



# **Molecular Recognition of Modified Nucleobases. Self-Complementarity and Base-Pairing of Betainic Guanine Model Compounds**

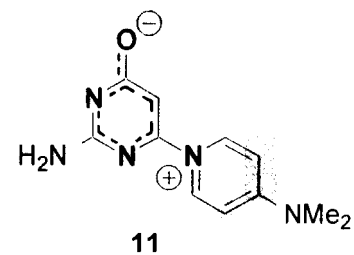
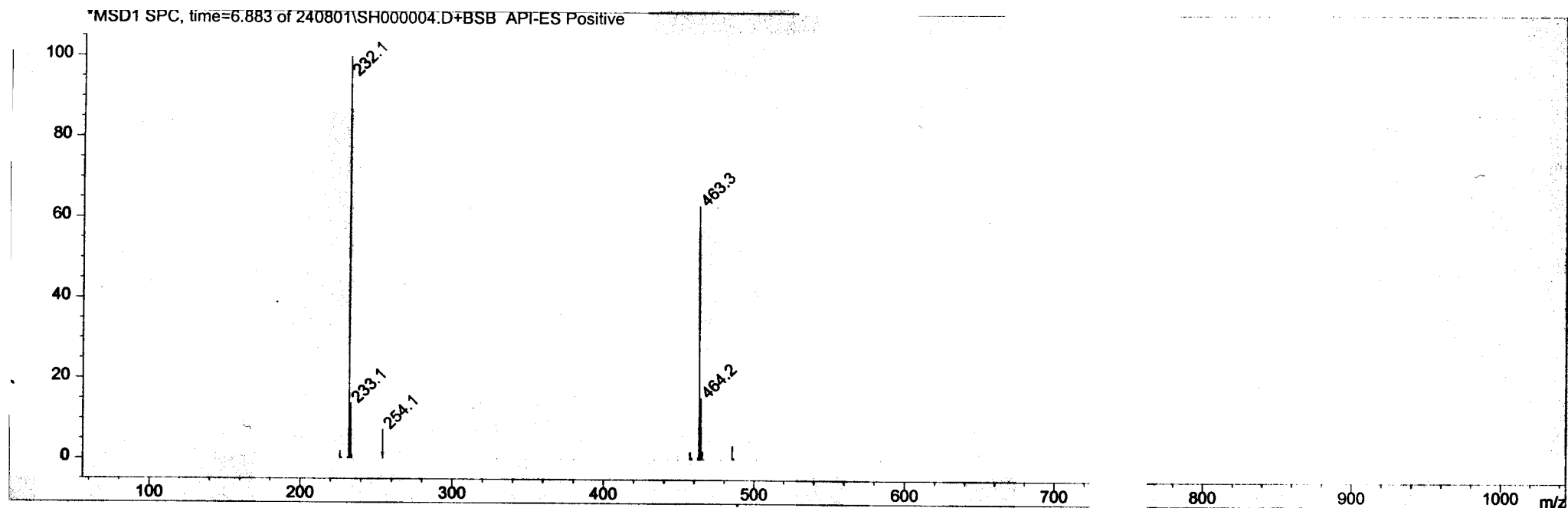
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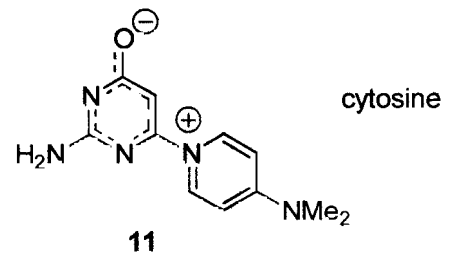
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Supplementary material

