SUPPLEMENTARY INFORMATION

Radiolabeled Pyridinyl Analogues of Dibenzylideneacetone as β-Amyloid Imaging Probes

Xiaomei Cui,[a] Xiaoyang Zhang,[a] Cheng Peng,[b] Jiapei Dai,[c] Boli Liu[a] and Mengchao Cui [a,*]

[a] Key Laboratory of Radiopharmaceuticals, Ministry of Education, College of Chemistry, Beijing Normal University, Beijing 100875, P. R. China.

[b] Department of Nuclear Medicine, Xuanwu Hospital, Capital Medical University, Beijing 100053, P. R. China.

[c] Wuhan Institute for Neuroscience and Neuroengineering, South-Central University for Nationalities, Wuhan 430074, P. R. China.

Corresponding Author:

*Tel/Fax: +86-10-58808891. E-mail: cmc@bnu.edu.cn (M. Cui)

Contents

1. Purity of key target compounds

Compounds	Flow rate (mL/min)	Mobile phase (CH_3CN %)	Column (Venusil MP C18)	Retention time (RT, min)	Purity (%)
15a	1	70	4.6 × 250 mm	10.08	95.3
15b	1	70	4.6 × 250 mm	7.54	98.0
15c	1	70	4.6 × 250 mm	7.06	98.3
16a	1	70	4.6 × 250 mm	9.24	96.3
16b	1	70	4.6 × 250 mm	7.36	96.0
16c	1	70	4.6 × 250 mm	6.55	98.5
17a	1	70	4.6 × 250 mm	8.56	95.4
17b	1	70	4.6 × 250 mm	7.16	98.4
17c	1	70	4.6 × 250 mm	6.30	97.9
18	1	70	4.6 × 250 mm	9.21	98.5
19	1	70	4.6 × 250 mm	16.02	95.8

2. Biodistribution of [^{18}F]17a, [^{18}F]18 and [^{125}I]19 in normal ICR mice[a]

Organ	2 min	10 min	30 min	60 min
	[^{18}F]**17a** (Log *D* = 2.36 ± 0.09)			
Blood	3.17 ± 0.22	2.06 ± 0.19	1.59 ± 0.18	1.35 ± 0.12
Brain	5.05 ± 0.55	1.80 ± 0.25	0.98 ± 0.17	0.83 ± 0.06
Heart	5.82 ± 0.42	2.44 ± 0.13	1.37 ± 0.18	1.20 ± 0.17
Liver	14.00 ± 1.16	12.55 ± 0.99	4.77 ± 1.19	2.44 ± 0.50
Spleen	4.69 ± 1.04	2.44 ± 0.30	1.18 ± 0.28	1.00 ± 0.22
Lung	10.30 ± 1.63	5.43 ± 1.31	1.66 ± 0.27	1.50 ± 0.51
Kidney	13.72 ± 1.89	7.59 ± 1.03	2.58 ± 0.76	1.55 ± 0.23
Pancreas	9.91 ± 1.48	3.09 ± 0.19	1.23 ± 0.18	0.95 ± 0.12
Muscle	3.23 ± 0.38	1.94 ± 0.38	1.12 ± 0.13	0.84 ± 0.08
Bone	2.04 ± 0.36	1.15 ± 0.34	1.49 ± 1.02	2.50 ± 0.42
Stomach[b]	2.87 ± 0.58	3.51 ± 0.52	2.02 ± 1.31	0.77 ± 0.38
Intestine[b]	10.51 ± 0.39	29.69 ± 2.75	48.02 ± 2.99	48.90 ± 4.96
	[^{18}F]**18** (Log *D* = 3.14 ± 0.03)			
Blood	2.57 ± 0.13	2.29 ± 0.13	2.12 ± 0.45	1.28 ± 0.34
Brain	6.24 ± 0.27	3.35 ± 0.32	1.35 ± 0.05	0.78 ± 0.07
Heart	5.41 ± 0.66	2.62 ± 0.13	1.67 ± 0.12	1.04 ± 0.33
Liver	15.73 ± 3.11	19.33 ± 1.16	13.2 ± 1.09	9.16 ± 2.40
Spleen	4.08 ± 0.44	4.98 ± 0.55	1.94 ± 0.16	1.48 ± 0.65
Lung	8.90 ± 0.99	4.70 ± 0.43	2.90 ± 0.27	2.14 ± 0.44
Kidney	10.68 ± 0.80	8.81 ± 0.71	7.79 ± 0.36	4.36 ± 1.27
Pancreas	10.30 ± 0.82	7.20 ± 1.60	3.00 ± 0.12	1.77 ± 1.46
Muscle	3.17 ± 0.38	1.79 ± 1.17	1.04 ± 0.24	0.76 ± 0.19
Bone	2.66 ± 0.14	2.36 ± 0.15	3.78 ± 0.51	3.87 ± 0.62
Stomach[b]	2.36 ± 0.21	3.63 ± 0.36	3.57 ± 1.52	2.39 ± 0.72

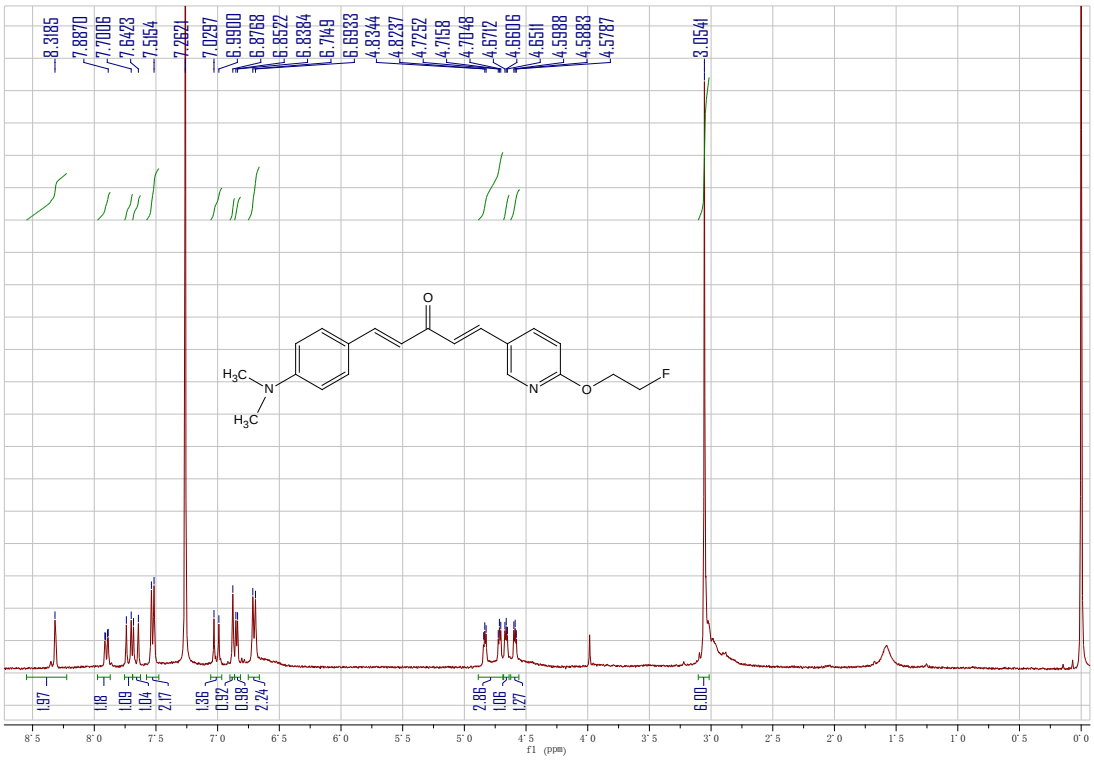
Intestine[b]	5.92 ± 0.79	15.09 ± 2.27	24.05 ± 7.87	36.62 ± 8.28
	[^{125}I]**19** (Log *D* = 3.31 ± 0.31)			
Blood	3.71 ± 0.75	1.80 ± 0.16	1.33 ± 0.21	1.02 ± 0.22
Brain	2.06 ± 0.16	1.72 ± 0.15	1.36 ± 0.18	1.04 ± 0.17
Heart	4.01 ± 0.19	2.13 ± 0.19	1.42 ± 0.18	1.09 ± 0.31
Liver	27.58 ± 1.55	23.98 ± 1.05	20.16 ± 1.61	14.78 ± 0.39
Spleen	5.16 ± 0.64	3.49 ± 0.27	2.86 ± 0.60	2.41 ± 0.61
Lung	6.73 ± 0.84	3.54 ± 0.38	3.04 ± 0.53	2.05 ± 0.46
Kidney	7.05 ± 0.50	5.55 ± 0.66	4.94 ± 0.88	3.88 ± 0.70
Pancreas	4.87 ± 034	3.75 ± 0.63	3.44 ± 0.29	2.64 ± 0.41
Muscle	2.44 ± 0.54	1.37 ± 0.15	1.02 ± 0.30	0.63 ± 0.09
Thyroid	0.07 ± 0.004	0.04 ± 0.01	0.03 ± 0.004	0.04 ± 0.01
Stomach[b]	1.52 ± 0.08	1.94 ± 0.21	3.15 ± 0.58	1.94 ± 0.46
Intestine[b]	5.24 ± 0.58	16.09 ± 2.57	33.41 ± 4.02	37.95 ± 3.89

[a] Expressed as % injected dose per gram. Each value represents the mean SD for 5-6 mice.

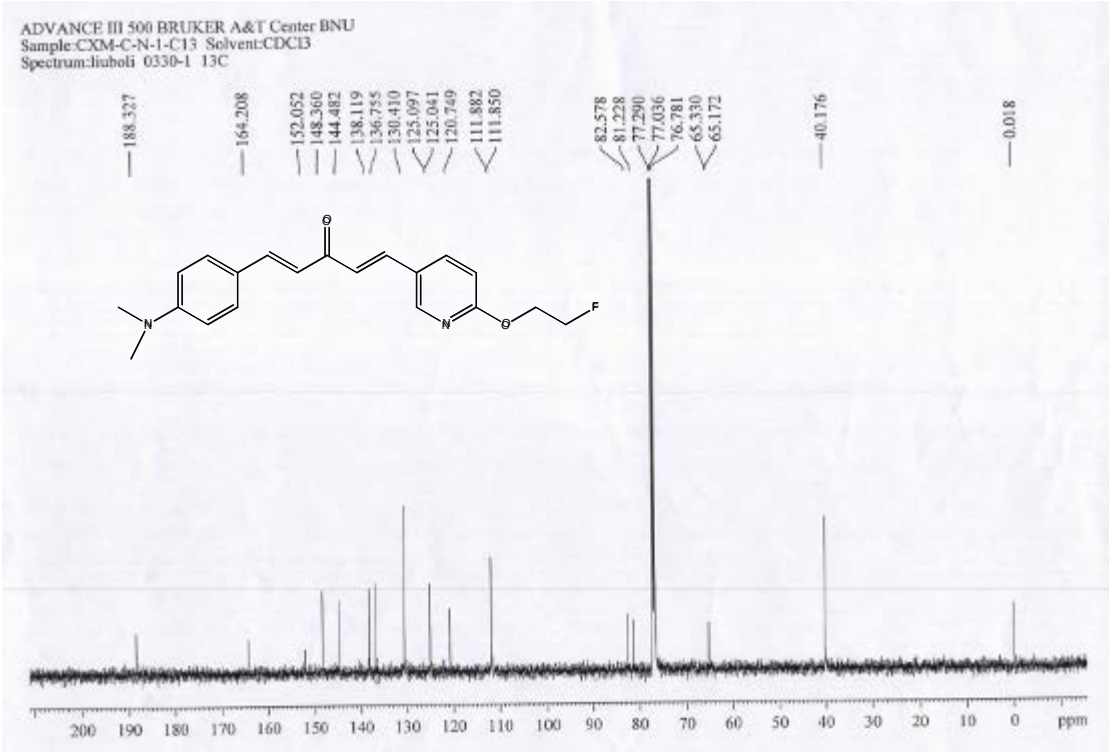
[b] Expressed as % injected dose per organ.

