Supporting Information

Efficient Amidation of Weak Amines: Synthesis, Chiral Separation by SFC, and Antimicrobial Activity of *N*-(9, 10-dioxo-9, 10-dihydro anthracene-1-yl) carboxamide

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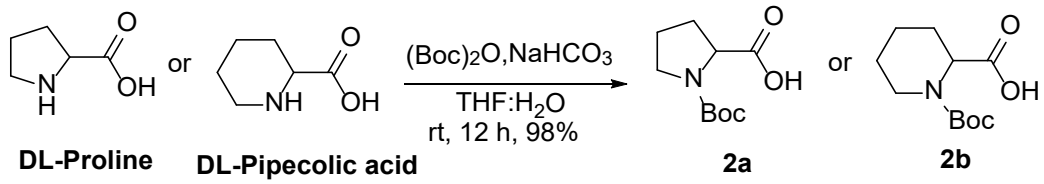
1. General Information:

All the reagents were purchased commercially and used without further purification. ^{1}H NMR and ^{13}C NMR were recorded with Bruker 400 MHz.^{1}H NMR (400MHz) and ^{13}C NMR (100MHz) spectra were recorded in $CDCl_3$ with tetramethylsilane as the internal standard. Multiplicities are reported using the following abbreviations: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, sep = septet, br = broad resonance. All the NMR spectra were acquired at ambient temperature. Analytical thin layer chromatography (TLC) was performed using Silica Gel 60 Å F_{254} pre-coated plates (0.25 mm thickness). Visualization was accomplished by irradiation with a UV lamp and staining with I_2 on silica gel. High resolution mass spectra (HRMS) were recorded on Bruker Compass Data Analysis 4.1, HRMS-ESI Mass Spectrometer with Orbitrap Exploris-240 Analyzer, Source Type ESI, in positive mode.

2. Experimental Procedure

2.1. General procedure for the synthesis of (*tert*-butoxycarbonyl)proline (2a) and 1-(*tert*-butoxycarbonyl)piperidine-2-carboxylic acid (2b)



To a suspension of DL-proline (1.0 equiv.) in THF: H_2O (1:1), sodium bicarbonate (3.0 equiv.) was added and stirred at room temperature for 30 min, then boc anhydride (1.05 equiv.) was added and stirred for 12 h. The reaction mixture was monitored by TLC. The reaction mixture was concentrated under reduced pressure. The residue was adjusted pH-2 by using aqueous citric acid solution. The aqueous layer was extracted with ethyl acetate (3 x 20 mL), washed with water, brine solution and combined organic layer was dried anhydrous sodium sulphate, filtered and concentrated under reduced pressure to get the desired product **2a or 2b.**

1-(*tert*-butoxycarbonyl)proline (DL-2a): ^{1}HNMR (400 MHz, DMSO-*d*6) δ 1.34-139 (d, *J* = 20.80 Hz, 9H), 1.80-1.86 (m, 3H), 2.14-2.18 (m, 1H), 3.26-3.30 (m, 2H), 4.03-4.08 (m, 1H), 12.40 (br, 1H). ELSD purity: 99.91% LCMS: 214.08 [M+H]+

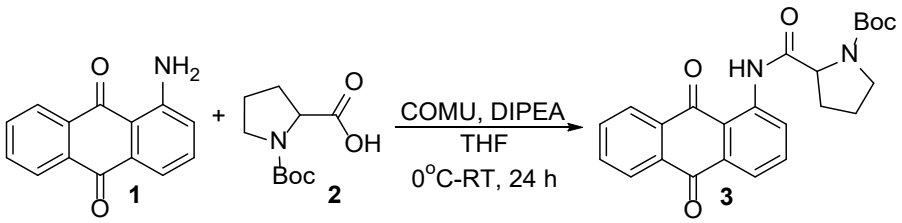
1-(*tert*-butoxycarbonyl)piperidine-2-carboxylic acid (DL-2b*)*: ^{1}HNMR (400 MHz, DMSO-*d*6) δ 1.05-1.15 (m, 1H), 1.23-1.39 (m, 10H), 1.59-1.62 (m, 3H), 2.06 (m, 1H), 2.74-2.96 (m, 1H), 3.78 (m, 1H), 4.53-4.61 (d, *J* = 29.20 Hz, 1H), 12.71 (s, 1H). ELSD purity: 99.95% LCMS: 228.14 [M+H]+

2.2. General procedure for synthesis of (±) 3a and (±) 3b

To a suspension of DL-pyrrolidine-1, 2-dicarboxylic acid 1-*tert*-butyl ester 2a (0.3 mmol) and DIPEA (0.5 mmol) in THF, COMU (0.25 mmol) was added at 0 ºC. After 30 min 1-aminoanthraquinone 1 (0.25 mmol) was added. The resulting reaction mixture was stirred at 0 ºC for 1 h and refluxed for 24 h. After completion of reaction (by TLC), reaction mixture was cooled to rt and diluted with water then extracted with ethyl acetate (3 x 20 mL). The combined organic layer was washed with water, brine solution, dried over anhydrous sodium sulphate, filtered and concentrated under reduced pressure. Crude product was purified through super critical fluid chromatography (Chiralcel-OX3, Methanol) to obtain the pair of enantiomers of (±)-**3a**.

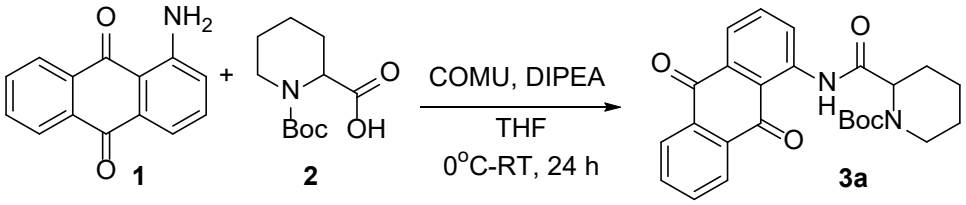
3. Experimental procedure and characterization of synthesized compounds

***tert*-Butyl 2-((9,10-dioxo-9,10-dihydroanthracen-1-yl)carbamoyl)pyrrolidine-1-carboxylate (±)-3a**



The reaction was carried out according to the general procedure A using **1**a (56 mg, 0.25 mmol), **2a** (64 mg, 0.3 mmol), DIPEA (87 mg, 0.5 mmol), COMU (107 mg, 0.25 mmol). Conditions: 0-55 ºC, 24 h. Yield: (70 mg, 66%). ^{1}HNMR (400 MHz, DMSO-d6) δ 1.23-1.45 (d, *J* = 87.9 Hz, 9H), 1.90-2.06 (m, 3H), 2.25-2.38 (m,1H), 3.48-3.55 (m,1H), 3.64-3.73 (m, 1H), 4.27-4.31 (m, 1H), 7.92-7.98 (m, 4H), 8.17-8.24 (m, 2H), 9.01-9.07 (m, 1H), 12.46-12.61 (d, *J* = 60.0 Hz, 1H).

***tert*-butyl 2-((9,10-dioxo-9,10-dihydroanthracen-1-yl)carbamoyl)piperidine-1-carboxylate (±)-3b**



The reaction was carried out according to the general procedure A using **1** (56 mg, 0.25 mmol), **2b** (69 mg, 0.3 mmol), DIPEA (87 mg, 0.5 mmol), COMU (107 mg, 0.25 mmol). Conditions: 0-55 ºC, 24 h. Yield: (69 mg, 63%). ^{1}HNMR (400 MHz, DMSO-*d*6) δ 1.23-1.64

(m, 15H), 2.97 (br, 1H), 4.05 (m, 1H), 4.92 (m, 1H), 7.91-7.99 (m, 4H), 8.18-8.19 (m, 2H), 9.07-9.09 (m, 1H), 12.60 (s,1H).

2.4 NMR studies

The ^{1}H and ^{13}CNMR values for compound (-)-**4a** and (+)-**4a'**, assigned on the basis of 2D NMR spectral data (HSQC and HMBC), and are given in Table 1.

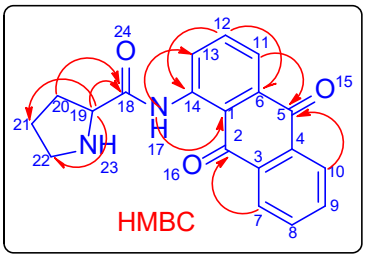


Figure 1. (a) General numbering and HMBC correlations for proline derivative

Table 1. **^{1}H NMR and ^{13}CNMR spectral data for proline derivative, assignments based on HSQC and HMBC correlations**

S.No.	Assignment	Type of atom	^{1}H Chemical shift (ppm)	^{13}C Chemical shift (ppm)
1	1	C	-	118.19
2	2	C	-	185.31
3	3	C	-	133.80
4	4	C	-	132.10
5	5	C	-	182.30
6	6	C	-	133.73
7	7	CH	8.23 (m)	126.94
8	8	CH	7.93 (m)	134.62
9	9	CH	7.93 (m)	134.31
10	10	CH	8.16 (m)	126.28
11	11	CH	7.92 (m)	121.60
12	12	CH	7.86 (t)	135.26
13	13	CH	9.12 (dd)	125.21

14	14	C	-	140.65
15	15	O	-	-
16	16	O	-	-
17	17	NH	13.18 (s)	-
18	18	C	-	176.27
19	19	CH	3.85 (m)	61.45
20	20	CH_2	2.15, 1.86 (m)	30.79
21	21	CH_2	1.69 (m)	25.96
22	22	CH_2	3.13, 2.96 (m)	46.87
23	23	NH	-	-
24	24	O	-	-

NOTE: m: multiplet, t: triplet d: doublet, s: singlet, dd: doublet of doublet, br: broad

b. Pipecolic acid analogue

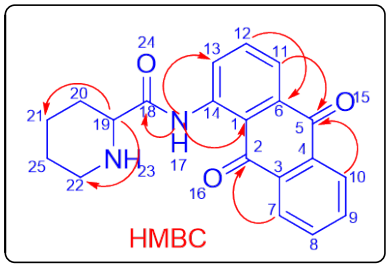


Figure 2. General numbering and HMBC correlations of pipecolic acid derivative

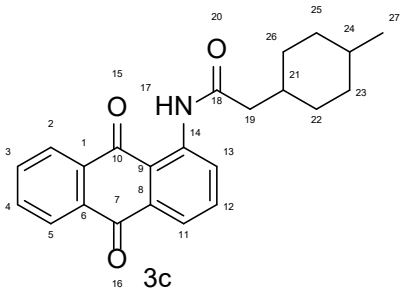
Table 2. ^{1}HNMR and ^{13}CNMR spectral data (chemical shifts) for pipecolic acid derivative

S.No.	Assignment	Type of atom	^{1}H Chemical shift (ppm)	^{13}C Chemical shift (ppm)
1	1	C	-	118.09
2	2	C	-	185.68
3	3	C	-	133.89
4	4	C	-	132.23
5	5	CO	-	182.37
6	6	C	-	133.75
7	7	CH	8.23 (m)	127.10
8	8	CH	7.93 (m)	134.74
9	9	CH	7.93 (m)	134.50
10	10	CH	8.16 (m)	126.39
11	11	CH	7.92 (m)	121.69
12	12	CH	7.86 (t)	135.47
13	13	CH	9.12 (dd)	125.50
14	14	C	-	141.04
15	15	O	-	-
16	16	O	-	-
17	17	NH	12.78 (s)	-
18	18	C	-	174.31
19	19	CH	3.36 (m)	66.42
20	20	CH_2	1.87, 1.56 (m)	29.00
21	21	CH_2	1.72, 1.46 (m)	23.57
22	22	CH_2	2.99, 2.69 (m)	44.92
23	23	NH	-	-
24	24	O	-	-

25	25	CH_2	1.52, 1.44 (m)	25.51

Note: Assignments made on the basis of HSQC and HMBC correlations, m: multiplet, t: triplet d: doublet, s: singlet, dd: doublet of doublet, br: broad.

***N*-(9,10-dioxo-9,10-dihydroanthracen-1-yl)-2-(4-methylcyclohexyl)acetamide (3c)**

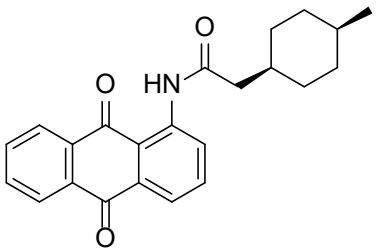


3c

N-(9,10-dioxo-9,10-dihydroanthracen-1-yl)-2-(4-methylcyclohexyl)acetamide

The reaction was carried out according to the general procedure A using **1a** (56 mg, 0.25 mmol), 2-((1s,4s)-4-methylcyclohexyl)acetic acid (**2c**) (47 mg, 0.3 mmol), DIPEA (87 mg, 0.5 mmol), COMU (107 mg, 0.25 mmol). Conditions: 0-55 ^{o}C, 24 h. Yield: (59 mg, 65%), the product **3c** was obtained as a *cis* and *trans* isomers and it was successfully separated by using SFC.

***N*-(9,10-dioxo-9,10-dihydroanthracen-1-yl)-2-((1s,4s)-4-methylcyclohexyl)acetamide (3c')**



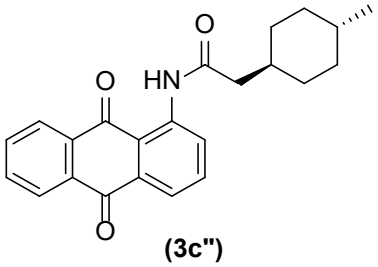
(3c')

^{1}HNMR (400 MHz, DMSO-*d*6) δ 12.10 (s, 1H), 8.99 (q, *J* = 3.2 Hz, 1H), 8.25 (m, *J* = 2.2 Hz, 1H), 8.18 (m, *J* = 2.2 Hz, 1H), 7.92 (m, *J* = 4.0 Hz, 4H), 2.50 (d, *J* = 1.4 Hz, 1H), 2.09 (q, *J* = 4.0 Hz, 1H), 1.53 (m, *J* = 6.8 Hz, 7H), 1.31 (m, *J* = 4.5 Hz, 2H), 0.94 (d, *J* = 6.8 Hz, 3H). ^{13}C NMR (DMSO-d6, 100 MHz) δ 24.8, 28.0, 55.3, 59.1, 60.9, 117.6, 121.7, 125.4, 126.4, 127.0, 132.3, 133.7, 133.8, 134.7, 134.7, 135.7, 141.4, 162.7, 172.2, 182.2, 186.6. HRMS (ESI), Calcd. for $C_{23}H_{24}O_3N$ $(M+H)^+$: 362.1751; found: 362.1741.

***N*-(9,10-dioxo-9,10-dihydroanthracen-1-yl)-2-(4-methylcyclohexyl)acetamide- Isomer-1 (3c')**

As Isomer-2 assigned as trans form, isomer-1 will be cis form. However H21 and H24 protons splitting pattern was not clear. Hence it is difficult to fix the relative stereo chemistry.

***N*-(9,10-dioxo-9,10-dihydroanthracen-1-yl)-2-((1r,4r)-4-methylcyclohexyl)acetamide (3c'')**



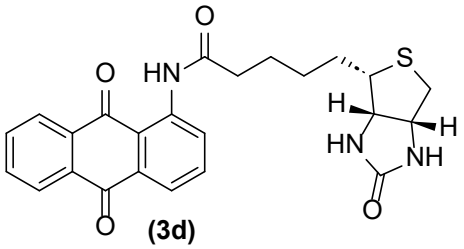
(3c")

^{1}HNMR (400 MHz, DMSO-*d*6) δ 12.10 (s, 1H), 9.00 (q, *J* = 3.2 Hz, 1H), 8.26 (q, *J* = 3.0 Hz, 1H), 8.19 (m, *J* = 2.2 Hz, 1H), 7.94 (m, *J* = 3.4 Hz, 4H), 2.40 (d, *J* = 6.7 Hz, 1H), 2.08 (d, *J* = 7.5 Hz, 1H), 1.78 (m, *J* = 10.5 Hz, 3H), 1.68 (d, *J* = 12.4 Hz, 2H), 1.31 (m, *J* = 4.8 Hz, H), 1.08 (m, *J* = 6.4 Hz, 2H), 0.96 (m, *J* = 12.1 Hz, 2H), 0.87 (m, *J* = 6.5 Hz, 4H). ^{13}C NMR (DMSO-*d*6, 100 MHz) δ 24.8, 28.0, 55.3, 59.1, 60.9, 117.6, 121.7, 125.4, 126.4, 127.0, 132.3, 133.7, 133.8, 134.7, 134.7, 135.7, 141.4, 162.7, 172.2, 182.2, 186.6.

***N*-(9,10-dioxo-9,10-dihydroanthracen-1-yl)-2-(4-methylcyclohexyl)acetamide-Isomer-2 (3c'')**

In HSQC, we could see CH21(1.92 ppm) at 35.00ppm and CH24(1.33 ppm) at 32.00 ppm. In COSY, H19(2.42 ppm)is coupling with H21 and H27(0.89 ppm) is coupling with H24. In ^{1}HNMR (Homo nuclear decoupling), we could see H21 (*J* value 11.60Hz) and H24 (*J* value 10.00Hz). Based on above *J* values H21 (Axial) and H24 (Axial) protons are in *trans* form.

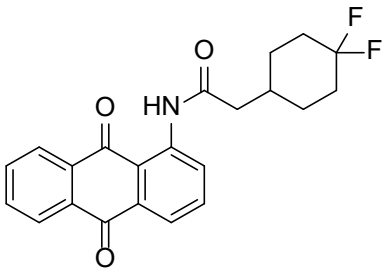
***N*-(9,10-dioxo-9,10-dihydroanthracen-1-yl)-5-((3aS,4S,6aR)-2-oxohexahydro-1H-thieno[3,4-d]imidazol-4-yl)pentanamide (3d)**



(3d)

The reaction was carried out according to the general procedure A using **1a** (57 mg, 0.25 mmol), biotin (**2d**) (73 mg, 0.3 mmol), DIPEA (87 mg, 0.5 mmol), COMU (107 mg, 0.25 mmol). Conditions: 0-55 ºC, 24 h. Yield: (80 mg, 71%), ^{1}HNMR (400 MHz, DMSO-*d*6) δ 12.11 (s, 1H), 9.00 (d, *J* = 8.0 Hz, 1H), 8.23 (m, *J* = 7.4 Hz, 2H), 7.94 (q, *J* = 8.5 Hz, 4H), 6.41 (d, *J* = 42.3 Hz, 2H), 4.25 (m, *J* = 16.2 Hz, 2H), 3.15 (d, *J* = 4.6 Hz, 1H), 2.83 (q, *J* = 5.8 Hz, 1H), 2.58 (t, *J* = 9.0 Hz, 4H), 1.72 (q, *J* = 7.3 Hz, 3H), 1.50 (m, *J* = 11.9 Hz, 4H). ^{13}C NMR (DMSO-*d*6, 100 MHz) δ 24.8, 28.0, 55.3, 59.1, 60.9, 117.6, 121.7, 125.4, 126.4, 127.0, 132.3, 133.7, 133.8, 134.7, 134.7, 135.7, 141.4, 162.7, 172.2, 182.2, 186.6. HRMS (ESI), Calcd. for $C_{24}H_{24}N_3O_4S$ $(M+H)^+$: 450.1482 ; found: 450.1478.

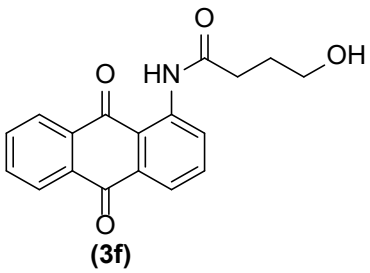
2-(4,4-difluorocyclohexyl)-N-(9,10-dioxo-9,10-dihydroanthracen-1-yl)acetamide (3e)



(3e)

The reaction was carried out according to the general procedure A using **1a** (60 mg, 0.25 mmol), 2-(4,4-difluorocyclohexyl)acetic acid (**2e**) (53 mg, 0.3 mmol), DIPEA (87 mg, 0.5 mmol), COMU (107 mg, 0.25 mmol). Conditions: 0-55 ºC, 24 h. Yield: (56 mg, 58%), ^{1}HNMR (400 MHz, DMSO-*d*6) δ 12.08 (s, 1H), 8.99 (q, *J* = 3.2 Hz, 1H), 8.26 (m, *J* = 2.2 Hz, 1H), 8.19 (m, *J* = 2.2 Hz, 1H), 7.93 (m, *J* = 3.1 Hz, 4H), 2.53 (s, 2H), 2.05 (q, *J* = 9.5 Hz, 4H), 1.85 (m, *J* = 6.0 Hz, 4H), 1.34 (q, *J* = 11.6 Hz, 1H). ^{13}C NMR (DMSO-*d*6, 100 MHz) δ 24.8, 28.0, 55.3, 59.1, 60.9, 117.6, 121.7, 125.4, 126.4, 127.0, 132.3, 133.7, 133.8, 134.7, 134.7, 135.7, 141.4, 162.7, 172.2, 182.2, 186.6. HRMS (ESI), Calcd. for $C_{22}H_{20}O_3NF_2$ $(M+H)^+$: 384.1399 ; found: 384.1399.

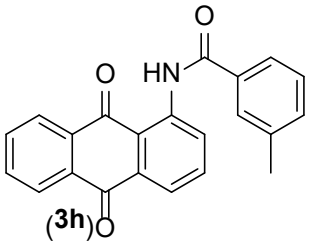
2-(4,4-difluorocyclohexyl)-N-(9,10-dioxo-9,10-dihydroanthracen-1-yl)acetamide (3f)



(3f)

The reaction was carried out according to the general procedure A using **1a** (56 mg, 0.25 mmol), 4-hydroxybutanoic acid (**2f**) (31 mg, 0.3 mmol), DIPEA (87 mg, 0.5 mmol), COMU (107 mg, 0.25 mmol). Conditions: 0-55 ºC, 24 h. Yield: (49 mg, 63%), ^{1}H NMR (400 MHz, DMSO-*d*6) δ 12.11 (s, 1H), 9.00 (d, *J* = 8.0 Hz, 1H), 8.23 (m, *J* = 7.4 Hz, 2H), 7.94 (q, *J* = 8.5 Hz, 4H), 6.41 (d, *J* = 42.3 Hz, 2H), 4.25 (m, *J* = 16.2 Hz, 2H), 3.15 (d, *J* = 4.6 Hz, 1H), 2.83 (q, *J* = 5.8 Hz, 1H), 2.58 (t, *J* = 9.0 Hz, 4H), 1.72 (q, *J* = 7.3 Hz, 3H), 1.50 (m, *J* = 11.9 Hz, 4H); ^{13}C NMR (DMSO-*d*6, 100 MHz) δ 24.8, 28.0, 55.3, 59.1, 60.9, 117.6, 121.7, 125.4, 126.4, 127.0, 132.3, 133.7, 133.8, 134.7, 134.7, 135.7, 141.4, 162.7, 172.2, 182.2, 186.6. HRMS (ESI), Calcd. for $C_{18}H_{14}O_4N$ $(M-H)^+$: 308.0922 ; found: 309.0918

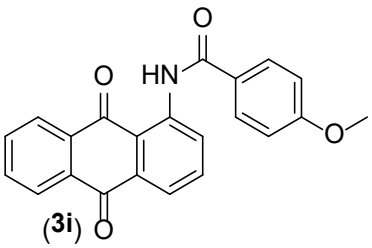
***N*-(9, 10-dioxo-9,10-dihydroanthracen-1-yl)-3-methylbenzamide (3h)**



(**3h**)

The reaction was carried out according to the general procedure A using **1**a (60 mg, 0.25 mmol), 3-methylbenzoic acid (**2h**) (41 mg, 0.3 mmol), DIPEA (87 mg, 0.5 mmol), COMU (107 mg, 0.25 mmol). Conditions: 0 - 55 ºC, 24 h. Yield : (64 mg, 75%). ^{1}HNMR (400 MHz, $CDCl_3$) δ 13.25 (s, 1H), 9.36 (q, *J* = 3.3 Hz, 1H), 8.37 (m, *J* = 1.8 Hz, 1H), 8.30 (m, *J* = 1.5 Hz, 1H), 8.11 (q, *J* = 2.9 Hz, 1H), 7.97 (t, *J* = 3.6 Hz, 2H), 7.83 (m, *J* = 2.5 Hz, 3H), 7.48 (m, *J* = 4.0 Hz, 1H), 7.43 (t, *J* = 3.9 Hz, 1H), 2.51 (s, 3H); ^{13}C NMR (DMSO-*d*6, 100 MHz) δ 21.7, 118.2, 122.8, 124.8, 126.5, 127.3, 127.7, 128.7, 129.0, 133.0, 133.3, 134.3, 134.5, 134.6, 134.8, 136.1, 139.0, 142.7, 167.0, 182.4, 187.8. HRMS (ESI), Calcd. for $C_{22}H_{15}NO_3$ $(M+H)^+$: 342.1125 ; found: 342.1121.

***N*-(9,10-dioxo-9,10-dihydroanthracen-1-yl)-4-methoxybenzamide (3i)**

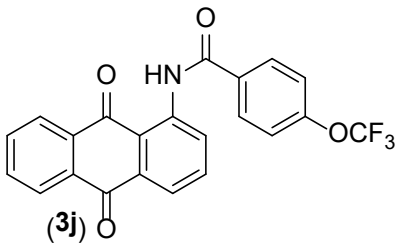


(**3i**)

The reaction was carried out according to the general procedure A using **1a** (55 mg, 0.25 mmol), 4-methoxybenzoic acid (**2i**) (46 mg, 0.3 mmol), DIPEA (87 mg, 0.5 mmol),

COMU (107 mg, 0.25 mmol). Conditions: 0 - 55 ºC, 24 h. Yield : (55 mg, 61%). ^{1}HNMR (400 MHz, $CDCl_3$) δ 13.25 (s, 1H), 9.37 (q, *J* = 3.2 Hz, 1H), 8.37 (m, *J* = 2.3 Hz, 1H), 8.31 (m, *J* = 2.3 Hz, 1H), 8.16 (d, *J* = 8.9 Hz, 2H), 8.10 (q, *J* = 2.9 Hz, 1H), 7.83 (m, *J* = 3.2 Hz, 3H), 7.08 (d, *J* = 8.8 Hz, 2H), 3.92 (s, 3H); ^{13}CNMR (DMSO-*d*6, 100 MHz) δ 55.7, 114.4, 118.0, 122.7, 126.4, 127.0, 127.3, 127.7, 129.9, 133.1, 134.3, 134.3, 134.5, 134.6, 136.1, 143.0, 163.2, 166.3, 183.0, 187.9. HRMS (ESI), Calcd. for $C_{22}H_{16}NO_4(M+H)^+$: 358.1074 ; found: 358.1069.

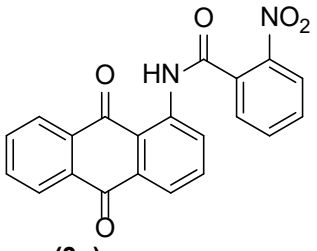
N-(9,10-dioxo-9,10-dihydroanthracen-1-yl)-4-(trifluoromethoxy)benzamide (3j)



(**3j**)

The reaction was carried out according to the general procedure A using **1a** (57 mg, 0.25 mmol), 4-(trifluoromethoxy)benzoic acid (**2j**) (62 mg, 0.3 mmol), DIPEA (87 mg, 0.5 mmol), COMU (107 mg, 0.25 mmol). Conditions: 0 - 55 ºC, 24 h. Yield : (57 mg, 55%). ^{1}HNMR (400 MHz, $CDCl_3$) δ 13.36 (s, 1H), 9.34 (q, *J* = 3.2 Hz, 1H), 8.36 (m, *J* = 2.3 Hz, 1H), 8.31 (m, *J* = 2.3 Hz, 1H), 8.23 (q, *J* = 2.9 Hz, 2H), 8.13 (q, *J* = 2.9 Hz, 1H), 7.85 (m, *J* = 2.4 Hz, 3H), 7.43 (d, *J* = 8.2 Hz, 2H); ^{13}C NMR (DMSO-*d*6, 100 MHz) δ 118.2, 121.1, 123.1, 126.4, 127.4, 127.7, 129.8, 133.1, 133.1, 134.2, 134.3, 134.6, 134.8, 136.3, 142.5, 152.4, 165.4, 182.8, 188.0. HRMS (ESI), Calcd. for $C_{22}H_{13}NF_3(M+H)^+$: 412.0791 ; found: 412.0788.

N-(9,10-dioxo-9,10-dihydroanthracen-1-yl)-2nitro benzamide (3k)

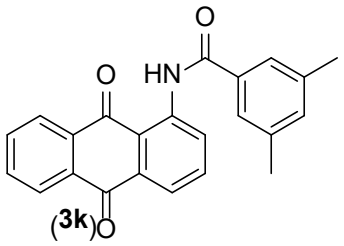


(3o)

The reaction was carried out according to the general procedure A using 1-aminoanthracene-9,10-dione (**1a**) (56 mg, 0.25 mmol), 2-nitrobenzoic acid (**2l**) (47.5 mg, 0.3 mmol), DIPEA (87 mg, 0.5 mmol), COMU (107 mg, 0.25 mmol). Conditions: 0 - 55 ºC, 24 h. Yield: 48% ; ^{1}HNMR (400 MHz, DMSO-*d*6) δ 12.59 (s, 1H), 8.97 (q, *J* = 3.1 Hz, 1H), 8.21 (q, *J* = 3.2 Hz, 3H), 8.08 (q, *J* = 3.0 Hz, 1H), 8.02 (q, *J* 5.3 Hz, 3H), 7.96 (m, *J* = 4.4 Hz, 2H),

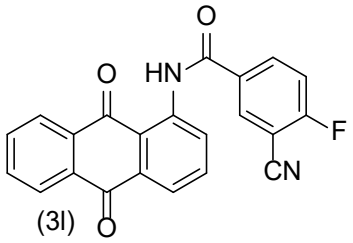
7.88 (m, *J* = 3.4 Hz, 1H), Ion trap LCMS(ESI), Calcd. for $C_{21}H_{12}N_2O_5(M+H)^+$: 373.07 ; found: 373.03.

***N*-(9,10-dioxo-9,10-dihydroanthracen-1-yl)-3,5-dimethylbenzamide (3l)**



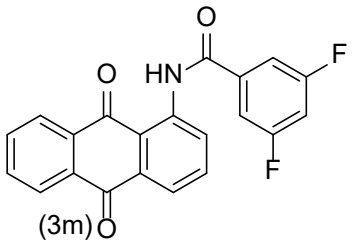
The reaction was carried out according to the general procedure A using **1a** (56 mg, 0.25 mmol), 3,5-dimethylbenzoic acid (**2l**) (45 mg, 0.3 mmol), DIPEA (87 mg, 0.5 mmol), COMU (107 mg, 0.25 mmol). Conditions: 0 - 55 °C, 24 h. Yield : (62 mg, 70%). ^{1}HNMR (400 MHz, DMSO-*d*6) δ 13.21 (s, 1H), 9.36 (d, *J* = 7.8 Hz, 1H), 8.39 (m, *J* = 2.2 Hz, 1H), 8.31 (m, *J* = 2.2 Hz, 1H), 8.11 (q, *J* = 2.8 Hz, 1H), 7.84 (m, *J* = 3.4 Hz, 3H), 7.76 (s, 2H), 4.09 (d, *J* = 6.4 Hz, 1H), 3.64 (s, 5H), 2.47 (s, 6H). ^{13}CNMR (DMSO-*d*6, 100 MHz) δ 21.6, 118.2, 122.8, 125.7, 126.6, 127.3, 127.7, 133.1, 134.2, 134.3, 134.5, 134.6, 134.8, 136.1, 138.8, 142.8, 167.3, 183.0, 187.7. HRMS (ESI), Calcd. for $C_{23}H_{18}NO_3(M+H)^+$: 356.1281 ; found: 356.1276.

3-cyano-N-(9,10-dioxo-9,10-dihydroanthracen-1-yl)-4-fluorobenzamide (3m)



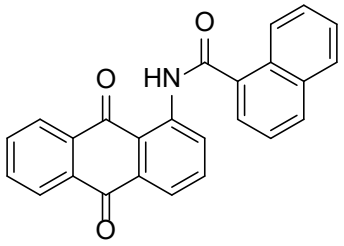
The reaction was carried out according to the general procedure A using 1-aminoanthracene-9,10-dione (**1a**) (60 mg, 0.25 mmol), 3-cyano-4-fluorobenzoic acid (**2m**) (50 mg, 0.3 mmol), DIPEA (87 mg, 0.5 mmol), COMU (107 mg, 0.25 mmol). Conditions: 0 - 55 °C, 24 h. Yield : (49 mg, 52%), ^{1}HNMR (400 MHz, DMSO-*d*6) δ 12.92 (s, 1H), 9.03 (d, *J* = 7.5 Hz, 1H), 8.53 (m, *J* = 4.1 Hz, 1H), 8.42 (m, *J* = 2.3 Hz, 1H), 8.28 (q, *J* = 3.0 Hz, 1H), 8.20 (q, *J* = 3.0 Hz, 1H), 8.00 (m, *J* = 4.6 Hz, 4H), 7.86 (t, *J* = 9.0 Hz, 1H);^{13}CNMR (DMSO-*d*6, 100 MHz) δ 101.2, 101.4, 113.4, 117.6, 117.8, 118.7, 122.6, 125.8, 126.5, 127.2, 131.8, 132.2, 133.5, 133.5, 134.7, 134.8, 134.9, 135.9, 140.7, 162.9, 163.2, 165.8, 182.0, 186.8. HRMS (ESI), Calcd. for $C_{22}H_{12}FN_2O_3(M+H)^+$: 371.0826 ; found: 371.0822.

***N*-(9,10-dioxo-9,10-dihydroanthracen-1-yl)-3,5-difluorobenzamide (3n)**



The reaction was carried out according to the general procedure A using 1 (56 mg, 0.25 mmol), 3,5-difluorobenzoic acid (**2n**) (47.5 mg, 0.3 mmol), DIPEA (87 mg, 0.5 mmol), COMU (107 mg, 0.25 mmol). Conditions: 0 - 55 ºC, 24 h. Yield: trace ; ^{1}HNMR (400 MHz, DMSO-*d*6) δ 13.38 (s, 1H), 9.33 (q, *J* = 3.2 Hz, 1H), 8.40 (m, *J* = 2.3 Hz, 1H), 8.34 (m, *J* = 2.2 Hz, 1H), 8.17 (q, *J* = 2.9 Hz, 1H), 8.03 (m, *J* = 3.7 Hz, 2H), 7.88 (m, *J* = 3.1 Hz, 3H), 7.41 (q, *J* = 8.6 Hz, 1H). HRMS (ESI), Calcd. for $C_{21}H_{12}NF_2O_3(M+H)^+$: 364.0780 ; found: 364.0775.

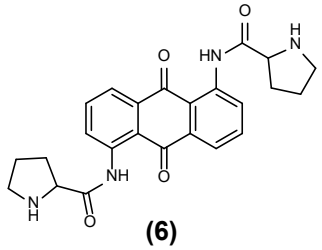
N-(9,10-dioxo-9,10-dihydroanthracen-1-yl)-1 naphthamide (3p)



(3p)

The reaction was carried out according to the general procedure A using **1** (56 mg, 0.25 mmol), 1-naphthoic acid (**2p**) (47.5 mg, 0.3 mmol), DIPEA (87 mg, 0.5 mmol), COMU (107 mg, 0.25 mmol). Conditions: 0 - 55 ºC, 24 h. Yield: 58 % ; ^{1}HNMR (400 MHz, DMSO-*d*6) δ 12.78 (s, 1H), 9.25 (q, *J* = 3.2 Hz, 1H), 8.43 (m, *J* = 1.6 Hz, 1H), 8.21 (m, *J* = 2.5 Hz, 3H), 8.05 (m, *J* = 3.8Hz, 4H), 7.93 (m, *J* = 2.7 Hz, 2H), 7.74(q, *J* = 5.1 Hz, 1H), 7.66 (m, *J* = 1.9 Hz, 2H).). Ion trap LCMS(ESI), Calcd. for $C_{21}H_{12}NF_2O_3(M+H)^+$: 378.10 ; found: 377.82.

***N,N'*-(9,10-dioxo-9,10-dihydroanthracene-1,5-diyl)bis(pyrrolidine-2-carboxamide)** (**5**)

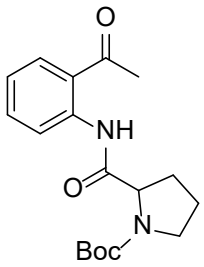


(6)

The reaction was carried out according to the general procedure A using 1,5-diaminoanthracene-9,10-dione (**1b**) (200 mg, 0.0.84 mmol), (tert-butoxycarbonyl)proline (**2a**) (398 mg, 1.85 mmol), DIPEA (542 mg, 4.2 mmol), COMU (540 mg, 1.26 mmol). Conditions: 0- 55 ºC, 24 h. Yield : 58 % ; ^{1}H NMR (400 MHz, DMSO-*d*6) δ 11.98 (s, 2H), 9.54 (br, 4H), 8.70 (q, J=3.0Hz, 2H), 7.98 (m, J=7.1Hz,4H), 4.67(t, *J* = 7.8 Hz 2H), 3.29 (q, J=5.6Hz, 4H), 2.55 (m, *J* = 5.3 Hz, 2H), 2.18 (m, J=7.0Hz,2H),2.03 (m, J=6.7Hz, 4H);^{13}CNMR(DMSO-*d*6,100MHz) δ185.14,167.99,139.09,135.84,134.49,126.88,

123.24118.99, 60.43, 45.45, 29.10, 23.58; HRMS (ESI): Calcd. for $C_{19}H_{16}N_2O_3$ (M+H)+, 433.180; found. 433.1868.

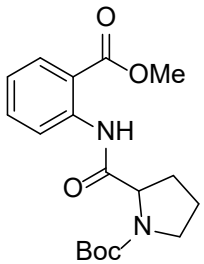
tert-butyl 2-((2-acetylphenyl)carbamoyl)pyrrolidine-1-carboxylate (5a)



5a (61%)

The reaction was carried out according to the general procedure A using 1-(2-aminophenyl)ethan-1-one (**1c**) (200 mg, 1.48 mmol), (tert-butoxycarbonyl)proline (**2a**) (382 mg, 1.78 mmol), DIPEA (573 mg, 4.44 mmol), COMU (951mg, 2.22 mmol). Conditions: 0-55 ºC, 24 h. Yield : 61% ; ^{1}H NMR (400 MHz, DMSO-*d*6) δ 10.47 (d, J=71.2 1H), 7.83 (q, J=23.5, 1H), 7.64 (m, J=6.5Hz, 4H), 7.48 (m, J=8.3Hz,3H), 7.28(t, *J* = 7.2 Hz 1H), 4.11 (m, J=6.4Hz, 1H), 3.32 (m, *J* = 14.44 Hz, 2H), 1.91 (t, J=9.7 Hz,1H),1.62(d, J=6.8Hz, 2H), 1.30 (d, J=32.1Hz, 10H).; ^{13}C NMR (DMSO-*d*6, 100MHz) δ 195.97, 195.56, 171.16, 170.89, 153.70, 153.04, 137.34, 136.73, 132.53, 132.21, 131.19, 130.75, 129.41, 129.25, 128.23, 127.94, 123.95, 123.63, 122.73, 122.18, 78.86, 78.58, 60.40, 46.58, 46.36, 29.97, 29.16, 27.95, 27.86, 23.78, 23.07.; HRMS (ESI): Calcd. for $C_{18}H_{24}N_2O_4$ (M+H)+, 334.40; found. 334.9854

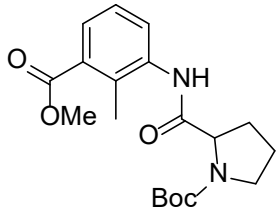
tert-butyl2-((2-(methoxycarbonyl)phenyl)carbamoyl)pyrrolidine-1-carboxylate (5b)



5c (48%)

The reaction was carried out according to the general procedure A using methyl 2-aminobenzoate (**1d**) (200 mg, 1.32 mmol), (tert-butoxycarbonyl)proline (**2a**) (342 mg, 1.59 mmol), DIPEA (513 mg, 3.97 mmol) COMU (850 mg, 1.95 mmol). Conditions: 0-55 ºC - rt, 24 h. Yield : 48%; ^{1}H NMR (400 MHz, DMSO-*d*6) δ 11.09 (d, J=7.7 Hz, 1H), 7.63 (q, J=5.2Hz,1H), 7.19 (t, J=7.5Hz, 1H), 4.20 (s,1H), 3.87 (s, *3*H), 3.45 (m, J=9.6Hz,2H), 2.26 (s,1H), 1.92 (m, J=12.8Hz, 3H), 1.34 (d, J+69.5Hz, 9H).; ^{13}CNMR (DMSO-*d*6,100MHz) 171.69, 171.47, 167.54, 154.04, 153.13, 139.73, 134.32, 130.70, 123.07, 120.10, 119.82, 116.49, 115.88, 79.23, 78.96, 61.84, 61.60, 52.47, 46.80, 46.55, 30.86, 29.97, 28.03, 27.76, 23.90, 23.30; HRMS (ESI): Calcd. for $C_{18}H_{24}N_2O_5$ (M+H)+, 349.3999; found. 349.1728.

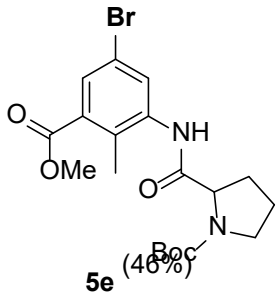
tert-butyl2-((3-(methoxycarbonyl)-2-methylphenyl)carbamoyl)pyrrolidine-1-carboxylate (5e)



5d (45%)

The reaction was carried out according to the general procedure A using methyl 3-amino-2-methylbenzoate (**1f**) (200 mg, 1.21 mmol), (tert-butoxycarbonyl)proline (**2a**) (313 mg, 1.45 mmol), DIPEA (469mg, 3.63 mmol), COMU (778 mg, 1.82 mmol). Conditions: 0-55 ºC - rt, 24 h. Yield : 45% ; ^{1}H NMR (400 MHz, CDCl3) δ 9.12 (s, 1H), 8.05(s, 1H), 7.60(s, 1H), 7.23 (t, J=7.9Hz,1H), 4.51(s, 1H), 3.88 (s, 3H), 3.45 (s, 2H), 2.60 (s, 1H),2.45(s,3H); 1.95 (s, 3H), 1.49 (s, 9H). ; ^{13}CNMR (CDCl3-101MHz) 170.30, 168.40, 156.51, 137.20, 131.40, 130.21, 126.39, 125.85, 80.99, 60.53, 52.05, 47.29, 28.41, 27.30, 24.65, 14.61; HRMS (ESI): Calcd. for $C_{19}H_{26}N_2O_5$ (M+H)+, 363.426; found. 363.1965.

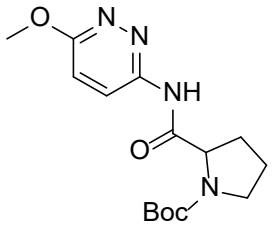
tert-butyl 2-((5-bromo-3-(methoxycarbonyl)-2-methylphenyl)carbamoyl)pyrrolidine-1-carboxylate (5e)



5e (46%)

The reaction was carried out according to the general procedure A using methyl 3-amino-5-bromo-2-methylbenzoate (**1g**) (200 mg, 0.82 mmol), (tert-butoxycarbonyl)proline (**2a**) (212 mg, 0.98 mmol), DIPEA (318 mg, 2.46 mmol), COMU (526 mg, 1.23 mmol). Conditions: 0 -55^{o}C - rt, 24 h. Yield: 46%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.12 (s, 1H), 8.05 (s, 1H), 7.60 (s, 1H), 7.23 (t, 4H), 4.67(t, *J* = 7.9 Hz, 1H), 4.51 (s, 1H), 3.88 (s, 3H), 3.45 (s, 9H). ^{13}CNMR ($CDCl_3$, 101MHz): δ 170.28, 167.07, 156.62, 138.56, 132.55, 128.69, 128.10, 119.02, 81.09, 60.50, 52.30, 47.30, 28.40, 2710, 24.64, 14.32. HRMS (ESI): Calcd.for $C_{19}H_{25}BrN_2O_5$ (M-H)-, 440.3220; found. 439.087 & 440.087.

tert-butyl 2-((6-methoxypyridazin-3-yl)carbamoyl)pyrrolidine-1-carboxylate (5f)



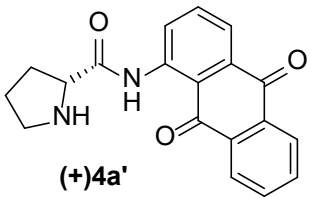
5d(53%)

The reaction was carried out according to the general procedure A using 6-methoxypyridazin-3-amine (**1h**) (200 mg, 1.60 mmol), (tert-butoxycarbonyl)proline (**2a**) (413 mg, 1.92 mmol), DIPEA (620 mg ,4.79 mmol), COMU (1.03 g, 2.40 mmol). Conditions: 0-55 ^{o}C - rt, 24 h. Yield : 53% ; ^{1}H NMR (400 MHz, DMSO-*d*6) δ 10.98 (d, J=20.8Hz,1H), 8.23 (t, J=9.5Hz, 1H), 7.26 (t, J=9.9Hz, 1H), 4.40 (m, J=6.1Hz 1H), 3.98 (s, *J* = 7.8 Hz 2H), 7.94-8.01 (m, 4H), 8.70 (dd, *J* = 7.9 Hz, 1.20 Hz 2H), 9.54 (br , 4H),11.98 (s, 3H) 3.39(q, J=5.6Hz,2H),2.21 (q, J=6.9Hz,1H),1.84 (m, J=7.0 Hz,3H)1.33 (d, J=51.7Hz,9H).; HRMS (ESI): Calcd. for $C_{15}H_{22}N_4O_4$ (M+H)+, 323.365; found. 323.170.

2.5. General procedure (B) for synthesis of (+)-4a', (-)-4a, (+)-4b'& (-)-4b.

To a stirred solution of compound (+)-**3a',** (-)-**3a,** (+)-**3b'&** (-)-**3** (1.0 equiv.) in THF (5 mL) at 0 ℃ was added 5M HCl (5 mL) and continued the stirring for 25 h at room temperature. After completion, the reaction mixture was concentrated under vacuum to obtain the residue, which was neutralized with aq. $NaHCO_3$ and extracted with DCM. The organic layer was dried over $NaSO_4$ and concentrated under vacuum to obtain (+)-**4a',** (-)-**4a,** (+)-**4b'&** (-)-**4b.**

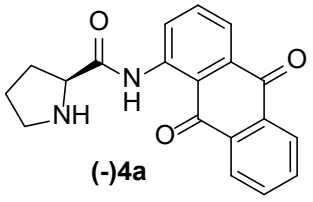
***(R)-N*-(9,10-dioxo-9,10-dihydroanthracen-1-yl)pyrrolidine-2-carboxamide**



(+)4a'

The reaction was carried out according to the general procedure B using (+)-**3a'** (105 mg, 0.25 mmol), COMU (107 mg, 0.25 mmol). Conditions: 0 ºC - rt, 25 h. Yield : 40% ; MP : 156-158 ºC; $[\alpha]_{D=}$+36.20 (c = 0.1, Acetonitrile); ^{1}HNMR (400 MHz, DMSO-*d*6) δ 1.65-1.72 (m, 2H), 1.83-1.91 (m, 1H), 2.07-2.17 (m,1H), 2.94-2.98 (m,1H), 3.07-3.13 (m, 1H), 3.84-3.88 (dd, *J* = 9.2 Hz,5.3 Hz, 1H), 7.86 (t, *J* = 7.8 Hz, 1H), 7.90-7.95 (m, 3H), 8.15-8.17(m, 1H), 8.22-8.24 (m,1H), 9.12 (dd, *J* = 8.3 Hz, 1.2Hz, 1H) 13.18 (s, 1H); ^{13}CNMR (DMSO-*d*6, 100 MHz): δ 25.9, 30.8, 46.8, 61.4, 118.2, 121.6, 125.2, 126.3, 126.9, 132.1, 133.7, 133.8, 134.3, 134.6, 135.2, 140.6, 176.2, 182.3, 185.3; Chiral purity (ee) by SFC: 98.40%; FT-IR (film cm-1) 3362,2964,1661,1497,1264,804. HRMS (ESI): Calcd. for $C_{19}H_{16}N_2O_3$ (M+H)+, 321.1234; found. 321.1228.

***(S)-N*-(9,10-dioxo-9,10-dihydroanthracen-1-yl)pyrrolidine-2-carboxamide**

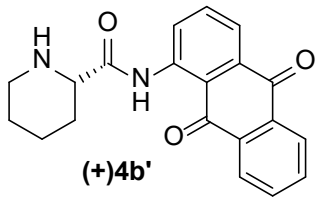


(-)4a

The reaction was carried out according to the general procedure B using (-)-**3a** (105 mg, 0.25 mmol), COMU (107 mg, 0.25 mmol). Conditions: 0 ºC - rt, 25 h. Yield 38%; MP: 162-164 0 ºC. $[\alpha]_{L=}$-41.72 (c = 0.1, Acetonitrile); ^{1}HNMR (400 MHz, DMSO-*d*6) δ 1.65-1.72 (m, 2H), 1.83-1.91 (m, 1H), 2.07-2.17 (m,1H), 2.94-2.98 (m,1H), 3.07-3.13 (m, 1H), 3.84-3.88 (dd,*J* = 9.2 Hz,5.3 Hz, 1H), 7.86 (t, *J* = 7.8 Hz, 1H), 7.90-7.95 (m, 3H),8.15-8.17 (m, 1H), 8.22-8.24 (m,1H), 9.12(dd,*J* = 8.3 Hz,1.2Hz, 1H) 13.18 (s, 1H); ^{13}CNMR (DMSO-D6, 100

MHz) δ 25.9, 30.8, 46.8, 61.4, 118.2, 121.6, 125.2, 126.3, 126.9, 132.1, 133.7, 133.8, 134.3, 134.6, 135.2, 140.6, 176.2, 182.3, 185.3; Chiral purity(ee) by SFC: 98.72 %, FT-IR (film) cm^{-1} 3362, 2964,1661,1497,1264,804 ; HRMS (ESI): Calcd. for $C_{19}H_{16}N_2O_3$ (M+H)+, 321.1234; found. 321.1224.

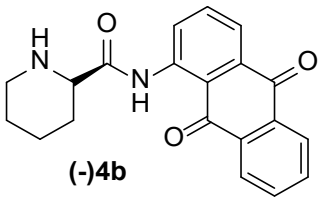
***(R)-N*-(9,10-dioxo-9,10-dihydroanthracen-1-yl)piperidine-2-carboxamide (+)4b'**



(+)4b'

The reaction was carried out according to the general procedure B using (-)-**3b'** (109 mg, 0.25 mmol), COMU (107 mg, 0.25 mmol). Conditions: 0 ºC - rt, 25 h. Yield : 35% ; MP; 160-162 ºC; $[\alpha]_D$ 25 = +26.78 (c = 0.1, Acetonitrile); ^{1}HNMR (400 MHz, DMSO-*d*6) δ 1.43-1.57 (m, 4H), 1.71-1.73 (m, 1H), 1.86-1.89 (m,1H), 2.67-2.70 (m,1H), 2.99-3.02 (m, 1H), 3.36 (m, 1H), 7.87-7.97 (m, *J* = 7.8 Hz, 4H), 8.17-8.19 (m, 1H), 8.25-8.27 (m, 1H), 9.12 (dd, *J* = 8.3 Hz,1.2Hz, 1H) 12.78 (br, 1H); ^{13}CNMR (DMSO-*d*6, 100 MHz) δ 23.5, 25.5, 29.0, 49.9, 60.4, 118.0, 121.6, 125.5, 126.3, 127.1, 132.2, 133.7, 133.8, 134.5, 134.7, 135.4, 141.0, 174.3, 182.3, 185.6; Chiral purity(ee)by SFC: 99.98%, FT-IR (film cm^{-1}) 3302, 2927,1697, 1508, 1264, 705; HRMS (ESI),Calcd.for $C_{20}H_{19}N_2O_3(M+H)^+$: 335.1390 ; found: 335.1352.

