

Electronic Supplementary Information (ESI)

Elucidation of substrate interaction effects in multicomponent systems containing 3-ring homocyclic and heterocyclic polynuclear aromatic hydrocarbons

by

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Table A1. HPLC method of identifying CBZ, FLU and DBT, individually and in mixtures

Time (min)	%A (Aqueous)	%B (Organic)	Flow (ml/min)
0	95	5	
1	95	5	
6	20	80	
9	20	80	
15	5	95	0.5
20	5	95	
21	95	5	
25	95	5	

Table A2. Summary of various parameter values associated with the simultaneous identification and quantification of CBZ, FLU and DBT in mixture

Compounds	Retention time (min)	Extraction efficiency (%)	LOD (mg/L)	LOQ (mg/L)
Carbazole	15.67 ± 0.19	100 ± 6	1.19	3.61
Fluorene	20.23 ± 0.17	97 ± 1	0.67	2.02
Dibenzothiophene	21.27 ± 0.21	100 ± 1	1.39	4.20

Table A3. Significant and insignificant effects influencing CBZ degradation based on multifactor ANOVA

Parameters	SS	DF	MS	F	p
Intercept	83119	1	83119	902	0.000
CBZ (mg/L)	338	1	338	4	0.092
FLU (mg/L)	515	1	515	6	0.046
DBT (mg/L)	205	1	205	2	0.174
CBZ (mg/L) *FLU (mg/L)	1	1	1	0.01	0.926
CBZ (mg/L) *DBT (mg/L)	90	1	90	1	0.352
FLU (mg/L) *DBT (mg/L)	288	1	288	3	0.115
CBZ (mg/L) *FLU (mg/L) *DBT (mg/L)	0.4	1	0.4	0.004	0.950
Error	737	8	92		

Table A4. Significant and insignificant effects influencing FLU degradation based on multifactor ANOVA

Parameters	SS	DF	MS	F	p
Intercept	110472	1	110472	12346	0.000
CBZ (mg/L)	425	1	425	48	0.000
FLU (mg/L)	56	1	56	6	0.037
DBT (mg/L)	126	1	126	14	0.006
CBZ (mg/L) *FLU (mg/L)	302	1	302	34	0.000
CBZ (mg/L) *DBT (mg/L)	673	1	673	75	0.000
FLU (mg/L) *DBT (mg/L)	1476	1	1476	165	0.000
CBZ (mg/L) *FLU (mg/L) *DBT (mg/L)	109	1	109	12	0.008
Error	72	8	9		

Table A5. Significant and insignificant effects influencing DBT degradation based on multifactor ANOVA

Parameters	SS	DF	MS	F	p
Intercept	57143	1	57143	3331	0.000
CBZ (mg/L)	437	1	437	25	0.001
FLU (mg/L)	3	1	3	0.2	0.693
DBT (mg/L)	220	1	220	13	0.007
CBZ (mg/L) *FLU (mg/L)	2965	1	2965	173	0.000
CBZ (mg/L) *DBT (mg/L)	46	1	46	3	0.141
FLU (mg/L) *DBT (mg/L)	1377	1	1377	80	0.000
CBZ (mg/L) *FLU (mg/L) *DBT (mg/L)	51	1	51	3	0.122
Error	137	8	17		

Note: p-value less than 0.05 is significant at 95% confidence level

Table A6. Tukey's HSD test results of main effects influencing CBZ degradation

CBZ main effect		
Cell No.	CBZ (mg/L)	p values
1	5	0.0917
2	30	0.0917
FLU main effect		
Cell No.	FLU (mg/L)	p values
1	5	0.0458
2	30	0.0458
DBT main effect		
Cell No.	DBT (mg/L)	p values
1	5	0.1745
2	30	0.1745

Table A7. Tukey's HSD test results of 2-way interactions influencing CBZ degradation

CBZ × FLU 2-way interaction effect						
Cell No.	CBZ (mg/L)	FLU (mg/L)	p-values			
1	5	5		0.3657	0.5206	0.0641
2	5	30	0.3657		0.9883	0.5948
3	30	5	0.5206	0.9883		0.4283
4	30	30	0.0641	0.5948	0.4283	
CBZ × DBT 2-way interaction effect						
Cell No.	CBZ (mg/L)	DBT (mg/L)	p-values			
1	5	5		0.3597	0.2462	0.1525
2	5	30	0.3597		0.9899	0.9104
3	30	5	0.2462	0.9899		0.9835
4	30	30	0.1525	0.9104	0.9835	
FLU × DBT 2-way interaction effect						
Cell No.	FLU (mg/L)	DBT (mg/L)	p-values			
1	5	5		0.1761	0.0744	0.0980
2	5	30	0.1761		0.9238	0.9733
3	30	5	0.0744	0.9238		0.9972
4	30	30	0.0980	0.9733	0.9972	

