

FIGURE 2

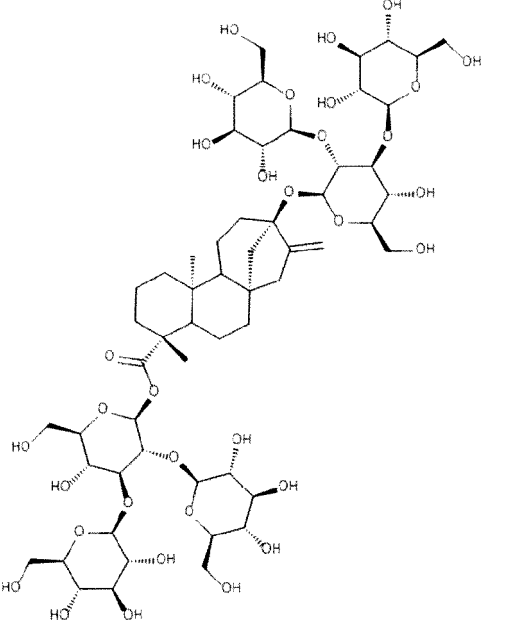
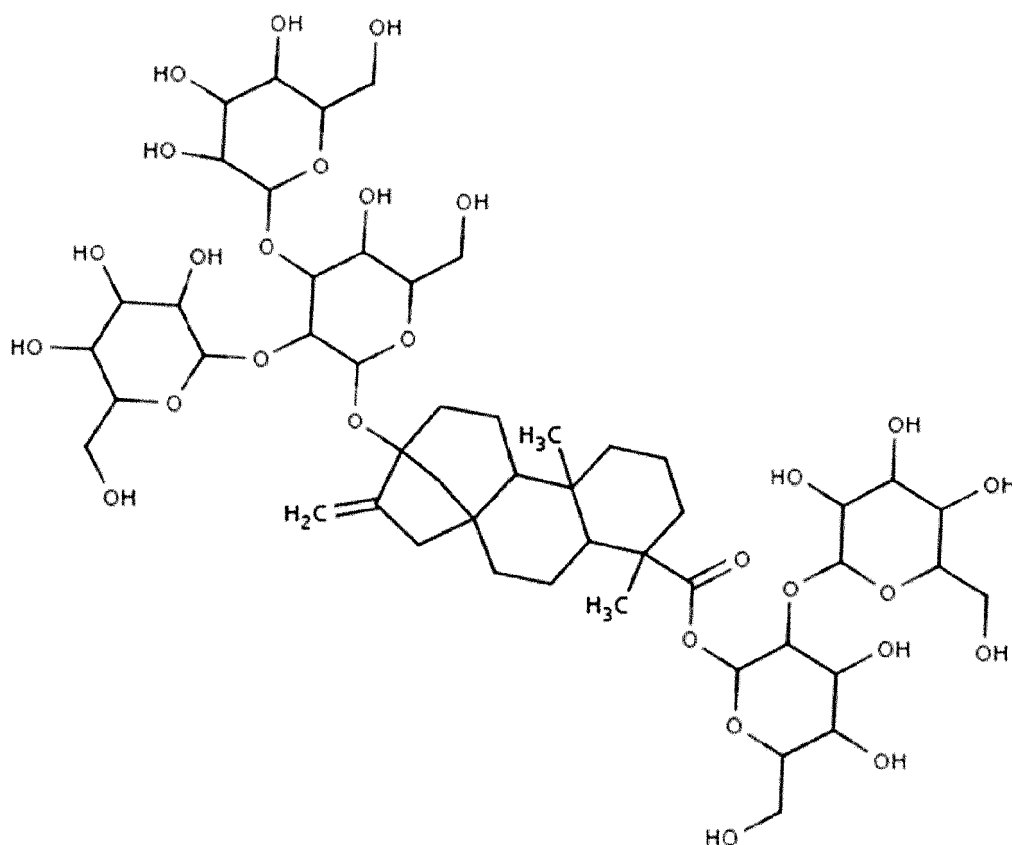
<i>Rebaudioside M</i>	Notation
	Glc-(1->2)Glc (1->3)Glc Glc-(1->2)Glc (1->3)Glc
ChemAxon IUPAC name from structure [JCIUPACName() function]: (2S,3R,4S,5R,6R)-5-hydroxy-6-(hydroxymethyl)-3,4-bis({[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy})oxan-2-yl(1R,5R,9S,13R)-13-{[(2S,3R,4S,5R,6R)-5-hydroxy-6-(hydroxymethyl)-3,4-bis({[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy})oxan-2-yl]oxy}-5,9-dimethyl-14-methylidenetetracyclo[11.2.1.0^{1,10}.0^{4,9}]hexadecane-5-carboxylate	
CambridgeSoft name from structure [CFW_CHEMICAL_NAME() function]: (4R,6aR,9S,11bS)-(3R,4S,5R,6R)-5-hydroxy-6-(hydroxymethyl)-3-(((2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-yl)oxy)-4-(((3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-yl)oxy)tetrahydro-2H-pyran-2-yl 9-(((3R,4S,5R,6R)-5-hydroxy-6-(hydroxymethyl)-3,4-bis(((3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-yl)oxy)tetrahydro-2H-pyran-2-yl)oxy)-4,11b-dimethyl-8-methylenetetradecahydro-6a,9-methanocyclohepta[a]naphthalene-4-carboxylate	

FIGURE 3

**Rebaudioside D:**

IUPAC Name: 4,5-dihydroxy-6-(hydroxymethyl)-3-[[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy]oxan-2-yl 13-[[5-hydroxy-6-(hydroxymethyl)-3,4-bis({[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy})oxan-2-yl]oxy]-5,9-dimethyl-14-methylidenetetracyclo[11.2.1.0^{1,10}.0^{4,9}]hexadecane-5-carboxylate

Synonym: (4 α)-13-[(O- β -D-Glucopyranosyl-(1 $\rightarrow$ 2)-O-[β -D-glucopyranosyl-(1 $\rightarrow$ 3)]- β -D-glucopyranosyl)oxy]kaur-16-en-18-oic acid 2-O- β -D-glucopyranosyl- β -D-glucopyranosyl ester

