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Supporting Information

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Neural Networks as a Tool to Classify Compounds According to Aromaticity Criteria

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Correlations for all compounds

Correlations

		ASE	Exaltation	NICS	NICS(1)	HOMA
ASE	Pearson Correlation	1	-.841(**)	-.893(**)	-.898(**)	.944(**)
	Sig. (2-tailed)		.000	.000	.000	.000
	N	107	107	107	107	57
Exaltation	Pearson Correlation	-.841(**)	1	.859(**)	.868(**)	-.900(**)
	Sig. (2-tailed)	.000		.000	.000	.000
	N	107	107	107	107	57
NICS	Pearson Correlation	-.893(**)	.859(**)	1	.971(**)	-.897(**)
	Sig. (2-tailed)	.000	.000		.000	.000
	N	107	107	110	110	59
NICS(1)	Pearson Correlation	-.898(**)	.868(**)	.971(**)	1	-.899(**)
	Sig. (2-tailed)	.000	.000	.000		.000
	N	107	107	110	110	59
HOMA	Pearson Correlation	.944(**)	-.900(**)	-.897(**)	-.899(**)	1
	Sig. (2-tailed)	.000	.000	.000	.000	
	N	57	57	59	59	59

** Correlation is significant at the 0.01 level (2-tailed).

Correlations for compounds classified as aromatic by the Kohonen network

Correlations

		ASE	Exaltation	NICS	NICS(1)	HOMA
ASE	Pearson Correlation	1	-.268(*)	-.297(*)	-.401(**)	.686(**)
	Sig. (2-tailed)		.023	.011	.000	.000
	N	72	72	72	72	30
Exaltation	Pearson Correlation	-.268(*)	1	.108	.189	-.495(**)
	Sig. (2-tailed)	.023		.366	.111	.005
	N	72	72	72	72	30
NICS	Pearson Correlation	-.297(*)	.108	1	.754(**)	-.474(**)
	Sig. (2-tailed)	.011	.366		.000	.006
	N	72	72	75	75	32
NICS(1)	Pearson Correlation	-.401(**)	.189	.754(**)	1	-.288
	Sig. (2-tailed)	.000	.111	.000		.110
	N	72	72	75	75	32
HOMA	Pearson Correlation	.686(**)	-.495(**)	-.474(**)	-.288	1
	Sig. (2-tailed)	.000	.005	.006	.110	
	N	30	30	32	32	32

* Correlation is significant at the 0.05 level (2-tailed).

** Correlation is significant at the 0.01 level (2-tailed).

Factor Analysis for all compounds (N = 107)

KMO and Bartlett's Test

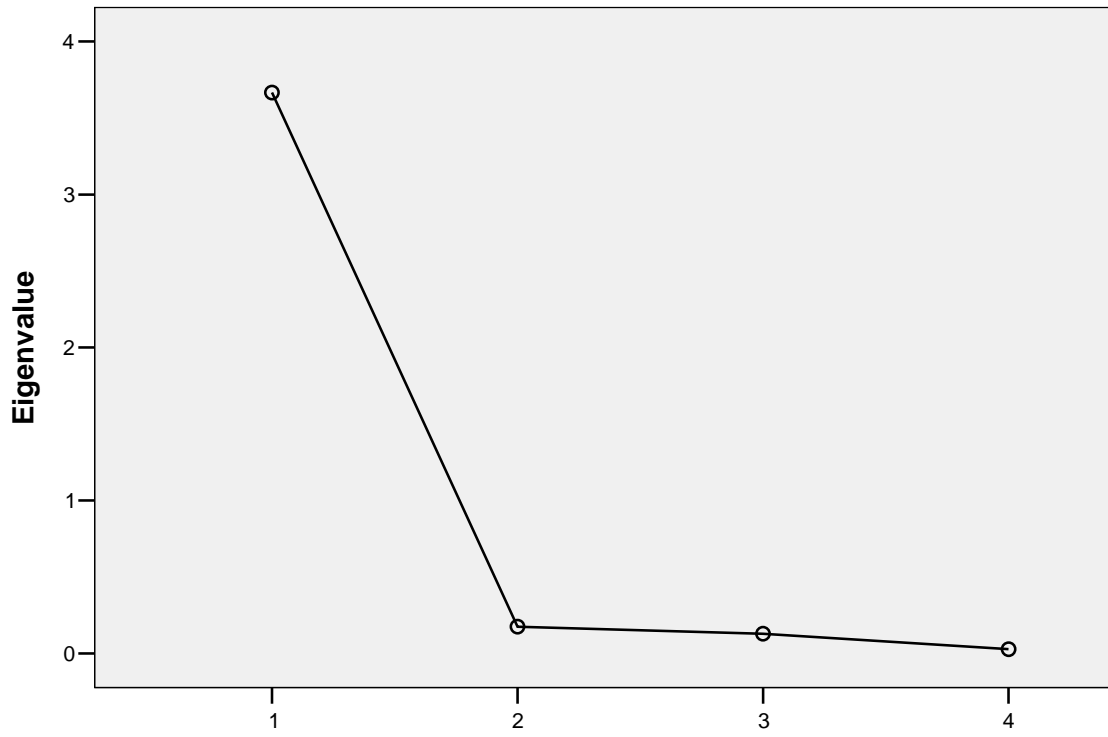
Kaiser-Meyer-Olkin Measure of Sampling Adequacy.		.846
Bartlett's Test of Sphericity	Approx. Chi-Square	627.863
	df	6
	Sig.	.000

Total Variance Explained

Component	Initial Eigenvalues			Extraction Sums of Squared Loadings		
	Total	% of Variance	Cumulative %	Total	% of Variance	Cumulative %
1	3.667	91.665	91.665	3.667	91.665	91.665
2	.176	4.394	96.059			
3	.129	3.231	99.290			
4	.028	.710	100.000			

Extraction Method: Principal Component Analysis.

