JO010302Z

Supporting Information Section

Table S1. Geometry of 6-[(4'-R_2-phenyl)amine]-3-hydroxy-1,4-benzoquinones (ABQs) and 6-[(4'-R_2-phenyl)amine]-3-methoxy-1,4-benzoquinones (ABQms). Distances in Å, angles in degrees.

R_1	OH	OMe	OH	OMe	OH	OMe	OMe	OH	OMe	OH	OMe	OH	OMe	OH	OMe
Bond R_2	OMe	OMe	Me	Me	H	H	H_{min}	F	F	CF_3	CF_3	CN	CN	NO_2	NO_2
C_1-C_7	1.442	1.449	1.442	1.449	1.443	1.449	1.449	1.442	1.449	1.443	1.449	1.442	1.449	1.443	1.449
C_2-C_3	1.355	1.358	1.355	1.358	1.355	1.358	1.358	1.355	1.358	1.355	1.358	1.355	1.358	1.355	1.359
C_3-C_4	1.515	1.521	1.514	1.520	1.514	1.520	1.523	1.515	1.520	1.514	1.520	1.514	1.519	1.516	1.521
C_4-C_5	1.427	1.448	1.429	1.449	1.430	1.450	1.449	1.430	1.406	1.434	1.453	1.435	1.445	1.436	1.455
C_5-C_6	1.376	1.368	1.375	1.367	1.374	1.366	1.366	1.374	1.366	1.371	1.364	1.370	1.363	1.369	1.362
C_6-C_1	1.542	1.525	1.542	1.526	1.543	1.526	1.522	1.542	1.526	1.543	1.526	1.542	1.526	1.538	1.522
C_1-O_1	1.233	1.233	1.233	1.232	1.232	1.232	1.232	1.232	1.232	1.232	1.232	1.232	1.232	1.232	1.232
C_4-O_4	1.242	1.228	1.241	1.227	1.240	1.227	1.227	1.240	1.227	1.239	1.225	1.238	1.225	1.237	1.224
C_3-O_3	1.326	1.333	1.326	1.333	1.326	1.332	1.332	1.325	1.332	1.325	1.331	1.325	1.331	1.325	1.331
C_6-N	1.348	1.356	1.349	1.358	1.350	1.359	1.358	1.350	1.358	1.353	1.362	1.355	1.364	1.356	1.365
C-R_2	1.362	1.365	1.509	1.510	1.085	1.085	1.085	1.347	1.349	1.503	1.502	1.431	1.431	1.466	1.463
H_5-$H_{6'}$	1.849	1.844	1.844	1.844	1.811	1.840	2.072	1.842	1.841	1.840	1.842	1.844	1.843	2.042	2.014
O_3-H or O_3-C	0.991	1.427	0.990	1.428	0.989	1.428	1.428	0.989	1.428	0.988	1.428	0.988	1.429	0.988	1.429
N-H	1.023	1.020	1.023	1.020	1.023	1.020	1.019	1.023	1.021	1.024	1.021	1.024	1.021	1.022	1.020
O_1-H(N)	1.939	1.978	1.943	1.980	1.944	1.978	2.031	1.938	1.973	1.937	1.973	1.933	1.965	1.979	2.013
O_4-H(O)	1.880		1.887		1.892			1.893		1.906		1.914		1.915	
N-$C_{1'}$	1.403	1.401	1.402	1.400	1.402	1.399	1.404	1.402	1.399	1.397	1.394	1.394	1.391	1.396	1.392
$C_{1'}$-$C_{2'}$	1.404	1.404	1.406	1.406	1.408	1.409	1.405	1.409	1.409	1.408	1.409	1.411	1.412	1.409	1.411
$C_{2'}$-$C_{3'}$	1.391	1.391	1.389	1.389	1.389	1.389	1.391	1.388	1.388	1.388	1.387	1.384	1.383	1.386	1.385
$C_{3'}$-$C_{4'}$	1.401	1.400	1.401	1.401	1.397	1.397	1.397	1.391	1.391	1.397	1.397	1.407	1.407	1.395	1.396
$C_{4'}$-$C_{5'}$	1.401	1.400	1.400	1.400	1.394	1.393	1.395	1.388	1.387	1.397	1.396	1.403	1.403	1.393	1.393
$C_{5'}$-$C_{6'}$	1.388	1.389	1.393	1.392	1.395	1.395	1.395	1.394	1.395	1.391	1.391	1.390	1.390	1.389	1.389
$C_{6'}$-$C_{1'}$	1.406	1.407	1.404	1.404	1.403	1.404	1.403	1.404	1.404	1.406	1.406	1.406	1.406	1.407	1.408
O_1-C_1-C_6	117.7	118.8	117.7	118.8	117.7	118.8	118.8	117.6	118.7	117.6	118.6	117.5	118.6	117.5	118.5
C_1-C_6-C_5	120.6	119.6	120.5	119.5	120.5	119.5	120.2	120.6	119.6	120.5	119.6	120.6	119.6	121.2	120.2
C_1-C_6-N	109.2	109.7	109.3	109.8	109.3	109.7	110.6	109.2	109.6	109.2	109.6	109.1	109.5	109.9	110.3
C_6-N-H	109.2	109.6	109.3	109.7	109.3	109.6	111.1	109.2	109.6	19.2	109.5	109.1	109.3	110.4	110.6
C_6-N-$C_{1'}$	135.3	134.8	135.2	134.8	135.2	134.8	131.6	135.1	134.8	135.1	134.8	135.1	134.8	132.3	132.3
C_6-C_5-C_4	119.9	122.1	119.9	122.1	119.9	122.0	121.8	119.8	122.0	119.8	122.0	119.8	121.9	119.5	121.6
O_1-C_1-C_2	124.5	122.4	123.4	122.4	123.4	124.4	122.8	123.5	122.5	123.5	122.5	123.5	122.6	123.9	122.9
O_4-C_4-C_5	125.9	123.3	125.8	123.2	125.7	123.1	123.4	125.7	123.1	125.4	122.9	125.3	122.7	125.5	122.9
O_4-C_4-C_3	115.0	119.3	115.1	119.4	115.2	119.4	119.3	115.2	119.4	115.4	119.6	115.6	119.7	115.6	119.7
O_3-C_3-C_4	112.7	112.2	112.8	112.2	112.9	112.2	112.1	112.9	112.2	113.0	112.2	113.1	112.2	113.1	112.1
O_3-C_3-C_2	124.7	126.3	124.7	126.3	124.7	126.4	126.3	124.7	126.4	124.7	126.5	124.6	126.5	124.5	126.5
H-N-$C_{1'}$	115.5	115.6	115.5	115.5	115.5	115.6	117.3	115.6	115.7	115.7	115.7	115.8	115.8	117.4	117.1
$C_{1'}$-$C_{2'}$-$C_{3'}$	121.6	121.7	120.8	120.9	120.7	120.8	120.4	121.2	121.2	120.9	121.0	121.0	121.1	120.6	120.8
$C_{1'}$-$C_{6'}$-$C_{5'}$	120.3	120.4	119.9	120.0	119.8	119.8	119.8	120.2	120.3	119.9	120.0	120.1	120.2	120.0	120.1
C_6-N-$C_{1'}$-$C_{2'}$	180.0	180.0	180.0	180.0	180.0	180.0	154.7	180.0	180.0	180.0	180.0	180.0	180.0	24.7	160.8
O_1-C_1-C_6-N	0.0	0.0	0.0	0.0	0.0	0.0	1.1	0.0	0.0	0.0	0.0	0.0	0.0	1.06	1.1
H-N-C_6-C_1	0.0	0.0	0.0	0.0	0.0	0.0	4.9	0.0	0.0	0.0	0.0	0.0	0.0	4.80	5.4
C_1-C_6-C_5-C_4	0.0	0.0	0.0	0.0	0.0	0.0	1.6	0.0	0.0	0.0	0.0	0.0	0.0	1.8	2.1
C_1-C_6-N-$C_{1'}$	180.0	180.0	180.0	180.0	180.0	180.0	176.4	180.0	180.0	180.0	180.0	180.0	180.0	175.6	174.5
O-C_1-C_4-O_4	180.0	180.0	180.0	180.0	180.0	180.0	126.8	180.0	180.0	180.0	180.0	180.0	180.0	152.9	120.2
O_3-C_3-C_2-C_1	180.0	180.0	180.0	180.0	180.0	180.0	179.9	180.0	180.0	180.0	180.0	180.0	180.0	179.6	179.9
O_4-C_4-C_5-C_6	180.0	180.0	180.0	180.0	180.0	180.0	179.0	180.0	180.0	180.0	180.0	180.0	180.0	179.6	179.2

Table S2. Wiberg Bond Indexes (WBI), and properties of the relevant bond critical points, in the electronic density of the referred quinones at Becke3LYP/6-31G(*d,p*) level.

