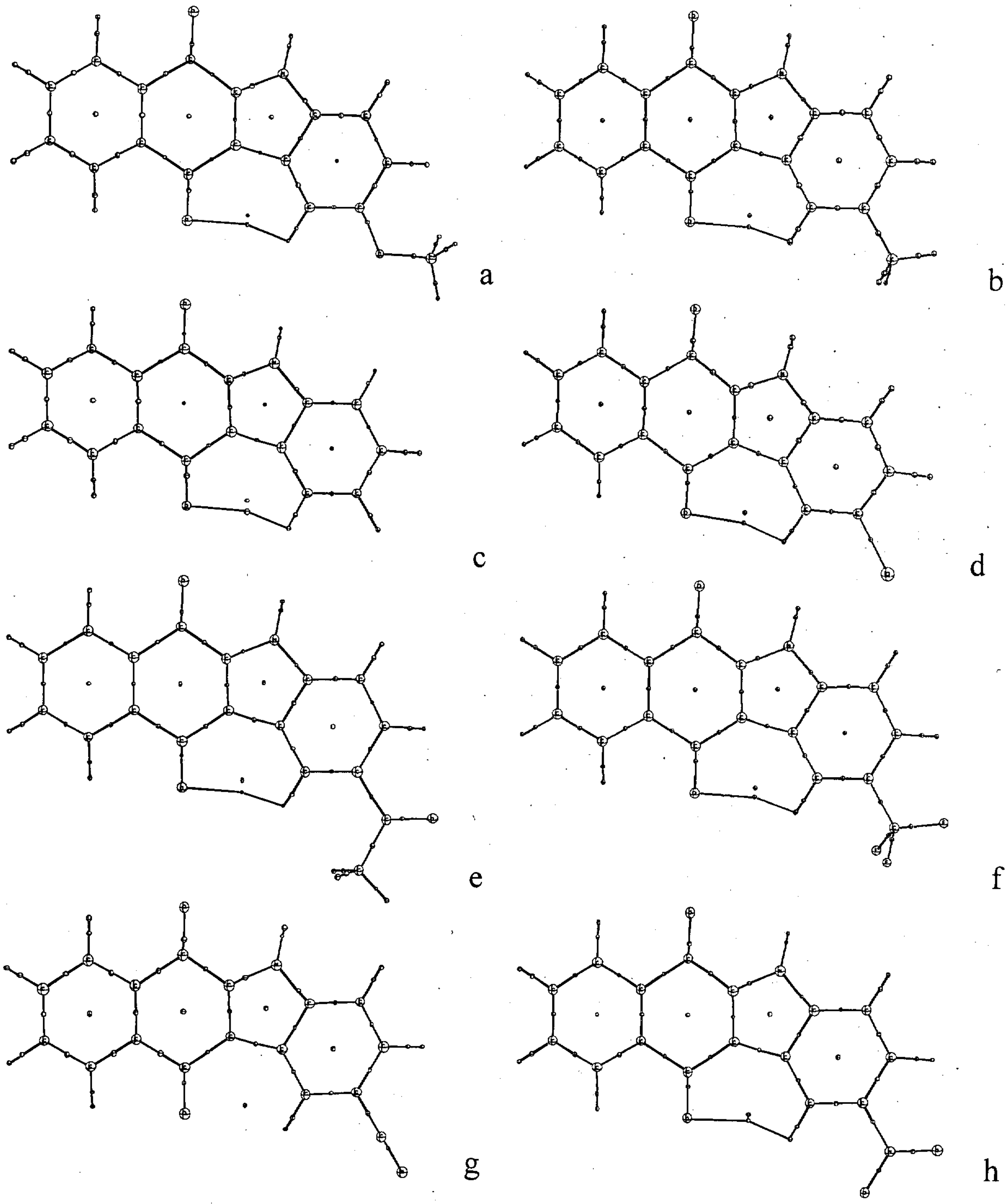

Figure S1. . Bond and ring critical points in the density of quinones: a) MeOBCD; b)MeBCD; c) BCD; d) ClBCD; e) COMeBCD; f) CF_3BCD; g) CNBCD and h) NO_2BCD. The values were obtained within the framework of the topological Theory of Atoms in Molecules at a level of B3LYP/6-31G(d,p).

