Towards net-zero adsorbents: A multi-factor selection approach considering performance, life cycle assessment, and end-of-life scenarios

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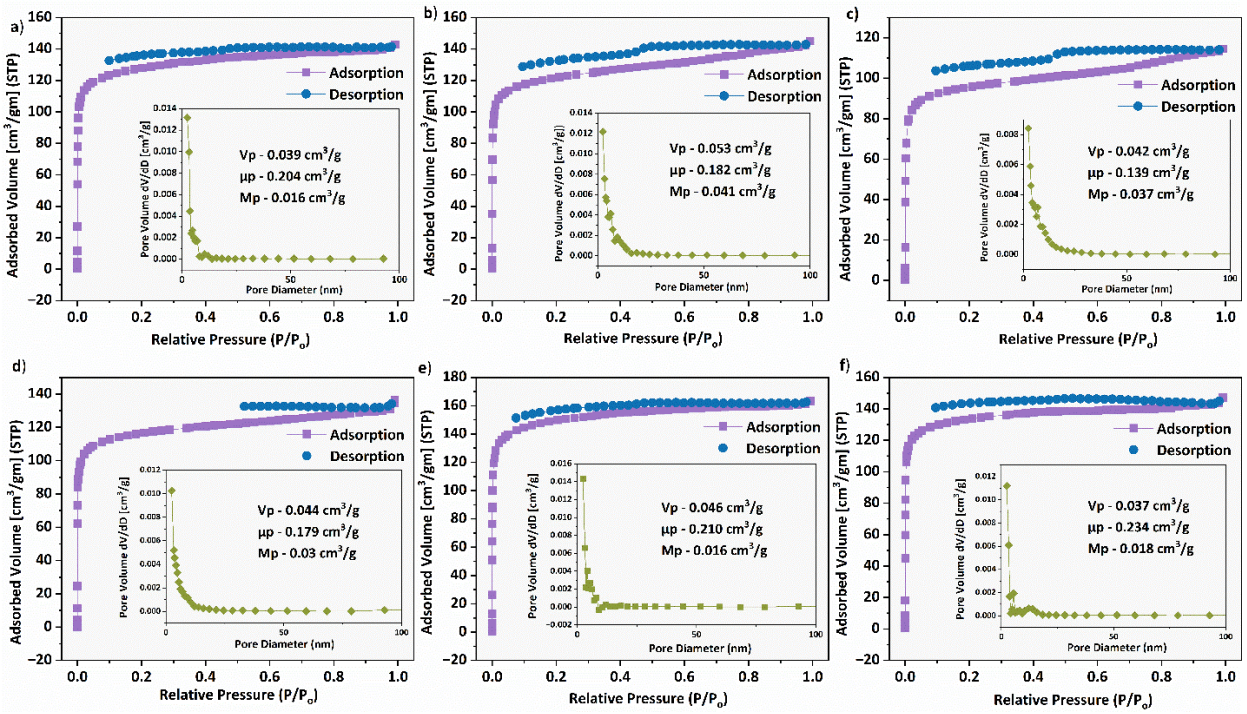

Fig. S1. N_2 adsorption desorption isotherm and pore size distribution with values of Vp (pore volume), μp (micropore volume) and Mp (mesopore volume) of (a) PB-N, (b) PB-H, (c) PB-NH, (d) PB-HN, (e) PB pristine and (f) PB-P.

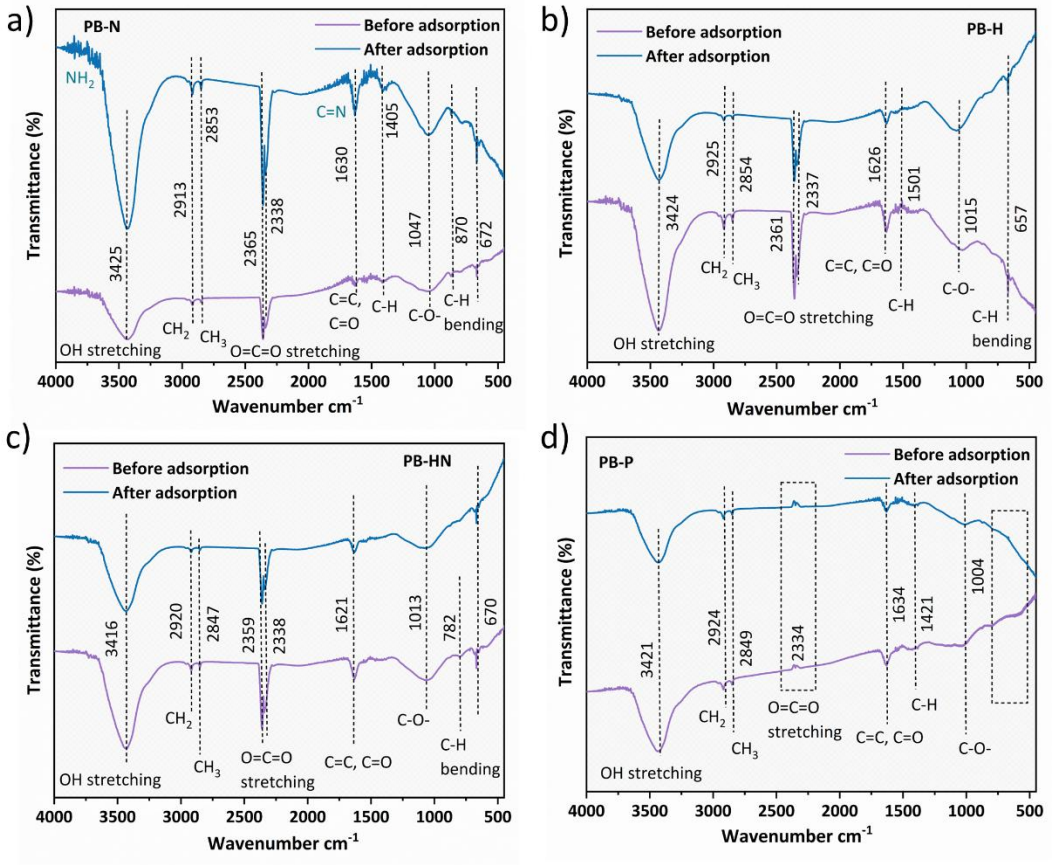

Fig. S2. FTIR analysis before and after adsorption for (a) PB-N, (b) PB-H, (c) PB-HN and (d) PB-P.

