Appendix

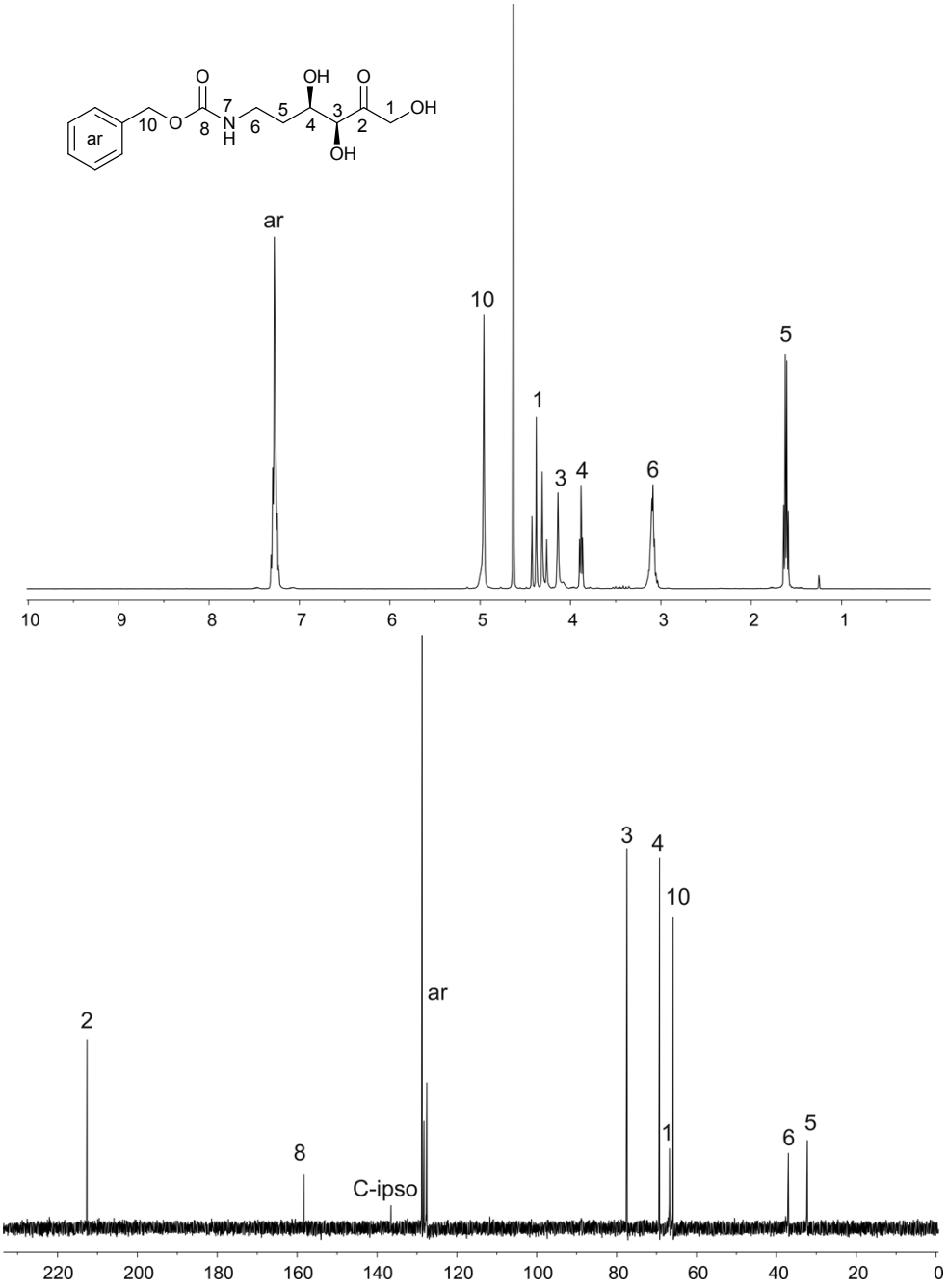

Figure 1 ^{1}H and ^{13}C NMR of the purified aldol adduct from the cascade oxidation-aldol addition reaction of *N*-Cbz-3-aminopropanol and dihydroxyacetone catalyzed by FSA A129S.

