

## Appendix E1

Table E1 shows the CT numbers (in Hounsfield units) measured on the CT images. For each sample, tube potential, and copper x-ray filter thickness, the mean is the mean of the CT number (in Hounsfield units) measured in the region of interest on the 16 images evaluated for each element (64 images for water and NaCl), and the standard deviation was calculated for the region of interest means between the 16 or 64 images.

In Table E1, the mean values of image contrast for the seven candidate elements ranged from 172 to 530 HU and averaged 293 HU. The standard deviations were typically approximately 10 HU and ranged from 2 to 22 HU. This means that after averaging the measured image contrast from 16 images, the uncertainties in the mean are on the order of a few Hounsfield units, or approximately less than 1% to 2% of the mean. Therefore, we did not perform detailed statistical analysis to assign error bars to each data point; instead, we considered any difference in the final results that exceeded 20 HU or 5% (corresponding to approximately 2 standard deviations) to be statistically significant.

With no added copper filter, the water values are 1–2 HU; therefore, the PMMA phantom has little effect on the water calibration. However, with added copper filters, the water values range from 11 to 93 HU, with the greatest effect occurring at lower tube potentials and with thicker filters. Therefore, correction for errors in the water values is clearly necessary. The mean water values for each tube potential and filter thickness combination in Table E1 were used to correct (by means of subtraction) each of the other measured values for that tube potential and filter combination. Note that the mean values for water were determined by averaging four sets of 16 images, so the precision of the water value is the square root of 4 or two times more precise than the value that it's being used to correct. Therefore, the precision of the result is only compromised by a factor of the square root of  $[1^2 + (1/2)^2]$  or 1.11 of the precision of the uncorrected result, which is in the range of 1% to 2%, so the precision of the corrected result is only degraded by approximately 0.1%.

Table E2 shows the corrections that we made for material concentration on the basis of measured concentrations. These were determined by multiplying the factors shown in Table 1 (of the primary article) by the raw data shown in Table E1, after correcting for water calibration. The values shown in Table E2 were then added to the water-corrected values from Table E1.

Table E3 shows the corrections that we made for presence of chlorine on the basis of our Hounsfield unit measurements of NaCl solutions and our calculation of chlorine concentration in the compounds that contained them. Because these corrections are approximately equal to our 20-HU limit of statistical significance and are a small fraction of the values we are correcting, and because the attenuation of sodium is a small fraction of the attenuation of chlorine, we did not “correct our correction” for the presence of sodium in our correction material, NaCl. Note that the mean values for NaCl were determined by averaging four sets of 16 images, so the precision of the NaCl value is the square root of 4 or two times more precise than the value that it's being used to correct. Therefore, the precision of the result is only compromised by a factor of the square root of  $[1^2 + (1/2)^2]$  or 1.11 of the precision of the uncorrected result, which is in

the range of 1%–2%, so the precision of the corrected result is only degraded by approximately 0.1%.

