Supporting Information

Baikalomycins A-C, New Aquamycin-Type Angucyclines Isolated from Lake Baikal Derived Streptomyces sp. IB201691-2A

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### Table S1. Primers used in this work.

| Primer | Sequence 5'-3' |
|--------|---------------|
|        | **bai gene cluster cloning** | |
| 91-2aTAR1-FNotI | atGCGGCGCAGACGTGTGATCTTCGCATG |
| 91-2aTAR1-RNheI | atGCTAGCTCTCGTGCGGGAGTCGAT |
| 91-2aCheck-FNotI | AGGTACGAGTCCGTCGGATA |
| 91-2aTAR2-FNheI | atGCTAGCATCGGATGAGCCGTCAA |
| 91-2aTAR2-RHindIII | atAAGCTTTCAACACCTGGATGGACGGA |
| 91-2aCheck-RHindIII | GTTATGAACCTGAGGCAG |
| pCLY10-FHindV | CTCTTGCAGTGAAGTCCGGG |
| pCLY10-RNotV | GTAGAGCTTCCGCTCGAT |
|        | **Disruption of glycosyltransferase genes** | |
| 3L-FHindIII | AAGCTTGATCTGGCGCTCTCGATG |
| 3L-REcoRV | GATATCTCAGGATACCGCAGTCTGA |
| 4R-FEcoRV | GATATCCCTACCTCGACAAGTG |
| 4R-RXbaI | TCTAGACGCGGTACATCAGAAGTCG |
| 5L-FHindIII | AAGCTTCAAAGATCTTCGGCAGGTACA |
| 5L-REcoRV | GATATCCGAAGGATCCTCAACATG |
| 6R-FEcoRV | GATATCGAACTCTCGGACAGATCGC |
| 6R-RXbaI | TCTAGAGCACTGCGCGAGATCGTG |
| CheckGT2F | CCCGTCGTTCCAGCTCGGTG |
| CheckGT2R | CGTGCAGTCGCGCATCGCCT |
| CheckGT3F | AGCTCGATCTCGGAGGAGAC |
| CheckGT3R | GCATCGAAATAACTGAAGGAT |
|        | **16S rRNA** | |
| 8F | AGAGTTTGATYMTGGCTCAG |
| 1492R | TACGGYTACCTGTTACGACTT |
**Table S2. 16S rRNA gene sequence used for phylogenetic analysis.**

| Related strain                        | Accessory N of isolates in NCBI database | Identity, % | Query cover, % |
|---------------------------------------|-----------------------------------------|-------------|----------------|
| *Streptomyces ederensis* NBRC 15410   | NR_112457.1                             | 99          | 97             |
| *Streptomyces phaeochromogenes* NRRL B-1248 | NR_116382.1                             | 99          | 98             |
| *Streptomyces umbrinus* NBRC 13091    | NR_041113.1                             | 99          | 97             |
| *Streptomyces aurantiacus* LMG 19358  | NR_114932.1                             | 99          | 97             |
| *Streptomyces bottropensis* ATCC 25435| NR_115571.2                             | 98          | 100            |
| *Streptomyces glomeroaurantiacus* NBRC 15418 | NR_041436.1                             | 99          | 95             |
| *Streptomyces avermitilis* MA-4680    | NR_074747.2                             | 98          | 100            |
| *Streptomyces durmitorensis* MS405    | NR_043520.1                             | 97          | 99             |
| *Rhodococcus phenolicus* DSM 44812    | NR_115082.1                             | 88          | 99             |
| *Rhodococcus zopfii* DSM 44108        | NR_041775.1                             | 88          | 99             |
| *Rhodococcus rhodochrous* DSM 43241   | NR_116689.1                             | 89          | 99             |
| *Rhodococcus pyridinivorans* PDB9     | NR_025033.1                             | 88          | 99             |
| *Rhodococcus marinonascens* DSM 43752 | NR_026183.1                             | 88          | 99             |
| *Rhodococcus erythropolis* N11       | NR_037024.1                             | 88          | 99             |
| *Rhodococcus coprophilus* CUB 687     | NR_029206.1                             | 90          | 99             |
**Figure S1.** Taxonomic relation of *Rhodococcus* sp. IB201691-2A2 based on 16S rRNA gene similarity. *Escherichia coli* U 5/41 was used as outgroup.
Figure S2. Taxonomic relation of *Streptomyces* sp. IB201691-2A based on 16S rRNA gene similarity. *Mycobacterium tuberculosis* ATCC 27294 was used as outgroup.
Table S3. Activity tests against bacterial and yeast test cultures of *Streptomyces* sp. IB201691-2A crude extracts from cultural liquid, cultivated in different media and conditions.

