How to Use Mol-Instincts

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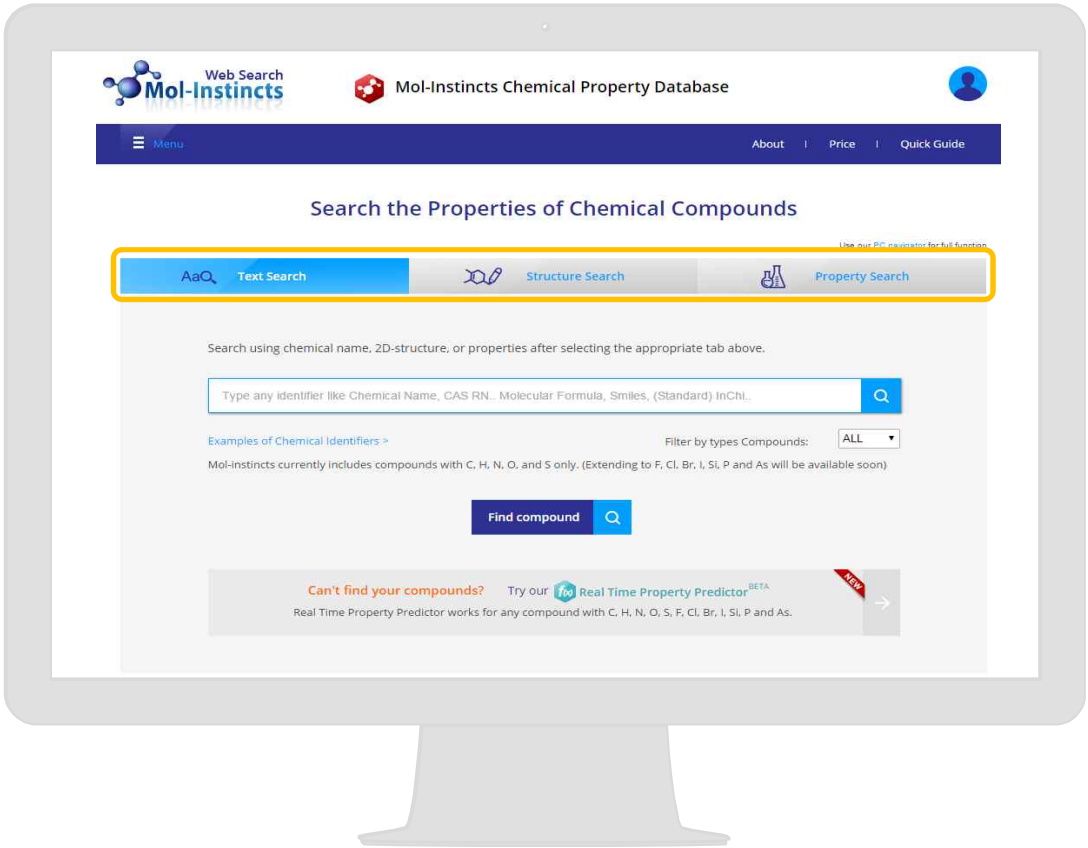
STEP 1



Select search method

- **Search a compound** : Three searching methods are available

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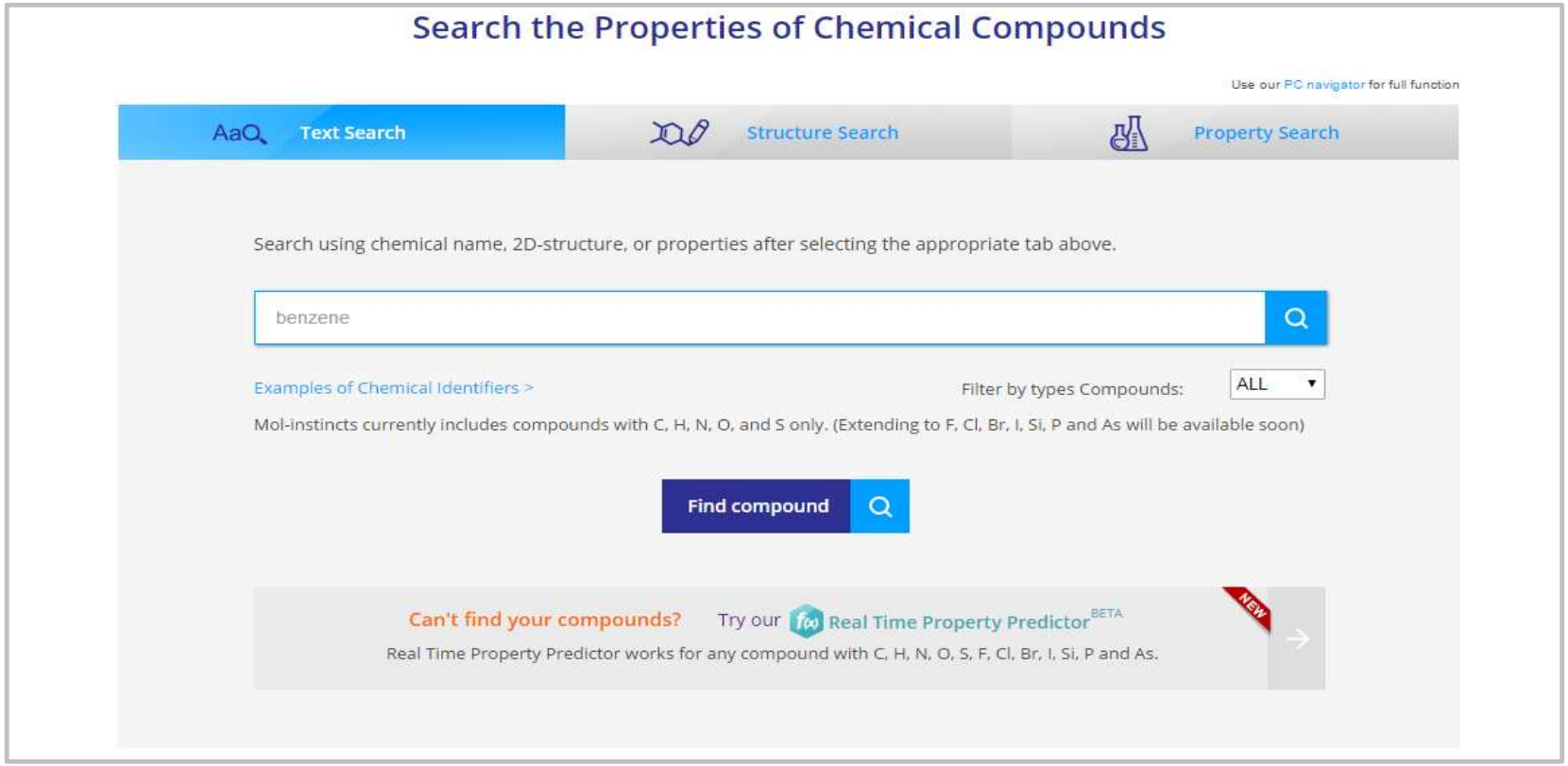
Compound search **TYPE 1**



