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SUPPLEMENTARY INFORMATION

How the surface chemical properties of nanoceria are related to its enzyme-like, antiviral and degradation activity

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Derivatization of choline

For the formation of choline-derivative, the same equivalent of choline (0.2 mmol/L) and SC4 (0.2 mmol/L) was mixed in water at room temperature for 2 hours. Time-resolved samples in kinetic studies (1000 µL) were derivatized by the addition of 1000 µL of SC4 solution (0.2 mmol/L).

XPS measurement protocol to minimize UHV and X-ray reduction of CeO_2

The samples are measured immediately after loading into the main chamber from the load lock chamber. In order to be able to insert the samples, the pressure in the load lock must be reduced to the level $3x10^{-7}$ mbar. The typical time to reach this pressure in the load lock is about 60 minutes and depends on the sample (humidity, surface area, etc.). Then, the first spectrum recorded is Ce3d in a high resolution to minimize X-ray irradiation effects which can cause CeO_2 reduction. Each high-resolution spectrum is accumulated five times to improve signal-to-noise ratio, the spectra accumulating immediately one after another. The difference between the first and the last data sets are negligible, which proves that the changes caused by X-ray are very low. The procedure for all samples is strictly the same, which allows their relative comparison.

HPLC measurements

To monitor catalytic hydrolysis of *p*-nitrophenyl phosphorylcholine (*p*-NPPC) and formation of its degradation products (choline and *p*-nitrophenol), HPLC system with a diode array detector (DAD) Dionex UltiMate 3000 (Thermo Scientific™, Palo Alto, USA) was used. Chromatographic analysis was carried out in a reverse phase system (RPLC-C18) on the AccucoreTM column, 2.6 µm, PFP, 150 x 4.6mm. For isocratic elution, mobile phase acetonitrile (ACN) and water (H_2O) acidified with formic acid (0.1%) in the ratio 45% ACN/55% H_2O (v/v) was used. The flow rate of the mobile phase was set to 1.0 $ml \cdot min^{-1}$, 30 °C column temperature, and 15 µL volume injection. Data were collected at the absorption maximum of the individual substances.

Wavelengths corresponding to 210 nm for *p*-NPPC, 315 nm for *p*-NP, and 277 nm for choline-derivate were set on the DAD detector. Data collection and evaluation was performed using the Chromeleon Chromatography Data System (CDS) software (Thermo Scientific). The same instrument was used to determine *p*-nitrophenyl thymidine 5'-monophosphate (*p*-NP-TMP), with slightly different ACN/H_2O ratio 35%/65% (v/v). The wavelengths corresponding to the absorption maximum of each analyte were set to 268 nm for thymidine, 272 nm for *p*-NP-TMP substrate, and 315 nm for *p*-nitrophenol. The other separation conditions were identical. Blank experiments were performed without the presence of the catalyst.

Deactivation of CWAs

The CWA substrate solution (150 µL) was added into a series of vials containing 50 mg of powder sorbent to obtain 1:50 mg CWA/sorbent ratio. The initial concentration of VX, GD and HD were 6876, 7107, and 6853 ng/µL. The sealed vials were protected from sunlight and kept at a constant temperature (25°C). The reaction was terminated by addition of 2-propanol (1.85 mL) at selected times and solid adsorbent was separated by centrifugation (5000 rpm, 5 min) before analysis of the supernatant aliquots on GC system Agilent 6890N with HP-5 column (5% phenyl methyl siloxane, 30 m ×0.32 mm ID ×0.25 µm film thickness) and FPD detector. All CWAs were synthesized in the Military Research institute, state enterprise, Brno, Czechia.

Preliminary cytotoxicity studies

Product test solutions were dissolved in distilled water at a concentration of 50 and 200 mg/mL. Dilution series in Dulbecco's Modified Eagle Medium (DMEM) (Lonza, Basel, Switzerland) supplemented with additional 2% Fetal Bovine Serum (FBS) and L-glutamine (Biological Industries, Kibbutz Beit-Haemek, Israel), 100 U/mL of penicillin and 100 g/mL of streptomycin (Sigma-Aldrich, Munich, Germany) from concentration 50 mg/mL to 5 x 10^{-7} mg/mL were transferred (50 µL) into cell culture units in a 96-well polystyrene plate (NUNC, Denmark) containing 50 µL of cells suspension. Two units were inoculated with each dilution. Plates were incubated in 37 °C/5%CO_2 and observed after 24 h for the development of cytotoxic effect, using an inverted microscope (Olympus Corp., Hamburg Germany; Axio Observer, Carl Zeiss MicroImaging GmbH).

