10.1071/CH09616_AC

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Australian Journal of Chemistry, 2010, 63(6), 886–894

Accessory Publication for

Dereplication of bromotyrosine-derived metabolites by LC-PDA-MS and analysis of the chemical profile of fourteen Aplysina species from the Brazilian coastline

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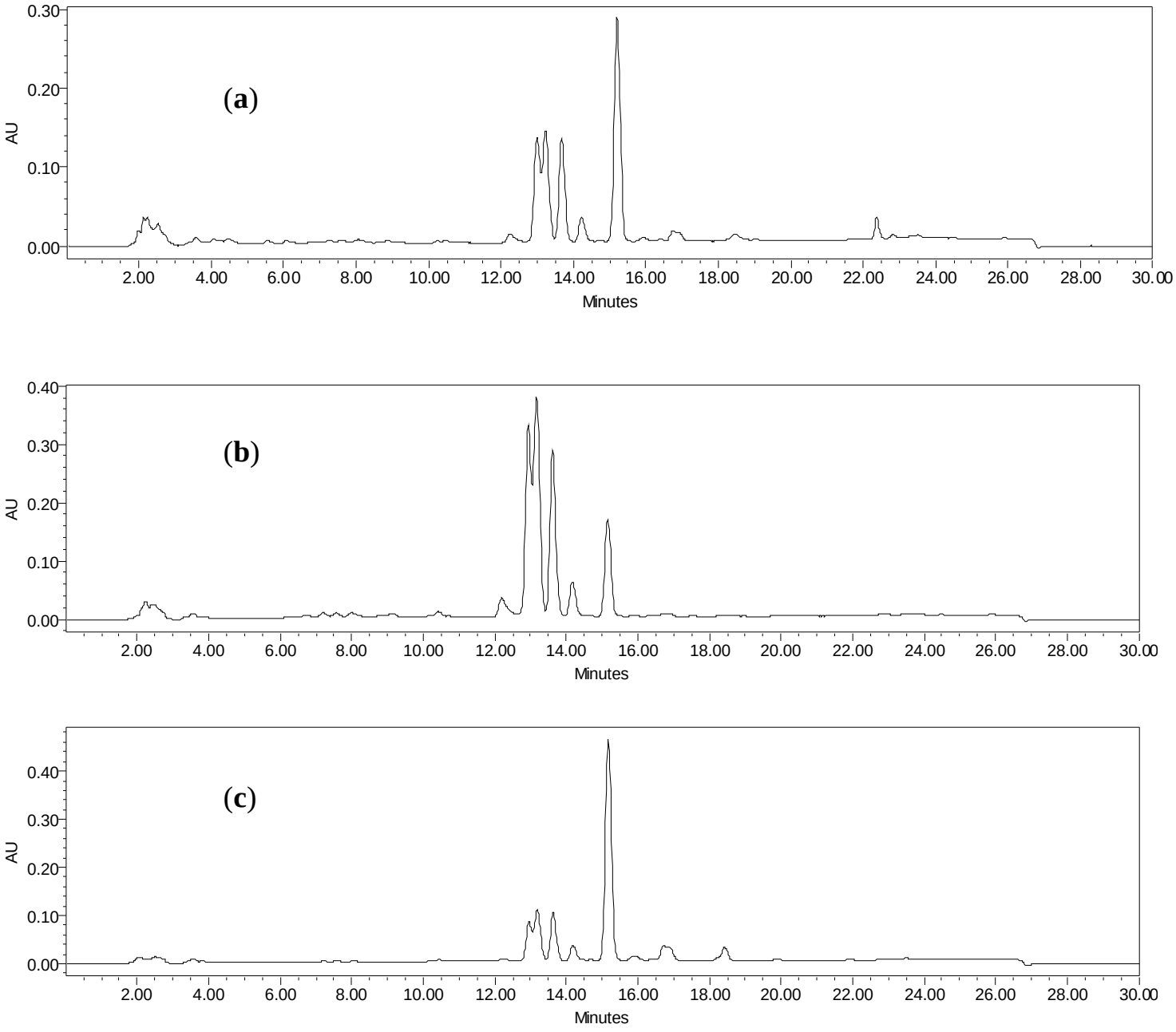

Figure S1 – Chromatographic analyses (LC-PDA-MS) of the SPE fractions (F1, F2 and F3) obtained from

the EtOAc crude extract of *Aplysina* cf. *lactuca* BA07ES-09. (a) Fraction F1 (eluted with 8:2 H_2O/MeOH); (b) Fraction F2 (eluted with 1:1 H_2O/MeOH); (c) Fraction F3 (eluted with 100% MeOH). LC-PDA-MS analyses were performed using the conditions as in the experimental section. Peak assignments: see Figure 2.

