

# Supporting Information

Towards less hazardous industrial compounds: coupling quantum mechanical computations, biomarker responses and behavioral profiles identify bioactivity of SN2 electrophiles in alternative vertebrate models

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### Supplemental Figures

Figure S1: Mean zebrafish dark (A) and light (B) swimming activity compared to mean fathead minnow dark (C) and light (D) activity after 96 h exposure to 3-Bromo-1-Propanol. Plotted data represents activity over two ten minute dark photoperiods and two ten minute light photoperiods for each fish model. Data is normalized to control, which is represented at the 0 axis in each figure. Behavioral parameters include distance swam, number of movements (counts), and duration of each movement across 3 speed levels, bursting ( $>20$  mm/sec), cruising (5-20 mm/sec), and freezing ( $<5$  mm/sec). In addition to movement patterns at each of the speed thresholds, total distance swam and total number of movements is represented.  $\uparrow$  represents a significant increase in activity in comparison to control and  $\downarrow$  indicates a significant decrease in activity in comparison to control. A total of 24 (N = 4 replicates of each treatment level, 6 larvae in each experimental unit) zebrafish and 12 (N = 3 replicates of each treatment level, 4 larvae in each experimental unit) fathead minnow were used in behavioral observations for each group. \* $p < 0.10$ ; \*\* $p < 0.05$ ; \*\*\* $p < 0.01$ .

Figure S1

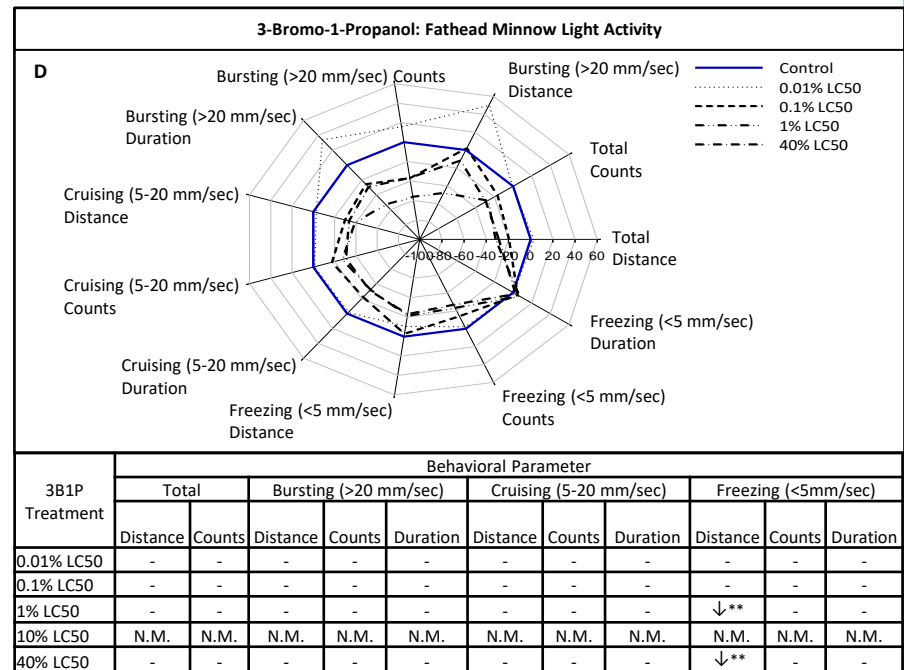
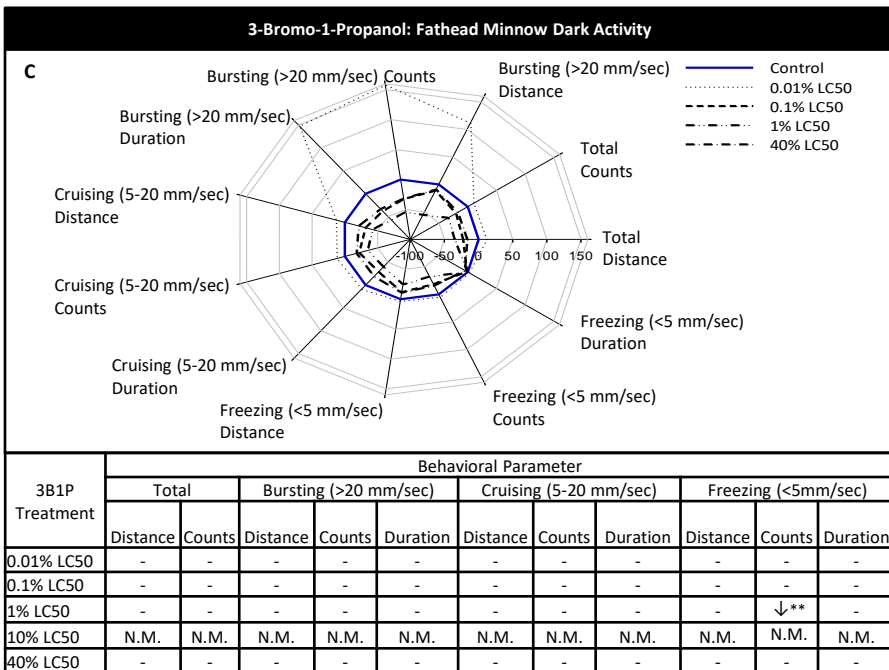
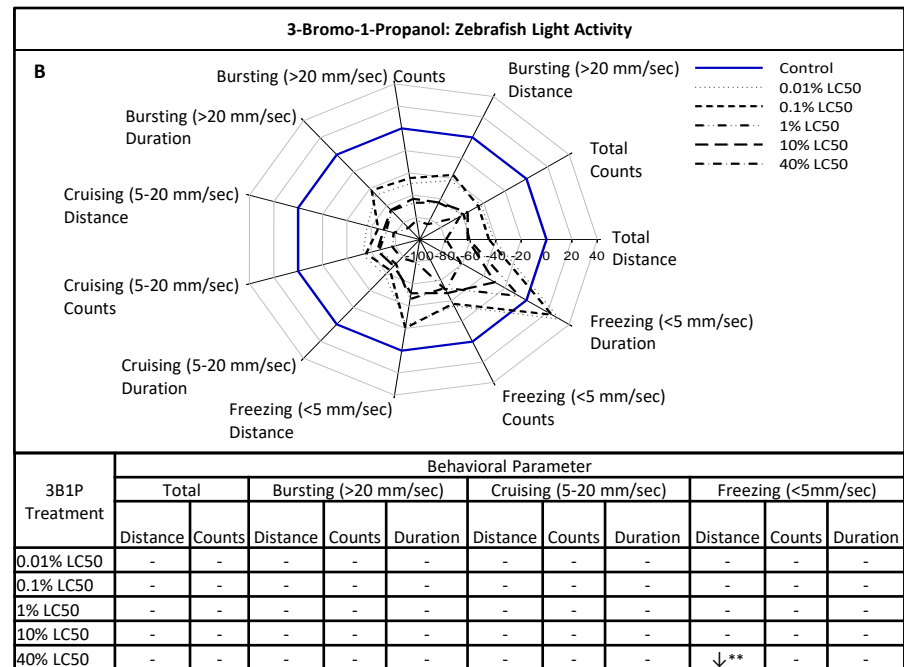
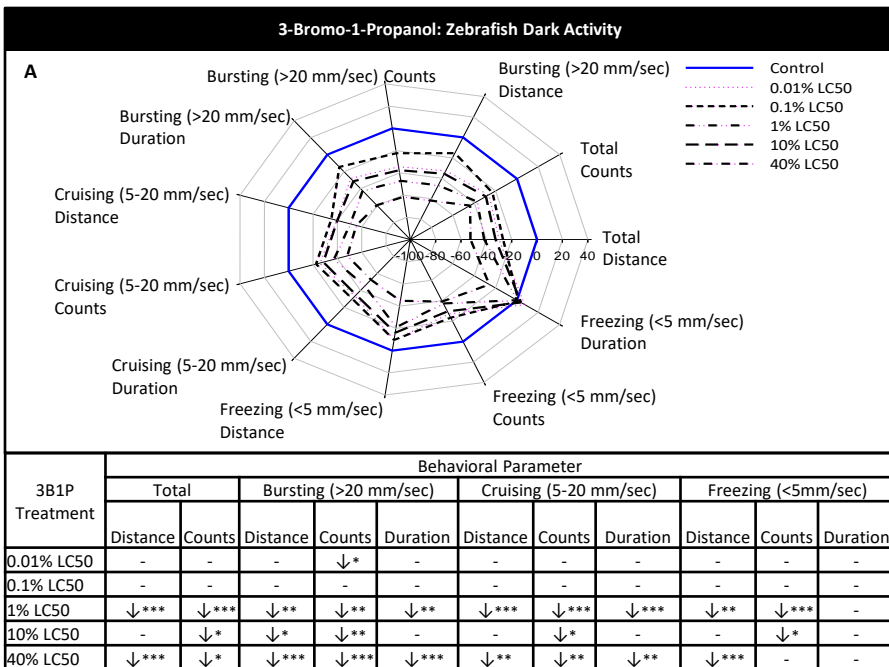
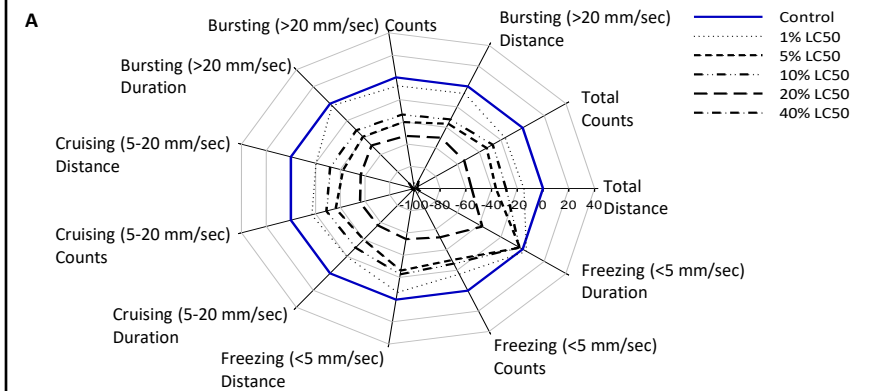


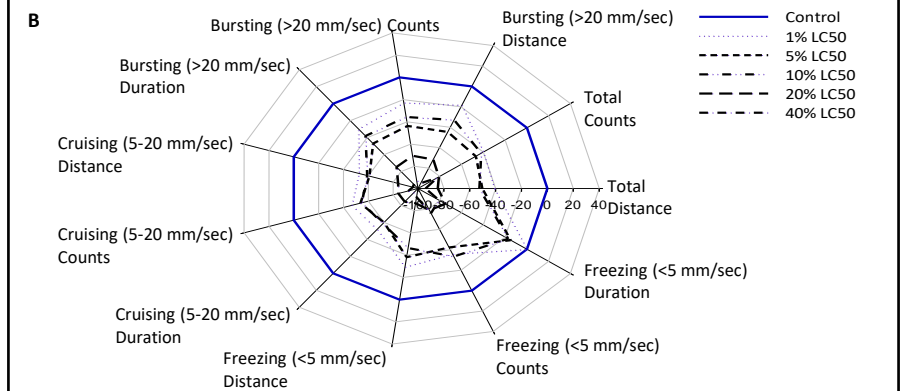
Figure S2: Mean zebrafish dark (A) and light (B) swimming activity compared to mean fathead minnow dark (C) and light (D) activity after 96 h exposure to 3-chloro-1,2-propanediol. Plotted data represents activity over two ten minute dark photoperiods and two ten minute light photoperiods for each fish model. Data is normalized to control, which is represented at the 0 axis in each figure. Behavioral parameters include distance swam, number of movements (counts), and duration of each movement across 3 speed levels, bursting (>20 mm/sec), cruising (5-20 mm/sec), and freezing (<5 mm/sec). In addition to movement patterns at each of the speed thresholds, total distance swam and total number of movements is represented. ↑ represents a significant increase in activity in comparison to control and ↓ indicates a significant decrease in activity in comparison to control. A total of 24 (N = 4 replicates of each treatment level, 6 larvae in each experimental unit) zebrafish and 12 (N = 3 replicates of each treatment level, 4 larvae in each experimental unit) fathead minnow were used in behavioral observations for each group. \*p<0.10; \*\*p<0.05; \*\*\*p<0.01.

## 3-chloro-1,2-propanediol: Zebrafish Dark Activity



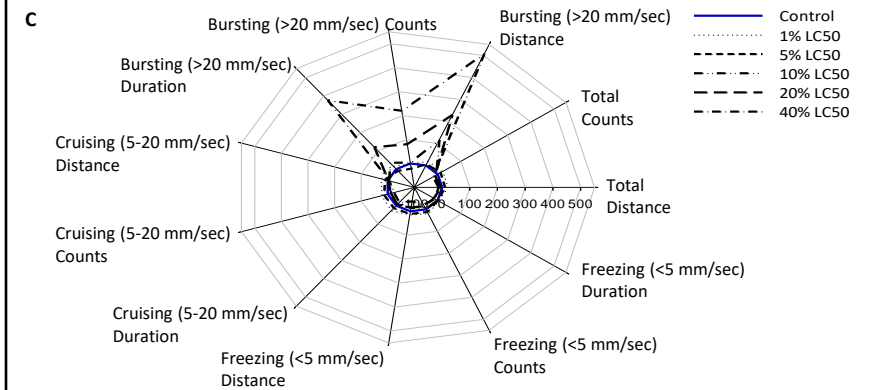
CPD Treatment	Behavioral Parameter										
	Total		Bursting (>20 mm/sec)			Cruising (5-20 mm/sec)			Freezing (<5mm/sec)		
	Distance	Counts	Distance	Counts	Duration	Distance	Counts	Duration	Distance	Counts	Duration
1% LC50	-	-	-	-	-	-	-	-	-	-	-
5% LC50	-	↓***	-	-	-	-	-	-	↓**	↓***	-
10% LC50	-	↓**	-	-	-	-	-	-	↓*	↓***	-
20% LC50	↓**	↓***	↓*	↓*	↓*	↓**	↓**	↓**	↓***	↓***	-
40% LC50	↓***	↓***	↓***	↓***	↓***	↓***	↓***	↓***	↓***	↓***	↓**

## 3-chloro-1,2-propanediol: Zebrafish Light Activity



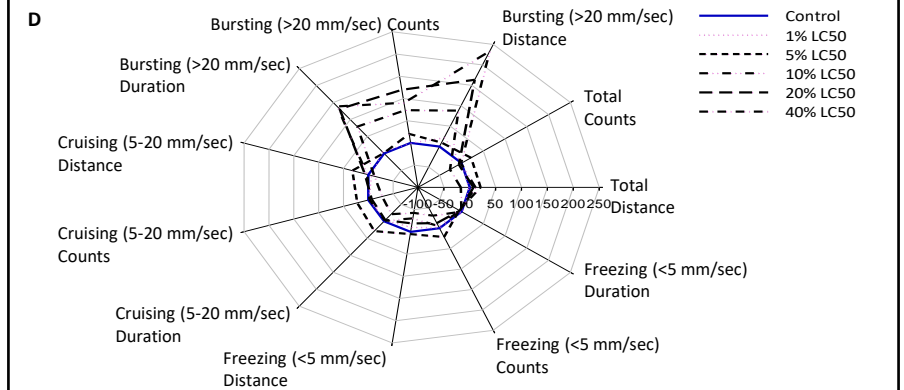
CPD Treatment	Behavioral Parameter										
	Total		Bursting (>20 mm/sec)			Cruising (5-20 mm/sec)			Freezing (<5mm/sec)		
	Distance	Counts	Distance	Counts	Duration	Distance	Counts	Duration	Distance	Counts	Duration
1% LC50	-	-	-	-	-	-	-	-	-	-	-
5% LC50	-	-	-	-	-	-	-	-	-	-	-
10% LC50	↓*	-	-	-	-	-	-	-	-	-	-
20% LC50	↓***	↓***	-	↓*	-	↓***	↓***	↓***	↓***	↓**	↓**
40% LC50	↓***	↓***	↓***	↓***	↓**	↓***	↓***	↓***	↓***	↓***	↓**

## 3-chloro-1,2-propanediol: Fathead Minnow Dark Activity



CPD Treatment	Behavioral Parameter										
	Total		Bursting (>20 mm/sec)			Cruising (5-20 mm/sec)			Freezing (<5mm/sec)		
	Distance	Counts	Distance	Counts	Duration	Distance	Counts	Duration	Distance	Counts	Duration
1% LC50	-	-	-	-	-	-	-	-	-	-	-
5% LC50	-	-	-	-	-	-	-	-	-	-	-
10% LC50	-	-	-	-	-	-	-	-	-	-	-
20% LC50	-	-	-	-	-	-	-	-	-	-	-
40% LC50	-	-	↑***	-	↑**	-	-	-	↓*	-	-

## 3-chloro-1,2-propanediol: Fathead Minnow Light Activity



CPD Treatment	Behavioral Parameter										
	Total		Bursting (>20 mm/sec)			Cruising (5-20 mm/sec)			Freezing (<5mm/sec)		
	Distance	Counts	Distance	Counts	Duration	Distance	Counts	Duration	Distance	Counts	Duration
1% LC50	-	-	-	-	-	-	-	-	-	-	-
5% LC50	-	-	-	-	-	-	-	-	-	-	-
10% LC50	-	-	-	-	-	-	-	-	↓*	-	-
20% LC50	-	-	-	-	-	-	-	-	-	-	-
40% LC50	-	-	-	-	-	-	-	-	↓**	-	-

Figure S3: Mean zebrafish dark (A) and light (B) swimming activity compared to mean fathead minnow dark (C) and light (D) activity after 96 h exposure to Dibromoacetonitrile. Plotted data represents activity over two ten minute dark photoperiods and two ten minute light photoperiods for each fish model. Data is normalized to control, which is represented at the 0 axis in each figure. Behavioral parameters include distance swam, number of movements (counts), and duration of each movement across 3 speed levels, bursting (>20 mm/sec), cruising (5-20 mm/sec), and freezing (<5 mm/sec). In addition to movement patterns at each of the speed thresholds, total distance swam and total number of movements is represented. ↑ represents a significant increase in activity in comparison to control and ↓ indicates a significant decrease in activity in comparison to control. A total of 24 (N = 4 replicates of each treatment level, 6 larvae in each experimental unit) zebrafish and 12 (N = 3 replicates of each treatment level, 4 larvae in each experimental unit) fathead minnow were used in behavioral observations for each group. \*p<0.10; \*\*p<0.05; \*\*\*p<0.01.

