SUPPORTING INFORMATION

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Elucidation of functions of human cytochrome P450 enzymes: Identification of endogenous substrates in tissue extracts using metabolomic and isotopic labeling approaches

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Table S-1. Main ion fragments of the oxidation products of human P450 1A2 and liver extract reaction mixture by UPLC-MS-MS (ESI negative mode)

$[M-H]^-$	Product number	$[M-H-18]^-$	$[M-H-44]^-$	$[M-H-18-44]^-$	Other ions
243	**1**	225	–	181	197, 183
271	**1**	253	–	209	225, 211
269	**1**	251	225	207	223, 211, 209, 195, 181
	2	251	225	–	171, 155
297	**1**	279	253	–	251, 237, 195, 173
	2	279	253	–	171, 155
295	**1**	277	251	–	237, 141
	2	277	251	–	195, 179, 171
319	**1**	301	275	257	219, 205, 175, 113
	2	301	275	257	219, 191, 179, 167
343	**1**	325	299	281	285, 271, 255, 241
	2	325	299	281	233, 221, 205, 193, 161

Figure S-1. GC-MS analysis of fatty acids in human liver extract. PFB ester derivatives were prepared and analyzed by GC-MS in the electron impact negative ion mode.

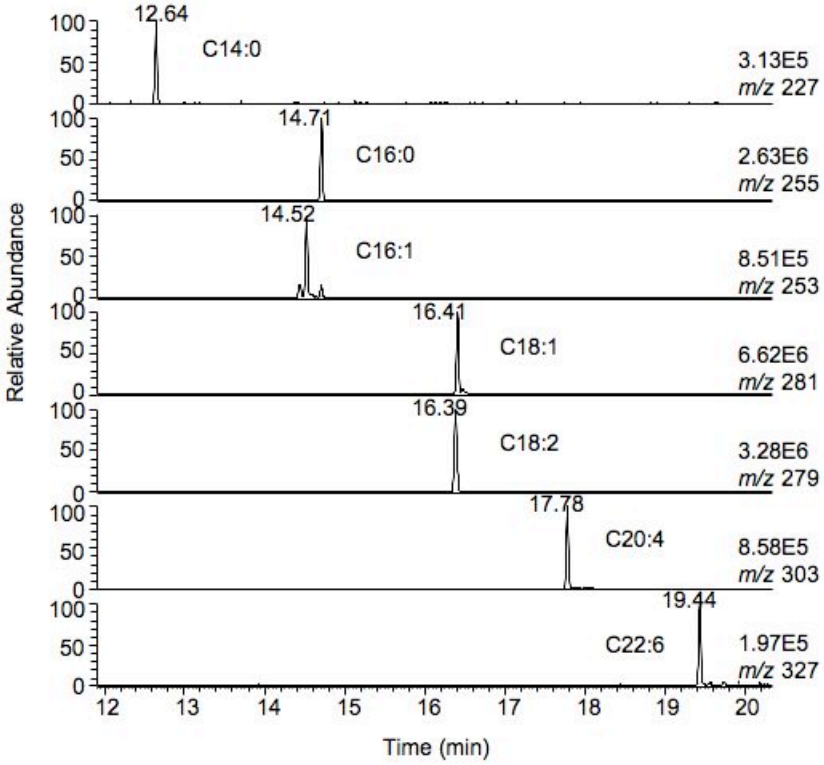

Figure S-2. Spectral changes induced by binding of C14:0 to P450 2C8. Purified P450 (2 μM) was titrated with C14:0 (in ethanol) in 100 mM phosphate buffer (pH 7.4). *A*, Absorbance difference spectra obtained from titration of P450 2C8. *B*, Plot of $\Delta A_{390} - A_{420}$ versus the concentration of C14:0. The value of K_s was estimated as 8.0 μM, using a hyperbolic equation in GraphPad Prism software (GraphPad Software, San Diego, CA).

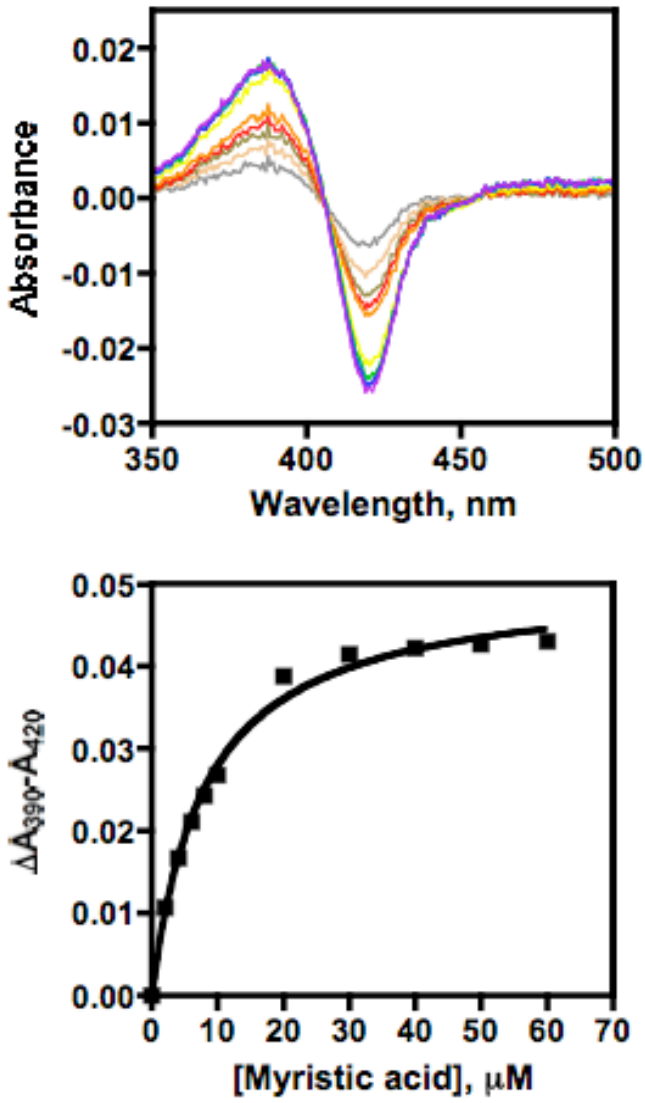

Figure S-3. GC-mass spectra of the hydroxylation product of the incubation of C14:0 with P450 1A2. The TMS derivatives were prepared for GC-MS assay in the electron impact mode.