Factual Searching in CrossFire Beilstein

DiscoveryGateSM Version 1.4 Participant's Guide

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Powering the process of Invention

Factual Searching in CrossFire Beilstein

Key points

- Welcome to the *Factual Searching in CrossFire Beilstein* module.
- In this module, you will search the Beilstein database through DiscoveryGate using the MDL Database Browser

Module objectives

- Conduct data searches to retrieve compounds based on their chemical name, CAS number, and physical or chemical properties
- Conduct searches using multiple data entries
- Conduct searches using data and structural entries
- Use predefined EDS forms and create custom forms to conduct the searches
- Review the search history, save a list, and create a report

Key points

- In this module, you will learn how to conduct data searches to retrieve compounds based on their chemical name, CAS number, and physical or chemical properties.
- You will learn how to use the predefined EDS forms, and create your own custom forms.

Search scenarios

Conduct a series of factual searches, in the CrossFire Beilstein database, to answer the following questions. In the process, you will learn how to use the MDL Database Browser in DiscoveryGate.

- How do I retrieve a compound from the database if I only have the chemical name or CAS number?
- How do I retrieve specific property data for a compound?
- How do I retrieve reactions without using a structural query?
- How do I conduct a search using a factual and structural entry?

Key points

- This module focuses on the capabilities of DiscoveryGate with respect to the individual capabilities of one of its main components, the MDL Database Browser.
- We will conduct a series of factual searches using the CrossFire Beilstein database.



- Launch the internet browser and enter the DiscoveryGate URL. To log in, enter your user name and password, and then click "go discover."
- DiscoveryGate uses the MDL Database Browser to search individual databases. Searching a specific database allows you to focus quickly on the information in a specific database and to search using data properties.

Configure CrossFire access information
Chris' DiscoveryGate Chris' Settings Company Settings
Edit your personal Discovery Gate settings Home Support Logout chrismarth EDIT PROFILE FOR CHRIS
My CrossFire Login Information To access CrossFire Beilstein and CrossFire Gmelin from MDL® Database Browser, enter missing information below and click Update. Enter login information User Name Password Confirm Password Group Confirm Group Update

Notes

• To search the CrossFire Beilstein database, you will need to enter the CrossFire login information. If this is not configured, return to the main screen and click the Settings tab. Enter your user name, password, and group for CrossFire Beilstein.

Select the Search of Interest



Key points

- The selections for data searching that we will use in this module are:
 - Find Compounds by Property
 - Find Reaction by Conditions
 - Custom Search

Define the search form

Find Compounds by Property and Custom Search

Find in Field Index: next	To add a structure to your query,	click Draw Structure.		
Field Index History	To add data to your query, double data criteria.	-click a field name in the Field	Index to add it to the query. Then, specify	the
Clasy bala search Substance Fields Reaction Fields Citation Fields	To locate a field, click in the Find closely matches what you type. C You can use the "=" (equals) ope	box and type part of the field na lick the Next button to search fi rator to search for a range of va	ame. The list scrolls to the field name that or the next field that meets the criteria. alues. For example, to search for substand	rnost
Use to access the predefined forms	With a molecular weight between You use the "<>" operator to sear "Molecular weight <> 141_7"	141 and 142, use "=141-142". ch for all values of a field excep	of the value that you specify. For example,	
or create a custom form.	Feaction If your query contains sev precedence, to avoid aml	n Find this reaction and its conditio	 Substitution as drawn, exclude tautomers Substitution as drawn, include tautomers Unlimited substitution on all atoms, exclude t 	tautomers
Find Reaction by (Conditions	Double-click in this box to edit structure	Allow: P Multi-component compounds Name (closure through substitution I isotopes P Charges P Radicals Grower atom mapping Neep Pagments separate Gearch Stereoinformation [As drawn	Resst Dates Into
	Reaction	n Details		
	AND 💌	Yield	Contains Data Lookup	Delete Duplicate Info
	AND 💌	Reagent	Contains Data Lookup	Delete Duplicate Info
	AND Y	Catalyst	Contains Data Lookup	Delete Duplicate Info
	AND 💌	Solvent	Contains Data Lookup	Delete Duplicate Info
	Chow Prov	inte	start search	
	Snow Brack	Kets		

Key points

- The "Find Compounds by Property" option allows you to select predefined EDS forms or individual data fields to create a search to retrieve properties of interest.
- The "Find Reaction by Conditions" option allows you to select predefined EDS forms or individual data fields to create a search to retrieve types of reactions.
- The "Custom Search" option allows you to select individual data fields to create your own search combination.

