CHEMISTRY
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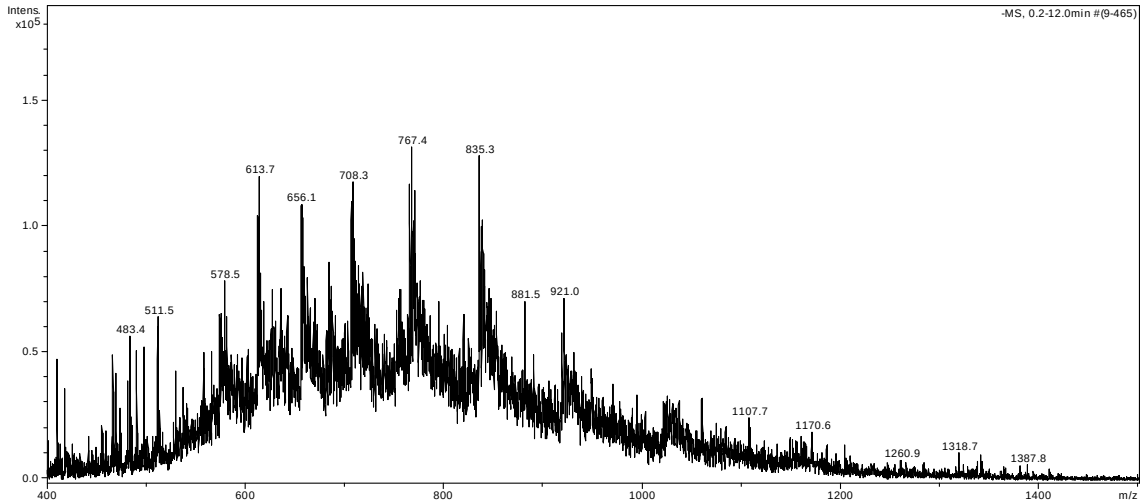
Supporting Information

Synthesis of DNA Strands site-specifically damaged by C8-Arylamine Purine Adducts and Effects on various DNA Polymerases

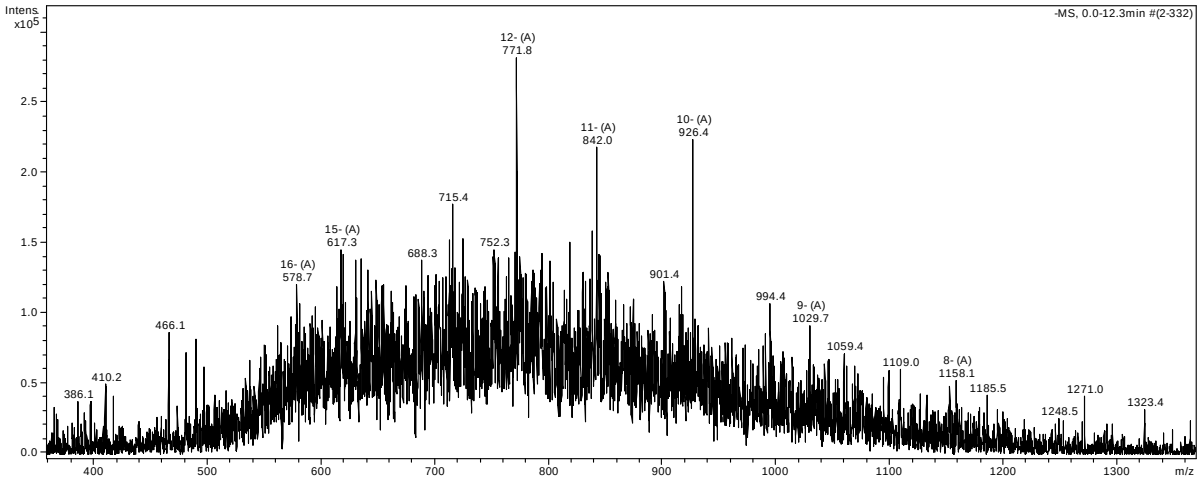
Nicolas Böge,[a] Maike I. Jacobsen,[a] Z. Szombati,[a] Sabrina Baerns,[b] Francesca Di Pasquale,[b] Andreas Marx,[b] and Chris Meier*[a]

[a] Organic Chemistry, Department of Chemistry, Faculty of Science, University of Hamburg, Martin-Luther-King-Platz 6, D-20146 Hamburg, Germany; phone: 040-42838-4324; fax: 040-42838-5592, e-mail: chris.meier@chemie.uni-hamburg.de; homepage: http://www.chemie.uni-hamburg.de/oc/meier/

[b] Department of Chemistry and Konstanz School of Chemical Biology, University of Konstanz, Universitätsstraße 10, D-78457 Konstanz, Germany

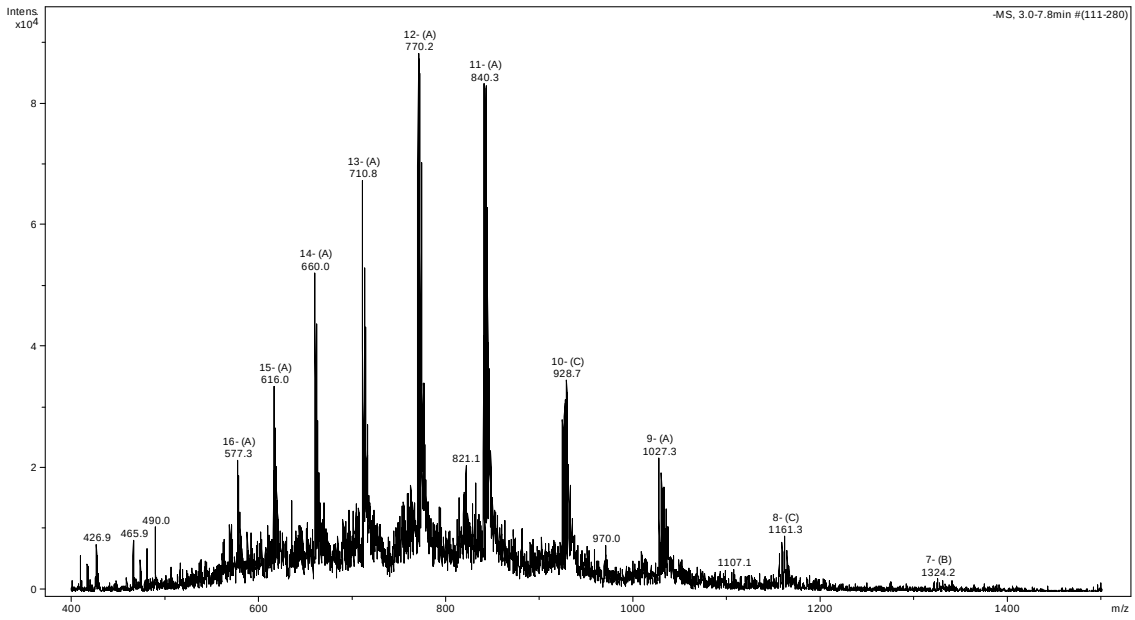


ESI-MS-spectra of **23b**

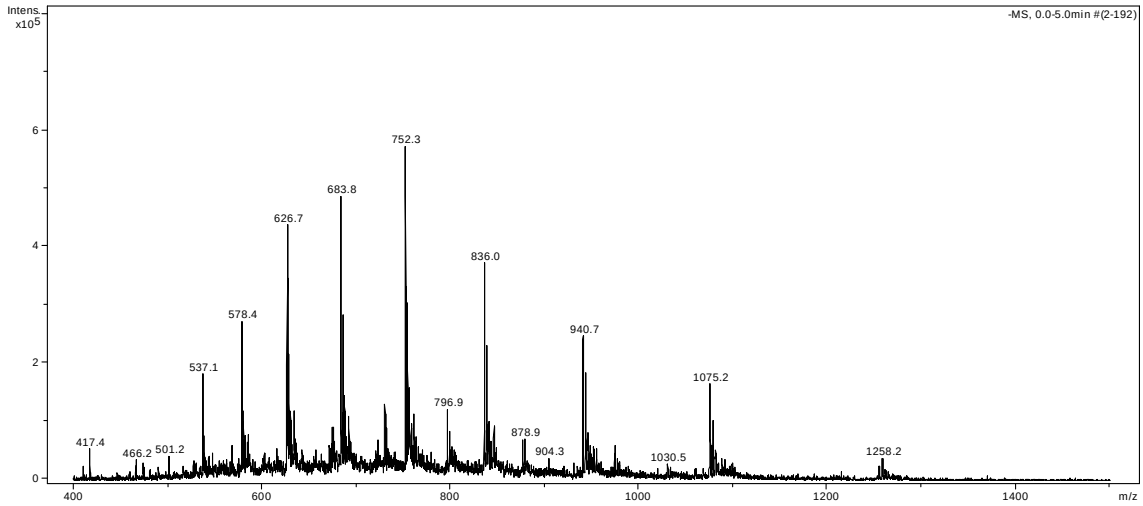


ESI-MS-spectra of **23c**

ESI-MS-spectra of **23e**


Intens.
x10^4
-MS, 3.0-7.8min #(111-280)
12- (A)
770.2
11- (A)
840.3
13- (A)
710.8
14- (A)
660.0
15- (A)
616.0
16- (A)
577.3
10- (C)
928.7
9- (A)
1027.3
821.1
426.9
465.9
490.0
970.0
1107.1
8- (C)
1161.3
7- (B)
1324.2
0
2
4
6
8
400
600
800
1000
1200
1400
m/z

