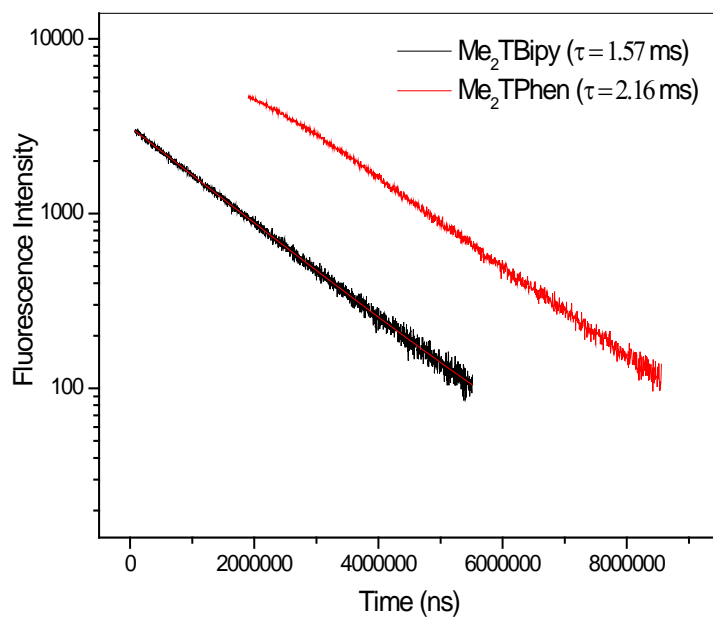


**ESI-1:** Lifetime spectra of Eu(III) complexes of Me<sub>2</sub>TBipy and Me<sub>2</sub>TPhen (M:L = 1:10) in acetonitrile ( $\lambda_{\text{ex}} = 247 \text{ nm}$ ,  $\lambda_{\text{em}} = 616 \text{ nm}$ )



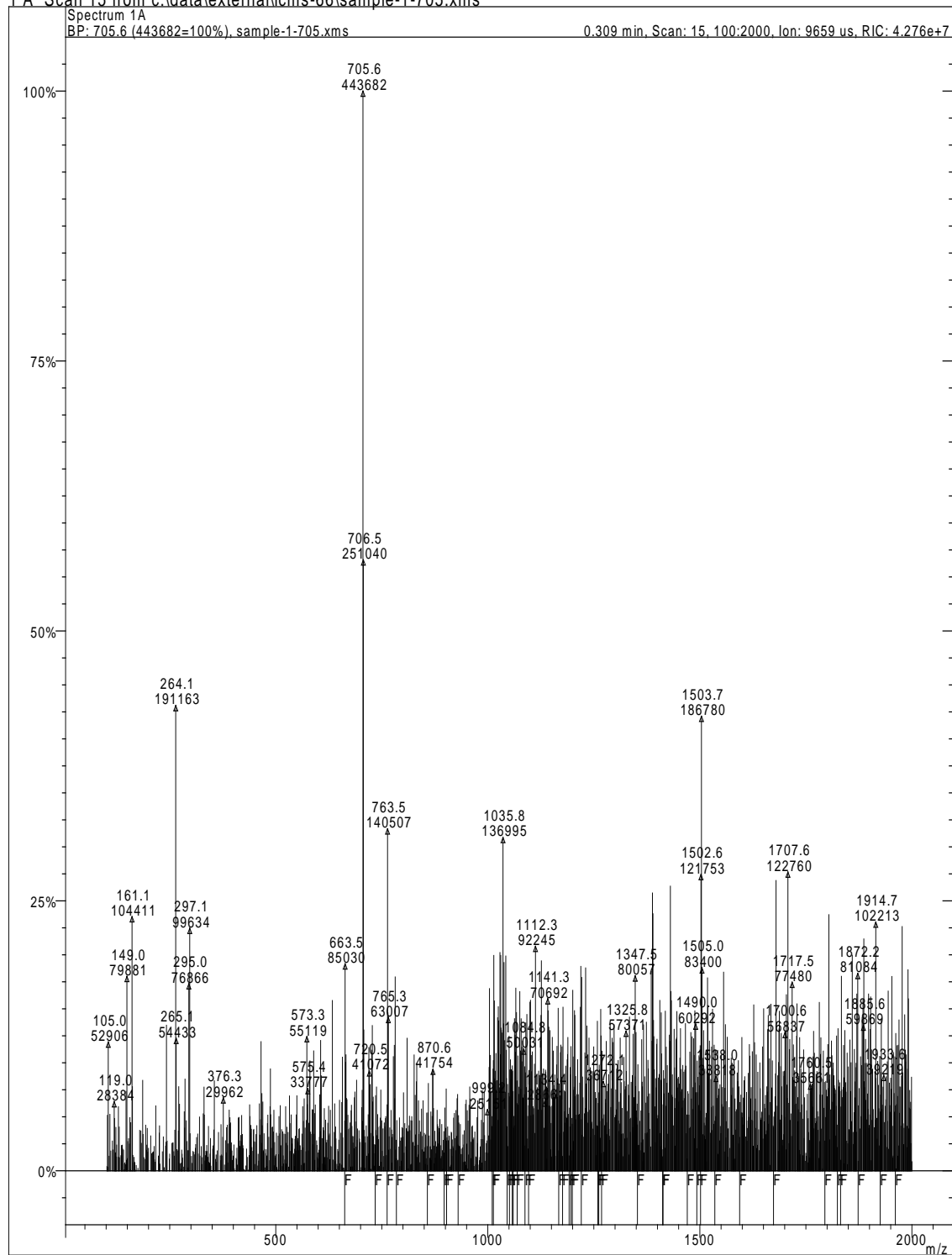
**ESI-2:** The species identified from the ESI-MS spectra of  $\text{Ln}^{3+}$  complexes of  $\text{Me}_2\text{TBipy}$  and  $\text{Me}_2\text{TPhen}$  in acetonitrile medium (L =  $\text{Me}_2\text{TBipy}/\text{Me}_2\text{TPhen}$ , S = acetonitrile, W = water)

