

Studying Scientific Discovery by Computer Simulation

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Scientists and artists sometimes direct their curiosity to studying their own mental processes. Perhaps they believe that a deeper understanding of their processes of discovery will allow them to be more creative. However that may be, a number of distinguished scientists have undertaken to speak and write on the topic of creativity (1). They have provided a rich description of the phenomena that are visible during the work of discovery, identifying and labeling such characteristic aspects as "preparation," "incubation," "intuition," and the "aha" experience.

Psychologists and sociologists, too, have studied invention, discovery, and the creative processes. They have interviewed and questioned scientists and artists, examined histories, biographies, and autobiographies, and even observed modest creativity in the laboratory. Their accounts agree well with those provided by the scientists themselves. In addition, they have learned something about how scientific discovery interacts with social environment.

None of this work, however, explains how a discovery actually comes about, and how it can be achieved by an information-processing system having the characteristics of the human brain. Words like "incubation" and "intuition" do not tell us what is going on; they merely emphasize that much occurs without detailed conscious awareness. These terms name processes that are not fully open to conscious reports.

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Computer Simulation of Creativity

During the past quarter century considerable success has been attained in constructing computer programs that simulate in some detail the processes that people use to solve relatively difficult problems, such as making a chess move or understanding the instructions for a puzzle. This progress has suggested extending computer simulation to study-

Summary. BACON is a computer program that simulates some of the important processes of scientific discovery. When provided with data about temperatures before and after two substances are brought into contact, the program infers the concept of specific heat and arrives at Black's law of temperature equilibrium. Comparison of BACON's discovery methods with historical records of Black's work casts light on the relation between data-driven and theory-driven discovery.

ing scientific discovery. As early as 1958 it had been proposed that the processes of creative thinking were essentially the same as those used to account for more ordinary garden varieties of problem-solving (2). What distinguished creative thinking from other thought, it was argued, was not qualitatively different processes, but the poorly structured character—the "vagueness"—of the problems attacked, and the creative person's persistence, over long periods of time, in attacking them.

Rather than speculate that creativity is problem-solving writ large, we can subject this hypothesis to empirical tests. One way to do this is through computer simulation. First, we specify the problem-solving processes we think are used in and required for discovery, defining

them with such specificity that we can write a computer program to execute them. Second, we confront the program with discovery problems that scientists have encountered, and we observe whether the program can make the discovery, starting from the same point the scientists did, using only processes that, from other psychological evidence, are known to be within human capabilities.

Our data about human creativity are historical accounts of actual scientific discoveries of first importance that were made by physicists and chemists in the 17th, 18th, and 19th centuries. Although these accounts provide only coarse-grained narratives of what took place, they define the initial conditions for the simulation by specifying what was already known at the time the discovery was made. They also disclose how the problem was conceptualized by the discoverer and his contemporaries and allow some conclusions to be drawn about similarities and differences between the computer simulation and the historical discovery.

Our approach is best illustrated by a concrete example. But first, one more caveat is in order. Scientific discovery involves a whole array of processes, including gathering data, finding parsimonious descriptions of the data, and formulating and testing explanatory theories. In this article, we will be concerned with just one subset of these processes—principally with data-driven discovery, that is, discovery that starts with given data, and derives new descriptive or explanatory laws from them. The generation of data, and even the invention of instruments to produce new kinds of data, are also important aspects of scientific discovery. And in many cases, existing theory as well as data steer the course of discovery. Later we will comment on these other components

of the discovery process, but initially we will consider the path from data to laws. Much important scientific work falls in this category. As an example, we turn now to the discovery of Black's law: the law describing the equilibrium temperature of a mixture of two liquids.

Black's Discovery

About 1760 Joseph Black made the first of the several important discoveries that have preserved his name (3). Using data reported in a standard chemistry textbook of his time (Boerhaave's) from an experiment performed at Boerhaave's request by Fahrenheit, Black reinterpreted the data to formulate what we now know as Black's law for the temperature of mixtures. Since Fahrenheit reported his invention of the mercury thermometer in 1724 and died in 1736, Black's data were 25 to 35 years old.

