SupplementaryTable 1

Identification the EM and EG metabolites in rats by UPLC-Q-Exactive MS

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No. | tR(min) | [M-H]- | Error(ppm) | Formula | fragment ions | identification | EM groups | | | | | | | | | EG groups | | | | | | | | |
| urine | bile | blood | heart | liver | spleen | lung | kidney | brain | urine | bile | blood | heart | liver | spleen | lung | kidney | brain |
| E1-1 | 6.82 | 237.0553 | -1.761 | C15H9O3 | 237.0553(100%) 209.0662(5%) | dideoxyemodin | √ |  |  |  |  |  |  |  |  | √ |  |  |  |  |  |  |  |  |
| E1-2 | 7.60 | 237.0553 | -1.761 | C15H9O3 | 237.0553(100%) 209.0662(5%) | dideoxyemodin | √ |  |  |  |  |  |  |  |  | √ |  |  |  |  |  |  |  |  |
| E2 | 8.08 | 253.0506 | -0.127 | C15H9O4 | 253.0501(100%) 225.0543(10%) 209.0593(15%) | deoxyemodin | √ | √ |  |  |  |  |  |  |  | √ |  |  |  |  |  |  |  |  |
| E3 | 8.49 | 269.0457 | 1.250 | C15H9O5 | 269.0456(100%) 241.0500(5%) 225.0547(20%) | EM | √ | √ | √ | √ | √ | √ | √ | √ | √ | √ | √ | √ | √ | √ | √ | √ | √ | √ |
| E4-1 | 6.63 | 271.0614 | 0.750 | C15H11O5 | 271.0614(85%) 253.0485(5%) 227.0694(10%) 165.0181 | ring open-deoxyemodin | √ |  |  | √ |  |  |  |  |  | √ |  |  | √ |  |  |  |  |  |
| E4-2 | 6.73 | 271.0614 | 0.750 | C15H11O5 | 271.0614(85%) 253.0485(5%) 227.0694(10%) 165.0181 | ring open-deoxyemodin | √ |  |  | √ | √ |  |  | √ |  | √ |  |  | √ | √ | √ |  | √ |  |
| E5 | 6.72 | 281.0463 | 0.901 | C16H9O5 | 281.0463(100%) 253.0507(45%) 225.0549(25%) | deoxyformylated emodin | √ |  |  |  |  |  |  |  |  | √ |  |  |  |  |  |  |  |  |
| E6 | 7.61 | 283.0249 | 0.314 | C15H7O6 | 283.0262(80%) 255.0299(40%) 239.0343(100%) | rhein | √ |  | √ | √ |  |  |  |  |  | √ |  | √ | √ |  |  |  |  |  |
| E7-1 | 7.46 | 283.0607 | 0.600 | C16H11O5 | 268.0376(60%) 240.0422(100%) | methylemodin | √ |  |  |  |  |  |  |  |  | √ |  |  |  |  |  |  |  |  |
| E7-2 | 7.59 | 283.0607 | 0.600 | C16H11O5 | 268.0376(60%) 240.0422(100%) | methylemodin | √ |  |  |  |  |  |  |  |  | √ |  | √ |  |  |  |  |  |  |
| E7-3 | 7.66 | 283.0607 | 0.600 | C16H11O5 | 268.0376(60%) 240.0422(100%) | methylemodin | √ |  |  | √ | √ |  |  | √ |  | √ |  |  | √ | √ |  | √ | √ |  |
| E8-1 | 5.86 | 285.0401 | 0.736 | C15H9O6 | 285.0405(100%) 257.0453(40%) 241.0499(90%) 226.0261(30%) 213.0546(40%) 198.0309(20%) | hydroxyemodin | √ | √ | √ | √ | √ |  | √ | √ |  | √ |  | √ | √ | √ |  | √ | √ |  |
| E8-2 | 6.18 | 285.0401 | 0.736 | C15H9O6 | 285.0405(100%) 257.0453(40%) 241.0499(90%) 226.0261(30%) 213.0546(40%) 198.0309(20%) | hydroxyemodin | √ |  | √ | √ | √ | √ | √ | √ |  | √ |  | √ | √ | √ | √ | √ | √ |  |
| E8-3 | 6.68 | 285.0401 | 0.736 | C15H9O6 | 285.0405(100%) 257.0453(40%) 241.0499(90%) 226.0261(30%) 213.0546(40%) 198.0309(20%) | hydroxyemodin |  |  | √ | √ | √ |  | √ |  |  |  |  | √ | √ | √ | √ | √ | √ |  |
| E8-4 | 6.91 | 285.0401 | 0.736 | C15H9O6 | 285.0405(100%) 257.0453(40%) 241.0499(90%) 226.0261(30%) 213.0546(40%) 198.0309(20%) | hydroxyemodin | √ |  | √ | √ | √ | √ | √ | √ |  | √ |  | √ | √ | √ | √ | √ | √ |  |
| E8-5 | 7.40 | 285.0401 | 0.736 | C15H9O6 | 285.0405(100%) 257.0453(40%) 241.0499(90%) 226.0261(30%) 213.0546(40%) 198.0309(20%) | hydroxyemodin | √ |  |  |  |  | √ |  | √ |  | √ |  |  |  |  |  |  | √ |  |
| E8-6 | 7.48 | 285.0401 | 0.736 | C15H9O6 | 285.0405(100%) 257.0453(40%) 241.0499(90%) 226.0261(30%) 213.0546(40%) 198.0309(20%) | hydroxyemodin | √ | √ | √ | √ |  |  | √ | √ |  | √ |  | √ | √ | √ | √ | √ |  |  |
| E8-7 | 8.78 | 285.0401 | 0.736 | C15H9O6 | 285.0405(100%) 257.0453(40%) 241.0499(90%) 226.0261(30%) 213.0546(40%) 198.0309(20%) | hydroxyemodin | √ | √ | √ |  | √ | √ |  | √ |  | √ |  | √ | √ | √ | √ |  | √ |  |
| E8-8 | 9.01 | 285.0401 | 0.736 | C15H9O6 | 285.0405(100%) 257.0453(40%) 241.0499(90%) 226.0261(30%) 213.0546(40%) 198.0309(20%) | hydroxyemodin | √ |  | √ |  | √ | √ |  | √ |  | √ |  |  |  |  | √ |  | √ |  |
| E9-1 | 5.54 | 287.0560 | 0.985 | C15H11O6 | 287.0561(100%) 269.0449(10%) 259.0604(5%) 243.0664(5%) 225.0557(5%) | ring open-emodin | √ |  |  |  |  |  |  |  |  | √ |  |  |  |  |  |  |  |  |
| E9-3 | 7.90 | 287.0560 | 0.985 | C15H11O6 | 287.0561(100%) 269.0449(10%) 259.0604(5%) 243.0664(5%) 225.0557(5%) | ring open-emodin | √ |  |  |  |  |  |  |  |  | √ |  |  |  |  |  |  |  |  |
| E9-2 | 7.76 | 287.0560 | 0.985 | C15H11O6 | 287.0561(100%) 269.0449(10%) 259.0604(5%) 243.0664(5%) 225.0557(5%) | ring open-emodin | √ |  |  |  |  |  |  |  |  | √ |  |  |  | √ |  |  |  |  |
