SUPPLEMENTARY MATERIAL

In Vitro Metabolite Profiling of ADB-FUBINACA, A New Synthetic Cannabinoid

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Table S1. Inclusion list of predicted biotransformations for information-dependent acquisition MS/MS mode with Analyst software. MS/MS, tandem mass spectrometry.

parent, oxidation (+O), carboxylation (+2O-2H), desaturation (-2H), hydrogenation (+2H), ketone formation (-2H+O), defluorination (-F+H), defluorobenzylation (-C7H6F), amide hydrolysis to carboxylic acid (-NH2+OH), internal hydrolysis (+2H+O), glucuronidation (+C6H8O6), sulfation (+SO3), di-oxidation (+2O), oxidation + defluorination (-F+OH), oxidation + amide hydrolysis (-NH2+OH+O), oxidation + internal hydrolysis (+2H+2O), oxidation + glucuronidation (+C6H8O7), oxidation + sulfation (+SO4), carboxylation + defluorination (-F-H+2O), di-hydrogenation (+4H), ketone formation + defluorination (-F-H+O), tri-oxidation (+3O), di-oxidation + ketone formation (-2H+3O), di-oxidation + defluorination (-F+H+2O), di-oxidation + internal hydrolysis (+2H+3O), di-oxidation + glucuronidation (+C6H8O8), oxidation + defluorination + glucuronidation (-F+OH+C6H8O6), carboxylation + defluorination + glucuronidation (-F-H+2O+C6H8O6), ketone formation + defluorination + glucuronidation (-F-H+O+C6H8O6), tetra-oxidation (+4O), tri-oxidation + defluorination (-F+H+3O), di-oxidation + defluorination + glucuronidation (-F+OH+C6H8O7), tetra-oxidation + defluorination (-F+H+4O), tri-oxidation + defluorination + glucuronidation (-F+OH+C6H8O8), tetra-oxidation + defluorination + glucuronidation (-F+OH+C6H8O9).

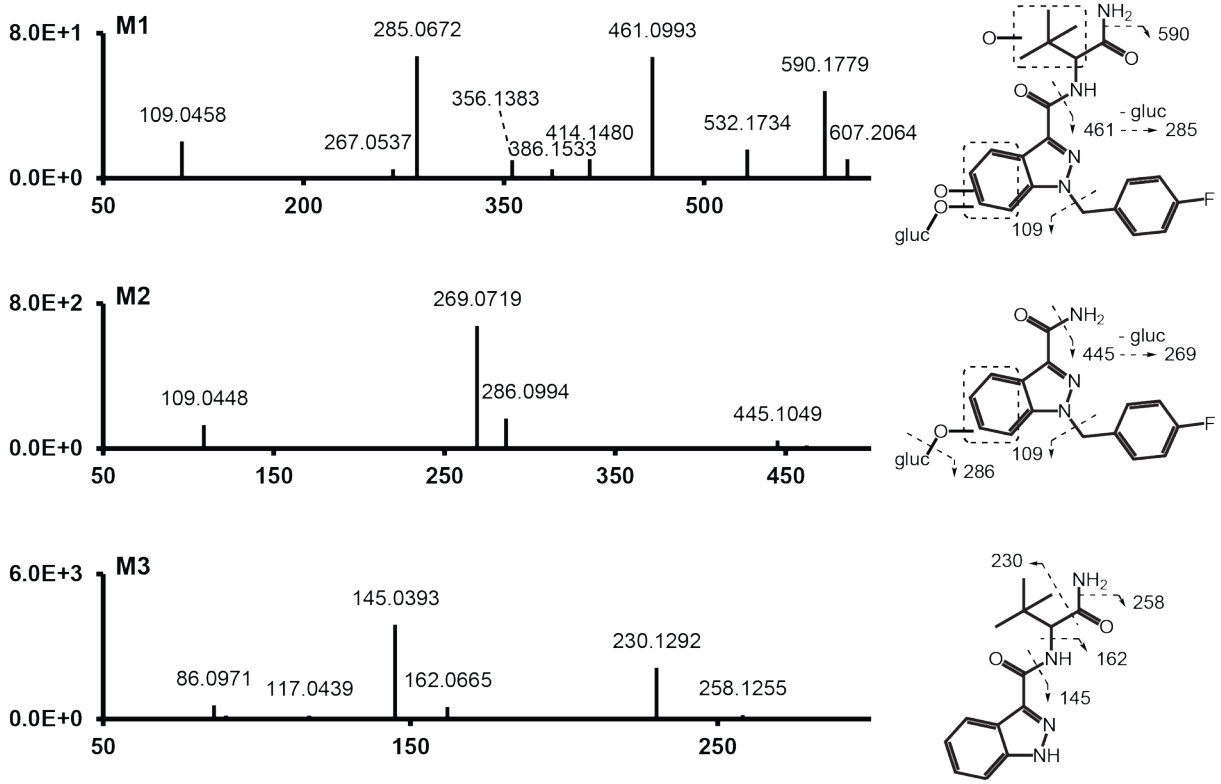

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Fig. (S1). contd….

