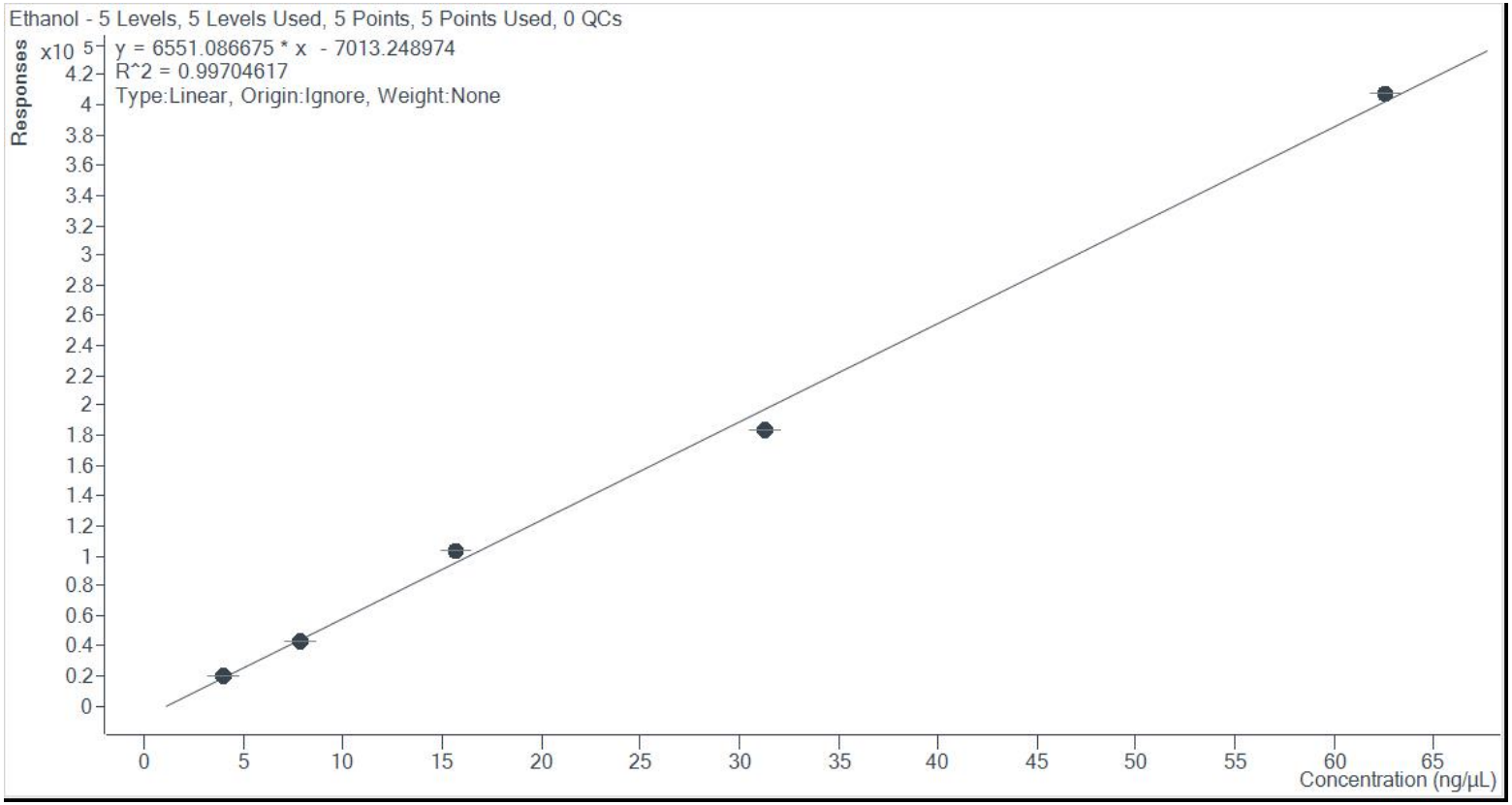
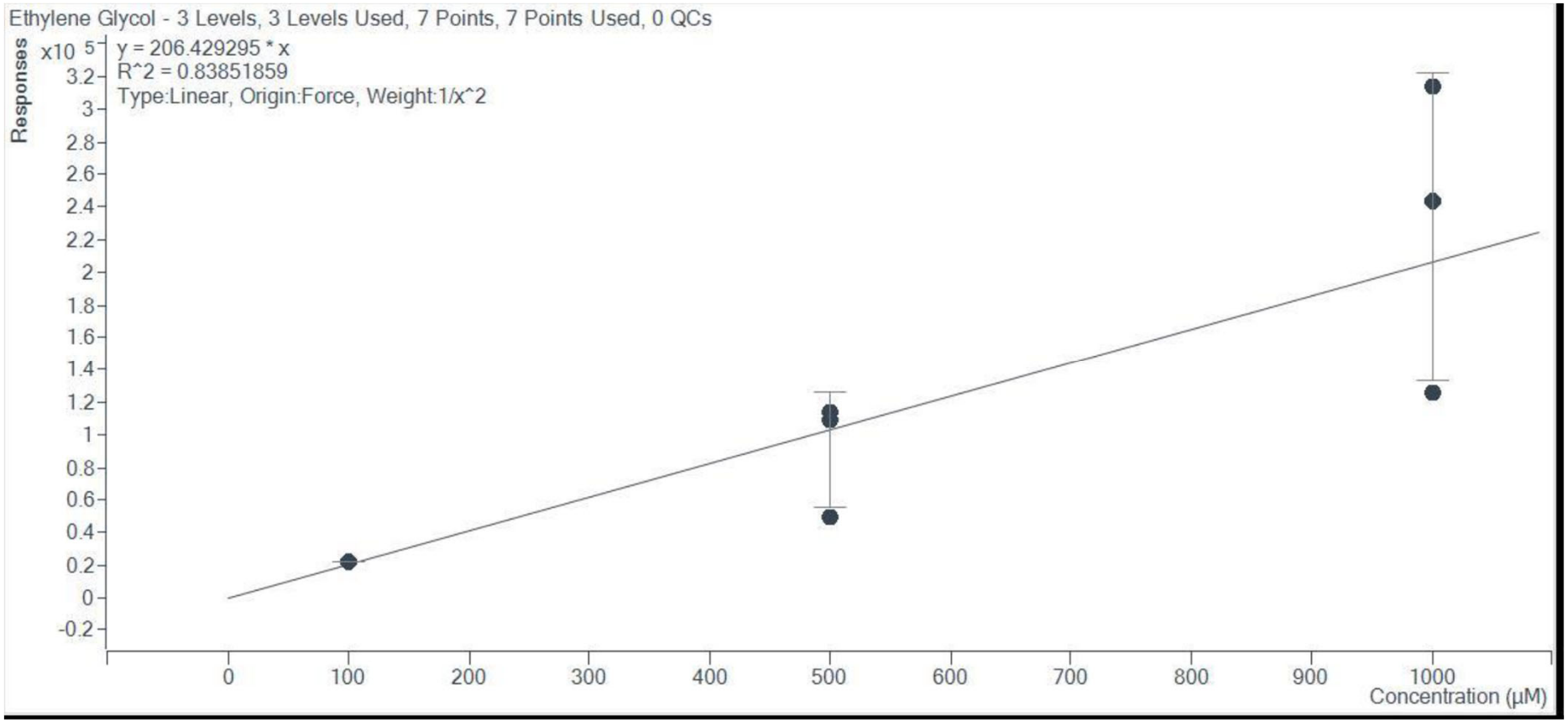
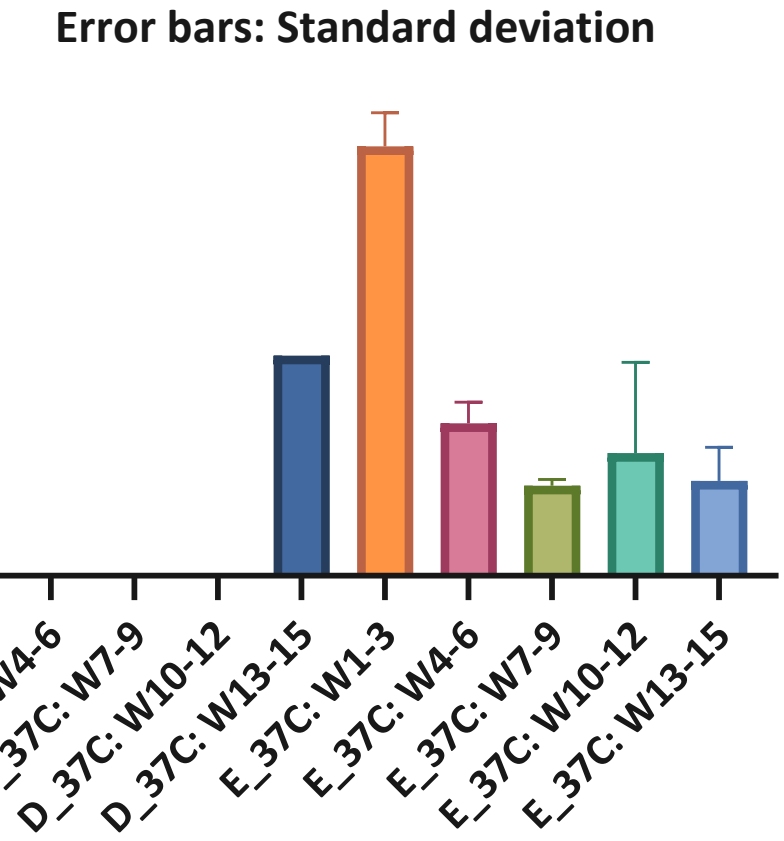
GC-MS by Kevin Murray ethanol Standard




