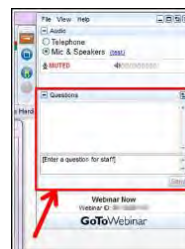




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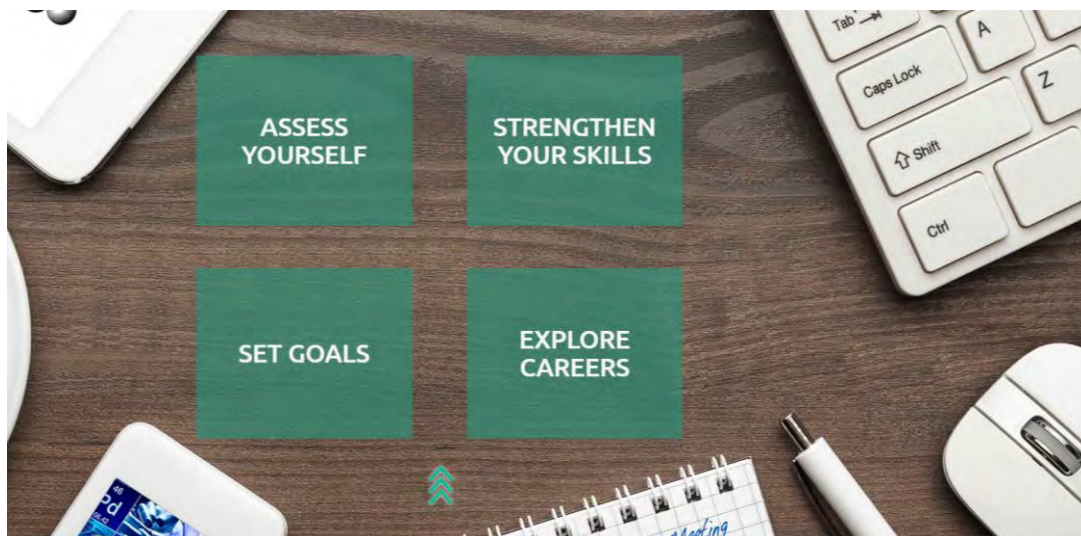


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WHO WE ARE

Founded in 1986, the American Association of Pharmaceutical Scientists (AAPS) is a professional, scientific organization of approximately 7,000 individual members and over 10,000 actively participating stakeholders employed in academia, industry, government, and other pharmaceutical science related research institutes worldwide.

Our mission:

To advance the capacity of pharmaceutical scientists to develop products and therapies that improve global health

Our vision:

Advancing the pharmaceutical sciences to drive prevention and cures.

Our five core values:

Learning, Innovation, Service, Inclusiveness and Integrity.

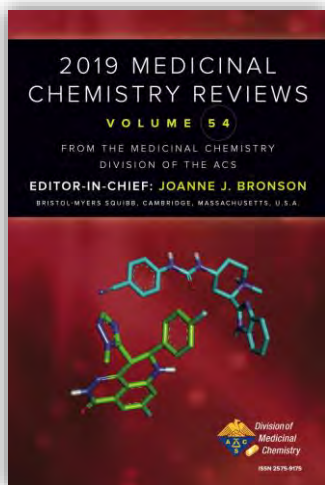
AAPS is incorporated as a not-for-profit organization under the U. S. Internal Revenue Service Code, 5501(c)3 in the District of Columbia.

Members of the American Association of Pharmaceutical Scientists (AAPS) gathered during the 2013 AAPS Annual Meeting and Exposition to discuss why they chose a career in pharmaceutical sciences and how AAPS has helped foster their journey. The I Am AAPS video series displays the diversity of AAPS membership while exhibiting one common goal: to impact global health.