3. NMR and HRMS (EI) spectra of key target compounds

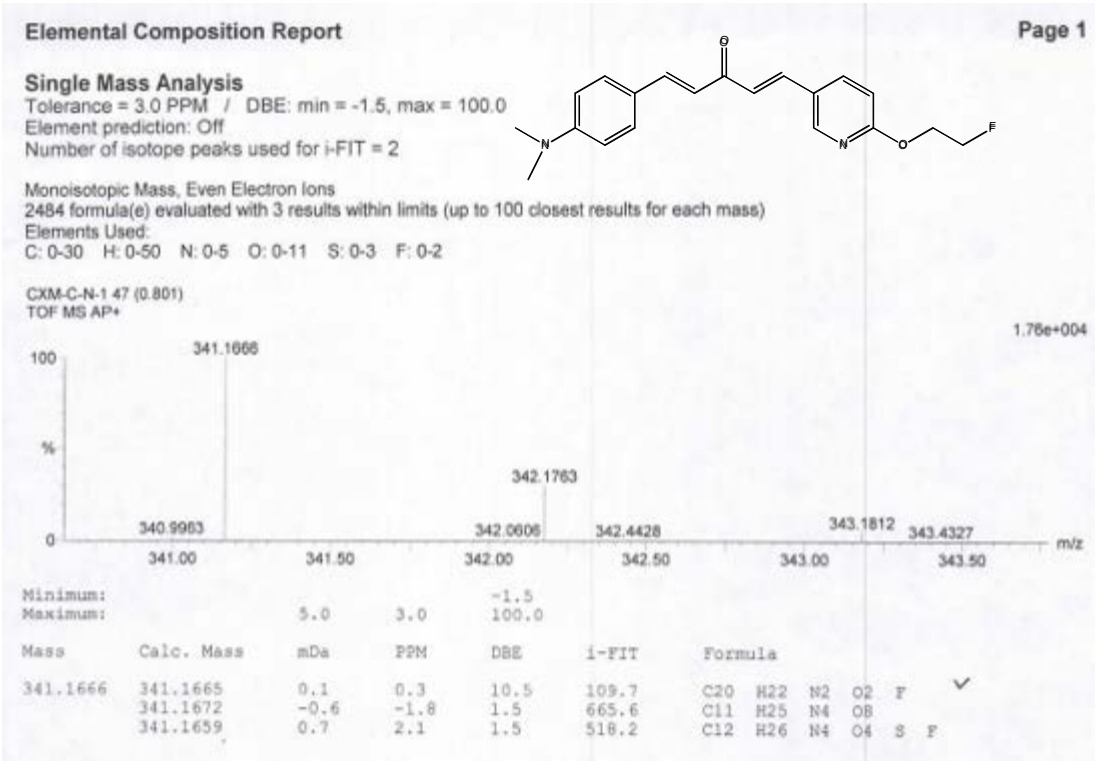
^{1}H-NMR for compound **15a**



^{13}C-NMR for compound **15a**



HRMS for compound **15a**



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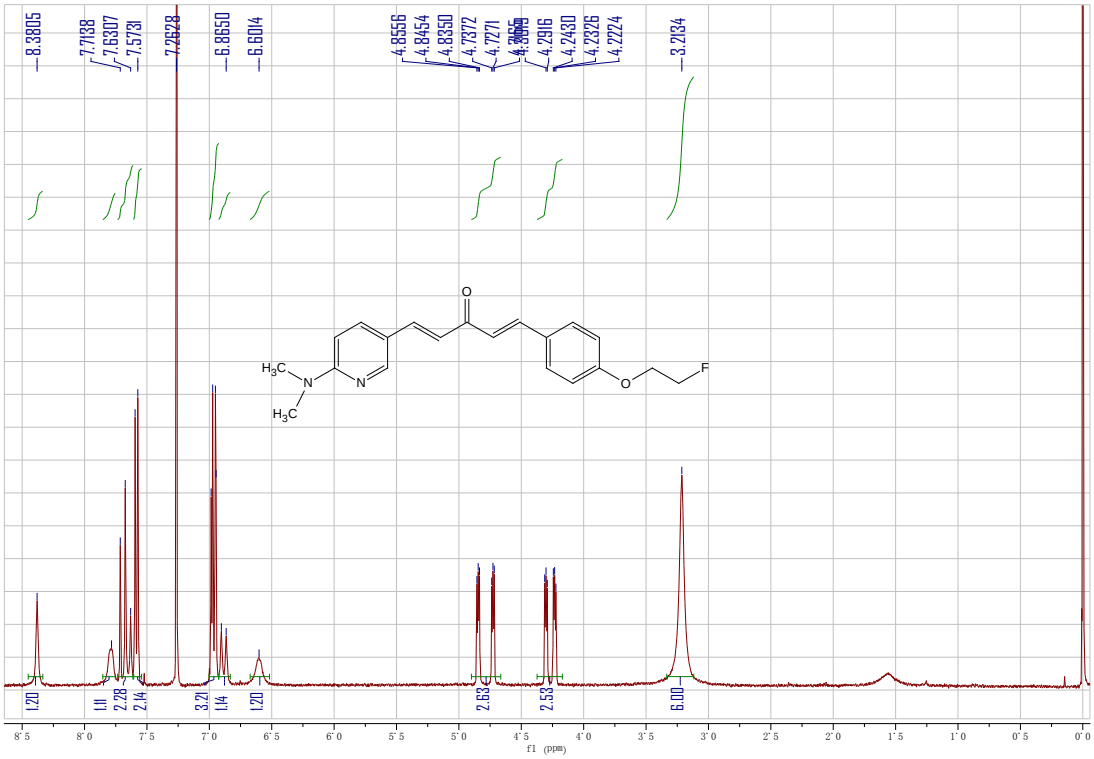

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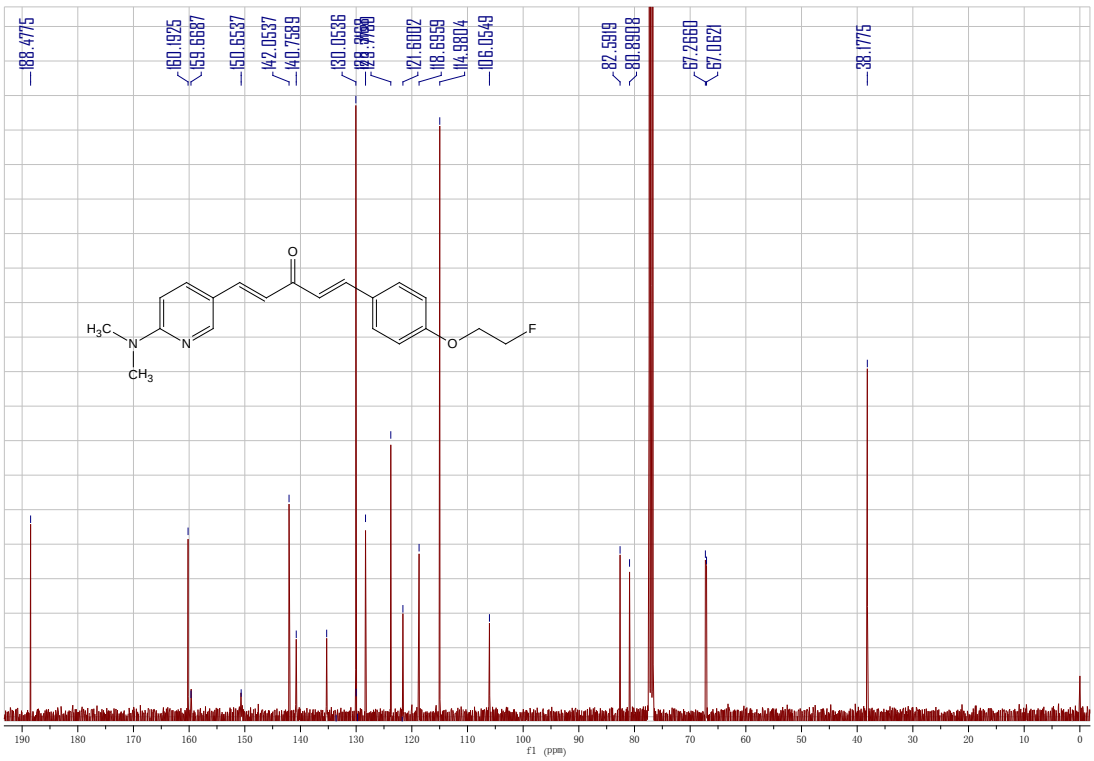

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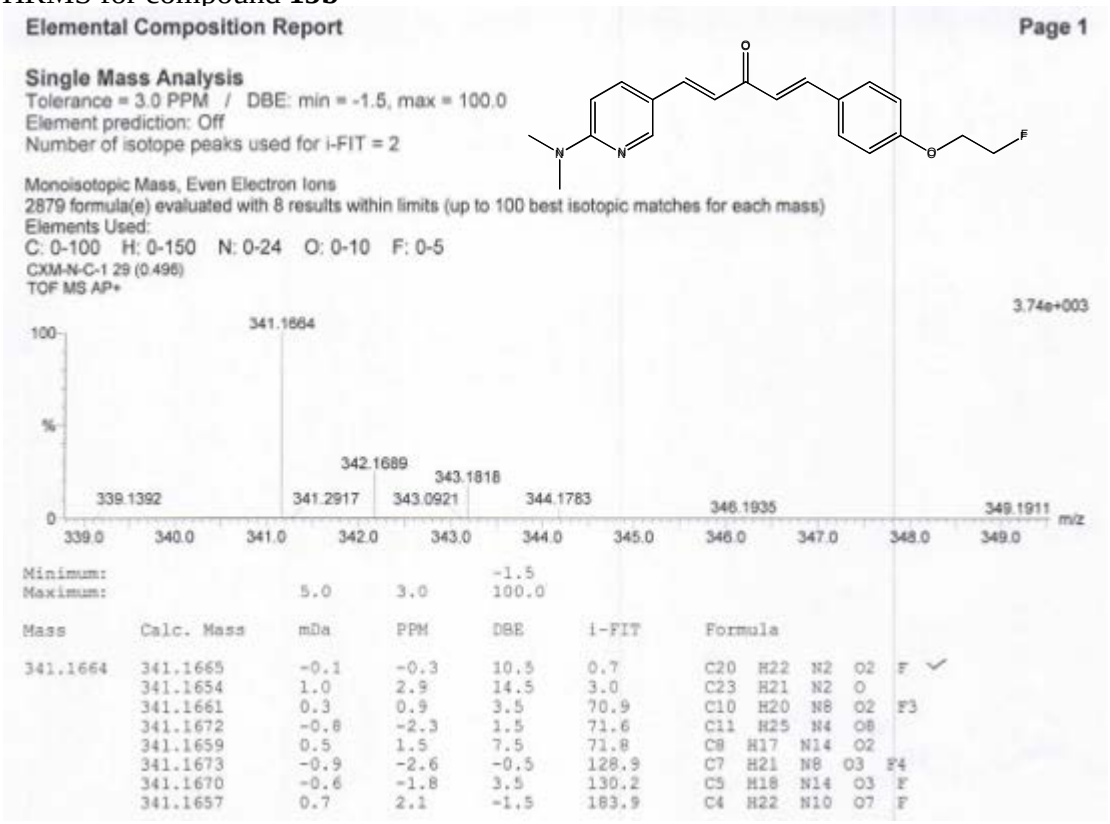

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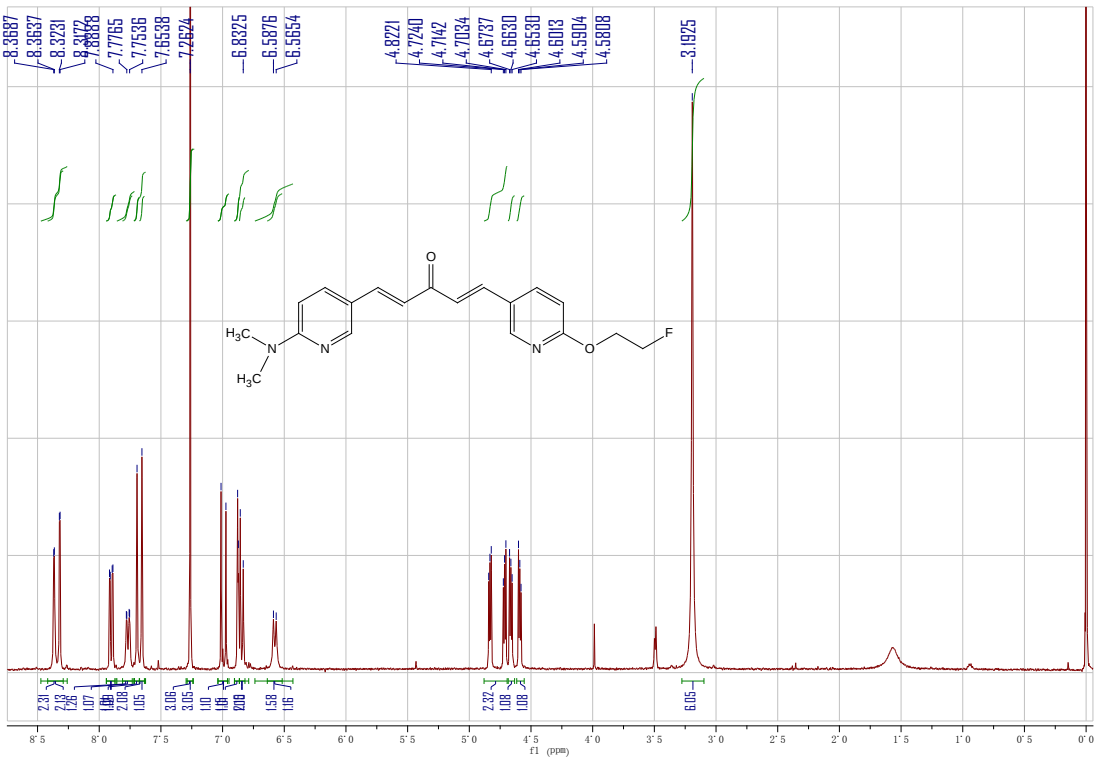

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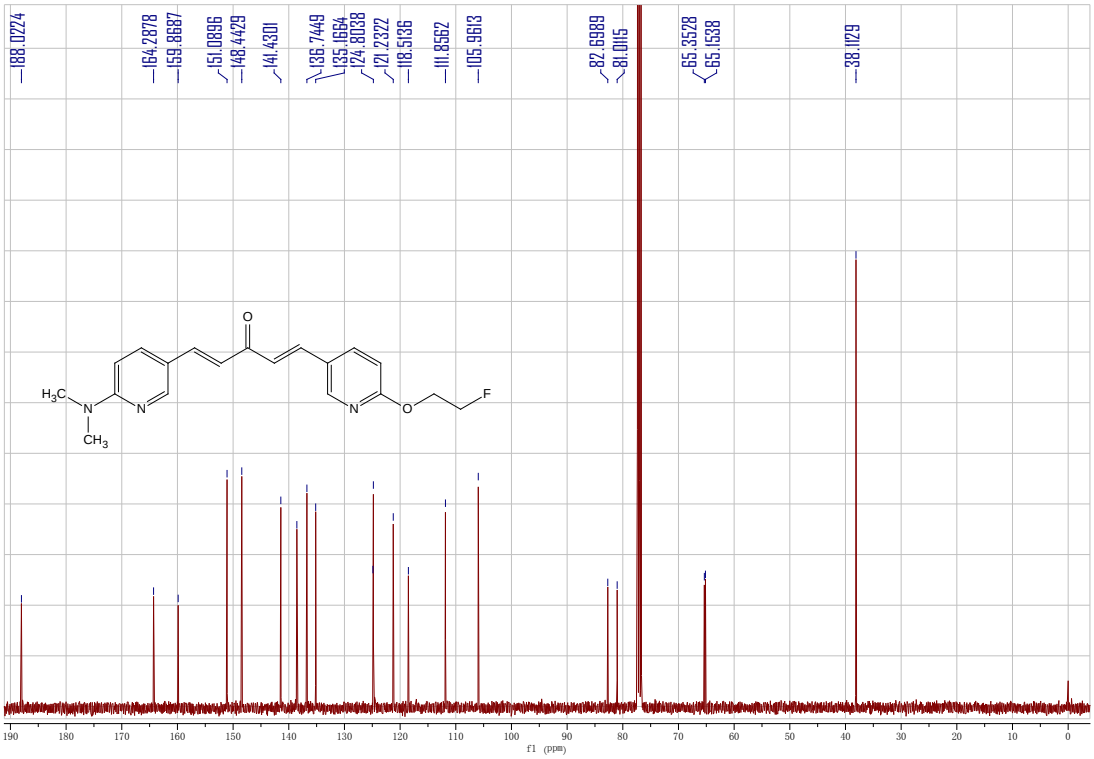

