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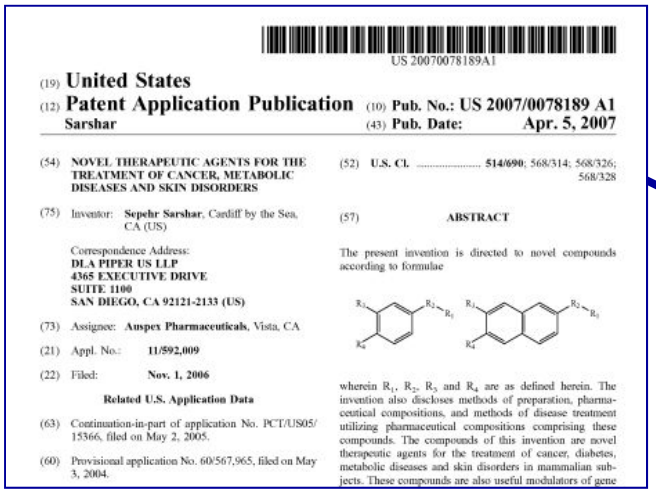

US 20070078189A1

(19) **United States**

(12) **Patent Application Publication** (10) **Pub. No.: US 2007/0078189 A1**

Sarshar (43) **Pub. Date: Apr. 5, 2007**

(54) **NOVEL THERAPEUTIC AGENTS FOR THE TREATMENT OF CANCER, METABOLIC DISEASES AND SKIN DISORDERS**

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(73) Assignee: **Auspex Pharmaceuticals**, Vista, CA

(21) Appl. No.: **11/592,009**

(22) Filed: **Nov. 1, 2006**

Related U.S. Application Data

(63) Continuation-in-part of application No. PCT/US05/15366, filed on May 2, 2005.

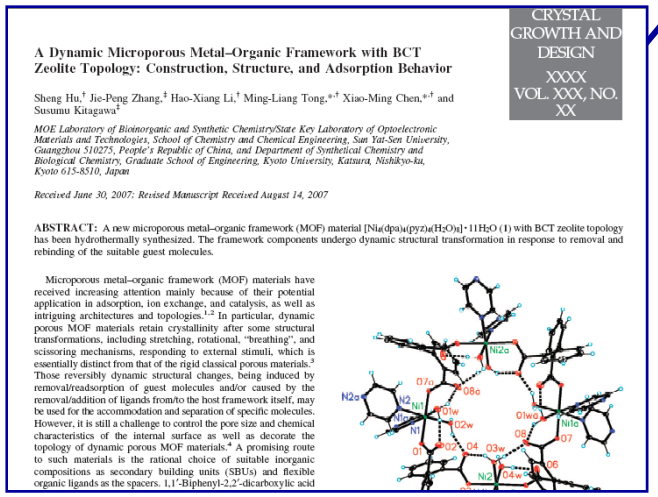
(60) Provisional application No. 60/567,965, filed on May 3, 2004.

(52) **U.S. Cl.** **514/690**; 568/314; 568/326; 568/328

(57) **ABSTRACT**

The present invention is directed to novel compounds according to formulae

wherein R_1, R_2, R_3 and R_4 are as defined herein. The invention also discloses methods of preparation, pharmaceutical compositions, and methods of disease treatment utilizing pharmaceutical compositions comprising these compounds. The compounds of this invention are novel therapeutic agents for the treatment of cancer, diabetes, metabolic diseases and skin disorders in mammalian subjects. These compounds are also useful modulators of gene



CRYSTAL GROWTH AND DESIGN
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A Dynamic Microporous Metal–Organic Framework with BCT Zeolite Topology: Construction, Structure, and Adsorption Behavior

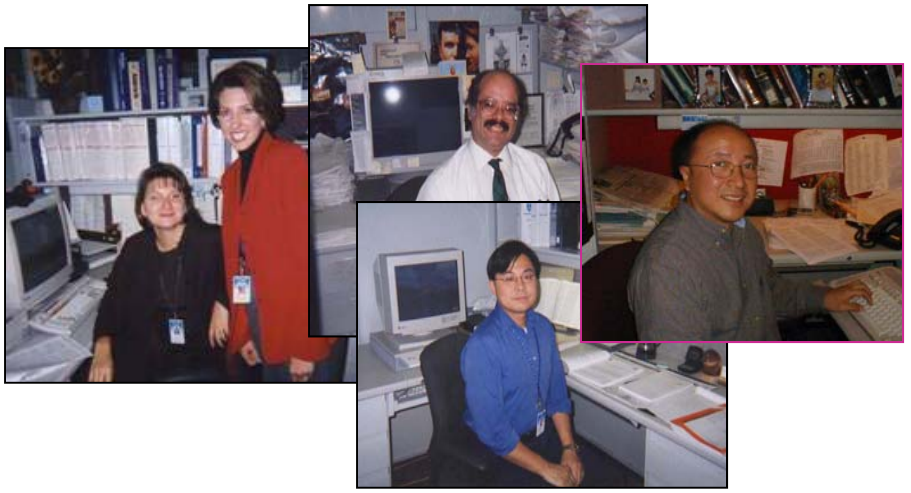
Sheng Hu,[†] Jie-Peng Zhang,[‡] Hao-Xiang Li,[†] Ming-Liang Tong,*[,†] Xiao-Ming Chen,*[,†] and Susumu Kitagawa[‡]

MOE Laboratory of Bioinorganic and Synthetic Chemistry/State Key Laboratory of Optoelectronic Materials and Technologies, School of Chemistry and Chemical Engineering, Sun Yat-Sen University, Guangzhou 510275, People's Republic of China, and Department of Synthetical Chemistry and Biological Chemistry, Graduate School of Engineering, Kyoto University, Katsura, Nishikyo-ku, Kyoto 615-8510, Japan

Received June 30, 2007; Revised Manuscript Received August 14, 2007

ABSTRACT: A new microporous metal–organic framework (MOF) material $[Ni_4(dpa)_4(pyz)_4(H_2O)_8]\cdot 11H_2O$ (1) with BCT zeolite topology has been hydrothermally synthesized. The framework components undergo dynamic structural transformation in response to removal and rebinding of the suitable guest molecules.