| Temperature of cultivation | 13°C |  |  |  | 28°C |  |  |  |  | 37°C |  |  |  |
|----------------------------|------|---|---|---|------|---|---|---|---|------|---|---|---|
| Medium                     | B.subtilis | P.putida | E.coli | S.cerevisiae | B.subtilis | P.putida | E.coli | S.cerevisiae | B.subtilis | P.putida | E.coli | S.cerevisiae |
| Sm1                        | 9 | - | - | - | 10 | - | - | - | - | - | - | - | - |
| Sm17                       | 9 | - | - | - | 8 | - | - | <7 | - | - | - | - | - |
| Sm12                       | <7 | - | - | - | - | - | - | 8 | - | - | - | - | - |
| Sm20                       | - | - | - | - | - | - | - | - | - | - | - | - | - |
| Sm24                       | - | - | - | - | - | - | - | - | - | - | - | - | - |
| Sm25                       | - | - | - | - | - | - | - | - | - | - | - | - | - |
| Sm27Ac                     | <7 | - | - | - | 13 | - | - | - | - | - | - | - | - |
| Sm27N                      | - | - | - | - | 15 | - | - | - | - | - | - | - | - |
| Sm27Al                     | - | - | - | - | - | - | - | - | - | - | - | - | - |
| R2                         | - | - | - | - | 12 | - | - | - | - | - | - | - | - |
| MM                         | 9 | - | - | - | 10 | - | - | - | - | - | - | - | - |

* zones of inhibition in mm
Figure S3. LC-MS chromatograms of pure compounds isolated in this work.
Purity of Baikalomycins A-C.

Despite MS and UV control during isolation, all $^1$H NMR spectra of Baikalomycins A-C still showed signals for long-chain alkyl moieties (methyl triplets at 0.90 and broad methylene singlets at 1.28 ppm), which are typical for saturated fats. According to the integration of the methyl proton signals, their content is about 15 mol% (baikalomycin A and B) or 20 mol% (baikalomycin C). In baikalomycin A and B even smaller amounts of an unspecified compound (< 5 mol%) with double bond protons at 6.08 and 6.18 ppm, both d, could be detected. All in all, the purity of Baikalomycins can be stated as follows: Baikalomycin A and C: > 80%, Baikalomycin B: > 85%.
Figure S4. (A) MS and UV absorption spectra of rabelomycin (1) (RT of 8.0 min; observed m/z 337.0738 [M-H], that corresponds to exact mass 338.081; calculated exact mass of rabelomycin 338.07904). (B) MS and UV absorption spectra of 5-hydroxy-rabelomycin (2) (RT of 6.8 min, observed m/z 353.0687 [M-H], that corresponds to exact mass 354.0759; calculated exact mass of 5-hydroxy-rabelomycin 354.07395).
Figure S5. MS and UV absorption spectra of baikalomycins A (A), B (B) and C (C).
Table S4. NMR spectroscopic data for rabelomycin (1) and 5-hydroxy-rabelomycin (2) in DMSO-d₆.

| Position | δC ₐ, ₐ | δH (J in Hz) | δC ₐ, ₐ | δH (J in Hz) |
|----------|--------|--------------|--------|--------------|
| 1        | 196.0, C | -            | 196.3, C | -            |
| 2        | 53.0, CH₂ | 2.92, d (14.4) | 52.6, CH₂ | 2.93, 2.63   |
| 3        | 71.1, C  | -            | 71.0, C  | -            |
| 4        | 43.4, CH₂ | 3.10, d (16.8) | 37.5, CH₂ | 3.06, 2.83   |
| 4a       | 152.0, C | -            | 147.5, C | -            |
| 5        | 121.4, CH | 7.11, s     | 135.4, C | -            |
| 6        | 162.0, C | -            | 162.3, C | -            |
| 6a       | 116.6, C | -            | 115.9, C | -            |
| 7        | 191.1, C | -            | 191.2, C | -            |
| 7a       | 115.4, C | -            | 115.3, C | -            |
| 8        | 160.4, C | -            | 160.4, C | -            |
| 9        | 123.4, CH | 7.32, d (8.3) | 122.4, CH | 7.30, d (8.5) |
| 10       | 137.4, CH | 7.76, t (8.3) | 136.7, CH | 7.75, t (7.9) |
| 11       | 118.5, CH | 7.46, d (7.4) | 117.9, CH | 7.46, d (7.4) |
| 11a      | 135.4, C | -            | 135.6, C | -            |
| 12       | 183.4, C | -            | 181.6, C | -            |
| 12a      | 137.6, C | -            | 135.4, C | -            |
| 12b      | 129.2, C | -            | 129.9, C | -            |
| 13       | 29.3, CH₃ | 1.30, s     | 29.9, CH₃ | 1.34, s     |

