INSTITUTO
UNIVERSITÁRIO
DE LISBOA

The Impact of Artificial Intelligence on the Pharmaceutical Industry

João Afonso Duarte Gonçalves e Santos Oliveira

M.Sc. in Business Administration

Supervisor:
Ph.D. Renato Jorge Lopes da Costa, Assistant Professor with Habilitation,
ISCTE-IUL

M.Sc. António Ângelo Machado Matos Pereira, Invited Professor,
ISCTE-IUL

June 2023

BUSINESS
SCHOOL

Department of Marketing, Strategy and Operations

The Impact of Artificial Intelligence on the Pharmaceutical Industry

João Afonso Duarte Gonçalves e Santos Oliveira

M.Sc. in Business Administration

Supervisor:
Ph.D. Renato Jorge Lopes da Costa, Assistant Professor with Habilitation,
ISCTE-IUL

M.Sc. António Ângelo Machado Matos Pereira, Invited Professor,
ISCTE-IUL

June 2023

Acknowledgements

This investigation represents the end of the most important academic stage of my life. A chapter that closes to give rise to blank pages in a future that I will always fight to be successful. It was an intense journey, with ups and downs and that would never have been possible to achieve without the very important people who have always surrounded me along the way and to whom I leave my deepest thanks.

To my grandparents, who not only now but throughout my life have always been figures of reference and a source of deep pride and admiration. Thanks for always being by my side.

To my parents and brother who never abandoned me and did everything to make this journey easier with motivation, patience and devotion. My deepest thanks for all your unconditional love and support throughout this entire process. Without you, this work would not exist and I am extremely proud to be able to call you family.

To my girlfriend Catarina, who was always by my side and encouraged me at all times, with love and patience, living this work as if it were her own. I will forever be grateful for all of your help and you have been a pillar of this journey. You will always be in my heart and thanks for being on my side at all times.

To my friends who never abandoned me and always cared about me, thank you for your support and patience and I am extremely proud to have shared this journey with you. A special thanks to José, João and Dinis for having lived up close and followed the whole process with care.

To my supervisor Professor Renato Lopes da Costa for all the shared knowledge and preparation, alongside with the interest for the topic.

To my co-supervisor Professor António Ângelo Pereira for all the motivation, precious help throughout this project and availability at all times.

To all interviewees and people who helped me, a deep thanks for the collaboration and insights provided.

Resumo

A Inteligência Artificial (IA) tem ganho grande importância em todos os setores empresariais, revelando enorme potencial na competitividade das empresas. Na indústria farmacêutica, inovação tem sido palavra-chave e está na linha da frente no que diz respeito à adoção de tecnologias vanguardistas (Malerba & Orsengio, 2015). Com o aparecimento da IA surgiu também a 'Pharma 4.0', caracterizada pela digitalização das estruturas desta indústria.

Esta investigação visa avaliar o estado de modernização e a influência que a IA tem nas empresas farmacêuticas. Pretende ainda avaliar as perspetivas futuras tendo em conta as tecnologias baseadas em IA e os benefícios que podem trazer para a indústria farmacêutica. Para este fim, os tópicos foram cuidadosamente considerados na revisão da literatura e aprofundados usando um método qualitativo por meio de entrevistas semiestruturadas a 17 intervenientes na indústria farmacêutica, incluído CEO's e profissionais de Estratégia Digital e R&D.

Os dados recolhidos revelaram que a indústria farmacêutica em Portugal se encontra numa fase inicial de implantação da IA, sendo Big Data, Machine Learning, Deep Learning e Robot Process Automation as tecnologias mais implementadas. Algumas barreiras que atrasam esta modernização estão relacionadas com razões financeiras e de fiabilidade, porém os benefícios que a IA traz são vários e espera-se que os investimentos cresçam futuramente. Globalmente, trabalhadores do setor farmacêutico português consideram a IA uma tecnologia disruptiva que pode potenciar os cuidados de saúde para um maior grau de qualidade e inovação, mas que também existem alguns constrangimentos que precisam de ser resolvidos.

Palavras-chave: Inteligência Artificial, Indústria Farmacêutica, Cuidados de Saúde

Classificação *JEL*:

I010 - *Analysis of Health Care Markets*
O320 - *Management of Technological Innovation and R&D*

Abstract

Artificial Intelligence (AI) has gained great importance in all business sectors, revealing enormous potential in the competitiveness of companies. In the pharmaceutical industry, innovation has been a keyword and it's at the forefront with regard to the adoption of cutting-edge technologies (Malerba & Orsengio, 2015). With the appearance of AI emerged 'Pharma 4.0', characterized by the digitization of the structures in the industry.

This investigation aims to assess the state of modernization and the influence that AI has on pharmaceutical companies. It also intends to assess future perspectives taking into account AI-based technologies and the benefits they can bring to the pharmaceutical industry. For this purpose, the topics were carefully considered in the literature review and deepened using a qualitative method through semi-structured interviews with 17 stakeholders in the pharmaceutical industry, including CEOs and Digital Strategy and R&D professionals.

The data collected revealed that the pharmaceutical industry in Portugal is in an early stage of AI deployment, with Big Data, Machine Learning, Deep Learning and Robot Process Automation being the most implemented technologies. Some barriers that delay this modernization are related to financial and reliability reasons, however the benefits that AI brings are several and it is expected that investments will grow in the future. Overall, workers in the Portuguese pharmaceutical sector consider AI to be a disruptive technology that can boost healthcare to a greater degree of quality and innovation, but that there are also some constraints that need to be resolved.

Keywords: Artificial Intelligence, Pharmaceutical Industry, Healthcare

JEL Classification:

I010 - Analysis of Health Care Markets
O320 - Management of Technological Innovation and R&D

General Index

Index of Tables

Index of Figures

List of Abbreviations

ADMET - Absorption, Distribution, Metabolism, and Excretion

AI - Artificial Intelligence

ANN - Artificial Neural Networks

AR - Augmented Reality

CEO - Chief Operating Office

CNN - Convolutional Network

CRPA - Cognitive Robotic Process Automation

DL - Deep Learning

DSRPAI - Dartmouth Summer Research Project on Artificial Intelligence

EBITDA - Earnings Before Interests, Tax, Depreciation and Amortization

GAN - Generative Adversarial Network

GPU - Graphic Processing Units

HTS - High-throughput Screening

IoT - Internet of Things

IT - Information Technology

KPI - Key Performance Indicators

ML - Machine Learning

MRI - Magnetic Resonance Imaging

NN - Neural Networks

OCR - Optical Character Recognition

OECD - Organization for Economic Co-operation and Development

PC - Portable Computer

QSAR - Quantitative Structure-Activity Relationship

R&D - Research & Development

RDA - Robotic Desktop Automation

RNN - Recurrent Neural Networks

RPA - Robotic Process Automation

SME - Small & Medium Enterprises

Chapter 1 - Introduction

1.1. Theme Framework

Today's modern world has been dominated by a digital era, which incorporates the well-known 'Industry 4.0', contributing to very technology-dependent industries in order to enable real-time optimization across the entire value chain and dynamic reactions to fluctuating product demand. This new 'Industry 4.0' brought a lot of differentiation factors to the present digital era, that includes Artificial Intelligence (AI) as one of the its biggest values. Its impact across a multidisciplinary world of industries is beyond measurable and can be applied in the majority of processes due to the incorporation of such broad technologies, like Big Data (BD), Machine Learning (ML), Deep Learning (DL) and Robotic Process Automation (RPA). (Peres *et al*., 2020)

In the pharmaceutical industry this is not an exception, and increasing needs of augmented manufacturing, personalized medicines and error reduction in production led to a natural evolution towards the use of vanguard technologies and AI. The pharmaceutical sector will also become more adaptable, intelligent, and personalized thanks to 'Industry 4.0', giving pharmaceutical firms a competitive edge (Reinhardt *et al*., 2021).

Examples that illustrate the uses of AI in the pharmaceutical industry exist in every step of the life-cycle of a drug, since the first stages of Research and Development (R&D), all the way through to its introduction in the market and beyond. But an overall analysis of the existing research of AI in pharma will show that "most of the work is focused on the research or drug discovery aspects" alongside with some initial efforts on clinical trials (Henstock, 2020, p. 26).

Taking a deeper look into the R&D stage of drug development, it should be no surprise on why this area is being so associated with AI technologies, given that it's where long-term profitability, competitiveness in the market and proficiency can more easily be found to companies, due to the high importance of innovation, cost reduction and efficient resource allocation. So, it's definitely undeniable the key role that R&D plays in the pharmaceutical industry, being considered the area that directly affects Key Performance Indicators (KPI) in the largest extent when compared to the rest of the business processes involved in the drug life-cycle. (Niño-Amézquita *et al*., 2018)

Taking into account all this, the present investigation has as primary objective to find answer to the questions directly related to the influence of one of the biggest and emergent

technologies on the pharmaceutical industry in Portugal, the AI. This will be done by understanding the state-of-the-art of AI in the Portuguese pharmaceutical market, more particularly in the initial stages of drug development, by exploring the way it affects R&D processes and enhances companies performance results, giving practical examples of its applications and by analyzing the importance those processes have in the value chain of the companies. From here, it will be possible to also perceive how does AI bring competitive advantages to companies in the pharmaceutical industry and if, in today's world and at the current moment is sustainable for companies to afford and adopt these technologies into their processes and if the returns of these investments will be seen in the short period or in a long-term perspective.

The secondary aim of the research is to understand the benefits and barriers of AI implementation in the pharmaceutical sector and also understand the short and long-term perspectives regarding the path that companies and governments will follow regarding the implementation of such technologies and what the industry can gain from this.

1.2. Research Problem

This investigation project will approach, more specifically, how the R&D processes in drug development are influenced by the use of AI technologies, in particular Big Data, Machine Learning, Deep Learning and Robotic Process Automation, that for some specific tasks can all be connected. This will allow us to investigate the market position of companies using these technologies and perceive similarities between them that represent a clear benefit taken from the application of AI in this stage. This is reasoned and supported by a literature review that is limited to the short existence of studies, reports and researches in the field of AI in Pharma, and also by interviews conducted to companies currently acting in the Portuguese pharmaceutical market, enabling a general perspective of what efforts are currently being made and how far can they go in a long run given the financial and resources limitations.

The pharmaceutical industry as always been characterized by its constant demand of finding new drugs that fit the needs of our world's populations, given the fact that, among many other factors, it's where companies find competitive advantages and higher financial returns. Innovation capacity and fearless approach to new technologies are key to these goals, and only those that can adapt and overcome these challenges are able to prevail in the market. In recent times, AI has been the newcomer into traditional industries, and in Pharma it has been used as an enormous stepping stone to reach the next level of differentiation between

companies, so it is only natural that these technologies are becoming more commonly used in drug discovering and development.

The more we move forward, more information is being generated that can be used in the R&D stage and bigger the datasets get, reaching a point where it's extremely expensive and time consuming to develop new medicines, given the huge error margins that exist, which lead to a lot of companies having no capacity to enroll in activities like these and many other that have to give up, fearing failure and loss of resources without any return. But AI technologies can become a new and fresh breeze in this stage, that help to spare time and money by reducing errors and enhancing the development speed of releasing a new medicine to the public, meaning faster returns on investment. Unfortunately, the pharma world finds itself in a very early stage of using AI due to high cost and uncertainty regarding its worth but by leaning on the existent literature, it's possible to find a variety of success cases.

The fear that is present in many occasions is mostly due to doubt and trusting issues towards AI, given that it is a relatively recent technology in the present and some fear to be substituted by it. As many other authors, Gunkel (2012) discussed this issue in a work that approaches the relation between humans and machines, stating that the introduction of intelligent machines is not supposed to substitute human workers, but to provide them more efficient and precise tools. And this especially true to the R&D world in pharma, where it's necessary a lot of rational thinking and scientific knowledge that only humans detain in nowadays. However, companies are now gaining perception about the potential of the technology and some are willing to put aside their fears and invest in this newer technologies in the short-term, while other that don't have the financial and human resources to do so, need to have a long-term perspective.

Following the presented, it's necessary to dig deeper in these various topics directly related to the research questions of this project, initiating by defining and understanding the history of AI and some of its principal ramifications, following by understanding the current state of this technology in pharma. Posteriorly, the relationship between AI and pharma will be studied analyzing how companies apply it to its strategies and processes and how these can leverage from the benefits this technology brings to the table.

1.3. Theoretical and Empirical Objectives

The topic definition for this master thesis dissertation project has 3 primary objectives. At the empirical level, the aim to is to enroll in a profound research with the goal of:

1) Understanding the relationship between AI, and other technologies, and the pharmaceutical industry in any of its stages, from the initial R&D phases, through clinical trials and all the processes associated with the entry and withdrawal of a drug from the market;
2) Identify and analyze the main intelligent tools being applied to R&D processes in the pharmaceutical industry in order to improve research processes and development techniques;
3) Identify the impacts and benefits of the use of AI in an intra-organizational environment of companies and in what forms it influences the market performance of the ones previously mentioned.

From these mains objectives, numerous research questions have emerged, such as: 1) What's the current level of technological development of the Portuguese pharmaceutical industry?; 2) What are the most commonly used AI technologies used in the Portuguese pharmaceutical industry?; 3) In which processes of the Portuguese pharmaceutical value chain are AI technologies more commonly used?; 4) What benefits does AI investment into R&D bring when compared to companies that don't do these investments?; 5) What are the impacts of AI investment on R&D in the short and long-term?

In order to materialize the objectives mentioned above, a deep literature review was conducted, which allows for a better understanding and comprehension of what type of intelligent tools are currently used in pharma and what impacts have been recorded from this practical implication, contributing for the evolution of the R&D of medicines and optimization of AI in this field. In addition, interviews were also conducted with professionals on the pharmaceutical industry in order to address these research questions from a practical point of view.

Posteriorly to the conclusion of this study, it will be possible for healthcare professionals and general population to perceive in detail what is AI and how it can be used to enhance the quality of new drugs and to decrease the time spent in introducing them into the market, given that the contact these previously mentioned have with the topic in question is mainly in the consumer perspective. It will also allow the analysis of a corporation perspective regarding the adopted strategies of companies in relation to business plans that aim to improve service quality and commercial performance, taking into consideration its limitations and market their inserted in, offering a first-hand vison that can help these to evolve and become more familiar with an industry that's technologically very developed.

1.4. Investigation Structure

This investigation will be divided into 6 different chapters, each one with a specific purpose.

In Chapter 1 will be provided an introduction to the study, explaining the theme framework, the research problem and also the theoretical and empirical objectives. In Chapter 2, a deep literature review will be conducted to raise awareness regarding the state-of-the-art about Artificial Intelligence, the Pharmaceutical Industry, and also the existing studies linking both of these main topics together. Chapter 3 presents an explanation on what led to the research questions that will be developed further within the investigation. Regarding Chapter 4, it explains the methodology applied in order to fulfil this research objectives and it also provides a sample characterization. Moving to Chapter 5, it will contain the results that originated from the chosen methodology and the consequent discussion between these results and the authors mentioned throughout the literature review presented earlier. The goal is to compare these perspectives and create new knowledge regarding the thematic of the study. Lastly, in Chapter 6, the main conclusions will be drowned, as well as the limitations of the investigations and further suggestions regarding future research.

Chapter 2 - Literature Review

2.1. Artificial Intelligence

2.1.1. A brief history of Artificial Intelligence

Humans are widely regarded as the most intelligent species on the planet. The feature that distinguishes humans from the rest of the living world is intelligence. On the other hand, human intelligence has its limitations. As a result, Artificial Intelligence (AI) is required, which is a technology that, when implemented in a system, allows it to acquire intellectual capabilities that can assist people in achieving greater human advancement. (Prasad & Choudhary, 2021).

The history of AI starts in 1942, when the American writer Isaac Asimov released a short fiction named “Runaround”, where the plot revolves around a robot developed by engineers. At the time, this fiction was considered revolutionary and Asimov’s work was an example for future generations of computer, AI, and robotics researchers. Around the same time, the mathematician Alan Turing, considered to be the father of computer science, was developing is work that he later published, in 1950, on a paper named “Computing Machinery and Intelligence”, offering what’s recognized as the "Turing Test", where a human interrogator attempts to differentiate between a computer-generated and human-written text response. It’s a remarkable milestone in the AI world, since it was the first experiment where a machine was able to exhibit intelligent behaviour. (Haenlein & Kaplan, 2019).

Marvin Minsky and John McCarthy established the Dartmouth Summer Research Project on Artificial Intelligence (DSRPAI) six years later, in 1956, which officially established the term Artificial Intelligence. The main objective of DSRPAI was to bring together experts from many fields to form a new study area targeted at creating machines that could mimic human intelligence (Haenlein & Kaplan, 2019). Here, Alien Newell, Herbert Simon and Cliff Shaw presented a reasoning program named “Logical Theorist”, that was able to solve *Principia Mathematica* complex problems and is considered to be the first AI program ever developed (Prasad & Choudhary, 2021). Years forward, these same scientists kept pushing boundaries, and developed the “General Problem Solver” in 1959, that automatically could solve math problems such as the ‘Towers of Hanoi’. Also on this same year, Arthur L.

Samuel, a computer scientist at IBM, developed the first checkers program on the IBM 701 which was considered a remarkable achievement for Machine Learning (ML). (Taulli, 2019).

