

Electronic Supplementary Information

Incorporation of deuterium oxide in MCF-7 cells to shed further mechanistic insights into benzo[*a*]pyrene-induced low-dose effects discriminated by ATR-FTIR spectroscopy

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A)

Trial	DMSO	10 ⁻¹⁰ M	10 ⁻⁶ M
1	372	310	0
2	304	221	0
2	362	213	0

B)

Parameter	Value			
One-way analysis of variance				
<i>P</i> -value	<i>P</i> < 0.0001			
<i>P</i> -value summary	***			
Means significantly different? (<i>P</i> < 0.05)	Yes			
Number of groups	3			
F	67.4			
R ²	0.9574			
ANOVA table				
	SS	df	MS	
Treatment (between columns)	190800	2	95410	
Residual (within columns)	8494	6	1416	
Total	199300	8		
Tukey's Multiple Comparison Test				
	Mean Diff.	q	<i>P</i> -value	95% CI of diff
10 ⁻⁶ M vs. 10 ⁻¹⁰ M	-248	11.42	<i>P</i> < 0.001	-342.3 to -153.7
10 ⁻⁶ M vs. DMSO	-346	15.93	<i>P</i> < 0.001	-440.3 to -251.7
10 ⁻¹⁰ M vs. DMSO	-98	4.511	<i>P</i> < 0.05	-192.3 to -3.744

Figure S1. Clonogenic assay: one-way ANOVA with Tukey's multiple comparison post-hoc test.

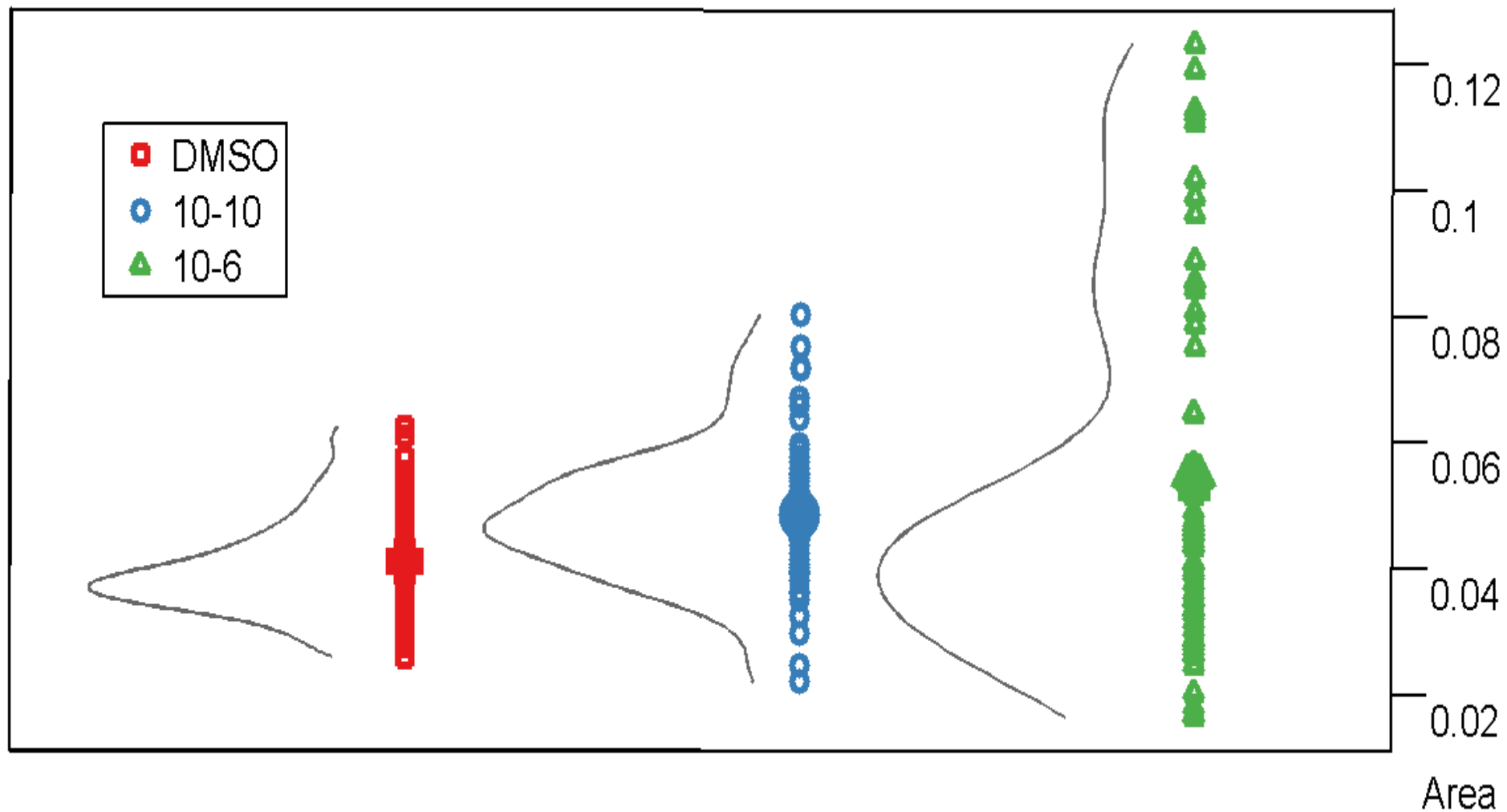


Figure S2. Protocol 1 - S-phase: protein-to-lipid ratio (1760-1720 cm⁻¹ vs. 1420-1380 cm⁻¹).

