Molecular Descriptors Family on Structure Activity Relationships

4. Molar Refraction of Cyclic Organophosphorus Compounds

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Abstract

The molecular descriptors family on structure activity relationships methodology was applied on ten cyclic organophosphorus compounds in order to predict theirs molar refraction. A number of 107692 significantly different MDF members enter into a multiple linear regression analysis. A pair of descriptors (lGDmSMt, lAmrfEt), which have the best performing ability in prediction of molar refraction of cyclic organophosphorus compounds, was found and a bi-varied MDF SAR model was built. After performing leave-one-out cross-validation, satisfactory result was obtained with cross-validation r^2_{cv} and r^2 values of 0.9999 and 0.9999. The external validation of the bi-varied MDF SAR model and its ability in prediction of molar refraction of cyclic organophosphorus compounds is demonstrated by the results obtained in training vs. test experiment. The correlated correlation results proved us that the ability in prediction of molar refraction of cyclic organophosphorus compounds with bi-varied MDF SAR model is significantly better compared with the previous reported SAR (see $p_Z = 0.0$ % from Steiger's Z test). The results showed clearly that the molar refraction of cyclic organophosphorus compounds is almost of topological nature (99.99%), and is strongly dependent on atomic relative mass and atomic electronegativity.

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Lorentz JÄNTSCHI and Sorana BOLBOACĂ

Keywords

Molecular Descriptors Family on Structure Activity Relationships, Molar refraction, Cyclic organophosphorus compounds

Introduction

In chemistry, the molar refraction is an approximate measure of the total volume (without free space) of the molecules in one mole of the compound. The molar refraction is calculated by the Lorenz-Lorentz formula [1]:

$$((n^2-1)/(n^2+2))\cdot(M/d)$$

where n is index of refraction (the ratio between the speed of light in a vacuum and the speed of light through the compound), M is the compound's molecular weight (the weight of one molecule, in atomic mass units), and d is the compound's density (in grams per cubic centimeter).

The molar refraction of ten cyclic organophosphorus compounds was previous studied using the Szeged topological indices [2]. The best reported SAR model has the following characteristics:
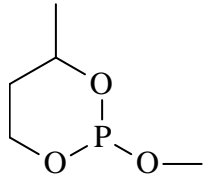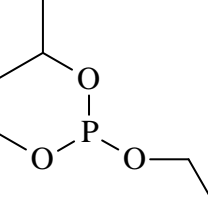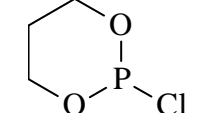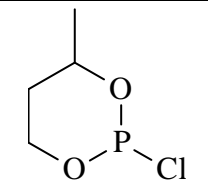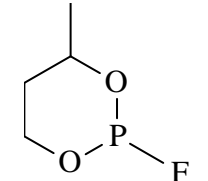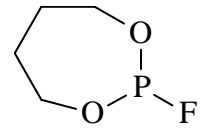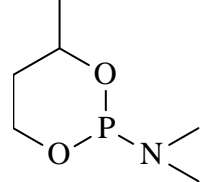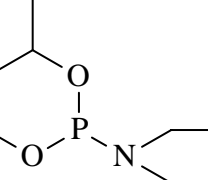
- Number of compounds: 10 and number of components: 2 (SZ_p = a topological descriptor, SZ_eX = an electronic descriptor);
- SAR model: $\hat{Y}$ = 36.821 + 0.016·SZ_p - 0.631·SZ_eX ($\hat{Y}$ = estimated molar refraction) and the correlation coefficient: r = 0.9755.
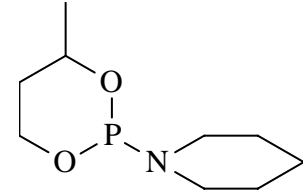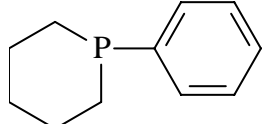
The aim of the research was to test the ability of MDF SAR methodology in prediction of the molar refraction of cyclic organophosphorus compounds and to compare the best performing MDF SAR model with the previous reported SAR model.

Material and Method

Ten cyclic organophosphorus compounds were studied [2]. The planar structure of the cyclic organophosphorus compounds, molar refraction (MR) and previous estimated molar refraction are in table 1.

Table 1. Planar structure of cyclic organophosphorus compounds, MR and previous estimated molar refraction

Mol.	Cyclic organophosphorus planar structure	MR	Estimated MR from ref. [2]
mr01		35.808	36.557
mr02		40.524	40.530
mr03		30.030	32.461
mr04		34.911	33.776
mr05		29.222	29.896
mr06		31.636	30.056
mr07		43.005	40.608
mr08		52.029	52.084

Molecular Descriptors Family on Structure Activity Relationships 4. Molar Refraction of Cyclic Organophosphorus Compounds

Lorentz JÄNTSCHI and Sorana BOLBOACĂ

mr09		49.971	53.864
mr10		58.323	54.714

The steps of molecular descriptors family on structure activity relationships (MDF SAD) modeling of molar refraction of cyclic organophosphorus compounds were [3]:

- Step 1: Sketch of the cyclic organophosphorus compounds;
- Step 2: Create the cyclic organophosphorus compounds molar refraction file;
- Step 3: Generate cyclic organophosphorus compounds MDF members;
- Step 4: Find the molar refraction SAR models;
- Step 5: Validate the MDF SAR models and compare with previous reported results;
- Step 6: Analyze the selected MDF SAR model.

Results

From a total number of 787968 calculated descriptors, 349553 had real and distinct values. Using a 10^{-9} significance selector to bias the values, the MDF members were reduced to a number of 107692 significantly different descriptors. In order to obtain the best performing bi-varied MDF SAR model, pairs of MDF members were included into multiple linear regression experiment. The pair of descriptors, which provide best performing prediction of molar refraction of cyclic organophosphorus compounds, contain *lGDmSMt* and *lAmrfEt* members. The resulted multiple linear regressions models are available at address:

http://vl.academicdirect.org/molecular_topology/mdf_findings/

A program was developed (*j_mdf_demo.php*) in order to demonstrate the validity and the complexity of the MDF SAR methodology in prediction of molar refraction of cyclic organophosphorus compounds. The calculations for the first considered cyclic organophosphorus compound (mr01) with *lGDmSMt* MDF member and for the last

considered cyclic organophosphorus compound (mr10) with *lAmrfEt* member are in Appendix.

The best performing bi-varied MDF SAR model, the calculated valued for the *lGDmSMt* and the *lAmrfEt* members, and estimated molar refraction are in table 2. The plot of the bi-varied MDF SAR model from table 2 is in figure 1.