Table A8. Tukey's HSD test results of 3-way interaction influencing CBZ degradation

Cell No.	CBZ (mg/L)	FLU (mg/L)	DBT (mg/L)	CBZ × FLU × DBT 3-way interaction effect							
				p-values							
1	5	5	5		0.4870	0.4917	0.3230	0.8052	0.2656	0.0876	0.2036
2	5	5	30	0.4870		1.0000	0.9999	0.9972	0.9988	0.8237	0.9910
3	5	30	5	0.4917	1.0000		0.9999	0.9975	0.9987	0.8194	0.9903
4	5	30	30	0.3230	0.9999	0.9999		0.9615	1.0000	0.9518	0.9999
5	30	5	5	0.8052	0.9972	0.9975	0.9615		0.9211	0.5071	0.8419
6	30	5	30	0.2656	0.9988	0.9987	1.0000	0.9211		0.9798	1.0000
7	30	30	5	0.0876	0.8237	0.8194	0.9518	0.5071	0.9798		0.9959
8	30	30	30	0.2036	0.9910	0.9903	0.9999	0.8419	1.0000	0.9959	

Table A9. Tukey's HSD test results of main effects influencing FLU degradation

CBZ main effect		
Cell No.	CBZ (mg/L)	p values
1	5	0.0003
2	30	0.0003
FLU main effect		
Cell No.	FLU (mg/L)	p values
1	5	0.0376
2	30	0.0376
DBT main effect		
Cell No.	DBT (mg/L)	p values
1	5	0.0057
2	30	0.0057

Table A10. Tukey's HSD test results of 2-way interactions influencing FLU degradation

CBZ × FLU 2-way interaction effect						
Cell No.	CBZ (mg/L)	FLU (mg/L)	p-values			
1	5	5	0.0018	0.8670	0.0567	
2	5	30	0.0018		0.0009	0.0003
3	30	5	0.8670	0.0009		0.1661
4	30	30	0.0567	0.0003	0.1661	
CBZ × DBT 2-way interaction effect						
Cell No.	CBZ (mg/L)	DBT (mg/L)	p-values			
1	5	5	0.0003	0.6109	0.1977	
2	5	30	0.0003		0.0005	0.0002
3	30	5	0.6109	0.0005		0.0341
4	30	30	0.1977	0.0002	0.0341	
FLU × DBT 2-way interaction effect						
Cell No.	FLU (mg/L)	DBT (mg/L)	p-values			
1	5	5	0.0011	0.0006	0.0097	
2	5	30	0.0011		0.8079	0.0002
3	30	5	0.0006	0.8079		0.0002
4	30	30	0.0097	0.0002	0.0002	

Table A11. Tukey's HSD test results of 3-way interaction influencing FLU degradation

Cell No.	CBZ (mg/L)	FLU (mg/L)	DBT (mg/L)	CBZ × FLU × DBT 3-way interaction effect							
				p-values							
1	5	5	5		0.5572	0.0464	0.0003	0.5074	0.0127	0.0331	0.4977
2	5	5	30	0.5572		0.4995	0.0002	0.0473	0.1430	0.3760	1.0000
3	5	30	5	0.0464	0.4995		0.0002	0.0043	0.9472	1.0000	0.5590
4	5	30	30	0.0003	0.0002	0.0002		0.0006	0.0002	0.0002	0.0002
5	30	5	5	0.5074	0.0473	0.0043	0.0006		0.0016	0.0033	0.0408
6	30	5	30	0.0127	0.1430	0.9472	0.0002	0.0016		0.9882	0.1658
7	30	30	5	0.0331	0.3760	1.0000	0.0002	0.0033	0.9882		0.4271
8	30	30	30	0.4977	1.0000	0.5590	0.0002	0.0408	0.1658	0.4271	

Table A12. Tukey's HSD test results of main effects influencing DBT degradation

CBZ main effect		
Cell No.	CBZ (mg/L)	p values
1	5	0.0012
2	30	0.0012
FLU main effect		
Cell No.	FLU (mg/L)	p values
1	5	0.6927
2	30	0.6927
DBT main effect		
Cell No.	DBT (mg/L)	p values
1	5	0.0074
2	30	0.0074

Table A13. Tukey's HSD test results of 2-way interactions influencing DBT degradation