Ethylene Glycol - 3 Levels, 3 Levels Used, 7 Points, 7 Points Used, 0 QCs
y = 206.429295 * x
R^2 = 0.83851859
Type:Linear, Origin:Force, Weight:1/x^2
Responses
x10 5
3.2
3
2.8
2.6
2.4
2.2
2
1.8
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
-0.2
0
100
200
300
400
500
600
700
800
900
1000
Concentration (µM)

nol quantification - GC-MS: Hydrolysis



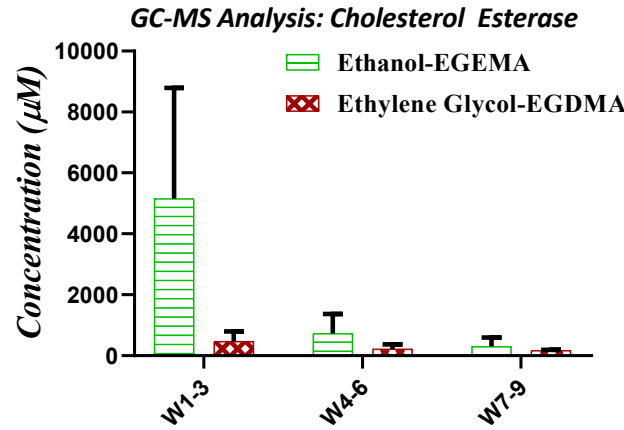
	Ethylene Glycol-EGDMA-Hydrolytic-1	Ethylene Glycol-EGDMA-Hydrolytic-2	Ethylene Glycol-EGDMA-Hydrolytic-3
37C: W1-3	12.1646	14.6926	12.3
37C: W4-6			
37C: W7-9			
37C: W10-12			
37C: W13-15	15.2705		
	Ethanol-EGEMA-Hydrolytic-1	Ethanol-EGEMA-Hydrolytic-2	Ethanol-EGEMA-Hydrolytic-3
37C: W1-3	27.2999	30.2291	31.89
37C: W4-6	9.3126	12.2003	10.2
37C: W7-9	6.0111	6.0068	6.73
37C: W10-12	15.726	4.0499	5.75
37C: W13-15	8.8094	6.7592	4.17