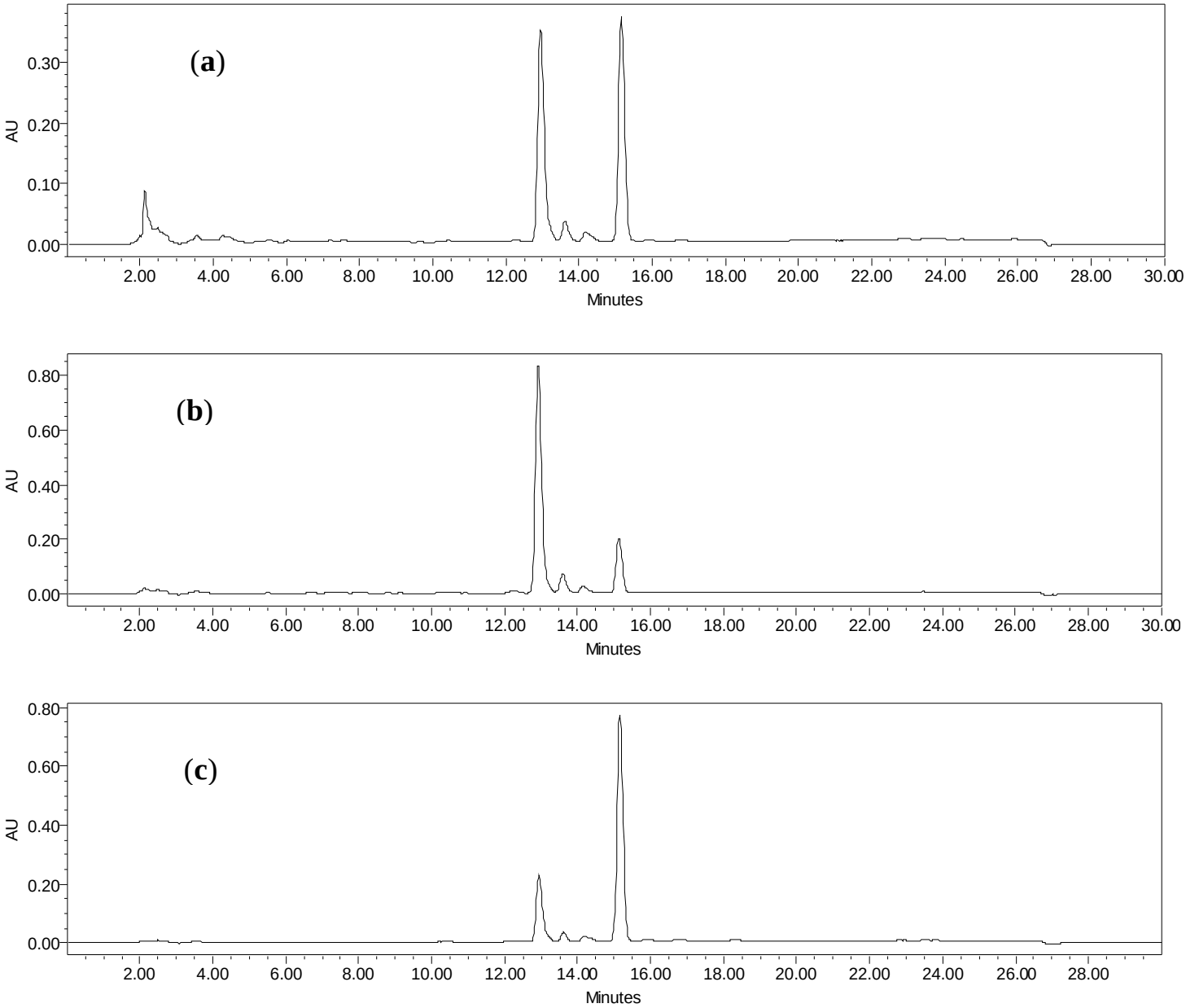

Figure S2 – Chromatographic analyses (LC-PDA-MS) of the SPE fractions (F1, F2 and F3) obtained from the EtOAc crude extract of *Aplysina* sp. BA07ES-20. (a) Fraction F1 (eluted with 8:2 H_2O/MeOH); (b) Fraction F2 (eluted with 1:1 H_2O/MeOH); (c) Fraction F3 (eluted with 100% MeOH). LC-PDA-MS analyses were performed using the conditions as in the experimental section. Peak assignments: see Figure 2.

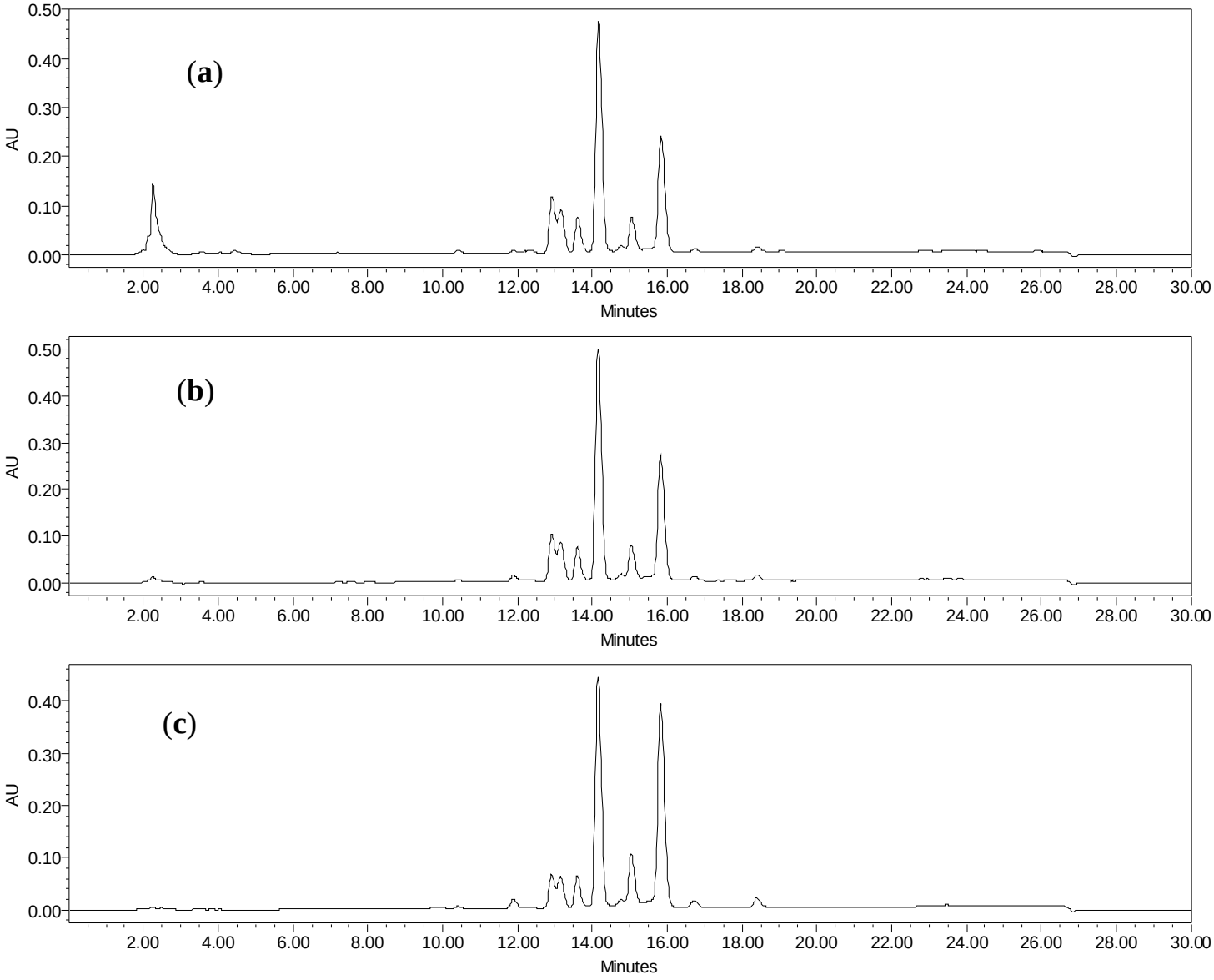

Figure S3 – Chromatographic analyses (LC-PDA-MS) of the SPE fractions (F1, F2 and F3) obtained from the EtOAc crude extract of *Aplysina fistularis* BA07ES-33. (a) Fraction F1 (eluted with 8:2 H_2O/MeOH); (b) Fraction F2 (eluted with 1:1 H_2O/MeOH); (c) Fraction F3 (eluted with 100% MeOH). LC-PDA-MS analyses were performed using the conditions as in the experimental section. Peak assignments: see Figure 2. Peak at 15.8 min corresponds to 11-keto-fistularin-3 (**13**).