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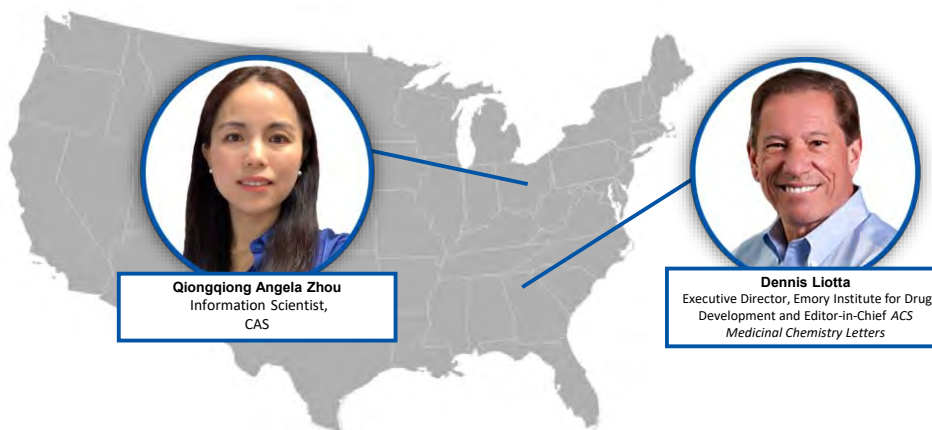
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A Groundwork for Therapeutic Agents and Vaccines

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Fighting COVID-19

A Groundwork for Therapeutic Agents and Vaccines

Qiongqiong Angela Zhou, Ph.D. (presenter)
Cynthia Liu, Ph.D.

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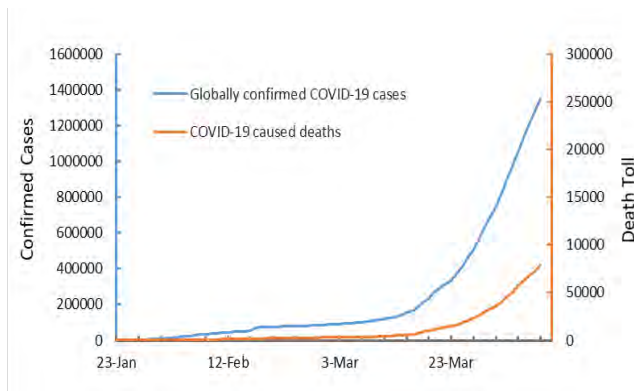
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The impact of COVID-19 is global and growing

- Confirmed cases and death toll are continuing to rise
- People's lives and global economy are being impacted significantly
- On-going worldwide effort to identify effective drugs and develop vaccines



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CAS recently published a report in *ACS Central Science* and an open source antiviral dataset



ACS Cent. Sci. 2020, 6, 3, 315-331
 Publication Date: March 12, 2020
<https://doi.org/10.1021/acscentsci.0c00272>

CAS COVID-19 Antiviral Candidate Compounds Dataset of nearly 50,000 compounds with known or potential antiviral activity and related metadata to support research, data mining, and analytics applications
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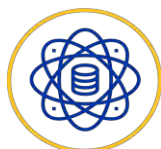
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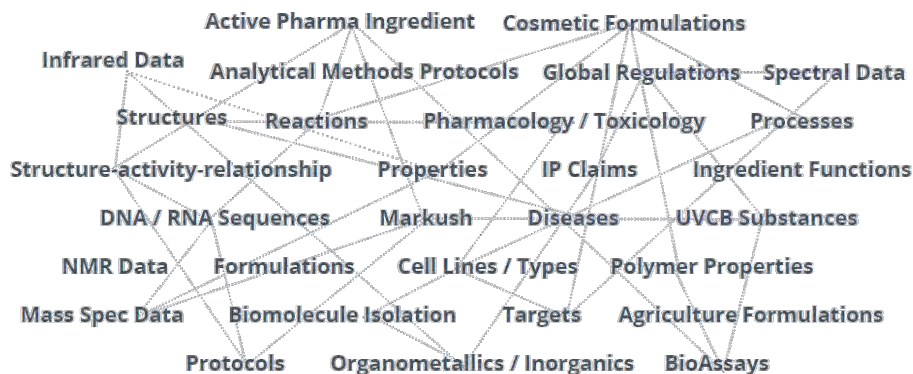
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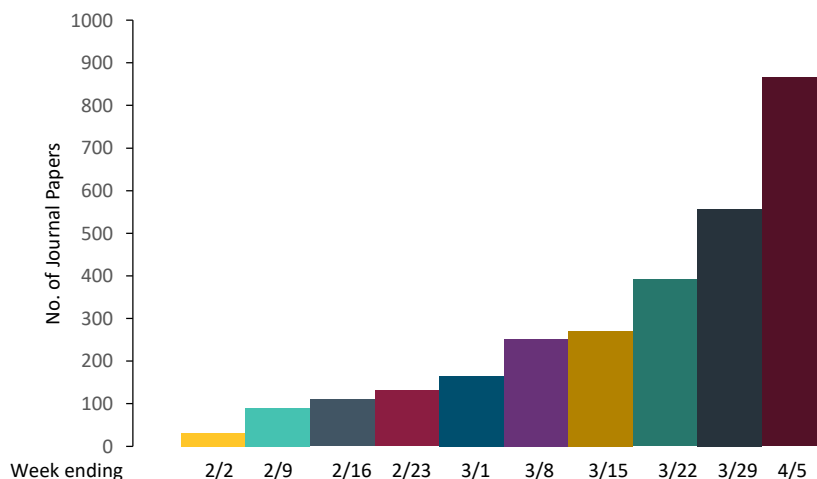


