

Supplementary Table 2. Chromatographic and spectral data used for the identification and relative quantification of benzyloisoquinoline alkaloids by LC-MS. The listed compounds were substrates and reaction products, or were major BIAs in opium poppy latex. Following liquid chromatography, molecular parent ions were generated, focused using positive-mode electrospray ionization (ESI[+]), and subjected to mass spectrometry. ESI[+]-CID spectra were compared with spectra obtained from authentic standards or from the indicated reference to identify or annotate compounds. The characterization of compounds without reference spectra was inferred as described in the Materials and Methods.

Compound	[M+H] ⁺	Ret. time (min)	CE (eV)	ESI-CID, <i>m/z</i> (Relative abundance)	Characterization criteria
Morphine	286	0.91	25	286 (100), 268 (4), 229 (10), 227 (4), 211 (10), 209 (6), 201 (23), 193 (5), 185 (10), 183 (12), 173 (11), 165 (7), 155 (6), 123 (1), 58 (7)	Authentic standard
Codeine	300	3.18	35	300 (100), 282 (5), 266 (2), 243 (8), 241 (1), 225 (3), 215 (24), 199 (14), 183 (14), 165 (8), 155 (1), 137 (3), 58 (11)	Authentic standard
Thebaine	312	6.4	25	312 (2), 281 (2), 266 (4), 255 (1), 251 (11), 249 (2), 237(1), 234 (2), 223 (2), 221 (7), 218 (4), 195 (2), 177 (1), 58 (100)	Authentic standard
Norreticuline	316	3.64	25	316 (1), 267 (1), 254 (1), 237 (1), 221 (1), 178 (100), 161 (12), 151 (5), 143 (19), 137 (22)	Gesell et al. 2009; Pienkny et al. 2009
Scoulerine	328	3.11	25	328 (25), 178 (100), 151 (5)	Authentic standard
Reticuline	330	2.77	25	330 (2), 298 (2), 267 (3), 239 (2), 227 (1), 207 (2), 192 (100), 175 (23), 151 (3), 143 (17), 137 (30)	Authentic standard
Norcodamine	330	3.07	25	178.2 (100), 175.2 (16), 163.3 (6), 151.2 (29), 143 (19)	Inferred
Papaverine	340	8.08	25	340 (86), 324 (59), 310 (2), 296 (9), 202 (100), 187 (3), 171 (11), 123 (2)	Authentic standard

Tetrahydrocolumbamine	342	3.93	25	342 (14), 327 (1), 265 (1), 192 (15), 178 (100), 165 (7), 163 (2), 151 (6), 58 (1)	Authentic standard
Codamine	344	3.14	25	192 (100), 177 (7), 175.2 (13), 151 (23), 143 (17)	Inferred
Tetrahydropapaverine	344	3.87	20	344 (1), 327 (2), 312 (2), 296 (10), 281 (4), 192 (100), 189 (38), 174 (17), 165 (3), 158 (8), 151 (46), 136 (1)	Authentic standard
Tetrahydropalmatine	356	4.44	20	356 (48), 192 (100), 176 (13), 165 (27), 150 (3)	Authentic standard
Laudanosine	358	3.44	25	358 (3), 327 (3), 312 (1), 296 (4), 206 (100), 189 (34), 174 (10), 165 (8), 158 (5), 151 (29), 44 (1)	Schmidt et al. 2007
Narcotoline	400	7.9	20	400 (65), 382 (5), 351 (16), 339 (47), 309 (4), 206 (100), 192 (4), 165 (13)	Authentic standard
Noscapine	414	10.17	25	414 (4), 365 (5), 353 (21), 323 (5), 220 (100), 206 (4), 179 (8)	Authentic standard