

Journal of Applicable Chemistry



2018, 7 (1):276-290 (International Peer Reviewed Journal)



ChemBiol– III (Science Direct) [#]			
(A consequence of evolution in nature)			
Reviews			
ChemBiol: Innovative Solutions for Diverse Challenges	Chemistry & Biology 12(6)(2005)617-620 doi = 10.1016/j.chembiol.2005.06.004		
biophysics, and molecular genetics] Joshua A. Kritzer, Nathan W. Luedtke	5		
ChemBiol: Innovative Solutions for Diverse Challenges	Cur OpiniChemBiol 6(3)(2002)359-366		
Miniaturization: [{biochemical assay + integration of microchip- technologies} + (combinatorial library screening)] Arrays : [Small-molecule micro-, protein ; cell-based; conventional \{DNA\}] microfluidic approaches in \{HTS\} Julia Kh,urina, , rásGuttman	doi = 10.1016/S1367-5931(02)00323-X		
Dynamic combinatorial chemistry	Drug Discovery Today		
[differences of dynamic & traditional combinatorial chemistries;]	7(2)(2002)-117-125		
Sijbren Otto, Ricardo L.E Furlan, Jeremy K.M S,ers			

# AAA (CNN)	JOAC, 2015, 4 (5), 1561-1573	Chemical biology-I
AAA (CNN)	JOAC, 2016, 5 (4) 894-896	Chemical biology-II

Applications of synthetic carbohydrates to ChemBiol	Current Opinion in ChemBiol 14(3)(2010)404-411
[synthetic diverse carbohydrate structures; glycobiology] [carbohydrate-based drugs, vaccines, adjuvants as well as novel	doi = 10.1016/j.cbpa.2010.02.016
drug delivery systems] "Bernd Lepenies and Jian Yin and Peter H Seeberg	ger
Combining functional genomics and ChemBiol to identify targets of bioactive compounds	Current Opinion in ChemBiol 15(1)2011)66-78
[yeast chemical genomic assays strategies for drug target identification]	doi = 10.1016/j.cbpa.2010.10.023
CheukHei Ho and Jeff Piotrowski and Scott J Dixon and Anastasia Baryshnikova and Boone	d Michael Costanzo and Charles
Drug Discovery ChemBiol	
Systems Biology and Systems Chemistry: New Directions for Drug Discovery	Chemistry & Biology 19(1)(2012)23-28
do	i = 10.1016/j.chembiol.2011.12.012
[systems-level research for drug design and discovery,awareness of multiple interactions from both ligand and protein perspectives.	
one-to-one drug design: adverse reactions in patients; → remedy multiple interactions from both ligand and protein J.B. Brown and Yasushi Okuno	
Structural genomics—Impact on biomedicine and drug discovery [Special Issue Celebrating the 60-Year Anniversary of \{ECR\} and the 200-Year Anniversary of the Karolinska Institute]	Exp Cell Research 316(8)(2010)1332-1338 doi = 10.1016/j.yexcr.2010.02.041
[structural genomics \rightarrow impact on biomedicine and drug discovery, ChemBiol [purified proteins \rightarrow generation of tool reagents, such as chemical probes and antibodies, \rightarrow explore protein function in the cell	
Johan Weigelt	
Established, Emerging Trends in Computational Drug Discovery in the Genomics Era	Structural Chemistry & Biology 19(1)(2012)29-41
[compound collection preparation; virtual screening, protein docking, - pharmacology→ChemBiol→ drug discovery;] [free software packages]	→ systems
Drug Discovery and ChemBiol of Cancer Epigenetics	Cell ChemBiol
[genetic mutations in epigenetic genes {CMP\}; inhibitors suitable for	24(9)(2017)1120-1147 doi =
preclinical studies]	10.1016/j.chembiol.2017.08.020
Bibliometry– PubChem	
PubChem applications in drug discovery: a bibliometric analysis	Drug Discovery Today 19(11)(2014)1751-1756
[PubChem (1132 research publications) \rightarrow lead identification and optimiza compound-target profiling, polypharmacology studies and unknown cherridentity elucidation] \rightarrow [drug innovation and repurposing.]	
[ChemBiol, medicinal chemistry and informatics] Tiejun Cheng and Yongmei Pan and Ming Hao and Yanli Wang and S	tephen H. Bryant