| E10-1 | 6.95 | 297.0407 | 0.804 | C16H9O6 | 297.0407(100%) 269.0457(50) 225.0556(10%) | formyl emodin | √ |  |  |  |  |  |  |  |  | √ |  |  |  |  |  |  |  |  |
| E10-2 | 7.48 | 297.0407 | 0.804 | C16H9O6 | 297.0407(100%) 269.0457(50) 225.0556(10%) | formyl emodin | √ |  |  |  |  | √ |  |  |  | √ |  |  |  |  |  |  |  |  |
| E11 | 7.05 | 299.0201 | 1.471 | C15H7O7 | 299.0193(100%) 255.0296(15%) 227.0340(10%) | emodic acid | √ |  | √ | √ | √ | √ | √ | √ |  | √ |  | √ | √ | √ | √ | √ | √ |  |
| E12 | 8.62 | 299.0552 | 0.185 | C16H11O6 | 299.0548(90%) 284.0320(100%) 256.0374(48%) | fallacinol | √ |  | √ |  | √ |  |  | √ |  | √ |  | √ |  | √ |  |  | √ |  |
| E13-1 | 6.94 | 301.0356 | 0.745 | C15H9O7 | 301.0378(100%) 283.0251(25%) 255.0297(22%) | dihydroxyemodin | √ |  |  |  |  |  |  |  |  | √ |  |  |  |  |  |  |  |  |
| E13-2 | 7.04 | 301.0356 | 0.745 | C15H9O7 | 301.0378(100%) 283.0251(25%) 255.0297(22%) | dihydroxyemodin | √ |  |  |  | √ | √ |  |  |  | √ |  |  | √ |  |  |  | √ |  |
| E13-3 | 7.20 | 301.0356 | 0.745 | C15H9O7 | 301.0378(100%) 283.0251(25%) 255.0297(22%) | dihydroxyemodin | √ |  |  |  |  |  |  |  |  | √ |  |  |  |  |  |  | √ |  |
| E14-1 | 7.85 | 311.0565 | 1.485 | C17H11O6 | 311.0565(100%) 283.0614(5%) 269.0457(8%) 225.0549(5%) | acetyl emodin | √ |  |  |  |  |  |  |  |  | √ |  |  |  |  |  |  | √ |  |
| E14-2 | 8.02 | 311.0565 | 1.485 | C17H11O6 | 311.0565(100%) 283.0614(5%) 269.0457(8%) 225.0549(5%) | acetyl emodin | √ |  | √ |  |  |  |  |  |  | √ |  |  |  |  |  |  |  |  |
| E14-3 | 8.14 | 311.0565 | 1.485 | C17H11O6 | 311.0565(100%) 283.0614(5%) 269.0457(8%) 225.0549(5%) | acetyl emodin | √ |  | √ |  |  |  |  |  |  | √ |  |  |  | √ | √ | √ | √ |  |
| E15-2 | 7.95 | 313.0358 | 0.716 | C16H9O7 | 313.0352(100%) 285.0404(10%) 269.0456(10%) | carboxyl emodin | √ |  |  |  |  |  |  |  |  | √ |  |  |  |  |  |  |  |  |
| E15-1 | 7.75 | 313.0358 | 0.716 | C16H9O7 | 313.0352(100%) 285.0404(10%) 269.0456(10%) | carboxyl emodin | √ |  |  |  | √ |  |  |  |  | √ |  |  |  | √ |  |  |  |  |
| E15-3 | 8.23 | 313.0358 | 0.716 | C16H9O7 | 313.0352(100%) 285.0404(10%) 269.0456(10%) | carboxyl emodin | √ |  |  |  | √ |  |  | √ |  | √ |  |  |  | √ |  | √ | √ |  |
| E16-1 | 5.17 | 313.0719 | 1.235 | C17H13O6 | 313.0709(100%) 295.0608(50%) 283.0611(75%) 269.0454(20%) | ethylene glycol emodin |  |  |  | √ | √ |  |  |  |  |  |  |  | √ | √ |  |  | √ |  |
| E16-2 | 6.86 | 313.0719 | 1.235 | C17H13O6 | 313.0709(100%) 295.0608(50%) 283.0611(75%) 269.0454(20%) | ethylene glycol emodin |  |  |  | √ | √ | √ | √ |  |  |  |  |  | √ | √ | √ | √ | √ |  |
| E16-3 | 7.33 | 313.0719 | 1.235 | C17H13O6 | 313.0709(100%) 295.0608(50%) 283.0611(75%) 269.0454(20%) | ethylene glycol emodin | √ |  |  | √ | √ | √ |  | √ |  | √ |  |  | √ | √ | √ |  | √ |  |
| E16-4 | 7.47 | 313.0719 | 1.235 | C17H13O6 | 313.0709(100%) 295.0608(50%) 283.0611(75%) 269.0454(20%) | ethylene glycol emodin |  |  |  | √ | √ |  |  | √ |  | √ |  |  | √ | √ | √ |  | √ |  |
| E16-5 | 7.62 | 313.0719 | 1.235 | C17H13O6 | 313.0709(100%) 295.0608(50%) 283.0611(75%) 269.0454(20%) | ethylene glycol emodin | √ |  |  | √ | √ | √ | √ | √ | √ | √ |  |  | √ | √ | √ | √ | √ | √ |
| E16-6 | 7.93 | 313.0719 | 1.235 | C17H13O6 | 313.0709(100%) 295.0608(50%) 283.0611(75%) 269.0454(20%) | ethylene glycol emodin | √ |  |  | √ | √ |  | √ | √ |  | √ |  | √ | √ | √ | √ | √ | √ |  |
| E17-1 | 6.91 | 315.0511 | 1.171 | C16H11O7 | 315.0511(95%) 300.0275(100%) 272.0372(38%) 244.0372(10%) | dihydroxymethylemodin | √ |  | √ | √ | √ |  |  | √ |  | √ |  | √ |  | √ | √ |  | √ |  |
| E17-2 | 7.43 | 315.0511 | 1.171 | C16H11O7 | 315.0511(95%) 300.0275(100%) 272.0372(38%) 244.0372(10%) | dihydroxymethylemodin | √ |  | √ |  |  |  |  |  |  | √ |  |  |  |  |  |  |  |  |
| E18-1 | 8.35 | 325.0722 | 1.535 | C18H13O6 | 325.0711(100%) 283.0610(42%) 254.0610(20%) 240.0426(5%) | methyl acetylemodin | √ |  |  |  |  |  |  |  |  | √ |  | √ |  |  |  |  |  |  |
| E18-2 | 8.83 | 325.0722 | 1.535 | C18H13O6 | 325.0711(100%) 283.0610(42%) 254.0610(20%) 240.0426(5%) | methyl acetylemodin | √ |  |  |  | √ |  |  | √ |  | √ |  |  |  | √ |  |  | √ |  |
| E19-1 | 5.13 | 327.0517 | 1.771 | C17H11O7 | 327.0511(5%) 283.0614(100%) 255.0660(5%) | methyl carboxylemodin | √ |  |  |  | √ |  |  |  |  | √ |  |  |  |  |  |  |  |  |
| E19-2 | 7.58 | 327.0517 | 1.771 | C17H11O7 | 327.0511(5%) 283.0614(100%) 255.0660(5%) 239.0709(10%) | methyl carboxylemodin | √ |  | √ |  |  |  |  |  |  | √ |  | √ |  |  |  |  |  |  |