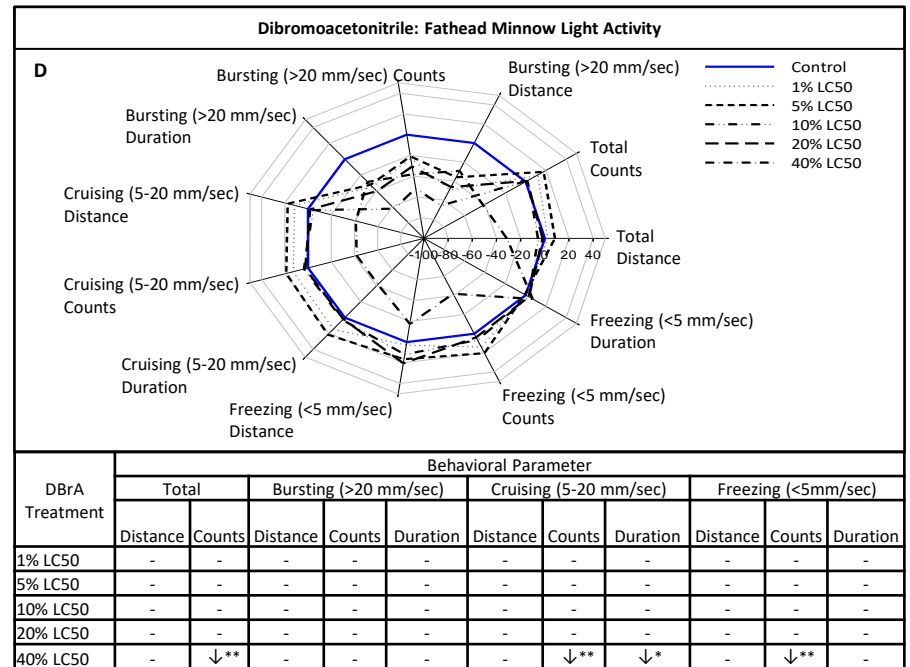
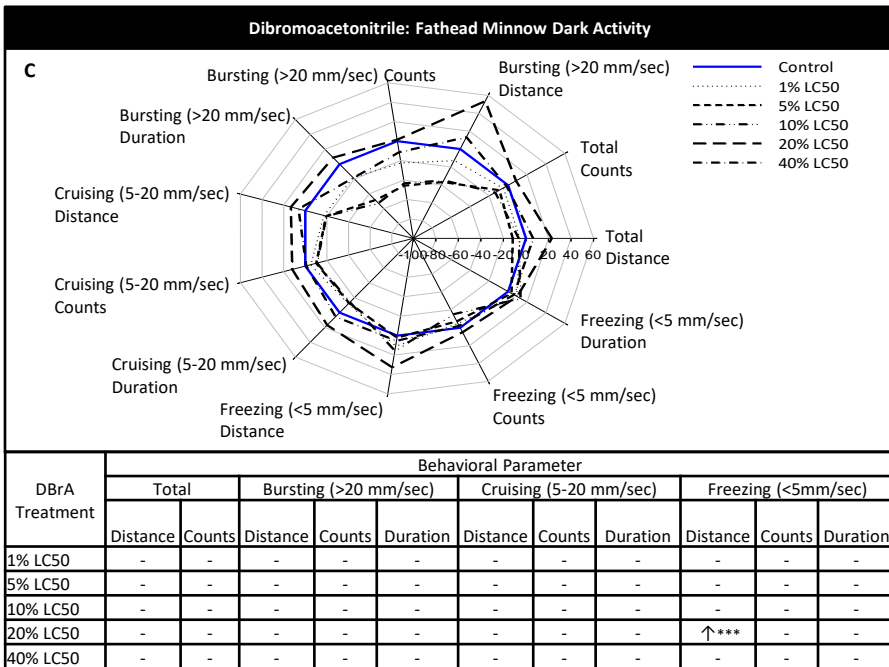
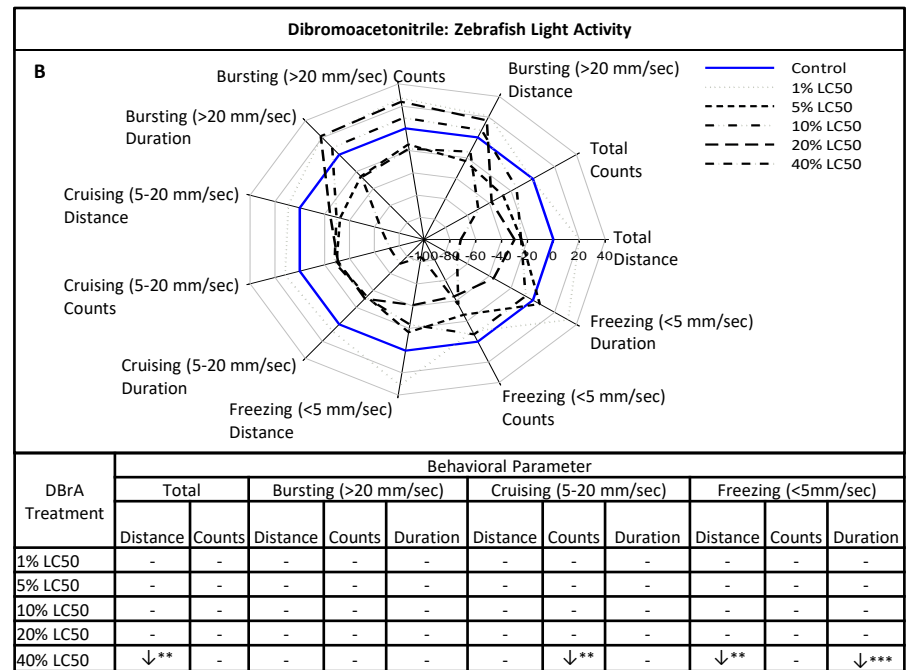
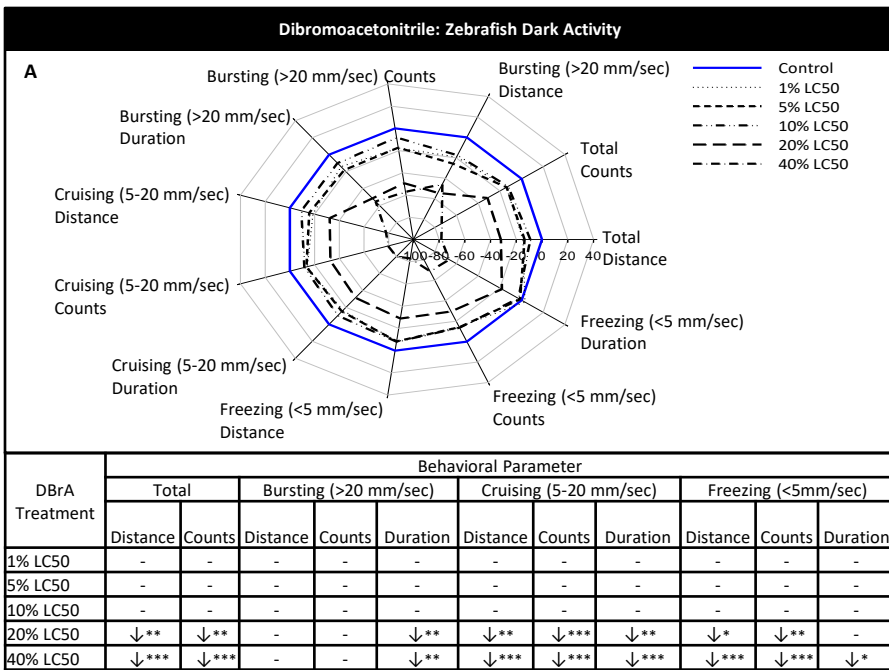




Figure S4: Mean zebrafish dark (A) and light (B) swimming activity compared to mean fathead minnow dark (C) and light (D) activity after 96 h exposure to Glycidol. Plotted data represents activity over two ten minute dark photoperiods and two ten minute light photoperiods for each fish model. Data is normalized to control, which is represented at the 0 axis in each figure. Behavioral parameters include distance swam, number of movements (counts), and duration of each movement across 3 speed levels, bursting (>20 mm/sec), cruising (5-20 mm/sec), and freezing (<5 mm/sec). In addition to movement patterns at each of the speed thresholds, total distance swam and total number of movements is represented. ↑ represents a significant increase in activity in comparison to control and ↓ indicates a significant decrease in activity in comparison to control. A total of 24 (N = 4 replicates of each treatment level, 6 larvae in each experimental unit) zebrafish and 12 (N = 3 replicates of each treatment level, 4 larvae in each experimental unit) fathead minnow were used in behavioral observations for each group. \*p<0.10; \*\*p<0.05; \*\*\*p<0.01.

Figure S4

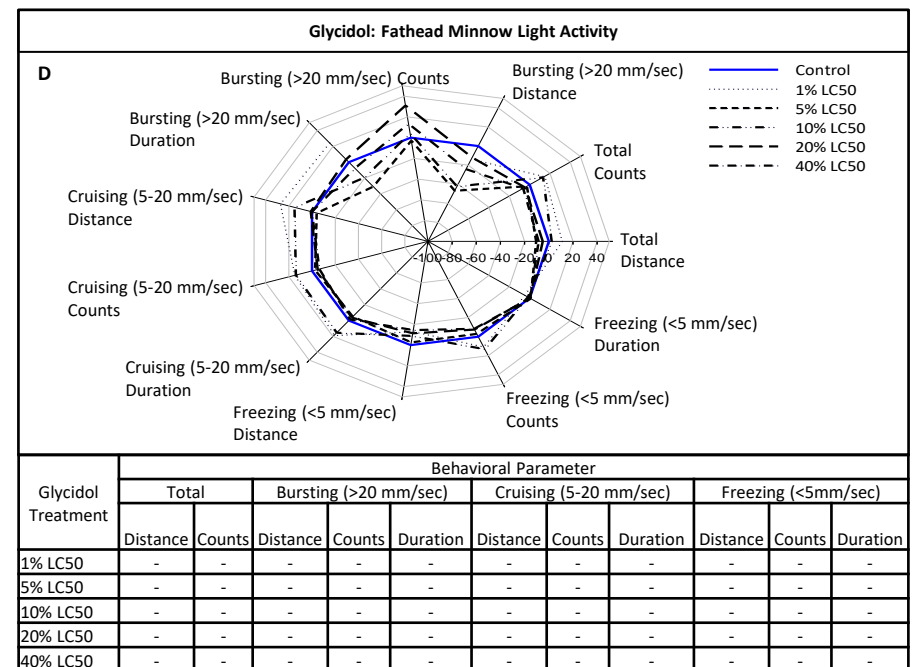
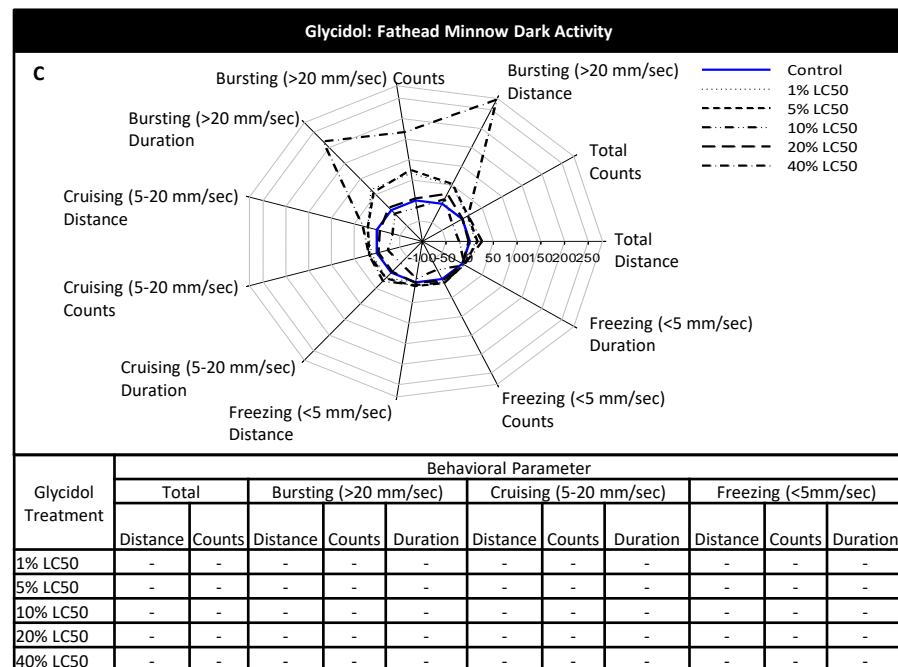
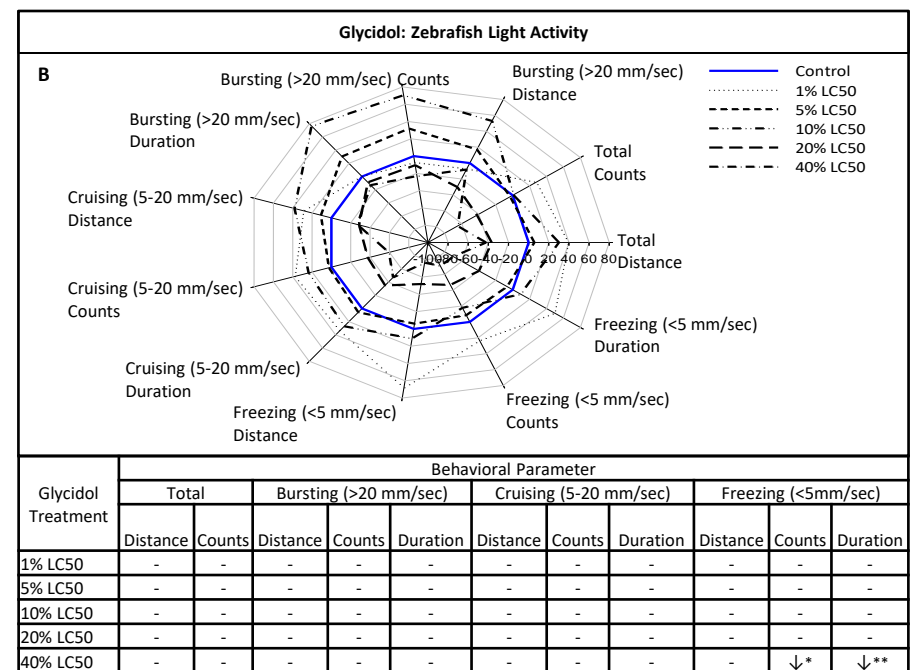
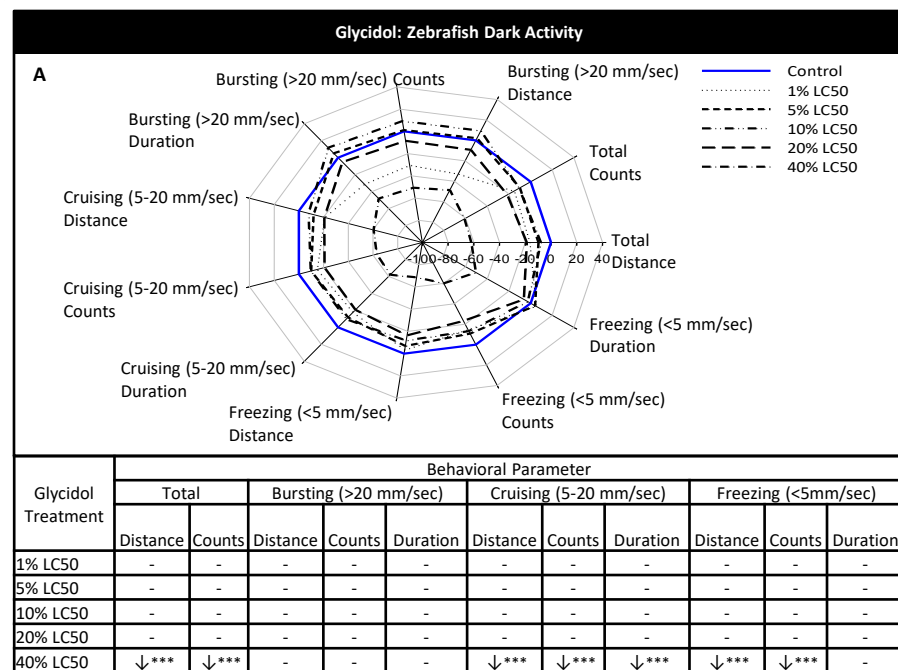
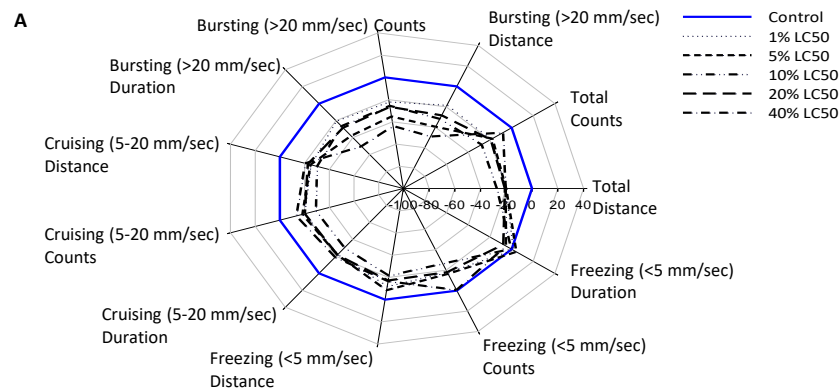


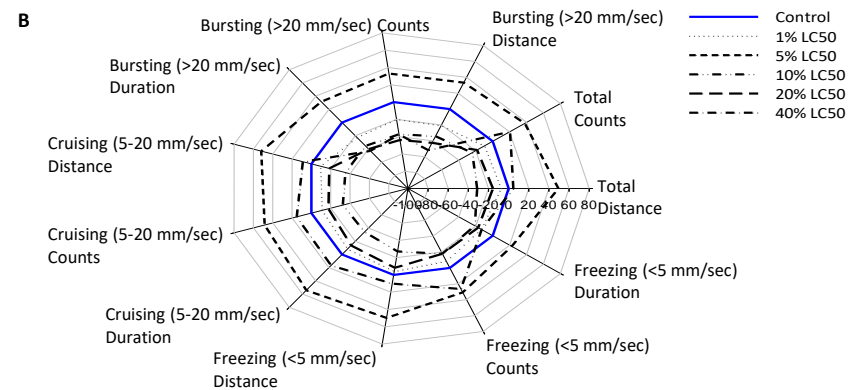
Figure S5: Mean zebrafish dark (A) and light (B) swimming activity compared to mean fathead minnow dark (C) and light (D) activity after 96 h exposure to Sodium decyl sulfate. Plotted data represents activity over two ten minute dark photoperiods and two ten minute light photoperiods for each fish model. Data is normalized to control, which is represented at the 0 axis in each figure. Behavioral parameters include distance swam, number of movements (counts), and duration of each movement across 3 speed levels, bursting (>20 mm/sec), cruising (5-20 mm/sec), and freezing (<5 mm/sec). In addition to movement patterns at each of the speed thresholds, total distance swam and total number of movements is represented. ↑ represents a significant increase in activity in comparison to control and ↓ indicates a significant decrease in activity in comparison to control. A total of 24 (N = 4 replicates of each treatment level, 6 larvae in each experimental unit) zebrafish and 12 (N = 3 replicates of each treatment level, 4 larvae in each experimental unit) fathead minnow were used in behavioral observations for each group. \*p<0.10; \*\*p<0.05; \*\*\*p<0.01.