***(S)-N*-(9,10-dioxo-9,10-dihydroanthracen-1-yl)piperidine-2-carboxamide**



(-)4b

The reaction was carried out according to the general procedure B using (-)-**3b** (109 mg, 0.25 mmol), COMU (107 mg, 0.25 mmol). Conditions: 0 ºC - rt, 25 h. Yield : 37%; MP 158-160 ºC; [α]D 25 = -27.06 (c =0.1, Acetonitrile); ^{1}HNMR (400 MHz, DMSO-*d*6) δ 1.43-1.57 (m, 4H), 1.71-1.73 (m, 1H), 1.86-1.89 (m,1H), 2.67-2.70 (m,1H), 2.99-3.02 (m, 1H), 3.36 (m, 1H), 7.87-7.97 (m, *J* = 7.8 Hz, 4H), 8.17-8.19 (m, 1H), 8.25-8.27 (m, 1H), 9.12 (dd, *J* = 8.3 Hz,1.2Hz, 1H) 12.78 (br, 1H); ^{13}CNMR (DMSO-*d*6, 100 MHz) δ 23.5, 25.5, 29.0, 49.9, 60.4, 118.0, 121.6, 125.5, 126.3, 127.1, 132.2, 133.7, 133.8, 134.5, 134.7, 135.4, 141.0, 174.3, 182.3, 185.6 Chiral purity (ee) by SFC: 99.86% FT-IR (film cm^{-1}) 3302, 2929, 1696, 1508, 1266, 707. HRMS (ESI), Calcd. for $C_{20}H_{19}N_2O_3(M+H)^+$: 335.1390 ; found: 335.1353.

NMR abbreviations: s-singlet, d-doublet, t-triplet, m-multiplet, q-quartet, br-broad, dd-doublet of doublet.

4. SFC Experimental Procedure

Materials

Reagents

Methanol (MeOH), acetonitrile (ACN), Trifluoroacetic acid (TFA), diethylamine (DEA) and 7N Methanolic ammonia, Isopropanol (IPA), were of HPLC grade and purchased from Sigma-Aldrich Co. (Merck-INDIA).

Compounds

L- or D-pyrrolidine-2-carboxylic acid (9,10-dioxo-9,10-dihydro-anthracen-1-yl)-amide (I-II), L& D piperidine-2-carboxylic acid (9,10-dioxo-9, 10-dihydro-anthracen-1-yl)-amide (III-IV) were synthesized internally. The purity of the compounds was at least 95%. Structures of four derivatives are listed in Fig. 1.

Columns

Four analytical coated and immobilized polysaccharide-based chiral SFC columns (Chiralpak- IA (4.6X150) mm,3µ, Chiralpak-IB(4.6X150) mm,3µ, Chiralpak-IC (4.6X150) mm,3µ, Chiralpak-ID (4.6X150)mm,3µ, Chiralpak-IE (4.6X150)mm,3µ, Chiralpak-IF and Chiralpak-IG (4.6X150) mm,3µ and Chiralcel-OX-3 (4.6X150) mm,3µ SFC columns were purchased from Chiral Technologies (West Chester, PA, USA). Lux-cellulose-2 and Lux-amylose -2 (4.6 X 250)mm,5µ were purchased from Phenomenex (Torrance, CA, USA). One Whelk-O 1 (RR) (4.6 X 250) mm,5µ was purchased from Regis (Morton Grove, IL, USA).

SFC instrumentation

Analytical Acquity UPC2 PDA (Waters) with a six-position modifier and column-switching valves, Thar SFC method development stations (SFC Method Station) with a six-position modifier and a ten-position column switching valves, and Waters SFC150Mgm prep were all purchased from Waters (WATERS GES MBH, W-Austria).

Methods

Analytical SFC methods

All analytical SFC experiments were performed either on Acquity UPC2 PDA or a Waters analytical SFC system. All method development work was performed on (4.6X150) mm, 3µ dimension columns under gradient or isocratic conditions at a back-pressure of 100 bar, a temperature of 30 ˚C, a flow rate of 3 ml/min, and a wavelength of 215 nm. The initial gradient program was run from 10% to 50% Co-solvents for 8 min, and 50% co-solvent for an additional 4 min. 30% of the Co-solvent ratio was stabilized for scale-up.

Preparative SFC methods

All preparative SFC separations were carried out on Chiralcel-OX-H (30X250)mm,5µ column on Waters 150Mgm SFC instrument under isocratic conditions at a back pressure of 100 bar and a temperature of 30 ºC.

Sample solution

Preparation For all the analytical SFC experiments, compounds **(±)-3a, (±)-3b** and **3d** were dissolved in MeOH at a concentration of ~1 mg/ml. For the preparative-scale SFC, 1-1.25 g of crude **(±)-3a, (±)-3b** and **3d** were dissolved in MeOH at 100 mg/ml. Total purification was completed within 2 hours of time with 50 mg/injection.

5.0 General Procedure for Antibacterial activity

The bacterial and fungal pathogens obtained from Microbial Type Culture Collection (MTCC), Chandigarh, and Government of India. The synthesized compounds were tested for their antibacterial efficacy against both gram positive and gram negative bacterial pathogens. The Gram-positive bacterial pathogens were Vibrio cholera (MTCC 3906), Salmonella typhi (MTCC 531) and Pseudomonas aeruginosa (MTCC 1688). The Gram negative bacterial pathogens were Rhodococcusrhodochrous (MTCC-265), Mycobacterium smegmatis (MTCC-994) and Micrococcus luteus (MTCC 1809). The synthesized compounds were tested for their antifungal efficacies against the fungal pathogens were Pichia jadinii MTCC 185, Candida parapsilosis MTCC 7043 and Candida glabrata MTCC 3019.

Determination of MIC and MBC values of synthesised compounds

The minimum inhibitory concentration (MIC) was determined to espouse the serial dilution technique using 96-well microplates.1 All the bacterial strains were prepared by Muller Hinton agar, and the turbidity of all the bacterial strains was adjusted to 0.5 McFarland Standard by making a bacterial suspension of three to five well-isolated colonies of the same morphological type selected from an agar plate culture. The cultures were further, diluted 1,000-fold to get an inoculums size of 1.5 x 10^5 CFU/mL 2 100 µL of sterilized Mueller Hinton broth added into the wells of a 96-well plate. The first row served as growth control. Then, the highest concentration (64 µg) of 100 µL of compounds (+)-**4a',** (-)-**4a,** (+)-**4b'&** (-)-**4b,** samples were poured in the second row of the plate. The compound dissolved in dimethyl sulfoxide (DMSO) serially diluted to create a concentration sequence from 64 to 1 mg/ml was tested against bacterial pathogens. The first row served as growth control. Finally, 10 µL of bacterial suspensions were added to deep wells of the plate incubated for 24 h at 37 °C. The streptomycin sulphate is used as a positive control. The resulting turbidity observed, and after 24 h, MIC determined as one where growth was no longer visible by assessment of turbidity by optical density reading at 600 nm in a microplate reader. The MBC values are the least concentration of an antibacterial compound that prevents the growth of the organism on the agar plates. It is evaluated by subculturing broth dilutions that of MIC values determined microplate. The dilutions are streaked onto sterilized Mueller Hinton agar plates and incubated for 24 hours. No growth on the plate implies that no viable organisms found in broth.

Determination of MIC and MFC values

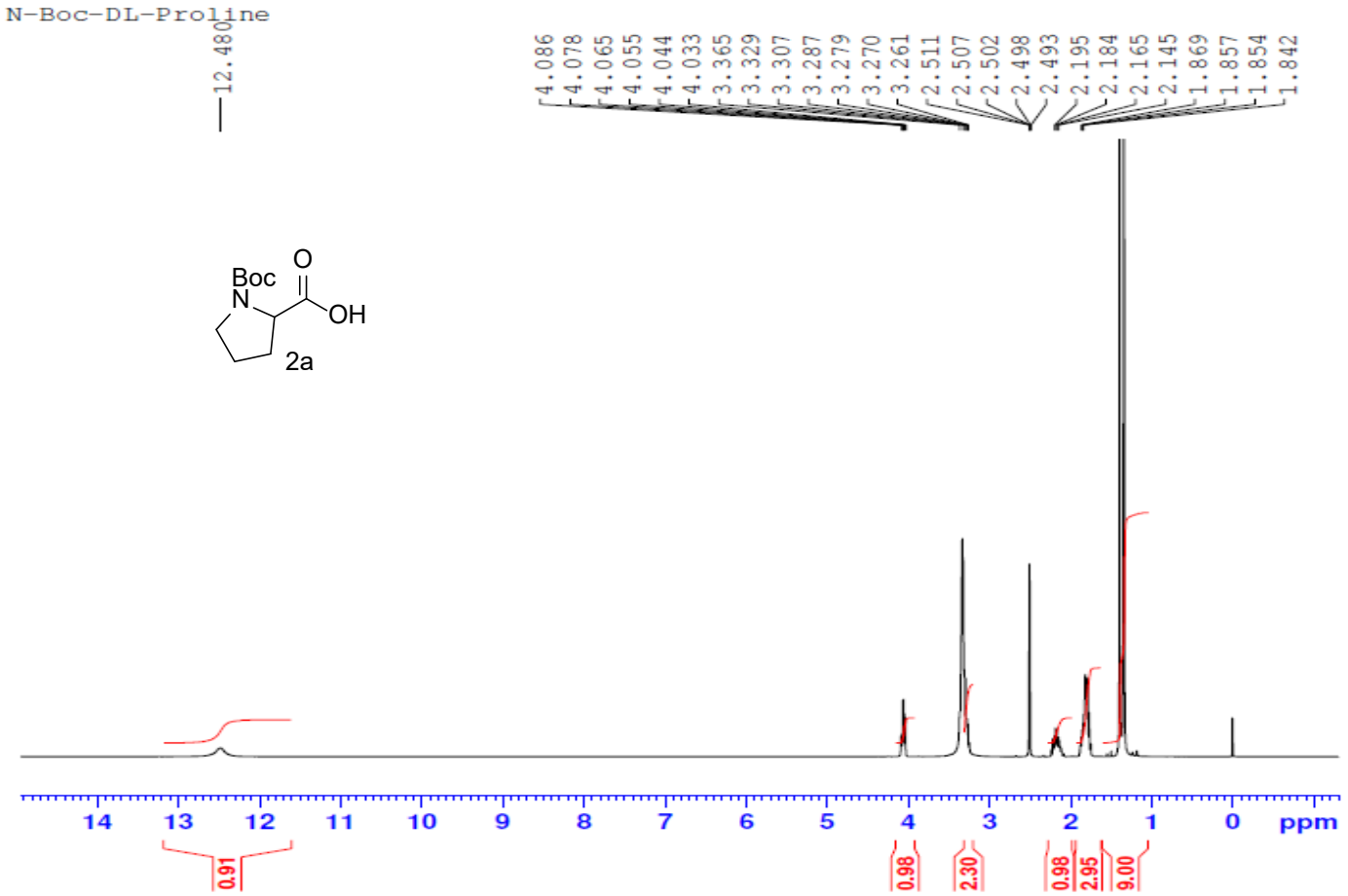
The determination of MIC and MFC for the synthesized compounds (+)-**4b'&** (-)-**4b** was assessed by the broth micro dilution method. 100 µL of YPD broth added into the wells of a 96-well plate. The first row served as growth control. Then, the highest concentration (64 µg) of 100 µL of compounds (+)-**4a',** (-)-**4a,** (+)-**4b'&** (-)-**4b** samples were poured in the second row of the plate. Doubled serial dilutions, where a 100 µL aliquot removed from the most concentrated well went to the next well, and yielded concentrations of 64 to 1µg/mL. Finally, 10 µL of yeast inoculum suspensions were added to each well of the plate and incubated at 37 °C for 24 h. After incubation the inhibition of visible growth defined as the MIC. This MIC value was further confirmed by Resozurin dye assay. The MFC defined as the minimal concentration of tested compounds required to kill 99.9% the yeast. The dilutions are streaked onto YPD agar plates and incubated for 24 h. No growth on the Petri dishes implies that no viable organisms found in the broth.

Resazurin dye assay

The 750 mg of Resazurin dye was dissolved in 100 ml sterile water. Vortex mixer used to homogenize the solution. This solution then referred to as Resazurin dye solution. After incubated followed by the serial dilution technique using 96-well microplates, 10 µl of Resazurin solution as the indicator added in each well. The plates were again incubated in a temperature-controlled incubator at 37 °C for 4 h. The colour change in the well then observed visually. The purple to pink colour changes taken indicates the growth inhibition of microbes. The lowest concentration of compound at which colour change occurred recorded as the MIC value.

6. Copies of ^{1}H NMR, ^{13}C NMR Spectra

(*tert*-butoxycarbonyl)proline (2a) -1HNMR spectra

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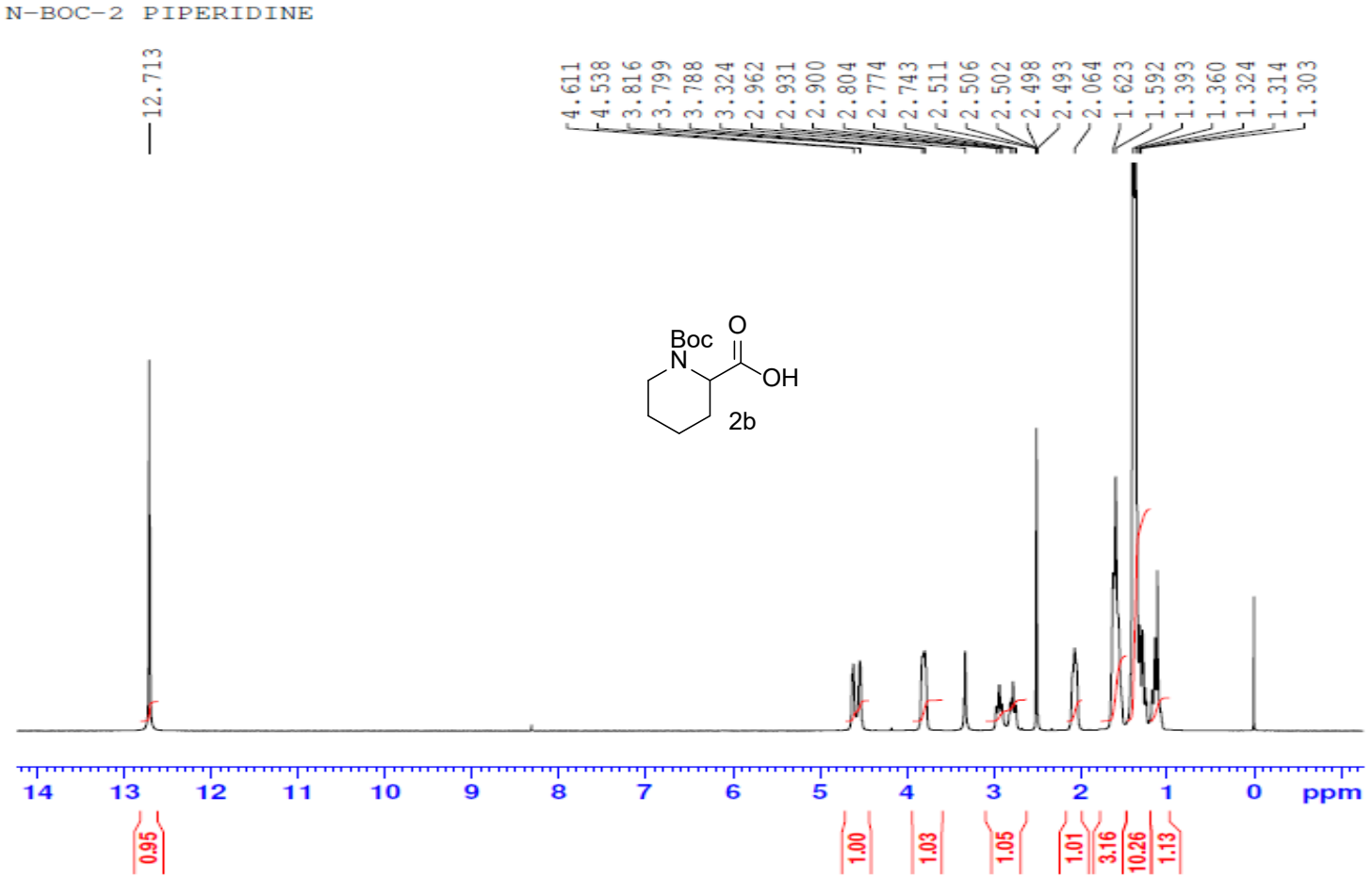
NMR-02

1-(*tert*-butoxycarbonyl)piperidine-2-carboxylic acid (DL-2b)- 1HNMR spectra

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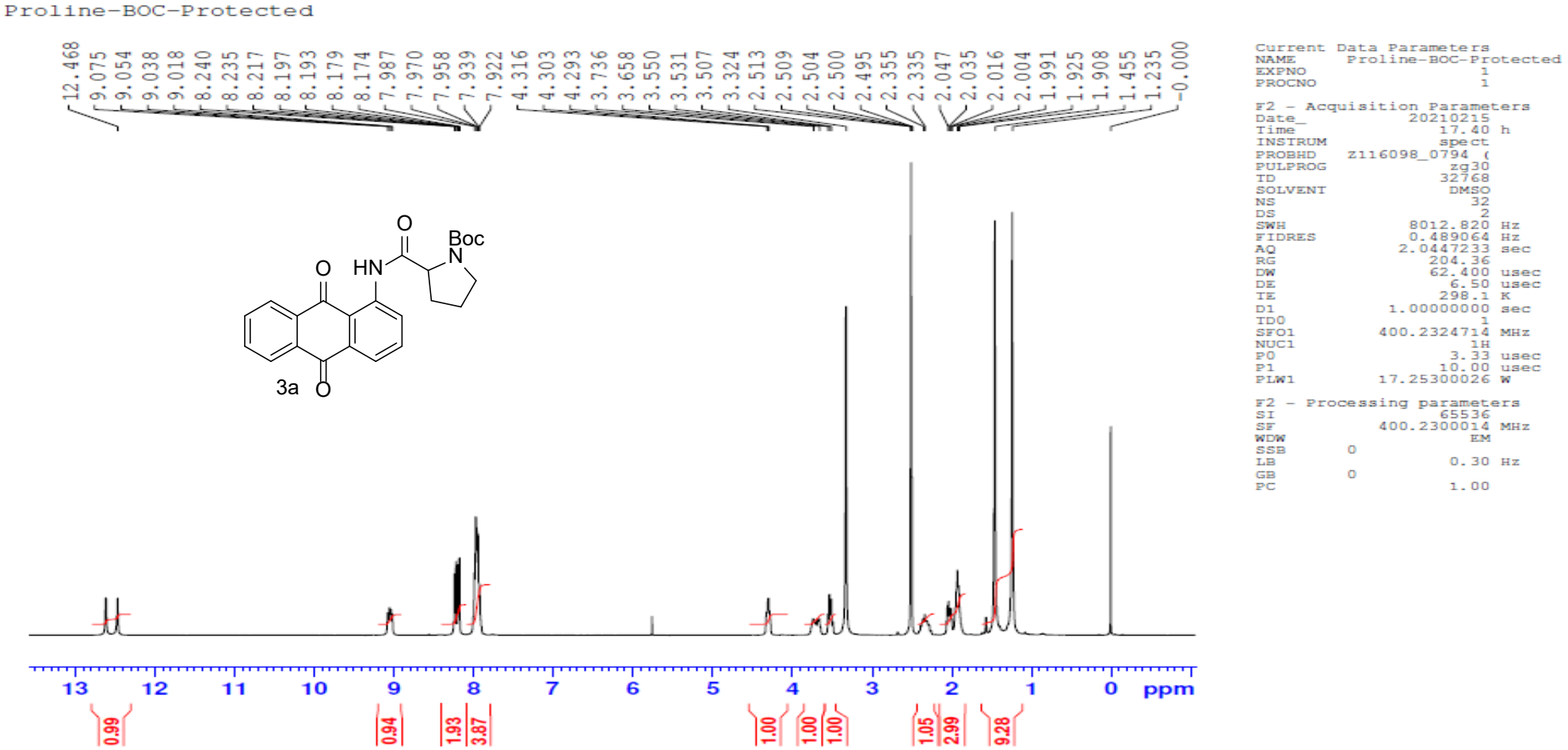
***tert*-Butyl 2-((9,10-dioxo-9,10-dihydroanthracen-1-yl)carbamoyl)pyrrolidine-1-carboxylate (±)-3a-1H NMR spectra**

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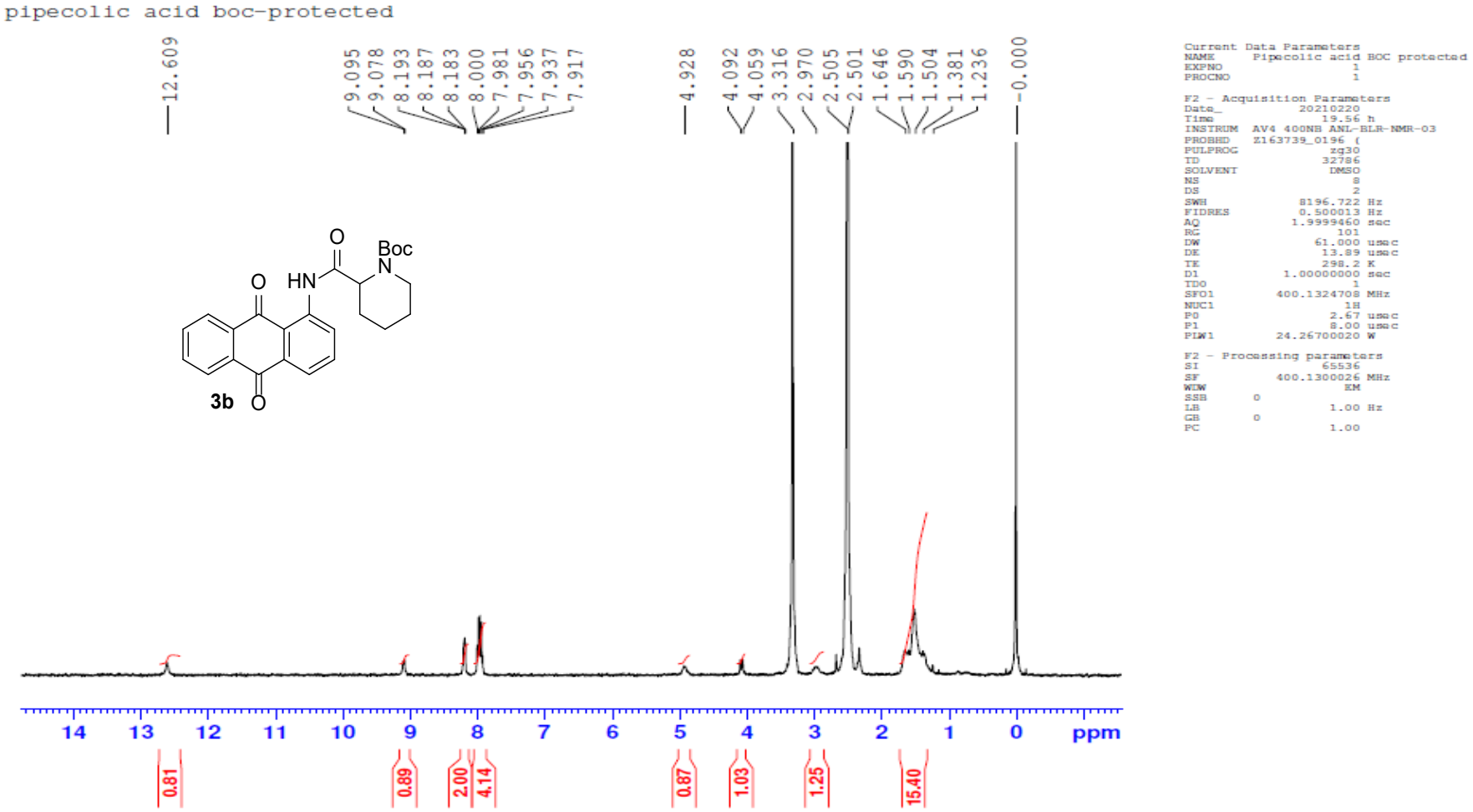
***tert*-butyl 2-((9,10-dioxo-9,10-dihydroanthracen-1-yl)carbamoyl)piperidine-1-carboxylate (±)3b- 1H NMR spectra**

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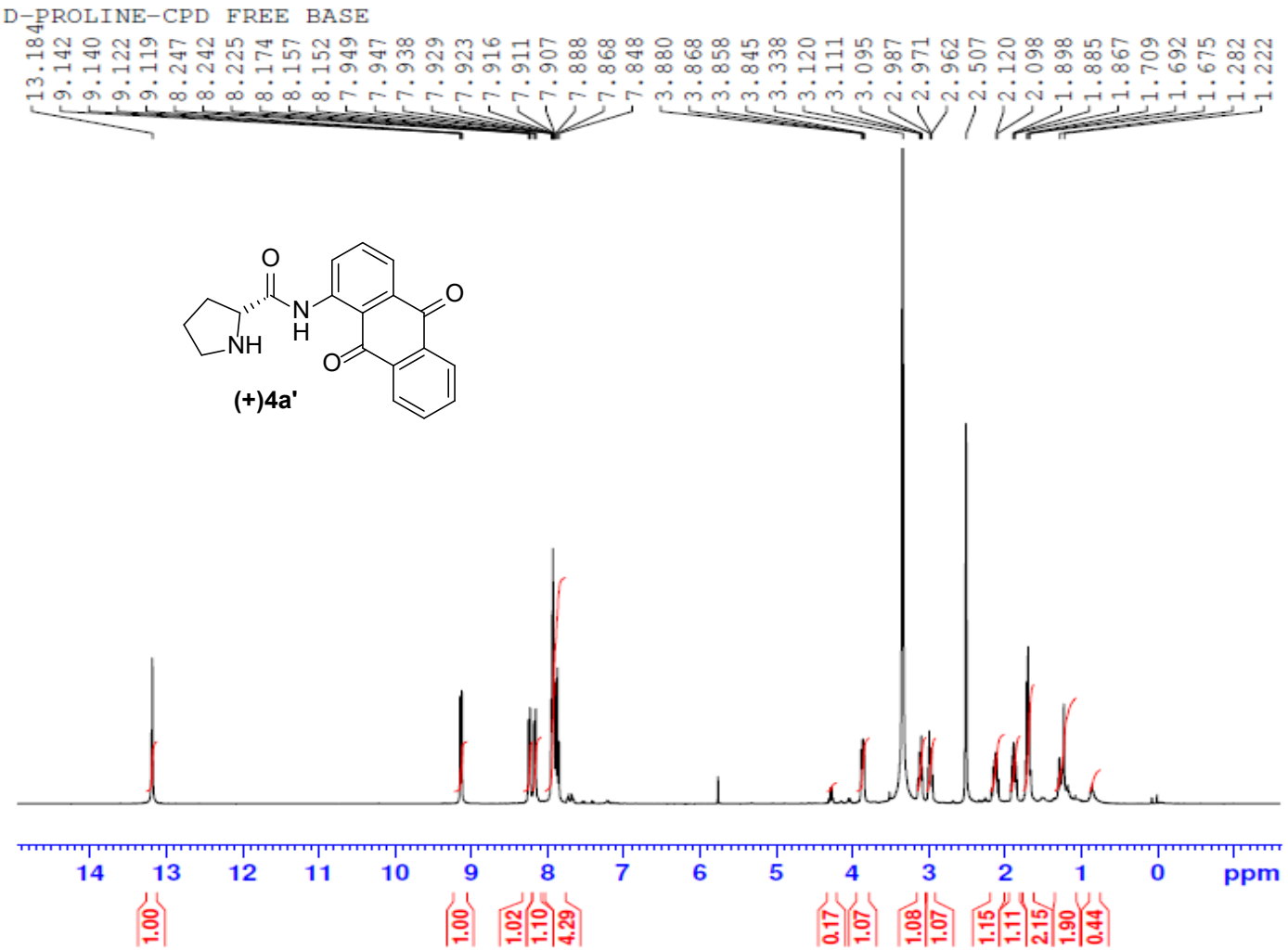
(R)-N-(9,10-dioxo-9,10-dihydroanthracen-1-yl)pyrrolidine-2-carboxamide -1HNMR spectra

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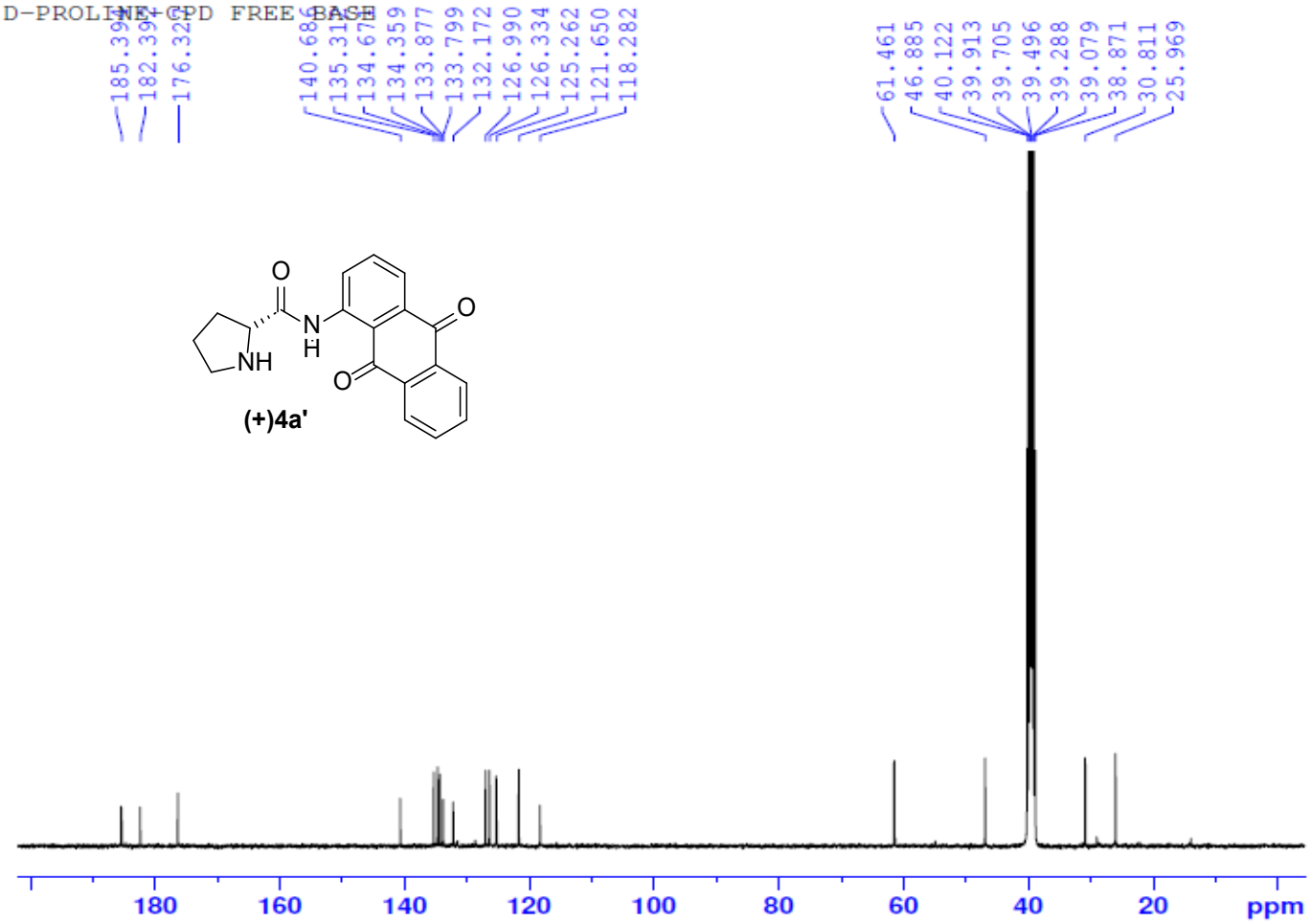
NMR-02

(R)-N-(9,10-dioxo-9,10-dihydroanthracen-1-yl)pyrrolidine-2-carboxamide -13C spectra

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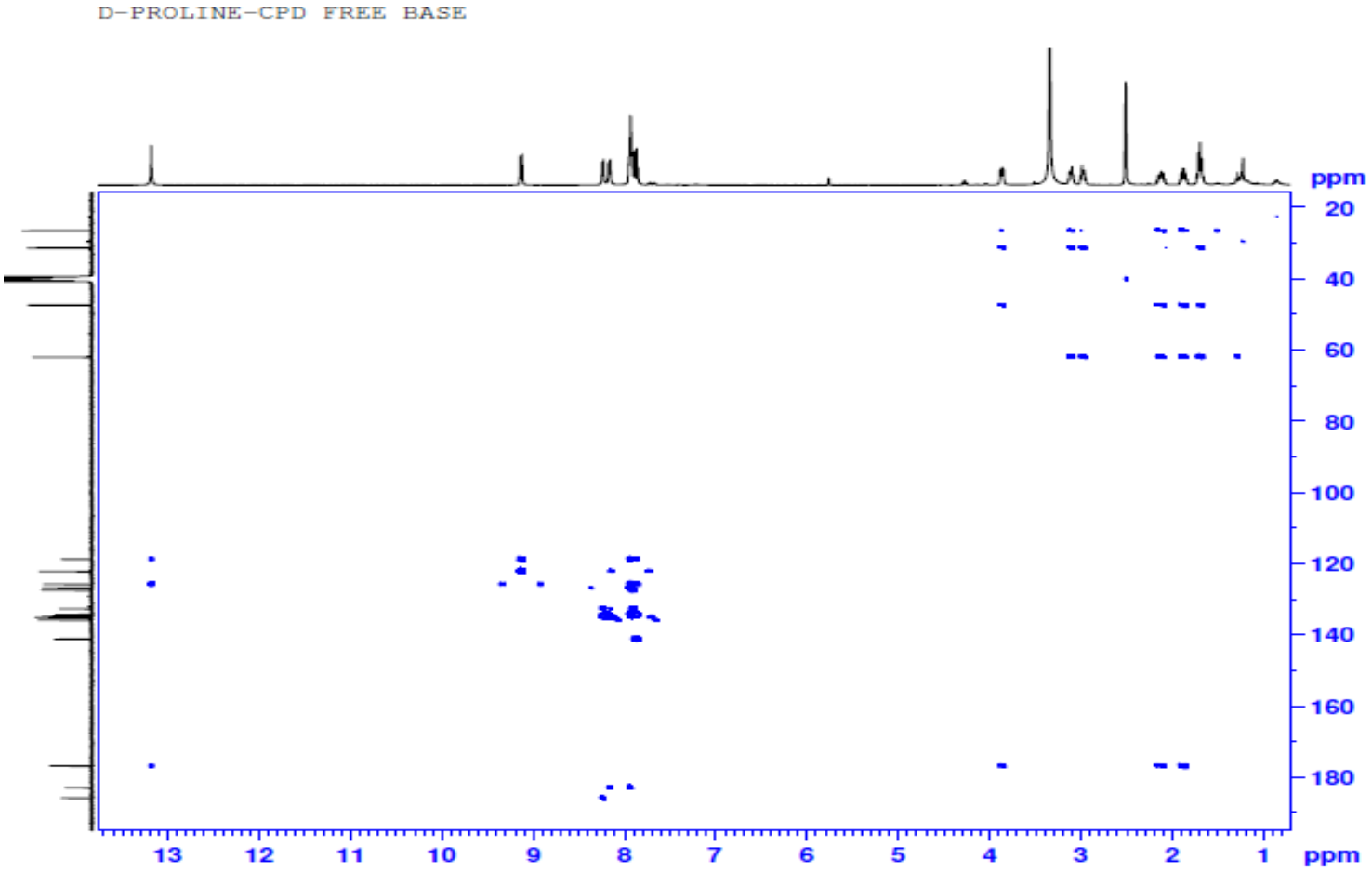
NMR-02

(R)-N-(9,10-dioxo-9,10-dihydroanthracen-1-yl)pyrrolidine-2-carboxamide -2D NMR data

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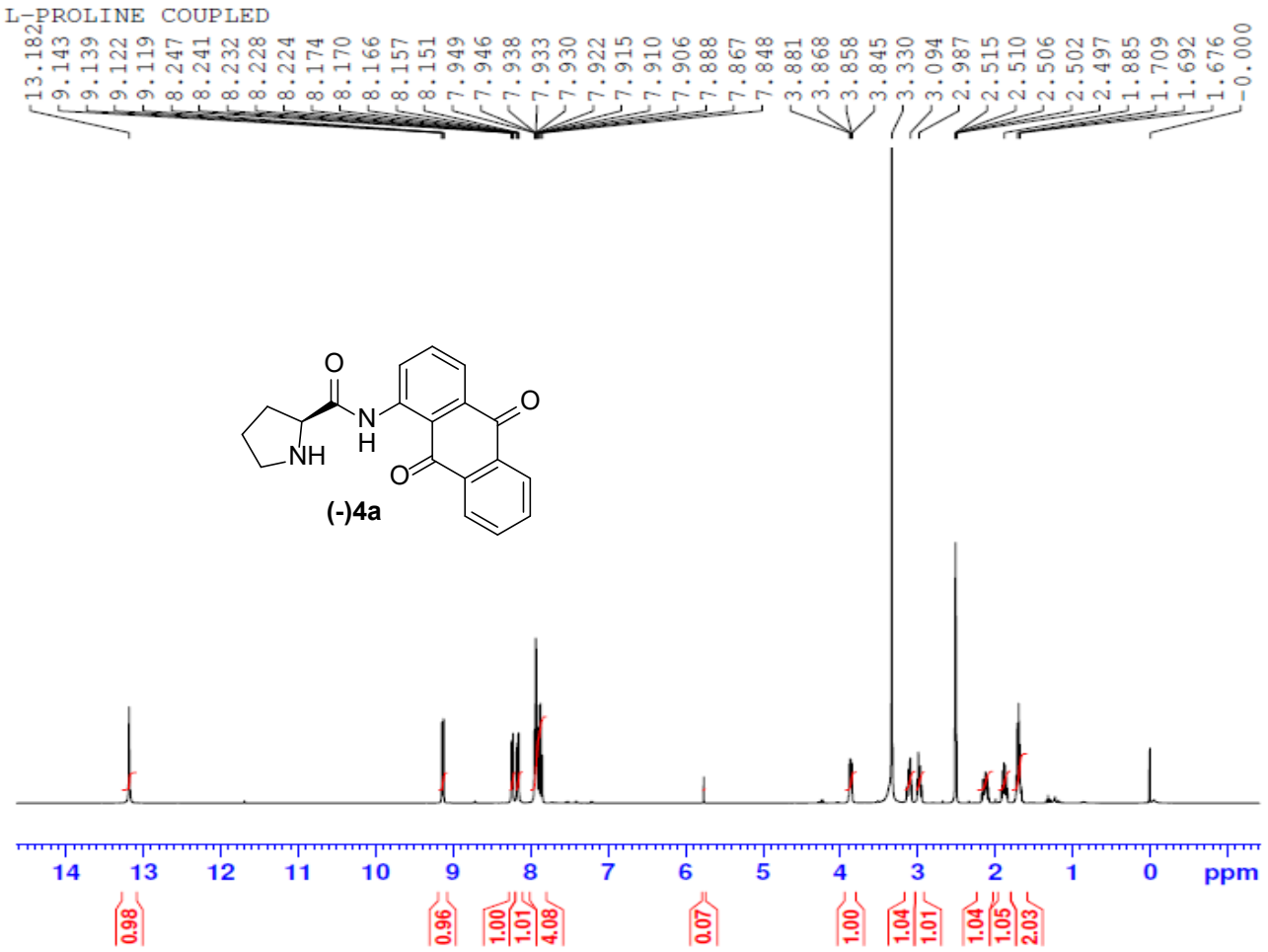
(S)-N-(9,10-dioxo-9,10-dihydroanthracen-1-yl)pyrrolidine-2-carboxamide -1HNMR spectra

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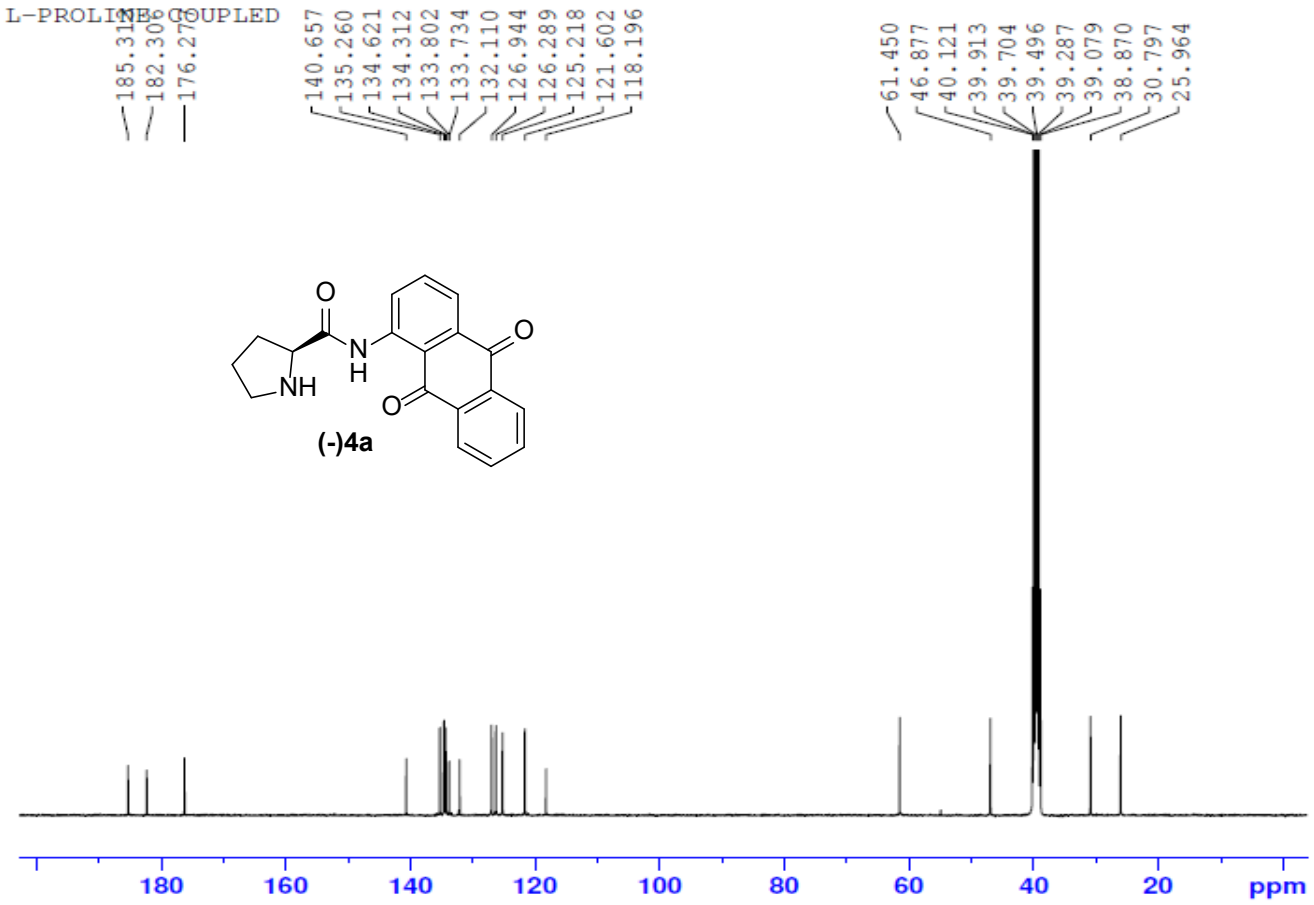
NMR-02

(S)-N-(9,10-dioxo-9,10-dihydroanthracen-1-yl)pyrrolidine-2-carboxamide -13C spectra

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DE                 6.50 usec
TE                298.2 K
D1             3.00000000 sec
D11            0.03000000 sec
TD0                      1
SFO1          100.7234199 MHz
NUC1                  13C
P0                 3.33 usec
P1                10.00 usec
PLW1          56.74499893 W
SFO2          400.5316021 MHz
NUC2                  1H
CPDPRG[2          waltz65
PCPD2             90.00 usec
PLW2          15.46500015 W
PLW12          0.18945029 W
PLW13          0.09495249 W

F2 - Processing parameters
SI                   32768
SF            100.7133985 MHz
WDW                     EM
SSB       0
LB                 2.00 Hz
GB        0
PC                 1.40
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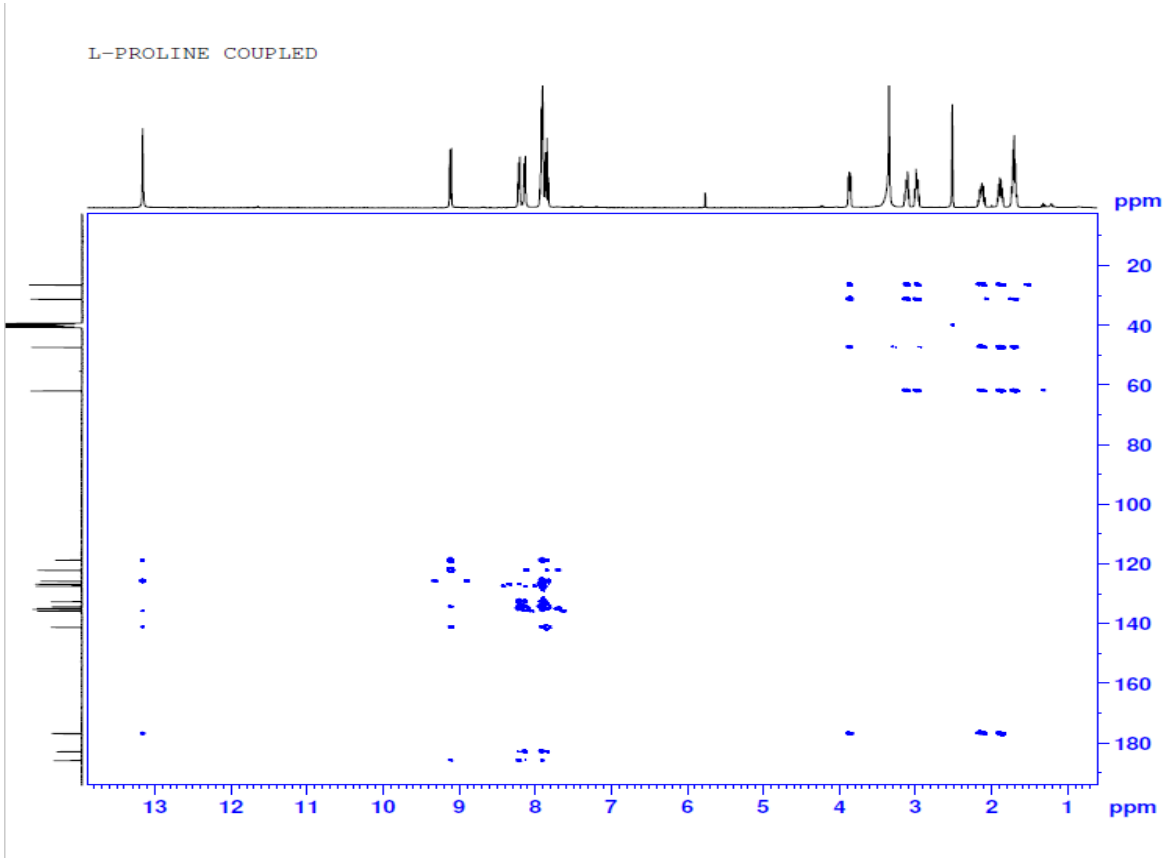
NMR-02

(S)-N-(9,10-dioxo-9,10-dihydroanthracen-1-yl)pyrrolidine-2-carboxamide -2D NMR data

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Current Data Parameters
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EXPNO                 4
PROCNO                1

F2 - Acquisition Parameters
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Time              22.23 h
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PULPROG    hmbcgplpndqf
TD                 2048
SOLVENT            DMSO
NS                   32
DS                   16
SWH           5882.353 Hz
FIDRES        5.744485 Hz
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RG                  101
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TE               298.1 K
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CNST13        10.0000000
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D1            1.50000000 sec
D2            0.00344828 sec
D6            0.05000000 sec
D16           0.00020000 sec
IN0           0.00002256 sec
Thav                  1
SFO1         400.5328749 MHz
NUC1                1H
P1                10.00 usec
P2                20.00 usec
PLW1         15.46500015 W
SFO2         100.7234199 MHz
NUC2                13C
P3                10.00 usec
PLW2         56.74499893 W
GPNAM[1]      SMSQ10.100
GPZ1              50.00 %
GPNAM[2]      SMSQ10.100
GPZ2              30.00 %
GPNAM[3]      SMSQ10.100
GPZ3              40.10 %
P16             1000.00 usec

F1 - Acquisition parameters
TD                 600
SFO1         100.7234 MHz
FIDRES        73.868881 Hz
SW           220.015 ppm
FnMODE              QF

F2 - Processing parameters
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SF           400.5299981 MHz
WDW               SINE
SSB       0
LB        0 Hz
GB        0
PC                1.40

F1 - Processing parameters
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MC2                QF
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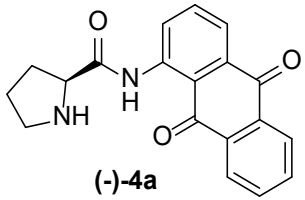
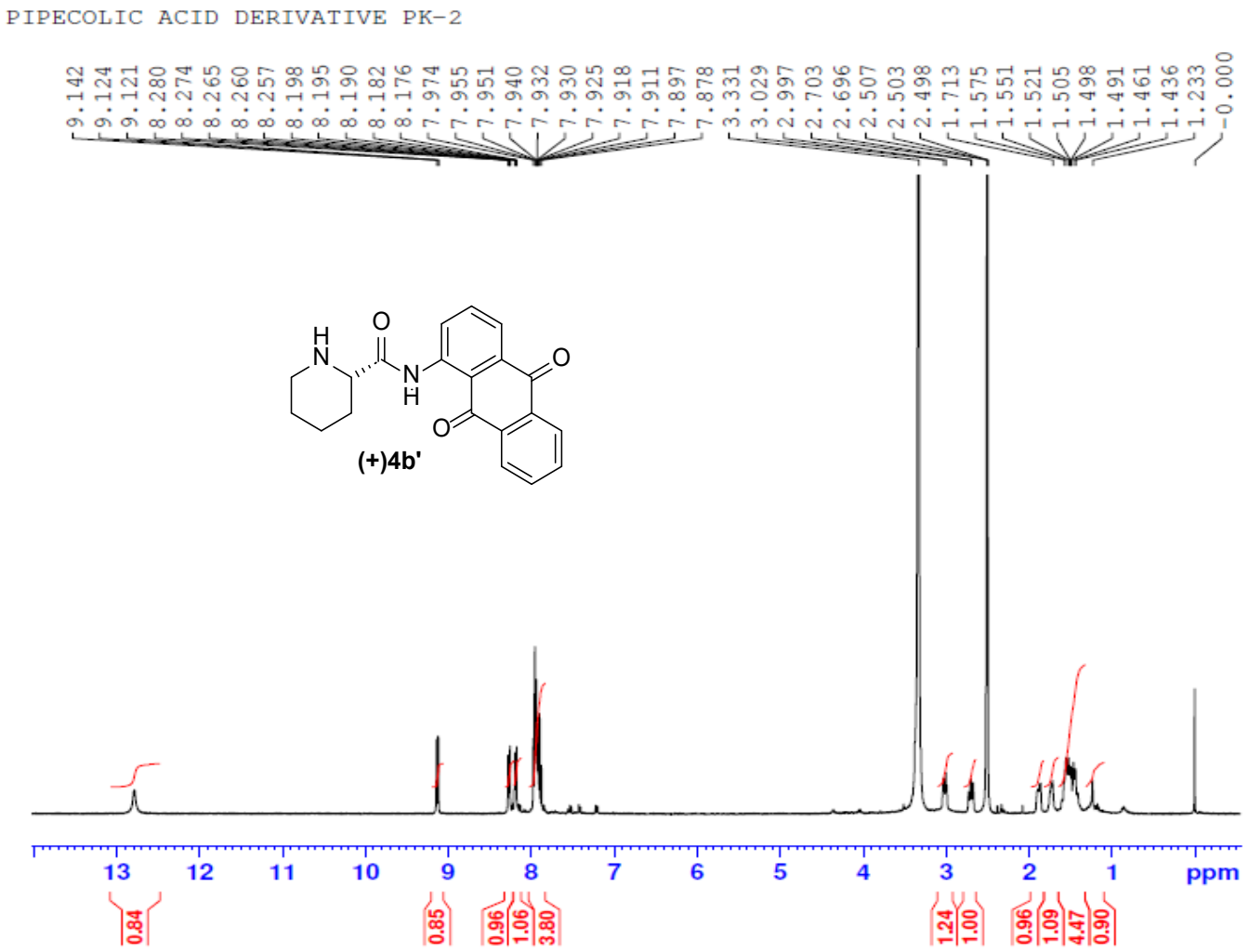


(-)-4a

(S)-N-(9,10-dioxo-9,10-dihydroanthracen-1-yl)piperidine-2-carboxamide- 1HNMR spectra

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Current Data Parameters
NAME      PIPECOLIC ACID DERIVATIVE PK-2
EXPNO                1
PROCNO               1