| E19-3 | 7.93 | 327.0517 | 1.771 | C17H11O7 | 327.0511(5%) 283.0614(100%) 255.0660(5%) 239.0709(10%) | methyl carboxylemodin | √ |  | √ |  |  |  |  |  |  | √ |  | √ |  | √ |  |  | √ |  |
| E20-1 | 6.28 | 329.0304 | 1.206 | C16H9O8 | 329.0305(100%) 285.0404(20%) | carboxyl hydroxyemodin | √ |  | √ |  |  |  |  |  |  | √ |  | √ |  |  |  |  |  |  |
| E20-2 | 6.55 | 329.0304 | 1.206 | C16H9O8 | 329.0305(100%) 285.0404(20%) | carboxyl hydroxyemodin | √ |  |  |  |  |  |  |  |  | √ |  | √ |  |  |  |  |  |  |
| E20-3 | 6.99 | 329.0304 | 1.206 | C16H9O8 | 329.0305(100%) 285.0404(20%) | carboxyl hydroxyemodin | √ |  | √ | √ |  |  |  | √ |  | √ |  | √ |  |  |  |  | √ |  |
| E20-4 | 7.72 | 329.0304 | 1.206 | C16H9O8 | 329.0305(100%) 285.0404(20%) | carboxyl hydroxyemodin | √ |  | √ |  |  |  |  |  |  | √ |  | √ |  |  |  |  | √ |  |
| E21-1 | 6.02 | 333.0076 | 0.461 | C15H9O7S | 333.0066(20%) 253.0504(100%) | deoxy sulfated-deoxyemodin | √ |  |  |  |  |  |  |  |  | √ |  |  |  |  |  |  |  |  |
| E21-2 | 6.72 | 333.0076 | 0.461 | C15H9O7S | 333.0066(20%) 253.0504(100%) | deoxy sulfated-deoxyemodin | √ |  |  |  |  |  |  |  |  | √ |  | √ |  |  |  |  |  |  |
| E22 | 8.01 | 339.0511 | 1.171 | C18H11O7 | 339.0503(100%) 311.0556(70%) 269.0453(35%) 241.0501(25%) 225.0547(15%) | formyl acetyl emodin | √ |  |  |  |  |  |  |  |  | √ |  | √ |  | √ | √ |  | √ |  |
| E23-1 | 6.98 | 341.0667 | 1.121 | C18H13O7 | 341.0659(100%) 323.0554(40%) 298.0478(60%) 281.0456(20%) 269.0451(20%) | lactated emodin | √ |  |  |  |  |  |  |  |  | √ |  |  |  |  |  |  |  |  |
| E23-2 | 7.58 | 341.0667 | 1.121 | C18H13O7 | 341.0659(100%) 323.0554(40%) 298.0478(60%) 281.0456(20%) 269.0451(20%) | lactated emodin | √ |  |  |  | √ |  |  |  |  | √ |  | √ |  |  |  |  |  |  |
| E23-3 | 7.86 | 341.0667 | 1.121 | C18H13O7 | 341.0659(100%) 323.0554(40%) 298.0478(60%) 281.0456(20%) 269.0451(20%) | lactated emodin | √ |  |  |  |  |  |  |  |  | √ |  |  |  |  |  |  | √ |  |
| E24-1 | 6.32 | 343.0463 | 1.048 | C17H11O8 | 343.0470(5%) 299.0561(55%) 281.0458(100%) 253.0505(26%) | carboxyl fallacinol | √ |  |  |  |  |  |  | √ |  | √ |  |  |  |  | √ | √ | √ |  |
| E24-2 | 6.75 | 343.0463 | 1.048 | C17H11O8 | 343.0470(5%) 299.0561(55%) 281.0458(100%) 253.0505(26%) | carboxyl fallacinol | √ |  |  |  |  |  |  | √ |  | √ |  |  |  |  | √ | √ | √ |  |
| E25-1 | 7.32 | 343.0825 | 1.271 | C18H15O7 | 343.0817(90%) 325.0711(20%) 283.0612(100%) 269.0465(10%) | glycerol emodin | √ |  |  | √ | √ |  |  | √ |  | √ |  |  |  |  |  |  | √ |  |
| E25-2 | 7.46 | 343.0825 | 1.271 | C18H15O7 | 343.0817(90%) 325.0711(20%) 283.0612(100%) 269.0465(10%) | glycerol emodin |  |  |  | √ |  | √ |  | √ |  |  |  |  | √ | √ | √ |  | √ |  |
| E25-3 | 7.67 | 343.0825 | 1.271 | C18H15O7 | 343.0817(90%) 325.0711(20%) 283.0612(100%) 269.0465(10%) | glycerol emodin | √ |  |  | √ | √ | √ |  | √ |  | √ |  | √ | √ | √ | √ | √ | √ |  |
| E25-4 | 7.86 | 343.0825 | 1.271 | C18H15O7 | 343.0817(90%) 325.0711(20%) 283.0612(100%) 269.0465(10%) | glycerol emodin | √ |  |  | √ |  |  |  |  |  | √ |  | √ |  | √ |  |  |  |  |
| E26-1 | 5.73 | 349.0027 | 0.971 | C15H9O8S | 349.0014(65%) 269.0454(100%) | sulfated emodin | √ | √ | √ | √ |  | √ | √ | √ | √ | √ |  | √ | √ |  |  | √ | √ |  |
| E26-2 | 5.83 | 349.0027 | 0.971 | C15H9O8S | 349.0014(65%) 269.0454(100%) | sulfated emodin |  |  |  |  |  |  |  |  |  |  |  |  | √ |  |  | √ | √ |  |
| E26-3 | 6.50 | 349.0027 | 0.971 | C15H9O8S | 349.0014(65%) 269.0454(100%) | sulfated emodin | √ | √ | √ | √ |  | √ | √ | √ |  | √ |  | √ | √ |  |  | √ | √ |  |
| E26-4 | 7.26 | 349.0027 | 0.971 | C15H9O8S | 349.0014(65%) 269.0454(100%) | sulfated emodin |  | √ |  |  |  |  |  |  |  |  | √ |  |  |  |  |  |  |  |
| E26-5 | 7.74 | 349.0027 | 0.971 | C15H9O8S | 349.0014(45%) 269.0454(100%) | sulfated emodin | √ | √ | √ | √ | √ | √ | √ | √ |  | √ | √ |  |  |  |  |  |  |  |
| E26-6 | 7.99 | 349.0027 | 0.971 | C15H9O8S | 349.0017(10%) 269.0456(100%) 225.0547(16%) | sulfated emodin | √ |  |  |  |  |  |  |  |  |  |  | √ | √ | √ |  | √ | √ |  |
| E27-1 | 6.54 | 355.0463 | 1.012 | C18H11O8 | 355.0455(100%) 327.0507(90%) 311.0573(10%) 296.0325(80%) 283.0611(15%) 269.0459(20%) 240.0426(30%) | malonyl emodin | √ |  |  |  |  |  |  |  |  | √ |  | √ |  |  |  |  |  |  |
| E27-2 | 7.19 | 355.0463 | 1.012 | C18H11O8 | 355.0455(100%) 327.0507(90%) 311.0573(10%) 296.0325(80%) 283.0611(15%) 269.0459(20%) 240.0426(30%) | malonyl emodin | √ |  |  |  |  |  |  |  |  | √ |  |  |  |  |  | √ |  |  |
| E27-3 | 7.95 | 355.0463 | 1.012 | C18H11O8 | 355.0455(100%) 327.0507(90%) 311.0573(10%) 296.0325(80%) 283.0611(15%) 269.0459(20%) 240.0426(30%) | malonyl emodin | √ |  |  |  |  |  |  |  |  | √ |  |  |  |  |  |  |  |  |