- **TYPE 1 : Text Search** using textual identification of compound

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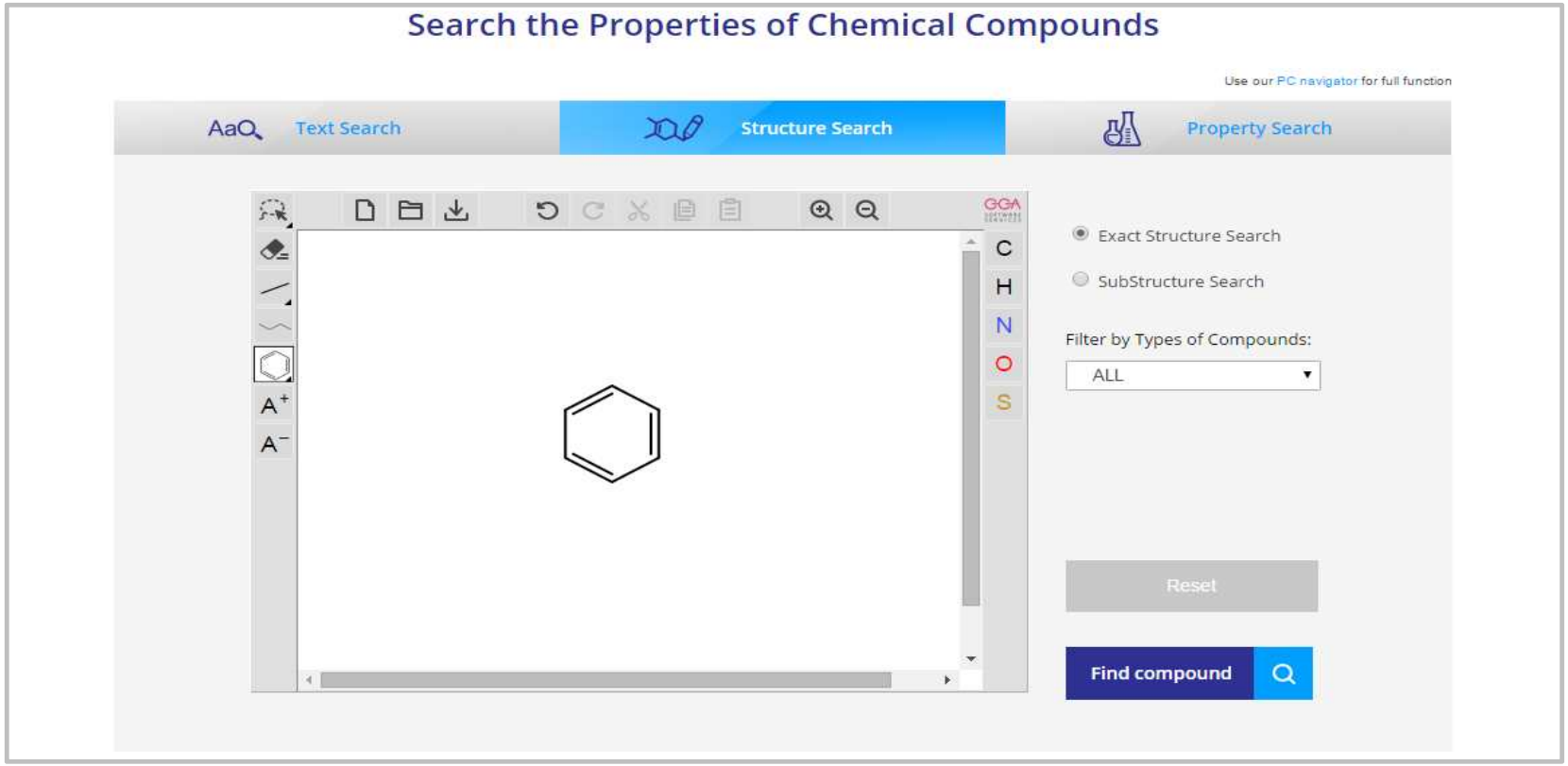
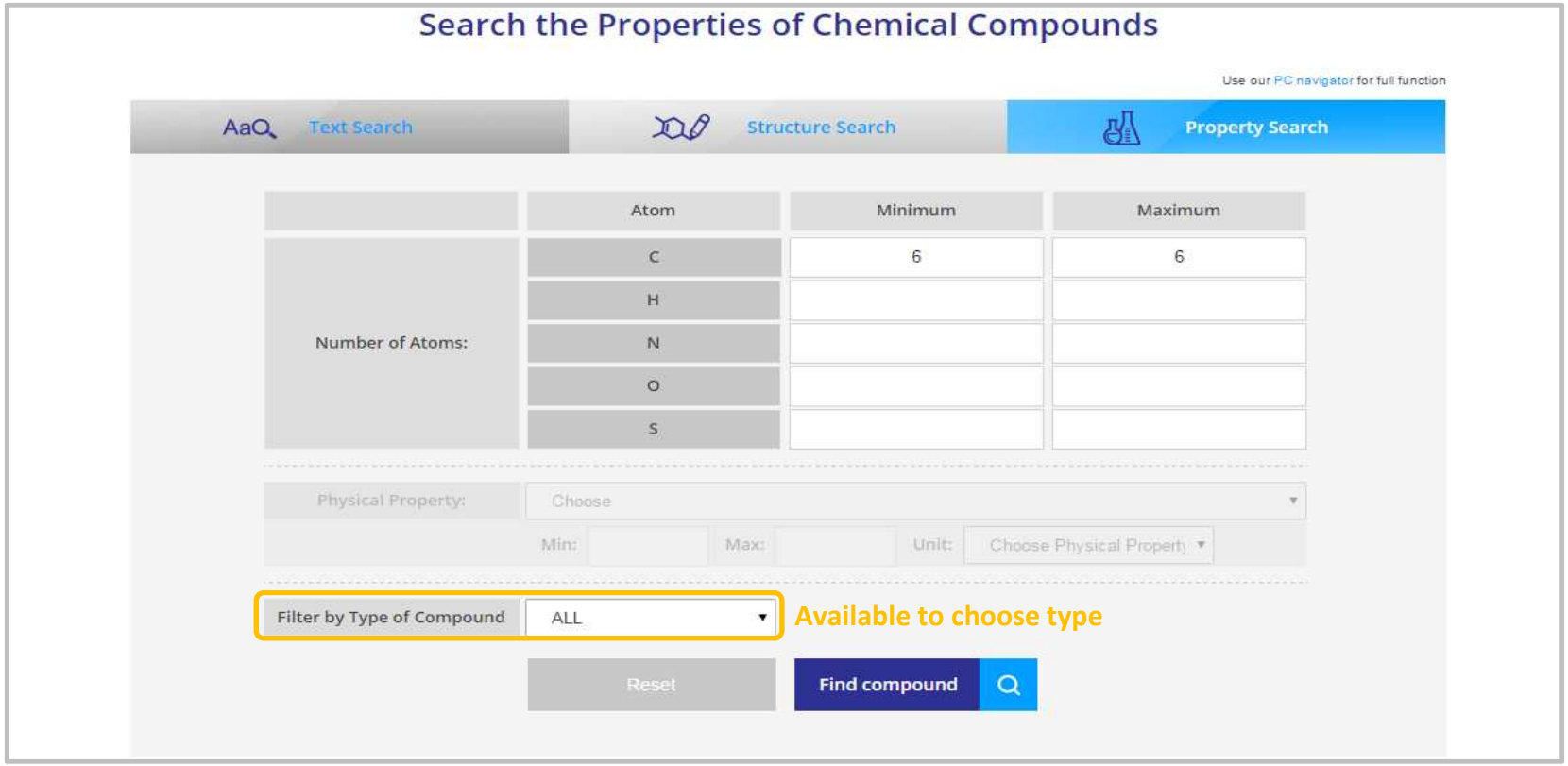
Compound search **TYPE 2**



