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CHARACTERIZATION OF MARINE SEDIMENTS TOXICITY BASED ON STRUCTURAL INFORMATION

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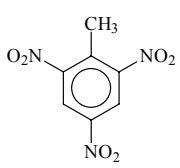
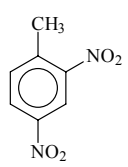
ABSTRACT

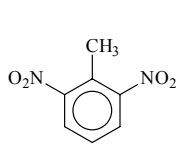
The poster presents the abilities in estimation and prediction of the ordnance compounds toxicity on five marine species through the integration of complex structures information by the use of an original molecular descriptor family on the structure-activity relationships approach.

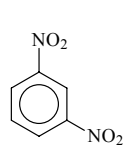
INTRODUCTION

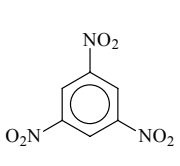
The molecular descriptors family on the structure-activity relationship, an original approach that based on the information obtained exclusively from the compound structures has been introduced [1]. The approach proved its abilities in estimation and prediction of activity of different classes ob biologic active compounds [2].
The marine sediment toxicity of eight ordnance compounds using five marine species had been previous studied [3]. The investigated ordnance compounds and marine species were:

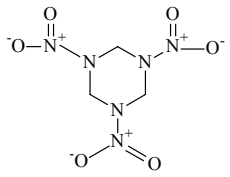

2,4,6-trinitrotoluene
2,4,6 TNT

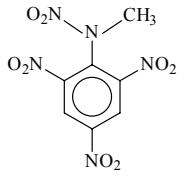

2,4-dinitrotoluene
2,4-DNT

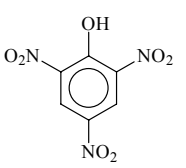

2,6-dinitrotoluene
2,6-DNT


1,3-dinitrobenzene
1,3-DNB

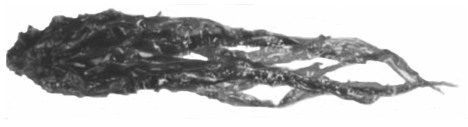

1,3,5-trinitrobenzene
1,3,5-TNB


Royal Demolition Explosive
RDX

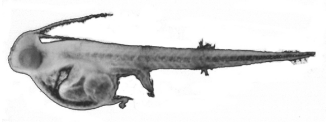

Tetryl
Te


Picric acid
PAc


Sea urchin (ms_01)
-Arbacia punctulata-


Green macroalgea (ms_02)
- Ulva fasciata-


Polychaete (ms_03)
- Dinophilus gyrociliatus-


Redfish (ms_04)
- Sciaenops ocellatus-


Opossum shrimp (ms_05)
- Mysidopsis bahia-

The poster presents the results of the ordnance compounds toxicity on marine species obtained by applying of the molecular descriptors family on the structure-activity relationships.

MATERIAL

The toxicity of ordnance compounds on five marine species express as the lethal concentration to 50% (LC_{50}) and the effective concentration to 50% (EC_{50}) previously reported by Carr & Nipper constituted the material of our investigation (see Table 1).

Table 1. Experimental data

Specie	*End point*	*2,4,6-TNT*	*2,4-DNT*	*2,6-DNT*	*1,3-DNB*	*1,3,5-TNB*	*RDX*	*Te*	*PAc*
Sea urchin	Fertilization (1)	>103	68.0	>84	258	84.0	>75	3	349
	Embryological development (2)	12.0	51.4	6.70	92.0	1.30	>75	0.08	281
	Germination (3)	2.50	2.50	6.70	0.85	0.08	12.0	0.67	415
Green macro-alga	Zoospore germination (4)	0.76	1.70	2.90	0.41	0.05	8.10	0.34	94
	Germling length (5)	1.40	2.10	4.20	0.45	0.06	9.80	0.40	118
	Germling cell number (6)	7.70	210	13.0	15.0	2.10	>49	0.06	265
Polychaete	Survival and reproductive success (7)	1.80	5.70	2.10	3.70	0.60	26.0	0.02	155
Redfish	Larvae survival (8)	8.20	48.0	34.0	46.0	1.40	>68	1.80	127
Opossum shrimp	Juveniles survival (9)	0.98	5.40	5.60	7.10	1.30	>47	1.30	13

MDF-SAR METHOD

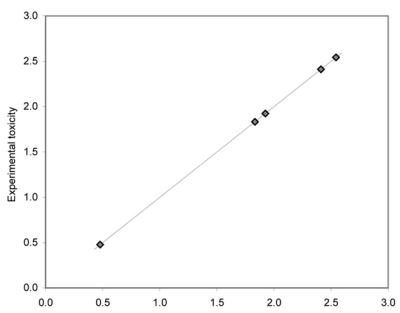
The MDF-SAR approach uses the complex information obtained from ordnance structures in order to generate and calculate the molecular descriptors family for each experiment (from (1) to (9), see Table 1).