## Sodium decyl sulfate: Zebrafish Dark Activity



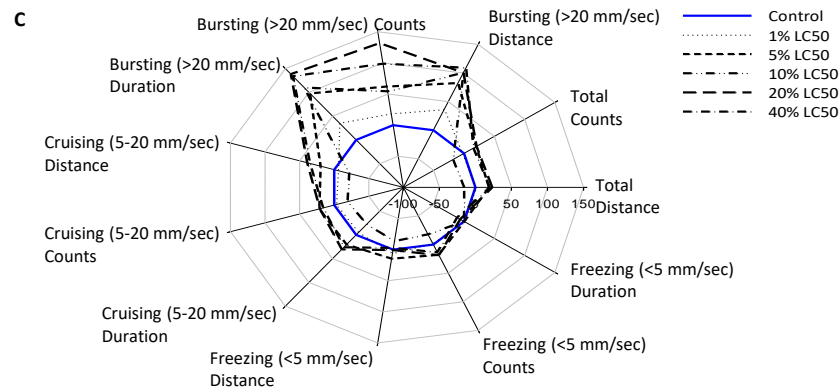
SDS Treatment	Behavioral Parameter										
	Total		Bursting (>20 mm/sec)			Cruising (5-20 mm/sec)			Freezing (<5mm/sec)		
	Distance	Counts	Distance	Counts	Duration	Distance	Counts	Duration	Distance	Counts	Duration
1% LC50	-	-	↓**	↓**	↓*	-	-	-	-	-	-
5% LC50	-	-	-	-	-	-	-	-	-	-	-
10% LC50	-	-	-	-	-	-	-	-	-	-	-
20% LC50	-	-	-	-	-	-	-	-	-	-	-
40% LC50	-	-	↓**	↓**	↓***	-	-	-	-	-	-

## Sodium decyl sulfate: Zebrafish Light Activity



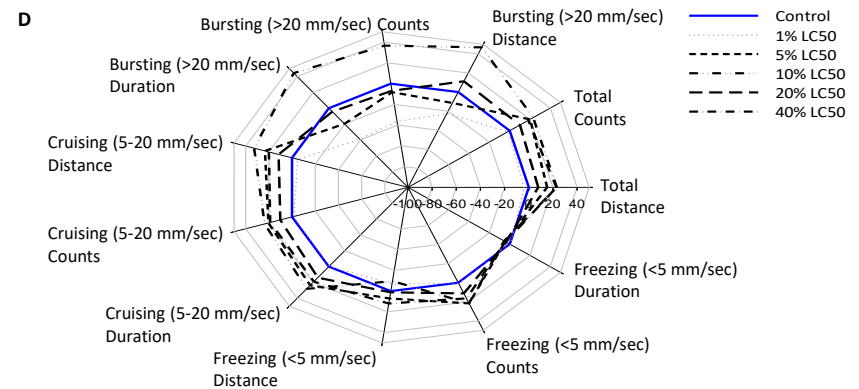
SDS Treatment	Behavioral Parameter										
	Total		Bursting (>20 mm/sec)			Cruising (5-20 mm/sec)			Freezing (<5mm/sec)		
	Distance	Counts	Distance	Counts	Duration	Distance	Counts	Duration	Distance	Counts	Duration
1% LC50	-	-	-	-	-	-	-	-	-	-	-
5% LC50	-	-	-	-	-	-	-	-	-	-	-
10% LC50	-	-	-	-	-	-	-	-	-	-	-
20% LC50	-	-	-	-	-	-	-	-	-	-	-
40% LC50	-	-	-	-	-	-	-	-	-	-	-

## Sodium decyl sulfate: Fathead Minnow Dark Activity



SDS Treatment	Behavioral Parameter										
	Total		Bursting (>20 mm/sec)			Cruising (5-20 mm/sec)			Freezing (<5mm/sec)		
	Distance	Counts	Distance	Counts	Duration	Distance	Counts	Duration	Distance	Counts	Duration
1% LC50	-	-	-	-	-	-	-	-	-	-	-
5% LC50	-	-	-	-	-	-	-	-	-	-	-
10% LC50	-	-	-	-	-	-	-	-	-	-	-
20% LC50	-	-	-	-	-	-	-	-	-	-	-
40% LC50	-	-	-	-	-	-	-	-	-	-	-

## Sodium decyl sulfate: Fathead Minnow Light Activity



SDS Treatment	Behavioral Parameter										
	Total		Bursting (>20 mm/sec)			Cruising (5-20 mm/sec)			Freezing (<5mm/sec)		
	Distance	Counts	Distance	Counts	Duration	Distance	Counts	Duration	Distance	Counts	Duration
1% LC50	-	-	-	-	-	-	-	-	-	-	-
5% LC50	-	-	-	-	-	-	-	-	-	-	-
10% LC50	-	-	-	-	-	-	-	-	-	-	-
20% LC50	-	-	-	-	-	-	-	-	-	-	-
40% LC50	-	-	-	-	-	-	-	-	-	-	-

Figure S6: Mean zebrafish dark (A) and light (B) swimming activity compared to mean fathead minnow dark (C) and light (D) activity after 96 h exposure to Styrene Oxide. Plotted data represents activity over two ten minute dark photoperiods and two ten minute light photoperiods for each fish model. Data is normalized to control, which is represented at the 0 axis in each figure. Behavioral parameters include distance swam, number of movements (counts), and duration of each movement across 3 speed levels, bursting (>20 mm/sec), cruising (5-20 mm/sec), and freezing (<5 mm/sec). In addition to movement patterns at each of the speed thresholds, total distance swam and total number of movements is represented. ↑ represents a significant increase in activity in comparison to control and ↓ indicates a significant decrease in activity in comparison to control. A total of 24 (N = 4 replicates of each treatment level, 6 larvae in each experimental unit) zebrafish and 12 (N = 3 replicates of each treatment level, 4 larvae in each experimental unit) fathead minnow were used in behavioral observations for each group. \*p<0.10; \*\*p<0.05; \*\*\*p<0.01.

Figure S6

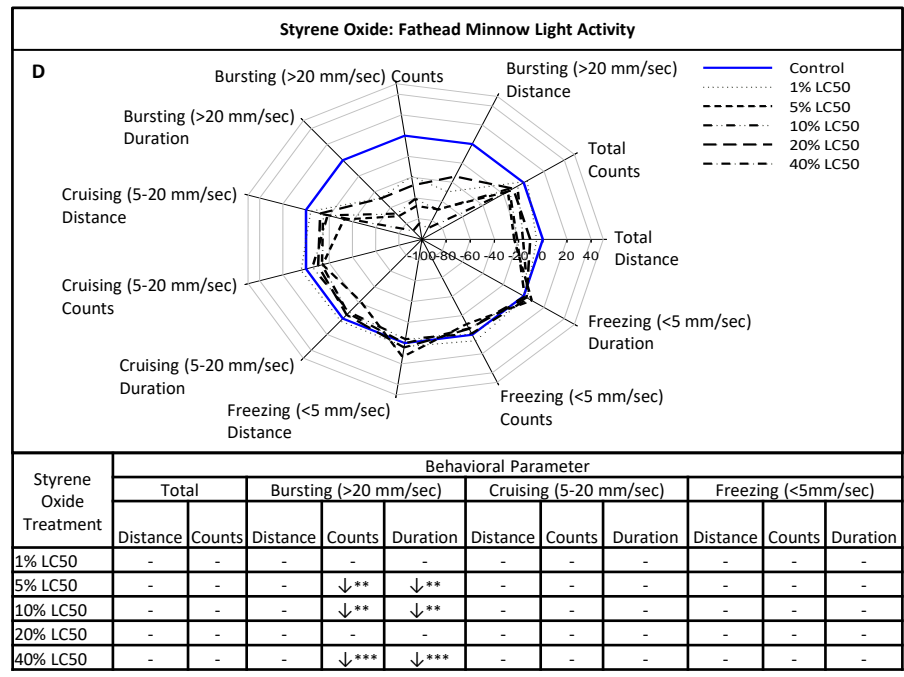
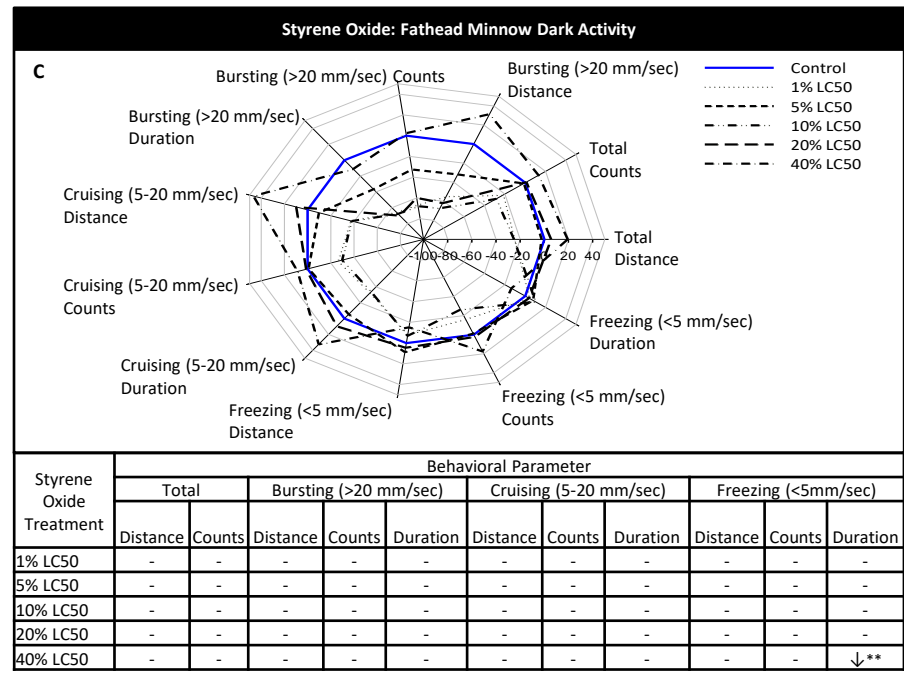
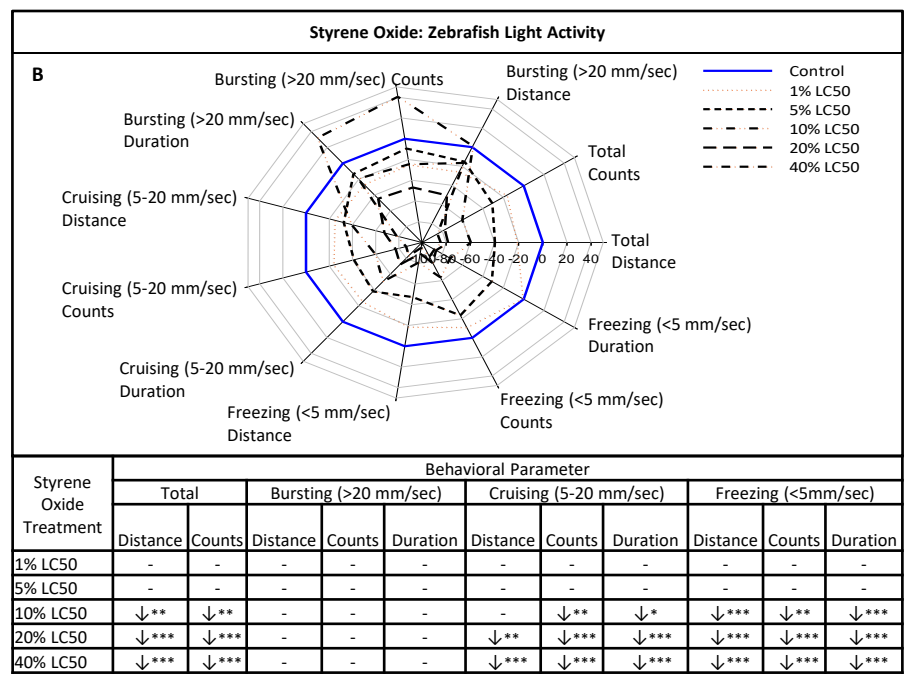
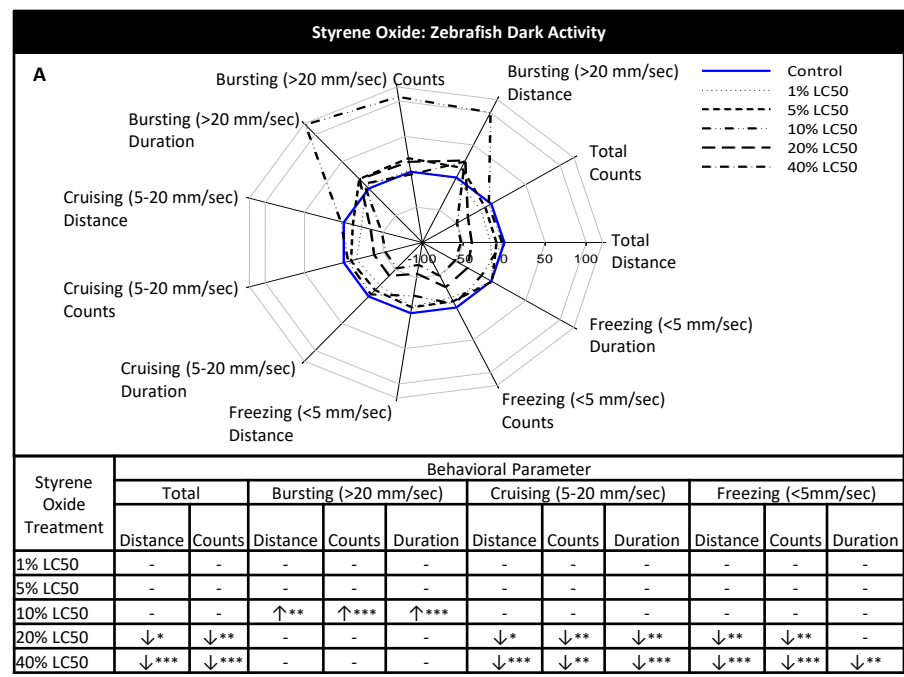
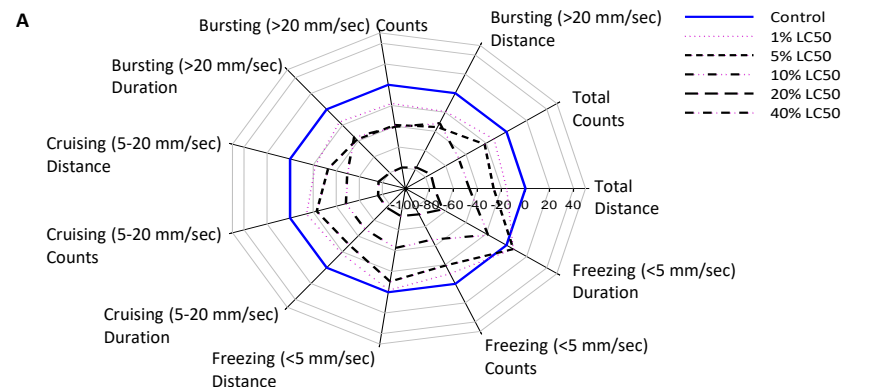


Figure S7: Mean zebrafish dark (A) and light (B) swimming activity compared to mean fathead minnow dark (C) and light (D) activity after 96 h exposure to TBPP. Plotted data represents activity over two ten minute dark photoperiods and two ten minute light photoperiods for each fish model. Data is normalized to control, which is represented at the 0 axis in each figure. Behavioral parameters include distance swam, number of movements (counts), and duration of each movement across 3 speed levels, bursting ( $>20$  mm/sec), cruising (5-20 mm/sec), and freezing ( $<5$  mm/sec). In addition to movement patterns at each of the speed thresholds, total distance swam and total number of movements is represented.  $\uparrow$  represents a significant increase in activity in comparison to control and  $\downarrow$  indicates a significant decrease in activity in comparison to control. A total of 24 (N = 4 replicates of each treatment level, 6 larvae in each experimental unit) zebrafish and 12 (N = 3 replicates of each treatment level, 4 larvae in each experimental unit) fathead minnow were used in behavioral observations for each group. \* $p<0.10$ ; \*\* $p<0.05$ ; \*\*\* $p<0.01$ .

