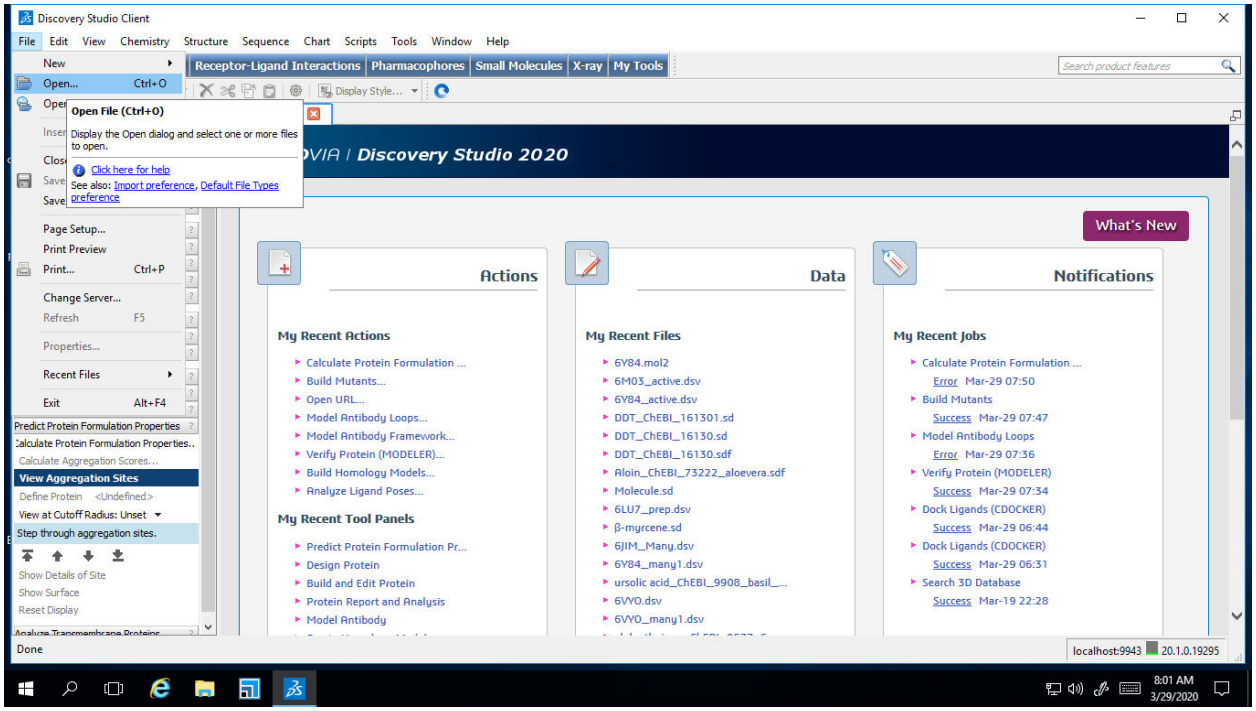
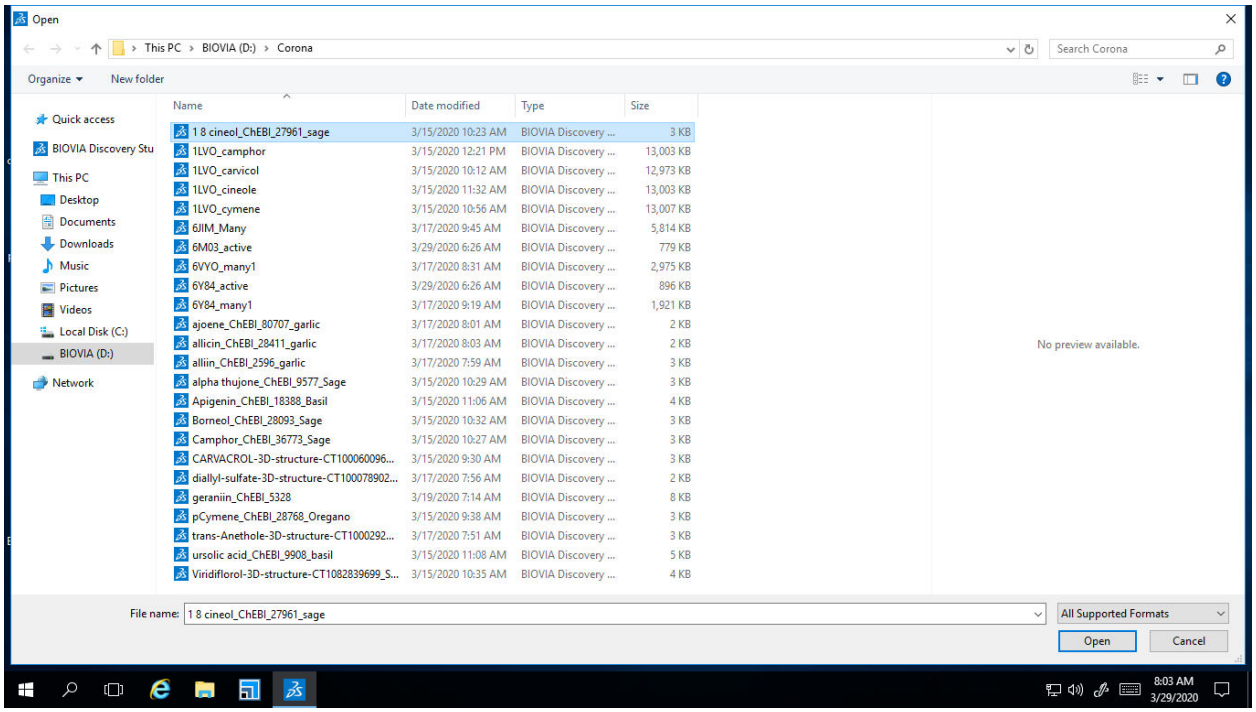
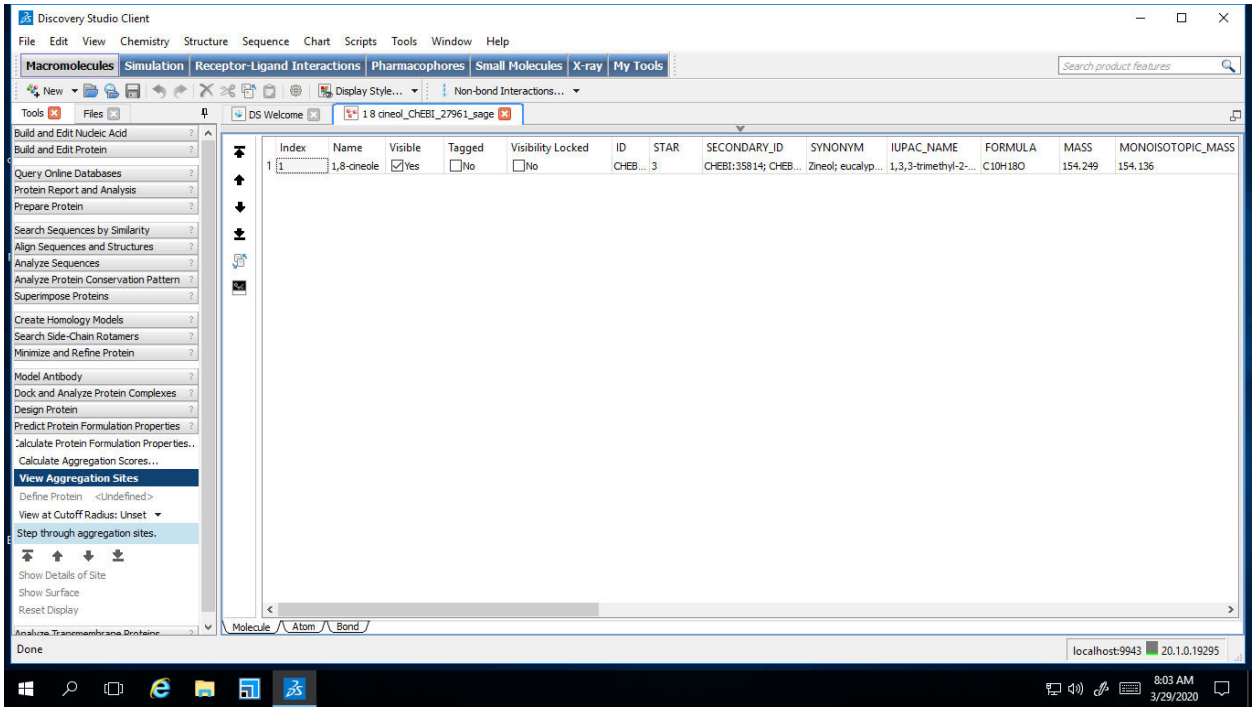
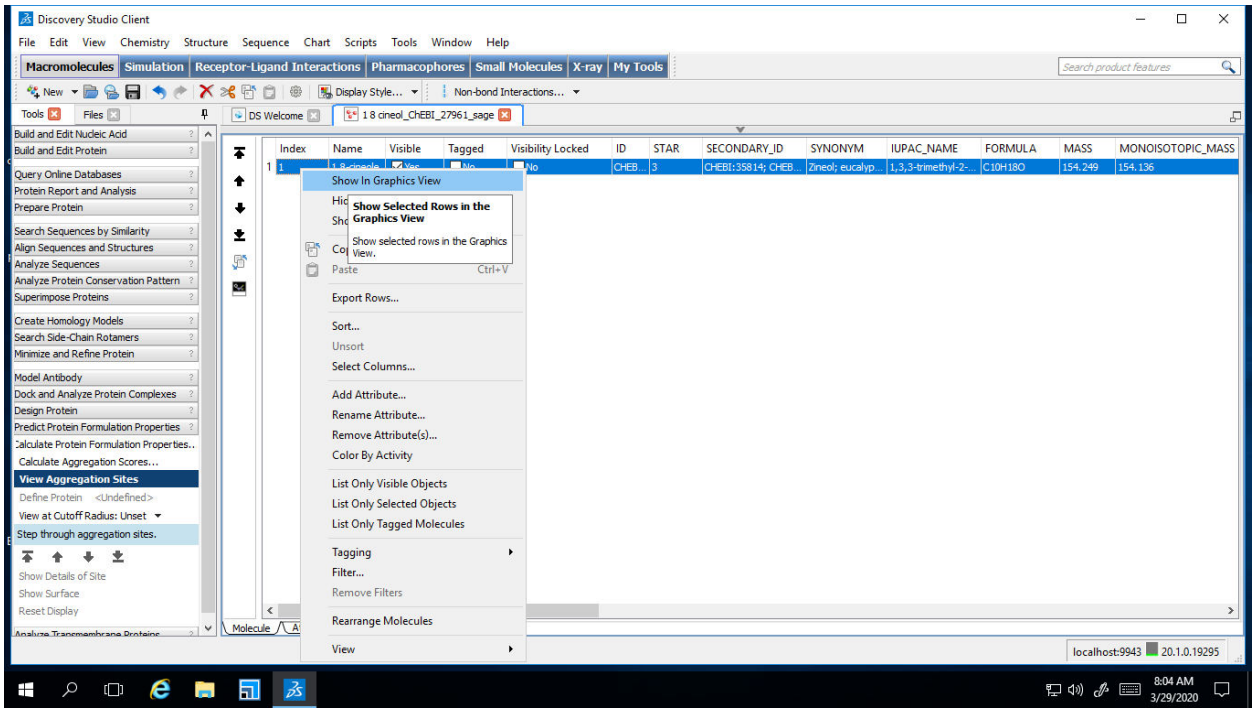
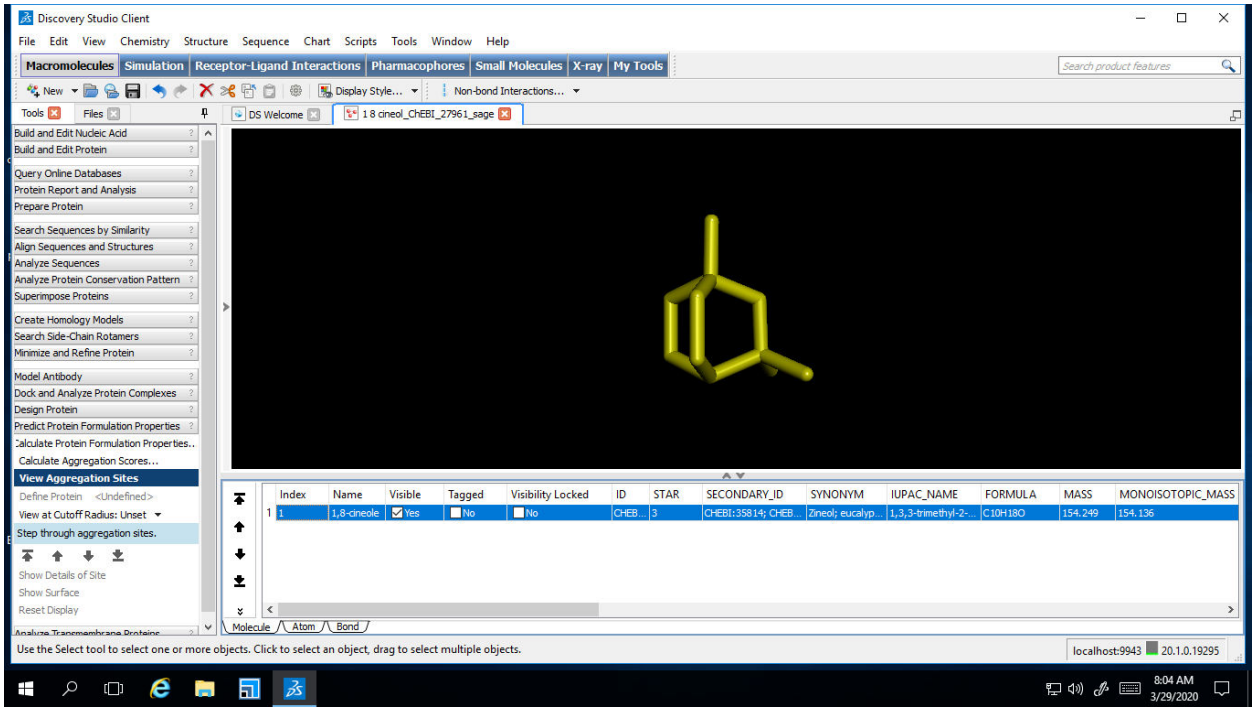
Pharmacophore search, Basis of aptamer

