Powerful Potential of Polyfluoroalkyl-containing 4-Arylhydrazinylidenepyrazol-3-ones for Pharmaceuticals

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Table of contents

Table S1. *In silico* ADME predictions of pyrazolones **5-9**

ID of ligand	dipole	IP (eV)	EA (eV)	SASA	FOSA	FISA	PISA	WPSA	volume	glob	QPpolrz	QPlogPC16	QPlogPoct
min	1.0	7.9	0.9	300	0	7	0	0	500	0.75	13.0	4.0	8.0
max	12.5	10.5	1.7	1000	750	330	450	175	2000	0.95	70.0	18.0	35.0
5a	2.2	8.9	1.6	456	1	128	212	115	742	0.87	23.6	6.9	12.0
5b	2.6	8.7	1.5	621	89	64	354	114	1054	0.81	37.5	10.2	15.2
5c	2.5	9.0	1.7	485	1	128	164	192	795	0.86	25.3	7.6	12.9
5d	2.5	8.8	1.6	523	179	73	156	115	865	0.84	28.0	7.0	11.7
5e	2.6	8.8	1.5	589	1	64	410	115	994	0.82	35.6	10.0	14.6
5f	2.4	8.8	1.6	488	89	128	157	115	802	0.85	25.5	7.0	12.6
5g	1.3	8.5	1.5	627	94	64	354	115	1070	0.81	37.5	10.3	15.5
5h	3.8	8.9	1.6	598	1	64	372	161	1010	0.81	35.9	9.5	15.0
5i	0.9	8.9	1.6	604	1	57	373	173	1031	0.82	36.7	10.4	15.2
5j	2.7	8.9	1.6	609	1	54	348	207	1057	0.82	37.5	10.8	15.7
5k	3.5	8.9	1.6	618	1	64	361	192	1047	0.81	37.3	10.7	15.6
5l	2.1	9.1	1.8	714	142	118	340	114	1218	0.77	42.6	12.1	18.1
5m	7.7	9.3	1.8	675	84	142	333	115	1161	0.79	40.9	11.6	19.5
5n	9.0	9.4	1.9	660	1	205	338	116	1130	0.79	39.1	12.3	22.6
5o	8.5	9.4	1.9	658	1	201	340	117	1124	0.79	38.8	12.0	20.6
5p	6.4	8.9	1.8	688	89	202	281	116	1184	0.79	40.7	12.4	22.5
5r	5.2	8.9	1.7	702	172	140	275	115	1214	0.78	42.5	11.7	19.5
5s	2.9	8.7	1.5	653	177	64	298	115	1114	0.80	39.3	10.4	15.7
6a	2.7	8.8	1.6	521	89	122	149	162	876	0.85	27.8	7.4	13.5
6b	2.7	8.8	1.6	649	89	56	343	161	1121	0.80	39.4	10.4	16.0
6c	1.2	8.9	1.7	631	0	50	361	219	1097	0.82	38.6	10.7	16.0
6d	4.4	9.0	1.7	641	0	56	351	233	1105	0.81	38.9	10.8	16.3
6e	3.6	9.3	1.5	650	0	45	336	269	1139	0.81	40.1	11.2	16.8
6f	1.8	8.9	1.8	655	0	50	314	291	1142	0.81	40.0	11.3	16.7
6g	2.1	9.1	1.8	746	141	112	332	161	1292	0.77	44.9	12.5	19.0
6h	7.1	9.4	1.9	703	84	135	323	161	1229	0.79	42.9	11.9	20.1
7a	2.8	8.8	1.7	551	89	118	149	195	937	0.84	29.6	7.7	14.3
7b	2.9	8.8	1.6	687	88	56	343	200	1198	0.79	41.9	10.9	17.0
8a	2.9	8.8	1.7	597	88	121	149	239	1031	0.83	32.7	8.3	15.5

8b	3.4	8.7	1.6	738	88	53	352	245	1290	0.78	45.0	11.6	18.3
9a	1.7	8.6	1.2	470	174	134	161	0	763	0.86	24.0	7.5	11.5
9b	1.3	8.5	1.1	602	174	70	358	0	1015	0.81	36.0	10.6	14.1

dipole – computed dipole moment of the molecule;
IP (ev) – PM3 calculated ionization potential (negative of HOMO energy);
EA (eV) – PM3 calculated electron affinity (negative of LUMO energy);
SASA – total solvent accessible surface area (SASA) in square angstroms using a probe with a 1.4 Å radius;
FOSA – hydrophobic component of the SASA (saturated carbon and attached hydrogen);
FISA – hydrophilic component of the SASA (SASA on N. O. H on heteroatoms. carbonyl C);
PISA – π (carbon and attached hydrogen) component of the SASA;
WPSA – weakly polar component of the SASA (halogens. P. and S);
volume – total solvent-accessible volume in cubic angstroms using a probe with a 1.4 Å radius;
glob – globularity descriptor.$(4\pi r^2)/(SASA)$. where r is the radius of a sphere with a volume equal to the molecular volume. Globularity is 1.0 for a spherical molecule;
QPpolrz – predicted polarizability in cubic angstroms;
QPlogPC16 – predicted hexadecane/gas partition coefficient;
QPlogPoct – predicted octanol/gas partition coefficient.

Table S2. Antifungal activity of 4-arylhydrazinylidenepyrazolones **5-9**

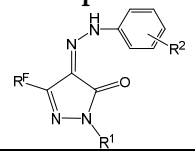
No	Compounds 			MIC (μg/ml) for fungi strains inhibition			
	R^F	R^1	R^2	*T. rubrum*	*E. floccosum*	*M. canis*	*C. albicans*
5b	CF_3	H	Me-4	50	>200	100	200
5c	CF_3	H	Br-4	**12.5**	**12.5**	**25**	>200
5d	CF_3	Me	Me-4	200	200	200	>200
5e	CF_3	Ph	H	200	200	200	>200
5f	CF_3	Ph	Me-4	>200	200	200	200
5h	CF_3	Ph	F-4	>200	>200	>200	>200
5i	CF_3	Ph	Cl-2	>200	>200	>200	>200
5j	CF_3	Ph	Cl_2-2,6	>200	>200	>200	>200
5k	CF_3	Ph	Br-4	>200	>200	>200	>200
5m	CF_3	Ph	SO_2Me-4	100	>200	>200	>200
5p	CF_3	$C_6H_4SO_2NH_2$-4	Me-4	>200	>200	>200	>200
5r	CF_3	$C_6H_4SO_2Me$-4	Me-4	>200	>200	>200	>200
6c	C_2F_5	Ph	Cl-2	200	>200	>200	>200
6d	C_2F_5	Ph	Cl-3	>200	200	>200	>200
6e	C_2F_5	Ph	Cl_2-2,6	>200	200	>200	>200
6f	C_2F_5	Ph	Cl_2-2,4	>200	200	>200	>200
6g	C_2F_5	Ph	CO_2Et-4	>200	>200	>200	>200
6h	C_2F_5	Ph	SO_2Me-4	>200	>200	>200	>200
7a	C_3F_7	H	Me-4	>200	200	>200	>200
8a	C_4F_9	H	Me-4	>200	>200	>200	>200
9b	Me	Ph	Me-4	>200	>200	>200	>200
Fluconazole				3.12	1.56	3.12	1.56

Figure S1. Z, E isomers of compound **5a**.

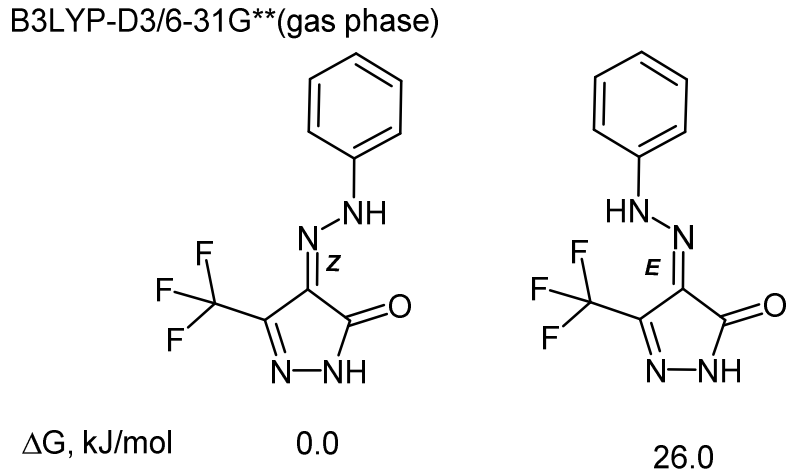
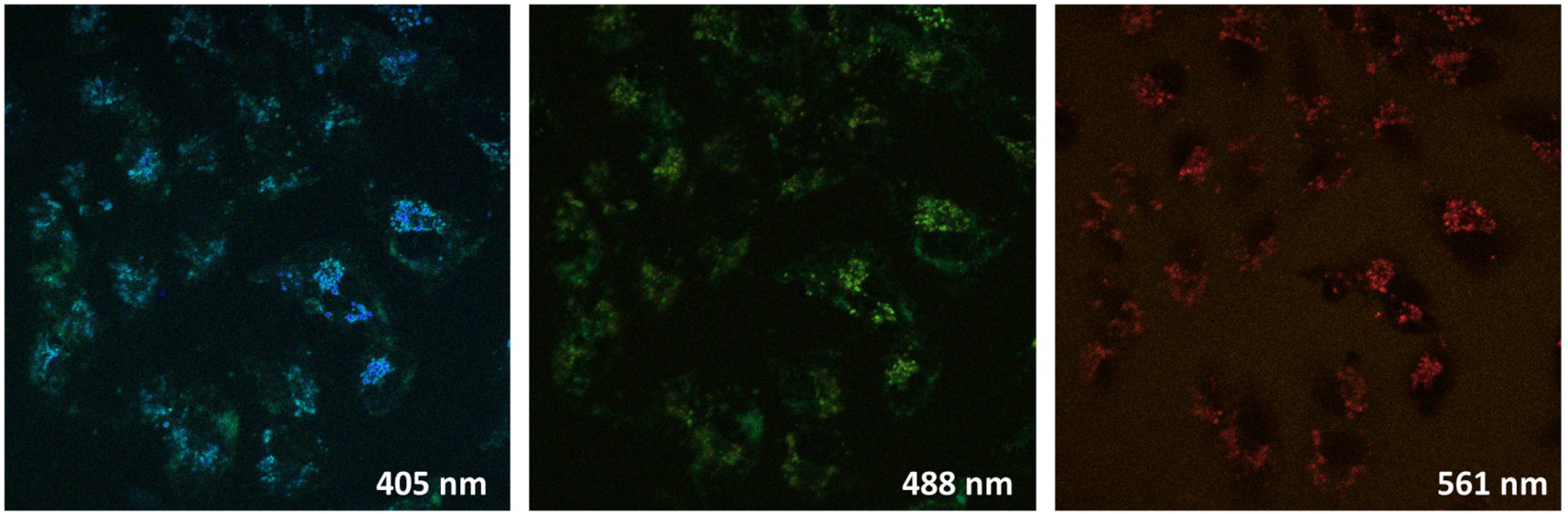
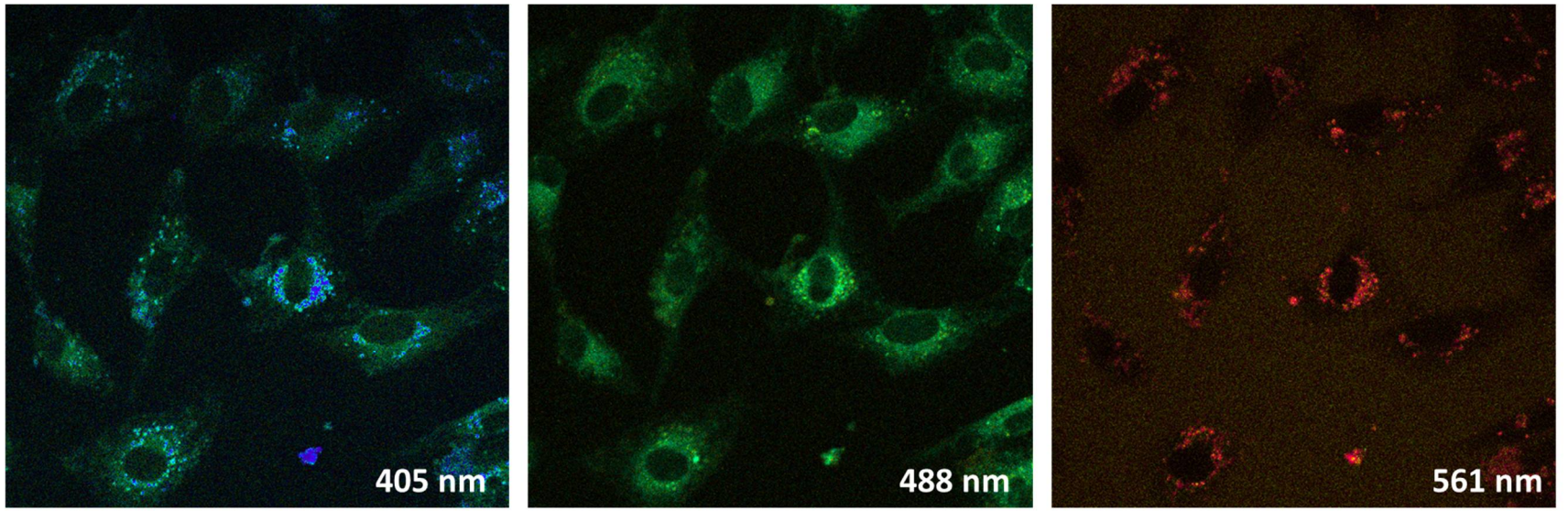


Figure S2. Images of Vero cells stained with compounds **5f** (**A**) and **9a** (**B**) exciting by lasers with different wavelengths.



(**A**)



(**B**)