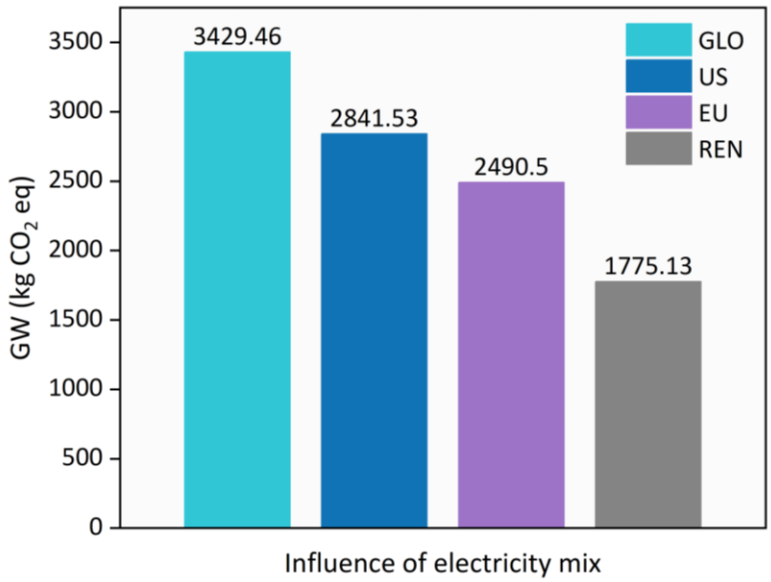

Fig S3. Influence of electricity mix on GW impact

Table S1. LCI consisting of inputs and outputs for the synthesis of PB-N, PB-H, PB-NH, PB-HN and PB-P.

Major Steps	Inputs	Outputs	Amt	Unit	Corresponding input from Ecoinvent	Comments
	Pine bark		2.4	kg	Bark {GLO}| market for bark | Cut-off, S	The amount of precursor material required for 1 kg of biochar was standardized based on the yield.
	DI water		4.92	L	Water, deionised {RoW}| market for water, deionised | Cut-off, S	
	Electricity (Oven, 6h, 120°)		9	kWh	Electricity, medium voltage {GLO}| market group for electricity, medium voltage | Cut-off, S	To remove moisture. DS-520M 1400-watt
Pretreatment		Wastewater	3.94	L	Wastewater, average {RoW}| market for wastewater, average | Cut-off, S	
Pyrolysis	Electricity (Tube Furnace)		10.2	kWh	Electricity, medium voltage {GLO}| market group for electricity, medium voltage | Cut-off, S	For pyrolysis at heating rate 5°C/min)OTF-1200X-UL furnace 3000-watt power.
	N2 gas (Flow rate – 70m^3/h)		2.67	kg	Nitrogen, liquid {RoW}| market for nitrogen, liquid | Cut-off, S	As an inert gas for pyrolysis
		Released N_2 gas	2.67	kg	Ecoinvent	Released from the tube furnace
		Syngas	0.36	kg	Pyrolysis fuel gas {GLO}| market for pyrolysis fuel gas | Cut-off, S	Syngas can be used as a combustion fuel and can be considered as avoided emission.
		Biochar	1	kg	Ecoinvent	Major precursor for the chemical activation
		Bio-oil	0.96	kg	Pyrolysis fuel oil {GLO}| market for pyrolysis fuel oil | Cut-off, S	Bio-oil is an avoided emission/product due to its versatile applications
Acid treatment	NaOH (PB-N)		0.5	kg	Neutralising agent, sodium hydroxide-equivalent {RER}| sodium hydroxide to generic market for neutralising agent | Cut-off, S	
	HCl (PB-H)		1.67	kg	Hydrochloric acid, without water, in 30% solution state {RoW}| market for hydrochloric acid, without water.	
	NaOH + HCl (PB-NH)		0.5 +1.67	kg	Neutralising agent, sodium hydroxide-equivalent {RER}| sodium hydroxide to generic market for neutralising agent | Cut-off, S	
	HCl + NaOH (PB-HN)		1.67+ 0.5	kg	Hydrochloric acid, without water, in 30% solution state {RoW}| market for hydrochloric acid, without water	
	H_2O_2 (PB-P)		1.6	kg	Hydrogen peroxide, without water, in 50% solution state {RoW}| market for hydrogen peroxide, without water, in 50% solution state | Cut-off, S	
	Electricity (magnetic stirrer,3h& 6h)		0.4, 0.8	kWh	Electricity, medium voltage {GLO}| market group for electricity, medium voltage | Cut-off, S	MS-MP8 20-watt power hot plate
	DI water		24	L	Water, deionised {RoW}| market for water, deionised | Cut-off, S	For diluting and washing
		Wastewater	24.8	L	Wastewater, average {RoW}| market for wastewater, average | Cut-off, S	

Post activation drying	Electricity (Oven, 12 h)		18	kWh	Electricity, medium voltage {GLO}| market group for electricity, medium voltage | Cut-off, S	To remove the moisture content post washing. DS-520M 1400-watt
		PB adsorbent	1	kg		Measured dry weight
Adsorption	Electricity		1.12	kWh	Electricity, medium voltage {GLO}| market group for electricity, medium voltage | Cut-off, S	