Within this initial efforts, the systems relied heavily on complex searching techniques rather than finding solutions based on their understanding of the problem. But this paradigm changed with the creation of DENDRAL, the first knowledge-intensive system created by Edward Feigenbaum and Joshua Lederberg in 1965, that emphasized the advantage of specialized expertise over a generic problem-solving approach. This kind of systems became known as Expert Systems[1]. After this, other expert systems started to appear in the medical field like MYCIN and INTERNIST-I, but also in other areas of expertise with systems like Macsyma, R1, PROSPECTOR and LUNAR (Prasad & Choudhary, 2021).

However, expert systems struggled in areas where formalization isn't possible. For particular activities, a system must be able to accurately understand external data, learn from it, and apply what it has learned to fulfill specified goals and tasks through flexible adaptation. These systems lack these properties and so are not considered real AI. Statistical techniques for creating true AI have been debated since the 1940s, when Donald Hebb, a Canadian psychologist, established Hebbian Learning, a learning theory that mimics the human brain's neuronal processes. As a result, it was given birth to the Artificial Neural Networks[2] (ANN) - widely known as Deep Learning (DL) (Haenlein & Kaplan, 2019). Frank Rosenblatt concurred that neural networks and other comparable brain-inspired technologies should be used in AI and so, he created in 1957, the Mark I Perceptron, the first computer program that could help differentiate between two images (Taulli, 2019). This work, however, came to a halt in 1969, when Seymour Papert and Marvin Minsky demonstrated that computers lacked the processing capability needed to handle the job required by ANN (Haenlein & Kaplan, 2019).

During the next decade, came what is known as the “AI Winter” that would go as far as 1980, as the enthusiasm for AI started to decrease. This was due to a variety of complex aspects regarding the understanding of intelligence and reasoning and also to the economic environment during this period, that was far from favorable to investments in this field. Nonetheless, AI still accomplished some significant progress like the backpropagation, crucial to establish connections between input and output layers in ANN, but it was primarily

[1]A computer software that mimics the decisions and actions of a human having in-depth subject matter expertise and experience. They are built on a foundation of learned experience and have a set of guidelines that they use in every situation (Gupta & Nagpal, 2018).

[2]Mathematical simulation of the composition and operation of organic brain networks. An input layer, one or more hidden layers, and an output layer make up this structure (Suzuki, 2011).

academic and limited to controlled conditions. During the 1980's and early 1990's, expert systems became a central topic once more due to the exponential growth of PC's and minicomputers, allowing them to enter the industry and have commercial use. One of the systems created in this period was John McDermott's XCON, launched in 1980, considered to be the first recommendation engine. After this huge success, the expert systems turned into a billion-dollar industry and many companies and governments started investing in them, such as IBM that developed Deep Blue in 1985 and Japan that invested hundreds of millions to frost its home market. Nonetheless, there were problems with expert systems that caused them to lose traction in the business world. For instance, the lack of ability to learn autonomously overtime implied great costs and the complexity to update them as these got larger, it became harder to feed them data. This boosted the reappearance of ANN, that were in a growing spiral since 1986 due to the work of Geoffrey Hinton in the paper "Learning Representations by Back-propagating Errors" (Taulli, 2019).

From here on, a lot of developments were made regarding ANN that culminated in the creation of AlphaGo, developed by Google in 2015. This was a tremendous milestone for AI, as the program was able to reach this high performance due to the use of specific type of ANN called Deep Learning. Nowadays, these "form the basis of most applications we know under the label of AI" (Haenlein & Kaplan, 2019, p. 4).

As of today, AI as a lot of different technological drivers besides some new models or approaches, that help it to grow and prevail in the modern era. Some of the main ones are the increase in massive datasets, the Graphic Processing Units (GPU's) that are extremely important in Deep Learning research, and the infrastructure that is supported by major companies like Google that have made significant advances is AI in the past decade (Taulli, 2019).

2.1.2. Modern Artificial Intelligence

Artificial Intelligence has made huge progresses since its early days but it's still on a very embryonic stage of reaching its full potential. Lots of derivate technologies from Artificial Intelligence have been on constant evolution like the ones that are going to be mentioned forward. These, upon deep research on the topic, are the most mentioned technologies to be used in the pharmaceutical industry, more specifically on R&D processes and investigation.

2.1.2.1. Big Data

The volume of digital data is rapidly increasing as a result of rapid digital technology innovation. Consequently, massive quantities of data are generated from a wide range of sources, including social media, smartphones, sensors, and so on. Big Data is known for massive amounts of data containing diverse formats that can be structured, unstructured and semi-structured data and that traditional relational databases and analytical algorithms have no capacity to store and interpret (Rahmani *et al*., 2021).

However, there isn't a consensual and clear definition of Big Data and this is a very broad way of defining it. Nevertheless, there are characteristics that are crucial for Big Data to be considered as it, normally described by three main V's. The first one stands for Volume, which as stated by Rahmani, *et al*. (2021) represents the scale and enormous amounts of data produced in the smallest scale of time. It is a major challenge for Big Data to cope and store all this information but next-generation databases and cloud computing have been extremely helpful regarding this task (Taulli, 2019).

Next, there's Variety which describes the diversity of the data that can be in different formats, as mentioned above. In the procedure of managing this, ML is often very useful to streamline the process (Taulli, 2019). Lastly but not least is Velocity and it "denotes the speed of data production and processing to extract valuable insights" (Rahmani *et al*., 2021, p. 3).

Besides these mentioned V's, currently some more have been added such as Veracity, Value, Variability and Visualization. This shows how complex and difficult it is to manage Big Data and in fact, about 85% of Big Data projects are dropped in early stages due to various reasons such as dirty data, wrong investments on information technology (IT) tools or problems with data collection. This illustrates the importance of the role AI can play in this managing and analysis processes. But to succeed with AI there needs to be a data-driven culture because it increases the quality of decision making (Taulli, 2019). A research conducted by Rahmani, *et al*. (2021) on Big Data analysis using AI mechanisms concluded that various subfields of AI can be applied such as "machine learning, knowledge-based and reasoning methods, decision-making algorithms, and search methods" (Rahmani *et al*., 2021, p. 19). Furthermore, the four most significant qualitative parameters - scalability, efficiency, precision and privacy - were defined to access each analysis method. The conclusions were that each method have advantages and drawbacks but it sets the ground for future research and reveals that AI is, nowadays, the only technology with the necessary potential to fully exploit Big Data and its applications.

An avant-garde and every day more popular approach to Big Data are smart cities, "as it offers the potential for cities to obtain valuable insights from a large amount of data collected through various sources (…)" (Hashem *et al.*, 2016, p. 1).

2.1.2.2. Machine Learning

Ever since, humans have used various tools to meet diverse life needs in simpler ways and this evolutive process led to many innovations that our species still use nowadays. According to Arthur L. Samuel, previously mentioned as a pioneer in AI, "machine learning is defined as the field of study that gives computers the ability to learn without being explicitly programmed" (Mahesh, 2019, p. 1).

Machine Learning is a technique for teaching machines how to better handle data, as sometimes, upon collecting the required data, we are unable to evaluate the extracted information. In that instance, Machine Learning is used relying on different algorithms to solve related problems. However, there isn't a "one-size-fits-all" type of algorithm that answers all the questions. In fact, depending on the problem intended to solve, there are different kinds of algorithms that can be employed to have a more suitable and efficient resolution (Mahesh, 2019).

It's important to acknowledge that algorithms specific for ML are normally different from the traditional ones and the main reason is that the first thing to do in ML is process the data in order for the computer to start learning autonomously. In addition, there are hundreds of algorithms available, and some are easier to calculate than others but usually there's no need to compute them, as there are a variety of languages that make this process straightforward (Taulli, 2019).

Despite the wide range and variety of existing algorithms, they can be divided into four main groups. The first is Supervised Learning, characterized by the existence of a supervisor, which in actual algorithms is provided by a training set composed of input and expected output that allows the agent to correct its parameters and reduce global loss function. Nevertheless, the ultimate goal is to train a system to work with samples never seen before and avoid overfitting[3]. Some common uses for supervised learning are pattern detection, natural language processing or even automatic sequence processing (Bonaccorso, 2017).

[3]A model that is overly capable but unable to generalize when the training set's original dynamics are taken into account (Bonaccorso, 2017).

Next, there's Unsupervised Learning which is normally used when working with unlabeled data, meaning that Deep Learning algorithms are used to detect patterns on the information (Taulli, 2019). This means that few features are learnt from the data itself but instead from previously learned features for recognition of different classes of data (Mahesh, 2019). There are two main uses for Unsupervised Learning. One of them is for clustering, which takes unlabeled data and groups the related objects together using algorithms. The other one is for sentiment analysis, that uses social media data to discover trends (Taulli, 2019). Some examples of unsupervised applications are object segmentation, similarity detection or automatic labeling commonly used in logistics (Bonaccorso, 2017).

Another group is Reinforced Learning, that's similar to Supervised Learning because even if there isn't a supervisor, it's based on inputs from the outside world. Regardless, "this information is more qualitative and doesn't help the agent determining a precise measure of its error" (Bonaccorso, 2017, p. 14). This algorithm its supported on positive and negative reinforcement, and makes its way through a trial-and-error process. Common examples of its applications are in games or robotics (Taulli, 2019).

Lastly, the final main group is Semi-supervised Learning, a conjugation of Supervised and Unsupervised Learning, and it's useful when the data available is a mixture of unlabeled and labeled. A practical application of this is the interpretation of Magnetic Resonance Imaging (MRI), where the radiologist first label the scans and afterwards can apply this algorithm to find the rest of the patterns (Taulli, 2019).

Within each one of these four main groups there are sub-groups of algorithms with particular properties that are applied in more specific situations. Besides this, almost every one of us uses machine learning every day, whether knowingly or unknowingly, in situation as getting recommended products when shopping online or updating photos in social media (Mahesh, 2019).

2.1.2.3. Deep Learning

It is not uncommon to confuse Deep Learning with Machine Learning because both share several similarities, given the fact that the first is a subfield of the second, but some differences can still be found. For instance, in the development of a conventional ML project, the identification or design of features that are required to the seeking project can be very time consuming due to the fact that the it's necessary to humanly provide training to the machine for it to know what to measure and how to do it. On the other hand, DL approaches this

process in a different way, given the fact that it learns automatically the required features from the raw data without the need for human-engineered features (Kelleher, 2019).

This ability to learn autonomously is what ultimately distinguishes DL from the traditional ML approaches. The way this is achieved, is through the previously mentioned Neural Networks (NN) and its hidden layers, which provide a greater power to learn. To better understand this process, it's critical to gather knowledge of the mechanisms behind this process and for this effect let's use the most basic form of a NN, the Artificial Neural Network, a function that incorporates units or neurons, each one with a value and weight that represent its importance, that will then be linked into the hidden layers of the NN and result in an outcome. On the other hand, there's a drawback on this process which are the adjustments to the weights and values of the units but with the use of backpropagation[4] it was possible to correct this, as the function would automatically adjust them and integrate the new values, constantly optimizing the model (Taulli, 2019).

Besides ANN being the most basic form of a neural network, it's possible to find other types such as the Convolutional Neural Network (CNN), the Recurrent Neural Network (RNN), or even the Generative Adversarial Network (GAN). Regarding the RNNs, these are designed to process sequential data. The way it processes a stream of data is by going through each element one at a time. Also, this network has only one hidden layer, but also features a memory buffer capable of saving the hidden layer's output for one input, enabling it to re-enter the hidden layer with the following input in the sequence. This means that each input is evaluated within the context that was created by evaluating the prior input. On the other hand, CNNs were originally designed for tasks related with image recognition and were first used for the specific case of handwritten digit recognition. The main design aim of was to develop a network in which early-layer neurons extracted local visual features[5], while later-layer neurons combined these features to form higher-order features. The critical task here is learning the feature detection functions but there's another challenge in the architectural design of this type of network, which is to guarantee that the network is able to recognize a local visual feature irrespectively of where it appears in the image and this requires a "translation invariance", as stated by Yann LeCun in 1989. Lastly, there's also the GANs,

[4]An algorithm used to calculate derivates within a feedforward neural network and it allows to calculate the gradient of the loss function regarding each weight of the function, enabling an individual update and, therefore, reducing the loss function over many different interactions (Thomas Wood, 2020).

[5]Feature is an image whose scope is restricted to a small patch, representing only a fraction of the total product (Kelleher, 2019).

which are composed by two neural networks, a generative model and a discriminative model. When fed with a real set of data, the generator must learn the distribution of this data and be able to synthesize fake information that will be passed to the discriminative model, that on the other hand, must learn to discriminate between the real and false data inputs. This is particularly helpful in supervised learning and the GANs have gained a lot of attention in recent years (Kelleher, 2019).

As stated before, DL as the ability to learn by itself without human intervention and it does so by relying on hidden layers analysis and hierarchical methods. For this reason, it has multiple applications to real life. One of the most avant-garde examples is in image processing, with facial recognition but a company named Sighthound Inc. took this a step further and developed a DL based software capable of recognizing not only gender and age but also emotions. Another area that can benefit a lot from DL is medicine, for example in disease prediction, as it's possible to process an image retrieved from a MRI of a human brain to make a prediction about the possibility of Alzheimer's disease (Vargas *et al*., 2017).

2.1.2.4 Robotic Process Automation

Three of the main fixtures of AI have already been addressed, but there's yet another field related to AI that is extremely useful in diverse areas of expertise, called Robotic Process Automation. Although the term may sound complex, it refers to software-based robots, or bots, that enable the workflow automatization of a process by utilizing a low-code visual drag-and-drop systems. As a matter of fact, this can be achieved with the RPA program simply recording the working processes of an employee for a specific task, and this is the reason why this technology is sometimes referred to as a digital employee. (Taulli, 2019).

The RPA can act in two distinct ways, depending on the functions that are necessary to develop. It can play an unattended role by automatizing activities or tasks in the background such as changing values on specific cells of a spreadsheet, only requiring human intervention when the bot finds something it doesn't understand or it can act as a Robotic Desktop Automation (RDA), functioning with the goal of assisting humans in particular tasks like in a contact center, where it guides the employees through the workflow depending on the answers that are registered (Hofmann *et al*., 2018).

Understandably, there can be a lot of advantages coming from the correct implementation of RPA, such as minimization of errors, scalability, compliance with specific rules or regulations, which leads to a more cleaner and higher quality data. In addition, it is also

possible to gain a lot of insights and analytics, given the fact that this bots can measure KPI's for the companies and alert when something goes off track. However, on the other side of the equation, there are also some landmines to note. For instance, RPA can be extremely fragile and break if there are any alterations to underlaying applications or procedures and it can be somehow difficult to implement due to resistance and fear that jobs will be lost and replaced by this technology, which can backfire to the company. Nevertheless, even though RPA is still on its initial stages, the advantages it brings to the table can be numerous, mainly by helping companies on process optimization and to achieve better results overall. As expected, these kinds of tools are already being developed with AI, which has recently resulted in the appearance of software bots known as Cognitive Robotic Process Automation (CRPA). This joint venture means that new optimization possibilities were unlocked, especially for the processes that involve large datasets, by implementing systems such as ML, DL, speech recognition or Natural Language Processing (Taulli, 2019).

Nowadays, there are already some RPA tools that operate with AI support like *AssistEdge*, owned by EdgeVerve Systems, that process documents through Optical Character Recognition (OCR) and allows automatic data extraction and analysis with the help of Artificial Neural Networks. Operating similarly to this software, there are some other such as *Automagica*, *WinAutomation* or *Automation Anywhere* (Ribeiro *et al.,* 2021).

These software robots are a changing of events for companies, by autonomously executing workflows of processes that once were made exclusively by human-hands with relatively low costs of implementation. It can definitely bring advantages to organizations, although some claim that this "is only a provisional step between human work and process re-engineering". Regardless, it is undeniable that RPA can solve diverse problems and create new solutions that improve performance and results for the companies that are able to integrate them into the usual operations (Hofmann *et al*., 2018, p. 103).

2.1.3. Artificial Intelligence applications and challenge

According to Cubric (2020), regarding a study conducted to understand Artificial Intelligence adoption rate across multiple business sectors, the author shows an analysis from 2017 conducted by PwC that reveals that the potential contribution of AI to the global economy in 2030 may exceed the combined output of China and India today. This tells us that these AI derivate technologies are being adopted more and more across a wide range of sectors, mainly because it allows businesses and employees to improve outcomes and general performance on

recurrent tasks (Shabbir & Anwer, 2018). The drivers of these growing adoption rate are mostly economic instead of social, as expected on a widely capitalist culture but there are also barriers, some of technical nature and others of financial nature, such as costs and infrastructures (Cubric, 2020). According to authors like Shabbir & Anwer (2018), as a new production element, AI will become essential for establishing a competitive edge and it has the potential to dramatically increase business profitability. Several solutions have already been implemented in a variety of industries, including finance, healthcare, manufacturing, retail, among many others.

For instance, in healthcare, AI has the potential to enhance patient care, diagnoses and interpretation of medical imaging, which could be crucial in areas like radiology (Dwivedi *et al.,* 2021). In addition, the creation of AI algorithms based on, for instance, machine learning, help doctors to make better and more certain decisions (Dreyer & Allen, 2018).