ₐ = followed by multiplicity;  
ₐ = ¹³C chemical shifts taken from 2D spectra HSQC/HMBC
Table S5. NMR spectroscopic data for baikalomycins A-C (3-5) in CD$_3$OD.

| Position | $\delta_{C}$ | $\delta_{H}$ (J in Hz) | $\delta_{C}$ | $\delta_{H}$ (J in Hz) | $\delta_{C}$ | $\delta_{H}$ (J in Hz) |
|----------|--------------|------------------------|--------------|------------------------|--------------|------------------------|
| 1        | 207.0, C     | -                      | 207.0, C     | -                      | 179.18, C    | -                      |
| 2        | 49.0, CH$_2$ | 2.48 (m, 2H)           | 49.0, CH$_2$ | 2.49 (m, 2H)           | 47.56, CH$_2$| 2.41 (d, 15)           |
|          |              |                        |              |                        |              | 2.36 (d, 15)           |
| 3        | 76.5, C      | -                      | 76.5, C      | -                      | 73.00, C     | -                      |
| 4        | 48.0, CH$_2$ | 2.38 (dd, 14.8, 2 Hz)  | 48.0, CH$_2$ | 2.38 (dd, 14.8, 2 Hz)  | 41.16, CH$_2$| 3.05 (d, 13.3 Hz)      |
|          |              | 1.87 (d, 14.8 Hz)      |              | 1.87 (d, 14.8)         |              | 3.03 (d, 13.3 Hz)      |
| 4a       | 72.5, C      | -                      | 72.5, C      | -                      | 136.73, C    | -                      |
| 5        | 30.0, CH$_2$ | 2.21 (m)               | 30.0, CH$_2$ | 2.20 (m)               | 140.82, CH$_2$| 7.76 (d, 8 Hz)         |
|          |              | 1.65 (m)               |              | 1.64 (m)               |              |                        |
| 6        | 26.0, CH$_2$ | 2.47 (m)               | 26.0 CH$_2$  | 2.47 (m)               | 119.55, CH$_2$| 7.80 (d, 8 Hz)         |
|          |              | 2.18 (m)               |              | 2.18 (m)               |              |                        |
| 6a       | 78.0, C      | -                      | 78.5, C      | -                      | 133.01, C    | -                      |
| 7        | 201.0, C     | -                      | 201.0, C     | -                      | 189.65, C    | -                      |
| 7a       | 116.0, C     | -                      | 116.0, C     | -                      | 116.74, C    | -                      |
| 8        | 159.0, C     | -                      | 159.0, C     | -                      | 160.00, C    | -                      |
| 9        | 140.0, C     | -                      | 140.0, C     | -                      | 140.15, C    | -                      |
| 10       | 134.0, CH    | 7.84 (dd, 8, 0.6 Hz)   | 134.0, CH    | 7.85 (dd, 8, 0.6 Hz)   | 134.22, CH   | 7.91 (d, 8 Hz)         |
