SUPPORTING MATERIAL

for

Hydrogen-bonding in phenolic nitronylnitroxides: 2-(3',5'-Dimethoxy-4'-hydroxyphenyl)-4,4,5,5-tetramethyl-4,5-dihydro-*1H*-imidazole-1-oxyl

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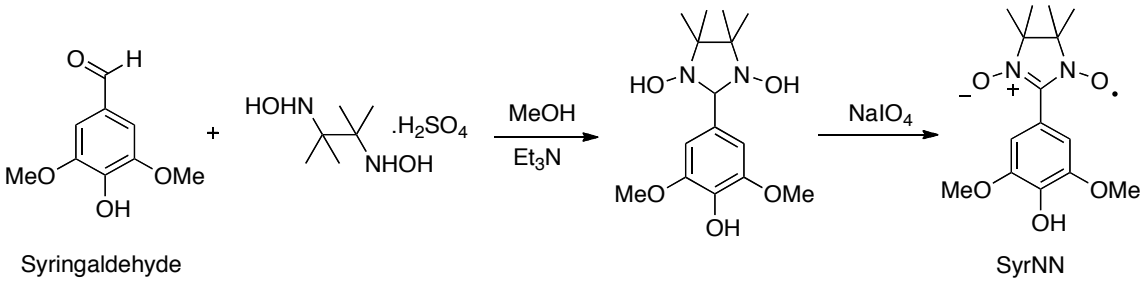
Synthesis. 2,3-Bis(hydroxylamino)-2,3-dimethylbutane hydrogensulfate (4.06 g, 8.23 mmol) was dissolved in 40 mL of methanol and triethylamine (2.22 mL, 8.2 3mmol) was added. This mixture was stirred for 10 min, then 2 g (5.4 8mmol) of syringaldehyde was added. The reaction mixture was stirred under reflux for 48 h. The solvent was removed and multiple extractions were done with ethyl acetate/water. The layers were separated, and the combined organic layers dried over $MgSO_4$, filtered, and evaporated under reduced pressure to yield crude 2-(4-hydroxy-3,5-dimethoxy-phenyl)-4,4,5,5-tetramethylimidazolidine-1,3-diol which was then dissolved in minimum amount of dichloromethane. To this solution was added 0.25 M aqueous solution of sodium periodate as a deep blue color formed at room temperature under argon. The dichloromethane layer was separated and the aqueous layer was extracted with 2 × 20 mL of dichloromethane. The combined organic layers were dried over $MgSO_4$, filtered, and evaporated to dryness. The crude product was purified by chromatography (silica gel with ethyl acetate:hexanes, 1:1) to afford **SyrNN (**0.25 g, 15%) which was crystallized by evaporation at room temperature from ethyl acetate in the hood air flow, to give blue-black, prism shaped crystals of product. Sometimes, red crystallites form during crystallization -- these show additional peaks in the EPR spectrum that are not due to SyrNN, but these crystallites typically can be manually separated from the distinguishable dark blue-black **SyrNN** crystals.

SyrNN. Melting point: 137-141 °C[d]. IR(KBr, cm^{-1}): 3285 [br, OH]; 2990, 2942, 2928, 2890 [all sh, wk, C-H]; 2841 [sh, wk, MeO]; 1387 [m, N–O]; 1241 [s]; 1102 [s, C-O]; 654, 544, 449 [all s]. EPR (toluene, 9.6083 GHz): 7.56 G (2N), 0.27 (at least 12H); g = 2.0677. MS (EI+): calculated for $C_{15}H_{21}N_2O_5$ m/z = 309.34, found = 309.1.



Syringaldehyde SyrNN

Figure S1. FTIR spectrum of SyrNN (ATR, neat solid sample, room temperature).

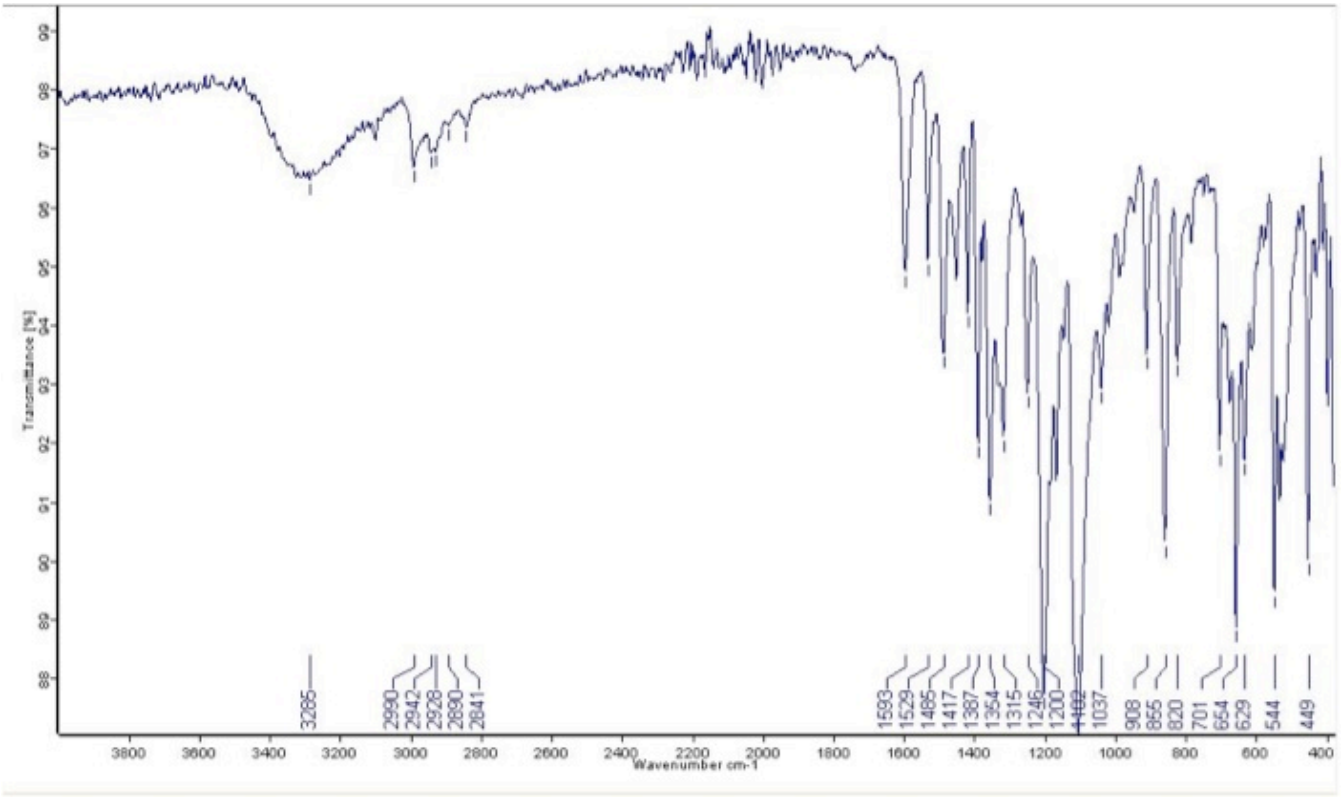


Figure S2. ORTEP diagram of SyrNN. Thermal ellipsoids shown at 50% probability.