Antiviral assay

EN 14476 standard describes a quantitative suspension test for the evaluation of virucidal activity in the medical area (Phase 2/Step 1), mixing one part by volume of test virus suspension (0.1 mL of $1x10^8 TCID_{50}$ Ad 5 virus or HSV1), one part by volume of interfering substance (0.1 mL of PBS), and eight parts by volume of disinfectant (investigated substances in concentration 50 and 200 mg/mL). After specified contact time (60 min), aliquots were taken, and serial dilutions up to 10^{-8} of each mixture were prepared. In four repeats, 50 µL of each dilution was added to the microtiter plate containing a monolayer of confluent A549 or HeLa cells. The plates were observed daily for up to 4 days for the development of viral cytopathic effect, using an inverted microscope. Then, residual infectivity was determined. According to EN 14476, a disinfectant is considered as having virucidal effectiveness if within the recommended exposure time the titer is reduced by ≥4 log10 steps (inactivation ≥ 99.99%).

Cell viability assay

Neoplastic cell line A549 in concentration of 3.000 cells per well and normal cell line MDCK in a concentration of 10^5 cells per well were seeded in a 96-well plate (NUNC, Denmark). Compounds dissolved in distilled water at a concentration of 200 mg/mL and diluted in the culture medium to afford concentrations of 200, 180, 160, 140, 120, 100, 80, 60, 40 and 20 mg/mL were added to the wells with cells. The cells were incubated (37 °C/5%CO_2) for 24 h, after which the MST assay was carried out. 20 µL of MST (MTS Assay Kit (Cell Proliferation) (Colorimetric) (ab197010), Abcam, Cambridge, MA, USA) was added to each well and incubation for 4 h at 37 °C was implemented. The test is based on the enzymatic reduction of the tetrazolium salt MTT in living, metabolically active cells. The metabolite, purple-colored formazan is measured colorimetrically, using a multiwell plate reader. The optical density (OD) was measured using a spectrophotometric microplate reader (ELx800, BioTek, USA) with reference wavelength of 490 nm. The percentage of viability was calculated using following formula: % viability = (average OD for test group/ average OD for control group) x 100. The control group was constituted by untreated cells and cells treated with DMSO.

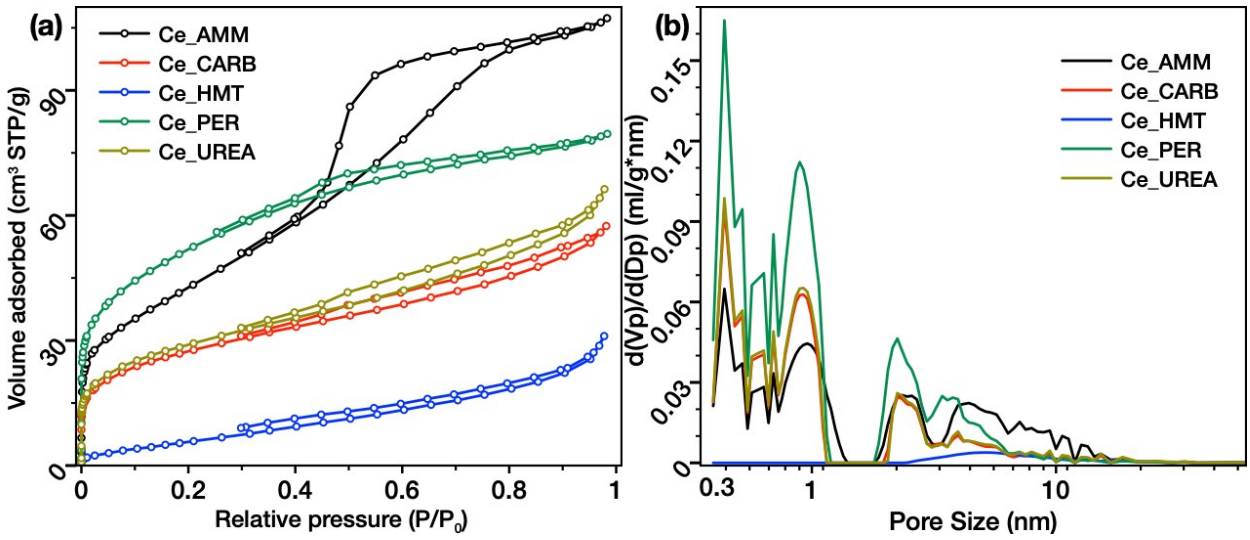

Figure S1. (a) The sorption isotherms and pore size distribution (NLDFT method) obtained from N_2 physisorption