$\text{Ln}^{3+}$	$\text{Me}_2\text{TBipy}$		$\text{Me}_2\text{TPhen}$	
	Species	m/z	Species	m/z
$\text{La}^{3+}$	$[\text{LaL}(\text{NO}_3)_2(\text{S})_3(\text{W})_3]^+$	705.0 (100%)	$[\text{HL}]^+$	288.1 (100%)
	$[\text{HL}]^+$	264.1	$[(\text{HL})_2.\text{HNO}_3]^{2+}$	319.1
			$[\text{LaL}(\text{NO}_3)_2(\text{W})(\text{S})_3]^+$	690.8
$\text{Eu}^{3+}$	$[\text{HL}]^+$	264.1 (100%)	$[(\text{HL})_2.\text{HNO}_3]^{2+}$	319.1 (100%)
	$[(\text{HL})_2.\text{HNO}_3]^{2+}$	295.1	$[\text{HL}]^+$	288.1
	$[\text{EuL}_2(\text{NO}_3)_2(\text{S})_2(\text{W})_3]^+$	938.8	$[\text{EuL}_2(\text{NO}_3)_2]^+$	851.5
	$[\text{EuL}_2(\text{NO}_3)_2(\text{W})]^+$	821.4	$[\text{EuL}_2(\text{NO}_3)]^{2+}$	395.1
$\text{Er}^{3+}$	$[\text{HL}]^+$	264.1 (100%)	$[(\text{HL})_2.\text{HNO}_3]^{2+}$	319.1 (100%)
	$[(\text{HL})_2.\text{HNO}_3]^{2+}$	295.1	$[\text{HL}]^+$	288.1
	$[\text{ErL}(\text{NO}_3)_2(\text{W})_2]^+$	589.4		
	$[\text{ErL}_2(\text{NO}_3)_2(\text{W})_2]^+$	853.8	$[\text{ErL}_2(\text{NO}_3)_2]^+$	865.8

ESI-3: ESI-MS spectra of  $1 \times 10^{-3} \text{M}$   $\text{La}(\text{NO}_3)_3$  and  $1 \times 10^{-3} \text{M}$  of  $\text{Me}_2\text{TBipy}$  in acetonitrile

