

SUPPLEMENTARY INFORMATION

Radiolabeled Pyridinyl Analogues of Dibenzylideneacetone as β -Amyloid Imaging Probes

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1. Purity of key target compounds

Compounds	Flow rate (mL/min)	Mobile phase (CH ₃ CN %)	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 [¹⁸F]17a, [¹⁸F]18 and [¹²⁵I]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

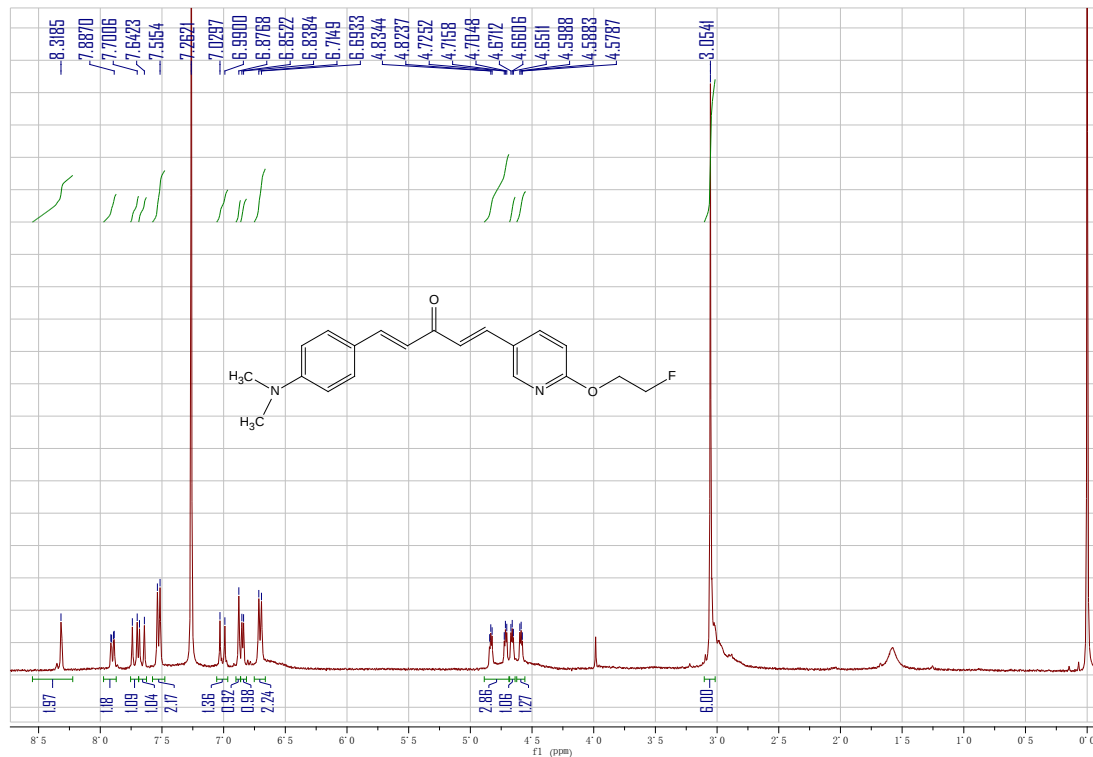
Intestine ^b	5.92 ± 0.79	15.09 ± 2.27	24.05 ± 7.87	36.62 ± 8.28
[¹²⁵ I] 19 (Log <i>D</i> = 3.31 ± 0.31)				
Blood	3.71 ± 0.75	1.80 ± 0.16	1.33 ± 0.21	1.02 ± 0.22
Brain	2.06 ± 0.16	1.72 ± 0.15	1.36 ± 0.18	1.04 ± 0.17
Heart	4.01 ± 0.19	2.13 ± 0.19	1.42 ± 0.18	1.09 ± 0.31
Liver	27.58 ± 1.55	23.98 ± 1.05	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 ± 0.34	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.

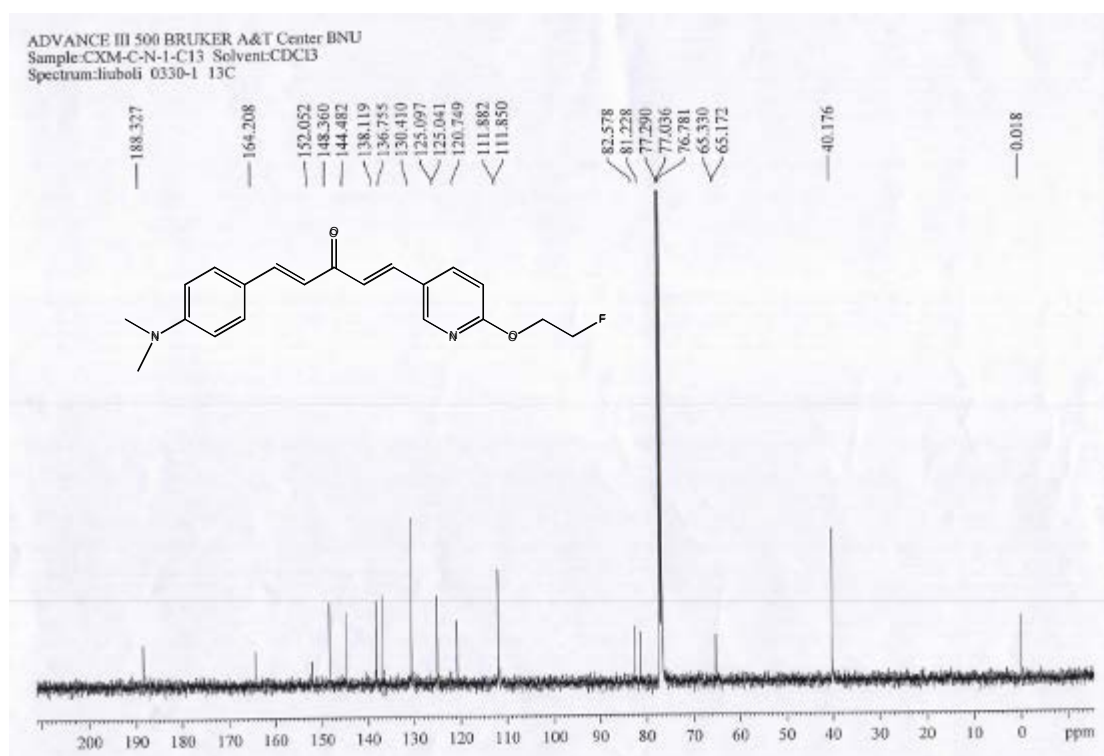
^b Expressed as % injected dose per organ.

