Supplementary Information

Evaluation of green chemistry metrics for sustainable recycling of platinum group metals from spent automotive catalysts via bioleaching

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Table S1 Concentration of PGM in pretreated SAC

Metal	**SAC Batch I for *P. fluorescens* and *B. megaterium* (mg/kg)**	**SAC Batch II for *C. violaceum* (mg/kg)**
Pt	1908	1112
Pd	1451	743
Rh	535	184

Table S2 The mass-based calculations

Mass-based Calculations	Equation
	Concentration of glycine 5 g/L
Initial mass of glycine	$\text{Initial mass of glycine} = \text{Concentration of glycine} \times \text{Volume of solution}$
	$\text{Initial mass of glycine} = 5\left(\frac{\text{g}}{\text{L}}\right) \times \frac{100\ \text{mL}}{1000\ \text{mL/L}} = 0.5\ \text{g}$
Mass of SAC used	$\text{Mass of SAC sample} = \text{Pulp density of SAC} \times \text{Volume of solution}$
Initial mass of PGM in the SAC	$\text{Mass of PGM} = \frac{\text{Mass of PGM (g)}}{\text{Mass of SAC (g)}} \times \text{Mass of SAC sample (g)}$
Initial mass of free CN ion	$\text{Mass of free CN ion} = \text{Conc. of free CN } ion \left(\frac{\text{mg}}{\text{L}}\right) \times 10^{-3}\left(\frac{\text{g}}{\text{mg}}\right) \times \text{Vol}ume \text{ of sol}ution \text{ (L)}$
Mass of metal-cyanide complex produced	$\text{Mass of metal recovered (g)} = \frac{\%\ \text{Recovery}}{100\ \%} \times \text{Initial mass of PGM in the SAC (g)}$
	$\text{No. of moles of metal recovered (mol)} = \frac{\text{Mass of metal recovered (g)}}{\text{Molar mass of metal}\left(\frac{\text{g}}{\text{mol}}\right)}$
	$\text{No. of moles of metal - cyanide (mol)} = \text{No. of moles of metal (mol)} \times \frac{\text{Stoichiometric coeffi. of metal - cyanide}}{\text{Stoichiometric coeffi. of metal}}$
	$\text{Mass of metal - cyanide (g)} = \text{No. of mol of metal} - \text{cyanide (mol)} \times \text{Molar mass of metal - cyanide } (\frac{\text{g}}{\text{mol}})$

Table S3 Green chemistry metrics for metal limiting reactions for *P. fluorescens* and *B. megaterium* at pulp density 0.5 % w/v

Limiting reagent (Metal)									
		***P. fluorescens* (0.5 % w/v)**				***B. megaterium* (0.5 % w/v)**			
		Pt	**Pd**	**Rh**	**Overall**	**Pt**	**Pd**	**Rh**	**Overall**
Percentage Yield	Y	44.00	54.00	96.00	58.19	40.00	51.00	94.00	55.03
Effective Mass Yield	YE	3.41	4.11	3.42	10.93	3.10	3.88	3.34	10.32
Percentage Conversion	C1a	44.00	54.00	96.00	58.19	40.00	51.00	94.00	55.03
	C1b	44.00	54.00	96.00	58.19	40.00	51.00	94.00	55.03
Selectivity	S1	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
	S2	0.35	0.80	0.43		0.33	0.79	0.45	
Atom Economy	AE1	89.79	86.07	83.55	85.80	89.79	86.07	83.55	85.80
	AE2	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00
	AE2 (glycine)	60.40	51.72	46.84	51.17	60.40	51.72	46.84	51.17
Atom Utilization	AU	89.79	86.07	83.55	86.37	89.79	86.07	83.55	86.30
Stoichiometric Factor	SF	1.34	1.48	1.58	1.78	1.27	1.39	1.47	1.63
Maximum RME (Kernel's RME)	Kernel's RME	44.00	54.00	96.00	58.19	40.00	51.00	94.00	55.03
Curzon's RME	Curzon's RME 1	32.92	36.50	60.64	40.13	31.43	36.74	63.86	40.24
	Curzon's RME 2	32.92	36.50	60.64	32.63	31.43	36.74	63.86	33.68
Simple E-Factor	sEF				0.53				0.59
Simple E-Factor (account for pretreatment)	sEF (pretreatment)				9.68				10.28
Complex E-Factor	cEF				222.70				235.84
Complex E-Factor (account for pretreatment)	cEF (pretreatment)				231.85				245.53
Carbon Efficiency	CE1	22.36	27.44	48.78	31.16	22.43	28.59	52.70	32.67
	CE2	0.13	0.22	0.22	0.58	0.12	0.21	0.22	0.55
Mass Intensity	MI	3.04	2.74	1.65	2.49	3.18	2.72	1.57	2.49
Mass Intensity (account for pretreatment)	MI (pretreatment)				11.64				12.18
Process Mass Intensity	PMI1				1.53				1.59
	PMI2				48414.66				51271.49
Process Mass Intensity	PMI1 (pretreatment)				10.68				11.28

