

Supporting information:

Ultrafast Dynamics in Spatially Confined
Photoisomerization: Accelerated Simulations
through Machine Learning Models

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Coordinates of I, II and III

Table S1: Coordinates of the optimized structure of I at the QM(B3LYP-D3/cc-pVDZ)/MM level.

N	-2.6075183792	3.8396577647	1.2156382342
N	-0.0613214286	3.9116172160	1.1484725672
C	-1.3624218806	4.4891467194	0.8620262664
C	-3.3616578262	3.4772006833	0.1765036850
C	0.7101119814	3.7787799463	0.0633984716
C	-1.4028953224	4.4511119823	-0.6585200396
N	-2.6532577234	3.7667255959	-0.9159782389
O	-4.4726383503	2.9827655217	0.2167895802
N	-0.1185679040	3.8591622848	-0.9838151887
O	1.9278567431	3.5991672779	0.0347329468
C	-3.3487145883	-1.1507589626	-3.6796379363
C	0.0785461849	-1.2845111220	-3.7476514897
C	-3.1220580324	3.5095814885	-2.2587287750
C	0.2281993347	3.4184551634	-2.3279269189
N	-2.8355621416	0.1661816990	-3.3757875634
N	-0.3558296826	0.0564760615	-3.3795985534
N	-2.7570363707	2.2164113398	-2.7910345401
N	-0.2780793225	2.1259741171	-2.7730536340
C	-1.5760494770	0.5995824741	-3.9311512861
C	-3.5131172032	1.1155081644	-2.7211650202
C	0.4262440380	0.9844678169	-2.8091694303
C	-1.5181042068	2.0523542422	-3.5099868154
O	-4.6168369977	1.0134456391	-2.2135357129
O	1.5790612740	0.8419503485	-2.4827650284
N	-2.8996138054	-2.2079294818	-2.8013705906
N	-0.3832164678	-2.3964664770	-2.9290441115
N	-2.6240159120	2.2404998753	3.0310800524
N	-0.1377119259	2.1254743480	2.9072704341
C	-1.7036291140	-2.9712799085	-3.0865893980
C	-3.6304252821	-2.6836802019	-1.7914366488
C	0.3980240134	-3.0954214777	-2.0972275700
C	-1.3567756387	1.9899446938	3.6704438667
C	-3.3898132905	1.1572662347	2.8651832752
C	0.5788538674	0.9923419933	2.8545603246
C	-1.7265453668	-4.0321104626	-1.9983848406
N	-2.9377260873	-3.7046744575	-1.2808463218
O	-4.7164599998	-2.2770984158	-1.4203966326
N	-0.4147803534	-3.8951138732	-1.3935224200
O	1.6176524120	-3.0418001558	-2.0254375200
C	-1.4185693391	0.5018072530	3.9448078414
N	-2.6942074806	0.1354055555	3.3753044127
O	-4.5121773536	1.1175806449	2.3925218369
N	-0.2036202713	0.0129932754	3.3311426713
O	1.7406068598	0.8855258338	2.5273347497
C	-3.3017256669	-4.3989489477	-0.0685098904
C	-0.0686847632	-4.5467028720	-0.1313609711
C	-3.2311571716	-1.1905838299	3.5836365037
C	0.2413573466	-1.3546666806	3.5661179561
N	-2.8898741892	-3.6869463862	1.1180884526
N	-0.3773091535	-3.8593939054	1.1216411137
N	-2.7896185353	-2.1961015528	2.6427363364
N	-0.2778669467	-2.3947322608	2.6883691365
C	-1.6546866305	-4.0179671898	1.7864848744

C	-3.5578665939	-2.6618640992	1.6544930720
C	0.4674725715	-3.0807229597	1.8117900047
C	-1.5920951593	-2.9715455923	2.8848456140
O	-4.6580493081	-2.2524945712	1.3279415227
O	1.6852812587	-3.0459543597	1.7053924973
C	-2.9639525738	3.5733619671	2.5895775872
C	0.3193350939	3.4419294688	2.4750632107
H	-3.0910814591	-1.4064529616	-4.7073449545
H	-4.4329133682	-1.1024716739	-3.5731465222
H	1.1666754972	-1.2924412939	-3.6761376457
H	-0.2108251432	-1.4664407349	-4.7827295071
H	-2.7571622586	4.2913134741	-2.9246767162
H	-4.2114767549	3.5379270436	-2.2166123709
H	1.3167139780	3.3599937434	-2.3493924060
H	-0.1008502073	4.1666495336	-3.0490947525
H	-2.8738439919	-5.4015530163	-0.0687504134
H	-4.3904788450	-4.4534800794	-0.0494554406
H	1.0134478407	-4.6794989814	-0.1509436797
H	-0.5451769530	-5.5268186408	-0.1139425371
H	-4.3131110702	-1.1114481313	3.4723896154
H	-2.9898606248	-1.5207273641	4.5939912540
H	0.0090122588	-1.6230081689	4.5965975916
H	1.3239023586	-1.3567659379	3.4346912570
H	-2.4885766390	4.3088192867	3.2386460597
H	-4.0488215825	3.6632866844	2.6547997031
H	1.4092951355	3.4140906208	2.4742427680
H	-0.0164493745	4.1698223788	3.2137689993
H	-1.3831535502	5.5243118509	1.2026367811
H	-1.4532624134	5.4670480152	-1.0503075813
H	-1.5781804335	0.5151307680	-5.0177740661
H	-1.4849139622	2.7040033491	-4.3829515062
H	-1.7875574954	-3.4430362152	-4.0656020725
H	-1.2834461941	2.5467115106	4.6045675841
H	-1.8141711962	-5.0206308593	-2.4494824608
H	-1.4067215382	0.3118994596	5.0180209031
H	-1.7187518160	-5.0139023259	2.2248854408
H	-1.6462829010	-3.4526117536	3.8613257185
C	-2.4696203885	0.6513001704	0.0843851191
C	-1.2522740246	1.3246447920	0.1522405837
C	-0.0539310846	0.6224329783	0.0606639379
C	-0.0501596276	-0.7685623136	-0.0852636567
C	-1.2831913146	-1.4282645492	-0.1406171343
C	-2.4869683919	-0.7315083742	-0.0668775276
C	1.2589002354	-1.4019125594	-0.1343811725
C	2.3977123237	-0.7035495684	-0.0784567480
C	2.3809838119	0.7854044239	0.0230671942
O	1.0986435512	1.3331020249	0.1482557759
H	-3.4123977904	1.1960206092	0.1576649953
H	-1.2114570798	2.3977904444	0.2841070212
H	-1.3110281106	-2.5110765264	-0.2268342982
H	-3.4428909303	-1.2532590169	-0.1085541869
H	1.3061432851	-2.4901062902	-0.1842467848
H	3.3712583689	-1.2000840733	-0.1044551837
H	2.9693570841	1.1185844579	0.8997697141
H	2.8653124080	1.2437934707	-0.8634236943

Table S2: Coordinates of the optimized structure of II at the QM(B3LYP-D3/cc-pVDZ)/MM level.

