Supplementary Material (ESI) for Organic and Biomolecular Chemistry

Intermediates in the reduction of the antituberculosis drug PA-824, (6*S*)-2-nitro-6-{[4-(trifluoromethoxy)benzyl]oxy}-6,7-dihydro-5*H*-imidazo[2,1-*b*][1,3]oxazine, in aqueous solution.

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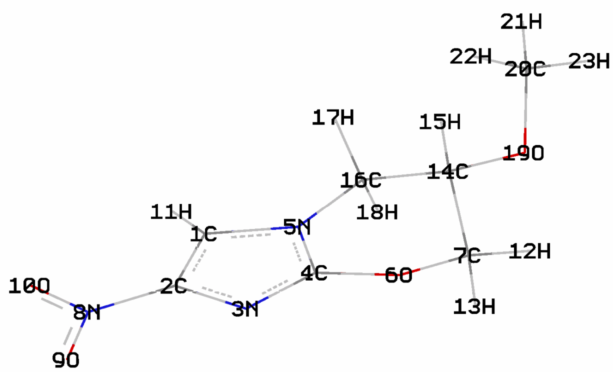
Supplementary Data

Method: UB3LYP/6-31G(d,p)

Isotropic Fermi Contact Couplings for PA-824 radical anion (spin=2, charge=-1)



	Atom	a.u.	MegaHertz	Gauss	10^{-4} cm^{-1}
1	C(13)	0.02929	32.92502	11.74847	10.98261
2	C(13)	-0.01292	-14.52537	-5.18301	-4.84514
3	N(14)	0.00314	1.01455	0.36202	0.33842
4	C(13)	-0.00725	-8.14949	-2.90794	-2.71838
5	N(14)	0.00398	1.28615	0.45893	0.42901
6	O(17)	-0.00190	1.15317	0.41148	0.38465
7	C(13)	-0.00071	-0.79286	-0.28291	-0.26447
8	N(14)	0.04528	14.63141	5.22085	4.88051
9	O(17)	0.03696	-22.40773	-7.99563	-7.47441
10	O(17)	0.02911	-17.64850	-6.29742	-5.88691
11	H(1)	-0.00546	-24.42359	-8.71494	-8.14683
12	H(1)	0.00016	0.70917	0.25305	0.23656
13	H(1)	0.00005	0.22430	0.08004	0.07482
14	C(13)	-0.00073	-0.82025	-0.29268	-0.27361
15	H(1)	0.00014	0.62072	0.22149	0.20705
16	C(13)	-0.00212	-2.37984	-0.84919	-0.79383
17	H(1)	0.00137	6.11767	2.18294	2.04063
18	H(1)	0.00236	10.54397	3.76235	3.51709
19	O(17)	0.00177	-1.07133	-0.38228	-0.35736
20	C(13)	0.00246	2.76291	0.98588	0.92161
21	H(1)	-0.00002	-0.10613	-0.03787	-0.03540
22	H(1)	-0.00002	-0.08752	-0.03123	-0.02919
23	H(1)	0.00001	0.06435	0.02296	0.02147