ELECTRONIC SUPPORTING INFORMATION

Highly Efficient Cr(VI) Removal from Water Using Deep Eutectic Solvents: A Sustainable and Comprehensive Approach

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TABLE CONTENTS

Table S1. Selected physical properties of the deep eutectic solvents (DESs) prepared with a 1:4 HBA:HBD molar ratio (n=3).

HBA	HBD	Appearence	pH	Density (g/mL)
N8888Br	HCOOH	Colourless	1.1 ± 0.1	1.107 ± 0.003
	CH_3COOH	Yellowish	2.3 ± 0.2	0.955 ± 0.005
	C_2H_5COOH	Colourless	4.2± 0.2	0.998 ± 0.002
	C_2H_5OH	Colourless	6.8 ± 0.4	0.885 ± 0.004

Table S2. Chemical shift assignments for HBA, HBD, and DES

Compound	Functional group	Chemical shift (ppm)	Explanation
HBA	CH_3 (a)	3H, triplet, δ = 0.871 ppm	Protons of the terminal methyl group in the alkyl chain.
	CH_2 (b)	10H, quartet, δ = 1.277 ppm):	Protons of the methylene groups within the alkyl chain.
	CH_2 (c)	1.583	Protons of the methylene group adjacent to the nitrogen atom.
	CH_2 (d)	2H, triplet, δ = 3.184 ppm	Protons of the methylene group adjacent to the nitrogen atom, significantly influenced by the positive charge on the nitrogen.
HBD	CH_3	3H (singlet, 1.91 ppm):	Protons of the methyl group adjacent to the carbonyl group.
	COOH	1H singlet, 11.913 ppm	Proton of the carboxyl group. This position is typically broad and may vary depending on the solvent and

			concentration.
HDES 4	CH_3 (from HBA)	3H, triplet, δ = 0,870 ppm	Similar to HBA
	CH_2 (from HBA)	10H, multiplet, δ = 1.280 ppm: 5 methylene (CH2) groups of the HBA	Similar to HBA
	CH_2 (from HBA)	2H, singlet, δ = 1.573 ppm: 1 methylene (CH2) group of the HBA.	Similar to HBA
	CH_2 (from HBA)	2H, triplet, δ 3.173 ppm: methylene group adjacent to the electronegative nitrogen of the HBA	Similar to HBA
	CH_3 (from HBD)	3H, singlet, δ 1.908 ppm: methyl group of the HBD.	Similar to HBD
	COOH (from HBD)	1H, singlet, δ 11.921 ppm (downfield): labile proton of the carboxylic acid group in the HBD.	This position may shift significantly compared to neat acetic acid due to hydrogen bonding interactions with the HBA.

Table S3. Absorbance measurements of Cr(VI) standard solutions at 540 nm (Water Matrix)

Conc.Cr(VI) (mg/L)	**Abs 1 (a.u)**	**Abs 2 (a.u)**	**Abs 3 (a.u)**	**Mean**	**SD**
0.1	0.0791	0.0783	0.0793	0.0789	0.0005
0.25	0.1962	0.1903	0.1893	0.1920	0.0037
0.5	0.2810	0.2791	0.2901	0.2834	0.0059
0.75	0.4527	0.4412	0.4531	0.4490	0.0067
1	0.5893	0.5902	0.5821	0.5872	0.0044
Slope	0.56606 ± 0.02061				
Interceps	0.02266 ± 0.0035				
R^2	0.9992				
LOD	0.0297 ± 0.001				

LOQ	0.0993 ± 0.004

Table S4. Absorbance measurements of Cr(VI) standard solutions at 540 nm (HDES Matrix)

Conc.Cr(VI) (mg/L)	**Abs 1 (a.u)**	**Abs 2 (a.u)**	**Abs 3 (a.u)**	**Mean**	**SD**
0.1	0.0795	0.0783	0.0801	0.0793	0.0009
0.25	0.1492	0.1501	0.1462	0.1485	0.0021
0.5	0.2636	0.2519	0.2662	0.2606	0.0076
0.75	0.3826	0.4189	0.3891	0.3969	0.0193
1	0.4755	0.4812	0.4593	0.4720	0.0114
Slope	0.44565 ± 0.00688				
Interceps	0.03511 ± 0.00139				
R^2	0.9960				
LOD	0.0378 ± 0.001				
LOQ	0.1258 ± 0.002				

Table S5. Effect of temperature on EE %

Temperature	**C_i (mg/L)**	**C_p (mg/L)**	**EE %**
30 °C	250	26.4 ± 1.8	89.4 ± 1.8
40 °C	250	2.0 ± 0.2	99.2 ± 1.6
50 °C	250	1.7 ± 0.1	99.3 ± 2.3