Table 2. The calculated values of the lGDmSMt and lAmrfEt descriptors and estimated by MDF SAR molar refraction

$\hat{Y}= 17.39 + 28.25 \cdot lGDmSMt - 83.96 \cdot lAmrfEt$			
Mol	lGDmSMt	lAmrfEt	Estimated MR, $\hat{Y}$
mr01	4.2161	1.1978	35.912
mr02	4.0257	1.0788	40.526
mr03	4.7052	1.4330	29.979
mr04	4.4888	1.3004	35.001
mr05	4.3624	1.3271	29.188
mr06	4.4222	1.3185	31.600
mr07	4.0972	1.0740	42.949
mr08	3.8446	0.8820	51.939
mr09	3.9102	0.9270	50.028
mr10	3.7941	0.7890	58.336
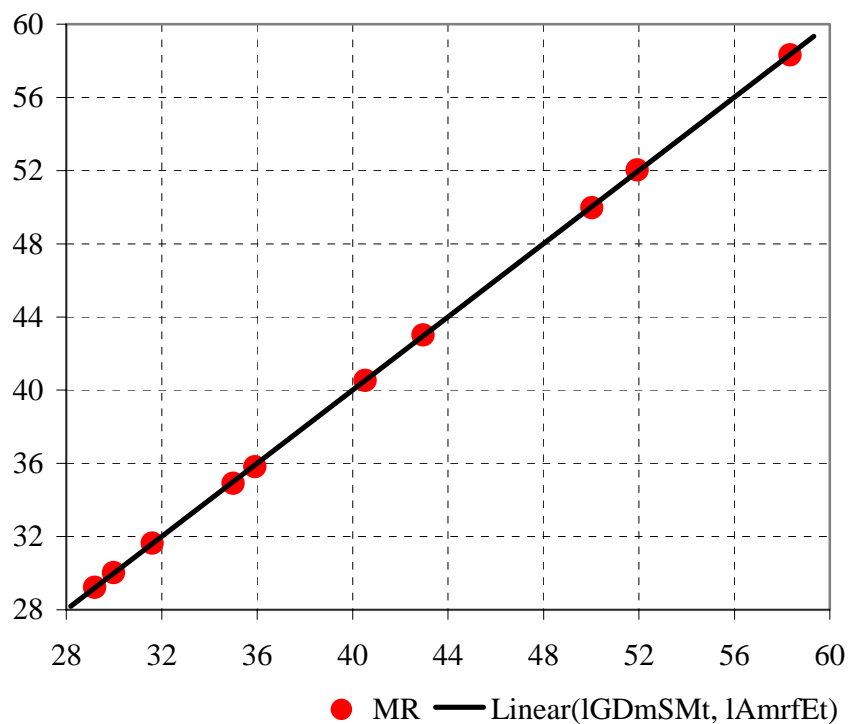
Figure 1. Molar refraction vs. bi-varied MDF SAR estimated molar refraction

Molecular Descriptors Family on Structure Activity Relationships 4. Molar Refraction of Cyclic Organophosphorus Compounds

Lorentz JÄNTSCHI and Sorana BOLBOACĂ

The training vs. test experiment was performed in order to validate the bi-varied MDF SAR model. The cyclic organophosphorus compounds were successively split into training and test sets. The experiment run twice times for training sample sizes equal with four, five, six and seven. Corresponding to the training tests sample sizes, the test sets sample sizes were respectively equal with six, five, four, and three. The Multiple Linear Regression results of the experiment are in table 3.

Table 3. Training vs. test sets results using bi-varied MDF SAR model

No.	Training set					Test set
	Molecules	Intercept	lGDmSMt	lAmrfEt	$(1-r^2)$	$(1-r^2)$
1	10, 4, 9, 7	19.411	27.516	-83.055	$2.5 \cdot 10^{-5}$	$1.5 \cdot 10^{-4}$
2	9, 6, 5, 7	16.578	28.473	-84.066	$1.5 \cdot 10^{-5}$	$4.3 \cdot 10^{-5}$
3	6, 2, 1, 8, 3	15.465	29.079	-85.31	$3.1 \cdot 10^{-5}$	$6.2 \cdot 10^{-5}$
4	1, 9, 3, 7, 10	15.707	28.853	-84.739	$2.2 \cdot 10^{-5}$	$1.0 \cdot 10^{-4}$
5	8, 1, 9, 4, 5, 6	18.617	27.821	-83.489	$5.8 \cdot 10^{-5}$	$2.4 \cdot 10^{-5}$
6	7, 8, 2, 3, 10, 5	17.293	28.287	-83.993	$1.0 \cdot 10^{-5}$	$5.7 \cdot 10^{-5}$
7	3, 4, 6, 5, 2, 8, 1	17.153	28.386	-84.258	$7.9 \cdot 10^{-5}$	$3.6 \cdot 10^{-5}$
8	10, 9, 4, 7, 3, 6, 5	17.908	28.024	-83.591	$2.2 \cdot 10^{-5}$	$6.4 \cdot 10^{-6}$

The MDF SAR model (Estimated MR, Ŷ from table 2) has the following associated statistics:

$$r = 0.9999, r^2 = 0.9999, r^2_{adj} = 0.9999, r^2_{cv} = 0.9999, F = 83012, p_F = 4.8 \cdot 10^{-14} \%,$$

$$r^2(MR, lGDmSMt) = 0.864, r^2(MR, lAmrfEt) = 0.969, r^2(lGDmSMt, lAmrfEt) = 0.948$$

where r is the correlation coefficient, r^2 is the squared correlation coefficient, r^2_{adj} is the adjusted r^2, r^2_{cv} is the cross-validation leave-one-out squared correlation score, F is the Fissssher parameter, and p_F is the Fisrer's associated p-value.

A correlated correlations analysis using the Steiger's Z test was applied in order to compare the bi-varied MDF SAR model with previous reported SAR model. The correlated correlations results are:

$$r(MR, MDF\ SAR) = 0.99998; r(MR, SAR) = 0.97537; r(MDF\ SAR, SAR) = 0.97555;$$

$$Z = 9.25276; p_Z = 0.0 \%$$

where Z is the Steiger's Z test parameter and p_Z is the associated p-value.

Discussions

The pair of MDF members that have the best ability in prediction of the molar refraction of cyclic organophosphorus compounds contain *lGDmSMt* and *lAmrfEt* members. Both members consider the topological shape of the molecules (t), one descriptor takes into consideration atomic relative mass (M) of the molecules while the other takes into consideration atomic electronegativity (E). The squared correlation coefficients computed between molar refraction and MDF members showed that 86% in variation of molar refraction is explainable by its linear relation with *lGDmSMt* member and almost 97% in variation of molar refraction is explainable by its linear relation with *lAmrfEt* member. Ninety-nine percent in variation of molar refraction is explainable by its linear relation with the pair (*lGDmSMt, lAmrfEt*) of MDF members. The probability of a wrong MDF SAR model is equal with $4.8 \cdot 10^{-14}$ %.

The cross-validation leave-one-out correlation score of bi-varied MDF SAR model demonstrate the power of the model in molar refraction of cyclic organophosphorus compounds prediction ($r^2_{cv} = 0.9999$).