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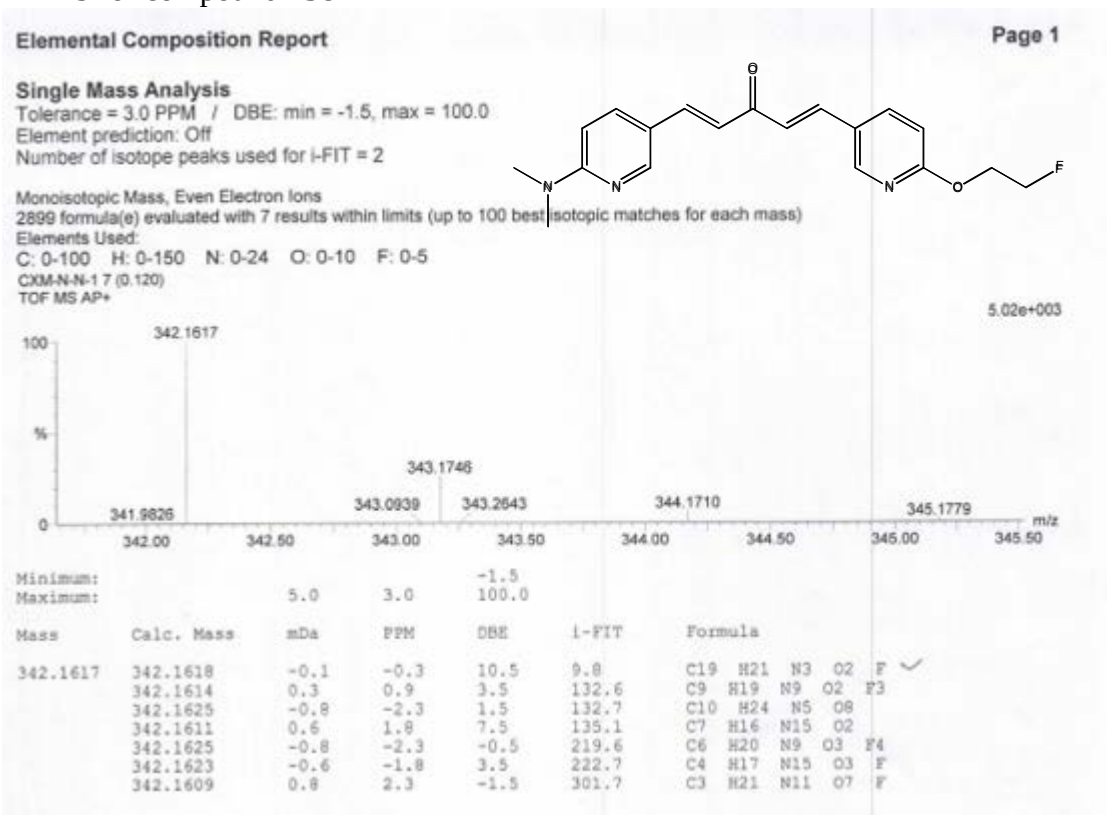

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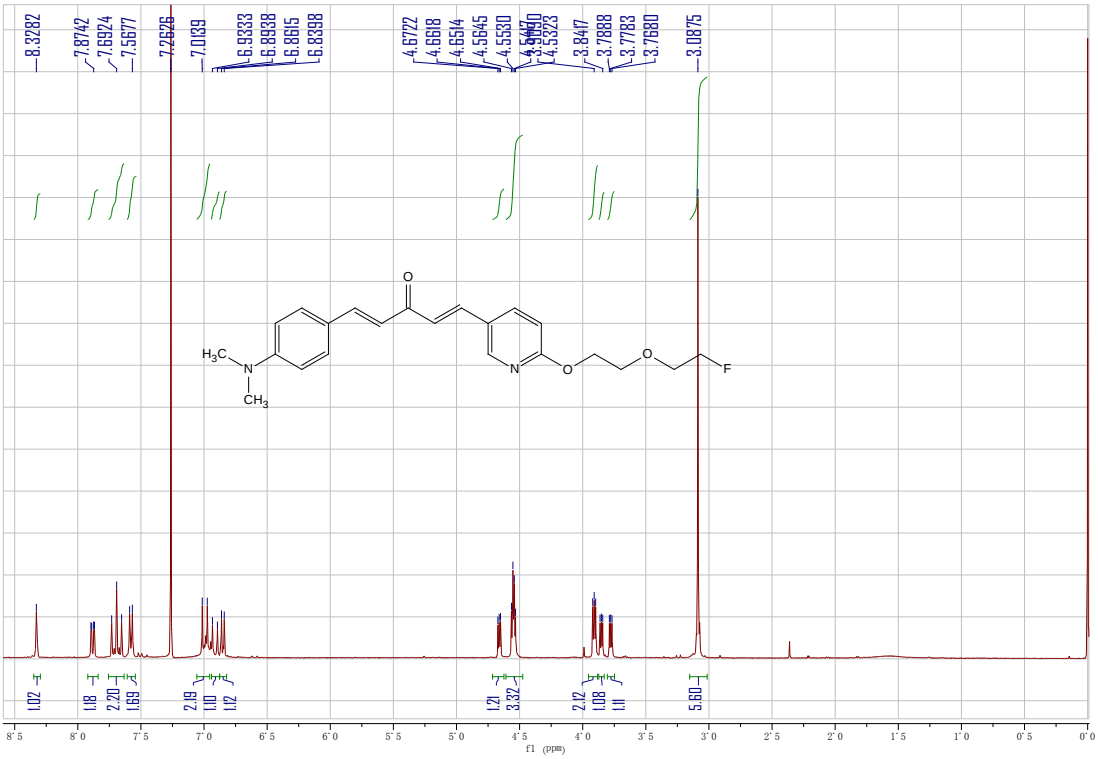

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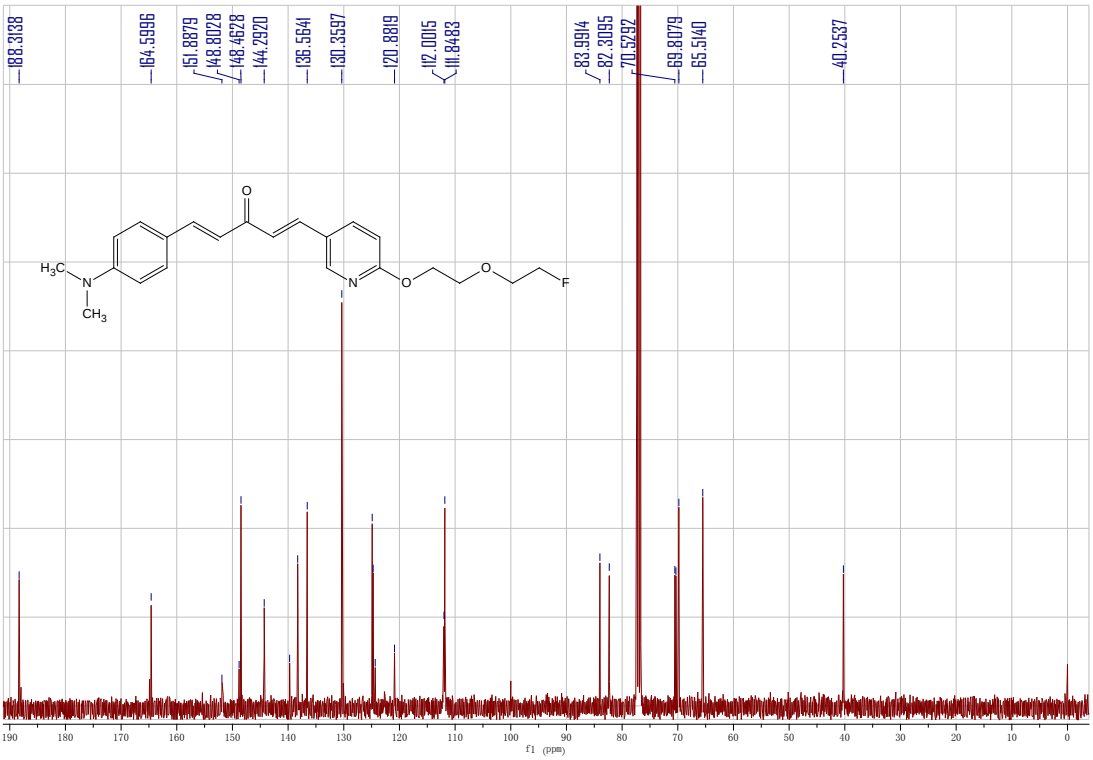

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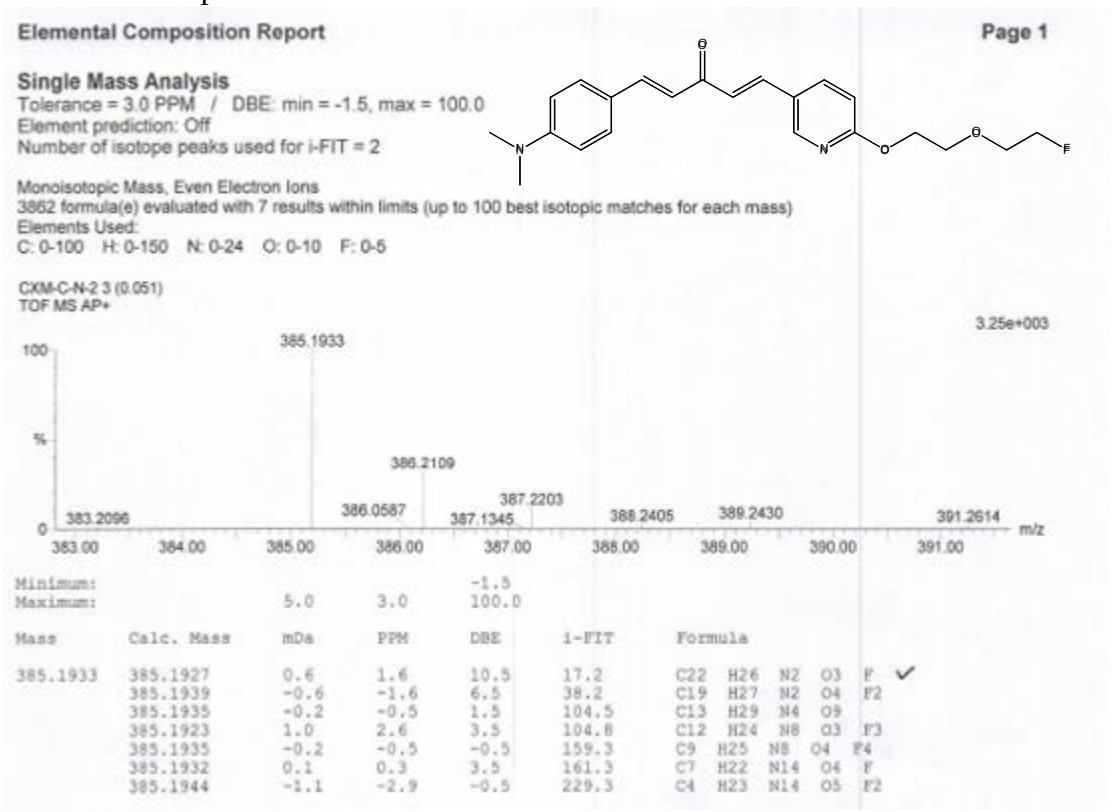


Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 3.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

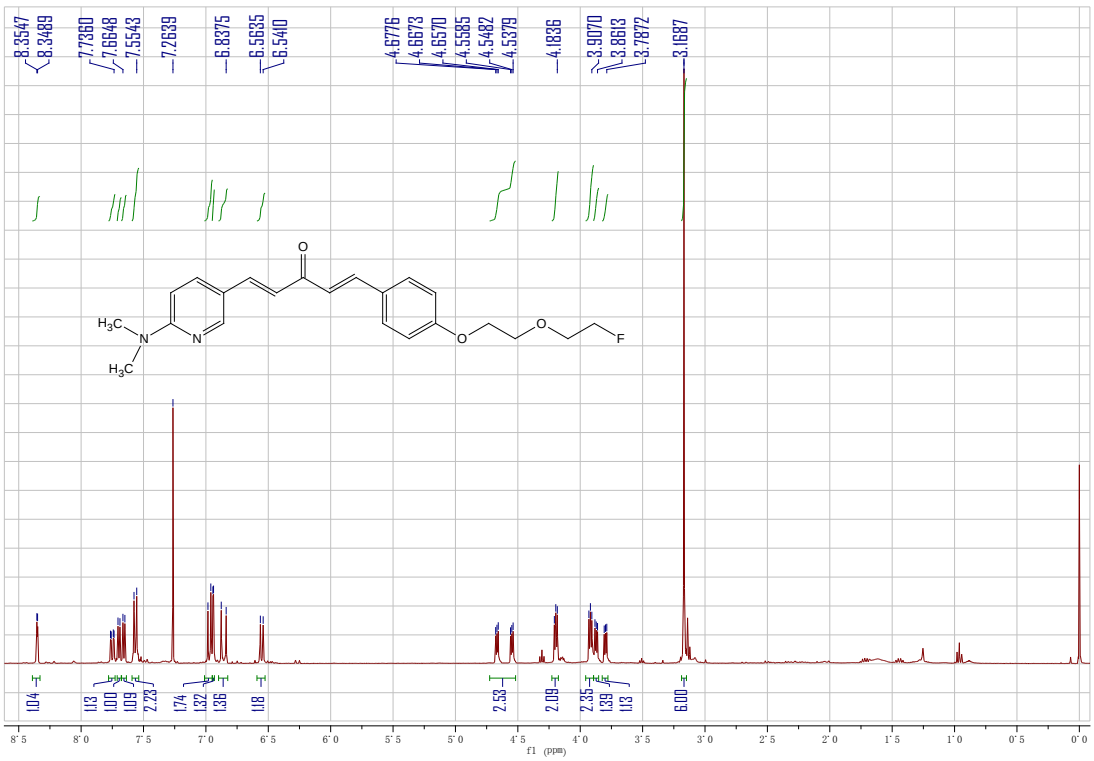
Monoisotopic Mass, Even Electron Ions
3862 formula(e) evaluated with 7 results within limits (up to 100 best isotopic matches for each mass)
Elements Used:
C: 0-100 H: 0-150 N: 0-24 O: 0-10 F: 0-5