Table S2. LCI of AR-KOH

Major Steps	Inputs	Outputs	Amt	Unit	Corresponding input from Ecoinvent	Comments
	Corn Straw		2.4	kg	Straw {RER}| market for straw | Cut-off, S	The amount of precursor material required for 1 kg of BC was standardized based on the yield.
	DI water		4.92	L	Water, deionised {RoW}| market for water, deionised | Cut-off, S	
	Electricity (Oven, 6h, 120°)		9	kWh	Electricity, medium voltage {GLO}| market group for electricity, medium voltage | Cut-off, S	To remove moisture. DS-520M 1400-watt
Pretreatment		Wastewater	3.94	L	Wastewater, average {RoW}| market for wastewater, average | Cut-off, S	
Pyrolysis	Electricity (Tube Furnace, 1 hr)		11.5	kWh	Electricity, medium voltage {GLO}| market group for electricity, medium voltage | Cut-off, S	For pyrolysis at heating rate 5°C/min)OTF-1200X-UL furnace 3000-watt power.
	N2 gas (Flow rate – 70m^3/h)		2.67	kg	Nitrogen, liquid {RoW}| market for nitrogen, liquid | Cut-off, S	As an inert gas for pyrolysis
		Released N_2 gas	2.67	kg	Ecoinvent	Released from the tube furnace
		Syngas	0.68	kg	Pyrolysis fuel gas {GLO}| market for pyrolysis fuel gas | Cut-off, S	Syngas can be used as a combustion fuel and can be considered as avoided emission.
		Biochar	0.56	kg	Ecoinvent	Major precursor for the chemical activation
		Bio-oil	1.13	kg	Pyrolysis fuel oil {GLO}| market for pyrolysis fuel oil | Cut-off, S	Bio-oil is an avoided emission/product due to its versatile applications
Acid treatment	KOH		0.84	kg	Potassium hydroxide {GLO}| market for potassium hydroxide | Cut-off, S	Chemical activation take 1:3 ratio with AC
	Electricity (magnetic stirrer,3 h)		0.4	kWh	Electricity, medium voltage {GLO}| market group for electricity, medium voltage | Cut-off, S	MS-MP8 20-watt power hot plate
	DI water		24	L	Water, deionised {RoW}| market for water, deionised | Cut-off, S	For diluting H2O2 concentration and washing
		Wastewater	24.8	L	Wastewater, average {RoW}| market for wastewater, average | Cut-off, S	Wastewater with high levels of H2O2
Post activation drying	Electricity (Oven, 12 h)		18	kWh	Electricity, medium voltage {GLO}| market group for electricity, medium voltage | Cut-off, S	To remove the moisture content post washing. DS-520M 1400-watt
		PB adsorbent	1	kg		Measured dry weight
Adsorption	Electricity		1.12	kWh	Electricity, medium voltage {GLO}| market group for electricity, medium voltage | Cut-off, S	

Table S3. LCI of AR-H_3PO_4

Major Steps	Inputs	Outputs	Amt	Unit	Corresponding input from Ecoinvent	Comments
	Palm kennel shells		2.4	kg	Palm kernel {GLO}| market for palm kernel meal | Cut-off, S	The amount of precursor material required for 1 kg of BC was standardized based on the yield.
	DI water		4.92	L	Water, deionised {RoW}| market for water, deionised | Cut-off, S	
	Electricity (Oven, 6h, 120°)		9	kWh	Electricity, medium voltage {GLO}| market group for electricity, medium voltage | Cut-off, S	To remove moisture. DS-520M 1400-watt
Pretreatment		Wastewater	3.94	L	Wastewater, average {RoW}| market for wastewater, average | Cut-off, S	
Pyrolysis	Electricity (Tube Furnace, 3 hr)		10.4	kWh	Electricity, medium voltage {GLO}| market group for electricity, medium voltage | Cut-off, S	For pyrolysis at heating rate 10°C/min)OTF-1200X-UL furnace 3000-watt power.
	N2 gas (Flow rate – 70m^3/h)		2.67	kg	Nitrogen, liquid {RoW}| market for nitrogen, liquid | Cut-off, S	As an inert gas for pyrolysis
		Released N_2 gas	2.67	kg	Ecoinvent	Released from the tube furnace
		Syngas	0.77	kg	Pyrolysis fuel gas {GLO}| market for pyrolysis fuel gas | Cut-off, S	Syngas can be used as a combustion fuel and can be considered as avoided emission.
		Biochar	0.86	kg	Ecoinvent	Major precursor for the chemical activation
		Bio-oil	0.77	kg	Pyrolysis fuel oil {GLO}| market for pyrolysis fuel oil | Cut-off, S	Bio-oil is an avoided emission/product due to its versatile applications
Acid treatment	H3PO4		1.68	kg	Phosphoric acid, industrial grade, without water, in 85% solution state {GLO}| market for phosphoric acid, industrial grade, without water, in 85% solution state | Cut-off, S	Chemical activation take 1:3 ratio with AC
	Electricity (magnetic stirrer,3 h)		0.4	kWh	Electricity, medium voltage {GLO}| market group for electricity, medium voltage | Cut-off, S	MS-MP8 20-watt power hot plate
	DI water		24	L	Water, deionised {RoW}| market for water, deionised | Cut-off, S	For diluting H2O2 concentration and washing
		Wastewater	26.8	L	Wastewater, average {RoW}| market for wastewater, average | Cut-off, S	Wastewater with high levels of H2O2
Post activation drying	Electricity (Oven, 12 h)		18	kWh	Electricity, medium voltage {GLO}| market group for electricity, medium voltage | Cut-off, S	To remove the moisture content post washing. DS-520M 1400-watt
		PB adsorbent	1	kg		Measured dry weight
Adsorption	Electricity		1.12	kWh	Electricity, medium voltage {GLO}| market group for electricity, medium voltage | Cut-off, S	

Table S4. LCI of AR-Steam

Major Steps	Inputs	Outputs	Amt	Unit	Corresponding input from Ecoinvent	Comments
	Saw dust		2.4	kg	Sawdust, loose, wet, measured as dry mass {GLO}| market for sawdust, loose, wet, measured as dry mass | Cut-off, S	The amount of precursor material required for 1 kg of BC was standardized based on the yield.
	DI water		4.92	L	Water, deionised {RoW}| market for water, deionised | Cut-off, S	
	Electricity (Oven, 6h, 120°C)		9	kWh	Electricity, medium voltage {GLO}| market group for electricity, medium voltage | Cut-off, S	To remove moisture. DS-520M 1400-watt
Pretreatment		Wastewater	3.94	L	Wastewater, average {RoW}| market for wastewater, average | Cut-off, S	
Pyrolysis	Electricity (Tube Furnace, 2h,700°C)		12.6	kWh	Electricity, medium voltage {GLO}| market group for electricity, medium voltage | Cut-off, S	For pyrolysis at heating rate 5°C/min)OTF-1200X-UL furnace 3000-watt power.
	N2 gas (Flow rate – 70m^3/h)		2.67	kg	Nitrogen, liquid {RoW}| market for nitrogen, liquid | Cut-off, S	As an inert gas for pyrolysis
		Released N_2 gas	2.67	kg	Ecoinvent	Released from the tube furnace
		Syngas	0.77	kg	Pyrolysis fuel gas {GLO}| market for pyrolysis fuel gas | Cut-off, S	Syngas can be used as a combustion fuel and can be considered as avoided emission.
		Biochar	0.57	kg	Ecoinvent	Major precursor for the chemical activation
		Bio-oil	1.05	kg	Pyrolysis fuel oil {GLO}| market for pyrolysis fuel oil | Cut-off, S	Bio-oil is an avoided emission/product due to its versatile applications
Acid treatment	Steam		0.3	kg	Steam, in chemical industry {RoW}| market for steam, in chemical industry | Cut-off, S	Chemical activation take 1:3 ratio with AC
	Electricity (activation, 1h, 700°C)		3	kWh	Electricity, medium voltage {GLO}| market group for electricity, medium voltage | Cut-off, S	For pyrolysis at heating rate 5°C/min)OTF-1200X-UL furnace 3000-watt power.
	DI water		24	L	Water, deionised {RoW}| market for water, deionised | Cut-off, S	For diluting H2O2 concentration and washing
		Wastewater	26.8	L	Wastewater, average {RoW}| market for wastewater, average | Cut-off, S	Wastewater with high levels of H2O2
Adsorption	Electricity		1.12	kWh	Electricity, medium voltage {GLO}| market group for electricity, medium voltage | Cut-off, S	