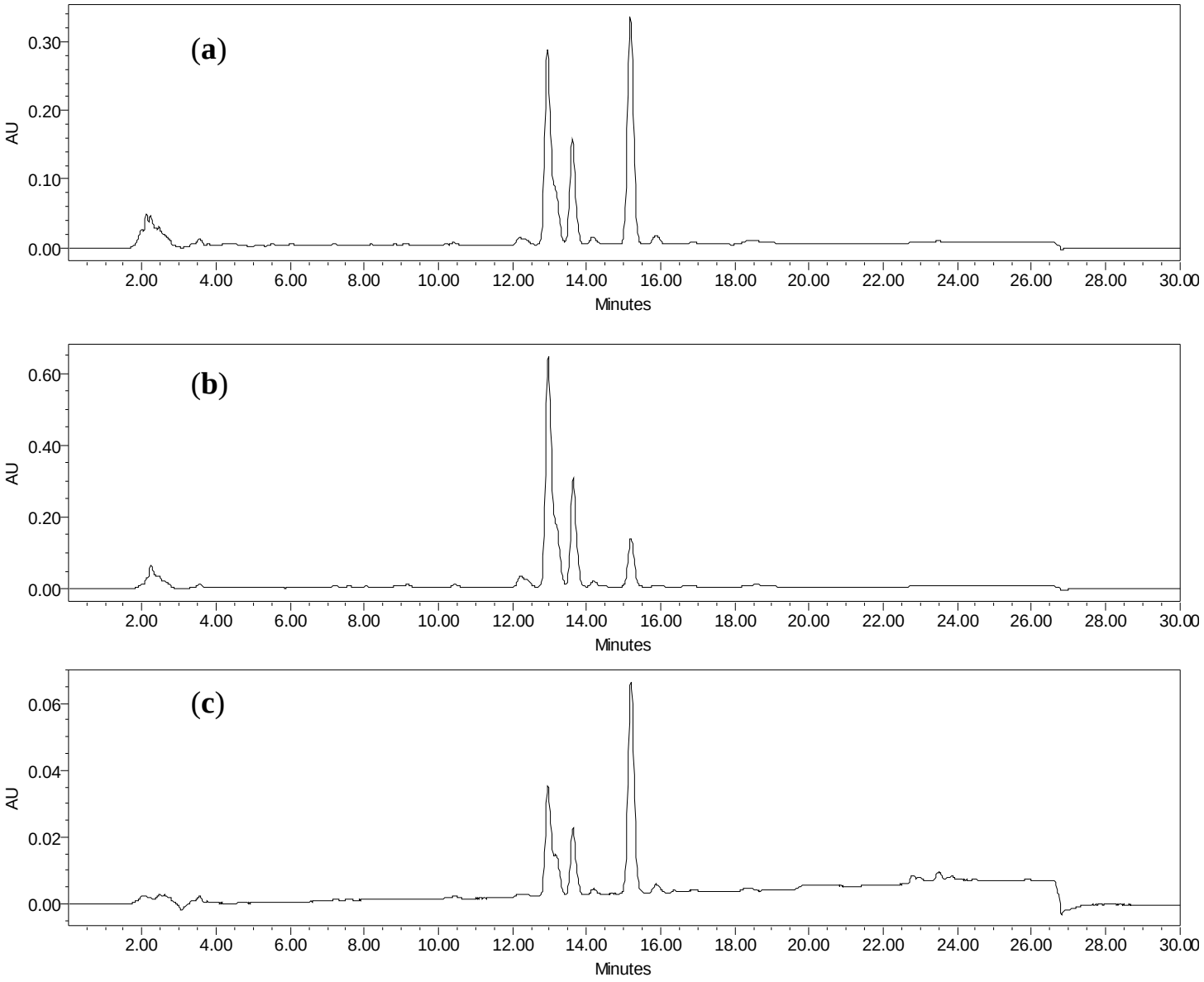

Figure S4 – Chromatographic analyses (LC-PDA-MS) of the SPE fractions (F1, F2 and F3) obtained from the EtOAc crude extract of *Aplysina solangeae* BA07ES-67. (a) Fraction F1 (eluted with 8:2 H_2O/MeOH); (b) Fraction F2 (eluted with 1:1 H_2O/MeOH); (c) Fraction F3 (eluted with 100% MeOH). LC-PDA-MS analyses were performed using the conditions as in the experimental section. Peak assignments: see Figure 2.

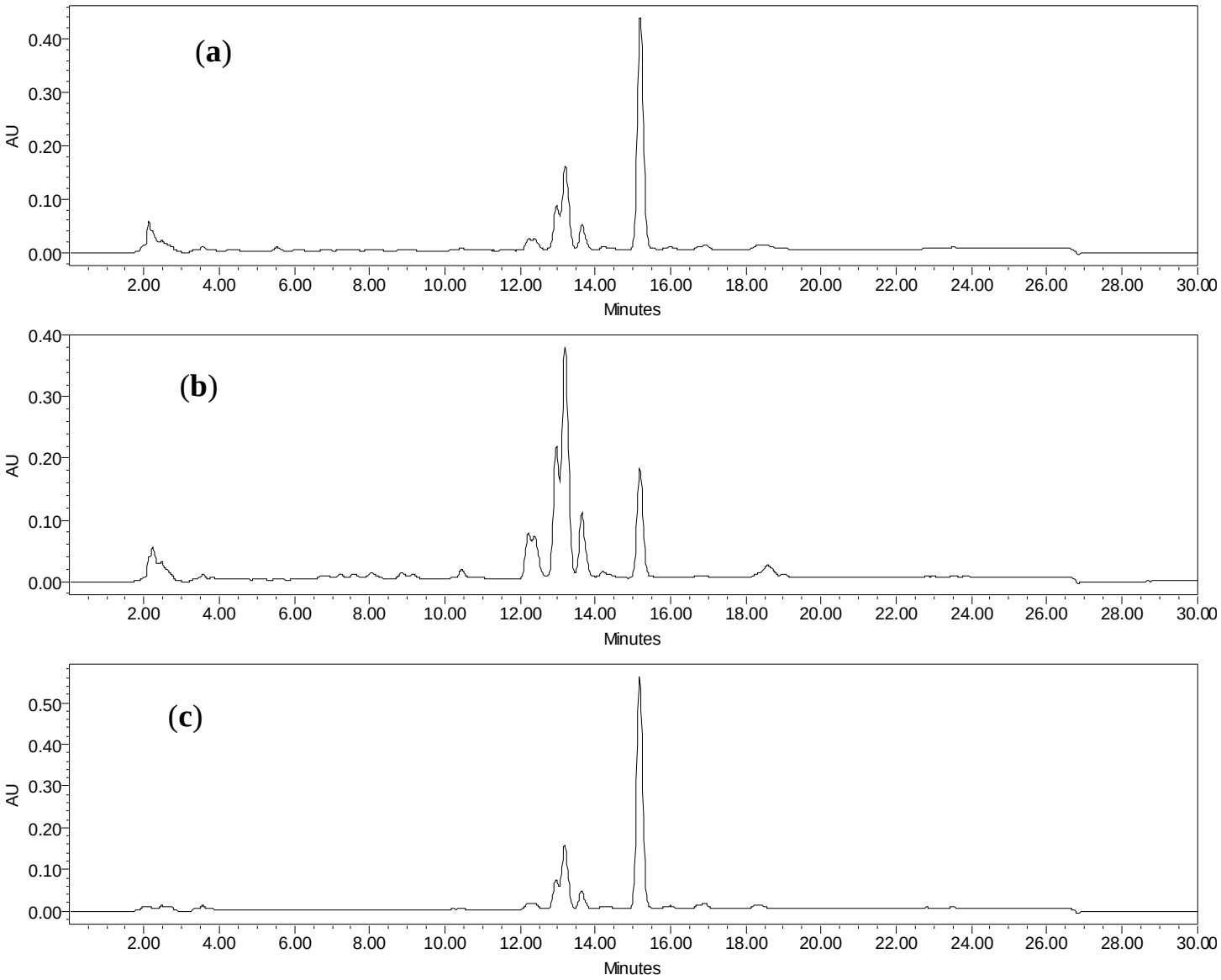

Figure S5 – Chromatographic analyses (LC-PDA-MS) of the SPE fractions (F1, F2 and F3) obtained from the EtOAc crude extract of *Aplysina fulva* BA07ES-70. (a) Fraction F1 (eluted with 8:2 H_2O/MeOH); (b) Fraction F2 (eluted with 1:1 H_2O/MeOH); (c) Fraction F3 (eluted with 100% MeOH). LC-PDA-MS analyses were performed using the conditions as in the experimental section. Peak assignments: see Figure 2.