CXM-C-N-2 3 (0.051)
TOF MS AP+

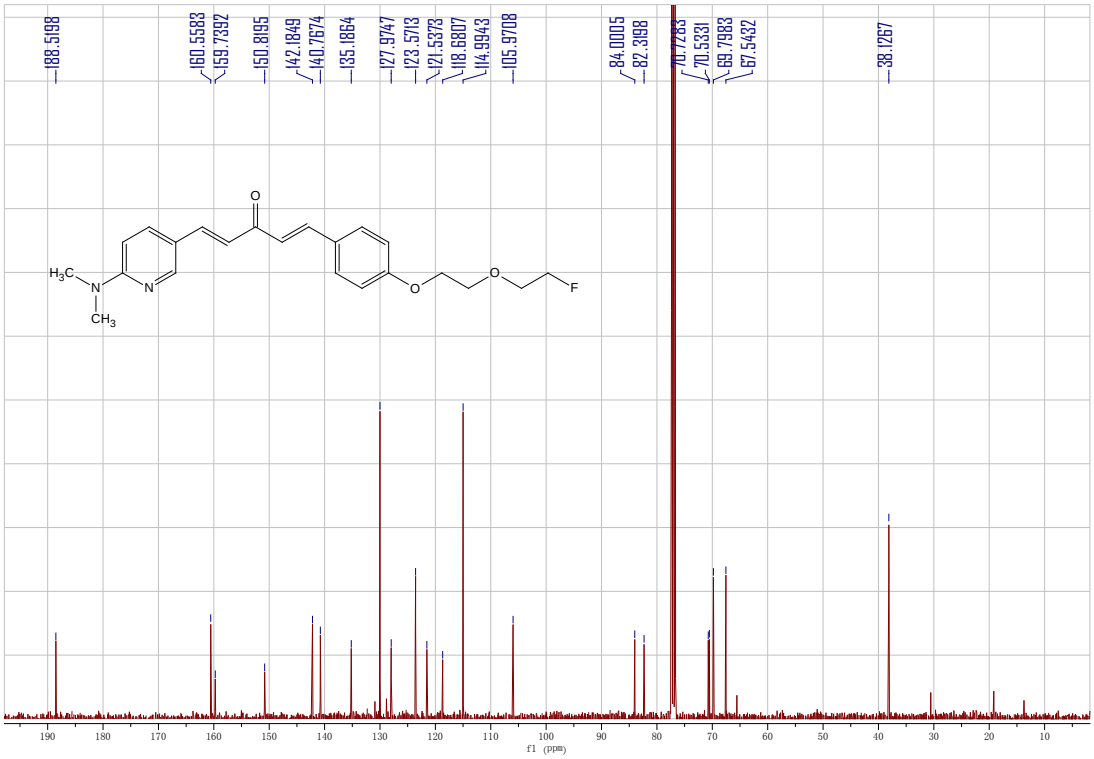
3.25e+003

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
Minimum:				-1.5		
Maximum:		5.0	3.0	100.0		
385.1933	385.1927	0.6	1.6	10.5	17.2	C22 H26 N2 O3 F ✓
	385.1939	-0.6	-1.6	6.5	38.2	C19 H27 N2 O4 F2
	385.1935	-0.2	-0.5	1.5	104.5	C13 H29 N4 O9
	385.1923	1.0	2.6	3.5	104.8	C12 H24 N8 O3 F3
	385.1935	-0.2	-0.5	-0.5	159.3	C9 H25 N8 O4 F4
	385.1932	0.1	0.3	3.5	161.3	C7 H22 N14 O4 F
	385.1944	-1.1	-2.9	-0.5	229.3	C4 H23 N14 O5 F2

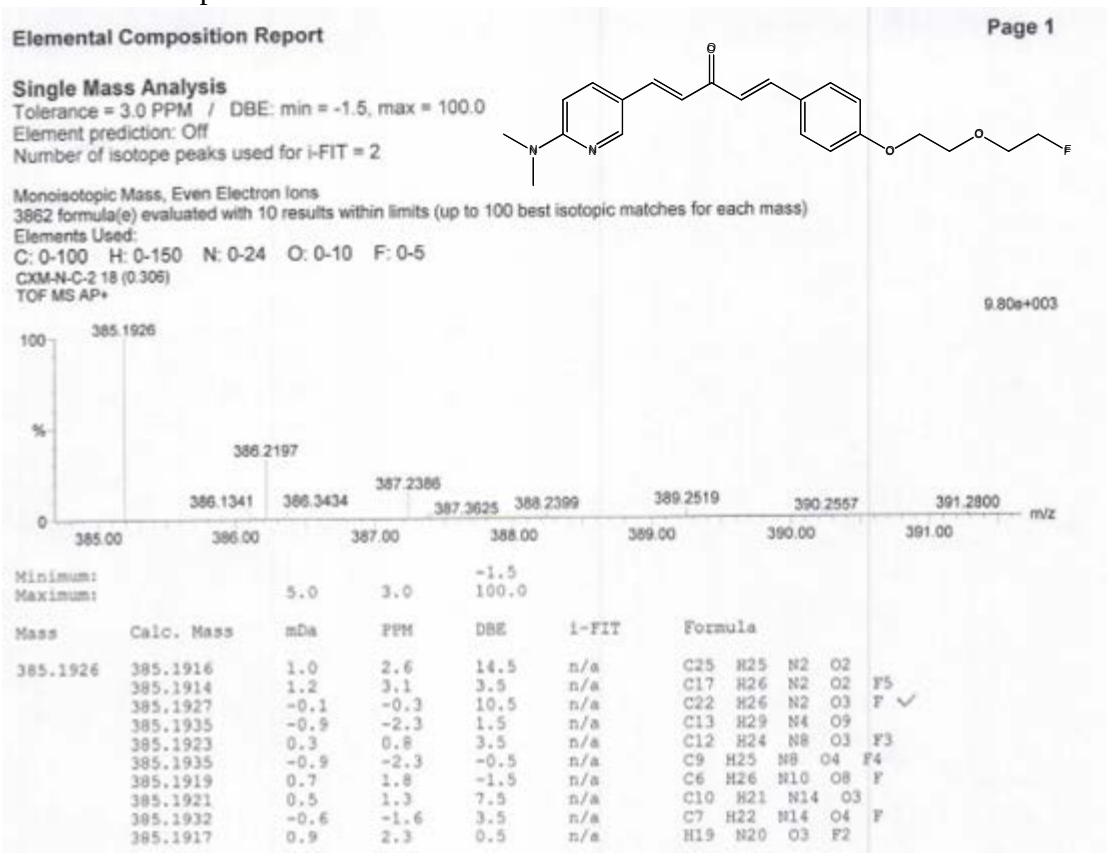
^{1}H-NMR for compound **16b**



^{13}C-NMR for compound **16b**



HRMS for compound **16b**



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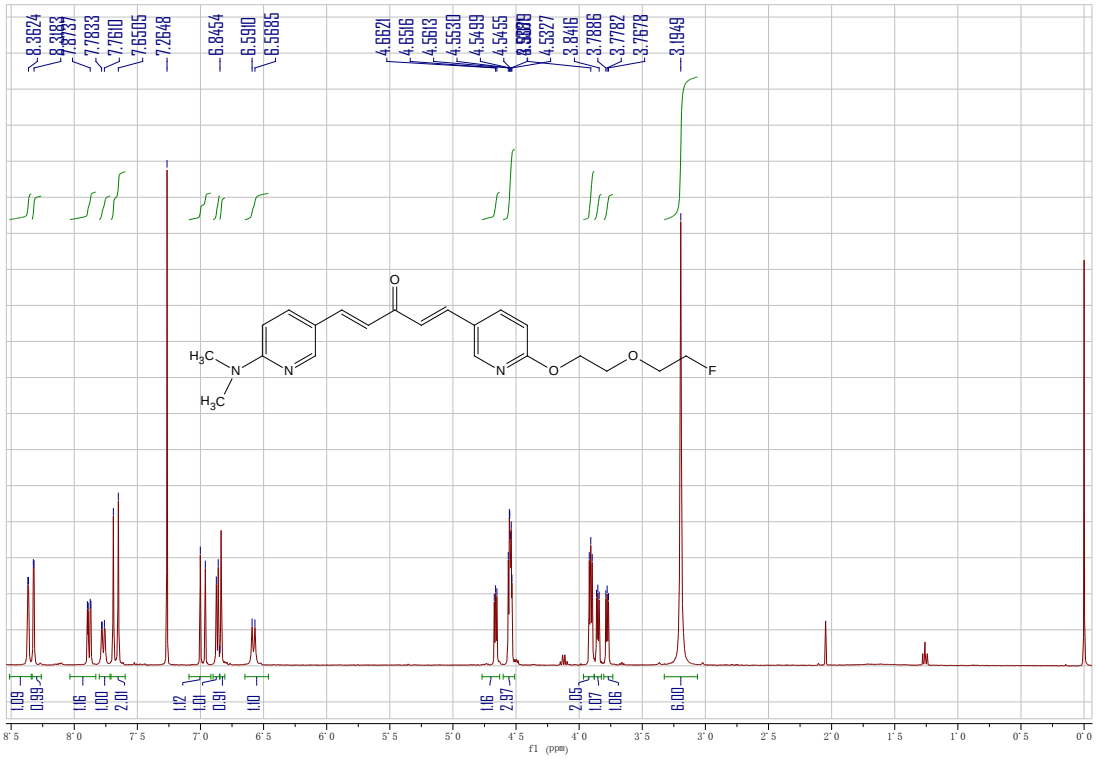

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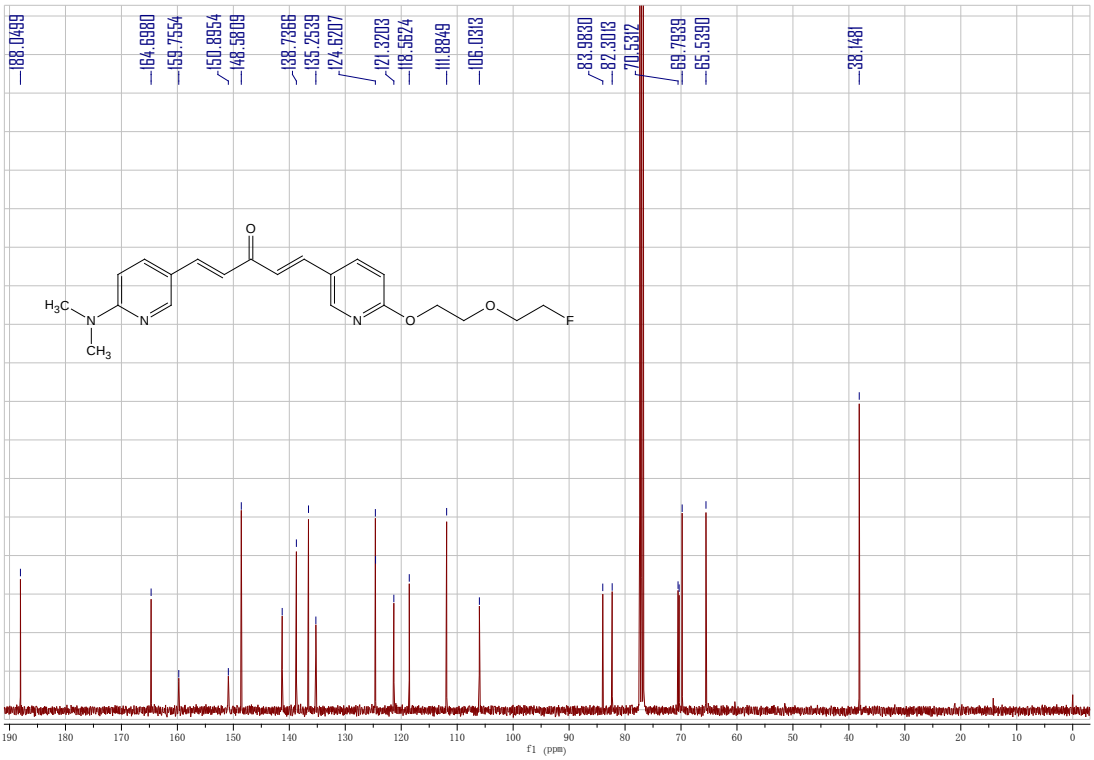