ESI mass spectra

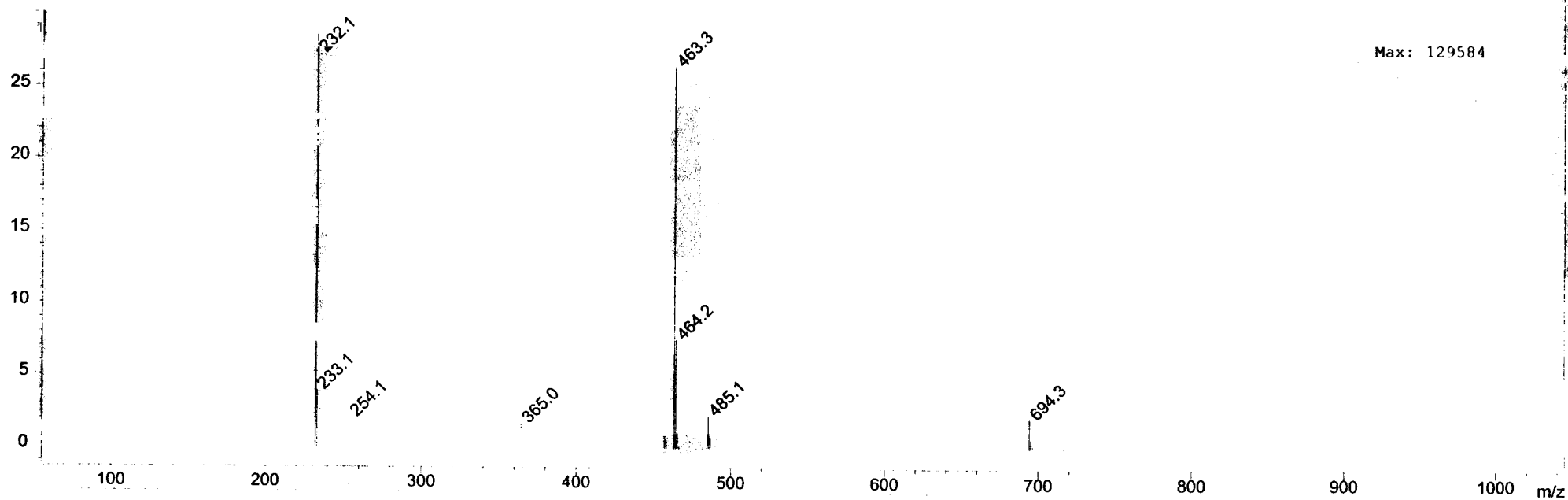


Injection date: 8 / 24 / 01  
Fragmentor voltage: 15 V  
Solvent flow : 0.8 mL/min.  
Solvent mixture: Water / MeCN = 1 : 9  
Positive detection mode  
Drying gas temp. 300°C  
Drying gas flow: 10 L/min  
Noise Cutoff: 5000 counts  
Reportable Ion Abundance: > 10%