Figure S3. ^{1}H NMR spectrum of compound **5a**

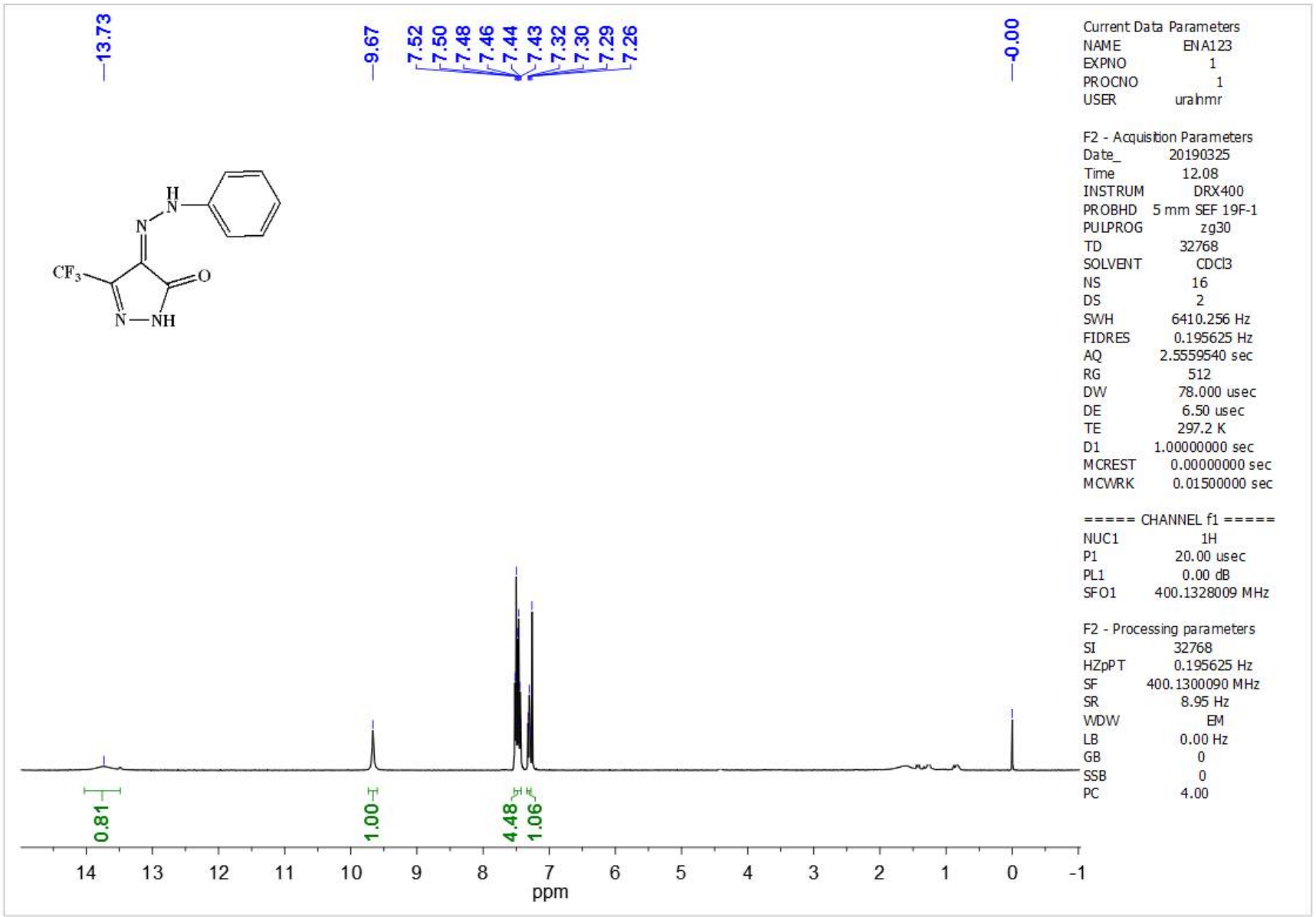


Figure S4. ^{13}C NMR spectrum of compound **5a**

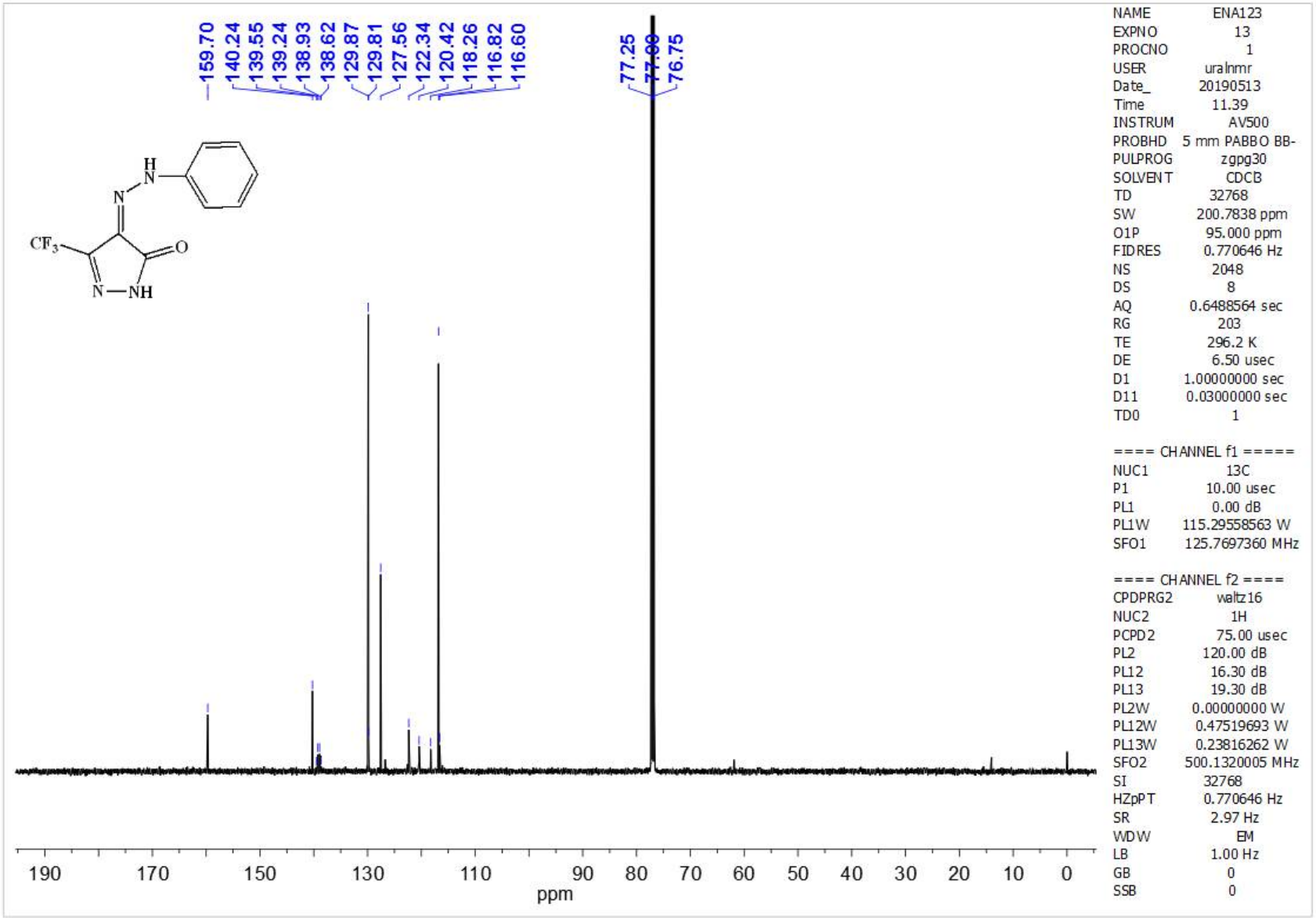


Figure S5. ^{19}F NMR spectrum of compound **5a**

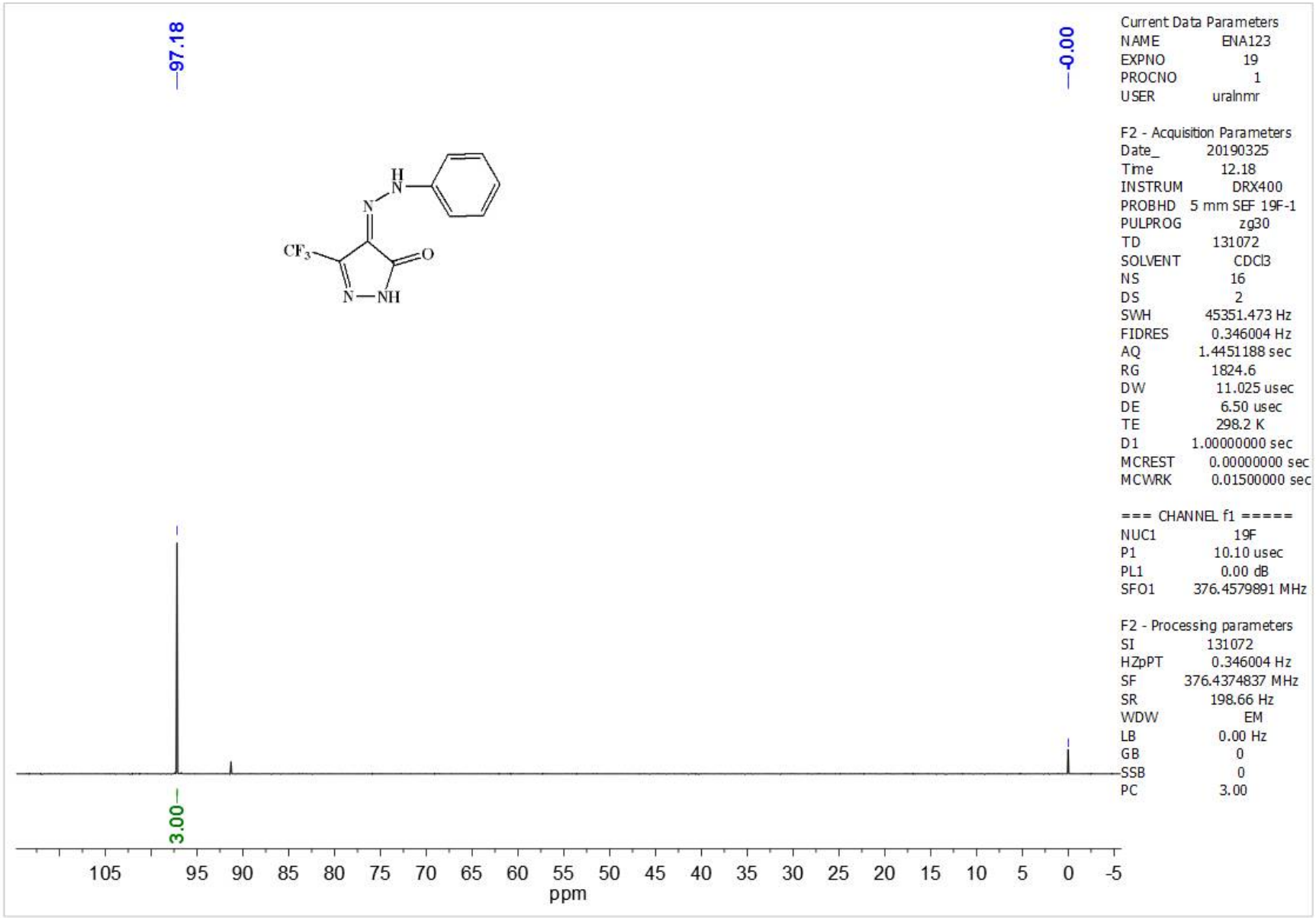


Figure S6. ^{1}H NMR spectrum of compound **5b**

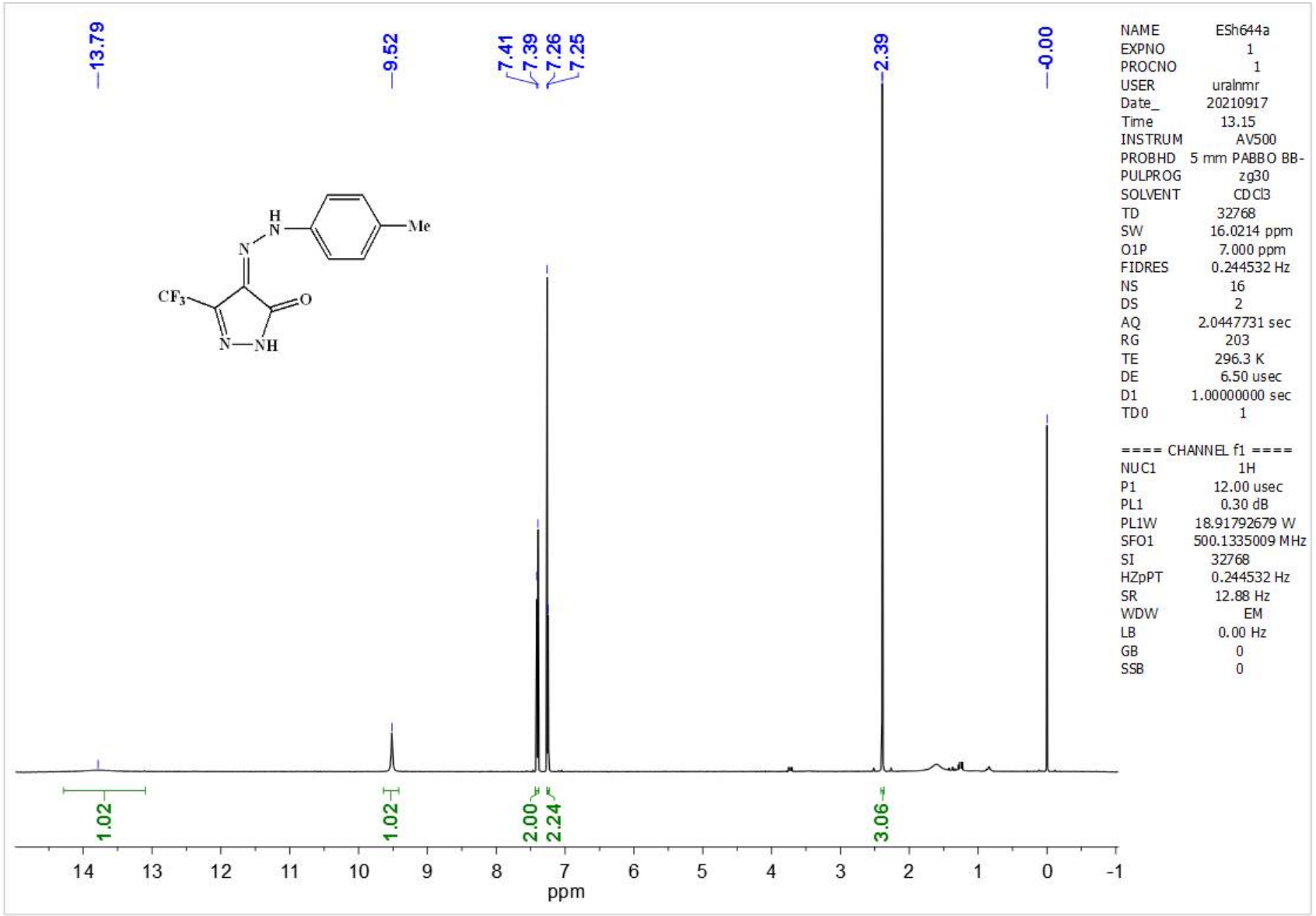


Figure S7. ^{19}F NMR spectrum of compound **5b**

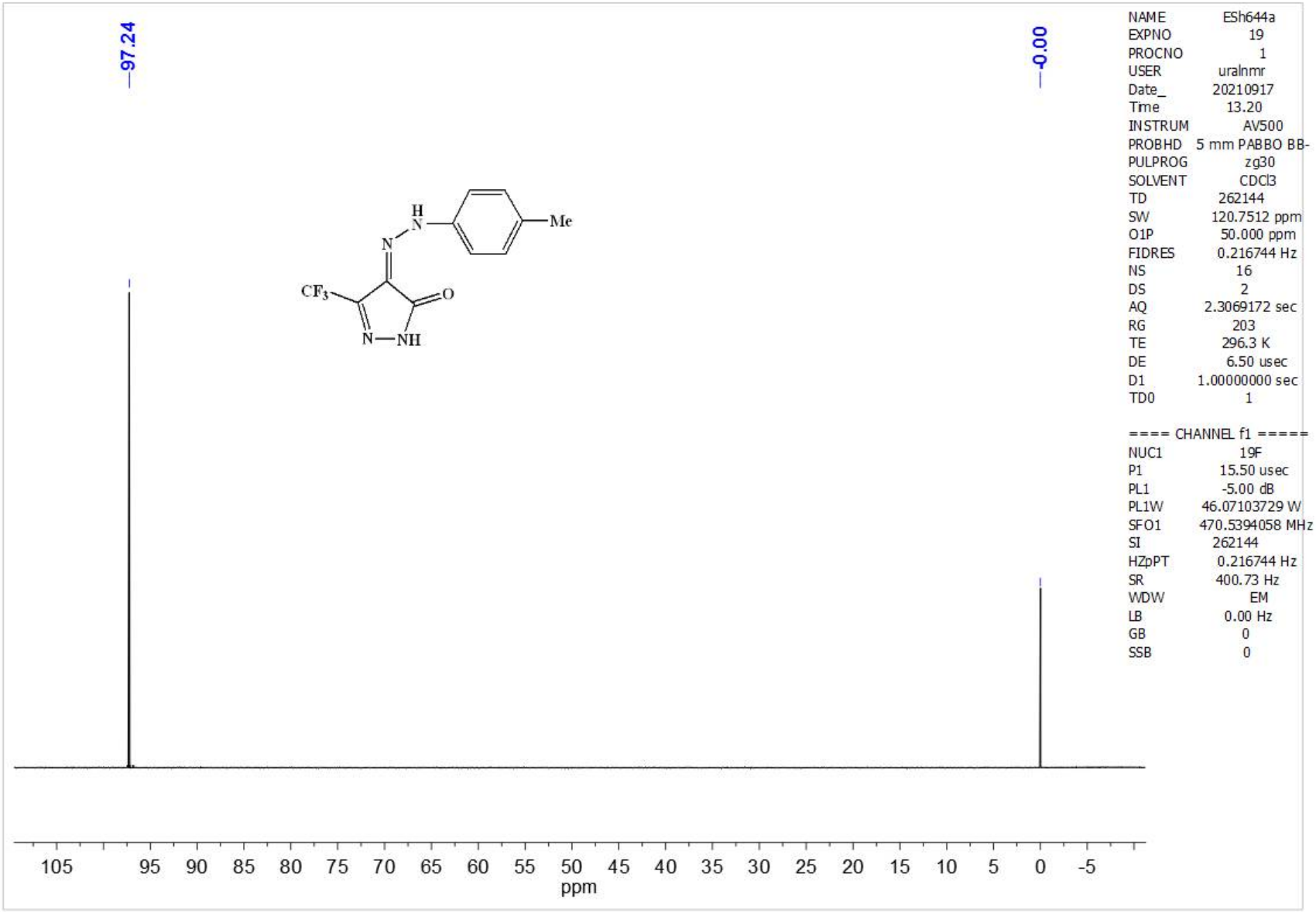


Figure S8. ^{1}H NMR spectrum of compound **5c**

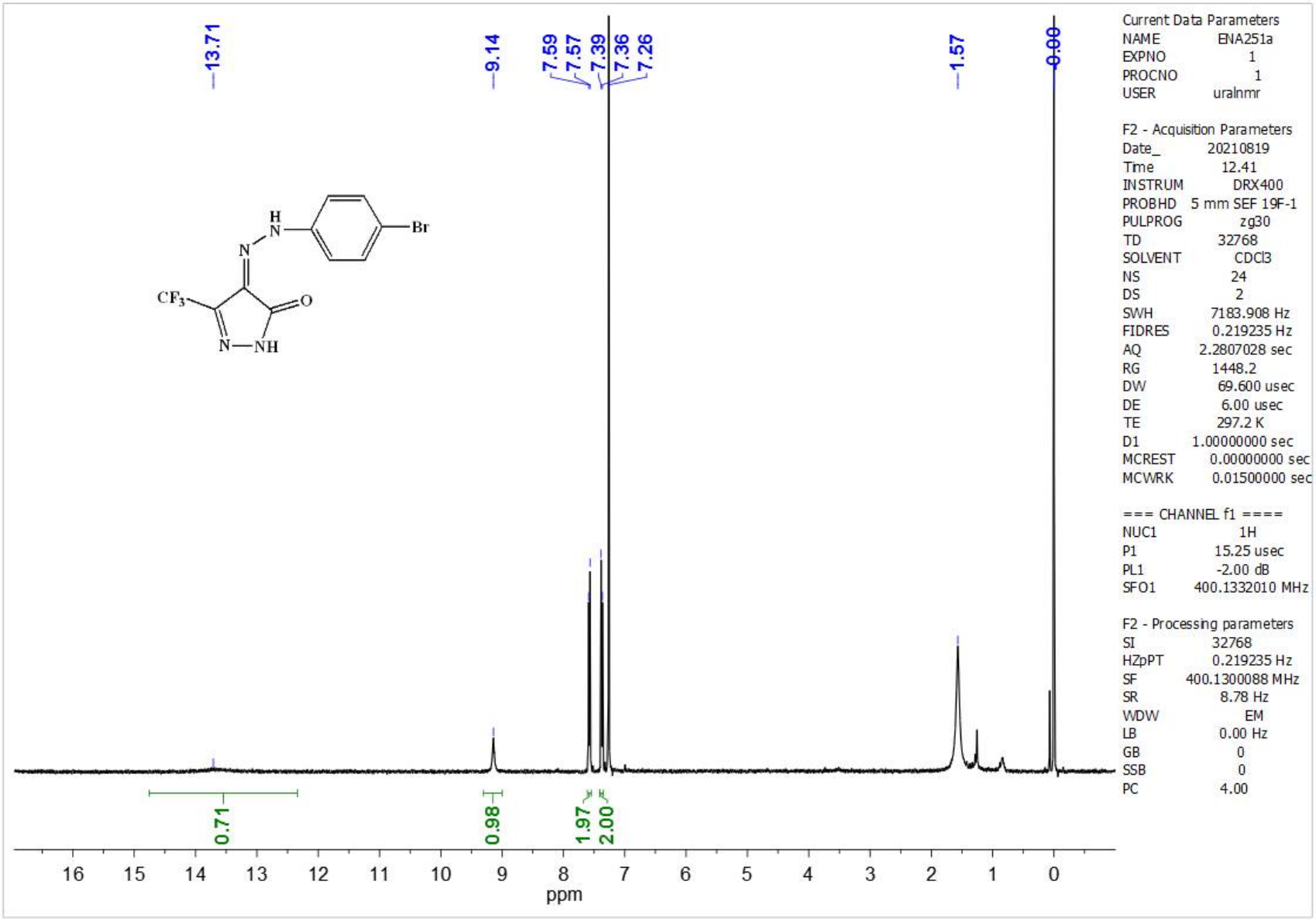


Figure S9. ^{13}C NMR spectrum of compound **5c**

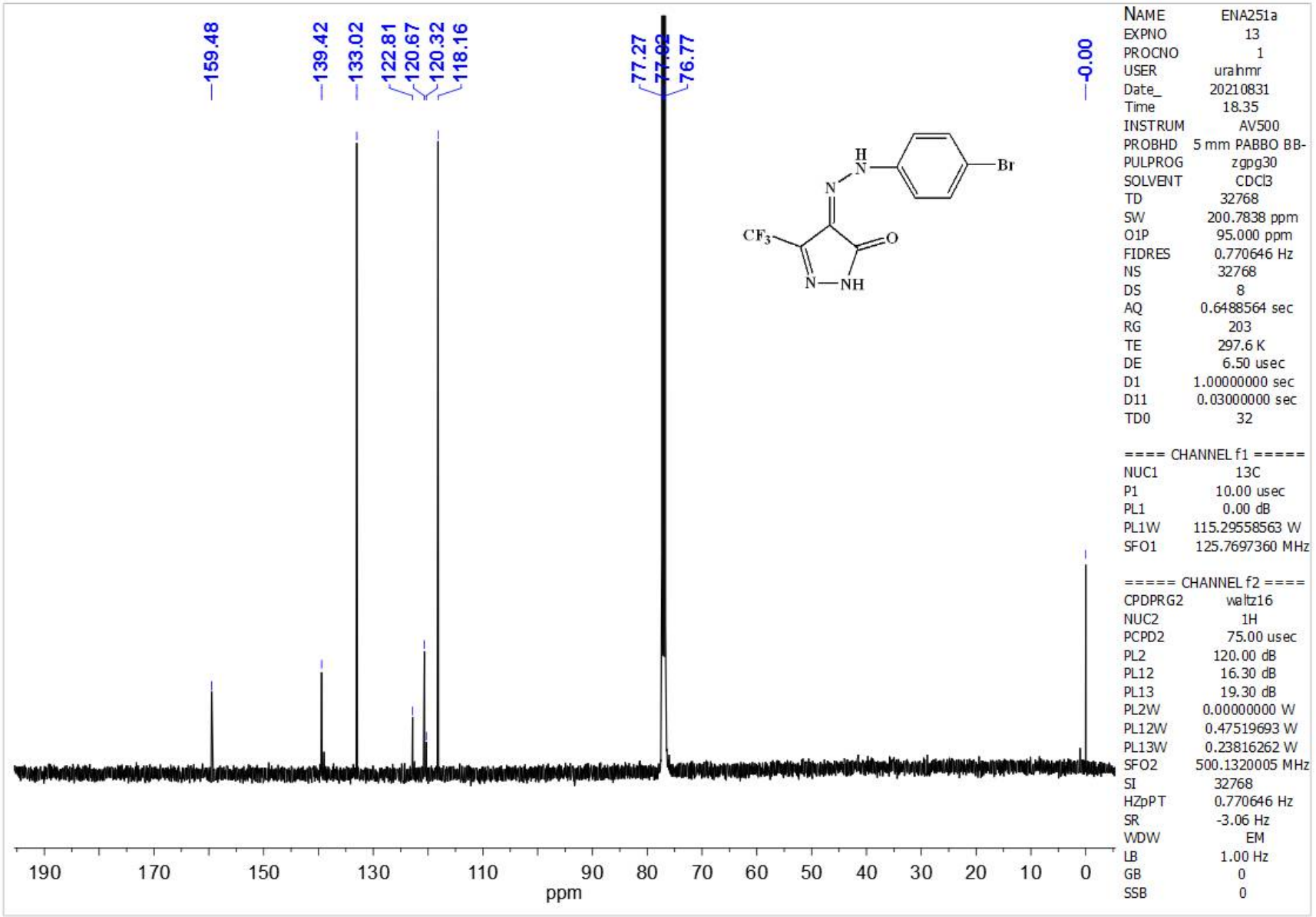


Figure S10. ^{19}F NMR spectrum of compound **5c**

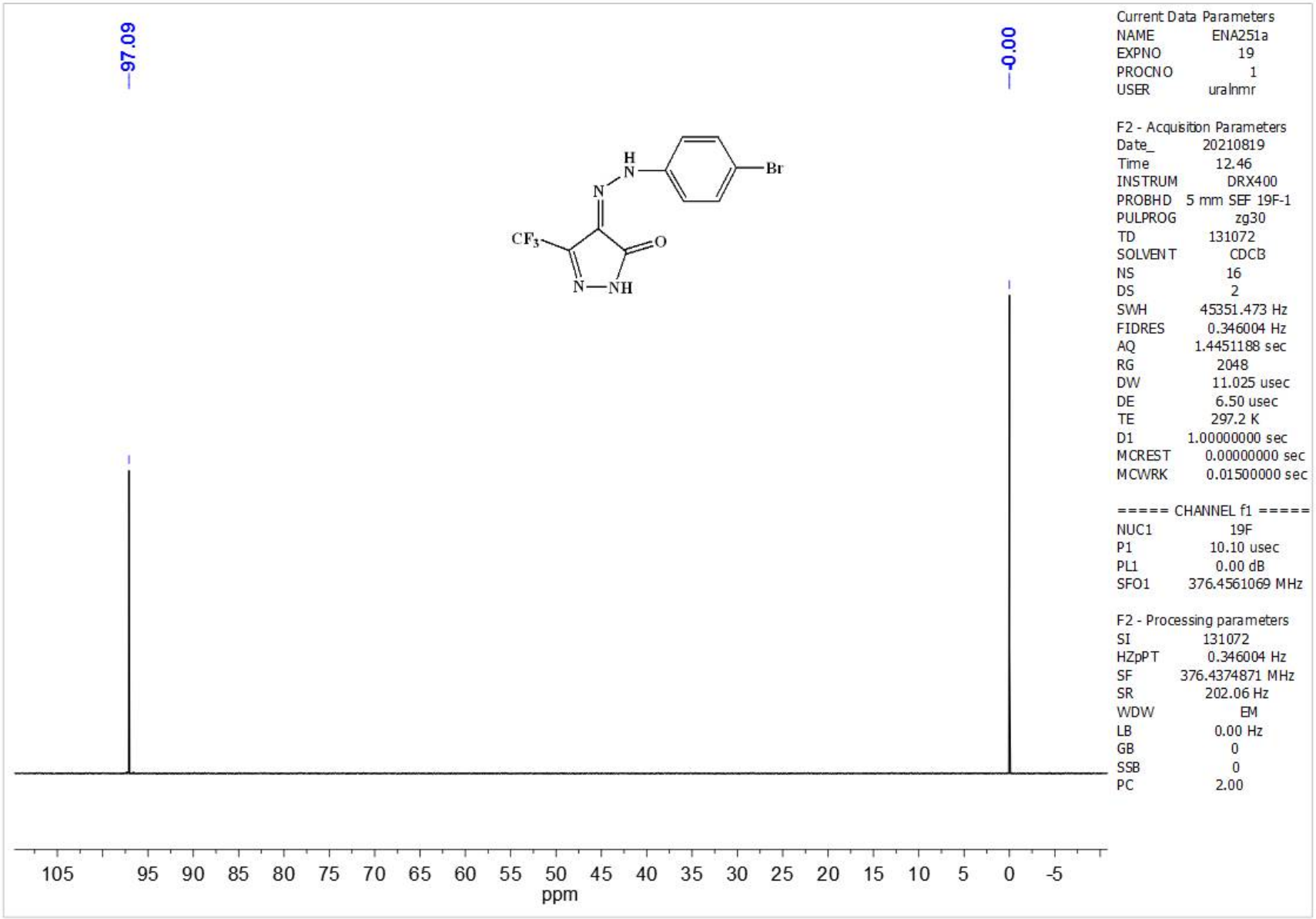


Figure S11. ^{1}H NMR spectrum of compound **5d**

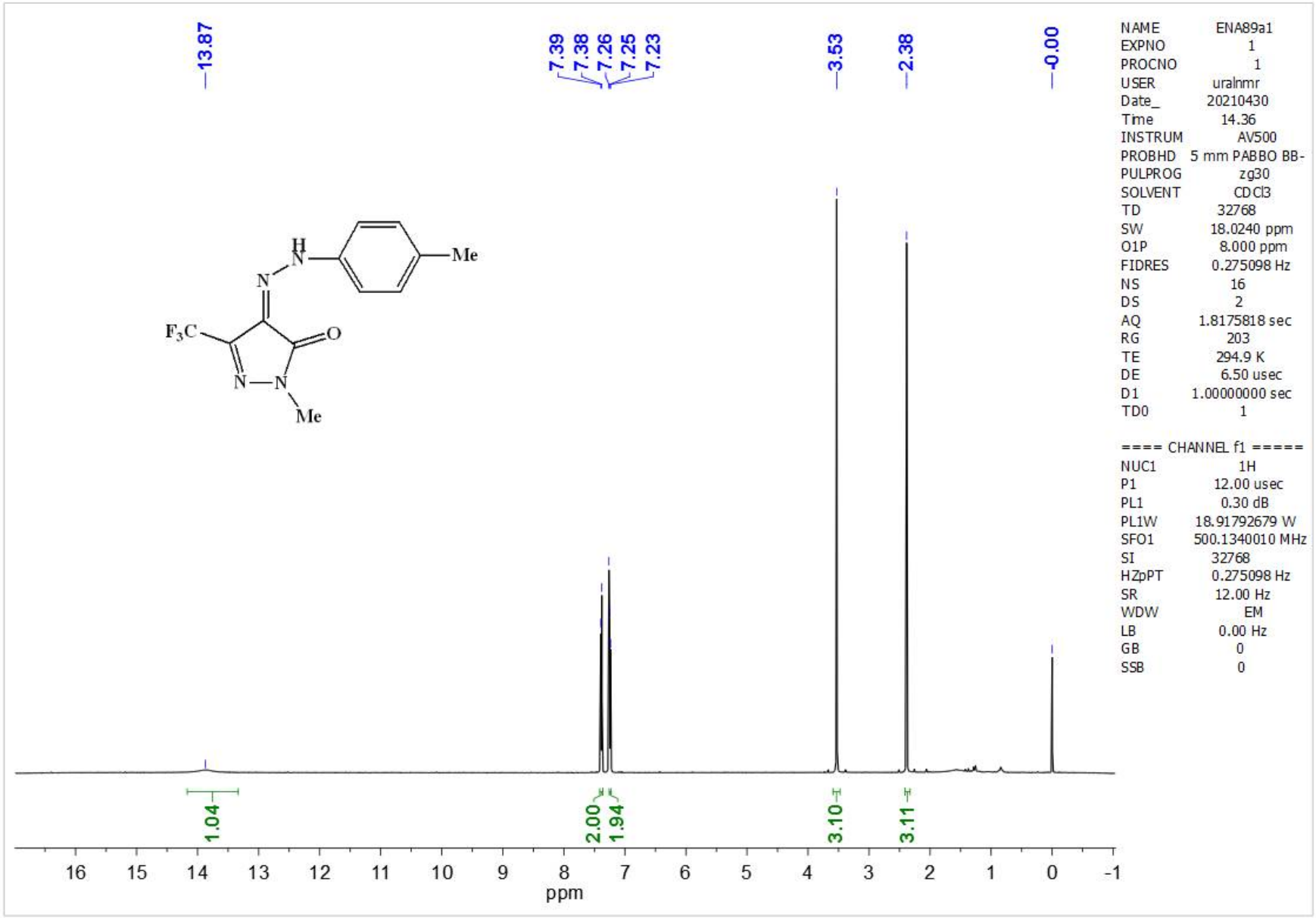


Figure S12. ^{19}F NMR spectrum of compound **5d**

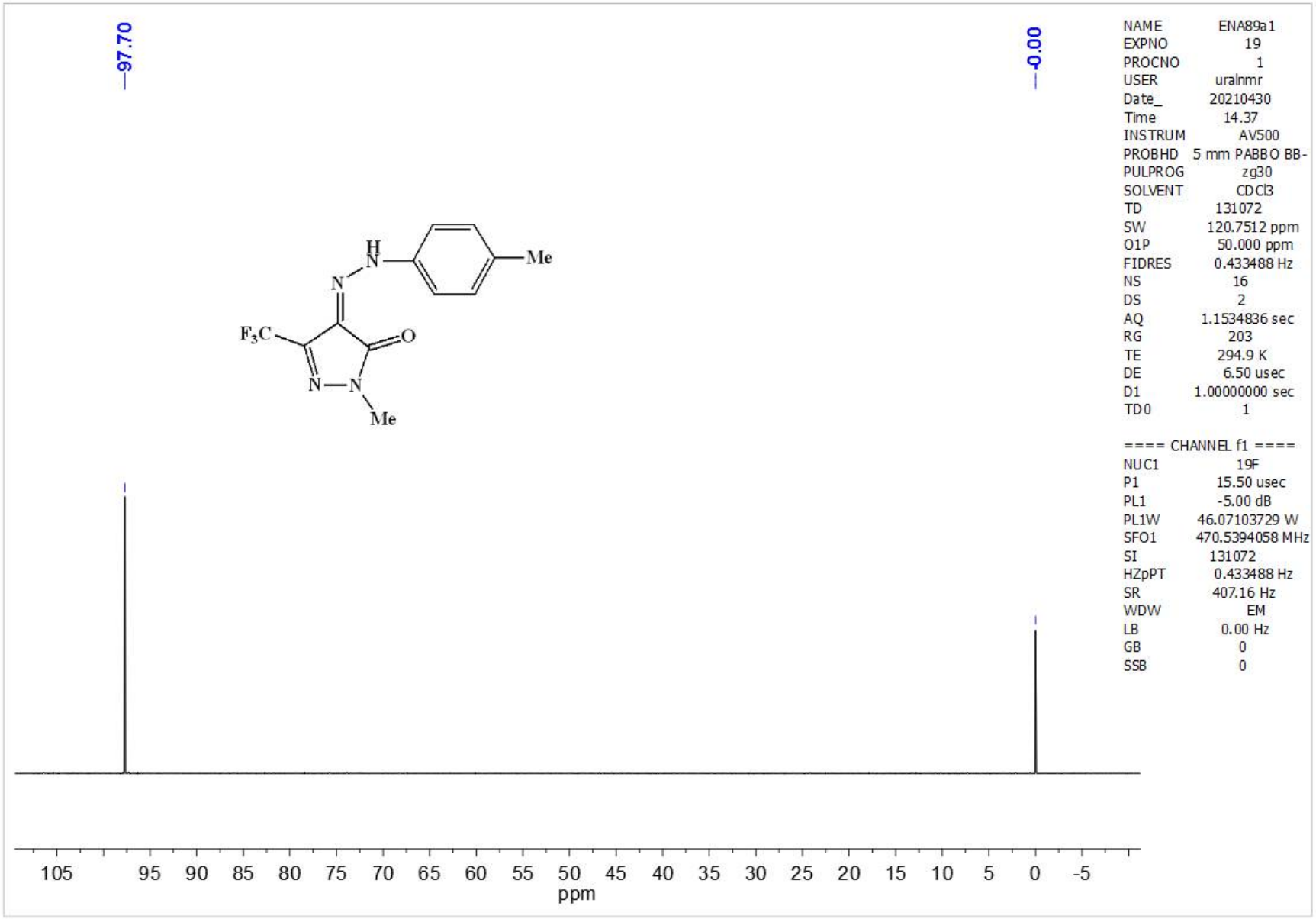


