Article title: Climatic history, constraints, and the plasticity of phytochemical traits under water stress
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Appendix S2. Table S1. Analytical information for the UV-absorbent chemistry of plants in the glasshouse drought experiment.

Species	Tissue	Retention time (min)-LCUV	RT-LCMS	m/z neg*	m/z pos*	MW	sum formula	UV spectra	fragments neg m/z	fragments pos m/z	**Tentative** ID	References
Asclepias fascicularis	leaf	6.82	7.3	***609.1462***[a]	***611.1609***[c]	610	C27H30O16			303 465	Quercetin-glucoside-rhamnoside	Haribal, M. & J. A. A. Renwick. 1996. Oviposition stimulants for the monarch butterfly: flavonol glycosides from *Asclepias curassavica*. Phytochemistry 41: 139-144. compound #3
Asclepias fascicularis	leaf	7.958	8.2	***593.1514***[a]	***595.166***[c]	594	C27H30O15			387 449	Kaempferol-glucoside-rhamnoside	El-Askary, H. 2003. Pregnene glycoside and monoterpene derivative from *Solenostemma argel* Hayne. Bull Fac Pharm Cairo University. 41: 131-137. compound #3
Asclepias fascicularis	leaf	17.366	17.8	***962.4746***[b]	***918.4838***[c]	917	C48H71N1O16				pregnane glycoside	Warashina, T., & N. Tadataka. 1996. Steroidal glycosides from roots of *Cynanchum caudatum*. III. Chemical & Pharmaceutical Bulletin 44: 358-363. compound #3
Asclepias fascicularis	leaf	20.354										
Asclepias fascicularis	leaf	21.461	22.5	***931.4667***[a] ***/977.4763***[b] ***950.5091***[d]		932	C49H72O17		809	309 327 345	benzoylated pregnane glycoside	Oberai, K., M. P. Khare, A. Khare. 1985. A pregnane ester triglycoside from *Sarcostemma brevistigma*. Phytochemistry. 24: 3011-3013. compound #1
Asclepias fascicularis	leaf	21.947	22.9	***931.4673***[a] ***/977.4735***[b] ***950.5103***[d]		932	C49H72O17		809		benzoylated pregnane glycoside	Oberai, K., M. P. Khare, A. Khare. 1985. A pregnane ester triglycoside from *Sarcostemma brevistigma*. Phytochemistry. 24: 3011-3013. compound #1
Asclepias fascicularis	leaf	22.237	23.3	915.6[a]	939.5[e]	916	C49H72O16		731 749	311 329	benzoylated pregnane glycoside	Vleggar, R., F. R. Van Heerden, L. A. P. Anderson, G. L. Erasmus. 1993. Toxic constituents of the Asclepiadaceae. Structure elucidation of sarcovimiside A-C, pregnane glycosides of *Sarcostemma viminale*. Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999). 483-487. compound #A6
Asclepias fascicularis	leaf	24.009	25.1	1075.6[a]	1099.6[e]	1076	C63H80O15		953	309 327 345	benzoylated pregnane glycoside	
Asclepias fascicularis	leaf	24.823	25.9	1059.7[a]	1083.6[e]	1060	C63H80O14		937	311	saponin	Sylla, B., S. Levoie, J. Legault, C. Gauthier, A. Pichette. 2019. Synthesis, cytotoxicity and anti-inflammatory activity of rhamnose-containing ursolic and betulinic acid saponins. RSC Advances 9: 39743-39757.compound #18
Asclepias fascicularis	root	6.351		***565.1924***[b]	***538.2288***[d]***; 543.1845***[e]***; 559.1578***[f]	520	C26H32O11				phenolic	
Asclepias fascicularis	root	7.307		***581.2236***[a]	***600.2655***[d]***; 543.1845***[e]***; 559.1578***[f]	582	C28H38O13				phenolic	
Asclepias fascicularis	root	11.32										
Asclepias fascicularis	root	11.527										
Asclepias fascicularis	root	15.991	16.6	841.5[b]	819.5[e]	796	C42H68O14				pregnane glycoside	Warashina, T. & T. Noro. 2000. Cardenolide and oxypregnane glycosides from the root of *Asclepias incarnata* L. Chemical & Pharmaceutical Bulletin. 48: 516-524. compound #3
Asclepias fascicularis	root	17.554	18.3	939.6[a]	963.5[e]	940	C49H80O17				pregnane glycoside	Fumiko, A. & T. Yamauchi. 2000. Pregnane glycosides from the roots of *Asclepias tuberosa*. Chemical & Pharmaceutical Bulletin. 48: 1017-1022. compound #13