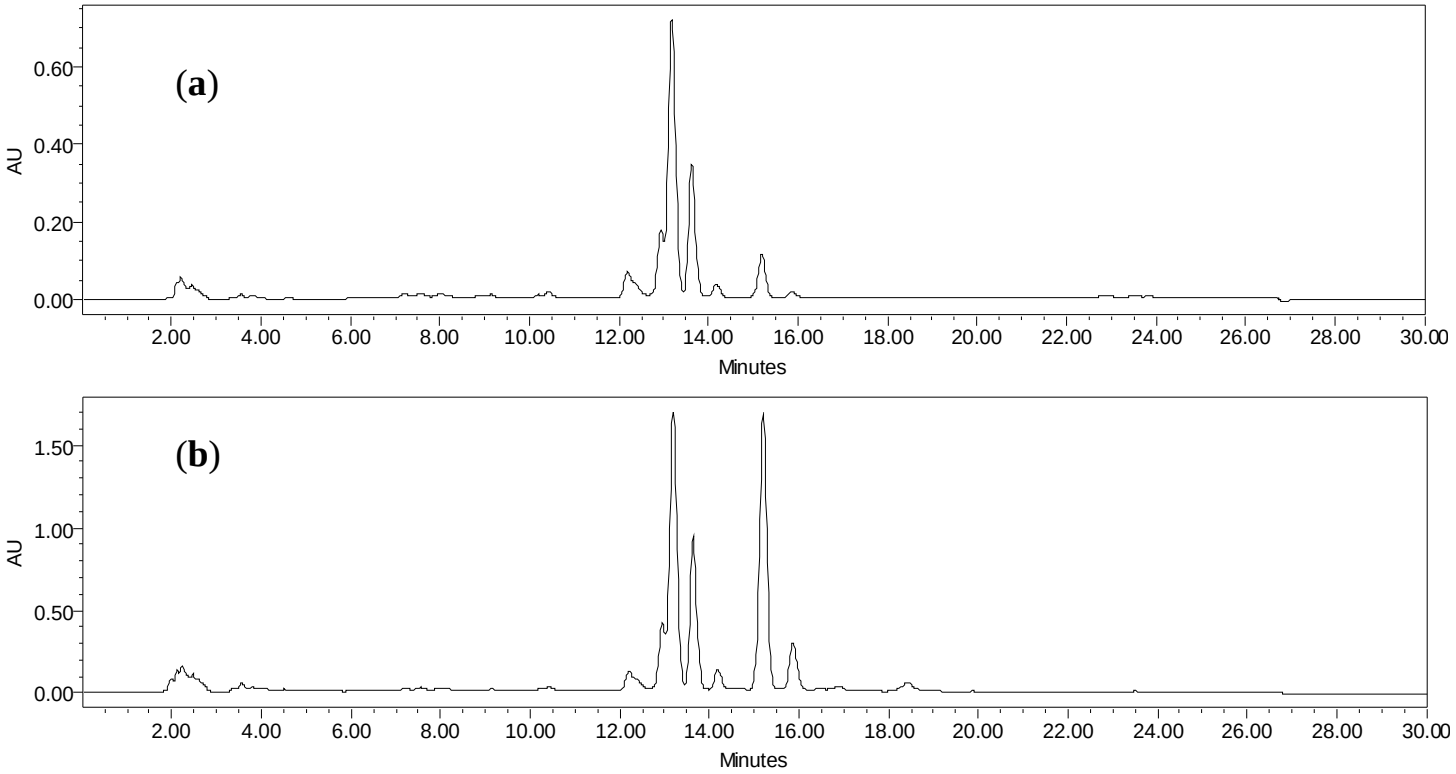

Figure S6 – Chromatographic analyses (LC-PDA-MS) of the SPE fractions (F1, F2 and F3) obtained from the EtOAc crude extract of *Aplysina* sp. BA07ES-72. (a) Fraction F2 (eluted with 1:1 H_2O/MeOH); (b) Fraction F3 (eluted with 100% MeOH). LC-PDA-MS analyses were performed using the conditions as in the experimental section. Peak assignments: see Figure 2. Peak at 15.8 min corresponds to 11-keto-fistularin-3 (**13**).

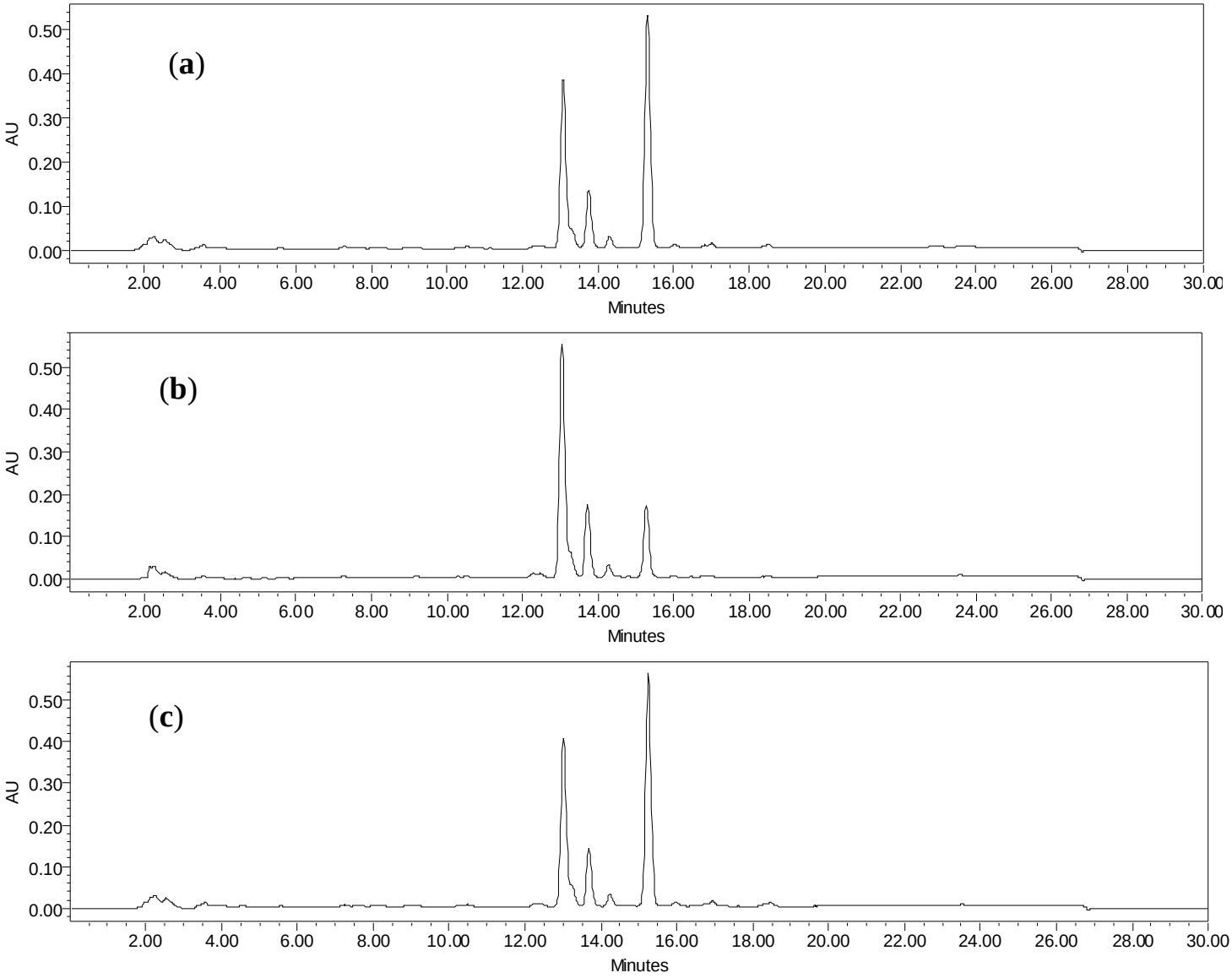

Figure S7 – Chromatographic analyses (LC-PDA-MS) of the SPE fractions (F1, F2 and F3) obtained from the EtOAc crude extract of *Aplysina solangeae* BA07ES-82. (a) Fraction F1 (eluted with 8:2 H_2O/MeOH); (b) Fraction F2 (eluted with 1:1 H_2O/MeOH); (c) Fraction F3 (eluted with 100% MeOH). LC-PDA-MS analyses were performed using the conditions as in the experimental section. Peak assignments: see Figure 2.

