

2025.8.21 蛋白研CSDセミナー



ConQuest & Mercury

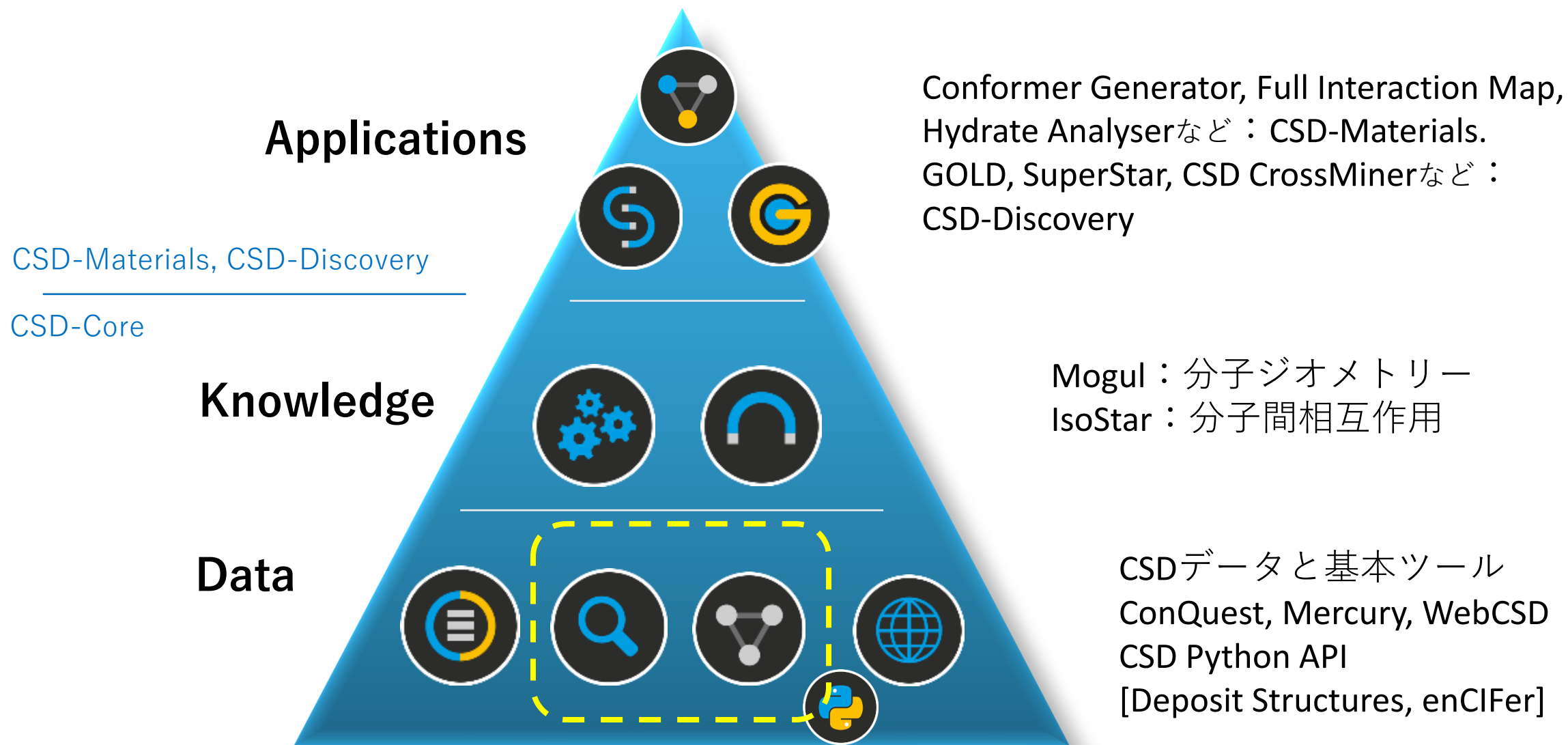
— 結晶構造の検索と分析 —

日本原子力研究開発機構 J-PARCセンター

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ConQuestとMercuryの位置付け

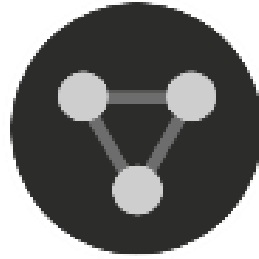


ConQuestとMercuryで何ができる？



[ConQuest](#)

結晶構造の検索



[Mercury](#)

Hitした結晶構造の表示、分析

- ❑ この化合物、結晶構造未知？
- ❑ 新規に解析した結晶構造、類似化合物とどこが違う？
- ❑ ある類似化合物群の構造的特徴は？
- ❑ この分子間/分子内相互作用の構造的特徴は？
- ❑ X線構造解析と中性子構造解析ではどこが違う？
- ❑ etc.

この発表で示す検索と表示の実例

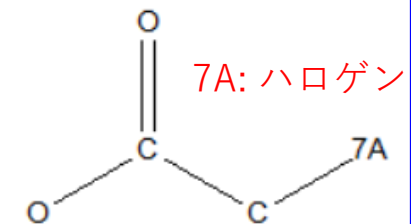
- 単純な検索と表示の一連の流れ
- 元素、結合の種類指定法
- 構造情報の追加による検索の絞り込み
- 分子間N—H $\cdots$ O水素結合を持つ構造の検索と、構造的特徴の分析
- 実験条件(線源：中性子)を指定した検索

この発表で示す検索と表示の実例

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部分構造(Fragment)の入力から検索、表示まで

Fragment



- ConQuest立上げ
- 上記の部分構造を持つ構造の検索
- Hitした構造の論文リストの出力
- Mercuryでの表示

Cambridge Structural Databases

OneDrive > 高志 - 個人用 > デスクトップ > Cambridge Structural Database

名前	状態	更新日時	種類	サイズ
Activate in-house Database	●	2025/06/05 13:30	ショートカット	
ConQuest	●	2025/06/05 13:30	ショートカット	
CrossMiner	●	2025/06/04 10:03	ショートカット	
CSD Python API	●	2025/06/04 10:04	ショートカット	
CSD-Editor	●	2025/06/04 10:03	ショートカット	

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- 実験条件を指定した検索

元素、結合の指定法

複数種の元素、結合の指定も可能

Other Atom Type

Other Atom Type

1A																	8A				
H																	He				
HD	D	2A																			
Li	Be															B	C	N	O	F	Ne
Na	Mg	3B	4B	5B	6B	7B	8X	8Y	8Z	1B	2B	Al	Si	P	S	Cl	Ar				
1R	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr			
TR	2R	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe		
3R	Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn			
Fr	Ra	Ac																			
			LN	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu				
			AN	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr				

Previous Selections

Picking Mode

☒ Single Pick

☐ Multi Pick

Current Selection: TR

Reset

Cancel

Apply

OK

Bond: Single

Single

Double

Triple

Quadruple

Aromatic

Polymeric

Delocalised

Pi

Any

Variable...

Variable Bond Type

☒ Single

☒ Double

☐ Triple

☐ Quadruple

☒ Aromatic

☐ Polymeric

☐ Delocalised

☐ Pi

Apply

OK

Cancel

Current Definition: 1, 2, ar

元素、結合の指定法

複数種の元素、結合の指定も可能

Other Atom Type

Other Atom Type

1A																	8A		
H																			
1M	2M	3M	4M	NM	Not H		Any												
HD	D	2A											3A	4A	5A	6A	7A	He	
Li		Be						8B	B		C	N	O	F	Ne				
Na		Mg	3B	4B	5B	6B	7B	8X	8Y	8Z	1B	2B	Al	Si	P	S	Cl	Ar	
1R	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr	
TR	2R	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
3R	Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn	
Fr		Ra	Ac																
LN	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu					
AN	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr					

Previous Selections

Picking Mode

☐ Single Pick

☒ Multi Pick

Current Selection: C N O H

ResetCancelApplyOK

Bond: Single

Single

Double

Triple

Quadruple

Aromatic

Polymeric

Delocalised

Pi

Any

Variable...

Variabl...

Variable Bond Type

☒ Single

☒ Double

☐ Triple

☐ Quadruple

☒ Aromatic

☐ Polymeric

☐ Delocalised

☐ Pi

ApplyOKCancel

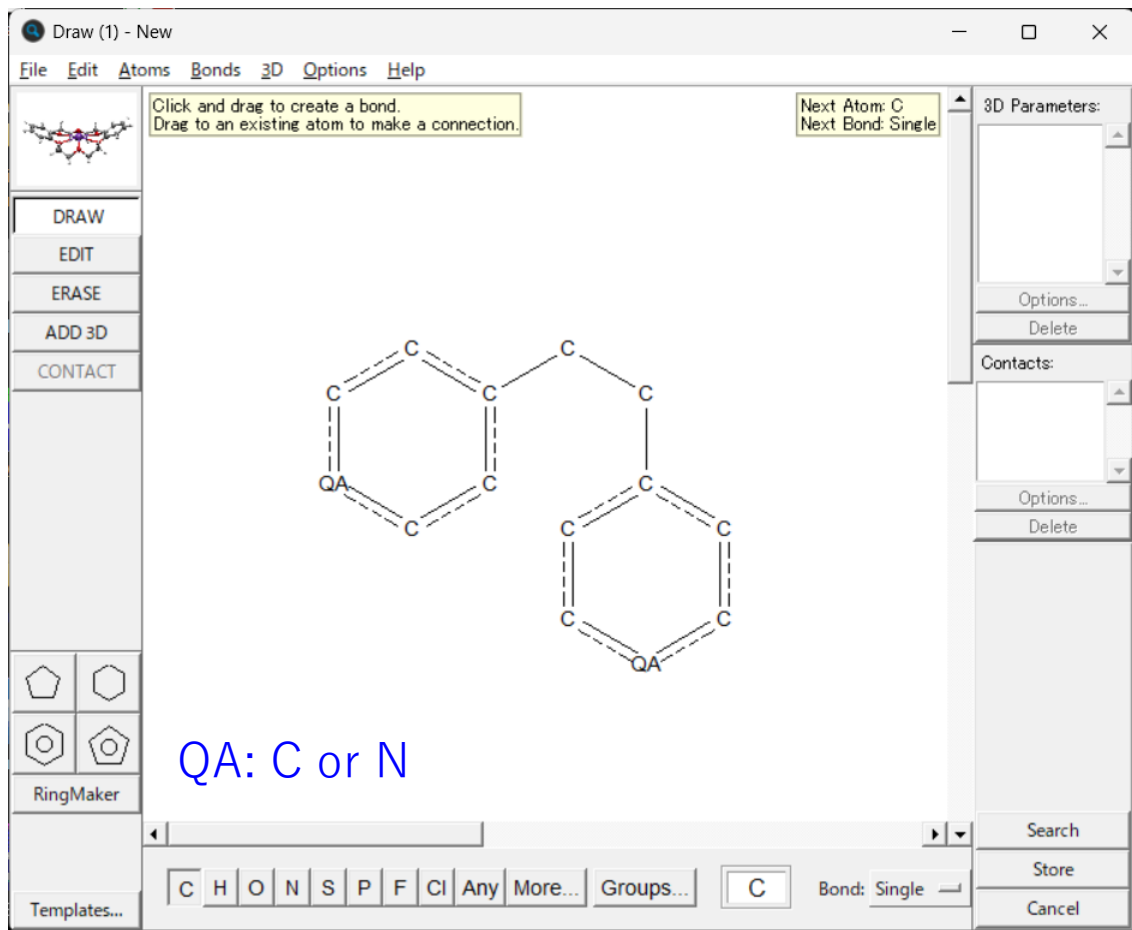
Current Definition: 1, 2, ar

この発表で示す検索と表示の実例

- 単純な検索と表示の一連の流れ
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検索結果の絞り込み

Fragmentに様々な条件を追加する



検索結果の絞り込み

Fragmentに様々な条件を追加する

The screenshot shows the 'Draw (1) - New' window with a chemical structure of a bicyclic compound. The structure consists of two fused six-membered rings. The left ring has a dashed bond labeled 'QA' between two carbon atoms. The right ring also has a dashed bond labeled 'QA' between two carbon atoms. The 'Search Setup' dialog is open, showing the 'Filters' tab. The 'Available Databases' section has 'CSD version 6.00 (Apr 2025)' selected. The 'Single query being used' section has 'Query 1' highlighted. The 'Filters' section includes several checkboxes and radio buttons for refining the search results.

QA: C or N

Search Setup

Search Name: search1

Available Databases:

- ☒ CSD version 6.00 (Apr 2025)

You can search complete database(s) or a subset (e.g., hits found in a previous search)

Select Subset Clear Subset

Single query being used. Search will find structures:

where this query is true:

Query 1

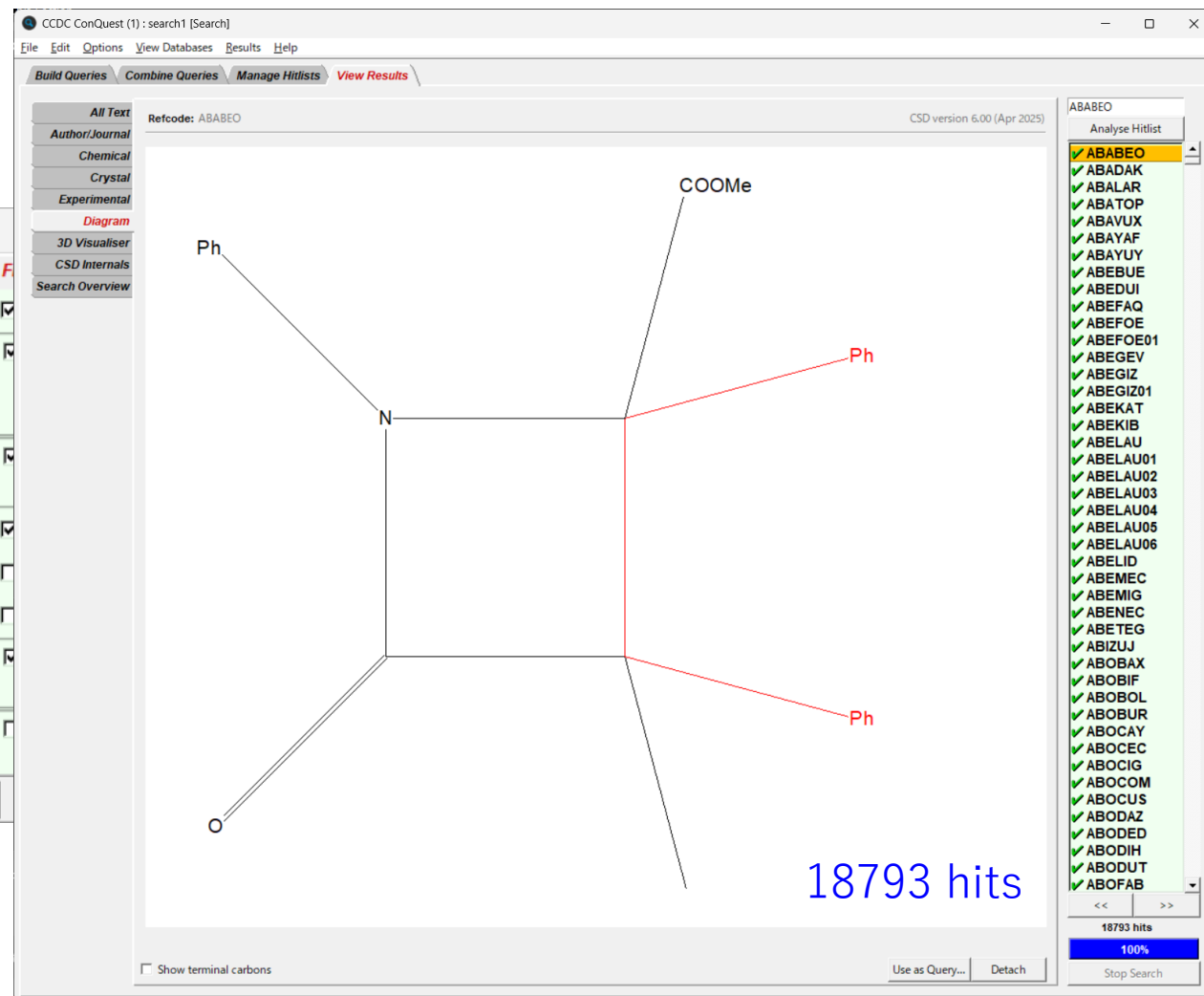
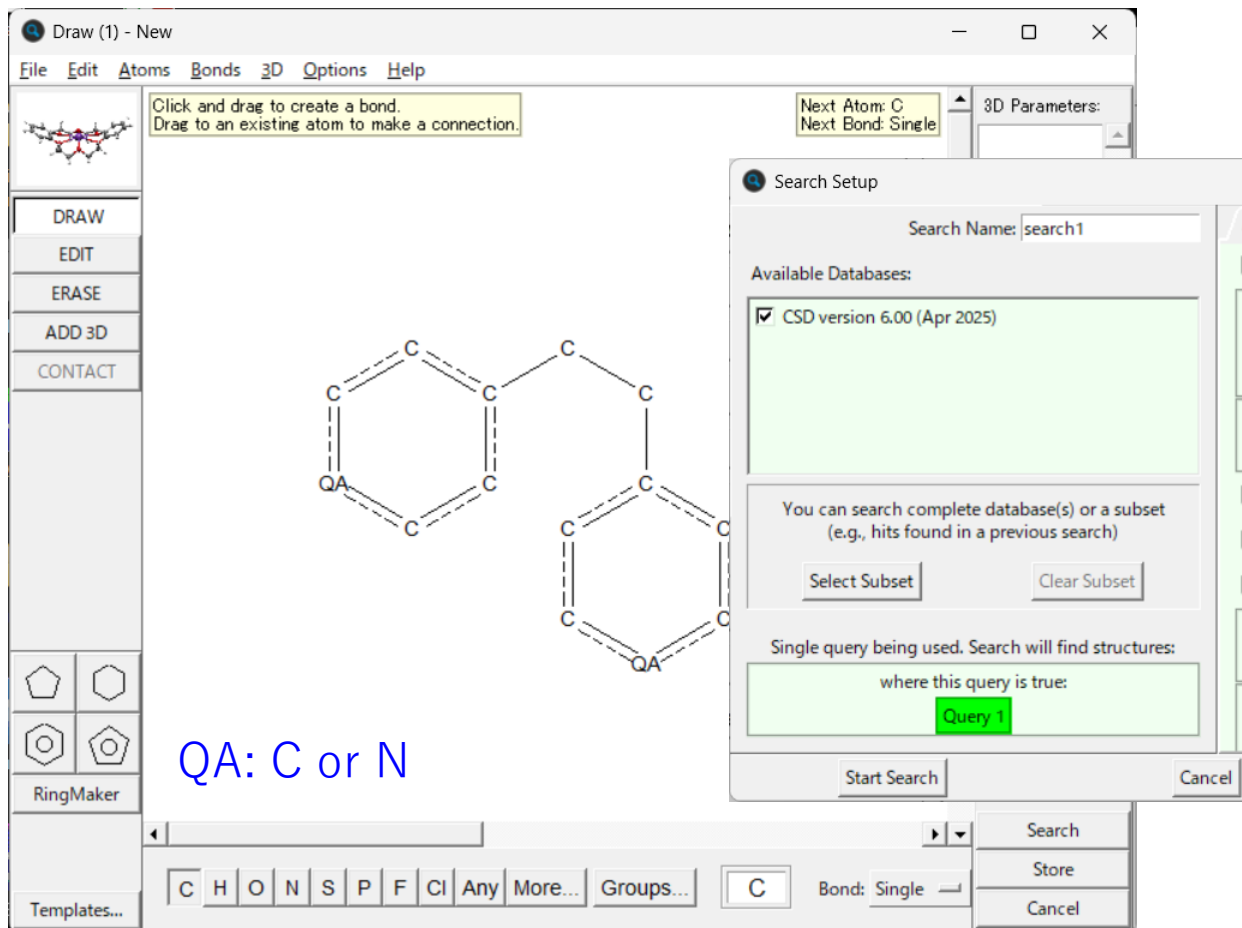
Start Search Cancel Reset

Filters Advanced Options

- ☒ 3D coordinates determined
- ☒ R factor ☐ <= 0.05 ☒ <= 0.075 ☐ <= 0.1
- ☒ Only ☒ Non-disordered ☐ Disordered
- ☒ No errors
- ☐ Not polymeric
- ☐ No ions
- ☒ Only ☒ Single crystal structures ☐ Powder structures
- ☐ Only ☒ Organics ☐ Organometallic

