

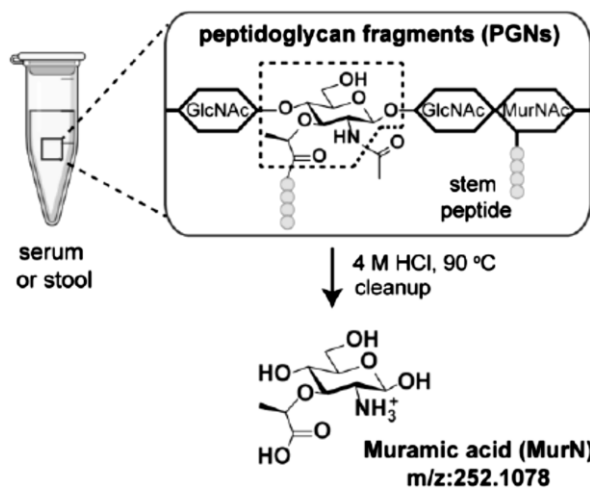


FIG. 1A

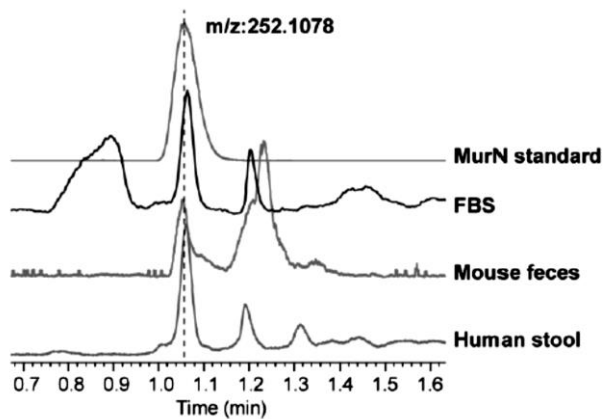


FIG. 1B

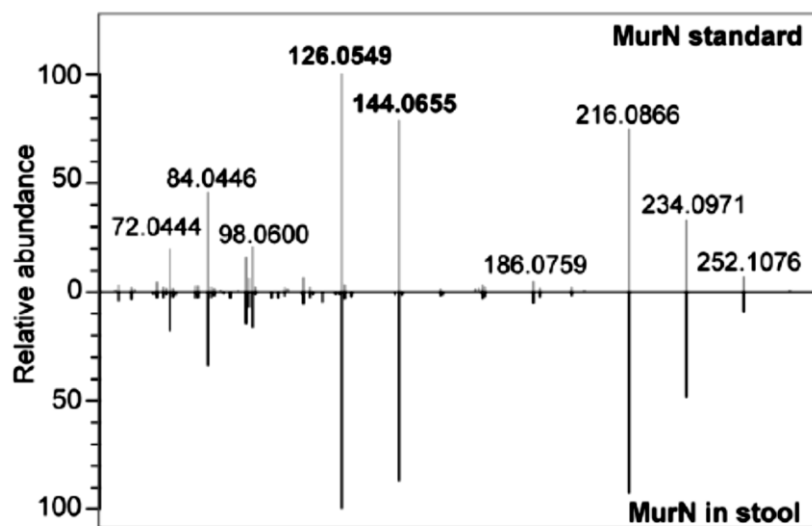


FIG. 1C

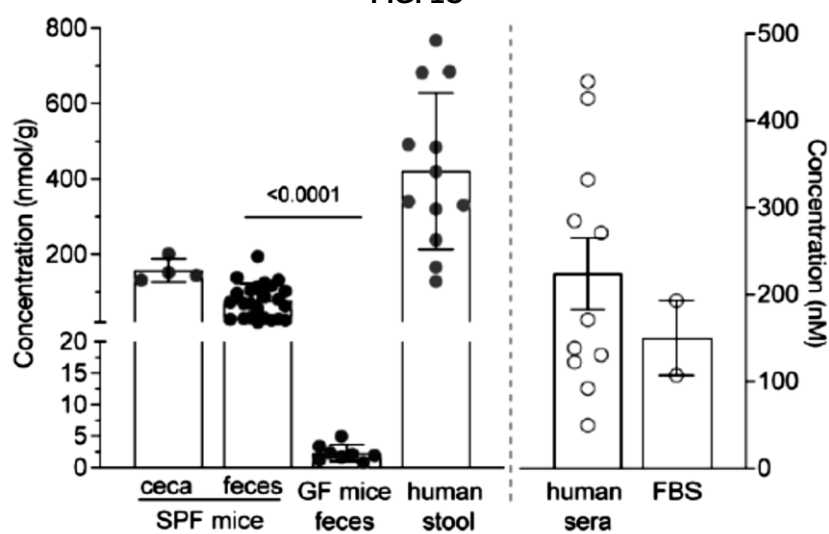


FIG. 1D

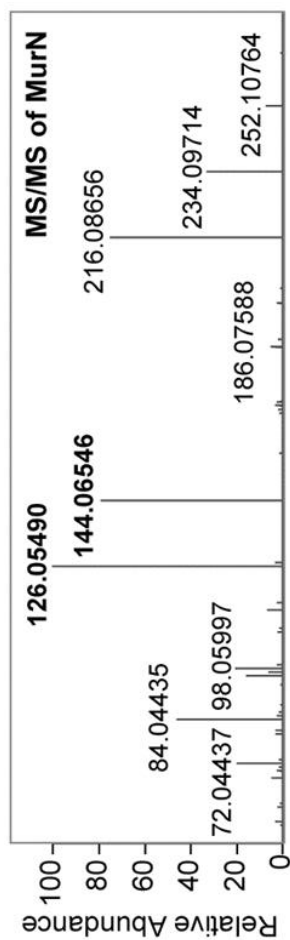
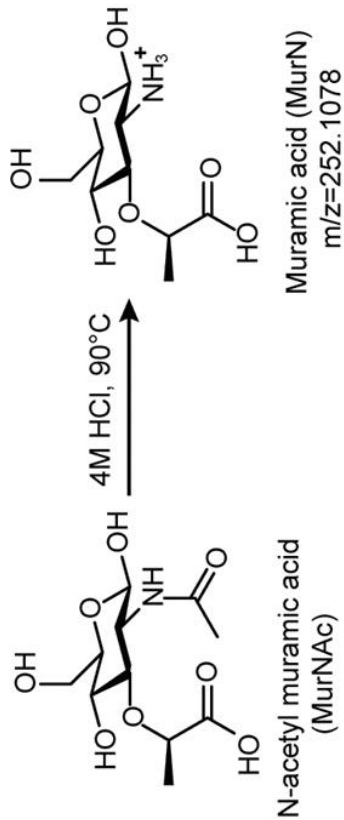
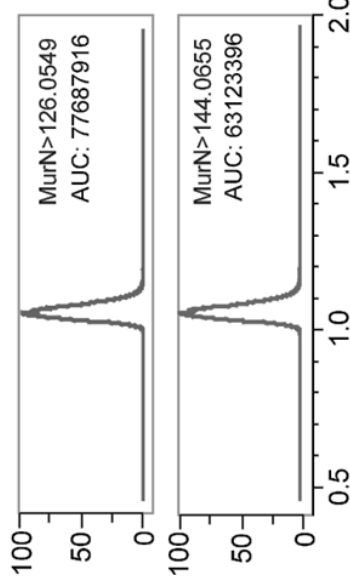


FIG. 2A

Area under curve (AUC) of MurN MS/MS peaks (126.0549 and 144.0655)



PRM mode (m/z : 252.1078)
EIC of 126.05490

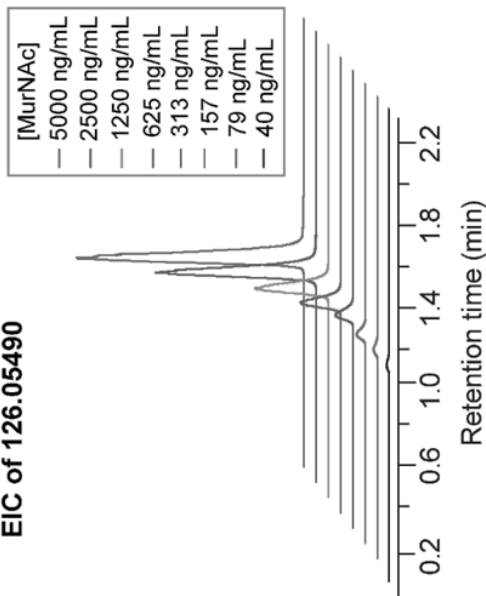
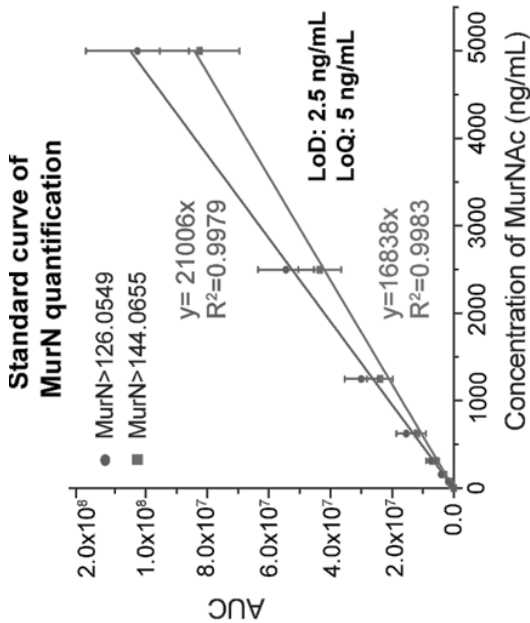


FIG. 2B



For evaluation of matrix effects of biological samples

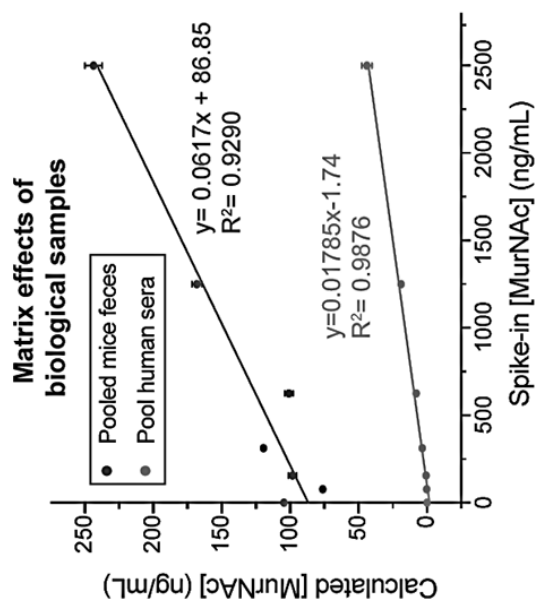
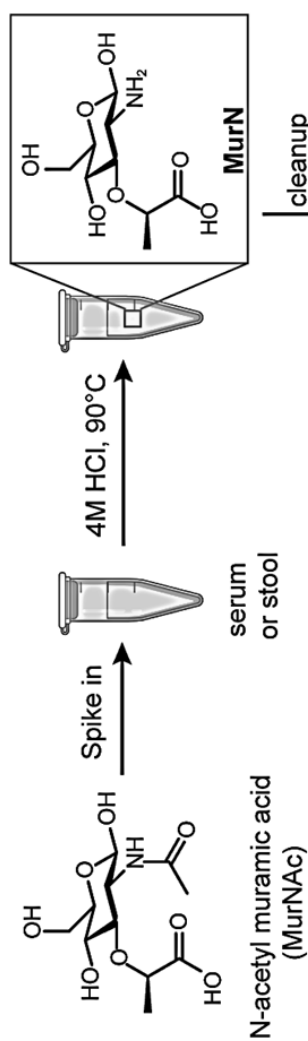


FIG. 2C

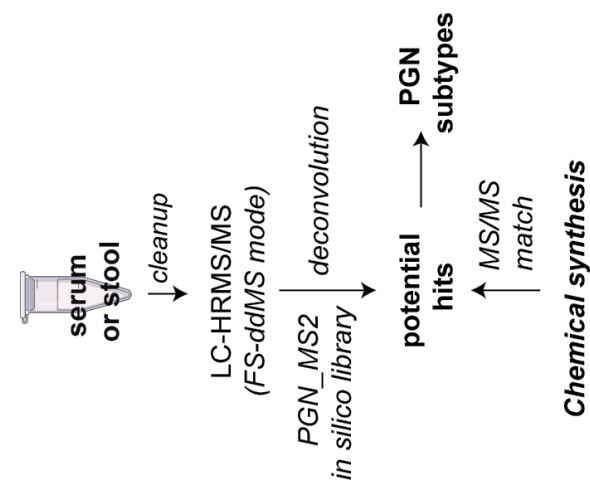


FIG. 3A

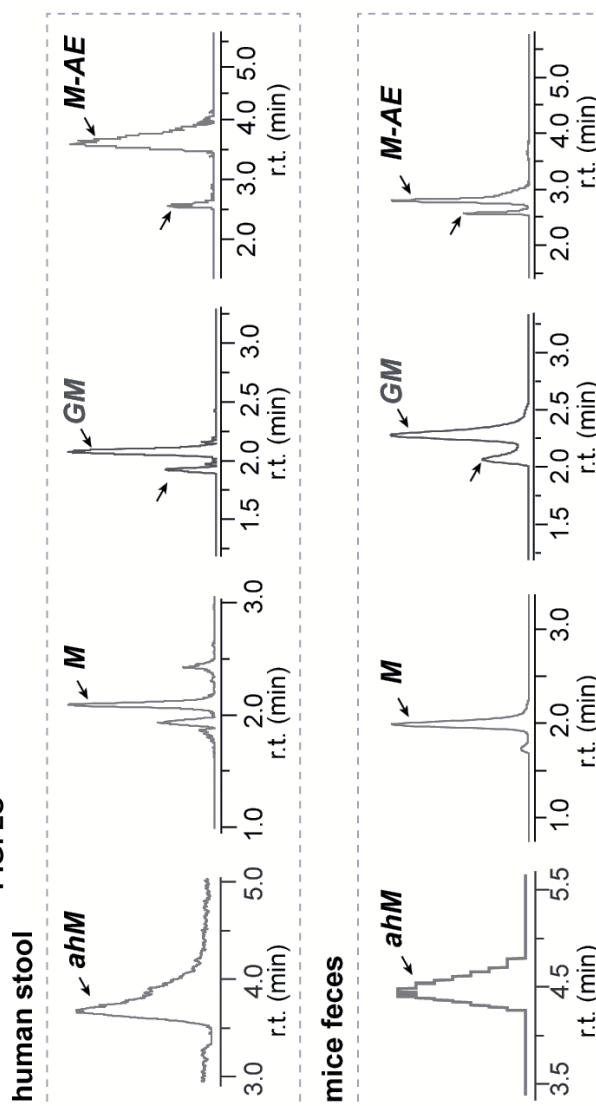


FIG. 3B

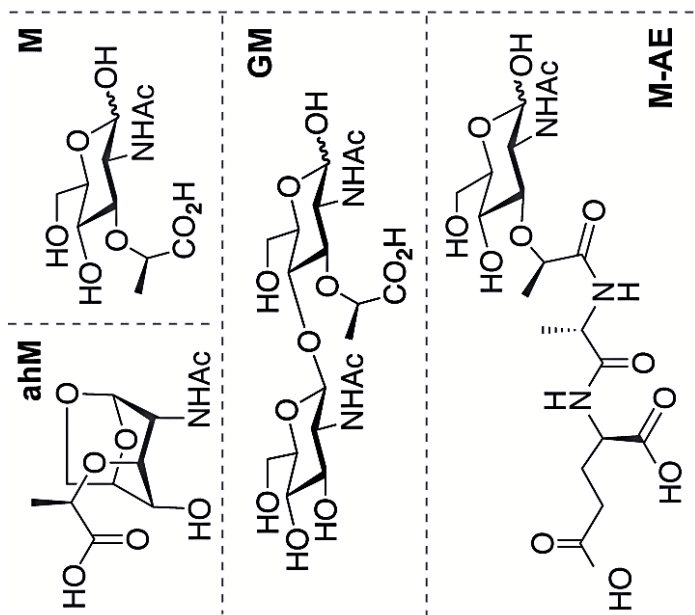


FIG. 3C

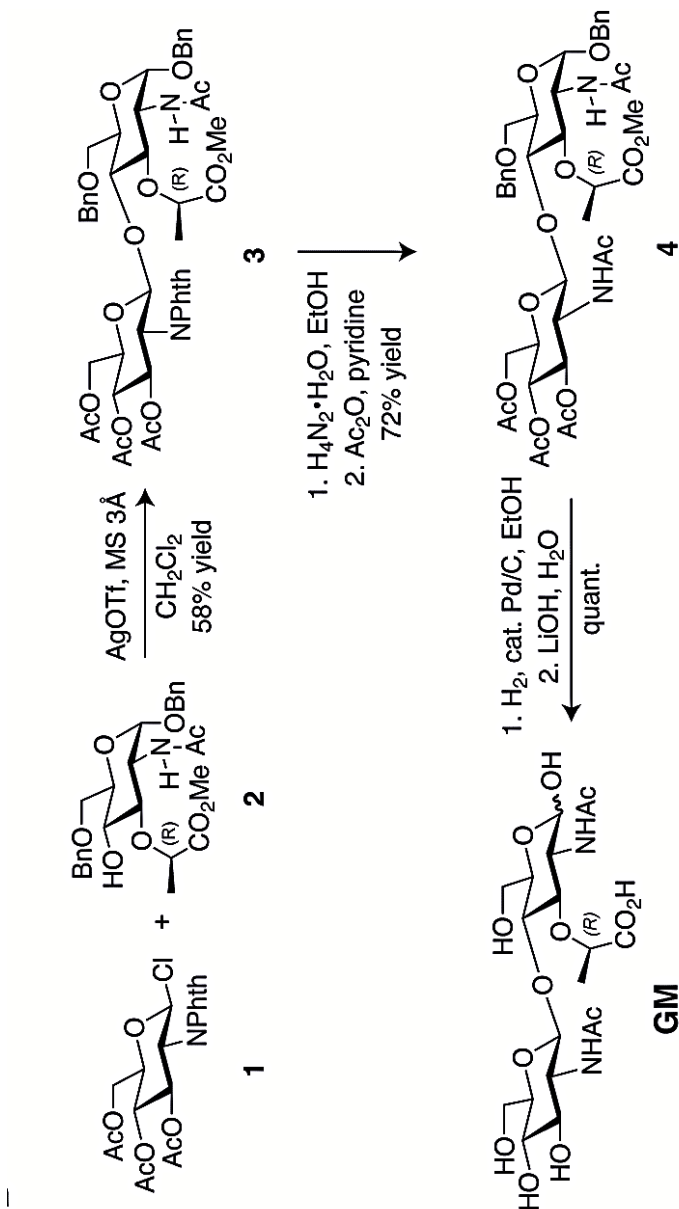


FIG. 3D

Sample	Compound	Formula	[M+H] ⁺ (Da)	Concentration (nmol/g)
Mice feces (steady-state)	GM	C ₁₉ H ₃₂ N ₂ O ₁₃	497.19772	2-10
	G-ahM	C ₁₉ H ₃₀ N ₂ O ₁₂	479.18715	1-3
	M	C ₁₁ H ₁₉ NO ₈	294.11834	6-40
	ahM	C ₁₁ H ₁₇ NO ₇	276.10778	2-15
	M-AE	C ₁₉ H ₃₁ N ₃ O ₁₂	494.19805	0.2-4
	ahM-AE	C ₁₉ H ₂₉ N ₃ O ₁₁	476.18749	0.2-3
	GM-AE	C ₂₇ H ₄₄ N ₄ O ₁₇	697.27742	n.d.-0.6
	GM-AEm	C ₃₄ H ₅₆ N ₆ O ₂₀	869.36221	n.d.-1
	M-AEmA	C ₂₉ H ₄₈ N ₆ O ₁₆	737.31996	n.d.-2
	GahM-AEmA	C ₃₇ H ₅₉ N ₇ O ₂₀	921.38149	n.d.-0.6
	M-AEmAA	C ₃₂ H ₅₃ N ₇ O ₁₇	808.35707	n.d.-2
	GM-AEmAA	C ₄₀ H ₆₆ N ₈ O ₂₂	1011.4364	n.d.-0.6
	G(DM)-AE	C ₂₈ H ₄₇ N ₅ O ₁₇	738.30397	n.d.-2
	(DG)M-AE	C ₂₉ H ₄₇ N ₅ O ₁₇	738.30397	n.d.-3
	(DG)M-AEm	C ₃₆ H ₅₈ N ₆ O ₂₁	911.37278	n.d.-2
	M-A	C ₁₄ H ₂₄ N ₂ O ₉	365.15555	n.d.-0.6
Human stool (healthy)	GM	C ₁₉ H ₃₂ N ₂ O ₁₃	497.19772	1-15
	M	C ₁₁ H ₁₉ NO ₈	294.11834	10-400
	ahM	C ₁₁ H ₁₇ NO ₇	276.10778	5-300
	M-AE	C ₁₉ H ₃₁ N ₃ O ₁₂	494.19805	n.d.-500
	ahM-AE	C ₁₉ H ₂₉ N ₃ O ₁₁	476.18749	n.d.-180
	GM-AE	C ₂₇ H ₄₄ N ₄ O ₁₇	697.27742	n.d.-60
	M-AEmA	C ₂₉ H ₄₈ N ₆ O ₁₆	737.31996	n.d.-500
	ahM-AEmA	C ₂₉ H ₄₆ N ₆ O ₁₅	719.30939	n.d.-70
	M-AEmAA	C ₃₂ H ₅₃ N ₇ O ₁₇	808.35707	n.d.-120

FIG. 4A

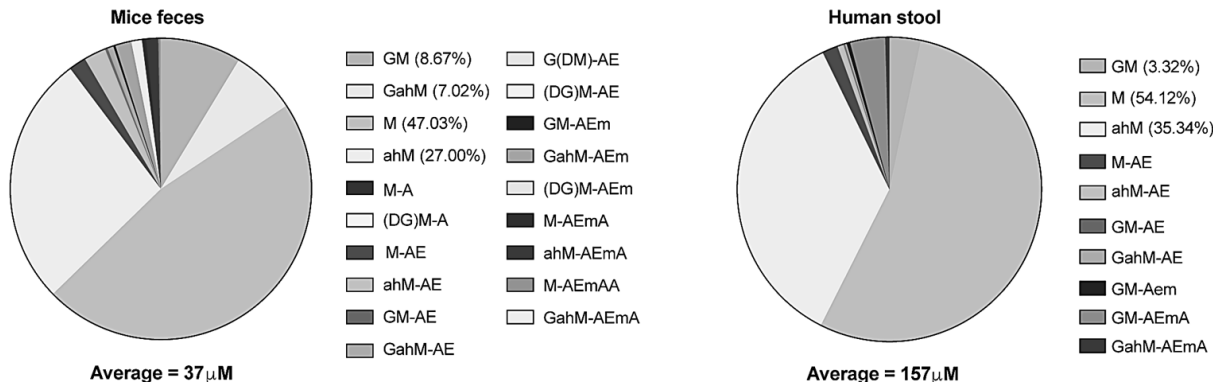


FIG. 4B

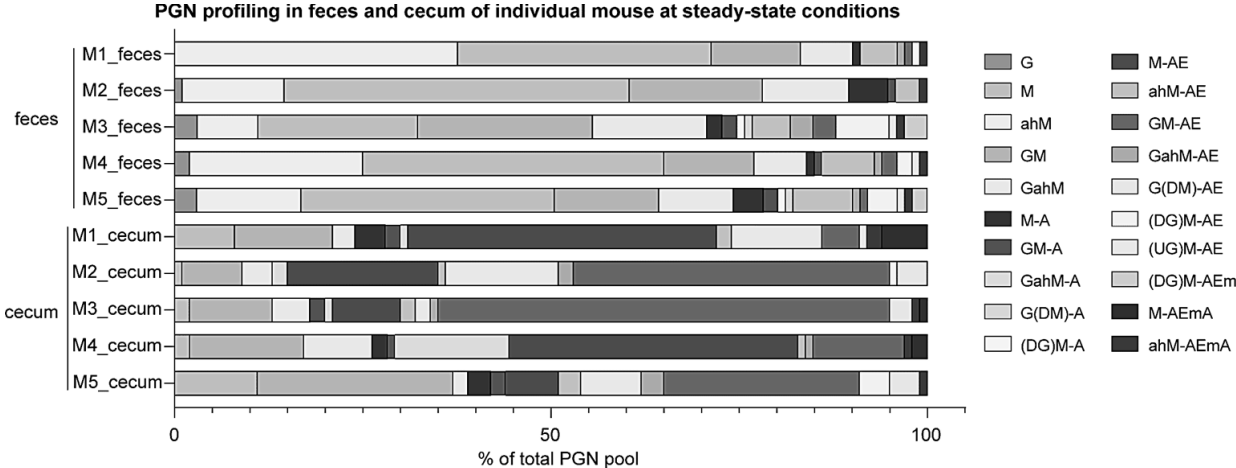


FIG. 4C

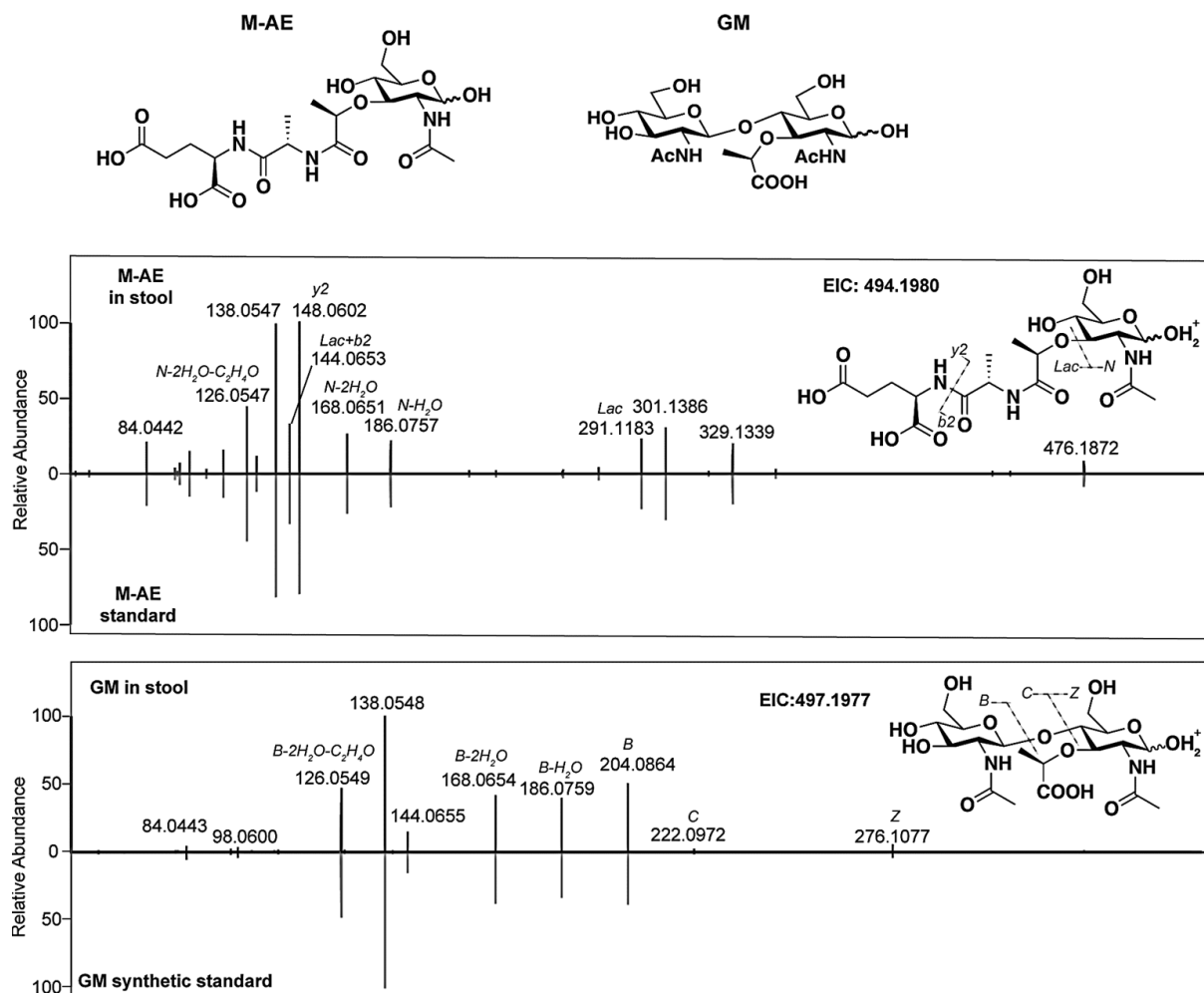


FIG. 5A

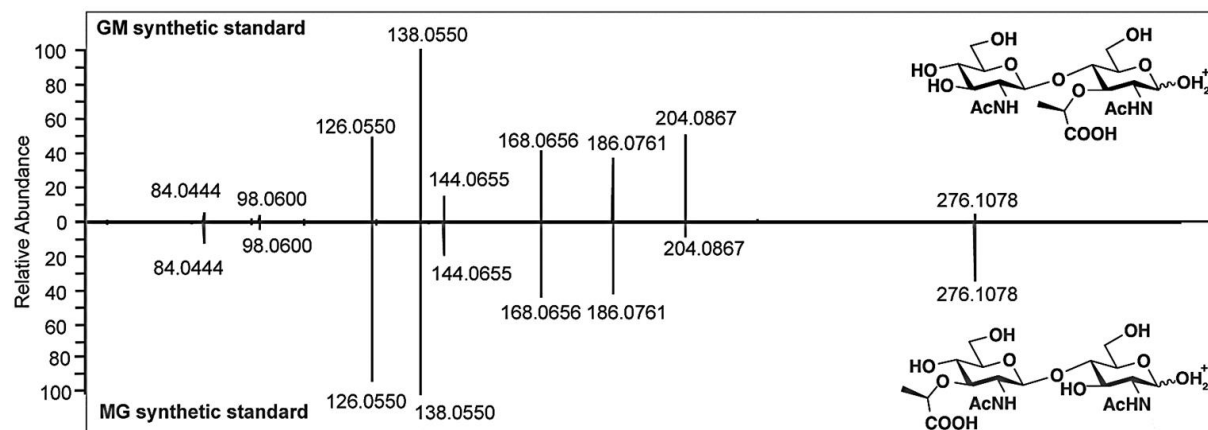
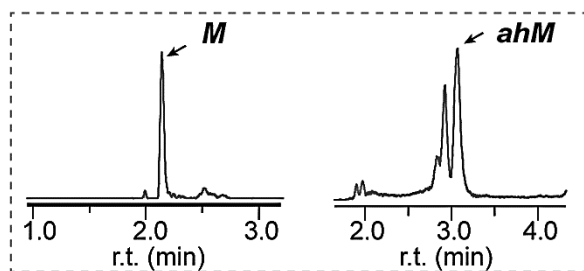


