

Supplementary Figures

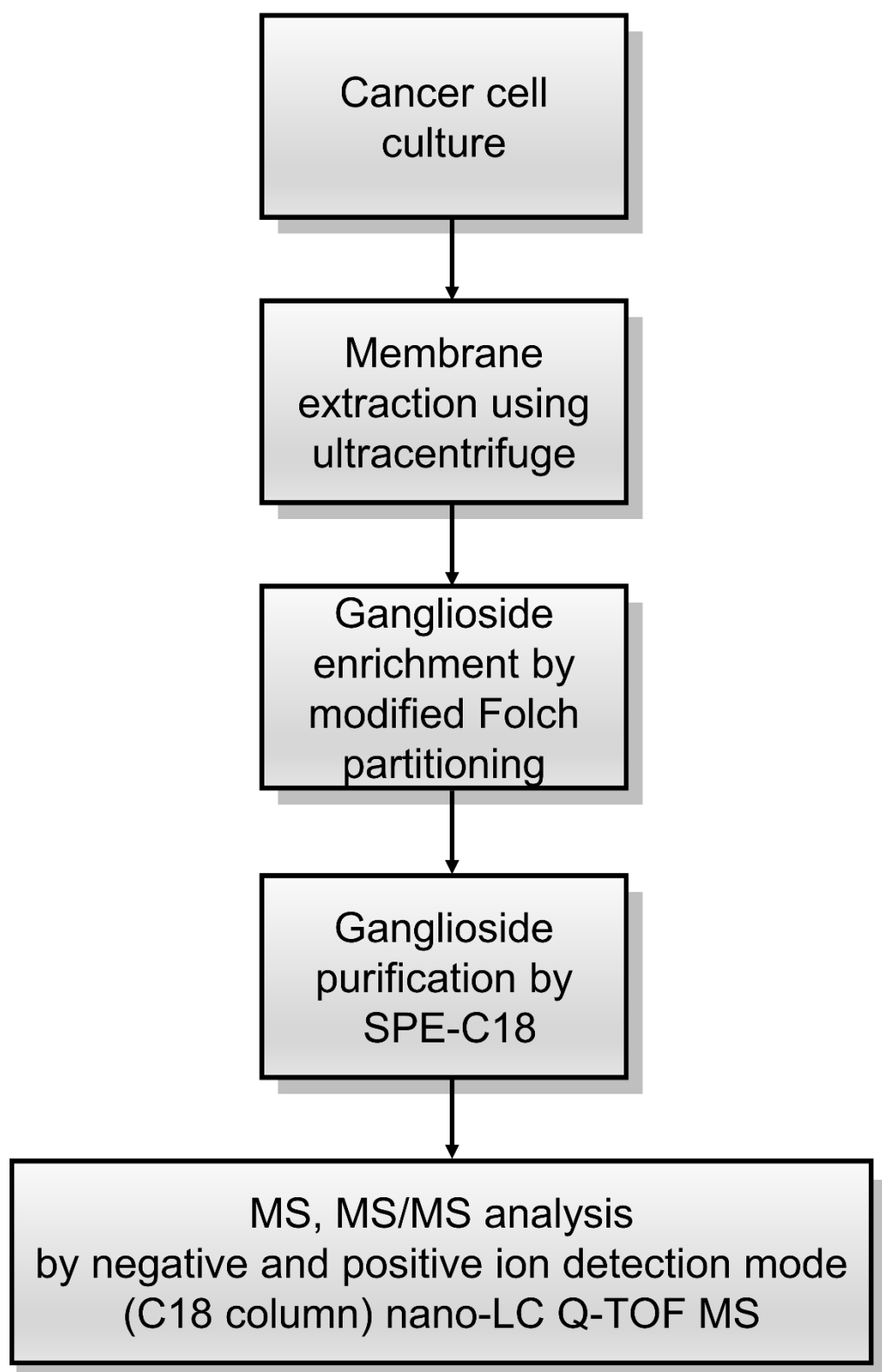
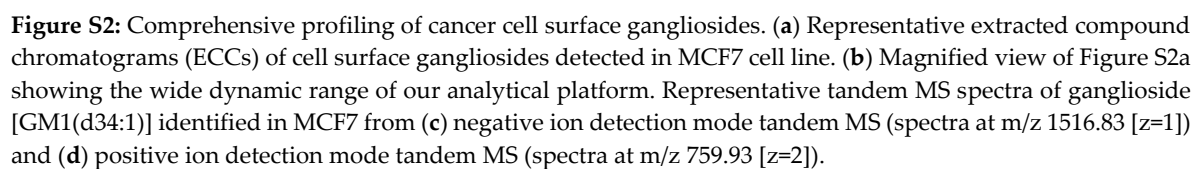


Figure S1: LC-MS based workflow for investigation of gangliosides extracted from cancer cell surfaces.