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Thousands of relevant journal articles have been published since the outbreak of COVID-19



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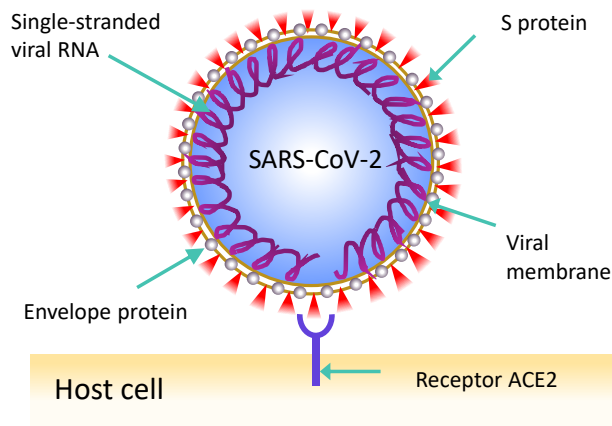
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What is the SARS-CoV-2 virus?

- Belongs to the beta-coronavirus genus
- Has a single-stranded, positive-sense **RNA genome**
- Encapsulated by the **viral membrane**
- Coated with **S protein** (glycoprotein) on the surface
- Viral entrance through S protein binding to **ACE2** on host cells



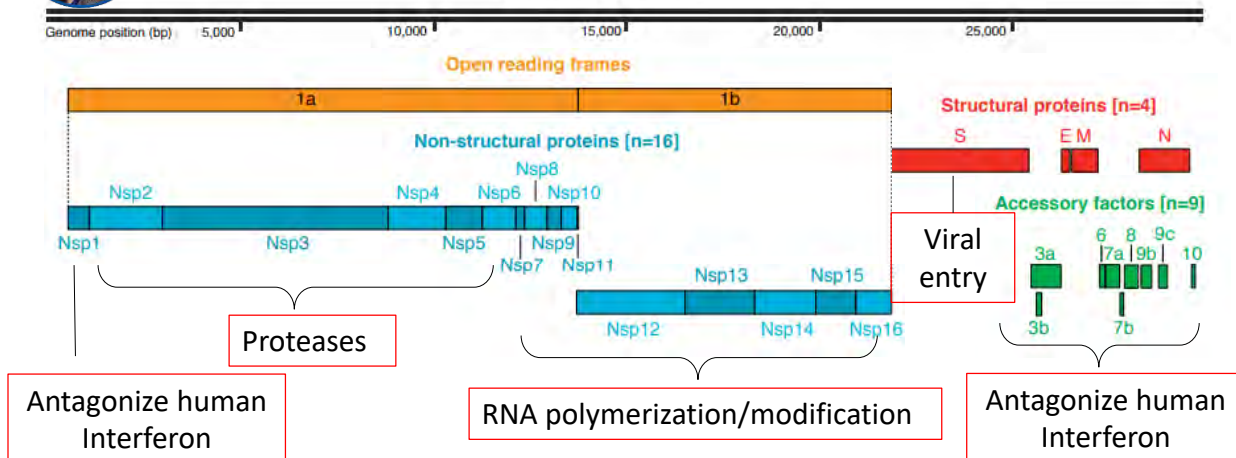
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The genomic organization of SARS-CoV-2

SARS-CoV-2 Genome



Source: Gorden et al. *Biorxiv* (03 2020) <https://www.biorxiv.org/content/10.1101/2020.03.22.002386v1>