**Table E1. Raw Data**

| Copper X-ray Filter Thickness (mm) | Atomic No. | Material        | Measured Values at Peak X-ray Tube Energy (HU) |    |         |    |         |    |         |    |
|------------------------------------|------------|-----------------|--|----|---------|----|---------|----|---------|----|
|                                    |            |                 | 80 kVp   |    | 100 kVp |    | 120 kVp |    | 140 kVp |    |
|                                    |            |                 | Mean   | SD | Mean    | SD | Mean    | SD | Mean    | SD |
| 0.0                                | 8          | Water           | 1  | 8  | 2       | 3  | 2       | 3  | 1       | 2  |
| 0.0                                | 15         | NaCl (6 mg/mL)  | 14   | 7  | 14      | 4  | 13      | 3  | 10      | 2  |
| 0.0                                | 53         | Iodine          | 367  | 9  | 273     | 4  | 218     | 3  | 179     | 3  |
| 0.0                                | 56         | Barium          | 360  | 7  | 273     | 4  | 218     | 3  | 180     | 3  |
| 0.0                                | 64         | Gadolinium      | 450  | 7  | 385     | 4  | 326     | 2  | 279     | 3  |
| 0.0                                | 70         | Ytterbium       | 342  | 10 | 342     | 3  | 309     | 4  | 276     | 3  |
| 0.0                                | 73         | Tantalum        | 269  | 10 | 304     | 4  | 285     | 3  | 258     | 4  |
| 0.0                                | 79         | Gold            | 222  | 8  | 228     | 5  | 237     | 3  | 227     | 3  |
| 0.0                                | 83         | Bismuth         | 282  | 6  | 232     | 5  | 248     | 4  | 246     | 3  |
| 0.2                                | 8          | Water           | 21   | 15 | 18      | 9  | 15      | 10 | 11      | 10 |
| 0.2                                | 15         | NaCl (25 mg/mL) | 70   | 11 | 57      | 10 | 49      | 10 | 43      | 10 |
| 0.2                                | 53         | Iodine          | 365  | 11 | 271     | 10 | 214     | 11 | 176     | 11 |
| 0.2                                | 56         | Barium          | 358  | 17 | 270     | 8  | 216     | 8  | 177     | 10 |
| 0.2                                | 64         | Gadolinium      | 474  | 17 | 392     | 11 | 325     | 9  | 277     | 11 |
| 0.2                                | 70         | Ytterbium       | 374  | 14 | 357     | 12 | 317     | 9  | 280     | 11 |
| 0.2                                | 73         | Tantalum        | 293  | 11 | 320     | 9  | 299     | 8  | 266     | 10 |
| 0.2                                | 79         | Gold            | 227  | 12 | 237     | 8  | 245     | 7  | 233     | 7  |
| 0.2                                | 83         | Bismuth         | 286  | 16 | 235     | 10 | 254     | 9  | 253     | 10 |
| 0.5                                | 8          | Water           | 51   | 13 | 38      | 13 | 33      | 12 | 26      | 14 |
| 0.5                                | 15         | NaCl (25 mg/mL) | 96   | 14 | 76      | 10 | 63      | 11 | 55      | 12 |
| 0.5                                | 53         | Iodine          | 367  | 13 | 272     | 10 | 216     | 10 | 175     | 10 |
| 0.5                                | 56         | Barium          | 361  | 14 | 271     | 11 | 213     | 11 | 174     | 11 |
| 0.5                                | 64         | Gadolinium      | 497  | 11 | 399     | 9  | 323     | 9  | 271     | 10 |
| 0.5                                | 70         | Ytterbium       | 405  | 11 | 380     | 11 | 329     | 10 | 285     | 10 |
| 0.5                                | 73         | Tantalum        | 320  | 11 | 346     | 11 | 314     | 9  | 275     | 11 |
| 0.5                                | 79         | Gold            | 237  | 12 | 255     | 11 | 264     | 10 | 246     | 12 |
| 0.5                                | 83         | Bismuth         | 291  | 11 | 244     | 11 | 267     | 10 | 263     | 10 |
| 1.0                                | 8          | Water           | 93   | 17 | 70      | 11 | 54      | 10 | 44      | 11 |
| 1.0                                | 15         | NaCl (25 mg/mL) | 134  | 17 | 103     | 12 | 83      | 12 | 70      | 12 |
| 1.0                                | 53         | Iodine          | 379  | 19 | 276     | 12 | 213     | 12 | 172     | 13 |
| 1.0                                | 56         | Barium          | 381  | 13 | 277     | 10 | 214     | 12 | 172     | 10 |

|     |    |            |     |    |     |    |     |    |     |    |
|-----|----|------------|-----|----|-----|----|-----|----|-----|----|
| 1.0 | 64 | Gadolinium | 530 | 16 | 404 | 12 | 320 | 12 | 262 | 13 |
| 1.0 | 70 | Ytterbium  | 467 | 17 | 408 | 12 | 341 | 10 | 289 | 12 |
| 1.0 | 73 | Tantalum   | 375 | 20 | 384 | 12 | 332 | 12 | 284 | 14 |
| 1.0 | 83 | Bismuth    | 313 | 22 | 261 | 10 | 286 | 11 | 278 | 11 |

Note.—SD = standard deviation.