Field Index: Field Index: Field Index: Field Index: Field Index: History Field Index: Field I	ical	Easy Da predeter	ta Search for mined data f	rms have a serie fields set up for s	s of searching.
Identification Data Physical Data Reaction Conditions	Subs	tance Beilstein Regist	ry = 💌		Delete Duplics
Solubility Data Spectral Data	OR	CAS Registry Nu	umber Contains 💌	Data Lookup	Info Delete Duplica
Citation Fields	OR	Chemical Name	Contains -	Data Lookup	<u>Delete</u> <u>Duplics</u> Info
	OR	Molecular Form	ula Contains 🔽	Data Lookup	Delete Duplica Info
	OR	 Molecular Weight 	nt 😑 💌		<u>Delete</u> Duplica

- There is a section on the Field Index tab called Easy Data Search. This category contains a number of predefined forms that have common search criteria.
- The forms are organized by search area.

Factual search features



Key points

- The data fields on an EDS (Easy Data Search) form are predefined and are listed. The fields can be text or numeric fields.
- When using text or numeric fields, you can use any of the operators shown in the slide.
- In our example, you are interested in retrieving all compounds having the chemical name *acyclovir*. The Data Lookup feature allows you to view the contents of the database.

Data operators and wildcards

Operators	Use to retrieve records that:
AND	satisfy both criteria
OR	satisfy either criterion
NOT	do not satisfy the criterion
=	satisfy the exact entry
<	are less than the specified entry
<=	are less than or equal to the specified entry
>	are greater that the specified entry
>=	are greater than or equal to the specified entry
<>	are not included as an entry
ls	have the exact entry
Starts with	begin with the entry
Ends with	end with the entry
Contains	have the term contained within
Wildcards	Use in text string to represent
?	One character
??	Two characters

Key points

Notes

• When using multiple fields, you must use some of the data operators.

Data Lookup tables

Chemical Name search		CAS number search	
🗿 Data Look up - Chemical Name		🗿 Data Look up - CAS Registry Number	
Find:		Find:	
acyclovir	Find	59277-89-3	Find
Frequency: Values:		Frequency: Values:	
6 acyclovir 1 acyclovir (sb-glucoside 1 acyclovir (na salt) 1 acyclovir carboxyphosphonate armonium 1 acyclovir diphosphate 1 acyclovir diphosphate 1 acyclovir diphosphate 1 acyclovir elaidate 1 acyclovir elaidate 1 acyclovir elaidate 1 acyclovir diphosphate diphosphonate ar ✓ ✓ Double-click the values you want to add to your query:	Start ↑ End	2 59277-89-3 1 59277-90-6 1 59277-91-7 1 59277-92-8 1 59277-93-9 1 59277-93-9 1 59277-95-1 1 59277-95-1 2 59277-96-2 Double-Click the values you want to add to your query: Your Query:	Start ↑ End
e Find any of these terms (OR operator) Find all of these terms (AND operator) Find all of these terms adjacent to one another in order	Clear OK Cancel	Find any of these terms (OR operator) Find all of these terms (AND operator) Find all of these terms adjacent to one another in order	Clear OK Cancel

Data Lookup tables display the specified value and the number of occurrences found in the database.

Key points

- The Data Lookup feature indicates the number of occurrences for that data entry.
- By default, "Find any of these terms (OR operator)" is selected. This means that an OR operator will be used to connect each value you have selected.
- Select "Find all of these terms (AND operator)" to require that every value is present.
- Select "Find all of these terms adjacent to one another in order" to search for a string of values adjacent to one another.