In manufacturing, diverse studies conclude that organizations are likely to adopt AI in the perspective of this technology act as a co-worker for key tasks or even to solve problems (Haeffner & Panuwatwanich, 2017). It is possible to experience examples of these on "smart factories", where a wide variety of processes is controlled via robots programmed using RPA technology (Dwivedi *et al*., 2021).

Moving to retail, it is very common to find examples of AI applications that are around us on our everyday life without us even realizing it. For instance, ML is widely used by companies to help them predict and analyze shopping habits of consumers, helping them with marketing and targeting campaigns (Shabbir & Anwer, 2018).

Concerning the financial sector, trading has recently become a very popular area for AI and this industry has seen a major transformation thanks to this technologies, which has automated the trading process and enabled numerous trading algorithms to generate profits without the need for human interaction. Also, the area of cybercrime has seen a major evolution due to AI, that has been used to fight against this practices, by using Machine Learning to detect intrudes, analyze malwares and search for phishing schemes (Ghimire *et al*., 2020).

Despite all these examples, that belong to an exhaustive list of sectors with examples of AI applications, and the opportunities that are created, there are challenges in what concerns to the application of these technologies in any sector. These barriers can be social, economic, data related, organizational, political or ethic (Dwivedi *et al.,* 2021). For instance, some problems that have been appointed to AI are the expensive and high investments that are necessary, the low reliability that it can provide under certain tasks and the structural changes

that would be necessary to accommodate this technology into companies (Bhbosale *et al.*, 2020).

2.2. Characterization of the Pharmaceutical Industry

2.2.1 Evolution of the Pharmaceutical Industry

The pharmaceutical industry is, undeniably, in continuous change since its existence as a consequence of diverse interactions between various exogenous events and endogenous responses to multiple factors such as scientific and technological evolution, political changes and economic factors. Despite the fast paced changes in our world, this industry has remained as one of the most innovative and on the vanguard of technology, due to the importance both these factors play in the competitiveness of the companies and ability to gain the biggest advantages over the competition (Malerba & Orsengio, 2015).

The birth of the pharmaceutical industry was in the final stages of the nineteenth century as a branch of the chemical sector and the pioneers were mainly German and Swiss companies such as Bayer, Sandoz and Ciba, that exploited their knowledge regarding organic chemistry and dyestuffs. In the United States, the industry started later in the turn of the century and the major companies relied heavily in technologies developed by the European companies and they could be distinguished in two main groups. The first one that focused on production and marketing of already existing drugs and a second group that developed chemically based prescriptions.

The industry experienced a fast growth and development that was supported by high demand for drugs, a consequence of population growth and unmeet medication needs. Alongside with these factors, the appearance of patent legislation in 1946 for pharma products also helped to reduce imitation and price competition, which induced the major companies to invest in R&D and contributing to this evolution with new discoveries and medicines. As consequence of this, the take-off of the industry started in the 50's, the beginning of the "Golden Age", with the innovation growth, where the R&D to sales ratio arise from 3,7% in 1951 to around 10% in the 60's and several hundreds of new chemical entities were discovered and new drug classes introduced in the following two decades. During this period, the pharmaceutical industry became truly international, mostly due to the high expenditures involved in the R&D and marketing, which obligated the companies to look for new markets

in order to cope with the average costs. The industry saw strong rates of innovation, expansion, and profitability within this favorable environment. From the 1950s to the 1980s, annual growth rates were far above 10 percent on average and the industry was highly profitable.

Despite all this, in the middle of the 70's, the majority of the factors that sustained the "Golden Age" have suffered fundamental changes. For instance, there were drastic changes in technological world that largely changed the way R&D was done and it was in 1976 that biotechnology was born, with the company Genetech, to change everything in the pharma environment, from intellectual property rights to expenditures and all that comes with this. The next years were extraordinary for the industry, with significant investments being made by incumbents and a vast range of new firms entering the market.

With all the evolution experienced, the 80s and 90's were marked with strong economic and financial performances from the industry. In this period, with the appearance of high-throughput screening (HTS) and combinatorial chemistry, R&D became more industrialized, enabling the creation of new compounds and the creation of more precise and effective drugs. In addition, further progress in R&D was made in the various "-omics", bioinformatic, synthetical and structural biology that led to continuously add new limits to progress. But the turn of the century brought changes in these perspectives, with stagnation in innovation, disputes over intellectual property rights and withdrawal of successful drugs from the market. All this hurt most companies financially and the cost of bringing a new medicine to the market was more than 1 billion dollars, and in 2002, the general expenditures for a company in the industry were thirty times higher than in the mid 80's and new regulations also brought rising costs. This raised concerns regarding innovation and research for the turn of the century, alongside with the increasing difficulties of finding new drugs, as "the low hanging fruits have already been picked and now the challenge becomes harder." (Malerba & Orsengio, 2015, p. 15).

Throughout the past two decades, there have been impactful changes to the operational model and footprint of the pharmaceutical and biopharmaceutical business (Gautam & Pan, 2016, as cited in Reinhardt *et al.,* 2020). Nowadays, the pharmaceutical market is already in the new industrial stage of Industry 4.0, where technologies are converging to provide digital solutions, focusing on a lean and more research oriented industry, with focus on innovation, aiming to generate growing streams of revenue. This is consequence of the emergence of new technologies such as Artificial Intelligence and Augmented Reality (AR) (Reinhardt *et al.,* 2020). But there are fundamental pillars to the Industry 4.0 which allow its proliferation

across industries such as Internet of Things (IoT), Big Data and data analysis, autonomous robots, among many others (Pereira *et al.,* 2022).

In the pharmaceutical industry there's no exception and there's been a growing number of applications of these rising technologies on the diverse processes of the R&D value chain of the pharmaceutical industry, leading to the creation of Pharma 4.0[6], whose implementation has been successful around many big pharma companies such as AstraZeneca, Roche and Novartis, but an assessment of the literature on Industry 4.0, Pharma 4.0, and related issues found that there was a dearth of published information on how ready the industry was to implement 4.0 technologies (Reinhardt *et al.,* 2020).

However, Pharma 4.0 still has a long way ahead and a survey of 80 pharmaceutical professionals in Ireland showed that only 42% of participants were aware about this recent trend. On the other hand, it also revealed that most pharmaceutical companies are adopting elements that serve as a base for Pharma 4.0, such as newer technologies as AI and modern infrastructures. Some these elements enable the evolution in innovation, efficiency, quality in development and much more. The COVID-19 pandemic also helped to speed the integration of Pharma 4.0, and revealed that the industry is ready to make the transition to this new era in a global scale. Unfortunately, it could take two or three more decades until Pharma 4.0 becomes a full reality, mainly for financial and human reasons, but also because "the pharmaceutical industry in general has a risk-averse attitude towards the adoption of new technology due to its strong emphasis on regulatory compliance". Only when these barrier is crossed, can this era be fully developed at an innovative-like speed. (Sharifzadeh, 2022, p. 314).

2.2.2. Pharmaceutical Industry in Portugal

In Portugal, the problematic is the same as abroad, given the lack of research and literature, still being somehow unknown the degree of integration of Pharma 4.0 into the industry. In despite, a study conducted by Mendes (2020) with two Portuguese pharmaceutical companies concludes that there's still a relative unfamiliarity of this reality within the company's employees and a big resistance to change in the Portuguese national market, hampering the implementation of this digital transformation in the short-term. It's not possible to generalize this investigation given the small sample in analysis, yet, it transmits the idea that is very

[6] The framework known as "Pharma 4.0" allows for the customization of digital strategies to the particular conditions of pharmaceutical manufacture.

difficult to assess the level of technological development and digital transformation among the pharmaceutical industry in Portugal and that the country is still in very early stages in the this transition phase. In fact, according to Oxford Insights & International Development Research Centre (2019), Portugal is ranked 15 out of 23 countries in Western Europe in level of readiness to receive AI technologies and the classification is based on criteria such as governance; infrastructure and data; education; and government and public services.

2.3. Artificial Intelligence and the Pharmaceutical Industry

2.3.1. Artificial Intelligence driven transformation in pharma

Technologies based on AI tend to impact a broad range of industries, bringing new opportunities and challenges wherever they are implemented in and the pharmaceutical industry represents no exception to this. In fact, All pharmaceutical businesses seek ways to make their operations more efficient in order to, among other things, research and develop new medicines, adhere to the stringent regulations set by the sector, and meet the required financial thresholds (Kulkov, 2021). In addition, the increasing data-driven demands combined with scientific decision-making that govern modern pharma, make the industry a strong candidate for the application of AI technologies (Henstock, 2019).

As stated by Paul, *et al*. (2021), this technology can be key to solve healthcare complex problems and it's not a threat to humans, as it cannot replace them completely. Also, the uses for AI in the pharmaceutical industry are various and can be applied in different sectors. For instance, AI can be applied in drug discovery and development, drug repurposing, improving pharmaceutical productivity and clinical trials, among many other.

Thus, the importance of automation will increase as a result of the use of the most advanced AI-based technologies, which will not only shorten the time it takes for products to reach the market but will also increase product quality, production process safety, and resource efficiency (Paul *et al*., 2021).

All the examples mentioned above make it clear that the application of AI, through Machine Learning, Deep Learning and other technologies, can improve the diagnosis, quality of healthcare, and the development of new drugs based on algorithms capable of enhancing analytical analysis, revolutionizing the field of medicine and life sciences as a whole (Leite *et*

al., 2021). This conclusion is also corroborated by Henstock (2020) stating that AI has the potential to completely transform the pharmaceutical industry.

According to McKinsey, investing in AI might yield 39% more value for the pharmaceutical sector than doing so with conventional analytics methods like statistics and visualization. Such an investment in AI would result in double digit gains in research, clinical trials, and commercial domains, and a 45-75% boost in companies' EBITDA. However, a recent study by ThoughtLab on AI spending across various sectors discovered that the pharma/life sciences sector's investment is significantly less than the industry average of 0.75% of revenue (Henstock, 2020).

Nonetheless, AI investments increased from US$200 million in 2015 to US$700 million in 2018, and the prediction is to increase all the way up to $5 billion by 2024. This evidences that pharmaceutical companies are beginning to understand the potential and influence of AI in the sector. AI is predicted to disrupt the pharmaceutical and medical industries, with a 40% estimated rise between 2017 and 2024 (Paul *et al*., 2021).

2.3.2 Artificial Intelligence investment by pharmaceutical companies

It's important to notice that there's a lack of studies and literature regarding the investment decisions of pharmaceutical companies on AI, what can be a limitation to fully understand the supporting reasons behind how and why these companies implement this technology into their different departments but besides this, it's clear that this is an unavoidable step to take for the industry to keep along with modern era of technological evolution.

Nevertheless, Kulkov (2021) conducted a study with the goal of identifying specifically the impact of AI on the core business operations and supporting systems of pharmaceutical firms with the goal of identify where this technology could be more useful. For this purpose, fifteen different sized pharmaceutical companies were surveyed in order to understand how they choose in what departments and business processes to invest in AI, based on the practical impact it would have for the company. The results showed that size and specialization are two key factors that affect this decision and also that R&D is the field that can benefit more from AI, as the companies unanimously claimed that this technology can have a major impact on the business processes inherent to this stage, such as target and leads identification, screening or even in the prediction of structure-activity relationships.

What this means is that, in practice, pharmaceutical companies are allocating more financial resources on AI to support R&D, independently of the business processes inside of

it, because "this expenditure affects SME growth", helping with "the goal of generate maximum profits and increase sales" (Niño-Amézquita *et al*., 2018, p. 162).

In addition, various authors agree that R&D is the area where pharmaceutical companies have invested more in recent years, due to the great influence it has over the companies proficiency when compared to other areas. Also, "larger companies (…) use AI more than midsized or small companies, which is not surprising given their budgets and staffing. In addition, larger companies also seek innovation and new approaches to drug development given the high cost of development and the desire to differentiate treatments in increasingly competitive disease areas" (Lamberti *et al.,* 2019, p. 1423).

Despite the few studies on this matter, it's possible to conclude that size and specialization are important to decide the business processes in which to implement AI, but there seems to be a pattern among companies that R&D is the most influential area to develop due to its overall influence on KPI's of the companies. Nonetheless, all the other areas are important as well but the impact they have on the performance is not that crucial when compared to R&D, and that might be a reason that justifies the increasing investment on this stage's processes (Niño-Amézquita *et al*., 2018)

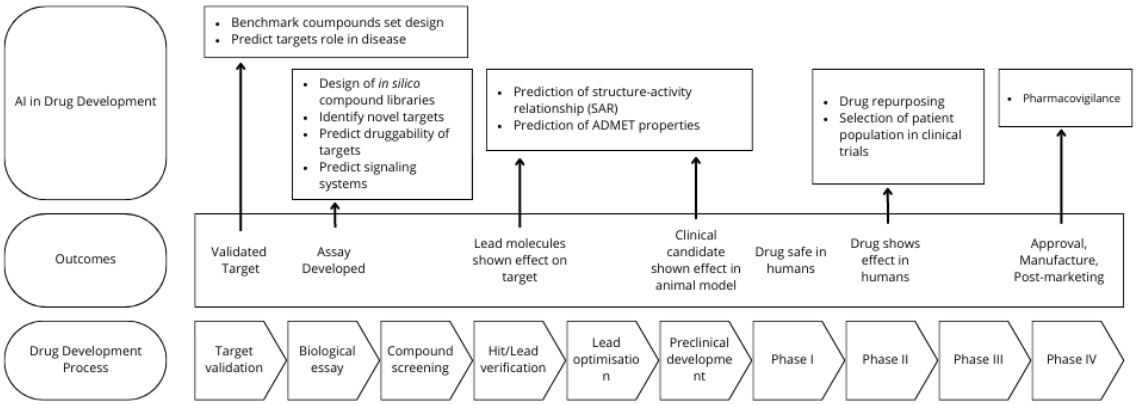
2.3.3. Impact of Artificial Intelligence in the R&D stage

Pharmaceutical R&D has become more difficult for a variety of reasons, including the proliferation of promising therapeutic targets brought about by molecular biology advancements, the majority of which have not yet been confirmed. Finding effective new medications is a demanding undertaking, and it is typically the most challenging aspect of drug development (Pammolli *et al.,* 2011).

The pharmaceutical business faces issues due to rising R&D expenses and high attrition rates during the creation of a new medicines. Currently, it takes 15 years and up to US$3 billion to bring a new medication to market. Consumers are unwilling to pay more for medications and the expense of failures, thus this trend cannot continue and a change is unavoidable. Consequently, the business model is required to change, and AI provides such a chance. The AI-infused technologies have evolved into adaptable tools that can be used anywhere and at different phases of R&D and, more specifically, in drug development, as shown in Figure 1, in processes such as discovery and validation of pharmacological targets, the development of novel medications, the repurposing of existing pharmaceuticals, increasing the effectiveness of R&D, the gathering and analysis of biomedical data, and the

improvement of the selection of patients for clinical trials. These prospective applications of AI provide the chance to mitigate the bias and human interference in the process while addressing the inefficiencies and uncertainties that emerge in the traditional drug development approaches (Mak & Pichika, 2019).

Figure 2.1 - Utilization of Artificial intelligence (AI) in the drug development process.



Adapted from: "Artificial Intelligence in drug development: present status and future prospects" by Mak & Pichika, 2019*, Drug Discovery Today,* 24(3), p.776.

Nowadays, as stated by Schuhmacher, *et al.* (2020) leading pharmaceutical businesses are currently adopting AI in R&D at a 'early mature' stage. The results of its application have not yet been established - R&D productivity, efficacy, or efficiency have not yet been sufficiently boosted by AI. Regardless, the study conducted by these same authors identified ongoing projects using AI on leading pharmaceutical companies. For instance, Johnson&Johnson offers an AI-based product to monitor infants' sleeping behavior (NodTM), whereas Novartis, alongside Microsoft, is supporting physicians in disease diagnosing with Assess MS. In addition, the authors noted 18 AI-related patents applications over the last few years. Within the same study, it was possible to conclude that the whole R&D value chain for the pharmaceutical sector is using AI, from drug discovery to drug development (Schuhmacher *et al*., 2020).

In order to understand and examine which were the most common areas of expertise, within pharmaceutical and biotechnology companies, where AI is being adopted and in what activities it is being implemented, Lamberti *et al*., (2019) conducted a study exploring the use of AI to support drug development. To do so, 8 companies were selected to make part of a working group with the role of providing relevant information to the study regarding the pharmaceutical industry. In the first stage of a two-part project, 11 AI experts were

interviewed to give their perceptions about technology definitions, industry AI investments, effects of AI, as well as challenges and expectations related to AI implementation. The second and last stage included a survey designed to collect data on AI and its subcategories, capturing the utilization of these within the respondent's organization and their thoughts on the use of AI for drug development. The results were conclusive and the majority reported that recruitment of patients to clinical trials was the most common AI activity. Regarding the planning phases of drug development, a large percentage claimed to use AI to identify medicinal products and data gathering. However, there are barriers that make the implementation of AI a complex process, such as regulations and regulatory constraints regarding unstructured data, and even unskilled staff or low budgets for small and medium companies when compared to larger players in the pharmaceutical industry.

In addition, several pharmaceutical corporations have invested in and formed joint ventures with AI businesses in the wake of the growing adoption of AI in healthcare, particularly in the years 2016 and 2017 with the aim of creating better healthcare solutions (Mak & Pichika, 2019). Due to this, "revenues of US$2.199 billion will be created by 2022 through AI-based solutions in the pharmaceutical sector, with an investment exceeding US$7.20 billion across 300+ deals between 2013 and 2018 by the pharmaceutical industry" (Paul *et al.,* 2021, p. 10).