Protein (Function) -- ChemBiol

Chemical Strategies for Controlling Protein Folding, Elucidating the Molecular Mechanisms of Amyloid Formation, Toxicity	Journal of Molecular Biology 421(2-3)(2012)204-236 doi = 10.1016/j.jmb.2012.01.051		
[protein folding/misfolding/ aggregation →effect in health/ disease]→ [chemistry, biology interface] Timothy N Lambert, Bradley D Smir	th		
Helix mimetics: Recent developments	Progress in Biophysics, Molecular Biology 119(1)(2015)33-40		
[small molecule α-helix mimetics (proteomimetic); protein– protein interaction (PPIs) inhibitors]	doi = 10.1016/j.pbiomolbio.2015.05.001		
The recombinant protein array: use in target identification and validation	Drug Discovery Today: \{TARGETS\} 3(6)(2004)246-252		
[protein function recombinant protein arrays] [diversity of proteins produced]	doi = 10.1016/S1741-8372(04)02460-0		
[human genome : \sim 30,000 genes \rightarrow encode up to a million			
different proteins] Mark J. Schofield and Neil Sharma and Hu	i Ge		
The ChemBiol of Apoptosis: Exploring Protein-Protein Interactions and the Life and Death of Cells with Small Molecules	Chemistry & Biology 9(10)(2002)1059-1072 doi = 10.1016/S1074-5521(02)00247-8		
[small molecules targeted to proteins of the Bcl-2 and $\{IAP\}\$ families.			
[basic mechanism of molecule recognition underling the life and death of cells]			
Ziwei Huang			
Chemical 'omics' approaches for understanding protein cysteine oxid biology	15(1)(2011)88-102		
[redox proteomics: oxidative biochemistry in health and disease] [ChemBiol \rightarrow direct detection of specific cysteine oxoforms based on their distinct chemical attributes] doi = 10.1016/j.cbpa.2010.11.012			
Stephen E Leonard and Kate S Carroll			
Membrane binding of lipidatedRas peptides and proteins — The structural point of view	Biochimica et BiophysicaActa (BBA) – Biomembranes 1788(1)(2009)273-288		
[ChemBiol of Ras: biophysical and structural features of the membrane bound C-terminus of the protein] Luc Brunsveld and Herbert Waldmann and Daniel	doi = 10.1016/j.bbamem.2008.08.006		
The ChemBiol of Molecular Chaperones—Implications for Modulation of Proteostasis	J Mol Biology 427(18) (2015) 2931-2947 doi = 10.1016/j.jmb. 2015.05.010		
aberrant regulation of cell stress responses;] \rightarrow [increasing the risk for diseases] [role of molecular chaperones in [protein synthesis, folding, disaggregation degradation:	unctional proteome		
ChemBiol of proteostasis;]	ilular chaperone activity nostasis restored nimoto		





