On the NICS limitations to predict local and global current pathways in polycyclic systems

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Table S1. Comparison of RCS [nA T^{-1}] with different NICSzz (ppm) computations, for the studied molecules. The values at ring centers in ppm calculated at PBE0/Def2-TZVP level of theory. (in parentheses the normalized values)

Molecule	Ring	RCS	NICSzz		NICSπzz (ppm)	
			0.0Å	1.0Å	0.0Å	1.0Å
benzene	-	12.1 (0.9)	-16.1 (1.0)	-30.2 (1.0)	-37.0 (1.0)	-29.9 (1.0)
II	-	13.1 (1.0)	-14.7 (0.9)	-30.1 (1.0)	-36.3 (1.0)	-30.0 (1.0)
III	-	10.6 (0.8)	-8.8 (0.5)	-24.8 (0.8)	-30.5 (0.8)	-24.6 (0.8)
IV	4MR	-12.3 (-0.9)	91.9 (-5.7)	38.9 (-1.3)	42.0 (-1.1)	36.0 (-1.2)
	6MR	5.4 (0.4)	4.0 (-0.2)	-12.0 (0.4)	-16.3 (0.4)	-12.4 (0.4)
V	4MR	-17.1 (-1.3)	105.3 (-6.5)	50.2 (-1.7)	54.6 (-1.5)	47.2 (-1.6)
	6MR	2.7 (0.2)	10.8 (-0.7)	-5.9 (0.2)	-8.9 (0.2)	-6.2 (0.2)
VI	-	-110.0 (-8.4)	96.1 (-6.0)	60.4 (-2.0)	70. 2 (-1.9)	62.4 (-2.1)

Table S2. RCS obtained from different integration planes (see Figure S2).

	Plane	Net (nA/T)	Diatropic	Paratropic	RCS (nA/T)
I	a	12.14	17.1	-5.01	12.14

	Plane	Net (nA/T)	Diatropic	Paratropic	RCS (nA/T)
II	a	20.84	23.90	-3.06	13.12
	b	12.95	25.42	-12.48	
	c	13.43	18.07	-4.64	
	d	13.06	17.91	-4.85	
	e	12.86	17.60	-4.74	
	f	0.00	7.77	-7.77	

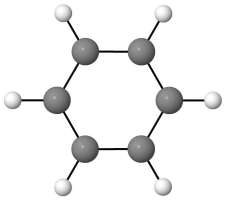
	Plane	Net (nA/T)	Diatropic	Paratropic	RCS (nA/T)
III	a	10.46	15.77	-5.31	10.56
	b	10.93	16.42	-5.49	
	c	10.31	15.93	-5.63	
	d	0	7.42	-7.42	

	Plane	Net (nA/T)	Diatropic	Paratropic	RCS (nA/T)
IV	a	5.5	12.29	-6.78	5.37
	b	5.22	11.86	-6.64	
	c	5.39	11.72	-6.33	
	d	-17.69	3.23	-20.92	
	e	-12.29	3.89	-16.18	-12.29

	Plane	Net (nA/T)	Diatropic	Paratropic	RCS (nA/T)
V	a	2.74	10.73	-8	2.67
	b	2.62	10.05	-7.43	
	c	2.66	10.28	-7.63	
	d	-19.8	2.97	-22.77	
	e	-17.05	3.42	-20.47	-17.15
	f	-17.25	4.24	-21.49	

	Plane	Net (nA/T)	Diatropic	Paratropic	RCS (nA/T)
VI	a	-7.66	7.68	-15.34	-20.50
	b	-20.96	7.08	-28.04	
	c	-20.39	5.08	-25.47	
	d	-20.15	4.46	-24.61	
	e	-20.50	5.58	-26.08	
	f	0.05	13.56	-13.51	
	g	-20.53	5.01	-25.54	

Table S3. Cartesian coordinates of the studied systems.