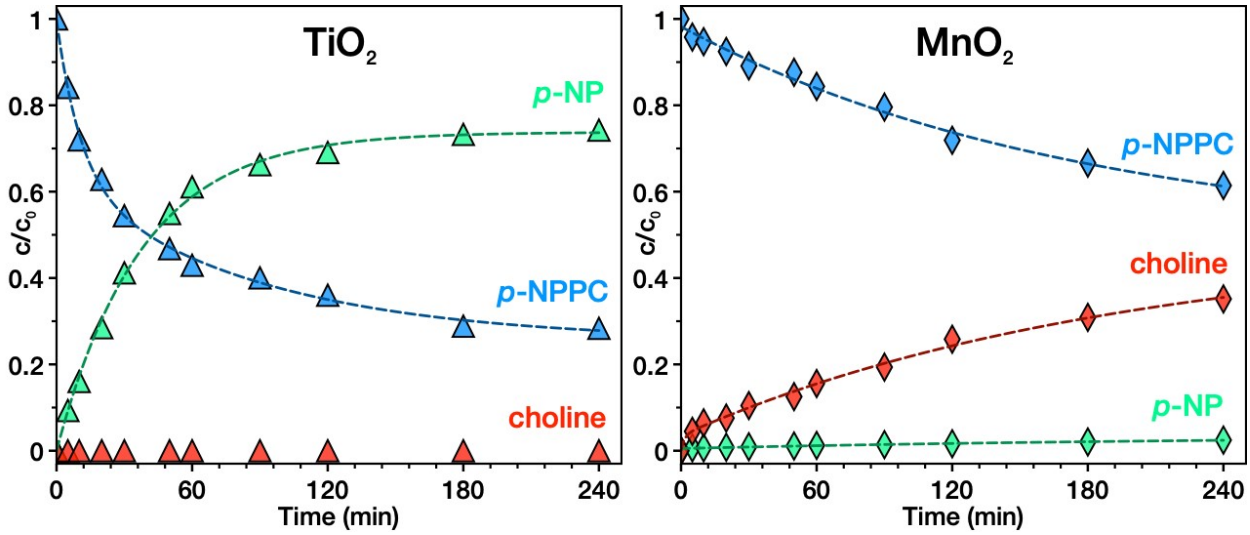

Figure S2. The kinetic curves for hydrolysis of *p*-nitrophenylphosphorylcholine (1.25 mmol/L) with concomitant formation of its products *p*-nitrophenol (green) and choline (red) on TiO_2 and MnO_2. Conditions: TRIS buffer at pH~ 7; temp. =37 °C, TiO_2 (MnO_2) conc. 25 mg/mL.

Table S1. The fitting parameters - rate constant (*k*), initial rate of conversion (IRC) and degree of conversion (DOC) of the pseudo-first-order kinetics model on ceria-catalyzed hydrolysis of *p*-NPPC and concomitant formation of *p*-NP and choline as hydrolysis products. In-house-prepared TiO_2 and MnO_2 added for comparison.

Sample	*p*-NPPC hydrolysis				formation of *p*-NP				formation of choline			
	k, [a] min^{-1}	SSA norm. $k \times 10^3$, min^{-1}	IRC, µmol/L × min^{-1}	DOC at t=60 min, %	*k*, [a] min^{-1}	SSA norm. $k \times 10^3$, min^{-1}	IRC, µmol/L× min^{-1}	DOC at t=60 min, %	*k*, [a] min^{-1}	SSA norm. $k \times 10^3$, min^{-1}	IRC µmol/L × min^{-1}	DOC at t=60 min, %
Ce_AMM	0.0321 (0.0024)	0.2045	255.5	81.3	0.0331 (0.0016)	0.2108	410.4	81.3	0.0305 (0.0216)	0.1942	193.9	80.5
Ce_CARB	0.0230 (0.0038)	0.2421	90.8	86.1	0.0243 (0.0015)	0.2558	156.4	77.9	0.0113 (0.0052)	0.1189	66.1	69.9
Ce_HMT	0.0182 (0.0079)	1.1375	77.4	53.6	0.0167 (0.0028)	1.0438	66.7	53.6	0.0135 (0.0074)	0.8438	37.2	53.6
Ce_PER	0.2738 (0.0072)	1.5043	1008.8	94.0	0.2786 (0.0061)	1.5308	933.1	92.9	0.2889 (0.0021)	1.5874	772.3	94.0
Ce_UREA	0.0345 (0.0141)	0.3450	168.0	90.1	0.0356 (0.0055)	0.3416	155.3	90.1	0.0245 (0.0014)	0.2426	145.0	90.1

