# Supporting Information for

## Six new diterpenoids from Croton laevigatus

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Figure S1. Key 2D NMR correlations for compound 2.



Figure S2. Key 2D NMR correlations for compound 3.



Figure S3. Key 2D NMR correlations for compound 4.



Figure S4. Key 2D NMR correlations for compound 7.



Figure S5. <sup>1</sup>H NMR spectrum of compound 1 in CDCl<sub>3</sub>



Figure S6. <sup>13</sup>C NMR spectrum of compound 1 in CDCl<sub>3</sub>



Figure S7. HSQC spectrum of compound 1 in CDCl<sub>3</sub>



Figure S8. HMBC spectrum of compound 1 in CDCl<sub>3</sub>



Figure S9. NOESY spectrum of compound 1 in CDCl<sub>3</sub>



Figure S10. ESI(+)MS spectrum of compound 1

#### Figure S11. HRESI(+)MS spectrum of compound 1





Figure S12. IR spectrum of compound 1



Figure S13. <sup>1</sup>H NMR spectrum of compound 2 in CD<sub>3</sub>OD







Figure S15. HSQC spectrum of compound 2 in CD<sub>3</sub>OD



Figure S16. HMBC spectrum of compound 2 in CD<sub>3</sub>OD



**Figure S17.** <sup>1</sup>H–<sup>1</sup>H COSY spectrum of compound **2** in CD<sub>3</sub>OD



Figure S18. NOESY spectrum of compound 2 in CD<sub>3</sub>OD



Figure S19. ESI(–)MS spectrum of compound 2

#### Figure S20. HRESI(-)MS spectrum of compound 2





Figure S21. IR spectrum of compound 2



Figure S22. <sup>1</sup>H NMR spectrum of compound 3 in CDCl<sub>3</sub>

Figure S23. <sup>13</sup>C NMR spectrum of compound 3 in CDCl<sub>3</sub>





Figure S24. HSQC spectrum of compound 3 in CDCl<sub>3</sub>



Figure S25. HMBC spectrum of compound 3 in CDCl<sub>3</sub>



Figure S26. <sup>1</sup>H–<sup>1</sup>H COSY spectrum of compound 3 in CDCl<sub>3</sub>



Figure S27. NOESY spectrum of compound 3 in CDCl<sub>3</sub>



Figure S28. ESI(–)MS spectrum of compound 3

#### Figure S29. HRESI(-)MS spectrum of compound 3





Figure S30. IR spectrum of compound 3











Figure S33. HSQC spectrum of compound 4 in CDCl<sub>3</sub>



Figure S34. HMBC spectrum of compound 4 in CDCl<sub>3</sub>



Figure S35. <sup>1</sup>H–<sup>1</sup>H COSY spectrum of compound 4 in CDCl<sub>3</sub>



Figure S36. NOESY spectrum of compound 4 in CDCl<sub>3</sub>



Figure S37. ESI(+)MS spectrum of compound 4

#### Figure S38. HRESI(+)MS spectrum of compound 4





Figure S39. IR spectrum of compound 4



Figure S40. <sup>1</sup>H NMR spectrum of compound 5 in CDCl<sub>3</sub>

Figure S41. <sup>13</sup>C NMR spectrum of compound 5 in CDCl<sub>3</sub>





Figure S42. HSQC spectrum of compound 5 in CDCl<sub>3</sub>



Figure S43. HMBC spectrum of compound 5 in CDCl<sub>3</sub>



Figure S44. <sup>1</sup>H–<sup>1</sup>H COSY spectrum of compound 5 in CDCl<sub>3</sub>



Figure S45. NOESY spectrum of compound 5 in CDCl<sub>3</sub>



Figure S46. ESI(+)MS spectrum of compound 5



Figure S47. ESI(–)MS spectrum of compound 5

### Figure S48. HRESI(+)MS spectrum of compound 5

#### **Elemental Composition Report** Page 1 Single Mass Analysis Tolerance = 3.0 PPM / DBE: min = -1.5, max = 50.0 Element prediction: Off Number of isotope peaks used for i-FIT = 3 Monoisotopic Mass, Even Electron Ions 113 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass) Elements Used: C: 0-100 H: 0-1000 O: 0-500 Na: 0-1 LCT PXE KE324 25-Sep-2017 25-Sep-2017 1: TOF MS ES+ 15:09:58 LCL-31-3-H 40 (0.847) Cm (38:43) 100-1.28e+004 315.1935 % 316.1971 313.8715 314.2213 314.7755 317.0182 317.1995 317.4459 318.1579 312.3571312.8365 0-315.7091 318.9698 312.00 313.00 314.00 315.00 --- m/z 316.00 317.00 318.00 319.00 Minimum: Maximum: -1.5 50.0 5.0 3.0 Mass Calc. Mass mDa PPM DBE i-FIT i-FIT (Norm) Formula 315.1935 315.1936 -0.1 -0.3 4.5 315.1 0.0 C18 H28 O3 Na



Figure S49. IR spectrum of compound 5



Figure S50. <sup>1</sup>H NMR spectrum of compound 6 in CDCl<sub>3</sub>







Figure S52. HSQC spectrum of compound 6 in CDCl<sub>3</sub>



Figure S53. HMBC spectrum of compound 6 in CDCl<sub>3</sub>



Figure S54. <sup>1</sup>H–<sup>1</sup>H COSY spectrum of compound 6 in CDCl<sub>3</sub>



Figure S55. NOESY spectrum of compound 6 in CDCl<sub>3</sub>



Figure S56. ESI(–)MS spectrum of compound 6



Figure S57. HRESI(–)MS spectrum of compound 6



Figure S58. IR spectrum of compound 6



Figure S59. <sup>1</sup>H NMR spectrum of compound 7 in CDCl<sub>3</sub>







Figure S61. HSQC spectrum of compound 7 in CDCl<sub>3</sub>



Figure S62. HMBC spectrum of compound 7 in CDCl<sub>3</sub>



Figure S63. <sup>1</sup>H–<sup>1</sup>H COSY spectrum of compound 7 in CDCl<sub>3</sub>



Figure S64. NOESY spectrum of compound 7 in CDCl<sub>3</sub>



Figure S65. ESI(+)MS spectrum of compound 7

#### Figure S66. HRESI(+)MS spectrum of compound 7



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Figure S67. IR spectrum of compound 7