| E28-1 | 7.50 | 355.0815 | 0.271 | C19H15O7 | 355.0806(100%) 337.0696(20%) 325.0702(30%) 307.0600(35%) 282.0523(50%) 269.0450(15%) | hydroxybutyryl emodin | √ |  |  |  |  | √ |  | √ |  | √ |  |  |  | √ | √ | √ | √ |  |
| E28-2 | 7.81 | 355.0815 | 0.271 | C19H15O7 | 355.0806(100%) 337.0696(20%) 325.0702(30%) 307.0600(35%) 282.0523(50%) 269.0450(15%) | hydroxybutyryl emodin | √ |  |  |  |  |  |  |  |  | √ |  |  |  |  |  |  |  |  |
| E28-3 | 7.98 | 355.0815 | 0.271 | C19H15O7 | 355.0806(100%) 337.0696(20%) 325.0702(30%) 307.0600(35%) 282.0523(50%) 269.0450(15%) | hydroxybutyryl emodin | √ |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| E28-4 | 8.10 | 355.0815 | 0.271 | C19H15O7 | 355.0806(100%) 337.0696(20%) 325.0702(30%) 307.0600(35%) 282.0523(50%) 269.0450(15%) | hydroxybutyryl emodin | √ |  |  |  |  |  |  |  |  | √ |  |  |  |  |  |  |  |  |
| E29-1 | 6.27 | 357.0258 | 1.666 | C17H9O9 | 313.0352(100%) 269.0457(25%) 241.0503(13%) 225.0547(5%) | dicarboxyl emodin | √ |  |  |  |  |  |  |  |  | √ |  |  |  |  |  |  |  |  |
| E29-2 | 6.48 | 357.0258 | 1.666 | C17H9O9 | 313.0352(100%) 269.0457(25%) 241.0503(13%) 225.0547(5%) | dicarboxyl emodin | √ |  |  |  |  |  |  |  |  | √ |  |  |  |  |  |  |  |  |
| E30-4 | 7.89 | 357.0611 | 0.606 | C18H13O8 | 357.0603(60%) 313.0704(40%) 295.0600(35%) 283.0603(50%) 269.0449(100%) | glyceryl acid emodin | √ |  |  |  |  |  |  |  |  | √ |  |  |  |  |  |  |  |  |
| E30-1 | 6.02 | 357.0611 | 0.606 | C18H13O8 | 357.0603(60%) 313.0704(40%) 295.0600(35%) 283.0603(50%) 269.0449(100%) | glyceryl acid emodin | √ |  |  |  |  | √ |  |  |  | √ |  |  |  |  |  |  |  |  |
| E30-2 | 6.80 | 357.0611 | 0.606 | C18H13O8 | 357.0603(60%) 313.0704(40%) 295.0600(35%) 283.0603(50%) 269.0449(100%) | glyceryl acid emodin | √ |  | √ | √ | √ | √ | √ | √ | √ | √ |  | √ | √ | √ | √ | √ | √ | √ |
| E30-3 | 7.21 | 357.0611 | 0.606 | C18H13O8 | 357.0603(60%) 313.0704(40%) 295.0600(35%) 283.0603(50%) 269.0449(100%) | glyceryl acid emodin | √ |  |  |  | √ | √ | √ |  |  | √ |  |  |  | √ |  |  |  |  |
| E31-1 | 6.56 | 363.0174 | -1.684 | C16H11O8S | 363.0160(25%) 283.0605(100%) 240.0418(50%) | sulfated methylemodin | √ |  |  |  |  |  |  |  |  | √ |  |  |  |  |  |  |  |  |
| E31-2 | 7.04 | 363.0174 | -1.684 | C16H11O8S | 363.0160(25%) 283.0605(100%) 240.0418(50%) | sulfated methylemodin | √ |  | √ |  |  |  |  |  |  | √ |  |  |  |  |  |  |  |  |
| E31-3 | 7.23 | 363.0174 | -1.684 | C16H11O8S | 363.0160(25%) 283.0605(100%) 240.0418(50%) | sulfated methylemodin | √ |  | √ |  |  |  |  |  |  |  |  | √ |  |  |  |  |  |  |
| E32-1 | 1.39 | 364.9972 | -0.208 | C15H9O9S | 285.0403(100%) 241.0500(5%) | sulfated hydroxyemodin | √ |  | √ |  |  |  |  |  |  | √ |  |  |  |  |  |  |  |  |
| E32-2 | 3.81 | 364.9972 | -0.208 | C15H9O9S | 285.0403(100%) 241.0500(5%) | sulfated hydroxyemodin | √ |  |  |  |  |  |  |  |  | √ |  |  |  |  |  |  |  |  |
| E32-3 | 4.46 | 364.9972 | -0.208 | C15H9O9S | 285.0403(100%) 241.0500(5%) | sulfated hydroxyemodin | √ |  | √ |  |  | √ | √ | √ |  | √ |  | √ |  |  |  |  | √ |  |
| E32-4 | 5.91 | 364.9972 | -0.208 | C15H9O9S | 285.0403(100%) 241.0500(5%) | sulfated hydroxyemodin | √ | √ | √ | √ | √ | √ | √ | √ | √ | √ |  | √ | √ | √ |  | √ | √ |  |
| E32-5 | 7.77 | 364.9972 | -0.208 | C15H9O9S | 285.0403(100%) 241.0500(5%) | sulfated hydroxyemodin |  | √ | √ |  |  |  |  | √ |  | √ |  |  |  |  |  |  |  |  |
| E32-6 | 8.01 | 364.9972 | -0.208 | C15H9O9S | 285.0403(100%) 241.0500(5%) | sulfated hydroxyemodin | √ |  |  |  |  |  |  |  |  |  |  | √ |  |  |  |  | √ |  |
| E33-1 | 7.81 | 369.0985 | 1.419 | C20H17O7 | 369.0977(100%) 351.0875(20%) 325.0715(58%) 283.0612(60%) 269.0457(15%) | hydroxyvaleryl emodin | √ |  |  |  |  |  |  |  |  | √ |  |  |  |  |  |  |  |  |
| E33-2 | 7.64 | 369.0985 | 1.419 | C20H17O7 | 369.0977(100%) 351.0875(20%) 283.0612(60%) 269.0457(15%) | hydroxyvaleryl emodin | √ |  |  |  |  |  |  |  |  | √ |  |  |  |  |  |  |  |  |
| E34-1 | 6.82 | 371.0767 | 0.556 | C19H15O8 | 371.0757(100%) 353.0658(15%) 341.0650(5%) 323.0556(20%) 311.0550(15%) 295.0603(15%) 283.0609(70%) 269.0447(58%) 225.0542(10%) | erythrose emodin | √ |  |  |  |  | √ | √ |  |  | √ |  |  |  |  | √ | √ | √ |  |
| E34-2 | 7.64 | 371.0767 | 0.556 | C19H15O8 | 371.0757(100%) 353.0658(15%) 341.0650(5%) 323.0556(20%) 311.0550(15%) 295.0603(15%) 283.0609(70%) 269.0447(58%) 225.0542(10%) | erythrose emodin | √ |  | √ | √ | √ | √ | √ | √ | √ | √ |  | √ | √ | √ | √ | √ | √ | √ |
