**Supplementary material**

**Anti-SARS-CoV-2 *in vitro* potential of Castor Oil Plant *(Ricinus communis*) Leaf Extract: *In-Silico* Virtual Evidence**

**Content**

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| **Table S2** | |
| **Table S2a** | UPLC- triple TOF -MS/MS analysis of the methylene chloride fraction of *Ricinus communis* leaf extract **(negative mode)** |
| **Table S2b** | UPLC- triple TOF -MS/MS analysis of the methylene chloride fraction of *Ricinus communis* leaf extract **(positive mode)** |

**Table S2 of *UPLC- Triple TOF -MS/MS analysis:***

**Table S2a: UPLC- triple TOF -MS/MS analysis of the methylene chloride fraction of *Ricinus communis* leaf extract (negative mode)**

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| **Identification** | **Fragments** | **Formula** | **[M-H]+ (*m/z*)** | **RT/min** | **Area** |
| Daidzein-8-C-glucoside | 343.08441:36 415.13312:250 | C21H20O9 | 415.1451 | 1.26 | 35263.71 |
| Esculin | 204.9803:107 339.086:214 | C15H16O9 | 339.0958 | 1.30 | 61670.23 |
| Naringenin | 161.08022:36 169.0154:143 271.04971:143 | C15H12O5 | 271.0457 | 1.39 | 26312.68 |
| Caffeic acid | 179.05421:71 | C9H8O4 | 179.0365 | 1.41 | 11179.17 |
| Myricetin | 80.965:71 94.97707:73 112.98393:398 164.98943:36 180.96033:71 180.96793:107 225.01334:107 248.9525:143 248.97701:112 317.03513:149 317.05527:1372 | C15H10O8 | 316.946 | 1.46 | 201030.9 |
| Quercitrin | 101.02283:7 220.96645:7 259.0737:7 401.14227:136 447.13373:57 447.15762:50 447.17255:36 447.19345:14 | C21H20O11 | 447.1526 | 5.16 | 32162.96 |
| Luteolin | 111.01701:18 124.01885:71 125.02428:54 140.0105:54 168.0033:54 169.01341:71 183.03688:18 211.01299:107 285.05991:1074 | C15H10O6 | 285.0608 | 5.23 | 94189.34 |
| Kaempferol-3-O-alpha-L-rhamnoside | 104.95534:2 112.98396:12 145.05669:2 179.05234:12 212.11203:2 286.92996:5 294.91483:7 324.91116:7 341.86649:2 357.17627:5 362.88651:5 369.16281:2 430.86612:5 431.1857:60 431.19745:64 | C21H20O10 | 431.1896 | 5.41 | 8426.313 |
| Kaempferol-3-O-alpha-L-arabinoside | 97.46767:7 151.0065:14 172.94479:7 211.04379:7 218.93065:14 218.94737:50 221.0798:7 227.02814:36 240.93182:14 249.17534:7 255.03214:93 256.03448:29 258.93964:21 281.14648:14 284.03088:243 285.03616:86 286.9324:107 310.92688:7 326.92282:21 349.17999:14 354.92465:43 379.11404:7 415.89899:15 417.08063:1038 417.18448:14 | C20H18O10 | 417.0814 | 7.18 | 133285.1 |
| Daphnetin | 77.0452:20 89.03659:10 105.02775:20 105.03209:71 117.02448:54 117.03517:1052 118.04262:299 121.02869:199 133.02657:36 134.03671:51 145.01767:48 145.02788:988 146.02962:26 162.03165:230 176.4917:36 176.49921:26 177.05687:2058 | C9H6O4 | 177.056 | 10.59 | 813628.6 |
| Apigenin | 151.11259:161 195.10025:36 251.19931:36 269.12106:36 269.16971:107 269.21606:234 | C15H10O5 | 269.212 | 12.01 | 60136.72 |
