

SUPPLEMENTARY MATERIAL

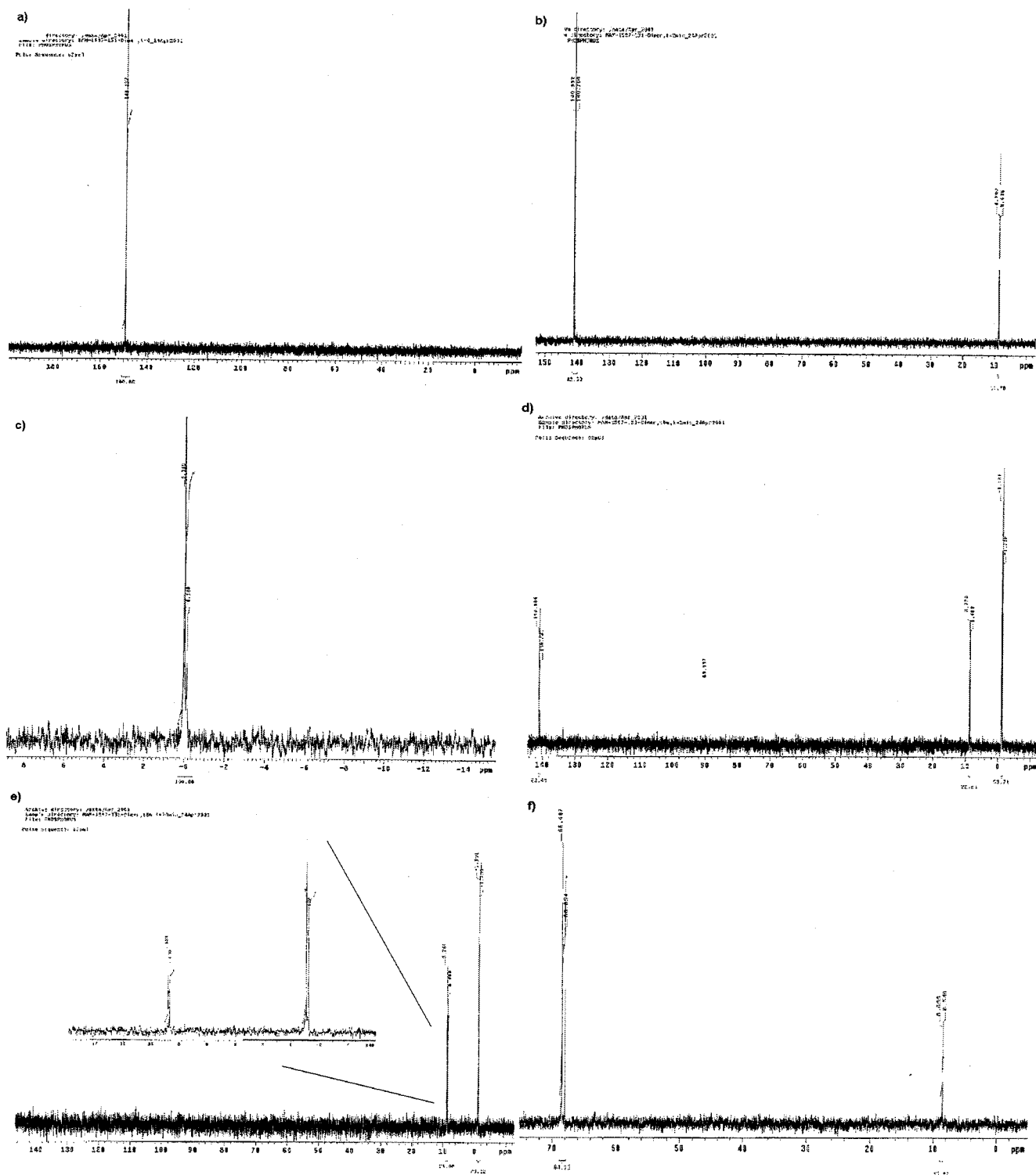
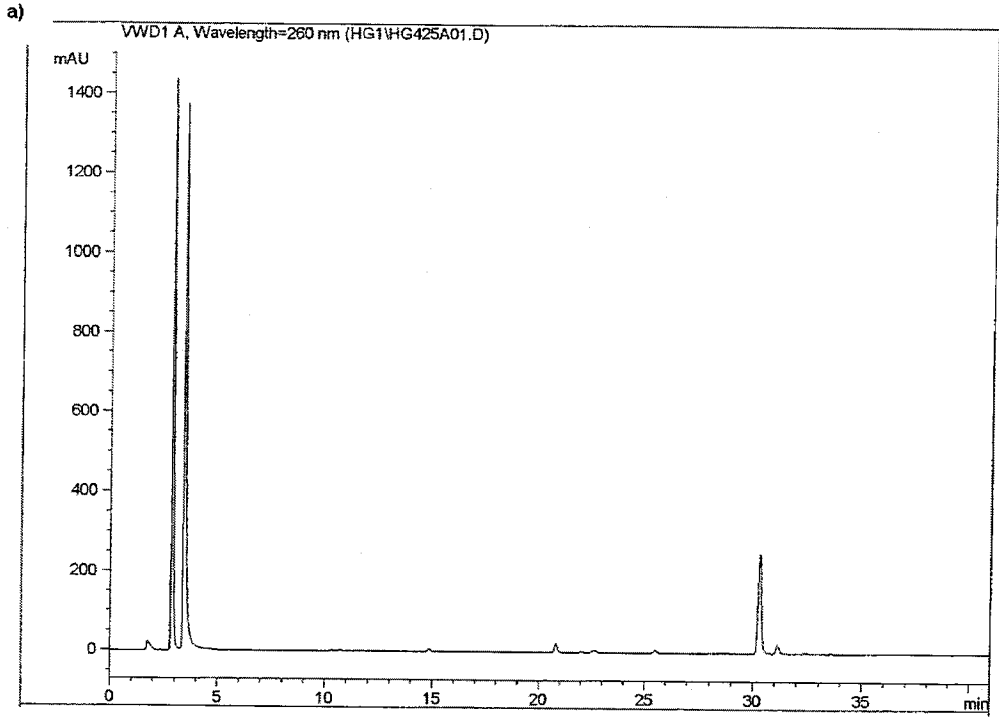
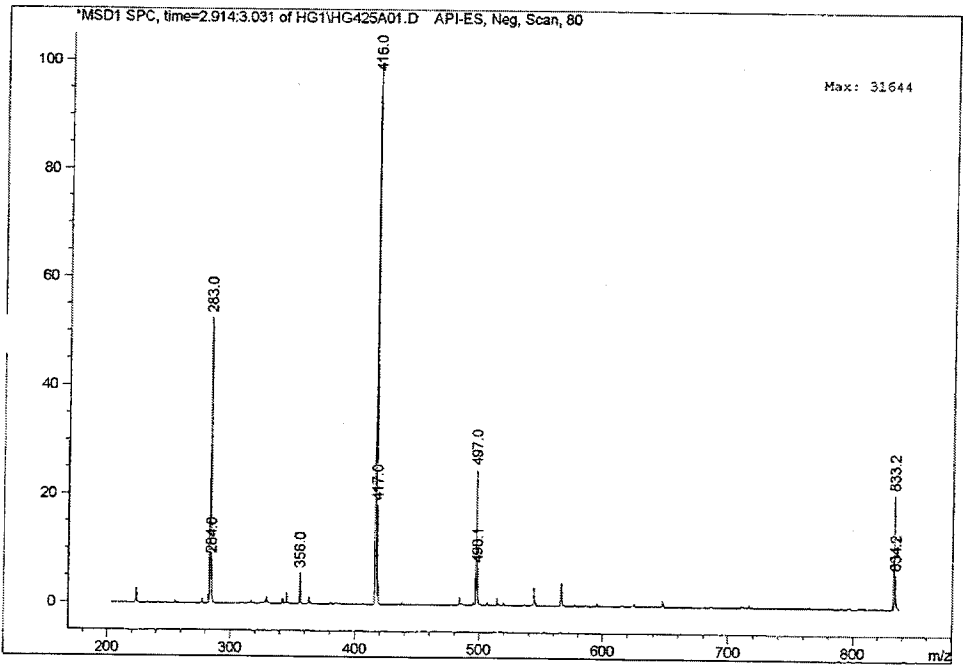


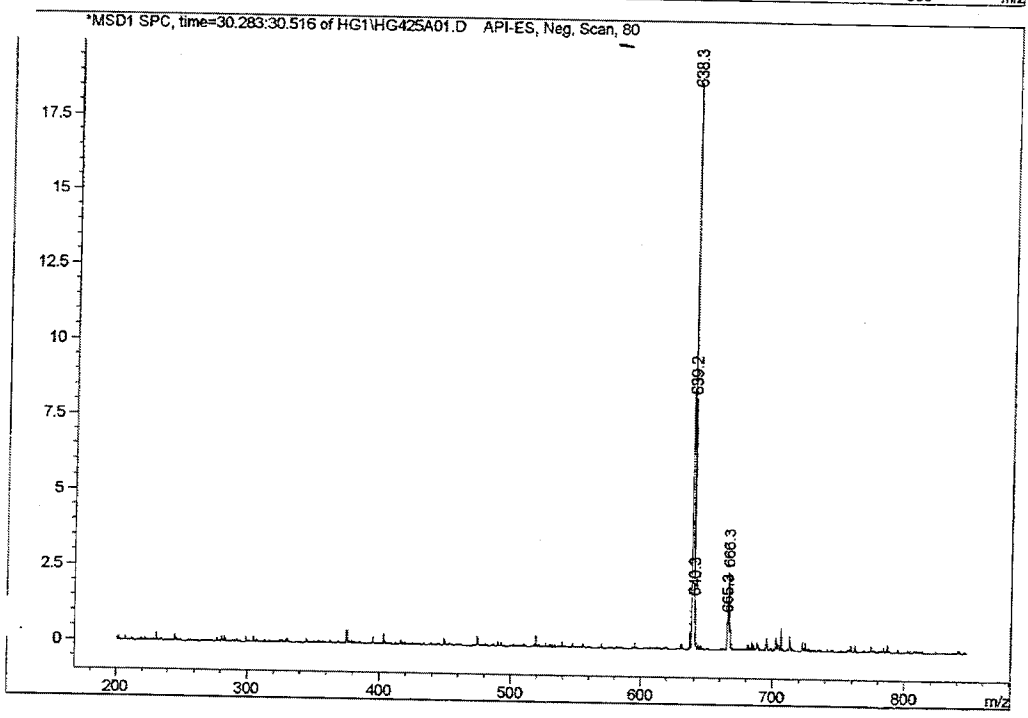
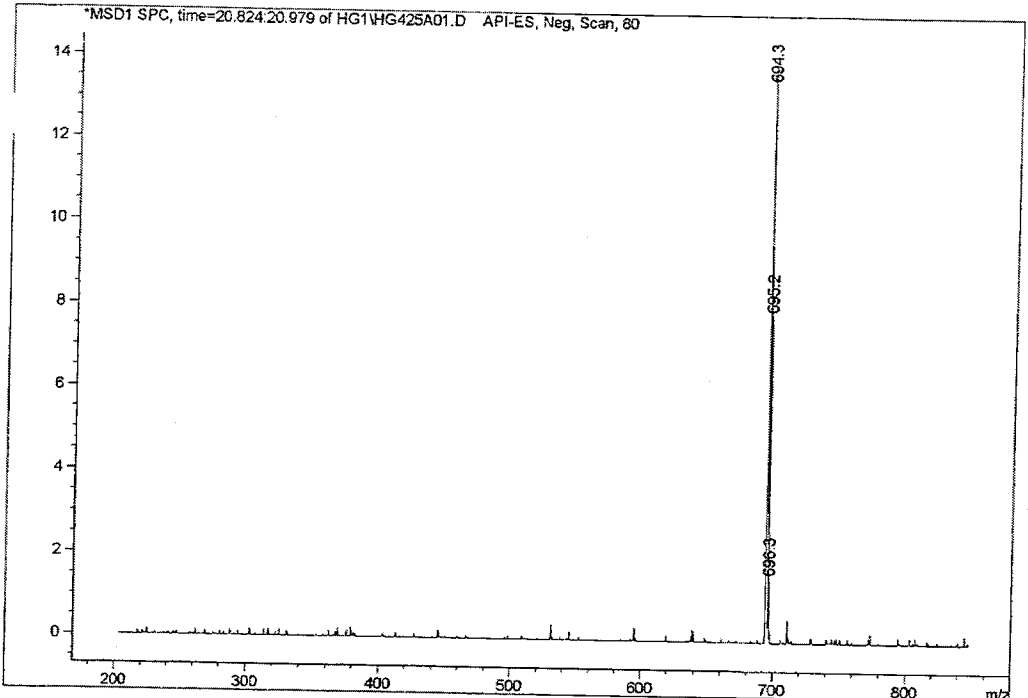
Figure 1. Oxidation of the A*pT dimer: ^{31}P -NMR of the reaction mixtures; (a) 2b and T-OAc before the addition of tetrazole, (b) 2 min after the addition of tetrazole, (c) 2 min after the addition of I_2 solution, (d) 2 min after the addition t-BuOOH solution, (e) 20 min after the addition t-BuOOH solution, (f) 2 min after the addition of Beaucage's sulfurizing reagent.