Chemical name or CAS number results

Chemical Name search results



Key points

- Results are displayed on a separate form in a structural format. To obtain detailed data, click the "Details" link.
- In some of the result panels, you will notice the green BIO indicator. This label indicates that the compound has pharmacological or toxicological data associated with it.

	esults Record # 1 of 6	1
CrossFire Beils	tein Substance 4257573	
Use as Query	Available Data Cifick on a fink to add the information to this page LiquidLiquid Systems (MCS) Weiting Point (1) (1) Nuclear Magnetic Partition octan-1-olivater Pharmacological Data (9) Related Structure (1) Substance (1) Substance for this Substance Substance	Click a link to obtain — specific data for the retrieved compound.
Substance (hide) Beilstein Registry Number	Substance record 1 of 1 4257573	
Beilstein Preferred RN	59277-89-3	
CAS Registry Number	59277-89-3	
Autoname	2-amino-9-(2-hydroxy-ethoxymethyl)-9/H-purin-6-ol	
Molecular Formula	C8H11N5O3	
Lawson Number	30725, 689, 514	Outpeter and date
Constitution ID	3789454	Substance data
Tautomer ID	1194427	
Beilstein Reference	6-26	
Entry Date	1992/07/20	
Commound Teno	2002/04/29	
Compound type		
Chemical Manie	and a second sec	
	Molecular Meight 226-21	
Molecular	MUIECUIAI YYEIYIN 220.21	

- The Substance data is shown, which includes identification information, such as registry numbers, molecular formula, CAS number, and chemical name.
- To obtain specific data for the compound, click a link in the Available Data box.
- If you would like to use this structure in a new query, click the "Use as Query" link.

Link t	o additi	onal da	ta	
Pharmacological [Data (hide)			
	Pharmacological Data reco	rd 1 of 9		
Comment	antiviral activity against HSV-1 in cell (0.18 µg/ml)	Vero cell (EC50: 0.41 µg/ml) and l	HSV-2 in Vero	
Pharmacological Data Citations	Journal; Sato, Yoshiko: Maruvar 43; 1; 1995; 91-95; LitLink	na, Tokumi; CPBTAL; Chem.Pharr	n.Bull.; EN;	 Links to the journal.
	Pharmacological Data reco	rd 2 of 9		
Comment	Chemoterapeutic activity agains	t Herpes simplex (HSV-1) infection	in mouse i.p.	
Pharmacological Data Citations	Journal; Winkelmann, E.; Winkle ARZNAD; Arzneim.Forsch.; EN;	e, G.;		
	Pharmacological Data reco	rd 3 of 9		
Comment	activity against Herpes Simplex 50 = 0.5 μM; cytoxicity against no	virus, type 1, strain McIntyre, in SIR rmal uninfected SIRC cells: CD 50	C cells:ED I=>50 µM	
Pharmacological Data Citations	Journal; El-Kousy, S.; Pedersen EN; 125; 6/7; 1994; 713-722;	, E. B.; Nielsen, C.; MOCMB7; Mon . <u>itLink</u>	atsh.Chem.;	
	Dharmacological Data reco	rd 4 of 9		
	antiviral activity (MIC = 2.42 and	Nuclear Magneti	c Reson	ance (hide)
Comment	respectively)		Nuclear N	Agnetic Resonance record 1 of 1
	Journal; Jaehne, Gerhard; Kroh	Description	Chemical :	shifts
Pharmacological Data Citations	Winkler, Irvin; et al.; ANCEAD; A	Solvents	dimethylsu	Ifoxide-d6
	<u>unum</u>	Nucleus	1H	
		Nuclear Magnetic Resonance Citations	Journal; B J.Med.Che Journal; B Satyamurt 10408-104	arrio, Jorge R.; Bryant, Jerry D.; Keyser, Gene E.; JMCMAR; am.; EN; 23; 5; 1980; 572-574; <u>LitLink</u> arrio, Jorge R.; Namavari, Mohammad; Phelps, Michael E.; hy, Nagichettiar; JACSAT; JAmer.Chem.Soc.; EN; 118; 43; 1996; 411; <u>LitLink</u>

- Using MDL LitLink, you can obtain the original literature reference.
- When you are in LitLink, click the publication link to view the abstract.
- You must have the appropriate access rights in order to view the primary literature using LitLink.