Spectrum Plot - 1/8/2014 10:56 AM

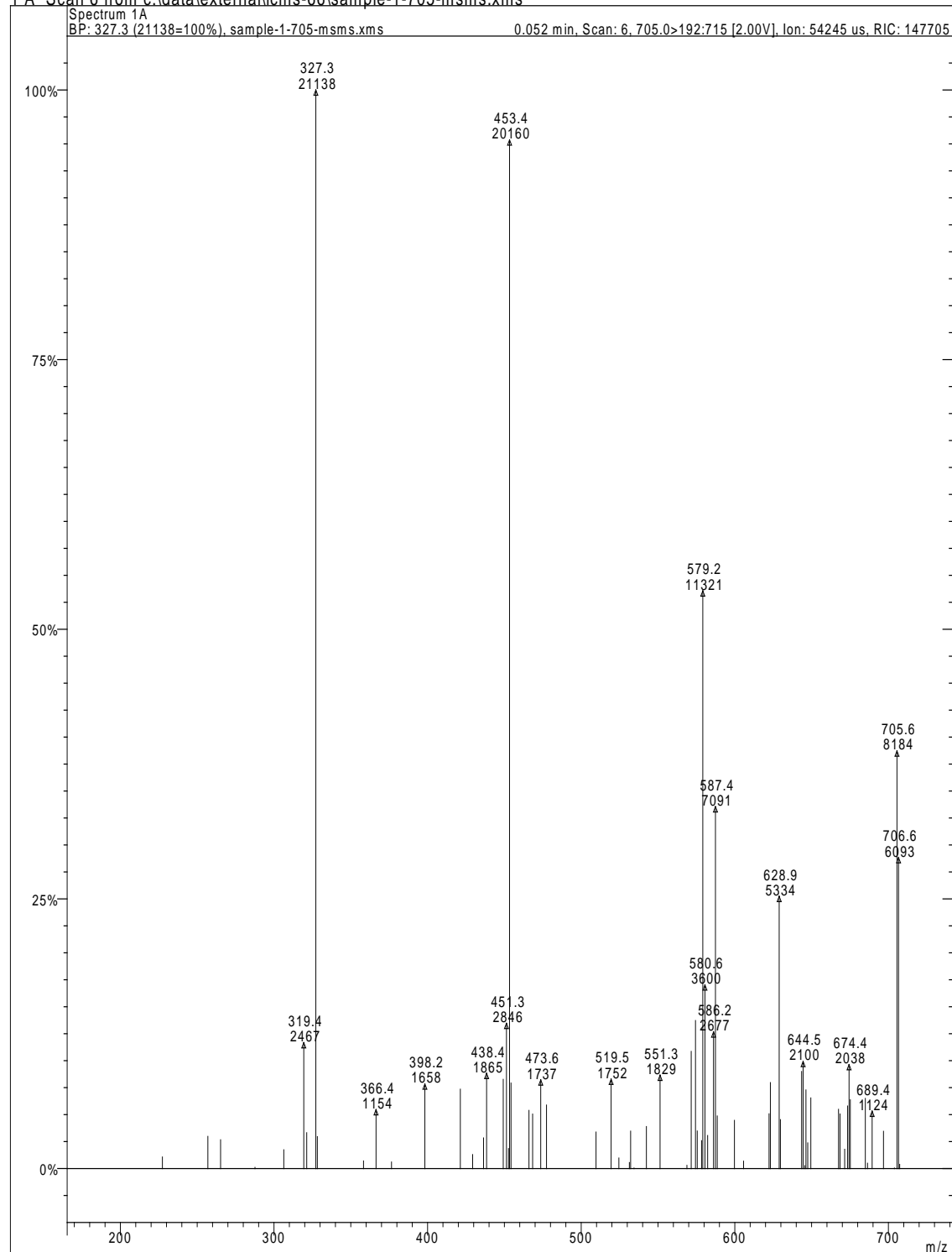
1 A Scan 15 from c:\data\external\lcms-66\sample-1-705.xms



**ESI -4:** MS-MS spectra for the peak at  $m/z = 705.6$  of  $1 \times 10^{-3} \text{M}$   $\text{La}(\text{NO}_3)_3$  and  $1 \times 10^{-3} \text{M}$  of  $\text{Me}_2\text{TBipy}$  in acetonitrile