CBZ × FLU 2-way interaction effect						
Cell No.	CBZ (mg/L)	FLU (mg/L)	p-values			
1	5	5		0.0003	0.0021	0.0450
2	5	30	0.0003		0.0203	0.0002
3	30	5	0.0021	0.0203		0.0003
4	30	30	0.0450	0.0002	0.0003	
CBZ × DBT 2-way interaction effect						
Cell No.	CBZ (mg/L)	DBT (mg/L)	p-values			
1	5	5		0.0256	0.1520	0.7338
2	5	30	0.0256		0.0015	0.0066
3	30	5	0.1520	0.0015		0.5470
4	30	30	0.7338	0.0066	0.5470	
FLU × DBT 2-way interaction effect						
Cell No.	FLU (mg/L)	DBT (mg/L)	p-values			
1	5	5		0.0003	0.0009	0.0858
2	5	30	0.0003		0.1920	0.0015
3	30	5	0.0009	0.1920		0.0218
4	30	30	0.0858	0.0015	0.0218	

Table A14. Tukey's HSD test results of 3-way interaction influencing DBT degradation

Cell No.	CBZ (mg/L)	FLU (mg/L)	DBT (mg/L)	CBZ × FLU × DBT 3-way interaction effect							
				p-values							
1	5	5	5		0.0037	0.0003	0.0004	0.0473	0.0003	0.1741	0.8381
2	5	5	30	0.0037		0.0383	0.1378	0.4265	0.0420	0.1247	0.0010
3	5	30	5	0.0003	0.0383		0.9606	0.0031	1.0000	0.0012	0.0002
4	5	30	30	0.0004	0.1378	0.9606		0.0090	0.9730	0.0031	0.0003
5	30	5	5	0.0473	0.4265	0.0031	0.0090		0.0033	0.9574	0.0089
6	30	5	30	0.0003	0.0420	1.0000	0.9730	0.0033		0.0013	0.0002
7	30	30	5	0.1741	0.1247	0.0012	0.0031	0.9574	0.0013		0.0298
8	30	30	30	0.8381	0.0010	0.0002	0.0003	0.0089	0.0002	0.0298	

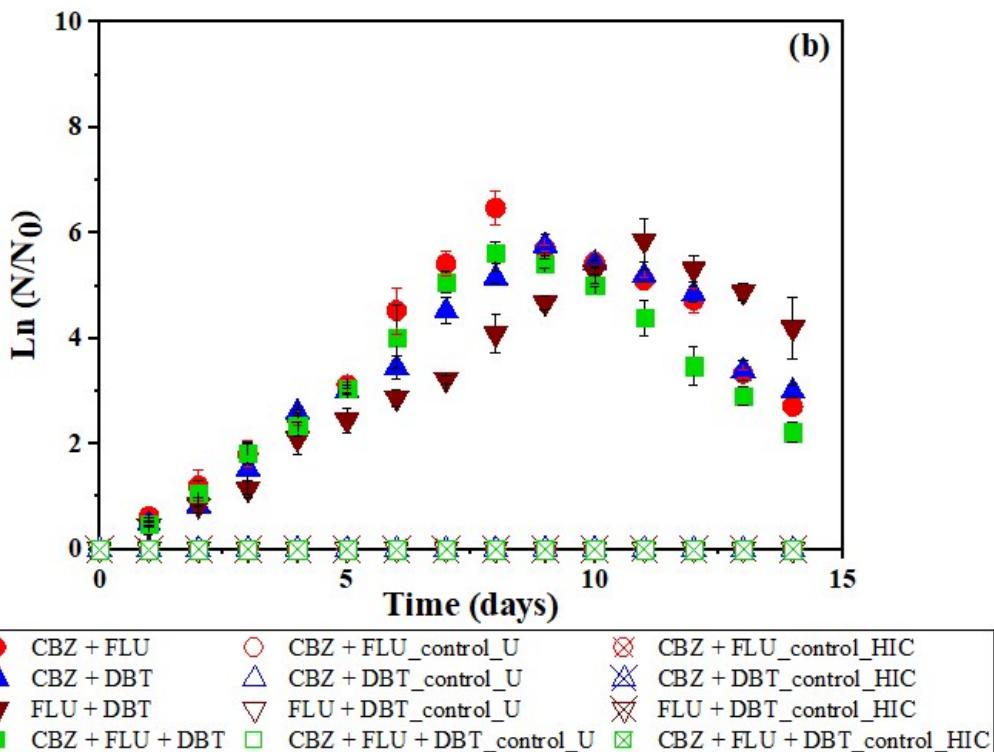
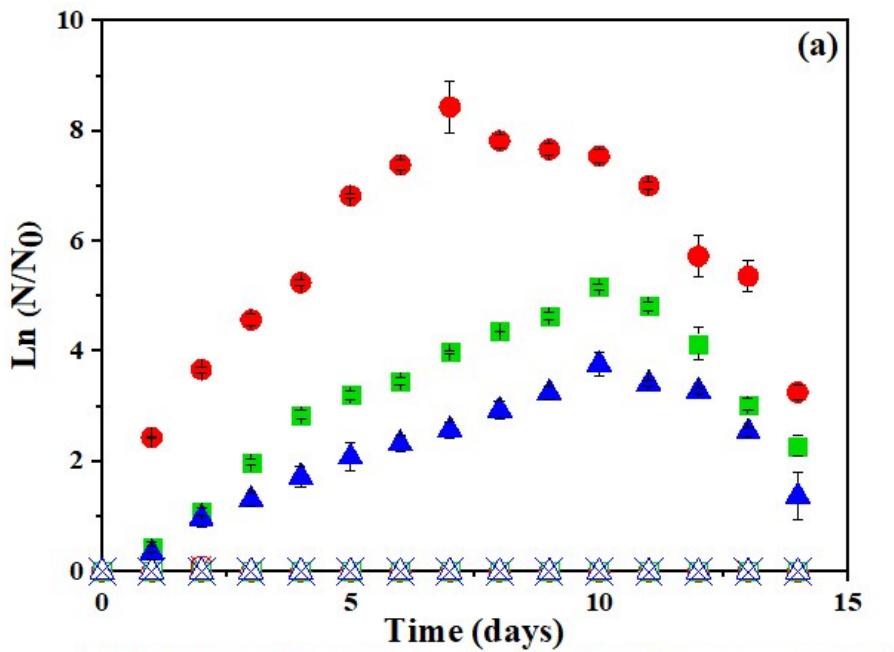