Figure S13. ^{1}H NMR spectrum of compound **5e**

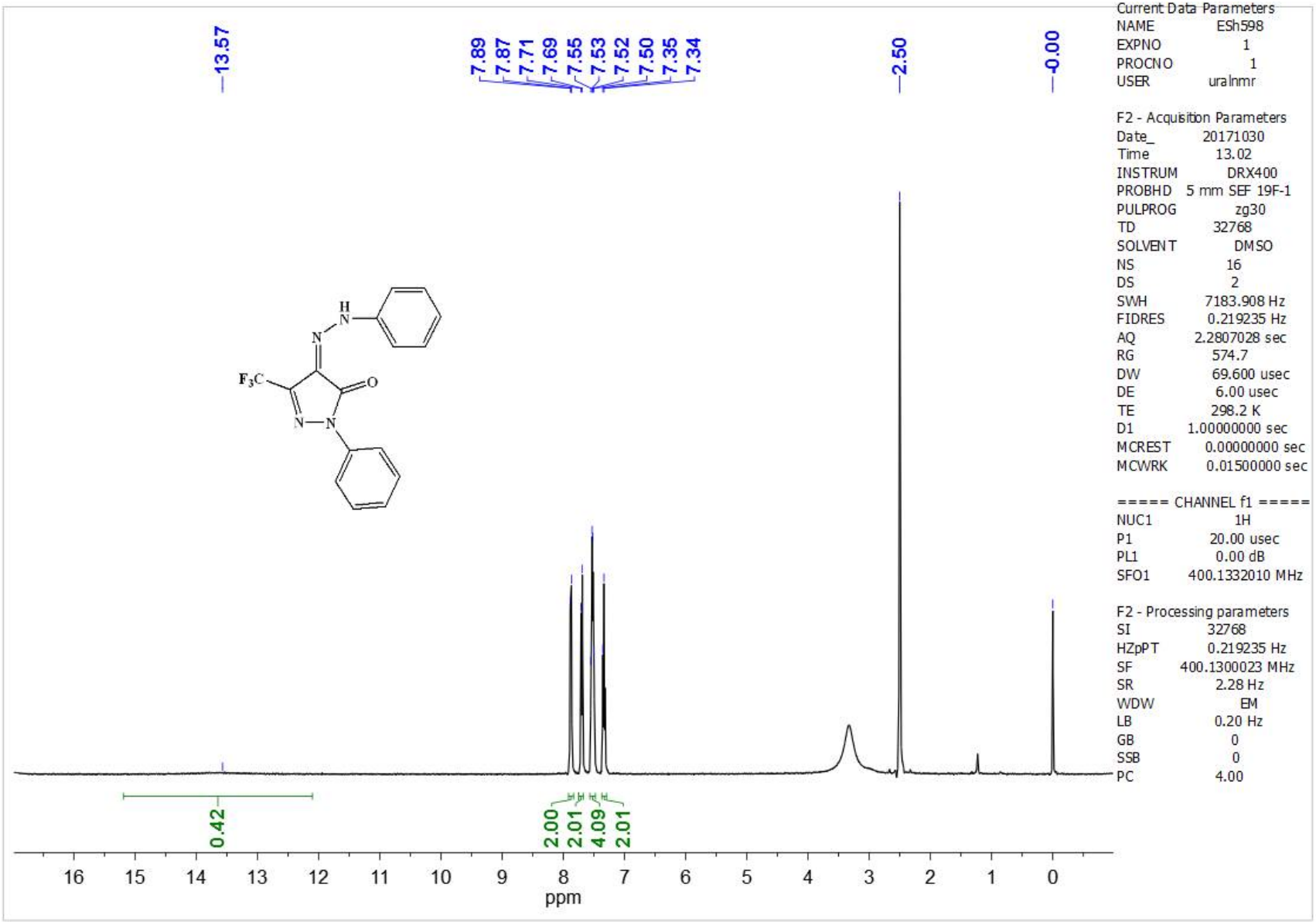


Figure S14. ^{19}F NMR spectrum of compound **5e**

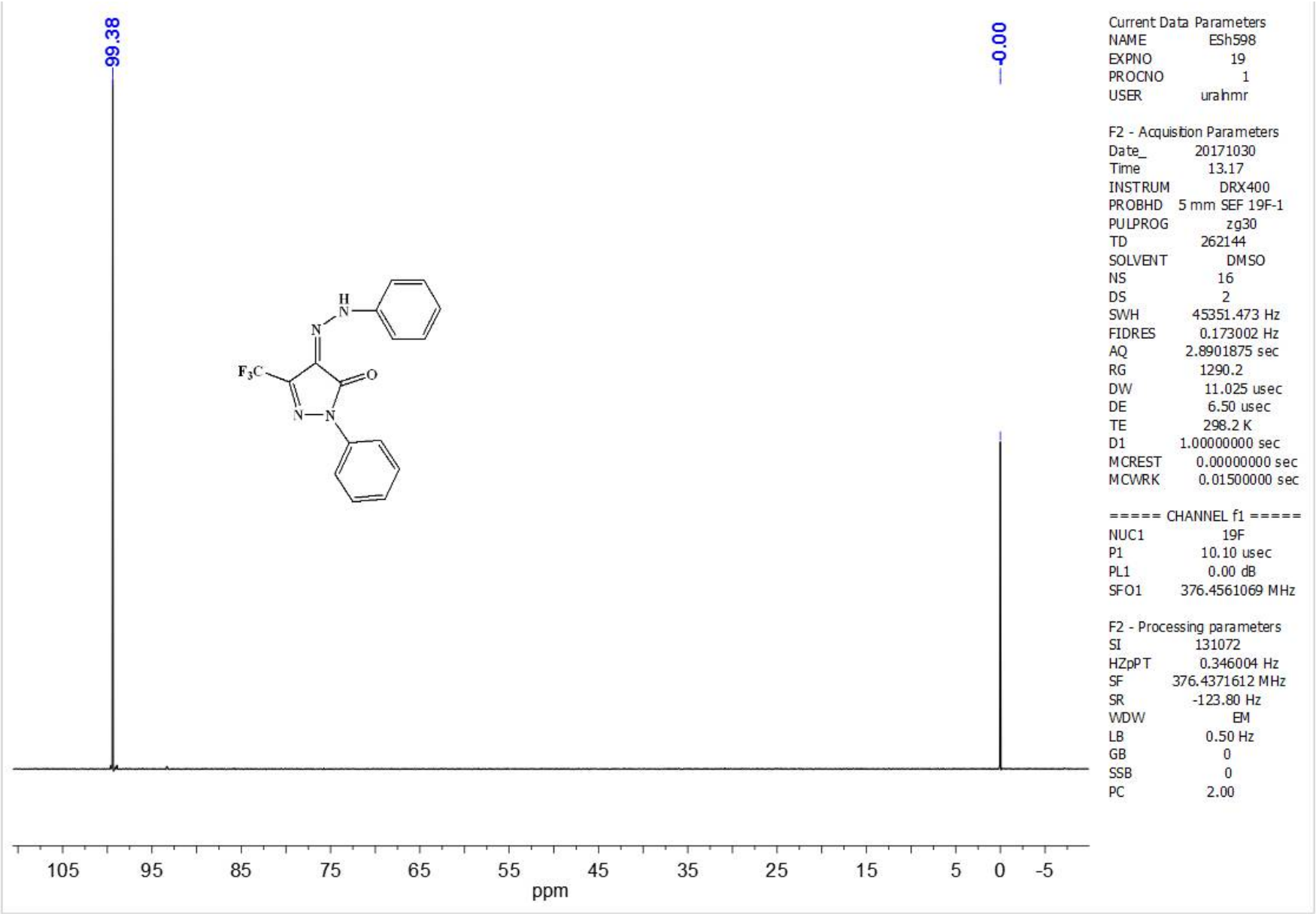
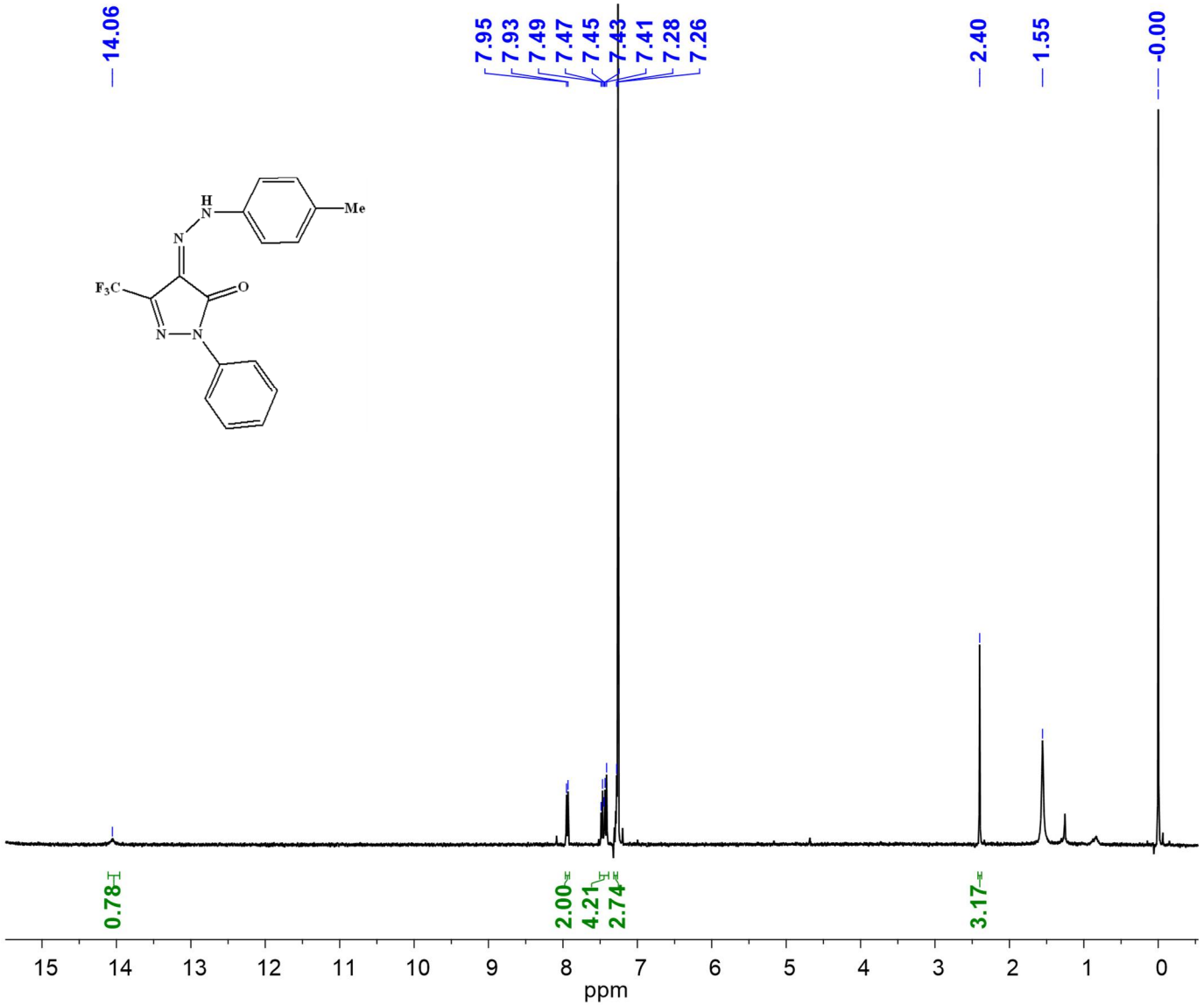


Figure S15. ^{1}H NMR spectrum of compound **5f**



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PROCNO 1
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FIDRES 0.195625 Hz
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DE 6.00 usec
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MCWRK 0.01500000 sec

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PL1 0.00 dB
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Figure S16. ^{13}C NMR spectrum of compound **5f**

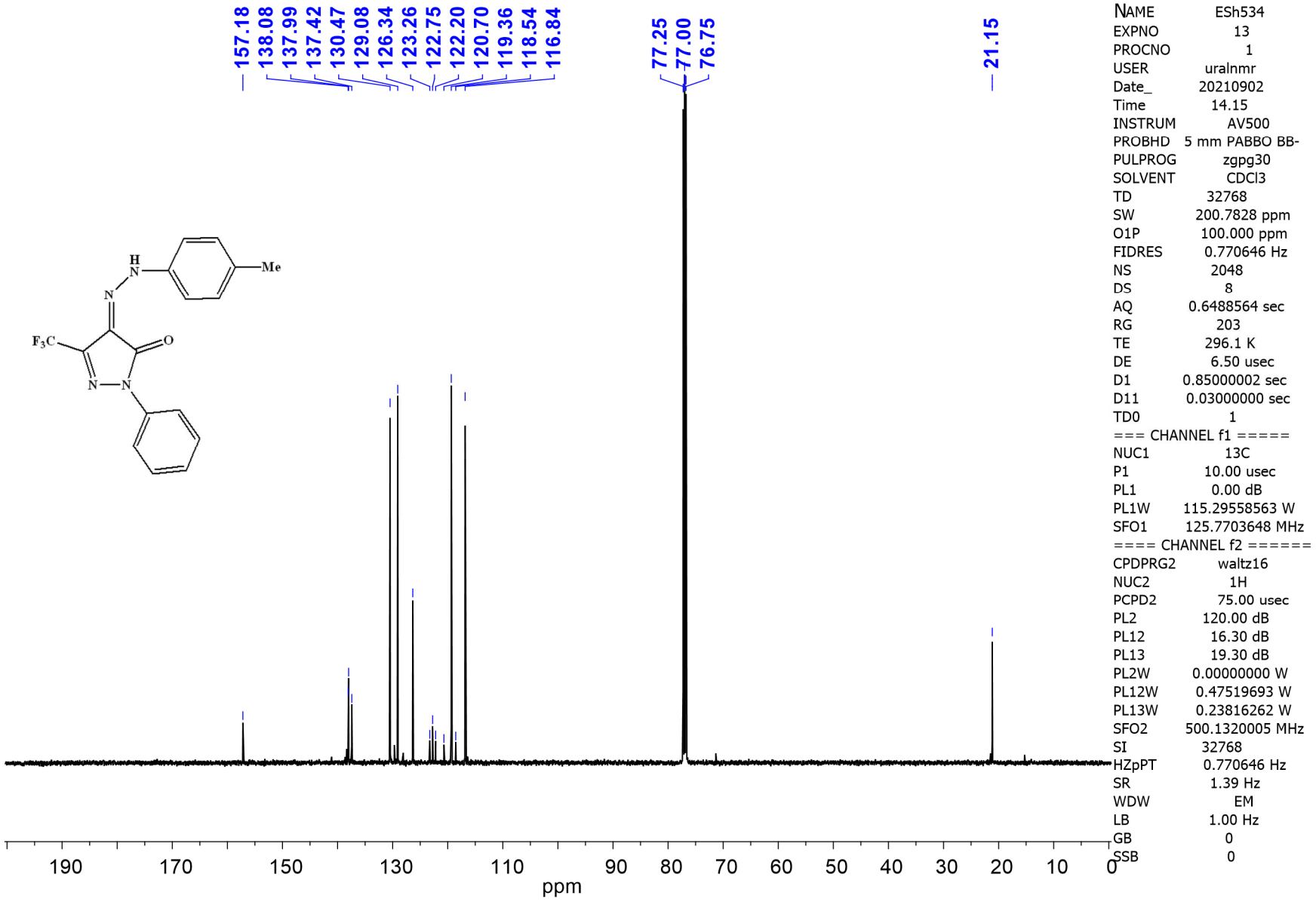

Figure S17. ^{19}F NMR spectrum of compound **5f**

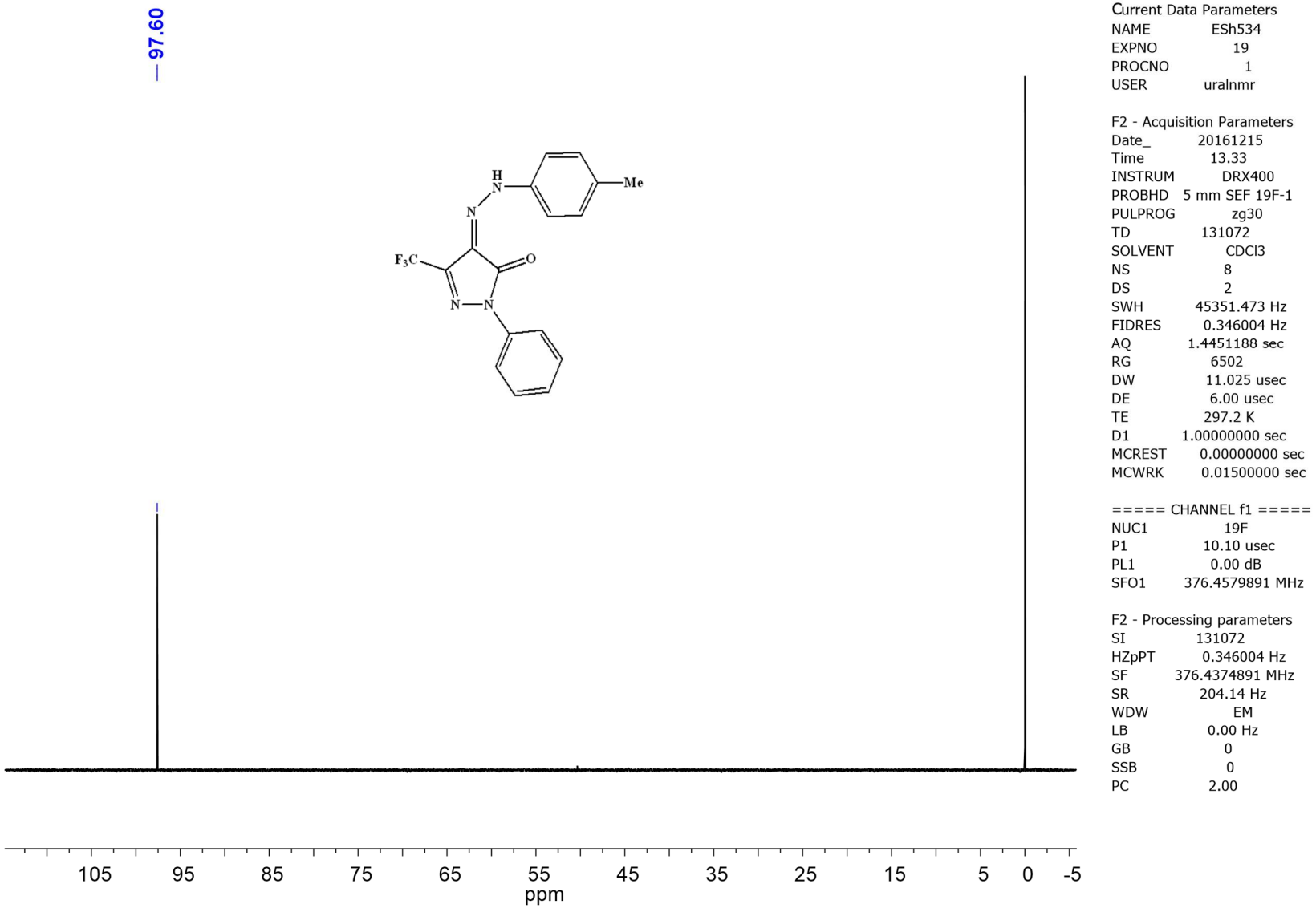

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Figure S18. ^{1}H NMR spectrum of compound **5g**