Spectrum Plot - 1/8/2014 10:55 AM

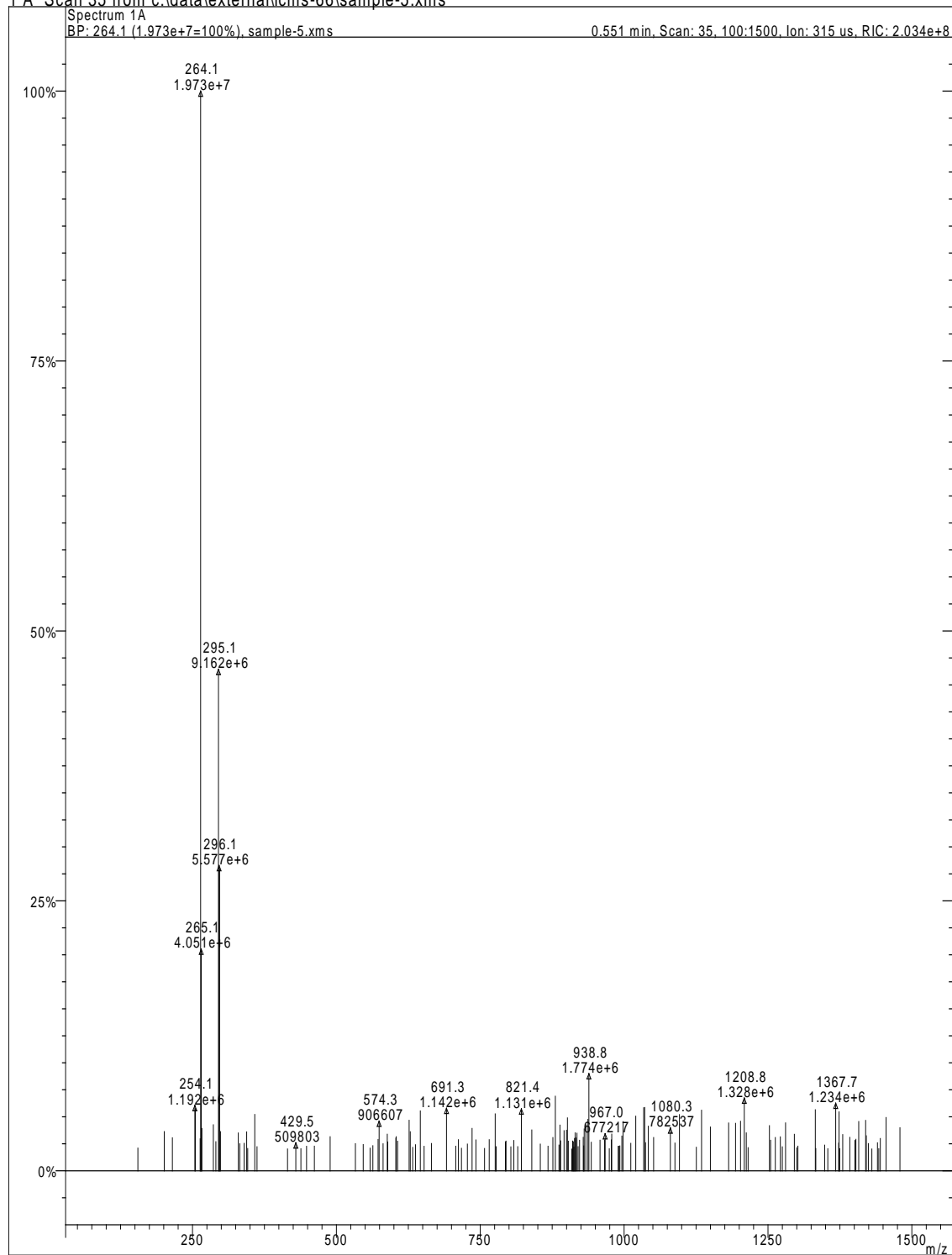
1 A Scan 6 from c:\data\external\lcms-66\sample-1-705-msms.xms



**ESI-5:** ESI-MS spectra of  $1 \times 10^{-3} \text{M}$   $\text{Eu}(\text{NO}_3)_3$  and  $1 \times 10^{-3} \text{M}$  of  $\text{Me}_2\text{TBipy}$  in acetonitrile