Empirical Formula (Hill Notation) C₅₀H₈₀O₂₈
Average Molecular Weight 1129.15

FIGURE 4

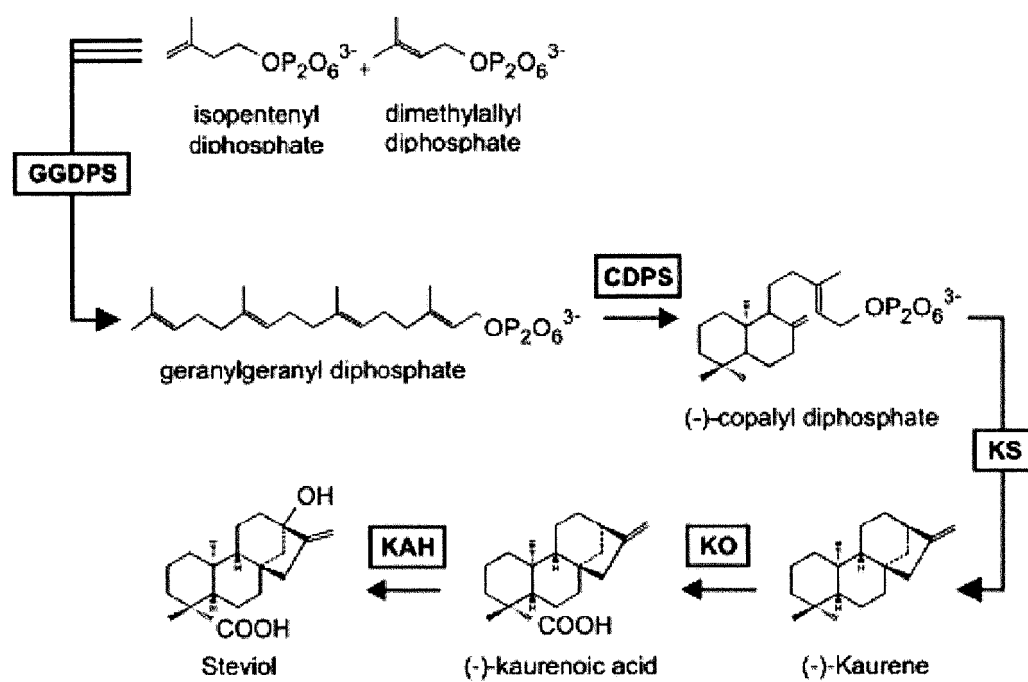


FIGURE 5

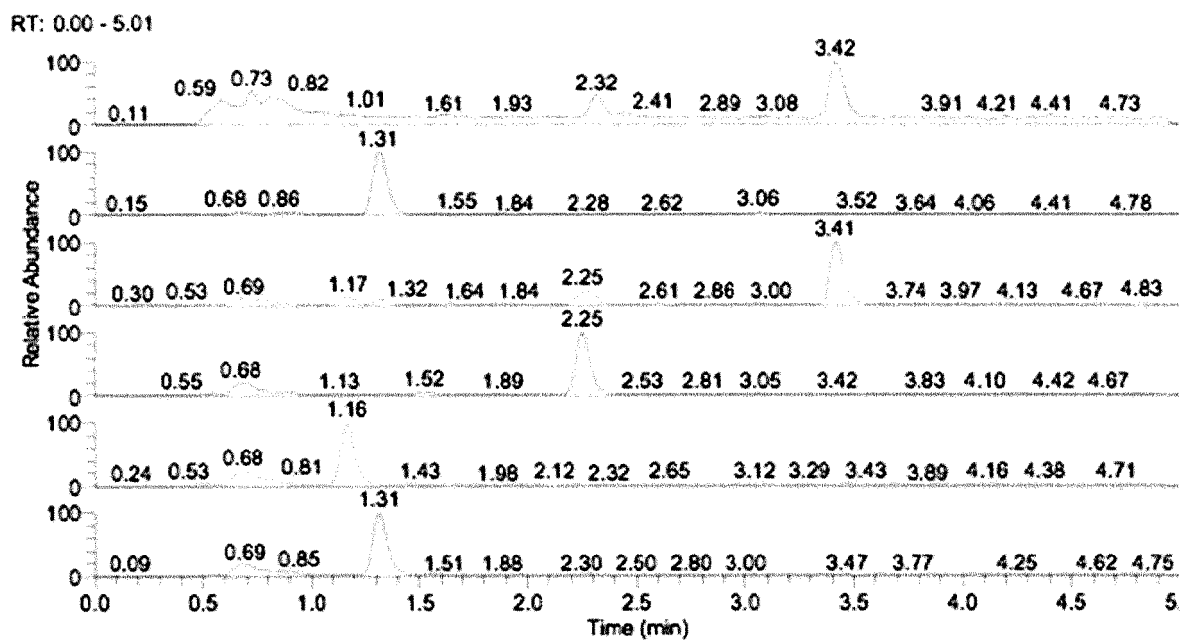


FIGURE 6

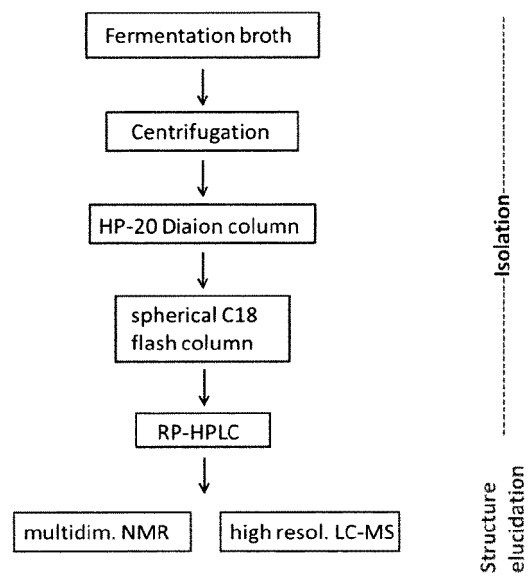
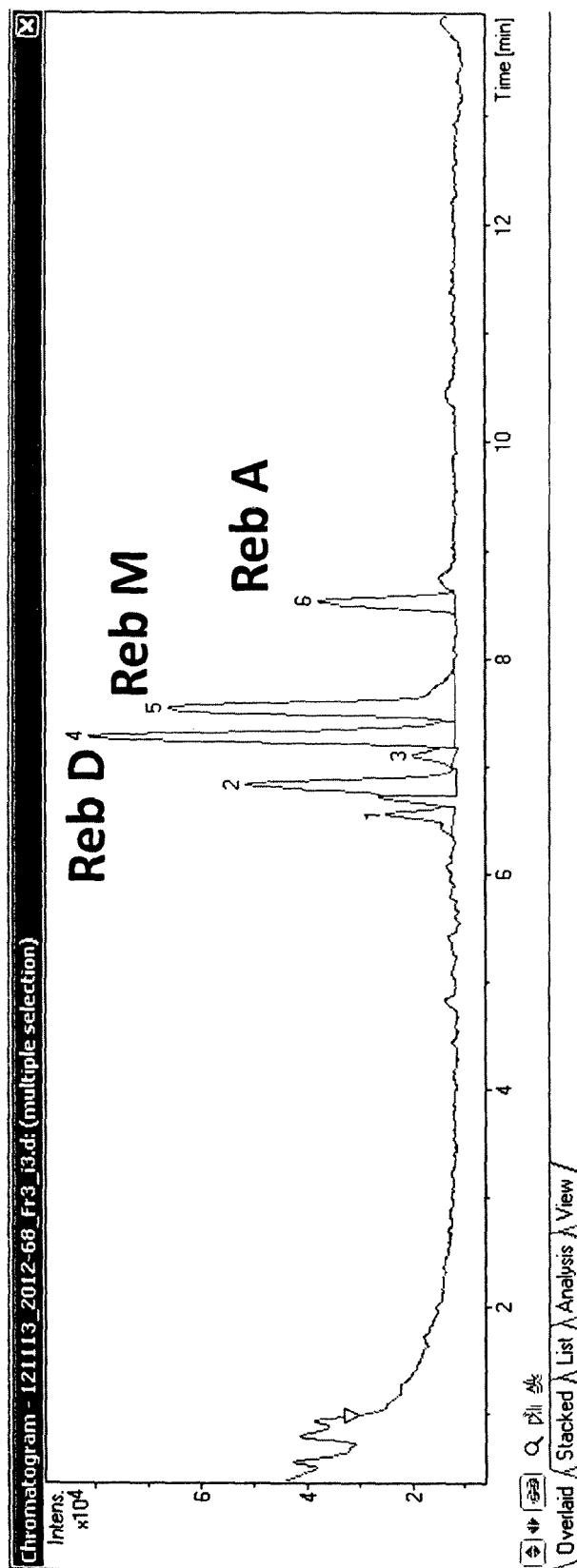