Omics - ChemBiol	
'Omic' approaches for unraveling signaling networks	Current Opinion in Cell Biology
[genomics + proteomics → global analysis of cell signaling] [gene expression, protein-protein interaction methods, protein microarrays, mass spectroscopy and gene-disruption] Heng Zhu and Michael Snyder	14(2)(2002)173-179 doi = 10.1016/S0955-0674(02)00315-0
RNA/ DNA ChemBio	bl
Targeting the eIF4A $\{$ RNA $\}$ helicase as an anti-neoplastic approach	Biochimica et BiophysicaActa (BBA) - Gene Regulatory Mechanisms 1849(7)(2015)781-791
[eIF: eukaryotic initiation factor] [<mark>cellular regulation of eIF4A activity</mark> and its potential as a therapeutic target] [Translation and Cancer]	doi = 10.1016/j.bbagrm.2014.09.006
Jennifer Chu and Jerry Pelletier	
Mechanism of interaction of small transcription inhibitors with {DNA\} in the context of chromatin and telomere	Biochimica et BiophysicaActa (BBA) - Gene Regulatory Mechanisms 1799(10-12)(2010)795-809
[prokaryotic and eukaryotic organisms] → transcription apparatus in the cell genomic \{DNA\}association withproteins[ChemBiol] Saptaparni Ghosh and ParijatMajumder and Suman Kal Labeled ChemBiol tools for investigating sphingolipid metabolism, trat and interaction with lipids and proteins	ffickingBiochimica et BiophysicaActa (BBA) - Molecular and Cell
[fluorescent and/or radio-labeled and other artificial substrates, (mech based) enzyme inhibitors, cross-linking probes or artificial membrane n [Tools to study lipid functions]	nodels doi =
Paul Workman and Ian Collins	10.1016/j.bbalip.2013.12.011
Mimicry of bioactive peptides via non-natural, sequence-speptidomimetic oligomers	6(6)(2002)872-877
[Non-natural, sequence-specific peptidomimetic oligomers are being due to mimic bioactive peptides, with potential therapeutic application] [Pseudo-tertiary structure in β -peptides and peptoids may herald the constraint of perturbation]	5951(02)00385-A
of entirely artificial proteins] James A Patch and Annelise E Barron	n
Protein-X interactio	
X: [protein; small molecule; [metal ion complex]	, organic sorvent; annuo aclu]]

Post-translational myristoylation: Fat matters in cellular life, death

Biochimie 93(1)(2011)-18-31 doi = 10.1016/j.biochi.2010.10.018

[Myristoylation; protein-membrane interactions as well as proteinprotein interactions] \rightarrow [health; disease] [functions of Myristoylated proteins: signalling pathways, oncogenesis or viral replication]

Dale D.O. Martin, Erwan Beauchamp, Luc G. Berthiaume

Neutralizing endogenous chemokines with small molecules: Pharmacology & Therapeutics Principles and potential therapeutic applications 126(1)(2010)39-55 doi = 10.1016/j.pharmthera.2009.12.003 [Regulation of cellular responses to external stimuli such as hormones, neurotransmitters, or cytokines is achieved through the control of all steps of the complex cascade starting with synthesis, going through maturation steps, release, distribution, degradation and/or uptake of the signalling molecule interacting with the target protein [ligand neutralization and tries to determine to what extent small chemical molecules could substitute for neutralizing antibodies in therapeutic approaches] Jean-Luc Galzi and Muriel Hachet-Haas and Dominique Bonnet and Francois Daubeuf and Sandra Lecat and Marcel Hibert and Jacques Haiech and Nelly Frossard Synthetic receptors for phospholipidheadgroups;35 Years of Synthetic Coordination Chemistry Reviews Anion Receptor Chemistry 1968-2003 240(1-2)(2003)129-141 doi = 10.1016/S0010-8545(02)00257-6 [biological phospholipid receptors; synthetic receptors reported;] [tools of ChemBiol→pharmaceuticals; Small molecules that recognize phospholipids selectively] Timothy N Lambert, Bradley D Smith Revisiting bleomycin from pathophysiology to safe clinical use Critical Reviews in Oncology/Hematology 87(1)(2013)90-100; [molecular pharmacology; bleomycin; curative chemotherapydoi = 10.1016/j.critrevonc.2012.12.003 Hodgkin lymphoma (HL), testicular germ-cell tumours (GCT)] MariosFroudarakis, EleftheriaHatzimichael, LydiaKyriazopoulou, Konstantinos Lagos, Periklis Pappas, , reas G. Tzakos, Vasilis Karavasilis, DanaiDaliani, Christos Pap, reou, Evangelos Briasoulis ChemBiol – III (ACS) Chemical Modifications to ACS Chem. Biol., 2017, 12 (2), pp 316–325 **RNA**: A New Layer of Gene DOI: 10.1021/acschembio.6b00960 **Expression Regulation** Epitranscriptomics: multitude of **RNA** m¹A hm⁵C m⁵C m⁶A modifications NH.

chemical modifications to mRNA; dynamic modifications to RNA have been identified in the transcriptome, including N6methyladenosine (m6A), inosine (I), 5methylcytosine (m5C), pseudouridine (Ψ), 5hydroxymethylcytosine (hm5C), and N1methyladenosine (m1A) – collectively called pre-mRNA processing pri-miRNA processing epitranscriptome mRNA stability mRNA translation (m⁶A, Ψ, m⁶C, hm⁶C, m¹A (m[°]A, Ψ)