Scree Plot



Component Matrix^(a)

	Component
	1
ASE	-.948
Exaltation	.931
NICS	.973
NICS(1)	.977

Extraction Method: Principal Component Analysis.

^a 1 components extracted.

**Factor Analysis for compounds classified as aromatic by the Kohonen network
(N = 72)**

KMO and Bartlett's Test

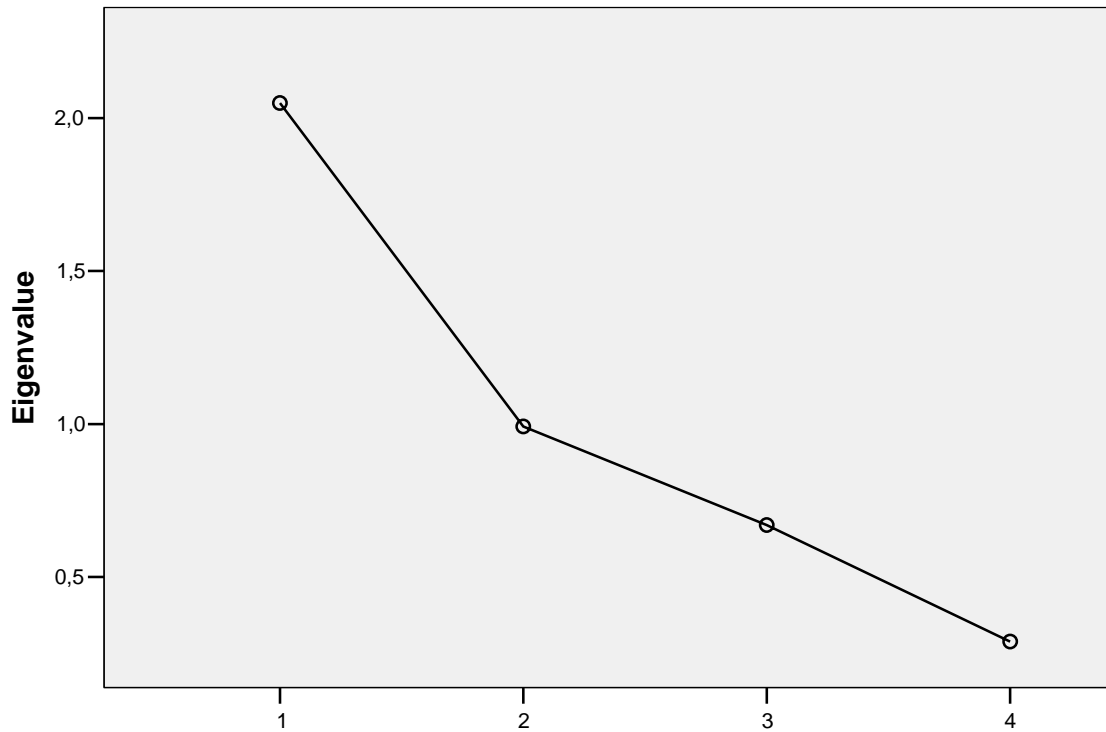
Kaiser-Meyer-Olkin Measure of Sampling Adequacy.		.604
Bartlett's Test of Sphericity	Approx. Chi-Square	64.148
	df	6
	Sig.	.000

Total Variance Explained

Component	Initial Eigenvalues			Extraction Sums of Squared Loadings		
	Total	% of Variance	Cumulative %	Total	% of Variance	Cumulative %
1	2.049	51.227	51.227	2.049	51.227	51.227
2	.992	24.795	76.022			
3	.670	16.746	92.768			
4	.289	7.232	100.000			

Extraction Method: Principal Component Analysis.

Scree Plot



Component Matrix^(a)

	Component
	1
ASE	-.671
Exaltation	.413
NICS	.815
NICS(1)	.874

Extraction Method: Principal Component Analysis.

^a 1 components extracted.

T-Test between NICS-NICS(1) for all compounds

Paired Samples Statistics

		Mean	N	Std. Deviation	Std. Error Mean
Pair 1	NICS	-8.3157	110	7.83410	.74695
	NICS(1)	-8.5331	110	5.57448	.53151

Paired Samples Correlations

		N	Correlation	Sig.
Pair 1	NICS & NICS(1)	110	.971(**)	.000

** Correlation is significant at the 0.01 level (2-tailed).

Paired Samples Test

	Paired Differences					t	df	Sig. (2-tailed)
	Mean	Std. Deviation	Std. Error Mean	95% Confidence Interval of the Difference				
				Lower	Upper			
Pair NICS - NICS(1)	.21736	2.75871	.26303	-.30396	.73869	.826	109	.410

T-Test between NICS-NICS(1) for compounds classified as aromatic by the Kohonen network

Paired Samples Statistics

		Mean	N	Std. Deviation	Std. Error Mean
Pair 1	NICS	-12.8505	75	2.25489	.26037
	NICS(1)	-11.6395	75	1.92493	.22227

Paired Samples Correlations

		N	Correlation	Sig.
Pair 1	NICS & NICS(1)	75	.754(**)	.000

** Correlation is significant at the 0.01 level (2-tailed).

Paired Samples Test

	Paired Differences					t	df	Sig. (2-tailed)
	Mean	Std. Deviation	Std. Error Mean	95% Confidence Interval of the Difference				
				Lower	Upper			
Pair NICS - NICS(1)	-1.21107	1.49862	.17305	-1.55587	-.86627	-6.999	74	.000

The statistical analysis were performed with SPSS 13.0