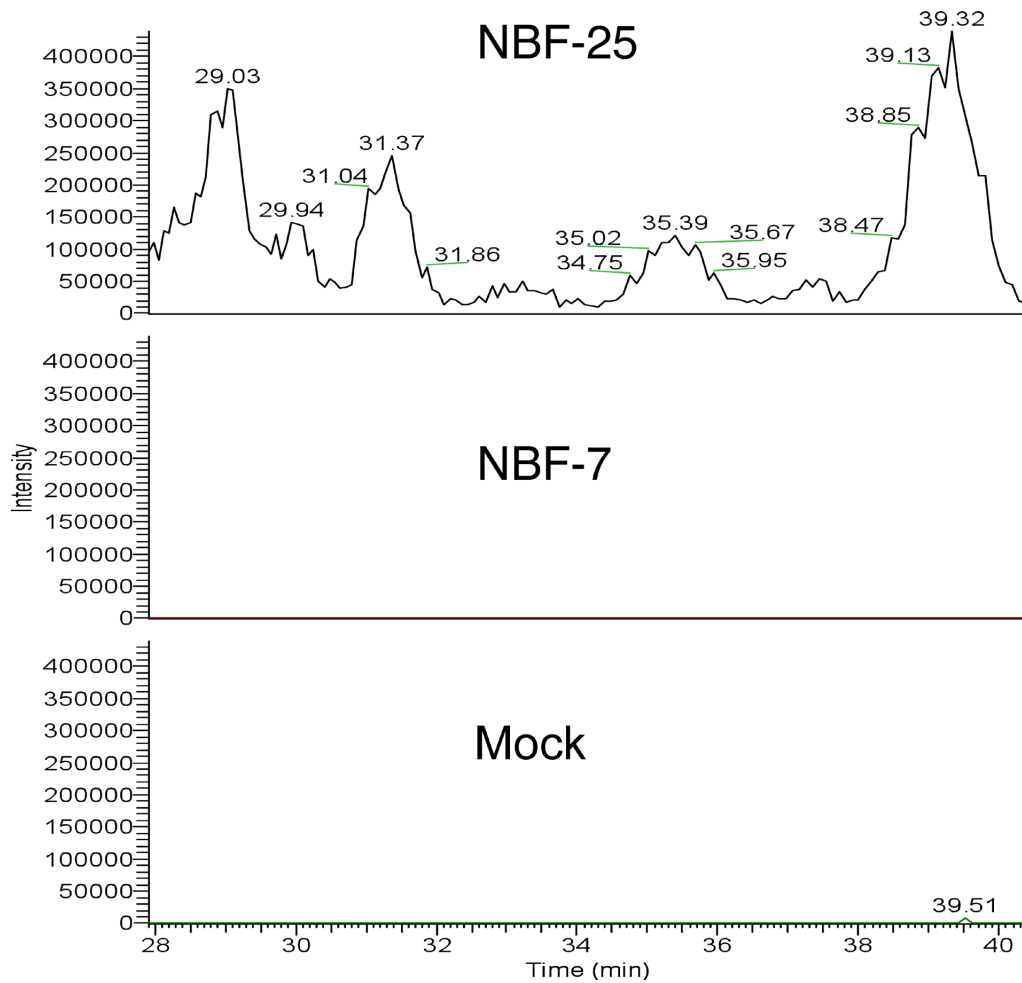


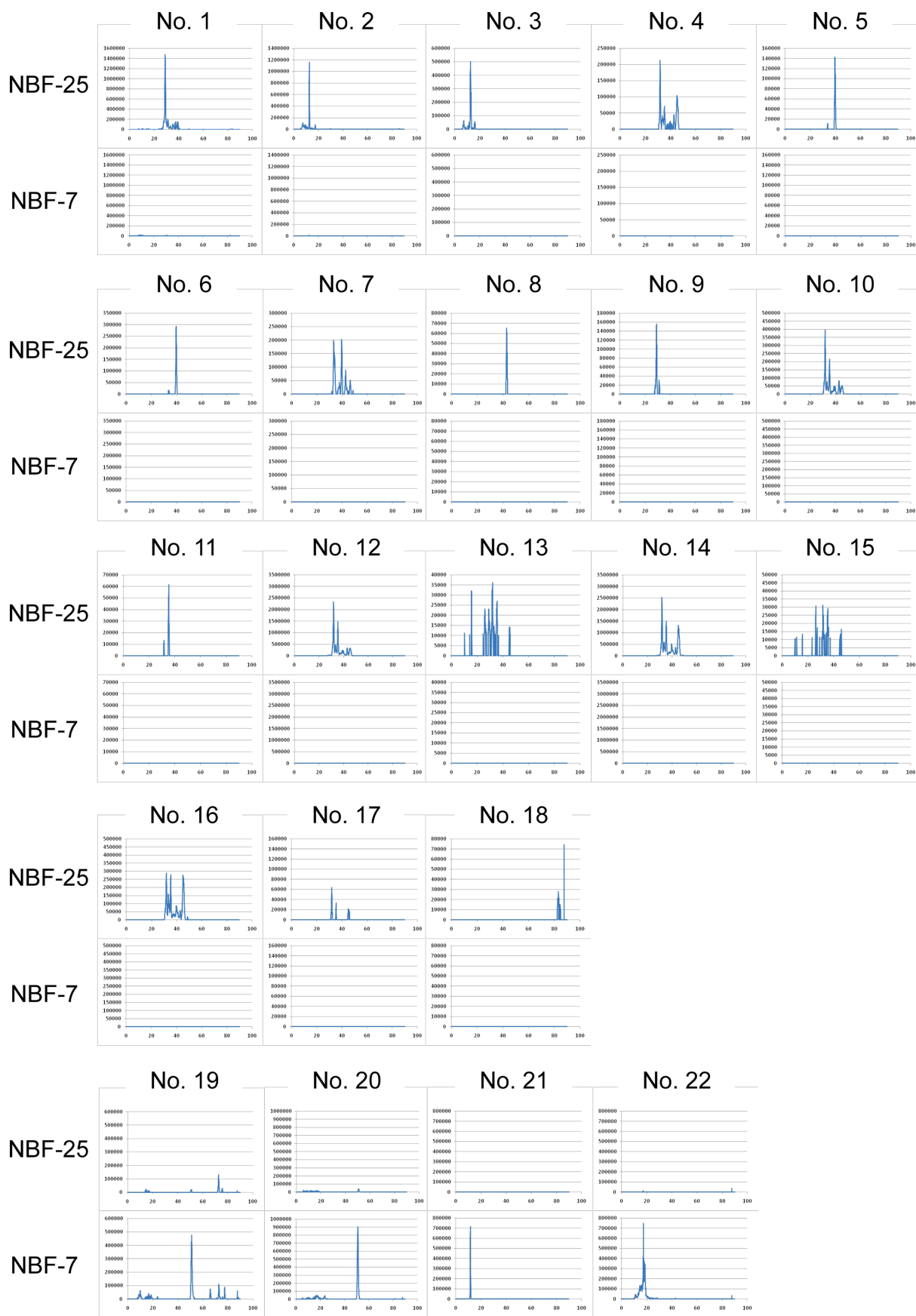
Supplemental Figure S1. Molecular structures of phorbol esters (PEs) found in *Jatropha curcas* L (adopted from Haas et al. 2002). (A) The common diterpene, 12-deoxy-16-hydroxyphorbol. (B-F) The acid moiety of C1 (B), C2 (C), C3 (E), C4 and C5 (D), and C6 (F).

LC Conditions	Analyzer	Agilent 1200 series	
	Buffer A/B	Water/Acetonitrile	
	Column	TOSOH TSKgel ODS-100V 5 µm Part no. 21456	
	Guard column	TOSOH TSKguardgel ODS-100V 5 µm Part no. 21453	
	Column Temperature	25°C	
	Flow rate ml/min	500 µl/min	
	Gradient B%	80%:0 min, 80%:60 min, 98%:70 min, 98%:80 min, 80%:80.1 min, 80%:90 min	
	Injection volume	40 arbitrary units	
Internal Standard Conditions	Materials	Lidcaine, Prochloraz, Reserpine, Rifampicin, Aureobasidin A	
	Flow rate	15 µl/min	
PDA		200-650nm	
MS Conditions	Analyzer	LTQ ORBITRAP XL	
	Ionization mode	APCI positive-ion	
	Scan type	Full	
	Vaporizer Temp(APCI)	300	
	DischargeCurrent(APCI)	6	
	Nitrogen Sheath Gas Flow rate	40 arbitrary units	
	Aux Gas Flow rate	15 arbitrary units	
	Spray Voltage(ESI)	-	
	Capillary Temp	200 °C	
	Spray position(x.y.z)	0,1,C	
	Lock mass on/off	on	