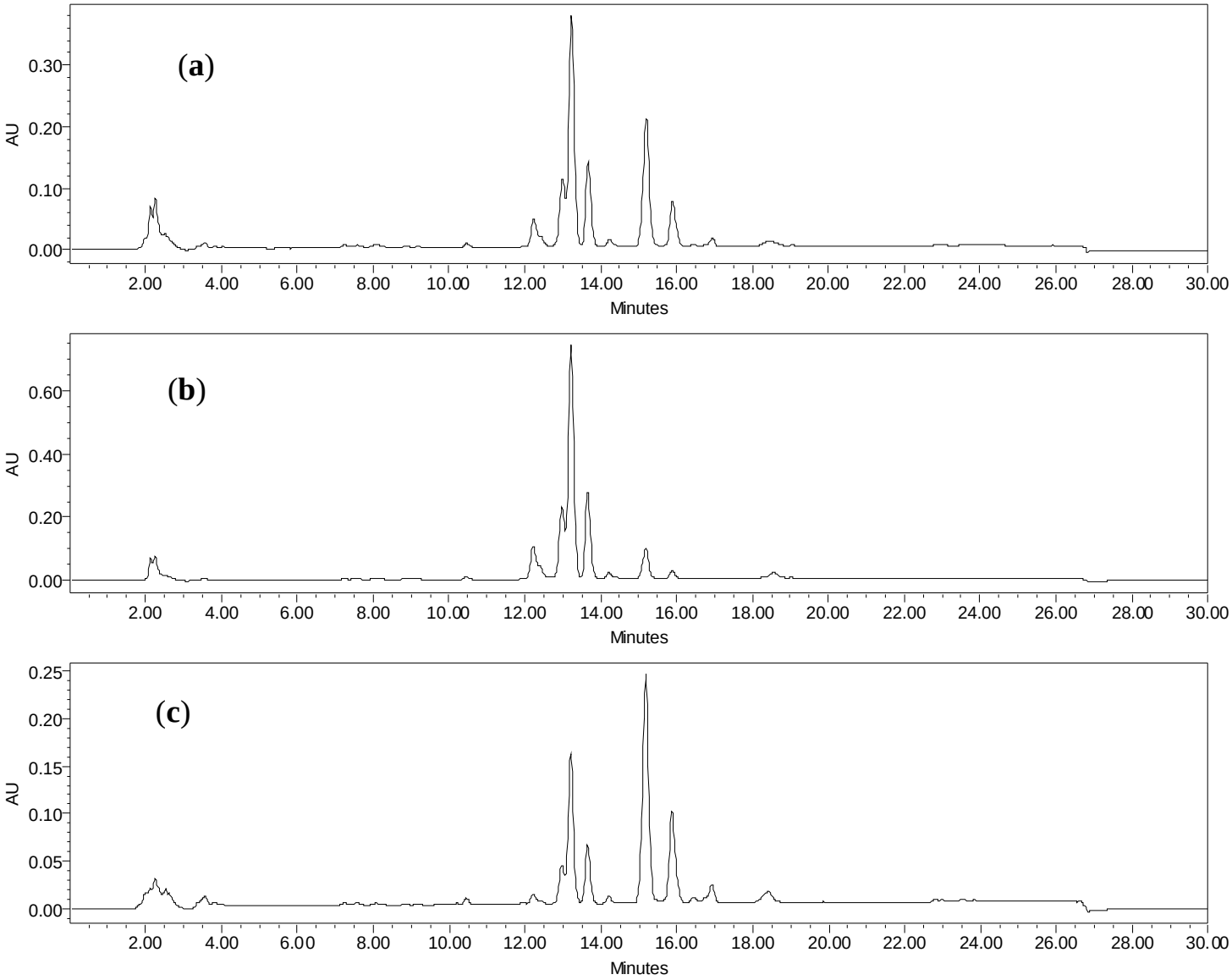

Figure S8 – Chromatographic analyses (LC-PDA-MS) of the SPE fractions (F1, F2 and F3) obtained from the EtOAc crude extract of *Aplysina* n. sp. BA07ES-85. (a) Fraction F1 (eluted with 8:2 H_2O/MeOH); (b) Fraction F2 (eluted with 1:1 H_2O/MeOH); (c) Fraction F3 (eluted with 100% MeOH). LC-PDA-MS analyses were performed using the conditions as in the experimental section. Peak assignments: see Figure 2. Peak at 15.8 min corresponds to 11-keto-fistularin-3 (**13**).

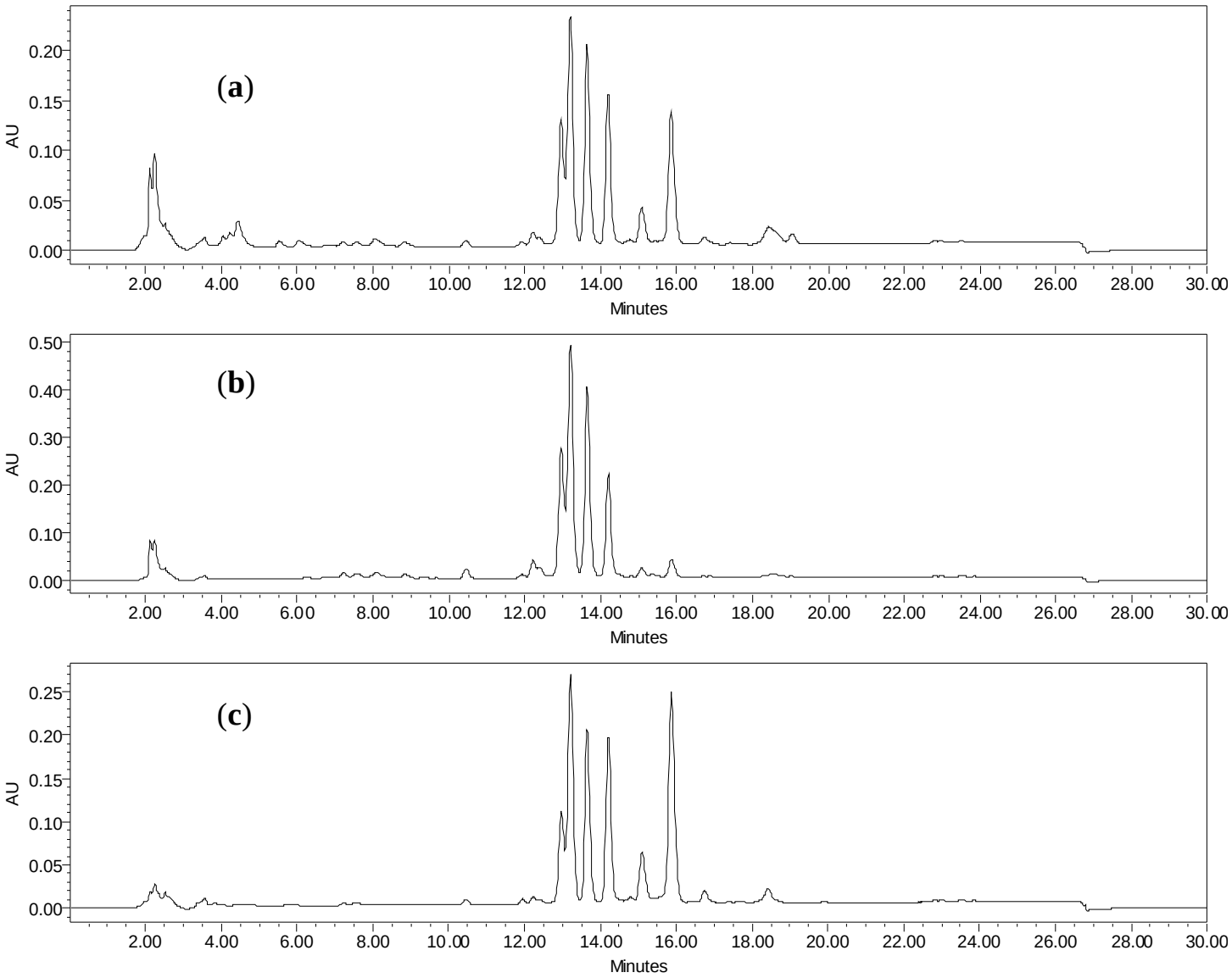

Figure S9 – Chromatographic analyses (LC-PDA-MS) of the SPE fractions (F1, F2 and F3) obtained from the EtOAc crude extract of *Aplysina lacuna* or *Aplysina insularis* BA07ES-90. (a) Fraction F1 (eluted with 8:2 H_2O/MeOH); (b) Fraction F2 (eluted with 1:1 H_2O/MeOH); (c) Fraction F3 (eluted with 100% MeOH). LC-PDA-MS analyses were performed using the conditions as in the experimental section. Peak assignments: see Figure 2. Peak at 15.8 min corresponds to 11-keto-fistularin-3 (**13**).