FIGURE 7A



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FIGURE 7B

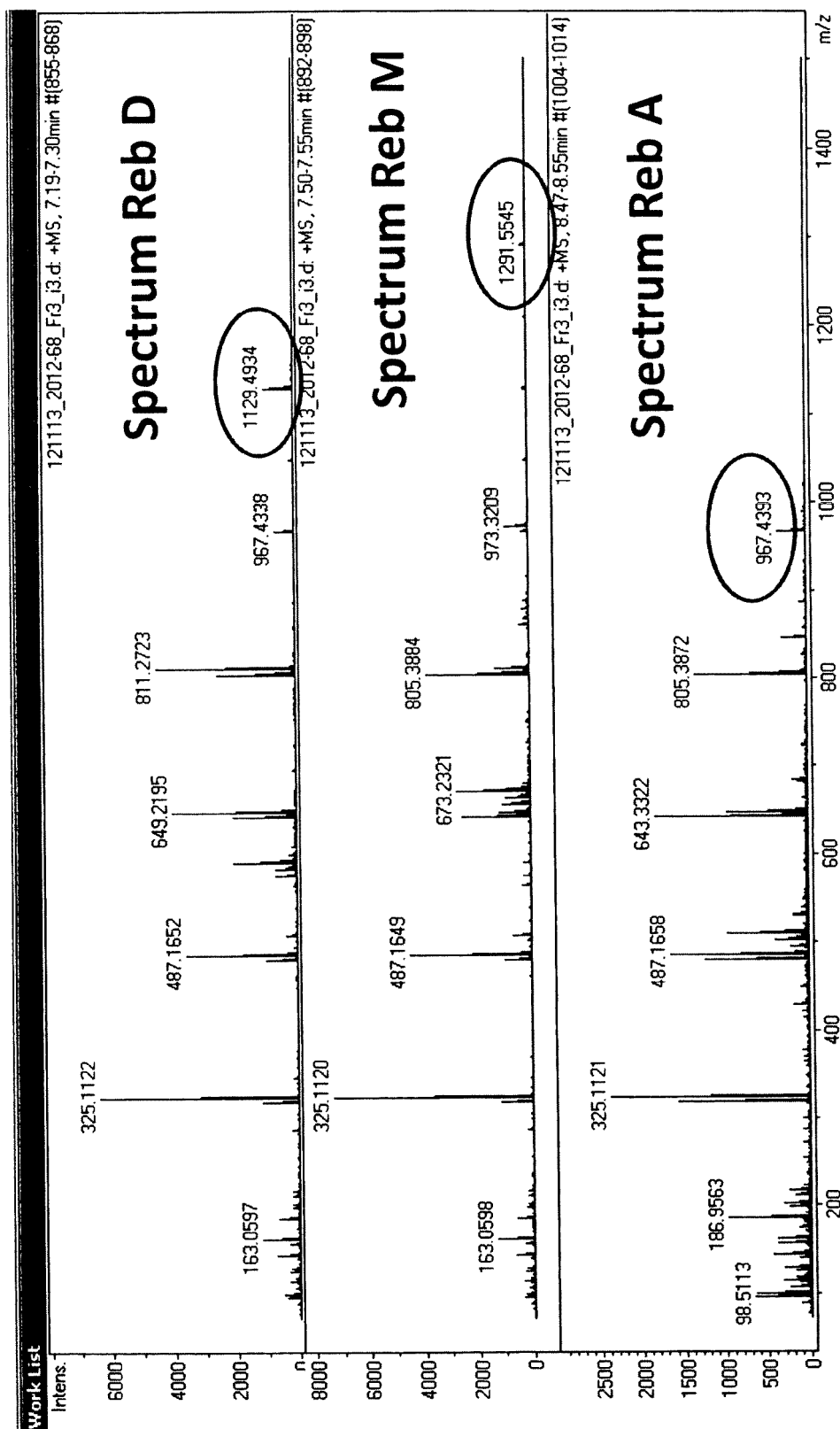


FIGURE 8

FIGURE 8A

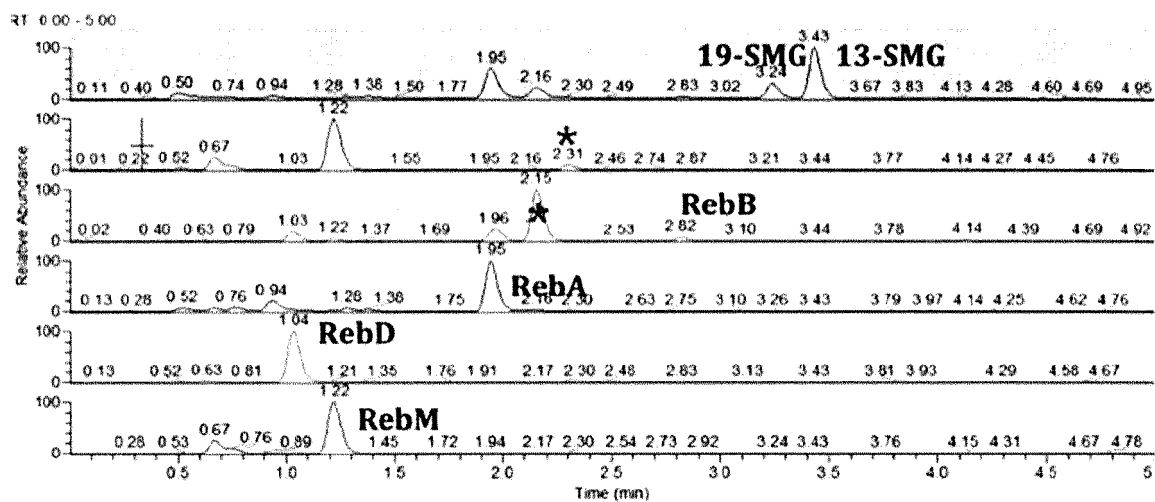


FIGURE 8B

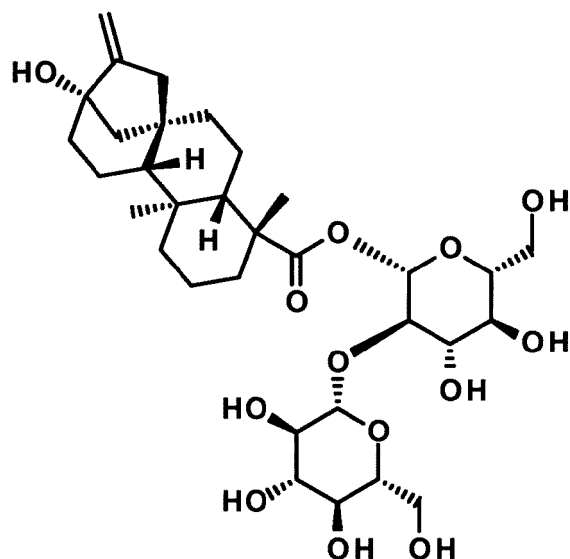


Figure 8C

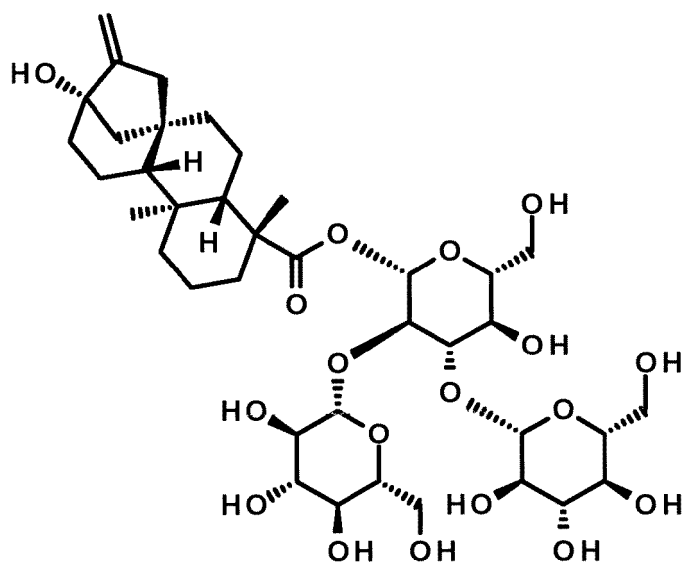


FIGURE 9

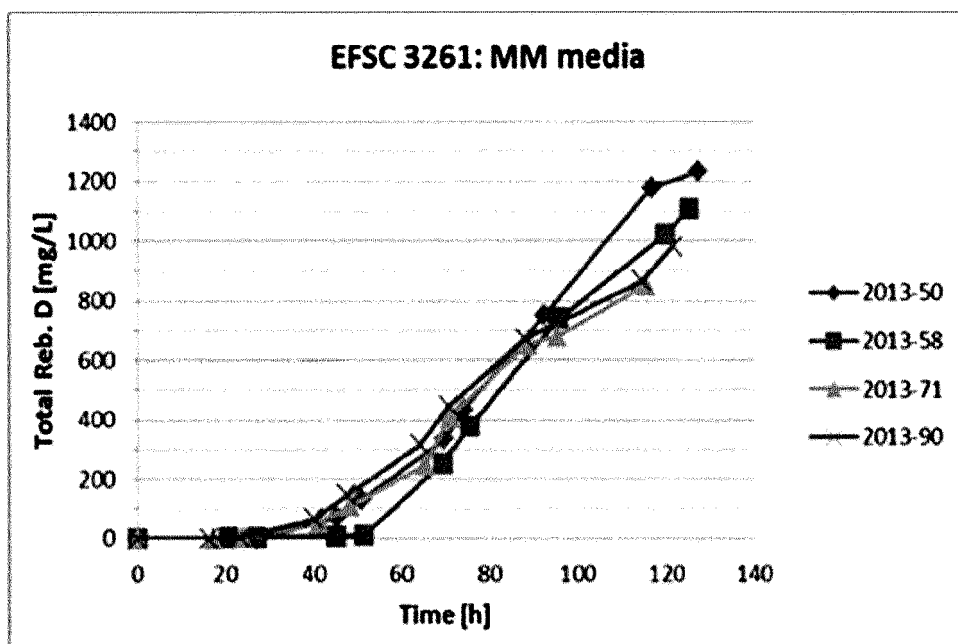


FIGURE 10

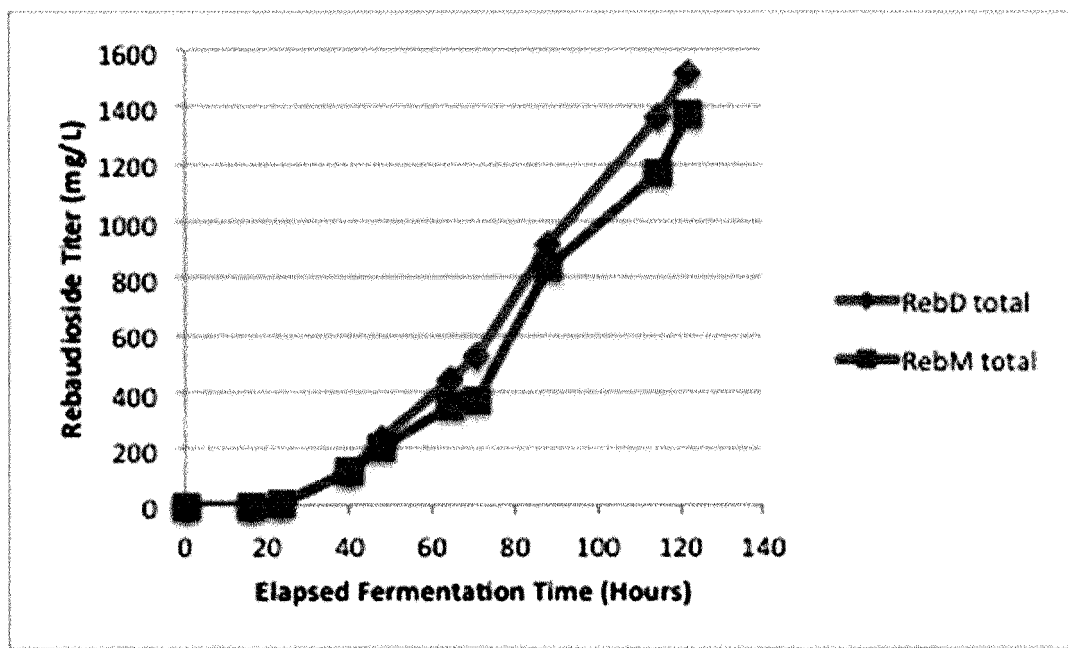


FIGURE 11

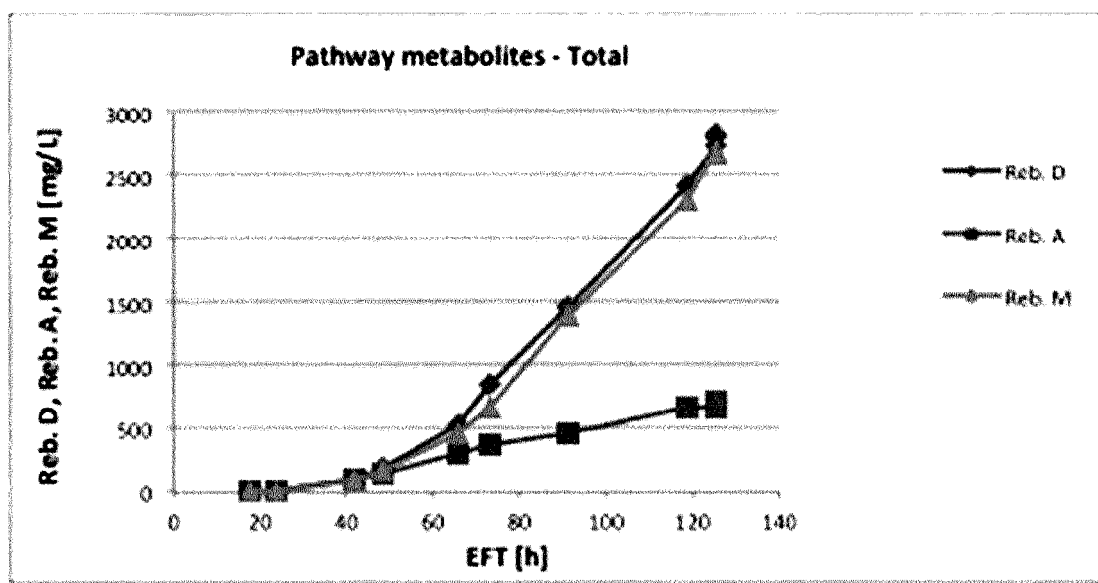


FIGURE 12

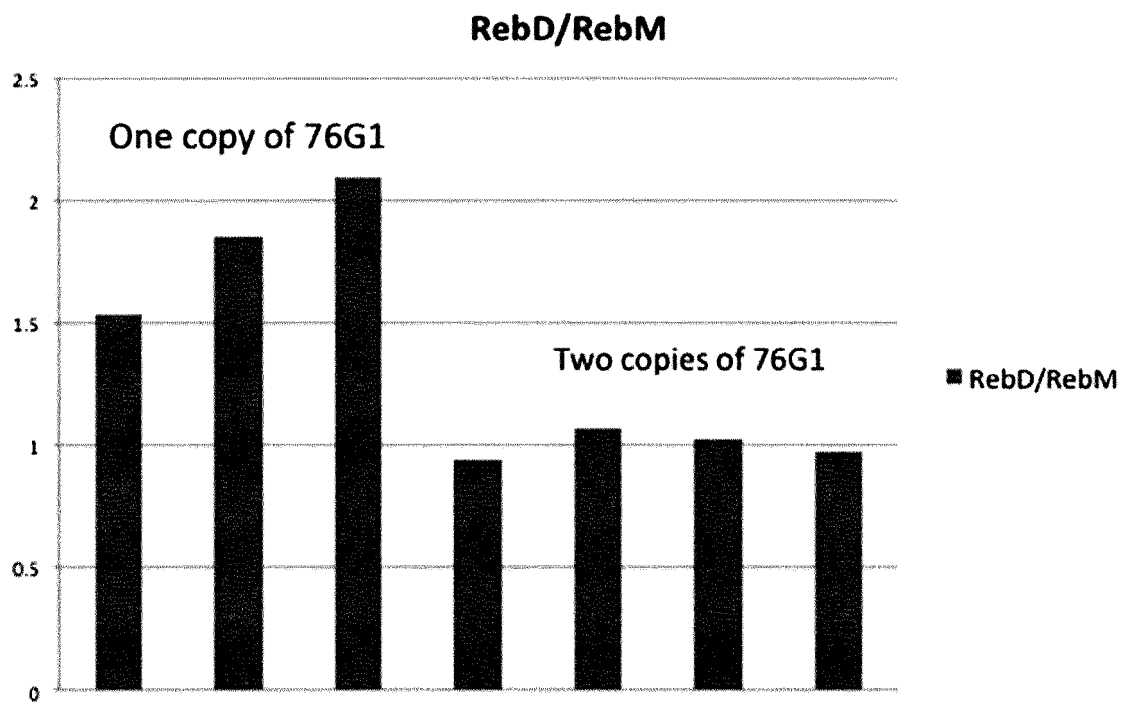


FIGURE 13

FIGURE 13A

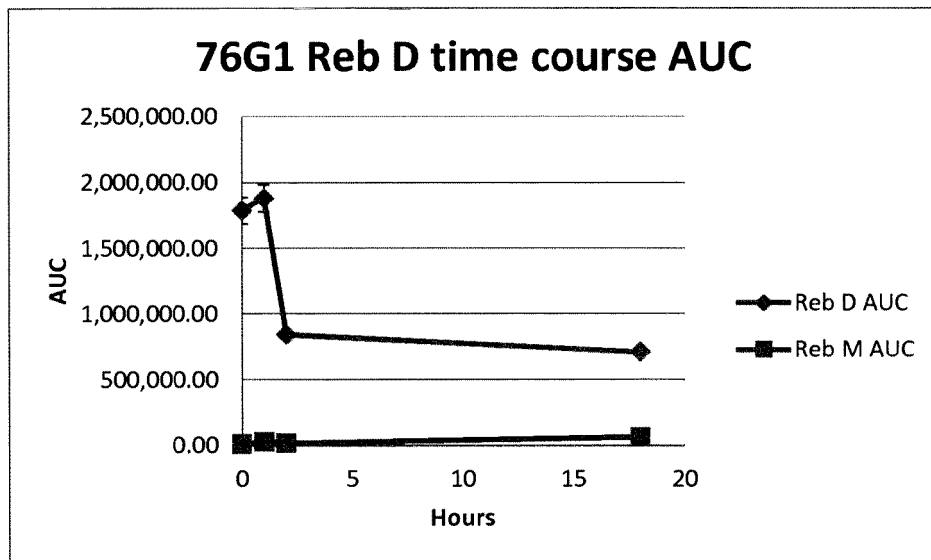


FIGURE 13B