Table S5. LCI of AR-CO_2

Major Steps	Inputs	Outputs	Amt	Unit	Corresponding input from Ecoinvent	Comments
	Barley malt bagasse		2.4	kg	Bagasse, from sugarcane {RoW}| market for bagasse, from sugarcane | Cut-off, S	The amount of precursor material required for 1 kg of BC was standardized based on the yield.
	DI water		4.92	L	Water, deionised {RoW}| market for water, deionised | Cut-off, S	
	Electricity (Oven, 6h, 120°C)		9	kWh	Electricity, medium voltage {GLO}| market group for electricity, medium voltage | Cut-off, S	To remove moisture. DS-520M 1400-watt
Pretreatment		Wastewater	3.94	L	Wastewater, average {RoW}| market for wastewater, average | Cut-off, S	
Pyrolysis	Electricity (Tube Furnace, 1h,800°C)		7.2	kWh	Electricity, medium voltage {GLO}| market group for electricity, medium voltage | Cut-off, S	For pyrolysis at heating rate 10°C/min) OTF-1200X-UL furnace 3000-watt power.
	N2 gas (Flow rate – 70m^3/h)		2.67	kg	Nitrogen, liquid {RoW}| market for nitrogen, liquid | Cut-off, S	As an inert gas for pyrolysis
		Released N_2 gas	2.67	kg	Ecoinvent	Released from the tube furnace
		Syngas	1.3	kg	Pyrolysis fuel gas {GLO}| market for pyrolysis fuel gas | Cut-off, S	Syngas can be used as a combustion fuel and can be considered as avoided emission.
		Biochar	0.6	kg	Ecoinvent	Major precursor for the chemical activation
		Bio-oil	0.5	kg	Pyrolysis fuel oil {GLO}| market for pyrolysis fuel oil | Cut-off, S	Bio-oil is an avoided emission/product due to its versatile applications
Acid treatment	CO2		9	kg	Carbon dioxide, liquid {RoW}| market for carbon dioxide, liquid | Cut-off, S	Chemical activation take 1:3 ratio with AC
	Electricity (activation, 1h, 900°C)		3.1	kWh	Electricity, medium voltage {GLO}| market group for electricity, medium voltage | Cut-off, S	For pyrolysis at heating rate of 5°C/min) OTF-1200X-UL furnace 3000-watt power.
	DI water		24	L	Water, deionised {RoW}| market for water, deionised | Cut-off, S	For diluting H2O2 concentration and washing
		Wastewater	26.8	L	Wastewater, average {RoW}| market for wastewater, average | Cut-off, S	Wastewater with high levels of H2O2
Adsorption	Electricity		1.12	kWh	Electricity, medium voltage {GLO}| market group for electricity, medium voltage | Cut-off, S	

Table S6. LCI inventory of IS-1000

Sl No	Input values	Quantity	Unit
	Precursors/Solvents		
1	Pine bark	2400	kg
2	Activator (NaOH+HCl)	500+1600	kg
3	DI water (pretreatment)	4428	kg
4	DI water (activation)	21600	kg
5	Nitrogen gas	2016	kg
	Energy		
6	Grinding	18+12	kWh
7	Drying (pretreatment)	513	kWh
8	Drying (Post activation)	648	kWh
	Cp, liq	3149.8	Kg
	Mliq	787.2	Kg
	Tboil	80	°C
	T0	25	°C
	hdry	0.8	kJ/mol
	Evaporization enthalpy (delta)	40.65	kJ/kg
	Hvap	2260	Kg
	mvap	734.79	
	Qdry	2439233340	J
	$Q_{dry} = \frac{C_{p,liq} \times m_{liq} \times (T_{boil} - T_0) + \Delta H_{vap} \times m_{vap}}{h_{dry}}$		
9	Stirring	220+76	kWh
10	Pyrolysis		
	Heating rate	10	°C/min
	Cp (dry PB)	1.8	KJ/kg
	Mmix (dry biomass weight)	2500	
	Tr (pyrolysis temperature)	840	°C
	T0 (initial temperature)	25	°C
	Tout (outside temperature)	25	°C
	A (surface area of the pyrolysis reactor)	17.25	m2
	S	0.075	M
	Ka	0.16	W/mK
	A*ka/s	36.8	W/K
	T (time for energy)	4.04	min
	Efficiency of heating element	0.77	
	Qreact	947.7	kWh
$Q_{react} = \frac{Q_{heat} + Q_{loss}}{h_{heat}} = \frac{C_p \times m_{mix} \times (T_r - T_0) + A \times \frac{k_a}{S}(T_r - T_{out}) \times t}{h_{heat}}$			
11	Filtration	5.54	kWh

12	Pumping (Pretreatment)	1.1	kWh
13	Pumping (activation)	1.6	kWh
14	Pumping (adsorption – tertiary treatment in WWTP)	2.7	kWh
15	Pumping (backwashing)	2.7	kWh
$E_{pump} = \frac{m \times g \times \Delta h}{\eta_{pump}}$			

Table S7. LCI inventory of EoL scenarios such as landfill, incineration and regeneration