TiO_2	0.0114 (0.0035)	-	46.5	57.1	0.0106 (0.0009)	-	24.6	57.1	-		-	-
MnO_2	0.0026 (0.0001)	-	3.5	15.6	0.0004 (0.0001)	-	4.2	1.6	0.0025 (0.0001)		23.2	15.6

[a)] Standard error given in parenthesis; adjusted R^2 >0.995 for all fits of the regression model

Table S2. The fitting parameters - rate constant (*k*), initial rate of conversion (IRC) and degree of conversion (DOC) of the pseudo-first-order kinetics model on ceria-catalyzed hydrolysis of *p*-NP-TMP and concomitant formation of *p*-NP and thymidine as hydrolysis products.

Sample	*p*-NP-TMP hydrolysis				formation of *p*-NP				formation of thymidine			
	k, [a] min^{-1}	SSA norm. $k \times 10^3$, min^{-1}	IRC, µmol/L × min^{-1}	DOC at t=60 min, %	*k*, [a] min^{-1}	SSA norm. $k \times 10^3$, min^{-1}	IRC, µmol/L × min^{-1}	DOC at t=60 min, %	*k*, [a] min^{-1}	SSA norm. $k \times 10^3$, min^{-1}	IRC, µmol/L × min^{-1}	DOC at t=60 min, %
Ce_AMM	0.1108 (0.0011)	0.7057	324.1	99.8	0.1060 (0.0022)	0.6752	349.3	97.4	0.0359 (0.0034)	0.2287	87.8	92.2
Ce_CARB	0.0292 (0.0027)	0.3074	92.3	77.7	0.0288 (0.0014)	0.3032	85.2	73.8	0.0122 (0.0011)	0.1284	22.4	63.0
Ce_HMT	0.0124 (0.0013)	0.7750	60.8	67.6	0.0121 (0.0016)	0.7563	49.2	65.2	0.0079 (0.0009)	0.4938	14.8	14.6
Ce_PER	0.1037 (0.0104)	0.5698	369.3	94.3	0.1094 (0.0102)	0.6011	510.8	92.0	0.0901 (0.0099)	0.4951	444.4	94.3
Ce_UREA	0.0795 (0.0068)	0.7871	91.3	99.3	0.0813 (0.0037)	0.8050	93.5	97.9	0.0334 (0.0014)	0.3307	38.8	82.7

[a] Standard error given in parenthesis; adjusted R^2 >0.995 for all fits of the regression model

