Table S1. UPLC-PDA-MS^n identifying features of bromination reaction products and substrates.

| Peak                  | $R_t$ (min) | $\lambda_{\text{max}}$ (nm) | [M - H]$^-$ | [M + H]$^+$ | MS/MS fragments$^+$ ($m/z$) |
|-----------------------|-------------|-------------------------------|-------------|-------------|--------------------------|
| apigenin$^a$          | 10.75       | 218, 267s, 335s               | 269.05      | 271.05      | 117.03                  |
| genkwanin$^a$         | 13.26       | 221, 267s, 334s               | 283.06      | 285.05      | 117.03                  |
| 6,8-dibromogenkwanin$^b$ | 17.52       | 222, 275s, 332s               | 440.88      | 442.88      | 425.86                  |
| tribromo-genkwanin    | 18.00       | 223, 272s, 331s               | 518.79      | 520.79      | 299.20                  |
| bromo-genkwanin A     | 15.28       | 220, 272s, 333s               | 360.97      | 362.97      | -                       |
| bromo-genkwanin B     | 16.12       | 221, 271s, 331s               | 360.97      | 362.97      | -                       |
| 6,8-dibromoapigenin$^b$ | 16.11       | 221, 276s, 332s               | 426.86      | 428.86      | -                       |

$^a$Peak identity based on comparison to an authentic standard.

$^b$Identity based on exact mass and proton NMR.
Table S2. 1H Chemical Shifts (ppm) of Brominated Flavone Derivatives.

|                  | 3-H | 5-OH  | 7-OR  | 4-OH  | 2'-H  | 3'-H  | \( J_{2'3'} \)^c |
|------------------|-----|-------|-------|-------|-------|-------|-----------------|
| 6,8-dibromo-apigenin (R = H) | 6.73 | 13.80^a | 10.97^a | 10.97^a | 7.85  | 6.87  | 8.8             |
| 6,8-dibromo-genkwanin (R = CH₃) | 7.16 | 13.98^c | 3.97  | 10.59^c | 8.09  | 7.02  | 8.8             |

*Solvent DMSO-d₆; a) broad singlet b) broad singlet; c) sharp singlet*
Table S3. Agilent 1290-QTRAP 5500 LC-MSn Settings

Quantitation Table:

Period 1:

------------------
Scans in Period: 3395
Relative Start Time: 60000.00 msec
Experiments in Period: 5

IDA Properties:

First Criteria:
Intense peaks from 1 to 3
Ions greater than: 260.000 m/z
Ions smaller than: 730.000 m/z
Which exceeds 5000.000 counts
Rolling collision energy: No
Exclude former target ions: Never
Mass Tolerance: 250.000 mDa
Exclude isotopes within 4.0 Da window
Use Enhanced Resolution scan to confirm Charge State and/or Isotope Pattern selection: Yes
Exclude 1+ precursors from Enhanced Resolution Scan confirmation and MS/MS: Yes
Dynamic Background Subtraction: Yes

Period 1 Experiment 1:
----------------------
Scan Type: Precursor Ion (Prec)
Polarity: Negative
Scan Mode: Profile
Ion Source: Turbo Spray
# Scans to Sum: 1
Precursor Of: 80.90 Da
Resolution Q1: Unit
Resolution Q3: Unit
Scan Rate: 1000 Da/s
Intensity Thres.: 0.00 cps
Settling Time: 0.0000 msec
MR Pause: 5.0070 msec
MCA: No
Center/Width: No
Step Size: 0.10 Da

Start (Da)  Stop (Da)  Time (sec)  Param  Start  Stop
260.00  730.00  0.47

Parameter Table(Period 1  Experiment 1)
CUR: 35.00
IS: -4500.00
TEM: 650.00
GS1:  60.00  
GS2:  60.00  
CAD:  High  
DP  -100.00  
EP  -10.00  
CE  -100.00  
CXP  -15.00  

Period 1  Experiment  2:

Scan Type:   Enhanced Resolution (ER)  
Polarity:   Negative  
Scan Mode:   Profile  
Ion Source:   Turbo Spray  
# Scans to Sum: 1  
Resolution Q1:  Open  
Scan Rate:   250 Da/s  
Intensity Thres.:  0.00 cps  
Settling Time:  0.0000 msec  
MR Pause:   15.0000 msec  
Q0 trapping:  No  
MCA:  No  
Center/Width:  Yes  
LIT fill time:  0.05 msec  
Dynamic Fill Time:  On  
TIC Target EMS Scan:  10.00 x1e7 cps.  
TIC Target ER Scan:  1.00 x1e7 cps.  
TIC Target EPI Scan:  10.00 x1e7 cps.  
Max Fill EMS Scan:  150.000 msec  
Max Fill ER Scan:  250.000 msec  
Max Fill EPI Scan:  250.000 msec  
Min Fill EMS Scan:  0.050 msec  
Min Fill ER Scan:  0.050 msec  
Min Fill EPI Scan:  0.050 msec  
Default Fill EMS Scan:  0.050 msec  
Default Fill ER Scan:  0.050 msec  
Default Fill EPI Scan:  1.000 msec  
Q3 Entry Barrier:  8.00  V  
Step Size:  0.02 Da  

Start (Da) Stop (Da) Time (sec) Param Start Stop
<Best ion>  
AF3  0.08  0.08  
EXB  158.78  158.72  

Start (Da) Stop (Da) Time (sec) Param Start Stop
<Best ion>  
AF3  0.08  0.08  
EXB  158.78  158.72
Parameter Table (Period 1 Experiment 2)

| Parameter | Value |
|-----------|-------|
| CUR       | 35.00 |
| IS        | -4500.00 |
| TEM       | 650.00 |
| GS1       | 60.00 |
| GS2       | 60.00 |
| CAD       | High |
| DP        | -100.00 |
| EP        | -10.00 |
| CE        | -10.00 |
| CES       | -0.00 |

Period 1 Experiment 3:

---

Scan Type: Enhanced Product Ion (EPI)
Polarity: Negative
Scan Mode: Profile
Ion Source: Turbo Spray
# Scans to Sum: 1
Product Of: 30.00 Da
Resolution Q1: Unit
Scan Rate: 10000 Da/s
Intensity Thres.: 0.00 cps
Settling Time: 0.0000 msec
MR Pause: 1.5000 msec
Q0 trapping: No
MCA: No
Center/Width: No
LIT fill time: 1.00 msec
Dynamic Fill Time: On

- TIC Target EMS Scan: 10.00 x1e7 cps.
- TIC Target ER Scan: 1.00 x1e7 cps.
- TIC Target EPI Scan: 10.00 x1e7 cps.
- Max Fill EMS Scan: 150.000 msec
- Max Fill ER Scan: 250.000 msec
- Max Fill EPI Scan: 250.000 msec
- Min Fill EMS Scan: 0.050 msec
- Min Fill ER Scan: 0.050 msec
- Min Fill EPI Scan: 0.050 msec
- Default Fill EMS Scan: 0.050 msec
- Default Fill ER Scan: 0.050 msec
- Default Fill EPI Scan: 1.000 msec
Q3 Entry Barrier: 8.00 V
Step Size: 0.12 Da

| Start (Da) | Stop (Da) | Time (sec) | Param | Start | Stop |
|-----------|-----------|------------|-------|-------|------|
| 50.00     | 102.87    | 0.0053     | AF3   | 2.98  | 3.06 |
|           |           |            | EXB   | 155.79| 153.89|

| Start (Da) | Stop (Da) | Time (sec) | Param | Start | Stop |
|-----------|-----------|------------|-------|-------|------|
| 102.87    | 308.63    | 0.0206     | AF3   | 3.06  | 3.40 |
|           |           |            | EXB   | 153.89| 146.52|

| Start (Da) | Stop (Da) | Time (sec) | Param | Start | Stop |
|-----------|-----------|------------|-------|-------|------|
| 308.63    | 730.00    | 0.0421     | AF3   | 3.40  | 4.10 |
|           |           |            | EXB   | 146.52| 131.41|