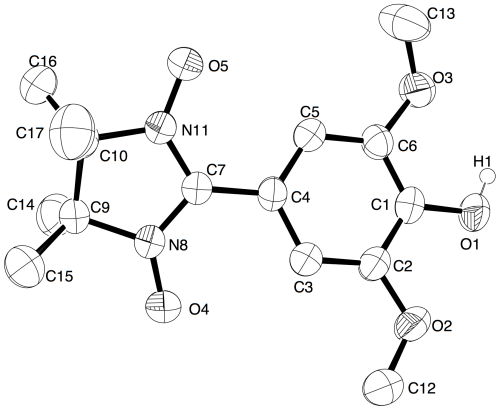
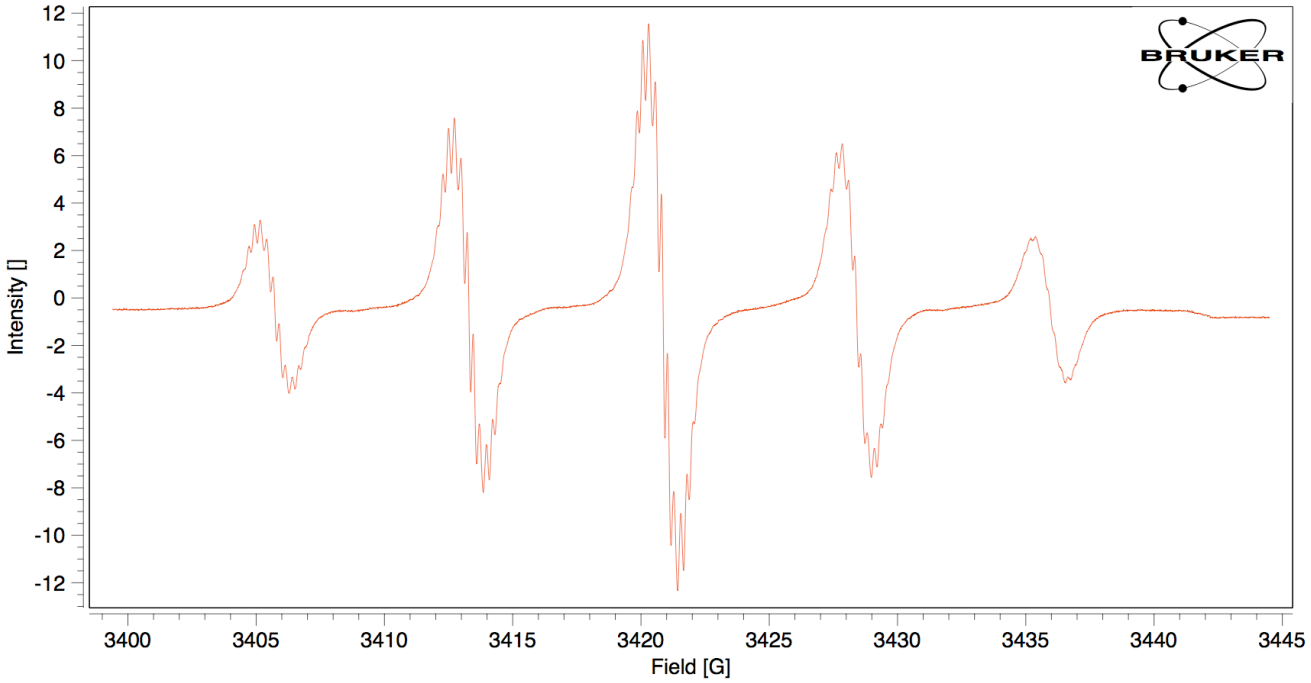
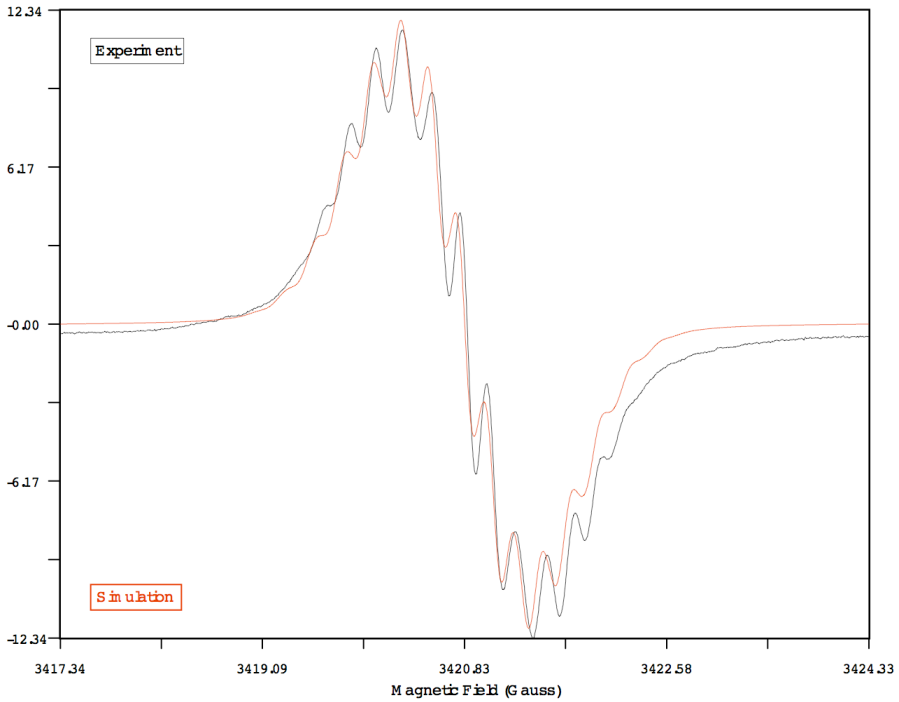


Figure S3. EPR spectrum for SyrNN in toluene at room temperature (9.6083 GHz, above), with expanded view of only the central experimental peak plus simulation using two equivalent I=1 atoms with twelve equivalent I = 0.5 atoms (below) and a single isotropic line broadening parameter.





Simulation using Winsim 2002 from the PEST program at NIEHS: Duling, D. R. *J. Magn. Reson.* **1994**, *B104*, 105.

Figure S4. Normalized molar magnetization versus field M/M_s versus H at 1.8 K (above) with corresponding second derivative plot (below). The Brillouin curve for isolated spin $S = 1/2$ is shown as a dashed line.

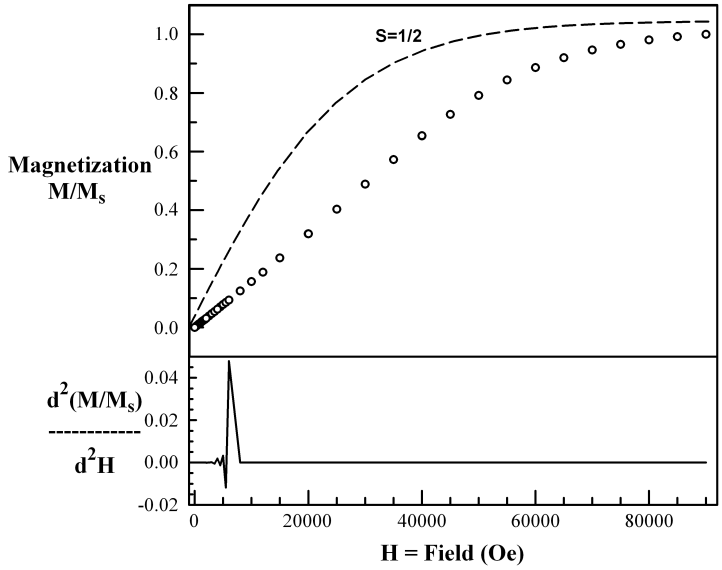


Figure S5. Normalized molar magnetization versus field M/M_s versus H at 0.55 K, with logarithmic ordinate. A Brillouin curve for isolated spin $S = 1/2$ is shown as a dashed line.

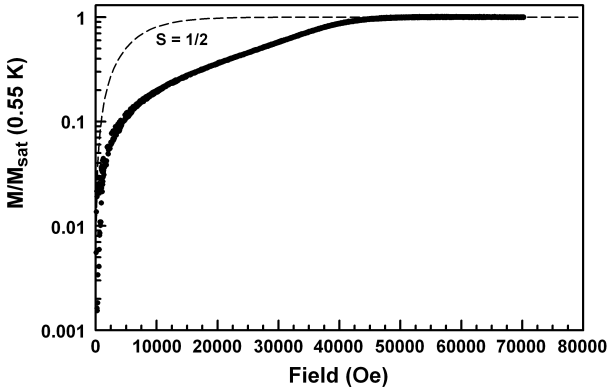
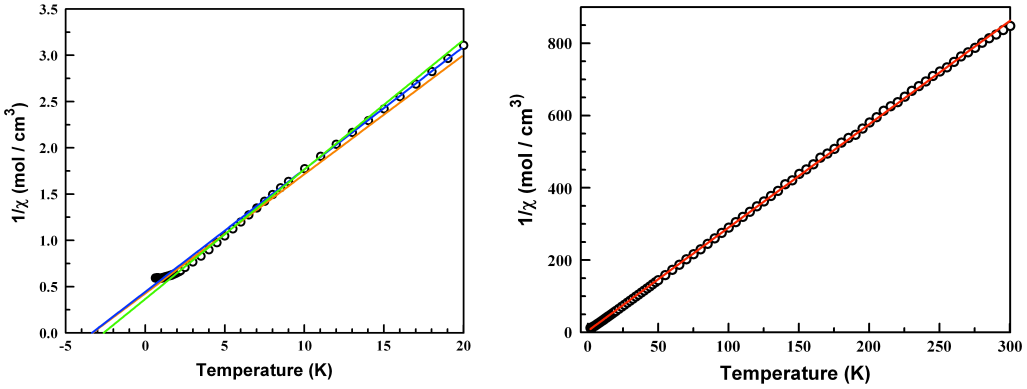


Figure S6. Curie plots from dc magnetic susceptibility versus temperature experiments (1000 Oe external field): left chart combines data from all experiments, showing $T < 20$ K data, right chart for data obtained in a 1.8-300 K temperature range experiment.