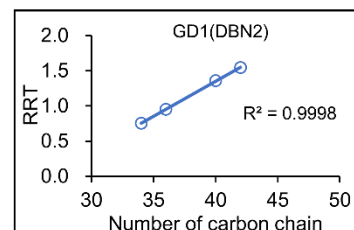
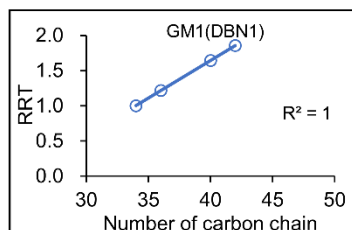
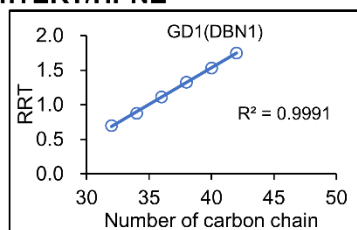
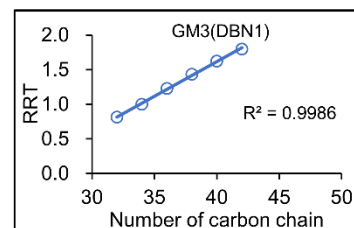
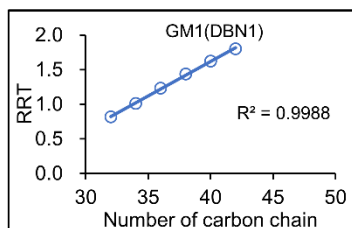
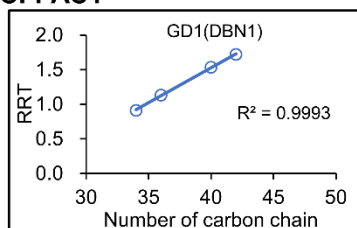
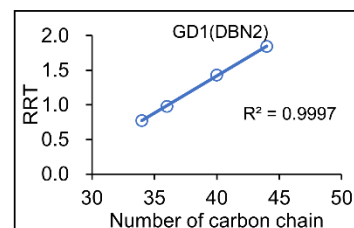
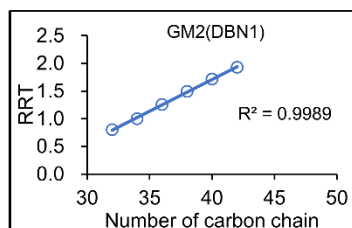
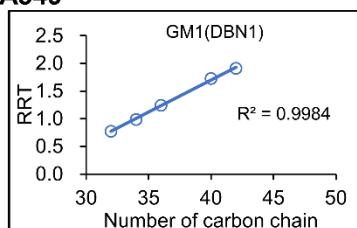
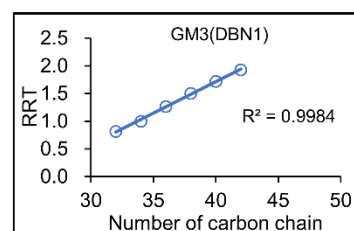
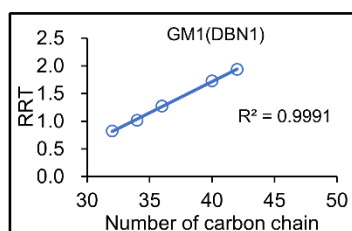
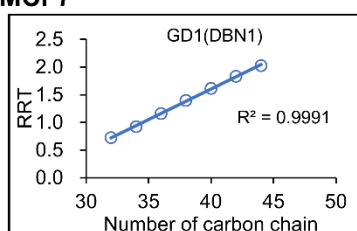
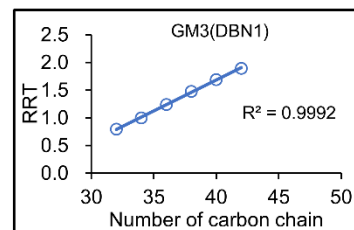
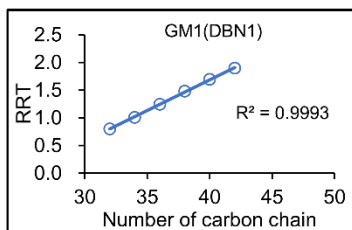
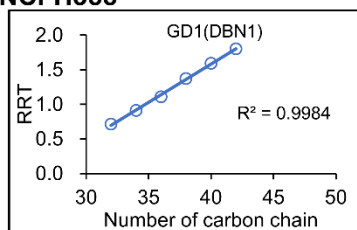
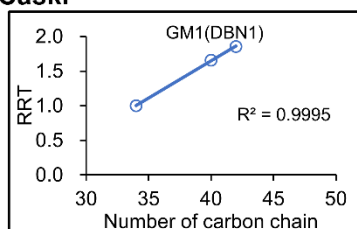
hTERT/HPNE**CFPAC1****A549****MCF7****NCI-H358****Caski**