F2 - Acquisition Parameters
Date_         20190906
Time              18.43 h
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PROBHD   Z163739_0079 (
PULPROG           zg30
TD               65536
SOLVENT           DMSO
NS                  16
DS                   2
SWH            8196.722 Hz
FIDRES         0.250144 Hz
AQ             3.9976959 sec
RG                 101
DW                61.000 usec
DE                13.54 usec
TE                298.2 K
D1             1.00000000 sec
TD0                  1
SFO1           400.5324733 MHz
NUC1                 1H
P0                 3.33 usec
P1                10.00 usec
PLW1          15.46500015 W

F2 - Processing parameters
SI               65536
SF            400.5300018 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
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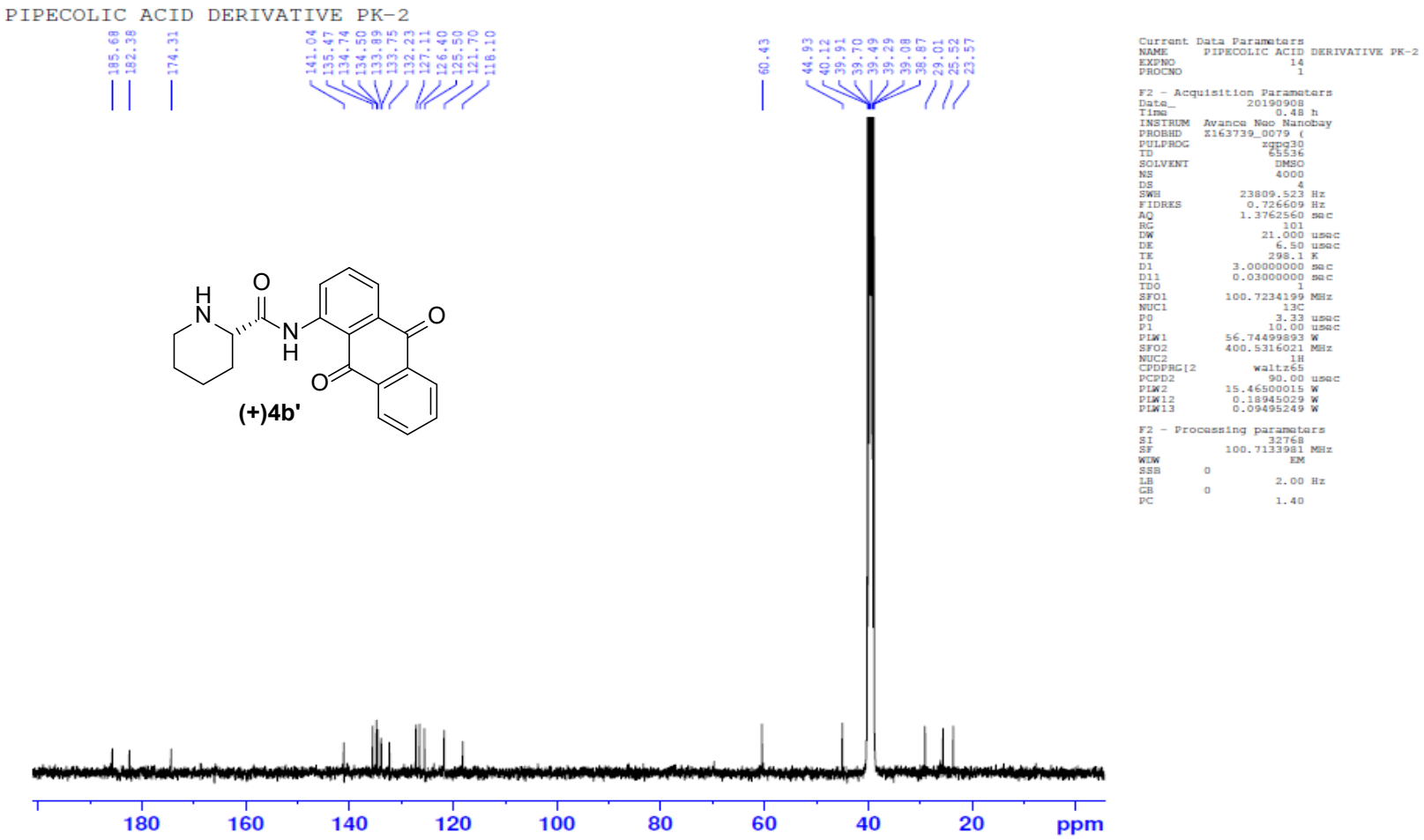
(S)-N-(9,10-dioxo-9,10-dihydroanthracen-1-yl)piperidine-2-carboxamide- 13C spectra

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Current Data Parameters
NAME      PIPECOLIC ACID DERIVATIVE PK-2
EXPNO                 14
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190908
Time               0.48 h
INSTRUM  Avance Neo Nanobay
PROBHD   Z163739_0079 (
PULPROG          zgpg30
TD              65536
SOLVENT            DMSO
NS                 4000
DS                    4
SWH           23809.523 Hz
FIDRES        0.726609 Hz
AQ            1.3762560 sec
RG                  101
DW               21.000 usec
DE                6.50 usec
TE               298.1 K
D1            3.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1         100.7234199 MHz
NUC1                13C
P0                 3.33 usec
P1                10.00 usec
PLW1         56.74499893 W
SFO2         400.5316021 MHz
NUC2                1H
CPDPRG[2         waltz65
PCPD2             90.00 usec
PLW2         15.46500015 W
PLW12         0.18945029 W
PLW13         0.09495249 W

F2 - Processing parameters
SI                 32768
SF           100.7133981 MHz
WDW                   EM
SSB       0
LB                 2.00 Hz
GB        0
PC                 1.40
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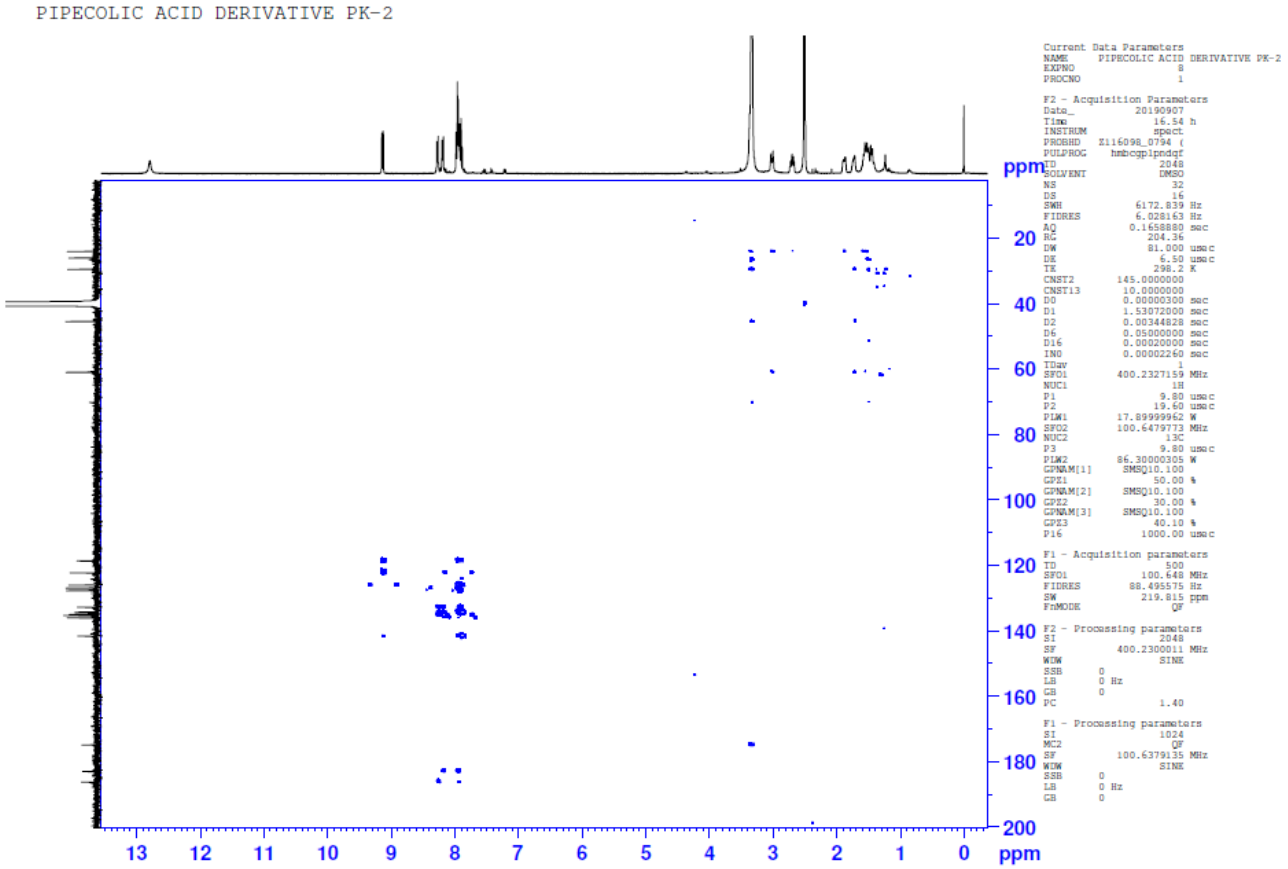
(S)-N-(9,10-dioxo-9,10-dihydroanthracen-1-yl)piperidine-2-carboxamide- 2D spectra



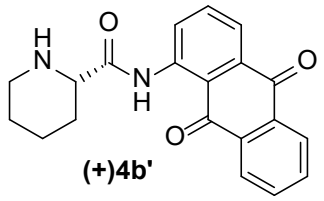
Current Data Parameters
NAME PIPECOLIC ACID DERIVATIVE PK-2
EXPNO 8
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190907
Time 16.54 h
INSTRUM spect
PROBHD Z116098_0794 (
PULPROG hmbcgplpndqf
TD 2048
SOLVENT DMSO
NS 32
DS 16
SWH 6172.839 Hz
FIDRES 6.028163 Hz
AQ 0.1658880 sec
RG 204.36
DW 81.000 usec
DE 6.50 usec
TE 298.2 K
CNST2 145.0000000
CNST13 10.0000000
D0 0.00000300 sec
D1 1.53072000 sec
D2 0.00344828 sec
D6 0.05000000 sec
D16 0.00020000 sec
IN0 0.00002260 sec
TD0 1
SFO1 400.2327159 MHz
NUC1 1H
P1 9.80 usec
P2 19.60 usec
PLW1 17.89999962 W
SFO2 100.6479773 MHz
NUC2 13C
P3 9.80 usec
PLW2 86.30000305 W
GPNAM[1] SMSQ10.100
GPZ1 50.00 %
GPNAM[2] SMSQ10.100
GPZ2 30.00 %
GPNAM[3] SMSQ10.100
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 500
SFO1 100.648 MHz
FIDRES 88.495575 Hz
SW 219.815 ppm
FnMODE QF

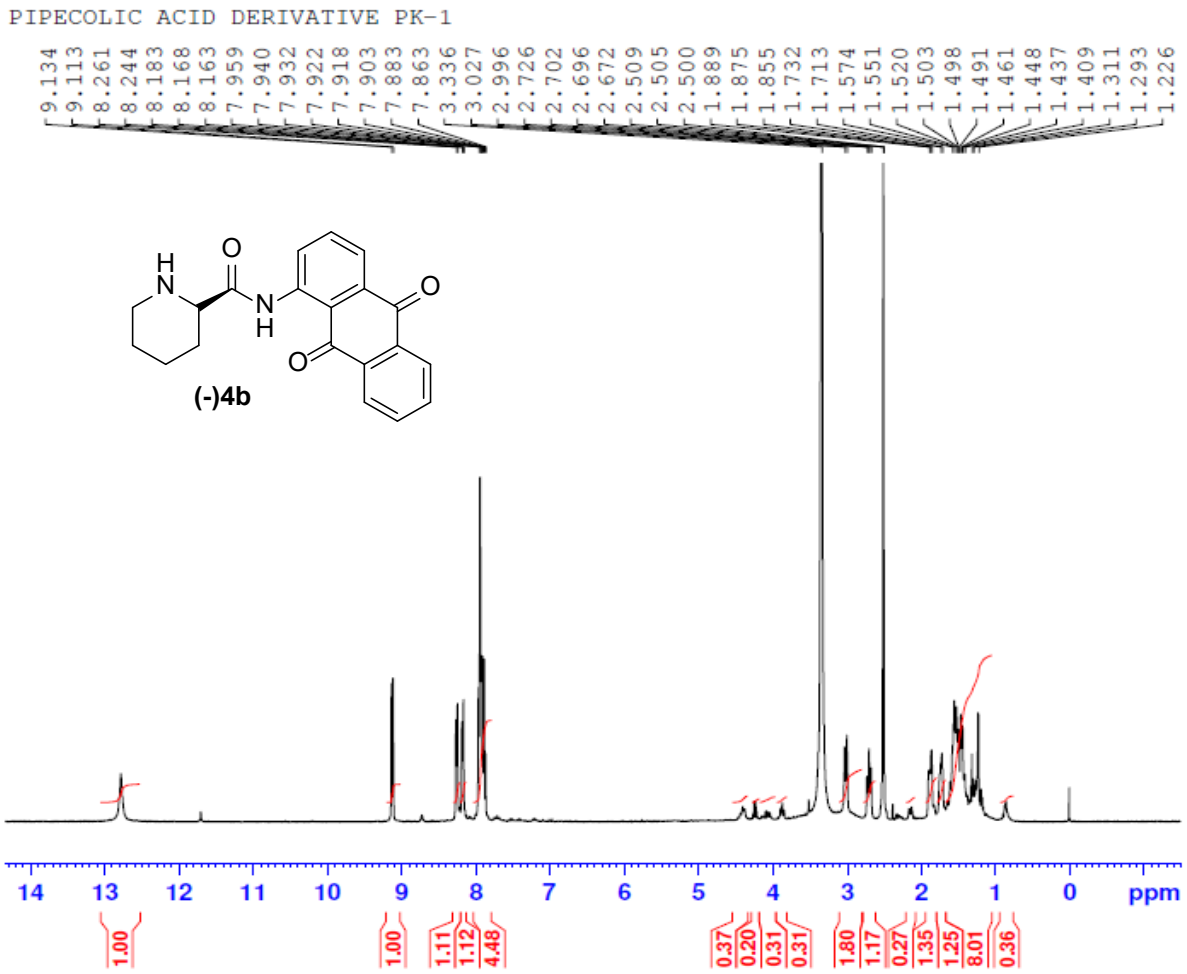
F2 - Processing parameters
SI 2048
SF 400.2300011 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 100.6379135 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0



(+)4b'

(R)-N-(9,10-dioxo-9,10-dihydroanthracen-1-yl)piperidine-2-carboxamide- 1HNMR spectra

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EXPNO                 6
PROCNO                1

F2 - Acquisition Parameters
Date_          20190907
Time              15.35 h
INSTRUM            spect
PROBHD   Z116098_0794 (
PULPROG            zg30
TD                65536
SOLVENT            DMSO
NS                    8
DS                    2
SWH            8012.820 Hz
FIDRES         0.244532 Hz
AQ             4.0894465 sec
RG                149.06
DW                62.400 usec
DE                 6.50 usec
TE                298.1 K
D1             1.00000000 sec
TD0                   1
SFO1         400.2324714 MHz
NUC1                 1H
P1                 9.80 usec
PLW1          17.89999962 W

F2 - Processing parameters
SI                65536
SF           400.2300011 MHz
WDW                  EM
SSB       0
LB                 0.50 Hz
GB        0
PC                 1.00
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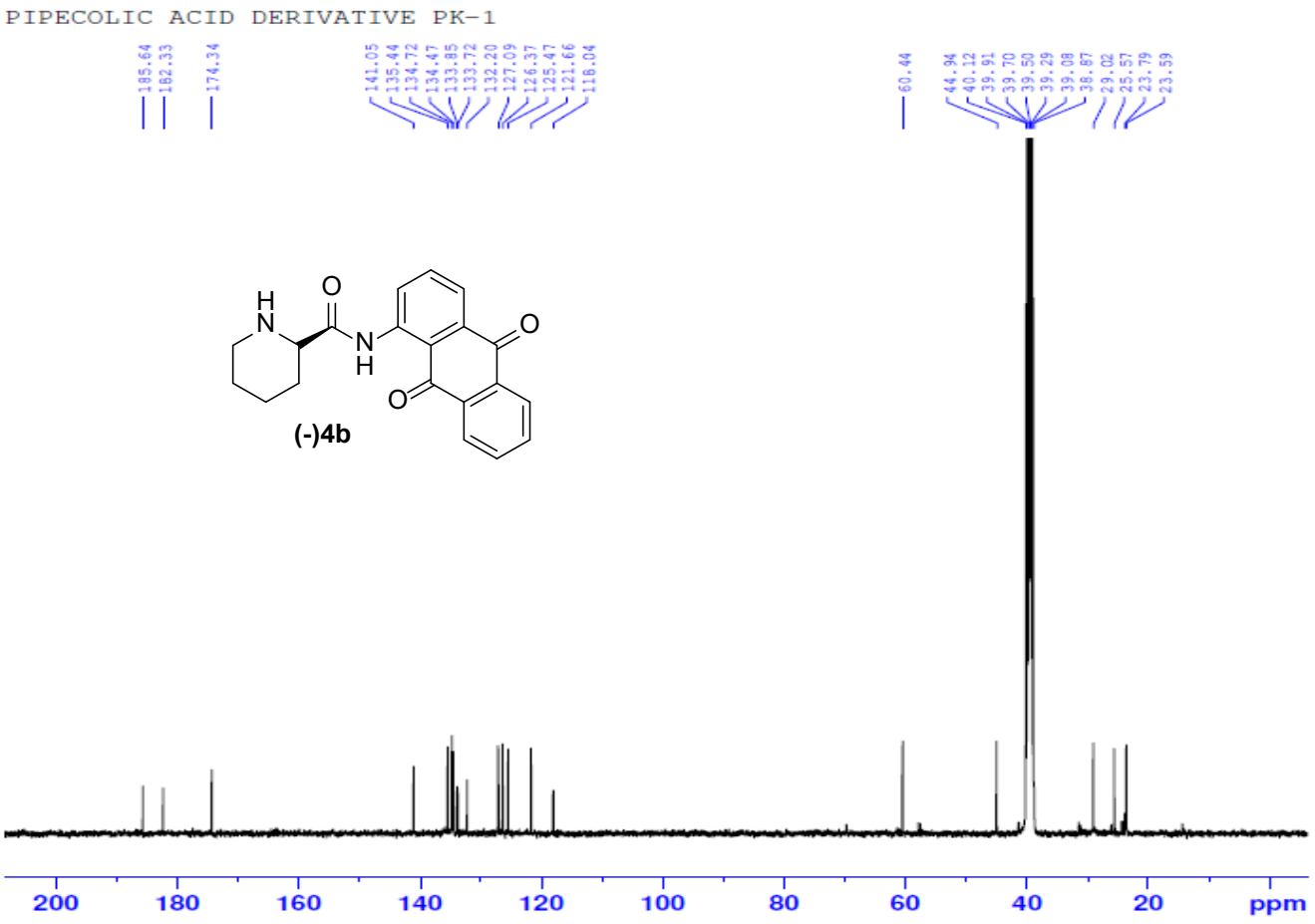
(R)-N-(9,10-dioxo-9,10-dihydroanthracen-1-yl)piperidine-2-carboxamide- 13C spectra

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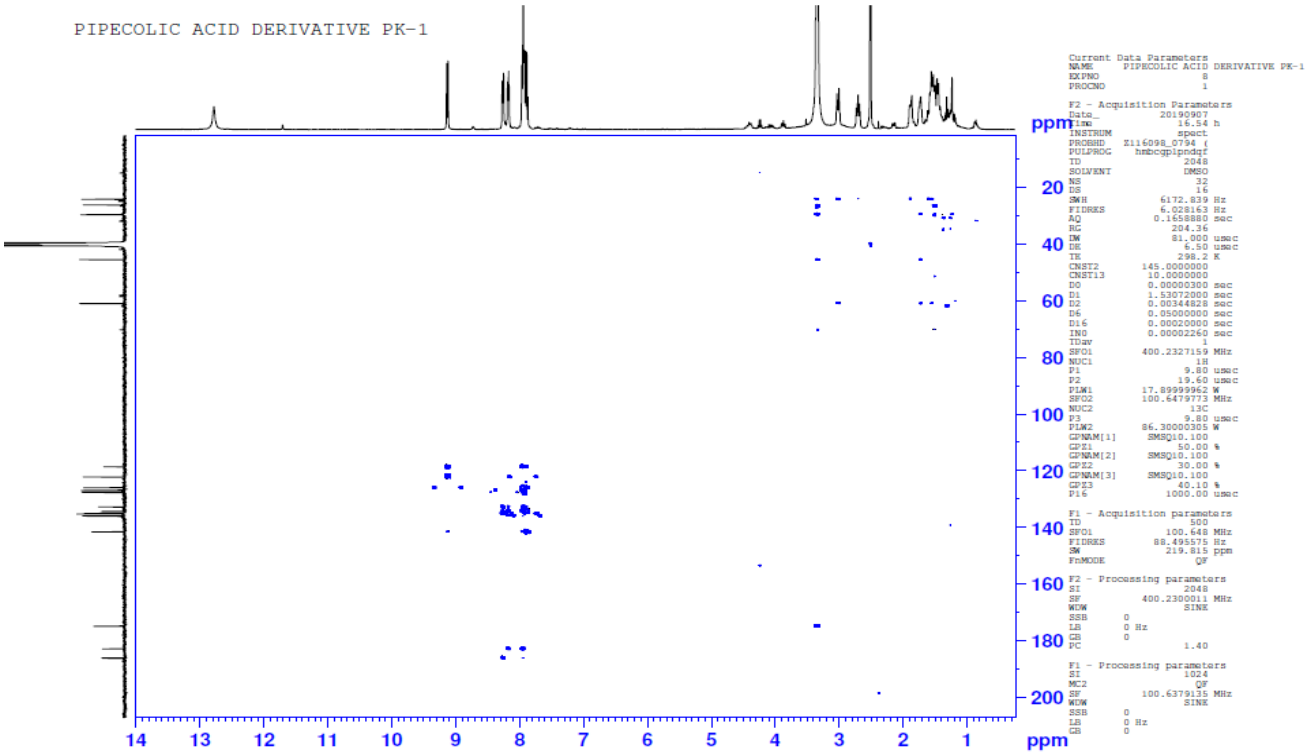
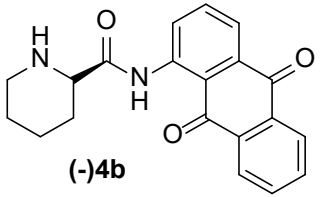
Current Data Parameters
NAME      PIPECOLIC ACID DERIVATIVE PK-1
EXPNO                 9
PROCNO                1

F2 - Acquisition Parameters
Data_              20190908
Time                  5.31 h
INSTRUM              spect
PROBHD    Z116098_0794 (
PULPROG           zgpg30
TD                 65536
SOLVENT              DMSO
NS                    5000
DS                       4
SWH               24038.461 Hz
FIDRES            0.733596 Hz
AQ                1.3631488 sec
RG                   204.36
DW                   20.800 usec
DE                    6.50 usec
TE                   298.1 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                      1
SFO1             100.6479773 MHz
NUC1                    13C
P1                    9.80 usec
PLW1             86.30000305 W
SFO2             400.2316009 MHz
NUC2                    1H
CPDPRG[2             waltz16
PCPD2                90.00 usec
PLW2             17.89999962 W
PLW12             0.21224000 W
PLW13             0.10659000 W

F2 - Processing parameters
SI                    32768
SF               100.6379632 MHz
WDW                     EM
SSB          0
LB                    2.00 Hz
GB           0
PC                    1.40
```

(R)-N-(9,10-dioxo-9,10-dihydroanthracen-1-yl)piperidine-2-carboxamide- 2D spectra

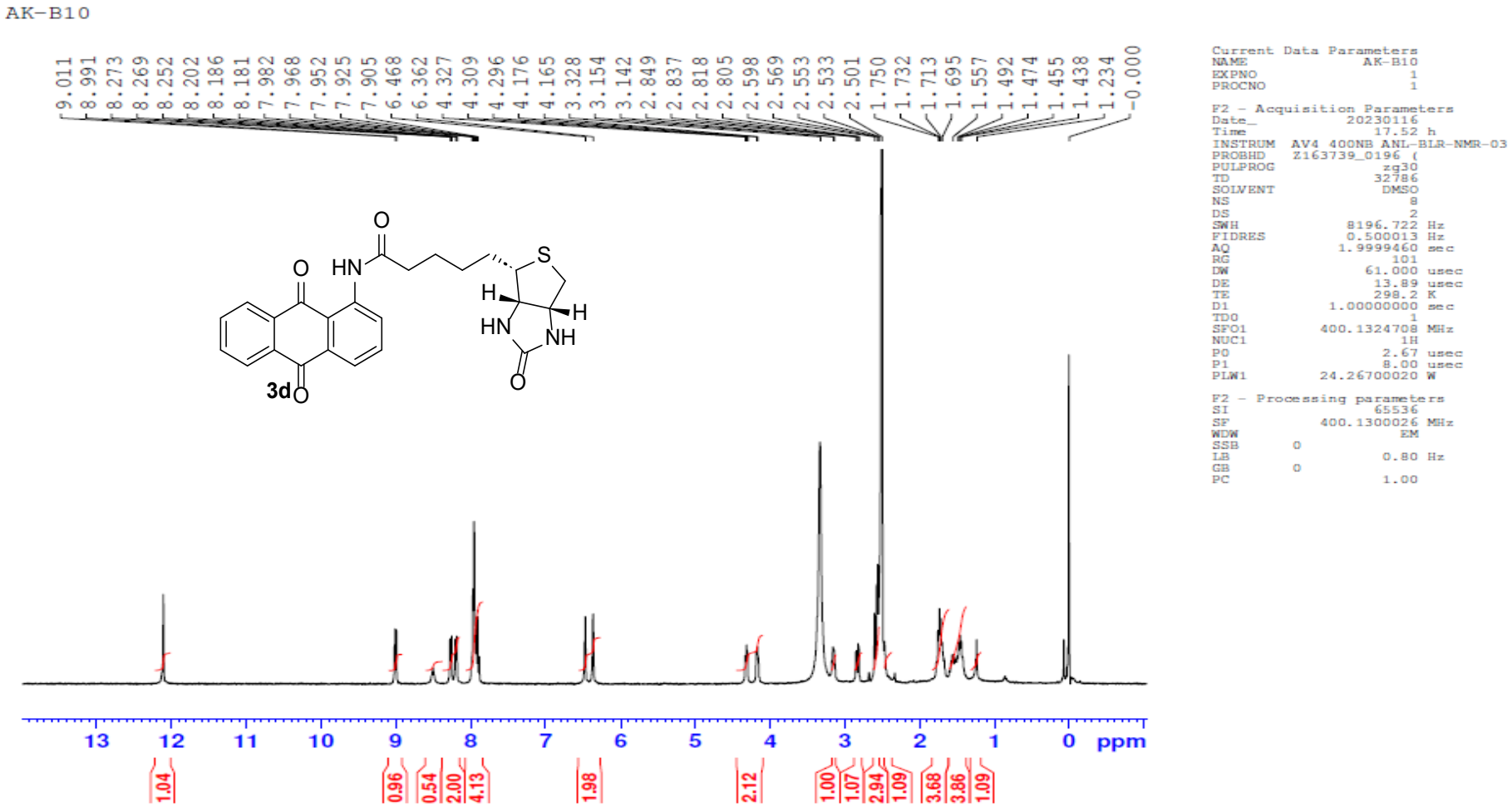




(-)4b

***N*-(9,10-dioxo-9,10-dihydroanthracen-1-yl)-5-((3aS,4S,6aR)-2-oxohexahydro-1H-thieno[3,4-d]imidazol-4-yl)pentanamide (3d)**

1H NMR spectra

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Current Data Parameters
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EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20230116
Time                 17.52 h
INSTRUM  AV4 400NB ANL-BLR-NMR-03
PROBHD   Z163739_0196 (
PULPROG                zg30
TD                    32786
SOLVENT                DMSO
NS                         8
DS                         2
SWH                8196.722 Hz
FIDRES             0.500013 Hz
AQ                 1.9999460 sec
RG                       101
DW                    61.000 usec
DE                    13.89 usec
TE                    298.2 K
D1                 1.00000000 sec
TD0                        1
SFO1             400.1324708 MHz
NUC1                      1H
P0                    2.67 usec
P1                    8.00 usec
PLW1            24.26700020 W

F2 - Processing parameters
SI                        65536
SF               400.1300026 MHz
WDW                       EM
SSB          0
LB                    0.80 Hz
GB           0
PC                    1.00
```
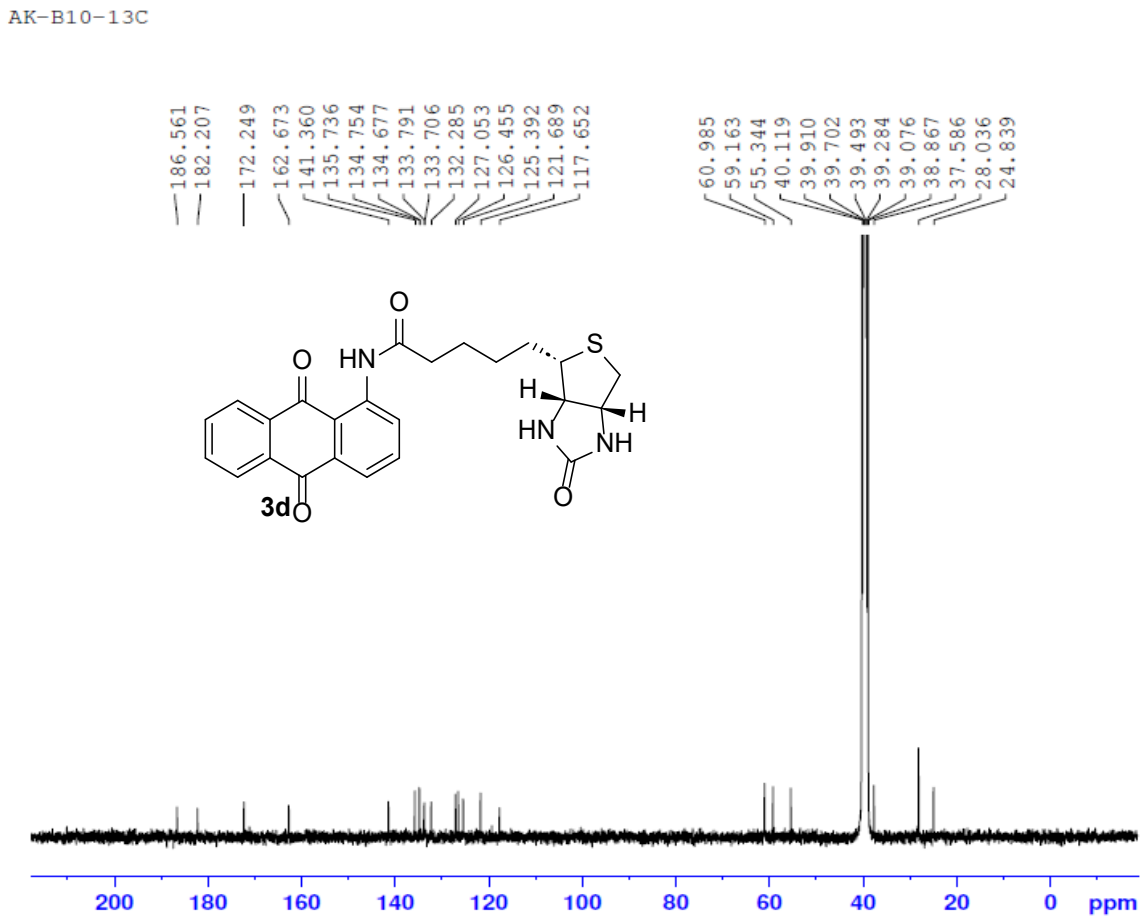

***N*-(9,10-dioxo-9,10-dihydroanthracen-1-yl)-5-((3aS,4S,6aR)-2-oxohexahydro-1H-thieno[3,4-d]imidazol-4-yl)pentanamide (3d)**

13C spectra

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Current Data Parameters
NAME                  AK-B10
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_              20230123
Time                   7.36 h
INSTRUM  AVNeo400-446284-Aragen
PROBHD   Z163739_0428 (
PULPROG              zgpg30
TD                    65536
SOLVENT                DMSO
NS                    10587
DS                        4
SWH               23809.523 Hz
FIDRES             0.726609 Hz
AQ                1.3762560 sec
RG                      101
DW                   21.000 usec
DE                    6.50 usec
TE                   299.8 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                       1
SFO1             100.6253446 MHz
NUC1                    13C
P0                    2.67 usec
P1                    8.00 usec
PLW1             97.26999664 W
SFO2             400.1416006 MHz
NUC2                    1H
CPDPRG[2             waltz65
PCPD2                90.00 usec
PLW2             24.83499908 W
PLW12             0.19622999 W
PLW13             0.09870100 W

F2 - Processing parameters
SI                     32768
SF               100.6153340 MHz
WDW                       EM
SSB          0
LB                    2.00 Hz
GB           0
PC                    1.40
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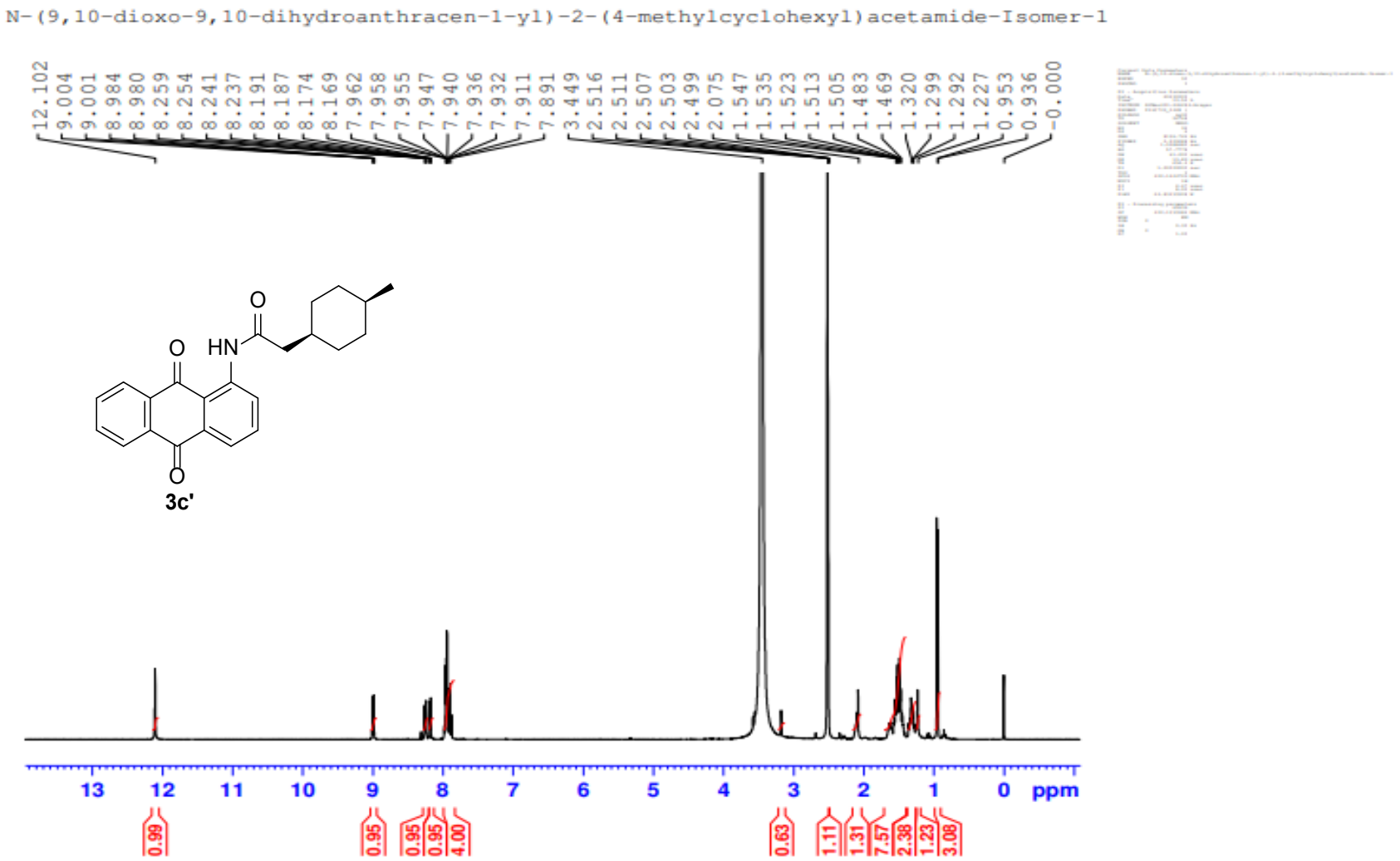
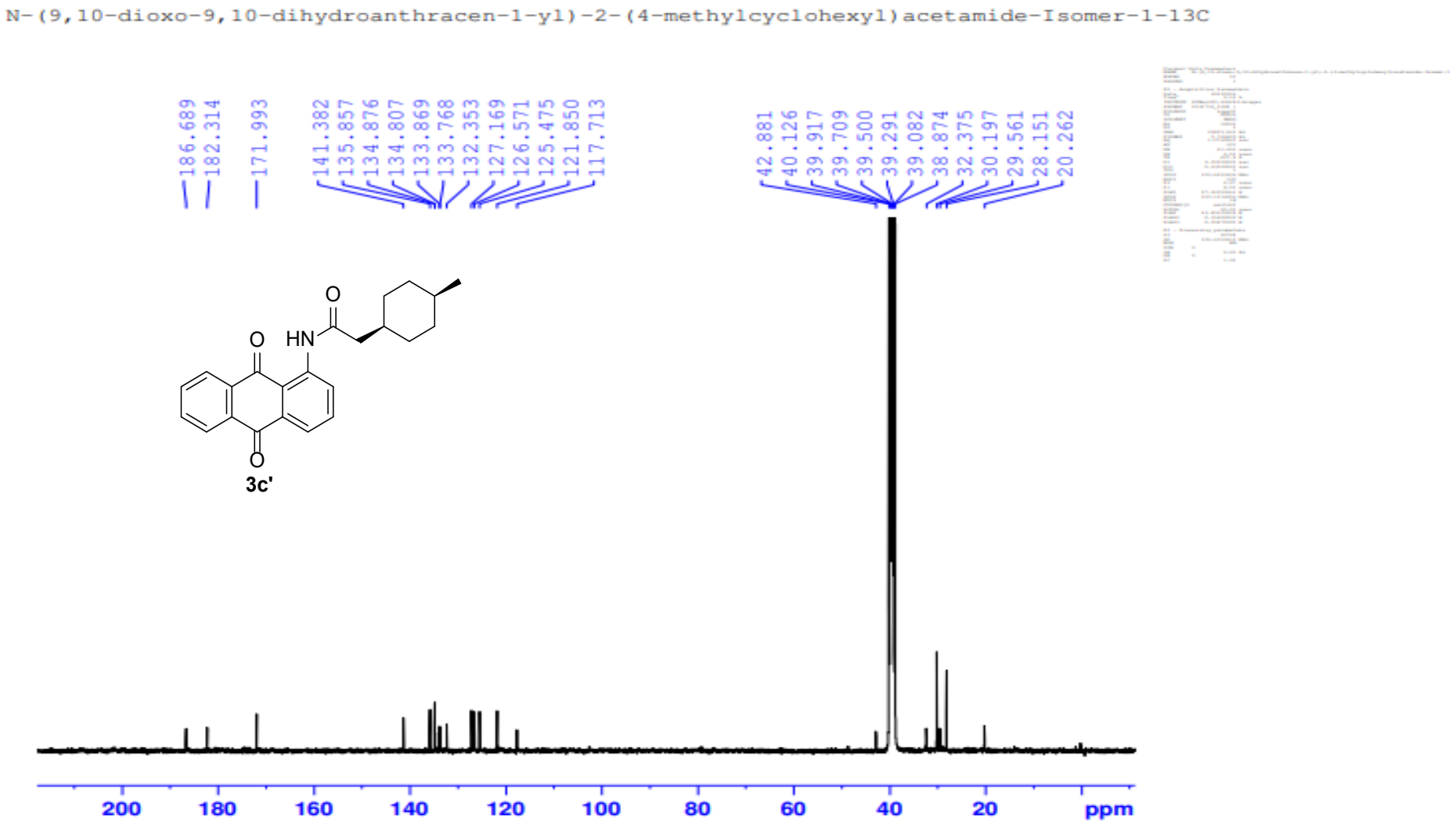
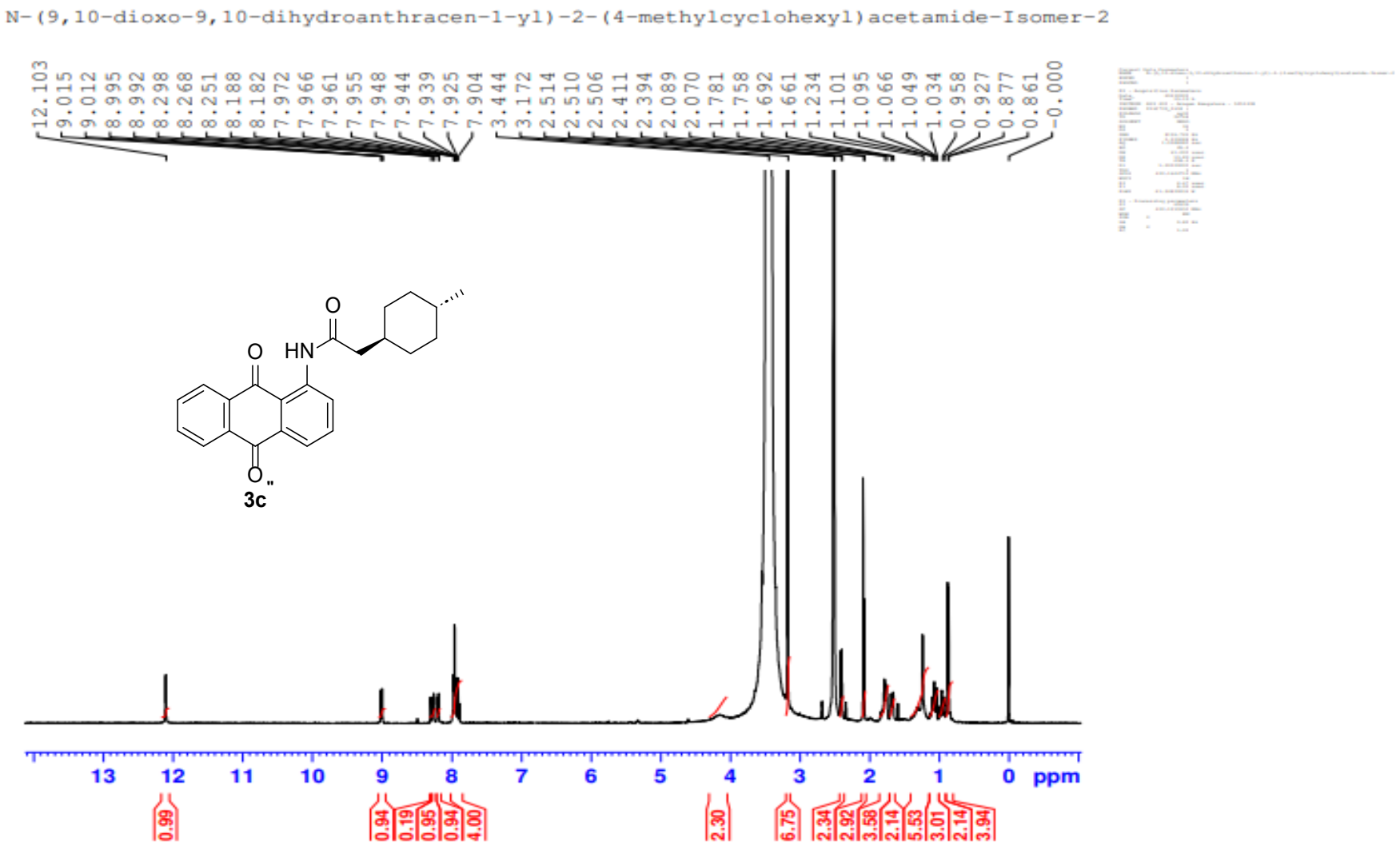
N-(9,10-dioxo-9,10-dihydroanthracen-1-yl)-2-((1s,4s)-4-methylcyclohexyl)acetamide (3c')-1H NMR spectra



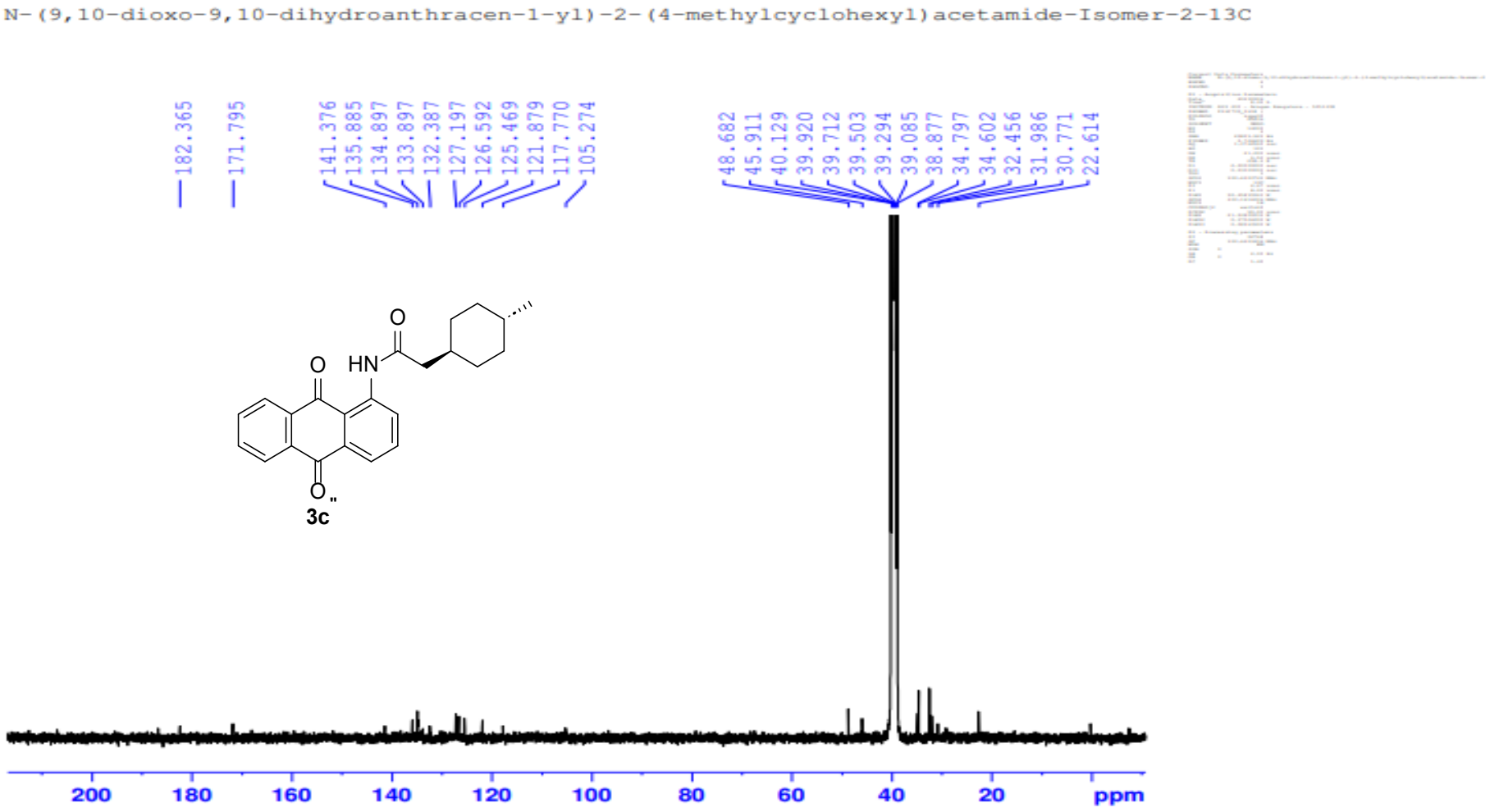
N-(9,10-dioxo-9,10-dihydroanthracen-1-yl)-2-((1s,4s)-4-methylcyclohexyl)acetamide (3c')-13C spectra



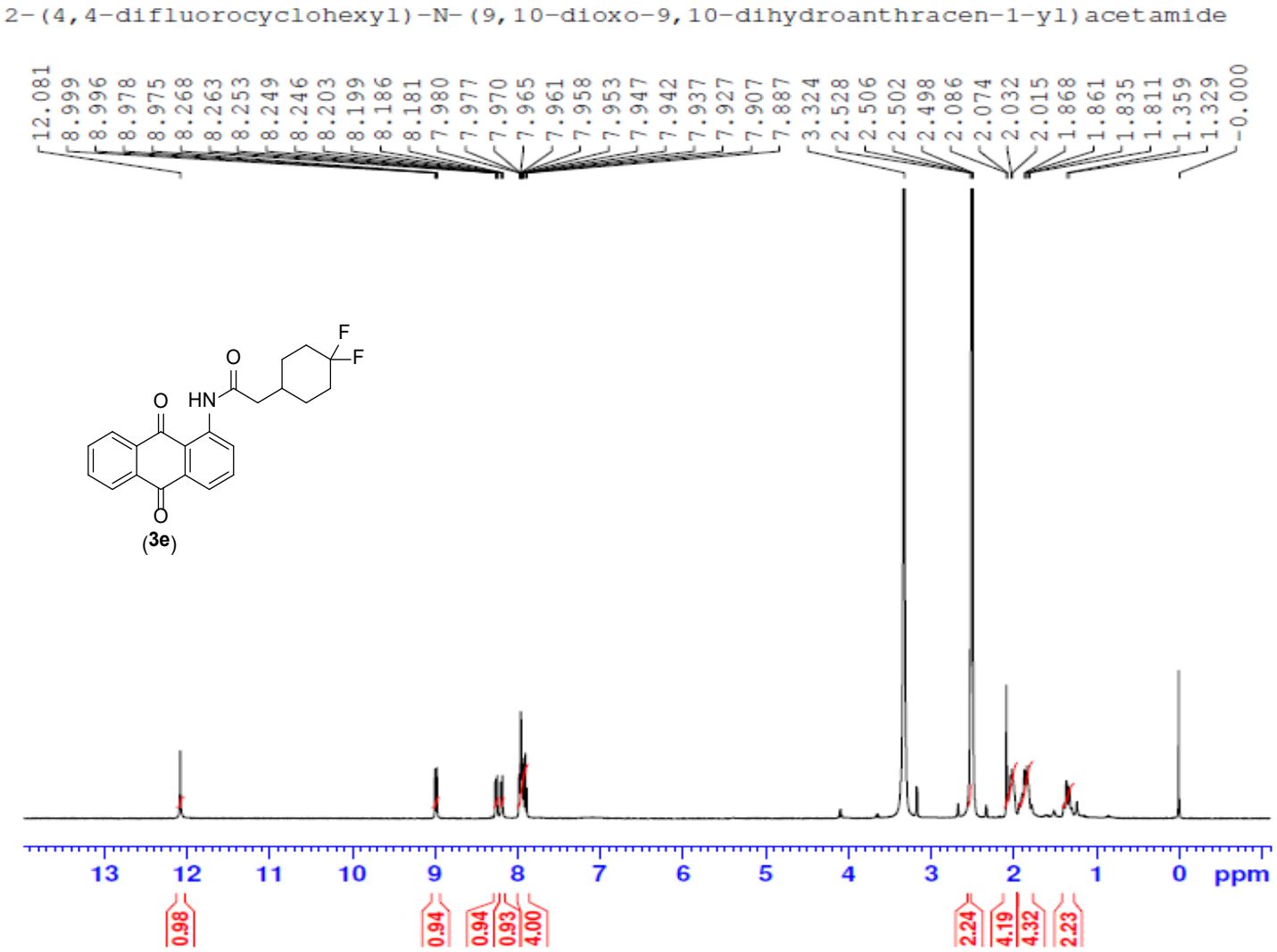
N-(9,10-dioxo-9,10-dihydroanthracen-1-yl)-2-((1r,4r)-4-methylcyclohexyl)acetamide-1H NMR spectra



N-(9,10-dioxo-9,10-dihydroanthracen-1-yl)-2-((1r,4r)-4-methylcyclohexyl)acetamide-13C spectra