Green line = linear fit to all data 2 K < T < 10 K, Weiss constant θ = (–)2.6 K from x-intercept.

Blue line = linear fit to all data T < 10 K, Weiss constant θ = (–)3.5 K from x-intercept.

Orange line left chart = linear fit to all data T < 20 K, Weiss constant θ = (–)3.3 K from x-intercept.

Red line right chart = linear fit to all data, Weiss constant θ = (–)1.4 K from x-intercept (only 1.8-300 K data fitted).

Figure S7. Fits to dc magnetic susceptibility data (1000 Oe external field) over full temperature ranges; see fitted parameters on next page.

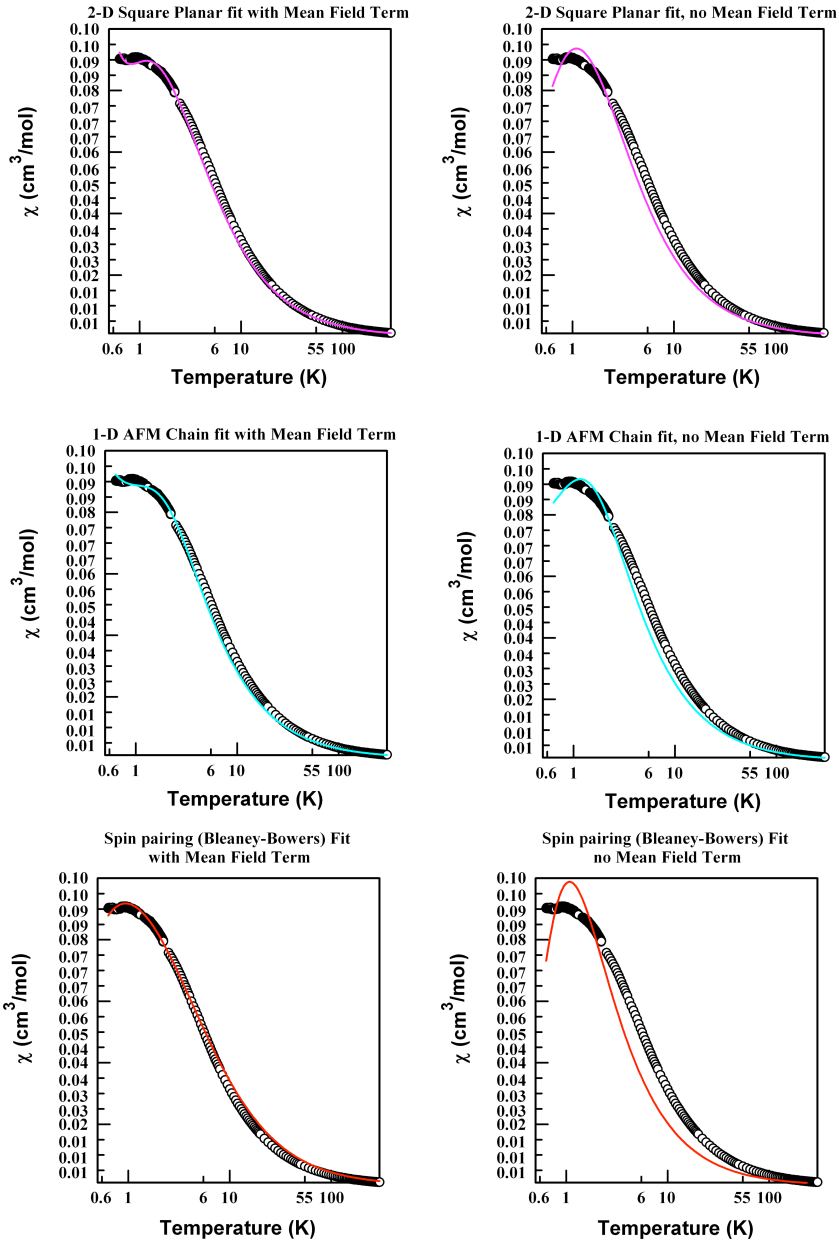


Table S1. Results of fitting SyrNN magnetic susceptibility versus temperature results for all data (full temperature range) to various models using PSI-Plot version 9.5 for Windows (Poly Software International, Pearl River NY 10965 USA). *Upper numbers* for fits with $T > 1$ K, lower numbers for fits with all data. The numbers in this table reflect the exchange hamiltonian ($H = -J\ S_1 \cdot S_2$). The uncertainties are 95% confidence intervals.

Model	**J/k**	θ_{MF}	**1000×Chisq goodness of fit**
Spin Pairing, no mean field	*–2.20±0.02 K*	fixed to 0 K	*6.8 (T > 1 K)*
	–1.74±0.02 K	fixed to 0 K	33.1
Spin Pairing	*–0.90±0.02 K*	*–2.39±0.04 K*	*0.20 (T > 1 K)*
	–0.57±0.01 K	–3.18±0.07 K	0.88
1-D AFM chain, no mean field*	*–1.02±0.005 K*	fixed to 0 K	*1.80 (T > 1 K)*
	–0.90±0.004 K	fixed to 0 K	5.34
1-D AFM chain*	*–1.46±0.005 K*	*+0.31±0.002 K*	*0.22 (T > 1 K)*
	–1.23±0.006 K	+0.18±0.013 K	1.06
2-D Square Planar, no mean field	*–1.38±0.005 K*	fixed to 0 K	*1.2 (T > 1 K)*
	–1.17±0.006 K	fixed to 0 K	7.5
2-D Square Planar	*–2.19±0.00[4]* K	*+0.45±0.00[1]* K	*0.05 (T > 1 K)*
	–1.79±0.006 K	+0.30±0.00[1	0.92

Spin pairing model Bleaney, B.; Bowers, K. D. *Proc. R. Soc. London A*, **1952**, *214*, 451-465.

$$\chi = \frac{2Ng^2\beta^2}{3k(T-\theta)} \times \frac{1}{3+\exp\left(-J/kT\right)}$$

$$H = -J_{ST} \cdot S_1 S_2$$

1-D model (a) Bonner, J. C.; Fisher, M. E. *Phys. Rev.*, **1964**, *135*, A640-A658. (b) J. C. Bonner, Ph. D. Dissertation, University of London, UK, 1968.)

$$\chi = \frac{Ng^2\beta^2}{k(T-\theta)} \cdot \frac{A + B\cdot\left(J/kT\right) + C\cdot\left(J/kT\right)^2}{1 + D\cdot\left(J/kT\right) + E\cdot\left(J/kT\right)^2 F\cdot\left(J/kT\right)^3}$$

$$H = -2J\sum_{N=1}^{\infty} S_1 S_{1+N}$$

A = 0.25, B = 0.14995, C = 0.30094, D = 1.9862, E = 0.68854 and F = 6.0626

***The values of *J/k* obtained from this fitting model *were doubled in Table 4 of the main article* to reflect the hamiltonian used elsewhere in the main article.**

2D model Square-planar antiferromagnetic sheet, all S = 1/2 units
Landee, C. P. private communication (2011).

