

SUPPLEMENTARY MATERIAL TO
**The role of molecular properties of mononitrofluoranthenes to
their mutagenic activity: Insight from *ab initio* and
DFT calculations**

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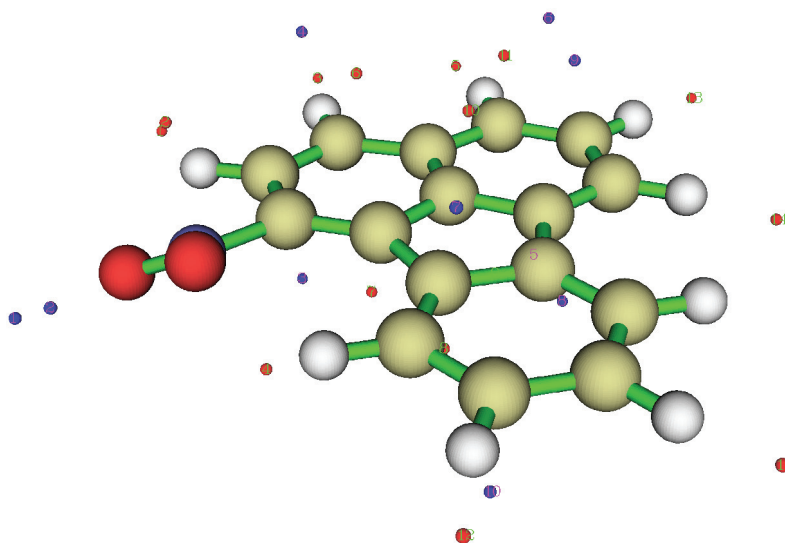


Fig. S-1. The surface extrema on the MEP surface of 1-NF (red and blue spheres are local maxima and minima, respectively) calculated at the B3LYP/6-311++G(2d,2p) level of theory.

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TABLE S-I. Energies of local minima and maxima obtained from the statistical analysis of the molecular electrostatic potential of 1-NF and their Cartesian coordinates calculated at the B3LYP/6-311++G(2d,2p) level of theory; *: the lowest minimum; **: the highest maximum

Number of surface minimum	Energy, kcal* mol ⁻¹	X,Y,Z coordinates, Å		
*1	-32.562269	-4.313678	-3.307358	-0.311412
2	-31.877230	-3.387944	-3.790251	0.346303
3	-3.700449	-2.448040	1.369519	-2.040790
4	-2.499955	-2.322553	1.498574	2.048844
5	-3.875406	0.749377	3.233367	-2.006918
6	-3.944228	0.847712	3.215092	2.041345
7	-11.031313	1.417569	2.449446	1.971289
8	-3.387652	1.554654	2.053474	-1.990502
9	-3.584547	1.600814	1.936398	2.017020
10	-9.785286	1.905954	-2.474086	-2.060622
1	17.207679	-4.814420	1.559752	0.019578
2	15.117982	-3.359182	-0.722482	1.463174
3	23.259853	-3.359182	4.215648	-0.001354
4	15.383660	-1.507062	-1.824947	-1.416096
5	22.940009	-1.383914	5.500043	-0.021042
6	1.572985	-1.261356	0.971306	1.789763
7	1.510522	-1.116409	0.975807	-1.762783
8	1.610662	0.365187	0.068847	-1.858611
9	-0.692757	0.448462	2.157176	-1.795500
10	0.760380	0.647194	0.217480	1.870740
11	-0.841163	0.501404	2.179649	1.823694
12	15.093827	2.557652	-5.424271	-0.176797
13	22.035003	2.615274	5.615887	-0.019703
**14	24.007609	4.556551	2.163114	-0.046266
15	17.798377	5.513386	-3.118207	-0.163579