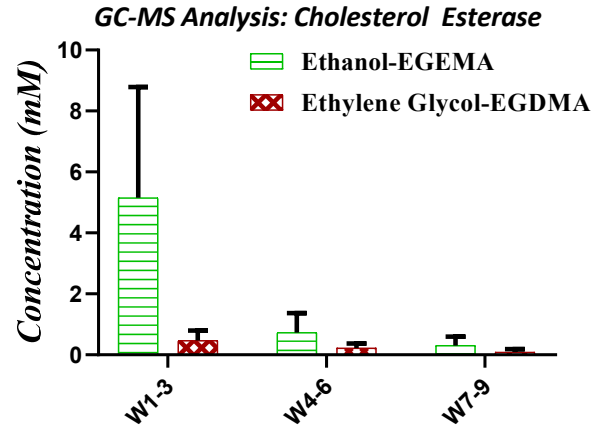
Quantification not reproducible

Ethylene Glycol and Ethanol – GC-MS

Quantification not reproducible

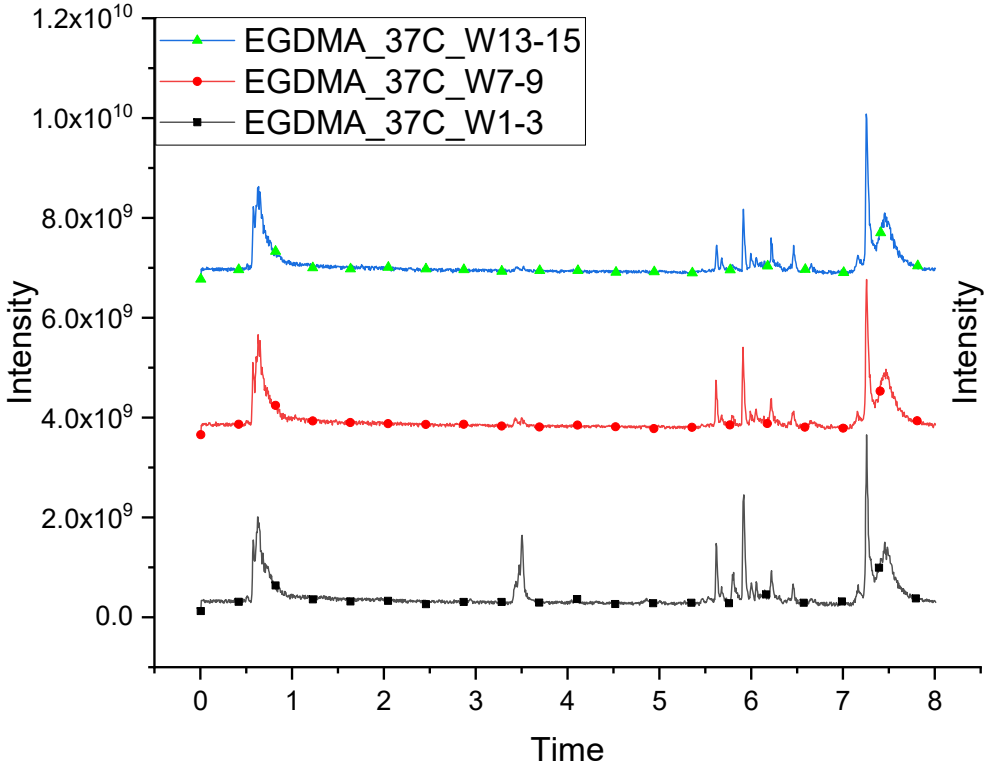
	Ethanol-EGEMA-Cholesterol Esterase-1	Ethanol-EGEMA-Cholesterol Esterase-2	Ethanol-EGEMA-Cholesterol Esterase-3	Ethanol-EGEMA-Cholesterol Esterase-4
W1-3	1.700757	2.383058	8.770868	7.768224
W4-6	0.621621	0.211314	0.419943	1.656754
W7-9	0.122239	0.095387	0.28898	0.715173
	Ethylene Glycol-EGDMA-Cholesterol Esterase-1	Ethylene Glycol-EGDMA-Cholesterol Esterase-2	Ethylene Glycol-EGDMA-Cholesterol Esterase-3	Ethylene Glycol-EGDMA-Cholesterol Esterase-4
W1-3	0.367798	0.951917	0.320914	0.237109
W4-6	0.101864	0.438683	0.15444	0.192651
W7-9	0	0.157699	0	0.188275