N	-2.8179565480	3.9260534661	0.4685347832
N	-0.2739712652	4.1386427493	0.4481226682
C	-1.5977962102	4.5913030956	0.0574138094
C	-3.5248233388	3.3944612596	-0.5317908491
C	0.5382471431	3.9158071707	-0.5910555320
C	-1.5880153981	4.3453843422	-1.4451172862
N	-2.7981067817	3.5713157145	-1.6378701763
O	-4.6051769964	2.8393772437	-0.4486871302
N	-0.2638071290	3.7862045479	-1.6536278057
O	1.7654434026	3.7837283996	-0.5633546046
C	-3.1966106389	-1.8028849920	-3.3875617090
C	0.2783200120	-1.7832235188	-3.3171541949
C	-3.1752141050	3.0550712107	-2.9349944053
C	0.1376734617	3.1119021449	-2.8815316462
N	-2.7279254510	-0.4362140407	-3.3209671858
N	-0.2434077970	-0.4253943603	-3.2252614982
N	-2.7554399224	1.6952799093	-3.1950360066
N	-0.2802168566	1.7274816160	-3.0722471270
C	-1.4635961129	-0.0731155775	-3.9163477327
C	-3.4725889930	0.6005079405	-2.9200617225
C	0.4775512118	0.6419905770	-2.8482366206
C	-1.4813577436	1.4372710374	-3.8185279255
O	-4.5938680856	0.5583541465	-2.4445526694
O	1.6270994599	0.6294657711	-2.4549194141
N	-2.7220203130	-2.6780950842	-2.3380799796
N	-0.1917639371	-2.7657540195	-2.3494816656
N	-2.8010625978	2.6202165022	2.5193639511
N	-0.3142595369	2.6108323226	2.4385732331
C	-1.4827464358	-3.4144309148	-2.4737281423
C	-3.4724281432	-3.0482912593	-1.2973183064
C	0.5804831180	-3.3164880853	-1.4047626672
C	-1.5352476325	2.5539915716	3.2065610746
C	-3.5170452413	1.4918134283	2.5624333002
C	0.4447162095	1.5107263300	2.5653319093
C	-1.5093982090	-4.3186916713	-1.2522910372
N	-2.7517176742	-3.9439504061	-0.6176706334
O	-4.5927412305	-2.6529410181	-1.0268444851
N	-0.2287849719	-4.0503804282	-0.6310120672
O	1.7897375424	-3.1881009659	-1.2819571559
C	-1.5285295158	1.1397891156	3.7468280068
N	-2.7836065260	0.6171739322	3.2599299542
O	-4.6303691133	1.3115792742	2.1012612423
N	-0.2920538980	0.6025934307	3.2237451016
O	1.6034833171	1.3831155843	2.2190899726
C	-3.1128499355	-4.4609500493	0.6828911044
C	0.0862366560	-4.5089166871	0.7185038394
C	-3.2643851878	-0.6671079165	3.7193581004
C	0.2205712410	-0.6661000266	3.7245182344
N	-2.7707932449	-3.5556809103	1.7564723266
N	-0.2558699093	-3.6372468014	1.8383789417
N	-2.7660995554	-1.8150457495	2.9937760631
N	-0.2438797002	-1.8865121584	3.0783792580
C	-1.5421878574	-3.7108818549	2.4992147380
C	-3.4983621871	-2.4908046302	2.1042013459
C	0.5422601166	-2.6953758412	2.3566265630
C	-1.5355164896	-2.4730353754	3.3796323427
O	-4.6110765815	-2.2005371178	1.7017653156

O	1.7528758736	-2.6063502790	2.2181710646
C	-3.2076062053	3.8410256855	1.8584008150
C	0.1036170987	3.8689174867	1.8299382364
H	-2.9266927221	-2.2261314876	-4.3549851422
H	-4.2824534710	-1.7705860377	-3.2922862653
H	1.3571162811	-1.7141960223	-3.1715832921
H	0.0801593819	-2.1588013278	-4.3209790445
H	-2.7792517709	3.7099686497	-3.7112758109
H	-4.2652658841	3.0612427332	-2.9652751540
H	1.2281697743	3.1169688827	-2.8794654219
H	-0.2162490186	3.6836543259	-3.7393054826
H	-2.6364024926	-5.4275510412	0.8460027840
H	-4.1973481765	-4.5726029240	0.6892465522
H	1.1686452889	-4.6395092616	0.7467208803
H	-0.3961774661	-5.4745845168	0.8709477751
H	-4.3469908731	-0.6604293221	3.5881877291
H	-3.0249259864	-0.7840448013	4.7762177033
H	0.0003327027	-0.7332218762	4.7898036166
H	1.3024120155	-0.6405012622	3.5881538860
H	-2.8087373344	4.6998518151	2.3982365573
H	-4.2976440277	3.8640506544	1.8779625846
H	1.1940309447	3.8780019033	1.8429726970
H	-0.2645891592	4.6803101134	2.4578172695
H	-1.6864444178	5.6602021369	0.2508300101
H	-1.6742469335	5.2955562294	-1.9719300812
H	-1.4190911104	-0.3887522470	-4.9585454349
H	-1.4345528509	1.8861968870	-4.8106532517
H	-1.5061409562	-4.0178473901	-3.3811688591
H	-1.5044370899	3.2745510548	4.0238472639
H	-1.5481530417	-5.3618246972	-1.5661428907
H	-1.5100085885	1.1475732484	4.8365288588
H	-1.5864901600	-4.6070329216	3.1182667659
H	-1.5769176114	-2.7625820130	4.4296695919
C	-2.6432614846	0.5977037393	-0.1116609718
C	-1.5431349301	1.3826198109	-0.2028551139
C	-0.1990392639	0.8430546525	-0.1094732906
C	-0.0574770575	-0.6049719144	0.0871577921
C	-1.2717358945	-1.3876915589	0.1860984474
C	-2.5016158005	-0.8183082855	0.0898970773
C	1.1713232183	-1.2150307313	0.1856574211
C	2.5848599896	-0.8879938837	0.1406333144
C	3.2702561793	0.2629746400	-0.0465186437
O	0.7951276098	1.5644572371	-0.1877784569
H	-3.6493648462	1.0169142476	-0.1865386089
H	-1.5759422161	2.4529891407	-0.3489749413
H	-1.1900498283	-2.4619514985	0.3421271526
H	-3.4103561091	-1.4141104795	0.1669537801
H	1.0630358914	-2.2902192948	0.3522980376
H	3.1896082869	-1.7904276526	0.2876353018
H	4.3642735674	0.2198107212	-0.0424773044
H	2.7655328473	1.2137767008	-0.1994093321

Table S3: Coordinates of the optimized structure of III at the QM(B3LYP-D3/cc-pVDZ)/MM level.