		ABQ's				ABQm's			
R_2	Bond	WBI	ρ	$\nabla^2\rho$	ε	WBI	ρ	$\nabla^2\rho$	ε
MeO	C_1-C_6	0.960	0.2489	-0.5826	0.0839	0.977	0.2569	-0.6187	0.0925
	C_6-C_5	1.493	0.3192	-0.8841	0.3030	1.540	0.3238	-0.9053	0.3189
	C_4-C_5	1.207	0.2982	-0.7978	0.1967	1.152	0.2880	-0.7470	0.1734
	C_4-C_3	0.973	0.2640	-0.6550	0.0886	0.965	0.2599	-0.6459	0.0971
	C_2-C_3	1.590	0.3365	-0.9903	0.3388	1.616	0.3343	-0.9616	0.3402
	C_1-C_2	1.164	0.2911	-0.7699	0.1682	1.137	0.2877	-0.7537	0.1511
	C_1-O	1.661	0.3919	0.1037	0.0394	1.672	0.3921	0.1103	0.0375
	C_4-O	1.600	0.3846	0.0346	0.0361	1.695	0.3970	0.1186	0.0676
	C_3-O	1.141	0.3158	-0.2573	0.0423	1.096	0.3057	-0.2120	0.0330
	N-H···O	0.050	0.0317	0.1057	0.1660	0.043	0.0293	0.1004	0.1997
	O_3-H	0.068	0.0353	0.1074	0.1651				
	C_6-N	1.250	0.3244	-0.8002	0.0841	1.208	0.3192	-0.8361	0.0899
	N-C_1·	1.059	0.2885	-0.8004	0.0960	1.064	0.2901	-0.8163	0.0956
	H_5-H_6·	0.004	0.0147	0.0509	0.1107	0.004	0.0149	0.0512	0.1090
Me	C_1-C_6	0.959	0.2487	-0.5822	0.0827	0.976	0.2566	-0.6177	0.0915
	C_6-C_5	1.503	0.3202	-0.8890	0.3045	1.549	0.3246	-0.9092	0.3196
	C_4-C_5	1.201	0.2974	-0.7948	0.1921	1.147	0.2874	-0.7452	0.1697
	C_4-C_3	0.973	0.2641	-0.6557	0.0884	0.965	0.2601	-0.6466	0.0970
	C_2-C_3	1.592	0.3367	-0.9916	0.3395	1.616	0.3344	-0.9621	0.3405
	C_1-C_2	1.162	0.2908	-0.7687	0.1669	1.136	0.2876	-0.7533	0.1505
	C_1-O	1.666	0.3924	0.1094	0.0403	1.675	0.3925	0.1143	0.0382
	C_4-O	1.607	0.3853	0.0439	0.0360	1.700	0.3974	0.1255	0.0674
	C_3-O	1.140	0.3158	-0.2584	0.0408	1.097	0.3059	-0.2132	0.0315
	N-H···O	0.049	0.0314	0.1052	0.1688	0.042	0.0292	0.1003	0.2005
	O_3-H	0.067	0.0348	0.1065	0.1718				
	C_6-N	1.244	0.3241	-0.8177	0.0801	1.203	0.3189	-0.8495	0.0864
	N-C_1·	1.062	0.2890	-0.8053	0.0771	1.069	0.2909	-0.8197	0.0780
	H_5-H_6·	0.004	0.0149	0.0513	0.1102	0.004	0.0149	0.0513	0.1090
H	C_1-C_6	0.958	0.2486	-0.5817	0.0822	0.976	0.2565	-0.6173	0.0911
	C_6-C_5	1.510	0.3208	-0.8923	0.3058	1.555	0.3251	-0.9118	0.3204
	C_4-C_5	1.196	0.2969	-0.7929	0.1892	1.144	0.2870	-0.7436	0.1674
	C_4-C_3	0.973	0.2642	-0.6563	0.0883	0.965	0.2602	-0.6470	0.0970
	C_2-C_3	1.593	0.3369	-0.9925	0.3397	1.616	0.3345	-0.9625	0.3405
	C_1-C_2	1.161	0.2907	-0.7681	0.1664	1.136	0.2875	-0.7533	0.1504
	C_1-O	1.667	0.3926	0.1119	0.0408	1.676	0.3926	0.1158	0.0385
	C_4-O	1.612	0.3858	0.0496	0.0363	1.703	0.3978	0.1300	0.0675
	C_3-O	1.140	0.3158	-0.2588	0.0400	1.097	0.2840	-1.0179	0.0340
	N-H···O	0.049	0.0314	0.1051	0.1686	0.043	0.0293	0.1005	0.1988
	O_3-H	0.065	0.0344	0.1058	0.1769				
	C_6-N	1.240	0.3236	-0.8244	0.0777	1.200	0.3184	-0.8546	0.0843
	N-C_1·	1.064	0.2894	-0.8129	0.0715	1.071	0.2914	-0.8263	0.0730
	H_5-H_6·	0.004	0.0150	0.0515	0.1100	0.004	0.0151	0.0516	0.1088
F	C_1-C_6	0.958	0.2486	-0.5817	0.0825	0.975	0.2565	-0.6170	0.0913
	C_6-C_5	1.509	0.3207	-0.8913	0.3066	1.554	0.3250	-0.9110	0.3212
	C_4-C_5	1.196	0.2968	-0.7923	0.1895	1.144	0.2869	-0.7431	0.1677
	C_4-C_3	0.973	0.2641	-0.6560	0.0882	0.965	0.2602	-0.6470	0.0970
	C_2-C_3	1.592	0.3367	-0.9917	0.3391	1.615	0.3343	-0.9615	0.3399
	C_1-C_2	1.162	0.2910	-0.7694	0.1670	1.137	0.2878	-0.7544	0.1510
	C_1-O	1.666	0.3925	0.1097	0.0406	1.674	0.3925	0.1138	0.0385
	C_4-O	1.613	0.3860	0.0503	0.0367	1.704	0.3979	0.1309	0.0677
	C_3-O	1.141	0.3159	-0.2582	0.0398	1.099	0.3064	-0.2135	0.0303
	N-H···O	0.050	0.0318	0.1060	0.1642	0.043	0.0296	0.1011	0.1942
	O_3-H	0.065	0.0343	0.1056	0.1783				
	C_6-N	1.240	0.3234	-0.8140	0.0780	1.200	0.3181	-0.8449	0.0844
	N-C_1·	1.063	0.2899	-0.8217	0.0883	1.069	0.2918	-0.8356	0.0893
	H_5-H_6·	0.004	0.0149	0.0515	0.1111	0.004	0.0150	0.0516	0.1099
CF_3	C_1-C_6	0.958	0.2486	-0.5817	0.0819	0.975	0.2564	-0.6172	0.0909
	C_6-C_5	1.529	0.3226	-0.9004	0.3101	1.572	0.3267	-0.9198	0.3234
	C_4-C_5	1.182	0.2953	-0.7865	0.1809	1.133	0.2856	-0.7381	0.1601
	C_4-C_3	0.973	0.2645	-0.6580	0.0883	0.966	0.2606	-0.6489	0.0972
	C_2-C_3	1.594	0.3369	-0.9930	0.3394	1.615	0.3343	-0.9617	0.3399
	C_1-C_2	1.160	0.2908	-0.7687	0.1657	1.136	0.2876	-0.7538	0.1506
	C_1-O	1.669	0.3929	0.1140	0.0417	1.676	0.3929	0.1165	0.0397
	C_4-O	1.626	0.3874	0.0669	0.0375	1.714	0.3989	0.1454	0.0681
	C_3-O	1.140	0.3160	-0.2596	0.0372	1.100	0.3070	-0.2161	0.0272
	N-H···O	0.049	0.0318	0.1063	0.1628	0.043	0.0296	1.009	0.1930
	O_3-H	0.062	0.0334	0.1040	0.1933				
	C_6-N	1.224	0.3215	-0.8330	0.0707	1.185	0.3161	-0.8577	0.0774
	N-C_1·	1.076	0.2931	-0.8370	0.0680	1.085	0.2954	-0.8490	0.0701
	H_5-H_6·	0.004	0.0150	0.0518	0.1132	0.004	0.0149	0.0516	0.1123
CN	C_1-C_6	0.958	0.2487	-0.5825	0.0823	0.975	0.2564	-0.6171	0.0912
	C_6-C_5	1.538	0.3233	-0.9040	0.3120	1.580	0.3274	-0.9231	0.3244

C_4-C_5	1.175	0.2945	-0.7829	0.1766	1.128	0.2848	-0.7350	0.1564
C_4-C_3	0.974	0.2647	-0.6588	0.0885	0.966	0.2608	-0.6499	0.0974
C_2-C_3	1.594	0.3370	-0.9931	0.3392	1.613	0.3342	-0.9613	0.3394

Table S2. (continues) Wiberg Bond Indexes (WBI), and properties of the relevant bond critical points, in the electronic density of the referred quinones at Becke3LYP/6-31G(*d,p*) level.