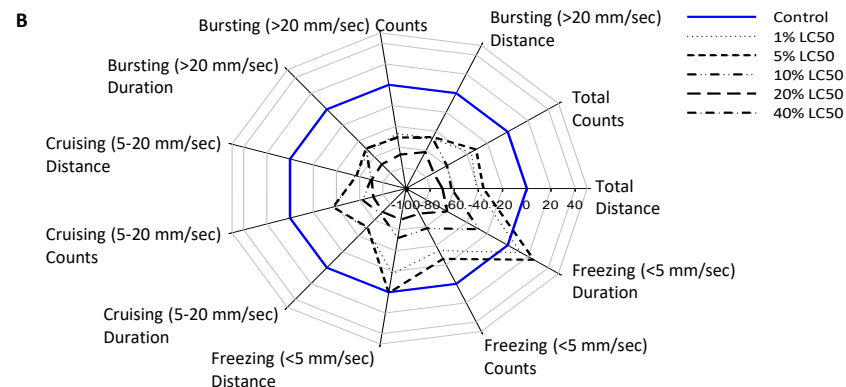
Figure S7

## Tris(2,3-dibromopropyl) phosphate: Zebrafish Dark Activity



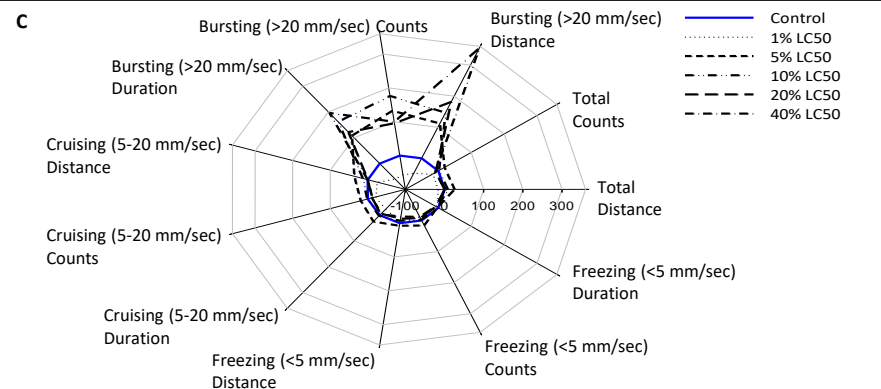
TBPP Treatment	Behavioral Parameter										
	Total		Bursting (>20 mm/sec)			Cruising (5-20 mm/sec)			Freezing (<5mm/sec)		
	Distance	Counts	Distance	Counts	Duration	Distance	Counts	Duration	Distance	Counts	Duration
1% LC50	-	-	-	-	-	-	-	-	-	-	-
5% LC50	↓*	-	-	-	-	-	↓*	↓**	-	-	-
10% LC50	↓***	↓***	-	-	-	-	↓*	↓***	↓***	↓***	-
20% LC50	↓***	↓***	↓***	↓***	↓***	↓***	↓***	↓***	↓***	↓***	-
40% LC50	↓***	↓***	↓***	↓***	↓***	↓***	↓***	↓***	↓***	↓***	-

## Tris(2,3-dibromopropyl) phosphate: Zebrafish Light Activity



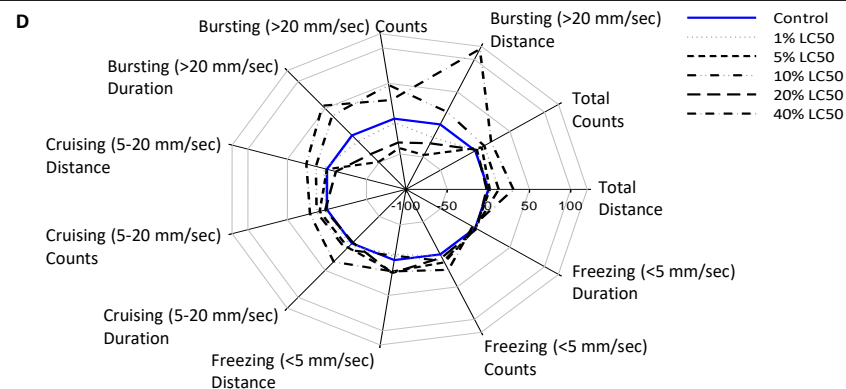
TBPP Treatment	Behavioral Parameter										
	Total		Bursting (>20 mm/sec)			Cruising (5-20 mm/sec)			Freezing (<5mm/sec)		
	Distance	Counts	Distance	Counts	Duration	Distance	Counts	Duration	Distance	Counts	Duration
1% LC50	-	-	↓*	-	-	-	-	-	-	↓*	-
5% LC50	-	-	-	-	-	-	-	-	-	-	-
10% LC50	↓*	-	↓*	-	-	↓**	-	↓*	↓*	↓***	-
20% LC50	↓**	↓**	↓**	-	-	↓*	↓**	↓*	↓***	↓***	↓***
40% LC50	↓***	↓***	↓***	↓***	↓***	↓***	↓***	↓***	↓***	↓***	↓***

## Tris(2,3-dibromopropyl) phosphate: Fathead Minnow Dark Activity



TBPP Treatment	Behavioral Parameter										
	Total		Bursting (>20 mm/sec)			Cruising (5-20 mm/sec)			Freezing (<5mm/sec)		
	Distance	Counts	Distance	Counts	Duration	Distance	Counts	Duration	Distance	Counts	Duration
1% LC50	-	-	-	-	-	-	-	-	-	-	-
5% LC50	-	-	-	-	-	-	-	-	-	-	-
10% LC50	-	-	-	-	-	-	-	-	-	-	-
20% LC50	-	-	-	-	-	-	-	-	-	-	-
40% LC50	-	-	-	-	-	-	-	-	-	-	-

## Tris(2,3-dibromopropyl) phosphate: Fathead Minnow Light Activity



TBPP Treatment	Behavioral Parameter										
	Total		Bursting (>20 mm/sec)			Cruising (5-20 mm/sec)			Freezing (<5mm/sec)		
	Distance	Counts	Distance	Counts	Duration	Distance	Counts	Duration	Distance	Counts	Duration
1% LC50	-	-	-	-	-	-	-	-	-	-	-
5% LC50	-	-	-	-	-	-	-	-	-	-	-
10% LC50	-	-	-	-	-	-	-	-	-	-	-
20% LC50	-	-	-	-	-	-	-	-	-	-	-
40% LC50	-	-	↑**	-	-	-	-	-	-	-	-



Figure S8: Mean zebrafish dark (A) and light (B) swimming activity compared to mean fathead minnow dark (C) and light (D) activity after 96 h exposure to TDCPP. Plotted data represents activity over two ten minute dark photoperiods and two ten minute light photoperiods for each fish model. Data is normalized to control, which is represented at the 0 axis in each figure. Behavioral parameters include distance swam, number of movements (counts), and duration of each movement across 3 speed levels, bursting (>20 mm/sec), cruising (5-20 mm/sec), and freezing (<5 mm/sec). In addition to movement patterns at each of the speed thresholds, total distance swam and total number of movements is represented. ↑ represents a significant increase in activity in comparison to control and ↓ indicates a significant decrease in activity in comparison to control. A total of 24 (N = 4 replicates of each treatment level, 6 larvae in each experimental unit) zebrafish and 12 (N = 3 replicates of each treatment level, 4 larvae in each experimental unit) fathead minnow were used in behavioral observations for each group. \*p<0.10; \*\*p<0.05; \*\*\*p<0.01.

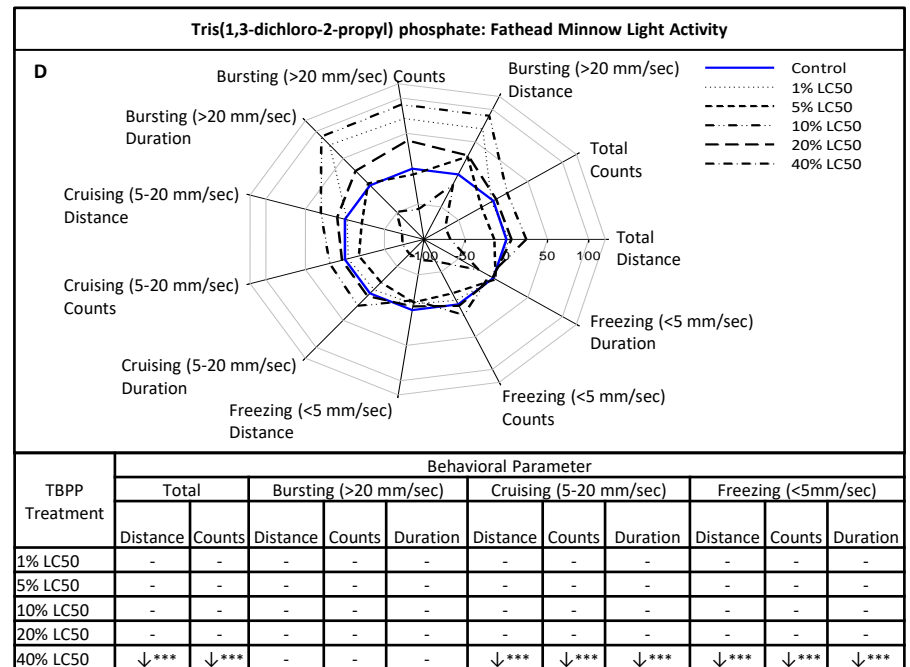
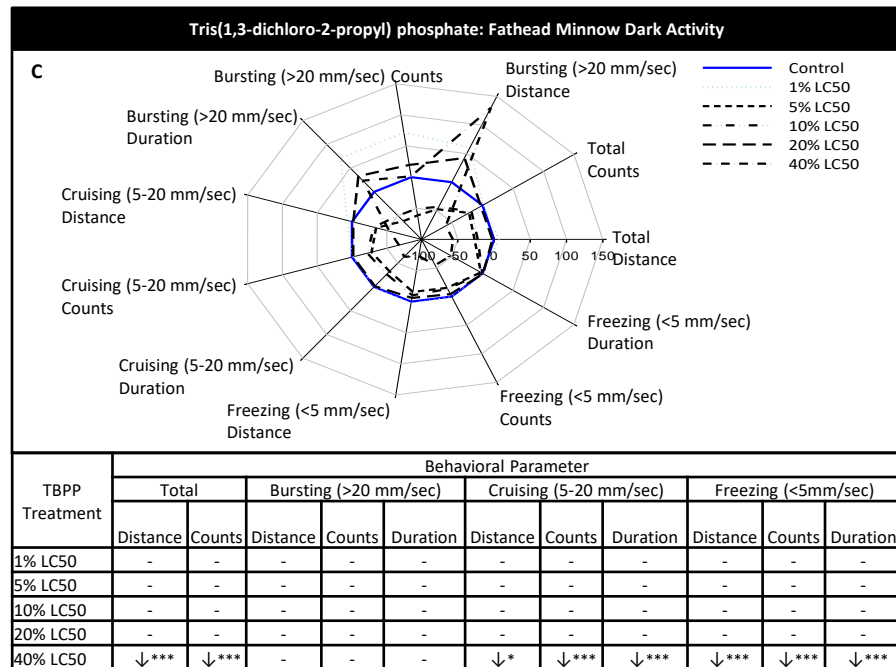
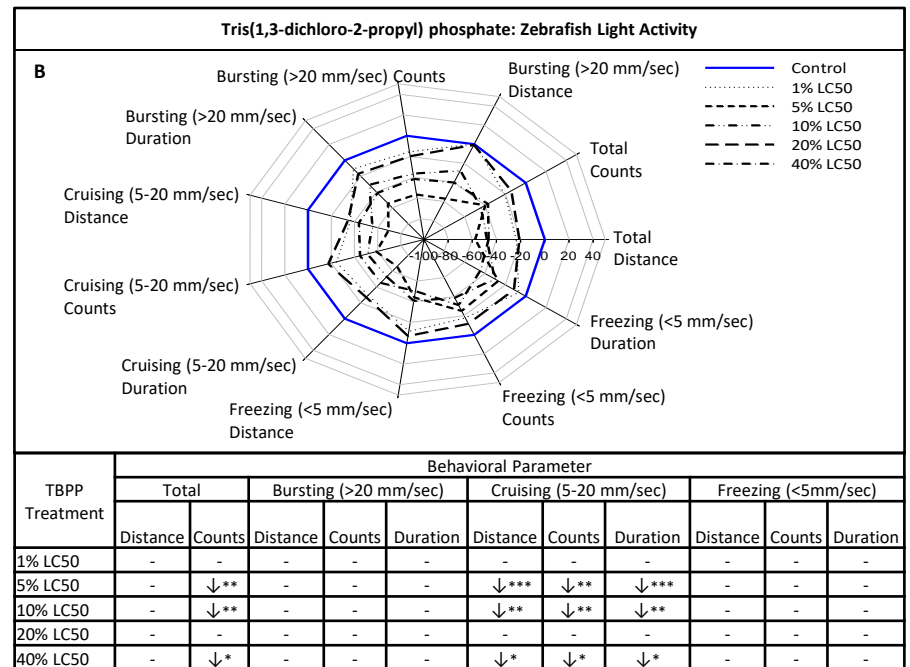
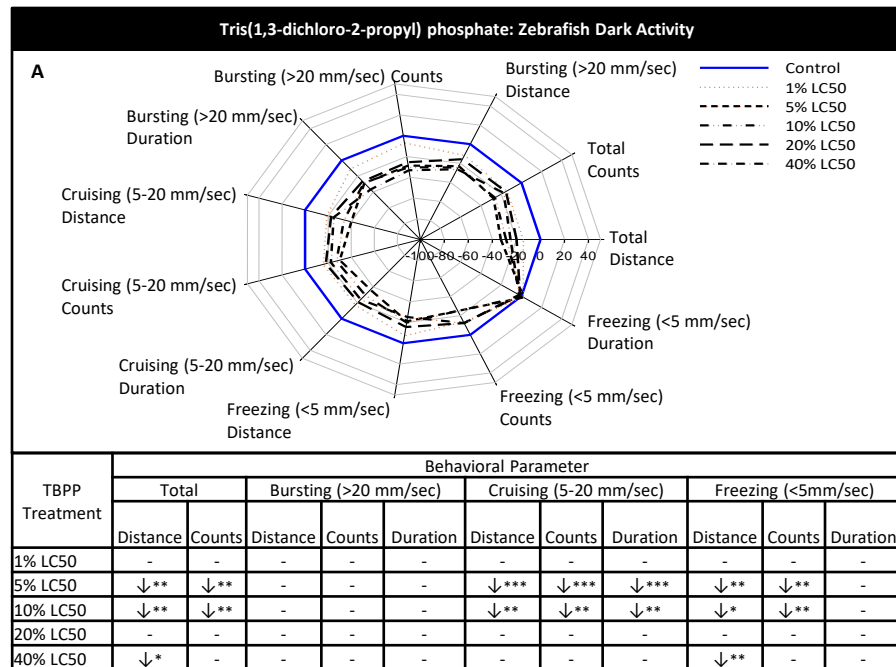


Figure S9: Activity of zebrafish (A and B) and fathead minnow (C and D) after 96 h exposure to 3-bromo-1-Propanol. The mean ( $\pm$ SE) distance swam for zebrafish (A) and fathead minnow (C) is given by dots each representing 1 minute intervals of activity. Photomotor responses of zebrafish (B) and fathead minnow (D) are measured as the change in mean ( $\pm$ SE) total distance traveled between the last minutes of an initial photoperiod and the first minute of the following period. Two dark and two light period photomotor responses were measured. A total of 24 (4 replicates each of 6 larvae) zebrafish and 12 (3 replicates of 4 larvae) fathead minnows were used for behavioral observation. \* $p < 0.10$ ; \*\* $p < 0.05$ ; \*\*\* $p < 0.01$ . N.M.: Not measured

## 3-Bromo-1-Propanol

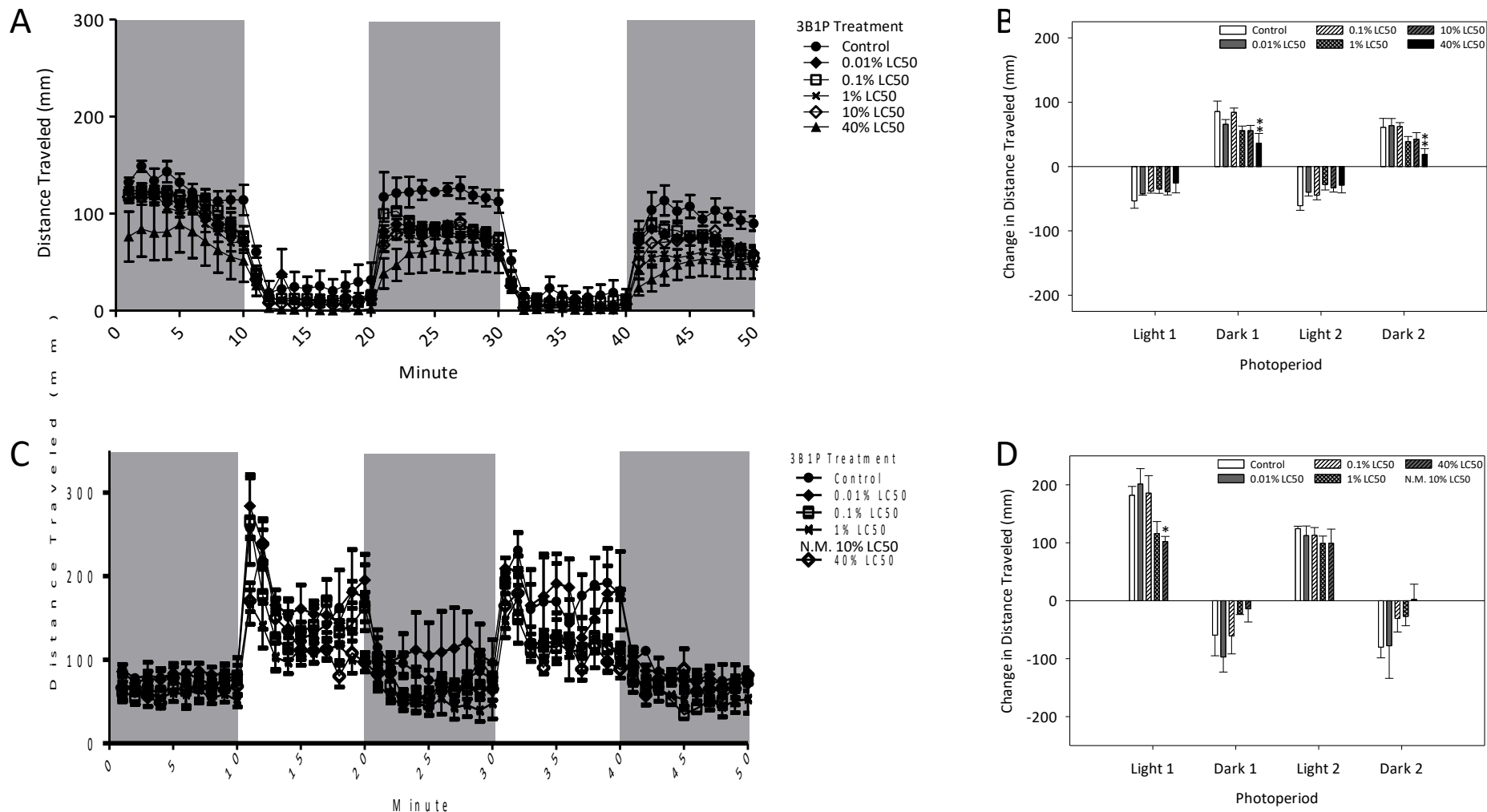


Figure S9 cont: Zebrafish (E,F, and G) and fathead minnow larvae (H,I, and J) photomotor responses were also measured across three speed thresholds (Freezing: <5 mm/s, Cruising: 5-20 mm/s, and Bursting >20 mm/s). Two dark and two light period photomotor responses were measured. A total of 24 (4 replicates each of 6 larvae) zebrafish and 12 (3 replicates of 4 larvae) fathead minnows were used for behavioral observation. \* $p < 0.10$ ; \*\* $p < 0.05$ ; \*\*\* $p < 0.01$ .