| E35-1 | 6.08 | 378.9758 | -1.953 | C15H7O10S | 378.9758(20%) 299.0194(100%) | sulfated emodic acid | √ |  | √ | √ |  |  | √ | √ |  | √ |  | √ |  |  |  |  |  |  |
| E35-2 | 6.78 | 378.9758 | -1.953 | C15H7O10S | 378.9758(20%) 299.0194(100%) | sulfated emodic acid | √ | √ | √ |  |  |  | √ |  |  | √ |  | √ | √ |  |  | √ | √ |  |
| E36-1 | 5.27 | 379.0133 | 0.987 | C16H11O9S | 299.0555(100%) 256.0377(40%) | sulfated fallacinol | √ |  |  | √ | √ |  |  |  |  | √ |  |  |  |  |  |  |  |  |
| E36-2 | 5.90 | 379.0133 | 0.987 | C16H11O9S | 299.0555(100%) 256.0377(40%) | sulfated fallacinol | √ |  |  | √ | √ |  |  | √ |  | √ |  |  | √ | √ |  |  | √ |  |
| E36-3 | 6.80 | 379.0133 | 0.987 | C16H11O9S | 299.0555(100%) 256.0377(40%) | sulfated fallacinol | √ |  |  | √ | √ |  |  |  |  |  |  |  |  |  |  |  |  |  |
| E36-4 | 7.19 | 379.0133 | 0.987 | C16H11O9S | 299.0555(100%) 256.0377(40%) | sulfated fallacinol | √ |  |  | √ | √ |  |  | √ |  |  |  |  | √ | √ |  |  | √ |  |
| E36-5 | 7.97 | 379.0133 | 0.987 | C16H11O9S | 299.0555(100%) 256.0377(40%) | sulfated fallacinol | √ |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| E37-1 | 4.97 | 380.9924 | 0.550 | C15H9O10S | 380.9906(10%) 301.0351(100%) | sulfated dihydroxyemodin | √ |  |  |  |  |  |  |  |  | √ |  | √ |  |  |  |  |  |  |
| E37-2 | 5.16 | 380.9924 | 0.550 | C15H9O10S | 380.9906(10%) 301.0351(100%) | sulfated dihydroxyemodin | √ |  | √ |  |  |  |  |  |  | √ |  | √ |  |  |  |  |  |  |
| E37-3 | 5.34 | 380.9924 | 0.550 | C15H9O10S | 380.9906(10%) 301.0351(100%) | sulfated dihydroxyemodin | √ |  | √ |  |  |  |  | √ |  | √ |  | √ |  |  |  |  |  |  |
| E38-1 | 7.28 | 383.0778 | 1.460 | C20H15O8 | 383.0765(20%) 339.0869(100%) 296.0689(55%) 281.0453(15%) | glutaryl emodin | √ |  |  |  |  |  |  |  |  | √ |  |  |  |  |  |  |  |  |
| E38-2 | 7.66 | 383.0778 | 1.460 | C20H15O8 | 383.0765(20%) 339.0869(100%) 321.0762(10%) 296.0689(55%) 281.0453(15%) 269.0463(10%) | glutaryl emodin | √ |  |  |  |  |  |  |  |  | √ |  |  |  |  |  |  |  |  |
| E38-3 | 7.94 | 383.0778 | 1.460 | C20H15O8 | 383.0765(20%) 339.0869(100%) 296.0689(55%) 281.0453(15%) | glutaryl emodin | √ |  |  | √ | √ | √ |  | √ |  | √ |  |  |  |  |  |  | √ |  |
| E39-1 | 7.41 | 389.0673 | 1.604 | C22H13O7 | 389.0660(100%) 269.0459(10%) | hydroxybenzoyl emodin | √ |  |  |  |  |  |  |  |  | √ |  |  |  |  |  |  |  |  |
| E39-2 | 7.84 | 389.0673 | 1.604 | C22H13O7 | 389.0660(100%) 269.0459(10%) | hydroxybenzoyl emodin | √ |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| E39-3 | 8.00 | 389.0673 | 1.604 | C22H13O7 | 389.0660(100%) 269.0459(10%) | hydroxybenzoyl emodin | √ |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| E40-1 | 5.54 | 392.9930 | 2.060 | C16H9O10S | 392.9916(5%) 313.0351(100%) 284.0411(8%) 269.0454(8%) | carboxyl sulfated emodin | √ |  | √ |  |  |  |  |  |  | √ |  | √ |  |  |  |  |  |  |
| E40-2 | 5.76 | 392.9930 | 2.060 | C16H9O10S | 392.9916(5%) 313.0351(100%) 284.0411(8%) 269.0454(8%) | carboxyl sulfated emodin | √ |  |  |  |  |  |  |  |  | √ |  |  |  |  |  |  |  |  |
| E40-3 | 7.75 | 392.9930 | 2.060 | C16H9O10S | 392.9916(5%) 313.0351(100%) 284.0411(8%) 269.0454(8%) | carboxyl sulfated emodin | √ | √ | √ |  |  |  |  |  |  | √ |  | √ |  |  |  |  | √ |  |
| E41-1 | 5.08 | 393.0293 | 1.842 | C17H13O9S | 393.0259(20%) 313.0709(20%) 295.0612(100%) 269.0453(10%) 255.0296(20%) | ethylene glycol sulfated emodin | √ |  |  |  |  |  |  |  |  | √ |  |  |  |  |  |  |  |  |
| E41-2 | 6.66 | 393.0293 | 1.842 | C17H13O9S | 393.0259(20%) 313.0709(20%) 295.0612(100%) 269.0453(10%) 255.0296(20%) | ethylene glycol sulfated emodin | √ |  |  |  |  |  |  |  |  | √ |  |  |  |  |  |  |  |  |
| E41-3 | 7.28 | 393.0293 | 1.842 | C17H13O9S | 393.0259(20%) 313.0709(20%) 295.0612(100%) 269.0453(10%) 255.0296(20%) | ethylene glycol sulfated emodin | √ |  |  |  |  |  |  |  |  |  |  |  |  | √ | √ | √ | √ |  |
| E42 | 6.03 | 395.0081 | 0.657 | C16H11O10S | 395.0081(5%) 315.0510(100%) 300.0277(80%) 272.0332(20%) | dihydroxymethyl sulfated emodin | √ |  | √ |  | √ |  |  |  |  | √ |  | √ |  |  |  |  |  |  |
| E43-1 | 5.41 | 398.0884 | 0.654 | C20H16O8N | 398.0870(100%) 381.0611(10%) 354.0978(5%) 337.0708(20%) 325.0724(6%) 311.0558(38%) 298.0723(10%) 283.0613(60%) 269.0456(25%) 225.0547(5%) | glutamyl emodin | √ |  |  |  |  |  |  |  |  | √ |  |  |  |  |  |  |  |  |
| E43-2 | 5.98 | 398.0884 | 0.654 | C20H16O8N | 398.0870(100%) 381.0611(10%) 354.0978(5%) 337.0708(20%) 325.0724(6%) 311.0558(38%) 298.0723(10%) 283.0613(60%) 269.0456(25%) 225.0547(5%) | glutamyl emodin | √ |  |  |  |  |  |  |  |  | √ |  |  |  |  |  |  |  |  |