		ABQ's				ABQm's			
R_2	Bond	WBI	ρ	$\nabla^2\rho$	ε	WBI	ρ	$\nabla^2\rho$	ε
	C_1-C_7	1.162	0.2908	-0.7691	0.1653	1.137	0.2879	-0.7549	0.1510
	C_1-O	1.669	0.3930	0.1146	0.0421	1.676	0.3929	0.1156	0.0400
	C_4-O	1.632	0.3881	0.0750	0.0384	1.719	0.3995	0.1538	0.0685
	C_3-O	1.140	0.3160	-0.2607	0.0357	1.102	0.3076	-0.2155	0.0257
	N-H···O	0.050	0.0321	0.1069	0.1597	0.045	0.0300	0.1021	0.1859
	O_3-H	0.060	0.0328	0.1028	0.2038				
	C_6-N	1.215	0.3201	-0.8338	0.0676	1.178	0.3148	-0.8567	0.0744
	N-C_1	1.085	0.2953	-0.8448	0.0693	1.095	0.2977	-0.8550	0.0716
	H_5-H_6	0.004	0.0148	0.0514	0.1148	0.004	0.0149	0.0515	0.1138
NO_2	C_1-C_6	0.959	0.2506	-0.5923	0.0801	0.976	0.2582	-0.6264	0.0896
	C_6-C_5	1.546	0.3245	-0.9116	0.3106	1.588	0.3286	-0.9302	0.3225
	C_4-C_5	1.173	0.2942	-0.7820	0.1746	1.125	0.2848	-0.7358	0.1543
	C_4-C_3	0.973	0.2637	-0.6539	0.0884	0.965	0.2600	-0.6458	0.0975
	C_2-C_3	1.595	0.3366	-0.9908	0.3393	1.614	0.3339	-0.9589	0.3395
	C_1-C_2	1.159	0.2906	-0.7678	0.1652	1.136	0.2876	-0.7533	0.1509
	C_1-O	1.673	0.3934	0.1145	0.0452	1.679	0.3933	0.1166	0.0429
	C_4-O	1.638	0.3887	0.0806	0.0389	1.723	0.3998	0.1578	0.0690
	C_3-O	1.140	0.3160	-0.2603	0.0351	1.102	0.3075	-0.2172	0.0248
	N-H···O	0.044	0.0293	0.1000	0.1943	0.039	0.0274	0.0958	0.2297
	O_3-H	0.060	0.0327	0.1028	0.2036				
	C_6-N	1.216	0.3205	-0.8502	0.0641	0.173	0.3150	-0.8682	0.0715
	N-C_1	1.074	0.2954	-0.8668	0.0662	0.088	0.2981	-0.8748	0.0692
	H_5-H_6	0.001	0.0116	0.0474	0.0729	0.001	0.0120	0.0486	0.0663

Table S3. Natural charges at Becke3LYP/6-31G(*d,p*) level of 6-[(R_2-phenyl)amine]-3-hydroxy-1,4-benzoquinones (ABQs) and 6-[(R_2-phenyl)amine]-3-methoxy-1,4-benzoquinones (ABQms).

	R_1	HO	OMe	HO	OMe	HO	OMe	HO	OMe	HO	OMe	HO	OMe	HO	OMe
Atom	R_2	MeO	OMe	Me	Me	H	H	F	F	CF_3	CF_3	CN	CN	NO_2	NO_2
C_1		0.50	0.51	0.50	0.51	0.50	0.51	0.50	0.51	0.50	0.51	0.50	0.51	0.50	0.51
C_2		-0.41	-0.43	-0.41	-0.43	-0.40	-0.43	-0.40	-0.43	-0.40	-0.43	-0.40	-0.43	-0.40	-0.43
C_3		0.35	0.35	0.35	0.35	0.35	0.35	0.35	0.35	0.35	0.35	0.35	0.35	0.35	0.35
C_4		0.44	0.46	0.45	0.46	0.45	0.46	0.45	0.46	0.45	0.47	0.45	0.47	0.46	0.47
C_5		-0.41	-0.40	-0.41	-0.39	-0.41	-0.39	-0.41	-0.39	-0.40	-0.38	-0.39	-0.38	-0.40	-0.38
C_6		0.19	0.16	0.19	0.16	0.19	0.16	0.19	0.16	0.19	0.16	0.19	0.16	0.19	0.16
O_1		-0.57	-0.57	-0.56	-0.56	-0.56	-0.56	-0.56	-0.56	-0.56	-0.56	-0.56	-0.56	-0.55	-0.56
O_3		-0.66	-0.47	-0.66	-0.47	-0.65	-0.47	-0.65	-0.47	-0.65	-0.47	-0.37	-0.47	-0.65	-0.47
O_4		-0.58	-0.52	-0.58	-0.52	-0.58	-0.52	-0.58	-0.52	-0.57	-0.51	-0.56	-0.51	-0.56	-0.50
N		-0.54	-0.56	-0.54	-0.56	-0.55	-0.56	-0.55	-0.56	-0.55	-0.56	-0.55	-0.56	-0.56	-0.56
C1'		0.13	0.14	0.15	0.15	0.16	0.16	0.14	0.15	0.17	0.18	0.18	0.18	0.18	0.19
C_2'		-0.23	-0.24	-0.24	-0.25	-0.25	-0.26	-0.24	-0.24	-0.25	-0.25	-0.25	-0.25	-0.24	-0.25
C_3'		-0.31	-0.31	-0.22	-0.22	-0.22	-0.22	-0.29	-0.29	-0.20	-0.20	-0.18	-0.20	-0.20	-0.20
C_4'		0.32	0.31	-0.04	-0.04	-0.25	-0.25	0.42	0.41	-0.18	-0.19	-0.18	-0.19	-0.05	0.04
C_5'		-0.26	-0.26	-0.22	-0.22	-0.22	-0.22	-0.29	-0.29	-0.19	-0.19	-0.17	-0.19	-0.20	-0.20
C_6'		-0.24	-0.25	-0.25	-0.25	-0.26	-0.26	-0.24	-0.25	-0.25	-0.26	-0.26	-0.26	-0.26	-0.27
H-N		0.45	0.44	0.45	0.44	0.45	0.44	0.45	0.44	0.45	0.45	0.45	0.45	0.45	0.45
H or (C)-O		0.52	-0.33	0.52	-0.33	0.52	-0.33	0.52	-0.33	0.52	-0.33	0.52	-0.33	0.52	-0.33
H_3		0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.26	0.25
H_8'		0.27	0.24	0.27	0.24	0.27	0.24	0.27	0.24	0.24	0.24	0.27	0.24	0.27	0.24

X-ray Structure Data.

Crystal Data

Empirical Formula	**$C_{22}H_{27}N\ O_3$**
Color, Habit	Deep purple, needle
Crystal size	0.7 x 0.1 x 0.1 mm^3
Crystal system	Orthorhombic
Space group	$P\ 2_1\ 2_1\ 2_1$
Unit cell dimensions	a = 7.563 (1) b = 11.966 (2) c = 21.207 (4) Å
Volume	1919.3 (7) $Å^3$
Z	4
Formula Weight	353.45
Density (calc.)	1.223 $g.cm^{-3}$
Absorption coefficient	0.08 mm^{-1}
F(000)	760

Data collection

Diffractometer used	**Siemens P4/PC**
Radiation	Mo-K_α (λ=0.71073 Å)
High-voltage and tube current	50 KV, 30 mA
Temperature	298 K
Monochromator	Highly oriented graphite crystal
2θ Range	4 – 42°
Scan type	θ / 2θ
Scan speed	Variable speed, 3 to 60°.mn-1 in ω
Scan range (ω)	0.72° + separation between the $K_{\alpha1}$ and the $K_{\alpha2}$ positions
Background measurement	Stationary crystal and stationary counter at beginning and end of scan, each for 25% of total scan time
Standard reflections	3 measured every 97 reflections: 1 2 2, 2 1 0, 0 1 4
Correction from standards	min: 0.99, max: 1.02
Index ranges	$-1<h<7$, $-1<k<12$, $-1<l<21$
Reflections collected	1698

Independent reflections[a]	1542 (R_{int}=2.62%)
Observed reflections	1118 (F>2 σ(F))
<I/σ(I)>(all data)	7.82
Absorption correction	Not applied

Solution and Refinement

System used	**SHELXTL**
Wilson's statistics	$< \lvert E^2-1 \rvert > = 0.780$
Solution	Patterson interpretation and difference Fourier maps
Refinement method	Full matrix least-squares
Quantity minimized	$\Sigma[w(F_o-F_c)^2]$
Absolute configuration	Not applied
Extinction correction	$\chi=0.0004$ (3) where $F^*=F[1+0.002\ \chi\ F^2 / \mathrm{Sin}(2\theta)]^{-¼}$
Hydrogen atoms	Idealized positions and riding refinement with fixed isotropic *U*, except for the Hydrogen atom of the Hydroxyl group (H2) which was found on a Fourier difference map and refined as previous Hydrogen atoms
Restraints, constraints[(d)]	None
Weighting scheme	$w^{-1}=\sigma^2(F)+0.0007\ F^2$
Parameters refined	236
Final *R* indices (obs. Data)[(b)]	*R* = 7.51%, *wR*=6.65%
Final *R* indices (all data)[(b)]	*R* = 11.14%, *wR*=7.37%
Goodness-of-fit[(c)]	1.22
Largest and mean Δ/σ	0.097, 0.026
Data-to-parameters ratio	4.7/1
Largest difference peak	0.38 eÅ^{-3}
Largest difference hole	-0.28 e.Å^{-3}

Table S4. Atomic coordinates (x 10^4) and equivalent isotropic displacement coefficients ($Å^2$ x 10^3)

