

Table 1-S Design matrix and the response of the PBD

Run No	A	B	C	D	E	F	Relative response
1	-1	-1	-1	1	-1	1	13.895
2	-1	-1	1	-1	1	1	21.456
3	1	-1	1	1	-1	1	15.018
4	-1	1	-1	1	1	-1	17.947
5	1	-1	1	1	1	-1	15.567
6	-1	-1	-1	-1	-1	-1	18.231
7	1	1	-1	-1	-1	1	20.378
8	-1	1	1	-1	1	1	24.078
9	-1	1	1	1	-1	-1	17.089
10	1	-1	-1	-1	1	-1	16.456
11	1	1	1	-1	-1	-1	21.127
12	1	1	-1	1	1	1	15.765

Table 2-S Design matrix and the response of the CCD

Run No	Blocks	A	B	C	D	Relative response	Comments
1	Block 1	5.6	48	2	38	23.005	Center- full factorial
2	Block 1	6.2	36	1	32	15.018	Full factorial
3	Block 1	6.2	36	3	44	17.174	Full factorial
4	Block 1	5	36	3	32	19.078	Full factorial
5	Block 1	5	60	3	44	18.067	Full factorial
6	Block 1	5	60	1	32	20.988	Full factorial
7	Block 1	5.6	48	2	38	24.356	Center- full factorial
8	Block 1	6.2	60	3	32	20.589	Full factorial
9	Block 1	6.2	60	1	44	19.015	Full factorial
10	Block 1	5	36	1	44	16.901	Full factorial
11	Block 2	6.2	36	3	32	18.349	Full factorial
12	Block 2	5	60	3	32	21.389	Full factorial
13	Block 2	5	36	1	32	18.578	Full factorial
14	Block 2	5	60	1	44	19.367	Full factorial
15	Block 2	5.6	48	2	38	23.045	Center- full factorial
16	Block 2	6.2	36	1	44	16.091	Full factorial
17	Block 2	6.2	60	1	32	20.234	Full factorial
18	Block 2	6.2	60	3	44	19.089	Full factorial
19	Block 2	5.6	48	2	38	23.609	Center- full factorial
20	Block 2	5	36	3	44	17.578	Full factorial
21	Block 3	5.6	48	2	50	14.267	Axial
22	Block 3	5.6	48	2	38	23.534	Center-axial
23	Block 3	4.4	48	2	38	18.089	Axial
24	Block 3	5.6	24	2	38	20.191	Axial
25	Block 3	5.6	48	0	38	19.012	Axial
26	Block 3	5.6	48	4	38	22.067	Axial

27	Block 3	5.6	48	2	26	15.987	Axial
28	Block 3	6.8	48	2	38	18.712	Axial
29	Block 3	5.6	72	2	38	24.005	Axial
30	Block 3	5.6	48	2	38	23.212	Center-axial

Table 3-S Analysis of variance for the fitted models in PBD

Source	SS ^a	d.f. ^b	MS ^c	F-value	p-value	
Model	100.17	6	16.70	20.93	0.0021	S
A	5.86	1	5.86	7.34	0.0423	S
B	20.70	1	20.70	25.95	0.0038	S
C	11.34	1	11.33	14.20	0.0130	S
D	58.28	1	58.28	73.05	0.0004	S
E	2.55	1	2.55	3.20	0.1339	NS
F	1.45	1	1.45	1.82	0.2353	NS
Residual	3.99	5	0.80			
Total	104.16	11				

^a SS: Sum of square; ^b d.f.: Degree of freedom; ^c MS: Mean square

Table 4-S The significance of each variable effect was showed by F and p values.

	Factor	SS ^a	d.f. ^b	MS ^c	F-value	p-value	
Linear effects	A	1.10	1	1.10	2.44	0.1424	NS
	B	31.74	1	31.74	70.26	< 0.0001	S
	C	5.26	1	5.26	11.64	0.0046	S
	D	8.62	1	8.62	19.08	0.0008	S
Interaction effects	AB	1.33	1	1.33	2.95	0.1095	NS
	AC	1.30	1	1.30	2.88	0.1133	NS
	AD	1.75	1	1.75	3.89	0.0704	NS
	BC	2.30	1	2.30	5.08	0.0421	S
	BD	1.20	1	1.20	2.66	0.1270	NS
	CD	1.03	1	1.03	2.27	0.1556	NS
Quadratic effects	A ²	49.21	1	49.21	108.94	< 0.0001	S
	B ²	4.73	1	4.73	10.46	0.0065	S
	C ²	17.76	1	17.76	39.32	< 0.0001	S
	D ²	127.71	1	127.71	282.74	< 0.0001	S

^a SS: Sum of square; ^b d.f.: Degree of freedom; ^c MS: Mean square

Table 5-S The repeatability and linearity of the proposed method

No	Aglycone compounds or m/z (Abundance) ^b	Repeatability/%	Reproducibility/%	Linearity/r
<i>Aliphatic alcohols</i>				
1	3-Methyl-butyl alcohol	8.1	9.5	0.995
<i>Fatty acids</i>				
2	3-Methylbutanoic acid	13.1	14.2	0.989
3	2-Methylbutanoic acid	11.6	11.8	0.991
4	3-Methylpentanoic acid	12.7	15.7	0.980
<i>Aromatic compounds</i>				
5	Benzaldehyde	7.8	8.5	0.997
6	Benzyl alcohol	4.1	5.3	0.999
7	Phenethyl alcohol	3.2	4.8	0.993
8	p-Vinylguaiacol	3.5	3.9	0.999
9	2-Hydroxyphenylethanol	10.2	13.5	0.988
10	4-Hydroxyphenylethanol (Tyrosol)	7.7	8.9	0.996
11	Homovanillyl alcohol	5.3	5.4	0.998
<i>Cl3 Norisoprenoids</i>				
12	3-Hydroxy- β -damascone	8.5	9.3	0.993
13	3-Hydroxy- β -ionol	7.0	8.5	0.992
14	3-Hydroxy-7,8-dehydro- β -ionol	3.6	4.9	0.995
15	181(100);125(91);163(39);145(7) 95(38); 83(35); 105(13)	6.5	7.8	0.990
16	3-Oxo- α -ionol	7.9	8.5	0.993
17	3-Hydroxy-5,6-epoxy- β -ionol	6.5	6.7	0.996
18	Blumenol C	6.2	7.1	0.993
19	9-Hydroxymegastigma-4,6-dien-3-one 1 9-Hydroxymegastigma-4,6-dien-3-one 2	5.3	6.2	0.995
20	Vomifoliol	8.2	9.5	0.994
<i>Terpenoids</i>				
21	2,6-Dimethyl-2,7-octadiene-1,6-diol	7.3	8.9	0.993
22	83(100);69(56);98(24);108(14);109(14); 55(49)	8.5	9.1	0.990
23	3 β -Hydroxysolanascone	9.0	11.8	0.992
24	256(3);241(11);223(7);181(21);163(11);153(27); 135(32);127(65);109(71);101(100);95(73); 81(72)	8.9	10.1	0.991
25	Rishitin	3.1	5.4	0.995
26	256(3);241(13);223(17);181(31);163(16);153(20); 135(22);127(100);109(56);101(59);95(78);81(74)	11.8	12.5	0.993
27	3 β -Hydroxysolavetivone	5.1	6.4	0.998
<i>Polyphenols</i>				
28	Scopoletin	13.6	15.4	0.985

Fig. 1-S Response surfaces of β -Glucosidase concentration (mg/mL) and agitation speed (rpm) for PBD