| 11       | 120.0, CH    | 7.58 (d, 8 Hz)         | 120.0, CH    | 7.58 (d, 8 Hz)         | 120.12, CH   | 7.86 (d, 8 Hz)         |
| 11a      | 133.0, C     | -                      | 133.0, C     | -                      | 133.37, C    | -                      |
| 12       | 193.0, C     | -                      | 193.0, C     | -                      | 189.50, C    | -                      |
| 12a      | 81.0, C      | -                      | 81.0, C      | -                      | 116.69, C    | -                      |
| 12b      | 79.5, C      | -                      | 79.5, C      | -                      | 162.56, C    | -                      |
| 13       | 25.0, CH$_3$ | 1.17 (s, 3H)           | 25.0, CH$_3$ | 1.17 (s, 3H)           | 27.36, CH$_3$| 1.21 (s, 3H)           |
| 1'       | 74.0, CH     | 4.77 (dd, 11, 2 Hz)    | 74.0, CH     | 4.79 (dd, 11, 2 Hz)    | 74.47, CH    | 4.85 (dd, 11, 2 Hz)    |
| 2'       | 33.0, CH$_2$ | 2.20 (m)               | 32.5, CH$_2$ | 2.23 (m)               | 32.83, CH$_2$| 2.27 (m)               |
|          |              | 1.43 (tdd, 13.5, 11, 3.7 Hz) | 32.5, CH$_2$ | 1.44 (tdd, 13.5, 11, 4 Hz) | 32.74, CH$_2$ | 1.52 (tdd, 13.5, 11, 4 Hz) |
| 3'       | 33.5, CH$_2$ | 2.11 (ddt, 12.5, 4.5, 3.5 Hz) | 32.5, CH$_2$ | 2.26 (m)               | 32.74, CH$_2$ | 2.36 (m)               |
|          |              | 1.63 (m)               |              | 1.75 (m)               |              | 1.82 (tdd, 13.5, 11, 4 Hz) |
| 4'       | 72.5, CH     | 3.22 (dddt, 11, 9, 4.5 Hz) | 81.0, CH     | 3.26 (dddt, 11, 9, 4.5 Hz) | 82.06, CH    | 3.45 (dddt, 11, 9, 4.5 Hz) |
| 5'       | 80.0, CH     | 3.37 (dq, 9, 6 Hz)     | 79.0, CH     | 3.48 (dq, 9, 6 Hz)     | 78.64, CH    | 3.54 (dq, 9, 6 Hz)     |
| 6'       | 18.5, CH$_3$ | 1.32 (d, 6 Hz)         | 18.0, CH$_3$ | 1.30 (d, 6 Hz)         | 18.81, CH$_3$| 1.37 (d, 6 Hz)         |
| 1''      | -            | 99.5, CH               | 4.80* (d, 2.5 Hz) | 96.21, CH | 5.40 (d, 3.5 Hz) |
| 2''      | -            | 31.0, CH$_2$           | 1.84 (m)     | 1.76 (m)               | 145.59, CH   | 6.98 (dd, 10, 3.5 Hz)  |
| 3''      | -            | 28.0, CH$_2$           | 1.78 (m)     | 1.74 (m)               | 127.64, CH   | 6.05 (d, 10 Hz)        |
| 4''      | -            | 72.5, CH               | 3.13 (m)     | -                      | 198.82, C    | -                      |
| 5''      | -            | 71.0, CH               | 3.70 (dq, 9, 6 Hz) | 71.44, CH | 4.61 (q, 6.8 Hz) |
| 6''      | -            | 18.5, CH$_3$           | 1.18 (d, 6 Hz) | 15.48, CH$_3$ | 1.32 (d, 6.8 Hz) |