	Lock mass	235.18049, 376.03808, 609.28065, 823.41240, 1101.69583	
	Full MS Conditions (ScanEvent 1)	Analyzer	Orbitrap
		mass range	100-1500
Data type		Centroid	
Scan type		Full	
Resolution		60,000	
MSMS Conditions (ScanEvent 2~6)	Analyzer	Ion Trap	
	Collision energy	35%	
	Target selection	5 most abundant precursor ions detected by Full MS	
	Reject Mass	102.09, 103.09, 113.07, 124.09, 140.08, 141.10, 155.12, 157.04, 233.17, 235.18, 308.00, 376.04, 379.04, 380.03, 391.28, 609.28, 641.27, 821.40, 822.40, 823.40, 823.41, 904.47, 1101.70, 1102.70	
	Data type	Centroid	
	Resolution	-	

Supplemental Figure S2.



Supplemental Figure S3. The m/z 711 mass chromatograms of the seed kernel extracts of NBF-25 (upper panel) and NBF-7 (middle panel). The vertical and horizontal axes represented the signal intensities and retention time, respectively. Black boxes in upper panel overlapped with peaks on PDA chromatogram (279.5 to 280.5 nm), which are shown in Figure 1G.



Supplemental Figure S4. Mass chromatograms of the accession-specific metabolites. The vertical and horizontal axes represented the signal intensities and retention times, respectively. For the m/z information of each peak, please see Table 1.