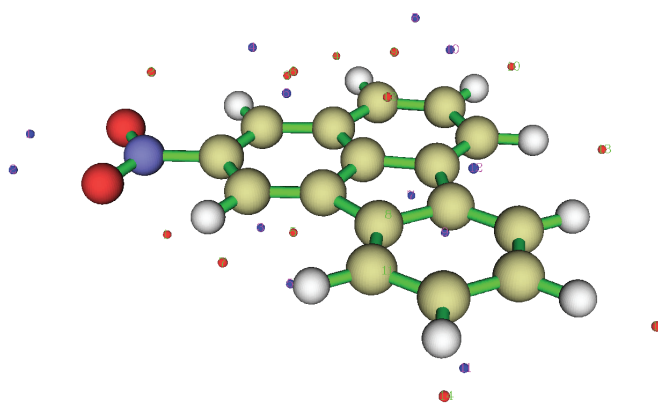


Fig. S-2. The surface extrema on the MEP surface of 2-NF (red and blue spheres are local maxima and minima, respectively) calculated at the B3LYP/6-311++G(2d,2p) level of theory.

* 1 kcal = 4184 J

TABLE S-II. Energies of local minima and maxima obtained from the statistical analysis of the molecular electrostatic potential of 2-NF and their Cartesian coordinates calculated at the B3LYP/6-311++G(2d,2p) level of theory; *: the lowest minimum; **: the highest maximum

Number of surface minimum	Energy, kcal mol ⁻¹		<i>X,Y,Z</i> coordinates, Å	
*1	-33.893202	-6.071951	-1.608978	0.009987
2	-33.849579	-5.413910	-2.791240	-0.017729
3	1.204224	2.072035	0.386665	-2.003669
4	1.204870	2.061712	0.391332	2.002460
5	-1.370354	-0.495409	-0.941030	-2.022442
6	-1.369990	-0.446246	-0.916305	2.021306
7	-2.986791	-0.061613	3.070647	-2.035905
8	-2.987689	-0.039971	3.061270	2.033907
9	-2.190148	1.233336	2.104355	-2.010926
10	-2.191492	1.188138	2.144517	2.004863
11	-8.003356	3.495598	-1.595194	-1.989415
12	-8.002052	3.500059	-1.591377	1.989651
1	13.090962	-3.330074	-1.026610	-1.779185
2	13.074301	-3.339990	-1.034593	1.778438
3	21.703367	-3.107847	3.062824	0.032072
4	22.543866	-2.749855	4.497487	-0.000718
5	3.015005	-1.218556	0.290378	-1.788181
6	3.025007	-1.090225	0.289739	1.779736
7	20.951807	-0.193908	-3.363683	-0.007345
8	0.653853	0.076245	1.854504	-1.819123
9	0.656592	0.131618	1.912538	1.801211
10	22.415120	0.836943	5.892579	0.020448
11	2.204875	0.983957	0.126887	-1.851682
12	2.204348	0.983962	0.126440	1.851676
**13	24.928017	3.876926	3.43286	0.001321
14	18.391343	4.568687	-4.561616	-0.010968
15	19.021158	6.671126	-1.459548	0.011594

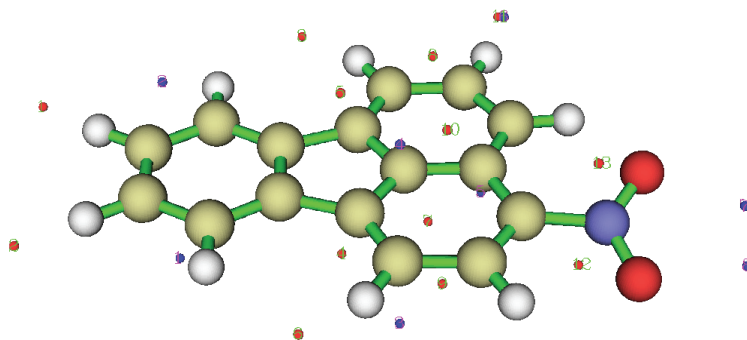


Fig. S-3. The surface extrema on the MEP surface of 3-NF (red and blue spheres are local maxima and minima, respectively) calculated at the B3LYP/6-311++G(2d,2p) level of theory.