ESI-MS-spectra of **23f**



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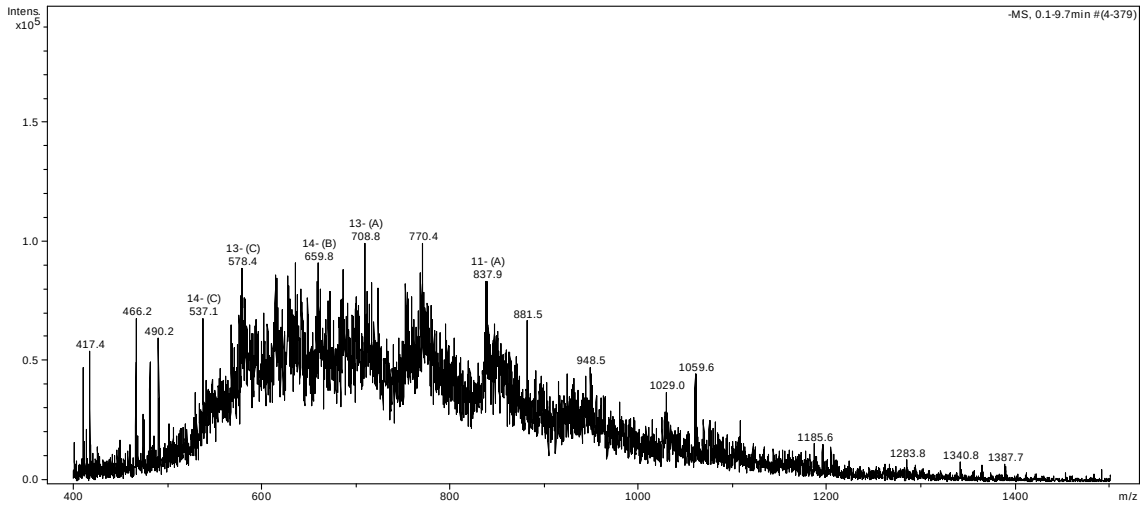

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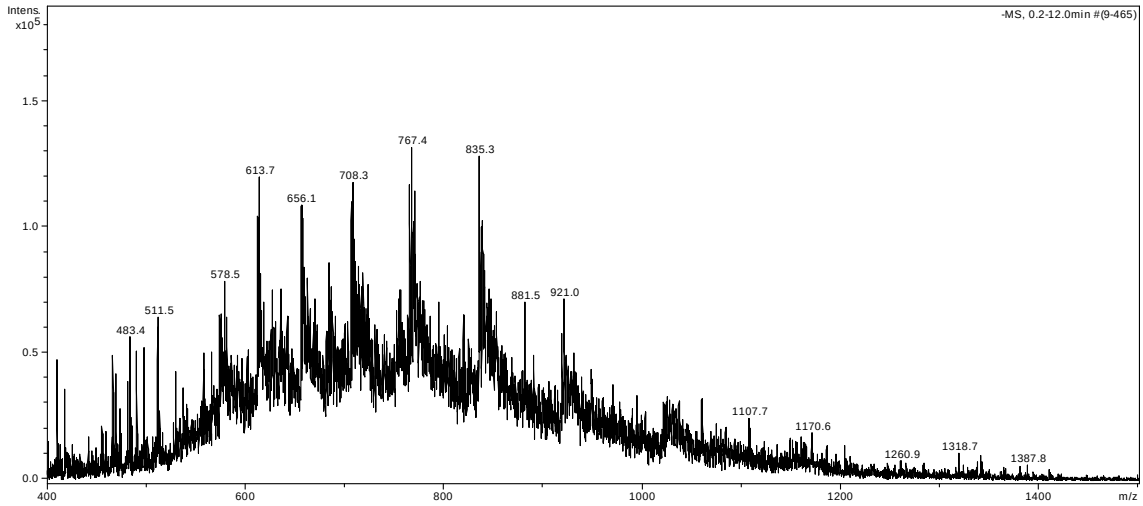
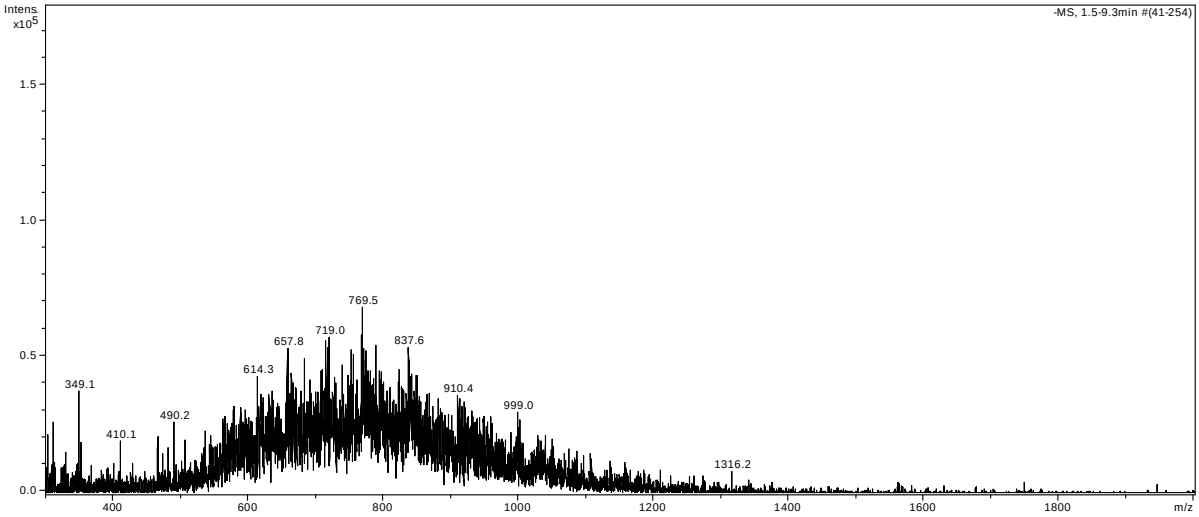


ESI-MS-spectra of **24d**



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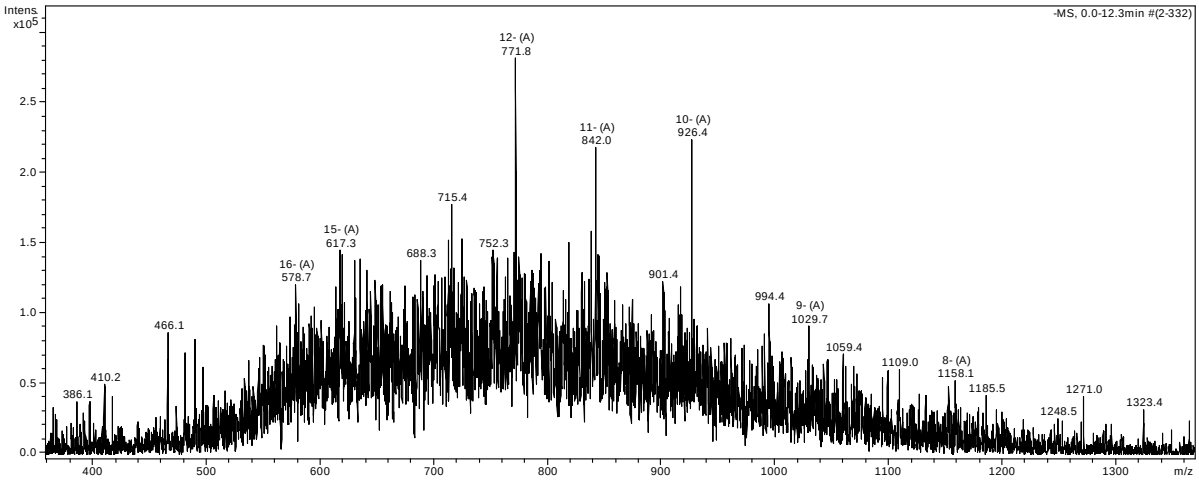

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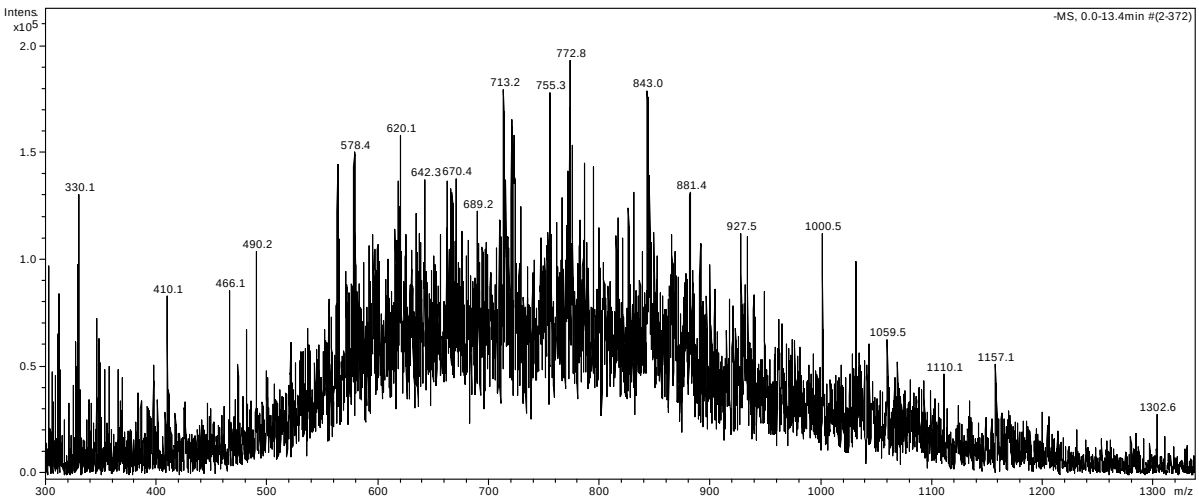