The experiment was simple: mixing two substances while measuring their initial and final temperatures. It is, of course, an everyday experience that the temperature of hot water can be moderated by mixing it with cold. What Fahrenheit, armed with the newly invented thermometer, showed was that if equal volumes of water at different temperatures are mixed, the temperature of the mixture is the arithmetic average of the initial temperatures. Other experiments showed that if the original amounts are unequal, the average has to be weighted by those amounts.

It also was reported by Boerhaave that if two objects of different substance are mixed, their final temperature will be some kind of average of their original temperatures. However, there was great confusion about that average, it being commonly maintained, in the face of contrary evidence, that the average depended on the masses or volumes involved, but not on the species of the substances. It was especially confusing that a heavy substance, like mercury, influenced the final temperature less than an equal volume of a lighter substance, like water. This result was highly counterintuitive.

Black cleared up the confusion and formulated his law by attributing a new property to the unit volume (or mass) (4) of each particular substance, its specific heat. The specific heat multiplied by the object's volume (or mass) gave its heat capacity. The final temperature of a mixture could be calculated from the average of the initial temperatures with the heat capacities as weights.

Different substances had different spe-

cific heats, determinable from the mixing experiment. No independent, converging procedures were available for estimating specific heats until Dulong and Petit in 1819 showed that they were approximately inversely proportional to atomic weights. And no theoretical basis for this relation was forthcoming until much later.

Inductive Derivation of Laws by BACON

It would seem, at first blush, that Black's accomplishment was a pure act of Baconian induction. Confronted with data on the equilibrium temperatures that resulted from mixing mercury and water, he introduced new constants, the specific heats. He then found that the final temperature could be predicted as a function of the initial temperatures, volumes, and specific heats of the substances. But how could this induction be achieved? The failure of Fahrenheit, Boerhaave, and others to arrive at it during the 30 years after the experiments were performed suggests that it was not trivial.

The technique of computer simulation allows us to answer at least part of this question. In particular, a program known as BACON, when provided with data like those that Black had, soon induces that they can be summarized parsimoniously by the formula we know as Black's law. While making the discovery, BACON also invents the concept that Black called specific heat.

BACON was not initially constructed with Black's law in mind (the initial versions were debugged mainly with data from Kepler's third law, Ohm's law, and Snell's law of refraction) but is a general data-driven system for inducing scientific laws (5). The program's inputs are data that may include both numerical and nominal values; its outputs are empirical laws that summarize those data. A number of versions of BACON have existed in the course of its development, later versions generally having richer sets of heuristics (rules to guide the induction process) than the earlier ones. Our description here will be based mainly on BACON.4 and BACON.5.

BACON begins to examine the independent variables, one at a time, while holding the others constant, with the aim of discovering a functional relation between independent and dependent variables. If a relation is found, additional variables are introduced, one at a time, and BACON attempts to generalize the function it has found. This process is continued until an invariant relation is

found that holds for the entire body of data, or until BACON runs out of time. BACON has a modest capacity to ignore noise in the data.

BACON does not engage in unrestricted, try-everything induction, since the goal of the research is to understand how humans can make difficult inductions after exploring relatively small numbers of possibilities that are selected intelligently. BACON's search is also highly selective, guided by a few powerful heuristics. It detects constancies in data. It looks for linear relations. When one variable varies monotonically with another, BACON examines the product or ratio of the two as a possible invariant. For example, if the current in a circuit varies inversely with the resistance, BACON computes their product, finding it to be constant. If the product or ratio is not constant, it is still introduced as a new variable (a theoretical term), and treated exactly like the observational variables.

When BACON discovers that a relation among variables depends on a nominal variable, it associates a new numerical variable (intrinsic property) with the nominal variable. For example, if the ratio of current to resistance in a circuit depends on which of several batteries is inserted in the circuit, BACON associates with the variable battery a new numerical variable, which we would call the voltage, and which is measured by the ratio of current to resistance. Once defined, the intrinsic properties are treated like the other variables and can be retrieved when useful for the analysis. This ability to introduce new intrinsic properties enables BACON to create the variable specific heat to account for the different effects of different substances on the equilibrium temperature in the mixture experiments.

In some situations, two objects (for example, two batteries) have exactly the same set of properties, although with different values. In this case, BACON.5 assumes that the law it is seeking will be symmetrical with respect to the objects. It orders the data so that variables attached to one of the objects are varied first. Once a constant function has been found incorporating all the variables associated with the one object, BACON will assume an analogous function for the other object. In this way, the symmetrical laws so common in physics are recognized with great saving in search. The assumption of symmetry can be very helpful in deriving Black's law of specific heat, but it is not essential.