**Table E2. Corrections (Additive) Required to Correct for Measured versus Nominal Elemental Concentrations**

| Copper X-ray Filter Thickness (mm) | Atomic No. | Material   | Correction at Peak X-ray Tube Energy (HU) |         |         |         |
|------------------------------------|------------|------------|---|---------|---------|---------|
|                                    |            |            | 80 kVp                                    | 100 kVp | 120 kVp | 140 kVp |
| 0.0                                | 53         | Iodine     | -33                                       | -25     | -20     | -16     |
| 0.0                                | 56         | Barium     | 95  | 72      | 57      | 47      |
| 0.0                                | 64         | Gadolinium | 29  | 24      | 21      | 18      |
| 0.0                                | 70         | Ytterbium  | 11  | 11      | 9       | 9       |
| 0.0                                | 73         | Tantalum   | 2   | 3       | 3       | 2       |
| 0.0                                | 79         | Gold       | 9   | 9       | 10      | 9       |
| 0.0                                | 83         | Bismuth    | 15  | 12      | 13      | 13      |
| 0.2                                | 53         | Iodine     | -31                                       | -23     | -18     | -15     |
| 0.2                                | 56         | Barium     | 90  | 67      | 53      | 44      |
| 0.2                                | 64         | Gadolinium | 29  | 24      | 20      | 17      |
| 0.2                                | 70         | Ytterbium  | 11  | 11      | 9       | 8       |
| 0.2                                | 73         | Tantalum   | 2   | 3       | 3       | 2       |
| 0.2                                | 79         | Gold       | 9   | 9       | 10      | 9       |
| 0.2                                | 83         | Bismuth    | 14  | 11      | 13      | 13      |
| 0.5                                | 53         | Iodine     | -29                                       | -21     | -17     | -14     |
| 0.5                                | 56         | Barium     | 82  | 62      | 48      | 39      |
| 0.5                                | 64         | Gadolinium | 28  | 23      | 19      | 16      |
| 0.5                                | 70         | Ytterbium  | 11  | 11      | 9       | 8       |
| 0.5                                | 73         | Tantalum   | 2   | 3       | 3       | 2       |
| 0.5                                | 79         | Gold       | 8   | 9       | 10      | 9       |
| 0.5                                | 83         | Bismuth    | 13  | 11      | 12      | 12      |
| 1.0                                | 53         | Iodine     | -26                                       | -19     | -14     | -12     |
| 1.0                                | 56         | Barium     | 77  | 55      | 43      | 34      |
| 1.0                                | 64         | Gadolinium | 28  | 21      | 17      | 14      |
| 1.0                                | 70         | Ytterbium  | 12  | 10      | 9       | 8       |
| 1.0                                | 73         | Tantalum   | 3   | 3       | 3       | 2       |
| 1.0                                | 83         | Bismuth    | 12  | 10      | 12      | 12      |

**Table E3. Corrections (Subtractive) Required to Correct for Chlorine Content in Formulations for Gadolinium, Ytterbium, and Gold**

| Copper X-ray Filter Thickness (mm) | Atomic No. | Material   | Correction at Peak X-ray Tube Energy (HU) |         |         |         |
|------------------------------------|------------|------------|---|---------|---------|---------|
|                                    |            |            | 80 kVp                                    | 100 kVp | 120 kVp | 140 kVp |
| 0.0                                | 64         | Gadolinium | 24  | 22      | 19      | 17      |
| 0.0                                | 70         | Ytterbium  | 22  | 20      | 17      | 16      |
| 0.0                                | 79         | Gold       | 19  | 18      | 15      | 14      |
| 0.2                                | 64         | Gadolinium | 22  | 18      | 15      | 15      |
| 0.2                                | 70         | Ytterbium  | 20  | 16      | 14      | 13      |
| 0.2                                | 79         | Gold       | 17  | 14      | 12      | 12      |
| 0.5                                | 64         | Gadolinium | 20  | 17      | 14      | 13      |
| 0.5                                | 70         | Ytterbium  | 18  | 15      | 12      | 12      |
| 0.5                                | 79         | Gold       | 16  | 13      | 11      | 10      |
| 1.0                                | 64         | Gadolinium | 18  | 15      | 13      | 12      |
| 1.0                                | 70         | Ytterbium  | 16  | 13      | 12      | 11      |