Atom	*X/a*	*Y/b*	*Z/c*	*U(eq)*
O(1)	-4190(8)	10350(5)	4465(3)	59(3)
O(2)	1912(8)	9831(5)	4619(3)	66(3)
O(3)	2330(9)	11875(5)	4317(3)	65(3)
N(1)	-3870(10)	12393(7)	4133(3)	48(3)
C(1)	754(15)	11591(9)	4334(4)	54(4)
C(2)	425(12)	10388(9)	4518(5)	54(4)
C(3)	-1189(11)	9954(9)	4569(4)	43(4)
C(4)	-2660(13)	10674(8)	4428(4)	40(4)
C(5)	-2342(13)	11899(8)	4239(4)	48(4)
C(6)	-683(12)	12327(8)	4220(4)	42(4)
C(7)	-175(12)	13520(8)	4064(5)	65(4)
C(8)	-1551(13)	8747(8)	4798(5)	66(5)
C(9)	-718(16)	7832(10)	4400(6)	92(5)
C(10)	-1338(19)	7641(13)	3805(5)	139(8)
C(11)	-643(17)	6597(11)	3459(69	86(6)
C(12)	-769(15)	6428(10)	2854(6)	65(5)
C(13)	47(13)	5442(8)	2528(5)	77(4)
C(14)	-1766(17)	7186(10)	2424(5)	104(6)
C(15)	-1053(16)	8617(9)	5483(5)	95(5)
C(16)	-4277(12)	13512(8)	3897(4)	50(4)
C(17)	-4218(12)	13643(10)	3185(5)	48(4)
C(18)	-3466(14)	12849(8)	2801(5)	56(4)
C(19)	-3440(14)	12993(9)	2142(5)	60(4)
C(20)	-4178(15)	13908(10)	882(6)	70(5)
C(21)	-4900(14)	14691(10)	2249(6)	77(5)
C(22)	-4927(14)	14575(10)	2903(6)	69(5)

Equivalent isotropic U defined as one third of the trace of the orthogonalized U_{ij} tensor

Table S5. Bond lengths (Å)

O(1)-C(4)	1.223(12)	O(2)-C(2)	1.325(12)
O(3)-C(1)	1.240(13)		
N(1)-C(5)	1.318(13)	N(1)-C(16)	1.462(12)
C(1)-C(2)	1.512(15)	C(1)-C(6)	1.420(14)
C(2)-C(3)	1.331(13)	C(3)-C(4)	1.439(13)
C(3)-C(8)	1.548(14)	C(4)-C(5)	1.538(13)
C(5)-C(6)	1.356(13)	C(6)-C(7)	1.514(14)
C(8)-C(9)	1.519(16)	C(8)-C(15)	1.510(16)
C(9)-C(10)	1.364(17)	C(10)-C(11)	1.541(20)
C(11)-C(12)	1.302(19)	C(12)-C(113)	1.501(15)
C(12)-C(14)	1.490(1)	C(16)-C(17)	1.518(14)
C(17)-C(18)	1.374(15)	C(17)-C(22)	1.375(16)
C(18)-C(19)	1.409(15)	C(19)-C(20)	1.347(16)
C(20)-C(21)	1.336(17)	C(21)-C(22)	1.392(18)

Hydrogen bonds:

O(3) ...H(1A)	2.165
O(1) ...H(2)	2.105

Table S6. Bond angles (°).

C(5)-N(1)-C(16)	139.9(8)	O(3)-C(1)-C(2)	115.3(9)
O(3)-C(1)-C(6)	124.1(10)	C(2)-C(1)-C(6)	120.6(9)
O(2)-C(2)-C(1)	112.4(8)	O(2)-C(2)-C(3)	124.7(9)
C(1)-C(2)-C(3)	122.9(9)	C(2)-C(3)-C(4)	117.3(9)
C(2)-C(3)-C(8)	123.5(9)	C(4)-C(3)-C(8)	119.2(8)
O(1)-C(4)C(3)	121.9(8)	O(1)-C(4)-C(5)	117.8(8)
C(3)-C(4)-C(5)	120.3(8)	N(1)-C(5)-C(4)	109.6(8)
N(1)-C(5)-C(6)	129.5(9)	C(4)-C(5)-C(6)	120.8(9)
C(1)-C(6)-C(5)	117.9(9)	C(1)-C(6)-C(7)	115.4(8)
C(5)-C(6)-C(7)	126.7(9)	C(3)-C(8)-C(9)	115.1(9)
C(3)-C(8)-C(15)	110.7(8)	C(9)-C(8)-C(15)	110.9(9)
C(8)-C(9)-C(10)	119.5(11)	C(9)-C(10)-C(11)	117.4(12)
C(10)-C(11)C(12)	124.8(12)	C(11)-C(12)-C(13)	123.2(11)
C(11)-C(12)-C(14)	123.0(11)	C(13)-C(12)-C(14)	113.8(11)
N(1)-C(16)-C(17)	115.4(8)	C(16)-C(17)-C(18)	122.0(10)
C(16)-C(17)-C(22)	120.3(10)	C(18)-C(17)-C(22)	117.6(10)
C(17)-C(18)-C(19)	120.6(9)	C(18)-C(19)-C(20)	120.0(10)
C(19)-C(20)-C(21)	120.0(11)	C(20)-C(21)-C(22)	121.1(11)
C(17)-C(22)-C(21)	120.6(10)		

Table S7. Anisotropic displacement coefficients ($Å^2 \times 10^3$)

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O(1)	37(4)	58(5)	81(5)	-1(4)	-4(4)	3(4)
O(2)	40(4)	78(5)	82(5)	11(4)	0(4)	2(4)
O(3)	43(4)	80(5)	71(5)	-6(4)	-6(4)	18(4)
N(1)	41(5)	48(6)	56(5)	-1(4)	-13(5)	13(5)
C(1)	33(6)	78(8)	51(8)	-6(7)	-1(6)	2(7)
C(2)	41(7)	63(8)	58(7)	10(7)	-7(6)	11(7)
C(3)	39(6)	49(7)	42(7)	9(6)	12(6)	-8(5)
C(4)	46(7)	49(7)	27(6)	-14(6)	10(6)	0(5)
C(5)	39(6)	68(8)	37(6)	8(6)	-5(6)	-16(6)
C(6)	31(6)	55(7)	40(6)	0(6)	4(5)	-4(6)
C(7)	41(6)	68(7)	84(9)	-5(6)	-13(6)	7(7)
C(8)	48(7)	66(8)	83(9)	1(7)	1(7)	-3(8)
C(9)	66(8)	98(9)	111(11)	17(8)	-4(9)	-9(10)
C(10)	123(13)	235(20)	59(9)	89(15)	15(9)	-22(11)
C(11)	100(11)	93(10)	65(9)	4(9)	9(9)	-23(8)
C(12)	56(7)	57(8)	81(10)	-10(7)	23(8)	-4(8
C(13)	84(8)	45(7)	102(8)	-9(7)	14(8)	-6(7)
C(14)	99(10)	122(11)	92(9)	15(10)	-18(9)	-17(9)
C(15)	99(9)	77(8)	110(11)	-18(8)	-4(9)	54(8)
C(16)	47(6)	56(7)	47(7)	5(7)	8(6)	-5(6)
C(17)	40(6)	48(7)	55(7)	3(6)	4(6)	5(7)
C(18)	61(7)	43(7)	64(8)	1(6)	-7(7)	3(6)
C(19)	60(7)	58(9)	62(8)	0(7)	-7(7)	-23(7)
C(20)	77(8)	60(8)	73(8)	5(7)	-9(8)	1(8)
C(21)	90(9)	57(8)	85(11)	17(8)	5(9)	7(8)
C(22)	86(9)	60(8)	62(9)	20(8)	4(8)	-17(7)

The anisotropic displacement exponent takes the form: $-2\pi^2(h^2 a^{*2} U_{11} + ... + 2hkabU_{12})$

Table S8. H-Atom coordinates (x 10^4) and isotropic displacement coefficients ($Å^2$ x 10^3)

Atom	*X/a*	*Y/b*	*Z/c*	*U(eq)*
H(2)	3237	9832	4707	80
H(1A)	-4825	11972	4220	80
H(7A)	-1223	13955	3995	80
H(7B)	487	13834	4407	80
H(7C)	536	13524	3689	80
H(8A)	-2807	8639	4774	80
H(9A)	-820	7146	4632	80
H(9B)	520	7996	4364	80
H(10A)	-2602	7579	3830	80
H(10B)	-1077	8285	3552	80
H(11A)	-67	6033	3707	80
H(13A)	669	4990	2829	80
H(13B)	-868	5005	2333	80
H(13C)	856	5700	2211	80
H(14A)	-2248	7796	2663	80
H(14B)	-985	7471	2106	80
H(14C)	-2709	6777	2228	80
H(15A)	-1286	7865	5617	80
H(15B)	182	8778	5536	80
H(15C)	-1737	9126	5734	80
H(16A)	-3452	14029	4080	80
H(16B)	-543	13717	4041	80
H(18A)	-2959	12189	2984	80
H(19A)	-2894	12441	1877	80
H(20A)	-4187	13999	1432	80
H(21A)	-5411	15345	2060	80
H(22A)	-5442	15152	3158	80

Table S9. Dependence of the density at bond critical point as a function of C_6-N-C_1'-C_6' dihedral angle (degrees).