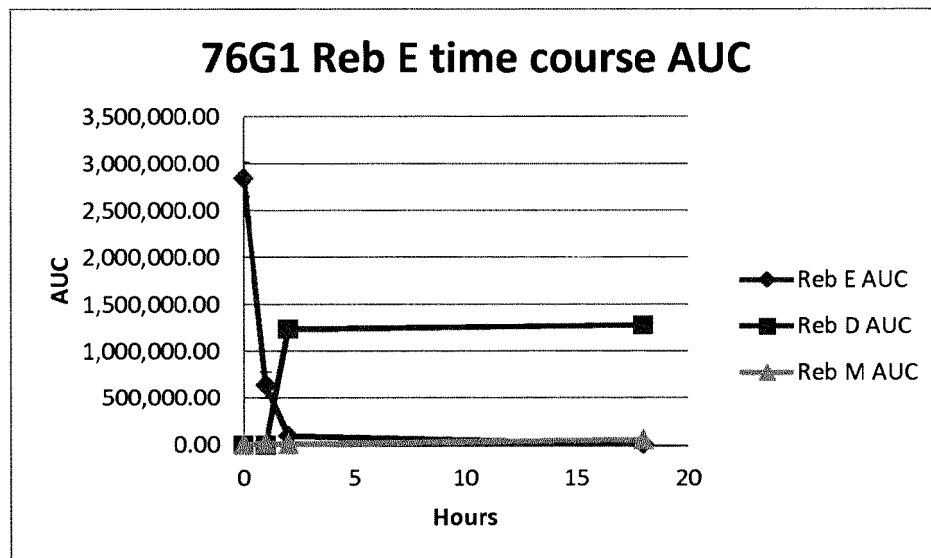


FIGURE 14

	1	11	21	31	41
76G1_1	--IILFPVPFQGHINPILQLANVLYSKGFSITIFHTFNKPKTSNYPHFT				
76G1_2	RRIILFPVPFQGHINPILQLANVLYSKGFSITIFHTNFNPKPKTSNYPH				
76G1_3	RRIILFPVPFQGHINPILQLANVLYSKGFSITIFHTNFSNYP				
	51	61	71	81	91
76G1_1	FRFILDNDPQDERISNLPTHGP AGMRIPiINEHGAD LRRELELLMLAS				
76G1_2	FILDNDPQDERISNLPTHGPLAGMRIPiINEHGADLRRELELLMLAS				
76G1_3	FILDNDPQDERISNLPTHGPLAGMRIPiINE A L EELLELM				
	101	111	121	131	141
76G1_1	EEDDEEVSLITDALWYFAQSV SLNLRRLVLMTSSLFNFHAHVSLPQFD				
76G1_2	EEDDEEVSLITD L NLRRLVLMTSSLFNFHAHVSLPQFD				
76G1_3	E EEVSLITDALWYFAQSVADS NLRRLVLMTSSLFNFHAHVSLPQFD				