Figure S3: Graphs of retention times (mins) vs the number of carbons in the ceramides for different glycan head groups in all cell lines.

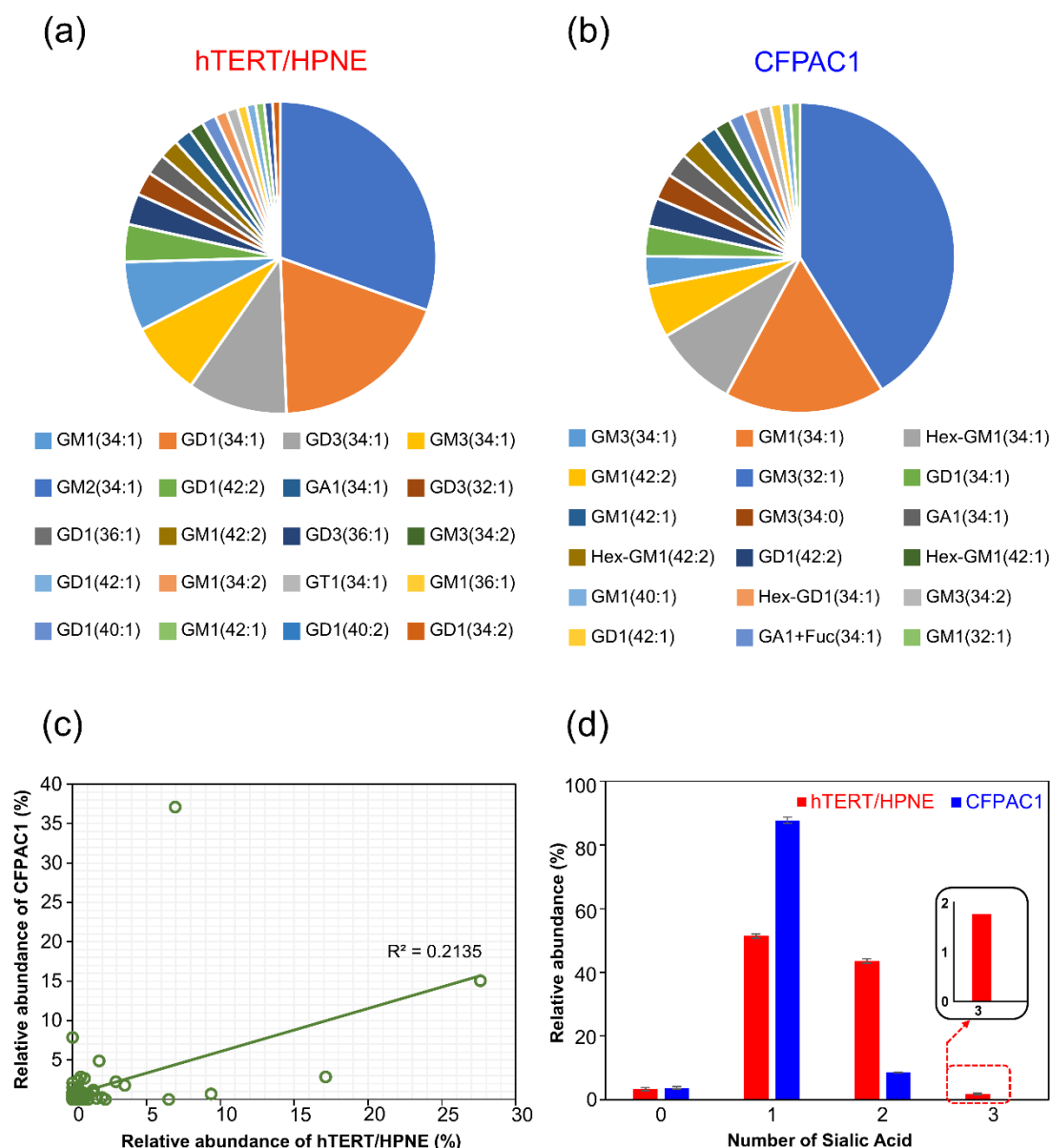


Figure S4: Differences in ganglioside distribution between cancerous (CFPAC1) and noncancerous (hTERT/HPNE) cell lines. Pie charts indicating the content distribution of gangliosides accounting for 90% (relative abundance) of total gangliosides in (a) hTERT/HPNE and (b) CFPAC1. (c) Graphs of relative abundances of total gangliosides from CFPAC1 vs hTERT/HPNE. (d) Relative abundances of gangliosides from CFPAC1 and hTERT/HPNE according to the number of sialic acids in their glycan heads.

Table S1: A complete list of the ganglioside compositions and relative abundances

Mas s[M]	Ganglioi de	hTER T/HP NE_1	hTER T/HP NE_2	CF PA C1_1	CF PA C1_2	CF PA C1_3	CF PA C1_4	A5 49 _1	A5 49 _2	A5 49 _3	A5 49 _4	MC F7 _1	MC F7 _2	MC F7 _3	MC F7 _4	NCI- H35 8_1	NCI- H35 8_2	NCI- H35 8_3	NCI- H35 8_4	Ca ski _1	Ca ski _2	Ca ski _3	Ca ski _4
106 4.69 709	GA2(34: 1)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	1.8 29 52	1.7 25 01	1.8 75 44	1.8 25 35
112 4.68 179	GM3(32: 1)	0.504 88	0.604 92	3.34 710	3.24 770	2.28 340	2.52 204	0.1 66 15	0.1 75 90	ND	0.1 95 87	1.3 20 22	0.9 31 59	1.4 02 05	1.4 25 92	2.35 043	2.39 932	3.54 500	2.89 447	ND	ND	ND	ND
115 0.69 744	GM3(34: 2)	1.431 82	1.383 60	1.42 884	1.43 805	0.91 762	0.89 411	0.2 09 43	0.2 05 25	0.1 99 27	0.2 67 54	1.8 98 19	1.3 55 98	2.3 20 47	2.5 82 82	0.97 891	1.02 667	1.50 844	1.41 526	ND	ND	ND	ND