Fig. A1. Growth profiles of *P. aeruginosa* RS1 on (a) individual substrates and (b) binary and ternary substrates mixtures

U and HIC indicate uninoculated and heat inactivated cultures, respectively for the controls

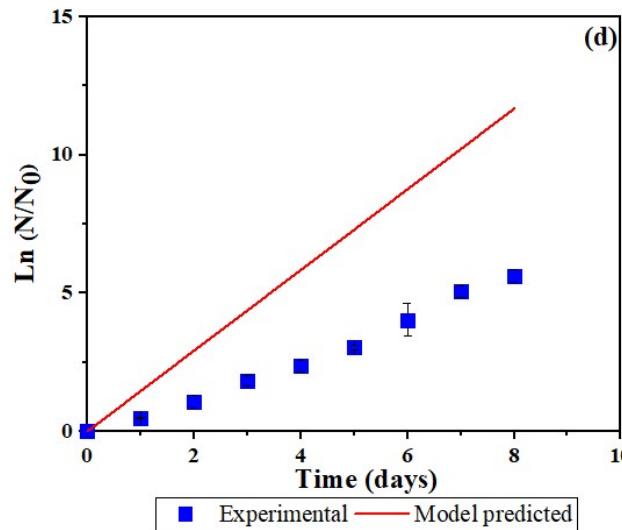
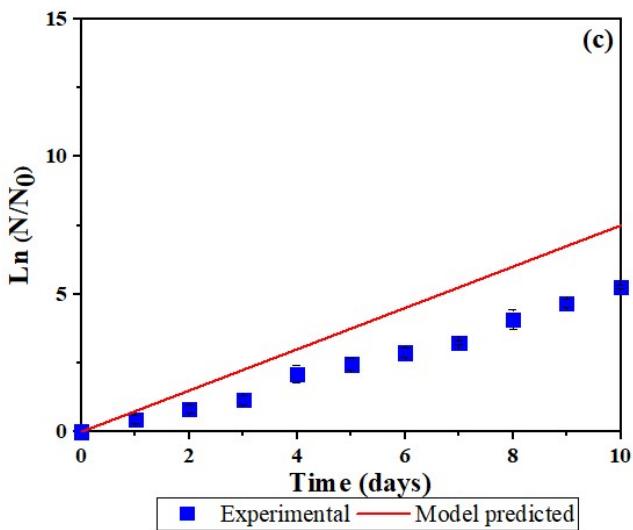
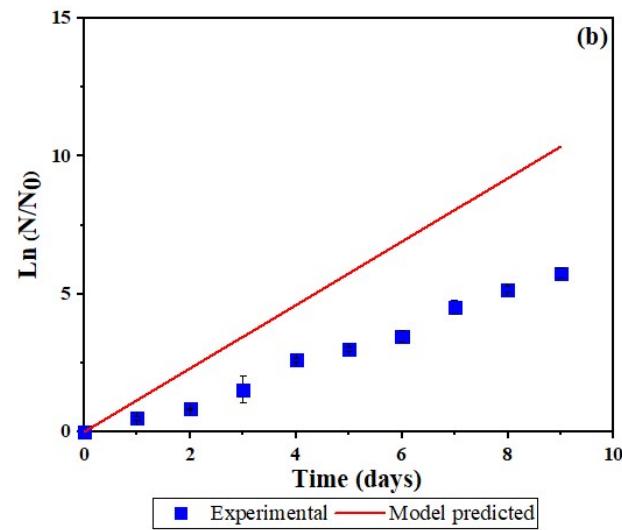
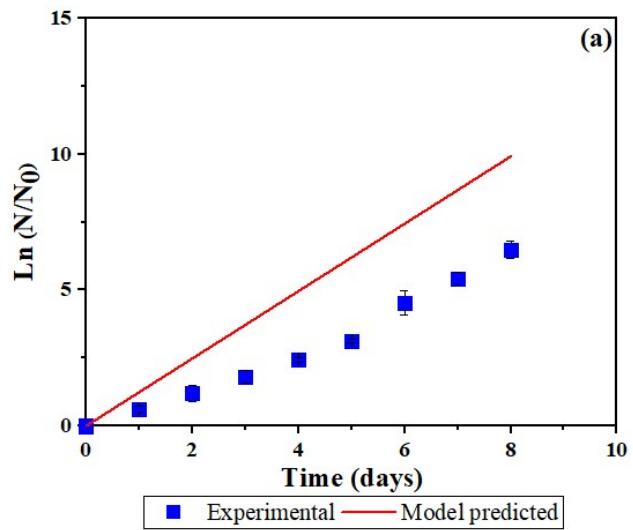