N	-3.2975899818	1.9554484358	3.2511206641
N	-0.7992571493	2.3603562686	3.5824324632
C	-2.1786142975	2.8155030201	3.5800815515
C	-3.9617000975	2.3067052158	2.1470338102
C	0.0028314757	3.0979206844	2.8073579607
C	-2.1851832405	3.8081287910	2.4254096442
N	-3.2931882459	3.3351529518	1.6192167266
O	-4.9615307815	1.7784658752	1.6971382673
N	-0.8079617309	3.7510348042	1.9681520984
O	1.2345273207	3.1157837138	2.8153978162
C	-3.0472135341	1.3314788732	-3.6975363314
C	0.3843775822	1.6445633040	-3.3469930742
C	-3.6522411062	3.9651541863	0.3671612204
C	-0.3581826770	4.3219312901	0.7058757981
N	-2.7636662403	2.1709416568	-2.5540484447
N	-0.3019799909	2.3560959397	-2.2765072510
N	-3.0595371764	3.3692492256	-0.8108298793
N	-0.6067395055	3.5620977410	-0.5132161954
C	-1.5752856188	2.9905285280	-2.5344722665
C	-3.6214437396	2.4105968982	-1.5555068726
C	0.2850937107	2.7851707058	-1.1485759985
C	-1.7858884276	3.8384015543	-1.2984906742
O	-4.7126703523	1.8941638143	-1.3852050140
O	1.4349617035	2.5729217266	-0.8098952390
N	-2.4407329413	0.0183702247	-3.6726842537
N	0.0777143752	0.2335058138	-3.5378985093
N	-3.0388787672	-0.4440984793	3.5348229778
N	-0.5737210768	-0.1353572113	3.6775701180
C	-1.1209910211	-0.2129634777	-4.2207264081
C	-3.1079530603	-1.0932629906	-3.3525931105
C	0.9439795494	-0.7590586719	-3.3025295595
C	-1.7551428264	-0.8936784370	4.0132388432
C	-3.6056944845	-1.2460202944	2.6271941397
C	0.3241515966	-0.8363729958	2.9668880816
C	-0.9966463825	-1.7256146456	-4.1362000111
N	-2.2585672281	-2.1062294025	-3.5439201554
O	-4.2614506035	-1.1678408507	-2.9661352693
N	0.2586157622	-1.9013648951	-3.4344666588
O	2.1301075348	-0.6455019793	-3.0354328654
C	-1.5540988090	-2.1856197970	3.2497348409
N	-2.7454974262	-2.2527906459	2.4360327742
O	-4.7033864137	-1.1125617296	2.1143577140
N	-0.2733093293	-1.9836824434	2.6087103329
O	1.4826912560	-0.5275067867	2.7480922412
C	-2.5152668224	-3.4706362662	-3.1392220818
C	0.6692953872	-3.1955564879	-2.8985047185
C	-3.0520647812	-3.4569259733	1.6952440251
C	0.4094249413	-3.1046565951	1.9753237941
N	-2.2570980846	-3.6956337015	-1.7341512357
N	0.2496437216	-3.5453618196	-1.5447874074
N	-2.4354851727	-3.5618592786	0.3905602679
N	0.0772770179	-3.4075989091	0.5892369229
C	-0.9956232316	-4.2364679024	-1.2851344012
C	-3.1043149757	-3.3778712684	-0.7514054067
C	0.9392434298	-3.2821218232	-0.4278349335
C	-1.1192706062	-4.1421541836	0.2260520685
O	-4.2581325767	-3.0044072547	-0.8716359406

O	2.1260070025	-3.0102260787	-0.3503977271
C	-3.6142751096	0.7841762164	4.0379528356
C	-0.3490809805	1.1688944757	4.2908303509
H	-2.7382885439	1.8498417806	-4.6051790303
H	-4.1258164625	1.1712699959	-3.7155780509
H	1.4498858630	1.6888290411	-3.1187031195
H	0.2003181310	2.1725834623	-4.2825007913
H	-3.3896800371	5.0222861814	0.4072311787
H	-4.7325737936	3.8571177373	0.2655763946
H	0.7227343394	4.4318853282	0.7988611708
H	-0.8041768256	5.3079234413	0.5752208750
H	-1.9184278589	-4.1562828290	-3.7409725442
H	-3.5773692340	-3.6552747096	-3.3047791173
H	1.7596727694	-3.1873135030	-2.8933237683
H	0.3211360733	-3.9714882994	-3.5799608129
H	-4.1303468716	-3.4582338927	1.5319974497
H	-2.7711795719	-4.3255992335	2.2907082322
H	0.2394789449	-3.9985518342	2.5752525758
H	1.4739533808	-2.8676467940	1.9887709263
H	-3.2951552429	0.9425972709	5.0680077726
H	-4.6976220908	0.6659066319	3.9999615412
H	0.7296264406	1.2845866806	4.4022530556
H	-0.8082154740	1.1543179426	5.2793774861
H	-2.3878067282	3.3399740088	4.5122689308
H	-2.4080023015	4.8060943825	2.8025127844
H	-1.5187642947	3.6175756507	-3.4242982978
H	-1.8333552821	4.8950839568	-1.5618999415
H	-1.0902080813	0.1024746899	-5.2635715721
H	-1.7914540399	-1.0862201108	5.0855235806
H	-0.9113781281	-2.1452471529	-5.1385072683
H	-1.5075666416	-3.0306319154	3.9366799878
H	-0.9046719210	-5.2799952269	-1.5863716723
H	-1.0898683171	-5.1397126745	0.6639703980
C	-2.7468251642	0.3031064794	0.3004757583
C	-1.7574766237	0.9598296974	0.9485122080
C	-0.3503393160	0.7029927780	0.6880388518
C	-0.0245544310	-0.3253507936	-0.3250583177
C	-1.1322787046	-0.9972446439	-0.9730118732
C	-2.4245101362	-0.6980696237	-0.6821324164
C	1.2750235900	-0.6375777577	-0.6317783086
C	2.5456126182	-0.1370785888	-0.1531407874
C	3.7075470767	-0.6477874015	-0.6301869757
O	0.5293620370	1.3139740355	1.2909571644
H	-3.7992637857	0.5102493914	0.5071950324
H	-1.9259900984	1.7174346825	1.7016073266
H	-0.9095553330	-1.7651592349	-1.7114640271
H	-3.2503819953	-1.2107785691	-1.1743143377
H	1.3900648841	-1.4323394792	-1.3749332209
H	2.5239533609	0.6536709607	0.5966028720
H	3.7103664261	-1.4432100662	-1.3818506906
H	4.6751221952	-0.2832652421	-0.2761296981