JinghuiSongandChengqi Yi

Deciphering the Functions of Protein O-GlcNAcylation with Chemistry

ACS Chem. Biol., 2017, 12 (2), pp 326–335 DOI: 10.1021/acschembio.6b01065

mRNA export

RNA structure

m°A.Ψ.m°C.m'A





Acs.org (ACS): Information Source (is)

Object Oriented Vocabulary of ChemBiology		
Biological system	 → Single_Speciesor organism [combination → cell → cell division → fetes]; → birth → growth [health; disease]; death; →] 	
Single_Species	→ Set of [organs; cells; tissues;; biological fluids;] at a specific instant of time	
Each organ Cell	 → Multiple cells [Multiple functions] → Composition:[[Two-thirds of a cell is water]; [mixture of proteins; lipids; carbohydrates] [DNA; multitude of compounds] ➡ Building blocks of life: basic structural, functional, and biological unit of all known living organisms; smallest unit of life that can replicate independently. ➡ Cells transform raw materials in the food eaten into the molecules the body needs, using thousands of different chemical reactions. Cell means "small room" from Latin word cella [living cells; dead cells] 	
Living cells	 → Composed of molecules that collectively provide a chemical environment. When energy provided, it continues function, adapts to the environment and reproduces 	
Dead cells	\rightarrow [Ex. Hair; finger nails; hard portion of bones]	
	\rightarrow	
Life	[Origin [Basic requirements]; evolution (past, present, future); [extinct in past; now existing; originating in future(near; far off)] Environment for habitability [necessities; Limits beyond which species die]	

		Environment for habitability [necessities, Ennits beyond which species die]
Life on \$\$	\rightarrow	[solar system; elsewhere [galaxy]]
Life on solar system	→	[Life_on earth; Life on (in) Sun; Life on Mars]
Life_on earth \$\$	\rightarrow	[terrestrial[surface; inside]; [arboreal(on trees)]; aquatic [marine; riverine;], atmospheric]
Life_ on Mars	\rightarrow	[Mars rover 2020]

... → Phenomenon → perceived → science → simulated → compared →

What is 'Life'? How much Science knows it today?	Life is what it is. Life is not what it is not. Wait to know more!!
Known with what accuracy	Truth value increases and falsehood decreases
	with time and perception

r	-	
Environment	\rightarrow	[Temperature, pressure, nutrient concentration, atmospheric composition
conditions		of gases; Light; gravity, electro-magnetic radiation;]
Terrestrial	\rightarrow	[normal environment; extreme env]
Extreme env	\rightarrow	[Temperature; Pressure; light; nutrient concentration]
Temperature_extreme	\rightarrow	[Hydro thermal vents (upto 400oC) [deep sea]; geo-thermal hot springs];
zones		extremely cold (sea ice); salt conc [high salinity; high con of compounds]
Habitable zones_life	\rightarrow	[Universe[[solar system [earth[moon]; Mars [];Jupitor]]
Habitable zone (HZ)	\rightarrow	A region of space where environmental conditions are best for life to form
		and survive. The synonyms of HZ are "life zone", "comfort zone", "green

	belt". \$\$_phile : [Mesophiles or Neutrophils; Extremophile] It is an organism that thrives and lives in physically or geochemically
Extremophile	extreme conditions of pressure and temperature that are detrimental to most life on Earth.
Mesophiles or \rightarrow Neutrophils	Ex.: Bacteria often form on the rocks near the hydrothermal vents. organisms that live in moderate environments prevalent on earth