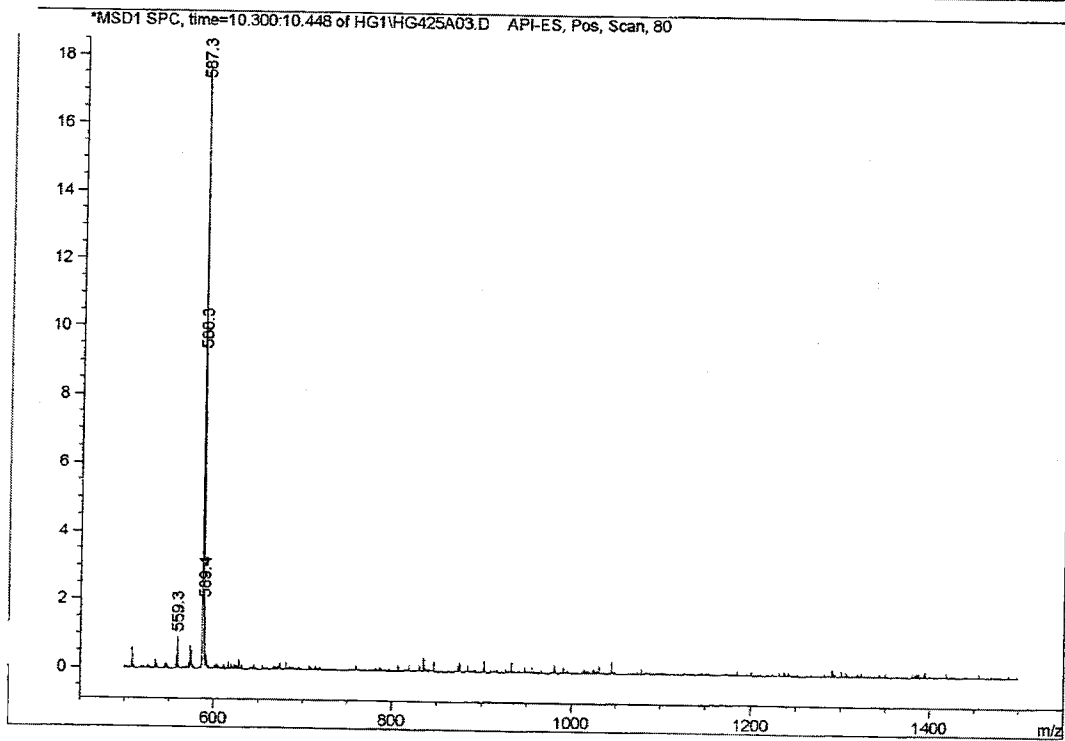
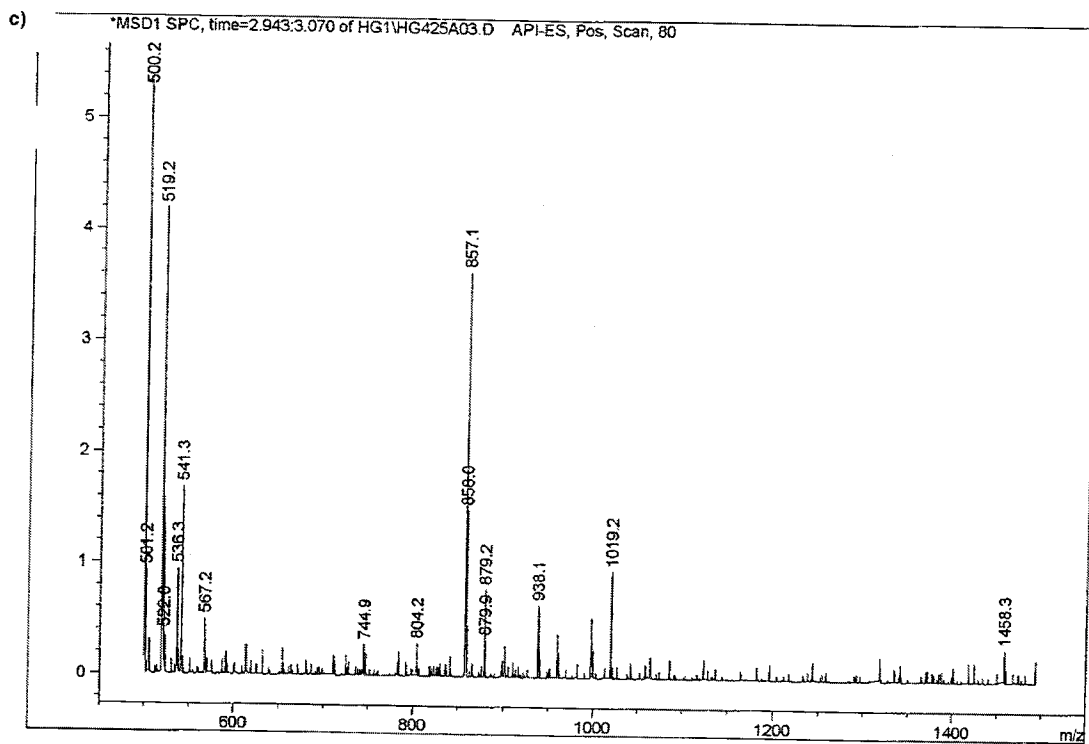


b) MS Signal: MSD1 TIC, MS File, API-ES, Neg, Scan, 80
 Spectra averaged over upper half of peaks.
 Noise Cutoff: 500 counts.
 Reportable Ion Abundance: > 50%.

Retention Time (MS)	MS Area	Mol. Weight or Ion
2.965	6116571	416.05 I 283.05 I
20.903	621754	695.15 I 694.25 I
30.397	1498954	638.25 I







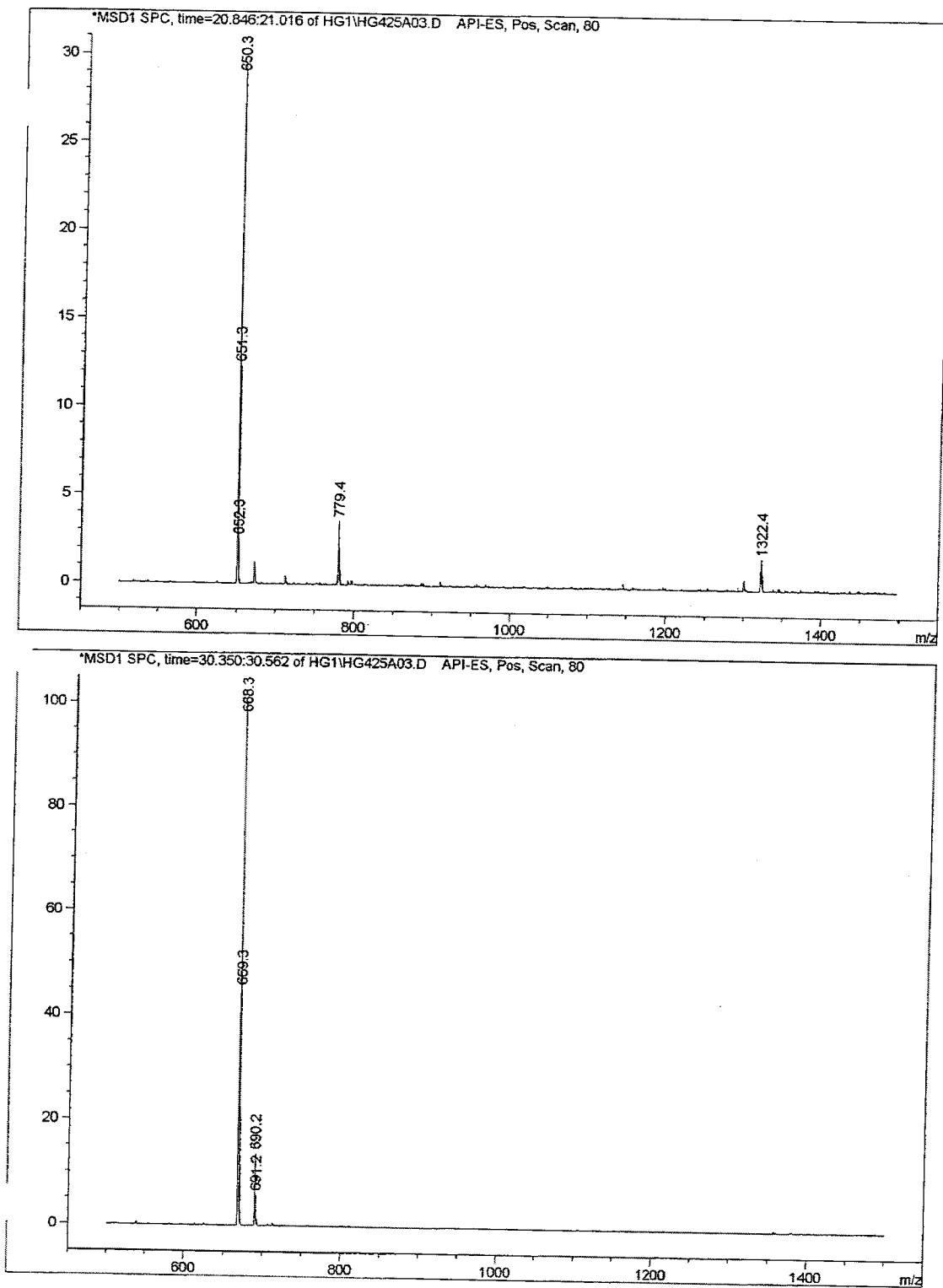
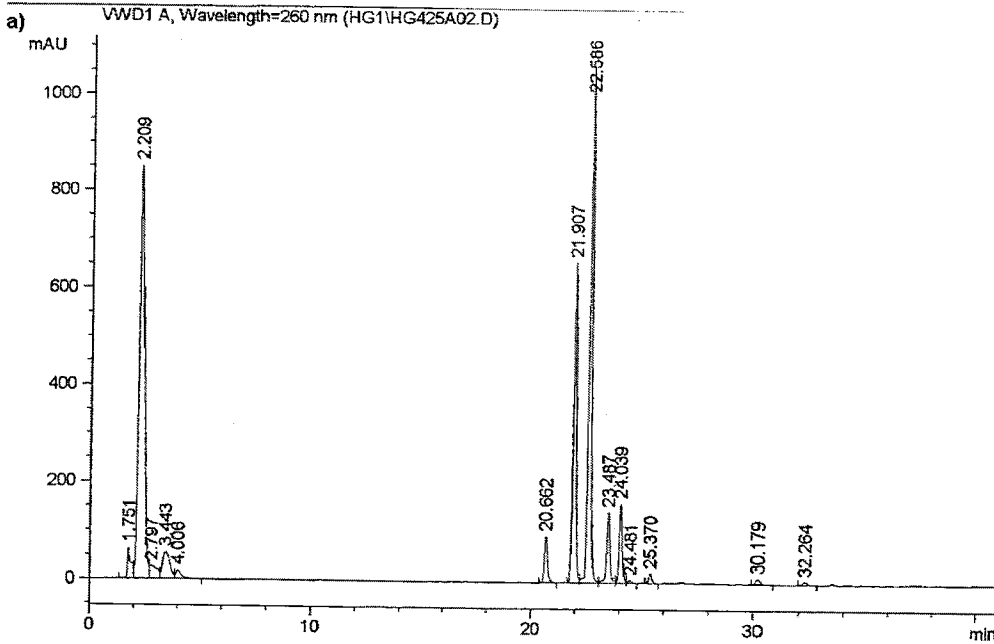
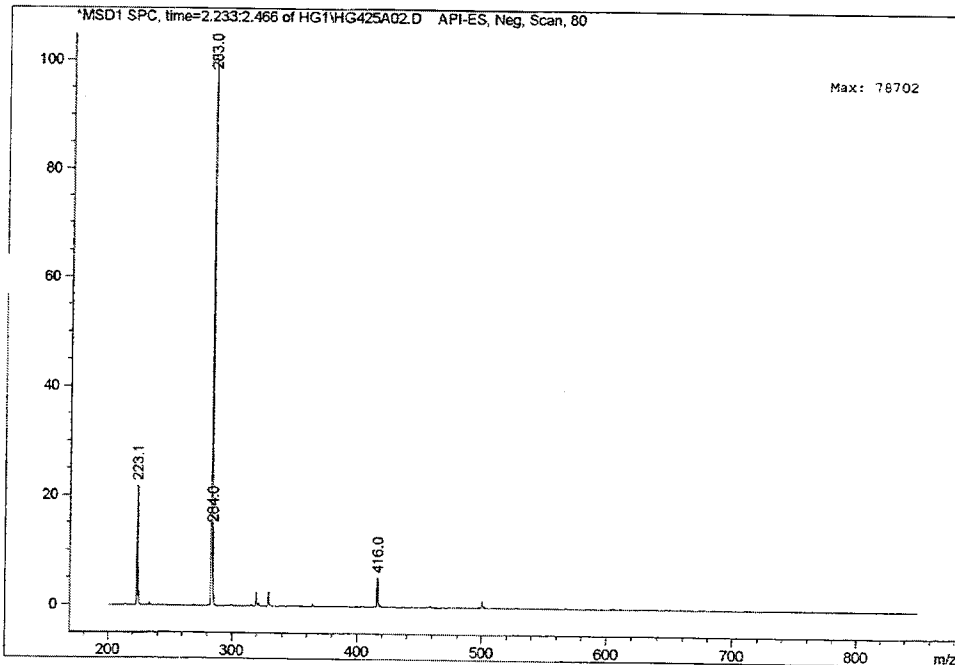