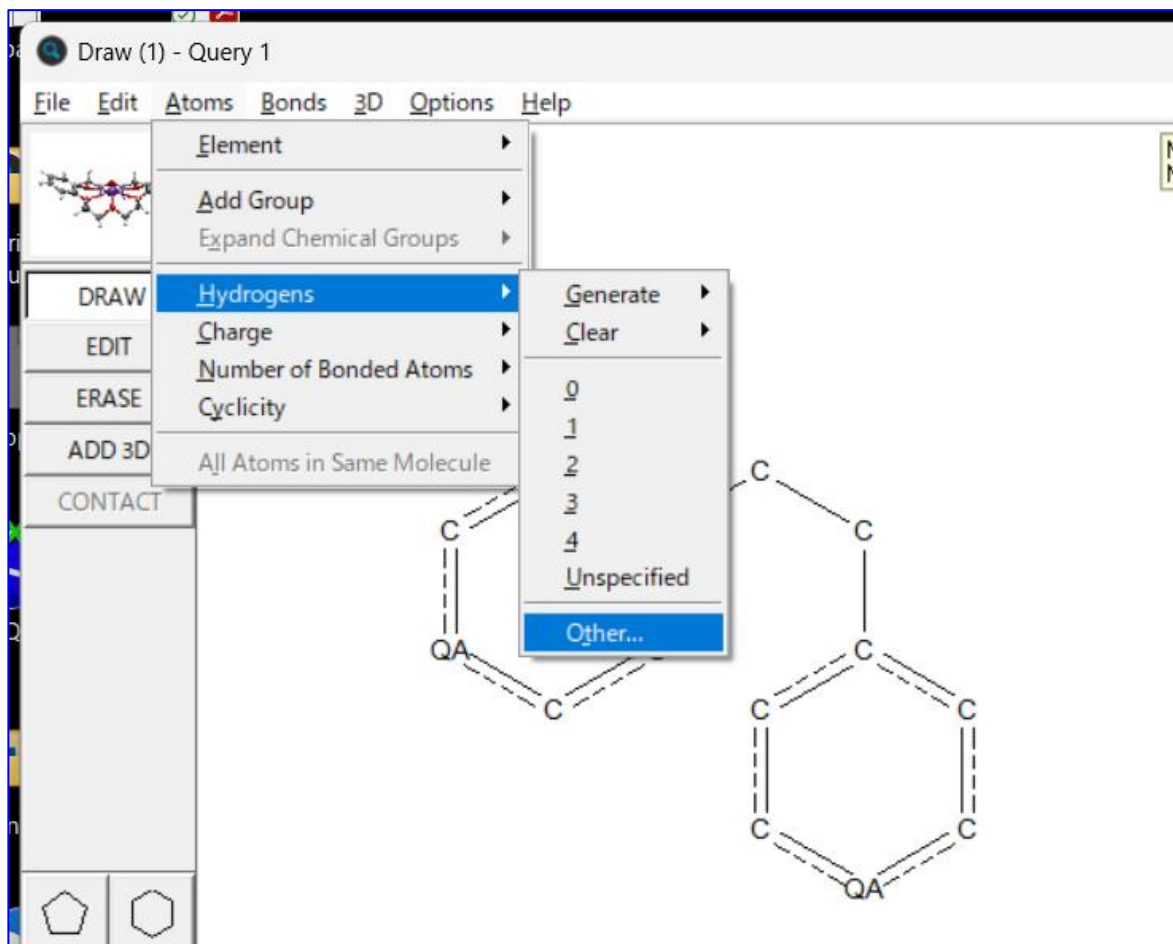
検索結果の絞り込み

Fragmentに様々な条件を追加する

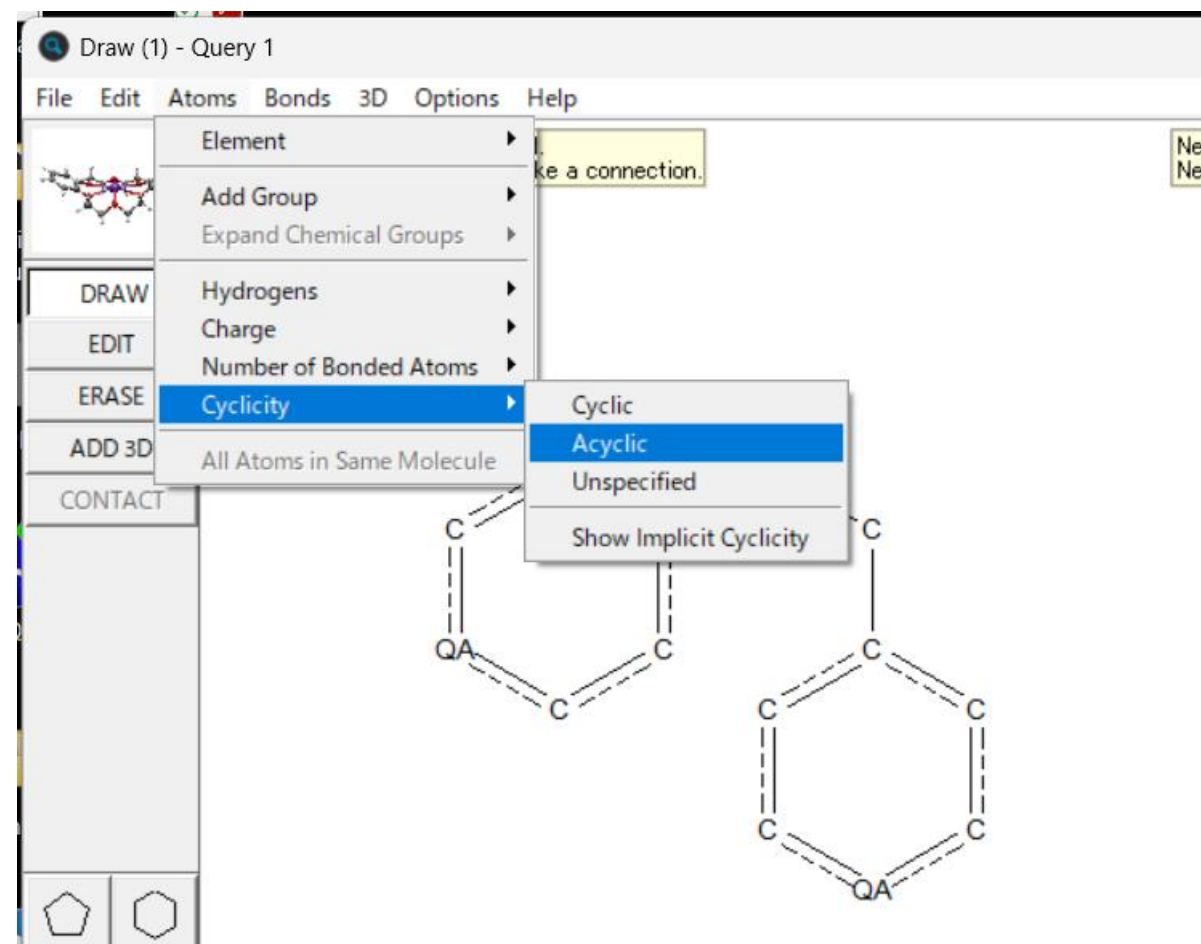


検索結果の絞り込み: 2次元構造の条件を追加

- ✓ 芳香環を繋ぐ炭素には水素が1個もしくは2個結合

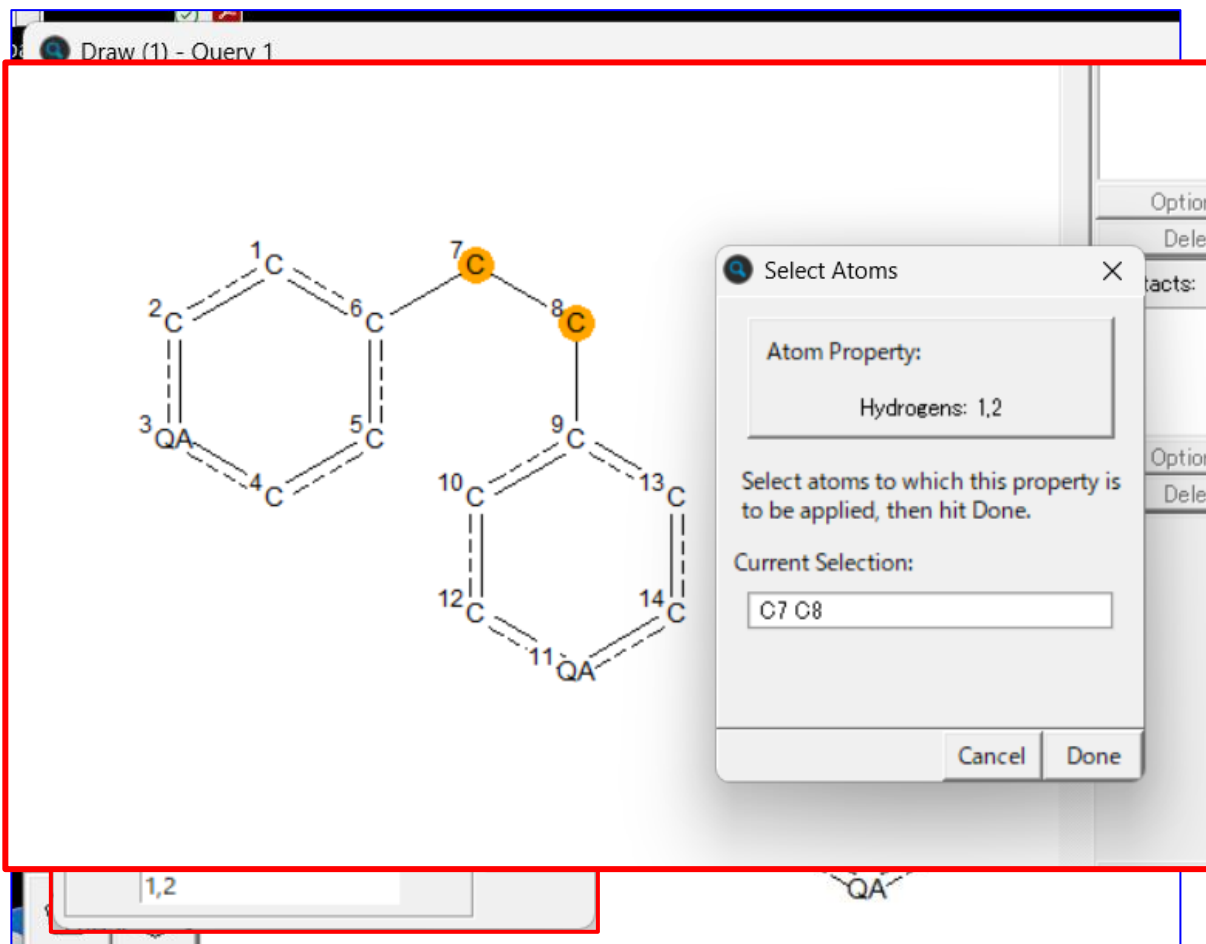


- ✓ 芳香環を繋ぐ炭素は環を構成しない

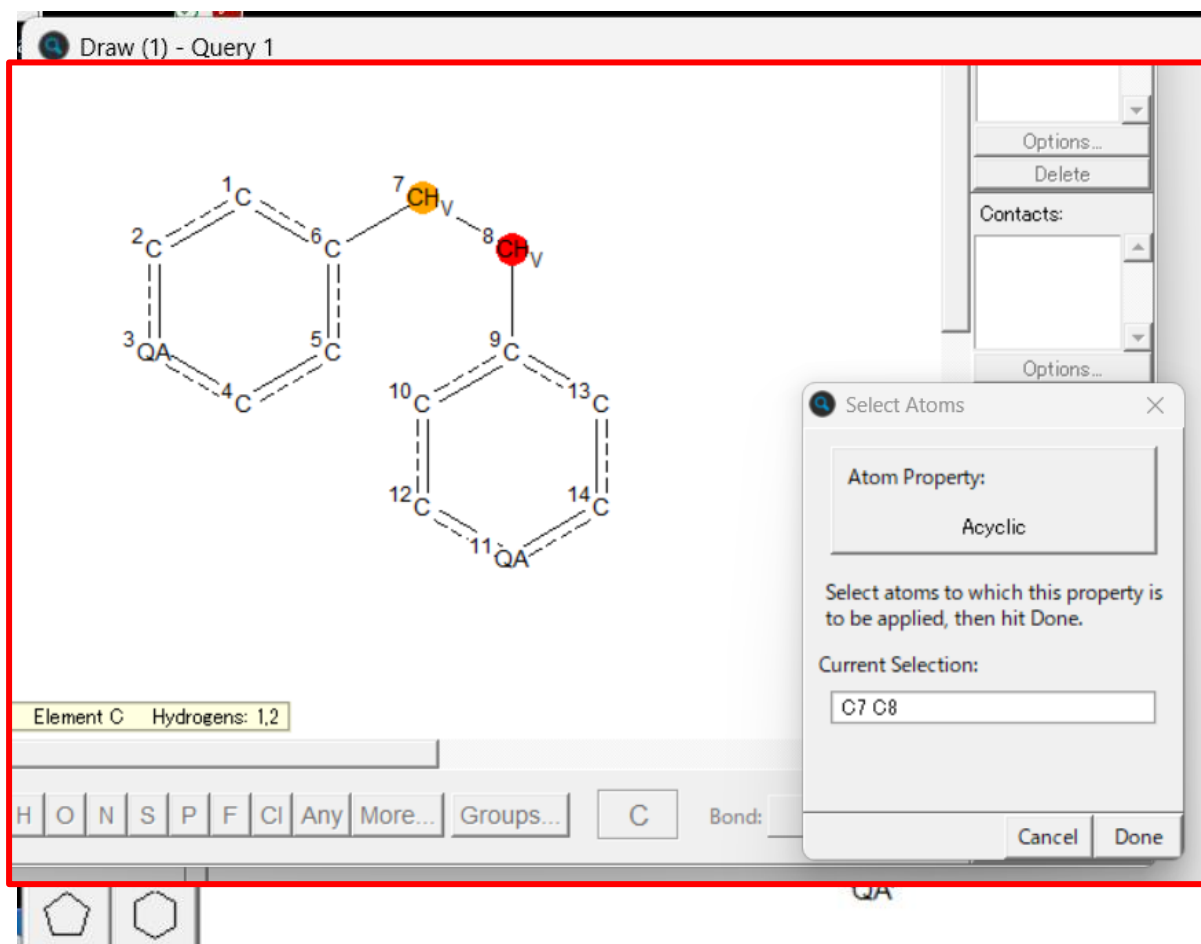


検索結果の絞り込み: 2次元構造の条件を追加

- ✓ 芳香環を繋ぐ炭素には水素が1個もしくは2個結合

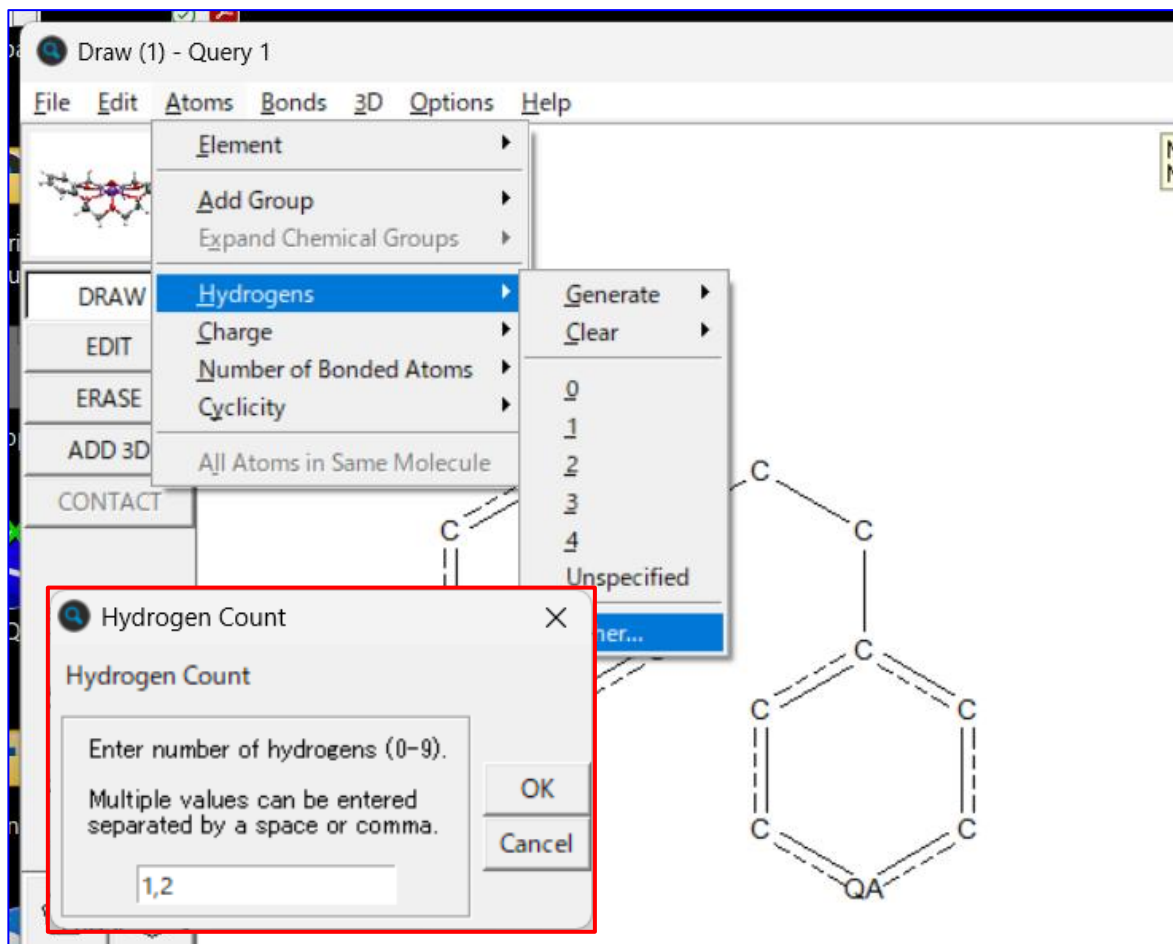


- ✓ 芳香環を繋ぐ炭素は環を構成しない

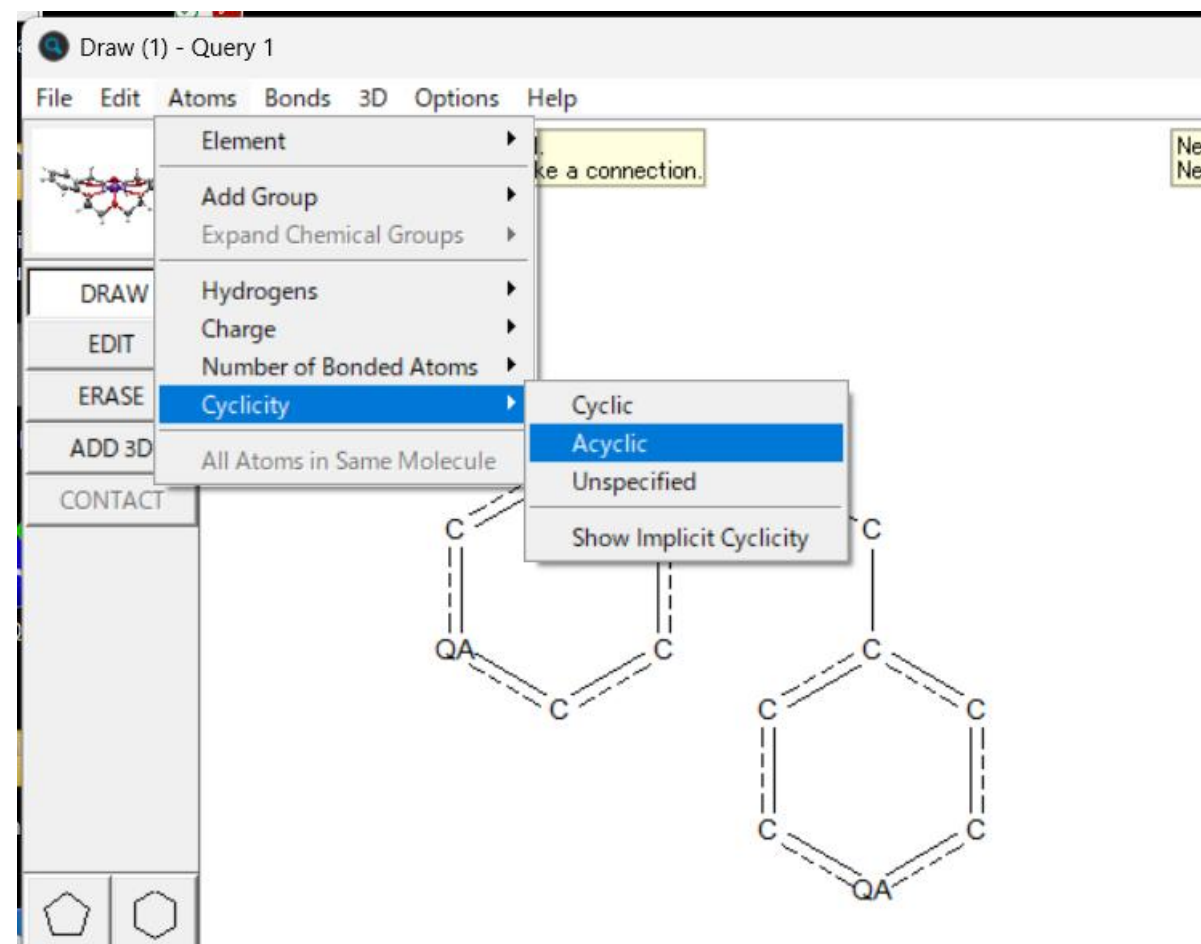


検索結果の絞り込み: 2次元構造の条件を追加

✓ 芳香環を繋ぐ炭素には水素が1個
もしくは2個結合

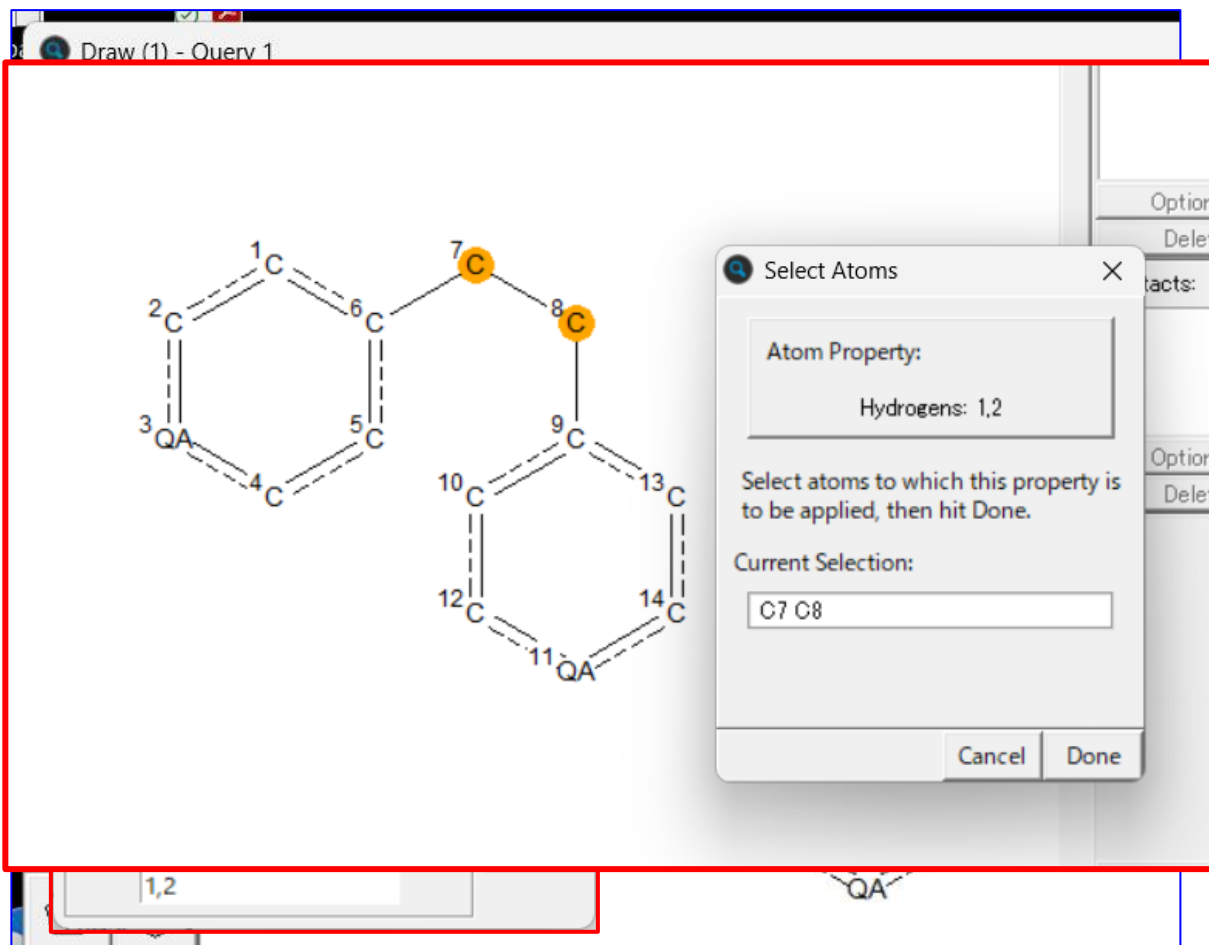