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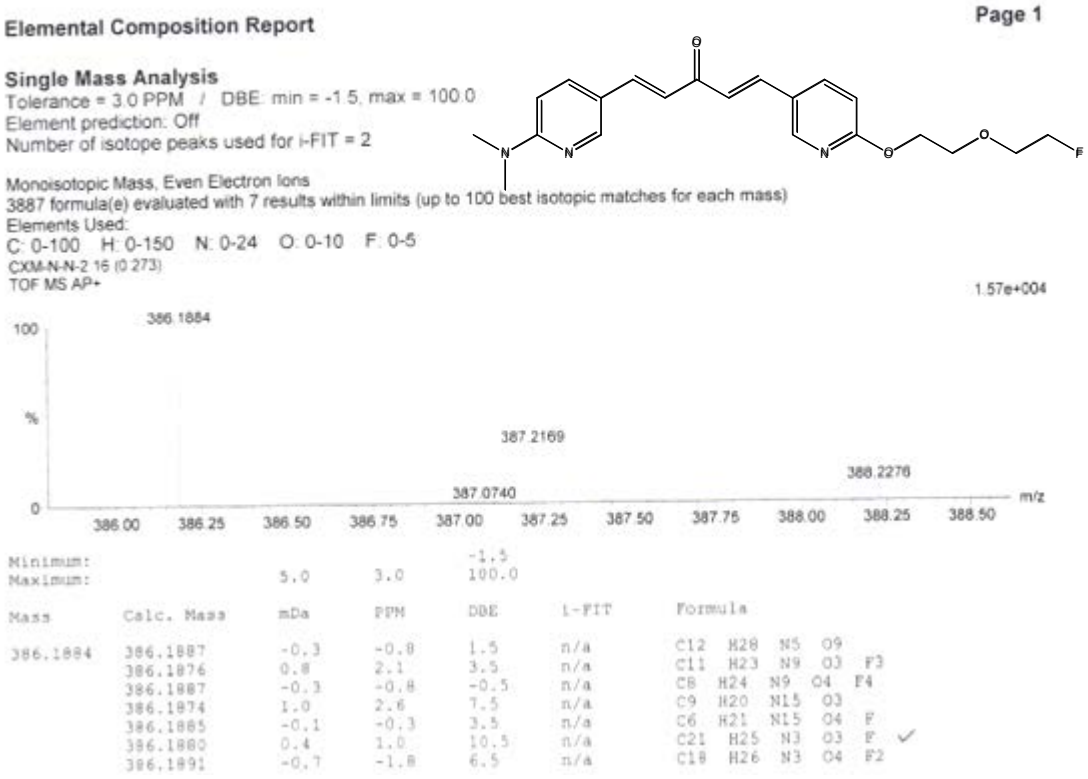
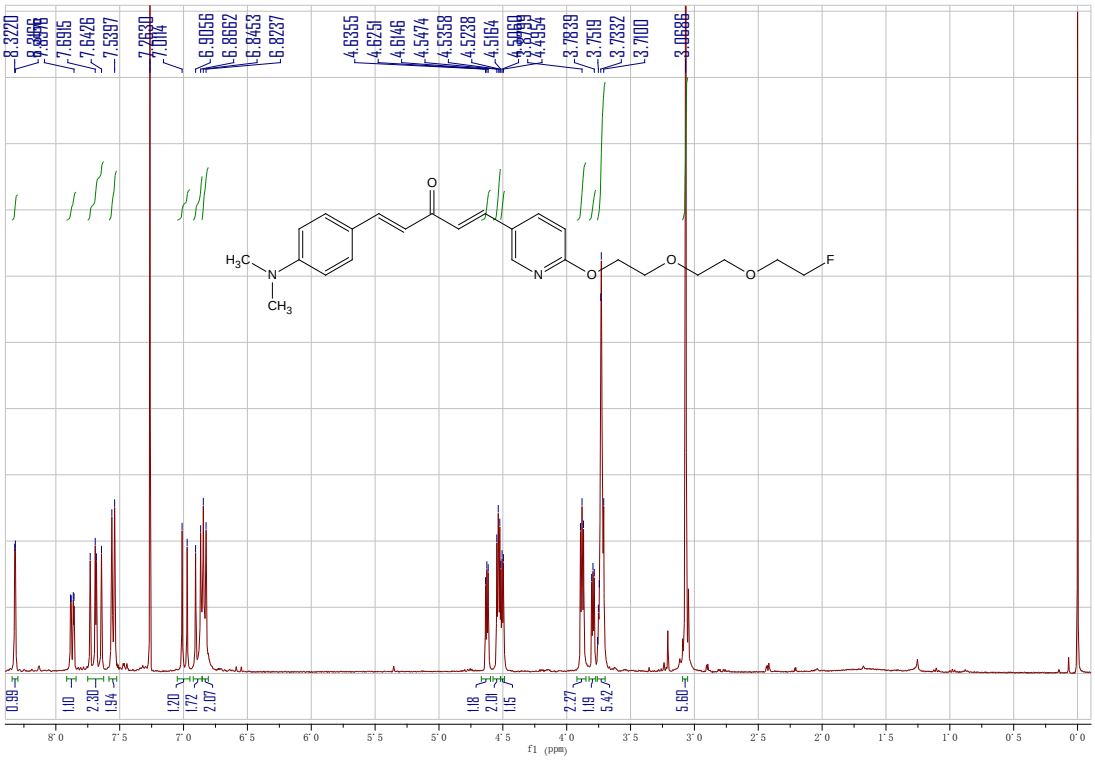


^{1}H-NMR for compound **17a**



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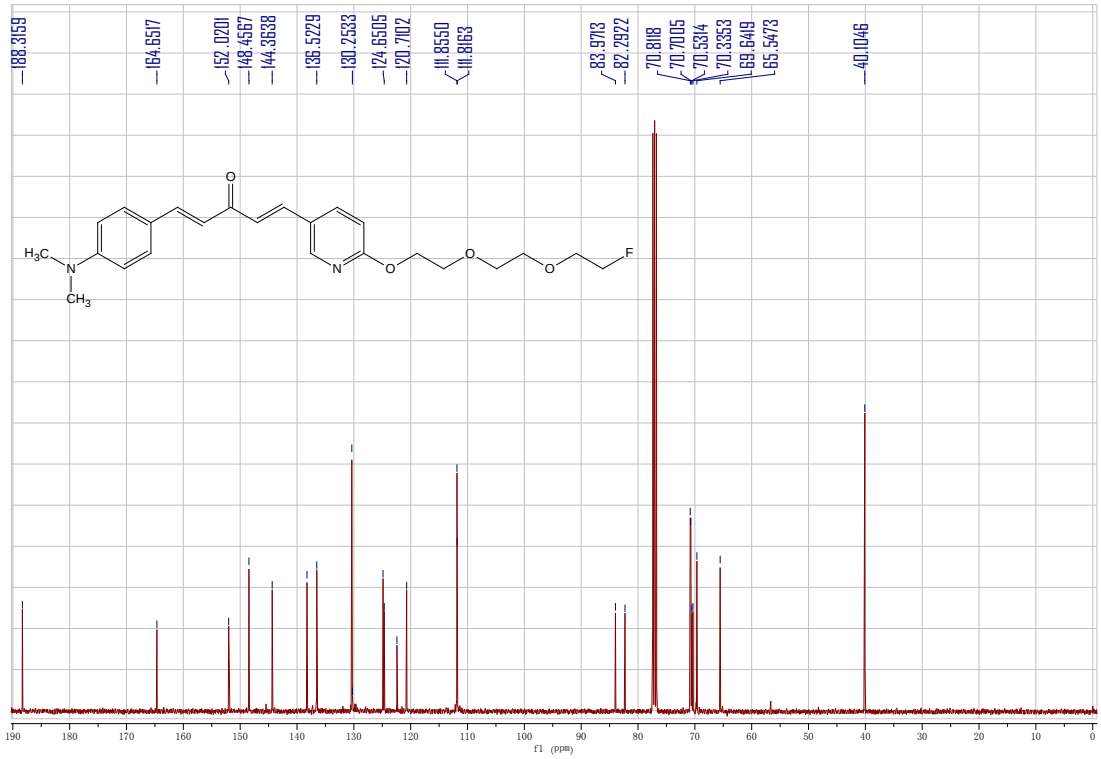

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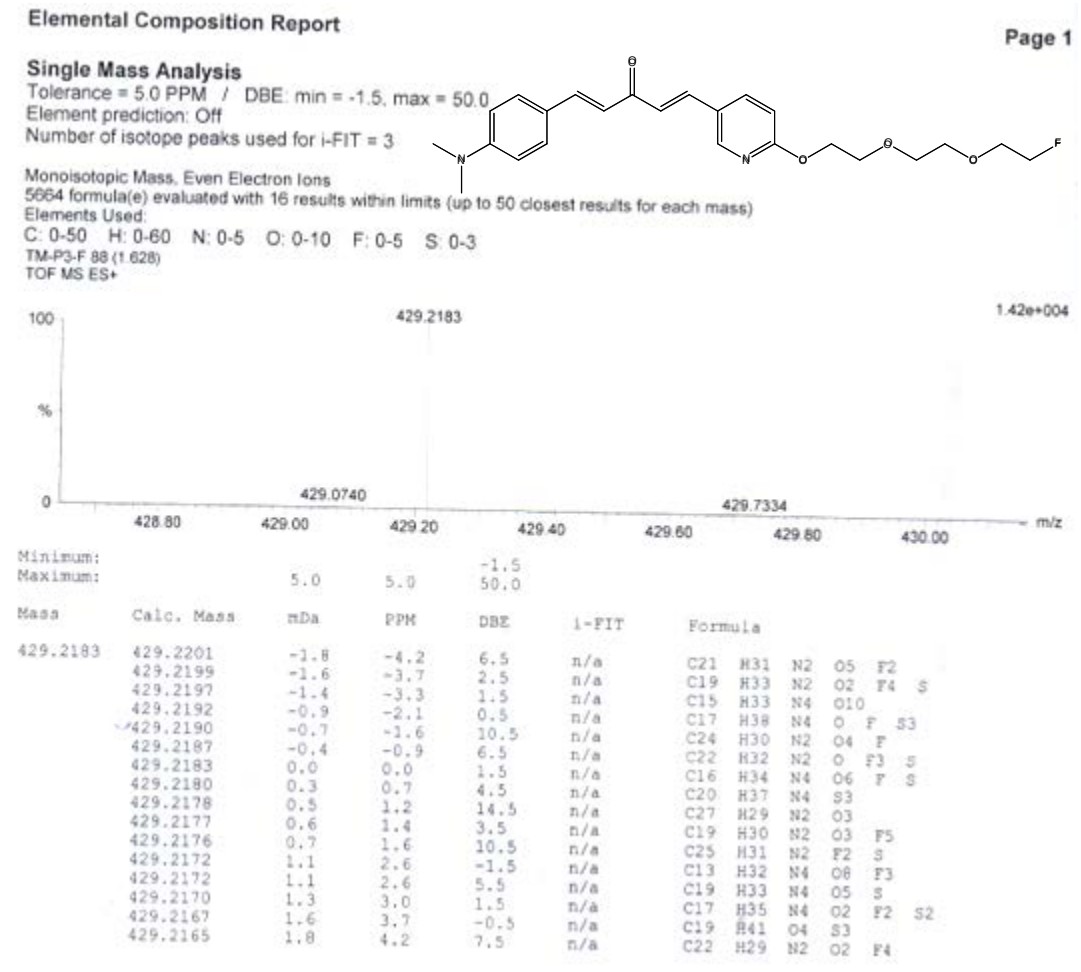

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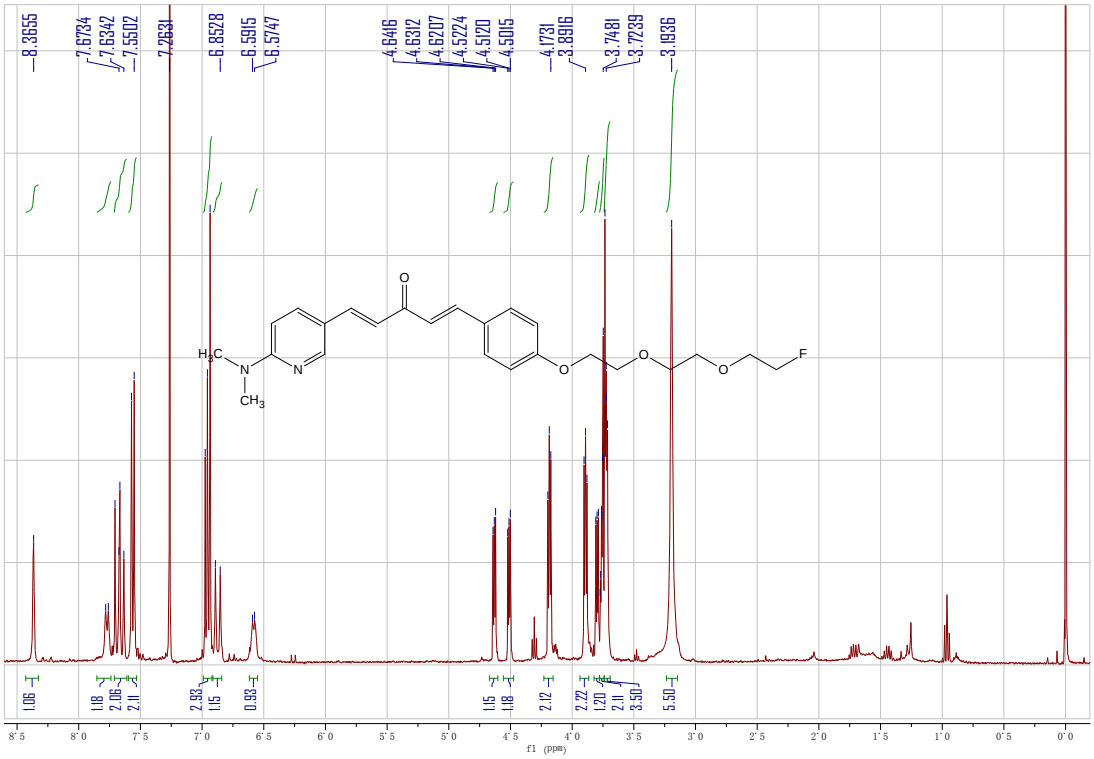

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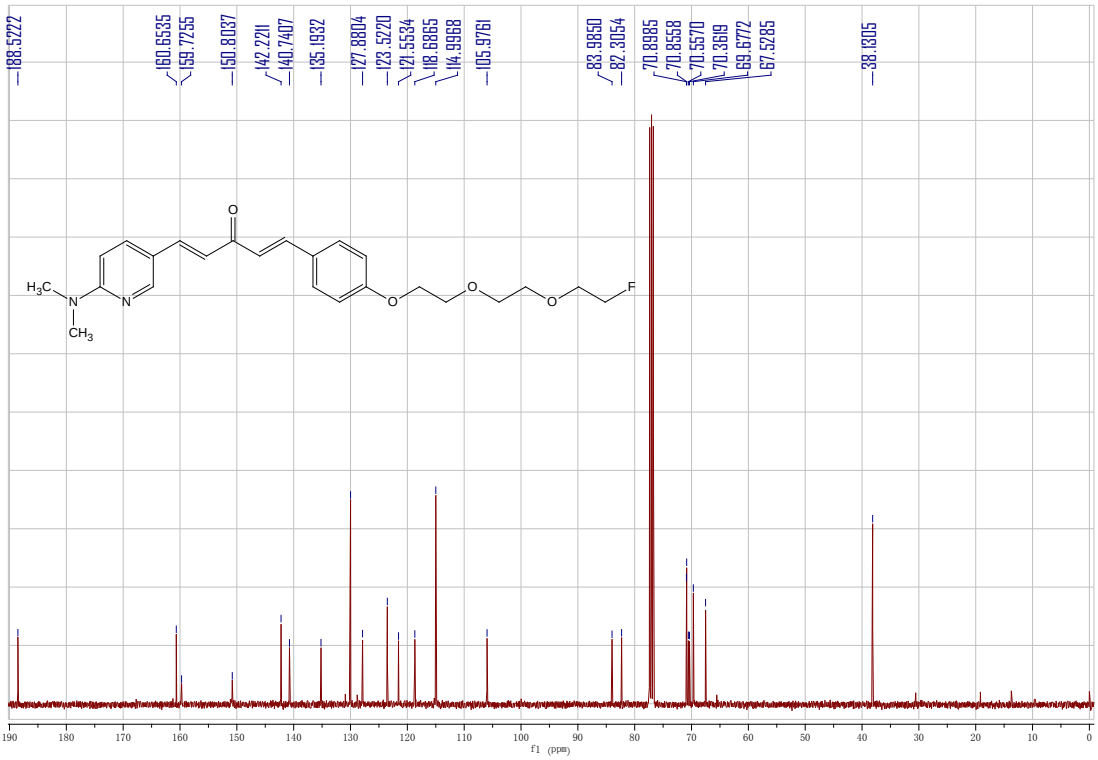