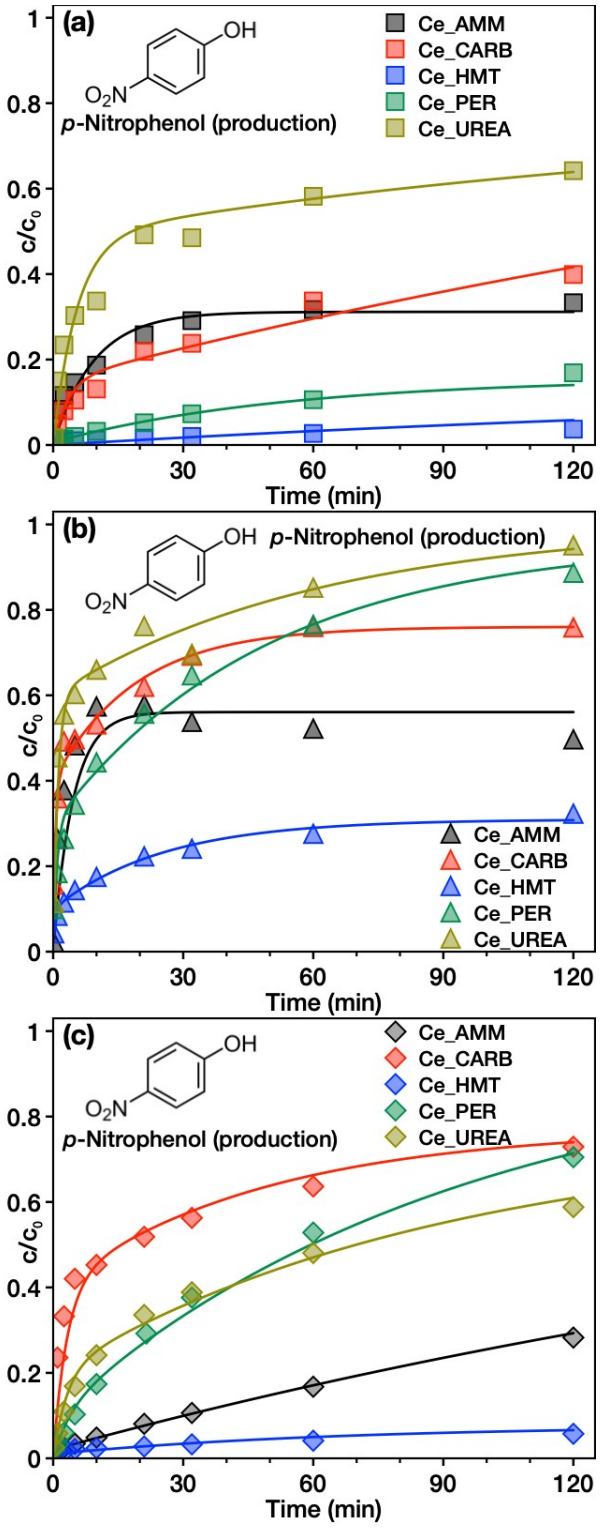

Figure S3. The kinetics of production of *p*-NP by reactive adsorption on nanoceria in degradation of MP in ACN, b) MPO in ACN, and c) MPO in water.

Table S3. The fitting parameters - rate constant (k), initial rate of conversion (IRC) and degree of conversion (DOC) of the kinetics model on ceria-catalyzed hydrolysis of MP in acetonitrile and concomitant formation of *p*-NP as hydrolysis product.

Sample	MP hydrolysis (ACN)					formation of *p*-NP				
	k_1, [a] min^{-1}	SSA norm. $k_1 \times 10^3$, min^{-1}	k_2, [a] min^{-1}	IRC, µmol/L × min^{-1}	DOC at t=60 min, %	k_1, [a] min^{-1}	SSA norm. $k_1 \times 10^3$, min^{-1}	k_2, [a] min^{-1}	IRC, µmol/L × min^{-1}	DOC at t=60 min, %
Ce_AMM	0.705 (0.048)	4.4904	0.044 (0.003)	531.0	90.1	0.166 (0.014)	1.0573	0.029 (0.002)	193.9	31.7
Ce_CARB	0.458 (0.018)	4.8211	0.011 (<0.001)	449.5	57.7	0.061 (0.006)	0.6421	0.015 (0.002)	94.1	33.7
Ce_HMT	0.011 (0.006)	0.6875	0.011 (0.006)	27.3	2.1	0.037 (0.013)	2.3125	0.009 (0.003)	1.2	2.1
Ce_PER	0.100 (0.014)	0.5495	0.015 (0.002)	124.0	21.4	0.016 (<0.001)	0.0879	0.011 (<0.001)	6.9	10.6
Ce_UREA	0.411 (0.011)	4.0693	0.012 (<0.001)	388.0	59.7	0.474 (0.006)	4.6930	0.037 (<0.001)	336.2	58.2

Table S4. The fitting parameters - rate constant (*k*), initial rate of conversion (IRC) and degree of conversion (DOC) of the kinetics model on ceria-catalyzed hydrolysis of MPO in acetonitrile and concomitant formation of *p*-NP as hydrolysis product.

Sample	MPO hydrolysis (ACN)					formation of *p*-NP				
	k_1, [a] min^{-1}	SSA norm. $k_1 \times 10^3$, min^{-1}	k_2, [a] min^{-1}	IRC, µmol/L × min^{-1}	DOC at t=60 min, %	k_1, [a] min^{-1}	SSA norm. $k_1 \times 10^3$, min^{-1}	k_2, [a] min^{-1}	IRC, µmol/L × min^{-1}	DOC at t=60 min, %
Ce_AMM	0.723 (0.006)	4.6050	0.146 (0.006)	1198.4	99.9	0.588 (0.047)	3.7452	<0.001 (<0.001)	654.2	52.2
Ce_CARB	0.497 (<0.001)	5.2316	0.018 (<0.001)	524.7	84.9	1.652 (0.021)	17.3895	0.042 (<0.001)	546.7	76.0
Ce_HMT	0.145 (<0.001)	9.0625	0.014 (<0.001)	38.5	20.2	0.203 (0.052)	12.6875	0.035 (0.001)	111.2	20.2
Ce_PER	0.169 (<0.001)	0.9285	0.016 (<0.001)	225.1	73.9	0.122 (0.024)	0.6703	0.027 (0.001)	224.1	73.9
Ce_UREA	0.852 (0.003)	8.4356	0.018 (0.002)	1132.3	77.2	1.245 (0.019)	12.3267	0.018 (<0.001)	919.5	77.2