Table S1. Geometry of the Quinones MeOBCD, MeBCD, BCD, ClBCD, COMeBCD, CF_3BCD, CNBCD and NO_2BCD Determined at the B3LYP/6-31G(d,p) Level of Theory. (Distances in Angstroms and angles in degrees).

Bond	OMe	Me	H	Cl	COMe	CF_3	CN	NO_2
C_1-O_1	1.229	1.230	1.230	1.229	1.229	1.229	1.228	1.228
C_1-C_2	1.462	1.461	1.461	1.463	1.463	1.464	1.465	1.465
C_2-C_3	1.388	1.387	1.386	1.386	1.384	1.384	1.383	1.382
C_3-C_4	1.457	1.459	1.459	1.460	1.460	1.461	1.462	1.463
C_4-O_2	1.229	1.229	1.229	1.228	1.229	1.228	1.228	1.227
C_4-C_{4a}	1.510	1.509	1.509	1.508	1.507	1.507	1.507	1.507
C_{4a}-C_5	1.396	1.396	1.396	1.396	1.396	1.396	1.396	1.396
C_5-C_6	1.395	1.395	1.395	1.395	1.395	1.395	1.395	1.395
C_6-C_7	1.397	1.397	1.397	1.397	1.397	1.397	1.397	1.397
C_7-C_8	1.394	1.394	1.394	1.394	1.394	1.394	1.394	1.394
C_8-C_{8a}	1.398	1.397	1.397	1.398	1.397	1.398	1.398	1.398
C_{4a}-C_{8a}	1.415	1.415	1.415	1.415	1.415	1.415	1.416	1.416
C_2-N	1.364	1.366	1.366	1.366	1.369	1.367	1.368	1.369
N-H	1.009	1.009	1.010	1.010	1.010	1.010	1.010	1.010
N-C_1'	1.385	1.384	1.383	1.382	1.380	1.381	1.379	1.378
C_3-C_6'	1.437	1.436	1.435	1.435	1.435	1.435	1.435	1.436
C_1'-C_2'	1.395	1.397	1.399	1.399	1.402	1.399	1.400	1.402

$C_{2'}$-$C_{3'}$	1.390	1.389	1.388	1.387	1.383	1.387	1.384	1.384
$C_{3'}$-$C_{4'}$	1.417	1.417	1.413	1.412	1.421	1.412	1.422	1.410
$C_{4'}$-R	1.367	1.517	1.086	1.760	1.499	1.506	1.434	1.471
$C_{1'}$-$C_{6'}$	1.427	1.426	1.426	1.426	1.426	1.427	1.427	1.428
$C_{6'}$-$C_{5'}$	1.399	1.403	1.405	1.405	1.402	1.401	1.400	1.400
$C_{5'}$-$C_{4'}$	1.393	1.393	1.387	1.385	1.394	1.390	1.397	1.386
O_1-H(N)	2.695	2.700	2.703	2.699	2.705	2.699	2.699	2.696
O_1-$H_{5'}$	2.790	2.769	2.777	2.772	2.749	2.775	2.770	2.797
O_1-C_1-C_2	121.9	121.9	121.9	121.7	121.8	121.6	121.6	121.5
C_1-C_2-C_3	125.6	125.6	125.6	125.5	125.6	125.5	125.5	125.6
C_1-C_2-N	124.4	124.5	124.6	124.6	124.7	124.5	124.5	124.5
C_2-N-H	123.2	123.2	123.2	123.2	123.2	123.2	123.2	123.2
C_2-N-$C_{1'}$	109.0	109.1	109.1	109.1	109.2	109.1	109.1	109.1
C_2-C_3-C_4	121.2	121.2	121.2	121.2	121.3	121.2	121.3	121.2
H-N-$C_{1'}$	127.8	127.7	127.6	127.8	127.6	127.7	127.7	127.7
$C_{1'}$-$C_{2'}$-$C_{3'}$	117.9	117.2	117.1	117.6	117.2	117.4	117.5	117.5
$C_{1'}$-$C_{6'}$-$C_{5'}$	120.0	119.7	119.5	119.9	119.7	119.6	119.8	119.8
C_{8a}-C_1-C_2	114.3	114.3	114.3	114.3	114.3	114.3	114.3	114.3
C_2-N-$C_{1'}$-$C_{2'}$	180.0	180.0	180.0	180.0	180.0	180.0	180.0	180.0
O_1-C_1-C_2-N	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H-N-C_2-C_1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