FIG. 5B

human serum



FBS

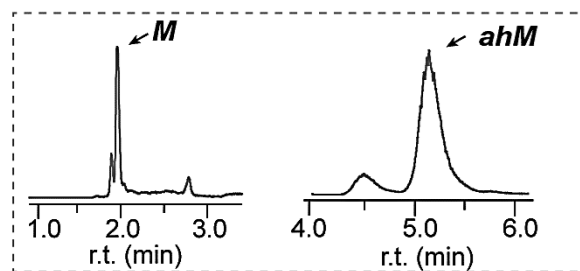


FIG. 6A

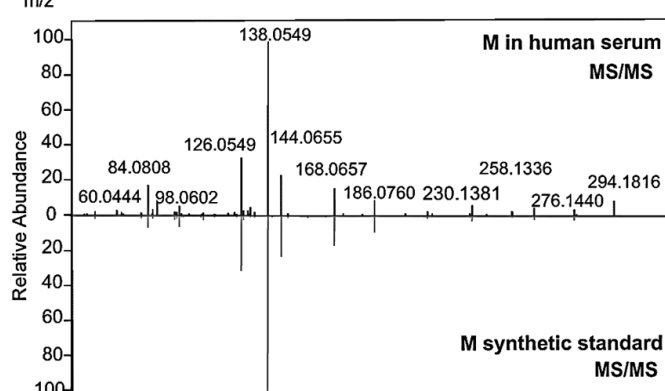
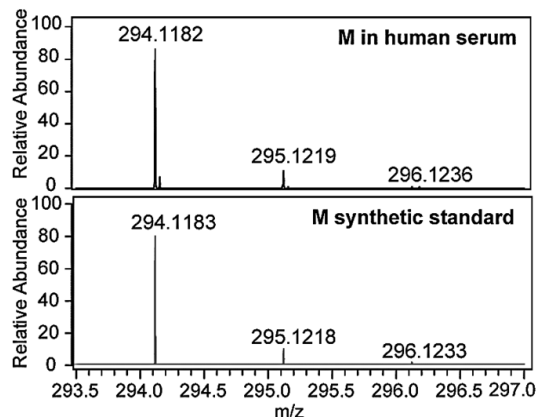
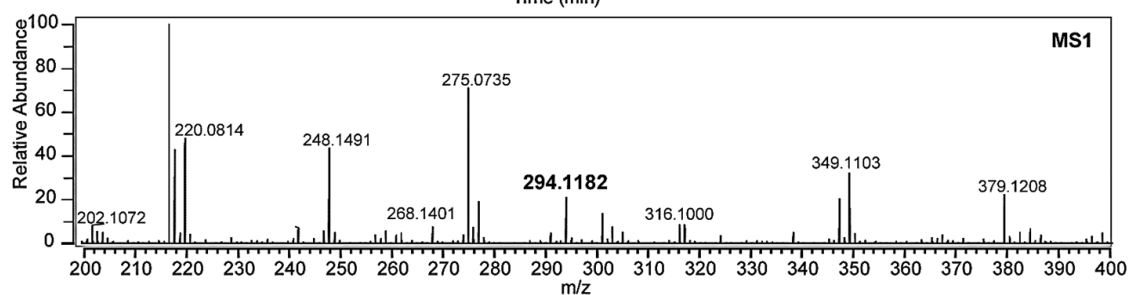
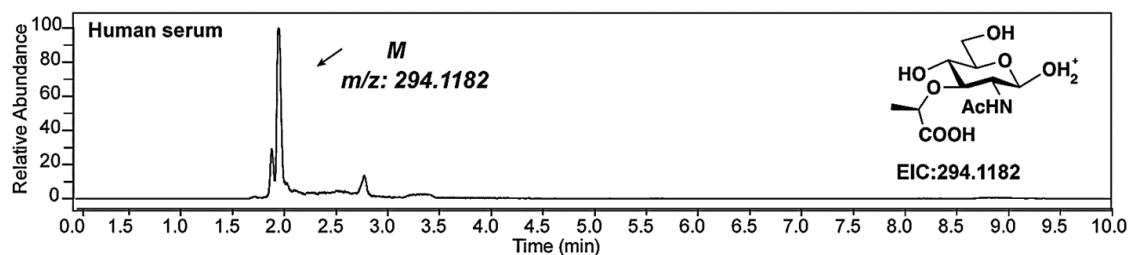


FIG. 6B

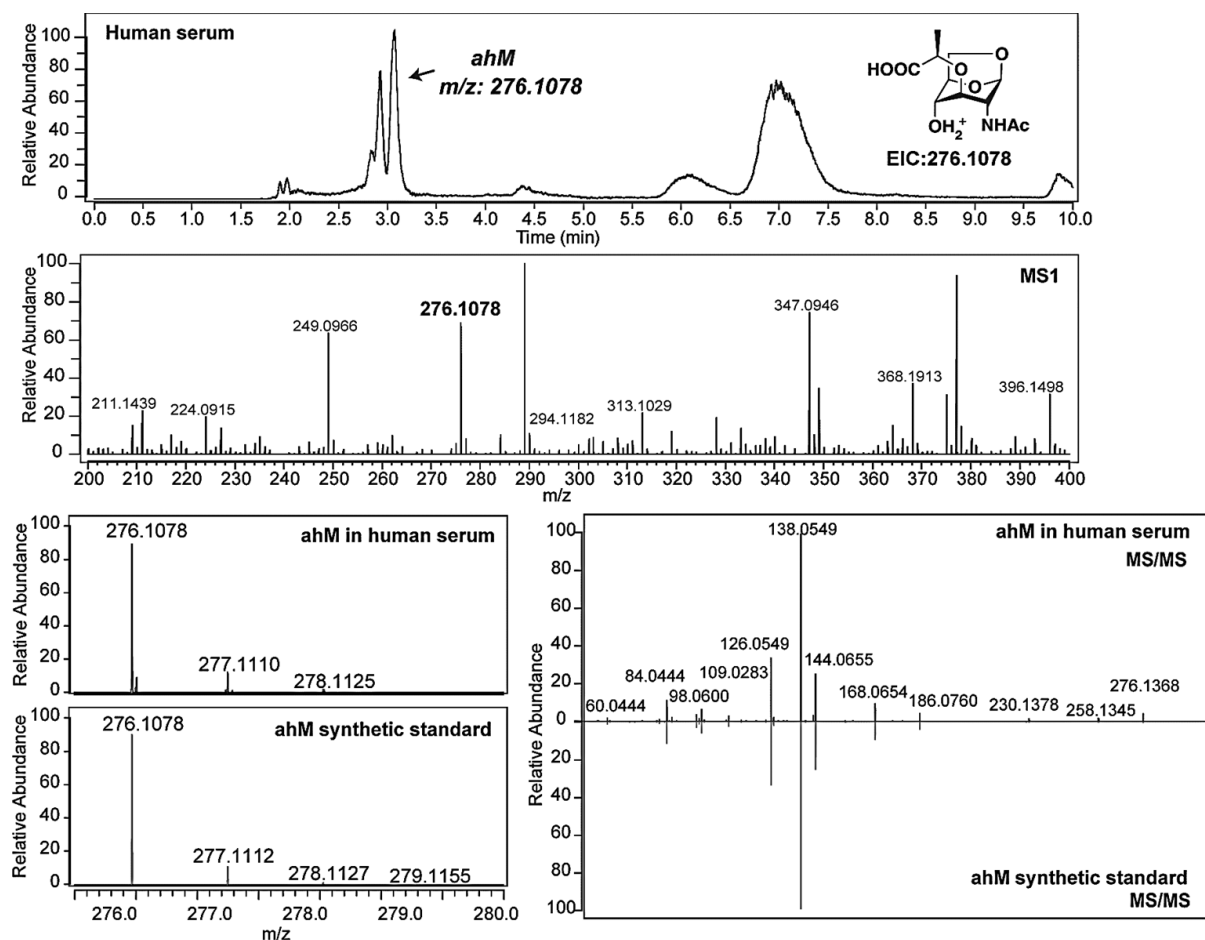


FIG. 6C

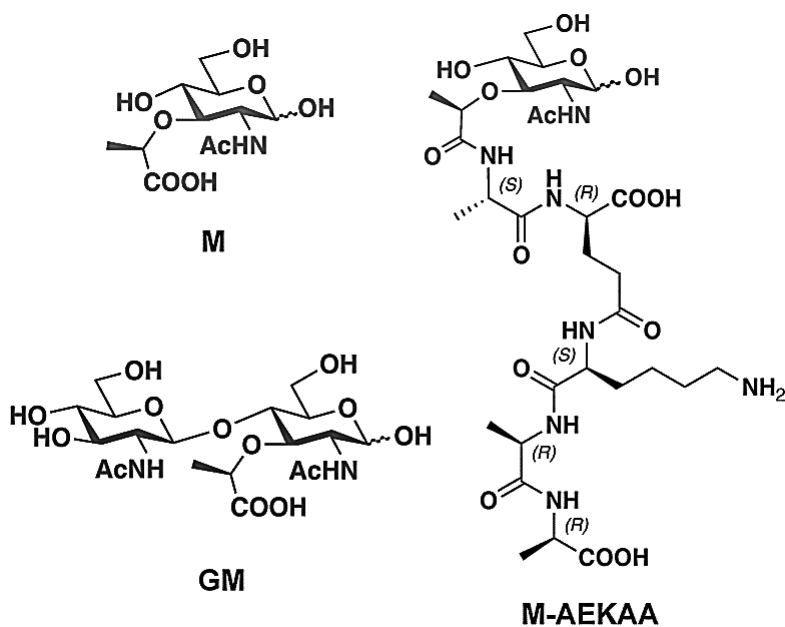


FIG. 7A

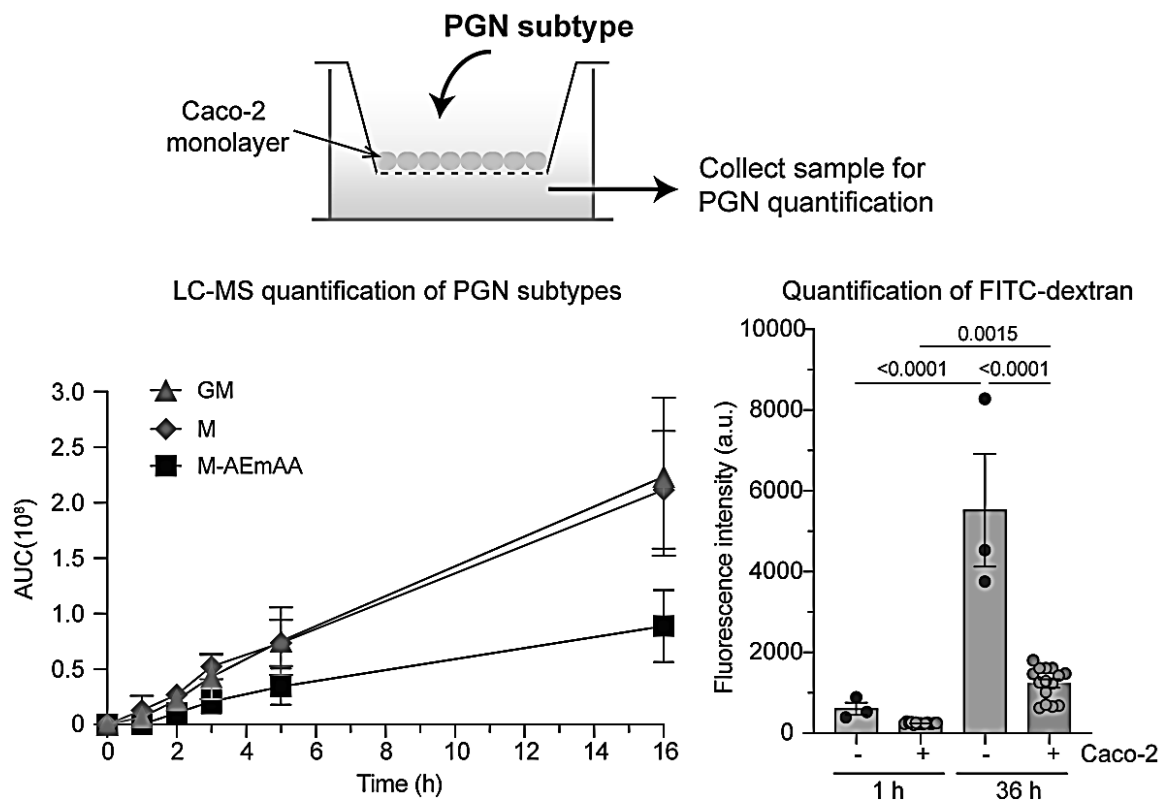


FIG. 7B

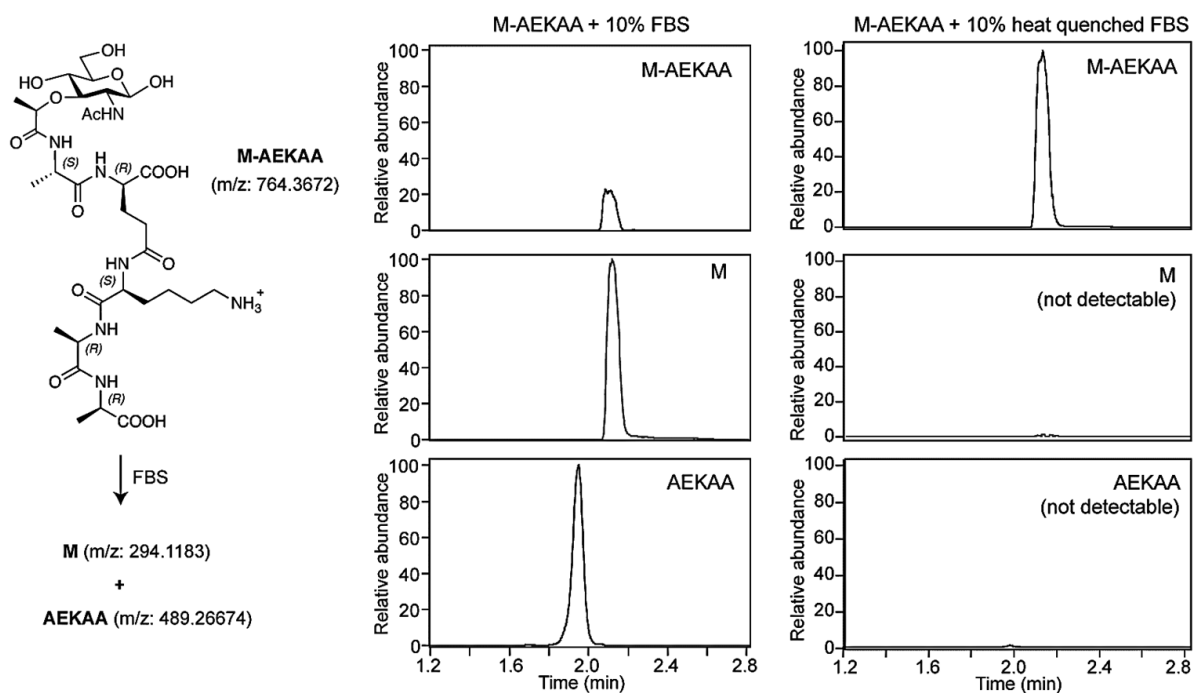


FIG. 7C

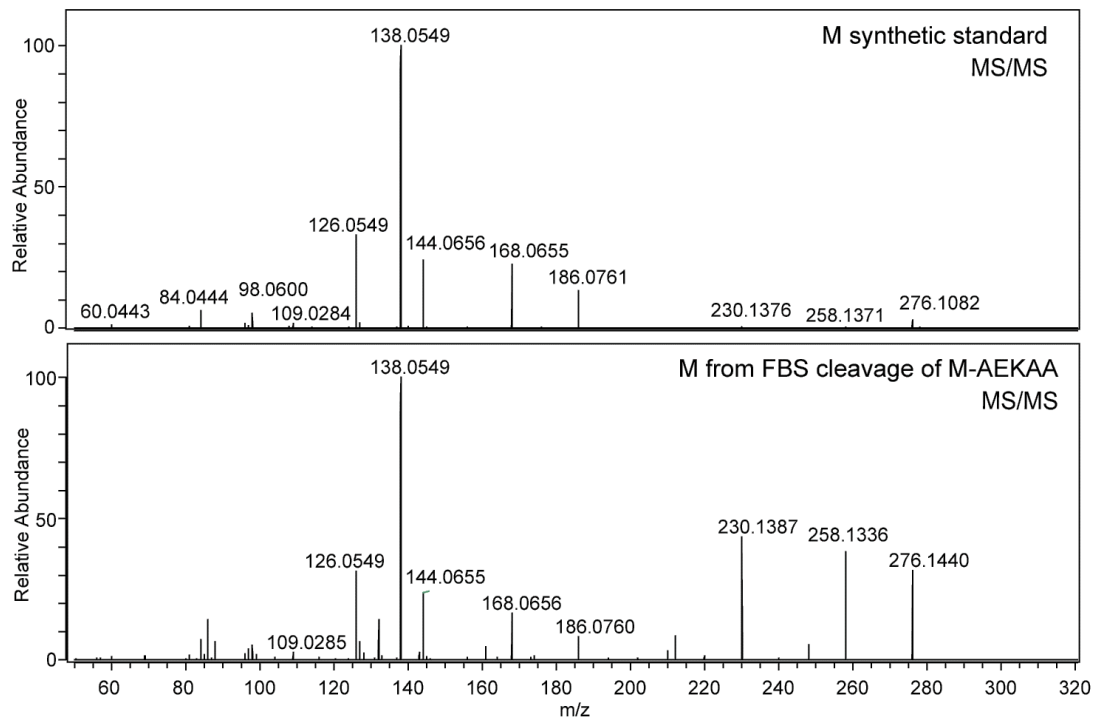


FIG. 7C (continued)

