

Table SII List of metabolites for which one-dimensional ^1H NMR signatures are available in a Chenomx NMR Suite compound database customized for opium poppy. An asterisk denotes a metabolite not present in the standard Chenomx library, but added to the customized database.

1.	Acetaldehyde	36.	<i>N</i> -Carbamoylaspartate
2.	Acetamide	37.	<i>N</i> -Carbamoyl- β -alanine
3.	Acetate	38.	Cholate
4.	Acetoacetate	39.	Choline
5.	Acetone	40.	Cinnamate *
6.	<i>N</i> -Acetylaspartate	41.	Citrate
7.	<i>N</i> -Acetylglutamate	42.	Citrulline
8.	Acetylsalicylate	43.	Codeine *
9.	<i>N</i> -Acetyltyrosine	44.	Coumarate *
10.	<i>cis</i> -Aconitate	45.	Cysteine
11.	<i>trans</i> -Aconitate	46.	Cystine
12.	Adenine	47.	Cytosine
13.	Adenosine	48.	2'-Deoxyadenosine
14.	Adenosine diphosphate *	49.	2'-Deoxyguanosine
15.	Adenosine triphosphate *	50.	2'-Deoxyinosine
16.	<i>S</i> -Adenosylhomocysteine	51.	1,3-Dihydroxyacetone
17.	<i>S</i> -Adenosylmethionine *	52.	5,6-Dihydrothymine
18.	Alanine	53.	5,6-Dihydrouracil
19.	β -Alanine	54.	Dihydroxyacetone phosphate *
20.	Alloisoleucine	55.	Dimethylamine
21.	2-Aminobutyrate	56.	<i>N,N</i> -Dimethylformamide
22.	4-Aminobutyrate	57.	<i>N,N</i> -Dimethylglycine
23.	3-Aminoisobutyrate	58.	1,7-Dimethylxanthine
24.	Anserine	59.	L-DOPA *
25.	Arginine	60.	Dopamine *
26.	Asparagine	61.	Erythrose-4-phosphate *
27.	Aspartate	62.	Ethanol
28.	Benzoate	63.	Ethanolamine
29.	Betaine	64.	Ethylene glycol
30.	Biotin	65.	Ethylmalonate
31.	Butanone	66.	Ferulate
32.	Butyrate	67.	Formate
33.	Caffeate *	68.	Fructose
34.	Caprate	69.	Fructose-1,6-bisphosphate *
35.	Caprylate	70.	Fructose-6-phosphate *

71. Fucose
72. Fumarate
73. 2-Furoate
74. Galactarate
75. Galactonate
76. Galactose
77. Glucarate
78. Glucitol
79. Gluconate
80. Glucose
81. Glucose-6-phosphate *
82. Glutamate
83. Glutamine
84. γ -Glutamylphenylalanine
85. Glutarate
86. Glutaric acid monomethyl ester
87. Glutathione
88. Glycerate
89. Glycerol
90. Glycine
91. Glycolate
92. Glycylproline
93. Guanidoacetate
94. Histadine
95. Homocitrulline
96. Homocysteine
97. Homoserine
98. Homovanillate
99. *trans*-4-Hydroxy-L-proline
100. 4-Hydroxybenzoate
101. 2-Hydroxybutyrate
102. 3-Hydroxybutyrate
103. 4-Hydroxybutyrate
104. 2-Hydroxyglutarate
105. 3-Hydroxyisovalerate
106. 5-Hydroxyindole-3-acetate
107. 5-Hydroxylysine
108. 3-Hydroxy-3-methylglutarate
109. 4-Hydroxy-3-methoxymandelate
110. 2-Hydroxy-3-methylvalerate
111. 3-Hydroxyphenylacetate
112. 4-Hydroxyphenylacetate
113. 2-Hydroxyvalerate
114. Hypoxanthine
115. Imidazole
116. Indole-3-acetate
117. Inosine
118. *myo*-Inositol
119. Isobutyrate
120. Isocaproate
121. Isocitrate
122. Isoeugenol
123. Isoleucine
124. Isopropanol
125. Isovalerate
126. *N*-Isovaleroylglycine
127. Lactate
128. Lactose
129. Leucine
130. Lysine
131. Malate
132. Maleate
133. Malonate
134. Mannitol
135. Mannose
136. Methanol
137. Methionine
138. Methylamine
139. 2-Methylglutarate
140. 3-Methylglutarate
141. Methylguanidine
142. π -Methylhistadine
143. τ -Methylhistadine
144. Methylmalonate
145. 3-Methyl-2-oxovalerate
146. 3-Methylxanthine
147. 5-Methoxysalicylate
148. Methylsuccinate
149. Morphine *
150. NAD⁺
151. Noscapine *
152. Ornithine
153. Oxaloacetate
154. 2-Oxobutyrate
155. 2-Oxoglutarate
156. 2-Oxovalerate

157. Panthothenate
158. Papaverine
159. Phenol
160. Phenylacetate
161. Phenylacetyl glycine
162. Phenylalanine
163. 3-Phenylpropionate
164. *O*-Phosphocholine
165. Phosphoenolpyruvate *
166. *O*-Phosphoethanolamine
167. 6-Phosphogluconic acid *
168. 2-Phosphoglycerate
169. 2-Phenylpropionate
170. 3-Phosphoserine *
171. *O*-Phosphoserine
172. Phthalate
173. Proline
174. Propionate
175. Propylene glycol
176. Pyridoxine
177. 4-Pyroxidate
178. Pyruvate
179. Quinolate
180. *S*-Reticuline *
181. Riboflavin
182. Ribose
183. Ribose-5-phosphate *
184. Salicylate
185. Sanguinarine *
186. Serine
187. Shikimate *
188. Stylopine *
189. Suberate
190. Succinate
191. Succinylacetone
192. Sucrose
193. *S*-Sulfocysteine
194. Tartrate
195. Tetrahydrofolic acid *
196. Thebaine *
197. Threonate
198. Threonine
199. Thymine
200. Trimethylamine
201. Trimethylamine-*N*-oxide
202. Tryptophan
203. Tyramine *
204. Tyrosine
205. Uracil
206. Uridine
207. Valerate
208. Valine
209. Vanillate
210. Xanthine
211. Xanthosine
212. Xylose