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

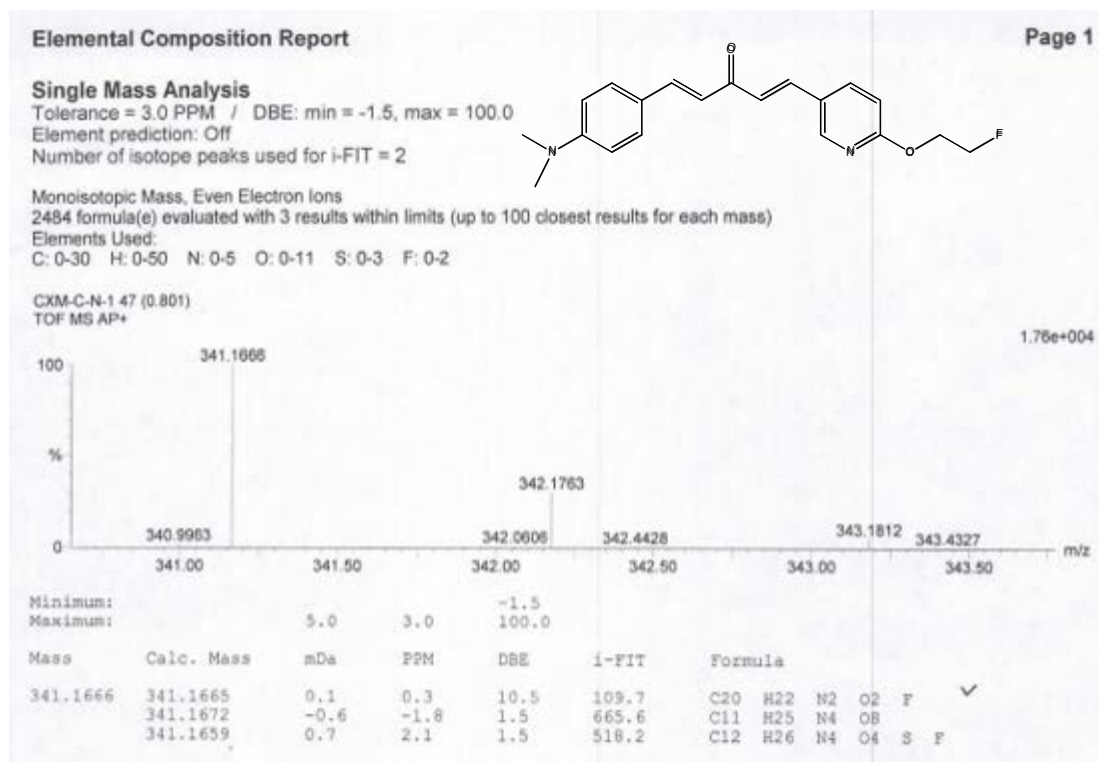
¹H-NMR for compound **15a**



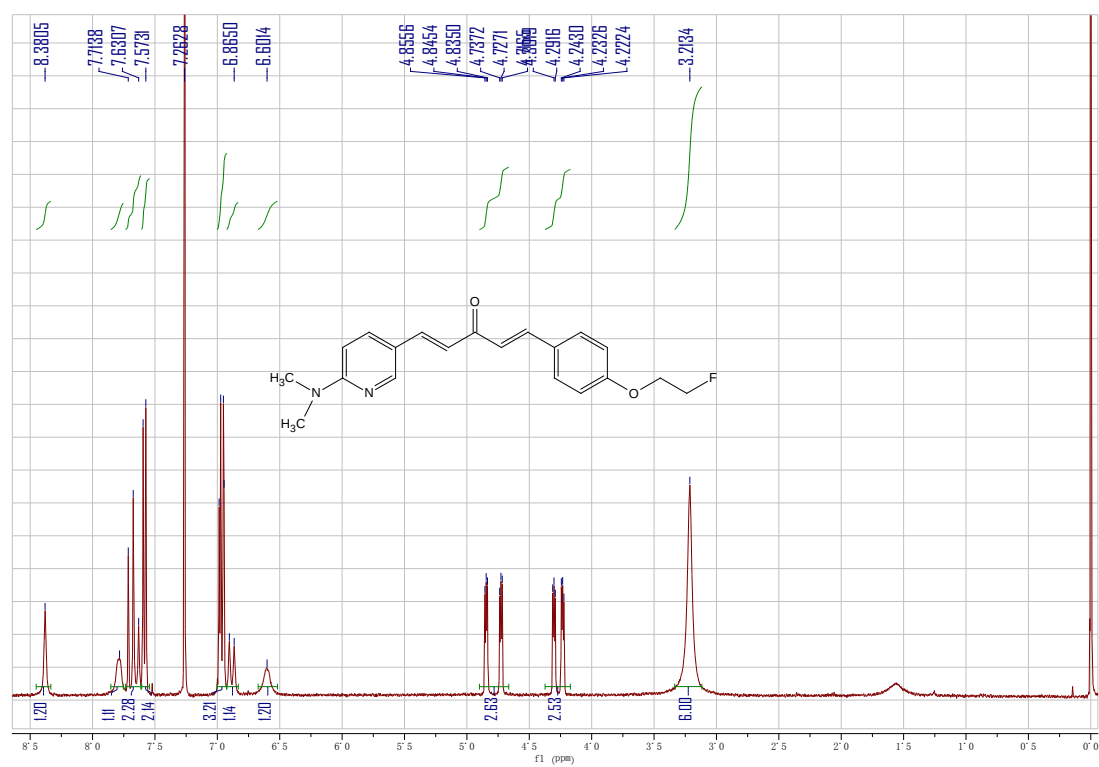
¹³C-NMR for compound **15a**



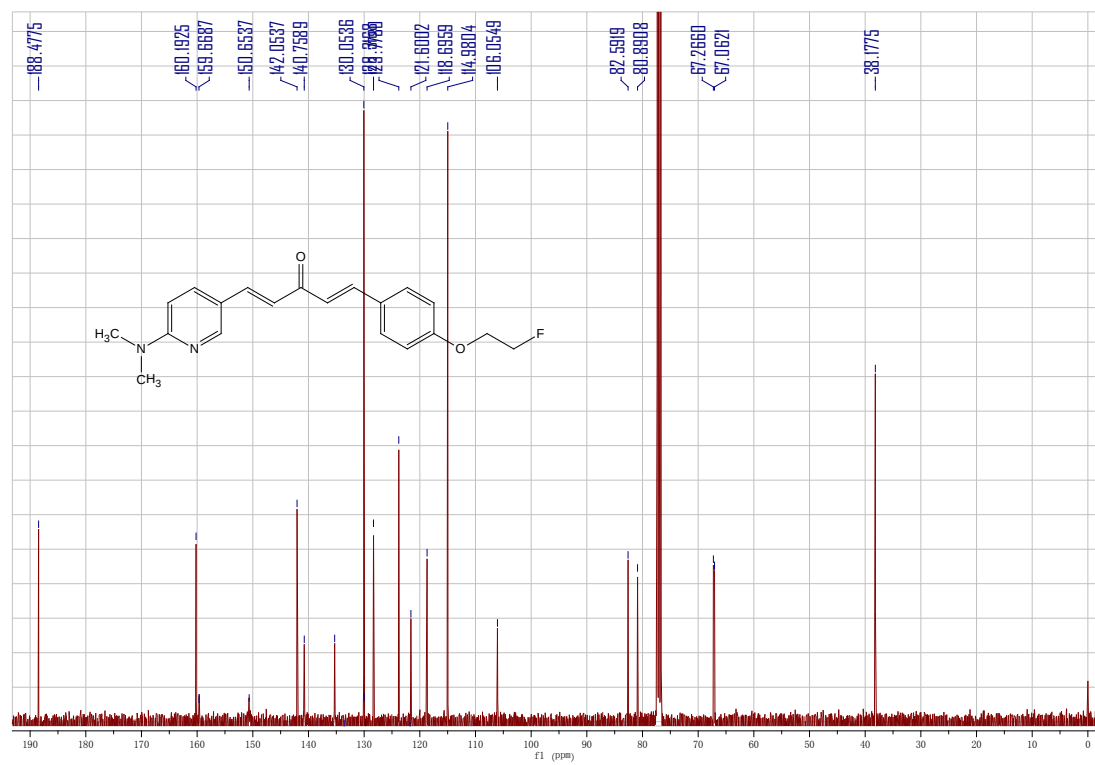
HRMS for compound **15a**



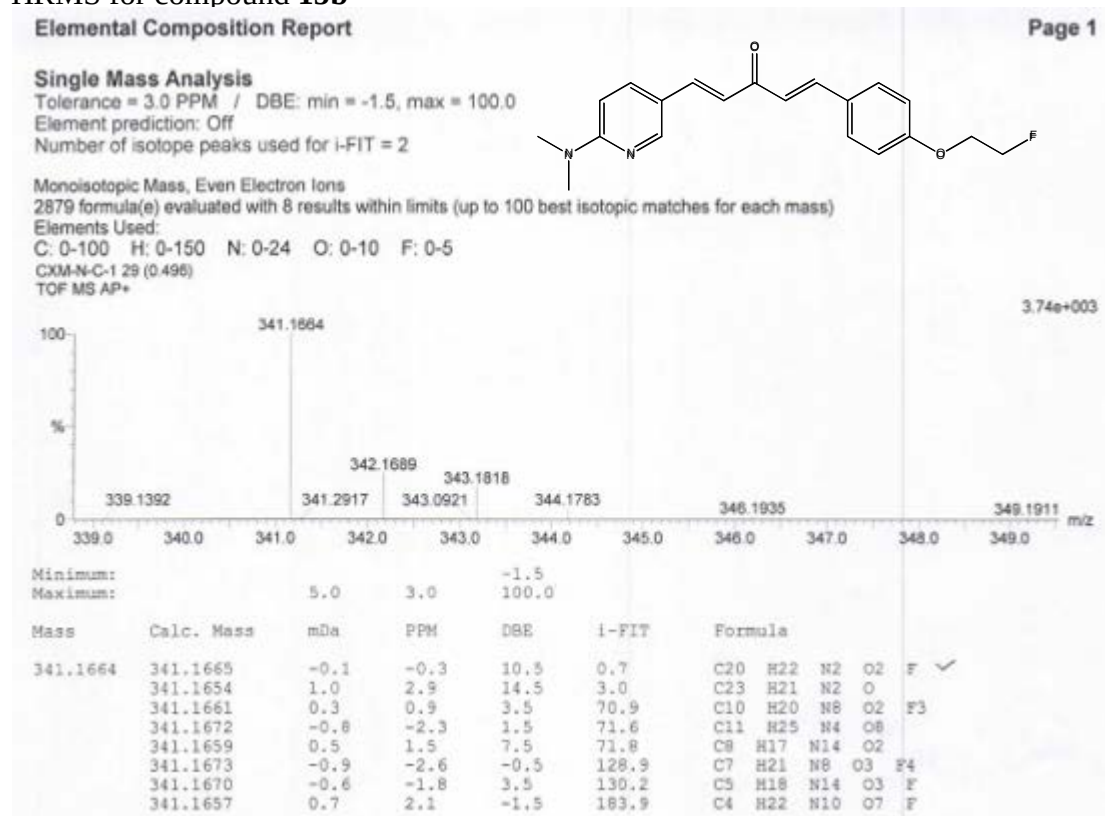
¹H-NMR for compound **15b**



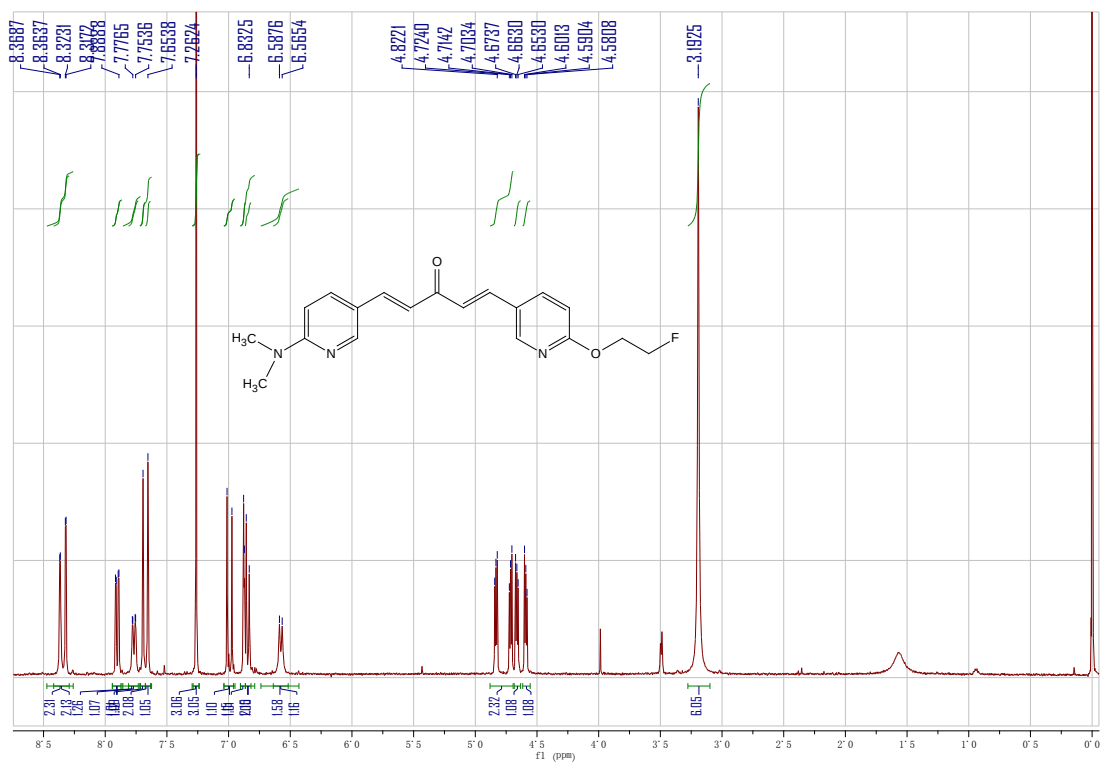
