Table S1: HPLC-PDA-ESI-MSn detection of phenolic compounds in leaves (L), stem (S) and roots (R) of *Moringa oleifera* grown under cadmium contaminated soils

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Tentative Identification of Compound** | **Rt, min** | **λmax (nm)** | **[M-H]-, *m/z*** | **MS2[M-H]- , *m/z* (Fragments)** | **Control** | **Cadmium (mM)** |
| **1** | **3** | **5** |
| **Flavonoids** |
| Quercetin-3,7-diglucoside | 12.86 | 255,295,355 | 625 | 505,463,301 | L/S/R | L/S/R | L/S/R | L/S/R |
| Apigenin-6-C-glucoside(isovitexin) | 15.46 | 235,270,335 | 431 | 341,311 | L/S/R | L/S/R | L/S/R | L/S/R |
| Quercetin-3-glucoside | 17.00 | 235,310,375 | 463 | 505,301 | L/S/R | L/S/R | L/S/R | L/S/R |
| Apigenin-7-C-glucoside (isorhoifolin) | 17.30 | 235,270,335 | 577 | 431,341,311 | L/S/R | L/S/R | L/S/R | L/S |
| Kaempferol-3,7-diglucoside | 19.58 | 240,255,295,355 | 609 | 431,341,311,283,269,225,156 | L/S/R | L/S/R | L/S/R | L/S/R |
| Apigenin-7-O- rutinoside | 20.34 | 270,300,335 | 577 | 431,341,311,283,269,225,156 | L/S/R | L/S/R | L/S/R | L/S/R |
| Quercetin-3-rhamanoside | 22.49 | 255,270,355 | 463 | 301,271,179,926 | L/S/R | L/S/R | L/S/R | L/S/R |
| Quercetin-3-sophoroside | 24.17 | 255,300,355 | 625 | 463,301,271,151 | L/S/R | L/S/R | L/S/R | L/S/R |
| Kaempferol-3-glucoside | 26.08 | 265,300,345 | 505 | 301 | L/S/R | L/S/R | L/S/R | L/S/R |
| Kaempferol-7-glucoside | 27.66 | 240,265,300,345 | 447 | 285,255,173 | L/S/R | L/S/R | L/S/R | L/S/R |
| **Hydroxycinamic acids** |
| Dicaffeoylquinic acid | 11.20 | 240,270,320 | 515 | 353,191,179,173,135 | L/S/R | L/S/R | L/S/R | L/S/R |
| 5-Caffeoylquinic acid | 11.86 | 245,295,325 | 353 | 179,173,135 | L/S/R | L/S/R | L/S/R | L/S/R |
| 3-Caffeoylquinic acid  | 12.48 | 245,265,315,325 | 353 | 191,179,135 | L/S/R | L/S/R | L/S/R | L/S/R |
| 3-*p*-coumaroylquinic acid | 13.59 | 245,270,305,315 | 337 | 191,179 | L/S/R | L/S/R | L/S/R | S/R |
| Feruloylquinic acid | 14.01 | 240,315,325 | 367 | 191,173,179,163 | L/S/R | L/S/R | L/S/R | L/S/R |

Table S2: HPLC-PDA-ESI-MSn detection of phenolic compounds in leaves (L), stem (S) and roots (R) of *Moringa oleifera* grown under lead contaminated soils

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Tentative Identification of Compound** | **Rt, min** | **λmax(nm)** | **[M-H]-, *m/z*** | **MS2[M-H]- , *m/z* (Fragments)** | **Control** | **Lead (mM)** |
| **5** | **10** | **20** |
| **Flavonoids** |
| Quercetin-3,7-diglucoside | 12.86 | 255,295,355 | 625 | 505,463,301 | L/S/R | L/S/R | L/S/R | L/S/R |
| Apigenin-6-C-glucoside(isovitexin) | 15.46 | 235,270,335 | 431 | 341,311 | L/S/R | L/S/R | L/S/R | S/R |
| Quercetin-3-glucoside | 17.00 | 235,310,375 | 463 | 505,301 | L/S/R | L/S/R | L/S/R | L/S/R |
| Apigenin-7-C-glucoside (isorhoifolin) | 17.30 | 235,270,335 | 577 | 431,341,311,283,269,225,156 | L/S/R | L/S/R | L/S/R | L/S/R |
| Kaempferol-3,7-diglucoside | 19.58 | 240,255,295,355 | 609 | 447,285 | L/S/R | L/S/R | L/S/R | S |
| Apigenin-7-O- rutinoside | 20.34 | 270,300,335 | 577 | 431,341,311,283,269,225,156 | L/S/R | L/S/R | L/S/R | R |
| Quercetin-3-rhamanoside | 22.49 | 255,270,355 | 463 | 301,271,179,926 | L/S/R | S/R | L/S/R | L/S/R |
| Quercetin-3-sophoroside | 24.17 | 255,300,355 | 625 | 463,301,271,151 | L/S/R | L/S/R | L/S/R | L/S/R |
| Kaempferol-3-glucoside | 26.08 | 265,300,345 | 505 | 301 | L/S/R | L/S/R | L/S/R | L/S/R |
| Kaempferol-7-glucoside | 27.66 | 240,265,300,345 | 447 | 285,255,173 | L/S/R | L/S/R | L/S/R | L/S/R |
| **Hydroxycinamic acids** |
| Dicaffeoylquinic acid | 11.20 | 240,270,320 | 515 | 353,191,179,173,135 | L/S/R | L/S/R | L/S/R | L/S/R |
| 5-Caffeoylquinic acid | 11.86 | 245,295,325 | 353 | 179,173,135 | L/S/R | L/S/R | L/S/R | L/S/R |
| 3-Caffeoylquinic acid  | 12.48 | 245,265,315,325 | 353 | 191,179,135 | L/S/R | L/S/R | L/S/R | L/S/R |
| 3-*p*-coumaroylquinic acid | 13.59 | 245,270,305,315 | 337 | 191,179 | L/S/R | L/S/R | L/S/R | L/S/R |
| Feruloylquinic acid | 14.01 | 240,315,325 | 367 | 191,173,179,163 | L/S/R | L/S/R | L/S/R | L/S/R |