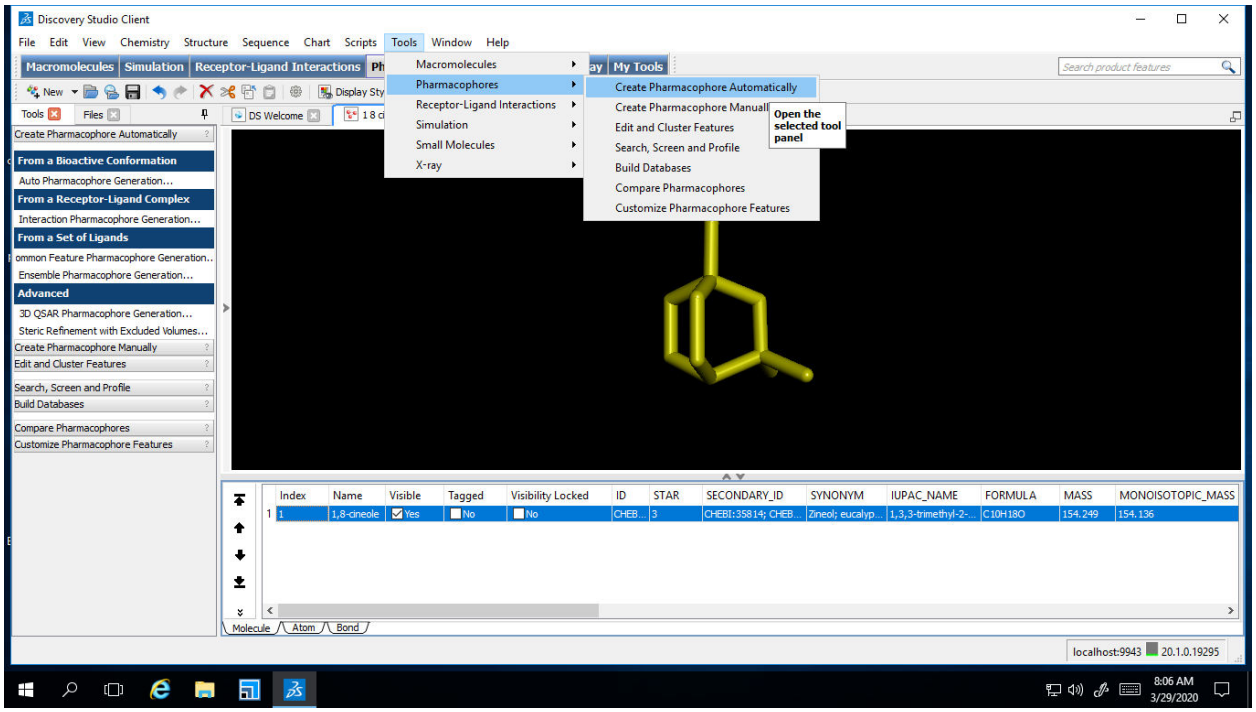


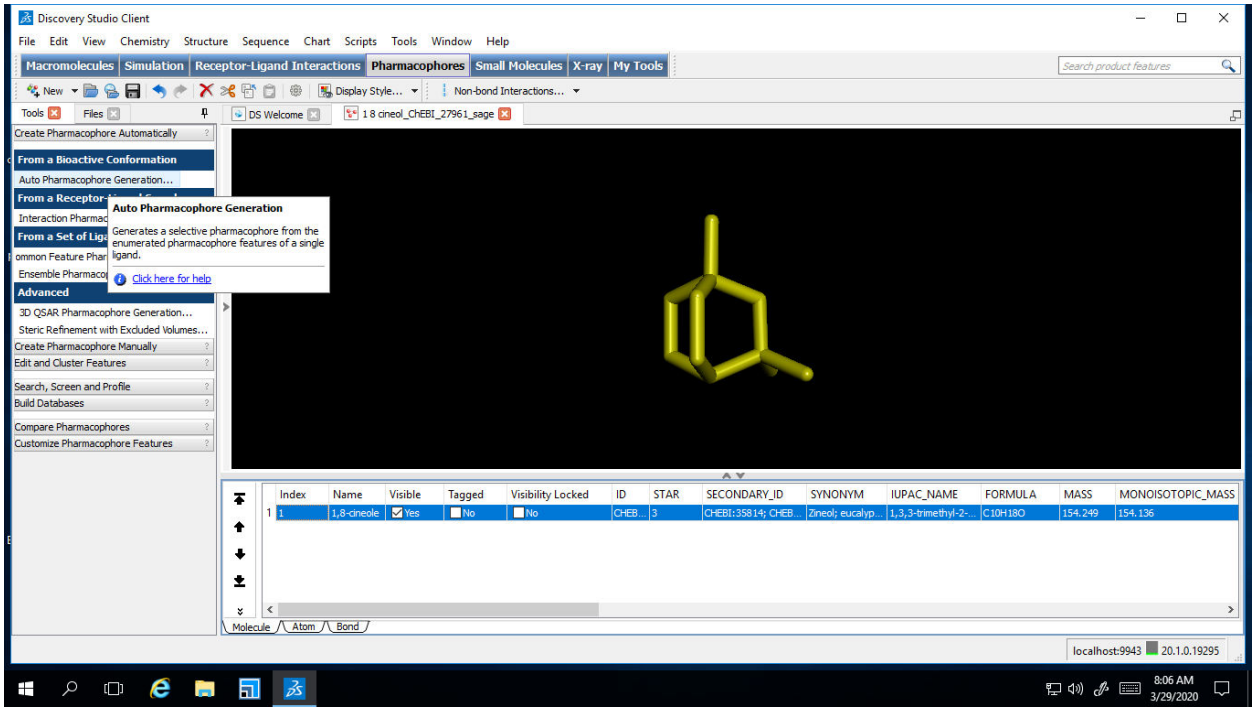


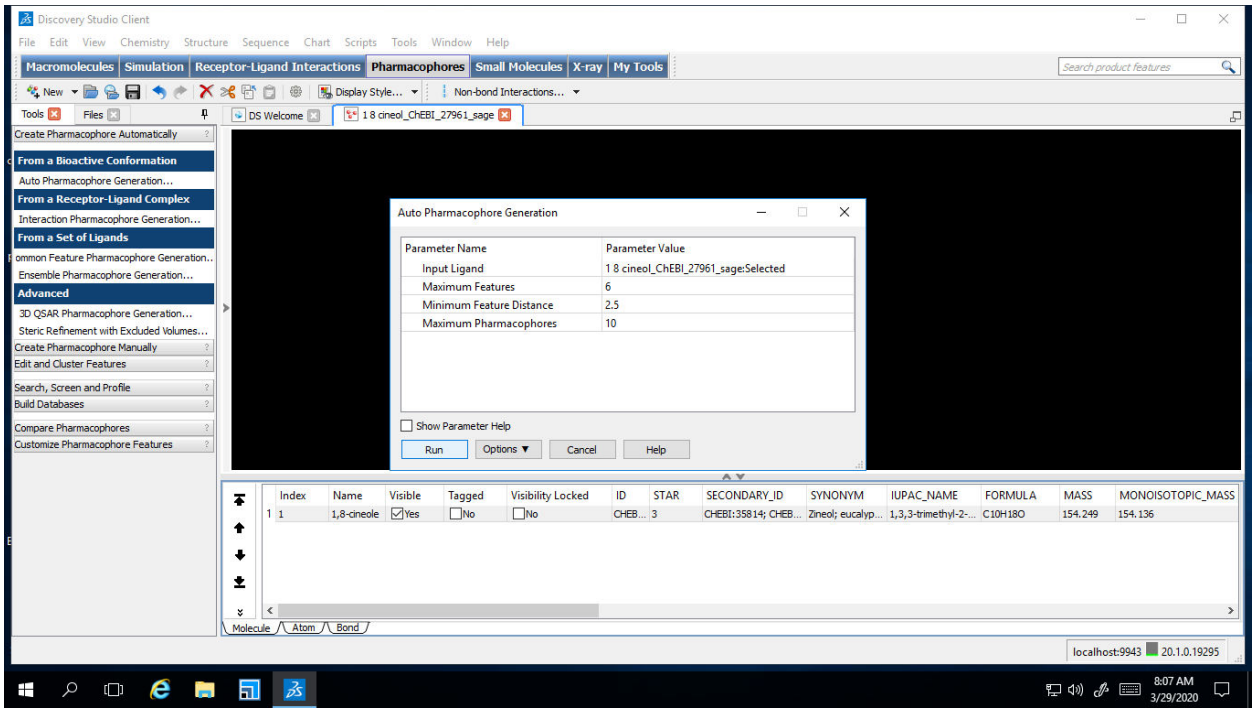

Discovery Studio Client
File Edit View Chemistry Structure Sequence Chart Scripts Tools Window Help
Macromolecules Simulation Receptor-Ligand Interactions Pharmacophores Small Molecules X-ray My Tools
Search product features
New Display Style... Non-bond Interactions...
Tools Files
DS Welcome 1 8 cineol_ChEBI_27961_sage
Build and Edit Nucleic Acid
Build and Edit Protein
Query Online Databases
Protein Report and Analysis
Prepare Protein
Search Sequences by Similarity
Align Sequences and Structures
Analyze Sequences
Analyze Protein Conservation Pattern
Superimpose Proteins
Create Homology Models
Search Side-Chain Rotamers
Minimize and Refine Protein
Model Antibody
Dock and Analyze Protein Complexes
Design Protein
Predict Protein Formulation Properties
Calculate Protein Formulation Properties..
Calculate Aggregation Scores...
View Aggregation Sites
Define Protein <Undefined>
View at Cutoff Radius: Unset
Step through aggregation sites.
Show Details of Site
Show Surface
Reset Display
Index Name Visible Tagged Visibility Locked ID STAR SECONDARY_ID SYNONYM IUPAC_NAME FORMULA MASS MONOISOTOPIC_MASS
1 1 1,8-cineole Yes No No CHEB... 3 CHEBI:35814; CHEB... Zineol; eucalyp... 1,3,3-trimethyl-2-... C10H18O 154.249 154.136
Molecule Atom Bond
Done
localhost:9943 20.1.0.19295
8:03 AM
3/29/2020

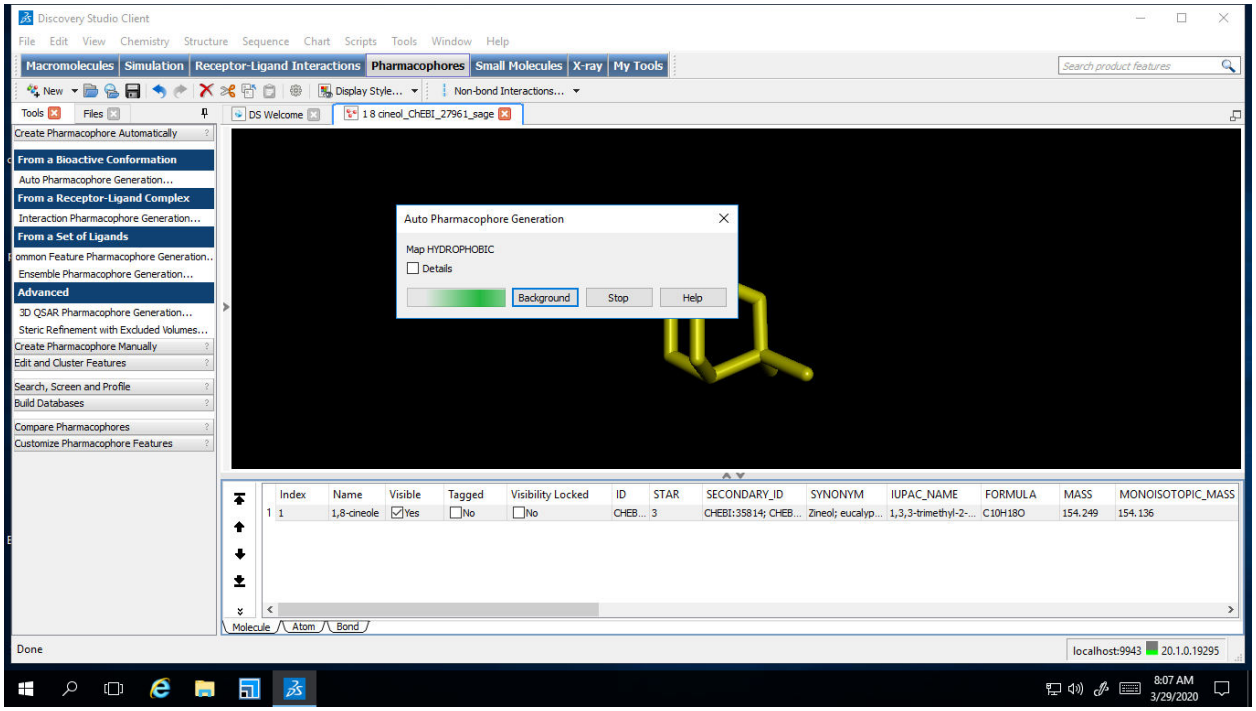

Discovery Studio Client
File Edit View Chemistry Structure Sequence Chart Scripts Tools Window Help
Macromolecules Simulation Receptor-Ligand Interactions Pharmacophores Small Molecules X-ray My Tools
Search product features
New Display Style... Non-bond Interactions...
Tools Files
DS Welcome 1 8 cineol_ChEBI_27961_sage
Index Name Visible Tagged Visibility Locked ID STAR SECONDARY_ID SYNONYM IUPAC_NAME FORMULA MASS MONOISOTOPIC_MASS
Show In Graphics View
Show Selected Rows in the Graphics View
Show selected rows in the Graphics View.
Paste Ctrl+V
Export Rows...
Sort...
Unsort
Select Columns...
Add Attribute...
Rename Attribute...
Remove Attribute(s)...
Color By Activity
List Only Visible Objects
List Only Selected Objects
List Only Tagged Molecules
Tagging
Filter...
Remove Filters
Rearrange Molecules
View
Molecule
localhost:9943 20.1.0.19295
8:04 AM
3/29/2020

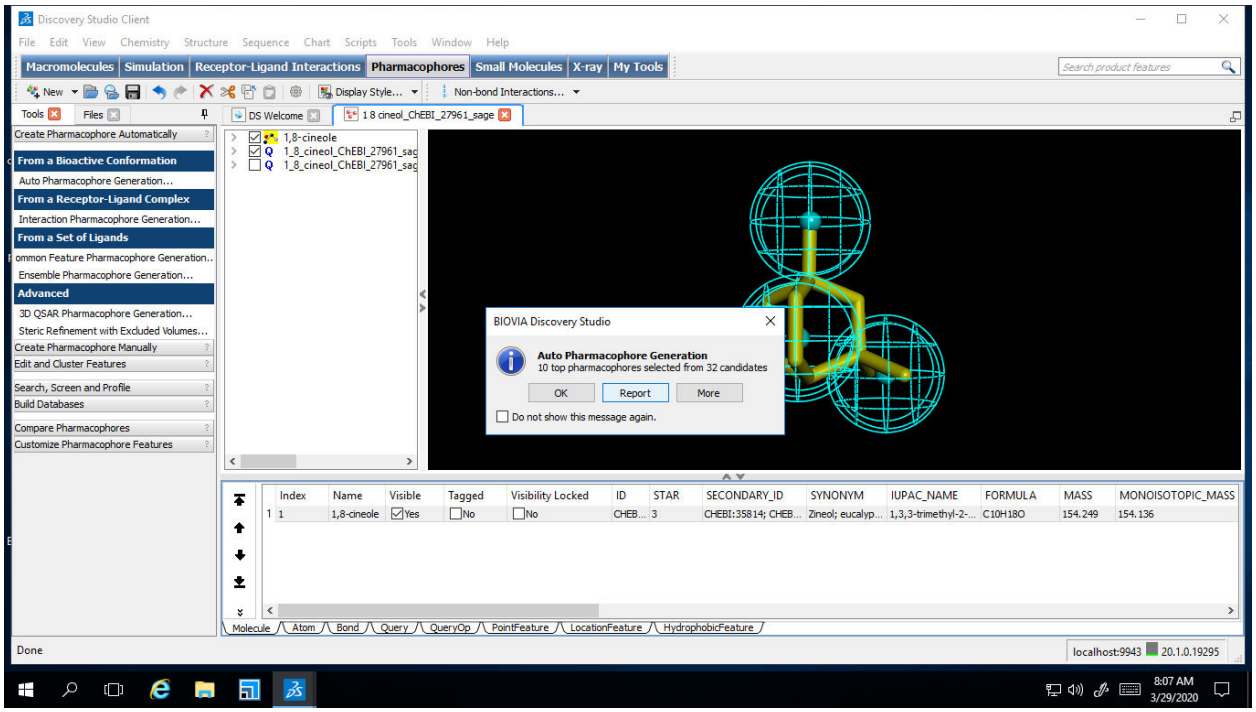

Discovery Studio Client
File Edit View Chemistry Structure Sequence Chart Scripts Tools Window Help
Macromolecules Simulation Receptor-Ligand Interactions Pharmacophores Small Molecules X-ray My Tools
Search product features
Tools Files
DS Welcome
1 8 cineol_ChEBI_27961_sage
Build and Edit Nucleic Acid
Build and Edit Protein
Query Online Databases
Protein Report and Analysis
Prepare Protein
Search Sequences by Similarity
Align Sequences and Structures
Analyze Sequences
Analyze Protein Conservation Pattern
Superimpose Proteins
Create Homology Models
Search Side-Chain Rotamers
Minimize and Refine Protein
Model Antibody
Dock and Analyze Protein Complexes
Design Protein
Predict Protein Formulation Properties
Calculate Protein Formulation Properties..
Calculate Aggregation Scores...
View Aggregation Sites
Define Protein <Undefined>
View at Cutoff Radius: Unset
Step through aggregation sites.
Show Details of Site
Show Surface
Reset Display
Index Name Visible Tagged Visibility Locked ID STAR SECONDARY_ID SYNONYM IUPAC_NAME FORMULA MASS MONOISOTOPIC_MASS
1 1,8-cineole Yes No No CHEB... 3 CHEBI:35814; CHEB... Zineol; eucalyp... 1,3,3-trimethyl-2-... C10H18O 154.249 154.136
Molecule Atom Bond
Use the Select tool to select one or more objects. Click to select an object, drag to select multiple objects.
localhost:9943 20.1.0.19295
8:04 AM
3/29/2020

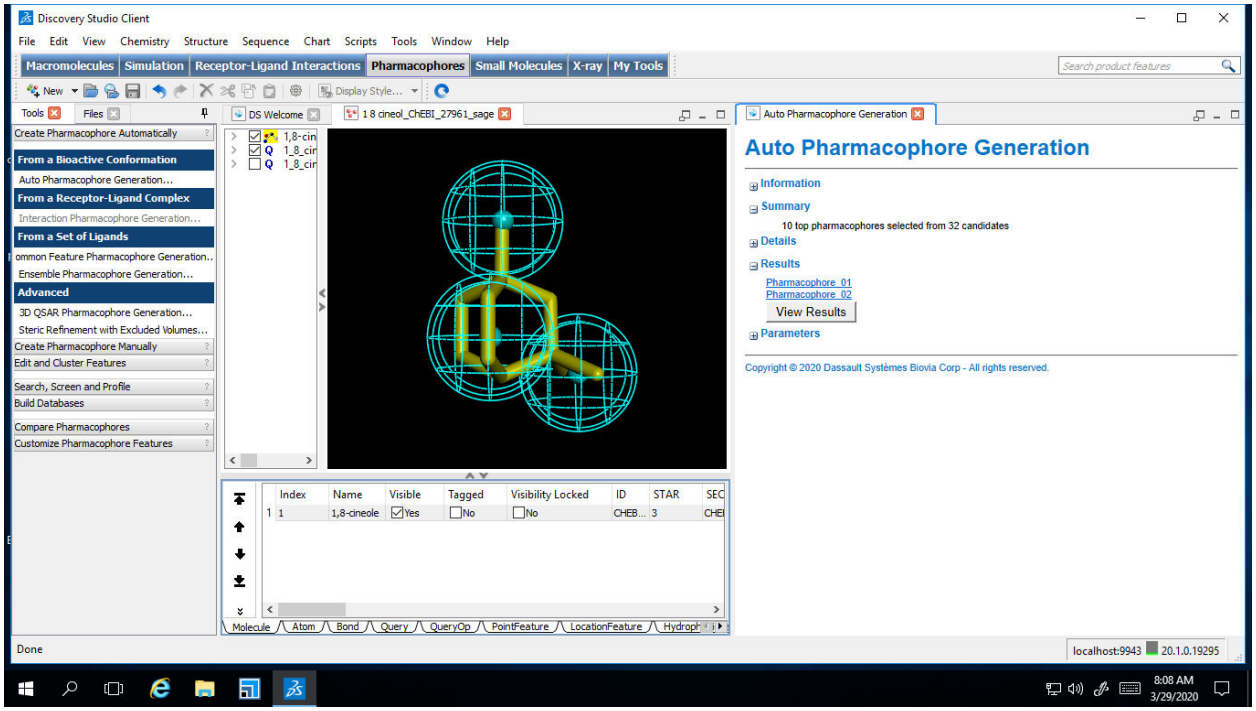

Discovery Studio Client
File Edit View Chemistry Structure Sequence Chart Scripts Tools Window Help
Macromolecules
Pharmacophores
Receptor-Ligand Interactions
Simulation
Small Molecules
X-ray
Create Pharmacophore Automatically
Create Pharmacophore Manuall
Edit and Cluster Features
Search, Screen and Profile
Build Databases
Compare Pharmacophores
Customize Pharmacophore Features
Open the selected tool panel
From a Bioactive Conformation
Auto Pharmacophore Generation...
From a Receptor-Ligand Complex
Interaction Pharmacophore Generation...
From a Set of Ligands
Ensemble Pharmacophore Generation...
Advanced
3D QSAR Pharmacophore Generation...
Steric Refinement with Excluded Volumes...
Create Pharmacophore Manually
Edit and Cluster Features
Search, Screen and Profile
Build Databases
Compare Pharmacophores
Customize Pharmacophore Features
Index Name Visible Tagged Visibility Locked ID STAR SECONDARY_ID SYNONYM IUPAC_NAME FORMULA MASS MONOISOTOPIC_MASS
1 1,8-cineole Yes No No CHEB... 3 CHEBI:35814; CHEB... Zineol; eucalyp... 1,3,3-trimethyl-2-... C10H18O 154.249 154.136
Molecule Atom Bond
localhost:9943 20.1.0.19295
8:06 AM
3/29/2020

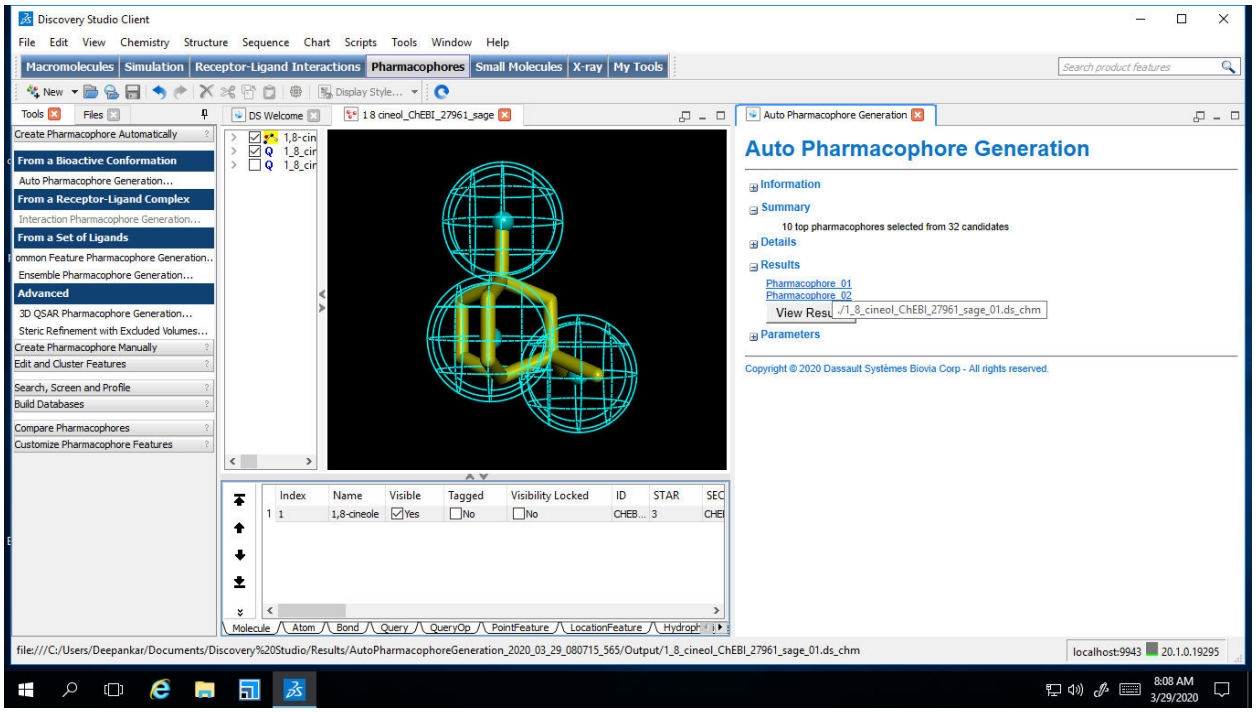

Discovery Studio Client
File Edit View Chemistry Structure Sequence Chart Scripts Tools Window Help
Macromolecules Simulation Receptor-Ligand Interactions Pharmacophores Small Molecules X-ray My Tools
Search product features
New Display Style... Non-bond Interactions...
Tools Files
DS Welcome 1 8 cineol_ChEBI_27961_sage
Create Pharmacophore Automatically
From a Bioactive Conformation
Auto Pharmacophore Generation...
From a Receptor-Ligand Complex
Interaction Pharmacophore Generation...
From a Set of Ligands
Ensemble Pharmacophore Generation...
Advanced
3D QSAR Pharmacophore Generation...
Steric Refinement with Excluded Volumes...
Create Pharmacophore Manually
Edit and Cluster Features
Search, Screen and Profile
Build Databases
Compare Pharmacophores
Customize Pharmacophore Features
Auto Pharmacophore Generation
Generates a selective pharmacophore from the enumerated pharmacophore features of a single ligand.
Click here for help
Index Name Visible Tagged Visibility Locked ID STAR SECONDARY_ID SYNONYM IUPAC_NAME FORMULA MASS MONOISOTOPIC_MASS
1 1 1,8-cineole Yes No No CHEB... 3 CHEBI:35814; CHEB... Zineol; eucalyp... 1,3,3-trimethyl-2-... C10H18O 154.249 154.136
Molecule Atom Bond
localhost:9943 20.1.0.19295
8:06 AM
3/29/2020