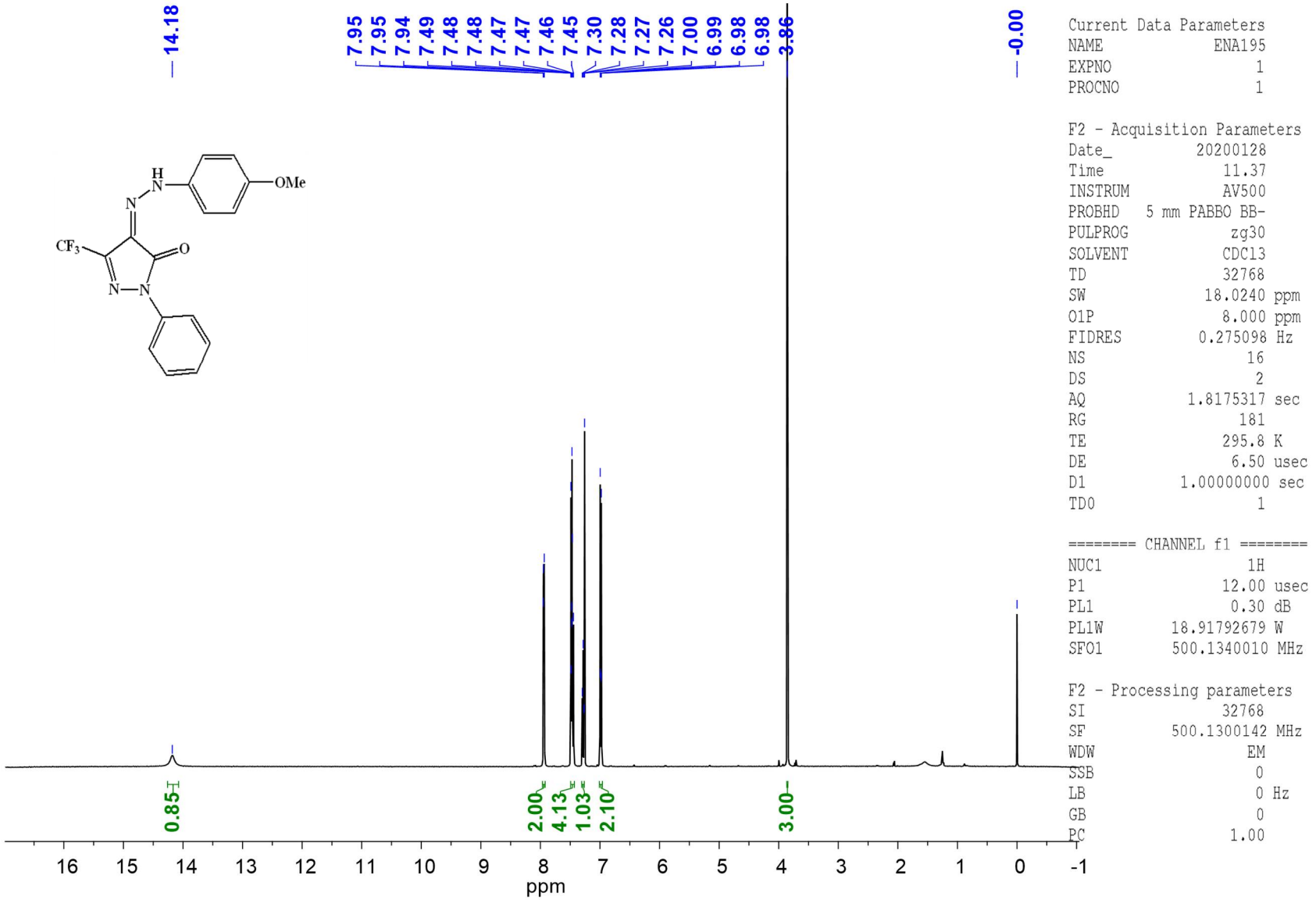

Figure S19. ^{13}C NMR spectrum of compound **5g**

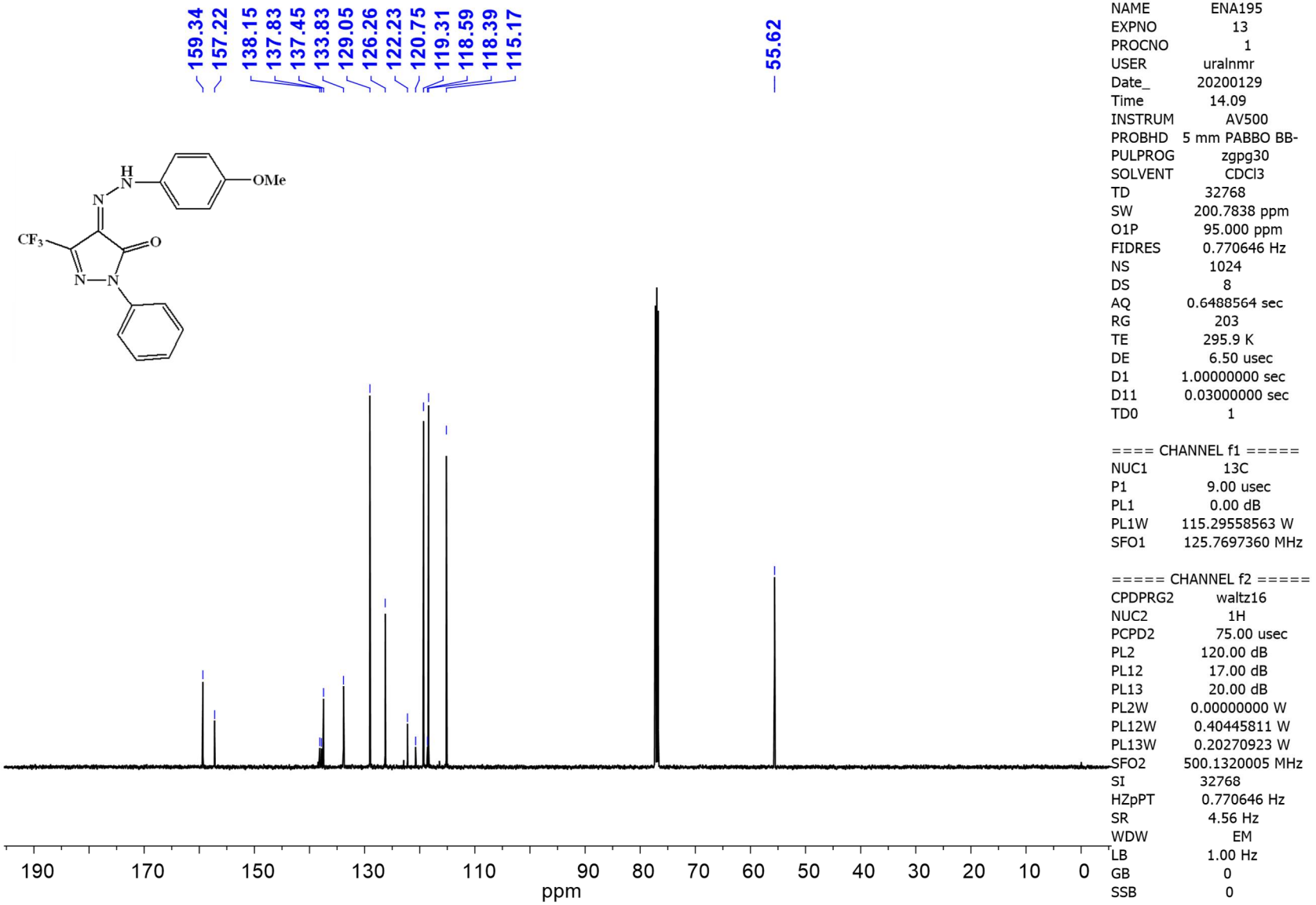

Figure S20. ^{19}F NMR spectrum of compound **5g**

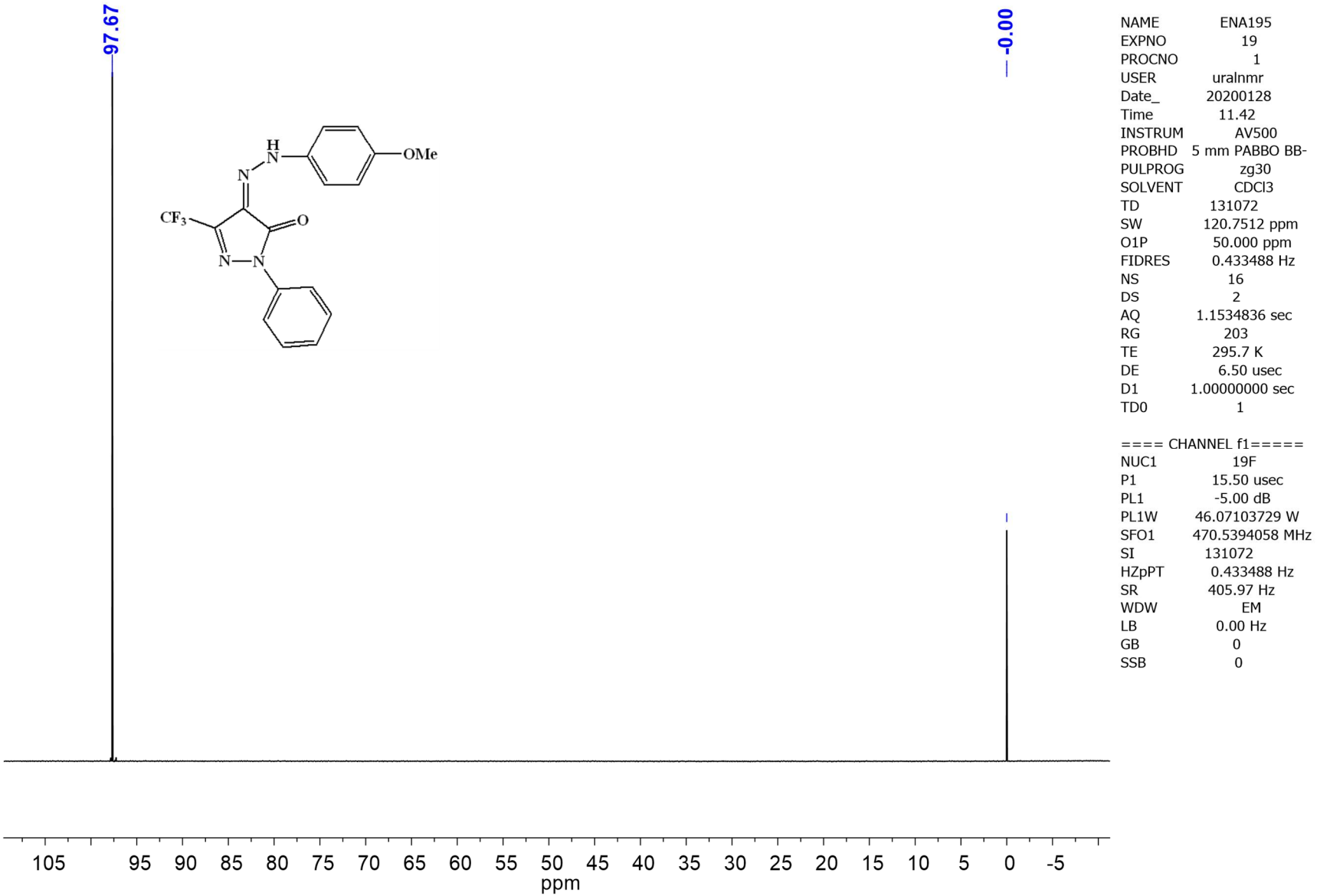

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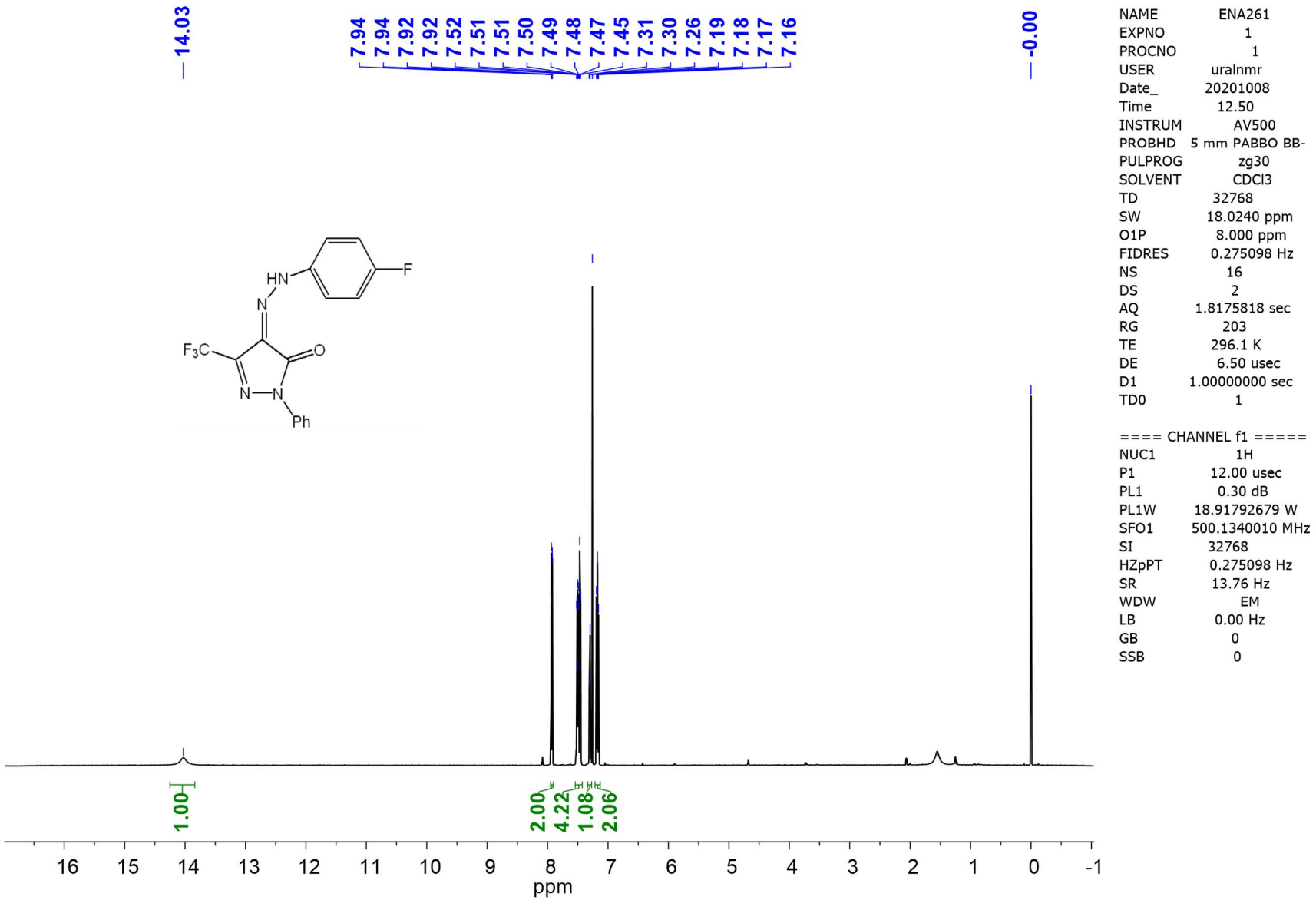
Figure S21. ^{1}H NMR spectrum of compound **5h**



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P1	12.00 usec
PL1	0.30 dB
PL1W	18.91792679 W
SFO1	500.1340010 MHz
SI	32768
HZpPT	0.275098 Hz
SR	13.76 Hz
WDW	EM
LB	0.00 Hz
GB	0
SSB	0

Figure S22. ^{13}C NMR spectrum of compound **5h**

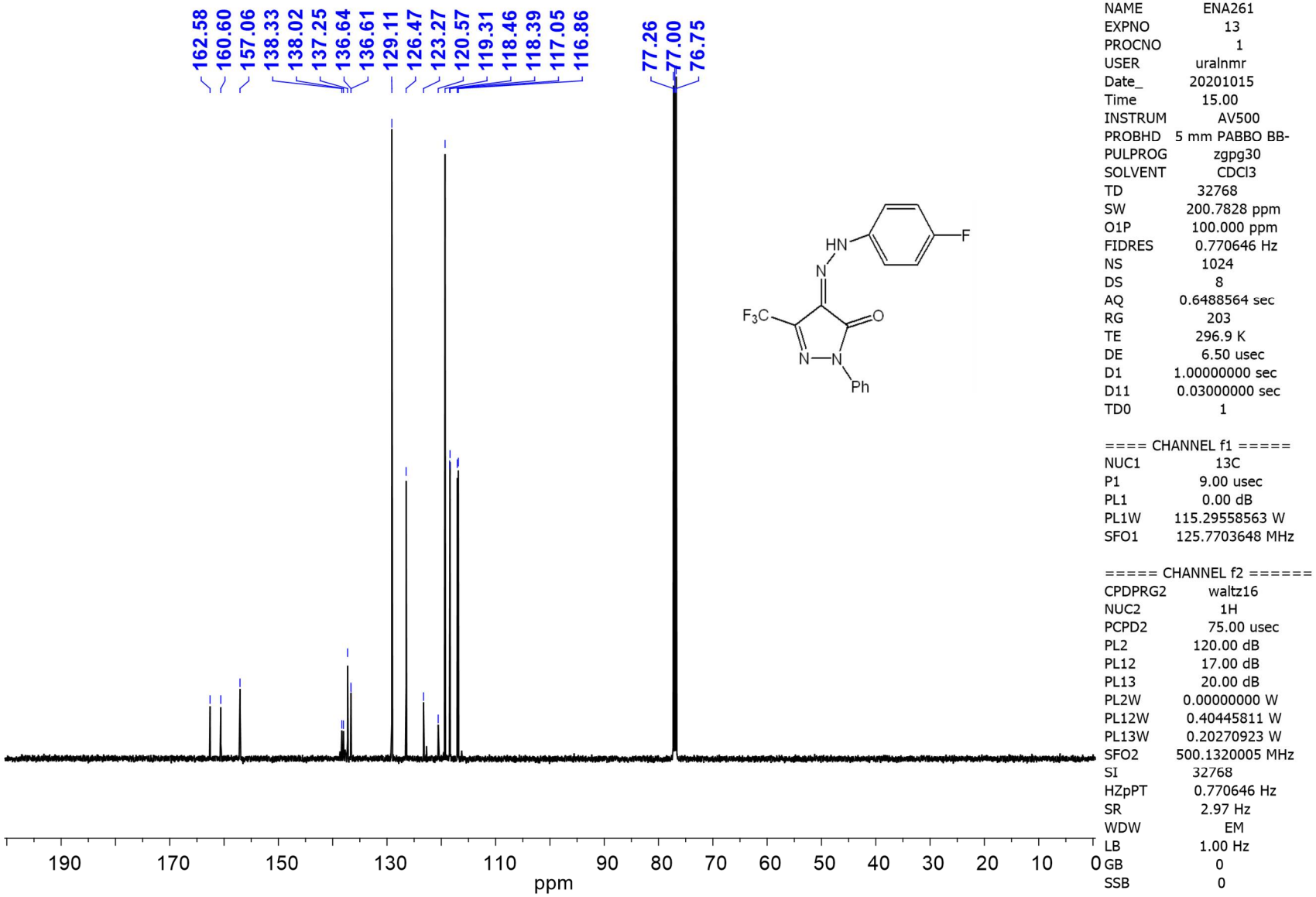
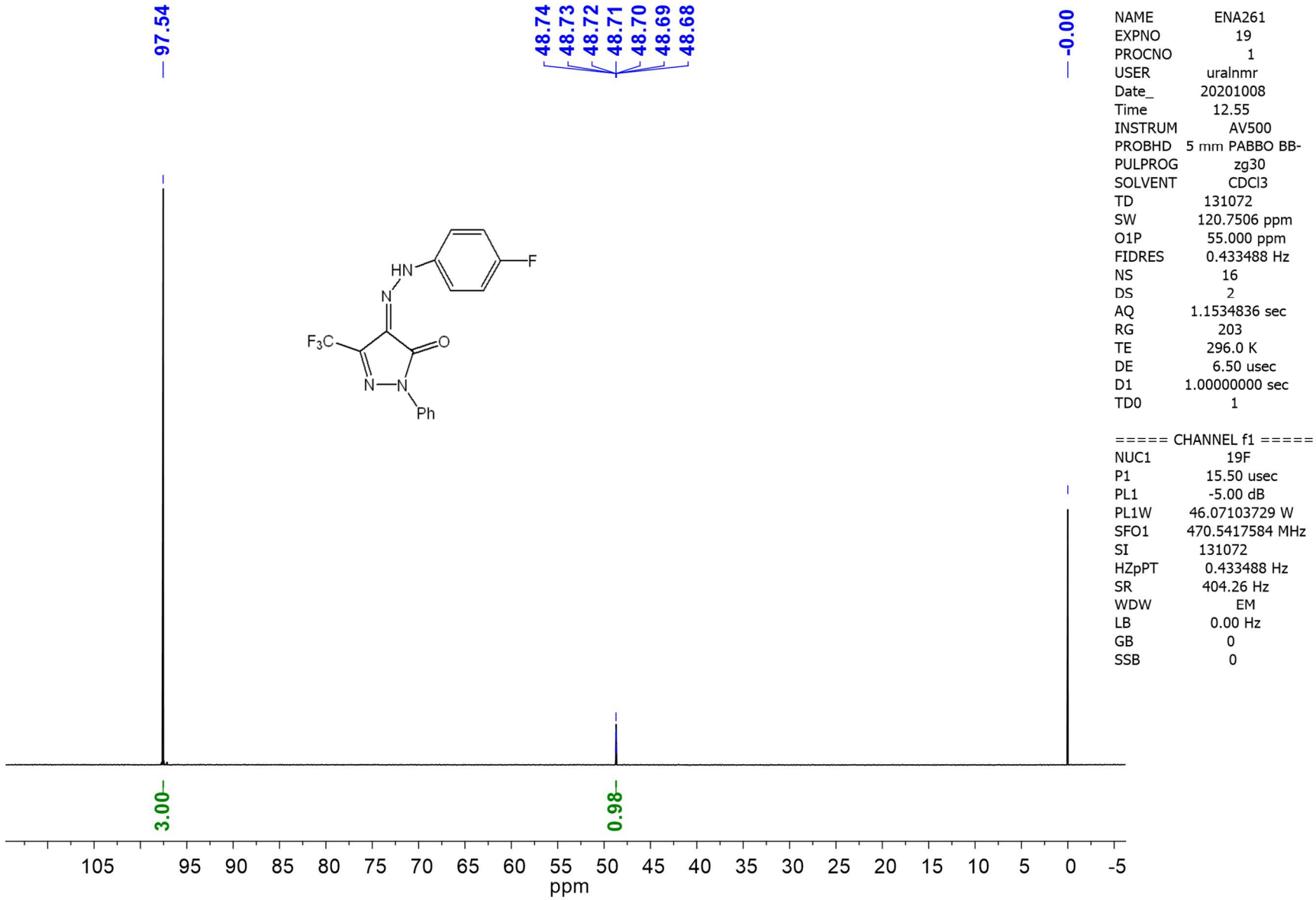


Figure S23. ^{19}F NMR spectrum of compound **5h**



NAME	ENA261
EXPNO	19
PROCNO	1
USER	uralnmr
Date_	20201008
Time	12.55
INSTRUM	AV500
PROBHD	5 mm PABBO BB-
PULPROG	zg30
SOLVENT	CDCl3
TD	131072
SW	120.7506 ppm
O1P	55.000 ppm
FIDRES	0.433488 Hz
NS	16
DS	2
AQ	1.1534836 sec
RG	203
TE	296.0 K
DE	6.50 usec
D1	1.00000000 sec
TD0	1
===== CHANNEL f1 =====	
NUC1	19F
P1	15.50 usec
PL1	-5.00 dB
PL1W	46.07103729 W
SFO1	470.5417584 MHz
SI	131072
HZpPT	0.433488 Hz
SR	404.26 Hz
WDW	EM
LB	0.00 Hz
GB	0
SSB	0

Figure S24. ^{1}H NMR spectrum of compound **5i**

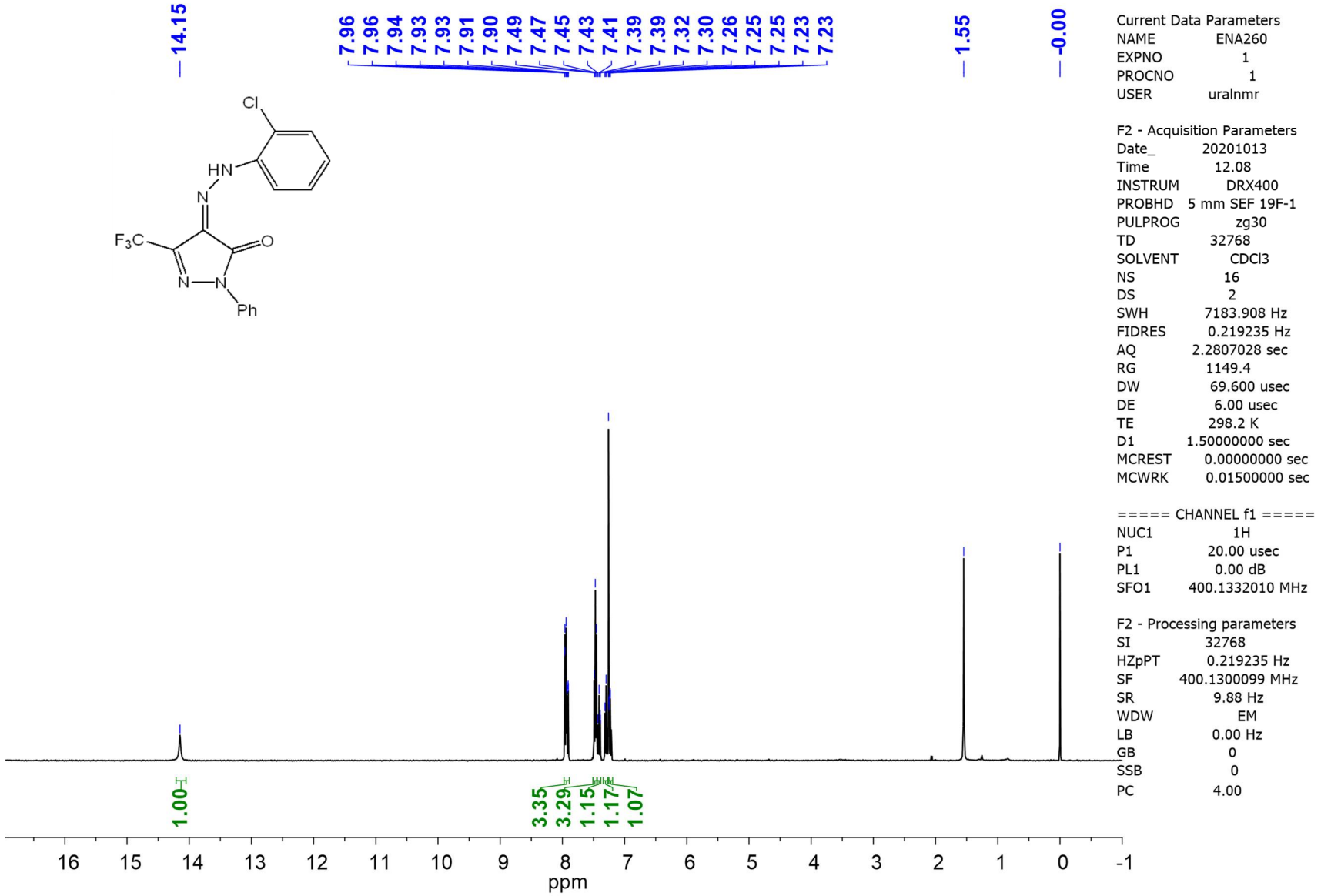
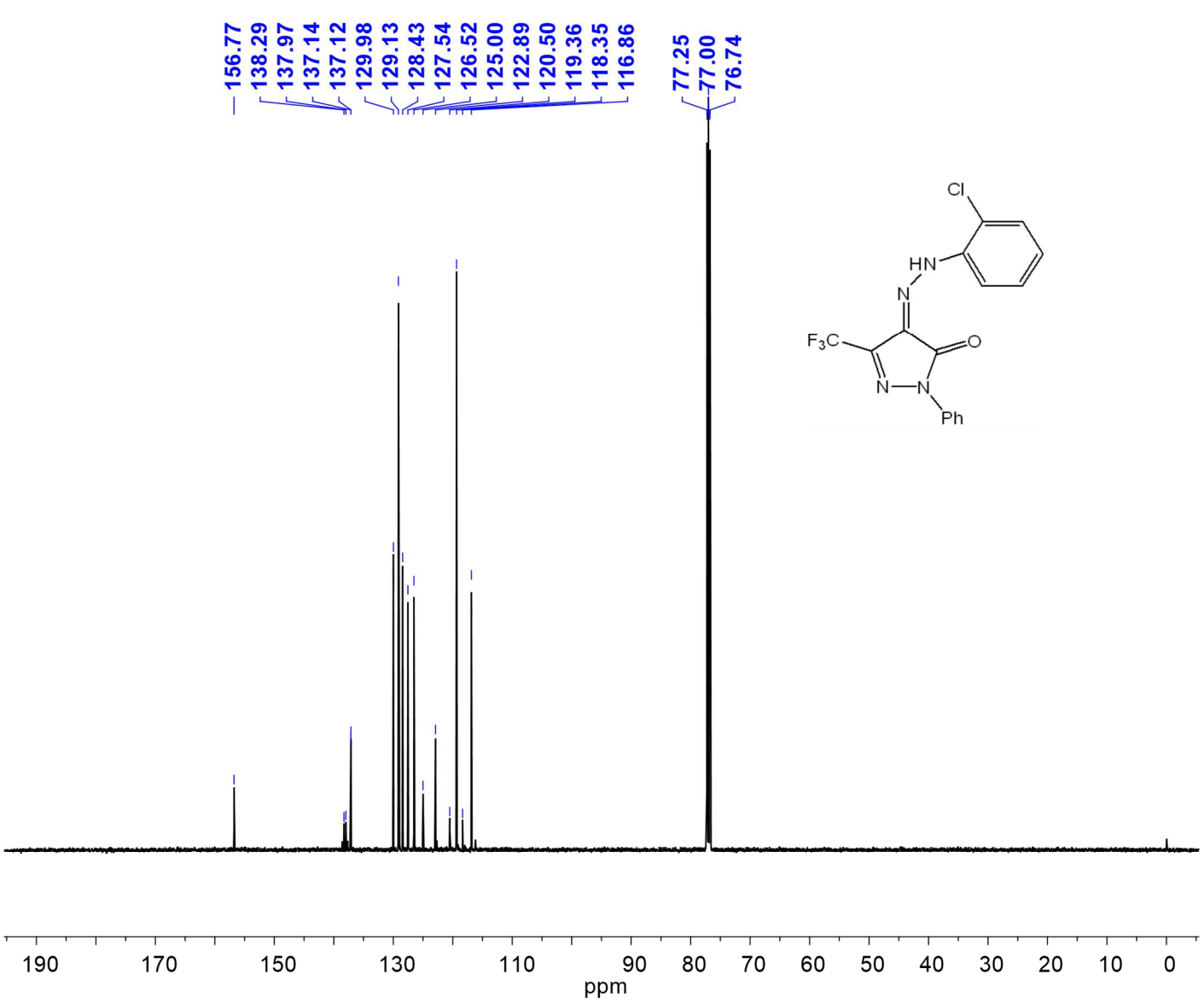


