

Scheme S1: Mechanism of hantzsch reaction of formaldehyde and 2-methyl acetoacetanilid

Figure captions

FIGURE S1: Response surface of the combined effect of reaction time, ethanol, acetate ammonium, 2-methylacetoacetanilid and temperature on derivitazation reaction of formaldehyde.

FIGURE S2: Counter plot of the combined effect of reaction time, ethanol, acetate ammonium, 2-methylacetoacetanilid and temperature on derivitazation reaction of formaldehyde.

FIGURE S3: ^1H NMR product of formaldehyde with 2-methyl acetoacetanilid.

FIGURE S4: Multiplicity ^1H NMR from 1.5-5.5 ppm product of formaldehyde with 2-methyl acetoacetanilid.

FIGURE S5: Multiplicity ^1H NMR from 6.7-8.4 ppm product of formaldehyde with 2-methyl acetoacetanilid

FIGURE S6: Effect of temperature on fluorescence intensity for derivitazation reaction of 1×10^{-6} M formaldehyde with 2-methylacetoacetanilid

FIGURE S7: Effect of PH on fluorescence intensity for derivitazation reaction of 1×10^{-6} M formaldehyde with 2-methylacetoacetanilid

FIGURE S8: Three dimension flourescence spectrum of a shampoo sample after derivitaztation of formaldehyde