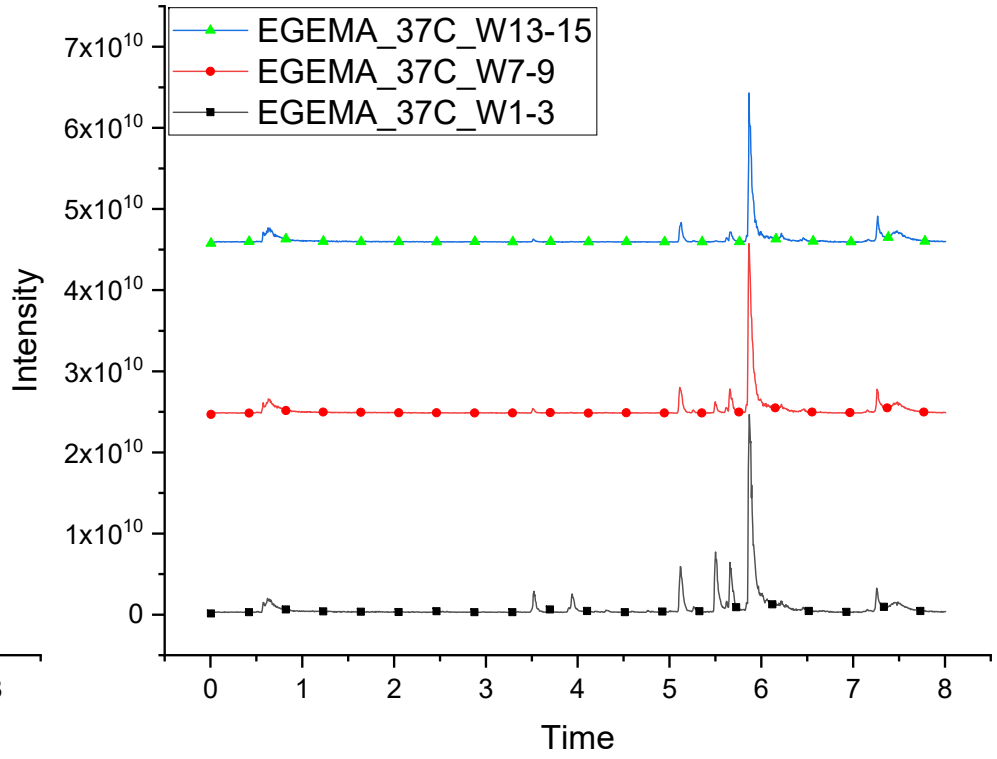




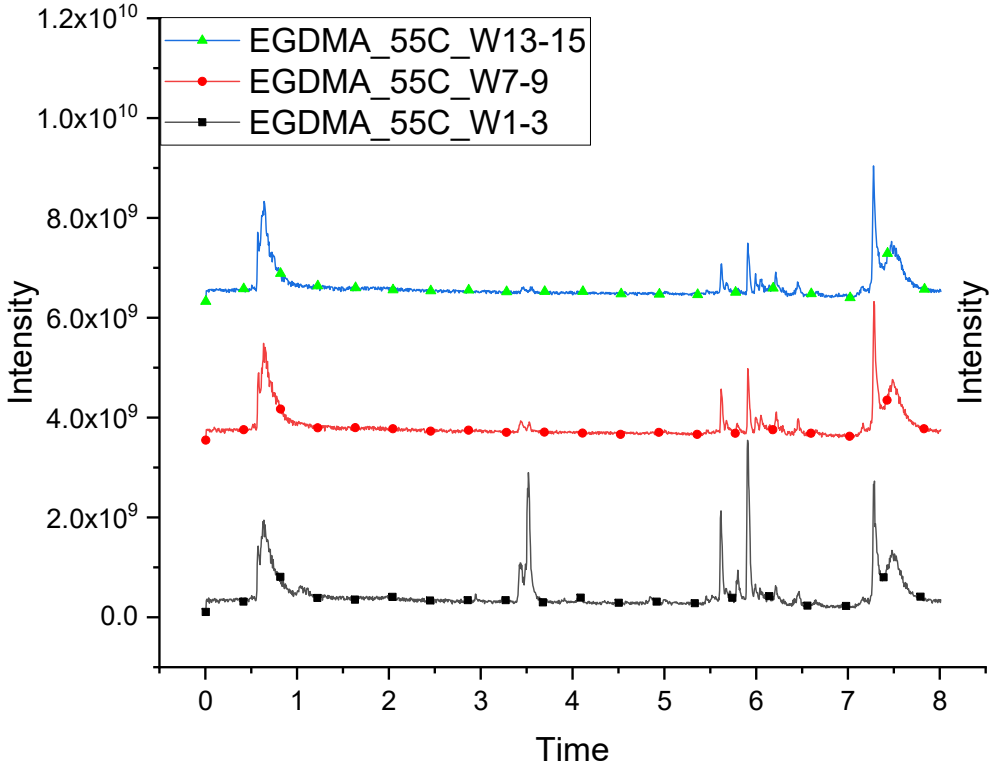
The quantification was not possible that why we went with the table reporting number of samples analyzed and said molecule detected in how many samples.