Figure S25. ^{13}C NMR spectrum of compound **5i**



NAME	ENA260
EXPNO	13
PROCNO	1
USER	uralnmr
Date_	20201016
Time	14.59
INSTRUM	AV500
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
SOLVENT	CDCl3
TD	32768
SW	200.7838 ppm
O1P	95.000 ppm
FIDRES	0.770646 Hz
NS	2048
DS	8
AQ	0.6488564 sec
RG	203
TE	296.5 K
DE	6.50 usec
D1	0.85000002 sec
D11	0.03000000 sec
TD0	1
==== CHANNEL f1 =====	
NUC1	13C
P1	9.00 usec
PL1	0.00 dB
PL1W	115.29558563 W
SFO1	125.7697360 MHz
==== CHANNEL f2 ====	
CPDPRG2	waltz16
NUC2	1H
PCPD2	75.00 usec
PL2	120.00 dB
PL12	17.00 dB
PL13	20.00 dB
PL2W	0.00000000 W
PL12W	0.40445811 W
PL13W	0.20270923 W
SFO2	500.1320005 MHz
SI	32768
HZpPT	0.770646 Hz
SR	3.09 Hz
WDW	EM
LB	1.00 Hz
GB	0
SSB	0

Figure S26. ^{19}F NMR spectrum of compound **5i**

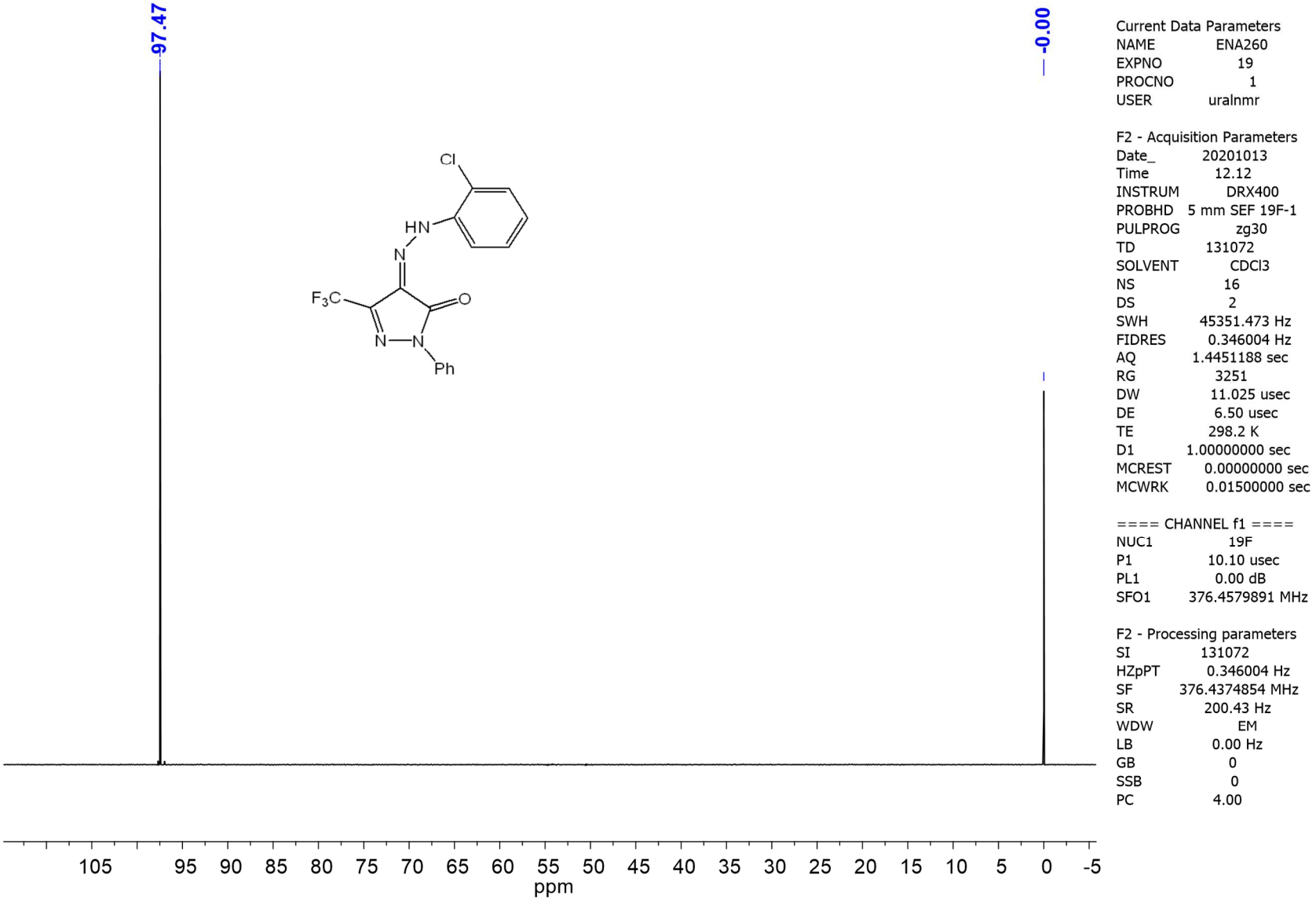


Figure S27. ^{1}H NMR spectrum of compound **5j**

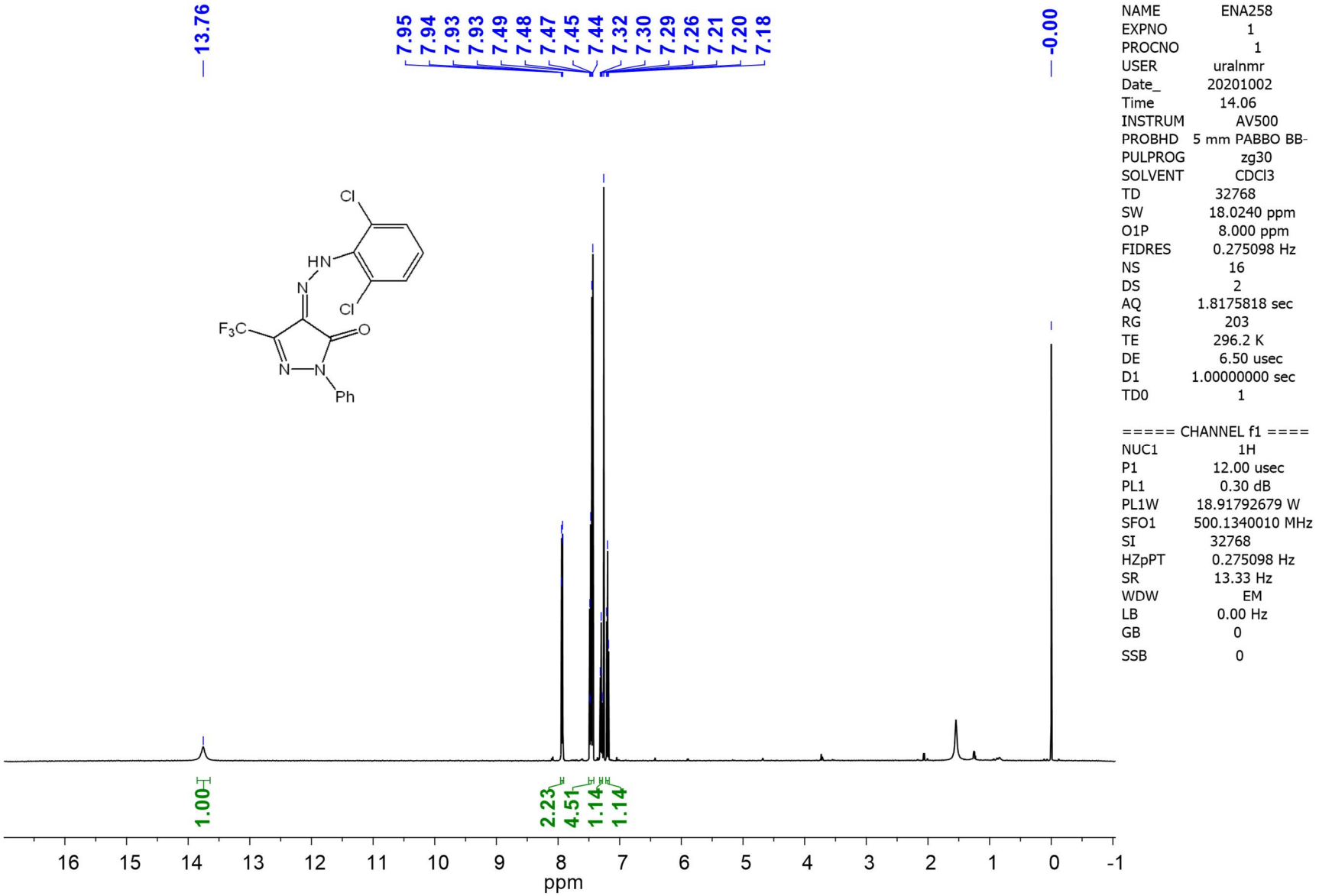
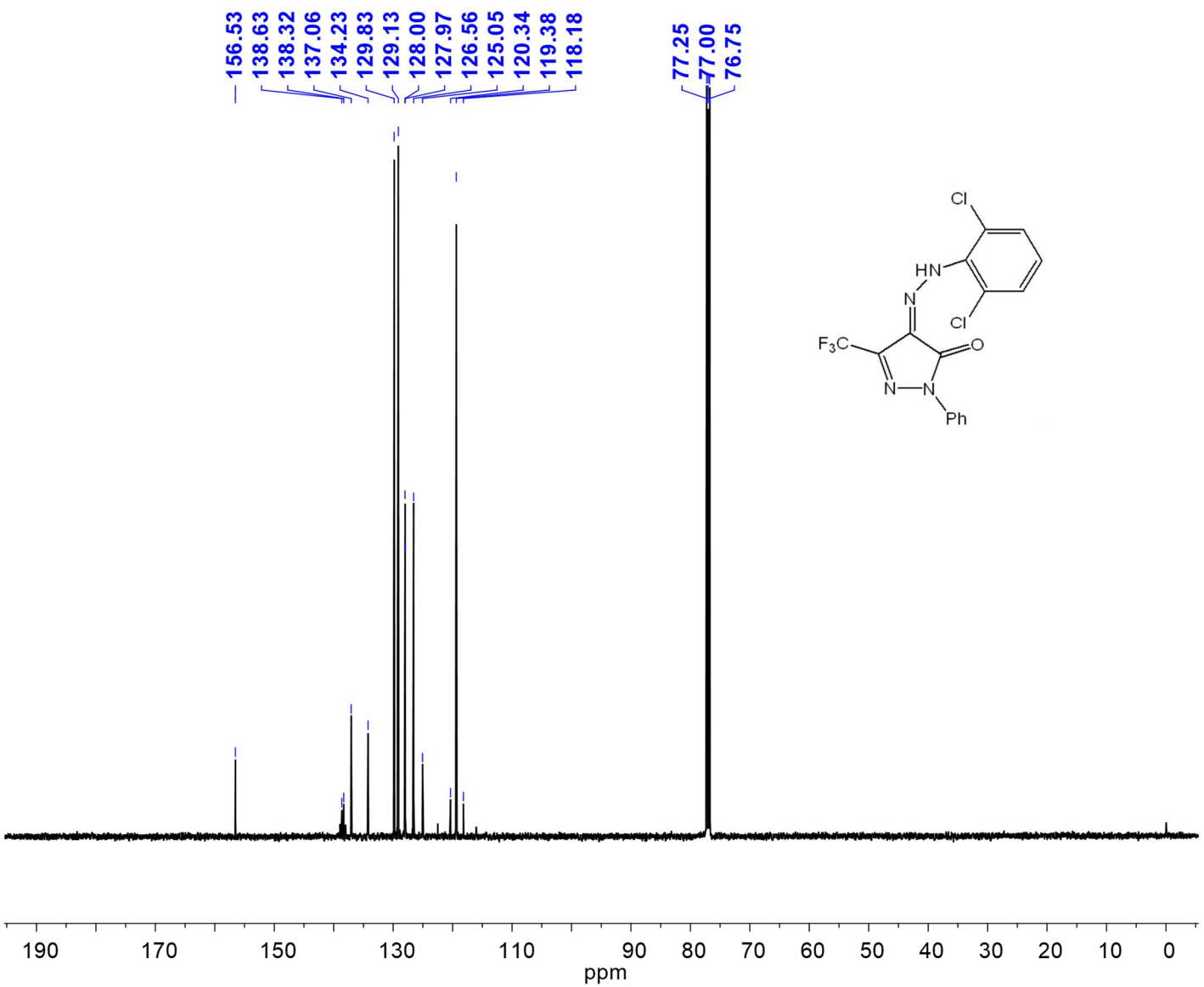
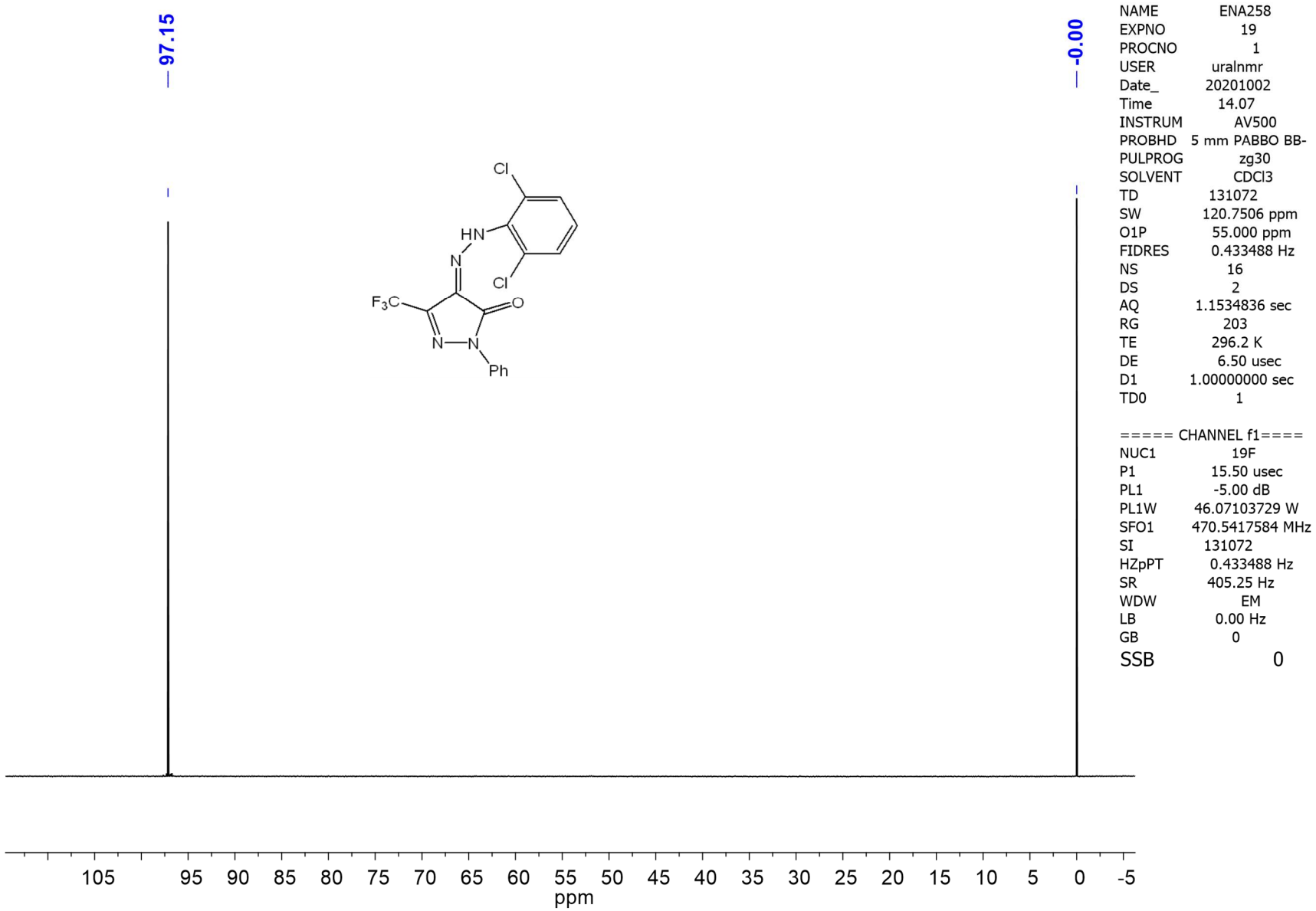


Figure S28. ^{13}C NMR spectrum of compound **5j**



NAME	ENA258
EXPNO	13
PROCNO	1
USER	uralnmr
Date_	20201008
Time	11.07
INSTRUM	AV500
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
SOLVENT	CDCl3
TD	32768
SW	200.7838 ppm
O1P	95.000 ppm
FIDRES	0.770646 Hz
NS	1024
DS	8
AQ	0.6488564 sec
RG	203
TE	296.8 K
DE	6.50 usec
D1	1.00000000 sec
D11	0.03000000 sec
TD0	1
=== CHANNEL f1 ====	
NUC1	13C
P1	9.00 usec
PL1	0.00 dB
PL1W	115.29558563 W
SFO1	125.7697360 MHz
==== CHANNEL f2 ====	
CPDPRG2	waltz16
NUC2	1H
PCPD2	75.00 usec
PL2	120.00 dB
PL12	17.00 dB
PL13	20.00 dB
PL2W	0.00000000 W
PL12W	0.40445811 W
PL13W	0.20270923 W
SFO2	500.1320005 MHz
SI	32768
HZpPT	0.770646 Hz
SR	4.06 Hz
WDW	EM
LB	1.00 Hz
GB	0
SSB	0

Figure S29. ^{19}F NMR spectrum of compound **5j**



NAME	ENA258
EXPNO	19
PROCNO	1
USER	uralnmr
Date_	20201002
Time	14.07
INSTRUM	AV500
PROBHD	5 mm PABBO BB-
PULPROG	zg30
SOLVENT	CDCl3
TD	131072
SW	120.7506 ppm
O1P	55.000 ppm
FIDRES	0.433488 Hz
NS	16
DS	2
AQ	1.1534836 sec
RG	203
TE	296.2 K
DE	6.50 usec
D1	1.00000000 sec
TD0	1
===== CHANNEL f1====	
NUC1	19F
P1	15.50 usec
PL1	-5.00 dB
PL1W	46.07103729 W
SFO1	470.5417584 MHz
SI	131072
HZpPT	0.433488 Hz
SR	405.25 Hz
WDW	EM
LB	0.00 Hz
GB	0
SSB	0

Figure S30. ^{1}H NMR spectrum of compound **5k**

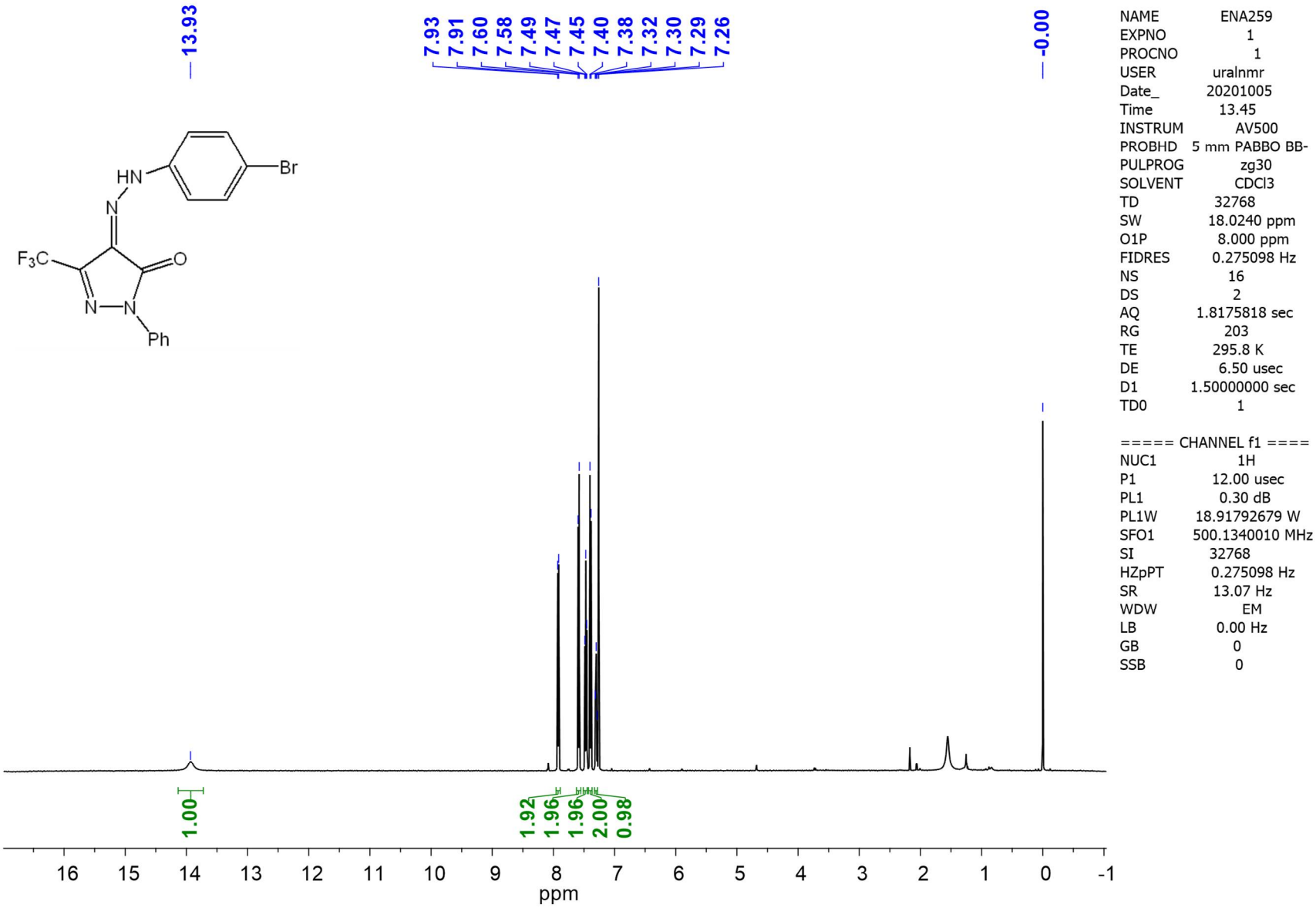
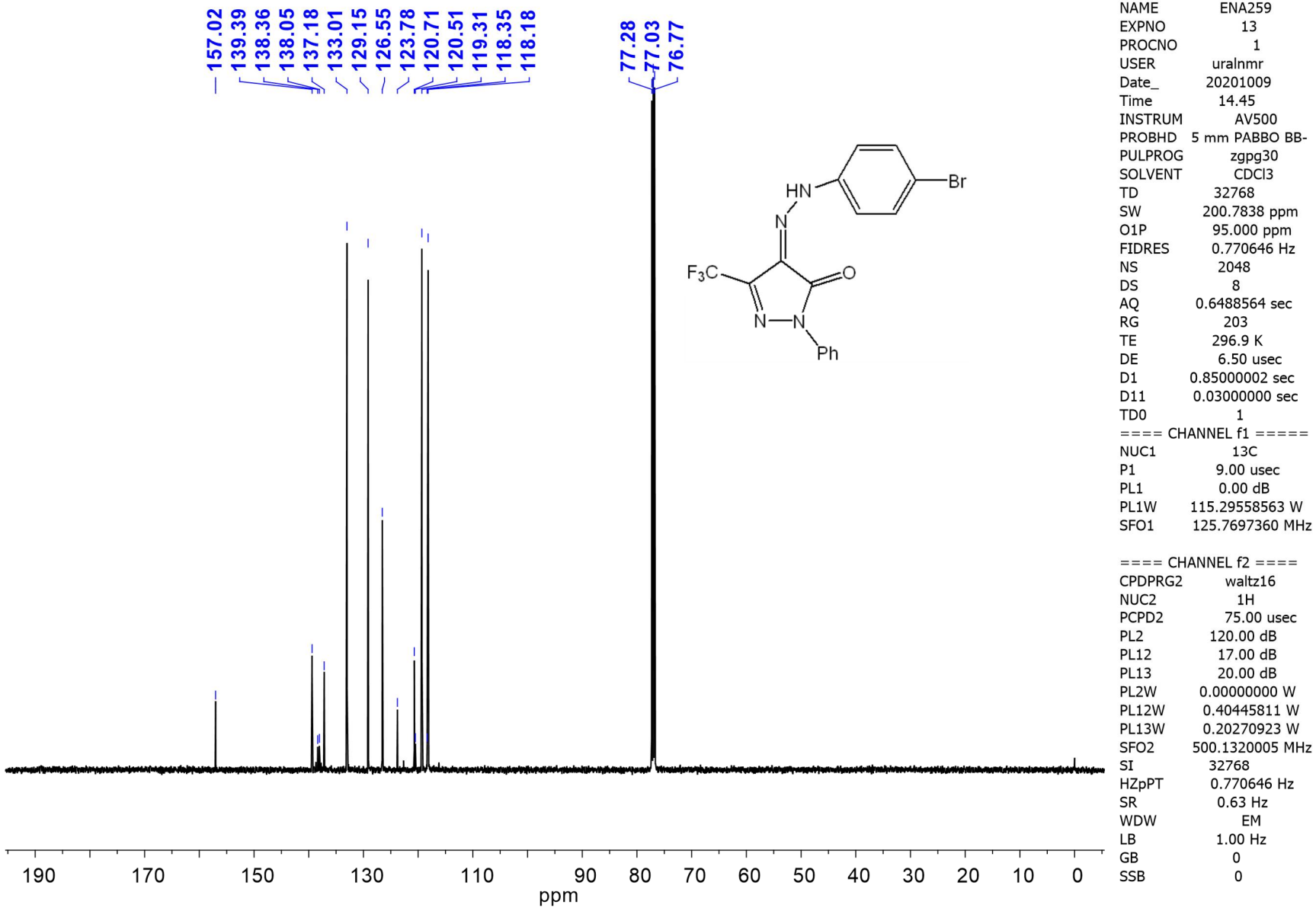