115 2.71 309	GM3(34: 1)	7.548 15	6.325 74	38.0 400 1	34.0 955 2	35.8 603 3	40.4 386 1	1.4 88 86	1.5 10 72	1.4 73 61	1.3 47 03	22. 20 22 0	15. 92 53 9	17. 20 66 7	15. 63 53 2	27.1 513 9	26.1 519 9	33.2 528 8	32.9 899 3	2.4 43 74	2.1 86 80	1.9 90 16	1.9 25 80
115 4.72 874	GM3(34: 0)	0.359 49	0.351 36	2.55 604	2.51 866	2.44 312	2.20 672	ND	ND	ND	ND	0.9 37 58	0.6 96 54	0.6 74 30	0.5 74 36	1.43 841	1.40 741	1.23 298	1.51 592	ND	ND	ND	ND
117 8.72 874	GM3(36: 2)	ND	ND	0.13 649	0.16 167	ND	0.05 813	ND	0.1 11 12	ND	ND	0.4 94 67	0.3 89 72	0.8 58 70	0.8 73 89	0.20 465	0.17 113	ND	ND	ND	ND	ND	ND
118 0.74 439	GM3(36: 1)	0.661 38	0.660 49	0.82 648	0.91 530	0.94 033	0.81 850	0.6 38 43	0.5 75 53	0.4 74 40	0.3 98 72	2.7 59 12	2.8 67 97	1.5 79 81	1.3 49 65	1.57 301	1.34 711	1.46 694	1.39 976	ND	ND	ND	ND
120 8.77 569	GM3(38: 1)	ND	ND	0.15 356	0.18 157	0.21 830	0.20 250	0.0 76 43	ND	ND	ND	0.2 85 70	0.3 69 05	0.2 17 12	0.2 01 05	0.89 283	1.18 810	1.04 919	1.01 124	ND	ND	ND	ND
122 6.74 989	GA1(34: 1)	2.356 32	3.491 99	2.03 077	2.16 310	2.62 124	2.18 696	0.5 42 83	ND	0.7 94 57	0.6 16 56	0.4 18 03	0.2 20 58	0.4 05 97	0.3 72 68	1.05 697	0.76 805	0.72 412	1.01 585	15. 86 72 9	15. 99 57 6	16. 61 57 0	15. 74 00 6
123 4.79 134	GM3(40: 2)	ND	ND	0.10 824	0.13 074	0.14 415	0.13 618	ND	0.1 27 31	ND	ND	0.4 91 76	0.6 43 86	0.6 65 10	0.6 09 99	0.92 404	0.95 619	1.18 331	1.16 836	ND	ND	ND	ND
123 6.80 699	GM3(40: 1)	ND	ND	0.62 209	0.76 594	0.75 655	0.76 860	ND	0.1 41 02	ND	ND	1.1 29 91	1.3 25 31	1.0 99 19	1.0 40 76	2.67 378	2.86 193	2.32 435	2.18 284	ND	ND	ND	ND