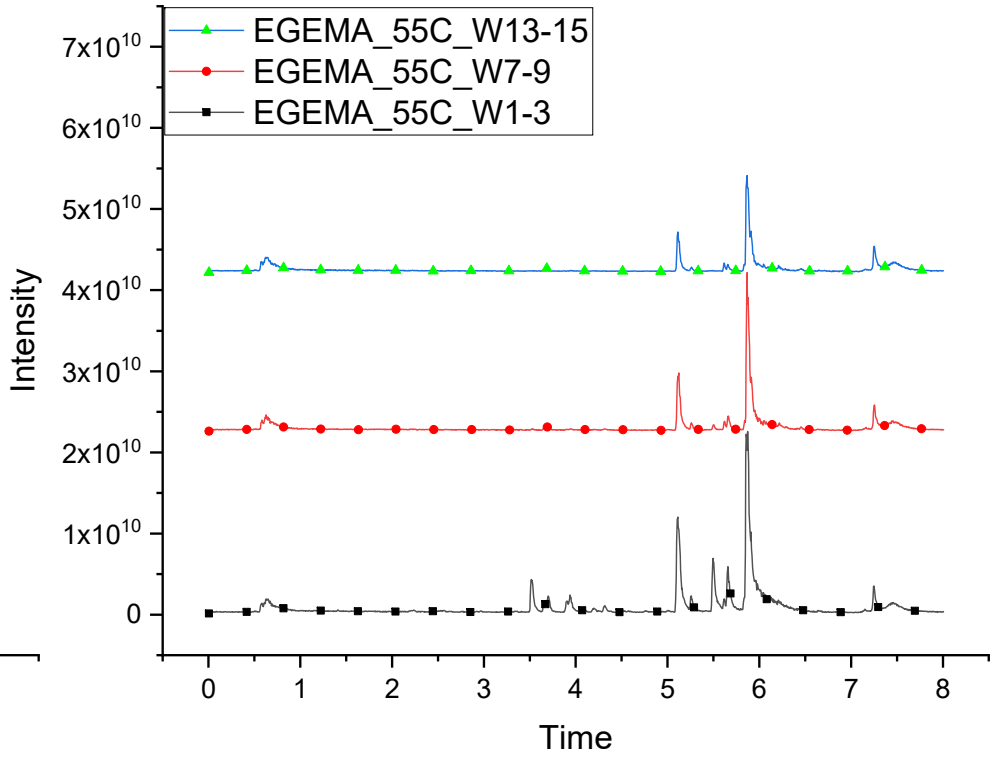
Chromatograph – LC MS



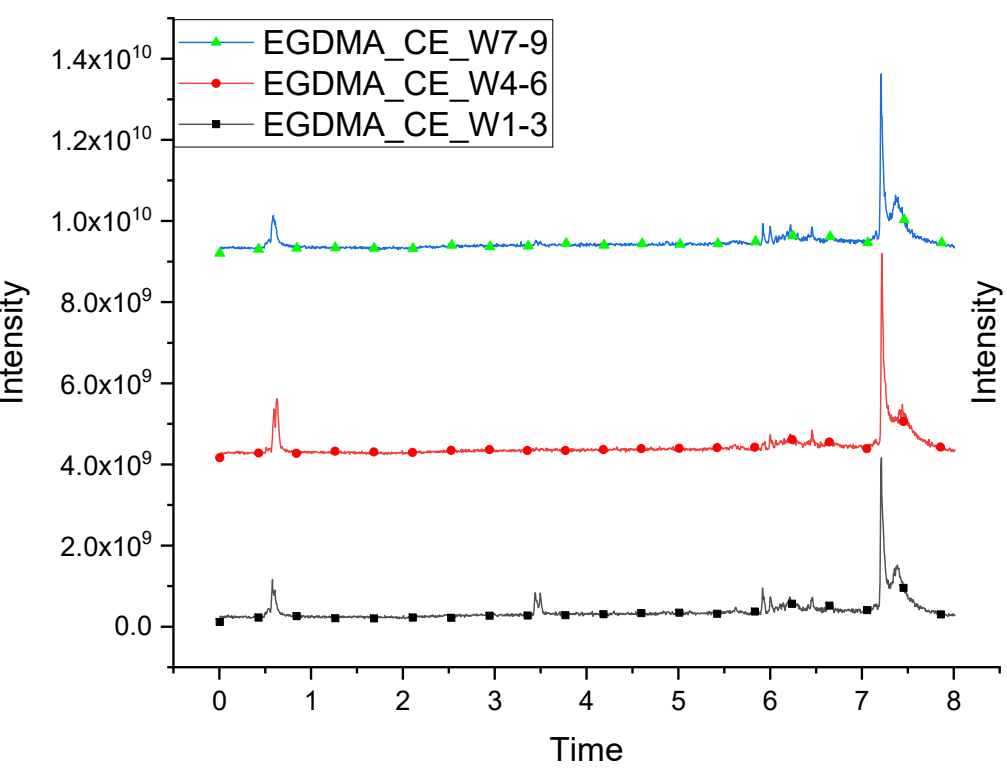


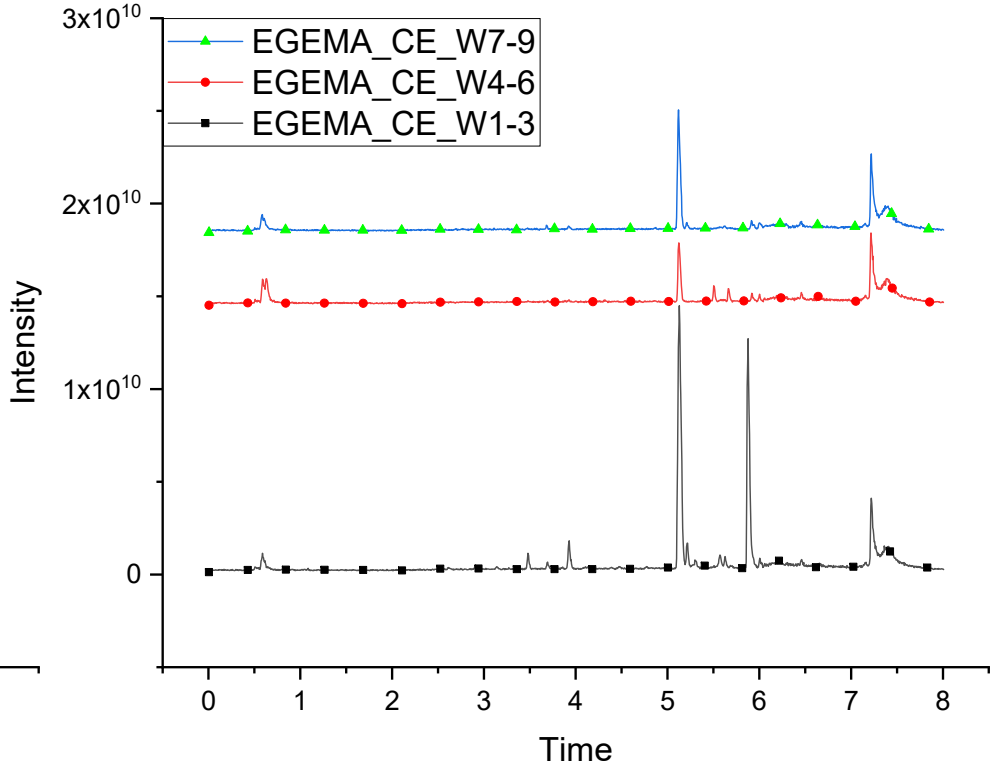
Chromatograph – LC MS





Chromatograph – LC MS Cholesterol Esterase





Serial number	Compound	Molecular weight	m/z (H+)	Retention time	Comments	Composition
1	EGDMA	198.08921	199.09649	5.80, 5.45	Two peaks are apparent.	C10H14O4
2	TEGDMA	286.14164	287.14891	5.73		C14H22O6
3	Ethylene glycol	62.03678	No	LC-MS		
4	EGEMA (L)	286.14164	287.14891	5.86		C14H22O6
5	EGEMA (D)	286.14164	287.14891	5.86		C14H22O6
6	Ethanol	46.041865	No	LC-MS		
7	EDMAB	193.110279	194.11756	5.91		C11H15NO2
8	CQ	166.09938	167.10666	5.54		C10H1402
9	Ph2I+PF6-	425.946908	280.98217	3.56	Pair of Ions. Diphenyliodonium mass observed.	C12H10I, F6P

molecule/EGDMA	37C W1-3			37C W4-6			37C W7-9			37C W10-12			37C W13-15		
	14F	6F	9F	4F	15F	7F	3F	13F	1F	2F	12F	5F	8F	11F	10F
CQ-167.10666	5.54	5.54	5.54	5.55	5.53	5.54	5.54	5.54 n							
EDMAB-194.11756	5.91	5.91	5.92	5.91	5.91	5.92	5.91	5.91	5.91	5.91	5.91	5.91	5.92	5.91	5.91
Ph2-280.98217	3.53	3.52	3.51	3.52	3.49	3.52	3.5	3.54	3.53	3.54	3.52	3.52	3.51	3.52	3.52
1: 199.097035	4.34 n 5.81	4.33 n 5.80	4.33 n 5.79	4.33 n 5.8	4.33 n 5.8	4.35 n 5.81	multiple								
2: 131.07082	3.46	3.45	3.44	3.44	3.42	3.45	3.43	3.46	3.45	3.46	3.45	3.44	3.43	3.44	3.45
3: 87.044605	3.46	3.45	3.44	3.44	3.42	3.45	3.43	3.46	3.45	3.46	3.45	3.44	3.43	3.44	3.45
4: 217.107600	4.1	4.09	4.09	4.1	4.09	4.1	4.09	4.1	4.1	4.11	4.1	4.09	4.09	4.1	4.09
5 and 12: 215.091950															