Microporous metal–organic framework (MOF) materials have received increasing attention mainly because of their potential application in adsorption, ion exchange, and catalysis, as well as intriguing architectures and topologies.[1,2] In particular, dynamic porous MOF materials retain crystallinity after some structural transformations, including stretching, rotational, "breathing", and scissoring mechanisms, responding to external stimuli, which is essentially distinct from that of the rigid classical porous materials.[3] Those reversibly dynamic structural changes, being induced by removal/readsorption of guest molecules and/or caused by the removal/addition of ligands from/to the host framework itself, may be used for the accommodation and separation of specific molecules. However, it is still a challenge to control the pore size and chemical characteristics of the internal surface as well as decorate the topology of dynamic porous MOF materials.[4] A promising route to such materials is the rational choice of suitable inorganic compositions as secondary building units (SBUs) and flexible organic ligands as the spacers. 1,1′-Biphenyl-2,2′-dicarboxylic acid



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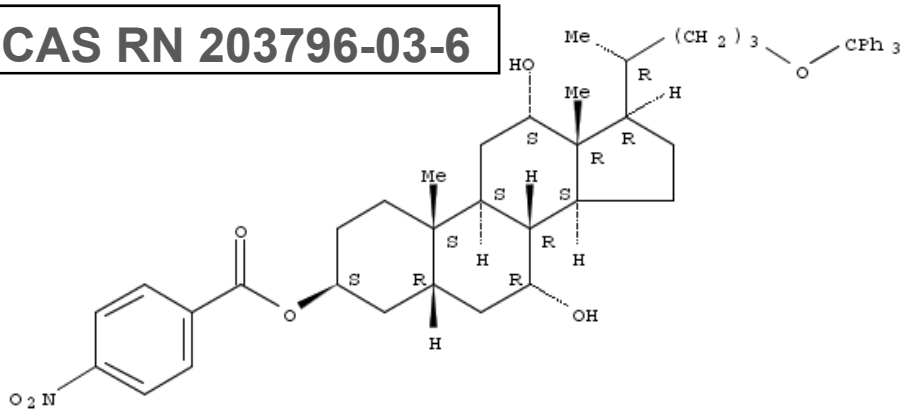
Compound 34: Diisopropyl azodicarboxylate (DIAD) (1.20 mL, 6.08 mmol) was added to triphenylphosphine (1.60 g, 6.08 mmol) in THF (100 mL) at 0 °C. and was stirred for half an hour during which time the yellow solution became a paste. Compound 14 (2.58 g, 4.06 mmol) and p-nitrobenzoic acid (0.81 g, 4.87 mmol) were dissolved in THF (50 mL) and added to the paste. The resulted mixture was stirred at ambient temperature overnight. Water (100 mL) was added and the mixture was made slightly basic by adding $NaHCO_3$ solution followed by extraction with EtOAc (3x50 mL). The combined extracts were washed with brine once and dried over anhydrous Na_2SO_4. The desired product (2.72 g, 85% yield) was obtained as white powder after SiO_2 chromatography (Et_2O/hexanes 1:2). m.p. 207-209 °C.; IR (KBr) 3434, 3056, 2940, 2868, 1722, 1608, 1529,1489, 1448, 1345 cm^{-1} ; ^1H NMR ($CDCl_3$, 300 MHz) δ 8.30-8.26 (m, 2 H), 8.21-8.16 (m, 2 H), 7.46-7.42 (m, 6 H), 7.31-7.18 (m, 9 H)5.33 (bs, 1 H), 4.02 (bs, 1 H), 3.90 (bs, 1 H), 3.09-2.97 (m, 2 H), 2.68 (td, J=14.95, 2.56 Hz, 1 H), 2.29-2.19 (m, 1 H), 2.07-1.06 (series of multiplets, 24 H), 1.01 (s, 3 H), 0.98 (d, J=6.6 Hz, 3 H), 0.70 (s, 3 H); ^{13}C NMR ($CDCl_3$, 75 MHz) δ 164.21, 150.56, 144.
64.
28.
(th

CAS RN 203796-03-6



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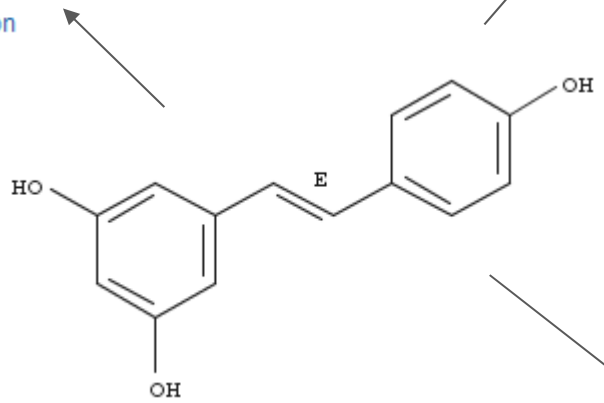

CAS Registry Number: 501-36-0

$C_{14}H_{12}O_3$

1,3-Benzenediol, 5-[(1E)-2-(4-hydroxyphenyl)ethenyl]-

1,3-Benzenediol, 5-[2-(4-hydroxyphenyl)ethenyl]-, (E)-; 3,4',5-Stilbenetriol (7CI,8CI); Resveratrol (6CI); (E)-2-(3,5-Dihydroxyphenyl)-1-(4-hydroxyphenyl)ethene; (E)-3,4',5-Trihydroxystilbene; (E)-5-(p-Hydroxystyryl)resorcinol; (E)-Resveratrol; 3,4',5-Trihydroxy-trans-stilbene; 5-[(1E)-2-(4-Hydroxyphenyl)ethenyl]-1,3-benzenediol; CA 1201; Resveratrol P 5; Resvida; Vineatrol 20M; trans-3,5,4'-Trihydroxystilbene; trans-Resveratrol

Biological Properties	Value	Note
ADME (Absorption, Distribution, Metabolism, Excretion)	See full text	(2) CAS
Half-Life (Biological)	See full text	(9) CAS
LC50	See full text	(13) CAS
Minimum Inhibitory Concentration	See full text	(43) CAS

Lipinski and Related Properties	Value
Freely Rotatable Bonds	5
H Acceptors	3
H Donors	3
H Donor/Acceptor Sum	6
logP	3.024±0.267
Molecular Weight	228.24

Spectra Properties	Value
Carbon-13 NMR Spectrum	See spectrum
Proton NMR Spectrum	See spectrum