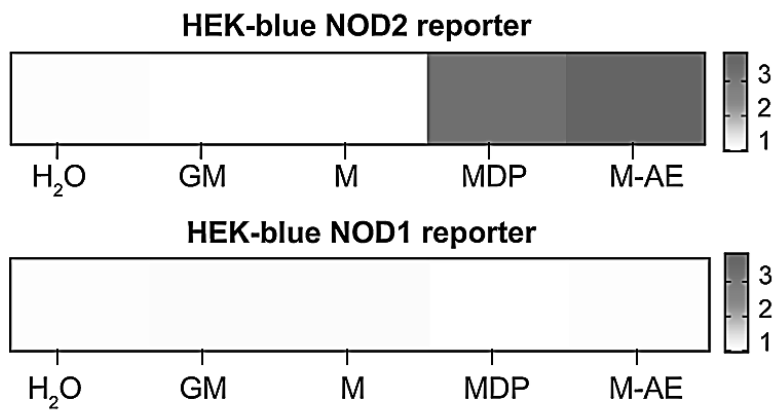


FIG. 8A

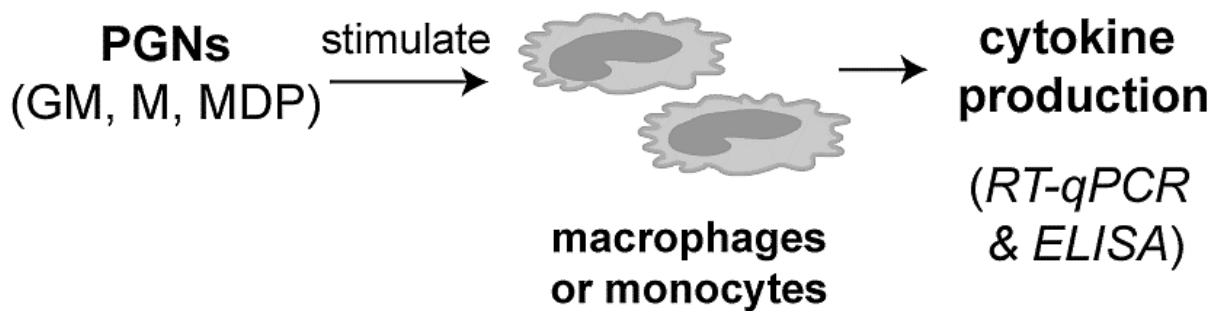


FIG. 8B

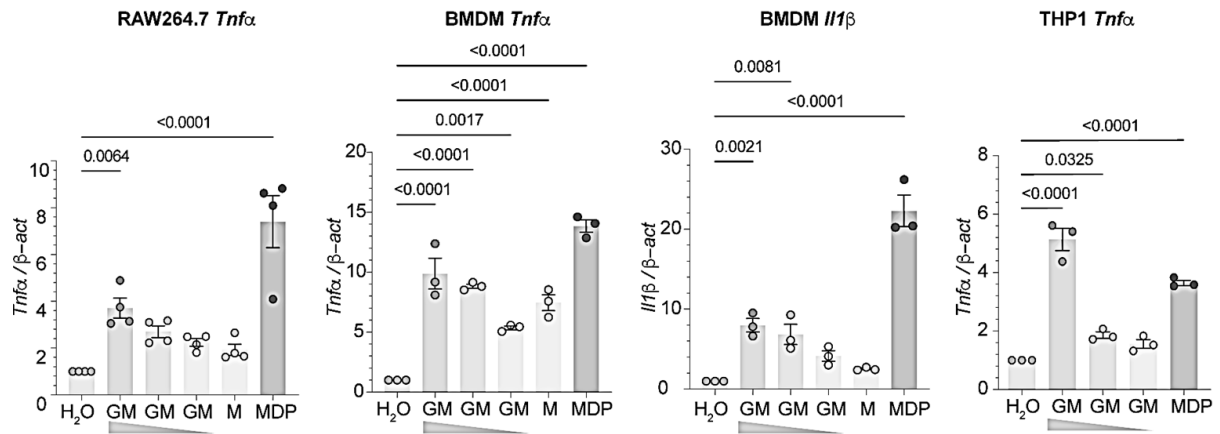


FIG. 8C

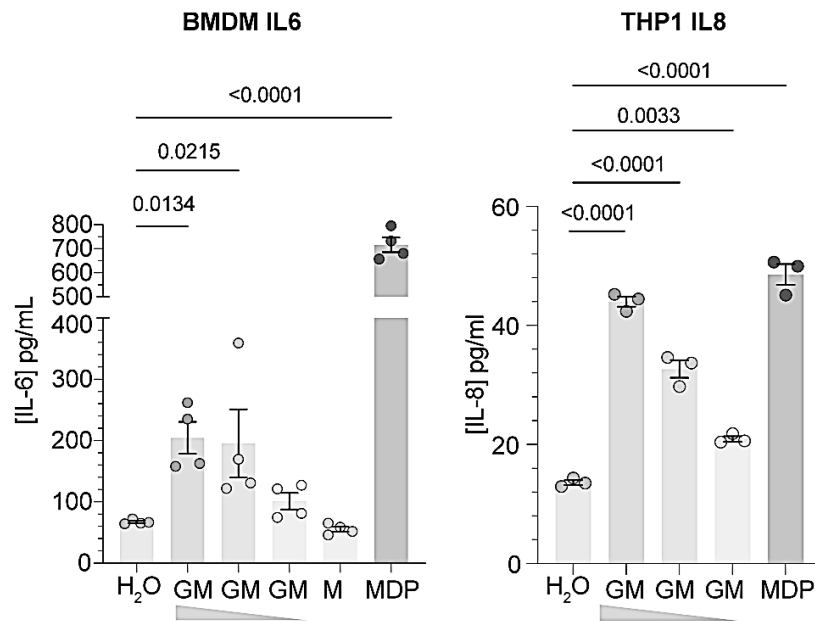


FIG. 8D

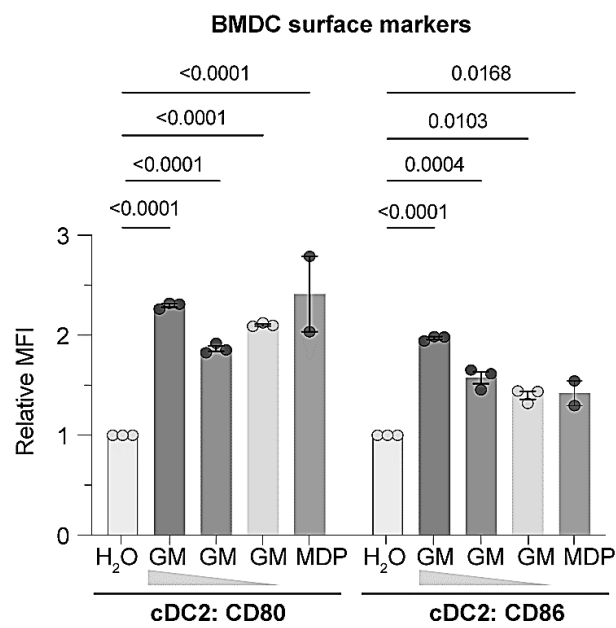


FIG. 8E

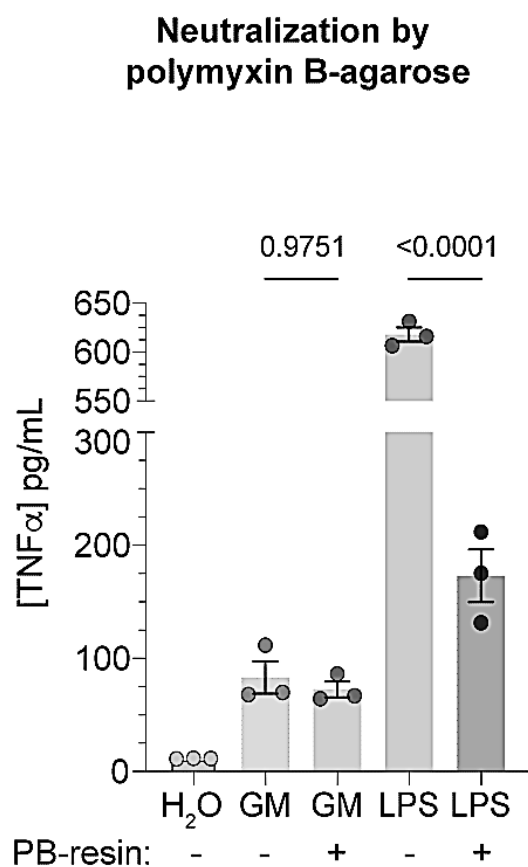


FIG. 8F

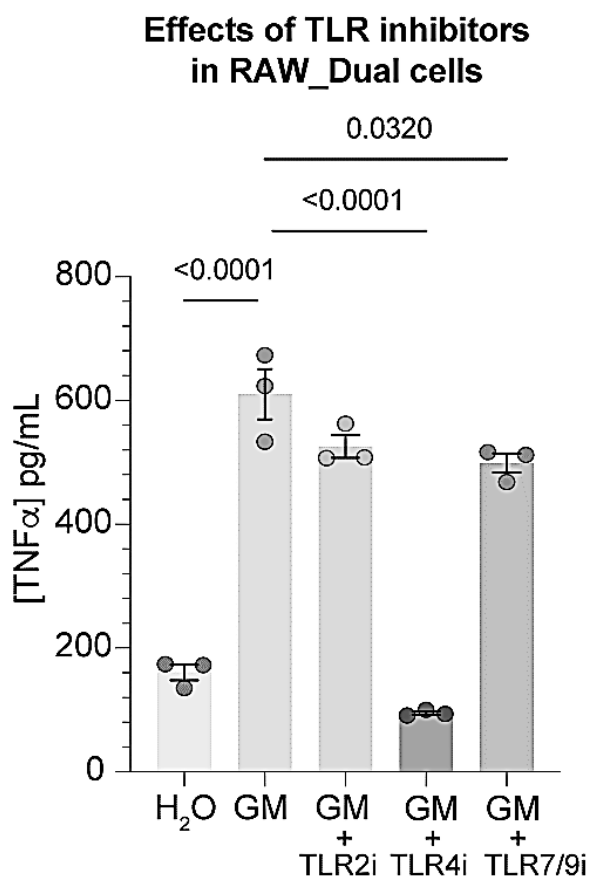


FIG. 8G

Polymyxin B titration in HEK-mTLR4 cells

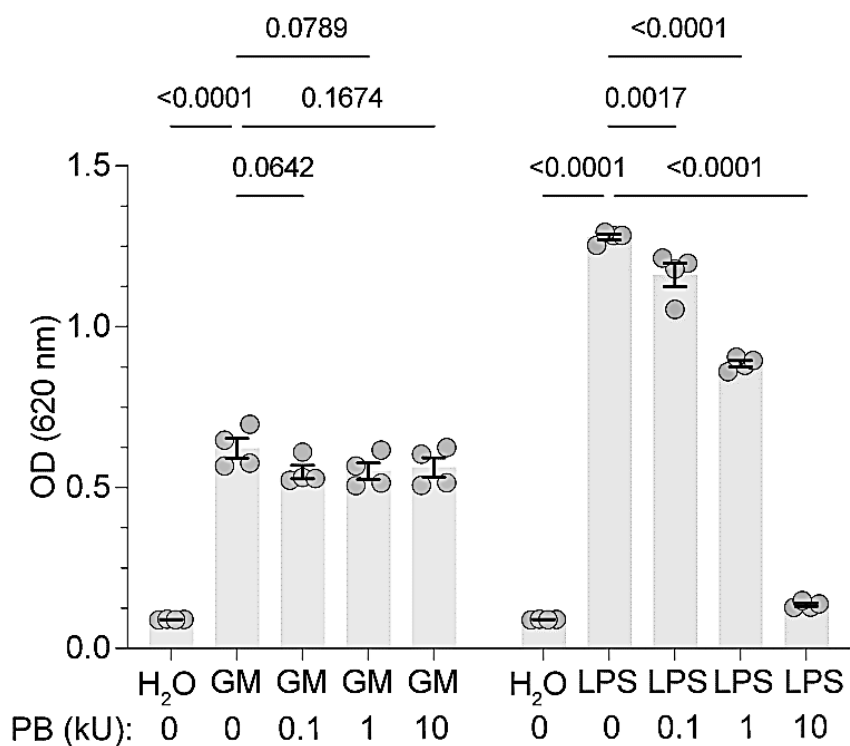


FIG. 8H

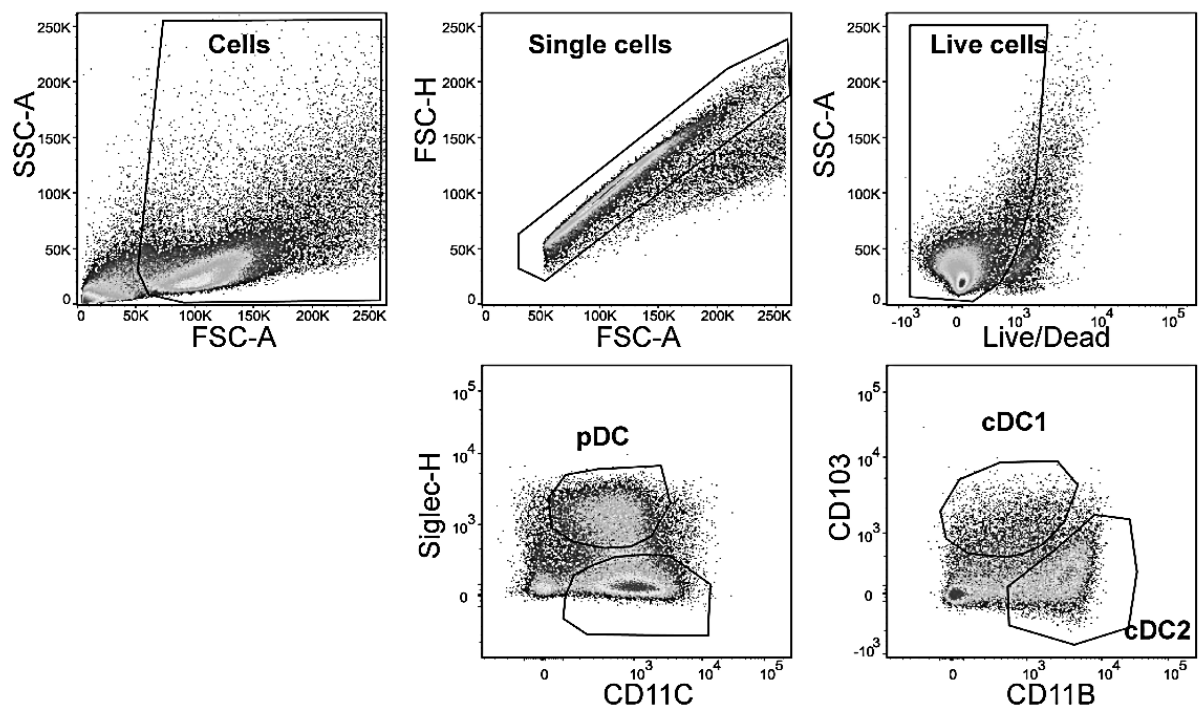


FIG. 9A

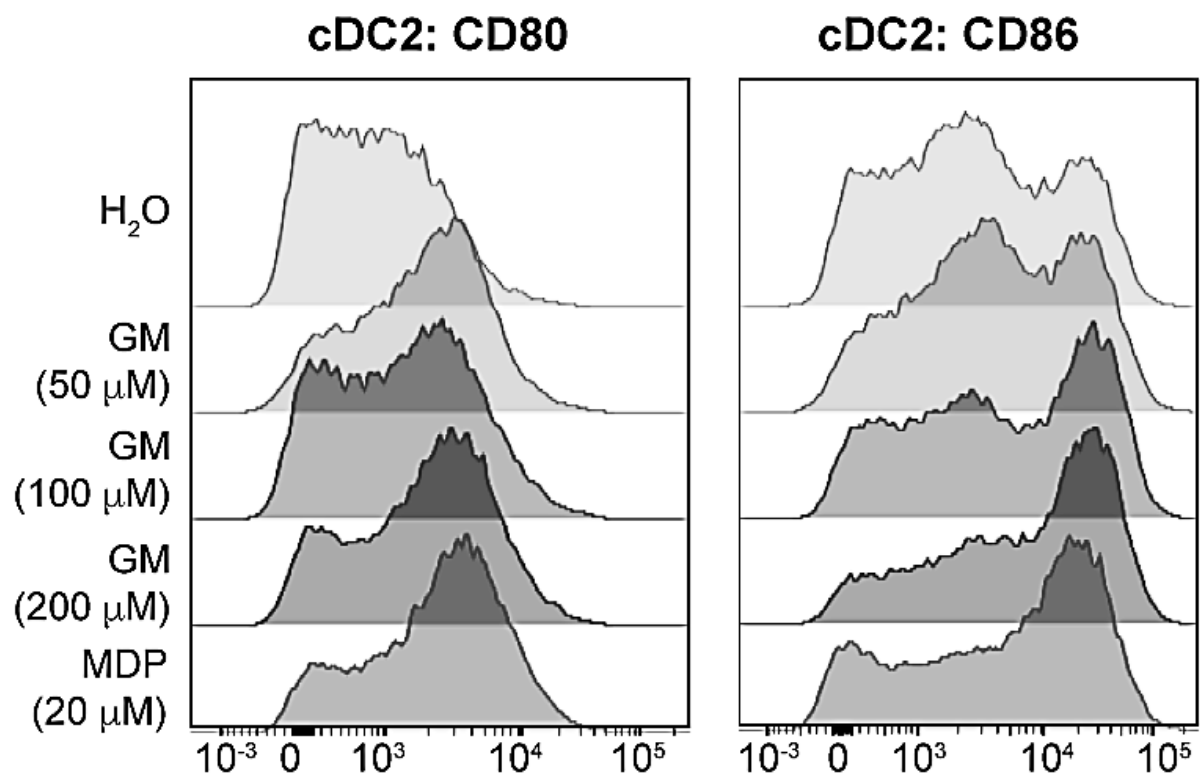


FIG. 9B

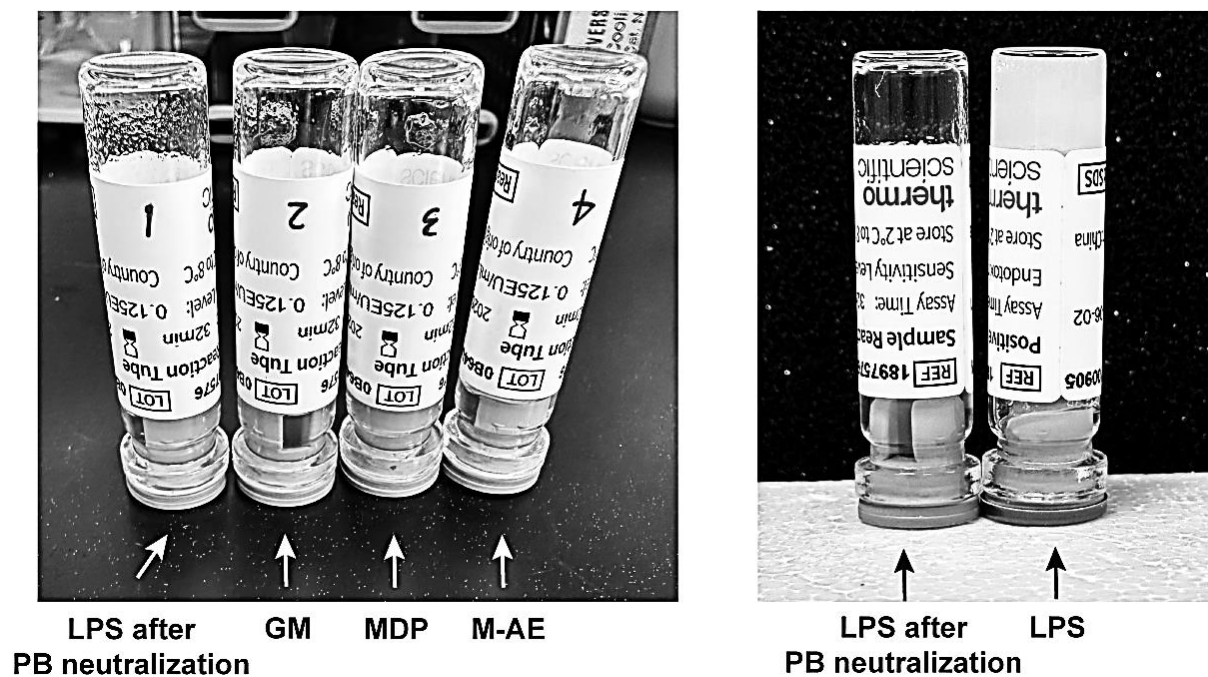


FIG. 10A

HEK-mTLR4 reporter assay of polymyxin B titration

LPS (100 ng/mL):	+	+	+	+	-
Polymyxin B (KU):	0	10	1	0.1	0



GM (1 mM):	+	+	+	+	-
Polymyxin B (KU):	0	10	1	0.1	0

FIG. 10B

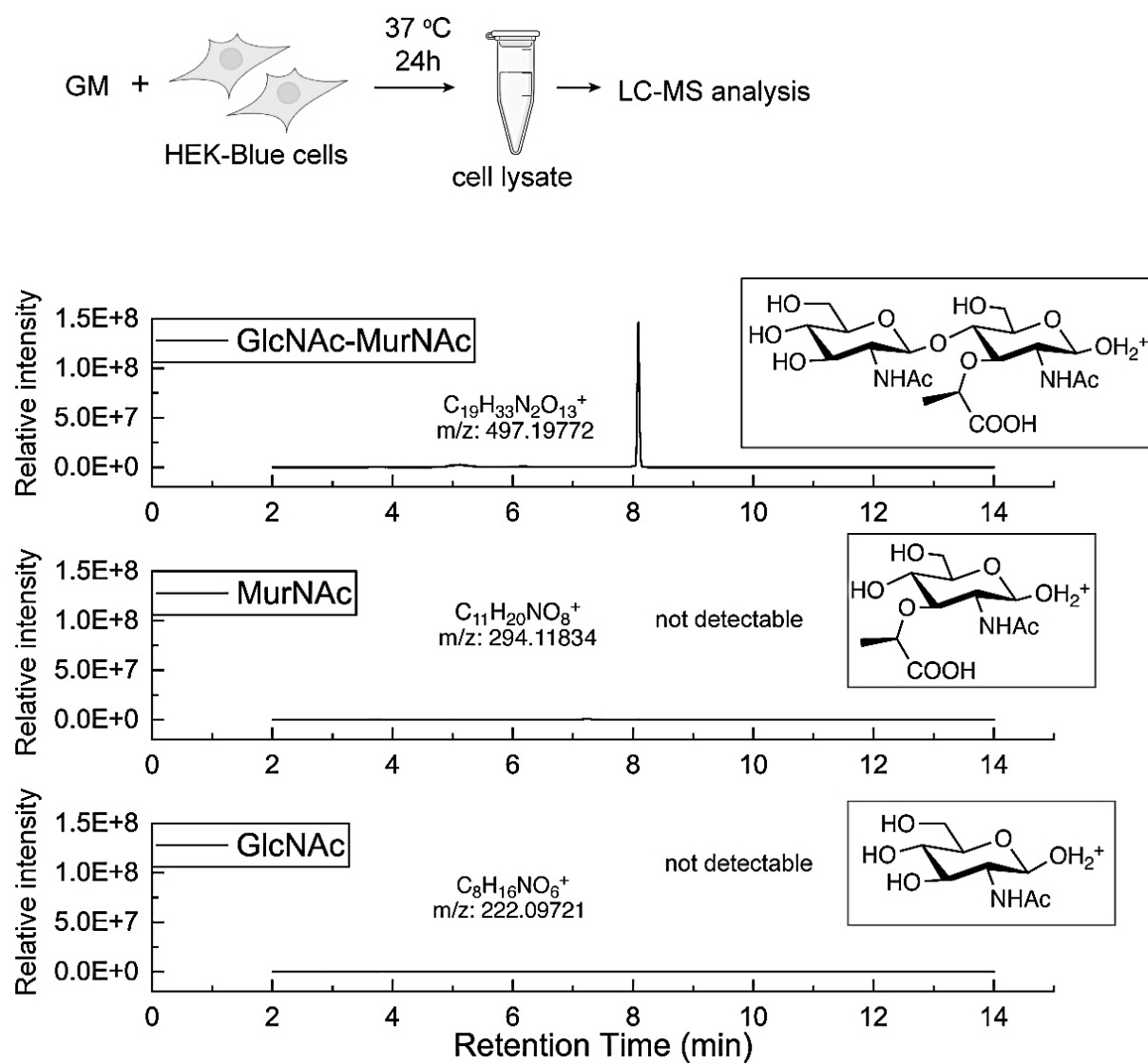


FIG. 11

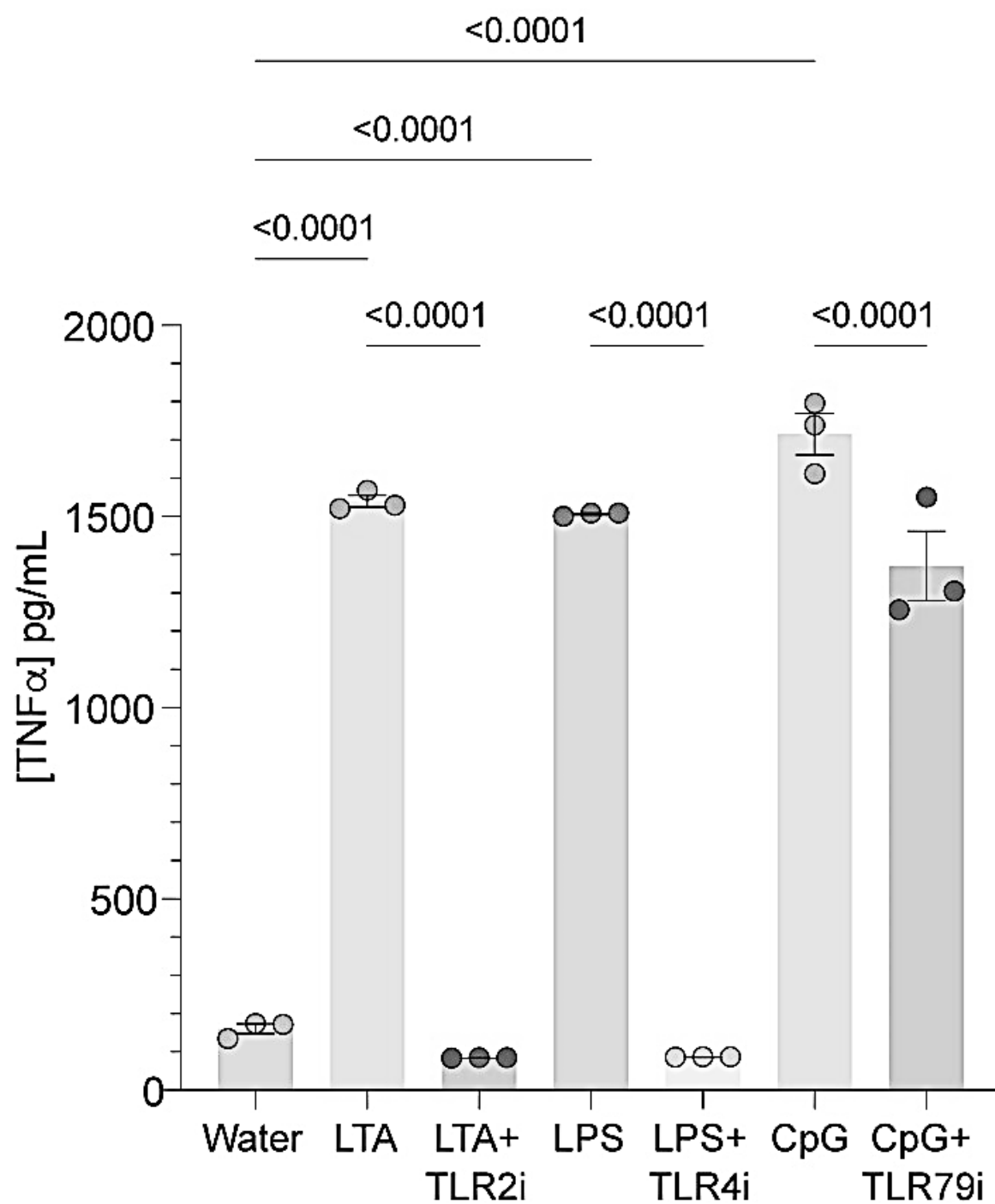
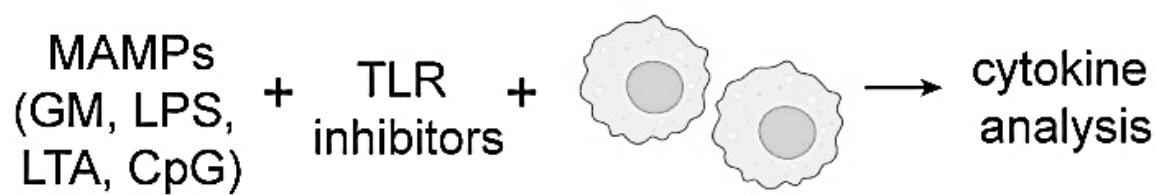