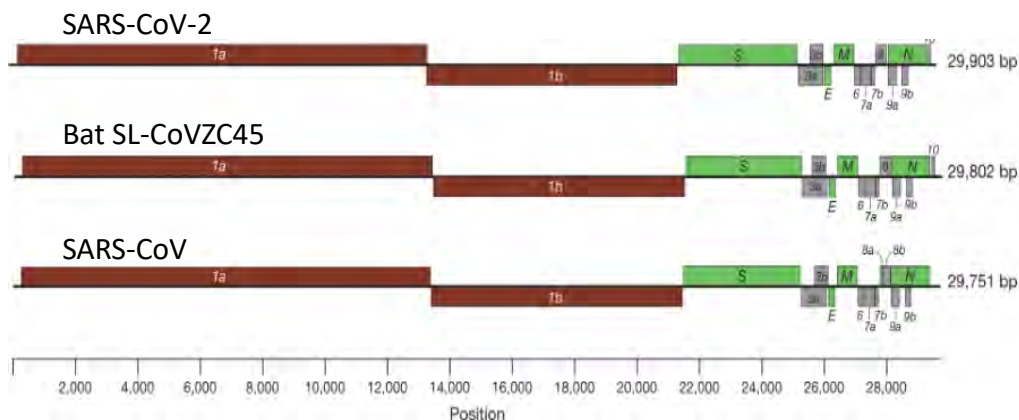
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Genomic structures of SARS-CoV-2 and SARS-CoV are similar



Source: Wu et al. *Nature* volume 579, pages265–269(2020)

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SARS-CoV-2 is similar to SARS-CoV and MERS-CoV

Virus	Disease	Host cell receptor	Viral surface protein	Viral proteases	Viral polymerase	Host protease
SARS-CoV-2	COVID-19	ACE2	S protein	3CLpro and PLpro	RdRp	TMPRSS2
SARS-CoV	SARS	ACE2	S protein (76%)	3CLpro and PLpro	RdRp	
MERS-CoV	MERS	DPP4	S protein	3CLpro and PLpro	RdRp	TMPRSS2

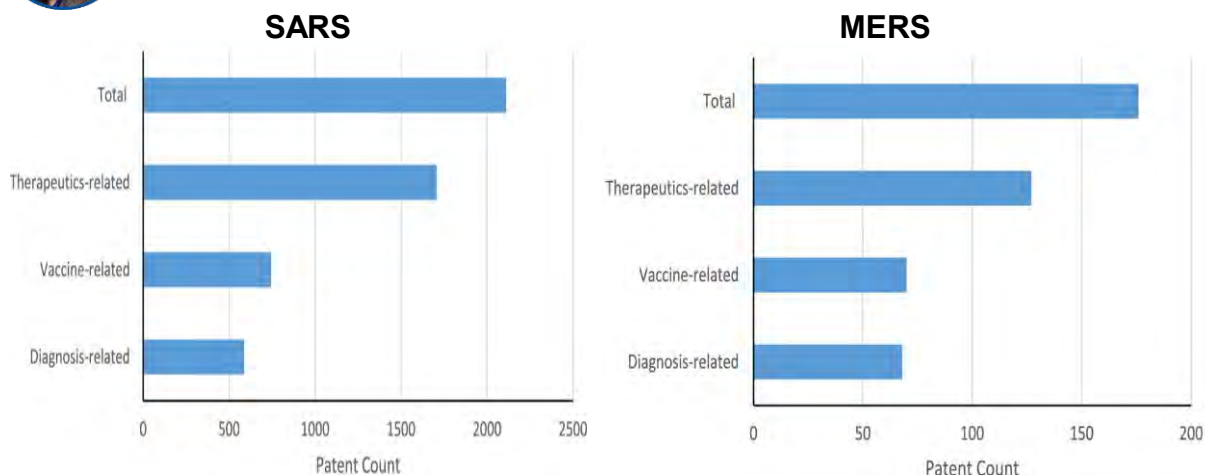
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Distribution of patents related to SARS and MERS



Source: Analysis of CAS content collection

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CAS data was analyzed for unique insights on potential drug candidates and vaccine strategies

Small molecule drugs and drug candidates

- Key proteins and their roles during SARS-CoV-2 infection
- Small molecules in R&D for SARS, MERS
- Repurposing existing drugs for COVID-19

Biologics

- Antibodies
- Cytokines
- Other recombinant proteins (e.g., rhsACE2)
- siRNA and antisense

