

Appendix 1. MS/MS Exclusion list. Contaminants and precursors with non-informative fragmentation.

Mass [m/z]	Polarity
200.0592	Positive
201.0241	Negative
201.0764	Negative
202.9694	Positive
203.0318	Negative
203.0522	Positive
204.9948	Positive
205.0855	Positive
206.9914	Positive
208.9905	Positive
209.0804	Positive
209.2012	Positive
210.1849	Positive
212.1435	Positive
213.0145	Negative
213.0764	Negative
213.1491	Negative
215.0921	Negative
215.1256	Positive
217.0026	Negative
217.0184	Positive
217.1046	Positive
217.1077	Negative
218.0060	Negative
219.0896	Positive
219.1750	Negative
222.0047	Positive
223.0196	Negative
224.0234	Negative
224.2002	Positive
225.1855	Negative
226.1799	Positive
227.0920	Negative
227.2011	Negative
227.2013	Negative
228.1956	Positive
229.1078	Negative
230.2476	Positive
231.0872	Negative

Mass [m/z]	Polarity
232.9752	Negative
233.0778	Positive
233.1543	Negative
234.1849	Positive
234.9757	Negative
235.2378	Positive
235.9734	Negative
237.0828	Positive
237.0913	Negative
238.0861	Positive
238.0940	Negative
239.0594	Negative
239.0933	Negative
239.1060	Positive
239.1470	Positive
239.2011	Negative
240.1086	Positive
240.9694	Negative
241.0353	Positive
241.0714	Negative
241.0834	Positive
241.1079	Negative
241.2168	Negative
242.1759	Negative
242.9663	Negative
243.0874	Negative
243.1234	Negative
244.1901	Positive
244.9538	Positive
244.9650	Negative
245.1029	Negative
245.1357	Positive
246.9508	Positive
248.9740	Negative
249.2533	Positive
250.1775	Positive
250.2564	Positive
250.9759	Negative
253.2168	Negative

Mass [m/z]	Polarity
253.2172	Negative
255.0874	Negative
255.2324	Negative
255.2328	Negative
256.2363	Negative
257.1031	Negative
257.1392	Negative
258.2787	Positive
259.0649	Positive
259.0826	Negative
259.1186	Negative
260.1168	Positive
260.9275	Positive
261.0874	Positive
261.1306	Positive
262.9807	Positive
263.2689	Positive
264.2721	Positive
264.9918	Negative
265.1479	Negative
265.2168	Negative
266.1511	Negative
266.1741	Positive
267.2324	Negative
268.9980	Positive
269.1375	Positive
269.2125	Negative
269.2481	Negative
269.2486	Negative
270.0014	Positive
271.1189	Negative
271.2307	Positive
271.9724	Positive
272.1494	Positive
273.0983	Negative
273.1344	Negative
273.1671	Positive
274.1650	Positive
275.2011	Negative

Mass [m/z]	Polarity
277.1050	Positive
277.2168	Negative
277.2846	Positive
278.9547	Positive
279.0917	Positive
279.1586	Positive
279.2324	Negative
279.2331	Negative
280.1617	Positive
280.9787	Negative
281.2481	Negative
281.2486	Negative
282.2519	Negative
282.9764	Negative
283.0693	Positive
283.1188	Negative
283.2637	Negative
283.2643	Negative
284.2677	Negative
284.3305	Positive
284.9717	Positive
285.2515	Positive
287.1137	Negative
287.9949	Negative
288.1497	Positive
288.9961	Negative
289.1295	Negative
290.1597	Positive
293.1790	Negative
296.0656	Negative
297.1535	Negative
297.1652	Positive
297.2431	Negative
297.2794	Negative
299.0061	Negative
299.0085	Positive
299.1137	Negative
299.1500	Negative
300.2038	Positive
301.1291	Negative

Mass [m/z]	Polarity
301.1405	Positive
301.2168	Negative
302.1441	Positive
302.1964	Positive
303.2324	Negative
304.1754	Positive
304.2995	Positive
305.0232	Negative
305.1568	Positive
305.2481	Negative
306.0265	Negative
307.2637	Negative
307.9977	Negative
309.1306	Positive
309.1746	Negative
309.2794	Negative
310.2349	Positive
311.1688	Negative
311.2950	Negative
312.1723	Negative
313.1291	Negative
313.1413	Positive
313.1669	Negative
315.1451	Negative
315.1850	Positive
316.1753	Positive
317.1146	Positive
317.1237	Negative
317.1606	Negative
318.1909	Positive
319.0947	Negative
320.1080	Negative
320.9967	Negative
321.1307	Positive
321.2104	Negative
322.9704	Negative
323.1457	Positive
325.1845	Negative
325.3107	Negative
326.1880	Negative

