

第七章 參考文獻

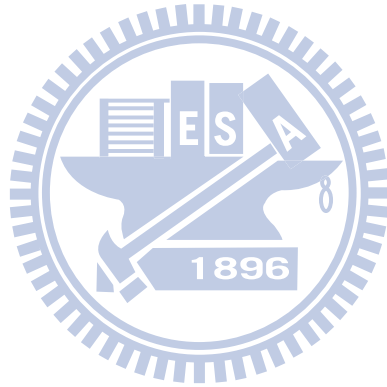
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附錄一、原始數據



實驗毒物: Ethyl fluoroacetate

初始細胞密度(cells/mL) : 15000

MCV (µm³) : 43.7

Initial pH : 7.48

EDTA(%):0

T(°C) :24

Test duration :48-h

Conc mg/L	Initial DO mg/L	Final DO mg/L	Final cells cells/ml	Delta DO mg/L	µspecific	µrelative	IR (growth rate)	IR (Biomass)	IR (DO)
Control	1.40	8.04	396400	6.64	1.64	1.00	0.00	0.00	0.00
0.1520	1.45	2.95	64900	1.50	0.73	0.45	0.55	0.87	0.77
0.0760	1.48	3.68	88100	2.20	0.89	0.54	0.46	0.81	0.67
0.0380	1.58	4.47	107100	2.89	0.98	0.60	0.40	0.76	0.56
0.0190	1.60	5.30	139700	3.70	1.12	0.68	0.32	0.67	0.44
0.0095	1.77	6.24	187900	4.47	1.26	0.77	0.23	0.55	0.33
0.0048	1.52	5.69	172000	4.17	1.22	0.75	0.25	0.59	0.37
Control	1.29	7.90	371500	6.61	1.60	1.00	0.00	0.00	0.00
0.1520	1.40	2.88	55100	1.48	0.65	0.41	0.59	0.89	0.78
0.0760	1.55	3.19	57000	1.64	0.67	0.42	0.58	0.88	0.75
0.0380	1.49	4.11	85700	2.62	0.87	0.54	0.46	0.80	0.60
0.0190	1.48	5.18	146100	3.70	1.14	0.71	0.29	0.63	0.44
0.0095	1.92	6.44	176700	4.52	1.23	0.77	0.23	0.55	0.32
0.0048	1.57	5.99	203000	4.42	1.30	0.81	0.19	0.47	0.33
Control	1.33	7.40	373700	6.07	1.61	1.00	0.00	0.00	0.00
0.1520	1.37	3.31	60500	1.94	0.70	0.43	0.57	0.87	0.68
0.0760	1.50	3.60	75700	2.10	0.81	0.50	0.50	0.83	0.65
0.0380	1.56	4.29	106500	2.73	0.98	0.61	0.39	0.74	0.55
0.0190	1.61	5.09	135000	3.48	1.10	0.68	0.32	0.67	0.43
0.0095	2.05	6.29	176600	4.24	1.23	0.77	0.23	0.55	0.30
0.0048	1.71	6.26	210100	4.55	1.32	0.82	0.18	0.46	0.25
Control	1.34	7.78	380533	6.44	1.62	1.00	0.00	0.00	0.00
0.1520	1.41	3.05	60167	1.64	0.69	0.43	0.57	0.88	0.75
0.0760	1.51	3.49	73600	1.98	0.79	0.49	0.51	0.84	0.69
0.0380	1.54	4.29	99767	2.75	0.94	0.58	0.41	0.77	0.57
0.0190	1.56	5.19	140267	3.63	1.12	0.69	0.31	0.66	0.44
0.0095	1.91	6.32	180400	4.41	1.24	0.77	0.23	0.55	0.32
0.0048	1.60	5.98	195033	4.38	1.28	0.79	0.21	0.51	0.32

IR : Inhibition rate

Biomass : Yield f (Final yield based on cell density)

實驗毒物: Ethyl chloroacetate

初始細胞密度(cells/mL) : 15000

MCV (µm³) : 41.0

Initial pH : 7.44

EDTA(%):0

T(°C) :24

Test duration :48-h

Conc mg/L	Initial DO mg/L	Final DO mg/L	Final cells cells/ml	Delta DO mg/L	µspecific	µrelative	IR (growth rate)	IR (Biomass)	IR (DO)
Control	1.62	6.34	249500	4.72	1.41	1.00	0.00	0.00	0.00
0.2115	2.54	2.59	18800	0.05	0.11	0.08	0.92	0.98	0.99
0.1058	2.10	2.77	46700	0.67	0.57	0.40	0.60	0.86	0.86
0.0529	1.90	5.51	171200	3.61	1.22	0.87	0.13	0.33	0.24
0.0264	1.63	5.12	166700	3.49	1.20	0.86	0.14	0.35	0.26
0.0132	1.71	6.62	253600	4.91	1.41	1.01	-0.01	-0.02	-0.04
0.0066	1.75	5.66	181600	3.91	1.25	0.89	0.11	0.29	0.17
Control	1.52	5.35	153300	3.83	1.16	1.00	0.00	0.00	0.00
0.2115	2.60	2.93	25200	0.33	0.26	0.22	0.78	0.93	0.91
0.1058	2.23	2.75	24400	0.52	0.24	0.21	0.79	0.93	0.86
0.0529	1.92	5.06	143300	3.14	1.13	0.97	0.03	0.07	0.18
0.0264	1.71	5.44	155700	3.73	1.17	1.01	-0.01	-0.02	0.03
0.0132	1.63	4.42	115300	2.79	1.02	0.88	0.12	0.27	0.27
0.0066	1.65	5.27	145500	3.62	1.14	0.98	0.02	0.06	0.05
Control	1.38	4.89	169400	3.51	1.21	1.00	0.00	0.00	0.00
0.2115	2.97	2.91	22900	-0.06	0.21	0.17	0.83	0.95	1.02
0.1058	2.39	3.30	29500	0.91	0.34	0.28	0.72	0.91	0.74
0.0529	2.22	5.76	166200	3.54	1.20	0.99	0.01	0.02	-0.01
0.0264	1.78	5.81	179100	4.03	1.24	1.02	-0.02	-0.06	-0.15
0.0132	1.74	4.20	109500	2.46	0.99	0.82	0.18	0.39	0.30
0.0066	1.62	5.31	159500	3.69	1.18	0.98	0.02	0.06	-0.05
Control	1.51	5.53	190733	4.02	1.26	1.00	0.00	0.00	0.00
0.2115	2.70	2.81	22300	0.11	0.19	0.16	0.84	0.96	0.97
0.1058	2.24	2.94	33533	0.70	0.38	0.30	0.68	0.89	0.83
0.0529	2.01	5.44	160233	3.43	1.18	0.94	0.07	0.17	0.15
0.0264	1.71	5.46	167167	3.75	1.20	0.96	0.05	0.13	0.07
0.0132	1.69	5.08	159467	3.39	1.14	0.90	0.07	0.18	0.16
0.0066	1.67	5.41	162200	3.74	1.19	0.95	0.06	0.16	0.07

IR : Inhibition rate

Biomass : Yield f (Final yield based on cell density)

實驗毒物: Ethyl bromoacetate

初始細胞密度(cells/mL) : 15000

MCV (µm³) : 39.8

Initial pH : 7.43

EDTA(%):0

T(°C) :24

Test duration :48-h

Conc mg/L	Initial DO mg/L	Final DO mg/L	Final cells cells/ml	Delta DO mg/L	µspecific	µrelative	IR (growth rate)	IR (Biomass)	IR (DO)
Control	1.38	5.99	225500	4.61	1.36	1.00	0.00	0.00	0.00
0.0580	1.74	1.72	29400	-0.02	0.34	0.25	0.75	0.93	1.00
0.0290	1.59	1.75	18600	0.16	0.11	0.08	0.92	0.98	0.97
0.0145	1.40	1.69	27900	0.29	0.31	0.23	0.77	0.94	0.94
0.0073	1.37	2.84	43200	1.47	0.53	0.39	0.61	0.87	0.68
0.0036	1.49	4.57	134900	3.08	1.10	0.81	0.19	0.43	0.33
0.0018	1.44	5.79	24400	4.35	0.24	0.18	0.82	0.96	0.06
0.0009	1.46	5.78	226500	4.32	1.36	1.00	0.00	0.00	0.06
Control	1.36	6.24	223600	4.88	1.35	1.00	0.00	0.00	0.00
0.0580	1.57	1.92	20100	0.35	0.15	0.11	0.89	0.98	0.93
0.0290	1.61	1.80	24000	0.19	0.24	0.17	0.83	0.96	0.96
0.0145	1.50	1.85	25800	0.35	0.27	0.20	0.80	0.95	0.93
0.0073	1.44	2.10	37100	0.66	0.45	0.34	0.66	0.89	0.86
0.0036	1.40	4.96	149600	3.56	1.15	0.85	0.15	0.35	0.27
0.0018	1.38	6.05	237200	4.67	1.38	1.02	-0.02	-0.07	0.04
0.0009	1.29	5.62	196900	4.33	1.29	0.95	0.05	0.13	0.11
Control	1.31	6.28	229700	4.97	1.36	1.00	0.00	0.00	0.00
0.0580	1.58	1.96	21300	0.38	0.18	0.13	0.87	0.97	0.92
0.0290	1.54	2.07	29500	0.53	0.34	0.25	0.75	0.93	0.89
0.0145	1.40	2.18	31200	0.78	0.37	0.27	0.73	0.92	0.84
0.0073	1.40	2.53	41800	1.13	0.51	0.38	0.62	0.88	0.77
0.0036	1.54	5.80	107300	4.26	0.98	0.72	0.28	0.57	0.14
0.0018	1.47	6.25	224400	4.78	1.35	0.99	0.01	0.02	0.04
0.0009	1.34	5.74	194500	4.40	1.28	0.94	0.06	0.16	0.11
Control	1.35	6.17	226267	4.82	1.36	1.00	0.00	0.00	0.00
0.0580	1.63	1.87	23600	0.24	0.22	0.16	0.83	0.96	0.95
0.0290	1.58	1.87	24033	0.29	0.23	0.17	0.83	0.96	0.94
0.0145	1.43	1.91	28300	0.47	0.32	0.23	0.77	0.94	0.90
0.0073	1.40	2.49	40700	1.09	0.50	0.37	0.63	0.88	0.77
0.0036	1.48	5.11	130600	3.63	1.08	0.79	0.20	0.45	0.25
0.0018	1.43	6.03	162000	4.60	0.99	0.73	0.12	0.30	0.05

IR : Inhibition rate

Biomass : Yield f (Final yield based on cell density)

實驗毒物: Ethyl iodoacetate

初始細胞密度(cells/mL) : 15000

MCV (µm³) : 42.7

Initial pH : 7.55

EDTA(%):0

T(°C) :24

Test duration :48-h

Conc mg/L	Initial DO mg/L	Final DO mg/L	Final cells cells/ml	Delta DO mg/L	µspecific	µrelative	IR (growth rate)	IR (Biomass)	IR (DO)
Control	1.80	5.07	200200	3.27	1.30	1.00	0.00	0.00	0.00
0.016	1.54	1.65	33600	0.11	0.40	0.31	0.69	0.90	0.97
0.008	1.41	2.12	45000	0.71	0.55	0.42	0.58	0.84	0.78
0.004	1.53	2.40	48800	0.87	0.59	0.46	0.54	0.82	0.73
0.002	1.47	3.77	134400	2.30	1.10	0.85	0.15	0.36	0.30
0.001	1.56	4.26	166600	2.70	1.20	0.93	0.07	0.18	0.17
0.0005	1.54	4.56	181100	3.02	1.25	0.96	0.04	0.10	0.08
Control	1.62	4.60	173300	2.98	1.22	1.00	0.00	0.00	0.00
0.016	1.53	2.23	40600	0.70	0.50	0.41	0.59	0.84	0.77
0.008	1.47	2.09	42000	0.62	0.51	0.42	0.58	0.83	0.79
0.004	1.54	2.43	34400	0.89	0.42	0.34	0.66	0.88	0.70
0.002	1.53	3.98	116600	2.45	1.03	0.84	0.16	0.36	0.18
0.001	1.55	4.43	178900	2.88	1.24	1.01	-0.01	-0.04	0.03
0.0005	1.54	4.71	199600	3.17	1.29	1.06	-0.06	-0.17	-0.06
Control	1.57	4.71	181900	3.14	1.25	1.00	0.00	0.00	0.00
0.0160	1.72	1.96	25900	0.24	0.27	0.22	0.78	0.93	0.92
0.0080	1.54	1.99	22600	0.45	0.20	0.16	0.84	0.95	0.86
0.0040	1.45	2.32	30400	0.87	0.35	0.28	0.72	0.91	0.72
0.0020	1.69	3.94	131100	2.25	1.08	0.87	0.13	0.30	0.28
0.0010	1.55	4.07	155500	2.52	1.17	0.94	0.06	0.16	0.20
0.0005	1.58	4.85	189500	3.27	1.27	1.02	-0.02	-0.05	-0.04
Control	1.66	4.79	185133	3.13	1.26	1.00	0.00	0.00	0.00
0.016	1.60	1.95	33367	0.35	0.39	0.31	0.68	0.89	0.89
0.008	1.47	2.07	36533	0.59	0.42	0.34	0.65	0.87	0.81
0.004	1.51	2.38	37867	0.88	0.45	0.36	0.63	0.87	0.72
0.002	1.56	3.90	127367	2.33	1.07	0.85	0.15	0.34	0.25
0.001	1.55	4.25	167000	2.70	1.20	0.96	0.04	0.11	0.14
0.0005	1.55	4.71	190067	3.15	1.27	1.01	-0.01	-0.03	-0.01

IR : Inhibition rate

Biomass : Yield f (Final yield based on cell density)

實驗毒物: Methyl bromoacetate

初始細胞密度(cells/mL) : 15000

MCV (µm3) : 41.0

Initial pH : 7.62

EDTA(%):0

T(°C) :24

Test duration :48-h

Conc mg/L	Initial DO mg/L	Final DO mg/L	Final cells cells/ml	Delta DO mg/L	µspecific	µrelative	IR (growth rate)	IR (Biomass)	IR (DO)
Control	1.42	6.95	305700	5.53	1.51	1.00	0.00	0.00	0.00
0.0420	1.74	2.04	20500	0.30	0.16	0.10	0.90	0.98	0.95
0.0210	1.54	2.16	25100	0.62	0.26	0.17	0.83	0.97	0.89
0.0105	1.46	2.25	35500	0.79	0.43	0.29	0.71	0.93	0.86
0.0053	1.40	5.07	188900	3.67	1.27	0.84	0.16	0.40	0.34
0.0026	1.38	6.69	284400	5.31	1.47	0.98	0.02	0.07	0.04
0.0013	1.56	6.77	298900	5.21	1.50	0.99	0.01	0.02	0.06
Control	1.40	6.70	312100	5.30	1.52	1.00	0.00	0.00	0.00
0.0420	1.62	2.34	15000	0.72	0.00	0.00	1.00	1.00	0.86
0.0210	1.60	2.23	21700	0.63	0.18	0.12	0.88	0.98	0.88
0.0105	1.50	2.29	31700	0.79	0.37	0.25	0.75	0.94	0.85
0.0053	1.28	4.54	188500	3.26	1.27	0.83	0.17	0.42	0.38
0.0026	2.15	6.93	293600	4.78	1.49	0.98	0.02	0.06	0.10
0.0013	1.89	6.87	295400	4.98	1.49	0.98	0.02	0.06	0.06
Control	1.40	6.98	313000	5.58	1.52	1.00	0.00	0.00	0.00
0.0420	1.68	2.43	33000	0.75	0.39	0.26	0.74	0.94	0.87
0.0210	1.69	2.12	24000	0.43	0.24	0.15	0.85	0.97	0.92
0.0105	1.56	2.01	36800	0.45	0.45	0.30	0.70	0.93	0.92
0.0053	1.37	4.98	184100	3.61	1.25	0.83	0.17	0.43	0.35
0.0026	1.45	6.70	289500	5.25	1.48	0.97	0.03	0.08	0.06
0.0013	1.73	7.01	291800	5.28	1.48	0.98	0.02	0.07	0.05
Control	1.41	6.88	310267	5.47	1.51	1.00	0.00	0.00	0.00
0.0420	1.68	2.27	22833	0.59	0.18	0.12	0.86	0.97	0.89
0.0210	1.61	2.17	23600	0.56	0.23	0.15	0.85	0.97	0.90
0.0105	1.51	2.18	34667	0.68	0.42	0.28	0.72	0.93	0.88
0.0053	1.35	4.86	187167	3.51	1.26	0.83	0.17	0.42	0.36
0.0026	1.66	6.77	289167	5.11	1.48	0.98	0.02	0.07	0.07
0.0013	1.73	6.88	295367	5.16	1.49	0.98	0.02	0.05	0.06

IR : Inhibition rate

Biomass : Yield f (Final yield based on cell density)

實驗毒物: Methyl 3-bromopropionate

初始細胞密度(cells/mL) : 15000

MCV (µm3) : 39.5

Initial pH : 7.49

EDTA(%):0

T(°C) :24

Test duration :48-h

Conc mg/L	Initial DO mg/L	Final DO mg/L	Final cells cells/ml	Delta DO mg/L	µspecific	µrelative	IR (growth rate)	IR (Biomass)	IR (DO)
Control	1.43	6.83	291100	5.40	1.48	1.00	0.00	0.00	0.00
708.6	2.50	3.23	28600	0.73	0.32	0.22	0.78	0.95	0.86
354.3	1.95	1.16	20200	-0.79	0.15	0.10	0.90	0.98	1.15
177.2	1.49	1.86	31400	0.37	0.37	0.25	0.75	0.94	0.93
88.6	1.49	5.04	108400	3.55	0.99	0.67	0.33	0.66	0.34
44.3	1.38	7.27	244200	5.89	1.39	0.94	0.06	0.17	-0.09
22.1	1.30	7.31	299000	6.01	1.50	1.01	-0.01	-0.03	-0.11
11.1	1.25	7.74	313700	6.49	1.52	1.03	-0.03	-0.08	-0.20
Control	1.26	7.66	312800	6.40	1.52	1.00	0.00	0.00	0.00
708.6	2.47	2.72	17300	0.25	0.07	0.05	0.95	0.99	0.96
354.3	1.96	0.80	20500	-1.16	0.16	0.10	0.90	0.98	1.18
177.2	1.51	2.02	29800	0.51	0.34	0.23	0.77	0.95	0.92
88.6	1.50	5.37	121100	3.87	1.04	0.69	0.31	0.64	0.40
44.3	1.43	6.97	239400	5.54	1.39	0.91	0.09	0.25	0.13
22.1	1.42	6.81	278500	5.39	1.46	0.96	0.04	0.12	0.16
11.1	1.42	6.78	269800	5.36	1.44	0.95	0.05	0.14	0.16
Control	1.22	6.86	307700	5.64	1.51	1.00	0.00	0.00	0.00
708.6	2.37	2.98	15800	0.61	0.03	0.02	0.98	1.00	0.89
354.3	2.01	1.76	24300	-0.25	0.24	0.16	0.84	0.97	1.04
177.2	1.45	2.02	33100	0.57	0.40	0.26	0.74	0.94	0.90
88.6	1.59	5.39	101100	3.80	0.95	0.63	0.37	0.71	0.33
44.3	1.44	6.63	249200	5.19	1.41	0.93	0.07	0.20	0.08
22.1	1.41	7.10	279500	5.69	1.46	0.97	0.03	0.10	-0.01
11.1	1.34	6.94	295400	5.60	1.49	0.99	0.01	0.04	0.01
Control	1.30	7.12	303867	5.81	1.50	1.00	0.00	0.00	0.00
708.6	2.45	2.98	20567	0.53	0.14	0.09	0.90	0.98	0.91
354.3	1.97	1.24	21667	-0.73	0.18	0.12	0.88	0.98	1.13
177.2	1.48	1.97	31433	0.48	0.37	0.25	0.75	0.94	0.92
88.6	1.53	5.27	110200	3.74	1.00	0.66	0.34	0.67	0.36
44.3	1.42	6.96	244267	5.54	1.40	0.93	0.07	0.21	0.05
22.1	1.38	7.07	285667	5.70	1.47	0.98	0.02	0.06	0.02
11.1	1.34	7.15	292967	5.82	1.49	0.99	0.01	0.04	0.00