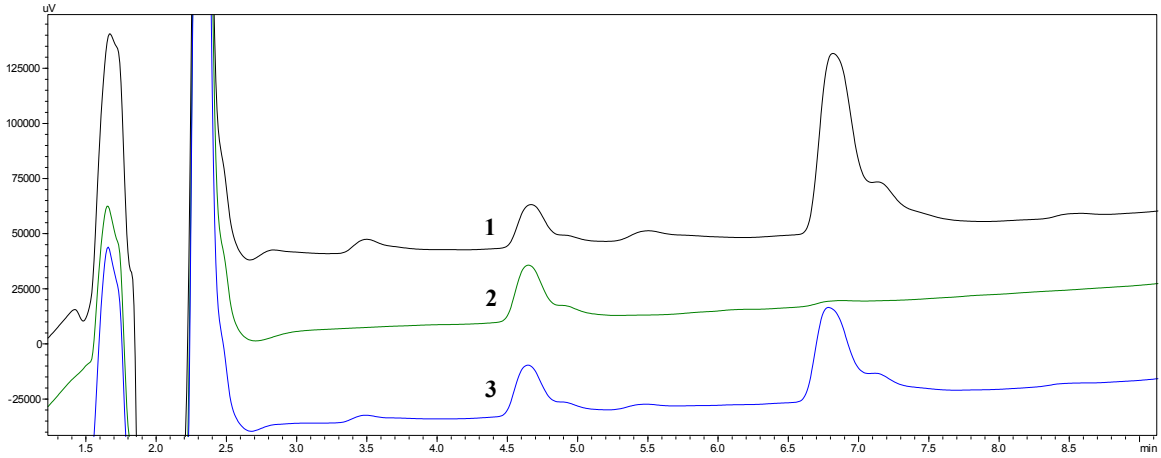

Figure 2 HPLC chromatograms of **1.** sample from cascade reaction, **2.** aldol adduct standard, **3.** mixed sample of reaction sample and aldol adduct standard. Retention time of the aldol adduct is 4.6 min.

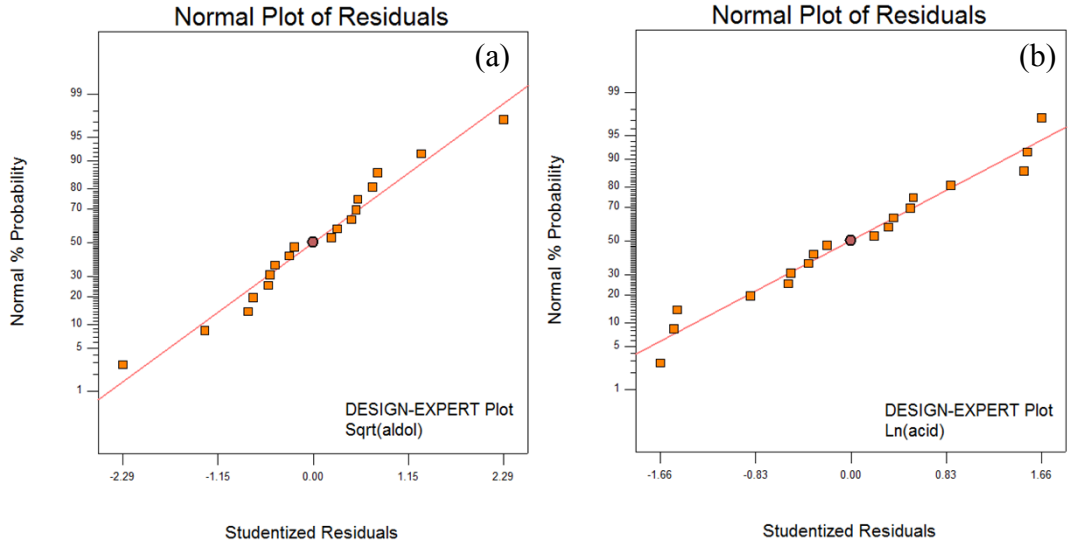

Figure 3 Normal plots of residuals for the aldol adduct (a) and amino acid concentration (b).

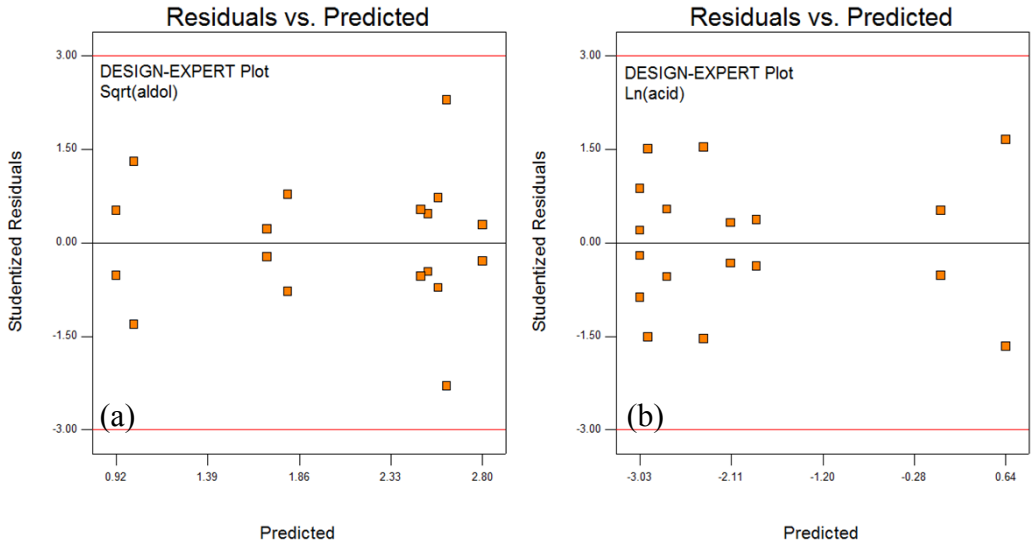

Figure 4 Residuals *vs* predicted plot for the aldol adduct (a) and amino acid concentration (b).