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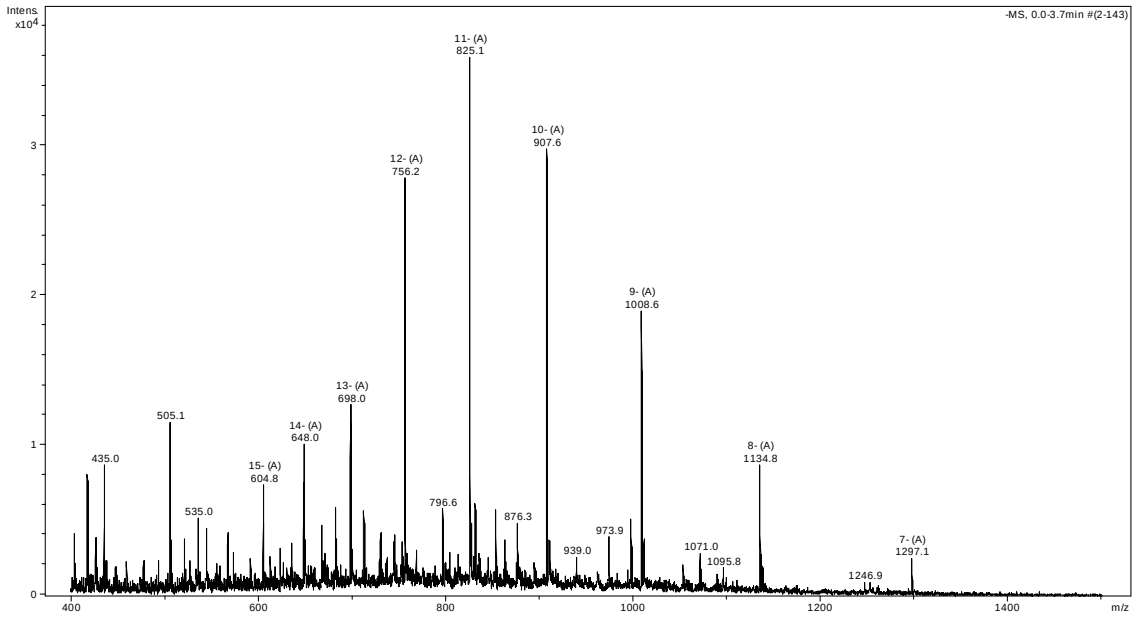

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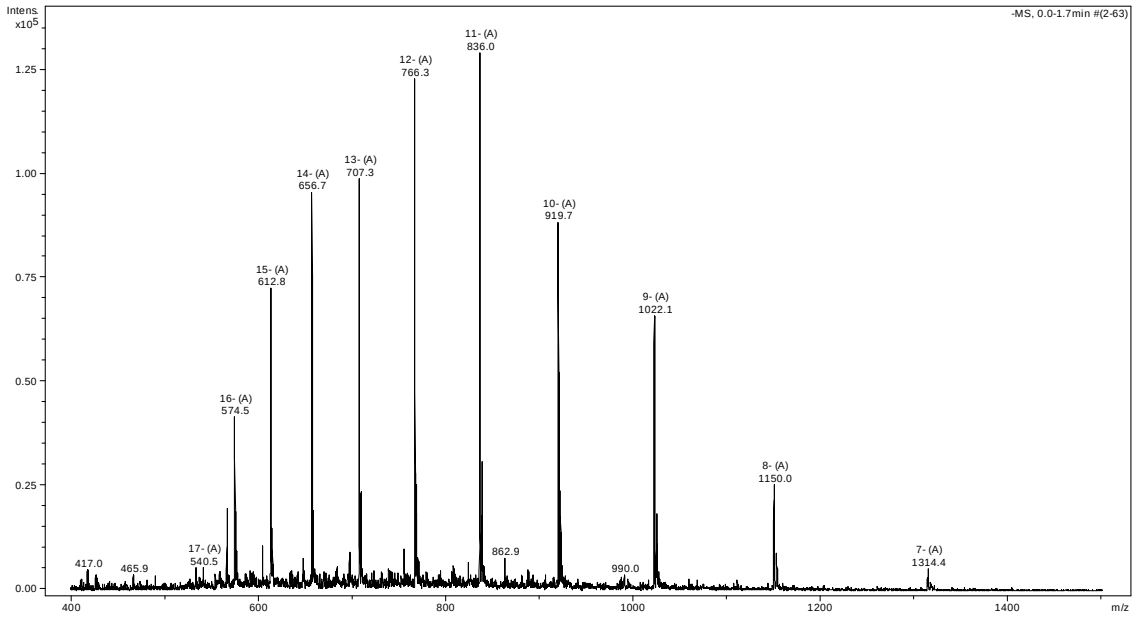

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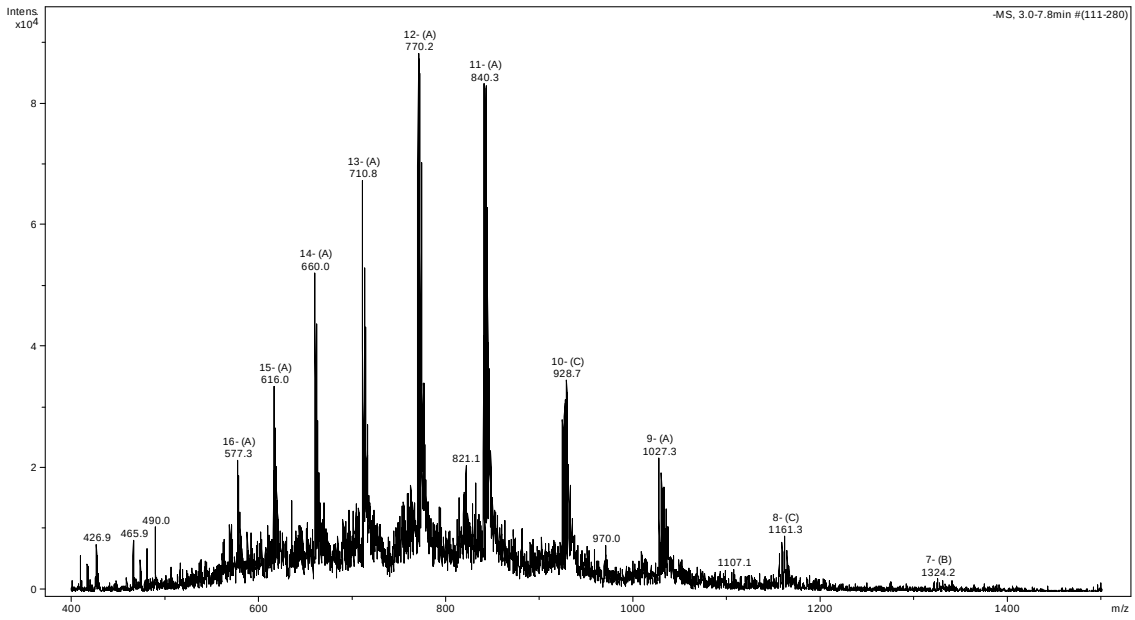

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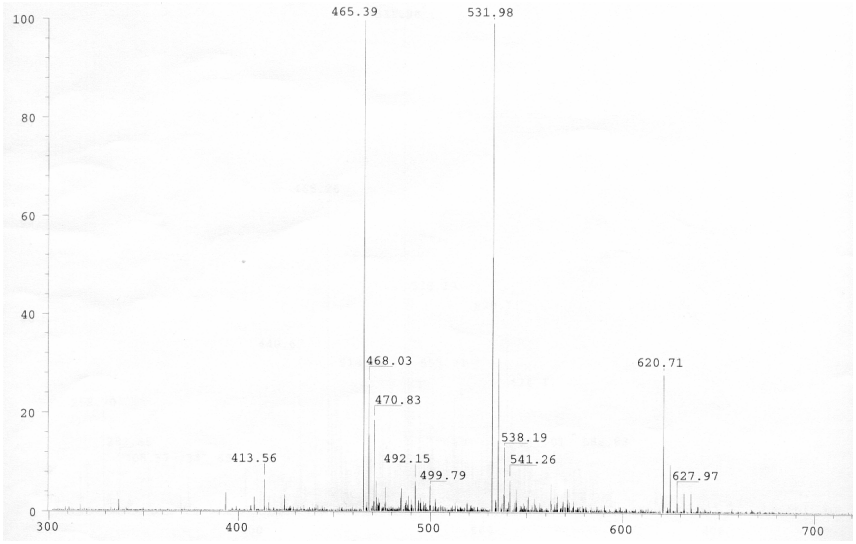

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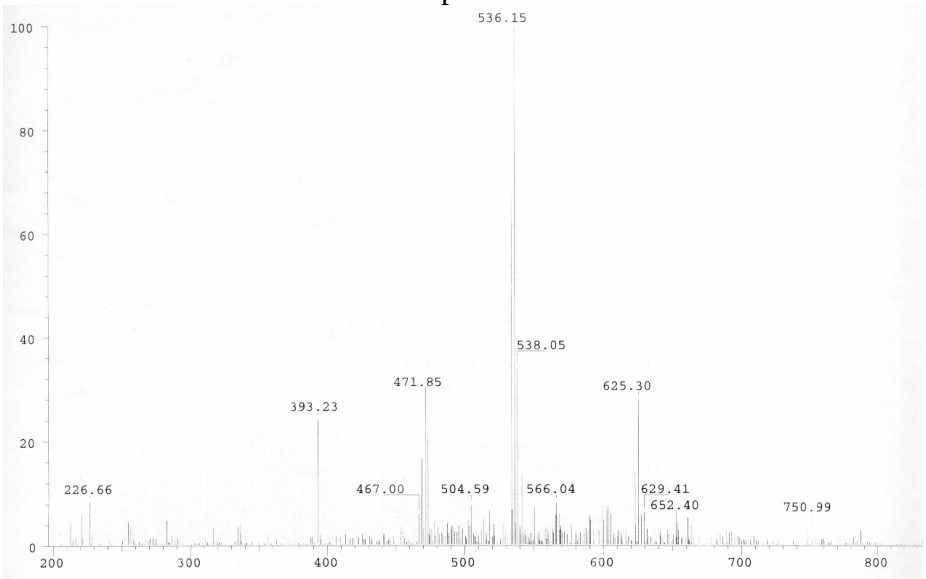

