Electronic Supporting Information

Carbon footprint and mitigation strategies of three chemistry laboratories

Andre Estevez-Torres,*[a, b] Fabienne Gauffre,[c] Guillaume Gouget,[c] Chloé Grazon,[d] Philippe Loubet*[d]

a. Université de Lille, CNRS, LASIRE (UMR 8516), Cité Scientifique, F-59655 Villeneuve d'Ascq, France
b. Sorbonne Université, CNRS, Institut de Biologie Paris-Seine (IBPS), Laboratoire Jean Perrin (LJP), F-75005 Paris, France.
c. Université de Rennes, CNRS, ISCR – UMR 6226, F-35000 Rennes, France
d. Univ. Bordeaux, CNRS, Bordeaux INP, ISM, UMR 5255, F-33400 Talence, France

Context of the study

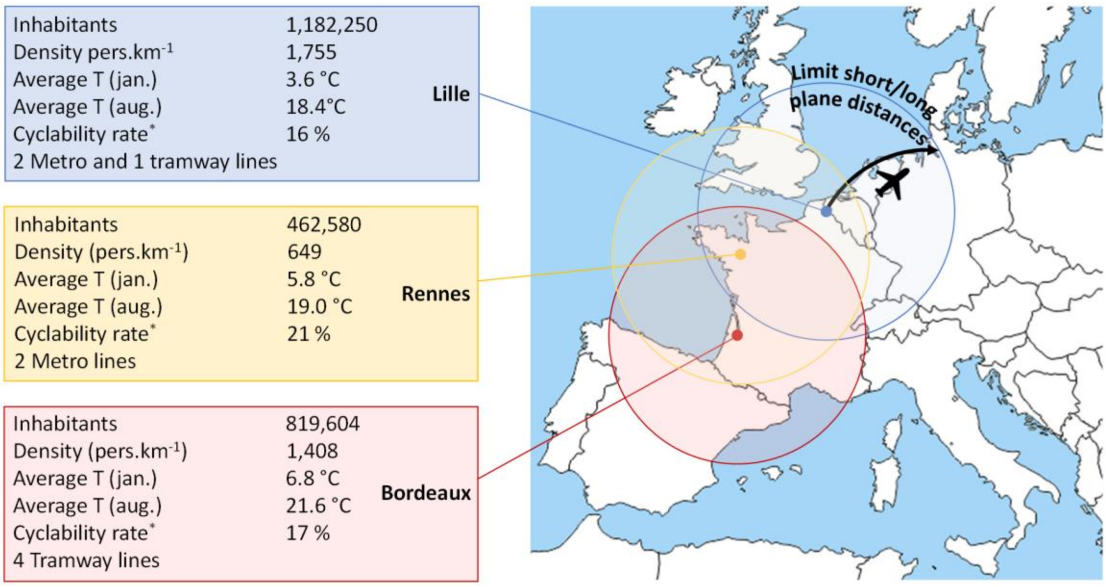

Figure S1. *Geographic and demographic data of three city areas hosting the chemistry labs: lab1, LASIRE in Lille Métropole; lab2, ISM in Bordeaux Métropole; lab3 ISCR in Rennes Métropole. Sources: Wikipedia pages of the cities; * https://www.velo-territoires.org/actualite/2022/05/11/indicateur-de-cyclabilite/. Data mostly from 2020, Rennes metro line B opened in 2022.*

Purchases/Equipment

Table S1. *Carbon intensities for different purchases categories*

Category	Subcategory	Carbon intensity (kgeqCO_2/€)
Purchases*		0.31
Consumables	All	0.44
IT**		0.14
Lab equipment		0.30
Lab life		0.51
Maintenance		0.23
Services		0.10
Hosting & transport***		0.37
Consumables	biochemistry	0.38
Consumables	chemicals	0.45
Consumables	gases	0.29
Consumables	glassware	0.23
Consumables	lab supplies	0.49
Consumables	solvents	0.45

Table S2. *Top 5 most expensive equipment bought in 2019 in Lab 2.*

Apparatus	Emissions (teqCO_2)	Cost (€)
MALDI spectrometer	47.9	199,500
Raman confocal microscope	27.2	100,784
NIR laser light source	15.0	50,000
Liquid-Phase Chromatography	13.2	55,000
UV-vis. spectrometer	11.5	48,000