Fig. A2. Summary of model fits of bacterial growth on (a) CBZ+FLU, (b) CBZ + DBT, (c) FLU + DBT and (d) CBZ +FLU +DBT

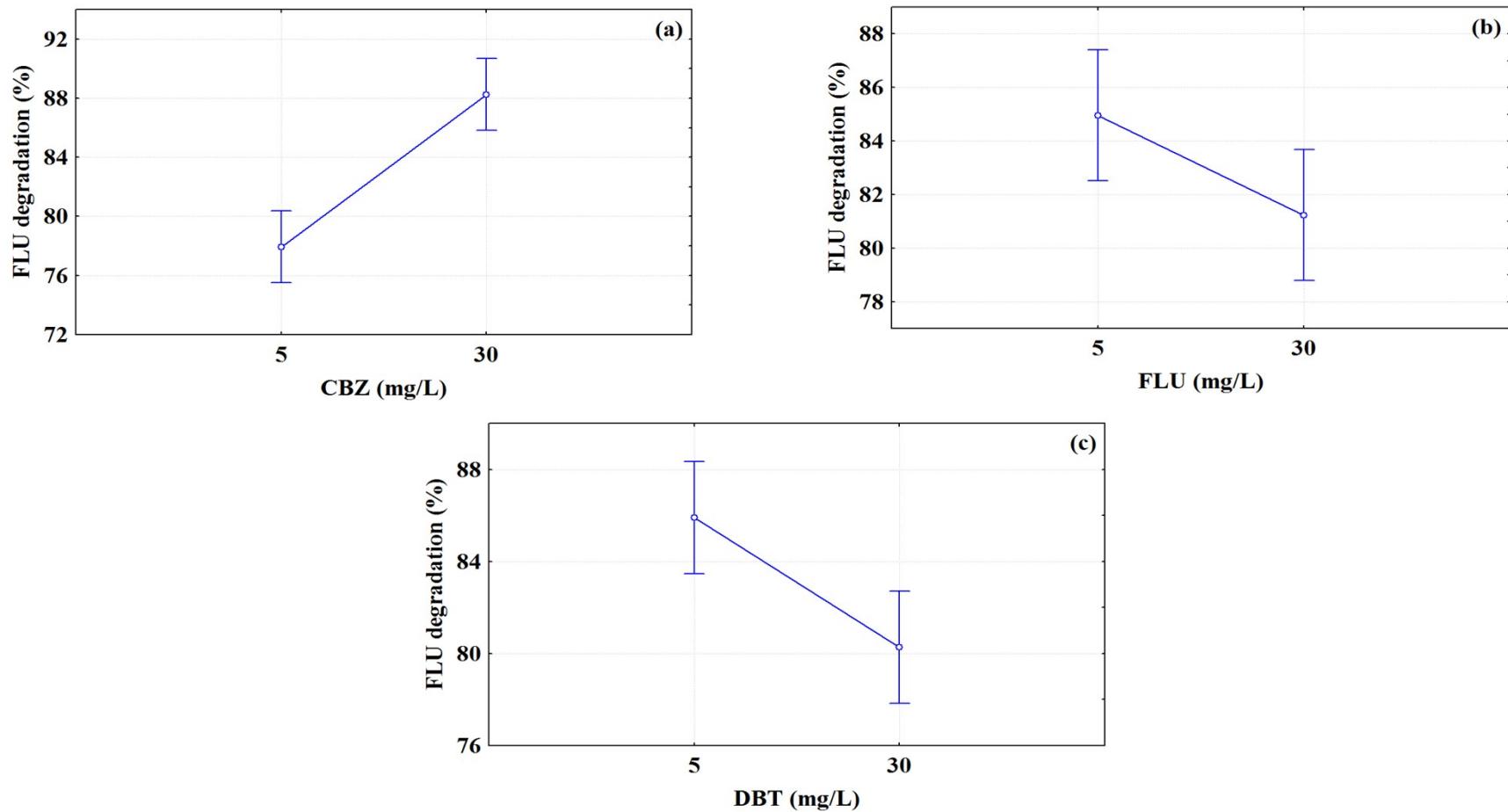


Fig. A3. Plots of main effects (a) CBZ, (b) FLU and (c) DBT influencing fluorene degradation