FIG. 12

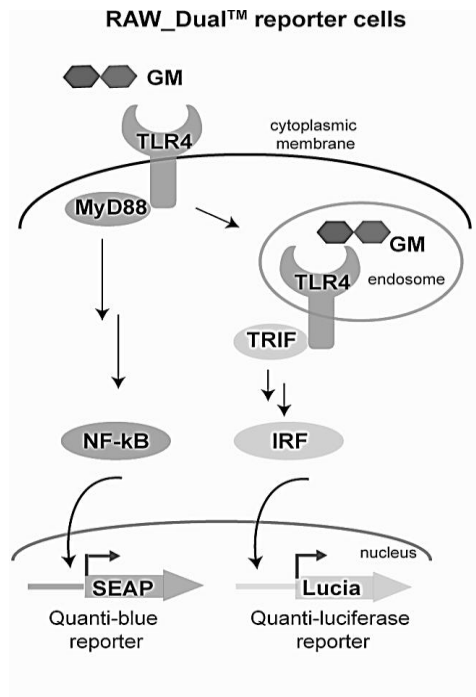


FIG. 13A

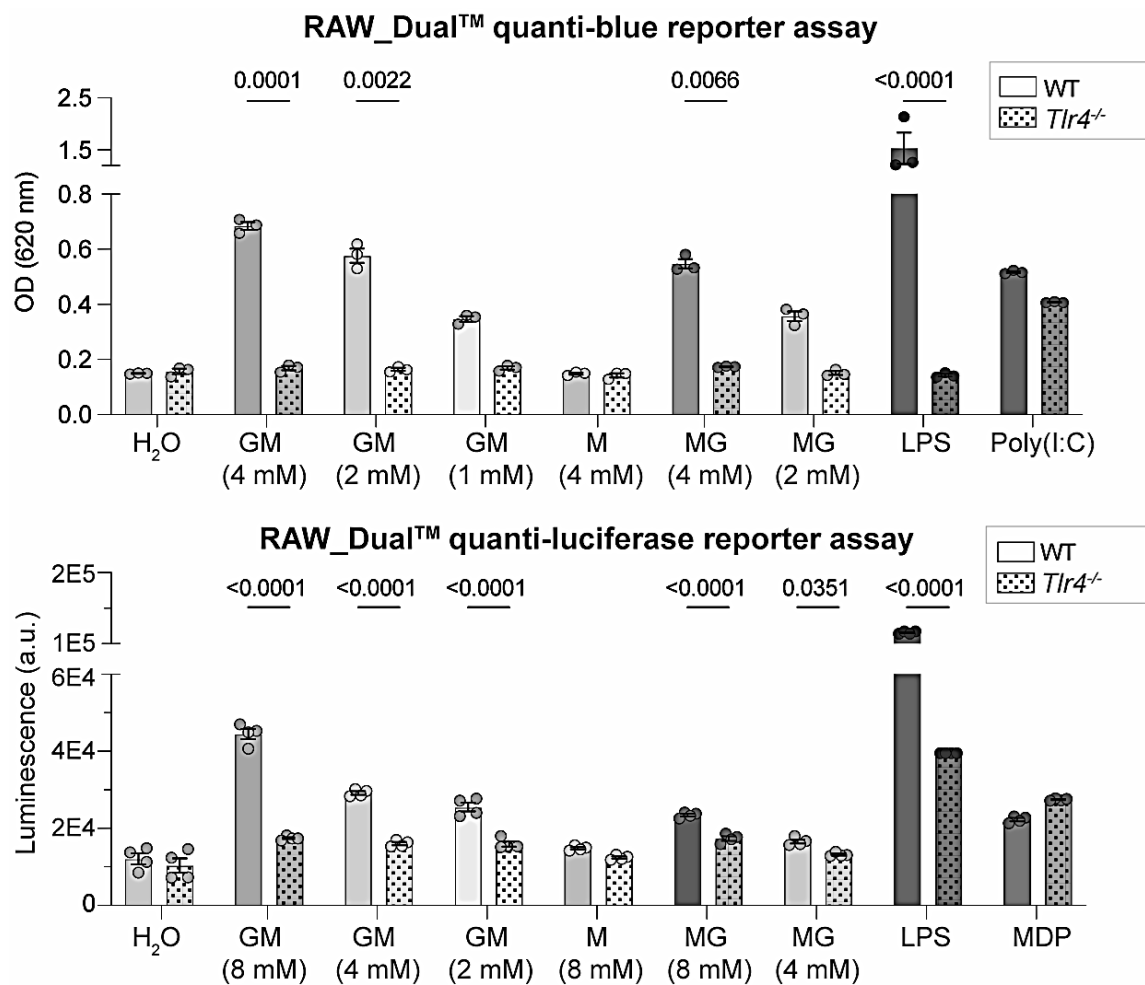


FIG. 13B

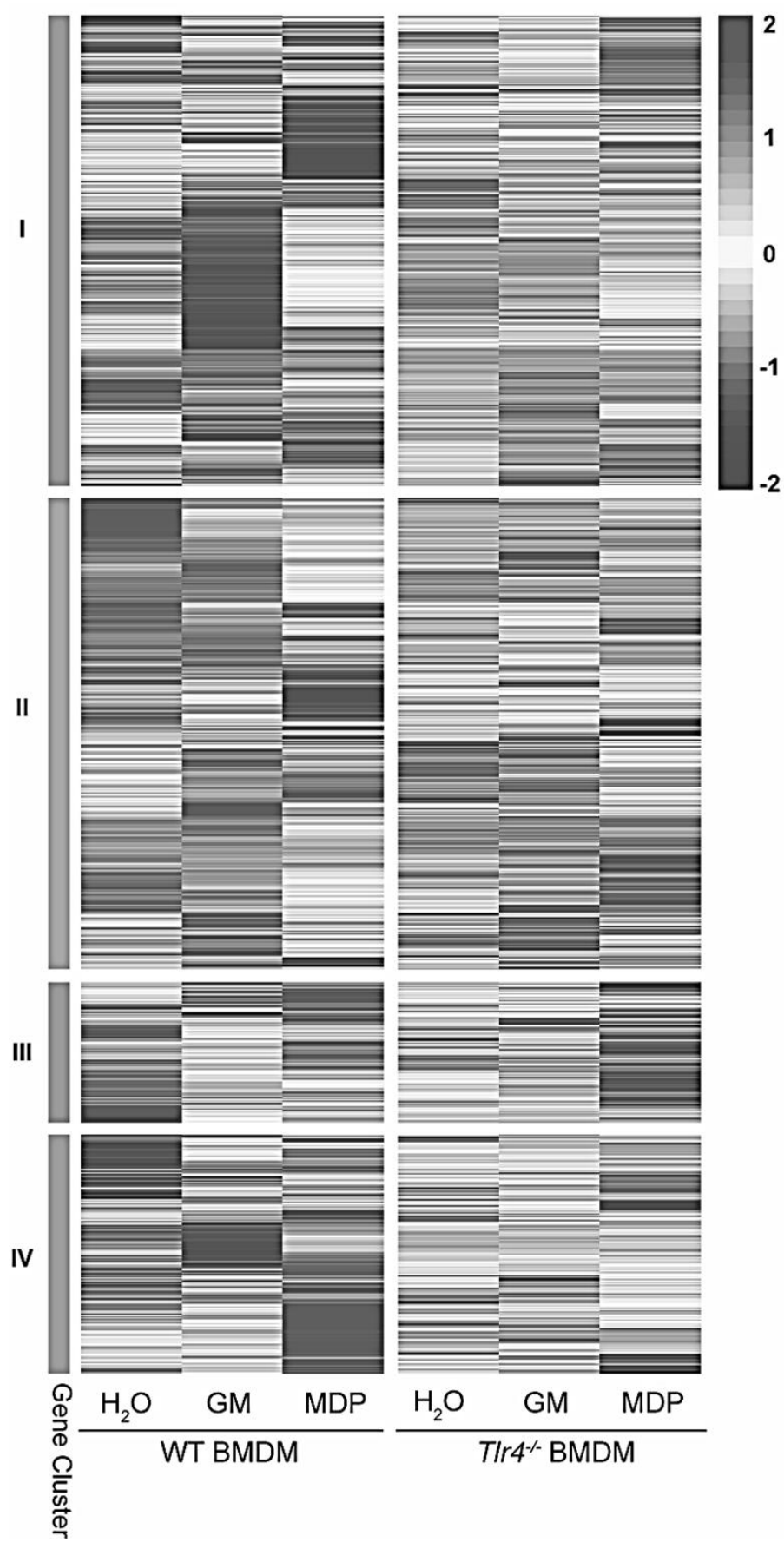


FIG. 13C

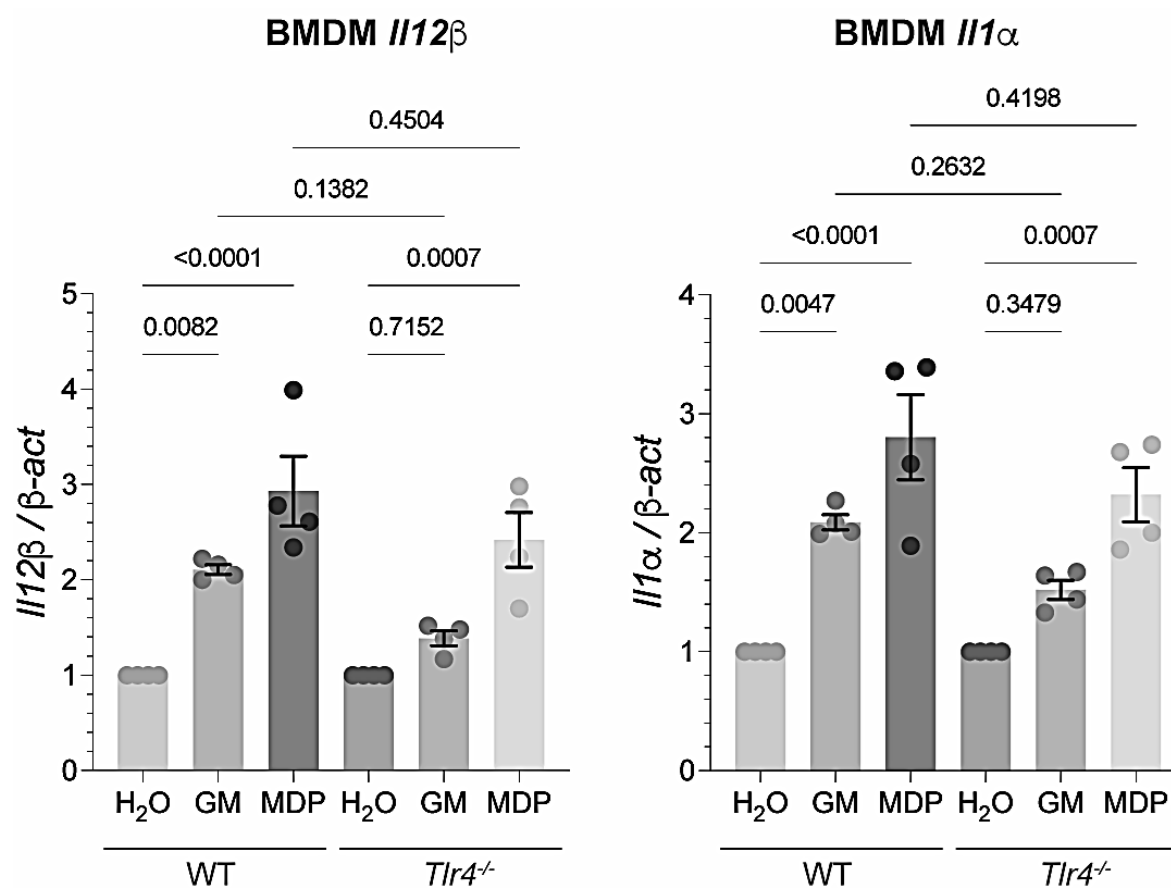


FIG. 13D

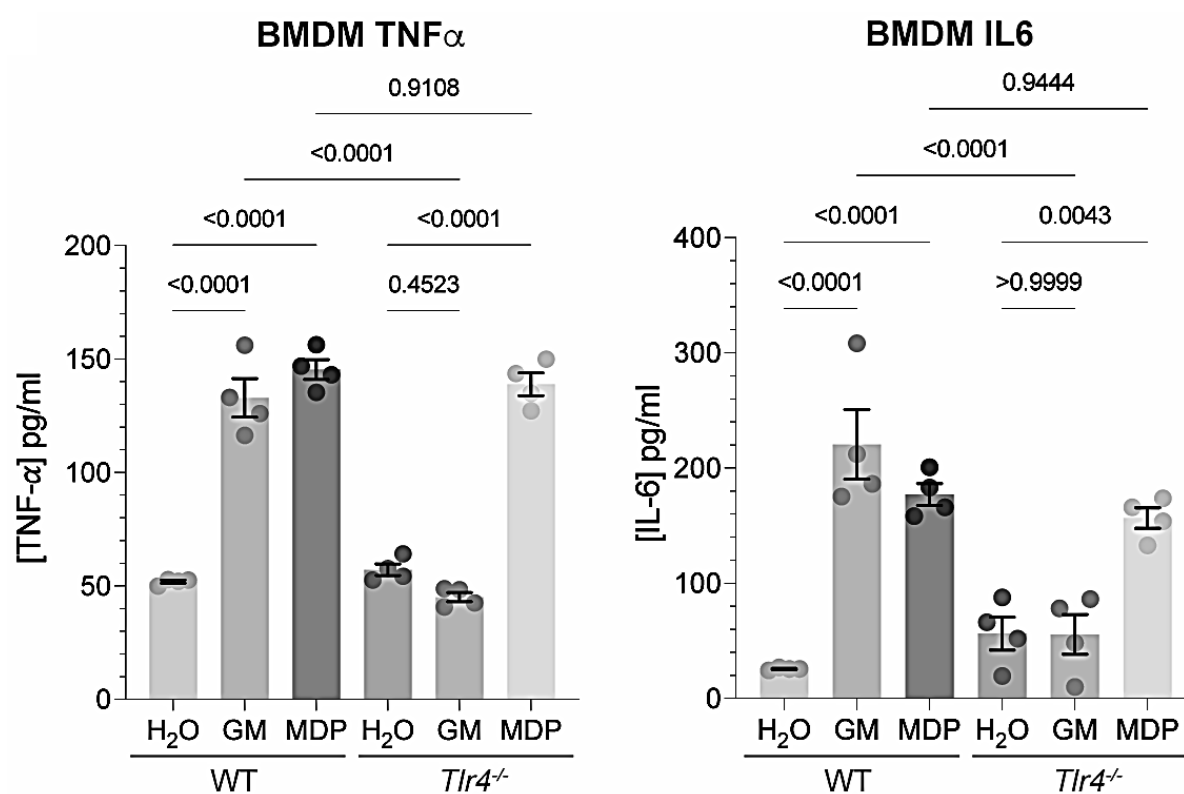


FIG. 13E

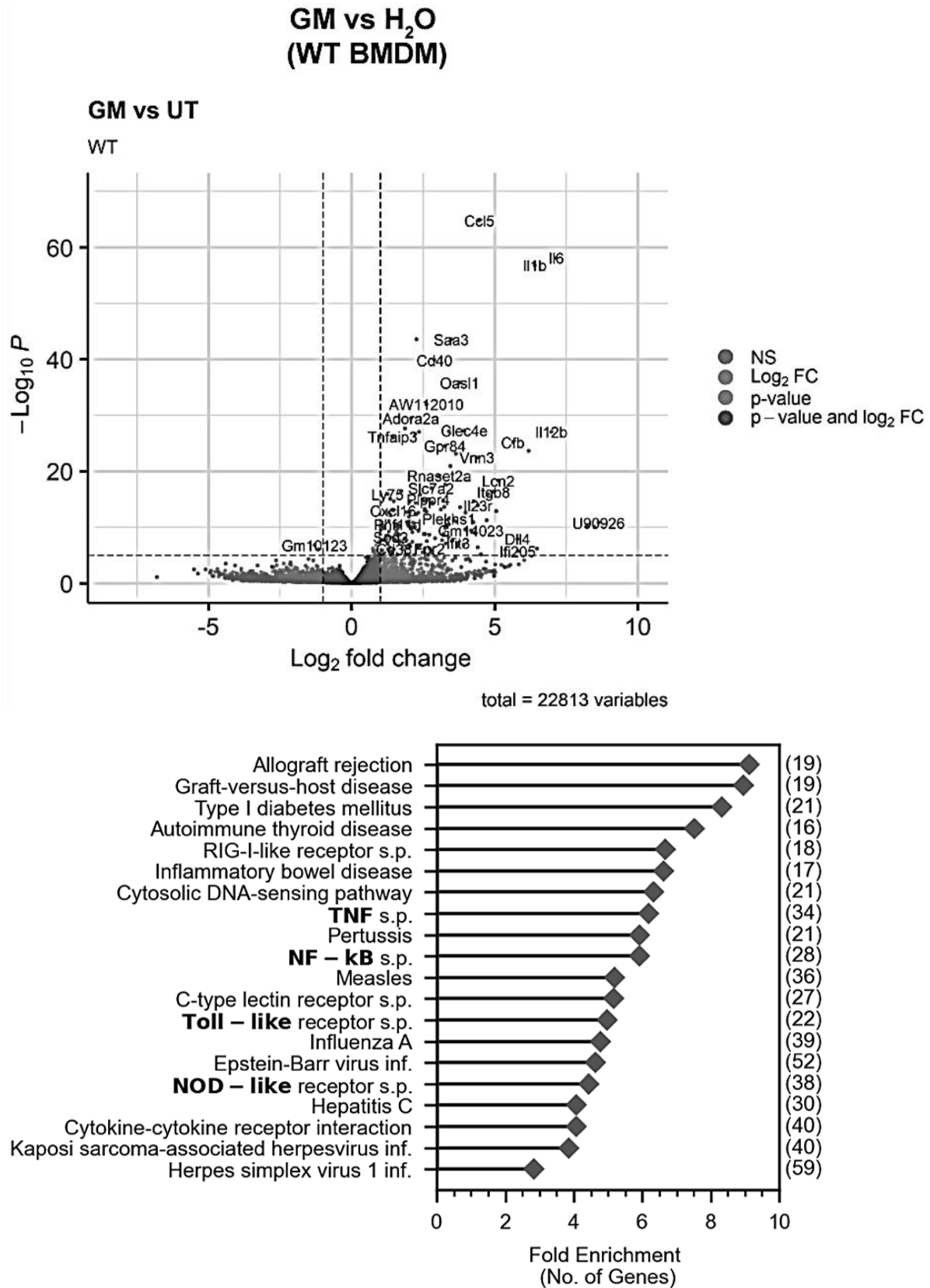


FIG. 14A

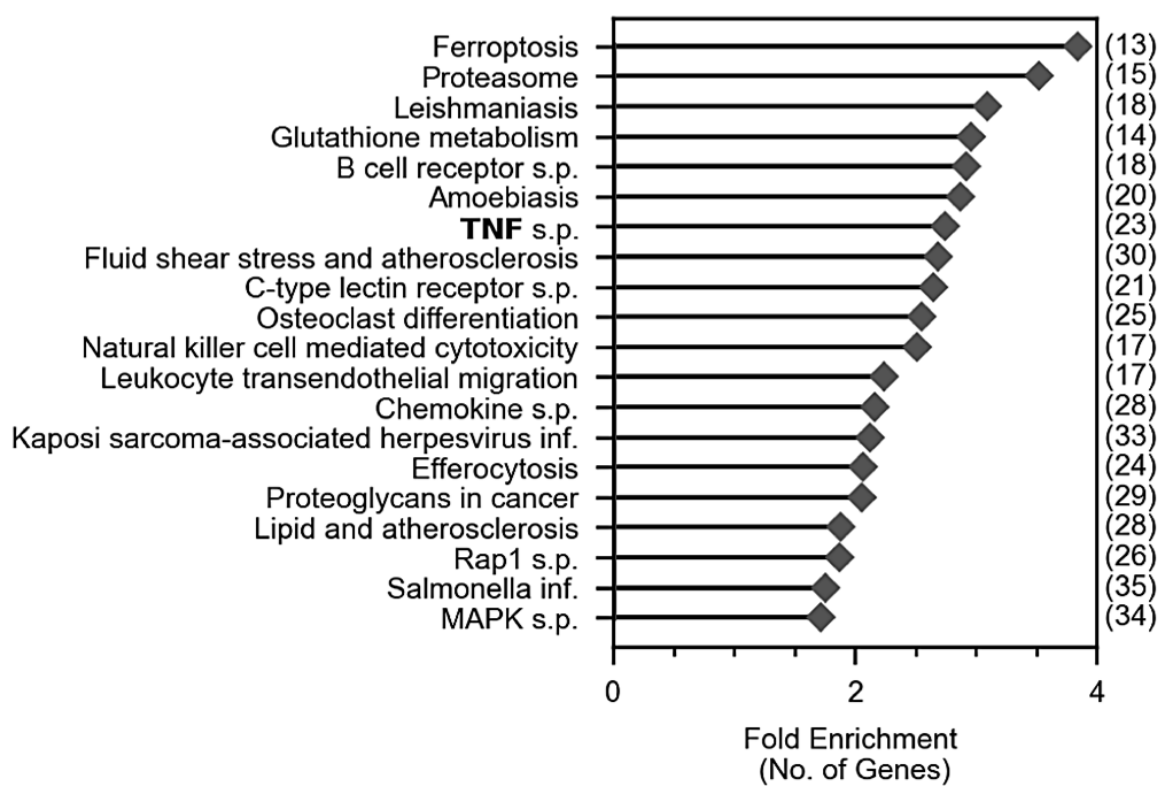
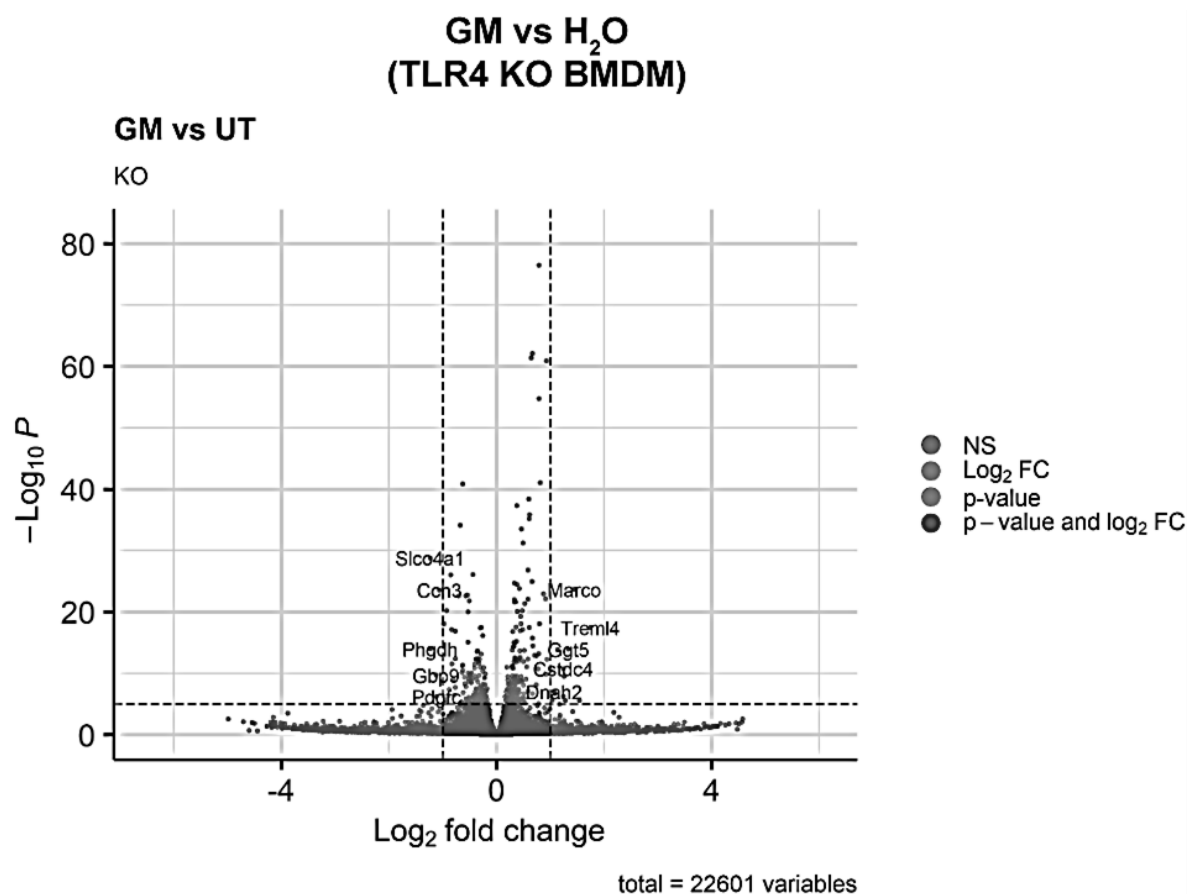


FIG. 14B

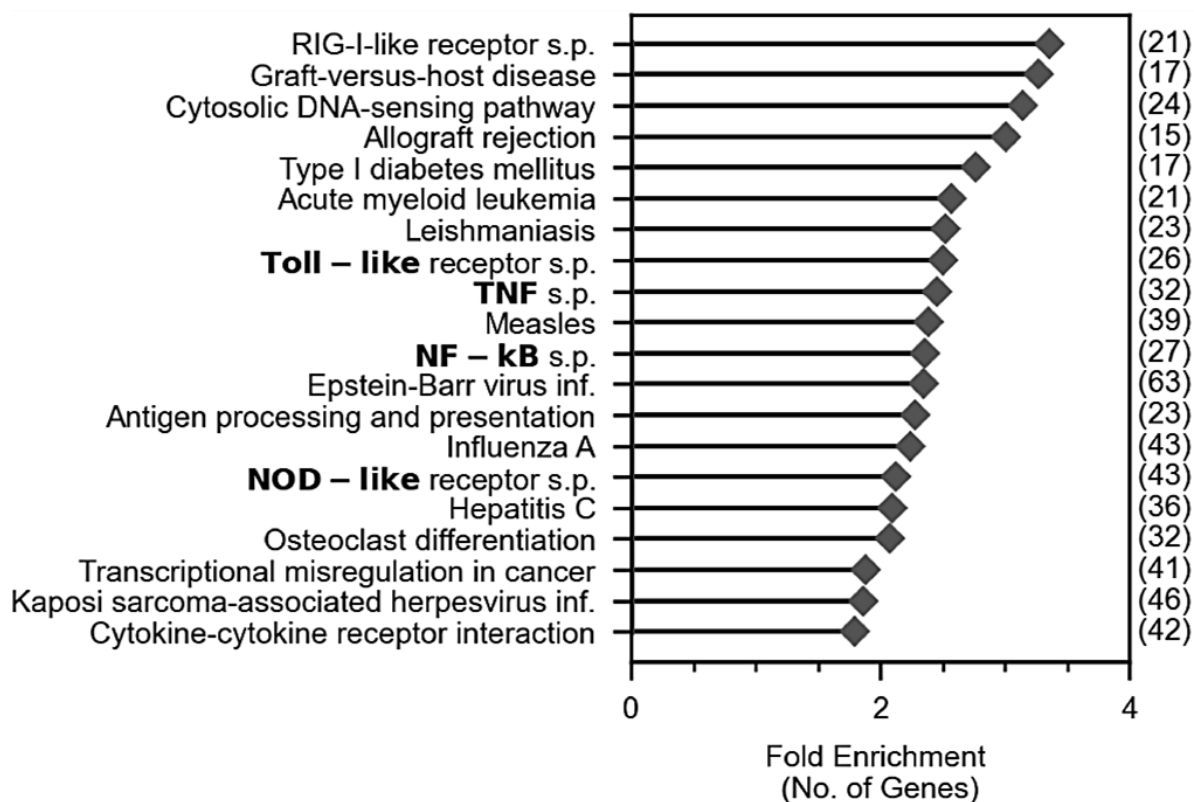
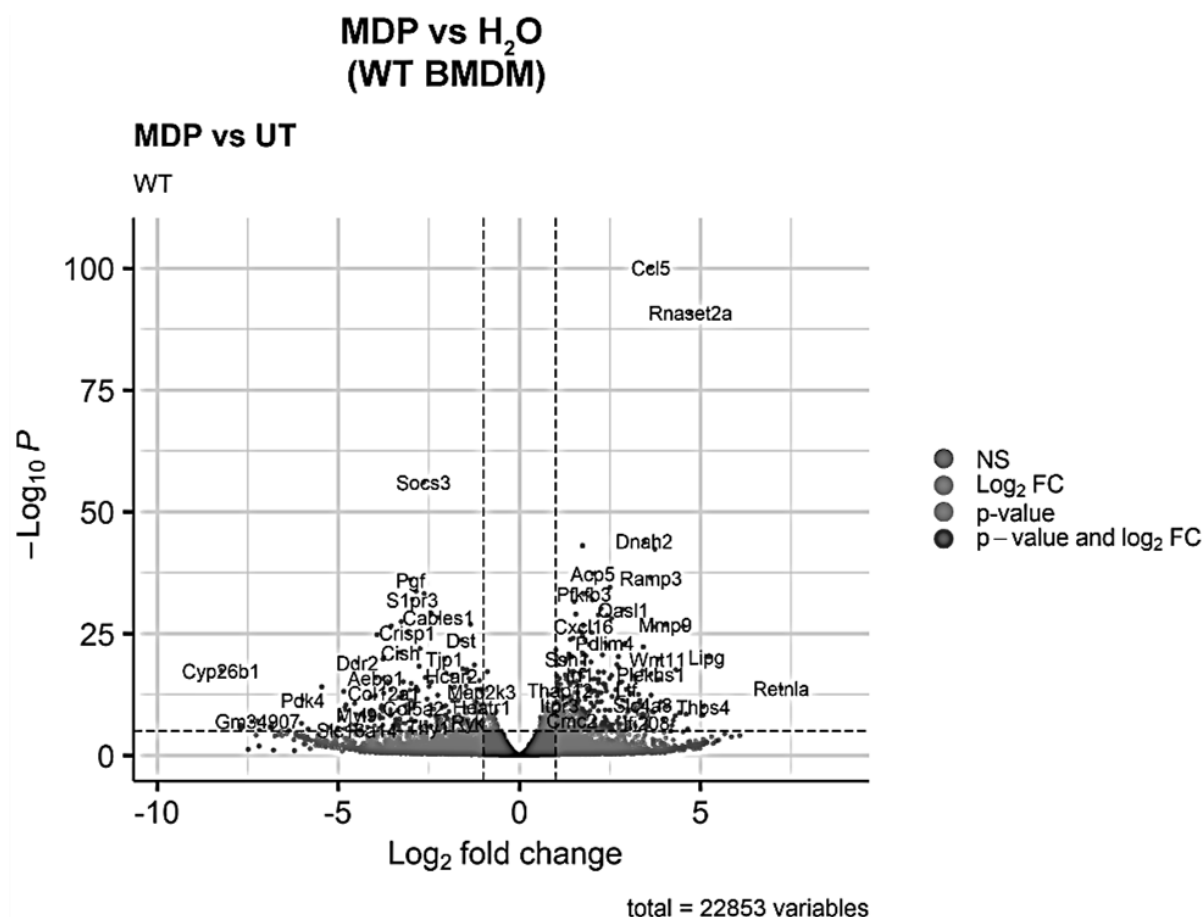


FIG. 14C

GO Term	Number of Genes
Graft-versus-host disease	19
Allograft rejection	18
RIG-I-like receptor s.p.	22
Type I diabetes mellitus	20
TNF s.p.	43
Amoebiasis	34
Leishmaniasis	29
Pertussis	25
C-type lectin receptor s.p.	36
NF – κB s.p.	33
Measles	44
IL-17 s.p.	26
NOD – like receptor s.p.	54
Influenza A	50
Osteoclast differentiation	40
Cell adhesion molecules	39
Fluid shear stress and atherosclerosis	43
Epstein-Barr virus inf.	65
Kaposi sarcoma-associated herpesvirus inf.	59
Cytokine-cytokine receptor interaction	55

FIG. 14D

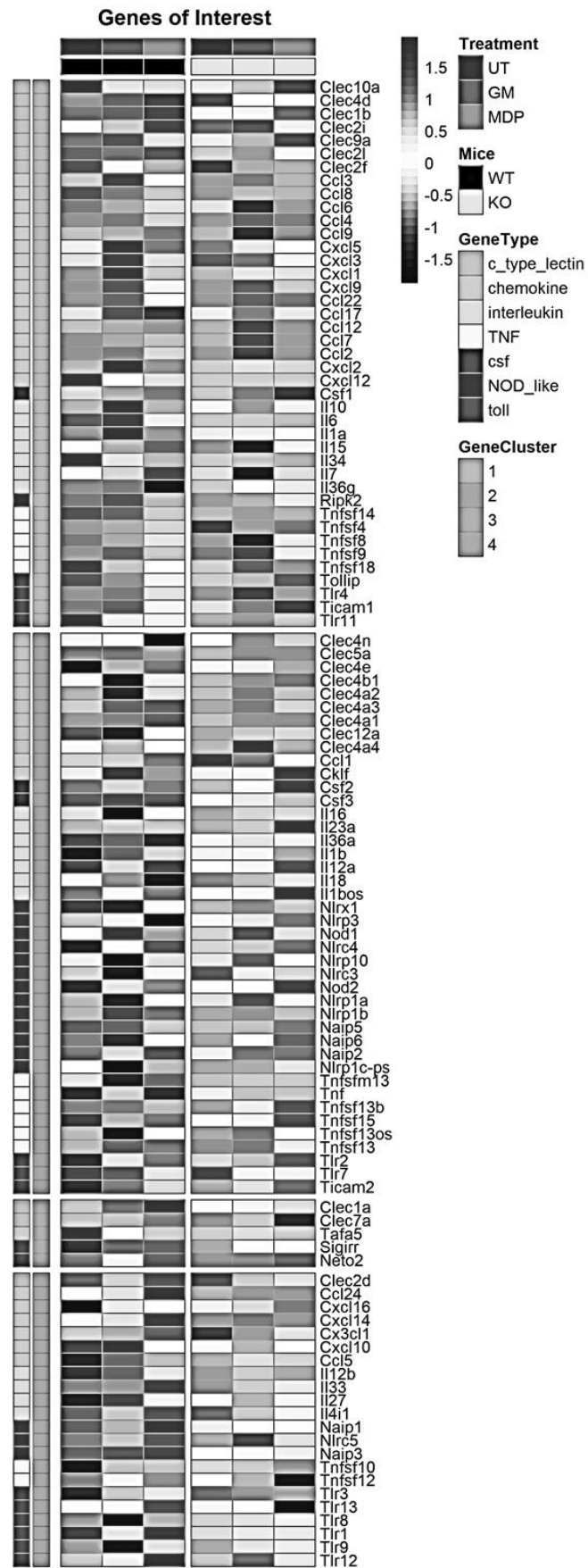


FIG. 15

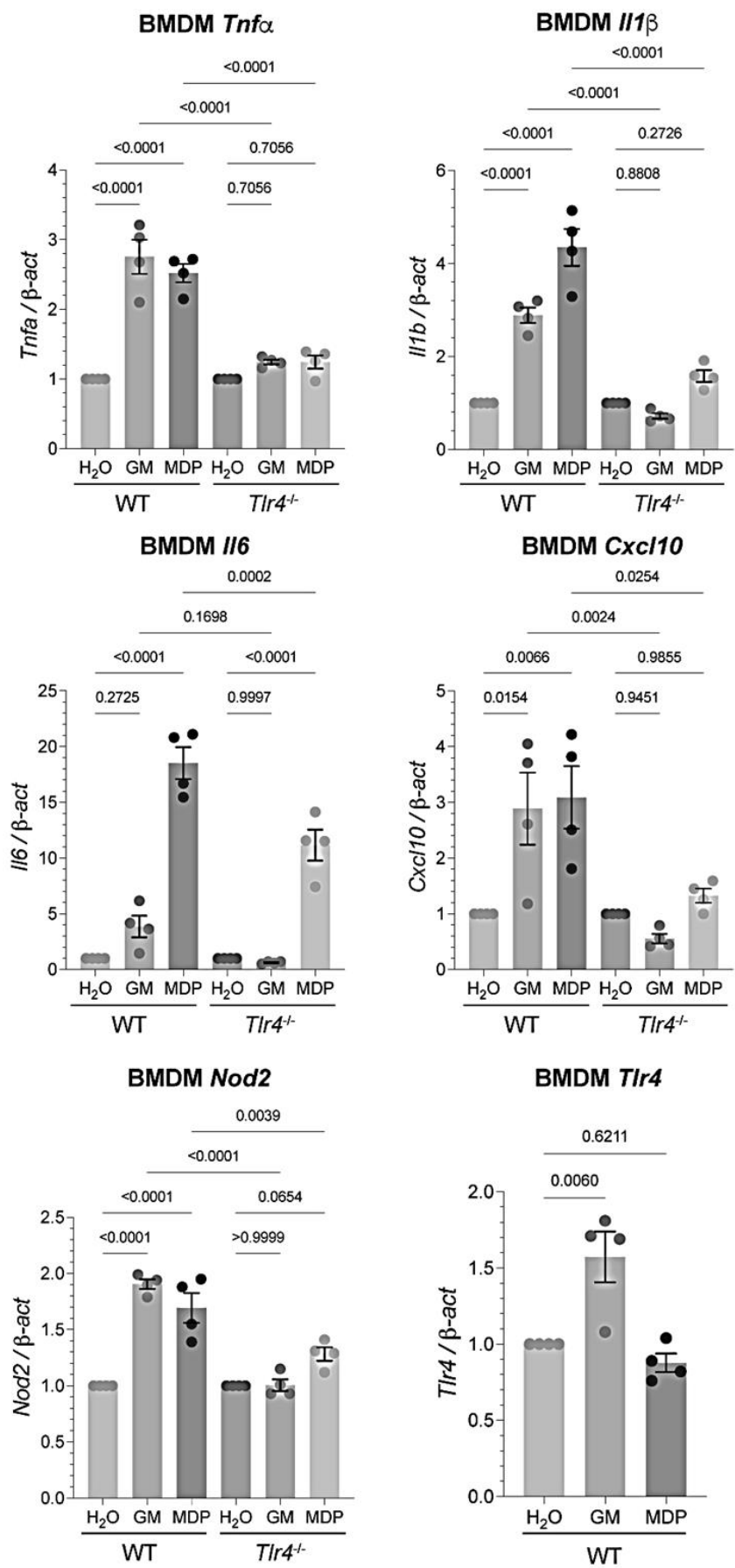


FIG. 16

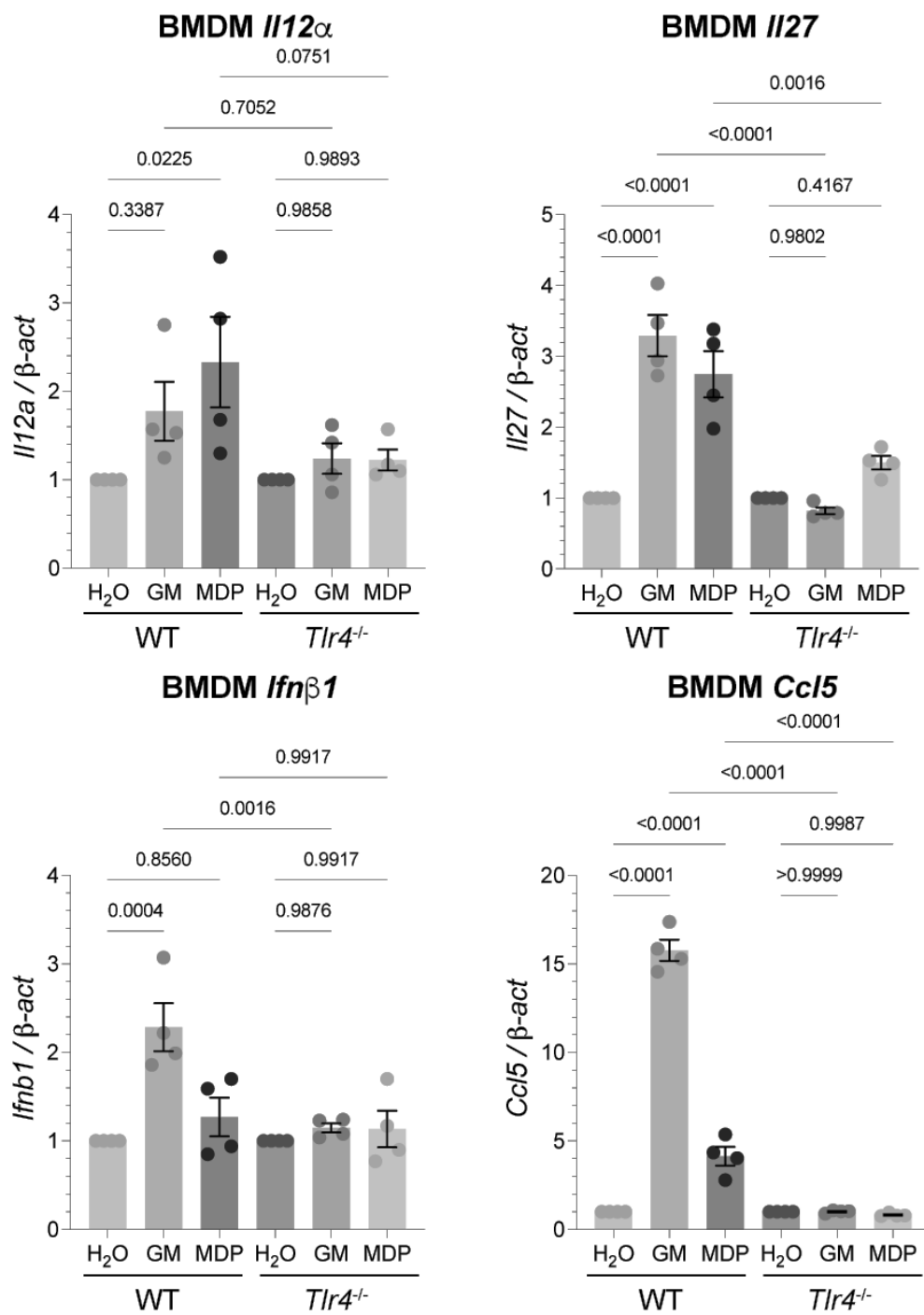


FIG. 16 (continued)