* taken from the $^1$H NMR in DMSO-d$_6$. This signal was overlapped by HDO in CD$_3$OD spectrum.

$^a$ = followed by multiplicity;

$^b$ = $^{13}$C chemical shifts taken from 2D spectra HSQC/HMBC.
Figure S6. $^1$H spectra of Baikalomycin A in CD$_3$OD.
Figure S7. $^1$H-$^1$H-Cosy spectra of Baikalomycin A in CD$_3$OD.
Figure S8. HSQC spectra of Baikalomycin A in CD$_2$OD.
Figure S9. HMBC spectra of Baikalomycin A in CD$_3$OD.
Figure S10. ROESY spectra of Baikalomycin A in CD$_3$OD.
Figure S11. $^1$H spectra of Baikalomycin B in CD$_3$OD.
Figure S12. \(^1\)H-\(^1\)H-Cosy spectra of Baikalomycin B in CD\(_3\)OD.
Figure S13. HSQC spectra of Baikalomycin B in CD$_3$OD.
Figure S14. HMBC spectra of Baikalomycin B in CD$_3$OD.
Figure S15. ROESY spectra of Baikalomycin B in CD$_3$OD.
Figure S16. $^1$H spectra of Baikalomycin C in CD$_3$OD.
Figure S17. $^{13}$C spectra of Baikalomycin C in CD$_3$OD.
Figure S18. $^1$H-$^1$H-Cosy spectra of Baikalomyacin C in CD$_3$OD.
Figure S19. HSQC spectra of Baikalomycin C in CD$_3$OD.
Figure S20. HMBC spectra of Baikalomycin C in CD$_3$OD.
Figure S21. ROESY spectra of Baikalomycin C in CD$_3$OD.
Figure S22. Anticancer activities. (A) Cancer cell viability was measured after 48 h treatment in an MTT assay normalized to the respective diluted solvent DMSO control (n=3, quadruplicates). (B) Cell proliferation was measured using the electric cell-substrate impedance sensing (ECIS®) system. Cells were treated 5 h after seeding. Control cells (vehicle) were treated with the diluted solvent DMSO. Impedance was normalized to values at 7 h after seeding (n=3, quadruplicates). Graphs show mean values ± SEM every ten hours and non-linear regression curves for all time points. * p < 0.05, ** p < 0.01, *** p < 0.001 compared to the control at the respective time point.
Table S6. Distribution of secondary metabolite gene clusters within genome of *Streptomyces* sp. IB201691-2A based on antiSMASH analysis.

| Cluster type      | Number of clusters |
|-------------------|--------------------|
| NRPS              | 6                  |
| NRPS, phenazine   | 1                  |
| NRPS, nucleoside  | 1                  |
| PKS I             | 2                  |
| PKS I-NRPS        | 3                  |
| hglE-KS           | 1                  |
| PKS II            | 1                  |
| PKS III           | 3                  |
| Melanin           | 2                  |
| Siderophore       | 4                  |
| Terpene           | 9                  |
| Bacteriocin       | 2                  |
| Cyanobactin       | 1                  |
| Ectoine           | 1                  |
| Phenazine         | 1                  |
Figure S23. Pairwise alignment of *bai* biosynthetic gene cluster from *Streptomyces* sp. IB201691-2A with *sch* Sch47554/47555 biosynthesis gene cluster from *Streptomyces* sp. SCC-2136. Scaffolds of *Streptomyces* sp. IB201691-2A genome covering entire *bai* gene cluster are shown.
Figure S24. Evolutional relationship between biosynthetic clusters.

*sqn* - saquayamycin gene cluster from *Streptomyces* sp. KY40-1, *spr* - saprolomycin gene cluster from *Streptomyces* sp. TK08046, *saq* - saquayamycin gene cluster from *S. nodosus* ATCC4899, *gcn* - grincamycin gene cluster from *S. lusitanus* SCSIO LR32, *sch* - Sch47554/47555 gene cluster from *Streptomyces* sp. SCC-2136, *bai* – baikalomycin gene cluster from *Streptomyces* sp. IB201691-2A, *urd* – urdamycin gene cluster from *Streptomyces fradiae* Tu2717.
Table S7. Baikalomycin gene cluster (bai) with predicted functions for each gene and homology to similar genes found within other *Streptomyces* sp.

