Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Electronic Supplementary Information for

6- and 14-Fluoro Farnesyl Diphosphate: Mechanistic Probes for Reaction Catalysed by Aristolochene Synthase

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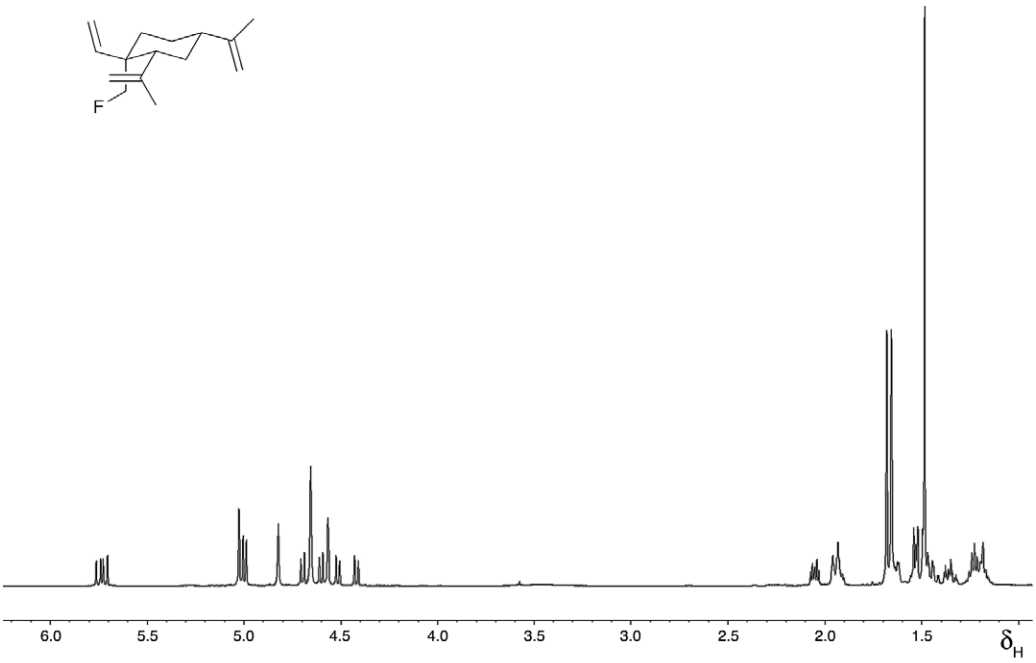

Figure S1. ^{1}H NMR spectrum (500 MHz, $C^{2}HCl_3$) of elemene derived from 14-fluorogermacrene A