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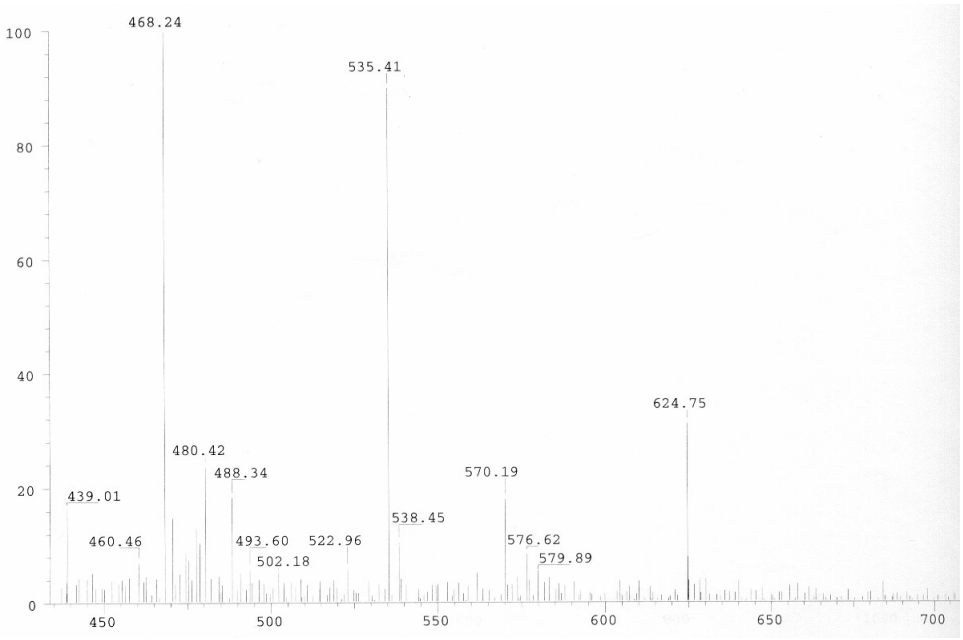

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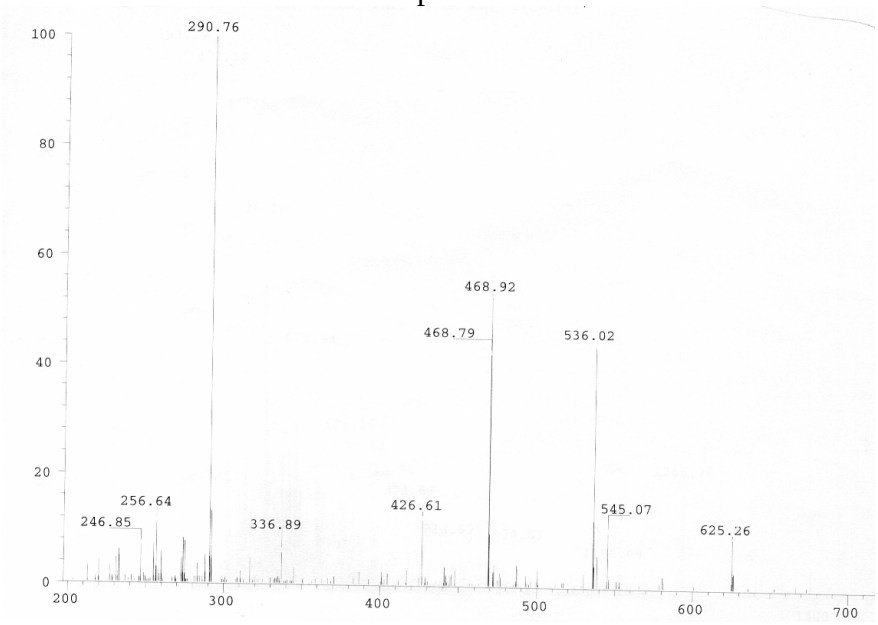

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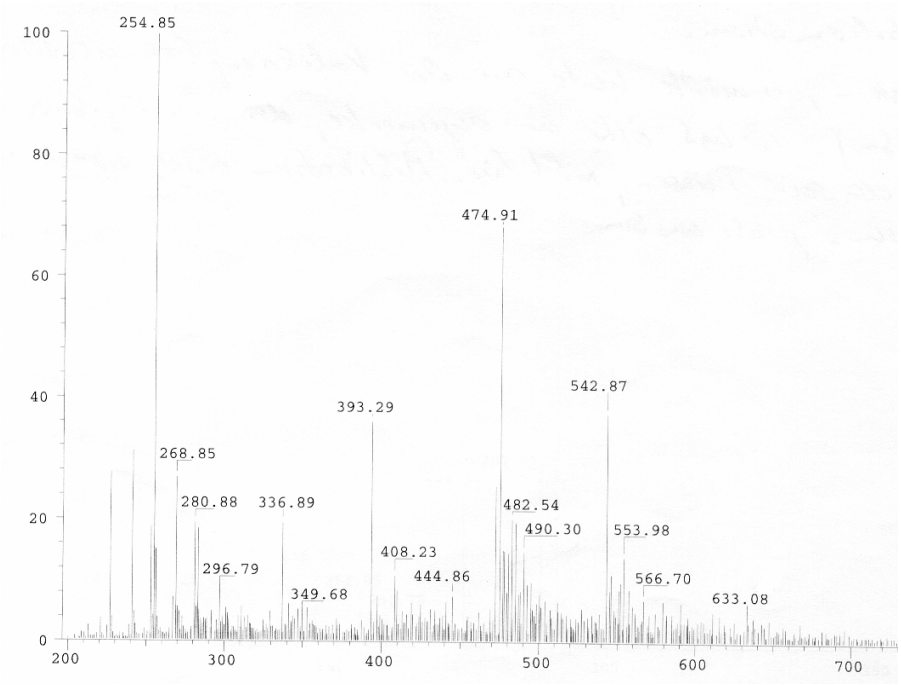

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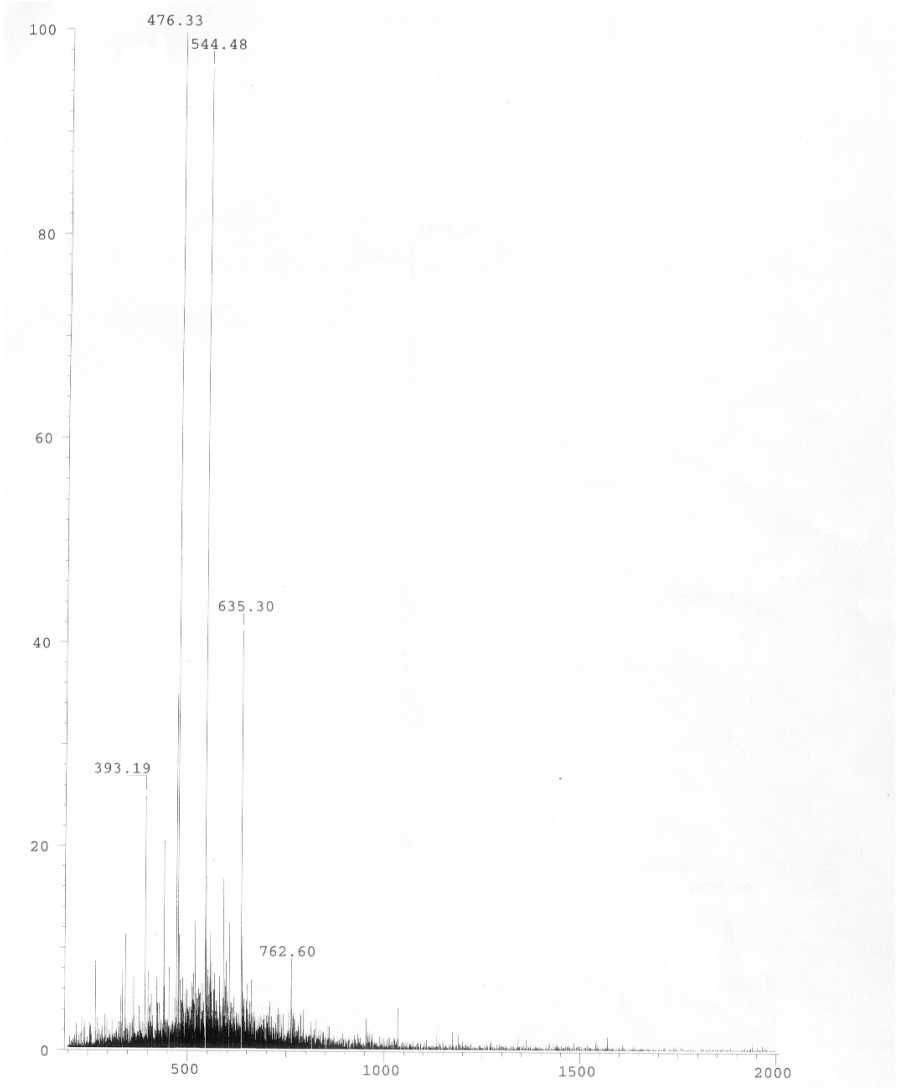