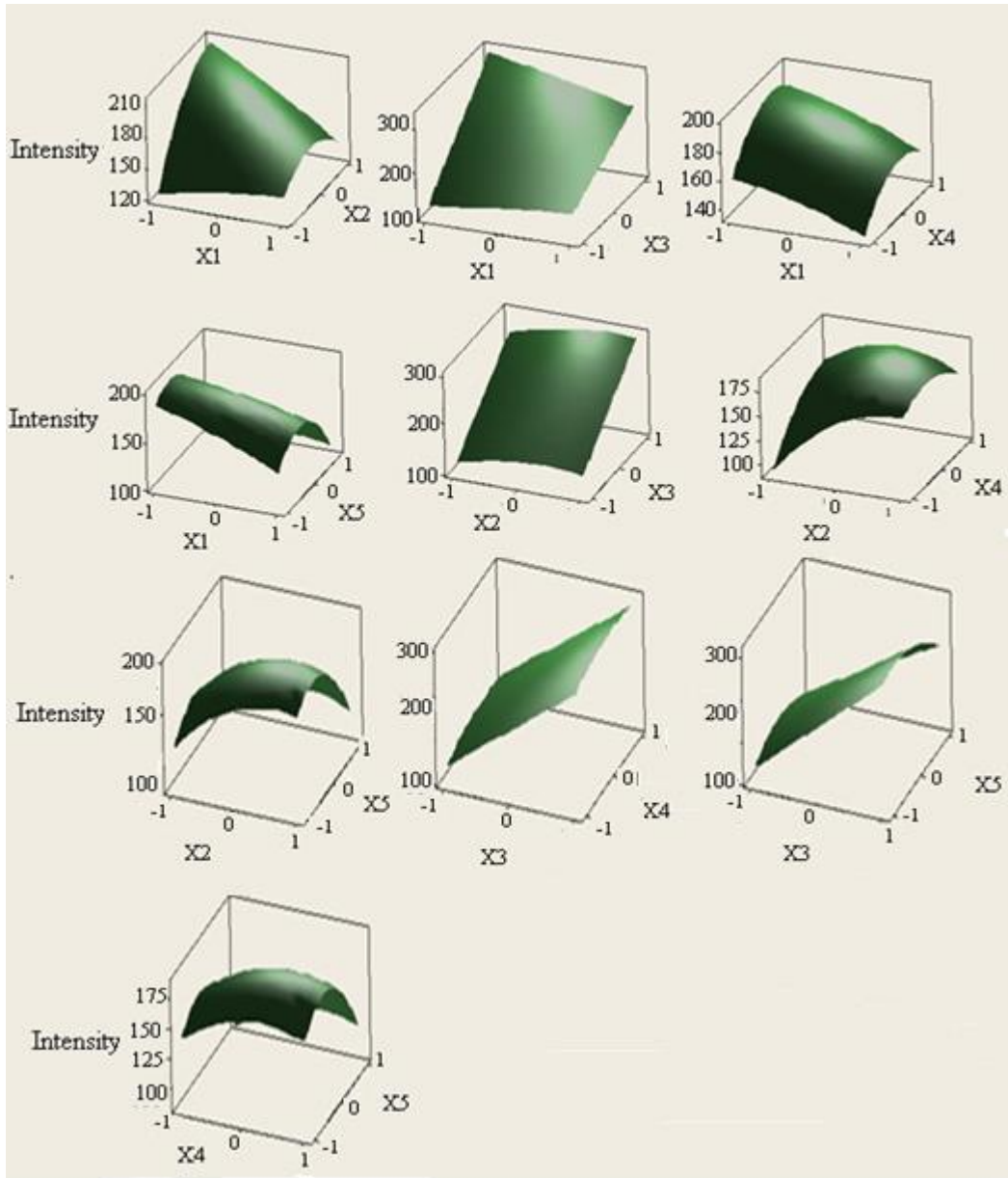


FIGURE S1

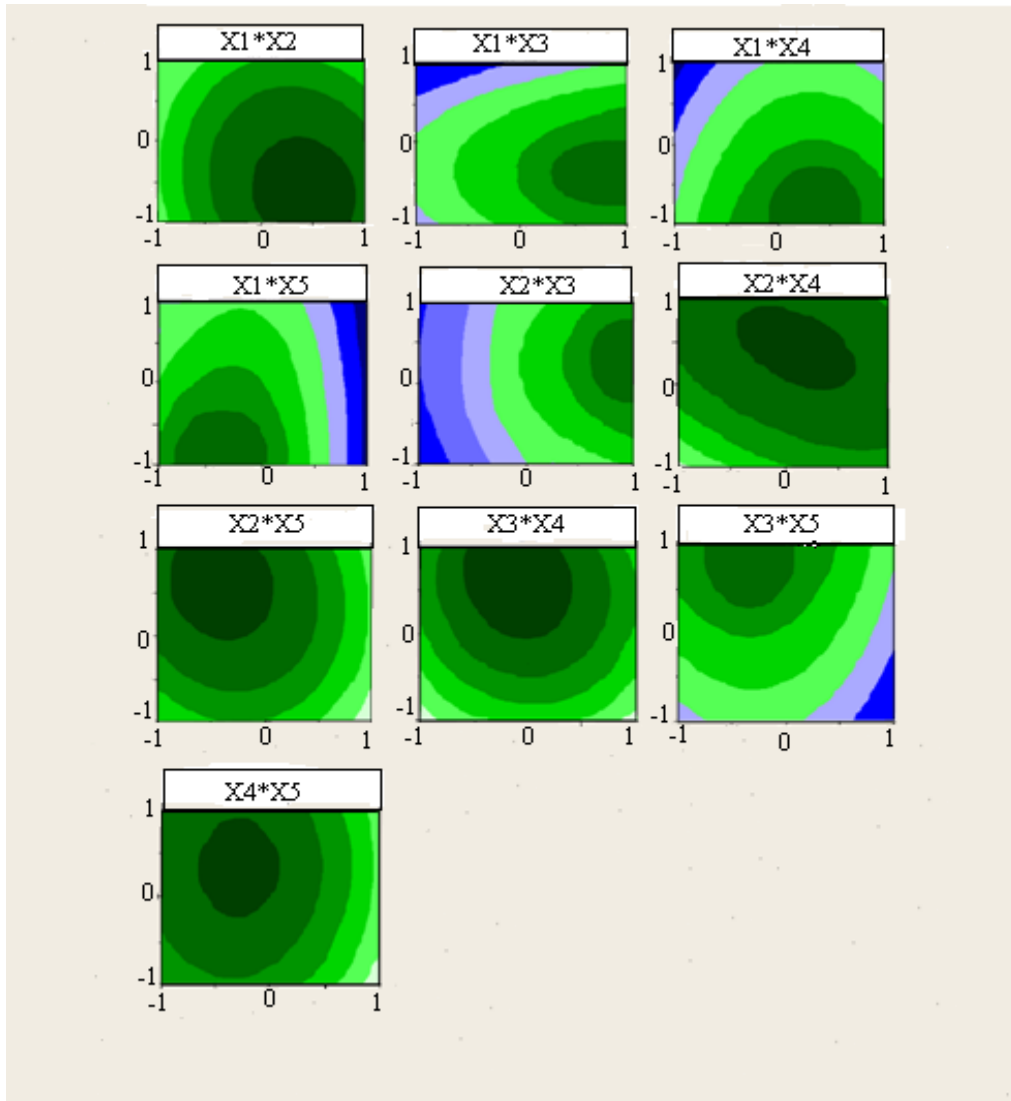