¹³C-NMR for compound **15b**



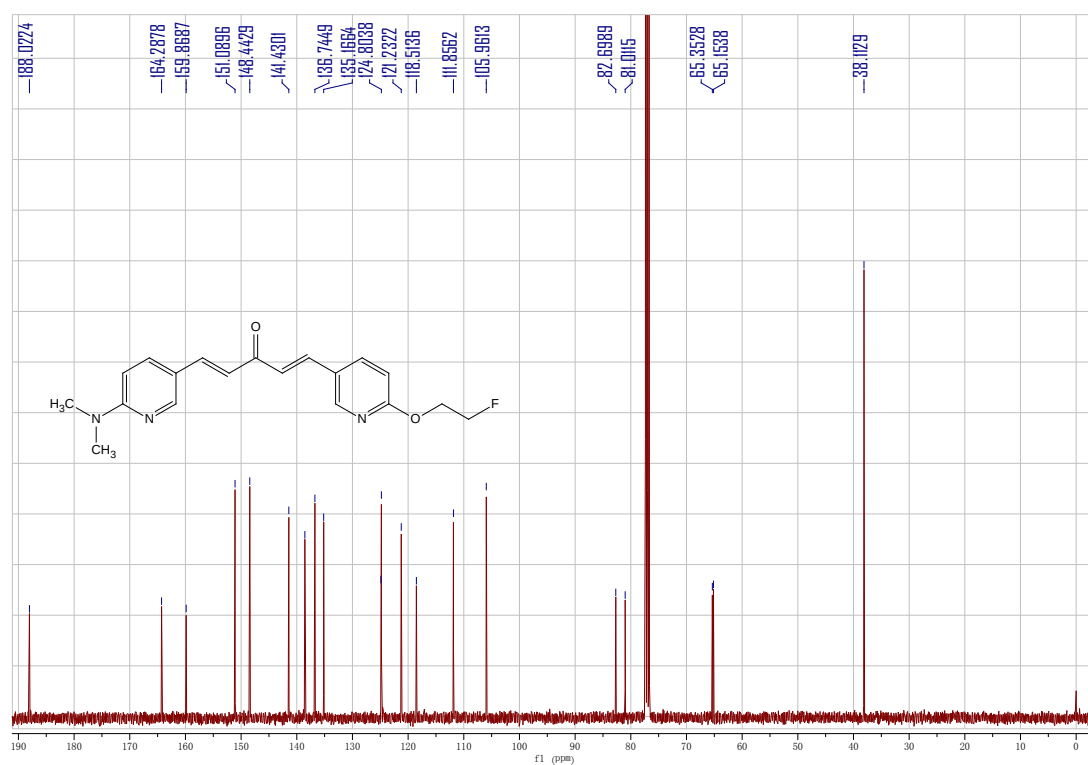
HRMS for compound 15b



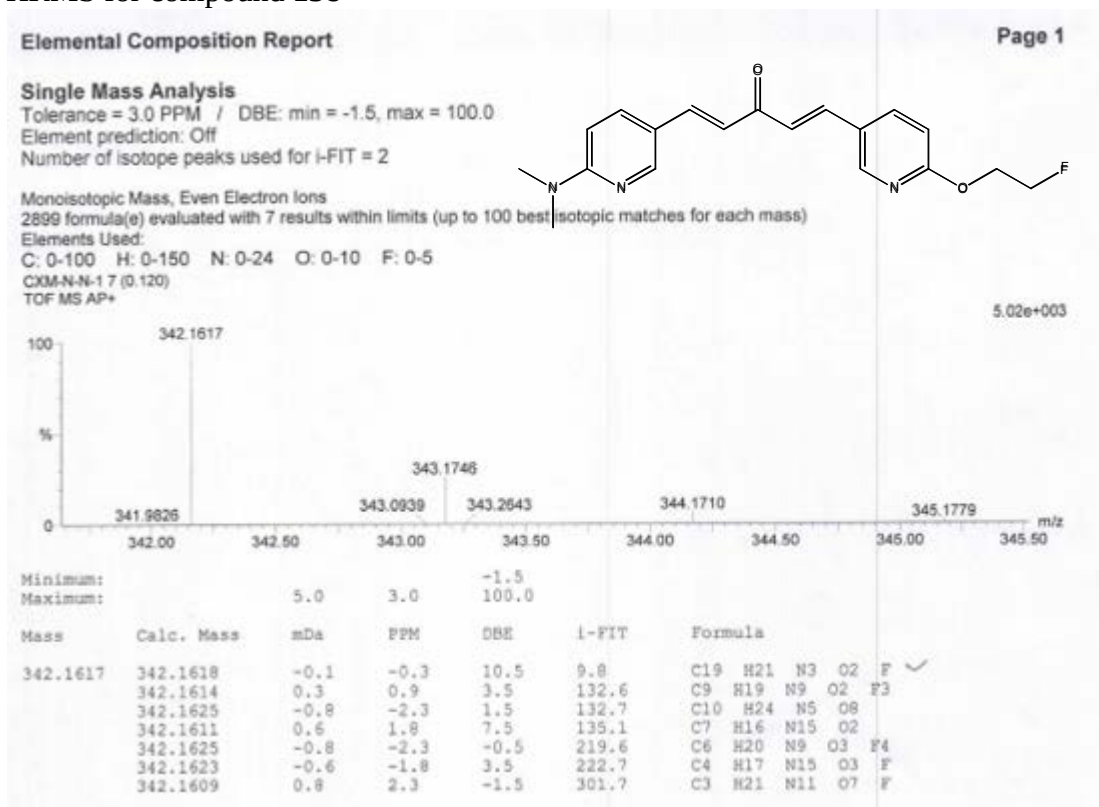
¹H-NMR for compound 15c



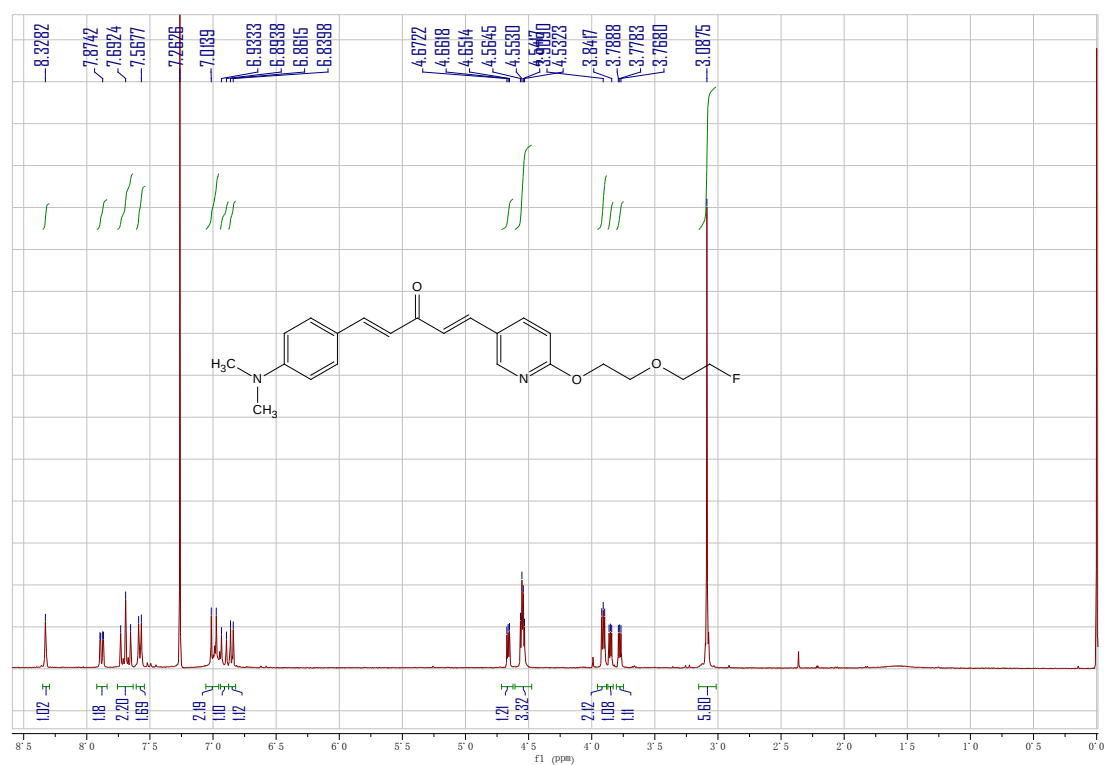
^{13}C -NMR for compound **15c**



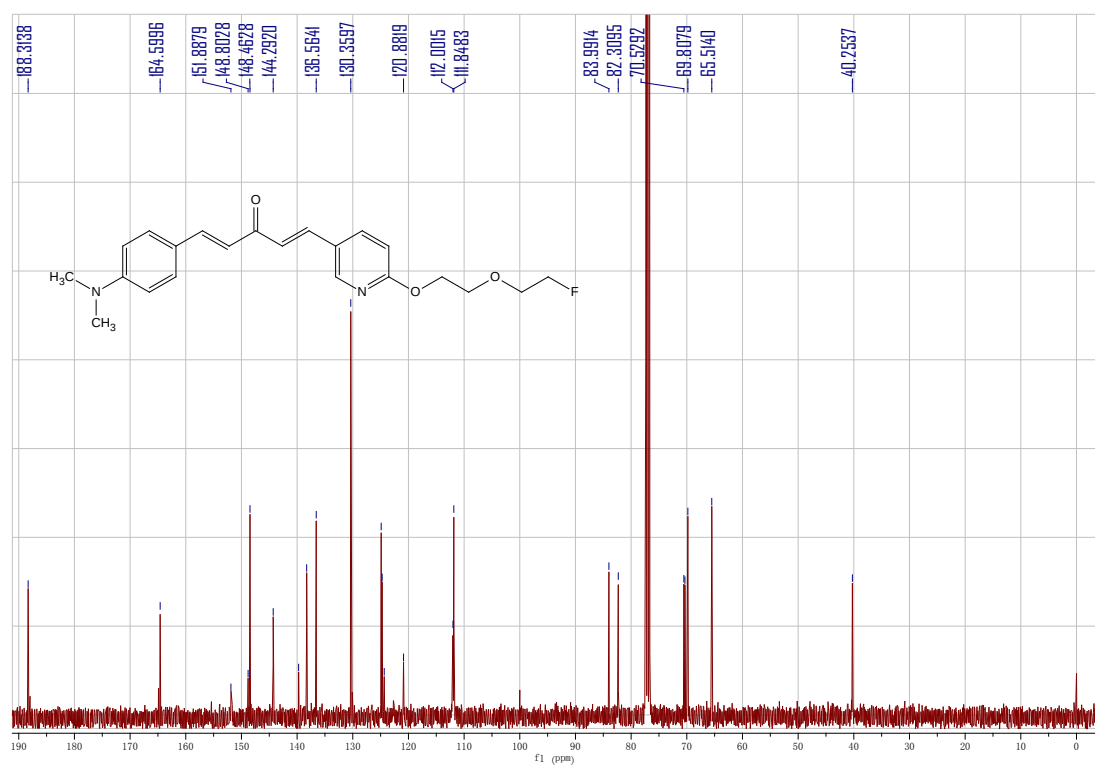
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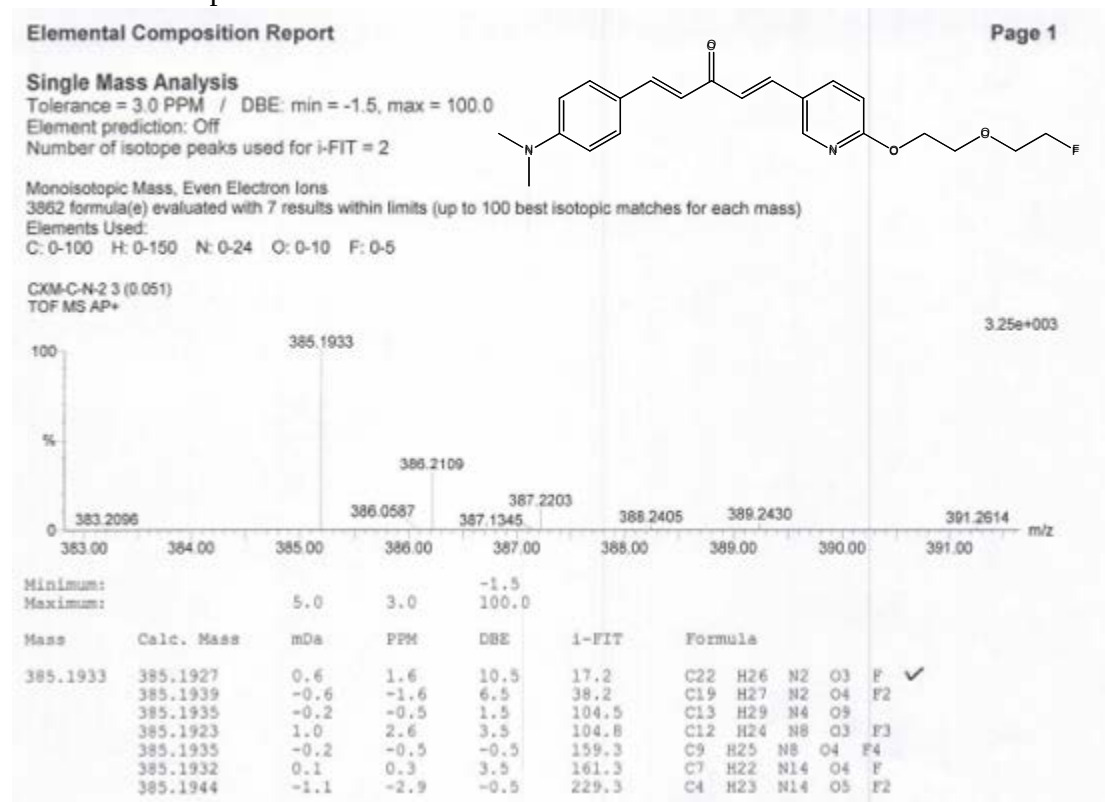
¹H-NMR for compound **16a**