✓ 芳香環を繋ぐ炭素は環を構成しない

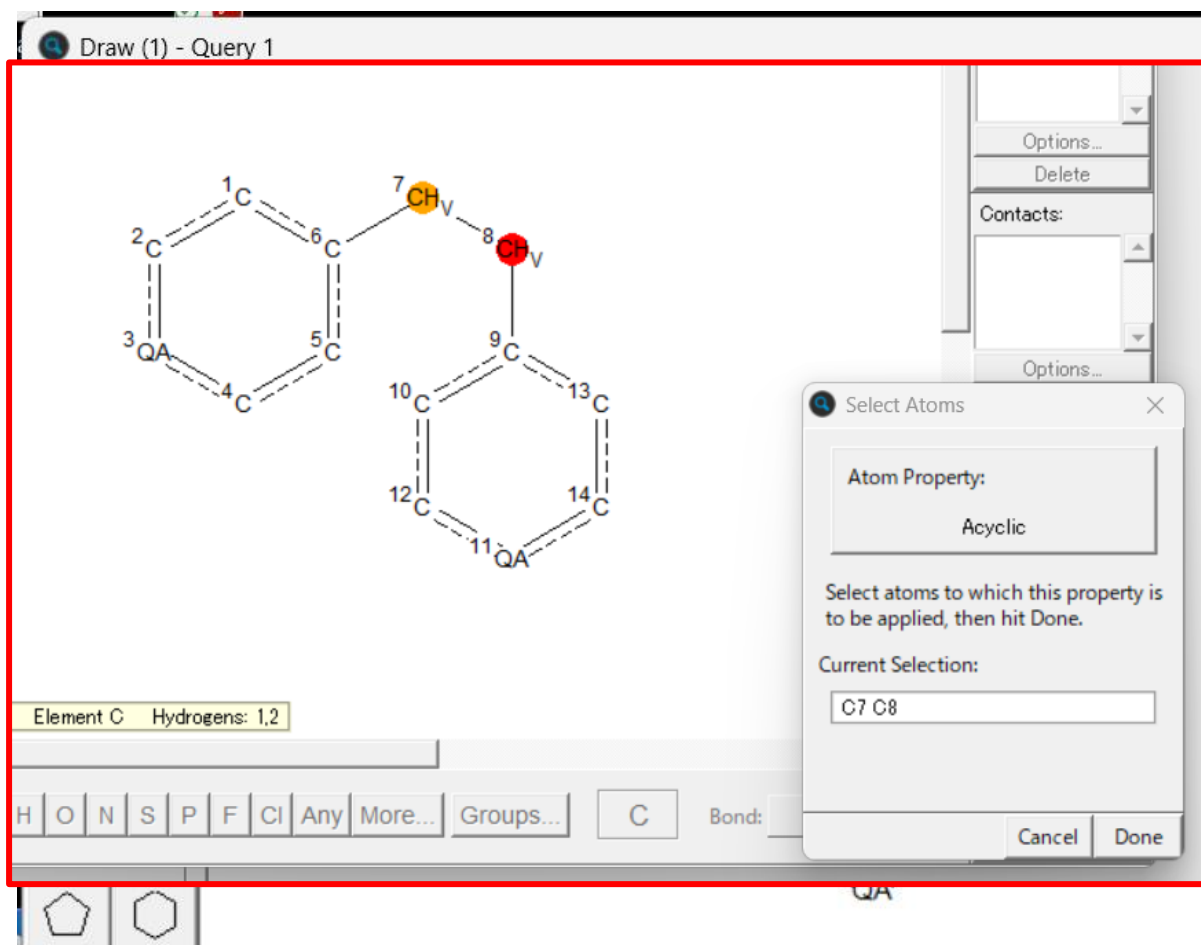


検索結果の絞り込み: 2次元構造の条件を追加

✓ 芳香環を繋ぐ炭素には水素が1個
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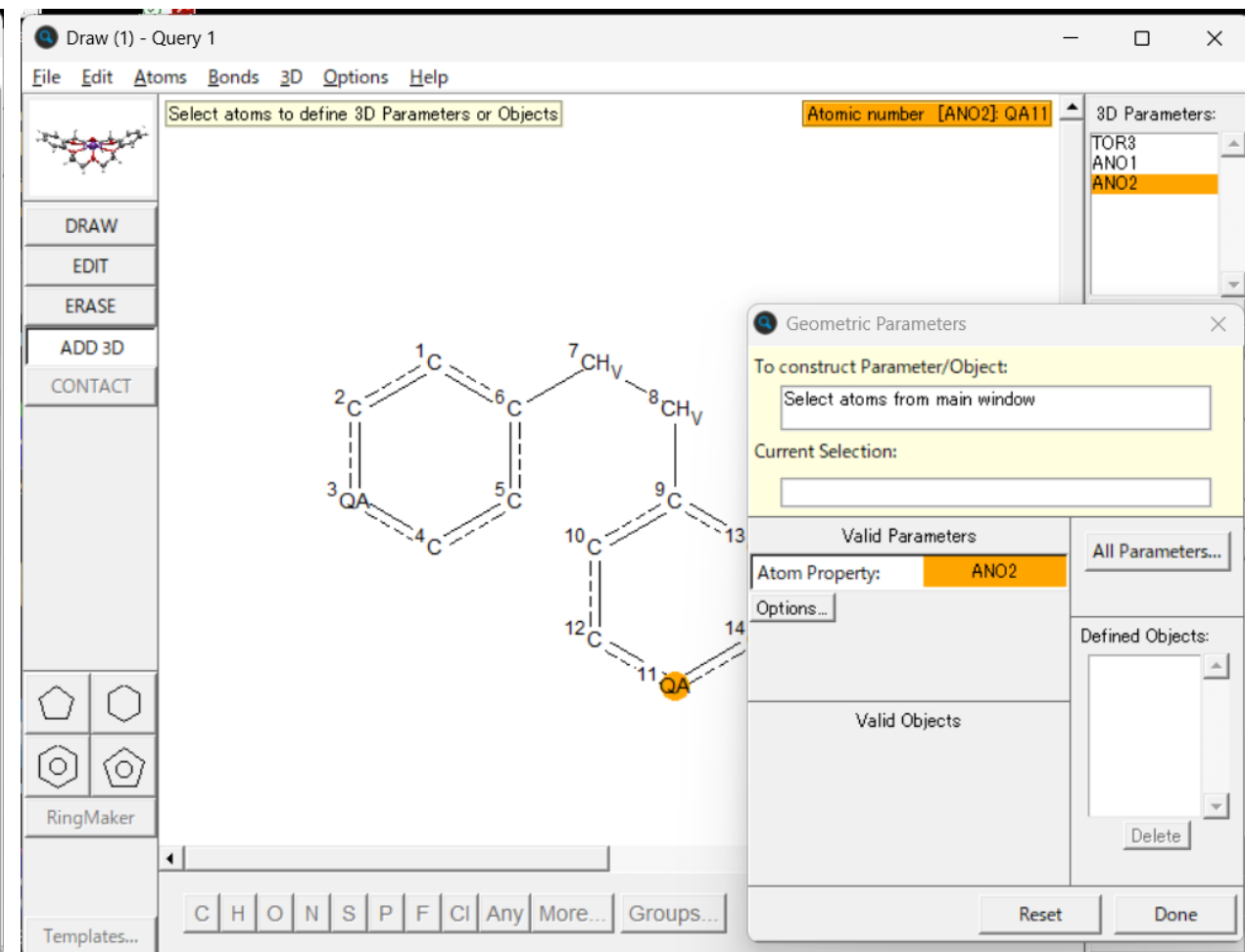
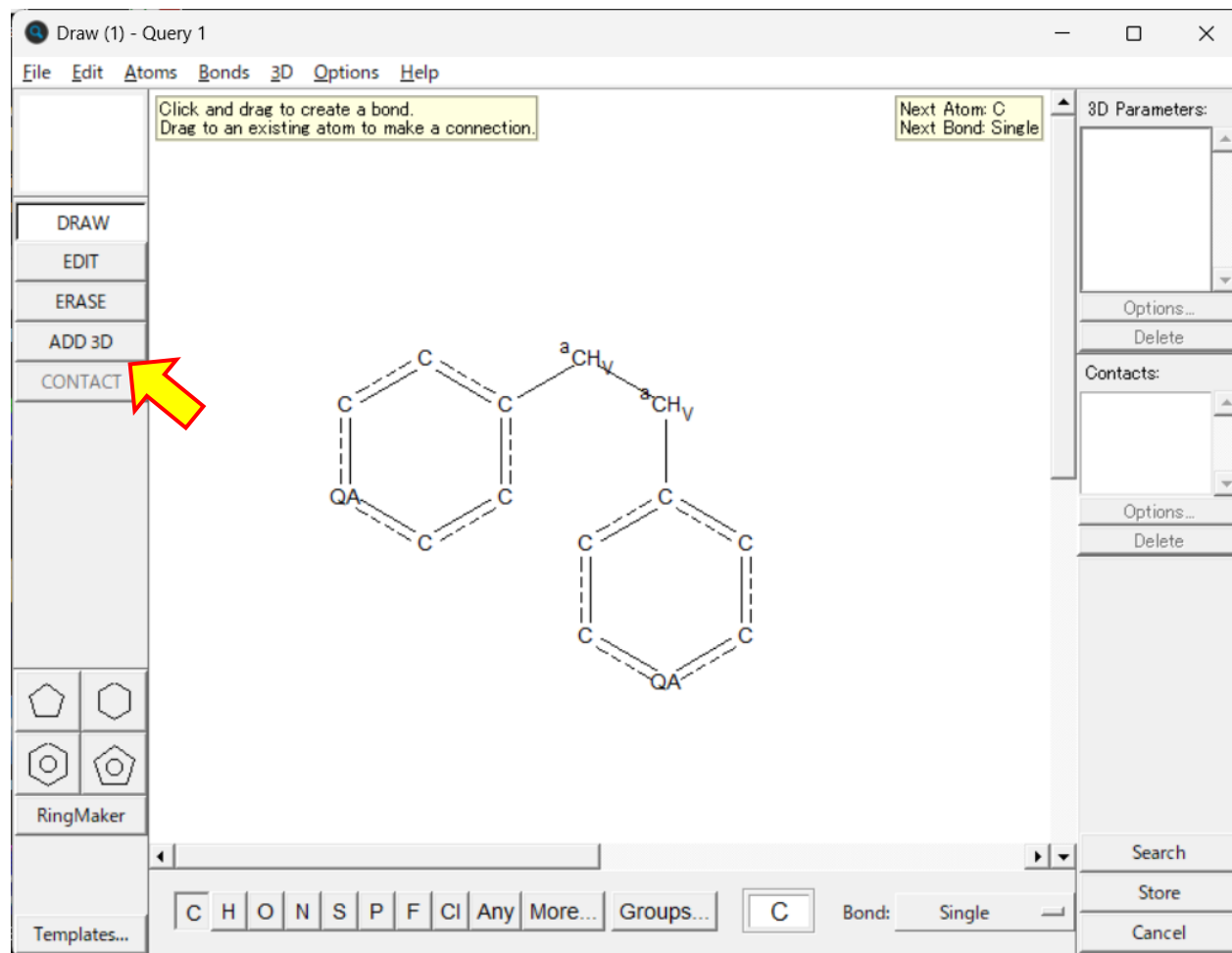
✓ 芳香環を繋ぐ炭素は環を構成しない



検索結果の絞り込み: 3次元構造の条件を追加

✓ 2個の芳香環がcisの相対関係

✓ QAはC?それともN?

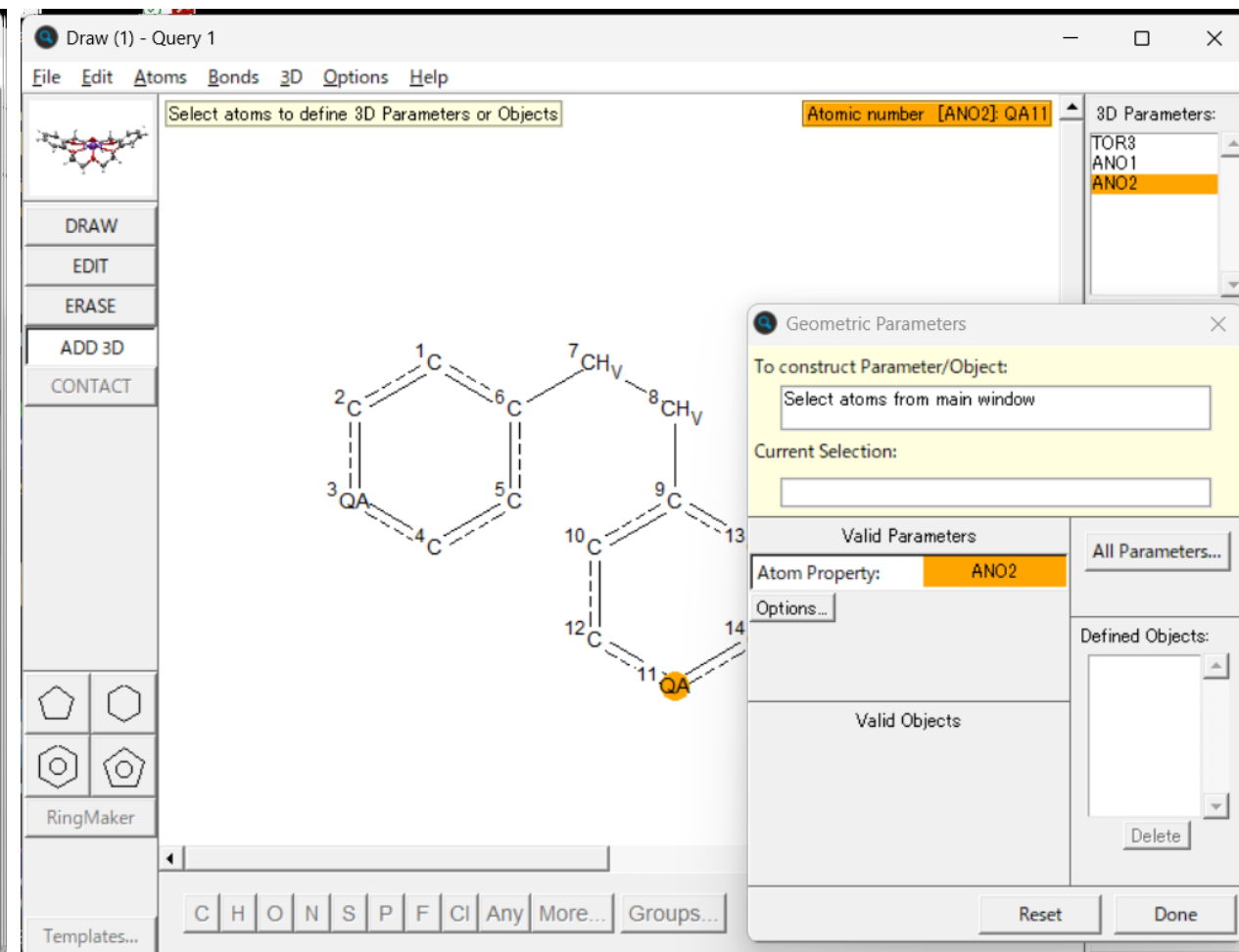
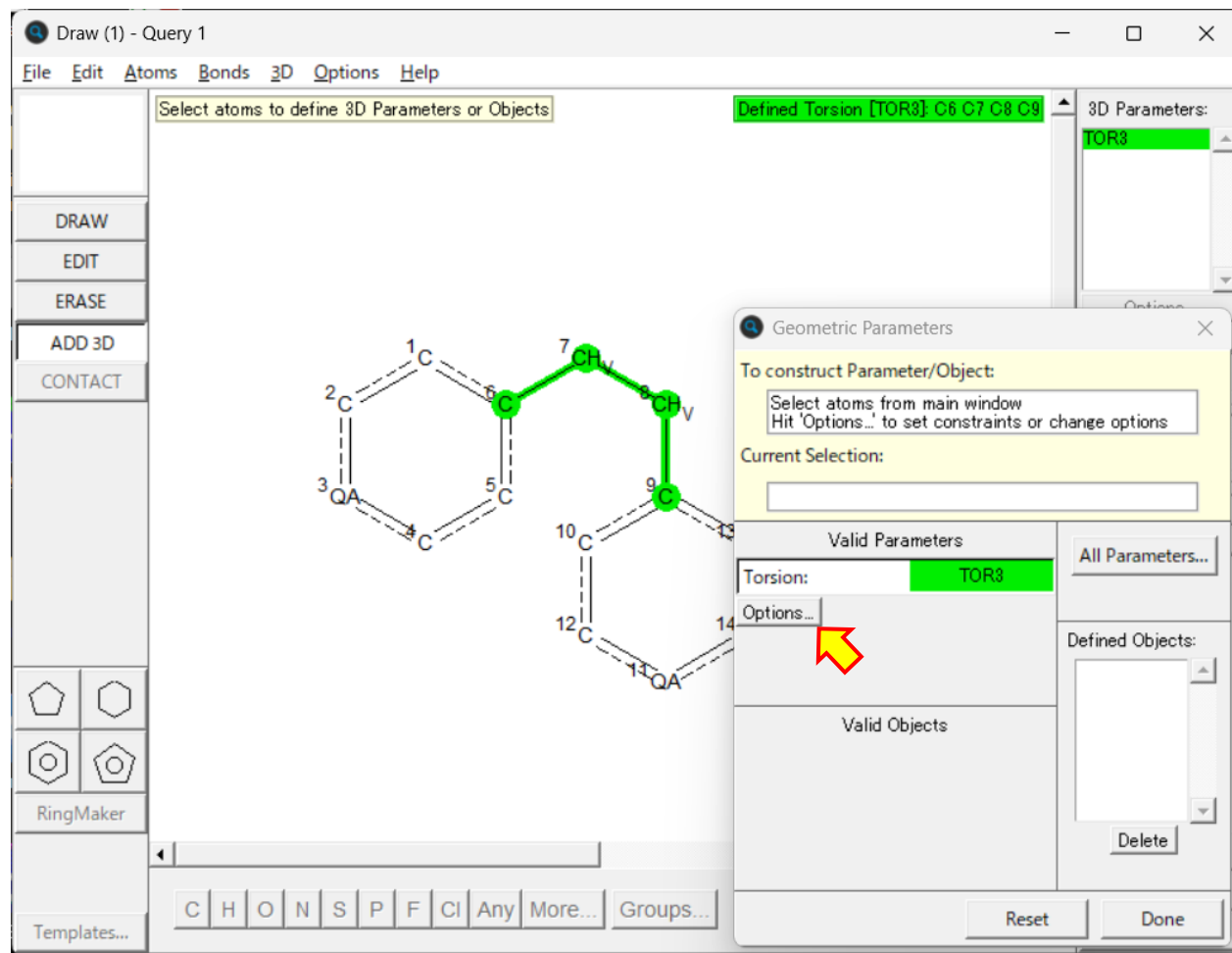


検索時に、“TOR3”, “ANO1”, “ANO2”の値も記録される

検索結果の絞り込み: 3次元構造の条件を追加

✓ 2個の芳香環がcisの相対関係

✓ QAはC?それともN?