(account for pretreatment)	PMI2 (pretreatment)				48423.81				51281.18
Mass productivity	MP1				0.40				0.40
	MP2				0.65				0.63
Mass productivity (account for pretreatment)	MP1 (pretreatment)				0.09				0.08
	MP2 (pretreatment)				0.09				0.09
Solvent intensity	SI				48412.17				51269.00
Solvent intensity (account for pretreatment)	SI (pretreatment)				48421.32				51278.69

Table S4 Green chemistry metrics for metal limiting reactions for *C. violaceum* at pulp densities 0.5 % w/v, 1 % w/v and 2 % w/v

Limiting reagent (Metal)													
		***C. violaceum* (0.5 % w/v)**				***C. violaceum* (1 % w/v)**				***C. violaceum* (2 % w/v)**			
		Pt	**Pd**	**Rh**	**Overall**	**Pt**	**Pd**	**Rh**	**Overall**	**Pt**	**Pd**	**Rh**	**Overall**
Percentage Yield	Y	69.00	74.00	99.00	75.11	62.00	69.00	96.00	69.57	42.00	49.00	84.00	50.56
Effective Mass Yield	YE	2.20	2.03	0.86	5.09	1.97	1.90	0.83	4.70	1.34	1.35	0.73	3.41
Percentage Conversion	C1a	69.00	74.00	99.00	75.11	62.00	69.00	96.00	69.57	42.00	49.00	84.00	50.56
	C1b	69.00	74.00	99.00	75.11	62.00	69.00	96.00	69.57	42.00	49.00	84.00	50.56
Selectivity	S1	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
	S2	0.57	0.91	0.19		0.54	0.92	0.20		0.49	0.88	0.26	
Atom Economy	AE1	89.79	86.07	83.55	85.80	89.79	86.07	83.55	85.80	89.79	86.07	83.55	85.80
	AE2	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00
	AE2 (glycine)	60.40	51.72	46.84	51.17	60.40	51.72	46.84	51.17	60.40	51.72	46.84	51.17
Atom Utilization	AU	89.79	86.07	83.55	87.19	89.79	86.07	83.55	87.12	89.79	86.07	83.55	86.92
Stoichiometric Factor	SF	3.04	3.91	4.54	5.47	1.85	2.21	2.47	2.86	1.25	1.36	1.43	1.55
Maximum RME (Kernel's RME)	Kernel's RME	69.00	74.00	99.00	75.11	62.00	69.00	96.00	69.57	42.00	49.00	84.00	50.56
Curzon's RME	Curzon's RME 1	22.68	18.94	21.82	20.89	33.56	31.27	38.91	33.39	33.61	36.15	58.64	38.13
	Curzon's RME 2	22.68	18.94	21.82	13.72	33.56	31.27	38.91	24.36	33.61	36.15	58.64	32.68
Simple E-Factor	sEF				0.39				0.35				0.63
Simple E-Factor (account for pretreatment)	sEF (pretreatment)				20.05				21.63				29.96
Complex E-Factor	cEF				308.39				361.54				506.56
Complex E-Factor (account for pretreatment)	cEF (pretreatment)				328.05				382.82				535.89
Carbon Efficiency	CE1	10.04	10.77	14.41	11.13	18.04	20.08	27.94	20.70	24.45	28.52	48.89	30.56
	CE2	0.12	0.16	0.08	0.35	0.21	0.29	0.15	0.66	0.29	0.41	0.27	0.97
Mass Intensity	MI	4.41	5.28	4.58	4.79	2.98	3.20	2.57	3.00	2.98	2.77	1.71	2.62
Mass Intensity (account for pretreatment)	MI (pretreatment)				24.45				24.27				31.95
Process Mass Intensity	PMI1				1.39				1.35				1.63
	PMI2				73431.22				39733.14				27384.13
Process Mass Intensity (account for	PMI1 (pretreatment)				21.05				22.63				30.96