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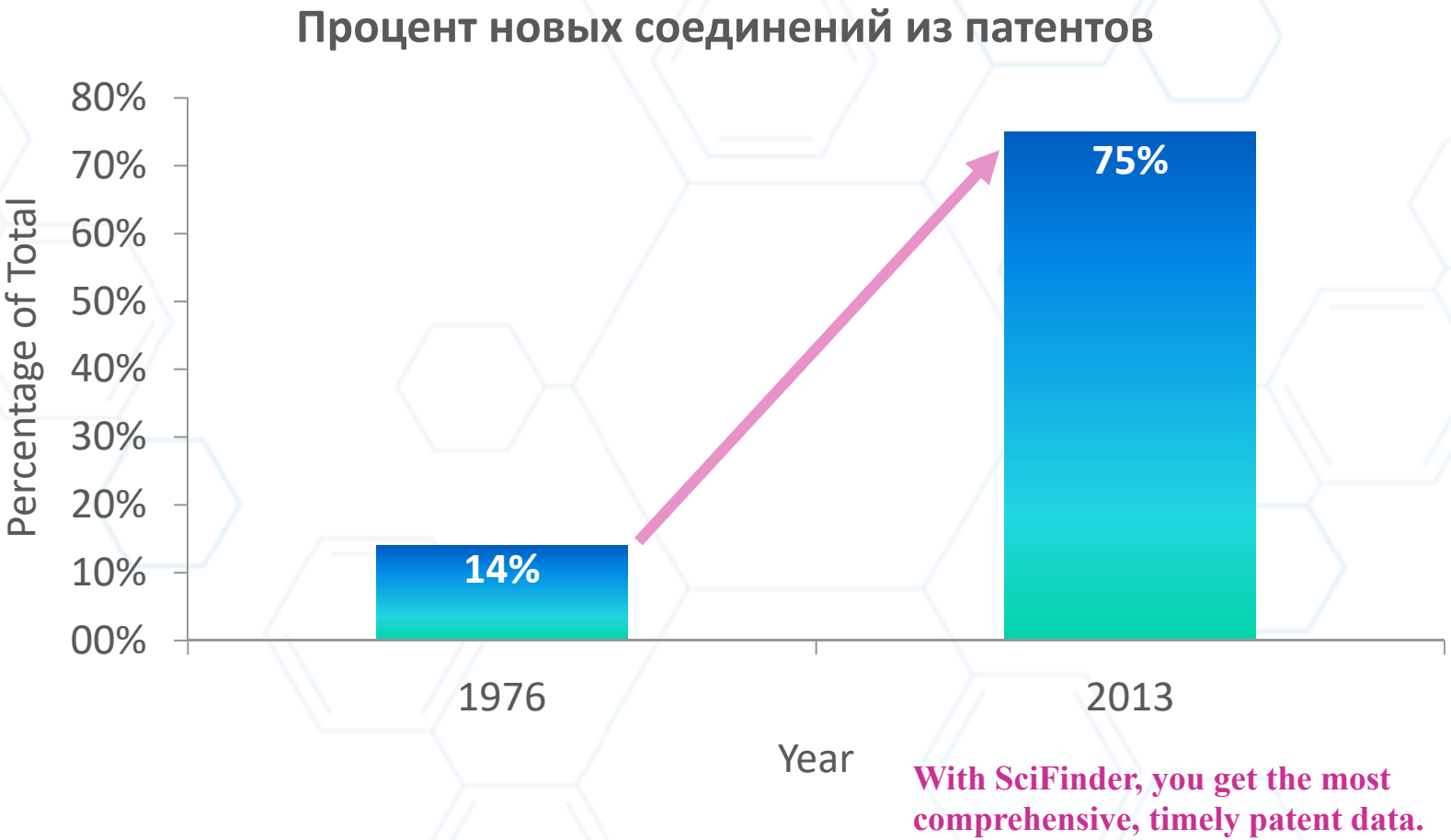

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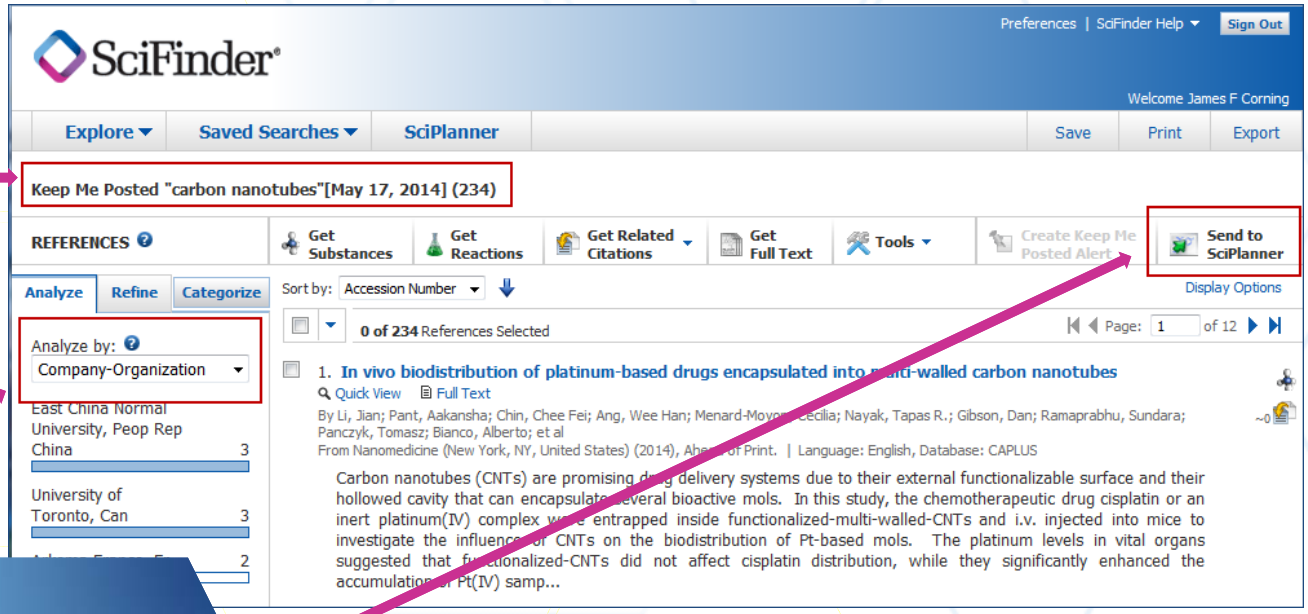