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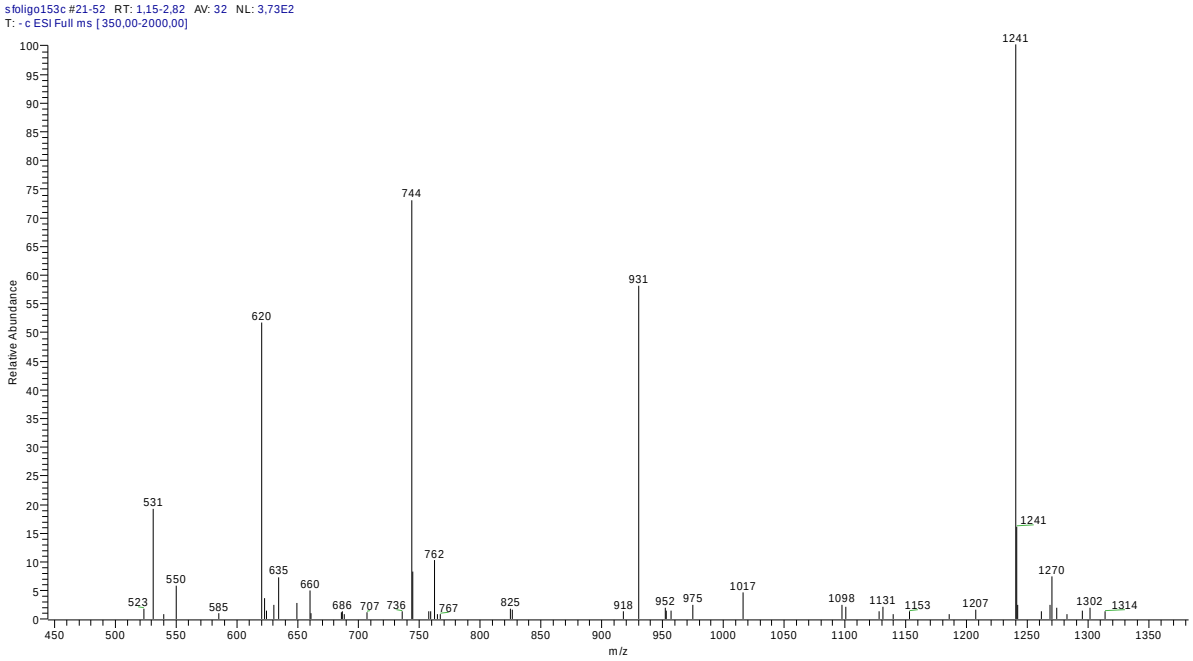

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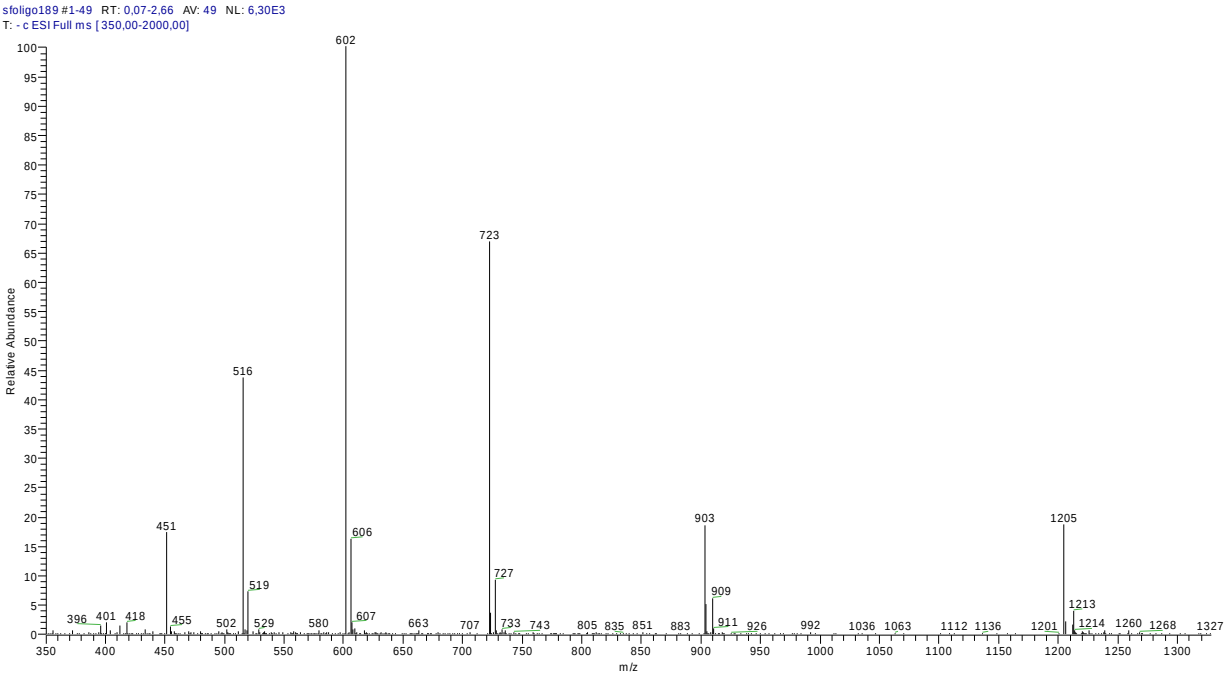

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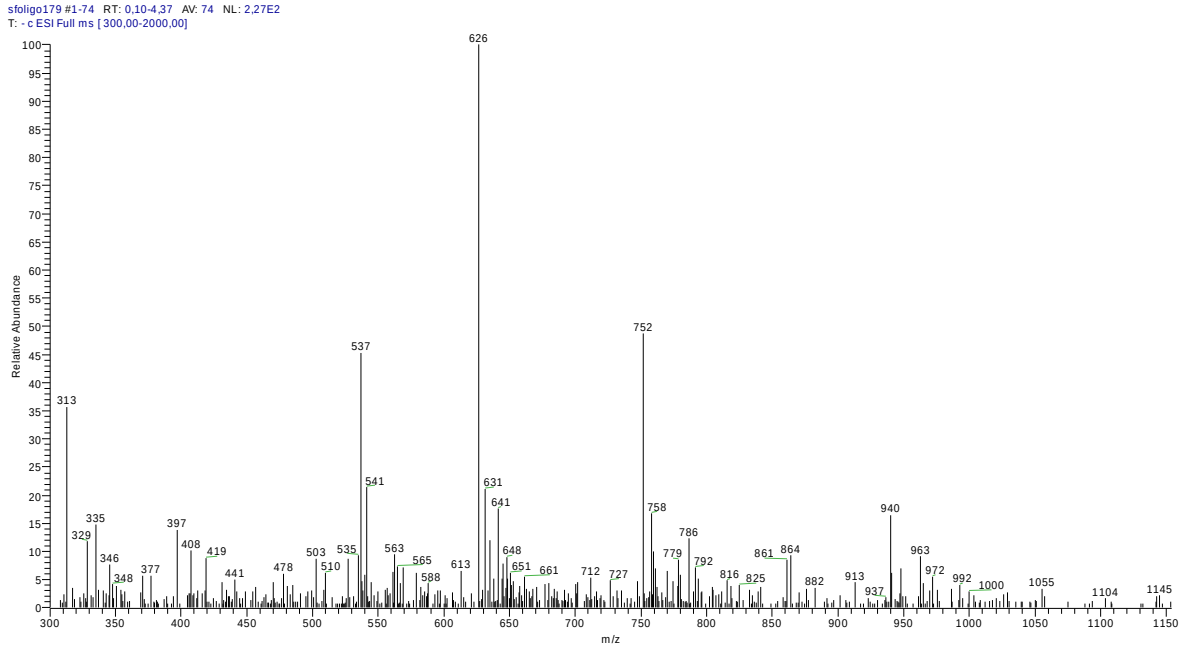

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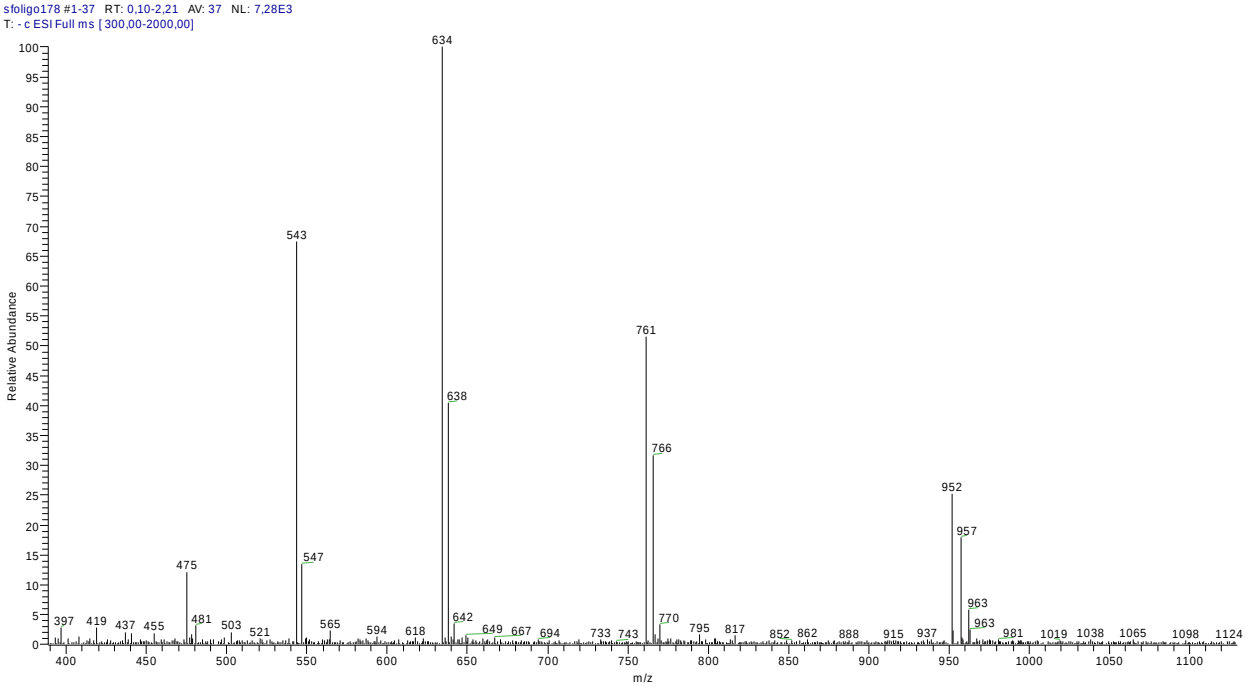