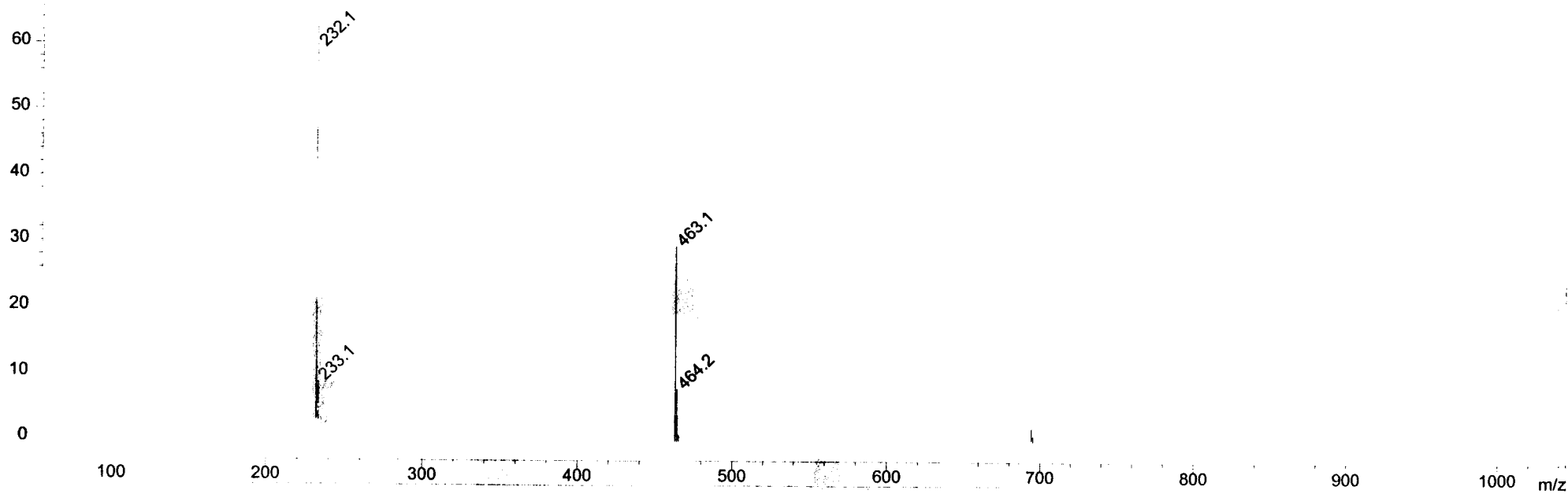


Injection date: 8 / 24 / 01  
Fragmentor voltage: 0, 0 V  
Solvent flow : 0.8 mL/min.  
Solvent mixture: Water / MeCN = 1 : 9  
Positive detection mode  
Drying gas temp. 140°C  
Drying gas flow: 10 L/min  
Noise Cutoff: 5000 counts  
Reportable Ion Abundance: > 10%