C_1-C_2-C_3-C_4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C_2-C_3-C_4-C_{4a}	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C_2-C_1-C_{8a}-C_8	180.0	180.0	180.0	180.0	180.0	180.0	180.0	180.0
C_{8a}-C_1-C_2-N	180.0	180.0	180.0	180.0	180.0	180.0	180.0	180.0
C_1-C_2-N-$C_{1'}$	180.0	180.0	180.0	180.0	180.0	180.0	180.0	180.0
O_1-C_2-C_4-O_2	180.0	180.0	180.0	180.0	180.0	180.0	180.0	180.0

Table S2. Wiberg Bond Indexes (WBI) and Properties of the Relevant Critical Bond Points, in the Electronic Density at the B3LYP/6-31G(*d,p*) Level for the Molecules: MeOBCD, MeBCD, BCD, ClBCD, COMeBCD, CF_3BCD, CNBCD and NO_2BCD.

R	**Bond**	**WBI**	ρ	$\nabla^2\rho$	ε
MeO	C_1-O1	1.70	0.3947	0.1028	0.0548
	C_1-C_2	1.06	0.2854	-0.7581	0.1258
	C_2-C_3	1.40	0.3208	-0.8861	0.2616
	C_3-C_4	1.08	0.2848	-0.7448	0.1271
	C_4-O	1.70	0.3952	0.1109	0.0584
	C_2-N	1.19	0.3143	-0.7395	0.1197
	N-C_1'	1.13	0.2994	-0.7416	0.1180
	C_3-C_6'	1.19	0.2870	-0.7174	0.1503
	O_2-H_5'	0.003	0.0060	0.0235	1.3236
	N-H	0.76	0.3432	-1.8595	0.0395
Me	C_1-O	1.70	0.3948	0.1034	0.0552
	C_1-C_2	1.06	0.2855	-0.7586	0.1267
	C_2-C_3	1.40	0.3213	-0.8886	0.2613
	C_3-C_4	1.08	0.2842	-0.7429	0.1237
	C_4-O	1.70	0.3953	0.1136	0.0576
	C_2-N	1.18	0.3134	-0.7465	0.1190

	N-C_1'	1.14	0.3004	-0.7428	0.1039
	C_3-C_6'	1.19	0.2873	-0.7185	0.1508
	O_2-H_5'	0.003	0.0062	0.0239	0.9054
	N-H	0.76	0.3432	-1.8595	0.0393
H	C_1-O	1.70	0.3950	0.1053	0.0555
	C_1-C_2	1.06	0.2854	-0.7579	0.1262
	C_2-C_3	1.41	0.3217	-0.8908	0.2614
	C_3-C_4	1.07	0.2839	-0.7417	0.1217
	C_4-O	1.71	0.3955	0.1165	0.0579
	C_2-N	1.18	0.3131	-0.7472	0.1183
	N-C_1'	1.14	0.3010	-0.7462	0.1010
	C_3-C_6'	1.20	0.2878	-0.7207	0.1519
	O_2-H_5'	0.003	0.0061	0.0238	1.0361
	N-H	0.76	0.3431	-1.8598	0.0392
Cl	C_1-O	1.70	0.3955	0.1086	0.0564
	C_1-C_2	1.06	0.2845	-0.7544	0.1231
	C_2-C_3	1.41	0.3222	-0.8935	0.2630
	C_3-C_4	1.07	0.2836	-0.7408	0.1212
	C_4-O	1.71	0.3960	0.1183	0.0591
	C_2-N	1.19	0.3133	-0.7421	0.1160
	N-C_1'	1.14	0.3019	-0.7557	0.1099
	C_3-C_6'	1.19	0.2879	-0.7211	0.1529

