

## Supplementary Material

### Antiviral and ROS Scavenging Potential of *Carica papaya* Linn and *Psidium guajava* Leaves Extract against HIV-1 Infection

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Table S1. Phytochemical constituents of methanolic leaves extract of *Carica papaya* and *Psidium guajava*

| Phytochemicals     | Name of the test                                 | <i>Carica papaya</i> | <i>Psidium guajava</i> |
|--------------------|--|----------------------|------------------------|
| Carbohydrates      | Molisch test                                     | +                    | +                      |
| Flavonoids         | Alkaline reagent test                            | +                    | -                      |
| Saponins           | Foam test  | -                    | -                      |
| Tannins            | Ferric chloride test                             | -                    | -                      |
| Terpenoids         | Chloroform-H <sub>2</sub> SO <sub>4</sub> method | +                    | +                      |
| Cardiac glycosides | Keller Kilani test                               | +                    | +                      |
| Steroids           | Salkowki test                                    | +                    | +                      |
| Coumarins          | Alkaline test                                    | +                    | +                      |
| Quinones           | H <sub>2</sub> SO <sub>4</sub> method            | +                    | +                      |

(+) Shows positive and (-) negative results.

**Table S2: Identified Compound from *Carica papaya* extract using HR-ESI-MS.** *Carica papaya* extract shows 25% of alkaloids (Peptide, Amino acids), 5% of Glycoside, 10% lipids, 20% of Phenolic compounds (Aromatic Phenol, Quinone, Flavonoids), and 20% of Terpenes, 15% of Aliphatic Compounds (Fatty acids, alcohol and saturated, Unsaturated Alkenes) as well as 5% of other. We observed that both extracts have a higher percentage of alkaloids, Terpenes.

| Formula  | Mass      | RT     | Height  | Area     | Score | Name   |
|--|-----------|--------|---------|----------|-------|--|
| C <sub>54</sub> H <sub>101</sub> NO <sub>8</sub> P               | 922.7262  | 13.853 | 5118    | 25518    | 91.33 | PC(22:4(7Z,10Z,13Z,16Z)/24:0)                |
| C <sub>38</sub> H <sub>75</sub> NO <sub>8</sub> P                | 704.5241  | 17.422 | 24137   | 96926    | 90.42 | PC(14:0/16:1(9Z))                            |
| C <sub>36</sub> H <sub>73</sub> NO <sub>8</sub> P                | 678.5067  | 5.635  | 3083596 | 17150362 | 90.85 | PC(14:0/14:0)                                |
| CH <sub>5</sub> N <sub>3</sub>                                   | 59.0482   | 1.051  | 10433   | 20987    | 85.33 | Guanidine                                    |
| C <sub>10</sub> H <sub>16</sub> N <sub>2</sub> O <sub>8</sub>    | 292.0902  | 7.25   | 49721   | 849686   | 86.85 | Edetate                                      |
| C <sub>10</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub>    | 208.0853  | 5.97   | 34521   | 259885   | 89.44 | Formyl-5-hydroxykynurenamine                 |
| C <sub>41</sub> H <sub>78</sub> NO <sub>8</sub> P                | 743.5457  | 15.717 | 43806   | 217552   | 85.44 | PE(18:2(9Z,12Z)/18:0)                        |
| C <sub>40</sub> H <sub>78</sub> NO <sub>8</sub> P                | 731.5484  | 18.337 | 38288   | 174844   | 86.37 | PE(20:1(11Z)/15:0)                           |
| C <sub>40</sub> H <sub>72</sub> NO <sub>8</sub> P                | 725.4994  | 14.649 | 20248   | 49069    | 85.23 | PE(20:4(5Z,8Z,11Z,14Z)/15:0)                 |
| C <sub>39</sub> H <sub>78</sub> NO <sub>8</sub> P                | 719.5402  | 16.868 | 15159   | 21555    | 84.37 | PE(14:0/20:0)                                |
| C <sub>10</sub> H <sub>13</sub> N <sub>5</sub> O                 | 219.1125  | 18.214 | 36427   | 766036   | 85.27 | cis-Zeatin                                   |
| C <sub>5</sub> H <sub>9</sub> N <sub>3</sub>                     | 111.0795  | 1.253  | 101510  | 32024    | 83.95 | Betazole                                     |
| C <sub>4</sub> H <sub>8</sub> N <sub>4</sub> O <sub>4</sub>      | 176.0548  | 16.215 | 8068    | 18897    | 86.12 | Allantoic acid                               |
| C <sub>2</sub> H <sub>7</sub> NO <sub>2</sub> S                  | 109.0196  | 5.117  | 14233   | 25483    | 96.28 | Hypotaurine                                  |
| C <sub>14</sub> H <sub>25</sub> NO <sub>11</sub>                 | 383.1414  | 6.112  | 20482   | 40775    | 91.68 | Beta-1,4-mannose-N-acetylglucosamine         |
| C <sub>7</sub> H <sub>11</sub> NO <sub>5</sub>                   | 189.0634  | 5.83   | 49522   | 207388   | 89.67 | AminoDHQ                                     |
| C <sub>18</sub> H <sub>29</sub> D <sub>5</sub> O <sub>2</sub>    | 287.2879  | 11.89  | 23706   | 69201    | 91.08 | Oleic acid (d5)                              |
| C <sub>16</sub> H <sub>24</sub> N <sub>2</sub> O <sub>4</sub>    | 308.173   | 15.147 | 36019   | 484368   | 94.25 | Bestatin                                     |
| C <sub>21</sub> H <sub>34</sub> O                                | 302.2588  | 11.87  | 25076   | 45717    | 97.34 | (15:1)-Cardanol                              |
| C <sub>7</sub> H <sub>8</sub> NO <sub>2</sub>                    | 138.0567  | 1.383  | 650136  | 1689048  | 90.47 | Trigonelline                                 |
| C <sub>11</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub>    | 220.0846  | 15.236 | 7163    | 18959    | 86.24 | N-Hydroxy-L-tryptophan                       |
| C <sub>5</sub> H <sub>13</sub> O <sub>8</sub> P                  | 232.0346  | 1.575  | 217384  | 1116976  | 91.87 | D-Ribitol 5-phosphate                        |
| C <sub>23</sub> H <sub>30</sub> N <sub>2</sub> O <sub>5</sub>    | 414.2131  | 12.165 | 618110  | 5092427  | 85.44 | Desacetylvindoline                           |
| C <sub>8</sub> H <sub>19</sub> N <sub>6</sub> O <sub>7</sub> P   | 342.107   | 16.148 | 19380   | 96868    | 81.17 | Streptidine 6-phosphate                      |
| C <sub>12</sub> H <sub>21</sub> NO <sub>4</sub> S <sub>2</sub>   | 307.09    | 3.774  | 56692   | 426609   | 85.2  | S-Succinylidihydrolipoamide                  |
| C <sub>4</sub> H <sub>8</sub> O <sub>3</sub>                     | 104.0482  | 1.097  | 90102   | 427813   | 85.52 | D(-)-β-hydroxy butyric acid                  |
| C <sub>30</sub> H <sub>52</sub> O <sub>7</sub> P <sub>2</sub>    | 586.3229  | 19.014 | 662649  | 1850028  | 86.72 | Presqualene diphosphate                      |
| C <sub>31</sub> H <sub>55</sub> O <sub>9</sub> P                 | 602.3587  | 19.498 | 369234  | 1821060  | 92.08 | dolichyl beta-D-glucosyl phosphate           |
| C <sub>63</sub> H <sub>105</sub> NO <sub>12</sub> P <sub>2</sub> | 1129.7118 | 12.58  | 9764    | 48529    | 96.83 | N-Acetyl-D-glucosaminyldiphosphoundecaprenol |
| C <sub>9</sub> H <sub>8</sub> O                                  | 132.0586  | 1.25   | 652170  | 709649   | 93.05 | Atropaldehyde                                |
| C <sub>21</sub> H <sub>38</sub> N <sub>4</sub> O <sub>8</sub>    | 474.2691  | 17.03  | 510494  | 3495956  | 91.17 | Amastatin                                    |
| C <sub>6</sub> H <sub>15</sub> N <sub>4</sub> O <sub>6</sub> P   | 270.0726  | 7.638  | 60066   | 573842   | 86.82 | D-Lombricine                                 |
| C <sub>5</sub> H <sub>11</sub> N                                 | 85.0896   | 1.791  | 550113  | 630076   | 91.13 | Piperidine                                   |
| C <sub>30</sub> H <sub>47</sub> N <sub>3</sub> O <sub>9</sub> S  | 625.3143  | 16.171 | 43403   | 252787   | 85.46 | Leukotriene C4                               |