126 2.82 264	GM3(42:2)	ND	ND	0.69 691	0.87 781	1.06 305	0.78 168	0.1 20 36	0.3 45 91	0.4 18 29	0.4 60 10	2.2 40 64	2.8 63 41	2.8 50 58	2.8 12 90	1.67 278	1.66 637	1.86 890	1.76 608	ND	ND	ND	ND
126 4.83 829	GM3(42:1)	ND	ND	0.54 240	0.79 332	0.39 549	0.50 405	ND	ND	ND	ND	1.2 37 77	1.6 40 03	1.4 54 07	1.2 25 74	1.24 312	1.30 984	0.73 466	0.87 143	ND	ND	ND	ND
132 7.76 119	GM2(32:1)	0.608 24	0.523 57	ND	ND	ND	ND	1.0 92 06	0.9 20 19	1.1 80 39	1.2 61 20	0.1 38 48	0.0 97 07	0.1 90 44	0.1 92 17	ND	ND	ND	ND	ND	ND	ND	ND
135 3.77 684	GM2(34:2)	0.419 04	0.610 94	ND	ND	ND	ND	1.6 12 35	1.3 70 22	1.6 89 50	2.0 21 86	0.2 73 30	0.2 02 59	0.3 34 30	0.3 94 63	ND	ND	ND	ND	ND	ND	ND	ND
135 5.79 249	GM2(34:1)	7.131 44	5.896 03	ND	ND	ND	ND	14. 33 24 3	14. 95 70 5	12. 79 23 2	11. 55 68 6	2.1 65 06	1.5 68 86	2.3 05 16	2.0 21 55	0.21 480	ND	0.29 167	0.26 751	9.7 36 86	10. 48 49 2	6.7 54 96	7.6 14 31
135 7.80 814	GM2(34:0)	ND	ND	0.24 710	0.22 111	0.24 188	0.25 258	0.9 57 93	0.5 15 48	1.1 93 95	0.7 88 31	0.1 07 49	ND	ND	0.0 68 95	ND	ND	ND	ND	0.9 32 88	1.1 10 42	0.7 38 59	0.8 40 78
137 1.78 739	GM2(NeuGc)(34:1)	ND	ND	ND	ND	ND	ND	2.1 67 78	1.2 27 67	0.8 63 62	1.8 76 29	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
137 2.80 779	GA1+Fu c(34:1)	ND	ND	0.79 457	0.82 180	1.02 622	0.89 899	ND	ND	ND	ND	ND	ND	ND	ND	0.71 060	0.48 718	0.42 682	0.64 128	9.7 34 76	9.8 94 52	10. 30 96 5	9.7 61 20
137 3.80 304	GM2(NeuGc)(34:0)	ND	ND	ND	ND	ND	ND	0.4 66 69	ND	0.2 43 04	0.3 23 48	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
138 3.82 379	GM2(36:1)	0.500 35	0.691 80	ND	ND	ND	ND	2.6 18 36	2.5 77 96	1.8 21 91	1.3 66 62	0.3 54 54	0.3 49 11	0.2 71 28	0.2 10 14	ND	ND	ND	ND	ND	ND	ND	ND
141 1.85 509	GM2(38:1)	ND	ND	ND	ND	ND	ND	0.3 80 17	0.5 34 55	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
141 5.77 719	GD3(32:1)	2.452 89	1.992 21	ND	ND	ND	ND	ND	ND	ND	ND	0.0 59 72	0.0 37 68	ND	0.0 62 22	ND	ND	ND	ND	ND	ND	ND	ND
143 7.87 074	GM2(40:2)	ND	ND	ND	ND	ND	ND	1.0 18 24	1.5 69 18	1.5 48 93	1.4 89 64	0.0 54 34	0.1 25 53	0.1 20 08	ND	ND	ND	ND	ND	ND	ND	ND	ND
143 9.88 639	GM2(40:1)	ND	ND	ND	ND	ND	ND	1.2 58 20	1.4 86 73	1.6 59 45	1.4 09 90	0.2 26 07	0.2 54 55	0.2 69 37	0.1 85 33	ND	ND	ND	ND	ND	ND	ND	ND