Table S5. The fitting parameters - rate constant (k), initial rate of conversion (IRC) and degree of conversion (DOC) of the kinetics model on ceria-catalyzed hydrolysis of MPO in water and concomitant formation of *p*-NP as hydrolysis product.

Sample	MPO hydrolysis (water)					formation of *p*-NP				
	k_1, [a] min^{-1}	SSA norm. $k_1 \times 10^3$, min^{-1}	k_2, [a] min^{-1}	IRC, µmol/L × min^{-1}	DOC at t=60 min, %	k_1, [a] min^{-1}	SSA norm. $k_1 \times 10^3$, min^{-1}	k_2, [a] min^{-1}	IRC, µmol/L × min^{-1}	DOC at t=60 min, %
Ce_AMM	0.015 (<0.001)	0.0955	0.006 (<0.001)	100.1	14.3	0.018 (<0.001)	0.1146	0.005 (<0.001)	2.8	14.3
Ce_CARB	0.482 (0.024)	5.0737	0.016 (<0.001)	618.5	59.5	0.558 (0.014)	5.8737	0.009 (<0.001)	568.4	59.5
Ce_HMT	0.008 (<0.001)	0.5000	0.007 (<0.001)	4.0	0.9	0.003 (<0.001)	0.1875	0.002 (<0.001)	1.9	0.9
Ce_PER	0.009 (<0.001)	0.0495	0.055 (<0.001)	34.1	48.7	0.025 (<0.001)	0.1374	0.009 (<0.001)	34.2	48.7
Ce_UREA	0.451 (0.022)	4.4653	0.017 (<0.001)	468.8	52.7	0.064 (0.004)	0.6337	0.015 (<0.001)	89.8	48.0

Table S6. The fitting parameters - rate constant (*k*), initial rate of conversion (IRC) and degree of conversion (DOC) of the kinetics model on the degradation of CWAs.

Sample	VX					GD					HD				
	k_1×10[2], [a)] min[-1]	SSA norm. k_1×10[5], min[-1]	k_2×10[2], [a)] min[-1]	IRC, µmol/L × min[-1]	DOC at t=60 min, %	k_1×10[2], [a)] min[-1]	SSA norm. k_1×10[5], min[-1]	k_2×10[2], [a)] min[-1]	IRC, µmol/L × min[-1]	DOC at t=60 min, %	k_1×10[2], [a)] min[-1]	SSA norm. k_1×10[5], min[-1]	k_2×10[2], [a)] min[-1]	IRC, µmol/L × min[-1]	DOC at t=60 min, %
Ce_AMM	8.05 (0.14)	51.27	1.20 (0.03)	1141.1	99.2	52.15 (3.37)	332.17	1.36 (0.32)	2265.8	95.7	0.325 (0.125)	2.070	0.024 (0.005)	16.2	23.0
Ce_CARB	2.38 (0.70)	25.05	0.20 (0.05)	203.2	84.7	0.36 (0.02)	3.79	0.04 (0.004)	1019.3	52.2	0.015 (0.005)	0.158	0.005 (0.001)	5.0	5.4
Ce_HMT	0.41 (0.05)	25.63	0.15 (0.01)	32.6	31.8	0.09 (0.001)	5.63	0.004 (0.0002)	38.9	14.8	0.017 (0.002)	1.063	0.005 (0.0004)	4.5	3.3
Ce_PER	4.95 (0.14)	27.20	2.42 (0.54)	1519.9	99.2	1.30 (0.33)	7.14	0.10 (0.03)	1204.5	80.0	0.816 (0.026)	4.484	0.048 (0.001)	57.9	60.0
Ce_UREA	4.62 (0.90)	45.74	0.57 (0.05)	150.4	95.9	0.70 (0.02)	6.93	0.06 (0.01)	1209.3	67.1	0.018 (0.003)	0.178	0.006 (0.003)	11.2	10.2