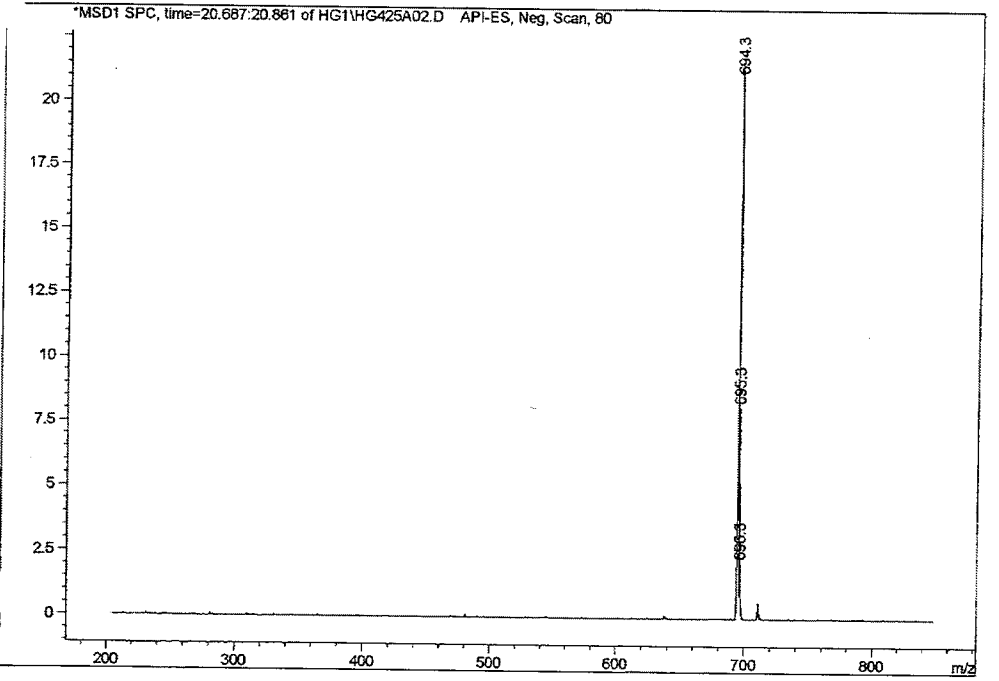
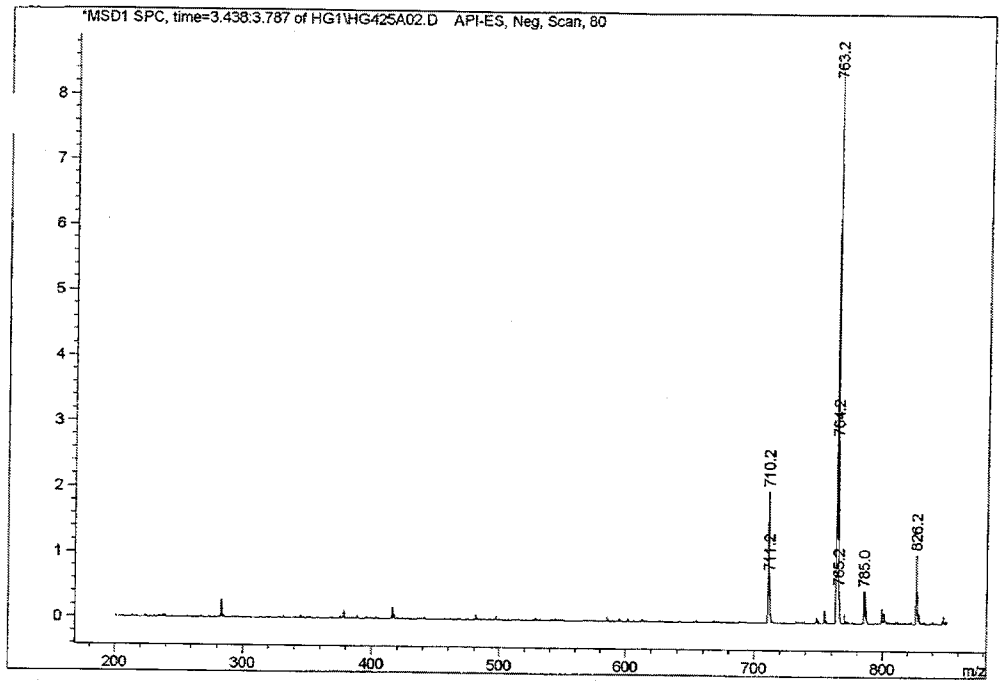
Figure 2. Oxidation of A*pT dimer with iodine: LC-MS of the reaction mixture (a) UV profile at 260 nm, (b) negative mode detection, (c) positive mode detection.



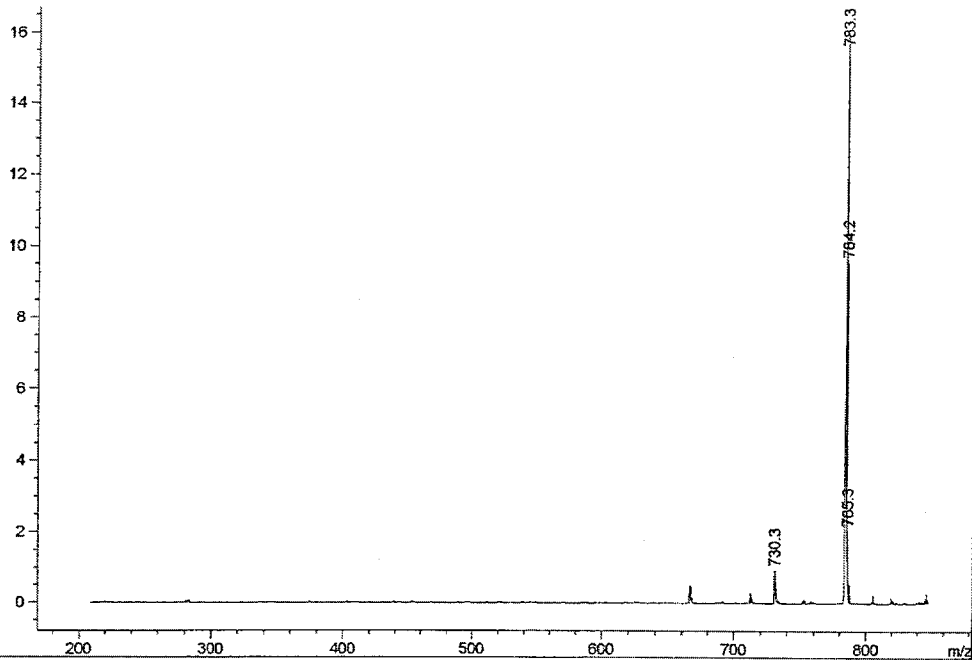
b) MS Signal: MSD1 TIC, MS File, API-ES, Neg, Scan, 80
 Spectra averaged over upper half of peaks.
 Noise Cutoff: 500 counts.
 Reportable Ion Abundance: > 50%.

Retention Time (MS)	MS Area	Mol. Weight or Ion
2.308	12560284	283.05 I
3.626	1663551	763.15 I
20.767	2882230	694.25 I
23.581	3548295	784.25 I 783.25 I
24.153	3153805	783.25 I