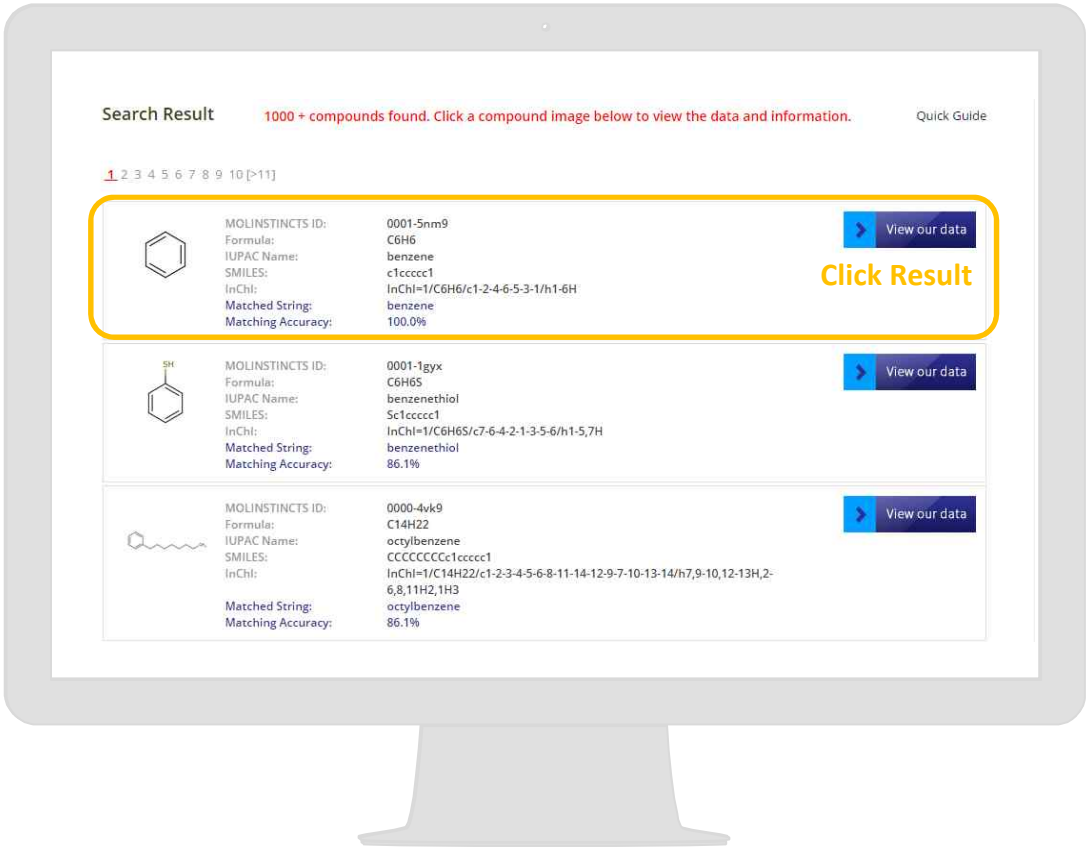
- **TYPE 2 : Structure Search** using 2D structure of compound

Compound search **TYPE 3**



- **TYPE 3 : Property Search** using physical property of compound

STEP 2



- **Select the compound from the result list**

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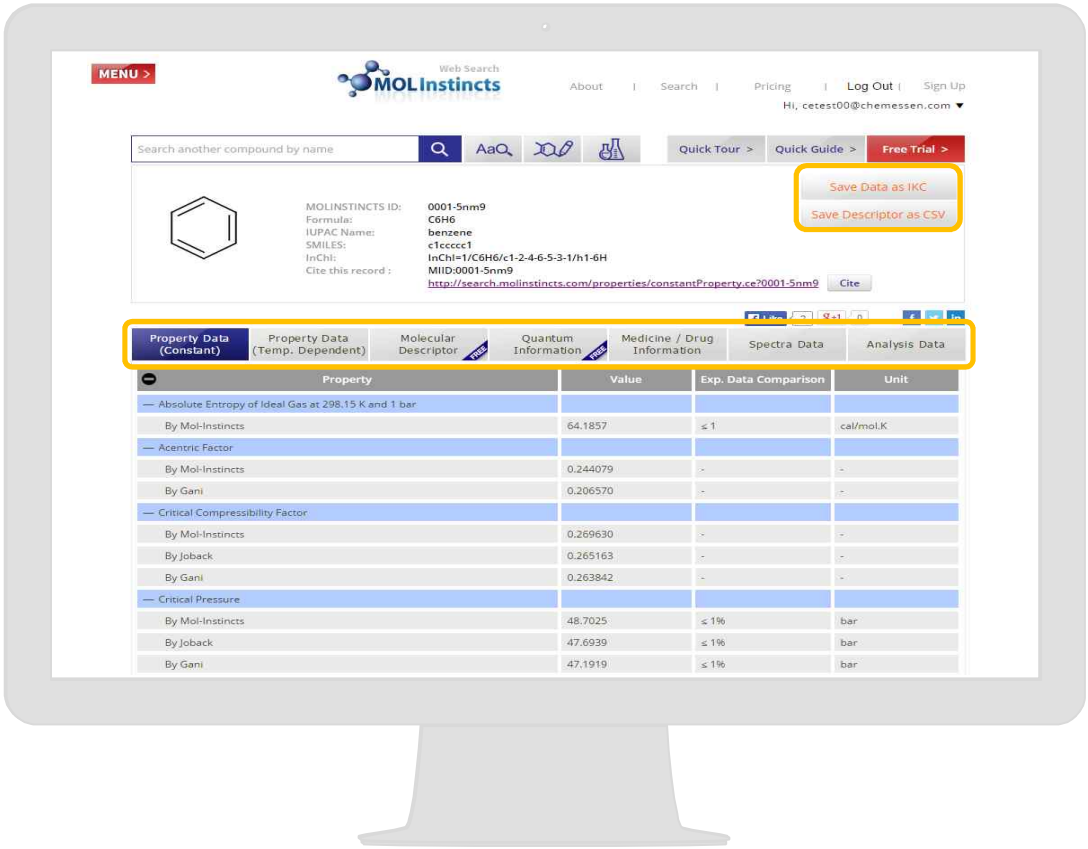
STEP 3