Experts strongly believe that AI will fundamentally alter how medications are discovered and the pharmaceutical business as an all. However, humans need to have domain expertise in order to train algorithms, which is necessary for efficient AI-assisted drug development. Because the latter may train computers, design algorithms, or improve the examined data for a quicker and more accurate drug development process, this offers the ideal environment for AI and medicinal chemists to collaborate together (Mak & Pichika, 2019).

All this that was previously mentioned, and given the fact that data management and patient selection are a part of the drug development stage, leads us to conclude that R&D is, definitely, one of the most suitable area to invest in AI, at least in this early stages. It's where pharmaceutical companies can really gain advantage over the others in the industry, given the fact that "in an AI- driven world, the pharmaceutical company with the best data and the best abilities to analyze it will be able to develop the best products" (Schuhmacher *et al.,* 2020, p. 5).

2.3.4. Uses of Artificial Intelligence on the pharma industry

With the theoretical ground settled, it's necessary to see how AI is helping the pharma industry achieving its best potential in the present and how it can scale up in the future. It's reasonable to admit that the pharmaceutical industry can evolve by a great margin by implementing AI into their processes, especially if these are involved in the drug discovery and production operations, i.e., on the Research and Development stage.

It's known for a fact that developing new drugs is an expensive, time and resource consuming process that most of the time leads to a hand full of nothing, as between phase I of clinical trials and regulatory approval, 9 out of 10 drug candidates will fail. One of the main objectives of AI is to help minimize this extremely high failure rate while, and consequently, reduce the costs of production and this starts precisely in the first step of the pharmaceutical workflow, the drug discovery phase. For instance, as an example, new lead compounds that display desirable action *in silico* have been created using AI. Combining computational *de novo* design with AI might enable the creation of chemically accurate and synthesizable molecules with a desired biological activity by allowing a "computer chemist" to learn from previously discovered beneficial chemicals (Lake, 2019).

Because of this and the natural evolution of knowledge, the amounts of biological data that are being produced during the initial research phases have moved this stage into the era of Big Data and from here grows the need for advanced computation techniques to process all the information, such as data mining, storage and management. For instance, the amount of compounds available on PubChem, a repository of chemical structures and their properties, increased from 25 million in 2008 to an expressive 96 million over the period of 10 years, and the same has happened in similar platforms. Thankfully, the development of AI enabled the use of novel modeling techniques, such as neural networks, to address this challenges and help humans to link all the relevant information for specific projects and substantially reduce errors. Over the past few years, a number of projects were developed using Deep Learning as resource to explore and retrieve data from this huge data sets and Wen, *et al*. (2017) for example, created a DL model that was capable of predicting interactions between drugs and their biological targets. But computational modeling can also be used in other research areas such as Rational Nanomaterials Design, responsible for using nanotechnology to discover biocompatible nanomaterials capable of delivering drugs to treat systemic diseases, with high reliability (Zhu, 2019).

Also, several reports "have demonstrated that Machine Learning and Deep Learning have substantial implications in virtual screening, peptide synthesis, drug ADMET screening and biomarker discovery" (Kumar *et al.,* 2022, p. 1). For instance, over the past several decades, various ML tools have been developed to facilitate the drug discovery processes such as Quantitative Structure-Activity Relationship (QSAR) modelling. This procedure as now become standardized practice to rational drug discovery, with applications in all stages of preclinical trials and it's still being developed to be "more applicable for drug discovery by integrating new modeling techniques" (Zhang *et al.,* 2017, p. 1680).

When it comes to the clinical trials phase, AI has also proved itself to be very productive and helpful, with a great influence in the management of processes. RPA, a technology based on Artificial Intelligence, is being commonly used to automate and facilitate processes in clinical trial management, such as patient data entry, patient matching to relevant trials based on their provided data and reports generation (Dilmegani, 2023).

These few examples show that Big Data, Machine Learning, Deep learning and RPA are very commonly examples of Artificial Intelligence uses in Pharma industry. An investigation conducted by Bhattamisra, *et al.* (2023) claims that Artificial Intelligence, Machine Learning, Big Data and Deep Learning are set to shape the future of the healthcare sector, including Pharma.

2.4. R&D and Business Proficiency

One of the industries with the highest value addition is the pharmaceutical industry. According to an OECD data from 2017, the pharmaceutical business has the highest R&D expenditure. However, there is little previous research in this field looking at the connection between R&D spending and corporate success. According to the available research, one of the sectors with the greatest frequency of R&D performers and large return is the pharmaceutical business. R&D and innovative activities are seen as essential to the success and growth of businesses. They increase profitability, turnover, and employment, which have an impact on economic processes both directly and indirectly. (Kounnou & Kyrkilis, 2020).

To illustrate the positive impact of R&D investment over the company profitability, a study was conducted by Mishra (2018) over the Indian pharmaceutical industry. The results suggest that "the greater intensity on R&D, increases a firm's innovation capabilities and therefore increases the firm's profitability" (Mishra, 2018, p. 67). On the other hand, a study by Kounnou and Kyrkilis (2020) on the Greek pharmaceutical industry showed that "due to

the lack of domestic production of new molecular drugs, the value-added of the Greek pharmaceutical industry is regarded as low. Therefore, the expenditures on R&D cannot affect considerably the profitability" (Kounnou and Kyrkilis, 2020, p. 54). Both these examples tell that R&D plays a key role on the company ability to be profitable.

In addition, Mishra (2018) also mentioned that R&D can be used as a measure of innovation, given the fact that providing researches with more resources and funds will increase the likelihood of successful innovation. As a result, companies will receive more patents and gain temporary monopoly advantages over the remaining market, which also helps the company proficiency, increasing their market value. So, the fact that there is a beneficial relationship between market value and R&D spending, supports the idea that innovation in R&D can also serve as the engine in a capitalist economy.

Overall, the existing literature reveals a positive impact of R&D expenditure in strategic and financial outcomes. It can increase a company profitability by affecting innovation, reduction of costs and increasing operating performance. All this leads R&D, especially in pharmaceuticals, to be critical when it comes to growth and prevalence of a company in the industry.

Chapter 3 - Theoretical Approach

Considering the literature review carried out across the previous chapter, and the various opinions from the different authors mentioned on Artificial Intelligence and its impacts on the pharmaceutical industry, it was possible to develop 5 research questions that will be further deepened in the present chapter.

Artificial intelligence as the power to impact a large variety of industries in a lot of different ways, and the implementation of Industry 4.0 helped these technologies to gain traction in a technology-dependent world. The pharmaceutical industry is also being impacted by these transformations and Pharma 4.0 is now a reality with AI being more present in the value chain than ever, however there's still a lack of investigation regarding this matter (Reinhardt *et al.,* 2020). Nonetheless, this new technological era for the industry is already taking place on major players of the pharmaceutical industry and even smaller companies are adopting AI into their operations, but in the present, the adoption in a larger scale is only available to those that have the financial, human and infrastructural resources (Sharifzadeh, 2022). In reality, due to the companies' necessity of gaining market value, this industry is one of the most innovative and relies on modern technologies to remain this way, so it's only natural that companies look at AI solutions with good eyes (Malerba & Orsengio, 2015). However, in Portugal, the research extension about the subject is also very short but, according to Mendes (2020), there's a relative unfamiliarity within the Portuguese pharmaceutical industry regarding the new era technologies which evolve very rapidly, a fact that can be directly correlated with the country's low rating regarding AI readiness, ranked only 15 out of 23 countries in Western Europe (Oxford Insights & International Development Research Centre, 2019). So, these facts joint with the importance of understanding the current technological level in Portugal lead me to my first research question:

RQ1) What's the current level of technological development of the Portuguese pharmaceutical industry?

On the other hand, Artificial Intelligence is rapidly spreading across the globe in every industry due to the fact that it improves the general performance on recurrent activities (Shabbir & Anwer, 2018). Also, AI is seen by many as a powerful driver of economic growth and McKinsey Global Institute predicts that around 70% of the companies worldwide will adopt any form of AI by 2030 (Szczepański, 2019). In addition, a PwC report demonstrates countries in Europe can experience gains on GDP of around 9,5-11,5% in the same period of time (Gillham *et al.*, 2018).

In healthcare, more specifically in the pharmaceutical industry, the impact of AI technologies is already making a statement, resulting in the creation of Pharma 4.0, meaning that the industry is embracing newer digital solutions to improve its value chain (Reinhardt *et al.,* 2020). Many authors such as Leite, *et al.* (2021), Henstock (2020) and Paul, *et al*. (2021) have claimed that AI derivate technologies as Machine Learning, Deep Learning, Robot Process Automation and others have the potential to revolutionize the pharmaceutical industry and solve complex problems by creating new innovative solutions. In Portugal, there's very little knowledge regarding the stage of AI adoption and the technologies being applied in practice on the pharmaceutical industry and for these reasons, my second research question was developed:

RQ2) What are the most commonly used AI technologies used in the Portuguese pharmaceutical industry?

However, the pharmaceutical value chain is very wide and complex, with lots of different stages as can be perceived by Figure 1, and AI has a role to play in every stage of the industry (Mak & Pichika, 2019). Perhaps, it can be used in processes like data mining, creation of novel modeling techniques, automation of clinical trials management and so much more (Zhu, 2019).

Besides these facts, many authors such as Schuhmacher, *et al.* (2020); Mak & Pichika (2019); Paul, *et al.* (2021); Niño-Amézquita, *et al*. (2018); Lamberti, *et al.* (2019) and Malerba & Orsengio (2015) state that the R&D stage is the one that can benefit more from AI technologies due to importance it plays in the overall performance of companies that create and manufacture medicines, having a major impact in profitability. This was demonstrated by a research conducted by Kulkov (2021) with 15 different sized pharmaceutical companies and R&D proved to be the area where most companies would invest more due to high returns and increase in profitability. In fact, this represents no surprise, given that the pharmaceutical industries is one of the most R&D intensive and innovation is a key factor for firm growth and prosperity (Kounnou & Kyrkilis, 2020). For Portugal, there's a wide gap to fill regarding these topic and so, in order to understand in what stages and processes of the Portuguese pharmaceutical value chain these technologies were being applied, the third research question aroused as follows:

RQ3) In which processes of the Portuguese pharmaceutical value chain are AI technologies more commonly used?

From the literature review, it's was possible to understand that the application of AI in the pharmaceutical industry have both advantages and challenges to overcome in next few years.

For instance, a study conducted by PwC shows that "AI contribution to the global economy in 2030 could be more than the current output of China and India combined" (Cubric, 2020, p. 1). For the companies themselves, McKinsey estimates that investments in AI can result in a 45-75% gain in EBITDA's (Henstock, 2020). Alongside this, another benefits arouse from the adoption of these technologies such as bigger innovation capacity, competitive advantages and cost reduction, as claimed by Mishra, (2018), Malerba & Orsengio (2015), Reinhardt, *et al*. (2021) and Shabbir & Anwer (2018). However, there are challenges and barriers that come along with the implementation of AI solutions and these can be social, economic, data related, organizational, political or ethic, as mentioned by Dwivedi, *et al.* (2021) and Bhbosale, *et al.* (2020).

In the case of Portugal, there is no specific data regarding the challenges and benefits of the implementation of AI in the national pharmaceutical industry and it's crucial to know the perspectives of professionals in the industry about what they believe to be main advantages and barriers to the adoption of AI technologies in the sector and understand if they follow the same path as in Europe. For these reason, the fourth research questions reads as follows:

RQ4) What benefits does AI investment bring when compared to companies that don't do these investments and what challenges can be expected?

Nowadays, pharmaceutical companies are in a 'early mature' phase of AI investing, meaning that the impacts in the long run are not as visible as they might be for other industries (Schuhmacher *et al.,* 2020). Nonetheless, Mak & Pichika (2019); Lamberti, *et al*. (2019) and Pammolli, *et al.* (2011) believe that the investments will become larger as time progresses due to the potential that AI has to dramatically change the drug development process and help to bring new drugs to the market.

On the other hand, in the short term it's already possible to verify some effects of AI on pharmaceutical industry. For instance, there have been an increase in investments made in these technologies, with the values going from US$200 million in 2015 to US$700 million in 2018 (Paul *et al.,* 2021). Also, companies are trying to beat the market and be in the frontline of AI adoption, so that they can experience all the benefits it can bring and gain competitive advantages, which justifies the increasing investments (Mak and Pichika, 2019).

This way, and because the effects of AI adoption in Portugal are not very known, it's important to understand what to expect in the short and long-term in order to have a perspective on why the investments in the national pharmaceutical industry are slower than in other European countries. Within this line of thought, the fifth research question is the following:

RQ5) What are the impacts of AI investment on R&D in the short and long-term?

Chapter 4 - Methodology

4.1. Research Model

The act of doing research is a logical and systematic path to found new knowledge on a topic of interest. The investigation process itself is as important as the act of defining its structure. As stated by Vilelas (2009, p. 24), investigation is an activity that requires us to discipline though and action.

There are a variety of steps that need to be defined in order to structure the investigation. Diverse authors have drawn the path for a successful investigation and all of them agree that the first checkpoint is to acknowledge what is the object of the investigation. In order to answer this problematic, according to Carmo & Ferreira (2008), there are four answers that need to be answered, which are who, what, when and where to investigate. To reach this conclusions, it's important to define a set of questions or hypothesis that narrow our study object, and also to design a suitable strategy for data collection. Meanwhile, all this must be described using a rigorous but clear speech.

Depending on the extent and purpose of the investigation, there are distinct ways to gather the necessary information and, due to this, it's possible to characterize the investigation into two large groups: the bibliographic investigation and the field investigation (Vilelas, 2009). The first is mainly defined as a form of gather data through a rigorous bibliographic review, that later will support the questions in the interview script. In the second one, the data is generated in a direct way and by the author of the investigation (Becker, 1997).

Considering the approach that is chosen, the investigation can either be qualitative or quantitative, depending on the type of data collected to suit the study purposes. Qualitative approaches focus on an interpretative analysis of the observations in a non-numeric path, with the goal of understanding and finding connections between the answers to the problematic under investigation. It's a more subjective perspective that depends on where the data was secured, always keeping in mind the dynamism of our surroundings. On the other hand, quantitative approaches rely on numeric manipulation of the observations, typically helping to get to more concrete and direct conclusions (Vilelas, 2009).

For this investigation in particular, it has an exploratory dimension as the field of applying Artificial Intelligence to the pharmaceutical industry, especially in the Portuguese market, is yet a broad space to be explored with lots of unknown answers. Also, the factors that influence the perceptions and views of those connected to the R&D of medicines

regarding the implementation of Artificial Intelligence into processes of this field, have not yet been explored. Based on these facts and the research questions that were designed, it's easy to understand that the right approach was a qualitative study to achieve the investigation goals, assuming that the emphasis of the study is on the interpretation of this phenomena. As a matter of fact, and as stated by Vilelas (2020), the focus of the branch of social science known as qualitative research is on how individuals interpret and make meaning of their life circumstances.

In addition, due to this investigation having an inductive[7] character, it was conducted through a non-probabilistic sample[8] defined by convenience, taking into consideration the relevance of the approached elements to the research problematic. Although the participants' involvement and responses to the interviews were highly satisfying, the investigation's findings and key lessons should be carefully considered, given the relatively small sample size and the broad range of answers, which does not allow generalization for the overall population. This is one of the principal limitations to this approach, alongside the gap of information on literature but this was already acknowledge in the beginning stages of the study.

According to the methodology classification criteria designed by Vilelas (2009), it's possible to categorize the methodology used to gather investigation documents in two distinct ways: by the ends and by the means. In the first scenario, this investigation tries to explore the use of a modern age vanguard technology in real life context, which was supported by exploratory data, given the lack of knowledge of the practical impacts of Artificial Intelligence on the Portuguese pharmaceutical industry. In the second case, the primary source of information was the application of semi-structured interviews to R&D and innovation specialists working directly with the pharmaceutical industry in Portugal, and secondary source was through literature review and personal market knowledge.