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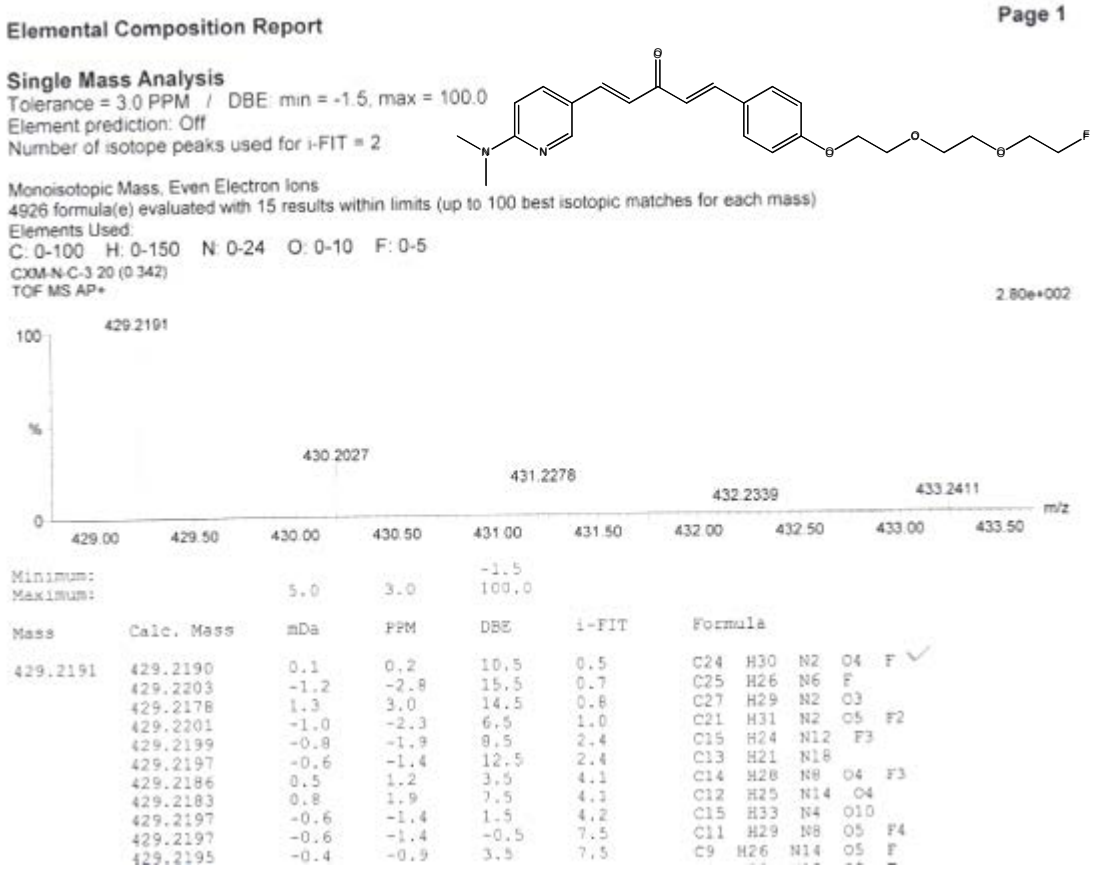

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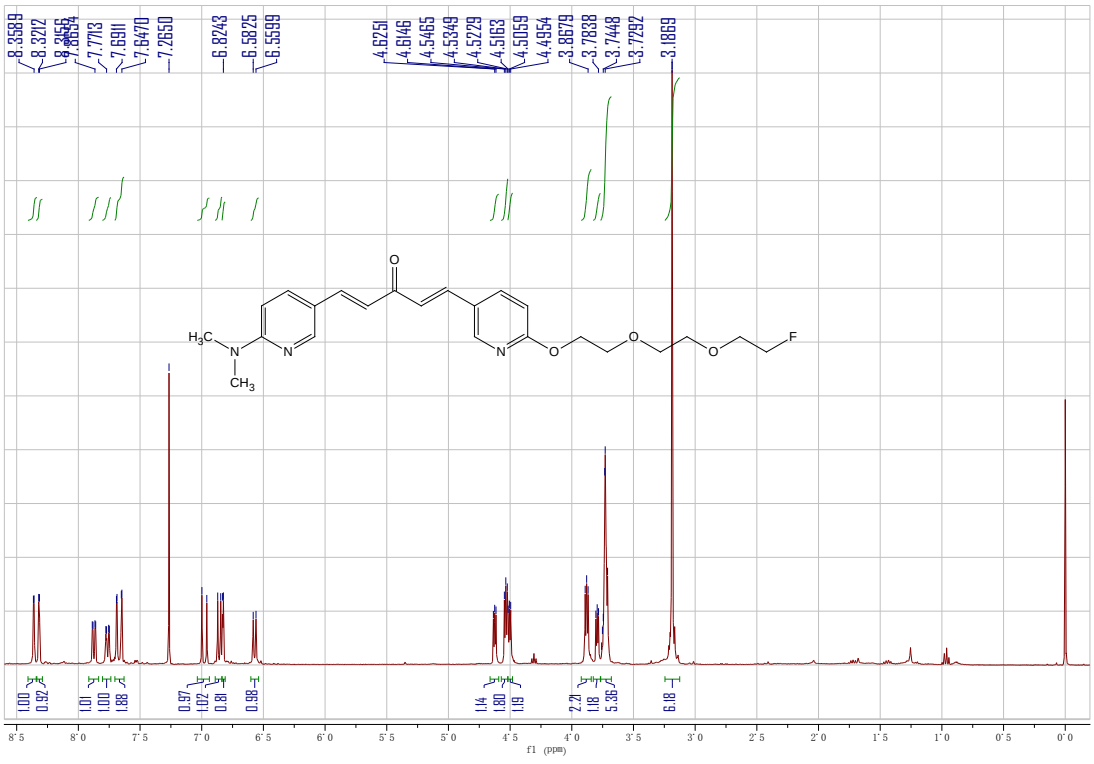

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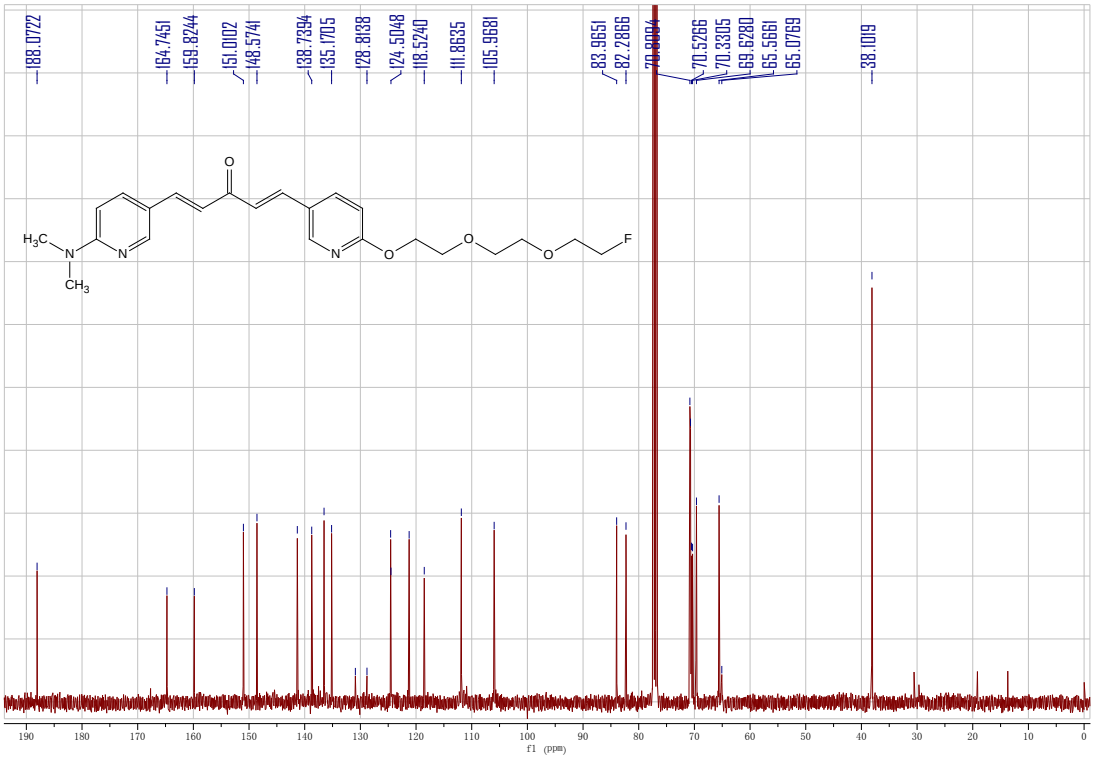

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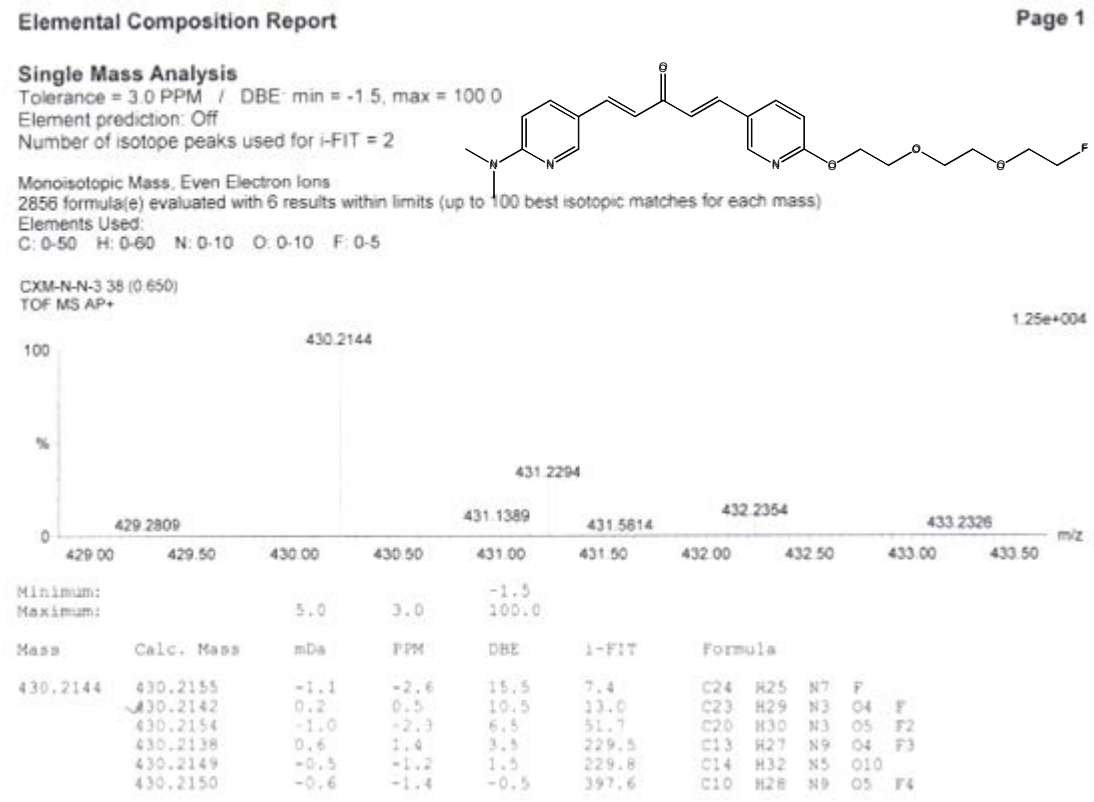

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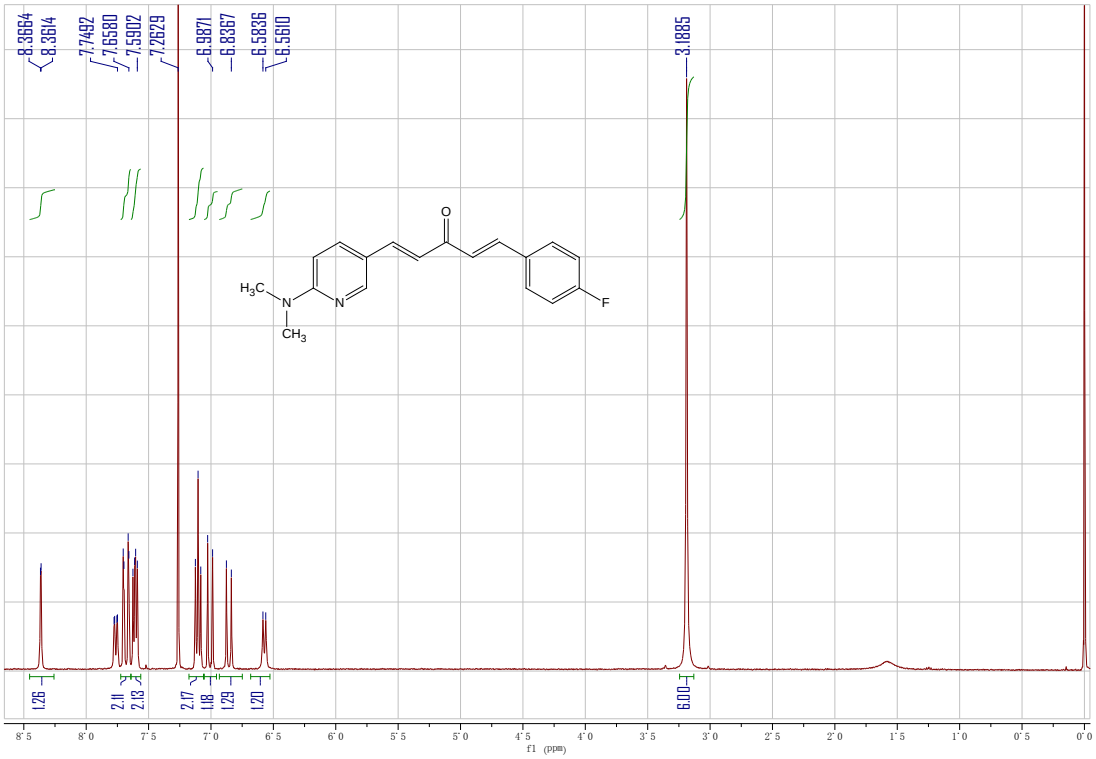