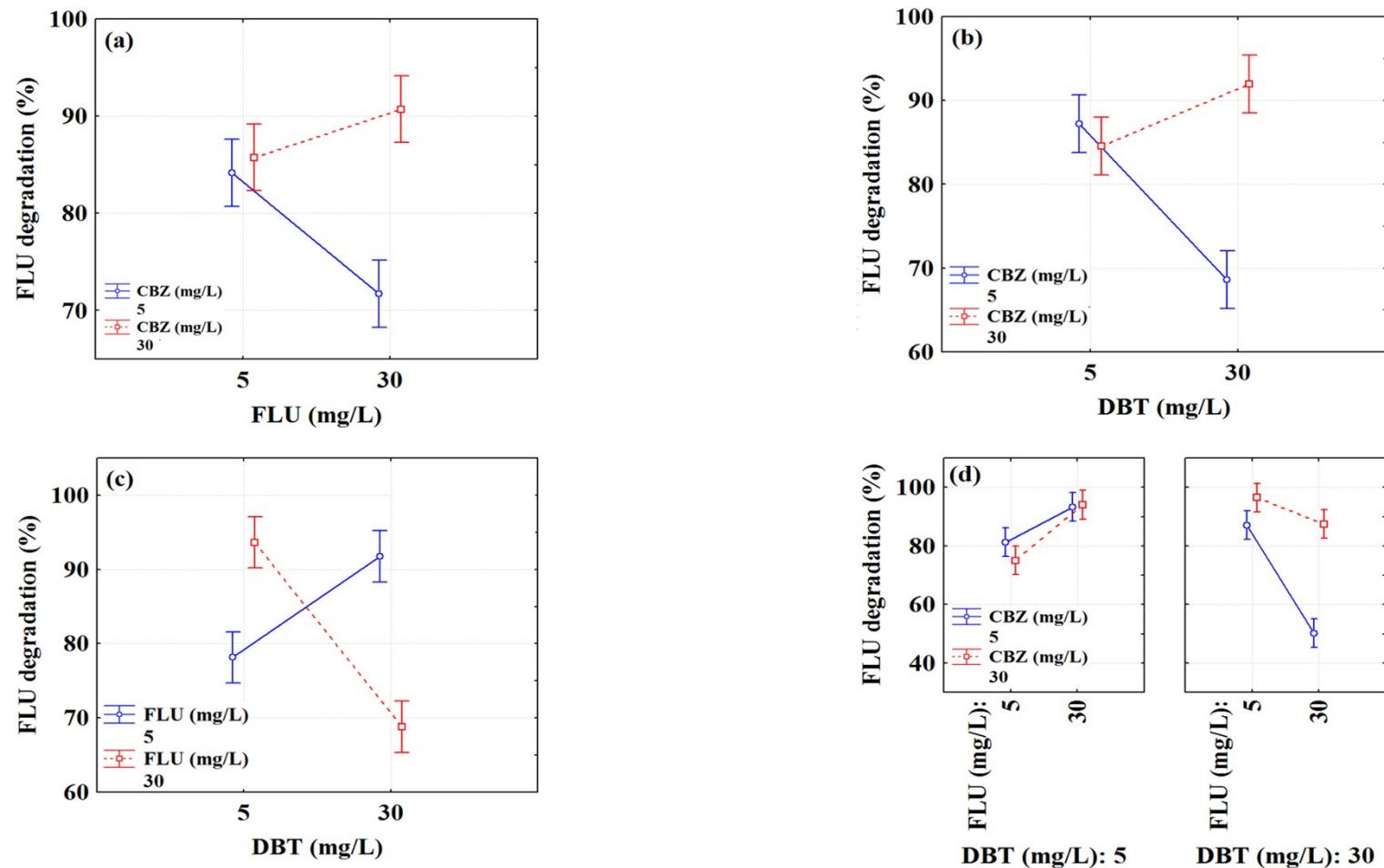


Fig. A4. Plots of 2-way interactions (a) CBZ × FLU, (b) CBZ × DBT, (c) FLU × DBT and 3-way interaction (d) CBZ × FLU × DBT influencing