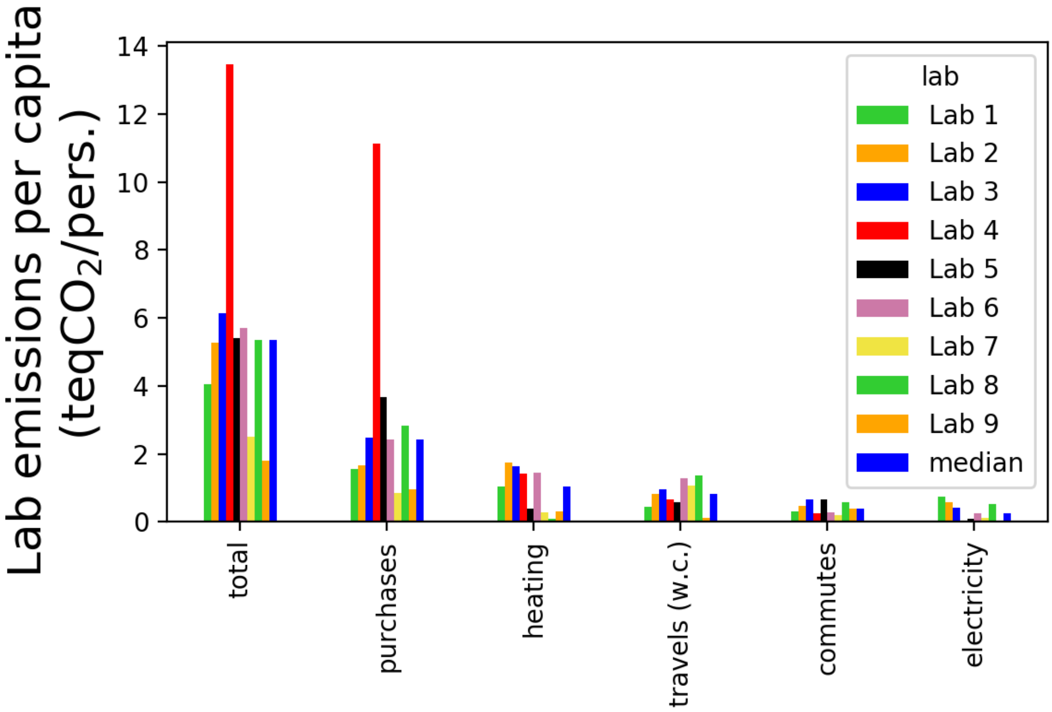

Figure S2. *GHG emissions per capita and per emission category for the all the chemistry laboratories having submitted 2019 data to the Labos 1point5 carbon footprint database. It includes Labs 1-3 thoroughly analysed in the Main Text. The median corresponds to the values called Chem 1p5 in Figure 1 of the Main Text. (w.c.) indicates that plane travel emissions take into account contrails as we do throughout the texte.*

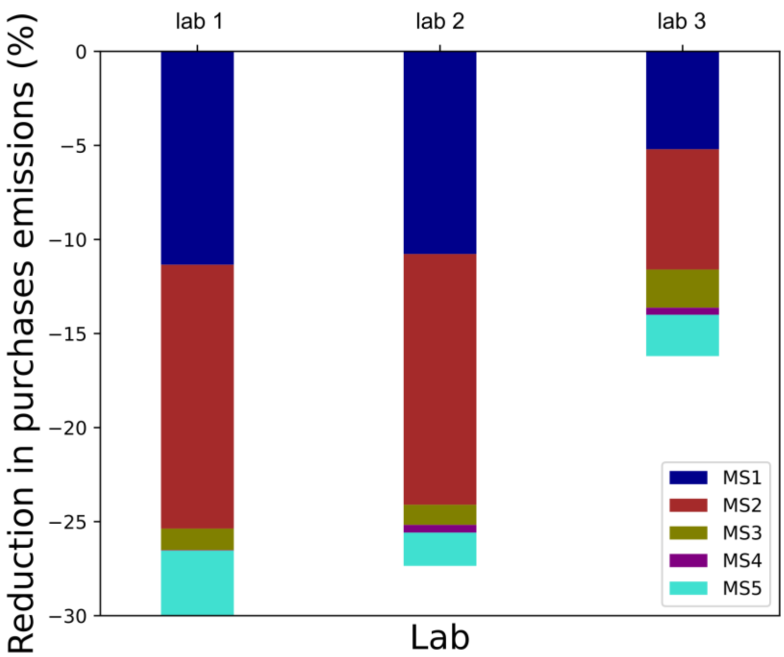

Figure S3. *Relative reduction in purchases emissions induced by each mitigation strategy (MS) per laboratory. MS1: increase the lifetime of equipment by 25 %; MS2: and further reducing by 25 % lab equipment by pooling; MS3: reducing by 10 % the use of chemicals by pooling; MS4: reducing acetone purchases by recycling; MS5: increasing by 50 % the lifetime of IT equipment.*

Acetone is one of the main solvents used in laboratories. For instance, Lab 2 and Lab 3 consume annually 3 700 and 10 000 liters of acetone, respectively. Their incineration induces the emission of 6.6 and 18.1 teqCO_2, respectively.