Available to save

Available to select

- **View the property data:** 7 different types of compound property information
- **Save data as IKC :** Compatible with other simulation software such as Aspen Plus
- **Save descriptors as CSV :** More than 2,000 descriptors exported to a CSV file by open in MS Excel

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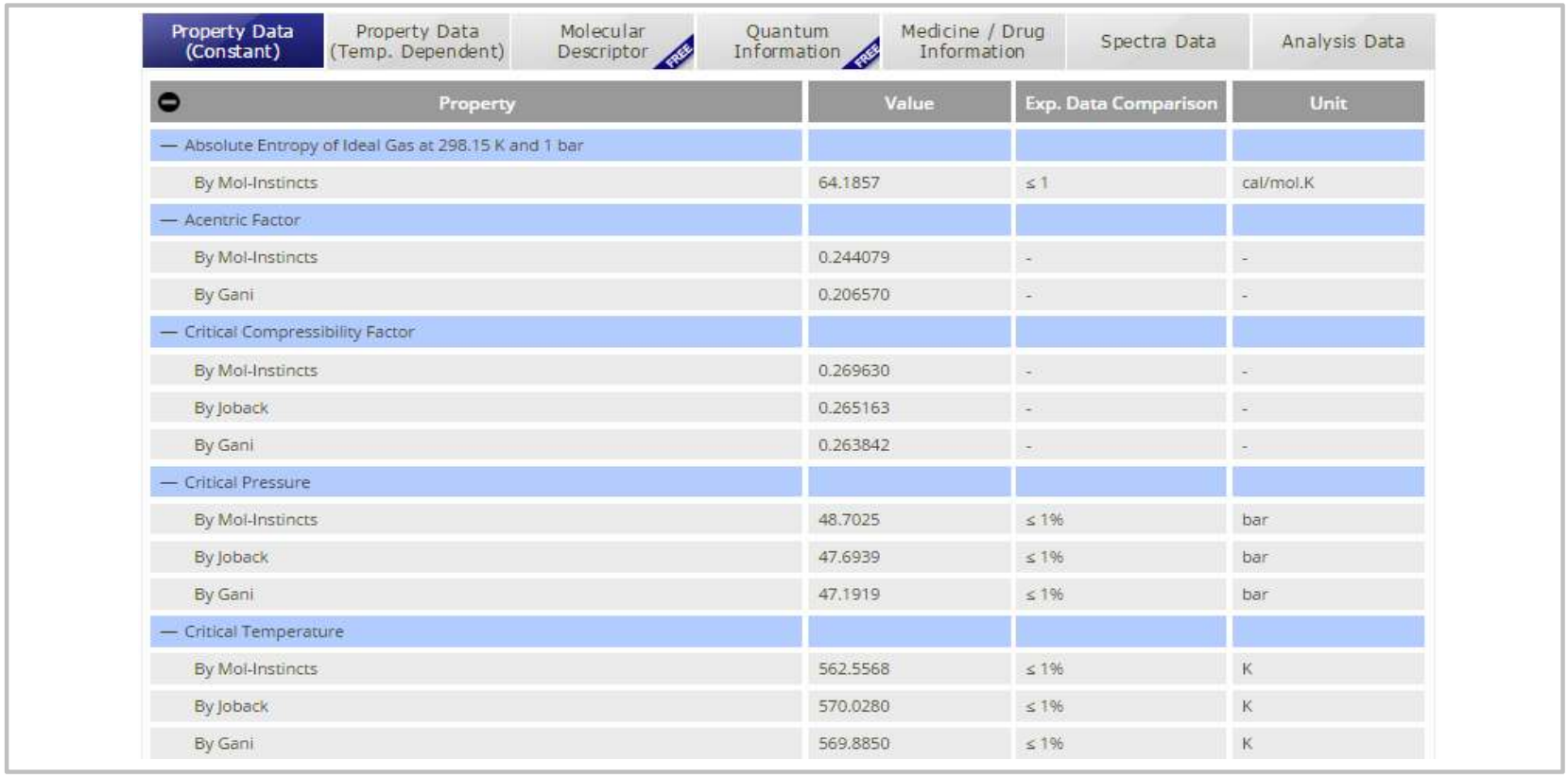
Property View **TYPE 1**



Property Data (Constant) | Property Data (Temp. Dependent) | Molecular Descriptor FREE | Quantum Information FREE | Medicine / Drug Information | Spectra Data | Analysis Data

Property	Value	Exp. Data Comparison	Unit
— Absolute Entropy of Ideal Gas at 298.15 K and 1 bar			
By Mol-Instincts	64.1857	≤ 1	cal/mol.K
— Acentric Factor			
By Mol-Instincts	0.244079	-	-
By Gani	0.206570	-	-
— Critical Compressibility Factor			
By Mol-Instincts	0.269630	-	-
By Joback	0.265163	-	-
By Gani	0.263842	-	-
— Critical Pressure			
By Mol-Instincts	48.7025	≤ 1%	bar
By Joback	47.6939	≤ 1%	bar
By Gani	47.1919	≤ 1%	bar
— Critical Temperature			
By Mol-Instincts	562.5568	≤ 1%	K
By Joback	570.0280	≤ 1%	K
By Gani	569.8850	≤ 1%	K

- **TYPE 1 : Thermo-Physical Property - Constant** (35 different categories)
  - Comparison with experimental value
  - Comparison with the existing method as JOBACK, GANI METHOD
  - Prediction value of the compound as Gas/Liquid/Solid