Multiple search criteria

Conduct a search to retrieve substances with a melting point between 300 - 310, where the solvent used is water. Restrict the list to those compounds that display data for the density of the liquid.

- use a predefined EDS search form
- use Available Data links to view retrieved data

Key points

- To search for compounds that have defined physical or chemical properties, use a multiple factual query.
- You want to retrieve substances with a melting point between 300-310, where the solvent used is water. A final requirement is to restrict the list to those compounds that display data for the density of the liquid.

Enter physical data search criter

Find in Field Index:	next						
Field Index History							
Structure	Melting Poi	nt					
Easy Data Search							Delete Duplicato
Bibliographic Data		I menting Point data exi	sis				Info
Bioactivity, Phai macological				200.210			Delete Duplicate
Emironmental Data		Value of Range	=	1000-010	•C		Info
					_		Delete
-E Physical Data	AND 🔳	From Solvent	Contains 💌	Data Lookup			Duplicate Info
Reaction Conditions	Dissociatio	n Exponent					
- 🖂 Solubility Data			at (pl/ value) data oviete				Delete Dunlicate
Spectral Data			it (pr< value) data exists			· · · · · ·	Info
🕂 🗀 Substance Fields	Boiling Poir	nt					
₽-C Reaction Fields ₽-C Citation Fields	AND 💌	Boiling Point data exis	sts			•	Delete Duplicate Info
	OR 💌	Value or Range	= 💌		•c		Delete Duplicate Info
	AND 💌	At Pressure	= •		Torr		Delete Duplicate Info
	Density of t	he Liquid					
	AND 💌	🔽 🔽 Density data exists					Delete Duplicate Info
	OR 💌	Value or Range	= •				Delete Duplicate Info
			st	art search			
	Remove Bracke	ts					

- This query form provides search criteria specific to fields related to physical data.
- You can search the database using fields with listed values.
- You can search some fields in the database without specifying a value. This technique is used to retrieve all records that have an entry in any subfield.
- Click the check mark next to the area of interest. This is a broad search for the occurrence of a fact in the database.

		1001		
		Availa	ble Data	
	۰ <i>"</i> ۴	Click on a link to add the informat	ion to this page	
	1	Crystal Phase (1)	Crystal System (1)	
	~N	Density of the Liquid (1)	Melting Point (1)	
	Query Curthopire	Solubility (MCS) (2)	Substance (1)	
Use as	uuery Synthesize	Show Reactions for this Substance	e Show Citations for thi	s Substance
		1		
Malting Daint				
			1	
Melting Point (C)		Solvent	Comment	Citation
307	m20		P. Contraction of the second s	12
		<u> </u>		
		Comments		
1 Handbook		Comments		
1 Handbook		Comments Citations		
1 Handbook 1 Journal; Pyman; Ravald; JCSOA	9; J.Chem.Soc.; 117; 1920; 1430; Litt.	Comments Citations		
1 Handbook 1 Journal; Pyman; Ravald; JCSOA	9; J.Chem.Soc.; 117; 1920; 1430; Litt.	Comments Citations ink Top of Page		
1 Handbook 1 Journal; Pyman; Ravald; JCSOA	9; J.Chem.Soc.; 117; 1920; 1430; L <u>itt.</u>	Comments Citations ink Top of Page		
1 Handbook 1 Journal; Pyman; Ravald; JCSOA Density of the Liqu	9; J.Chem.Soc.; 117; 1920; 1430; <u>Litt</u> I <mark>İČ</mark> (hide)	Comments Citations ink Top of Page		
1 Handbook 1 Journal; Pyman; Ravald; JCSOA Density of the Liqu Density of the Liquid	9; J.Chem.Soc.; 117; 1920; 1430; Litt Jid (hide) Reference Temperature (C)	Comments Citations ink <u>Top of Page</u> Measurement Temperatur	e (C) Comme	ent Citatio
1 Handbook 1 Journal; Pyman; Ravald; JCSOA Density of the Liqu Density of the Liquid 1.838	9; J.Chem.Soc.; 117; 1920; 1430; Litt. Jid (hide) Reference Temperature (C)	Comments Citations ink Top of Page Measurement Temperatur	e (C) Comme	nt Citati
1 Handbook 1 Journal; Pyman; Ravald; JCSOA Density of the Liquid 1.838	9; J.Chem.Soc.; 117; 1920; 1430; Litt JiC (hide) Reference Temperature (C)	Comments Citations ink Top of Page Measurement Temperatur Comments	e (C) Comme	nt Citat
1 Handbook 1 Journal; Pyman; Ravald; JCSOA Density of the Liquid 1.838 1 g/cm**3	9; J.Chem.Soc.; 117; 1920; 1430; Lift Jid (hide) Reference Temperature (C)	Comments Citations Ink Top of Page Measurement Temperatur Comments	e (C) Comme 1, 2	nt Citati