The practical terms of the qualitative methodology used in the present investigation, came from the analysis of a collection of interviews, which sought to gauge the study's focus on the level of social, personal, and holistic human dynamics, applied to the use of Artificial Intelligence on pharmaceutical R&D. In order to enable the analysis of the collected

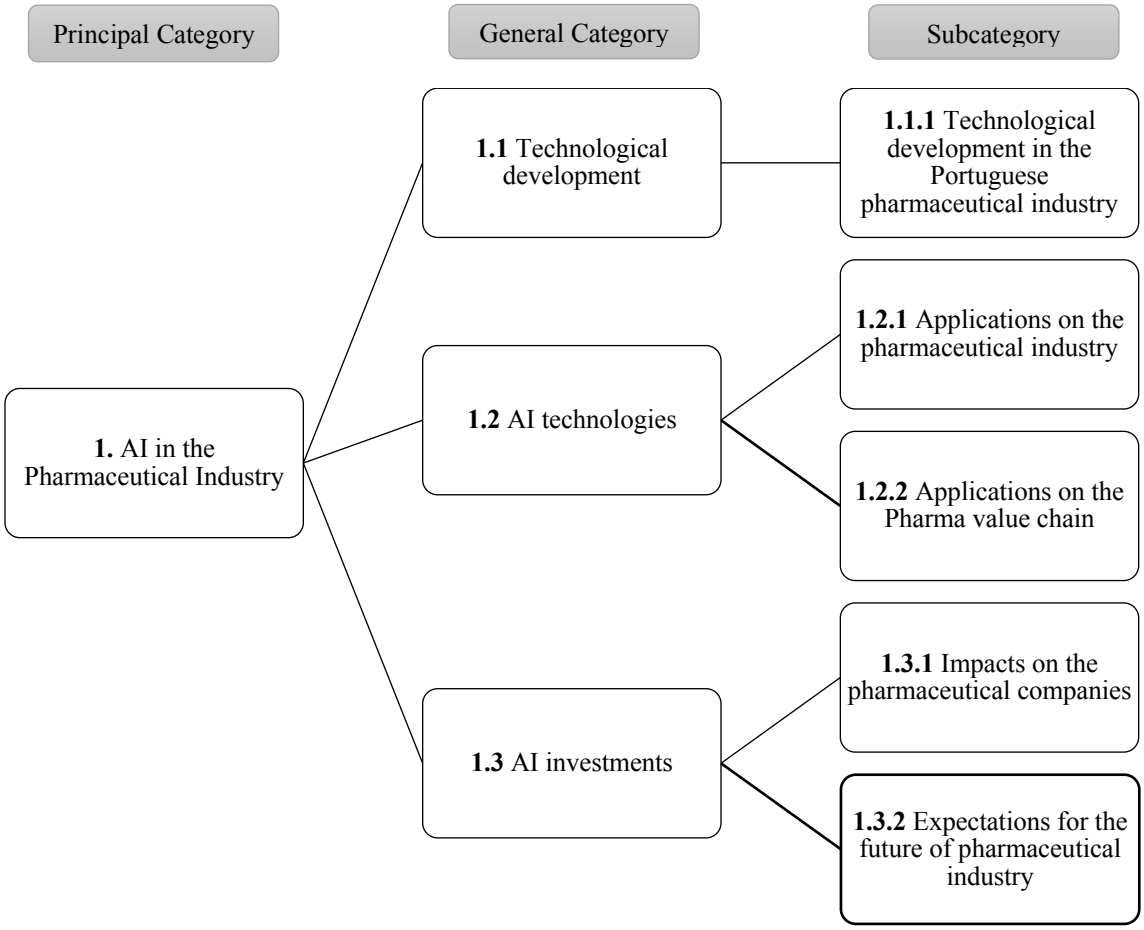
[7]The final aim isn't to reach truthful conclusions based on equally truthful premises, but to measure a group of phenomena related to the investigation in order to achieve conclusions that allow for comparisons and the discover of relations between them.

[8]Instead of choosing samples at random, the researcher uses this sampling strategy to choose samples based on their own evaluation. Researchers frequently utilize it for qualitative research because it is carried out through observation.

information, it's necessary to consider that it was obtained *in loco,* meaning that it's crucial to comprehend the context of the perspectives provided by the interviewees, given the fact that acts, words and gestures can only be comprehended in their context (Vilelas, 2020).

Regarding the qualitative analysis technique, it resulted in the establishment of relationships between the semantical structures of the answers with the social and professional environment. This provided a connection between the perspectives and all the variables that affect them, understanding that interpretation and awareness is key. In Figure 4.1, it's carefully characterized the interview corpus's classification and coding that originated the qualitative analysis.

Figure 4.1 - Categorization and codification of the interview qualitative analysis



Source: Author's elaboration

The exploitation, systematization and content expression process was done according to Bardin (2018) chronology, that asserts that content analysis must go through three stages, beginning with a pre-analysis, which implies organizing and systematizing the concepts from

the interviews. The examination of the information or substance is the next step, where the information is coded and categorized. Finally, it is important to handle the results and apply the appropriate interpretation. MAXQDA 2020 was used in this inquiry to carry out the data analysis retrieved from the interviews. MAXQDA 2020.1 is a specialized program for analyzing qualitative data that offers interview transcription and analysis as well as the ability to classify pertinent material using codes.

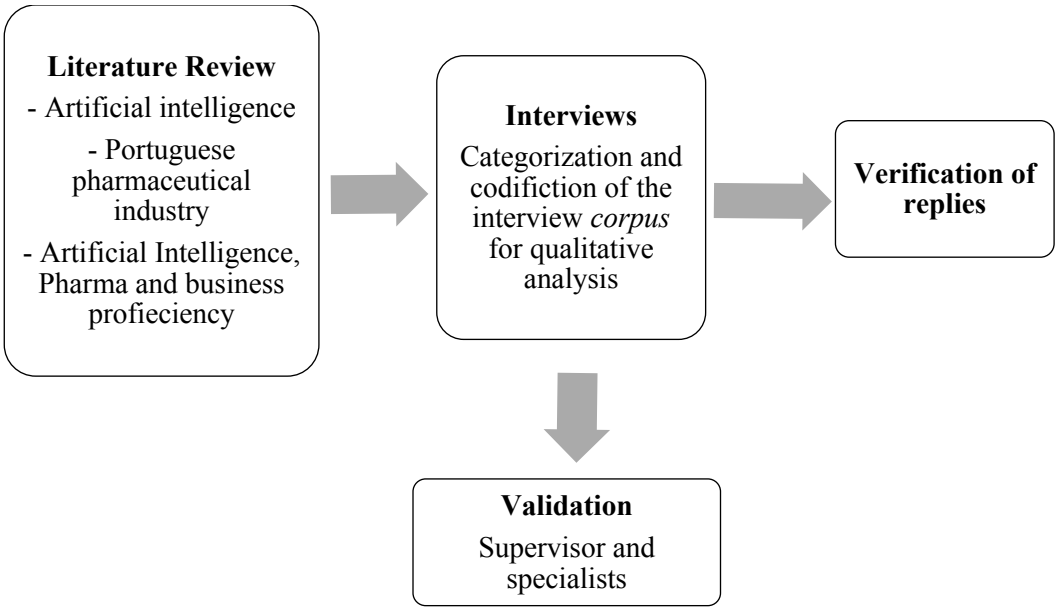
Taking into account the objectives of this investigation, the interview seemed the most appropriate method to gather primary data. Although the analysis might be, somehow, subjective and submissive to interpretation of the answers provided, it's a method that allows that the main social protagonists provide the data regarding the phenomena in study. In addition, the 17 interviews that were conducted provide a reliable value, as this number is within the parameters recognized by diverse authors as acceptable.

It's important to mention that the interviews had a semi-structured nature, has they were constructed based on predefined questions related to the investigation but were susceptible to an adaptable character, allowing the conversations between both parties to run smoothly (Carmo & Ferreira, 2008). The great advantage of this structuring method is that is enables other relevant topics to be brought to the interview, and to be more deeply exploited if they are relevant and in accordance with our goals. Besides this, the interviews were still prepared but flexible, generating data that proved relevant and that otherwise, wouldn't be included. On the other hand, the biggest disadvantage of this technique is the increased difficulty to cluster and compare the answers, due to their heterogeneity, leading to harder data synthesis (Vilelas, 2009).

In sum, this investigation has developed itself into four stages: the first one, focused on a bibliographic research and information selection; the second stage, based on the transfer of theoretical knowledge into the working field; the third, taking things to the working field and gather data provided by interviews; and the fourth and final phase, the quantitative analysis of the data collected, leading to the construction of new theoretical approaches combined with empirical data based on Artificial Intelligence impacts on the pharmaceutical industry.

Regarding to external validation, meaning the possibility of apply the obtained results to other contexts or populations, this study supports some theory that already exists regarding Artificial Intelligence impacts on the general pharmaceutical industry worldwide and also generates new data regarding the Portuguese market, which allows for future comparisons and analysis between different fields of expertise within the pharma industry in Portugal and in other countries. The figure 4.2 shows the investigation model used on this research.

Figure 4.2 - Investigation model



Source: Author's elaboration

In Table 4.1, the link between the goals of this study, the research questions created in the theoretical approach chapter, and the appropriate connection with the literature review conducted at the outset of the inquiry are all discussed.

Table 4.1 - Relationship between objectives, research questions and literature review

Objectives	Research Questions	Literature
(O1) - Understand the current state-of-the-art regarding technological development and use of AI in the Portuguese pharmaceutical industry	(RQ1) - What's the current level of technological development of the Portuguese pharmaceutical industry?	Mendes (2020); Reinhardt *et al.,* (2020); Sharifzadeh (2022); Malerba
	(RQ2) - What are the most commonly used AI technologies used in the Portuguese pharmaceutical industry?	Leite *et al.*, (2021); Reinhardt *et al.,* (2020); Henstock (2020); Paul *et al.,* (2021)

	(RQ3) - In which processes of the Portuguese pharmaceutical value chain are AI technologies more commonly used?	Schuhmacher *et al.,* (2020); Mak & Pichika (2019); Paul *et al.,* (2021); Niño-Amézquita *et al*., (2018); Lamberti *et al.,* (2019); Kulkov (2021);
(O2) - Analyze the practical impacts of AI in the present and the future	(RQ4) - What benefits does AI investment bring when compared to companies that don't do these investments and what challenges can be expected?	Henstock (2020); Malerba & Orsengio (2015); Reinhardt *et al*., (2021); Shabbir & Anwer (2018); Bhbosale *et al.*, (2020); Dwivedi *et al.,* (2021); Cubric (2020); Mishra (2018)
	(RQ5) - What are the impacts of AI investment on R&D in the short and long-term?	Paul *et al.,* (2021); Mak and Pichika (2019); Lamberti *et al*., (2019); Pammolli *et al.,* (2011):

Source: Author's elaboration

4.2 Sample Characterization

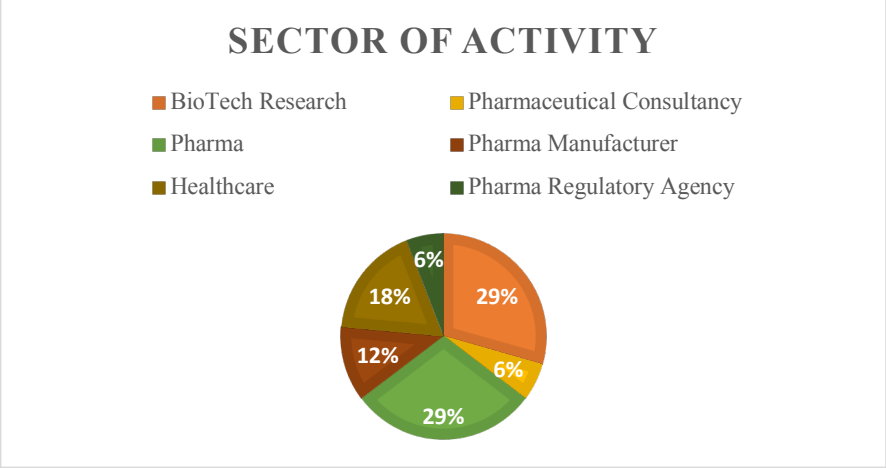
For the investigation, the participants in the current study were selected from a specified demographic, hence the sample size was non-probabilistic, related with the sectors of activity that are relevant for the study itself within the pharmaceutical industry. This comprehends big

pharmaceutical companies, investigation centers, pharmaceutical manufacturers and pharmaceutical consultancy companies, as well as big healthcare companies. All these are key to understand the level of Artificial Intelligence integrated by in the pharmaceutical industry in its R&D processes.

This way, in order to characterize the sample, factors such the sample's industry of activity, present occupation, age, and firm classification were taken into account. As the majority of participants required confidentiality in the data treatment, parameters like names or gender were not consider.

The interviews were conducted with 17 professionals from the areas referred to above, and Figure 4.3 shows how these were distributed among the different sector. As observed, 29% work in the BioTech research field and other 29% on Pharmaceutical companies, while 18% work on Healthcare companies. From the remaining interviewees, 6% work on pharmaceutical consulting, 12% on pharmaceutical manufacturers and 6% on Pharmaceutical Regulatory Agencies. An option that was made was to distinguish between Pharmaceutical Companies and General Healthcare companies due to the fact that many Healthcare companies work towards the pharmaceutical market but have different perspectives regarding the industry, so these professionals can offer a variable range of opinions for working with the industry but without been directly related to it.

Figure 4.3 - Companies Sector of Activity

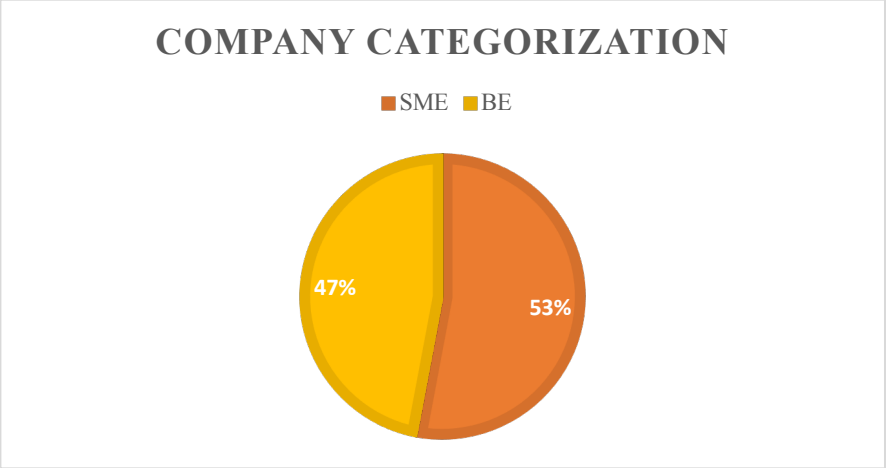


Source: Author's elaboration

Regarding the categorization of the companies, as Figure 4.4 reveals, 53% of the companies are SME's and the remaining 47% are BE. Some of the factors that were considered to distinguish between both groups were number of employees, size of operations

and business volume. This is important because it allows for a better interpretation of the results, given that the perspectives can vary based on the size of the companies themselves.

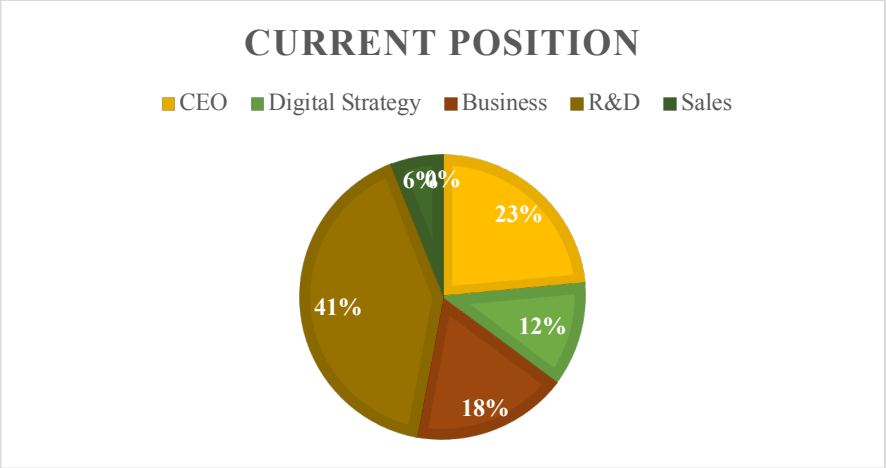
Figure 4.4 - Interviewees Current Position in the Company



Source: Author's elaboration

Concerning the interviewees themselves and their current positions occupied within the companies, the majority works in R&D (41%), while in the remaining population, 24% are CEO's, 18% work in Business related activities, 12% work as Digital Strategists and 6% work in Sales departments, as shown in Figure 4.5.

Figure 4.5 - Interviewees Current Position in the Company

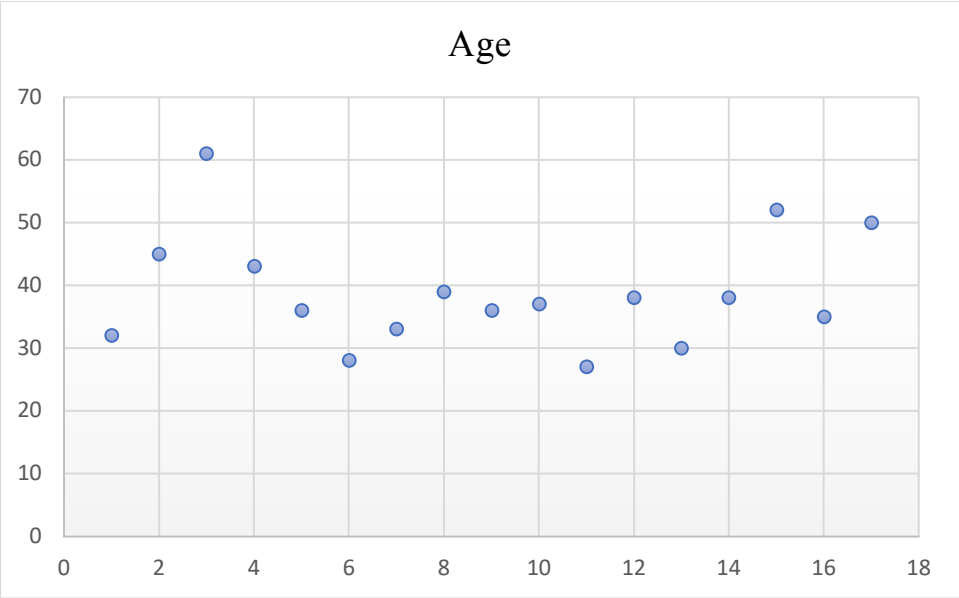


Source: Author's elaboration

Lastly, the age range of the interviewees goes from 27 years-old all the way up to 61 years-old. Figure 4.6 shows this dispersion of ages in no particular order or number

attribution to the interviewees, where the *x* represents a randomized number attributed to each participant and the *y* represents the age of the participants.

