Supplementary Material

Effect of biofortification with iodine by 8-hydroxy-7-iodo-5-quinolinesulfonic acid and 5-chloro-7-iodo-8-quinolinol on the chemical composition and antioxidant properties of potato tubers (Solanum Tuberosum L.) in a pot experiment

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Table S1. Chromatographic gradient (A – 0.3% FA in H2O; B – 0.3% FA in MetOH for 5-Cl-7-I-8-Q or 0.3% FA in ACN for 8-OH-7-I-5QSA.
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Table S1. Chromatographic gradient (A – 0.3% FA in H2O; B – 0.3% FA in MetOH for 5-Cl-7-I-8-Q or 0.3% FA in ACN for 8-OH-7-I-5QSA.

No.	Retention time, min.	%A	%B
1.	0.0	60	40
2.	2.0	60	40
3.	5.0	30	70
4.	8.0	2	98
5.	13.5	2	98
6.	13.6	60	40
7.	16.0	60	40

Injection volume was 10 μL and total analysis time was 16 min. The HPLC column effluent was introduced directly into a mass spectrometer. Electrospray ionization (ESI) in positive ion mode was used. Spray voltage and source temperature was set to 4500 V and 500 °C. Parameters of Turbo Spray ion source are listed in Table S2.

Table S2. Parametres of Turbo Spray Ion Source

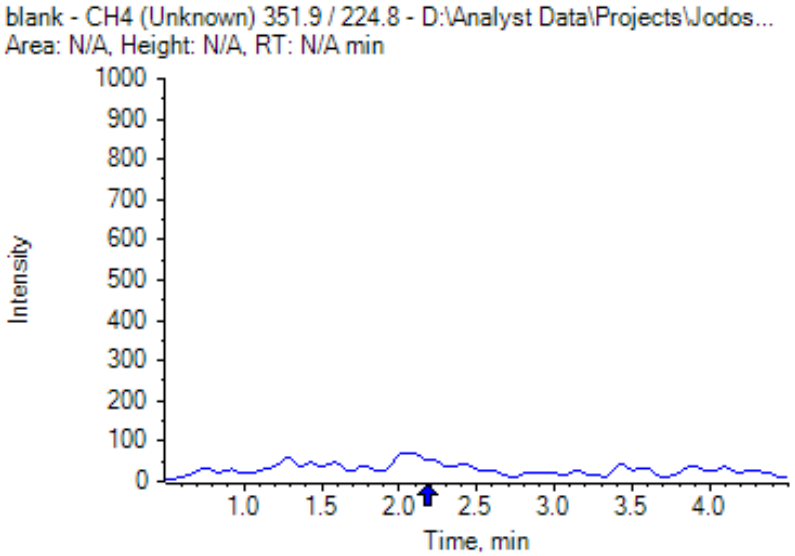
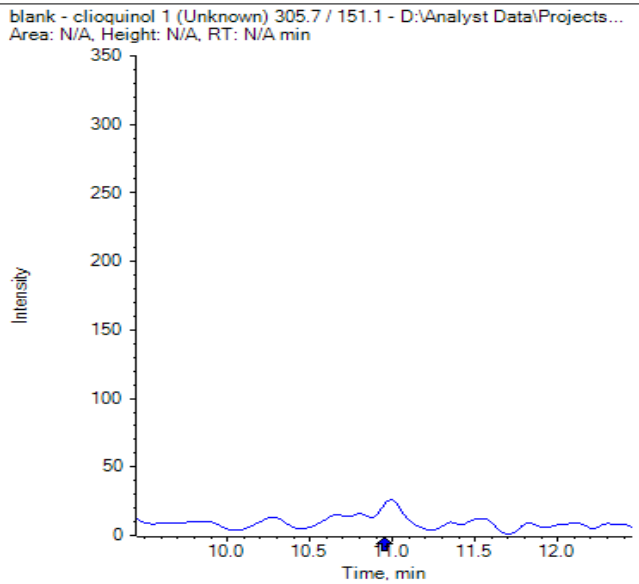
Parameter	Value
IonSpray Voltage	4500 V
temperature	500 °C
Curtain gas (CUR)	30
Collision Gas	medium
Ion source gas (GS1)	50
Ion source gas (GS2)	65

Scheduled MRM mode was used for quantitative studies and transitions in the Table S3. Precursor/Product Transitions of Analytes were monitored. The LC-MS/MS system was controlled using Analyst 1.7 with HotFix 3 software, which was also used for data processing.