## 3-Bromo-1-Propanol

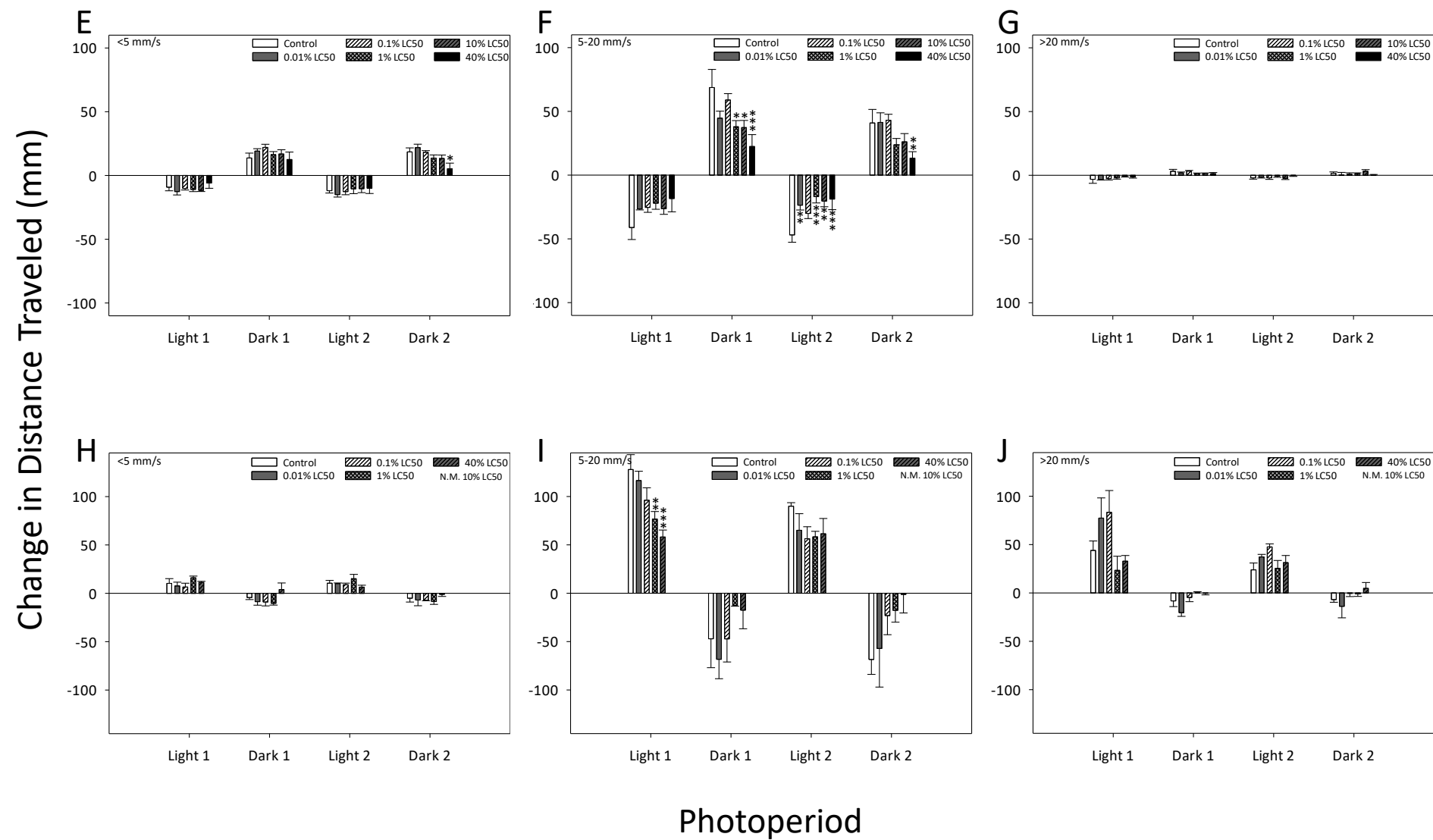


Figure S10: Activity of zebrafish (A and B) and fathead minnow (C and D) after 96 h exposure to 3-chloro-1,2-propanediol. The mean ( $\pm$ SE) distance swam for zebrafish (A) and fathead minnow (C) is given by dots each representing 1 minute intervals of activity. Photomotor responses of zebrafish (B) and fathead minnow (D) are measured as the change in mean ( $\pm$ SE) total distance traveled between the last minutes of an initial photoperiod and the first minute of the following period. Two dark and two light period photomotor responses were measured. A total of 24 (4 replicates each of 6 larvae) zebrafish and 12 (3 replicates of 4 larvae) fathead minnows were used for behavioral observation. \* $p < 0.10$ ; \*\* $p < 0.05$ ; \*\*\* $p < 0.01$ .

## 3-chloro-1,2-propanediol

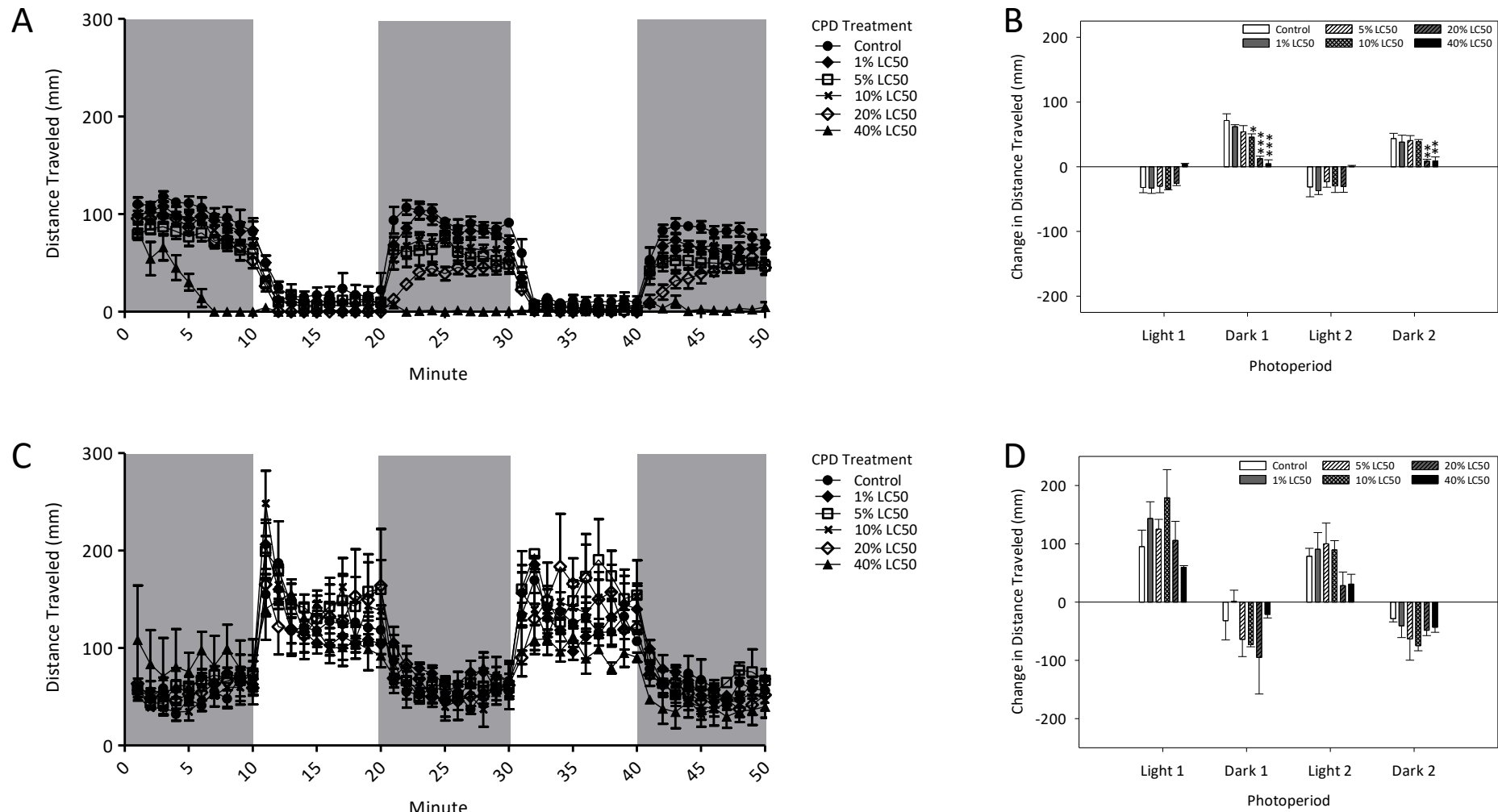
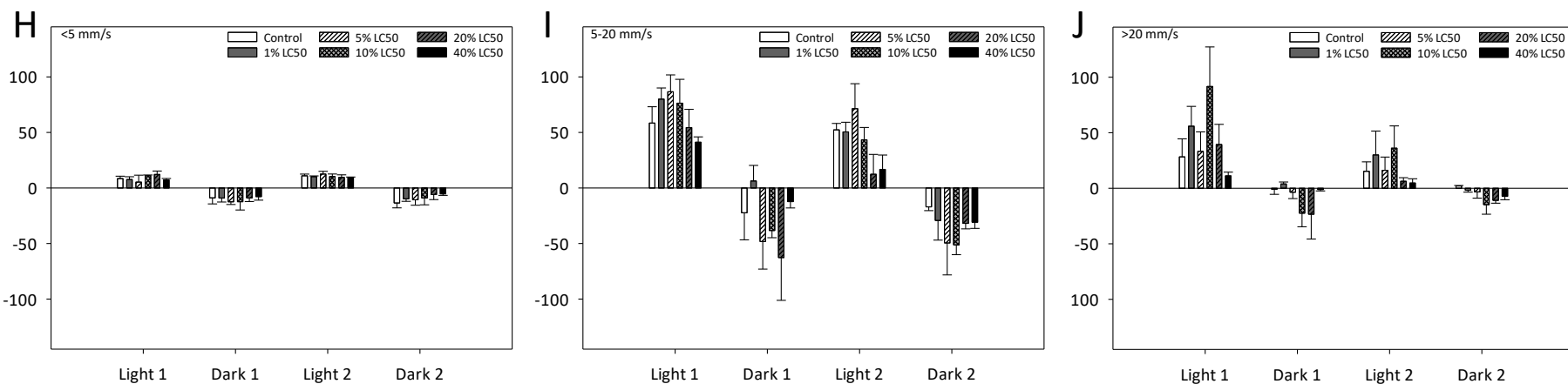
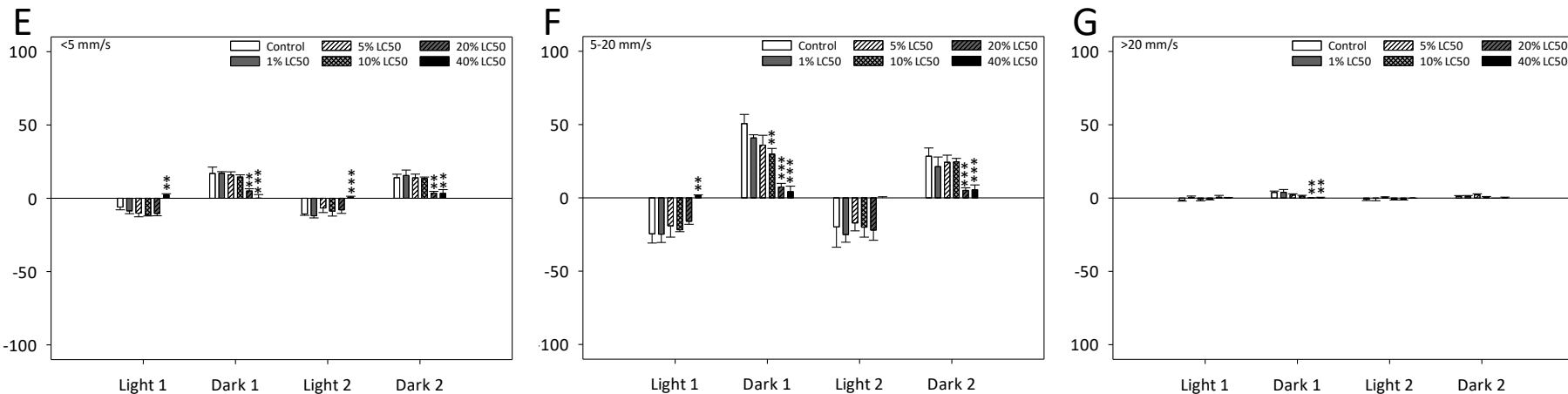




Figure S10 cont: Zebrafish (E,F, and G) and fathead minnow larvae (H,I, and J) photomotor responses were also measured across three speed thresholds (Freezing: <5 mm/s, Cruising: 5-20 mm/s, and Bursting >20 mm/s). Two dark and two light period photomotor responses were measured. A total of 24 (4 replicates each of 6 larvae) zebrafish and 12 (3 replicates of 4 larvae) fathead minnows were used for behavioral observation. \* $p < 0.10$ ; \*\* $p < 0.05$ ; \*\*\* $p < 0.01$ .

## 3-chloro-1,2-propanediol



## Photoperiod

Figure S11: Activity of zebrafish (A and B) and fathead minnow (C and D) after 96 h exposure to dibromoacetonitrile. The mean ( $\pm$ SE) distance swam for zebrafish (A) and fathead minnow (C) is given by dots each representing 1 minute intervals of activity. Photomotor responses of zebrafish (B) and fathead minnow (D) are measured as the change in mean ( $\pm$ SE) total distance traveled between the last minutes of an initial photoperiod and the first minute of the following period. Two dark and two light period photomotor responses were measured. A total of 24 (4 replicates each of 6 larvae) zebrafish and 12 (3 replicates of 4 larvae) fathead minnows were used for behavioral observation. \* $p < 0.10$ ; \*\* $p < 0.05$ ; \*\*\* $p < 0.01$ .

## Dibromoacetonitrile

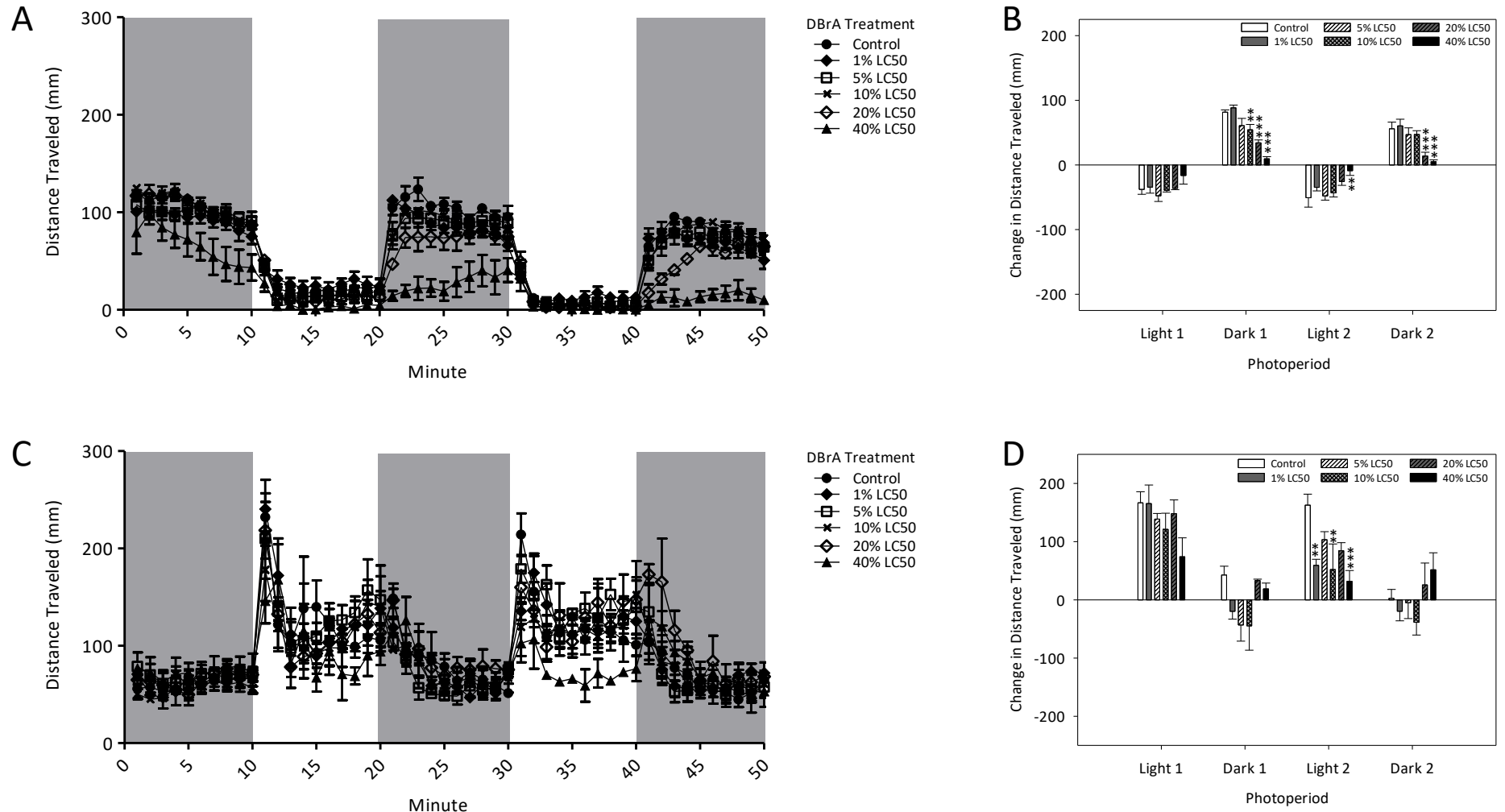


Figure S11 cont: Zebrafish (E,F, and G) and fathead minnow larvae (H,I, and J) photomotor responses were also measured across three speed thresholds (Freezing: <5 mm/s, Cruising: 5-20 mm/s, and Bursting >20 mm/s). Two dark and two light period photomotor responses were measured. A total of 24 (4 replicates each of 6 larvae) zebrafish and 12 (3 replicates of 4 larvae) fathead minnows were used for behavioral observation. \* $p < 0.10$ ; \*\* $p < 0.05$ ; \*\*\* $p < 0.01$ .