The external validation of the bi-varied MDF SAR model and its ability in prediction of molar refraction of cyclic organophosphorus compounds is demonstrated by the results of training vs. test experiment (table 3). The averages of squared correlation coefficients from training (0.9999) and test (0.9999) are equal, which prove its ability in prediction.

The correlated correlation experiment proved us that the ability in prediction of molar refraction of cyclic organophosphorus compounds with bi-varied MDF SAR model is significantly better compared with the previous reported SAR (see $p_Z = 0.0$ % from Steiger's Z test).

Conclusions

The molar refraction of cyclic organophosphorus compounds is almost of topological nature (99.99%), and is strongly dependent on atomic relative mass and atomic electronegativity.

Molecular Descriptors Family on Structure Activity Relationships 4. Molar Refraction of Cyclic Organophosphorus Compounds

Lorentz JÄNTSCHI and Sorana BOLBOACĂ

Even if the MDF SAR methodology is complex and time consuming the result worth the effort because the ability in prediction of the molar refraction of cyclic organophosphorus compounds with bi-varied MDF SAR model is significantly better comparing with previous reported SAR model.

References

[1] Vakili-Nezhaad G. R., Modarress H., A New Characterization Factor for Hydrocarbons and Petroleum Fluids Fractions, Oil & Gas Science and Technology – Rev. IFP, Vol. 57, No. 2, 2002, p. 149-154.

[2] Jäntschi L., Mureşan S., Diudea M.V., Modeling molar refraction and chromatographic retention by Szeged Indices, Studia Universitatis Babeş-Bolyai, Chemia, 2000, XLV(1-2), p. 313-318.

[3] Jäntschi L., Molecular Descriptors Family on Structure Activity Relationships 1. The review of Methodology, Leonardo Electronic Journal of Practices and Technologies, AcademicDirect, 2005, Issue 6, p. 76-98.

Appendix

The appendix are from output of *j_mdf_demo.php* program.

Demonstrative calculations for mr01 molecule and lGDmSMt MDF member

```
POST data: Array
(
    [hin] => 01_mr1001.hin
    [Do] => t
    [Ap] => M
    [Df] => S
    [Im] => m
    [Fc] => D
    [Sf] => G
    [Lo] => l
)
Molecule's data: m_c Object
(
    [a] => 9
    [b] => 9
    [atom] => Array
        (
            [1] => Array
                (
                    [0] => 1
                    [1] => -
                    [2] => C
                    [3] => C4
                    [4] => -
                    [5] => -0.1095657
                    [6] => 0.4318282
                    [7] => 0.6380987
                    [8] => 2.849884
                    [9] => 1
                    [10] => 2
                    [11] => 1
                )

            [2] => Array
                (
                    [0] => 2
                    [1] => -
                    [2] => C
                    [3] => C4
                    [4] => -
                    [5] => 0.5250869
                    [6] => -0.2941397
                    [7] => 0.1247597
                    [8] => 1.592484
                    [9] => 3
                    [10] => 1
                    [11] => 1
                    [12] => 3
                    [13] => 1
```

Molecular Descriptors Family on Structure Activity Relationships 4. Molar Refraction of Cyclic Organophosphorus Compounds

Lorentz JÄNTSCHI and Sorana BOLBOACĂ

```
            [14] => 7
            [15] => 1
        )

    [3] => Array
        (
            [0] => 3
            [1] => -
            [2] => C
            [3] => C4
            [4] => -
            [5] => -0.0686326
            [6] => -0.2920918
            [7] => -1.415741
            [8] => 1.596032
            [9] => 2
            [10] => 2
            [11] => 1
            [12] => 4
            [13] => 1
        )

    [4] => Array
        (
            [0] => 4
            [1] => -
            [2] => C
            [3] => C4
            [4] => -
            [5] => 0.4661818
            [6] => -1.039482
            [7] => -1.962821
            [8] => 0.3649576
            [9] => 2
            [10] => 3
            [11] => 1
            [12] => 5
            [13] => 1
        )

    [5] => Array
        (
            [0] => 5
            [1] => -
            [2] => O
            [3] => O2
            [4] => -
            [5] => -0.9945602
            [6] => -0.3896529
            [7] => -1.532219
            [8] => -0.8337278
            [9] => 2
            [10] => 4
            [11] => 1
            [12] => 6
            [13] => 1
        )

    [6] => Array
```

```
            (
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                [1] => -
                [2] => P
                [3] => P5
                [4] => -
                [5] => 1.883921
                [6] => -0.5882888
                [7] => 0.2352459
                [8] => -1.032513
                [9] => 3
                [10] => 5
                [11] => 1
                [12] => 7
                [13] => 1
                [14] => 8
                [15] => 1
            )

        [7] => Array
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                [3] => O2
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                [6] => 0.3748803
                [7] => 0.6139225
                [8] => 0.4270911
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                [10] => 6
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                [12] => 2
                [13] => 1
            )

        [8] => Array
            (
                [0] => 8
                [1] => -
                [2] => O
                [3] => O2
                [4] => -
                [5] => -1.019472
                [6] => 0.6156649
                [7] => 1.142236
                [8] => -1.997664
                [9] => 2
                [10] => 6
                [11] => 1
                [12] => 9
                [13] => 1
            )

        [9] => Array
            (
                [0] => 9
                [1] => -
```

Molecular Descriptors Family on Structure Activity Relationships 4. Molar Refraction of Cyclic Organophosphorus Compounds

Lorentz JÄNTSCHI and Sorana BOLBOACĂ

```
                    [2] => C
                    [3] => C4
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                    [6] => 0.2612277
                    [7] => 2.5274
                    [8] => -2.022074
                    [9] => 1
                    [10] => 8
                    [11] => 1
                )

        )

    [prop] => Array
        (
            [1] => Array
                (
                    [0] => 1
                    [1] => 4
                    [2] => 12
                    [3] => 2.746
                    [4] => 2.6296707827796
                    [5] => -0.1095657
                )

            [2] => Array
                (
                    [0] => 1
                    [1] => 2
                    [2] => 12
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                    [4] => 2.6678890531654
                    [5] => 0.5250869
                )

            [3] => Array
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                    [0] => 1
                    [1] => 3
                    [2] => 12
                    [3] => 2.746
                    [4] => 2.6423489837131
                    [5] => -0.0686326
                )

            [4] => Array
                (
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                    [1] => 3
                    [2] => 12
                    [3] => 2.746
                    [4] => 2.6423489837131
                    [5] => 0.4661818
                )

            [5] => Array
                (
                    [0] => 1
```

```
                            [1] => 1
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                            [5] => -0.9945602
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                            [3] => 2.515
                            [4] => 2.515
                            [5] => 1.883921
                    )

            [7] => Array
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                            [0] => 1
                            [1] => 1
                            [2] => 15.99491464
                            [3] => 3.654
                            [4] => 3.654
                            [5] => -1.095338
                    )

            [8] => Array
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                            [1] => 1
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                            [4] => 3.654
                            [5] => -1.019472
                    )

            [9] => Array
                    (
                            [0] => 1
                            [1] => 4
                            [2] => 12
                            [3] => 2.746
                            [4] => 2.6296707827796
                            [5] => 0.4202826
                    )

        )

    [e] => seed 0
    [f] => forcefield mm+
    [m] => mol 1
    [s] => sys 0 0 1
)
Fragments tree structure: Array
(
    [1] => Array
        (
                [2] => Array
```