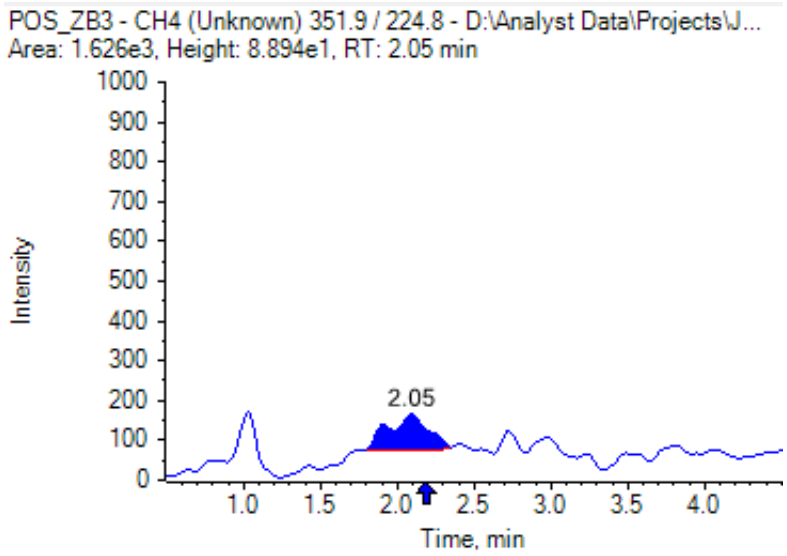
Table S3. Precursor/Product Transitions of Analytes

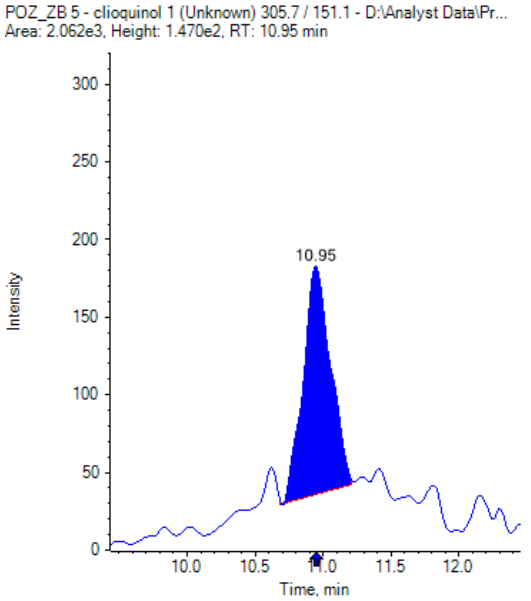
Analyte	Precursor ion (m/z)	Product ion (m/z)	Transition
5-Cl-7-I-8-Q 1	305.7	151.1	quantifying
5-Cl-7-I-8-Q 2	305.7	115.8	qualifying
8-OH-7-I-5QSA 1	351.9	224.8	quantifying
8-OH-7-I-5QSA 2	351.9	126.1	qualifying

Table S4. Chromatograms from the analysis of the content of 8-OH-7-I-5 QSA and 5-Cl-7-I-8-Q in potato tubers.

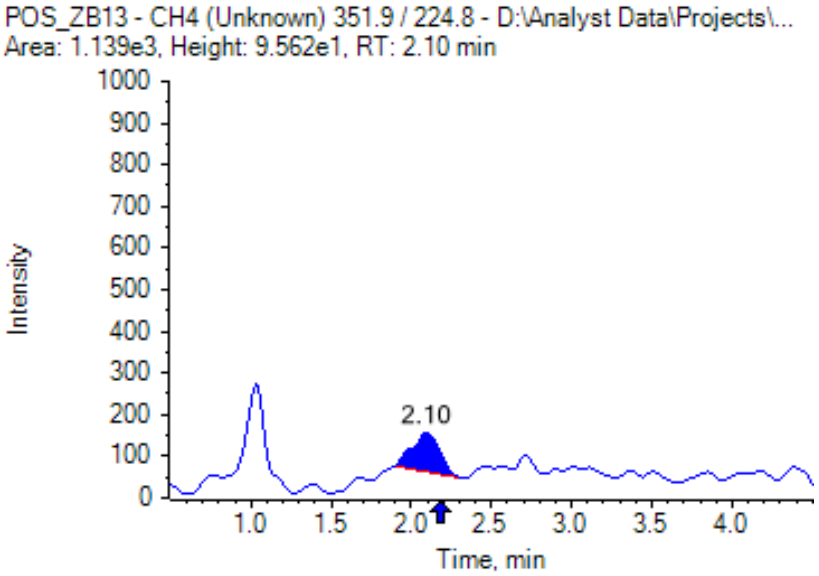
Treatments/type of sample	Chromatograms for determnation **8-Hydroxy-7-iodo-5-quinolinesulfonic acid** by LC-MS/MS methods	Chromatograms for determnation **5-chloro-7-iodo-8-quinolinol** by LC-MS/MS methods
Blank – chromatogram of blank sample		