FIGURE S2

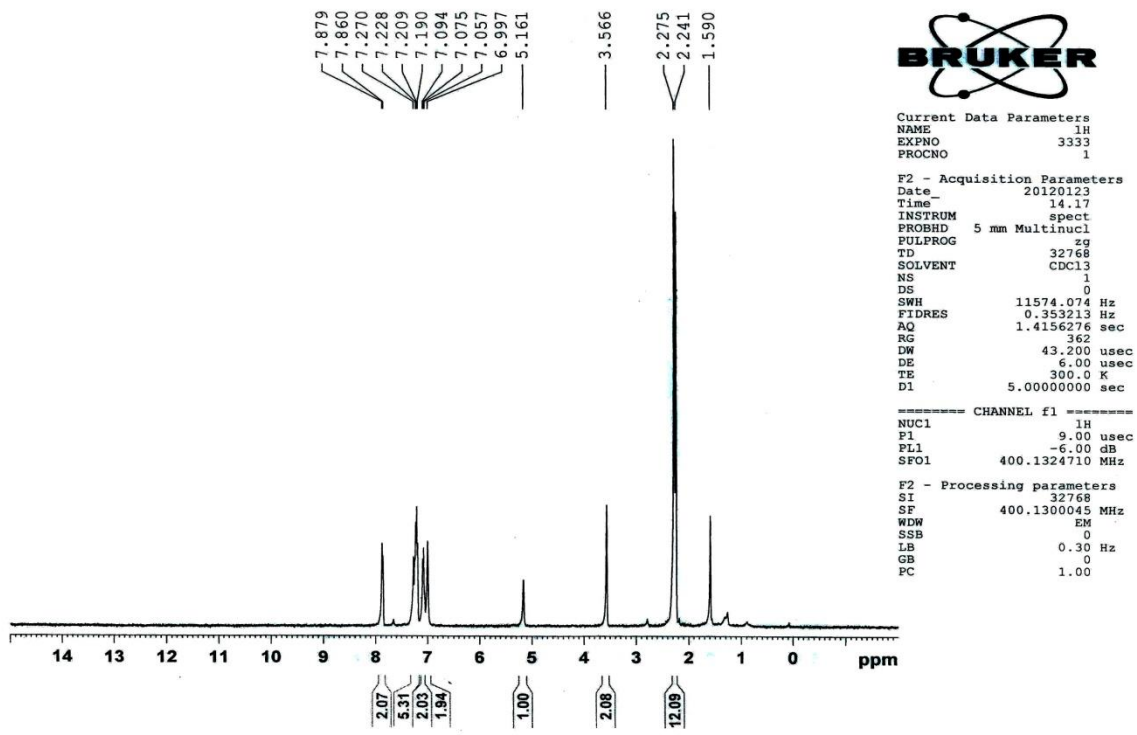
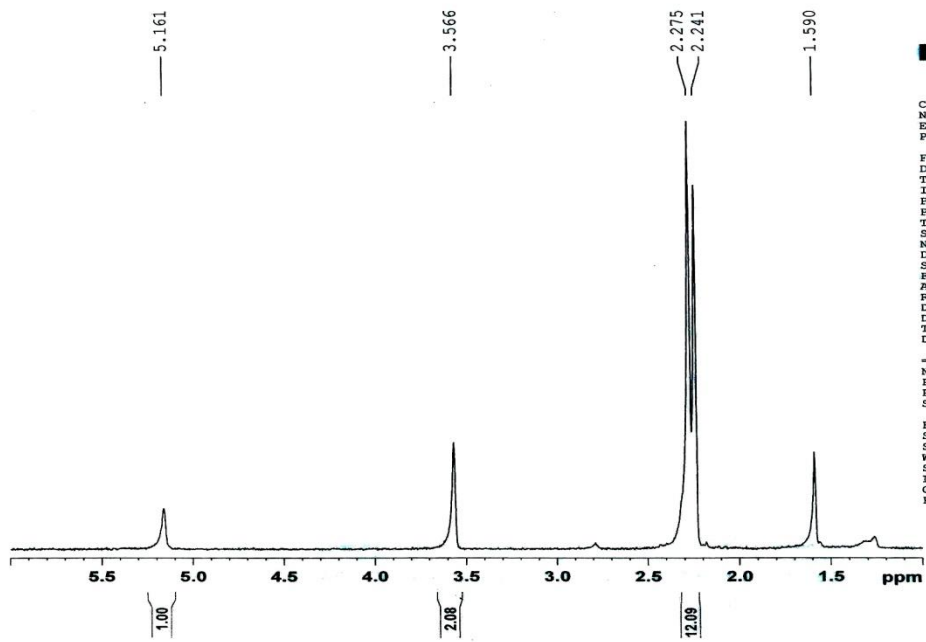