| Cholic acid | 343.22351:12 407.30414:48 | C24H40O5 | 407.2931 | 12.66 | 4218.2 |
| E-3,4,5'-Trihydroxy-3'-glucopyranosylstilbene | 405.18054:89 405.22318:36 | C20H22O9 | 405.1667 | 12.98 | 28736.67 |
| 3'-methoxy-4',5,7- trihydroxyflavonol | 297.03635:36 315.16003:107 | C16H12O7 | 315.1588 | 13.37 | 31033.78 |
| Neohesperidin dihydrochalcone | 561.21417:36 611.14313:71 | C28H36O15 | 611.1729 | 15.18 | 65008.11 |
| Phlorizin | 222.89384:36 349.983:36 367.19055:1034 372.88724:36 433.85306:78 435.16891:726 435.24551:71 | C21H24O10 | 435.1792 | 15.22 | 837598.4 |
| Acacetin-7-O-rutinoside | 271.2222:36 310.94739:107 347.23312:71 455.21863:107 489.18158:36 545.18488:107 559.35248:74 591.14447:73 591.18909:375 | C28H32O14 | 591.186 | 15.37 | 106312.1 |
| Acacetin | 240.04327:54 240.06078:18 268.04526:54 283.0636:161 283.26559:54 | C16H12O5 | 283.0575 | 15.73 | 16257.76 |
| 1-Myristoyl-2-hydroxy-sn-glycero-3-phosphate | 96.96135:71 305.27347:18 381.19101:112 381.23514:1878 | C17H35O7P | 381.2322 | 17.89 | 378724.7 |
| 2'-Deoxyinosine | 148.08665:36 251.19969:291 | C10H12N4O4 | 251.1999 | 17.98 | 75997.59 |
| gamma-Linolenic acid | 59.01659:250 127.07301:107 141.09064:71 182.12686:107182.13068:214 205.1929:214 208.15092:107 231.22017:74 233.23021:712257.19055:109 259.21017:557 261.19205:73 272.93842:73 275.20389:560 275.45932:73 276.32959:600 277.04605:89 277.21768:13698 | C18H30O2 | 277.2186 | 20.02 | 1.53E+08 |
| Sodium Deoxycholate | 345.30389:54 391.29556:89 | C24H40O4 | 391.304 | 21.02 | 26472.99 |

**Table S2b: UPLC- triple TOF -MS/MS analysis for methylene chloride fraction of *Ricinus communis* leaf extract (positive mode)**

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| **Identification** | **Fragments** | **Formula** | **[M+H]+ (*m/z*)** | **RT/min** | **Area** |
| 3 5 7-trihydroxy-4'-methoxyflavone | 121.07944:72 124.05583:36 147.10567:36 211.10869:143 228.10925:72 253.12735:36 297.9032:73 301.14362:837 | C16H12O6 | 301.1417 | 1.25 | 20810.04 |
| Acacetin | 285.00696:72 285.01172:251 | C16H12O5 | 285.0173 | 1.31 | 67633.05 |
| 4'-hydroxyisoflavone-7-O-glucoside | 112.89754:107 255.11269:72 417.17789:72 | C21H20O9 | 417.1629 | 1.33 | 49204.63 |
| Trigonelline | 50.01662:1026 51.02224:2433 52.03176:1636 53.00386:334 53.03883:3401 53.99742:107 55.05467:107 63.0246:72 64.8423:172 65.03802:7875 66.03479:1372 67.05534:2115 68.05109:143 76.01514:108 77.02551:182 77.04038:516 78.03507:8091 79.03363:292 79.04116:3386 80.05117:1047 90.03168:36 91.76562:265 92.0499:18176 93.05785:4380 93.77572:335 94.06583:13213 95.04067:72 102.45649:36 105.02216:143 110.05307:179 110.06493:375 120.04371:823 123.03248:74 136.03931:1068 137.62495:538 138.05598:30849 | C7H7NO2 | 138.0566 | 1.38 | 6508700 |