Vaccines

- Attenuated vaccines
- DNA-based vaccines
- Protein-based vaccines
- Virus-like particle vaccines
- mRNA-based vaccines

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Key proteins and their roles during SARS-CoV-2 infection were analyzed

Target Candidate	Full Name	Role during Viral Infection	Drug Candidate
3CLpro	Coronavirus main protease 3CLpro	A protease for the proteolysis of viral polyprotein into functional units	Lopinavir/Ritonavir
PLpro	Papain-like protease PLpro	A protease for the proteolysis of viral polyprotein into functional units	Lopinavir/Ritonavir
RdRp	RNA-dependent RNA polymerase	A RNA-dependent RNA polymerase for replicating viral genome	Remdesivir
S protein	Viral spike glycoprotein	A viral surface protein for binding to host cell receptor ACE2	Arbidol
TMPRSS2	Transmembrane serine protease 2	A host cell-produced protease that primes S protein to facilitate its binding to ACE2	Camostat mesylate
ACE2	Angiotensin-Converting Enzyme 2	A viral receptor protein on the host cells which binds to viral S protein	

Source: Analysis of CAS content collection

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Key protein targets were analyzed for numbers of related patents and potential drug candidates

Target	No. of Patents	No. of Potential Drug Candidates
3CLpro	49	2178
PLpro	4	189
RdRp	26	570
S protein	46	333
ACE2	5	97

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Existing drugs with therapeutic potential for COVID-19 (drug repurposing) were identified

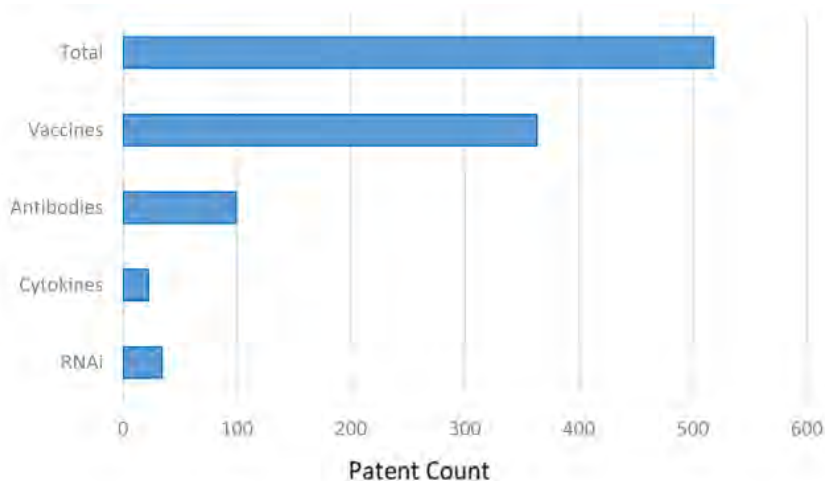
Drug Candidate	CAS Registry No.	Targets	Possible Mechanisms of Actions on COVID-19	Disease indication
Baricitinib	1187594-09-7	JAK kinase	A JAK inhibitor that may interfere with the inflammatory processes	Approved drug for rheumatoid arthritis
Ruxolitinib	941678-49-5			Myelofibrosis
Lopinavir	192725-17-0	Viral proteases: 3CLpro or PLpro	Protease inhibitors that may inhibit the viral proteases: 3CLpro or PLpro	Lopinavir and ritonavir are approved drug combination for HIV infection
Ritonavir	155213-67-5			Approved drug for HIV infection
Darunavir	206361-99-1			
Favipiravir (Favilavir)	259793-96-9	RdRp	A purine nucleoside that acts as an alternate substrate leading to inaccurate viral RNA synthesis	Viral infections
Remdesivir	1809249-37-3			Ebola virus infection
Ribavirin	36791-04-5			A nucleotide analogue that may block viral nucleotide synthesis to stop viral replication
Arbidol	131707-23-8	Spike/ACE2	An inhibitor that may disrupt the binding of viral envelope protein to host cells and prevent viral entry to the target cell	Influenza antiviral drug
Chloroquine	54-05-7	Endosome/ACE2	A drug that can elevate endosomal pH and interfere with ACE2 glycosylation	Malarial parasite infection

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Distributions of biologics patents related to SARS and MERS