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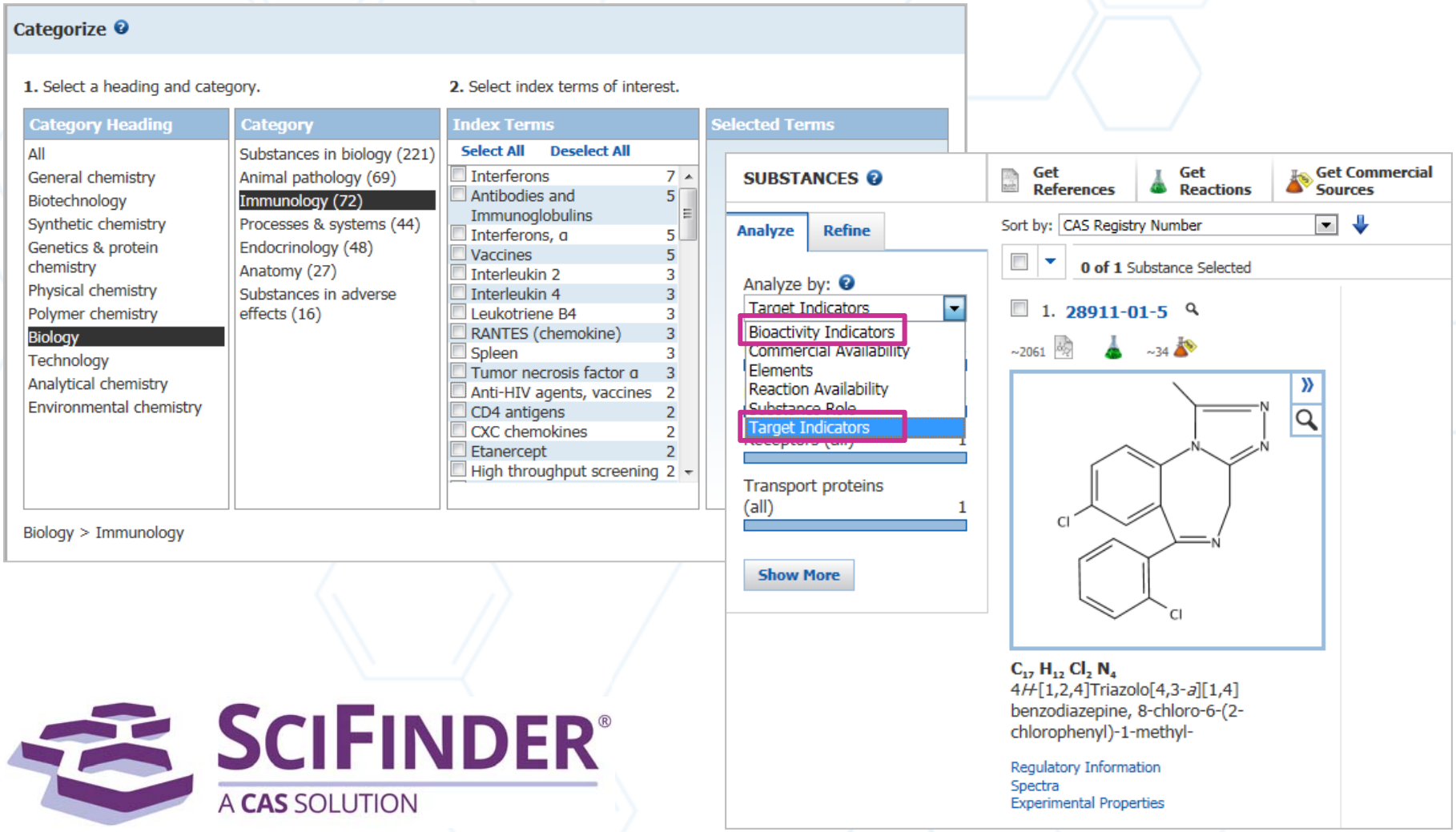

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CAS Registry Number 13292-46-1

~17,438 ~124

$C_{43}H_{58}N_4O_{12}$

Rifamycin, 3-[[(4-methyl-1-piperazinyl)imino]methyl]-

Molecular Weight
822.94

pKa (Predicted)
Value: 4.81±0.70 | Condition: Most Acidic Temp: 25 °C

Melting Point (Experimental)
Value: See full text | Condition: 1 of 2

Boiling Point (Predicted)
Value: 937.4±65.0 °C | Condition: Press: 760 Torr

Density (Predicted)
Value: 1.34±0.1 g/cm3 | Condition: Temp: 20 °C Press: 760 Torr

