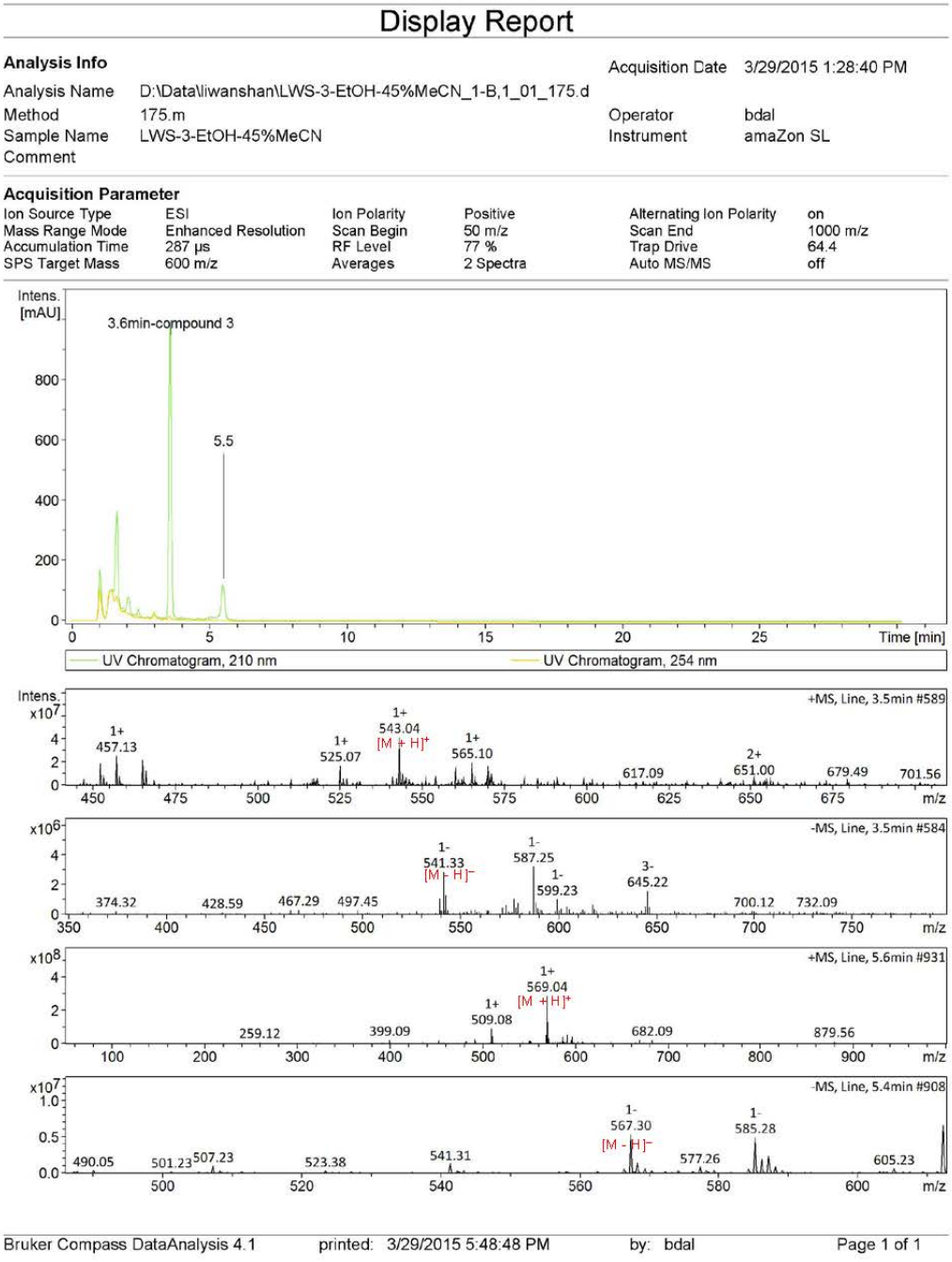

Figure S10. UPLC-MS analysis of thaixylomolin I (**3**) maintained in EtOH (1.0 mg of thaixylomolin I (**3**) was dissolved and maintained in 1.0 mL EtOH at room temperature for a week)