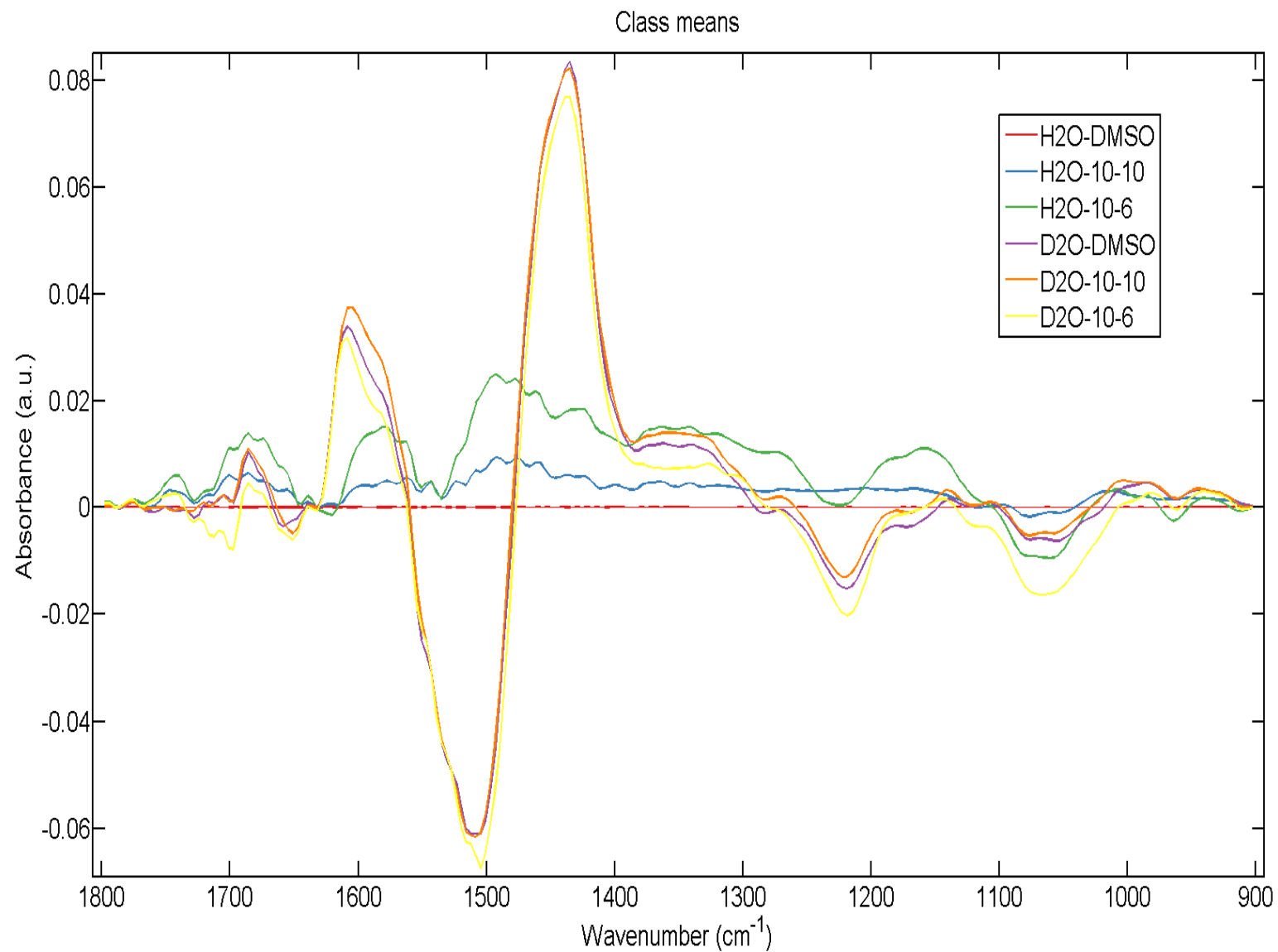


Figure S3. Protocol 2 – D₂O- vs. H₂O-fixed class means with a reference mean subtracted (H₂O: DMSO).