	O_2-H_5'	0.003	0.0061	0.0241	1.1456
	N-H	0.76	0.3429	-1.8605	0.0389
COMe	C_1-O	1.70	0.3956	0.1088	0.0568
	C_1-C_2	1.06	0.2848	-0.7559	0.1244
	C_2-C_3	1.42	0.3232	-0.8982	0.2634
	C_3-C_4	1.07	0.2834	-0.7403	0.1188
	C_4-O	1.71	0.3956	0.1175	0.0580
	C_2-N	1.18	0.3117	-0.7515	0.1137
	N-C_1'	1.15	0.3035	-0.7532	0.0943
	C_3-C_6'	1.19	0.2877	-0.7210	0.1508
	O_2-H_5'	0.004	0.0064	0.0246	0.8065
	N-H	0.76	0.3428	-1.8609	0.0384
CF_3	C_1-O	1.71	0.3957	0.1117	0.0568
	C_1-C_2	1.05	0.2841	-0.7533	0.1212
	C_2-C_3	1.42	0.3234	-0.8994	0.2644
	C_3-C_4	1.07	0.2831	-0.7386	0.1188
	C_4-O	1.71	0.3964	0.1225	0.0598
	C_2-N	1.18	0.3126	-0.7527	0.1112
	N-C_1'	1.15	0.3029	-0.7632	0.0974
	C_3-C_6'	1.19	0.2877	-0.7213	0.1499
	O_2-H_5'	0.003	0.0061	0.0239	1.1944
	N-H	0.76	0.3428	-1.8604	0.0388

CN	C_1-O	1.71	0.3960	0.1135	0.0576
	C_1-C_2	1.05	0.2838	-0.7518	0.1200
	C_2-C_3	1.43	0.3241	-0.9028	0.2656
	C_3-C_4	1.07	0.2827	-0.7372	0.1172
	C_4-O	1.72	0.3967	0.1240	0.0604
	C_2-N	1.18	0.3119	-0.7498	0.1090
	N-C_1'	1.15	0.3043	-0.7665	0.0998
	C_3-C_6'	1.19	0.2876	-0.7209	0.1494
	O_2-H_5'	0.003	*	*	*
	N-H	0.76	0.3426	-1.8610	0.0384
NO_2	C_1-O	1.71	0.3962	0.1147	0.0577
	C_1-C_2	1.05	0.2836	-0.7513	0.1193
	C_2-C_3	1.43	0.3247	-0.9059	0.2665
	C_3-C_4	1.06	0.2821	-0.7345	0.1153
	C_4-O	1.72	0.3973	0.1289	0.0615
	C_2-N	1.17	0.3114	-0.7520	0.1070
	N-C_1'	1.16	0.3054	-0.7706	0.0968
	C_3-C_6'	1.19	0.2876	-0.7213	0.1498
	O_2-H_5'	0.003	0.0059	0.0236	2.4702
	N-H	0.75	0.3425	-1.8613	0.0382

* Not determined.

Table S3. Natural Charges of the Quinones: MeOBCD, MeBCD, BCD, ClBCD, COMeBCD, CF_3BCD, CNBCD and NO_2BCD at the Level of B3LYP/6-31G(*d,p*).

R_2	NO_2	CN	CF_3	COMe	Cl	H	Me	MeO
C1	0.52	0.52	0.51	0.51	0.51	0.51	0.51	0.51
C2	0.13	0.13	0.13	0.13	0.13	0.12	0.13	0.13
C3	-0.14	-0.14	-0.14	-0.14	-0.15	-0.15	-0.15	-0.15
C4	0.54	0.54	0.54	0.54	0.54	0.54	0.53	0.53
C4a	-0.11	-0.11	-0.10	-0.11	-0.10	-0.10	-0.10	-0.10
C5	-0.19	-0.19	-0.19	-0.19	-0.19	-0.19	-0.19	-0.19
C6	-0.21	-0.21	-0.21	-0.21	-0.21	-0.22	-0.22	-0.22
C7	-0.22	-0.22	-0.22	-0.22	-0.22	-0.22	-0.22	-0.22
C8	-0.18	-0.18	-0.19	-0.19	-0.19	-0.19	-0.19	-0.19
C8a	-0.12	-0.12	-0.12	-0.12	-0.12	-0.12	-0.12	-0.12
O1	-0.54	-0.54	-0.54	-0.54	-0.54	-0.55	-0.55	-0.55
O2	-0.53	-0.54	-0.54	-0.54	-0.54	-0.54	-0.55	-0.55
N	-0.52	-0.52	-0.53	-0.52	-0.52	-0.53	-0.53	-0.52
C1'	0.19	0.19	0.18	0.19	-0.17	0.17	0.17	-0.15
C2'	-0.26	-0.26	-0.26	-0.27	-0.25	-0.27	-0.26	-0.25
C3'	-0.21	-0.19	-0.21	-0.18	-0.24	-0.23	-0.22	-0.30
C4'	0.04	-0.18	-0.18	-0.16	-0.05	-0.25	-0.04	0.31