|  |          |        |          |          |       |  |
|--|----------|--------|----------|----------|-------|--|
| <b>C<sub>20</sub>H<sub>40</sub>O</b>                           | 296.3121 | 15.014 | 18947    | 42611    | 92.36 | Phytol                                   |
| <b>C<sub>25</sub>H<sub>27</sub>N<sub>4</sub>O</b>              | 399.2168 | 17.216 | 168809   | 1984843  | 91.11 | Z-Phe-Phe-CHN2                           |
| <b>C<sub>6</sub>H<sub>5</sub>NO<sub>4</sub></b>                | 155.0216 | 16.496 | 6682     | 14307    | 87.56 | 2,4-Dihydroxy-nitrophenol                |
| <b>C<sub>6</sub>H<sub>13</sub>NO<sub>2</sub></b>               | 131.0948 | 2.441  | 738395   | 7496636  | 87.12 | L-Norleucine                             |
| <b>C<sub>18</sub>H<sub>22</sub>O<sub>5</sub>S</b>              | 350.1194 | 17.846 | 17078    | 118070   | 88.28 | Estrone 3-sulfate                        |
| <b>C<sub>8</sub>H<sub>7</sub>NS</b>                            | 149.03   | 19.216 | 10936    | 25357    | 91.91 | 2-Methylbenzothiazole                    |
| <b>C<sub>6</sub>H<sub>12</sub>O<sub>6</sub></b>                | 180.0654 | 1.515  | 2073667  | 14057729 | 85.83 | D-Tagatose                               |
| <b>C<sub>20</sub>H<sub>20</sub>N<sub>2</sub>O<sub>3</sub></b>  | 336.1473 | 16.155 | 91052    | 959692   | 93.25 | Nb-Feruloyltryptamine                    |
| <b>C<sub>4</sub>H<sub>9</sub>N<sub>3</sub>O<sub>2</sub></b>    | 131.07   | 4.706  | 27260    | 69423    | 87.51 | Creatine                                 |
| <b>C<sub>6</sub>H<sub>15</sub>N<sub>2</sub>O<sub>6</sub>P</b>  | 242.0665 | 15.259 | 4623     | 14189    | 87.96 | 2-Deoxystreptamine 4-phosphate           |
| <b>C<sub>26</sub>H<sub>53</sub>NO<sub>7</sub>P</b>             | 522.363  | 19.123 | 2361701  | 23273042 | 84.91 | LysoPC(18:1(11Z))                        |
| <b>C<sub>7</sub>H<sub>8</sub>O<sub>8</sub></b>                 | 220.0231 | 1.257  | 641808   | 2174634  | 88.57 | 4-Carboxy-4-hydroxy-2-oxoadipate         |
| <b>C<sub>18</sub>H<sub>22</sub>O<sub>3</sub></b>               | 286.1566 | 11.24  | 14705    | 54917    | 88.4  | Furamethrin                              |
| <b>C<sub>4</sub>H<sub>5</sub>N<sub>3</sub>O<sub>2</sub></b>    | 127.0387 | 1.074  | 64087    | 299394   | 94.29 | I-Methyl-4-nitro-imidazole               |
| <b>C<sub>14</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub></b>  | 278.1268 | 14.036 | 25368    | 250598   | 96.89 | Prolyl-Tyrosine                          |
| <b>C<sub>12</sub>H<sub>12</sub>N<sub>2</sub>O<sub>4</sub></b>  | 248.0812 | 17.17  | 46386    | 319594   | 90.78 | 5-Hydroxyindoleacetyl glycine            |
| <b>C<sub>9</sub>H<sub>13</sub>NO<sub>6</sub></b>               | 231.0748 | 5.973  | 37806    | 218952   | 87.5  | N-Acetyl-L-2-amino-6-oxopimelate         |
| <b>C<sub>5</sub>H<sub>9</sub>NO<sub>4</sub></b>                | 147.0546 | 5.137  | 30042    | 118981   | 88.26 | O-Acetyl-L-serine                        |
| <b>C<sub>20</sub>H<sub>14</sub>NO<sub>4</sub></b>              | 332.094  | 2.003  | 179742   | 1002099  | 86.14 | SANGUINARINE                             |
| <b>C<sub>21</sub>H<sub>29</sub>FO<sub>5</sub></b>              | 380.1928 | 5.014  | 131003   | 927867   | 92.33 | Fludrocortisone                          |
| <b>C<sub>19</sub>H<sub>25</sub>N<sub>5</sub>O<sub>4</sub></b>  | 387.1888 | 11.359 | 291256   | 2290450  | 91.71 | Terazosin                                |
| <b>C<sub>7</sub>H<sub>8</sub>N<sub>4</sub>O<sub>2</sub></b>    | 180.0654 | 1.515  | 1910783  | 12571886 | 88.83 | Paraxanthine                             |
| <b>C<sub>15</sub>H<sub>25</sub>NO<sub>3</sub></b>              | 267.1839 | 4.713  | 23798    | 42883    | 87.29 | Metoprolol                               |
| <b>C<sub>31</sub>H<sub>33</sub>N<sub>3</sub>O<sub>6</sub>S</b> | 575.2095 | 1.963  | 49640    | 185737   | 85.12 | Zafirlukast                              |
| <b>C<sub>13</sub>H<sub>17</sub>N</b>                           | 187.1363 | 4.467  | 49475    | 347892   | 88.83 | (+/-)-2-(4'-Isobutylphenyl)propionitrile |
| <b>C<sub>26</sub>H<sub>29</sub>N<sub>3</sub>O<sub>6</sub></b>  | 479.208  | 19.704 | 67070    | 772269   | 85.77 | Nicardipine                              |
| <b>C<sub>8</sub>H<sub>7</sub>N<sub>3</sub>O<sub>5</sub></b>    | 225.0382 | 14.394 | 10851    | 83045    | 86.99 | Dinitolmide                              |
| <b>C<sub>6</sub>H<sub>14</sub>NO<sub>2</sub></b>               | 132.1027 | 2.441  | 423197   | 3332548  | 93.79 | beta-Alaninebetaine                      |
| <b>C<sub>22</sub>H<sub>42</sub>O<sub>2</sub></b>               | 338.3192 | 17.024 | 48028    | 215179   | 91.45 | cis-Cetoleic acid                        |
| <b>C<sub>14</sub>H<sub>17</sub>NO<sub>10</sub></b>             | 359.0866 | 10.596 | 97016    | 1310489  | 90.63 | TRIBOA-glucoside                         |
| <b>C<sub>17</sub>H<sub>11</sub>NO<sub>7</sub></b>              | 341.0521 | 10.633 | 75539    | 997278   | 93.19 | Aristolochic Acid                        |
| <b>C<sub>11</sub>H<sub>13</sub>N<sub>3</sub>O<sub>6</sub></b>  | 283.0823 | 14.036 | 25847    | 259607   | 87.95 | Cucumopine                               |
| <b>C<sub>32</sub>H<sub>46</sub>N<sub>2</sub>O<sub>8</sub></b>  | 586.3254 | 18.855 | 395562   | 2550746  | 87.51 | Inuline                                  |
| <b>C<sub>24</sub>H<sub>39</sub>NO<sub>7</sub></b>              | 453.2737 | 19.475 | 69955    | 374036   | 88.66 | Delcosine                                |
| <b>C<sub>32</sub>H<sub>44</sub>N<sub>2</sub>O<sub>8</sub></b>  | 584.3122 | 18.695 | 11774919 | 81571602 | 86.75 | Lappaconitine                            |
| <b>C<sub>33</sub>H<sub>42</sub>N<sub>4</sub></b>               | 494.3313 | 11.571 | 26792    | 107536   | 91.22 | Auricularine                             |
| <b>C<sub>38</sub>H<sub>40</sub>N<sub>4</sub>O<sub>2</sub></b>  | 584.3218 | 18.957 | 329092   | 257280   | 95.98 | Caracurine V                             |
| <b>C<sub>43</sub>H<sub>52</sub>N<sub>4</sub>O<sub>6</sub></b>  | 720.3896 | 17.107 | 59036    | 360925   | 92.52 | Epivoacorine                             |
| <b>C<sub>17</sub>H<sub>22</sub>O<sub>6</sub></b>               | 322.14   | 19.153 | 12819    | 59200    | 89.11 | Tetraneurin A                            |
| <b>C<sub>21</sub>H<sub>21</sub>NO<sub>7</sub></b>              | 399.1322 | 3.432  | 12715    | 159803   | 90.3  | Adlumidiceine                            |

|   |          |        |        |         |       |   |
|---|----------|--------|--------|---------|-------|---|
| <b>C<sub>28</sub>H<sub>36</sub>N<sub>2</sub>O<sub>4</sub></b>             | 464.2669 | 17.163 | 17638  | 11790   | 90.02 | Ipecac (Psychotrine)  |
| <b>C<sub>18</sub>H<sub>22</sub>O<sub>11</sub></b>                         | 414.1167 | 7.565  | 17408  | 106656  | 86.06 | Asperuloside  |
| <b>C<sub>11</sub>H<sub>13</sub>NO<sub>3</sub></b>                         | 207.089  | 1.704  | 596508 | 2145255 | 86.9  | Cantleyine  |
| <b>C<sub>39</sub>H<sub>49</sub>N<sub>5</sub>O<sub>7</sub></b>             | 699.3676 | 13.157 | 66131  | 57463   | 94.01 | Lasiodine A   |
| <b>C<sub>24</sub>H<sub>26</sub>O<sub>6</sub></b>                          | 410.1725 | 8.039  | 60279  | 572023  | 86.67 | $\alpha$ -Mangostin   |
| <b>C<sub>8</sub>H<sub>15</sub>NO<sub>2</sub></b>                          | 157.1121 | 11.949 | 14981  | 47673   | 86.8  | Tranexamic acid   |
| <b>C<sub>41</sub>H<sub>28</sub>O<sub>26</sub></b>                         | 936.0906 | 4.225  | 93182  | 307822  | 96.79 | Casuarinin  |
| <b>C<sub>31</sub>H<sub>45</sub>NO<sub>8</sub></b>                         | 559.313  | 19.17  | 138319 | 476544  | 91.39 | Auriculine  |
| <b>C<sub>20</sub>H<sub>27</sub>NO<sub>7</sub></b>                         | 393.1768 | 5.708  | 64573  | 541061  | 85.12 | Latifoline  |
| <b>C<sub>16</sub>H<sub>11</sub>NO<sub>3</sub></b>                         | 265.0744 | 12.324 | 16053  | 100789  | 91.45 | Piperolactam A  |
| <b>C<sub>45</sub>H<sub>73</sub>NO<sub>14</sub></b>                        | 851.4994 | 12.941 | 13053  | 24540   | 85.77 | alpha-Chaconine   |
| <b>C<sub>27</sub>H<sub>48</sub>N<sub>2</sub>O</b>                         | 416.378  | 16.778 | 93673  | 950044  | 88.11 | Cyclovirobuxine C   |
| <b>C<sub>27</sub>H<sub>48</sub>N<sub>2</sub>O<sub>2</sub></b>             | 432.3714 | 15.77  | 239536 | 429354  | 94.97 | Solacapine  |
| <b>C<sub>22</sub>H<sub>24</sub>O<sub>6</sub></b>                          | 384.1566 | 18.41  | 6822   | 17897   | 91.4  | 12-Dehydroporson  |
| <b>C<sub>7</sub>H<sub>7</sub>N<sub>3</sub></b>                            | 133.0645 | 1.489  | 598515 | 1670793 | 86.54 | 3-Methylpyrrolo[1,2-a]pyrazine  |
| <b>C<sub>19</sub>H<sub>17</sub>NO<sub>2</sub></b>                         | 291.1272 | 18.078 | 8267   | 29057   | 88.11 | Naproanilide  |
| <b>C<sub>13</sub>H<sub>7</sub>F<sub>3</sub>N<sub>2</sub>O<sub>5</sub></b> | 328.0307 | 8.304  | 8037   | 53567   | 95.53 | Fluorodifen   |
| <b>C<sub>23</sub>H<sub>36</sub>N<sub>4</sub>O<sub>5</sub></b>             | 448.267  | 17.657 | 24643  | 253155  | 90.83 | N-Acetyl-leu-leu-tyr-amide  |
| <b>C<sub>10</sub>H<sub>15</sub>O<sub>4</sub>P</b>                         | 230.0705 | 6.908  | 8638   | 23658   | 87.76 | Diethyl phenyl phosphate  |
| <b>C<sub>26</sub>H<sub>44</sub>O<sub>9</sub></b>                          | 500.2982 | 13.495 | 217030 | 1101659 | 92.21 | Mupirocin   |
| <b>C<sub>26</sub>H<sub>35</sub>NO<sub>4</sub></b>                         | 425.2568 | 7.124  | 76746  | 828491  | 88.61 | Diprenorphine   |
| <b>C<sub>41</sub>H<sub>60</sub>O<sub>11</sub></b>                         | 728.4131 | 16.37  | 41283  | 153480  | 94.19 | Avermectin A1b monosaccharide   |
| <b>C<sub>26</sub>H<sub>35</sub>N<sub>5</sub>O<sub>12</sub>S</b>           | 641.1981 | 11.432 | 154630 | 1598893 | 87.48 | Cyclothialidine   |
| <b>C<sub>36</sub>H<sub>48</sub>N<sub>2</sub>O<sub>8</sub></b>             | 636.3415 | 18.413 | 449009 | 3257077 | 92.9  | Ansatrienin A   |
| <b>C<sub>16</sub>H<sub>14</sub>N<sub>2</sub>O<sub>3</sub></b>             | 282.1009 | 12.324 | 17490  | 105725  | 91.45 | Saphenic acid methyl ester  |
| <b>C<sub>16</sub>H<sub>19</sub>NO<sub>4</sub></b>                         | 289.13   | 2.321  | 45572  | 1548787 | 92.04 | Balfourodine  |
| <b>C<sub>26</sub>H<sub>33</sub>NO<sub>5</sub></b>                         | 439.2342 | 12.556 | 79780  | 768359  | 87    | Militarinone B  |
| <b>C<sub>30</sub>H<sub>31</sub>NO<sub>9</sub></b>                         | 549.1988 | 9.532  | 22305  | 187050  | 87.29 | Jadomycin B   |
| <b>C<sub>19</sub>H<sub>14</sub>O<sub>5</sub></b>                          | 322.0868 | 6.285  | 44577  | 318028  | 96.59 | 11-Deoxylandomycinone   |
| <b>C<sub>17</sub>H<sub>14</sub>N<sub>2</sub>O<sub>7</sub></b>             | 358.0789 | 10.596 | 82135  | 1165905 | 94.84 | Coumeroic acid  |
| <b>C<sub>15</sub>H<sub>22</sub>FN<sub>3</sub>O<sub>6</sub></b>            | 359.1494 | 1.28   | 154769 | 343989  | 93.09 | Capecitabine  |
| <b>C<sub>32</sub>H<sub>32</sub>O<sub>16</sub>S<sub>4</sub></b>            | 800.0559 | 1.333  | 171790 | 624862  | 87.78 | TS-TM-calix(4)arene   |
| <b>C<sub>32</sub>H<sub>61</sub>NO<sub>10</sub>P</b>                       | 650.4025 | 17.359 | 122294 | 1671973 | 87.28 | 1-Palmitoyl-2-(5-hydroxy-8-oxo-6-octenoyl)-sn-glycero-3-phosphatidylcholine |
| <b>C<sub>12</sub>H<sub>11</sub>N<sub>3</sub></b>                          | 197.0945 | 1.721  | 117523 | 951786  | 86.64 | 2-Amino-3-methyl-9H-pyrido[2,3-b]indole                                     |
| <b>C<sub>8</sub>H<sub>6</sub>N<sub>2</sub>O</b>                           | 146.047  | 5.134  | 32262  | 199294  | 88.86 | 1(2H)-Phthalazinone   |
| <b>C<sub>15</sub>H<sub>23</sub>NOS</b>                                    | 265.1512 | 4.769  | 466119 | 2648362 | 86.86 | Esprocarb   |
| <b>C<sub>35</sub>H<sub>43</sub>NO<sub>11</sub></b>                        | 653.2855 | 17.226 | 38938  | 162008  | 86.4  | Rifamycin W-hemiacetal  |
| <b>C<sub>20</sub>H<sub>30</sub>O<sub>2</sub></b>                          | 302.2247 | 11.233 | 46768  | 588657  | 85.78 | Cascarillone  |
| <b>C<sub>22</sub>H<sub>30</sub>F<sub>2</sub>O<sub>3</sub></b>             | 380.216  | 11.306 | 58711  | 614770  | 92.28 | 4,4-Difluoro-17beta-hydroxyandrost-5-en-3-one propionate                    |
| <b>C<sub>13</sub>H<sub>21</sub>O<sub>3</sub>PS</b>                        | 288.0954 | 19.906 | 10737  | 38469   | 90.24 | Iprobenfos  |