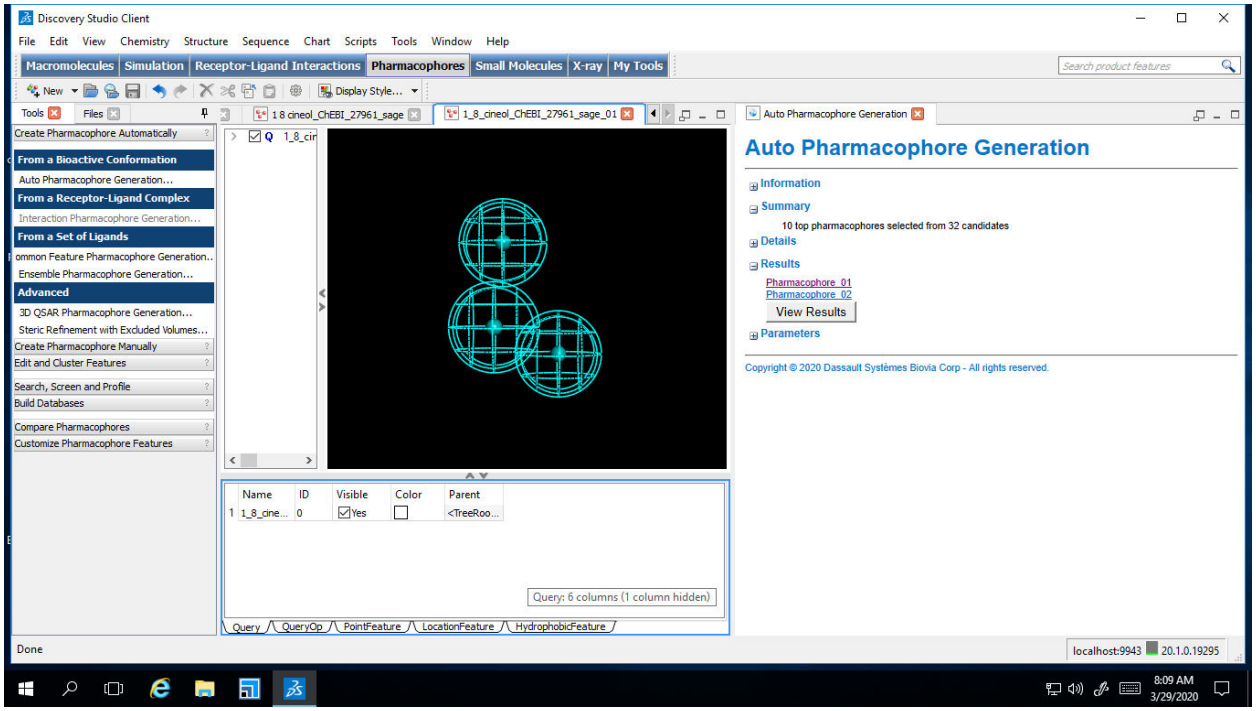

Discovery Studio Client
File Edit View Chemistry Structure Sequence Chart Scripts Tools Window Help
Macromolecules Simulation Receptor-Ligand Interactions Pharmacophores Small Molecules X-ray My Tools
Search product features
New Display Style... Non-bond Interactions...
Tools Files
DS Welcome 1 8 cineol_ChEBI_27961_sage
Create Pharmacophore Automatically
From a Bioactive Conformation
Auto Pharmacophore Generation...
From a Receptor-Ligand Complex
Interaction Pharmacophore Generation...
From a Set of Ligands
Ensemble Pharmacophore Generation...
Advanced
3D QSAR Pharmacophore Generation...
Steric Refinement with Excluded Volumes...
Create Pharmacophore Manually
Edit and Cluster Features
Search, Screen and Profile
Build Databases
Compare Pharmacophores
Customize Pharmacophore Features
Auto Pharmacophore Generation
Parameter Name Parameter Value
Input Ligand 1 8 cineol_ChEBI_27961_sage:Selected
Maximum Features 6
Minimum Feature Distance 2.5
Maximum Pharmacophores 10
Show Parameter Help
Run Options ▼ Cancel Help
Index Name Visible Tagged Visibility Locked ID STAR SECONDARY_ID SYNONYM IUPAC_NAME FORMULA MASS MONOISOTOPIC_MASS
1 1 1,8-cineole Yes No No CHEB... 3 CHEBI:35814; CHEB... Zineol; eucalyp... 1,3,3-trimethyl-2-... C10H18O 154.249 154.136
Molecule Atom Bond
localhost:9943 20.1.0.19295
8:07 AM
3/29/2020

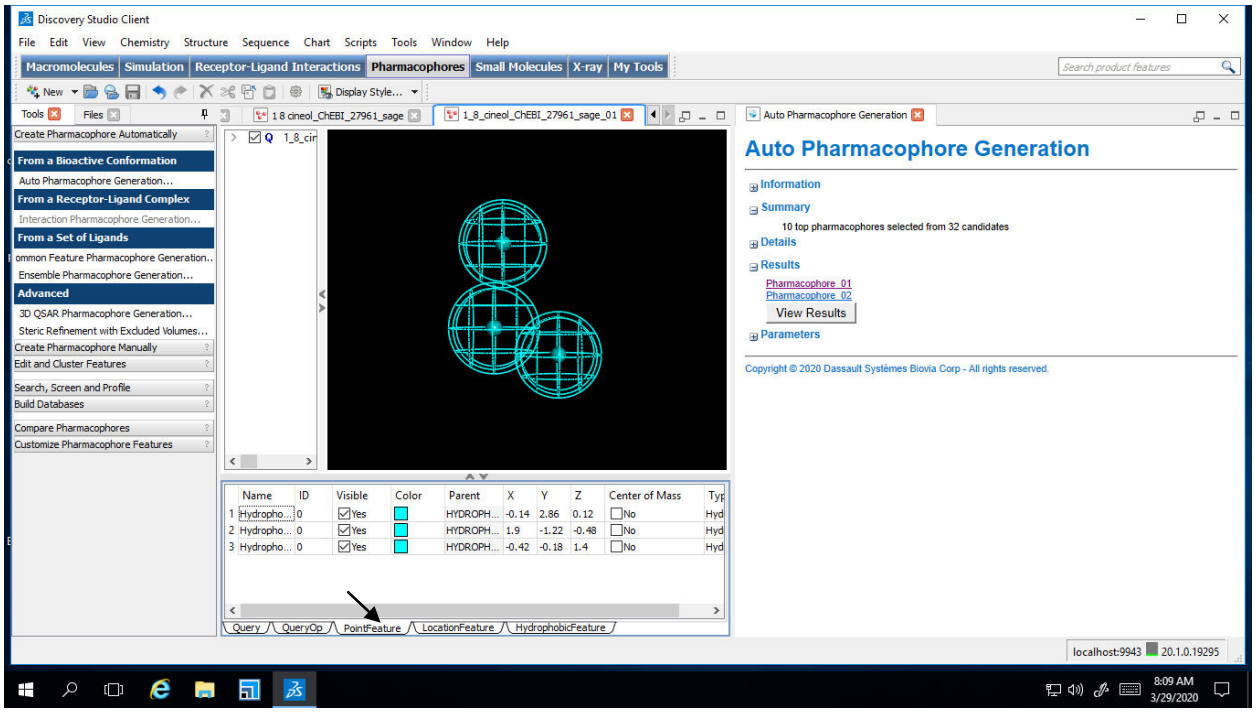

Discovery Studio Client
File Edit View Chemistry Structure Sequence Chart Scripts Tools Window Help
Macromolecules Simulation Receptor-Ligand Interactions Pharmacophores Small Molecules X-ray My Tools
Search product features
New Display Style... Non-bond Interactions...
Tools Files
DS Welcome 1 8 cineol_ChEBI_27961_sage
Create Pharmacophore Automatically
From a Bioactive Conformation
Auto Pharmacophore Generation...
From a Receptor-Ligand Complex
Interaction Pharmacophore Generation...
From a Set of Ligands
ommon Feature Pharmacophore Generation...
Ensemble Pharmacophore Generation...
Advanced
3D QSAR Pharmacophore Generation...
Steric Refinement with Excluded Volumes...
Create Pharmacophore Manually
Edit and Cluster Features
Search, Screen and Profile
Build Databases
Compare Pharmacophores
Customize Pharmacophore Features
Auto Pharmacophore Generation
Map HYDROPHOBIC
Details
Background
Stop
Help
Index Name Visible Tagged Visibility Locked ID STAR SECONDARY_ID SYNONYM IUPAC_NAME FORMULA MASS MONOISOTOPIC_MASS
1 1 1,8-cineole Yes No No CHEB... 3 CHEBI:35814; CHEB... Zineol; eucalyp... 1,3,3-trimethyl-2-... C10H18O 154.249 154.136
Molecule Atom Bond
Done
localhost:9943 20.1.0.19295
8:07 AM
3/29/2020


Discovery Studio Client
File Edit View Chemistry Structure Sequence Chart Scripts Tools Window Help
Macromolecules Simulation Receptor-Ligand Interactions Pharmacophores Small Molecules X-ray My Tools
Search product features
New Display Style... Non-bond Interactions...
Tools Files
DS Welcome 1 8 cineol_ChEBI_27961_sage
Create Pharmacophore Automatically
From a Bioactive Conformation
Auto Pharmacophore Generation...
From a Receptor-Ligand Complex
Interaction Pharmacophore Generation...
From a Set of Ligands
ommon Feature Pharmacophore Generation...
Ensemble Pharmacophore Generation...
Advanced
3D QSAR Pharmacophore Generation...
Steric Refinement with Excluded Volumes...
Create Pharmacophore Manually
Edit and Cluster Features
Search, Screen and Profile
Build Databases
Compare Pharmacophores
Customize Pharmacophore Features
1,8-cineole
1_8_cineol_ChEBI_27961_sag
1_8_cineol_ChEBI_27961_sag
BIOVIA Discovery Studio
Auto Pharmacophore Generation
10 top pharmacophores selected from 32 candidates
OK
Report
More
Do not show this message again.
Index Name Visible Tagged Visibility Locked ID STAR SECONDARY_ID SYNONYM IUPAC_NAME FORMULA MASS MONOISOTOPIC_MASS
1 1 1,8-cineole Yes No No CHEB... 3 CHEBI:35814; CHEB... Zineol; eucalyp... 1,3,3-trimethyl-2-... C10H18O 154.249 154.136
Molecule Atom Bond Query QueryOp PointFeature LocationFeature HydrophobicFeature
Done
localhost:9943 20.1.0.19295
8:07 AM
3/29/2020

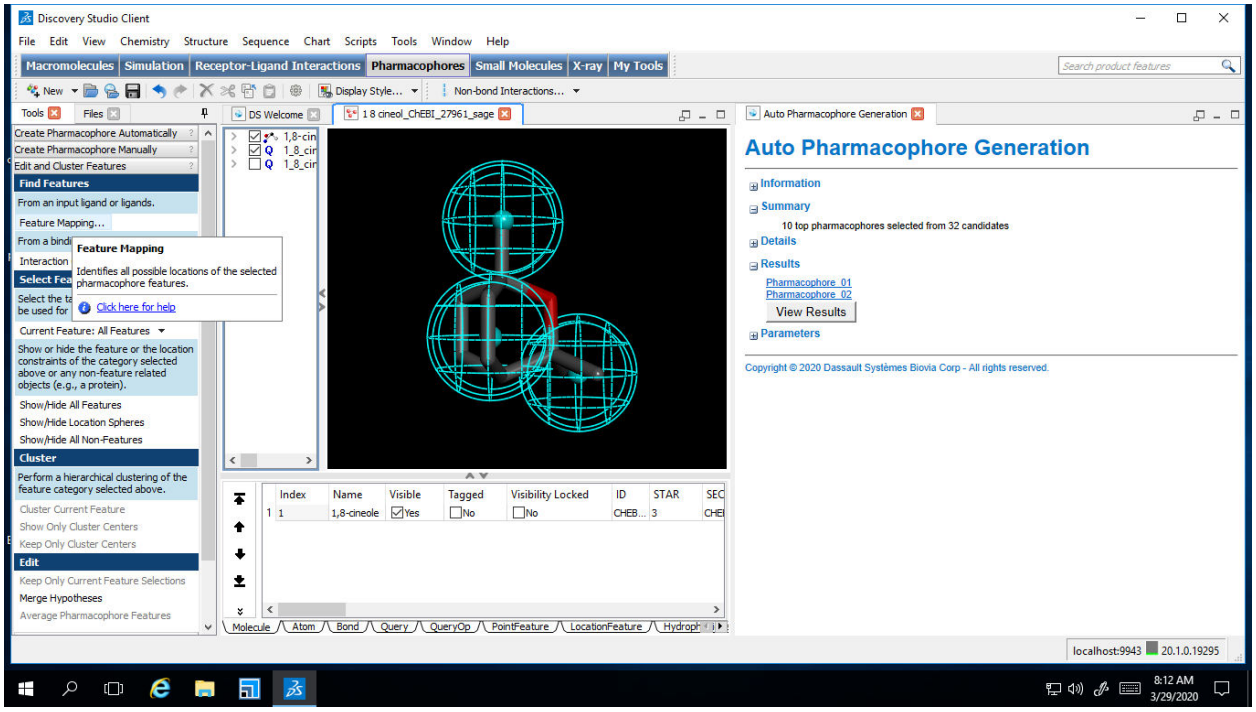

Discovery Studio Client
File Edit View Chemistry Structure Sequence Chart Scripts Tools Window Help
Macromolecules Simulation Receptor-Ligand Interactions Pharmacophores Small Molecules X-ray My Tools
Search product features
Tools Files
DS Welcome
1 8 cineol_ChEBI_27961_sage
Auto Pharmacophore Generation
Create Pharmacophore Automatically
From a Bioactive Conformation
Auto Pharmacophore Generation...
From a Receptor-Ligand Complex
Interaction Pharmacophore Generation...
From a Set of Ligands
ommon Feature Pharmacophore Generation..
Ensemble Pharmacophore Generation...
Advanced
3D QSAR Pharmacophore Generation...
Steric Refinement with Excluded Volumes...
Create Pharmacophore Manually
Edit and Cluster Features
Search, Screen and Profile
Build Databases
Compare Pharmacophores
Customize Pharmacophore Features
Auto Pharmacophore Generation
Information
Summary
10 top pharmacophores selected from 32 candidates
Details
Results
Pharmacophore_01
Pharmacophore_02
View Results
Parameters
Copyright © 2020 Dassault Systèmes Biovia Corp - All rights reserved.
Index Name Visible Tagged Visibility Locked ID STAR
1 1,8-cineole Yes No No
Molecule Atom Bond Query QueryOp PointFeature LocationFeature
Done
localhost:9943 20.1.0.19295
8:08 AM
3/29/2020

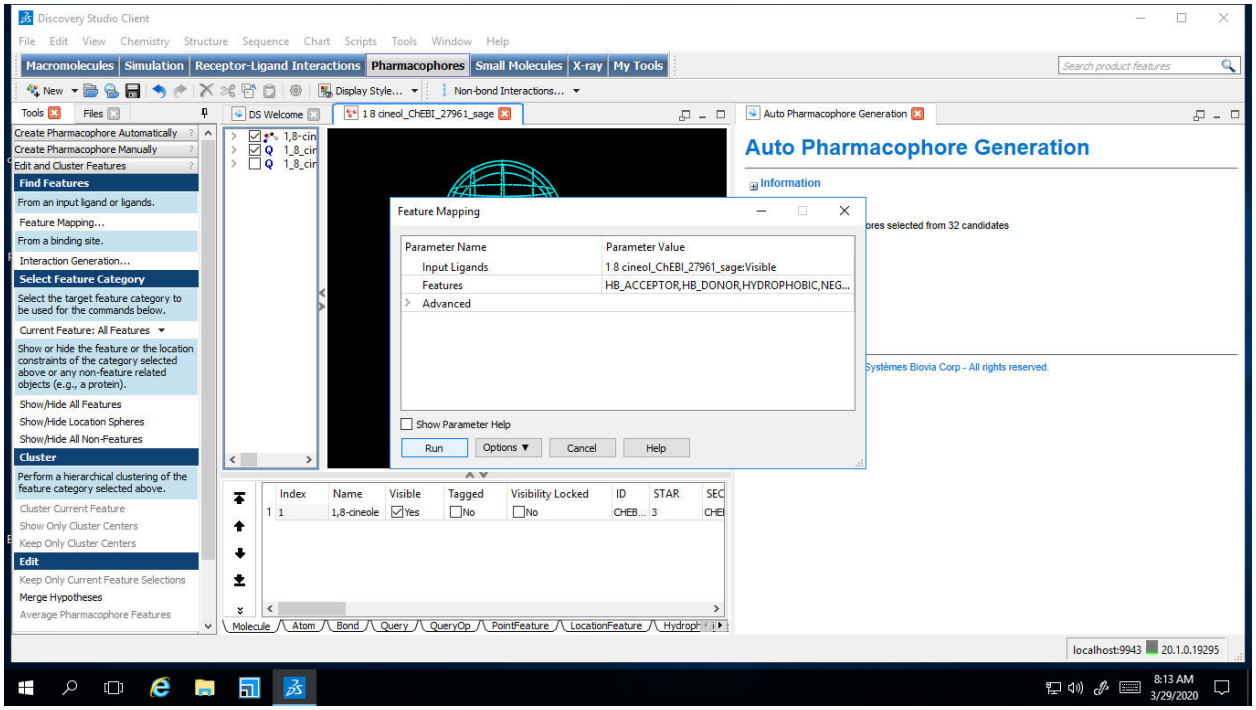

Discovery Studio Client
File Edit View Chemistry Structure Sequence Chart Scripts Tools Window Help
Macromolecules Simulation Receptor-Ligand Interactions Pharmacophores Small Molecules X-ray My Tools
Search product features
Tools Files
DS Welcome
1 8 cineol_ChEBI_27961_sage
Auto Pharmacophore Generation
Create Pharmacophore Automatically
From a Bioactive Conformation
Auto Pharmacophore Generation...
From a Receptor-Ligand Complex
Interaction Pharmacophore Generation...
From a Set of Ligands
ommon Feature Pharmacophore Generation..
Ensemble Pharmacophore Generation...
Advanced
3D QSAR Pharmacophore Generation...
Steric Refinement with Excluded Volumes...
Create Pharmacophore Manually
Edit and Cluster Features
Search, Screen and Profile
Build Databases
Compare Pharmacophores
Customize Pharmacophore Features
Auto Pharmacophore Generation
Information
Summary
10 top pharmacophores selected from 32 candidates
Details
Results
Pharmacophore_01
Pharmacophore_02
View Resu
./1_8_cineol_ChEBI_27961_sage_01.ds_chm
Parameters
Copyright © 2020 Dassault Systèmes Biovia Corp - All rights reserved.
Index Name Visible Tagged Visibility Locked ID STAR
1 1,8-cineole Yes No No
Molecule Atom Bond Query QueryOp PointFeature LocationFeature
file:///C:/Users/Deepankar/Documents/Discovery%20Studio/Results/AutoPharmacophoreGeneration_2020_03_29_080715_565/Output/1_8_cineol_ChEBI_27961_sage_01.ds_chm
localhost:9943 20.1.0.19295
8:08 AM
3/29/2020