	151	161	171	181	191
76G1_1	ELGYLD DKTRLEEQASGFPMK K AYS QI EILGKMIKQTK				
76G1_2	ELGYLDPD LEEQASGFPMKVKD SAYS WQILK LGKMIKQT				
76G1_3	ELGYLDPD T LEEQASGFP KVKDIKSA NWQ KEILGKMIKQTK				
	201	211	221	231	241
76G1_1	ASSGVIWNSFKELEEESELETVI APSFLIP PKHLTASSSSLLDHDR				
76G1_2	ASSGVIWNSFKELEEESELETVIREIPAPSFLI H TASSSSLLDHDR				
76G1_3	ASSGVIWNSFKELEEESELETVIREIPAPSFLI LP TASSSSL R				
	251	261	271	281	291
76G1_1	T F WLDQQPPSSVLVVSFGSTSEVDEKDFLEIARGLVDSKQSFLLWVVRP				
76G1_2	TV L QQQPPSSVLVVSFG T VDEKDFLEIARGLVDSKQSFLLWVVR				
76G1_3	T FQWLDQQPPSSVLVVSFGSTSEVDEKDFLEIARGLVDSKQSFLLWVVRP				
	301	311	321	331	341
76G1_1	G S WVEPL DGFLGERG IVKWVPQQEVLAH GAFWTHSGWNST				
76G1_2	FVKGS VEPLPD GE RIVKWVPQQEVLAHGAIGAFWTHSGWNST				
76G1_3	GF TWVEP PDG L ER RIVKWVPQQEVLAHGAIGAFWTHSGWNST				
	351	361	371	381	391
76G1_1	LESVCEGVPMIFSDFGLDQPLNARYMSDVLKV-----				
76G1_2	LESVCEGVPMIFSDFGLDQPLNARYMSDVLKVGVYLENGWERGEIANAIR				
76G1_3	LESVCEGVPMIFSDFGLDQPLNARYMSDVLKVGVYLENGWERGEIANAIR				

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	401	411	421	431	441
76G1_1	-----KSSYESLESLVSY--				
76G1_2	RVDEEGEYIRQNARVLKQKADVSLMKGSSYESLESLVSYIQL				
76G1_3	RVDEEGEYIRQNARVLKQKADVSLMKGSSYESLESLVSYQL				

