

SAX fractions 22 and 27: CID fragments and identifications

m/z	Rel. Int.		charge	M_exp	I.D.	M_theo
	Fr. 22	Fr. 27				
277.06	0.6	2.0	1	278.07	0,2 A2 (0S)	278.06
286.54	2.6	3.1	2	575.09	B3 (1S)	575.08
326.51	5.7	7.0	2	655.04	B3(2S)	655.04
329.71	0.1	6.9	3	992.15	B5 (2S)	992.14
335.71	6.1	37.2	3	1010.14	C5 (2S)	1010.15
349.71	8.0	29.3	3	1052.16	2,4 A6 (2S)	1052.16
356.36	0.1	15.8	3	1072.11	B5 (3S)	1072.09
362.37	1.6	7.0	3	1090.13	C5(3S)	1090.10
367.08	15.2	7.5	2	736.17	B4(1S)	736.15
369.72	13.3	37.6	3	1112.17	0,2 A6 (2S)	1112.18
376.08	0.7	5.4	2	754.18	2,4 X3 (1S, Ac)	754.16
391.38	0.9	1.3	3	1177.17	0,2 X5 (3S, Ac)	1177.17
396.38	14.1	33.4	3	1192.16	0,2 A6 (3S)	1192.14
403.40	14.0	22.1	3	1213.24	precursor - SO3	1213.23
407.05	75.0	43.8	2	816.12	B4 (2S)	816.10
416.06	3.9	36.9	2	834.13	C4(2S)	834.12
424.06	2.4	5.8	3	1275.19	precursor - H2O	1275.17
430.05	100	100	3	1293.18	precursor	1293.18
447.03	4.3	3.4	2	896.08	B4 (3S)	896.06
455.09	1.7	6.8	2	912.20	B5(1S)	912.18
486.62	1.5	1.7	2	975.26	Y5 (1S, Ac)	975.25
495.07	3.7	15.2	2	992.15	B5 (2S)	992.14
504.08	1.1	2.8	2	1010.17	C5 (2S)	1010.15
515.11	14.9	19.0	2	1032.24	0,2 A6 (1S)	1032.22
526.61	9.9	9.6	2	1055.23	Y5 (2S, Ac)	1055.21
547.61	1.5	1.6	2	1097.23	0,2 X5 (2S, Ac)	1097.22
555.09	55.7	79.1	2	1112.20	0,2 A6 (2S)	1112.18
595.07	1.4	2.0	2	1192.15	0,2 A6 (3S)	1192.14

Supplemental Table 1. All fragment ions from fractions 22 and 27 present above 1% relative abundance are listed using the Domon and Costello nomenclature⁶⁸.

Experimental and theoretical masses are listed as M_exp and M_theo, respectively.