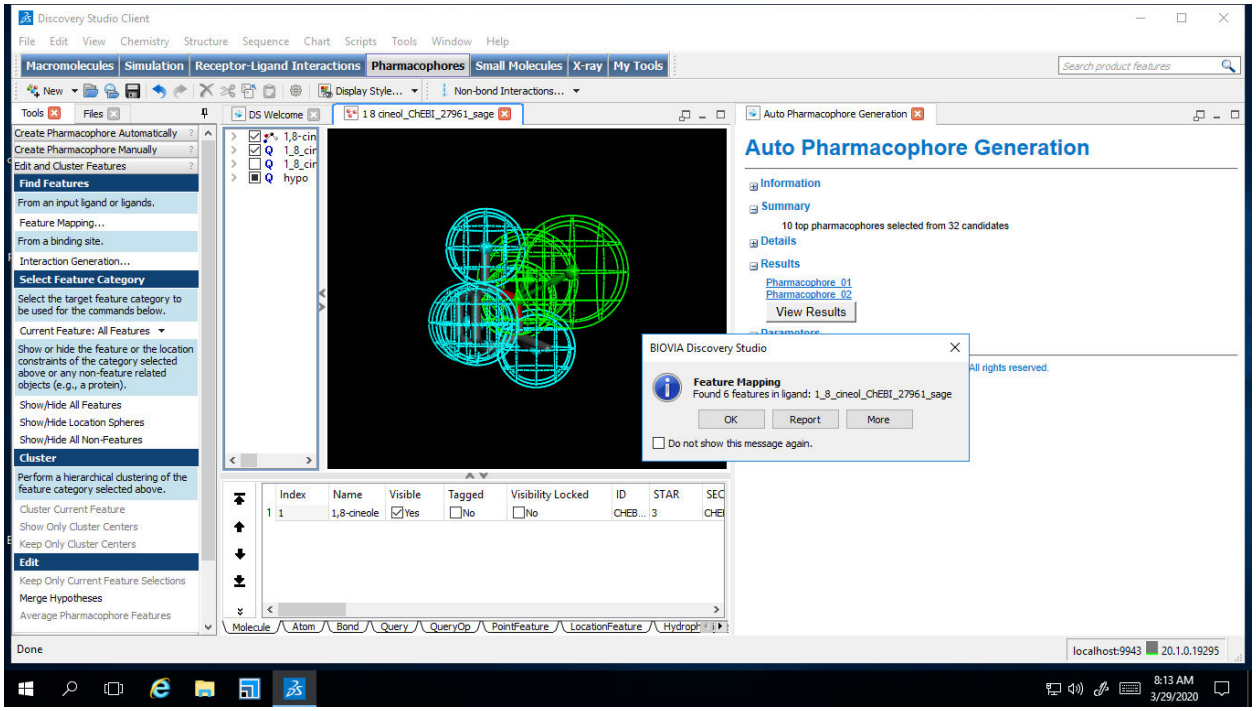

Discovery Studio Client
File Edit View Chemistry Structure Sequence Chart Scripts Tools Window Help
Macromolecules Simulation Receptor-Ligand Interactions Pharmacophores Small Molecules X-ray My Tools
Search product features
New
Display Style...
Tools
Files
1 8 cineol_ChEBI_27961_sage
1_8_cineol_ChEBI_27961_sage_01
Auto Pharmacophore Generation
Create Pharmacophore Automatically
From a Bioactive Conformation
Auto Pharmacophore Generation...
From a Receptor-Ligand Complex
Interaction Pharmacophore Generation...
From a Set of Ligands
ommon Feature Pharmacophore Generation...
Ensemble Pharmacophore Generation...
Advanced
3D QSAR Pharmacophore Generation...
Steric Refinement with Excluded Volumes...
Create Pharmacophore Manually
Edit and Cluster Features
Search, Screen and Profile
Build Databases
Compare Pharmacophores
Customize Pharmacophore Features
Auto Pharmacophore Generation
Information
Summary
10 top pharmacophores selected from 32 candidates
Details
Results
Pharmacophore_01
Pharmacophore_02
View Results
Parameters
Copyright © 2020 Dassault Systèmes Biovia Corp - All rights reserved.
Name ID Visible Color Parent
1 1_8_cine... 0 Yes <TreeRoo...
Query: 6 columns (1 column hidden)
Query QueryOp PointFeature LocationFeature HydrophobicFeature
Done
localhost:9943 20.1.0.19295
8:09 AM
3/29/2020

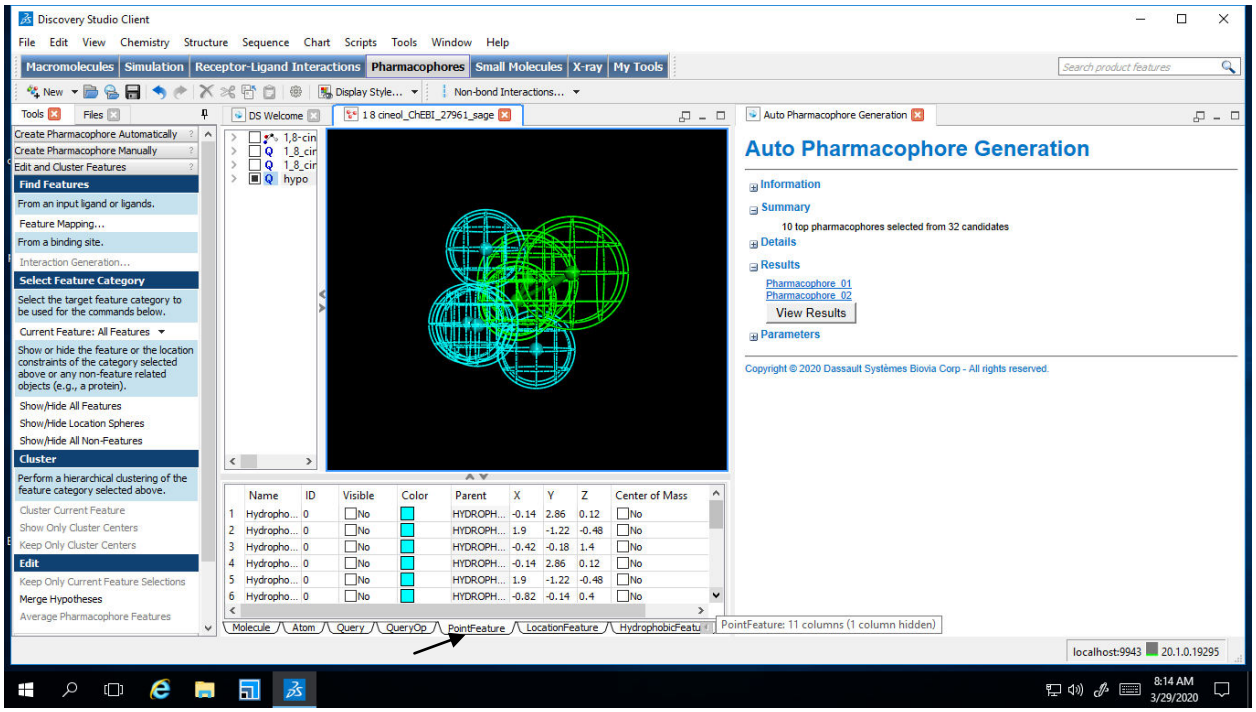

Discovery Studio Client
File Edit View Chemistry Structure Sequence Chart Scripts Tools Window Help
Macromolecules Simulation Receptor-Ligand Interactions Pharmacophores Small Molecules X-ray My Tools
Search product features
New
Display Style...
Tools
Files
1 8 cineol_ChEBI_27961_sage
1_8_cineol_ChEBI_27961_sage_01
Auto Pharmacophore Generation
Create Pharmacophore Automatically
From a Bioactive Conformation
Auto Pharmacophore Generation...
From a Receptor-Ligand Complex
Interaction Pharmacophore Generation...
From a Set of Ligands
ommon Feature Pharmacophore Generation...
Ensemble Pharmacophore Generation...
Advanced
3D QSAR Pharmacophore Generation...
Steric Refinement with Excluded Volumes...
Create Pharmacophore Manually
Edit and Cluster Features
Search, Screen and Profile
Build Databases
Compare Pharmacophores
Customize Pharmacophore Features
Auto Pharmacophore Generation
Information
Summary
10 top pharmacophores selected from 32 candidates
Details
Results
Pharmacophore_01
Pharmacophore_02
View Results
Parameters
Copyright © 2020 Dassault Systèmes Biovia Corp - All rights reserved.
Name ID Visible Color Parent X Y Z Center of Mass
1 Hydropho... 0 Yes HYDROPH... -0.14 2.86 0.12 No
2 Hydropho... 0 Yes HYDROPH... 1.9 -1.22 -0.48 No
3 Hydropho... 0 Yes HYDROPH... -0.42 -0.18 1.4 No
Query QueryOp PointFeature LocationFeature HydrophobicFeature
localhost:9943 20.1.0.19295
8:09 AM
3/29/2020

Pharmacophore feature






Discovery Studio Client
Auto Pharmacophore Generation
Information
Summary
10 top pharmacophores selected from 32 candidates
Details
Results
Pharmacophore_01
Pharmacophore_02
View Results
BIOVIA Discovery Studio
Feature Mapping
Found 6 features in ligand: 1_8_cineol_ChEBI_27961_sage
OK
Report
More
Do not show this message again.
Done
localhost:9943
20.1.0.19295
8:13 AM
3/29/2020


Discovery Studio Client
Auto Pharmacophore Generation
Information
Summary
10 top pharmacophores selected from 32 candidates
Details
Results
Pharmacophore_01
Pharmacophore_02
View Results
Parameters
Copyright © 2020 Dassault Systèmes Biovia Corp - All rights reserved.
PointFeature: 11 columns (1 column hidden)
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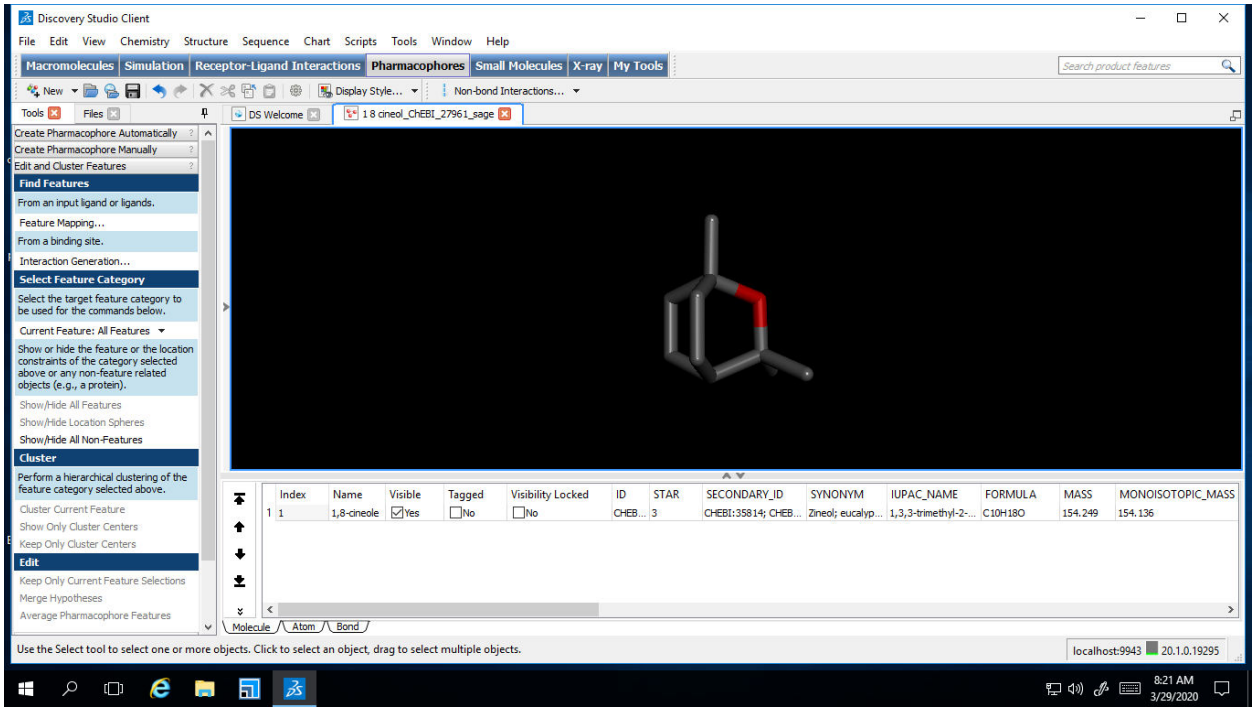
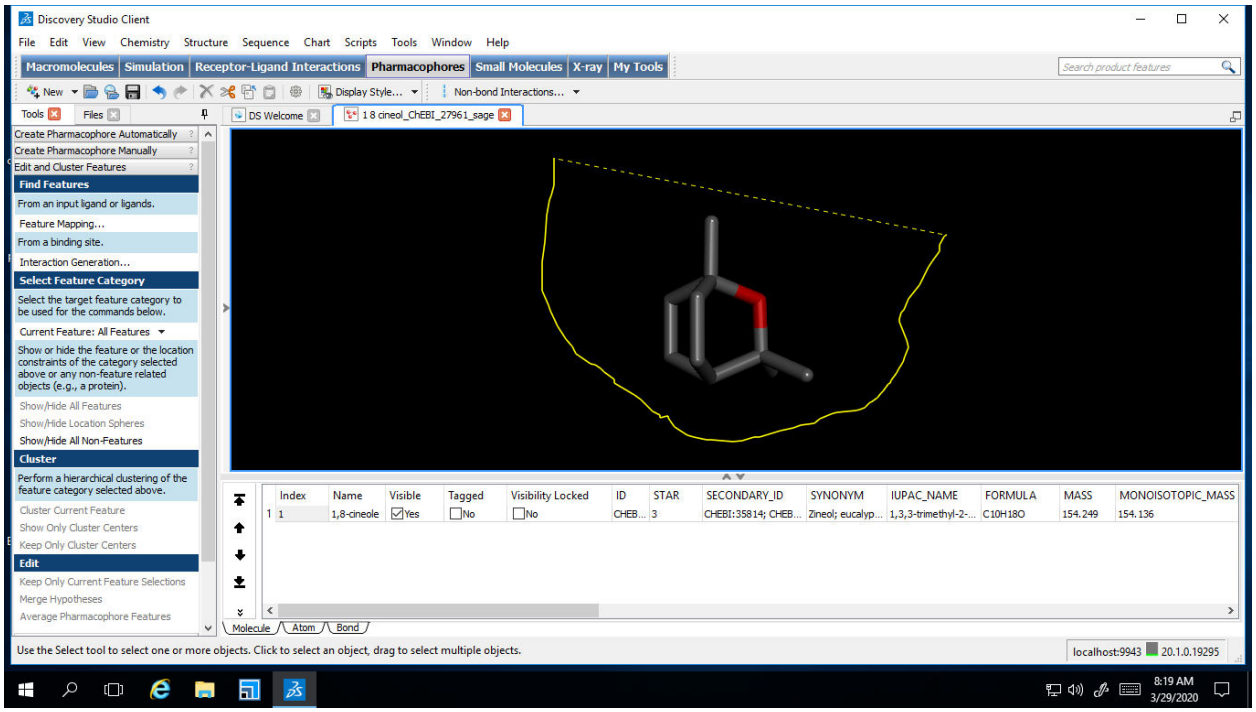
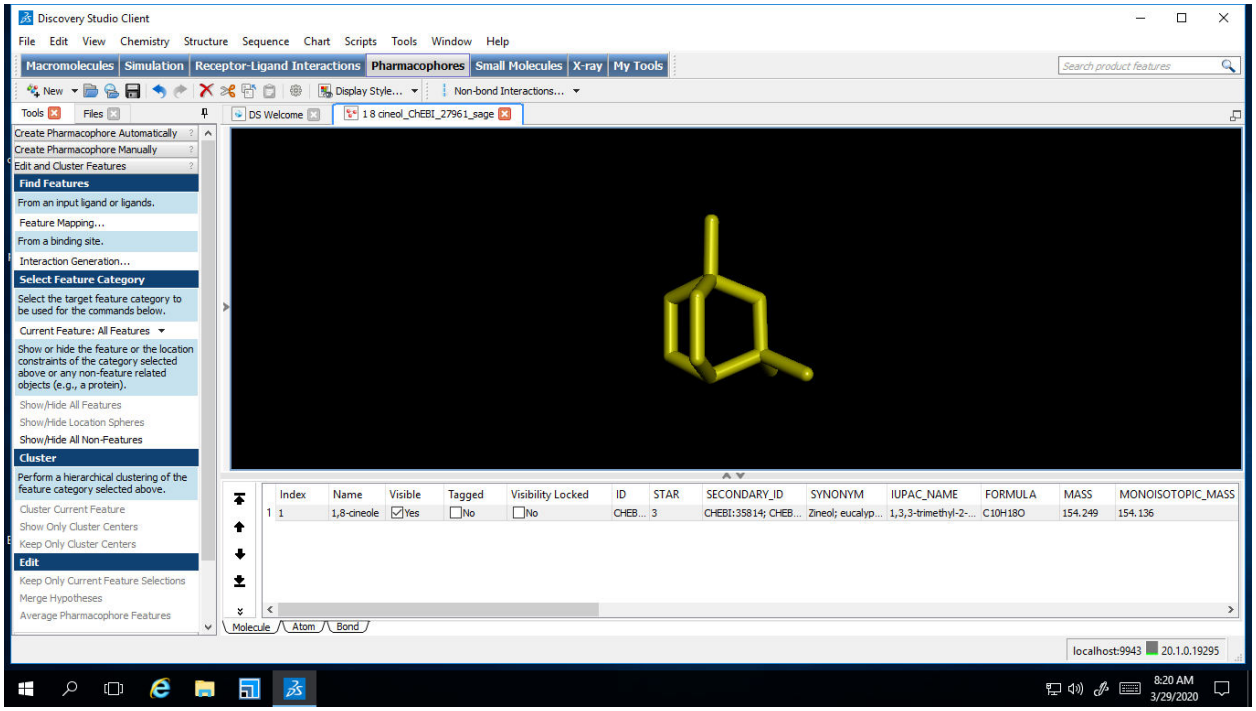
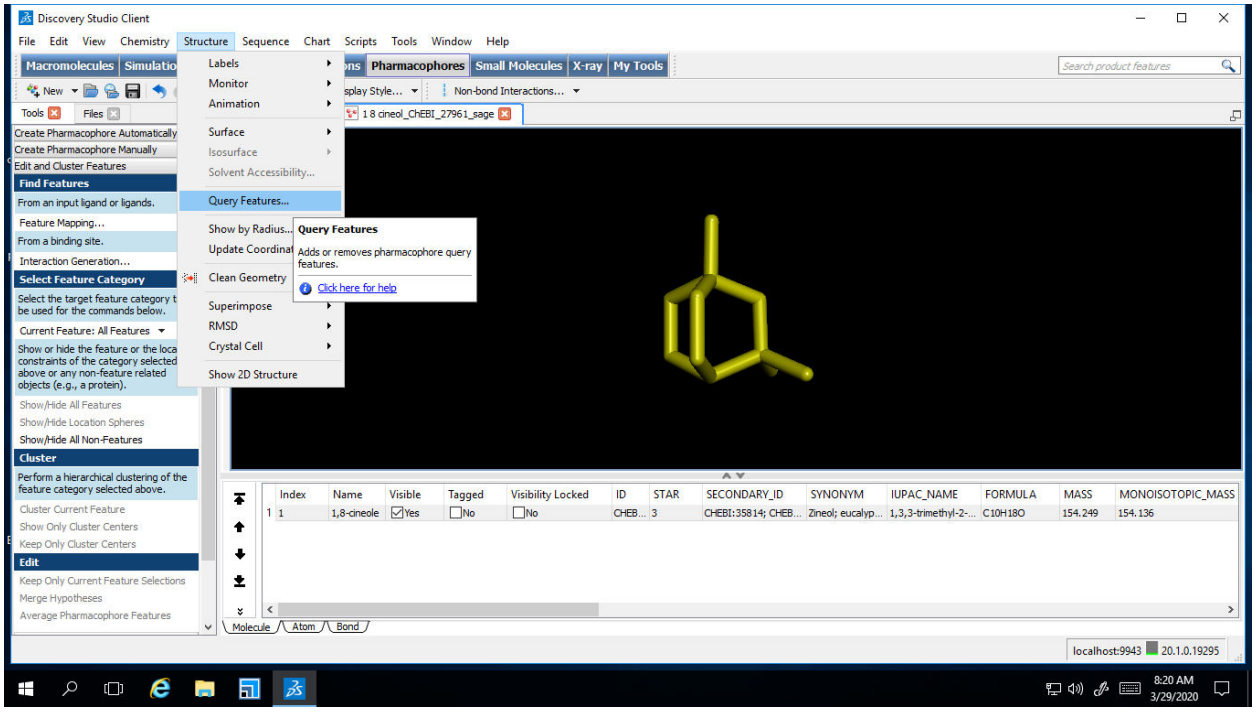
20.1.0.19295
8:14 AM
3/29/2020