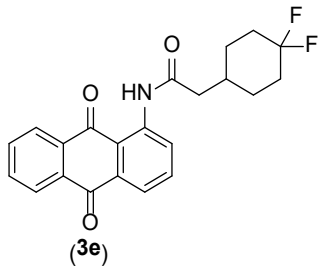


(4,4-difluorocyclohexyl)-N-(9,10-dioxo-9,10-dihydroanthracen-1-yl)acetamide (3e)-1HNMR spectra

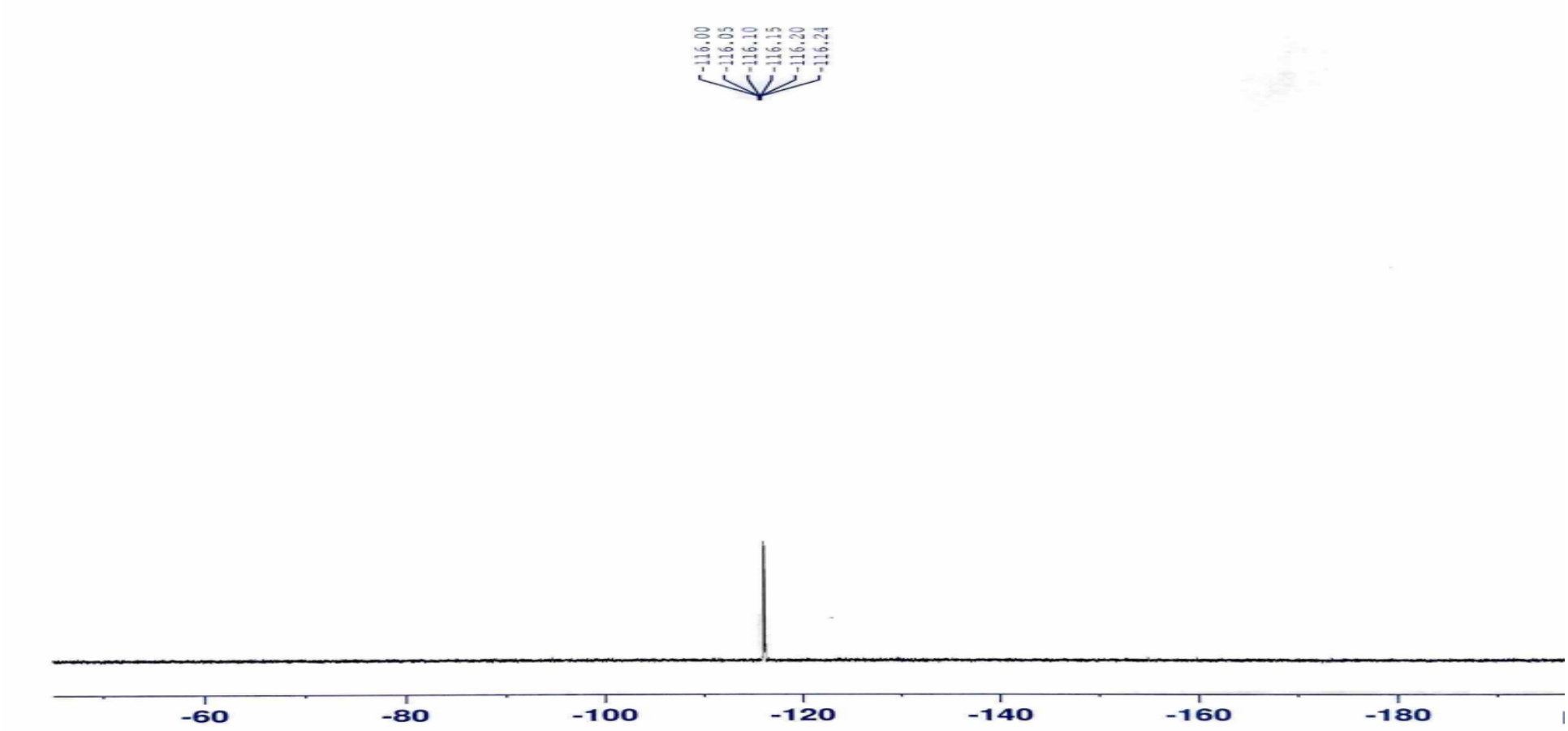


-1

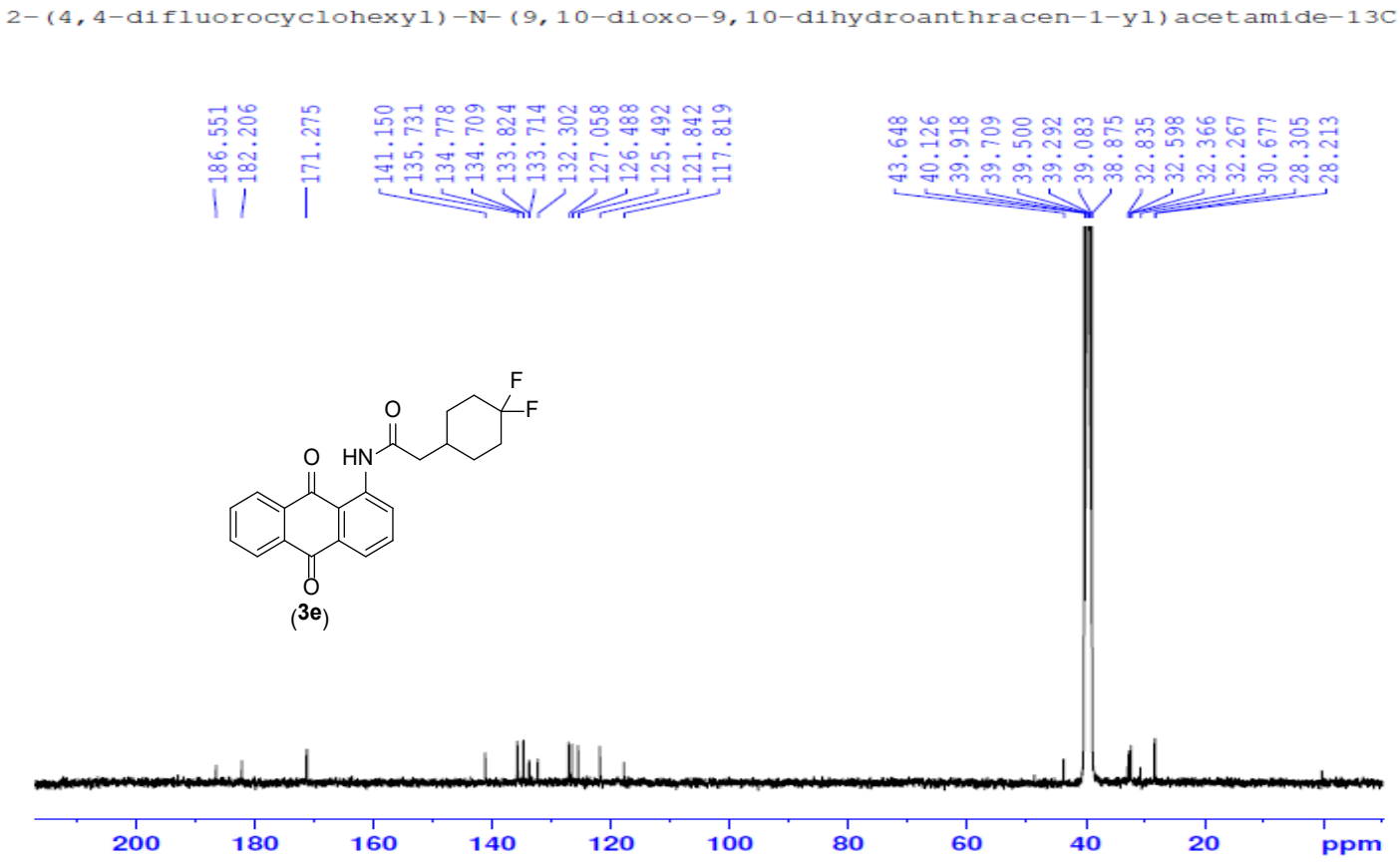
4,4-difluorocyclohexyl)-N-(9,10-dioxo-9,10-dihydroanthracen-1-yl)acetamide (3e)-19F



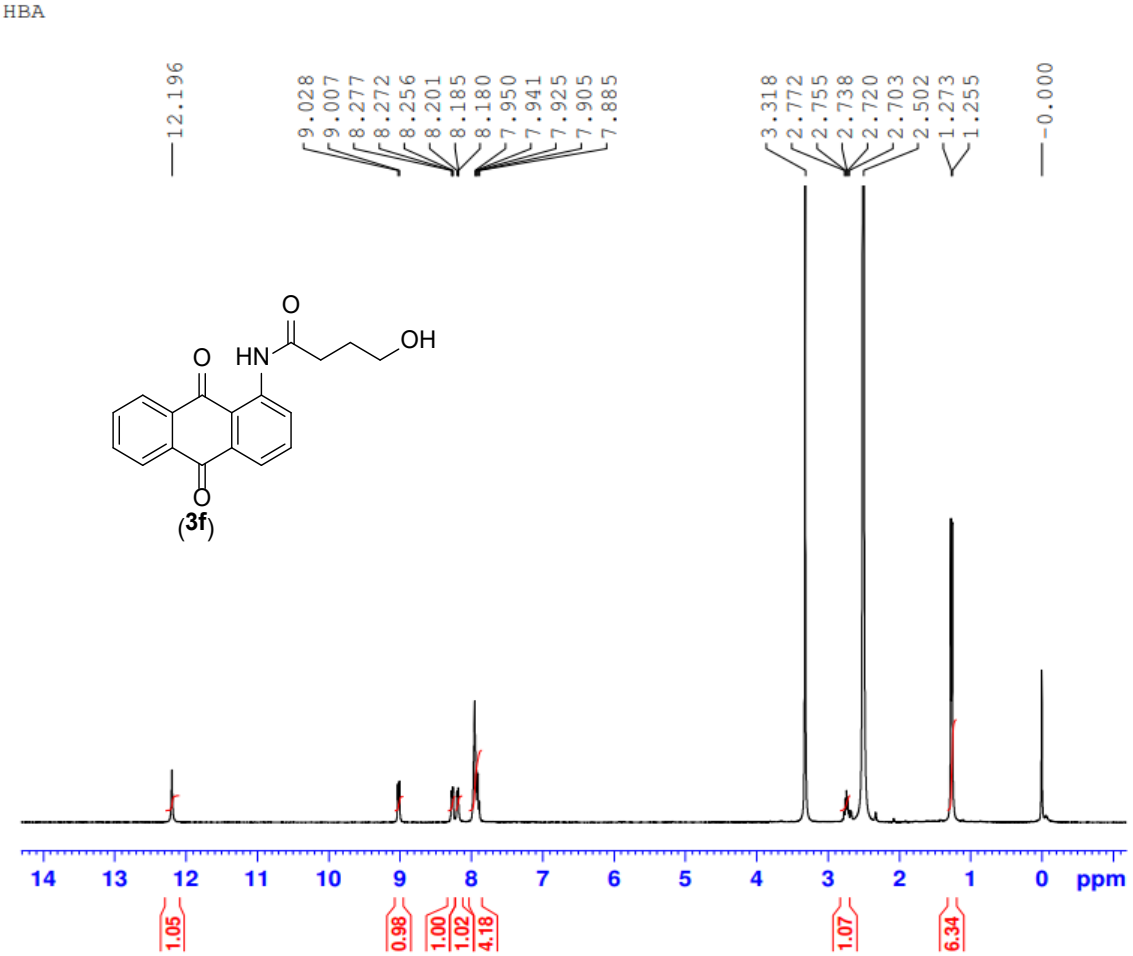
(**3e**)



4,4-difluorocyclohexyl)-N-(9,10-dioxo-9,10-dihydroanthracen-1-yl)acetamide (3e)-13C spectra



N-(9,10-dioxo-9,10-dihydroanthracen-1-yl)-4-hydroxybutanamide(3f)-1H NMR spectra

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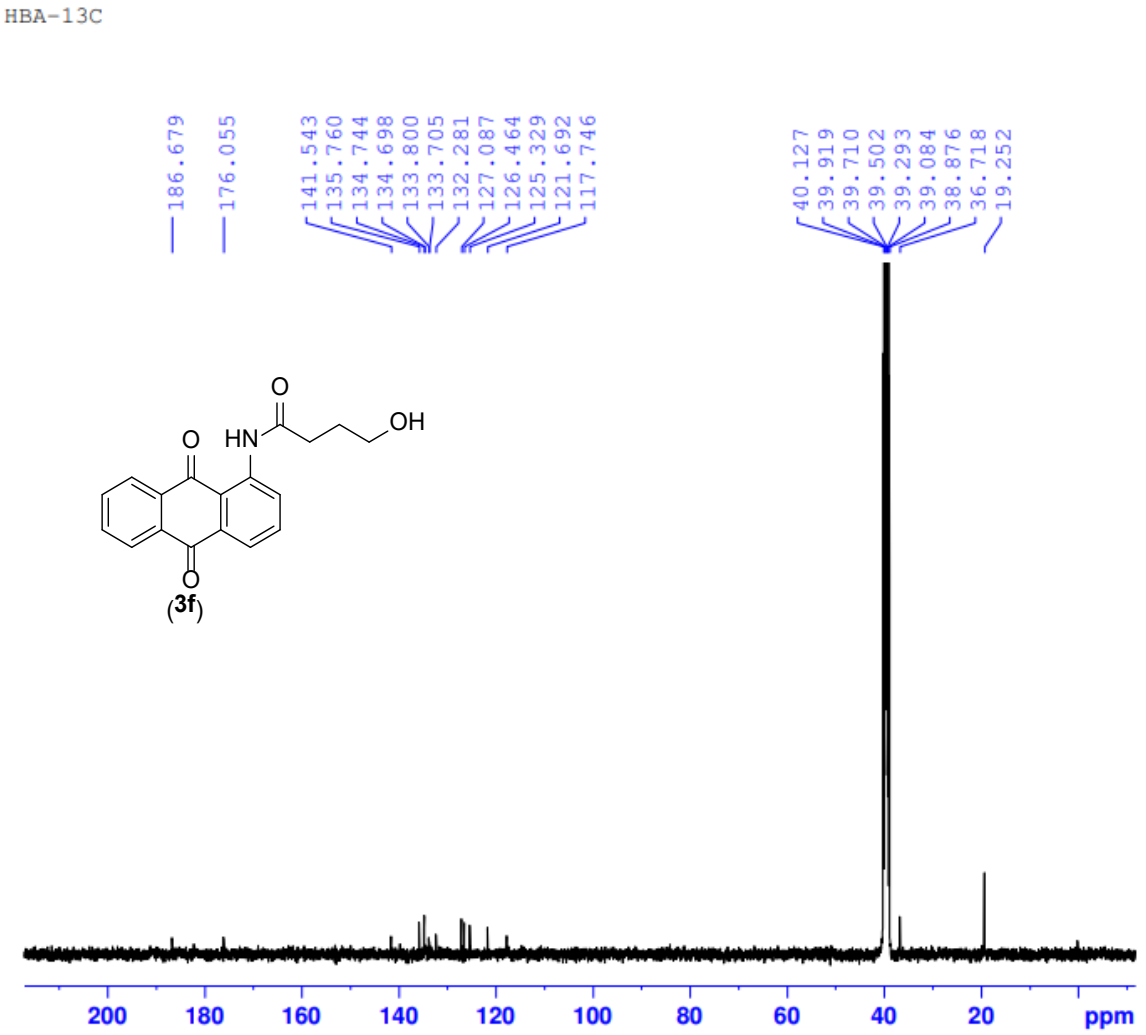
Current Data Parameters
NAME                  HBA
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20230308
Time              17.23 h
INSTRUM  AV4 400NB ANL-BLR-NMR-03
PROBHD   Z163739_0195 (
PULPROG             zg30
TD                 32786
SOLVENT             DMSO
NS                    64
DS                     2
SWH             8196.722 Hz
FIDRES          0.500013 Hz
AQ              1.9999460 sec
RG                   101
DW                61.000 usec
DE                13.89 usec
TE                298.2 K
D1             1.00000000 sec
TD0                    1
SFO1          400.1324708 MHz
NUC1                  1H
P0                 2.67 usec
P1                 8.00 usec
PLW1          24.03499985 W

F2 - Processing parameters
SI                 65536
SF            400.1300024 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

N-(9,10-dioxo-9,10-dihydroanthracen-1-yl)-4-hydroxybutanamide(3f)-13C spectra

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Current Data Parameters
NAME                  HBA-13C
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_               20230309
Time                   11.48 h
INSTRUM                spect
PROBHD    Z116098_0561 (
PULPROG              zgpg30
TD                    65536
SOLVENT                DMSO
NS                      1800
DS                         4
SWH               24038.461 Hz
FIDRES             0.733596 Hz
AQ                 1.3631488 sec
RG                    204.36
DW                    20.800 usec
DE                     6.50 usec
TE                    298.1 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                         1
SFO1            100.6479773 MHz
NUC1                     13C
P0                     3.33 usec
P1                    10.00 usec
PLW1            71.33300018 W
SFO2            400.2316009 MHz
NUC2                     1H
CPDPRG[2            waltz65
PCPD2                 90.00 usec
PLW2            16.51199913 W
PLW12            0.20385000 W
PLW13            0.10253000 W

F2 - Processing parameters
SI                      32768
SF              100.6379634 MHz
WDW                        EM
SSB         0
LB                     2.00 Hz
GB          0
PC                     1.40
```
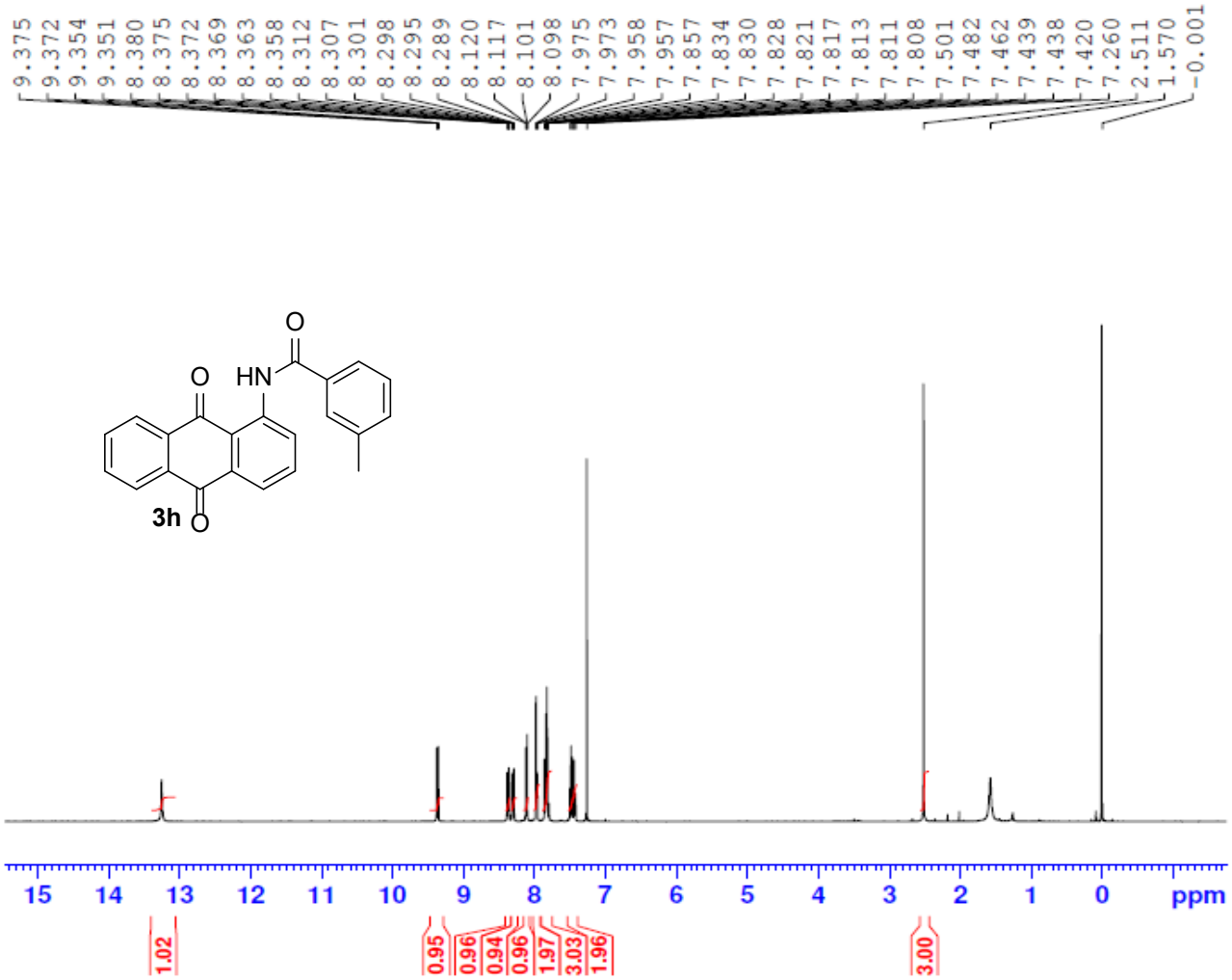

***N*-(9, 10-dioxo-9,10-dihydroanthracen-1-yl)-3-methylbenzamide (3h)- 1H NMR spectra**

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Current Data Parameters
NAME                  AC-28
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20230202
Time                   5.29 h
INSTRUM  AVNeo400-446284-Aragen
PROBHD   Z163739_0428 (
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                        8
DS                        2
SWH               8196.722 Hz
FIDRES            0.500288 Hz
AQ                1.9988480 sec
RG                      101
DW                 61.000 usec
DE                 13.89 usec
TE                 298.2 K
D1              1.00000000 sec
TD0                       1
SFO1           400.1424709 MHz
NUC1                    1H
P0                 2.67 usec
P1                 8.00 usec
PLW1           24.83499908 W

F2 - Processing parameters
SI                    65536
SF             400.1400093 MHz
WDW                      EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
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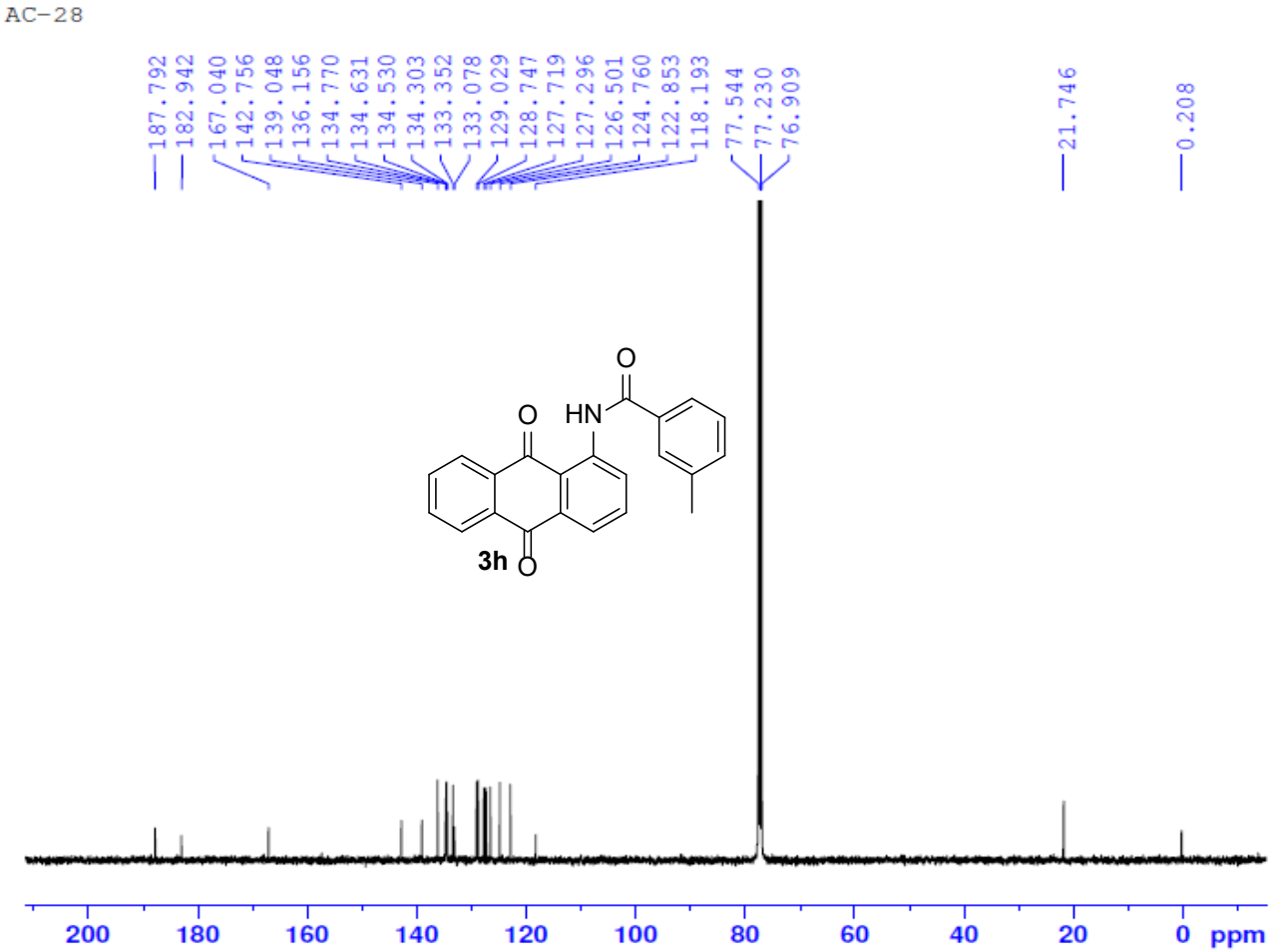
***N*-(9, 10-dioxo-9,10-dihydroanthracen-1-yl)-3-methylbenzamide (3h)- 13C spectra**

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Current Data Parameters
NAME                  AC-28
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_              20230202
Time                  7.59 h
INSTRUM  AVNeo400-446284-Aragen
PROBHD   Z163739_0428 (
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     2602
DS                        4
SWH               23809.523 Hz
FIDRES             0.726609 Hz
AQ                 1.3762560 sec
RG                      101
DW                   21.000 usec
DE                    6.50 usec
TE                   298.4 K
D1                2.00000000 sec
D11               0.03000000 sec
ID0                       1
SFO1             100.6253446 MHz
NUC1                    13C
P0                    2.67 usec
P1                    8.00 usec
PLW1             97.26999664 W
SFO2             400.1416006 MHz
NUC2                    1H
CPDPRG[2             waltz65
PCPD2                90.00 usec
PLW2             24.83499908 W
PLW12             0.19622999 W
PLW13             0.09870100 W

F2 - Processing parameters
SI                    32768
SF               100.6152620 MHz
WDW                      EM
SSB          0
LB                    2.00 Hz
GB           0
PC                    1.40
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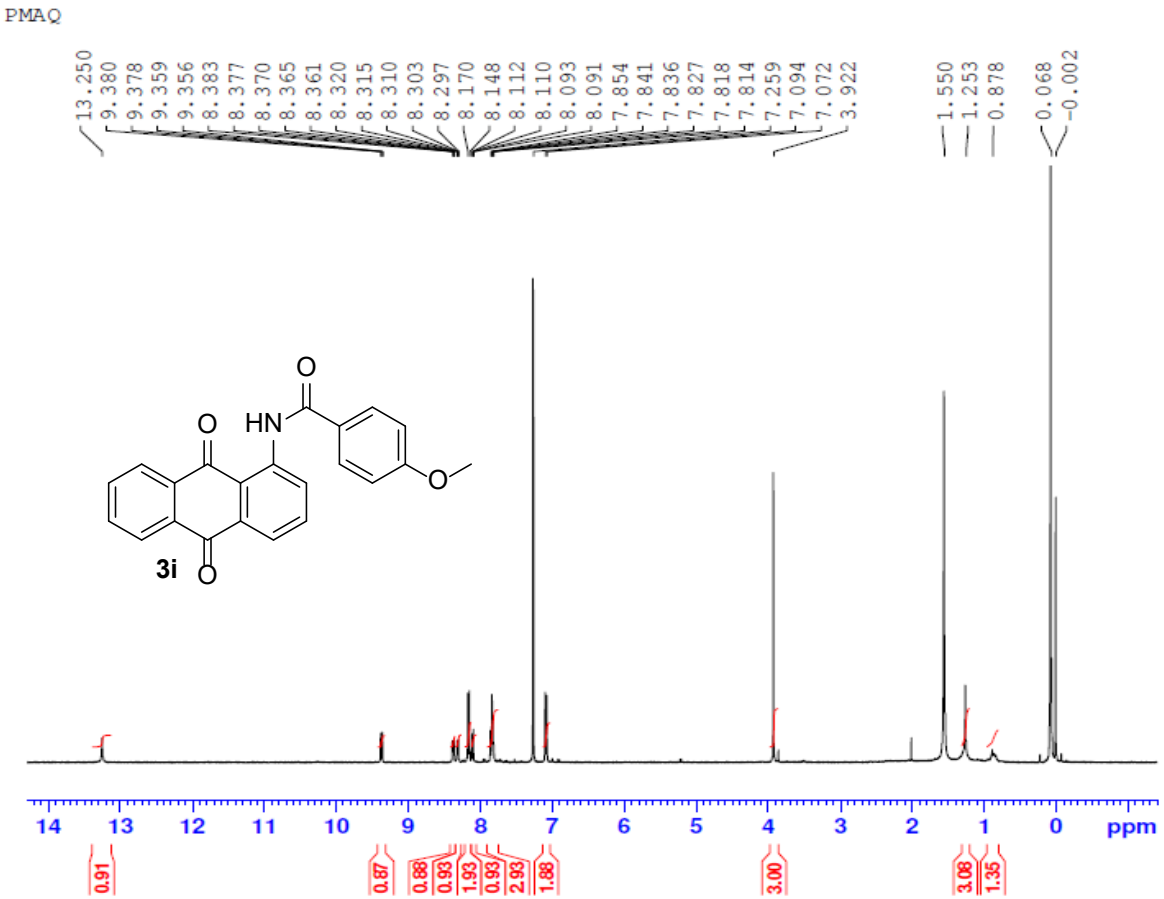
***N*-(9,10-dioxo-9,10-dihydroanthracen-1-yl)-4-methoxybenzamide (3i)-1H NMR spectra**

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Current Data Parameters
NAME                  PMAQ
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_              20230111
Time                 18.34 h
INSTRUM  AV4 400NB ANL-BLR-NMR-03
PROBHD   Z163739_0196 (
PULPROG                zg30
TD                    32786
SOLVENT               CDCl3
NS                        8
DS                        2
SWH                8196.722 Hz
FIDRES            0.500013 Hz
AQ                1.9999460 sec
RG                      101
DW                   61.000 usec
DE                   13.89 usec
TE                   298.2 K
D1                1.00000000 sec
TD0                       1
SFO1           400.1324708 MHz
NUC1                     1H
P0                    2.67 usec
P1                    8.00 usec
PLW1           24.26700020 W

F2 - Processing parameters
SI                    65536
SF             400.1300099 MHz
WDW                      EM
SSB       0
LB                    0.30 Hz
GB        0
PC                    1.00
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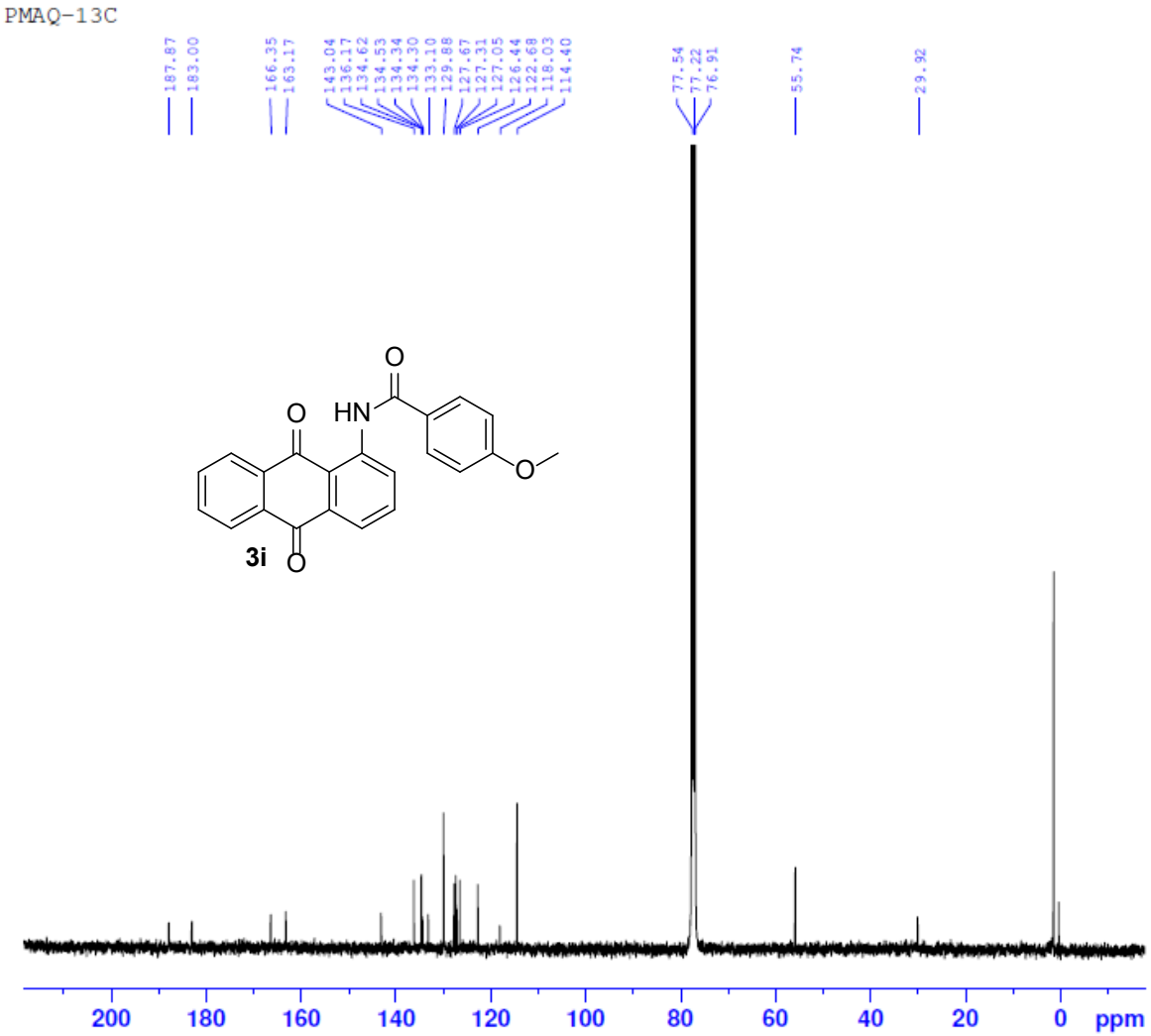
***N*-(9,10-dioxo-9,10-dihydroanthracen-1-yl)-4-methoxybenzamide (3i)- 13C spectra**

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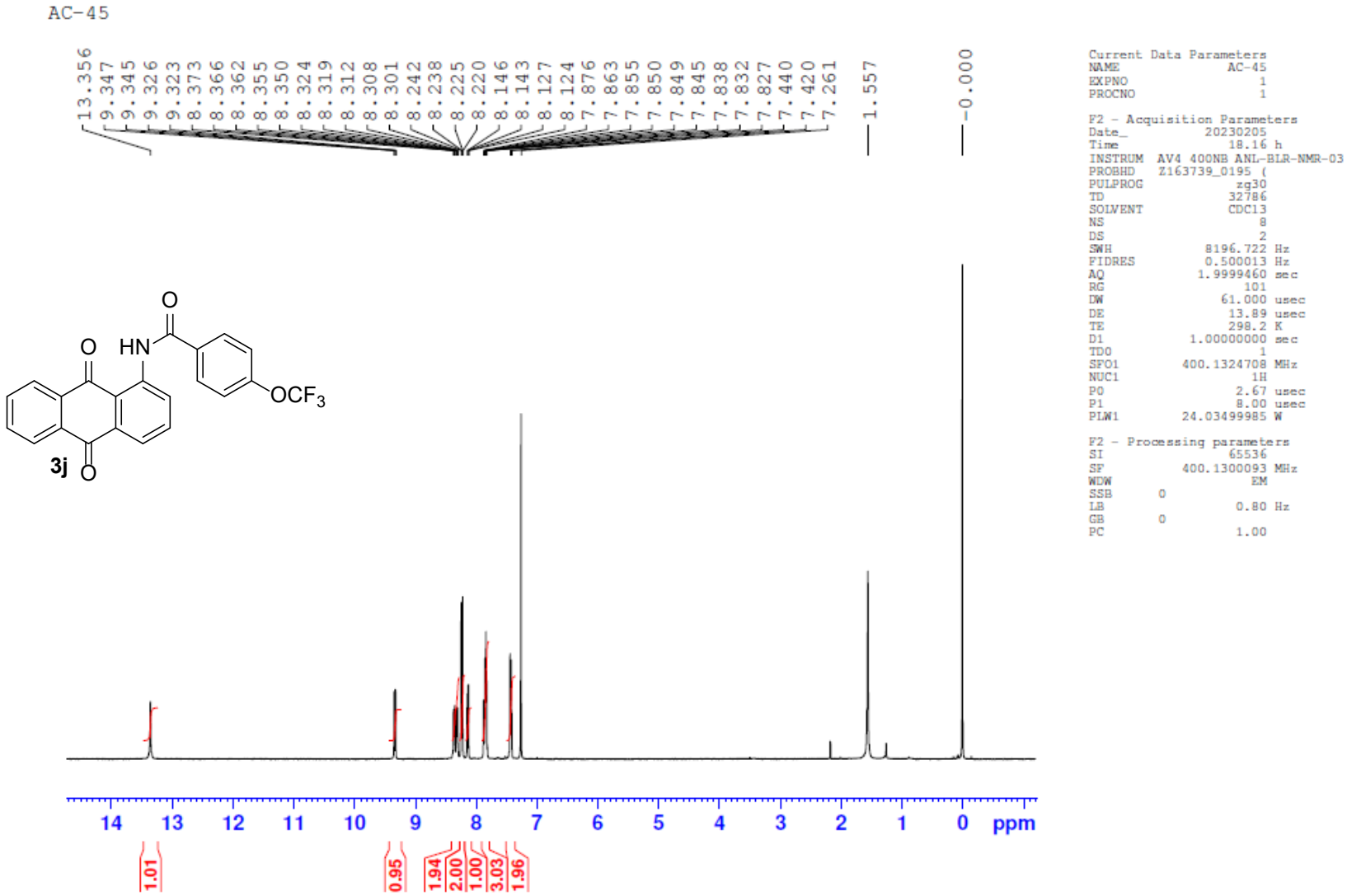
Current Data Parameters
NAME                  PMAQ
EXPNO                   12
PROCNO                   1

F2 - Acquisition Parameters
Date_              20230115
Time                  4.38 h
INSTRUM  Avance Neo Nanobay
PROBHD   Z163739_0079 (
PULPROG              zgpg30
TD                    65536
SOLVENT               CDC13
NS                    12000
DS                        4
SWH              23809.523 Hz
FIDRES            0.726609 Hz
AQ                1.3762560 sec
RG                      101
DW                   21.000 usec
DE                    6.50 usec
TE                   298.2 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                       1
SFO1           100.7234199 MHz
NUC1                    13C
P0                    3.33 usec
P1                   10.00 usec
PLW1           59.21300125 W
SFO2           400.5316021 MHz
NUC2                    1H
CPDPRG[2             waltz65
PCPD2                90.00 usec
PLW2           15.97799969 W
PLW12           0.19618130 W
PLW13           0.09832609 W

F2 - Processing parameters
SI                    32768
SF           100.7133280 MHz
WDW                     EM
SSB       0
LB                    2.00 Hz
GB        0
PC                    1.40
```

_N_-(9,10-dioxo-9,10-dihydroanthracen-1-yl)-4-(trifluoromethoxy)benzamide (3j)-1H NMR spectra

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Current Data Parameters
NAME                  AC-45
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20230205
Time                 18.16 h
INSTRUM  AV4 400NB ANL-BLR-NMR-03
PROBHD   Z163739_0195 (
PULPROG               zg30
TD                   32786
SOLVENT              CDCl3
NS                       8
DS                       2
SWH               8196.722 Hz
FIDRES            0.500013 Hz
AQ                1.9999460 sec
RG                     101
DW                  61.000 usec
DE                  13.89 usec
TE                  298.2 K
D1                1.00000000 sec
TD0                      1
SFO1           400.1324708 MHz
NUC1                    1H
P0                   2.67 usec
P1                   8.00 usec
PLW1           24.03499985 W

F2 - Processing parameters
SI                   65536
SF             400.1300093 MHz
WDW                     EM
SSB       0
LB                   0.80 Hz
GB        0
PC                   1.00
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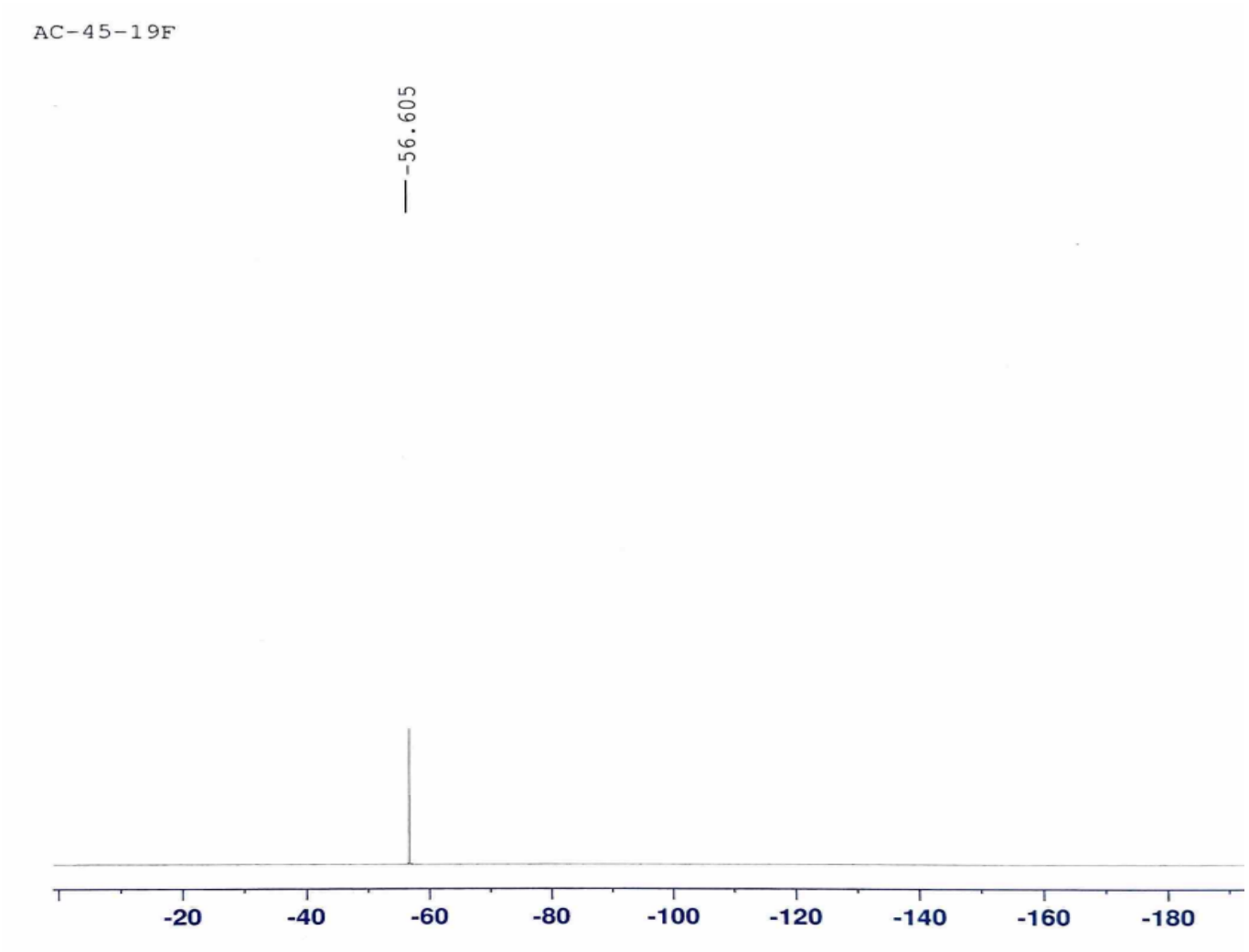
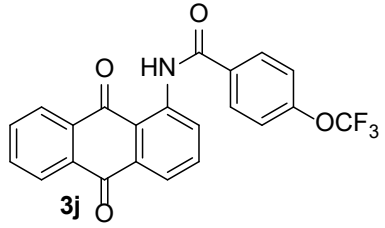
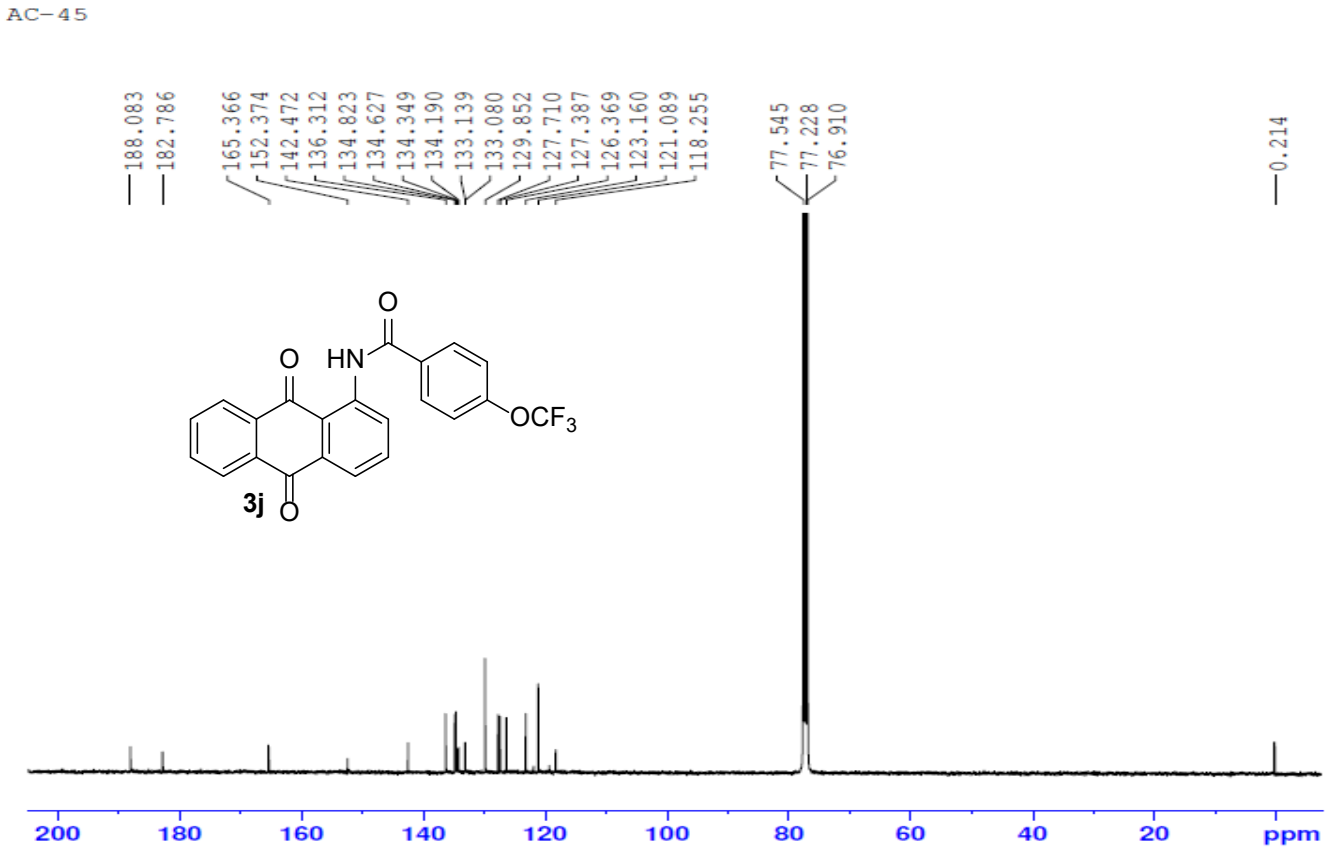
***N*-(9,10-dioxo-9,10-dihydroanthracen-1-yl)-4-(trifluoromethoxy)benzamide (3j)-19F spectra**





***N*-(9,10-dioxo-9,10-dihydroanthracen-1-yl)-4-(trifluoromethoxy)benzamide (3j)-13C spectra**

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Current Data Parameters
NAME                  AC-45
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_              20230206
Time                   5.45 h
INSTRUM  AV4 400NB ANL-BLR-NMR-03
PROBHD   Z163739_0195 (
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                    12000
DS                        4
SWH               23809.523 Hz
FIDRES             0.726609 Hz
AQ                1.3762560 sec
RG                      101
DW                   21.000 usec
DE                    6.50 usec
TE                  298.1 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                       1
SFO1            100.6228298 MHz
NUC1                    13C
P0                    2.67 usec
P1                    8.00 usec
PLW1             99.25000000 W
SFO2            400.1316005 MHz
NUC2                    1H
CPDPRG[2             waltz65
PCPD2                90.00 usec
PLW2             24.03499985 W
PLW12             0.19059330 W
PLW13             0.09552535 W