Figure S31. ^{13}C NMR spectrum of compound **5k**



NAME	ENA259
EXPNO	13
PROCNO	1
USER	uralnmr
Date_	20201009
Time	14.45
INSTRUM	AV500
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
SOLVENT	CDCl3
TD	32768
SW	200.7838 ppm
O1P	95.000 ppm
FIDRES	0.770646 Hz
NS	2048
DS	8
AQ	0.6488564 sec
RG	203
TE	296.9 K
DE	6.50 usec
D1	0.85000002 sec
D11	0.03000000 sec
TD0	1
==== CHANNEL f1 =====	
NUC1	13C
P1	9.00 usec
PL1	0.00 dB
PL1W	115.29558563 W
SFO1	125.7697360 MHz
==== CHANNEL f2 ====	
CPDPRG2	waltz16
NUC2	1H
PCPD2	75.00 usec
PL2	120.00 dB
PL12	17.00 dB
PL13	20.00 dB
PL2W	0.00000000 W
PL12W	0.40445811 W
PL13W	0.20270923 W
SFO2	500.1320005 MHz
SI	32768
HZpPT	0.770646 Hz
SR	0.63 Hz
WDW	EM
LB	1.00 Hz
GB	0
SSB	0

Figure S32. ^{19}F NMR spectrum of compound **5k**

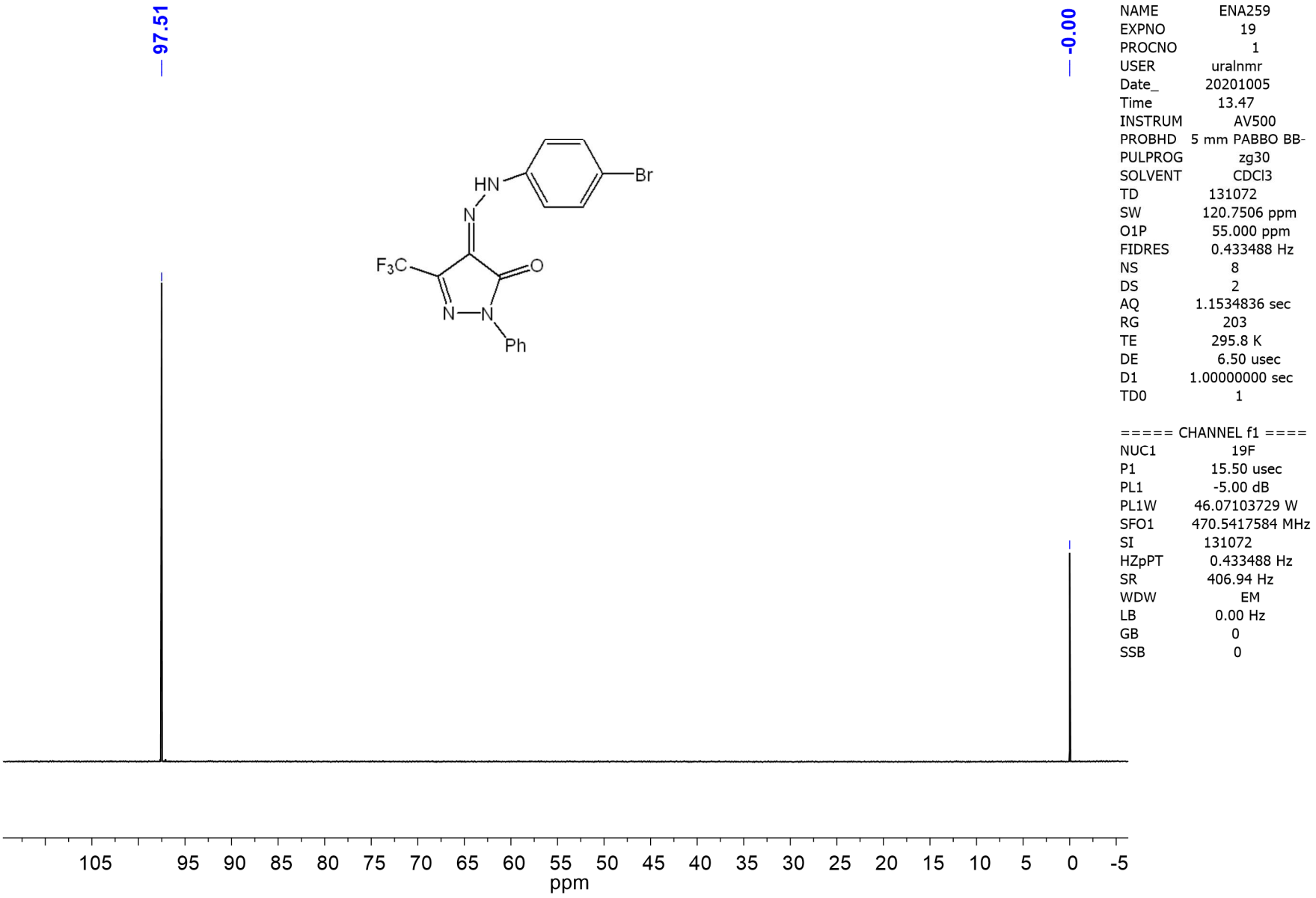


Figure S33. ^{1}H NMR spectrum of compound **51**

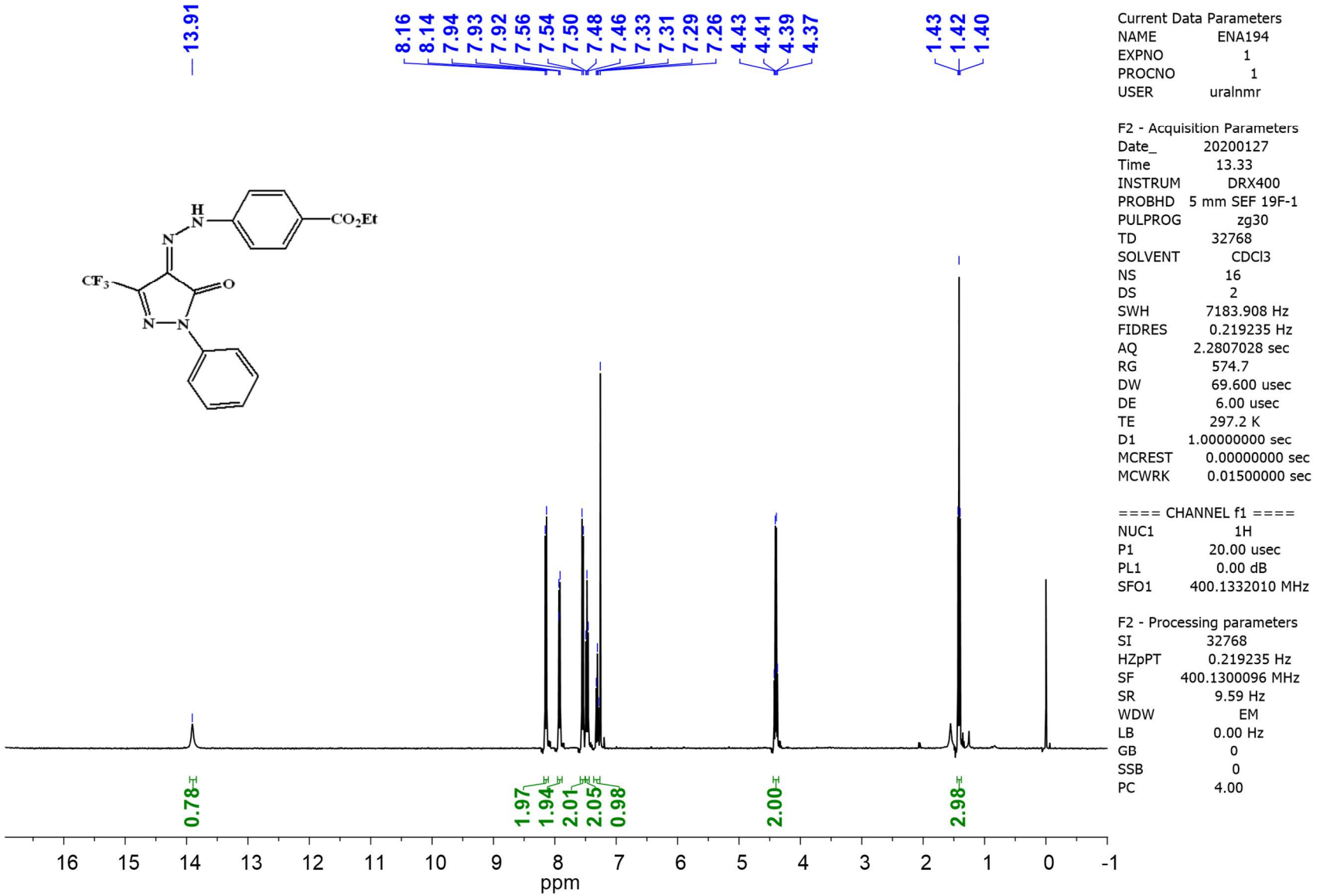


Figure S34. ^{13}C NMR spectrum of compound **5l**

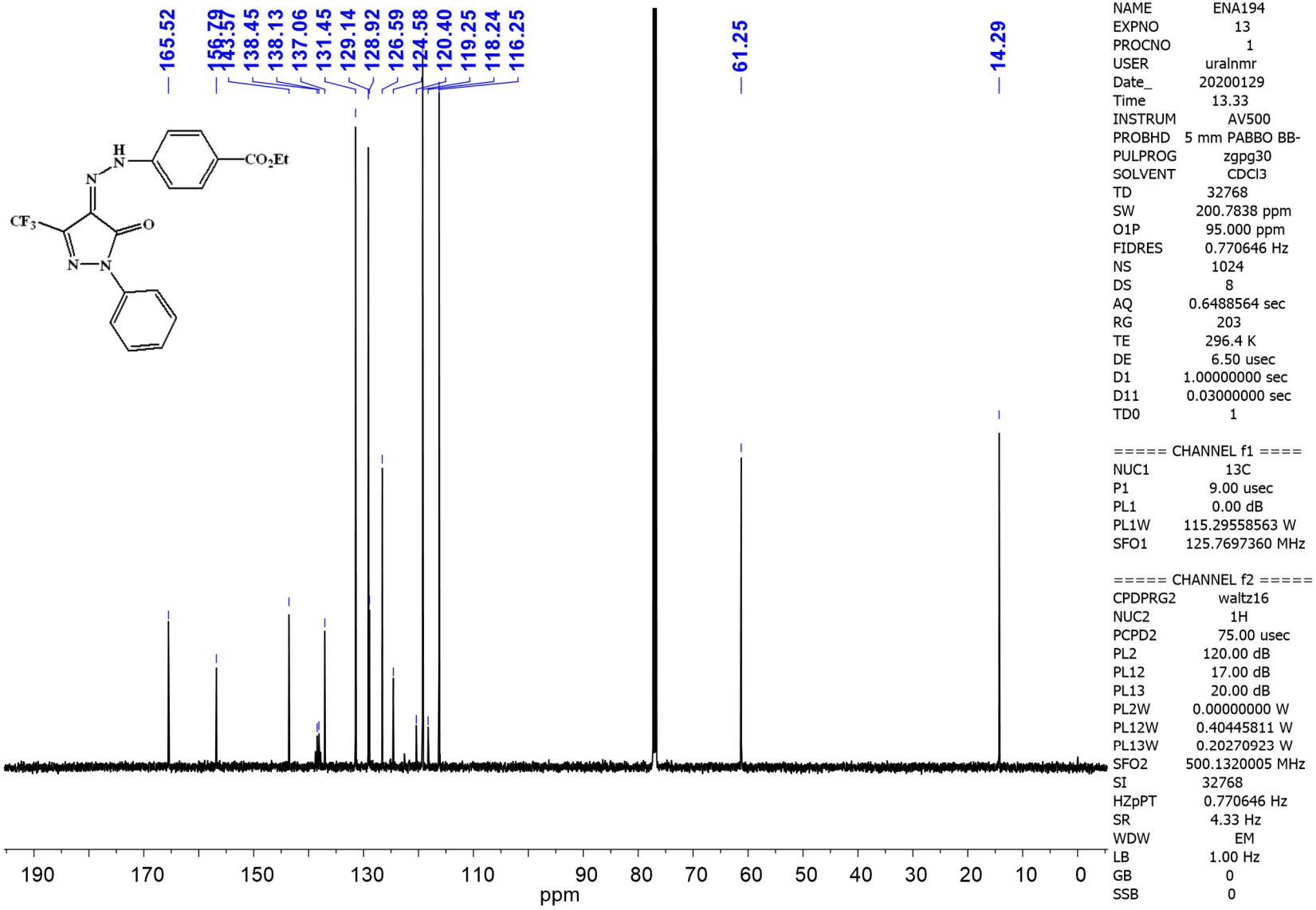
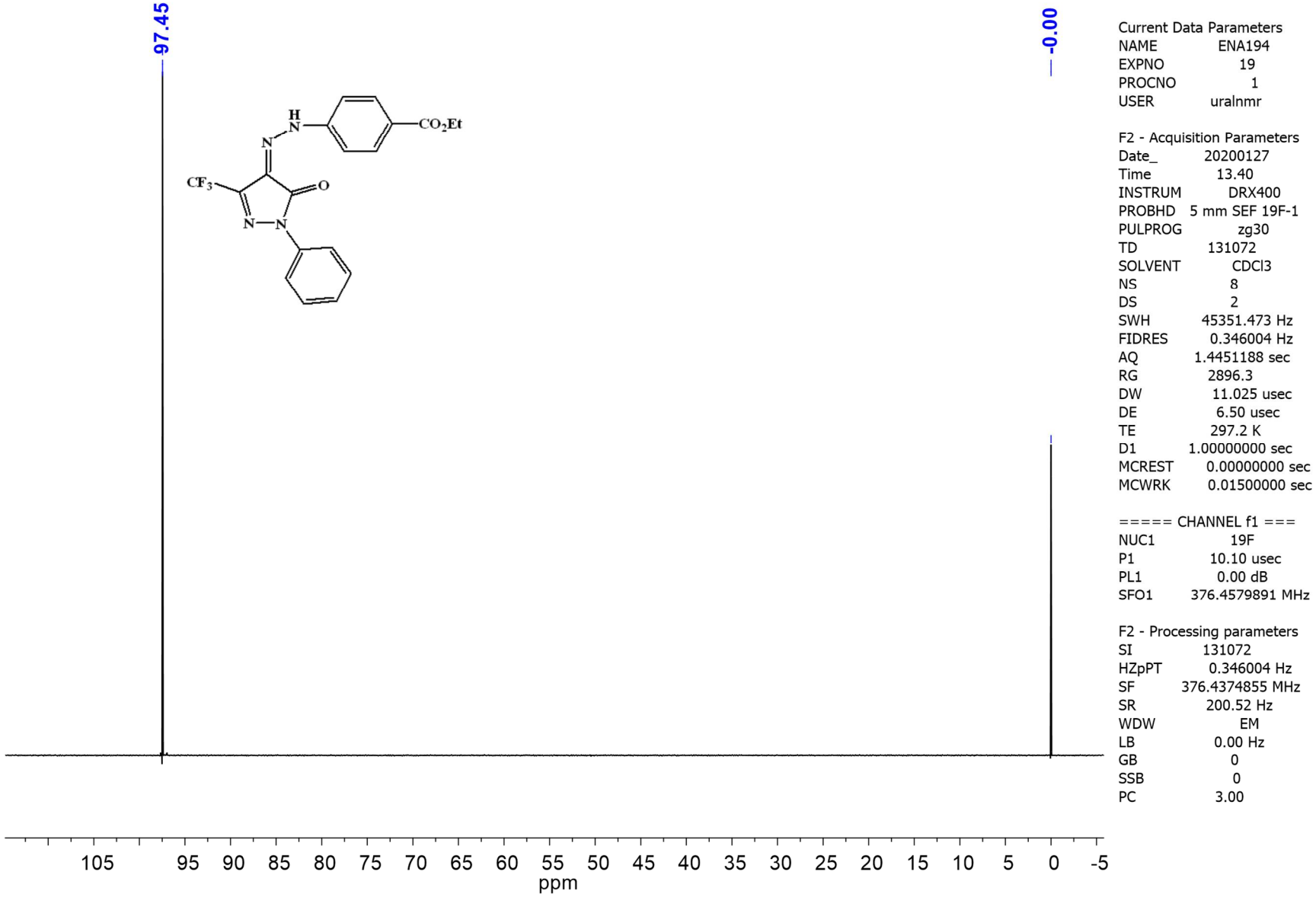


Figure S35. ^{19}F NMR spectrum of compound **5l**



Current Data Parameters
NAME ENA194
EXPNO 19
PROCNO 1
USER uralnmr

F2 - Acquisition Parameters
Date_ 20200127
Time 13.40
INSTRUM DRX400
PROBHD 5 mm SEF 19F-1
PULPROG zg30
TD 131072
SOLVENT CDCl3
NS 8
DS 2
SWH 45351.473 Hz
FIDRES 0.346004 Hz
AQ 1.4451188 sec
RG 2896.3
DW 11.025 usec
DE 6.50 usec
TE 297.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 ===
NUC1 19F
P1 10.10 usec
PL1 0.00 dB
SFO1 376.4579891 MHz

F2 - Processing parameters
SI 131072
HZpPT 0.346004 Hz
SF 376.4374855 MHz
SR 200.52 Hz
WDW EM
LB 0.00 Hz
GB 0
SSB 0
PC 3.00

Figure S36. ^{1}H NMR spectrum of compound **5m**

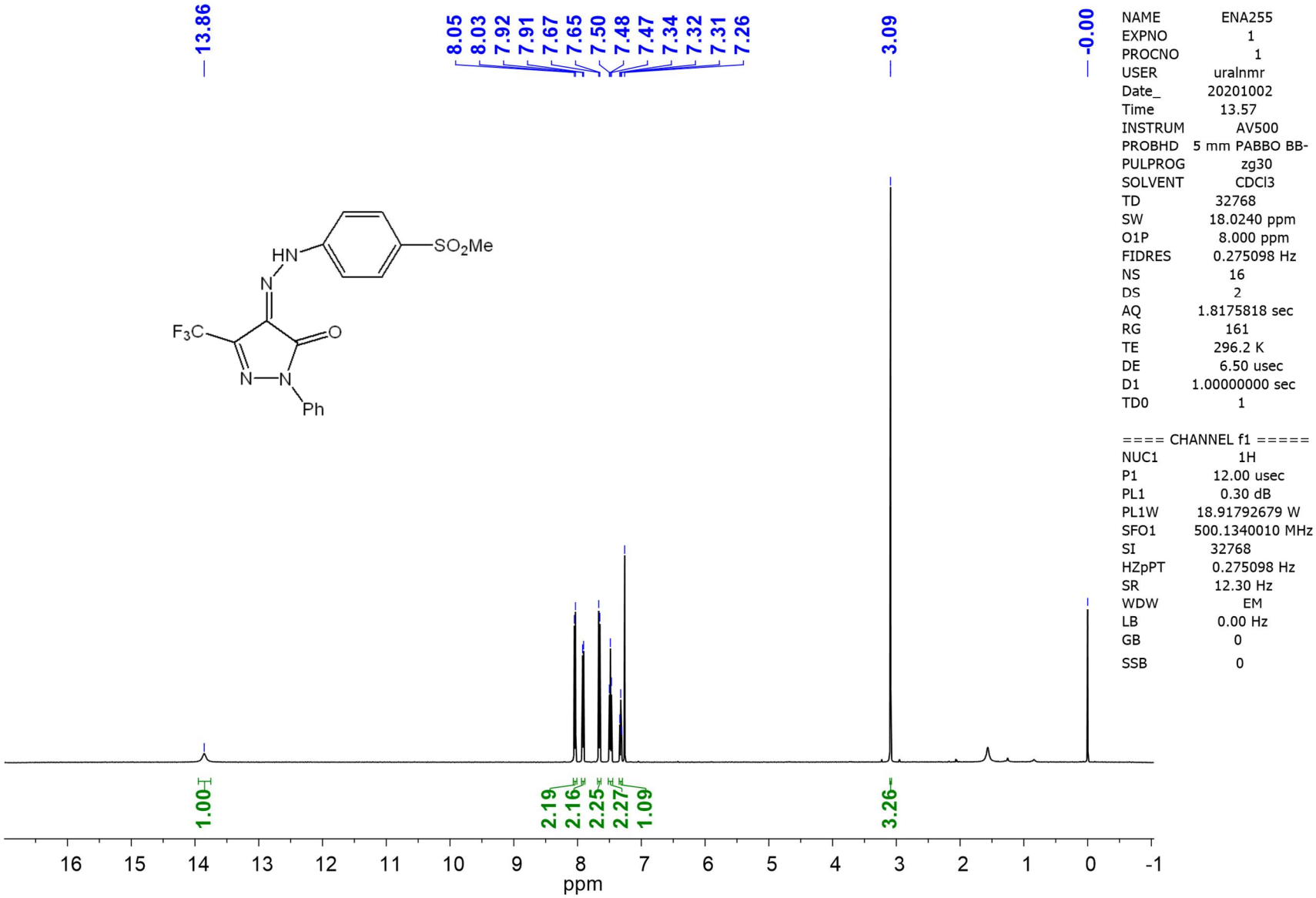
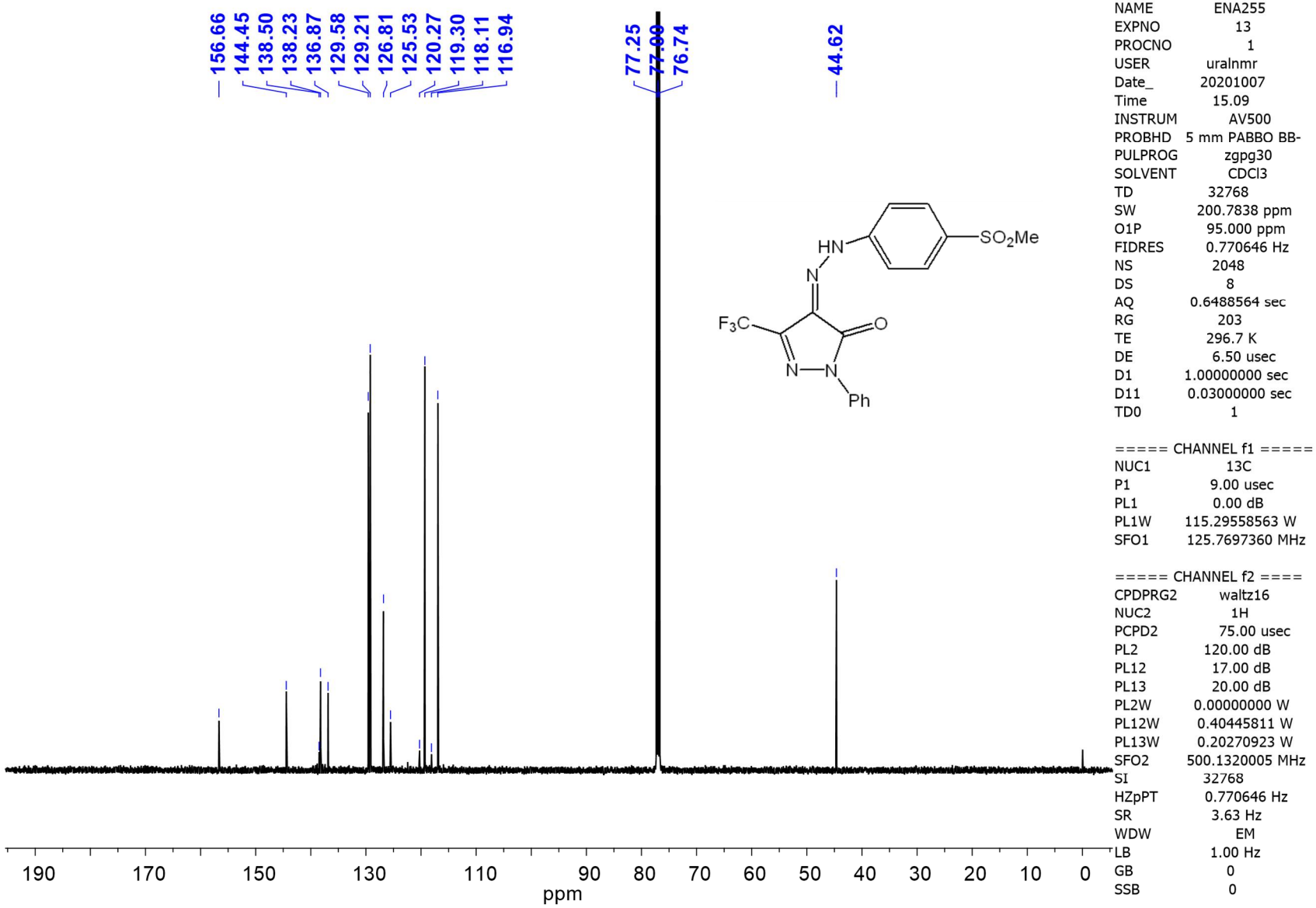
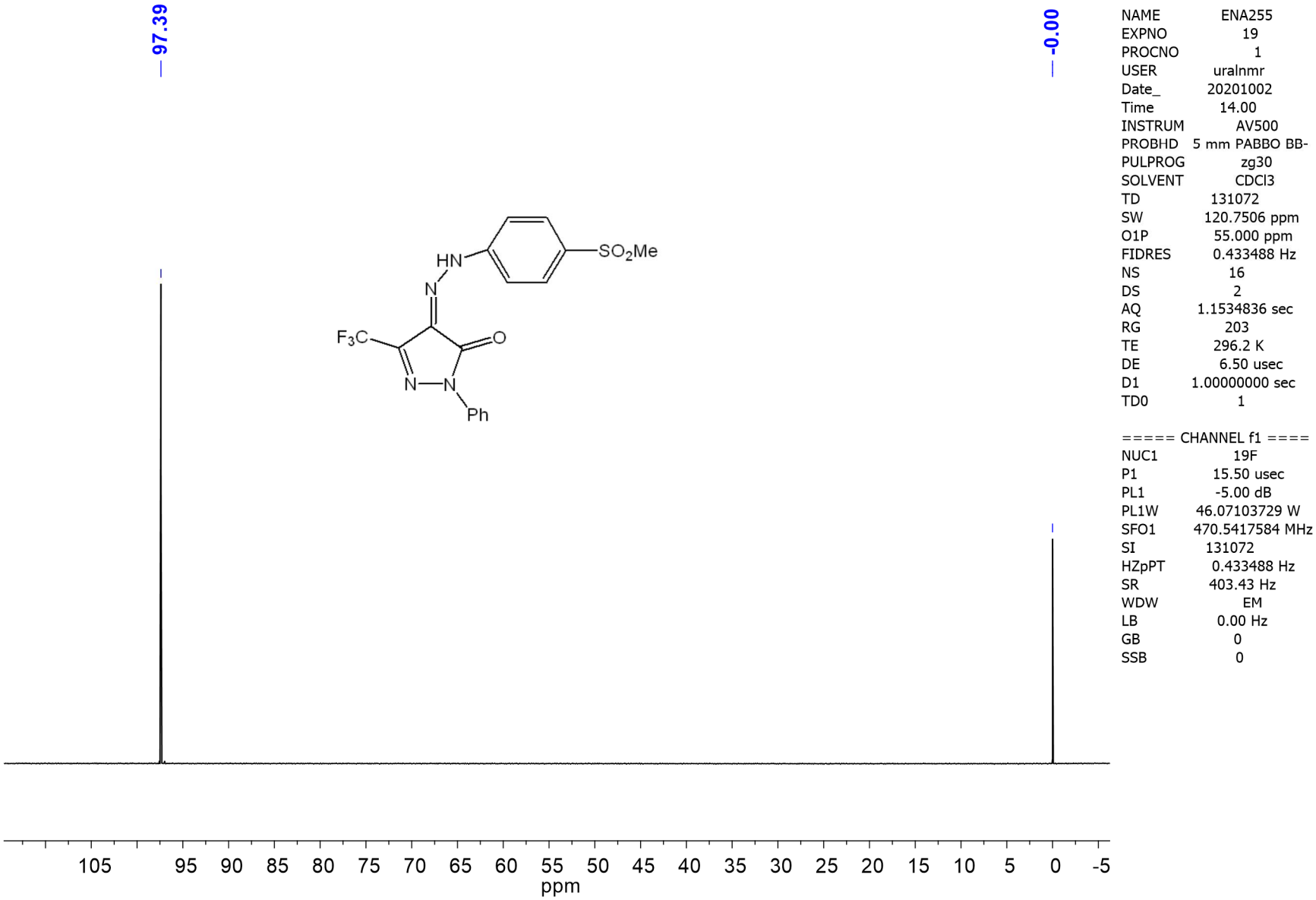