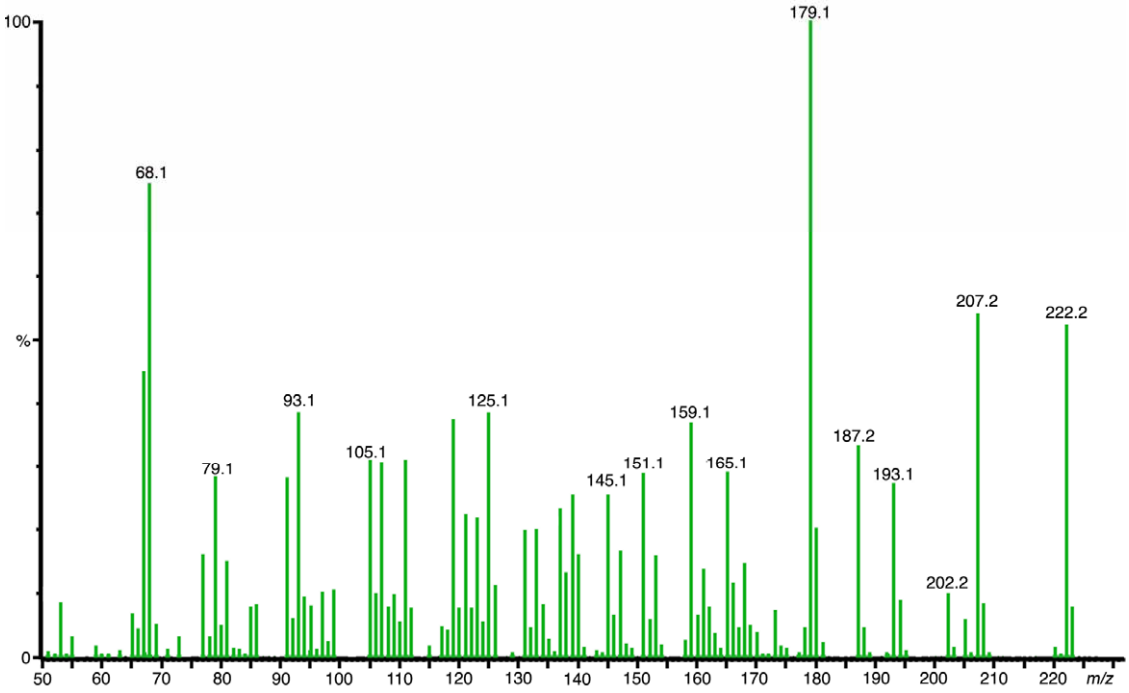

Figure S2. Mass spectrum of compound eluting at 27.4 min from incubation of 6F-FPP (**1b**) with PR-AS.

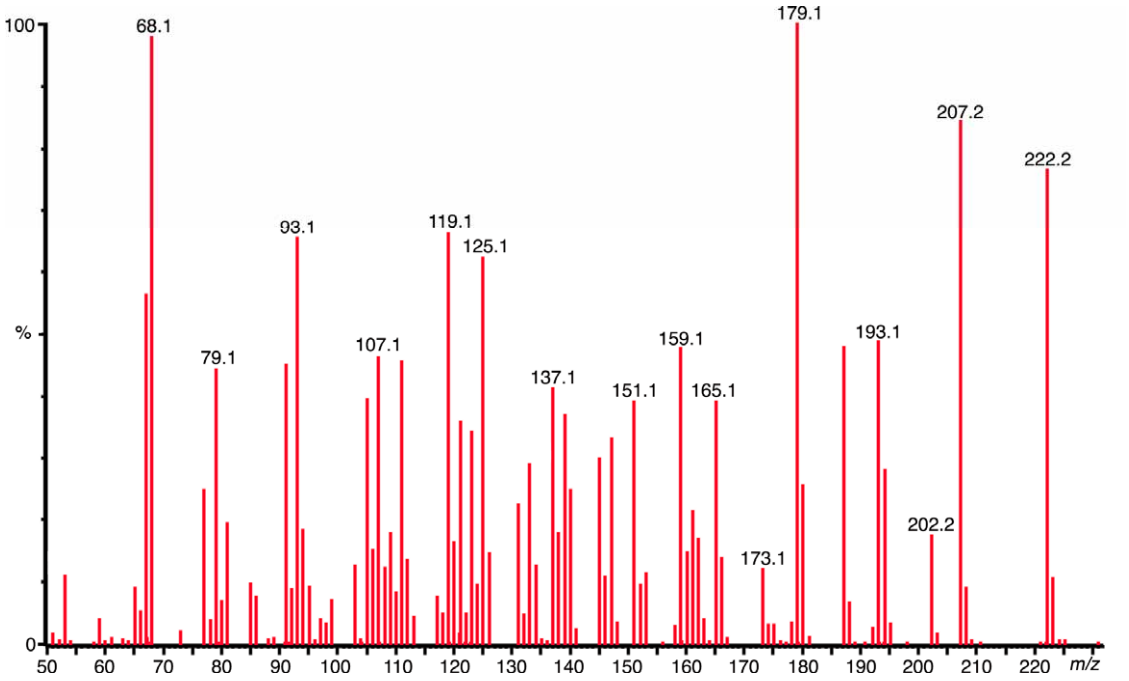

Figure S3. Mass spectrum of compound eluting at 28.0 min from incubation of 6F-FPP (**1b**) with PR-AS.