TABLE S-III. Energies of local minima and maxima obtained from statistical analysis of the molecular electrostatic potential of 3-NF and their Cartesian coordinates calculated at the B3LYP/6-311++G(2d,2p) level of theory; *: the lowest minimum; **: the highest maximum

Number of surface minimum	Energy, kcal mol ⁻¹	X,Y,Z coordinates, Å		
1	-6.677654	-3.970909	-0.631119	-1.962197
2	-6.696598	-4.048307	-0.503758	2.000112
3	-0.695482	0.289333	-1.565891	-1.988678
4	-0.472932	0.230055	-1.468847	2.024294
5	-5.576115	1.250955	2.310074	-2.093521
6	-6.687012	1.489443	2.410115	1.994340
7	34.534486	6.028666	0.115069	0.199028
*8	-34.766494	6.13171	-1.025476	-0.142211
1	19.995966	-6.870946	0.930716	-0.037913
2	19.920614	-6.130962	-2.935372	0.086560
3	23.988869	-2.572736	3.967514	-0.067699
4	2.618484	-1.033089	0.110274	1.854298
5	2.509195	-1.018936	0.100543	1.867459
**6	25.741516	-0.975861	-4.110780	0.061402
7	-1.033355	0.399804	1.060033	-1.877615
8	-1.539021	0.369275	1.296488	1.800944
9	2.595193	0.916968	0.665448	1.770370
10	2.585589	0.906165	0.670104	1.784588
11	19.282032	1.121995	5.290457	-0.070597
12	13.355371	3.291722	0.123573	-1.648272
13	11.716327	3.471496	-1.028046	1.726761

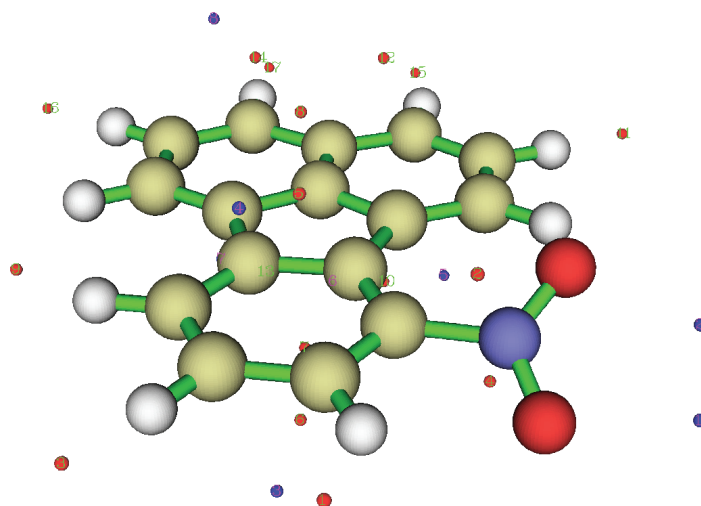


Fig. S-4. The surface extrema on the MEP surface of 7-NF (red and blue spheres are local maxima and minima, respectively) calculated at the B3LYP/6-311++G(2d,2p) level of theory.

TABLE S-IV. Energies of local minima and maxima obtained from statistical analysis of the molecular electrostatic potential of 7-NF and their Cartesian coordinates calculated at the B3LYP/6-311++G(2d,2p) level of theory; *: the lowest minimum; **: the highest maximum

Number of surface minimum	Energy, kcal mol ⁻¹	<i>X,Y,Z</i> coordinates, Å		
*1	-33.178530	-4.90421	-2.712881	-0.335613
2	32.302778	-4.01362	-3.158128	0.378116
3	-4.366100	2.455497	1.851599	-2.017195
4	-3.584358	2.092705	2.112421	2.016593
5	-7.443992	1.745000	2.253291	2.082338
6	-4.632554	2.055927	0.518373	-1.998761
7	-6.431629	3.336383	0.915174	2.029680
8	-6.617609	3.493034	0.821650	2.008159
1	16.663241	-5.100422	2.116947	-0.037832
2	13.069195	-3.673803	-0.274296	1.519493
3	21.536378	-3.518565	4.680685	-0.011362
4	15.130468	-1.931033	-1.354046	-1.427003
5	-0.961651	-1.654971	1.219337	1.814832
6	-0.828912	-1.416652	1.179030	-1.783706
7	1.070864	0.247007	0.554643	-1.829708
8	0.148726	0.350625	0.524889	1.880192
**9	25.560215	0.661915	4.440781	0.067022
10	-4.183951	1.534908	-1.155095	-1.835147
11	16.769586	1.808664	-5.250066	-0.142679
12	-4.895051	1.762206	-1.200177	1.796212
13	-3.697897	2.407576	0.508862	-1.814361
14	-3.944792	2.422371	0.519936	1.792383
15	20.336378	5.012742	-3.047057	-0.138611
16	20.078650	5.523622	3.084654	-0.015802
17	20.699730	6.066319	-0.798054	-0.140520