pretreatment)	PMI2 (pretreatment)				73450.88				39754.42				27413.46
Mass productivity	MP1				0.21				0.33				0.38
	MP2				0.72				0.74				0.61
Mass productivity (account for pretreatment)	MP1 (pretreatment)				0.04				0.04				0.03
	MP2 (pretreatment)				0.05				0.04				0.03
Solvent intensity	SI				73426.43				39730.14				27381.51
Solvent intensity (account for pretreatment)	SI (pretreatment)				73446.09				39751.42				27410.84

Table S5 Green chemistry metrics for cyanide limiting reactions for *P. fluorescens* at pulp density 1 %w/v, *B. megaterium* at pulp density 1 % w/v, and *C. violaceum* at pulp densities 4 % w/v

Limiting Reagent (Cyanide)													
		***P. fluorescens* (1 % w/v)**				***B. megaterium* (1 % w/v)**				***C. violaceum* (4 % w/v)**			
		Pt	**Pd**	**Rh**	**Overall**	**Pt**	**Pd**	**Rh**	**Overall**	**Pt**	**Pd**	**Rh**	**Overall**
Percentage Yield	Y1	12.09	19.58	23.04	54.70	12.28	20.13	24.02	56.44	12.94	18.03	12.57	43.53
	Y2	38.61	44.71	92.47	54.70	39.24	45.97	96.43	56.44	34.92	39.58	72.18	43.53
Effective Mass Yield	YE	2.94	3.35	3.24	9.52	2.71	3.12	3.06	8.89	0.96	0.93	0.54	2.43
Percentage Conversion	C1a	38.61	44.71	92.47	54.70	39.24	45.97	96.43	56.44	34.92	39.58	72.18	43.53
	C1b	38.61	44.71	92.47	54.70	39.24	45.97	96.43	56.44	34.92	39.58	72.18	43.53
	C2				94.72				95.03				97.82
Selectivity	S1	0.13	0.21	0.24	0.58	0.13	0.21	0.25	0.59	0.13	0.18	0.13	0.45
	S2	0.35	0.71	0.49		0.34	0.71	0.49		0.49	0.85	0.27	
Atom Economy	AE1	89.79	86.07	83.55	85.80	89.79	86.07	83.55	85.80	89.79	86.07	83.55	85.80
	AE2	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00
	AE2 (Glycine)	60.40	51.72	46.84	51.17	60.40	51.72	46.84	51.17	60.40	51.72	46.84	51.17
Atom Utilization	AU	89.79	86.07	83.55	86.29	89.79	86.07	83.55	86.26	89.79	86.07	83.55	86.91
Stoichiometric Factor	SF	1.01	1.01	1.01	1.01	1.08	1.06	1.05	1.07	1.11	1.08	1.06	1.09
Maximum RME (Kernel's RME)	Kernel's RME	38.61	44.71	92.47	54.70	39.24	45.97	96.43	56.44	34.92	39.58	72.18	43.53
Curzon's RME	Curzon's RME 1	38.21	44.35	91.88	50.76	36.37	43.32	91.99	49.45	31.55	36.55	67.75	38.04
	Curzon's RME 2	38.21	44.35	91.89	54.22	36.37	43.32	92.04	52.94	31.55	36.55	67.80	39.87
Simple E-Factor	sEF				0.61				0.69				1.05
Simple E-Factor (account for pretreatment)	sEF (pretreatment)				11.11				11.94				42.29
Complex E-Factor	cEF				261.05				279.80				731.41
Complex E-Factor (account for pretreatment)	cEF (pretreatment)				271.55				291.05				772.65
Carbon Efficiency	CE	38.61	44.71	92.47	54.70	39.24	45.97	96.43	56.44	34.92	39.58	72.18	43.53
	CE (glycine)	0.22	0.36	0.43	1.01	0.21	0.34	0.40	0.94	0.41	0.57	0.40	1.38
Mass Intensity	MI	2.62	2.25	1.09	1.97	2.75	2.31	1.09	2.02	3.17	2.74	1.48	2.63