Bond/dihedral angle.	0	10	20	27.94	30	40	50	60	70	80	90
C_1-C_6	0.2565	0.2578	0.2582	0.2584	0.2585	0.2588	0.2592	0.2569	0.2599	0.2600	0.2601
C_6-C_5	0.3251	0.3257	0.3258	0.3259	0.326	0.3264	0.3269	0.3274	0.3277	0.3276	0.3269
C_4-C_5	0.2870	0.2871	0.2873	0.2874	0.2874	0.2875	0.2876	0.2877	0.2879	0.2881	0.2887
C_4-C_3	0.2602	0.2595	0.2592	0.2589	0.2588	0.2585	0.2583	0.2579	0.2576	0.2572	0.2567
C_2-C_3	0.3345	0.3342	0.3341	0.3341	0.3340	0.3340	0.3339	0.3339	0.3339	0.3338	0.3337
C_1-C_2	0.2875	0.2873	0.2873	0.2873	0.2873	0.2872	0.2870	0.2869	0.2868	0.2868	0.2870
C_1-O	0.3926	0.3928	0.3929	0.3930	0.3930	0.3931	0.3932	0.3933	0.3934	0.3934	0.3933
C_4-O	0.3978	0.3980	0.3979	0.3979	0.3979	0.3980	0.3980	0.3980	0.3981	0.3980	0.3978
C_3-O	0.2840	0.3060	0.3059	0.3058	0.3059	0.3058	0.3057	0.3056	0.3055	0.3054	0.3053
N-H	0.3387	0.3387	0.3387	0.3387	0.3388	0.3388	0.3388	0.3387	0.3384	0.3380	0.3374
C_6-N	0.3184	0.3190	0.3194	0.3196	0.3197	0.3198	0.3199	0.3202	0.3209	0.3219	0.3238
N-C_1	0.2914	0.2908	0.2905	0.2900	0.2898	0.2888	0.2874	0.2856	0.2834	0.2812	0.2795
H_5-H_6	0.0151	0.0133	0.0122	0.0112	0.0109	0.0096					
NH-O	0.0282	0.0277	0.0271	0.0235	0.0264	0.0257	0.0251	0.0243	0.0237	0.0232	0.0229

Cartesian Coordinates and Energies (Hartrees) of calculated compounds and conformations.

OMe-ABQ R1 = H, R2 = OMe (Figure 7)

C	-0.3753	0.0000	-3.3774
C	-0.4441	0.0000	-1.9518
C	0.7151	0.0000	-1.2097
C	2.0916	0.0000	-1.9041
C	2.1423	0.0000	-3.3451
C	0.9832	0.0000	-4.0477
O	-1.3446	0.0000	-4.1540
H	-1.4351	0.0000	-1.5260
N	0.8917	0.0000	0.1263
O	3.0956	0.0000	-1.1882
H	1.8939	0.0000	0.3338
C	0.0434	0.0000	1.2434
C	-1.3621	0.0000	1.2012
C	-2.0977	0.0000	2.3783
C	-1.4642	0.0000	3.6281
C	0.6700	0.0000	2.4999
C	-0.0645	0.0000	3.6812
H	-1.8970	0.0000	0.2642
H	-3.1819	0.0000	2.3484
O	-2.2858	0.0000	4.7145
H	1.7557	0.0000	2.5531
H	0.4616	0.0000	4.6277
C	-1.6938	0.0000	6.0057
H	-2.5218	0.0000	6.7154
H	-1.0791	-0.8943	6.1683
H	-1.0791	0.8943	6.1683
H	3.1138	0.0000	-3.8231
O	0.9020	0.0000	-5.3707
H	-0.0740	0.0000	-5.5394

Energy: =-857.65195

Me-ABQ R1 = H, R2 = Me (Figure 7)

C	-0.4749	0.0000	-2.9802
C	-0.5420	0.0000	-1.5527
C	0.6169	0.0000	-0.8128
C	1.9922	0.0000	-1.5105
C	2.0413	-0.0000	-2.9521
C	0.8819	-0.0000	-3.6535
O	-1.4466	-0.0001	-3.7523
H	-1.5331	-0.0000	-1.1271
N	0.7953	0.0000	0.5243
O	2.9970	-0.0000	-0.7967
H	1.7972	0.0000	0.7321
C	-0.0527	0.0000	1.6410
C	-1.4558	0.0000	1.5972
C	-2.1873	0.0000	2.7821
C	-1.5702	0.0000	4.0391
C	0.5774	0.0000	2.8978
C	-0.1698	0.0000	4.0689
H	-1.9898	0.0000	0.6596
H	-3.2726	0.0000	2.7208
C	-2.3886	0.0000	5.3073
H	1.6632	0.0000	2.9501
H	0.3469	0.0000	5.0248
H	-1.7498	0.0000	6.1944
H	-3.0379	0.8811	5.3636
H	-3.0379	-0.8811	5.3636
H	3.0127	-0.0000	-3.4306
O	0.7995	0.0000	-4.9766
H	-0.1757	0.0001	-5.1466

Energy: =-782.44815

ABQ R1 = H, R2 = H (Figure 7)

C	-0.6606	0.0000	-2.5874
C	-0.7249	0.0000	-1.1587

C	0.4343	0.0000	-0.4213
C	1.8085	0.0000	-1.1222
C	1.8548	-0.0000	-2.5642
C	0.6945	-0.0000	-3.2637
O	-1.6344	-0.0001	-3.3558
H	-1.7153	-0.0000	-0.7318
N	0.6157	0.0000	0.9164
O	2.8144	-0.0000	-0.4104
H	1.6181	0.0000	1.1218
C	-0.2295	0.0000	2.0350
C	-1.6323	0.0000	1.9908
C	-2.3629	0.0000	3.1792
C	-1.7251	0.0000	4.4183
C	0.4113	0.0000	3.2891
C	-0.3287	0.0000	4.4643
H	-2.1659	0.0000	1.0532
H	-3.4474	0.0000	3.1261
H	-2.3055	0.0000	5.3352
H	1.4974	0.0000	3.3312
H	0.1880	0.0000	5.4192
H	2.8253	-0.0000	-3.0442
O	0.6105	0.0000	-4.5867
H	-0.3642	0.0001	-4.7573

Energy: =--743.12730

F-ABQ R1 = H, R2 = F (Figure 7)

HF=-842.357379

C	-0.4966	0.0000	-2.9573
C	-0.5622	0.0000	-1.5285
C	0.5970	0.0000	-0.7909
C	1.9717	0.0000	-1.4906
C	2.0192	-0.0000	-2.9319
C	0.8592	-0.0000	-3.6323

O	-1.4699	-0.0001	-3.7261
H	-1.5538	-0.0000	-1.1039
N	0.7795	0.0000	0.5464
O	2.9765	-0.0000	-0.7768
H	1.7826	0.0000	0.7495
C	-0.0659	0.0000	1.6645
C	-1.4691	0.0000	1.6198
C	-2.2092	0.0000	2.8014
C	-1.5512	0.0000	4.0233
C	0.5719	0.0000	2.9207
C	-0.1620	0.0000	4.0990
H	-2.0022	0.0000	0.6823
H	-3.2932	0.0000	2.7771
F	-2.2719	0.0000	5.1619
H	1.6574	0.0000	2.9675
H	0.3258	0.0000	5.0671
H	2.9901	-0.0000	-3.4114
O	0.7765	0.0000	-4.9551
H	-0.1978	0.0001	-5.1275

Energy: =-842.35738

CF_3-ABQ R1 = H, R2 = CF_3 (Figure 7)

C	-0.0477	0.0000	-3.9262
C	-0.1090	0.0000	-2.4939
C	1.0501	0.0000	-1.7616
C	2.4222	0.0000	-2.4666
C	2.4657	0.0000	-3.9085
C	1.3047	0.0000	-4.6066
O	-1.0255	0.0000	-4.6864
H	-1.1001	0.0000	-2.0683
N	1.2391	0.0000	-0.4215
O	3.4285	0.0000	-1.7558
H	2.2434	0.0000	-0.2239
C	0.4007	0.0000	0.6964
C	-1.0042	0.0000	0.6541

C	-1.7332	0.0000	1.8382
C	-1.0908	0.0000	3.0780
C	1.0407	0.0000	1.9505
C	0.3049	0.0000	3.1269
H	-1.5397	0.0000	-0.2819
H	-2.8174	0.0000	1.7928
C	-1.9205	0.0000	4.3310
H	2.1263	0.0000	1.9948
H	0.8134	0.0000	4.0838
F	-1.1613	0.0000	5.4468
F	-2.7286	1.0843	4.3905
F	-2.7286	-1.0843	4.3905
H	3.4359	0.0000	-4.3901
O	1.2199	0.0000	-5.9293
H	0.2473	0.0000	-6.1046

Energy: =-1080.16221

CN-ABQ R1 = H, R2 = CN (Figure 7)

C	-0.3905	0.0000	-3.1928
C	-0.4543	0.0000	-1.7588
C	0.7031	0.0000	-1.0261
C	2.0759	0.0000	-1.7289
C	2.1222	-0.0000	-3.1706
C	0.9626	-0.0000	-3.8712
O	-1.3684	-0.0001	-3.9515
H	-1.4468	-0.0000	-1.3359
N	0.8922	0.0000	0.3159
O	3.0805	0.0000	-1.0158
H	1.8971	0.0000	0.5121
C	0.0562	0.0000	1.4315
C	-1.3488	0.0000	1.3910
C	-2.0800	0.0000	2.5730
C	-1.4368	0.0000	3.8196
C	0.6992	0.0000	2.6873
C	-0.0307	0.0000	3.8626

