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Data Article

Dataset from analytical pyrolysis assays for converting waste tires into valuable chemicals in the presence of noble-metal catalysts

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ABSTRACT

About 25.7 million tons of waste tires (WT) are discarded each year worldwide causing important environmental, and health problems. This waste is difficult to manage and dispose due to its huge rate of generation and its extremely slow biodegradation. Therefore, many efforts are being made to valorise WTs into a series of marketable products under a circular economy framework. In the attempt to convert WT into higher-value products, thermochemical decomposition by pyrolysis has emerged as a promising process [1]. The pyrolysis is a thermochemical transformation (under an oxygen-depleted atmosphere) of the tireś polymeric constituents: natural rubber (NR), styrene-butadiene rubber (SBR), and butadiene rubber (BR) into three major fractions. These fractions are a gas (10–35%, TPG) which is usually used as a heat source (50 MJ kg^{-1}), a solid consisting mainly of recovered carbon black (12–45%, rCB), and a liquid fraction (35-65%, TPO) containing a complex mixture of organic compounds. Among the high-value compounds that can be found

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in the TPO are D,L-limonene, isoprene, benzene, toluene, mixed-xylene, ethylbenzene, styrene, p-cymene, and some polycyclic aromatic hydrocarbons. This mixture is commonly used as a diesel substitute and owing to its complex composition it rarely is seen as a source for more valuable products. To overcome such a complexity, and selectively produce specific chemical identities, different types of catalysts have been used [2,3].

Herein, we provide a dataset from a systematic study about catalytic pyrolysis of WT for selectively producing benzene, toluene, and xylenes (BTX) and p-cymene on noble metals (Pd, Pt, Au) supported on titanate nanotubes (NT-Ti). The comprehensive analysis of this data was recently published, thus, the analytical techniques, experimental conditions and dataset are given in the present paper as a complement to that publication [1]. The reaction was evaluated in an analytical pyrolysis unit consisting in a micropyrolizer coupled to a mass spectrometer (Py-GC/MS) operating at temperatures between 400 and 450 °C in a fast pyrolysis regime (12 s). The effectivity of catalysts was measured in terms of selectivity to monoaromatics as BTX and p-cymene, under non-catalytic and for catalytic pyrolysis conditions. Moreover, the reaction was conducted on individual rubbers (Polyisoprene, Polybutadiene, and Styrene-Butadiene) and DL-limonene, to get deep insights into the transformation behaviour and reaction pathways. Therefore, the reader will find a data-in-brief paper containing some characterizations of the WTs used for the investigation, along with a complete dataset of Py-GC/MS results. Finally, the original files for the interpretation of the MS results are also provided, so that the reader can easily use this information to further expand the study to their own interest (industrial or scientific).

Specifications Table

Subject	Chemistry: Chemical Engineering, Catalysis
Specific subject area	Conversion of wastes into valuable chemicals via catalytic fast pyrolysis.
Type of data	Tables and Figures
How the data were acquired	The data was measured in a micro-pyrolysis reactor (CDS5200, CDS Analytical Co Ltd.) coupled to a gas chromatograph (Clarus 690, Perkin Emer) equipped with a quadrupole mass detector (SQ8, Perkin Emer). The waste tires were characterized in an elemental analyser (CHNS 628, Leco) and thermogravimetric analysis (Netzsch, model STA 409 PC). Compound identification was done by comparison with the National Institute of Standards and Technology database (NIST, v2016) with the software TurboMass™ v5.4.
Data format	Raw (TurboMass files and *.xls files). Filtered (Tables with compounds ids, retention times, etc.).
Description of data collection	The experiments were done for waste tires coming from vehicles. Three metals Pd, Pt, Au deposited on titanate nanotubes (NT-Ti) were used as catalysts for fast pyrolysis. Experimental factors were the metal nature and reaction temperature (400 – 450 °C). Moreover, the pyrolysis was investigated for three individual polymers (polyisoprene, butadiene, and styrene-butadiene).
Data source location	Institution: Universidad del Bio-Bio City/Town/Region: Concepción/Concepción/Biobio Country: Chile

(*continued on next page*)

Data accessibility	All data can be accessed in the following MendeleyData repository. Repository name: Dataset for waste tire and constituent polymers pyrolysis on Me/NT-Ti (Me = Pd, Au, Pt). [4] Data identification number: doi: 10.17632/m72tyjb8nr.1 Direct URL to data: https://data.mendeley.com/datasets/m72tyjb8nr/1
Related research article	P. Osorio-Vargas, C.H. Campos, C.C. Torres, C. Herrera, K. Shanmugaraj, T.M. Bustamante, J.N. Diaz de Leon, F. Medina, L.E. Arteaga-Pérez, Catalytic pyrolysis of used tires on noble-metal-based catalysts to obtain high-value chemicals: Reaction pathways, Cat. Today. In Press.