Although BACON's search is primarily driven by the data, its use of symmetry shows that it can also respond to

theoretical considerations—as presumably human scientists can. We shall presently outline a system that also can entertain hypotheses of conservation (in this case, conservation of heat) to facilitate its discovery of laws.

BACON's Derivation of Black's Law

Black's Law can be stated quite simply. The quantitative relation is

$$c_1 m_1 t_1 + c_2 m_2 t_2 = (c_1 m_1 + c_2 m_2) f$$

where t_1 and t_2 are the initial temperatures, f is the final temperature, m_1 and m_2 are the masses of the two liquids, and c_1 and c_2 are the specific heats associated with the two species of liquid. If we call the coefficients of the two temperatures on the left side of the equation A and B , respectively, then the final temperature is the weighted average of the temperatures of the components, with weights of $A/(A+B)$ and $B/(A+B)$, respectively. The coefficients A and B are the heat capacities of the two substances, At_1 and Bt_2 are their total heats, and $(A+B)f$ is the total heat of the mixture. Hence, the equation can be interpreted as saying that total heat is conserved, where the heat capacity of the mixture is the sum of the heat capacities of the components.

Now we can sketch out an inductive path, involving almost no extraneous search, that will lead from the data to Black's law. For simplicity, we will not follow exactly the path used by any single version of BACON but will describe one that does not differ in essential respects from those that were tested.

Initially, we employ identical volumes of the same substance (for example, water). In the first experiment, we vary the temperature of the first component, holding all other variables constant. We discover that the equilibrium temperature is a linear function of the independent variable, with a slope of 1/2. In the second experiment, we vary the second temperature, using symmetry between the two volumes to conjecture that the equilibrium temperature will also vary linearly with this new independent variable, with a slope of 1/2. The data confirm this relation.

In the third experiment, we vary the mass of the first component to determine how that mass enters the function determining the equilibrium. We now conjecture that a symmetric function will describe the joint effects of both masses. The data confirm this conjecture.

In the fifth experiment, we change the composition of the first component (for

example, substitute mercury for water). BACON finds that a new coefficient must be introduced into the equation, whose value changes with change in the composition of the component. In the sixth experiment, we change the composition of the second component, and, by symmetry, introduce another new coefficient into the equation. The equation, thus modified, again fits the data. The coefficients introduced in the fifth and sixth experiments are, of course, the quantities that Black called specific heats (6).

Data-Driven Induction

Black's law is not an isolated example of data-driven induction. In modern science, it has been common for the discovery of laws of first importance to precede, sometimes by many years, the discovery of theoretical conceptions that could account for them. Let us cite a few examples.

Kepler's third law, expressing the periods of revolution of the planets about the sun as the 3/2 power of their distances from it, was a product of pure Baconian induction. It was 100 years later that Newton produced the gravitational theory from which Kepler's law could be deduced.

Ohm's law is another clear-cut case where data preceded any substantial theoretical framework (7, pp. 465–472), although the analogy of hydraulic flow may have been helpful. The invention of the voltaic cell around 1800 transformed electricity from a transient phenomenon—a spark produced by a Leyden jar—into a continuous one—a current. Later, Seebeck's thermopile provided reasonably constant voltages. The subsequent invention by Ampère, about 1820, of an instrument for measuring current provided a quantifiable observable for experiments with circuits. The second observable (the independent variable) that Ohm selected was the length of the resistance wire in the circuit. The discovery of Ohm's law in 1826 became then a straightforward task of inducing the relation between current and resistance.

This by no means exhausts the list of scientific laws that were induced from data before any theory was available to discover the regularities. We could add Balmer's formula for the hydrogen spectrum, Prout's hypothesis of atomic structure, Mendel's laws of inheritance, the law of Gay-Lussac for gaseous reactions, the law of atomic heats of Dulong and Petit, the derivation of atomic

weights by Avogadro and Cannizzaro, and the construction of the periodic table by Mendeleev. Experiments with BACON have indicated paths along which most of these discoveries (excluding those of Mendel and Mendeleev, which we have not simulated) could have been made, with only plausible heuristics to guide the search.