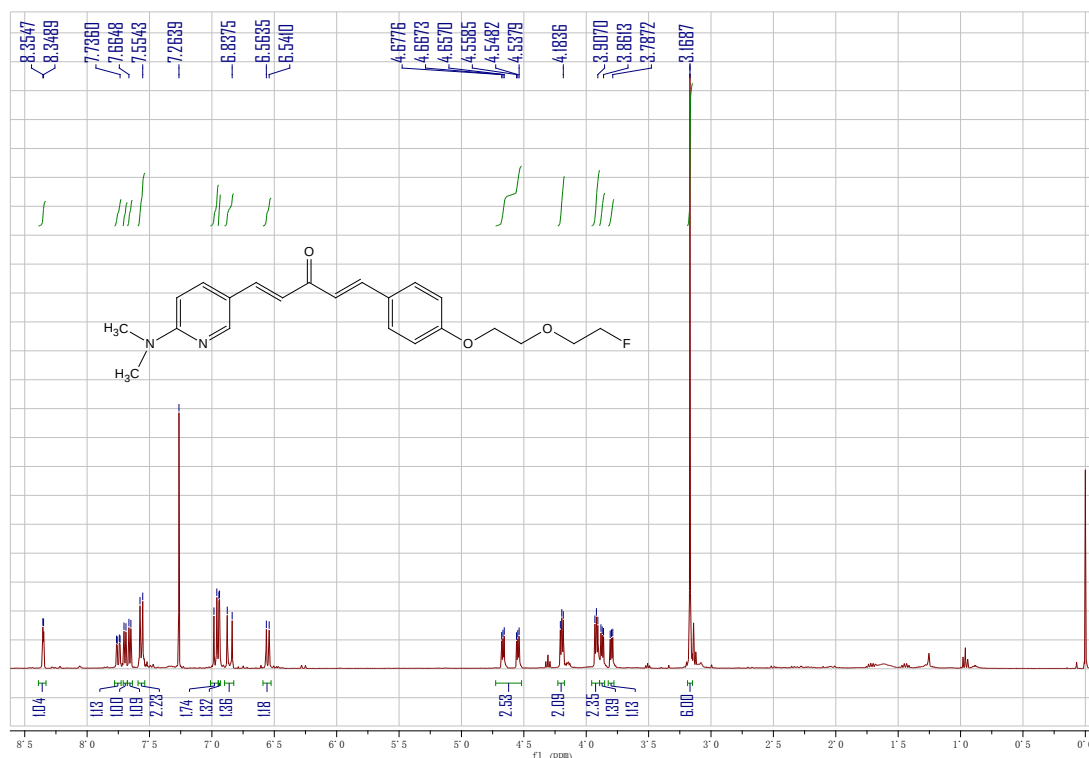
¹³C-NMR for compound **16a**



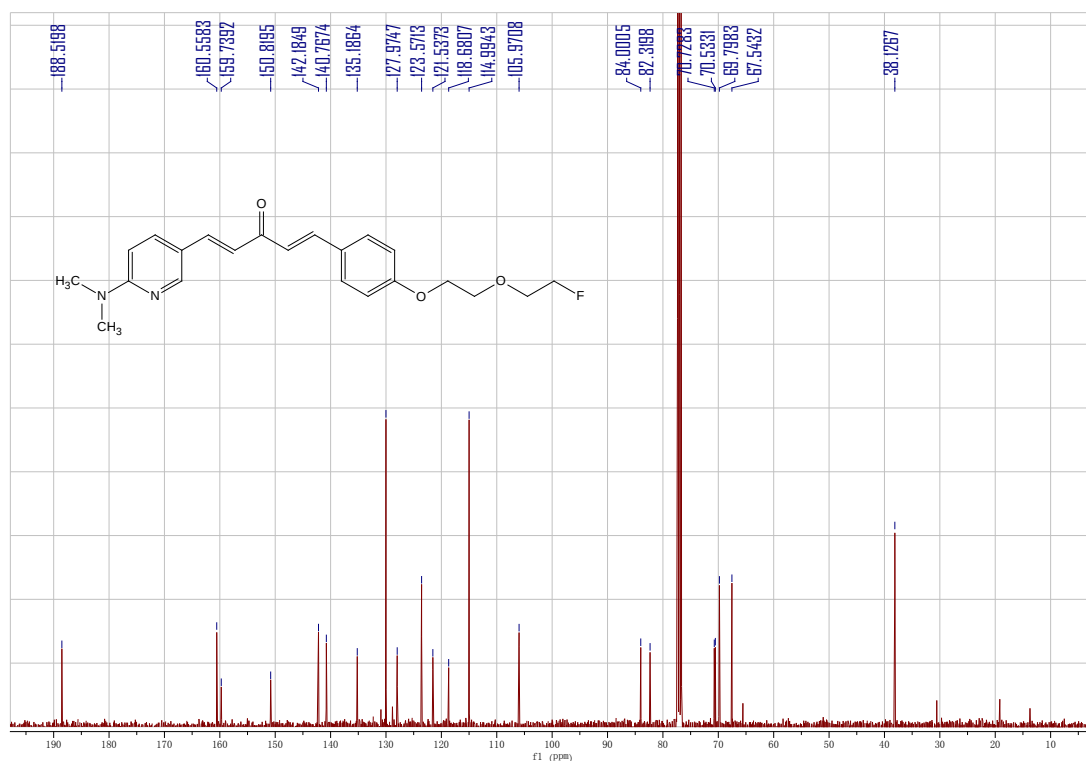
HRMS for compound 16a



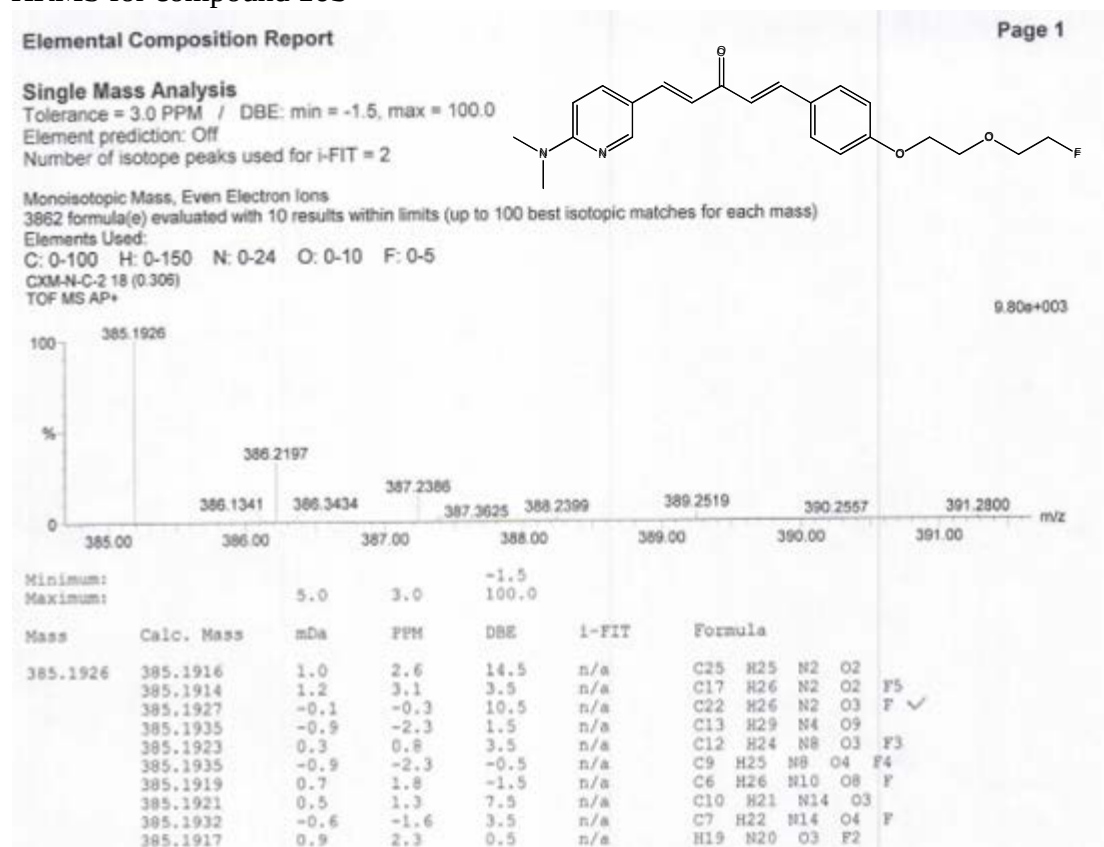
¹H-NMR for compound 16b



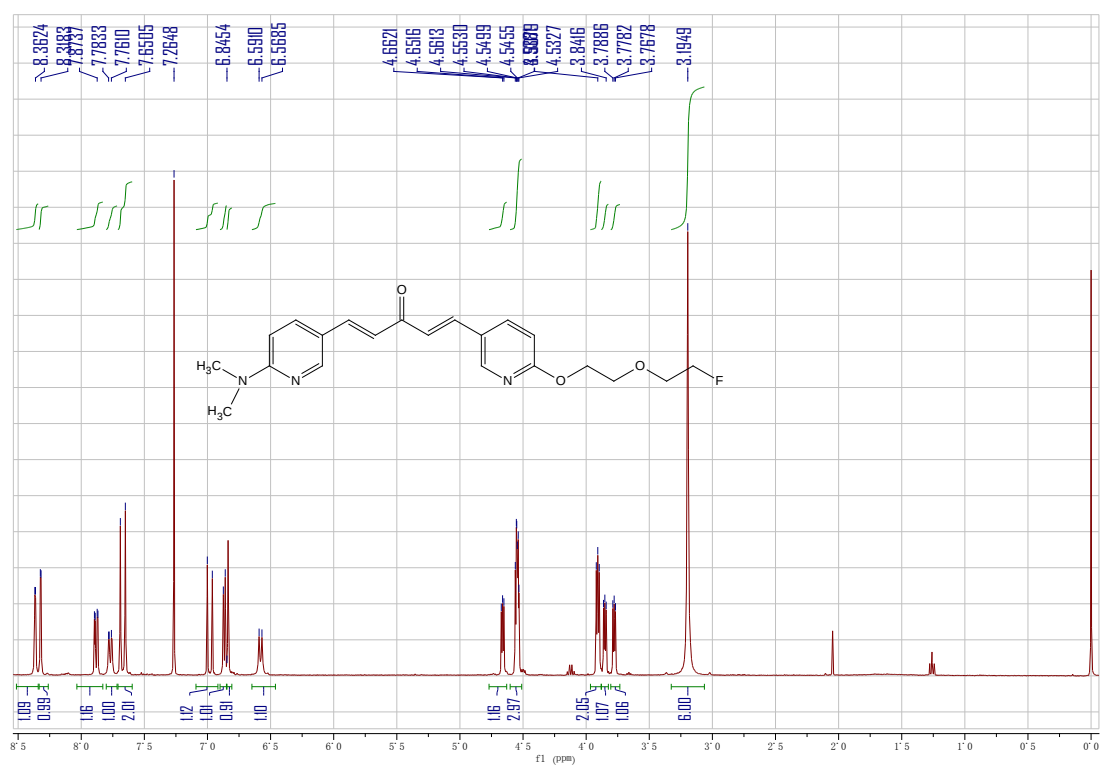
¹³C-NMR for compound **16b**



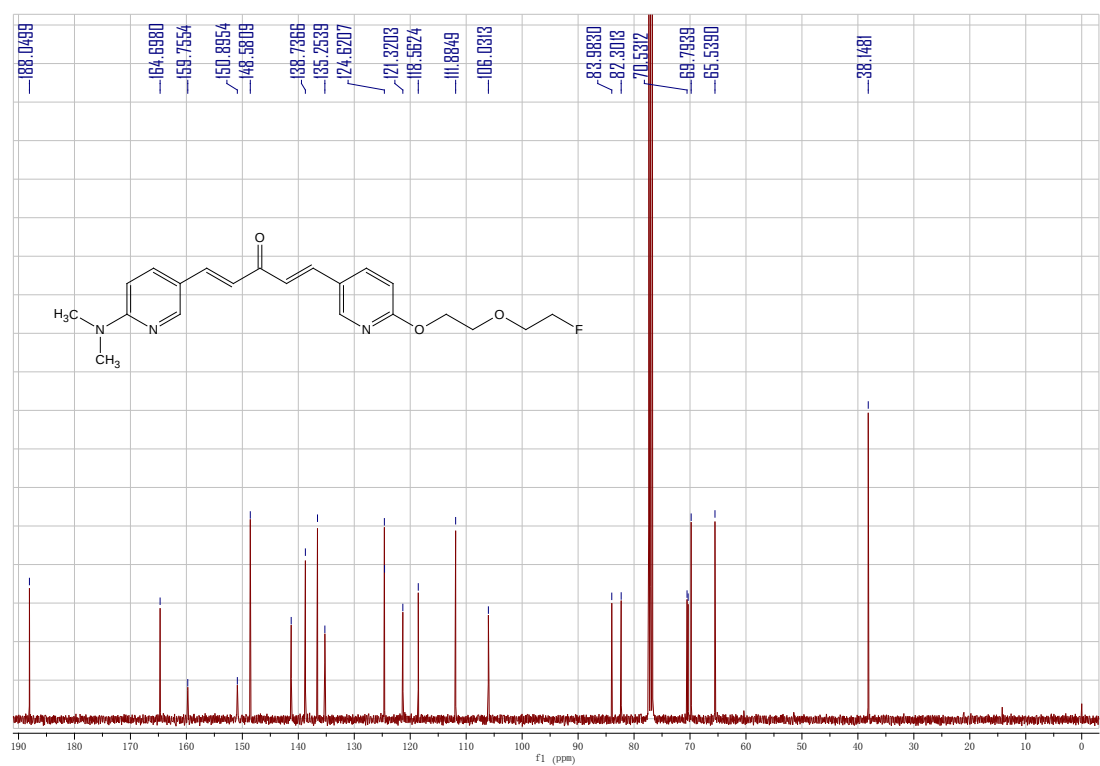
HRMS for compound **16b**



¹H-NMR for compound **16c**



¹³C-NMR for compound **16c**



HRMS for compound 16c

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

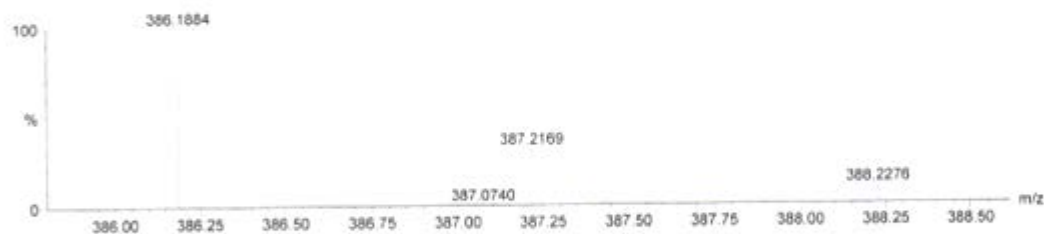
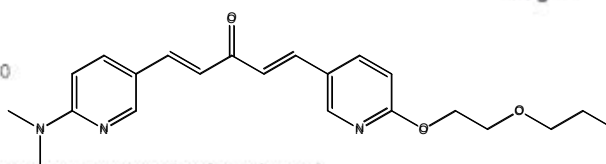
3887 formula(e) evaluated with 7 results within limits (up to 100 best isotopic matches for each mass)

Elements Used:

C: 0-100 H: 0-150 N: 0-24 O: 0-10 F: 0-5

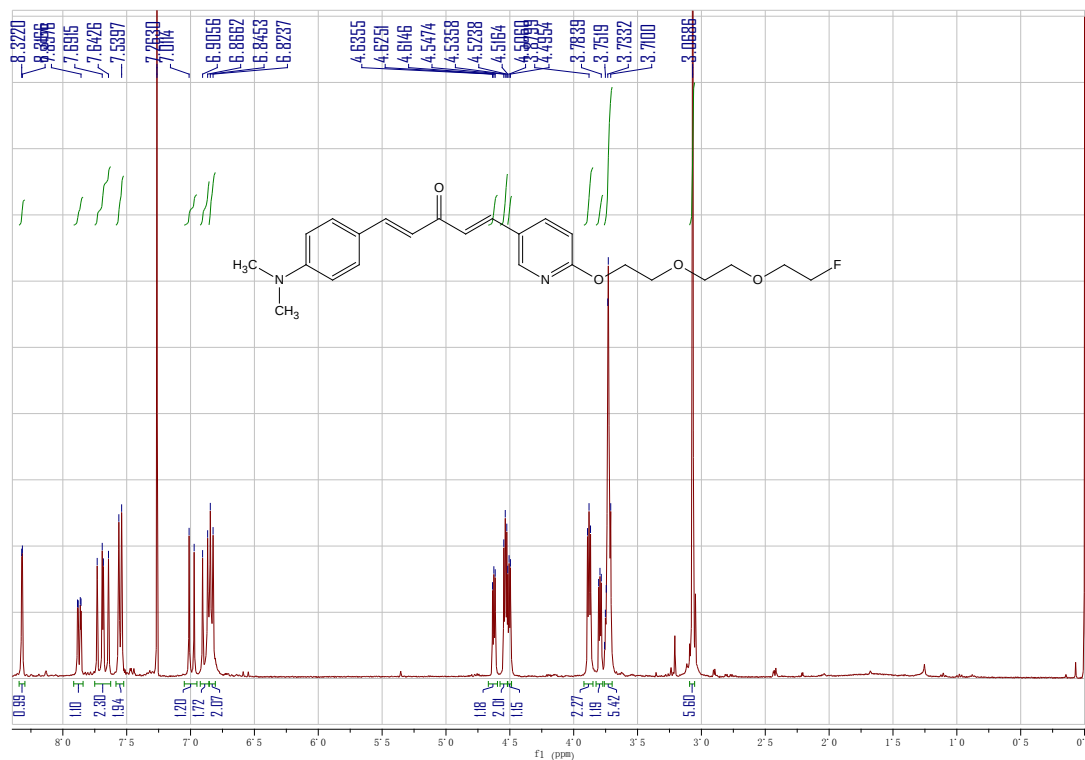
CXMM-N-2 16 (0.273)

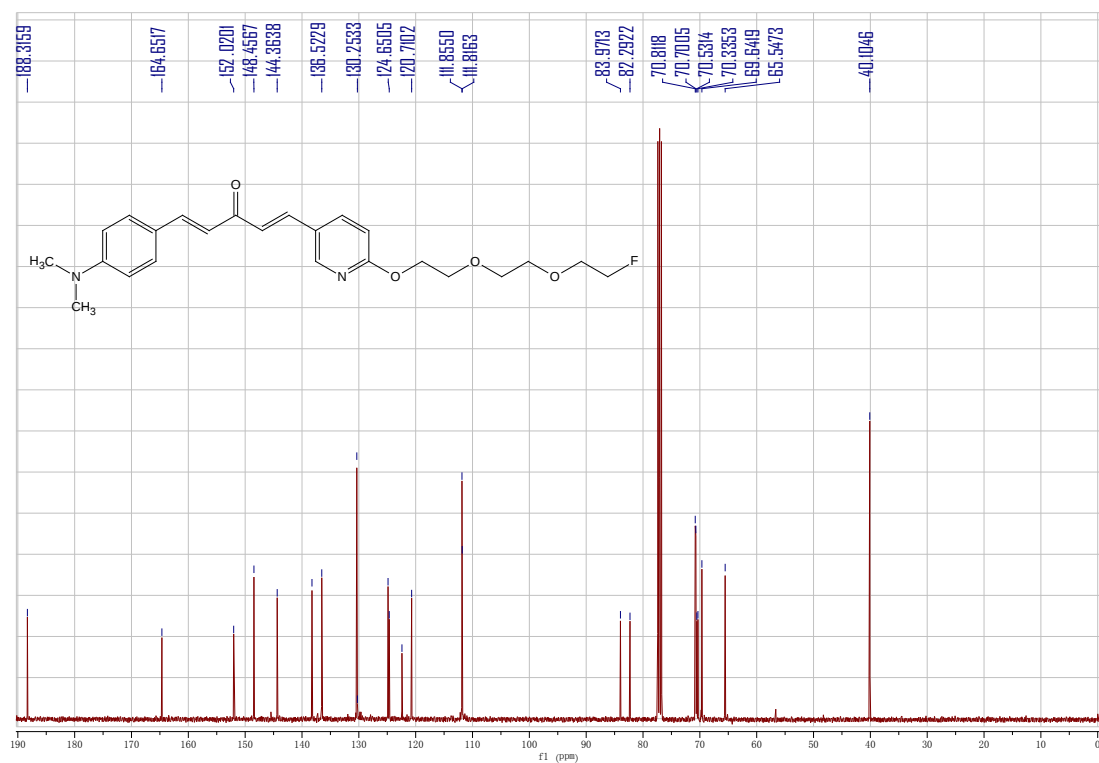
TOF MS AP+



Minimum:				-1.5		
Maximum:	5.0	3.0		100.0		
Mass	Calc. Mass	mDa	PPM	DBE	I-FIT	Formula
386.1884	386.1887	-0.3	-0.8	1.5	n/a	C12 H28 N5 O9
	386.1876	0.8	2.1	3.5	n/a	C11 H23 N9 O3 F3
	386.1887	-0.3	-0.8	-0.5	n/a	C8 H24 N9 O4 F4
	386.1874	1.0	2.6	7.5	n/a	C9 H20 N15 O3
	386.1885	-0.1	-0.3	3.5	n/a	C6 H21 N15 O4 F
	386.1880	0.4	1.0	10.5	n/a	C21 H25 N3 O3 F
	386.1891	-0.7	-1.8	6.5	n/a	C18 H26 N3 O4 F2

¹H-NMR for compound 17a



^{13}C -NMR for compound **17a**

HRMS for compound **17a**

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

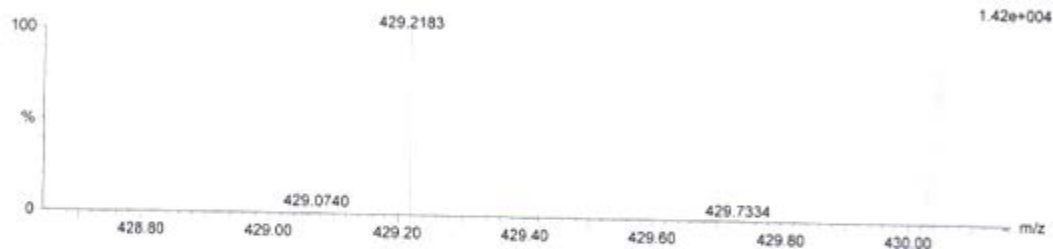
5664 formula(e) evaluated with 16 results within limits (up to 50 closest results for each mass)
Elements Used:

Elements Used:

C: 0-50 H: 0-60 N: 0-5 O: 0-10 F: 0-5 S: 0-3

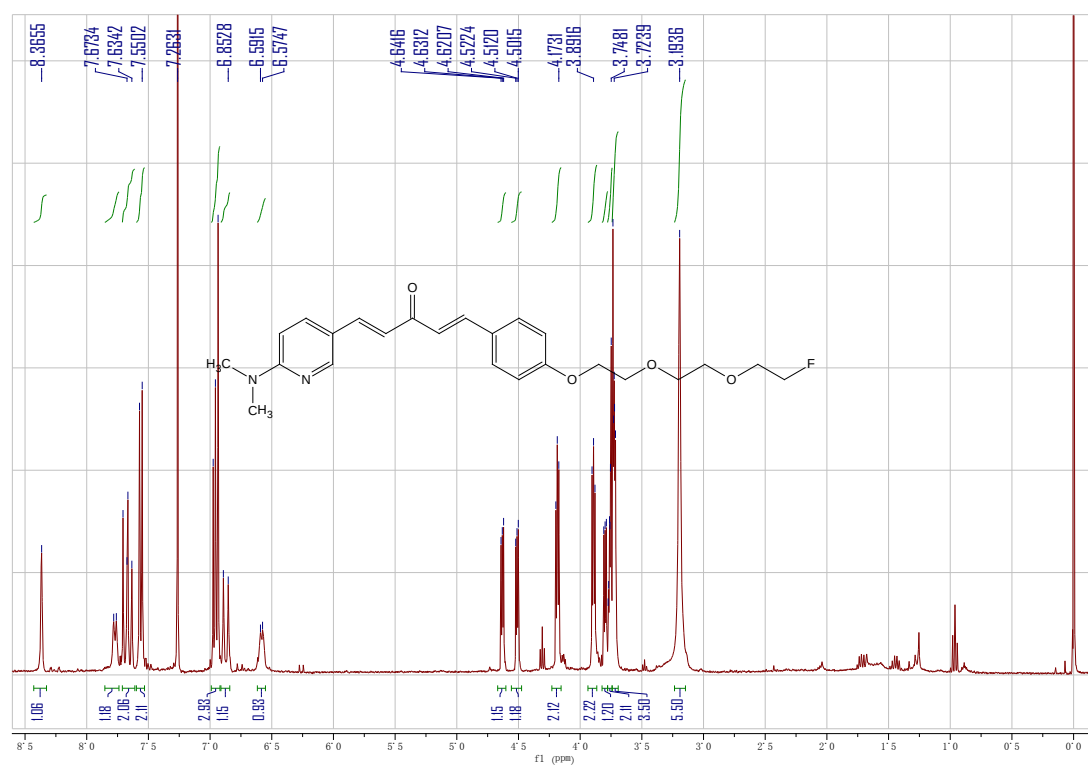
TM-P3-F 88 (1.628)

TOF MS ES+

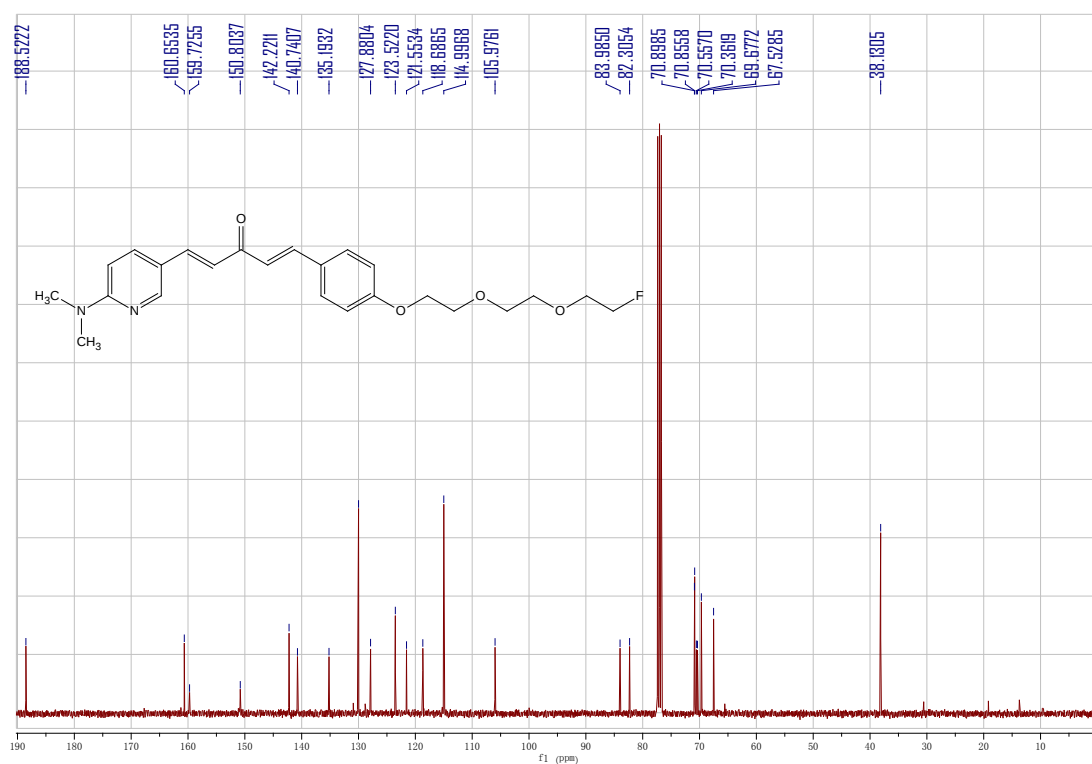


Minimum:					-1.5						
Maximum:	5.0	5.0			50.0						
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula					
429.2183	429.2201	-1.8	-4.2	6.5	n/a	C21	H31	N2	O5	F2	
	429.2199	-1.6	-3.7	2.5	n/a	C19	H33	N2	O2	F4	\$
	429.2197	-1.4	-3.3	1.5	n/a	C15	H33	N4	O10		
	429.2192	-0.9	-2.1	0.5	n/a	C17	H38	N4	O	F	S3
	429.2190	-0.7	-1.6	10.5	n/a	C24	H30	N2	O4	F	
	429.2187	-0.4	-0.9	6.5	n/a	C22	H32	N2	O	F3	\$
	429.2183	0.0	0.0	1.5	n/a	C16	H34	N4	O6	F	\$
	429.2180	0.3	0.7	4.5	n/a	C20	H37	N4	S3		
	429.2178	0.5	1.2	14.5	n/a	C27	H29	N2	O3		
	429.2177	0.6	1.4	3.5	n/a	C19	H30	N2	O3	F5	
	429.2176	0.7	1.6	10.5	n/a	C25	H31	N2	F2	\$	
	429.2172	1.1	2.6	-1.5	n/a	C13	H32	N4	O8	F3	
	429.2172	1.1	2.6	5.5	n/a	C19	H33	N4	O5	\$	
	429.2170	1.3	3.0	1.5	n/a	C17	H35	N4	O2	F2	\$2
	429.2167	1.6	3.7	-0.5	n/a	C19	H41	O4	S3		
	429.2165	1.8	4.2	7.5	n/a	C22	H29	N2	O2	F4	