Value of the Data

- Waste tire pyrolysis is a sustainable solution to the problems associated to WTs management and valorisation. Therefore, analytical data is of paramount importance to defining potential marketable products.
- Industrials and scientific groups devoted to the understanding and analysis of pyrolysis processes can benefit from this data, which includes regular and catalytic pyrolysis experiments of WTs and its constituent polymers.
- The data presented here can be used for expanding analysis on product distribution, kinetics and as a basis for scaling-up the process.

1. Data Description

Waste tire pyrolysis is attracting the attention of industrials and the scientific community worldwide, hence the availability of experimental data is mandatory for defining production strategies in a circular economy framework. Here we provide raw data (linked) and filtered results for analytical pyrolysis experiments.

1.1. Material characterization

This paper presents the composition, and the thermal characterization parameters -gathered from thermogravimetric analysis- for waste tires coming from light vehicles (Table 1 and Fig. 1). Moreover, the area-related composition of pyrolysis vapours produced from natural rubber (CAS N° 104389-31-3), butadiene rubber (CAS N° 9003-17-2) and styrene-butadiene rubber (CAS N° 9003-55-8) is also provided for two temperatures (400 °C and 450 °C) in Tables 2 and 3. Deconvolution of DTG curves allows estimating the polymeric composition of the tires which is fundamental to understand reaction pathways, thus the TGA data and characteristic DTG temperatures are also provided [5].

1.2. Catalytic pyrolysis assays

The Tables 4 to 5 presents the results of catalytic pyrolysis experiments for waste tires on Pd/NT-Ti, Pt/NT-Ti and Au/NT-Ti at 400 °C and 450 °C, respectively. Each table indicate the retention times, chromatographic area percentage and the assignation of compounds ids according to the comparison of the ionization patterns with the NIST database.

Supplementary datafiles: The Supplementary information to this manuscript includes raw data in (*.xls) format along with the original TruboMass v5.6 data files, both can be freely used by expert to re-process the results. In addition, TGA and DTG data are also included, which could

Table 1
Elemental and proximate composition of waste tires.

Proximate Analysis (wt.%)$_{a.r.}$		Ultimate Analysis (wt.%)$_{d.b.}$		Alkali Metals (mg/kg) $_{d.b.}$	
Moisture content (MC)	1.2	C	79.54 ± 0.17	Al	1352
Volatile matter (VM)	58.76	H	7.33 ± 0.03	Ca	1152
Fixed carbon (FC)	30.15	N	0.47 ± 0.03	Fe	1117
Ash	9.89	S	1.48± 0.06	K	509
HHV* (MJ/kg)$_{d.b.}$	36.55	O**	1.29	Na	508
Natural Rubber (BR)	22.9	T_{peak} (°C)	380		
Butadiene Rubber (BR)	43.4	$T_{initial}$ (°C)	327		
Styrene-Butadiene (SBR)	33.7	T_{f1} /T_{f2} (°C)	456/506		

* HHV (MJ/kg) = 35.2C +116.2H + 6.3N + 10.5S - 11.1O, where C, H, O, S, N are fractional elemental composition of carbon, hydrogen and oxygen, respectively [6].

** Oxygen is calculated by difference from O = 100 – C%– N% – H% – S% – ASH%***Metal content was measured by inductively coupled plasma optical emission spectrometry (ICP-OES) using a PerkinElmer Optima 7000 DV ICP-OES series instrument.

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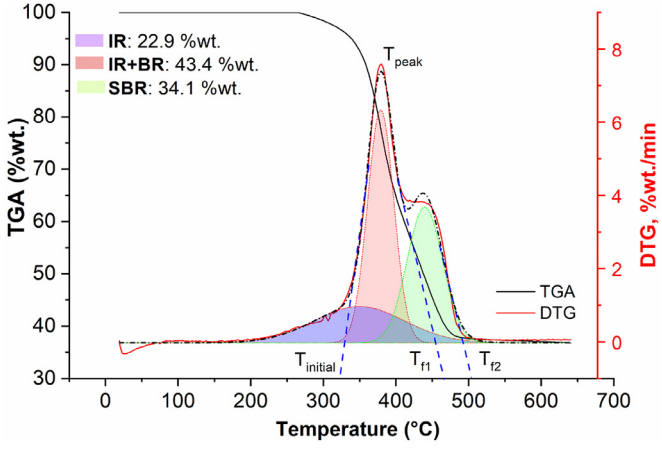

Fig. 1. TGA/DTG characterization of waste tires with characteristic peaks identification (T_{peak}, $T_{initial}$ and T_{final}).

allow performing further kinetic analyses or other valuable interpretation of the results. This is shared as a MendeleyData repository to facilitate the access and sharing of the information.

2. Experimental Design, Materials and Methods

Sample preparation: The waste tires were provided by a local enterprise as polymeric granules (free of steel). Then, the WT granules were crushed, and sieved in sizes between 180 and 300 µm (Gilson ASTME11), before being dried at 100 °C, during 12 h in static air (LabTech, LDO-150F). Dry samples were stored until use in hermetic plastic bags.