FIGURE S3



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PROCNO    1

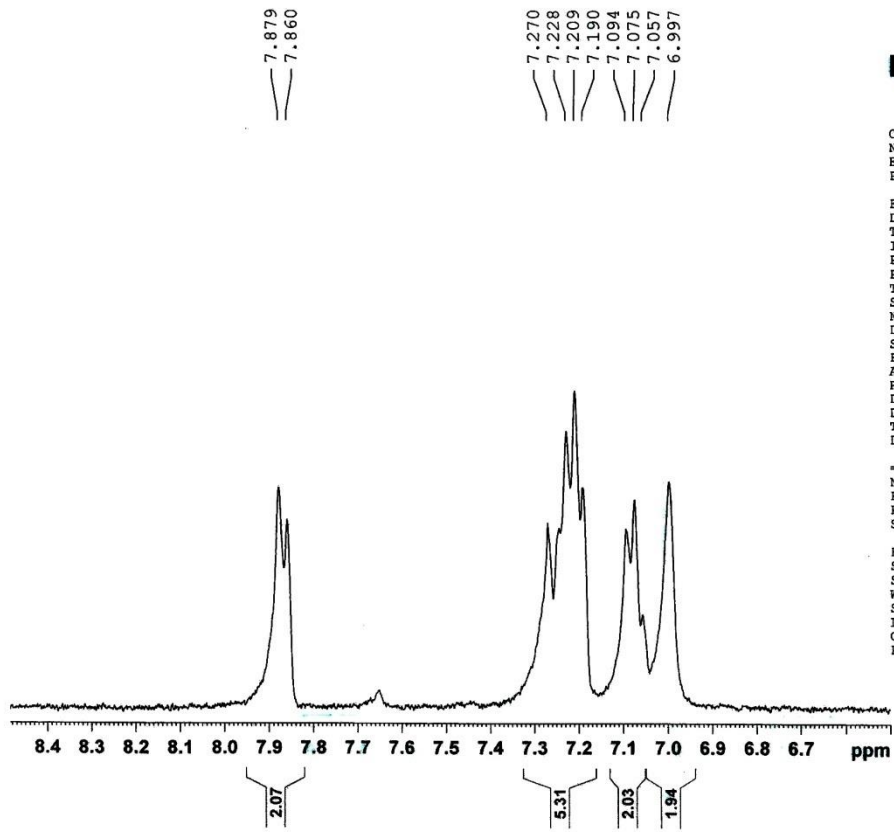
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Time      14.17
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PROBHD    5 mm Multinucl
PULPROG   zg
TD         32768
SOLVENT   CDCl3
NS         1
DS         0
SWH        11574.074 Hz
FIDRES     0.353213 Hz
AQ         1.4156276 sec
RG         362
DW         43.200 usec
DE         6.00 usec
TE         300.0 K
D1         5.0000000 sec

----- CHANNEL f1 -----
NUC1      1H
P1         9.00 usec
PL1       -6.00 dB
SFO1      400.1324710 MHz

F2 - Processing parameters
SI         32768
SF         400.1300045 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00

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FIGURE S4



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Current Data Parameters
NAME          1H
EXPNO         3333
PROCNO        1

F2 - Acquisition Parameters
Date_         20120123
Time_         14.17
INSTRUM       spect
PROBHD        5 mm Multinucl
PULPROG       zg
TD            32768
SOLVENT       CDC13
NS            1
DS            0
SWH           11574.074 Hz
FIDRES        0.353213 Hz
AQ            1.4156276 sec
RG            362
DW            43.200 usec
DE            6.00 usec
TE            300.0 K
D1            5.00000000 sec

===== CHANNEL f1 =====
NUC1          1H
P1            9.00 usec
PL1          -6.00 dB
SFO1         400.1324710 MHz

F2 - Processing parameters
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SF           400.1300045 MHz
WDW          EM
SSB          0
LB           0.30 Hz
GB           0
PC           1.00
  