A life cycle assessment (LCA) has been conducted in order to compare the carbon footprint and costs of three acetone recycling scenarios in Lab 2. The functional unit of this comparative LCA is “to provide 3 710 L of acetone to Lab 2”, which is equivalent to the yearly demand of this solvent. The assessed scenarios are: 1) business-as-usual 0% recycling, 2) 10% recycling, and 3) 50% recycling.
The boundaries are “cradle-to-grave” and include the production and transport of acetone, distillation of the solvent (manufacture and use of the distillation/chiller unit), evaporation of acetone during distillation, transport and incineration of the waste solvent. Lice cycle inventory (LCI) related to the background processes (acetone production, lorry transport, machine manufacturing) has been retrieved from ecoinvent 3.9 database. The manufacture of the distillation/chiller unit has been built through an estimation of the metal/plastics/electronic content of the machines. The method for life cycle impact assessment is IPCC in order to compute climate change impacts in compliance with carbon footprint calculation of GES1point5. Cost has been retrieved from invoices of electricity, machines and waste treatment purchased by Lab 2 .
Main results and data used in this LCA are shown in Table S3.

Table S3. *Life cycle assessment conducted to compare the carbon footprint and cost related to three scenarios of acetone supply in Lab 2.*

Inventory data	**Scenario recycling 0**	**Scenario recycling 0.1**	**Scenario recycling 0.5**
Yearly purchase of acetone (L)	3 710	3 346	1 892
Yearly purchase of acetone (kg)	2 909	2 618	1 454
Acetone recycling rate	0%	10%	50%
Yearly amount of recycled acetone (L)	-	371	1 855
Electricity consumption distiller/chiller (kWh)		285	1 425
GHG emissions (kgCO2eq/year)	**12 416**	**11 202**	**6 349**
Acetone production	5 535	4 993	2 823
Waste transport	336	302	168
Waste incineration	6 544	5 890	3 272
Electricity distiller/chiller	-	17	85
Manufacturing distiller/chiller		123	123
Acetone evaporation and degradation	-	17	84
Cost (€/year)	**6 245**	**6 407**	**4 121**
Acetone purchase	5 194	4 685	2 649
Waste treatment	1 051	946	526
Electricity distiller/chiller	-	43	214
Purchases distiller/chiller		733	733

Unitary cost and emission factors	**€**	**kgCO2eq**	**per**	**Source**
Electricity (FR)	0.15	0.0599	kWh	ADEME
Acetone production	1.4	1.492	L	ecoinvent 3.9 + IPCC
Acetone incineration	0.36	2.25	kg	stoechiometric combustion
Lorry transport		0.21	tkm	ecoinvent 3.9 + IPCC
Distiller manufacturing	7000	1589	unit	ecoinvent 3.9 + IPCC
Chiller manufacturing	3500	260	unit	ecoinvent 3.9 + IPCC

Other data		
Evaporation rate of acetone during distil.	2%	
Acetone density	0.784	kg/L
Waste treatment plant distance (Bdx/Lyon)	550	km
Power of the chiller	0.52	kW
Power of the distiller	2.04	kW
Cadence distiller per run	4.5	h
Volume distiller per run (up to 30L)	15	L
Life time of the distiller	15	yr
Life time of the chiller	15	yr

Energy

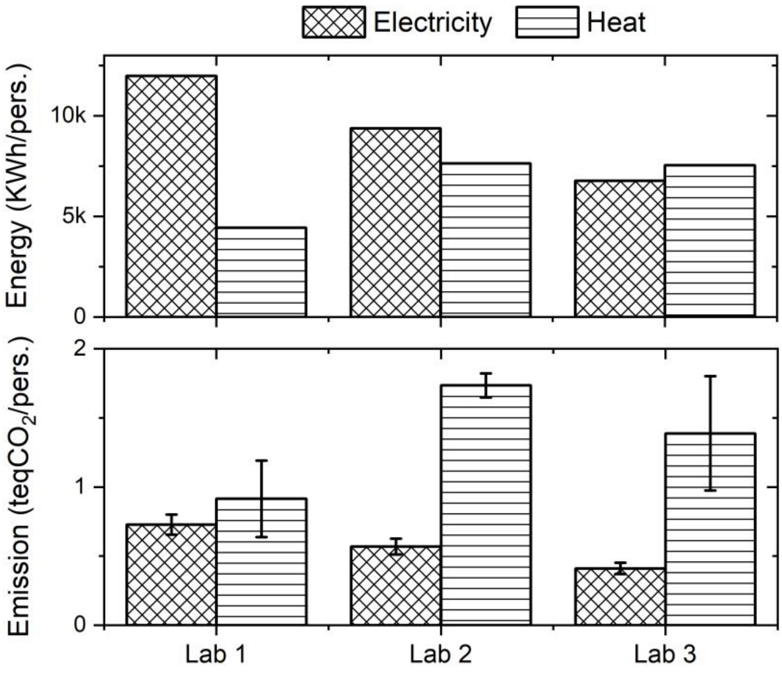

Figure S4. *Energy consumptions for year 2019 of the three labs (top) and associated emissions (down). Note that in France the electricity is mainly produced by nuclear fission.*