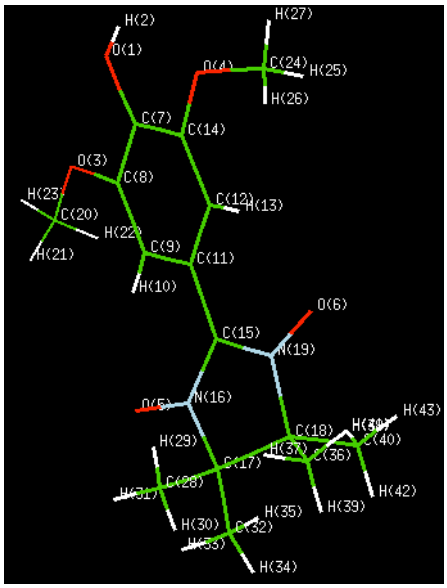
χ Layer

$N_1 = 0.998586$ $D_1 = -1.84279$
$N_2 = -1.28534$ $D_2 = 1.14141$
$N_3 = 0.656313$ $D_3 = -0.704192$
$N_4 = 0.235862$ $D_4 = -0.189044$
$N_5 = 0.277527$ $D_5 = -0.277545$

$$\chi_{layer}(T) = \left(\frac{C}{T}\right) * \left[\frac{\sum_{i=1}^{5} N_i * \left(\frac{-J}{T}\right)^i}{1 + \sum_{i=1}^{5} D_i * \left(\frac{-J}{T}\right)^i} + 1\right] + \frac{P * C}{T} \qquad (1)$$

$$H = -J\sum_{i,j}^{i\neq j} S_i S_j$$

Computational Spin Density Archive Summary




```
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  P DIRECT GFINPUT IOP(6/7=3) UB3LYP/EPR-III\\Syringyl NN xtl geom\\0,2
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 429,6.267\C,0,3.096,7.464,4.513\C,0,3.425,8.691,3.929\H,0,3.223,8.856,
 3.037\C,0,4.052,9.65,4.689\C,0,2.484,6.411,3.705\N,0,2.433,5.094,4.004
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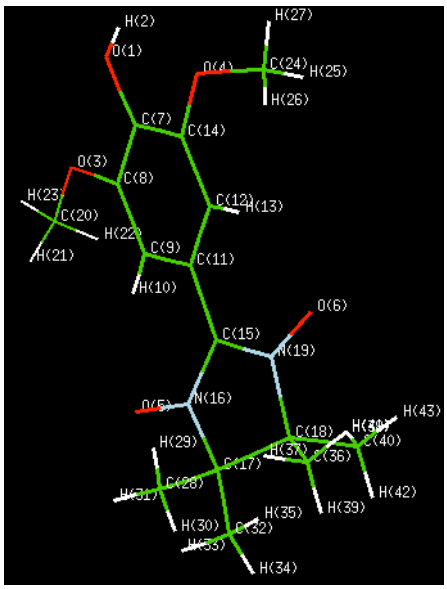
```


Isotropic Fermi Contact Couplings

	Atom	a.u.	MegaHertz	Gauss	10(-4) cm-1
1	O(17)	-0.00151	0.91772	0.32747	0.30612
2	H(1)	0.00011	0.51230	0.18280	0.17089
3	O(17)	0.00062	-0.37390	-0.13342	-0.12472
4	O(17)	0.00054	-0.33017	-0.11781	-0.11013
5	O(17)	0.04717	-28.59327	-10.20279	-9.53769
6	O(17)	0.04572	-27.71693	-9.89009	-9.24537
7	C(13)	-0.00300	-3.37518	-1.20435	-1.12584
8	C(13)	0.00277	3.11387	1.11111	1.03868
9	C(13)	-0.00337	-3.78735	-1.35142	-1.26332
10	H(1)	0.00051	2.26146	0.80695	0.75434
11	C(13)	0.00744	8.36599	2.98519	2.79059
12	C(13)	-0.00375	-4.21022	-1.50231	-1.40438
13	H(1)	0.00055	2.43848	0.87011	0.81339
14	C(13)	0.00281	3.15661	1.12636	1.05293
15	C(13)	-0.03319	-37.31469	-13.31481	-12.44684
16	N(14)	0.04904	15.84560	5.65410	5.28552
17	C(13)	-0.00584	-6.56916	-2.34404	-2.19124
18	C(13)	-0.00613	-6.88877	-2.45808	-2.29785
19	N(14)	0.04784	15.45755	5.51564	5.15608
20	C(13)	-0.00001	-0.01288	-0.00460	-0.00430
21	H(1)	0.00002	0.09710	0.03465	0.03239
22	H(1)	0.00001	0.06011	0.02145	0.02005
23	H(1)	0.00000	-0.01668	-0.00595	-0.00556
24	C(13)	0.00018	0.19881	0.07094	0.06632
25	H(1)	-0.00002	-0.09534	-0.03402	-0.03180
26	H(1)	0.00004	0.16917	0.06036	0.05643
27	H(1)	0.00000	-0.01718	-0.00613	-0.00573
28	C(13)	0.00839	9.42704	3.36380	3.14452
29	H(1)	-0.00025	-1.13860	-0.40628	-0.37980
30	H(1)	0.00020	0.88409	0.31546	0.29490
31	H(1)	-0.00043	-1.90004	-0.67798	-0.63379
32	C(13)	0.00306	3.44148	1.22801	1.14795
33	H(1)	-0.00018	-0.79510	-0.28371	-0.26522
34	H(1)	-0.00018	-0.81626	-0.29126	-0.27228
35	H(1)	-0.00017	-0.75562	-0.26963	-0.25205
36	C(13)	0.00277	3.11060	1.10994	1.03758
37	H(1)	-0.00013	-0.59080	-0.21081	-0.19707
38	H(1)	-0.00021	-0.94238	-0.33626	-0.31434
39	H(1)	-0.00019	-0.86154	-0.30742	-0.28738
40	C(13)	0.00793	8.91086	3.17962	2.97234
41	H(1)	-0.00023	-1.00672	-0.35922	-0.33581
42	H(1)	0.00020	0.87878	0.31357	0.29313
43	H(1)	-0.00042	-1.86509	-0.66551	-0.62213

Computed spin densities using EPR-III method in Gaussian 09*

Mulliken atomic spin densities:												
1	O	-0.007349	12	C	-0.030077	24	C	0.000637	35	H	-0.000384
2	H	0.000049	13	H	-0.001462	25	H	0.000173	36	C	-0.009466
3	O	0.001651	14	C	0.014879	26	H	0.000022	37	H	-0.000496
4	O	0.001061	15	C	-0.159467	27	H	0.000021	38	H	-0.000977
5	O	0.374196	16	N	0.216621	28	C	0.006675	39	H	-0.000904
6	O	0.357396	17	C	0.035315	29	H	-0.000639	40	C	0.003270
7	C	-0.032644	18	C	0.034677	30	H	-0.000012	41	H	-0.000599
8	C	0.014827	19	N	0.206363	31	H	-0.000532	42	H	0.000089
9	C	-0.027079	20	C	0.000326	32	C	-0.008324	43	H	-0.000187
10	H	-0.002303	21	H	0.000097	33	H	-0.000912	Sum of Mulliken atomic spin densities = 1.00000		
11	C	0.016152	22	H	0.000250	34	H	-0.000951			
			23	H	0.000019						



* *Full citation for Gaussian 09*: Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.,; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Keith, T.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J.; Gaussian 09 Revision B.01 ed.; Gaussian, Inc: Wallingford CT, 2010.

Archival summaries for dyad singlet triplet splittings.

OH to ON Contact A

Singlet broken-symmetry, UB3LYP/6-31G*


```
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 \\0,1\O,0,4.577962,0.13952,4.247308\O,0,3.937962,-2.11348,5.400308\O,0
 ,3.938962,0.69352,1.708308\O,0,2.413962,-5.66948,2.544308\O,0,1.294962
 ,-2.54048,-0.686692\C,0,3.925962,-0.78448,3.493308\C,0,3.577962,-1.999
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 98692\O,0,-3.148038,2.54152,-4.829692\C,0,-0.517038,0.78552,-0.649692\
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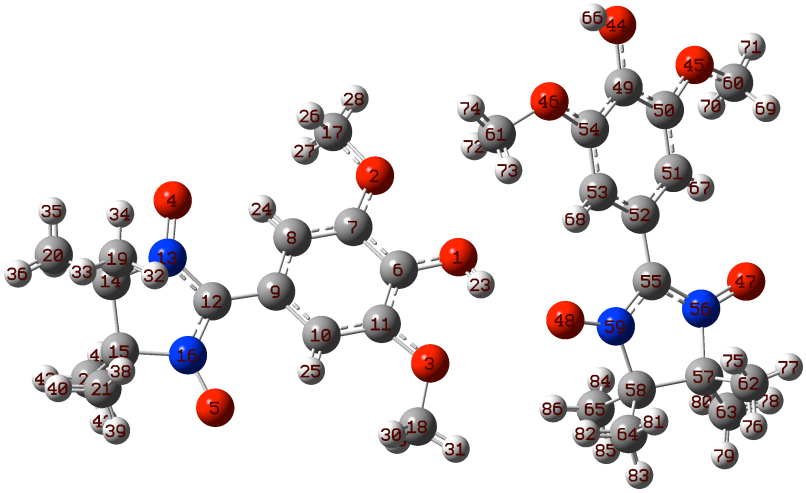
 8,0.55452,-1.971692\C,0,-2.436038,3.79352,-2.955692\N,0,-2.486038,5.11
 052,-2.656692\C,0,-2.957038,5.94052,-3.810692\C,0,-3.676038,4.87752,-4
 .662692\N,0,-3.019038,3.63152,-4.161692\H,0,0.322962,-0.78748,-0.36069
 2\H,0,-0.785457,3.001485,1.601839\H,0,-0.785324,-0.787541,-3.381399\H,
 0,-1.755038,3.77652,-0.393692\H,0,-1.697038,1.34852,-3.623692\H,0,-2.0
 70908,6.335568,-4.374235\H,0,-3.70229,6.69699,-3.448445\H,0,-3.418657,
 5.027686,-5.744392\H,0,-4.765962,4.85904,-4.396994\\Version=EM64L-G09R
 evB.01\State=1-A\HF=-1667.5189246\S2=1.117295\S2-1=0.\S2A=0.923979\RMS
 D=5.245e-09\Dipole=-0.9955263,-0.2965183,-2.1533574\Quadrupole=-9.3152
 036,18.7851759,-9.4699723,-6.0015325,-4.5960398,-5.9310601\PG=C01 [X(C
 18H18N4O10)]\\@
```