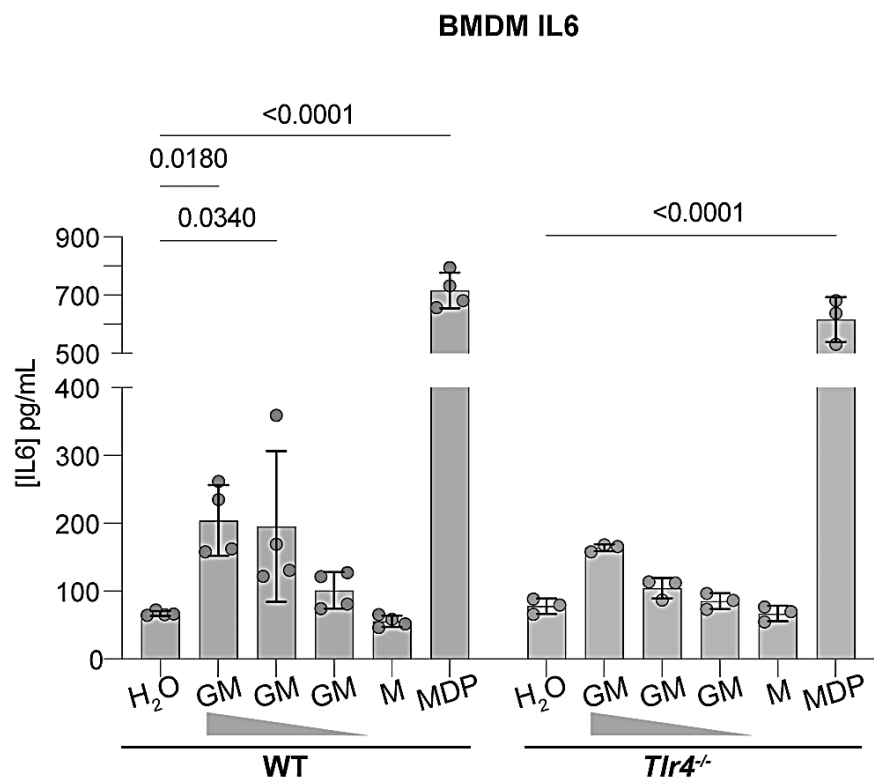


FIG.17A

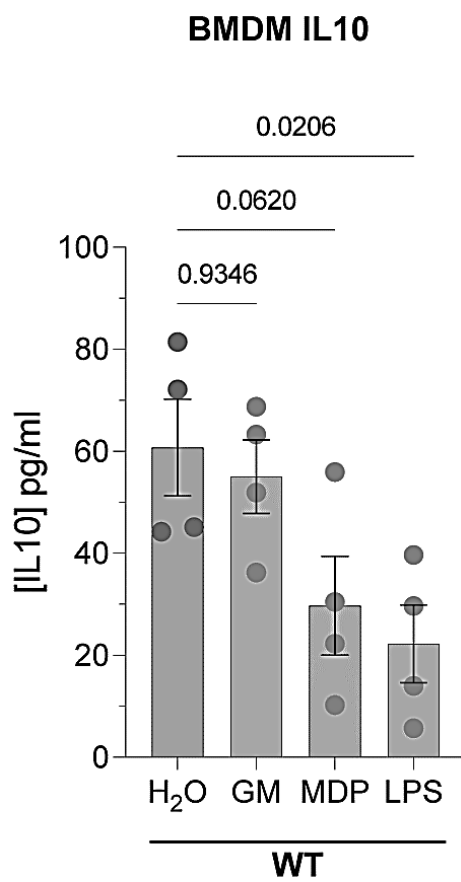


FIG. 17B

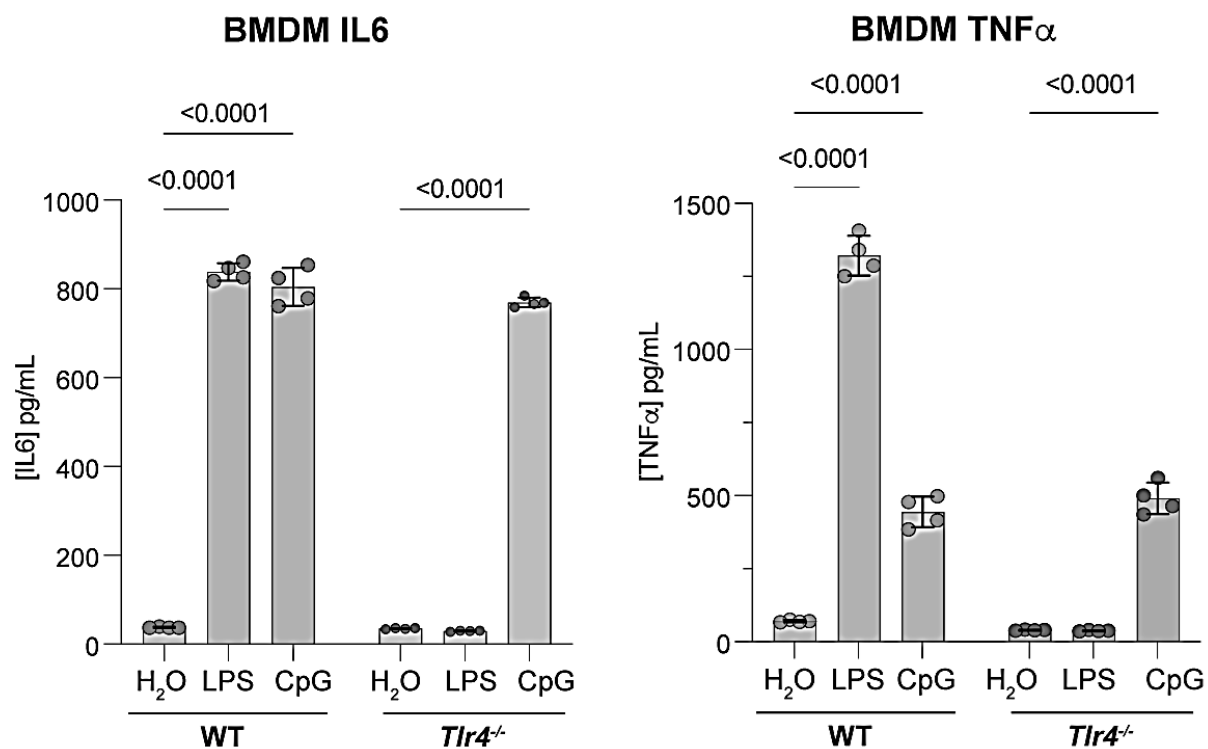


FIG. 17C

RAW_Dual™ reporter cells TNF α

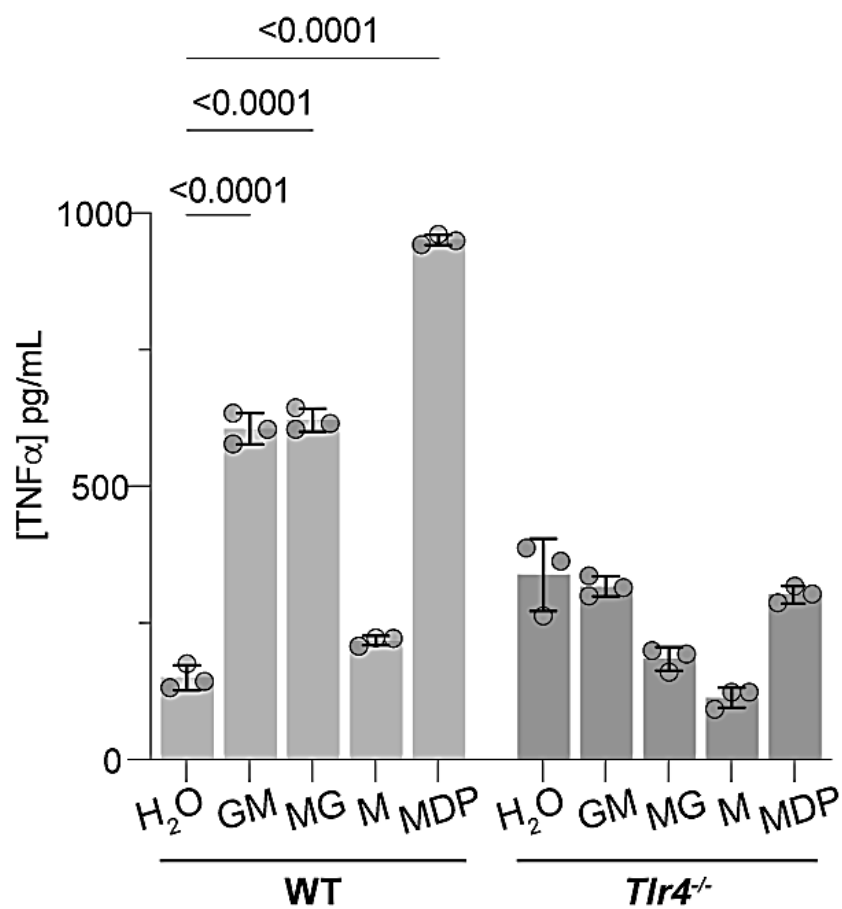


FIG. 17D

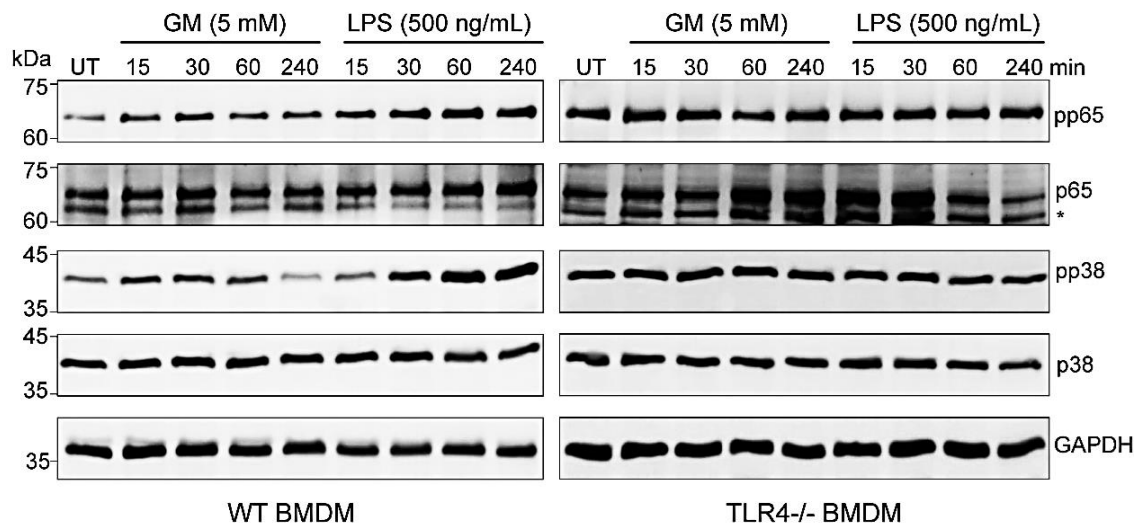


FIG. 18A

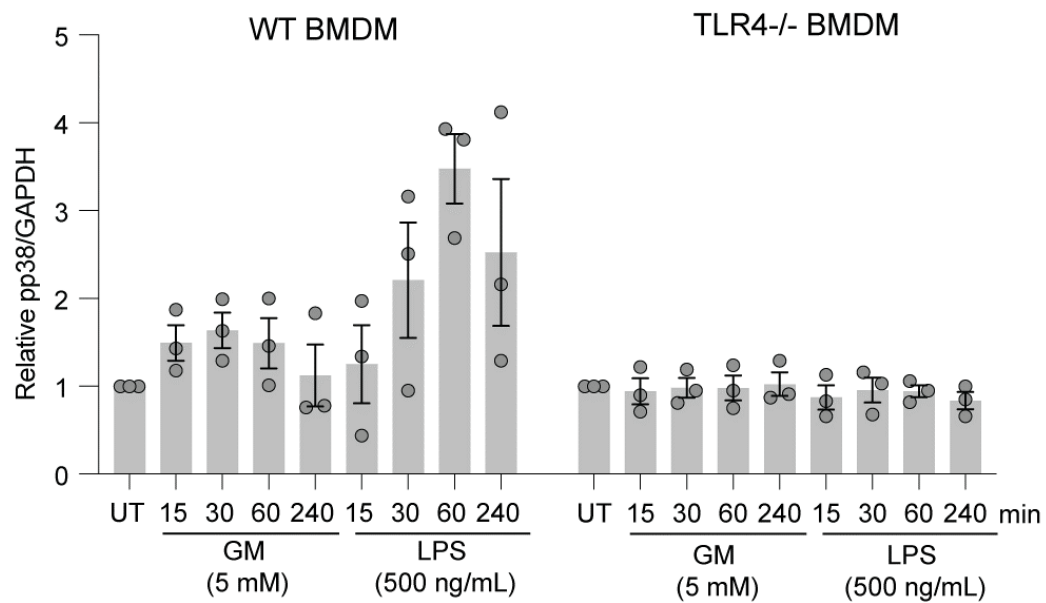
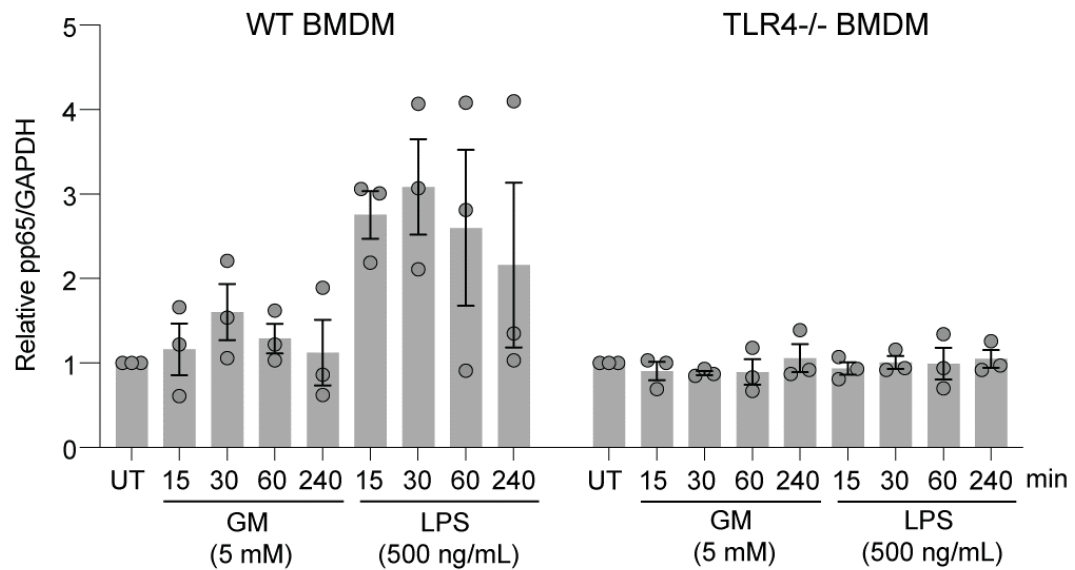


FIG. 18B

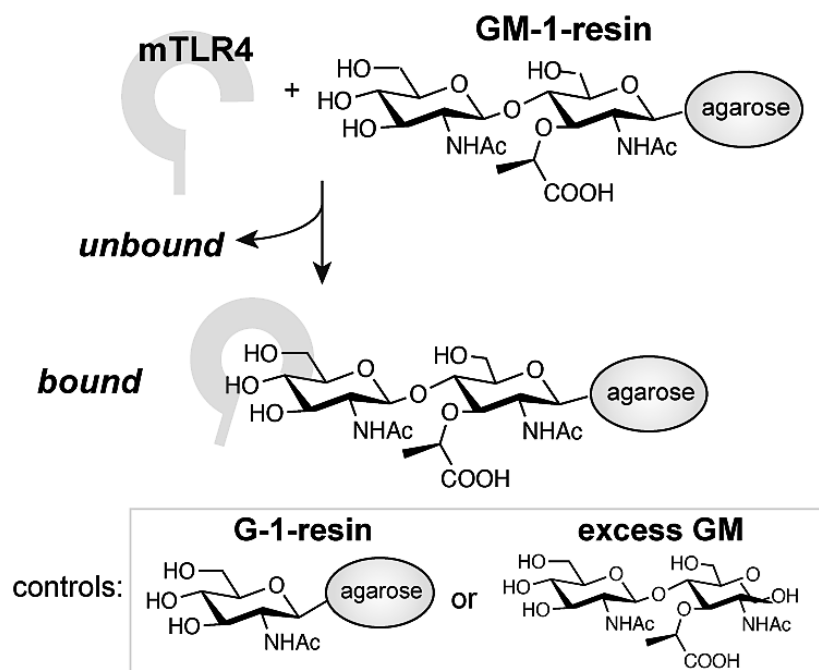


FIG. 19A

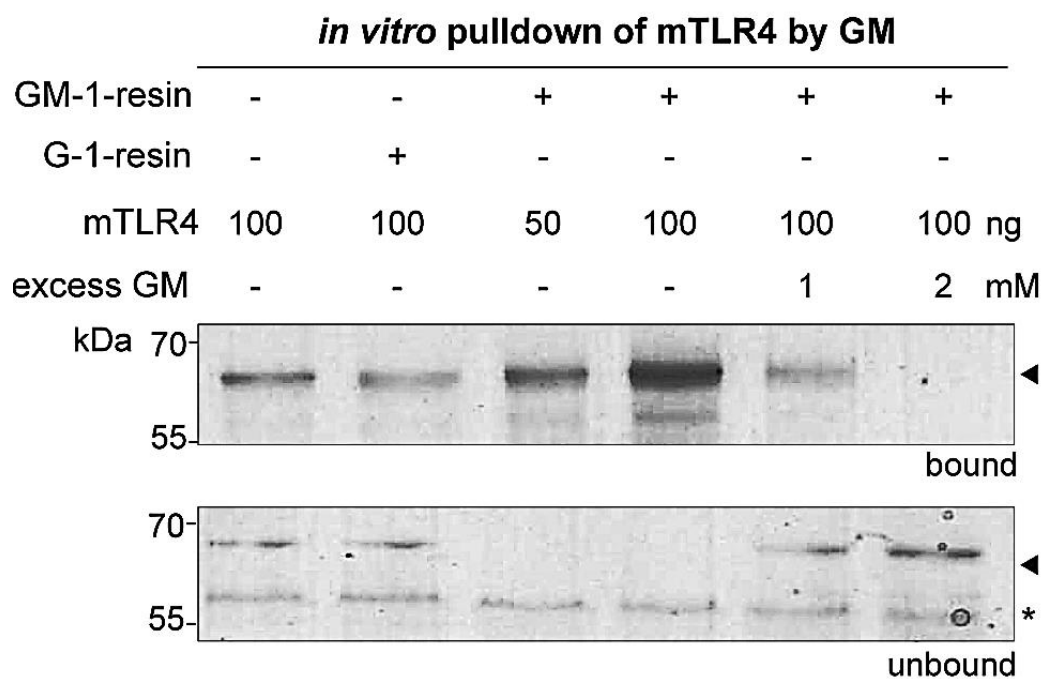
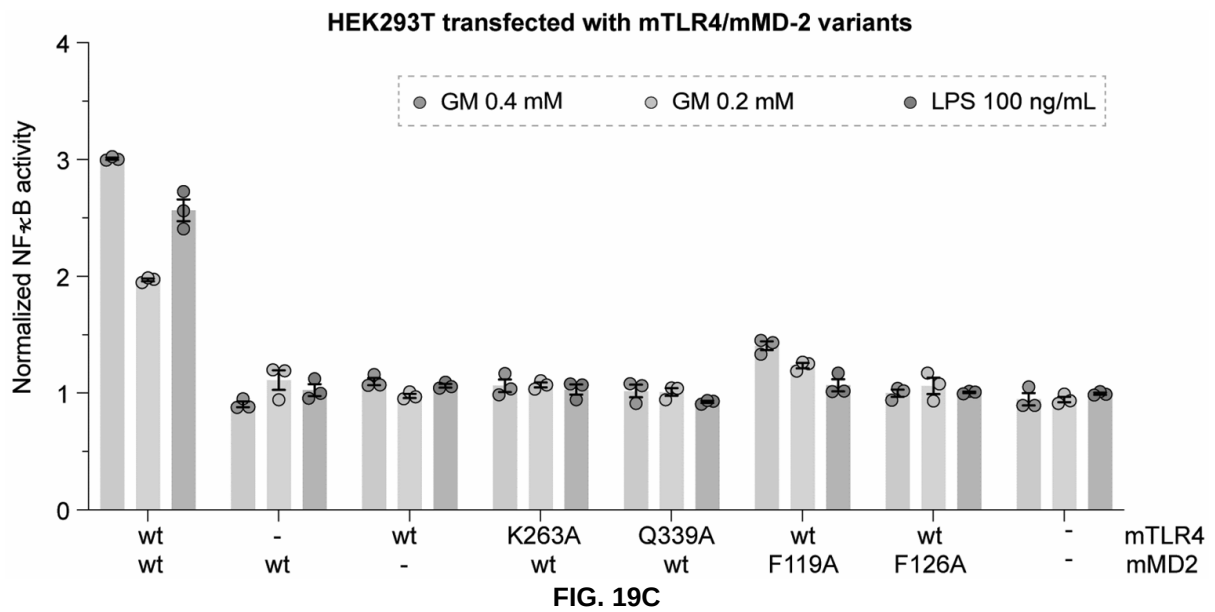


FIG. 19B



Structures of GM analogs

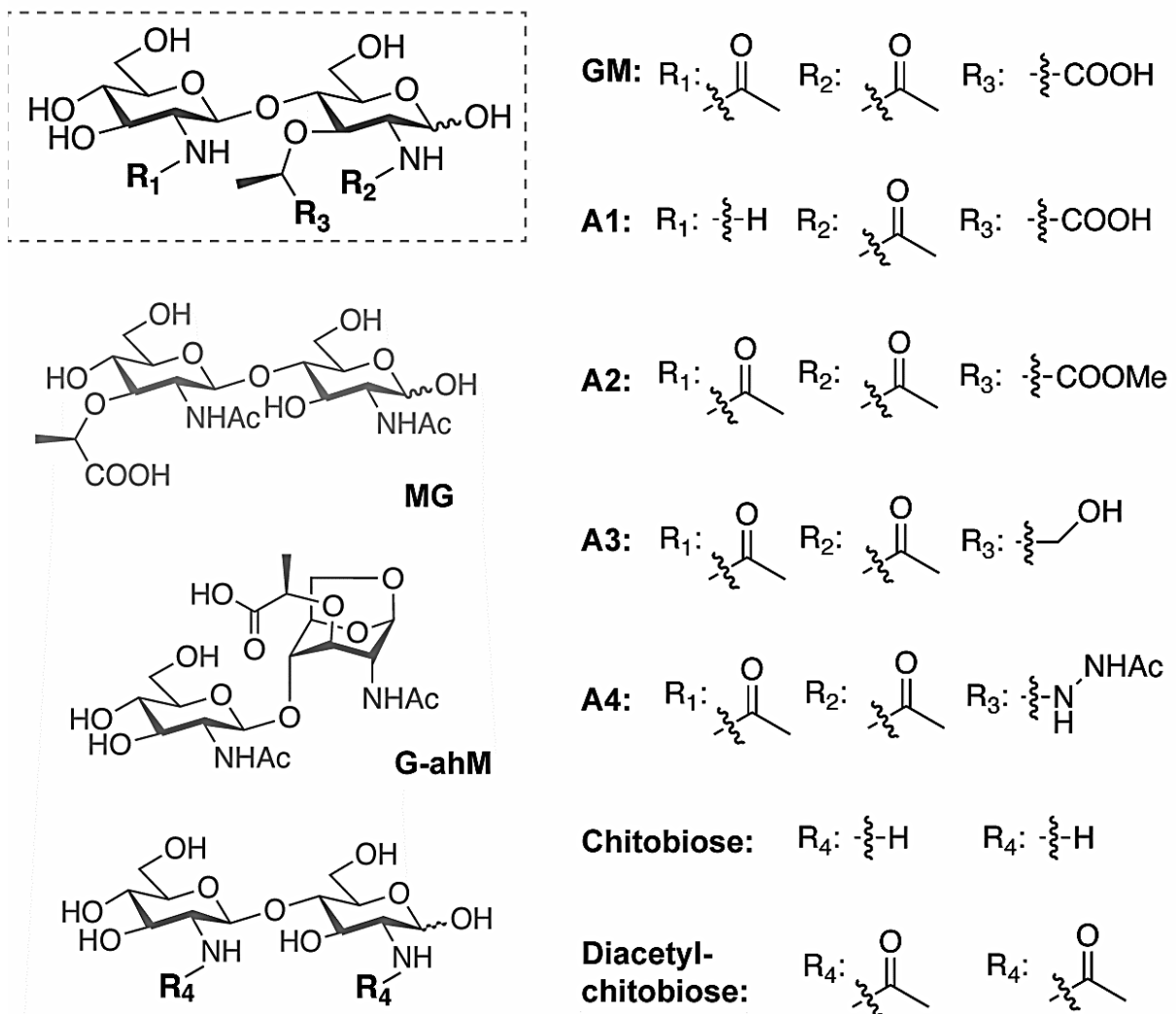


FIG. 19D

HEK-mTLR4 reporter

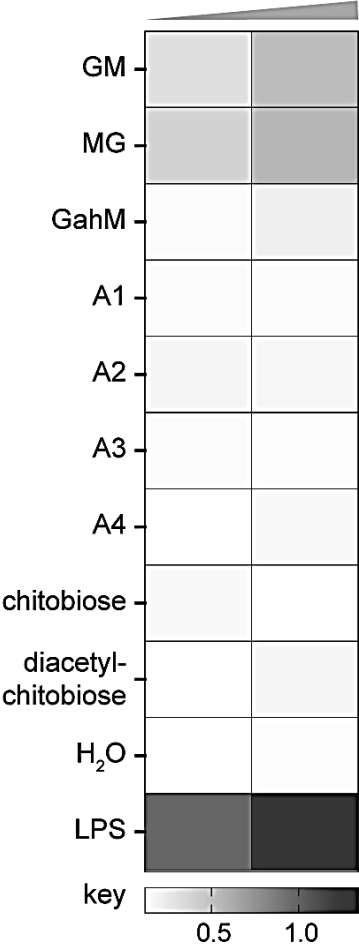


FIG. 19E

In vitro pulldown of mTLR4 by GM

	bound						unbound					
GM-1-resin	-	-	+	+	+	+	-	-	+	+	+	+
G-1-resin	-	+	-	-	-	-	-	+	-	-	-	-
mTLR4(ng)	100	100	50	100	100	100	100	100	50	100	100	100
excess GM (mM)	-	-	-	-	1	2	loading ctrl	-	-	-	-	1 2