IR : Inhibition rate

Biomass : Yield f (Final yield based on cell density)

實驗毒物: Methyl 2-bromopropionate

初始細胞密度(cells/mL) : 15000

MCV (µm3) : 42.4

Initial pH : 7.60

EDTA(%):0

T(°C) :24

Test duration :48-h

Conc mg/L	Initial DO mg/L	Final DO mg/L	Final cells cells/ml	Delta DO mg/L	µspecific	µrelative	IR (growth rate)	IR (Biomass)	IR (DO)
Control	1.33	5.32	205200	3.99	1.31	1.00	0.00	0.00	0.00
0.927	1.52	2.92	59700	1.40	0.69	0.53	0.47	0.76	0.65
0.463	1.62	3.81	100100	2.19	0.95	0.73	0.27	0.55	0.45
0.232	1.38	4.18	124600	2.80	1.06	0.81	0.19	0.42	0.30
0.116	1.37	4.74	169300	3.37	1.21	0.93	0.07	0.19	0.16
0.058	1.64	5.65	229600	4.01	1.36	1.04	-0.04	-0.13	-0.01
0.029	1.36	4.95	228000	3.59	1.36	1.04	-0.04	-0.12	0.10
0.014	1.45	5.41	233400	3.96	1.37	1.05	-0.05	-0.15	0.01
Control	1.36	5.17	227600	3.81	1.36	1.00	0.00	0.00	0.00
0.9267	1.57	3.51	79600	1.94	0.83	0.61	0.39	0.70	0.49
0.4634	1.61	4.17	116500	2.56	1.02	0.75	0.25	0.52	0.33
0.2317	1.50	4.57	147400	3.07	1.14	0.84	0.16	0.38	0.19
0.1158	1.53	5.21	209400	3.68	1.32	0.97	0.03	0.09	0.03
0.0579	1.49	4.40	188400	2.91	1.27	0.93	0.07	0.18	0.24
0.0290	1.38	4.75	204600	3.37	1.31	0.96	0.04	0.11	0.12
0.0145	1.45	5.17	239300	3.72	1.38	1.02	-0.02	-0.06	0.02
Control	1.54	5.21	212700	3.67	1.33	1.00	0.00	0.00	0.00
0.9267	1.31	3.01	66800	1.70	0.75	0.56	0.44	0.74	0.54
0.4634	1.46	3.76	100900	2.30	0.95	0.72	0.28	0.57	0.37
0.2317	1.63	4.79	153400	3.16	1.16	0.88	0.12	0.30	0.14
0.1158	1.51	3.89	140200	2.38	1.12	0.84	0.16	0.37	0.35
0.0579	1.56	4.28	143400	2.72	1.13	0.85	0.15	0.35	0.26
0.0290	1.41	5.43	235100	4.02	1.38	1.04	-0.04	-0.11	-0.10
0.0145	1.34	4.67	209900	3.33	1.32	1.00	0.00	0.01	0.09
Control	1.41	5.23	215167	3.82	1.33	1.00	0.00	0.00	0.00
0.9267	1.47	3.15	68700	1.68	0.76	0.57	0.43	0.73	0.56
0.4634	1.56	3.91	105833	2.35	0.98	0.73	0.27	0.55	0.39
0.2317	1.50	4.51	141800	3.01	1.12	0.84	0.16	0.37	0.21
0.1158	1.47	4.61	172967	3.14	1.22	0.91	0.08	0.21	0.18
0.0579	1.56	4.78	187133	3.21	1.25	0.94	0.05	0.14	0.16
0.0290	1.38	5.04	222567	3.66	1.35	1.01	-0.01	-0.04	0.04
0.0145	1.41	5.08	227533	3.67	1.36	1.02	-0.02	-0.06	0.04

IR : Inhibition rate

Biomass : Yield f (Final yield based on cell density)

實驗毒物: Ethyl-2-bromopropionate

初始細胞密度(cells/mL) : 15000

MCV (µm3) : 44.2

Initial pH : 7.40

EDTA(%):0

T(°C) :24

Test duration :48-h

Conc mg/L	Initial DO mg/L	Final DO mg/L	Final cells cells/ml	Delta DO mg/L	µspecific	µrelative	IR (growth rate)	IR (Biomass)	IR (DO)
Control	1.29	5.69	271000	4.40	1.45	1.00	0.00	0.00	0.00
4.480	1.54	1.74	30700	0.20	0.36	0.25	0.75	0.94	0.95
2.240	1.23	1.42	24000	0.19	0.24	0.16	0.84	0.96	0.96
1.120	1.31	2.17	40100	0.86	0.49	0.34	0.66	0.90	0.80
0.560	1.12	3.08	57200	1.96	0.67	0.46	0.54	0.84	0.55
0.280	1.38	4.06	124600	2.68	1.06	0.73	0.27	0.57	0.39
0.140	1.20	5.25	229500	4.05	1.36	0.94	0.06	0.16	0.08
0.070	1.26	5.70	288200	4.44	1.48	1.02	-0.02	-0.07	-0.01
Control	1.31	6.01	276600	4.70	1.46	1.00	0.00	0.00	0.00
4.480	1.62	1.93	35700	0.31	0.43	0.30	0.70	0.92	0.93
2.240	1.23	1.71	21100	0.48	0.17	0.12	0.88	0.98	0.90
1.120	1.19	2.40	39300	1.21	0.48	0.33	0.67	0.91	0.74
0.560	1.15	2.75	54800	1.60	0.65	0.44	0.56	0.85	0.66
0.280	1.26	3.99	113200	2.73	1.01	0.69	0.31	0.62	0.42
0.140	1.20	5.53	248200	4.33	1.40	0.96	0.04	0.11	0.08
0.070	1.13	5.34	268700	4.21	1.44	0.99	0.01	0.03	0.10
Control	1.21	5.86	275800	4.65	1.46	1.00	0.00	0.00	0.00
4.480	1.69	2.40	32800	0.71	0.39	0.27	0.73	0.93	0.85
2.240	1.31	2.20	31200	0.89	0.37	0.25	0.75	0.94	0.81
1.120	1.28	1.74	30400	0.46	0.35	0.24	0.76	0.94	0.90
0.560	1.16	2.94	37600	1.78	0.46	0.32	0.68	0.91	0.62
0.280	1.20	3.42	81400	2.22	0.85	0.58	0.42	0.75	0.52
0.140	1.16	5.61	271700	4.45	1.45	0.99	0.01	0.02	0.04
0.070	1.32	5.75	274100	4.43	1.45	1.00	0.00	0.01	0.05
Control	1.27	5.85	274467	4.58	1.45	1.00	0.00	0.00	0.00
4.480	1.62	2.02	33067	0.41	0.39	0.27	0.73	0.93	0.91
2.240	1.26	1.78	25433	0.52	0.26	0.18	0.82	0.96	0.89
1.120	1.26	2.10	36600	0.84	0.44	0.30	0.69	0.92	0.82
0.560	1.14	2.92	49867	1.78	0.59	0.41	0.59	0.87	0.61
0.280	1.28	3.82	106400	2.54	0.97	0.67	0.33	0.65	0.45
0.140	1.19	5.46	249800	4.28	1.41	0.97	0.03	0.10	0.07
0.070	1.24	5.60	277000	4.36	1.46	1.00	0.00	-0.01	0.05

IR : Inhibition rate

Biomass : Yield f (Final yield based on cell density)

實驗毒物: Methyl 2-bromobutyrate

初始細胞密度(cells/mL) : 15000

MCV (µm3) : 41.3

Initial pH : 7.55

EDTA(%):0

T(°C) :24

Test duration :48-h

Conc mg/L	Initial DO mg/L	Final DO mg/L	Final cells cells/ml	Delta DO mg/L	µspecific	µrelative	IR (growth rate)	IR (Biomass)	IR (DO)
Control	1.25	6.20	243200	4.95	1.39	1.00	0.00	0.00	0.00
5.990	1.79	1.69	21000	-0.10	0.17	0.12	0.88	0.97	1.02
2.995	1.46	1.85	29600	0.39	0.34	0.24	0.76	0.94	0.92
1.498	1.29	4.70	159700	3.41	1.18	0.85	0.15	0.37	0.31
0.749	1.32	5.85	221800	4.53	1.35	0.97	0.03	0.09	0.08
0.374	1.40	6.15	239700	4.75	1.39	0.99	0.01	0.02	0.04
0.187	1.42	6.31	251100	4.89	1.41	1.01	-0.01	-0.03	0.01
0.094	1.35	6.20	240900	4.85	1.39	1.00	0.00	0.01	0.02
Control	1.19	5.97	241500	4.78	1.39	1.00	0.00	0.00	0.00
5.990	1.88	1.96	22100	0.08	0.19	0.14	0.86	0.97	0.98
2.995	1.56	1.88	31200	0.32	0.37	0.26	0.74	0.93	0.93
1.498	1.30	4.63	159700	3.33	1.18	0.85	0.15	0.36	0.30
0.749	1.33	5.80	233800	4.47	1.37	0.99	0.01	0.03	0.06
0.374	1.31	5.78	242200	4.47	1.39	1.00	0.00	0.00	0.06
0.187	1.42	5.93	251700	4.51	1.41	1.01	-0.01	-0.05	0.06
0.094	1.34	6.34	244700	5.00	1.40	1.00	0.00	-0.01	-0.05
Control	1.12	6.67	258700	5.55	1.42	1.00	0.00	0.00	0.00
5.990	2.12	2.17	25500	0.05	0.27	0.19	0.81	0.96	0.99
2.995	1.52	1.83	20300	0.31	0.15	0.11	0.89	0.98	0.94
1.498	1.24	4.59	126800	3.35	1.07	0.75	0.25	0.54	0.40
0.749	1.33	5.70	230100	4.37	1.37	0.96	0.04	0.12	0.21
0.374	1.25	5.86	251100	4.61	1.41	0.99	0.01	0.03	0.17
0.187	1.38	6.55	252200	5.17	1.41	0.99	0.01	0.03	0.07
0.094	1.44	6.45	234900	5.01	1.38	0.97	0.03	0.10	0.10
Control	1.19	6.28	247800	5.09	1.40	1.00	0.00	0.00	0.00
5.990	1.93	1.94	22867	0.01	0.21	0.15	0.85	0.97	1.00
2.995	1.51	1.85	27033	0.34	0.29	0.20	0.79	0.95	0.93
1.498	1.28	4.64	148733	3.36	1.14	0.82	0.18	0.43	0.34
0.749	1.33	5.78	228567	4.46	1.36	0.97	0.03	0.08	0.13
0.374	1.32	5.93	244333	4.61	1.40	1.00	0.01	0.01	0.09
0.187	1.41	6.26	251667	4.86	1.41	1.01	-0.01	-0.02	0.05
0.094	1.38	6.33	240167	4.95	1.39	0.99	0.01	0.03	0.03

IR : Inhibition rate

Biomass : Yield f (Final yield based on cell density)

實驗毒物: Ethyl-2-di-bromoisobutyrate

初始細胞密度(cells/mL) : 15000

MCV (µm³) : 40.8

Initial pH : 7.58

EDTA(%):0

T(°C) :24

Test duration :48-h

Conc mg/L	Initial DO mg/L	Final DO mg/L	Final cells cells/ml	Delta DO mg/L	µspecific	µrelative	IR (growth rate)	IR (Biomass)	IR (DO)
Control	1.25	8.28	287600	7.03	1.48	1.00	0.00	0.00	0.00
104.0	2.59	2.32	21900	-0.27	0.19	0.13	0.87	0.97	1.04
52.0	1.92	1.69	29900	-0.23	0.34	0.23	0.77	0.95	1.03
26.0	1.69	2.76	164000	1.07	1.20	0.81	0.19	0.45	0.85
13.0	1.44	5.50	234000	4.06	1.37	0.93	0.07	0.20	0.42
6.5	1.37	6.60	249300	5.23	1.41	0.95	0.05	0.14	0.26
3.3	1.40	6.59	272100	5.19	1.45	0.98	0.02	0.06	0.26
1.6	1.27	7.54	305000	6.27	1.51	1.02	-0.02	-0.06	0.11
Control	1.25	7.70	285900	6.45	1.47	1.00	0.00	0.00	0.00
104.0	2.38	2.21	20200	-0.17	0.15	0.10	0.90	0.98	1.03
52.0	1.93	2.01	28700	0.08	0.32	0.22	0.78	0.95	0.99
26.0	1.61	2.58	91700	0.97	0.91	0.61	0.39	0.72	0.85
13.0	1.51	5.36	222600	3.85	1.35	0.92	0.08	0.23	0.40
6.5	1.31	6.45	259300	5.14	1.42	0.97	0.03	0.10	0.20
3.3	1.36	6.72	276300	5.36	1.46	0.99	0.01	0.04	0.17
1.6	1.27	7.40	291500	6.13	1.48	1.01	-0.01	-0.02	0.05
Control	1.31	6.97	274400	5.66	1.45	1.00	0.00	0.00	0.00
104.0	2.44	2.40	25300	-0.04	0.26	0.18	0.82	0.96	1.01
52.0	1.89	2.66	31200	0.77	0.37	0.25	0.75	0.94	0.86
26.0	1.61	3.13	80200	1.52	0.84	0.58	0.42	0.75	0.73
13.0	1.49	5.71	250300	4.22	1.41	0.97	0.03	0.09	0.25
6.5	1.45	6.68	268000	5.23	1.44	0.99	0.01	0.02	0.08
3.3	1.33	7.52	259100	6.19	1.42	0.98	0.02	0.06	-0.09
1.6	1.24	7.57	285800	6.33	1.47	1.01	-0.01	-0.04	-0.12
Control	1.27	7.65	282633	6.38	1.47	1.00	0.00	0.00	0.00
104.0	2.47	2.31	22467	-0.16	0.20	0.14	0.86	0.97	1.03
52.0	1.91	2.12	29933	0.21	0.35	0.24	0.76	0.94	0.97
26.0	1.64	2.82	111967	1.19	0.98	0.67	0.32	0.64	0.81
13.0	1.48	5.52	235633	4.04	1.38	0.94	0.06	0.18	0.37
6.5	1.38	6.58	258867	5.20	1.42	0.97	0.03	0.09	0.18
3.3	1.36	6.94	269167	5.58	1.44	0.98	0.02	0.05	0.13
1.6	1.26	7.50	294100	6.24	1.49	1.01	-0.01	-0.04	0.02

IR : Inhibition rate

Biomass : Yield f (Final yield based on cell density)

實驗毒物: tert-Butyl bromoacetate

初始細胞密度(cells/mL) : 15000

MCV (µm³) : 43.2

Initial pH : 7.46

EDTA(%):0

T(°C) :24

Test duration :48-h

Conc mg/L	Initial DO mg/L	Final DO mg/L	Final cells cells/ml	Delta DO		µrelative	IR (growth rate)	IR (Biomass)	IR (DO)
				mg/L	µspecific				
Control	1.28	8.26	369700	6.98	1.60	1.00	0.00	0.00	0.00
0.1050	2.39	3.45	28700	1.06	0.32	0.20	0.80	0.96	0.85
0.0525	1.57	2.52	21500	0.95	0.18	0.11	0.89	0.98	0.86
0.0263	1.37	3.37	58400	2.00	0.68	0.42	0.58	0.88	0.71
0.0131	1.19	6.36	264000	5.17	1.43	0.89	0.11	0.30	0.26
0.0066	1.35	7.31	301000	5.96	1.50	0.94	0.06	0.19	0.15
0.0033	1.44	8.56	384800	7.12	1.62	1.01	-0.01	-0.04	-0.02
0.0016	1.37	8.33	376500	6.96	1.61	1.01	-0.01	-0.02	0.00
Control	1.49	8.42	339800	6.93	1.56	1.00	0.00	0.00	0.00
0.1050	2.19	2.67	20700	0.48	0.16	0.10	0.90	0.98	0.93
0.0525	1.63	2.80	43900	1.17	0.54	0.34	0.66	0.91	0.83
0.0263	1.30	3.68	68700	2.38	0.76	0.49	0.51	0.83	0.66
0.0131	1.29	6.76	284500	5.47	1.47	0.94	0.06	0.17	0.21
0.0066	1.25	7.12	321600	5.87	1.53	0.98	0.02	0.06	0.15
0.0033	1.44	8.72	389500	7.28	1.63	1.04	-0.04	-0.15	-0.05
0.0016	1.31	8.21	332400	6.90	1.55	0.99	0.01	0.02	0.00
Control	1.28	8.50	375800	7.22	1.61	1.00	0.00	0.00	0.00
0.1050	2.35	3.01	17400	0.66	0.07	0.05	0.95	0.99	0.91
0.0525	1.73	2.18	31100	0.45	0.36	0.23	0.77	0.96	0.94
0.0263	1.27	3.64	85100	2.37	0.87	0.54	0.46	0.81	0.67
0.0131	1.29	6.78	292700	5.49	1.49	0.92	0.08	0.23	0.24
0.0066	1.28	7.67	304900	6.39	1.51	0.94	0.06	0.20	0.11
0.0033	1.35	8.58	388000	7.23	1.63	1.01	-0.01	-0.03	0.00
0.0016	1.38	8.78	335700	7.40	1.55	0.96	0.04	0.11	-0.02
Control	1.35	8.39	361767	7.04	1.59	1.00	0.00	0.00	0.00
0.1050	2.31	3.04	22267	0.73	0.19	0.12	0.88	0.98	0.90
0.0525	1.64	2.50	32167	0.86	0.36	0.23	0.76	0.95	0.88
0.0263	1.31	3.56	70733	2.25	0.77	0.48	0.51	0.84	0.68
0.0131	1.26	6.63	280400	5.38	1.46	0.92	0.08	0.23	0.24
0.0066	1.29	7.37	309167	6.07	1.51	0.95	0.05	0.15	0.14
0.0033	1.41	8.62	387433	7.21	1.63	1.02	-0.02	-0.07	-0.02
0.0016	1.35	8.44	348200	7.09	1.57	0.99	0.01	0.04	-0.01

IR : Inhibition rate

Biomass : Yield f (Final yield based on cell density)