|  |          |        |         |          |       |   |
|--|----------|--------|---------|----------|-------|---|
| <b>C<sub>14</sub>H<sub>10</sub>N<sub>2</sub>O<sub>4</sub></b>  | 270.0636 | 17.17  | 46631   | 327290   | 93.51 | 4,4'-dinitrostilbene  |
| <b>C<sub>4</sub>H<sub>8</sub>FNO<sub>3</sub></b>               | 137.0493 | 1.383  | 658341  | 1730519  | 97.64 | 4-Fluoro-L-threonine  |
| <b>C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>9</sub>P</b> | 381.069  | 10.629 | 5883    | 12340    | 86.51 | 2-Amino-5-formylamino-6-(5-phospho-D-riboseylamino)pyrimidin-4(3H)-one  |
| <b>C<sub>39</sub>H<sub>56</sub>N<sub>6</sub>O<sub>8</sub></b>  | 736.4164 | 17.654 | 33197   | 200941   | 87.93 | Myxochromide S2   |
| <b>C<sub>25</sub>H<sub>45</sub>NO<sub>9</sub></b>              | 503.309  | 18.629 | 67677   | 340461   | 85.06 | Pederin   |
| <b>C<sub>7</sub>H<sub>17</sub>N<sub>3</sub></b>                | 143.1432 | 17.77  | 9370    | 12333    | 86.57 | Dehydrospermidine   |
| <b>C<sub>30</sub>H<sub>42</sub></b>                            | 402.3311 | 9.999  | 19428   | 85537    | 85.14 | 4,4'-Diaponeurosporene  |
| <b>C<sub>5</sub>H<sub>8</sub></b>                              | 68.063   | 1.791  | 550074  | 630027   | 91.13 | Isoprene  |
| <b>C<sub>25</sub>H<sub>27</sub>NO</b>                          | 357.2104 | 5.038  | 85480   | 513344   | 90.72 | N-Desmethyltamoxifen  |
| <b>C<sub>14</sub>H<sub>22</sub>N<sub>2</sub>O<sub>2</sub></b>  | 250.1673 | 3.728  | 30199   | 207053   | 87.83 | Rivastigmine  |
| <b>C<sub>23</sub>H<sub>27</sub>NO<sub>9</sub></b>              | 461.1682 | 8.285  | 20146   | 197687   | 85.29 | Morphine 3-glucuronide  |
| <b>C<sub>7</sub>H<sub>16</sub>NO<sub>4</sub></b>               | 178.1072 | 1.326  | 22311   | 21505    | 86.98 | Anthopleurine   |
| <b>C<sub>25</sub>H<sub>43</sub>NO<sub>10</sub></b>             | 517.2878 | 17.183 | 2915546 | 47362111 | 88    | Mycalamide B  |
| <b>C<sub>26</sub>H<sub>34</sub>O<sub>8</sub></b>               | 474.2254 | 18.029 | 35581   | 127559   | 93.17 | Agrimophol  |
| <b>C<sub>26</sub>H<sub>34</sub>O<sub>8</sub></b>               | 474.2249 | 17.803 | 44549   | 346048   | 85.72 | Agrimophol  |
| <b>C<sub>9</sub>H<sub>18</sub>N<sub>2</sub>O<sub>2</sub>S</b>  | 218.1083 | 4.868  | 52158   | 165755   | 88.31 | Thiofanox   |
| <b>C<sub>18</sub>H<sub>35</sub>NO</b>                          | 281.2726 | 17.455 | 158415  | 1727696  | 96.13 | Oleamide  |
| <b>C<sub>12</sub>H<sub>19</sub>N<sub>3</sub>O<sub>5</sub></b>  | 285.1332 | 5.144  | 17730   | 29789    | 86.04 | Glycylprolylhydroxyproline  |
| <b>C<sub>24</sub>H<sub>35</sub>NO<sub>5</sub></b>              | 417.2507 | 12.201 | 95660   | 654263   | 89.33 | Batrachotoxinin A   |
| <b>C<sub>23</sub>H<sub>28</sub>O<sub>8</sub></b>               | 432.1771 | 8.092  | 45860   | 446413   | 90.97 | (2S,4S,6S)-2-[2-(4-Hydroxy-3-methoxyphenyl)ethyl]tetrahydro-6-(4,5-dihydroxy-3-methoxyphenyl)-2H-pyran-4-yl 4-acetate |
| <b>C<sub>22</sub>H<sub>31</sub>NO</b>                          | 325.2416 | 11.598 | 17206   | 107463   | 87.29 | Tolterodine   |
| <b>C<sub>18</sub>H<sub>36</sub>O<sub>3</sub></b>               | 300.2669 | 12.735 | 25843   | 104107   | 88.14 | (R)-10-hydroxystearic acid  |
| <b>C<sub>41</sub>H<sub>28</sub>O<sub>27</sub></b>              | 952.0994 | 4.109  | 968912  | 7530433  | 95.18 | Geraniin  |
| <b>C<sub>41</sub>H<sub>30</sub>O<sub>26</sub></b>              | 938.0987 | 4.354  | 102890  | 328235   | 85.09 | Eugeniin  |
| <b>C<sub>41</sub>H<sub>26</sub>O<sub>26</sub></b>              | 934.0718 | 3.926  | 1454647 | 10557650 | 90.28 | 2-O-Galloylpunicalin  |
| <b>C<sub>41</sub>H<sub>64</sub>O<sub>19</sub></b>              | 860.4062 | 12.327 | 93398   | 847262   | 91.93 | Corchoroside E  |
| <b>C<sub>42</sub>H<sub>74</sub>O<sub>15</sub></b>              | 818.503  | 12.692 | 24968   | 156236   | 87.6  | Quinquenoside F1  |
| <b>C<sub>41</sub>H<sub>62</sub>O<sub>15</sub></b>              | 794.4069 | 13.561 | 15198   | 41760    | 95.52 | Betavulgaroside IV  |
| <b>C<sub>34</sub>H<sub>26</sub>O<sub>22</sub></b>              | 786.0953 | 4.305  | 144479  | 865815   | 92.53 | Heterophylliin A  |
| <b>C<sub>42</sub>H<sub>79</sub>O<sub>10</sub>P</b>             | 774.5383 | 19.879 | 108970  | 589250   | 92.83 | PG(18:0/18:2(9Z,12Z))   |
| <b>C<sub>42</sub>H<sub>61</sub>NO<sub>7</sub></b>              | 691.445  | 15.316 | 79676   | 2848823  | 96.01 | 13-Demethylspirolide C  |
| <b>C<sub>45</sub>H<sub>66</sub>O<sub>5</sub></b>               | 686.4881 | 15.306 | 60953   | 799562   | 93.05 | DG(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/20:5(5Z,8Z,11Z,14Z,17Z)/0:0)   |
| <b>C<sub>33</sub>H<sub>60</sub>O<sub>14</sub></b>              | 680.3922 | 12.825 | 609372  | 4726320  | 95.09 | Gingerglycolipid C  |
| <b>C<sub>33</sub>H<sub>58</sub>O<sub>14</sub></b>              | 678.3772 | 14.152 | 109454  | 474530   | 87.28 | Gingerglycolipid B  |
| <b>C<sub>42</sub>H<sub>30</sub>O<sub>9</sub></b>               | 678.1885 | 4.945  | 16024   | 56792    | 83.18 | alpha-Viniferin   |
| <b>C<sub>36</sub>H<sub>58</sub>O<sub>11</sub></b>              | 666.3939 | 16.002 | 84645   | 393522   | 88.61 | Quercilicoside A  |
| <b>C<sub>43</sub>H<sub>64</sub>O<sub>5</sub></b>               | 660.4724 | 8.573  | 36464   | 413546   | 91.13 | DG(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/18:4(6Z,9Z,12Z,15Z)/0:0)   |
| <b>C<sub>36</sub>H<sub>62</sub>O<sub>10</sub></b>              | 654.4334 | 16.629 | 47407   | 115424   | 88.14 | Vinaginsenoside R10   |
| <b>C<sub>36</sub>H<sub>58</sub>O<sub>10</sub></b>              | 650.4025 | 17.193 | 155843  | 638402   | 85.16 | Saponin H   |