Theory and Law Induction

BACON's derivation of Black's law is truly data-driven. It was achieved simply by carrying out a succession of controlled experiments, from which emerged not only the law, but a new theoretical concept, the specific heat. Theoretical presuppositions (symmetry) played only a minor role in the discovery. The assumption of symmetry reduced the search required to find the law, but other versions of BACON have found the same law, more tediously, without this assumption.

However, data-driven induction is not the only route to discovery. At the opposite extreme, there may already exist a theory so complete and powerful that the laws can be deduced from it without any induction at all. Lying somewhere between pure induction and pure deduction are situations where incomplete theoretical constructs can guide and channel somewhat the course of the induction but fall short of permitting a priori deduction of the actual laws.

The circumstances surrounding the discovery of Black's law provide evidence that the actual discovery was, indeed, aided by some conceptual framework and was not as completely data-driven as the pathway taken by BACON. In a textbook published posthumously, Black observed that the nature of temperature equilibrium was not well understood, in particular, that it was sometimes supposed to imply an equal amount of heat per unit volume of each body. "But," he wrote, "this is taking a very hasty view of the subject. It is confounding the quantity of heat in different bodies with its general strength or intensity, although it is plain that these are two different things, and should always be distinguished, when we are thinking of the distribution of heat" (7, p. 135).

Although the equilibrium experiments measured only one physical variable, the temperature, Black was contrasting quantity of heat with general strength or intensity, and attributed the difficulties of his predecessors to their failure to make a sharp distinction between these

and to identify temperature only with the latter. The idea of quantity of heat predated Black, playing a central role in the caloric theory. Although the very terms "hot" and "cold" as used in everyday language refer to heat intensity, it is not clear that this idea had been equally clearly conceptualized before the time of Black. Let us see, however, how he might have used a very general conceptual framework, involving the relation between extensive and intensive quantities, to clarify these notions.

We are familiar with extensive quantities like mass and volume, which are additive: the volume (mass) of the combination of two objects is the sum of the volumes (masses) of the individual objects. The density, the mass per unit volume, behaves differently. The density of the combined object is a weighted average of the densities of the components, their volumes constituting the weights.

But there is an easier way to think of the density in terms of conservation principles. When objects are combined, mass and volume are conserved (8). Density is simply the ratio of mass to volume. Hence, to compute the density of the combination, simply divide the total mass by the total volume. The notion of weighted averages need not enter if the extensive, conserved quantities are given primary position in the representation, and intensive quantities only a secondary position.

With this general framework, one can reconsider the heat experiments. Black may well have approached the experimental data with the idea already somewhat in mind that quantity of heat is an extensive magnitude and one that is conserved. He could also have had the idea that large quantities of substances would contain, other things being equal, greater quantities of heat than would small quantities of substances. Hence, one could define an intensive quantity by dividing the total heat by a substance's capacity for heat. Black identified this ratio with temperature.

Black's predecessors were clearly prepared to admit that large quantities of water would have a greater influence on the equilibrium temperature than small quantities. Their problem came from identifying a large quantity of volume or weight with "heat capacity." Before the fact, both volume and mass were plausible candidates for the measure of heat capacity, volume because it defined the space within which the heat, or caloric, was held, and mass because it defined the "quantity of matter" of the heat-bearing substance.

Black was the first to perceive that neither of these extensive measures of heat capacity was consistent with the data from the experiments. By introducing a new property, with a different value for each substance, he could express total heat as the product of the extensive variable, heat capacity, and the intensive variable, temperature. Heat capacity, in turn, could be expressed as a product of the traditionally accepted variables, mass or volume, by a new intensive quantity, specific heat. The key to Black's success was the idea of introducing this new intrinsic property.

We would not like to insist on the detailed accuracy of this account of how Black arrived at the concept of specific heat for his textbook enjoys the clarity of hindsight and does not necessarily represent his state of mind at the time of the discovery. What is important for our purposes here is that this somewhat hypothetical sequence shows how the ideas of preceding theory could guide the interpretation of new data. In the next section, we outline a system that is capable of making use of conceptualizations of this kind to aid data analysis.