¹H-NMR for compound **17b**



¹³C-NMR for compound **17b**



HRMS for compound **17h**

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Elemental Composition Report

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

4926 formula(e) evaluated with 15 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

COM-N-C-3 20 (0.342)

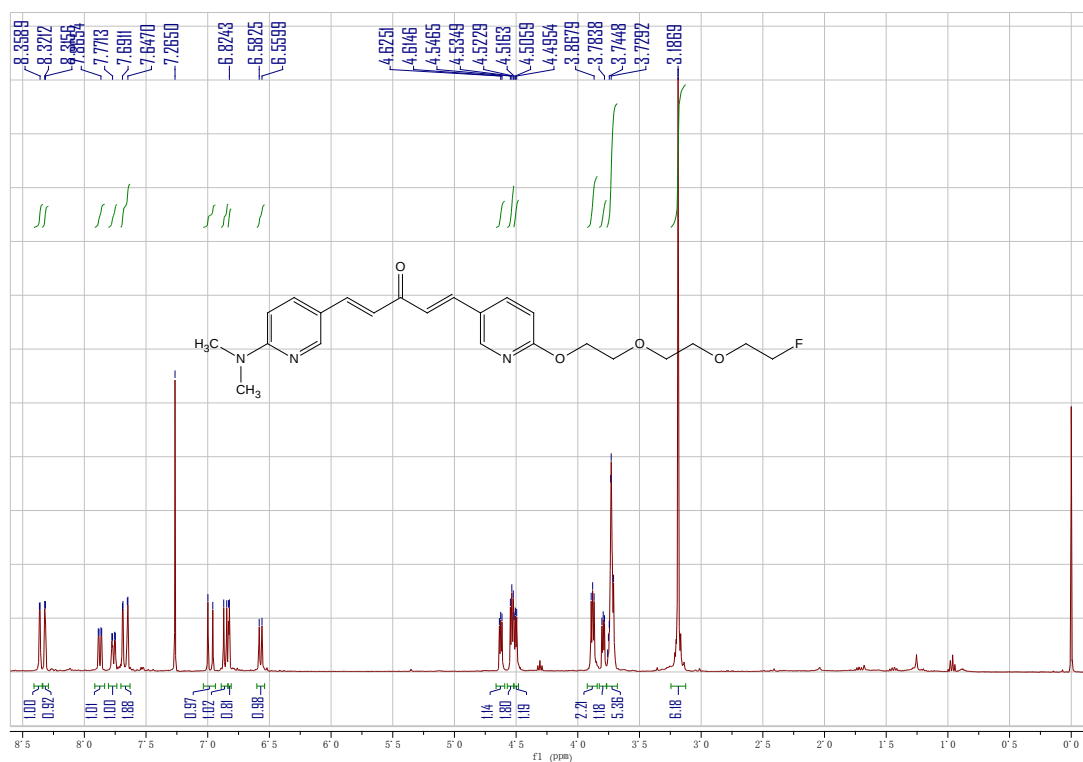
TOF MS AP+

2.80e+002

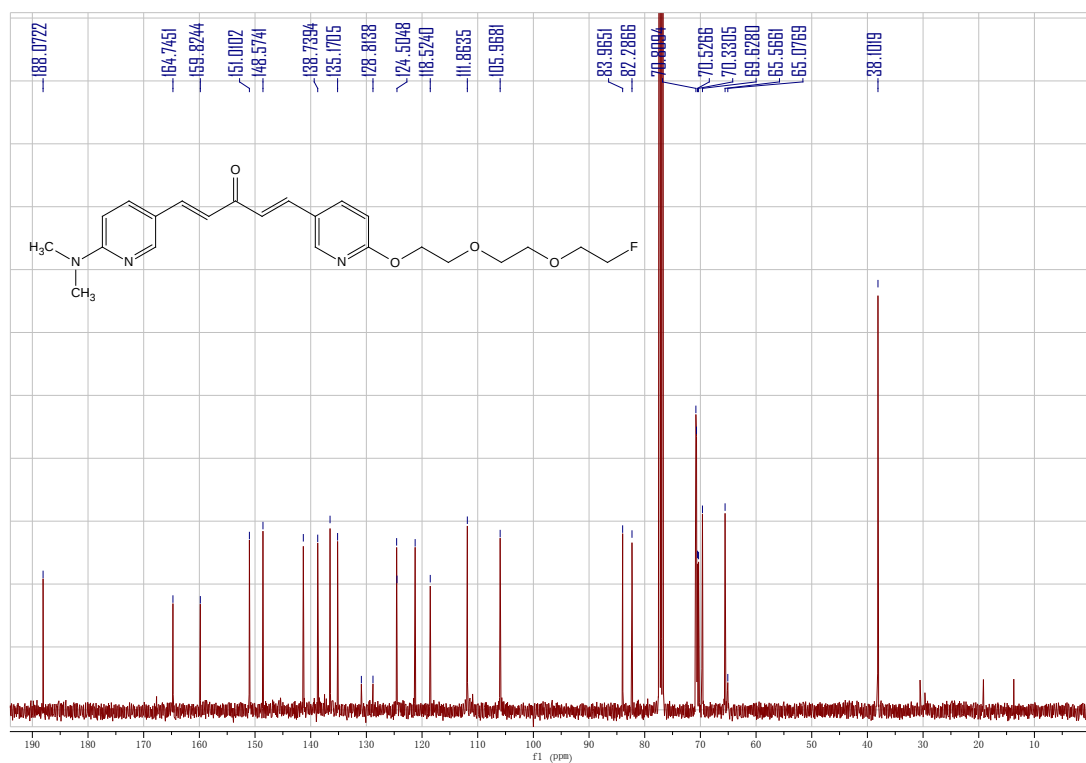


Minimum:				-1.5		
Maximum:		5.0	3.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
429.2191	429.2190	0.1	0.2	10.5	0.5	C24 H30 N2 O4 F ✓
	429.2203	-1.2	-2.8	15.5	0.7	C25 H26 N6 F
	429.2178	1.3	3.0	14.5	0.8	C27 H29 N2 O3
	429.2201	-1.0	-2.3	6.5	1.0	C21 H31 N2 O5 F2
	429.2199	-0.8	-1.9	8.5	2.4	C15 H24 N12 F3
	429.2197	-0.6	-1.4	12.5	2.4	C13 H21 N18
	429.2186	0.5	1.2	3.5	4.1	C14 H28 N8 O4 F3
	429.2183	0.8	1.9	7.5	4.1	C12 H25 N14 O4
	429.2197	-0.6	-1.4	1.5	4.2	C15 H33 N4 O10
	429.2197	-0.6	-1.4	-0.5	7.5	C11 H29 N8 O5 F4
	429.2195	-0.4	-0.9	3.5	7.5	C9 H26 N14 O5 F

¹H-NMR for compound **17c**



¹³C-NMR for compound **17c**



HRMS for compound **17c**

Elemental Composition Report

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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

2856 formula(e) evaluated with 6 results within limits (up to 100 best isotopic matches for each mass)

Elements Used:

C: 0-50 H: 0-60 N: 0-10 O: 0-10 F: 0-5

CXM-N-N-3 38 (0.650)

TOF MS AP+

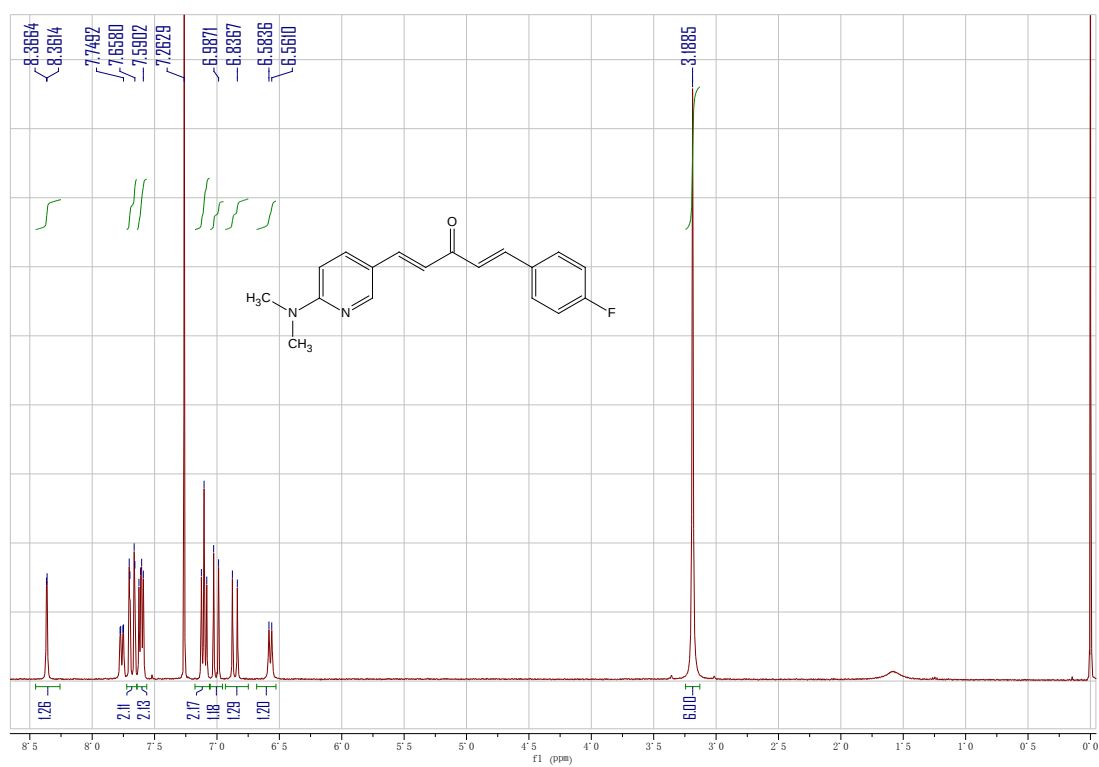


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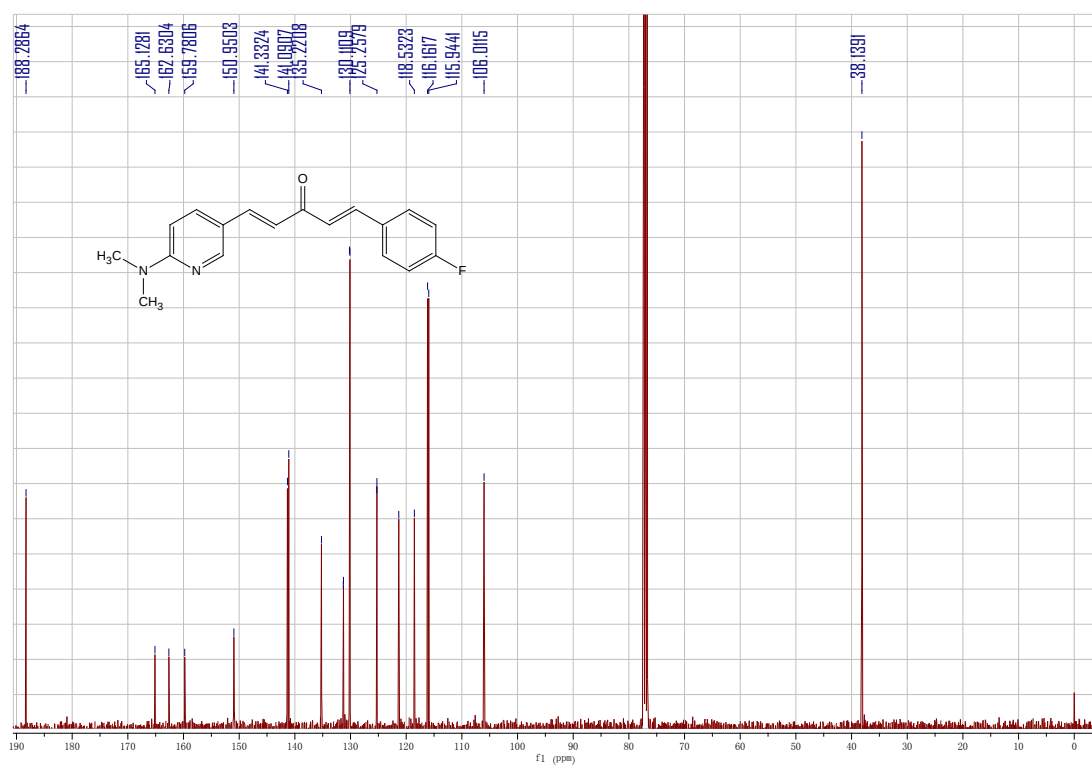
Maximum:

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
430.2144	430.2155	-1.1	-2.6	15.5	7.4	C24 H25 N7 F
	430.2142	0.2	0.5	10.5	13.0	C23 H29 N3 O4 F
	430.2154	-1.0	-2.3	6.5	51.7	C20 H30 N3 O5 F2
	430.2138	0.6	1.4	3.5	229.5	C13 H27 N9 O4 F3
	430.2149	-0.5	-1.2	1.5	229.8	C14 H32 N5 O10
	430.2150	-0.6	-1.4	-0.5	397.6	C10 H28 N9 O5 F4

¹H-NMR for compound **18**



¹³C-NMR for compound **18**



HRMS for compound 18

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

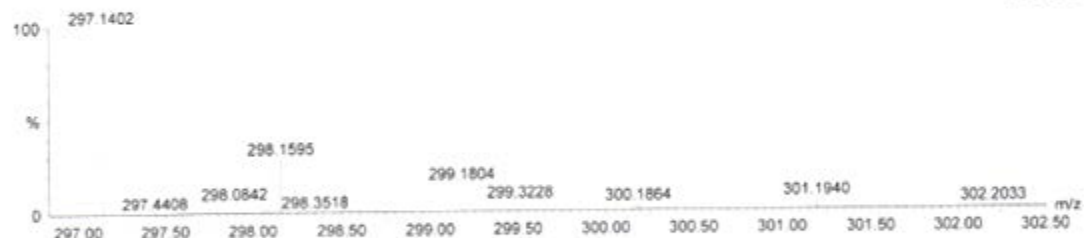
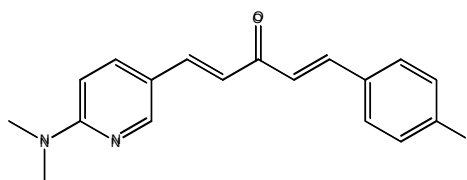
2032 formula(e) evaluated with 7 results within limits (up to 100 best isotopic matches for each mass)

Elements Used:

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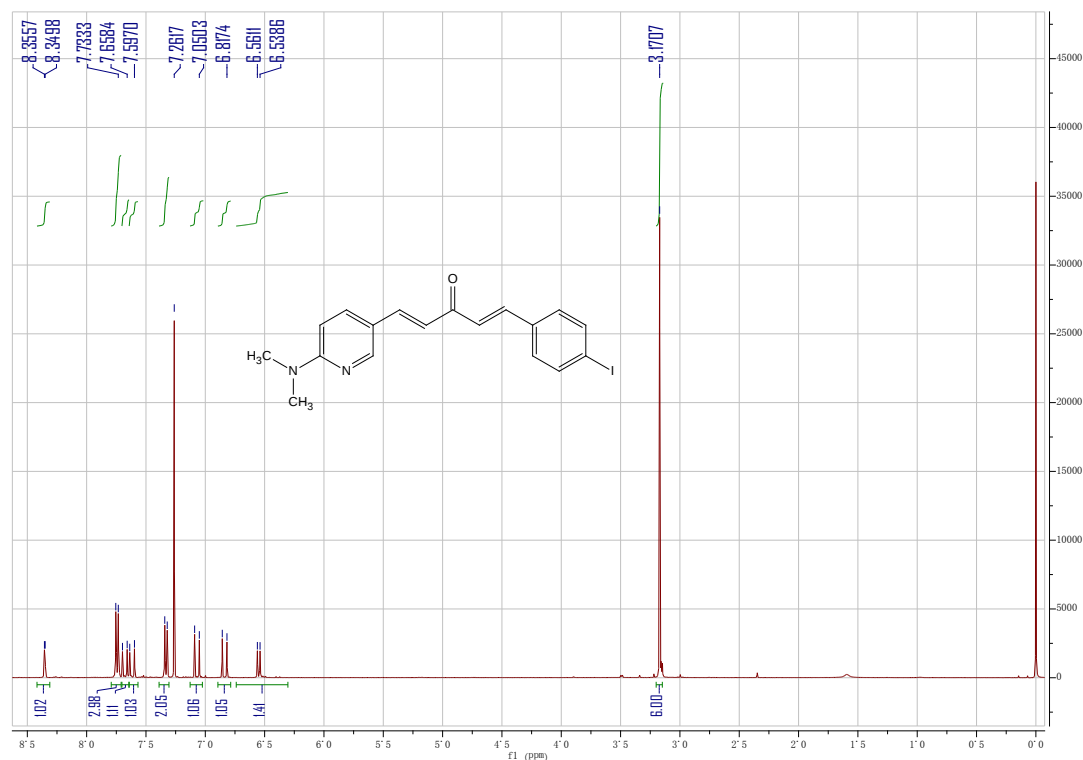
CXM-N-C-F 5 (0.085)

TOF MS AP+

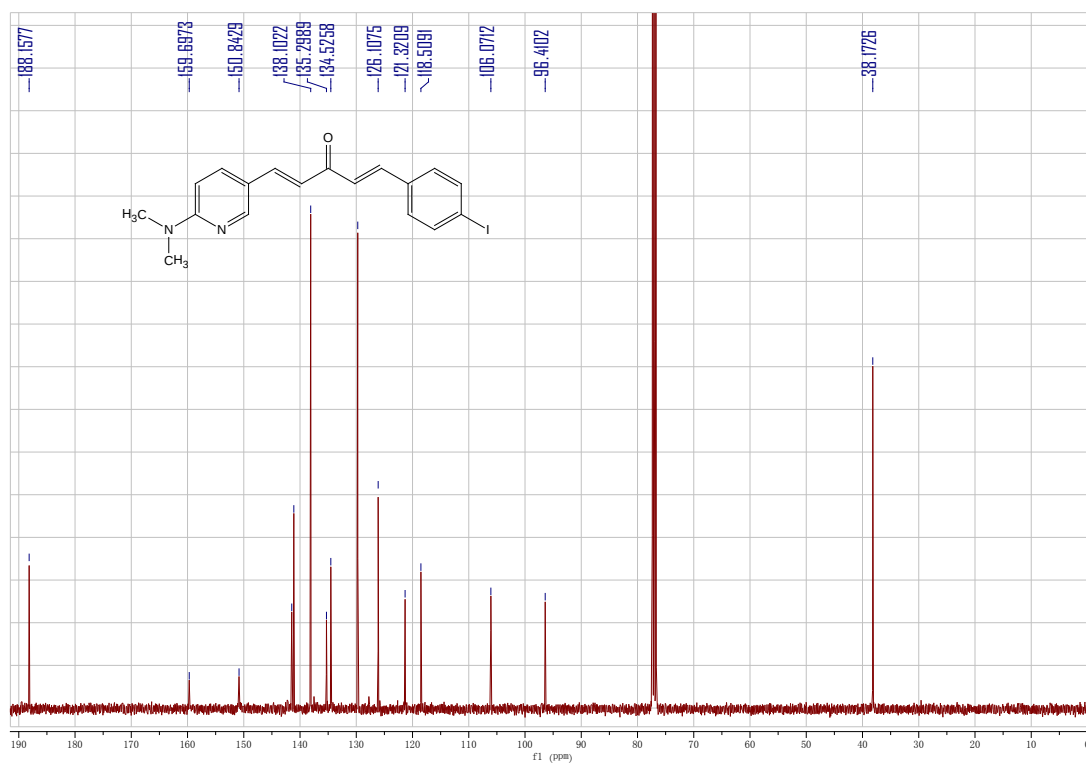


Minimum:				-1.5						
Maximum:		5.0	3.0	100.0						
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula				
297.1402	297.1403	-0.1	-0.3	10.5	255.6	C18	H18	N2	O	F ✓
	297.1410	-0.8	-2.7	1.5	1077.1	C9	H21	N4	O7	
	297.1399	0.3	1.0	3.5	1082.1	C8	H16	N8	O	F3
	297.1411	-0.9	-3.0	-0.5	1548.7	C5	H17	N8	O2	F4
	297.1408	-0.6	-2.0	3.5	n/a	C3	H14	N14	O2	F
	297.1397	0.5	1.7	7.5	n/a	C6	H13	N14	O	
	297.1395	0.7	2.4	-1.5	n/a	C2	H18	N10	O6	F

¹H-NMR for compound 19



¹³C-NMR for compound **19**



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)

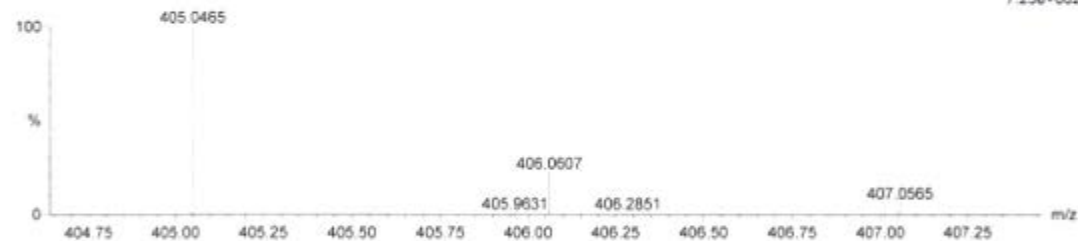
Elements Used:

C: 0-100 H: 0-150 N: 0-24 O: 0-10 I: 0-4

CXM-N-C-13 (0.051)

TOF MS AP+

7.23e+002



Minimum:

Maximum:

5.0

3.0

-1.5

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 H18 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