H	-1.8848	0.0000	0.4554
H	-3.1637	0.0000	2.5309
C	-2.2001	0.0000	5.0305
H	1.7848	0.0000	2.7291
H	0.4790	0.0000	4.8197
N	-2.8192	0.0000	6.0158
H	3.0931	-0.0000	-3.6502
O	0.8818	-0.0000	-5.1940
H	-0.0892	0.0001	-5.3755

Energy: =-835.36797

NO_2-ABQ R1 = H, R2 = NO_2 (Figure 7)

C	-0.0997	0.1735	-3.4757
C	-0.1597	0.1481	-2.0413
C	1.0020	0.1569	-1.3175
C	2.3720	0.2356	-2.0124
C	2.4161	0.2400	-3.4547
C	1.2554	0.2071	-4.1535
O	-1.0763	0.1749	-4.2349
H	-1.1437	0.1530	-1.5940
N	1.1679	0.1464	0.0284
O	3.3711	0.2952	-1.2949
H	2.1540	0.2730	0.2661
C	0.2651	0.0070	1.0842
C	-0.9757	-0.6434	0.9594
C	-1.8117	-0.7640	2.0627
C	-1.4067	-0.2440	3.2897
C	0.6605	0.5069	2.3407
C	-0.1706	0.3846	3.4427
H	-1.2704	-1.0913	0.0205
H	-2.7677	-1.2665	1.9892
N	-2.2946	-0.3696	4.4493
H	1.6208	1.0039	2.4395
H	0.1144	0.7706	4.4131
O	-3.3823	-0.9212	4.2792

O	-1.8982	0.0841	5.5234
H	3.3849	0.2839	-3.9374
O	1.1741	0.2151	-5.4763
H	0.2037	0.2004	-5.6588

Energy: =-794.62737

OMe-ABQm R1 = Me, R2 = OMe (Figure 7)

C	-0.6454	0.0000	-3.0017
C	-0.6139	0.0000	-1.5540
C	0.5609	0.0000	-0.8525
C	1.8873	0.0000	-1.6050
C	1.8667	0.0000	-3.0539
C	0.6892	0.0000	-3.7303
O	-1.6857	0.0000	-3.6535
H	-1.5897	0.0000	-1.0940
N	0.7925	0.0000	0.4840
O	2.9375	0.0000	-0.9592
H	1.7980	0.0000	0.6580
C	-0.0184	0.0000	1.6263
C	-1.4249	0.0000	1.6276
C	-2.1256	0.0000	2.8266
C	-1.4565	0.0000	4.0566
C	0.6435	0.0000	2.8650
C	-0.0563	0.0000	4.0676
H	-1.9872	0.0000	0.7068
H	-3.2103	0.0000	2.8278
O	-2.2470	0.0000	5.1689
H	1.7304	0.0000	2.8867
H	0.4977	0.0000	4.9984
C	-1.6153	0.0000	6.4397
H	-2.4200	0.0000	7.1759
H	-0.9951	-0.8940	6.5837
H	-0.9951	0.8940	6.5837
H	2.8353	0.0000	-3.5378
O	0.5402	0.0000	-5.0547

C	1.7138	0.0000	-5.8669
H	2.3183	0.8944	-5.6804
H	2.3183	-0.8944	-5.6804
H	1.3614	0.0000	-6.8978

Energy: =-896.94255

Me-ABQm R1 = Me, R2 = Me (Figure 7)

C	-0.6604	0.0000	-2.6237
C	-0.6696	0.0000	-1.1744
C	0.4841	0.0000	-0.4409
C	1.8309	0.0000	-1.1576
C	1.8510	0.0000	-2.6067
C	0.6932	0.0000	-3.3160
O	-1.6829	0.0000	-3.3020
H	-1.6583	0.0000	-0.7426
N	0.6793	0.0000	0.9027
O	2.8623	0.0000	-0.4829
H	1.6796	0.0000	1.1044
C	-0.1616	0.0000	2.0217
C	-1.5655	0.0000	1.9838
C	-2.2940	0.0000	3.1709
C	-1.6745	0.0000	4.4263
C	0.4704	0.0000	3.2781
C	-0.2740	0.0000	4.4510
H	-2.1016	0.0000	1.0475
H	-3.3796	0.0000	3.1117
H	1.5564	0.0000	3.3284
H	0.2458	0.0000	5.4054
H	2.8331	0.0000	-3.0625
O	0.5804	0.0000	-4.6437
C	1.7764	0.0000	-5.4232
H	2.3752	0.8946	-5.2197
H	2.3752	-0.8946	-5.2197
H	1.4525	0.0000	-6.4634
C	-2.4883	0.0000	5.6977

H	-3.1375	0.8810	5.7582
H	-3.1375	-0.8810	5.7582
H	-1.8454	0.0000	6.5820

Energy: =-821.73910

F-ABQm R1 = Me, R2 = F (Figure 7)

C	-0.7326	0.0001	-2.5874
C	-0.7116	0.0001	-1.1371
C	0.4575	0.0000	-0.4297
C	1.7891	-0.0000	-1.1749
C	1.7786	-0.0001	-2.6237
C	0.6059	0.0000	-3.3084
O	-1.7696	0.0002	-3.2424
H	-1.6918	0.0002	-0.6863
N	0.6838	-0.0000	0.9097
O	2.8336	-0.0001	-0.5209
H	1.6890	-0.0000	1.0863
C	-0.1318	-0.0000	2.0466
C	-1.5362	-0.0001	2.0358
C	-2.2491	-0.0001	3.2347
C	-1.5644	0.0000	4.4411
C	0.5331	0.0001	3.2893
C	-0.1738	0.0001	4.4841
H	-2.0903	-0.0003	1.1106
H	-3.3334	-0.0002	3.2344
F	-2.2591	0.0000	5.5976
H	1.6195	0.0002	3.3117
H	0.3365	0.0002	5.4407
H	2.7507	-0.0002	-3.1007
O	0.4645	-0.0000	-4.6328
C	1.6434	-0.0001	-5.4385
H	2.2464	0.8944	-5.2479
H	2.2462	-0.8948	-5.2479
H	1.2968	-0.0001	-6.4712

Energy: =-881.64866

CF_3-ABQm R1 = Me, R2 = CF_3 (Figure 7)

C	-0.3154	0.0000	-3.5764
C	-0.2896	0.0000	-2.1232
C	0.8801	0.0000	-1.4217
C	2.2088	0.0000	-2.1721
C	2.1936	0.0000	-3.6211
C	1.0193	0.0000	-4.3030
O	-1.3563	0.0000	-4.2229
H	-1.2687	0.0000	-1.6702
N	1.1125	0.0000	-0.0796
O	3.2547	0.0000	-1.5210
H	2.1187	0.0000	0.0920
C	0.3053	0.0000	1.0570
C	-1.1010	0.0000	1.0521
C	-1.8001	0.0000	2.2544
C	-1.1280	0.0000	3.4783
C	0.9748	0.0000	2.2968
C	0.2689	0.0000	3.4906
H	-1.6599	0.0000	0.1298
H	-2.8852	0.0000	2.2348
C	-1.9228	0.0000	4.7523
H	2.0612	0.0000	2.3145
H	0.8015	0.0000	4.4344
F	-1.1328	0.0000	5.8474
F	-2.7299	1.0842	4.8371
F	-2.7299	-1.0842	4.8371
H	3.1644	0.0000	-4.1004
O	0.8722	0.0000	-5.6263
C	2.0478	0.0000	-6.4379
H	2.6510	0.8947	-6.2497
H	2.6510	-0.8947	-6.2497
H	1.6960	0.0000	-7.4687

Energy: =-1119.45424

CN-ABQm R1 = Me, R2 = CN (Figure 7)

C	-0.6356	0.0003	-2.8220
C	-0.6128	0.0002	-1.3670
C	0.5552	0.0001	-0.6649
C	1.8853	0.0001	-1.4129
C	1.8732	-0.0000	-2.8613
C	0.7002	0.0000	-3.5459
O	-1.6758	-0.0000	-3.4682
H	-1.5936	0.0001	-0.9169
N	0.7879	0.0001	0.6791
O	2.9290	0.0000	-0.7582
H	1.7952	0.0001	0.8473
C	-0.0171	0.0000	1.8130
C	-1.4235	-0.0000	1.8080
C	-2.1261	-0.0001	3.0071
C	-1.4545	-0.0000	4.2387
C	0.6543	0.0001	3.0551
C	-0.0474	0.0000	4.2469
H	-1.9814	-0.0001	0.8852
H	-3.2106	-0.0001	2.9901
C	-2.1881	-0.0001	5.4674
H	1.7406	0.0001	3.0713
H	0.4853	0.0001	5.1916
N	-2.7827	-0.0001	6.4679
H	2.8447	-0.0001	-3.3394
O	0.5552	-0.0001	-4.8686
C	1.7315	-0.0003	-5.6796
H	2.3344	0.8945	-5.4911
H	2.3342	-0.8953	-5.4909
H	1.3799	-0.0004	-6.7104

Energy: =-874.66038

NO_2-ABQm R1 = Me, R2 = NO_2 (Figure 7)