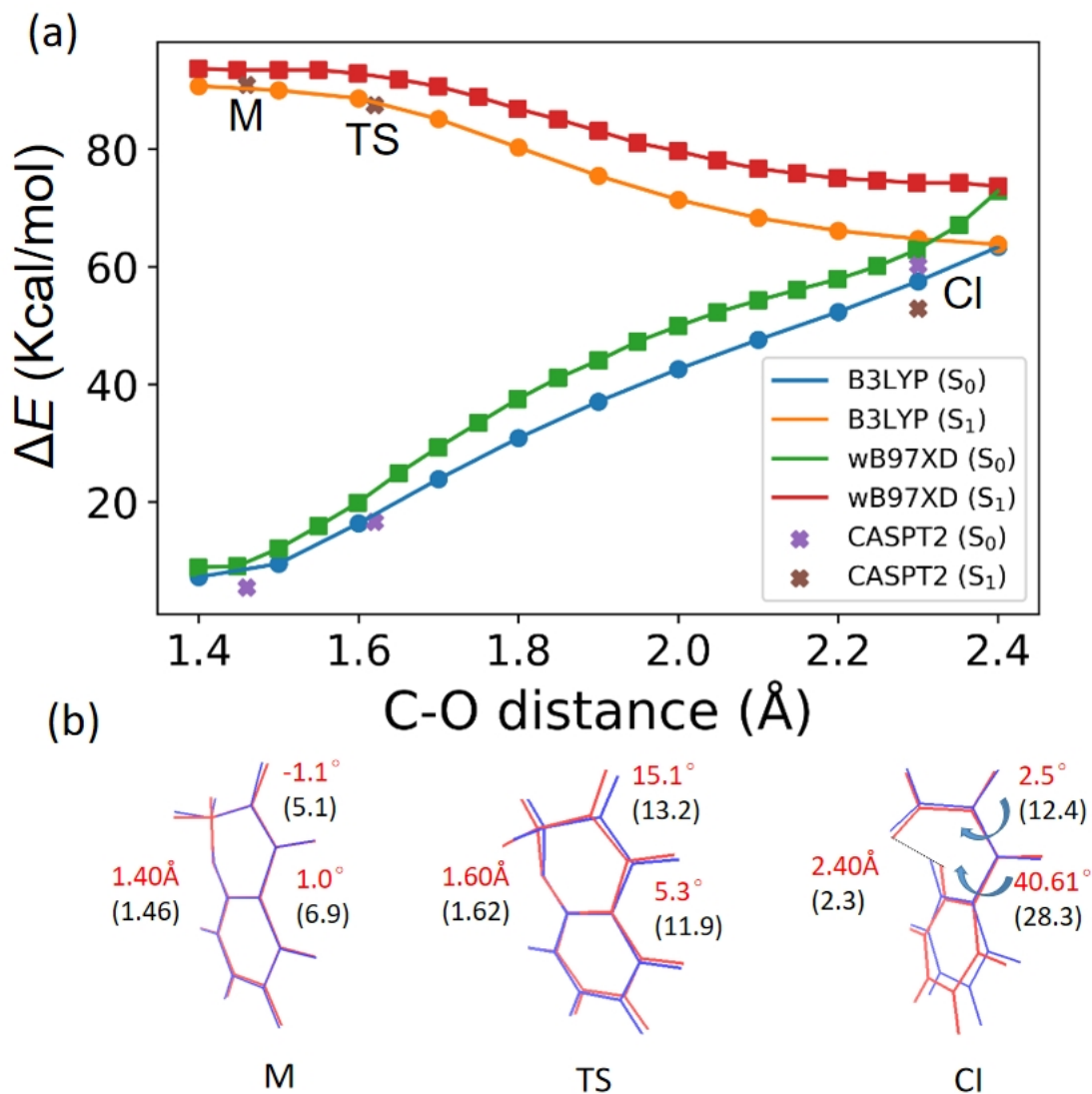
Table S4: Vertical excitation energies (eV), oscillator strengths of G@CB[5]

	MO (weight %)	Energy (eV)	Osc.
$S_0 \rightarrow S_1$	HOMO $\rightarrow$ LUMO+1 (54)	4.06	0.02
$S_0 \rightarrow S_2$	HOMO $\rightarrow$ LUMO+1 (43)	4.09	0.03

Table S5: Modified force field parameters

element	$-\epsilon$ (kcal/mol)	element	$-\epsilon$ (kcal/mol)	element	$-\epsilon$ (kcal/mol)
N	-0.169996	O	-0.209995	H	-0.00314
N	-0.169996	N	-0.169996	H	-0.00314
C	-0.109397	O	-0.209995	H	-0.00314
C	-0.085998	C	-0.109397	H	-0.00314
C	-0.085998	N	-0.169996	H	-0.00314
C	-0.109397	O	-0.209995	H	-0.00314
N	-0.169996	N	-0.169996	H	-0.00314
O	-0.209995	O	-0.085998	H	-0.00314
N	-0.169996	C	-0.109397	H	-0.00314
O	-0.209995	C	-0.109397	H	-0.00314
C	-0.109397	C	-0.109397	H	-0.00314
C	-0.109397	C	-0.109397	H	-0.00314
C	-0.109397	N	-0.169996	H	-0.00314
C	-0.109397	N	-0.169996	H	-0.00314
N	-0.169996	N	-0.169996	H	-0.00314
N	-0.169996	N	-0.169996	H	-0.00314
N	-0.169996	C	-0.109397	H	-0.00314
N	-0.169996	C	-0.085998	H	-0.00314
C	-0.109397	C	-0.085998	C	-0.085998
C	-0.085998	C	-0.109397	C	-0.085998
C	-0.085998	O	-0.209995	C	-0.085998
C	-0.109397	O	-0.209995	C	-0.085998
O	-0.209995	C	-0.109397	C	-0.085998
O	-0.209995	C	-0.109397	C	-0.085998
N	-0.169996	H	-0.00314	C	-0.085998
N	-0.169996	H	-0.00314	C	-0.085998
N	-0.169996	H	-0.00314	C	-0.085998
N	-0.169996	H	-0.00314	O	-0.209995
C	-0.109397	H	-0.00314	H	-0.00314
C	-0.085998	H	-0.00314	H	-0.00314
C	-0.085998	H	-0.00314	H	-0.00314
C	-0.109397	H	-0.00314	H	-0.00314
C	-0.085998	H	-0.00314	H	-0.00314
C	-0.085998	H	-0.00314	H	-0.00314
C	-0.085998	H	-0.00314	H	-0.00314
C	-0.109397	H	-0.00314	H	-0.00314
N	-0.169996	H	-0.00314	H	-0.00314