Pharmacophore database search






Discovery Studio Client
File Edit View Chemistry Structure Sequence Chart Scripts Tools Window Help
Macromolecules Simulation Receptor-Ligand Interactions Pharmacophores Small Molecules X-ray My Tools
Search product features
New Display Style... Non-bond Interactions...
Tools Files
DS Welcome 1 8 cineol_ChEBI_27961_sage
Create Pharmacophore Automatically
Create Pharmacophore Manually
Edit and Cluster Features
Find Features
From an input ligand or ligands.
Feature Mapping...
From a binding site.
Interaction Generation...
Select Feature Category
Select the target feature category to be used for the commands below.
Current Feature: All Features
Show or hide the feature or the location constraints of the category selected above or any non-feature related objects (e.g., a protein).
Show/Hide All Features
Show/Hide Location Spheres
Show/Hide All Non-Features
Cluster
Perform a hierarchical clustering of the feature category selected above.
Cluster Current Feature
Show Only Cluster Centers
Keep Only Cluster Centers
Edit
Keep Only Current Feature Selections
Merge Hypotheses
Average Pharmacophore Features
Index Name Visible Tagged Visibility Locked ID STAR SECONDARY_ID SYNONYM IUPAC_NAME FORMULA MASS MONOISOTOPIC_MASS
1 1 1,8-cineole Yes No No CHEB... 3 CHEBI:35814; CHEB... Zineol; eucalyp... 1,3,3-trimethyl-2-... C10H18O 154.249 154.136
Molecule Atom Bond
localhost:9943 20.1.0.19295
8:20 AM
3/29/2020


Discovery Studio Client
File Edit View Chemistry Structure Sequence Chart Scripts Tools Window Help
Labels
Monitor
Animation
Surface
Isosurface
Solvent Accessibility...
Query Features...
Show by Radius...
Update Coordinat
Clean Geometry
Superimpose
RMSD
Crystal Cell
Show 2D Structure
Query Features
Adds or removes pharmacophore query features.
Click here for help
Macromolecules Pharmacophores Small Molecules X-ray My Tools
Search product features
New Non-bond Interactions...
Tools Files
1 8 cineol_ChEBI_27961_sage
Create Pharmacophore Automatically
Create Pharmacophore Manually
Edit and Cluster Features
Find Features
From an input ligand or ligands.
Feature Mapping...
From a binding site.
Interaction Generation...
Select Feature Category
Current Feature: All Features
Show/Hide All Features
Show/Hide Location Spheres
Show/Hide All Non-Features
Cluster
Perform a hierarchical clustering of the feature category selected above.
Cluster Current Feature
Show Only Cluster Centers
Keep Only Cluster Centers
Edit
Keep Only Current Feature Selections
Merge Hypotheses
Average Pharmacophore Features
Index Name Visible Tagged Visibility Locked ID STAR SECONDARY_ID SYNONYM IUPAC_NAME FORMULA MASS MONOISOTOPIC_MASS
1 1 1,8-cineole Yes No No CHEB... 3 CHEBI:35814; CHEB... Zineol; eucalyp... 1,3,3-trimethyl-2-... C10H18O 154.249 154.136
Molecule Atom Bond
localhost:9943 20.1.0.19295
8:20 AM
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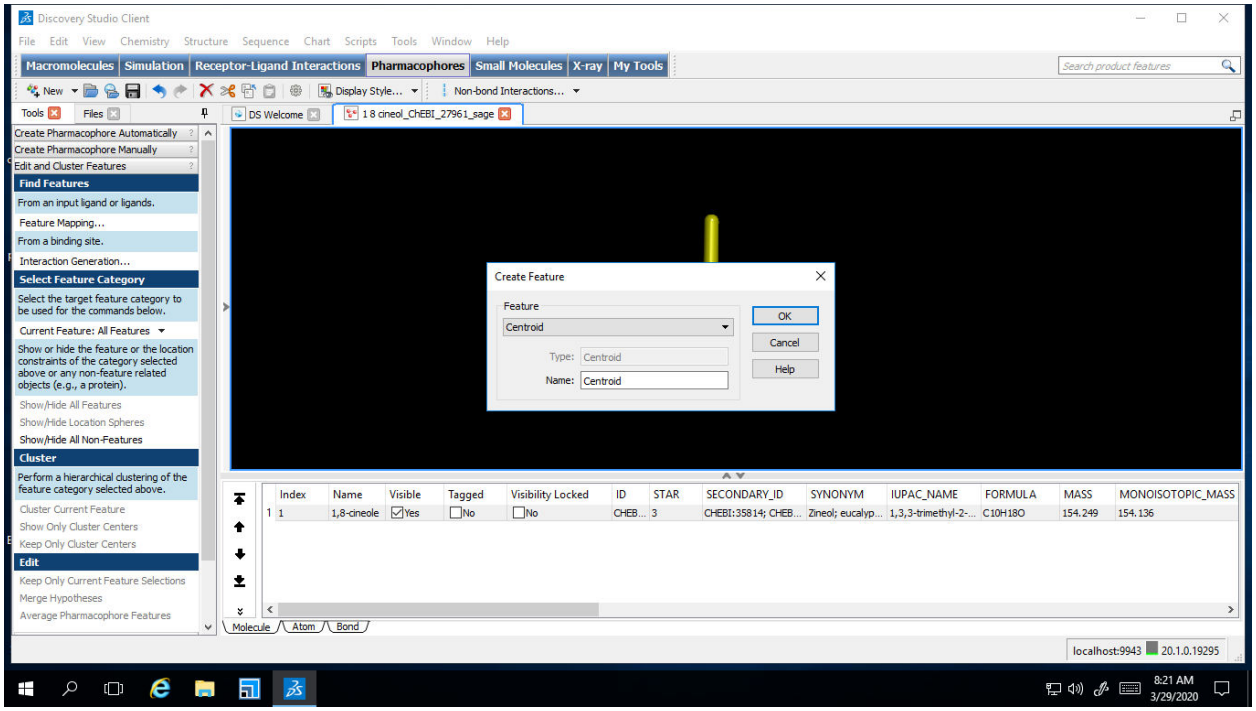
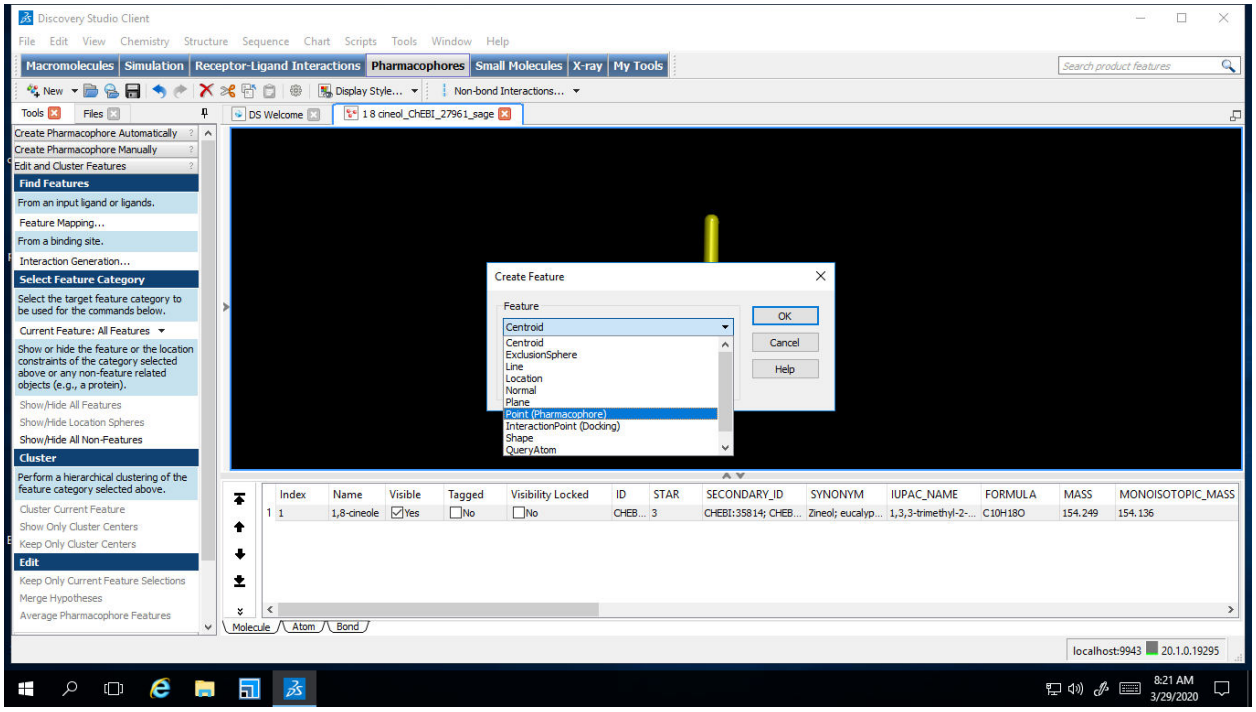

Discovery Studio Client
File Edit View Chemistry Structure Sequence Chart Scripts Tools Window Help
Macromolecules Simulation Receptor-Ligand Interactions Pharmacophores Small Molecules X-ray My Tools
Search product features
New Display Style... Non-bond Interactions...
Tools Files
DS Welcome 1 8 cineol_ChEBI_27961_sage
Create Pharmacophore Automatically
Create Pharmacophore Manually
Edit and Cluster Features
Find Features
From an input ligand or ligands.
Feature Mapping...
From a binding site.
Interaction Generation...
Select Feature Category
Select the target feature category to be used for the commands below.
Current Feature: All Features
Show or hide the feature or the location constraints of the category selected above or any non-feature related objects (e.g., a protein).
Show/Hide All Features
Show/Hide Location Spheres
Show/Hide All Non-Features
Cluster
Perform a hierarchical clustering of the feature category selected above.
Cluster Current Feature
Show Only Cluster Centers
Keep Only Cluster Centers
Edit
Keep Only Current Feature Selections
Merge Hypotheses
Average Pharmacophore Features
Create Feature
Feature
Centroid
OK
Cancel
Help
Type: Centroid
Name: Centroid
Index Name Visible Tagged Visibility Locked ID STAR SECONDARY_ID SYNONYM IUPAC_NAME FORMULA MASS MONOISOTOPIC_MASS
1 1 1,8-cineole Yes No No CHEB... 3 CHEBI:35814; CHEB... Zineol; eucalyp... 1,3,3-trimethyl-2-... C10H18O 154.249 154.136
Molecule Atom Bond
localhost:9943 20.1.0.19295
8:21 AM
3/29/2020


Discovery Studio Client
File Edit View Chemistry Structure Sequence Chart Scripts Tools Window Help
Macromolecules Simulation Receptor-Ligand Interactions Pharmacophores Small Molecules X-ray My Tools
Search product features
New Display Style... Non-bond Interactions...
Tools Files
DS Welcome 1 8 cineol_ChEBI_27961_sage
Create Pharmacophore Automatically
Create Pharmacophore Manually
Edit and Cluster Features
Find Features
From an input ligand or ligands.
Feature Mapping...
From a binding site.
Interaction Generation...
Select Feature Category
Select the target feature category to be used for the commands below.
Current Feature: All Features
Show or hide the feature or the location constraints of the category selected above or any non-feature related objects (e.g., a protein).
Show/Hide All Features
Show/Hide Location Spheres
Show/Hide All Non-Features
Cluster
Perform a hierarchical clustering of the feature category selected above.
Cluster Current Feature
Show Only Cluster Centers
Keep Only Cluster Centers
Edit
Keep Only Current Feature Selections
Merge Hypotheses
Average Pharmacophore Features
Create Feature
Feature
Centroid
Centroid
ExclusionSphere
Line
Location
Normal
Plane
Point (Pharmacophore)
InteractionPoint (Docking)
Shape
QueryAtom
OK
Cancel
Help
Index Name Visible Tagged Visibility Locked ID STAR SECONDARY_ID SYNONYM IUPAC_NAME FORMULA MASS MONOISOTOPIC_MASS
1 1 1,8-cineole Yes No No CHEB... 3 CHEBI:35814; CHEB... Zineol; eucalyp... 1,3,3-trimethyl-2-... C10H18O 154.249 154.136
Molecule Atom Bond
localhost:9943 20.1.0.19295
8:21 AM
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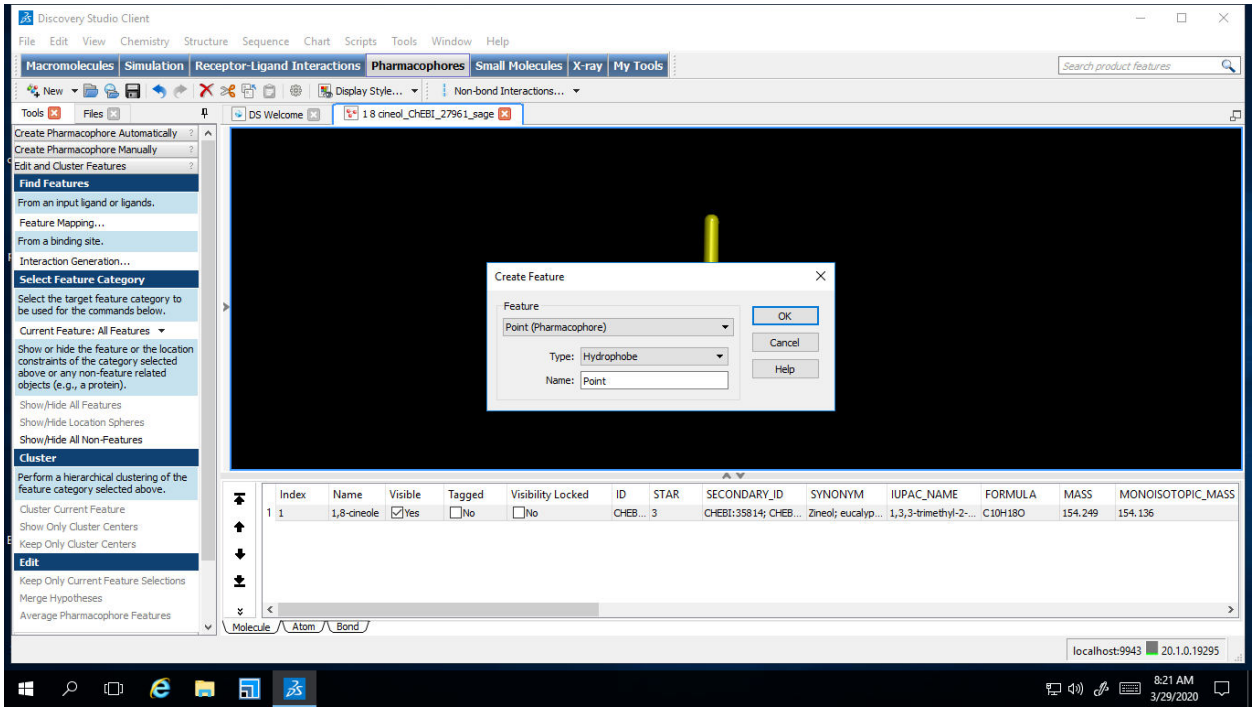
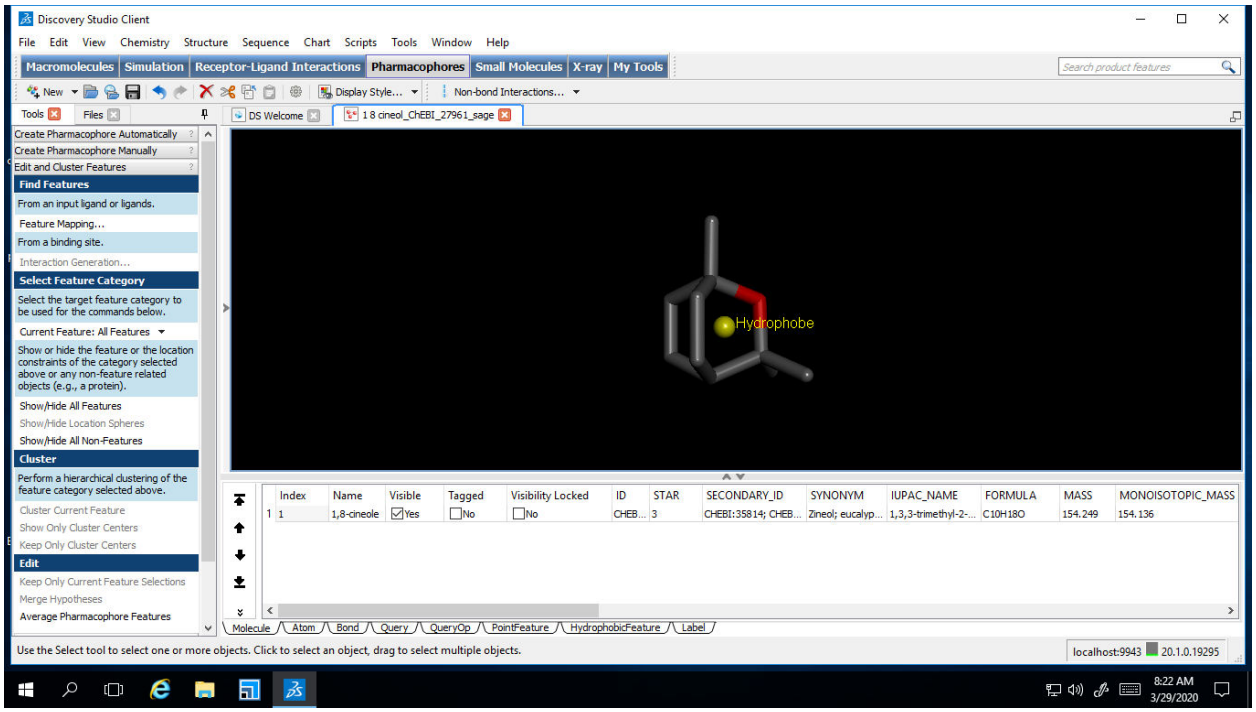