C	-0.3469	0.1101	-3.1387
C	-0.3341	0.1238	-1.6835
C	0.8317	0.1391	-0.9797
C	2.1662	0.1897	-1.7103
C	2.1653	0.1511	-3.1590
C	0.9970	0.1047	-3.8508
O	-1.3805	0.1098	-3.7947
H	-1.3101	0.1525	-1.2198
N	1.0296	0.1636	0.3705
O	3.1989	0.2646	-1.0434
H	2.0172	0.2998	0.5858
C	0.1563	0.0385	1.4472
C	-1.1084	-0.5732	1.3571
C	-1.9126	-0.6801	2.4847
C	-1.4570	-0.1847	3.7044
C	0.6016	0.5150	2.6980
C	-0.1981	0.4064	3.8232
H	-1.4474	-1.0019	0.4247
H	-2.8851	-1.1533	2.4350
N	-2.3108	-0.2955	4.8878
H	1.5787	0.9830	2.7726
H	0.1279	0.7750	4.7875
O	-3.4195	-0.8144	4.7484
O	-1.8696	0.1367	5.9543
H	3.1391	0.1713	-3.6316
O	0.8618	0.0643	-5.1741
C	2.0439	0.0633	-5.9772
H	2.6261	0.9766	-5.8133
H	2.6640	-0.8122	-5.7558
H	1.6996	0.0230	-7.0097

Energy: =-956.91991

ABQm R_1 = Me R_2 = H .$C_{6'}$-N-C_1-C_6 dihedral angle = 0 degrees (Figure 7)

C	-0.8691	0.0000	-2.2192

C	-0.8574	0.0001	-0.7689
C	0.3067	-0.0001	-0.0534
C	1.6429	-0.0002	-0.7902
C	1.6418	-0.0002	-2.2395
C	0.4739	-0.0000	-2.9317
O	-1.9018	0.0004	-2.8812
H	-1.8397	0.0003	-0.3231
N	0.5227	-0.0001	1.2879
O	2.6836	-0.0003	-0.1306
H	1.5261	-0.0001	1.4736
C	-0.3004	-0.0000	2.4195
C	-1.7043	-0.0002	2.3995
C	-2.4159	-0.0001	3.5997
C	-1.7597	0.0001	4.8289
C	0.3588	0.0002	3.6649
C	-0.3624	0.0003	4.8515
H	-2.2519	-0.0004	1.4701
H	-3.5012	-0.0003	3.5632
H	-2.3253	0.0001	5.7550
H	1.4456	0.0003	3.6901
H	0.1700	0.0004	5.7979
H	2.6172	-0.0002	-2.7097
O	0.3410	0.0000	-4.2574
C	1.5249	-0.0000	-5.0555
H	2.1268	0.8946	-4.8614
H	2.1267	-0.8947	-4.8615
H	1.1848	0.0001	-6.0905

Energy: =-782.4185212

ABQm R_1 = Me R_2 = H .C_6-N-C_1-C_6 dihedral angle = 10 degrees (Figure 7)

C	1.9274	-1.3280	-0.1909
C	0.5249	-0.9603	-0.2210
C	0.1151	0.3362	-0.0881
C	1.1470	1.4481	0.0489

C	2.5510	1.0901	0.0987
C	2.9391	-0.2076	-0.0003
O	2.3241	-2.4813	-0.3203
H	-0.1555	-1.7821	-0.3904
N	-1.1401	0.8564	-0.1039
O	0.7561	2.6146	0.1159
H	-1.1020	1.8746	-0.0687
C	-2.4151	0.2817	-0.0168
C	-2.6571	-1.0600	0.3173
C	-3.9681	-1.5321	0.3839
C	-5.0500	-0.6929	0.1224
C	-3.5095	1.1291	-0.2719
C	-4.8102	0.6453	-0.2007
H	-1.8421	-1.7233	0.5688
H	-4.1381	-2.5710	0.6505
H	-6.0653	-1.0727	0.1729
H	-3.3272	2.1683	-0.5329
H	-5.6398	1.3164	-0.4021
H	3.2429	1.9148	0.2146
O	4.1909	-0.6623	0.0385
C	5.2487	0.2823	0.2034
H	5.2684	0.9954	-0.6281
H	5.1429	0.8262	1.1487
H	6.1685	-0.3012	0.2127

Energy: -782.41922

ABQm R_1 = Me R_2 = H .C_6-N-C_1-C_6 dihedral angle = 20 degrees (Figure 7)

C	1.9023	-1.3254	-0.2021
C	0.5041	-0.9426	-0.1950
C	0.1132	0.3572	-0.0400
C	1.1580	1.4569	0.0901
C	2.5585	1.0828	0.1086
C	2.9298	-0.2176	-0.0173
O	2.2848	-2.4806	-0.3550
H	-0.1935	-1.7526	-0.3535

N	-1.1376	0.8864	-0.0204
O	0.7798	2.6261	0.1773
H	-1.0992	1.9042	0.0115
C	-2.4110	0.3002	0.0132
C	-2.6522	-1.0172	0.4334
C	-3.9569	-1.5100	0.4527
C	-5.0324	-0.7117	0.0651
C	-3.4983	1.1077	-0.3655
C	-4.7940	0.6047	-0.3374
H	-1.8408	-1.6407	0.7831
H	-4.1284	-2.5299	0.7837
H	-6.0432	-1.1066	0.0807
H	-3.3144	2.1283	-0.6906
H	-5.6201	1.2431	-0.6361
H	3.2621	1.8983	0.2200
O	4.1773	-0.6860	-0.0116
C	5.2484	0.2447	0.1454
H	5.2606	0.9682	-0.6773
H	5.1665	0.7774	1.0993
H	6.1618	-0.3489	0.1297

Energy: -782.41960

ABQm R_1 = Me R_2 = H .C_6-N-C_1-C_6 dihedral angle = 27.94 degrees. (Figure 7)

C	0.0046	0.0909	0.0866
C	0.0588	0.1217	1.5345
C	1.2447	0.0810	2.2112
C	2.5601	0.0379	1.4467
C	2.5168	-0.0190	-0.0014
C	1.3287	-0.0037	-0.6594
O	-1.0416	0.1428	-0.5514
H	-0.8980	0.2070	2.0309
N	1.4708	0.1098	3.5501
C	3.6156	0.0539	2.0817
H	2.4667	0.1773	3.7528
C	0.5917	0.0875	4.6443

C	-0.6733	-0.5185	4.6015
C	-1.4770	-0.5253	5.7411
C	-1.0370	0.0522	6.9320
C	1.0393	0.6573	5.8483
C	0.2310	0.6364	6.9801
H	-1.0129	-1.0138	3.7013
H	-2.4530	-0.9992	5.6947
H	-1.6703	0.0426	7.8132
H	2.0204	1.1232	5.8840
H	0.5918	1.0842	7.9012
H	3.4766	-0.0655	-0.5004
O	1.1578	-0.0535	-1.9801
C	2.3171	-0.1355	-2.8092
H	2.9573	0.7431	-2.6732
H	2.8908	-1.0428	-2.5900
H	1.9474	-0.1693	-3.8335

Energy: -782.41967

ABQm R_1 = Me R_2 = H C_6-N-C_1-C_6 dihedral angle = 30 degrees (Figure 7)

C	1.8733	-1.3240	-0.2051
C	0.4808	-0.9246	-0.1608
C	0.1111	0.3787	0.0121
C	1.1702	1.4652	0.1299
C	2.5662	1.0740	0.1145
C	2.9182	-0.2295	-0.0334
O	2.2394	-2.4819	-0.3770
H	-0.2342	-1.7235	-0.3017
N	-1.1347	0.9170	0.0660
O	0.8074	2.6379	0.2323
H	-1.0955	1.9344	0.0907
C	-2.4056	0.3199	0.0434
C	-2.6577	-0.9645	0.5492
C	-3.9537	-1.4783	0.5195
C	-5.0104	-0.7274	0.0047

C	-3.4730	1.0807	-0.4623
C	-4.7626	0.5596	-0.4785
H	-1.8592	-1.5435	0.9949
H	-4.1356	-2.4731	0.9153
H	-6.0155	-1.1364	-0.0149
H	-3.2791	2.0771	-0.8502
H	-5.5754	1.1598	-0.8762
H	3.2822	1.8795	0.2193
O	4.1597	-0.7129	-0.0612
C	5.2454	0.2035	0.0785
H	5.2453	0.9359	-0.7363
H	5.1941	0.7265	1.0398
H	6.1510	-0.4005	0.0331

Energy: -782.41967

ABQm R_1 = Me R_2 = H .C_6-N-C_1-C_6 dihedral angle = 40 degrees (Figure 7)

C	1.8426	-1.3243	-0.1989
C	0.4570	-0.9079	-0.1205
C	0.1092	0.3995	0.0636
C	1.1825	1.4727	0.1647
C	2.5731	1.0645	0.1154
C	2.9047	-0.2425	-0.0485
O	2.1914	-2.4859	-0.3805
H	-0.2747	-1.6960	-0.2388
N	-1.1315	0.9457	0.1541
O	0.8358	2.6490	0.2796
H	-1.0908	1.9629	0.1659
C	-2.3989	0.3399	0.0737
C	-2.6753	-0.9036	0.6612
C	-3.9609	-1.4371	0.5816
C	-4.9850	-0.7387	-0.0590
C	-3.4326	1.0484	-0.5583
C	-4.7152	0.5112	-0.6203
H	-1.9000	-1.4345	1.2000
H	-4.1630	-2.4013	1.0385