Comparison of methods



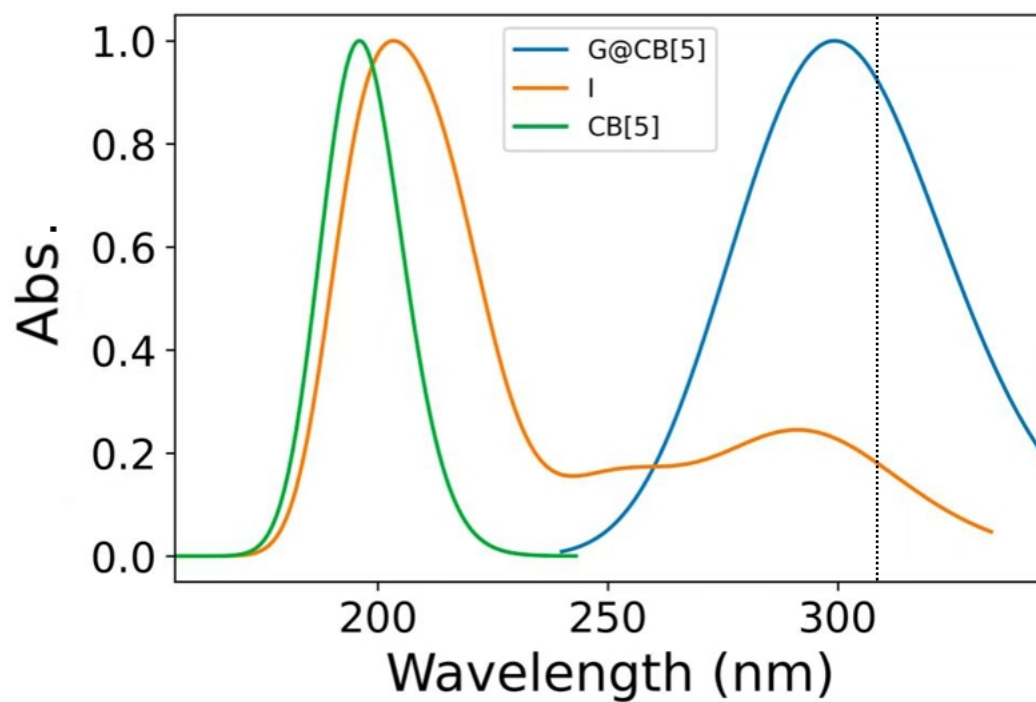


Figure S2: Theoretical absorption spectrum of benzopyran(I), host(CB[5]) and host-guest(G@CB[5]) computed using B3LYP/cc-pVDZ. The experimental absorption spectrum, obtained from 2,2-diethyl-2H-chromene where the vinyl group is replaced by C-(CH₂-CH₃)₂ (black).

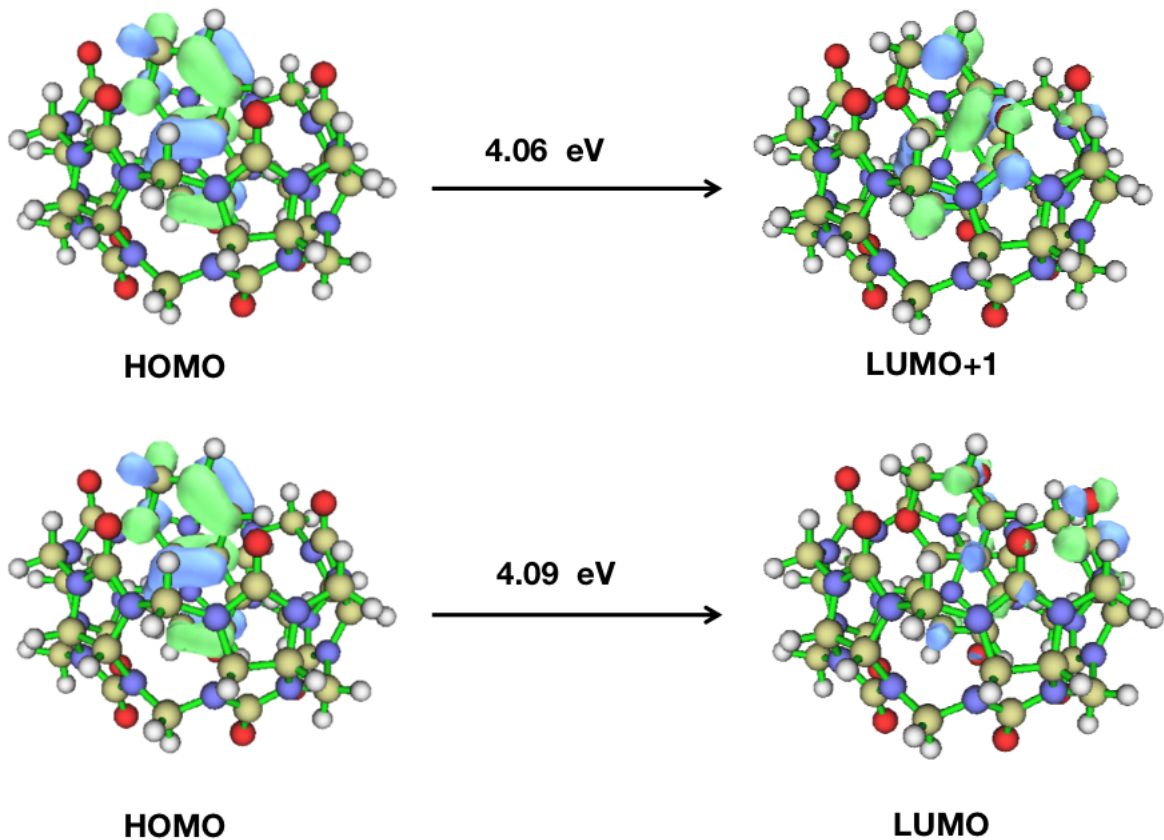


Figure S3: Vertical excitation energy (in eV), relevant molecular orbitals, and corresponding electronic characters at G@CB[5] calculated with the B3LYP-D3/cc-pVDZ method.

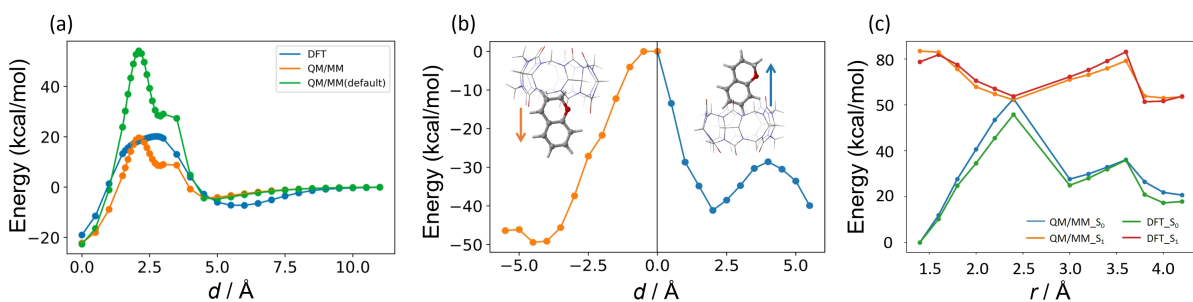


Figure S4: (a) Calibration of the force field by adjusting the distance between the host-guest center of mass, denoted as d . (b) QM/MM energy profiles along different directions with arrows indicating the directions of movement. (c) Potential energy surfaces for both S_1 and S_0 states along the r coordinate, as calculated using both QM/MM and DFT methods.