Waste tire characterization: Elemental composition and proximate analysis of waste tire were carried out in an elemental analyzer (Leco CHNS 628), and a muffle (Thermo Scientific F6020C) following the ASTM D3176 and D3172 standards, respectively. The inorganic elements were determined by inductively coupled plasma optical emission spectrometry (ICP-OES) using a PerkinElmer Optima 7000 DV series instrument and the UOP389-15. Thermogravimetric analysis (TGA) was carried out for 25 mg of WTs between 20 and 650 °C at 10 °C min^{-1} heating

Table 2
Py-GC/MS results for individual polymers and waste tires under regular pyrolysis conditions (non-catalytic). Conditions T = 400 °C, time = 12 s, mass = 1 mg.

Peak N°	time (min)	NR	BR	SBR	WT	IUPAC Compound id
1	1.718	0.0%	4.71%	4.93%	0.0%	1,3-Butadiene
2	1.922	19.30%	1.28%	1.60%	21.82%	Isoprene
3	2.486	0.05%	0.64%	0.69%	0.03%	cyclohexene
4	3.136	0.07%	1.20%	1.83%	0.15%	Benzene
5	4.05	0.49%	0.33%	0.10%	0.55%	3,5-Dimethylcyclopentene
6	4.789	0.92%	0.30%	0.09%	0.57%	1-Methyl-1,4-cyclohexadiene
7	5.378	0.35%	0.79%	1.05%	0.61%	Toluene
8	6.961	0.0%	69.47%	59.99%	0.52%	4-Ethenyl- cyclohexene
9	7.6	0.02%	0.58%	0.47%	0.09%	2,6-Dimethyl-1,6-heptadiene
10	8.4	0.15%	0.01%	0.01%	0.08%	(E,E,E)-2,4,6-Octatriene
11	10.2	0.08%	0.01%	0.06%	0.01%	Ethylbenzene
12	10.726	0.55%	0.40%	0.41%	2.77%	Xylenes
13	12.2	0.0%	0.29%	0.07%	0.00%	1,5,5,6-tetramethyl-1,3-cyclohexadiene
14	12.912	0.39%	1.06%	0.42%	0.09%	Styrene
15	13.009	0.37%	0.01%	0.73%	0.02%	2,5,5-trimethyl-1,6-Heptadiene
16	13.414	5.03%	0.69%	0.01%	1.99%	4-ethenyl-1,4-dimethyl- cyclohexene
17	14.024	0.23%	0.01%	0.31%	1.08%	2,5,6-trimethyl-1,3,6-Heptatriene
18	14.497	0.45%	0.29%	0.03%	0.13%	2,6-dimethyl-2,6-Octadiene
19	14.747	0.76%	0.09%	0.08%	0.35%	Benzene, 1-ethyl-3-methyl-
20	15.0	0.13%	0.01%	0.14%	0.16%	5-ethyl-1,5-dimethyl-1,3-cyclohexadiene
21	15.192	0.32%	0.14%	0.04%	0.10%	3,7-dimethyl 2,4,6-octatriene
22	15.4	0.24%	0.0%	0.00%	0.00%	2,6-dimethyl-1,6-octadiene
23	15.501	0.97%	0.0%	0.16%	0.43%	2,6-Dimethyl1,3,5,7octatetr
24	15.6	0.0%	0.11%	0.00%	0.21%	1,6-Dimethyl-hepta-1,3,5-triene
25	15.8	0.06%	0.04%	2.81%	0.74%	3,7-dimethyl-1,3,6-octatriene

(*continued on next page*)

Table 2 (*continued*)