$C_{6'}$	-0.17	-0.15	-0.17	-0.17	-0.22	-0.20	-0.20	-0.25
$C_{5'}$	-0.07	-0.07	-0.07	-0.07	-0.06	-0.07	-0.06	-0.06

Energies

2-Methoxy-5H-benzo[b]-carbazole-6,11-dione (MeOBCD)

C	-0.0212	0.0000	-1.5807
C	0.0082	0.0000	-0.1237
C	1.2098	-0.0000	0.5705
C	2.5412	-0.0000	-0.0325
C	2.5392	-0.0000	-1.5255
C	1.3283	-0.0000	-2.2575
O	-1.0627	0.0000	-2.2336
N	0.9717	-0.0000	1.9138
O	3.5636	-0.0000	0.6512
C	3.7626	-0.0000	-2.2013
C	1.3741	-0.0000	-3.6525
C	3.7943	-0.0000	-3.5949
H	4.6746	-0.0000	-1.6135
C	2.5997	-0.0000	-4.3195
H	0.4337	0.0000	-4.1934
H	4.7472	-0.0000	-4.1154
H	2.6234	-0.0000	-5.4052
H	1.7071	-0.0000	2.6050
C	-0.3966	0.0000	2.1298
C	-1.0418	0.0000	0.8569
C	-2.4390	0.0000	0.7806
C	-3.1689	0.0000	1.9676
C	-1.1295	0.0000	3.3170
C	-2.5169	0.0000	3.2255
H	-2.9467	0.0000	-0.1758
H	-0.6413	0.0000	4.2865
H	-3.0977	0.0000	4.1394
O	-4.5286	0.0000	1.8251
C	-5.3384	-0.0000	2.9890
H	-5.1698	0.8944	3.6030

H	-5.1698	-0.8944	3.6030
H	-6.3707	-0.0000	2.6354

Total energy = -934.89465 Hartrees

2-Methy-5H-benzo[b]-carbazole-6,11-dione (MeBCD)

C	-0.2992	0.0000	-1.4010
C	-0.2964	0.0000	0.0576
C	0.8919	0.0000	0.7728
C	2.2336	0.0000	0.1941
C	2.2586	0.0000	-1.2992
C	1.0616	0.0000	-2.0535
O	-1.3294	0.0000	-2.0716
N	0.6269	0.0000	2.1126
O	3.2440	0.0000	0.8951
C	3.4940	0.0000	-1.9524
C	1.1326	0.0000	-3.4475
C	3.5510	0.0000	-3.3454
H	4.3952	0.0000	-1.3482
C	2.3701	0.0000	-4.0919
H	0.2023	0.0000	-4.0057
H	4.5133	0.0000	-3.8482
H	2.4138	0.0000	-5.1770
H	1.3486	0.0000	2.8184
C	-0.7438	0.0000	2.3026
C	-1.3633	0.0000	1.0187
C	-2.7632	0.0000	0.9234
C	-3.5286	0.0000	2.0867
C	-1.4982	0.0000	3.4788
C	-2.8807	0.0000	3.3469
H	-3.2284	0.0000	-0.0569
H	-1.0272	0.0000	4.4569

H	-3.4921	0.0000	4.2450
C	-5.0392	0.0000	2.0080
H	-5.4106	0.8811	1.4726
H	-5.4927	0.0000	3.0029
H	-5.4106	-0.8811	1.4726

Total energy = -859.69225 Hartrees

5H-benzo[b]-carbazole-6,11-dione (BCD)