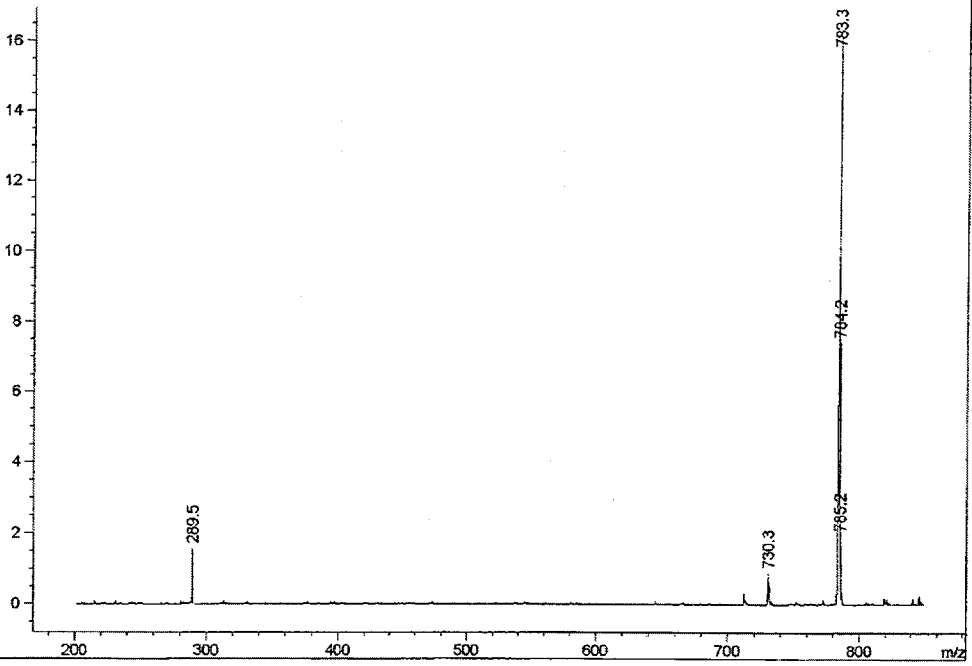




*MSD1 SPC, time=23.484:23.717 of HG1\HG425A02.D API-ES, Neg, Scan, 80

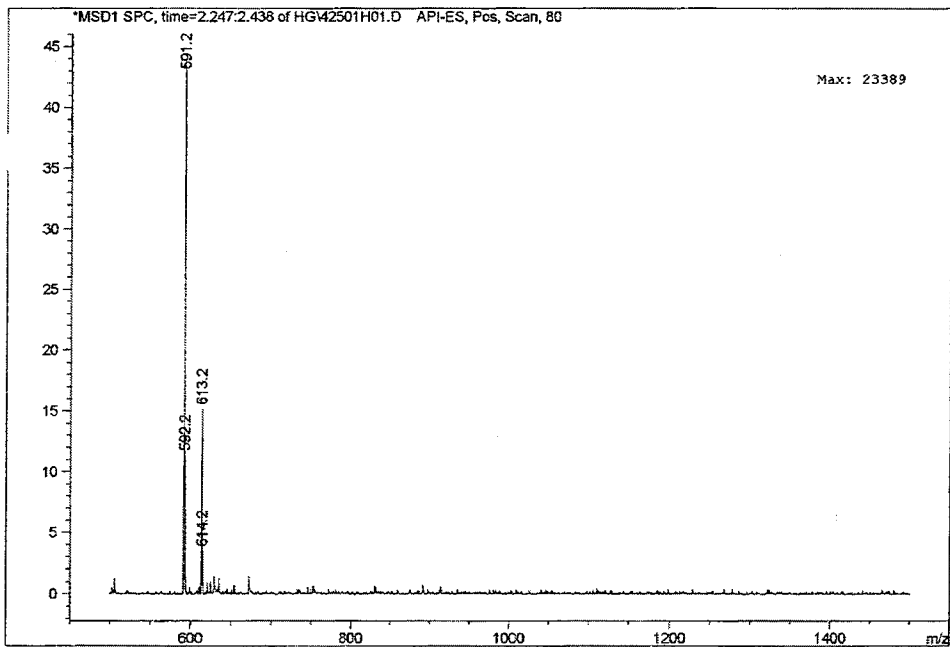


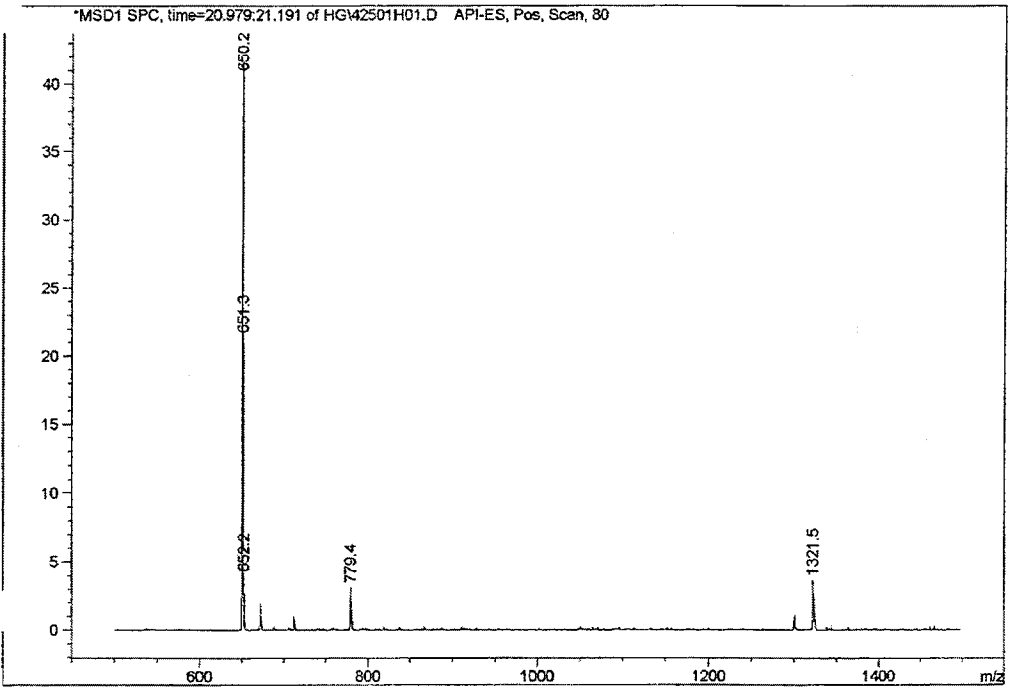
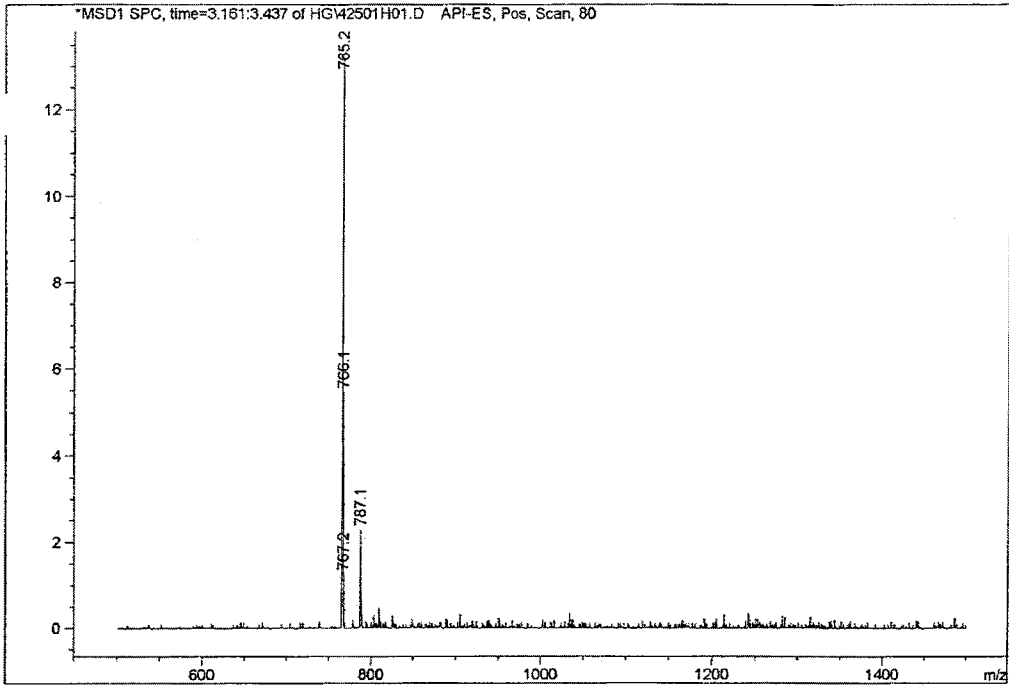
*MSD1 SPC, time=24.047:24.280 of HG1\HG425A02.D API-ES, Neg, Scan, 80

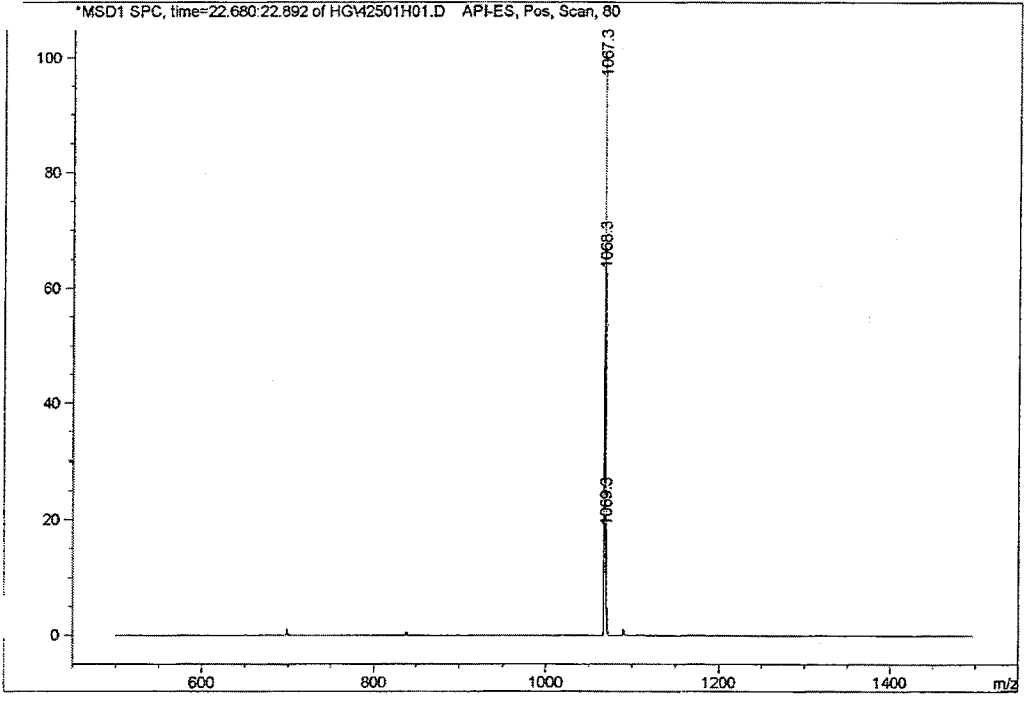
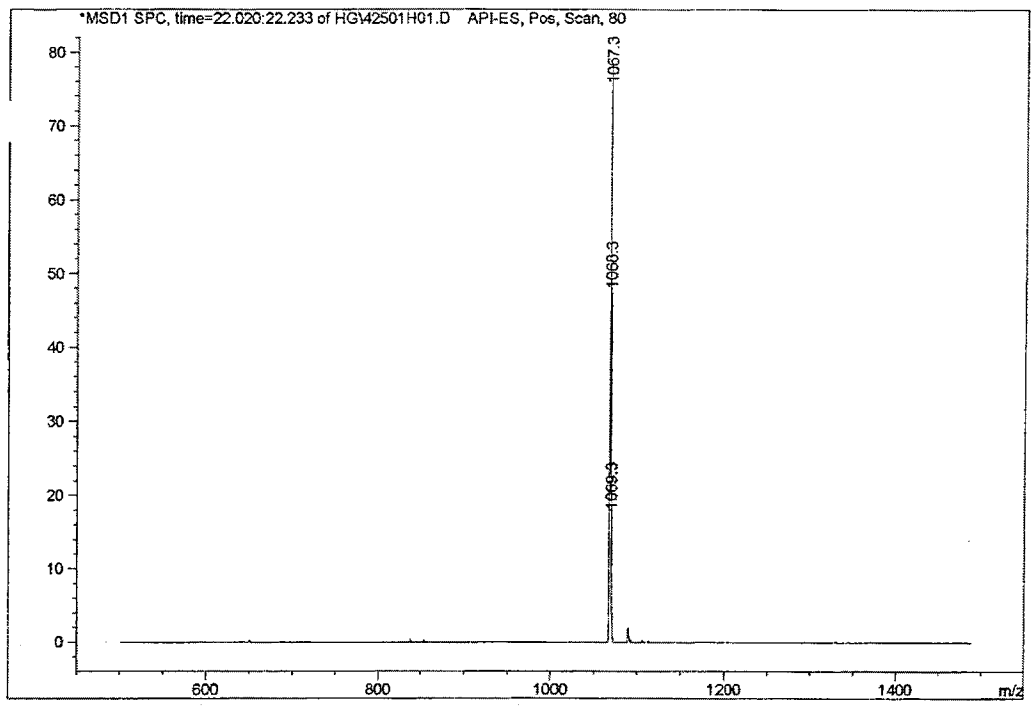


c) MS Signal: MSD1 TIC, MS File, API-ES, Pos, Scan, 80
 Spectra averaged over upper half of peaks.
 Noise Cutoff: 500 counts.
 Reportable Ion Abundance: > 50%.