## Dibromoacetonitrile

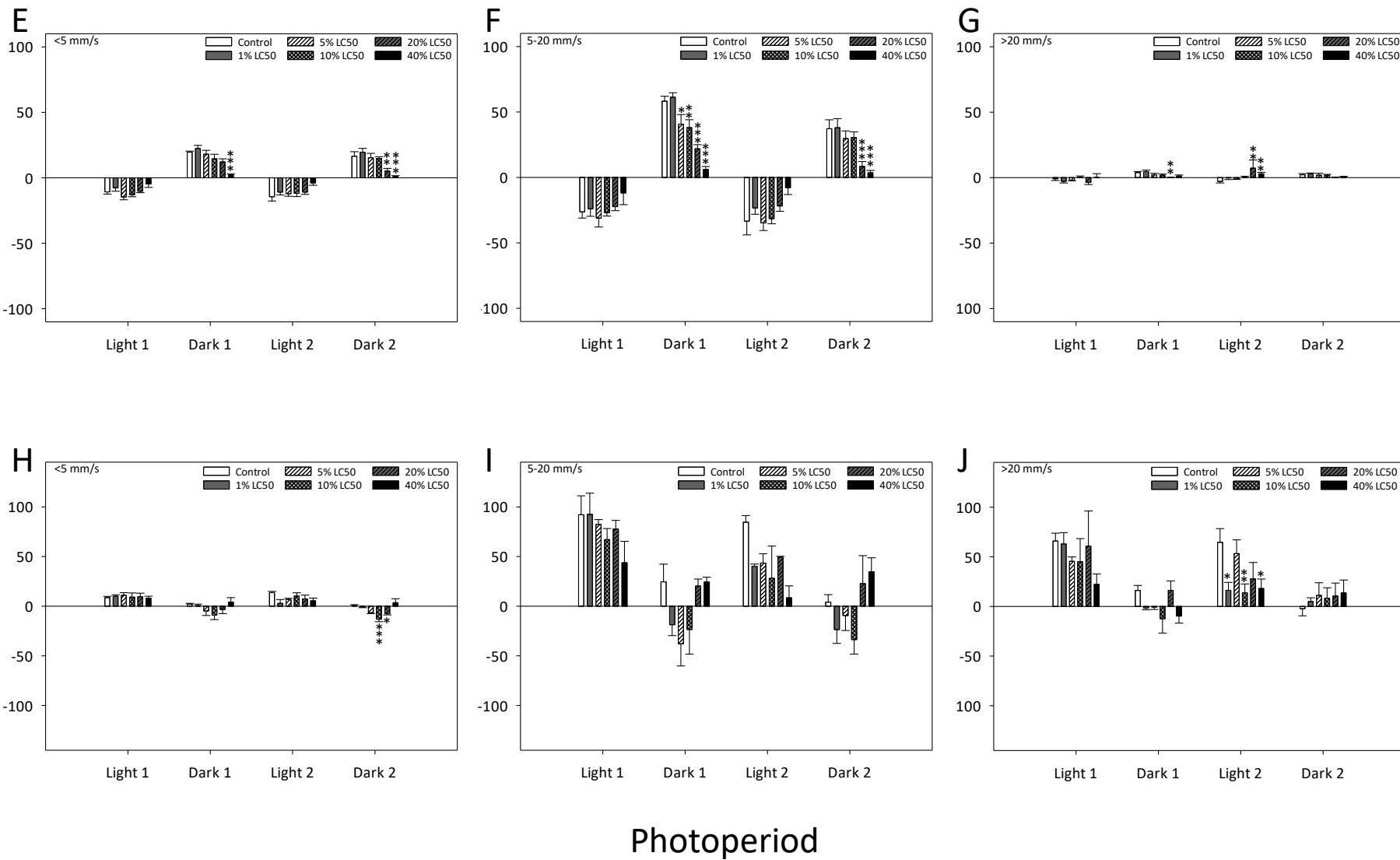


Figure S12: Activity of zebrafish (A and B) and fathead minnow (C and D) after 96 h exposure to glycidol. The mean ( $\pm$ SE) distance swam for zebrafish (A) and fathead minnow (C) is given by dots each representing 1 minute intervals of activity. Photomotor responses of zebrafish (B) and fathead minnow (D) are measured as the change in mean ( $\pm$ SE) total distance traveled between the last minutes of an initial photoperiod and the first minute of the following period. Two dark and two light period photomotor responses were measured. A total of 24 (4 replicates each of 6 larvae) zebrafish and 12 (3 replicates of 4 larvae) fathead minnows were used for behavioral observation. \* $p < 0.10$ ; \*\* $p < 0.05$ ; \*\*\* $p < 0.01$ .

## Glycidol

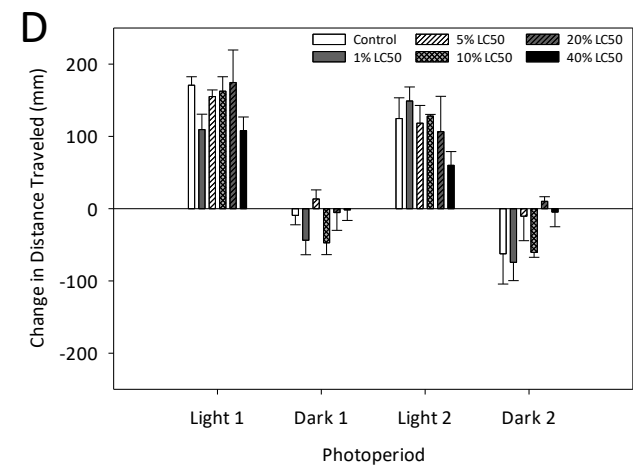
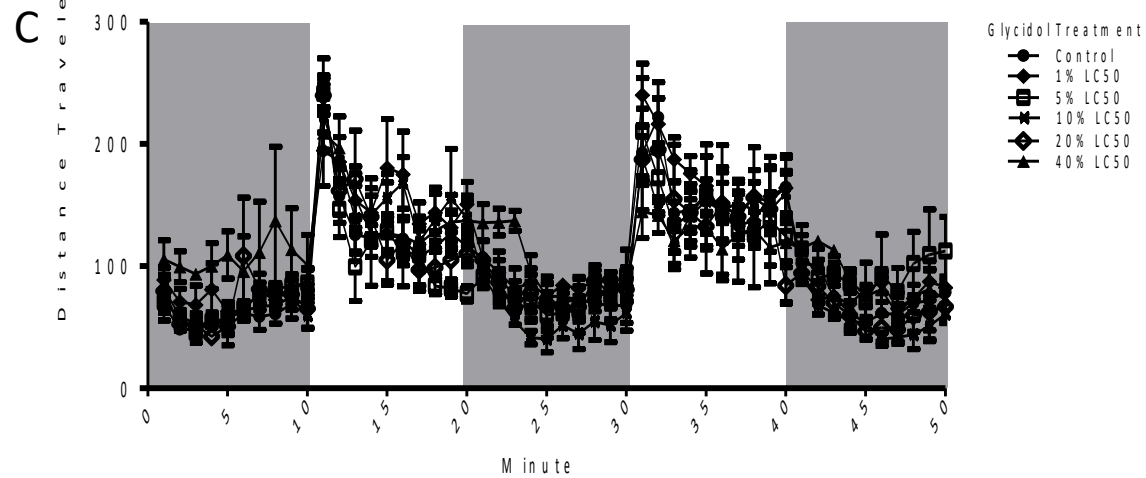
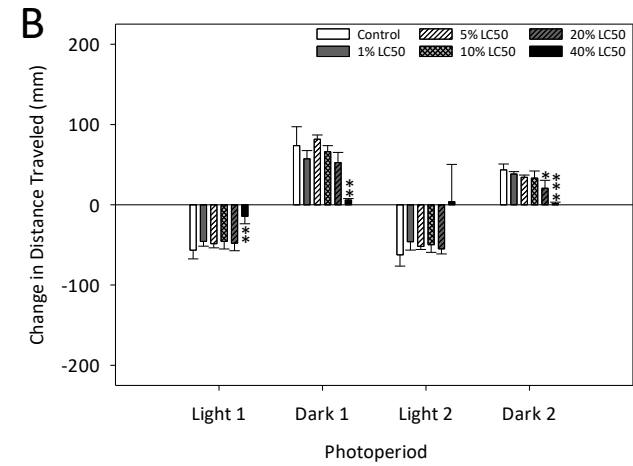
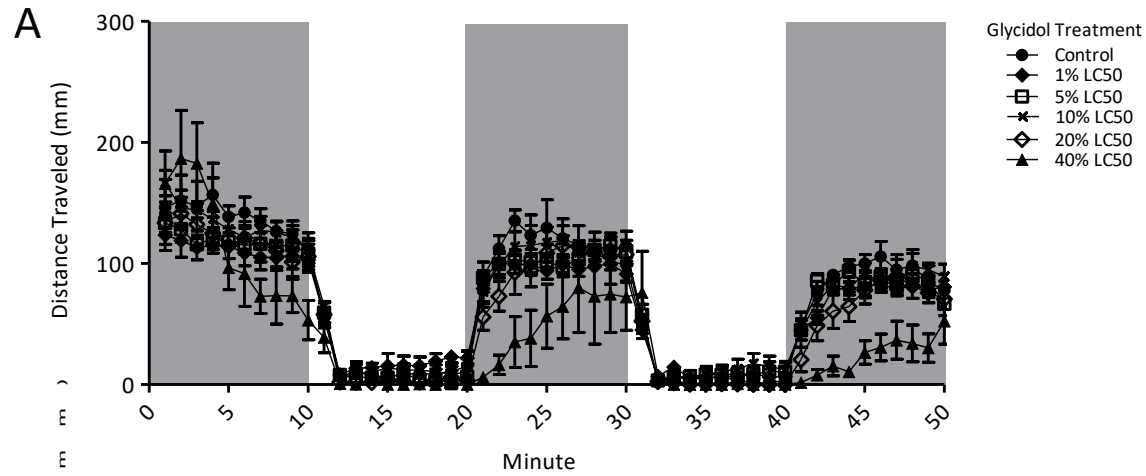
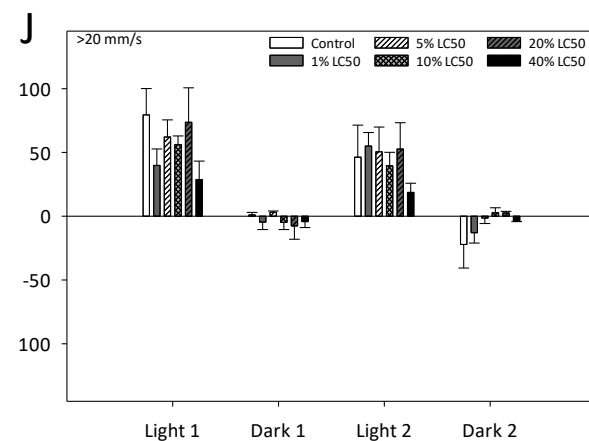
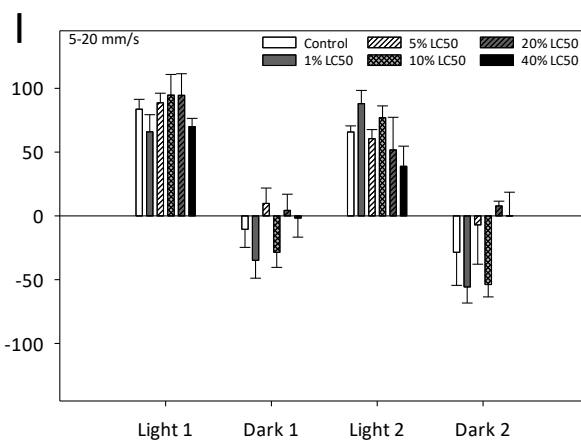
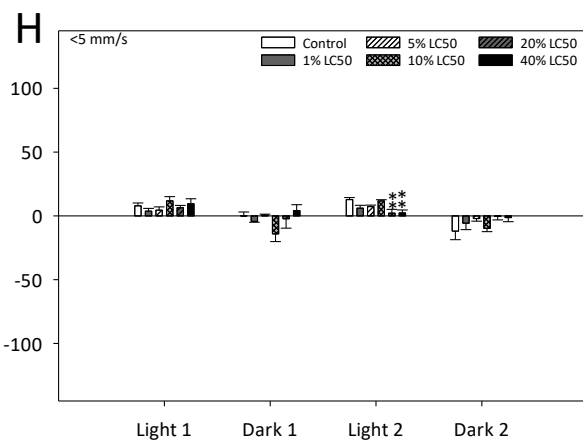
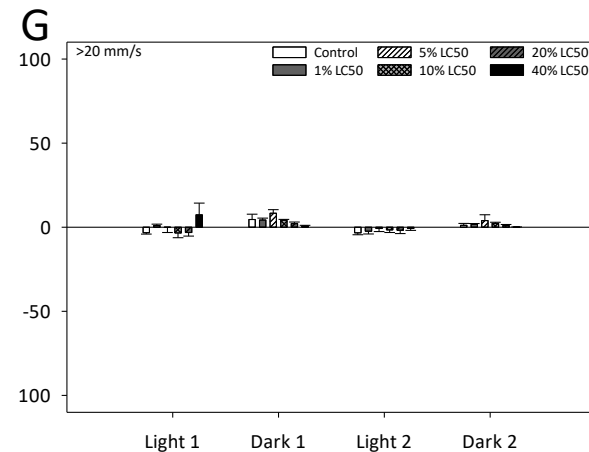
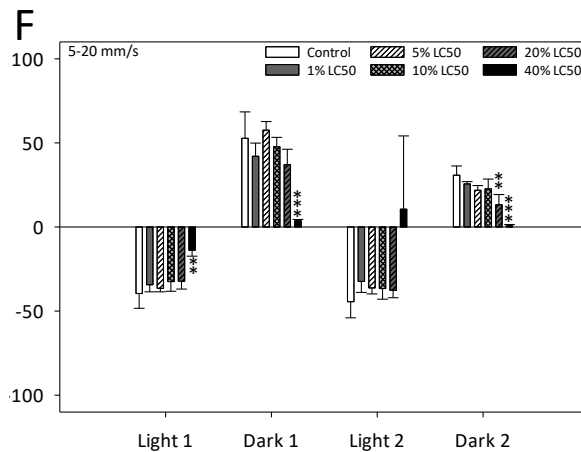
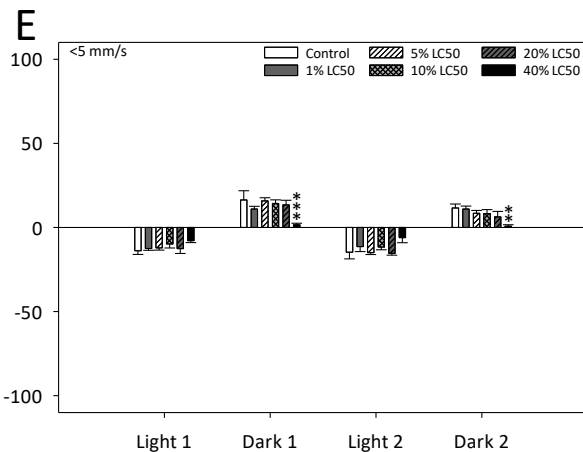




Figure S12 cont: Zebrafish (E,F, and G) and fathead minnow larvae (H,I, and J) photomotor responses were also measured across three speed thresholds (Freezing: <5 mm/s, Cruising: 5-20 mm/s, and Bursting >20 mm/s). Two dark and two light period photomotor responses were measured. A total of 24 (4 replicates each of 6 larvae) zebrafish and 12 (3 replicates of 4 larvae) fathead minnows were used for behavioral observation. \* $p < 0.10$ ; \*\* $p < 0.05$ ; \*\*\* $p < 0.01$ .