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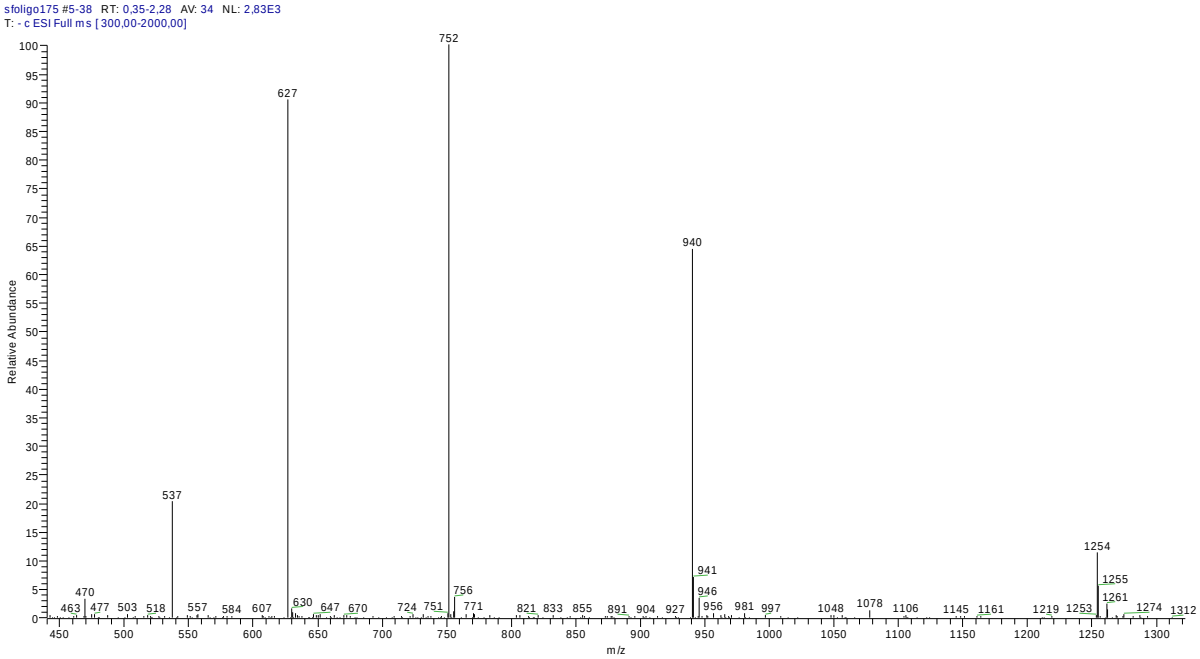

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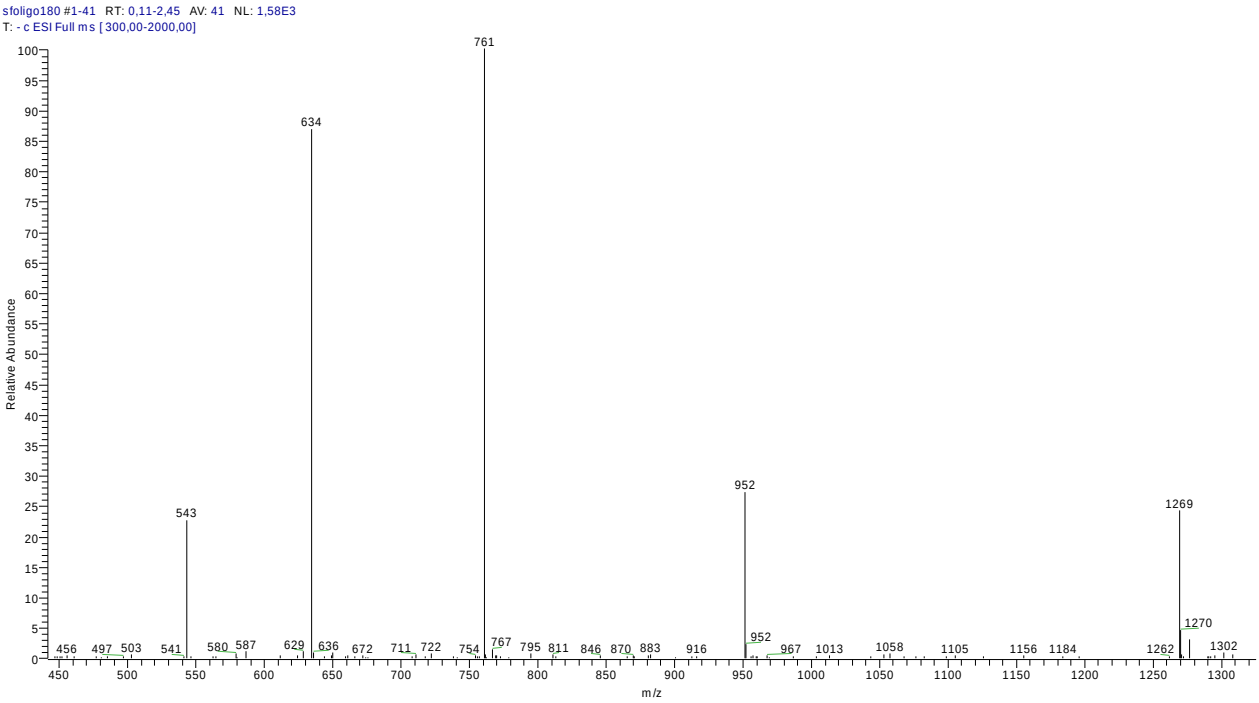

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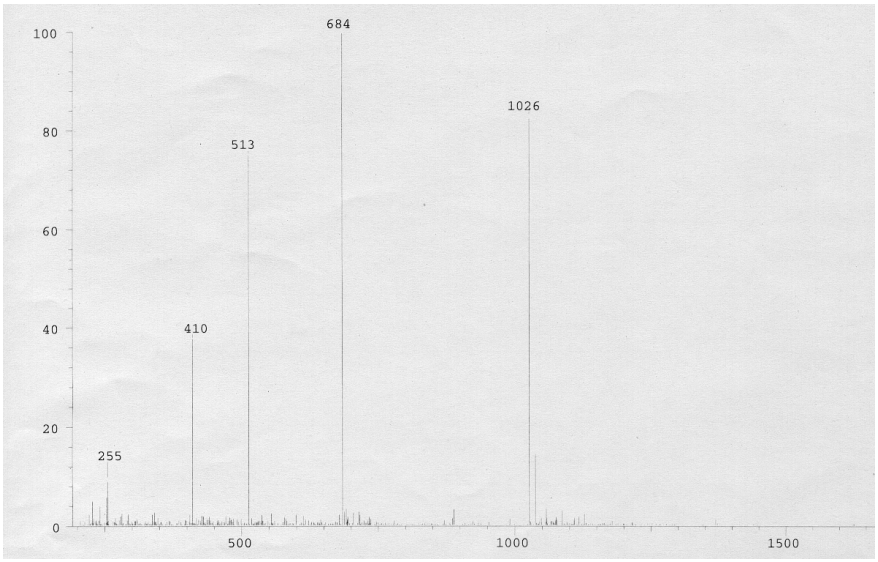
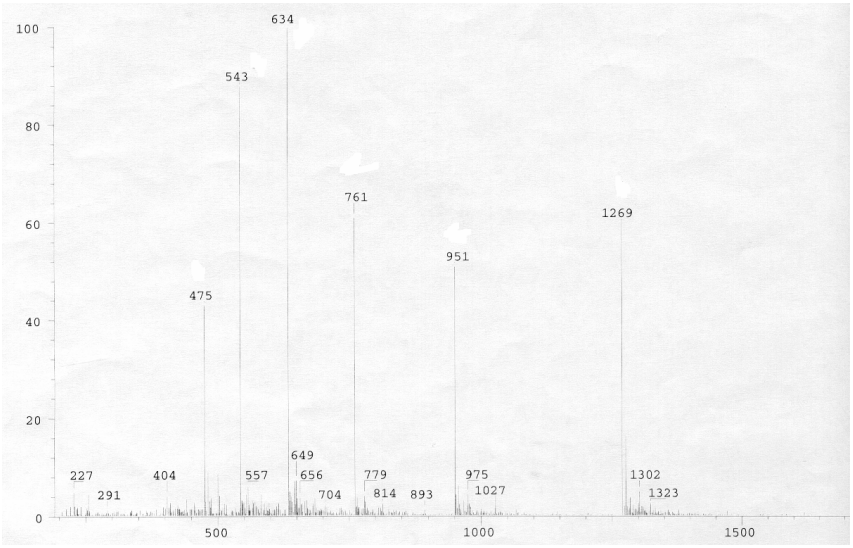