|  |          |        |         |          |       |  |
|--|----------|--------|---------|----------|-------|--|
| <b>C<sub>36</sub>H<sub>54</sub>O<sub>10</sub></b>              | 646.3695 | 16.155 | 38235   | 174209   | 85.45 | abrusoside A   |
| <b>C<sub>35</sub>H<sub>68</sub>NO<sub>7</sub>P</b>             | 645.4727 | 7.17   | 58199   | 644992   | 90.25 | PE(14:1(9Z)/P-16:0)  |
| <b>C<sub>39</sub>H<sub>51</sub>NO<sub>7</sub></b>              | 645.3656 | 16.274 | 119794  | 1073156  | 94.07 | Janthitrem F   |
| <b>C<sub>11</sub>H<sub>22</sub>O<sub>22</sub>P<sub>4</sub></b> | 629.9575 | 1.535  | 18495   | 75236    | 90.25 | Phosphatidylinositol-3,4,5-trisphosphate   |
| <b>C<sub>28</sub>H<sub>33</sub>O<sub>16</sub></b>              | 625.1771 | 11.432 | 44834   | 316559   | 86.14 | Petunidin 3-rhamnoside 5-glucoside   |
| <b>C<sub>28</sub>H<sub>33</sub>O<sub>15</sub></b>              | 609.1823 | 15.06  | 45915   | 275871   | 90.11 | Peonidin 3-rhamnoside 5-glucoside  |
| <b>C<sub>30</sub>H<sub>53</sub>NO<sub>11</sub></b>             | 603.3627 | 18.861 | 83688   | 518503   | 91.75 | Fumonisin AK1  |
| <b>C<sub>35</sub>H<sub>54</sub>N<sub>2</sub>O<sub>6</sub></b>  | 598.3975 | 5.296  | 104638  | 503114   | 92.97 | 3'-N-Acetyl-4'-O-(9-octadecenoyl)fusarochromanone  |
| <b>C<sub>30</sub>H<sub>28</sub>O<sub>13</sub></b>              | 596.1579 | 7.764  | 74085   | 379945   | 90.31 | Eriodictyol 7-(6-trans-p-coumaroylglucoside)   |
| <b>C<sub>26</sub>H<sub>29</sub>N<sub>2</sub>O<sub>14</sub></b> | 593.1725 | 13.966 | 44272   | 43403    | 90.9  | 2-Decarboxyphyllactin  |
| <b>C<sub>34</sub>H<sub>56</sub>O<sub>8</sub></b>               | 592.3991 | 15.455 | 79441   | 1651922  | 85.51 | Tuberoside   |
| <b>C<sub>29</sub>H<sub>36</sub>O<sub>13</sub></b>              | 592.2151 | 18.032 | 2196637 | 10506288 | 87.88 | 8-Acetoxy-4'-methoxypinoresinol 4-glucoside  |
| <b>C<sub>29</sub>H<sub>36</sub>O<sub>13</sub></b>              | 592.2178 | 17.86  | 1529307 | 13406469 | 85.13 | 8-Acetoxy-4'-methoxypinoresinol 4-glucoside  |
| <b>C<sub>28</sub>H<sub>30</sub>O<sub>14</sub></b>              | 590.1642 | 14.802 | 56817   | 166182   | 85.27 | Maysin 3'-methyl ether   |
| <b>C<sub>37</sub>H<sub>48</sub>O<sub>6</sub></b>               | 588.3456 | 19.714 | 84797   | 438794   | 91.21 | Hydratopyrrophanthol   |
| <b>C<sub>26</sub>H<sub>30</sub>O<sub>15</sub></b>              | 582.1607 | 7.346  | 25355   | 178789   | 89.84 | Asperuloside tetraacetate  |
| <b>C<sub>38</sub>H<sub>56</sub>O<sub>4</sub></b>               | 576.4165 | 5.31   | 71958   | 314071   | 87.34 | 2-Hexaprenyl-3-methyl-5-hydroxy-6-methoxy-1,4-benzoquinone   |
| <b>C<sub>37</sub>H<sub>66</sub>O<sub>4</sub></b>               | 574.5002 | 17.428 | 268925  | 2449230  | 92.63 | Montecristin   |
| <b>C<sub>33</sub>H<sub>28</sub>O<sub>9</sub></b>               | 568.1732 | 4.245  | 45129   | 175152   | 91.31 | Asticolorin C  |
| <b>C<sub>29</sub>H<sub>58</sub>NO<sub>7</sub>P</b>             | 563.3949 | 18.924 | 149859  | 100375   | 90.3  | LysoPE(0:0/24:1(15Z))  |
| <b>C<sub>28</sub>H<sub>34</sub>O<sub>12</sub></b>              | 562.2036 | 6.188  | 44184   | 235913   | 86.76 | 5,7-Dihydroxy-3',4'-dimethoxy-8-(3-hydroxy-3-methylbutyl)-isoflavone 7-glucoside                           |
| <b>C<sub>35</sub>H<sub>60</sub>O<sub>5</sub></b>               | 560.4428 | 5.296  | 74401   | 330471   | 89.18 | Corepoxylone   |
| <b>C<sub>24</sub>H<sub>32</sub>O<sub>15</sub></b>              | 560.1698 | 7.16   | 39055   | 132047   | 87.78 | 5''-(4-Hydroxy-(E)-cinnamoyl) alpha-L-arabinofuranosyl-(1->3)-beta-D-xylopyranosyl-(1->4)-D-xylopyranoside |
| <b>C<sub>33</sub>H<sub>38</sub>N<sub>2</sub>O<sub>5</sub></b>  | 542.2764 | 18.34  | 1134745 | 4047772  | 90.44 | Chaetoglobosin N   |
| <b>C<sub>25</sub>H<sub>30</sub>O<sub>13</sub></b>              | 538.1752 | 7.429  | 61102   | 542703   | 86.94 | Lippioside I   |
| <b>C<sub>30</sub>H<sub>47</sub>NO<sub>4</sub>S</b>             | 517.3251 | 13.495 | 244935  | 1241072  | 86.2  | Retapamulin  |
| <b>C<sub>23</sub>H<sub>39</sub>N<sub>3</sub>O<sub>8</sub></b>  | 485.2751 | 18.075 | 37970   | 139892   | 91.84 | Sarcodon scabrosus Depsipeptide  |
| <b>C<sub>31</sub>H<sub>48</sub>O<sub>4</sub></b>               | 484.3531 | 15.525 | 64335   | 434271   | 87.32 | 3b,18b-3-Methoxy-11-oxo-12-oleanen-30-oic acid   |
| <b>C<sub>30</sub>H<sub>44</sub>O<sub>5</sub></b>               | 484.3193 | 17.432 | 22380   | 73701    | 90.06 | Propapyriogenin A2   |
| <b>C<sub>21</sub>H<sub>30</sub>O<sub>12</sub></b>              | 474.1756 | 7.256  | 17044   | 119736   | 85.54 | 6-Feruloylglucose 2,3,4-trihydroxy-3-methylbutylglycoside  |
| <b>C<sub>31</sub>H<sub>42</sub>O<sub>3</sub></b>               | 462.3136 | 16.646 | 72852   | 348161   | 91.16 | Hydroxysintaxanthin 5,6-epoxide  |
| <b>C<sub>22</sub>H<sub>20</sub>O<sub>11</sub></b>              | 460.1005 | 1.618  | 43337   | 119003   | 86.59 | Glycitein 4'-O-glucuronide   |
| <b>C<sub>20</sub>H<sub>23</sub>N<sub>7</sub>O<sub>6</sub></b>  | 457.1726 | 9.542  | 13721   | 132294   | 90.29 | 5,10-Methylenetetrahydrofolate   |
| <b>C<sub>18</sub>H<sub>32</sub>N<sub>8</sub>O<sub>6</sub></b>  | 456.2372 | 17.684 | 1288131 | 14369689 | 90.12 | Rigin  |
| <b>C<sub>22</sub>H<sub>20</sub>O<sub>10</sub></b>              | 444.1062 | 6.689  | 21041   | 409463   | 89.11 | Betavulgarin xyloside  |
| <b>C<sub>23</sub>H<sub>39</sub>NO<sub>5</sub>S</b>             | 441.2527 | 6.165  | 62219   | 283472   | 91.07 | Leukotriene E3   |
| <b>C<sub>29</sub>H<sub>58</sub>O<sub>2</sub></b>               | 438.4434 | 19.435 | 16368   | 45594    | 80.95 | Nonacosanoic acid  |
| <b>C<sub>22</sub>H<sub>42</sub>O<sub>8</sub></b>               | 434.2882 | 7.177  | 25134   | 202413   | 90.23 | Polysorbate 60   |
| <b>C<sub>21</sub>H<sub>36</sub>O<sub>9</sub></b>               | 432.2306 | 15.415 | 97534   | 910459   | 92.35 | Glucosyl (2E,6E,10x)-10,11-dihydroxy-2,6-farnesadienoate   |

|  |          |        |        |         |       |   |
|--|----------|--------|--------|---------|-------|---|
| <b>C<sub>29</sub>H<sub>46</sub>O<sub>2</sub></b>               | 426.3471 | 12.546 | 27335  | 148159  | 88.86 | Stigmast-4-ene-3,6-dione                      |
| <b>C<sub>19</sub>H<sub>14</sub>O<sub>11</sub></b>              | 418.053  | 1.525  | 55134  | 297886  | 86.6  | Shoyuflavone C                                |
| <b>C<sub>23</sub>H<sub>28</sub>N<sub>8</sub></b>               | 416.2435 | 17.216 | 136891 | 1970985 | 97.39 | Forasartan                                    |
| <b>C<sub>29</sub>H<sub>50</sub>O</b>                           | 414.3871 | 5.227  | 265994 | 1563669 | 85.96 | β-Sitosterol                                  |
| <b>C<sub>24</sub>H<sub>48</sub>NO<sub>4</sub></b>              | 414.3588 | 15.899 | 117382 | 19854   | 95.31 | Heptadecanoyl carnitine                       |
| <b>C<sub>27</sub>H<sub>40</sub>O<sub>3</sub></b>               | 412.2962 | 12.218 | 108692 | 838456  | 88.79 | (9E)-Valenciananthin                          |
| <b>C<sub>21</sub>H<sub>30</sub>O<sub>8</sub></b>               | 410.2015 | 8.079  | 59053  | 754502  | 88.12 | Scorzoside                                    |
| <b>C<sub>19</sub>H<sub>34</sub>O<sub>9</sub></b>               | 406.2174 | 4.593  | 205678 | 2446898 | 87.1  | Kiwiionoside                                  |
| <b>C<sub>19</sub>H<sub>30</sub>O<sub>9</sub></b>               | 402.189  | 2.169  | 9173   | 14927   | 86.41 | Methyl 7-epi-12-hydroxyjasmonate glucoside    |
| <b>C<sub>21</sub>H<sub>23</sub>NO<sub>7</sub></b>              | 401.1489 | 14.914 | 8422   | 43838   | 92.29 | Margrapine A                                  |
| <b>C<sub>24</sub>H<sub>28</sub>O<sub>4</sub></b>               | 380.1928 | 5.014  | 123041 | 831029  | 89.38 | Tokinolide A                                  |
| <b>C<sub>19</sub>H<sub>29</sub>N<sub>3</sub>O<sub>3</sub>S</b> | 379.1897 | 5.021  | 83804  | 192503  | 87.61 | Thaumatococin b, recombinant                  |
| <b>C<sub>22</sub>H<sub>26</sub>O<sub>5</sub></b>               | 370.1764 | 5.532  | 115876 | 324788  | 92.89 | 3,17beta-Diacetoxystera-1,3,5(10)-trien-6-one |
| <b>C<sub>22</sub>H<sub>44</sub>O<sub>2</sub></b>               | 340.3343 | 14.881 | 18012  | 25750   | 88.47 | Docosanoic acid                               |
| <b>C<sub>20</sub>H<sub>41</sub>NO<sub>2</sub></b>              | 327.3188 | 16.195 | 27259  | 166395  | 88.59 | N,N-Dimethylsphingosine                       |
| <b>C<sub>18</sub>H<sub>18</sub>O<sub>5</sub></b>               | 314.117  | 18.042 | 8806   | 39015   | 88.28 | 6-Hydroxyenterolactone                        |
| <b>C<sub>18</sub>H<sub>14</sub>O<sub>5</sub></b>               | 310.0844 | 5.492  | 17037  | 83652   | 88.91 | 6-Deoxyjacareubin                             |
| <b>C<sub>15</sub>H<sub>12</sub>O<sub>7</sub></b>               | 304.0578 | 5.419  | 484823 | 2678026 | 87.22 | (±)-Taxifolin                                 |
| <b>C<sub>16</sub>H<sub>28</sub>N<sub>2</sub>O<sub>2</sub></b>  | 280.2105 | 8.235  | 12571  | 59858   | 86.86 | Phygrine                                      |
| <b>C<sub>18</sub>H<sub>19</sub>NO</b>                          | 265.146  | 7.028  | 43646  | 223054  | 89.45 | Mukoening A                                   |
| <b>C<sub>18</sub>H<sub>32</sub>O</b>                           | 264.2461 | 17.455 | 165784 | 1783055 | 96.13 | (±)-(Z)-2-(5-Tetradecenyl)cyclobutanone       |
| <b>C<sub>9</sub>H<sub>12</sub>O<sub>7</sub>S</b>               | 264.0287 | 1.23   | 56189  | 146424  | 96.02 | 3-Methoxy-4-Hydroxyphenylglycol Sulfate       |
| <b>C<sub>15</sub>H<sub>28</sub>O<sub>3</sub></b>               | 256.2044 | 5.247  | 10892  | 12807   | 90.33 | Ipomeatetrahydrofuran                         |
| <b>C<sub>12</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub></b>  | 254.1247 | 7.631  | 41803  | 313464  | 87.09 | Midodrine                                     |
| <b>C<sub>8</sub>H<sub>10</sub>O<sub>7</sub>S</b>               | 250.0123 | 0.746  | 5280   | 11554   | 95.87 | 3,4-Dihydroxyphenylglycol O-sulfate           |
| <b>C<sub>12</sub>H<sub>24</sub>N<sub>2</sub>O<sub>3</sub></b>  | 244.1784 | 1.243  | 72724  | 96556   | 99.12 | N-(6-aminohexanoyl)-6-aminohexanoic acid      |
| <b>C<sub>12</sub>H<sub>15</sub>NO<sub>4</sub></b>              | 237.0999 | 7.688  | 40045  | 369318  | 87.09 | 3-Hydroxy-carbofuran                          |
| <b>C<sub>16</sub>H<sub>28</sub>O</b>                           | 236.2134 | 19.458 | 9137   | 20096   | 85.98 | Ambroside                                     |
| <b>C<sub>10</sub>H<sub>20</sub>N<sub>2</sub>O<sub>4</sub></b>  | 232.143  | 7.664  | 37960  | 260081  | 93.8  | Isoleucyl-Threonine                           |
| <b>C<sub>9</sub>H<sub>17</sub>N<sub>3</sub>O<sub>4</sub></b>   | 231.1217 | 7.246  | 24558  | 207870  | 93.68 | Asparaginyl-Valine                            |
| <b>C<sub>15</sub>H<sub>26</sub>O</b>                           | 222.1982 | 11.183 | 26195  | 133933  | 88.18 | Faurinone                                     |
| <b>C<sub>13</sub>H<sub>17</sub>NS</b>                          | 219.1078 | 6.049  | 28356  | 215913  | 86.03 | 2-Hexylbenzothiazole                          |
| <b>C<sub>12</sub>H<sub>22</sub>O<sub>3</sub></b>               | 214.1577 | 12.583 | 18458  | 111416  | 87.67 | 4-Acetoxy-2-hexyltetrahydrofuran              |
| <b>C<sub>5</sub>H<sub>12</sub>NO<sub>6</sub>P</b>              | 213.0405 | 5.97   | 33352  | 222527  | 82.66 | N-Lactoyl ethanolamine phosphate              |
| <b>C<sub>14</sub>H<sub>28</sub>O</b>                           | 212.2113 | 13.429 | 46108  | 321939  | 86.32 | 12-Methyltridecanal                           |
| <b>C<sub>13</sub>H<sub>25</sub>NO</b>                          | 211.1924 | 16.48  | 9472   | 11014   | 85.66 | Ethyl menthane carboxamide                    |
| <b>C<sub>15</sub>H<sub>28</sub></b>                            | 208.2178 | 15.465 | 12184  | 160728  | 86.14 | Cadinene                                      |
| <b>C<sub>14</sub>H<sub>24</sub>O</b>                           | 208.1839 | 19.8   | 9400   | 41479   | 85.36 | 2-Decylfuran                                  |
| <b>C<sub>15</sub>H<sub>22</sub></b>                            | 202.1714 | 6.775  | 32932  | 60246   | 95.82 | beta-vatirene                                 |
| <b>C<sub>10</sub>H<sub>10</sub>N<sub>4</sub>O</b>              | 202.0859 | 18.214 | 36727  | 736458  | 85.28 | Metamitron                                    |

|  |          |        |        |         |       |                                    |
|--|----------|--------|--------|---------|-------|------------------------------------|
| C <sub>9</sub> H <sub>14</sub> N <sub>2</sub> O <sub>3</sub> | 198.0997 | 1.532  | 429271 | 1944774 | 86.36 | Metharbital                        |
| C <sub>6</sub> H <sub>8</sub> OS <sub>2</sub>                | 160.0022 | 18.423 | 8251   | 86561   | 87.27 | (2-Furanylmethyl) methyl disulfide |
| C <sub>6</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub>  | 138.0431 | 1.618  | 136387 | 469588  | 88.56 | para-Benzoquinone dioxime          |
| C <sub>7</sub> H <sub>7</sub> NO <sub>2</sub>                | 137.0473 | 7.094  | 15236  | 24829   | 91.35 | Salicylamide                       |
| C <sub>6</sub> H <sub>10</sub> O <sub>2</sub>                | 114.0682 | 2.447  | 715759 | 7259424 | 87.12 | Allyl propionate                   |
| C <sub>6</sub> H <sub>14</sub> O                             | 102.1045 | 18.423 | 318262 | 502355  | 94.75 | 3-Hexanol                          |
| C <sub>5</sub> H <sub>12</sub> N                             | 86.0974  | 1.791  | 566325 | 768345  | 91.13 | Neurine                            |