Table S4. *Measures for the reduction of heat-related GHG emissions, from reduction plan of the University of Bordeaux*[1]*, host of Lab 2.*

Daily-life operations	■ removal of hot water for sanitary purposes (except showers), ■ removal of auxiliary electric heaters in favor of a collective regulation, ■ optimization of outdoor lightning (e.g., turning off parking lot lightning from 1.00 to 5.00 AM), ■ reduction of heating at night, on weekends and for summer and winter breaks, ■ schedules of heating times accorded to room booking tools, temperature at 19° C in winter when the buildings are occupied and 16° C when not, ■ end of comfort air-conditioning, ■ minimum 26 °C air-conditioning when necessary.
Infrastructures	■ switch from natural gas to biomass and geothermy for heating systems, ■ installation of photovoltaic panels, ■ insulation of buildings.

[1] Univ Bordeaux. Le plan de sobriété énergétique de l’université de Bordeaux. https://www.u-bordeaux.fr/actualites/plan-sobriete-energetique (2022).

Table S5. *Measures for the reduction of electricity-related GHG emissions that are specific to chemistry activities.*

Fume hoods management	The work from Posner *et al*. indicate that a clever use of the fume hoods could reduce the electrical consumption of the extraction system by 30 % (direct reduction by less air pumping and indirect reduction by air compensation, possibly heated or cooled in winter/summer),[2] which is in line with previous estimations.[3] Since 2023, the recommendations given to all chemists in Labs 2 and 3 are the following: *(i) fume hoods must have their sash down in the absence of operator,* which is also a safety requirement, and *(ii) fume hoods must be turned off when all containers stored underneath are closed.*
Ultra-low temperature freezers	Regular cleaning/defrost of the freezers and their maintenance and location in a room at less than 25° C allow to decrease their energy consumption down to 25 % and increases their life time.[4] In addition, following the recommendations of MyGreenLab[5], shifting ultra-low freezer from - 80° C to - 70° C reduces the energy consumption of those machines by 30-40 %, without damaging the cell lines.[6],[7]
Lasers	Replacing gas lasers with diode lasers in spectroscopy devices, such as Raman and infrared spectrometers, is a significant step towards achieving energy savings for equipment. Diode lasers offer higher electrical-to-optical conversion efficiency, resulting in reduced energy consumption and lower operating costs. In Lab 2, two gas lasers with power outputs of 15 kW and 21 kW, along with a water consumption rate of 10 L/min, were recently replaced by two diode lasers with power outputs of 30 W and 63 W, eliminating the need for water consumption entirely. This transition allows for a remarkable 99 % reduction in both energy and water usage for these specific applications. However, further LCA studies must be conducted to ensure the avoidance of any potential burden shifting during manufacturing of diode lasers. One main issue is that diode lasers lifetime might be reduced compared to gas lasers.

[2] Posner, S., Stuart, R. & Thompson, G. A conceptual model for laboratory ventilation greenhouse gas planning. J. Chem. Health Saf. 18, 34–42 (2011).
[3] International Institute for Sustainable Laboratories. The Laboratory Benchmarking Tool. https://lbt.i2sl.org/.
[4] Gumapas, L. A. M. & Simons, G. Factors affecting the performance, energy consumption, and carbon footprint for ultra low temperature freezers: case study at the National Institutes of Health. *World Rev. Sci. Technol. Sustain. Dev.* **10**, 129–141 (2013).
[5] My green lab. https://www.mygreenlab.org/. ; Drahl, C. A Matter of Degree. *ACS Cent. Sci.* **4**, 1294–1297 (2018).
[6] Espinel-Ingroff, A., Montero, D. & Martin-Mazuelos, E. Long-Term Preservation of Fungal Isolates in Commercially Prepared Cryogenic Microbank Vials. J. Clin. Microbiol. 42, 1257–1259 (2004).
[7] Biological Samples Stored Long Term at -70 C or Warmer database. https://docs.google.com/spreadsheets/u/1/d/13UvBeoXAhwSHshSYoUDHwcxWiW7qYLnUb-eLwxJbCYs/pubhtml.

Estimating solar energy production potential

The average electricity produced by a photovoltaic panel in France in a year is 1000 kWh/(kWp.yr), where kWh correspond to electric energy generated and kWp to the maximum electric power delivered by the panel at peak. Knowing that the power of a photovoltaic cell per unit surface is 0.2 kWp/m^2, we get 200 kWh/(m^2.yr). Table S6 estimates the electric production for each of the labs from the surface data of the labs in Tab 1. We suppose that a building has 3 stories and thus that de surface of the building roof, S_r, is 1/3 of the total surface of the building S_b we get S_r = 1/3 S_b. From the commuting data we know that 50% of the staff number, noted N_s, comes by car to the laboratory. Taking 10 m^2 for a single parking slot at the ground floor level on campus the parking surface is S_p = 5 N_s. Our estimate of the surface available for solar panels is

$$S_s = S_b + S_p = 1/3S_b + 5N_s. \qquad \text{(S1)}$$

Table S6 summarizes the estimates for the potential electric production per laboratory using photovoltaics. Note that this potential should be considered an upper limit and taken with caution because the roof surfaces on chemistry buildings are often filled with hood exhausts and air conditioning which could reduce the effective available surface. In addition, covering parking lots with photovoltaic panels may be in contradiction with the reductions in car use considered in the *Commutes* section.

