

**Table S4.** Intercorrelations between the variables of DF for the group of active compounds.

	J <sub>1</sub>	J <sub>1</sub> <sup>v</sup>	J <sub>3</sub> <sup>v</sup>	<sup>1</sup> D	<sup>4</sup> C <sub>c</sub>
J <sub>1</sub>	1	-0.3959151	0.19469083	0.12647627	0.06154102
J <sub>1</sub> <sup>v</sup>	-0.3959151	1	0.42390454	0.13859051	-0.27254996
J <sub>3</sub> <sup>v</sup>	0.19469083	0.42390454	1	0.36881239	0.09421997
<sup>1</sup> D	0.12647627	0.13859051	0.36881239	1	0.15407574
<sup>4</sup> C <sub>c</sub>	0.06154102	-0.27254996	0.09421997	0.15407574	1