Other Names
2,7-(Epoxypentadeca[1,11,13]trienimino)naphtho[2,1-*b*]furan-1,11(2*H*)-dione, 5,6,9,17,19,21-hexahydroxy-23-methoxy-2,4,12,16,18,20,22-heptamethyl-8-[*N*-(4-methyl-1-piperazinyl)formimidoyl]-, 21-acetate (8CI)
2,7-(Epoxypentadeca[1,11,13]trienimino)naphtho[2,1-*b*]furan-1,11(2*H*)-dione, 5,6,9,17,19,21-hexahydroxy-23-methoxy-2,4,12,16,20,22-heptamethyl-8-[*N*-(4-methyl-1-piperazinyl)formimidoyl]-, 21-acetate (7CI)
2,7-(Epoxypentadeca[1,11,13]trienimino)naphtho[2,1-*b*]furan, rifamycin deriv.
3-[(4-Methyl-1-piperazinyl)iminomethyl]rifamycin SV
5,6,9,17,19,21-Hexahydroxy-23-methoxy-2,4,12,16,18,20,22-heptamethyl-8-[*N*-(4-methyl-1-piperazinyl)formimidoyl]-2,7-(epoxypentadeca[1,11,13]trienimino)-naphtho[2,1-*b*]furan-1,11(2*H*)-dione 21-acetate
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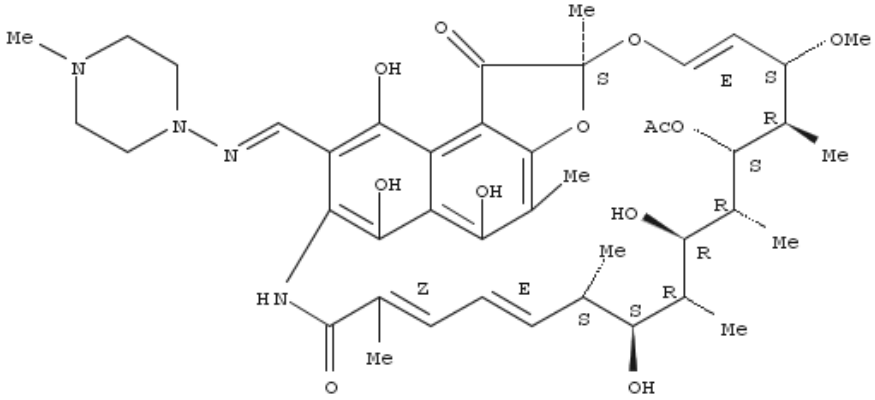
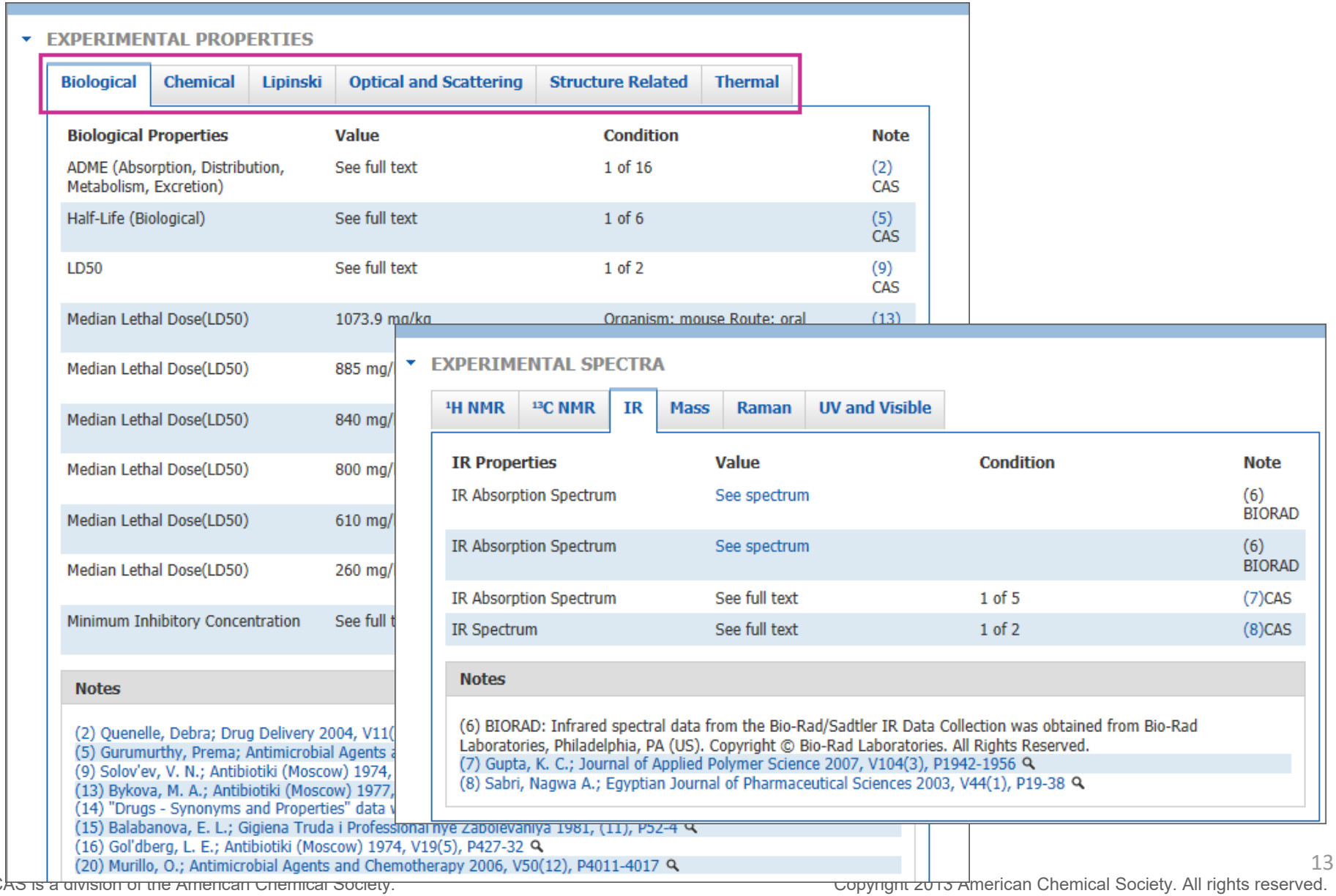


Absolute stereochemistry. Double bond geometry as described by E or Z.

Property and Spectra Data Collated tabs organize information scientifically



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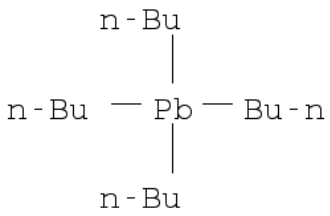
tetrabutylplumbane (REACH, EINECS)
Tetrabutylplumbat (German) (EINECS)
tetrabutilplumbato (Spanish) (EINECS)
Lead, tetrabutyl-
NSC 179770
Tetrabutyllead



File Segment

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Restricted Chemical Lists: RSTR
USA: TSCA

Regulatory List Number

EC No.: 217-649-2
EINECS No.: 217-649-2
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ХИРАЛЬНЫЕ ЖИДКИЕ КРИСТАЛЛЫ НА ОСНОВЕ ОПТИЧЕСКИ АКТИВНОГО ИЗОАМИЛОВОГО СПИРТА

Ивановский государственный университет, НИИ Наноматериалов
153025 Иваново, ул. Ермака, 39. E-mail: nv_usoltseva@mail.ru

С целью изучения влияния строения каламитных соединений на их мезоморфные свойства осуществлен синтез и изучены текстурные характеристики пяти производных изоамилового спирта. Установлено, что из пяти соединений только два (алкилзамещенные) проявляют хиральную нематическую фазу. Алкоксизамещенные и производные со сложноэфирной связью формируют нематическую фазу без признаков хиральности.

Ключевые слова: *синтез, хиральные жидкие кристаллы, мезоморфизм, оптически активный изоамиловый спирт. (С. 43 – 47)*

1. **Chiral liquid crystals based on optical active isoamyl alcohol** Full Text

By Bykova, V. V.; Anan'eva, G. A.; Usol'tseva, N. V.
From Zhidkie Kristally i Ikh Prakticheskoe Ispol'zovanie (2011), (1), 43-47. | Language: Russian, Database: CAPLUS

To study the influence of the calamitic compds. structure on their mesomorphic properties, the synthesis and study of the texture characteristics of 5 isoamil alc. derivs. were carried out. Only two (alkyl substituted) from 5 compds. possess chiral nematic phase. The alkoxy substituted and the ester derivs. from nematic phase without chirality features.