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FIGURE S5

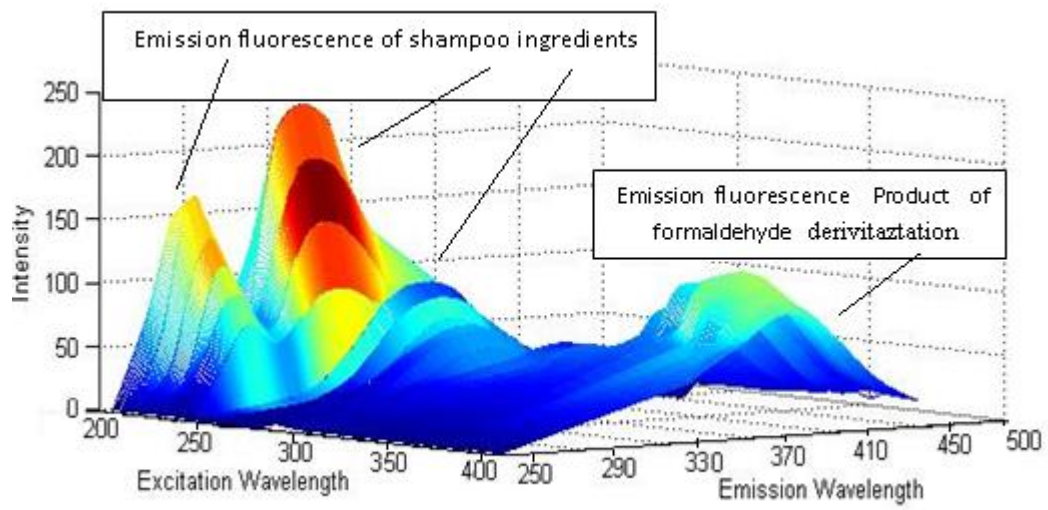


FIGURE S6

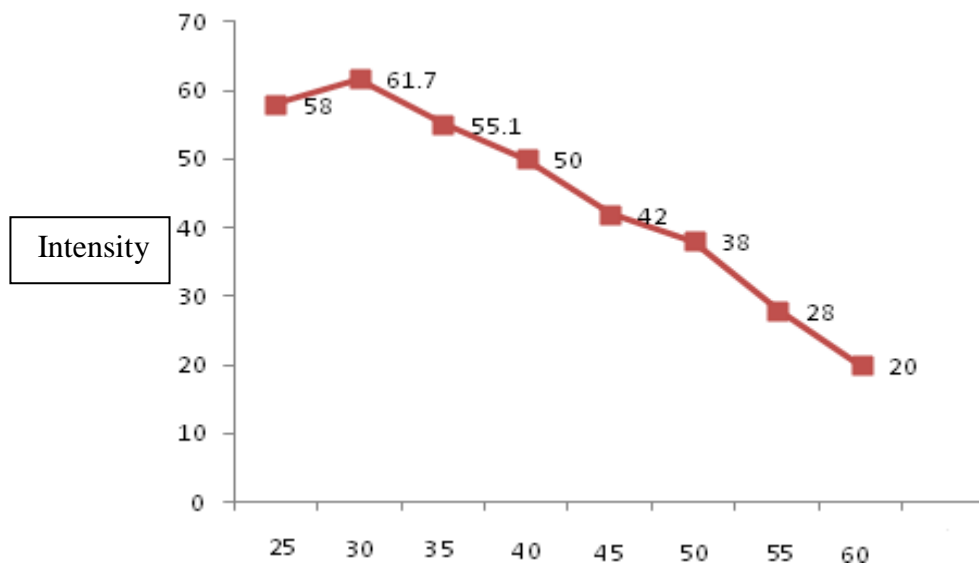


FIGURE S7

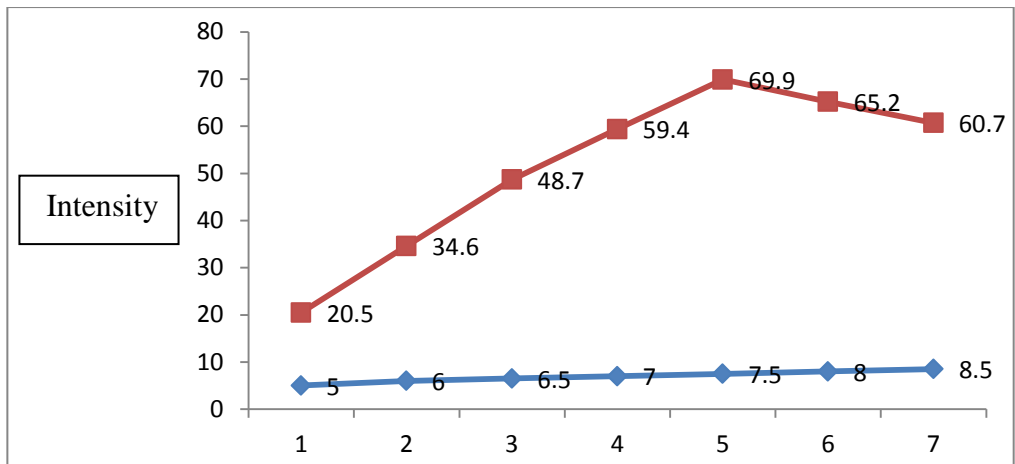


FIGURE S8

TABLE captions

TABLE S1: Scheme of independent variables (X_i) for Box- Behnken design

TABLE S2: Estimated regression coefficients for derivitazation reaction of formaldehyde

TABLE S1: Scheme of independent variables (X_i) for Box- Behnken design

Std Order	Run Order	X_1	X_2	X_3	X_4	X_5
11	1	1	0	-1	0	1
30	2	0	0	1	0	-1
33	3	-1	0	0	0	-1
20	4	0	0	0	1	1
18	5	0	0	0	1	-1
3	6	-1	1	0	0	0
5	7	0	0	-1	-1	0
40	8	0	1	0	1	0
22	9	0	1	-1	0	0
34	10	1	0	0	0	-1
7	11	0	0	-1	1	0
26	12	1	0	0	-1	0
38	13	0	1	0	-1	0
23	14	0	-1	1	0	0
35	15	-1	0	0	0	1
37	16	0	-1	0	-1	0
10	17	0	1	0	0	-1
13	18	-1	0	-1	0	0
14	19	1	0	-1	0	0
43	20	0	0	0	0	0
1	21	-1	-1	0	0	0
24	22	0	1	1	0	0
31	23	0	0	-1	0	1
15	24	-1	0	1	0	0
29	25	0	0	-1	0	-1
32	26	0	0	1	0	1
28	27	0	-1	-1	0	0
2	29	1	-1	0	0	0
41	30	0	0	0	0	0
44	31	0	0	0	0	0
27	32	-1	0	0	1	0
36	33	1	0	0	0	1
39	34	0	-1	0	1	0
9	35	0	-1	0	0	-1
17	36	0	0	0	-1	-1
6	37	0	0	1	-1	0