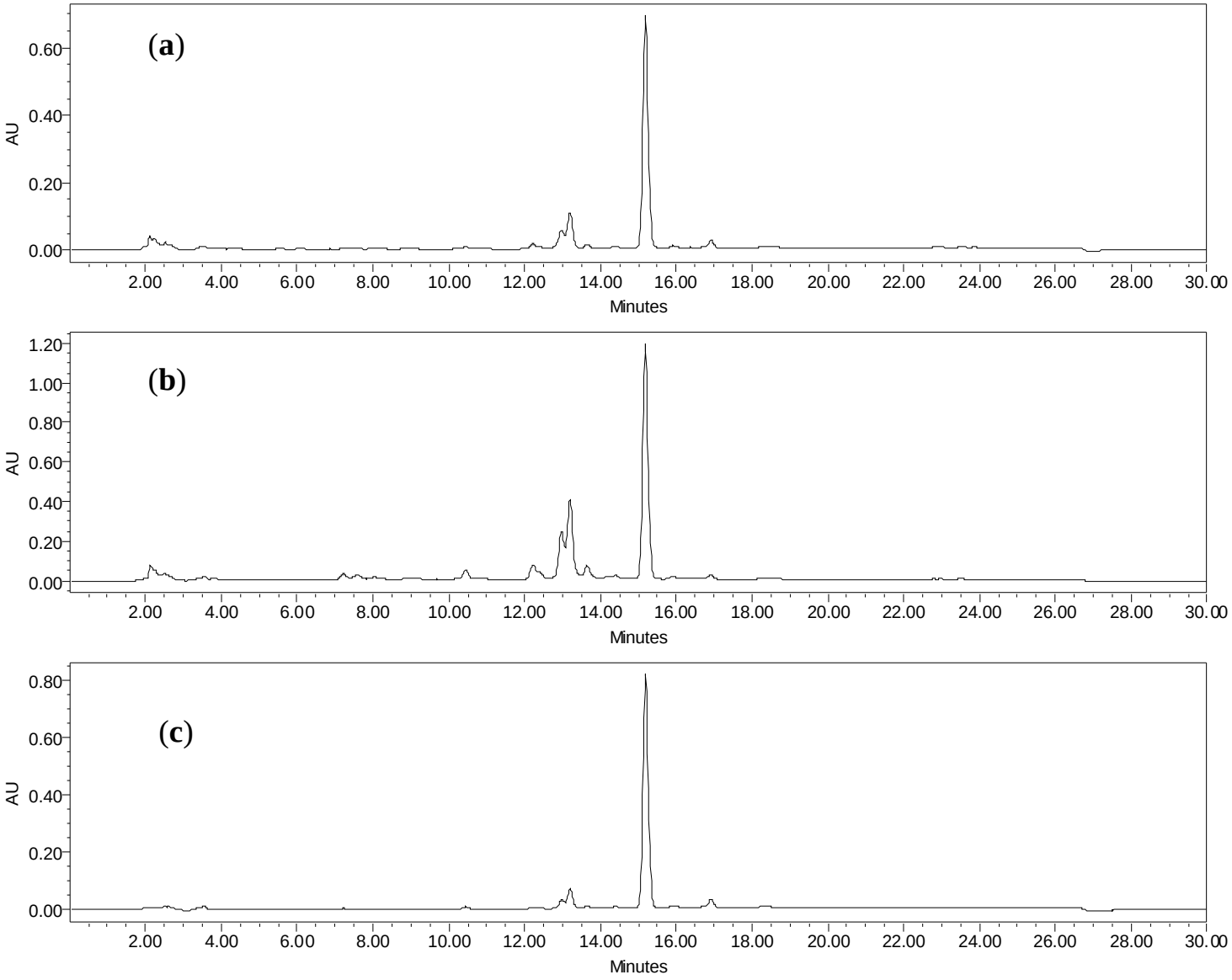

Figure S10 – Chromatographic analyses (LC-PDA-MS) of the SPE fractions (F1, F2 and F3) obtained from the EtOAc crude extract of *Aplysina* sp. BA07ES-91. (a) Fraction F1 (eluted with 8:2 H_2O/MeOH); (b) Fraction F2 (eluted with 1:1 H_2O/MeOH); (c) Fraction F3 (eluted with 100% MeOH). LC-PDA-MS analyses were performed using the conditions as in the experimental section. Peak assignments: see Figure 2.