Figure S37. ^{13}C NMR spectrum of compound **5m**



NAME	ENA255
EXPNO	13
PROCNO	1
USER	uralnmr
Date_	20201007
Time	15.09
INSTRUM	AV500
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
SOLVENT	CDCl3
TD	32768
SW	200.7838 ppm
O1P	95.000 ppm
FIDRES	0.770646 Hz
NS	2048
DS	8
AQ	0.6488564 sec
RG	203
TE	296.7 K
DE	6.50 usec
D1	1.00000000 sec
D11	0.03000000 sec
TD0	1
===== CHANNEL f1 =====	
NUC1	13C
P1	9.00 usec
PL1	0.00 dB
PL1W	115.29558563 W
SFO1	125.7697360 MHz
===== CHANNEL f2 ====	
CPDPRG2	waltz16
NUC2	1H
PCPD2	75.00 usec
PL2	120.00 dB
PL12	17.00 dB
PL13	20.00 dB
PL2W	0.00000000 W
PL12W	0.40445811 W
PL13W	0.20270923 W
SFO2	500.1320005 MHz
SI	32768
HZpPT	0.770646 Hz
SR	3.63 Hz
WDW	EM
LB	1.00 Hz
GB	0
SSB	0

Figure S38. ^{19}F NMR spectrum of compound **5m**



NAME	ENA255
EXPNO	19
PROCNO	1
USER	uralnmr
Date_	20201002
Time	14.00
INSTRUM	AV500
PROBHD	5 mm PABBO BB-
PULPROG	zg30
SOLVENT	CDCl3
TD	131072
SW	120.7506 ppm
O1P	55.000 ppm
FIDRES	0.433488 Hz
NS	16
DS	2
AQ	1.1534836 sec
RG	203
TE	296.2 K
DE	6.50 usec
D1	1.00000000 sec
TD0	1
===== CHANNEL f1 ====	
NUC1	19F
P1	15.50 usec
PL1	-5.00 dB
PL1W	46.07103729 W
SFO1	470.5417584 MHz
SI	131072
HZpPT	0.433488 Hz
SR	403.43 Hz
WDW	EM
LB	0.00 Hz
GB	0
SSB	0

Figure S39. ^{1}H NMR spectrum of compound **5n**

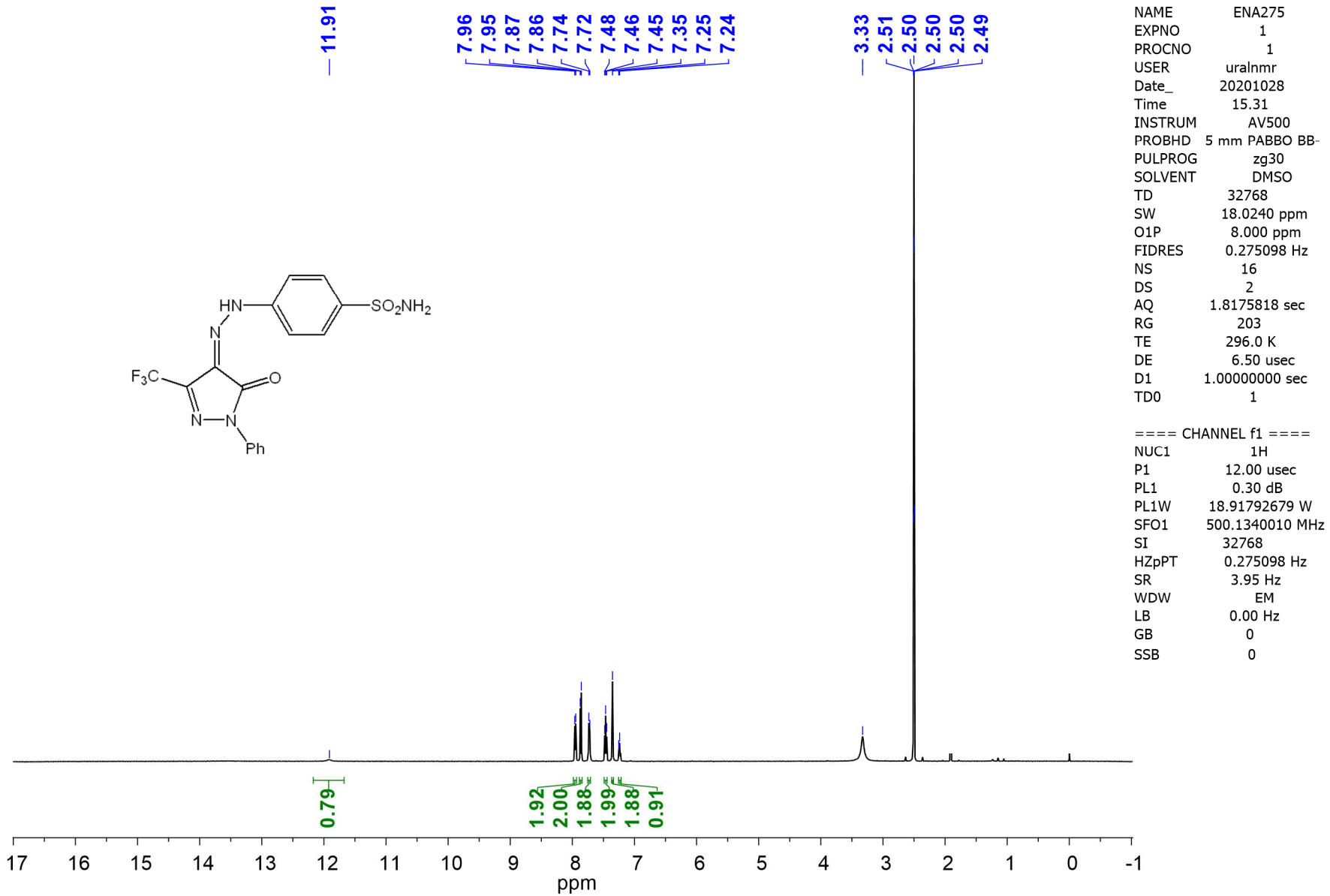


Figure S40. ^{13}C NMR spectrum of compound **5n**

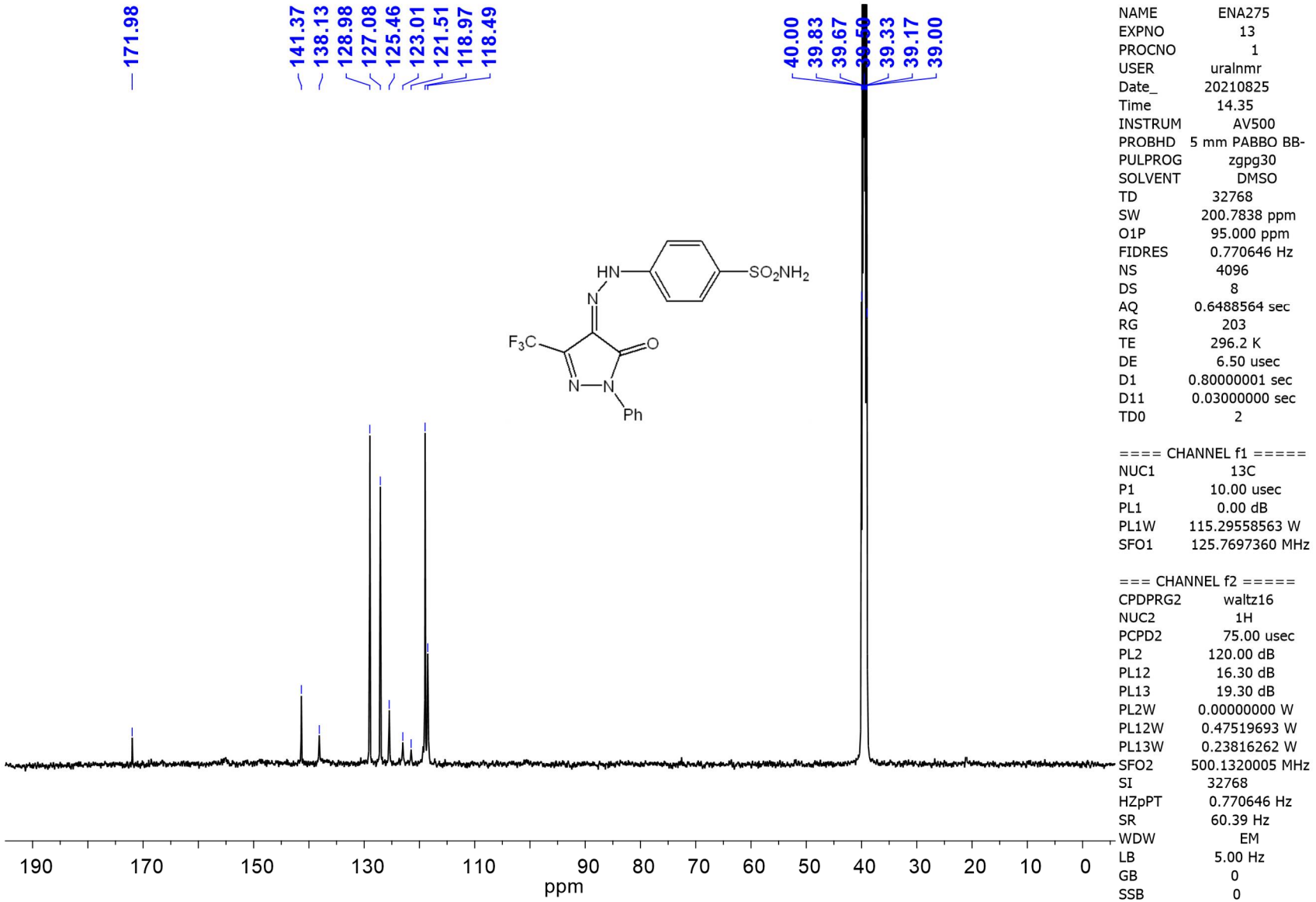


Figure S41. ^{19}F NMR spectrum of compound **5n**

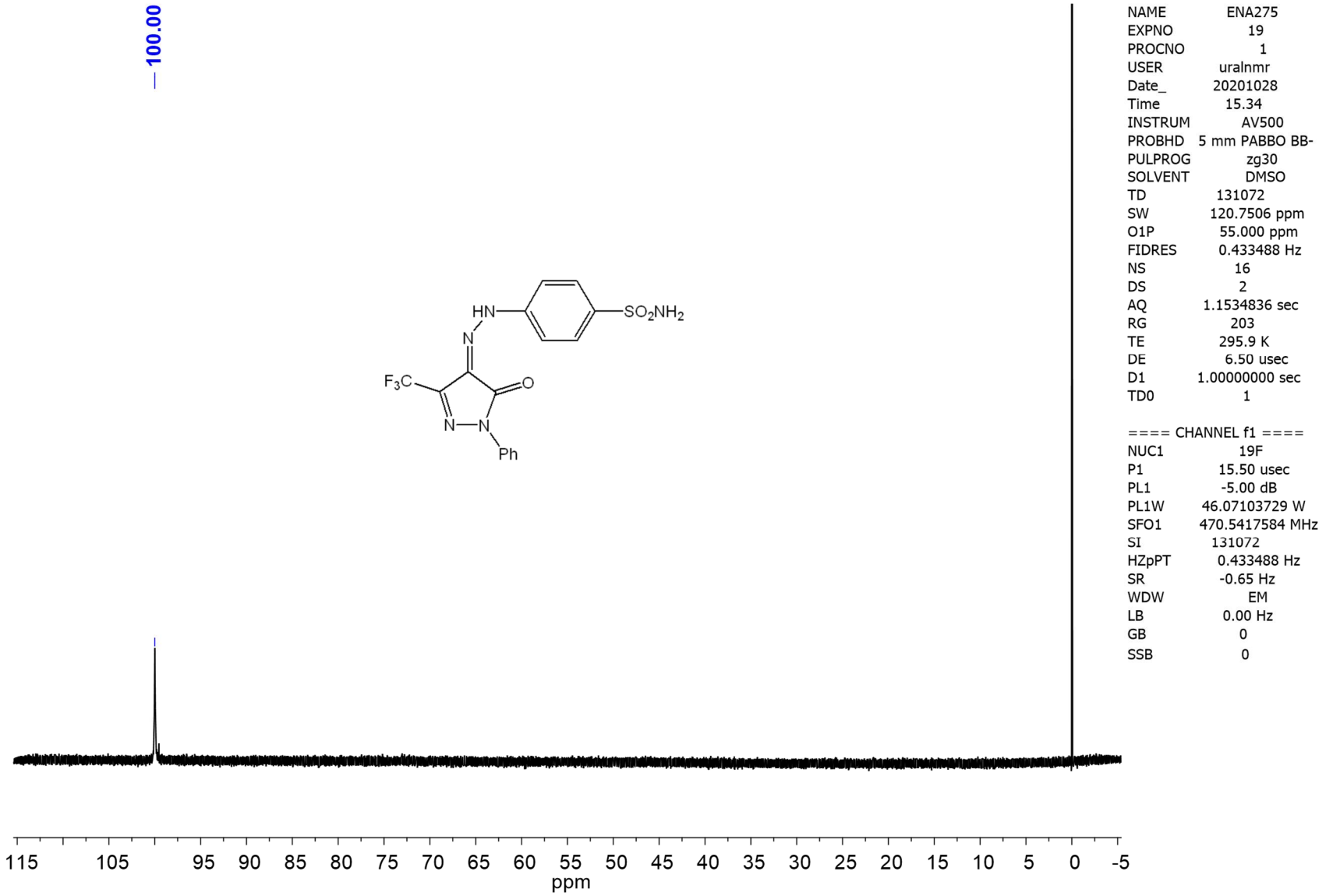


Figure S42. ^{1}H NMR spectrum of compound **5o**

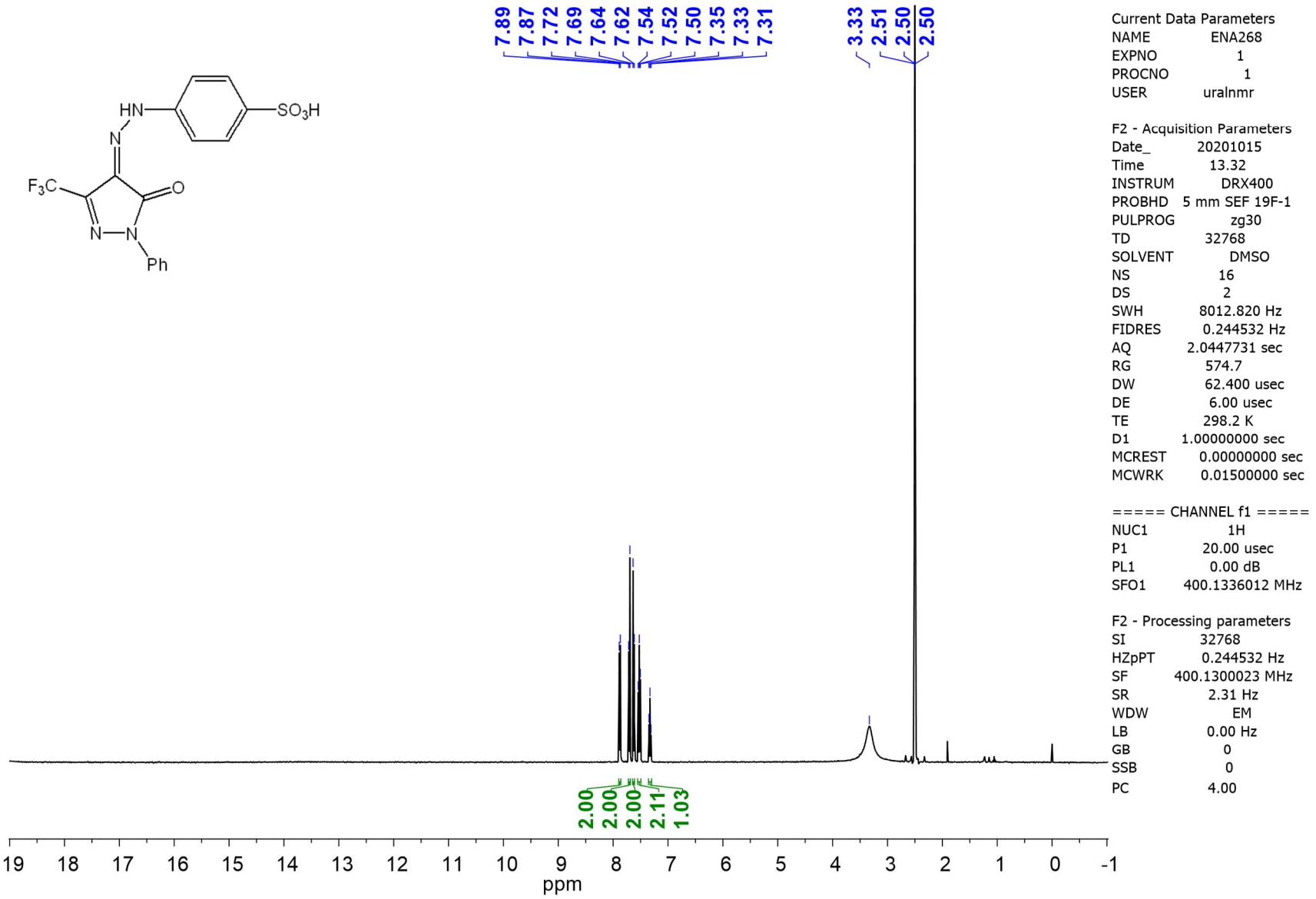
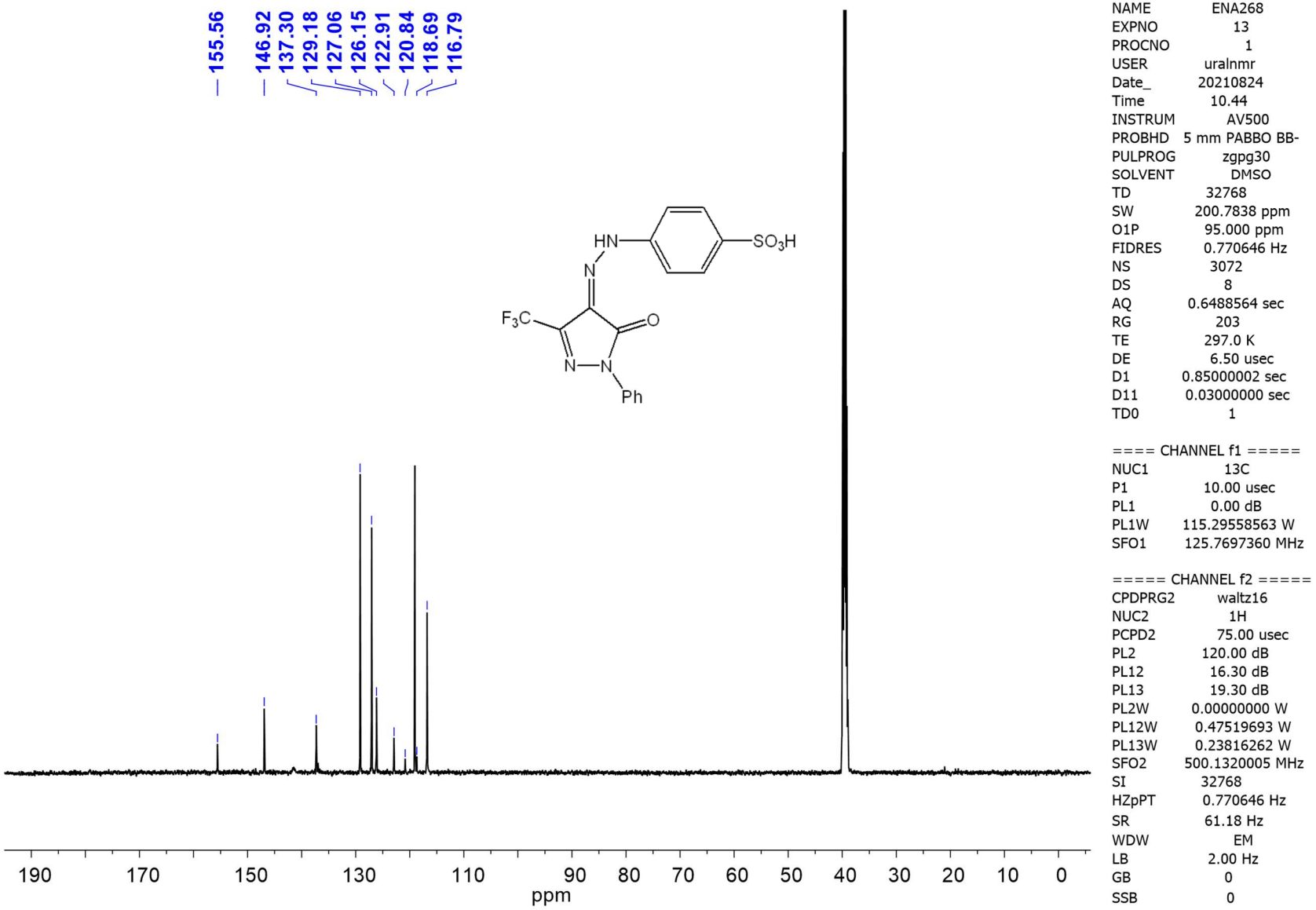