C	-0.6164	0.0000	-1.2843
C	-0.6268	0.0000	0.1751
C	0.5542	0.0000	0.9011
C	1.9014	0.0000	0.3345
C	1.9400	0.0000	-1.1587
C	0.7500	0.0000	-1.9241
O	-1.6409	0.0000	-1.9629
N	0.2752	0.0000	2.2387
O	2.9049	0.0000	1.0450
C	3.1813	0.0000	-1.8007
C	0.8337	0.0000	-3.3173
C	3.2511	0.0000	-3.1930
H	4.0769	0.0000	-1.1882
C	2.0771	0.0000	-3.9504
H	-0.0913	0.0000	-3.8841
H	4.2180	0.0000	-3.6869
H	2.1308	0.0000	-5.0351
H	0.9891	0.0000	2.9525
C	-1.0965	0.0000	2.4161
C	-1.7025	0.0000	1.1251
C	-3.1038	0.0000	1.0180
C	-3.8541	0.0000	2.1842
C	-1.8549	0.0000	3.5922

C	-3.2365	0.0000	3.4548
H	-3.5666	0.0000	0.0379
H	-4.9381	0.0000	2.1252
H	-1.3843	0.0000	4.5705
H	-3.8572	0.0000	4.3456

Total energy = -820.37233 Hartrees

2-Chloro-5H-benzo[b]-carbazole-6,11-dione (ClBCD)

C	-0.0015	0.0000	-1.5161
C	-0.0005	0.0000	-0.0563
C	1.1846	0.0000	0.6616
C	2.5290	0.0000	0.0838
C	2.5557	0.0000	-1.4085
C	1.3596	0.0000	-2.1652
O	-1.0326	0.0000	-2.1839
N	0.9171	0.0000	2.0011
O	3.5355	0.0000	0.7892
C	3.7922	0.0000	-2.0599
C	1.4327	0.0000	-3.5590
C	3.8510	0.0000	-3.4527
H	4.6928	0.0000	-1.4549
C	2.6714	0.0000	-4.2012
H	0.5036	0.0000	-4.1190
H	4.8141	0.0000	-3.9540
H	2.7169	0.0000	-5.2862
H	1.6376	0.0000	2.7084
C	-0.4525	0.0000	2.1880
C	-1.0680	0.0000	0.9022
C	-2.4685	0.0000	0.7942
C	-3.1984	0.0000	1.9710

C	-1.2068	0.0000	3.3662
C	-2.5886	0.0000	3.2444
H	-2.9458	0.0000	-0.1776
H	-0.7367	0.0000	4.3443
H	-3.2145	0.0000	4.1291
Cl	-4.9564	0.0000	1.8944

Total energy = -1279.96543 Hartrees

2-Acethyl-5H-benzo[b]-carbazole-6,11-dione (COMe BCD)

C	-1.0745	-1.1703	-0.0000
C	-0.2643	0.0449	-0.0000
C	-0.8501	1.2989	0.0000
C	-2.2881	1.5658	0.0000
C	-3.1400	0.3392	0.0000
C	-2.5664	-0.9548	-0.0000
O	-0.5862	-2.2979	-0.0000
N	0.1206	2.2639	0.0000
O	-2.7339	2.7110	0.0000
C	-4.5297	0.4848	0.0000
C	-3.4017	-2.0730	-0.0000
C	-5.3529	-0.6405	0.0000
H	-4.9419	1.4884	0.0000
C	-4.7885	-1.9184	-0.0000
H	-2.9411	-3.0552	-0.0000
H	-6.4321	-0.5219	0.0000
H	-5.4293	-2.7950	-0.0000
H	-0.0833	3.2530	0.0000
C	1.3607	1.6595	-0.0000
C	1.1564	0.2485	-0.0000
C	2.2627	-0.6130	-0.0000
C	3.5431	-0.0620	-0.0000

C	2.6456	2.2211	-0.0000
C	3.7176	1.3481	-0.0000
H	2.0930	-1.6828	-0.0000
H	2.7939	3.2964	0.0000
H	4.7358	1.7209	-0.0000
C	4.7791	-0.9099	-0.0000
O	5.8870	-0.3930	-0.0000
C	4.6313	-2.4217	0.0001
H	4.0787	-2.7634	0.8819
H	4.0787	-2.7635	-0.8816
H	5.6257	-2.8681	0.0001

Total energy = -973.02320 Hartrees

2-Trifluoromethy-5H-benzo[b]-carbazole-6,11-dione (CF_3 BCD)