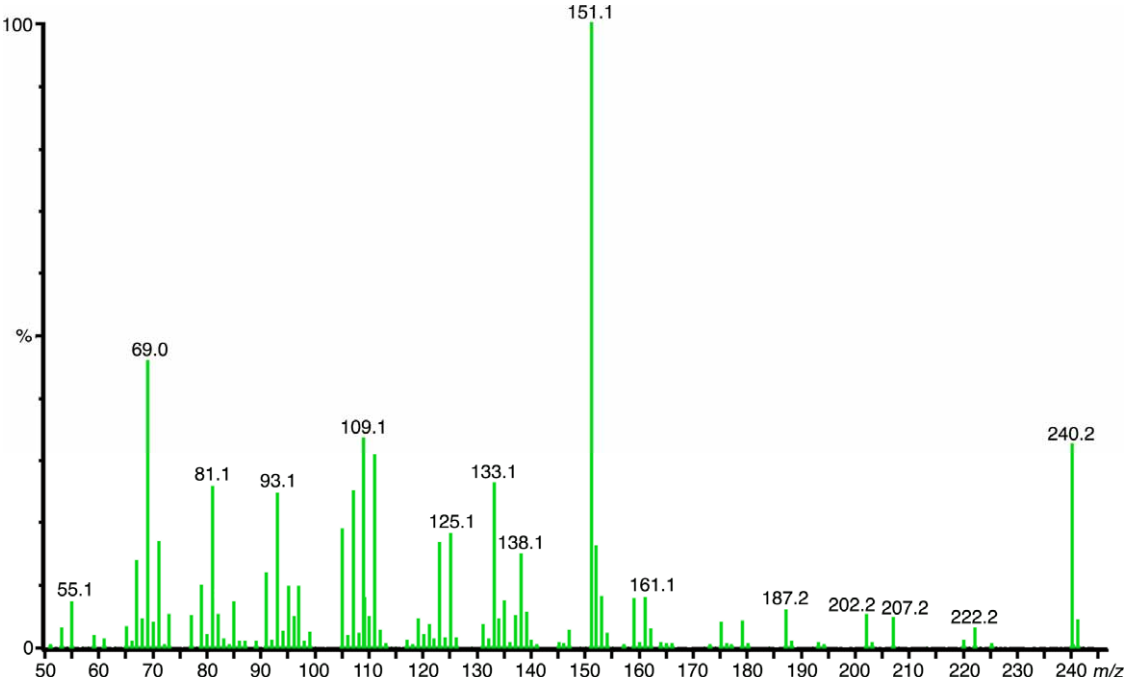

Figure S4. Mass spectrum of compound eluting at 29.4 min from incubation of 6F-FPP (**1b**) with PR-AS.

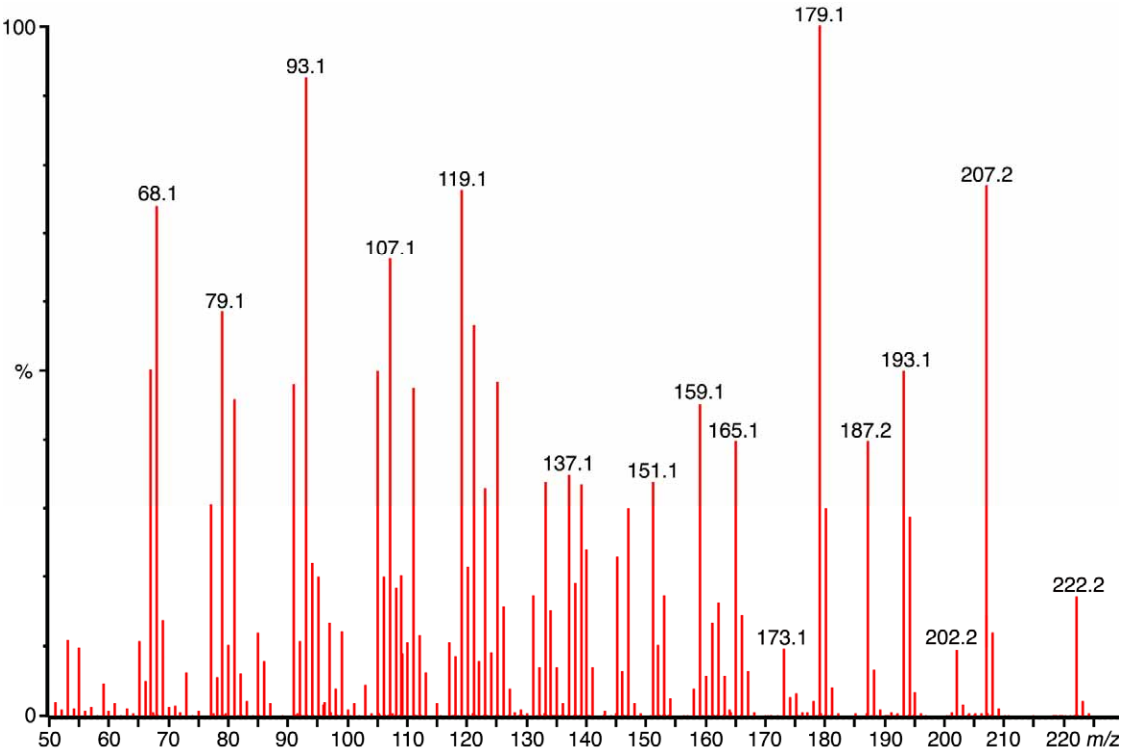

Figure S5 Mass spectrum of compound eluting at 23.6 min from incubation of 6F-FPP (**1b**) with PR-AS and after thermal rearrangement at 300 °C.