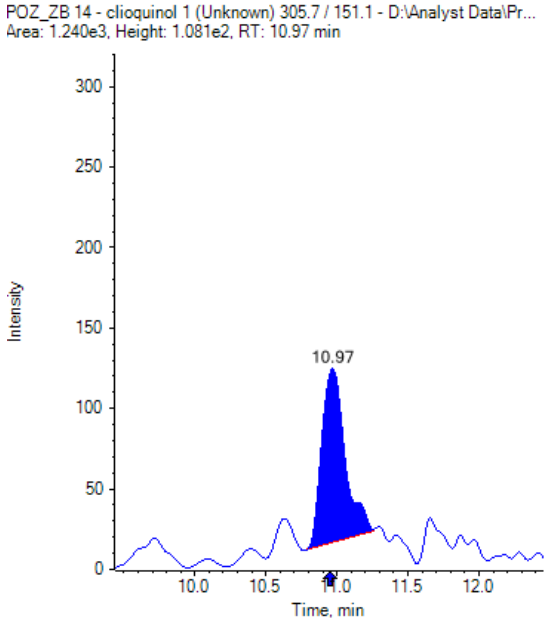
Control - chromatogram for the control tuber extract





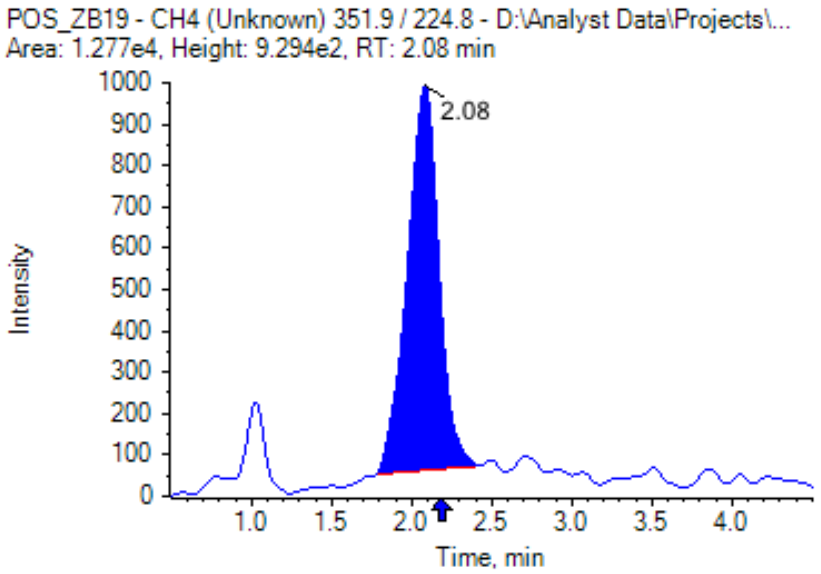
KIO3 - chromatogram for tuber extract of plants enriched in KIO3

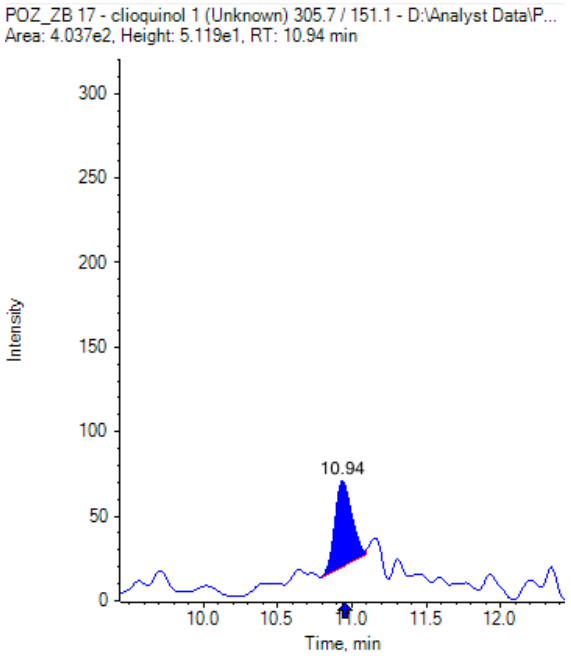




8-OH-7-I-5QSA

- chromatogram for tuber extract of plants enriched in 8-OH-7-I-5QSA





5-Cl-7-I-8-Q - chromatogram for tuber extract of plants enriched in 5-Cl-7-I-8-Q