Triplet, UB3LYP/6-31G*

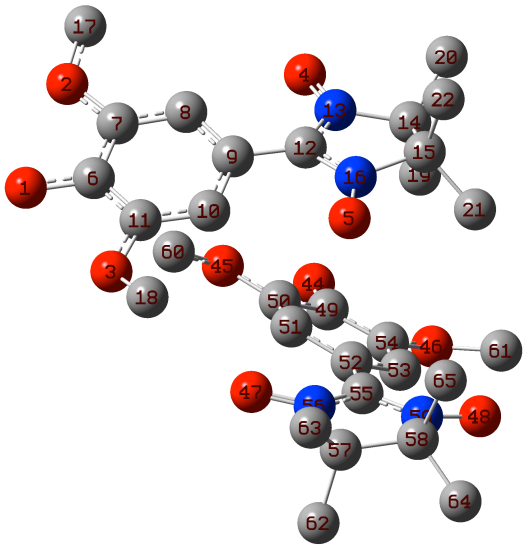

```
1\1\GINC-SKYNET\SP\UB3LYP\6-31G(d)\C18H18N4O10(3)\LAHTI\10-May-2012\0\
 \#p UB3LYP/6-31G* test\\SyrNN HO to ON contact, xtl geom\\0,3\O,0,4.57
 7962,0.13952,4.247308\O,0,3.937962,-2.11348,5.400308\O,0,3.938962,0.69
 352,1.708308\O,0,2.413962,-5.66948,2.544308\O,0,1.294962,-2.54048,-0.6
 86692\C,0,3.925962,-0.78448,3.493308\C,0,3.577962,-1.99948,4.078308\C,
 0,2.924962,-2.96948,3.348308\C,0,2.619962,-2.73948,1.995308\C,0,2.9489
 62,-1.51248,1.411308\C,0,3.575962,-0.55348,2.171308\C,0,2.007962,-3.79
 248,1.187308\N,0,1.956962,-5.10948,1.486308\C,0,1.486962,-5.93948,0.33
 1308\C,0,0.766962,-4.87648,-0.519692\N,0,1.424962,-3.63048,-0.018692\H
 ,0,4.765962,0.78852,3.782308\H,0,3.658059,-3.000781,5.744392\H,0,3.659
 327,0.789479,0.761398\H,0,2.687962,-3.77448,3.749308\H,0,2.746962,-1.3
 4748,0.519308\H,0,0.742446,-6.69699,0.692895\H,0,2.373636,-6.332959,-0
 .232477\H,0,-0.322627,-4.857984,-0.252627\H,0,1.023327,-5.026333,-1.60
 1677\O,0,0.134962,-0.13848,0.104308\O,0,-0.505038,2.11452,1.257308\O,0
 ,-0.505038,-0.69148,-2.434692\O,0,-2.029038,5.67052,-1.598692\O,0,-3.1
 48038,2.54152,-4.829692\C,0,-0.517038,0.78552,-0.649692\C,0,-0.866038,
 2.00052,-0.064692\C,0,-1.518038,2.97152,-0.794692\C,0,-1.823038,2.7415
 2,-2.147692\C,0,-1.494038,1.51452,-2.731692\C,0,-0.868038,0.55452,-1.9
 71692\C,0,-2.436038,3.79352,-2.955692\N,0,-2.486038,5.11052,-2.656692\
 C,0,-2.957038,5.94052,-3.810692\C,0,-3.676038,4.87752,-4.662692\N,0,-3
 .019038,3.63152,-4.161692\H,0,0.322962,-0.78748,-0.360692\H,0,-0.78545
 7,3.001485,1.601839\H,0,-0.785324,-0.787541,-3.381399\H,0,-1.755038,3.
 77652,-0.393692\H,0,-1.697038,1.34852,-3.623692\H,0,-2.070908,6.335568
 ,-4.374235\H,0,-3.70229,6.69699,-3.448445\H,0,-3.418657,5.027686,-5.74
 4392\H,0,-4.765962,4.85904,-4.396994\\Version=EM64L-G09RevB.01\State=3
 -A\HF=-1667.5189243\S2=2.117275\S2-1=0.\S2A=2.006036\RMSD=6.144e-09\Di
 pole=-0.9955541,-0.2964723,-2.1533678\Quadrupole=-9.3151875,18.7851093
 ,-9.4699218,-6.0016516,-4.5959124,-5.9312459\PG=C01 [X(C18H18N4O10)]\\
 @
```

NO to ON Contact B

Singlet broken-symmetry, UB3LYP/6-31G*

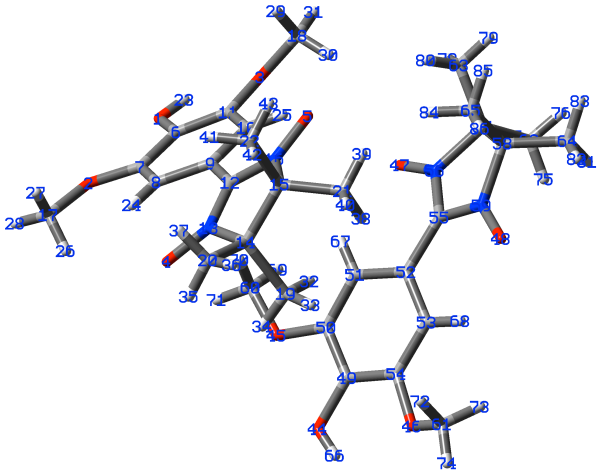

```
1\1\GINC-SKYNET\SP\UB3LYP\6-31G(d)\C18H18N4O10\LAHTI\11-May-2012\0\\#p
  UB3LYP/6-31G* test GUESS=(READ,MIX)\\SyrNN ON to ON contact, xtl geom
 \\0,1\O,0,3.70933,3.539637,0.104451\O,0,3.06933,1.286637,1.257451\O,0,
 3.07033,4.093637,-2.434549\O,0,1.54533,-2.269363,-1.598549\O,0,0.42633
 ,0.859637,-4.829549\C,0,3.05733,2.615637,-0.64955\C,0,2.70933,1.400637
 ,-0.064549\C,0,2.05633,0.430637,-0.794549\C,0,1.75133,0.660637,-2.1475
 49\C,0,2.08033,1.887637,-2.731549\C,0,2.70733,2.846637,-1.971549\C,0,1
 .13933,-0.392363,-2.955549\N,0,1.08833,-1.709363,-2.656549\C,0,0.61833
 ,-2.539363,-3.811549\C,0,-0.10167,-1.476363,-4.662549\N,0,0.55633,-0.2
 30363,-4.161549\H,0,3.89733,4.188637,-0.360549\H,0,2.789427,0.399336,1
 .601535\H,0,2.790695,4.189596,-3.381459\H,0,1.81933,-0.374363,-0.39355
 \H,0,1.87833,2.052637,-3.623549\H,0,-0.126186,-3.296873,-3.449962\H,0,
 1.505004,-2.932842,-4.375334\H,0,-1.191259,-1.457867,-4.395485\H,0,0.1
 54695,-1.626216,-5.744534\O,0,1.00333,-3.541363,4.24645\O,0,0.36333,-1
 .288363,5.40045\O,0,0.36433,-4.094362,1.707451\O,0,-1.16067,2.268637,2
 .543451\O,0,-2.27967,-0.861363,-0.687549\C,0,0.35133,-2.617363,3.49345
 \C,0,0.00333,-1.402363,4.078451\C,0,-0.64967,-0.431363,3.34845\C,0,-0.
 95467,-0.661363,1.995451\C,0,-0.62567,-1.888363,1.411451\C,0,0.00133,-
 2.848363,2.171451\C,0,-1.56667,0.390637,1.187451\N,0,-1.61767,1.707637
 ,1.486451\C,0,-2.08767,2.537637,0.331451\C,0,-2.80767,1.474637,-0.5205
 49\N,0,-2.14967,0.228637,-0.019549\H,0,1.19133,-4.189363,3.78145\H,0,0
 .083427,-0.401062,5.744534\H,0,0.084356,-4.189596,0.760568\H,0,-0.8866
 7,0.373637,3.74945\H,0,-0.82767,-2.053363,0.518451\H,0,-1.200991,2.931
 575,-0.232006\H,0,-2.832269,3.295074,0.69302\H,0,-2.550791,1.62483,-1.
 602365\H,0,-3.89733,1.455983,-0.253783\\Version=EM64L-G09RevB.01\State
 =1-A\HF=-1667.5178924\S2=1.120678\S2-1=0.\S2A=0.950611\RMSD=9.142e-09\
 Dipole=-1.1646518,0.0194714,-2.3384099\Quadrupole=-2.5520373,5.3399849
 ,-2.7879476,-3.9765796,-4.2764492,6.6514936\PG=C01 [X(C18H18N4O10)]\\@
```