| (+-)-Taxifolin | 55.01692:36 120.07148:143 121.08241:251 123.05746:251 126.05474:36 131.06569:107 133.07462:215 135.05614:107 136.06229:107 137.07216:394 145.07458:107 149.06438:215 149.07127:322 160.06963:72 161.07521:215 162.08034:179 163.08498:322 171.05656:36 173.07547:287 175.09126:287 177.11122:107 179.07851:179 187.0872:72 191.07916:473 197.08269:72 197.09457:143 205.09969:179 207.0903:36 209.0946:468 215.08675:107 221.09216:145 225.08662:145 225.09933:73 227.10789:1258 231.0273:37 233.09657:430 251.10939:394 269.12036:471 287.12784:985 304.17487:38 305.14099:4002 | C15H12O7 | 305.1398 | 1.39 | 694411.9 |
| Hypotaurine | 52.99774:18 110.05611:90 | C2H7NO2S | 110.061 | 4.18 | 5813.906 |
| Ricinine | 53.03677:107 55.01696:107 56.04815:251 64.033:36 67.04146:143 68.04875:251 80.05621:109 82.02901:974 83.01154:179 84.04394:941 92.04716:72 93.04148:215 94.04936:72 105.04528:143 108.04475:322 110.05599:398 121.03894:107 122.0508:251 136.07219:292 138.05592:2087 150.05214:251 165.06731:6600 | C8H8N2O2 | 165.0682 | |  | | --- | | 4.25 | |  | | 41406780 |
| Phenylephrine | 57.02916:18 68.05339:36 83.03211:36 90.90462:36 141.05843:54 168.07422:143 | C9H13NO2 | 168.0788 | |  | | --- | | 4.27 | | 18085.97 |
| Para aminobenzoic acid | 55.01908:48 60.98331:24 82.02907:48 83.00904:48 103.01186:12 138.01959:48 138.05609:322 | C7H7NO2 | 138.0581 | 4.30 | 119338 |
| L-(-)-Phenylalanine | 50.0166:54 51.02423:161 52.02562:90 53.00385:170 53.02235:54 53.04086:287 54.0057:161 54.03476:399 55.01904:557 55.03999:251 56.02065:331 56.05024:170 57.05476:72 58.02946:107 59.01459:90 59.03411:72 64.01716:99 65.02432:161 65.04027:134 66.04165:251 67.00906:63 67.04374:516 68.05106:721 69.0471:120 69.05415:534 70.03621:72 70.06693:170 71.07043:170 73.06503:54 76.01756:36 77.02052:54 78.03503:197 79.0361:287 80.05366:260 81.05483:453 82.03154:2922 82.06735:118 82.77497:36 83.0321:2896 83.06814:227 84.04651:2397 85.04883:2088 91.02312:72 92.04985:188 93.04691:513 94.04112:179 94.05208:773 95.03236:206 96.04264:143 97.03043:90 97.0499:72 98.03167:99 105.04526:215 106.04911:351 107.03145:152 108.04472:521 109.04803:1411 110.02338:72 110.0619:518 111.02987:63 111.06557:1402 119.01858:27 120.0622:45 121.04824:81 122.04767:439 123.05433:701 124.03683:36 125.04533:72 127.06186:36 134.0472:90 136.03593:36 136.05899:54 137.0424:179 138.05589:1853 139.05981:9212 145.1188:9 149.03336:45 150.04175:206 151.0466:1123 152.05829:134 165.07092:197 165.54659:197 166.07022:21469 | C9H11NO2 | 165.9953 | 4.31 | 7422.022 |

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| Lupeol | 137.11504:9 185.11458:18 409.18677:18 425.8219:18 426.99988:18 427.18079:3157 | C30H50O | 427.1806 | 5.63 | 256517.4 |