Discovery Studio Client
File Edit View Chemistry Structure Sequence Chart Scripts Tools Window Help
Macromolecules Simulation Receptor-Ligand Interactions Pharmacophores Small Molecules X-ray My Tools
Search product features
New Display Style... Non-bond Interactions...
Tools Files
DS Welcome 1 8 cineol_ChEBI_27961_sage
Create Pharmacophore Automatically
Create Pharmacophore Manually
Edit and Cluster Features
Find Features
From an input ligand or ligands.
Feature Mapping...
From a binding site.
Interaction Generation...
Select Feature Category
Select the target feature category to be used for the commands below.
Current Feature: All Features
Show or hide the feature or the location constraints of the category selected above or any non-feature related objects (e.g., a protein).
Show/Hide All Features
Show/Hide Location Spheres
Show/Hide All Non-Features
Cluster
Perform a hierarchical clustering of the feature category selected above.
Cluster Current Feature
Show Only Cluster Centers
Keep Only Cluster Centers
Edit
Keep Only Current Feature Selections
Merge Hypotheses
Average Pharmacophore Features
Create Feature
Feature
Point (Pharmacophore)
OK
Cancel
Help
Type: Hydrophobe
Name: Point
Index Name Visible Tagged Visibility Locked ID STAR SECONDARY_ID SYNONYM IUPAC_NAME FORMULA MASS MONOISOTOPIC_MASS
1 1 1,8-cineole Yes No No CHEB... 3 CHEBI:35814; CHEB... Zineol; eucalyp... 1,3,3-trimethyl-2-... C10H18O 154.249 154.136
Molecule Atom Bond
localhost:9943 20.1.0.19295
8:21 AM
3/29/2020


Discovery Studio Client
File Edit View Chemistry Structure Sequence Chart Scripts Tools Window Help
Macromolecules Simulation Receptor-Ligand Interactions Pharmacophores Small Molecules X-ray My Tools
Search product features
New Display Style... Non-bond Interactions...
Tools Files
DS Welcome 1 8 cineol_ChEBI_27961_sage
Create Pharmacophore Automatically
Create Pharmacophore Manually
Edit and Cluster Features
Find Features
From an input ligand or ligands.
Feature Mapping...
From a binding site.
Interaction Generation...
Select Feature Category
Select the target feature category to be used for the commands below.
Current Feature: All Features
Show or hide the feature or the location constraints of the category selected above or any non-feature related objects (e.g., a protein).
Show/Hide All Features
Show/Hide Location Spheres
Show/Hide All Non-Features
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Perform a hierarchical clustering of the feature category selected above.
Cluster Current Feature
Show Only Cluster Centers
Keep Only Cluster Centers
Edit
Keep Only Current Feature Selections
Merge Hypotheses
Average Pharmacophore Features
Hydrophobe
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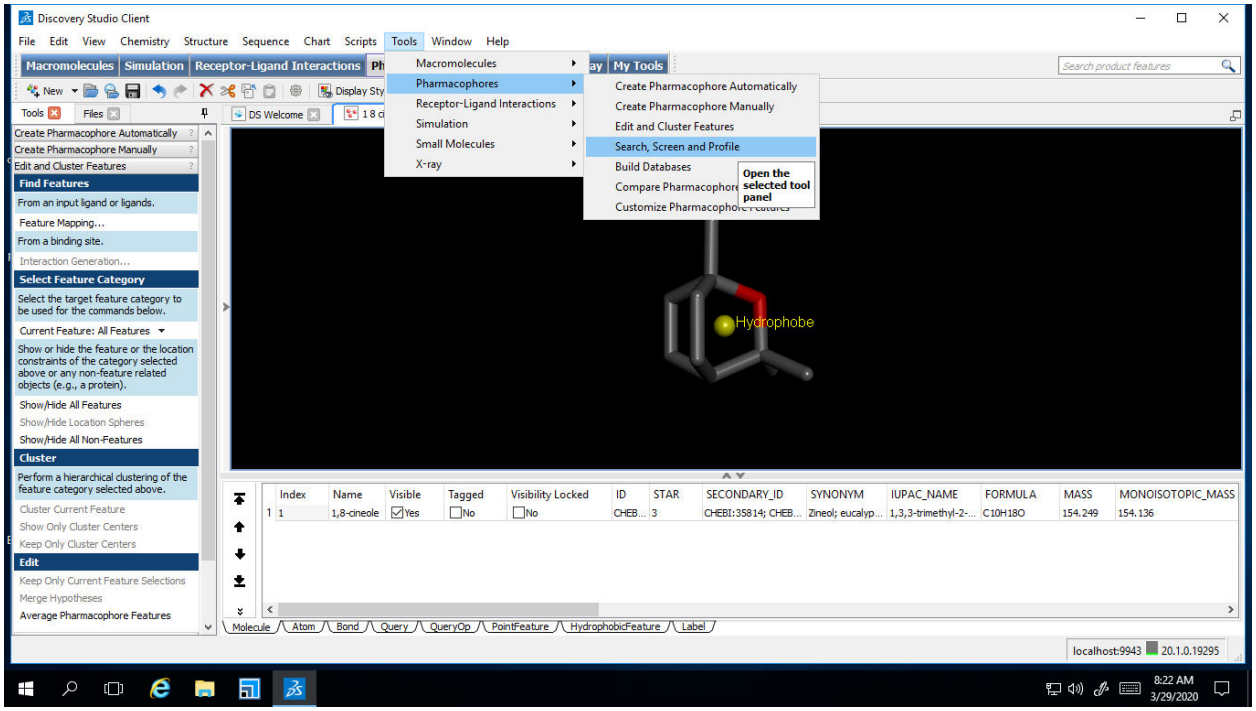
Molecule Atom Bond Query QueryOp PointFeature HydrophobicFeature Label
Use the Select tool to select one or more objects. Click to select an object, drag to select multiple objects.
localhost:9943 20.1.0.19295
8:22 AM
3/29/2020


Discovery Studio Client
File Edit View Chemistry Structure Sequence Chart Scripts Tools Window Help
Macromolecules Simulation Receptor-Ligand Interactions Pharmacophores Small Molecules X-ray My Tools
Search product features
Macromolecules
Pharmacophores
Receptor-Ligand Interactions
Simulation
Small Molecules
X-ray
Create Pharmacophore Automatically
Create Pharmacophore Manually
Edit and Cluster Features
Search, Screen and Profile
Build Databases
Compare Pharmacophore
Customize Pharmacophore Features
Open the selected tool panel
Tools Files
DS Welcome
Create Pharmacophore Automatically
Create Pharmacophore Manually
Edit and Cluster Features
Find Features
From an input ligand or ligands.
Feature Mapping...
From a binding site.
Interaction Generation...
Select Feature Category
Select the target feature category to be used for the commands below.
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Show/Hide Location Spheres
Show/Hide All Non-Features
Cluster
Perform a hierarchical clustering of the feature category selected above.
Cluster Current Feature
Show Only Cluster Centers
Keep Only Cluster Centers
Edit
Keep Only Current Feature Selections
Merge Hypotheses
Average Pharmacophore Features
Hydrophobe
Index Name Visible Tagged Visibility Locked ID STAR SECONDARY_ID SYNONYM IUPAC_NAME FORMULA MASS MONOISOTOPIC_MASS
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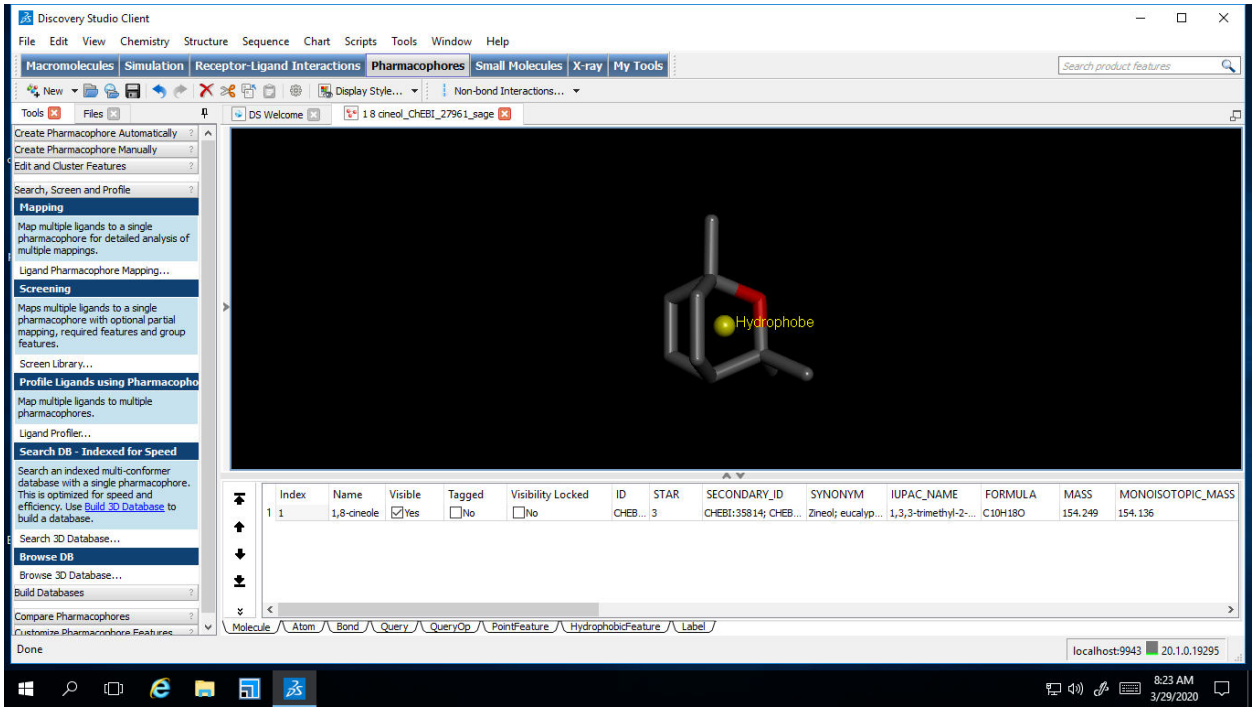
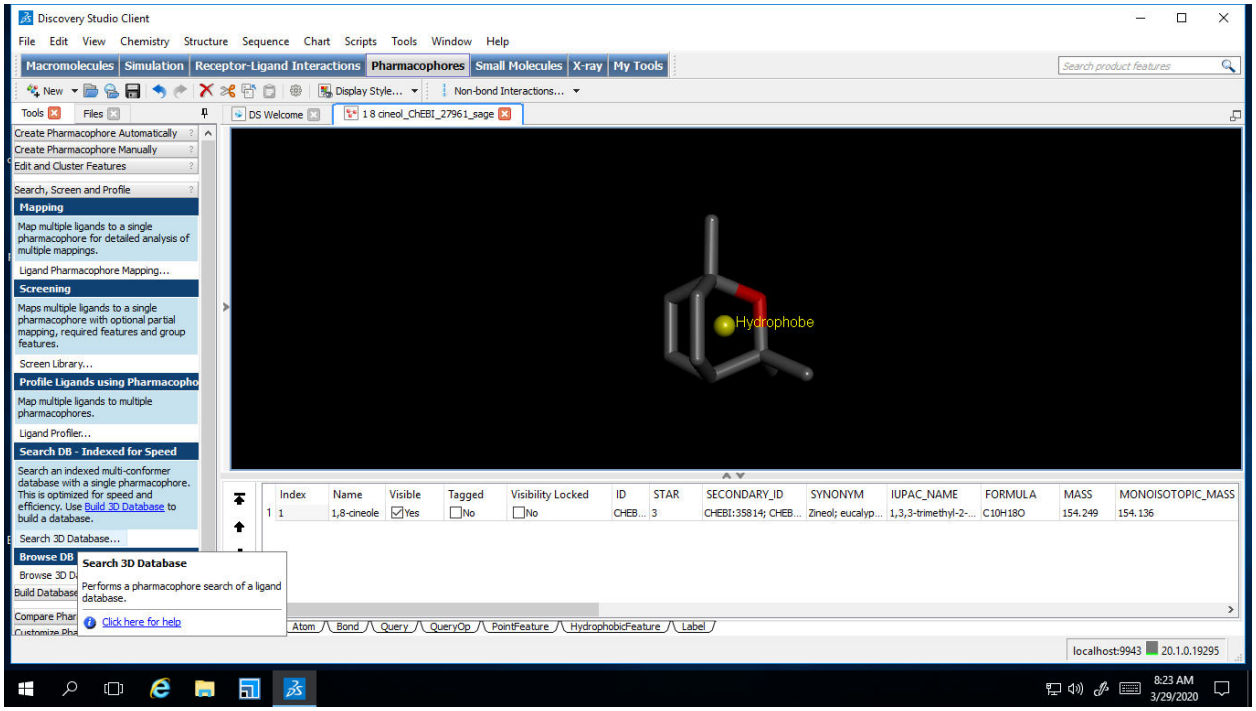
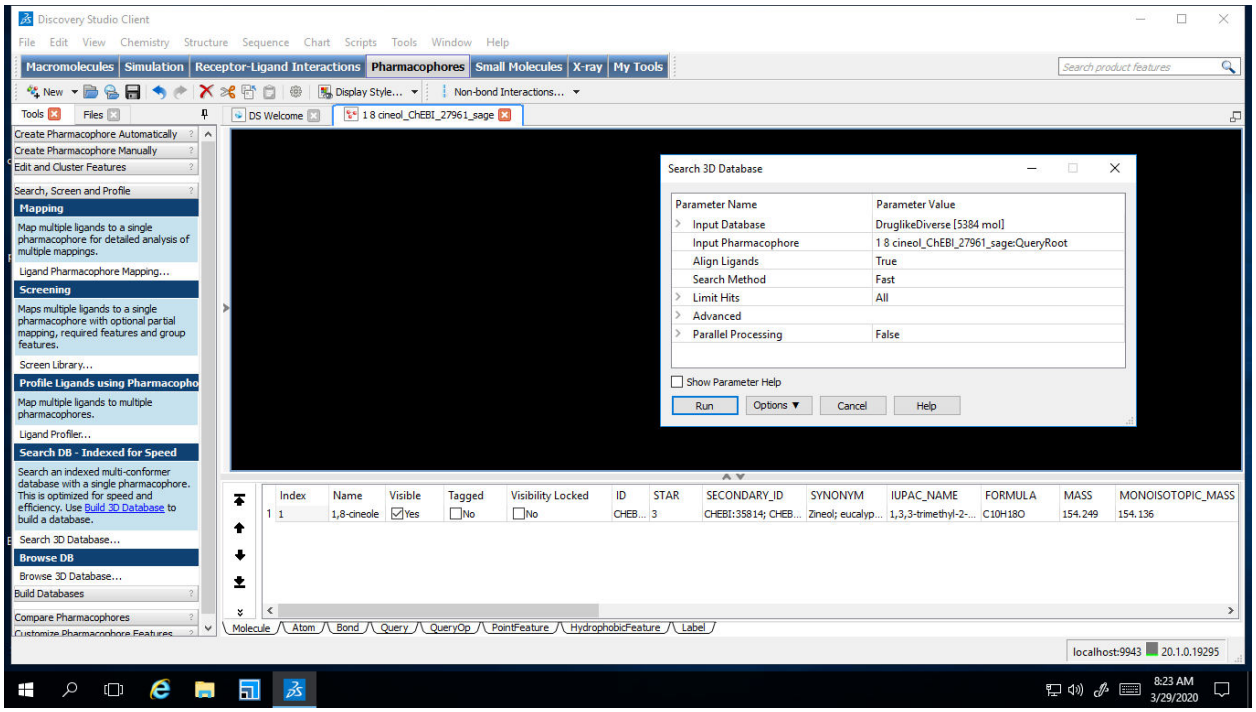
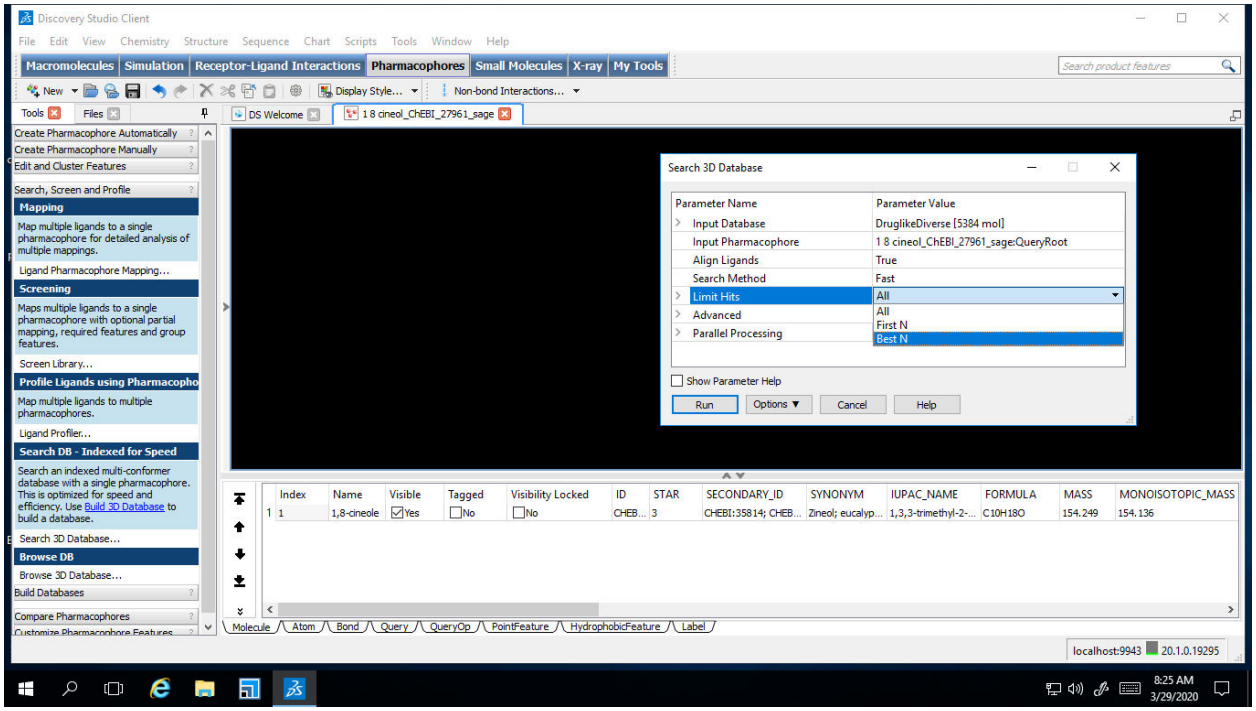
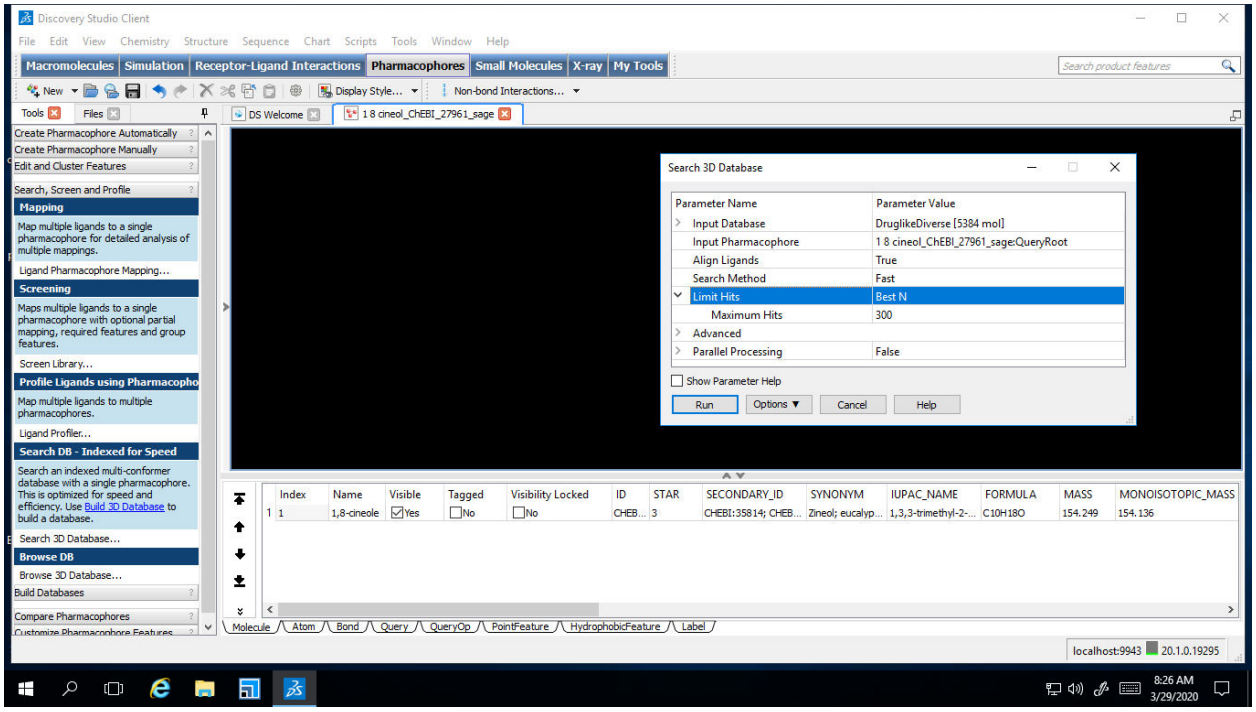
Molecule Atom Bond Query QueryOp PointFeature HydrophobicFeature Label
localhost:9943 20.1.0.19295
8:22 AM
3/29/2020