實驗毒物: Ethyl dibromoacetate

初始細胞密度(cells/mL) : 15000

MCV (µm3) : 42.2

Initial pH : 7.56

EDTA(%):0

T(°C) :24

Test duration :48-h

Conc mg/L	Initial DO mg/L	Final DO mg/L	Final cells cells/ml	Delta DO mg/L	µspecific	µrelative	IR (growth rate)	IR (Biomass)	IR (DO)
Control	1.55	5.67	272600	4.12	1.45	1.00	0.00	0.00	0.00
0.640	2.12	2.21	31000	0.09	0.36	0.25	0.75	0.94	0.98
0.320	1.48	1.8	28700	0.32	0.32	0.22	0.78	0.95	0.92
0.160	1.54	2.53	55900	0.99	0.66	0.45	0.55	0.84	0.76
0.080	1.28	4.55	214100	3.27	1.33	0.92	0.08	0.23	0.21
0.040	1.33	5.54	268900	4.21	1.44	1.00	0.00	0.01	-0.02
0.020	1.38	4.88	251500	3.5	1.41	0.97	0.03	0.08	0.15
0.010	1.61	5.41	273800	3.8	1.45	1.00	0.00	0.00	0.08
Control	1.26	5.66	292800	4.4	1.49	1.00	0.00	0.00	0.00
0.640	1.86	2.24	33800	0.38	0.41	0.27	0.73	0.93	0.91
0.320	1.61	1.57	25100	-0.04	0.26	0.17	0.83	0.96	1.01
0.160	1.41	2.12	53300	0.71	0.63	0.43	0.57	0.86	0.84
0.080	1.37	4.81	220500	3.44	1.34	0.90	0.10	0.26	0.22
0.040	1.35	4.56	245300	3.21	1.40	0.94	0.06	0.17	0.27
0.020	1.35	5.13	268800	3.78	1.44	0.97	0.03	0.09	0.14
0.010	1.34	5.13	302500	3.79	1.50	1.01	-0.01	-0.03	0.14
Control	1.34	5.56	291200	4.22	1.48	1.00	0.00	0.00	0.00
0.640	2.11	2.04	35600	-0.07	0.43	0.29	0.71	0.93	1.02
0.320	1.63	1.68	28400	0.05	0.32	0.22	0.78	0.95	0.99
0.160	1.45	2.71	57500	1.26	0.67	0.45	0.55	0.85	0.70
0.080	1.52	5.11	238700	3.59	1.38	0.93	0.07	0.19	0.15
0.040	1.39	5.07	255700	3.68	1.42	0.96	0.04	0.13	0.13
0.020	1.35	5.35	293000	4	1.49	1.00	0.00	-0.01	0.05
0.010	1.45	5.23	272500	3.78	1.45	0.98	0.02	0.07	0.10
Control	1.38	5.63	285533	4.25	1.47	1.00	0.00	0.00	0.00
0.640	2.03	2.16	33467	0.13	0.40	0.27	0.73	0.93	0.97
0.320	1.57	1.68	27400	0.11	0.30	0.20	0.80	0.95	0.97
0.160	1.47	2.45	55567	0.99	0.65	0.44	0.56	0.85	0.77
0.080	1.39	4.82	224433	3.43	1.35	0.92	0.08	0.23	0.19
0.040	1.36	5.06	256633	3.70	1.42	0.96	0.04	0.11	0.13
0.020	1.36	5.12	271100	3.76	1.45	0.98	0.02	0.05	0.11
0.010	1.47	5.26	282933	3.79	1.47	1.00	0.00	0.01	0.11

IR : Inhibition rate

Biomass : Yield f (Final yield based on cell density)

實驗毒物: Ethyl tribromoacetate

初始細胞密度(cells/mL) : 15000

MCV (µm3) : 40.5

Initial pH : 7.47

EDTA(%):0

T(°C) :24

Test duration :48-h

Conc mg/L	Initial DO mg/L	Final DO mg/L	Final cells cells/ml	Delta DO mg/L	µspecific	µrelative	IR (growth rate)	IR (Biomass)	IR (DO)
Control	1.28	5.58	195700	4.3	1.28	1.00	0.00	0.00	0.00
1.280	2.89	3.05	31500	0.16	0.37	0.29	0.71	0.91	0.96
0.640	2.12	2.92	57300	0.8	0.67	0.52	0.48	0.77	0.81
0.320	1.42	2.79	81600	1.37	0.85	0.66	0.34	0.63	0.68
0.160	1.26	3.99	135100	2.73	1.10	0.86	0.14	0.34	0.37
0.080	1.28	4.75	161400	3.47	1.19	0.92	0.08	0.19	0.19
0.040	1.29	5.69	175000	4.4	1.23	0.96	0.04	0.11	-0.02
0.020	1.25	6.25	208800	5	1.32	1.03	-0.03	-0.07	-0.16
Control	1.32	5.84	189800	4.52	1.27	1.00	0.00	0.00	0.00
1.280	2.57	2.71	32000	0.14	0.38	0.30	0.70	0.90	0.97
0.640	2.07	2.82	58700	0.75	0.68	0.54	0.46	0.75	0.83
0.320	1.45	3.52	100000	2.07	0.95	0.75	0.25	0.51	0.54
0.160	1.28	3.82	114800	2.54	1.02	0.80	0.20	0.43	0.44
0.080	1.29	4.81	177900	3.52	1.24	0.97	0.03	0.07	0.22
0.040	1.24	5.92	205200	4.68	1.31	1.03	-0.03	-0.09	-0.04
0.020	1.41	6.3	210300	4.89	1.32	1.04	-0.04	-0.12	-0.08
Control	1.27	6	215200	4.73	1.33	1.00	0.00	0.00	0.00
1.280	3.17	1.36	34800	-1.81	0.42	0.32	0.68	0.90	1.38
0.640	1.89	2.71	52000	0.82	0.62	0.47	0.53	0.82	0.83
0.320	1.43	3.23	96000	1.8	0.93	0.70	0.30	0.60	0.62
0.160	1.3	3.54	133100	2.24	1.09	0.82	0.18	0.41	0.53
0.080	1.26	5.12	166200	3.86	1.20	0.90	0.10	0.24	0.18
0.040	1.29	6.22	219100	4.93	1.34	1.01	-0.01	-0.02	-0.04
0.020	1.21	5.49	193900	4.28	1.28	0.96	0.04	0.11	0.10
Control	1.29	5.81	200233	4.52	1.29	1.00	0.00	0.00	0.00
1.280	2.88	2.37	32767	-0.50	0.39	0.30	0.70	0.90	1.11
0.640	2.03	2.82	56000	0.79	0.66	0.51	0.49	0.78	0.83
0.320	1.43	3.18	92533	1.75	0.91	0.70	0.30	0.58	0.61
0.160	1.28	3.78	127667	2.50	1.07	0.83	0.17	0.39	0.45
0.080	1.28	4.89	168500	3.62	1.21	0.93	0.07	0.17	0.20
0.040	1.27	5.94	199767	4.67	1.29	1.00	0.00	0.00	-0.03
0.020	1.29	6.01	204333	4.72	1.31	1.01	-0.01	-0.02	-0.05

IR : Inhibition rate

Biomass : Yield f (Final yield based on cell density)

實驗毒物: Ethyl-2,3-di-bromopropionate

初始細胞密度(cells/mL) : 15000

MCV (µm3) : 39.5

Initial pH : 7.62

EDTA(%):0

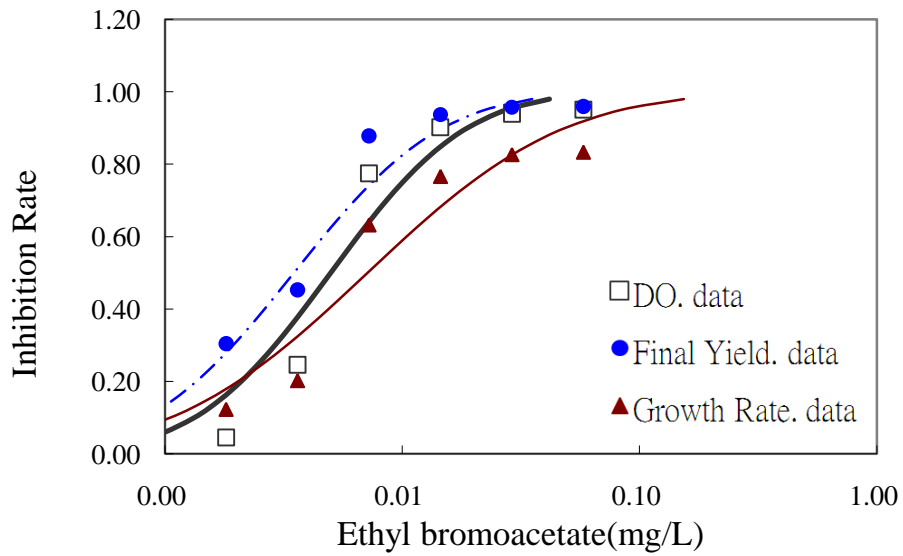
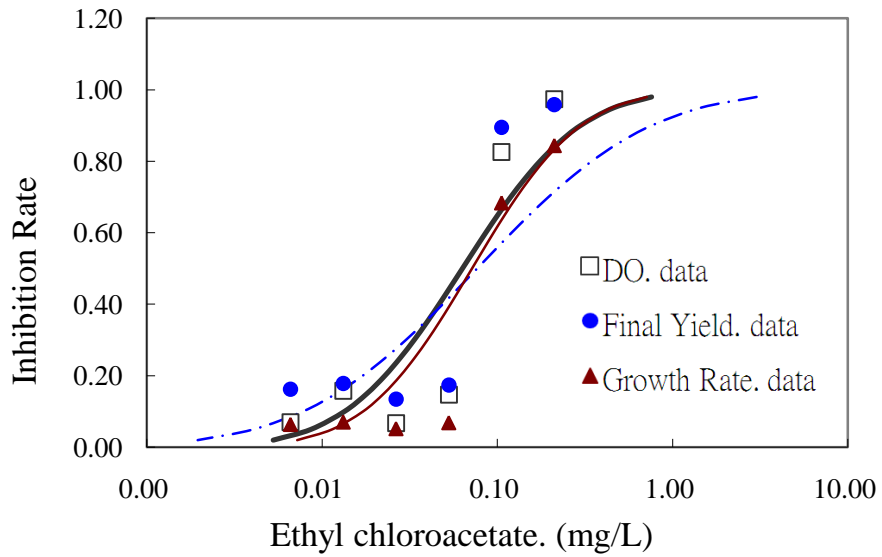
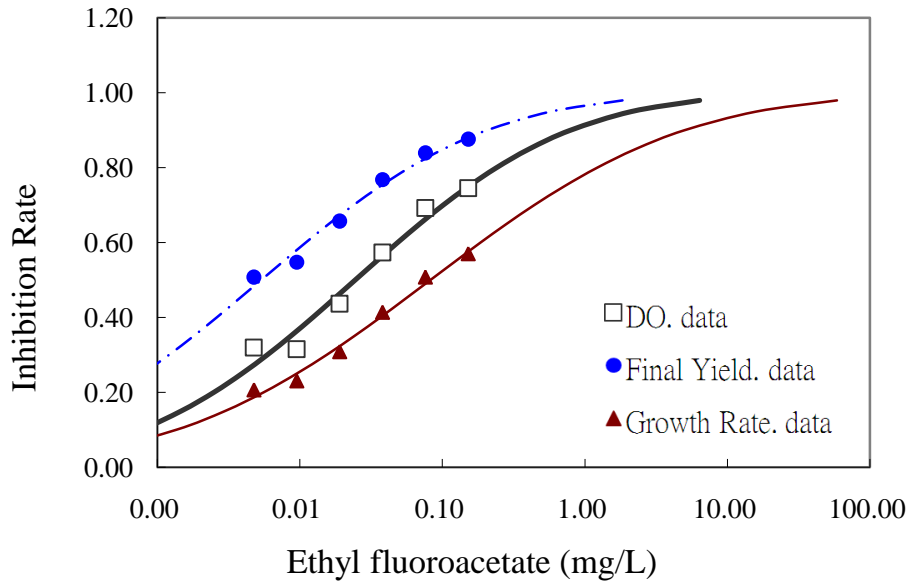
T(°C) :24

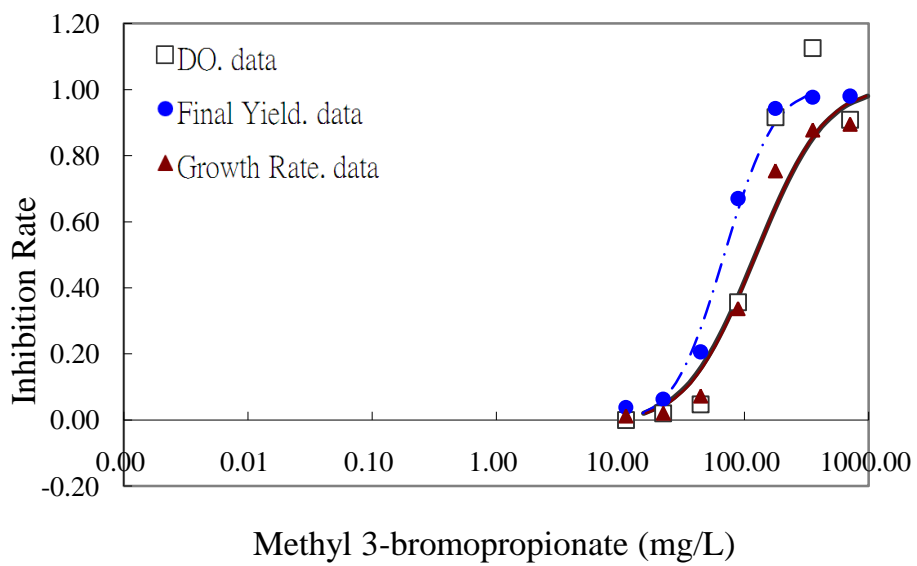
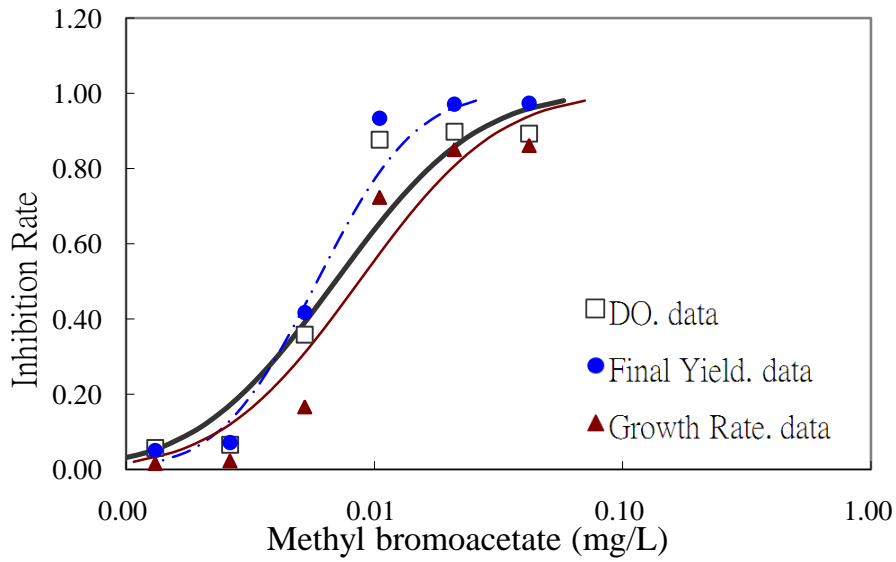
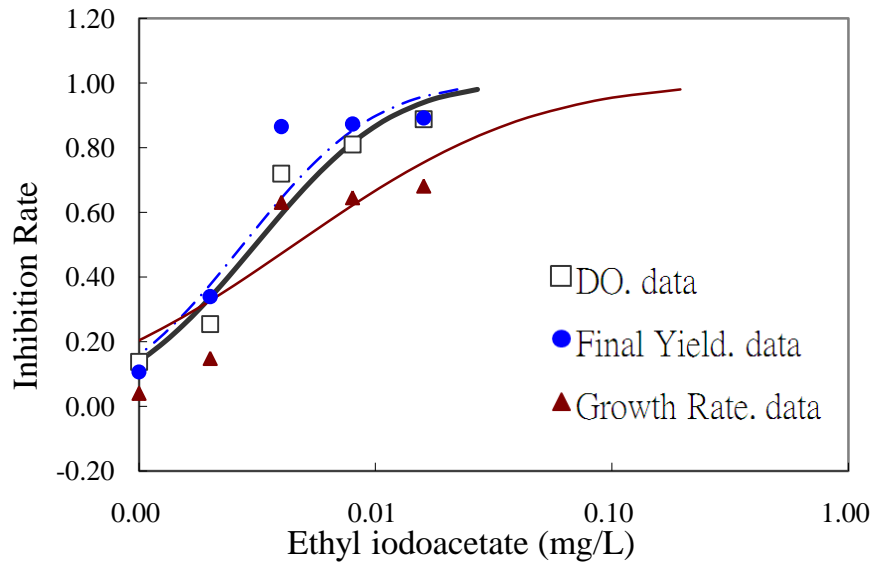
Test duration :48-h