Retention Time (MS)	MS Area	Mol. Weight or Ion
2.316	5571722	591.20 I
3.280	2237881	765.20 I
21.085	6693614	651.30 I 650.20 I
22.115	10639256	1068.30 I 1067.30 I
22.782	13606527	1068.30 I 1067.30 I
23.678	8460878	785.20 I
24.235	8612253	785.20 I







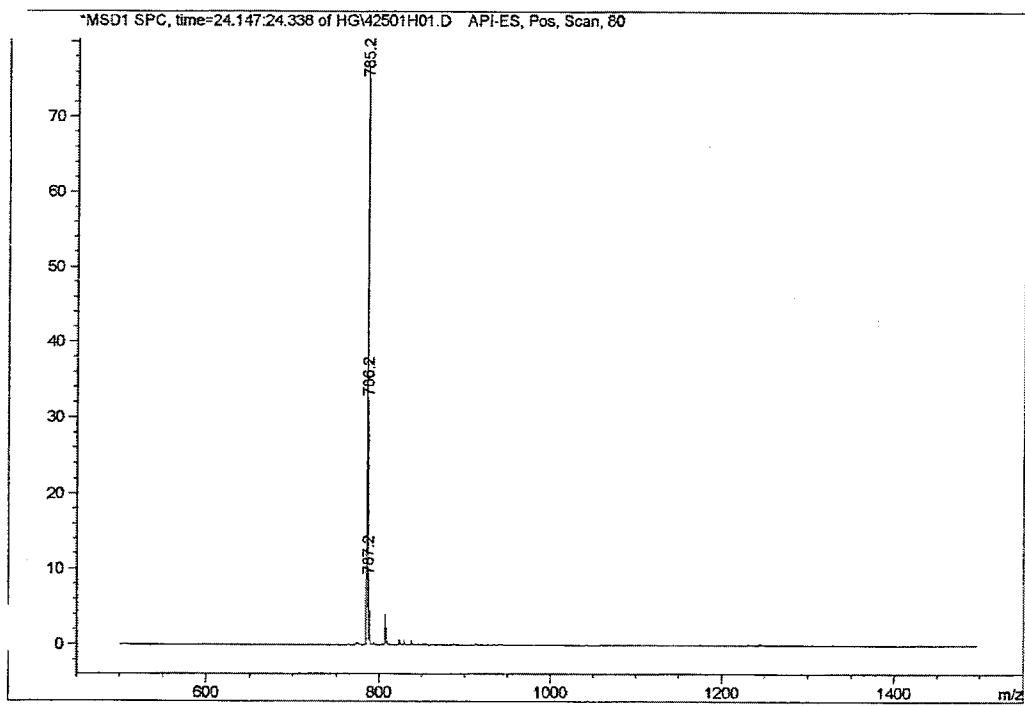
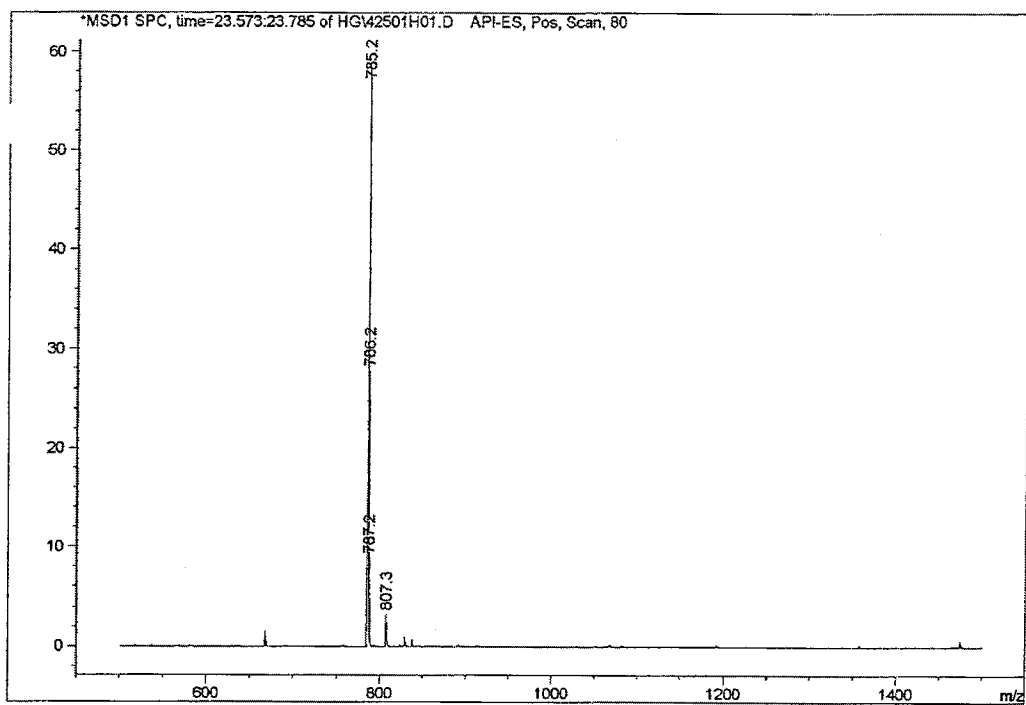


Figure 3. Oxidation of A*pT dimer with t-butylhydroperoxide: LC-MS of the reaction mixture (a) UV profile at 260 nm, (b) negative mode detection, (c) positive mode detection.

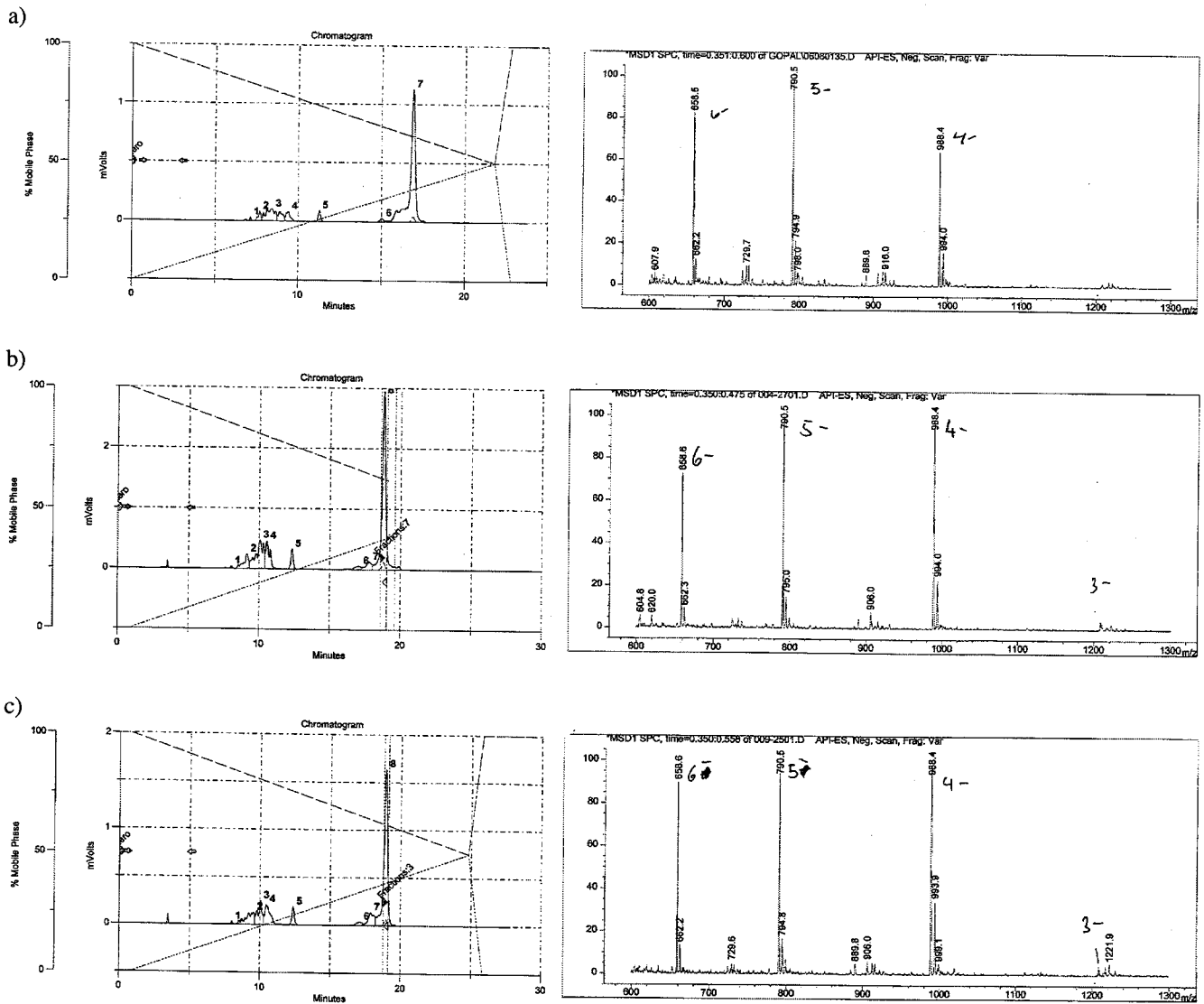
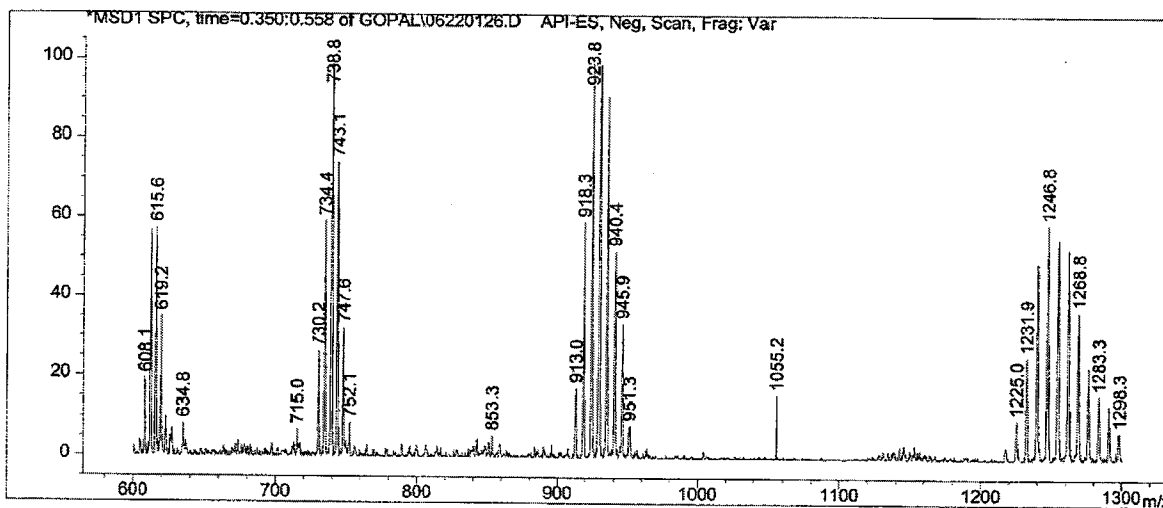
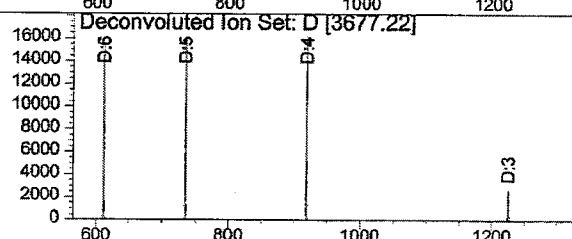
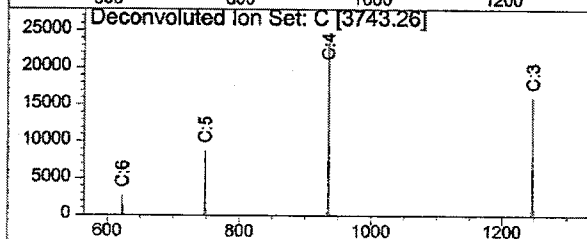
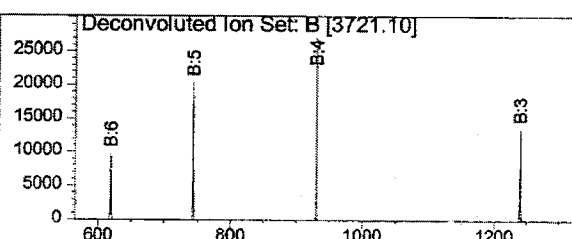
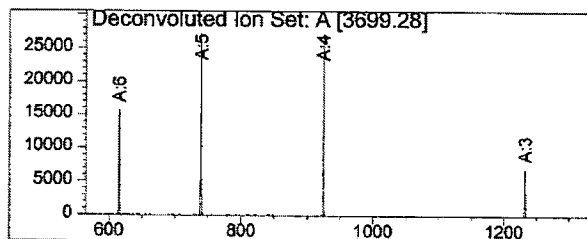
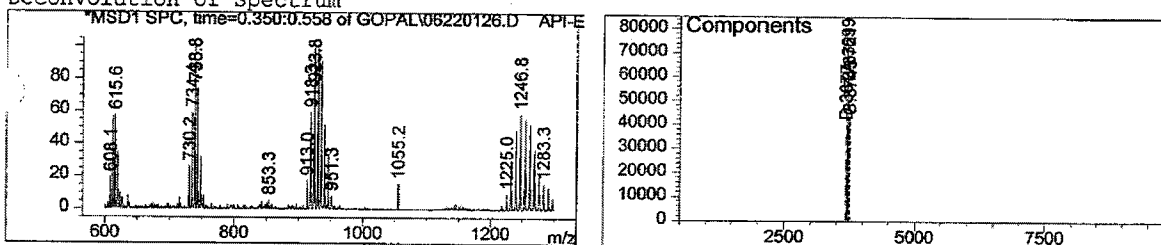