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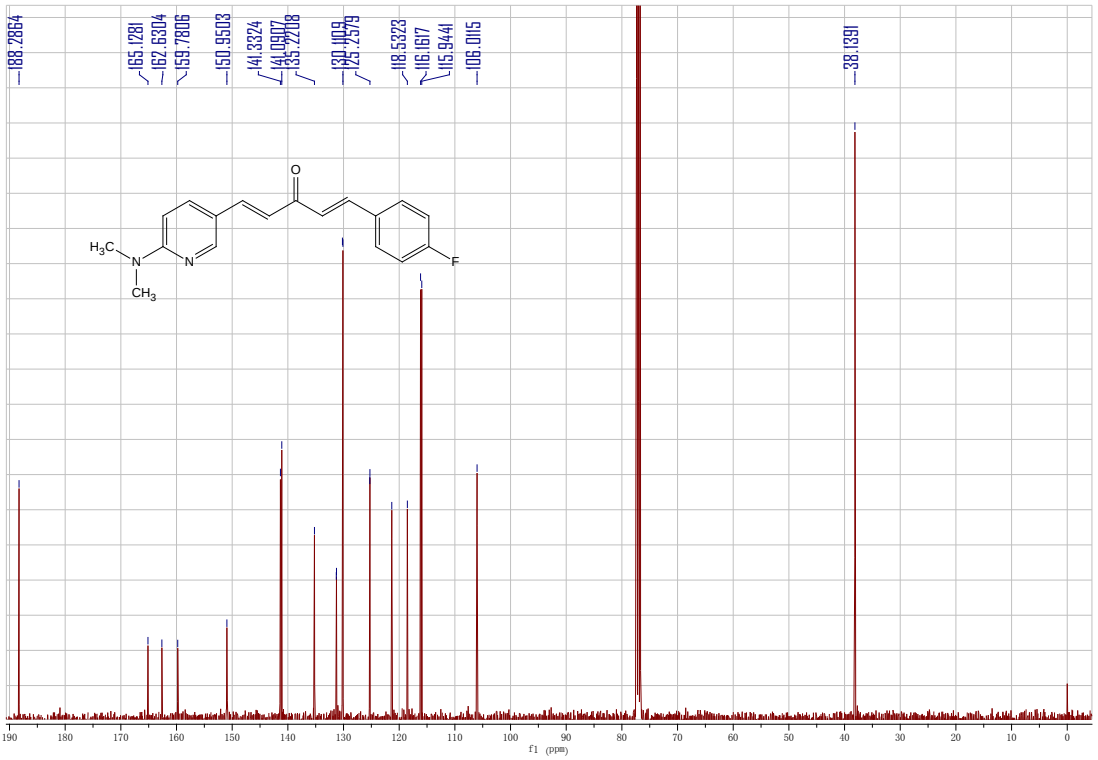

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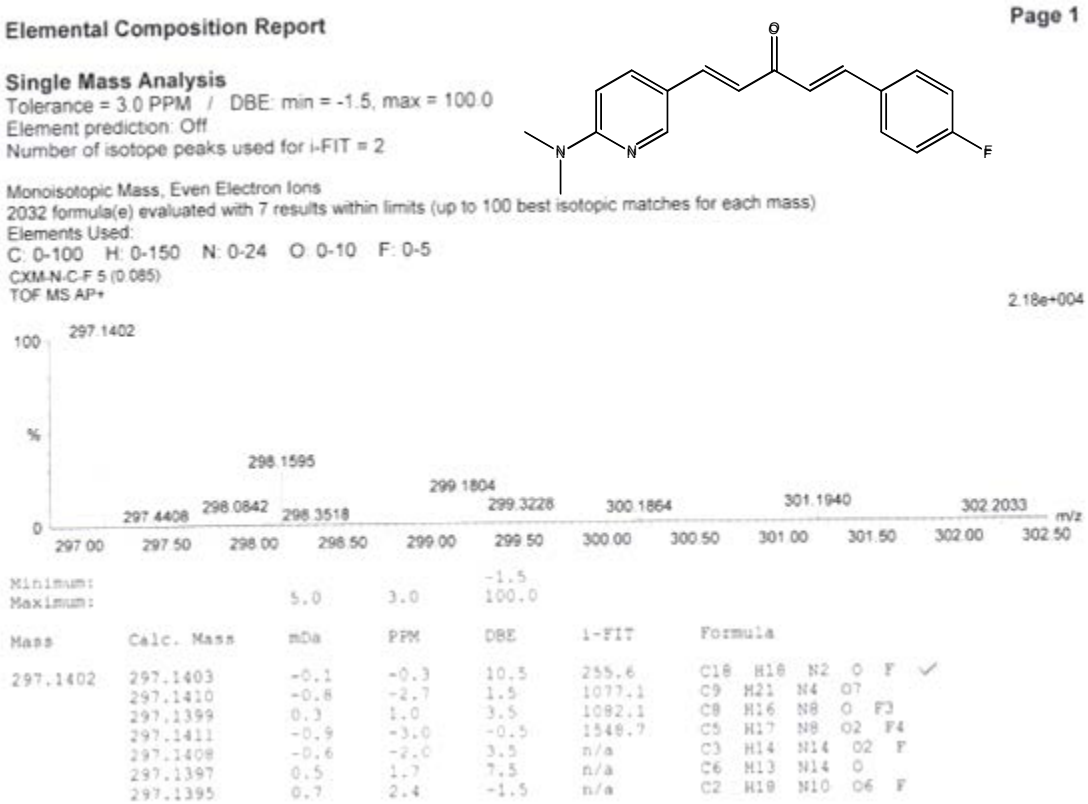

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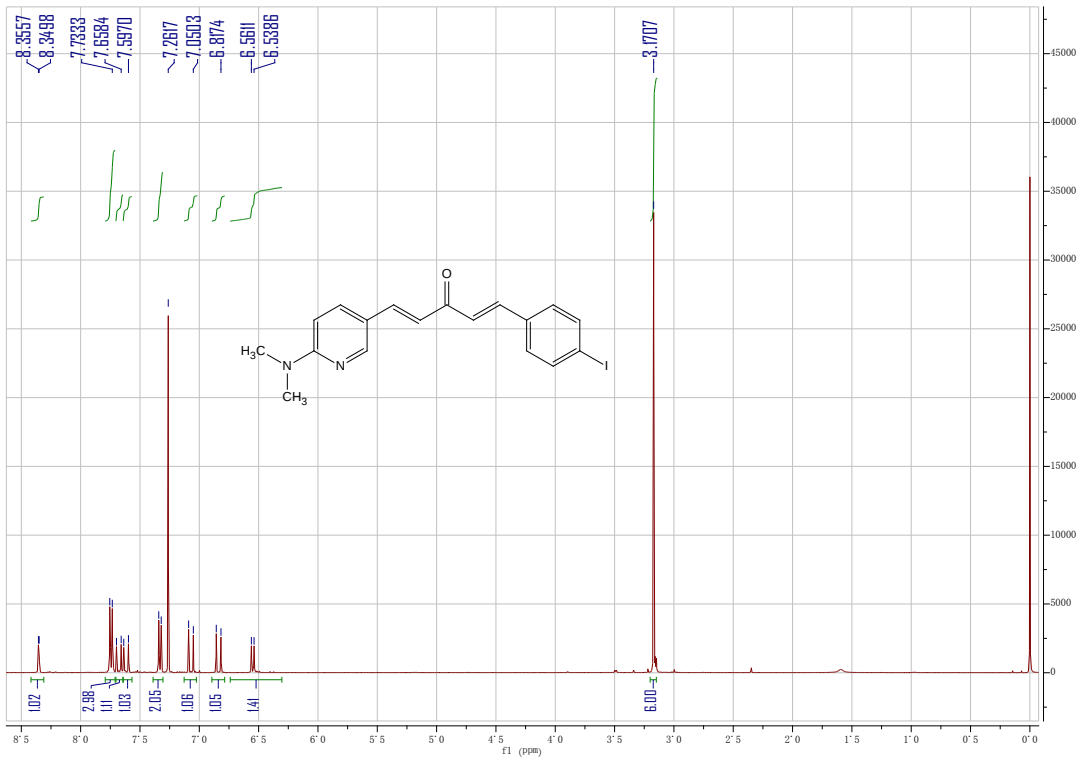

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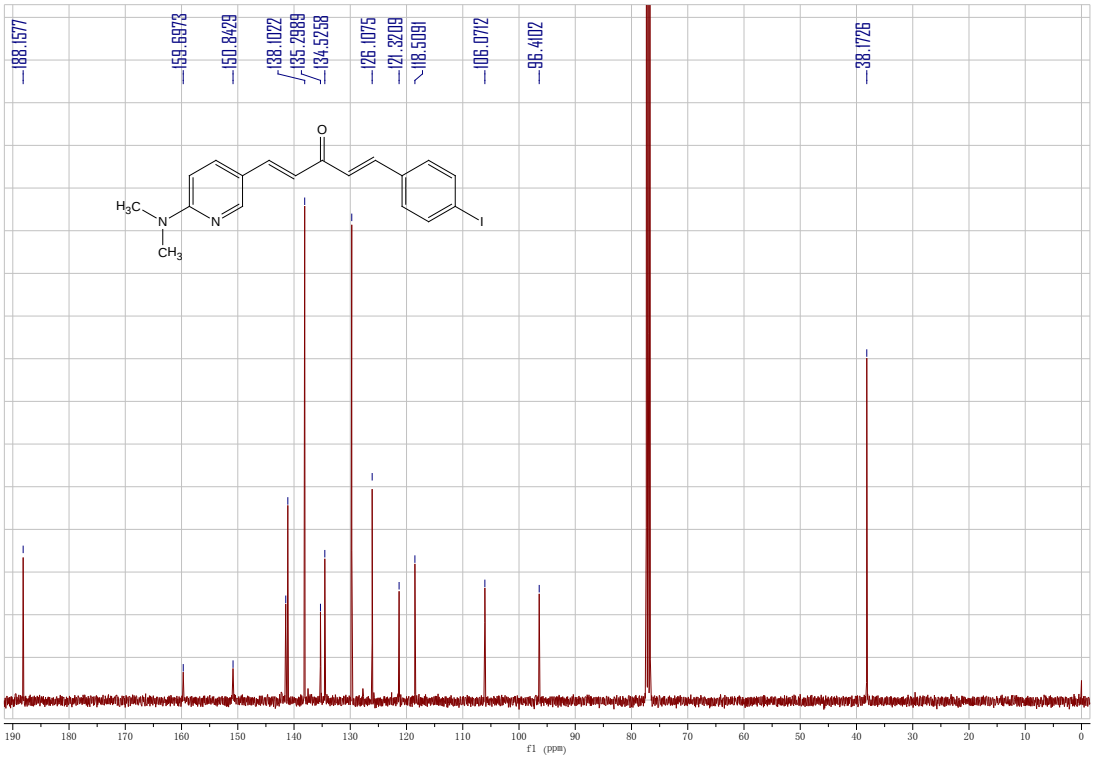
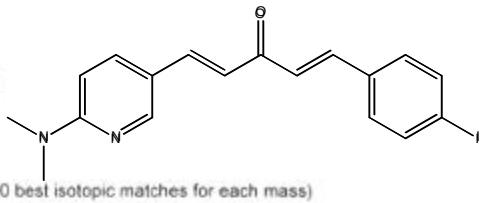


HRMS for compound **19**

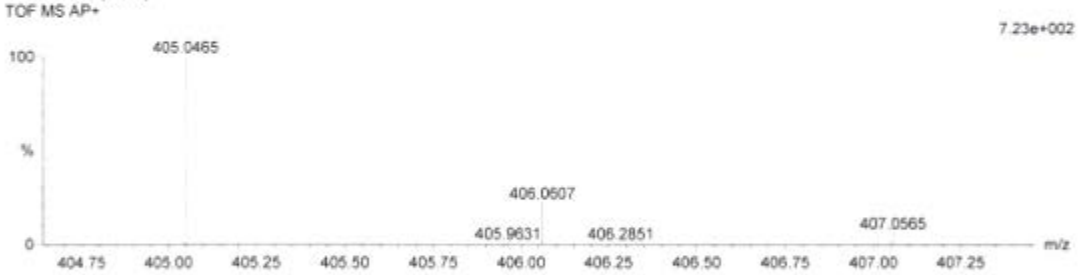
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 3.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2