F2 - Processing parameters
SI                    32768
SF              100.6127472 MHz
WDW                      EM
SSB         0
LB                    2.00 Hz
GB          0
PC                    1.40
```
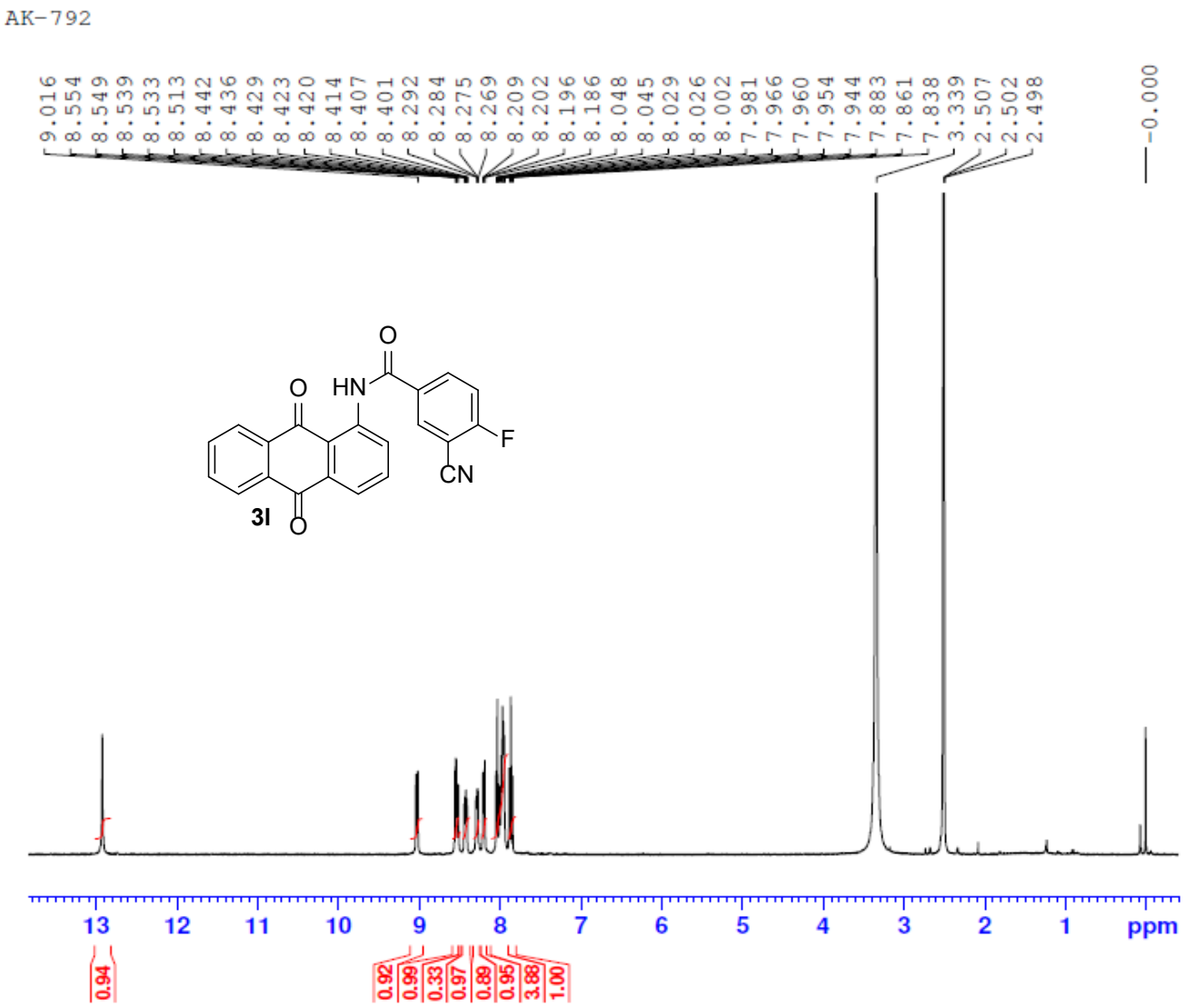

3-cyano-N-(9,10-dioxo-9,10-dihydroanthracen-1-yl)-4-fluorobenzamide (3l) -1 H NMR spectra

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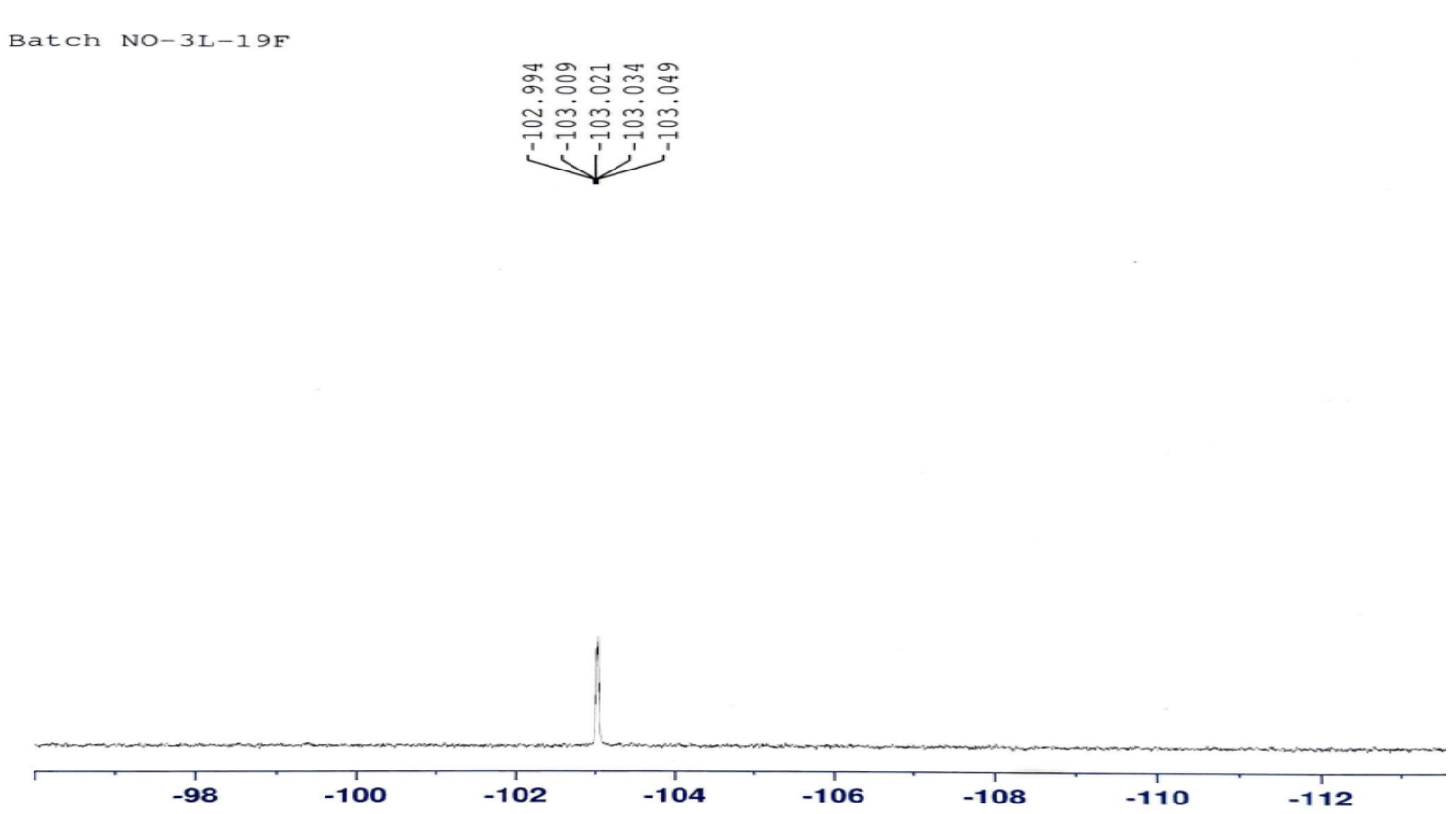
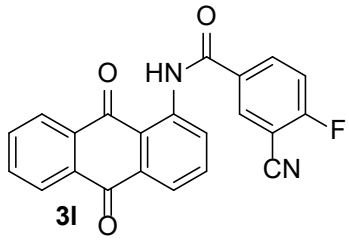
Current Data Parameters
NAME                  AK-792
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20230113
Time                 17.26 h
INSTRUM              spect
PROBHD    Z116098_0561 (
PULPROG              zg30
TD                   32768
SOLVENT              DMSO
NS                      16
DS                       2
SWH               8012.820 Hz
FIDRES            0.489064 Hz
AQ                2.0447233 sec
RG                  204.36
DW                  62.400 usec
DE                   6.50 usec
TE                  298.2 K
D1              1.00000000 sec
TD0                      1
SFO1           400.2324714 MHz
NUC1                    1H
P0                   3.33 usec
P1                  10.00 usec
PLW1           16.45199966 W

F2 - Processing parameters
SI                    65536
SF             400.2300024 MHz
WDW                     EM
SSB       0
LB                   0.30 Hz
GB        0
PC                   1.00
```

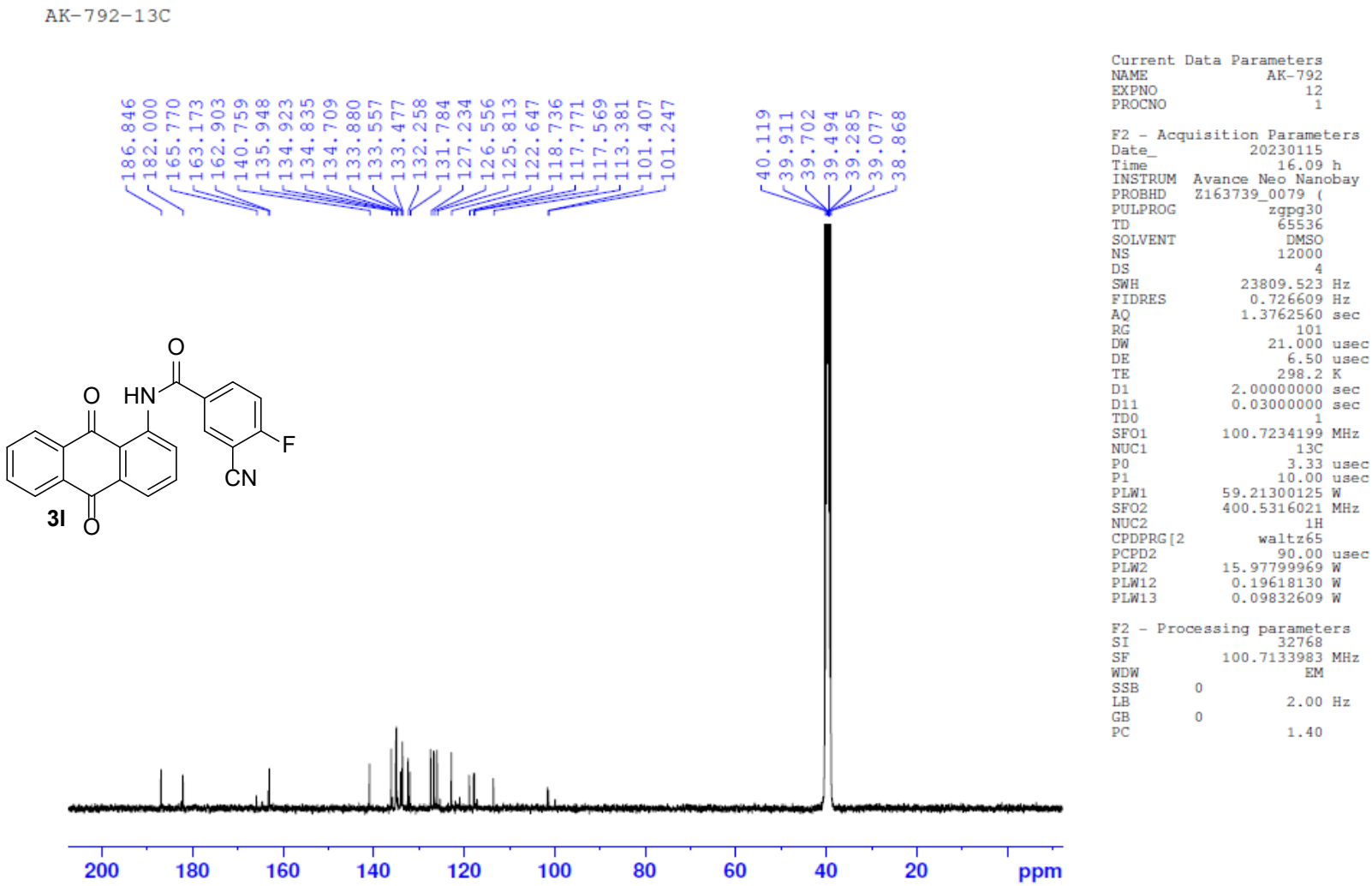
3-cyano-N-(9,10-dioxo-9,10-dihydroanthracen-1-yl)-4-fluorobenzamide (3l) -19F spectra





3l

3-cyano-N-(9,10-dioxo-9,10-dihydroanthracen-1-yl)-4-fluorobenzamide (3l) -13C spectra

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Current Data Parameters
NAME                 AK-792
EXPNO                    12
PROCNO                    1

F2 - Acquisition Parameters
Date_              20230115
Time                 16.09 h
INSTRUM  Avance Neo Nanobay
PROBHD   Z163739_0079 (
PULPROG              zgpg30
TD                    65536
SOLVENT                DMSO
NS                    12000
DS                        4
SWH              23809.523 Hz
FIDRES            0.726609 Hz
AQ                1.3762560 sec
RG                      101
DW                   21.000 usec
DE                    6.50 usec
TE                   298.2 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                       1
SFO1            100.7234199 MHz
NUC1                    13C
P0                    3.33 usec
P1                   10.00 usec
PLW1           59.21300125 W
SFO2           400.5316021 MHz
NUC2                    1H
CPDPRG[2             waltz65
PCPD2                90.00 usec
PLW2           15.97799969 W
PLW12           0.19618130 W
PLW13           0.09832609 W

F2 - Processing parameters
SI                    32768
SF              100.7133983 MHz
WDW                      EM
SSB          0
LB                    2.00 Hz
GB           0
PC                    1.40
```
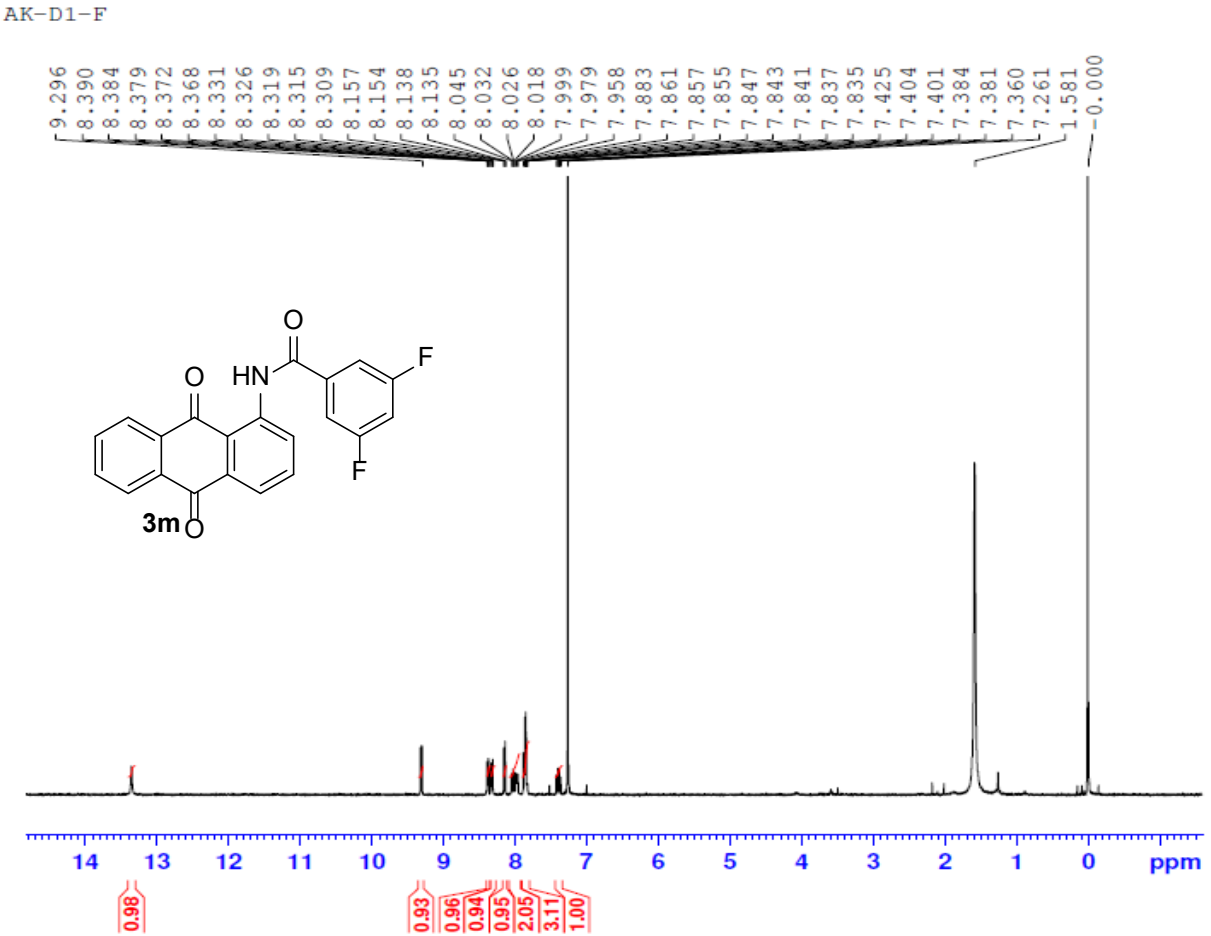

***N*-(9,10-dioxo-9,10-dihydroanthracen-1-yl)-3,5-difluorobenzamide (3m)- 1H NMR spectra**

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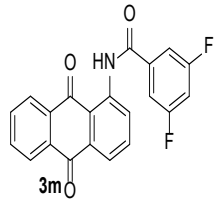
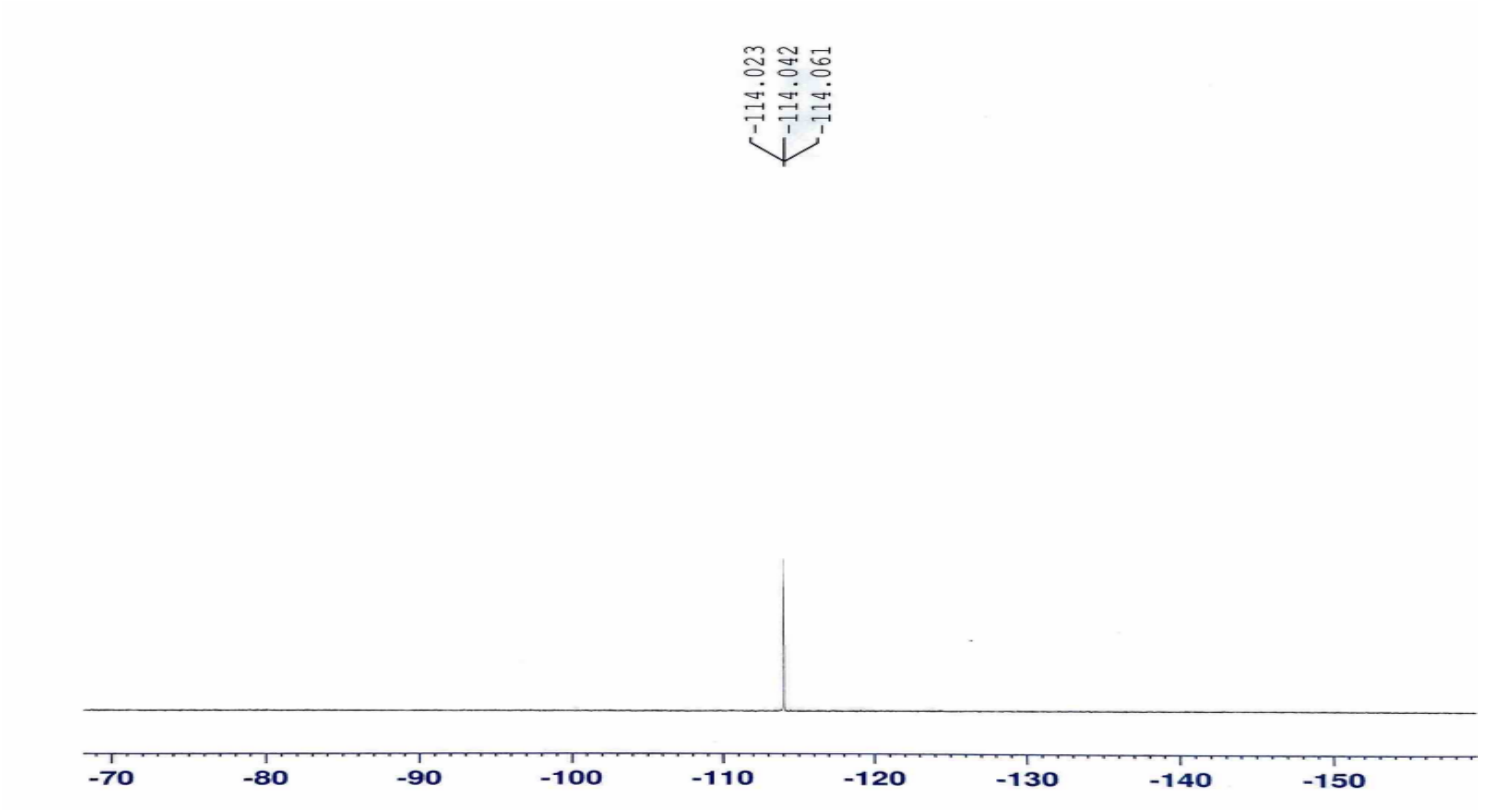
Current Data Parameters
NAME                  AK-D1-F
EXPNO                      10
PROCNO                      1

F2 - Acquisition Parameters
Date_               20230202
Time                    2.03 h
INSTRUM  AVNeo400-446284-Aragen
PROBHD   Z163739_0428 (
PULPROG                 zg30
TD                     32768
SOLVENT                CDCl3
NS                         8
DS                         2
SWH                 8196.722 Hz
FIDRES              0.500288 Hz
AQ                  1.9988480 sec
RG                       101
DW                    61.000 usec
DE                    13.89 usec
TE                    298.1 K
D1                  1.00000000 sec
TD0                        1
SFO1               400.1424709 MHz
NUC1                       1H
P0                    2.67 usec
P1                    8.00 usec
PLW1               24.83499908 W

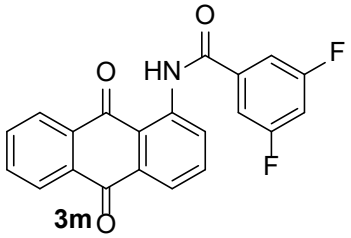
F2 - Processing parameters
SI                         65536
SF                 400.1400090 MHz
WDW                        EM
SSB          0
LB                    0.30 Hz
GB           0
PC                    1.00
```

_N_-(9,10-dioxo-9,10-dihydroanthracen-1-yl)-3,5-difluorobenzamide (3m)- 19F spectra



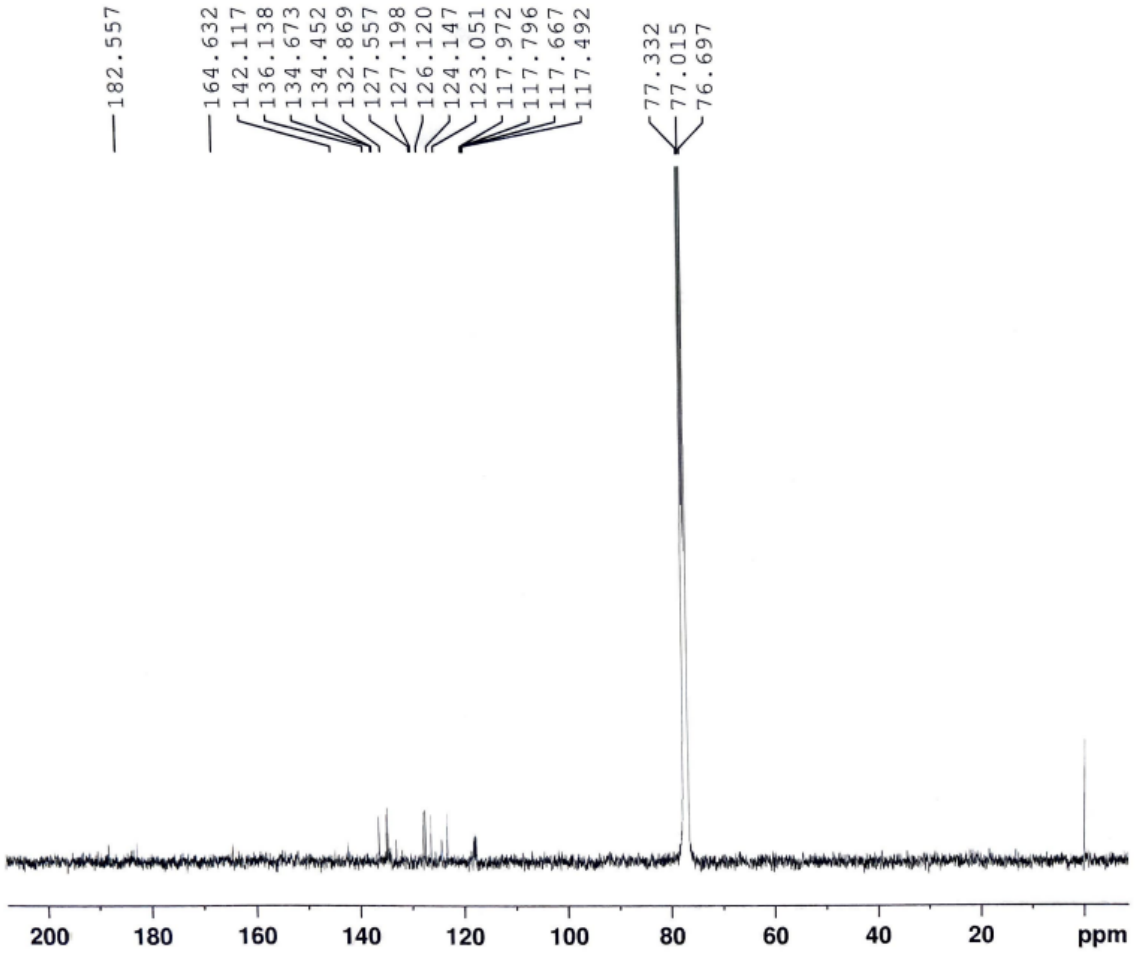


_N_-(9,10-dioxo-9,10-dihydroanthracen-1-yl)-3,5-difluorobenzamide (3m)- 13C spectra



3m

AK-D1-F

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Current Data Parameters
NAME                  AK-D1-F
EXPNO                      66
PROCNO                      1

F2 - Acquisition Parameters
Date_               20230205
Time                   18.12 h
INSTRUM   AV4 400NB ANL-BLR-1
PROBHD    Z163739_0195 (
PULPROG               zgpg30
TD                     65536
SOLVENT                CDCl3
NS                     12000
DS                         4
SWH                23809.523 Hz
FIDRES             0.726609 Hz
AQ                 1.3762560 sec
RG                       101
DW                    21.000 usec
DE                     6.50 usec
TE                    298.2 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        1
SFO1             100.6228298 MHz
NUC1                     13C
P0                     2.67 usec
P1                     5.00 usec
PLW1              99.25000000 W
SFO2             400.1316005 MHz
NUC2                     1H
CPDPRG[2              waltz65
PCPD2                 90.00 usec
PLW2              24.03499985 W
PLW12              0.19059330 W
PLW13              0.09552535 W

F2 - Processing parameters
SI                       32768
SF               100.6127686 MHz
WDW                         EM
SSB          0
LB                     3.00 Hz
GB           0
PC                     1.40
```
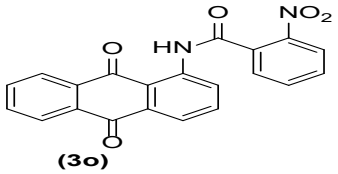
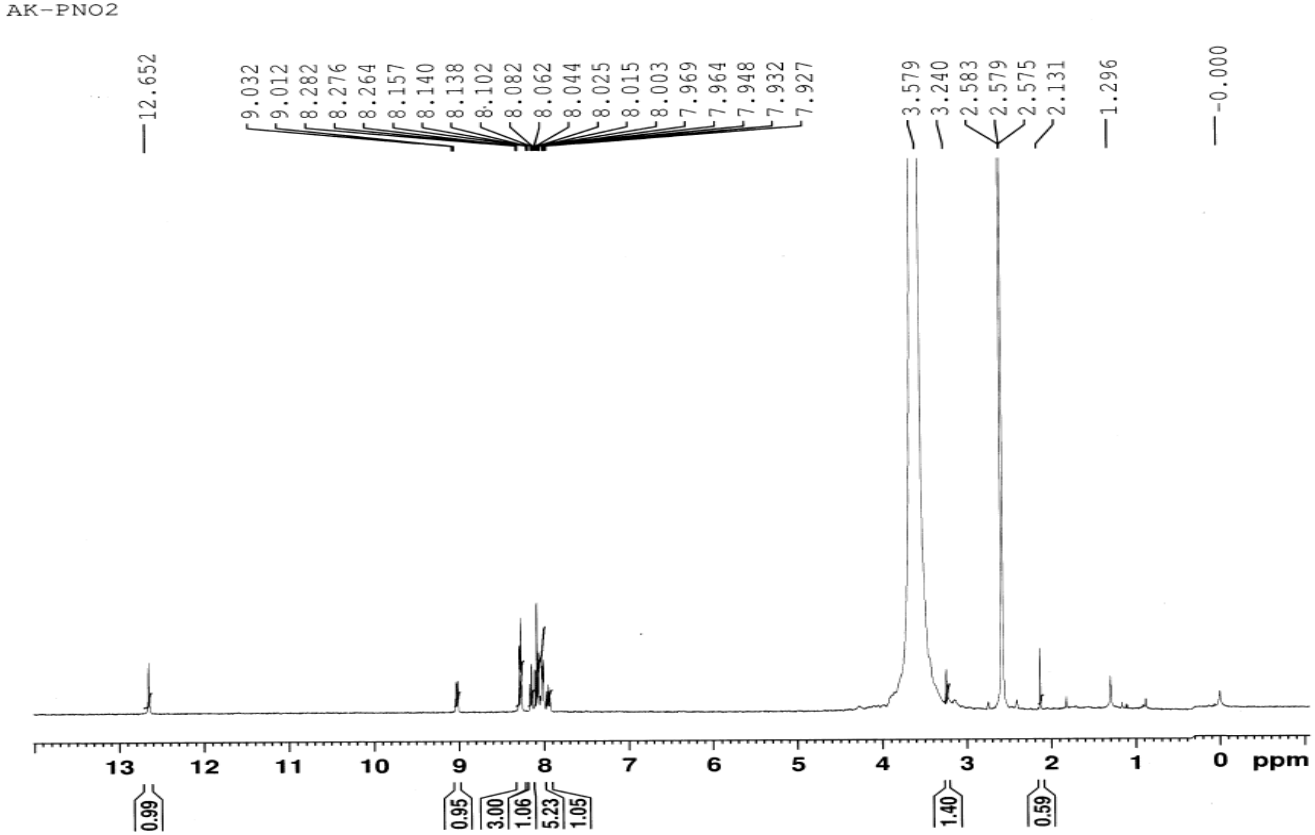

N-(9,10-dioxo-9,10-dihydroanthracen-1-yl)-2nitro benzamide (3o)-1H NMR spectra



(3o)

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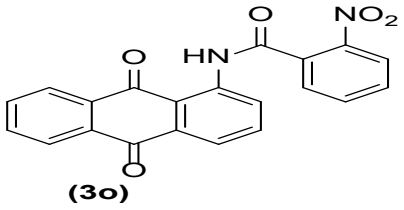
Current Data Parameters
NAME                  AK-PNO2
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_                20230818
Time                    17.16 h
INSTRUM  Avance Neo Nanobay
PROBHD   Z163739_0078 (
PULPROG                 zg30
TD                     32768
SOLVENT             DMSO-D6
NS                          8
DS                          2
SWH                8196.722 Hz
FIDRES             0.500288 Hz
AQ                 1.9988480 sec
RG                    38.1287
DW                    61.000 usec
DE                    13.54 usec
TE                    298.2 K
D1                 1.00000000 sec
TD0                         1
SFO1           400.5324733 MHz
NUC1                       1H
P0                    3.33 usec
P1                   10.00 usec
PLW1           14.34099960 W

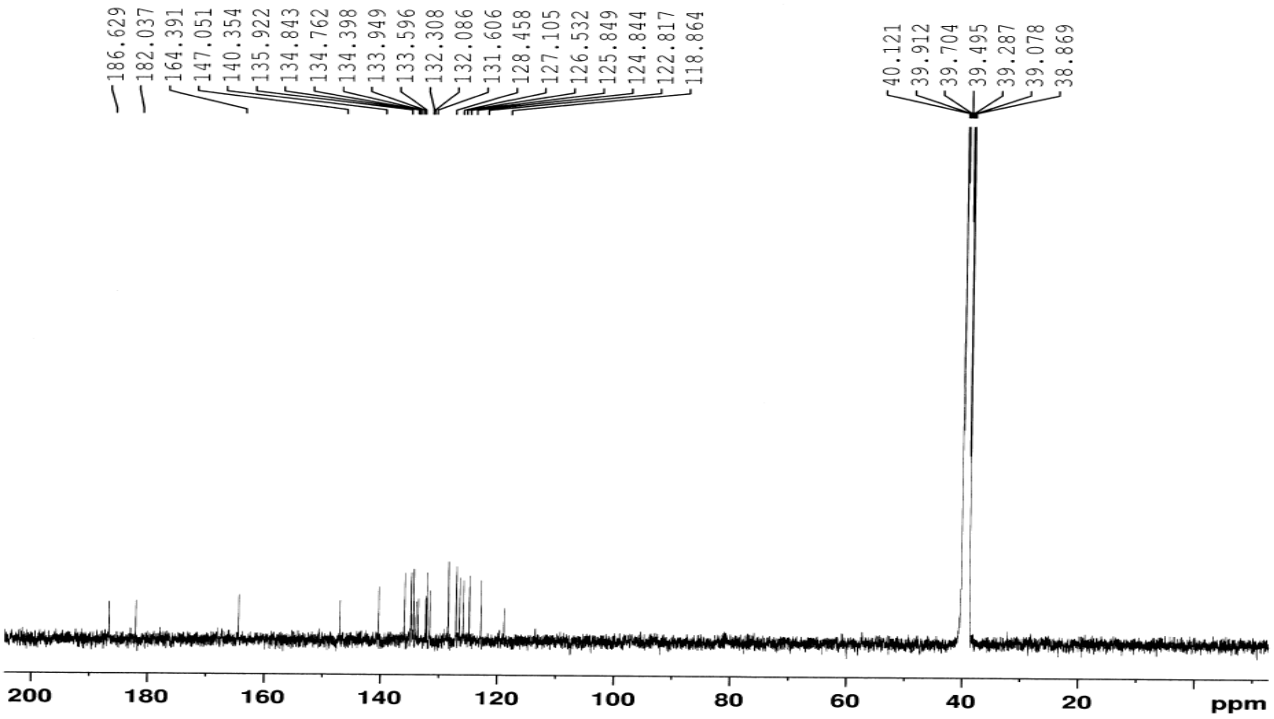
F2 - Processing parameters
SI                      65536
SF             400.5299715 MHz
WDW                        EM
SSB          0
LB                    0.30 Hz
GB           0
PC                    1.00
```

N-(9,10-dioxo-9,10-dihydroanthracen-1-yl)-2nitro benzamide (3o)-13C spectra



(3o)

AK-P-NO2

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Current Data Parameters
NAME                  AK-P-NO2A003
EXPNO                           11
PROCNO                           1

F2 - Acquisition Parameters
Date_                     20230823
Time                          8.02 h
INSTRUM                      spect
PROBHD     Z116098_0561 (
PULPROG                    zgpg30
TD                            65536
SOLVENT                        DMSO
NS                             7000
DS                                4
SWH                   24038.461 Hz
FIDRES                    0.733596 Hz
AQ                        1.3631488 sec
RG                           204.36
DW                           20.800 usec
DE                            6.50 usec
TE                           300.9 K
D1                    2.00000000 sec
D11                   0.03000000 sec
TD0                               1
SFO1                100.6479773 MHz
NUC1                         13C
P0                            3.33 usec
P1                           10.00 usec
PLW1                71.33300018 W
SFO2                400.2316009 MHz
NUC2                         1H
CPDPRG[2                 waltz65
PCPD2                        90.00 usec
PLW2                16.51199913 W
PLW12                0.20385000 W
PLW13                0.10253000 W

F2 - Processing parameters
SI                            32768
SF                  100.6379647 MHz
WDW                             EM
SSB                0
LB                            2.00 Hz
GB                 0
PC                            1.40
```
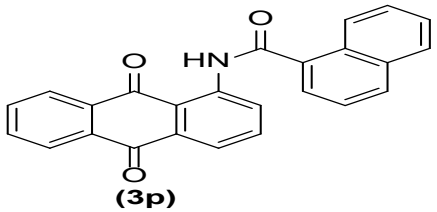
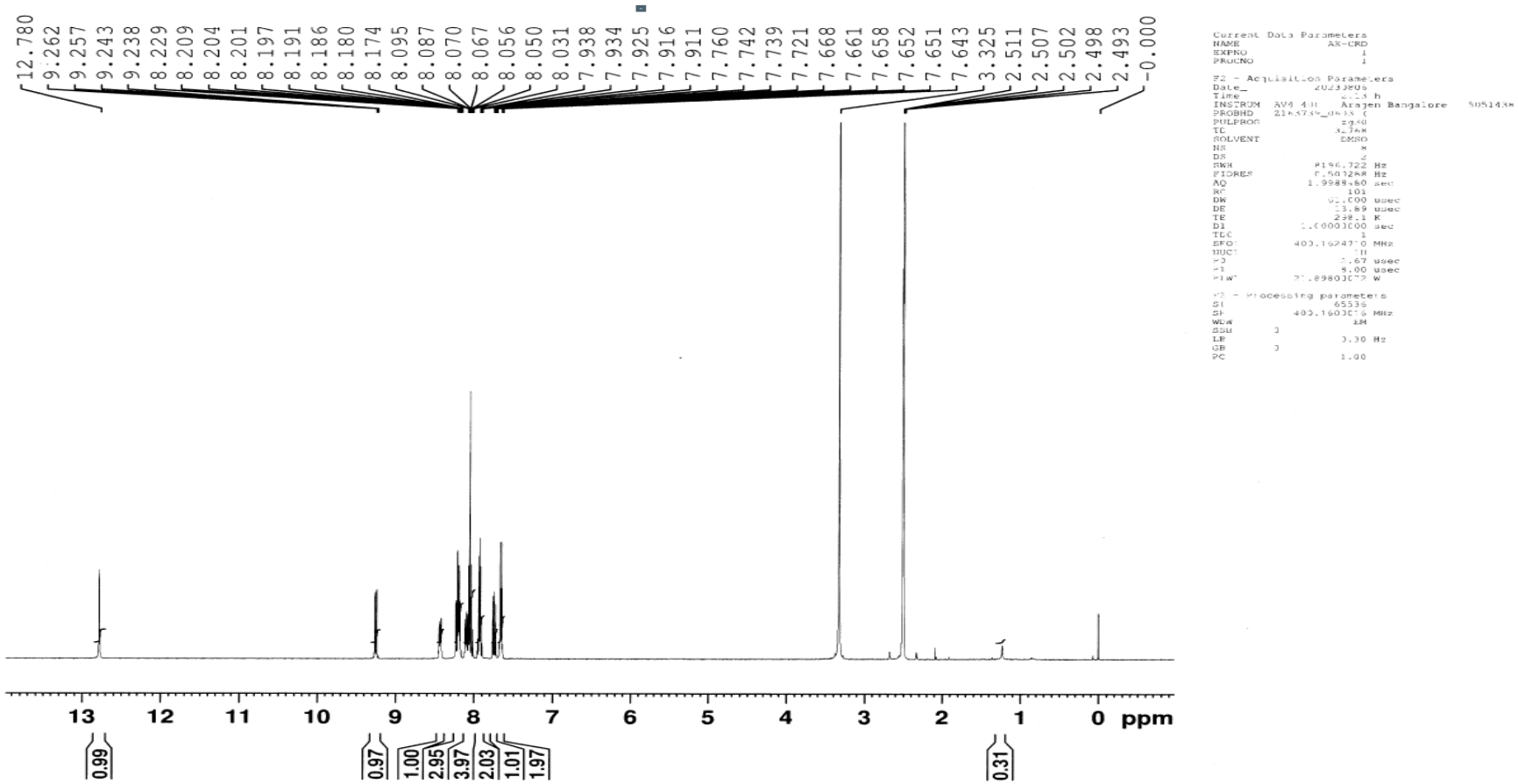
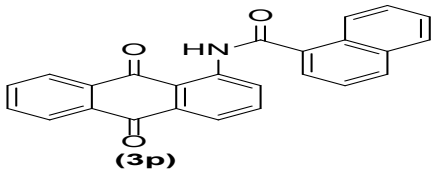

N-(9,10-dioxo-9,10-dihydroanthracen-1-yl)-1 naphthamide (3p)- 1H NMR spectra



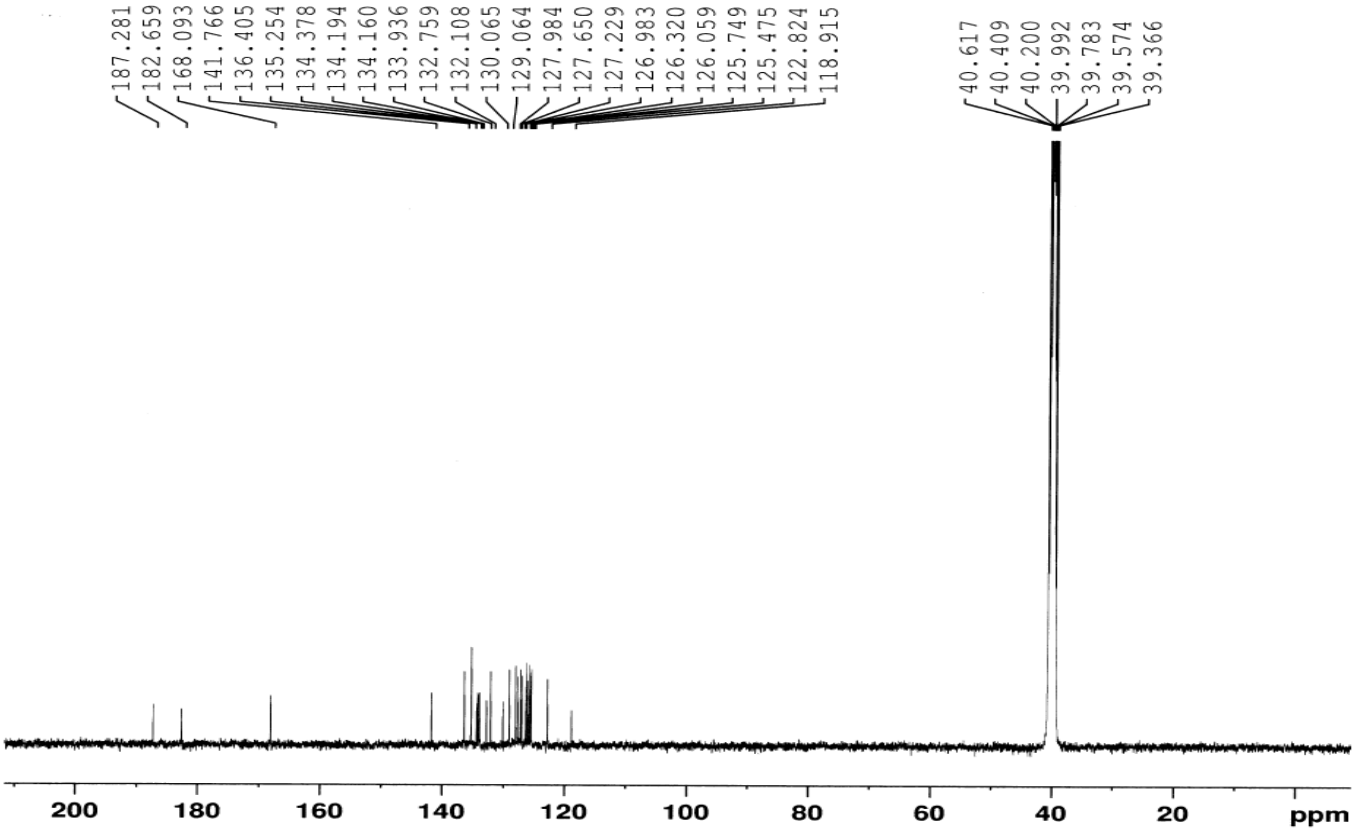
(3p)



N-(9,10-dioxo-9,10-dihydroanthracen-1-yl)-1 naphthamide (3p)-13C spectra



(3p)

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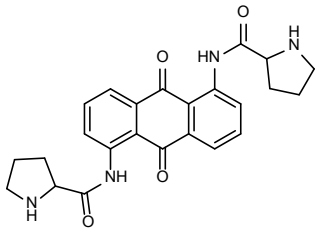
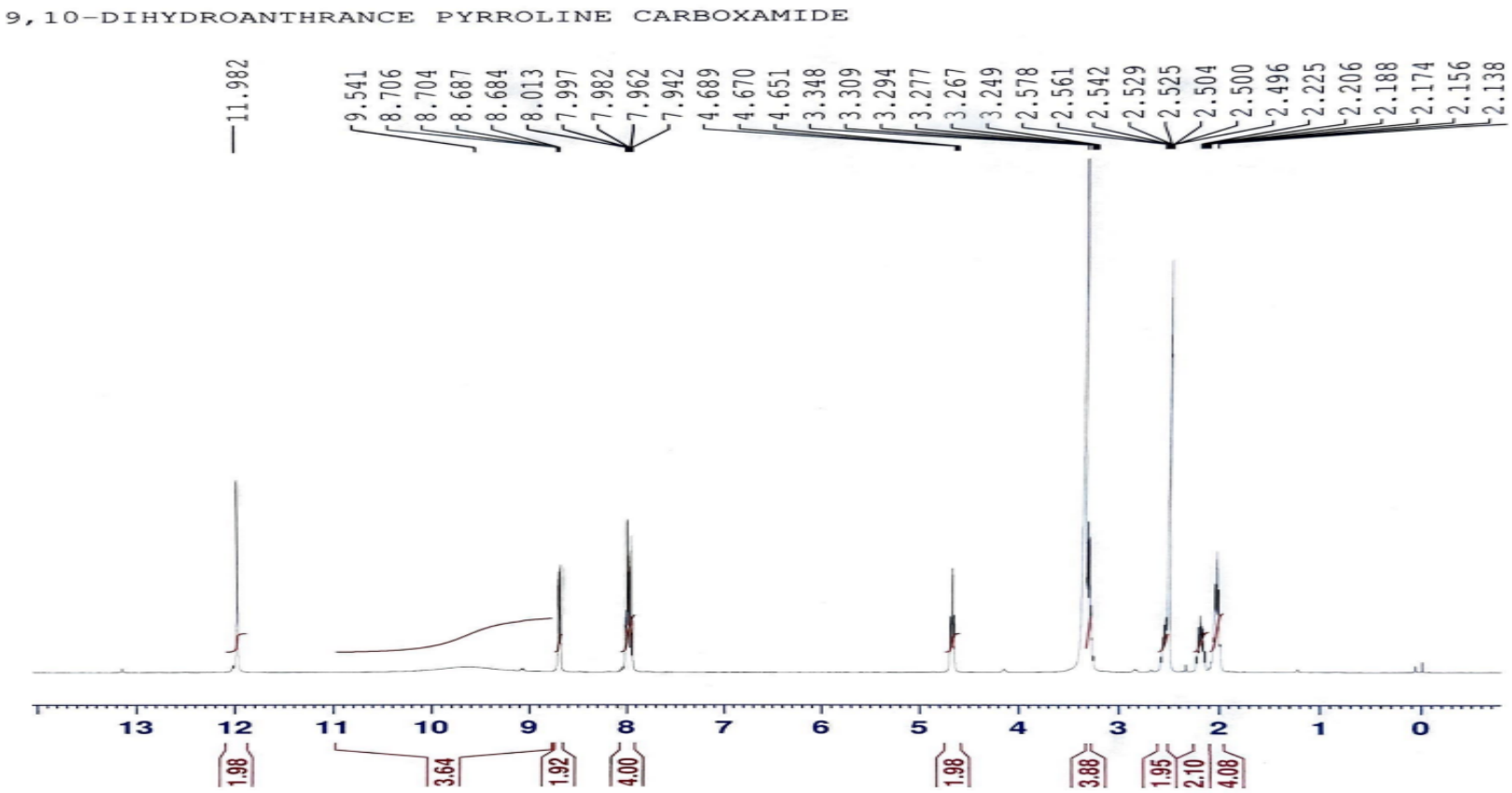
Current Data Parameters
NAME                  AS-CRD
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_              20231005
Time                  13.41 h
INSTRUM   AV4 400   Aragen Bangalore   5051438
PROBHD    216374_0613 (
PULPROG                zgpg30
TD                     65536
SOLVENT                DMSO
NS                      1600
DS                         4
SWH               23809.523 Hz
FIDRES             0.725609 Hz
AQ                 1.3762560 sec
RG                       101
DW                    21.000 usec
DE                     6.50 usec
TE                   298.1 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        1
SFO1             100.6303743 MHz
NUC1                     13C
P3                     15.67 usec
P1                     9.00 usec
PLW1            59.34303237 W
SFO2            400.1615006 MHz
NUC2                     1H
CPDPRG[2          waltz65
PCPD2                 93.00 usec
PLW2            25.89803072 W
PLW12            0.13020101 W
PLW13            0.05702700 W

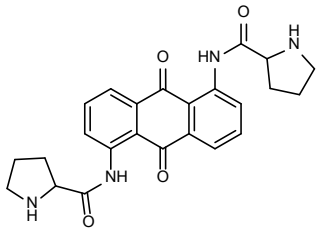
F2 - Processing parameters
SI                      32768
SF               100.6203120 MHz
WDW                        EM
SSB                        0
LB                      2.00 Hz
GB                         0
PC                      1.40
```

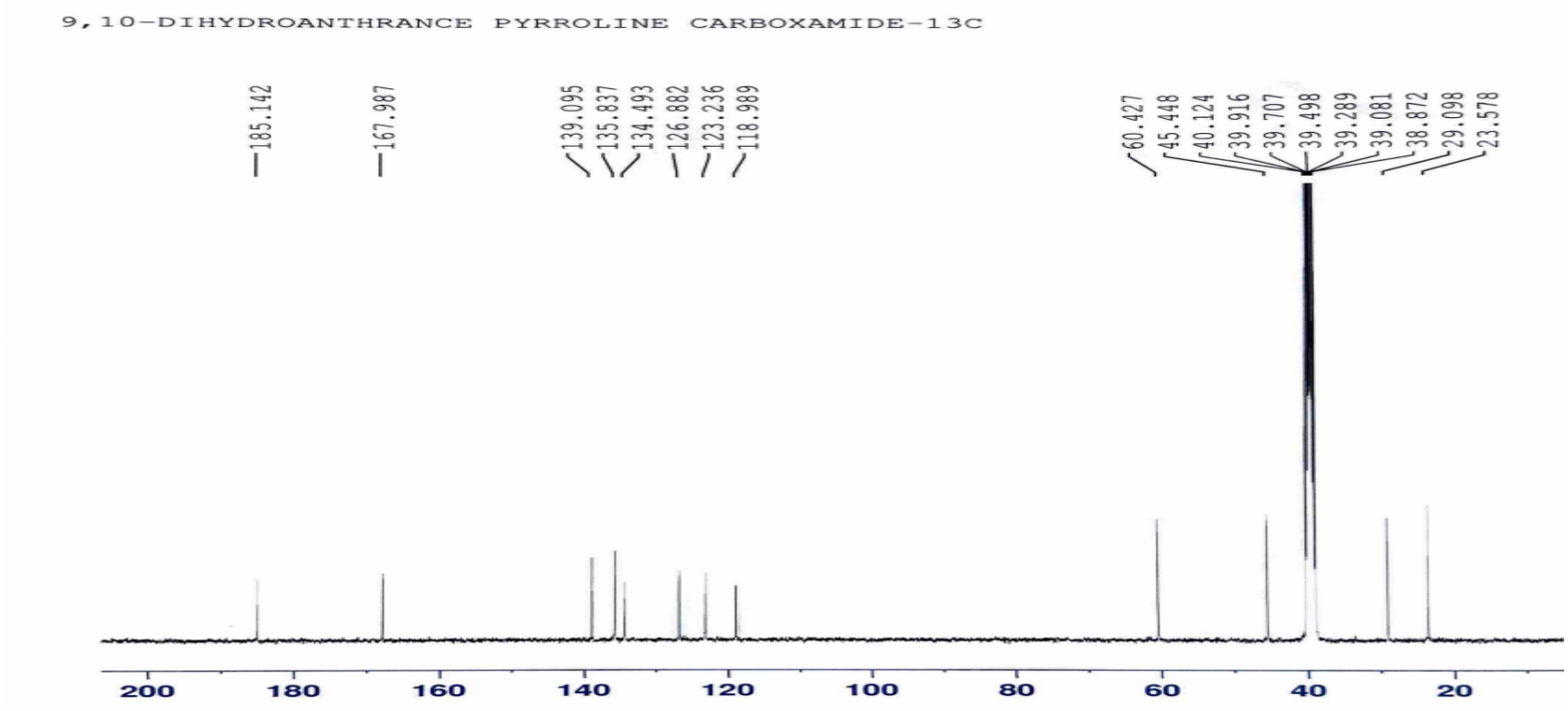
_N,N′_-(9,10-dioxo-9,10-dihydroanthracene-1,5-diyl)bis(pyrrolidine-2-carboxamide) -1H NMR spectra