**Table S3: Identified Compound from *Psidium guajava* extract using HR-ESI-MS.** The HR-ESI-MS data of *Psidium guajava* extract shows 40% of alkaloids (Peptide, Amino acids), 10% of Glycoside, 10% lipids, 10% of Phenolic compound (Aromatic Phenol, Quinone), and 10% of Terpenes, 15% of aliphatic Compounds (Fatty acids, alcohol and saturated, Unsaturated Alkenes) as well as 5% of other compounds were observed.

| Formula  | Mass     | RT     | Area     | Height  | Score | Chemical Name   |
|--|----------|--------|----------|---------|-------|---|
| C <sub>18</sub> H <sub>18</sub> N <sub>2</sub> O <sub>5</sub>    | 342.1228 | 1.346  | 36328701 | 6341465 | 89.77 | Dictyoquinazol C  |
| C <sub>11</sub> H <sub>23</sub> N <sub>2</sub> O <sub>7</sub> PS | 358.0967 | 1.346  | 33637932 | 5795375 | 92.01 | D-Pantetheine 4'-phosphate  |
| C <sub>14</sub> H <sub>20</sub> O <sub>10</sub> S                | 380.0785 | 1.346  | 32567359 | 5651386 | 93.02 | 4-Methoxybenzyl O-(2-sulfoglucoside)                                  |
| C <sub>12</sub> H <sub>14</sub> O                                | 174.1042 | 1.313  | 5277170  | 2359957 | 86.12 | (R)-11,12,13-Trinor-1(5),6,9-guaiatrien-8-one                         |
| C <sub>10</sub> H <sub>16</sub> O                                | 152.1211 | 1.376  | 4236221  | 942093  | 91.27 | alpha-Cyclocitral   |
| C <sub>7</sub> H <sub>16</sub> NO                                | 130.1233 | 1.134  | 785693   | 636421  | 93.51 | 4-Trimethylammoniobutanal   |
| C <sub>21</sub> H <sub>40</sub> O <sub>9</sub>                   | 436.2684 | 14.928 | 4200628  | 778494  | 87.29 | (R)-1-O-[b-D-Apiofuranosyl-(1->2)-b-D-glucopyranoside]-1,3-octanediol |
| C <sub>18</sub> H <sub>35</sub> N <sub>3</sub> O <sub>13</sub>   | 501.2158 | 1.648  | 3215465  | 973292  | 90.38 | D-Glucosaminide   |
| C <sub>6</sub> H <sub>14</sub> O                                 | 102.1048 | 18.284 | 254648   | 253617  | 93.23 | 3-Hexanol   |
| C <sub>42</sub> H <sub>77</sub> O <sub>10</sub> P                | 772.5257 | 17.495 | 3092491  | 338911  | 90.72 | PG(18:3(6Z,9Z,12Z)/18:0)  |
| C <sub>35</sub> H <sub>56</sub> O <sub>7</sub>                   | 588.4054 | 12.636 | 1173809  | 345953  | 84.08 | 22-Angeloyltheasapogenol A  |
| C <sub>20</sub> H <sub>30</sub> O <sub>10</sub>                  | 430.1826 | 19.001 | 2293200  | 396140  | 87.96 | Phenethyl rutinoside  |
| C <sub>6</sub> H <sub>8</sub> N <sub>2</sub> O                   | 124.0629 | 5.18   | 42056    | 212958  | 87.08 | Methylimidazole acetaldehyde  |
| C <sub>13</sub> H <sub>28</sub> NO <sub>2</sub>                  | 230.2103 | 6.218  | 392328   | 213161  | 86.07 | Capryloylcholine  |
| C <sub>8</sub> H <sub>12</sub> O                                 | 124.0888 | 19.03  | 131368   | 37006   | 86.13 | trans, trans-3,5-Octadien-2-one                                       |
| C <sub>36</sub> H <sub>72</sub> NO <sub>7</sub> P                | 661.5047 | 18.642 | 2232877  | 459799  | 92.35 | PE(P-16:0/15:0)   |
| C <sub>29</sub> H <sub>32</sub> O <sub>13</sub>                  | 588.1835 | 4.812  | 2728670  | 421837  | 88.22 | Etoposide   |
| C <sub>15</sub> H <sub>17</sub> NO <sub>4</sub>                  | 275.1139 | 5.247  | 553250   | 123903  | 87.75 | 5-Amino-6-(4-hydroxy-2-butenyl)-2,2-dimethyl-4- chromanone            |
| C <sub>12</sub> H <sub>15</sub> N <sub>3</sub> O <sub>6</sub>    | 297.0958 | 5.247  | 552765   | 123005  | 95.83 | Musk xylene   |
| C <sub>42</sub> H <sub>75</sub> O <sub>10</sub> P                | 770.5104 | 15.362 | 606510   | 178893  | 91.34 | PG(18:3(9Z,12Z,15Z)/18:1(9Z))   |
| C <sub>25</sub> H <sub>50</sub> NO <sub>7</sub> P                | 507.3329 | 6.265  | 888928   | 175901  | 85.77 | LysoPE(20:1(11Z)/0:0)   |
| C <sub>41</sub> H <sub>62</sub> O <sub>2</sub>                   | 586.4755 | 15.147 | 2724165  | 201701  | 94.3  | 3',4'-Dihydrorhodovibrin  |