Asclepias fascicularis	root	19.17	19.5	939.6[a]	963.5[e]	940	C49H80O17				pregnane glycoside	Fumiko, A. & T. Yamauchi. 2000. Pregnane glycosides from the roots of Asclepias tuberosa. Chemical & Pharmaceutical Bulletin. 48: 1017-1022. compound #13
Asclepias fascicularis	root	20.354										
Asclepias fascicularis	root	21.461		***931.4667***[a] ***/977.4763***[b] ***950.5091***[c]		932	C49H72O17				benzoylated pregnane glycoside	Oberai, K., M. P. Khare, A. Khare. 1985. A pregnane ester triglycoside from *Sarcostemma brevistigma*. Phytochemistry. 24: 3011-3013. compound #1
Asclepias fascicularis	root	21.947		***931.4673***[a] ***/977.4735***[b] ***950.5103***[c]		932	C49H72O17				benzoylated pregnane glycoside	Oberai, K., M. P. Khare, A. Khare. 1985. A pregnane ester triglycoside from *Sarcostemma brevistigma*. Phytochemistry. 24: 3011-3013. compound #1
Asclepias fascicularis	root	22.197									benzoylated pregnane glycoside	
Asclepias fascicularis	root	22.237		915.6[a]	939.5[e]	916	C49H72O16				benzoylated pregnane glycoside	Vleggar, R., F. R. Van Heerden, L. A. P. Anderson, G. L. Erasmus. 1993. Toxic constituents of the Asclepiadaceae. Structure elucidation of sarcovimiside A-C, pregnane glycosides of *Sarcostemma viminale*. Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999). 483-487. compound #A6
Asclepias speciosa	leaf	6.82	7.3	***609.1462***[a]	***611.1609***[c]	610	C27H30O16				Quercetin-glucoside-rhamnoside	Haribal, M. & J. A. A. Renwick. 1996. Oviposition stimulants for the monarch butterfly: flavonol glycosides from *Asclepias curassavica*. Phytochemistry 41: 139-144. compound #3
Asclepias speciosa	leaf	7.774	8.3	463.0[a]	465.0[c]	464	C21H20O12			303	Quercetin-glucoside	
Asclepias speciosa	leaf	8.766	9.4	477.1[a]	479.1[c]	478	C22H22O12			317	Isorhamnetin-glucoside	
Asclepias speciosa	leaf	17.366	18.3	807.5[b]	785.5[e]	762			613			
Asclepias speciosa	leaf	17.841										
Asclepias speciosa	leaf	20.354	21.4	675.4[a]	699.3[e]	676	C33H56O14		397 415			
Asclepias speciosa	root	7.307										
Asclepias speciosa	root	7.572	8.1	***581.2238***[a]	***600.2651***[d]	582	C28H38O13		401			
Asclepias speciosa	root	7.774	8.4	***551.2132***[a]	***570.2554***[d]	552	C27H36O12					
Asclepias speciosa	root	11.527	12	953.3[a]	977.3[e]	954			757			
Asclepias speciosa	root	13.93	14.5	843.5[b]	821.5[e]	798	C42H70O14					
Asclepias speciosa	root	15.991	16.5	***616.2216***[a]		617	C31H39N1O10S1		491	311	labriformin (cardenolide)	Cardenolides in the latex and leaves of seven Asclepias species and Calotropis procera: Seiber, James N.; Nelson, Carolyn J.; Lee, S. Mark; Phytochemistry,Volume21, Issue9, Pages2343-8, 1982. compound #10
Asclepias speciosa	root	17.554	18.1	939.6[a]	963.5[e]	940	C49H80O17				pregnane glycoside	Fumiko, A. & T. Yamauchi. 2000. Pregnane glycosides from the roots of *Asclepias tuberosa*. Chemical & Pharmaceutical Bulletin. 48: 1017-1022. compound #13
Asclepias speciosa	root	18.532	19.5	939.6[a]	963.5[e]	940	C49H80O17			617	cinnamoylated pregnane glycoside	Fumiko, A. & T. Yamauchi. 2000. Pregnane glycosides from the roots of *Asclepias tuberosa*. Chemical & Pharmaceutical Bulletin. 48: 1017-1022. compound #13
Asclepias speciosa	root	19.77	20.8	1265.7[a]	1289.7[e]	1266					cinnamoylated pregnane glycoside	
Asclepias speciosa	root	20.354	21.4	947.5[b]	925.5[e]	902			679			

**Values for m/z of molecular ion and fragment ions from low resolution mass spectrometry (LC-ESI-IonTrap-MS); values in bold and italics from high-resolution mass spectrometry (LC-ESI-Q-ToF-MS)*

[a] $[M-H]^-$
[b] $[M+HCOOH-H]^-$
[c] $[M+H]^+$
[d] $[M+NH4]^+$
[e] $[M+Na]^+$
[f] $[M+K]^+$