Spectrum Plot - 1/8/2014 11:03 AM

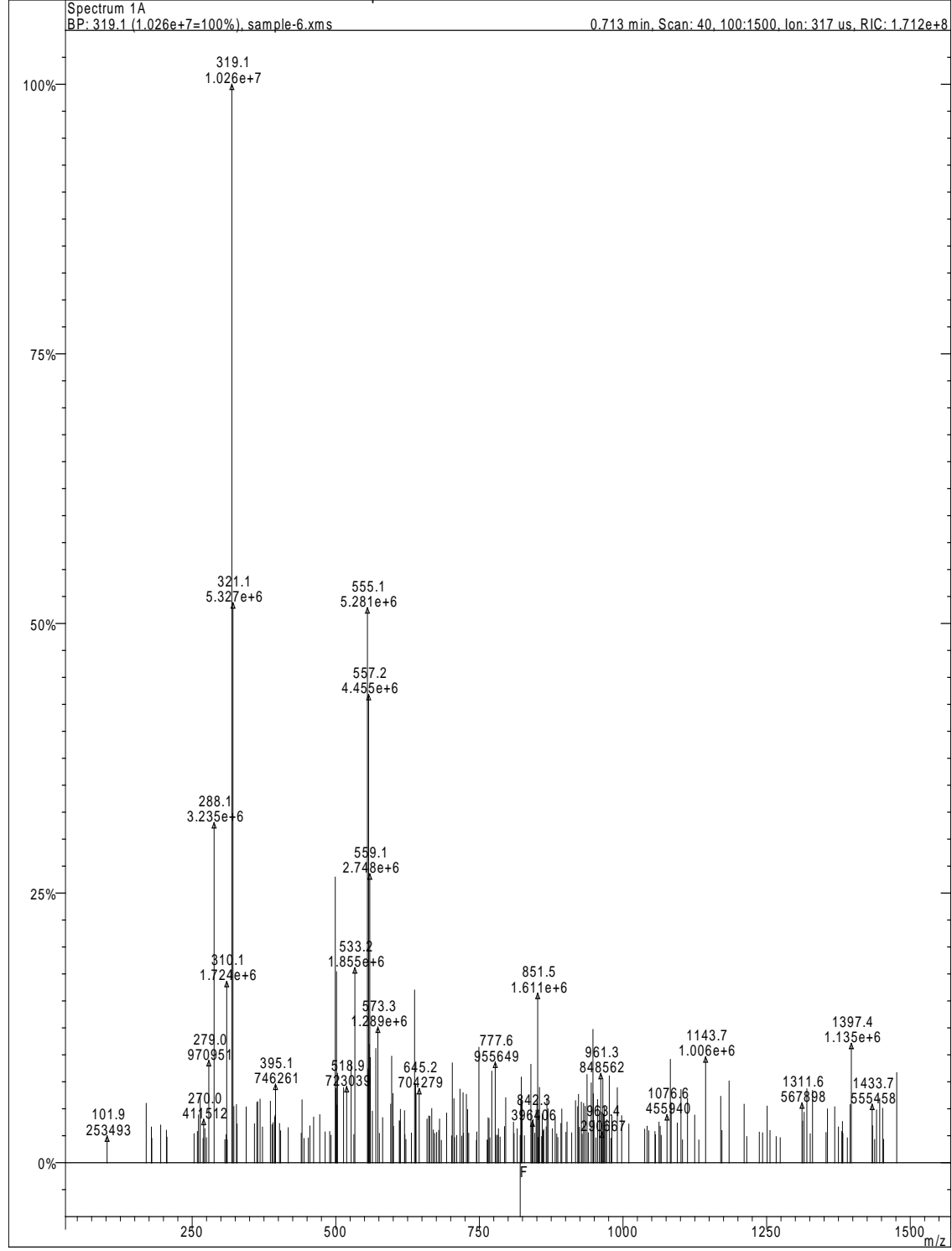
1 A Scan 35 from c:\data\external\lcms-66\sample-5.xms



ESI-6: ESI-MS spectra of  $1 \times 10^{-3}$  M  $\text{Eu}(\text{NO}_3)_3$  and  $1 \times 10^{-3}$  M of  $\text{Me}_2\text{TPhen}$  in acetonitrile