Table S3: HPLC-PDA-ESI-MSn detection of phenolic compounds in leaves (L), stem (S) and roots (R) of *Moringa oleifera* grown under cadmium and lead contaminated soils

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Tentative Identification of Compound** | **Rt, min** | **λmax (nm)** | **[M-H]-, *m/z*** | **MS2[M-H]- , *m/z* (Fragments)** | **Control** | **Cadmium × Lead (mM)** |
| **1×1** | **1×10** | **1×20** | **3×1** | **3×10** | **3×20** | **5×1** | **5×10** | **5×20** |
| **Flavonoids** |
| Quercetin-3,7-diglucoside | 12.86 | 255,295,355 | 625 | 505,463,301 | L/S/R | L/S/R | L/S/R | L/S/R | L/S/R | L/S/R | S | L/S/R | L/S/R | L |
| Apigenin-6-C-glucoside(isovitexin) | 15.46 | 235,270,335 | 431 | 341,311 | L/S/R | L/S/R | L/S/R | S/R | L/S/R | L/S | L/S/R | L/S/R | L/S/R | L/S |
| Quercetin-3-glucoside | 17.00 | 235,310,375 | 463 | 505,301 | L/S/R | L/S/R | L/S/R | L/S/R | L/S/R | S/R | L/S/R | L/S/R | L/S | L |
| Apigenin-7-C-glucoside (isorhoifolin) | 17.30 | 235,270,335 | 577 | 431,341,311,283,269,225,156 | L/S/R | L/S/R | L/S/R | R | S/R | L/S/R | --- | L/S/R | L/S | L |
| Kaempferol-3,7-diglucoside | 19.58 | 240,255,295,355 | 609 | 447,285 | L/S/R | L/S/R | L/S/R | S/R | S/R | S | --- | S | L/S | L/S |
| Apigenin-7-O- rutinoside | 20.34 | 270,300,335 | 577 | 431,341,311,283,269,225,156 | L/S/R | L/S/R | L/S/R | S/R | L/S/R | L/S/R | L/R | L/S/R | R | R |
| Quercetin-3-rhamanoside | 22.49 | 255,270,355 | 463 | 301,271,179,926 | L/S/R | L/S/R | L/S/R | L/S | S/R | L/S/R | L | L/S/R | S | --- |
| Quercetin-3-sophoroside | 24.17 | 255,300,355 | 625 | 463,301,271,151 | L/S/R | L/S/R | L/S/R | L/S/R | L/S/R | L/S/R | L/S/R | L/S/R | L/S/R | --- |
| Kaempferol-3-glucoside | 26.08 | 265,300,345 | 505 | 301 | L/S/R | L/S/R | L/S/R | L/S/R | L/S/R | L/S/R | S/R | L/S/R | L/S | L/S |
| Kaempferol-7-glucoside | 27.66 | 240,265,300,345 | 447 | 285,255,173 | L/S/R | L/S/R | L/S/R | L/S/R | L/S/R | L/S/R | L/S/R | L/R | L/R | L/R |
| **Hydroxycinamic acids** |
| Dicaffeoylquinic acid | 11.20 | 240,270,320 | 515 | 353,191,179,173,135 | L/S/R | L/S/R | L/S/R | L/S/R | L/S/R | L/S/R | L/S/R | L/S/R | L/S/R | L/S/R |
| 5-Caffeoylquinic acid | 11.86 | 245,295,325 | 353 | 179,173,135 | L/S/R | L/S/R | L/S/R | L/S/R | L/S/R | L/S/R | L/R | R | R | R |
| 3-Caffeoylquinic acid  | 12.48 | 245,265,315,325 | 353 | 191,179,135 | L/S/R | L/S/R | L/S/R | S/R | L/S/R | L/S/R | L/S/R | S/R | R | R |
| 3-*p*-coumaroylquinic acid | 13.59 | 245,270,305,315 | 337 | 191,179 | L/S/R | L/S/R | L/S/R | L/S/R | L/S/R | L/S/R | L/S | L/S/R | L/S/R | --- |
| Feruloylquinic acid | 14.01 | 240,315,325 | 367 | 191,173,179,163 | L/S/R | L/S/R | L/S/R | L/S/R | L/S/R | L/S/R | L/S/R | L/S/R | L/S/R | L/S/R |