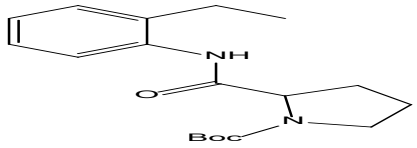


***N,N′*-(9,10-dioxo-9,10-dihydroanthracene-1,5-diyl)bis(pyrrolidine-2-carboxamide) -13C spectra**

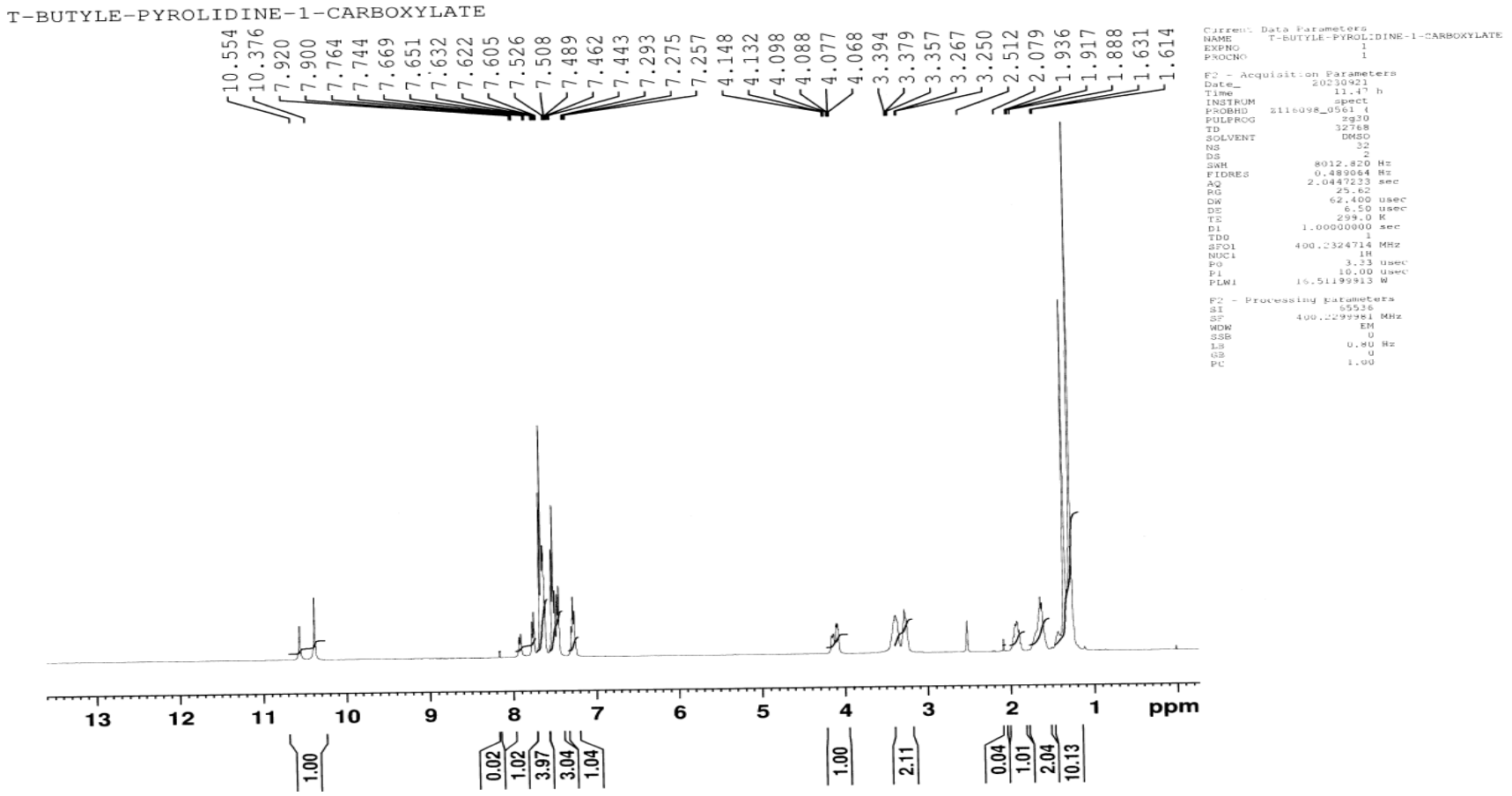




tert-butyl 2-((2-ethylphenyl)carbamoyl)pyrrolidine-1-carboxylate (5a)



5a

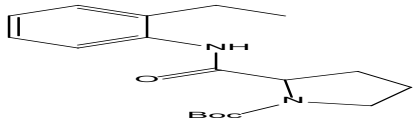


Current Data Parameters
NAME T-BUTYLE-PYROLIDINE-1-CARBOXYLATE
EXPNO 1
PROCNO 1

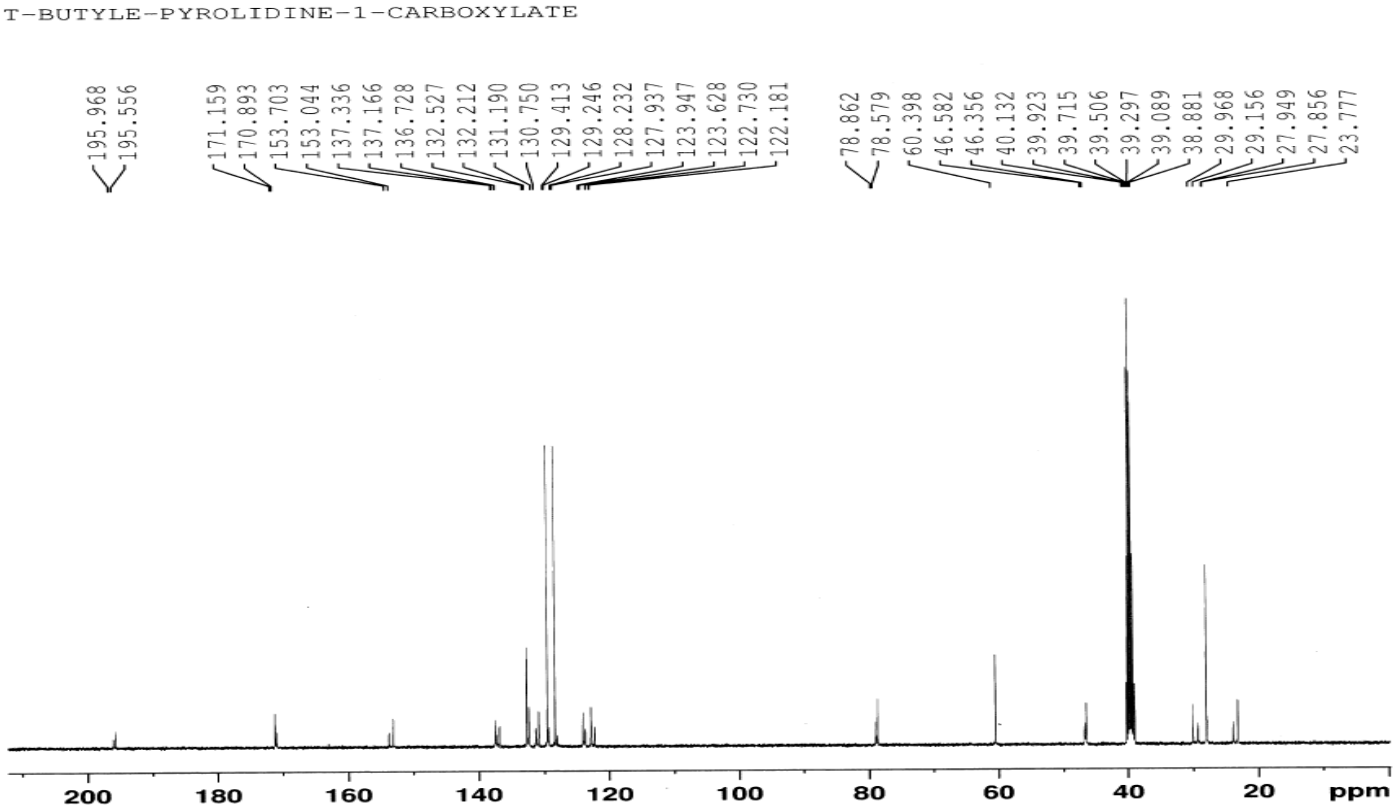
F2 - Acquisition Parameters
Date_ 20230921
Time 11.47 h
INSTRUM spect
PROBHD 2116098_0561 (
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.489064 Hz
AQ 2.0447233 sec
RG 25.62
DW 62.400 usec
DE 6.50 usec
TE 299.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324714 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 16.51199913 W

F2 - Processing parameters
SI 65536
SF 400.2299981 MHz
WDW EM
SSB 0
LB 0.80 Hz
GB 0
PC 1.00

tert-butyl 2-((2-ethylphenyl)carbamoyl)pyrrolidine-1-carboxylate (5a)



5a

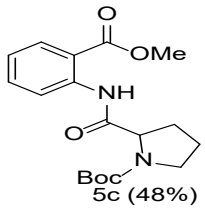



```
Current Data Parameters
NAME        T-BUTYLE-PYROLIDINE-1-CARBOXYLATE
EXPNO                 21
PROCNO                 1

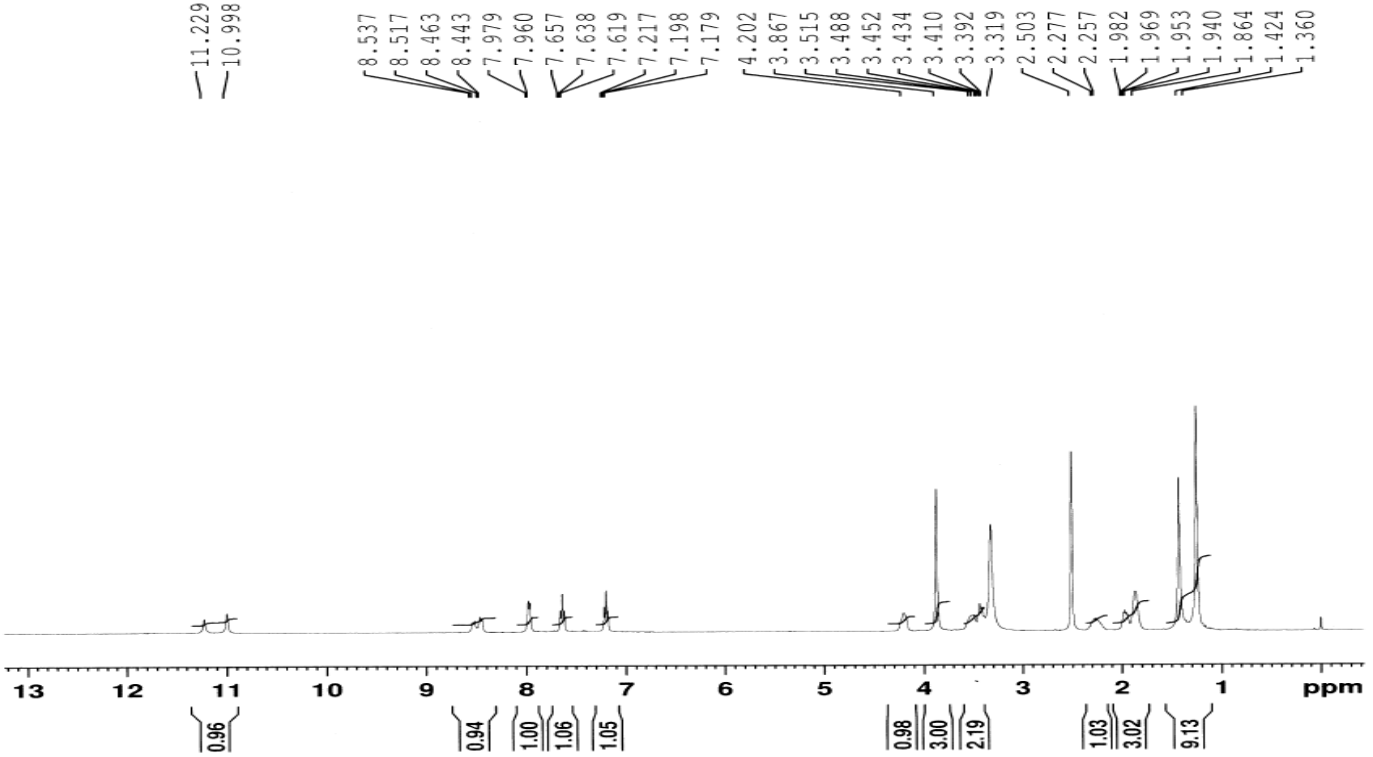
F2 - Acquisition Parameters
Date_           20230921
Time              23.13 h
INSTRUM             spect
PROBHD     Z116098_0561 (
PULPROG          zgpg30
TD                65536
SOLVENT            DMSO
NS                  1001
DS                     4
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ             1.3631488 sec
RG                204.36
DW                20.800 usec
DE                 6.50 usec
TE                300.4 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1
SFO1          100.6479773 MHz
NUC1                  13C
P0                  3.33 usec
P1                 10.00 usec
PLW1          71.32300018 W
SFO2          400.2316009 MHz
NUC2                  1H
CPDPRG[2          waltz65
PCPD2              90.00 usec
PLW2          19.51198913 W
PLW12          0.20385000 W
PLW13          0.10253000 W

F2 - Processing parameters
SI                 32768
SF            100.6379659 MHz
WDW                   EM
SSB                    0
LB                  0.90 Hz
GB                     0
PC                  1.40
```

tert-butyl2-((2-(methoxycarbonyl)phenyl)carbamoyl)pyrrolidine-1-carboxylate (5c)



COMPOUND-10-DMSO

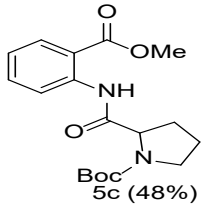



```
Current Data Parameters
NAME        COMPOUND-10-DMSO
EXPNO                      1
PROCNO                     1

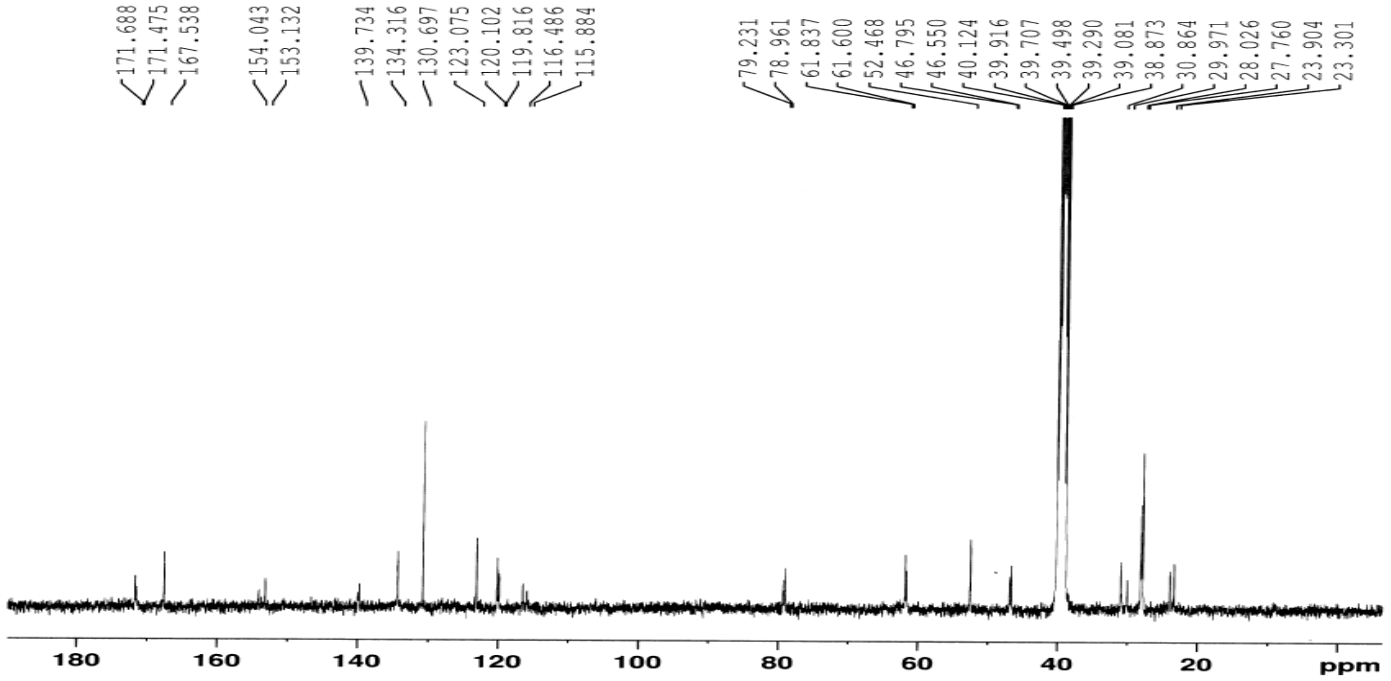
F2 - Acquisition Parameters
Date_                20230922
Time                    12.08 h
INSTRUM                 spect
PROBHD    Z116098_0561 (
PULPROG                 zg30
TD                     32768
SOLVENT                 DMSO
NS                        32
DS                         2
SWH                  8012.820 Hz
FIDRES               0.489064 Hz
AQ                   2.0447233 sec
RG                      149.06
DW                      62.400 usec
DE                       6.50 usec
TE                      300.2 K
D1                1.00000000 sec
TD0                        1
SFO1             400.2324714 MHz
NUC1                       1H
P0                      3.33 usec
P1                     10.00 usec
PLW1             16.51199913 W

F2 - Processing parameters
SI                     65536
SF               400.2300021 MHz
WDW                       EM
SSB                  0
LB                      0.80 Hz
GB                   0
PC                      1.00
```

tert-butyl2-((2-(methoxycarbonyl)phenyl)carbamoyl)pyrrolidine-1-carboxylate (5c)



COMPOUND-10

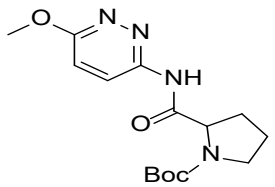



```
Current Data Parameters
NAME                  Compound-10
EXPNO                         191
PROCNO                          1

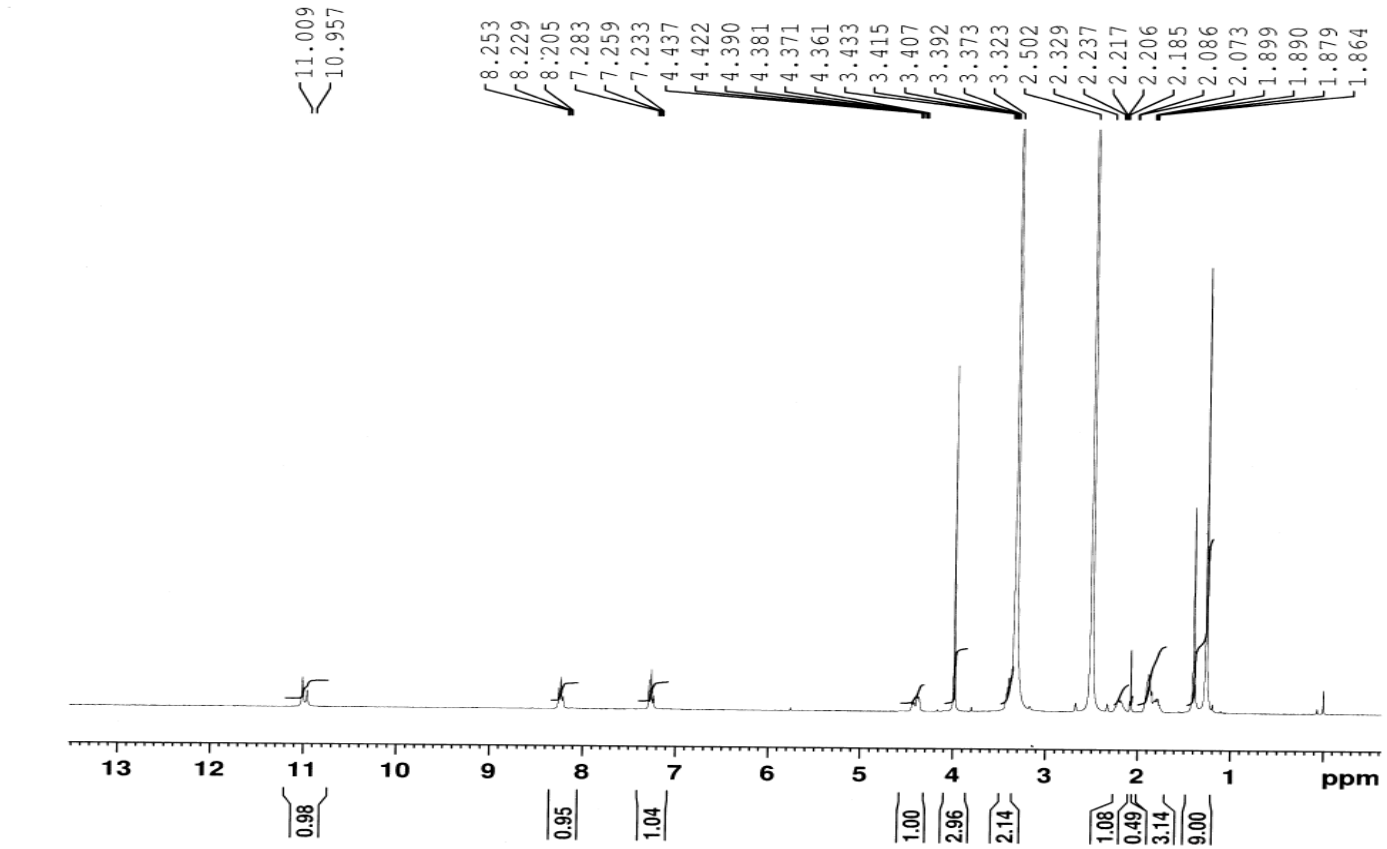
F2 - Acquisition Parameters
Date_                    20230923
Time                         0.51 h
INSTRUM                      spect
PROBHD     Z116098_0561 (
PULPROG                  zgpg30
TD                            65536
SOLVENT                       DMSO
NS                            3072
DS                               4
SWH                   24038.461 Hz
FIDRES                 0.733596 Hz
AQ                    1.3631488 sec
RG                          204.36
DW                          20.800 usec
DE                           6.50 usec
TE                          300.5 K
D1                    2.00000000 sec
D11                   0.03000000 sec
TD0                             1
SFO1                100.6479773 MHz
NUC1                         13C
P0                           3.33 usec
P1                          10.00 usec
PLW1                71.33300018 W
SFO2                400.2316009 MHz
NUC2                         1H
CPDPRG[2                waltz65
PCPD2                       90.00 usec
PLW2                16.51199913 W
PLW12                0.20385000 W
PLW13                0.10253000 W

F2 - Processing parameters
SI                           32768
SF                  100.6379654 MHz
WDW                             EM
SSB                  0
LB                           2.00 Hz
GB                   0
PC                           1.40
```

tert-butyl 2-((6-methoxypyridazin-3-yl)carbamoyl)pyrrolidine-1-carboxylate (5d)



5d(53%)

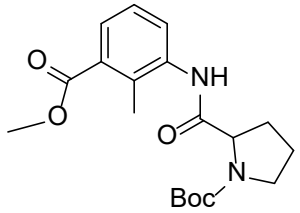



```
Current Data Parameters
NAME      COMPOUND-12-DMSO
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20230925
Time                11.34 h
INSTRUM              spect
PROBHD    Z116098_0561 (
PULPROG              zg30
TD                  32768
SOLVENT              DMSO
NS                     64
DS                      2
SWH              8012.820 Hz
FIDRES           0.489064 Hz
AQ              2.0447233 sec
RG                 204.36
DW                 62.400 usec
DE                  6.50 usec
TE                 298.9 K
D1            1.00000000 sec
TD0                     1
SFO1         400.2324714 MHz
NUC1                   1H
P0                  3.33 usec
P1                 10.00 usec
PLW1         16.51199913 W

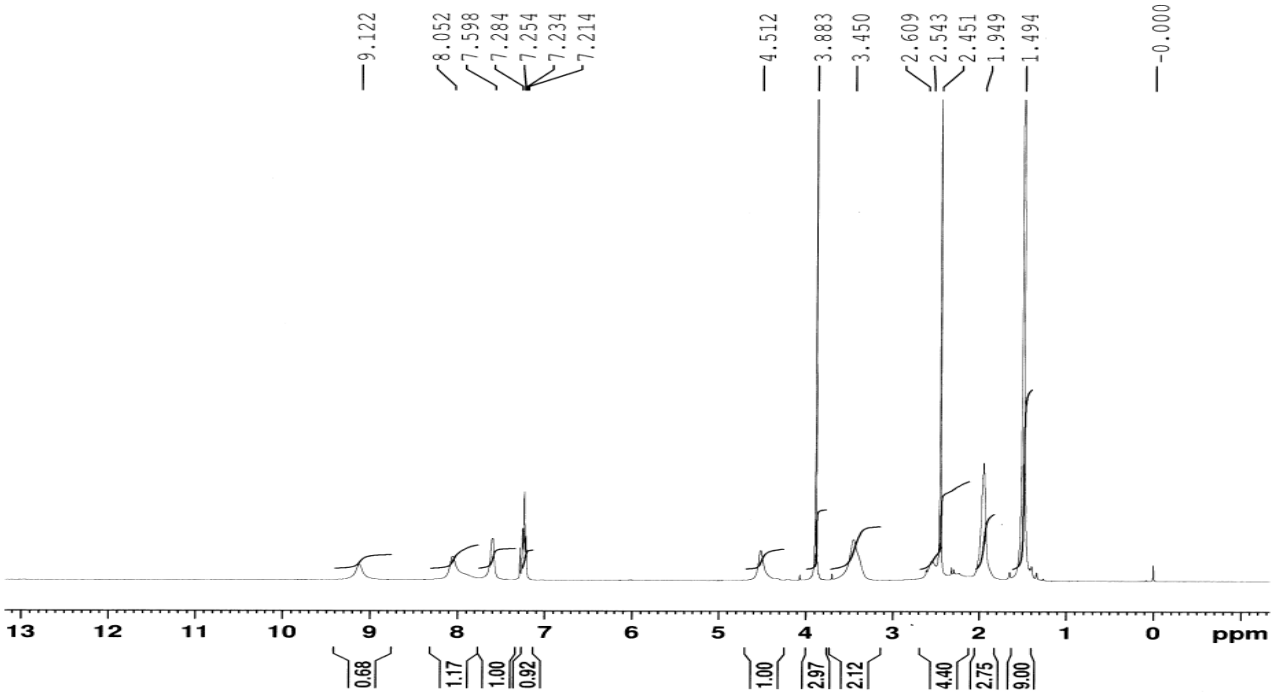
F2 - Processing parameters
SI                  65536
SF           400.2300025 MHz
WDW                    EM
SSB                 0
LB                   0.80 Hz
GB                  0
PC                   1.00
```

tert-butyl 2-((3-(methoxycarbonyl)-2-methylphenyl)carbamoyl)pyrrolidine-1-carboxylate



5e

WITHOUT-BROMO COMPOUND-CDCL3

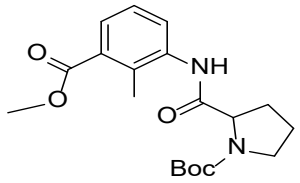



```
Current Data Parameters
NAME      WITHOUT-BROMO COMPOUND-CDCL3
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20230927
Time              12.42 h
INSTRUM           spect
PROBHD    Z116098_0561 (
PULPROG           zg30
TD               32768
SOLVENT          CDCl3
NS                   64
DS                    2
SWH            8012.820 Hz
FIDRES         0.489064 Hz
AQ             2.0447233 sec
RG                28.21
DW               62.400 usec
DE                6.50 usec
TE               299.4 K
D1            1.00000000 sec
TD0                   1
SFO1         400.2324714 MHz
NUC1                 1H
P0                3.33 usec
P1               10.00 usec
PLW1         16.51199913 W

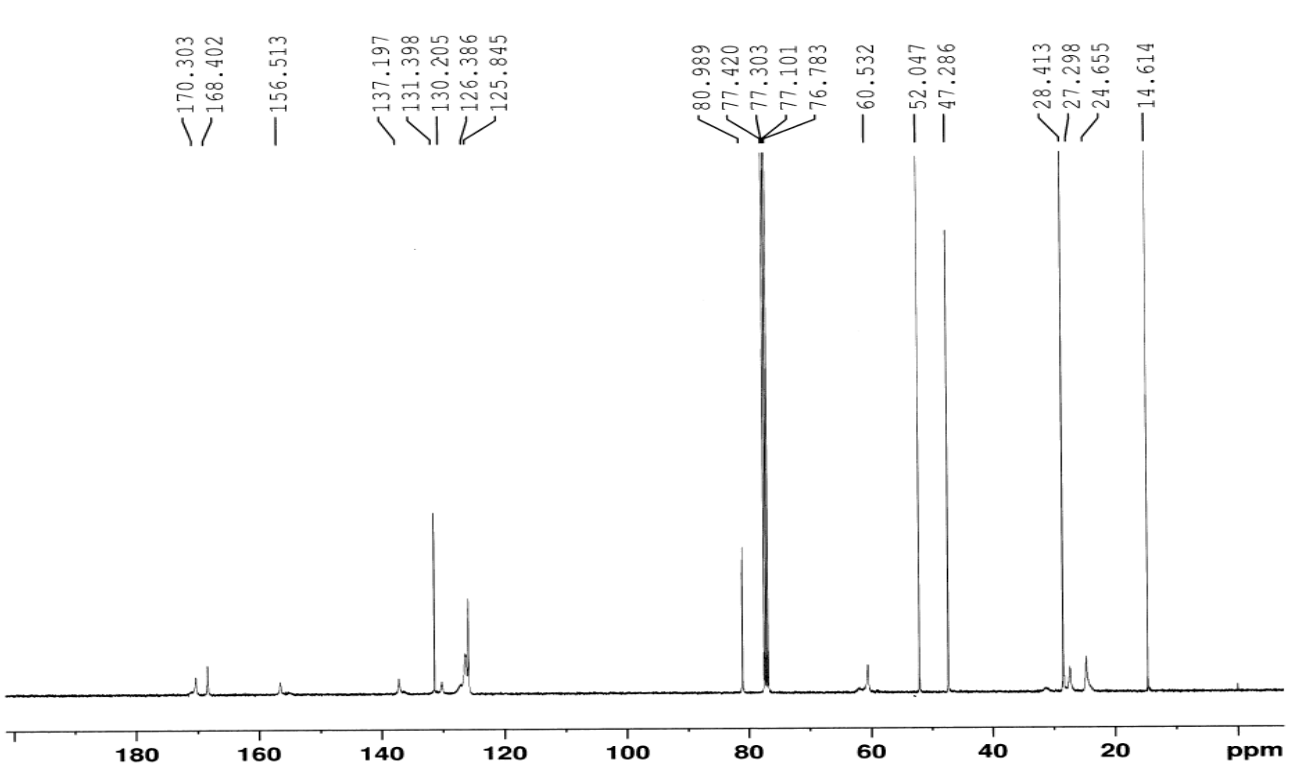
F2 - Processing parameters
SI                65536
SF           400.2299998 MHz
WDW                  EM
SSB          0
LB                0.80 Hz
GB           0
PC                1.00
```

tert-butyl 2-((3-(methoxycarbonyl)-2-methylphenyl)carbamoyl)pyrrolidine-1-carboxylate



5e

WITHAOUT BROMO COMPOUND

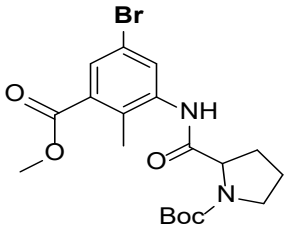



```
Current Data Parameters
NAME      WITHAOUT BROMO COMPOUND
EXPNO                 22
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230929
Time              23.21 h
INSTRUM             spect
PROBHD   Z116098_0561 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                 4000
DS                    4
SWH           24038.461 Hz
FIDRES        0.733596 Hz
AQ            1.3631488 sec
RG                204.36
DW                20.800 usec
DE                 6.50 usec
TE                298.1 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1         100.6479773 MHz
NUC1                 13C
P0                  3.33 usec
P1                 10.00 usec
PLW1         71.33300018 W
SFO2         400.2316009 MHz
NUC2                 1H
CPDPRG[2          waltz65
PCPD2              90.00 usec
PLW2         16.51199913 W
PLW12         0.20385000 W
PLW13         0.10253000 W

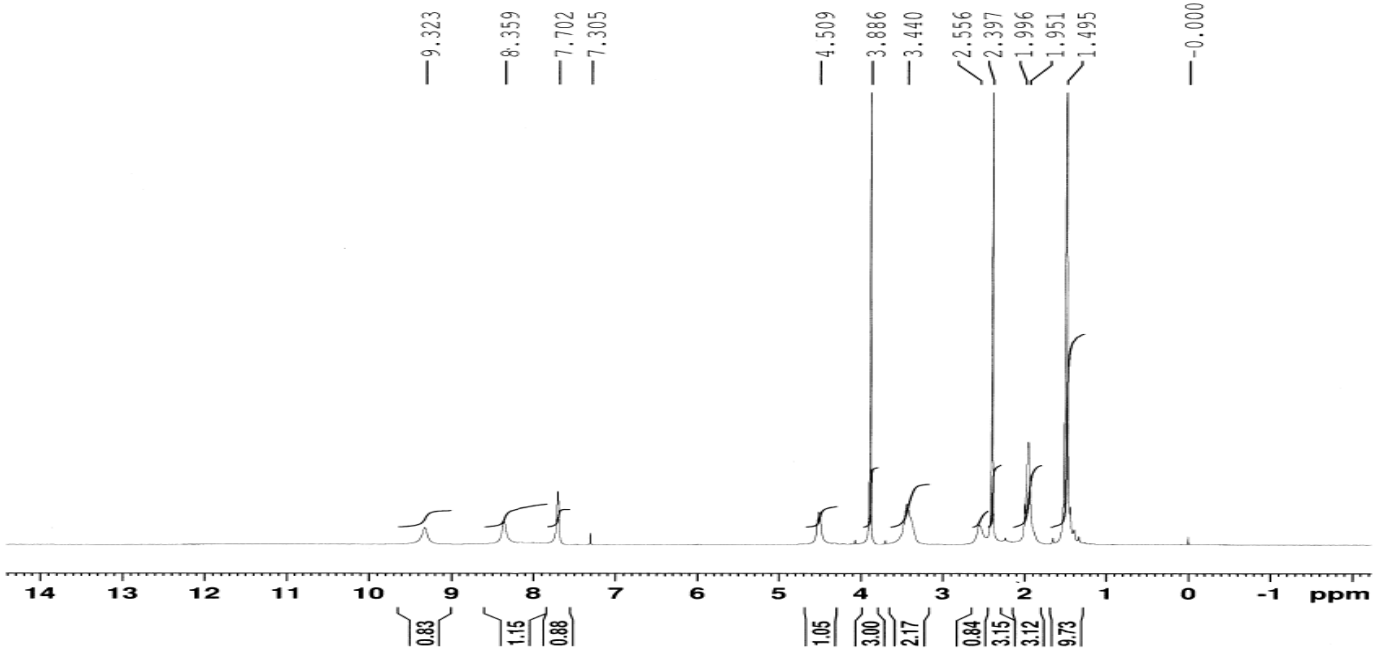
F2 - Processing parameters
SI                32768
SF           100.6379135 MHz
WDW                  EM
SSB       0
LB                0.80 Hz
GB        0
PC                1.40
```

tert-butyl 2-((5-bromo-3-(methoxycarbonyl)-2-methylphenyl)carbamoyl)pyrrolidine-1-carboxylate



5f

WITH-BROMO COMPOUND-CDCL3

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Current Data Parameters
NAME        WITH-BROMO COMPOUND-CDCL3
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20230927
Time              12.36 h
INSTRUM           spect
PROBHD    Z116098_0561 (
PULPROG           zg30
TD               32768
SOLVENT          CDCl3
NS                   64
DS                    2
SWH            8012.820 Hz
FIDRES         0.489064 Hz
AQ             2.0447233 sec
RG                 19.8
DW                62.400 usec
DE                 6.50 usec
TE                299.4 K
D1             1.00000000 sec
TD0                   1
SFO1          400.2324714 MHz
NUC1                  1H
P0                 3.33 usec
P1                10.00 usec
PLW1          16.51199913 W

F2 - Processing parameters
SI                65536
SF            400.2299913 MHz
WDW                  EM
SSB                   0
LB                 0.80 Hz
GB                    0
PC                 1.00
```
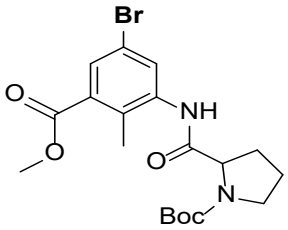
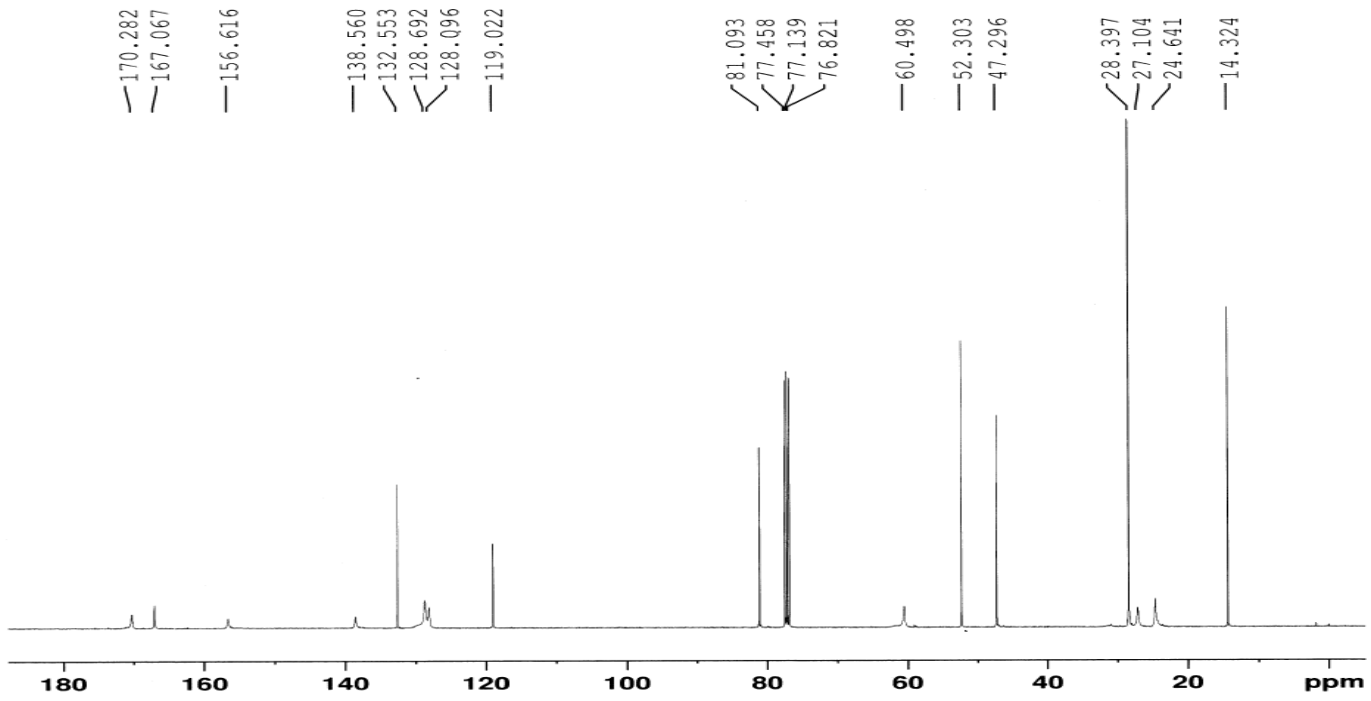

tert-butyl 2-((5-bromo-3-(methoxycarbonyl)-2-methylphenyl)carbamoyl)pyrrolidine-1-carboxylate



5f

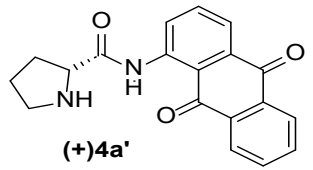
Bromo COMPUND-CDCL3



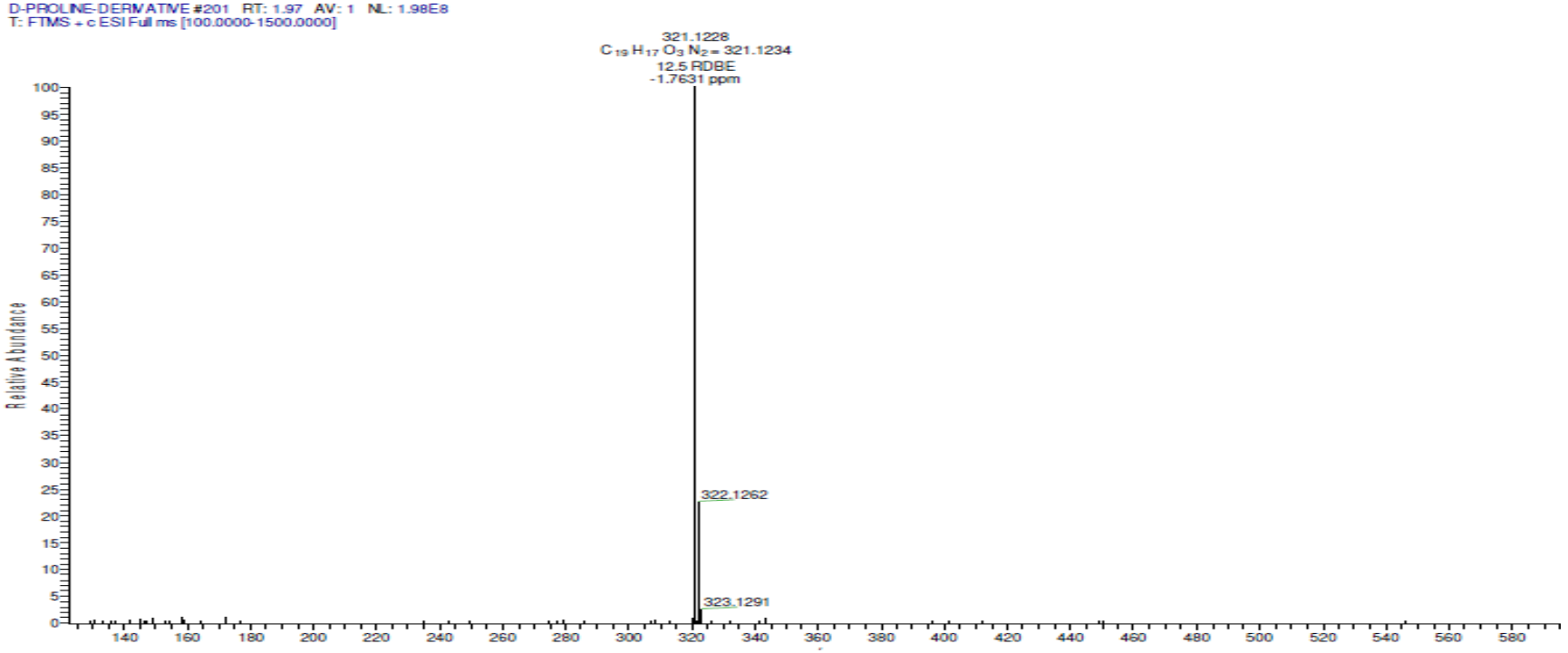

```
Current Data Parameters
NAME       Bromo COMPUND-CDCL3
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_             20230929
Time                23.20 h
INSTRUM   AV4 400NB ANL-BLR-NMR-03
PROBHD   2163739_0195 (
PULPROG             zgpg30
TD                  65536
SOLVENT             CDCl3
NS                   4000
DS                      4
SWH              23809.523 Hz
FIDRES           0.726609 Hz
AQ               1.3762560 sec
RG                    101
DW                 21.000 usec
DE                  6.50 usec
TE                 298.1 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                     1
SFO1         100.6228298 MHz
NUC1                  13C
P0                  2.67 usec
P1                  8.00 usec
PLW1         99.25000000 W
SFO2         400.1316005 MHz
NUC2                  1H
CPDPRG[2          waltz65
PCPD2              90.00 usec
PLW2         24.03499985 W
PLW12         0.19059330 W
PLW13         0.09552535 W