| E43-3 | 7.04 | 398.0884 | 0.654 | C20H16O8N | 398.0870(100%) 381.0611(10%) 354.0978(5%) 337.0708(20%) 325.0724(6%) 311.0558(38%) 298.0723(10%) 283.0613(60%) 269.0456(25%) 225.0547(5%) | glutamyl emodin | √ |  |  |  |  |  |  |  |  | √ |  |  |  |  |  |  |  |  |
| E44-1 | 6.89 | 399.0726 | 1.114 | C20H15O9 | 399.0717(40%) 355.0823(100%) 311.0919(40%) 283.0610(45%) 269.0458(20%) 254.0585(30%) | hydroxyglutaryl emodin | √ |  |  | √ | √ |  |  |  |  | √ |  |  | √ | √ |  |  |  |  |
| E44-2 | 7.03 | 399.0726 | 1.114 | C20H15O9 | 399.0717(40%) 355.0823(100%) 311.0919(40%) 283.0610(45%) 269.0458(20%) 254.0585(30%) | hydroxyglutaryl emodin | √ |  |  | √ | √ |  |  |  |  | √ |  |  | √ | √ |  |  |  |  |
| E44-3 | 7.21 | 399.0726 | 1.114 | C20H15O9 | 399.0717(40%) 355.0823(100%) 311.0919(40%) 283.0610(45%) 269.0458(20%) 254.0585(30%) | hydroxyglutaryl emodin | √ |  |  | √ |  |  |  |  |  |  |  |  | √ |  |  |  |  |  |
| E45 | 6.14 | 405.0277 | -2.163 | C18H13O9S | 405.0269(25%) 325.0704(100%) 283.0597(10%) 254.0576(20%) | methyl sulfated acetylemodin | √ |  |  |  |  |  |  |  |  | √ |  |  |  |  |  |  |  |  |
| E46 | 5.13 | 407.0084 | 1.375 | C17H11O10S | 327.0508(40%) 283.0615(100%) 255.0662(5%) 239.0708(10%) | methyl sulfated carboxyl emodin | √ |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| E47-1 | 4.92 | 408.9875 | 0.966 | C16H9O11S | 408.9875(10%) 329.0309(100%) 314.0067(65%) 286.0124(10%) | sulfated carboxyl hydroxyemodin | √ |  |  |  |  |  |  |  |  | √ |  |  |  |  |  |  |  |  |
| E47-2 | 5.28 | 408.9875 | 0.966 | C16H9O11S | 408.9875(10%) 329.0309(100%) 314.0067(65%) 286.0124(10%) | sulfated carboxyl hydroxyemodin | √ |  |  |  |  |  |  |  |  | √ |  |  |  |  |  |  |  |  |
| E47-3 | 6.19 | 408.9875 | 0.966 | C16H9O11S | 408.9875(10%) 329.0309(100%) 314.0067(65%) 286.0124(10%) | sulfated carboxyl hydroxyemodin | √ |  |  |  |  |  |  |  |  | √ |  |  |  |  |  |  |  |  |
| E48 | 7.16 | 409.0686 | -0.657 | C20H13O8N2 | 409.0675(35%) 329.0291(15%) 269.0457(100%) | unknown | √ |  |  |  |  |  |  |  |  | √ |  |  |  | √ |  |  |  |  |
| E49-1 | 7.11 | 416.0777 | 0.300 | C23H14O7N | 416.0771(100%) 398.0674(8%) 370.0728(16%) 354.0769(25%) 326.0817(10%) 269.0455(32%) | unknown | √ |  |  |  |  |  |  |  |  | √ |  |  |  |  |  |  |  |  |
| E49-2 | 8.13 | 416.0777 | 0.300 | C23H14O7N | 416.0771(100%) 398.0674(8%) 370.0728(16%) 354.0769(25%) 326.0817(10%) 269.0455(32%) | unknown | √ |  |  |  |  |  |  |  |  | √ |  |  |  |  |  | √ |  |  |
| E50 | 5.07 | 421.0245 | 2.398 | C18H13O10S | 341.0662(100%) 323.0557(35%) 298.0481(50%) 281.0458(20%) 269.0457(10%) 225.0549(5%) | lactated sulfated emodin | √ |  |  |  |  |  |  |  |  | √ |  |  |  |  |  |  |  |  |
| E51 | 4.24 | 423.0033 | 1.288 | C17H11O11S | 343.0453(25%) 325.0351(45%) 299.0559(28%) 281.0457(100%) 253.0507(10%) | sulfated carboxyl fallacinol | √ |  |  |  |  |  |  |  |  | √ |  |  |  |  |  |  |  |  |
| E52-1 | 6.69 | 427.0673 | 1.327 | C21H15O10 | 427.0649(5%) 269.0457(100%) | ascorbyl emodin | √ |  |  |  |  |  |  |  |  | √ |  |  |  |  |  |  |  |  |
| E52-2 | 6.96 | 427.0673 | 1.327 | C21H15O10 | 427.0649(5%) 269.0457(100%) | ascorbyl emodin | √ |  | √ | √ | √ |  |  | √ |  | √ |  | √ | √ | √ |  | √ | √ |  |
| E53-1 | 6.16 | 429.0835 | 1.818 | C21H17O10 | 253.0505 | glucuronide deoxyemodin | √ |  |  |  |  |  |  |  |  | √ |  |  |  |  |  |  | √ |  |
| E53-2 | 6.28 | 429.0835 | 1.818 | C21H17O10 | 253.0505 | glucuronide deoxyemodin | √ |  | √ |  |  |  |  |  |  | √ |  | √ |  |  |  |  |  |  |
| E53-3 | 6.83 | 429.0835 | 1.818 | C21H17O10 | 253.0505 | glucuronide deoxyemodin | √ |  |  |  |  |  |  |  |  | √ |  |  |  |  |  |  |  |  |
| E53-4 | 7.31 | 429.0835 | 1.818 | C21H17O10 | 429.0820(100%) 411.0675(5%) 401.0883(5%) 383.0770(10%) 351.0511(15%) 311.0557(30%) 269.0458(28%) | glucosone emodin | √ |  |  |  |  |  |  |  |  | √ |  |  |  |  |  |  |  |  |
| E54 | 6.11 | 431.0979 | 0.627 | C21H19O10 | 431.0981(79%) 269.0454(100%) 225.0548(20%) | EG | √ |  | √ | √ | √ | √ | √ | √ | √ | √ | √ | √ | √ | √ | √ | √ | √ | √ |
| E55 | 7.57 | 434.0872 | -0.253 | C23H16O8N | 434.0866(100%) 416.0754(10%) 389.1027(10%) 372.0863(20%) 354.0757(25%) 325.0343(10%) 308.0316(25%) 297.0394(45%) 281.0448(30%) 269.0449(65%) | dihydroxyphenylglycine emodin | √ |  |  |  |  |  |  |  |  | √ |  |  |  |  |  |  |  |  |
| E56 | 6.75 | 437.0993 | 0.895 | C22H17O8N2 | 437.0994(50%) 419.0883(90%) 376.0822(35%) 358.0715(20%) 269.0457(100%) | unknown | √ |  |  |  |  |  |  |  |  | √ |  |  |  |  |  |  |  |  |