| 3' 4' 5 7-tetrahydroxyflavanone | 87.04253:12 130.08496:36 214.07361:12 272.15454:12 289.10324:48 289.16565:131 | C15H12O6 | 289.1086 | 5.91 | 8176.653 |
| Apigenin 8-C-glucoside | 416.27277:36 433.15567:399 | C21H20O10 | 433.1524 | 6.23 | 16123.15 |
| Rutin | 57.02906:24 57.03546:96 69.03528:60 71.04891:586 73.05046:24 84.76771:25 85.03052:980 87.04751:37 93.03593:12 97.03036:72 101.05196:12 111.03873:36 124.35465:12 127.03954:215 129.05276:665 137.02585:72 145.04056:36 145.05077:227 147.06784:688 153.02094:60 163.06334:36 165.02739:60 229.05707:96 250.00534:12 255.87552:12 257.05139:119 268.00974:24 275.67365:12 281.05438:60 285.04538:96 302.09027:191 302.14426:48 303.05307:50348 309.12027:60 345.06348:60 355.06549:119 356.07727:155 401.99286:36 413.11563:12 447.09604:48 449.12262:334 464.05734:37 465.11041:4236 611.1712:2514 611.33179:40 | C27H30O16 | 611.1697 | 6.63 | 980015.8 |
| Quercetin | 69.00267:18 115.05634:18 127.04612:54 137.02606:143 145.05096:54 153.02463:107 165.02396:72 170.0941:90 173.05708:36 179.02956:18 195.09767:36 198.10706:18 229.04863:107 230.11838:54 245.04703:18 257.03336:36 257.04694:72 285.04541:90 286.11441:72 301.05548:37 303.05801:1448 303.14648:72 | C15H10O7 | 303.0541 | 6.64 | 97103.82 |
| Baicalein-7-O-glucuronide | 62.03764:18 149.01979:36 165.06029:18 429.25034:73 447.19171:620 447.26337:54 | C21H18O11 | 447.192 | 6.70 | 21673.55 |
| Hyperoside | 83.01138:36 85.02785:287 95.046:36 97.02753:143 127.03312:107 131.04298:36 145.05412:143 149.06432:36 153.0139:107 163.04167:36 257.04688:215 275.06912:36 297.08496:36 302.10501:169 303.0531:14394 335.33371:46 343.01541:72 432.08685:107 448.09393:72 465.11053:394 465.17142:107 | C21H20O12 | 465.1075 | 6.96 | 292431.7 |
| Isosakuranetin-7-O-neohesperidoside | 53.03071:12 69.03786:12 71.04916:299 85.02816:374 112.54388:12 125.02974:12 129.0466:48 129.05621:203 145.0544:72 147.06465:131 165.02036:36 284.13553:12 286.14795:96 287.0563:12984 427.25729:12 433.11459:96 449.07468:36 449.11057:889 595.17047:442 595.2876:36 | C28H34O14 | 595.1757 | 7.24 | 244765.1 |
| Scopoletin | 50.01637:358 51.01796:94 51.02401:1405 52.03151:134 53.00568:55 53.04064:1824 55.01881:143 62.01283:45 62.0195:27 65.04004:1316 66.03913:114 66.04831:3537 67.01578:27 67.05508:45 68.02754:143 68.99761:376 70.00763:18 75.02096:45 76.03458:116 76.80482:55 77.04013:3275 78.04978:242 79.01831:278 79.05346:215 81.03428:2987 82.04156:27 83.01131:18 88.02765:18 89.04005:461 91.05256:206 93.0358:179 93.75906:45 94.04366:5517 95.04868:45 97.02745:36 102.04502:18 104.02582:36 105.0248:98 105.03349:1796 106.04311:116 107.04879:197 109.03015:63 109.06554:72 117.03339:313 118.04375:18 119.04921:81 120.65069:27 121.02943:1311 121.66093:57 122.03813:11016 122.7317:21 123.04476:27 126.03239:18 