Disposal method	Inventory	Unit	Quantity
Landfill	*Input*		
	Electricity	kWh	132.35
	Output		
	CH_4	kg	31.1
	CO_2	kg	0.058
	NO_2	kg	69.8
Incineration	*Input*		
	Electricity	kWh	13.79
	Lime	kg	10.2
	NaOH	kg	1.96
	Output		
	Electricity	kWh	125.05
	CO2	kg	357.73
	CO	kg	0.4
	NO2	kg	1.6
	Flyash/bottom ash	kg	250
Steam regeneration	*Input*		
	Natural gas	m^3	216
	Electricity	kWh	452.2
	Water	kg	3045
	Steam	kg	720
	Outputs		
	CO_2	kg	498.66
	CO	kg	0.39
	NO_2	kg	1.47
	Regenerated AC	kg	864
Thermal regeneration	*Input*		
	Natural gas	m^3	314
	Electricity	kWh	196.62
	Water	kg	1047.3
	$Ca(OH)_2$	kg	3.5
	NaOH	kg	3.5
	Outputs		
	CO_2	kg	869.7
	NO_2	kg	3.02
	SO_2	kg	0.5
	Regenerated AC	kg	762.8
Chemical regeneration	*Input*		
	KOH	kg	250
	Electricity (stirring+filtration+drying	kWh	729.54
	Water	kg	4400
	Outputs		
	CO_2	kg	498.66
	CO	kg	0.39
	NO_2	kg	1.47
	Regenerated AC	kg	800

Table S8. Kinetics and isotherm parameters of the PBAs

Kinetics							
		PB	**PB-P**	**PB-N**	**PB-HN**	**PB-H**	**PB-NH**
PFO	K1	0.0121	0.0126	0.0105	0.0147	0.0143	0.0134
	Qe (mg/g)	0.79373	0.64120	0.87985	1.86190	1.96108	2.11530
	R2	0.9885	0.9601	0.9733	0.9639	0.9882	0.9668
PSO	K2	0.01846	0.02206	0.02272	0.01078	0.00591	0.00593
	Qe (mg/g)	1.63612	0.70392	1.18161	0.98541	2.42600	2.46852
	R2	0.9862	0.9818	0.993	0.9815	0.9918	0.9957
Isotherm							
		PB	**PB-P**	**PB-N**	**PB-HN**	**PB-H**	**PB-NH**
Langmuir	KL	0.01756	0.01918	0.03558	0.01013	0.01210	0.00514
	Qmax	1.88964	3.63372	5.67536	6.69792	8	15.8478
	R2	0.9904	0.9927	0.9874	0.989	0.9946	0.9974
Freundlich	KF	0.17304	0.35519	1.07583	0.26767	0.48495	0.16342
	1/n	0.3887	0.3788	0.2704	0.5073	0.438	0.7411
	R2	0.9348	0.9587	0.944	0.9395	0.9269	0.9958

Table S9. Life cycle impacts of PBAs using ReCiPe Midpoint (H) method.

Impact category	**Unit**	**PB-N**	**PB-H**	**PB-NH**	**PB-HN**	**PB-P**
Global warming	kg CO2 eq	28.93984	30.17148	30.92121	30.92121	32.41225
Stratospheric ozone depletion	kg CFC11 eq	0.00001	0.00001	0.00001	0.00001	0.00001
Ionizing radiation	kBq Co-60 eq	3.46142	3.44485	3.59450	3.59450	3.47302
Ozone formation, Human health	kg NOx eq	0.06477	0.06767	0.06924	0.06924	0.07023
Fine particulate matter formation	kg PM2.5 eq	0.05797	0.06077	0.06194	0.06194	0.06161
Ozone formation, Terrestrial	kg NOx eq	0.06519	0.06819	0.06980	0.06980	0.07111
Terrestrial acidification	kg SO2 eq	0.09261	0.09856	0.10089	0.10089	0.09943
Freshwater eutrophication	kg P eq	0.01732	0.01782	0.01834	0.01834	0.01838
Marine eutrophication	kg N eq	0.00116	0.00119	0.00125	0.00125	0.00130
Terrestrial ecotoxicity	kg 1,4-DCB	69.50250	84.97747	90.46256	90.46256	86.81626
Freshwater ecotoxicity	kg 1,4-DCB	0.70012	0.81573	0.86206	0.86206	0.83361
Marine ecotoxicity	kg 1,4-DCB	0.99264	1.15291	1.21762	1.21762	1.18366
Human carcinogenic toxicity	kg 1,4-DCB	3.06448	3.30549	3.45936	3.45936	4.15534
Human non-carcinogenic toxicity	kg 1,4-DCB	26.17075	28.58951	29.65784	29.65784	29.20183
Land use	m2a crop eq	0.89038	0.91947	0.94354	0.94354	0.92751
Mineral resource scarcity	kg Cu eq	0.01942	0.02728	0.03005	0.03005	0.02534
Fossil resource scarcity	kg oil eq	5.53434	5.87188	6.06709	6.06709	6.55002
Water consumption	m3	0.21257	0.21725	0.22568	0.22568	0.31607

Table S10. Breakdown of impacts associated with PB-NH using the ReCiPe Midpoint (H) method.

Impact	Pine bark	DI water	E-Drying	E-Pyrolysis	N2 gas	NaOH	HCl	E-Stirring	DI water	E-drying	E-adsorption	Syngas	Bio-oil
GW	0.019458	0.002537	6.672922	7.562645	1.227759	0.453159	1.689952	0.593149	0.012375	13.345843	0.830408	-0.408597	-1.089591
SOD	0.000000	0.000000	0.000002	0.000002	0.000000	0.000000	0.000001	0.000000	0.000000	0.000004	0.000000	0.000000	0.000000
IR	0.000992	0.000143	0.760849	0.862296	0.095742	0.115825	0.099549	0.067631	0.000696	1.521698	0.094683	-0.007078	-0.018874
OFHH	0.000104	0.000006	0.015104	0.017117	0.002896	0.000894	0.003808	0.001343	0.000029	0.030207	0.001880	-0.001137	-0.003033
FPM	0.000032	0.000006	0.013110	0.014858	0.002427	0.000579	0.003391	0.001165	0.000030	0.026220	0.001631	-0.000416	-0.001110
OFTE	0.000113	0.000006	0.015398	0.017451	0.002947	0.000927	0.003944	0.001369	0.000030	0.030796	0.001916	-0.001395	-0.003719
TA	0.000062	0.000016	0.021120	0.023936	0.003881	0.001394	0.007371	0.001877	0.000076	0.042241	0.002628	-0.001020	-0.002719
FE	0.000011	0.000001	0.003788	0.004293	0.000664	0.000355	0.000856	0.000337	0.000006	0.007575	0.000471	-0.000056	-0.000151
ME	0.000001	0.000000	0.000207	0.000235	0.000035	0.000044	0.000081	0.000018	0.000001	0.000414	0.000026	-0.000012	-0.000033
TT	0.321114	0.032553	18.023052	20.426125	3.464667	4.684064	20.225206	1.602049	0.158797	36.046103	2.242869	-4.627445	-12.339852
FT	0.000492	0.000363	0.153546	0.174018	0.026920	0.039503	0.155847	0.013649	0.001768	0.307091	0.019108	-0.008592	-0.022912
MT	0.000977	0.000488	0.221175	0.250665	0.039086	0.054871	0.216143	0.019660	0.002381	0.442350	0.027524	-0.016257	-0.043352
HCT	0.007289	0.000834	0.712127	0.807077	0.133754	0.122213	0.364922	0.063300	0.004068	1.424253	0.088620	-0.074812	-0.199498
HNCT	0.011406	0.007380	5.767605	6.536619	1.037381	0.812001	3.245756	0.512676	0.036001	11.535210	0.717746	-0.171630	-0.457679
LU	0.372751	0.000075	0.120887	0.137005	0.021619	0.018700	0.047937	0.010745	0.000364	0.241773	0.015044	-0.011887	-0.031700
MRS	0.000068	0.000029	0.004620	0.005236	0.000821	0.002567	0.010482	0.000411	0.000141	0.009241	0.000575	-0.001147	-0.003060
FRS	0.005460	0.000617	1.652537	1.872875	0.299730	0.121767	0.460555	0.146892	0.003009	3.305074	0.205649	-0.547903	-1.461074
WC	0.000094	0.005098	0.039928	0.045251	0.027695	0.006658	0.021695	0.003549	0.024870	0.079855	0.004969	-0.001100	-0.002934