fluorene degradation

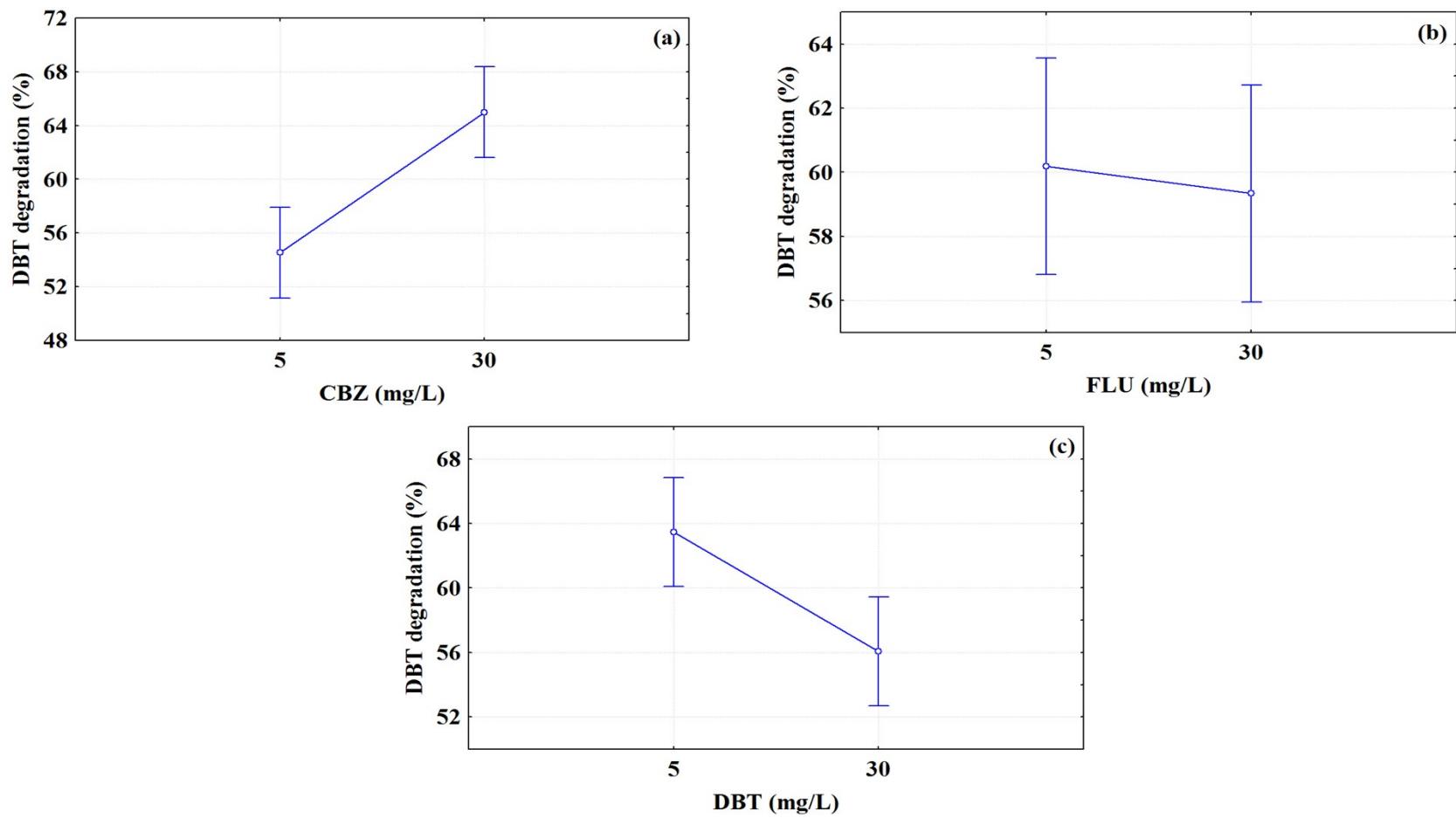


Fig. A5. Plots of main effects (a) CBZ, (b) FLU and (c) DBT influencing dibenzothiophene degradation