| E57 | 6.04 | 441.0944 | 0.446 | C21H17O9N2 | 441.0941(50%) 296.0565(100%) 269.0457(90%) | aspartylglycine emodin | √ |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| E58-1 | 6.58 | 445.0773 | 0.762 | C21H17O11 | 445.0774(45%) 269.0452(100%) | glucuronide emodin | √ | √ | √ | √ | √ | √ | √ | √ | √ | √ | √ | √ | √ | √ | √ | √ | √ | √ |
| E58-2 | 5.25 | 445.0778 | 1.262 | C21H17O11 | 445.0774(45%) 269.0452(100%) | glucuronide emodin | √ | √ | √ | √ | √ |  | √ | √ | √ | √ |  | √ | √ | √ | √ | √ | √ | √ |
| E58-3 | 6.04 | 445.0778 | 1.262 | C21H17O11 | 445.0774(45%) 269.0452(100%) | glucuronide emodin | √ | √ | √ | √ | √ | √ | √ | √ | √ | √ | √ | √ | √ | √ | √ | √ | √ | √ |
| E59-1 | 5.12 | 447.0933 | 1.112 | C21H19O11 | 447.0930(100%) 285.0401(25%) 268.0377(20%) 201.0216(30%) | hydroxyemodin-O-glucoside | √ |  |  |  |  |  |  |  |  | √ | √ |  |  |  |  |  | √ |  |
| E59-2 | 5.47 | 447.0933 | 1.112 | C21H19O11 | 447.0930(100%) 285.0401(25%) 268.0377(20%) 201.0216(30%) | hydroxyemodin-O-glucoside | √ |  |  |  |  |  |  |  |  | √ |  |  |  |  |  |  |  |  |
| E60-1 | 5.21 | 449.1093 | 1.462 | C21H21O11 | 449.1086(30%) 431.0978(35%) 254.0583(100%) 230.0576(10%) | open ring emodin-O-glucoside | √ |  |  |  |  |  | √ | √ |  | √ |  | √ |  |  |  |  |  |  |
| E60-2 | 5.31 | 449.1093 | 1.462 | C21H21O11 | 449.1086(30%) 431.0978(35%) 254.0583(100%) 230.0576(10%) | open ring emodin-O-glucoside | √ |  |  |  | √ |  |  | √ |  | √ |  | √ |  |  |  |  |  |  |
| E60-3 | 5.59 | 449.1093 | 1.462 | C21H21O11 | 449.1086(30%) 431.0978(35%) 254.0583(100%) 230.0576(10%) | open ring emodin-O-glucoside |  |  |  |  |  |  |  |  |  |  |  | √ |  |  |  |  |  |  |
| E61-1 | 6.56 | 450.0823 | -1.676 | C23H16O9N | 450.0818(100%) 432.0702(8%)388.0803(5%) 370.0692(5%) 325.0345(5%) 297.0396(42%) 281.0488(30%) 269.0458(52%) | trihydroxyphenylglycine emodin | √ |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| E61-2 | 6.97 | 450.0823 | -1.676 | C23H16O9N | 450.0818(100%) 432.0702(8%) 388.0803(5%) 370.0692(5%) 325.0345(5%) 297.0396(42%) 281.0488(30%) 269.0458(52%) | trihydroxyphenylglycine emodin | √ |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| E62-1 | 6.31 | 459.0937 | 0.905 | C22H119O11 | 283.0614(100%) | methylemodin-O-glucuronide | √ |  | √ |  |  |  |  |  |  | √ |  |  |  |  |  |  |  |  |
| E62-2 | 6.52 | 459.0937 | 0.905 | C22H119O11 | 283.0614(100%) 240.0418(60%) | methylemodin-O-glucuronide |  |  |  |  |  |  |  | √ |  |  |  |  |  |  |  |  | √ |  |
| E62-3 | 6.62 | 459.0937 | 0.905 | C22H119O11 | 283.0614(100%) 240.0418(60%) | methylemodin-O-glucuronide |  |  |  |  |  |  |  | √ |  |  |  |  |  |  |  |  | √ |  |
| E62-4 | 6.99 | 459.0937 | 0.905 | C22H119O11 | 283.0614(100%) 240.0418(60%) | methylemodin-O-glucuronide |  |  |  |  |  |  |  | √ | √ |  |  |  |  |  |  |  | √ | √ |
| E63-1 | 4.19 | 461.0728 | 1.208 | C21H17O12 | 461.0727(30%) 285.0404(100%) | hydroxyemodin-O-glucuronide | √ | √ | √ |  | √ |  |  | √ |  | √ | √ | √ |  |  |  |  | √ |  |
| E63-2 | 4.87 | 461.0728 | 1.208 | C21H17O12 | 461.0727(30%) 285.0404(100%) | hydroxyemodin-O-glucuronide | √ | √ | √ | √ | √ |  | √ | √ | √ | √ |  | √ | √ | √ |  | √ | √ |  |
| E63-3 | 5.67 | 461.0728 | 1.208 | C21H17O12 | 461.0727(30%) 285.0404(100%) | hydroxyemodin-O-glucuronide | √ |  | √ |  | √ |  |  | √ |  | √ |  | √ |  | √ |  |  | √ |  |
| E63-4 | 6.14 | 461.0728 | 1.208 | C21H17O12 | 461.0727(30%) 285.0404(100%) | hydroxyemodin-O-glucuronide | √ |  | √ |  | √ |  |  | √ |  | √ |  | √ | √ | √ |  | √ | √ |  |
| E63-5 | 6.49 | 461.0728 | 1.208 | C21H17O12 | 461.0727(30%) 285.0404(100%) | hydroxyemodin-O-glucuronide | √ |  | √ |  | √ |  |  | √ |  | √ |  | √ |  |  |  | √ | √ |  |
| E63-6 | 6.77 | 461.0728 | 1.208 | C21H17O12 | 461.0727(30%) 285.0404(100%) | hydroxyemodin-O-glucuronide | √ |  | √ | √ | √ |  | √ | √ |  |  |  | √ | √ | √ | √ | √ | √ | √ |
| E64 | 7.54 | 464.0974 | -2.810 | C24H18O9N | 464.0970(100%) 446.0861(5%) 387.0733(20%) 369.0618(5%) 338.0400(5%) 308.0312(15%) 297.0393(40%) 281.0447(25%) 269.0447(55%) | dihydroxy-methoxyphenylglycine emodin | √ |  |  |  |  |  |  |  |  | √ |  |  |  |  |  |  | √ |  |
| E65-1 | 4.27 | 475.0521 | 1.383 | C21H15O13 | 299.0193 | emodic acid-O-glucuronide | √ |  | √ |  |  |  |  | √ |  | √ |  | √ |  |  |  |  | √ |  |
| E65-2 | 5.00 | 475.0521 | 1.383 | C21H15O13 | 299.0193 | emodic acid-O-glucuronide | √ | √ | √ | √ | √ |  | √ | √ | √ | √ |  | √ | √ | √ |  | √ | √ |  |