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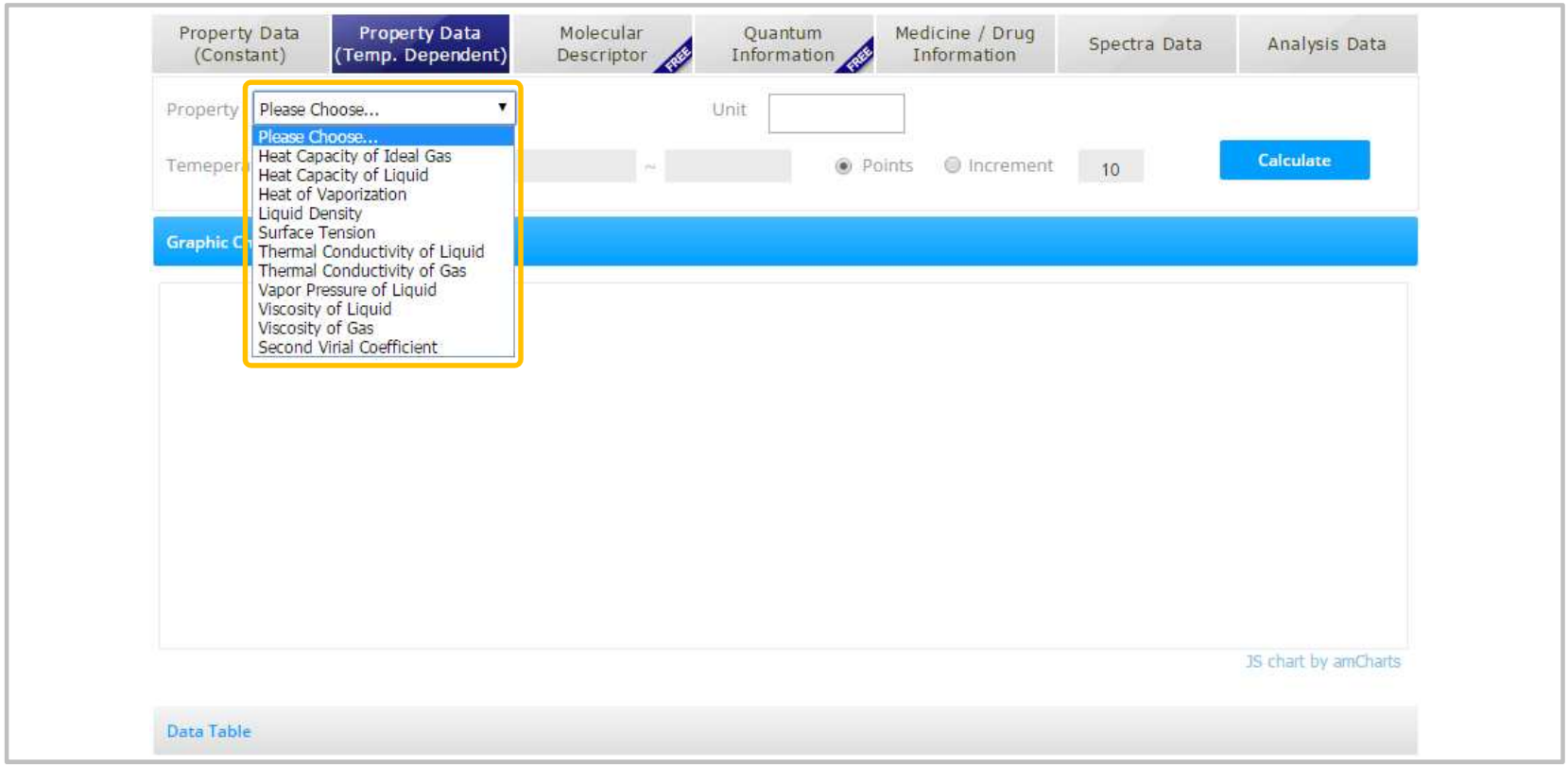
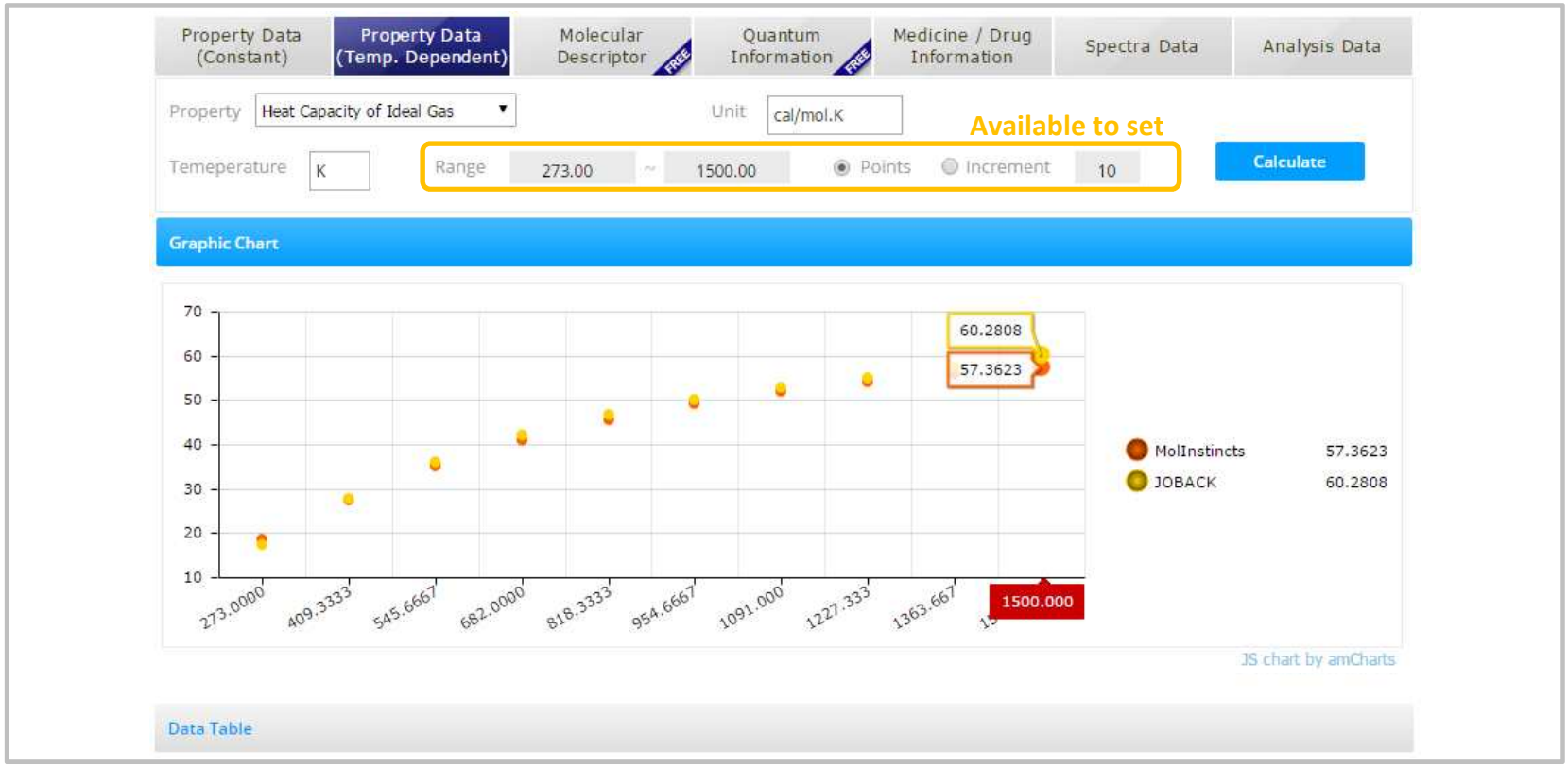
Property View **TYPE 2**