Triplet, UB3LYP/6-31G*


```
1\1\GINC-SKYNET\SP\UB3LYP\6-31G(d)\C18H18N4O10(3)\LAHTI\11-May-2012\0\
 \#p UB3LYP/6-31G* test\\SyrNN ON to ON contact, xtl geom\\0,3\O,0,3.70
 933,3.539637,0.104451\O,0,3.06933,1.286637,1.257451\O,0,3.07033,4.0936
 37,-2.434549\O,0,1.54533,-2.269363,-1.598549\O,0,0.42633,0.859637,-4.8
 29549\C,0,3.05733,2.615637,-0.64955\C,0,2.70933,1.400637,-0.064549\C,0
 ,2.05633,0.430637,-0.794549\C,0,1.75133,0.660637,-2.147549\C,0,2.08033
 ,1.887637,-2.731549\C,0,2.70733,2.846637,-1.971549\C,0,1.13933,-0.3923
 63,-2.955549\N,0,1.08833,-1.709363,-2.656549\C,0,0.61833,-2.539363,-3.
 811549\C,0,-0.10167,-1.476363,-4.662549\N,0,0.55633,-0.230363,-4.16154
 9\H,0,3.89733,4.188637,-0.360549\H,0,2.789427,0.399336,1.601535\H,0,2.
 790695,4.189596,-3.381459\H,0,1.81933,-0.374363,-0.39355\H,0,1.87833,2
 .052637,-3.623549\H,0,-0.126186,-3.296873,-3.449962\H,0,1.505004,-2.93
 2842,-4.375334\H,0,-1.191259,-1.457867,-4.395485\H,0,0.154695,-1.62621
 6,-5.744534\O,0,1.00333,-3.541363,4.24645\O,0,0.36333,-1.288363,5.4004
 5\O,0,0.36433,-4.094362,1.707451\O,0,-1.16067,2.268637,2.543451\O,0,-2
 .27967,-0.861363,-0.687549\C,0,0.35133,-2.617363,3.49345\C,0,0.00333,-
 1.402363,4.078451\C,0,-0.64967,-0.431363,3.34845\C,0,-0.95467,-0.66136
 3,1.995451\C,0,-0.62567,-1.888363,1.411451\C,0,0.00133,-2.848363,2.171
 451\C,0,-1.56667,0.390637,1.187451\N,0,-1.61767,1.707637,1.486451\C,0,
 -2.08767,2.537637,0.331451\C,0,-2.80767,1.474637,-0.520549\N,0,-2.1496
 7,0.228637,-0.019549\H,0,1.19133,-4.189363,3.78145\H,0,0.083427,-0.401
 062,5.744534\H,0,0.084356,-4.189596,0.760568\H,0,-0.88667,0.373637,3.7
 4945\H,0,-0.82767,-2.053363,0.518451\H,0,-1.200991,2.931575,-0.232006\
 H,0,-2.832269,3.295074,0.69302\H,0,-2.550791,1.62483,-1.602365\H,0,-3.
 89733,1.455983,-0.253783\\Version=EM64L-G09RevB.01\State=3-A\HF=-1667.
 5178886\S2=2.120769\S2-1=0.\S2A=2.006403\RMSD=8.048e-09\Dipole=-1.1645
 993,0.0196204,-2.3387861\Quadrupole=-2.551462,5.3387302,-2.7872681,-3.
 975683,-4.2755774,6.6506129\PG=C01 [X(C18H18N4O10)]\\@
```

NO to methyl Contact C1



Singlet broken-symmetry, UB3LYP/6-31G*


```
1\1\GINC-SKYNET\SP\UB3LYP\6-31G(d)\C30H42N4O10\LAHTI\12-May-2012\0\\#P
  GFINPUT IOP(6/7=3) UB3LYP/6-31G* test GUESS=(READ,MIX)\\SyrNN Me to O
 N contact, xtl geom\\0,1\O,0,1.4385,-3.541,4.0425\O,0,0.7985,-1.287,5.
 1955\O,0,0.7985,-4.094,1.5035\O,0,-0.7255,2.269,2.3395\O,0,-1.8445,-0.
 86,-0.8915\C,0,0.7865,-2.617,3.2885\C,0,0.4375,-1.401,3.8735\C,0,-0.21
 45,-0.431,3.1435\C,0,-0.5195,-0.661,1.7905\C,0,-0.1905,-1.888,1.2065\C
 ,0,0.4355,-2.847,1.9665\C,0,-1.1325,0.392,0.9825\N,0,-1.1825,1.709,1.2
 815\C,0,-1.6535,2.539,0.1275\C,0,-2.3725,1.475,-0.7245\N,0,-1.7155,0.2
 29,-0.2235\C,0,0.4345,-0.147,5.8895\C,0,0.0465,-4.658,0.4755\C,0,-0.36
 85,3.082,-0.5535\C,0,-2.5255,3.672,0.6165\C,0,-2.1745,1.604,-2.2115\C,
 0,-3.8565,1.321,-0.4095\H,0,1.6265,-4.189,3.5775\H,0,-0.4515,0.374,3.5
 445\H,0,-0.3935,-2.053,0.3145\H,0,0.8125,0.623,5.4585\H,0,-0.5225,-0.0
 71,5.9015\H,0,0.7615,-0.203,6.7905\H,0,-0.8795,-4.68,0.7325\H,0,0.1445
 ,-4.132,-0.3205\H,0,0.3525,-5.552,0.3085\H,0,0.1685,2.347,-0.8565\H,0,
 -0.6105,3.633,-1.3015\H,0,0.1325,3.604,0.0795\H,0,-1.9945,4.283,1.1345
 \H,0,-2.9015,4.135,-0.1365\H,0,-3.2315,3.32,1.1615\H,0,-1.2395,1.702,-
 2.4025\H,0,-2.5095,0.816,-2.6475\H,0,-2.6505,2.374,-2.5325\H,0,-3.9755
 ,1.242,0.5385\H,0,-4.3325,2.09,-0.7305\H,0,-4.1935,0.533,-0.8415\O,0,4
 .1445,3.541,-0.1005\O,0,3.5045,1.287,1.0525\O,0,3.5045,4.094,-2.6395\O
 ,0,1.9805,-2.269,-1.8035\O,0,0.8615,0.86,-5.0345\C,0,3.4925,2.617,-0.8
 535\C,0,3.1435,1.401,-0.2685\C,0,2.4915,0.431,-0.9985\C,0,2.1865,0.661
 ,-2.3515\C,0,2.5155,1.888,-2.9365\C,0,3.1415,2.847,-2.1765\C,0,1.5735,
 -0.392,-3.1605\N,0,1.5235,-1.709,-2.8615\C,0,1.0525,-2.539,-4.0155\C,0
 ,0.3335,-1.475,-4.8675\N,0,0.9905,-0.229,-4.3665\C,0,3.1405,0.147,1.74
 65\C,0,2.7525,4.658,-3.6665\C,0,2.3375,-3.082,-4.6955\C,0,0.1805,-3.67
 2,-3.5255\C,0,0.5315,-1.604,-6.3545\C,0,-1.1505,-1.321,-4.5525\H,0,4.3
 325,4.189,-0.5655\H,0,2.2545,-0.374,-0.5975\H,0,2.3125,2.053,-3.8285\H
 ,0,3.5185,-0.623,1.3165\H,0,2.1835,0.071,1.7585\H,0,3.4675,0.203,2.647
 5\H,0,1.8265,4.68,-3.4105\H,0,2.8505,4.132,-4.4635\H,0,3.0585,5.552,-3
 .8345\H,0,2.8745,-2.347,-4.9995\H,0,2.0955,-3.633,-5.4445\H,0,2.8385,-
 3.604,-4.0635\H,0,0.7115,-4.283,-3.0085\H,0,-0.1955,-4.135,-4.2795\H,0
 ,-0.5255,-3.32,-2.9805\H,0,1.4665,-1.702,-6.5455\H,0,0.1965,-0.816,-6.
 7905\H,0,0.0555,-2.374,-6.6755\H,0,-1.2695,-1.242,-3.6035\H,0,-1.6265,
 -2.09,-4.8735\H,0,-1.4875,-0.533,-4.9845\\Version=EM64L-G09RevB.01\Sta
 te=1-A\HF=-2138.7581863\S2=1.110879\S2-1=0.\S2A=0.87568\RMSD=5.767e-09
 \Dipole=-1.5908581,-0.0275681,-1.9788516\Quadrupole=-7.1708644,11.6408
 525,-4.4699881,-3.5565295,-3.1461055,5.8438254\PG=C01 [X(C30H42N4O10)]
 \\@
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Triplet, UB3LYP/6-31G*