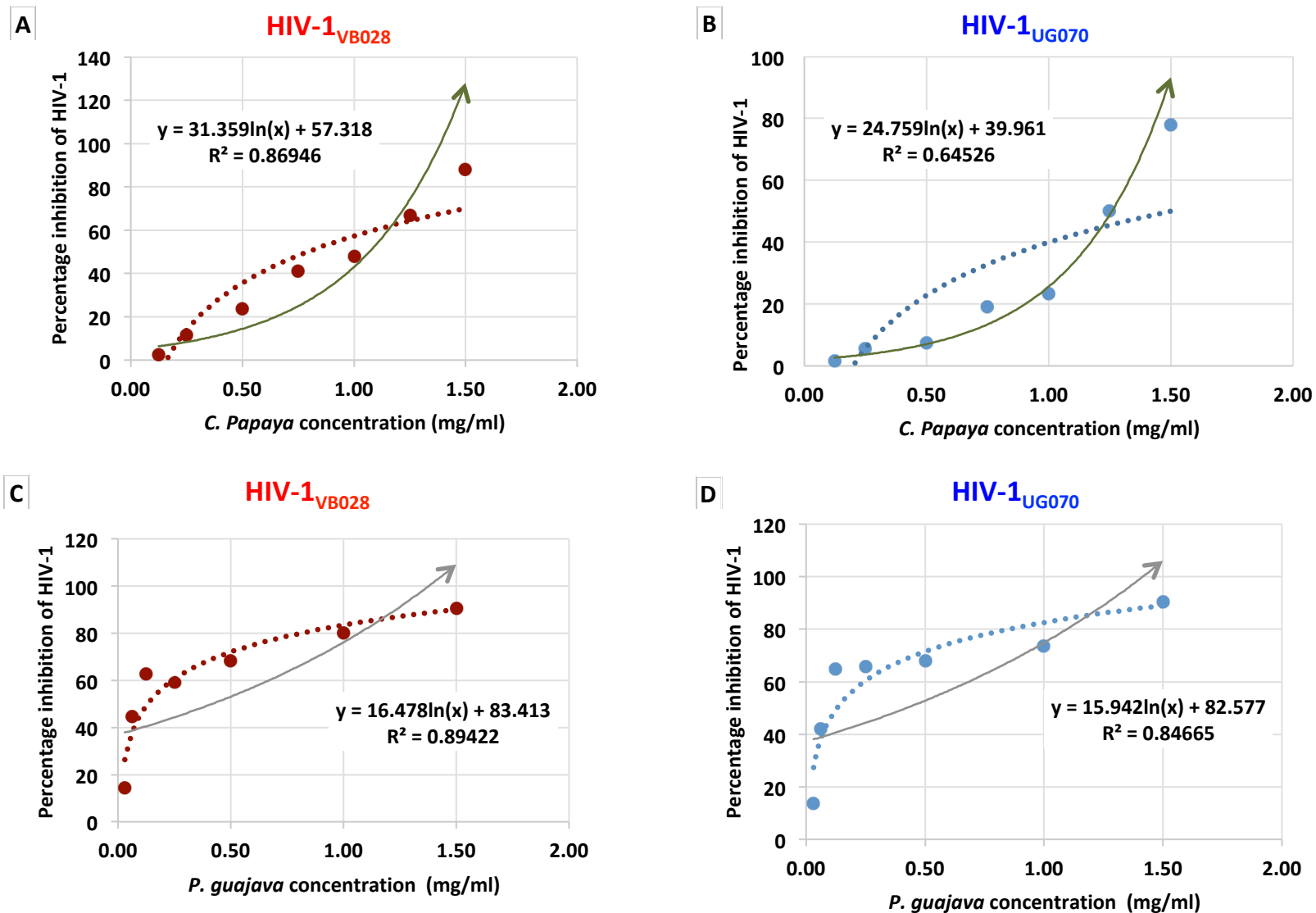


|  |          |        |         |        |       |   |
|--|----------|--------|---------|--------|-------|---|
| <b>C<sub>26</sub>H<sub>36</sub>O<sub>13</sub></b>              | 556.2159 | 5.021  | 876596  | 187931 | 81.73 | 11-Hydroxyiridodial glucoside pentaacetate  |
| <b>C<sub>6</sub>H<sub>8</sub>N<sub>2</sub>O<sub>2</sub></b>    | 140.0588 | 4.806  | 1523345 | 208006 | 85.06 | 1,3-Dimethyluracil  |
| <b>C<sub>42</sub>H<sub>75</sub>O<sub>10</sub>P</b>             | 770.5094 | 14.994 | 122114  | 59904  | 88.93 | PG(18:3(9Z,12Z,15Z)/18:1(9Z))   |
| <b>C<sub>23</sub>H<sub>38</sub>O</b>                           | 330.2907 | 12.59  | 925396  | 142637 | 89.02 | Teprenone   |
| <b>C<sub>13</sub>H<sub>18</sub>N<sub>2</sub>O<sub>2</sub></b>  | 234.136  | 9.25   | 2158813 | 164833 | 84.41 | Lenacil   |
| <b>C<sub>28</sub>H<sub>40</sub>O<sub>2</sub></b>               | 408.3019 | 11.734 | 1305114 | 195772 | 86.57 | Ganodosterone   |
| <b>C<sub>16</sub>H<sub>25</sub>NO<sub>3</sub></b>              | 279.183  | 6.553  | 1612887 | 162125 | 87.9  | Serratine   |
| <b>C<sub>18</sub>H<sub>35</sub>NO<sub>3</sub></b>              | 313.2614 | 14.795 | 733022  | 147582 | 92.05 | (+)-Prosopinine   |
| <b>C<sub>18</sub>H<sub>24</sub>O</b>                           | 256.1811 | 15.001 | 1605689 | 129942 | 85.26 | Phenolic steroid  |
| <b>C<sub>15</sub>H<sub>22</sub>N<sub>2</sub>O<sub>3</sub></b>  | 278.1632 | 14.997 | 2101442 | 169261 | 92.61 | Isoleucyl-Phenylalanine   |
| <b>C<sub>42</sub>H<sub>75</sub>O<sub>10</sub>P</b>             | 770.5119 | 16.148 | 2129780 | 162690 | 83.76 | PG(18:3(9Z,12Z,15Z)/18:1(9Z))   |
| <b>C<sub>15</sub>H<sub>19</sub>NO<sub>3</sub></b>              | 261.1366 | 14.988 | 1766250 | 134516 | 91.44 | cis-1,3,4,6,7,11b-Hexahydro-9-methoxy-2H-benzo[a]quinolizine-3-carboxylic acid  |
| <b>C<sub>22</sub>H<sub>31</sub>NO<sub>3</sub></b>              | 357.23   | 15.853 | 994179  | 76849  | 87.51 | Dihydroretrofractamide B  |
| <b>C<sub>6</sub>H<sub>14</sub>NO<sub>2</sub></b>               | 132.1029 | 2.421  | 209487  | 40245  | 85.14 | beta-Alaninebetaine   |
| <b>C<sub>22</sub>H<sub>42</sub>O<sub>4</sub></b>               | 370.3076 | 11.306 | 2135413 | 171477 | 87.28 | Di(2-ethylhexyl) adipate  |
| <b>C<sub>15</sub>H<sub>22</sub>N<sub>2</sub>O<sub>3</sub></b>  | 278.1636 | 15.313 | 1322964 | 159426 | 95.13 | Isoleucyl-Phenylalanine   |
| <b>C<sub>21</sub>H<sub>29</sub>FO<sub>4</sub></b>              | 364.2035 | 11.339 | 668712  | 115939 | 86.74 | 6alpha-Fluoro-11beta,17-dihydroxypregn-4-ene-3,20-dione   |
| <b>C<sub>24</sub>H<sub>28</sub>O<sub>3</sub></b>               | 364.2035 | 11.339 | 668712  | 115939 | 94.67 | 3-(1,1-Dimethyl-2-propenyl)-8-(3-methyl-2-butenyl)xanthyletin   |
| <b>C<sub>21</sub>H<sub>23</sub>NO<sub>5</sub></b>              | 369.1588 | 11.339 | 858486  | 126597 | 86.73 | 7-Hydroxydehydroglucine   |
| <b>C<sub>14</sub>H<sub>15</sub>N</b>                           | 197.1207 | 5.754  | 1219640 | 153120 | 94.12 | 2-(3-Phenylpropyl)pyridine  |
| <b>C<sub>24</sub>H<sub>36</sub>O<sub>8</sub></b>               | 452.2402 | 1.774  | 130107  | 38500  | 85.47 | Rhodojaponin I  |
| <b>C<sub>37</sub>H<sub>64</sub>O<sub>8</sub></b>               | 636.4612 | 12.573 | 1477672 | 199545 | 86.17 | 9-Oxoasimicinone  |
| <b>C<sub>20</sub>H<sub>12</sub></b>                            | 252.0931 | 5.137  | 739252  | 135740 | 88.66 | Benzpyrene  |
| <b>C<sub>43</sub>H<sub>66</sub>O<sub>16</sub></b>              | 838.4363 | 12.328 | 3571429 | 429579 | 92.21 | Talinumoside I  |
| <b>C<sub>17</sub>H<sub>12</sub>O<sub>4</sub></b>               | 280.0726 | 4.593  | 762048  | 121373 | 93.1  | 3-Hydroxy-2-(4-methylbenzoyl)-4H-1-benzopyran-4-one   |
| <b>C<sub>11</sub>H<sub>23</sub>N<sub>3</sub>O<sub>2</sub></b>  | 229.1789 | 9.668  | 585172  | 96268  | 89.48 | n1,n8-diacetylspermidine  |
| <b>C<sub>21</sub>H<sub>23</sub>NO<sub>5</sub></b>              | 369.1587 | 10.898 | 972916  | 99631  | 89.4  | 7-Hydroxydehydroglucine   |
| <b>C<sub>34</sub>H<sub>38</sub>N<sub>4</sub>O<sub>6</sub></b>  | 598.2778 | 1.446  | 398273  | 72867  | 87.29 | Hematoporphyrin   |
| <b>C<sub>38</sub>H<sub>76</sub>NO<sub>7</sub>P</b>             | 689.536  | 18.626 | 371315  | 97293  | 88.77 | PE(15:0/P-18:0)   |
| <b>C<sub>9</sub>H<sub>12</sub>FN<sub>2</sub>O<sub>9</sub>P</b> | 342.0267 | 1.227  | 155814  | 107774 | 96.78 | 5-Fluorouridine monophosphate   |
| <b>C<sub>35</sub>H<sub>54</sub>O<sub>3</sub></b>               | 522.4061 | 9.943  | 633677  | 67322  | 85.43 | Panaxydol linoleate   |
| <b>C<sub>15</sub>H<sub>22</sub>N<sub>2</sub>O<sub>4</sub></b>  | 294.1585 | 1.947  | 186551  | 52028  | 89.59 | Isoleucyl-Tyrosine  |
| <b>C<sub>23</sub>H<sub>28</sub>O<sub>8</sub></b>               | 432.1779 | 1.28   | 98921   | 45449  | 91.77 | (2S,4S,6S)-2-[2-(4-Hydroxy-3-methoxyphenyl)ethyl]tetrahydro-6-(4,5-dihydroxy-3-methoxyphenyl)-2H-pyran-4-yl 4-acetate |
| <b>C<sub>12</sub>H<sub>23</sub>N<sub>3</sub>O<sub>6</sub></b>  | 305.159  | 3.844  | 5408947 | 114969 | 86.95 | Syndesine   |
| <b>C<sub>18</sub>H<sub>19</sub>NO</b>                          | 265.1466 | 1.227  | 27834   | 63219  | 96.02 | Mukoening A   |
| <b>C<sub>22</sub>H<sub>32</sub>O<sub>9</sub></b>               | 440.205  | 1.496  | 842774  | 73812  | 87.25 | 3'-Hydroxy-HT2 toxin  |
| <b>C<sub>8</sub>H<sub>13</sub>NS</b>                           | 155.0759 | 1.234  | 895750  | 95467  | 87.95 | 4-Ethyl-5-propylthiazole  |
| <b>C<sub>19</sub>H<sub>27</sub>NO<sub>11</sub></b>             | 445.159  | 1.313  | 134420  | 40229  | 85.36 | Lucuminamide  |
| <b>C<sub>24</sub>H<sub>35</sub>NO<sub>5</sub></b>              | 417.2516 | 16.55  | 1437955 | 52978  | 85.9  | Batrachotoxinin A   |