Molecular Descriptors Family on Structure Activity Relationships 4. Molar Refraction of Cyclic Organophosphorus Compounds

Lorentz JÄNTSCHI and Sorana BOLBOACĂ

```
                        (
                            [0] => 1
                        )

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                        )

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                        )

                    [5] => Array
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                            [0] => 1
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                        )

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                        (
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                            [1] => 2
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                    [7] => Array
                        (
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                            [1] => 2
                            [2] => 3
                        )

                    [9] => Array
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                            [0] => 1
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                            [2] => 3
                            [3] => 4
                            [4] => 7
                        )

                    [1] => Array
                        (
                            [0] => 0
                        )

                )

        [2] => Array
                (
```

```
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        [7] => 9
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[3] => Array
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        [2] => 6
        [3] => 7
        [4] => 8
        [5] => 9
    )

[4] => Array
    (
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        [1] => 1
        [2] => 7
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    (
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        [1] => 1
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        [3] => 7
    )

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    (
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        [1] => 1
        [2] => 3
    )

[7] => Array
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        [0] => 2
        [1] => 1
        [2] => 3
        [3] => 4
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[8] => Array
    (
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        [1] => 1
        [2] => 3
        [3] => 4
        [4] => 7
```

Molecular Descriptors Family on Structure Activity Relationships 4. Molar Refraction of Cyclic Organophosphorus Compounds

Lorentz JÄNTSCHI and Sorana BOLBOACĂ

```
                )

        [9] => Array
            (
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                [1] => 1
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                [3] => 4
                [4] => 7
            )

        [2] => Array
            (
                [0] => 0
            )

    )

[3] => Array
    (
        [1] => Array
            (
                [0] => 3
                [1] => 4
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            )

        [2] => Array
            (
                [0] => 3
                [1] => 4
                [2] => 5
            )

        [4] => Array
            (
                [0] => 3
                [1] => 1
                [2] => 2
                [3] => 7
            )

        [5] => Array
            (
                [0] => 3
                [1] => 1
                [2] => 2
            )

        [6] => Array
            (
                [0] => 3
                [1] => 1
                [2] => 2
                [3] => 4
            )

        [7] => Array
            (
```

```
            [0] => 3
            [1] => 4
        )

    [8] => Array
        (
            [0] => 3
            [1] => 1
            [2] => 2
            [3] => 4
        )

    [9] => Array
        (
            [0] => 3
            [1] => 1
            [2] => 2
            [3] => 4
            [4] => 5
            [5] => 7
        )

    [3] => Array
        (
            [0] => 0
        )

)

[4] => Array
    (
        [1] => Array
            (
                [0] => 4
                [1] => 3
                [2] => 5
                [3] => 6
                [4] => 8
                [5] => 9
            )

        [2] => Array
            (
                [0] => 4
                [1] => 5
            )

        [3] => Array
            (
                [0] => 4
                [1] => 5
                [2] => 6
                [3] => 8
                [4] => 9
            )

        [5] => Array
            (
                [0] => 4
```

Molecular Descriptors Family on Structure Activity Relationships 4. Molar Refraction of Cyclic Organophosphorus Compounds

Lorentz JÄNTSCHI and Sorana BOLBOACĂ

```
                    [1] => 1
                    [2] => 2
                    [3] => 3
                )

        [6] => Array
            (
                    [0] => 4
                    [1] => 3
            )

        [7] => Array
            (
                    [0] => 4
                    [1] => 3
                    [2] => 5
            )

        [8] => Array
            (
                    [0] => 4
                    [1] => 1
                    [2] => 2
                    [3] => 3
                    [4] => 5
            )

        [9] => Array
            (
                    [0] => 4
                    [1] => 1
                    [2] => 2
                    [3] => 3
                    [4] => 5
            )

        [4] => Array
            (
                    [0] => 0
            )

    )

[5] => Array
    (
        [1] => Array
            (
                    [0] => 5
                    [1] => 4
                    [2] => 6
                    [3] => 8
                    [4] => 9
            )

        [2] => Array
            (
                    [0] => 5
                    [1] => 4
                    [2] => 6
```

```
                [3] => 8
                [4] => 9
            )

        [3] => Array
            (
                [0] => 5
                [1] => 6
                [2] => 8
                [3] => 9
            )

        [4] => Array
            (
                [0] => 5
                [1] => 6
                [2] => 7
                [3] => 8
                [4] => 9
            )

        [6] => Array
            (
                [0] => 5
                [1] => 3
                [2] => 4
            )

        [7] => Array
            (
                [0] => 5
                [1] => 4
            )

        [8] => Array
            (
                [0] => 5
                [1] => 3
                [2] => 4
            )

        [9] => Array
            (
                [0] => 5
                [1] => 1
                [2] => 2
                [3] => 3
                [4] => 4
                [5] => 6
                [6] => 7
            )

        [5] => Array
            (
                [0] => 0
            )

    )
```

Molecular Descriptors Family on Structure Activity Relationships 4. Molar Refraction of Cyclic Organophosphorus Compounds

Lorentz JÄNTSCHI and Sorana BOLBOACĂ

```
[6] => Array
    (
        [1] => Array
            (
                [0] => 6
                [1] => 4
                [2] => 5
                [3] => 7
                [4] => 8
                [5] => 9
            )

        [2] => Array
            (
                [0] => 6
                [1] => 5
                [2] => 8
                [3] => 9
            )

        [3] => Array
            (
                [0] => 6
                [1] => 5
                [2] => 7
                [3] => 8
                [4] => 9
            )

        [4] => Array
            (
                [0] => 6
                [1] => 7
                [2] => 8
                [3] => 9
            )

        [5] => Array
            (
                [0] => 6
                [1] => 1
                [2] => 2
                [3] => 7
                [4] => 8
                [5] => 9
            )

        [7] => Array
            (
                [0] => 6
                [1] => 4
                [2] => 5
                [3] => 8
                [4] => 9
            )

        [8] => Array
            (
                [0] => 6
```

```
            [1] => 1
            [2] => 2
            [3] => 3
            [4] => 4
            [5] => 5
            [6] => 7
        )

    [9] => Array
        (
            [0] => 6
            [1] => 1
            [2] => 2
            [3] => 3
            [4] => 4
            [5] => 5
            [6] => 7
        )

    [6] => Array
        (
            [0] => 0
        )

)

[7] => Array
    (
        [1] => Array
            (
                [0] => 7
                [1] => 5
                [2] => 6
                [3] => 8
                [4] => 9
            )

        [2] => Array
            (
                [0] => 7
                [1] => 5
                [2] => 6
                [3] => 8
                [4] => 9
            )

        [3] => Array
            (
                [0] => 7
                [1] => 6
                [2] => 8
                [3] => 9
            )

        [4] => Array
            (
                [0] => 7
                [1] => 1
                [2] => 2
```