Notes

• When used, the two connected search terms will only be retrieved as a hit if they are present in the same occurrence of a fact.

Custom form search for reactions

Conduct a search to retrieve hydrogenation reactions where Raney-Ni is used as a reagent or catalyst and acetic acid is used as a reagent.

- create a Custom Search form
- use data operators and wildcards

Key points

• In this example, you are interested in retrieving hydrogenation reactions that use the Raney-Ni as a reagent or a catalyst, as well as acetic acid as a reagent.

Search for reactions

Find in Field Index: maxt Field Index History Structure Easy Data Search Stubstance Fields Reaction Fields Reaction Fields Reaction Defails (RX) Reaction Defails (RX) Reaction Defails (RX) Stage Reaction Classification Stage Solvent (RX.CAT) Catalyst (RX.CAT) Solvent (RX,SOL) Time (RX.TM) Pressure (RX.P) PH4ue (RX.PH) Pressure (RX.P)	Custom Search forms contain only those data fields specifically selected for the search. Select data field twice or click <i>Duplicat</i> e to add the same data field to the form.	
Other Conditions (RX.COND)	Reaction Details	
Subject Studied (RX.SUB) Reaction Type (RX.TYP) Prototype Reaction (RX.PRT	Reagent (RX.RGT) Contains Data Lookup Data Lookup	<u>ete</u> plicate 2
Citation Fields	OR Y Reagent (RX.RGT) Contains Y Data Lookup	<u>ete</u> plicate
F	AND V Catalyst (RX.CAT) Contains V Data Leakup	<u>ete</u> plicate
F	AND V Other Conditions (RX.COND) Contains V Data Lookep	<u>ete</u> plicate
<u>P</u>	start search	

Key points

- Due to the inconsistencies of how authors report various reagents and catalysts in the literature, catalyst information can be stored in the catalyst and/or reagent field.
- To obtain a complete listing of information, you must search both data fields.

			start	search		
AND 🗾	Other Conditions (F	& COND) Contains	<u>•</u>	hydrogenation Data Lookup		Duplica Info
	Other Cand ¹¹¹			Data Lookup		Info Delete
OR 💌	Catalyst (RX.CAT)	Contains	•	ran?y]	<u>Delete</u> Duplica
AND 💌	Reagent (RX.RGT)	Contains	•	ran?y Data Lookup		Delete Duplica Info
	Reagent (RX.RGT)	Contains	<u> </u>	acetic acid Data Lookup		Duplica Info

• The substance, Raney Ni, occurs in the database using different entries. Use wildcards to include all occurrences of the catalyst and the reagent in the query.

• Use parentheses to force your search condition. You want to create an OR between the reagent and catalyst fields for Raney Ni.

Structure/data combination search

Conduct a search for the synthesis of para-halo-acetophenone compounds. Limit the list of reactions to those where methanol is used as the solvent.

- use the Find Reaction by Conditions form
- combine structure and data components

Key points

- Factual searching is most effective when combined with a structure or reaction query.
- In the next example, we want to conduct a search for the synthesis of paraacetophenone compounds, limiting the list to only those reactions that use methanol as a solvent.