\*MSD1 SPC, time=2.155 of 240801\SH000008.D+BSB API-ES Positive

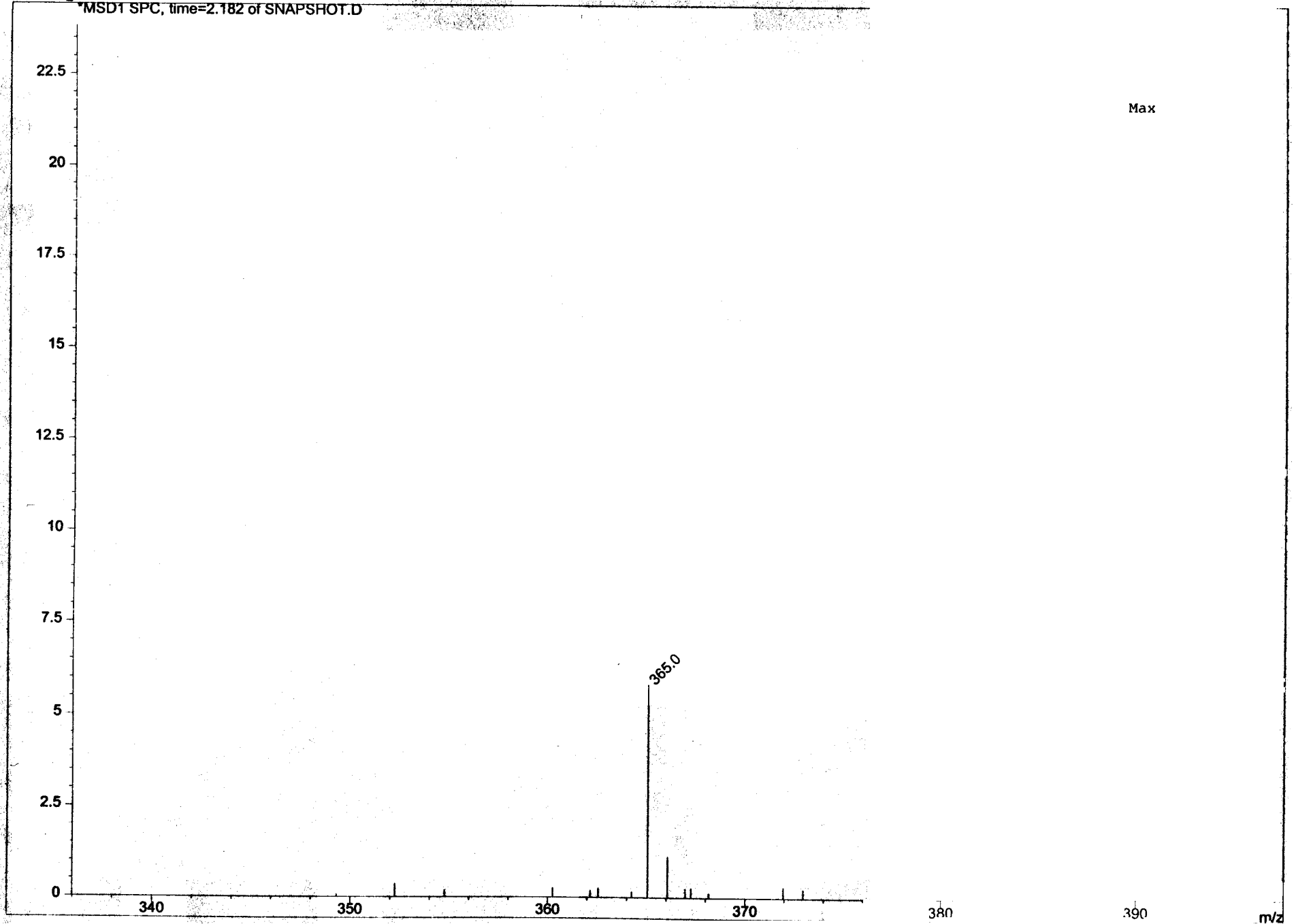


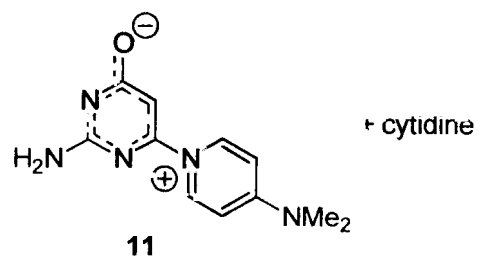
\*MSD1 SPC, time=4.479 of 240801\SH000008.D+BSB API-ES Positive