Parameter Table (Period 1 Experiment 3)
CUR: 35.00
IS: -4500.00
TEM: 650.00
GS1: 60.00
GS2: 60.00
CAD: High
DP -100.00
EP -10.00
CE -100.00
CES 40.00

Period 1 Experiment 4:
-----------------------------
Scan Type: Enhanced Product Ion (EPI)
Polarity: Negative
Scan Mode: Profile
Ion Source: Turbo Spray
# Scans to Sum: 1
Product Of: 30.00 Da
Resolution Q1: Unit
Scan Rate: 10000 Da/s
Intensity Thres.: 0.00 cps
Settling Time: 0.0000 msec
MR Pause: 1.5000 msec
Q0 trapping: No
MCA: No
Center/Width: No
LIT fill time: 1.00 msec
Dynamic Fill Time: On
TIC Target EMS Scan: 10.00 x 1e7 cps.
TIC Target ER Scan: 1.00 x 1e7 cps.
TIC Target EPI Scan: 10.00 x 1e7 cps.
Max Fill EMS Scan: 150.000 msec
Max Fill ER Scan: 250.000 msec
Max Fill EPI Scan: 250.000 msec
Min Fill EMS Scan: 0.050 msec
Min Fill ER Scan: 0.050 msec
Min Fill EPI Scan: 0.050 msec
Default Fill EMS Scan: 0.050 msec
Default Fill ER Scan: 0.050 msec
Default Fill EPI Scan: 1.000 msec
Q3 Entry Barrier: 8.00 V
Step Size: 0.12 Da

Start (Da) Stop (Da) Time (sec) Param Start Stop
50.00 102.87 0.0053 AF3 2.98 3.06
   EXB 155.79 153.89

Start (Da) Stop (Da) Time (sec) Param Start Stop
102.87 308.63 0.0206 AF3 3.06 3.40
   EXB 153.89 146.52

Start (Da) Stop (Da) Time (sec) Param Start Stop
308.63 730.00 0.0421 AF3 3.40 4.10
   EXB 146.52 131.41

Parameter Table (Period 1 Experiment 4)
CUR: 35.00
IS: -4500.00
TEM: 650.00
GS1: 60.00
GS2: 60.00
CAD: High
DP -100.00
EP -10.00
CE -100.00
CES 40.00

Period 1 Experiment 5:
-----------------------------------------------
Scan Type: Enhanced Product Ion (EPI)
Polarity: Negative
Scan Mode: Profile
Ion Source: Turbo Spray
# Scans to Sum: 1
Product Of: 30.00 Da
Resolution Q1: Unit
Scan Rate: 10000 Da/s
Intensity Thres.: 0.00 cps
Settling Time: 0.0000 msec
MR Pause: 1.5000 msec
Q0 trapping: No
MCA: No
Center/Width: No
LIT fill time: 1.00 msec
Dynamic Fill Time: On
TIC Target EMS Scan: 10.00 x1e7 cps.
TIC Target ER Scan: 1.00 x1e7 cps.
TIC Target EPI Scan: 10.00 x1e7 cps.
Max Fill EMS Scan: 150.000 msec
Max Fill ER Scan: 250.000 msec
Max Fill EPI Scan: 250.000 msec
Min Fill EMS Scan: 0.050 msec
Min Fill ER Scan: 0.050 msec
Min Fill EPI Scan: 0.050 msec
Default Fill EMS Scan: 0.050 msec
Default Fill ER Scan: 0.050 msec
Default Fill EPI Scan: 1.000 msec
Q3 Entry Barrier: 8.00 V
Step Size: 0.12 Da

| Start (Da) | Stop (Da) | Time (sec) | Param | Start | Stop |
|------------|-----------|------------|-------|-------|------|
| 50.00      | 102.87    | 0.0053 AF3 | EXB   | 155.79| 153.89 |
|            |           |            |       |       |      |
| 102.87     | 308.63    | 0.0206 AF3 | EXB   | 153.89| 146.52 |
|            |           |            |       |       |      |
| 308.63     | 730.00    | 0.0421 AF3 | EXB   | 146.52| 131.41 |