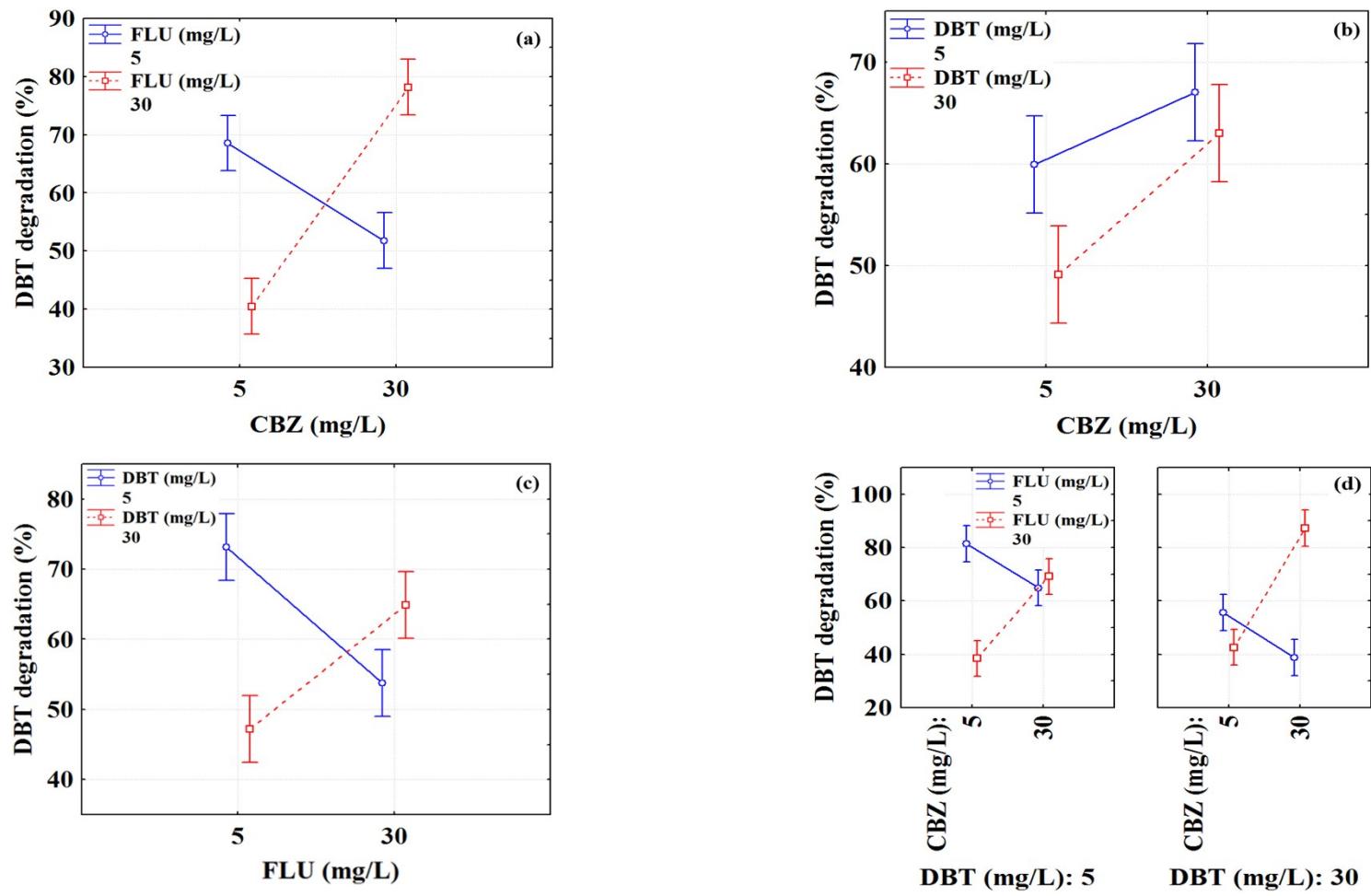


Fig. A6. Plots of 2-way interactions (a) CBZ × FLU, (b) CBZ × DBT, (c) FLU × DBT and 3-way interaction (d) CBZ × FLU × DBT influencing dibenzothiophene degradation