132.01454:18 132.60576:161 133.02885:20803 134.04051:331 135.04286:63 136.64252:57 137.0125:29 137.06209:7263 137.9131:18 147.0369:18 147.04033:36 148.59225:18 149.02977:118 149.06081:1125 149.55771:76 150.0347:8703 151.03952:20 154.45296:18 161.02133:900 164.04198:18 164.52701:37 165.0563:1922 177.00966:18 177.02469:27 177.46835:107 178.02934:16645 179.03685:18 180.68056:18 192.44:233 192.89864:21 193.05164:15762 | C10H8O4 | 193.0512 | 7.33 | 3005504 |
| Pantothenate | 57.07194:50 63.0247:7 77.03802:14 91.05025:64 99.01015:7 103.05208:21 105.06863:50 107.08426:21 115.05034:64 117.05824:466 118.06564:2865 119.07428:64 120.07792:43 121.06712:21 127.05256:7 128.06364:72 129.06911:50 130.06561:430 131.07565:179 132.08311:981 133.09117:179 134.09651:136 137.09557:21 144.07317:57 144.08334:244 145.10208:100 146.09712:901 147.10582:36 148.11456:50 150.09393:21 157.08626:21 158.10019:50 160.10924:143 161.09343:43 161.11494:43 162.09143:935 163.09612:21 172.11488:36 174.09155:72 175.58521:36 176.1095:430 176.14323:2713 177.11906:150 178.12776:36 179.1053:36 188.10483:14 189.13264:29 190.1243:509 192.14673:21 202.16629:86 204.13861:57 205.16478:394 219.48721:64 220.16971:6320 | C9H17NO5 | 220.1734 | 8.06 | 386672.8 |
| Hypoxanthine | 77.03796:36 91.05557:143 137.02605:143 | C5H4N4O | 137.0977 | 12.81 | 74672.97 |
| Daphnetin | 55.05302:36 65.04532:36 77.04087:36 81.06554:36 105.06612:107 133.0948:72 179.10565:143 | C9H6O4 | 179.1086 | 15.08 | 31639.17 |
| DL-alpha,epsilon-Diaminopimelic acid | 67.05782:107 69.07548:107 77.0381:72 81.07542:36 83.05295:143 91.05305:179 93.06898:72 95.05193:72 105.07742:143 115.05652:143 117.07365:36 121.07036:143 128.06058:179 129.06924:72 131.09196:145 133.09782:72 135.08282:398 143.08861:143 156.08635:36 161.0972:179 173.13544:107 175.13664:72 191.14221:759 | C7H14N2O4 | 191.1435 | 16.02 | 85056.15 |
| all-trans-Retinoic acid | 67.05312:107 77.04794:36 81.07281:107 91.05837:143 93.06892:107 95.08215:143 99.07764:36 107.08431:251 109.066:143 117.07053:143 119.08668:287 121.06409:143 128.07332:72 130.08502:36 133.10429:215 135.08606:287 142.08029:72 145.0988:107 147.07854:143 147.12991:72 149.09583:287 156.09691:107 157.10056:215 159.11397:143 161.09358:107 173.09825:143 189.09789:72 203.14343:72 223.15097:107 241.19467:107 259.17545:143 269.21384:36 283.20392:143 301.21799:1347 | C20H28O2 | 301.2188 | 17.68 | 623206.5 |
| 4- Methoxy cinnamic acid | 65.03577:36 131.08859:36 161.14009:72 179.10916:72 | C10H10O3 | 179.1522 | 17.89 | 23934.5 |
| D-(-)-Erythrose | 67.05817:36 77.03845:215 105.06618:36 121.02407:72 | C4H8O4 | 121.1005 | 20.72 | 359604.6 |
| Nicotinamide | 123.09566:72 | C6H6N2O | 123.1179 | 20.78 | 21498.16 |