Peak N°	time (min)	NR	BR	SBR	WT	IUPAC Compound id
26	16.042	55.50%	1.48%	0.06%	50.37%	Limonene
27	16.323	2.21%	0.07%	0.01%	0.82%	1,3,6-Heptatriene, 2,5,6-trimethyl-
28	16.53	0.27%	0.06%	0.00%	0.40%	p-Cymene
29	17.616	0.30%	0.07%	0.12%	0.29%	γ-Terpinene
30	17.8	0.12%	0.10%	3.31%	0.30%	Toluene, p-ethynyl-
31	17.9	0.06%	4.01%	0.76%	0.05%	α-Terpinene
32	18.515	0.38%	0.30%	5.62%	0.97%	p-Cymenene
33	19.5	0.02%	0.83%	0.19%	0.05%	Dodecane
34	20.911	1.06%	0.36%	5.34%	0.04%	Dodecane, 2,6,11-trimethyl-
35	21.1	0.02%	5.80%	2.85%	0.01%	Dodecane, 2,6,10-trimethyl-
36	21.308	0.02%	0.21%	0.56%	0.06%	Benzene, 1,4-bis(1,1-dimethylethyl)-
37	22.507	0.40%	0.50%	0.35%	2.03%	Benzothiazole
38	22.615	0.37%	0.15%	0.06%	0.23%	1,5-Cycloundecadiene, 8,8-dimethyl-9-methylene-
39	22.694	0.61%	0.0%	0.06%	0.32%	1,5-Cycloundecadiene, 9-(1-methylethylidene)-
40	23.074	0.31%	0.07%	0.01%	0.06%	Tetradecane
41	23.443	0.71%	0.01%	0.11%	0.28%	1,5-Cyclodecadiene, 1,5-dimethyl-8-(1-methylethylidene)-, (E,E)-
42	23.687	1.22%	0.10%	0.04%	0.52%	1-Cycloheptene, 1,4-dimethyl-3-(2-methyl-1-propene-1-yl)-4-vinyl-
43	23.84	1.71%	0.01%	0.02%	0.46%	Bicyclo[5.2.0]nonane, 4-methylene-2,8,8-trimethyl-2-vinyl-
44	24.015	0.45%	0.01%	0.63%	0.26%	Cyclohexane, 1-ethenyl-1-methyl-2,4-bis(1-methylethenyl)-, [1S-(1α,2β,4β)]-
45	24.183	1.26%	0.04%	0.33%	0.81%	Cyclohexane, 1-ethenyl-1-methyl-2-(1-methylethenyl)-4-(1-methylethylidene)-
46	26.2	0.12%	0.08%	1.05%	0.23%	Hexadecane
47	26.346	0.59%	0.31%	0.38%	5.74%	Quinoline, 1,2-dihydro-2,2,4-trimethyl-
48	28.91	0.04%	0.32%	0.30%	0..25%	Octadecane
49	30.245	0.19%	0.25%	0.06%	1.02%	β-D-Glucopyranose, 1,6-anhydro-
50	30.534	0.11%	0.27%	0.15%	0.22%	(E,E,E)-3,7,11,15-Tetramethylhexadeca-1,3,6,10,14-pentaene
51	30.645	0.13%	0.48%	1.08%	0.29%	1,5,5-Trimethyl-6-(3-methyl-buta-1,3-dienyl)-cyclohexene
52	31.008	0.88%	1.64%	0.53%	1.41%	Cyclohexane, 1-ethenyl-1-methyl-2-(1-methylethenyl)-4-(1-methylethylidene)-

Table 3
Py-GC/MS results for individual polymers and waste tires under regular pyrolysis conditions (non-catalytic). Conditions T = 450 °C, time = 12 s, mass = 1 mg.

Peak N°	time (min)	NR	BR	SBR	WT	IUPAC Compound id
1	1.718	0.00%	5.19%	4.00%	0.00%	1,3-Butadiene
2	1.922	19.39%	1.41%	1.30%	22.56%	Isoprene
3	2.486	0.05%	0.71%	0.56%	0.01%	cyclohexene
4	3.136	0.07%	0.00%	1.49%	0.19%	Benzene
5	4.05	0.49%	0.36%	0.04%	0.68%	3,5-Dimethylcyclopentene
6	4.789	0.92%	0.33%	0.07%	0.62%	1-Methyl-1,4-cyclohexadiene
7	5.378	0.35%	0.87%	0.85%	0.72%	Toluene
8	6.961	0.01%	76.60%	48.74%	1.04%	4-Ethenyl- cyclohexene
9	7.6	0.02%	0.64%	0.38%	0.13%	2,6-Dimethyl-1,6-heptadiene
10	8.4	0.15%	0.01%	0.01%	0.17%	(E,E,E)-2,4,6-Octatriene
11	10.2	0.08%	0.53%	0.08%	0.14%	Ethylbenzene
12	10.726	0.55%	0.44%	0.34%	2.12%	Xylenes
13	12.2	0.00%	0.32%	0.05%	0.00%	1,5,5,6-tetramethyl-1,3-cyclohexadiene
14	12.912	0.39%	1.17%	17.51%	0.30%	Styrene
15	13.009	0.37%	0.01%	0.34%	0.25%	2,5,5-trimethyl-1,6-Heptadiene
16	13.414	5.05%	0.77%	0.59%	3.69%	4-ethenyl-1,4-dimethyl- cyclohexene
17	14.024	0.23%	0.01%	0.01%	0.21%	2,5,6-trimethyl-1,3,6-Heptatriene
18	14.497	0.45%	0.32%	0.25%	0.39%	2,6-dimethyl-2,6-Octadiene
19	14.747	0.77%	0.01%	0.07%	0.71%	Benzene, 1-ethyl-3-methyl-
20	15.0	0.53%	0.01%	0.03%	0.45%	5-ethyl-1,5-dimethyl-1,3-cyclohexadiene
21	15.192	0.32%	0.16%	0.11%	0.34%	3,7-dimethyl 2,4,6-octatriene
22	15.4	0.24%	0.01%	0.03%	0.00%	2,6-dimethyl-1,6-octadiene
23	15.501	0.98%	0.02%	0.00%	0.63%	2,6-Dimethyl1,3,5,7octatetr
24	15.6	0.00%	0.12%	0.01%	0.27%	1,6-Dimethyl-hepta-1,3,5-triene
25	15.8	0.06%	0.05%	0.03%	0.19%	3,7-dimethyl-1,3,6-octatriene
26	16.042	55.76%	1.63%	2.28%	47.79%	Limonene
27	16.323	2.23%	0.08%	0.04%	1.48%	1,3,6-Heptatriene, 2,5,6-trimethyl-