19	38	0	0	0	-1	1
16	39	1	0	1	0	0
4	40	1	1	0	0	0
46	41	0	0	0	0	0
8	42	0	0	1	1	0
45	43	0	0	0	0	0
25	44	-1	0	0	-1	0
12	45	0	1	0	0	1
42	46	0	0	0	0	0

TABLE S2: Estimated regression coefficients for derivitazation reaction of formaldehyde

Term	Coef ^a .	SE coef ^b .	t ^c	p-value ^d
Constant	188.890	7.263	26.006	0.000
x ₁	-29.086	4.448	-6.539	0.000
x ₂	19.144	4.448	4.304	0.000
x ₃	116.579	4.448	26.210	0.000
x ₄	8.094	4.448	1.820	0.081
x ₅	-11.167	4.448	-2.511	0.019
x ₁ *x ₁	-38.974	6.023	-6.471	0.000
x ₂ *x ₂	-22.639	6.023	-3.759	0.001
x ₃ *x ₃	2.118	6.023	0.352	0.728
x ₄ *x ₄	-25.145	6.023	-4.175	0.000
x ₅ *x ₅	-20.514	6.023	-3.406	0.002
x ₁ *x ₂	-21.202	8.896	-2.383	0.025
x ₁ *x ₃	-22.313	8.896	-2.508	0.019
x ₁ *x ₄	0.777	8.896	0.087	0.931
x ₁ *x ₅	10.498	8.896	1.180	0.249
x ₂ *x ₃	7.751	8.896	0.871	0.392
x ₂ *x ₄	-39.969	8.896	-4.493	0.000
x ₂ *x ₅	-20.762	8.896	-2.334	0.028
x ₃ *x ₄	-1.809	8.896	-0.203	0.841
x ₃ *x ₅	-13.945	8.896	-1.568	0.130
x ₄ *x ₅	8.557	8.896	0.962	0.345
Adj-R square	97.19%			
Pred-R square	89.35%			
R square	94.94%			

a= coefficient, b=standard error of the coefficient, c=t test, d=p value