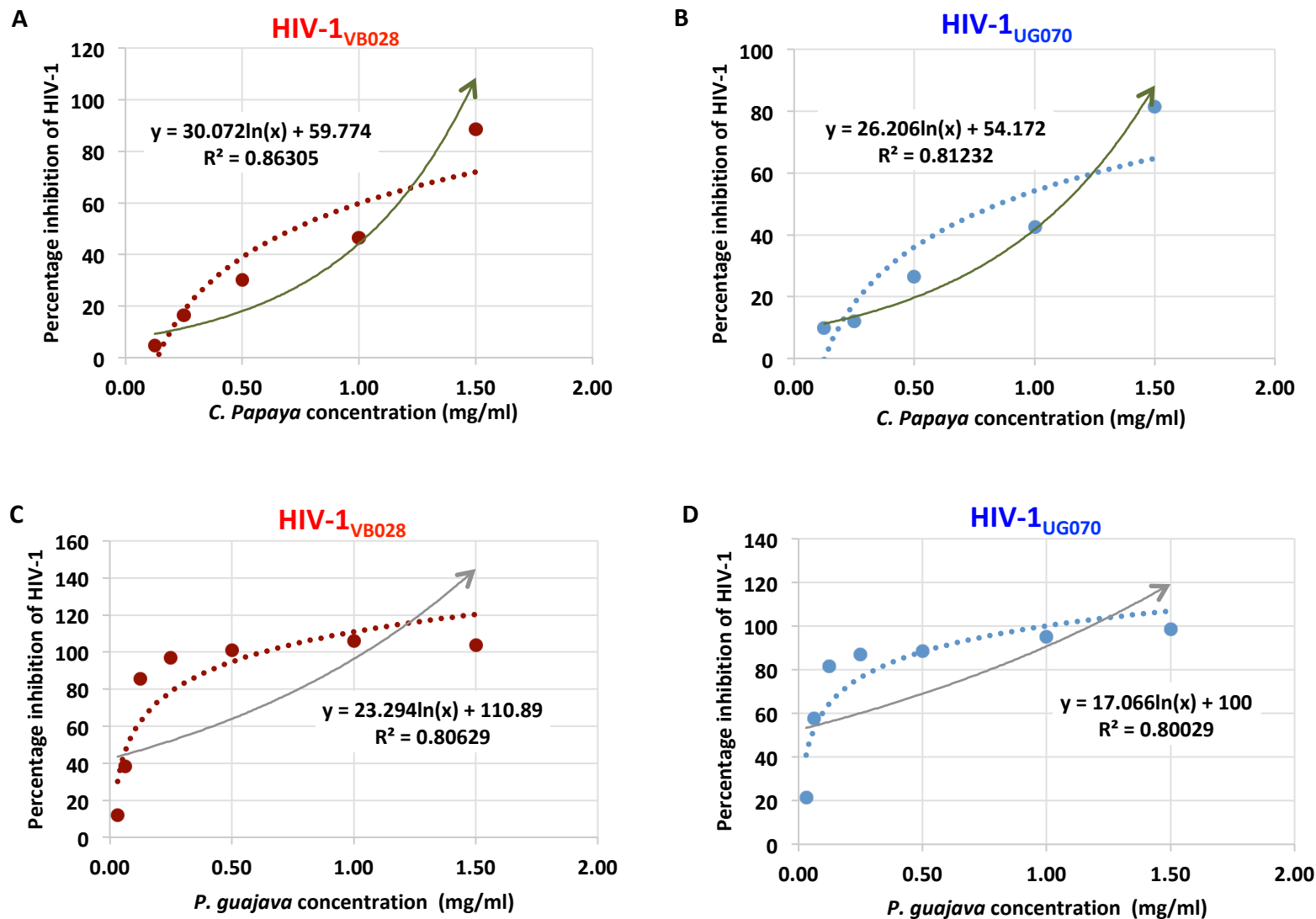
|   |          |        |         |        |       |   |
|---|----------|--------|---------|--------|-------|---|
| <b>C<sub>15</sub>H<sub>26</sub>O</b>                            | 222.1985 | 1.237  | 132821  | 77578  | 87.79 | Faurinone (T)   |
| <b>C<sub>10</sub>H<sub>20</sub>N<sub>2</sub>O<sub>3</sub>S</b>  | 248.1201 | 1.224  | 60498   | 88218  | 85.84 | Valyl-Methionine  |
| <b>C<sub>17</sub>H<sub>27</sub>NO<sub>2</sub></b>               | 277.2032 | 14.533 | 1670288 | 56186  | 85.64 | Terbucarb   |
| <b>C<sub>33</sub>H<sub>42</sub>O<sub>20</sub></b>               | 758.2306 | 4.587  | 1113213 | 127885 | 87.15 | Rubrofusarin 6-[glucosyl-(1->3)-glucosyl-(1->6)-glucoside]  |
| <b>C<sub>39</sub>H<sub>62</sub>O<sub>15</sub></b>               | 770.4085 | 5.107  | 358696  | 85984  | 89.96 | Scopoloside II  |
| <b>C<sub>27</sub>H<sub>47</sub>N<sub>7</sub>O<sub>6</sub></b>   | 565.3591 | 19.007 | 388663  | 39100  | 86.26 | JSTX-3  |
| <b>C<sub>59</sub>H<sub>90</sub>O<sub>8</sub></b>                | 926.6661 | 5.92   | 152744  | 42573  | 88.68 | Thermozeaxanthin-13   |
| <b>C<sub>40</sub>H<sub>56</sub>O<sub>2</sub></b>                | 568.4286 | 11.25  | 516119  | 55290  | 84.29 | Deoxymyxol/ ((2'S)-Plectaniaxanthin)                        |
| <b>C<sub>8</sub>H<sub>10</sub>N<sub>2</sub>O<sub>4</sub></b>    | 198.0638 | 4.444  | 308802  | 52505  | 86.18 | Mimosine  |
| <b>C<sub>42</sub>H<sub>48</sub>N<sub>4</sub>O<sub>16</sub></b>  | 864.3064 | 4.713  | 963411  | 155639 | 92.5  | Precorin 2  |
| <b>C<sub>6</sub>H<sub>8</sub>OS<sub>2</sub></b>                 | 160.0018 | 1.121  | 209032  | 53737  | 84.64 | (2-Furanylmethyl) methyl disulfide                          |
| <b>C<sub>14</sub>H<sub>27</sub>NO<sub>10</sub>S<sub>3</sub></b> | 465.0819 | 1.23   | 141751  | 83672  | 85.98 | Glucohesperalin   |
| <b>C<sub>5</sub>H<sub>15</sub>N<sub>4</sub>O<sub>3</sub>P</b>   | 210.0882 | 1.257  | 89144   | 48372  | 84.72 | N4-Phosphoagmatine  |
| <b>C<sub>4</sub>H<sub>10</sub>OS</b>                            | 106.0449 | 1.117  | 135143  | 46014  | 90.53 | 3-(Methylthio)-1-propanol                                   |
| <b>C<sub>15</sub>H<sub>16</sub>O<sub>7</sub></b>                | 308.0915 | 6.716  | 456251  | 50963  | 85.12 | Allamandin  |
| <b>C<sub>15</sub>H<sub>23</sub>NO<sub>9</sub></b>               | 361.1358 | 1.509  | 211133  | 41362  | 88.48 | De-O-methylsimmondsin                                       |
| <b>C<sub>39</sub>H<sub>36</sub>N<sub>4</sub>O<sub>7</sub></b>   | 672.2583 | 8.225  | 808056  | 103426 | 96.82 | 4-[N-(p-Coumaroyl)serotonin-4"-yl]-N-feruloylserotonin      |
| <b>C<sub>12</sub>H<sub>18</sub>O<sub>2</sub>S</b>               | 226.1026 | 6.388  | 46404   | 27650  | 88.77 | 3-[(2-Methyl-3-furanyl)thio]-4-heptanone                    |
| <b>C<sub>17</sub>H<sub>28</sub></b>                             | 232.2192 | 12.294 | 157414  | 36670  | 90.36 | 5alpha-Gonane   |
| <b>C<sub>21</sub>H<sub>32</sub>O<sub>6</sub></b>                | 380.221  | 11.303 | 410176  | 39811  | 84.27 | [6]-Gingerdiol 3,5-diacetate                                |
| <b>C<sub>13</sub>H<sub>14</sub>N<sub>2</sub>O<sub>7</sub></b>   | 310.0799 | 5.286  | 537181  | 52436  | 97.64 | Acromelic acid A  |
| <b>C<sub>38</sub>H<sub>46</sub>O<sub>8</sub></b>                | 630.3211 | 18.818 | 157871  | 40671  | 91.35 | (R)-6'-O-(4-Geranyloxy-2-hydroxycinnamoyl)-marmin           |
| <b>C<sub>18</sub>H<sub>29</sub>D<sub>5</sub>O<sub>2</sub></b>   | 287.2884 | 11.575 | 259092  | 41158  | 85.55 | Oleic acid (d5)   |
| <b>C<sub>11</sub>H<sub>14</sub>N<sub>2</sub>O<sub>2</sub></b>   | 206.1053 | 4.275  | 457291  | 51283  | 86.43 | Pheneturide   |
| <b>C<sub>13</sub>H<sub>16</sub>O<sub>2</sub></b>                | 204.1141 | 6.394  | 50903   | 25120  | 85.61 | Isobutyl cinnamate  |
| <b>C<sub>11</sub>H<sub>11</sub>NO<sub>2</sub></b>               | 189.0786 | 4.262  | 538896  | 60264  | 98.48 | 1,3-Dimethyl-6,8-isoquinolinediol)                          |
| <b>C<sub>20</sub>H<sub>31</sub>NO<sub>2</sub></b>               | 317.236  | 13.983 | 244326  | 30280  | 87.31 | 17beta-Hydroxy-4,17-dimethyl-4-azaandrost-5-en-3-one        |
| <b>C<sub>12</sub>H<sub>22</sub>O<sub>6</sub></b>                | 262.1415 | 15.007 | 299934  | 26250  | 91.55 | Triethylene glycol diglycidyl ether (Aliphatic epo)         |
| <b>C<sub>19</sub>H<sub>24</sub>N<sub>7</sub>O<sub>8</sub>P</b>  | 509.1423 | 1.678  | 60796   | 19199  | 88.38 | N6,N6,O-Tridemethylpuromycin-5'-phosphate                   |
| <b>C<sub>7</sub>H<sub>9</sub>O<sub>3</sub>P</b>                 | 172.0291 | 1.114  | 189927  | 45069  | 80.17 | Monomethyl phenylphosphonate                                |
| <b>C<sub>15</sub>H<sub>15</sub>N<sub>3</sub>O<sub>2</sub></b>   | 269.1174 | 1.605  | 72593   | 36090  | 85.86 | Disperse Yellow 3   |
| <b>C<sub>15</sub>H<sub>12</sub>N<sub>2</sub>O<sub>2</sub></b>   | 252.0909 | 1.605  | 64520   | 31759  | 85.86 | 2-Hydroxycarbamazepine                                      |
| <b>C<sub>10</sub>H<sub>12</sub></b>                             | 132.0932 | 4.414  | 100924  | 24239  | 86.25 | Dicyclopentadiene   |
| <b>C<sub>14</sub>H<sub>18</sub>N<sub>2</sub>O<sub>7</sub></b>   | 326.1123 | 1.937  | 152580  | 47048  | 87.67 | Dinobuton   |
| <b>C<sub>27</sub>H<sub>34</sub>O<sub>8</sub></b>                | 486.226  | 1.496  | 254266  | 56580  | 89.65 | Austalide I   |
| <b>C<sub>19</sub>H<sub>21</sub>NO<sub>5</sub></b>               | 343.1408 | 1.456  | 125439  | 151603 | 86.94 | N-trans-Feruloyl-4-O-methyldopamine                         |
| <b>C<sub>24</sub>H<sub>34</sub>O</b>                            | 338.2614 | 1.234  | 38636   | 33560  | 88.68 | 3-(2,4-Cyclopentadien-1-ylidene)-5alpha-androstan-17beta-ol |
| <b>C<sub>15</sub>H<sub>20</sub>O<sub>9</sub></b>                | 344.1104 | 1.681  | 141461  | 28881  | 80.86 | Domesticoside   |
| <b>C<sub>10</sub>H<sub>17</sub>N<sub>3</sub>O<sub>2</sub></b>   | 211.132  | 1.432  | 65295   | 36976  | 96.4  | Isouron   |
| <b>C<sub>25</sub>H<sub>48</sub>O<sub>2</sub></b>                | 380.364  | 15.886 | 38661   | 25573  | 85.6  | 10,12-Pentacosanedione                                      |

|  |          |        |         |        |       |   |
|--|----------|--------|---------|--------|-------|---|
| <b>C<sub>13</sub>H<sub>26</sub>NO<sub>4</sub></b>              | 260.1858 | 11.552 | 112524  | 22891  | 86.33 | O-hexanoyl-R-carnitine                                      |
| <b>C<sub>26</sub>H<sub>24</sub>O<sub>5</sub></b>               | 416.1604 | 18.195 | 294458  | 32538  | 87.77 | Calophyllolide  |
| <b>C<sub>7</sub>H<sub>16</sub>N<sub>4</sub>O<sub>4</sub></b>   | 220.118  | 14.6   | 140303  | 16035  | 96.52 | 1D-1-Guanidino-3-amino-1,3-dideoxy-scylo-inositol           |
| <b>C<sub>5</sub>H<sub>5</sub>NOS</b>                           | 127.0102 | 1.214  | 96682   | 41071  | 87.75 | 2-Acetylthiazole  |
| <b>C<sub>18</sub>H<sub>19</sub>NO<sub>4</sub></b>              | 313.1296 | 3.887  | 71266   | 26992  | 88    | Acetylcaranine  |
| <b>C<sub>6</sub>H<sub>11</sub>NO<sub>2</sub></b>               | 129.0797 | 1.605  | 121319  | 74780  | 84.89 | 2-Pyrrolidineacetic acid                                    |
| <b>C<sub>20</sub>H<sub>39</sub>NO</b>                          | 309.3029 | 4.68   | 10308   | 7704   | 94.21 | N-Hexadecanoylpyrrolidine                                   |
| <b>C<sub>5</sub>H<sub>11</sub>O<sub>5</sub></b>                | 151.0606 | 1.631  | 82602   | 28630  | 90.23 | L-(+)-Arabinose   |
| <b>C<sub>22</sub>H<sub>33</sub>NO<sub>8</sub></b>              | 439.2206 | 16.211 | 452170  | 22429  | 90.52 | Parsonsine  |
| <b>C<sub>16</sub>H<sub>21</sub>NO</b>                          | 243.1629 | 4.6    | 25266   | 16990  | 85.53 | Isobutylphendienamide                                       |
| <b>C<sub>9</sub>H<sub>12</sub>N<sub>2</sub></b>                | 148.0991 | 18.195 | 9027    | 17089  | 87.12 | Nornicotine   |
| <b>C<sub>20</sub>H<sub>28</sub>N<sub>2</sub>O</b>              | 312.2197 | 12.805 | 34300   | 12498  | 96.37 | Fruticosonine   |
| <b>C<sub>7</sub>H<sub>16</sub>OS</b>                           | 148.0917 | 18.38  | 2707    | 13897  | 89.13 | R-3-(Methylthio)-1-hexanol                                  |
| <b>C<sub>6</sub>H<sub>9</sub>N<sub>5</sub>O<sub>2</sub></b>    | 183.0741 | 1.25   | 75765   | 27543  | 93.17 | 2,6-Diamino-4-hydroxy-5-N-methylformamidopyrimidine         |
| <b>C<sub>18</sub>H<sub>19</sub>N<sub>2</sub>O<sub>2</sub></b>  | 295.1449 | 1.303  | 43355   | 22329  | 86.84 | Nigellidine   |
| <b>C<sub>20</sub>H<sub>19</sub>NO<sub>3</sub></b>              | 321.1359 | 3.963  | 71661   | 17940  | 87.49 | Acronycine  |
| <b>C<sub>25</sub>H<sub>44</sub>N<sub>2</sub></b>               | 372.3511 | 14.928 | 20335   | 22394  | 83.3  | Kurchessine   |
| <b>C<sub>45</sub>H<sub>54</sub>N<sub>8</sub>O<sub>10</sub></b> | 866.3915 | 4.272  | 67120   | 18982  | 87.96 | Pristinamycin IA  |
| <b>C<sub>23</sub>H<sub>44</sub>O<sub>4</sub></b>               | 384.3233 | 17.153 | 118058  | 13151  | 87.55 | MG(20:1(11Z)/0:0/0:0)                                       |
| <b>C<sub>20</sub>H<sub>26</sub>O<sub>12</sub></b>              | 458.1401 | 6.182  | 122230  | 17193  | 88.03 | 7-Hydroxy-4-methylphthalide O-[arabinosyl-(1->6)-glucoside] |
| <b>C<sub>12</sub>H<sub>11</sub>NO</b>                          | 185.0844 | 0.832  | 56431   | 19372  | 88.47 | 4-Hydroxydiphenylamine                                      |
| <b>C<sub>30</sub>H<sub>24</sub>O<sub>13</sub></b>              | 592.1199 | 4.812  | 1235671 | 304798 | 84.25 | Protoleucomelone  |
| <b>C<sub>11</sub>H<sub>11</sub>NO<sub>3</sub></b>              | 205.0724 | 10.835 | 152026  | 14061  | 87.04 | Swietenidin B   |
| <b>C<sub>11</sub>H<sub>14</sub>N<sub>2</sub>O<sub>3</sub></b>  | 222.0993 | 10.852 | 228582  | 20860  | 86.86 | Glycyl-Phenylalanine  |
| <b>C<sub>6</sub>H<sub>8</sub>N<sub>2</sub>O<sub>2</sub></b>    | 140.0589 | 4.739  | 659506  | 201486 | 98.28 | 1,3-Dimethyluracil  |
| <b>C<sub>28</sub>H<sub>24</sub>N<sub>2</sub>O<sub>7</sub></b>  | 500.1579 | 17.223 | 323503  | 17216  | 88.22 | Orcein  |
| <b>C<sub>4</sub>H<sub>8</sub>N<sub>4</sub>O<sub>4</sub></b>    | 176.0551 | 10.749 | 158477  | 14125  | 89.23 | Allantoic acid  |
| <b>C<sub>15</sub>H<sub>16</sub></b>                            | 196.1247 | 13.047 | 36196   | 14863  | 89.42 | 1,3-Diphenylpropane   |
| <b>C<sub>4</sub>H<sub>5</sub>O<sub>7</sub>P</b>                | 195.9766 | 5.273  | 28131   | 6218   | 94.77 | 1-Carboxyvinyl carboxyphosphonate                           |
| <b>C<sub>9</sub>H<sub>15</sub>NS</b>                           | 169.0925 | 5.141  | 3404    | 6657   | 87.8  | 4-ethyl-5-methyl-2-propylthiazole                           |
| <b>C<sub>9</sub>H<sub>12</sub>O<sub>2</sub>S</b>               | 184.056  | 0.557  | 57219   | 13484  | 94.46 | (+/-)-3-[(2-methyl-3-furyl)thio]-2-butanone                 |
| <b>C<sub>4</sub>H<sub>8</sub>NO<sub>7</sub>P</b>               | 213.0037 | 5.273  | 45915   | 11984  | 94.46 | 4-Phospho-L-aspartate                                       |
| <b>C<sub>18</sub>H<sub>10</sub></b>                            | 226.0779 | 1.469  | 37715   | 18096  | 88.59 | Benzo[ghi]fluoranthene                                      |
| <b>C<sub>19</sub>H<sub>27</sub>FO<sub>2</sub></b>              | 306.1989 | 10.835 | 85657   | 12472  | 95.31 | 2alpha-Fluoro-17beta-hydroxyandrost-4-en-3-one              |
| <b>C<sub>32</sub>H<sub>44</sub>N<sub>2</sub>O<sub>8</sub></b>  | 584.3099 | 15.266 | 131280  | 14337  | 90.74 | Lappaconitine   |
| <b>C<sub>4</sub>H<sub>5</sub>O<sub>7</sub>P</b>                | 195.977  | 5.094  | 15068   | 5438   | 93.6  | 1-Carboxyvinyl carboxyphosphonate                           |
| <b>C<sub>37</sub>H<sub>38</sub>N<sub>2</sub>O<sub>7</sub></b>  | 622.2658 | 15.266 | 164052  | 16251  | 85.76 | O-Methylsomniferine   |
| <b>C<sub>23</sub>H<sub>34</sub>O<sub>14</sub></b>              | 534.1922 | 5.35   | 37259   | 16904  | 87.79 | • Isosyringinoside  |
| <b>C<sub>4</sub>H<sub>8</sub>NO<sub>7</sub>P</b>               | 213.0052 | 5.482  | 11068   | 7672   | 98.27 | 4-Phospho-L-aspartate                                       |
| <b>C<sub>2</sub>H<sub>7</sub>N<sub>3</sub>O</b>                | 89.0594  | 1.234  | 9867    | 10119  | 87.41 | N-(Aminomethyl)urea   |