Explaining Concept-Guided Induction

Volume, mass, and density constitute a system of related quantities, two extensive and one intensive. When two objects are combined, the volumes and masses combine additively, and the density of the combined object is a weighted average of the densities of the components. The weights are the volumes of the components. The same relations hold among any triad of extensive (conservative) and intensive variables where the third is the ratio of the first two.

Suppose that we give our system the information that C and H are extensive and conservative quantities and that $T = H/C$. We also provide data, as in the experiments previously described, for the initial and equilibrium values of T under different conditions. The system can then employ the relations

$$H_1 + H_2 = C_1 T_1 + C_2 T_2 = C_f T_f = H_f$$

$$C_f = C_1 + C_2$$

Fitting the data to these relations, we find that the C 's vary proportionately with the masses of their respective objects, but that they are different for equal masses of different substances. If mass is also accepted as an extensive, conservative measure, then the variations in C can be explained in introducing $c = C/M$, where c , the specific heat, is a property of the substance employed in the

experiment (9). With these definitional identities, Black's law can now be stated in precisely the form that was displayed earlier.

The conservation assumptions are therefore very powerful, allowing the system to predict the form of the law and requiring the data only to show the need for specific heats and to estimate their values. Inductive search is essentially eliminated.

There were at least two paths—a purely inductive one and a deductive one—that could have been used to discover Black's law. The historical evidence does not make clear their relative roles in the discovery, and hindsight does not settle the matter. Our main motive in introducing the historical example was to illustrate a few of the routes that scientific discovery can take and the kinds of mechanisms that can be used to traverse these routes.

Conclusion

The experiments with the BACON program show how major scientific discoveries can be made with only data-driven induction, unaided by theory. In fact, the inductive processes, in the course of discovering laws, themselves create new theoretical terms, including new intrinsic properties. The BACON experiments help to explain, thereby, how some of the important laws of modern science could antecede by decades or even generations the theoretical structures that subsequently rationalized them and took them out of the category of brute empirical generalizations.

On the other hand, the experiments also show that introducing pretheoretical constructs, like symmetry and conservation, may reduce significantly the amount of search required to detect empirical regularities in data. In fact, if sufficiently strong hypotheses are available, the roles of theory and data may be reversed, so that laws are now deduced directly from theoretical assumptions and subsequently tested by data. The history of the discovery of Black's law suggests that it was neither wholly data-driven nor wholly deduced from theoretical assumptions, but that both induction from experimental observations and deduction from notions of the conservation of extensive properties played a role in the discovery.

More generally, the experiments with BACON provide hypotheses about how scientific discovery comes about. The processes that BACON uses are much the same as those that have emerged

from other research on human problem-solving and that are usually described as processes for selective heuristic search through spaces of possible solutions. The less blind the search—that is, the more existing theoretical knowledge is available to guide it and turn it from unprofitable directions—the more readily and directly are the regularities hidden in empirical data discovered.

References and Notes

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2. A. Newell, J. C. Shaw, H. A. Simon, in *Models of Thought*, H. A. Simon, Ed. (Yale Univ. Press, New Haven, Conn., 1979), pp. 144–174; H. A. Simon, in *Mind and Cosmos*, R. Colodny,

Ed. (Univ. of Pittsburgh Press, Pittsburgh, 1966), pp. 22–40.

3. Many of the source documents relating to this and most of the other scientific discoveries discussed in this paper can be found in H. M. Leicester and H. S. Klockstein [A *Source Book in Chemistry* (McGraw-Hill, New York, 1952)] and W. F. Magie (7); Black's law is described by Magie (7), pp. 134–139.
4. Black saw that it did not matter which of the two measures of amount was used.
5. A description of the basic BACON program will be found in H. A. Simon, P. W. Langley, G. L. Bradshaw [Synthese 47, 1 (1981)]. BACON.4's heuristics were devised before our work on Black's law; BACON.5 incorporates modifications partly motivated by our experience with that law. There are a number of programs antecedent to BACON that are capable of inducing laws from data. Early examples include a program for extrapolating letter series [H. A. Simon and K. Kotovsky, *Psychol. Rev.* 70, 534 (1963)] and a program for fitting functions to data [D. G. Gerwin, *Behav. Sci.* 19, 314 (1974)]. The METADENDRAL program [B. G. Buchanan, G. Sutherland, E. B. Feigenbaum, in *Machine Intelligence 4*, B. Meltzer and D. Michie, Eds. (Elsevier, New York, 1969)] constructs rules for explaining mass spectrogram data. The AM and EURISKO programs [D. B. Lenat, *Proc. 5th*

Int. Jt. Conf. Artif. Intell. (1977), p. 833; *Artif. Intell.* 21, 31 (1983)] discover new concepts and make conjectures. This is by no means an exhaustive list of programs with such inductive capabilities.