Mass Intensity (account for pretreatment)	MI (pretreatment)				12.47				13.28				43.86
Process Mass Intensity	PMI1				1.61				1.69				2.05
	PMI2				27773.06				29767.62				19250.40
Process Mass Intensity (account for pretreatment)	PMI1 (pretreatment)				12.11				12.94				43.29
	PMI2 (pretreatment)				27783.56				29778.88				19291.60
Mass productivity	MP1				0.51				0.49				0.38
	MP2				0.62				0.59				0.49
Mass productivity (account for pretreatment)	MP1 (pretreatment)				0.08				0.08				0.02
	MP2 (pretreatment)				0.08				0.08				0.02
Solvent intensity	SI				27771.09				29765.60				19247.70
Solvent intensity (account for pretreatment)	SI (pretreatment)				27781.59				29776.85				19289.00

Table S6 Green chemistry metrics for cyanide limiting reactions (Rh99) for *P. fluorescens* and *B. megaterium* at pulp density 2 % w/v

Limiting Reagent (Cyanide) (Rh99)									
		***P. fluorescens* (2 % w/v)**				***B. megaterium* (2 % w/v)**			
		Pt	**Pd**	**Rh**	**Overall**	**Pt**	**Pd**	**Rh**	**Overall**
Percentage Yield	Y1	19.08	32.04	42.02	93.14	19.65	31.42	43.02	94.09
	Y2	79.55	95.45	99.00	93.14	83.38	95.29	99.00	94.09
Effective Mass Yield	YE	2.32	2.74	2.95	8.01	2.17	2.43	2.74	7.34
Percentage Conversion	C1a	79.55	95.45	99.00	93.14	83.38	95.29	99.00	94.09
	C1b	79.55	95.45	99.00	93.14	83.38	95.29	99.00	94.09
	C2				95.41				96.31
Selectivity	S1	0.20	0.34	0.44	0.98	0.20	0.33	0.45	0.98
	S2	0.32	0.68	0.55		0.33	0.65	0.56	
Atom Economy	AE1	89.79	86.07	83.55	85.80	89.79	86.07	83.55	85.80
	AE2	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00
	AE2 (Glycine)	60.40	51.72	46.84	51.17	60.40	51.72	46.84	51.17
Atom Utilization	AU	89.79	86.07	83.55	86.14	89.79	86.07	83.55	86.15
Stoichiometric Factor	SF	2.08	1.83	1.08	1.66	2.29	2.00	1.11	1.78
Maximum RME (Kernel's RME)	Kernel's RME	79.55	95.45	99.00	93.14	83.38	95.29	99.00	94.09
Curzon's RME	Curzon's RME 1	38.30	52.06	91.95	55.13	36.41	47.68	88.90	51.92
	Curzon's RME 2	38.30	52.06	91.95	56.20	36.41	47.68	88.90	52.72
Simple E-Factor	sEF				0.80				0.91
Simple E-Factor (account for pretreatment)	sEF (pretreatment)				13.28				14.54
Complex E-Factor	cEF				313.62				342.35
Complex E-Factor (account for pretreatment)	cEF (pretreatment)				326.10				355.97
Carbon Efficiency	CE	79.55	95.45	99.00	93.14	83.38	95.29	99.00	94.09
	CE (glycine)	0.35	0.59	0.78	1.72	0.33	0.53	0.72	1.57
Mass Intensity	MI	2.74	2.08	0.84	1.81	2.88	2.27	0.86	1.93
Mass Intensity (account for pretreatment)	MI (pretreatment)				14.29				15.55
Process Mass Intensity	PMI1				1.80				1.91
	PMI2				16507.98				18020.30
Process Mass Intensity (account for pretreatment)	PMI1 (pretreatment)				14.28				15.54