<1 2 >4 Å variance between models

FIGURE 15

FIGURE 15A

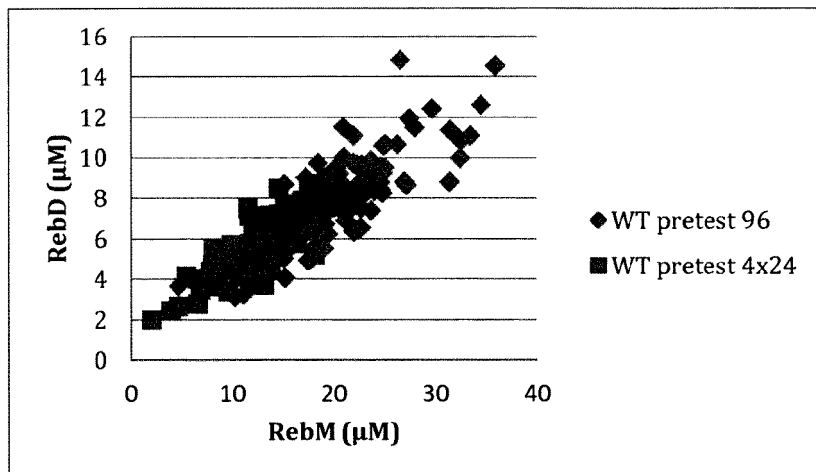


FIGURE 15B

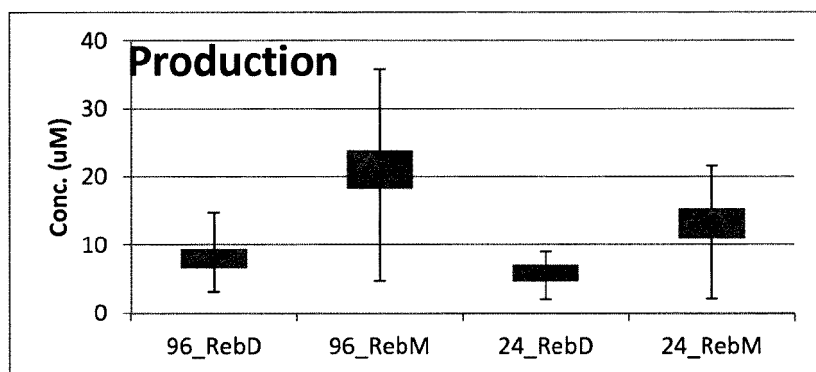


FIGURE 15C

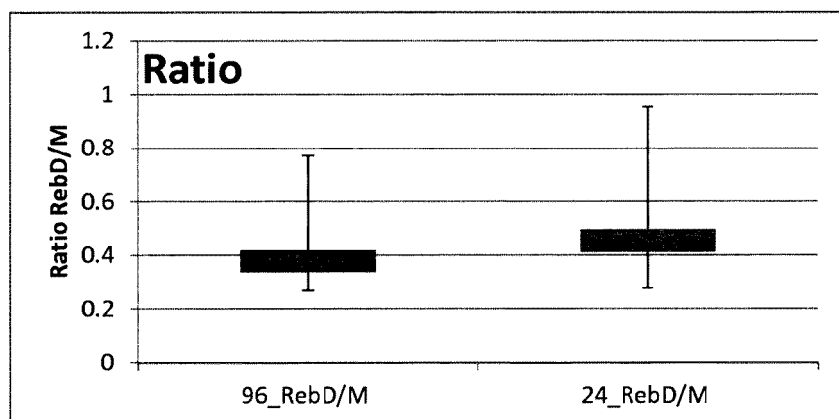


FIGURE 16

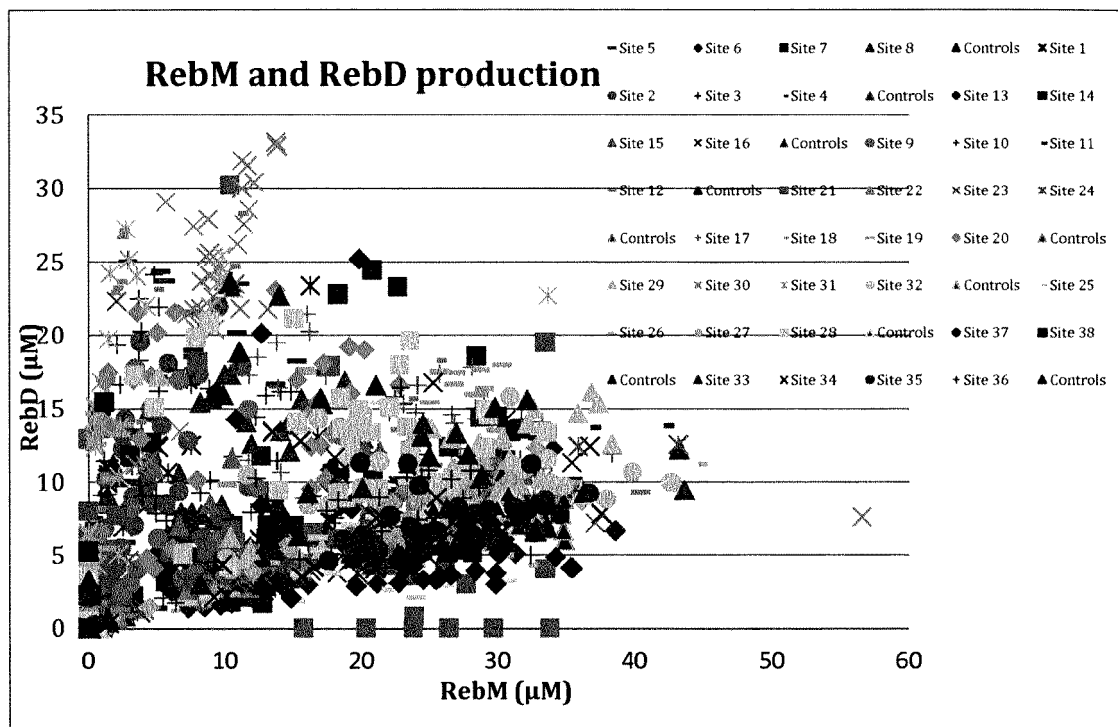


FIGURE 17