Chromosome DNA	\rightarrow \rightarrow	[Chromosomes are strings of genes]; protein +single molecule DNA] [DNA molecule stores the code for building living bodies in genes]→ DNA chain made from nucleotide subunits (adenine, cytosine, guanine, and thymine which are nitrogen-containing bases), each composed of: a five-carbon sugar (2'- deoxyribose), a phosphate group and nucleic acids of joined by sugar-phosphate backbone (specific instructions that make each type of living creature unique)
Genes	\rightarrow	[gene is segment of DNA]
	\rightarrow	instruct cells to produce particular proteins, which in turn determine traits DNA copied to RNA
RNA	\rightarrow	RNA [directly functional or intermediate template] for a protein
Protein		Performs a function \rightarrow amino-acid \rightarrow functional groups \rightarrow atoms
	\rightarrow	[nature (in vivo of Biosystems);
Protein		Laboratory (in vitro);
machine:		Virtual PM (computational);]
Protein design methods	÷	[De novo] [biotechnology and chemical biology] Computational;
Protein	\rightarrow	fold, fold faster, catalyze, catalyze faster,
characteristics		signal, adopt preferred conformational states
Protein functions	\rightarrow	[structural, catalytic, sensory, regulatory]



Chromosome (10 ⁷ - 10 ¹⁰ bp)	DNA AXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
DNA Gene (10 ³ - 10 ⁶ bp) Function	Function Function

	Quantifies the function and regulation of enzymes and proteins at the cellular
Physiological	level
enzymology,	Special Issue entitled: Physiological Enzymology and Protein Functions. "
	doi = "https://doi.org/10.1016/j.bbapap.2015.07.011",
	Mars [Phoenix: pathfinder; Global surveyor;]
Projects_Life exploration	Titan [Cssini Huygens]
	Mars Exploration Rovers, the Mars Phoenix Lander
	(Kepler, James Webb Space Telescope) \rightarrow searching for Earth-like planets around other stars
	[temperature and mineralogy on Mars] \leftarrow Mars Odyssey and the Mars
Probes (instruments)	Reconnaissance Orbiter
	[signs of past life on Mars] ←Mars Science Laboratory [sources and sinks of CO2 on Earth] ←Orbiting Carbon Observatory-2





Disciplines in different bands energy and surroundings

From	\rightarrow	То		From			\rightarrow	То
Blobology		Chemistry		Chemistry			Physics	
BioChemistr	/	Chemistry		Physical chemistry			Physics	
				Chemica	l Phy	sics		Physics
From →	То			From	\rightarrow	То		
Physics	Quai	ntum Physics]	Physics		Energ	gу	





Glowing flash in the middle: WHL J24.3324-8.477 A brightest galaxy Each glowing speck is a distinct galaxy (Detector: NASA/ESA Hubble Space Telescope);



	DefBase.ChemBiol
Astronomy	 Formation, functioning and interaction of stars, galaxies, planets, moons, asteroids, comets and nebulae Explains supernovae explosions, gamma ray bursts, and cosmic microwave background radiation. The physics, chemistry, and evolution of such objects, and phenomena that originate outside the atmosphere of Earth. Probes of research: Telescopes and radio dishes are used from the surface of the Earth to study visible light, near infrared light, and radio waves (E-M Band) Exoplanet (extrasolar planet) is a planet that orbits a star other than our own
Astrophysics	Space science probing with laws of physics to explain the birth, life and death of stars, planets, galaxies, nebulae and other objects in the universe.
Astro (or Cosmo) chemistry	Processes and chemical composition of matterprimarily through the study of the chemical composition of meteorites and other physical samples in the universe over time. The basis is that the asteroid parent bodies of meteorites were some of the first solid material to condense from the early solar nebula.
Astrobiology	 Search for life beyond the Earth in our solar system and then in universe (Exobiology) Tools in vogue are knowledge in astronomy, biology, chemistry, geology, atmospheric science, oceanography and m g of planetary/ stellar processes Search for and study of life elsewhere in the universe.
Bioorthogonal chemistry	Chemical reaction that can occur inside of living systems without interfering with native biochemical processes. The term was coined by Carolyn R. Bertozzi in 2003.
Chemical genetics	Complementary approach involving the use of small molecules capable of either inactivating or activating their targets Use of small molecule compounds to perturb a biological system to explore the outcome. Chemical genetics is also used to describe the technique of screening for small molecule modulators.