MS Spectrum

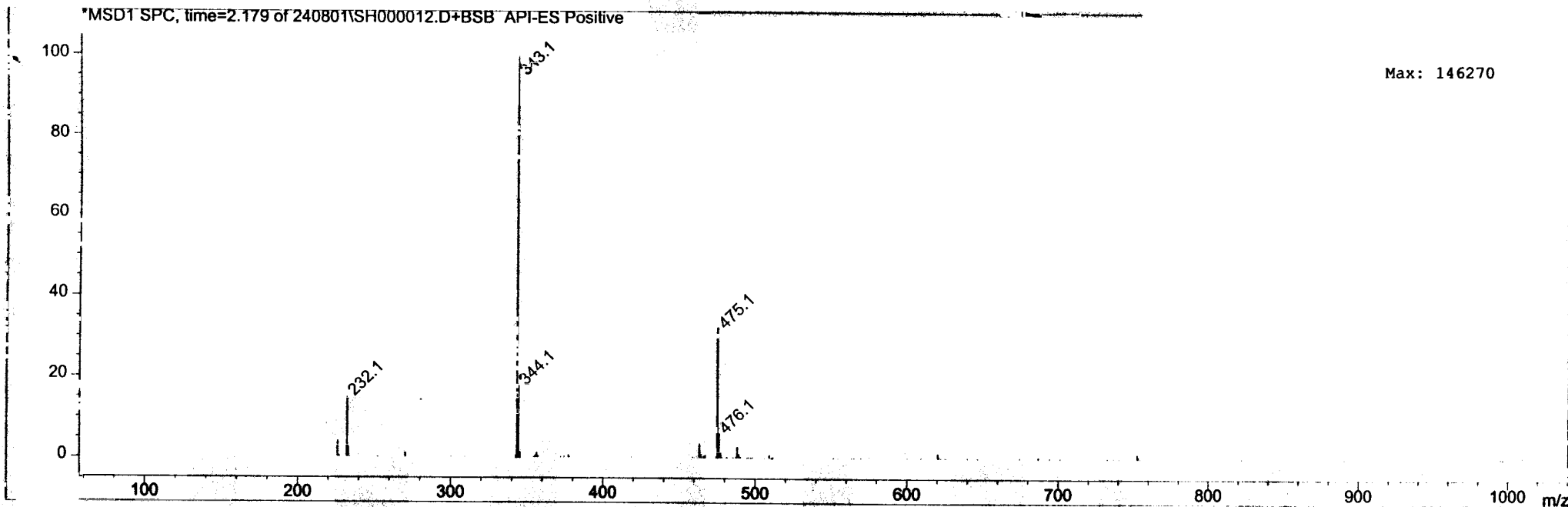
MSD1 SPC, time=2.182 of SNAPSHOT.D

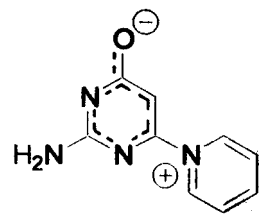




**Injection date: 8 / 24 / 01**  
**Fragmentor voltage: 0 V**  
**Solvent flow : 0.8 mL/min.**  
**Solvent mixture: Water / MeCN =**  
**Positive detection mode**  
**Drying gas temp. 140°C**  
**Drying gas flow: 10 L/min**  
**Noise Cutoff: 5000 counts**  
**Reportable Ion Abundance: > 10%**

Retention Time (MS)	MS Area	Mol. Weight or Ion
2.179	2696495	475.15 I 344.15 I 343.15 I 232.15 I
2.441	3356708	344.15 I 343.15 I
3.126	1813394	343.15 I