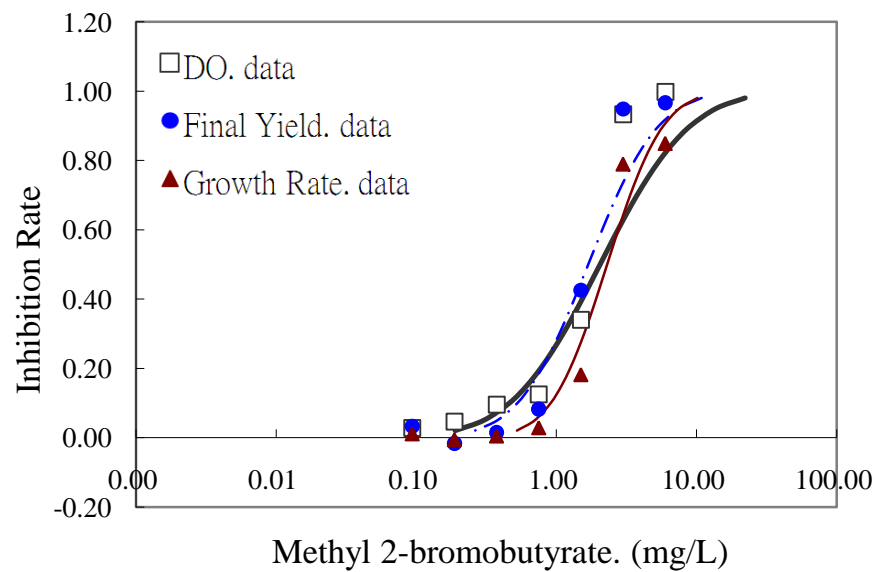
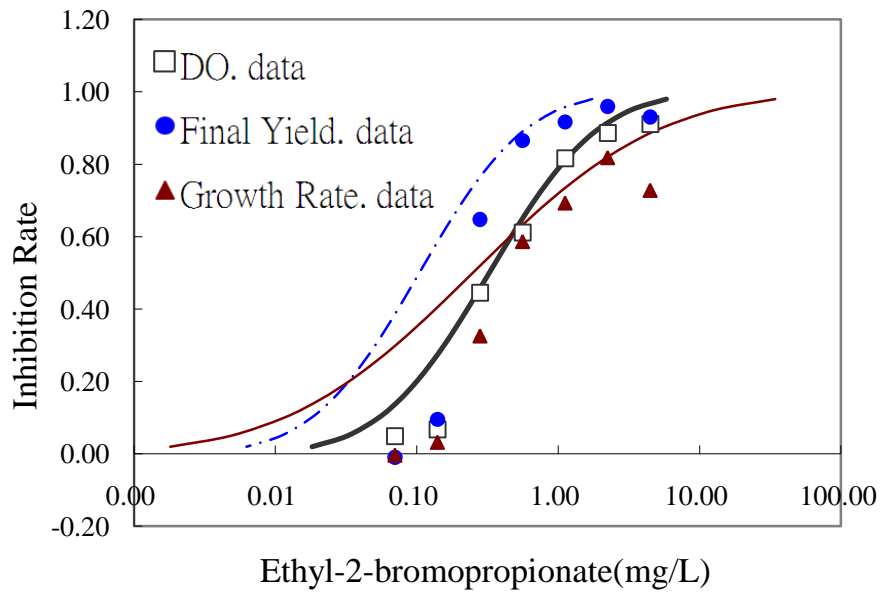
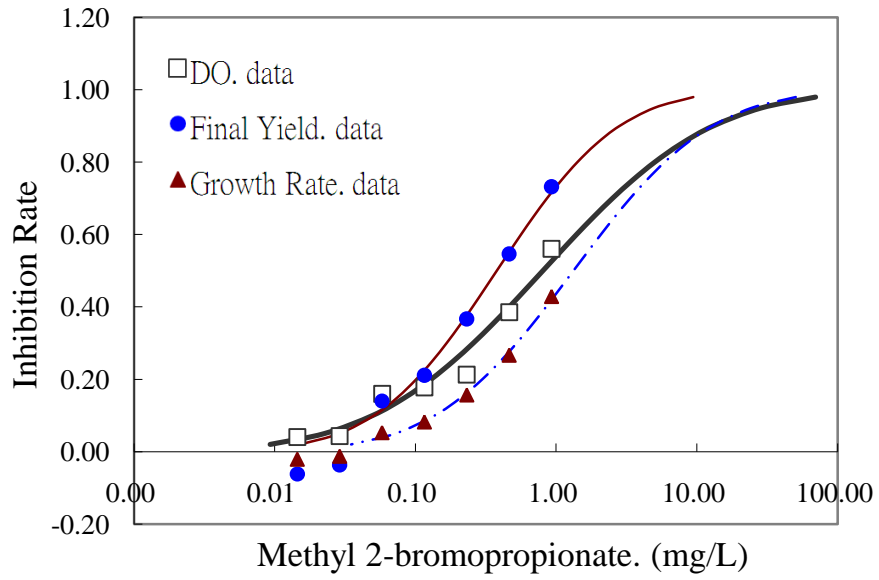
Conc mg/L	Initial DO mg/L	Final DO mg/L	Final cells cells/ml	Delta DO		µrelative	IR (growth rate)	IR (Biomass)	IR (DO)
				mg/L	µspecific				
Control	1.85	5.75	242200	3.9	1.39	1.00	0.00	0.00	0.00
0.2340	2.09	3.41	48400	1.32	0.59	0.42	0.58	0.85	0.66
0.1170	1.71	4.12	106800	2.41	0.98	0.71	0.29	0.60	0.38
0.0585	1.4	4.21	147700	2.81	1.14	0.82	0.18	0.42	0.28
0.0293	1.79	6.27	243600	4.48	1.39	1.00	0.00	-0.01	-0.15
0.0146	1.76	5.05	223100	3.29	1.35	0.97	0.03	0.08	0.16
0.0073	1.91	5.94	241200	4.03	1.39	1.00	0.00	0.00	-0.03
0.0037	2.11	6.06	240500	3.95	1.39	1.00	0.00	0.01	-0.01
Control	1.75	5.69	237900	3.94	1.38	1.00	0.00	0.00	0.00
0.2340	2.62	3.92	48100	1.3	0.58	0.42	0.58	0.85	0.67
0.1170	1.67	4.82	126600	3.15	1.07	0.77	0.23	0.50	0.20
0.0585	1.43	4.74	185000	3.31	1.26	0.91	0.09	0.24	0.16
0.0293	1.52	5.2	213000	3.68	1.33	0.96	0.04	0.11	0.07
0.0146	1.79	5.68	226600	3.89	1.36	0.98	0.02	0.05	0.01
0.0073	2	6.23	234400	4.23	1.37	0.99	0.01	0.02	-0.07
0.0037	2.12	6.19	232100	4.07	1.37	0.99	0.01	0.03	-0.03
Control	1.59	5.78	234900	4.19	1.38	1.00	0.00	0.00	0.00
0.2340	2.44	3.68	51300	1.24	0.61	0.45	0.55	0.83	0.70
0.1170	1.75	4.48	101200	2.73	0.95	0.69	0.31	0.61	0.35
0.0585	1.45	4.93	185300	3.48	1.26	0.91	0.09	0.23	0.17
0.0293	1.45	5.44	223800	3.99	1.35	0.98	0.02	0.05	0.05
0.0146	1.68	5.62	236000	3.94	1.38	1.00	0.00	-0.01	0.06
0.0073	1.8	5.69	230900	3.89	1.37	0.99	0.01	0.02	0.07
0.0037	1.91	5.92	245000	4.01	1.40	1.02	-0.02	-0.05	0.04
Control	1.73	5.74	238333	4.01	1.38	1.00	0.00	0.00	0.00
0.2340	2.38	3.67	49267	1.29	0.59	0.43	0.57	0.85	0.68
0.1170	1.71	4.47	111533	2.76	1.00	0.72	0.27	0.57	0.31
0.0585	1.43	4.63	172667	3.20	1.22	0.88	0.12	0.29	0.20
0.0293	1.59	5.64	226800	4.05	1.36	0.98	0.02	0.05	-0.01
0.0146	1.74	5.45	228567	3.71	1.36	0.98	0.02	0.04	0.08
0.0073	1.90	5.95	235500	4.05	1.38	1.00	0.00	0.01	-0.01
0.0037	2.05	6.06	239200	4.01	1.38	1.00	0.00	0.00	0.00

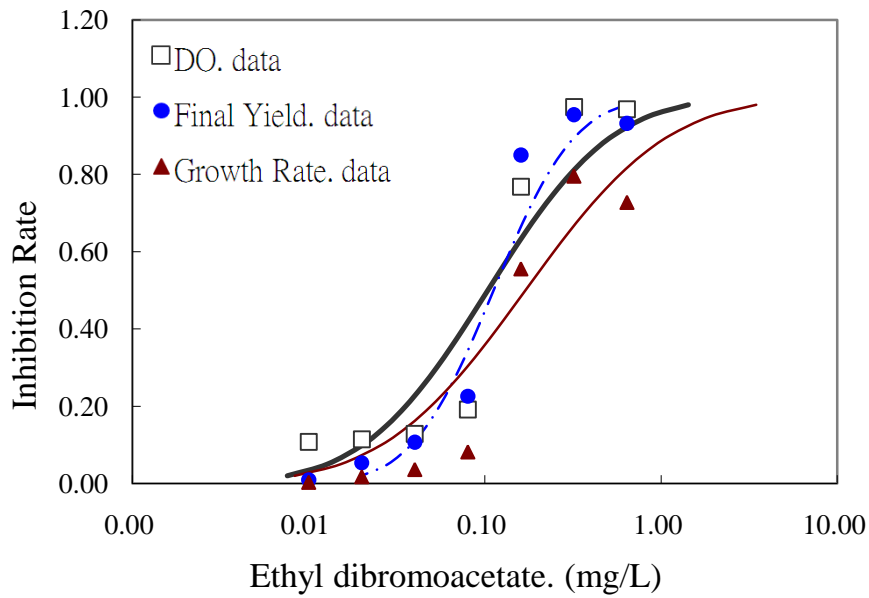
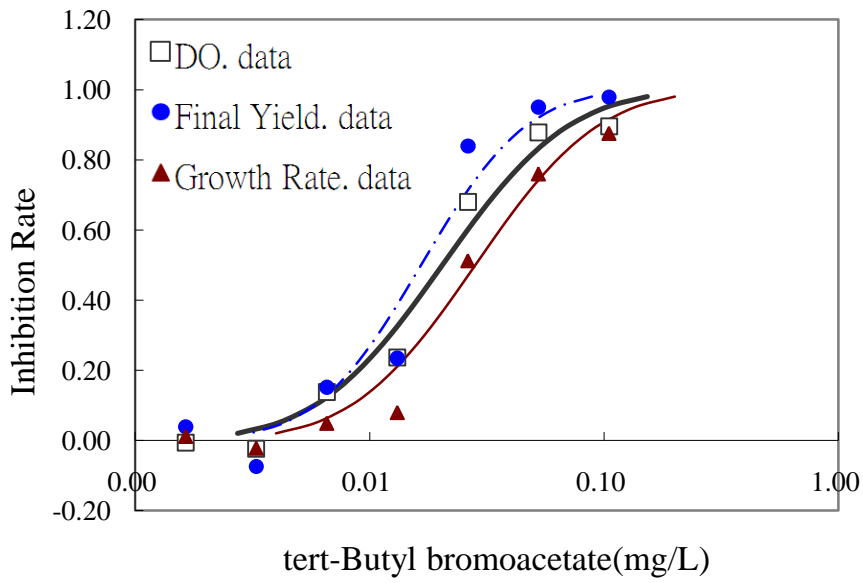
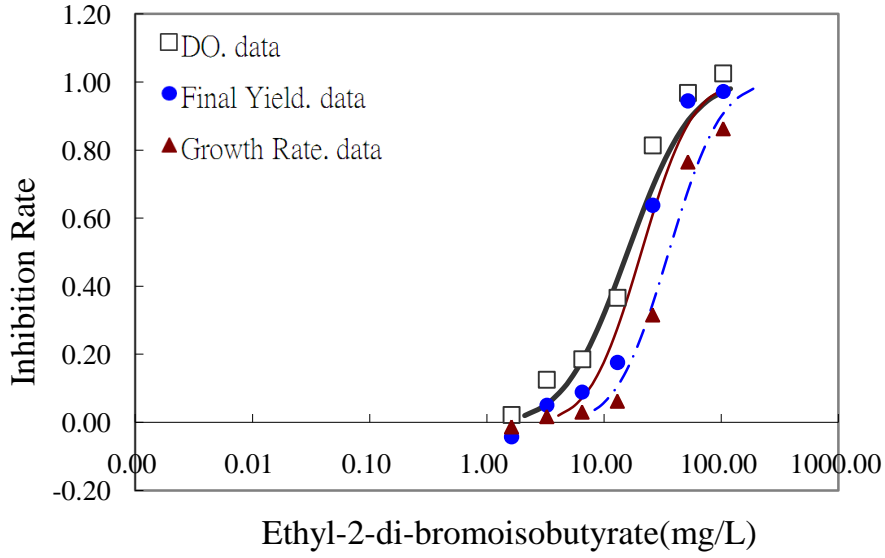
IR : Inhibition rate

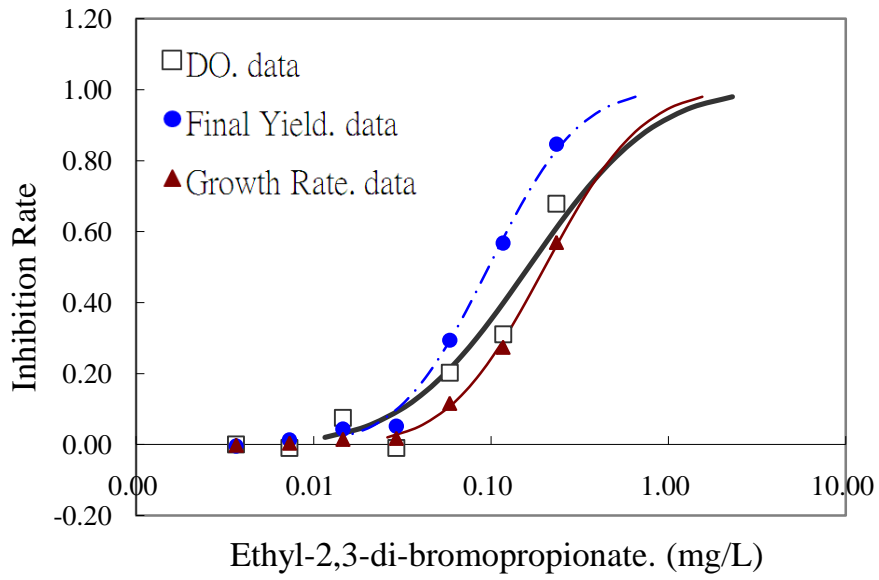
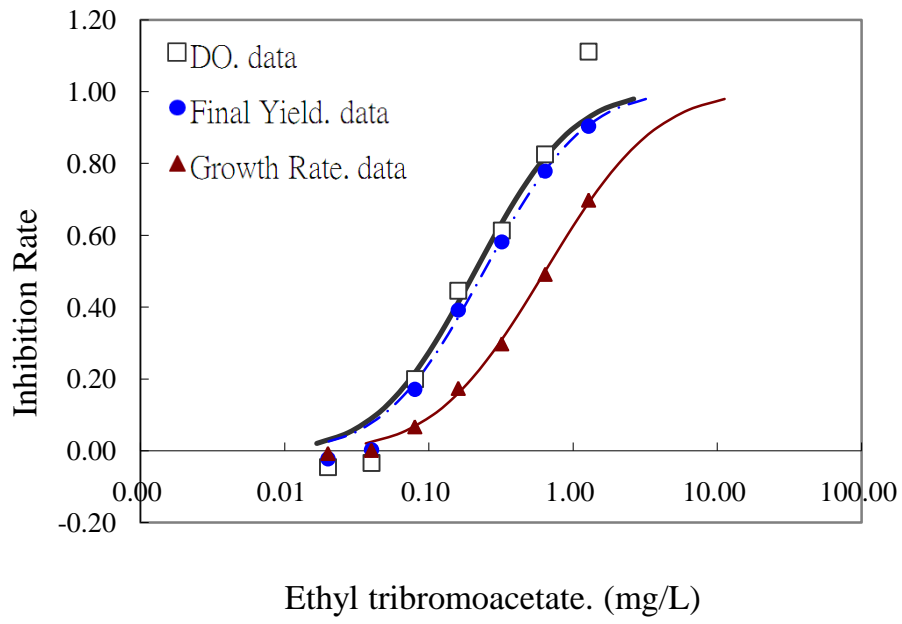
Biomass : Yield f (Final yield based on cell density)











附錄二、其他迴歸



(一) N=12(去掉 Ethyl fluoroacetate(1)、Methyl 3-bromopropionate(6))

$$\text{Log}(1/\text{EC}_{50, \Delta\text{DO}}) = 4.09 + 0.829 \text{Log}(1/\text{RC}_{50}) - 0.684 \text{Log Kow}$$
$$R^2 = 0.824, R_{\text{pred}}^2 = 0.687, S = 0.493, F = 21.3$$

$$\text{Log}(1/\text{EC}_{50, \text{FY}}) = 4.14 + 0.882 \text{Log}(1/\text{RC}_{50}) - \text{Log Kow}$$
$$R^2 = 0.832, R_{\text{pred}}^2 = 0.692, S = 0.506, F = 22.3$$

$$\text{Log}(1/\text{EC}_{50, \text{GR}}) = 4.02 + 0.856 \text{Log}(1/\text{RC}_{50}) - 0.781 \text{Log Kow}$$
$$R^2 = 0.790, R_{\text{pred}}^2 = 0.624, S = 0.489, F = 40.2$$

※Log Kow 的係數為負，不合理，故不收錄於討論中。

$$\text{Log}(1/\text{EC}_{50, \Delta\text{DO}}) = 3.46 + 0.960 \text{Log}(1/\text{RC}_{50}) + 0.644 \text{E}_{\text{LUMO}}$$
$$R^2 = 0.787, R_{\text{pred}}^2 = 0.630, S = 0.541, F = 16.6$$

$$\text{Log}(1/\text{EC}_{50, \text{FY}}) = 3.52 + 1.02 \text{Log}(1/\text{RC}_{50}) + 0.692 \text{E}_{\text{LUMO}}$$
$$R^2 = 0.761, R_{\text{pred}}^2 = 0.568, S = 0.614, F = 14.3$$

$$\text{Log}(1/\text{EC}_{50, \text{GR}}) = 3.33 + 1.02 \text{Log}(1/\text{RC}_{50}) + 0.784 \text{E}_{\text{LUMO}}$$
$$R^2 = 0.805, R_{\text{pred}}^2 = 0.640, S = 0.546, F = 22.3$$

※E_{LUMO} 的係數為正，不合理，故不收錄於討論中。

$$\text{Log}(1/\text{EC}_{50, \Delta\text{DO}}) = 4.04 + 0.876 \text{Log}(1/\text{RC}_{50}) + 0.231 \text{E}_{\text{LUMO}} - 0.551 \text{Log Kow}$$
$$R^2 = 0.829, R_{\text{pred}}^2 = 0.633, S = 0.514, F = 12.9$$

$$\text{Log}(1/\text{EC}_{50, \text{FY}}) = 4.08 + 0.942 \text{Log}(1/\text{RC}_{50}) + 0.292 \text{E}_{\text{LUMO}} - 0.532 \text{Log Kow}$$
$$R^2 = 0.840, R_{\text{pred}}^2 = 0.652, S = 0.524, F = 14.0$$

$$\text{Log}(1/\text{EC}_{50, \text{GR}}) = 3.94 + 0.928 \text{Log}(1/\text{RC}_{50}) + 0.349 \text{E}_{\text{LUMO}} - 0.579 \text{Log Kow}$$
$$R^2 = 0.802, R_{\text{pred}}^2 = 0.575, S = 0.593, F = 10.8$$

※Log Kow 的係數為負，E_{LUMO} 的係數為正，不合理，故不收錄於討論中。

(二) N=10(去掉 Ethyl fluoroacetate(1)、Methyl 3-bromopropionate(6)、

Ethyl-2,3-di-bromopropionate(14))

$$\text{Log}(1/\text{EC}_{50, \Delta\text{DO}}) = -0.397 - 14.6 \text{H-carbon}$$
$$R^2 = 0.721, R_{\text{pred}}^2 = 0.642, S = 0.619, F = 23.3$$

$$\text{Log}(1/\text{EC}_{50, \text{FY}}) = -0.514 - 15.1 \text{H-carbon}$$
$$R^2 = 0.702, R_{\text{pred}}^2 = 0.610, S = 0.675, F = 21.1$$

$$\text{Log}(1/\text{EC}_{50, \text{GR}}) = -0.931 - 15.8 \text{H-carbon}$$
$$R^2 = 0.737, R_{\text{pred}}^2 = 0.664, S = 0.643, F = 25.2$$

$$\text{Log}(1/\text{EC}_{50, \Delta\text{DO}}) = -0.400 - 14.6 \text{H-carbon} - 0.006 \text{E}_{\text{LUMO}}$$
$$R^2 = 0.721, R_{\text{pred}}^2 = 0.652, S = 0.657, F = 10.4$$

$$\text{Log}(1/\text{EC}_{50,\text{FY}}) = -0.506 - 15.2 \text{ H-carbon} + 0.018 E_{\text{LUMO}}$$

$$R^2 = 0.702, R_{\text{pred}}^2 = 0.442, S = 0.715, F = 9.42$$

$$\text{Log}(1/\text{EC}_{50,\text{GR}}) = -0.877 - 15.9 \text{ H-carbon} + 0.127 E_{\text{LUMO}}$$

$$R^2 = 0.740, R_{\text{pred}}^2 = 0.523, S = 0.679, F = 11.4$$

※ E_{LUMO} 的係數為正，不合理，故不收錄於討論中。

$$\text{Log}(1/\text{EC}_{50, \Delta\text{DO}}) = 0.09 - 14.0 \text{ H-carbon} - 0.229 \text{ Log Kow}$$

$$R^2 = 0.733, R_{\text{pred}}^2 = 0.631, S = 0.643, F = 11.0$$

$$\text{Log}(1/\text{EC}_{50,\text{FY}}) = 0.03 - 14.6 \text{ H-carbon} - 0.257 \text{ Log Kow}$$

$$R^2 = 0.715, R_{\text{pred}}^2 = 0.594, S = 0.657, F = 10.0$$

$$\text{Log}(1/\text{EC}_{50,\text{GR}}) = -0.26 - 15.1 \text{ H-carbon} - 0.317 \text{ Log Kow}$$

$$R^2 = 0.756, R_{\text{pred}}^2 = 0.695, S = 0.658, F = 12.4$$

※ Log Kow 的係數為負，不合理，故不收錄於討論中。

(三) $N=9$ (去掉 Ethyl fluoroacetate(1)、Methyl 3-bromopropionate(6)、Ethyl dibromoacetate(12)、Ethyl tribromoacetate(13)、Ethyl-2,3-di-bromopropionate(14))