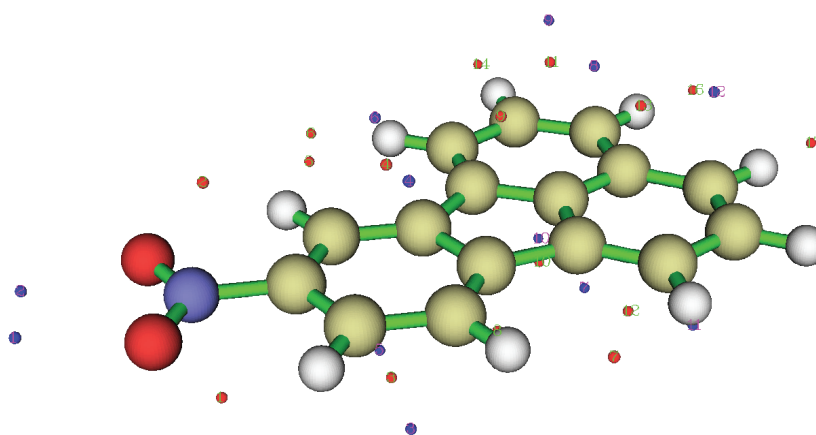


Fig. S-5. The surface extrema on the MEP surface of 8-NF (red and blue spheres are local maxima and minima, respectively) calculated at the B3LYP/6-311++G(2d,2p) level of theory.

TABLE S-V. Energies of local minima and maxima obtained from statistical analysis of the molecular electrostatic potential of 8-NF and their Cartesian coordinates calculated at the B3LYP/6-311++G(2d,2p) level of theory; *: the lowest minimum; **: the highest maximum

Number of surface minimum	Energy, kcal mol ⁻¹		<i>X,Y,Z</i> coordinates, Å	
*1	-35.728083	-6.657665	0.454461	0.052304
2	-35.681122	-6.222462	1.636816	0.000892
3	-2.519452	-1.726669	-1.544525	-2.017655
4	-2.519498	-1.685821	-1.524092	2.014658
5	-1.834833	-1.192734	0.443534	-2.010139
6	-1.838580	-1.195053	0.384740	2.004828
7	-2.256863	2.530607	0.318099	-1.979619
8	-2.257226	2.524477	0.316136	1.979714
9	-4.862517	2.822425	2.056929	2.027374
10	-4.860652	2.774069	2.109762	-2.028527
11	-4.027812	3.434446	-1.412434	-2.018554
12	-4.032397	3.481442	-1.385819	2.024236
1	10.746224	-3.904467	0.221714	-1.780773
2	10.730671	-3.911460	0.215066	1.780535
3	0.065668	-1.524681	-0.573798	-1.784064
4	0.062885	-1.528299	-0.576758	1.784140
5	21.816185	-1.031714	3.088923	0.022345
6	21.593412	-0.552938	4.026408	-0.004764
**7	25.408913	0.062652	-3.920121	0.039470
8	2.798204	0.542507	0.212339	-1.852626
9	2.798319	0.543588	0.211947	1.852458
10	-1.716946	2.166564	1.136314	-1.801749
11	-1.692616	2.234326	1.101973	1.807167
12	-1.126035	2.571818	-0.843721	-1.790539
13	-1.123284	2.577628	-0.835449	1.791149
14	20.662807	3.270295	5.021001	-0.011573
15	21.809205	4.920522	-4.051721	0.021344
16	22.353156	5.959750	2.169758	0.007732
17	22.801221	6.450427	-0.397997	-0.009016