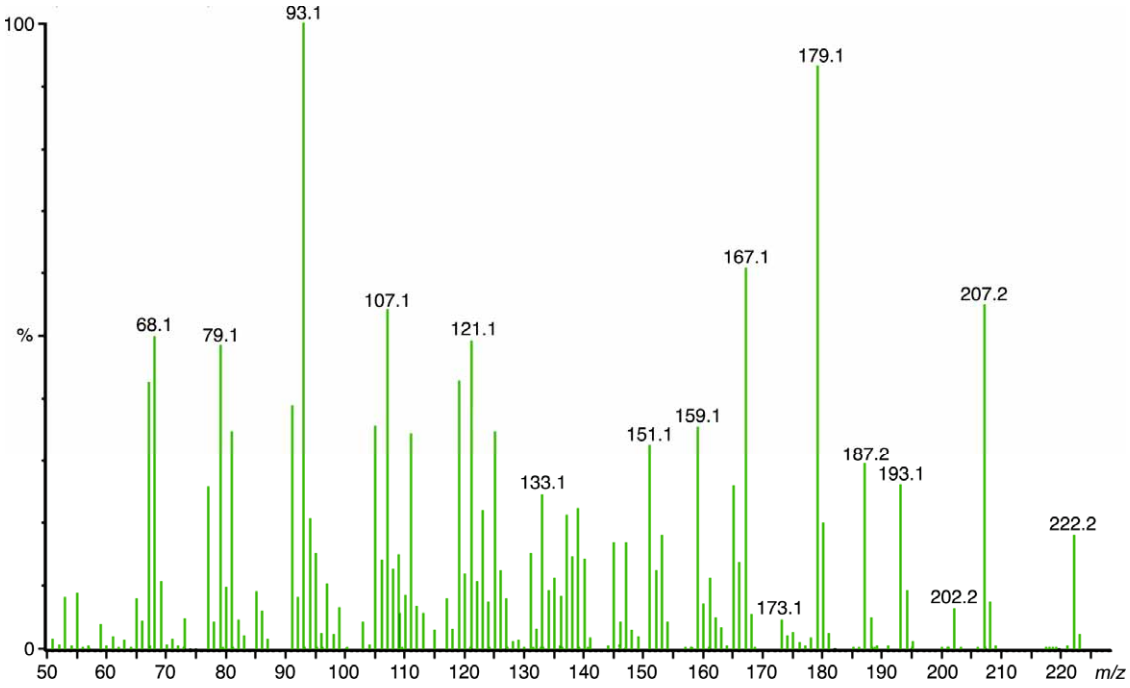

Figure S6. Mass spectrum of compound eluting at 23.5 min from incubation of 6F-FPP (**1b**) with PR-AS and after thermal rearrangement at 300 °C.