	PMI2 (pretreatment)				16520.46				18033.90
Mass productivity	MP1				0.55				0.52
	MP2				0.55				0.52
Mass productivity (account for pretreatment)	MP1 (pretreatment)				0.07				0.06
	MP2 (pretreatment)				0.07				0.06
Solvent intensity	SI				16506.17				18018.40
Solvent intensity (account for pretreatment)	SI (pretreatment)				16518.65				18032.00

Table S7 Correlation between green chemistry metrics for metal limiting reactions

Pulp density and bacteria	Product	Metal limiting reactions							
P. fluorescens (0.5 % w/v)	Individual	Y = C1a = C1b = Kernel's RME	S1 > S2	Curzon's RME1 = Curzon's RME2	AE1 < AE2	sEF < cEF	CE1 > CE2	PMI1 < MI < PMI2	MPI < MP2
P. fluorescens (0.5 % w/v)	Overall	Y = C1a = C1b = Kernel's RME		Curzon's RME1 > Curzon's RME2	AE1 < AE2	sEF < cEF	CE1 > CE2	PMI1 < MI < PMI2	MPI < MP2
B. megaterium (0.5 % w/v)	Individual	Y = C1a = C1b = Kernel's RME	S1 > S2	Curzon's RME1 = Curzon's RME2	AE1 < AE2	sEF < cEF	CE1 > CE2	PMI1 < MI < PMI2	MPI < MP2
B. megaterium (0.5 % w/v)	Overall	Y = C1a = C1b = Kernel's RME		Curzon's RME1 > Curzon's RME2	AE1 < AE2	sEF < cEF	CE1 > CE2	PMI1 < MI < PMI2	MPI < MP2
C. violaceum (0.5 % w/v)	Individual	Y = C1a = C1b = Kernel's RME	S1 > S2	Curzon's RME1 = Curzon's RME2	AE1 < AE2	sEF < cEF	CE1 > CE2	PMI1 < MI < PMI2	MPI < MP2
C. violaceum (0.5 % w/v)	Overall	Y = C1a = C1b = Kernel's RME		Curzon's RME1 > Curzon's RME2	AE1 < AE2	sEF < cEF	CE1 > CE2	PMI1 < MI < PMI2	MPI < MP2
C. violaceum (1 % w/v)	Individual	Y = C1a = C1b = Kernel's RME	S1 > S2	Curzon's RME1 = Curzon's RME2	AE1 < AE2	sEF < cEF	CE1 > CE2	PMI1 < MI < PMI2	MPI < MP2
C. violaceum (1 % w/v)	Overall	Y = C1a = C1b = Kernel's RME		Curzon's RME1 > Curzon's RME2	AE1 < AE2	sEF < cEF	CE1 > CE2	PMI1 < MI < PMI2	MPI < MP2
C. violaceum (2 % w/v)	Individual	Y = C1a = C1b = Kernel's RME	S1 > S2	Curzon's RME1 = Curzon's RME2	AE1 < AE2	sEF < cEF	CE1 > CE2	PMI1 < MI < PMI2	MPI < MP2
C. violaceum (2 % w/v)	Overall	Y = C1a = C1b = Kernel's RME		Curzon's RME1 > Curzon's RME2	AE1 < AE2	sEF < cEF	CE1 > CE2	PMI1 < MI < PMI2	MPI < MP2

Table S8 Correlation between green chemistry metrics for cyanide limiting reactions