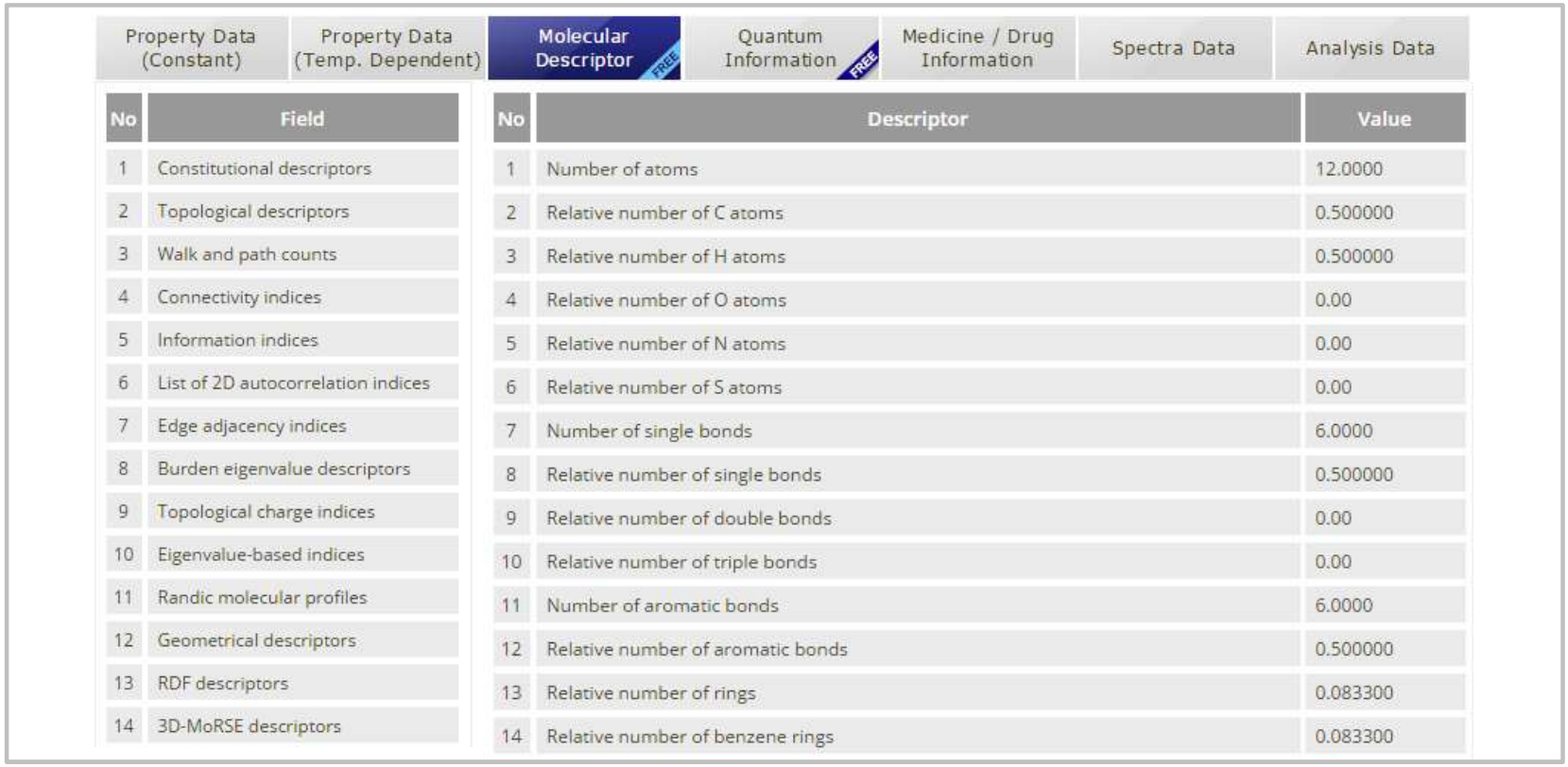
- **TYPE 2 : Thermo-Physical Property Temperature dependent** (11 different categories)

Property View **TYPE 2**



- Available to set the number of points or temperature range
- Point value on a graph
- Prediction value pursuant to temperature in data table