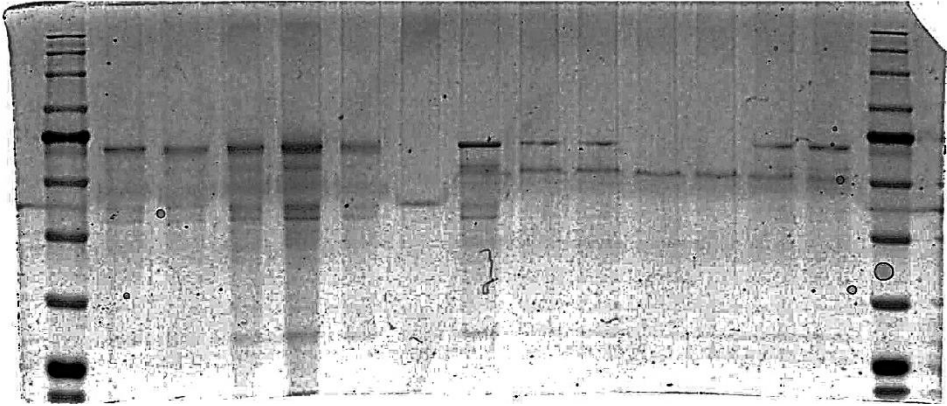


FIG. 20

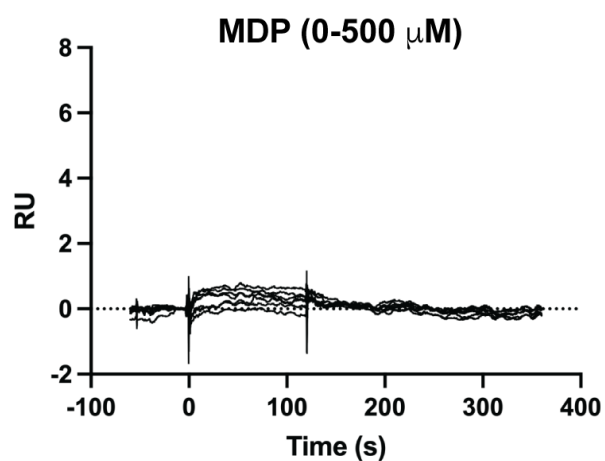


FIG. 21A

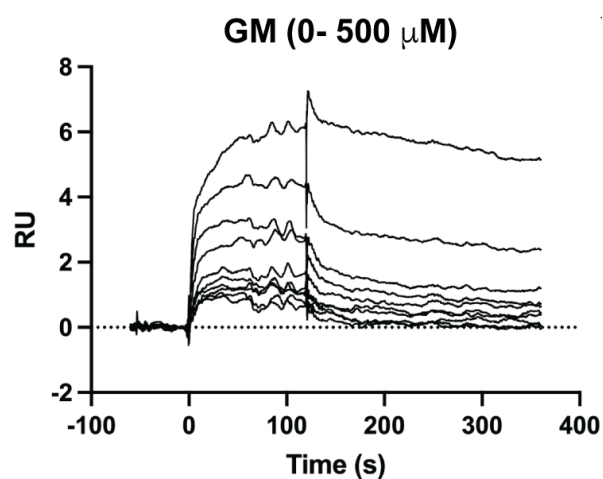


FIG. 21B

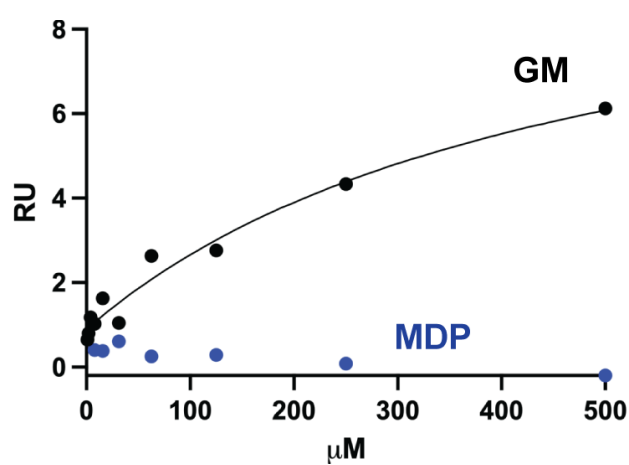


FIG. 21C

Compounds	K_D (μM)
MDP	ND
GM	383 ± 95

FIG. 21D

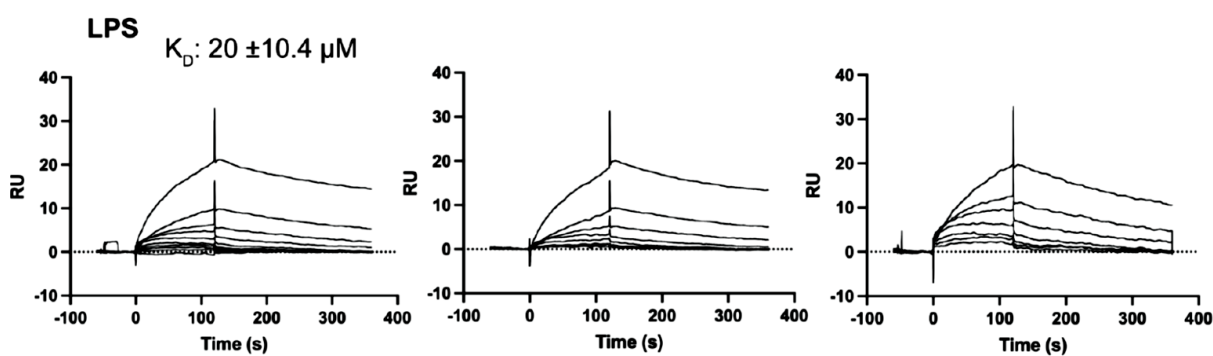
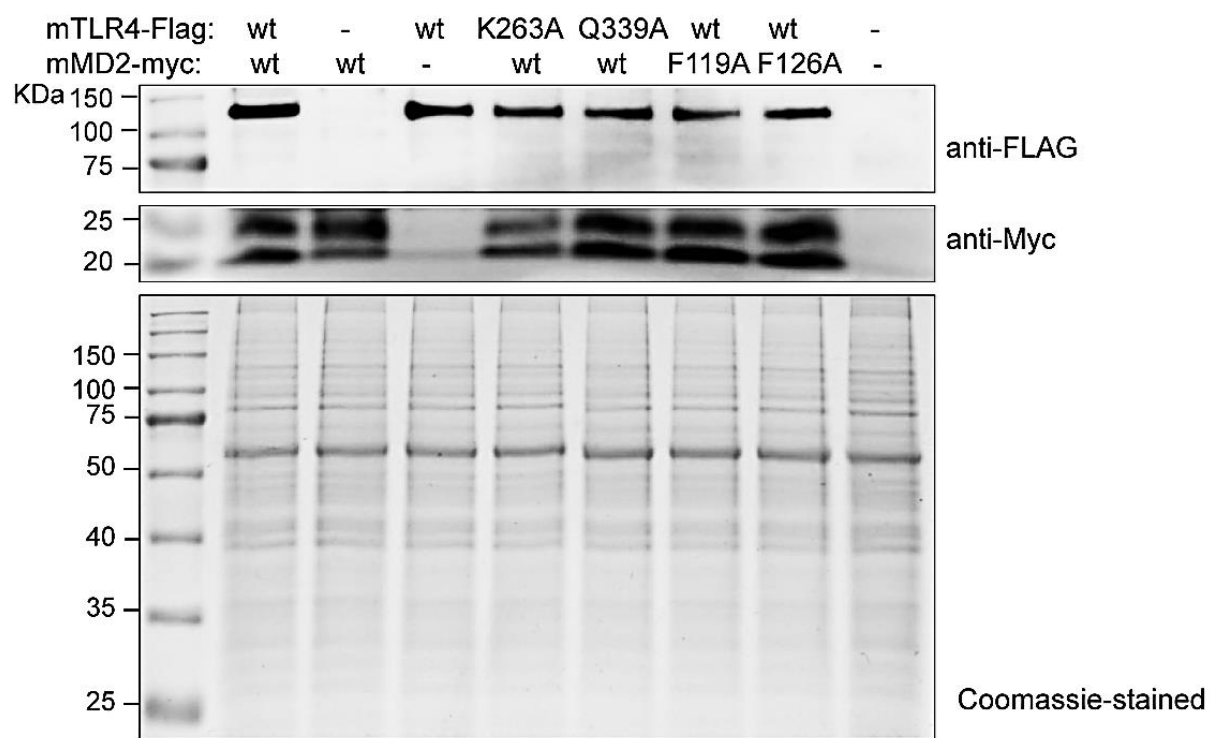
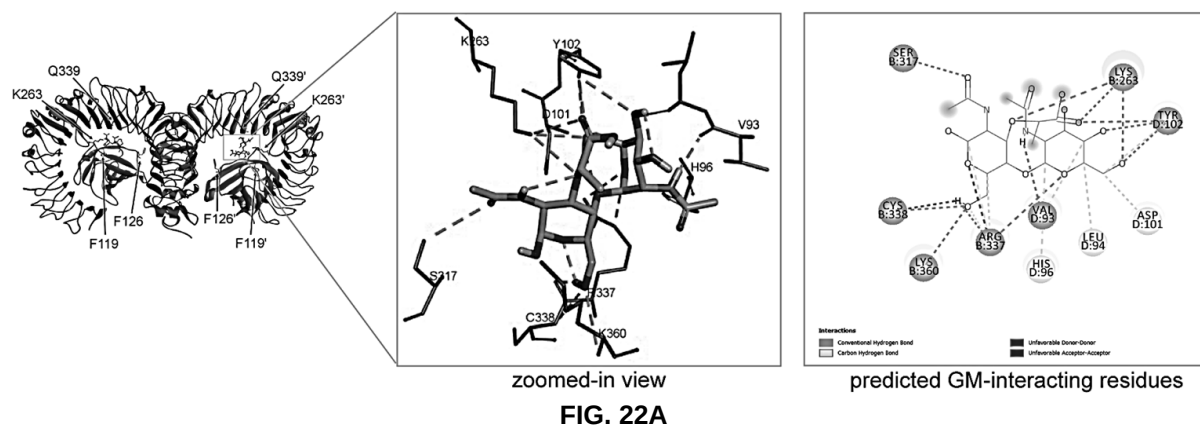