Figure 4. Oxidation of A* during synthesis of ON-1 with (a) t-butylhydroperoxide, (b) CSO and (c) t-butylhydroperoxide followed by iodine: HPLC and mass spectrometrical analysis of the crude samples.



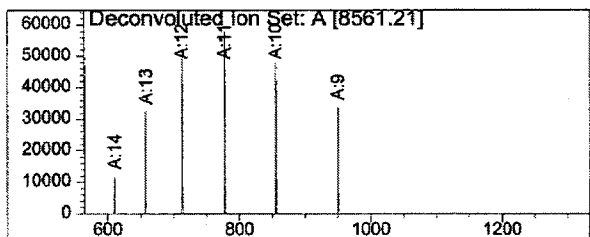
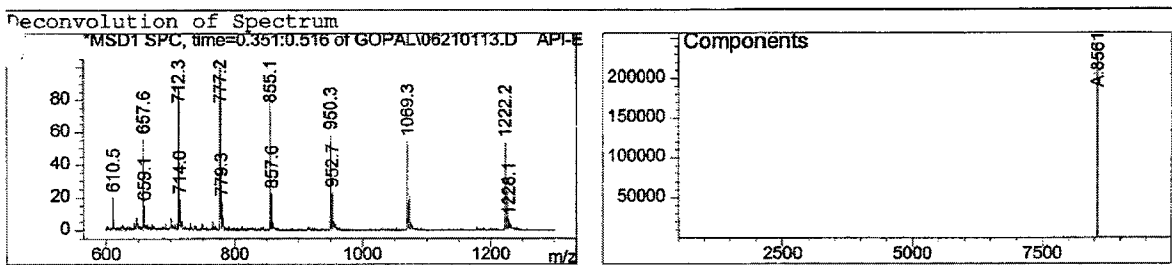
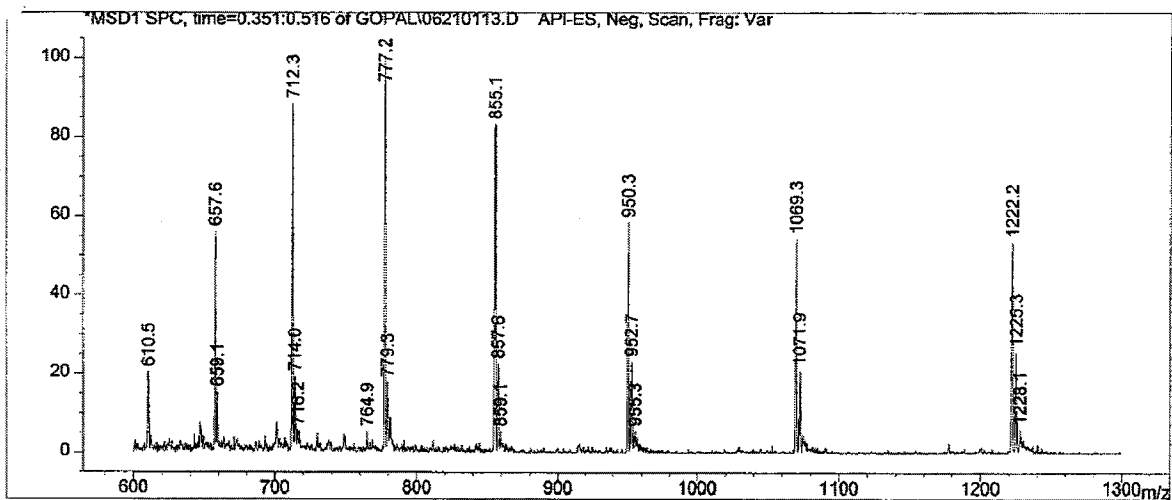
Deconvolution of Spectrum



Component	Molecular Weight	Absolute Abundance	Relative Abundance
A	3699.28	75992	100.00
B	3721.10	68750	90.47
C	3743.26	52109	68.57
D	3677.22	49646	65.33

*** End of Report ***

Figure 5. ESI-MS analysis of ON-1 (MW_{calc} : 3656.5). The deconvoluted ion sets correspond to various Na^+ -adducts of the oligonucleotide (A, $M + 2 \text{Na}^+$; B, $M + 3 \text{Na}^+$; C, $M + 4 \text{Na}^+$; D, $M + \text{Na}^+$).



Component	Molecular Weight	Absolute Abundance	Relative Abundance
A	8561.21	229719	100.00

*** End of Report ***

Figure 6. ESI-MS analysis of ON-2 (MW_{calc} : 8563.7).

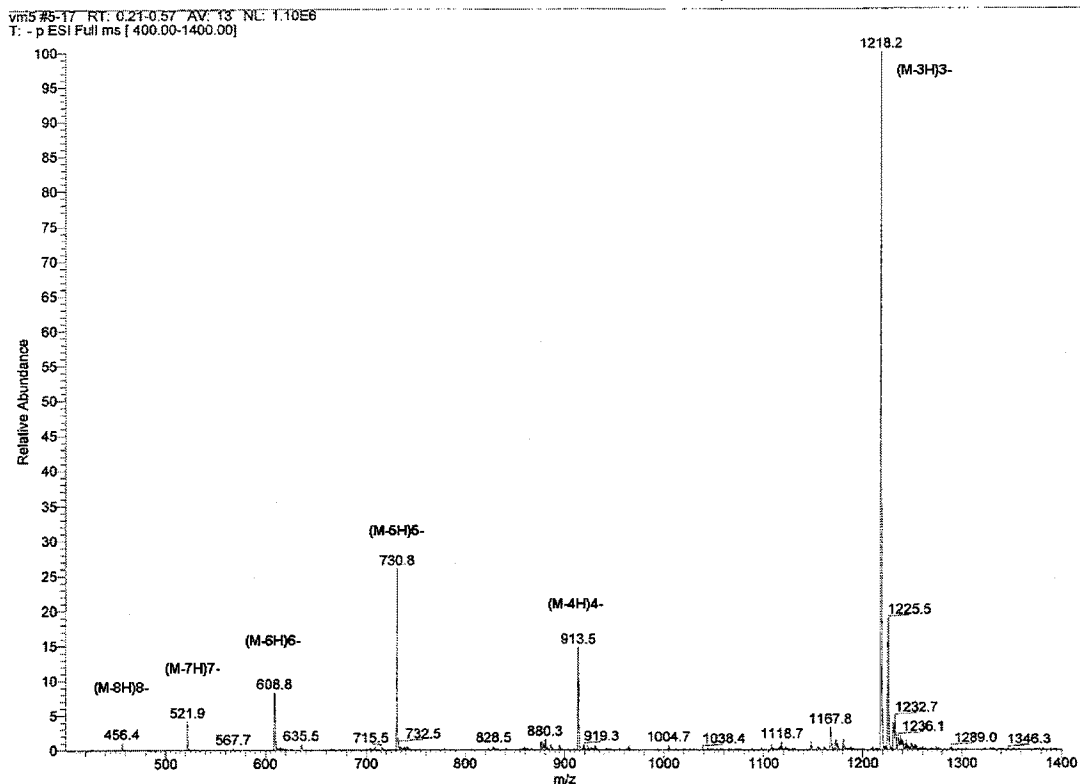


Figure 7. ESI-MS analysis of ON-3 (MW_{calc} : 3656.5).