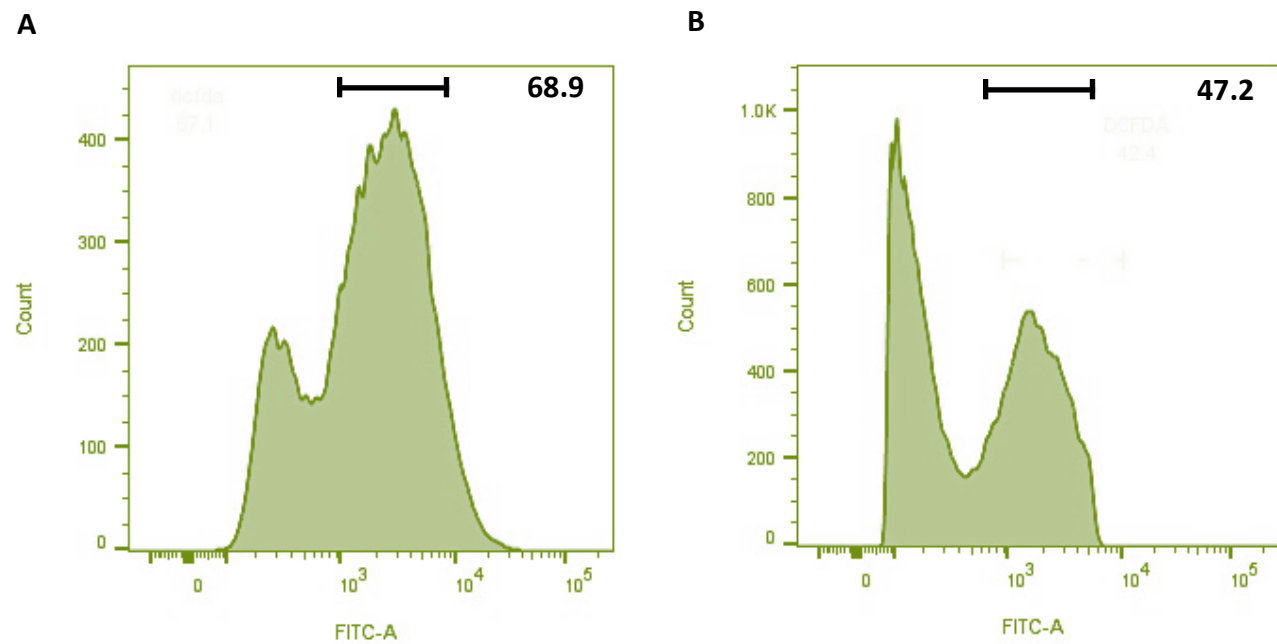
|   |          |        |         |        |       |  |
|---|----------|--------|---------|--------|-------|--|
| <b>C<sub>11</sub>H<sub>13</sub>NO<sub>3</sub></b>                           | 207.0898 | 3.519  | 5239    | 7204   | 85.42 | Cantleyine   |
| <b>C<sub>7</sub>H<sub>11</sub>NO</b>  | 125.0841 | 17.555 | 6019    | 8651   | 85.36 | 2-Ethyl-4,5-dimethyloxazole                                  |
| <b>C<sub>29</sub>H<sub>54</sub>O<sub>2</sub></b>                            | 434.4121 | 13.764 | 27623   | 15115  | 85.17 | Ximenoylacetone  |
| <b>C<sub>14</sub>H<sub>24</sub>O</b>  | 208.1838 | 19.75  | 22472   | 9711   | 91.72 | 2-Decylfuran   |
| <b>C<sub>16</sub>H<sub>30</sub>O<sub>7</sub></b>                            | 334.1988 | 10.56  | 25751   | 8365   | 89.5  | trans-p-Menthane-7,8-diol 8-glucoside                        |
| <b>C<sub>11</sub>H<sub>22</sub>O</b>  | 170.1672 | 8.275  | 3727    | 7837   | 86.7  | 6-Undecanone   |
| <b>C<sub>17</sub>H<sub>23</sub>N<sub>3</sub>O<sub>3</sub></b>               | 317.1728 | 10.56  | 28616   | 8531   | 85.23 | Isoleucyl-Tryptophan   |
| <b>C<sub>14</sub>H<sub>10</sub>F<sub>4</sub>N<sub>4</sub>O<sub>7</sub>S</b> | 454.0207 | 17.448 | 63392   | 8952   | 88.28 | Primisulfuron  |
| <b>C<sub>10</sub>H<sub>12</sub>N<sub>2</sub></b>                            | 160.0994 | 11.558 | 62031   | 16110  | 84.73 | 2-(2-Aminoethyl)indole                                       |
| <b>C<sub>23</sub>H<sub>38</sub>O</b>  | 330.2899 | 12.324 | 641409  | 67984  | 85.62 | Teprenone  |
| <b>C<sub>5</sub>H<sub>7</sub>N</b>  | 81.0571  | 7.21   | 5781    | 6804   | 87.78 | 1-Methylpyrrole  |
| <b>C<sub>14</sub>H<sub>20</sub>N<sub>4</sub>O<sub>2</sub></b>               | 276.1579 | 1.131  | 18059   | 11493  | 88.92 | p-Coumaroylagmatine  |
| <b>C<sub>14</sub>H<sub>16</sub>N<sub>2</sub>O<sub>8</sub></b>               | 340.091  | 5.439  | 15016   | 7733   | 89.2  | Vulgaxanthin-II  |
| <b>C<sub>10</sub>H<sub>12</sub>N<sub>5</sub>O<sub>7</sub>P</b>              | 345.0466 | 5.439  | 14601   | 7621   | 85.71 | 2',3'-Cyclic GMP   |
| <b>C<sub>7</sub>H<sub>4</sub>O<sub>7</sub></b>                              | 199.9971 | 19.883 | 13005   | 5262   | 90.91 | Poppy acid   |
| <b>C<sub>24</sub>H<sub>40</sub>N<sub>2</sub></b>                            | 356.319  | 19.299 | 10861   | 10211  | 86.26 | Conessine  |
| <b>C<sub>14</sub>H<sub>12</sub>N<sub>4</sub>O<sub>2</sub></b>               | 268.0962 | 9.8    | 3240    | 6159   | 85.09 | Disperse Blue 1  |
| <b>C<sub>17</sub>H<sub>20</sub>O<sub>5</sub></b>                            | 304.1316 | 2.762  | 4890    | 6777   | 87.86 | 3'-Deoxyoleacein   |
| <b>C<sub>10</sub>H<sub>20</sub>N<sub>2</sub>O<sub>4</sub></b>               | 232.1412 | 10.225 | 10100   | 10361  | 85.55 | Isoleucyl-Threonine  |
| <b>C<sub>47</sub>H<sub>86</sub>O<sub>16</sub>P<sub>2</sub></b>              | 968.5384 | 19.903 | 9958    | 4682   | 88.41 | PIP(18:2(9Z,12Z)/20:1(11Z))                                  |
| <b>C<sub>6</sub>H<sub>6</sub>O<sub>5</sub>S</b>                             | 189.9937 | 1.197  | 1917    | 3751   | 94.95 | 4-Sulfocatechol  |
| <b>C<sub>15</sub>H<sub>19</sub>NO<sub>10</sub></b>                          | 373.1016 | 18.012 | 8810    | 2812   | 87.24 | DIMBOA-glucoside   |
| <b>C<sub>13</sub>H<sub>27</sub>N<sub>3</sub>O<sub>7</sub></b>               | 337.1859 | 2.806  | 3713    | 8035   | 93.42 | Istamycin AO   |
| <b>C<sub>19</sub>H<sub>20</sub>O<sub>12</sub></b>                           | 440.0915 | 1.804  | 2699    | 4277   | 90.33 | 3,5-Dihydroxyphenyl 1-O-(6-O-galloyl-beta-D-glucopyranoside) |
| <b>C<sub>54</sub>H<sub>109</sub>NO<sub>8</sub>P</b>                         | 930.7885 | 17.972 | 5970    | 5481   | 89.66 | PC(22:0/24:0)  |
| <b>C<sub>11</sub>H<sub>16</sub>O<sub>10</sub></b>                           | 308.0736 | 1.23   | 13396   | 8527   | 87.6  | D-Erythroascorbic acid 1'-a-D-glucoside                      |
| <b>C<sub>9</sub>H<sub>11</sub>ClN<sub>2</sub>O<sub>2</sub></b>              | 214.0508 | 8.361  | 238960  | 25930  | 85.53 | Monolinuron  |
| <b>C<sub>27</sub>H<sub>33</sub>NO<sub>5</sub></b>                           | 451.2352 | 1.781  | 1763478 | 436445 | 77.56 | 14alpha-Hydroxypaxilline                                     |



**Figure S1:** Anti-HIV-1 activity of *C. papaya* and *P. guajava* in cell associated study. Dose-dependent inhibition of (A) HIV-1<sub>VB028</sub> and (B) HIV-1<sub>UG070</sub> replication in presence of *C. papaya* extract (0.125-1.500mg/ml). The effect of different concentrations of *P. guajava* extract (0.03125-1.500mg/ml) on (C) HIV-1<sub>VB028</sub> and (D) HIV-1<sub>UG070</sub> replication.



**Figure S2:** Effects of *C. papaya* and *P. guajava* on HIV-1 suppression through cell-free assays. Percentage of inhibition observed in dose dependent manner for (A) HIV-1<sub>VB028</sub> and (B) HIV-1<sub>UG070</sub> in presence of *C. papaya* extract (0.125-1500mg/ml). The effect of different concentrations of *P. guajava* extract (0.03125-1.500mg/ml) on (C) HIV-1<sub>VB028</sub> and (D) HIV-1<sub>UG070</sub> isolates.



**Figure S3:** (A) ROS generator  $15\mu\text{M H}_2\text{O}_2$  ( $\text{H}_2\text{O}_2$  generator) for 6 h served as positive control. (B)  $15\mu\text{M H}_2\text{O}_2$  ( $\text{H}_2\text{O}_2$  generator) and 250U Catalase served as scavenger/inhibitor of ROS generation in the experiment.