Molecular Descriptors Family on Structure Activity Relationships 4. Molar Refraction of Cyclic Organophosphorus Compounds

Lorentz JÄNTSCHI and Sorana BOLBOACĂ

```
                        [3] => 6
                        [4] => 8
                        [5] => 9
                    )

            [5] => Array
                    (
                        [0] => 7
                        [1] => 1
                        [2] => 2
                    )

            [6] => Array
                    (
                        [0] => 7
                        [1] => 1
                        [2] => 2
                        [3] => 3
                    )

            [8] => Array
                    (
                        [0] => 7
                        [1] => 1
                        [2] => 2
                        [3] => 3
                    )

            [9] => Array
                    (
                        [0] => 7
                        [1] => 1
                        [2] => 2
                        [3] => 3
                        [4] => 4
                        [5] => 5
                        [6] => 6
                    )

            [7] => Array
                    (
                        [0] => 0
                    )

        )

    [8] => Array
        (
            [1] => Array
                    (
                        [0] => 8
                        [1] => 5
                        [2] => 6
                        [3] => 9
                    )

            [2] => Array
                    (
                        [0] => 8
```

```
                    [1] => 5
                    [2] => 6
                    [3] => 9
                )

        [3] => Array
            (
                    [0] => 8
                    [1] => 6
                    [2] => 9
                )

        [4] => Array
            (
                    [0] => 8
                    [1] => 6
                    [2] => 7
                    [3] => 9
                )

        [5] => Array
            (
                    [0] => 8
                    [1] => 9
                )

        [6] => Array
            (
                    [0] => 8
                    [1] => 9
                )

        [7] => Array
            (
                    [0] => 8
                    [1] => 9
                )

        [9] => Array
            (
                    [0] => 8
                    [1] => 1
                    [2] => 2
                    [3] => 3
                    [4] => 4
                    [5] => 5
                    [6] => 6
                    [7] => 7
                )

        [8] => Array
            (
                    [0] => 0
                )

    )

[9] => Array
    (
```

Molecular Descriptors Family on Structure Activity Relationships 4. Molar Refraction of Cyclic Organophosphorus Compounds

Lorentz JÄNTSCHI and Sorana BOLBOACĂ

```
        [1] => Array
            (
                [0] => 9
                [1] => 5
                [2] => 6
                [3] => 8
            )

        [2] => Array
            (
                [0] => 9
                [1] => 8
            )

        [3] => Array
            (
                [0] => 9
                [1] => 6
                [2] => 8
            )

        [4] => Array
            (
                [0] => 9
                [1] => 8
            )

        [5] => Array
            (
                [0] => 9
                [1] => 8
            )

        [6] => Array
            (
                [0] => 9
            )

        [7] => Array
            (
                [0] => 9
                [1] => 8
            )

        [8] => Array
            (
                [0] => 9
            )

        [9] => Array
            (
                [0] => 0
            )

    )

)
Fragments: 72
Fragmental properties: Array
```

```
(
    [0] => 144
    [1] => 18
    [2] => 32.808788679292
    [3] => 7.5833333333333
    [4] => 28.666666666667
    [5] => 18
    [6] => 9.8333333333333
    [7] => 16.279455345959
    [8] => 243.99228165407
    [9] => 234.66149059666
    [10] => 32.808788679292
    [11] => 57.562995125944
    [12] => 28.666666666667
    [13] => 185.33333333333
    [14] => 47.146328459277
    [15] => 16.279455345959
    [16] => 27.33079105741
    [17] => 171.47545534596
    [18] => 176.80878867929
    [19] => 25.583333333333
    [20] => 46.666666666667
    [21] => 23.333333333333
    [22] => 15.166666666667
    [23] => 25.754910691918
    [24] => 68.012619861456
    [25] => 27.475455345959
    [26] => 216.66149059666
    [27] => 169.58333333333
    [28] => 23.333333333333
    [29] => 55.312995125944
    [30] => 47.146328459277
    [31] => 16.279455345959
    [32] => 50.012619861456
    [33] => 159.12266308681
    [34] => 72.661490596657
    [35] => 396.9599574277
    [36] => 279.17062767422
    [37] => 37.312995125944
    [38] => 39.562995125944
    [39] => 145.67666308681
    [40] => 81.992281654066
    [41] => 141.12266308681
    [42] => 104.64115238927
    [43] => 141.12266308681
    [44] => 1036.2500094111
    [45] => 1034.0000094111
    [46] => 1038.5000094111
    [47] => 145.67666308681
    [48] => 76.658948320733
    [49] => 396.9599574277
    [50] => 72.661490596657
    [51] => 164.45599642015
    [52] => 39.562995125944
    [53] => 284.50396100755
    [54] => 41.812995125944
    [55] => 145.67666308681
    [56] => 44.679286528122
    [57] => 141.12266308681
```

Molecular Descriptors Family on Structure Activity Relationships 4. Molar Refraction of Cyclic Organophosphorus Compounds

Lorentz JÄNTSCHI and Sorana BOLBOACĂ

```
    [58] => 40.681828804046
    [59] => 141.12266308681
    [60] => 37.312995125944
    [61] => 273.83729434089
    [62] => 37.312995125944
    [63] => 401.5139574277
    [64] => 44.679286528122
    [65] => 11.725455345959
    [66] => 40.681828804046
    [67] => 11.725455345959
    [68] => 37.312995125944
    [69] => 18
    [70] => 37.312995125944
    [71] => 144
)
GDmSMt = 67.772137360531
lGDmSMt = 4.2161511570974
```

Demonstrative calculations for mr10 molecule and lAmrfEt MDF member

```
POST data: Array
(
    [hin] => 10_mr1010.hin
    [Do] => t
    [Ap] => E
    [Df] => f
    [Im] => r
    [Fc] => m
    [Sf] => A
    [Lo] => l
)
Molecule's data: m_c Object
(
    [a] => 12
    [b] => 13
    [atom] => Array
        (
            [1] => Array
                (
                    [0] => 1
                    [1] => -
                    [2] => C
                    [3] => C4
                    [4] => -
                    [5] => -0.01363325
                    [6] => -1.374815
                    [7] => -2.525667
                    [8] => -1.163645
                    [9] => 2
                    [10] => 2
                    [11] => 1
                    [12] => 6
                    [13] => 1
                )

            [2] => Array
```

```
            (
                [0] => 2
                [1] => -
                [2] => C
                [3] => C4
                [4] => -
                [5] => -0.03494024
                [6] => -0.6541022
                [7] => -3.076405
                [8] => 0.08466685
                [9] => 2
                [10] => 1
                [11] => 1
                [12] => 3
                [13] => 1
            )

        [3] => Array
            (
                [0] => 3
                [1] => -
                [2] => C
                [3] => C4
                [4] => -
                [5] => -0.01286221
                [6] => 0.8641648
                [7] => -2.810718
                [8] => 0.0138855
                [9] => 2
                [10] => 2
                [11] => 1
                [12] => 4
                [13] => 1
            )

        [4] => Array
            (
                [0] => 4
                [1] => -
                [2] => C
                [3] => C4
                [4] => -
                [5] => -0.2916856
                [6] => 1.165918
                [7] => -1.313278
                [8] => 0.1745337
                [9] => 2
                [10] => 3
                [11] => 1
                [12] => 5
                [13] => 1
            )

        [5] => Array
            (
                [0] => 5
                [1] => -
                [2] => P
                [3] => P5
```