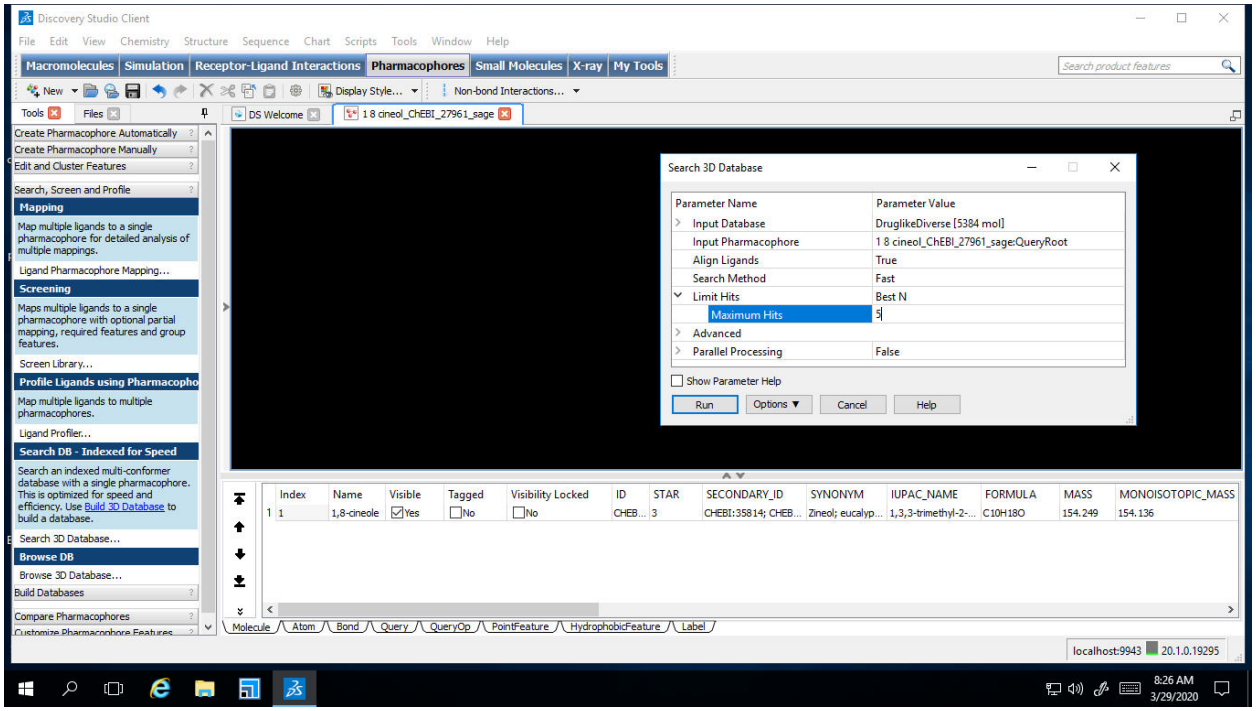

Discovery Studio Client
File Edit View Chemistry Structure Sequence Chart Scripts Tools Window Help
Macromolecules Simulation Receptor-Ligand Interactions Pharmacophores Small Molecules X-ray My Tools
Search product features
New Display Style... Non-bond Interactions...
Tools Files
DS Welcome
1 8 cineol_ChEBI_27961_sage
Create Pharmacophore Automatically
Create Pharmacophore Manually
Edit and Cluster Features
Search, Screen and Profile
Mapping
Map multiple ligands to a single pharmacophore for detailed analysis of multiple mappings.
Ligand Pharmacophore Mapping...
Screening
Maps multiple ligands to a single pharmacophore with optional partial mapping, required features and group features.
Screen Library...
Profile Ligands using Pharmacopho
Map multiple ligands to multiple pharmacophores.
Ligand Profiler...
Search DB - Indexed for Speed
Search an indexed multi-conformer database with a single pharmacophore. This is optimized for speed and efficiency. Use Build 3D Database to build a database.
Search 3D Database...
Browse DB
Browse 3D Database...
Build Databases
Compare Pharmacophores
Customize Pharmacophore Features
Hydrophobe
Index Name Visible Tagged Visibility Locked ID STAR SECONDARY_ID SYNONYM IUPAC_NAME FORMULA MASS MONOISOTOPIC_MASS
1 1 1,8-cineole Yes No No CHEB... 3 CHEBI:35814; CHEB... Zineol; eucalyp... 1,3,3-trimethyl-2-... C10H18O 154.249 154.136
Molecule Atom Bond Query QueryOp PointFeature HydrophobicFeature Label
Done
localhost:9943 20.1.0.19295
8:23 AM
3/29/2020

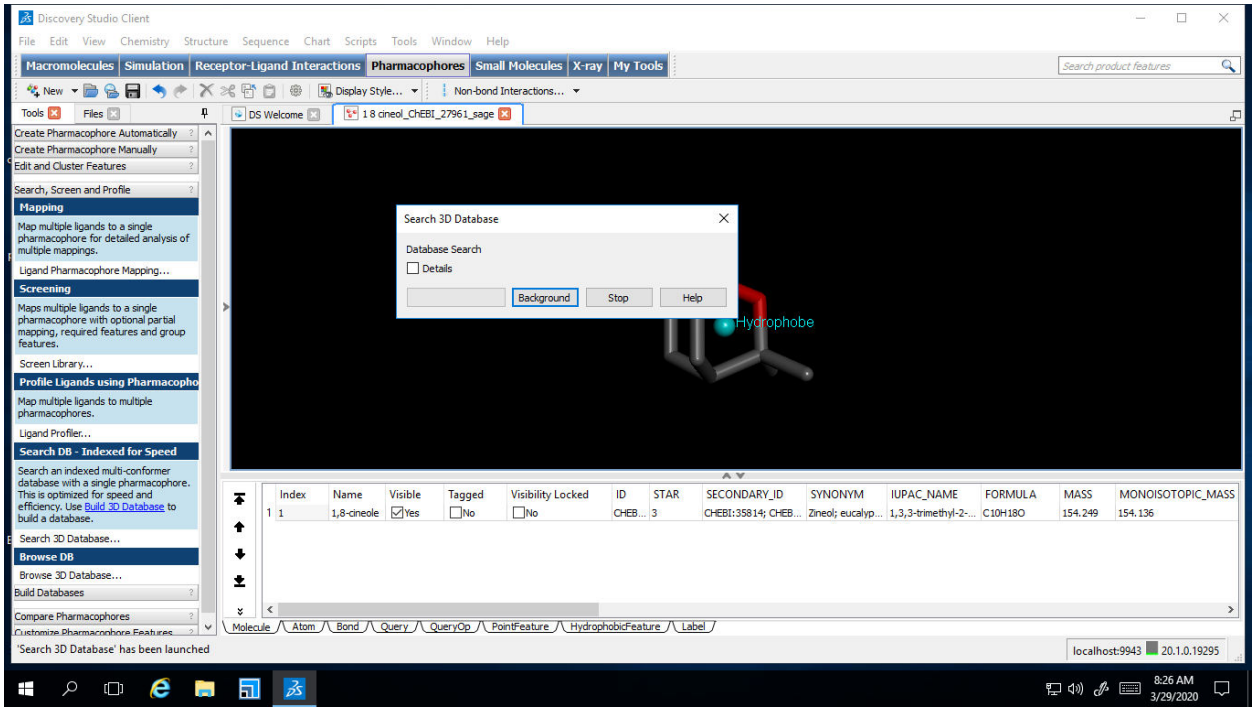

Discovery Studio Client
File Edit View Chemistry Structure Sequence Chart Scripts Tools Window Help
Macromolecules Simulation Receptor-Ligand Interactions Pharmacophores Small Molecules X-ray My Tools
Search product features
New Display Style... Non-bond Interactions...
Tools Files
DS Welcome 1 8 cineol_ChEBI_27961_sage
Create Pharmacophore Automatically
Create Pharmacophore Manually
Edit and Cluster Features
Search, Screen and Profile
Mapping
Map multiple ligands to a single pharmacophore for detailed analysis of multiple mappings.
Ligand Pharmacophore Mapping...
Screening
Maps multiple ligands to a single pharmacophore with optional partial mapping, required features and group features.
Screen Library...
Profile Ligands using Pharmacopho
Map multiple ligands to multiple pharmacophores.
Ligand Profiler...
Search DB - Indexed for Speed
Search an indexed multi-conformer database with a single pharmacophore. This is optimized for speed and efficiency. Use Build 3D Database to build a database.
Search 3D Database...
Browse DB
Build Database
Compare Phar
Search 3D Database
Performs a pharmacophore search of a ligand database.
Click here for help
Hydrophobe
Index Name Visible Tagged Visibility Locked ID STAR SECONDARY_ID SYNONYM IUPAC_NAME FORMULA MASS MONOISOTOPIC_MASS
1 1 1,8-cineole Yes No No CHEB... 3 CHEBI:35814; CHEB... Zineol; eucalyp... 1,3,3-trimethyl-2-... C10H18O 154.249 154.136
Atom Bond Query QueryOp PointFeature HydrophobicFeature Label
localhost:9943 20.1.0.19295
8:23 AM
3/29/2020

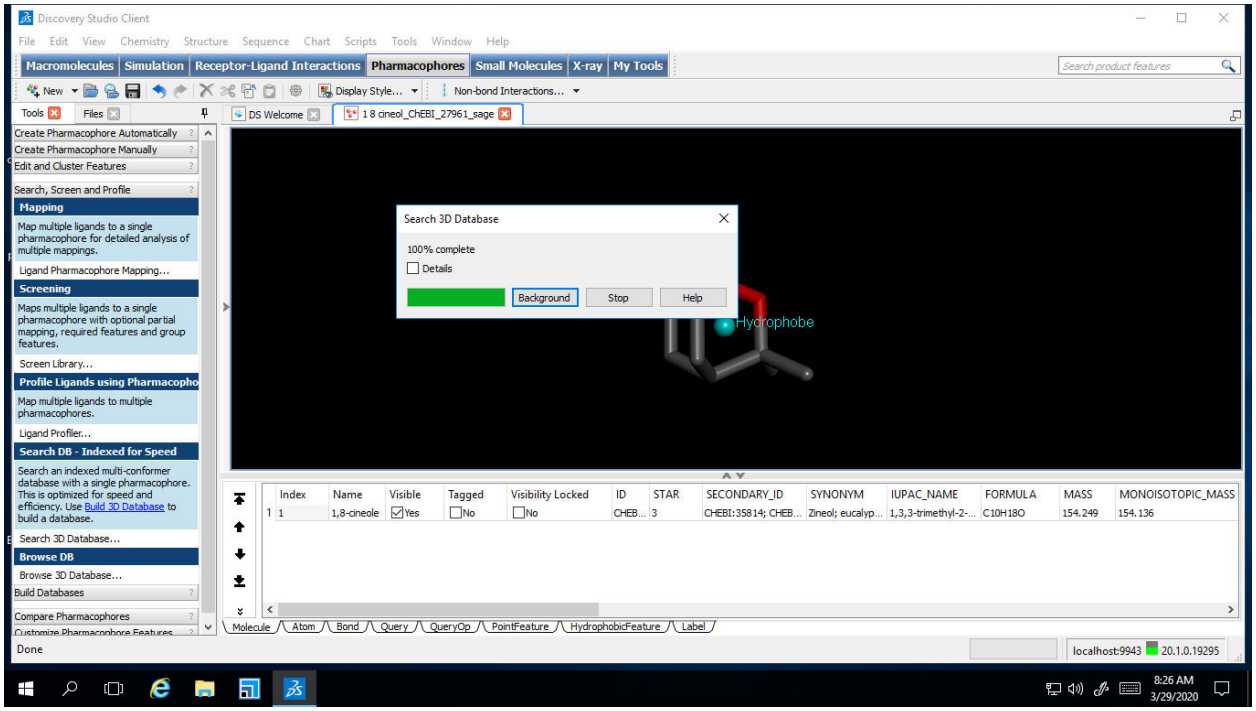

Discovery Studio Client
File Edit View Chemistry Structure Sequence Chart Scripts Tools Window Help
Macromolecules Simulation Receptor-Ligand Interactions Pharmacophores Small Molecules X-ray My Tools
Search product features
New Display Style... Non-bond Interactions...
Tools Files
DS Welcome 1 8 cineol_ChEBI_27961_sage
Create Pharmacophore Automatically
Create Pharmacophore Manually
Edit and Cluster Features
Search, Screen and Profile
Mapping
Map multiple ligands to a single pharmacophore for detailed analysis of multiple mappings.
Ligand Pharmacophore Mapping...
Screening
Maps multiple ligands to a single pharmacophore with optional partial mapping, required features and group features.
Screen Library...
Profile Ligands using Pharmacopho
Map multiple ligands to multiple pharmacophores.
Ligand Profiler...
Search DB - Indexed for Speed
Search an indexed multi-conformer database with a single pharmacophore. This is optimized for speed and efficiency. Use Build 3D Database to build a database.
Search 3D Database...
Browse DB
Browse 3D Database...
Build Databases
Compare Pharmacophores
Customize Pharmacophore Features
Search 3D Database
Parameter Name Parameter Value
Input Database DruglikeDiverse [5384 mol]
Input Pharmacophore 1 8 cineol_ChEBI_27961_sage:QueryRoot
Align Ligands True
Search Method Fast
Limit Hits All
Advanced
Parallel Processing False
Show Parameter Help
Run Options ▼ Cancel Help
Index Name Visible Tagged Visibility Locked ID STAR SECONDARY_ID SYNONYM IUPAC_NAME FORMULA MASS MONOISOTOPIC_MASS
1 1 1,8-cineole Yes No No CHEB... 3 CHEBI:35814; CHEB... Zineol; eucalyp... 1,3,3-trimethyl-2-... C10H18O 154.249 154.136
Molecule Atom Bond Query QueryOp PointFeature HydrophobicFeature Label
localhost:9943 20.1.0.19295
8:23 AM
3/29/2020

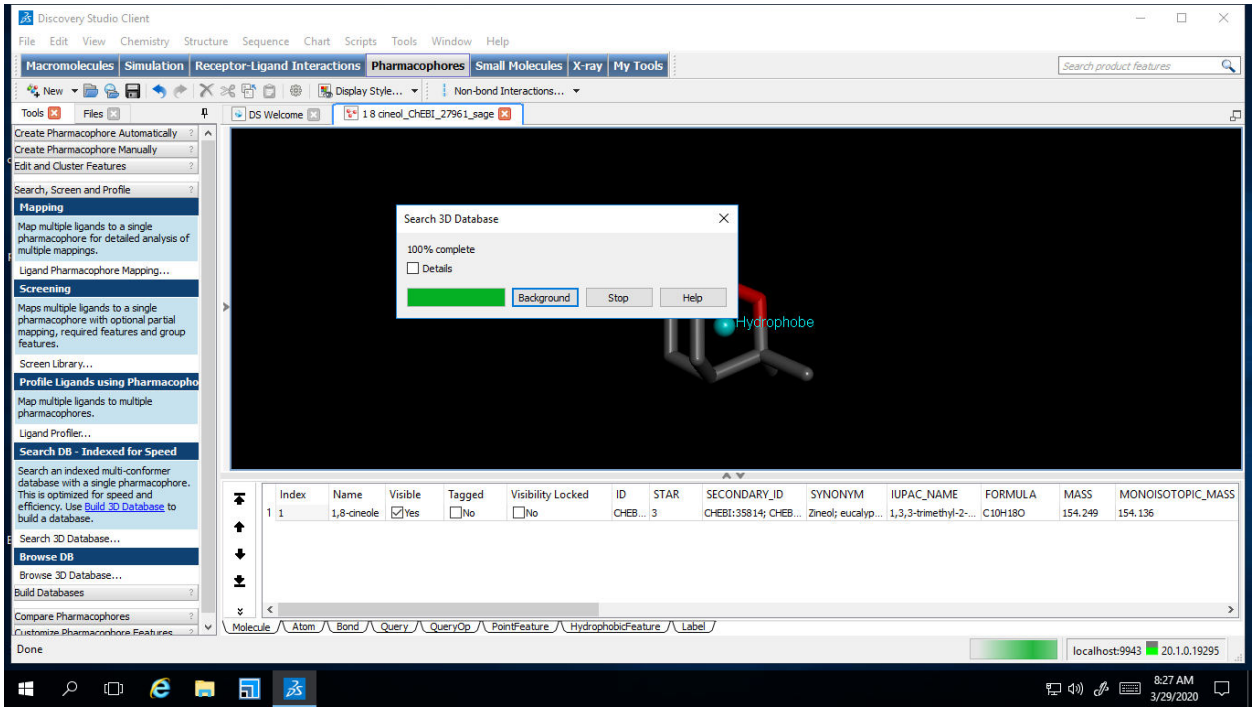

Discovery Studio Client
Search 3D Database
Parameter Name
Parameter Value
Input Database
DruglikeDiverse [5384 mol]
Input Pharmacophore
1 8 cineol_ChEBI_27961_sage:QueryRoot
Align Ligands
True
Search Method
Fast
Limit Hits
All
All
First N
Best N
Advanced
Parallel Processing
Show Parameter Help
Run
Options
Cancel
Help
Index
Name
Visible
Tagged
Visibility Locked
ID
STAR
SECONDARY_ID
SYNONYM
IUPAC_NAME
FORMULA
MASS
MONOISOTOPIC_MASS
1 1,8-cineole
Yes
No
No
CHEB...
3
CHEBI:35814; CHEB...
Zineol; eucalyp...
1,3,3-trimethyl-2-...
C10H18O
154.249
154.136
localhost:9943
20.1.0.19295
8:25 AM
3/29/2020


Discovery Studio Client
Search 3D Database
Parameter Name
Parameter Value
Input Database
DruglikeDiverse [5384 mol]
Input Pharmacophore
1 8 cineol_ChEBI_27961_sage:QueryRoot
Align Ligands
True
Search Method
Fast
Limit Hits
Best N
Maximum Hits
300
Advanced
Parallel Processing
False
Show Parameter Help
Run
Options
Cancel
Help
Index
Name
Visible
Tagged
Visibility Locked
ID
STAR
SECONDARY_ID
SYNONYM
IUPAC_NAME
FORMULA
MASS
MONOISOTOPIC_MASS
1 1,8-cineole
Yes
No
No
CHEB...
3
CHEBI:35814; CHEB...
Zineol; eucalyp...
1,3,3-trimethyl-2-...
C10H18O
154.249
154.136
localhost:9943
20.1.0.19295
8:26 AM
3/29/2020