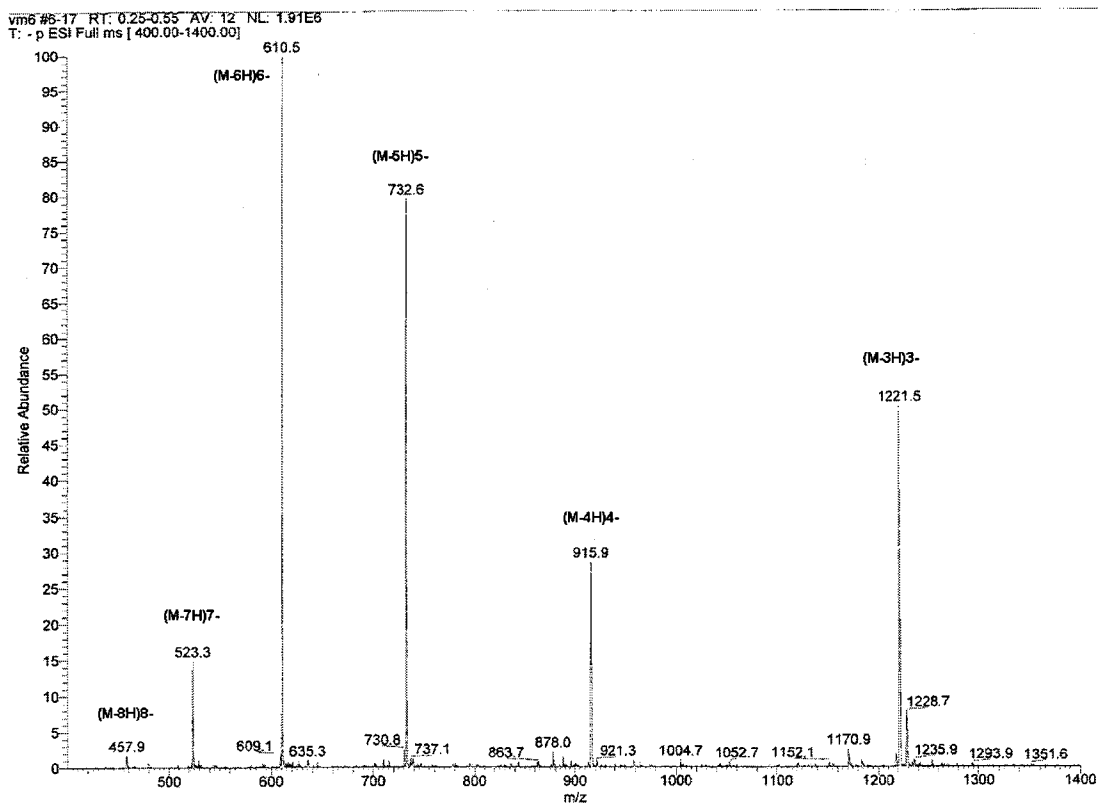
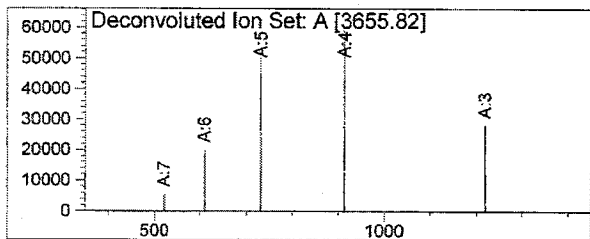
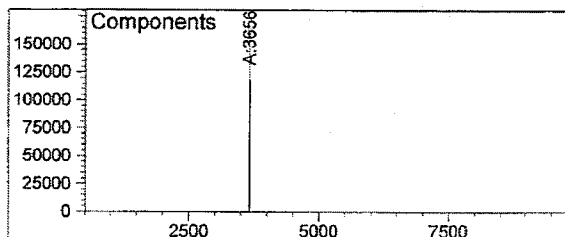
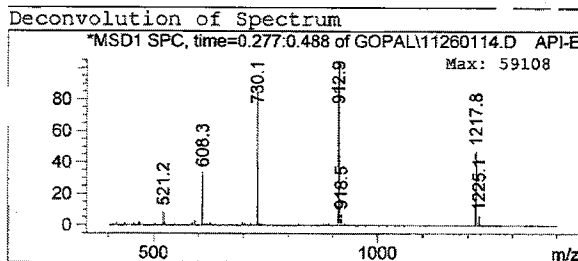
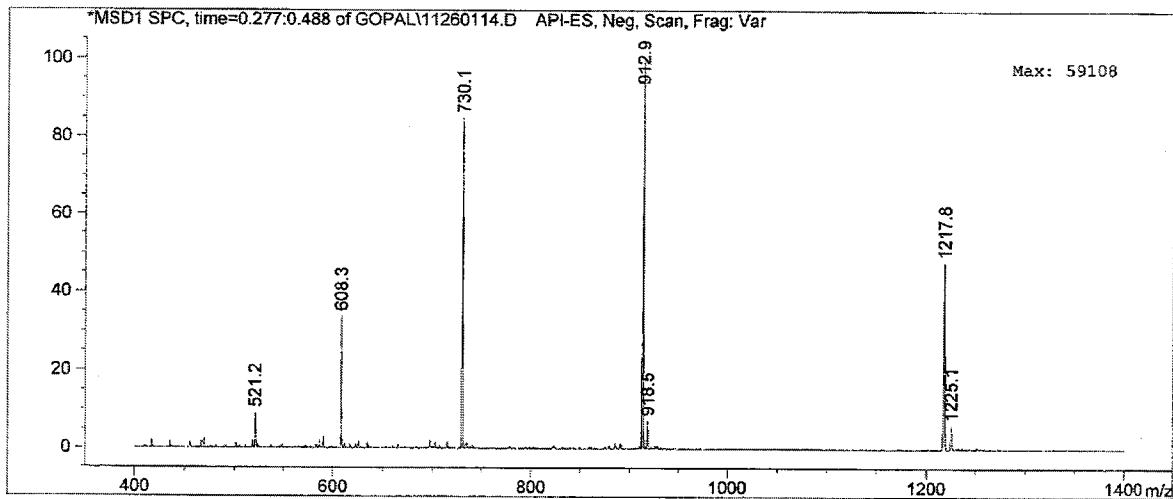


Figure 8. ESI-MS analysis of ON-4 (MW_{calc} : 3656.5).

Retention Time (MS)	MS Area	Mol. Weight or Ion
0.337	44030912	3655.82 M

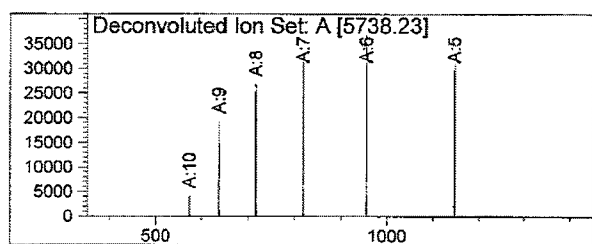
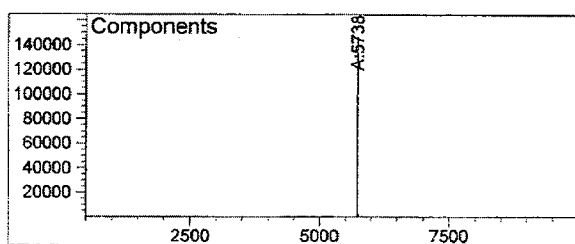
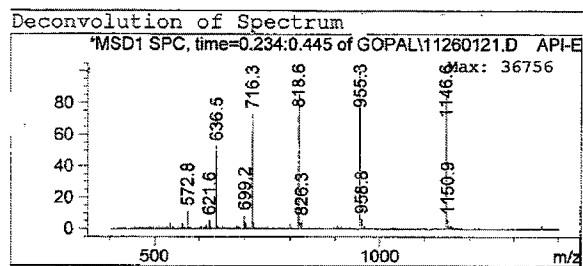
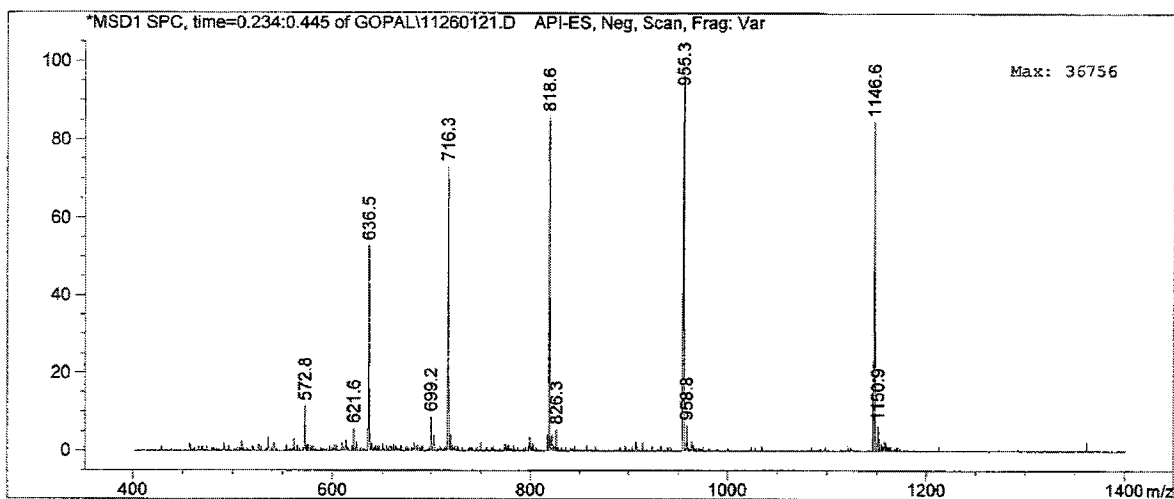


Component	Molecular Weight	Absolute Abundance	Relative Abundance
A	3655.82	161548	100.00

*** End of Report ***

Figure 9. ESI-MS analysis of ON-5 (MW_{calc}: 3656.5).

Retention Time (MS)	MS Area	Mol. Weight or Ion
0.309	35818392	5738.23 M



Component	Molecular Weight	Absolute Abundance	Relative Abundance
A	5738.23	147064	100.00

*** End of Report ***

Figure 10. ESI-MS analysis of ON-6 (MW_{calc}: 5738.9).

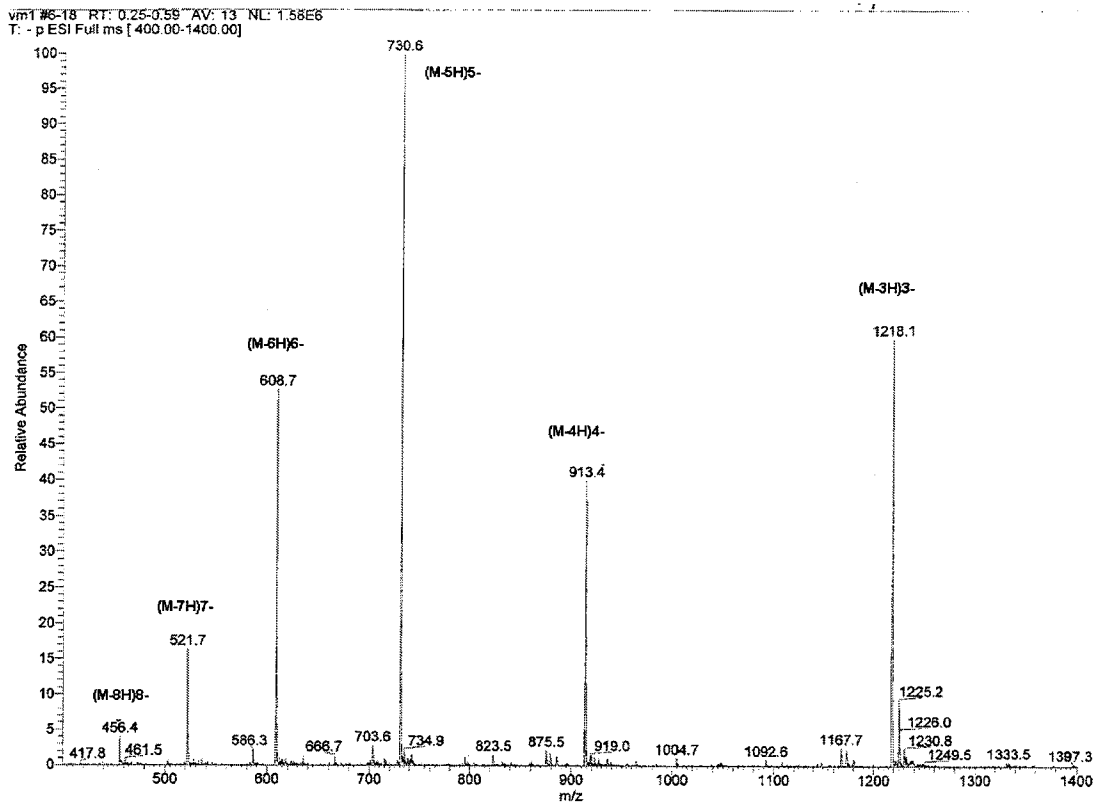


Figure 11. ESI-MS analysis of ON-7 (MW_{calc} : 3656.5).