144 1.79 284	GD3(34: 2)	0.456 60	0.498 65	ND	ND	ND	ND	ND	ND	ND	ND	0.1 53 40	0.1 08 18	0.1 67 63	0.1 90 92	0.18 602	0.19 069	0.21 238	0.18 607	ND	ND	ND	ND
144 3.80 849	GD3(34: 1)	10.20 449	8.549 68	0.84 814	0.75 043	0.66 283	0.52 844	1.3 35 53	1.4 22 56	0.7 37 67	1.0 47 17	0.6 75 15	0.4 72 21	0.3 07 40	0.3 32 11	1.71 538	1.62 310	1.70 370	1.85 713	1.6 37 85	2.2 05 51	1.5 17 54	1.6 49 27
144 5.82 414	GD3(34: 0)	0.184 22	0.138 35	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
146 5.90 204	GM2(42: 2)	ND	ND	ND	ND	ND	ND	5.8 65 35	5.1 47 28	6.9 49 42	9.0 10 07	0.5 39 15	0.6 30 01	0.7 11 80	0.7 53 85	ND	ND	ND	ND	1.5 44 31	1.3 07 46	1.5 46 13	1.4 56 53
146 7.91 769	GM2(42: 1)	ND	ND	ND	ND	ND	ND	1.5 33 00	1.4 49 84	2.5 60 48	0.8 57 30	0.2 39 28	0.3 79 70	0.2 95 17	0.3 44 12	ND	ND	ND	ND	0.5 12 51	0.4 63 66	0.5 10 04	0.6 15 75
146 9.82 414	GD3(36: 2)	0.339 25	0.335 37	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
147 1.83 979	GD3(36: 1)	1.820 71	1.441 76	ND	0.20 340	0.17 432	0.12 059	0.3 81 02	0.3 65 93	0.2 36 00	0.2 24 54	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
148 9.81 399	GM1(32: 1)	ND	ND	0.92 380	0.99 352	0.67 717	0.94 292	0.1 31 81	ND	0.2 43 90	ND	0.4 34 60	0.2 03 50	0.2 21 37	0.4 03 60	1.28 615	0.98 521	1.39 947	0.77 789	ND	ND	ND	ND
151 5.82 964	GM1(34: 2)	1.506 13	0.734 23	0.59 116	0.64 943	0.49 261	0.39 252	0.7 52 44	0.4 22 06	0.3 13 54	0.8 13 79	0.6 68 85	0.4 79 72	0.9 53 12	0.8 21 02	0.44 302	0.46 121	0.64 728	0.70 824	ND	ND	ND	ND
151 7.84 529	GM1(34: 1)	25.67 669	29.55 495	15.3 177 1	13.5 223 7	15.7 285 5	15.6 598 6	5.7 79 38	3.6 09 36	2.5 55 94	2.4 70 28	6.3 62 95	4.4 84 77	5.6 88 55	5.4 41 91	10.0 184 2	9.89 856	8.39 569	10.4 315 5	19. 99 29 6	20. 66 56 0	15. 76 86 8	16. 27 45 4
151 9.86 094	GM1(34: 0)	0.667 09	0.524 74	0.97 974	0.79 339	0.73 565	0.93 321	ND	ND	ND	ND	0.1 63 96	0.1 00 81	ND	0.1 04 31	0.37 924	0.41 133	0.37 974	0.56 299	ND	ND	ND	ND
154 3.86 094	GM1(36: 2)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	0.3 18 19	0.1 70 36	0.4 02 51	0.5 88 67	ND	ND	ND	ND	ND	ND	ND	ND
154 5.87 659	GM1(36: 1)	0.894 21	0.875 25	0.67 136	0.75 292	0.75 257	0.60 848	1.2 14 97	0.8 46 57	0.5 09 68	ND	1.3 17 97	1.3 66 32	0.8 58 64	0.7 48 08	1.10 945	1.08 376	0.85 958	0.71 733	ND	ND	ND	ND
155 3.91 804	GD3(42: 2)	0.266 78	0.378 30	ND	ND	ND	ND	0.2 68 56	0.0 38 16	0.2 94 02	0.3 22 87	ND	ND	ND	ND	1.09 427	1.17 101	1.14 095	1.03 458	ND	ND	ND	ND