(*continued on next page*)

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28	16.53	0.27%	0.07%	0.05%	0.62%	p-Cymene
29	17.616	0.30%	0.08%	0.15%	0.51%	γ-Terpinene
30	17.8	0.12%	0.11%	0.10%	0.29%	Toluene, p-ethynyl-
31	17.9	0.06%	0.00%	2.69%	0.08%	α-Terpinene
32	18.515	0.57%	0.97%	2.56%	1.03%	p-Cymenene
33	19.5	0.02%	0.91%	4.56%	0.02%	Dodecane
34	20.911	1.07%	0.53%	0.15%	0.03%	Dodecane, 2,6,11-trimethyl-
35	21.1	0.12%	0.50%	4.34%	0.24%	Dodecane, 2,6,10-trimethyl-
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38	22.615	0.37%	0.17%	0.28%	0.24%	1,5-Cycloundecadiene, 8,8-dimethyl-9-methylene-
39	22.694	0.61%	0.00%	0.05%	0.34%	1,5-Cycloundecadiene, 9-(1-methylethylidene)-
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42	23.687	1.23%	0.05%	0.09%	0.83%	1-Cycloheptene, 1,4-dimethyl-3-(2-methyl-1-propene-1-yl)-4-vinyl-
43	23.84	0.72%	0.02%	0.14%	0.67%	Bicyclo[5.2.0]nonane, 4-methylene-2,8,8-trimethyl-2-vinyl-
44	24.015	0.45%	0.01%	0.01%	0.48%	Cyclohexane, 1-ethenyl-1-methyl-2,4-bis(1-methylethenyl)-, [1S-(1α,2β,4β)]-
45	24.183	1.26%	0.54%	0.07%	0.91%	Cyclohexane, 1-ethenyl-1-methyl-2-(1-methylethenyl)-4-(1-methylethylidene)-
46	26.2	0.12%	0.09%	0.27%	0.30%	Hexadecane
47	26.346	0.70%	0.36%	0.85%	3.48%	Quinoline, 1,2-dihydro-2,2,4-trimethyl-
48	28.91	0.04%	0.35%	0.30%	0.15%	Octadecane
49	30.245	0.19%	0.21%	0.24%	0.55%	β-D-Glucopyranose, 1,6-anhydro-
50	30.534	0.11%	0.09%	0.05%	0.30%	(E,E,E)-3,7,11,15-Tetramethylhexadeca-1,3,6,10,14-pentaene
51	30.645	0.13%	0.53%	0.12%	0.35%	1,5,5-Trimethyl-6-(3-methyl-buta-1,3-dienyl)-cyclohexene
52	31.008	0.88%	1.80%	0.88%	1.27%	Cyclohexane, 1-ethenyl-1-methyl-2-(1-methylethenyl)-4-(1-methylethylidene)-

Table 4
Py-GC/MS results for waste tires under catalytic pyrolysis on Pd/NT-Ti, Pt/NT-Ti and Au/NT-Ti. Conditions T = 400 °C, time = 12 s, mass of WT = 1 mg, Catalyst-to-WT ratio = 4.

Peak N°	time (min)	Pd/NT-Ti	Pt/NT-Ti	Au/NT-Ti	IUPAC Compound id
1	1.8	0.00%	4.44%	4.49%	Butadiene
2	2.1	13.52%	16.17%	16.34%	Isoprene
3	2.97	0.71%	1.04%	1.05%	Cyclohexene
4	3.14	6.96%	0.70%	0.71%	Benzene
5	4.05	0.25%	0.45%	0.45%	3,5-Dimethylcyclopentene
6	4.79	0.26%	0.46%	0.47%	1-Methyl-1,4-cyclohexadiene
7	5.38	9.99%	7.35%	7.43%	Toluene
8	6.98	0.05%	0.34%	0.35%	4-Ethenyl- cyclohexene
9	7.6	0.05%	0.09%	0.09%	2,6-Dimethyl-1,6-heptadiene
10	8.4	0.01%	0.01%	0.01%	(E,E,E)-2,4,6-Octatriene
11	10.2	0.30%	0.01%	0.01%	Ethylbenzene
12	10.7	3.61%	3.22%	3.26%	Xylenes
13	12.2	0.00%	0.01%	0.00%	1,5,5,6-tetramethyl-1,3-cyclohexadiene
14	12.9	0.14%	0.03%	0.02%	Styrene
15	13.0	0.04%	0.01%	0.01%	2,5,5-trimethyl-1,6-Heptadiene
16	13.4	0.09%	0.76%	0.76%	4-ethenyl-1,4-dimethyl- cyclohexene
17	14.0	0.96%	0.01%	0.01%	2,5,6-trimethyl-1,3,6-Heptatriene
18	14.5	0.13%	0.00%	0.00%	2,6-dimethyl-2,6-Octadiene
19	15.0	0.13%	0.16%	0.03%	5-ethyl-1,5-dimethyl-1,3-cyclohexadiene
20	15.2	0.04%	0.32%	0.05%	3,7-dimethyl 2,4,6-octatriene
21	15.4	0.12%	0.04%	0.21%	2,6-dimethyl-1,6-octadiene
22	15.5	0.04%	0.21%	0.10%	2,6-Dimethyl1,3,5,7octatetriene
23	15.6	0.06%	0.10%	0.01%	1,6-Dimethyl-hepta-1,3,5-triene
24	15.8	0.26%	0.39%	0.40%	3,7-dimethyl-1,3,6-octatriene
25	16.0	21.32%	26.15%	26.43%	DL-Limonene
26	16.5	13.12%	11.05%	11.17%	p-Cymene
27	17.6	0.13%	1.33%	1.34%	γ-Terpinene