Spectrum Plot - 1/8/2014 11:04 AM

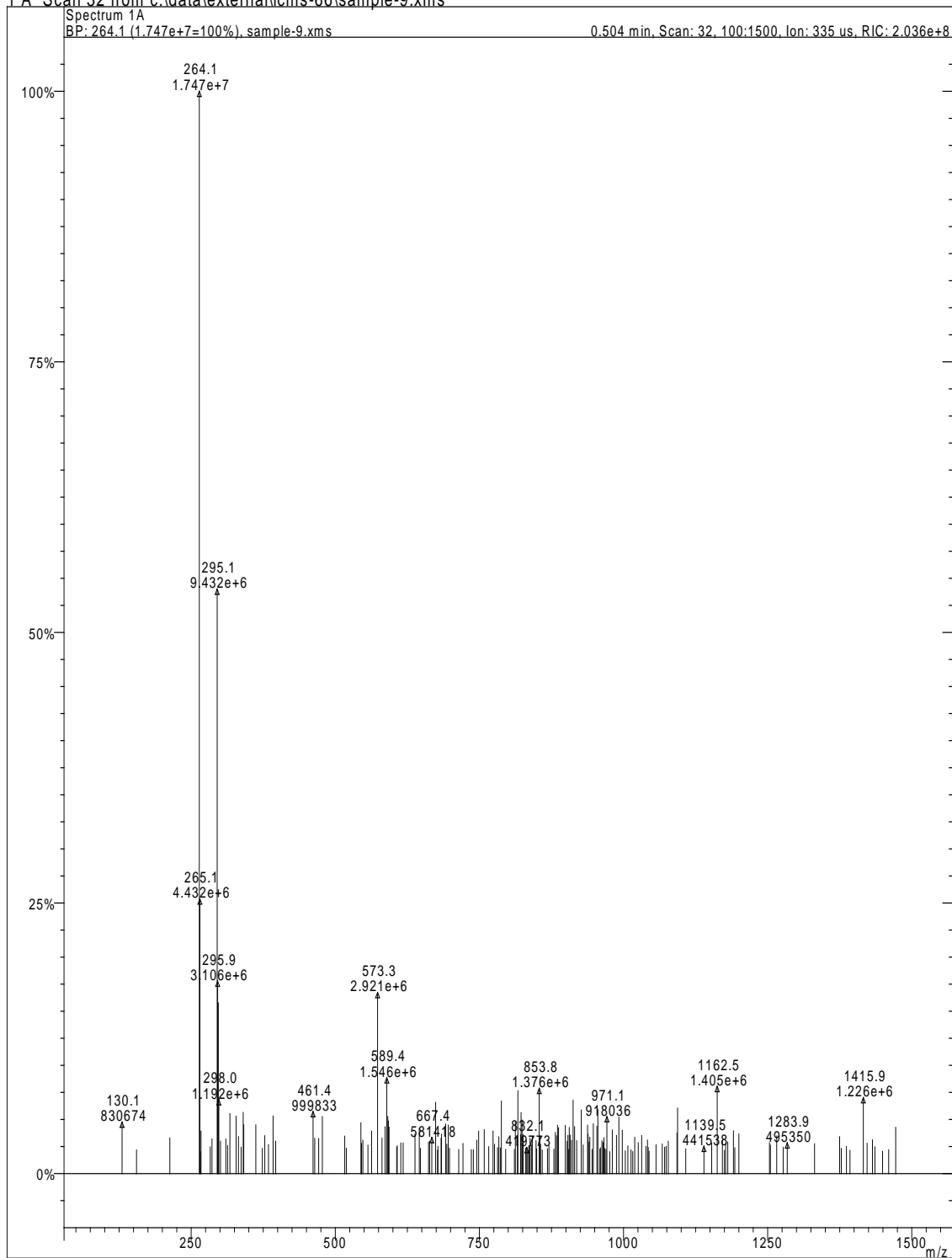
1 A Scan 40 from c:\data\external\lcms-66\sample-6.xms



**ESI-7:** ESI-MS spectra of  $1 \times 10^{-3} \text{ M Er(NO}_3)_3$  and  $1 \times 10^{-3} \text{ M}$  of  $\text{Me}_2\text{TBipy}$  in acetonitrile