Nevertheless the potential electric production is significant, amounting to 30-50% of the electrical consumption in 2019, depending on the laboratory. Note, however, that the carbon intensity of solar electricity is 40 geqCO_2/kWh, which is only 30 % lower than the carbon intensity of the electricity from the French electric grid. As a result, a 50% switch from electricity consumed from the grid to photovoltaics would result in a 30 % reduction in electricity-related emissions.

Table S6. *Estimate of the maximum potential of electric production for each laboratory if photovoltaic panels covering the surface S_s, calculated using eq. S1, were used. The ratio of potential production vs. consumption uses 2019 data for the consumption (Fig. S3).*

Lab #	Staff number (N_s)	Indoor building surface (S_b, m^2)	Maximal surface available for solar panels (S_s, m^2)	Potential electric production (kWh/yr)	Potential electric production (kWh/yr/pers)	Ratio potential vs. consumption
Lab 1	76	3570	1570	3.14E+05	4132	0.34
Lab 2	222	10000	4443	8.89E+05	4003	0.43
Lab 3	468	16447	7822	1.56E+06	3343	0.50

Travel/business trips

Table S7. *Distribution of transportation uses for professional travels in the three chemistry laboratories for year 2019. Bottom lines: distance ratio made by long distance flights or train over the total distance travelled. Long distance: > 600 km.*

		Lab 1	Lab 2	Lab 3
distance (km/pers.)	plane (long dist.)	2464	4418	5390
	plane (short dist.)	50	268	190
	car	50	152	119
	train	678	1011	844
distance ratio	plane (long dist.)	0.76	0.76	0.82
	train	0.21	0.17	0.13

Table S8. *Duration of several trips by train, according to the French Railway Service SNCF. Other tools (example https://www.chronotrains.com) enable to estimate the duration of train trips from one city to another.*

Departure	Arrival	Geodesic distance (km)	Duration (hh:mm)
Lille	Brest	600	05:30
Lille	Hamburg (DE)	560	07:30
Lille	Geneva (CH)	570	05:20
Bordeaux	Valencia (ES)	590	10:30
Bordeaux	Marseille	500	06:10
Bordeaux	Geneva (CH)	540	06:20
Rennes	Antwerp (BE)	570	05:30
Rennes	Liverpool (UK)	590	09:00
Rennes	Grenoble	650	05:40