The structure-activity relationship models are built using the generated descriptors. The obtained models were validated by computing a series of statistical parameters: the squared correlation coefficient (r^2); the standard error of estimated (s); the Fisher parameter (F); the cross-validation leave-one-out score ($r_{cv\text{-}loo}^2$) [4].

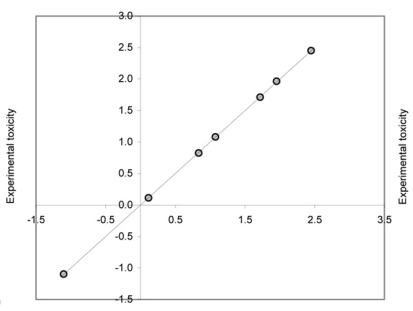
The experimental toxicity expressed with the sign greater than … (see Table 1) were not included into the model.

RESULTS

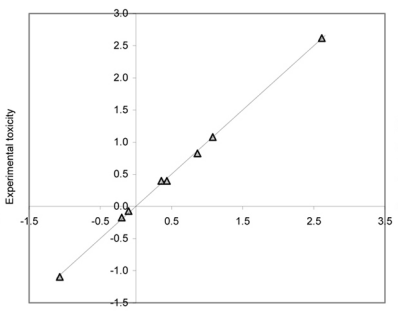
The obtained MDF-SAR models and associated statistical characteristics were:



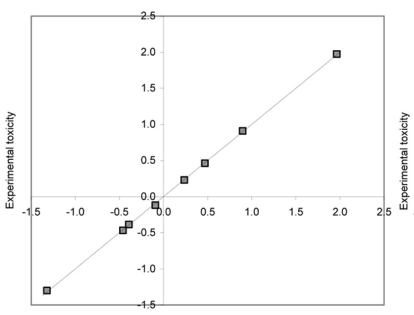
$\hat{Y}_{(1)} = -5.2+7.4\cdot10^{-4}\cdot IAPMLMt+2.7\cdot ImPmlQg$ (1)
n = 5; s = $3.83\cdot10^{-5}$; F = $9.16\cdot10^{8}$†;
r^2 = 0.9999; $r_{cv\text{-}loo}^2$ = 0.9999



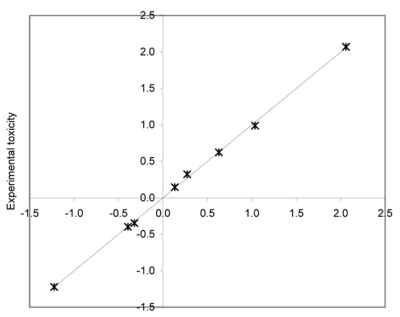
$\hat{Y}_{(2)} = 8.6-6.2\cdot10^{-2}\cdot anPrdQg+234\cdot IsmRLQt$ (2)
n = 7; s = $8.64\cdot10^{-3}$; F = $5.86\cdot10^{4}$†;
r^2 = 0.9999; $r_{cv\text{-}loo}^2$ = 0.9998



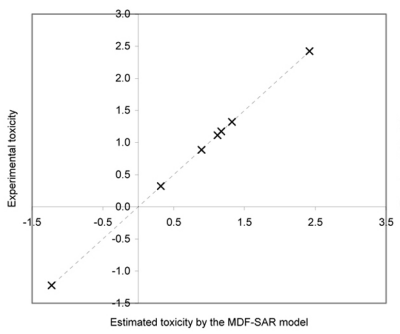
$\hat{Y}_{(3)} = 21.6-4.3\cdot10^{-3}\cdot iHDRkMg+11.1\cdot inMrPQg$ (3)
n = 8; s = $3.75\cdot10^{-2}$; F = $2.95\cdot10^{3}$†;
r^2 = 0.9991; $r_{cv\text{-}loo}^2$ = 0.9976