Spectrum Plot - 1/8/2014 11:08 AM

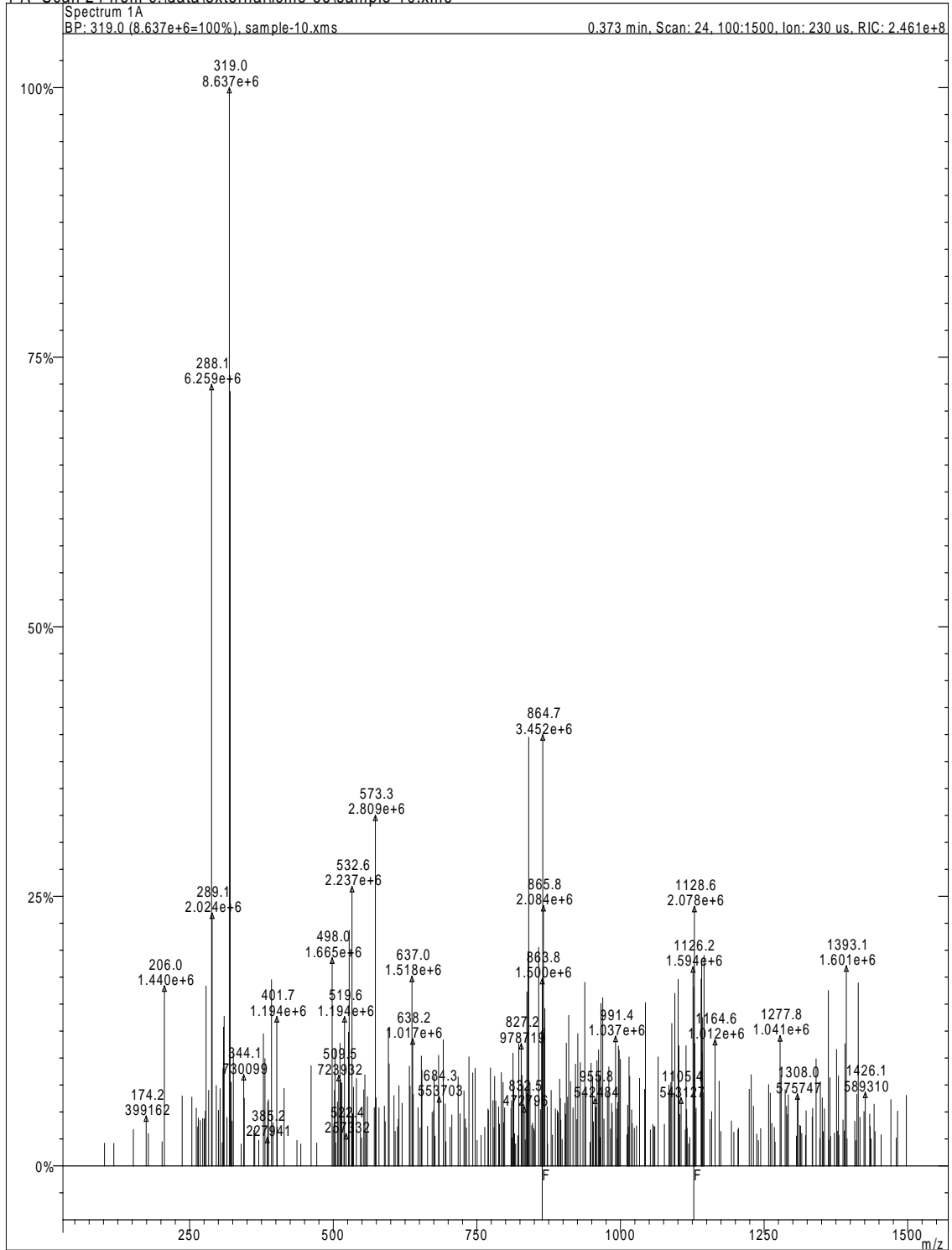
1 A Scan 32 from c:\data\external\lcms-66\sample-9.xms



**ESI-8:** ESI-MS spectra of  $1 \times 10^{-3}$  M  $\text{Er}(\text{NO}_3)_3$  and  $1 \times 10^{-3}$  M of  $\text{Me}_2\text{TPhen}$  in acetonitrile