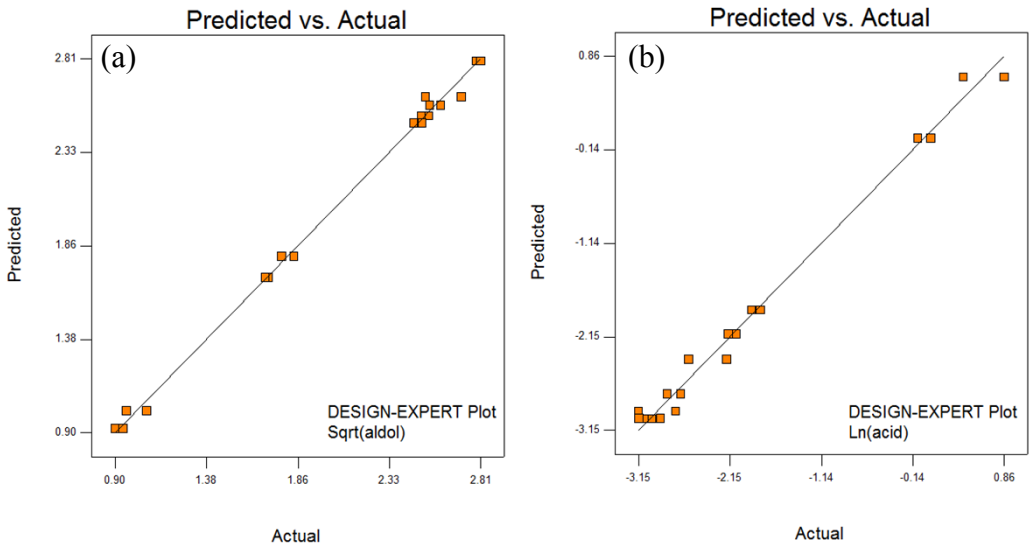

Figure 5 Predicted *vs* actual plot for the aldol adduct (a) and amino acid concentration (b).

Table 1 Optimal conditions for achieving maximum aldol adduct concentration suggested by the software.

Name	Goal	Lower Limit	Upper Limit	Lower Weight	Upper Weight	Importance
NAD	is in range	0.1	1	1	1	3
FSA	is in range	1	3	1	1	3
HLADH	is in range	1	10	1	1	3
aldol adduct	maximize	0.81	7.91	1	1	5

Solutions

Number	NAD^+	FSA	HLADH	aldol adduct	Desirability	$Y_{\text{aldol adduct}}$ / %
1	1.00	3.00	10.00	7.85	0.9939	78.49
2	1.00	2.95	10.00	7.82	0.9915	78.23
3	1.00	2.90	10.00	7.80	0.9893	77.99
4	0.99	2.99	10.00	7.79	0.9883	77.89
5	0.99	3.00	10.00	7.76	0.9855	77.58
6	1.00	2.77	10.00	7.73	0.9827	77.29
7	1.00	2.04	10.00	7.37	0.9481	73.65
8	1.00	1.82	10.00	7.25	0.9373	72.54
9	1.00	1.00	4.02	6.70	0.8830	67.05

Table 2 Optimal conditions for achieving minimum amino acid concentration suggested by the software.

Name	Goal	Lower Limit	Upper Limit	Lower Weight	Upper Weight	Importance
NAD	is in range	0.1	1	1	1	3
FSA	is in range	1	3	1	1	3
HLADH	is in range	1	10	1	1	3
amino acid	minimize	0.04272	2.37326	1	1	5

Solutions

Number	NAD^+	FSA	HLADH	amino acid	Desirability	$Y_{\text{amino acid}}$ / %
1	0.10	1.15	10.00	0.04825	0.9697	0.4825
2	0.10	1.00	9.96	0.04825	0.9697	0.4825
3	0.10	1.46	10.00	0.04828	0.9696	0.4828
4	0.10	1.58	10.00	0.04829	0.9695	0.4829
5	0.10	1.07	9.85	0.04832	0.9694	0.4832
6	0.10	1.90	10.00	0.04832	0.9694	0.4832
7	0.10	2.31	10.00	0.04836	0.9692	0.4836
8	0.10	2.51	10.00	0.04838	0.9691	0.4838
9	0.10	1.00	5.39	0.05060	0.9579	0.5056
10	0.10	1.00	4.10	0.05092	0.9563	0.5092