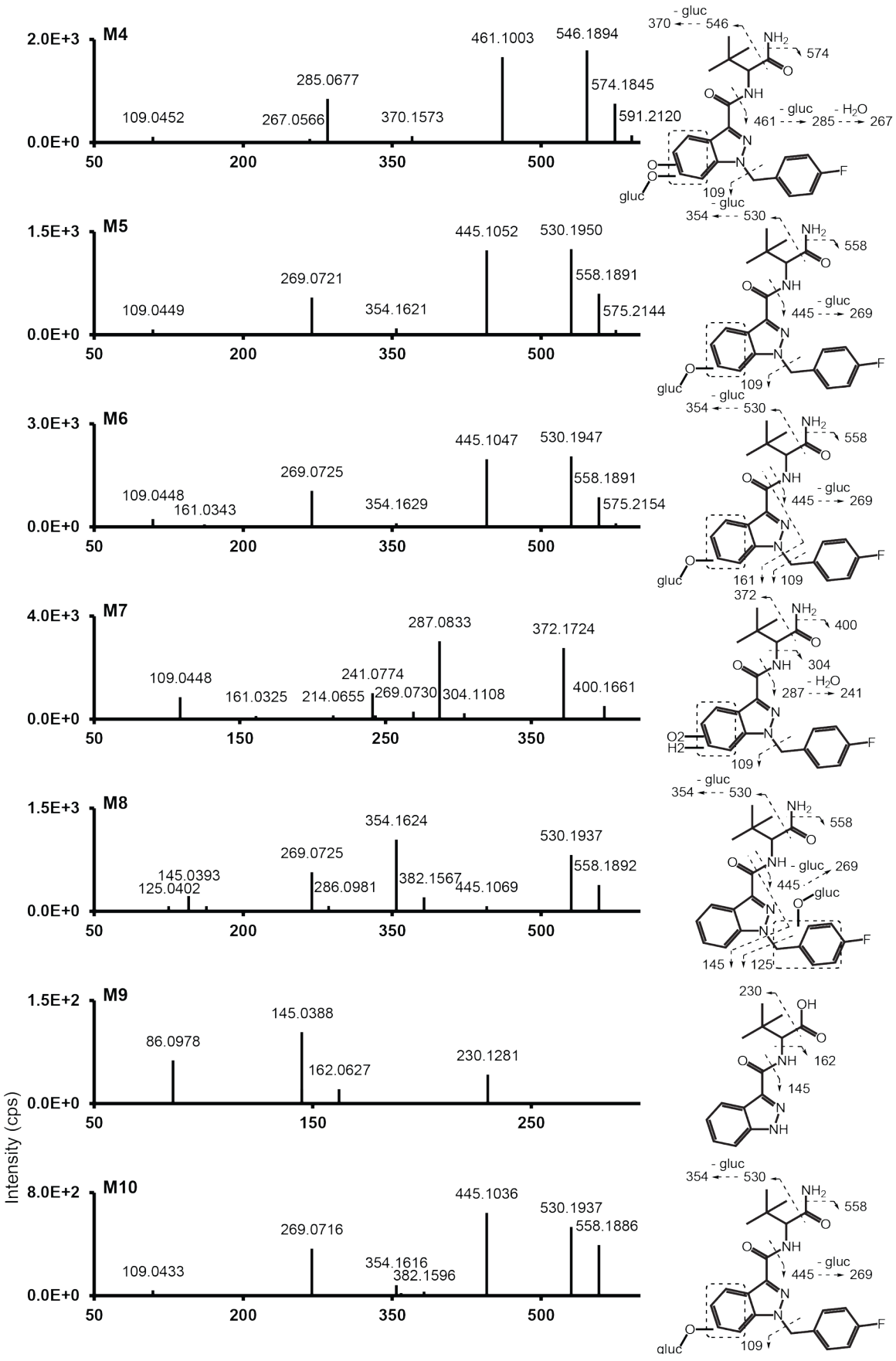
M4
2.0E+3
0.0E+0
109.0452
267.0566
285.0677
370.1573
461.1003
546.1894
574.1845
591.2120
M5
1.5E+3
0.0E+0
109.0449
269.0721
354.1621
445.1052
530.1950
558.1891
575.2144
M6
3.0E+3
0.0E+0
109.0448
161.0343
269.0725
354.1629
445.1047
530.1947
558.1891
575.2154
M7
4.0E+3
0.0E+0
109.0448
161.0325
214.0655
241.0774
269.0730
287.0833
304.1108
372.1724
400.1661
M8
1.5E+3
0.0E+0
125.0402
145.0393
269.0725
286.0981
354.1624
382.1567
445.1069
530.1937
558.1892
M9
1.5E+2
0.0E+0
86.0978
145.0388
162.0627
230.1281
M10
8.0E+2
0.0E+0
109.0433
269.0716
354.1616
382.1596
445.1036
530.1937
558.1886
Intensity (cps)
50
150
200
250
350
500
- gluc
- H2O
gluc

Fig. (S1). contd….