$$\text{Log}(1/\text{EC}_{50, \Delta\text{DO}}) = 3.17 + 1.07 \text{ Log}(1/\text{RC}_{50})$$

$$R^2 = 0.939, R_{\text{pred}}^2 = 0.893, S = 0.328, F = 108$$

$$\text{Log}(1/\text{EC}_{50,\text{FY}}) = 3.20 + 1.13 \text{ Log}(1/\text{RC}_{50})$$

$$R^2 = 0.947, R_{\text{pred}}^2 = 0.916, S = 0.323, F = 124$$

$$\text{Log}(1/\text{EC}_{50,\text{GR}}) = 2.96 + 1.13 \text{ Log}(1/\text{RC}_{50})$$

$$R^2 = 0.916, R_{\text{pred}}^2 = 0.879, S = 0.410, F = 76.8$$

$$\text{Log}(1/\text{EC}_{50, \Delta\text{DO}}) = 3.02 - 3.41 \text{ Halo} + 1.06 \text{ Log}(1/\text{RC}_{50})$$

$$R^2 = 0.940, R_{\text{pred}}^2 = 0.798, S = 0.350, F = 47.3$$

$$\text{Log}(1/\text{EC}_{50,\text{FY}}) = 3.03 - 4.18 \text{ Halo} + 1.12 \text{ Log}(1/\text{RC}_{50})$$

$$R^2 = 0.948, R_{\text{pred}}^2 = 0.869, S = 0.343, F = 55.0$$

$$\text{Log}(1/\text{EC}_{50,\text{GR}}) = 3.04 + 1.8 \text{ Halo} + 1.13 \text{ Log}(1/\text{RC}_{50})$$

$$R^2 = 0.917, R_{\text{pred}}^2 = 0.719, S = 0.441, F = 33.0$$

$$\text{Log}(1/\text{EC}_{50, \Delta\text{DO}}) = 0.81 - 12.9 \Delta\text{Halo} - 0.093 \text{ Log Kow}$$

$$R^2 = 0.630, R_{\text{pred}}^2 = 0.283, S = 0.874, F = 5.10$$

$$\text{Log}(1/\text{EC}_{50,\text{FY}}) = 0.65 - 13.6 \Delta\text{Halo} - 0.055 \text{ Log Kow}$$

$$R^2 = 0.622, R_{\text{pred}}^2 = 0.213, S = 0.929, F = 4.93$$

$$\text{Log}(1/\text{EC}_{50,\text{GR}}) = 0.15 - 14.6 \Delta\text{Halo} - 0.011 \text{ Log Kow}$$

$$R^2 = 0.679, R_{\text{pred}}^2 = 0.226, S = 0.868, F = 6.33$$

※ Log Kow 的係數為負，不合理，故不收錄於討論中。

附錄三、統計方法



(一)一般迴歸分析法

- 1.先安裝好 Minitab 15 統計軟體
- 2.打開軟體，新建立一個檔案
- 3.將所有參數值鍵入，以及試驗毒化物名稱

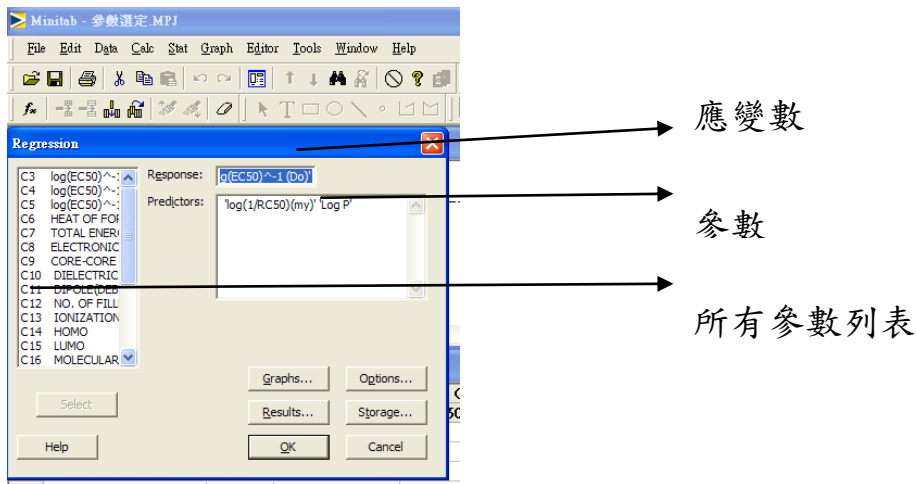
輸入參數名稱

輸入參數值

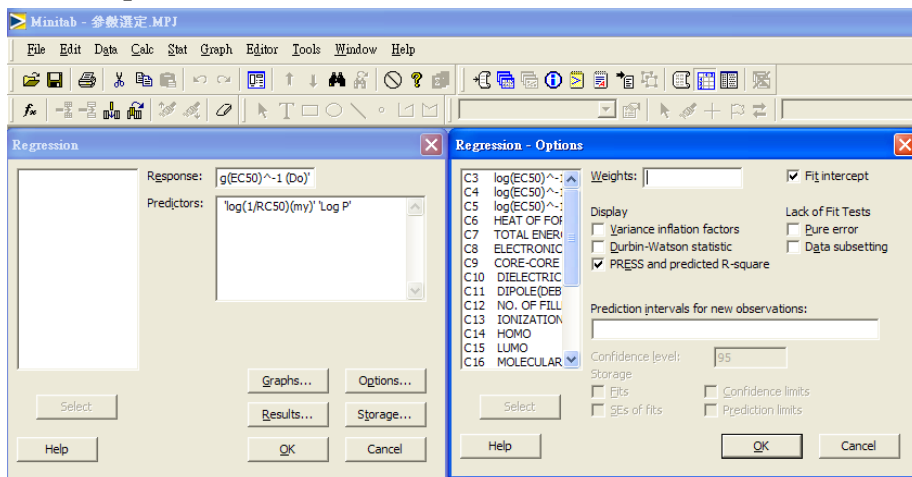
	C1-T	C2-T	C3	C4	C5	C6	C7	C8
	chemical	CAS No.	log(EC50)-1 (G6)	log(EC50)-1 (D6)	log(EC50)-1 (G6)	HEAT OF FORMATION(B)	TOTAL ENERGY	ELECTRONIC ENER
1	3-hexyn-2-one	1679-36-3	2.84614	2.66899	2.50574		102.686	-1196.22
2	3-buten-2-one	1423-60-5	3.92993	3.71908	3.68689	*	*	
3	3-methyl-3-pentene-2-one	565-62-8	0.22726	0.22507	0.13384	-147.401	-1226.13	-15
4	5-hexen-2-one	109-49-9	0.12229	-0.12012	-0.26393	-165.873	-1226.32	-14
5	3-hepten-2-one	1119-44-4	1.64351	1.47747	1.52992	-192.423	-1382.13	-16
6	4-methyl-3-pentene-2-one	141-79-7	-0.16658	-0.26506	-0.33749	226.371	-1222.25	-15
7	4-hexen-3-one	2497-21-4	1.55122	1.46075	1.36781	-170.489	-1226.36	-14
8	3-nonene-2-one	14309-57-0	1.6681	1.706	0.94605	-248.552	-1693.79	-21
9	3-pentene-2-one	625-33-2	1.4937	1.32295	1.32295	-138.732	-1070.50	-12
10	3-buten-2-one	78-94-4	3.02611	2.84133	2.88661	-97.193	-914.53	-10
11	5-methyl-5-hexene-2-one	3240-09-3	-0.25573	-0.37984	-0.53549	-187.180	-1382.08	-17
12	3-octene-2-one	1669-44-9	1.82642	1.48654	1.48900	-221.505	-1537.97	-19
13	2-cyclopenten-1-one	930-30-3	1.21408	0.94348	0.97387	-73.702	-1042.51	-12
14	6-methyl-5-heptene-2-one	110-93-0	0.25730	0.24466	-0.00021	-215.986	-1537.91	-20
15	2-methyl-2-cyclopenten-1-one	1120-73-6	-0.13042	-0.20387	-0.30940	-76.412	-1198.08	-14
16	3-methyl-2-cyclopenten-1-one	2758-18-1	-0.54162	-0.62666	-0.68577	-109.961	-1198.43	-14
17	Methyl ethyl ketone*	78-93-3	*	*	*	-242.296	-943.34	-10

4.一般迴歸分析，選擇 Stat→Regression

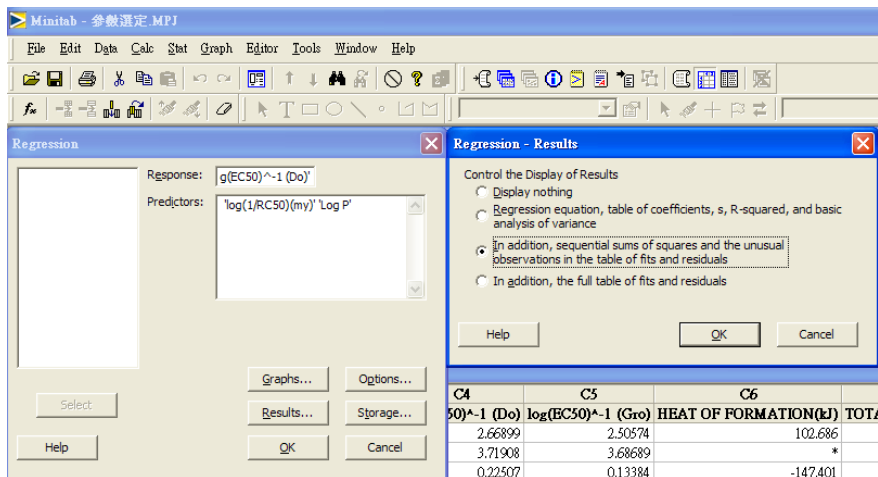
5. 挑選應變數與參數



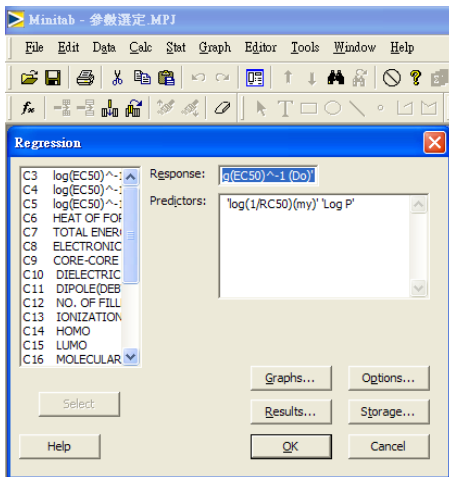
6. 點選 options → 勾選其圖片勾選處 → 點 OK



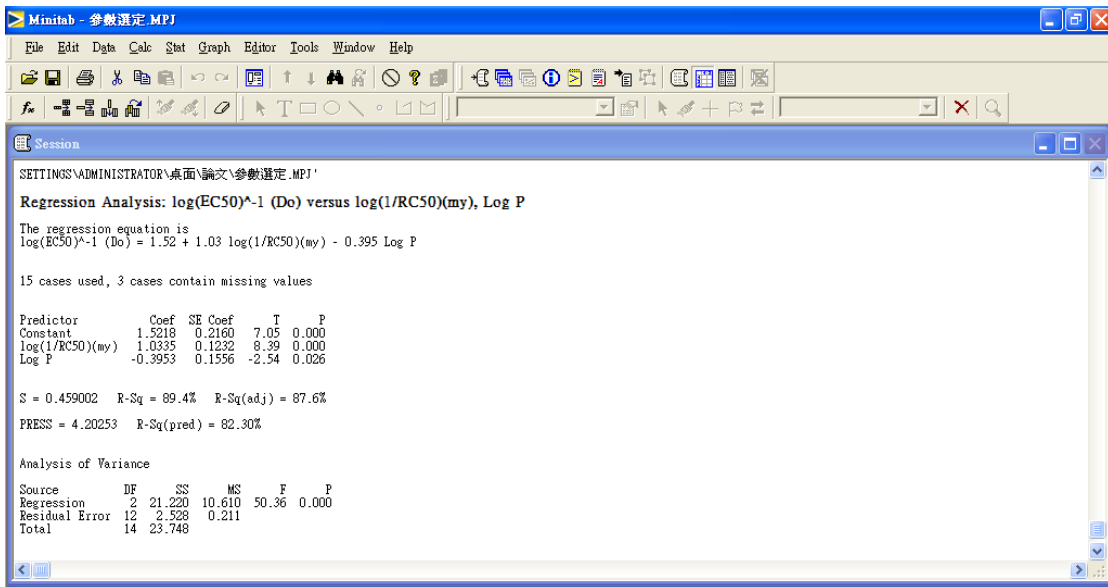
7. 點選 Results → 勾選其圖片勾選處 → 點 OK



8. 回畫面之後→點選 OK

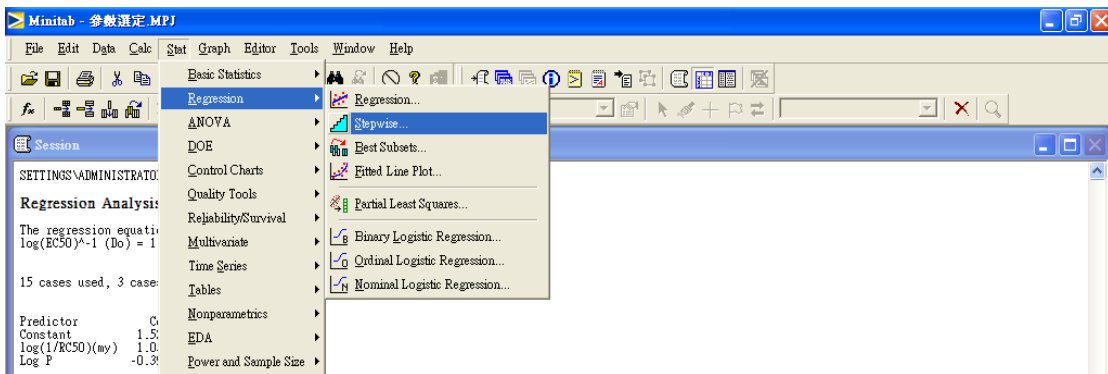


9. 結果如下

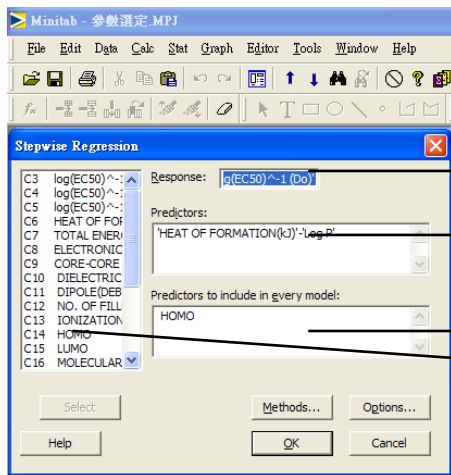


(二) 逐步迴歸分析法適用挑選參數

1. 逐步迴歸分析選擇 Stat→Regression→Stepwise



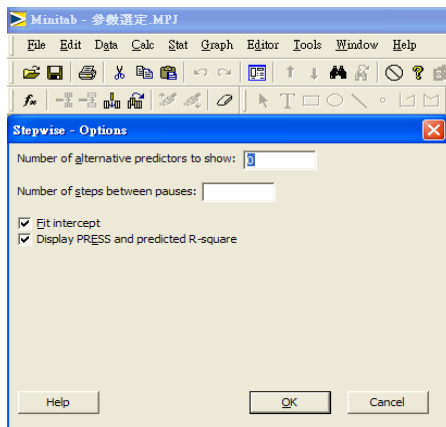
2. 挑選應變數與參數



The screenshot shows the Minitab Stepwise Regression dialog box. The 'Response' field contains 'log(EC50)^-1 (Co)'. The 'Predictors' list contains 'HEAT OF FORMATION(kJ)^-Log P'. The 'Predictors to include in every model' list contains 'HOMO'. A list of variables (C3 to C16) is shown on the left. Three arrows point from the dialog box to the following text:

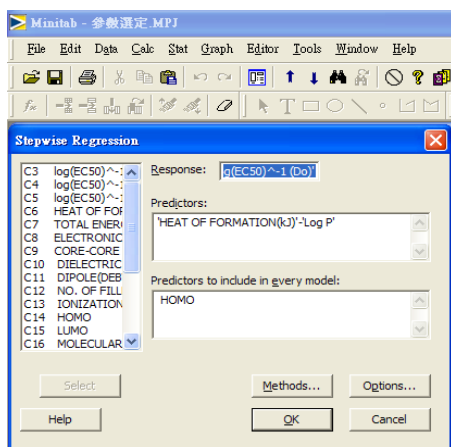
- 應變數(毒性數據)
- 選擇參數選列
- 所有參數列表

3. 點選 options → 勾選其圖片勾選處 → 點 OK



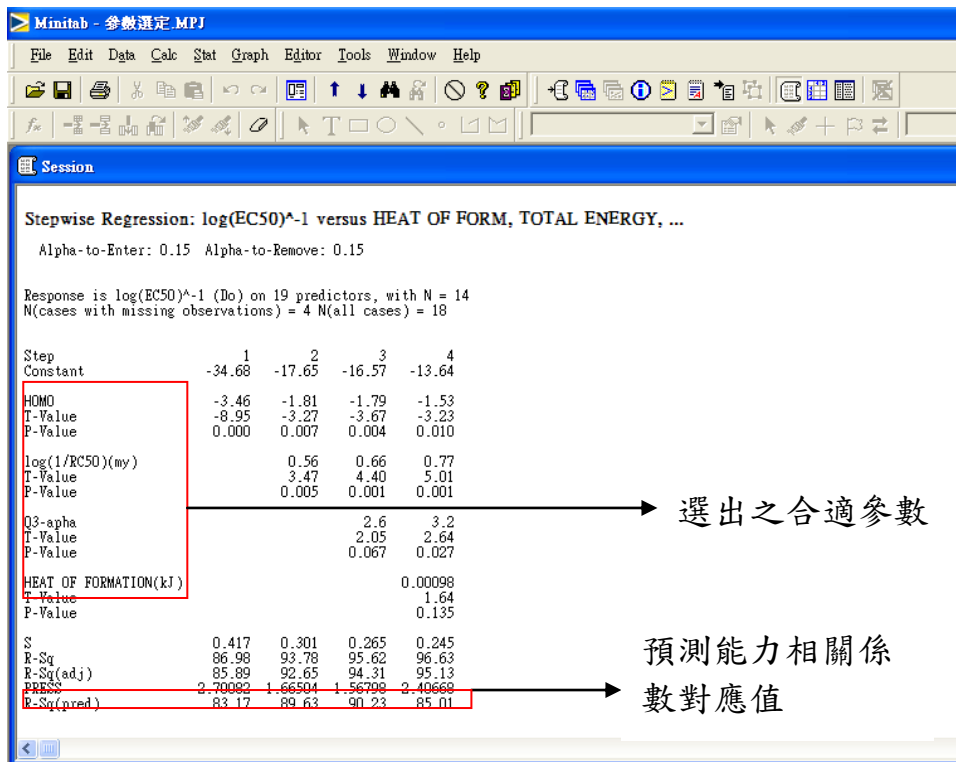
The screenshot shows the Minitab Stepwise - Options dialog box. The 'Number of alternative predictors to show' is set to 1. The 'Number of steps between pauses' is set to 1. The 'Fit intercept' and 'Display PRESS and predicted R-square' checkboxes are checked. A large watermark logo is visible in the background.