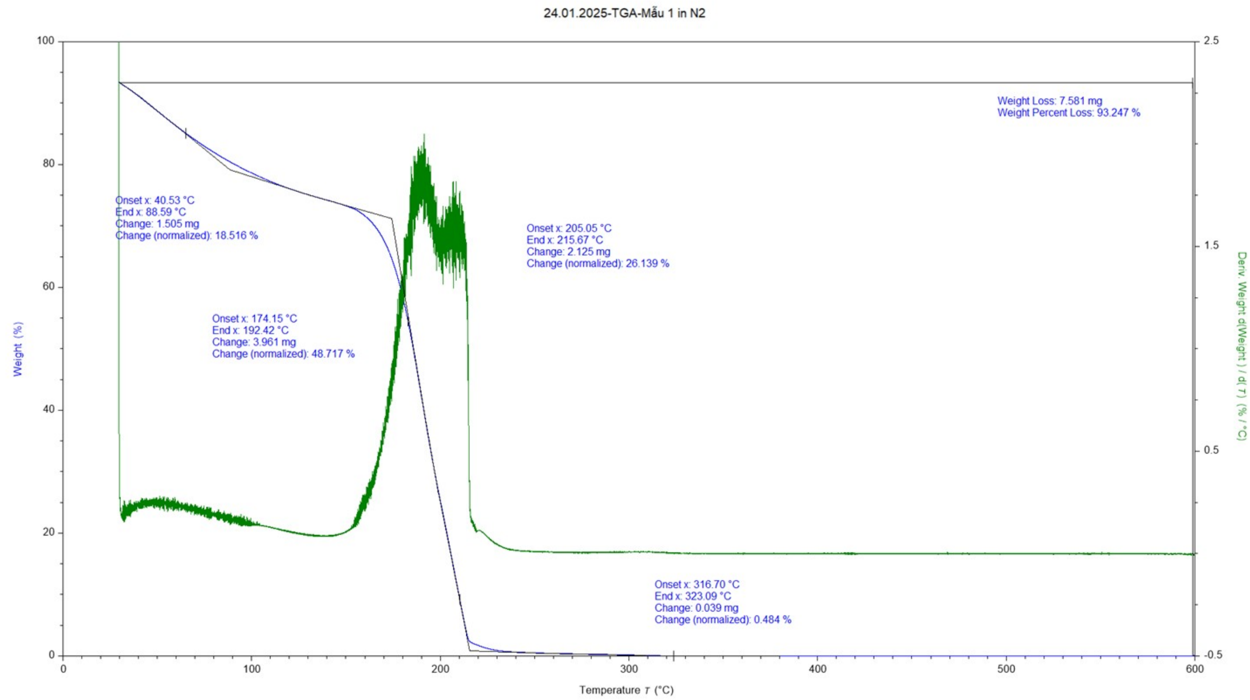

Figure S1. TGA of HDES 4

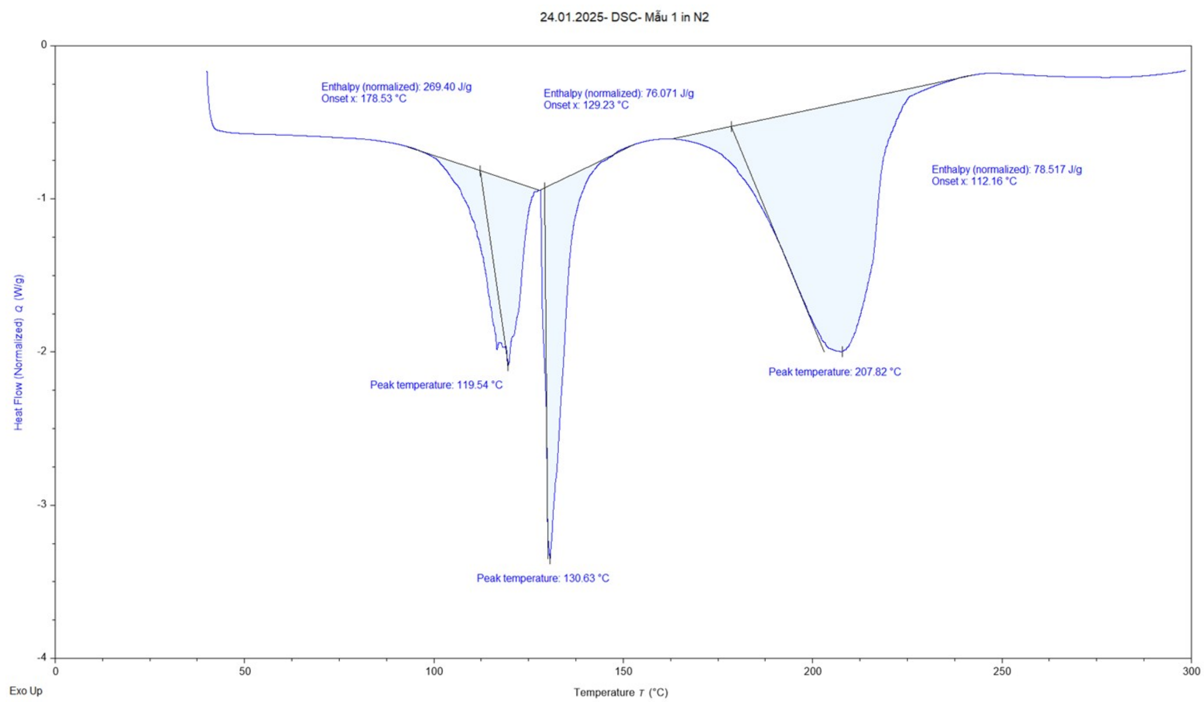

Figure S2. DSC of HDES 4

Analytical Greenness report sheet

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Criteria	Score	Weight
1. Direct analytical techniques should be applied to avoid sample treatment.	0.85	2
2. Minimal sample size and minimal number of samples are goals.	0.32	2
3. If possible, measurements should be performed in situ.	0.0	2
4. Integration of analytical processes and operations saves energy and reduces the use of reagents.	1.0	2
5. Automated and miniaturized methods should be selected.	0.75	2
6. Derivatization should be avoided.	1.0	2
7. Generation of a large volume of analytical waste should be avoided, and proper management of analytical waste should be provided.	0.39	2
8. Multi-analyte or multi-parameter methods are preferred versus methods using one analyte at a time.	0.84	2
9. The use of energy should be minimized.	1.0	2
10. Reagents obtained from renewable sources should be preferred.	1.0	2
11. Toxic reagents should be eliminated or replaced.	1.0	2
12. Operator's safety should be increased.	1.0	2

Figure S3. Analytical Greeness Report sheet