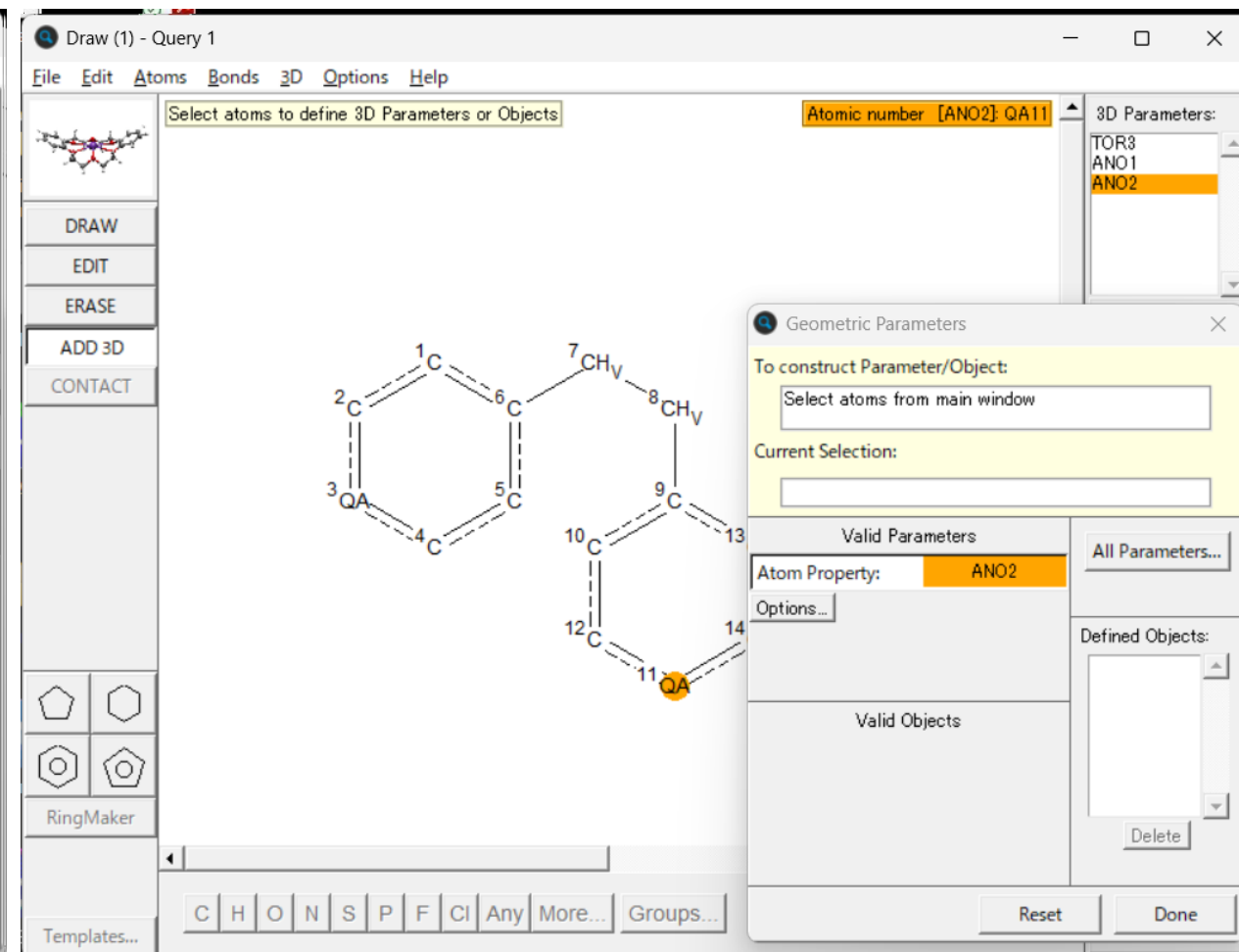
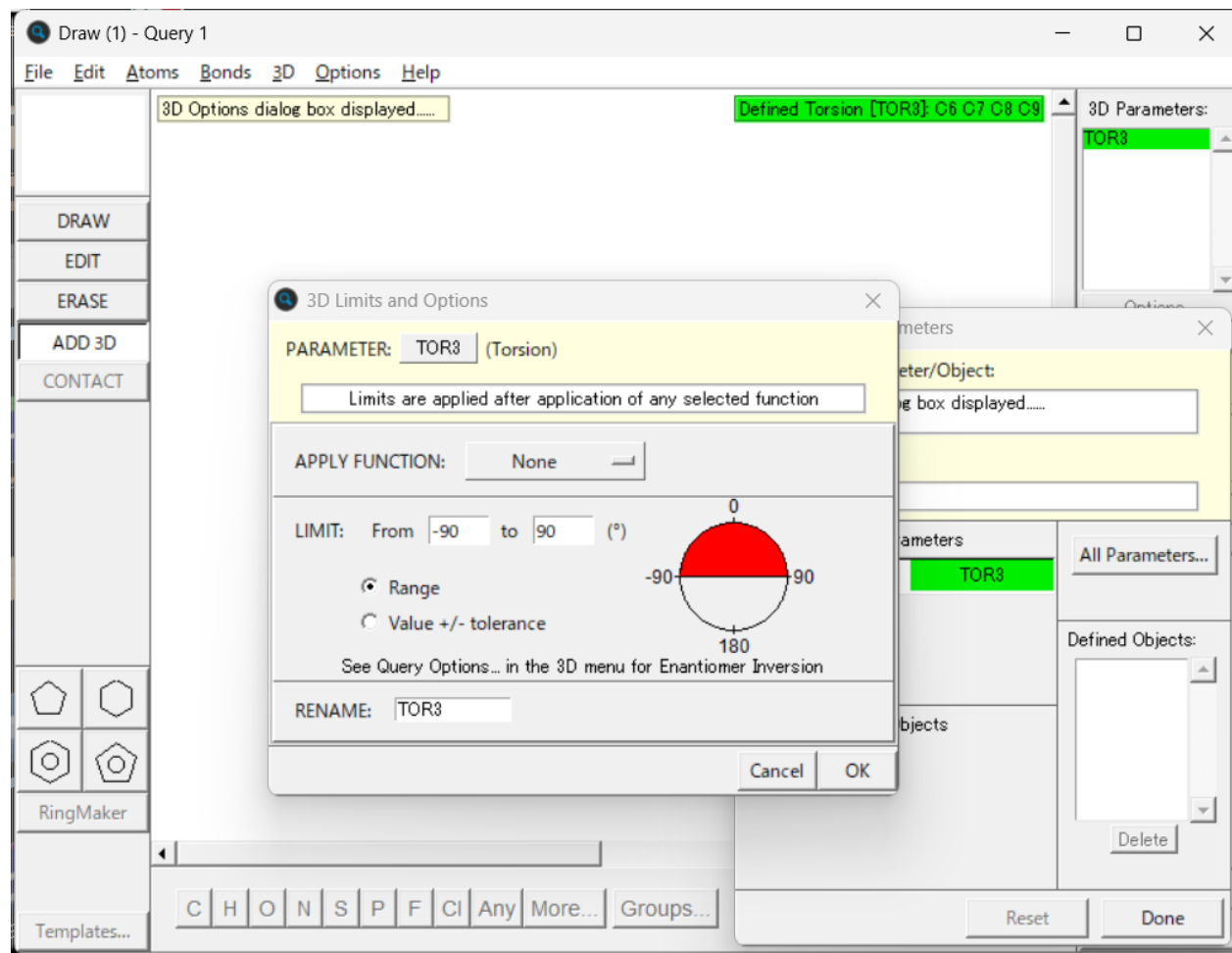


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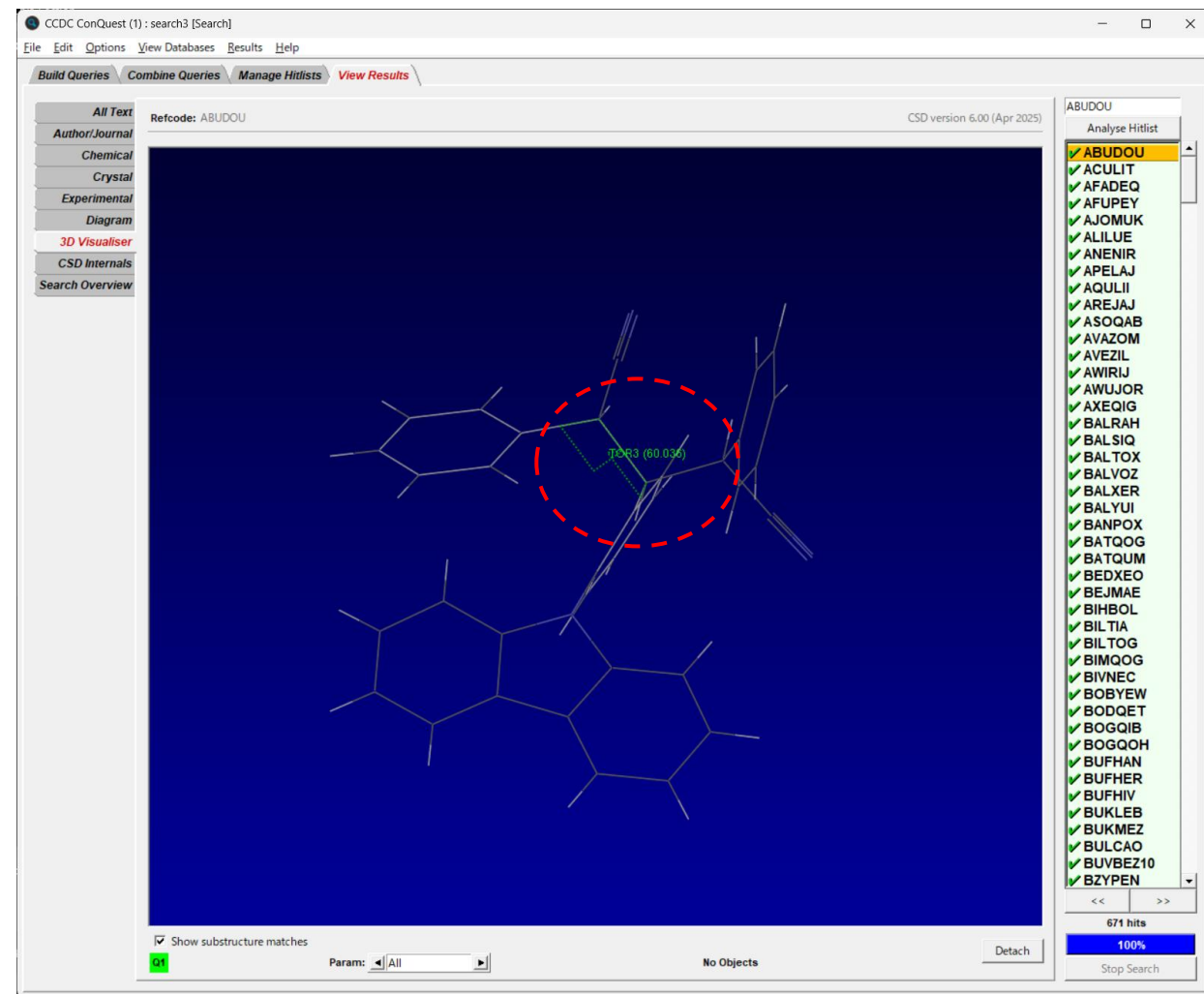
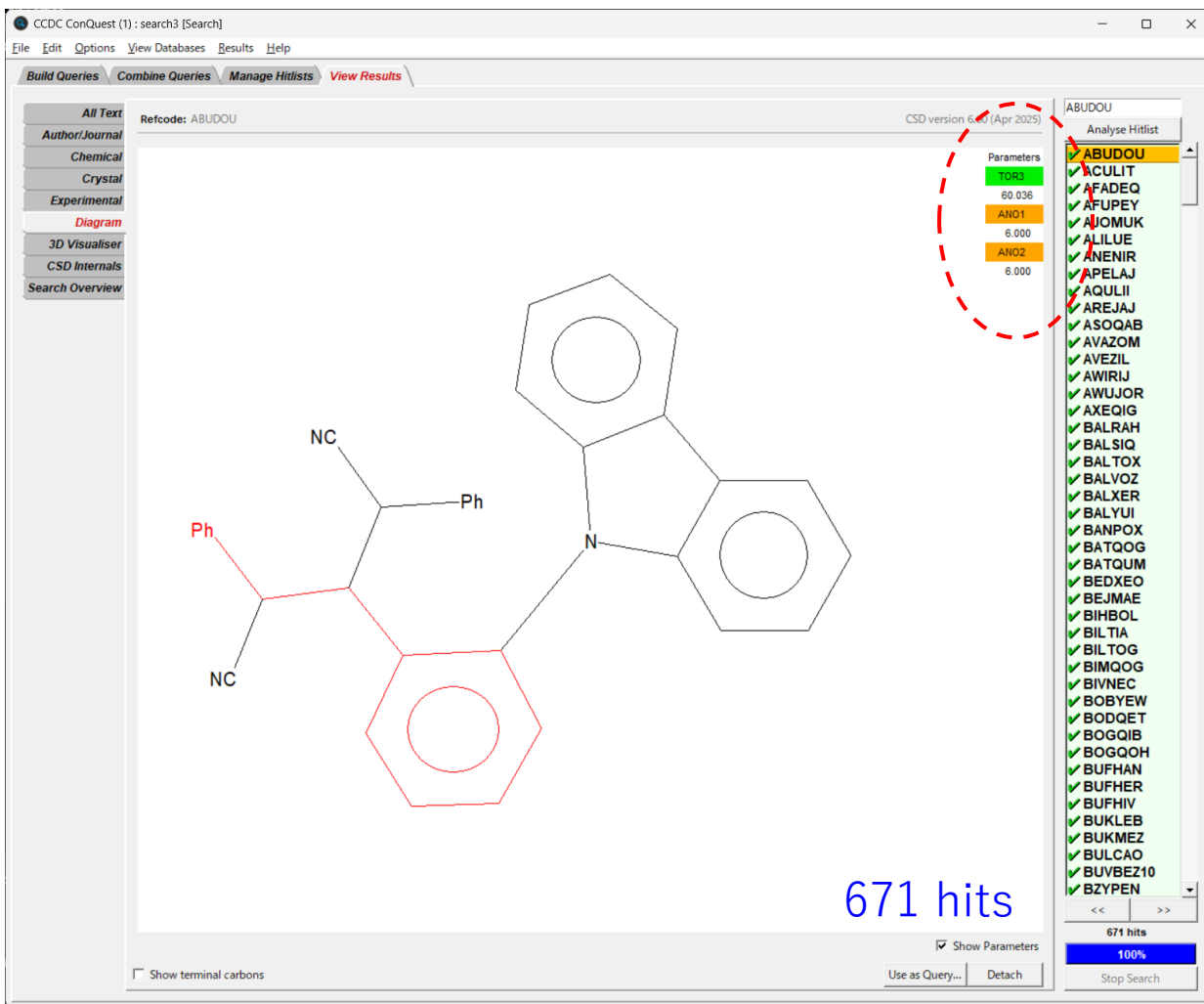
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✓ QAはC?それともN?



検索時に、“TOR3”, “ANO1”, “ANO2”の値も記録される

検索結果



“TOR3”, “ANO1”, “ANO2”の値が表示される

検索結果のMercuryでの表示

Entry

TOR3

ANO1,2

Identifier	NAME	Query	Fragment	TOR3	ano(ANO1)	ano(ANO2)
search3 ABUDOU 0	ABUDOU	1	1	60.0360	6.0000	6.0000
search3 ACULIT 1	ACULIT	1	1	-71.8430	6.0000	6.0000
search3 AFADQ2	AFADQ2	1	1	61.2970	6.0000	6.0000
search3 AFUPEY 3	AFUPEY	1	1	62.3940	6.0000	6.0000
search3 AJOMUK 4	AJOMUK	1	1	-56.5690	6.0000	6.0000
search3 ALILUE 5	ALILUE	1	1	61.7910	7.0000	7.0000
search3 ANENIR 6	ANENIR	1	1	-63.5410	6.0000	6.0000
search3 ANENIR 7	ANENIR	1	2	54.8450	6.0000	6.0000
search3 APELAJ 8	APELAJ	1	1	-66.7510	6.0000	6.0000
search3 AQULIJ 9	AQULIJ	1	1	55.0050	6.0000	6.0000
search3 AREJAJ 10	AREJAJ	1	1	50.8770	6.0000	6.0000
search3 ASOQAB 11	ASOQAB	1	1	-48.3840	6.0000	6.0000
search3 AVAZOM 12	AVAZOM	1	1	-85.6170	6.0000	6.0000
search3 AVEZIL 13	AVEZIL	1	1	-60.5830	6.0000	6.0000
search3 AWIRIJ 14	AWIRIJ	1	1	-55.3070	6.0000	6.0000
search3 AWIRIJ 15	AWIRIJ	1	2	54.0660	6.0000	6.0000
search3 AWUJOR 16	AWUJOR	1	1	-66.0520	6.0000	6.0000
search3 AWUJOR 17	AWUJOR	1	2	74.4550	6.0000	6.0000
search3 AXEQIG 18	AXEQIG	1	1	73.2200	7.0000	6.0000
search3 BALRAH 19	BALRAH	1	1	-55.2940	6.0000	6.0000
search3 BALSIQ 20	BALSIQ	1	1	-56.7680	6.0000	6.0000
search3 BALTOX 21	BALTOX	1	1	-55.3940	6.0000	6.0000
search3 BALTOX 22	BALTOX	1	2	-57.3480	6.0000	6.0000
search3 BALVOZ 23	BALVOZ	1	1	-67.1090	6.0000	6.0000
search3 BALXER 24	BALXER	1	1	-49.5200	6.0000	6.0000
search3 BALYUI 25	BALYUI	1	1	-57.3050	6.0000	6.0000
search3 BANPOX 26	BANPOX	1	1	48.0480	6.0000	6.0000
search3 BATQOG 27	BATQOG	1	1	-55.1460	6.0000	6.0000
search3 BATQUM 28	BATQUM	1	1	-66.2840	6.0000	6.0000
search3 BEDXEO 29	BEDXEO	1	1	-44.2750	6.0000	6.0000
search3 BEDXEO 30	BEDXEO	1	2	52.9310	6.0000	6.0000
search3 BEJMAE 31	BEJMAE	1	1	69.4070	6.0000	6.0000
search3 BIHBOL 32	BIHBOL	1	1	59.1980	6.0000	6.0000
search3 BILTIA 33	BILTIA	1	1	-65.5890	6.0000	6.0000
search3 BILTQ34	BILTQ34	1	1	76.7080	6.0000	6.0000
search3 BIMQOG 35	BIMQOG	1	1	-58.4970	6.0000	6.0000
search3 BIVNEC 36	BIVNEC	1	1	53.9060	6.0000	6.0000
search3 BOBYEW 37	BOBYEW	1	1	-70.5350	6.0000	6.0000
search3 BODQET 38	BODQET	1	1	-66.2600	6.0000	6.0000
search3 BOGQIB 39	BOGQIB	1	1	-42.9900	6.0000	6.0000
search3 BOGQOH 40	BOGQOH	1	1	-70.0000	6.0000	6.0000
search3 BUFHAN 41	BUFHAN	1	1	-60.0240	6.0000	6.0000
search3 BUFHER 42	BUFHER	1	1	-60.9540	6.0000	6.0000
search3 BUFHIV 43	BUFHIV	1	1	61.0880	6.0000	6.0000
search3 BUKLEB 44	BUKLEB	1	1	-48.3490	6.0000	6.0000
search3 BUKMEZ 45	BUKMEZ	1	1	72.5810	6.0000	6.0000
search3 BULCAO 46	BULCAO	1	1	59.3110	6.0000	6.0000
search3 BUVBEZ10 47	BUVBEZ10	1	1	61.6400	6.0000	6.0000
search3 BZYPEN 48	BZYPEN	1	1	-55.1620	6.0000	6.0000
search3 CAMKOT 49	CAMKOT	1	1	71.1380	6.0000	6.0000

Hit Fragment Display Options

Fragment Selection

Fragment Highlighting

☒ Tree view

☐ Load multiple structures

Select all

☐ Show only hit atoms

Structure	Value
AWIRIJ	
Query 1	
Fragment...	
...	-55.307
...	6.0
...	6.0
Fragment...	
...	54.066
...	6.0
...	6.0

☒ Show parameters: All

Data Analysis... Close

AWIRIJ (P-1) - Mercury

File Edit Selection Display Calculate CSD-Community CSD-Core CSD-Materials CSD-Theory CSD-Particle CSD-Discovery CSD Python API Help

Picking Mode: Pick Atoms Clear Measurements Show Labels for All atoms with Atom Label

Style: Ellipsoid Colour: by Element Manage Styles... Publication Atom lists: Select by SMARTS: [c]

Animate... Default view: b a b c a* b* c* x- x+ y- y+ z- z+ x-90 x+90 y-90 y+90 z-90 z+90 zoom- zoom+ Disorder: None

Structure Navigator

Crystal Structures	Spacegroup
AWIRIJ	P-1
AWUJOR	P2/c
AWUJOR	P2/c
AXEQIG	P21
BALRAH	P212121
BALSIQ	P21
BALTOX	P21
BALTOX	P21
BALVOZ	P212121
BALXER	P212121
BALYUI	P212121
BANPOX	P21/n
BATQOG	P21
BATQUM	P212121
BEDXEO	P-1
BEDXEO	P-1
BEJMAE	Pbca
BIHBOL	P212121
BILTIA	P212121
BILTQ	P212121

Tree View

☐ Multiple Structures Structures...

Searches

0 hits # motifs % frequency

View Options

View results: by motif

☐ List all matches ☐ Multi-view mode ☐ Show negative results

Display Options

Display

☐ Packing ☐ Short Contact < (sum of vdW radii) ☐ Asymmetric Unit ☐ H-Bond Default definition ☐ Auto centre

Reset

Options

☒ Show hydrogens ☐ Depth cue ☐ Show cell axes ☐ Z-Clipping ☐ Label atoms ☐ Stereo

Contacts... More Info Powder...