155 5.93 369	GD3(42:1)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	0.70 457	0.84 990	0.47 445	0.49 851	ND	ND	ND	ND
157 3.90 789	GM1(38:1)	ND	ND	0.20 012	0.22 501	0.24 019	ND	ND	ND	ND	ND	ND	ND	ND	ND	1.08 154	1.26 434	0.71 946	1.01 105	ND	ND	ND	ND
159 1.88 209	GA1+Hexnac+Hex(34:1)	0.315 07	0.417 29	0.53 756	0.61 757	0.67 715	0.52 426	0.6 02 13	0.6 31 00	0.6 61 76	ND	ND	ND	ND	ND	ND	ND	ND	ND	1.9 79 10	2.7 60 22	2.3 78 79	2.2 68 18
159 9.92 354	GM1(40:2)	ND	ND	0.25 110	0.32 696	0.35 599	0.28 021	0.3 92 86	0.7 54 53	0.6 74 87	1.2 47 05	0.5 89 14	0.6 99 79	0.7 77 68	1.0 40 65	2.04 988	1.82 829	1.77 971	1.72 699	ND	ND	ND	ND
160 1.93 919	GM1(40:1)	0.376 88	0.371 91	1.28 196	1.56 362	1.61 303	1.43 396	0.9 15 51	1.0 90 38	1.1 66 54	1.1 50 96	1.7 37 83	2.0 44 08	2.0 79 32	1.7 11 26	5.02 056	5.59 851	3.62 101	3.64 864	3.4 05 42	2.5 40 56	4.0 18 26	4.7 35 26
162 7.95 484	GM1(42:2)	1.291 01	2.305 16	3.67 409	4.62 831	5.78 074	5.44 040	7.0 38 58	7.3 06 19	10. 62 02	11. 70 53 5	5.9 28 56	8.0 05 72	8.0 58 02	7.7 10 68	5.59 905	5.65 023	5.39 258	4.97 267	9.6 77 84	8.8 05 57	13. 21 5	12. 39 7
162 9.97 049	GM1(42:1)	0.350 42	1.265 17	2.50 458	3.97 789	1.92 749	2.29 096	1.3 98 73	2.0 88 83	1.3 80 82	1.4 35 83	3.4 24 46	4.6 93 09	3.9 52 05	3.9 06 29	4.55 899	4.01 633	3.13 603	2.75 947	4.3 33 87	3.7 71 98	5.4 31 23	5.7 78 57
165 1.86 679	Hex-GM1(32:1)	0.157 67	ND	0.39 542	0.45 681	0.48 997	0.38 980	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
165 5.98 614	GM1(44:2)	ND	ND	ND	ND	ND	ND	ND	ND	0.2 21 95	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
167 4.91 919	GD2(36:1)	0.596 56	0.448 65	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
167 9.89 809	Hex-GM1(34:1)	ND	ND	7.85 048	8.26 779	8.09 509	7.23 206	ND	ND	ND	ND	1.3 43 79	0.9 11 74	0.9 42 63	1.4 14 78	1.02 212	1.01 560	1.15 557	1.13 155	ND	ND	ND	ND
173 4.90 389	GT3(34:1)	0.357 80	0.308 96	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
173 7.97 634	Hex-GM1(38:0)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	5.3 18 45	5.3 08 26	5.6 79 98	5.8 30 28
176 3.99 199	Hex-GM1(40:1)	ND	ND	0.53 537	0.61 193	0.62 447	0.51 023	ND	ND	ND	ND	0.3 02 05	0.3 37 63	0.3 13 43	0.2 73 70	0.41 982	0.55 012	0.33 196	0.30 530	ND	ND	ND	ND