(*continued on next page*)

Table 4 (*continued*)

Peak N°	time (min)	Pd/NT-Ti	Pt/NT-Ti	Au/NT-Ti	IUPAC Compound id
28	17.8	0.07%	0.13%	0.02%	Toluene, p-ethynyl-
29	17.9	0.00%	0.04%	0.04%	α-Terpinene
30	18.5	1.51%	1.84%	1.86%	p-Cymenene
31	19.5	0.00%	0.04%	0.43%	Dodecane
32	20.9	1.38%	0.41%	0.42%	Dodecane, 2,6,11-trimethyl-
33	21.1	0.04%	0.12%	0.01%	Dodecane, 2,6,10-trimethyl-
34	21.3	0.06%	0.63%	0.64%	Benzene, 1,4-bis(1,1-dimethylethyl)-
35	22.5	6.25%	9.41%	9.51%	Benzothiazole
36	22.6	0.08%	0.15%	0.15%	1,5-Cycloundecadiene, 8,8-dimethyl-9-methylene-
37	22.7	0.04%	0.12%	0.02%	1,5-Cycloundecadiene, 9-(1-methylethylidene)-
38	23.1	0.08%	0.70%	0.06%	Tetradecane
39	23.4	0.04%	0.10%	0.10%	1,5-Cyclodecadiene, 1,5-dimethyl-8-(1-methylethylidene)-, (E,E)-
40	23.7	0.02%	0.01%	0.01%	1-Cycloheptene, 1,4-dimethyl-3-(2-methyl-1-propene-1-yl)-4-vinyl-
41	23.8	0.31%	0.29%	0.30%	Bicyclo[5.2.0]nonane, 4-methylene-2,8,8-trimethyl-2-vinyl-
42	24.0	0.25%	0.18%	0.18%	Cyclohexane, 1-ethenyl-1-methyl-2,4-bis(1-methylethenyl)-, [1S-(1α,2β,4β)]-
43	24.2	0.49%	0.33%	0.33%	Cyclohexane, 1-ethenyl-1-methyl-2-(1-methylethenyl)-4-(1-methylethylidene)-
44	26.2	0.13%	0.12%	0.12%	Hexadecane
45	26.346	7.31%	9.57%	9.67%	Quinoline, 1,2-dihydro-2,2,4-trimethyl-
46	28.9	0.67%	0.34%	0.35%	Octadecane
47	30.245	2.40%	0.18%	0.18%	β-D-Glucopyranose, 1,6-anhydro-
48	30.5	2.28%	0.06%	0.06%	(E,E,E)-3,7,11,15-Tetramethylhexadeca-1,3,6,10,14-pentaene
49	30.7	0.36%	0.03%	0.03%	1,5,5-Trimethyl-6-(3-methyl-buta-1,3-dienyl)-cyclohexene
50	31.0	3.94%	0.34%	0.34%	Cyclohexane, 1-ethenyl-1-methyl-2-(1-methylethenyl)-4-(1-methylethylidene)-

Table 5
Py-GC/MS results for waste tires under catalytic pyrolysis on Pd/NT-Ti, Pt/NT-Ti and Au/NT-Ti. Conditions T = 450 °C, time = 12 s, mass of WT = 1 mg, Catalyst-to-WT ratio = 4.