Figure 4.6 - Interviewees Age Range



Source: Author's elaboration

Chapter 5 - Data Analysis and Discussion

In the current chapter, the gathered data through-out the interviews will be presented and analyzed, as well as discussed according to the literature presented in Chapter 1, regarding Artificial Intelligence and the its relation with the pharmaceutical industry. In more detail, it will be discussed the intentionality of implementation of Artificial Intelligence and it's impacts on the diverse processes surrounding the Research and Development of medicines.

5.1. Technological development level of the pharmaceutical industry

In order to fulfil the objective of this research, the first category aims to explore the current state-of-the-art regarding the technological development of pharmaceutical companies in Portugal. This is relevant to understand the context surrounding Artificial Intelligence technologies in the country, as this will give a perception about how prepared and advanced is the industry to receive and implement vanguard AI technology. In addition, this is a problematic that has not yet been deeply studied in Portugal, so it bring new relevant information to this investigation. To do so, general technological development of the Portuguese pharmaceutical industry was explored.

In Table 5.1 is possible to see the perceptions of the interviewees regarding the level of technological development in the Portuguese pharmaceutical industry. Many authors like Henstock (2020); Mak & Pichika (2019) and Schuhmacher, *et al.* (2020) claim that Pharma 4.0 is a new reality across multiple countries in the sector, with companies implementing new and innovative technologies. In addition, as mentioned by Malerba & Orsengio (2015) the pharmaceutical industry is one of the most innovative that exist, by adopting modern technological solutions as need to respond to the market necessities and gain competitive advantages over their rivals. But in Portugal this evolution seems to be a little bit different, according to Mendes (2020), that mentioned that there is still a relative unfamiliarity with newer technologies across the industry and its stakeholders, with companies being in general, somewhat resistant to change. Also, the lack of investments and opportunities is a factor that influence the slow development in the Portuguese industry in adopting modern technologies like AI.

Table 5.1 - Level of technological development in the Portuguese pharmaceutical industry

Text	Generic Category	Subcategory	Times Mentioned	Interviewees
Relatively Developed	1.1.	1.1.1	8	3, 7, 8, 10, 12, 14, 15, 16
Low Development	1.1.	1.1.1	6	1, 2, 6, 9, 11, 13
Very Developed	1.1.	1.1.1	3	4, 5,17

Source: Author's elaboration

As it can be seen in Table 5.1, the majority of answers is split between a low technological development and a relative development in the Portuguese pharmaceutical industry, supporting the arguments of the previously mentioned authors of a natural evolution but less evident in Portugal. Yet, there's still a minority claiming that Portugal is very technologically developed, going against Mendes (2020) conclusions. The reasons that support the interviewees opinions are reflected in Table 5.2.

Table 5.2 - Perceptions technological development in the Portuguese pharmaceutical industry

Text	Generic Category	Subcategory	Times Mentioned	Interviewees
Low innovation capacity and slow development in comparison to other countries	1.1.	1.1.1	7	1,6,7,10,11,13,14
Low investments	1.1.	1.1.1	7	1,2,9,12,13,15,16
Many companies that operate in Portugal have their operations centers outside the country	1.1.	1.1.1	3	4,11,14
Good infrastructures and laboratorial techniques	1.1.	1.1.1	3	9,10,12
Front line regarding innovation in some therapeutical areas	1.1.	1.1.1	2	4,5
In comparison to other European countries, Portugal is very similar but still not at the same level	1.1.	1.1.1	2	8,16
Lack of qualified professionals due to emigration	1.1.	1.1.1	2	3,9

Fast Development	1.1.	1.1.1	1	17

Source: Author's elaboration

Sharifzadeh (2022) and Reinhardt, *et al.* (2020) claim that Pharma 4.0 is the new technological era for the pharmaceutical industry and it's already being applied in big Pharma corporations in their operational centers, which have the necessary financial, human and infrastructural resources available. According to the authors, this evolution will bring innovation, efficiency and enhanced quality of products and it's an unavoidable step to take in the direction of progress. As mentioned before, the perceptions of the interviewees are only centered on the Portuguese pharmaceutical industry and from Table 5.2, it's possible to the see that a vast number of participants referred low investments, low innovation and slow development as crucial reasons for low technological development, which means, in accordance to the authors claims regarding their perception of evolution and technological progress in the pharmaceutical industry as a whole, that the majority of participants agrees that Portugal is not a very technologically developed country concerning the pharmaceutical industry. Some other reasons that were mentioned concern the lack of qualified professionals that stay in the country to go to foreign territory in pursuit of better career options and the fact that most of big pharmaceutical companies operating in the country have their R&D and manufacturing centers outside of Portugal. On the other hand, a smaller percentage of interviewees also mentioned positive aspects observed in the Portuguese pharmaceutical industry, such as the good quality of infrastructures and laboratorial techniques; and frontline appearances in some therapeutical areas.

Kounnou & Kyrkilis (2020); Mishra (2018) and many others authors mentioned that R&D is the stage that pharmaceutical companies gain a significant advantage to their competitors, due to innovation capacity and drug development speed, and these features are only driven by large financial, human and material investments. The majority of justifications presented by the interviewees is related to this stage and they all mentioned innovation, investment, development capacity, qualified professionals and infrastructures as reasons for low, medium and high technological development. Kounnou & Kyrkilis, (2020); Mishra (2018); Schuhmacher, *et al.* (2020); Niño-Amézquita, *et al*. (2018) and Lamberti, *et al.* (2019) defended that this stage is one of the most impactful and important in the pharmaceutical industry due to the reasons mentioned earlier and the interviewees all agreed with this claims,

as they recognize that the difference between success and failure can be pointed to R&D in companies that heavily depend on this department.

5.2. Artificial Intelligence on the Portuguese pharmaceutical industry

After understanding the state-of-the-art regarding technological development in the Portuguese pharmaceutical industry, the second research category is proposed to explore the current Artificial Intelligence technologies being used in the industry and their current applications. To do so, it was considered the perspectives of the interviewees concerning AI technologies currently being in practice on the industry in Portugal and in which processes or areas were these being implemented.

Table 5.3 - Artificial Intelligence technologies in the Portuguese pharmaceutical industry

Text	Generic Category	Subcategory	Times Mentioned	Interviewees
Machine Learning	1.2.	1.2.1	8	1,4,6,7,9,11,14,17
Big Data	1.2.	1.2.1	7	4,8,9,11,12,13,14
Not aware of any AI related technology	1.2.	1.2.1	5	2,3,15,16
Robot Process Automation (RPA)	1.2.	1.2.1	3	5,12,14
Natural Language Processing (NLP)	1.2.	1.2.1	2	7,10
Deep Learning	1.2.	1.2.1	1	11

Source: Author's elaboration

In Table 5.3 are summarized the AI related technologies that the interviewees recognize that exist in the Portuguese pharmaceutical industry, either by practical knowledge within their companies or by empirical knowledge from reliable sources that these technologies are being used.

According to Reinhardt, *et al.* (2020), the proliferation of Industry 4.0 have positively impacted the pharmaceutical industry and that resulted in the creation of Pharma 4.0. This means that the industry has now embraced the latest technological developments and adopted digital strategies to reformulate and modernize all of its value chain. Pereira, *et al.* (2020) also claims that there are fundamental pillars that support the proliferation of industry 4.0, and consequently Pharma 4.0, some being the Internet of Things (allows the self-management of objects by extending network connectivity and processing capability to artifacts that are not often thought of as computers), Big Data, Autonomous Robots and others. Taking a deeper look into the answers provided, it's possible to conclude that all the technologies mentioned fit into the fundamental pillars of Industry 4.0 and Pharma 4.0, given that Machine learning, Deep learning and NLP are integrated with IoT to make the networks more efficient and autonomous (Zikria *et al.,* 2020). About RPA, it is one of the fundamental pillars itself, being in accordance to what was stated before. In addition, Leite, *et al.* (2021) and Henstock (2020) claim that ML, DL, RPA and other derivate technologies have the potential to transform the pharmaceutical industry. Also, retrieving to the literature review made in Chapter 2, the numerous references to these technologies by a large amount of authors, also reveals that these AI based technologies are indeed, the most used and with biggest transforming potential. The provided answers by the interviewees are in the same line of thought as the authors mentioned, proving that indeed the mentioned technologies are the most commonly used in the industry and the ones with the biggest potential to have an impact on the evolution of Pharma as we know it. It's also important to underline that 5 of the respondents are not aware of any of the AI technologies being in use in the Portuguese pharmaceutical industry.

5.3. Artificial Intelligence applications on the Portuguese pharmaceutical industry

At this moment, it's perceptible what modern Artificial Intelligence solutions are most used in the Portuguese pharmaceutical industry but it is important to understand where are these technologies being applied. The third research category comes in the continuation of the previous one, which aims to explore the applications of these Artificial Intelligence based technologies. In order to accomplish this goal, the interviewees were questioned regarding the areas and processes of practical use of these previously mentioned technologies.

Table 5.4 - Artificial Intelligence applications in the Portuguese pharmaceutical industry

Text	Generic Category	Subcategory	Times Mentioned	Interviewees
Chemical Structures Library Analysis	1.2.	1.2.2.	8	2,5,6,11,12,13,14,17
Target / Lead Discovery	1.2.	1.2.2.	7	5,6,10,11,12,17
Screening	1.2.	1.2.2.	6	1,5,11,12,13,17
In Vitro / *In Silico* Testing	1.2.	1.2.2.	6	2,5,8,11,12,17
Bioinformatic Analysis	1.2.	1.2.2.	5	1,4,11,12,17
Clinical Trial Management	1.2.	1.2.2.	2	4,12
Pharmacovigilance	1.2.	1.2.2.	2	10,12
Not aware of any applications	1.2.	1.2.2.	2	3,7

Source: Author's elaboration

Table 5.4 illustrates the perspectives of the interviewees regarding the processes that are impacted in a greater extent by the application of Artificial Intelligence technologies. It's important to disclosure that this particular question was not influenced by the previous answers and the respondents were free to mention any process with no relation to the technologies that were referred previously.

Schuhmacher, *et al.* (2020); Mak & Pichika (2019); Paul, *et al.* (2021); Niño-Amézquita, *et al*. (2018); Lamberti, *et al.* (2019) and Malerba & Orsengio (2015) stated that Artificial Intelligence is having and will have even more impact on the R&D stage of the pharmaceutical industry that in any other stage, due to multiple positive outcomes that this phase has on the performance of the companies operating in the industry, such as competitive advantage, innovative capacity, increase on profitability and many others. By observing Figure 1, it's possible to understand some of the applications of Artificial Intelligence across the R&D stage and according to the perceptions provided by the interviewees, it's notorious that 6 out of the 8 answers are directly related to this stage.

Paul, *et al.* (2021); Kulkov (2021) and Mak & Pichika (2019) are some of the many authors that converge into the opinion that the first steps into drug discovery and development are critical to the success of the investigation. It's in this early stages that the investigation goes from very generic to very specific in short period but it's also the phase where most failures happen. So, the authors believe that AI can play an important role in minimizing these failure rate. Lake (2019) supports this with an example of an AI based tool that combines with of *de novo* computational design to generate chemically accurate and synthesizable molecules with a desired biological activity. Niño-Amézquita, *et al*. (2018) provides us with some other options of AI application on these earlier stages or R&D, such as the design of *in silico* compound libraries and target identification. Kumar, *et al.* (2022) also mentions that virtual screening, peptide synthesis, drug ADMET screening, and biomarker development are all significantly impacted by ML and DL. Table 5.4 is showing that 3 out of the 8 answers are referent to these firsts steps in drug R&D, which are "Hit / Lead Identification", "Screening" and "*In Vitro / In Silico* Testing". The authors mentioned provide clear examples of AI application into each process mentioned by the interviewees, meaning that the parties have and agreement regarding this matter.

Zhu (2019) mentioned in one of is publications that the repository of chemical structures by PubMed, increased its database from 25 million structures in 2008 to over 96 million structures in 2018, with the same happening across different platforms. In the author's words, it's only due to the development of Deep Learning and Neural Networks that it's possible to address the challenge of analyzing and combine such a large data set in favor of drug development. Wen, *et al.* (2017) was also invested into this field and trough one of his articles, the author explains his creation of a Deep Learning model that was capable of predicting interactions between biological targets. In addition, Niño-Amézquita, *et al*. (2018), mentions that the prediction of structure-activity relationship of compounds is also one of the potential uses of Artificial Intelligence in the industry. Moving to Table 5.4, it's clear that the majority of the interviewees would agree with the authors, given that 10 of them stated "Chemical Structures Library Analysis" and "Bioinformatic Analysis" as two of the main processes where Artificial Intelligence technologies were having a higher impact in the Portuguese pharmaceutical industry.

Dilmegani (2023) and Niño-Amézquita, *et al*. (2018) also mention Clinical trials and Pharmacovigilance as one of the areas with a good potential for AI application, where these technologies have already proven themselves to be helpful and productive. For instance, RPA is commonly used to automate and facilitate processes in clinical trial management and in

pharmacovigilance, ML is used to help in the design of questionnaires and transcription of data collected during this stage. Respondents also are in accordance with the authors, as 3 out of the 17 people referred these areas as being suitable and with present applications of Artificial intelligence.

Lastly, 2 of the interviewees also claimed to not be aware of any application of AI in the Portuguese pharmaceutical industry, which is in the same line of thought as Mendes (2020), as the author mentions that there's a relative unfamiliarity with these modern technologies and it's practical uses within the Portuguese industry.

5.4. Artificial Intelligence positive and negative impacts across Pharmaceutical companies

As expected, inherent to any modern technology, there will be advantages and disadvantages of its applications and Artificial intelligence is no exception to this. Pharma 4.0 it's in very early stages of its implementation and having a relatively modern implementation, it's perceptible that the benefits and problems that may arouse are not well exploit. Nevertheless, to understand the interviewees perspectives, they were questioned regarding this matter and the answers are reflected in Table 5.5.

Table 5.5 - Artificial Intelligence benefits on the pharmaceutical industry

Text	Generic Category	Subcategory	Times Mentioned	Interviewees
Data Analysis Speed	1.3.	1.3.1.	9	2,4,6,7,10,11,12, 15
R&D processes optimization	1.3.	1.3.1.	5	1,3,4,11,12
Increase of final product quality	1.3.	1.3.1.	4	7,11,14,15
Less R&D time spent	1.3.	1.3.1.	4	9,11,14,15
Competitive advantages	1.3.	1.3.1.	3	1,8,9
R&D costs reduction	1.3.	1.3.1.	3	1,11,16
R&D success	1.3.	1.3.1.	2	3,11

Innovation capacity	1.3.	1.3.1.	2	4,5
Decrease of human mistakes	1.3.	1.3.1.	2	5, 12
Better human resources allocation	1.3.	1.3.1.	2	7,12

Source: Author's elaboration

Paul, *et al*. (2021); Leite, *et al.* (2021) and Henstock, (2020) claim that AI-based technologies can bey key to solve healthcare complex problems, from the pharmaceutical industry to the delivery of personalized healthcare. These solutions not have the capacity to speed-up the time for a new medicine to reach the market but also improve the quality of the final products, while it allows to optimize the core processes of R&D along the Pharma value chain and to enhance the overall success rate of this very same stage. With all of these is also associated more cost-effective practices, which could translate to gaining's of 39% just from implementing AI into core processes of the value chain. Also, such investments in AI-based solutions could result in a 45 to 75% increase in the companies' EBITDA, with most of this growth coming from stages like research and clinical trials. All this benefits are in accordance to what was mentioned by the majority of the respondents, that mentioned reduced time-to-market of drugs, improve quality of the products, data analysis speed and process optimization, cost reduction and increased success in R&D.

Malerba & Orsengio (2015); Reinhardt, *et al*. (2021) and Shabbir & Anwer (2018) all defend that AI will be increasingly important for companies in order for them to win competitive advantages over their rivals, given that pharma industry is highly dependent on innovation and new solutions. Given that this industry is already in an era where AI is the present, it's crucial that the companies adopt these sort of technologies to keep in the frontline or to maintain competitiveness, because in a few decades AI tools will become standard practice and those that do not adopt it in time, can go down before this happens. Some interviewees agreed with this perspective and mentioned innovation capacity and competitive advantages as two of the reasons of AI's beneficial implementation.

Mak & Pichika (2019) also referred the reduction of human intervention in some processes as an advantage, as it would reduce the bias and mistakes caused by human hand. This a perspective shared with 2 of the interviewees that also see this factor as one of the most relevant when it comes AI implementation. Regarding the answer "Better human resources allocation", no literature was found on the topic to confront this perspective with.

Despite all the good things AI bring to the table, there are also some perspectives that are not so positive, as it can be perceived in Table 5.6, where the opinions of the interviewees regarding the disadvantages of AI were collected. Not every respondent choose to answer this question, as they thought AI had much more advantages than its opposite and choose not answer this part of the question.