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  - абревиатура : **HPLC**
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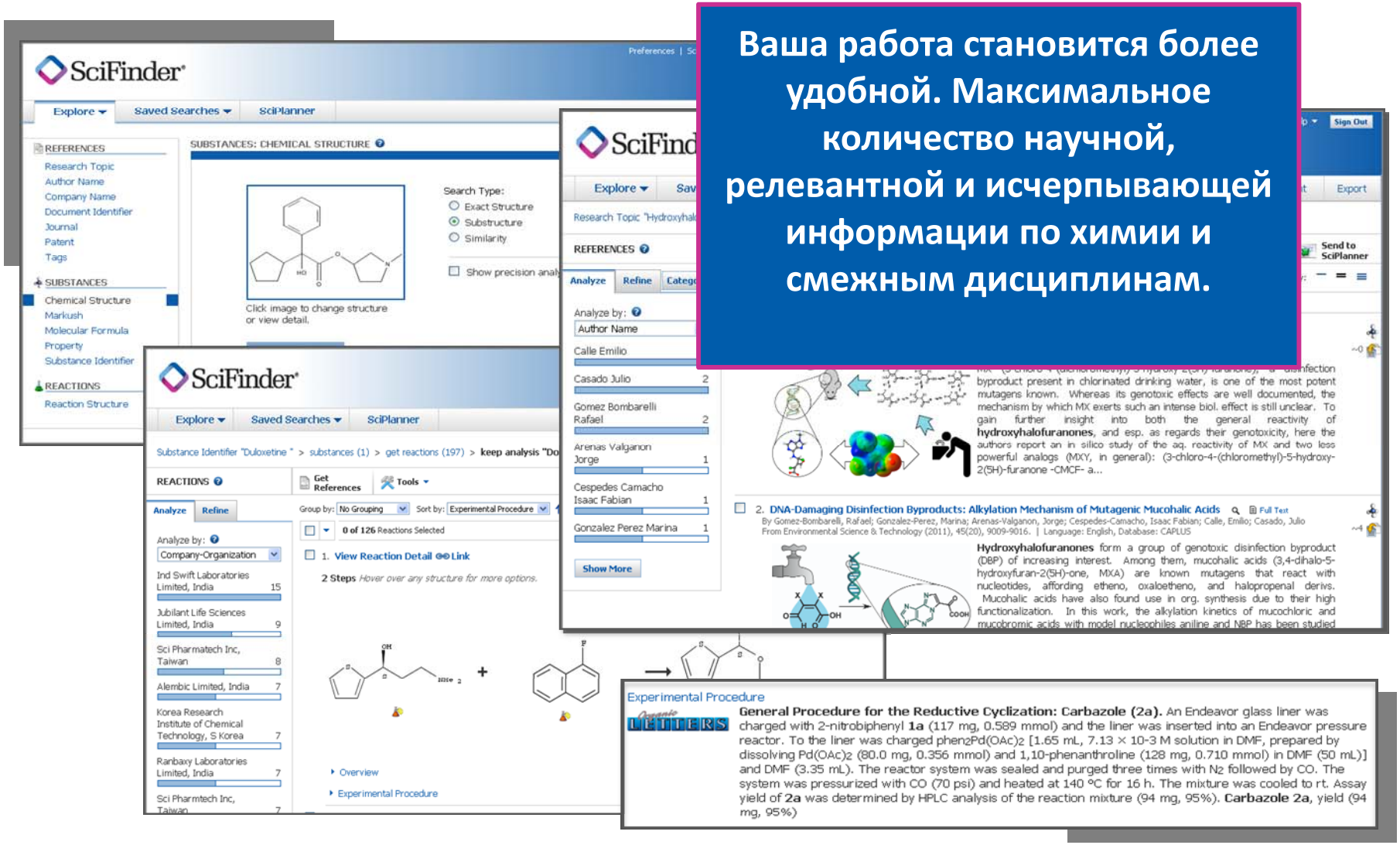

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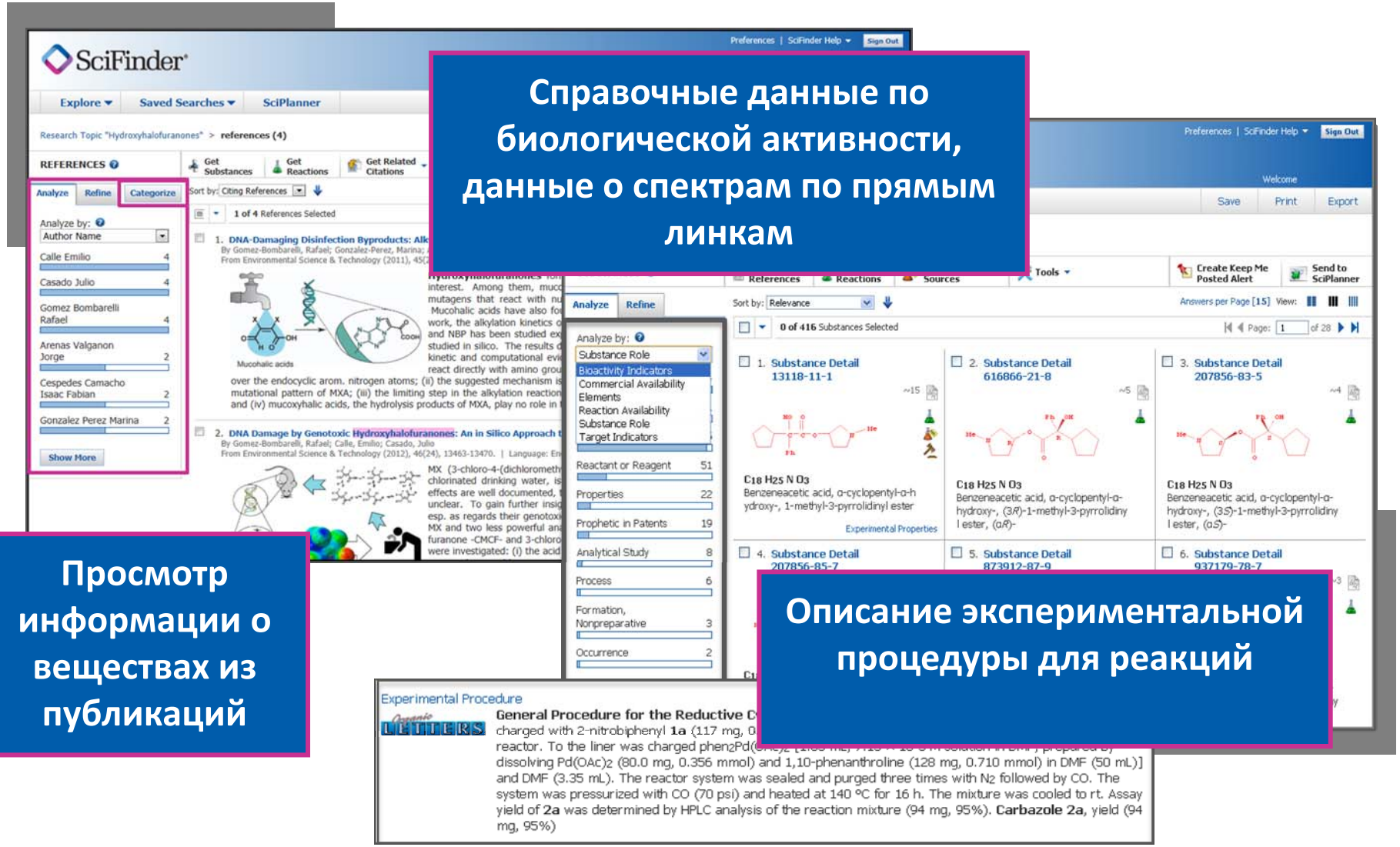