Pulp density and bacteria	Product	Cyanide limiting reactions							
P. fluorescens (1 % w/v)	Individual	Y2 = C1a = C1b = Kernel's RME = CE	S1 < S2	Curzon's RME1 = Curzon's RME2	AE1 < AE2	sEF < cEF	CE1 > CE2	PMI1 < MI < PMI2	MPI < MP2
P. fluorescens (1 % w/v)	Overall	Y2 = C1a = C1b = Kernel's RME = CE		Curzon's RME1 < Curzon's RME2	AE1 < AE2	sEF < cEF	CE1 > CE2	PMI1 < MI < PMI2	MPI < MP2
B. megaterium (1 % w/v)	Individual	Y2 = C1a = C1b = Kernel's RME = CE	S1 < S2	Curzon's RME1 = Curzon's RME2	AE1 < AE2	sEF < cEF	CE1 > CE2	PMI1 < MI < PMI2	MPI < MP2
B. megaterium (1 % w/v)	Overall	Y2 = C1a = C1b = Kernel's RME = CE		Curzon's RME1 < Curzon's RME2	AE1 < AE2	sEF < cEF	CE1 > CE2	PMI1 < MI < PMI2	MPI < MP2
C. violaceum (4 % w/v)	Individual	Y2 = C1a = C1b = Kernel's RME = CE	S1 < S2	Curzon's RME1 = Curzon's RME2	AE1 < AE2	sEF < cEF	CE1 > CE2	PMI1 < MI < PMI2	MPI < MP2
C. violaceum (4 % w/v)	Overall	Y2 = C1a = C1b = Kernel's RME = CE		Curzon's RME1 < Curzon's RME2	AE1 < AE2	sEF < cEF	CE1 > CE2	PMI1 < MI < PMI2	MPI < MP2
P. fluorescens (2 % w/v)	Individual	Y2 = C1a = C1b = Kernel's RME = CE	S1 < S2	Curzon's RME1 = Curzon's RME2	AE1 < AE2	sEF < cEF	CE1 > CE2	PMI1 < MI < PMI2	MPI < MP2
P. fluorescens (2 % w/v)	Overall	Y2 = C1a = C1b = Kernel's RME = CE		Curzon's RME1 < Curzon's RME2	AE1 < AE2	sEF < cEF	CE1 > CE2	PMI1 < MI < PMI2	MPI < MP2
B. megaterium (2 % w/v)	Individual	Y2 = C1a = C1b = Kernel's RME = CE	S1 < S2	Curzon's RME1 = Curzon's RME2	AE1 < AE2	sEF < cEF	CE1 > CE2	PMI1 < MI < PMI2	MPI < MP2
B. megaterium (2 % w/v)	Overall	Y2 = C1a = C1b = Kernel's RME = CE		Curzon's RME1 < Curzon's RME2	AE1 < AE2	sEF < cEF	CE1 > CE2	PMI1 < MI < PMI2	MPI < MP2

Detailed explanation on the cyanide split in:

The steps regarding the splitting of cyanide are explained using the results of *P. fluorescens* at 1 % w/v pulp density. Once the limiting reagent is determined, the percentage difference between the initial number of moles of free cyanide present in the system and the theoretical number of moles of cyanide required for the complete reaction of Pt, Pd and Rh was calculated. The percentage difference was found to be -1.59 %, implying that the amount of cyanide split between the PGM should give a percentage yield which is slightly higher than the percentage recovery of each metal. Hence, to obtain the number of moles of cyanide available for each metal, the theoretical number of moles of cyanide required for the complete reaction of each metal was reduced proportionately by the percentage difference. This approach was used for all metal-limiting reactions and when the percentage difference was less than -15 % for cyanide-limiting reactions.

However, the method was modified for cyanide-limiting reactions with large percentage differences namely, *P. fluorescens* at 2 % w/v pulp density and *B. megaterium* 2 % w/v pulp density. If the aforementioned method of splitting was used for these two experiments, the percentage yield of Rh would be 100 % (Table 3, Part 1). A percentage yield of 100 % was obtained because the number of moles of cyanide allocated to Rh was not sufficient. Since having a percentage yield equal to 100 % is not realistic from a practical perspective, an alternative method was conducted which is shown in Table 3, Part 2. The percentage yield of Rh was assumed to be 99 % (named "Rh99") as Rh has the highest percentage recovery among the three bacteria. Emphasis was also given to Rh because Rh requires 6 moles of cyanide to react with one mole of Rh while Pt and Pd each only require 4 moles of cyanide for one mole of the metal. After determining the number of moles of cyanide allocated to Rh using the percentage yield equation, the number of moles of free cyanide left was calculated. To split the cyanide to Pt and Pd, E1 and E2 were used as shown in Table 3, Part 1.