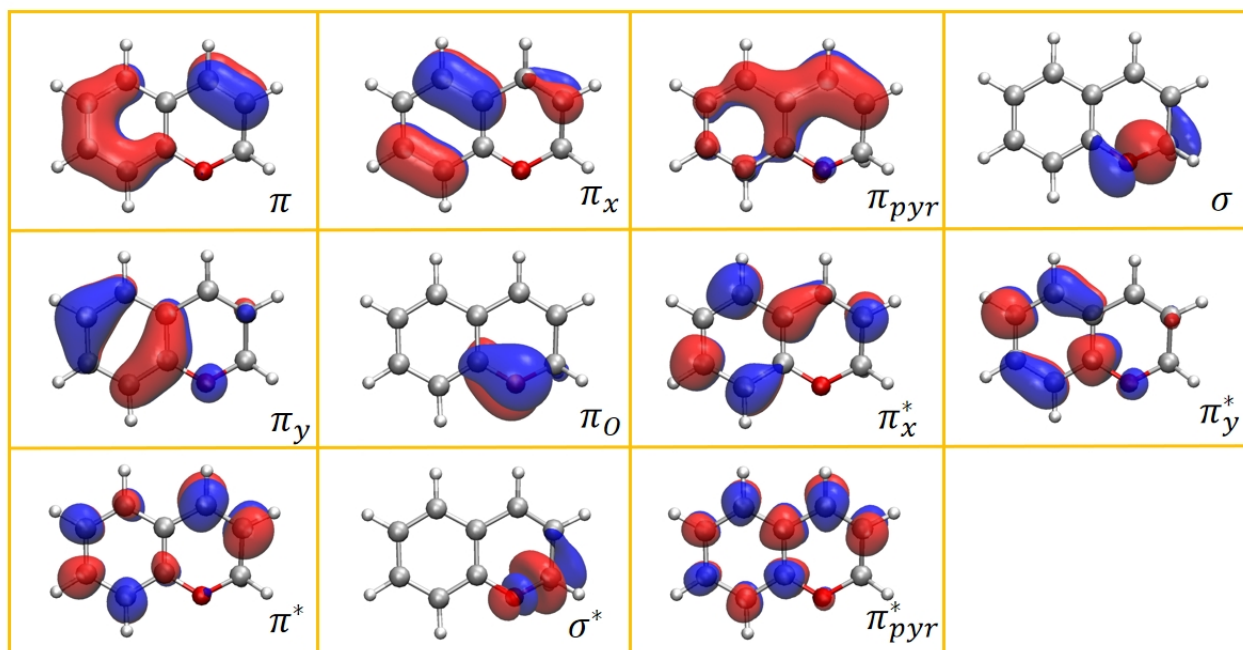


Figure S5: The active space obtained from state-average CASSCF(12,11)/cc-pVDZ calculations.

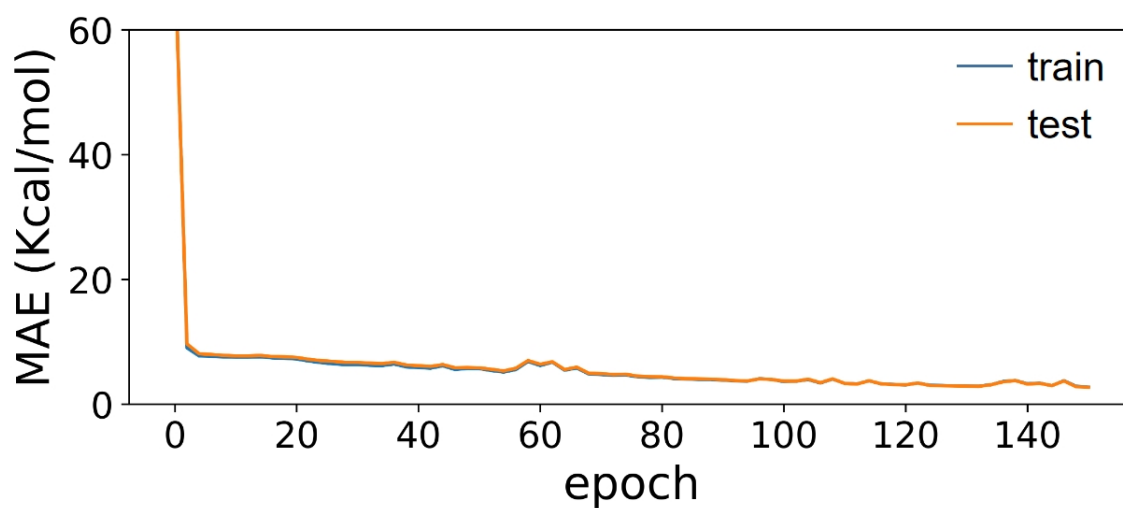


Figure S6: The number of epochs against ML-G@CB[5] model accuracy on the training and testing sets.