4. 回畫面之後 → 點選 OK



The screenshot shows the Minitab Stepwise Regression dialog box after the options dialog box has been closed. The 'Response' field contains 'log(EC50)^-1 (Co)'. The 'Predictors' list contains 'HEAT OF FORMATION(kJ)^-Log P'. The 'Predictors to include in every model' list contains 'HOMO'. The 'OK' button is highlighted.

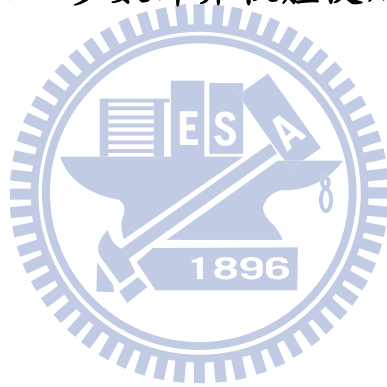
5. 結果如下



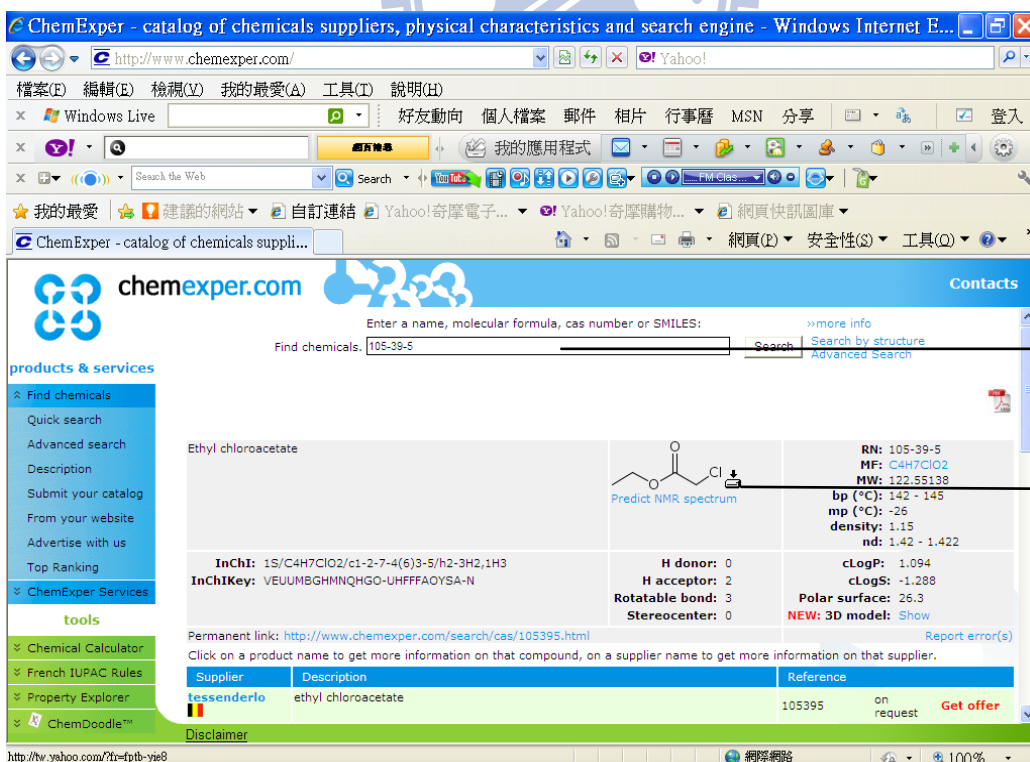
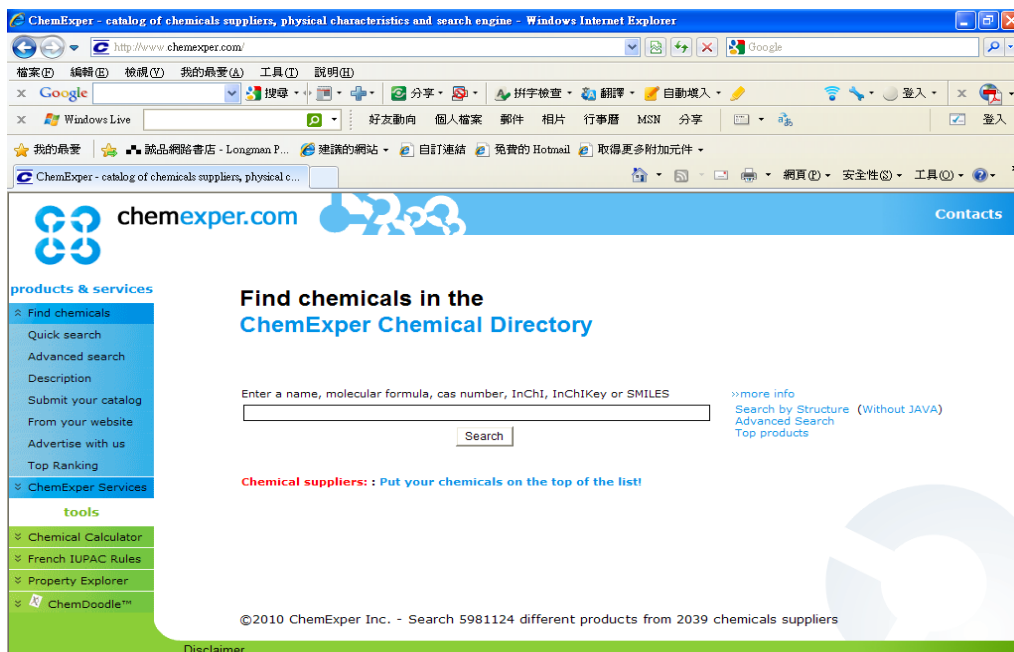
6. 將逐步迴歸分析法所挑出之合適參數→跑一般迴歸分析即可。



附錄四、參數計算軟體使用方法



- 1.先安裝好 CS Chem3D Pro 計算軟體
- 2.開啟檔案並建立一新檔
- 3.選擇欲分析之毒化物，至網站 <http://www.chemexper.com/> 下載其分析結構式圖檔。以 Ethyl chloroacetate 為例，輸入 CAS No.



The screenshot shows the ChemExper website interface. A dialog box titled "檔案下載" (File Download) is open, asking if the user wants to save the file "download.mol" (703 bytes) from "mastersearch.chemexper.com". The dialog includes a warning icon and text: "雖然來自網際網路的檔案可能是有用的，但是某些檔案有可能會傷害您的電腦。如果您不信任其來源，請不要搜尋開啟此檔案的程式，或是儲存此檔案。有什麼樣的風險?" (Although files from the internet may be useful, some files may harm your computer. If you do not trust the source, do not search for or open this file, or save it. What are the risks?). Buttons for "尋找(F)" (Find), "儲存(S)" (Save), and "取消" (Cancel) are visible.

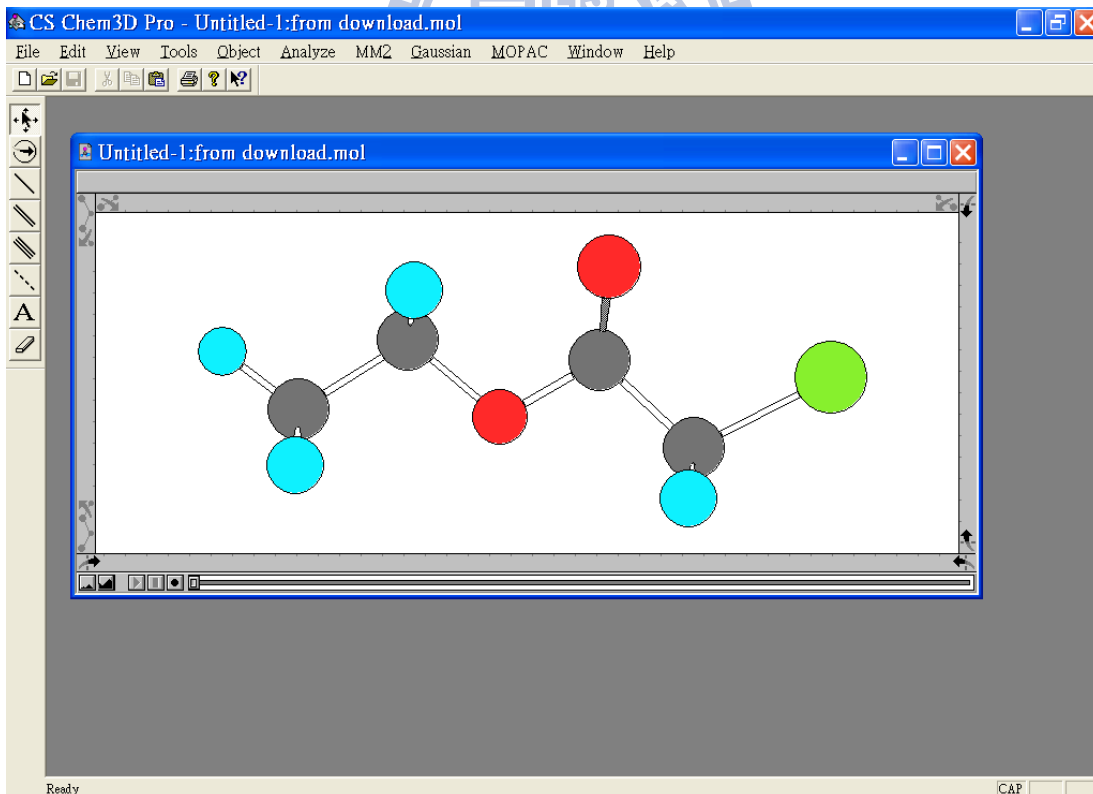
The background website shows the ChemExper logo and navigation menus. The main content area displays the chemical structure and properties of ethyl chloroacetate:

- InChI:** 1S/C4H7ClO2/c1-2-7-4(6)3-5/h2-3H2,1H3
- InChIKey:** VEUUMBGHMNQHG0-UHFFFAOYSA-N
- Properties:**
 - MF: C4H7ClO2
 - MW: 122.55138
 - bp (°C): 142 - 145
 - mp (°C): -26
 - density: 1.15
 - nd: 1.42 - 1.422
- LogP:** 1.094
- cLogS:** -1.288
- Polar surface:** 26.3
- NEW: 3D model:** Show

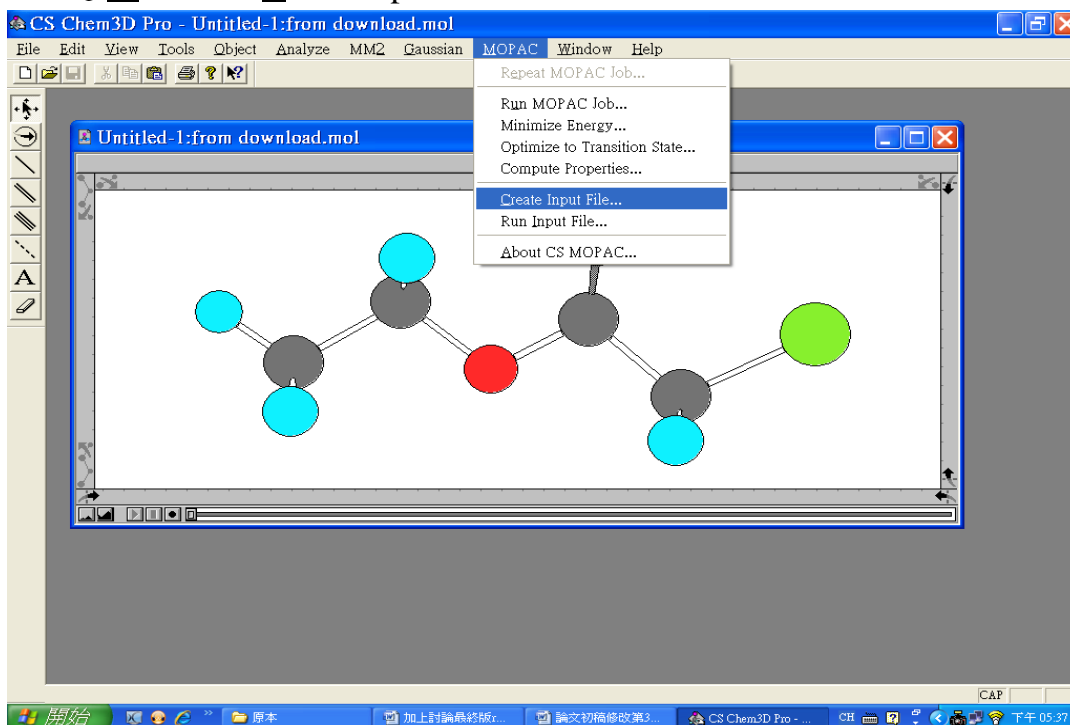
A table below lists suppliers and references:

Supplier	Description	Reference
tessenderlo	ethyl chloroacetate	105395 on request Get offer

4. 將所下載之圖檔利用 CS Chem3D Pro 開啟



5. 點選 MOPAC → Create Input File



6. 設定依照下面圖示設定

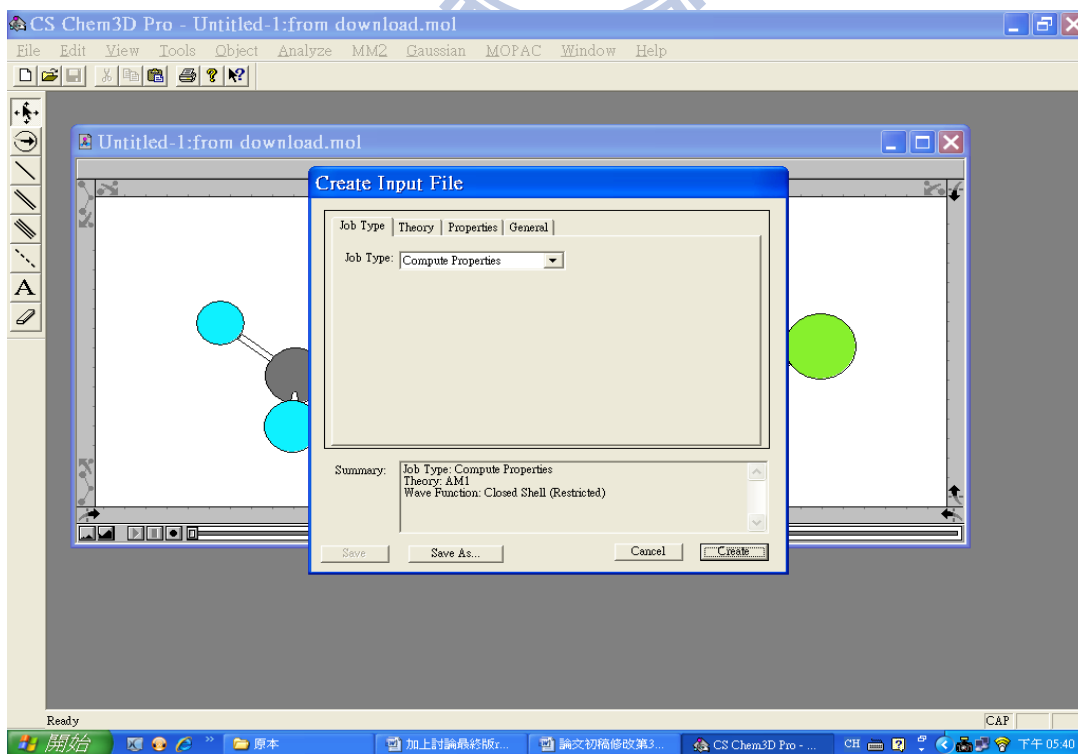
Job Type: Compute Properties

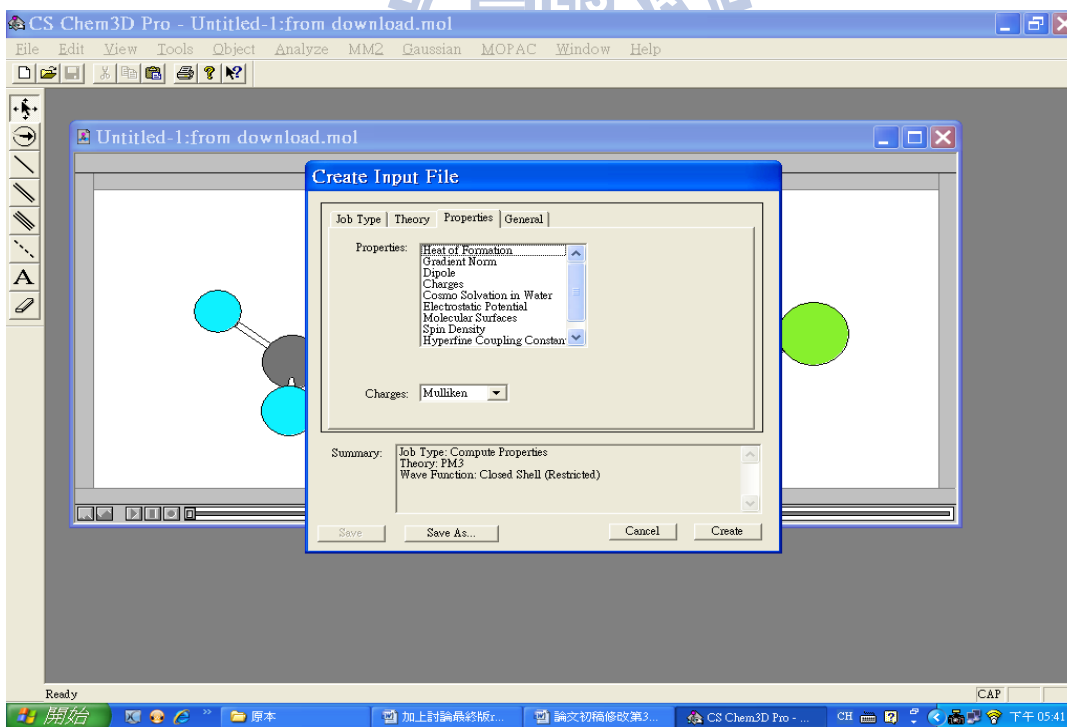
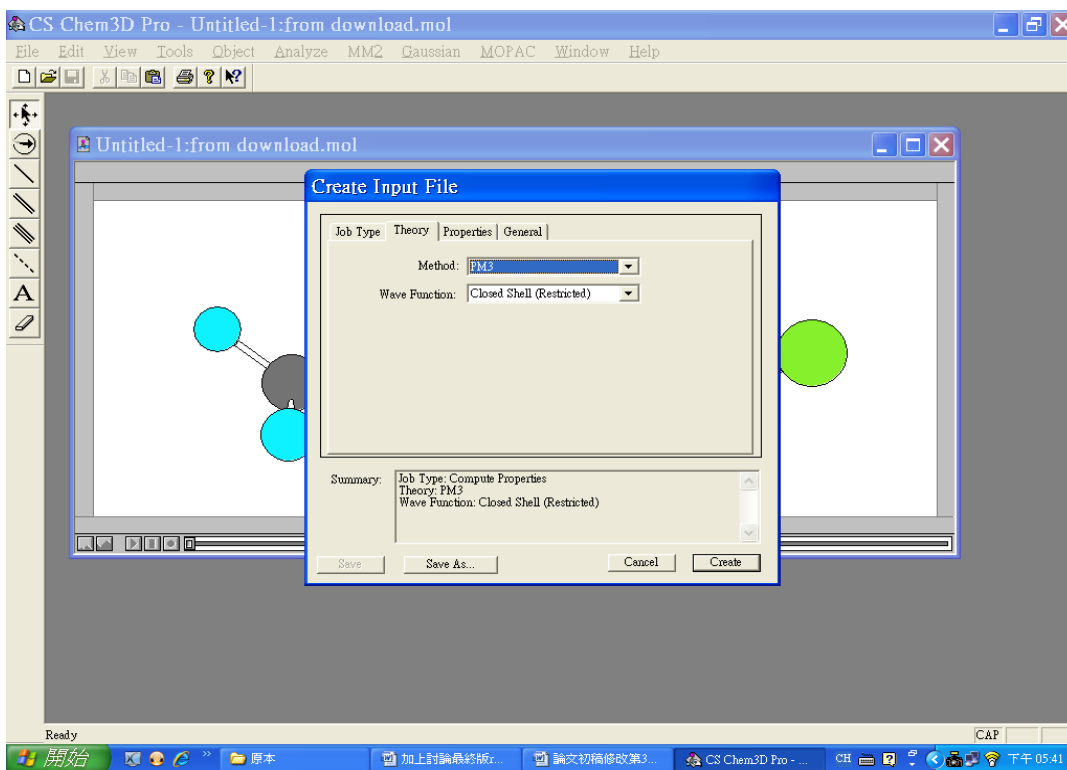
Theory: PM3