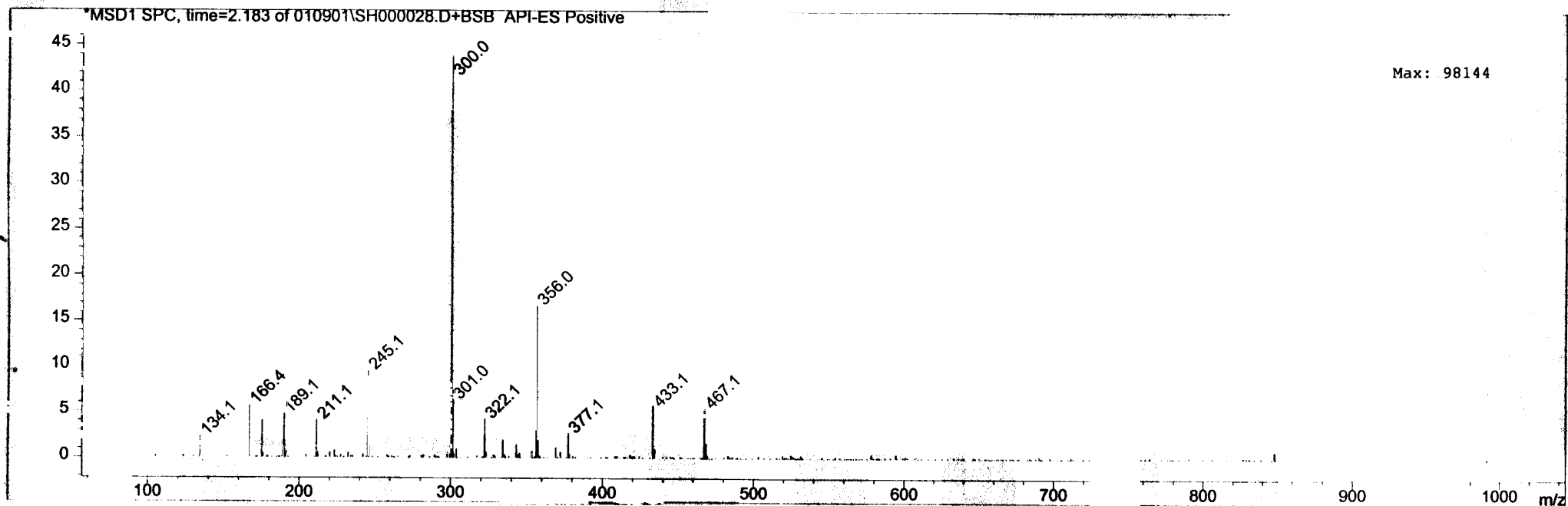
+ cytosine

12

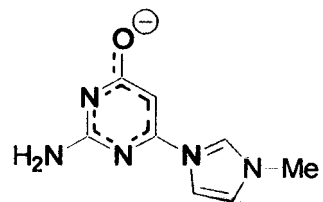
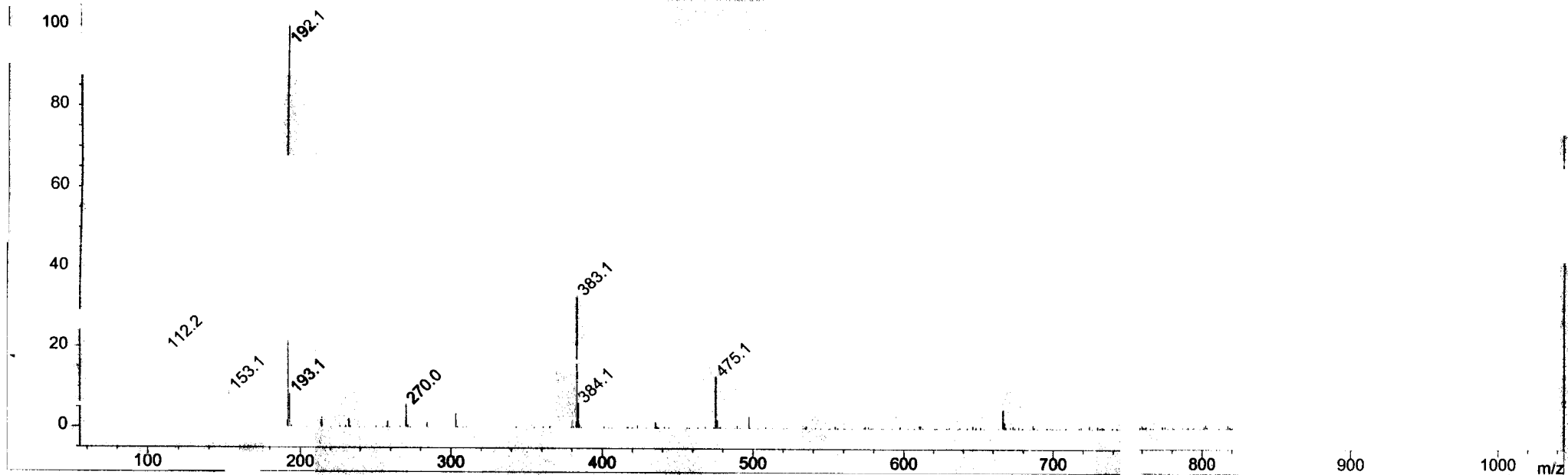
Injection date: 8 / 24 / 01  
Fragmentor voltage: 0 V  
Solvent flow : 0.8 mL/min.  
Solvent mixture: Water / MeCN = 1 : 9  
Positive detection mode  
Drying gas temp. 140°C  
Drying gas flow: 10 L/min  
Noise Cutoff: 5000 counts  
Reportable Ion Abundance: > 10%



192.05 I  
190.05 I  
189.05 I  
134.05 I  
105.85 I



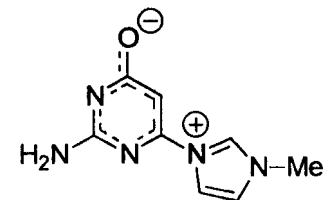
\*MSD1 SPC, time=4.825 of 010901\SH000025.D+BSB API-ES Positive



13

Injection date: 8 / 24 / 01  
Fragmentor voltage: 0 V  
Solvent flow : 0.8 mL/min.  
Solvent mixture: Water / MeCN = 1 : 9  
Positive detection mode  
Drying gas temp. 140°C  
Drying gas flow: 10 L/min  
Noise Cutoff: 5000 counts  
Reportable Ion Abundance: > 10%