Find	Reaction	bv	Conditions
1 11 14	noadion	~ J	Contantione

Reaction							
ſ	Find this r	eaction and its conditions • •	Substitutio Substitutio Substitutio Unlimited Allow: Multi-com; Ring closu Isotopes Ignore ato Keep fragm Search Stereoc	in as drawn, exclude tautomers in as drawn, include tautomers substitution on all atoms, exclud ponent compounds ire through substitution ire Charges ir Radicals m mapping ments separate pinformation Off	e tautomers	_	<u>Reset</u> Delete Info
Reaction Det	ails					-	
	▼ Yield	Contains	•	Data Lookup		•	<u>Delete</u> Duplicate Info
AND	▼ Reagent	Contains	•	Data Lookup		•	<u>Delete</u> Duplicate Info
	💌 Catalyst	Contains	•	Data Lookup		•	<u>Delete</u> Duplicate Info
	✓ Solvent	[Is	•	methanol Data Lookup		•	<u>Delete</u> Duplicate Info
			start searc	h			

Notes

• When searching for reaction conditions, it is best to use the "Find Reaction by Conditions" form.

Structure/data search results

CrossFire Beilstein Reac	tion 2037355		~			
$c \mapsto \bigcup_{v \in \mathcal{V}} f \mapsto $						
Reaction Details			1			
	Reaction Detail	s record 1 of 1				
Yield	24 percent (BRN=386014) 63 percent (BRN=1564310)					
Reaction Details Citations	Reaction Details Citations Journal; Nishinaga, Akira; Yamazaki, Shigekazu, Matsuura, Teruo, TELEAY; Tetrahedron Lett.; EN; 27; 23; 1986; 2649-2652; LitLink					
Reaction Classification	Preparation					
	Reagent	Co(salen)(OH), O2				
Stano	Solvent	methanol				
Staye	Time	1 hour(s)				
	Other Conditions	Ambient temperature				

Conducting the structural search retrieves greater than 300 records. Conducting the structure/data search retrieves approximately 20 records.

Key points

- Using a partial reaction query does not limit use to a specific type of reaction.
- Doing this portion of the search alone could retrieve too many results. The inclusion of the data parameter keeps the list focused.

Create a	report and save a list
discoverygate	MDL [®] database browser queries results reports rxn schemes CrossFire Bellstein age setup print save refine query new query change database help logout
Copy to Report Select copy destination Create new report Append to existing report View report now Find	Sove As File name: Enter file name here Okt Cancel Notime: Search results 1 to 12 of 14
	History This Report Search results 1 to 12 of 14 Reaction ID: 92708 □ → → ↓ → Br → ↓ ↓ ↓ ↓

- You can copy your search results to a report that can be printed or exported.
- To create a report, click "copy to report" on the menu bar.
- You have the option of creating a new report or appending the data to an existing report. If you want to view the report immediately, check the box.
- To save a search, click the save button on the top menu bar.
- Saved searches are placed in the Saved Searches folder and stored permanently.

The following descriptions explain the goal of each exercise. If you like to figure things out on your own, use the descriptions to conduct the exercises. If you prefer step-by- step instructions, go to the page listed below the description.
Conduct a Chemical Name search to retrieve ibuprofen. Review the results. Conduct a second search for only those ibuprofen compounds that display pharmacological data. Review the results and link to the pharmacological data.
For a step-by-step solution, see page 1-26.
Conduct a combination factual/structure search to retrieve all compounds that have a phenobarbital core structure and a melting point restriction greater than or equal to 150° C.
For a step-by-step solution, see page 1-28.
Conduct a factual search to retrieve reactions where the product was derived from a demethylation of various groups.
For a step-by-step solution, see page 1-30.

	Conduct a Chemical Name search to retrieve ibuprofen
Exercise 1	Conduct a Chemical Name search to retrieve ibuprofen. Review the results. Conduct a second search for only those ibuprofen compounds that display pharmacological data. Review the results and link to the pharmacological data.
Start DiscoveryGate	 If you have already started the application, go to Step 3. Launch your internet browser and enter the DiscoveryGate URL (www.discoverygate.com).
	 Enter your user name and password. If necessary, enter your company id. Click go discover.
	3. Under Applications, click Search individual databases.
Open the CrossFire Beilstein database	4. Under Chemistry Information, click CrossFire Beilstein.
	5. Click the Find Compounds by Property link.
Open the Easy Data Search form	 In the Field Index pane, open the Easy Data Search folder. Double-click the Substance Identification Data folder.
	7. For the Chemical Name field, select the Contains operator.
	8. Click the Data Lookup link below the text entry box.
Use the Data Lookup table	 In the Data Look up – Chemical Name dialog box, type ibuprofen in Find text box and click Find.
	10. In the Frequency: Values: box, double-click the ibuprofen entry.
	11. When the entry appears in the Query box, click OK .

start search

Isolate the list of compounds refine query 12. Click start search.