| E66-1 | 3.63 | 478.0450 | 0.096 | C20H16O11NS | 398.0870(100%) 381.0611(10%) 354.0978(5%) 337.0708(20%) 325.0724(6%) 311.0558(38%) 298.0723(10%) 283.0613(60%) 269.0456(25%) 225.0547(5%) | sulfated glutamyl emodin | √ |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| E66-2 | 3.86 | 478.0450 | 0.096 | C20H16O11NS | 398.0870(100%) 381.0611(10%) 354.0978(5%) 337.0708(20%) 325.0724(6%) 311.0558(38%) 298.0723(10%) 283.0613(60%) 269.0456(25%) 225.0547(5%) | sulfated glutamyl emodin | √ |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| E67 | 6.65 | 501.1040 | 1.248 | C24H21O12 | 325.0711(100%) 283.0609(30%) 254.0582(10%) | methyl acetylemodin-O-glucuronide | √ |  |  |  | √ |  |  | √ |  | √ |  | √ |  |  |  |  |  |  |
| E68-1 | 4.06 | 525.0344 | -0.093 | C21H17O14S | 525.0334(5%) 445.0773(10%) 269.0456(100%) | sulafed emodin-O-glucuronide | √ | √ | √ | √ |  |  |  | √ | √ | √ | √ | √ | √ |  |  | √ | √ |  |
| E68-2 | 4.43 | 525.0344 | -0.093 | C21H17O14S | 525.0334(5%) 445.0773(10%) 269.0456(100%) | sulafed emodin-O-glucuronide | √ |  |  |  |  |  |  | √ |  | √ |  | √ |  |  |  |  |  |  |
| E68-3 | 5.02 | 525.0344 | -0.093 | C21H17O14S | 525.0334(5%) 445.0773(10%) 269.0456(100%) | sulafed emodin-O-glucuronide |  | √ | √ |  |  |  |  | √ |  |  |  |  |  |  |  |  |  |  |
| E68-4 | 6.81 | 525.0344 | -0.093 | C21H17O14S | 525.0334(100%) 445.0773(75%) 269.0456(10%) | sulafed emodin-O-glucuronide | √ |  | √ |  |  |  |  | √ |  |  |  |  |  |  |  |  |  |  |
| E69 | 4.61 | 527.0504 | 0.571 | C21H19O14S | 527.0497(15%) 447.0933(100%) 285.0404(20%) | sulfated hydroxyemodin-O-glucoside | √ |  |  |  |  |  |  |  |  | √ |  |  |  |  |  |  |  |  |
| E70-1 | 3.86 | 541.0295 | 0.252 | C21H17O15S | 541.0291(5%) 461.0730(45%) 285.0406(100%) 237.0554(10%) | sulafed hydroxyemodin-O-glucuronide |  | √ | √ |  |  |  |  |  |  | √ | √ |  |  |  |  |  |  |  |
| E70-2 | 4.75 | 541.0295 | 0.252 | C21H17O15S | 541.0291(5%) 461.0730(45%) 285.0406(100%) 237.0554(10%) | sulafed hydroxyemodin-O-glucuronide | √ | √ | √ |  |  |  |  |  |  | √ | √ | √ |  |  |  |  |  |  |
| E70-3 | 5.55 | 541.0295 | 0.252 | C21H17O15S | 541.0291(5%) 461.0730(45%) 285.0406(100%) 237.0554(10%) | sulafed hydroxyemodin-O-glucuronide | √ |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| E71-1 | 4.40 | 607.1315 | 1.717 | C27H27O16 | 607.1309(20%) 445.0764(12%) 431.0987(25%) 269.0455(100%) 225.0548(10%) | emodin-O-glucoside-O-glucuronide |  |  | √ |  | √ |  |  | √ |  | √ |  |  | √ | √ |  | √ | √ |  |
| E71-2 | 4.58 | 607.1315 | 1.717 | C27H27O16 | 607.1309(20%) 445.0764(12%) 431.0987(25%) 269.0455(100%) 225.0548(10%) | emodin-O-glucoside-O-glucuronide |  |  |  | √ | √ |  |  |  |  |  |  |  | √ | √ |  | √ |  |  |
| E71-3 | 4.81 | 607.1315 | 1.717 | C27H27O16 | 607.1309(20%) 445.0764(12%) 431.0987(25%) 269.0455(100%) 225.0548(10%) | emodin-O-glucoside-O-glucuronide | √ |  | √ | √ | √ | √ | √ | √ | √ | √ | √ | √ | √ | √ | √ | √ | √ | √ |
| E71-4 | 5.12 | 607.1315 | 1.717 | C27H27O16 | 607.1309(20%) 445.0764(12%) 431.0987(25%) 269.0455(100%) 225.0548(10%) | emodin-O-glucoside-O-glucuronide | √ |  |  | √ | √ | √ |  |  |  | √ |  |  | √ | √ |  | √ |  |  |
| E71-5 | 5.30 | 607.1315 | 1.717 | C27H27O16 | 607.1309(20%) 445.0764(12%) 431.0987(25%) 269.0455(100%) 225.0548(10%) | emodin-O-glucoside-O-glucuronide | √ |  |  | √ | √ |  |  |  |  | √ |  |  | √ | √ |  | √ |  |  |
| E72-1 | 3.41 | 621.1101 | 0.608 | C27H25O17 | 621.1087(10%) 445.0771(35%) 269.0456(100%) 225.0547(10%) | emodin-O-diglucuronide | √ |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| E72-2 | 3.75 | 621.1101 | 0.608 | C27H25O17 | 621.1087(10%) 445.0771(35%) 269.0456(100%) 225.0547(10%) | emodin-O-diglucuronide |  | √ | √ |  | √ |  | √ | √ | √ | √ | √ | √ |  | √ |  |  | √ |  |
| E72-3 | 4.36 | 621.1101 | 0.608 | C27H25O17 | 621.1087(10%) 445.0771(35%) 269.0456(100%) 225.0547(10%) | emodin-O-diglucuronide | √ |  | √ |  | √ |  |  | √ |  | √ | √ | √ |  | √ |  |  | √ |  |
| E72-4 | 4.82 | 621.1101 | 0.608 | C27H25O17 | 621.1087(10%) 445.0771(35%) 269.0456(100%) 225.0547(10%) | emodin-O-diglucuronide | √ | √ | √ | √ | √ | √ | √ | √ | √ | √ | √ | √ | √ | √ | √ | √ | √ |  |
| E73-1 | 3.07 | 637.1050 | 1.460 | C27H25O18 | 637.1050(5%) 461.0725(50%) 285.0404(100%) | hydroxyemodin-O-diglucuronide | √ | √ | √ |  |  |  |  | √ |  | √ | √ |  |  |  |  |  |  |  |
| E73-2 | 5.07 | 637.1050 | 1.460 | C27H25O18 | 637.1050(5%) 461.0725(50%) 285.0404(100%) | hydroxyemodin-O-diglucuronide | √ | √ | √ |  |  |  |  |  |  | √ |  | √ |  |  |  |  | √ |  |