Change in Distance Traveled (mm)

Glycidol

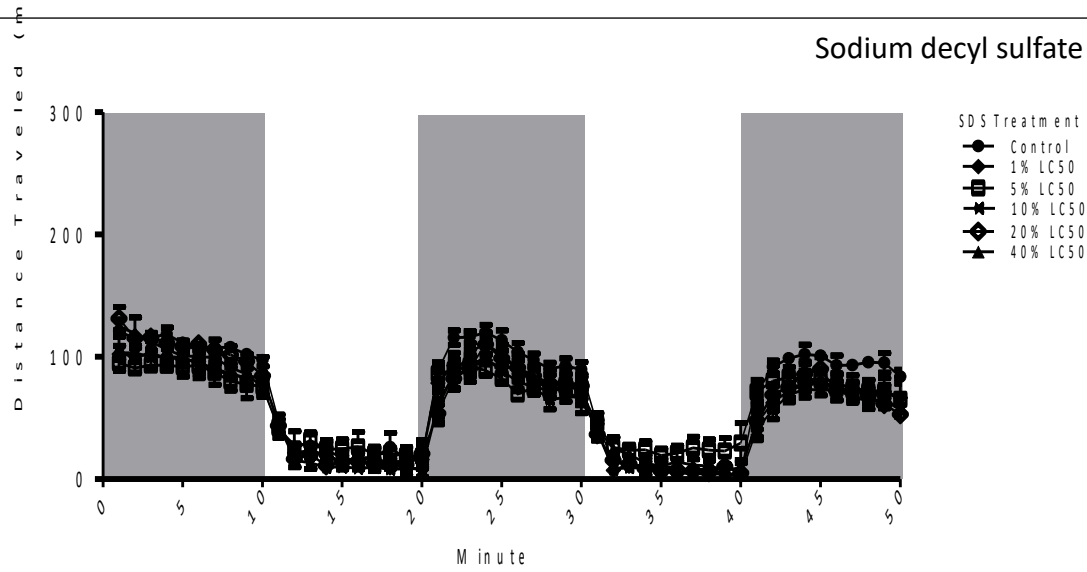


Photoperiod

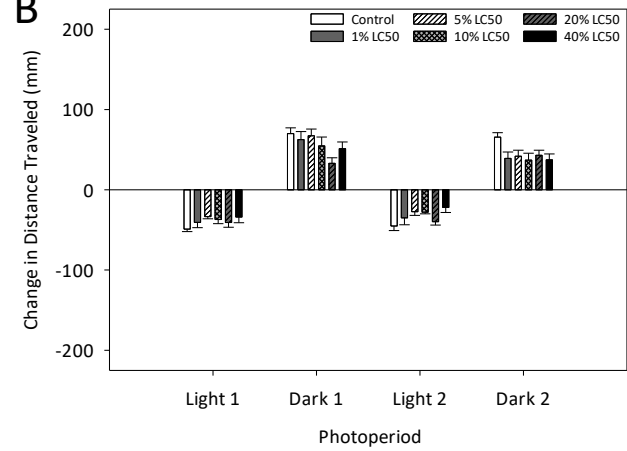
Figure S13: Activity of zebrafish (A and B) and fathead minnow (C and D) after 96 h exposure to sodium decyl sulfate. The mean ( $\pm$ SE) distance swam for zebrafish (A) and fathead minnow (C) is given by dots each representing 1 minute intervals of activity. Photomotor responses of zebrafish (B) and fathead minnow (D) are measured as the change in mean ( $\pm$ SE) total distance traveled between the last minutes of an initial photoperiod and the first minute of the following period. Two dark and two light period photomotor responses were measured. A total of 24 (4 replicates each of 6 larvae) zebrafish and 12 (3 replicates of 4 larvae) fathead minnows were used for behavioral observation. \* $p < 0.10$ ; \*\* $p < 0.05$ ; \*\*\* $p < 0.01$ .

## Sodium decyl sulfate

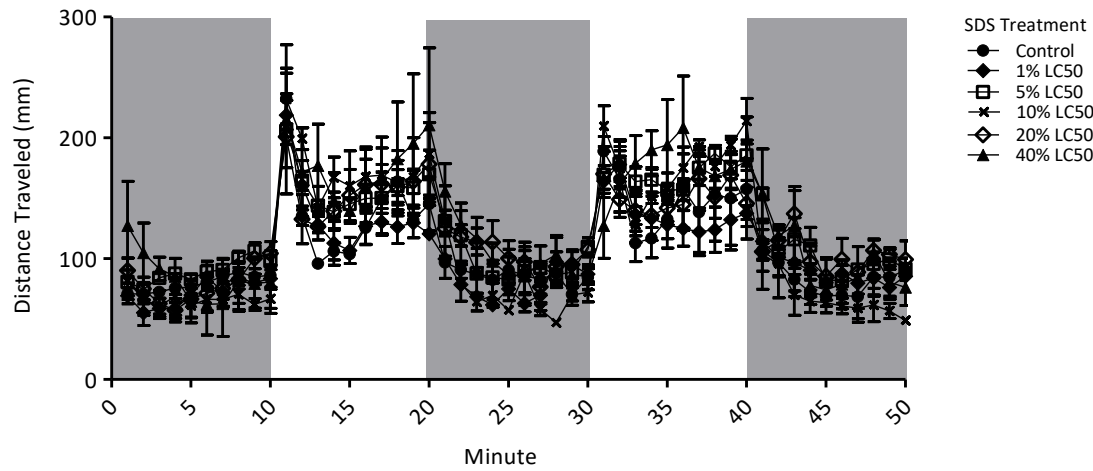
A



B



C



D

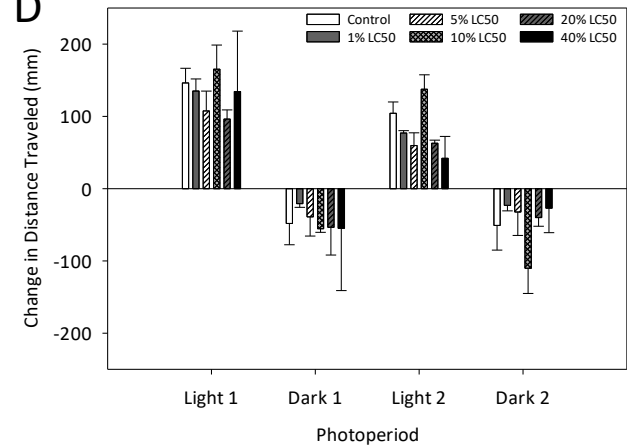
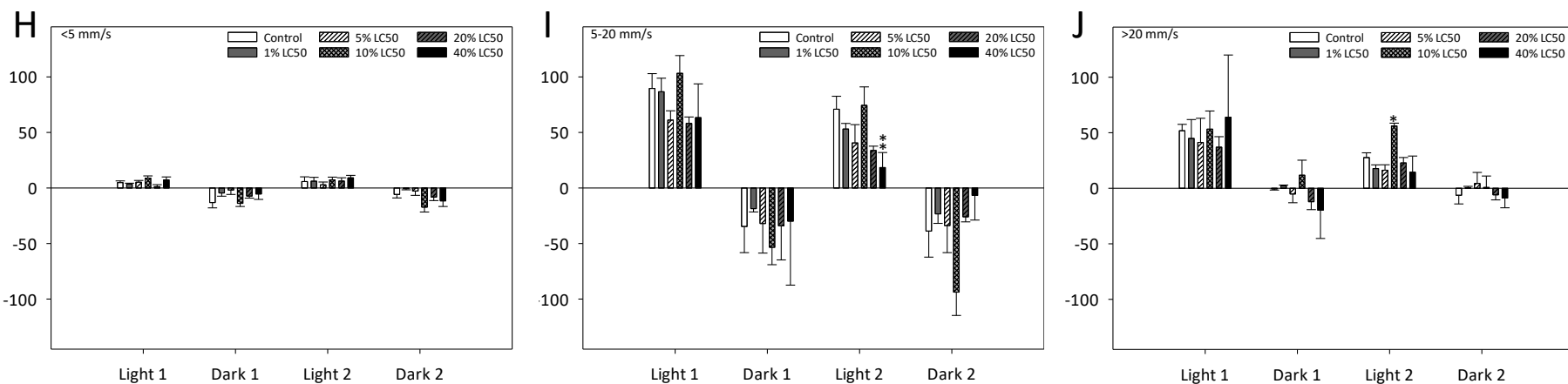
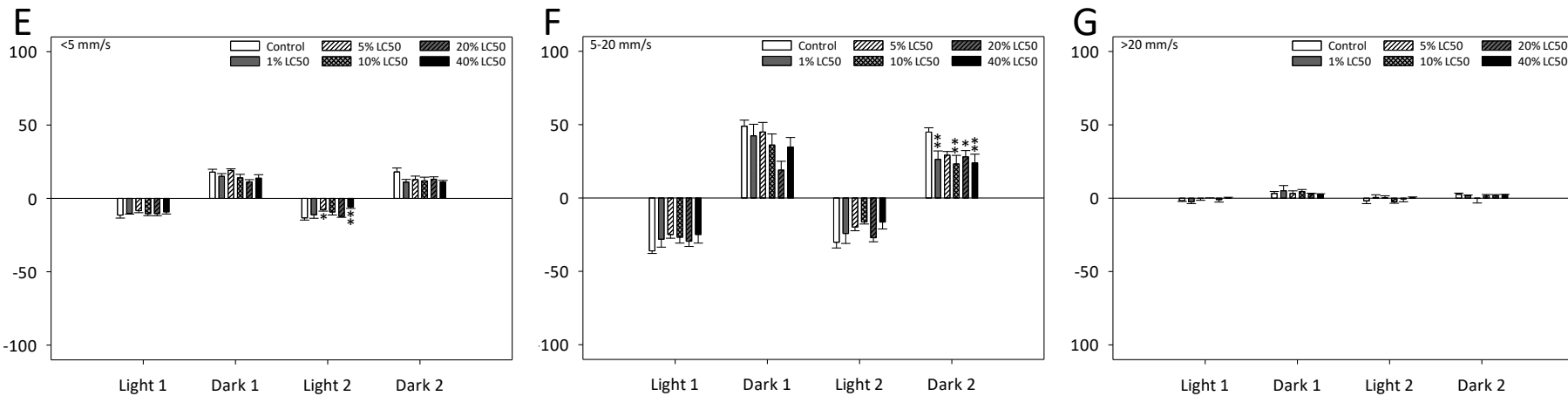


Figure S13 cont: Zebrafish (E,F, and G) and fathead minnow larvae (H,I, and J) photomotor responses were also measured across three speed thresholds (Freezing: <5 mm/s, Cruising: 5-20 mm/s, and Bursting >20 mm/s). Two dark and two light period photomotor responses were measured. A total of 24 (4 replicates each of 6 larvae) zebrafish and 12 (3 replicates of 4 larvae) fathead minnows were used for behavioral observation. \* $p < 0.10$ ; \*\* $p < 0.05$ ; \*\*\* $p < 0.01$ .

## Sodium decyl sulfate



## Photoperiod

Figure S14: Activity of zebrafish (A and B) and fathead minnow (C and D) after 96 h exposure to styrene oxide. The mean ( $\pm$ SE) distance swam for zebrafish (A) and fathead minnow (C) is given by dots each representing 1 minute intervals of activity. Photomotor responses of zebrafish (B) and fathead minnow (D) are measured as the change in mean ( $\pm$ SE) total distance traveled between the last minutes of an initial photoperiod and the first minute of the following period. Two dark and two light period photomotor responses were measured. A total of 24 (4 replicates each of 6 larvae) zebrafish and 12 (3 replicates of 4 larvae) fathead minnows were used for behavioral observation. \* $p < 0.10$ ; \*\* $p < 0.05$ ; \*\*\* $p < 0.01$ .

## Styrene Oxide

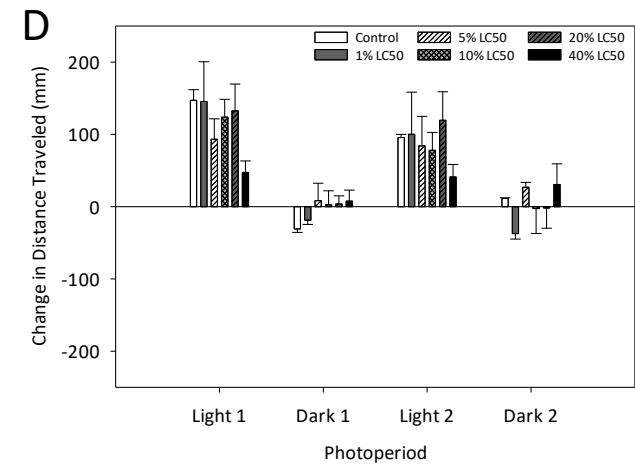
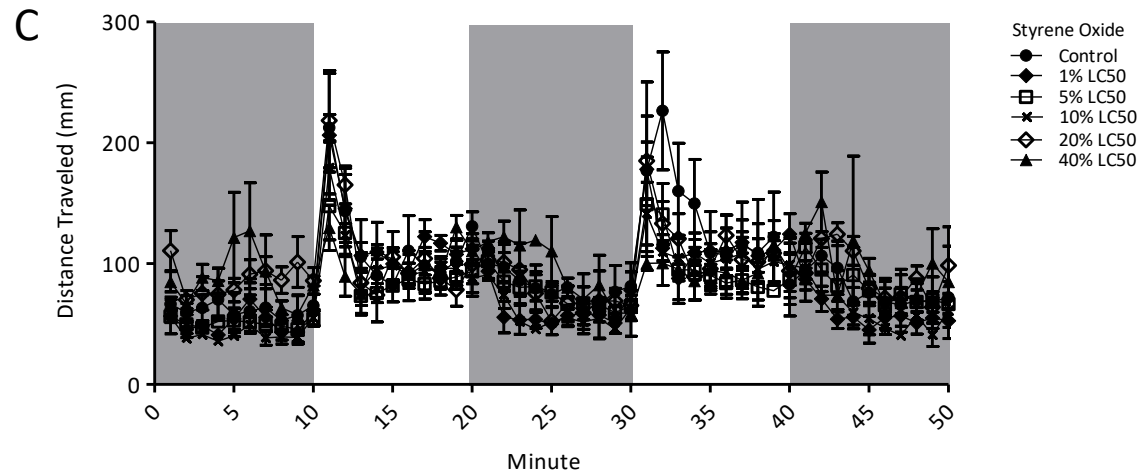
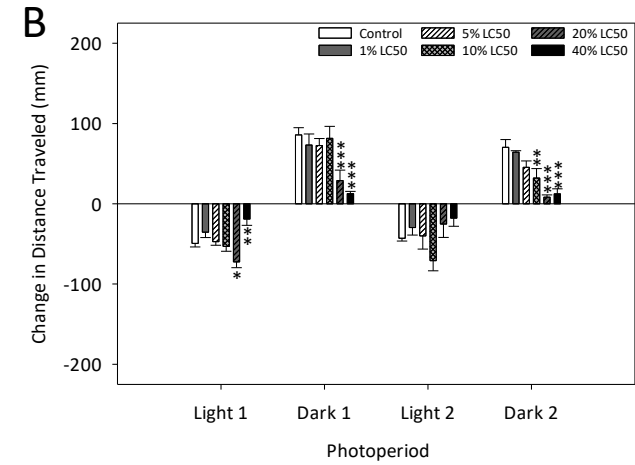
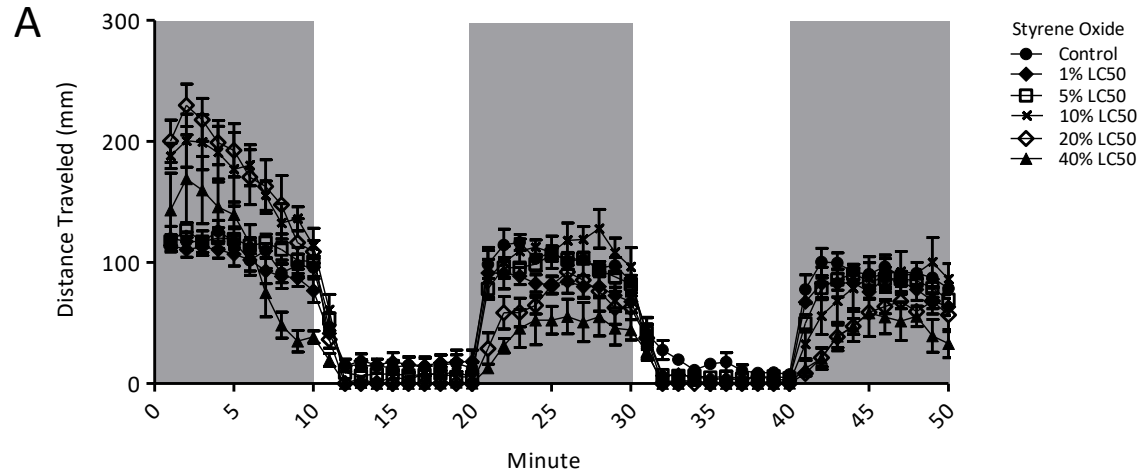
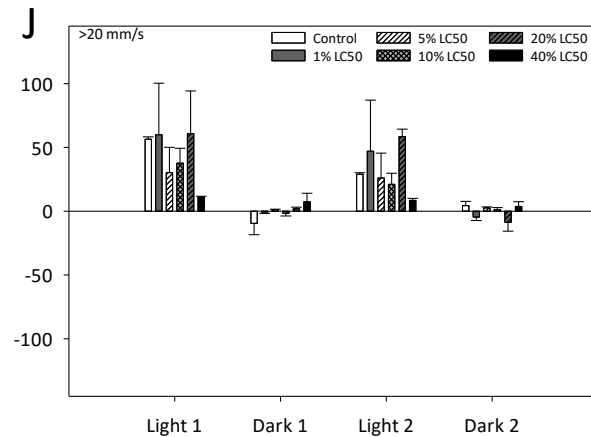
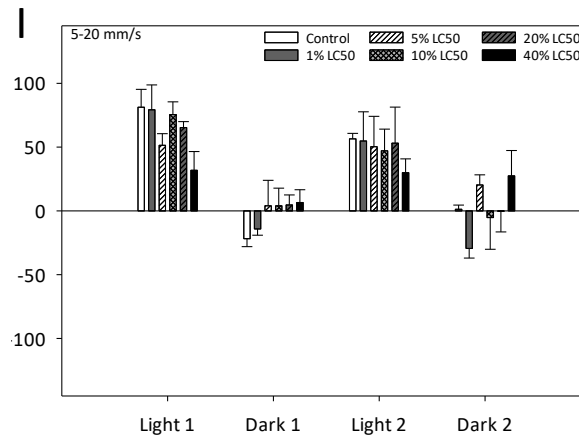
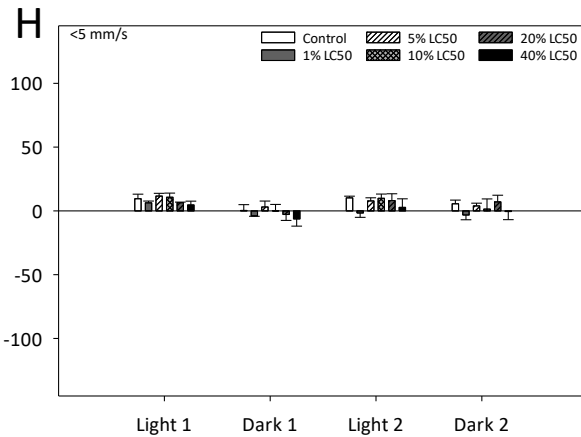
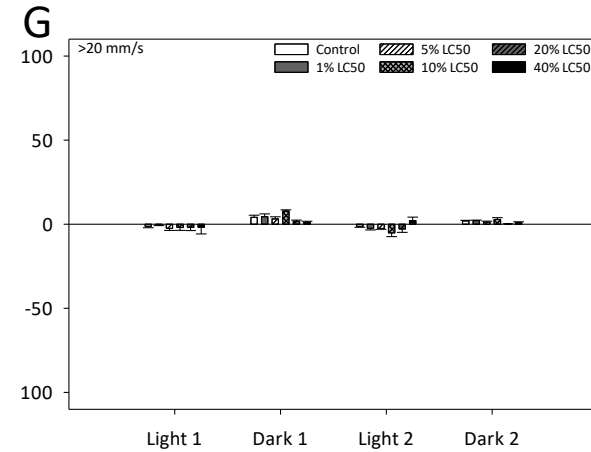
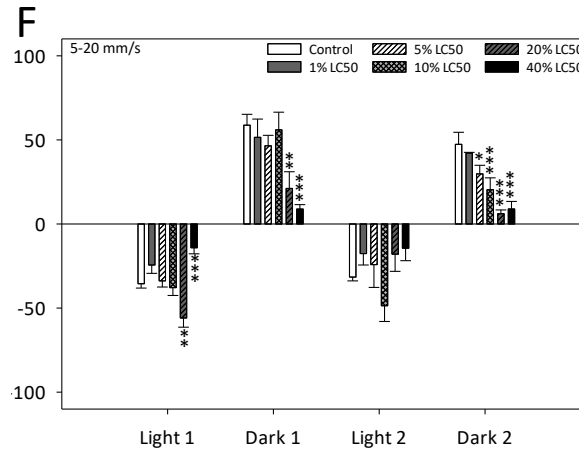
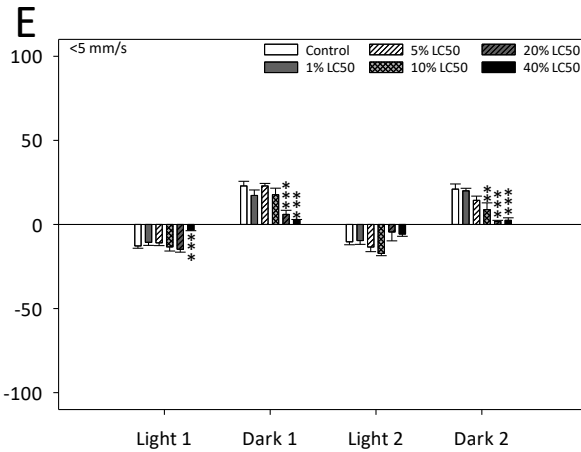




