Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Non-covalent interactions of the carcinogen (+)-*anti*-BPDE with exon 1 of the human K-ras proto-oncogene

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Supplementary Material

Table S1. Cartesian coordinates of (+)-*anti*-BPDE with rotatable hydroxyl groups corresponding to type **I** site.

C	-1.81600	28.25900	388.91000
C	-2.17700	29.19900	388.04600
C	-1.59000	30.41000	387.86400
C	-0.52100	30.74700	388.75300
C	0.09600	32.02300	388.64200
C	1.12000	32.40300	389.46800
C	1.61500	31.44600	390.48100
C	2.60200	31.78100	391.33900
C	3.11800	30.87700	392.21600
C	4.33200	31.28800	393.09400
C	4.47900	30.40600	394.33500
C	4.30900	28.98000	394.07100
C	3.38300	28.54200	393.06600
C	2.64200	29.56100	392.28000
C	1.51100	29.22600	391.45000
C	0.88200	27.91600	391.60000
C	-0.19300	27.63100	390.76800
C	-0.71600	28.54000	389.78900
C	-0.07700	29.83600	389.69200
C	1.01200	30.16500	390.54200
O	4.79900	28.51500	392.77600
O	4.20000	32.66300	393.50000
H	3.22900	32.75600	393.90000
O	5.74800	30.71600	394.93000
H	5.31900	31.19700	395.77200

Table S2. Cartesian coordinates of (+)-*anti*-BPDE with rotatable hydroxyl groups corresponding to type **IIa** site.

C	2.44200	24.24300	211.58600
C	2.22100	25.52500	211.32700
C	1.27200	26.31900	211.88500
C	0.35700	25.69100	212.78700
C	-0.69000	26.46200	213.36200
C	-1.59800	25.91500	214.22900
C	-1.46500	24.48900	214.59800
C	-2.35000	23.89300	215.42500
C	-2.18400	22.60500	215.83400
C	-3.17100	22.01400	216.87800
C	-3.18600	20.48400	216.86600
C	-1.85800	19.88100	216.79700
C	-0.81200	20.52900	216.05700
C	-1.09600	21.83300	215.40700
C	-0.20900	22.42200	214.43400
C	0.84500	21.60000	213.84400
C	1.68600	22.21300	212.92400
C	1.57500	23.58600	212.52300
C	0.50200	24.35600	213.11700
C	-0.38700	23.75300	214.04500
O	-0.80000	20.60000	217.50100
O	-4.50100	22.50500	216.62900
H	-5.09800	22.14100	217.41800
O	-3.93500	20.05600	218.01300
H	-4.85800	20.41800	217.63600

Table S3. Cartesian coordinates of (+)-*anti*-BPDE with rotatable hydroxyl groups corresponding to type **IIb** site.

C	-1.30300	11.52800	189.42300
C	-2.09400	10.48400	189.22100
C	-2.00300	9.26300	189.80900
C	-0.88500	9.05000	190.67600
C	-0.71000	7.77300	191.27800
C	0.34300	7.50900	192.11300
C	1.30400	8.59000	192.41800
C	2.37500	8.37400	193.21100
C	3.21500	9.38600	193.56200
C	4.35900	9.09800	194.57300
C	5.48300	10.13300	194.49100
C	5.01200	11.51300	194.40300
C	3.79700	11.81200	193.70000
C	3.01700	10.69600	193.10800
C	1.94400	10.91500	192.16900
C	1.80000	12.23000	191.54800
C	0.74400	12.40000	190.66300
C	-0.19500	11.37000	190.32400
C	0.00000	10.07600	190.94500
C	1.08200	9.86500	191.83900
O	3.79100	11.81100	195.14600
O	4.90200	7.78600	194.33800
H	5.74600	7.70400	194.96400
O	6.35000	9.91000	195.61200
H	7.20200	10.31700	195.12800