I		C	-0.693815000	1.201630000	0.000000000
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		C	1.387636000	0.000001000	0.000000000
		C	0.693815000	-1.201630000	0.000000000
		C	-0.693813000	-1.201631000	0.000000000
		C	-1.387636000	-0.000001000	0.000000000
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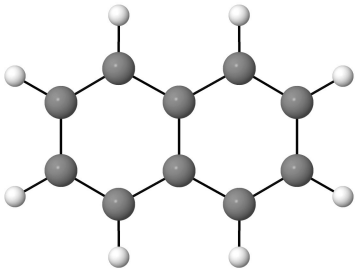
		H	1.235886000	2.140590000	0.000000000
		H	2.471828000	0.000002000	0.000000000
		H	1.235889000	-2.140588000	0.000000000
		H	-1.235886000	-2.140590000	0.000000000
		H	-2.471828000	-0.000002000	0.000000000
II		C	1.236246000	-1.393915000	0.000000000
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		C	1.236246000	1.393915000	0.000000000
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		C	0.000000000	-0.711132000	0.000000000
		C	-1.236246000	-1.393915000	0.000000000
		C	-2.417004000	-0.704289000	0.000000000
		C	-2.417004000	0.704289000	0.000000000
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		H	-1.233071000	2.479011000	0.000000000
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		H	-3.359268000	-1.240207000	0.000000000
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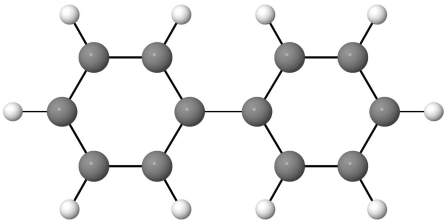
		H	1.233071000	-2.479011000	0.000000000
III		C	-0.742860000	0.000000000	0.000000000
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		H	-0.928141000	2.148377706	0.026262328
		C	-2.859282000	-1.205423772	0.001088911
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		C	0.742860000	0.000000000	0.000000000
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		C	1.465445000	-1.205092205	0.000363444
		H	0.928141000	-2.148361263	0.027574693
		H	0.928141000	2.148361263	-0.027574693
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		C	2.859282000	1.205424213	0.000352558
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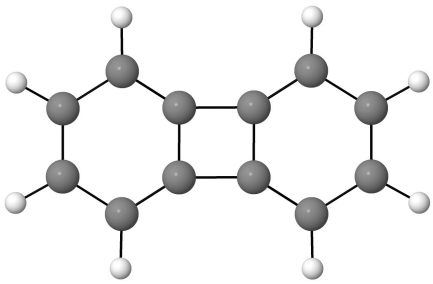
IV		C	1.455478000	1.928377000	0.000389000
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		C	-1.420661000	1.954602000	0.000460000
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		C	0.700571000	-0.718382000	-0.000382000
		C	1.420681000	-1.878371000	-0.000454000
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		C	-0.719208000	-3.056101000	-0.000689000
		C	-1.455456000	-1.852084000	-0.000506000
		C	0.714200000	0.781867000	0.000116000
		C	-0.700577000	0.794615000	0.000141000
		H	1.252848000	4.076218000	0.001013000
		H	-1.178852000	4.098309000	0.001069000
		H	-2.503818000	1.984225000	0.000461000

		H	-2.538975000	-1.861687000	-0.000456000
		H	-1.252796000	-3.999906000	-0.000829000
		H	1.178705000	-4.022109000	-0.000789000
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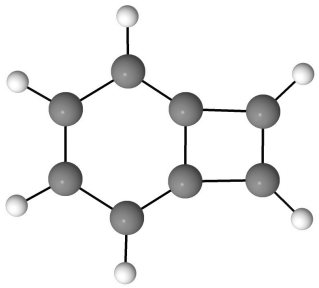
		H	2.538989000	1.938047000	0.000361000
V		C	0.703049000	-0.496861000	0.000031000
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		C	1.443603000	0.636000000	-0.000157000
		H	2.527257000	0.645934000	-0.000141000
		H	1.240278000	2.796073000	-0.000498000
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		H	-2.515021000	0.691847000	0.000152000
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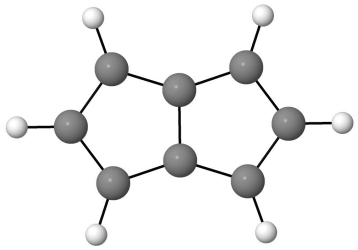
		C	0.654071000	-2.010994000	0.000576000
		H	1.397590000	-2.796208000	0.000881000
		H	-1.448105000	-2.770419000	0.000617000
VI		C	-1.155612084	1.271586088	0.000000000
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		H	2.174759156	1.765672128	0.000000000
		C	0.724603052	0.005802000	0.000000000
		C	1.155612084	-1.271586088	0.000000000
		H	2.178325154	-1.628045116	0.000000000
		C	-1.155612084	-1.406759098	0.000000000
		C	-0.037597003	-2.159481153	0.000000000
		H	-2.174759156	-1.765672128	0.000000000
		H	-0.009308001	3.239653231	0.000000000
		H	0.009308001	-3.239653231	0.000000000
		C	-0.724603052	-0.005802000	0.000000000
		H	-2.178325154	1.628045116	0.000000000