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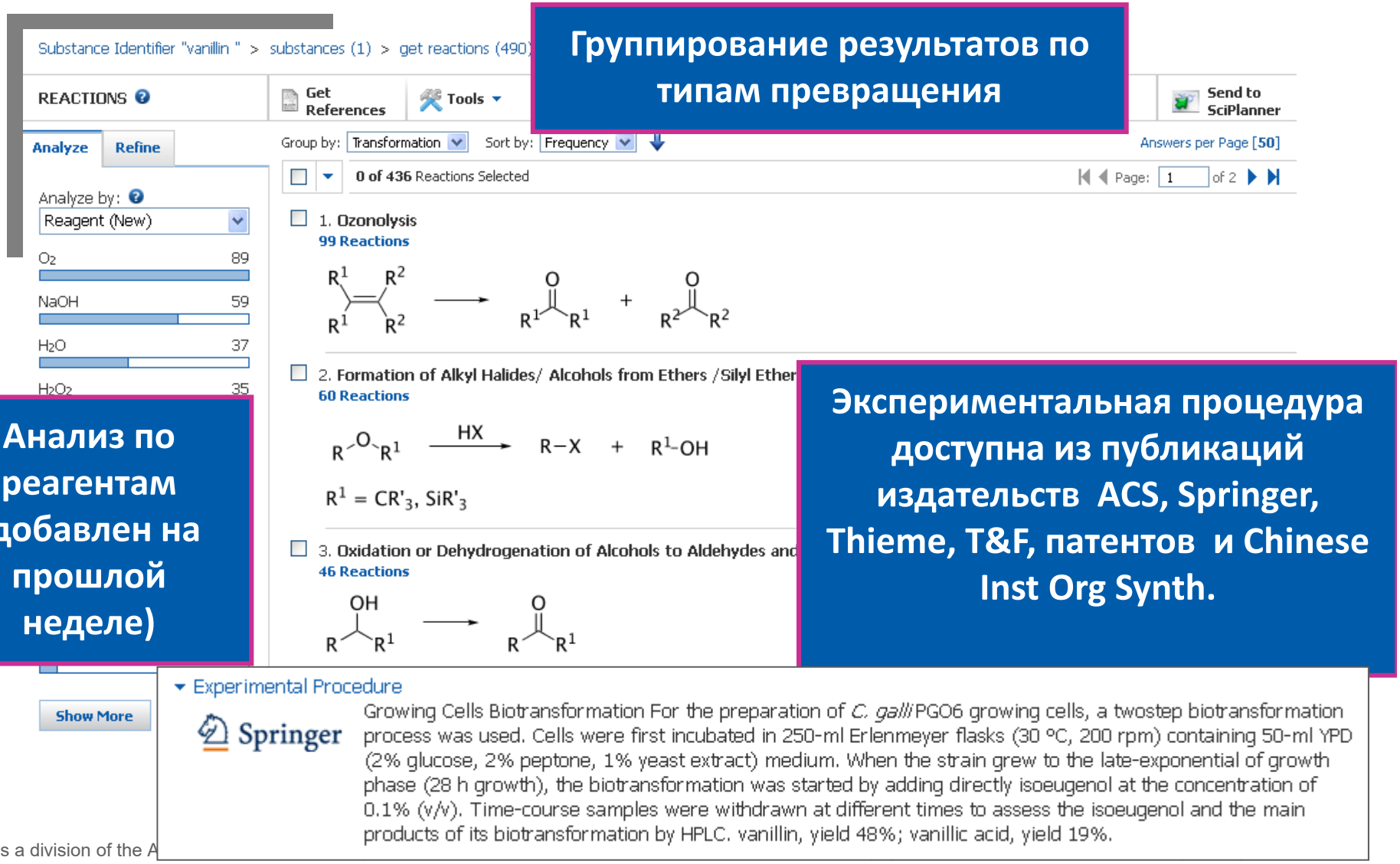