Discovery Studio Client
Search 3D Database
Parameter Name
Parameter Value
Input Database
DruglikeDiverse [5384 mol]
Input Pharmacophore
1 8 cineol_ChEBI_27961_sage:QueryRoot
Align Ligands
True
Search Method
Fast
Limit Hits
Best N
Maximum Hits
5
Advanced
Parallel Processing
False
Show Parameter Help
Run
Options
Cancel
Help


Discovery Studio Client
Search 3D Database
Database Search
Details
Background
Stop
Help
Hydrophobe
'Search 3D Database' has been launched


Discovery Studio Client
File Edit View Chemistry Structure Sequence Chart Scripts Tools Window Help
Macromolecules Simulation Receptor-Ligand Interactions Pharmacophores Small Molecules X-ray My Tools
Search product features
New Display Style... Non-bond Interactions...
Tools Files
DS Welcome 1 8 cineol_ChEBI_27961_sage
Create Pharmacophore Automatically
Create Pharmacophore Manually
Edit and Cluster Features
Search, Screen and Profile
Mapping
Map multiple ligands to a single pharmacophore for detailed analysis of multiple mappings.
Ligand Pharmacophore Mapping...
Screening
Maps multiple ligands to a single pharmacophore with optional partial mapping, required features and group features.
Screen Library...
Profile Ligands using Pharmacopho
Map multiple ligands to multiple pharmacophores.
Ligand Profiler...
Search DB - Indexed for Speed
Search an indexed multi-conformer database with a single pharmacophore. This is optimized for speed and efficiency. Use Build 3D Database to build a database.
Search 3D Database...
Browse DB
Browse 3D Database...
Build Databases
Compare Pharmacophores
Search 3D Database
100% complete
Details
Background Stop Help
Hydrophobe
Index Name Visible Tagged Visibility Locked ID STAR SECONDARY_ID SYNONYM IUPAC_NAME FORMULA MASS MONOISOTOPIC_MASS
1 1 1,8-cineole Yes No No CHEB... 3 CHEBI:35814; CHEB... Zineol; eucalyp... 1,3,3-trimethyl-2-... C10H18O 154.249 154.136
Molecule Atom Bond Query QueryOp PointFeature HydrophobicFeature Label
Done
localhost:9943 20.1.0.19295
8:26 AM
3/29/2020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Macromolecules Simulation Receptor-Ligand Interactions Pharmacophores Small Molecules X-ray My Tools
Search product features
New Display Style... Non-bond Interactions...
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DS Welcome 1 8 cineol_ChEBI_27961_sage
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Map multiple ligands to multiple pharmacophores.
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Search 3D Database...
Browse DB
Browse 3D Database...
Build Databases
Compare Pharmacophores
Search 3D Database
100% complete
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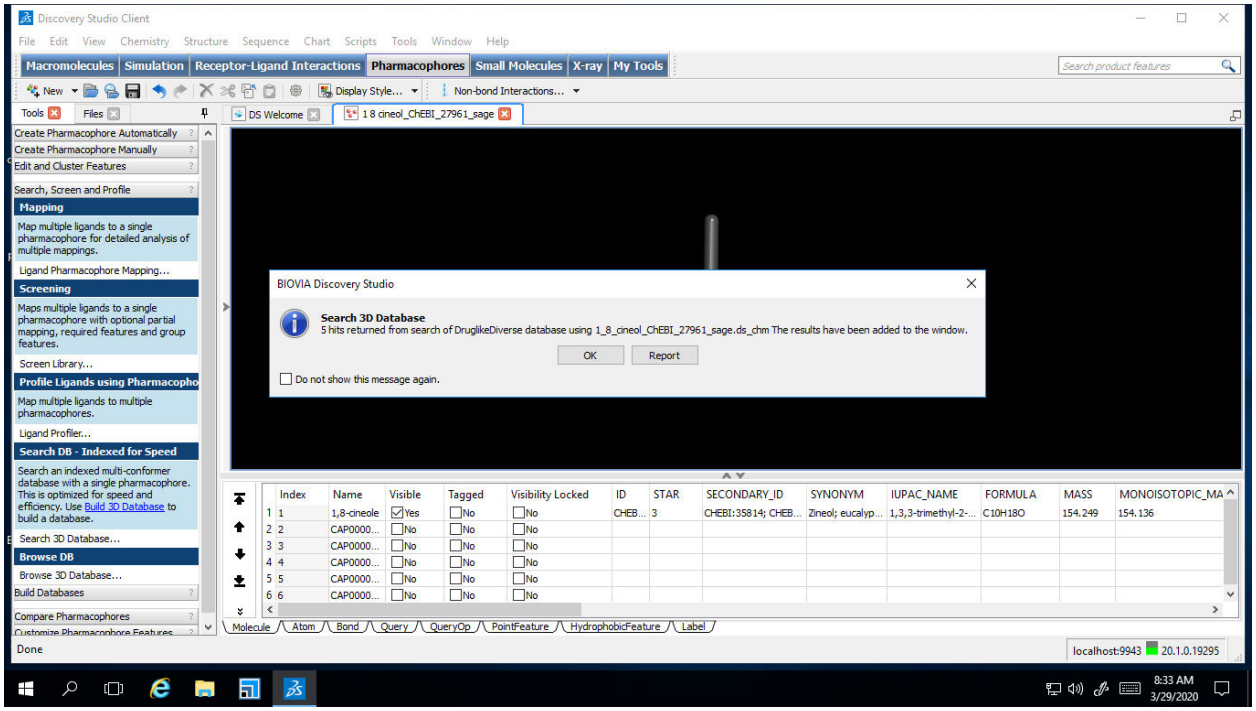
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Map multiple ligands to multiple pharmacophores.
Ligand Profiler...
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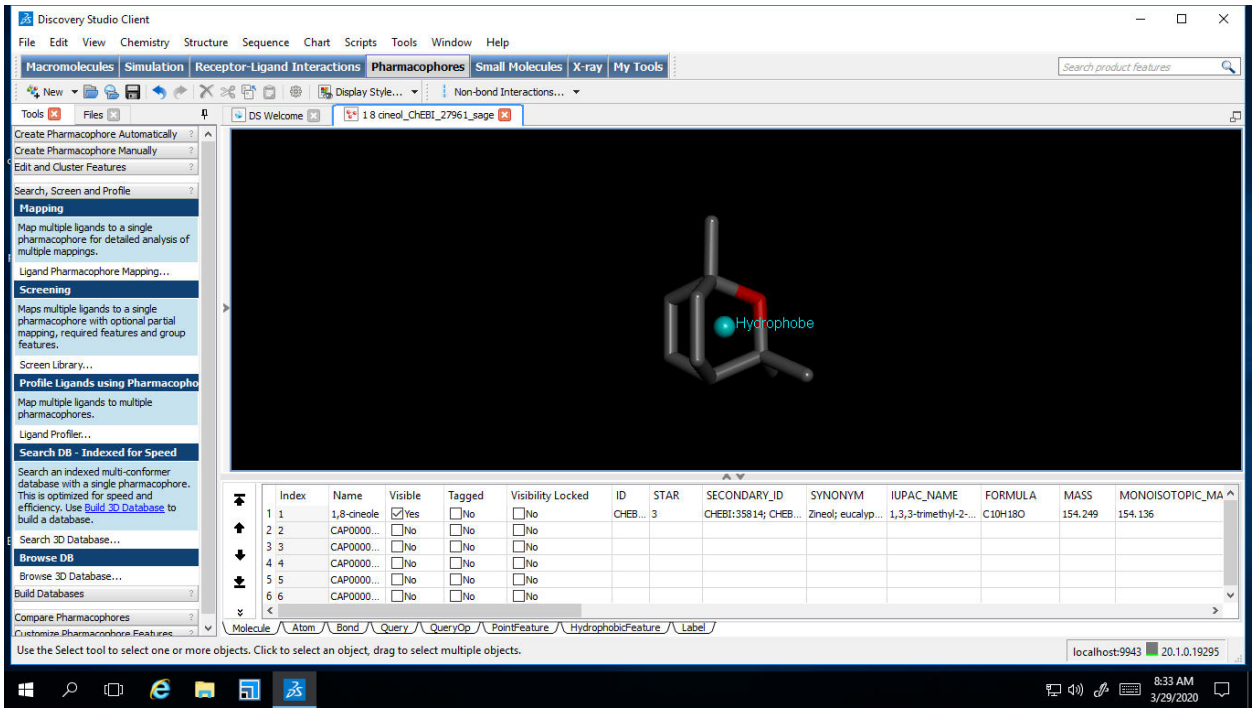
Search 3D Database...
Browse DB
Browse 3D Database...
Build Databases
Compare Pharmacophores
BIOVIA Discovery Studio
Search 3D Database
5 hits returned from search of DruglikeDiverse database using 1_8_cineol_ChEBI_27961_sage.ds_chm The results have been added to the window.
OK Report
Do not show this message again.
Index Name Visible Tagged Visibility Locked ID STAR SECONDARY_ID SYNONYM IUPAC_NAME FORMULA MASS MONOISOTOPIC_MA
1 1 1,8-cineole Yes No No CHEB... 3 CHEBI:35814; CHEB... Zineol; eucalyp... 1,3,3-trimethyl-2-... C10H18O 154.249 154.136
2 2 CAP0000... No No No
3 3 CAP0000... No No No
4 4 CAP0000... No No No
5 5 CAP0000... No No No
6 6 CAP0000... No No No
Molecule Atom Bond Query QueryOp PointFeature HydrophobicFeature Label
Done
localhost:9943 20.1.0.19295
8:33 AM
3/29/2020


Discovery Studio Client
File Edit View Chemistry Structure Sequence Chart Scripts Tools Window Help
Macromolecules Simulation Receptor-Ligand Interactions Pharmacophores Small Molecules X-ray My Tools
Search product features
New Display Style... Non-bond Interactions...
Tools Files
DS Welcome 1 8 cineol_ChEBI_27961_sage
Create Pharmacophore Automatically
Create Pharmacophore Manually
Edit and Cluster Features
Search, Screen and Profile
Mapping
Map multiple ligands to a single pharmacophore for detailed analysis of multiple mappings.
Ligand Pharmacophore Mapping...
Screening
Maps multiple ligands to a single pharmacophore with optional partial mapping, required features and group features.
Screen Library...
Profile Ligands using Pharmacopho
Map multiple ligands to multiple pharmacophores.
Ligand Profiler...
Search DB - Indexed for Speed
Search an indexed multi-conformer database with a single pharmacophore. This is optimized for speed and efficiency. Use Build 3D Database to build a database.
Search 3D Database...
Browse DB
Browse 3D Database...
Build Databases
Compare Pharmacophores
Hydrophobe
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Use the Select tool to select one or more objects. Click to select an object, drag to select multiple objects.
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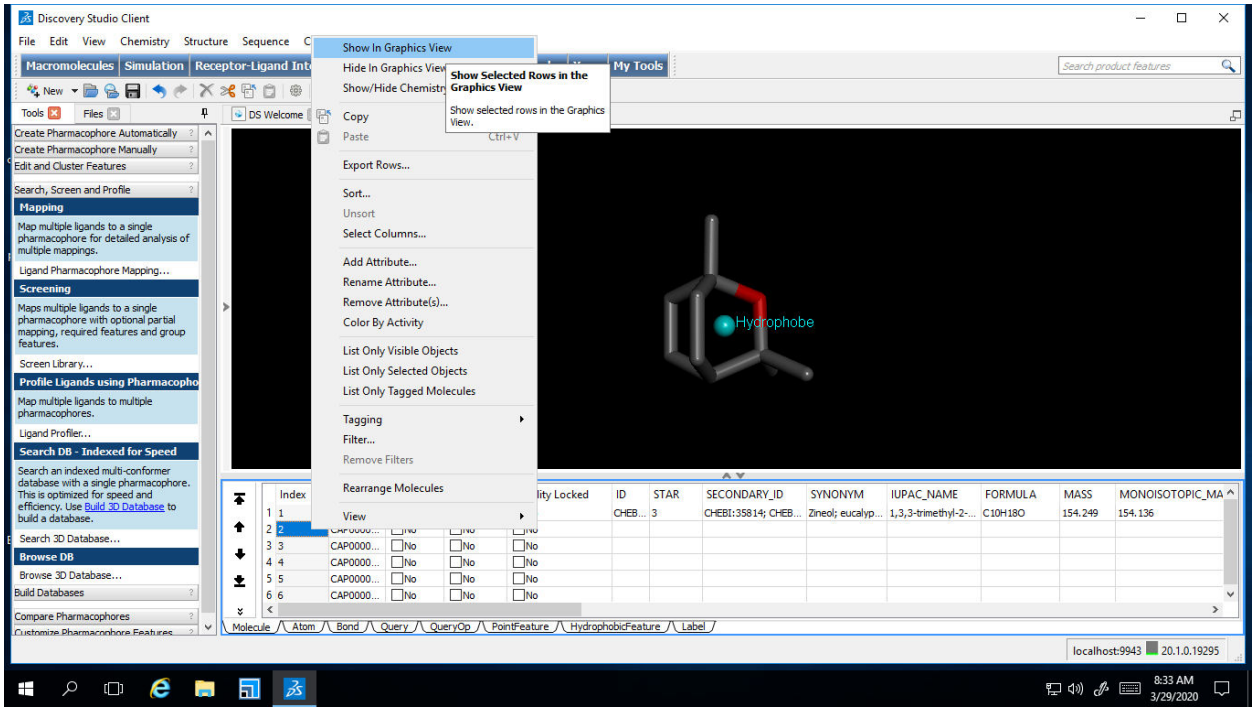
Discovery Studio Client
File Edit View Chemistry Structure Sequence
Show In Graphics View
Hide In Graphics View
Show/Hide Chemistry
Show Selected Rows in the Graphics View
Show selected rows in the Graphics View.
Copy
Paste
Export Rows...
Sort...
Unsort
Select Columns...
Add Attribute...
Rename Attribute...
Remove Attribute(s)...
Color By Activity
List Only Visible Objects
List Only Selected Objects
List Only Tagged Molecules
Tagging
Filter...
Remove Filters
Rearrange Molecules
View
Hydrophobe
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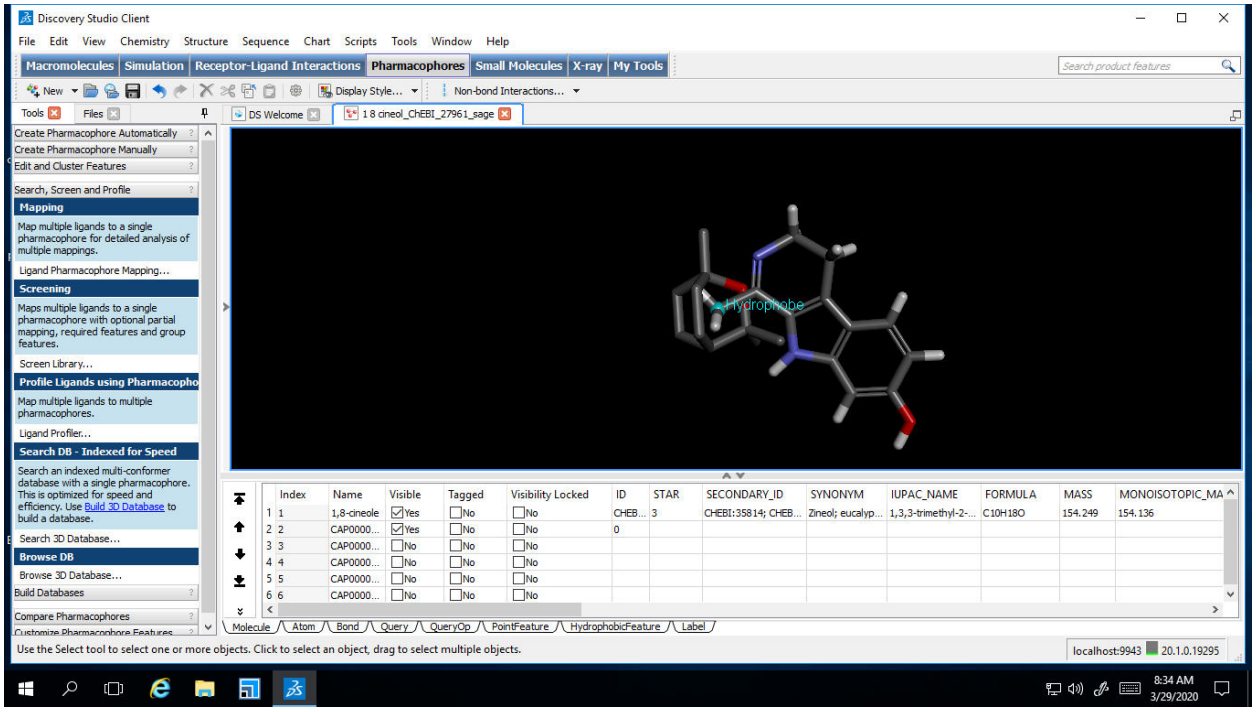
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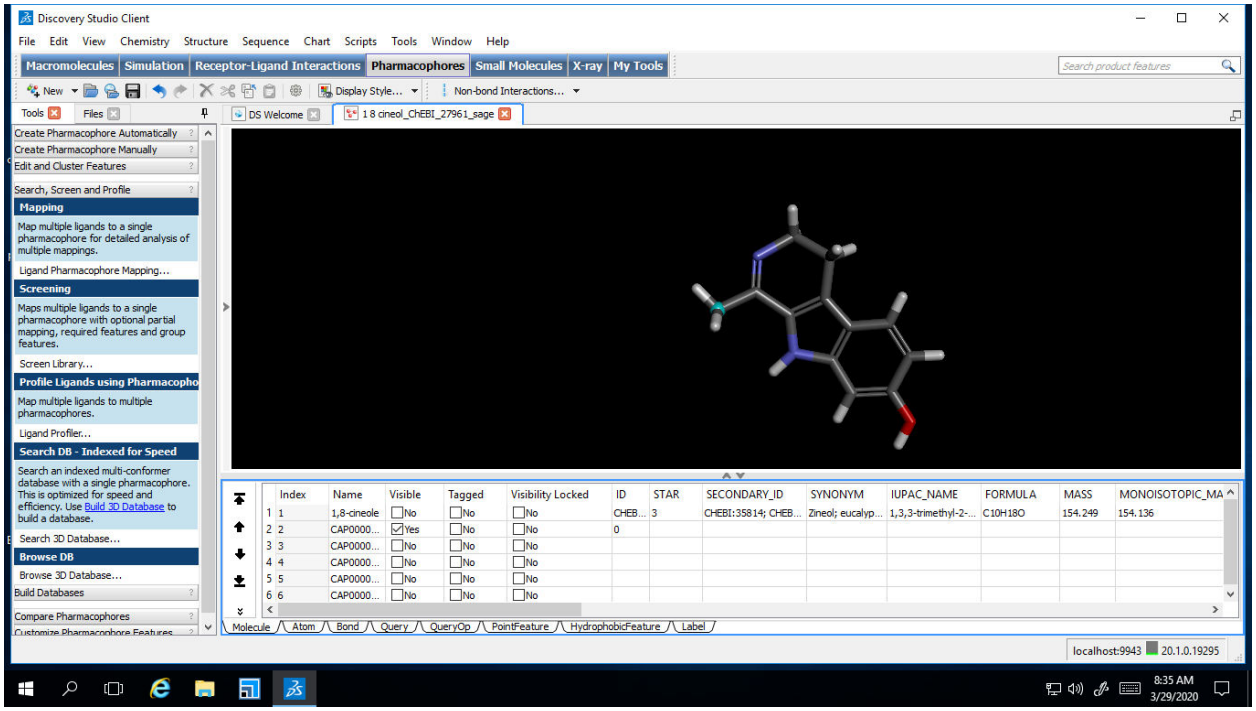
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