Table S11. Comparison of PB-NH against AR-KOH, AR-H3PO4, AR-Steam and AR-CO2 using ReCiPe Midpoint (H) method.

Impact category	**Unit**	**PB-NH**	**AR-KOH**	**AR-H3PO4**	**AR-Steam**	**AR-CO2**
Global warming	kg CO2 eq	30.92121	59.22112	36.94127	32.24212	53.71393
Stratospheric ozone depletion	kg CFC11 eq	1.10E-05	2.30E-05	1.56E-05	1.06E-05	1.09E-05
Ionizing radiation	kBq Co-60 eq	3.594496	6.740093	4.025843	3.924466	3.502064
Ozone formation, Human health	kg NOx eq	0.069237	0.13471	0.084008	0.071229	0.07283
Fine particulate matter formation	kg PM2.5 eq	0.061936	0.118964	0.083715	0.066587	0.066173
Ozone formation, Terrestrial ecosystems	kg NOx eq	0.069805	0.13539	0.084754	0.070551	0.072657
Terrestrial acidification	kg SO2 eq	0.100889	0.194889	0.156938	0.10438	0.109283
Freshwater eutrophication	kg P eq	0.018341	0.034993	0.023317	0.019883	0.019456
Marine eutrophication	kg N eq	0.001247	0.004359	0.003198	0.001198	0.001811
Terrestrial ecotoxicity	kg 1,4-DCB	90.46256	170.3031	137.3322	57.41251	173.1221
Freshwater ecotoxicity	kg 1,4-DCB	0.862059	1.622419	1.679416	0.747735	1.235501
Marine ecotoxicity	kg 1,4-DCB	1.217616	2.291091	2.33425	1.04397	1.694082
Human carcinogenic toxicity	kg 1,4-DCB	3.459357	6.793855	11.98383	3.177006	4.407695
Human non-carcinogenic toxicity	kg 1,4-DCB	29.65784	56.70032	47.20618	29.42088	35.70874
Land use	m2a crop eq	0.943541	3.712039	2.061959	1.140501	0.792706
Mineral resource scarcity	kg Cu eq	0.030052	0.057711	0.152444	0.014983	0.056422
Fossil resource scarcity	kg oil eq	6.067091	10.70161	6.635112	4.023746	4.741609
Water consumption	m3	0.225681	0.464329	0.482095	0.265631	0.299274

Table S12. Breakdown of impacts associated with IS1000.

Category	Total	PB	NaOH	HCl	DI water	N2 gas	E-Grinding	E-Drying (pre)	E-Drying (post)	E-Stirring	E-Pyrolysis	E-Filtration	E-Adsorption	Syngas	Bio-oil
GW	3429.46	19.46	453.16	1689.95	13.42	927.03	22.24	380.36	480.45	219.46	702.66	4.11	6.01	-408.60	-1089.59
SOD	0.00	0.00001	0.00020	0.00146	0.00001	0.00026	0.0000	0.00012	0.00015	0.00007	0.00023	0.0000	0.0000	-0.0001	-0.0002
IR	470.79	0.99199	115.8254	99.54874	0.75517	72.29034	2.5361	43.36840	54.78114	25.0234	80.11742	0.4683	0.6847	-7.0777	-18.8740
OFHH	6.98	0.10448	0.89387	3.80825	0.03097	2.18640	0.05035	0.86090	1.08745	0.49674	1.59040	0.0093	0.0135	-1.1374	-3.0331
FPM	7.92	0.03152	0.57885	3.39080	0.03297	1.83247	0.0437	0.74726	0.94391	0.43117	1.38046	0.0080	0.0118	-0.4163	-1.1101
OFTE	6.34	0.11285	0.92718	3.94359	0.03200	2.22538	0.0513	0.87768	1.10865	0.50642	1.62140	0.0094	0.0138	-1.3947	-3.7191
TA	13.87	0.06228	1.39361	7.37071	0.08207	2.93037	0.0704	1.20386	1.52066	0.69462	2.22397	0.0130	0.0190	-1.0196	-2.7190
FE	2.75	0.01092	0.35487	0.85611	0.00687	0.50119	0.0126	0.21590	0.27271	0.12457	0.39884	0.0023	0.0034	-0.0564	-0.1505
ME	0.40	0.00093	0.04432	0.08055	0.00058	0.02624	0.0006	0.01181	0.01492	0.00681	0.02182	0.0001	0.0001	-0.0123	-0.0328
TT	16161	321	4684	20225	172	2616	60	1027	1298	593	1898	11	16	-4627	-12340
FT	229.63	0.49193	39.50318	155.84727	1.91789	20.32599	0.5118	8.75210	11.05529	5.04995	16.16836	0.0945	0.1381	-8.5920	-22.9119
MT	306.58	0.97740	54.87134	216.14302	2.58227	29.51226	0.7372	12.60698	15.92461	7.27420	23.28974	0.1361	0.1990	-16.2568	-43.3515
HCT	524.54	7.28875	122.2132	364.92190	4.41223	100.9914	2.3737	40.59122	51.27312	23.4210	74.98693	0.4383	0.6409	-74.8119	-199.4983
HNCT	5899.7	11.4	812.0	3245.8	39.0	783.3	19.2	328.8	415.3	189.7	607.3	3.6	5.2	-171.6	-457.7
LU	445.64	372.75	18.70046	47.93652	0.39515	16.32365	0.4029	6.89053	8.70383	3.97582	12.72936	0.0744	0.1088	-11.8874	-31.6997
MRS	11.01	0.06806	2.56695	10.48219	0.15263	0.62026	0.0154	0.26336	0.33266	0.15196	0.48652	0.0028	0.004	-1.1473	-3.0595
FRS	-740.13	5.46	121.77	460.56	3.26	226.31	5.51	94.19	118.98	54.35	174.01	1.02	1.49	-547.90	-1461.07
WC	52.70	0.09378	6.65773	21.69458	26.9717	20.91098	0.1330	2.27587	2.87478	1.31317	4.20437	0.0245	0.0359	-1.1002	-2.9338