177 4.01 274	Fuc- GM1(42: 2)	ND	ND	0.42 157	0.46 010	0.63 719	0.63 033	ND	ND	ND	ND	ND	ND	ND	ND	1.05 859	1.12 012	0.89 323	0.84 938	3.1 12 49	2.7 67 99	3.9 97 15	4.0 24 66
178 0.90 939	GD1(32: 1)	0.626 04	0.671 72	ND	ND	ND	ND	0.3 09 18	0.3 89 79	0.7 05 80	0.7 34 32	0.2 81 27	0.1 85 31	0.3 58 13	0.3 80 85	0.16 108	0.18 957	0.22 096	0.20 697	ND	ND	ND	ND
179 0.00 764	Hex- GM1(42: 2)	ND	ND	1.85 686	2.29 750	2.66 945	1.53 717	ND	ND	ND	ND	ND	ND	ND	ND	0.68 068	0.61 769	0.62 285	0.68 125	ND	ND	ND	ND
179 2.02 329	Hex- GM1(42: 1)	ND	ND	1.38 719	1.90 017	1.29 496	1.39 456	ND	ND	ND	ND	0.8 44 59	0.8 65 24	0.9 03 68	0.9 65 27	0.39 462	0.46 811	ND	0.30 887	ND	ND	ND	ND
180 6.92 504	GD1(34: 2)	0.578 29	0.896 50	ND	ND	ND	ND	0.8 83 28	0.8 10 08	1.3 38 53	1.2 30 75	0.7 20 25	0.5 06 51	0.9 81 02	1.0 27 31	ND	ND	ND	ND	ND	ND	ND	ND
180 8.94 069	GD1(34: 1)	18.13 750	16.13 164	3.36 541	3.27 467	2.65 445	2.04 538	12. 72 50 4	13. 90 32 1	10. 42 09 3	10. 98 81 9	6.2 46 86	4.2 61 66	5.7 99 30	5.6 15 81	2.92 429	2.84 881	3.35 230	3.41 032	ND	ND	ND	ND
181 0.95 634	GD1(34: 0)	0.719 66	0.543 24	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
183 4.95 634	GD1(36: 2)	0.368 10	0.353 50	ND	ND	ND	ND	0.3 17 92	0.2 83 06	0.4 62 72	0.4 03 44	0.2 68 00	0.1 99 59	0.4 61 92	0.4 73 99	ND	ND	ND	ND	ND	ND	ND	ND
183 6.97 199	GD1(36: 1)	2.208 08	1.761 94	0.27 034	0.27 971	0.22 740	0.13 909	1.6 33 61	1.7 99 01	1.2 10 84	1.3 61 92	1.1 71 39	0.7 61 40	0.9 48 31	0.9 87 69	0.53 676	0.46 598	0.51 837	0.55 285	1.8 67 61	1.5 77 01	2.0 69 03	2.0 05 60
186 5.00 329	GD1(38: 1)	0.310 48	ND	ND	ND	ND	ND	0.5 76 74	0.5 45 25	0.4 87 15	ND	0.2 99 18	0.3 97 94	0.3 25 52	0.3 01 85	0.72 884	0.71 869	0.70 907	0.66 887	1.1 46 80	1.3 02 66	1.3 42 63	1.7 67 14
189 1.01 894	GD1(40: 2)	0.718 02	0.830 19	ND	ND	ND	ND	2.6 75 76	3.4 66 17	3.3 66 58	2.0 32 87	1.3 25 45	1.9 28 27	1.9 90 62	1.9 86 87	0.99 899	1.09 167	1.19 447	1.10 162	ND	ND	ND	ND
189 3.03 459	GD1(40: 1)	0.789 84	0.908 66	0.41 352	0.44 305	0.48 181	0.43 477	1.4 87 05	1.3 52 71	1.0 91 88	1.0 72 52	2.6 97 40	3.2 95 75	2.2 78 26	2.2 57 89	2.71 041	2.86 853	1.95 423	1.82 325	ND	ND	ND	ND
191 9.05 024	GD1(42: 2)	3.394 92	3.650 50	1.56 058	1.81 774	1.97 251	1.76 077	14. 28 48 5	14. 17 46 1	14. 07 56 0	16. 28 82 3	12. 45 55 4	16. 42 90 7	14. 89 51 0	17. 08 62 8	4.35 033	4.26 112	4.23 240	4.05 090	ND	ND	ND	ND
192 1.06 589	GD1(42: 1)	0.801 10	1.863 35	0.91 020	1.17 171	0.87 288	1.00 970	6.9 76 75	8.4 58 80	9.4 80 48	8.4 80 38	7.0 34 48	10. 00 08 5	7.0 20 51	7.1 67 29	1.80 790	3.03 289	1.78 568	1.44 314	ND	ND	ND	ND

[illegible]

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