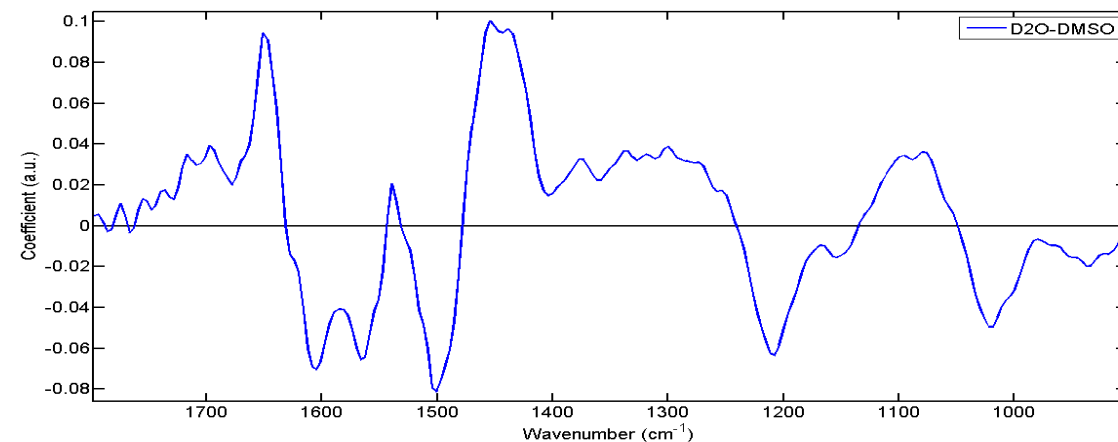


Figure S4A. Protocol 2: Vehicle control DMSO treatments fixed in 70% EtOH + 30% D₂O compared to fixation in 70% EtOH + 30% dH₂O alone.

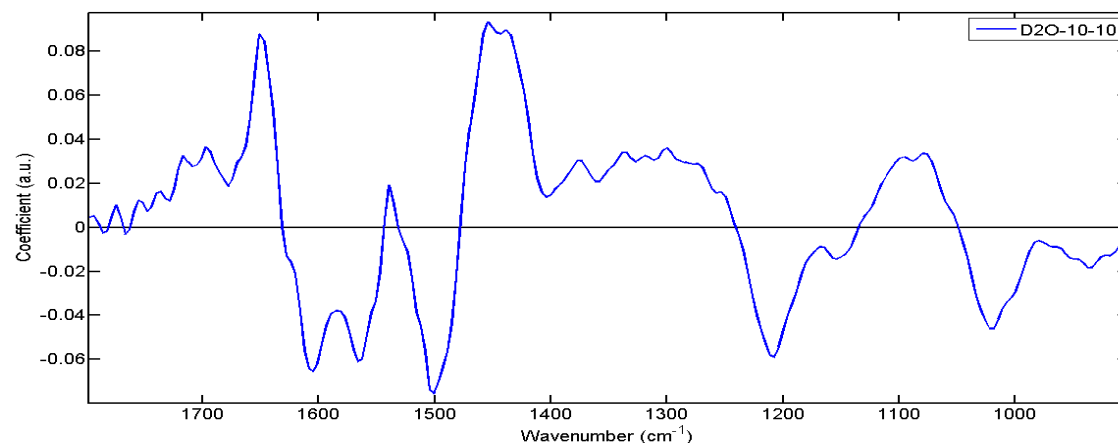


Figure S4B. Protocol 2: Low-dose 10⁻¹⁰ M B[a]P treatments fixed in 70% EtOH + 30% D₂O compared to fixation in 70% EtOH + 30% dH₂O alone.

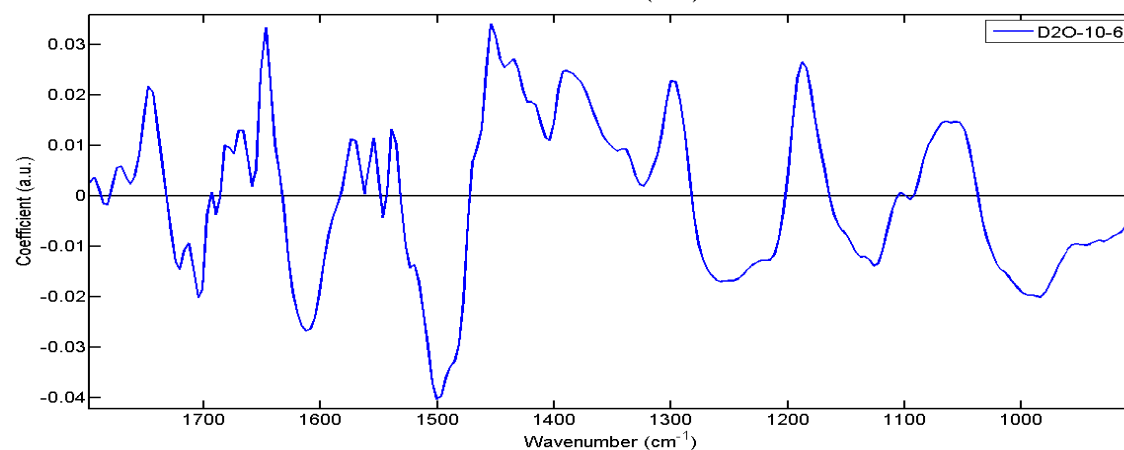


Figure S4C. Protocol 2: High-dose 10⁻⁶ M B[a]P treatments fixed in 70% EtOH + 30% D₂O compared to fixation in 70% EtOH + 30% dH₂O alone.