Spectrum Plot - 1/8/2014 11:08 AM

1 A Scan 24 from c:\data\external\lcms-66\sample-10.xms

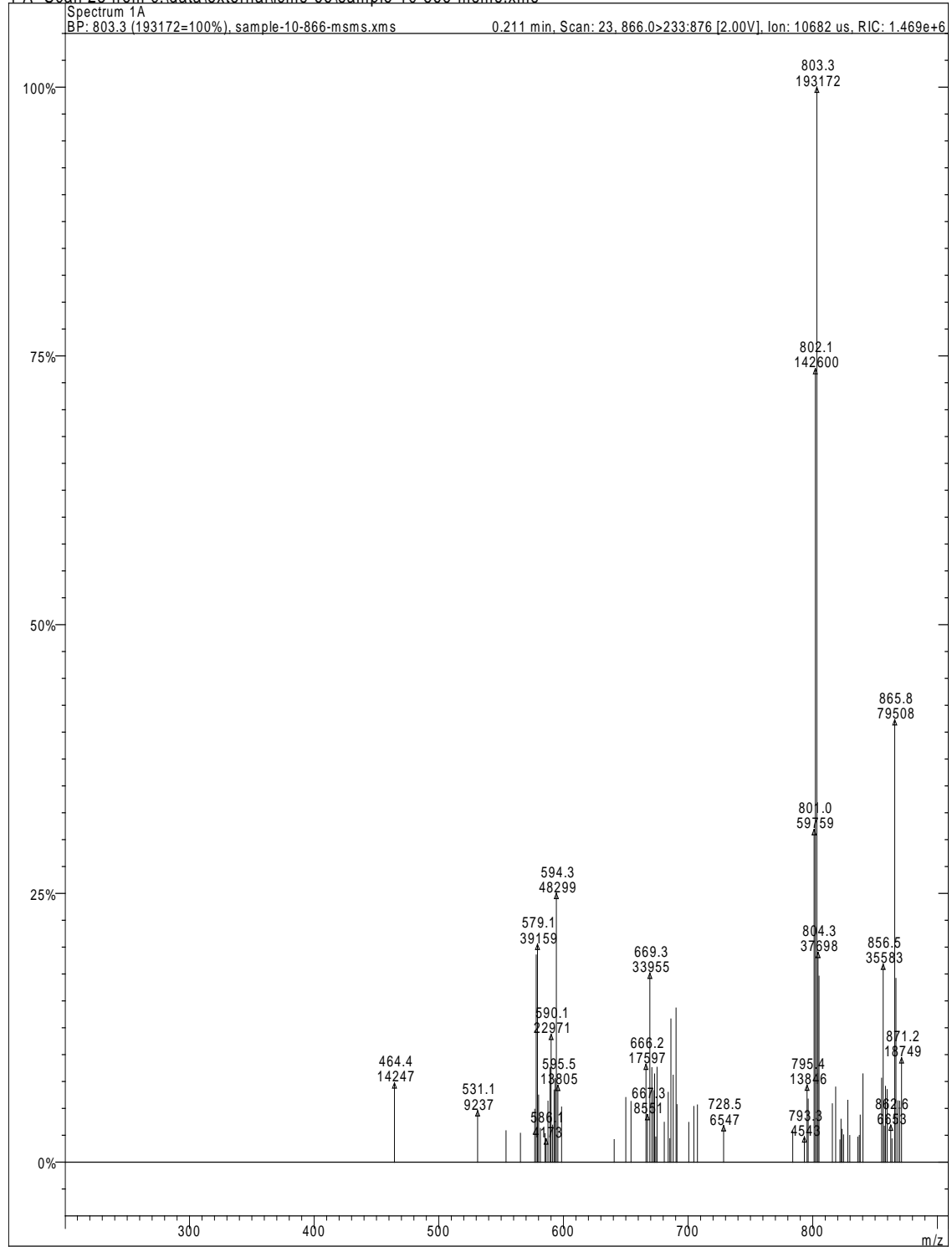




**ESI -9:** MS-MS spectra for the peak at  $m/z = 705.6$  of  $1 \times 10^{-3} \text{ M Er(NO}_3)_3$  and  $1 \times 10^{-3} \text{ M}$  of  $\text{Me}_2\text{TPhen}$  in acetonitrile

Spectrum Plot - 1/8/2014 11:08 AM

1 A Scan 23 from c:\data\external\cms-66\sample-10-866-msms.xms



**ESI-10:** The optimized geometries and relative energies of the  $\text{Eu}^{3+}$  complex of  $\text{Me}_2\text{TBipy}$  having mono dentate nitrate ions with respect to that having bidentate nitrate ions