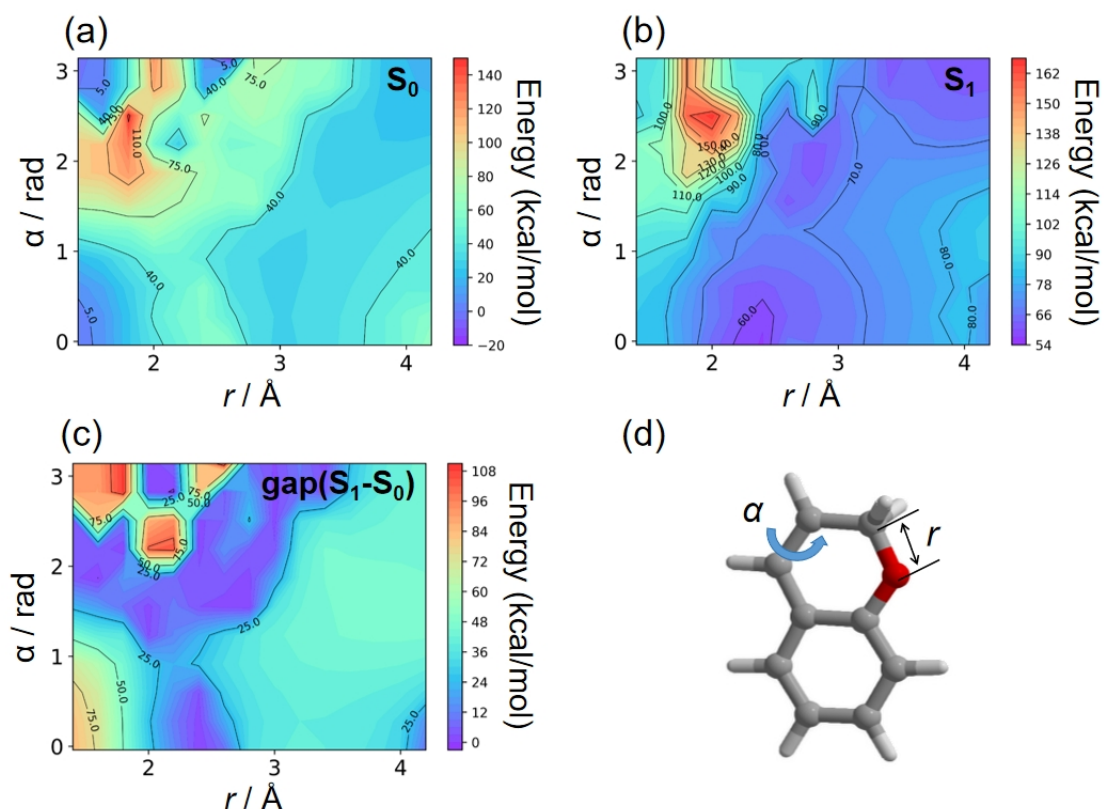


Figure S7: DFT calculations for PESs of benzopyran along r and α in the S_0 (a) and S_1 (b). (c) Contour map of the energy difference between the S_1 and S_0 states. (d) A schematic diagram of r and dihedral angle α .

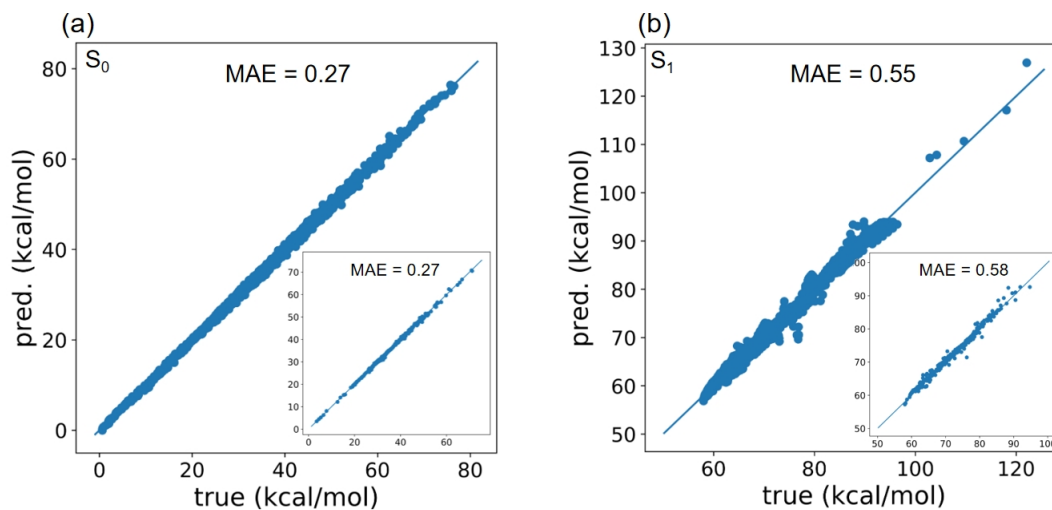


Figure S8: Validation of the ML-gas model for (a) the S_0 state and (b) the S_1 state, based on the training and test datasets (shown in the inset plot)

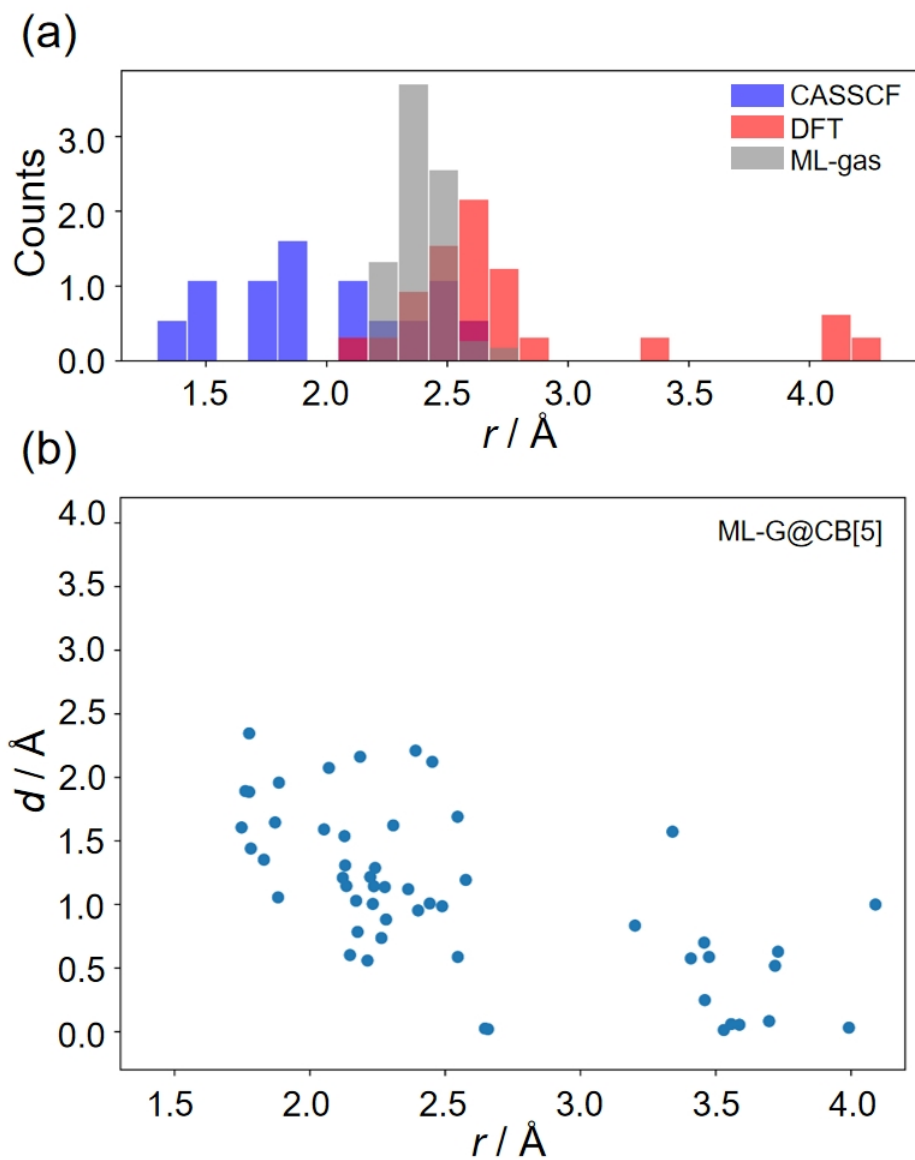


Figure S9: Counts of surface crossing points in gas-phase (a) and along r and d in host-guest (b).