Property View **TYPE 3**



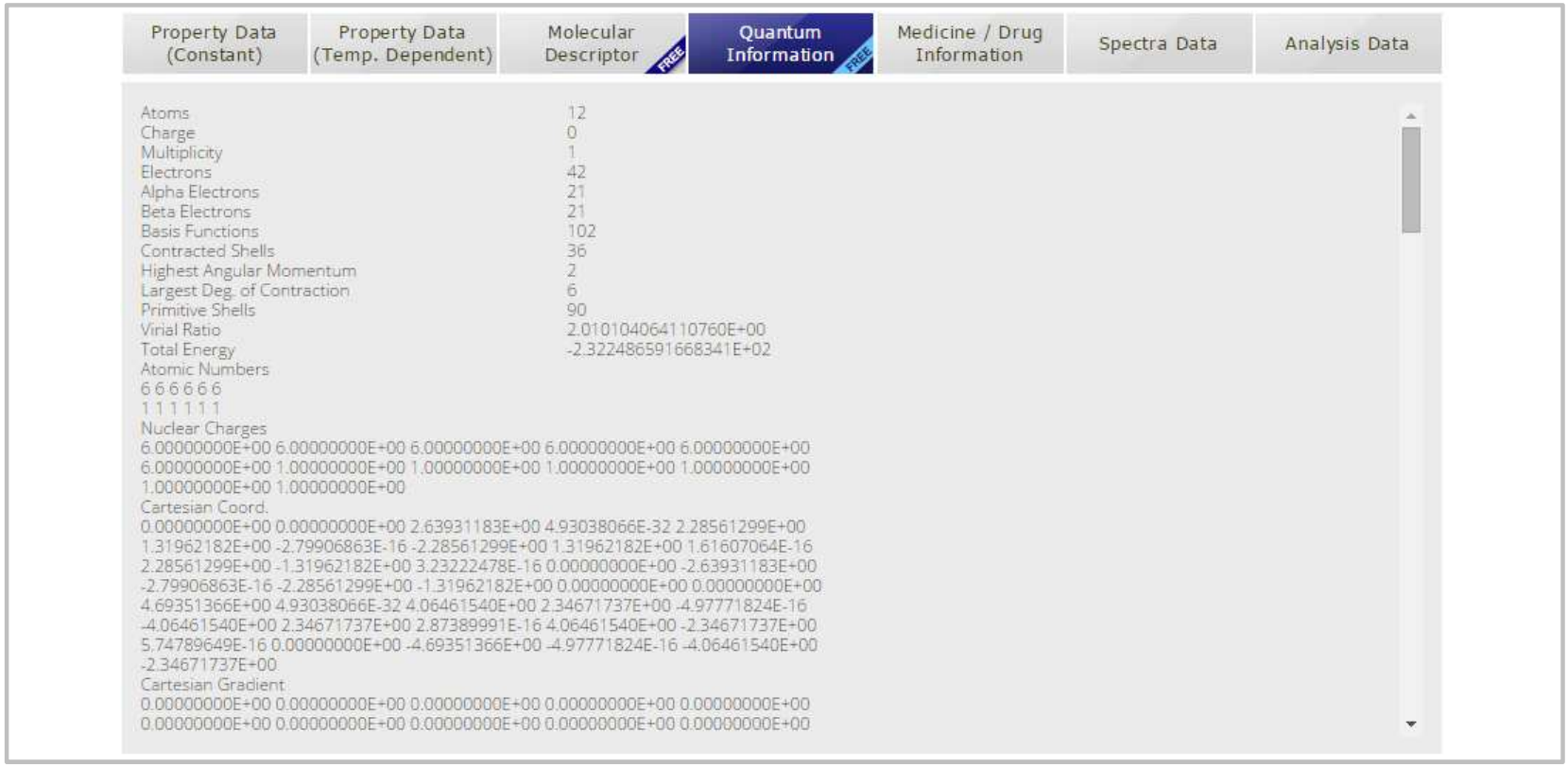
Property Data (Constant) | Property Data (Temp. Dependent) | **Molecular Descriptor** FREE | Quantum Information FREE | Medicine / Drug Information | Spectra Data | Analysis Data

No	Field
1	Constitutional descriptors
2	Topological descriptors
3	Walk and path counts
4	Connectivity indices
5	Information indices
6	List of 2D autocorrelation indices
7	Edge adjacency indices
8	Burden eigenvalue descriptors
9	Topological charge indices
10	Eigenvalue-based indices
11	Randic molecular profiles
12	Geometrical descriptors
13	RDF descriptors
14	3D-MoRSE descriptors

No	Descriptor	Value
1	Number of atoms	12.0000
2	Relative number of C atoms	0.500000
3	Relative number of H atoms	0.500000
4	Relative number of O atoms	0.00
5	Relative number of N atoms	0.00
6	Relative number of S atoms	0.00
7	Number of single bonds	6.0000
8	Relative number of single bonds	0.500000
9	Relative number of double bonds	0.00
10	Relative number of triple bonds	0.00
11	Number of aromatic bonds	6.0000
12	Relative number of aromatic bonds	0.500000
13	Relative number of rings	0.083300
14	Relative number of benzene rings	0.083300

- **TYPE 3 : Molecular Descriptor** (24 different fields)

Property View **TYPE 4**



- **TYPE 4 : Quantum data**

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Property View **TYPE 5**

Property Data (Constant) | Property Data (Temp. Dependent) | Molecular Descriptor FREE | Quantum Information FREE | **Medicine / Drug Information** | Spectra Data | Analysis Data

No	Property Name	Value
1	Number of atoms	12.0000
2	molecular weight	78.1118
3	dipole moment	0.00
4	LogP (Octanol-Water Partition Coefficient)	2.1520 (≤ 0.1)
5	LogS (Water Solubility)	-1.6622 (≤ 0.1)
6	number of acceptor atoms for H-bonds (N,O)	0.00
7	number of donor atoms for H-bonds (N,O)	0.00
8	Ghose-Crippen molar refractivity	26.0580
9	Ghose-Crippen octanol-water partition coeff. (logP)	1.8300
10	Moriguchi octanol-water partition coeff. (logP)	2.2550
11	Lipinski Alert index	0.00
12	Drug-likeness	non-drug
13	Activity Score for GPCR ligands	-3.6930
14	Activity Score for Ion Channel Modulators	-3.6410
15	Activity Score for Kinase Inhibitors	-3.8030
16	Activity Score for Nuclear receptor ligands	-3.9990

- **TYPE 5 : Drug-Related Property** (16 different data)