| 3-(4-Hydroxyphenyl)Prop-2-Enoic acid | 57.02721:36 79.05644:107 91.04767:72 107.08438:72 119.08675:143 147.11627:107 165.06419:107 | C9H8O3 | 165.1685 | 21.69 | 24401.07 |
| L-beta-Homotryptophan-HCl | 57.07231:36 93.06935:72 105.07201:36 112.13733:36 119.08712:107 127.05309:36 201.16434:36 219.17839:215 | C12H14N2O2 | 219.1799 | 21.71 | 19864.9 |
| 4-Hydroxy-3-methoxycinnamaldehyde | 55.05309:24 65.04085:36 67.05128:72 73.02462:12 79.04679:24 79.05683:96 81.07075:72 88.01529:12 91.05346:60 93.07758:12 95.08263:48 105.07205:36 117.06491:12 119.09024:48 123.08334:24 131.08592:12 133.10803:24 136.01701:24 161.13705:24 164.03578:12 179.06435:36 179.13994:96 | C10H10O3 | 179.1448 | 22.32 | 100183.2 |
| Leupeptin hemisulfate salt | 57.03402:36 80.05184:36 81.07844:107 91.05083:36 93.07492:36 95.08546:179 105.08371:36 109.1049:72 121.10194:179 123.11788:72 133.10161:107 137.13261:251 139.11072:72 144.07047:107 146.10805:107 151.11006:72 151.1552:72 158.06184:36 163.15092:107 171.12041:72 175.15585:107 177.16867:72 183.11554:36 185.11195:107 189.17223:72 191.18178:143 193.19411:72 201.16045:36 205.15746:107 229.20781:107 247.17021:72 257.19293:72 269.23749:36 281.22128:72 299.15848:36 391.34149:107 409.31436:179 427.25281:251 427.31119:251 427.35788:664 | C20H38N6O4 | 427.3577 | 23.47 | 87204.86 |
| Acacetin-7-O-rutinoside | 95.0826:36 121.10186:72 149.09978:36 224.13551:54 249.14993:54 283.15213:54 315.18375:72 333.23868:54 335.26776:72 360.17236:54 372.14706:36 373.16104:36 375.20413:36 382.19455:54 389.18262:54 400.18445:54 401.18503:54 402.19818:54 404.21695:72 405.21118:90 416.19946:36 417.20831:107 418.21835:54 419.22388:197 420.23059:54 421.19794:36 428.84808:36 431.17886:314 431.19058:1039 432.20569:251 433.24548:1119 434.25122:251 444.2002:72 445.21262:628 446.20828:627 447.22299:1348 448.24481:73 449.24985:125 458.2189:54 459.229:1094 460.23416:2964 461.24042:2645 462.21741:90 462.24777:251 463.21976:90 464.22318:72 471.24692:36 472.2467:54 473.24142:897 474.24335:181 475.18475:72 476.2627:433 477.24313:452 478.2431:107 485.23483:54 487.2587:639 488.22543:107 488.26288:90 489.26181:305 490.23676:90 490.69333:54 491.22522:381 492.26477:1085 493.24271:90 499.23801:72 501.23395:72 503.24655:107 504.26068:270 505.23776:2018 506.26028:72 515.25293:412 517.28058:125 518.23804:305 519.24786:453 520.25867:233 521.21246:90 532.24359:125 533.11047:68 533.26044:21265 534.25873:106 535.2644:72 540.38593:54 543.23883:90 546.23126:72 547.28119:412 549.23853:161 550.25818:179 551.27222:125 557.38928:36 558.39655:90 560.99548:36 561.26306:547 563.23181:108 564.25098:1023 565.29797:961 575.27228:711 575.44165:90 576.36334:36 578.25647:215 590.49683:37 591.40302:903 592.13123:54 592.26178:36 592.39923:54 592.83234:54 593.15558:215 593.27936:90507 | C28H32O14 | 593.2808 | 24.41 | 5925746 |