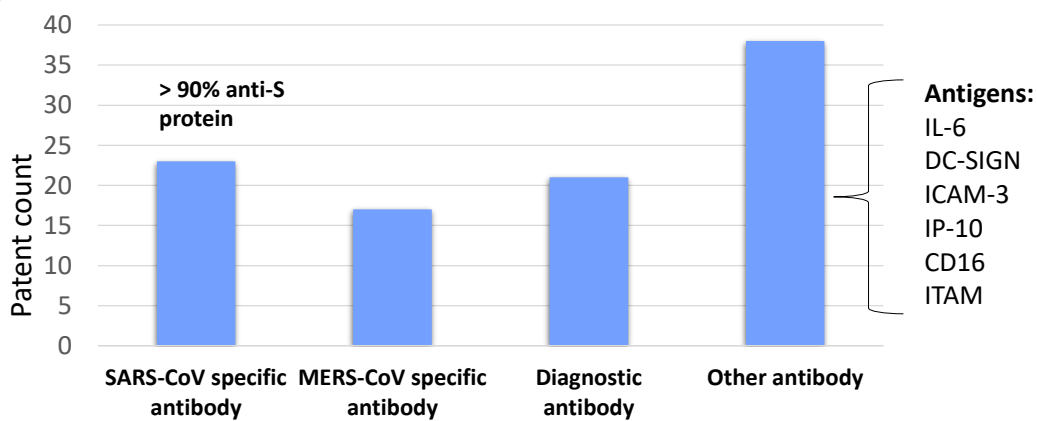
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Distributions of antibody patents related to SARS and MERS



An anti-S protein human antibody 47D11 showed inhibitory effect on SARS-CoV-2 in cultured kidney cells.

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Source: Wang et al. *BioRxiv* doi: <https://doi.org/10.1101/2020.03.11.987958>

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Cytokines in R&D for treating SARS

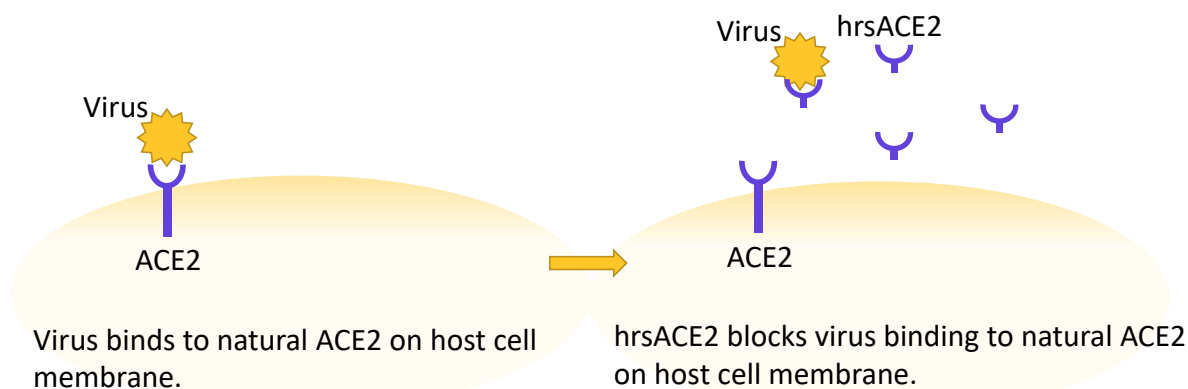
Cytokine	Registered Name	CAS RN	Disease indication
Recombinant interferon	rSIFN-co	2043378-94-3	SARS
	rhIFN- ω	791910-34-4	SARS
	MetIL-29C172S-PEG	867228-40-8	viral infection
Human serum albumin fused interferon	IFN- α 1b	1122730-20-4	SARS
	IFN- α 2b	1122730-23-7	SARS
	IFN- β	1122730-25-9	SARS
	IFN- ω	1122730-27-1	SARS
	IFN- γ	1122730-29-3	SARS

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Human recombinant soluble ACE2 (hrsACE2) inhibits SARS-CoV-2 infection