- 13. Click the **Details** link. Note that a number of records have the BIO label in the structure result box.
- 14. Click the **refine query** button.
- 15. In the Field Index pane, click to expand the **Easy Data Search** category.
- 16. Double-click the **Pharmacological Data** form.
- 17. Check the **Pharmacological data exists** box.
- 18. Click start search.
- 19. Click the **Details** link for any record.

Combination factual/structure search

Exercise 2 Conduct a combination factual/structure search to retrieve all compounds that have a phenobarbital core structure and a melting point restriction greater than or equal to 150°C.



Prepare for a new search

- 1. Click the **new query** button.
- 2. Click the **Custom Search** link.
- 3. In the Field Index pane, double-click the **Structure** field.
- 4. In the Find Field Index text box, type melting point.
- 5. Open the **Melting Point** (**MP**) folder and double-click the **Melting Point** (**MP**) data field.
- 6. Double-click the structure box and draw phenobarbital using MDL Draw. Click **Done**.
- 7. In the MDL Database Browser select:
 - Find this compound and its properties
 - Substitution as drawn, exclude tautomers
 - Under Allow, check **Multi-component substances**, **Ring closure through substitution**, **Isotopes**, **Charges**, and **Radicals**.
 - Search Stereoinformation, select Off

- 8. If necessary, choose the **AND** operator between the fields.
- 9. For the melting point field, select the **greater than or** equal to (>=) operator and enter 150 in the text box.
- 10. Click start search and view the results.

start search

- 11. Click the **Details** link for BRN 551715.
- 12. Under Available Data, click the **Melting Point** link.

	Retrieve reactions using a factual query
Exercise 3	Conduct a factual search to retrieve reactions where the product was derived from a demethylation of various groups.
Prepare for a new search	1. Click the new query button.
	2. Click the Custom Search link.
	3. In the Field Index pane, type conditions in the Find Field Index text box, if necessary. Click the Next button until you obtain the Other Conditions (RX.COND) data field.
	 In the Field Index pane, double-click the Other Conditions (RX.COND) data field. If necessary, select the Contains operator and type demethylation in the text box on the form.
start search	5. Click start search and view the results.

To launch the DiscoveryGate application

- 1. Launch your internet browser and enter the DiscoveryGate URL (<u>www.discoverygate.com</u>).
- 2. Enter your username and password.
- 3. If necessary, enter your company ID.

discov	ery gate
about	contact
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4. Click go discover.

To select an individual database

1. Under Applications, click Search individual databases.



To select CrossFire Beilstein

1. Under Chemistry Information, click CrossFire Beilstein.



To configure CrossFire

- 1. Click the personal **Settings** tab.
- 2. In the My CrossFire Login Information box, enter your User Name, Password, Confirm Password, Group, and Confirm Group information.

My CrossFire Login	Information	?			
To access CrossFire Beilstein and CrossFire Gmelin from MDL [®] Database Browser, enter missing information below and click Update.					
Enter login information:					
User Name					
Password					
Confirm Password					
Group					
Confirm Group					
	Update				

3. Click Update.

To create a factual query

1. In the Select the Search of Interest window, click **Find Compounds by Property, Find Reaction by Conditions**, or **Custom Search**.



- 2. In the Field Index pane, open a predefined EDS form, or open a folder and double-click to select individual data fields.
- 3. Select a data operator and enter a text or numeric data entry into the associated text box.
- 1. Enter a query into one or more data fields.
- 2. Click start search.
- 1. After a query is launched, click Cancel.