Peak N°	time (min)	Pd/NT-Ti	Pt/NT-Ti	Au/NT-Ti	IUPAC Compound id
1	1.8	0.00%	0.00%	0.00%	Butadiene
2	2.1	19.87%	19.23%	21.71%	Isoprene
3	2.97	0.12%	0.09%	0.47%	Cyclohexene
4	3.14	2.91%	1.62%	0.66%	Benzene
5	4.05	1.11%	1.43%	0.86%	3,5-Dimethylcyclopentene
6	4.79	0.48%	0.49%	0.42%	1-Methyl-1,4-cyclohexadiene
7	5.38	2.25%	2.39%	3.49%	Toluene
8	6.98	1.01%	0.80%	0.75%	4-Ethenyl- cyclohexene
9	7.6	0.34%	0.37%	0.33%	2,6-Dimethyl-1,6-heptadiene
10	8.4	0.00%	0.00%	0.00%	(E,E,E)-2,4,6-Octatriene
11	10.2	1.10%	0.49%	0.14%	Ethylbenzene
12	10.7	4.34%	3.91%	2.72%	Xylenes
13	12.2	0.03%	0.00%	0.00%	1,5,5,6-tetramethyl-1,3-cyclohexadiene
14	12.9	0.26%	0.48%	0.33%	Styrene
15	13.0	0.55%	0.55%	0.24%	2,5,5-trimethyl-1,6-Heptadiene
16	13.4	4.98%	4.80%	2.70%	4-ethenyl-1,4-dimethyl- cyclohexene
17	14.0	0.20%	0.11%	0.01%	2,5,6-trimethyl-1,3,6-Heptatriene
18	14.5	0.69%	0.00%	0.30%	2,6-dimethyl-2,6-Octadiene
19	15.0	0.78%	0.66%	0.39%	5-ethyl-1,5-dimethyl-1,3-cyclohexadiene
20	15.2	0.31%	0.27%	1.09%	3,7-dimethyl 2,4,6-octatriene
21	15.4	0.00%	0.00%	0.00%	2,6-dimethyl-1,6-octadiene
22	15.5	1.12%	0.91%	0.79%	2,6-Dimethyl1,3,5,7octatetriene
23	15.6	0.41%	0.44%	0.22%	1,6-Dimethyl-hepta-1,3,5-triene
24	15.8	0.26%	0.99%	1.12%	3,7-dimethyl-1,3,6-octatriene
25	16.0	31.40%	31.90%	29.39%	DL-Limonene
26	16.5	9.84%	9.81%	13.32%	p-Cymene
27	17.6	0.89%	2.03%	1.86%	γ-Terpinene

(*continued on next page*)

Table 5 (*continued*)

Peak N°	time (min)	Pd/NT-Ti	Pt/NT-Ti	Au/NT-Ti	IUPAC Compound id
28	17.8	0.04%	0.30%	0.12%	Toluene, p-ethynyl-
29	17.9	0.17%	0.23%	0.15%	α-Terpinene
30	18.5	4.50%	4.49%	2.65%	p-Cymenene
31	19.5	0.07%	0.19%	0.03%	Dodecane
32	20.9	0.17%	0.24%	0.17%	Dodecane, 2,6,11-trimethyl-
33	21.1	0.00%	0.00%	0.00%	Dodecane, 2,6,10-trimethyl-
34	21.3	0.18%	0.36%	0.25%	Benzene, 1,4-bis(1,1-dimethylethyl)-
35	22.5	2.33%	2.36%	4.52%	Benzothiazole
36	22.6	0.12%	0.18%	0.14%	1,5-Cycloundecadiene, 8,8-dimethyl-9-methylene-
37	22.7	0.07%	0.08%	0.19%	1,5-Cycloundecadiene, 9-(1-methylethylidene)-
38	23.1	0.19%	0.15%	0.47%	Tetradecane
39	23.4	0.52%	0.48%	0.32%	1,5-Cyclodecadiene, 1,5-dimethyl-8-(1-methylethylidene)-, (E,E)-
40	23.7	0.80%	0.39%	0.47%	1-Cycloheptene, 1,4-dimethyl-3-(2-methyl-1-propene-1-yl)-4-vinyl-
41	23.8	1.11%	1.14%	0.44%	Bicyclo[5.2.0]nonane, 4-methylene-2,8,8-trimethyl-2-vinyl-
42	24.0	0.27%	0.27%	0.34%	Cyclohexane, 1-ethenyl-1-methyl-2,4-bis(1-methylethenyl)-, [1S-(1α,2β,4β)]-
43	24.2	0.87%	0.82%	0.38%	Cyclohexane, 1-ethenyl-1-methyl-2-(1-methylethenyl)-4-(1-methylethylidene)-
44	26.2	0.30%	0.32%	0.21%	Hexadecane
45	26.346	2.17%	2.68%	3.87%	Quinoline, 1,2-dihydro-2,2,4-trimethyl-
46	28.9	0.29%	0.22%	0.25%	Octadecane
47	30.245	0.01%	0.02%	0.02%	β-D-Glucopyranose, 1,6-anhydro-
48	30.5	0.19%	0.35%	0.40%	(E,E,E)-3,7,11,15-Tetramethylhexadeca-1,3,6,10,14-pentaene
49	30.7	0.02%	0.07%	0.05%	1,5,5-Trimethyl-6-(3-methyl-buta-1,3-dienyl)-cyclohexene
50	31.0	0.33%	0.88%	1.25%	Cyclohexane, 1-ethenyl-1-methyl-2-(1-methylethenyl)-4-(1-methylethylidene)-