Press the left mouse button and move the mouse to rotate the structure

BUVBEZ10

BZYPEN

671 hits

Data Analysis window

Data Analysis

File Options

search3 Spreadsheet 1

File Tools Descriptors Display Selection Plots Statistics

Find identifier Find next

Identifier	NAME	Query	Fragment	TOR3	ano(ANO1)	ano(ANO2)
search3 ALILUE 5	ALILUE	1	1	61.7910	7.0000	
search3 BULCAO 46	BULCAO	1	1	59.3110	7.0000	
search3 CAMKOT 49	CAMKOT	1	1	71.1280	7.0000	
search3 CEHNEI 55	CEHNEI	1	1	-55.8560	7.0000	
search3 CODGIO 68	CODGIO	1	1	53.6640	7.0000	
search3 DEBJIE 83	DEBJIE	1	1	-54.8820	7.0000	
search3 DEJYID 89	DEJYID	1	1	-65.6940	7.0000	
search3 DUQHEF 106	DUQHEF	1	1	-72.4370	7.0000	7.0000
search3 EDUPAW 115	EDUPAW	1	1	62.1960	7.0000	7.0000
search3 EMURUA 128	EMURUA	1	1	-52.3440	7.0000	7.0000
search3 EQERUP 129	EQERUP	1	1	-49.9200	7.0000	7.0000
search3 EWOTAM 134	EWOTAM	1	1	-64.5020	7.0000	7.0000
search3 EWOTAM 135	EWOTAM	1	2	-61.3400	7.0000	7.0000
search3 GEYXOA 175	GEYXOA	1	1	-72.7920	7.0000	7.0000
search3 GOGFOA 183	GOGFOA	1	1	55.8680	7.0000	7.0000
search3 GOGFOA01 184	GOGFOA...	1	1	-56.6290	7.0000	7.0000
search3 HEQREB 193	HEQREB	1	1	-70.7530	7.0000	7.0000
search3 HEQREB 194	HEQREB	1	2	62.8130	7.0000	7.0000
search3 HIBSOD 197	HIBSOD	1	1	-63.1350	7.0000	7.0000
search3 HIBSOD 198	HIBSOD	1	2	-68.1180	7.0000	7.0000
search3 HOZTIA 203	HOZTIA	1	1	69.2460	7.0000	7.0000
search3 HOZTIA 204	HOZTIA	1	2	-49.6590	7.0000	7.0000
search3 ILOVOV 221	ILOVOV	1	1	-47.9630	7.0000	7.0000
search3 ILOVUB 222	ILOVUB	1	1	46.5910	7.0000	7.0000
search3 ISICOD 223	ISICOD	1	1	-54.3250	7.0000	7.0000
search3 ISIKIE 224	ISIKIE	1	1	53.1000	7.0000	7.0000
search3 ISIKOK 225	ISIKOK	1	1	53.1950	7.0000	7.0000
search3 ISIKUQ 226	ISIKUQ	1	1	51.7880	7.0000	7.0000
search3 ISIIYT 227	ISIIYT	1	1	62.4960	7.0000	7.0000
search3 JITHUQ 251	JITHUQ	1	1	-62.2500	7.0000	7.0000
search3 JITJAY 252	JITJAY	1	1	64.2700	7.0000	7.0000
search3 JITJIG 253	JITJIG	1	1	63.1770	7.0000	7.0000
search3 KAVDUH 273	KAVDUH	1	1	-67.5430	7.0000	7.0000

Sort

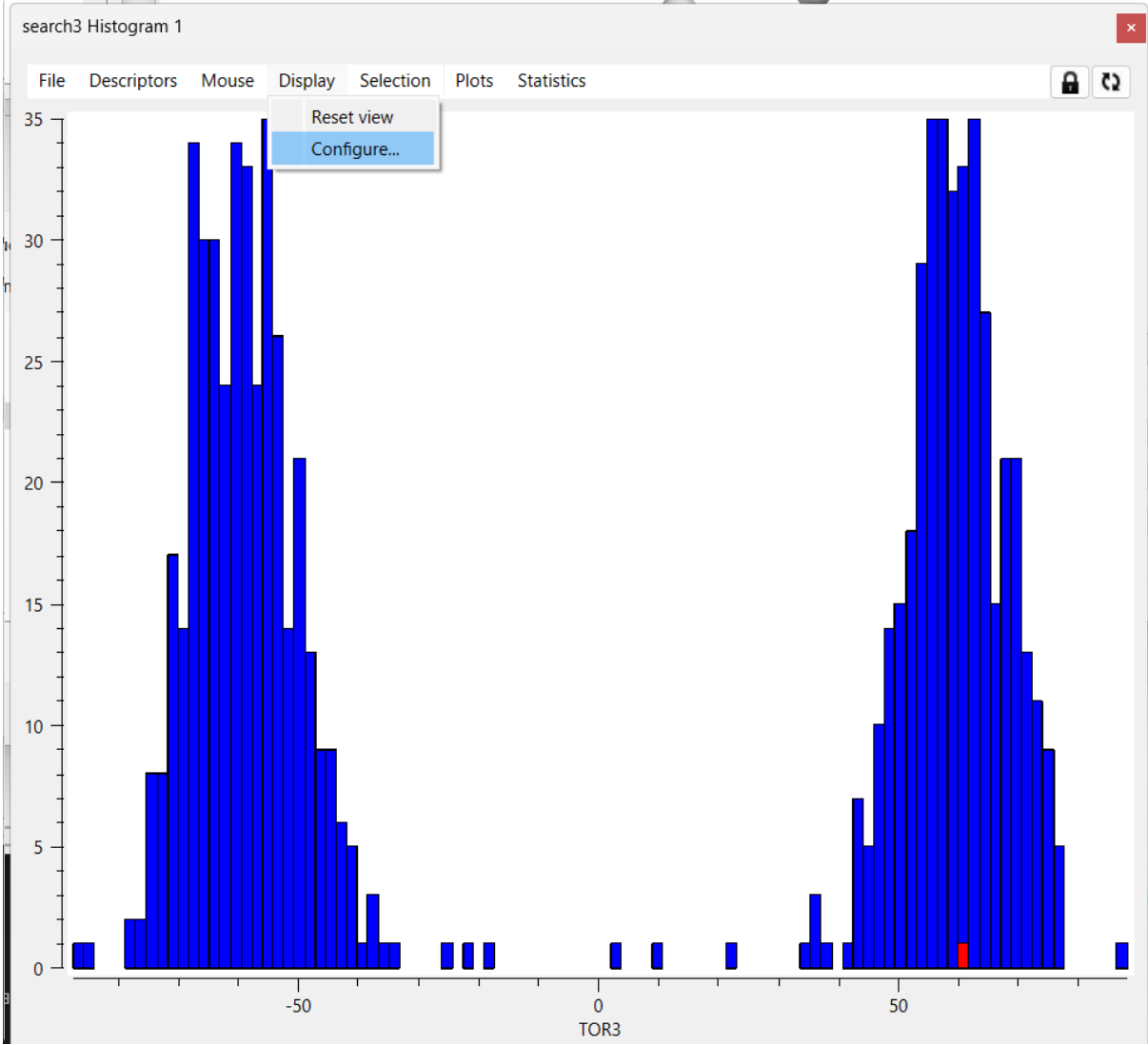
Filter

Hide

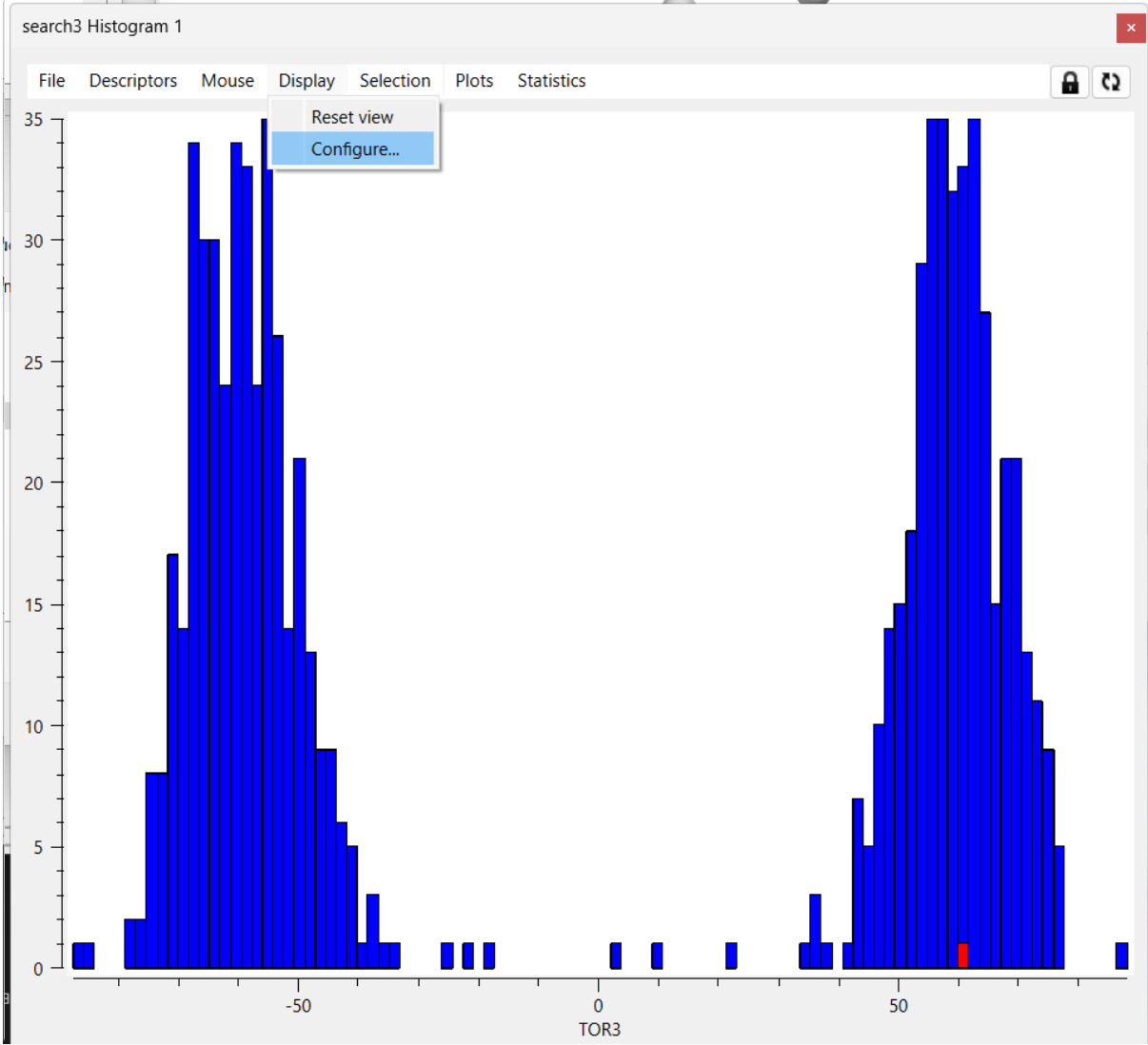
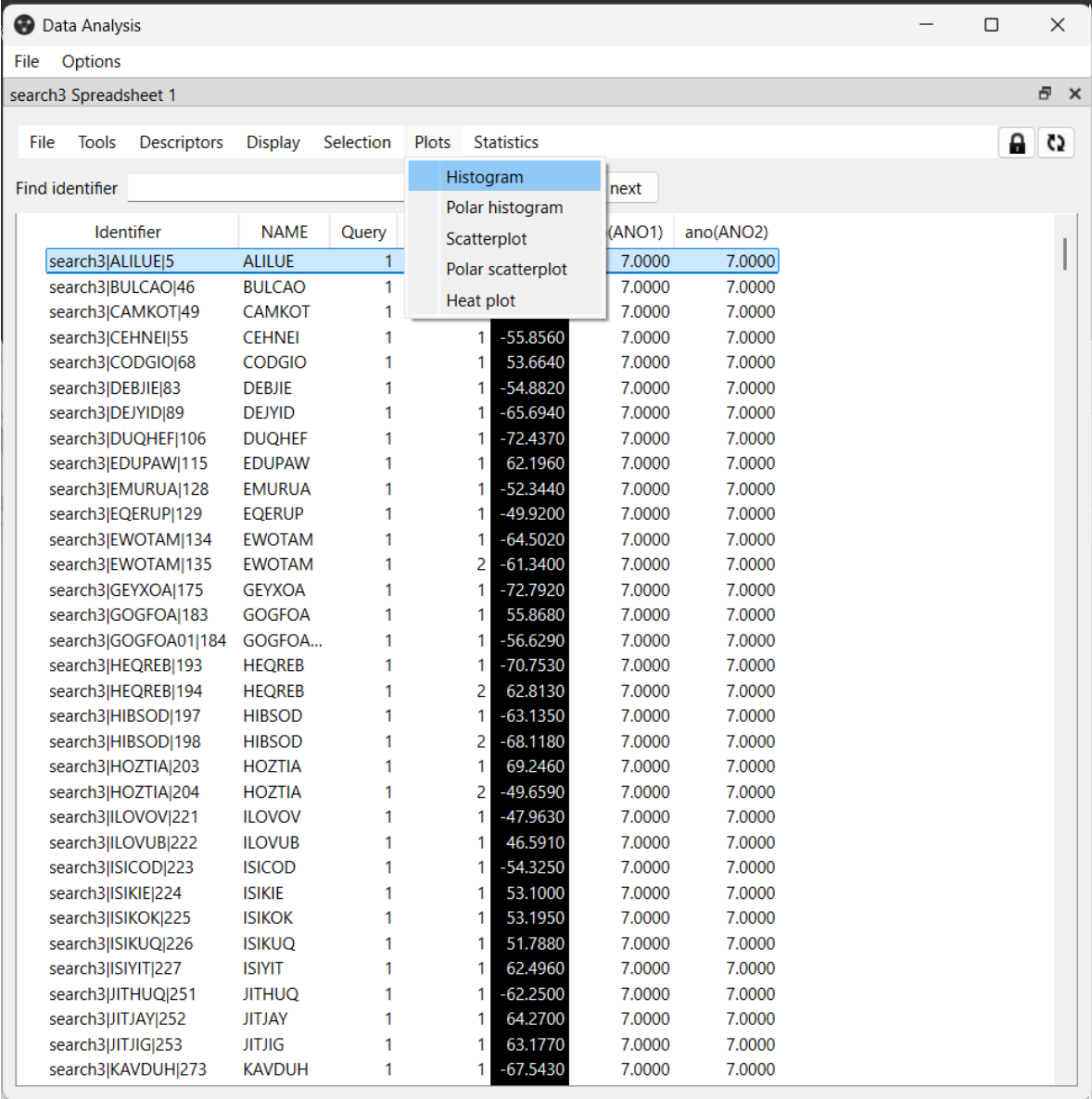
Colour

Categorise

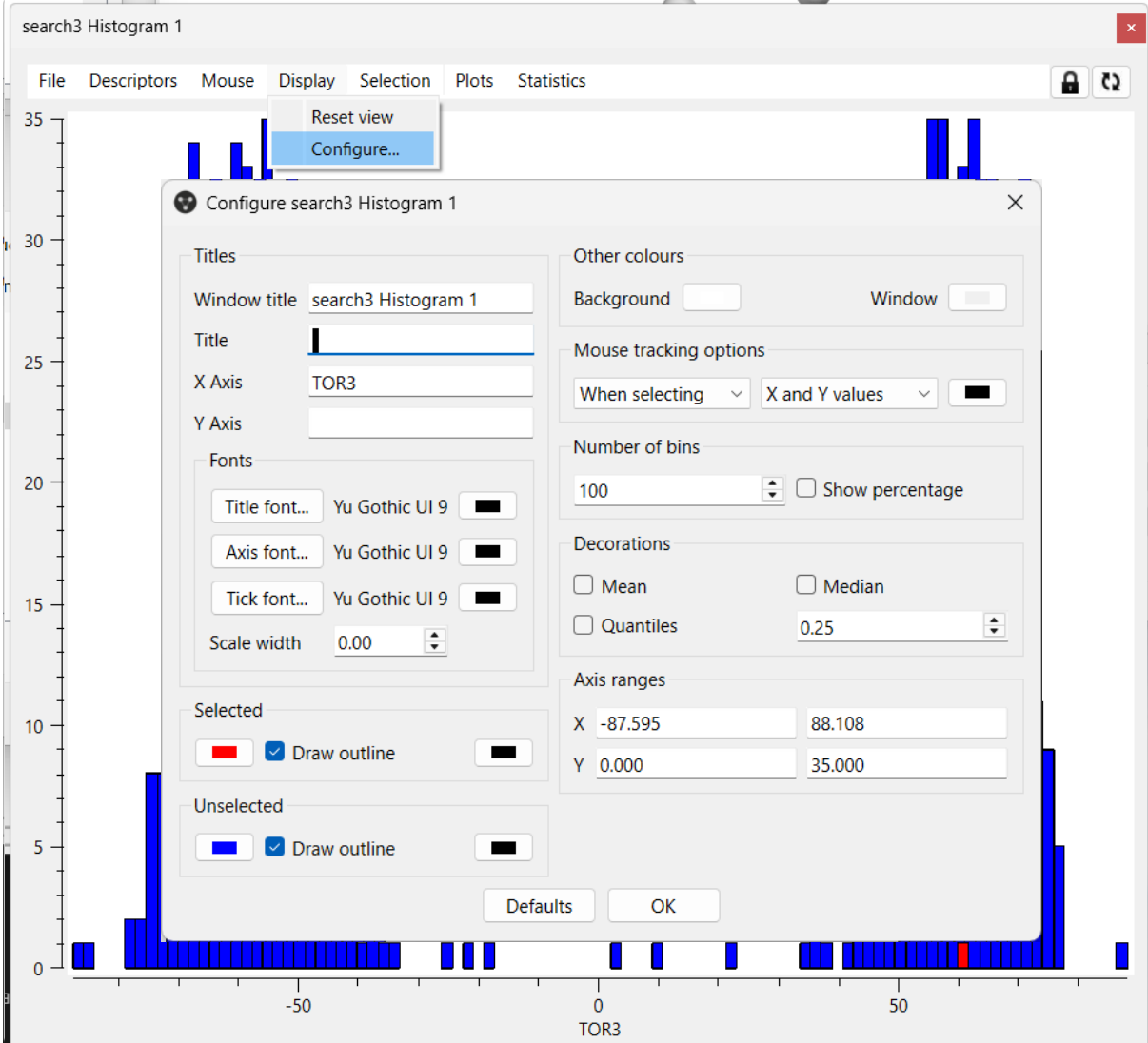
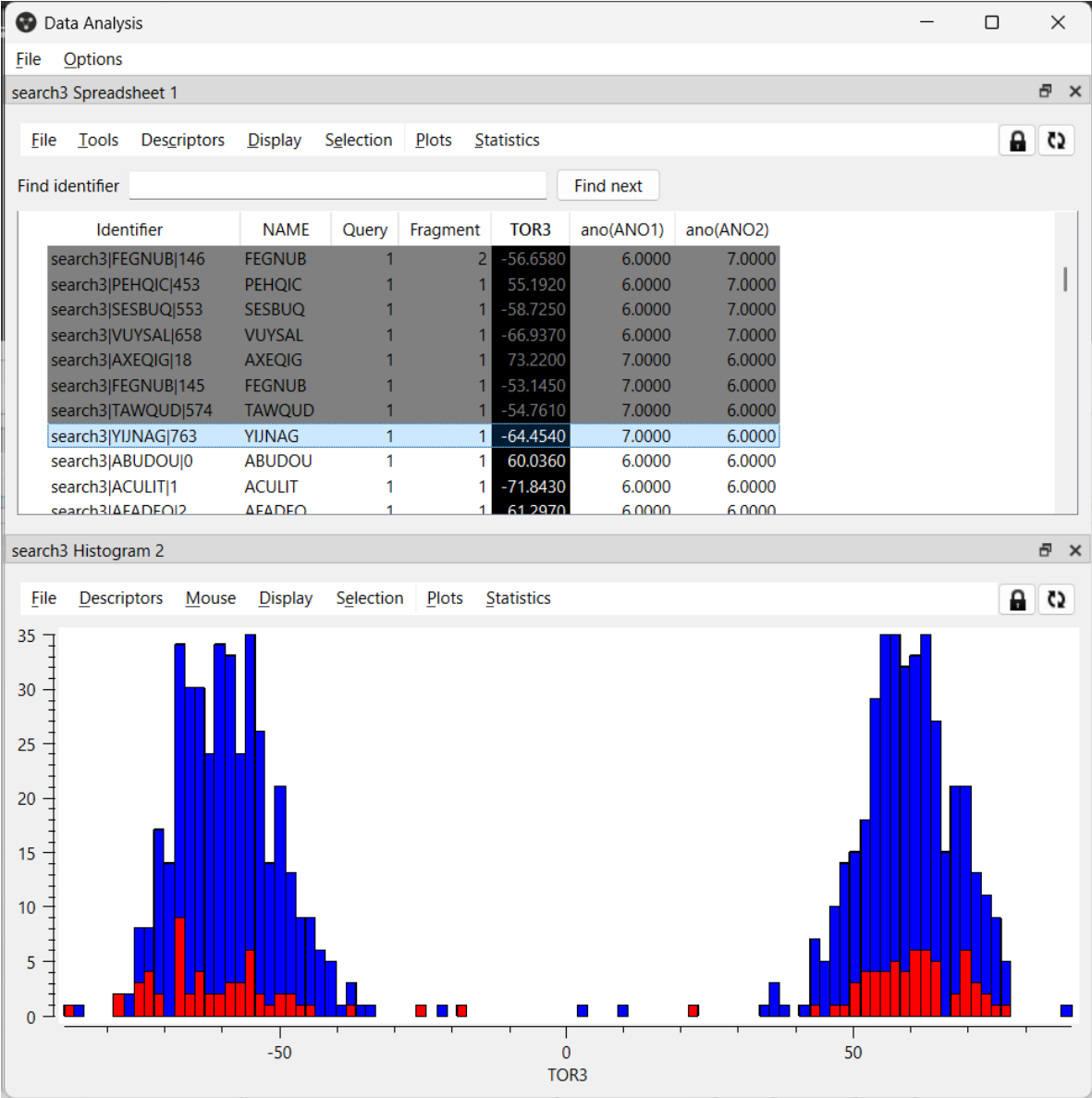
Group by