C	0.5255	0.0000	-1.6965
C	0.5287	0.0000	-0.2355
C	1.7134	0.0000	0.4797
C	3.0575	0.0000	-0.1009
C	3.0822	0.0000	-1.5931
C	1.8849	0.0000	-2.3478
O	-0.5069	0.0000	-2.3612
N	1.4487	0.0000	1.8213
O	4.0641	0.0000	0.6037
C	4.3177	0.0000	-2.2462
C	1.9556	0.0000	-3.7418
C	4.3743	0.0000	-3.6392
H	5.2192	0.0000	-1.6426
C	3.1934	0.0000	-4.3858
H	1.0258	0.0000	-4.3006
H	5.3365	0.0000	-4.1421

H	3.2371	0.0000	-5.4708
H	2.1709	0.0000	2.5270
C	0.0808	0.0000	2.0119
C	-0.5372	0.0000	0.7258
C	-1.9349	0.0000	0.6296
C	-2.6758	0.0000	1.8057
C	-0.6684	0.0000	3.1929
C	-2.0503	0.0000	3.0720
H	-2.4117	0.0000	-0.3436
H	-0.1921	0.0000	4.1679
H	-2.6692	0.0000	3.9608
C	-4.1778	0.0000	1.7010
F	-4.7775	0.0000	2.9128
F	-4.6297	1.0848	1.0304
F	-4.6297	-1.0848	1.0304

Total energy = -1157.40724 Hartrees

2-Cyano-5H-benzo[b]-carbazole-6,11-dione (CNBCD)

C	-0.1103	0.0000	-1.4654
C	-0.1120	0.0000	-0.0036
C	1.0689	0.0000	0.7159
C	2.4159	0.0000	0.1404
C	2.4457	0.0000	-1.3512
C	1.2512	0.0000	-2.1111
O	-1.1418	0.0000	-2.1313
N	0.7982	0.0000	2.0572
O	3.4184	0.0000	0.8503
C	3.6836	0.0000	-1.9999
C	1.3272	0.0000	-3.5047
C	3.7454	0.0000	-3.3926
H	4.5832	0.0000	-1.3934

C	2.5676	0.0000	-4.1439
H	0.3998	0.0000	-4.0674
H	4.7096	0.0000	-3.8917
H	2.6155	0.0000	-5.2287
H	1.5174	0.0000	2.7663
C	-0.5685	0.0000	2.2420
C	-1.1819	0.0000	0.9534
C	-2.5779	0.0000	0.8472
C	-3.3286	0.0000	2.0249
C	-1.3215	0.0000	3.4228
C	-2.7000	0.0000	3.3004
H	-3.0529	0.0000	-0.1263
H	-0.8479	0.0000	4.3990
H	-3.3223	0.0000	4.1883
C	-4.7610	0.0000	1.9588
N	-5.9237	0.0000	1.9146

Total energy = -912.61332 Hartrees

2-Nitro-5H-benzo[b]-carbazole-6,11-dione (NO_2BCD)

C	0.2100	0.0000	-1.5983
C	0.2110	0.0000	-0.1353
C	1.3931	0.0000	0.5805
C	2.7394	0.0000	0.0023
C	2.7666	0.0000	-1.4889
C	1.5704	0.0000	-2.2462
O	-0.8225	0.0000	-2.2613
N	1.1265	0.0000	1.9237
O	3.7422	0.0000	0.7116
C	4.0034	-0.0000	-2.1399
C	1.6436	-0.0000	-3.6400
C	4.0623	-0.0000	-3.5327

H	4.9040	-0.0000	-1.5350
C	2.8828	-0.0000	-4.2815
H	0.7152	0.0000	-4.2013
H	5.0253	-0.0000	-4.0339
H	2.9285	-0.0000	-5.3663
H	1.8484	0.0000	2.6302
C	-0.2381	0.0000	2.1133
C	-0.8559	0.0000	0.8254
C	-2.2522	0.0000	0.7229
C	-2.9707	-0.0000	1.9086
C	-0.9869	-0.0000	3.2982
C	-2.3660	-0.0000	3.1827
H	-2.7520	0.0000	-0.2365
H	-0.5091	-0.0000	4.2722
H	-3.0041	-0.0000	4.0565
N	-4.4399	-0.0000	1.8400
O	-5.0623	-0.0000	2.9037
O	-4.9622	-0.0000	0.7261

Total energy = -1024.87154 Hartrees