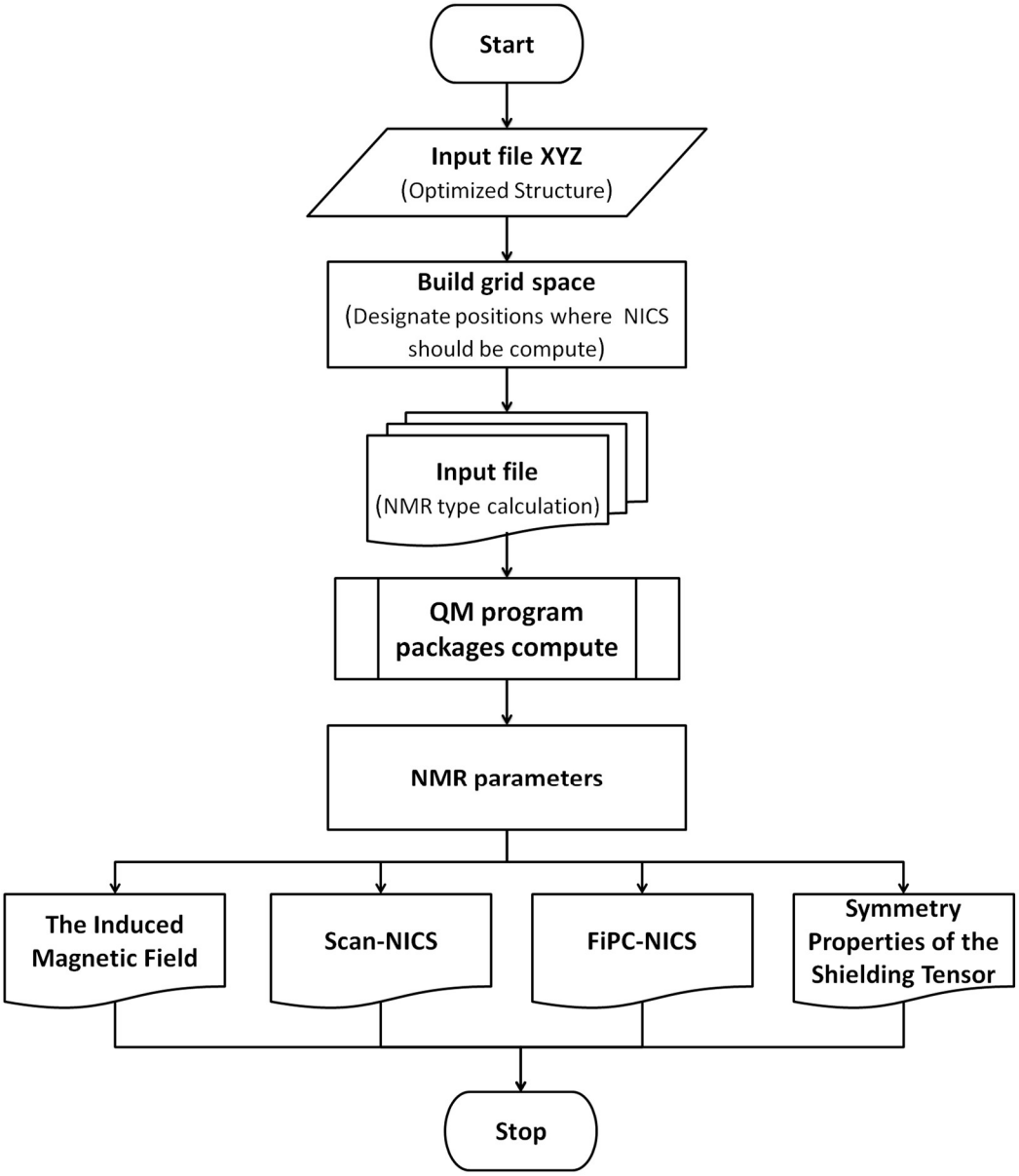

Figure S1. NICSall program flowchart. Manual and source code can be found in https://github.com/HumanOsv/NICSall.

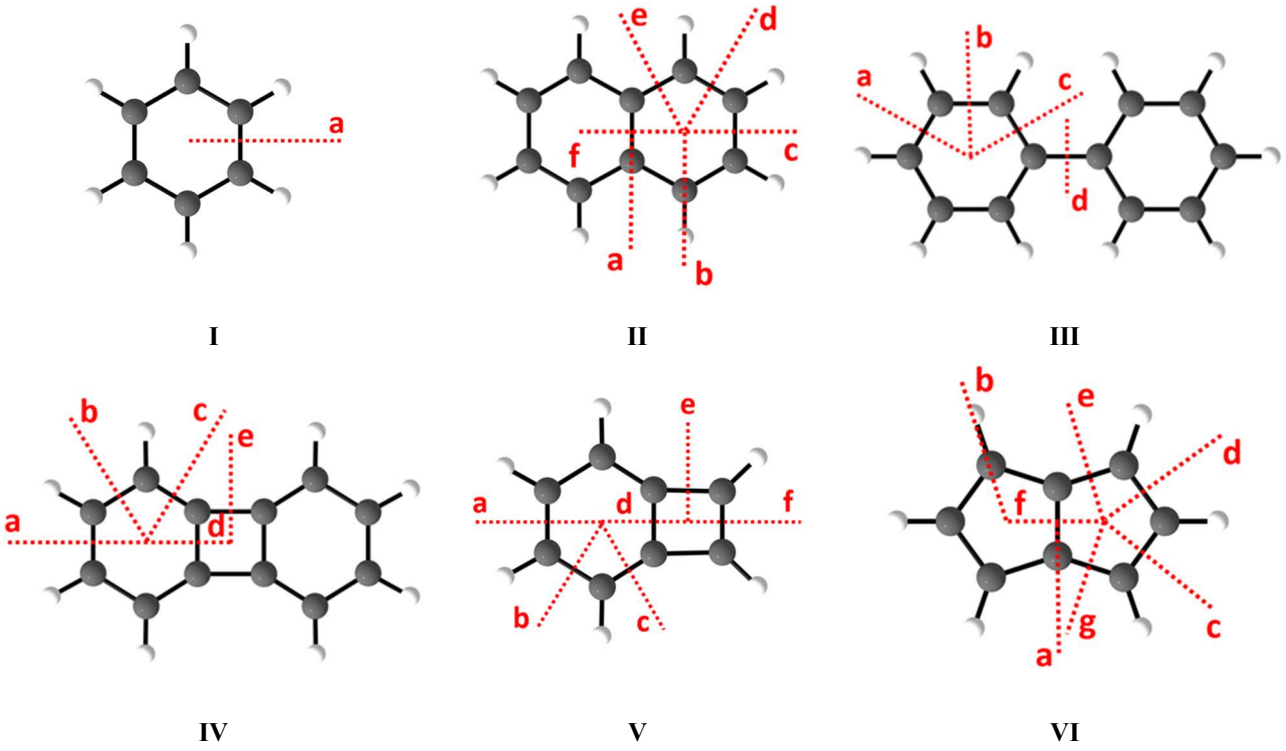

Figure S2. Top view of integration planes considered to average the RCS (in red dotted lines) for **I** Benzene, **II** Naphthalene, **III** planar Biphenyl, **IV** Biphenylene, **V** Benzocyclobutadiene, **VI** Pentalene.