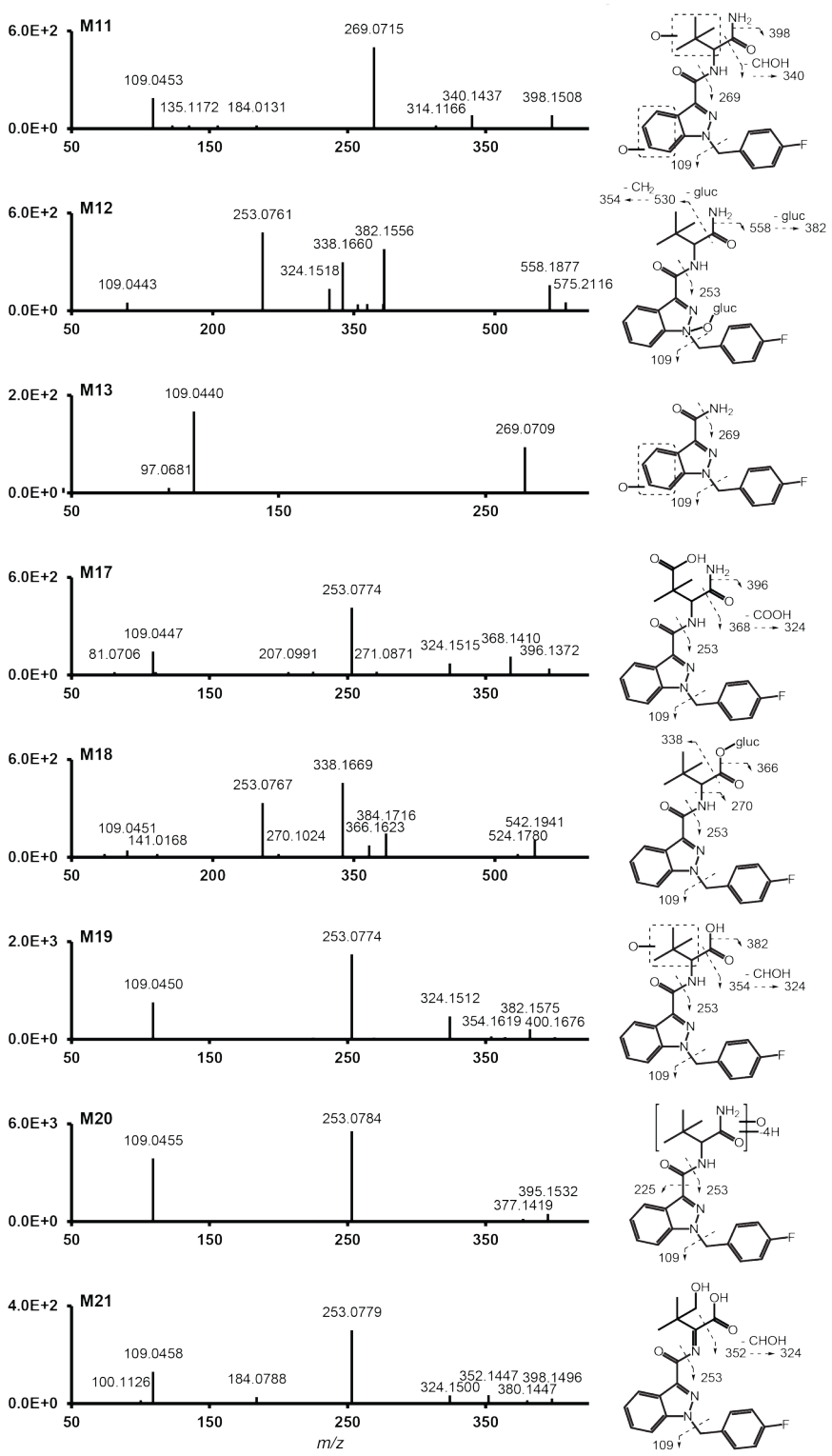

Fig. (S1). ADB-FUBINACA minor metabolites' MS/MS spectrum and assigned fragmentation patterns. Metabolites are presented in ascending retention time order.