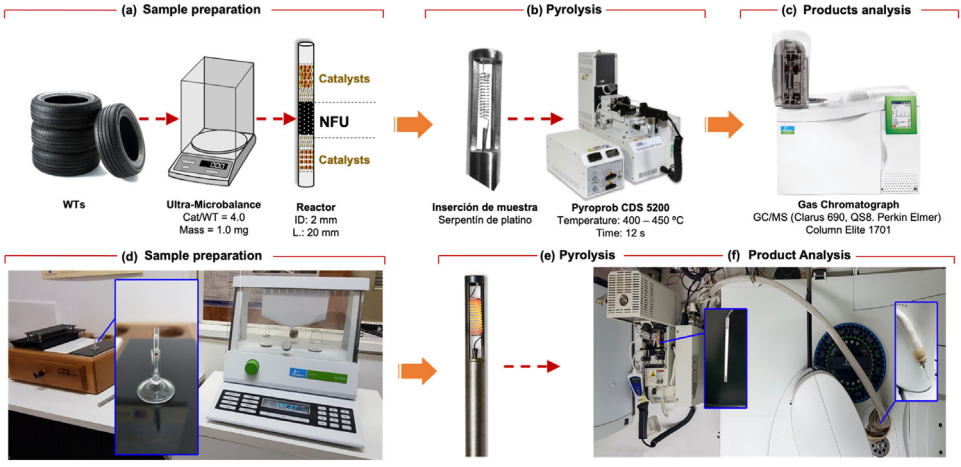

Fig. 2. Flow diagram for Py-GC/MS experiments.

ramp and using (50 mL/min) N_2 as the carrier gas in a thermobalance (Netzsch, model STA 409 PC).

Micropyrolysis Assays (Py-GC/MS): The Fig. 2 (a–f) summarizes the experimental protocol for performing analytical pyrolysis experiments. Moreover, a detailed explanation on the experimental design and equipment's conditions/protocols is provided below.

In a typical experiment, around 1 ± 0.1 mg of waste tire were weighted in an AD 6000 Ultra MicroBalance (Perkin Elmer, $\pm 10^{-6}$ mg) and placed in the pyrolysis reactor Fig. 2**d**), supported by glass wool. Fast pyrolysis experiments for waste tires, with and without catalysts, were carried out in a CDS 5200 pyroprobe (CDS Analytical). The quartz tube reactor (25 mm length and 1.9 mm ID) was inserted inside a probe and electrically heated using a resistively heating Pt filament (**Fig. 2e**). For the catalytic pyrolysis, a fixed catalyst-to-tire mass ratio of 4:1 was used. In this case, the tire and the catalyst were separated by glass wool to perform the experiment in an ex-situ regime. All the experiments were done under a constant flow of He (pure 99.996%, Iconsa, Chile) of 20 mL min^{-1} to transport the volatiles to the analysis area (GC/MS) (**Fig. 2f**). The heating rate was varied according to the reaction temperature (400 and 450 °C), considering a residence time of 12 s, and the kinetically-controlled regime was confirmed by the dimensionless numbers of Biot, Py^{I} and Py^{II} (See Eqs. ((1)–(3)).

$$Bi = h \cdot R/\lambda \tag{1}$$

$$Py^{I} = \lambda/\left(k \cdot \rho \cdot C_p \cdot R^2\right) \tag{2}$$

$$Py^{II} = h/\left(k \cdot \rho \cdot C_p \cdot R\right) \tag{3}$$

Here λ, is the thermal conductivity ($Wm^{-1}K^{-1}$), R is the characteristic length (m), h is the heat transfer coefficient ($Wm^{-2}K^{-1}$), ρ is the mass density of the WT (kgm^{-3}), Cp is the specific heat $Jkg^{-1}K^{-1}$ and k is the apparent kinetic constant for the solid conversion (s^{-1}).

Before entering the GC, the volatiles passed by a Sorbent Tube, packed with 20:35 mesh Tenax-TA (pre column Perkin Elmer), which was kept at 280 °C to release the volatiles through a heated transfer line (CDS Analytical) to the gas chromatograph (Clarus, 690, Perkin Elmer) (**Fig. 2f**). Then the volatiles were separated in an Elite 1701 column (30 m × 0.25 mm × 0.25 μm) using He as carrier gas at 15 mL min^{-1} and using a heating ramp from 45 to 280 °C at 2.5 °C min^{-1}. The chromatograph is equipped with a quadrupole mass

detector (SQ8S, Perkin Elmer) working in electron ionization mode. The compounds were ionized and the resulting mass spectra were compared with the standard spectra database from the NIST library in a m/z range of 30–600 Da. Because the amount of tire was strictly controlled, the relative peak area (R_A) (Eq. (4)) was used as a measured of the products selectivity.

$$R_A = Apeak_i / \sum_{i=1}^{n} (Apeak_i) \quad (4)$$

R_A is the relative peak area, $Apeak_i$ peak area for the *i*th compound and n is the total number of identified compounds.

Ethics Statement

Provided dataset do not involve human subjects nor experiments with animals. Furthermore, it represents original data gathered by the research team thus it does not imply the collection of information from social media or any other public database.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

CRediT Author Statement

Beatriz Smith Azócar: Conceptualization, Methodology, Writing – original draft; **Paula Osorio Vargas:** Data curation, Writing – original draft; **Cristian Campos:** Investigation, Formal analysis; **Francisco Medina:** Methodology, Investigation; **Luis E. Arteaga-Pérez:** Conceptualization, Supervision, Writing – review & editing.

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