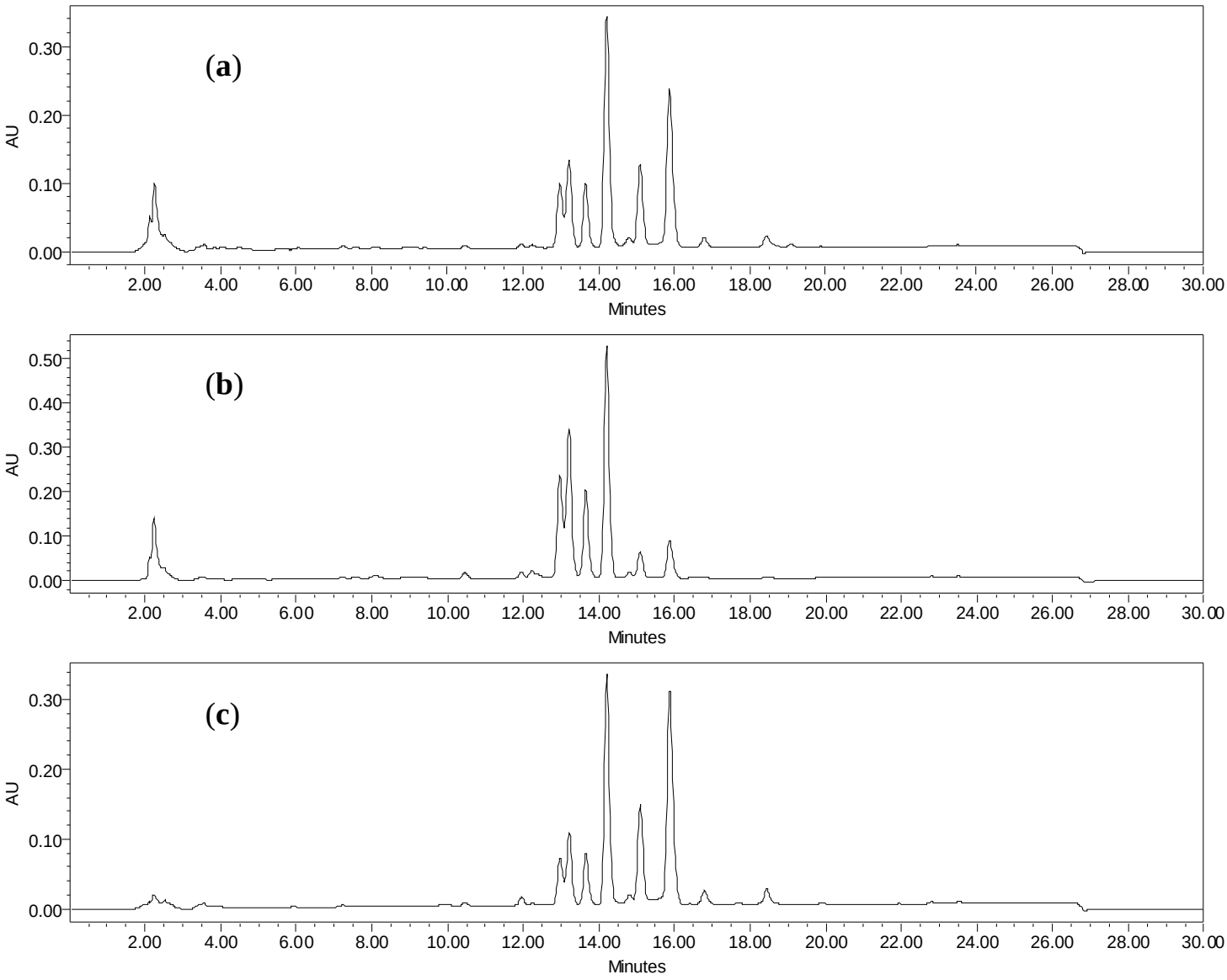

Figure S11 – Chromatographic analyses (LC-PDA-MS) of the SPE fractions (F1, F2 and F3) obtained from the EtOAc crude extract of *Aplysina* sp. BA07ES-92. (a) Fraction F1 (eluted with 8:2 H_2O/MeOH); (b) Fraction F2 (eluted with 1:1 H_2O/MeOH); (c) Fraction F3 (eluted with 100% MeOH). LC-PDA-MS analyses were performed using the conditions as in the experimental section. Peak assignments: see Figure 2. Peak at 15.8 min corresponds to 11-keto-fistularin-3 (**13**).

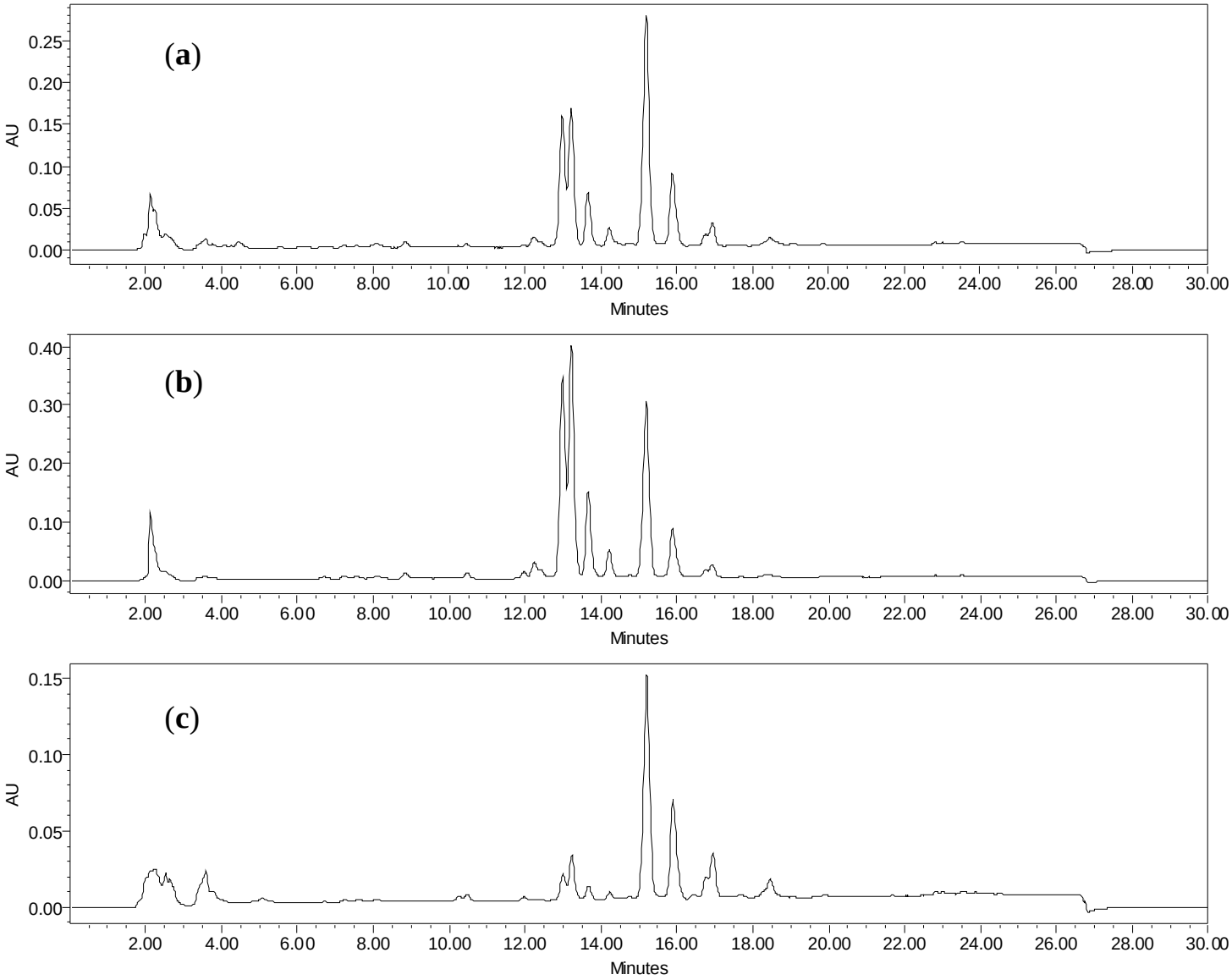

Figure S12 – Chromatographic analyses (LC-PDA-MS) of the SPE fractions (F1, F2 and F3) obtained from the EtOAc crude extract of *Aplysina* sp. BA07ES-94. (a) Fraction F1 (eluted with 8:2 H_2O/MeOH); (b) Fraction F2 (eluted with 1:1 H_2O/MeOH); (c) Fraction F3 (eluted with 100% MeOH). LC-PDA-MS analyses were performed using the conditions as in the experimental section. Peak assignments: see Figure 2. Peak at 15.8 min corresponds to 11-keto-fistularin-3 (**13**).