ESI-MS-spectra of **25n**



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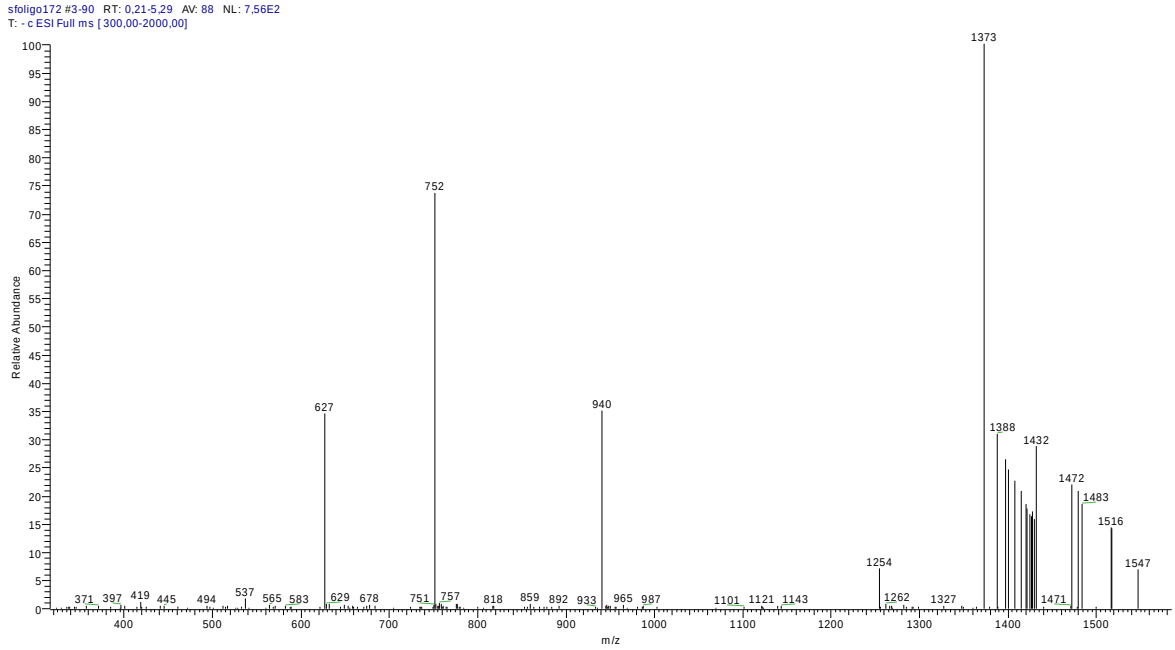
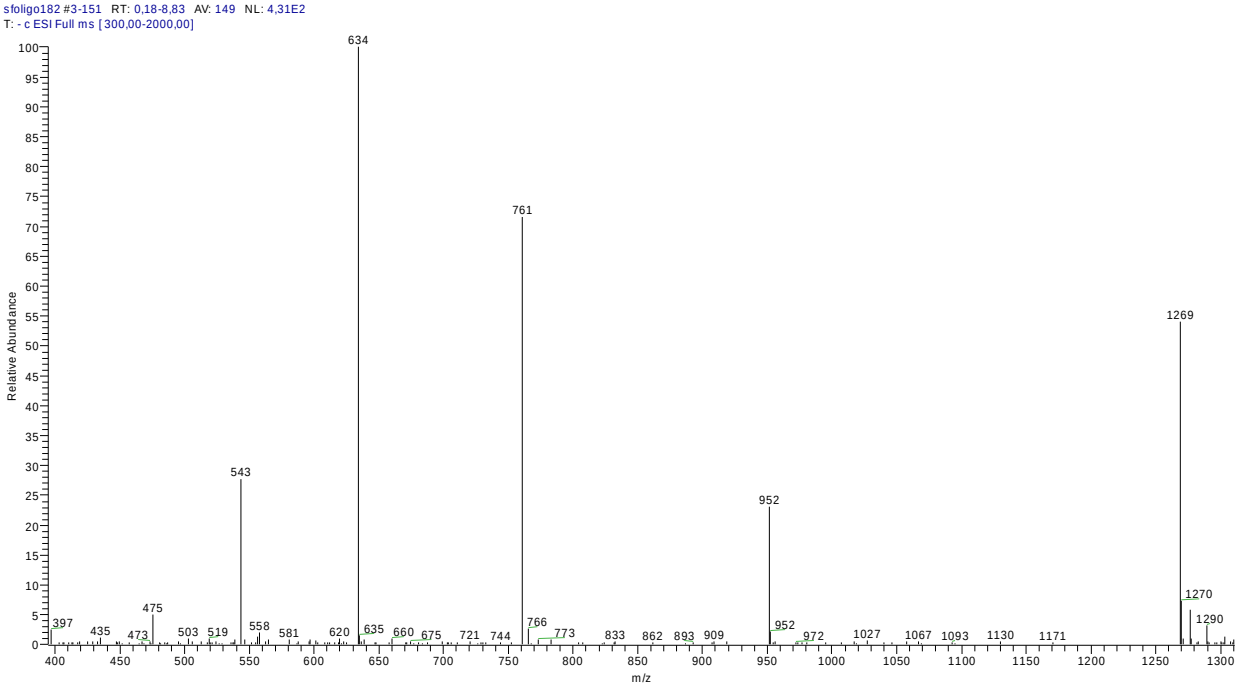
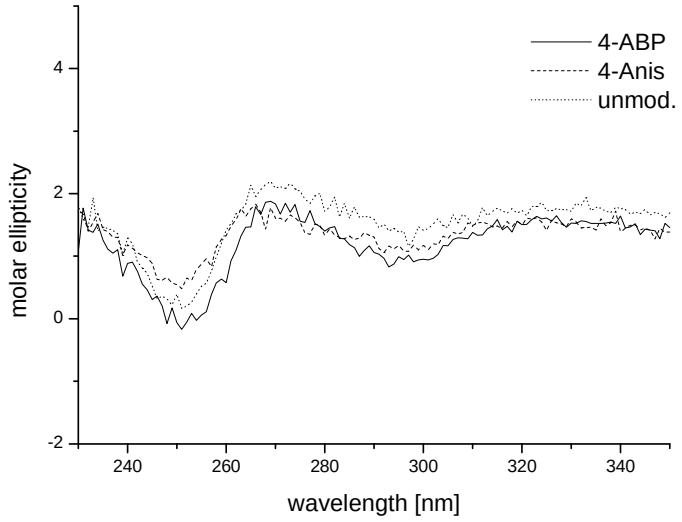