Molecular Descriptors Family on Structure Activity Relationships 4. Molar Refraction of Cyclic Organophosphorus Compounds

Lorentz JÄNTSCHI and Sorana BOLBOACĂ

```
            [4] => -
            [5] => 0.9998846
            [6] => 0.3477604
            [7] => -0.3762538
            [8] => -1.163645
            [9] => 3
            [10] => 4
            [11] => 1
            [12] => 6
            [13] => 1
            [14] => 7
            [15] => 1
        )

    [6] => Array
        (
            [0] => 6
            [1] => -
            [2] => C
            [3] => C4
            [4] => -
            [5] => -0.07605362
            [6] => -1.374815
            [7] => -0.9852762
            [8] => -1.163645
            [9] => 2
            [10] => 5
            [11] => 1
            [12] => 1
            [13] => 1
        )

    [7] => Array
        (
            [0] => 7
            [1] => -
            [2] => C
            [3] => C3
            [4] => -
            [5] => -0.2473259
            [6] => 0.2043564
            [7] => 1.029266
            [8] => -0.0003523827
            [9] => 3
            [10] => 5
            [11] => 1
            [12] => 8
            [13] => 2
            [14] => 9
            [15] => 1
        )

    [8] => Array
        (
            [0] => 8
            [1] => -
            [2] => C
            [3] => C3
            [4] => -
```

```
            [5] => -0.04595566
            [6] => -0.4518933
            [7] => 0.876143
            [8] => 1.157674
            [9] => 2
            [10] => 7
            [11] => 2
            [12] => 10
            [13] => 1
        )

    [9] => Array
        (
            [0] => 9
            [1] => -
            [2] => C
            [3] => C3
            [4] => -
            [5] => -0.04757643
            [6] => 0.7997317
            [7] => 2.319123
            [8] => -0.3369715
            [9] => 2
            [10] => 7
            [11] => 1
            [12] => 11
            [13] => 2
        )

    [10] => Array
        (
            [0] => 10
            [1] => -
            [2] => C
            [3] => C3
            [4] => -
            [5] => -0.04881668
            [6] => -0.5716058
            [7] => 1.999108
            [8] => 2.082884
            [9] => 2
            [10] => 8
            [11] => 1
            [12] => 12
            [13] => 2
        )

    [11] => Array
        (
            [0] => 11
            [1] => -
            [2] => C
            [3] => C3
            [4] => -
            [5] => -0.0406456
            [6] => 0.6907468
            [7] => 3.349581
            [8] => 0.5127543
            [9] => 2
```

Molecular Descriptors Family on Structure Activity Relationships 4. Molar Refraction of Cyclic Organophosphorus Compounds

Lorentz JÄNTSCHI and Sorana BOLBOACĂ

```
                    [10] => 9
                    [11] => 2
                    [12] => 12
                    [13] => 1
                )

        [12] => Array
            (
                    [0] => 12
                    [1] => -
                    [2] => C
                    [3] => C3
                    [4] => -
                    [5] => -0.05546284
                    [6] => -0.02339876
                    [7] => 3.182384
                    [8] => 1.775193
                    [9] => 2
                    [10] => 10
                    [11] => 2
                    [12] => 11
                    [13] => 1
                )

        )

    [prop] => Array
        (
            [1] => Array
                (
                    [0] => 1
                    [1] => 3
                    [2] => 12
                    [3] => 2.746
                    [4] => 2.6423489837131
                    [5] => -0.01363325
                )

            [2] => Array
                (
                    [0] => 1
                    [1] => 3
                    [2] => 12
                    [3] => 2.746
                    [4] => 2.6423489837131
                    [5] => -0.03494024
                )

            [3] => Array
                (
                    [0] => 1
                    [1] => 3
                    [2] => 12
                    [3] => 2.746
                    [4] => 2.6423489837131
                    [5] => -0.01286221
                )

            [4] => Array
```

```
        (
                [0] => 1
                [1] => 3
                [2] => 12
                [3] => 2.746
                [4] => 2.6423489837131
                [5] => -0.2916856
        )

    [5] => Array
        (
                [0] => 1
                [1] => 1
                [2] => 30.9737634
                [3] => 2.515
                [4] => 2.515
                [5] => 0.9998846
        )

    [6] => Array
        (
                [0] => 1
                [1] => 3
                [2] => 12
                [3] => 2.746
                [4] => 2.6423489837131
                [5] => -0.07605362
        )

    [7] => Array
        (
                [0] => 1
                [1] => 1
                [2] => 12
                [3] => 2.746
                [4] => 2.746
                [5] => -0.2473259
        )

    [8] => Array
        (
                [0] => 1
                [1] => 2
                [2] => 12
                [3] => 2.746
                [4] => 2.6678890531654
                [5] => -0.04595566
        )

    [9] => Array
        (
                [0] => 1
                [1] => 2
                [2] => 12
                [3] => 2.746
                [4] => 2.6678890531654
                [5] => -0.04757643
        )
```

Molecular Descriptors Family on Structure Activity Relationships 4. Molar Refraction of Cyclic Organophosphorus Compounds

Lorentz JÄNTSCHI and Sorana BOLBOACĂ

```
                        [10] => Array
                            (
                                [0] => 1
                                [1] => 2
                                [2] => 12
                                [3] => 2.746
                                [4] => 2.6678890531654
                                [5] => -0.04881668
                            )

                        [11] => Array
                            (
                                [0] => 1
                                [1] => 2
                                [2] => 12
                                [3] => 2.746
                                [4] => 2.6678890531654
                                [5] => -0.0406456
                            )

                        [12] => Array
                            (
                                [0] => 1
                                [1] => 2
                                [2] => 12
                                [3] => 2.746
                                [4] => 2.6678890531654
                                [5] => -0.05546284
                            )

                )

        [e] => seed 0
        [f] => forcefield mm+
        [m] => mol 1
        [s] => sys 0 0 1
    )
Fragments tree structure: Array
(
    [1] => Array
        (
            [1] => Array
                (
                    [0] => 0
                )

            [2] => Array
                (
                    [0] => 1
                )

            [3] => Array
                (
                    [0] => 1
                )

            [4] => Array
                (
                    [0] => 1
```

```
                )

        [5] => Array
            (
                [0] => 1
            )

        [6] => Array
            (
                [0] => 1
            )

        [7] => Array
            (
                [0] => 1
            )

        [8] => Array
            (
                [0] => 1
            )

        [9] => Array
            (
                [0] => 1
            )

        [10] => Array
            (
                [0] => 1
            )

        [11] => Array
            (
                [0] => 1
            )

        [12] => Array
            (
                [0] => 1
            )

    )

[2] => Array
    (
        [1] => Array
            (
                [0] => 2
            )

        [2] => Array
            (
                [0] => 0
            )

        [3] => Array
            (
                [0] => 2
```