Chemical probes for interrogating biological processes	 [Cell permeable small molecule tools] Objective : minimizing the generation of poor quality and misleading biological data, thus increasing understanding of the particular biological area Goal:basic research and drug discovery
Chemical proteomics	 ◇ Detects proteomes with specific chemical molecules that interact with target proteins ○ [Mass spectrometry-based affinity chromatography approach] → identifies proteome-wide small molecule-protein interactions.
	 Selectively perturb with external stimuli and observe (measure) the consequent response of a bio-system
How to	? With model systems; model compounds; model processes
understand	In-vitro studies
biology	In-vivo probes
	? Evolutionary knowledge
	? Synthetic(artificial) bio-systems

Interdisciplinary sciences (Binary,Ternary,Quaternary)

Sciences :	[Mathematic Physical Natural Applied]	al [Pure_Mathematics; Statitics; Nature_ mimicking algorithms] [Physics; chemistry; [Biology [Geology; Oceanography; Astronomy;
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Unary				<mark>Binary</mark>	
				$A + B \rightarrow physics \rightarrow chemistry$	$A + B \rightarrow$ chemistry physics \rightarrow
				Physics[of \$\$ in]	\$\$ [of Physics in]
Physics Chemistry	Physics Physics Physics	+ Chemistry+ Astronomy+ Biology	${\rightarrow}$ ${\rightarrow}$	Physical Chemistry Physical Astronomy Physical Biology	Chemical Physics Astro(logical) Physics Bio(logical) Physics
Astronomy Biology 	Chemistry Chemistry	+ Astronomy + Biology	${\rightarrow}$	Chemical Astronomy Chemical Biology	Astro Chemistry Biological Chemistry
	Astronomy	+ Biology	\rightarrow	Astro Biology	Biological Astronomy

				Te	rna	ry
Chemistry	+	Biology	+	Astronomy	>	 Chemistry of (biological astronomy) Chemistry of (astro biology) Chemistry of (chemical astronomy) Biology of (chemical astronomy) Biology of (astro chemistry) Astro (Chemical biology) Astro (Biological chemistry)
Chemistry	+	Biology	+	Physics	÷	 Chemistry of (biological physics) Chemistry of (physics of biology) Biology of (chemical physics) Biology of (physics of chemistry) Physics (Chemical biology) Physics (Biological chemistry)

				(<mark>)uatern</mark>	ary	7
Physics +	Chemistry	+	Astronomy	+	Biology	→	 Physics of (chemical (astro biology)) Physics of (astrochem biology) Physics & chemistry of (astro biology) Chemistry of (Physics of (astro biology)) Physics and/or Chemisty and/or PhysChem and/or ChemPhys/ (astrobiology)

	Mathematical Sciences
Mathematical Sciences	 [[Mathematics [Algebra [linear; Boolean; operator]; Functional analysis;]; Statistics; Fuzzy theory; Possibility [St+Fuzzy]; Nature_inspired_methods]

Omni_metrics	Discipline	Omni_omics	
		Gen_omics	Genetics
bio_metrics	Biology	Epige_omics	epigenetics

Medicino_metrics	Medicine	Prote_omics		Protein
Pharmaco_metrics	Pharmacy	Metabol_om	ics	metabolome
Pisci_metrics	Fisheries			(Small molecule
				metabolic
Chemo_metrics	Chemistry			products- metabolytes)
Environ_metrics	Environment	Splice_omics	S	splicing
Kineto_metrics	Kinetics	Pharmacoger	n_omics	Pharmacogenetics
Specio_metrics	Species	Transcript_o	mics]	Transcriptome
Biblio_metrics	Bibliography			
Performance_metrics	Performance	Omni_\$\$\$		omics; -istry; -ology;
			-metri	ics
Metrics_metrics]	Measurement			

Metrics + Co	mputation	\rightarrow parameters	→- Infe	→→ Informatics formation extraction
Chemistry	+	Informatics	\rightarrow	Chemo_informatics
Biology	+	Informatics	\rightarrow	Bio_informatics
Chemical biology	+	Informatics		ChemBiol_informatics
		ibes Kids (knowledg al links governed by		ligence and data systems) with meta) Kids

	[Chemometrics; System_Biology; Chemical Biology;	
	[Mensuration; Mensurometrics	
Tools or toolboxes	[Instrumentation;	
	[Models; solutionMethods	
	[Knowledge_eXtration]	

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