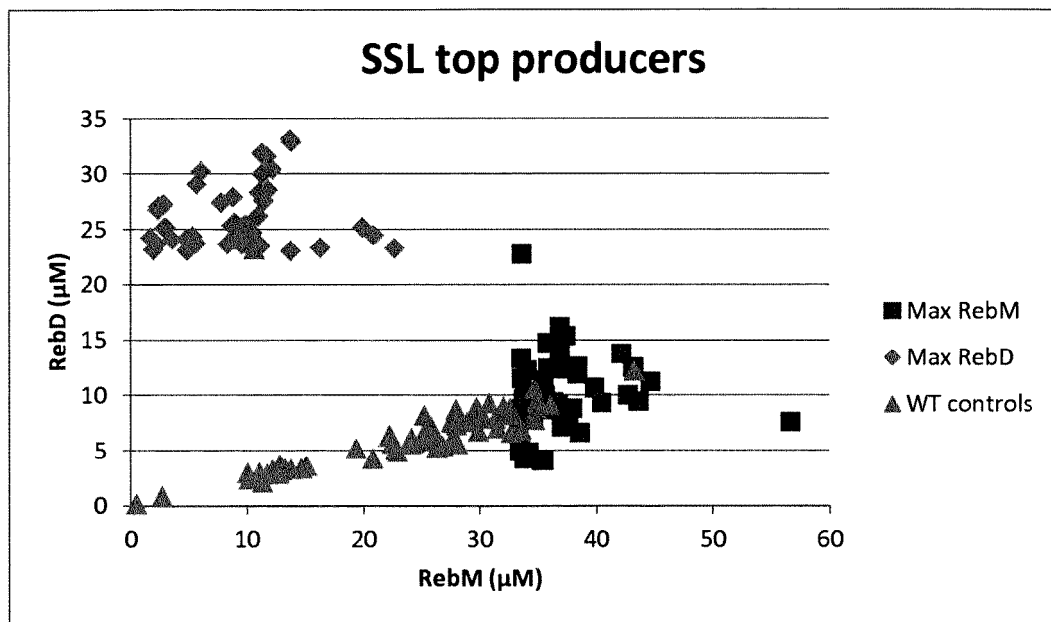


FIGURE 18

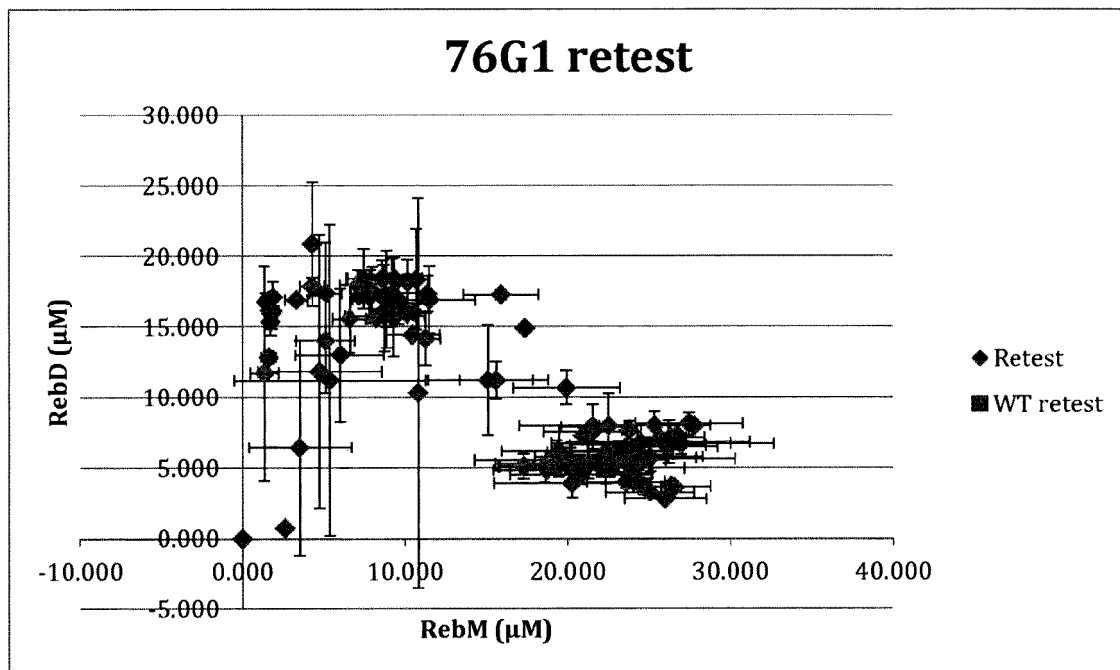


FIGURE 19

FIGURE 19A

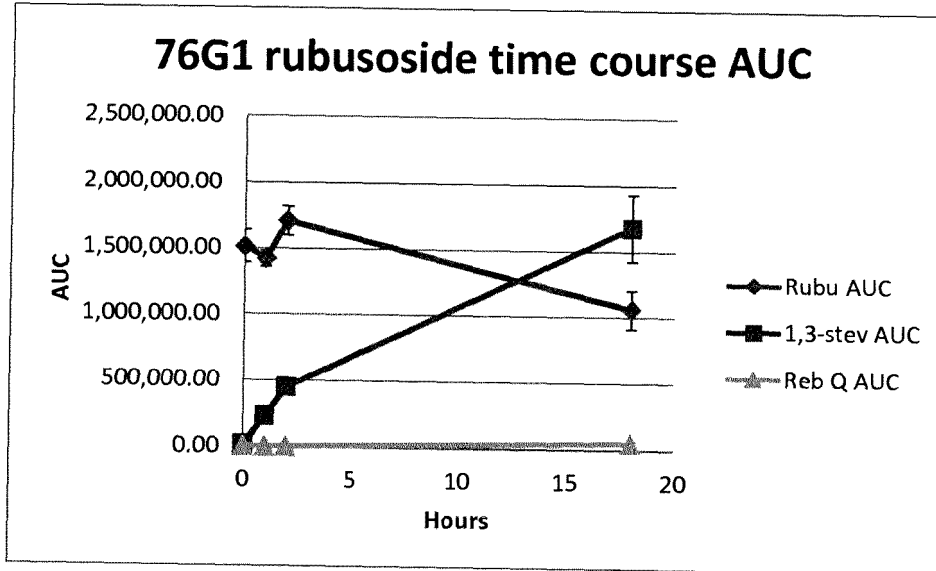


FIGURE 19B

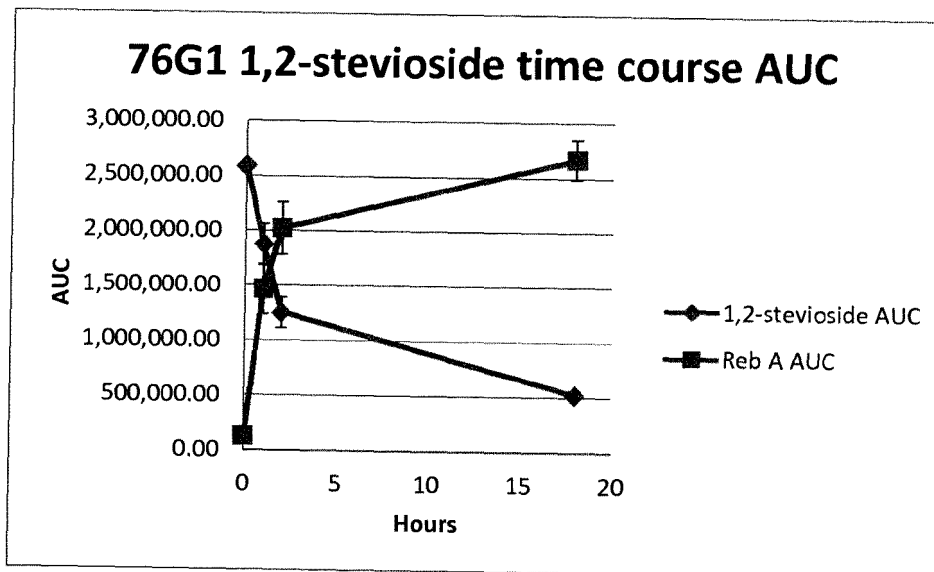


FIGURE 19C

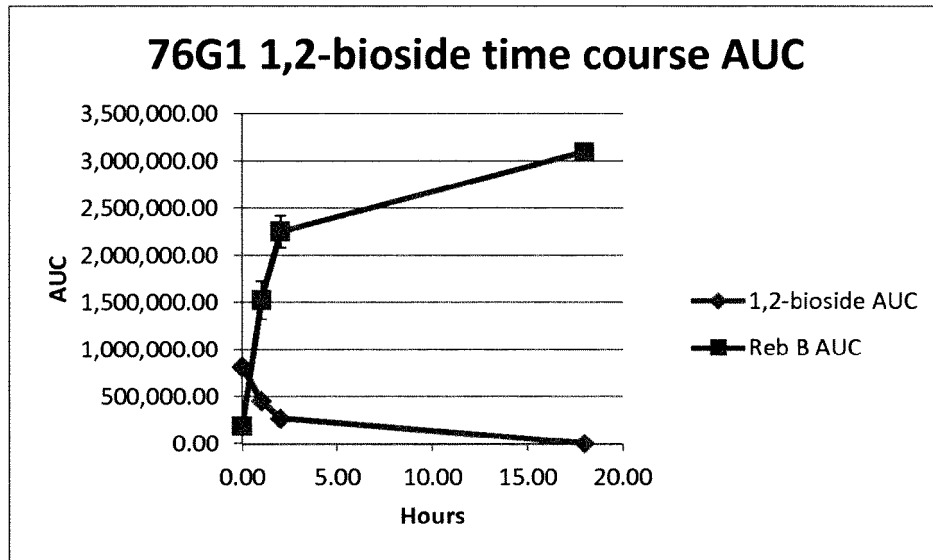


FIGURE 20