Molecular Descriptors Family on Structure Activity Relationships 4. Molar Refraction of Cyclic Organophosphorus Compounds

Lorentz JÄNTSCHI and Sorana BOLBOACĂ

```
            )

        [4] => Array
            (
                [0] => 2
            )

        [5] => Array
            (
                [0] => 2
            )

        [6] => Array
            (
                [0] => 2
            )

        [7] => Array
            (
                [0] => 2
            )

        [8] => Array
            (
                [0] => 2
            )

        [9] => Array
            (
                [0] => 2
            )

        [10] => Array
            (
                [0] => 2
            )

        [11] => Array
            (
                [0] => 2
            )

        [12] => Array
            (
                [0] => 2
            )

    )

[3] => Array
    (
        [1] => Array
            (
                [0] => 3
            )

        [2] => Array
            (
                [0] => 3
```

```
                    )

            [3] => Array
                (
                    [0] => 0
                )

            [4] => Array
                (
                    [0] => 3
                )

            [5] => Array
                (
                    [0] => 3
                )

            [6] => Array
                (
                    [0] => 3
                )

            [7] => Array
                (
                    [0] => 3
                )

            [8] => Array
                (
                    [0] => 3
                )

            [9] => Array
                (
                    [0] => 3
                )

            [10] => Array
                (
                    [0] => 3
                )

            [11] => Array
                (
                    [0] => 3
                )

            [12] => Array
                (
                    [0] => 3
                )

        )

    [4] => Array
        (
            [1] => Array
                (
                    [0] => 4
```

Molecular Descriptors Family on Structure Activity Relationships 4. Molar Refraction of Cyclic Organophosphorus Compounds

Lorentz JÄNTSCHI and Sorana BOLBOACĂ

```
                )

        [2] => Array
            (
                [0] => 4
            )

        [3] => Array
            (
                [0] => 4
            )

        [4] => Array
            (
                [0] => 0
            )

        [5] => Array
            (
                [0] => 4
            )

        [6] => Array
            (
                [0] => 4
            )

        [7] => Array
            (
                [0] => 4
            )

        [8] => Array
            (
                [0] => 4
            )

        [9] => Array
            (
                [0] => 4
            )

        [10] => Array
            (
                [0] => 4
            )

        [11] => Array
            (
                [0] => 4
            )

        [12] => Array
            (
                [0] => 4
            )

    )
```

```
[5] => Array
    (
        [1] => Array
            (
                [0] => 5
            )

        [2] => Array
            (
                [0] => 5
            )

        [3] => Array
            (
                [0] => 5
            )

        [4] => Array
            (
                [0] => 5
            )

        [5] => Array
            (
                [0] => 0
            )

        [6] => Array
            (
                [0] => 5
            )

        [7] => Array
            (
                [0] => 5
            )

        [8] => Array
            (
                [0] => 5
            )

        [9] => Array
            (
                [0] => 5
            )

        [10] => Array
            (
                [0] => 5
            )

        [11] => Array
            (
                [0] => 5
            )

        [12] => Array
            (
```

Molecular Descriptors Family on Structure Activity Relationships 4. Molar Refraction of Cyclic Organophosphorus Compounds

Lorentz JÄNTSCHI and Sorana BOLBOACĂ

```
                    [0] => 5
                )

        )

    [6] => Array
        (
            [1] => Array
                (
                    [0] => 6
                )

            [2] => Array
                (
                    [0] => 6
                )

            [3] => Array
                (
                    [0] => 6
                )

            [4] => Array
                (
                    [0] => 6
                )

            [5] => Array
                (
                    [0] => 6
                )

            [6] => Array
                (
                    [0] => 0
                )

            [7] => Array
                (
                    [0] => 6
                )

            [8] => Array
                (
                    [0] => 6
                )

            [9] => Array
                (
                    [0] => 6
                )

            [10] => Array
                (
                    [0] => 6
                )

            [11] => Array
                (
```

```
                    [0] => 6
                )

            [12] => Array
                (
                    [0] => 6
                )

        )

    [7] => Array
        (
            [1] => Array
                (
                    [0] => 7
                )

            [2] => Array
                (
                    [0] => 7
                )

            [3] => Array
                (
                    [0] => 7
                )

            [4] => Array
                (
                    [0] => 7
                )

            [5] => Array
                (
                    [0] => 7
                )

            [6] => Array
                (
                    [0] => 7
                )

            [7] => Array
                (
                    [0] => 0
                )

            [8] => Array
                (
                    [0] => 7
                )

            [9] => Array
                (
                    [0] => 7
                )

            [10] => Array
                (
```

Molecular Descriptors Family on Structure Activity Relationships 4. Molar Refraction of Cyclic Organophosphorus Compounds

Lorentz JÄNTSCHI and Sorana BOLBOACĂ

```
                    [0] => 7
                )

            [11] => Array
                (
                    [0] => 7
                )

            [12] => Array
                (
                    [0] => 7
                )

        )

    [8] => Array
        (
            [1] => Array
                (
                    [0] => 8
                )

            [2] => Array
                (
                    [0] => 8
                )

            [3] => Array
                (
                    [0] => 8
                )

            [4] => Array
                (
                    [0] => 8
                )

            [5] => Array
                (
                    [0] => 8
                )

            [6] => Array
                (
                    [0] => 8
                )

            [7] => Array
                (
                    [0] => 8
                )

            [8] => Array
                (
                    [0] => 0
                )

            [9] => Array
                (
```

```
                    [0] => 8
                )

        [10] => Array
            (
                    [0] => 8
                )

        [11] => Array
            (
                    [0] => 8
                )

        [12] => Array
            (
                    [0] => 8
                )

    )

[9] => Array
    (
        [1] => Array
            (
                    [0] => 9
                )

        [2] => Array
            (
                    [0] => 9
                )

        [3] => Array
            (
                    [0] => 9
                )

        [4] => Array
            (
                    [0] => 9
                )

        [5] => Array
            (
                    [0] => 9
                )

        [6] => Array
            (
                    [0] => 9
                )

        [7] => Array
            (
                    [0] => 9
                )

        [8] => Array
            (
```

Molecular Descriptors Family on Structure Activity Relationships 4. Molar Refraction of Cyclic Organophosphorus Compounds

