Supplementary material for the paper

Binding of Genistein to the Estrogen Receptor Based on an Experimental Electron Density Study

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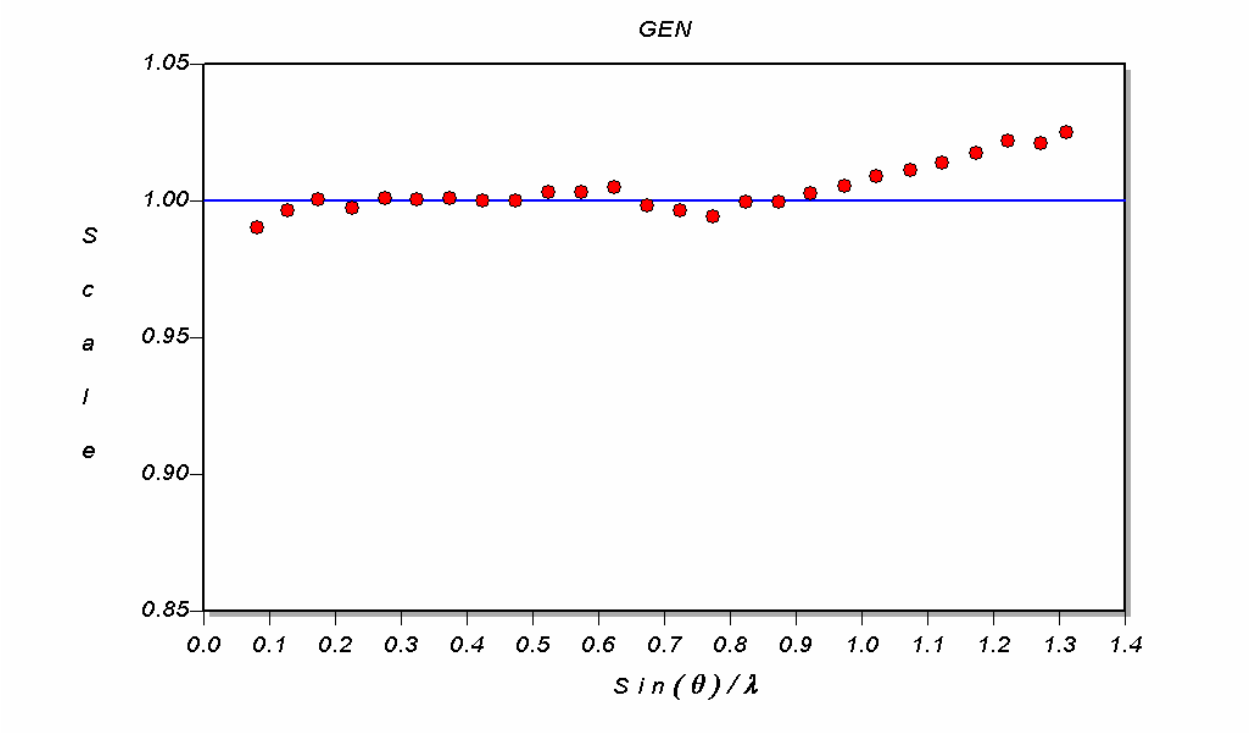
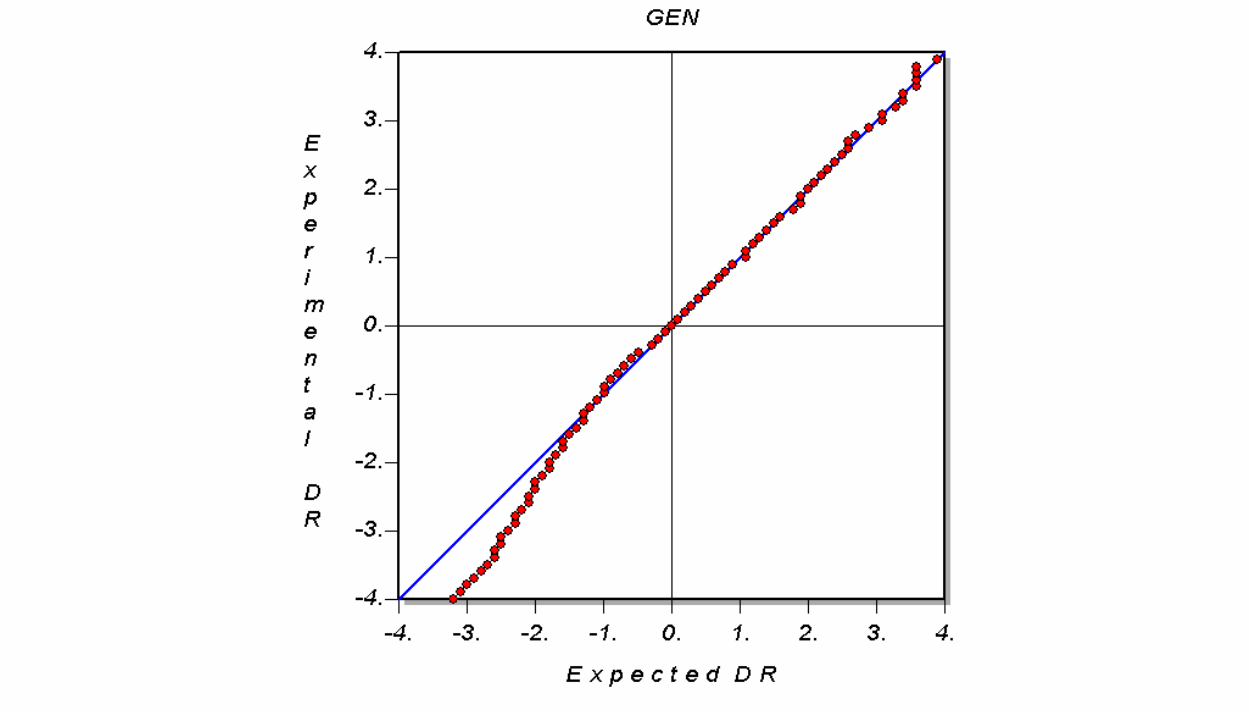
Reference 61:

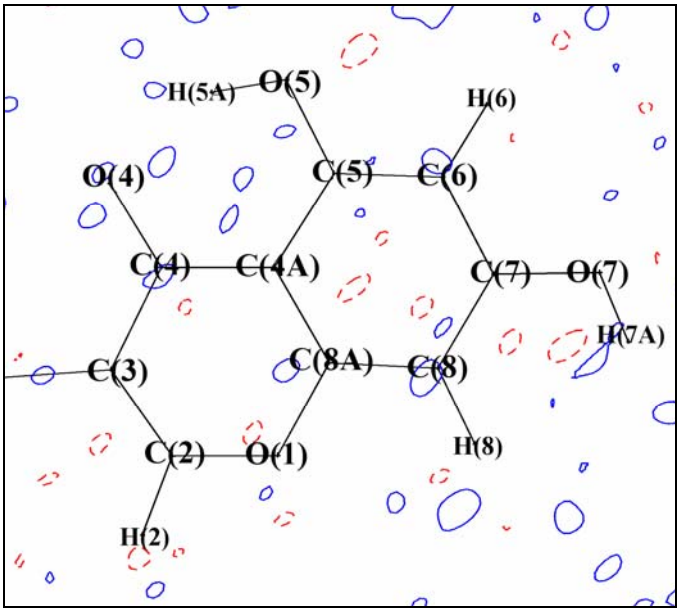
Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Gill, P. M. W.; Johnson, B. G.; Robb, M. A.; Cheeseman, T. K.; Petersson, G. A.; Montgomery, J. A.; Raghavachari, K.; AlLaham, M. A.; Zakrzewski, V. G.; Ortiz, J. V.; Foresman, J. B.; Cioslowski, J.; Nanavakkara, A.; Challacombe, M.; Peng, C. Y.; Ayala, P. Y.; Chen, W., Wong, M. W.; Andres, J. L.; Replogle, E. S.; Gomperts, R.; Martin, R. L.; Fox, D. J.; Binkley, J. S.; Defrees, D. J.; Baker, J.; Stewart, J. P.; Head-Gordon, M.; Gonzalez, C.; Pople, J. A. "Gaussian 98." **2004**, Gaussian, Inc., Pittsburgh, PA.



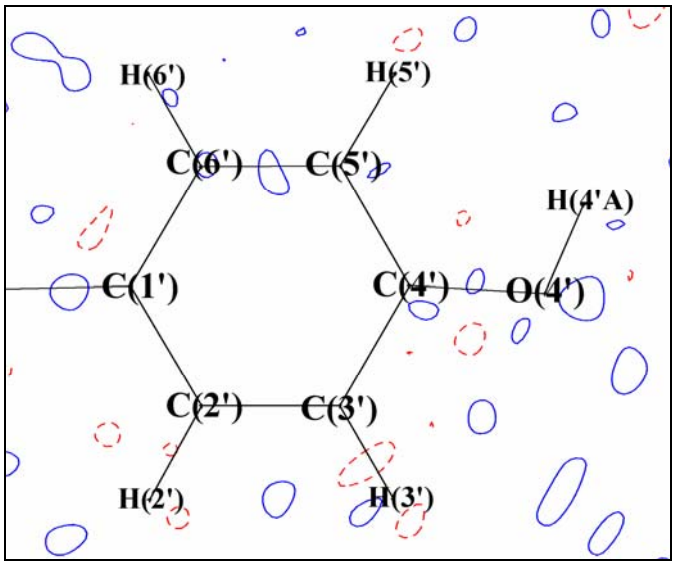
$\Sigma F_{ods}/ F_{calc}$ vs ($\sin\theta/\lambda$)