Searching	×
Click Cancel to stop the search.	
Cancel	

1. At the top of the window, click the **refine query** button.

To start a search

start search

To stop a search

To modify a search query

refine query

To clear the query clear query	1. On the query tab, click clear query .
To open an Easy Data Search form	 (Optional) Click clear query. In the Field Index pane, expand the Easy Data Search folder. Double-click the appropriate form.
To add a data field to the query	 In the Field Index pane, expand the folders to locate the field. Or – Type the name of the field and click Find. Double-click the field name to add it to the query.
To add the same data field to the query form twice	 In the Field Index pane, expand the folders to locate the field and double-click the field name. Or – If the data field is currently on the form, click the Duplicate command to the right of the data field. Reaction Details OR ■ Reagent (RXR0T) Contains ■ Data Lostop. Deter
	AND Catalyst (RX.CAT) Contains Catalyst (RX.CAT) Catalyst (RX.CAT) Contains Catalyst (RX.CAT) Contains Catalyst (RX.CAT) Contains Catalyst (RX.CAT) Catalyst (RX.CAT) Contains Catalyst (RX.CAT) Catalyst
Fo use a Data Lookup table	1. Click Data Lookup .

To use a Data Lookup table

1. Click Data Lookup.

- 2. Type the value of interest.
- 3. Click **Find**.
- 4. Double-click to add a value to your query.

	· · · · · · · · · · · · · · · · · · ·	
acyclovir	Fit	nd
Frequency: Va	alues:	
6	acyclovir Sta	art
1	acyclovir \$b-glucoside	
1	acyclovir (na salt)	
1	acyclovir carboxyphosphonate ammonium	
1	acyclovir diphosphate	
1	acyclovir diphosphate dimyristoylglyce	L.
1	acyclovir elaidate	
1	acyclovir ethoxycarbonylphosphonate ar	
Your Query: acyclovir 🗲		ar

- 5. Repeat Steps 2-4 until all of the desired values have been added.
- 6. Click **OK**.
- 1. Place a structure in the Structure box using MDL Draw.
- 2. Set the Structure and Global search options.
- 3. Under Allow, set the search limits.



4. In the Field Index pane, navigate to the data field and double-click to add it to the form.

To conduct a combination factual/structure search

To conduct a Chemical Name search 5. Select a data operator and type your search entry into the available text box.

- 6. Click start search.
- 1. Under Easy Data Search, double-click **Identification Data**.
- 2. For the Chemical Name field, select a data operator and type your data entry in the available text box.

Substance			
Beilstein Registry Number	= •		<u>Delete</u> Duplicate Info
OR 🔽 CAS Registry Numbe	r Contains 💌	Data Lookup	<u>Delete</u> <u>Duplicate</u> Info
OR 🔽 Chemical Name	Is 💌	acyclovir Data Lookup	<u>Delete</u> <u>Duplicate</u> Info
OR 🗾 Molecular Formula	Starts With Ends With	Data Lookup	<u>Delete</u> Duplicate Info
OR 💌 Molecular Weight	=		<u>Delete</u> Duplicate Info
	starts	search	
Show Brackets			

- 3. Click start search.
- 1. Under Easy Data Search, double-click **Identification Data**.
- 2. For the CAS Number field, select a data operator and type your data entry in the available text box.
- 3. Click start search.
- 1. When the search is complete, the system automatically displays the results tab.
- 2. If necessary, click the **results** tab at the top of the window.
- 3. On the History tab, double-click to open the **Today's Searches** folder.
- 4. Double-click to open a Search.

To conduct a CAS Number search

To view search results

To view details of a search

To save search results



To create a report

copy to report

To use MDL LitLink to

retrieve a publication

- 1. On the results tab, click the **Details** link found under the structure.
- 2. In the **Available Data** box, click a link to view the specific data.
- 3. Click the **Top of Page** link and repeat Step 2 to view more data.
- 1. At the top of the results tab, click the **save** button.
- 2. Type a name into the Save As box and click **OK**.
- 1. At the top of the results tab, click the **copy to report** button.
- 2. Select Create new report or Append to existing report.
- 3. Check the View report now box and click OK.

o Report	×
t copy destination	
Create new report	
Append to existing report	
w report now	
	create new report Create new report Append to existing report

- 1. On the results tab or in the Details window, click LitLink.
- 2. In the MDL LitLink window, click the data source from which you would like to retrieve the article.