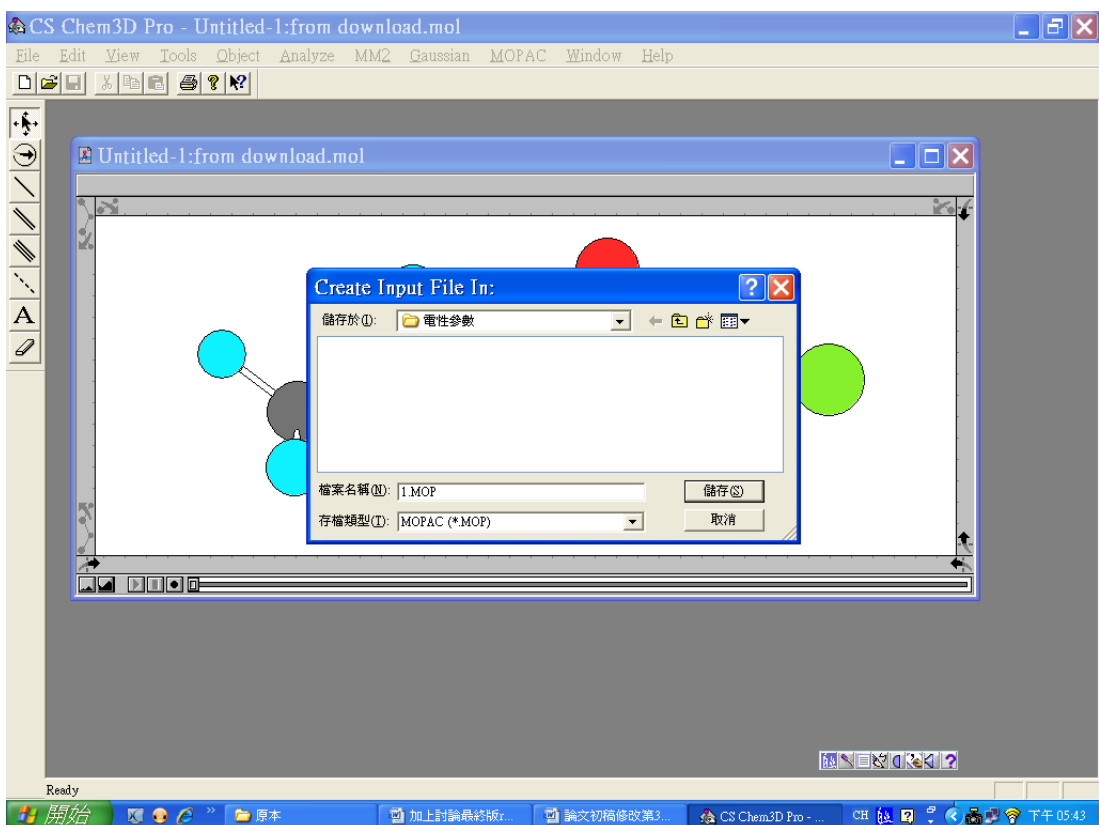
Wave Function: Closed Shell (Restricted)

Properties: Mulliken Charges

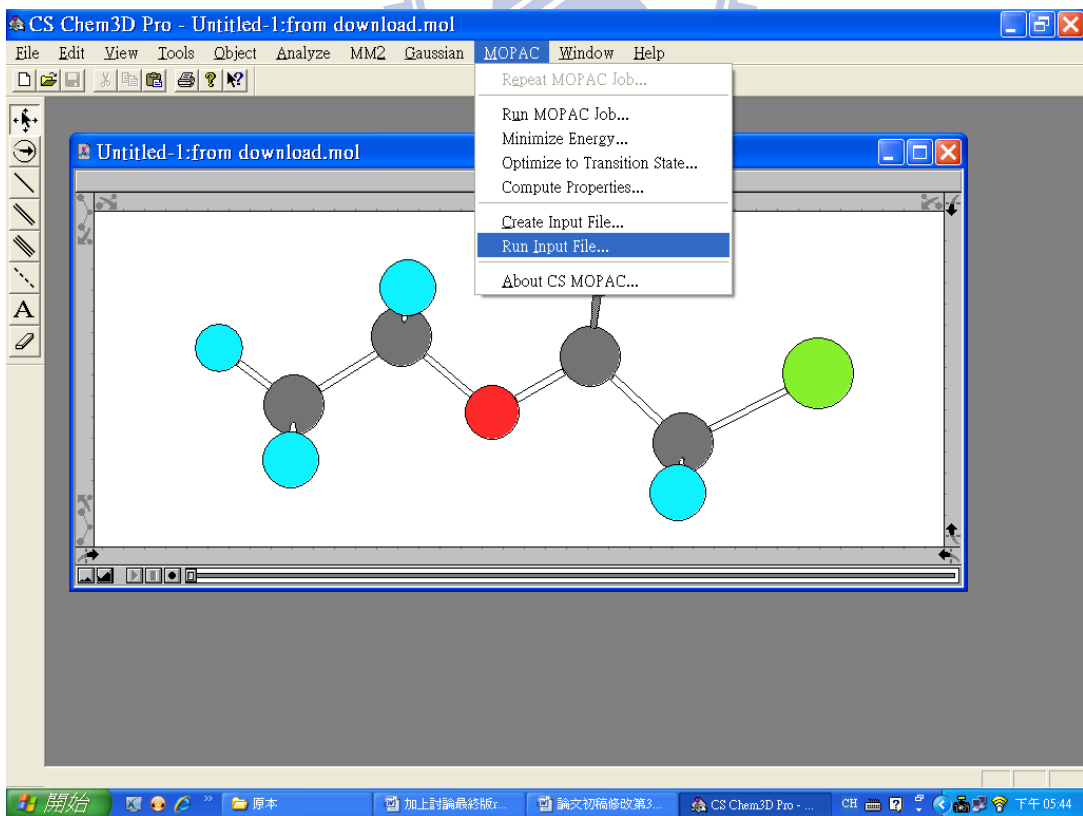
設定完成後 → 按 Create → 按儲存建檔(ex : 1.MOPAC Input File)

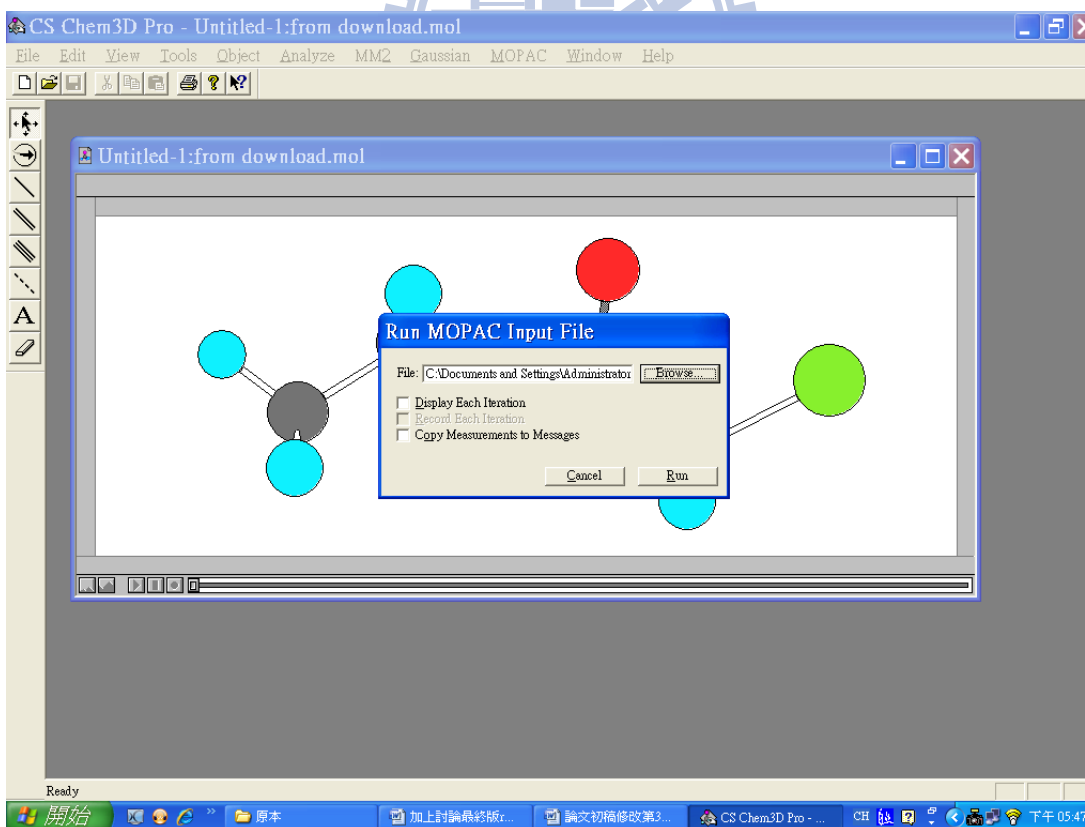
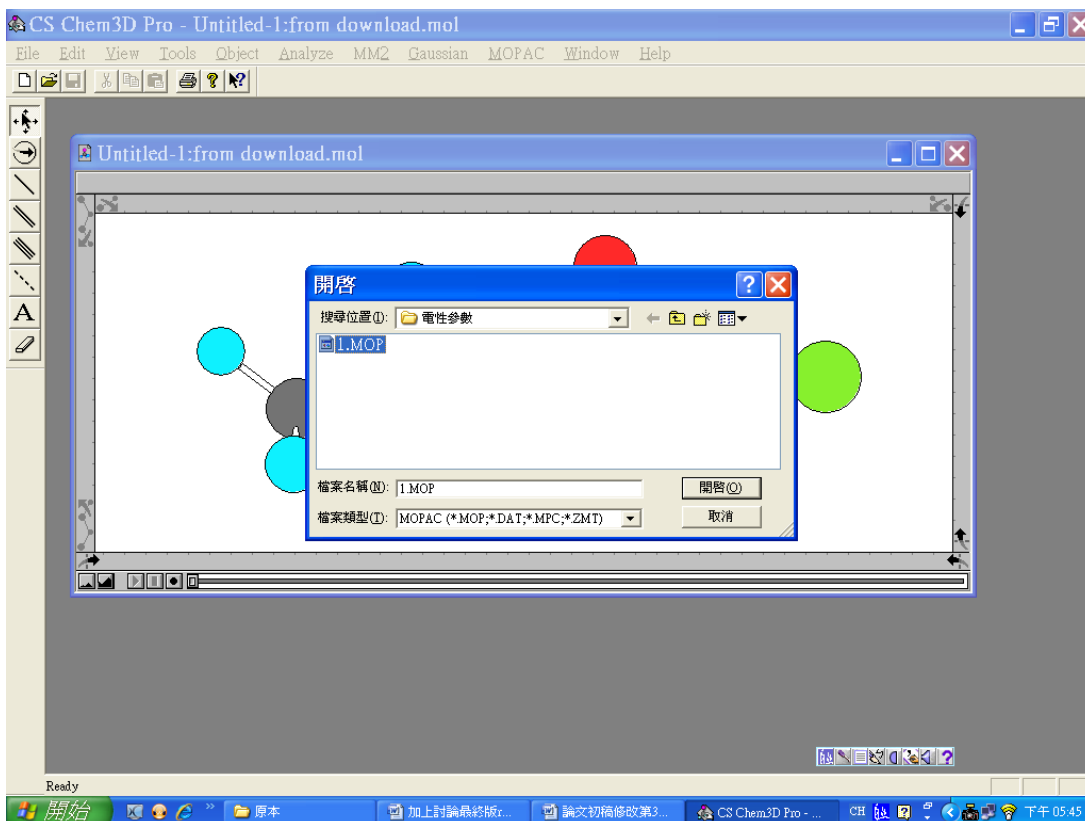


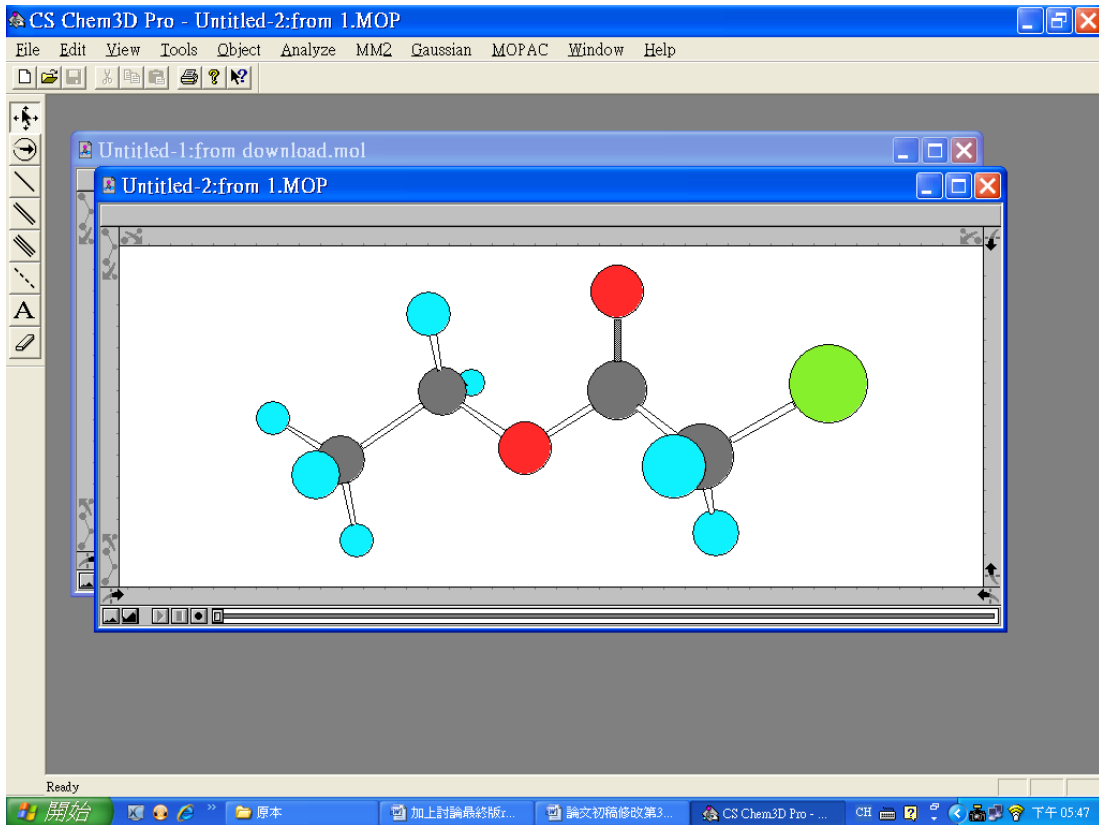




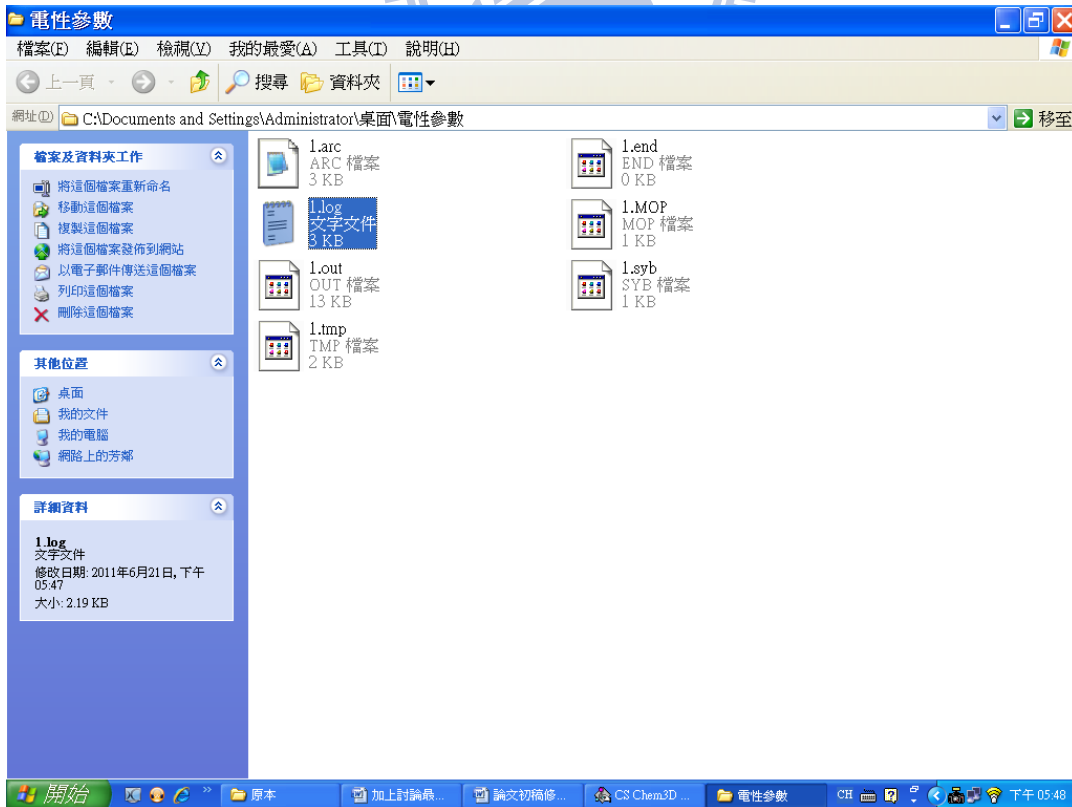
7. 依照前步驟所建製之 MOPAC 檔 → Run Input File
 (ex : Browse → 開啓 1.MOPAC Input File → Run)







8. 至所儲存資料夾→開啓記事本檔



1.arc - 記事本

檔案(F) 編輯(E) 格式(O) 檢視(V) 說明(H)

SUMMARY OF PM3 CALCULATION

MOPAC 97.00

C4 H7 O2 C1

2011/ 6/21

1SCF HMOK GEO-OK PM3

1SCF WAS SPECIFIED, SO BFGS WAS NOT USED
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION = -82.128252 KCAL = -343.62461 KJ
ELECTRONIC ENERGY = -5578.400355 EU
CORE-CORE REPULSION = 4092.646613 EU
DIPOLE = 2.62931 DEBYE SYMMETRY: C1
NO. OF FILLED LEVELS = 21
IONIZATION POTENTIAL = 10.500726 EU
HOMO LUMO ENERGIES (EU) = -10.589 0.194
MOLECULAR WEIGHT = 122.551
SCF CALCULATIONS = 1
COMPUTATION TIME = 0.129 SECONDS

FINAL GEOMETRY OBTAINED

1SCF HMOK GEO-OK PM3

CHARGE

C	0.00000000	0	0.00000000	0	0.00000000	0	0	0	0	0.3438
O	1.20797700	1	0.00000000	0	0.00000000	0	1	0	0	-0.3399
O	1.33799700	1	121.9983220	1	0.00000000	0	1	2	0	-0.2398
C1	2.70814500	1	88.3496400	1	-162.9960630	1	1	2	3	-0.0222
C	1.50897200	1	122.5001530	1	-144.0175320	1	1	2	3	-0.1169
C	1.40199300	1	109.9002530	1	31.2269740	1	3	1	2	0.0448
C	1.51399200	1	107.3998570	1	179.9996340	1	6	3	1	-0.1358