Normal probability plot for weighted residuals



(a)



(b)

Residual electron density maps of the (a) A and C rings **(**b) and the B ring. Contour intervals are 0.05 eÅ^{-3} with solid, blue lines positive and dotted, red lines negative. The Fourier series have been truncated at 1.0 Å^{-1}. For clarity, the zero-line has been omitted.

Critical Point Properties of All Closed-Shell Interactions

Bond Path	ρ (e Å^{-3})	$\nabla^2\rho$ (e Å^{-5})	λ_1 (e Å^{-5})	λ_2 (e Å^{-5})	λ_3 (e Å^{-5})	R_{ij} (Å)	d_1 (Å)	d_2 (Å)	g, a.u.	*v*, a.u.	h_e, a.u.
O(4)···H(5A)-O(5)	0.288	3.72	-1.840	-1.517	7.073	1.748	1.132	0.621	0.0406	-0.0427	-0.0021
O(4)···H(7A)-O(7)^{i}	0.242	2.41	-1.623	-1.473	5.509	1.801	1.167	0.635	0.0279	-0.0308	-0.0029
O(7)···H(4'A)-O(4')^{ii}	0.181	2.52	-1.132	-0.997	4.652	1.865	1.210	0.658	0.0243	-0.0225	0.0018
O(4)···H(8)-C(8)^{i}	0.049	1.34	-0.139	-0.073	1.552	2.387	1.441	0.960	0.0101	-0.0062	0.0039
O(4')···H(3')-C(3')^{iii}	0.058	1.17	-0.214	-0.194	1.583	2.303	1.414	0.908	0.0091	-0.0061	0.0030
O(4')···H(2)-C(2)^{iv}	0.054	0.96	-0.192	-0.142	1.293	2.437	1.465	0.979	0.0076	-0.0052	0.0024
O(5)···H(2')-C(2')^{v}	0.026	0.45	-0.109	-0.084	0.638	2.622	1.589	1.055	0.0034	-0.0021	0.0013
H(3')···H(3')^{iii}	0.051	0.67	-0.161	-0.132	0.963	2.179	1.089	1.089	0.0055	-0.0040	0.0015
H(6)···H(5')^{ii}	0.033	0.56	-0.112	-0.089	0.761	2.402	1.092	1.325	0.0043	-0.0027	0.0015
C(5)···C(4A)	0.048	0.48	-0.059	-0.045	0.584	3.358	1.669	1.726	00041	-0.0032	0.0010
C(8A)···C(8)	0.050	0.49	-0.089	-0.034	0.609	3.369	1.679	1.700	0.0042	-0.0033	0.0010
O(1)···C(6)	0.042	0.50	-0.064	-0.021	0.584	3.297	1.629	1.717	0.0041	-0.0029	0.0011
O(5)···C(4)	0.039	0.52	-0.065	-0.024	0.610	3.178	1.596	1.597	0.0041	-0.0029	0.0013
O(4')···C(5')	0.041	0.54	-0.096	-0.054	0.689	3.229	1.582	1.652	0.0043	-0.0030	0.0013
O(7)···C(2')	0.027	0.50	-0.061	-0.040	0.599	3.349	1.564	1.808	0.0037	-0.0023	0.0014
O(4)···H(8)-C(8)	0.012	0.17	-0.037	-0.015	0.223	3.252	1.770	1.532	0.0013	-0.0007	0.0005
C(3')···H(6')-C(6')	0.031	0.39	-0.063	-0.026	0.478	3.107	1.814	1.299	0.0030	-0.0021	0.0010

Symmetry operators: i – (1-x, y – ½, -z + ½); ii – (x, -y + ½, z + ½); iii – (-x, -y, -z); iv – (x – ½, -y + ½, -z); v – (x + ½, y, -z + ½)

ρ is the electron density; $\nabla^2\rho$ is the Laplacian where $\nabla^2\rho = \lambda_1 + \lambda_2 + \lambda_3$; λ_1, λ_2, and λ_3 are the principle curvatures; d_1 and d_2 are the distances from the bond critical point to atoms 1 and 2, respectively; R is the C···C, C···O, O···H, or C···H distance; g, *v*, h_e are the kinetic, potential, and total electronic energy densities.