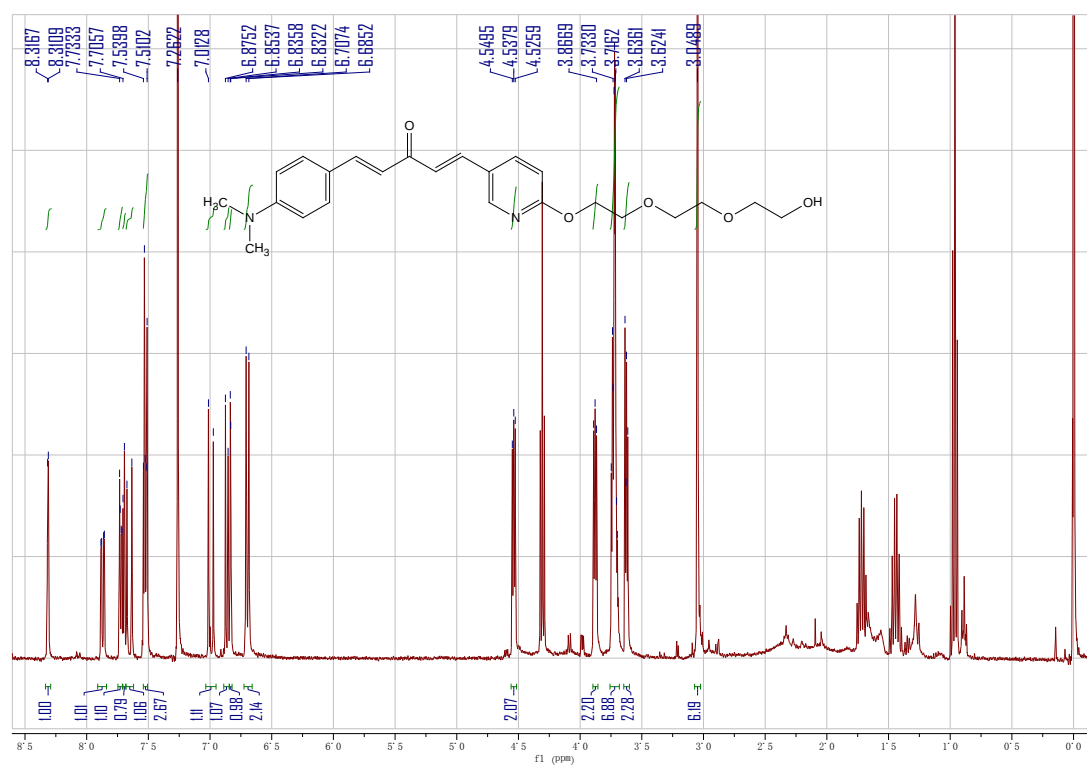
2.2

-1.5

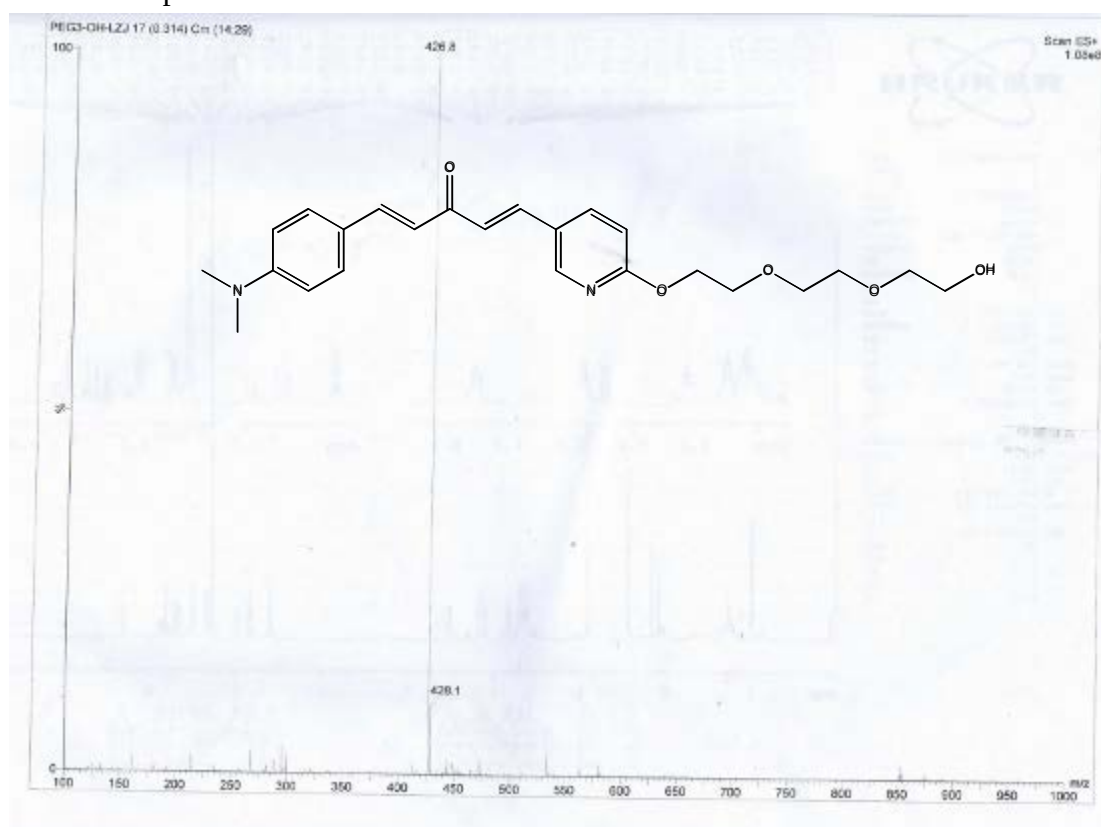
39.9

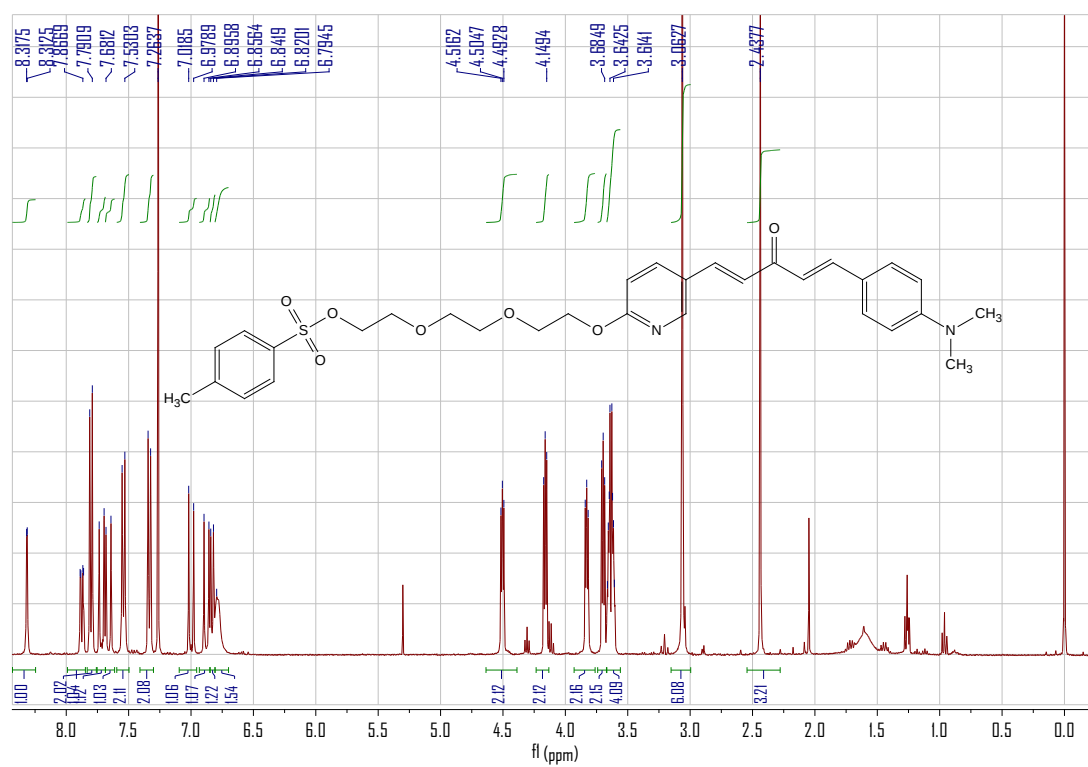
C2 H18 N10 O6 I

¹H-NMR for compound 20

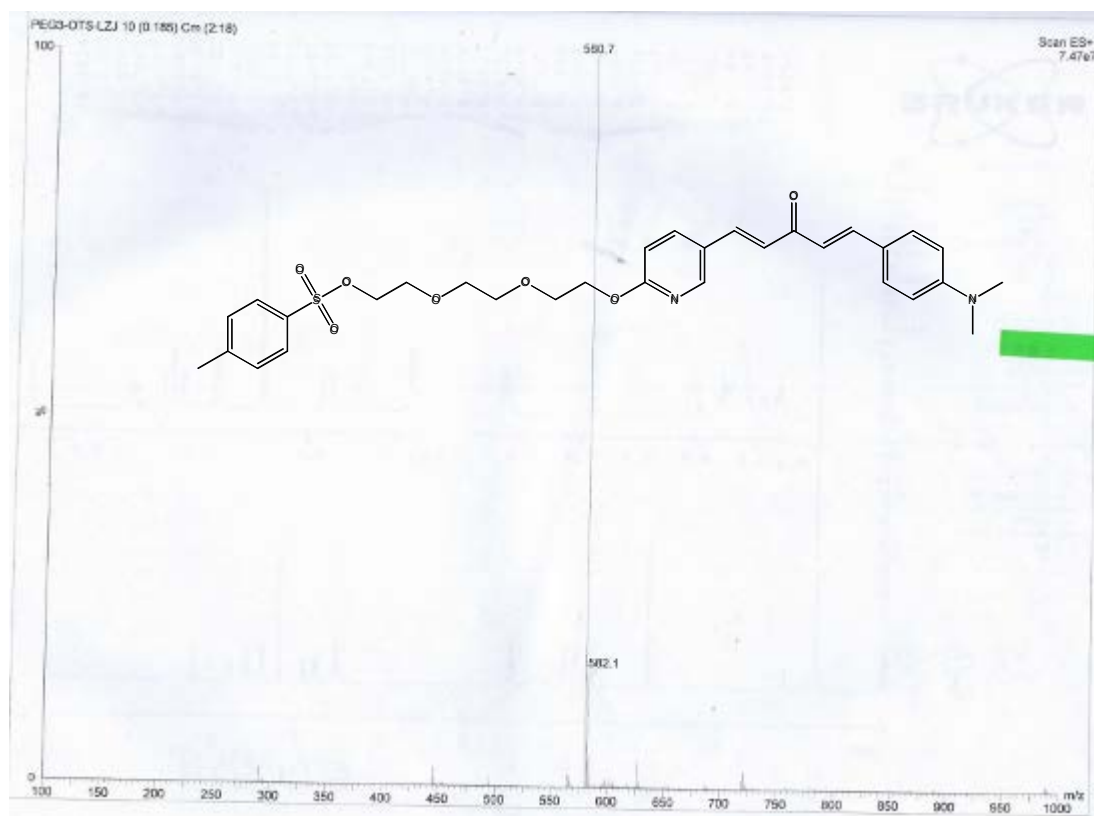


MS for compound 20

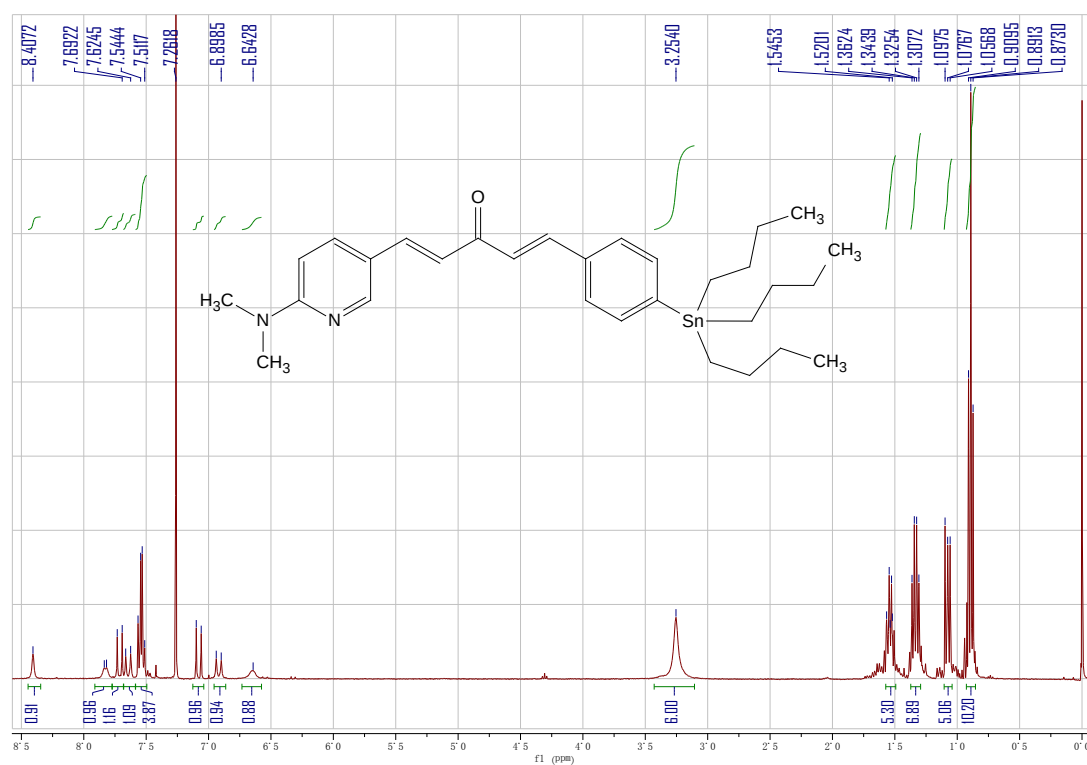


¹H-NMR for compound **21**

MS for compound **21**



¹H-NMR for compound 22



MS for compound