Data Analysis window



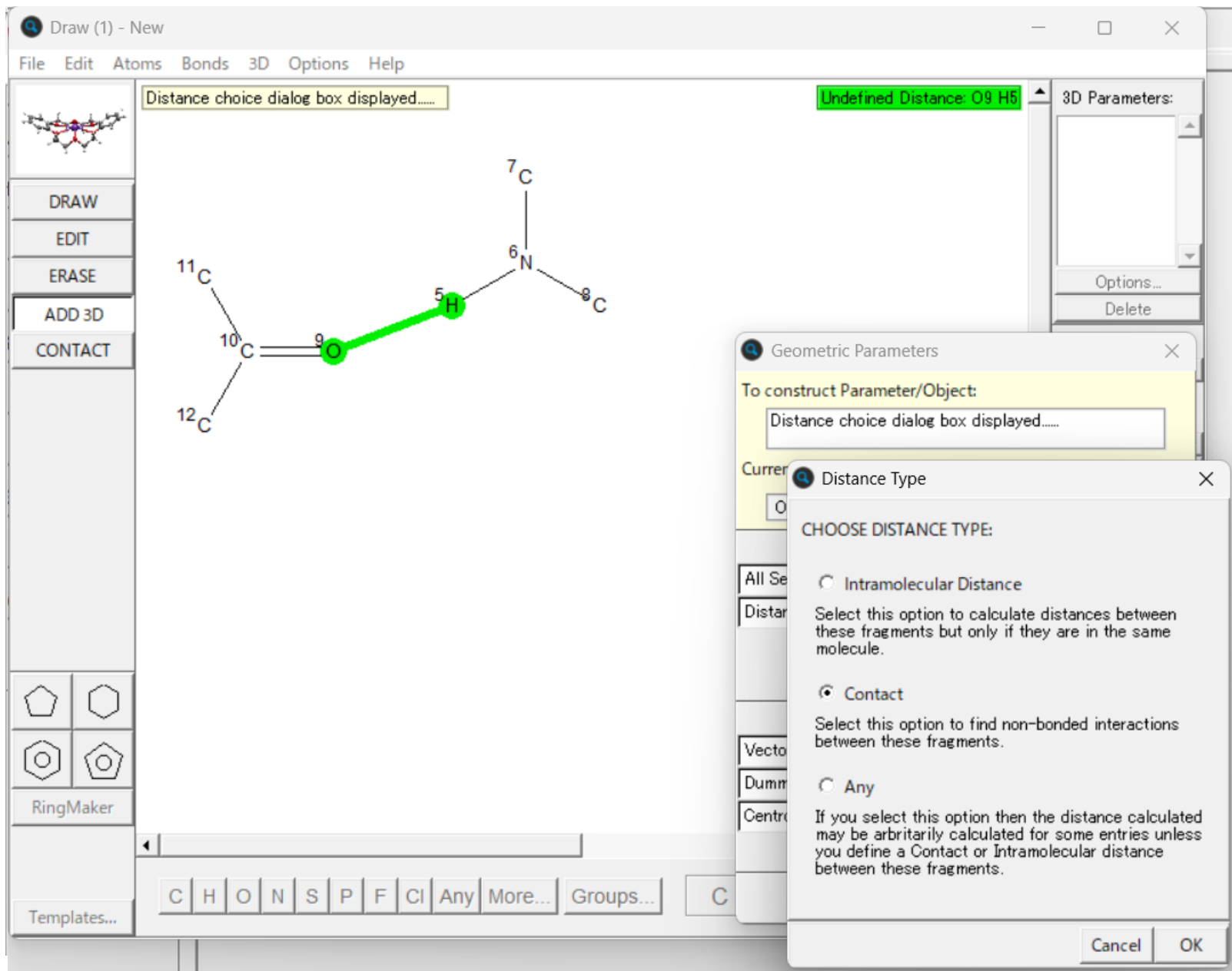
Data Analysis window



この発表で示す検索と表示の実例

- 単純な検索と表示の一連の流れ
- 元素、結合の種類の指定法
- 構造情報の追加による検索の絞り込み
- 分子間N—H $\cdots$ O水素結合を持つ構造の検索と、構造的特徴の分析
- 実験条件を指定した検索

分子間相互作用を用いた検索



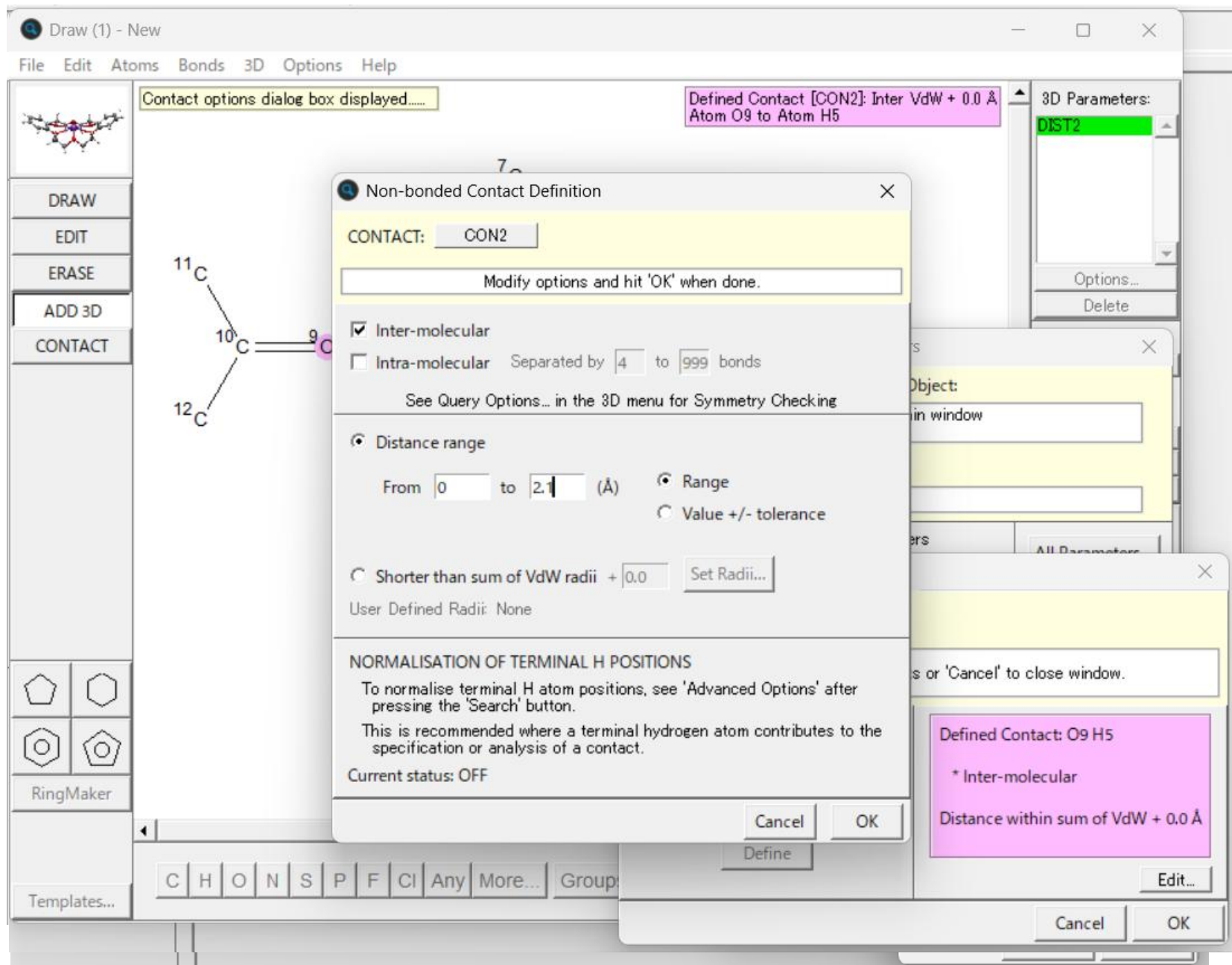
検索条件：

- ✓ 分子間O···Hコンタクト
- ✓ O···H距離 < 2.1 Å

記録するパラメータ：

- ☐ O···H 距離 (DIST2)
- ☐ O···N 距離 (DIST3)
- ☐ O···H-N 角 (ANG1)
- ☐ C-O···H 角 (ANG2)

分子間相互作用を用いた検索



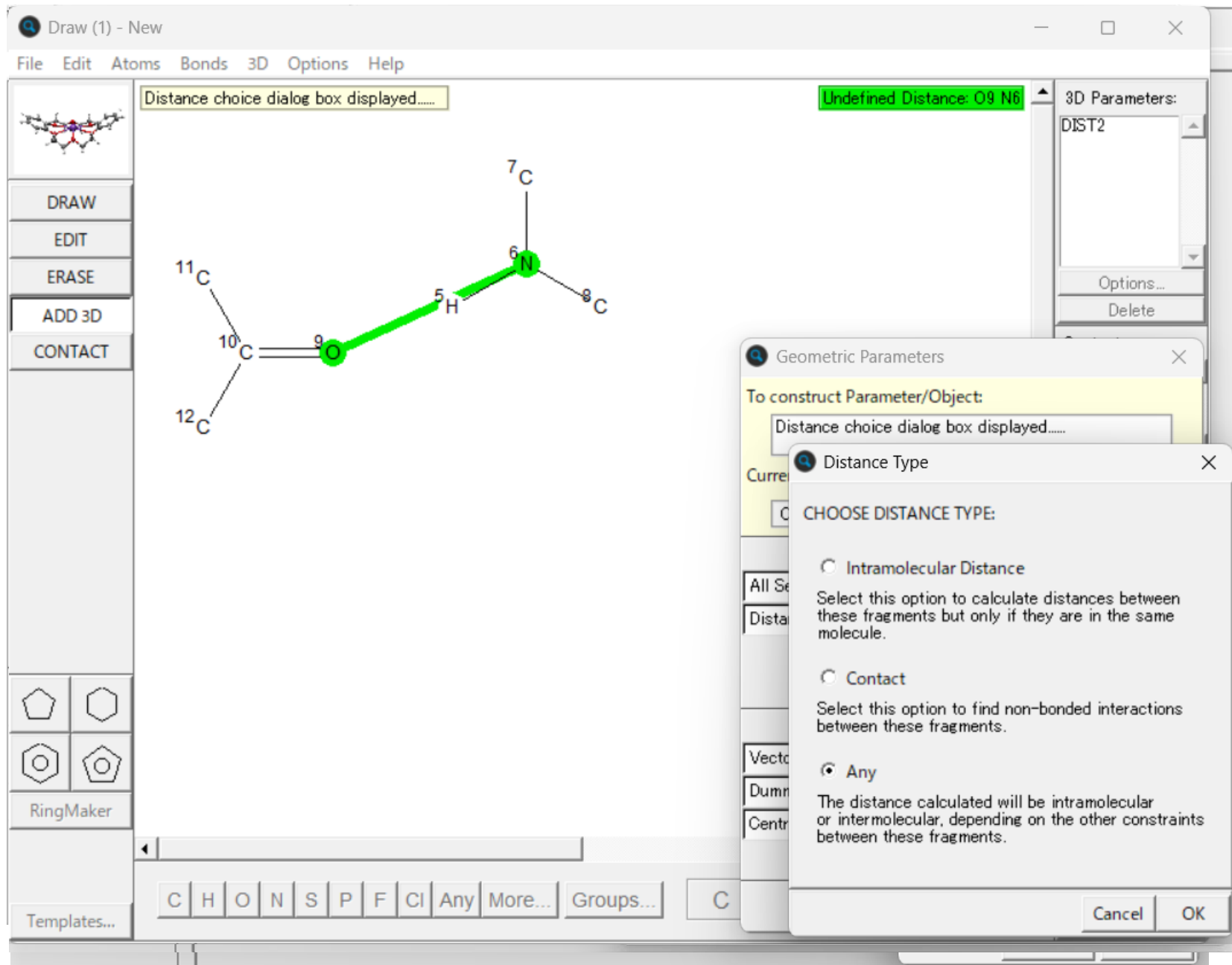
検索条件：

- ✓ 分子間O···Hコンタクト
- ✓ O···H距離 < 2.1 Å

記録するパラメータ：

- O···H 距離 (DIST2)
- O···N 距離 (DIST3)
- O···H-N 角 (ANG1)
- C-O···H 角 (ANG2)

分子間相互作用を用いた検索



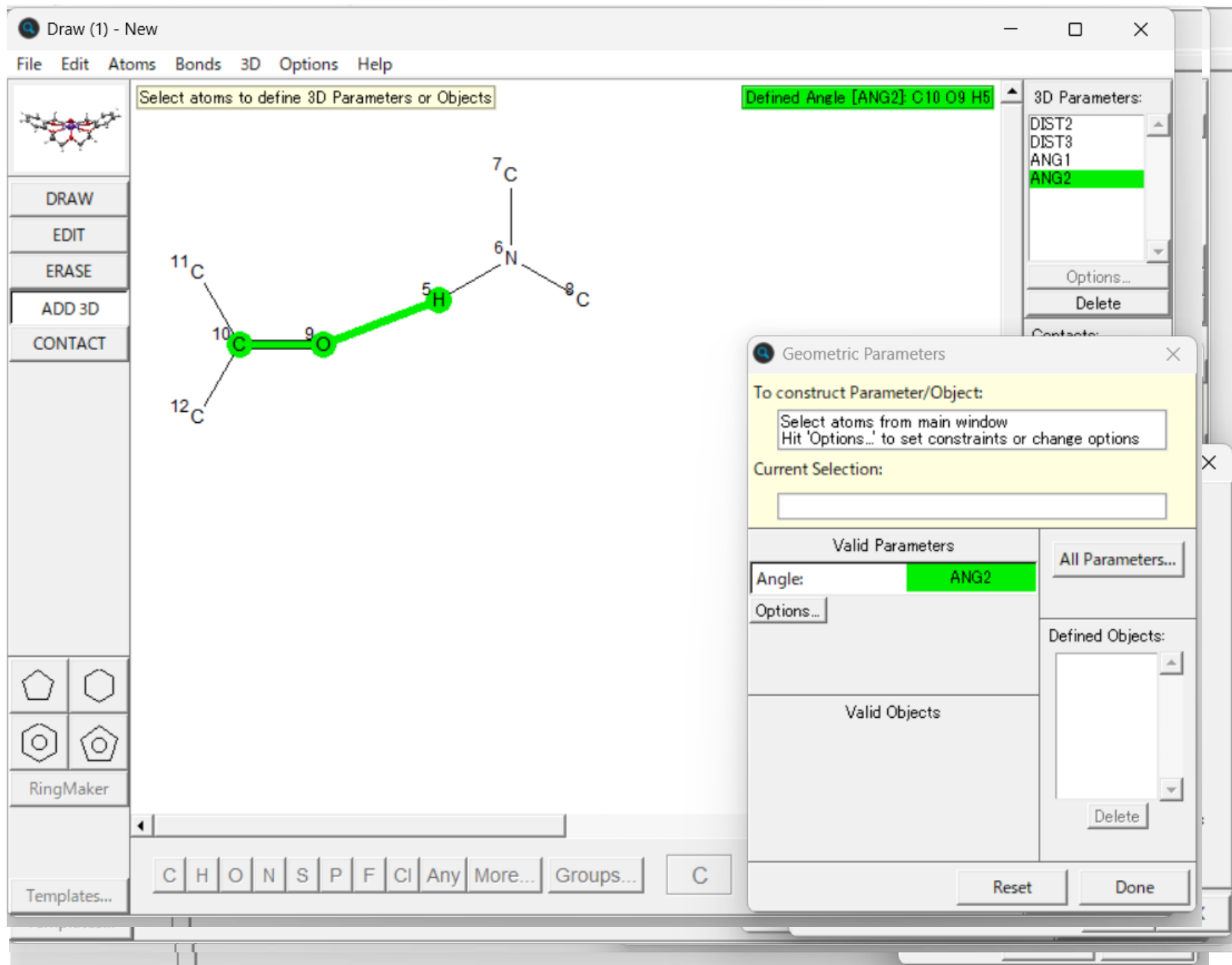
検索条件：

- ✓ 分子間O···Hコンタクト
- ✓ O···H距離 < 2.1 Å

記録するパラメータ：

- ☐ O···H 距離 (DIST2)
- ☐ O···N 距離 (DIST3)
- ☐ O···H-N 角 (ANG1)
- ☐ C-O···H 角 (ANG2)

分子間相互作用を用いた検索



検索条件：

- ✓ 分子間O $\cdots$ Hコンタクト
- ✓ O $\cdots$ H距離 < 2.1 Å

記録するパラメータ：

- ❑ O $\cdots$ H 距離 (DIST2)
- ❑ O $\cdots$ N 距離 (DIST3)
- ❑ O $\cdots$ H-N 角 (ANG1)
- ❑ C-O $\cdots$ H 角 (ANG2)

分子間相互作用を用いた検索

Search Setup

Search Name: search1

Available Databases:

☒ CSD version 6.00 (Apr 2025)

You can search complete database(s) or a subset (e.g., hits found in a previous search)

Select Subset Clear Subset

Single query being used. Search will find structures: where this query is true: Query 1

Start Search Cancel Reset

Filters **Advanced Options**

☒ 3D coordinates determined

☒ R factor ☐ <= 0.05 ☐ <= 0.075 ☒ <= 0.1

☒ Only ☒ Non-disordered ☐ Disordered

☒ No errors

☒ Not polymeric

☐ No ions

☐ Only ☒ Single crystal structures ☐ Powder structures

☐ Only ☒ Organics ☐ Organometallic

Search Setup

Search Name: search1

Available Databases:

☒ CSD version 6.00 (Apr 2025)

You can search complete database(s) or a subset (e.g., hits found in a previous search)

Select Subset Clear Subset

Single query being used. Search will find structures: where this query is true: Query 1

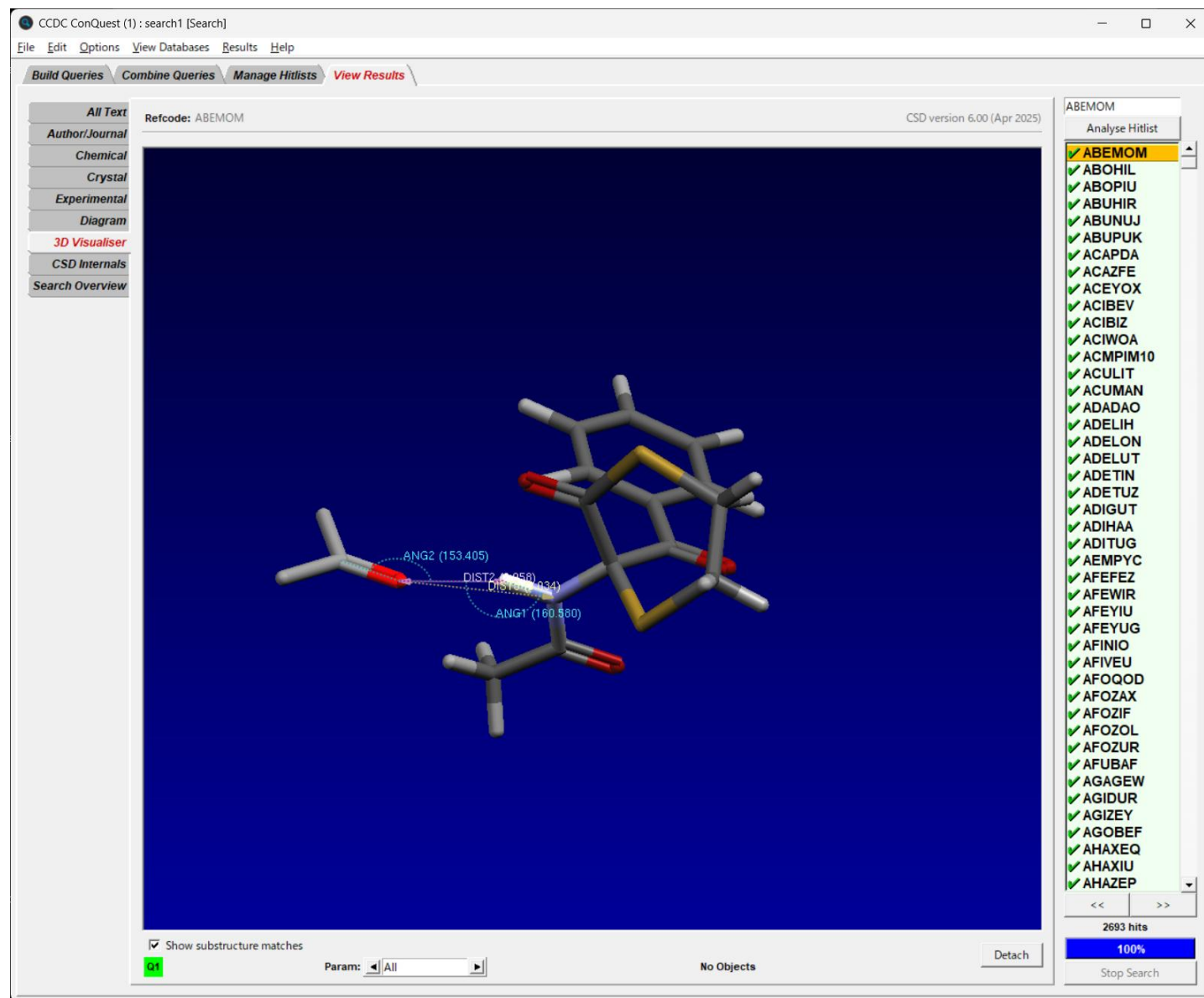
Start Search Cancel Reset

Filters **Advanced Options**

☒ Normalise terminal H positions

☒ C,N,O Defaults ☐ User Defined Edit...

C-H, N-H, O-Hを
固定値に修正



2693 hits

Mercuryを用いた構造的特徴の分析

Refcode: ABEMOM

Hit Fragment Display Options

Fragment Selection

Fragment Highlighting

☒ Tree view

☐ Load multiple structures

☐ Show only hit atoms

Structure

Value

ABEMOM

Query 1

Fragment

...

2.058

...

3.034

...

160.58

...

153.405

☒ Show parameters:

All

Data Analysis...