6. We have described the last stages of the inductive process only in the roughest terms. Parenthetically, it should be mentioned that the derivation of Black's law by BACON.4 [G. L. Bradshaw, P. W. Langley, H. A. Simon, *Proc. Natl. Conf. Can. Soc. Comput. Stud. Intell.* (1980), p. 19] is incomplete, but the derivation by BACON.5 [P. W. Langley, G. L. Bradshaw, H. A. Simon, *Proc. 7th Int. Jt. Conf. Artif. Intell.* (1981), p. 121] is correct.
7. W. F. Magie, *A Source Book in Physics* (McGraw-Hill, New York, 5/1935).
8. This is not always true; whether it is in any given case is a matter of physics and chemistry. But early in life we encounter many situations where such conservation holds, and we build up a representation for thinking about that broad class of situations.
9. A first crude version of a computer program capable of carrying out this kind of reasoning has been constructed, and our experiences with it will be reported in future publications.
10. Supported by NIMH grant MH-07722 and contract N00014-82-K-0168 from the Office of Naval Research.

Brain Peptides: What, Where, and Why?

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In recent years, a large number of peptides, many of which were originally characterized in nonneural tissues, have been reported to be present in the central nervous system. Table 1 indicates the rapidity of recent progress in this field. It can be seen that, in addition to those peptides that were originally termed "hypothalamic-releasing hormones," all of the other peptides identified within the central nervous system and which were previously known to occur within the gastrointestinal tract—that is, vasoactive intestinal polypeptide (VIP), cholecystokinin (CCK), insulin, and glucagon—and within the pituitary—that is, adrenocorticotrophic hormone (ACTH) and other peptides derived from its precursor, pro-opiomelanocortin (POMC), and possibly prolactin, thyrotropin-stimulating hormone (TSH), and a luteinizing hormone (LH)—have been described essentially within the last 10 years.

The detection of these peptides within the central nervous system has raised many questions regarding their source,

mechanism of action, and function. Many of the initial studies in this field focused on the delineation of the sites of peptide distribution and the demonstration of peptide synthesis within the central nervous system. Distribution studies were of value in delineating localization

source. Regulation of a neuronally synthesized peptide is governed by both "neuronal" and "metabolic" inputs impinging on the neuron; the synthesized material would be acting as a neurotransmitter—that is, being liberated at presynaptic terminals with subsequent postsynaptic membrane effects. In the case of a peripherally synthesized peptide having access to the central nervous system, its synthesis is regulated by the multiplicity of factors known to affect its tissue of origin, and its central nervous system actions would presumably be mediated via peptidergic receptors present on neurons or their terminals.

Until recently, the monoamines (norepinephrine, epinephrine, dopamine, and serotonin), acetylcholine, and the amino acids (such as glycine, glutamine,

Summary. Within the past decade, a large number of peptides have been described within the vertebrate central nervous system. Some of these peptides were previously known to be present in nonneural vertebrate tissues, as well as in lower species, in which they may serve as primitive elements of intercellular communication prior to the development of neuronal or endocrine systems. In vertebrates, these peptides are thought to have neurotransmitter or neuromodulatory roles and appear to be involved in the regulation of a number of homeostatic systems, although the mechanisms of their actions are still unclear.

of peptide-containing cell bodies in which synthesis could potentially occur, as well as delineating fiber pathways for investigation of possible physiological function (or functions). Demonstration of synthesis was deemed important since conceptually the mechanism of action and the function of a peptide detected in the central nervous system would differ if the peptide were locally synthesized or were transported thereto from another

and γ -aminobutyric acid) were thought to be the only neurotransmitters that classically mediated synaptic communication (1). Prior to the last decade, the only peptide chemically characterized within the brain was substance P (2), previously identified therein and in the gastrointestinal tract in terms of its biological activity. Table 1 indicates the time frame in the past decade during which some of the other peptides present

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