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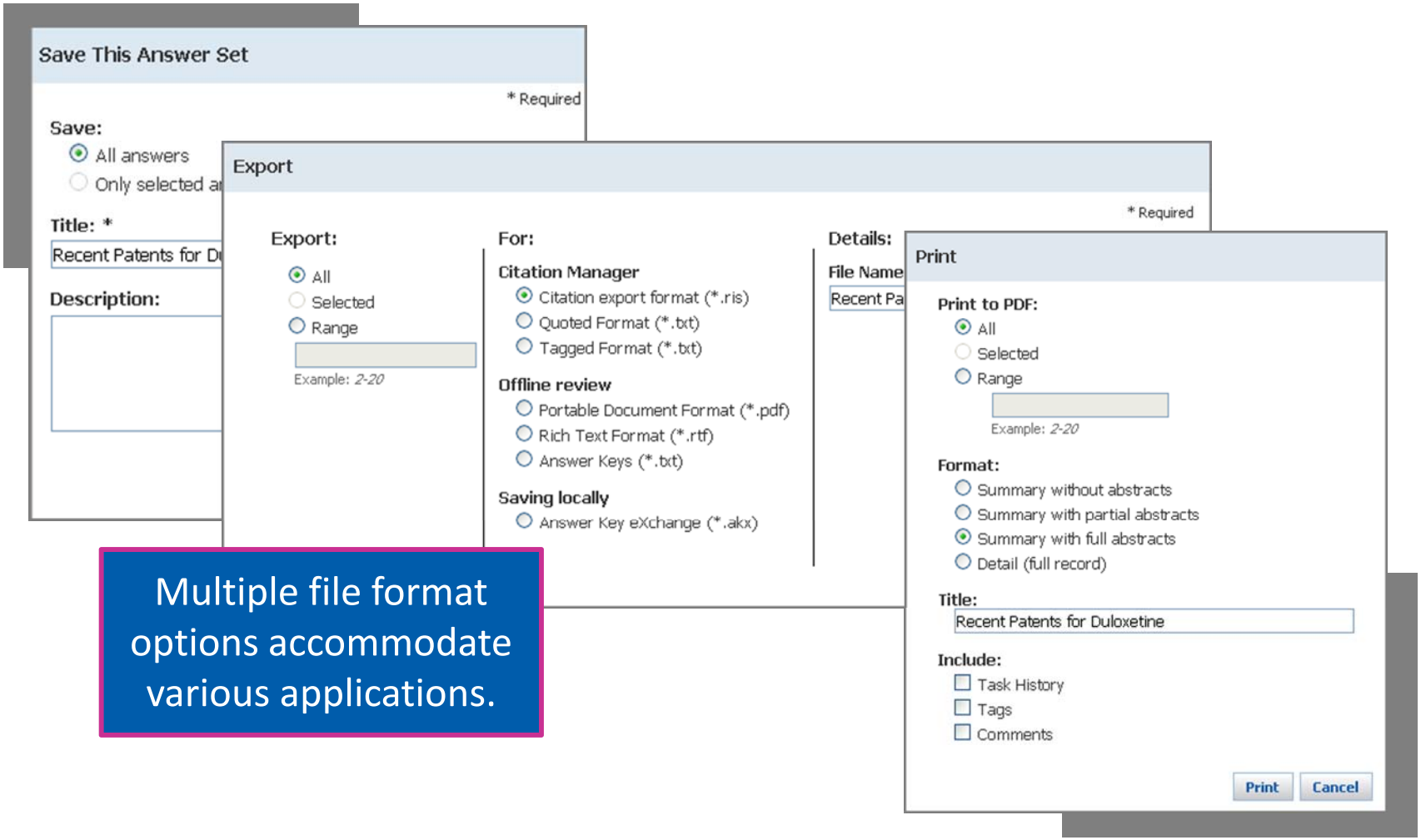

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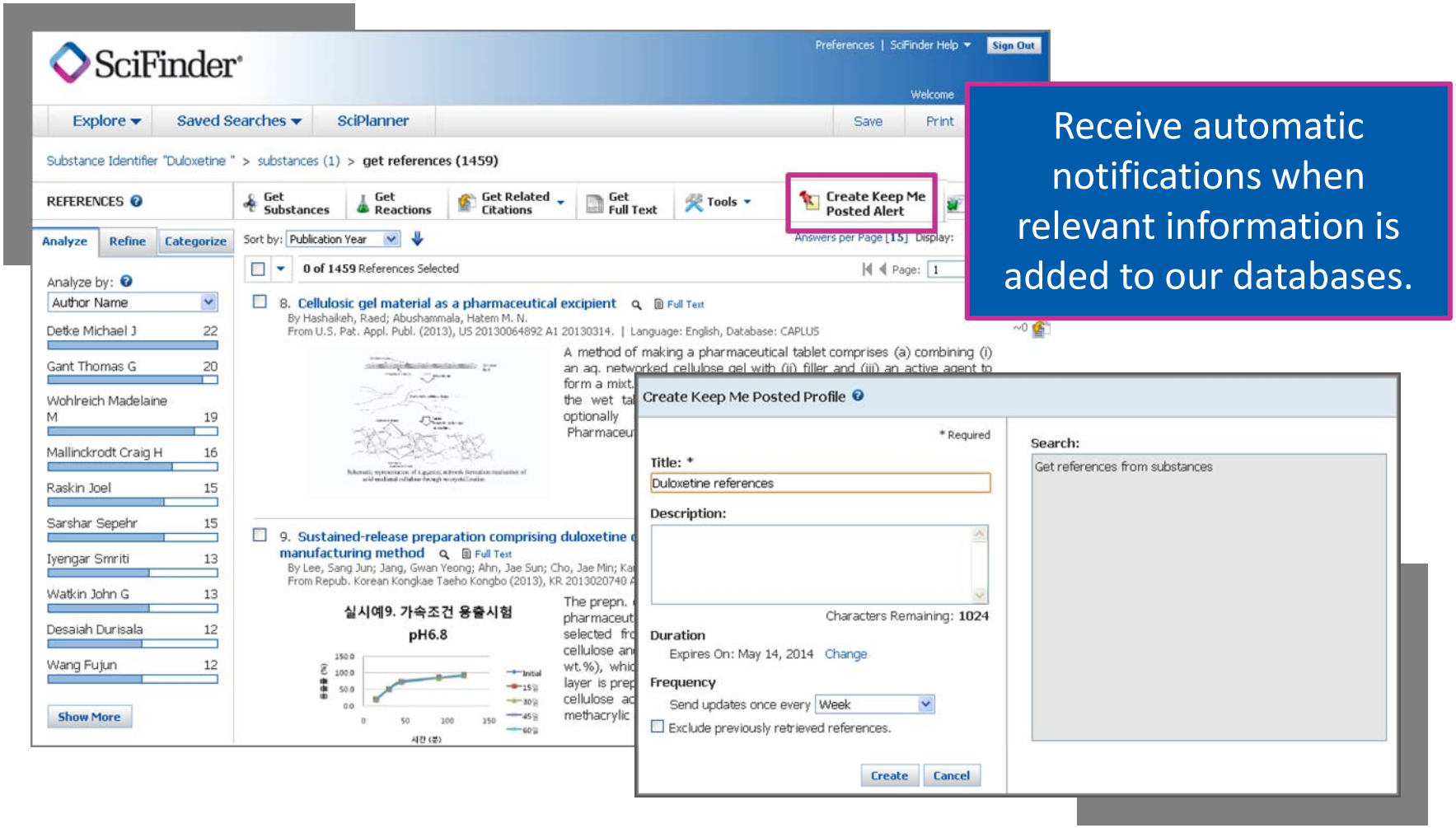

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