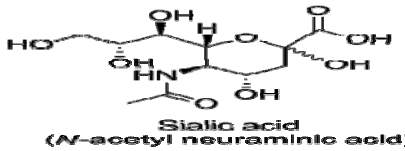
CHEMISTRY 133

Spring, 2015 Homework Set 3.2 - Additional Problem 1

Trisialic acid is a trimer from combining sialic acid (shown below):



Production of an oligomer of n monomers involves the loss of n-1 waters. Given the following ESI negative ion mass spectrum table (below),

a) Find three peaks that are due to due to the the sialic acid trimer. For each peak, give the ion (including alternative isotopes) that produces it. For ESI-MS, fragmentation normally doesn't occur, but multiple charging is possible as well as adducts (such as with Na^+).

b) what resolution is needed to distinguish a tetrasialic acid oligomer M – H peak, from an isotope peak (due to one ^{13}C) of the standard observed at 1180 amu (assume that that mass is exactly correct)?

Standards	Centroid Mass (amu)	Area (A)
HBAPE Std	213.0549	40602
	214.0586	42738
	255.2327	19173
	283.2635	17584
Gly Std M - 2H	410.1927	25372
	410.6936	10367
	411.1953	3462
	444.6382	10076
	445.1393	3664
	807.4159	3663
Gly Std M - H	821.3959	91828
	822.3988	41359
	823.4018	14402
	843.3774	7057
	844.3829	2879
	890.2878	12474
	891.2884	4145
	912.2659	3251
	1005.9724	3233
	1065.9959	4300
UM1080 Std	1080.0100	15741
	1081.0092	2891
	1105.9634	4106
	1120.6753	3153
	1165.9850	10333
	1170.6705	4122
	1171.1704	3373
UM1180 Std	1180.0033	36577
	1181.0048	8261
	1182.9806	4702
	1205.9556	4473
	1220.6664	4335