Close

Data Analysis

File Options

search1 Spreadsheet 1

File Tools Descriptors Display Selection Plots Statistics

Find identifier

Find next

Identifier	NAME	Query	Fragment	ANG1	ANG2	DIST2	DIST3
search1 ABEMOM 0	ABEMOM	1	1	160.5800	153.4050	2.0580	3.0340
search1 ABOHIL 1	ABOHIL	1	1	155.4180	144.9530	2.0940	3.0470
search1 ABOPIU 2	ABOPIU	1	1	144.1230	131.1740	2.0760	2.9590
search1 ABUHIR 3	ABUHIR	1	1	150.3230	127.4620	1.9090	2.8360
search1 ABUNUJ 4	ABUNUJ	1	1	167.6340	134.2580	1.7380	2.7380
search1 ABUPUK 5	ABUPUK	1	1	154.9080	161.9790	2.0600	3.0100
search1 ACAPDA 6	ACAPDA	1	1	158.0020	130.5310	1.9050	2.8710
search1 ACAZFE 7	ACAZFE	1	1	153.0770	152.7710	1.8840	2.8260
search1 ACEYOX 8	ACEYOX	1	1	169.4930	146.1370	1.8200	2.8240
search1 ACIBEV 9	ACIBEV	1	1	171.4930	136.3220	2.0280	3.0350
search1 ACIBIZ 10	ACIBIZ	1	1	160.6310	132.5150	2.0780	3.0540
search1 ACIWOA 11	ACIWOA	1	1	154.8820	137.0410	2.0030	2.9540
search1 ACMPIM10 12	ACMPIM10	1	1	176.4560	143.4650	1.8570	2.8710
search1 ACULIT 13	ACULIT	1	1	160.9530	111.3910	1.9290	2.9070
search1 ACUMAN 14	ACUMAN	1	1	152.5460	140.9590	1.9330	2.8720
search1 ADADAO 15	ADADAO	1	1	161.4880	152.6640	1.9790	2.9590
search1 ADELIH 16	ADELIH	1	1	153.5250	149.6260	2.0740	3.0160
search1 ADELIH 17	ADELIH	1	2	160.8310	129.4610	1.9730	2.9510
search1 ADELON 18	ADELON	1	1	170.9290	157.3390	1.8890	2.8960
search1 ADELUT 19	ADELUT	1	1	163.0600	149.4620	1.8260	2.8130
search1 ADELUT 20	ADELUT	1	2	156.9490	147.9130	1.9220	2.8830
search1 ADETIN 21	ADETIN	1	1	147.9920	141.9380	1.8290	2.7430
search1 ADETUZ 22	ADETUZ	1	1	130.7680	168.4700	2.0860	2.8540
search1 ADIGUT 23	ADIGUT	1	1	167.7050	159.8820	1.8340	2.8340
search1 ADIHAA 24	ADIHAA	1	1	164.1020	148.9190	2.0610	3.0500
search1 ADITUG 25	ADITUG	1	1	153.0240	119.2930	1.9530	2.8940
search1 AEMPYC 26	AEMPYC	1	1	169.6100	125.9930	1.9170	2.9220
search1 AFEFEZ 27	AFEFEZ	1	1	167.4590	162.0930	1.9500	2.9490
search1 AFEWIR 28	AFEWIR	1	1	146.2440	165.1560	2.0680	2.9660
search1 AFEYIU 29	AFEYIU	1	1	151.6480	131.4370	1.7090	2.6460
search1 AFEYUG 30	AFEYUG	1	1	154.5960	137.4880	1.9260	2.8760
search1 AFINIO 31	AFINIO	1	1	155.0280	172.6850	2.0640	3.0150
search1 AFIVEU 32	AFIVEU	1	1	163.2880	125.8620	2.0760	3.0620

ABEMOM (P-1) - Mercury

CSD version 6.00 (Apr 2025)

ABEMOM

Analyse Hitlist

File Edit Selection Display Calculate CSD-Community CSD-Core CSD-Materials CSD-Theory CSD-Particle CSD-Discovery CSD Python API Help

Picking Mode: Pick Atoms Clear Measurements Show Labels for All atoms with Atom Label

Style: Ellipsoid Colour: by Element Manage Styles... Publication Atom lists: Select by SMARTS: [c]

Animate... Default view: b a b c a* b* c* x- x+ y- y+ z- z+ x-90 x+90 y-90 y+90 z-90 z+90 zoom- zoom+ Disorder: None

Structure Navigator

ABEMOM

Find

Crystal Structures

Spacegroup

ABEMOM P-1

ABOHIL P21/c

ABOPIU Pna21

ABUHIR P212121

ABUNUJ P21/c

ABUPUK P-1

ACAPDA I2/c

ACAZFE P-1

ACEYOX Pna21

ACIBEV C2/c

ACIBIZ P-1

ACIWOA P21/n

ACMPIM10 Pbca

ACULIT P21

ACUMAN C2/c

ADADAO P-1

ADELIH P21/c

ADELIH P21/c

ADELON C2/c

ADELUT P-1

ADELUT P-1

<< >>

☒ Tree View

☐ Multiple Structures

Structures...

Searches

Options

0 hits # motifs % frequency

View Options

View results: by motif

☐ List all matches ☐ Multi-view mode

☐ Show negative results

Display Options

Display

☐ Packing

☐ Asymmetric Unit

☐ Auto centre

☐ Short Contact < (sum of vdW radii)

☐ H-Bond Default definition

Contacts... More Info Powder... Reset

Options

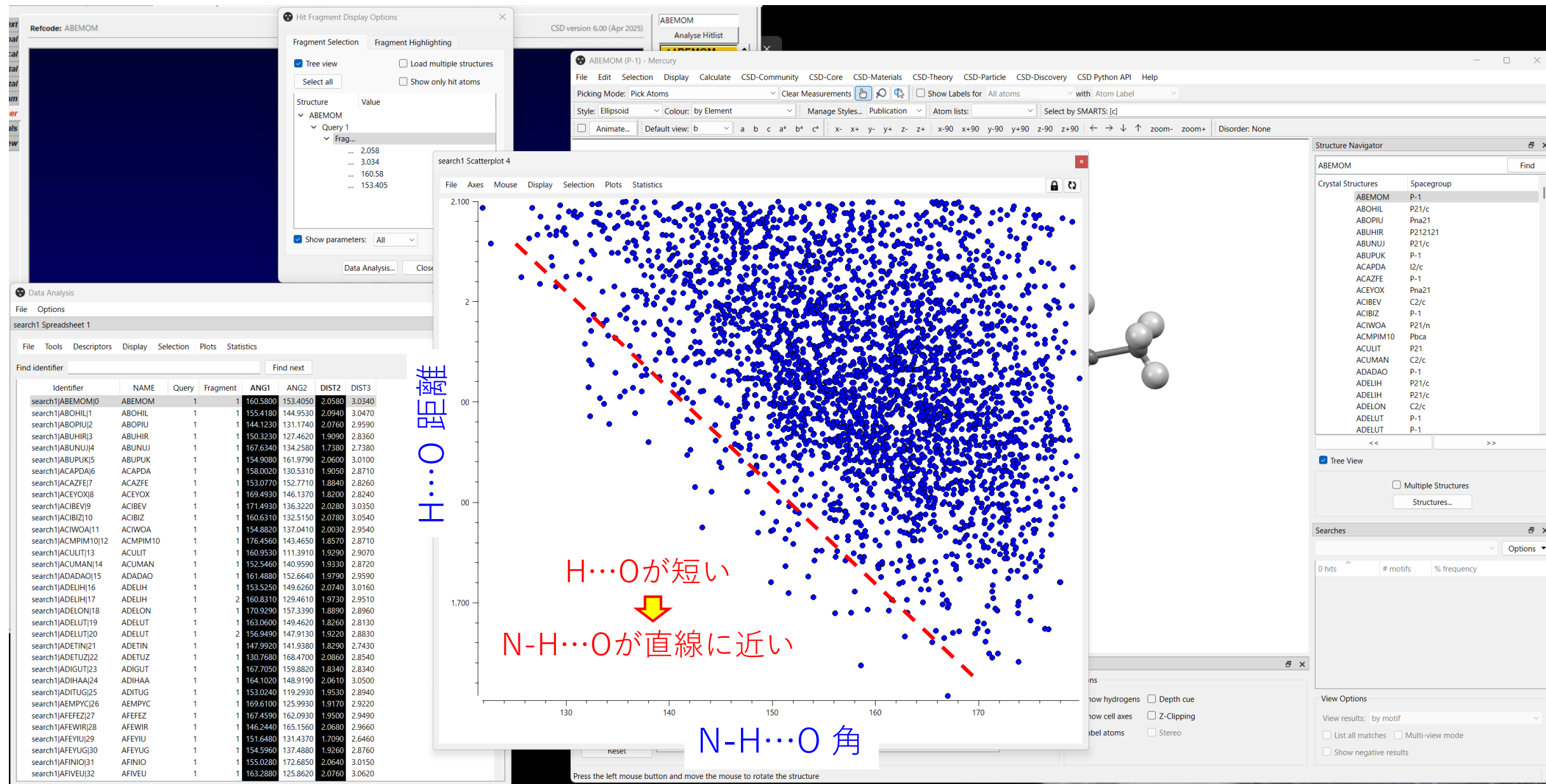
☒ Show hydrogens ☐ Depth cue

☐ Show cell axes ☐ Z-Clipping

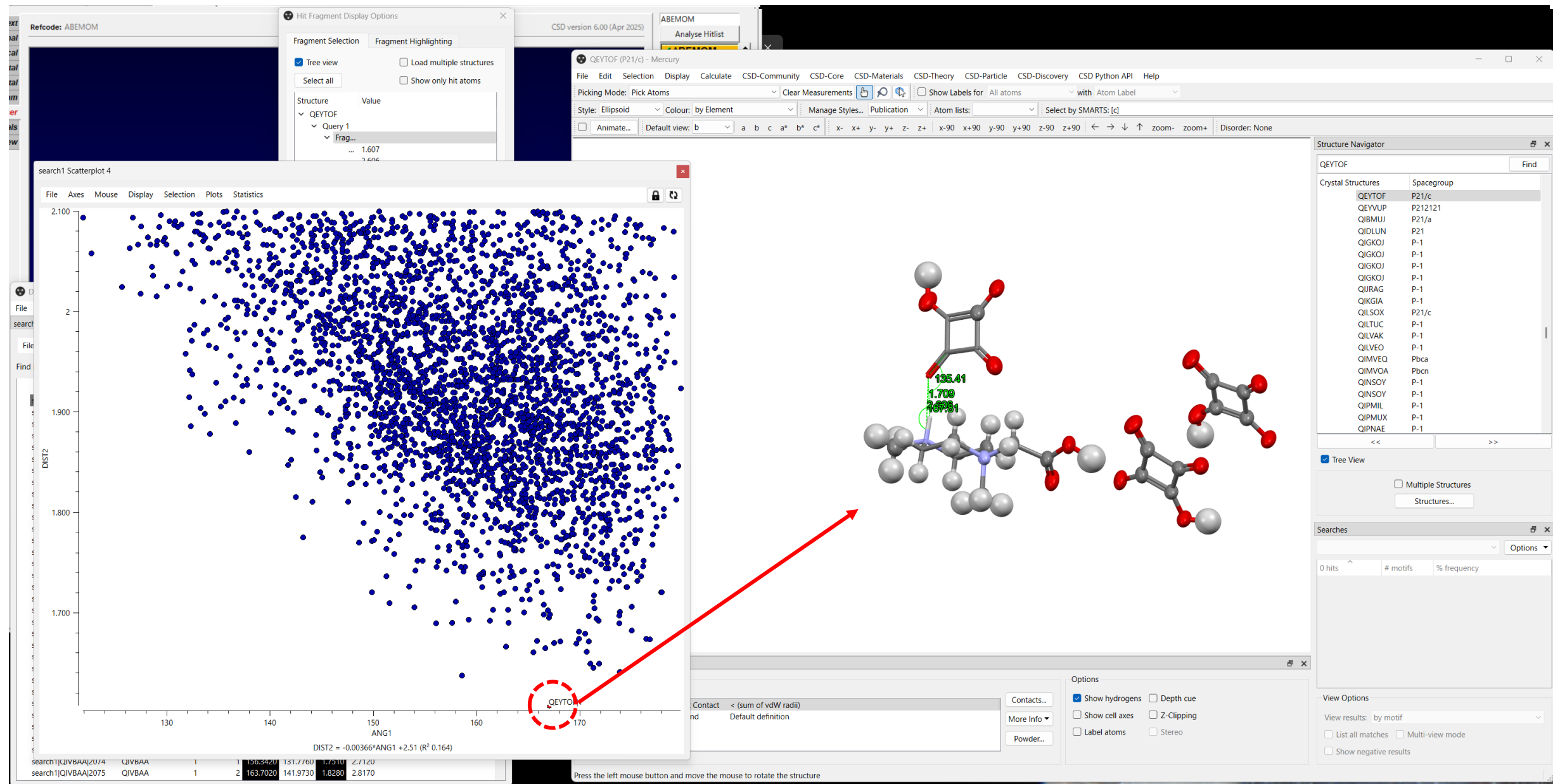
☐ Label atoms ☐ Stereo

Press the left mouse button and move the mouse to rotate the structure

Mercuryを用いた構造的特徴の分析



Mercuryを用いた構造的特徴の分析



この発表で示す検索と表示の実例

- 単純な検索と表示の一連の流れ
- 元素、結合の種類の指定法
- 構造情報の追加による検索の絞り込み
- 分子間N—H $\cdots$ O水素結合を持つ構造の検索と、構造的特徴の分析
- 実験条件を指定した検索

Fragment以外の条件を用いた検索

CCDC ConQuest (1)

File Edit Options View Databases Results Help

Build Queries Combine Queries Manage Hitlists View Results

Draw

- Author/Journal
- Name/Class
- Elements
- Formula
- Space Group
- Unit Cell
- Z/Density
- Experimental
- All Text
- Refcode (entry ID)

- 著者名、雑誌名
- 化合物名
- 構成元素
- 組成
- 空間群
- 格子定数
- 格子内分子数(Z)、密度
- 実験条件

Search Reset

Author/Journal (1) - New

Authors' Names New Box

☐ Exact surname

(Required format: F.H.Allen, O'Hara, Murray-Rust etc.
Brown will hit Browning unless 'Exact surname' is selected)

Journal Name

Type part of Journal name above to narrow list displayed
Select required journal in list below

2D Mat. [2017]
3 Biotech [2015]
A. J. Biomedical Sci. Res. [2021]
A. J. Quantum Chem. Molecular Spectroscopy [2019]
A.C.A.(Spring) [1974-1975]
A.C.S.Mtg.172,Inorg. [1976]
A.K.U.Intl.J.Engg.Tech.App.Sci. [2020]
AAPS PharmSciTech [2004-2020]
ACA Abstr.Papers(Winter) [1967-1986]
ACA, Ser.2 [1977-1984]

Volume (14, 1.2 etc.) Page (212,6-A etc.) Year (1998, 2001 etc.)

during

CCDC Number (Enter numeric part only, e.g. 123456 or 123/456)

Search Store Cancel Reset

著者名、雑誌名

Fragment以外の条件を用いた検索

The screenshot displays the CCDC ConQuest (1) search interface. On the left, a sidebar lists search criteria categories: Draw, Author/Journal, Name/Class, Elements, Formula, Space Group, Unit Cell, Z/Density, Experimental, All Text, and Refcode (entry ID). The 'Experimental' category is highlighted with a red dashed box. To the right of this box, a list of search criteria is provided in Japanese, each preceded by a blue dot:

- 著者名、雑誌名
- 化合物名
- 構成元素
- 組成
- 空間群
- 格子定数
- 格子内分子数(Z)、密度
- 実験条件

The main search area on the right is titled 'Experimental (1) - New'. It contains several search criteria with input fields and checkboxes:

- R-factor**: Input field with a dropdown menu, radio buttons for 'fractional' (selected) and '%', and a checkbox for 'Exclude disordered structures'.
- Exclude structures with unresolved errors**: Checkbox.
- Average e.s.d. of C-C Bonds**: Input field with a dropdown menu set to 'Any'.
- Exclude powder structures**: Checkbox.
- Temperature of Structure Determination**: Input field with a dropdown menu, radio buttons for 'K' (selected) and '°C', and a range slider from 0 to 610K. The slider is labeled 'Room Temperature' and has a note: 'All values in the range 283-303 K are stored as Room Temperature'.
- Radiation Source**: Input field with a dropdown menu set to 'Any', and a dropdown menu showing 'Any', 'X-Rays', and 'Neutron' (highlighted).

At the bottom of the search area are buttons for 'Search', 'Store', 'Reset', and 'Neutron' (highlighted).

実験条件

中性子回折の結果を用いた分子間O-H $\cdots$ N水素結合の分析

Draw (1) - Query 1

File Edit Atoms Bonds 3D Options Help

Contact options dialog box displayed.....

Defined Contact [CON1]: Inter 0.0 to 2.1 Å
Atom H3 to Atom N4

3D Parameters:
DIST1
DIST2
ANG1
DIST3

Options...
Delete

Contacts:
CON1: H3 N4

Non-bonded Contact Definition

CONTACT: CON1

Modify options and hit 'OK' when done.

☒ Inter-molecular
☐ Intra-molecular Separated by 4 to 999 bonds

See Query Options... in the 3D menu for Symmetry Checking

☒ Distance range
From 0.0 to 2.1 (Å) ☒ Range
☐ Value +/- tolerance

☐ Shorter than sum of VdW radii + 0.0 Set Radii...

User Defined Radii: None

NORMALISATION OF TERMINAL H POSITIONS
To normalise terminal H atom positions, see 'Advanced Options' after pressing the 'Search' button.
This is recommended where a terminal hydrogen atom contributes to the specification or analysis of a contact.
Current status: OFF

Cancel OK

検索条件：

- ✓ N $\cdots$ H距離 < 2.1 Å
- ✓ 分子間コンタクト
- ✓ 線源: 中性子

use this query? ☒ Query 2 ☒ Query 3

3D NB

Radiation Neutron

Edit... Delete

記録するパラメータ：

- N $\cdots$ H 距離 (DIST1)
- O—H 距離 (DIST2)
- O $\cdots$ N 距離 (DIST3)
- O—H $\cdots$ N角 (ANG1)

中性子回折の結果を用いたO-H...N水素結合の分析

Search Setup

Search Name: search3

Available Databases:

- ☒ CSD version 6.00 (Apr 2025)

You can search complete database(s) or a subset (e.g., hits found in a previous search)

Select Subset Clear Subset

Summary of queries to be used. Search will find structures: where these queries are true:

Query 2 Query 3

Start Search Cancel Reset

Filters **Advanced Options**

- ☒ 3D coordinates determined
- ☒ R factor
 - ☐ <= 0.05
 - ☐ <= 0.075
 - ☒ <= 0.1
- ☒ Only ☒ Non-disordered ☐ Disordered
- ☒ No errors
- ☒ Not polymeric
- ☐ No ions
- ☐ Only ☒ Single crystal structures ☐ Powder structures
- ☐ Only ☒ Organics ☐ Organometallic

Search Setup

Search Name: search3

Available Databases:

- ☒ CSD version 6.00 (Apr 2025)

You can search complete database(s) or a subset (e.g., hits found in a previous search)

Select Subset Clear Subset

Summary of queries to be used. Search will find structures: where these queries are true:

Query 2 Query 3

Start Search Cancel Reset

Filters **Advanced Options**

- ☐ Normalise terminal H positions
- ☒ C,N,O Defaults
- ☐ User Defined Edit...