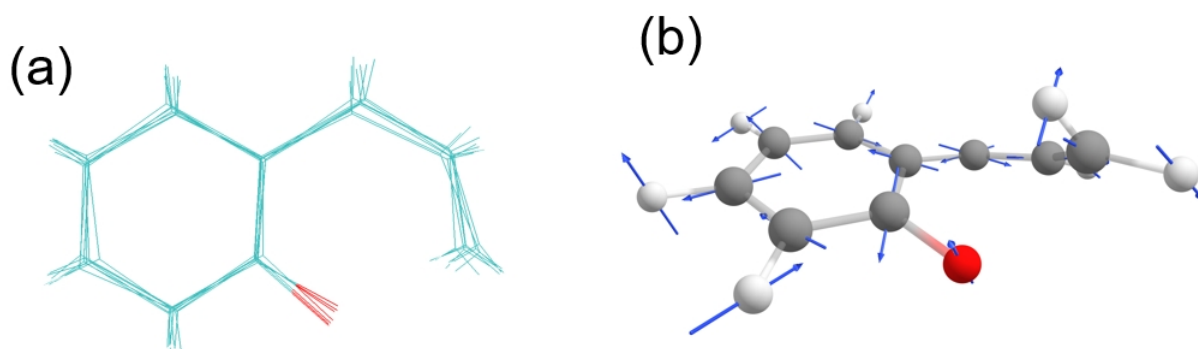


Figure S10: The structure (a) and h-vector direction (b) at the CI using the CASSCF trajectories.

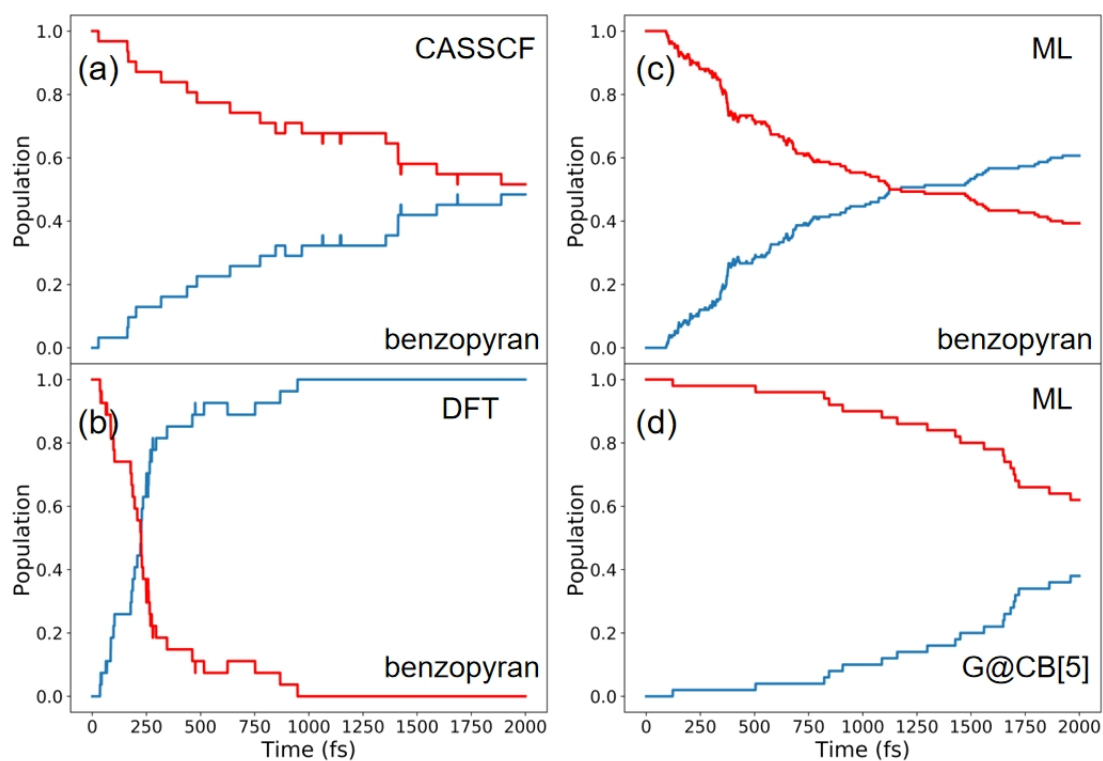


Figure S11: Evolution of the S_1 (red) and S_0 populations (blue) with CASSCF (a), DFT (b), ML-gas (c) for benzopyran and ML-G@CB[5] (d) for host-guest.

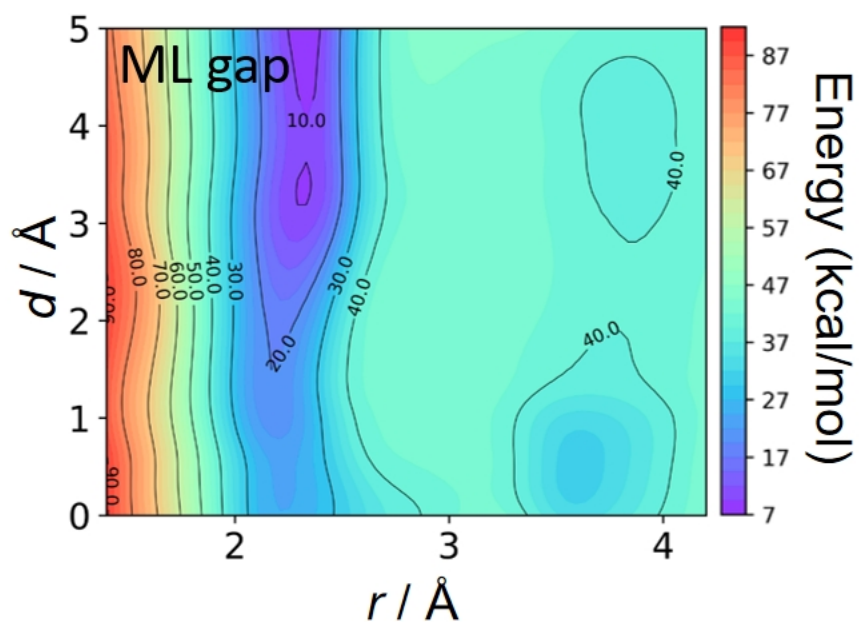


Figure S12: Countour map of the energy difference in the S_1 and S_0 states with ML-G@CB[5].