



Software for  
Business Intelligence

**BizInt Smart Charts**

# Smart Chat: ClinicalTrials.gov and Chemistry Features

*26 June 2024*



## *Classic.ClinicalTrials.Gov is gone*

- This week the NIH turned off classic.clinicaltrials.gov
- XML exports are no longer available
- JSON exports are now the preferred export
- BizInt Smart Charts Drug Development Suite Version 5.7.4 (or later) is required to use the JSON exports

## *Data compatibility*

- Most fields are identical (classic vs. new)
- Some differences in terminology  
Estimated vs Anticipated
- Cleaner handling of non-interventional trials
- As a result, updating charts from the classic system with JSON charts may show changes which aren't meaningful

## Normalized Phase

- All trial databases now have a Phase (Normalized) field - using the same vocabulary used in drug pipelines records for Highest Phase and Phase by Indication

Database	Phase (Normalized)	Phase
GlobalData Trials	Phase 2	Phase II
Citeline TrialTrove	Phase 2	II
ClinicalTrials.Gov	Phase 2	Phase 2

# *Trial Results and References*

- The new export includes Results and References
- Selected references are included in the chart
- Currently no results fields are included in the chart - **if there is a field that you would like to see in a table of results, let us know**

## *Chemistry in BizInt Smart Charts for Patents*

- Patent and non-patent chemistry supported on STN
- CAplus hit structures added in Version 4.8
- Support for PatentPAK locations added in Version 5.7
- Version 5.9 adds support for MARPAT assembled structures  
**MSTR support only works with BizInt exports from STNNext**



# MARPAT Assembled Structures

## Index of Markush Structures



Structure	Structure
<p>MSTR 1B Assembled</p> <p><a href="#">Reference 1</a></p>	<p>MSTR 1 Assembled</p> <p><a href="#">Reference 2</a></p>

## Markush Structures:

<p>MSTR 1A Assembled</p> <p><a href="#">Patent location: claim 1</a> Note: or pharmaceutically acceptable salts Note: additional derivatization also claimed <a href="#">(Cmpd. 8)</a></p>	
<p>MSTR 1B Assembled</p> <p><a href="#">Patent location: claim 1</a> Note: or pharmaceutically acceptable salts Note: additional derivatization also claimed <a href="#">(Cmpd. 9)</a></p>	

# Additional Columns in MARPAT

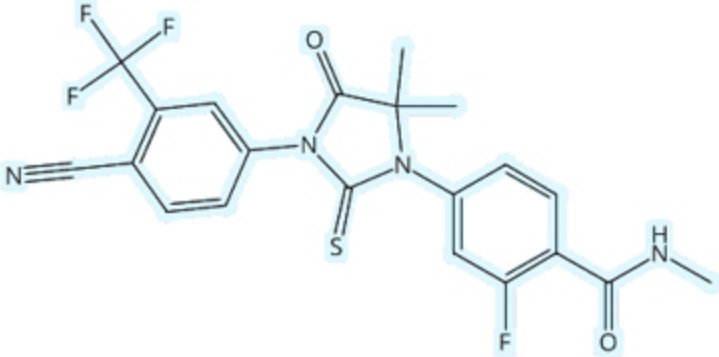
First Hit Structure	Num Hit Structures	Node Annotations	Additional G-groups	Structure Notes	Patent Location
147:427336+1 Assembled	1	316: carbon chain <containing 1-12 C> (opt. substd. by (1-4) G4) 398: carbon chain <containing 1-12 C> (opt. substd. by (1-4) G4)		Note: additional heteroatom interruptions also claimed	claim 1
145:505452+1 Assembled	1		G15 = Me G18 = F / CONHMe	Note: substitution is restricted Note: also incorporates other claims Note: also incorporates claim 38 Note: substitution is restricted	claim 45



## *Color structure images*

- Hit structure region highlights available in CAplus and MARPAT with version 5.8.5
- Higher resolution images
- Also available in REGISTRY
- Will extend color & high resolution images to other sources including drug pipelines

# Color structure images

	Substance	Structure	Reference
1	<p><b>915087-33-1</b></p> <p>Benzamide, 4-[3-[4-cyano-3-(trifluoromethyl)phenyl]-5,5-dimethyl-4-oxo-2-thioxo-1-imidazolidinyl]-2-fluoro-N-methyl- (CA INDEX NAME)</p>		<p><u><a href="#">compn. conta. beaverin in medicine for inhibiting proliferation of human prostate cancer cell</a></u> <u><a href="#">Reference 1</a></u></p> <p>treating metastatic castration-resistant prostate cancer with engineered bispecific PSMA x CD28 antibodies with anti-PD-1 antibodies <u><a href="#">Reference 2</a></u></p> <p>engineering of ERBB2/ERBB3 bispecific antibodies for treating castration-resistant prostate cancer <u><a href="#">Reference 3</a></u></p>

## *Enhanced Chemistry Support (still to come)*

- Adding support for REAXYSsub/bib, DCR on STN
- First HITSTR/QHIT column
- Improved index term handling
- New options for Index of Hit Structures - sections for **Exemplified**, **Markush**, and Non-exemplified structures; option for grid display of index (w/ # of columns)





Software for  
Business Intelligence

**BizInt Smart Charts**

**BIZINT**

THE JOURNEY CONTINUES...

Questions?  
Requests?

[support@bizint.com](mailto:support@bizint.com)