Table 5.6 - Artificial Intelligence disadvantages on the pharmaceutical industry

Text	Generic Category	Subcategory	Times Mentioned	Interviewees
Less working opportunities	1.3.	1.3.1.	4	2,7,12,13
High investments	1.3.	1.3.1.	3	4,12,13
Systematic errors	1.3.	1.3.1.	2	2,12
Reliability	1.3.	1.3.1.	1	11

Source: Author's elaboration

Bhbosale, *et al.* (2020) and Dwivedi, *et al.* (2021) referred that there also barriers in AI that difficult the implementation of these technologies in some companies that can be social, economic, data related, organizational, political or ethic. Some more specific examples of this are the high costs and investments that are necessary to adopt such a vanguard technology, the low reliability provided in certain tasks that can result in systematic errors and consequent backdrop to the company, or even structural changes that would be necessary to make in order to accommodate and apply AI into the companies processes. Some interviewees recognized these disadvantages and also mentioned high investments, reliability and systematic errors as examples of the bad side of AI. But concerning the opinion of 4 respondents regarding the problematic of less employment due to substitution by AI technologies, some authors would disagree with this. It's the case of Paul, *et al*. (2021), that mentioned that this technology would never be a threat to humans because it couldn't replace them at its fullest, due to human capacities that machines don't have like emotions, intelligence and critical spirit.

5.5. Artificial Intelligence in the short and long-term

Finally, it's important to understand what are the perceptions regarding the future implications of AI in the pharmaceutical industry, both in the short-term and in the long-term. It's necessary to disclaim that the periods of time in Pharma industry can be a bit different, so when talking about short-term, its referent to a period of 6 months to 1 year and long-term means 4 or more years. This last research category aims to do precisely that and the respondents provided theirs perspectives regarding the evolution of AI in the Portuguese pharmaceutical industry, which are exposed on Table 5.7.

Table 5.7 - Artificial Intelligence effects on the short-term

Text	Generic Category	Subcategory	Times Mentioned	Interviewees
Increasing investments	1.3.	1.3.2.	9	1, 3, 4, 6, 10, 14, 15, 16, 17
Creation of investment laws to support the adoption of AI	1.3.	1.3.2.	2	7, 2
Human Formation	1.3.	1.3.2.	2	8, 9
No changes	1.3.	1.3.2.	2	11, 12

Source: Author's elaboration

Paul, *et al.* (2021) concludes that the investments in AI made by companies in the Pharma industry raised from US$500 million between 2015 and 2017 and it's expected that this value will increase, in 2024, up to US$5 billion. This demonstrates that the predictions regarding AI investments are positive and will suffer an increment in the short-term. This point can be also be validated according to authors like Niño-Amézquita, *et al*. (2018) and Mak and Pichika (2019), that claim investments have been growing since 2013 and larger companies are relying on this newer technologies to beat the market. The majority of the interviewees also agree with these conclusions, stating that there will be an increase in investments related to the implementation of AI technologies in the Portuguese pharmaceutical industry.

Regarding the creation of laws to support AI investment and the increase in the theoretical formation of professionals there are no records or information's regarding

government policies or companies formation plans to address these issues but it's certain that AI will not take the place of humans in the near future (Paul *et al*., 2021). Also, it's important to mention that 2 of the respondents claimed that no changes will happen within a short-term period.

In Table 5.8 are mentioned the long-term perspectives of the interviewees regarding AI impacts on the Portuguese pharmaceutical industry.

Table 5.8 - Artificial Intelligence effects on the long-term

Text	Generic Category	Subcategory	Times Mentioned	Interviewees
New treatments and medicines available	1.3.	1.3.2.	7	1, 2, 3, 9, 10, 11, 12
Easier access to AI for SME	1.3.	1.3.2.	8	1, 4, 5, 6, 7, 13, 14, 15
AI implementation will be mandatory to maintain competitiveness	1.3.	1.3.2.	5	6, 7, 15, 16, 17
Creation of specific infrastructures to accommodate AI	1.3.	1.3.2.	2	8, 14

Source: Author's elaboration

Lamberti, *et al*. (2019) mentioned that in the present, larger companies tend to make more use of AI technologies than small and midsized companies. Also Niño-Amézquita, *et al*. (2018) concluded that AI would also help SME's to improve their growth and generate more profits. This aligns with the opinions of the interviewees that more investments will be made by smaller companies, but nowadays is something that is mainly accessible by larger enterprises. This is due to a necessity that will arouse from the competitiveness perspective, were companies will need to adopt this technologies to maintain themselves relevant in the industry.

Mak & Pichika (2019); Lamberti, *et al*. (2019) and Pammolli, *et al.* (2011), claim that AI has the potential to dramatically change the drug development process and certainly, new drugs and treatments will be available to the public that have been created using different AI technologies. Also, not only will these technologies help with innovation but also with the time spent to bring new medicines to the market. It's a known fact that the challenge of

finding new solutions in healthcare is becoming abruptly difficult but the joint venture of AI and professionals will lead the way to new paths that have never been explored before. This is a shared perspective with 7 of the respondents, who think AI will bring new medicines and treatments to the public in a long-term period.

The creation of specific infrastructures, mentioned by 2 of the interviewees, is not very documented in literature regarding the topic of AI in the long-term, but it's definitely an interesting point of view and something to take into consideration when approaching this matter.

Chapter 6 - Conclusion

6.1. Final Considerations

The primary conclusions of this research are presented in this concluding chapter, which seeks to draw conclusions from the earlier findings. It continues the prior examination of the information obtained from the interviews and the corresponding discussions regarding Artificial Intelligence and the pharmaceutical industry with earlier authors. Over the past few decades, studies about this technology have grown significantly across various sectors, putting it on the public's attention. Additionally, it has shown to assist individuals and businesses in enhancing their performance in regular tasks. In simultaneous, the pharmaceutical industry as evolved and is constant progress, with new challenges arising every day and the growing necessity to find better solutions relying on modern technologies.

The first research question of this study was designed to help understand the perceptions of the interviewees regarding the technological development levels in the Portuguese pharmaceutical industry. From the interview, it was possible to conclude that 47,1% of the interviewees perceive this technological development as relatively developed, while 35,3% claimed that development was low and the remaining 17,6% considered the industry to be very developed. The take away from these results is that the majority of the respondents consider the national pharmaceutical industry to be in a close level to other countries, mainly from Europe and that a third thinks this level is below other countries, while only a minority thinks that Portugal is more technologically developed than a vast group of European countries.

Following these opinions, the interviewees were asked to provide reasons that supported their answers. From the 17 respondents, 70,5% claimed that low investments, low innovation capacity and slow development were the main drivers for the Portuguese pharmaceutical industry not to be ‘pacesetter’ in comparison with other European countries. Some other reasons pointed out by a minority were the lack of qualified professionals and the fact that many companies operating in Portugal have their principal R&D operations outside the country. Concerning the positive reasons, only 35,3% of the sample pointed positive aspects regarding this matter, with the arguments that Portugal had good infrastructures and laboratorial practices, a fast development industry and it’s in the frontline in some therapeutical areas. As neutral reasons, 11,7% stated that Portugal is in same level as the majority of other European countries. It’s important to notice that 3 of the interviewees

provided both good and bad opinions regarding the technological development level in Portuguese Pharma. From these results, it's relevant to highlight that the Portuguese pharmaceutical industry is in a similar stage of technological development as other European countries with a tendency to be a pursuer rather than to be in the front line.

Moving to the second research question, the goal is to gather knowledge regarding the most common types of Artificial Intelligence technologies used in the Portuguese pharmaceutical industry. From the answers provided, it's clear that the majority consider Machine Learning to be the most applied, with 47% of the interviewees mentioning this technology. The second most mentioned was Big Data, with 41,2% of respondents and for the remaining ones was RPA, NLP and Deep Learning, with 17,6%, 11,7% and 5,9% of the respondents, respectively. Also, it's very important to highlight that 29,4% of the respondents claimed to not be aware of any AI technology in use in the national industry, which reveals a relative unfamiliarity with these modern technologies from some professionals in the industry. Overall, it's understandable that ML and Big Data are the two most common types of AI in present use in the industry, while there's still a space for technologies like RPA, NLP and DL on the Portuguese Pharma industry.

The third research question aimed to explore in what processes these previously mentioned technologies are being applied in practice throughout the industry's value chain. Considering the interviewees answers, a vast majority, 64,7%, mentioned processes related to the earlier stages of R&D, such as chemical structures analysis, targets / leads discovery, screening and *In Vitro* / *In Silico* testing. In addition, 29,4% mentioned bioinformatic analysis, which can be used in a larger variety of processes, and 17,6% mentioned later stages of R&D, such as clinical trials management and pharmacovigilance. Lastly, 11,7% claimed to not be aware of any specific process in which these technologies are applied, what does not mean that they are not aware of any technology in use.

The fourth research question of the investigation aims to discover what are the perceptions of the interviewees regarding the benefits and disadvantages of using Artificial Intelligence in pharmaceutical industry as a whole. The first thing to notice, is that far more positive reasons were pointed when compared to the reduced number of disadvantages. Data analysis speed, was the most pointed benefit, with more than half of the respondents mentioning it but R&D was the stage that had more potential advantages in absolute number, with 47% of the respondents pointing reasons within this area, such as optimization of R&D processes, reduction of R&D costs and time and enhancement of R&D success rate. The other reasons pointed were more general to the value chain, with 23,5% mentioning the increase in

the products final quality, 17,6% referring the gain of competitive advantages over other companies and 4 interviewees pointing the increase in innovation capacity, decrease in human mistakes and a better allocation of human resources.

Considering the disadvantages, these were far lower and with only 6 respondents mentioning their opinion. The biggest concern was the reduction in working opportunities, pointed by the majority of interviewees, while the high financial investments that were required to implement AI, the increased probability of systematic errors and consequent lack of reliability also being pointed out. In analysis, it's understandable that there will be good side and a bad side to everything but concerning AI application in the Pharma industry, the benefits that it brings can be a lot bigger than the possible disadvantages.

Finally, the last research question seeks to understand what are the perceptions regarding the short and long-term of the Artificial Intelligence evolution in the Portuguese pharmaceutical industry. For the short-term, most of the interviewees - 52,9% - mentioned an increase on the investments in AI technologies and some others also referred the creation of investment laws to support the adoption of AI in Portuguese companies and the increase in human formation, to capacitate professionals in this area. A small minority of 11,7% of the respondents claimed that no changes will be visible in the short-term. Regarding the long-term 8 out of the 17 interviewees believe that there will be an easier access to Artificial Intelligence for small and medium enterprises. In fact, 29,4% of the respondents claim that AI will be almost mandatory for firms to stay relevant in the industry and to not become obsolete. In addition, it's also a belief that innovative treatments and medicines become available to public and that companies create specific infrastructures to accommodate Artificial Intelligence centers. Overall, it's clear that changes will happen both in the near future and in more distant times but the changes that will occur in the period of 6 month to 1 year are far more minimal when compared with those that will occur in the period of 4 or more years.

In conclusion, taking into consideration all the content that was discussed and analyzed throughout this investigation, it's undoubtful that the pharmaceutical industry is evolving and modernizing itself due to the arrival of Industry 4.0 and AI is being explored and applied as a part of this revolution. In a general context, both areas are being merged to tackle the biggest gaps and flaws of the pharmaceutical industry but the application of AI in this industry is still in a very early stage and has not reached is full potential due to huge initial investments that are necessary and only available to the bigger companies.

This investigation had the purpose of filling the gaps raised by Mendes (2020) regarding the existing void over the implementation of AI in the Portuguese pharmaceutical industry and taking into consideration what Henstock (2019); Paul, *et al*. (2021); Leite, *et al.* (2021); Kulkov (2021); Niño-Amézquita, *et al*. (2018) and Mak & Pichika (2019) shared regarding the importance of linking AI to the pharmaceutical industry and the benefits it could bring to the table, which resulted in the five research questions mentioned on Table 4.3.

This study's research model was born due to the exploratory nature of this study, that led to the need for one-on-one semi-interviews, which allowed for the collection of more material than would have been possible with organized interviews. However, it's necessary to highlight that the sample is extremely small in order to allow for extrapolation and generalization of results.

6.2. Contributions to the Development of AI in the Pharmaceutical Industry

This investigation is not only academically interesting for research purposes, but also offers perspectives that can be very helpful for companies and professionals in the Portuguese pharmaceutical industry to understand how and where AI can impact their businesses and the sector itself.

As mentioned before, Portugal is one of the lowest rated countries in Western Europe regarding readiness to receive or implement AI-based technologies, even though the majority of the interviewees perceive the pharmaceutical industry in the country as not to far behind when compared to more developed countries in Europe. This can be due to two reasons, the first one being that the index previously mentioned is not specific to the pharmaceutical sector and the second is that this sector in is an early mature phase of implementing AI solutions, meaning that the discrepancies are not very visible yet.

Nonetheless, it's consensual that the Portuguese pharmaceutical industry is not as developed as in other countries throughout Europe, and the guilt can be attributed to both the lack of governmental policies to support investments and the fixation of R&D operation centers in the country, but also to the companies themselves that do not have the financial, human or structural resources to pursue AI based solutions. Also, there's still some aversion to risk and some unfamiliarity regarding to the implementation of AI within the professionals on the pharma sector.

Nontheless, AI has the potential to benefit pharmaceutical companies in a large scale regarding innovation, quality and proficiency. For these reasons, it's mandatory that

companies start to look at AI.based technologies not only as a helping hand but as requirement for the future.

Although, trough the next years, there's a generalized opinion that AI will become crucial to innovation and that the companies that do not adopt them will lose competitive advantages or become obsoletes, which can be a driver to change in the Portuguese pharmaceutical sector that can finally start to take advantage of the benefits that AI can bring to the table.

6.3. Limitations

This study was based on prior research on the subject as well as primary information obtained through interviews. The limited size of the sample is the primary drawback of this study. Although the results of the current study supported those of other studies, care must be used when drawing inferences from the interview data. It is crucial to keep in mind that this is an exploratory research and that, in large part because of the study's small sample size, it shouldn't be regarded as generalized or typical.

6.4. Suggestions for Future Research

Taking into account the relevance and impact that AI could have in the pharmaceutical industry, focusing on the major advantages it can bring to the companies and general public, and also the urgency of the industry to modernize itself in order to create disruptive innovative healthcare solutions, my suggestions are intended to encourage additional research into this topic.

Initially, the first option tackles the primary weakness of the current study, given that a bigger sample size would be quite useful. The second recommendation would be to explore this topic addressing financial parameters and results of companies within the industry to understand if the returns on investments are positive. Another proposal would be to go a step further and include other disruptive technologies, including Internet of Things (IoT), to the equation. Last but not least, considering the opinion of a lot of interviewees that AI in not a common standard practice in the industry, it should not be analyzed independently as an end but as a mean to an end.

References

Anagnoste, S. (2018). Robotic Process Automation in Pharma: Three Case Studies. In *BASIQ 2018 New Trends in Sustainable Business and Consumption*.

Angra, S., & Ahuja, S. (2017). Machine learning and its applications: A review. *International Conference on Big Data*. https://doi.org/10.1109/icbdaci.2017.8070809

Balas, V. E., Kumar, R., & Srivastava, R. (2019). *Recent Trends and Advances in Artificial Intelligence and Internet of Things* (Vol. 172). Springer Nature. https://doi.org/10.1007/978-3-030-32644-9

Baraniuk, R. G., Donoho, D. L., & Gavish, M. (2020). The science of deep learning. *Proceedings of the National Academy of Sciences of the United States of America*, *117*(48), 30029–30032. https://doi.org/10.1073/pnas.2020596117

Bhatnagar, N. (2019). Role of Robotic Process Automation in Pharmaceutical Industries. *Advances in Intelligent Systems and Computing*, 497–504. https://doi.org/10.1007/978-3-030-14118-9_50

Bhattamisra, S. K., Banerjee, P., Gupta, P., Mayuren, J., Patra, S., & Candasamy, M. (2023). Artificial Intelligence in Pharmaceutical and Healthcare Research. *Big Data and Cognitive Computing*, *7*(1), 10. https://doi.org/10.3390/bdcc7010010

Bhosale, S. S., Pujari, V., & Multani, Z. (2020). Advantages And Disadvantages Of Artificial Intellegence. In *National Seminar on "Trends in Geography, Commerce, IT And Sustainable Development."* Aayushi International Interdisciplinary Research Journal.

Bonaccorso, G. (2017). *Machine Learning Algorithms*. Packt Publishing.

Burbidge, R., Trotter, M., Buxton, B. F., & Holden, S. B. (2001). Drug design by machine learning: support vector machines for pharmaceutical data analysis. *Computers & Chemistry*, *26*(1), 5–14. https://doi.org/10.1016/s0097-8485(01)00094-8

Carmo, H., & Ferreira, M. M. (1998). *Metodologia da Investigação - Guia para auto-aprendizagem* (1st ed.). Universidade Aberta.

Chen, L. (2021). *Deep Learning and Practice with MindSpore*. Springer Nature.