FIG. 21E



HEK-mTLR4 reporter assay for various PGNs

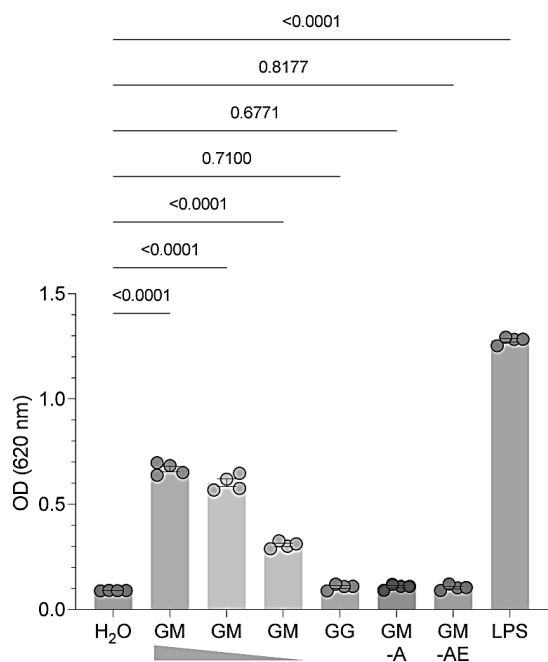


FIG. 23A

HEK-mTLR2 reporter assay for various PGNs

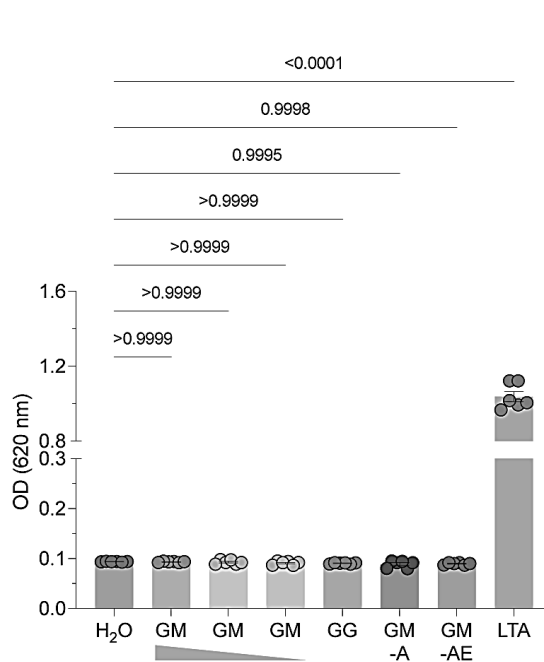


FIG. 23B

Pre-treatment of GM impedes LPS-induced TLR4 activation

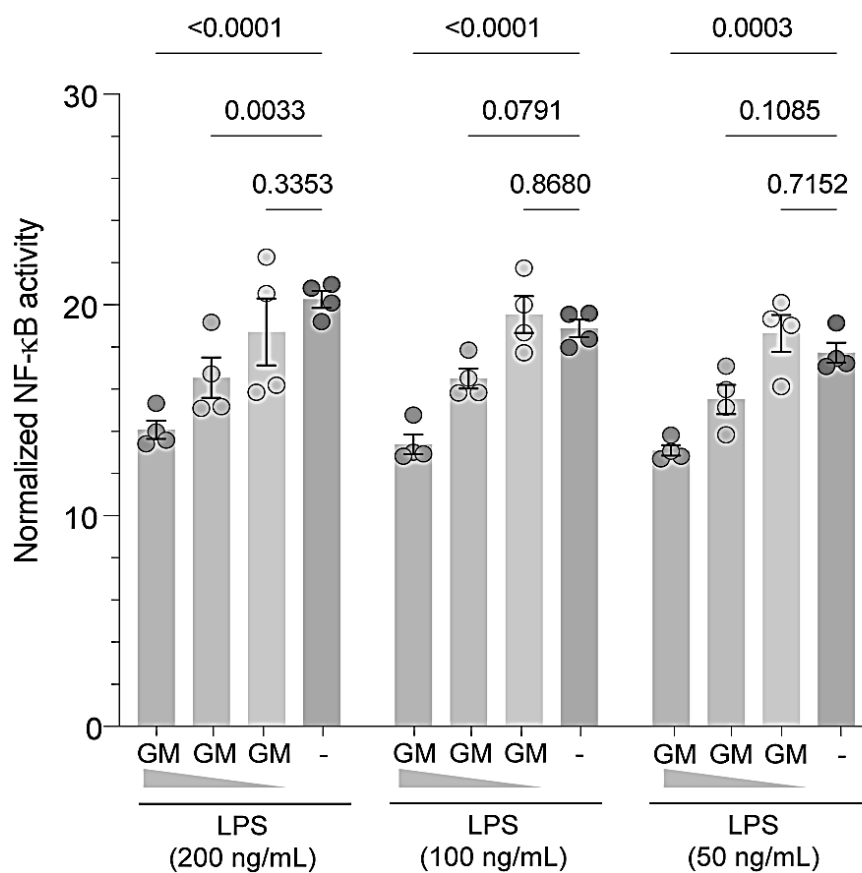


FIG. 23C

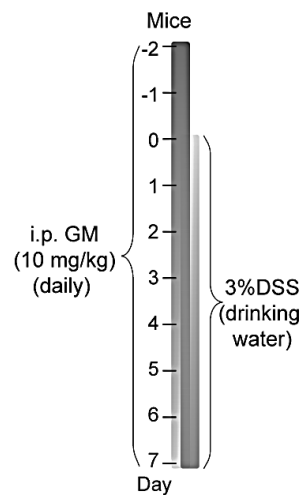


FIG. 24A

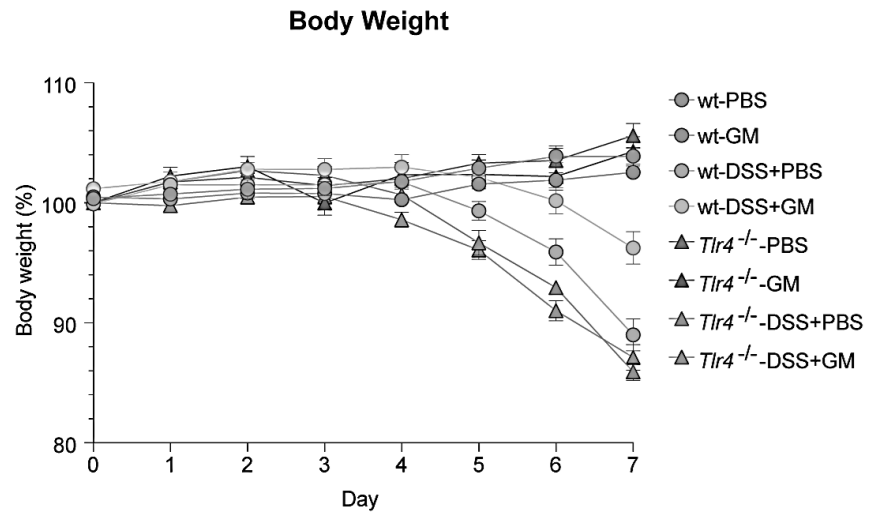


FIG.24B

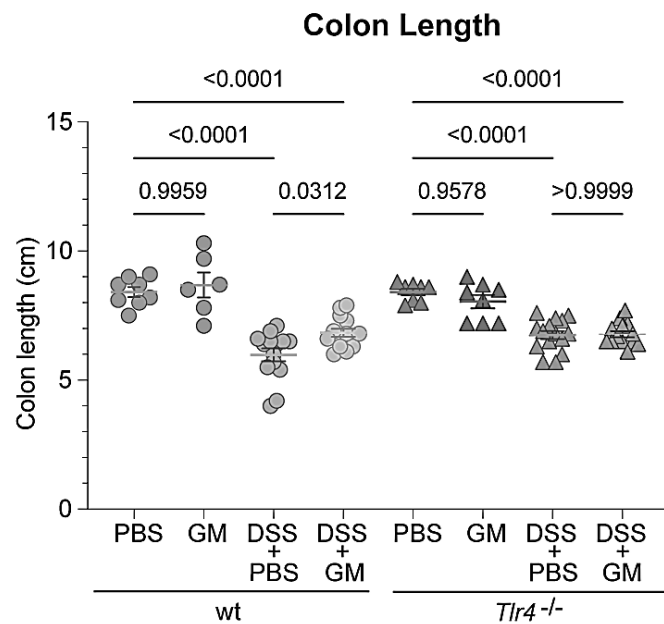


FIG. 24C

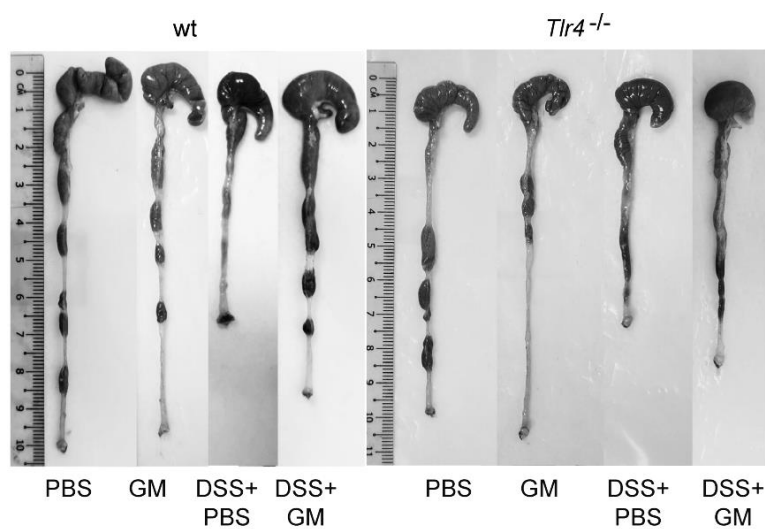


FIG. 24D

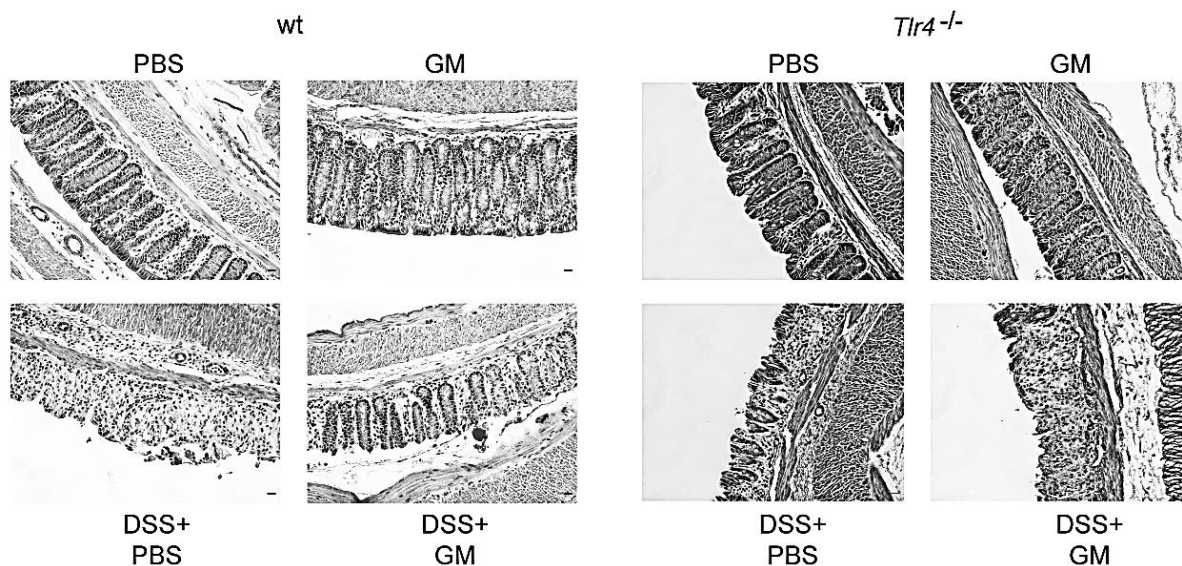


FIG. 24E

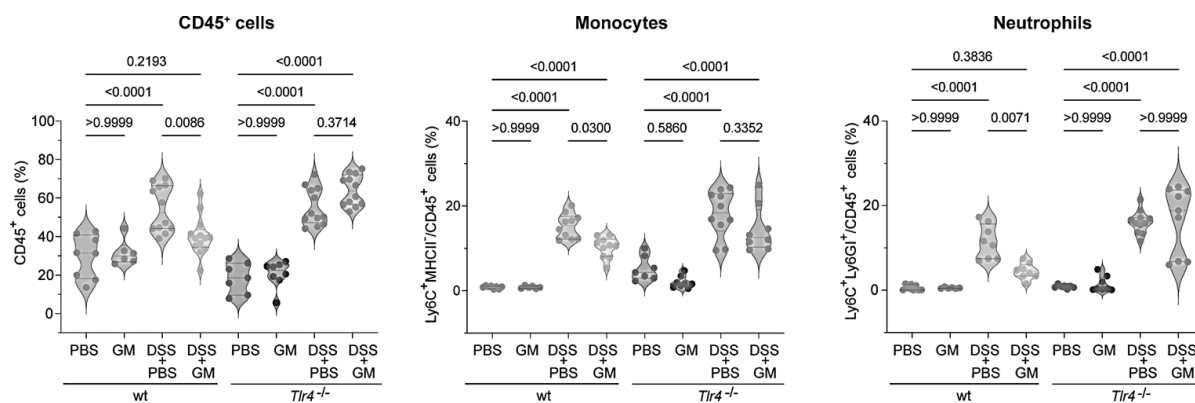


FIG. 24F

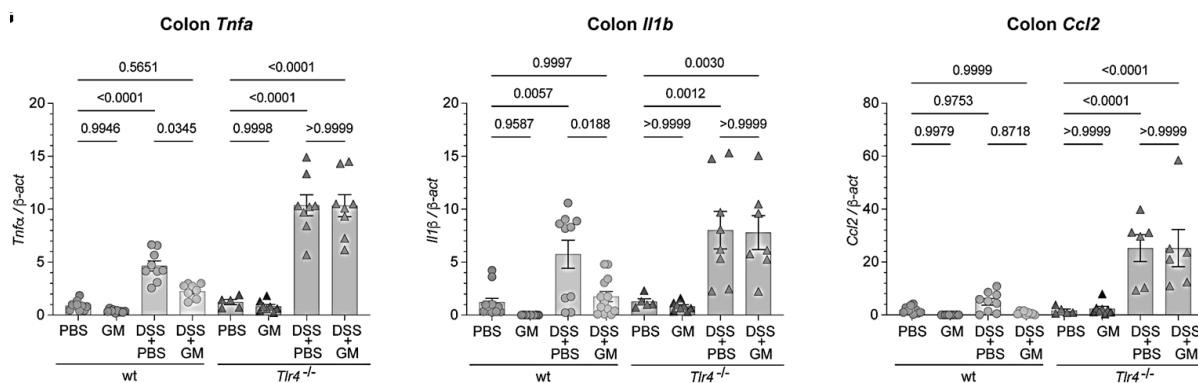


FIG. 24G

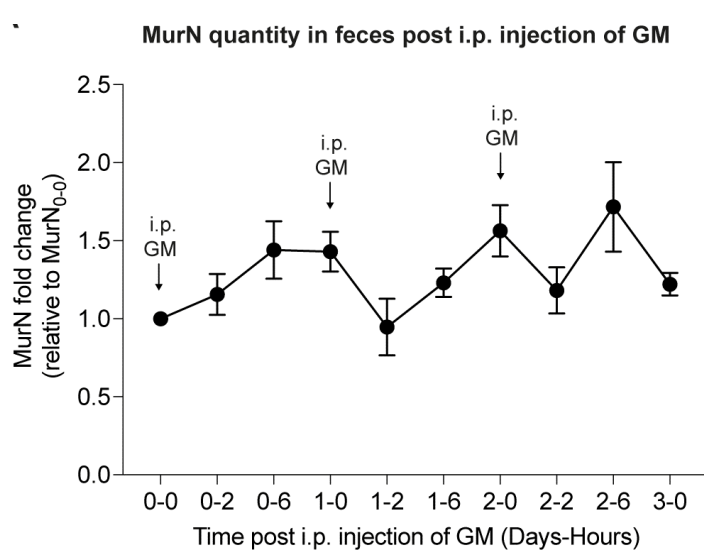


FIG. 25A

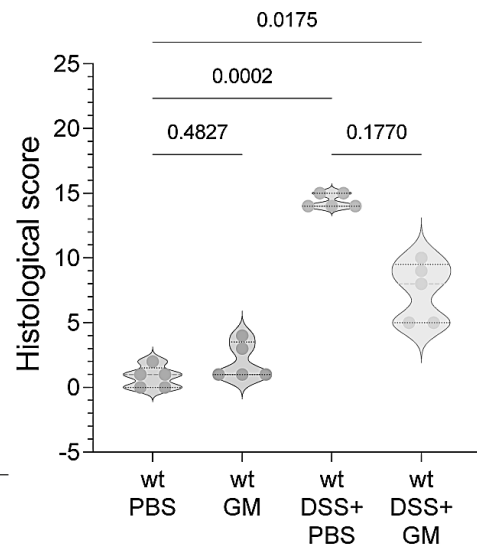


FIG. 25B

Gating for immune cell populations from mice colon

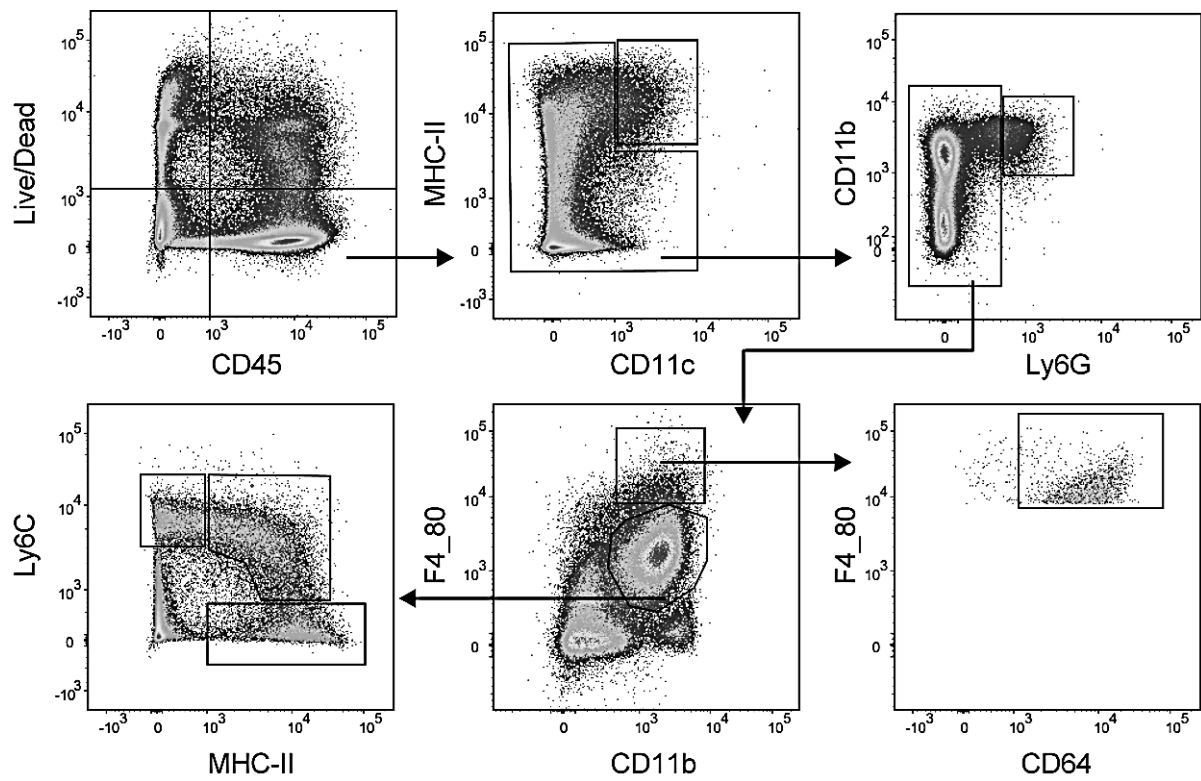


FIG. 25C

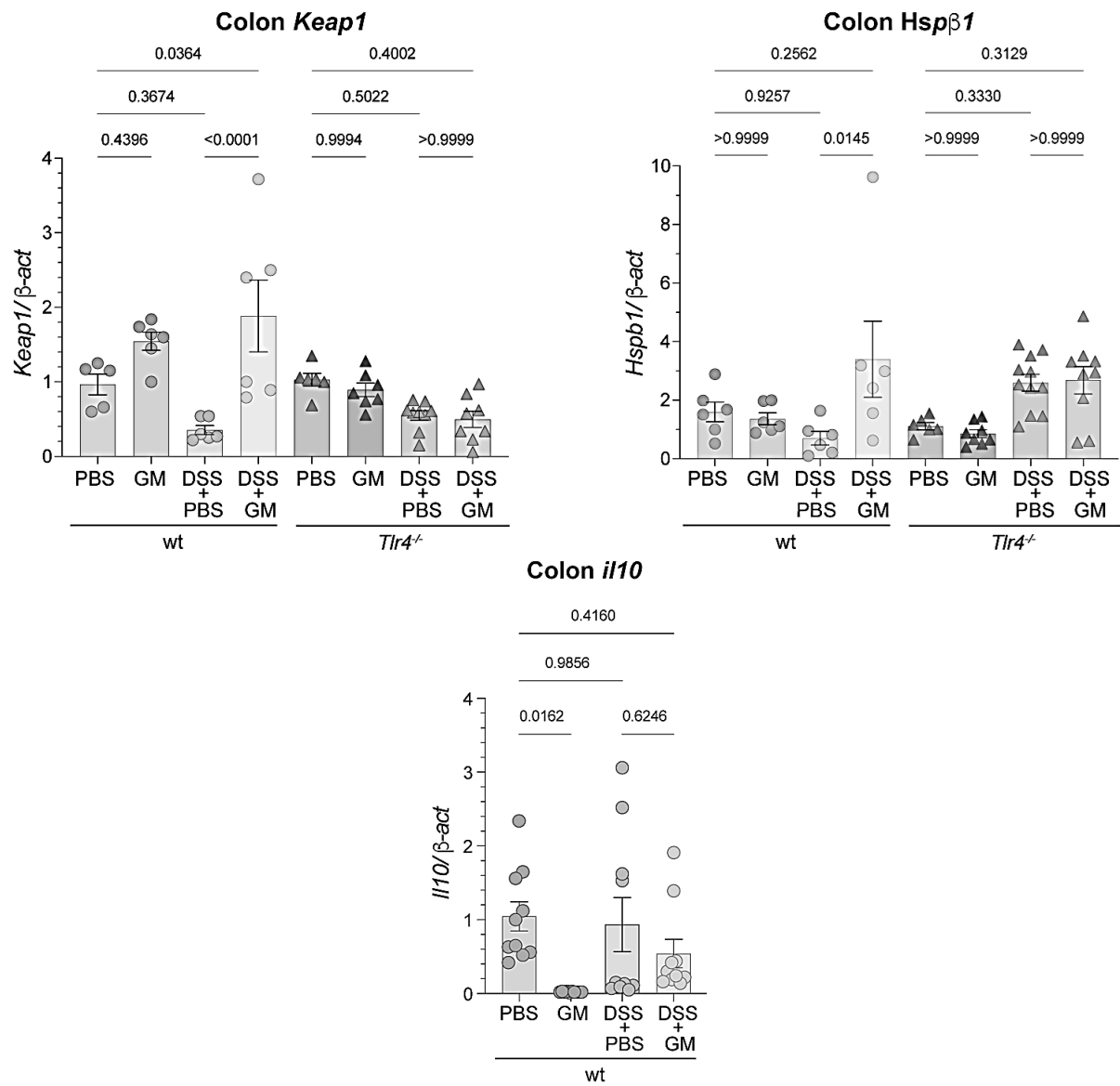


FIG. 25D

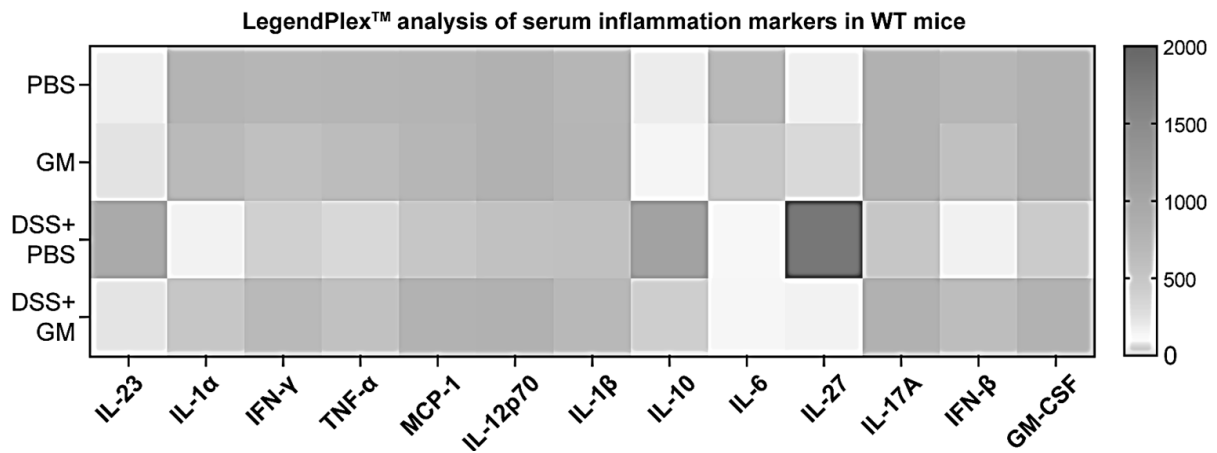


FIG. 25E

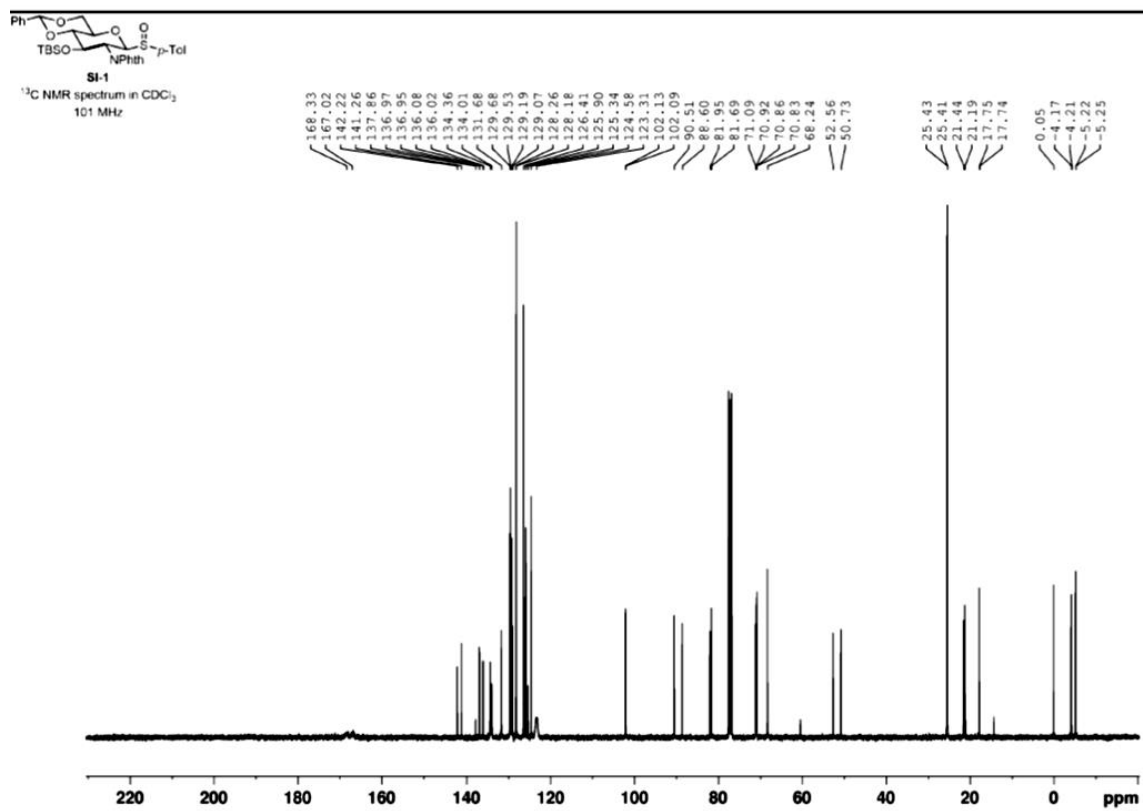
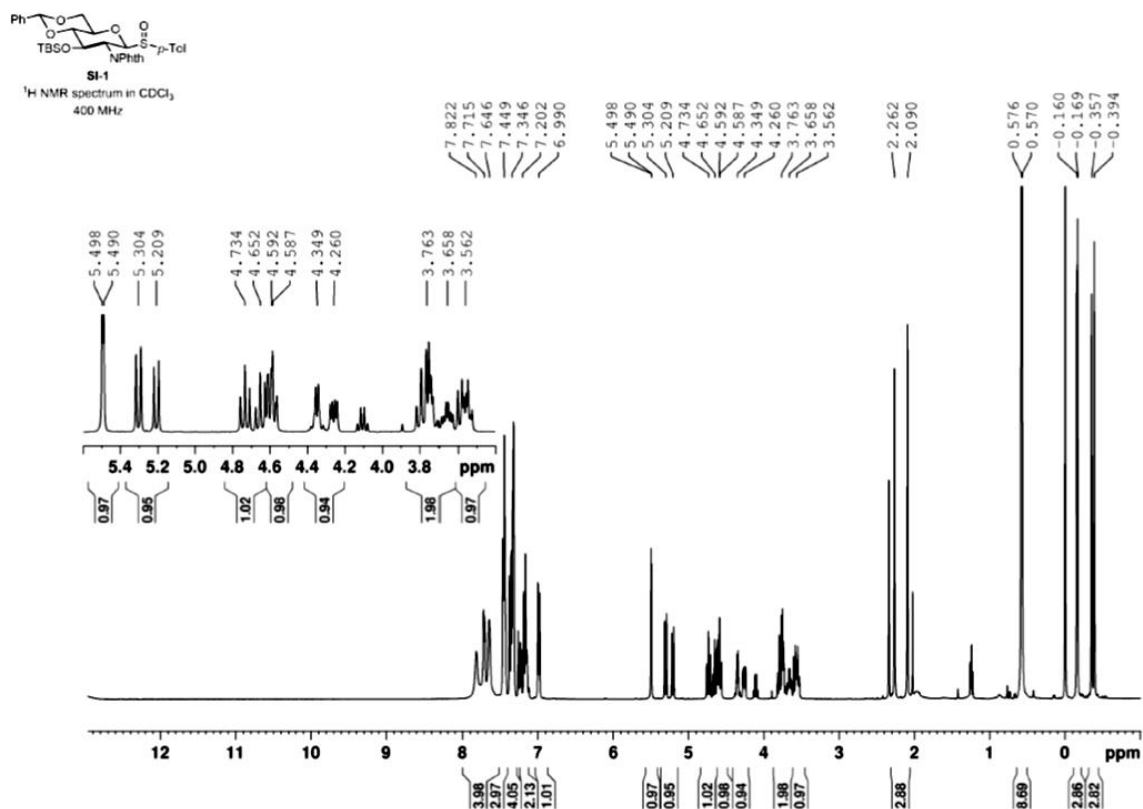


FIG. 26A

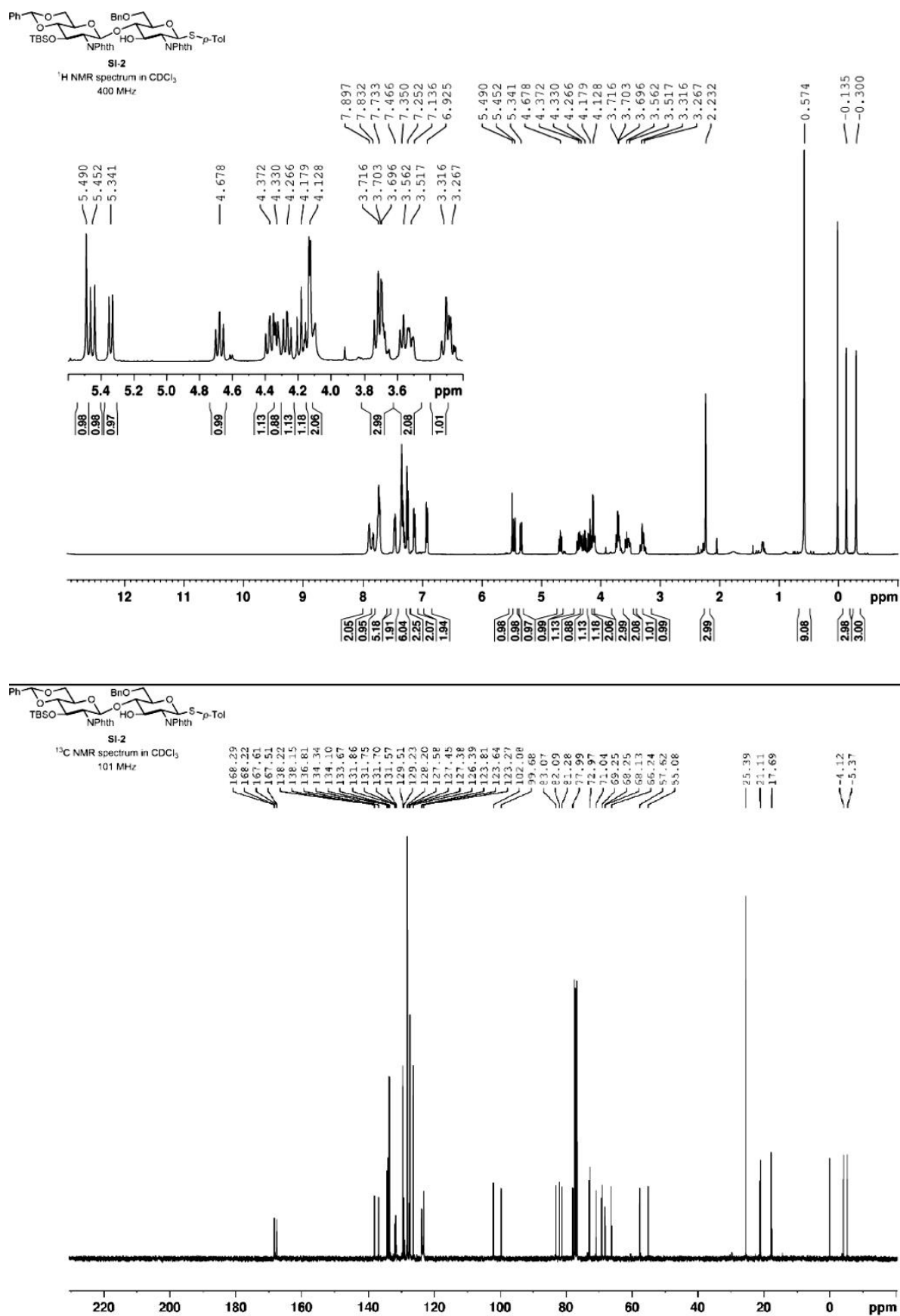


FIG. 26B

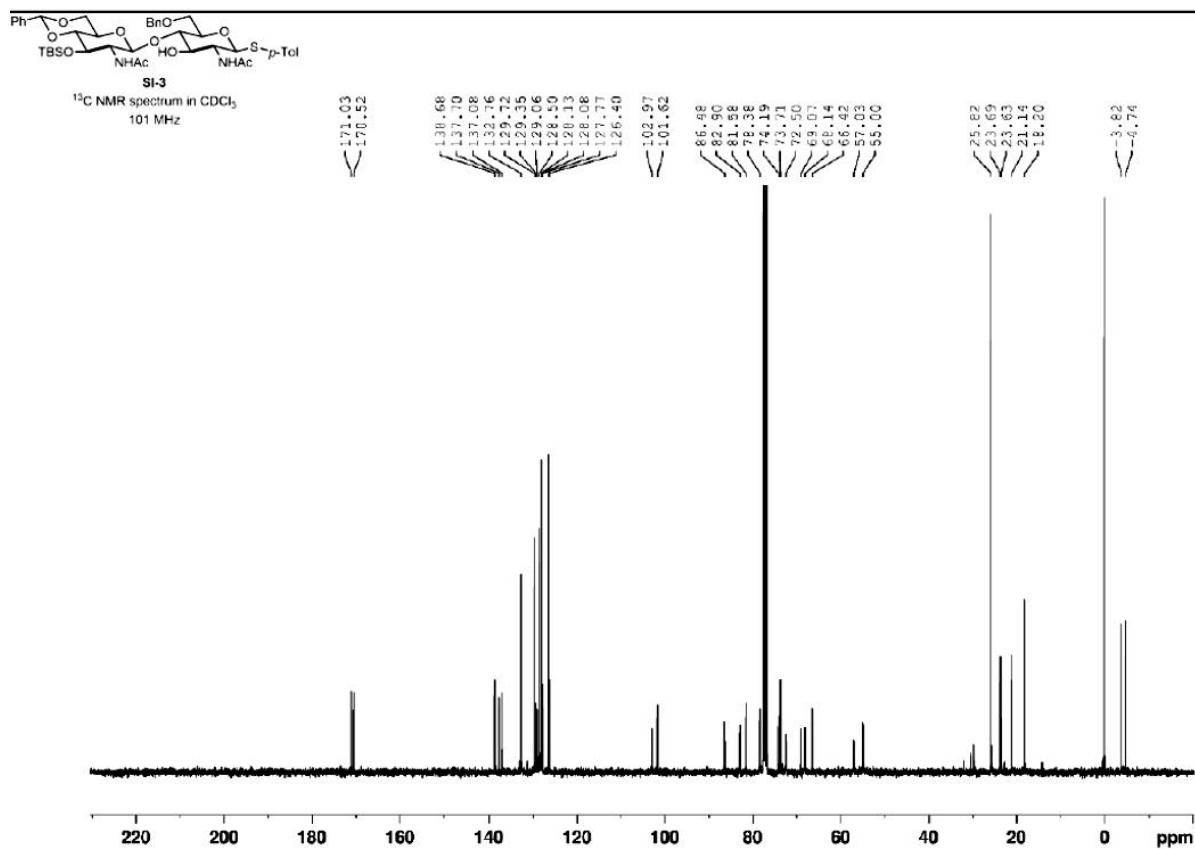
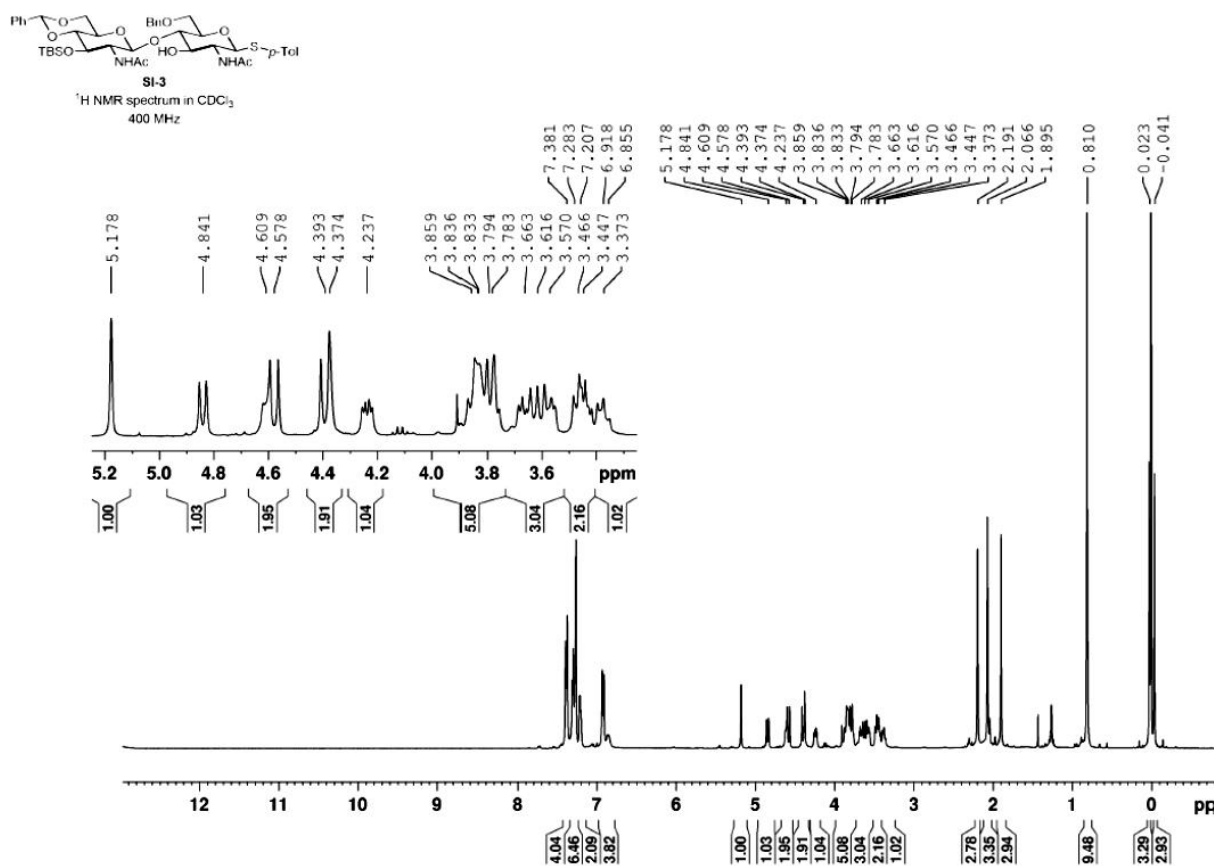


FIG. 26C

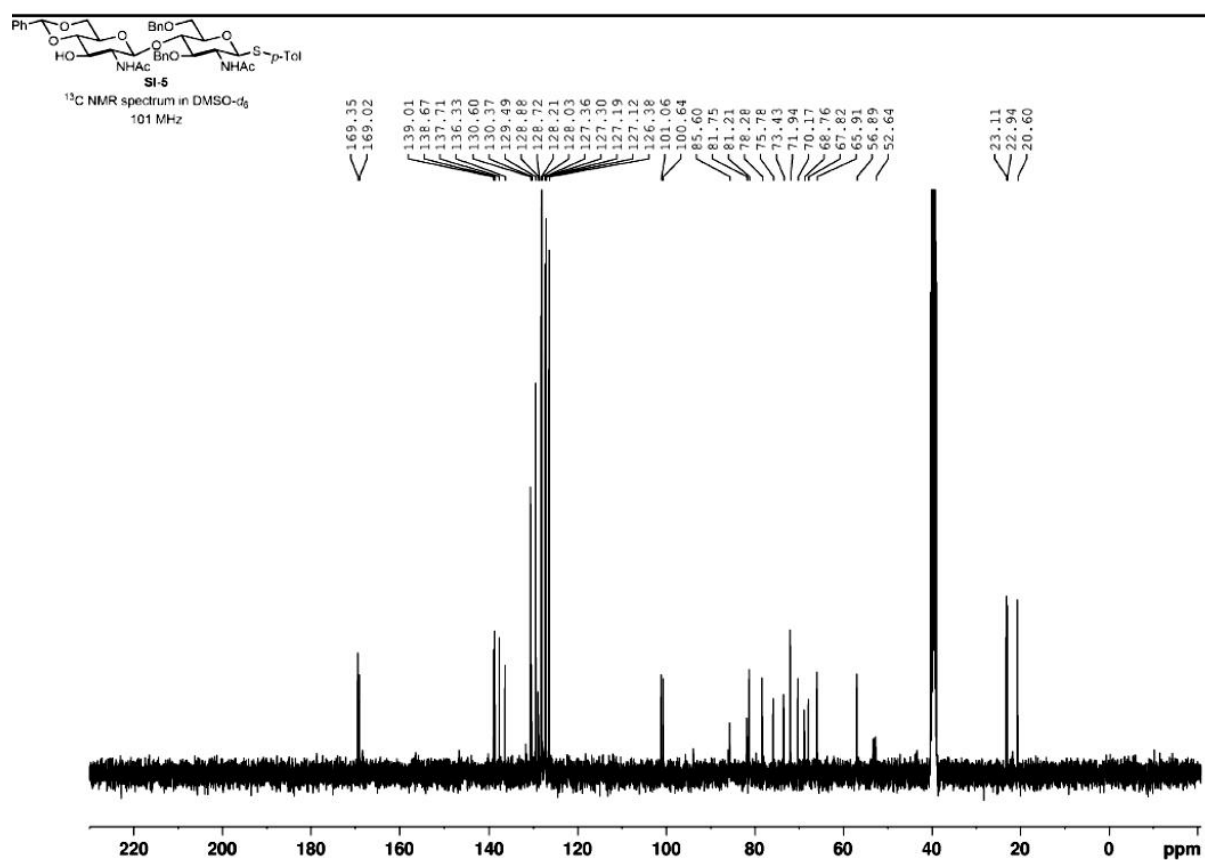
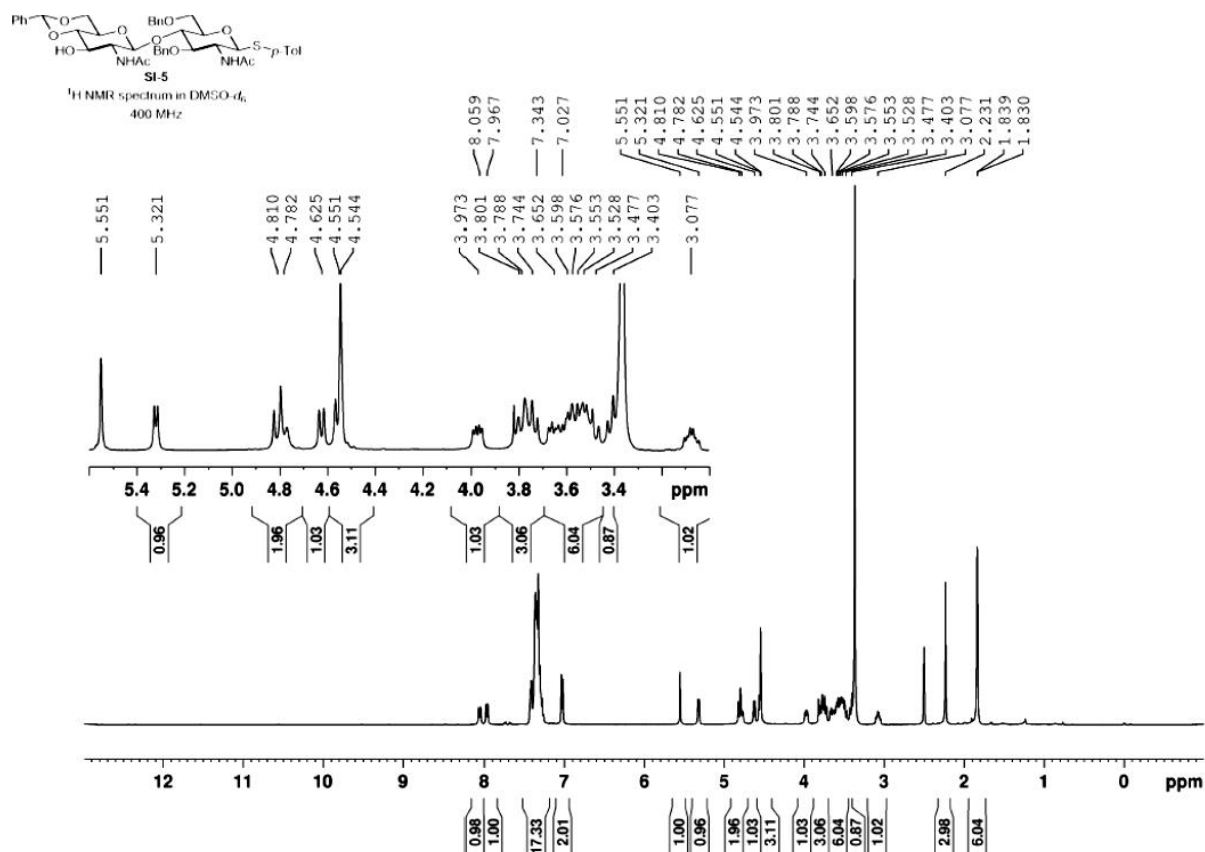