```
1\1\GINC-SKYNET\SP\UB3LYP\6-31G(d)\C30H42N4O10(3)\LAHTI\12-May-2012\0\
 \#P GFINPUT IOP(6/7=3) UB3LYP/6-31G* test\\SyrNN Me to ON contact, xtl
  geom\\0,3\O,0,1.4385,-3.541,4.0425\O,0,0.7985,-1.287,5.1955\O,0,0.798
 5,-4.094,1.5035\O,0,-0.7255,2.269,2.3395\O,0,-1.8445,-0.86,-0.8915\C,0
 ,0.7865,-2.617,3.2885\C,0,0.4375,-1.401,3.8735\C,0,-0.2145,-0.431,3.14
 35\C,0,-0.5195,-0.661,1.7905\C,0,-0.1905,-1.888,1.2065\C,0,0.4355,-2.8
 47,1.9665\C,0,-1.1325,0.392,0.9825\N,0,-1.1825,1.709,1.2815\C,0,-1.653
 5,2.539,0.1275\C,0,-2.3725,1.475,-0.7245\N,0,-1.7155,0.229,-0.2235\C,0
 ,0.4345,-0.147,5.8895\C,0,0.0465,-4.658,0.4755\C,0,-0.3685,3.082,-0.55
 35\C,0,-2.5255,3.672,0.6165\C,0,-2.1745,1.604,-2.2115\C,0,-3.8565,1.32
 1,-0.4095\H,0,1.6265,-4.189,3.5775\H,0,-0.4515,0.374,3.5445\H,0,-0.393
 5,-2.053,0.3145\H,0,0.8125,0.623,5.4585\H,0,-0.5225,-0.071,5.9015\H,0,
 0.7615,-0.203,6.7905\H,0,-0.8795,-4.68,0.7325\H,0,0.1445,-4.132,-0.320
 5\H,0,0.3525,-5.552,0.3085\H,0,0.1685,2.347,-0.8565\H,0,-0.6105,3.633,
 -1.3015\H,0,0.1325,3.604,0.0795\H,0,-1.9945,4.283,1.1345\H,0,-2.9015,4
 .135,-0.1365\H,0,-3.2315,3.32,1.1615\H,0,-1.2395,1.702,-2.4025\H,0,-2.
 5095,0.816,-2.6475\H,0,-2.6505,2.374,-2.5325\H,0,-3.9755,1.242,0.5385\
 H,0,-4.3325,2.09,-0.7305\H,0,-4.1935,0.533,-0.8415\O,0,4.1445,3.541,-0
 .1005\O,0,3.5045,1.287,1.0525\O,0,3.5045,4.094,-2.6395\O,0,1.9805,-2.2
 69,-1.8035\O,0,0.8615,0.86,-5.0345\C,0,3.4925,2.617,-0.8535\C,0,3.1435
 ,1.401,-0.2685\C,0,2.4915,0.431,-0.9985\C,0,2.1865,0.661,-2.3515\C,0,2
 .5155,1.888,-2.9365\C,0,3.1415,2.847,-2.1765\C,0,1.5735,-0.392,-3.1605
 \N,0,1.5235,-1.709,-2.8615\C,0,1.0525,-2.539,-4.0155\C,0,0.3335,-1.475
 ,-4.8675\N,0,0.9905,-0.229,-4.3665\C,0,3.1405,0.147,1.7465\C,0,2.7525,
 4.658,-3.6665\C,0,2.3375,-3.082,-4.6955\C,0,0.1805,-3.672,-3.5255\C,0,
 0.5315,-1.604,-6.3545\C,0,-1.1505,-1.321,-4.5525\H,0,4.3325,4.189,-0.5
 655\H,0,2.2545,-0.374,-0.5975\H,0,2.3125,2.053,-3.8285\H,0,3.5185,-0.6
 23,1.3165\H,0,2.1835,0.071,1.7585\H,0,3.4675,0.203,2.6475\H,0,1.8265,4
 .68,-3.4105\H,0,2.8505,4.132,-4.4635\H,0,3.0585,5.552,-3.8345\H,0,2.87
 45,-2.347,-4.9995\H,0,2.0955,-3.633,-5.4445\H,0,2.8385,-3.604,-4.0635\
 H,0,0.7115,-4.283,-3.0085\H,0,-0.1955,-4.135,-4.2795\H,0,-0.5255,-3.32
 ,-2.9805\H,0,1.4665,-1.702,-6.5455\H,0,0.1965,-0.816,-6.7905\H,0,0.055
 5,-2.374,-6.6755\H,0,-1.2695,-1.242,-3.6035\H,0,-1.6265,-2.09,-4.8735\
 H,0,-1.4875,-0.533,-4.9845\\Version=EM64L-G09RevB.01\State=3-A\HF=-213
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 07076,-0.0273952,-1.9792694\Quadrupole=-7.1700672,11.6398166,-4.469749
 4,-3.5550702,-3.1454783,5.8434013\PG=C01 [X(C30H42N4O10)]\\@
```

NO to methyl contact C2

Singlet broken-symmetry, UB3LYP/6-31G*