Figure S14 cont: Zebrafish (E,F, and G) and fathead minnow larvae (H,I, and J) photomotor responses were also measured across three speed thresholds (Freezing: <5 mm/s, Cruising: 5-20 mm/s, and Bursting >20 mm/s). Two dark and two light period photomotor responses were measured. A total of 24 (4 replicates each of 6 larvae) zebrafish and 12 (3 replicates of 4 larvae) fathead minnows were used for behavioral observation. \* $p < 0.10$ ; \*\* $p < 0.05$ ; \*\*\* $p < 0.01$ .

## Styrene Oxide



## Photoperiod

Figure S15: Activity of zebrafish (A and B) and fathead minnow (C and D) after 96 h exposure to TBPP. The mean ( $\pm$ SE) distance swam for zebrafish (A) and fathead minnow (C) is given by dots each representing 1 minute intervals of activity. Photomotor responses of zebrafish (B) and fathead minnow (D) are measured as the change in mean ( $\pm$ SE) total distance traveled between the last minutes of an initial photoperiod and the first minute of the following period. A total of 24 (4 replicates each of 6 larvae) zebrafish and 12 (3 replicates of 4 larvae) fathead minnows were used for behavioral observation. \* $p < 0.10$ ; \*\* $p < 0.05$ ; \*\*\* $p < 0.01$ .

## Tris(2,3-dibromopropyl) phosphate

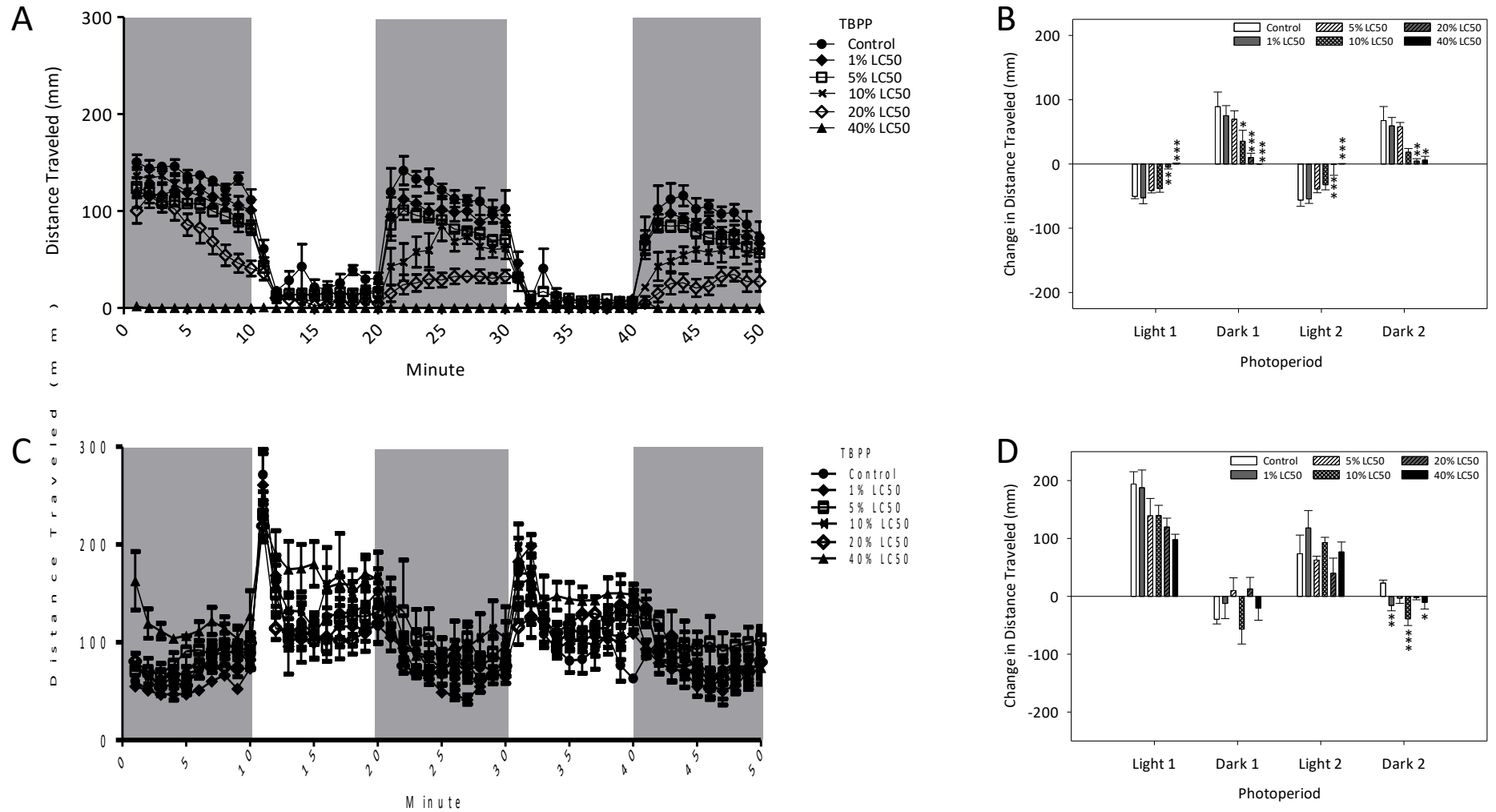
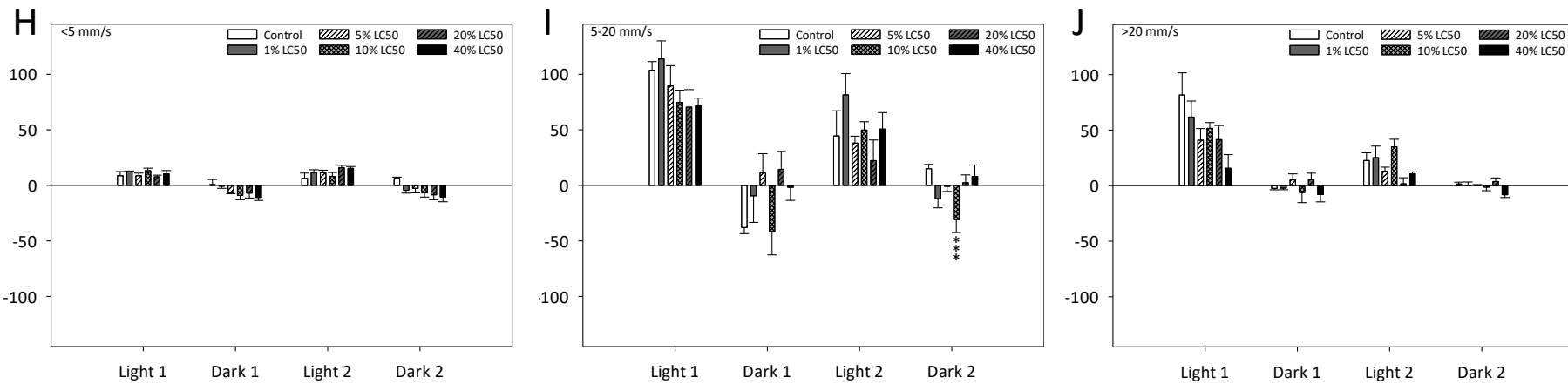
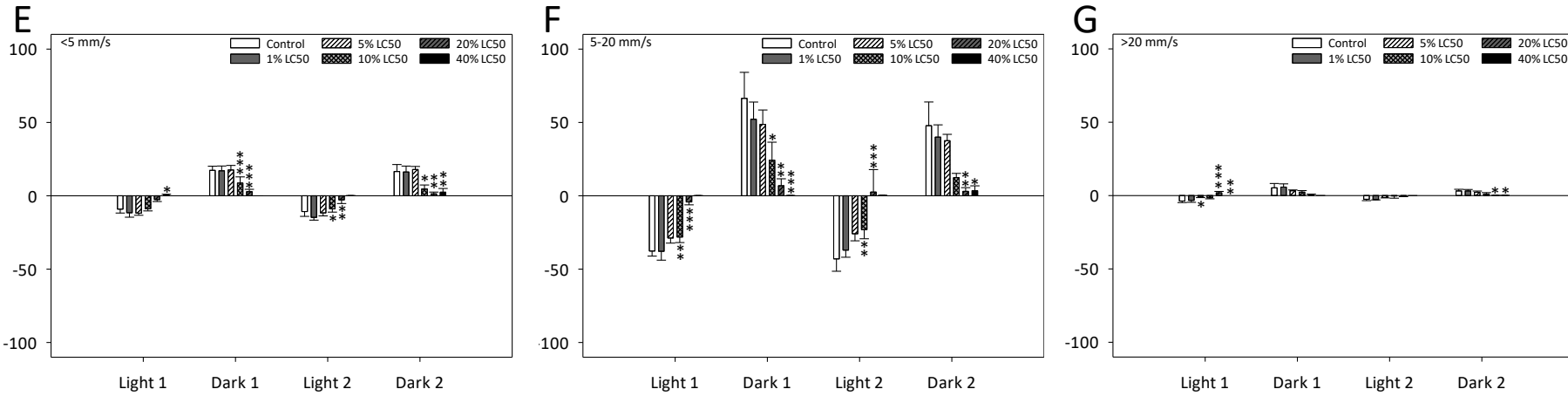


Figure S15 cont: Zebrafish (E,F, and G) and fathead minnow larvae (H,I, and J) photomotor responses were also measured across three speed thresholds (Freezing:  $<5$  mm/s, Cruising: 5-20 mm/s, and Bursting  $>20$  mm/s). Two dark and two light period photomotor responses were measured. A total of 24 (4 replicates each of 6 larvae) zebrafish and 12 (3 replicates of 4 larvae) fathead minnows were used for behavioral observation. \* $p<0.10$  ; \*\* $p<0.05$ ; \*\*\* $p<0.01$ .

## Tris(2,3-dibromopropyl) phosphate



## Photoperiod

Figure S16: Activity of zebrafish (A and B) and fathead minnow (C and D) after 96 h exposure to TDCPP. The mean ( $\pm$ SE) distance swam for zebrafish (A) and fathead minnow (C) is given by dots each representing 1 minute intervals of activity. Photomotor responses of zebrafish (B) and fathead minnow (D) are measured as the change in mean ( $\pm$ SE) total distance traveled between the last minutes of an initial photoperiod and the first minute of the following period. A total of 24 (4 replicates each of 6 larvae) zebrafish and 12 (3 replicates of 4 larvae) fathead minnows were used for behavioral observation. \* $p < 0.10$ ; \*\* $p < 0.05$ ; \*\*\* $p < 0.01$ .

## Tris(1,3-dichloro-2-propyl) phosphate

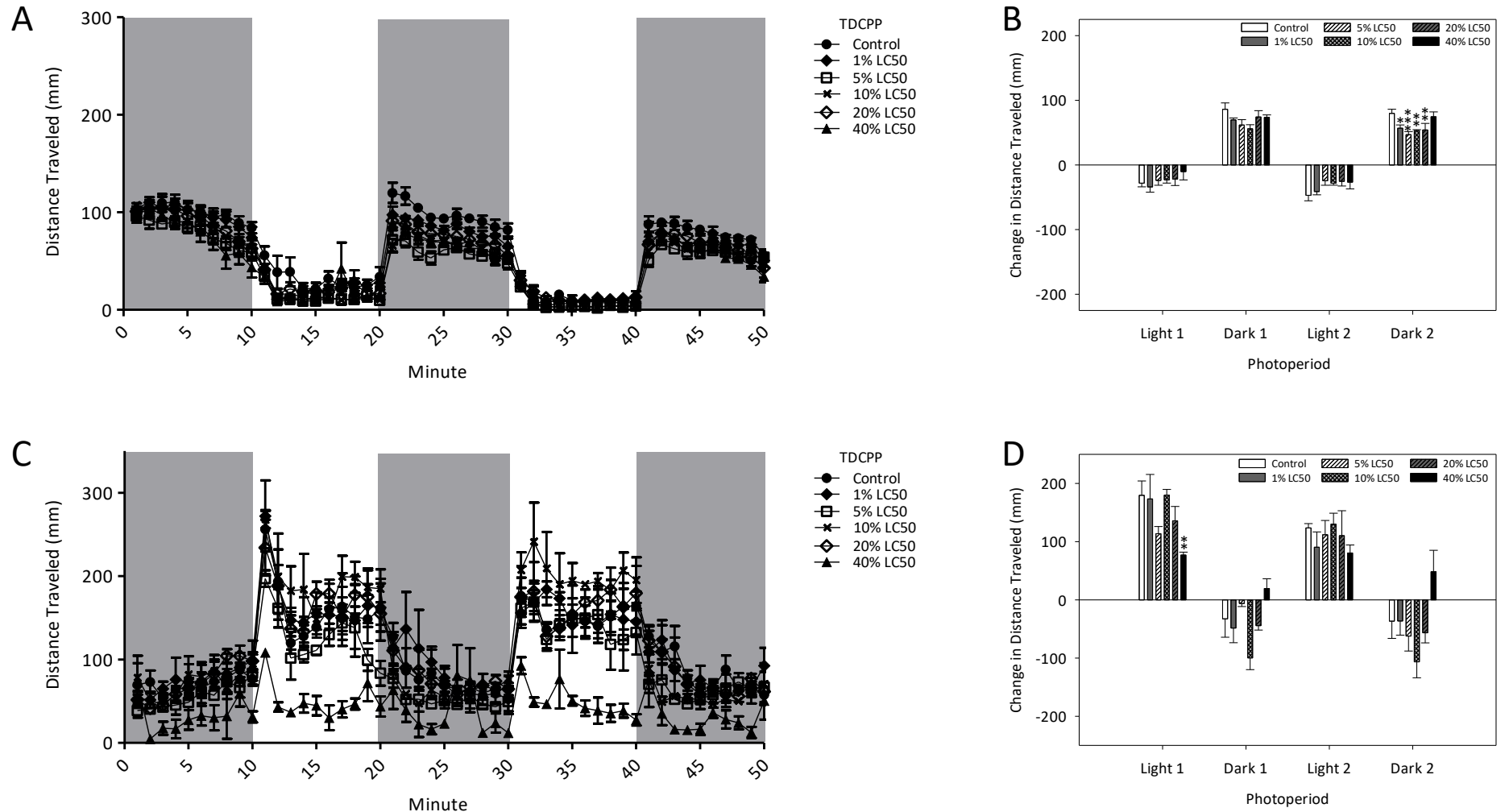




Figure S16 cont: Zebrafish (E,F, and G) and fathead minnow larvae (H,I, and J) photomotor responses were also measured across three speed thresholds (Freezing: <5 mm/s, Cruising: 5-20 mm/s, and Bursting >20 mm/s). Two dark and two light period photomotor responses were measured. A total of 24 (4 replicates each of 6 larvae) zebrafish and 12 (3 replicates of 4 larvae) fathead minnows were used for behavioral observation. \* $p < 0.10$ ; \*\* $p < 0.05$ ; \*\*\* $p < 0.01$ .

## Tris(1,3-dichloro-2-propyl) phosphate