Lorentz JÄNTSCHI and Sorana BOLBOACĂ

```
                    [0] => 9
                )

            [9] => Array
                (
                    [0] => 0
                )

            [10] => Array
                (
                    [0] => 9
                )

            [11] => Array
                (
                    [0] => 9
                )

            [12] => Array
                (
                    [0] => 9
                )

        )

    [10] => Array
        (
            [1] => Array
                (
                    [0] => 10
                )

            [2] => Array
                (
                    [0] => 10
                )

            [3] => Array
                (
                    [0] => 10
                )

            [4] => Array
                (
                    [0] => 10
                )

            [5] => Array
                (
                    [0] => 10
                )

            [6] => Array
                (
                    [0] => 10
                )

            [7] => Array
                (
```

```
                [0] => 10
            )

        [8] => Array
            (
                [0] => 10
            )

        [9] => Array
            (
                [0] => 10
            )

        [10] => Array
            (
                [0] => 0
            )

        [11] => Array
            (
                [0] => 10
            )

        [12] => Array
            (
                [0] => 10
            )

    )

[11] => Array
    (
        [1] => Array
            (
                [0] => 11
            )

        [2] => Array
            (
                [0] => 11
            )

        [3] => Array
            (
                [0] => 11
            )

        [4] => Array
            (
                [0] => 11
            )

        [5] => Array
            (
                [0] => 11
            )

        [6] => Array
            (
```

Molecular Descriptors Family on Structure Activity Relationships 4. Molar Refraction of Cyclic Organophosphorus Compounds

Lorentz JÄNTSCHI and Sorana BOLBOACĂ

```
                    [0] => 11
                )

            [7] => Array
                (
                    [0] => 11
                )

            [8] => Array
                (
                    [0] => 11
                )

            [9] => Array
                (
                    [0] => 11
                )

            [10] => Array
                (
                    [0] => 11
                )

            [11] => Array
                (
                    [0] => 0
                )

            [12] => Array
                (
                    [0] => 11
                )

        )

    [12] => Array
        (
            [1] => Array
                (
                    [0] => 12
                )

            [2] => Array
                (
                    [0] => 12
                )

            [3] => Array
                (
                    [0] => 12
                )

            [4] => Array
                (
                    [0] => 12
                )

            [5] => Array
                (
```

```
                        [0] => 12
                    )

            [6] => Array
                (
                        [0] => 12
                )

            [7] => Array
                (
                        [0] => 12
                )

            [8] => Array
                (
                        [0] => 12
                )

            [9] => Array
                (
                        [0] => 12
                )

            [10] => Array
                (
                        [0] => 12
                )

            [11] => Array
                (
                        [0] => 12
                )

            [12] => Array
                (
                        [0] => 0
                )

        )

)
Fragments: 132
Fragmental properties: Array
(
    [0] => 7.540516
    [1] => 1.885129
    [2] => 0.83783511111111
    [3] => 1.7265475
    [4] => 7.540516
    [5] => 0.83783511111111
    [6] => 0.47128225
    [7] => 0.47128225
    [8] => 0.30162064
    [9] => 0.30162064
    [10] => 0.20945877777778
    [11] => 7.540516
    [12] => 7.540516
    [13] => 1.885129
    [14] => 0.76735444444444
```

Molecular Descriptors Family on Structure Activity Relationships 4. Molar Refraction of Cyclic Organophosphorus Compounds

Lorentz JÄNTSCHI and Sorana BOLBOACĂ

```
[15] => 1.885129
[16] => 0.47128225
[17] => 0.30162064
[18] => 0.30162064
[19] => 0.20945877777778
[20] => 0.20945877777778
[21] => 0.15388808163265
[22] => 1.885129
[23] => 7.540516
[24] => 7.540516
[25] => 1.7265475
[26] => 0.83783511111111
[27] => 0.83783511111111
[28] => 0.47128225
[29] => 0.47128225
[30] => 0.30162064
[31] => 0.30162064
[32] => 0.20945877777778
[33] => 0.83783511111111
[34] => 1.885129
[35] => 7.540516
[36] => 6.90619
[37] => 1.885129
[38] => 1.885129
[39] => 0.83783511111111
[40] => 0.83783511111111
[41] => 0.47128225
[42] => 0.47128225
[43] => 0.30162064
[44] => 1.7265475
[45] => 0.76735444444444
[46] => 1.7265475
[47] => 6.90619
[48] => 6.90619
[49] => 6.90619
[50] => 1.7265475
[51] => 1.7265475
[52] => 0.76735444444444
[53] => 0.76735444444444
[54] => 0.431636875
[55] => 7.540516
[56] => 1.885129
[57] => 0.83783511111111
[58] => 1.885129
[59] => 6.90619
[60] => 1.885129
[61] => 0.83783511111111
[62] => 0.83783511111111
[63] => 0.47128225
[64] => 0.47128225
[65] => 0.30162064
[66] => 0.83783511111111
[67] => 0.47128225
[68] => 0.83783511111111
[69] => 1.885129
[70] => 6.90619
[71] => 1.885129
[72] => 7.540516
[73] => 7.540516
```

```
[74] => 1.885129
[75] => 1.885129
[76] => 0.83783511111111
[77] => 0.47128225
[78] => 0.30162064
[79] => 0.47128225
[80] => 0.83783511111111
[81] => 1.7265475
[82] => 0.83783511111111
[83] => 7.540516
[84] => 1.885129
[85] => 7.540516
[86] => 0.83783511111111
[87] => 1.885129
[88] => 0.47128225
[89] => 0.30162064
[90] => 0.47128225
[91] => 0.83783511111111
[92] => 1.7265475
[93] => 0.83783511111111
[94] => 7.540516
[95] => 1.885129
[96] => 0.83783511111111
[97] => 7.540516
[98] => 1.885129
[99] => 0.30162064
[100] => 0.20945877777778
[101] => 0.30162064
[102] => 0.47128225
[103] => 0.76735444444444
[104] => 0.47128225
[105] => 1.885129
[106] => 7.540516
[107] => 0.83783511111111
[108] => 1.885129
[109] => 7.540516
[110] => 0.30162064
[111] => 0.20945877777778
[112] => 0.30162064
[113] => 0.47128225
[114] => 0.76735444444444
[115] => 0.47128225
[116] => 1.885129
[117] => 0.83783511111111
[118] => 7.540516
[119] => 1.885129
[120] => 7.540516
[121] => 0.20945877777778
[122] => 0.15388808163265
[123] => 0.20945877777778
[124] => 0.30162064
[125] => 0.431636875
[126] => 0.30162064
[127] => 0.83783511111111
[128] => 1.885129
[129] => 1.885129
[130] => 7.540516
[131] => 7.540516
)
```

Molecular Descriptors Family on Structure Activity Relationships 4. Molar Refraction of Cyclic Organophosphorus Compounds

Lorentz JÄNTSCHI and Sorana BOLBOACĂ

```
AmrfEt = 2.2007209544439
lAmrfEt = 0.78878501324562
```