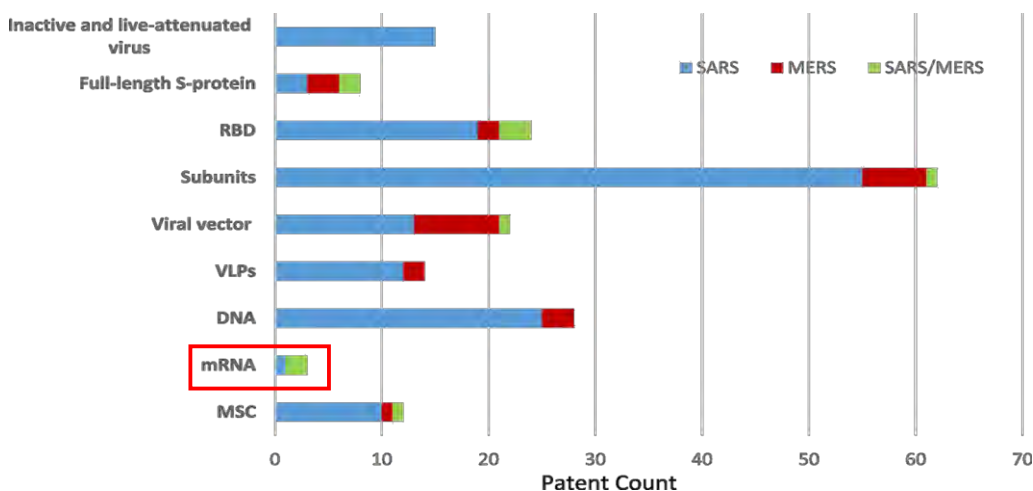
Source: *Monteil et al Cell 2020 DOI: 10.1016/j.cell.2020.04.004*

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Distribution of vaccine-related patents associated with SARS and MERS



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CAS is eager to help all organizations working on COVID-19 treatments and analysis

Learn more at www.cas.org

THANK YOU

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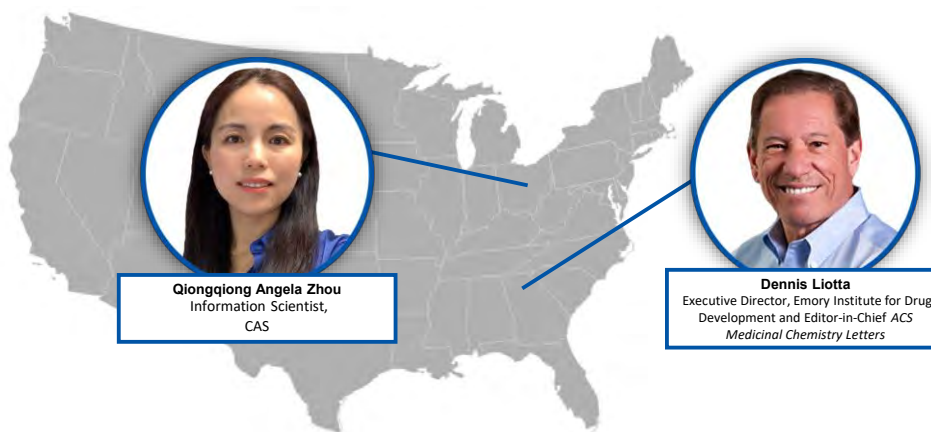
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COVID-19: A Groundwork for Therapeutic Agents and Vaccines



Qiongqiong Angela Zhou
Information Scientist,
CAS

Dennis Liotta
Executive Director, Emory Institute for Drug
Development and Editor-in-Chief ACS
Medicinal Chemistry Letters

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This ACS Webinar is co-produced with CAS, ACS Division of Medicinal Chemistry, American Association of Pharmaceutical Scientists, and ACS Publications.



Summary and perspectives

- Key protein targets
- Small molecules in R&D
- Drug repurposing candidates
- Biologics (antibodies, cytokines, RNA therapy and other recombinant proteins)
- Vaccine technologies

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Advancing the pharmaceutical sciences to drive prevention and cures.

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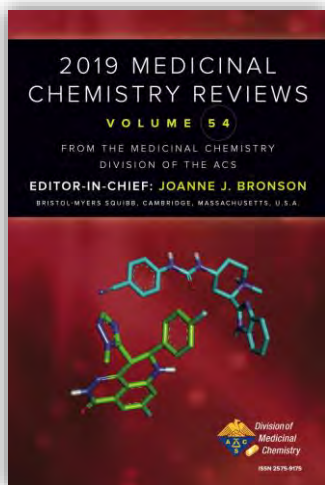
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