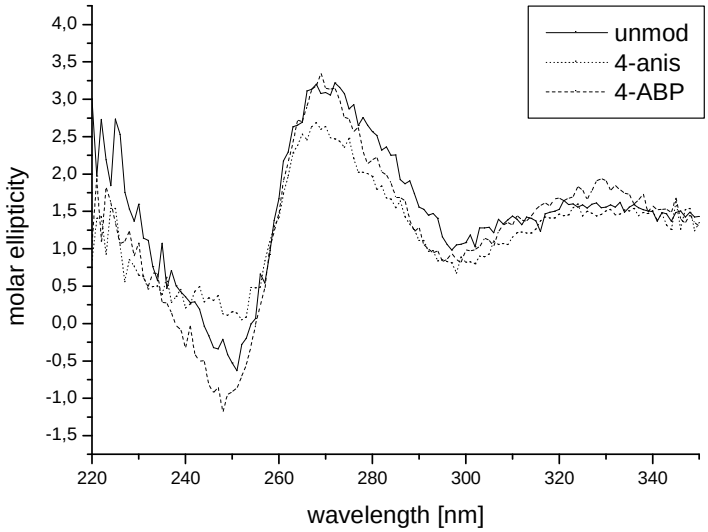
ESI-MS-spectra of **25p**



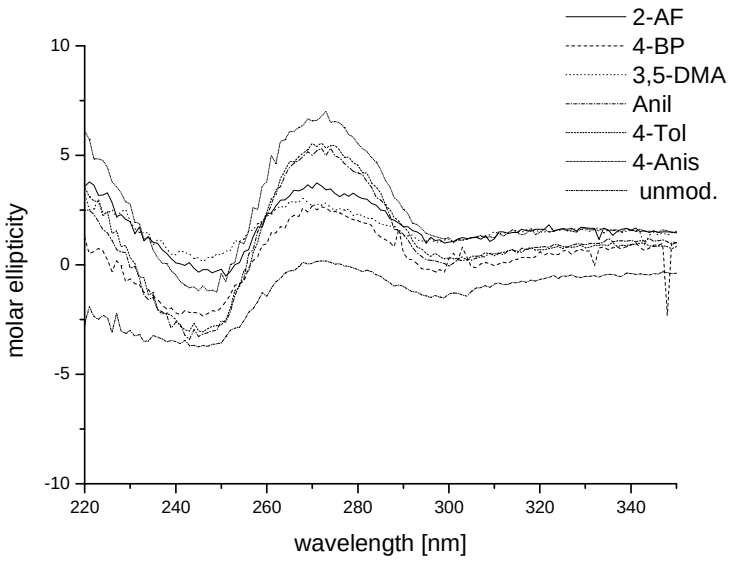
ESI-MS-spectra of **25q**



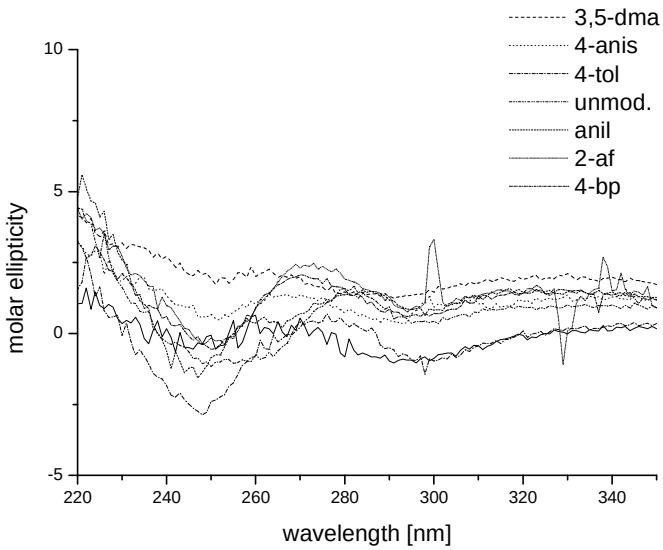
CD-spectra for **23a-c**



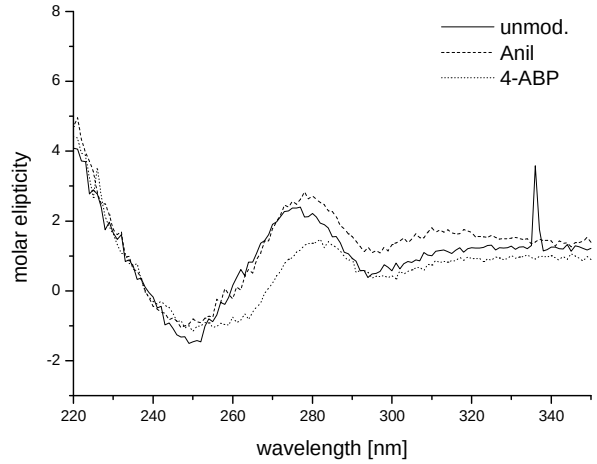
CD-spectra for **23d-f**



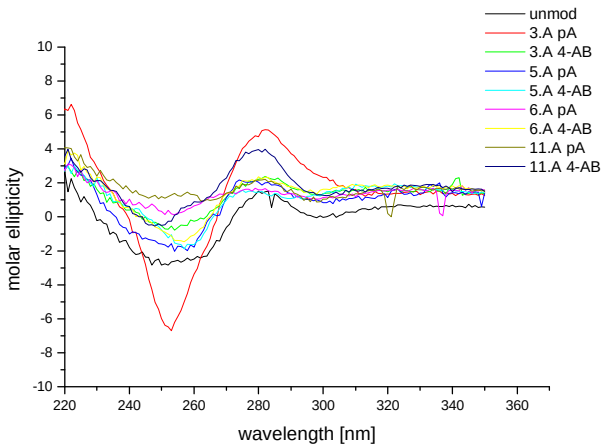
CD-spectra for **24a-g**



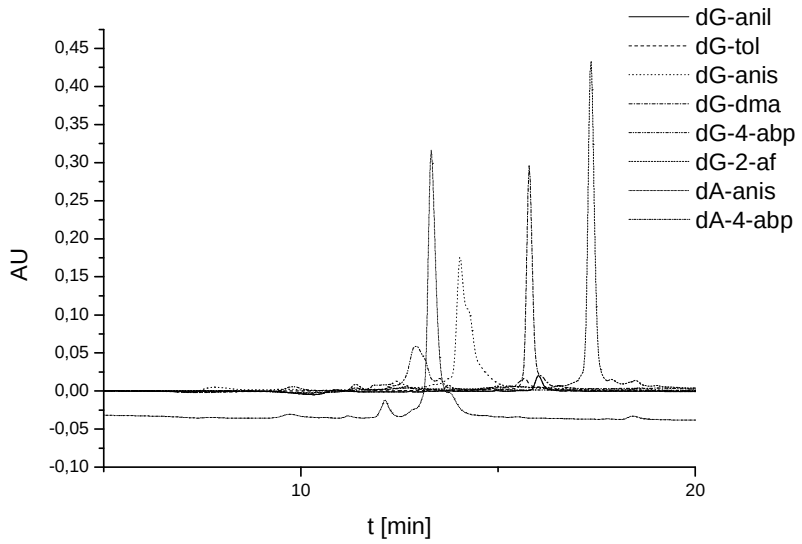
CD-spectra for **25a-g**



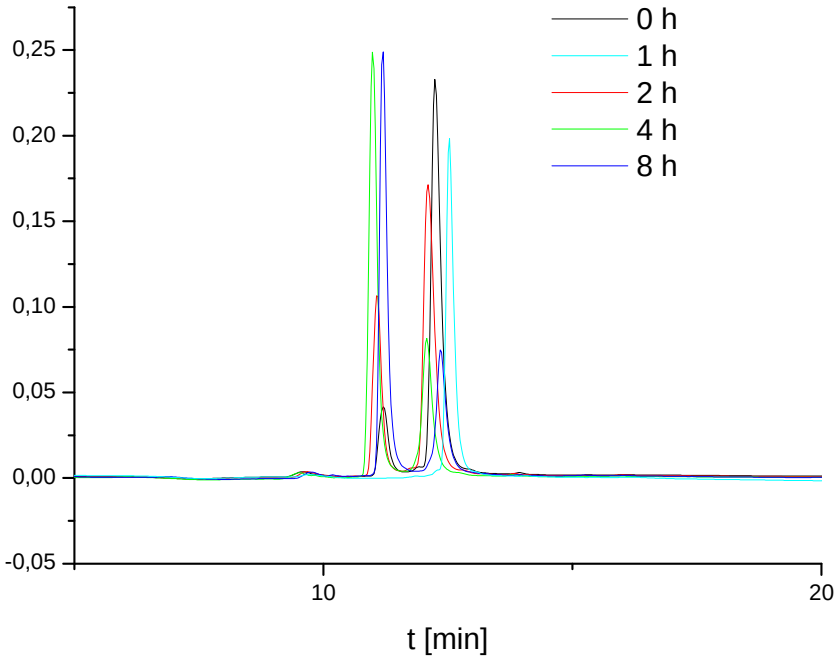
CD-spectra for **25h,i**



CD-spectra for **25j-q**



HPLC chromatograms of the EcoRI assay for oligonucleotides **25b-i** after 8 hours



HPLC chromatograms of the EcoRI assay with the modified oligonucleotide **25i**

Efficiencies of primer extension reactions

The primer extension reactions were quantified by phosphorimaging (BioRad FX) of the dried polyacrylamide gels. The ratio of primer extension was determined by subtracting the intensity of the band corresponding to the remaining primer from the total intensity in the lane. The results depicted below are averages from repeated experiments.

Pfu DNA polymerase (exo-):

Template Nucleobase	**dNTP**	**Extension [%]**	**Template Nucleobase**	**dNTP**	**Extension [%]**
G	A	21 ± 3	A	A	33 ± 4
	C	92 ± 1		C	31 ± 5
	G	13 ± 1		G	4 ± 1
	T	26 ± 2		T	95 ± 1
G(4-abp)	A	29 ± 3	A(4-abp)	A	78 ± 8
	C	60 ± 7		C	10 ± 1
	G	5 ± 1		G	11 ± 2
	T	10 ± 1		T	90 ± 1
G(anis)	A	54 ± 3	A(anis)	A	19 ± 3
	C	77 ± 8		C	7 ± 1
	G	10 ± 1		G	-
	T	60 ± 3		T	90 ± 1

human DNA polymerase β:

Template Nucleobase	dNTP	Extension [%]	Template Nucleobase	dNTP	Extension [%]
G	A	9 ± 1	A	A	10 ± 1
	C	73 ± 1		C	-
	G	-		G	-
	T	-		T	79 ± 2
G(4-abp)	A	7 ± 1	A(4-abp)	A	10 ± 1
	C	55 ± 1		C	-
	G	4 ± 1		G	-
	T	-		T	63 ± 1
G(anis)	A	7 ± 1	A(anis)	A	5 ± 1
	C	47 ± 1		C	-
	G	4 ± 1		G	-
	T	7 ± 1		T	84 ± 1

- : below 2%.

Dpo4 DNA polymerase:

Template Nucleobase	dNTP	Extension [%]	Template Nucleobase	dNTP	Extension [%]
G	A	-	A	A	20 ± 1
	C	80 ± 1		C	-
	G	-		G	-
	T	-		T	83 ± 1
G(4-abp)	A	-	A(4-abp)	A	-
	C	49 ± 4		C	-
	G	-		G	-
	T	7 ± 2		T	49 ± 3
G(anis)	A	-	A(anis)	A	-
	C	65 ± 2		C	-
	G	-		G	-
	T	11 ± 2		T	64 ± 2

- : below 2%.

Primer extension reactions employing *Pfu* (exo+) DNA polymerase

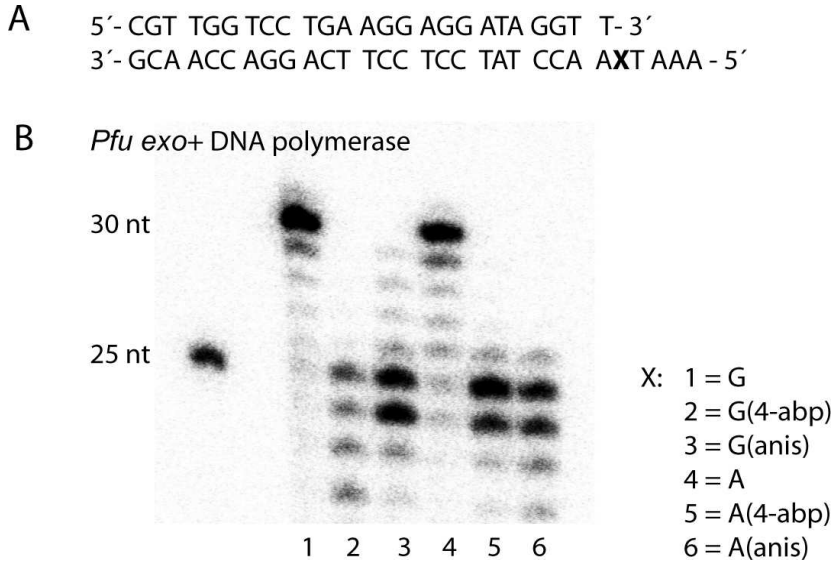


Figure: Action of C8-arylamine adducts on *Pfu* (exo+) DNA polymerase. (A): DNA sequences employed. X = modified dG or dA residues. (B): reactions catalyzed by the indicated *Pfu* (exo+) DNA polymerase in the presence of all four dNTPs and the indicated DNA template.