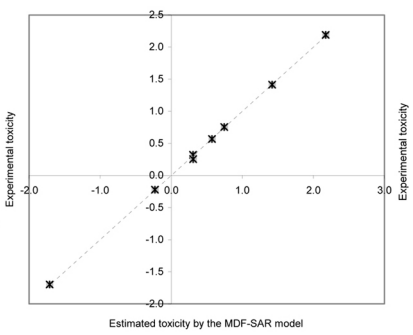
$\hat{Y}_{(4)} = 6.9-10.1\cdot iGDREHg-1.4\cdot lnDDVQg$ (4)
n = 8; s = $1.74\cdot10^{-2}$; F = $1.13\cdot10^{4}$†;
r^2 = 0.9998; $r_{cv\text{-}loo}^2$ = 0.9984



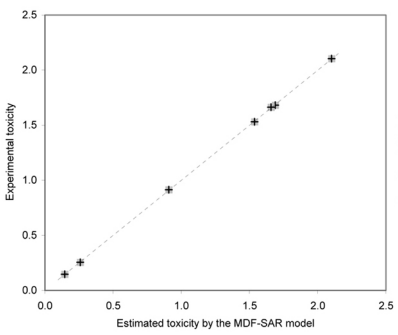
$\hat{Y}_{(5)} = 5.9+383\cdot AHDmtQg-5.2\cdot inMDqQg$ (5)
n = 8; s = $3.33\cdot10^{-2}$; F = $3.13\cdot10^{3}$†;
r^2 = 0.9992; $r_{cv\text{-}loo}^2$ = 0.9984



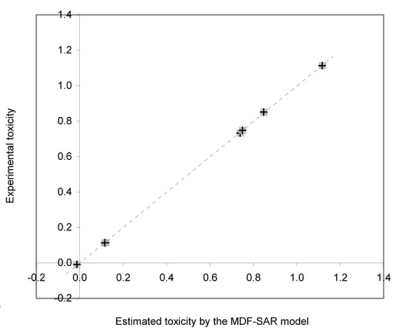
$\hat{Y}_{(6)} = 4.3-55.3\cdot lGPMqGg-1.6\cdot10^{-2}\cdot lBPrJHt$ (6)
n = 7; s = $5.88\cdot10^{-3}$; F = $1.08\cdot10^{5}$†;
r^2 = 0.9999; $r_{cv\text{-}loo}^2$ = 0.9999



$\hat{Y}_{(7)} = 17-14.7\cdot iAMrECt-0.1\cdot aAPmfQt$ (7)
n = 8; s = $2.70\cdot10^{-2}$; F = $6.31\cdot10^{3}$†;
r^2 = 0.9996; $r_{cv\text{-}loo}^2$ = 0.9991



$\hat{Y}_{(8)} = 2.3-1.2\cdot LsDmjQg-6.9\cdot lAMrDHt$ (8)
n = 7; s = $6.13\cdot10^{-3}$; F = $4.59\cdot10^{4}$†;
r^2 = 0.9999; $r_{cv\text{-}loo}^2$ = 0.9999



$\hat{Y}_{(9)} = 49.6-0.3\cdot lAMrDQg+31650\cdot iBPRwMt$ (9)
n = 7; s = $5.24\cdot10^{-3}$; F = $2.13\cdot10^{4}$†;
r^2 = 0.9999; $r_{cv\text{-}loo}^2$ = 0.9997

r^2 = squared correlation coefficient; s = standard error of estimated; F = Fisher parameter; $r_{cv\text{-}loo}^2$ = cross-validation leave-one-out score; n = sample size; † $p < 0.001$

CONCLUSIONS

The goodness-of-fit of the bi-varied MDF-SAR models and the internal validation results sustain that the obtained model are stable and valid. Thus, the MDF-SAR approach is able to provide valid and reliable model for marine sediments toxicity characterization.
The bi-varied MDF-SAR models can be used in order to predict the toxicity of ordnance compounds without any experiments and measurements, using the MDF-SAR Predictor application, available at: http://l.academicdirect.org/Chemistry/SARs/MDF_SARs/sar/.

REFERENCES

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[2] L. Jäntschi, S. Bolboaca. *International Journal of Molecular Sciences* 8 (2007) 189-203.
[3] R.S. Carr, M. Nipper. Final Report [online]. Available at: http://stinet.dtic.mil/cgi-bin/GetTRDoc?AD=ADA383554&Location=U2&doc=GetTRDoc.pdf (cited 2007 February)
[4] ***, Leave-one-out Analysis. ©2007 [cited 2007 March]. Available from: URL: http://l.academicdirect.org/Chemistry/SARs/MDF_SARs/loo/

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