| ORF   | Predicted function                              | Homologous                                                   | % Identity | Sequence ID   |
|-------|-------------------------------------------------|--------------------------------------------------------------|------------|---------------|
| baiS8 | flavin-dependent oxidoreductase                 | SchA26, *Streptomyces* sp. SCC 2136                          | 97         | CAH10126.1    |
| baiX1 | unknown                                         | *Streptomyces* sp. TK08046                                   | 61         | BAV17022.1    |
| baiR1 | repressor-response regulator                   | *IndI, Streptomyces globisporus*                             | 66         | AAU04840.1    |
| baiA10| NADH:flavin oxidoreductase                     | *Streptomyces* sp. AM-2504                                   | 76         | TBO55069.1    |
| baiT1 | transporter                                     | *Streptomyces* sp. HG99                                     | 86         | PIB12227.1    |
| baiA9 | flavin-reductase                                | *Streptomyces bingchenggensis* BCW-1                        | 80         | ADI11037.1    |
| baiR2 | TetR family transcriptional regulator          | *Streptomyces* sp. NBS 14/10                                 | 75         | OXL27454.1    |
| baiX2 | unknown                                         | *SaqP, Micromonospora* sp. Tu 6368                           | 48         | ACP19350.1    |
| baiA7 | hydroxylase                                     | *UrdE, Streptomyces fradiae Tü2717                          | 78         | CAA60567.1    |
| baiA5 | cyclase/aromatase                               | SchP4, *Streptomyces* sp. SCC 2136                          | 99         | CAH10113.1    |
| baiA1 | ketoacyl synthase alpha                         | SchP6, *Streptomyces* sp. SCC 2136                          | 99         | CAH10117.1    |
| baiA2 | chain length factor                             | SchP7, *Streptomyces* sp. SCC 2137                          | 98         | CAH10116.1    |
| baiA3 | acyl-carrier protein                            | SchP8, *Streptomyces* sp. SCC 2138                          | 97         | CAH10115.1    |
| baiA4 | ketoreductase                                    | SchP5, *Streptomyces* sp. SCC 2136                          | 98         | CAH10114.1    |
| baiA6 | cyclase/aromatase                               | SchP9, *Streptomyces* sp. SCC 2136                          | 99         | CAH10113.1    |
| baiA8 | oxygenase-reductase                             | *UrdM, Streptomyces fradiae Tü 217                          | 85         | AFU51427.1    |
| baiT2 | transporter                                      | PgaJ, *Streptomyces* sp. PGA64                               | 65         | AAK57531.1    |
| baiGT1| O-glycosyltransferase                           | SchS10, *Streptomyces* sp. SCC 2136                         | 97         | CAH10110.1    |
| baiGT2| O-glycosyltransferase                           | SchS9, *Streptomyces* sp. SCC 2136                          | 98         | CAH10109.1    |
| baiS7 | NDP-hexose 3,5-epimerase                        | UrdZ1, *Streptomyces fradiae* TÜ 2717                        | 71         | AAF00208.1    |
| baiGT3| C-glycosyltransferase                           | SchS7, *Streptomyces* sp. SCC 2136                          | 98         | CAF31363.2    |
| baiS1 | glucose-1-phosphate thymidylyltransferase      | *Streptomyces* sp. MJM1172                                  | 77         | OKI61982.1    |
| baiS2 | NDP-glucose 4,6-dehydratase                     | *Streptomyces* sp. SCC 2136                                  | 98         | CAF31365.1    |
| baiS3 | dTDP-6-deoxy-L-talose-4-dehydrogenase          | *Streptomyces hundungensis*                                  | 50         | AYG82949.1    |
| baiS4 | dTDP-4-amino-4,6-dideoxy-D-glucose transaminase| *Streptomyces bingchenggensis* BCW-1                        | 83         | ADI09991.1    |
| baiX3 | unknown                                         | *Streptomyces* sp. TK08046                                   | 76         | BAV17015.1    |
| baiS5 | NDP-hexose 2,3-dehydratase                      | *SaqS, Micromonospora* sp. Tu 6368                          | 73         | ACP19377.1    |
| baiS6 | glucose-fructose oxidoreductase                | *Streptomyces nodosus*                                      | 78         | AJE43663.1    |
| baiA11| phosphopantheine-transferase PgaX              | *Streptomyces dengpaensis*                                  | 77         | AVH55999.1    |
| baiA12| methylmalonyl-CoA carboxyltransferase          | *Streptomyces scabiei*                                      | 90         | KFF99397.1    |
Figure S25. Mass and UV absorption spectra of aglycone compound X1 found in the extract of the mutant strain *Streptomyces* sp. IB201691-2AΔGT3 and IB201691-2AΔGT2.
Figure S26. Baikalomycin trisaccharides found in the extract of cultivated host strains *S. albus* J1074/p8-13bai which contains the baikalomycin gene cluster closely related to SCH-47554/47555 gene cluster. Candidins and antimycin compounds were accumulated in *S. albus* J1074.
Figure S27. MS/MS fragmentation of Baikalomycins trisaccharides found in the extract of cultivated host strains *S. albus* J1074/p8-13bai which contains the baikalomycin gene cluster closely related to SCH-47554/47555 gene cluster. Fragmentation of compound with m/z 697.2882 [M-H]⁻ (RT 12.64, 12.89, and 13.11 min) (A) and of compound with m/z 695.2734 [M-H]⁻ (RT 14.83 min) (B). Loss of 113 Da coincides with the sugar cinerulose, loss of 115 da coincides to the sugar amacetose or rhodinose.