此為 E_{homo} 、 E_{lumo}
 $E_{\text{homo}} = -10.589$
 $E_{\text{lumo}} = 0.194$

開始 自己的... 加上討論... 論文初稿... 電性參數 1 arc - 記... CH 上午 11:02

9. 接著觀察部分電荷值

View → Settings → 依下列圖示設定

CS Chem3D Pro - Untitled-2:from 1.MOP

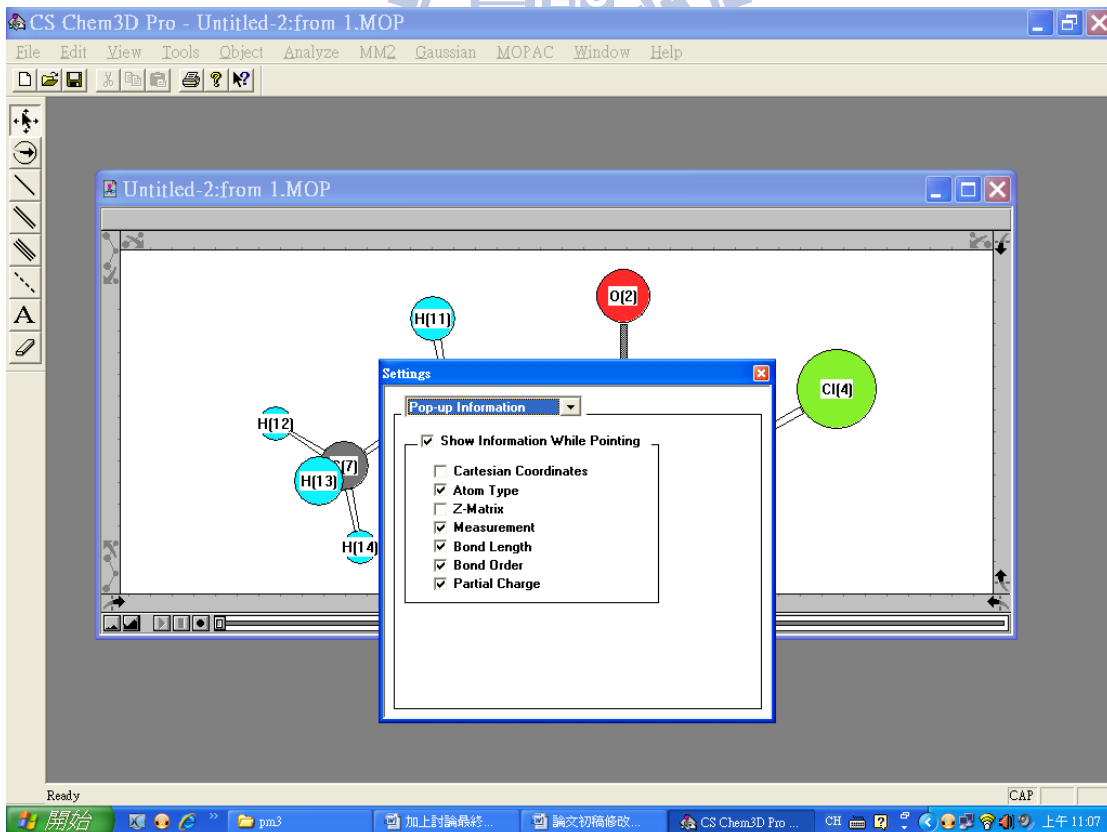
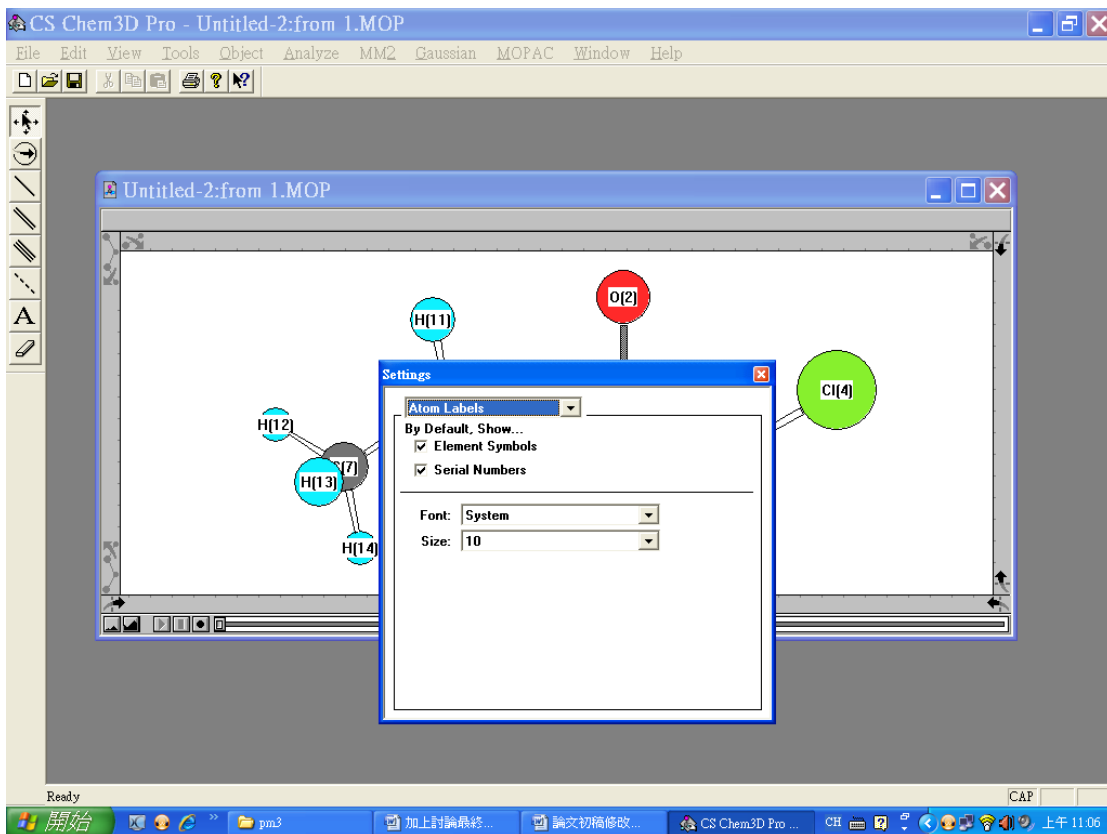
File Edit View Tools Object Analyze MM2 Gaussian MOPAC Window Help

Toolbar
Tools Palette
Settings

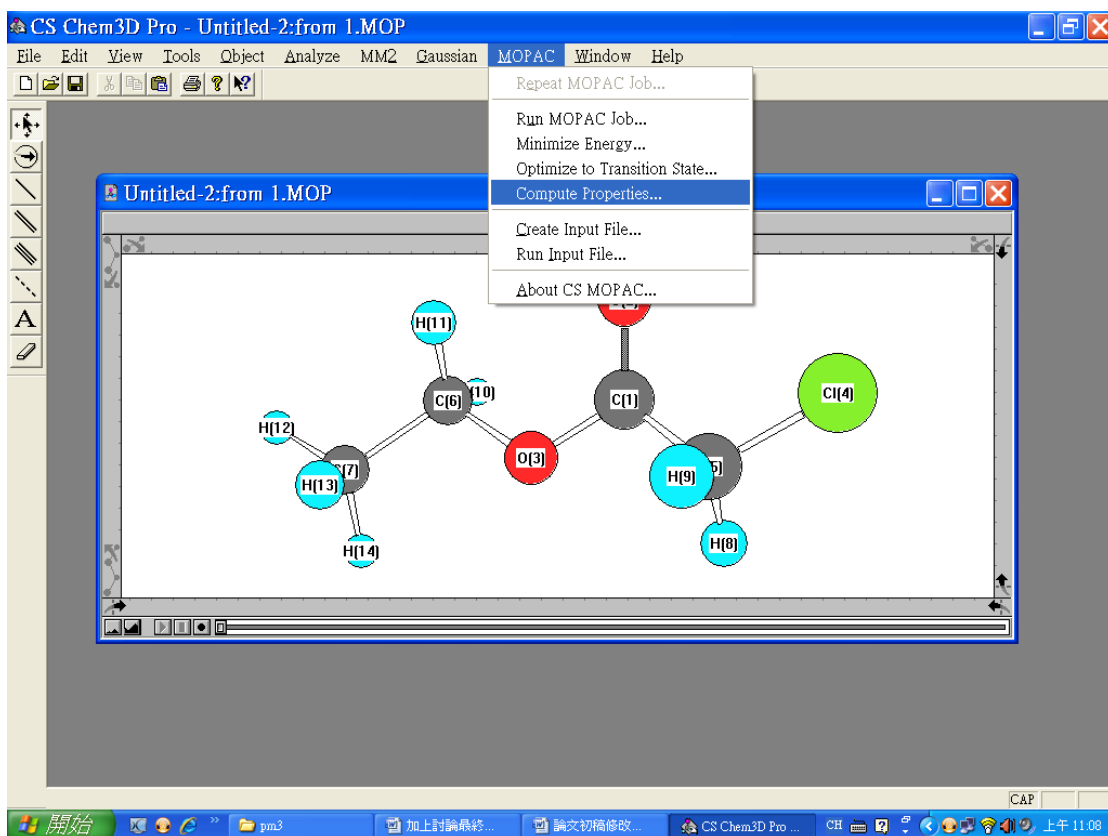
- Solvent Accessible...
- Total Charge Density...
- Total Spin Density...
- Molecular Electrostatic Potential...
- Molecular Orbitals...
- Partial Charges...
- 3-Membered Ring Angles.TBL
- 4-Membered Ring Angles.TBL
- 4-Membered Ring Torsionals.TBL
- Angle Bending Parameters.TBL
- Atom Types.TBL
- Bond Stretching Parameters.TBL
- Conjugated PIsystem Atoms.TBL
- Conjugated PIsystem Bonds.TBL
- Electronegativity Adjustments.TBL
- Elements.TBL
- MM2 Atom Type Parameters.TBL
- MM2 Constants.TBL
- Out-of-Plane Bending Parameters.TBL
- References.TBL
- Substructures.TBL
- Torsional Parameters.TBL
- VDW Interactions.TBL

Specify model settings CAP

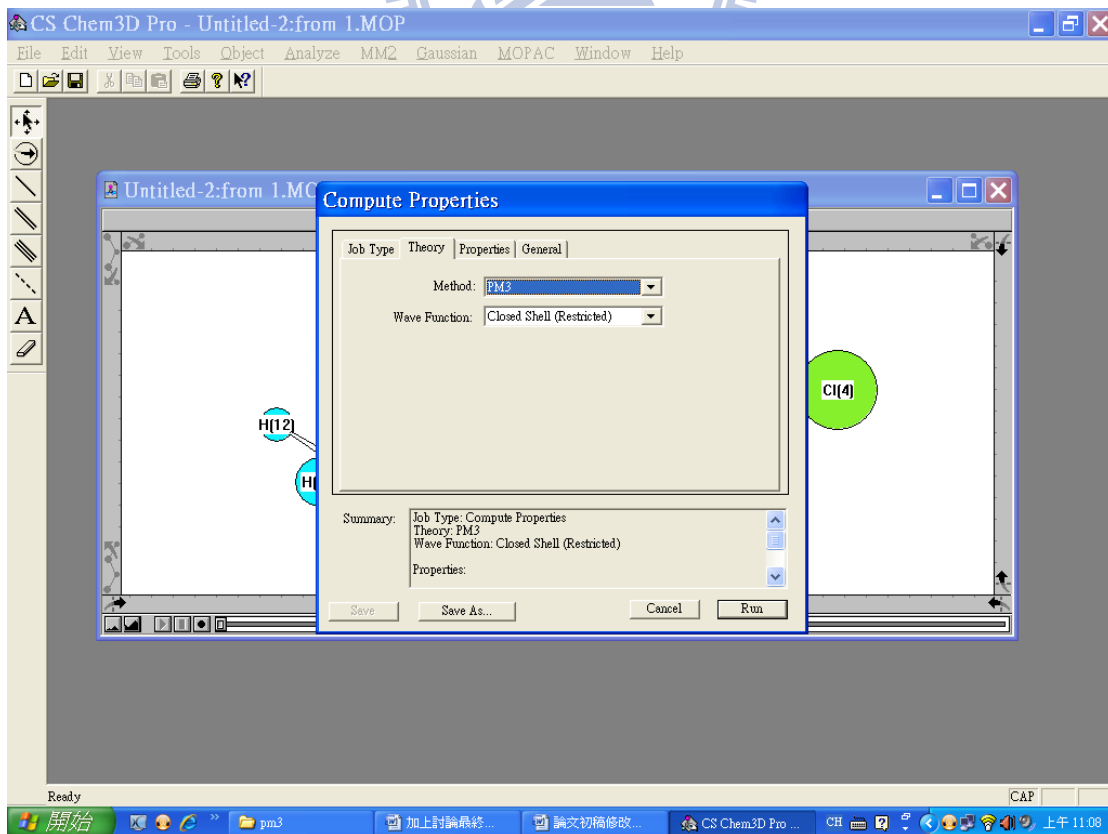
開始 自己的... 加上討論... 論文初稿修改... CS Chem3D Pro ... CH 上午 11:06



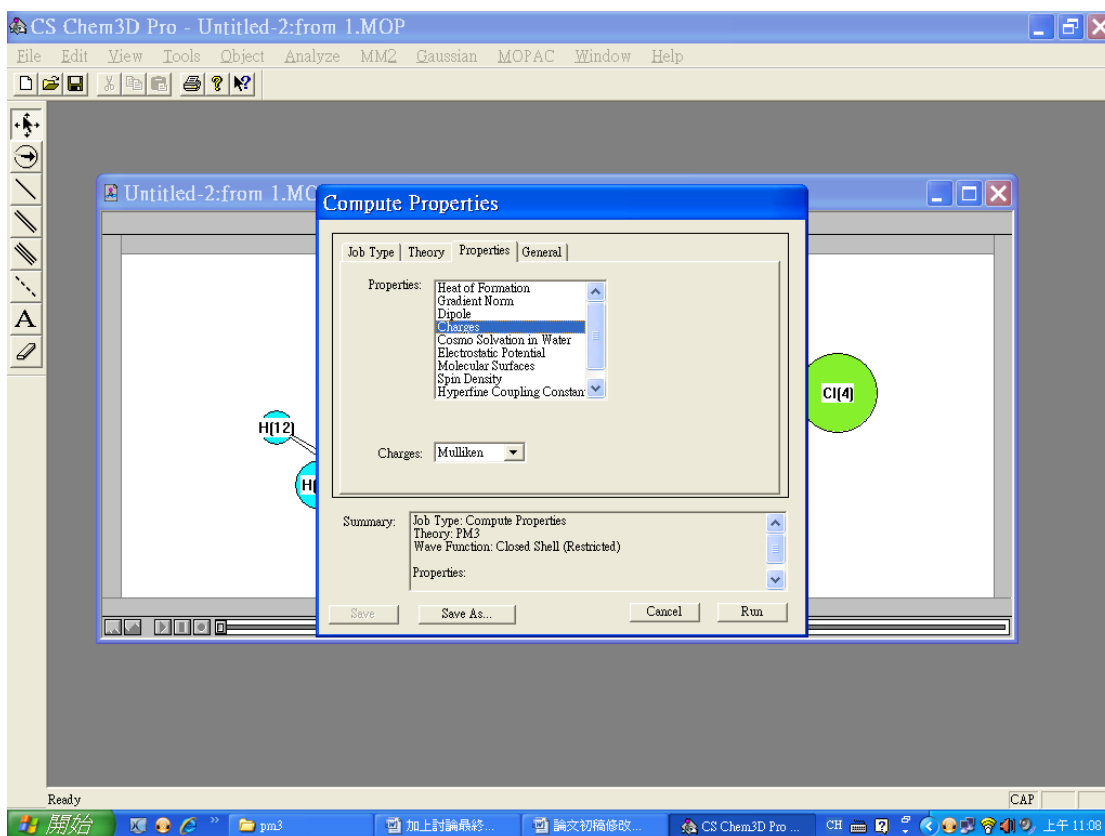
10. 點選 MOPAC → Compute Properties



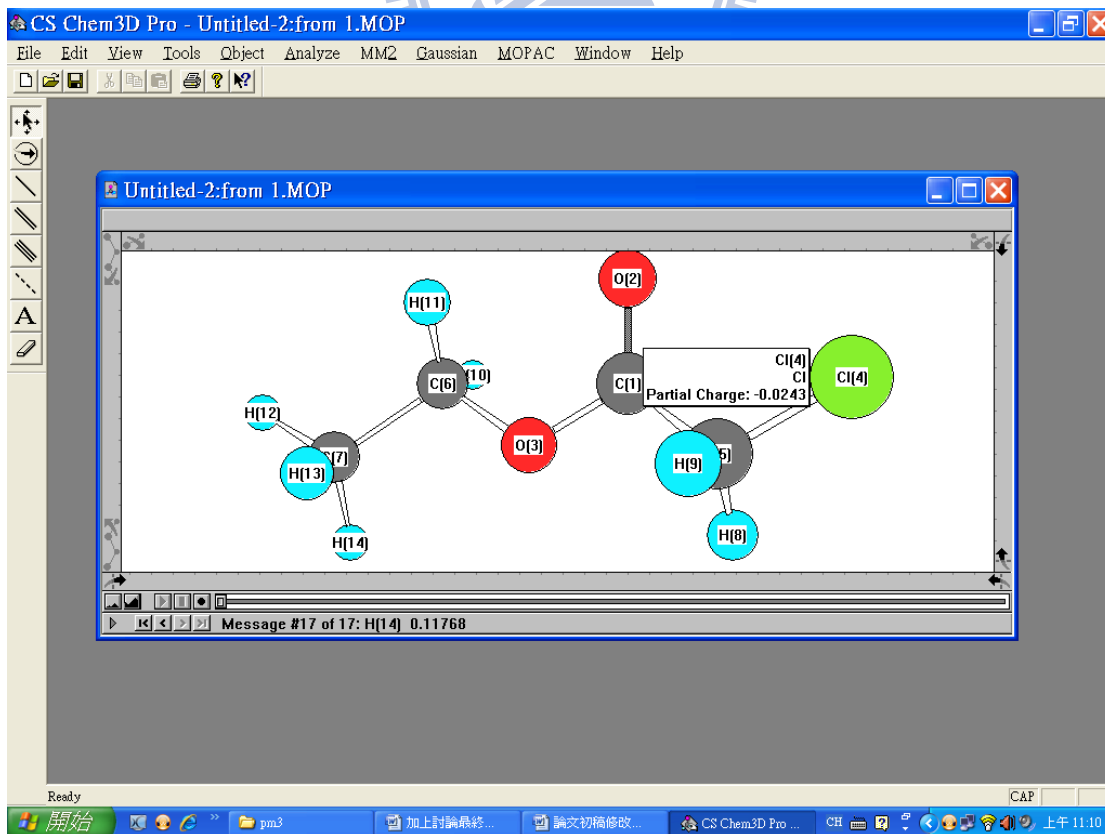
Theory: PM3



僅單選 Charge→Run



游標移至鹵素位置即為 Halo 部分電荷=-0.0243 即可求出



游標移至鍵結鹵素碳位置即為 H-carbon 部分電荷=-0.2922 即可求出