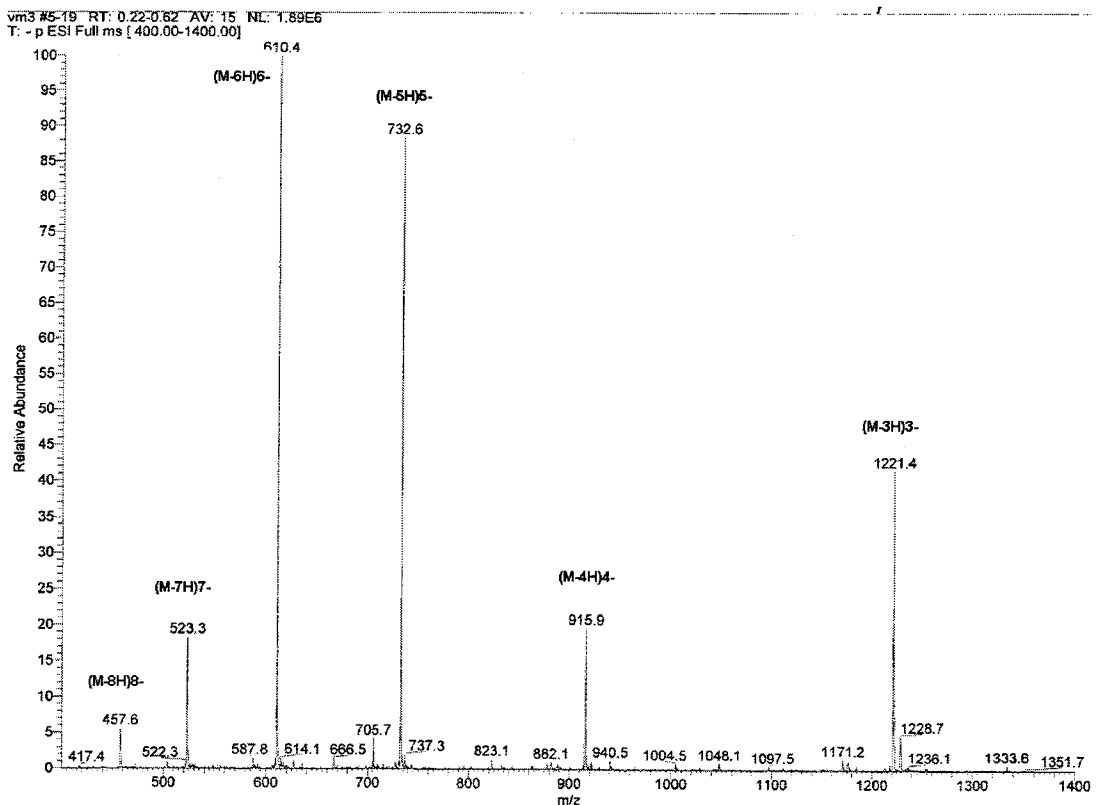
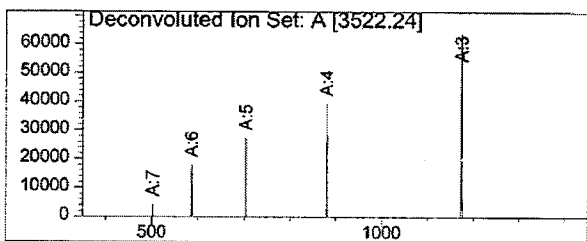
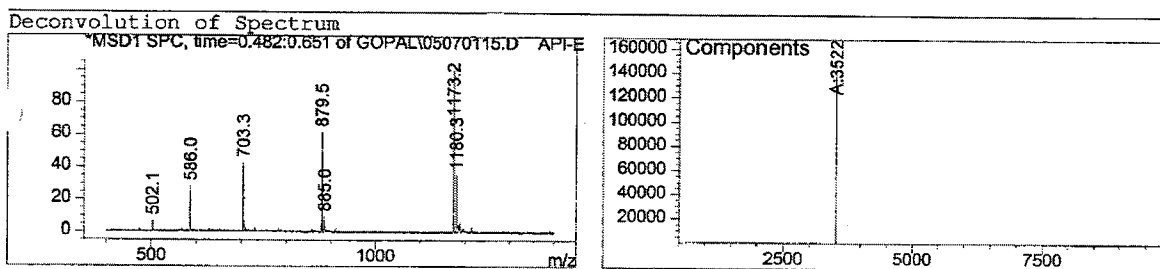
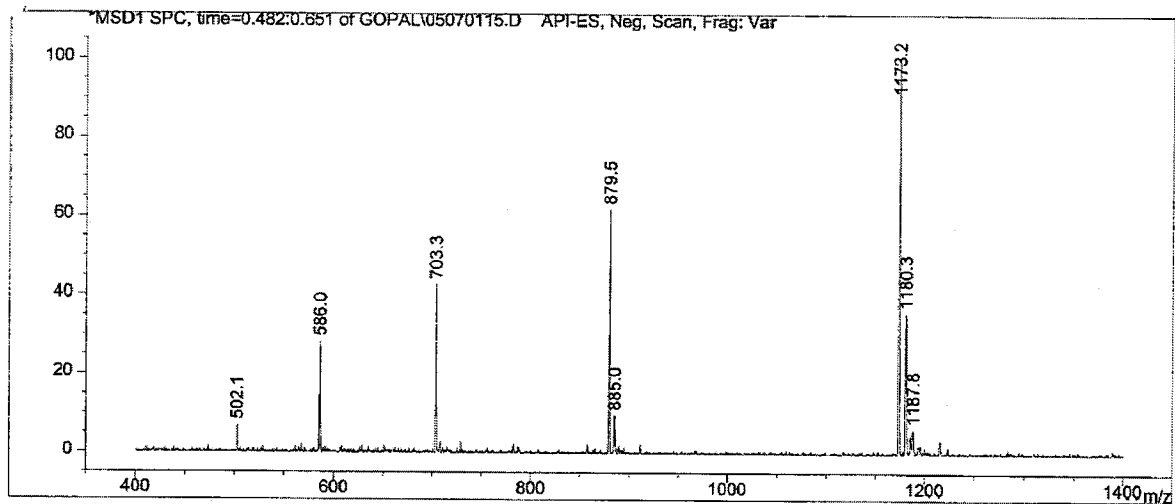


Figure 12. ESI-MS analysis of ON-8 (MW_{calc} : 3666.5).



Component	Molecular Weight	Absolute Abundance	Relative Abundance
A	3522.24	150583	100.00

*** End of Report ***

Figure 13. ESI-MS analysis of ON-9 (MW_{calc}: 3523.4).

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Operator : maier
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CurrentMeth: C:\HPCHEM\1\METHODS\OLIGO.M
Description: Average from 2.13 to 2.98 minutes

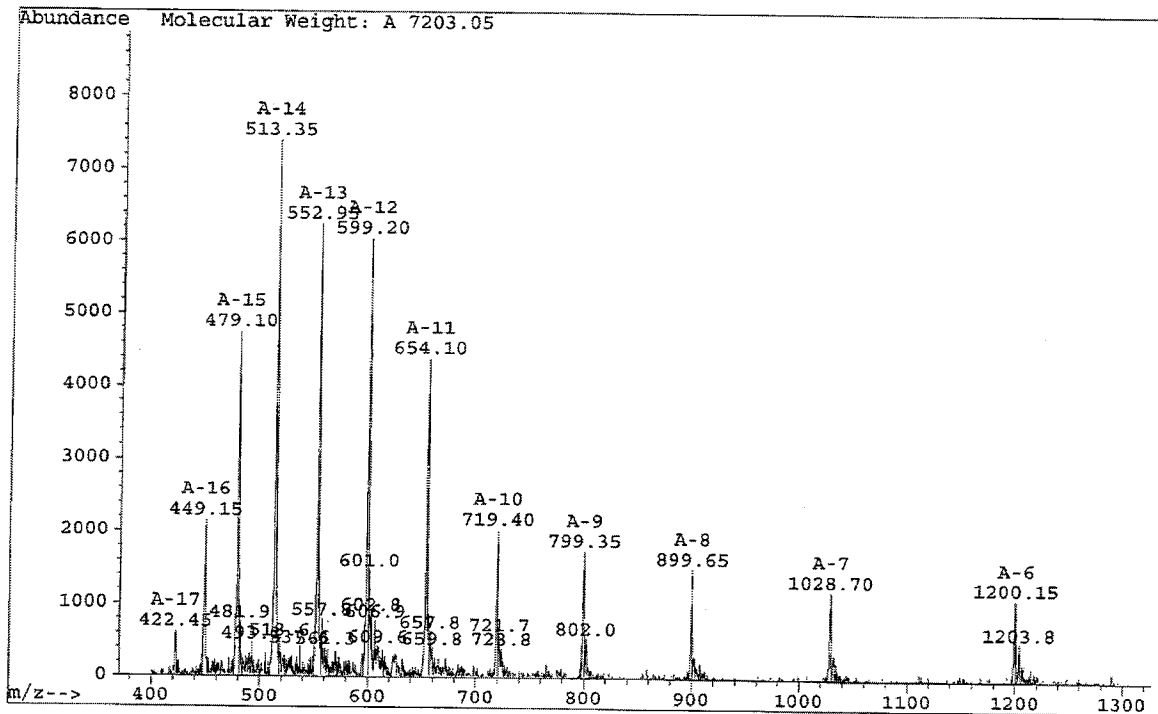
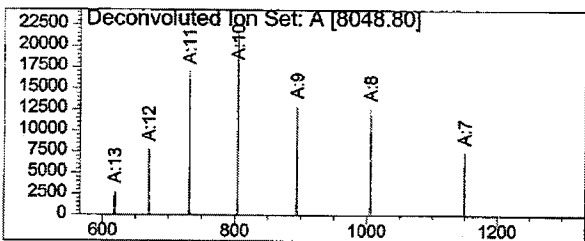
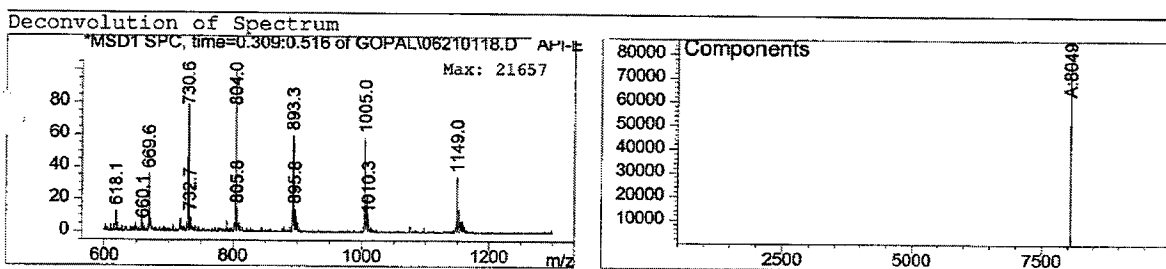
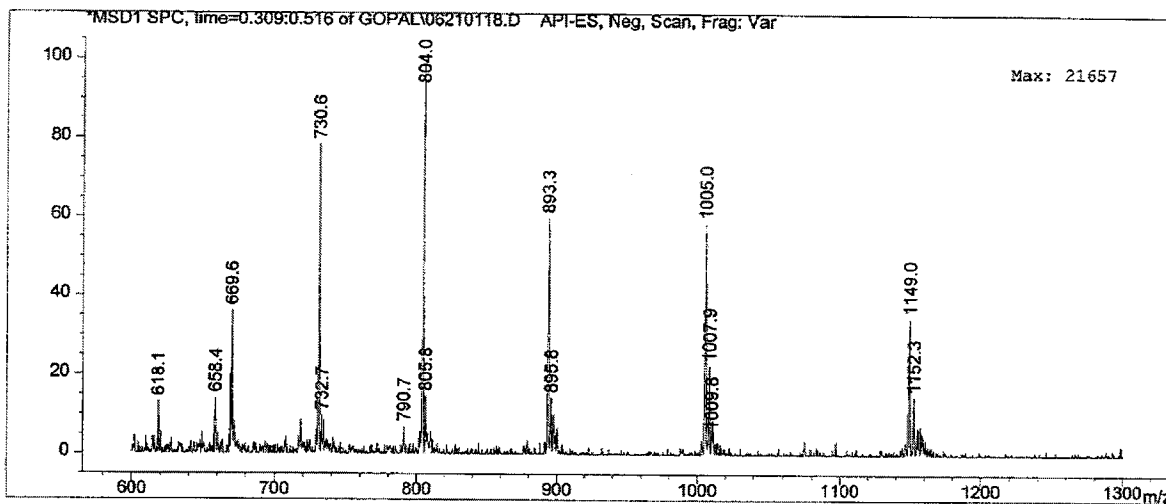


Figure 14. ESI-MS analysis of ON-10 (MW_{calc}: 7204.7).



Component	Molecular Weight	Absolute Abundance	Relative Abundance
A	8048.80	76934	100.00

*** End of Report ***

Figure 15. ESI-MS analysis of ON-11 (MW_{calc} : 8050.8).