F2 - Processing parameters
SI                  32768
SF           100.6127685 MHz
WDW                    EM
SSB         0
LB                  1.00 Hz
GB          0
PC                  1.40
```

7. HRMS DATA

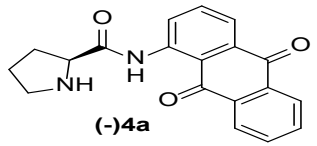
(R)-N-(9,10-dioxo-9,10-dihydroanthracen-1-yl)pyrrolidine-2-carboxamide



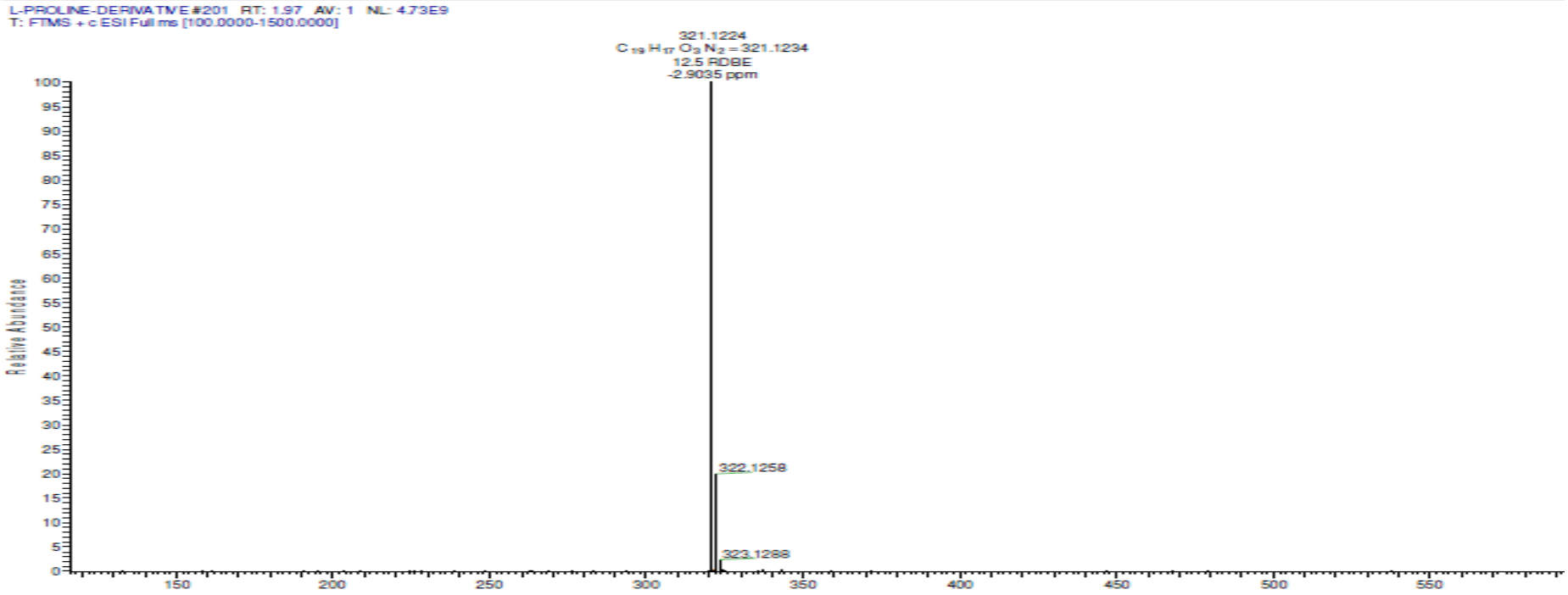
(+)4a'



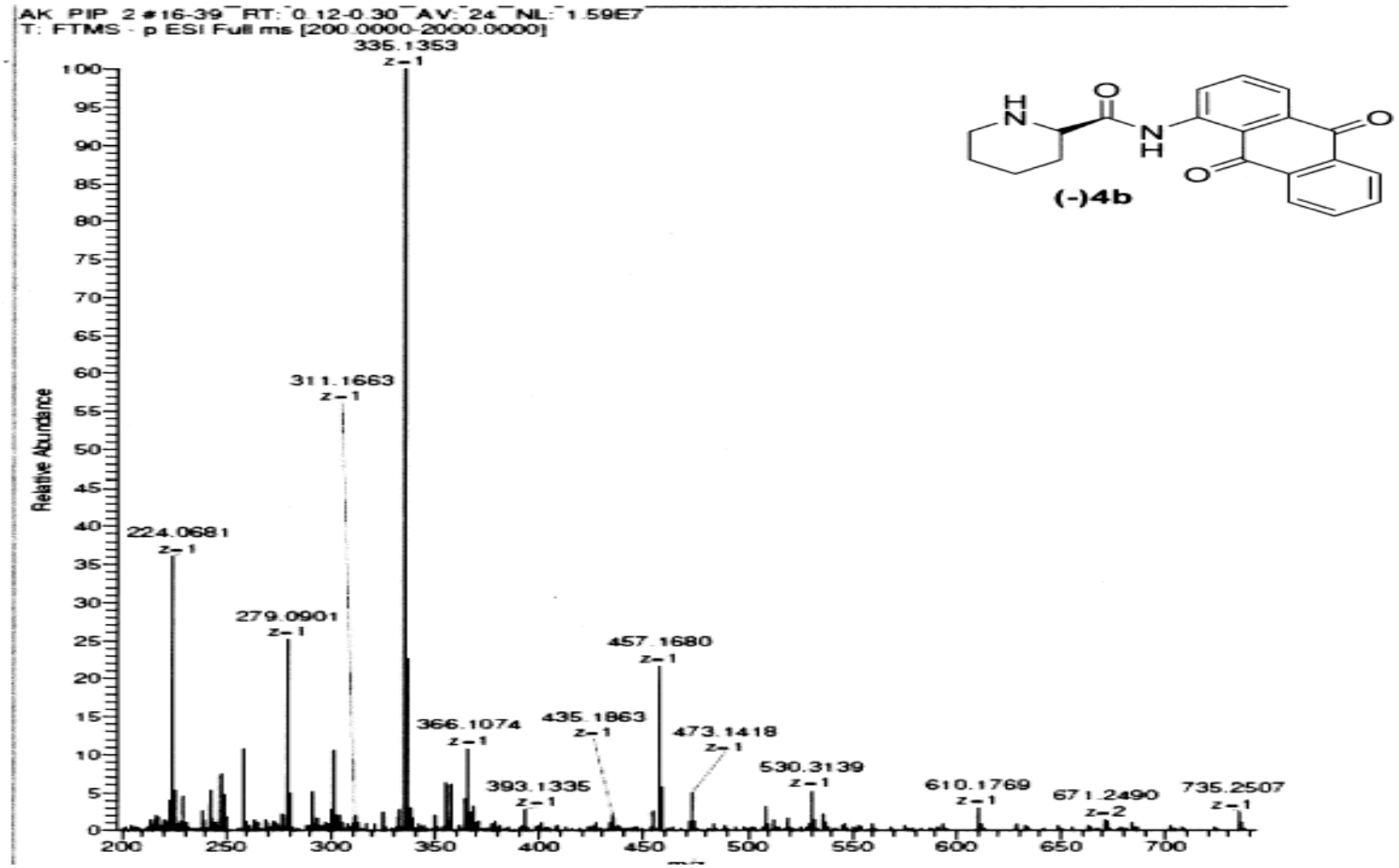
(S) -N-(9,10-dioxo-9,10-dihydroanthracen-1-yl)pyrrolidine-2-arboxamide



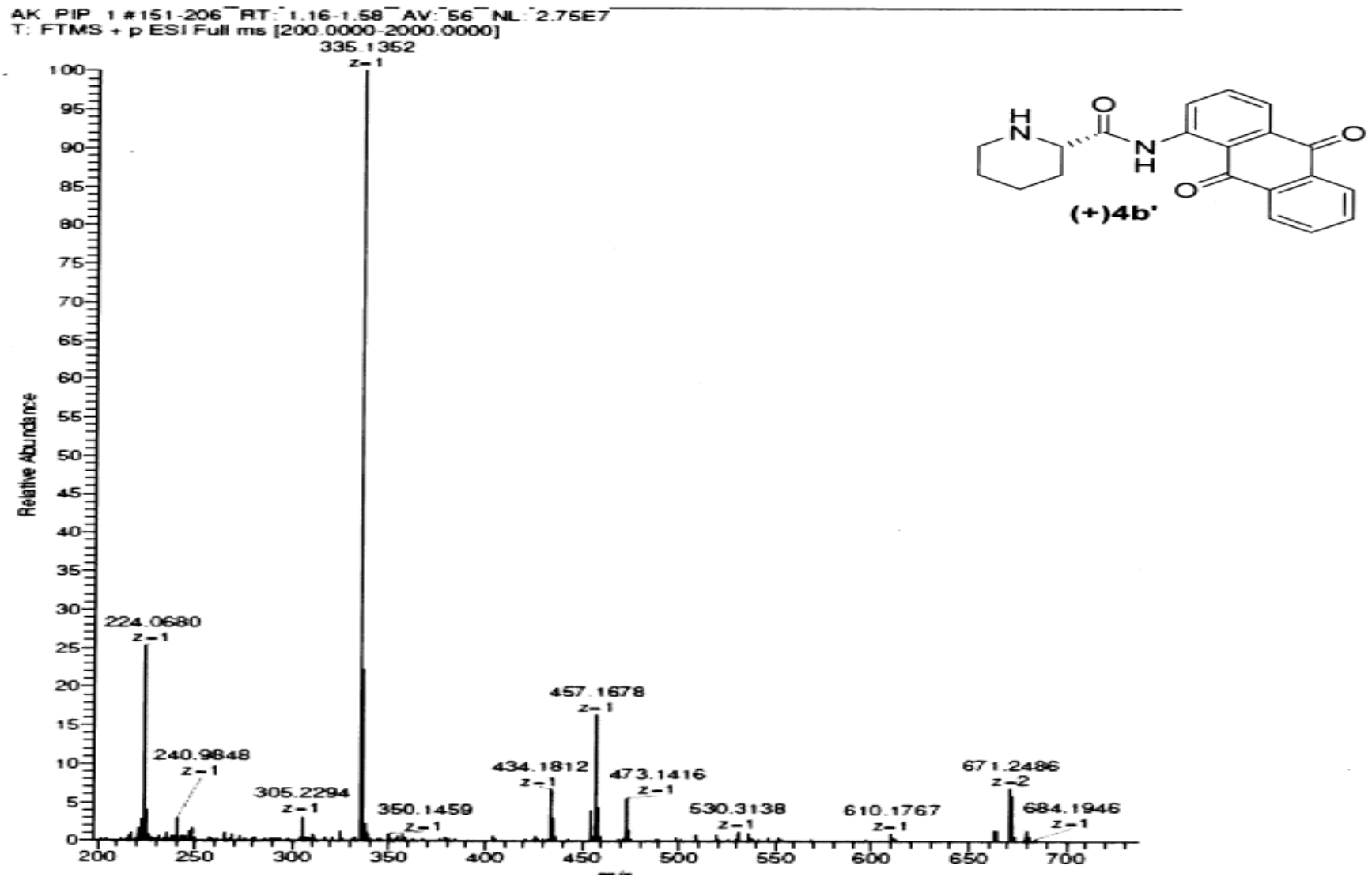
(-)4a



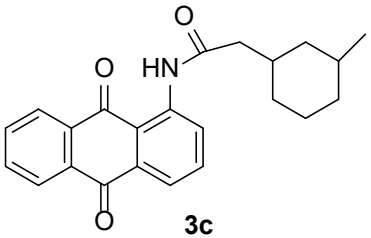
(R)-N-(9,10-dioxo-9,10-dihydroanthracen-1-yl)piperidine-2-carboxamide



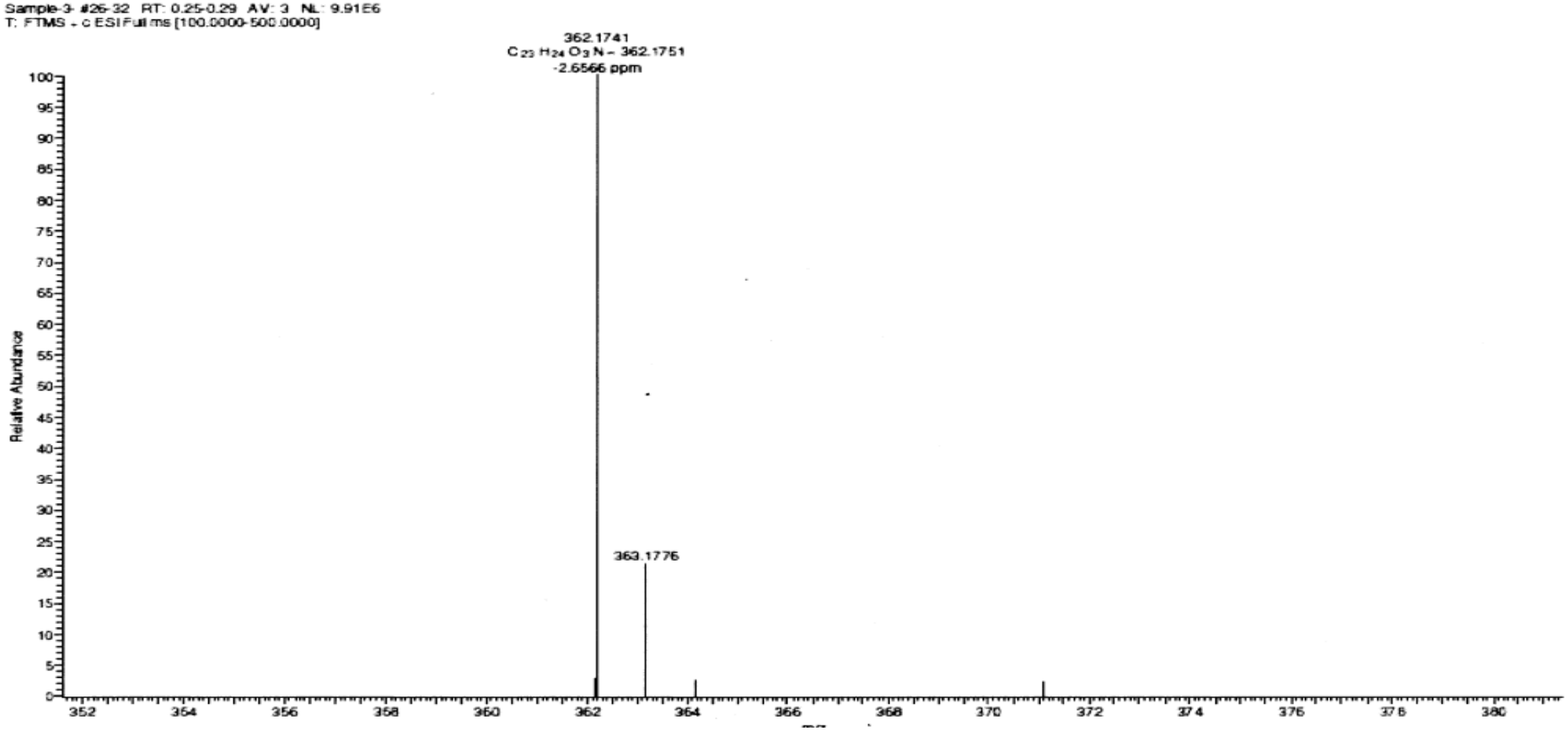
(S)-N-(9,10-dioxo-9,10-dihydroanthracen-1-yl)piperidine-2-carboxamide



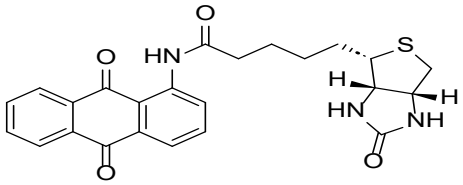
N-(9,10-dioxo-9,10-dihydroanthracen-1-yl)-2-((1s,4s)-4-methylcyclohexyl)acetamide (3c)



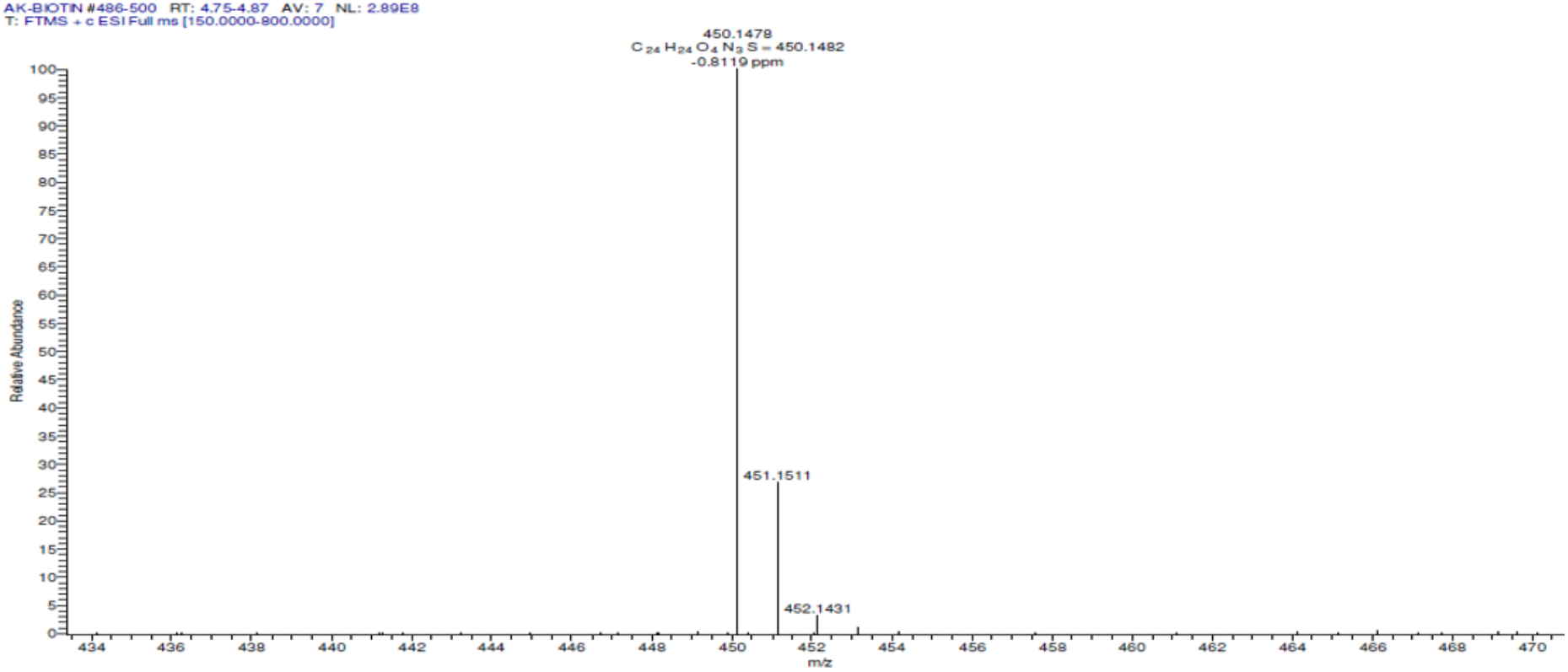
3c



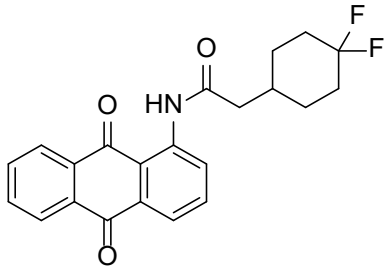
***N*-(9,10-dioxo-9,10-dihydroanthracen-1-yl)-5-((3aS,4S,6aR)-2-oxohexahydro-1H-thieno[3,4-d]imidazol-4-yl)pentanamide (3d)**



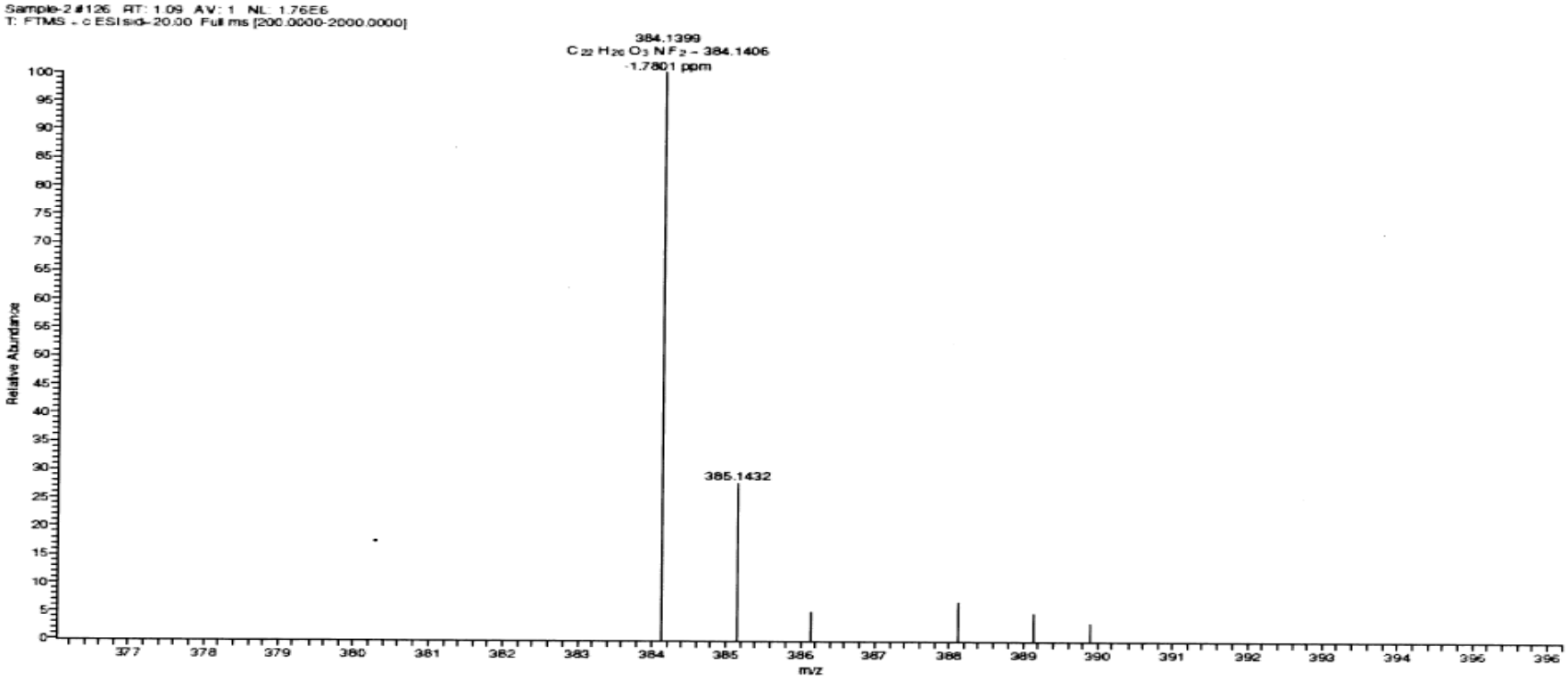
3d



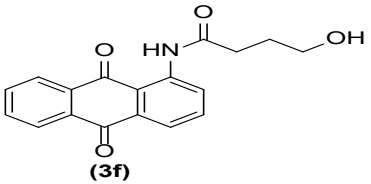
4,4-difluorocyclohexyl)-N-(9,10-dioxo-9,10-dihydroanthracen-1-yl)acetamide (3e)-



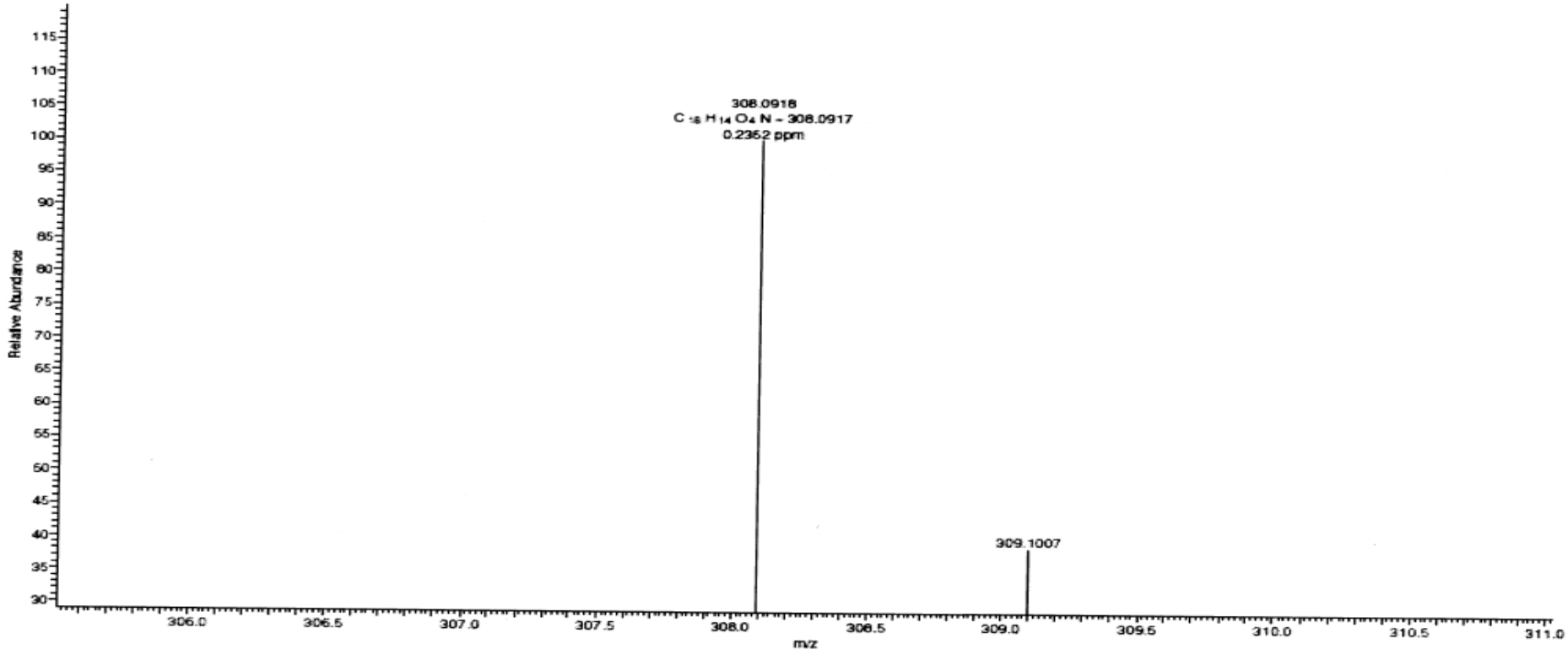
(**3e**)



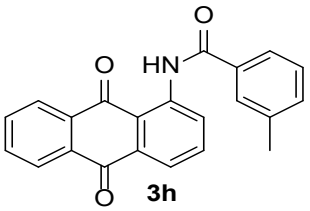
N-(9,10-dioxo-9,10-dihydroanthracen-1-yl)-4-hydroxybutanamide(3f)



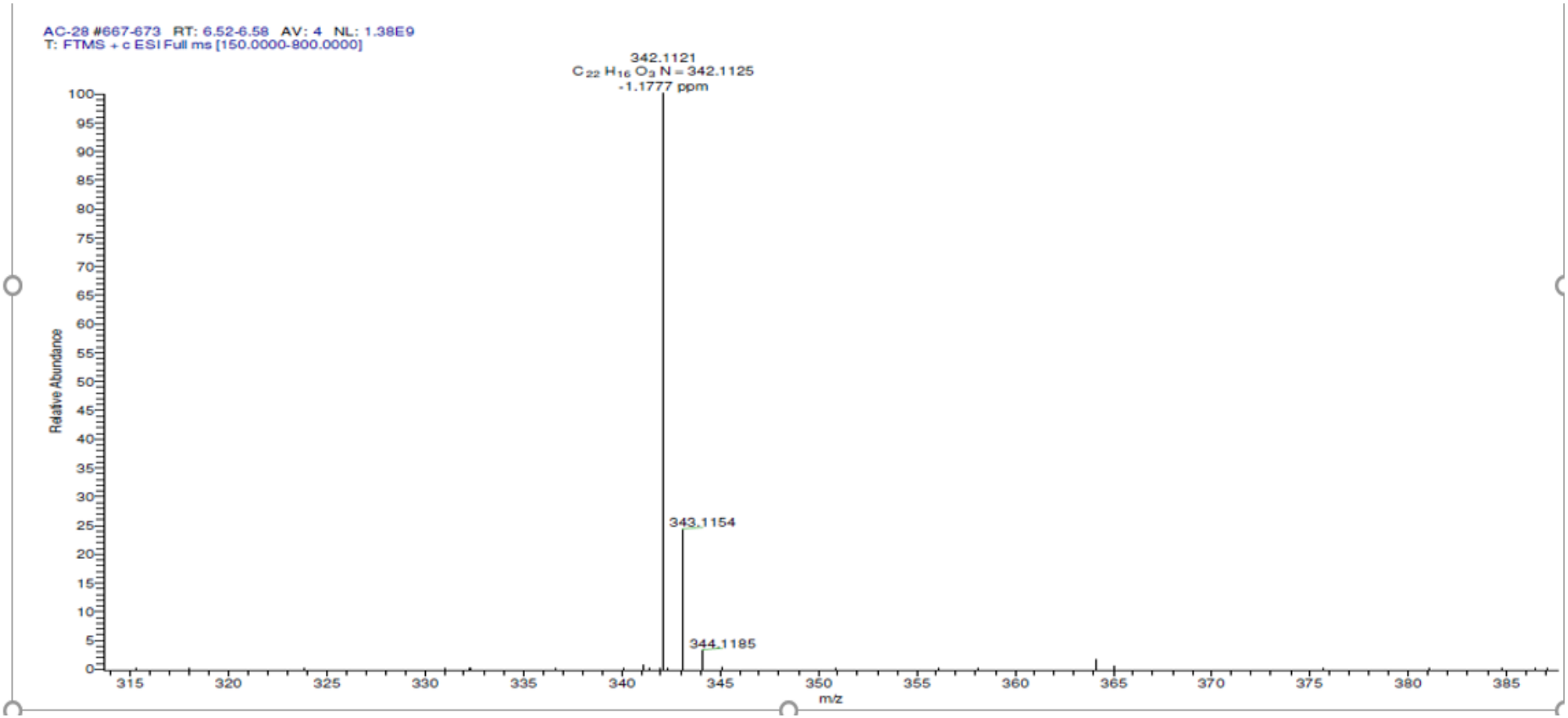
(3f)



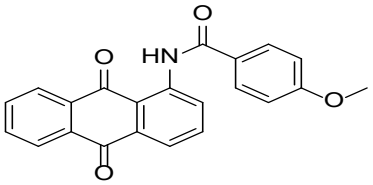
***N*-(9, 10-dioxo-9,10-dihydroanthracen-1-yl)-3-methylbenzamide (3h)**



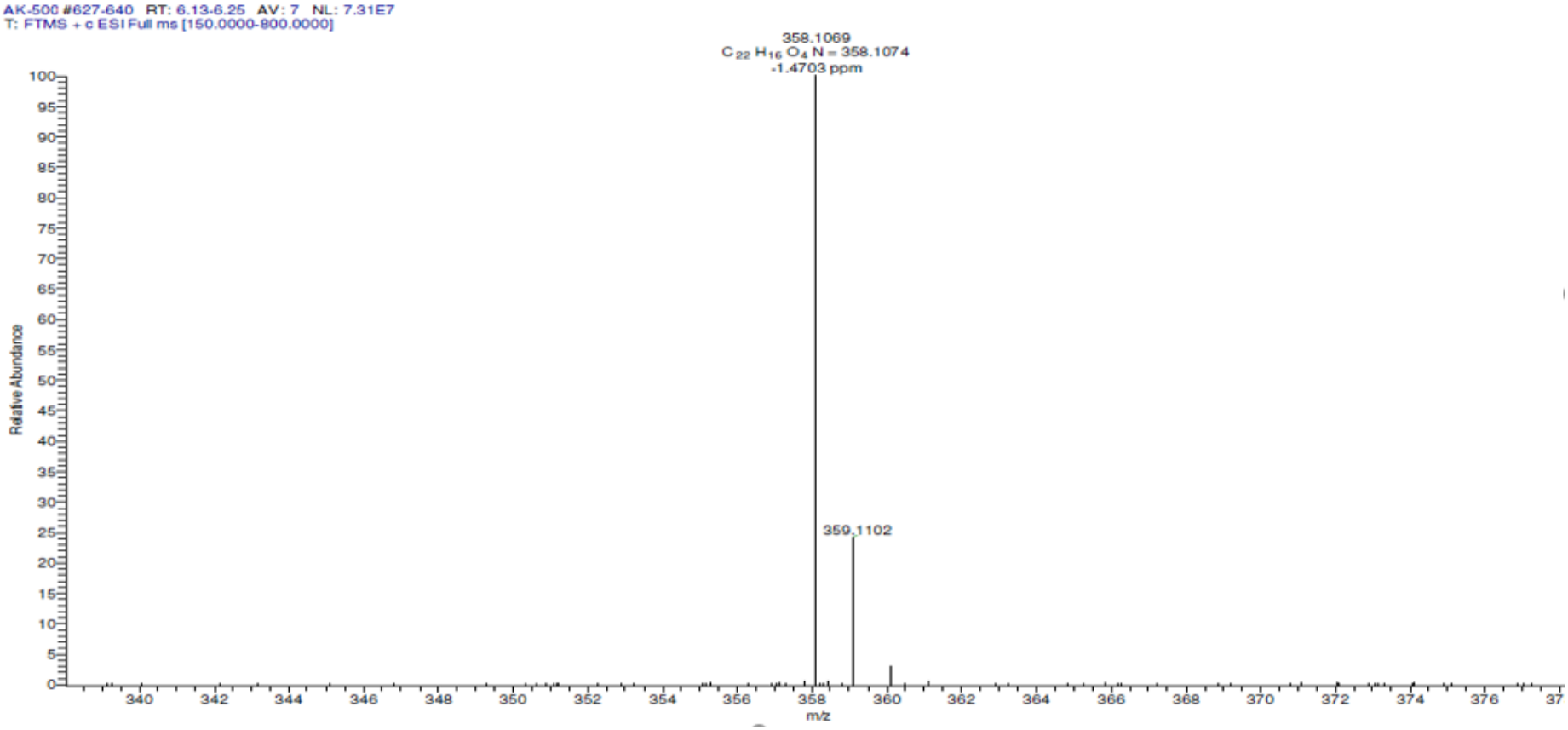
3h



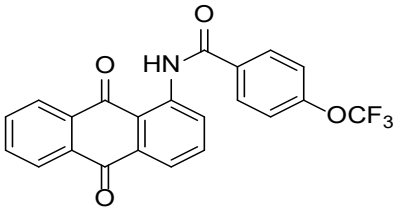
***N*-(9,10-dioxo-9,10-dihydroanthracen-1-yl)-4-methoxybenzamide (3i)**



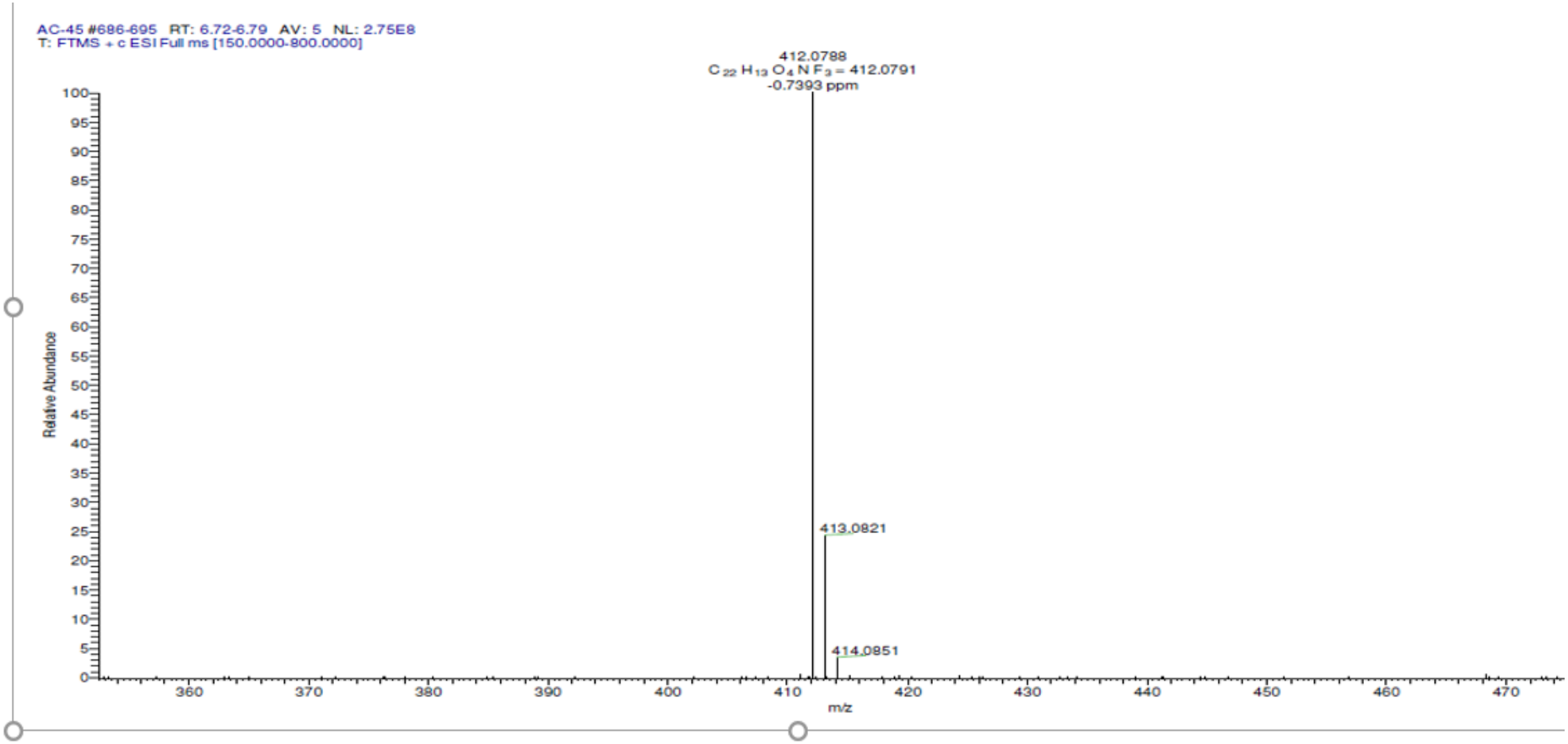
3i



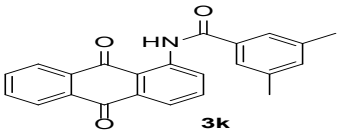
***N*-(9,10-dioxo-9,10-dihydroanthracen-1-yl)-4-(trifluoromethoxy)benzamide (3j)**

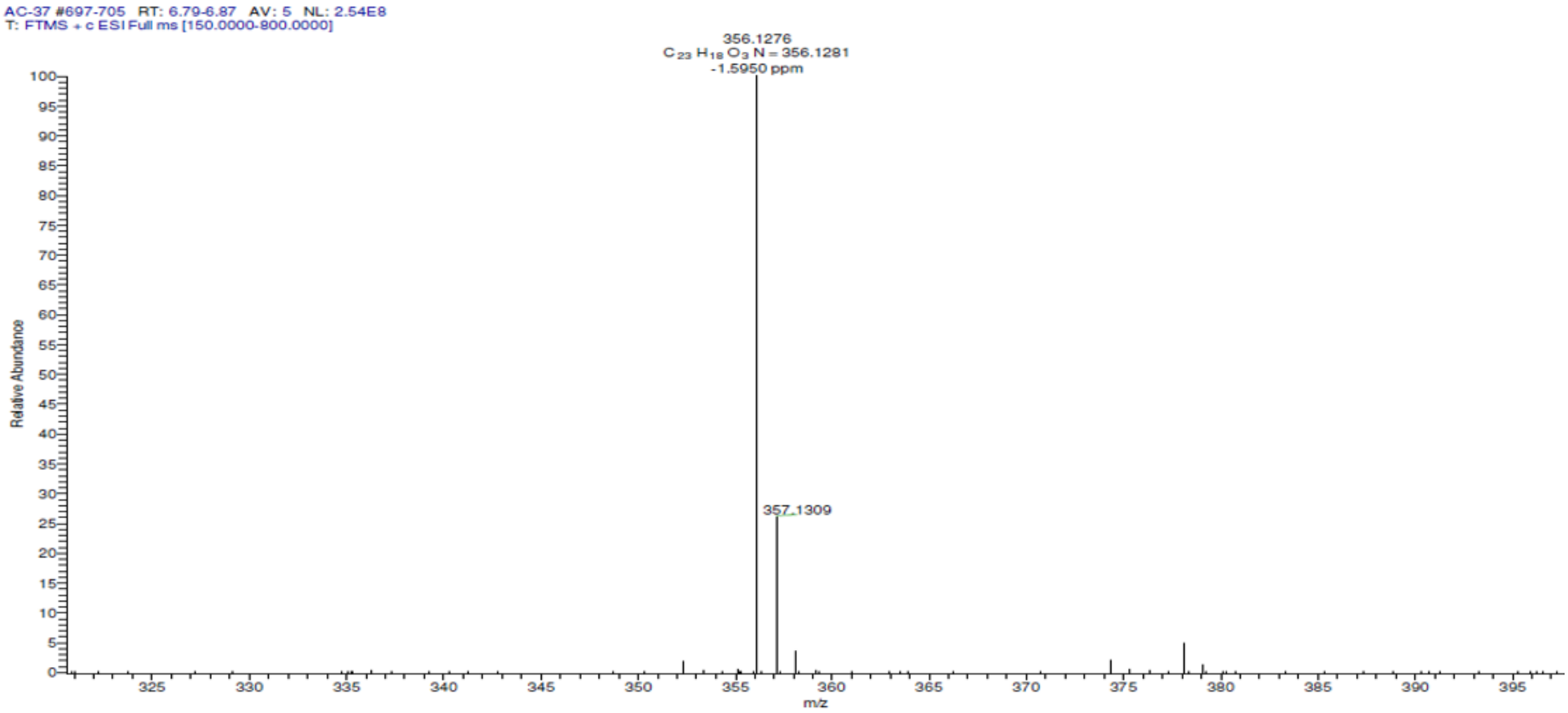


3j

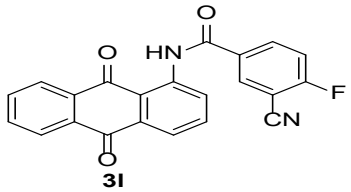


***N*-(9,10-dioxo-9,10-dihydroanthracen-1-yl)-3,5-dimethylbenzamide (3k)**

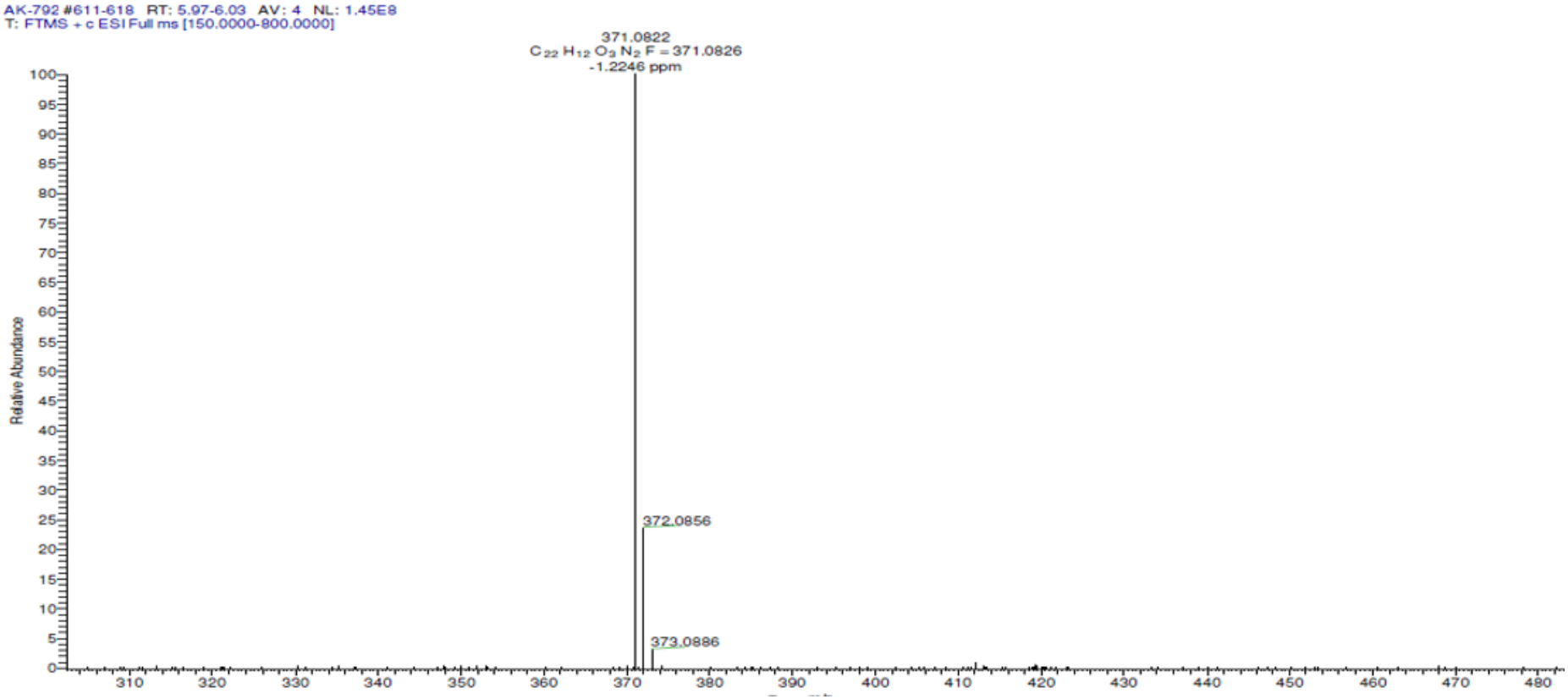




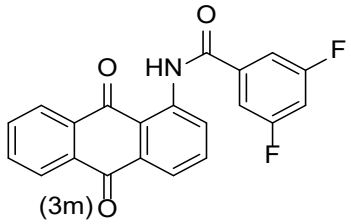
3-cyano-N-(9,10-dioxo-9,10-dihydroanthracen-1-yl)-4-fluorobenzamide (3l)

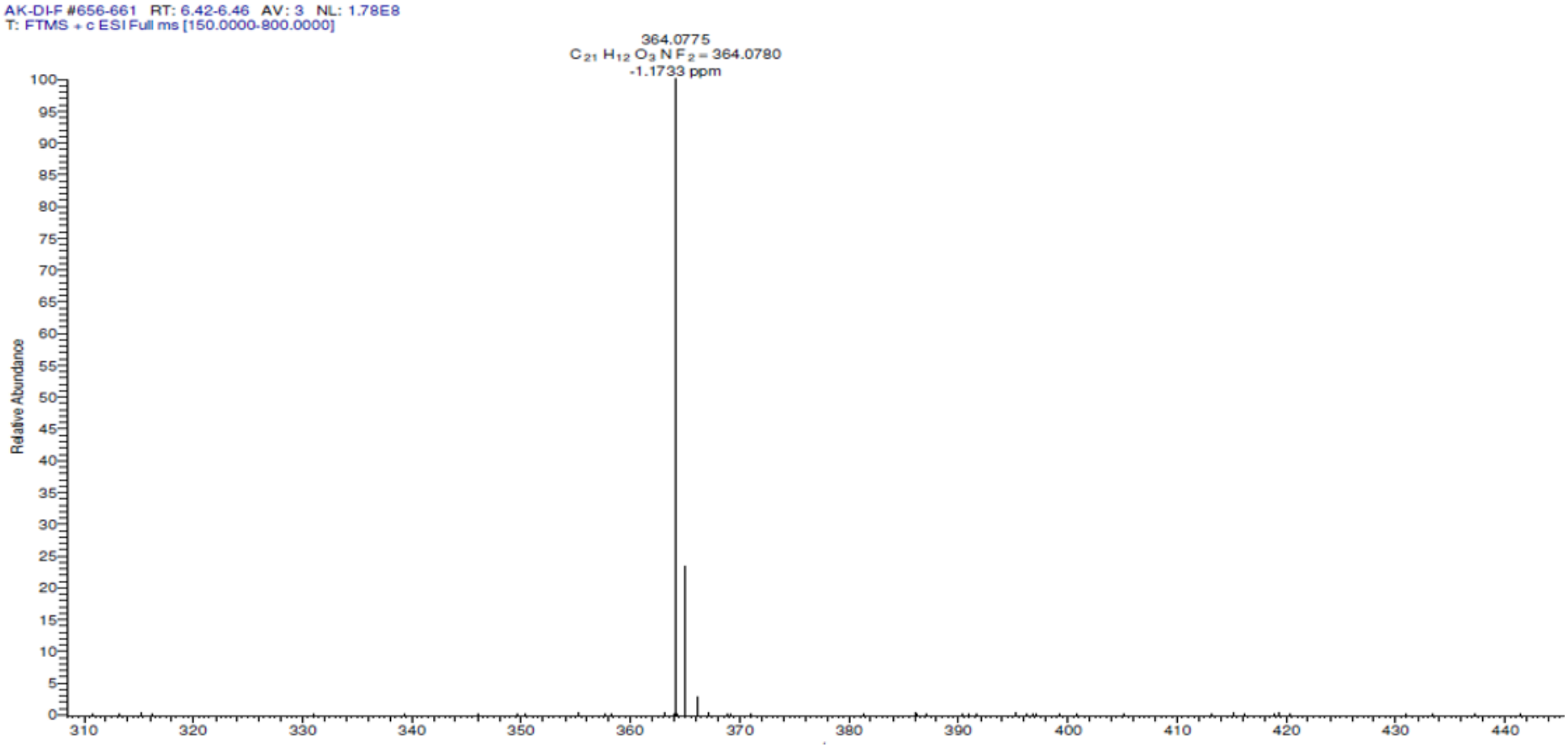


3l

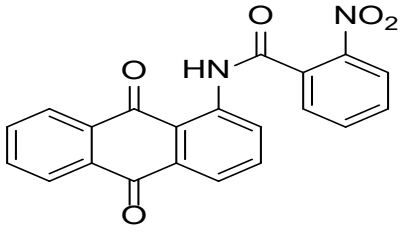


***N*-(9,10-dioxo-9,10-dihydroanthracen-1-yl)-3,5-difluorobenzamide (3m)**

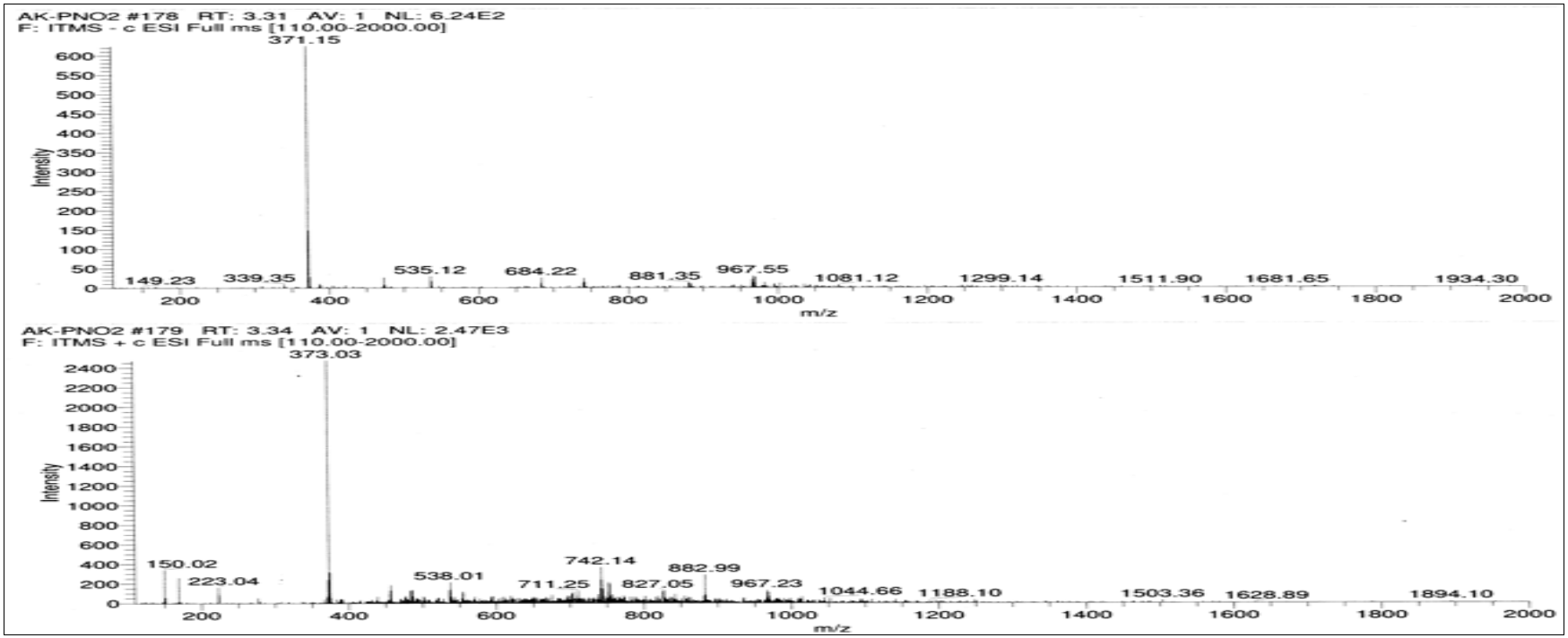




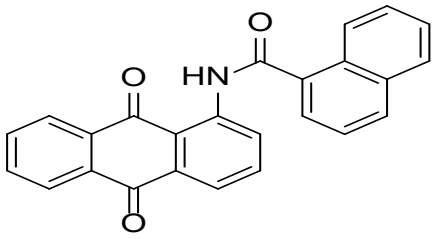
N-(9,10-dioxo-9,10-dihydroanthracen-1-yl)-2nitro benzamide (3o)



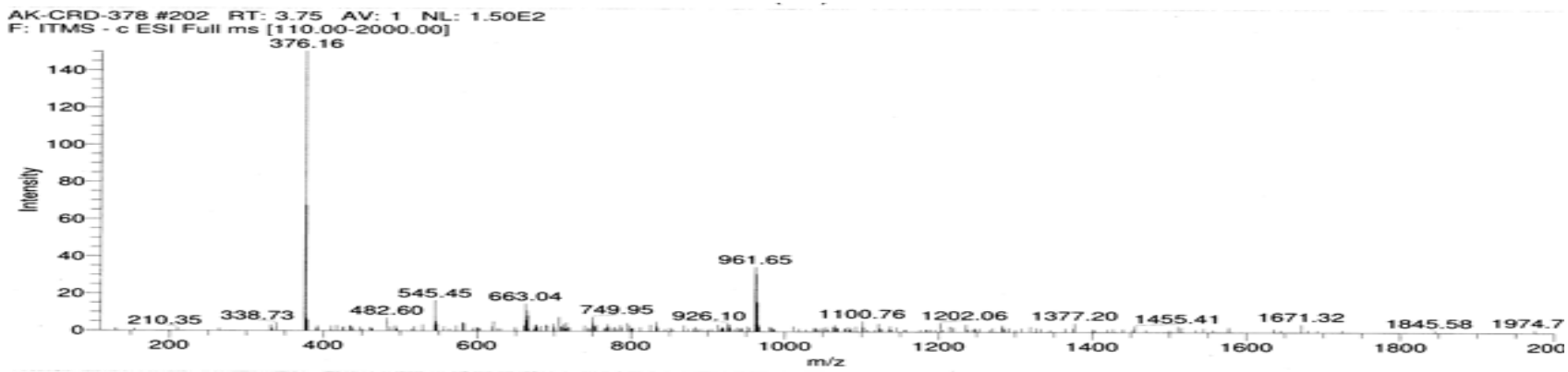
(3o)

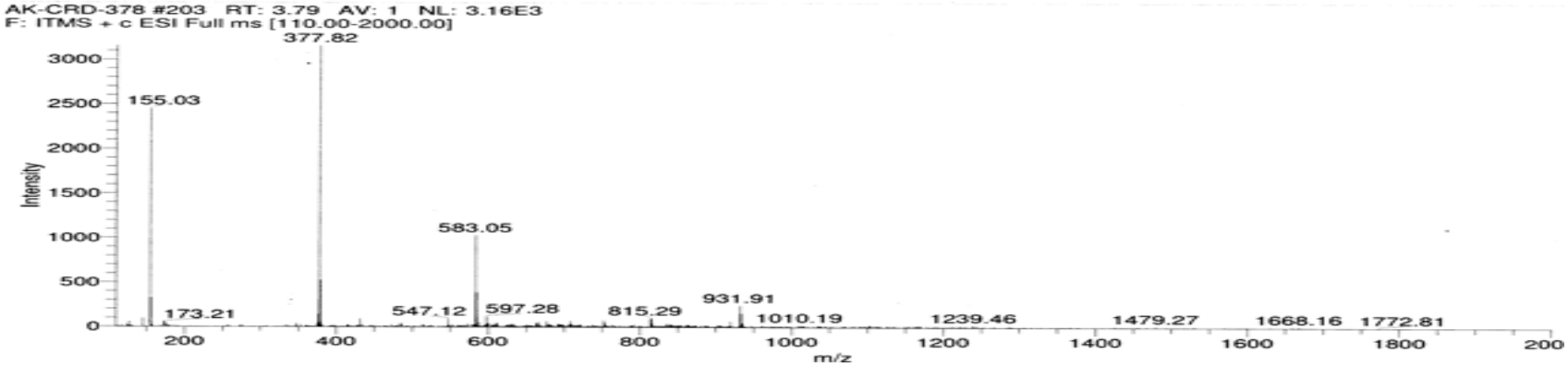


N-(9,10-dioxo-9,10-dihydroanthracen-1-yl)-1 naphthamide (3p)

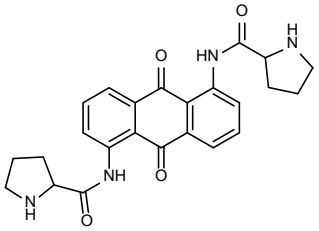


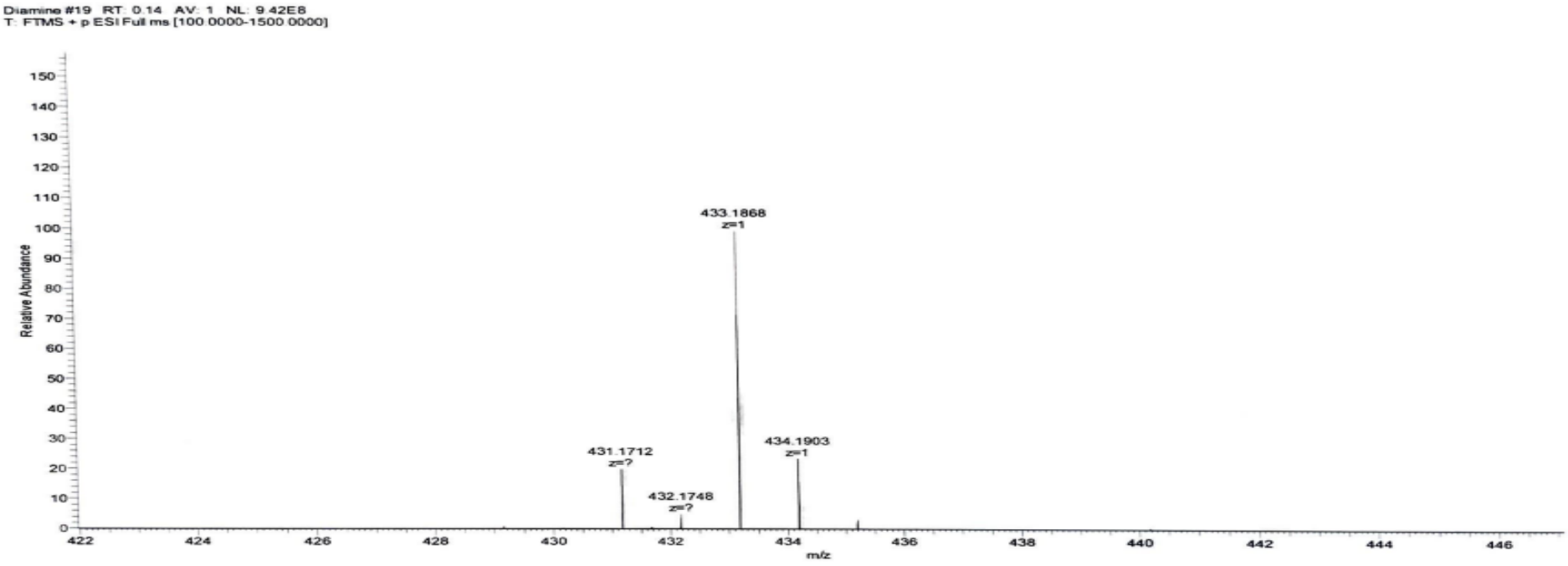
(3p)



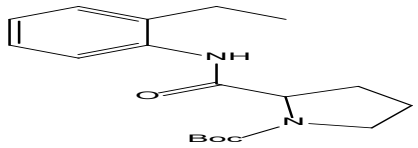


***N,N'*-(9,10-dioxo-9,10-dihydroanthracene-1,5-diyl)bis(pyrrolidine-2-carboxamide) (6)**



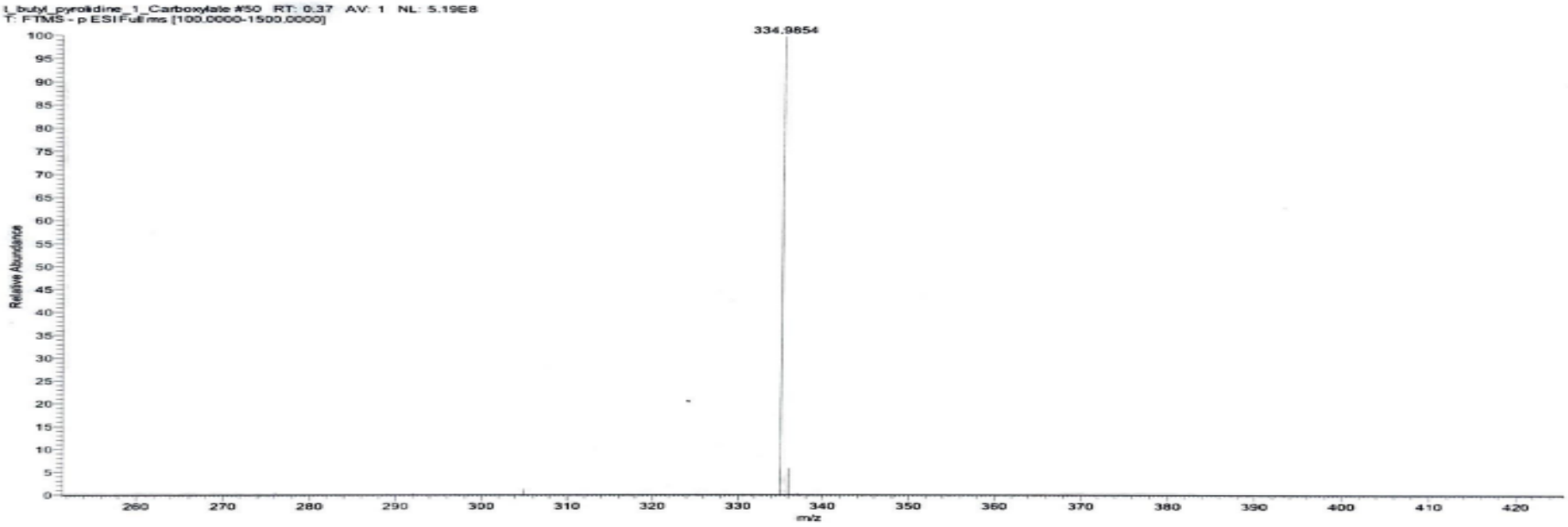


tert-butyl 2-((2-ethylphenyl)carbamoyl)pyrrolidine-1-carboxylate

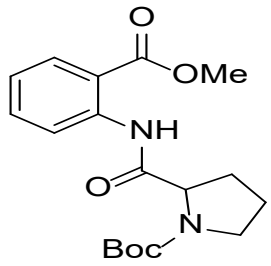


5a

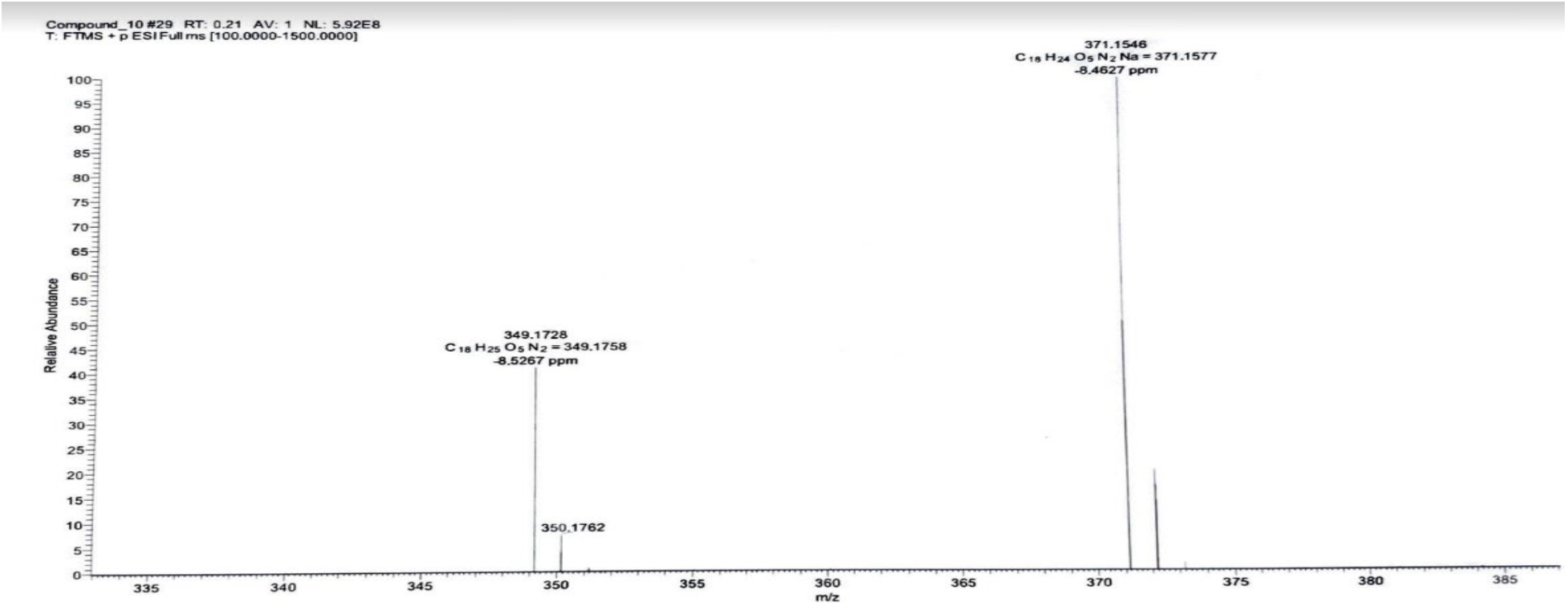
Sample ID : t_butyl_pyrolidine_1_Carboxylate **Instrument ID: ANL-BLR-LCMS-020**
Date : 21-09-2023



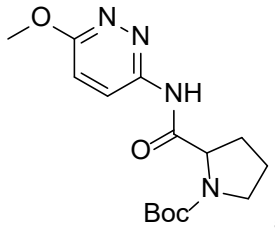
tert-butyl 2-((2-(methoxycarbonyl)phenyl)carbamoyl)pyrrolidine-1-carboxylate



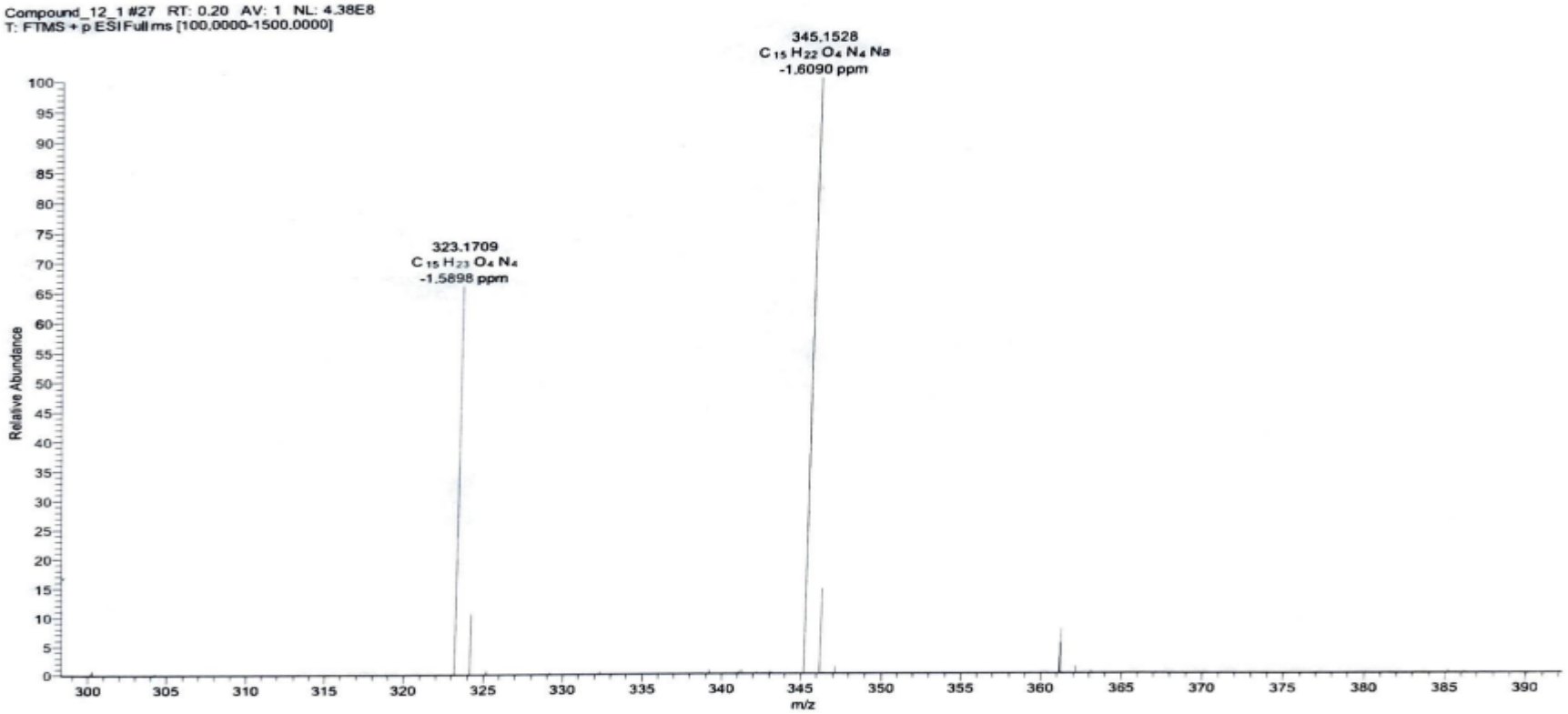
5c



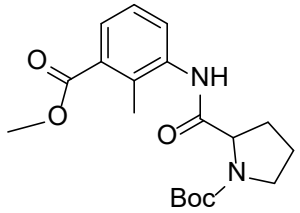
tert-butyl 2-((6-methoxypyridazin-3-yl)carbamoyl)pyrrolidine-1-carboxylate



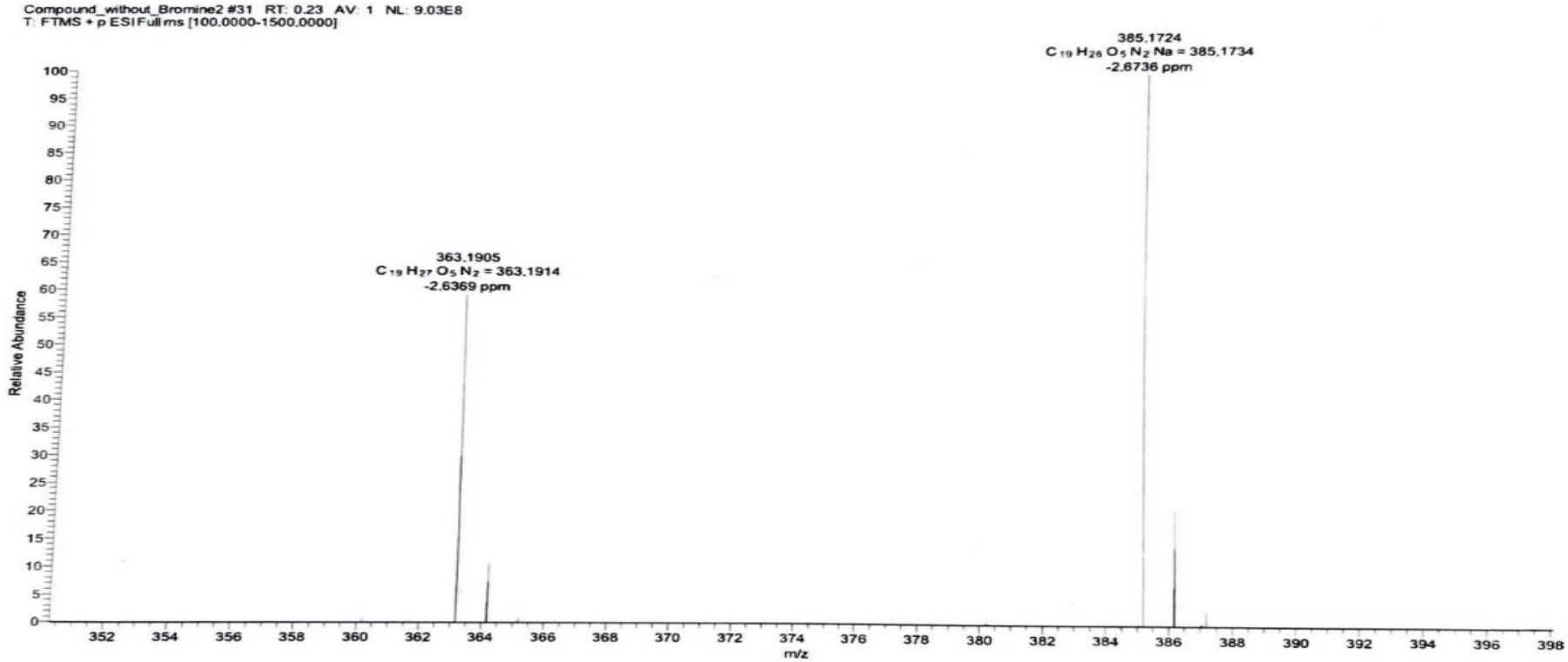
5d



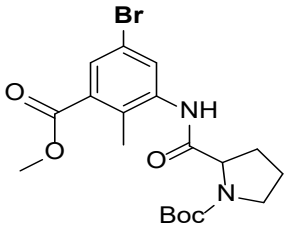
tert-butyl 2-((3-(methoxycarbonyl)-2-methylphenyl)carbamoyl)pyrrolidine-1-carboxylate



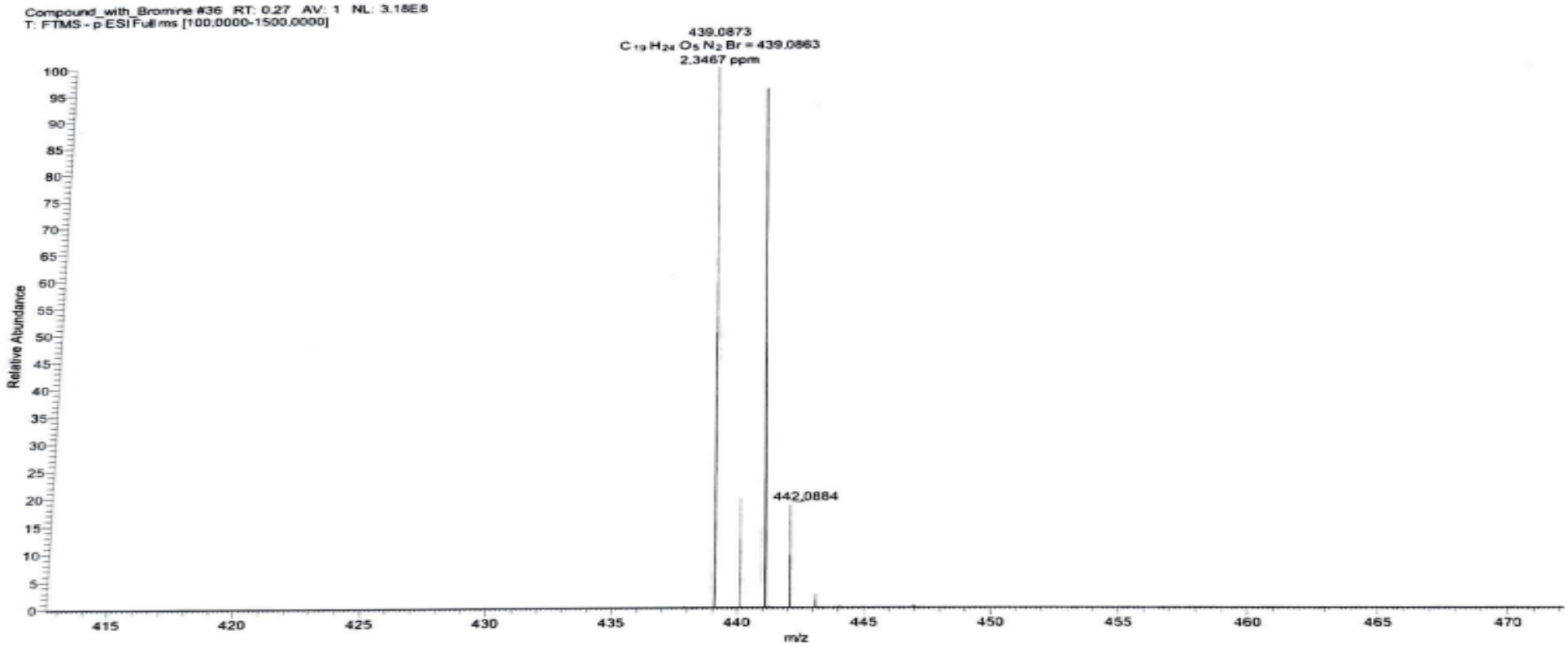
5e



tert-butyl 2-((5-bromo-3-(methoxycarbonyl)-2-methylphenyl)carbamoyl)pyrrolidine-1-carboxylate

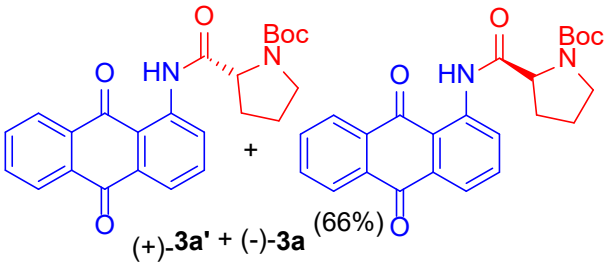


5f

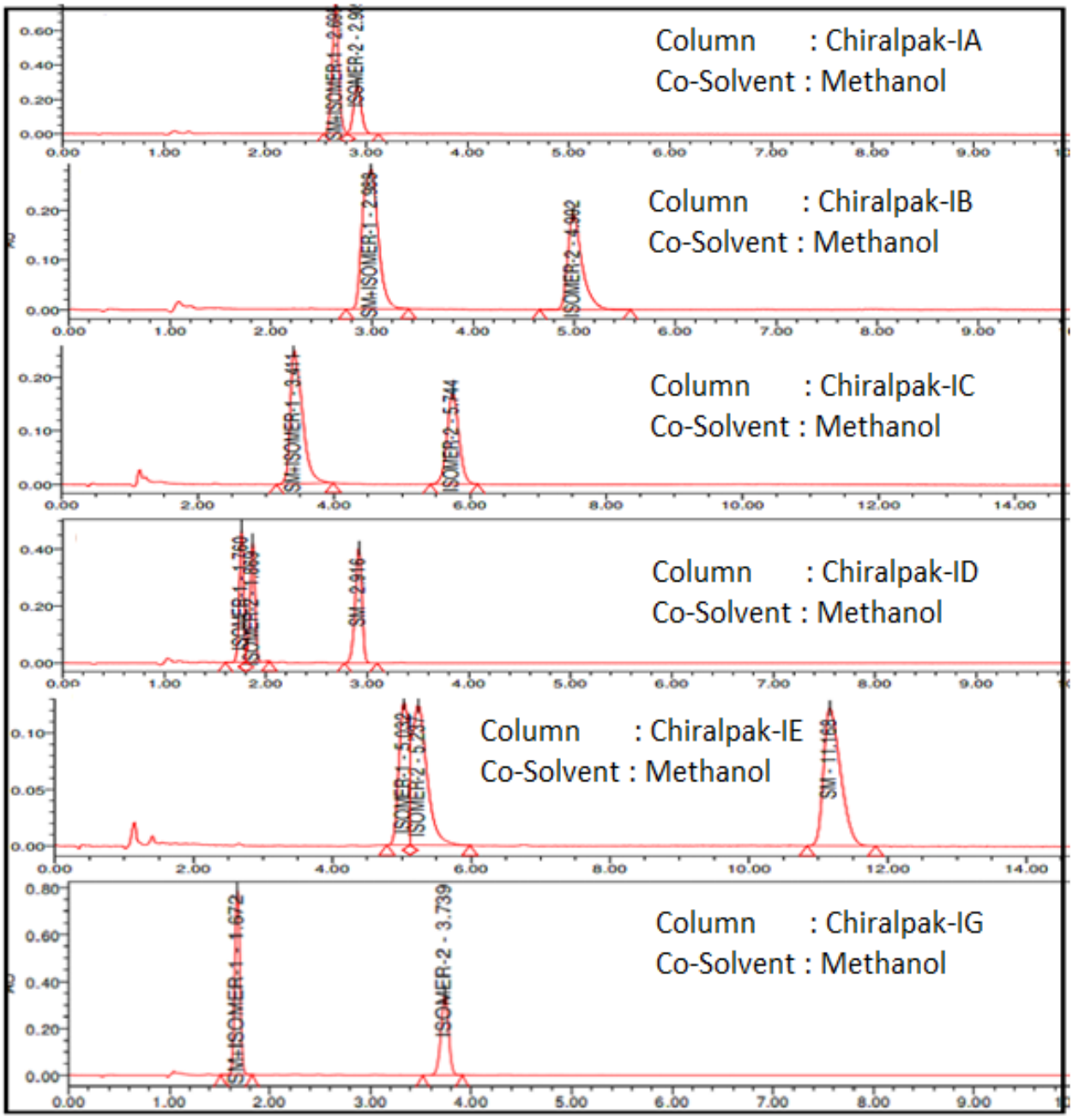


8. Super critical Fluid chromatography Data

Optimisation of condition for SFC separation of compounds (+)-3a' + (-)-3a

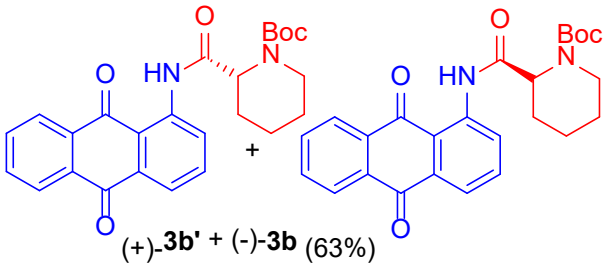


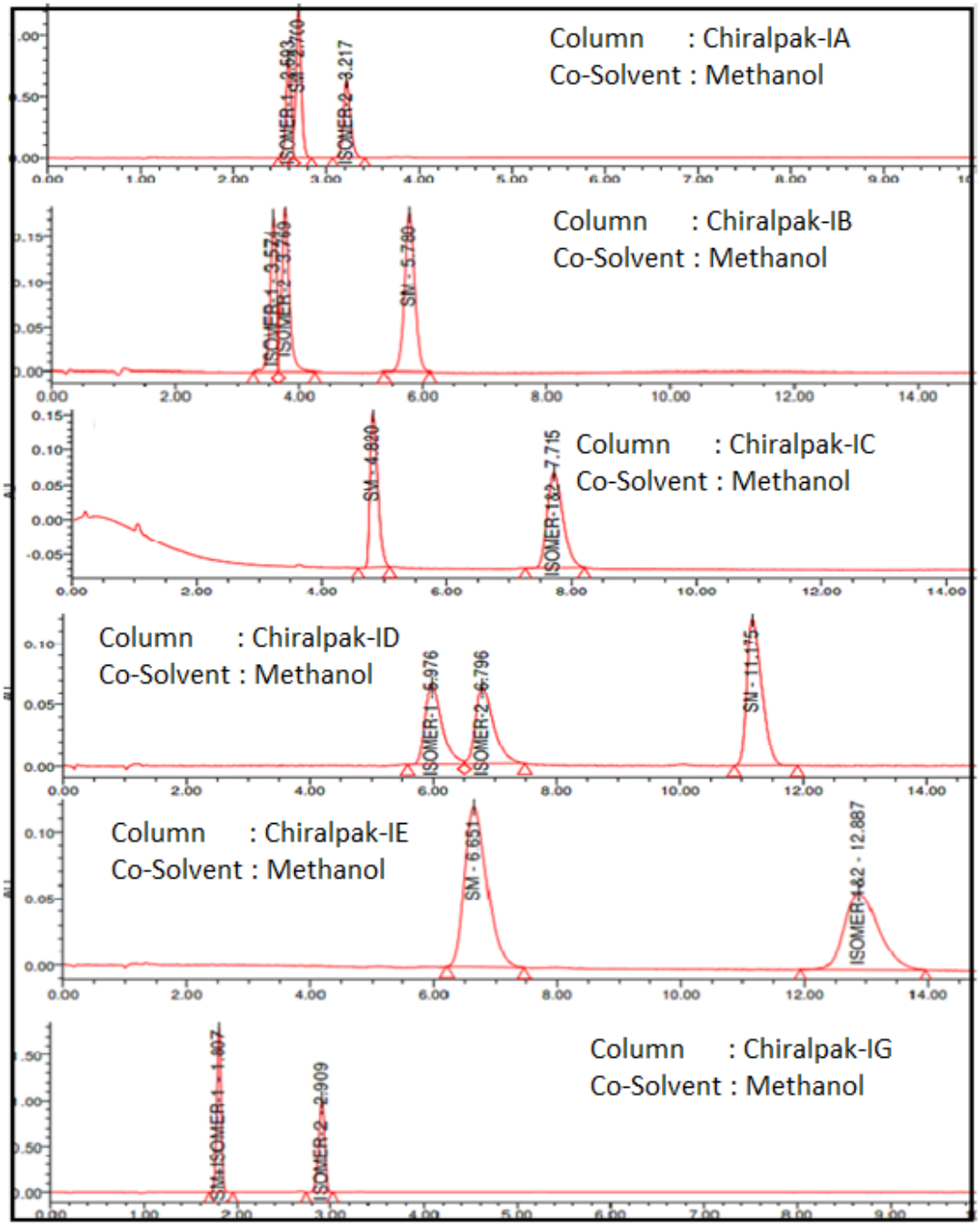
(+)-**3a'** + (-)-**3a** (66%)



SFC screening chromatogram of D and L-proline ((±)-**3a**) amide derivatives in different chiral columns.

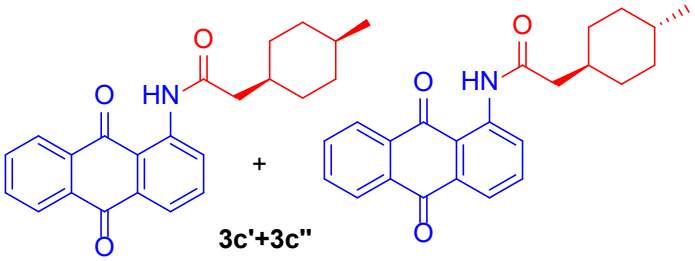
Optimisation of condition for SFC separation of compounds (+)-3b' and + **(-)-3b**

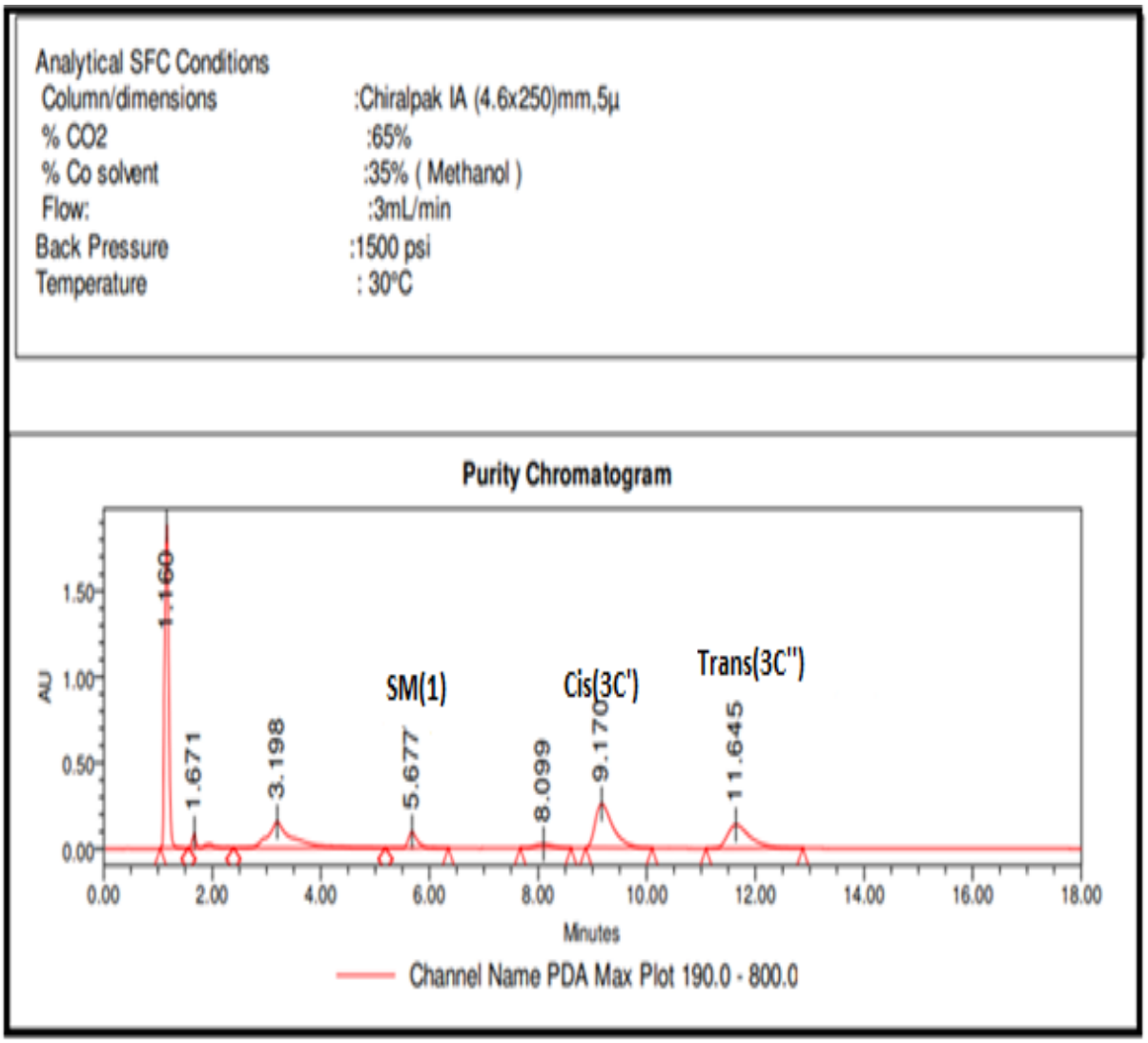




SFC screening chromatogram of D and L-Piperidine (±)-**3b**) amide derivatives in different chiral columns.

Optimisation of condition for SFC separation of compounds 3c' and **3c''**



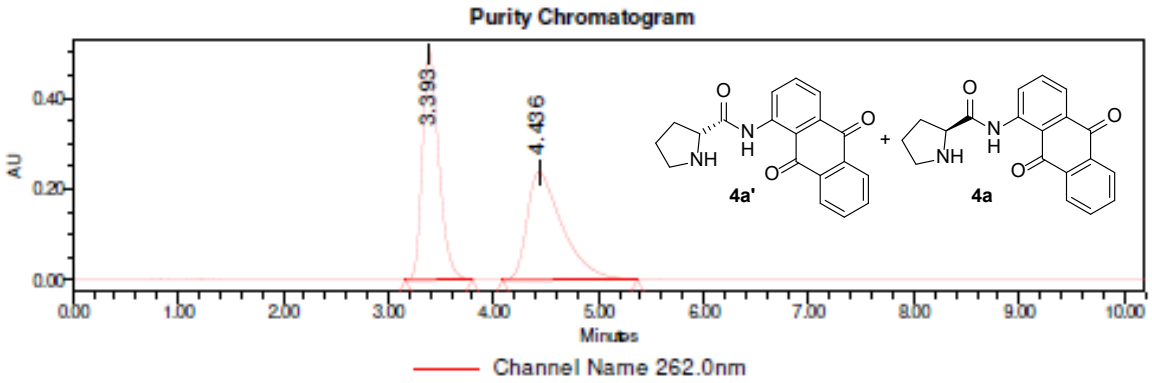


Successful separation of compound **1** and *cis* **3c'** and *trans* **3c''** isomers using Chiralpak IA column with Methanol as Co-solvent.

Chiral purity SFC method for 4a & 4a'

SampleName: DL-Proline	Date Acquired 25-Jul-2019 12:08:40 PM IST
Vial : 1:B,1	System Name: ANL_BLR_UPC2_01
Injection Volume : 8.00 uL	Method Set: 3g_30_1500PSI_B2_C1_C6
Column Name: Chiralpak IG-3(4.6X150)mm;3u	Processed Channel Descr: PDA Spectrum PDA 262.0 nm (PDA Spectrum (210-400)nm)
File Name: DL-Proline	

Analytical SFC Conditions	:
Column/dimensions	:Chiralpak IG-3(4.6X150)mm;3u
% CO2	:70%
% Co solvent	:30%(0.2% 7M Methanolic Ammonia in Acetonitrile:Methanol)(1:1)
Total Flow	:3.00 g/min
Back Pressure	:1500PSI
Temperature (degree)	:30



Peak Results

	RT	Area	% Area
1	3.393	5476142	50.03
2	4.436	5469549	49.97

Chiral purity SFC method for 4a1

SampleName: D-Proline

Vial : 1:B,6

Injection Volume : 8.00 uL

Column Name: Chiralpak IG-3(4.6X150)mm;3u

File Name: D-Proline

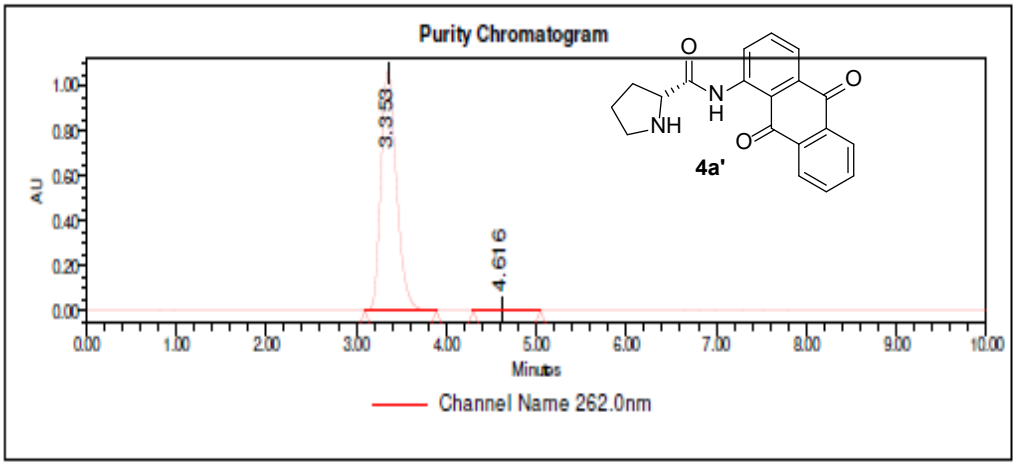
Date Acquired 25-Jul-2019 01:04:17 PM IST

System Name: ANL_BLR_UPC2_01

Method Set: 3g_30_1500PSI_B2_C1_C6

Processed Channel Descr: PDA Spectrum PDA 262.0 nm (PDA Spectrum (210-400)nm)

Analytical SFC Conditions	:
Column/dimensions	:Chiralpak IG-3(4.6X150)mm;3u
% CO2	:70%
% Co solvent	:30%(0.2% 7M Methanolic Ammonia in Acetonitrile:Methanol)(1:1)
Total Flow	:3.00 g/min
Back Pressure	:1500PSI
Temperature(degree)	:30



Peak Results

	RT	Area	% Area
1	3.353	12823747	99.20
2	4.616	103470	0.80

Chiral purity SFC method for 4a

SampleName: L-Proline

Vial : 1:B,2

Injection Volume : 8.00 uL

Column Name: Chiralpak IG-3(4.6X150)mm;3u

File Name: L-Proline

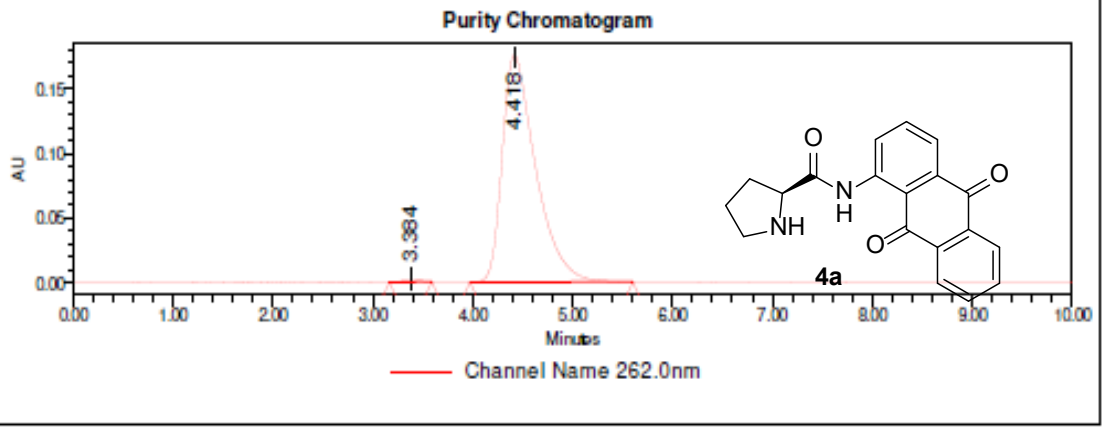
Date Acquired 25-Jul-2019 12:19:56 PM IST

System Name: ANL_BLR_UPC2_01

Method Set: 3g_30_1500PSI_B2_C1_C6

Processed Channel Descr: PDA Spectrum PDA 262.0 nm (PDA Spectrum (210-400)nm)

Analytical SFC Conditions	:
Column/dimensions	:Chiralpak IG-3(4.6X150)mm;3u
% CO2	:70%
% Co solvent	:30%(0.2% 7M Methanolic Ammonia in Acetonitrile:Methanol)(1:1)
Total Flow	:3.00 g/min
Back Pressure	:1500PSI
Temperature(degree)	:30



Peak Results

	RT	Area	% Area
1	3.384	26501	0.64
2	4.418	4093742	99.36

Chiral purity SFC method for 4b & 4b'

SampleName: pipecolic acid derivative

Vial : 2:C,3

Injection Volume : 10.00 uL

Column Name: Chiralpak IA-3(4.6X150)mm;3u

File Name:

Date Acquired 13-Aug-2019 05:08:43 PM IST

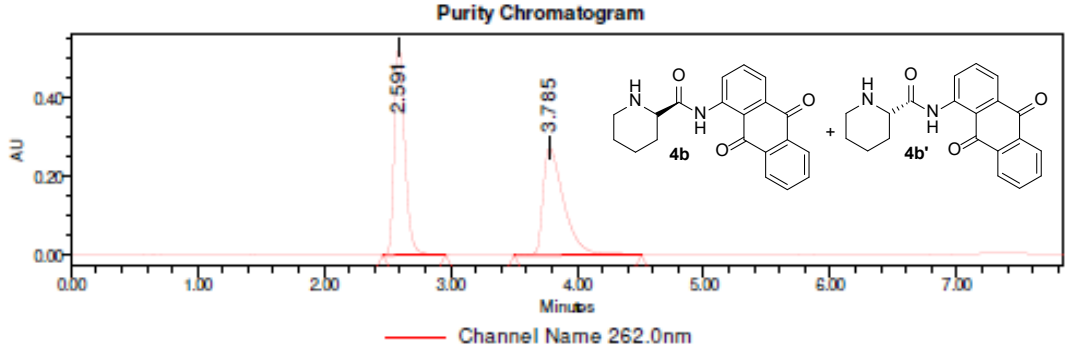
System Name: ANL_BLR_UPC2_01

Method Set: 3g_30_1500PSI_B1_C1_C4

Processed Channel Descr: PDA Spectrum PDA 262.0 nm (PDA Spectrum (210-400)nm)

Analytical SFC Conditions

Column/dimensions	:Chiralpak IA-3(4.6X150)mm;3u
% CO2	:70%
% Co solvent	:30% of (MEOH)
Total Flow	:3.00 g/min