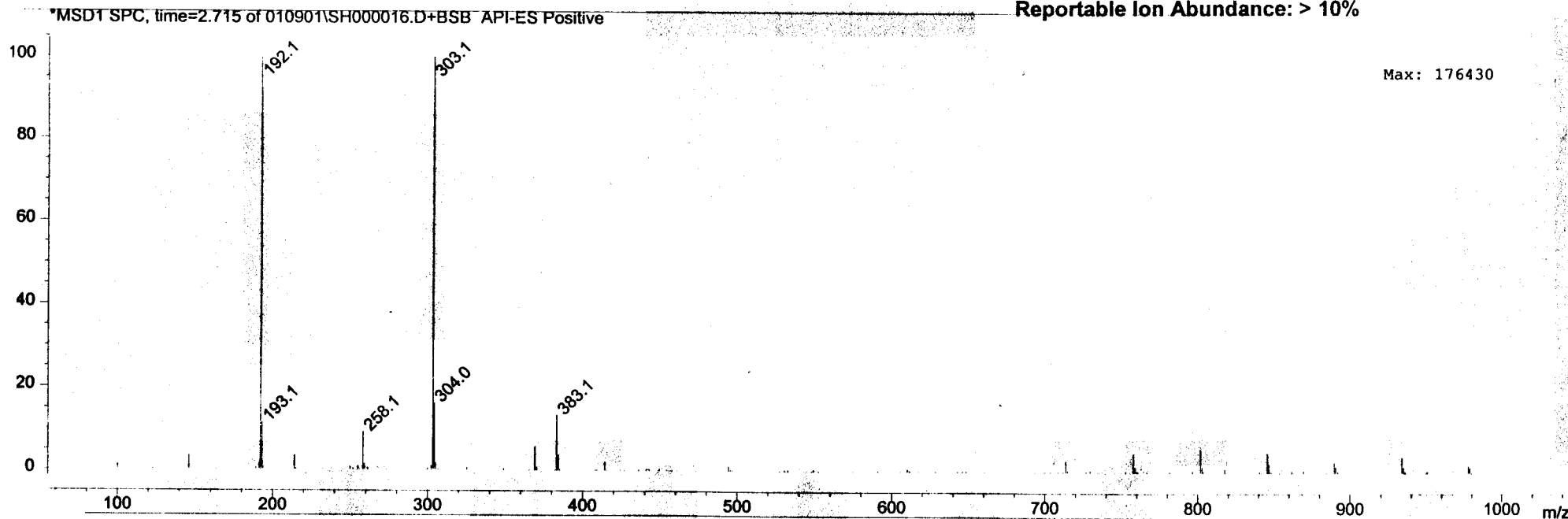
Retention Time (MS)	MS Area	Mol. Weight or Ion
2.724	4357882	383.15 I
		304.05 I
		303.15 I
		193.05 I
		192.05 I
2.818	15424062	383.15 I
		304.05 I
		303.15 I
		192.05 I
		153.15 I
		112.05 I
		105.05 I



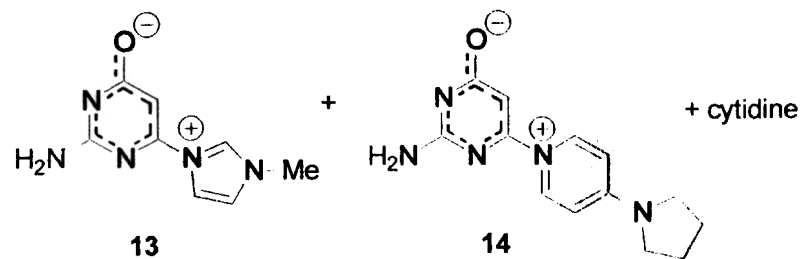
+ cytosine

13

Injection date: 8 / 24 / 01  
 Fragmentor voltage: 0 V  
 Solvent flow : 0.8 mL/min.  
 Solvent mixture: Water / MeCN = 1 : 9  
 Positive detection mode  
 Drying gas temp. 140°C  
 Drying gas flow: 10 L/min  
 Noise Cutoff: 5000 counts  
 Reportable Ion Abundance: > 10%



Retention Time (MS)	MS Area	Mol. Weight or Ion
2.177	4942993	501.15 I
		436.15 I
		435.15 I
		370.15 I
		369.15 I
		343.15 I
		304.05 I
		303.15 I
		270.25 I
		258.05 I
192.05 I		
4.730	4017986	757.45 I
		502.25 I
		501.25 I
		435.15 I
		258.15 I
		258.15 I



Injection date: 8 / 24 / 01  
 Fragmentor voltage: 0 V  
 Solvent flow : 0.8 mL/min.  
 Solvent mixture: Water / MeCN = 1 : 9  
 Positive detection mode  
 Drying gas temp. 140°C  
 Drying gas flow: 10 L/min  
 Noise Cutoff: 5000 counts  
 Reportable Ion Abundance: > 10%