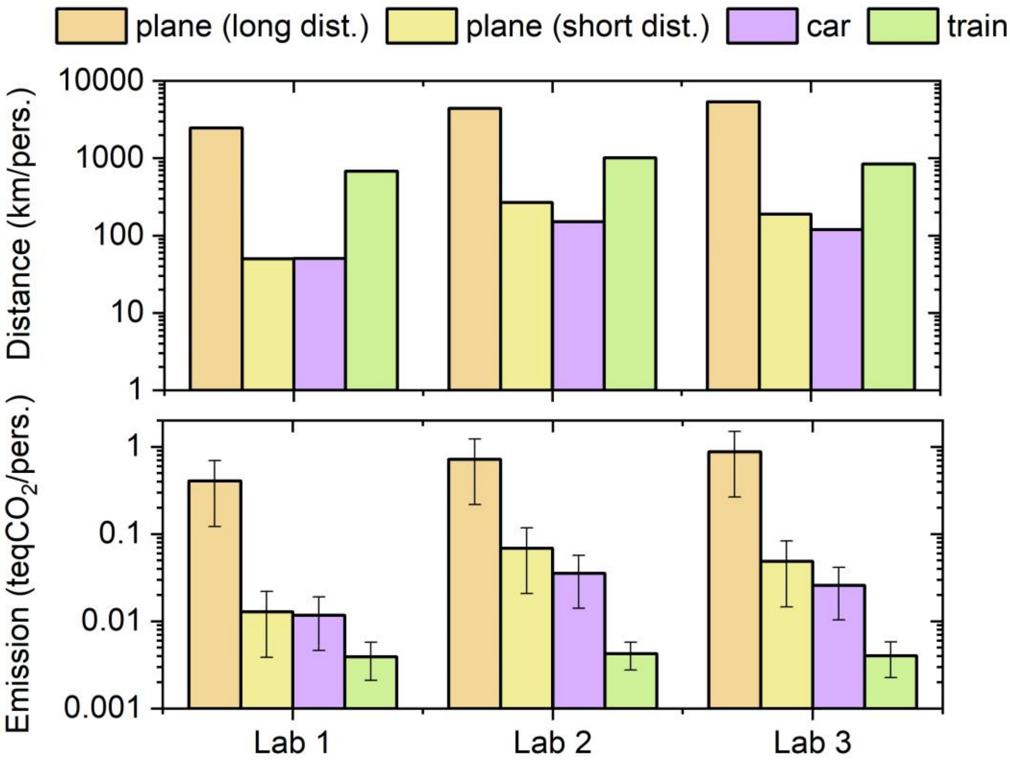

Figure S5. *Modes of transportation used during business trips (conferences, seminars, PhD committees...) for the three labs (top) and associated GES (down) for year 2019. Data are normalized per persons. Amplitudes are represented on a logarithmic scale.*

Commute

In order to know the mode of transportation of the employees of the different laboratories, an online survey (managed via the GAS 1point5 tool)[8] was sent to all the staff (PhD, post-doc, techs., researchers/teachers).

The questions were the following:

1. In 2019, on average, when you were not on vacation, how many days per week did you go to your workplace?
2. What modes of transportation did you use on the most frequent typical day in 2019? (Possibility to enter a 2nd typical day later if you have very different trips in the same week). (Choose between: walk, bike, electric bike, electric scooter, moto, car, city bus, long-distance bus, tramway, train, metro).
3. What were the total distances you traveled to and from on the most typical day in 2019?
4. Do you have another frequent typical day to report in 2019? (yes→go back to question 2 / no→question 5)
5. Simulation answer

Table S9. *Answers of the commuting survey. Category are: Researchers/teachers (α), technical staff/engineers (β), PhD and Post-doctoral fellows (γ)*

	Lab 1			Lab 2			Lab 3		
Category	α	β	γ	α	β	γ	α	β	γ
total	27	17	32	78	51	93	204	80	180
answers	24	10	8	46	35	26	113	61	46
% answers	90%	57%	25%	59%	69%	28%	55%	76%	26%

[8] Mariette, J.; Blanchard, O.; Berné, O.; Aumont, O.; Carrey, J.; Ligozat, A.; Lellouch, E.; Roche, P.-E.; Guennebaud, G.; Thanwerdas, J.; Bardou, P.; Salin, G.; Maigne, E.; Servan, S.; Ben-Ari, T. An Open-Source Tool to Assess the Carbon Footprint of Research. *Environ. Res.: Infrastruct. Sustain*. **2022**, 2 (3), 035008. https://doi.org/10.1088/2634-4505/ac84a4.