6: 129.05517	2.37	2.37	2.36		2.35			2.37 n 5.46	n	5.47 n	n	n		5.45 n	
7	no	LC	MS	data	low	MW									
8: 149.081385	2.65	2.66	2.64	2.65 n	2.64 lower										
9: 147.065735	1.5 n 5.46	1.57 n 5.47	1.5 n 5.47	5.47	5.46	5.47	5.46	5.46	5.46	5.47	5.47 multi	5.46	5.47	5.46	5.47
10															
11	broad lower RT														
13: 235.118165	5.51	5.51	5.5	5.5	5.5	5.51	5.5	5.5	5.5	5.5	5.5	5.5	5.51	5.5	5.5
14 and 15: 233.10252		4.06	4.05	4.06	4.05	4.07		4.07 lower							

13 may be more stable under hydrolysis but ester degrades.

molecule/EGDMA	1	2	3	4	5	6	7	8	9	10	11	12
Cholesterol Esterase	EGD_1_37C_W1_3	EGD_2_37C_W1_3	EGD_5_37C_W1_3	EGD_6_37C_W1_3	EGD_1_37C_W4_6	EGD_2_37C_W4_6	EGD_5_37C_W4_6	EGD_6_37C_W4_6	EGD_1_37C_W7_10	EGD_2_37C_W7_9	EGD_5_37C_W7_10	EGD_6_37C_W7_10
CQ-167.10666	4.71, 5.54	4.72	4.59 4.71 5.54	4.73, 5.54			multi	multi	multi			
EDMAB-194.11756	5.92	5.92	5.92	5.91	5.92	5.92	5.92	5.91	5.92	5.91	5.92	5.91
Ph2-280.98217	3.5	3.49	3.5	3.51	3.48	3.51	3.51	3.51	3.49	3.5	3.5	3.51
1: 199.097035	4.34, 4.92	multple	4.91	4.91				4.01, 4.91 multi	low			
2: 131.07082	3.43	3.43	3.44	3.46	3.43	3.45	3.45	3.45	3.44	3.44	3.45	3.45
3: 87.044605	3.44	3.43	3.44	3.46	3.43	3.45 multi	3.45	3.46	3.44 multi	3.44 multi	3.45	3.45
4: 217.107600			3.27									
5 and 12: 215.091950												
6: 129.05517	2.36	2.35	3.94	3.94				5.12				5.12
7	no	LC	MS	low	MW							
8: 149.081385												
9: 147.065735												
10												
11												
13: 235.118165			1.48									
14 and 15: 233.10252	4.4	4.4	4.4	4.4	low							