```
1\1\GINC-SKYNET\SP\UB3LYP\6-31G(d)\C30H42N4O10\LAHTI\12-May-2012\0\\#P
  GFINPUT IOP(6/7=3) UB3LYP/6-31G* test GUESS=(READ,MIX)\\SyrNN Me to O
 N contact, xtl geom\\0,1\O,0,5.013,6.9415,4.0425\O,0,4.373,4.6885,5.19
 55\O,0,4.374,7.4955,1.5035\O,0,2.849,1.1325,2.3395\O,0,1.73,4.2615,-0.
 8915\C,0,4.361,6.0175,3.2885\C,0,4.013,4.8025,3.8735\C,0,3.36,3.8325,3
 .1435\C,0,3.055,4.0625,1.7905\C,0,3.384,5.2895,1.2065\C,0,4.011,6.2485
 ,1.9665\C,0,2.443,3.0095,0.9825\N,0,2.392,1.6925,1.2815\C,0,1.922,0.86
 25,0.1265\C,0,1.202,1.9255,-0.7245\N,0,1.86,3.1715,-0.2235\C,0,4.01,3.
 5485,5.8895\C,0,3.621,8.0595,0.4755\C,0,3.206,0.3195,-0.5535\C,0,1.049
 ,-0.2705,0.6165\C,0,1.4,1.7975,-2.2125\C,0,-0.282,2.0805,-0.4095\H,0,5
 .201,7.5905,3.5775\H,0,3.123,3.0275,3.5445\H,0,3.182,5.4545,0.3145\H,0
 ,4.387,2.7785,5.4585\H,0,3.053,3.4715,5.9015\H,0,4.336,3.6035,6.7905\H
 ,0,2.695,8.0815,0.7325\H,0,3.719,7.5335,-0.3205\H,0,3.928,8.9535,0.308
 5\H,0,3.743,1.0545,-0.8565\H,0,2.964,-0.2315,-1.3015\H,0,3.707,-0.2025
 ,0.0785\H,0,1.581,-0.8815,1.1345\H,0,0.674,-0.7335,-0.1365\H,0,0.343,0
 .0815,1.1615\H,0,2.335,1.6995,-2.4025\H,0,1.066,2.5845,-2.6475\H,0,0.9
 25,1.0275,-2.5325\H,0,-0.401,2.1595,0.5385\H,0,-0.757,1.3115,-0.7305\H
 ,0,-0.619,2.8675,-0.8415\O,0,0.57,-6.9425,-0.1005\O,0,-0.07,-4.6885,1.
 0525\O,0,-0.07,-7.4955,-2.6395\O,0,-1.594,-1.1325,-1.8035\O,0,-2.713,-
 4.2615,-5.0345\C,0,-0.082,-6.0185,-0.8545\C,0,-0.431,-4.8025,-0.2695\C
 ,0,-1.083,-3.8325,-0.9995\C,0,-1.388,-4.0625,-2.3525\C,0,-1.059,-5.289
 5,-2.9365\C,0,-0.433,-6.2485,-2.1765\C,0,-2.001,-3.0095,-3.1605\N,0,-2
 .051,-1.6925,-2.8615\C,0,-2.522,-0.8625,-4.0155\C,0,-3.241,-1.9265,-4.
 8675\N,0,-2.584,-3.1725,-4.3665\C,0,-0.434,-3.5485,1.7465\C,0,-0.822,-
 8.0595,-3.6675\C,0,-1.237,-0.3195,-4.6965\C,0,-3.394,0.2705,-3.5265\C,
 0,-3.043,-1.7975,-6.3545\C,0,-4.725,-2.0805,-4.5525\H,0,0.758,-7.5905,
 -0.5655\H,0,-1.32,-3.0275,-0.5985\H,0,-1.262,-5.4545,-3.8285\H,0,-0.05
 6,-2.7785,1.3155\H,0,-1.391,-3.4725,1.7585\H,0,-0.107,-3.6045,2.6475\H
 ,0,-1.748,-8.0815,-3.4105\H,0,-0.724,-7.5335,-4.4635\H,0,-0.516,-8.953
 5,-3.8345\H,0,-0.7,-1.0545,-4.9995\H,0,-1.479,0.2315,-5.4445\H,0,-0.73
 6,0.2025,-4.0635\H,0,-2.863,0.8815,-3.0085\H,0,-3.77,0.7335,-4.2795\H,
 0,-4.1,-0.0815,-2.9815\H,0,-2.108,-1.6995,-6.5455\H,0,-3.378,-2.5855,-
 6.7905\H,0,-3.519,-1.0275,-6.6755\H,0,-4.844,-2.1595,-3.6045\H,0,-5.20
 1,-1.3115,-4.8735\H,0,-5.062,-2.8685,-4.9845\\Version=EM64L-G09RevB.01
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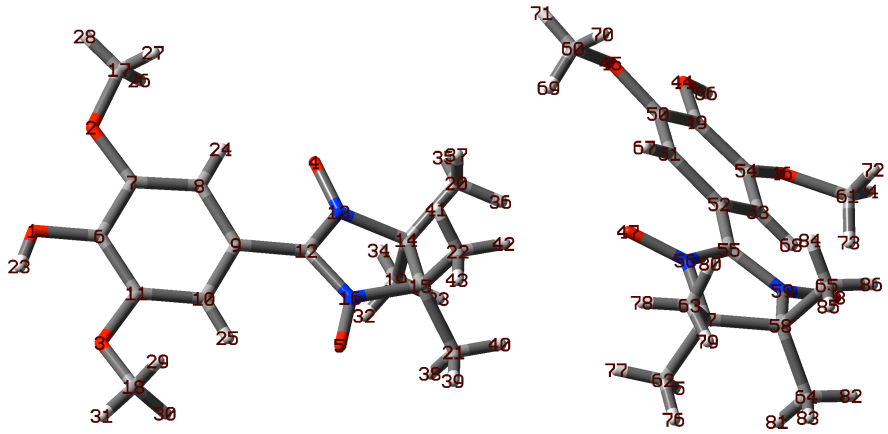
 1076843,1.7769579,-5.5559418,-2.0358348,-4.8618095\PG=C01 [X(C30H42N4O
 10)]\\@
```

Triplet, UB3LYP/6-31G*


```
1\1\GINC-SKYNET\SP\UB3LYP\6-31G(d)\C30H42N4O10(3)\LAHTI\12-May-2012\0\
 \#P GFINPUT IOP(6/7=3) UB3LYP/6-31G* test\\SyrNN Me to ON contact, xtl
  geom\\0,3\O,0,5.013,6.9415,4.0425\O,0,4.373,4.6885,5.1955\O,0,4.374,7
 .4955,1.5035\O,0,2.849,1.1325,2.3395\O,0,1.73,4.2615,-0.8915\C,0,4.361
 ,6.0175,3.2885\C,0,4.013,4.8025,3.8735\C,0,3.36,3.8325,3.1435\C,0,3.05
 5,4.0625,1.7905\C,0,3.384,5.2895,1.2065\C,0,4.011,6.2485,1.9665\C,0,2.
 443,3.0095,0.9825\N,0,2.392,1.6925,1.2815\C,0,1.922,0.8625,0.1265\C,0,
 1.202,1.9255,-0.7245\N,0,1.86,3.1715,-0.2235\C,0,4.01,3.5485,5.8895\C,
 0,3.621,8.0595,0.4755\C,0,3.206,0.3195,-0.5535\C,0,1.049,-0.2705,0.616
 5\C,0,1.4,1.7975,-2.2125\C,0,-0.282,2.0805,-0.4095\H,0,5.201,7.5905,3.
 5775\H,0,3.123,3.0275,3.5445\H,0,3.182,5.4545,0.3145\H,0,4.387,2.7785,
 5.4585\H,0,3.053,3.4715,5.9015\H,0,4.336,3.6035,6.7905\H,0,2.695,8.081
 5,0.7325\H,0,3.719,7.5335,-0.3205\H,0,3.928,8.9535,0.3085\H,0,3.743,1.
 0545,-0.8565\H,0,2.964,-0.2315,-1.3015\H,0,3.707,-0.2025,0.0785\H,0,1.
 581,-0.8815,1.1345\H,0,0.674,-0.7335,-0.1365\H,0,0.343,0.0815,1.1615\H
 ,0,2.335,1.6995,-2.4025\H,0,1.066,2.5845,-2.6475\H,0,0.925,1.0275,-2.5
 325\H,0,-0.401,2.1595,0.5385\H,0,-0.757,1.3115,-0.7305\H,0,-0.619,2.86
 75,-0.8415\O,0,0.57,-6.9425,-0.1005\O,0,-0.07,-4.6885,1.0525\O,0,-0.07
 ,-7.4955,-2.6395\O,0,-1.594,-1.1325,-1.8035\O,0,-2.713,-4.2615,-5.0345
 \C,0,-0.082,-6.0185,-0.8545\C,0,-0.431,-4.8025,-0.2695\C,0,-1.083,-3.8
 325,-0.9995\C,0,-1.388,-4.0625,-2.3525\C,0,-1.059,-5.2895,-2.9365\C,0,
 -0.433,-6.2485,-2.1765\C,0,-2.001,-3.0095,-3.1605\N,0,-2.051,-1.6925,-
 2.8615\C,0,-2.522,-0.8625,-4.0155\C,0,-3.241,-1.9265,-4.8675\N,0,-2.58
 4,-3.1725,-4.3665\C,0,-0.434,-3.5485,1.7465\C,0,-0.822,-8.0595,-3.6675
 \C,0,-1.237,-0.3195,-4.6965\C,0,-3.394,0.2705,-3.5265\C,0,-3.043,-1.79
 75,-6.3545\C,0,-4.725,-2.0805,-4.5525\H,0,0.758,-7.5905,-0.5655\H,0,-1
```

.32,-3.0275,-0.5985\H,0,-1.262,-5.4545,-3.8285\H,0,-0.056,-2.7785,1.31
55\H,0,-1.391,-3.4725,1.7585\H,0,-0.107,-3.6045,2.6475\H,0,-1.748,-8.0
815,-3.4105\H,0,-0.724,-7.5335,-4.4635\H,0,-0.516,-8.9535,-3.8345\H,0,
-0.7,-1.0545,-4.9995\H,0,-1.479,0.2315,-5.4445\H,0,-0.736,0.2025,-4.06
35\H,0,-2.863,0.8815,-3.0085\H,0,-3.77,0.7335,-4.2795\H,0,-4.1,-0.0815
,-2.9815\H,0,-2.108,-1.6995,-6.5455\H,0,-3.378,-2.5855,-6.7905\H,0,-3.
519,-1.0275,-6.6755\H,0,-4.844,-2.1595,-3.6045\H,0,-5.201,-1.3115,-4.8
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604,-5.5559225,-2.0357851,-4.8617568\PG=C01 [X(C30H42N4O10)]\\@