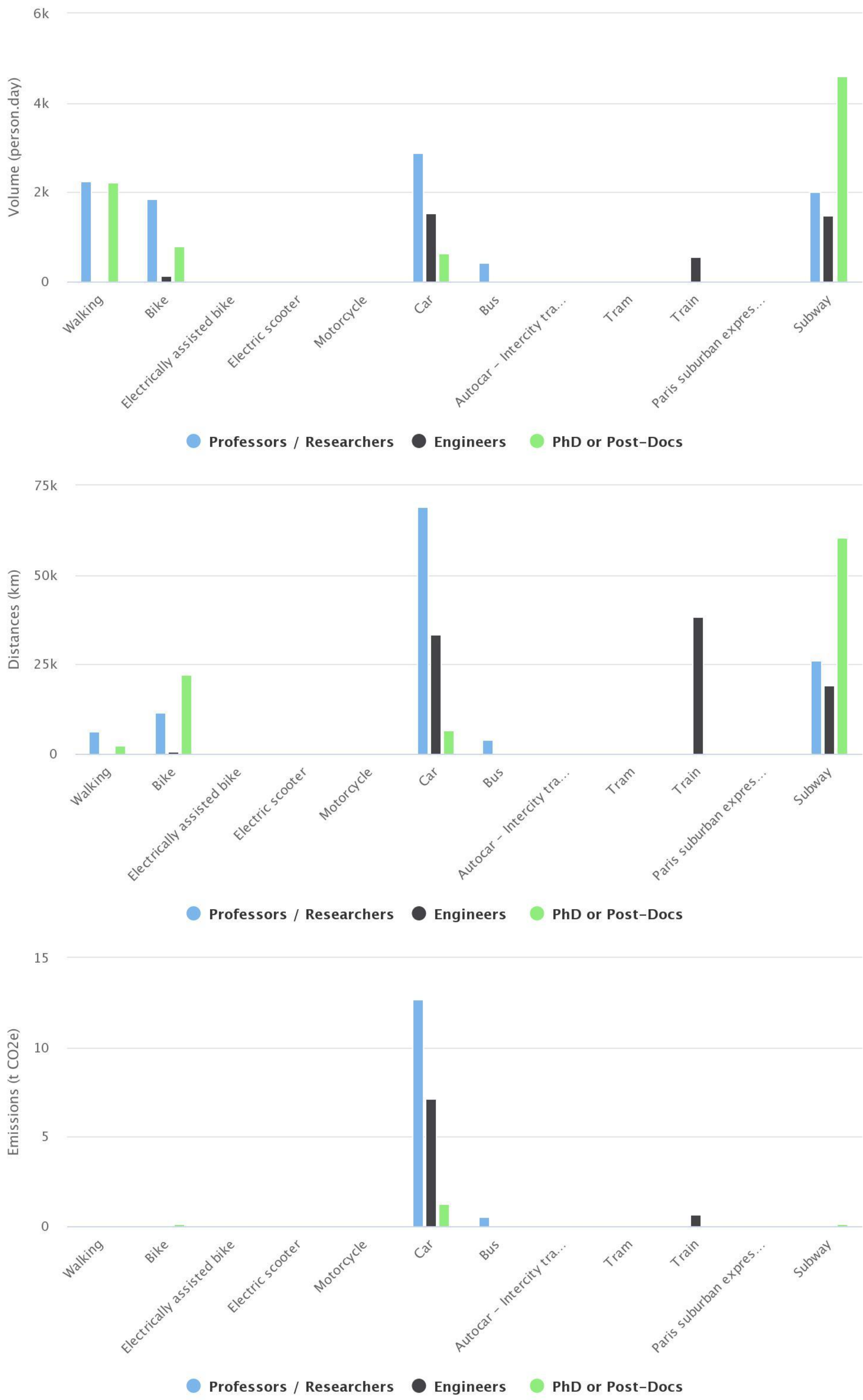

Figure S6. *Lab 1 commute survey results (year 2019). Answers rate: 55 %.*

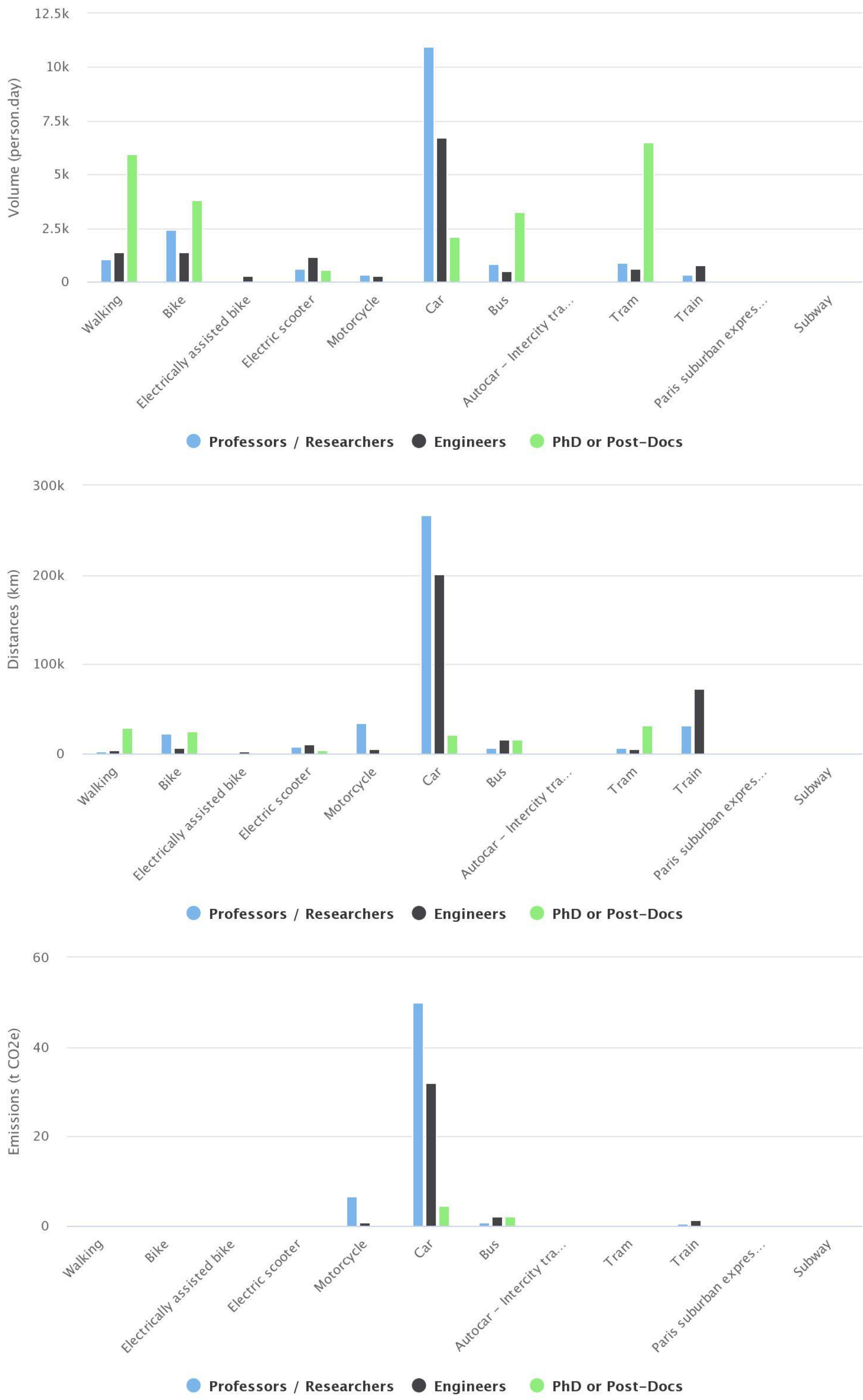