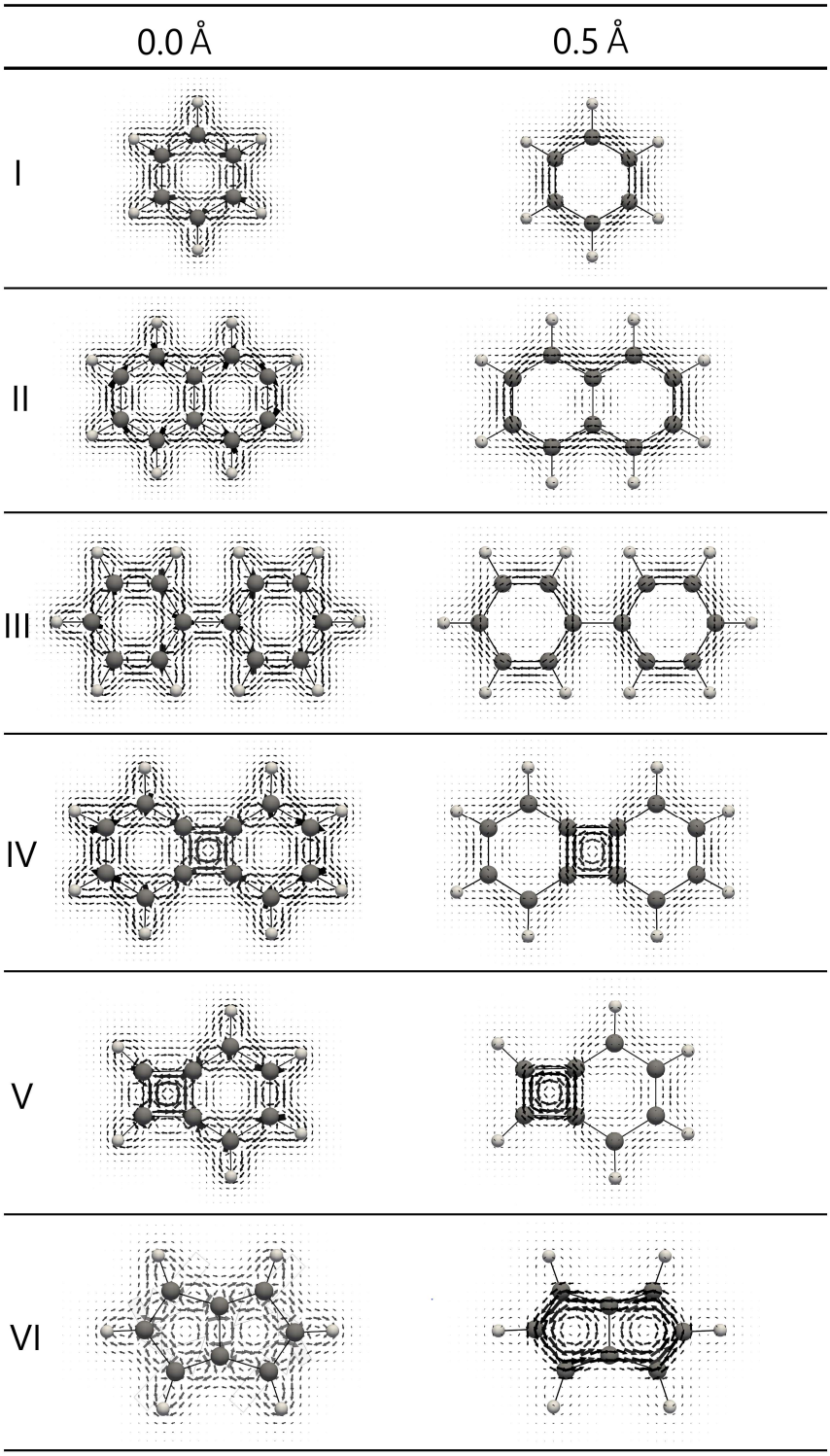

Figure S3. Vector plot visualization of the current density in the plane of the molecule and 0.5Å above for **I** Benzene, **II** Naphthalene, **III** planar Biphenyl, **IV** Biphenylene, **V** Benzocyclobutadiene and **VI** Pentalene. Diatropic currents are assumed to circle clockwise.