Table S13. Breakdown of impacts associated with landfilling, incineration and steam regeneration.

Category	Landfilling			Incineration						Steam Regeneration						
	Total	Emissions	Electricity	Total	Emissions	Electricity	Lime	NaOH	E-recovered	Total	Emissions	Natural gas	Electricity	Water	Steam	Recovered adsorbent
GW	1217.9	1119.65	98.2773	277.325	357.730	10.2244	0.43	1.652	-92.71	-1773.05	498.6600	127.6638	335.2777	1.5701	226.85	-2963.0560
SOD	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.00	0.000	0.0000	-0.0018	0.0000	0.0000	0.0001	0.0000	0.0000	-0.0019
IR	11.205	0.0000	11.2056	-9.0039	0.0000	1.1658	0.01	0.388	-10.57	-362.66	0.0000	1.0732	38.228	0.088	4.7049	-406.7610
OFHH	70.022	69.8000	0.2224	1.4182	1.6000	0.0231	0.00	0.003	-0.2099	-3.2193	1.4700	0.3040	0.7589	0.0036	0.2783	-6.0341
FPM	7.8711	7.6780	0.1931	0.0171	0.1760	0.0201	0.00	0.002	-0.1822	-5.8051	0.1617	0.0717	0.6587	0.0039	0.1419	-6.8430
OFTE	70.026	69.8000	0.2268	1.4147	1.6000	0.0236	0.00	0.003	-0.2139	-2.5360	1.4700	0.3873	0.7737	0.0037	0.3058	-5.4765
TA	25.439	25.1280	0.3111	0.3228	0.5760	0.0324	0.00	0.006	-0.2935	-9.8167	0.5292	0.1631	1.0612	0.0096	0.4058	-11.9857
FE	0.0558	0.0000	0.0558	-0.0454	0.0000	0.0058	0.00	0.001	-0.0526	-2.1452	0.0000	0.0093	0.1903	0.0008	0.0285	-2.3742
ME	0.0031	0.0000	0.0031	-0.0024	0.0000	0.0003	0.00	0.000	-0.0029	-0.3255	0.0000	0.0045	0.0104	0.0001	0.0035	-0.3439
TT	265.43	0.0000	265.439	-198.45	0.0000	27.6153	6.42	17.92	-250.42	-9702.48	0.0000	1581.10	905.55	20.147	1753.8	-13963.09
FT	2.2614	0.0000	2.2614	-1.6642	0.0000	0.2353	0.08	0.152	-2.1334	-187.709	0.0000	1.3121	7.7148	0.2244	1.4415	-198.4018
MT	3.2574	0.0000	3.2574	-2.4067	0.0000	0.3389	0.115	0.211	-3.0731	-246.266	0.0000	3.6130	11.1128	0.3021	3.5914	-264.8862
HCT	10.488	0.0000	10.4880	-8.2382	0.0000	1.0911	0.09	0.466	-9.8946	-380.168	0.0000	24.6468	35.78	0.5162	12.091	-453.2041
HNCT	84.944	0.0000	84.9440	-65.232	0.0000	8.8373	2.97	3.088	-80.137	-4731.46	0.0000	22.4044	289.79	4.5676	49.117	-5097.3415
LU	1.7804	0.0000	1.7804	-1.4012	0.0000	0.1852	0.01	0.076	-1.6797	-374.705	0.0000	1.7168	6.0739	0.0462	2.4889	-385.0313
MRS	0.0680	0.0000	0.0680	-0.0390	0.0000	0.0071	0.00	0.010	-0.0642	-8.8267	0.0000	0.3084	0.2321	0.0179	0.1264	-9.5116
FRS	24.338	0.0000	24.3382	-19.87	0.0000	2.5321	0.116	0.437	-22.961	1009.53	0.0000	212.712	83.03	0.3818	73.933	639.4726
WC	0.5880	0.0000	0.5880	-0.4531	0.0000	0.0612	0.01	0.030	-0.5548	-39.8595	0.0000	0.2424	2.0061	3.1554	0.2709	-45.5343

Table S14. Breakdown of impacts associated with thermal and chemical regeneration.