FIG. 26D

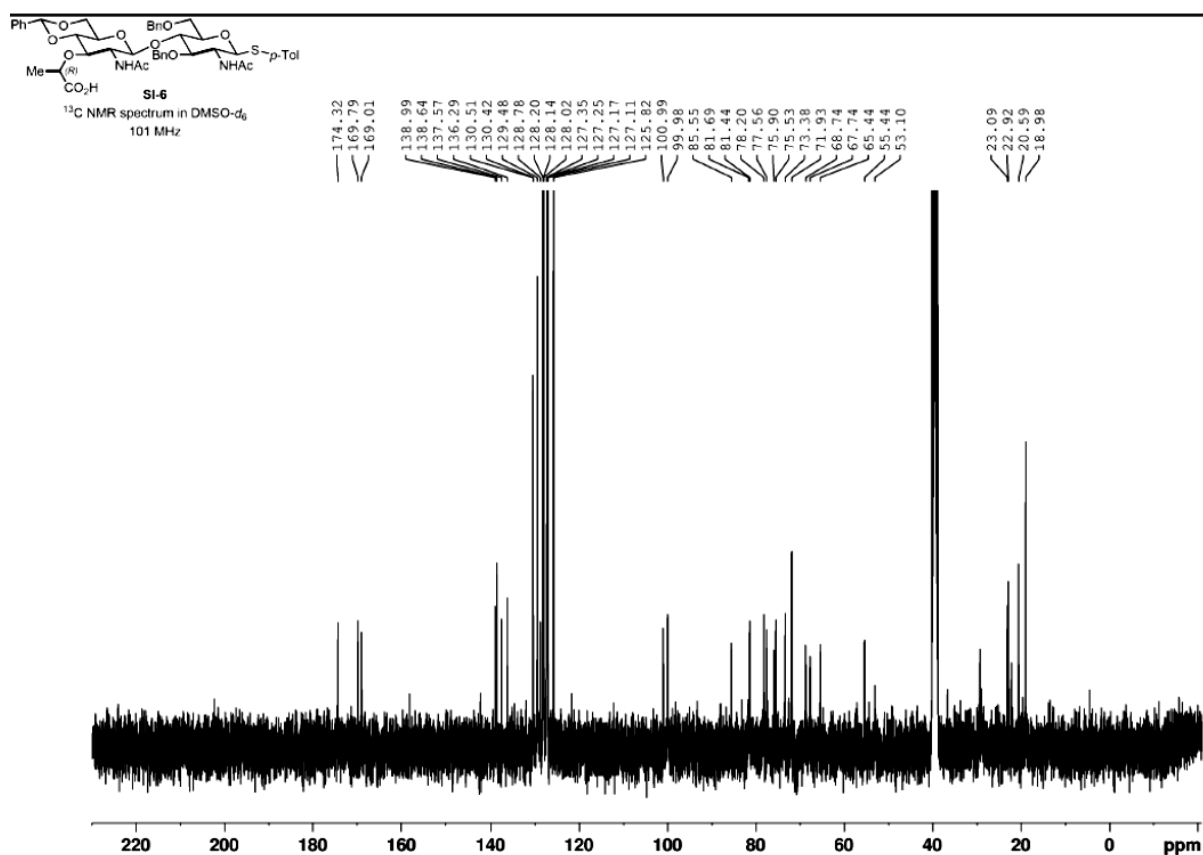
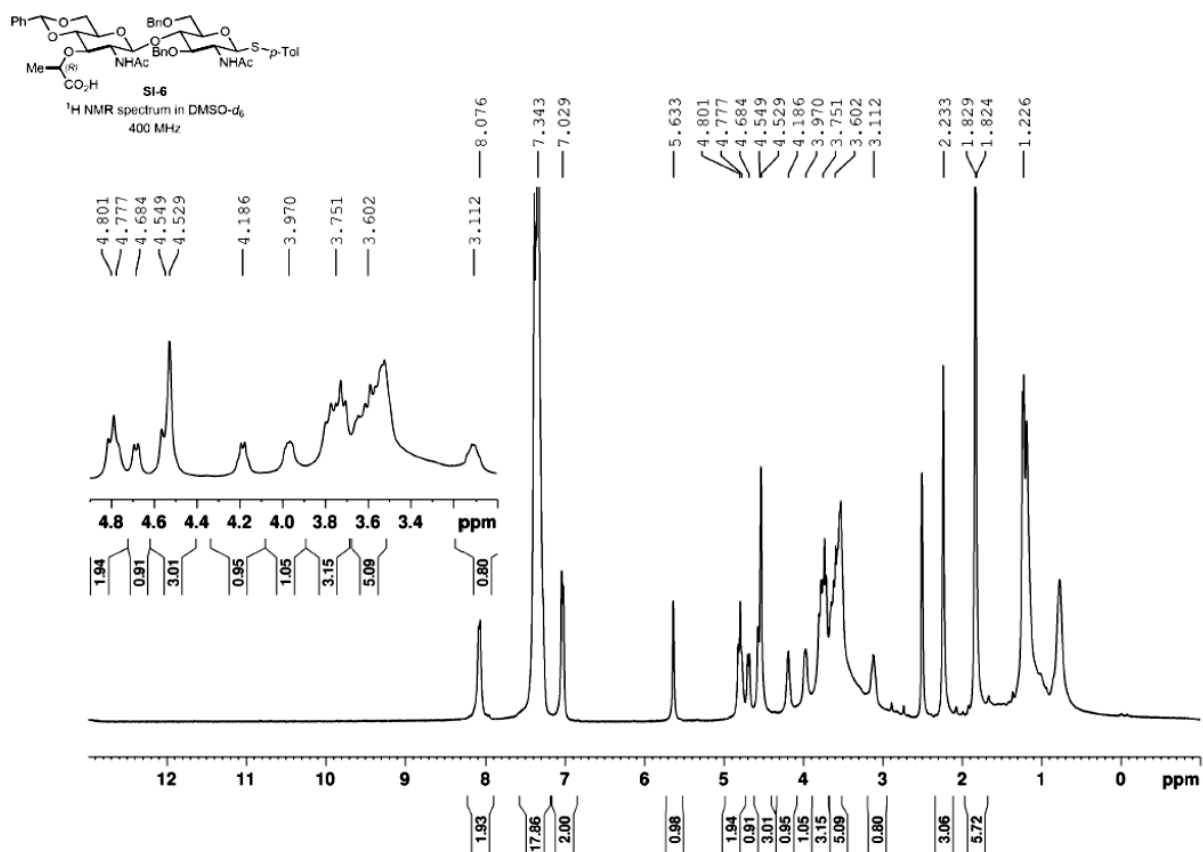


FIG. 26E

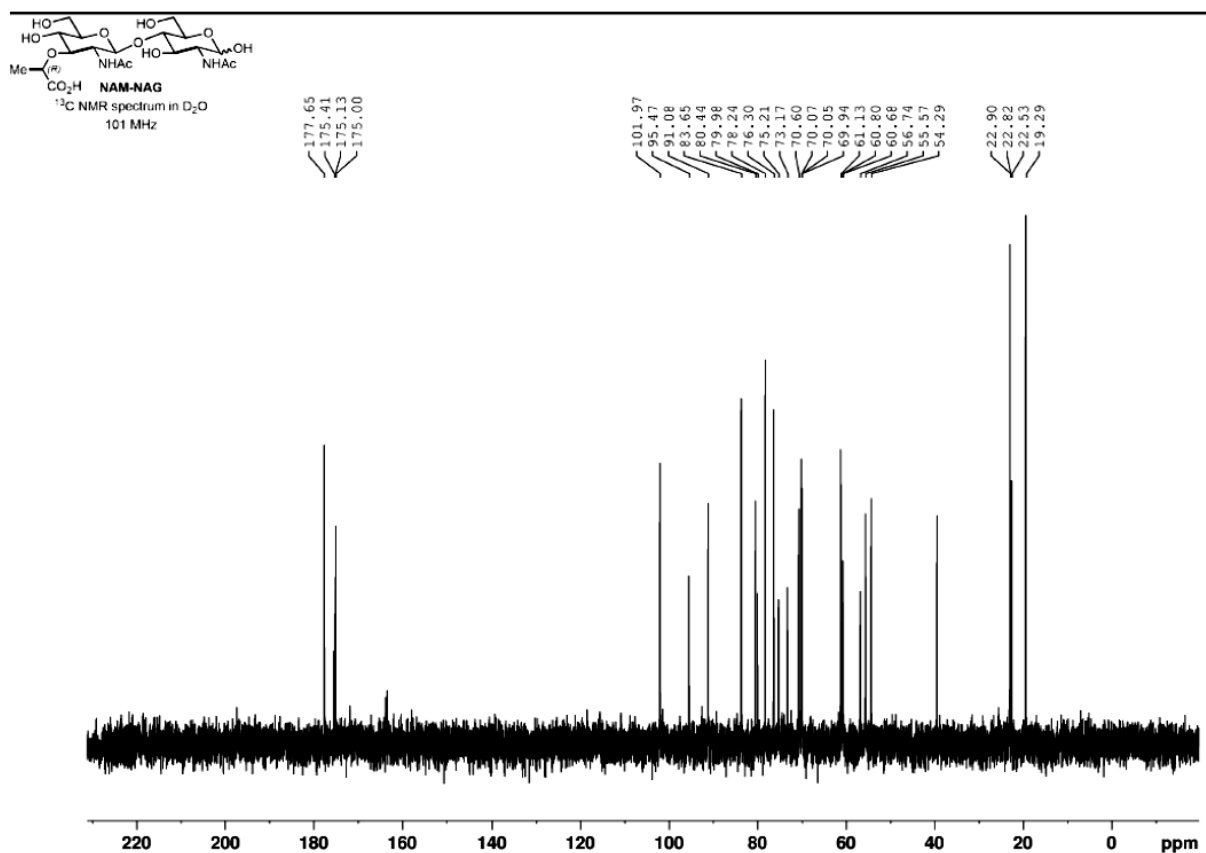
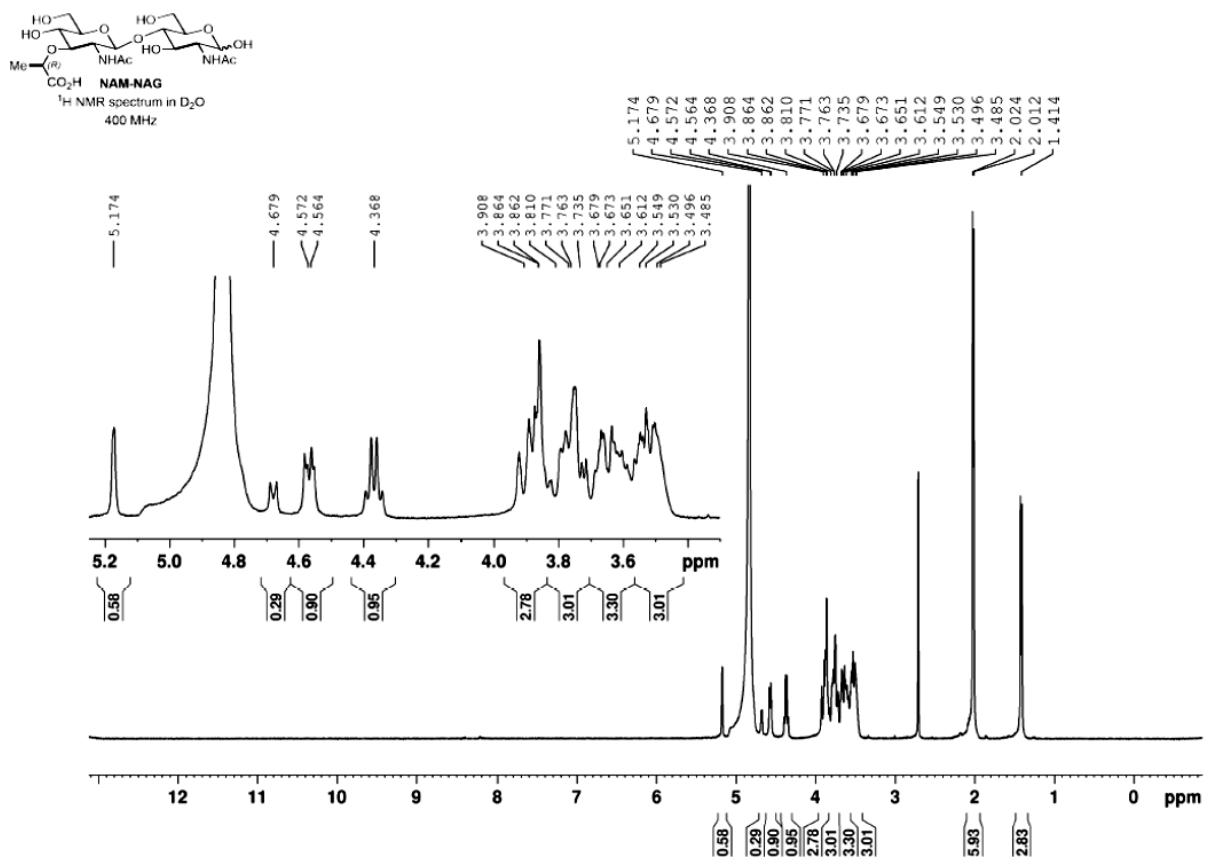


FIG. 26F

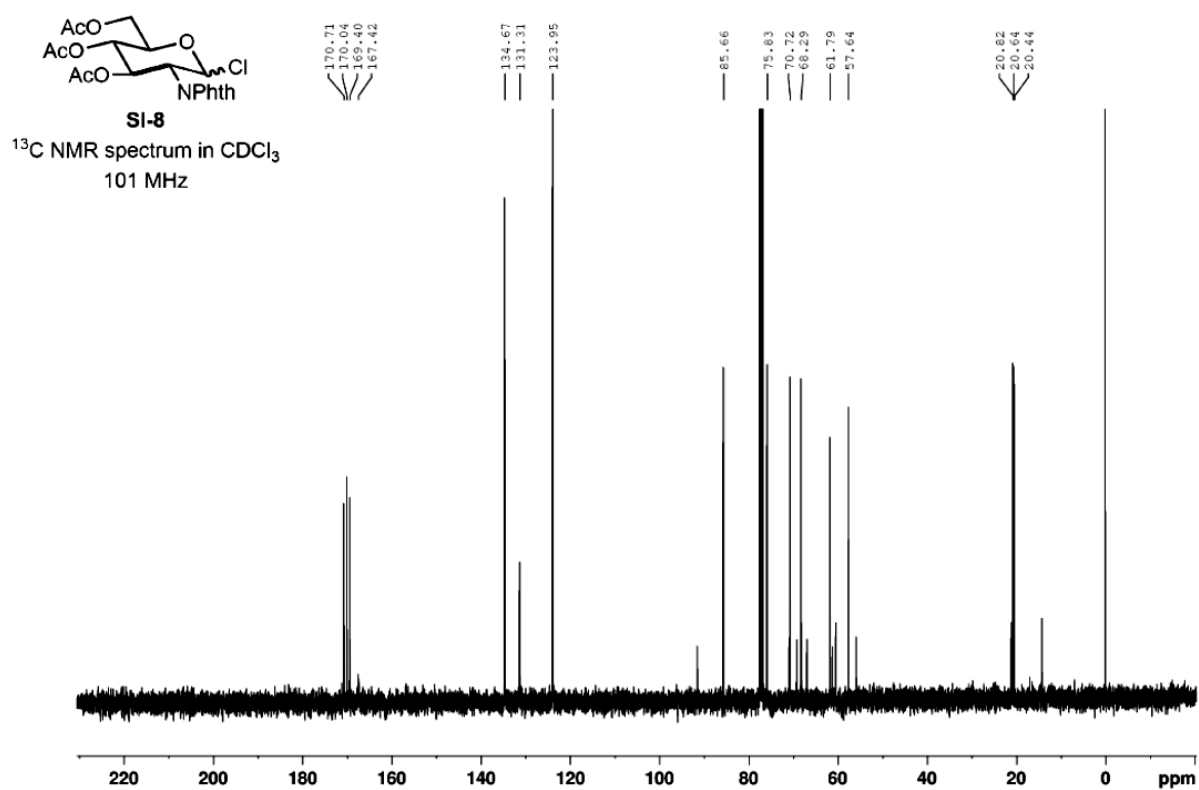
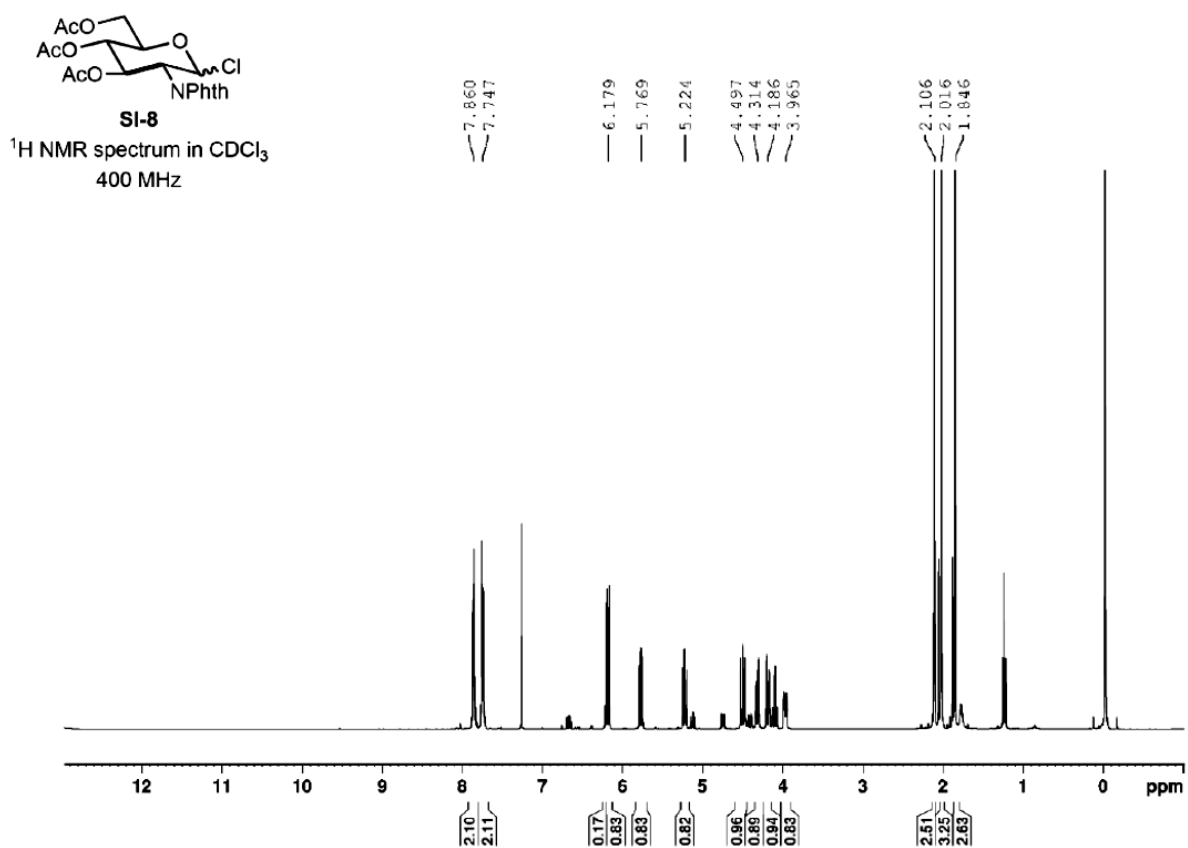


FIG. 26G

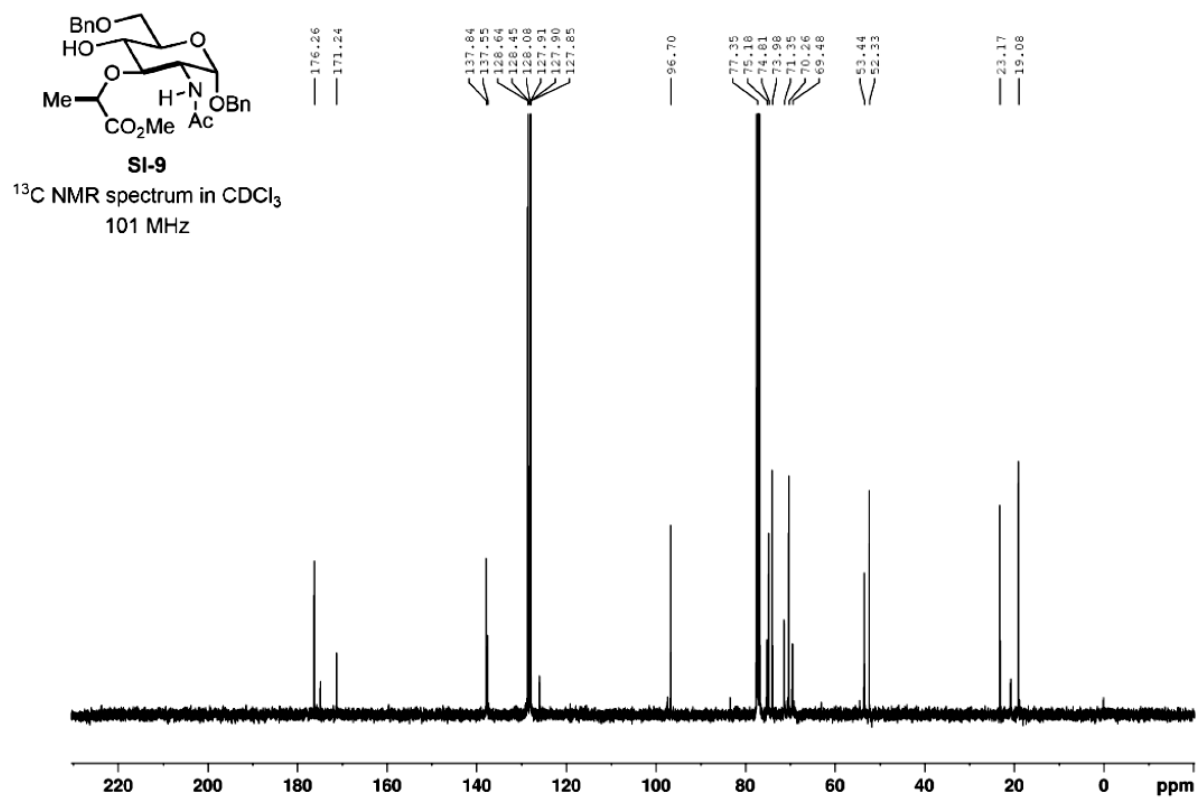
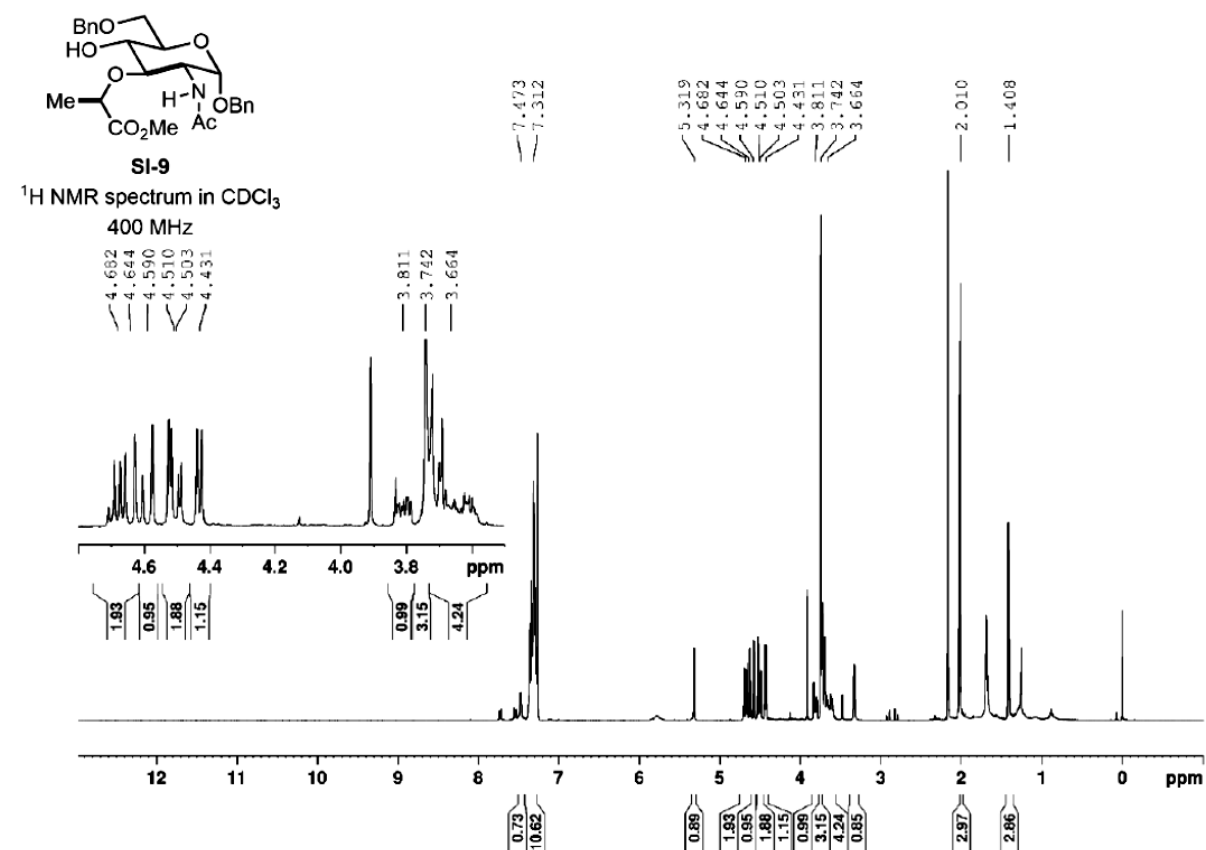


FIG. 26H

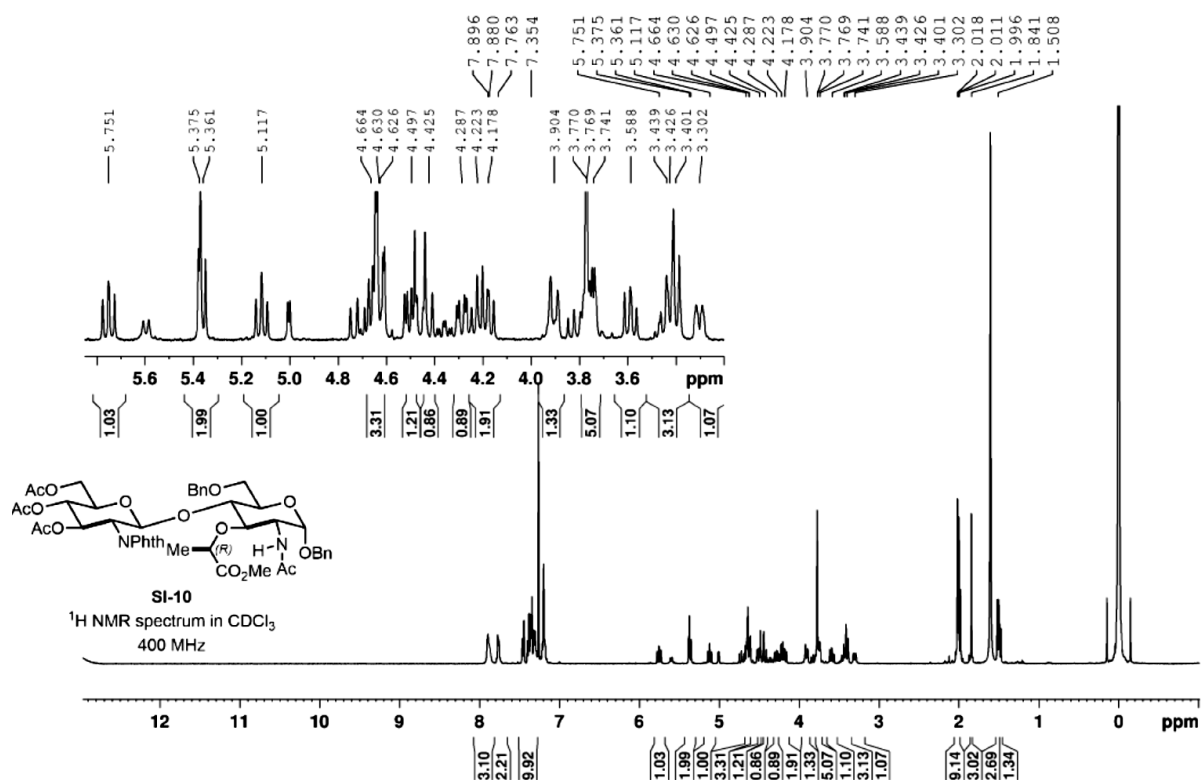


FIG. 261