H	-5.9836	-1.1601	-0.1147
H	-3.2191	2.0147	-1.0071
H	-5.5040	1.0691	-1.1160
H	3.3016	1.8604	0.2064
O	4.1392	-0.7408	-0.1103
C	5.2391	0.1614	0.0072
H	5.2278	0.8984	-0.8034
H	5.2180	0.6798	0.9722
H	6.1358	-0.4532	-0.0638

Energy: -782.41947

ABQm R_1 = Me R_2 = H .C_6-N-C_1-C_6 dihedral angle = 50 degrees (Figure 7)

C	1.8124	-1.3256	-0.1875
C	0.4340	-0.8926	-0.0821
C	0.1075	0.4185	0.1102
C	1.1934	1.4793	0.1926
C	2.5781	1.0549	0.1136
C	2.8902	-0.2555	-0.0606
O	2.1449	-2.4914	-0.3728
H	-0.3133	-1.6701	-0.1770
N	-1.1278	0.9713	0.2372
O	0.8613	2.6590	0.3137
H	-1.0863	1.9882	0.2356
C	-2.3908	0.3576	0.1013
C	-2.7056	-0.8336	0.7708
C	-3.9808	-1.3829	0.6458
C	-4.9580	-0.7441	-0.1190
C	-3.3763	1.0061	-0.6565
C	-4.6521	0.4570	-0.7616
H	-1.9627	-1.3126	1.3982
H	-4.2140	-2.3080	1.1643
H	-5.9505	-1.1746	-0.2082
H	-3.1321	1.9333	-1.1673
H	-5.4059	0.9664	-1.3544
H	3.3180	1.8418	0.1897

O	4.1170	-0.7686	-0.1517
C	5.2301	0.1200	-0.0580
H	5.2083	0.8597	-0.8659
H	5.2384	0.6355	0.9087
H	6.1175	-0.5050	-0.1523

Energy: -782.41894

ABQm R_1 = Me R_2 = H .C_6-N-C_1-C_6 dihedral angle = 60 degrees (Figure 7)

C	-1.7794	-1.3276	0.1755
C	-0.4090	-0.8743	0.0541
C	-0.1057	0.4413	-0.1423
C	-1.2057	1.4872	-0.2088
C	-2.5834	1.0434	-0.1098
C	-2.8740	-0.2715	0.0682
O	-2.0939	-2.4987	0.3582
H	0.3538	-1.6393	0.1299
N	1.1236	1.0018	-0.2965
O	-0.8908	2.6711	-0.3344
H	1.0807	2.0183	-0.2835
C	2.3822	0.3786	-0.1212
C	2.7486	-0.7327	-0.8923
C	4.0123	-1.2999	-0.7356
C	4.9284	-0.7500	0.1629
C	3.3047	0.9373	0.7728
C	4.5726	0.3747	0.9092
H	2.0483	-1.1378	-1.6147
H	4.2864	-2.1649	-1.3320
H	5.9139	-1.1908	0.2760
H	3.0197	1.8043	1.3618
H	5.2802	0.8132	1.6064
H	-3.3357	1.8196	-0.1741
O	-4.0918	-0.8017	0.1789
C	-5.2184	0.0714	0.1042
H	-5.1929	0.8118	0.9115
H	-5.2505	0.5864	-0.8623

H	-6.0954	-0.5656	0.2138

Energy: -782.41804

ABQm R_1 = Me R_2 = H .C_6-N-C_1-C_6 dihedral angle = 70 degrees (Figure 7)

C	-1.7471	-1.3316	0.1522
C	-0.3850	-0.8568	0.0244
C	-0.1040	0.4650	-0.1613
C	-1.2182	1.4961	-0.2078
C	-2.5885	1.0314	-0.1005
C	-2.8578	-0.2892	0.0680
O	-2.0444	-2.5091	0.3222
H	0.3926	-1.6092	0.0801
N	1.1186	1.0368	-0.3260
O	-0.9202	2.6853	-0.3226
H	1.0732	2.0528	-0.3004
C	2.3748	0.4028	-0.1321
C	2.8118	-0.5871	-1.0208
C	4.0653	-1.1722	-0.8469
C	4.9000	-0.7550	0.1917
C	3.2131	0.8259	0.9059
C	4.4733	0.2495	1.0619
H	2.1692	-0.8861	-1.8424
H	4.3961	-1.9440	-1.5352
H	5.8789	-1.2066	0.3191
H	2.8705	1.5985	1.5881
H	5.1184	0.5818	1.8696
H	-3.3529	1.7969	-0.1493
O	-4.0668	-0.8381	0.1865
C	-5.2064	0.0193	0.1320
H	-5.1824	0.7530	0.9454
H	-5.2567	0.5422	-0.8295
H	-6.0730	-0.6311	0.2457

Energy: -782.41708

ABQm R_1 = Me R_2 = H .C_6-N-C_1-C_6 dihedral angle =.80 degrees (Figure 7)

C	-1.7202	-1.3372	0.1074
C	-0.3650	-0.8405	-0.0045
C	-0.1025	0.4902	-0.1513
C	-1.2295	1.5075	-0.1716
C	-2.5935	1.0217	-0.0766
C	-2.8447	-0.3067	0.0554
O	-2.0034	-2.5231	0.2394
H	0.4244	-1.5821	0.0276
N	1.1135	1.0765	-0.3004
O	-0.9466	2.7028	-0.2567
H	1.0652	2.0917	-0.2625
C	2.3700	0.4287	-0.1209
C	2.8932	-0.3754	-1.1393
C	4.1402	-0.9787	-0.9769
C	4.8781	-0.7635	0.1885
C	3.1093	0.6463	1.0469
C	4.3630	0.0533	1.1964
H	2.3195	-0.5179	-2.0494
H	4.5404	-1.6061	-1.7676
H	5.8520	-1.2278	0.3093
H	2.6966	1.2750	1.8301
H	4.9339	0.2258	2.1038
H	-3.3683	1.7778	-0.1044
O	-4.0463	-0.8746	0.1596
C	-5.1973	-0.0314	0.1302
H	-5.1818	0.6802	0.9632
H	-5.2563	0.5168	-0.8166
H	-6.0550	-0.6962	0.2273

Energy: -782.41613

ABQm R_1 = Me R_2 = H .C_6-N-C_1-C_6 dihedral angle = 90 degrees (Figure 7)

C	1.6933	-1.3417	-0.0033
C	0.3450	-0.8177	-0.0039

C	0.1010	0.5256	-0.0013
C	1.2439	1.5255	0.0020
C	2.6011	1.0134	0.0016
C	2.8330	-0.3252	-0.0008
O	1.9627	-2.5383	-0.0046
H	-0.4572	-1.5462	-0.0058
N	-1.1075	1.1361	-0.0014
O	0.9784	2.7279	0.0053
H	-1.0524	2.1510	0.0025
C	-2.3707	0.4711	-0.0002
C	-2.9888	0.1466	1.2117
C	-4.2330	-0.4845	1.2102
C	-4.8604	-0.7933	0.0021
C	-2.9972	0.1589	-1.2112
C	-4.2415	-0.4718	-1.2073
H	-2.4903	0.3930	2.1439
H	-4.7114	-0.7336	2.1525
H	-5.8291	-1.2839	0.0028
H	-2.5049	0.4146	-2.1441
H	-4.7265	-0.7116	-2.1487
H	3.3881	1.7573	0.0037
O	4.0280	-0.9163	-0.0012
C	5.1910	-0.0893	0.0009
H	5.2216	0.5446	-0.8923
H	5.2208	0.5413	0.8964
H	6.0404	-0.7716	-0.0001

Energy: -782.41558

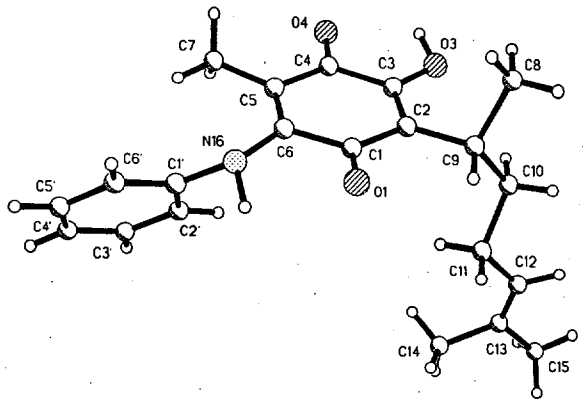

Figure S1. X-ray structure of APZ

$C_{21}H_{25}NO_3$

MW 339.4

Cryst. System Monoclinic

Space group $P2_1$

a(Å)	10.456(2)
b(Å)	7.558(2)
c(Å)	11.621(2)
α(deg)	90
β(deg)	90.8(3)
γ(deg)	90
V(Å)	918.3(5)
Z	2
Dx($mgcm^{-3}$)	1.228
F(000)	364

Reflections Collected 2136

Independent Reflections(%) 2013

(R_{int} = 16.74)

(Rint=16.74%)

Observed Reflections 981(F>3.0 sigma(F))

Absorption Coeff. 0.081mm^{-1}

Color: purple

Temperature: 293 K

Θ range: 3.0 to 45°

G-o-F on F^2 = 1.17

Final R indeces R = 6.91

[I>2σ(I)]% WR = 6.26%