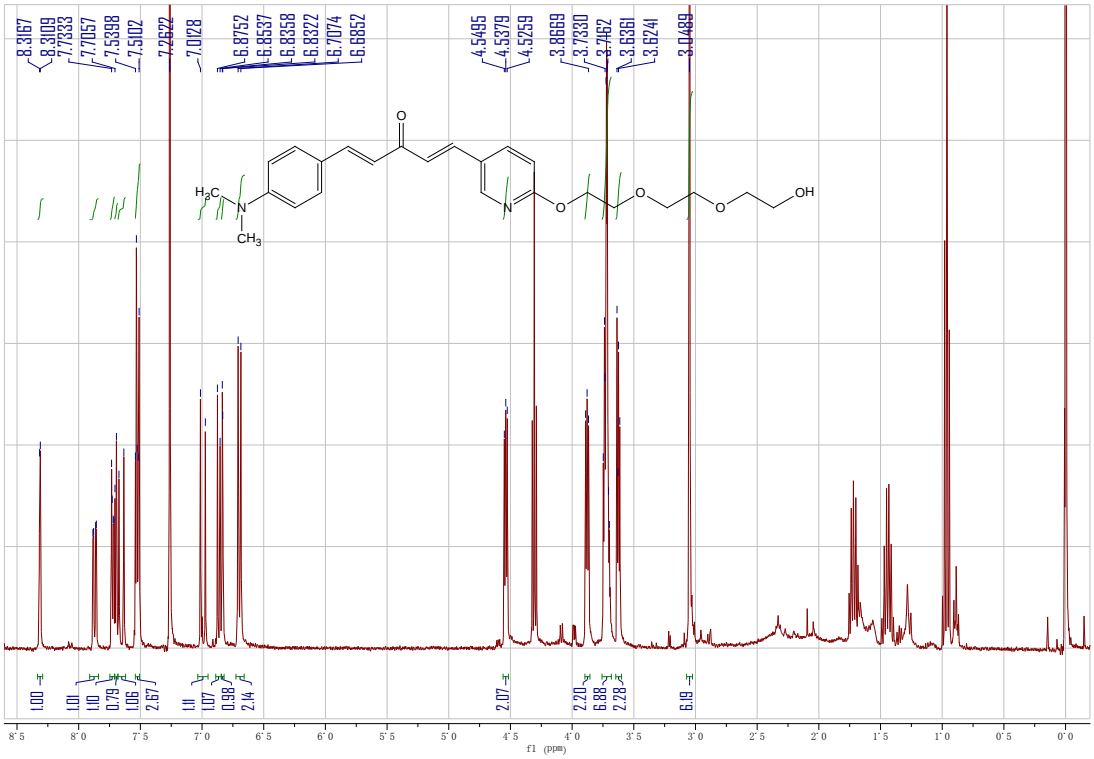
Monoisotopic Mass, Even Electron Ions
1514 formula(e) evaluated with 6 results within limits (up to 100 best isotopic matches for each mass)
Elements Used:
C: 0-100 H: 0-150 N: 0-24 O: 0-10 I: 0-4

CXM-N-C-I 3 (0.051)
TOF MS AP+

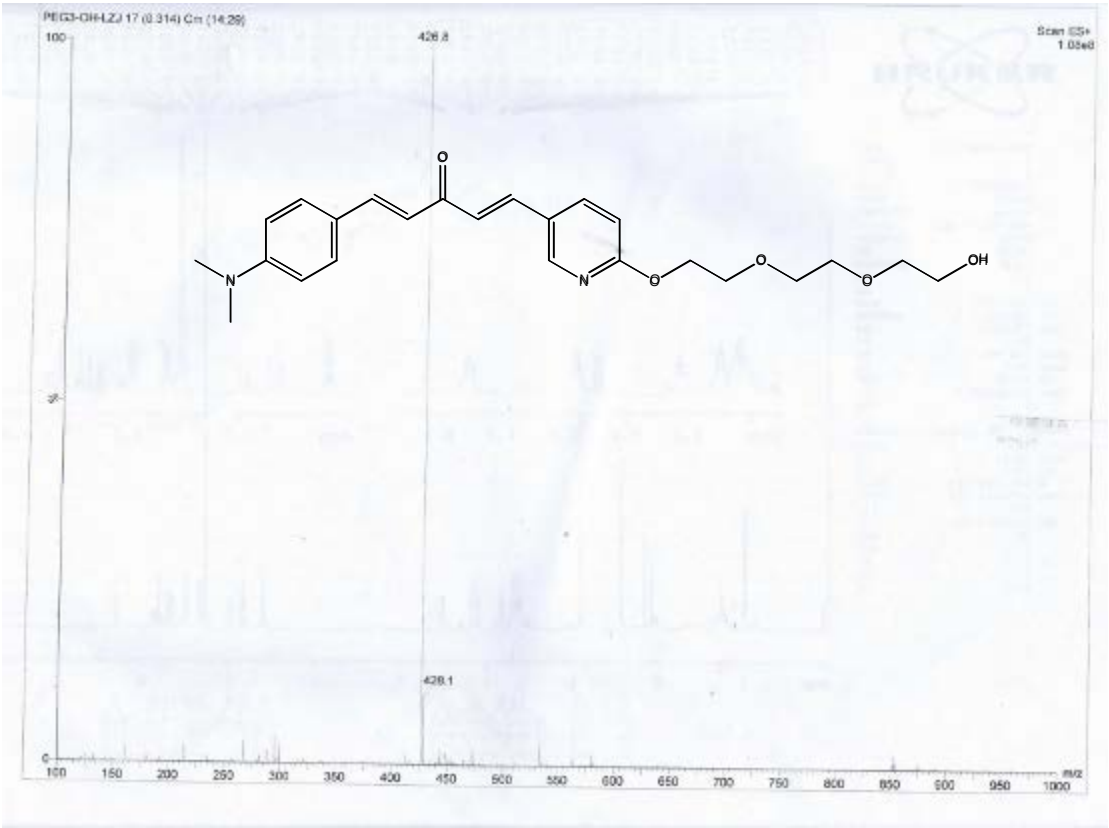


Minimum:				-1.5		
Maximum:		5.0	3.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
405.0465	405.0471	-0.6	-1.5	17.5	0.4	C19 H9 N4 O7
	405.0464	0.1	0.2	10.5	0.4	C18 H10 N2 O I ✓
	405.0458	0.7	1.7	23.5	0.6	C16 H N14 O
	405.0476	-1.1	-2.7	10.5	20.4	C4 H5 N16 O8
	405.0469	-0.4	-1.0	3.5	28.3	C3 H14 N14 O2 I
	405.0456	0.9	2.2	-1.5	39.9	C2 H10 N10 O6 I

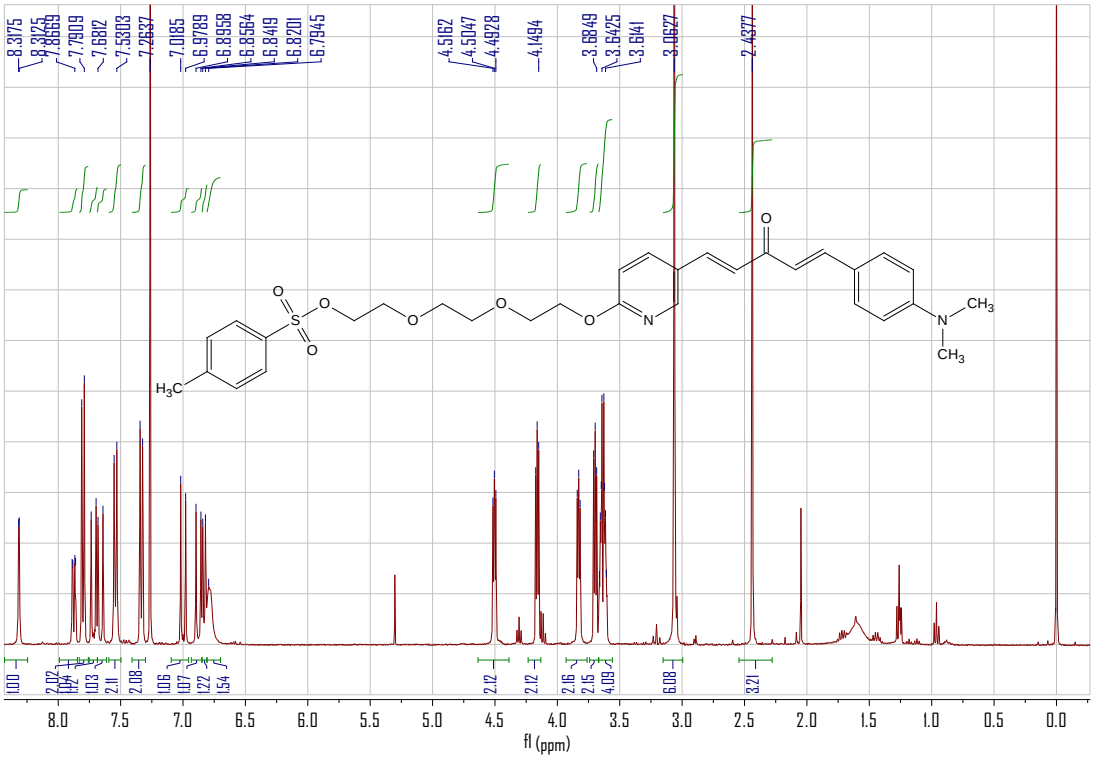
^{1}H-NMR for compound **20**



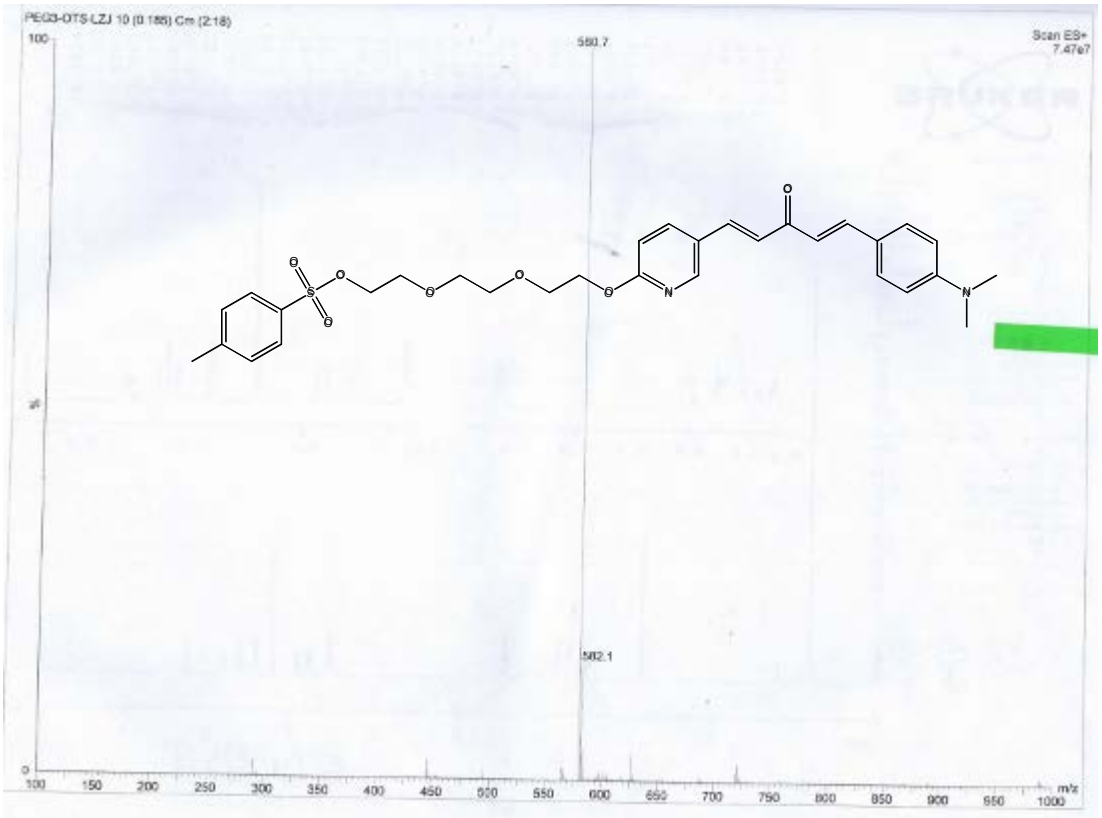
MS for compound **20**



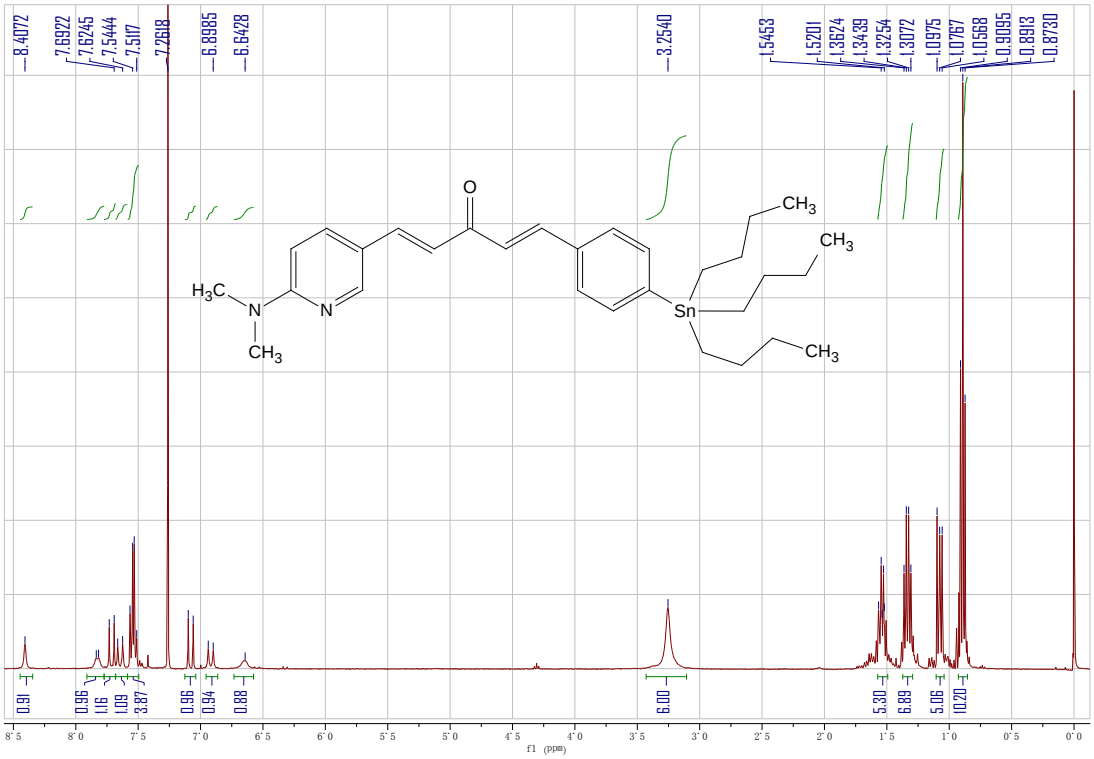
^{1}H-NMR for compound **21**



MS for compound **21**



^{1}H-NMR for compound **22**



MS for compound