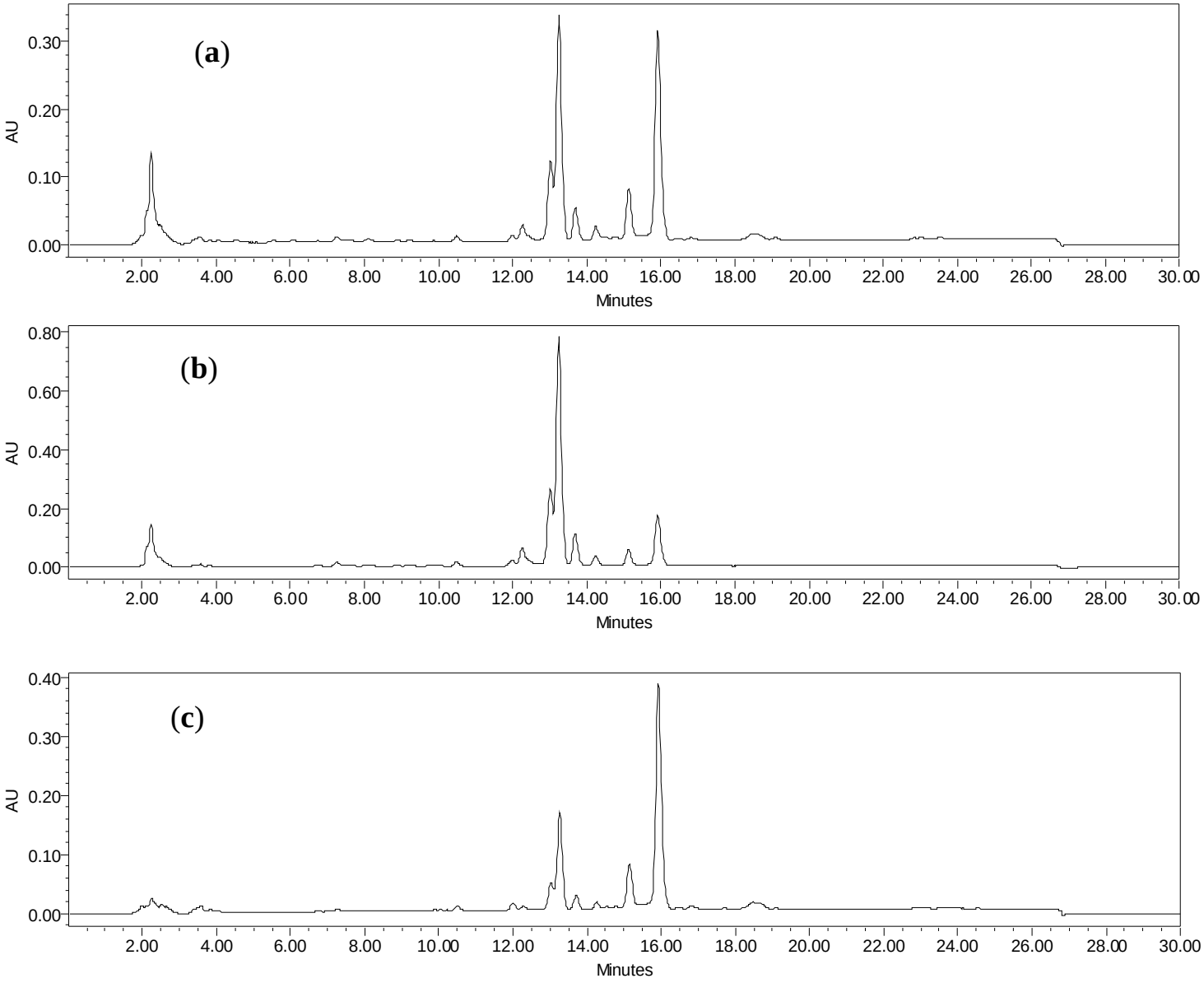

Figure S13 – Chromatographic analyses (LC-PDA-MS) of the SPE fractions (F1, F2 and F3) obtained from the EtOAc crude extract of *Aplysina* sp. BA07ES-108. (a) Fraction F1 (eluted with 8:2 H_2O/MeOH); (b) Fraction F2 (eluted with 1:1 H_2O/MeOH); (c) Fraction F3 (eluted with 100% MeOH). LC-PDA-MS analyses were performed using the conditions as in the experimental section. Peak assignments: see Figure 2. Peak at 15.8 min corresponds to 11-keto-fistularin-3 (**13**).

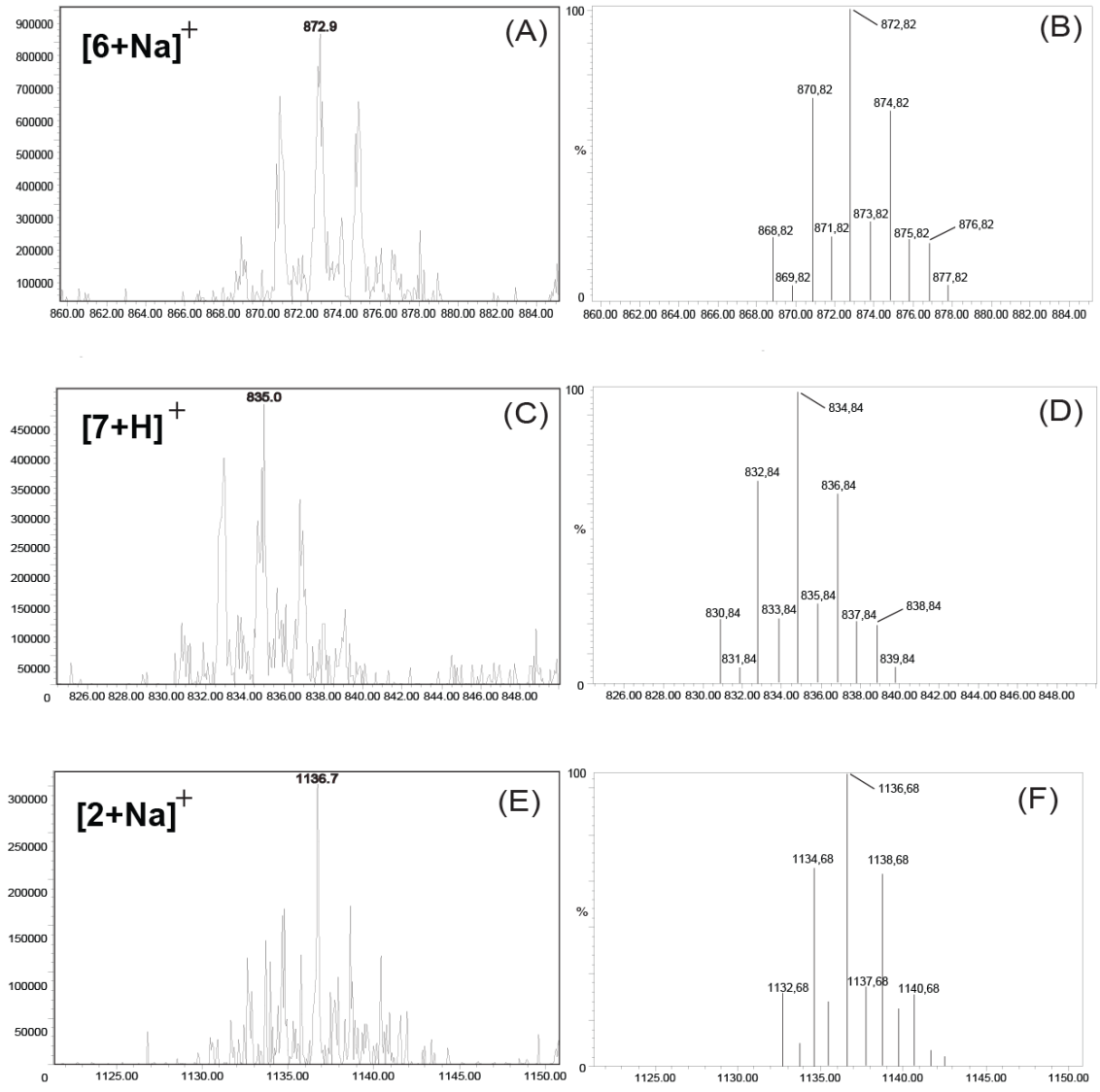

Figure S14. ESI-MS spectra (protonated or sodiated region) of **6**, **7** and **2**, as well as their respective theoretical isotopic distribution**.** [(B) - *m/z*: 872.8239 (100.0%), 870.8260 (68.5%), 874.8219 (64.9%), 873.8273 (26.0%), 871.8293 (17.8%), 868.8280 (17,6%), 875.8252 (16.9%), 876.8198 (15.8%), 869.8314 (4.6%), 877.8232 (4.1%], **7** [(D) - *m/z*: 834.8471 (100.0%), 832.8491 (68.5%), 836.8450 (64.9%), 835.8504 (26.0%), 833.8525 (17.8%), 830.8512 (17.6%), 837.8484 (16.8%), 838.8430 (15.8%), 831.8545 (4.6%), 839.8463 (4.1%)] and **2** [(F) - *m/z*: 1136.6848 (100.0%), 1134.6868 (77.1%), 1138.6827 (73.0%), 1137.6881 (33.6%), 1132.6889 (31.7%), 1140.6807 (28.4%), 1135.6902 (25.9%), 1139.6861 (24.5%), 1133.6922 (10.6%), 1141.6840 (9.5%), 1138.6915 (5.4%), 1130.6909 (5.4%), 1142.6786 (4.6%), 1136.6935 (4.2%), 1140.6894 (4.0%)].