CCDC ConQuest (1) : search3 [Search]

File Edit Options View Databases Results Help

Build Queries Combine Queries Manage Hitlists View Results

Refcode: ADENOS01

CSD version 6.00 (Apr 2025)

Analyse Hitlist

Parameters

- DIST1 1.994
- DIST2 0.986
- ANG1 158.327

ADENOS01

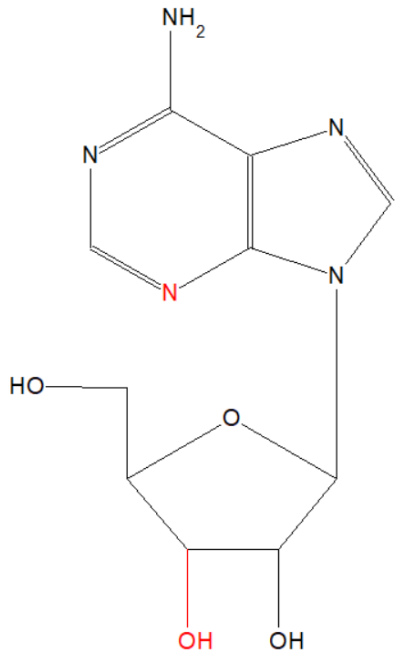
- ☒ ADENOS01
- ☒ AHXGLP
- ☒ AMPHOM03
- ☒ COZYOG01
- ☒ DINICA12
- ☒ DOZGUX
- ☒ ENALOU01
- ☒ EPHEDH03
- ☒ GADGUN03
- ☒ GADGUN04
- ☒ GADGUN05
- ☒ GOKQV07
- ☒ HOLJAU05
- ☒ HOLJAU06
- ☒ HOLJAU07
- ☒ LOLSUA
- ☒ MAMPOL02
- ☒ MAMPUM04
- ☒ MAMPUM05
- ☒ OPUNEU01
- ☒ QUQCUB
- ☒ QUQCUB02
- ☒ QUQCUB03
- ☒ RAKQOJ01
- ☒ THXMAM14
- ☒ THXMAM15
- ☒ ULAWAF03
- ☒ ULAWAF05
- ☒ WISNAN01
- ☒ WISNAN02
- ☒ WISNAN03
- ☒ WIVDUA04
- ☒ WIVDUA05

Multiple Hits: Show 1 of 2

Show terminal carbons

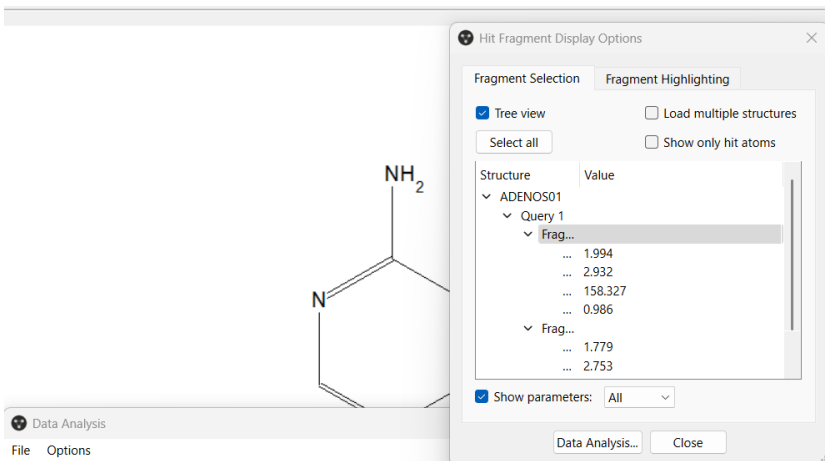
Show Parameters Use as Query... Detach

33 hits 100% Stop Search



33 hits

Mercuryを用いた分析



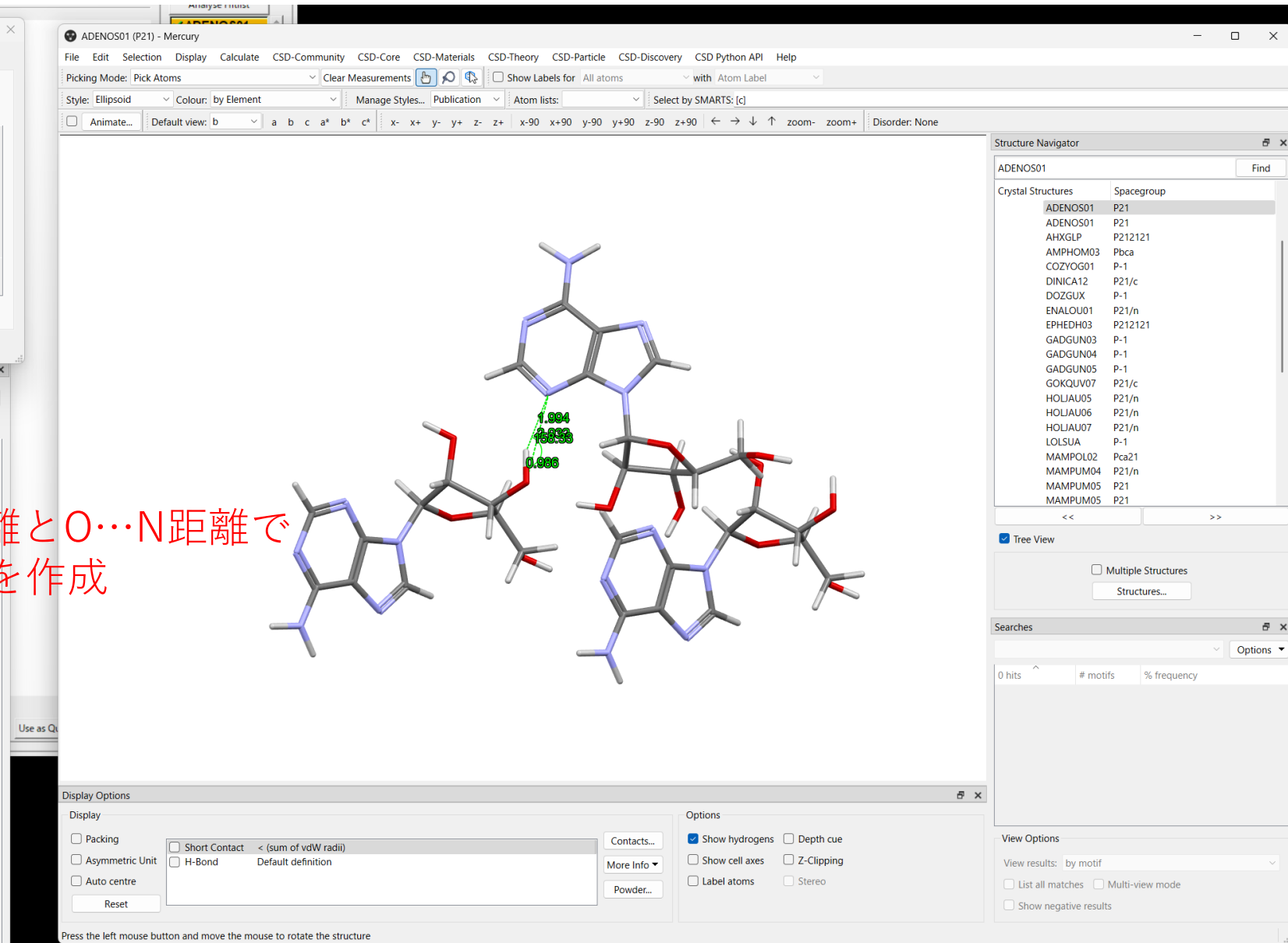
search2 Spreadsheet 1

File Tools Descriptors Display Selection Plots Statistics

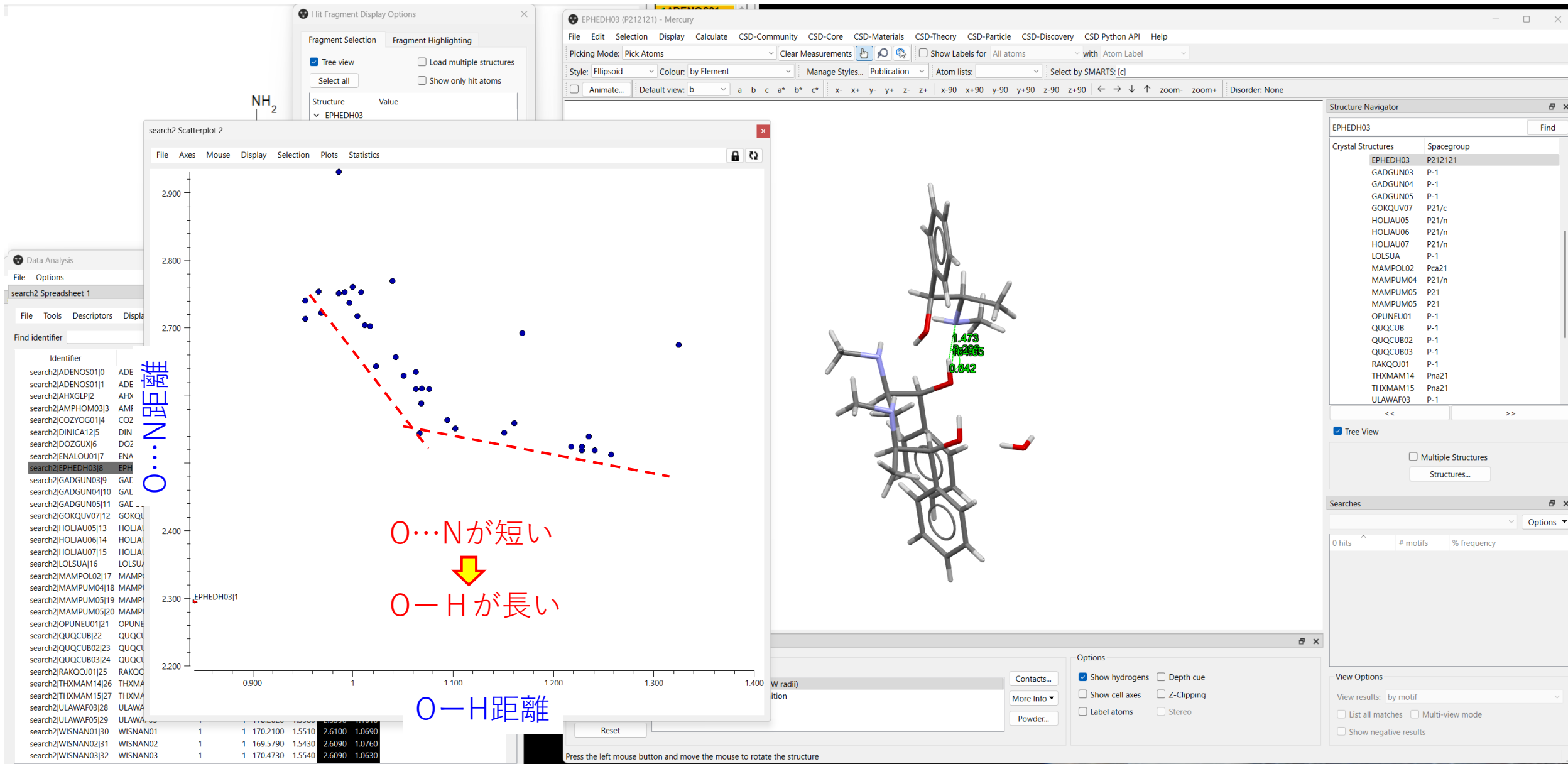
Find identifier Find next

Identifier	NAME	Query	Fragment	ANG1	DIST1	DIST2	DIST3
search2 ADENOS01 0	ADENOS01	1	1	158.3270	1.9940	2.9320	0.9860
search2 ADENOS01 1	ADENOS01	1	2	166.3810	1.7790	2.7530	0.9920
search2 AHXGLPI 2	AHXGLP	1	1	165.3820	1.7600	2.7370	0.9970
search2 AMPHOM03 3	AMPHOM03	1	1	172.6930	1.7660	2.7610	1.0000
search2 COZYOG01 4	COZYOG01	1	1	170.9140	1.7210	2.7180	1.0050
search2 DINICA12 5	DINICA12	1	1	177.8150	1.3070	2.5250	1.2180
search2 DOZGUX 6	DOZGUX	1	1	178.1230	1.6210	2.6440	1.0230
search2 ENALOU01 7	ENALOU01	1	1	167.8600	1.7690	2.7230	0.9690
search2 EPHEDH03 8	EPHEDH03	1	1	164.6510	1.4730	2.2960	0.8420
search2 GADGUN03 9	GADGUN03	1	1	169.5880	1.2880	2.5190	1.2410
search2 GADGUN04 10	GADGUN04	1	1	169.5970	1.3000	2.5190	1.2290
search2 GADGUN05 11	GADGUN05	1	1	170.5680	1.3040	2.5250	1.2290
search2 GOKQUV07 12	GOKQUV07	1	1	177.1150	1.3950	2.5450	1.1510
search2 HOLJAU05 13	HOLJAU05	1	1	176.6020	1.5790	2.6290	1.0510
search2 HOLJAU06 14	HOLJAU06	1	1	175.7860	1.6150	2.6570	1.0430
search2 HOLJAU07 15	HOLJAU07	1	1	174.9420	1.5740	2.6350	1.0630
search2 LOLSUA 16	LOLSUA	1	1	167.5130	1.5350	2.5890	1.0680
search2 MAMPOL02 17	MAMPOL02	1	1	167.9980	1.7580	2.7530	1.0090
search2 MAMPUM04 18	MAMPUM04	1	1	145.6560	1.8730	2.7140	0.9530
search2 MAMPUM05 19	MAMPUM05	1	1	142.7520	1.9000	2.7510	0.9860
search2 MAMPUM05 20	MAMPUM05	1	2	155.1940	1.4140	2.6750	1.3250
search2 OPUNEU01 21	OPUNEU01	1	1	176.5150	1.7310	2.7700	1.0400
search2 QUQCUB 22	QUQCUB	1	1	167.7380	1.4640	2.5510	1.1020
search2 QUQCUB02 23	QUQCUB02	1	1	167.7960	1.4840	2.5640	1.0940
search2 QUQCUB03 24	QUQCUB03	1	1	165.6490	1.4970	2.5440	1.0670
search2 RAKQJO1 25	RAKQJO1	1	1	170.1370	1.2650	2.5130	1.2580
search2 THXMAM14 26	THXMAM14	1	1	176.4100	1.6930	2.7040	1.0120
search2 THXMAM15 27	THXMAM15	1	1	175.7560	1.6880	2.7030	1.0170
search2 ULAWAF03 28	ULAWAF03	1	1	170.5210	1.3130	2.5390	1.2350
search2 ULAWAF05 29	ULAWAF05	1	1	178.2020	1.3980	2.5590	1.1610
search2 WISNAN01 30	WISNAN01	1	1	170.2100	1.5510	2.6100	1.0690
search2 WISNAN02 31	WISNAN02	1	1	169.5790	1.5430	2.6090	1.0760
search2 WISNAN03 32	WISNAN03	1	1	170.4730	1.5540	2.6090	1.0630

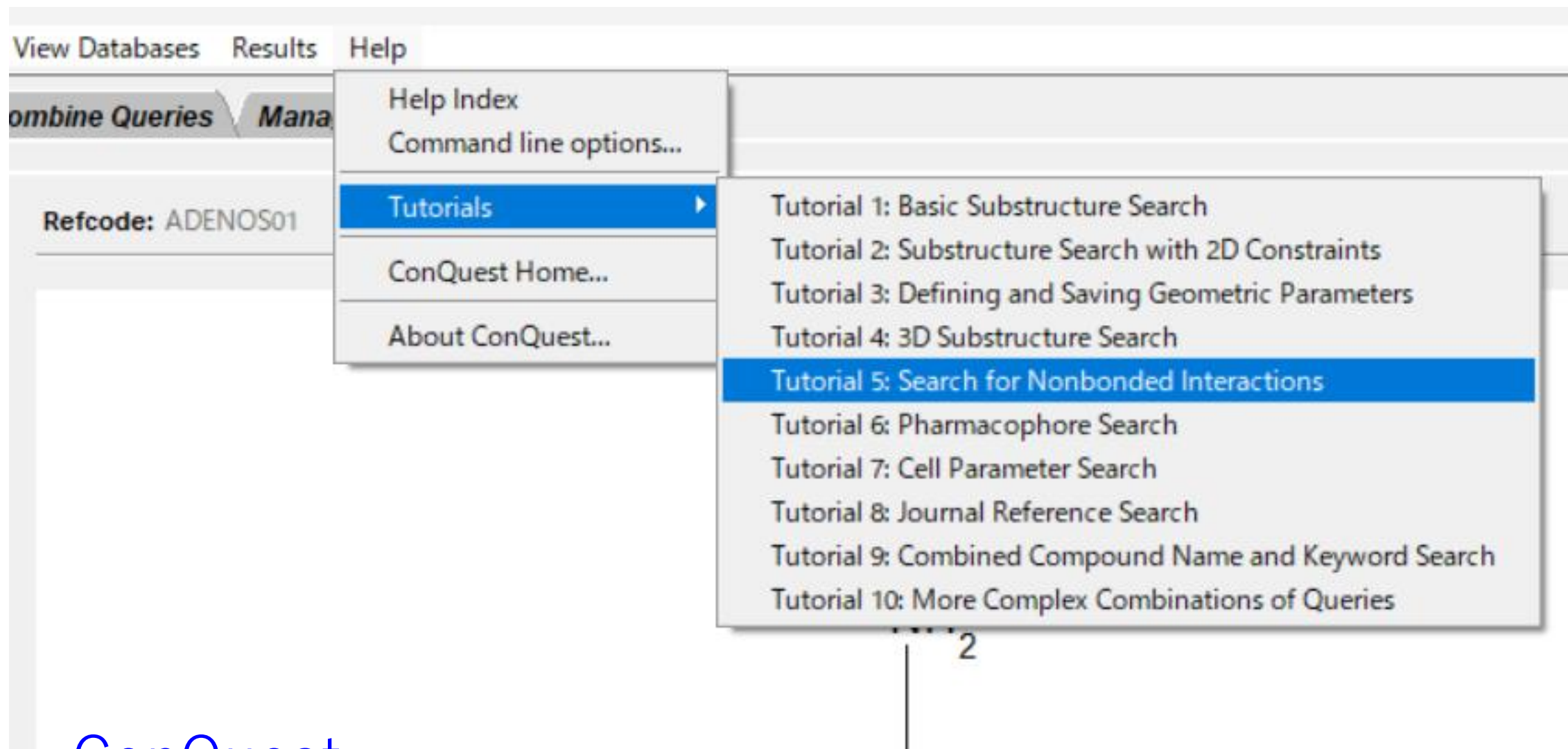
O-H距離とO...N距離で 散布図を作成



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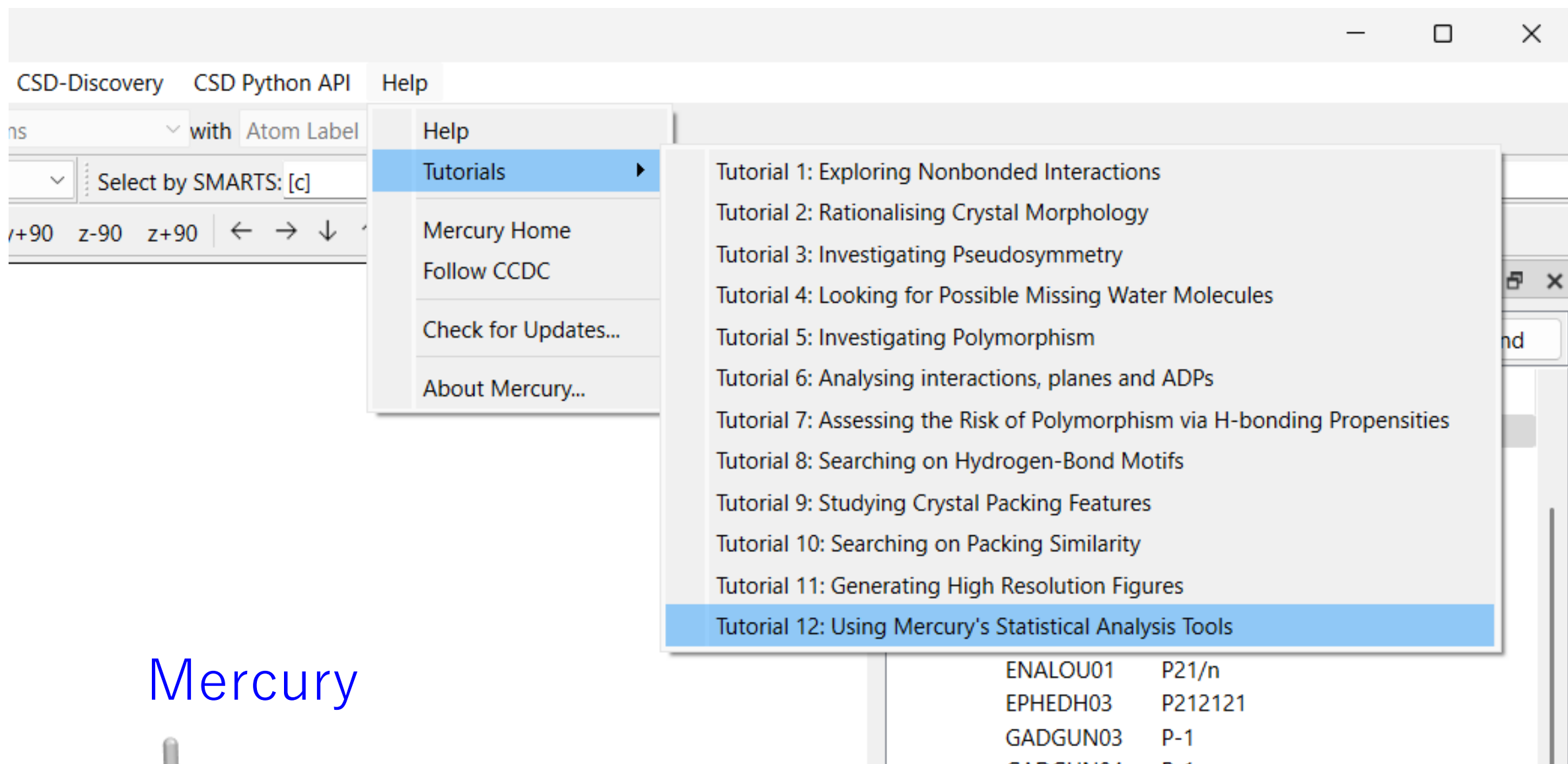


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interaction.
This ends the tutorial.

20.6 Tutorial 6: Pharmacophore Search

20.6.1 Objectives

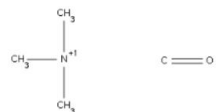
- To draw two chemical fragments (substructures).
- To specify the distance required between the two fragments, i.e. to specify a pharmacophore.
- To find molecules in the CSD containing the specified pharmacophore.

20.6.2 Steps Required

1. Draw the fragments.
2. Define one of the fragments as a *group* for use in non-bonded searching.
3. Specify the required distance between the fragments.
4. Ensure that the search is for intramolecular non-bonded distances only (i.e. both fragments must be in the same molecule).
5. Run the search.
6. Save the file of hits.

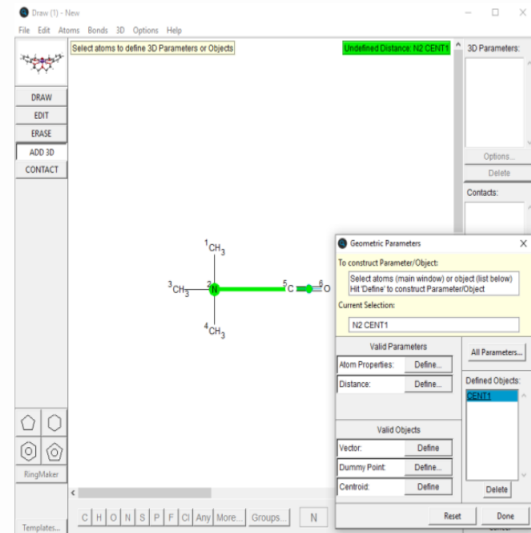
20.6.3 The Example

The tutorial explains how to search for the following pharmacophore:



4. Define the distance between the N atom and the centroid of the C=O group.

- Select the N atom by clicking on it.
- Select the centroid of the carbonyl group by clicking on *CENT1* in the box headed **Defined Objects**.
- Hit the **Define** button next to the word *Distance*:



- ◆ インストールされたチュートリアル用ファイルをブラウザで表示
- ◆ 「ConQuest tutorials」「Mercury tutorials」での検索で、それぞれのユーザーガイド(チュートリアル込み)を入手可能