Figure S7. *Lab 2 commute survey results (year 2019). Answers rate: 48 %.*

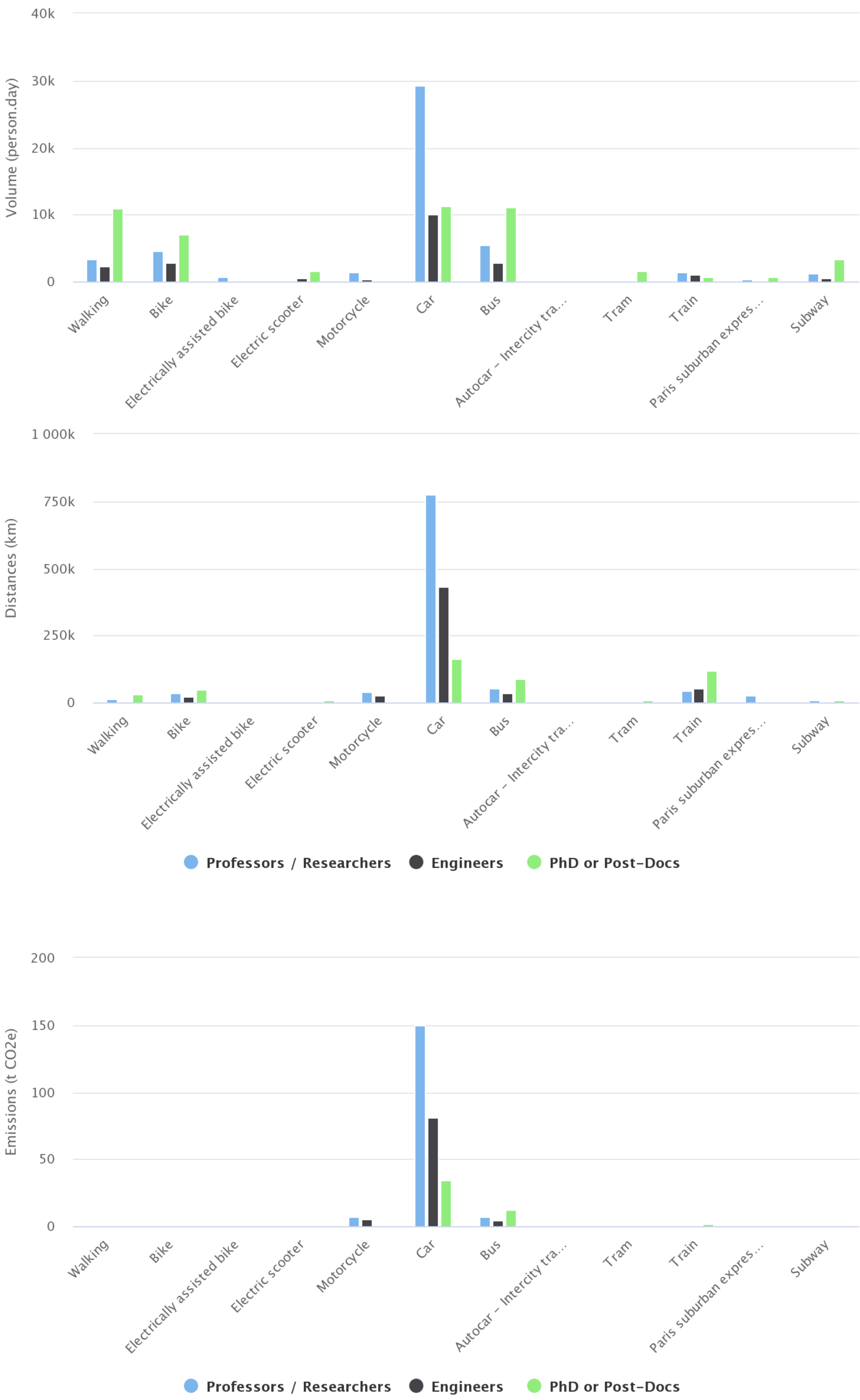

Figure S8. *Lab 3 commute survey results (year 2019). Answers rate: 47 %.*