			Thermal regeneration							Chemical regeneration					
Category	Total	Unit	Emissions	Natural gas	Electricity	Water	$Ca(OH)_2$	NaOH	Rec. adsor.	Total	Emissions	KOH	Electricity	Water	Rec. adsor.
GW	-1455.57	kg CO2 eq	869.730	154.997	140.222	0.5072	3.3017	5.8073	-2630.14	-570.201	498.600	1167.19	520.283	2.1309	-2758.41
SOD	-0.0001	kg CFC-11	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0001	-0.0001	0.0000	0.0000	0.0000	0.0000	-0.0001
TA	-11.0047	kg SO2 eq	0.0000	0.2866	0.5265	0.0035	0.0032	0.0220	-11.8465	-4.7826	0.8232	4.8501	1.9535	0.0148	-12.4242
FE	-1.4961	kg P eq	0.0000	0.0101	0.0616	0.0002	0.0001	0.0017	-1.5697	-0.9451	0.0000	0.4717	0.2285	0.0009	-1.6462
ME	-0.7500	kg N eq	0.0000	0.0180	0.0270	0.0001	0.0001	0.0145	-0.8097	-0.4317	0.0573	0.2594	0.1003	0.0004	-0.8492
HT	-1639.97	kg 1,4-DB	0.0000	11.4424	47.0938	0.3944	0.1135	2.0266	-1701.04	-1115.3	0.0000	492.227	174.737	1.6570	-1784.00
POF	-0.5435	kg VOC	0.0000	1.3968	0.4137	0.0018	0.0051	0.0170	-2.3779	4.5644	1.4878	4.0277	1.5350	0.0077	-2.4939
PMF	-6.4932	kg PM10	0.0000	0.1373	0.3372	0.0014	0.0016	0.0095	-6.9802	-3.0210	0.3234	2.7191	1.2512	0.0059	-7.3206
TE	-0.7161	kg 1,4-DB	0.0000	0.0348	0.0059	0.0001	0.0001	0.0015	-0.7586	-0.6180	0.0000	0.1554	0.0217	0.0005	-0.7956
FE	-101.352	kg 1,4-DB	0.0000	0.6506	1.6353	0.0421	0.0037	0.1974	-103.881	-65.5011	0.0000	37.2016	6.0678	0.1767	-108.94
ME	-86.8933	kg 1,4-DB	0.0000	0.6287	1.4953	0.0369	0.0042	0.1734	-89.2319	-55.0864	0.0000	32.7938	5.5482	0.1552	-93.5835
IR	-389.603	kBq U235	0.0000	1.9935	19.4075	0.0358	0.0197	0.2983	-411.358	-248.050	0.0000	111.2092	72.0096	0.1505	-431.419
ALO	-1006.07	m2a	0.0000	0.6445	3.6330	0.0164	0.0048	0.2170	-1010.58	-996.173	0.0000	50.1501	13.4800	0.0688	-1059.8
ULO	-39.3244	m2a	0.0000	0.6433	1.1327	0.0095	0.0135	0.0733	-41.1966	-17.1231	0.0000	21.8401	4.2027	0.0398	-43.2057
NLT	0.2015	m2	0.0000	0.0682	0.0117	0.0001	0.0002	0.0006	0.1208	0.2253	0.0000	0.0548	0.0436	0.0002	0.1267
WD	-347.351	m3	0.0000	-240.248	-11.642	1.0341	-0.0116	-0.7316	-95.7509	-236.60	0.0000	-97.3306	-43.199	4.3444	-100.420
MD	-150.321	kg Fe eq	0.0000	10.4785	1.9895	0.1039	0.0197	0.5469	-163.460	-71.7967	0.0000	91.8169	7.3819	0.4366	-171.432
FD	-461.960	kg oil eq	0.0000	2.9514	22.8532	0.0533	0.0261	0.5761	-488.420	-268.371	0.0000	158.8499	84.7945	0.2241	-512.239

Table S15. Sensitivity analysis with ±5%, ±10% and ±15% variation in yield, electricity and activation agent.

Category	Baseline	Yield						Electricity						Activation					
		5	10	20	-5	-10	-20	5	10	20	-5	-10	-20	5	10	20	-5	-10	-20
GW	3429.463	3257.990	3086.517	2743.570	3600.936	3772.409	4115.356	3520.222	3610.989	3792.514	3338.696	3247.937	3066.412	3899.670	4006.826	4221.137	3322.308	3215.152	3000.841
SOD	0.002	0.002	0.002	0.002	0.002	0.002	0.003	0.002	0.002	0.002	0.002	0.002	0.002	0.002	0.003	0.003	0.002	0.002	0.002
IR	470.788	447.249	423.709	376.631	494.328	517.867	564.946	481.137	491.486	512.184	460.439	450.091	429.393	522.952	533.721	555.258	460.020	449.251	427.713
OFHH	6.984	6.635	6.286	5.587	7.333	7.682	8.381	7.189	7.395	7.806	6.778	6.573	6.162	8.041	8.276	8.746	6.749	6.514	6.043
FPM	7.920	7.524	7.128	6.336	8.316	8.712	9.504	8.098	8.277	8.633	7.742	7.564	7.207	8.832	9.030	9.427	7.722	7.523	7.126
OFTE	6.339	6.022	5.705	5.071	6.655	6.972	7.606	6.548	6.757	7.176	6.129	5.920	5.501	7.420	7.663	8.150	6.095	5.851	5.364
TA	13.872	13.179	12.485	11.098	14.566	15.260	16.647	14.160	14.447	15.021	13.585	13.298	12.723	15.460	15.898	16.774	13.434	12.996	12.119
FE	2.748	2.610	2.473	2.198	2.885	3.023	3.297	2.799	2.851	2.954	2.696	2.645	2.542	3.014	3.075	3.196	2.687	2.627	2.506
ME	0.398	0.378	0.358	0.318	0.418	0.438	0.478	0.401	0.404	0.409	0.395	0.392	0.387	0.416	0.422	0.434	0.392	0.386	0.373
TT	16160.985	15352.936	14544.887	12928.788	16969.034	17777.084	19393.182	16406.119	16651.272	17141.559	15915.832	15670.698	15180.411	18387.023	19632.486	22123.413	14915.522	13670.058	11179.131
FT	229.632	218.150	206.669	183.705	241.113	252.595	275.558	231.720	233.809	237.986	227.543	225.455	221.278	247.753	257.521	277.056	219.864	210.097	190.562
MT	306.581	291.252	275.923	245.265	321.910	337.239	367.898	309.589	312.598	318.615	303.573	300.565	294.548	332.165	345.716	372.818	293.031	279.480	252.378
HCT	524.542	498.315	472.088	419.633	550.769	576.996	629.450	534.228	543.914	563.286	514.855	505.170	485.797	587.643	612.000	660.713	500.185	475.828	427.115
HNCT	5899	5604.	5309	4719	6194	6489	7079	5978	6056	6213	5821	5742	5585	6416	6619	7025	5696	5493	5088
LU	445.6	423.3	401.0	356.5	467.9	490.2	534.7	447.2	448.9	452.2	443.9	442.3	439.0	455.5	458.8	465.5	442.3	438.9	432.3
MRS	11.009	10.45	9.908	8.807	11.559	12.110	13.211	11.07	11.134	11.260	10.94	10.88	10.75	11.913	12.56	13.87	10.35	9.704	8.399
FRS	-740.1	-703.1	-666.1	-592.1	-777.1	-814.1	-888.1	-717.6	-695.1	-650.2	-762.6	-785.0	-830.0	-621.1	-591.9	-533.7	-769.2	-798.3	-856.5