molecule/EGEMA	37C W1-3			37C W4-6			37C W7-9			37C W10-12			37C W13-15		
	6D	13D	5D	4D		9D	7D	12D	2D	3D	11D	1D	empty	10D	8D
CQ-167.10666	4.7 n 4.83 n 4.91 n *5.55* n 5.95		5.55 n	4.91, 5.54, 5.95	5.53, 5.95	4.91, 5.54, 5.95	5.95	5.94	5.95	5.94	5.95	5.94		5.94	5.94
EDMAB-194.11756	5.91	5.92	5.92	5.91	5.91	5.91	5.91	5.91	5.91	5.91	5.91	5.91		5.91	5.92
Ph2-280.98217	3.53	3.53	3.52	3.53	3.51	3.52	3.54	3.53	3.51	3.52	3.53	3.5		3.53	3.52
1: 287.149465	5.86	5.87	5.87	5.86	5.87	5.87	5.87	5.86	5.86	5.86	5.87	5.86		5.86	5.87
2: no LC-MS															
3: 258.11034 (H)	2.87, 3.66, 3.96	2.87, 3.66, 3.96	3.65 n 3.96	2.84, 3.96	3.94	3.95, 7.27	3.95	3.95	3.94	3.94	3.96	3.93		3.95	3.94
3: 259.118165 (H+)	5.12	5.12	5.12	5.12	5.12	5.13	5.12	5.12	5.11	5.12	5.12	5.12		5.12	5.13
4: 305.16003	5.26	5.26	5.26	5.26	5.26	5.26	5.27	5.26	5.26	5.26	5.27	5.26		5.26	5.26
5 and 11: 303.14438	5.01 multi close peaks	5.09 multi close peaks	5.01 multiple	5.00 multi	5.00 multi	5.01 multi	5.00 multi	5.00 multi	5.00 multi	low					
6: 230.07904(2-) (2H)	2.57	2.58	2.57	2.56	2.56	2.56	2.58	2.57	2.56	2.56	2.57	2.55		2.56	2.56
6: 231.086865 (H+)	3.71, 4.27, 5.12, 5.5	3.71, 4.28, 5.12, 5.51	3.70, 5.12 5.50	3.69, 5.12, 5.5	3.68, 5.11	3.69, 5.12	3.72, 5.12	3.7, 5.12	3.69, 5.11	3.7, 5.12	3.7, 5.12	3.67, 5.13		3.69, 5.12	3.69, 5.13
7 and 8: 276.120905 (H)	2.49, 4.37, 5.3	2.51, 4.38, 5.32	4.38, 5.31	4.37, 5.31	4.37, 5.31	4.37, 5.31	4.38, 5.31	4.37	4.36, 5.3	4.38, 5.31	4.38	4.36		4.38	4.37
7 and 8: 277.12873 (H+)	3.95, 4.2, 4.58	3.96, 4.22, 4.59	3.96, 4.21, 4.59	3.96, 4.21, 4.58	3.94, 4.21, 4.59	3.95, 4.21, 4.59	3.95, 4.22, 4.60	3.95, 4.21, 4.59	3.94, 4.2, 4.58	3.95, 4.21, 4.58	3.96, 4.21	3.93, 4.2, 4.58		3.95, 4.22	3.95, 4.21
9 and 10: 274.10255 (H)	5.8	5.81	5.81	5.8 low											
9 and 10: 275.113079 (H+)	4.11, 4.51, 4.76	4.12, 4.51, 4.78	4.11, 4.51, 4.77	4.11, 4.51	4.1, 4.5	4.11, 4.51	4.12, 4.51, 4.77	4.5	4.1, 4.5	4.11, 4.51	4.51	4.5		4.5, 5.68	
12: 323.170595	3.71, 4.2, 5.03, 5.75	3.7, 4.21, 5.03, 5.76	4.19, 5.04, 5.75	4.2, 5.75 low	4.18, 5.75	5.75	5.75	5.75	5.75	5.75	low				
13 and 14: 321.154945	4.76	4.78	4.77	4.76	4.76	4.77	4.77	4.76	4.76	4.76	4.77	4.76		4.76	4.76

molecule/EGEMA	13	14	15	16	17	18	19	20	21	22	23	24
Cholesterol Esterase	EGE_1_37C_W1_3	EGE_2_37C_W1_3	EGE_5_37C_W1_3	EGE_6_37C_W1_3	EGE_1_37C_W4_6	EGE_2_37C_W4_6	EGE_5_37C_W4_6	EGE_6_37C_W4_6	EGE_1_37C_W7_9	EGE_2_37C_W7_9	EGE_5_37C_W7_10	EGE_6_37C_W7_10
CQ-167.10666	4.72, 5.95	4.72, 5.94	5.55 multi	5.55	5.94	5.96	multi	multi	5.95 multi	5.95		
EDMAB-194.11756	5.92	5.92	5.92	5.92	5.92	5.92	5.91	5.92	5.92	5.92	5.92	5.92
Ph2-280.98217	3.5	3.49	3.48	3.51	3.5	3.48	3.5	3.51	3.48	3.5	3.48	3.5
1: 287.149465	5.87	5.87	5.88	5.87	5.87	5.87	multi 5.87	4.13 multi	multi	4.08 multi		4.08 multi
2: no LC-MS												
3: 258.11034 (H)												
3: 259.118165 (H+)	5.12	5.12	5.13	5.12	5.13	5.13	5.12	5.13	5.13	5.13	5.12	5.13
4: 305.16003	3.01, 5.26	3.01, 5.27	5.27	5.27	3.01, 5.27 (low)	2.99	3.01, 5.27	3.02	2.99	3.02	2.98	3.02
5 and 11: 303.14438	5.01 multi	5.01 multi	5.01 multi	5.01 multi	low							
6: 230.07904(2-) (2H)												
6: 231.086865 (H+)	3.7, 5.12	3.71, 5.12	3.69, 5.13	3.71, 5.12	3.7, 5.13	3.69, 5.13	3.7, 5.12	3.72, 5.13	3.69, 5.13	3.72, 5.13	3.68, 5.12	3.71, 5.13
7 and 8: 276.120905 (H)	4.38	4.38	low		4.38				low			
7 and 8: 277.12873 (H+)	3.96	3.96	3.95	3.96	3.95	3.94	3.95	3.95	low		3.93 n	3.96 n
9 and 10: 274.10255 (H)												
9 and 10: 275.113079 (H+)	2.81, 2.84, 4.52, 4.77	2.85, 4.51, 4.77	4.51 multi	4.51, 4.13 n	2.83	2.82	2.83, 4.11, 4.51 multi	2.85 multi	2.83	2.85	2.82 multi	2.85 multi
12: 323.170595												
13 and 14: 321.154945	4.77	4.77	4.77	4.78	4.78	4.77	4.76	4.78	4.77	4.78	4.77	4.78