Back Pressure	:1500PSI
Temperature(degree)	:30



Peak Results

	RT	Area	% Area
1	2.591	3070357	49.68
2	3.785	3109648	50.32

Chiral purity SFC method for 4b'

SampleName: pipecolic acid derivative-PK-2

Vial : 2:D,6

Injection Volume : 10.00 uL

Column Name: Chiralpak IA-3(4.6X150)mm;3u

File Name: pipecolic acid derivative-PK-2

Date Acquired 14-Aug-2019 12:30:55 PM IST

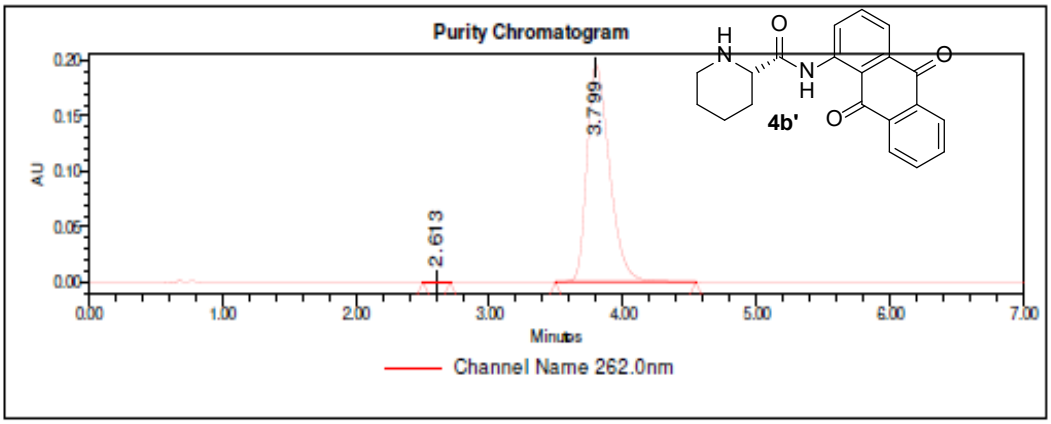
System Name: ANL_BLR_UPC2_01

Method Set: 3g_30_1500PSI_B1_C1_C4

Processed Channel Descr: PDA Spectrum PDA 262.0 nm (PDA Spectrum (210-400)nm)

Analytical SFC Conditions

Column/dimensions	:Chiralpak IA(4.6X150)mm;3u
% CO2	:70%
% Co solvent	:30%(Methanol)
Total Flow	:3.00 g/min
Back Pressure	:1500PSI
Temperature(degree)	:30



Peak Results

	RT	Area	% Area
1	2.613	1566	0.07
2	3.799	2301688	99.93

Chiral purity SFC method for 4b

SampleName: pipecolic acid derivative-PK-1

Vial : 2:D,5

Injection Volume : 10.00 uL

Column Name: Chiralpak IA-3(4.6X150)mm;3u

File Name: pipecolic acid derivative-PK-1

Date Acquired 14-Aug-2019 12:12:23 PM IST

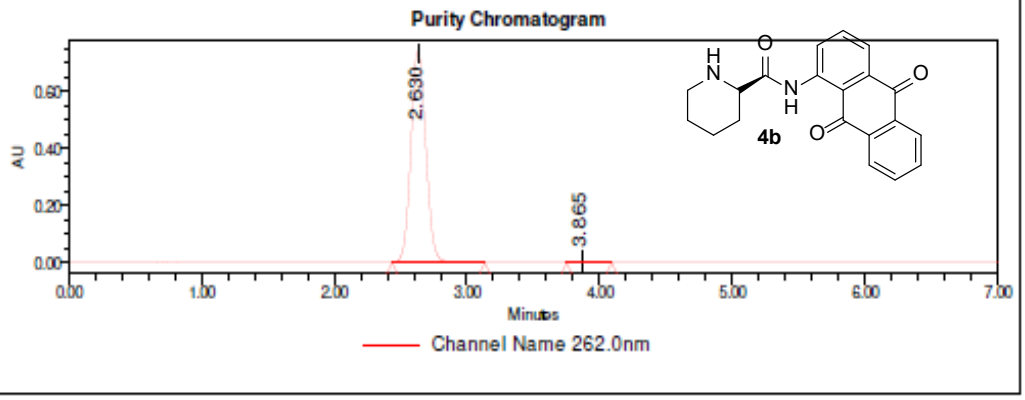
System Name: ANL_BLR_UPC2_01

Method Set: 3g_30_1500PSI_B1_C1_C4

Processed Channel Descr: PDA Spectrum PDA 262.0 nm (PDA Spectrum (210-400)nm)

Analytical SFC Conditions

Column/dimensions	:Chiralpak IA(4.6X150)mm;3u
% CO2	:70%
% Co solvent	:30%(Methanol)
Total Flow	:3.00 g/min
Back Pressure	:1500PSI
Temperature(degree)	:30



Peak Results

	RT	Area	% Area
1	2.630	5771310	99.99
2	3.865	841	0.01

9. Optical Rotation values for compounds 4a, 4a' 4b and 4b'

D-Proline derivative

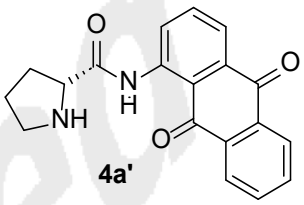
[Data Information]
Creation Date 05-Sep-2019 16:21

[Measurement Information]
Instrument Name Polarimeter
Model Name P-2000
Serial No. A112361232
Polarizer Dichrom
Faraday Cell Flint Glass

Accessory PTC-262
Accessory S/N B024761481
Temperature 25.00 C
Control Sonsor Holder
Monitor Sensor Holder
Start Mode Start immediately

Light Source WI
Monitor wavelength 589 nm
D.I.T. 5 sec
No. of cycle 5
Cycle interval 5 sec
Temp. Monitor Holder
Temp. Corr. Factor 0 at 25 C
Aperture(S) 3.0mm
Aperture(L) Auto
Mode Specific O.R.
Path Length 100 mm
Concentration 0.1 w/v%
Water content of sample 0 %
Factor 1

[Comment]
Sample name D-Proline derivative
Comment 0.1% in Acetonitrile
User Administrator
Workgroup QC
Division QC
Company GVK



4a'

		No.	Sample No.	Mode	Calc. Data	Meas. Data	PMT Voltage[V]	Temperature(C)	Blank	Comment
1	*	1	D-Proline derivative-1	Specific O.R.	+36.2800	+0.0363	352	25.00	+0.0051	0.1% in Acetonitrile
2	*	2	D-Proline derivative-2	Specific O.R.	+36.4800	+0.0365	383	24.99	+0.0051	0.1% in Acetonitrile
3	*	3	D-Proline derivative-3	Specific O.R.	+35.7800	+0.0358	362	24.99	+0.0051	0.1% in Acetonitrile
4	*	4	D-Proline derivative-4	Specific O.R.	+36.4800	+0.0365	382	24.99	+0.0051	0.1% in Acetonitrile
5	*	5	D-Proline derivative-5	Specific O.R.	+35.9800	+0.0360	386	24.99	+0.0051	0.1% in Acetonitrile
6	*	6	Avg.		+36.2000					
7		7	S.D		0.3114					
8		8	C.V		0.8604					

L-Proline derivative

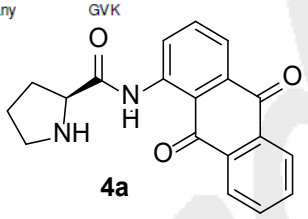
[Data Information]
Creation Date 05-Sep-2019 12:36

[Measurement Information]
Instrument Name Polarimeter
Model Name P-2000
Serial No. A112361232
Polarizer Dichrom
Faraday Cell Flint Glass

Accessory PTC-262
Accessory S/N B024761481
Temperature 25.00 C
Control Sonsor Holder
Monitor Sensor Holder
Start Mode Start immediately

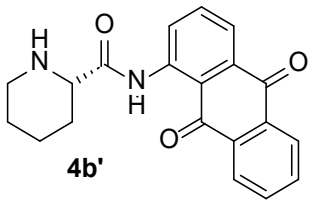
Light Source WI
Monitor wavelength 589 nm
D.I.T. 5 sec
No. of cycle 5
Cycle interval 5 sec
Temp. Monitor Holder
Temp. Corr. Factor 0 at 25 C
Aperture(S) 3.0mm
Aperture(L) Auto
Mode Specific O.R.
Path Length 100 mm
Concentration 0.1 w/v%
Water content of sample 0 %
Factor 1

[Comment]
Sample name L-Proline derivative
Comment 0.1% in Acetonitrile
User Administrator
Workgroup QC
Division QC
Company GVK



4a

		No.	Sample No.	Mode	Calc. Data	Meas. Data	PMT Voltage[V]	Temperature(C)	Blank	Comment
1	*	1	L-Proline derivative-1	Specific O.R.	-44.2200	-0.0442	422	25.01	+0.0051	0.1% in Acetonitrile
2	*	2	L-Proline derivative-2	Specific O.R.	-40.1200	-0.0401	427	25.01	+0.0051	0.1% in Acetonitrile
3	*	3	L-Proline derivative-3	Specific O.R.	-42.0200	-0.0420	430	25.00	+0.0051	0.1% in Acetonitrile
4	*	4	L-Proline derivative-4	Specific O.R.	-41.3200	-0.0413	412	25.00	+0.0051	0.1% in Acetonitrile
5	*	5	L-Proline derivative-5	Specific O.R.	-40.9200	-0.0409	285	24.99	+0.0051	0.1% in Acetonitrile
6	*	6	Avg.		-41.7200					
7		7	S.D		1.5572					
8		8	C.V		3.7326					



4b'

D-pipecolic acid derivative

[Data Information]
Creation Date 05-Sep-2019 14:49

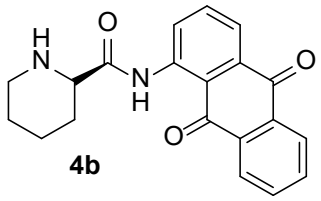
[Measurement Information]
Instrument Name Polarimeter
Model Name P-2000
Serial No. A112361232
Polarizer Dichrom
Faraday Cell Flint Glass

Accessory PTC-262
Accessory S/N B024761481
Temperature 25.00 C
Control Sonsor Holder
Monitor Sensor Holder
Start Mode Start immediately

Light Source WI
Monitor wavelength 589 nm
D.I.T. 5 sec
No. of cycle 5
Cycle interval 5 sec
Temp. Monitor Holder
Temp. Corr. Factor 0 at 25 C
Aperture(S) 3.0mm
Aperture(L) Auto
Mode Specific O.R.
Path Length 100 mm
Concentration 0.1 w/v%
Water content of sample 0 %
Factor 1

[Comment]
Sample name D-pipecolic acid derivative
Comment 0.1% in Acetonitrile
User Administrator
Workgroup QC
Division QC
Company GVK

		No.	Sample No.	Mode	Calc. Data	Meas. Data	PMT Voltage[V]	Temperature(C)	Blank	Comment
1	*	1	D-pipecolic acid derivative-1	Specific O.R.	+26.8800	+0.0269	411	24.99	+0.0051	0.1% in Acetonitrile
2	*	2	D-pipecolic acid derivative-2	Specific O.R.	+26.2800	+0.0263	410	24.99	+0.0051	0.1% in Acetonitrile
3	*	3	D-pipecolic acid derivative-3	Specific O.R.	+26.8800	+0.0269	328	24.99	+0.0051	0.1% in Acetonitrile
4	*	4	D-pipecolic acid derivative-4	Specific O.R.	+25.4800	+0.0255	370	25.00	+0.0051	0.1% in Acetonitrile
5	*	5	D-pipecolic acid derivative-5	Specific O.R.	+28.3800	+0.0284	403	25.00	+0.0051	0.1% in Acetonitrile
6	*	6	Avg.		+26.7800					
7		7	S.D		1.0630					
8		8	C.V		3.9694					



4b

L-pipecolic acid derivative

[Data Information]
Creation Date 05-Sep-2019 15:18

[Measurement Information]
Instrument Name Polarimeter
Model Name P-2000
Serial No. A112361232
Polarizer Dichrom
Faraday Cell Flint Glass

Accessory PTC-262
Accessory S/N B024761481
Temperature 25.00 C
Control Sonsor Holder
Monitor Sensor Holder
Start Mode Start immediately

Light Source WI
Monitor wavelength 589 nm
D.I.T. 5 sec
No. of cycle 5
Cycle interval 5 sec
Temp. Monitor Holder
Temp. Corr. Factor 0 at 25 C
Aperture(S) 3.0mm
Aperture(L) Auto
Mode Specific O.R.
Path Length 100 mm
Concentration 0.1 w/v%
Water content of sample 0 %
Factor 1

[Comment]
Sample name L-pipecolic acid derivative
Comment 0.1% in Acetonitrile
User Administrator
Workgroup QC
Division QC
Company GVK

		No.	Sample No.	Mode	Calc. Data	Meas. Data	PMT Voltage[V]	Temperature(C)	Blank	Comment
1	*	1	L-pipecolic acid derivative-1	Specific O.R.	-26.1200	-0.0261	397	25.01	+0.0051	0.1% in Acetonitrile
2	*	2	L-pipecolic acid derivative-2	Specific O.R.	-26.6200	-0.0266	355	25.01	+0.0051	0.1% in Acetonitrile
3	*	3	L-pipecolic acid derivative-3	Specific O.R.	-27.9200	-0.0279	296	25.00	+0.0051	0.1% in Acetonitrile
4	*	4	L-pipecolic acid derivative-4	Specific O.R.	-26.8200	-0.0268	367	25.00	+0.0051	0.1% in Acetonitrile
5	*	5	L-pipecolic acid derivative-5	Specific O.R.	-27.6200	-0.0276	411	24.99	+0.0051	0.1% in Acetonitrile
6	*	6	Avg.		-27.0200					
7		7	S.D		0.7382					
8		8	C.V		2.7322					