Mass [m/z]	Polarity
327.1837	Negative
327.2324	Negative
329.1611	Negative
329.2481	Negative
331.1397	Negative
331.2154	Positive
331.2637	Negative
332.2080	Positive
332.3306	Positive
333.2794	Negative
334.1853	Positive
335.0331	Negative
335.2950	Negative
337.3107	Negative
338.3414	Positive
339.1985	Negative
339.3263	Negative
340.2016	Negative
341.1117	Negative
341.1988	Negative
343.1389	Negative
344.2292	Positive
344.9840	Positive
345.1553	Negative
346.2255	Positive
347.1435	Negative
348.2007	Positive
349.1837	Positive
350.3407	Positive
351.0010	Positive
353.3420	Negative
357.1450	Positive
358.1527	Negative
359.1724	Negative
359.2168	Positive
362.2164	Positive
362.9818	Negative
364.9796	Negative
365.1054	Positive
365.1558	Positive

Mass [m/z]	Polarity
365.2687	Negative
365.3420	Negative
366.2639	Positive
366.9753	Positive
367.2450	Negative
367.3576	Negative
367.3582	Negative
368.4247	Positive
371.1621	Positive
373.1903	Negative
373.2366	Positive
375.1664	Negative
376.2377	Positive
377.2255	Positive
378.2103	Positive
378.9554	Negative
379.1556	Negative
381.0089	Negative
381.3733	Negative
381.3748	Negative
383.1490	Positive
385.1792	Positive
387.0263	Negative
388.0299	Negative
388.2549	Positive
389.1821	Negative
390.0005	Negative
391.2839	Positive
391.2888	Negative
392.2274	Positive
392.2869	Positive
392.2917	Negative
393.1723	Negative
393.2124	Positive
393.2867	Negative
393.2910	Positive
394.2896	Negative
395.3889	Negative
395.3896	Negative
399.2508	Positive

Mass [m/z]	Polarity
400.2550	Positive
401.0974	Negative
401.1347	Negative
403.0000	Negative
403.2406	Positive
404.9861	Negative
405.9750	Negative
407.1883	Negative
408.3092	Positive
408.9601	Positive
409.1796	Positive
413.2659	Positive
414.2694	Positive
415.2736	Positive
417.0345	Negative
417.2628	Positive
418.2431	Positive
418.9740	Negative
419.2337	Positive
419.3171	Positive
421.2027	Negative
421.2417	Positive
425.2134	Positive
429.2404	Positive
430.2420	Positive
431.2376	Positive
432.2818	Positive
433.0045	Positive
433.2528	Positive
433.3358	Negative
434.3386	Negative
437.2263	Positive
444.3807	Positive
444.9848	Negative
446.9811	Negative
448.9792	Positive
449.3371	Positive
450.3432	Positive
453.2088	Positive
457.3034	Positive

Mass [m/z]	Polarity
459.3276	Negative
460.3310	Negative
460.9585	Negative
461.2884	Positive
463.0140	Negative
463.3285	Negative
464.3305	Negative
465.3261	Negative
469.0291	Negative
470.0329	Negative
472.0037	Negative
475.1749	Negative
475.3266	Positive
476.3089	Positive
478.3889	Positive
479.3928	Positive
480.3946	Positive
481.2515	Positive
483.1213	Negative
485.0036	Negative
486.3569	Positive
486.9869	Negative
487.3887	Positive
487.9788	Negative
489.1899	Negative
491.2995	Positive
492.4049	Positive
493.4086	Positive
495.2692	Positive
497.2289	Positive
500.3760	Positive
500.9773	Negative
501.4106	Positive
505.3756	Negative
506.3776	Negative
507.3762	Negative
515.0082	Positive
515.4220	Positive
522.5971	Positive
526.9877	Negative

Mass [m/z]	Polarity
529.4402	Positive
532.4413	Positive
536.1657	Positive
537.1649	Positive
537.3962	Positive
538.1623	Positive
542.9632	Negative
544.3944	Positive
547.1023	Negative
549.1004	Negative
550.6282	Positive
551.0306	Negative
551.6313	Positive
552.0326	Negative
553.3811	Positive
554.0063	Negative
557.1822	Negative
565.1135	Negative
567.0074	Negative
571.1977	Negative
575.1344	Negative
577.1335	Negative
581.0541	Negative
582.9777	Negative

Mass [m/z]	Polarity
589.1509	Negative
591.1488	Negative
603.1671	Negative
605.1656	Negative
608.9911	Negative
609.0984	Negative
610.1847	Positive
611.0947	Negative
611.1844	Positive
612.1826	Positive
613.0923	Negative
623.1136	Negative
623.5721	Negative
624.2348	Positive
624.9662	Negative
625.1090	Negative
625.2358	Positive
633.0358	Negative
637.1278	Negative
638.6073	Positive
639.1241	Negative
641.1276	Negative
649.0102	Negative
663.4532	Positive

Mass [m/z]	Polarity
664.4594	Positive
673.0913	Negative
675.0933	Negative
680.4770	Positive
681.4817	Positive
684.2032	Positive
685.2031	Positive
685.4260	Positive
686.2022	Positive
690.9928	Negative
698.2538	Positive
715.0379	Negative
721.5054	Positive
723.5049	Positive
731.0144	Negative
750.5574	Positive
751.5619	Positive
764.5717	Positive
777.5931	Negative
797.0444	Negative
819.6404	Negative
820.6425	Negative
891.6800	Negative
933.7261	Negative