molecule/EGDMA	55C W1-3			55C W4-6			55C W7-9			55C W10-12			55C W13-15		
	7A	3A	5A	10A	14A	1A	11A	12A	6A	4A	13A	8A	2A	15A	9A
CQ-167.10666	5.54	5.55	5.54	5.55	5.55										
EDMAB-194.11756	5.91	5.91	5.91	5.91	5.91	5.91	5.91	5.91	5.91	5.91	5.91	5.9	5.91	5.92	5.91
Ph2-280.98217	3.53	3.55	3.52	3.51	3.54	3.54	3.53	3.54	3.54	3.51	3.54	3.54	3.55	3.55	3.54
1: 199.097035	4.34 n 5.8	4.34 n 5.81	4.33 n 5.8	3.98 n 5.80	3.99 n 5.81	3.99 n 5.81									
2: 131.07082	3.45	3.46	3.44	3.43	3.45	3.46	3.45	3.44	3.45	3.42	3.45	3.45	3.45	3.45	3.47
3: 87.044605	3.45	3.46	3.44	3.43	3.45	3.45	3.43	3.44	3.45	3.42	3.45	3.45	3.45 n	3.47	3.47
4: 217.107600	4.11 n 4.84	4.09 n 4.84	4.09 n 4.84	4.09	4.1	4.1	4.1	4.1	4.1	4.08	4.1	4.09	4.1	4.1	4.1
5 and 12: 215.091950															
6: 129.05517	2.37 n 5.47	2.37 n 5.46	2.36	2.3 n 5.46	5.46 n	n	n	n	n	n	5.47 n	5.46 n	5.46 n	5.46 n	5.46 n
7															
8: 149.081385	2.65	2.66	2.64	2.61 multi low											
9: 147.065735	1.56 n 5.47	5.46	5.46	1.51 n 5.46	5.46	5.47	5.46	5.46	5.46	5.47	5.47	5.46	5.46	5.47	5.47
10															
11	broad lower RT														
13: 235.118165	5.51	5.5	5.5	5.5 n	5.5	5.5 multi									
14 and 15: 233.10252	4.05	4.06	4.05	4.06 multi low											

molecule/EGEMA	55C W1-3			55C W4-6			55C W7-9			55C W10-12			55C W13-15		
	12E	7E	10E	4E	3E	13E	15E	11E	9E	14E	2E	6E	1E	5E	8E
CQ-167.10666	5.54, 5.95, n	5.54, 5.95, n	5.54, 5.95, n	5.53, 5.95	5.54, 5.94	5.54, 5.94	5.95	5.94	5.94	5.95	5.93	5.95	5.94	5.94	5.94
EDMAB-194.11756	5.92	5.91	5.91	5.91	5.91	5.91	5.92	5.91	5.91	5.91	5.9	5.91	5.91	5.91	5.91
Ph2-280.98217	3.5	3.51	3.52	3.53	3.53	3.52	3.52	3.55	3.52	3.52	3.52	3.51	3.52	3.54	3.54
1: 287.149465	5.87	5.87	5.87	5.86	5.87	5.87	5.87	5.87	5.87	5.87	5.87	5.86	5.86	5.86	5.86
2: no LC-MS															
3: 258.11034 (H)	2.83, 3.62 n	2.83, 3.62 n	2.83, 3.62 n	2.85 n		2.83 n									
3: 259.118165 (H+)	5.11	5.12	5.11	5.11	5.11	5.11	5.12	5.12	5.12	5.12	5.12	5.11	5.11	5.11	5.11
4: 305.16003	5.25	5.25	5.26	5.26	5.26	5.26	5.26	5.26	5.26	5.27	5.25	5.26	5.25	5.26	5.26
5 and 11: 303.14438	5.0, multi	5.0, multi	5.0, multi	5.0, multi	5.0, multi	5.0, multi	5.01 multi	5.01 multi	5.01 multi						
6: 230.07904(2-) (2H)	2.55	2.56	2.57	2.57	2.57	2.56									
6: 231.086865 (H+)	3.68	3.69	3.7	3.69	3.7	3.69	3.7	3.71	3.71	3.69	3.69	3.69	3.68	3.71	3.69
7 and 8: 276.120905 (H)	4.36, 5.3	4.36	4.37	4.37	4.37	4.37	4.37	4.37	4.37	4.37	4.36	4.37	4.36	4.37	4.37
7 and 8: 277.12873 (H+)	3.93, 4.2	3.94, 4.2	3.95, 4.21	3.95, 4.21	3.95, 4.21	3.95, 4.21	3.96, 4.21	3.95, 4.22	3.95, 4.22	3.95, 4.22	3.94, 4.2	3.93, 4.2	3.94, 4.2	3.95, 4.21	3.95, 4.21
9 and 10: 274.10255 (H)															
9 and 10: 275.113079 (H+)	4.5 multi	4.5 multi	4.5 multi	4.5 multi	4.5 multi	4.51 multi	4.51 multi	4.52 multi	4.52 multi						
12: 323.170595	4.18	4.19	4.19	4.19	4.19	4.19	4.19	4.2	4.2	4.19	4.18	4.18	4.19	4.19	4.19
13 and 14: 321.154945	4.76	4.76	4.76	4.76	4.76	4.77	4.77	4.78	4.76	4.76	4.76	4.77	4.76	4.76	4.76