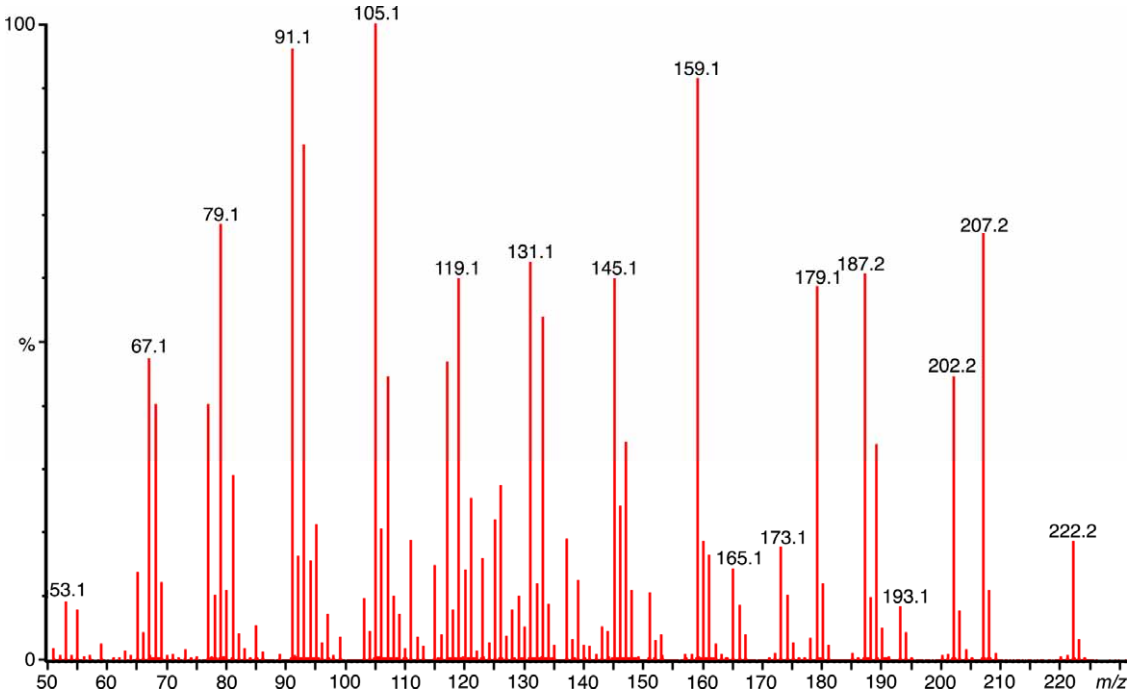

Figure S7. Mass spectrum of compound eluting at 29.1 min from incubation of 14F-FPP (**1c**) with PR-AS.

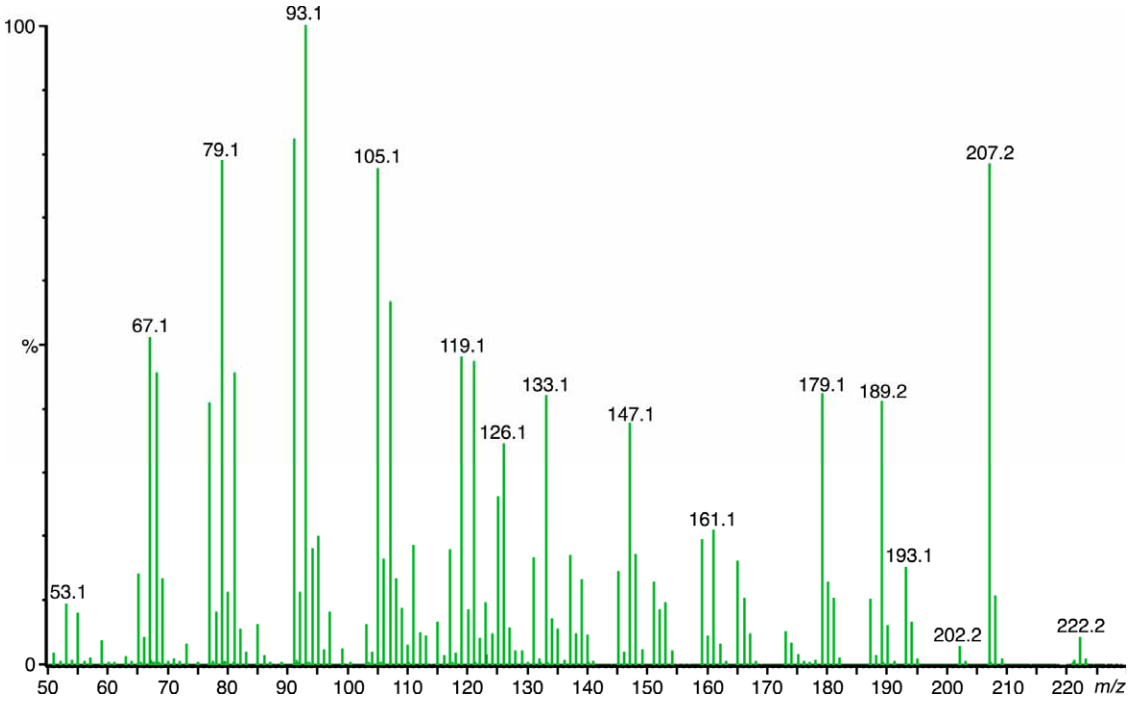

Figure S8. Mass spectrum of compound eluting at 24.8 min from incubation of 14F-FPP (**1c**) with PR-AS and after thermal rearrangement at 300 °C.