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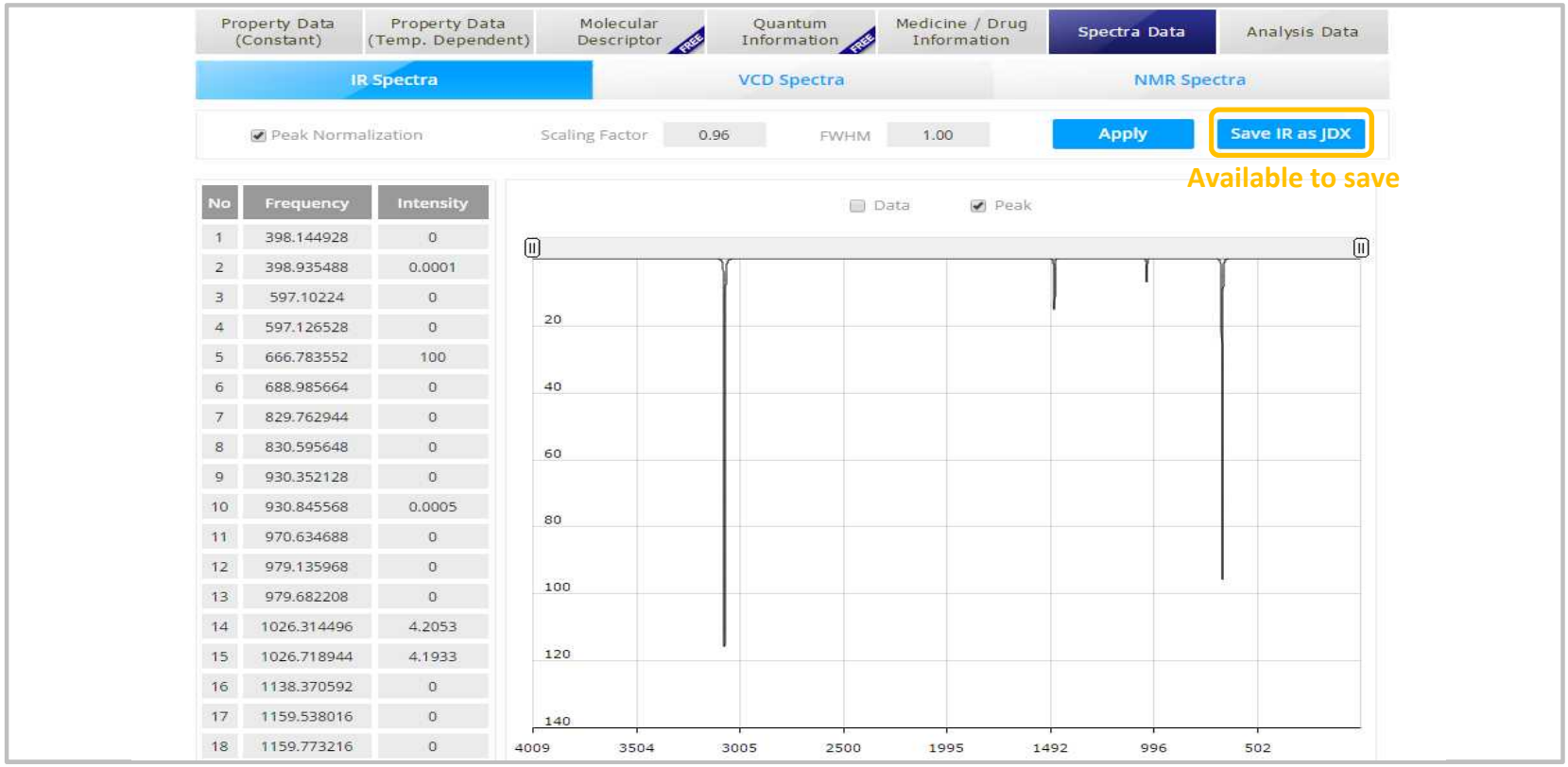
Property View **TYPE 6**



No	Frequency	Intensity
1	398.144928	0
2	398.935488	0.0001
3	597.10224	0
4	597.126528	0
5	666.783552	100
6	688.985664	0
7	829.762944	0
8	830.595648	0
9	930.352128	0
10	930.845568	0.0005
11	970.634688	0
12	979.135968	0
13	979.682208	0
14	1026.314496	4.2053
15	1026.718944	4.1933
16	1138.370592	0
17	1159.538016	0
18	1159.773216	0

- **TYPE 6 : IR / VCD / NMR spectra data**
  - Available to save IR data as JDX file accessible by open in MS Excel, Word, or Notepad

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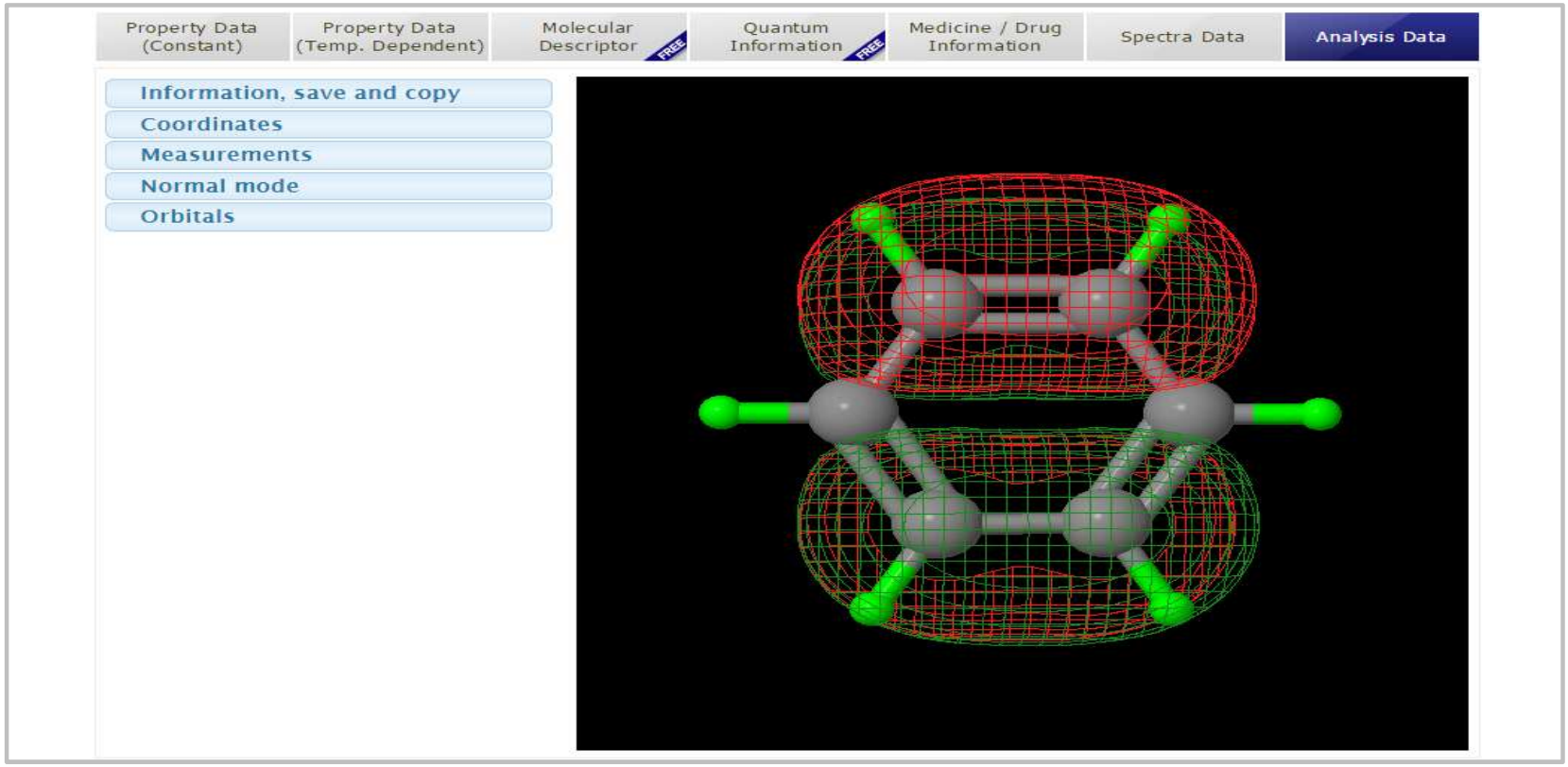
Property View **TYPE 7**



- TYPE 7 : **Molecular Orbital Information**