Cubric, M. (2020). Drivers, barriers and social considerations for AI adoption in business and management: A tertiary study. *Technology in Society*, *62*, 101257. https://doi.org/10.1016/j.techsoc.2020.101257

Davenport, T. H., & Kalakota, R. (2019). The potential for artificial intelligence in healthcare. *Future Healthcare Journal*, *6*(2), 94–98. https://doi.org/10.7861/futurehosp.6-2-94

Dilmegani, C. (2023, January 8). *Top 4 Use Cases of RPA in Pharma in 2023*. AIMultiple. Retrieved February 16, 2023, from https://research.aimultiple.com/rpa-pharma/

Dreyer, K. J., & Allen, B. (2018). Artificial Intelligence in Health Care: Brave New World or Golden Opportunity? *Journal of the American College of Radiology*, *15*(4), 655–657. https://doi.org/10.1016/j.jacr.2018.01.010

Dwivedi, Y. K., Hughes, L., Ismagilova, E., Aarts, G., Coombs, C., Crick, T., Duan, Y., Dwivedi, R., Edwards, J. E., Eirug, A., Galanos, V., Ilavarasan, P. V., Janssen, M., Jones, P. W., Kar, A. K., Kizgin, H., Kronemann, B., Lal, B., Lucini, B., . . . Williams, M. (2021). Artificial Intelligence (AI): Multidisciplinary perspectives on emerging challenges, opportunities, and agenda for research, practice and policy. *International Journal of Information Management*, *57*, 101994. https://doi.org/10.1016/j.ijinfomgt.2019.08.002

Ekins, S. (2016). The Next Era: Deep Learning in Pharmaceutical Research. *Pharmaceutical Research*, *33*(11), 2594–2603. https://doi.org/10.1007/s11095-016-2029-7

Ghimire, A., Thapa, S., Jha, A. K., Adhikari, S., & Kumar, A. (2020a). Accelerating Business Growth with Big Data and Artificial Intelligence. *2020 Fourth International Conference on I-SMAC (IoT in Social, Mobile, Analytics and Cloud) (I-SMAC)*. https://doi.org/10.1109/i-smac49090.2020.9243318

Ghimire, A., Thapa, S., Jha, A. K., Adhikari, S., & Kumar, A. (2020b). Accelerating Business Growth with Big Data and Artificial Intelligence. *2020 Fourth International Conference on I-SMAC (IoT in Social, Mobile, Analytics and Cloud) (I-SMAC)*, 441–448. https://doi.org/10.1109/i-smac49090.2020.9243318

Gillham, J., Rimmington, L., Dance, H., Verweij, G., Rao, A., Roberts, K. B., & Paich, M. (2018). *The macroeconomic impact of artificial intelligence*. PwC.

Gunkel, D. J. (2013). The machine question: critical perspectives on AI, robots, and ethics. *Choice Reviews Online*, *50*(09), 50–4929. https://doi.org/10.5860/choice.50- 4929

Gupta, I., & Nagpal, G. (2020). *Artificial Intelligence and Expert Systems*. Mercury Learning and Information.

Haeffner, M., & Panuwatwanich, K. (2017). Perceived Impacts of Industry 4.0 on Manufacturing Industry and Its Workforce: Case of Germany. *Lecture Notes in Mechanical Engineering*, 199–208. https://doi.org/10.1007/978-3-319-74123-9_21

Haenlein, M., & Kaplan, A. M. (2019). A Brief History of Artificial Intelligence: On the Past, Present, and Future of Artificial Intelligence. *California Management Review*, *61*(4), 5–14. https://doi.org/10.1177/0008125619864925

Hashem, I. a. T., Chang, V., Anuar, N. B., Adewole, K. S., Yaqoob, I., Gani, A., Ahmed, E., & Chiroma, H. (2016). The role of big data in smart city. *International Journal of Information Management*, *36*(5), 748–758. https://doi.org/10.1016/j.ijinfomgt.2016.05.002

Henstock, P. V. (2019). Artificial Intelligence for Pharma: Time for Internal Investment. *Trends in Pharmacological Sciences*, *40*(8), 543–546. https://doi.org/10.1016/j.tips.2019.05.003

Henstock, P. V. (2020). Artificial Intelligence in Pharma: Positive Trends but More Investment Needed to Drive a Transformation. *Archives of Pharmacology and Therapeutics*, *2*(2), 24–28. https://doi.org/10.33696/pharmacol.2.017

Hofmann, P., Samp, C., & Urbach, N. (2020). Robotic process automation. *Electronic Markets*, *30*(1), 99–106. https://doi.org/10.1007/s12525-019-00365-8

Horobet, A., Polychronidou, P., & Karasavvoglou, A. (Eds.). (2020). Business Performance and Financial Institutions in Europe. *Contributions to Economics*. https://doi.org/10.1007/978-3-030-57517-5

Kelleher, J. D. (2019). *Deep Learning*. MIT Press.

Khan, S., & Aoki, Y. (2018). A review on the application of deep learning in system health management. *Mechanical Systems and Signal Processing*, *107*, 241–265. https://doi.org/10.1016/j.ymssp.2017.11.024

Kounnou, V., & Kyrkilis, D. (2020). Competitiveness, Profitability and R/D Intensity: The Case of the Domestic Pharmaceutical Industry in Greece. *Business Performance and Financial Institutions in Europe*, 47-55. Springer Nature. https://doi.org/10.1007/978-3-030-57517-5_3

Kulkov, I. (2021). The role of artificial intelligence in business transformation: A case of pharmaceutical companies. *Technology in Society*, *66*, 101629. https://doi.org/10.1016/j.techsoc.2021.101629

Kumar, S. R., Kumar, T. S. S., Beeraka, N. M., Pujar, G. V., Singh, M., Akshatha, H. S. D., & Bhagyalalitha, M. (2021). Machine learning and deep learning in data-driven

decision making of drug discovery and challenges in high-quality data acquisition in the pharmaceutical industry. *Future Medicinal Chemistry*, *14*(4), 245–270. https://doi.org/10.4155/fmc-2021-0243

Lake, F. (2019). Artificial intelligence in drug discovery: what is new, and what is next? *Future Drug Discovery*, *1*(2). https://doi.org/10.4155/fdd-2019-0025

Lamberti, M. J., Wilkinson, M. H. F., Donzanti, B. A., Wohlhieter, G. E., Parikh, S., Wilkins, R. J., & Getz, K. A. (2019). A Study on the Application and Use of Artificial Intelligence to Support Drug Development. *Clinical Therapeutics*, *41*(8), 1414–1426. https://doi.org/10.1016/j.clinthera.2019.05.018

Leite, M. L., De Loiola Costa, L. S., Cunha, V. M., Kreniski, V., Silva, K. H. C. V. E., Da Cunha, N. B., & Costa, F. F. (2021). Artificial intelligence and the future of life sciences. *Drug Discovery Today*, *26*(11), 2515–2526. https://doi.org/10.1016/j.drudis.2021.07.002

Leone, D., Schiavone, F., Appio, F. P., & Chiao, B. (2021). How does artificial intelligence enable and enhance value co-creation in industrial markets? An exploratory case study in the healthcare ecosystem. *Journal of Business Research*, *129*, 849–859. https://doi.org/10.1016/j.jbusres.2020.11.008

Loureiro, S., Guerreiro, J. F., & Tussyadiah, I. P. (2021). Artificial intelligence in business: State of the art and future research agenda. *Journal of Business Research*, *129*, 911–926. https://doi.org/10.1016/j.jbusres.2020.11.001

Mahesh, B. (2020). Machine Learning Algorithms - A Review. *International Journal of Science and Research (IJSR)*, *9*(1). https://doi.org/10.21275/ART20203995

Mak, K., & Pichika, M. R. (2019). Artificial intelligence in drug development: present status and future prospects. *Drug Discovery Today*, *24*(3), 773–780. https://doi.org/10.1016/j.drudis.2018.11.014

Malerba, F., & Orsenigo, L. (2015). The evolution of the pharmaceutical industry. *Business History*, *57*(5), 664–687. https://doi.org/10.1080/00076791.2014.975119

Marques, C., Moniz, S., De Sousa, J. P., Barbosa-Póvoa, A. P., & Reklaitis, G. V. (2020). Decision-support challenges in the chemical-pharmaceutical industry: Findings and future research directions. *Computers & Chemical Engineering*, *134*, 106672. https://doi.org/10.1016/j.compchemeng.2019.106672

Mendes, J. D. T. (2020). *Digitalização: O impacto da Indústria 4.0 na Indústria Farmacêutica em Portugal* [MA Thesis]. Faculdade de Economia da Universidade do Porto.

Miller, H., & Stirling, R. (2019). *Government Artificial Intelligence Readiness Index*. Oxford Insights.

Mishra, R. (2018). Influence of Research and Development (R&D) Cost on Profitability: A Study of Indian Pharmaceutical Sector. *IOSR Journal of Economics and Finance (IOSR-JEF)*, *9*(2), 63–68. https://doi.org/10.9790/5933-0902026368

Niño-Amézquita, J. (2017). Economic success and sustainability in pharmaceutical sector: a case of Indian SMEs. *Hal.Science*. https://doi.org/10.9770/jesi.2017.5.1(13

Oliveira, A. L. (2019). Biotechnology, Big Data and Artificial Intelligence. *Biotechnology Journal*, *14*(8), 1800613. https://doi.org/10.1002/biot.201800613

Ostrowski, D. (2018). Artificial Intelligence with Big Data. *2018 First International Conference on Artificial Intelligence for Industries (AI4I)*, 125–126. https://doi.org/10.1109/AI4I.2018.8665678

Pammolli, F., Magazzini, L., & Riccaboni, M. (2011). The productivity crisis in pharmaceutical R&D. *Nature Reviews Drug Discovery*, *10*(6), 428–438. https://doi.org/10.1038/nrd3405

Paul, D., Sanap, G., Shenoy, S., Kalyane, D., Kalia, K., & Tekade, R. K. (2021). Artificial intelligence in drug discovery and development. *Drug Discovery Today*, *26*(1), 80– 93. https://doi.org/10.1016/j.drudis.2020.10.010

Pereira, A., D, R. L., Costa, A., Gonçalves, R., Pereira, L., & Dias, Á. (2023). Industry 4.0 in Portugal - the state of the art. *International Journal of Internet Manufacturing and Services*, *9*(1), 44–70. https://doi.org/10.1504/ijims.2023.129286

Peres, R. S., Jia, X., Lee, J. H., Sun, K., Colombo, A. W., & Barata, J. (2020). Industrial Artificial Intelligence in Industry 4.0 - Systematic Review, Challenges and Outlook. *IEEE Access*, *8*, 220121–220139. https://doi.org/10.1109/access.2020.3042874

PharmaNewsIntelligence. (2021, April 29). *AI in the Pharma Industry: Current Uses, Best Cases, Digital Future*. Retrieved July 3, 2022, from https://pharmanewsintel.com/news/ai-in-the-pharma-industry-current-uses-best- cases-digital-future

Prasad, R., & Choudhary, P. (2021). State-of-the-Art of Artificial Intelligence. *Journal of Mobile Multimedia*. https://doi.org/10.13052/jmm1550-4646.171322

Qin, T. (2021). *Dual Learning*. Springer. https://doi.org/10.1007/978-981-15-8884-6

Rahmani, A. M., Azhir, E., Ali, S., Mohammadi, M., Ahmed, O. H., Ghafour, M. Y., Ahmed, S. H., & Hosseinzadeh, M. (2021). Artificial intelligence approaches and

mechanisms for big data analytics: a systematic study. *PeerJ*, *7*, e488. https://doi.org/10.7717/peerj-cs.488

Reinhardt, I. C., Oliveira, J. C., & Ring, D. (2021). Industry 4.0 and the Future of the Pharmaceutical Industry. *Pharmaceutical Engineering*, *41*(2).

Reinhardt, I., Oliveira, J. M., & Ring, D. (2020). Current Perspectives on the Development of Industry 4.0 in the Pharmaceutical Sector. *Journal of Industrial Information Integration*, *18*, 100131. https://doi.org/10.1016/j.jii.2020.100131

Ribeiro, J. P., Lima, R., Eckhardt, T., & Paiva, S. (2021a). Robotic Process Automation and Artificial Intelligence in Industry 4.0 – A Literature review. *Procedia Computer Science*, *181*, 51–58. https://doi.org/10.1016/j.procs.2021.01.104

Ribeiro, J. P., Lima, R., Eckhardt, T., & Paiva, S. (2021b). Robotic Process Automation and Artificial Intelligence in Industry 4.0 – A Literature review. *Procedia Computer Science*, *181*, 51–58. https://doi.org/10.1016/j.procs.2021.01.104

Schuhmacher, A., Gatto, A., Hinder, M., Kuss, M., & Gassmann, O. (2020). The upside of being a digital pharma player. *Drug Discovery Today*, *25*(9), 1569–1574. https://doi.org/10.1016/j.drudis.2020.06.002

Shabbir, J., & Anwer, T. (2018). Artificial Intelligence and its Role in Near Future. *ArXiv (Cornell University)*. http://export.arxiv.org/pdf/1804.01396

Sharifzadeh, M. (2022). *Industry 4.0 Vision for the Supply of Energy and Materials: Enabling Technologies and Emerging Applications*. John Wiley & Sons.

Shinde, P. P., & Shah, S. K. (2018). A Review of Machine Learning and Deep Learning Applications. *International Conference on Computing Communication Control and Automation*. https://doi.org/10.1109/iccubea.2018.8697857

Suzuki, K. (2011). *Artificial Neural Networks: Methodological Advances and Biomedical Applications*. IntechOpen.

Szczepański, M. (2019). *Economic impacts of artificial intelligence (AI)*. European Parliamentary Research Service.

Taulli, T. (2019). *Artificial Intelligence Basics: A Non-Technical Introduction*. Apress. https://doi.org/10.1007/978-1-4842-5028-0

Turin, A. M. (1950). *Mind: A Quarterly Review of Psychology and Philosophy* (Vol. 59).

Vargas, R. R., Mosavi, A., & Ruiz, R. L. (2017). Deep Learning: A Review. *Advances in Intelligent Systems and Computing*. https://doi.org/10.20944/preprints201810.0218.v1

Vilelas, J. (2020). *Investigação - O Processo de Construção do Conhecimento* (3rd ed.). Edições Sílabo, Lda.

Wagner, A. K., Grootendorst, P., Lexchin, J., Cunningham, C., & Greyson, D. (2011). The cost of drug development: A systematic review. *Health Policy*, *100*(1), 4–17. https://doi.org/10.1016/j.healthpol.2010.12.002

Wang, F., & Preininger, A. M. (2019). AI in Health: State of the Art, Challenges, and Future Directions. *Yearbook of Medical Informatics*, *28*(01), 016–026. https://doi.org/10.1055/s-0039-1677908

Wang, S. S., Pershing, S., Lee, A. Y., & Ai, A. T. O. (2020). Big data requirements for artificial intelligence. *Current Opinion in Ophthalmology*, *31*(5), 318–323. https://doi.org/10.1097/icu.0000000000000676

Wang, X., Zhao, Y., & Pourpanah, F. (2020). Recent advances in deep learning. *International Journal of Machine Learning and Cybernetics*, *11*(4), 747–750. https://doi.org/10.1007/s13042-020-01096-5

What is Artificial Intelligence (AI)? | IBM. (n.d.). Retrieved June 11, 2022, from https://www.ibm.com/topics/artificial-intelligence

Wen, M., Zhang, Z., Niu, S., Sha, H., Yang, R., Yun, Y., & Lu, H. (2017). Deep-Learning Based Drug–Target Interaction Prediction. *Journal of Proteome Research*, *16*(4), 1401–1409. https://doi.org/10.1021/acs.jproteome.6b00618

Wood, T. (2020, September 2). *Backpropagation*. DeepAI. Retrieved January 5, 2023, from https://deepai.org/machine-learning-glossary-and-terms/backpropagation

Zhang, L., Tan, J., Han, D., & Zhu, H. (2017). From machine learning to deep learning: progress in machine intelligence for rational drug discovery. *Drug Discovery Today*, *22*(11), 1680–1685. https://doi.org/10.1016/j.drudis.2017.08.010

Zhu, H. (2020). Big Data and Artificial Intelligence Modeling for Drug Discovery. *Annual Review of Pharmacology and Toxicology*, *60*(1), 573–589. https://doi.org/10.1146/annurev-pharmtox-010919-023324

Zikria, Y. B., Afzal, M., Kim, S. W., Marin, A., & Guizani, M. (2020). Deep learning for intelligent IoT: Opportunities, challenges and solutions. *Computer Communications*, *164*, 50–53. https://doi.org/10.1016/j.comcom.2020.08.017

Kpayc, K. M., Kpayc, H. M., & Manzhura, O. (2021). Digitalization of Business Processes of Enterprises of the Ecosystem of Industry 4.0: Virtual-Real Aspect of Economic Growth Reserves. *WSEAS Transactions on Business and Economics*, *18*, 569–580. https://doi.org/10.37394/23207.2021.18.57

Annex A - Interview Script

Q1. - Qual é a sua perceção relativamente ao desenvolvimento tecnológico da indústria farmacêutica em Portugal?

Q2. - Na sua ótica, quais são as tecnologias de IA que são mais vulgarmente utilizadas na indústria farmacêutica portuguesa?

Q3. - Na sua perspetiva, em quais processos de Investigação e Desenvolvimento farmacêutico são as tecnologias de IA mais vulgarmente utilizados?

Q4. - Quais considera ser os impactos (riscos ou benefícios) dos investimentos em tecnologias IA face a empresas que não apliquem estas tecnologias?

Q5. - Quais são as suas expectativas relativamente aos investimentos nas tecnologias IA na indústria farmacêutica?