Parameter Table(Period 1 Experiment 5)
CUR: 35.00
IS: -4500.00
TEM: 650.00
GS1: 60.00
GS2: 60.00
CAD: High
DP -100.00
| Mass (Da) | Offset Value |
|-----------|--------------|
| 44.998    | -0.450       |
| 411.259   | -1.160       |
| 585.385   | -1.515       |
| 933.636   | -2.212       |

Quad 3 Negative  Unit  Scan Speed = 10 Da/s  
Last Modification Date Time: December 27, 2012 14:14:08

IE3  0.000

| Mass (Da) | Offset Value |
|-----------|--------------|
| 44.998    | -0.150       |
| 411.259   | -0.860       |
| 585.385   | -1.215       |
| 933.636   | -1.912       |

Calibration tables
Quad 1 Negative  Unit Resolution Scan Speed = 10 Da/s  
Last Modification Date Time: December 28, 2012 10:35:40

| Mass (Da) | Dac Value |
|-----------|-----------|
| 44.998    | 8087      |
| 585.385   | 106766    |
| 933.636   | 170369    |

Quad 1 Negative  Unit Resolution Scan Speed = 1000 Da/s  
Last Modification Date Time: December 28, 2012 10:46:48

Resolution tables
Quad 1 Negative  Unit  Scan Speed = 1000 Da/s  
Last Modification Date Time: June 20, 2012 12:07:02

IE1  -0.500

| Mass (Da) | Offset Value |
|-----------|--------------|
| 44.998    | -0.042       |
| 411.259   | 0.119        |
| 585.385   | 0.200        |
| 933.636   | 0.315        |

Quad 3 Negative  Low  Scan Speed = 10 Da/s  
Last Modification Date Time: August 13, 2013 09:56:00

| Mass (Da) | Offset Value |
|-----------|--------------|
| 44.998    | -0.450       |
| 411.259   | -1.160       |
| 585.385   | -1.515       |
| 933.636   | -2.212       |
| Mass (Da) | Dac Value |
|----------|-----------|
| 44.998   | 8115      |
| 411.259  | 75034     |
| 585.385  | 106853    |
| 933.636  | 170471    |

Quad 3 Negative Unit Resolution Scan Speed = 10 Da/s
Last Modification Date Time: December 27, 2012 14:14:34

| Mass (Da) | Dac Value |
|----------|-----------|
| 44.998   | 8183      |
| 411.259  | 75808     |
| 585.385  | 107961    |
| 933.636  | 172261    |

Quad 3 Negative Unit Resolution Scan Speed = 2000 Da/s
Last Modification Date Time: June 20, 2012 12:19:58

| Mass (Da) | Dac Value |
|----------|-----------|
| 44.998   | 8222      |
| 411.259  | 75883     |
| 585.385  | 108047    |
| 933.636  | 172388    |

Quad 3 Negative Scan Speed = 250 Da/s
Last Modification Date Time: June 20, 2012 14:59:12

| Mass (Da) | Dac Value |
|----------|-----------|
| 112.985  | 24976     |
| 431.982  | 95599     |
| 601.978  | 133225    |

Quad 3 Negative Scan Speed = 10000 Da/s
Last Modification Date Time: June 20, 2012 15:36:46

| Mass (Da) | Dac Value |
|----------|-----------|
| 112.985  | 25058     |
| 431.982  | 95853     |
| 601.978  | 133532    |

Instrument Parameters:
Detector Parameters (Negative):
CEM 2200.0