Figure S43. ^{13}C NMR spectrum of compound **5o**



NAME	ENA268
EXPNO	13
PROCNO	1
USER	uralnmr
Date_	20210824
Time	10.44
INSTRUM	AV500
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
SOLVENT	DMSO
TD	32768
SW	200.7838 ppm
O1P	95.000 ppm
FIDRES	0.770646 Hz
NS	3072
DS	8
AQ	0.6488564 sec
RG	203
TE	297.0 K
DE	6.50 usec
D1	0.85000002 sec
D11	0.03000000 sec
TD0	1
==== CHANNEL f1 =====	
NUC1	13C
P1	10.00 usec
PL1	0.00 dB
PL1W	115.29558563 W
SFO1	125.7697360 MHz
===== CHANNEL f2 =====	
CPDPRG2	waltz16
NUC2	1H
PCPD2	75.00 usec
PL2	120.00 dB
PL12	16.30 dB
PL13	19.30 dB
PL2W	0.00000000 W
PL12W	0.47519693 W
PL13W	0.23816262 W
SFO2	500.1320005 MHz
SI	32768
HZpPT	0.770646 Hz
SR	61.18 Hz
WDW	EM
LB	2.00 Hz
GB	0
SSB	0

Figure S44. ^{19}F NMR spectrum of compound **5o**

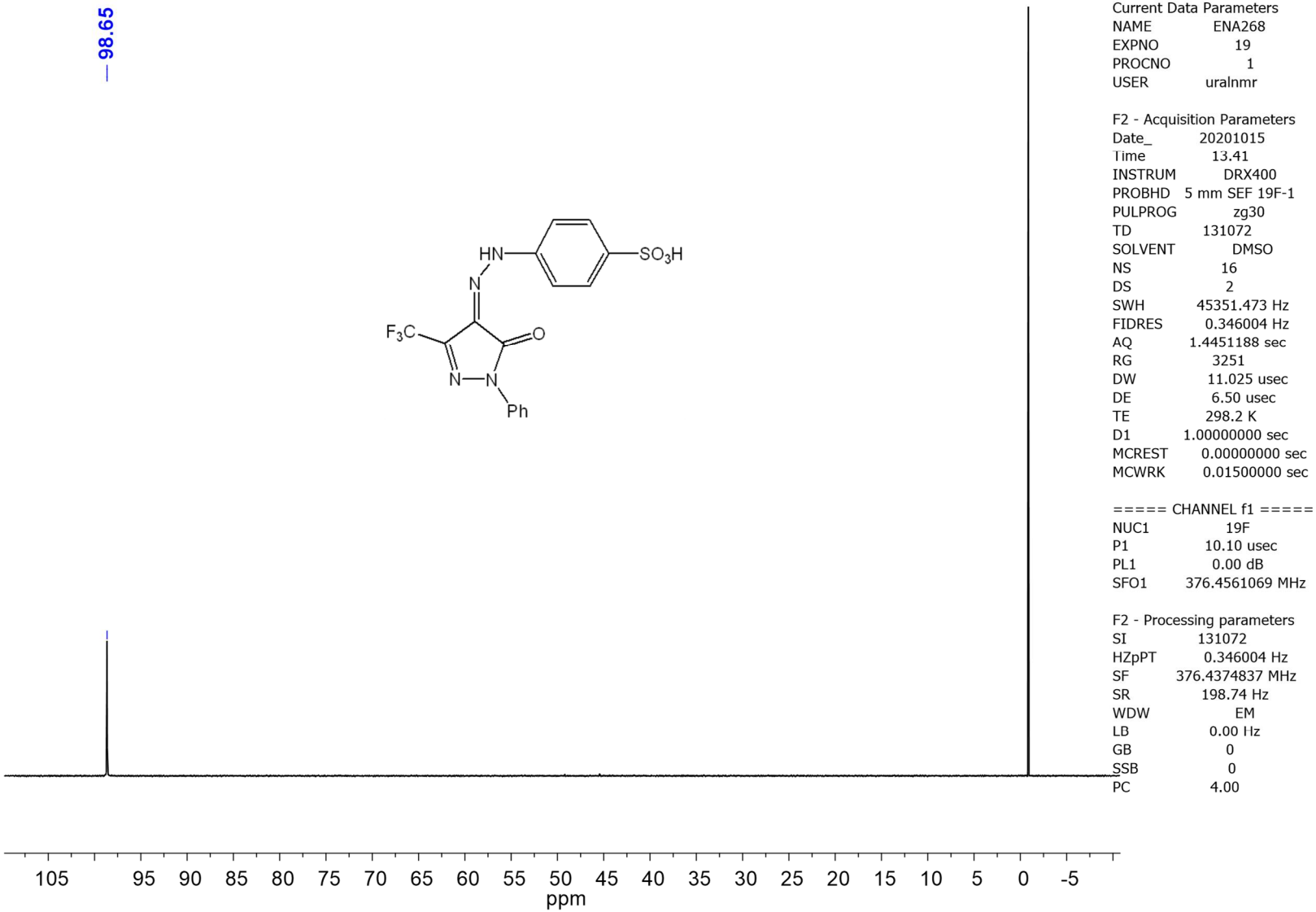


Figure S45. ^{1}H NMR spectrum of compound **5p**

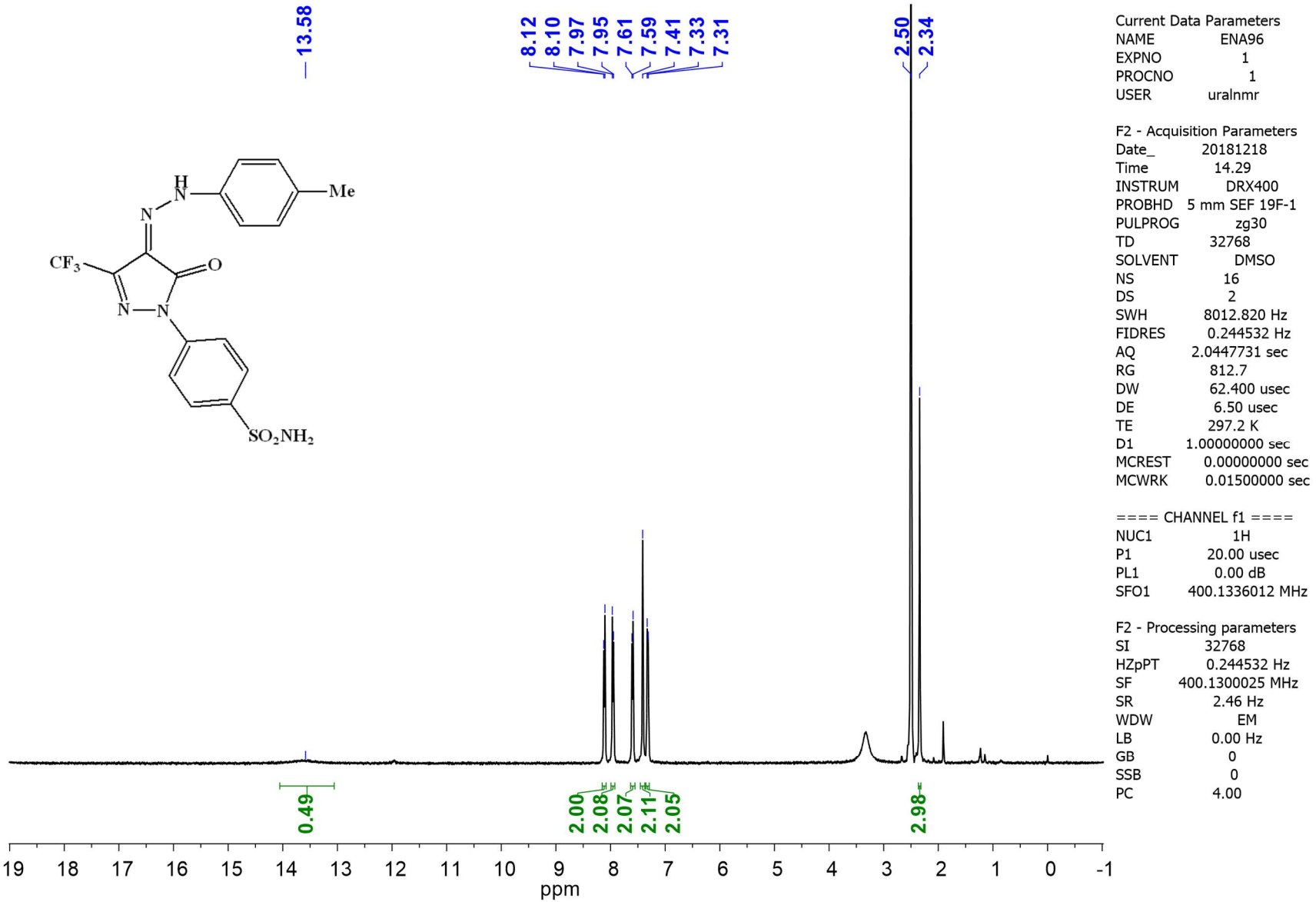
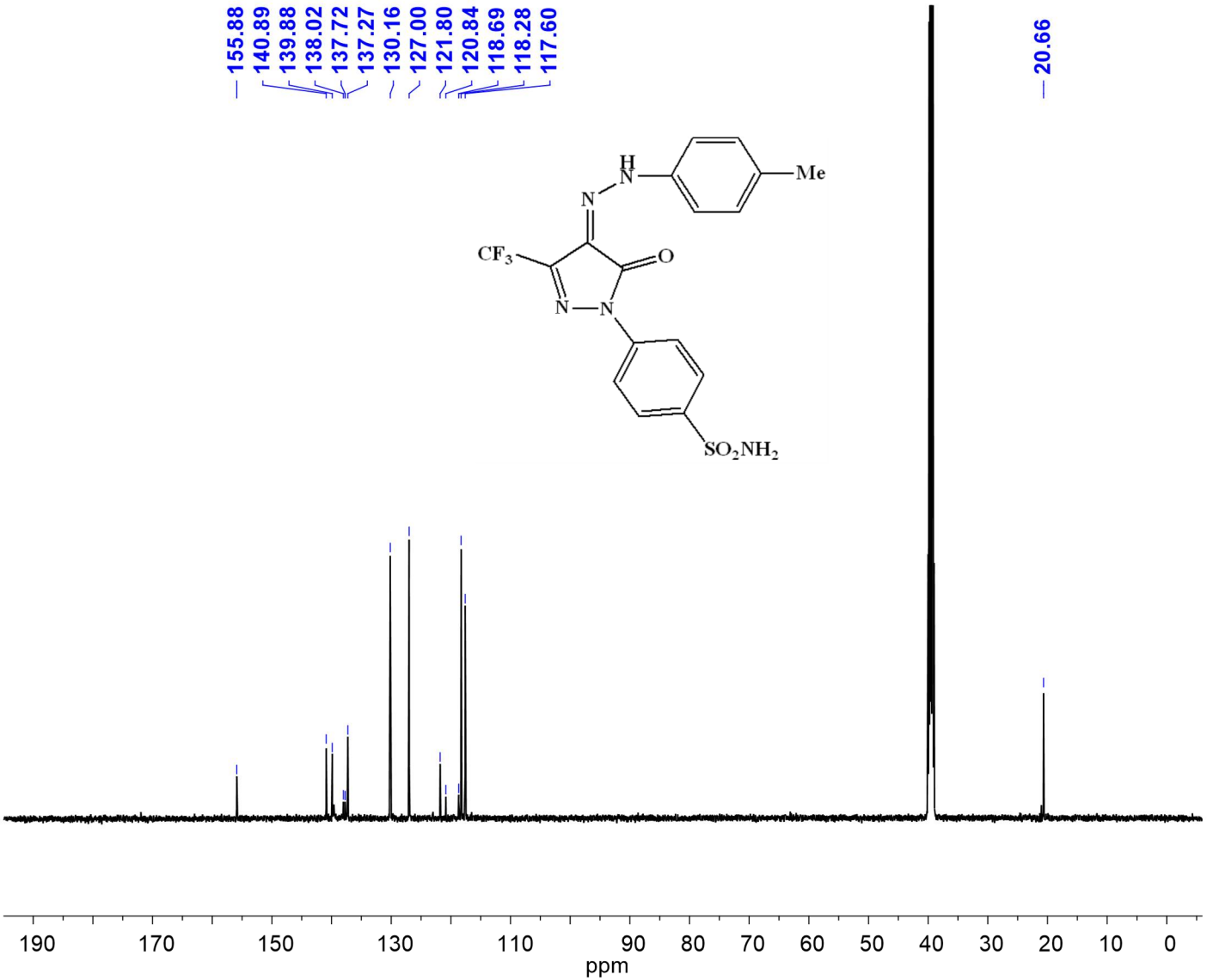
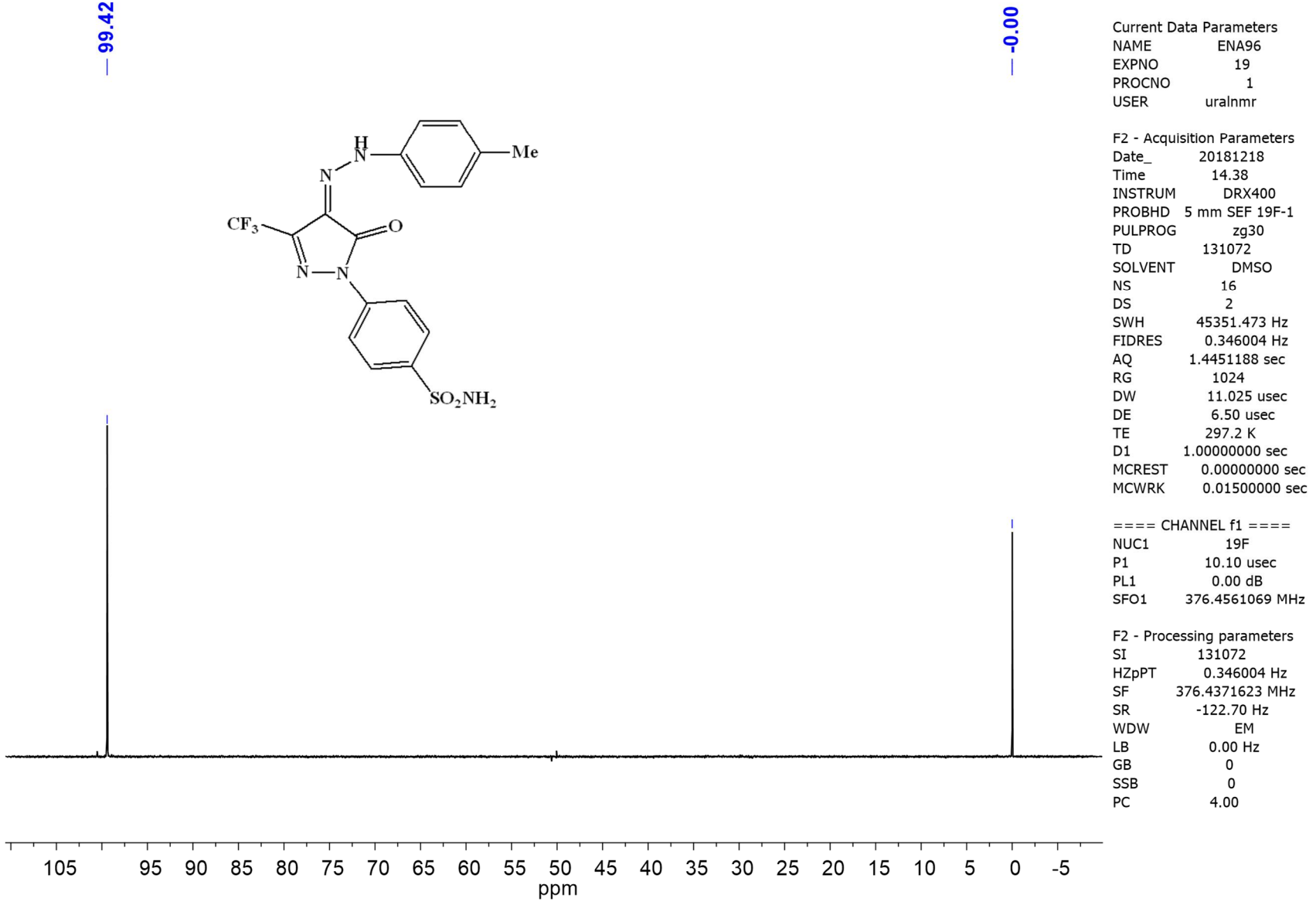


Figure S46. ^{13}C NMR spectrum of compound **5p**



NAME	ENA96
EXPNO	13
PROCNO	1
USER	uralnmr
Date_	20190516
Time	15.18
INSTRUM	AV500
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
SOLVENT	DMSO
TD	32768
SW	200.7838 ppm
O1P	95.000 ppm
FIDRES	0.770646 Hz
NS	3072
DS	8
AQ	0.6488564 sec
RG	203
TE	297.7 K
DE	6.50 usec
D1	0.80000001 sec
D11	0.03000000 sec
TD0	1
=== CHANNEL f1 =====	
NUC1	13C
P1	10.00 usec
PL1	0.00 dB
PL1W	115.29558563 W
SFO1	125.7697360 MHz
===== CHANNEL f2 =====	
CPDPRG2	waltz16
NUC2	1H
PCPD2	75.00 usec
PL2	120.00 dB
PL12	16.30 dB
PL13	19.30 dB
PL2W	0.00000000 W
PL12W	0.47519693 W
PL13W	0.23816262 W
SFO2	500.1320005 MHz
SI	32768
HZpPT	0.770646 Hz
SR	61.84 Hz
WDW	EM
LB	1.00 Hz
GB	0
SSB	0

Figure S47. ^{19}F NMR spectrum of compound **5p**



Current Data Parameters
NAME ENA96
EXPNO 19
PROCNO 1
USER uralnmr

F2 - Acquisition Parameters
Date_ 20181218
Time 14.38
INSTRUM DRX400
PROBHD 5 mm SEF 19F-1
PULPROG zg30
TD 131072
SOLVENT DMSO
NS 16
DS 2
SWH 45351.473 Hz
FIDRES 0.346004 Hz
AQ 1.4451188 sec
RG 1024
DW 11.025 usec
DE 6.50 usec
TE 297.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

==== CHANNEL f1 ====
NUC1 19F
P1 10.10 usec
PL1 0.00 dB
SFO1 376.4561069 MHz

F2 - Processing parameters
SI 131072
HZpPT 0.346004 Hz
SF 376.4371623 MHz
SR -122.70 Hz
WDW EM
LB 0.00 Hz
GB 0
SSB 0
PC 4.00

Figure S48. ^{1}H NMR spectrum of compound **5q**

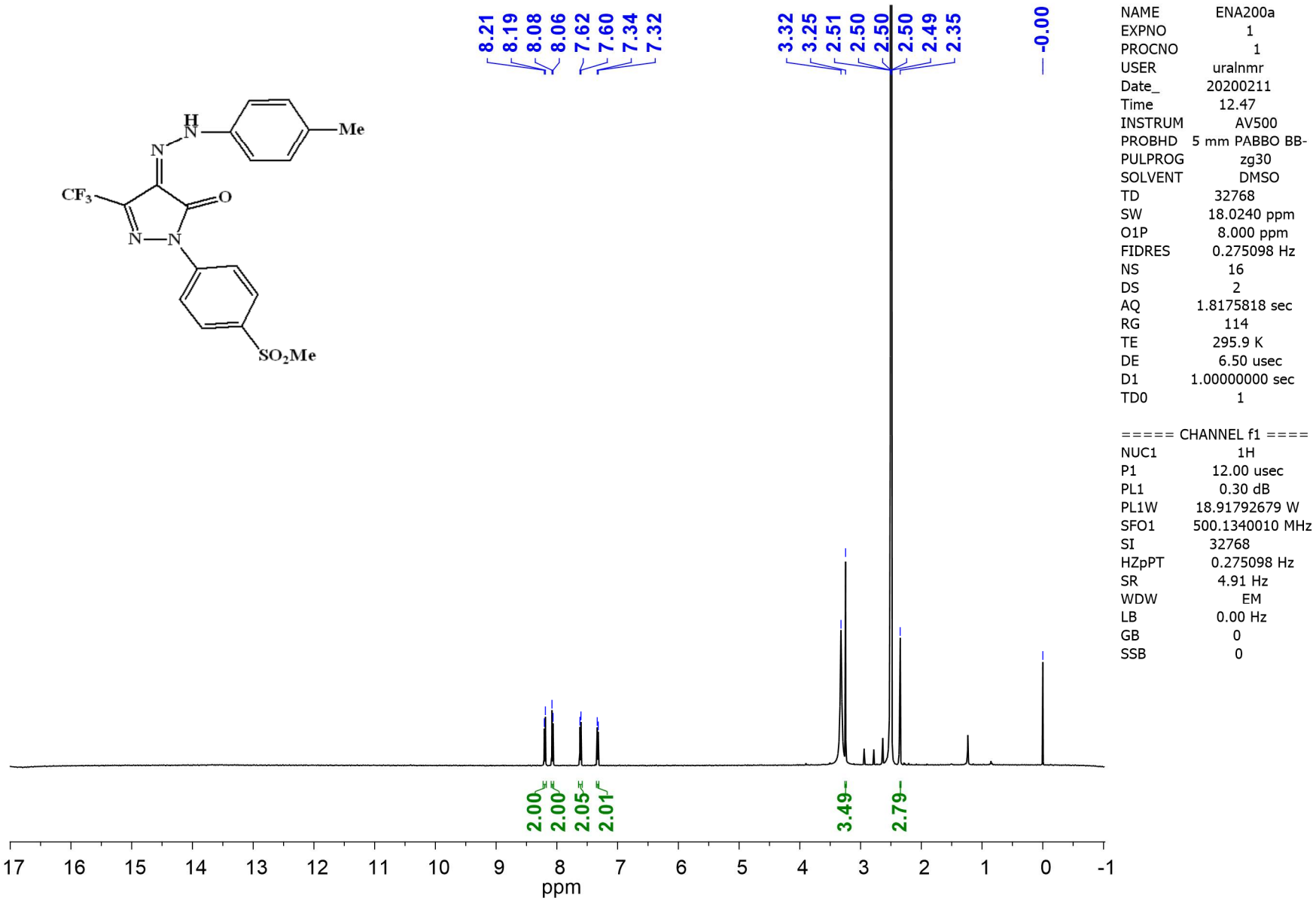


Figure S49. ^{19}F NMR spectrum of compound **5q**

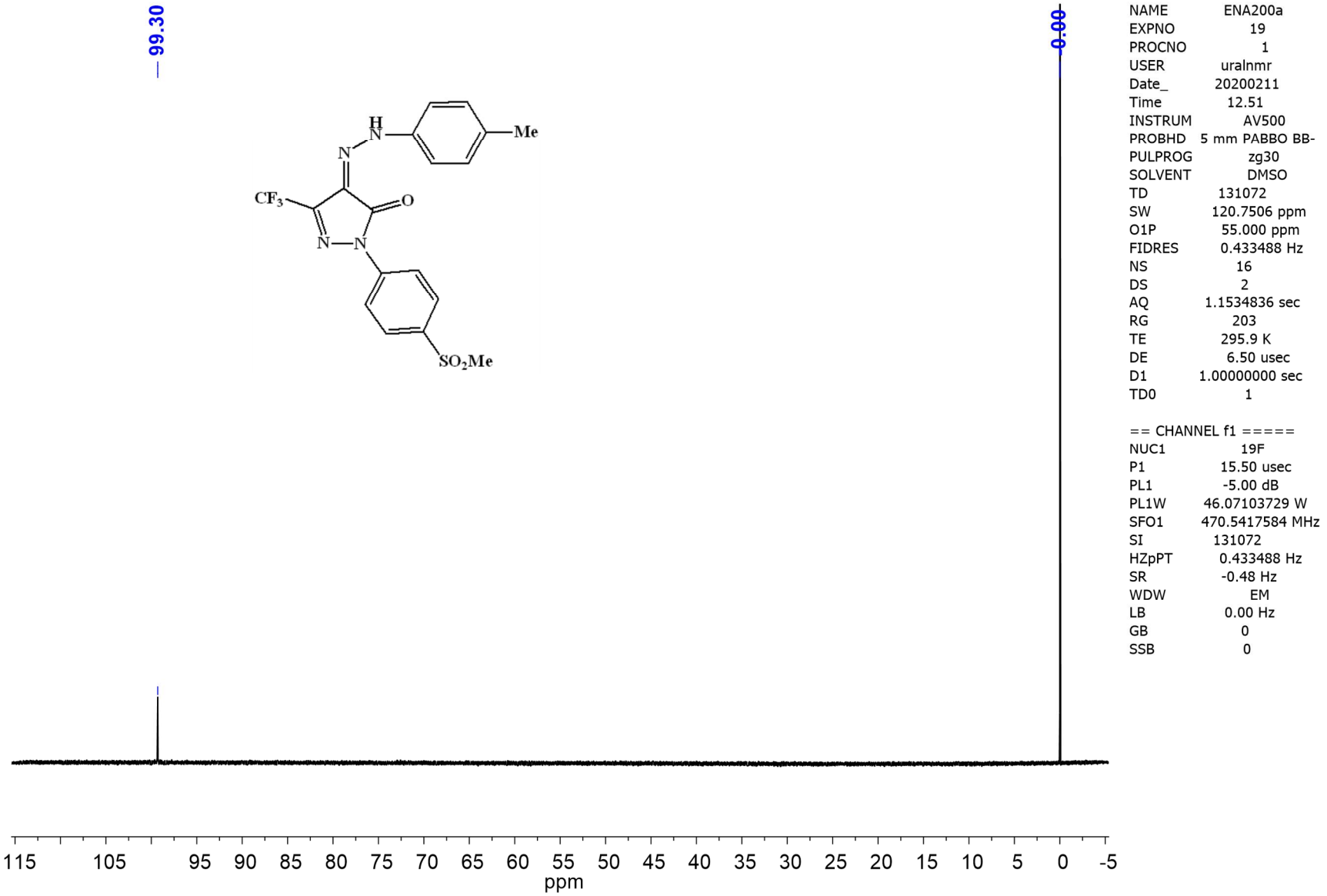


Figure S50. ^{1}H NMR spectrum of compound **5r**

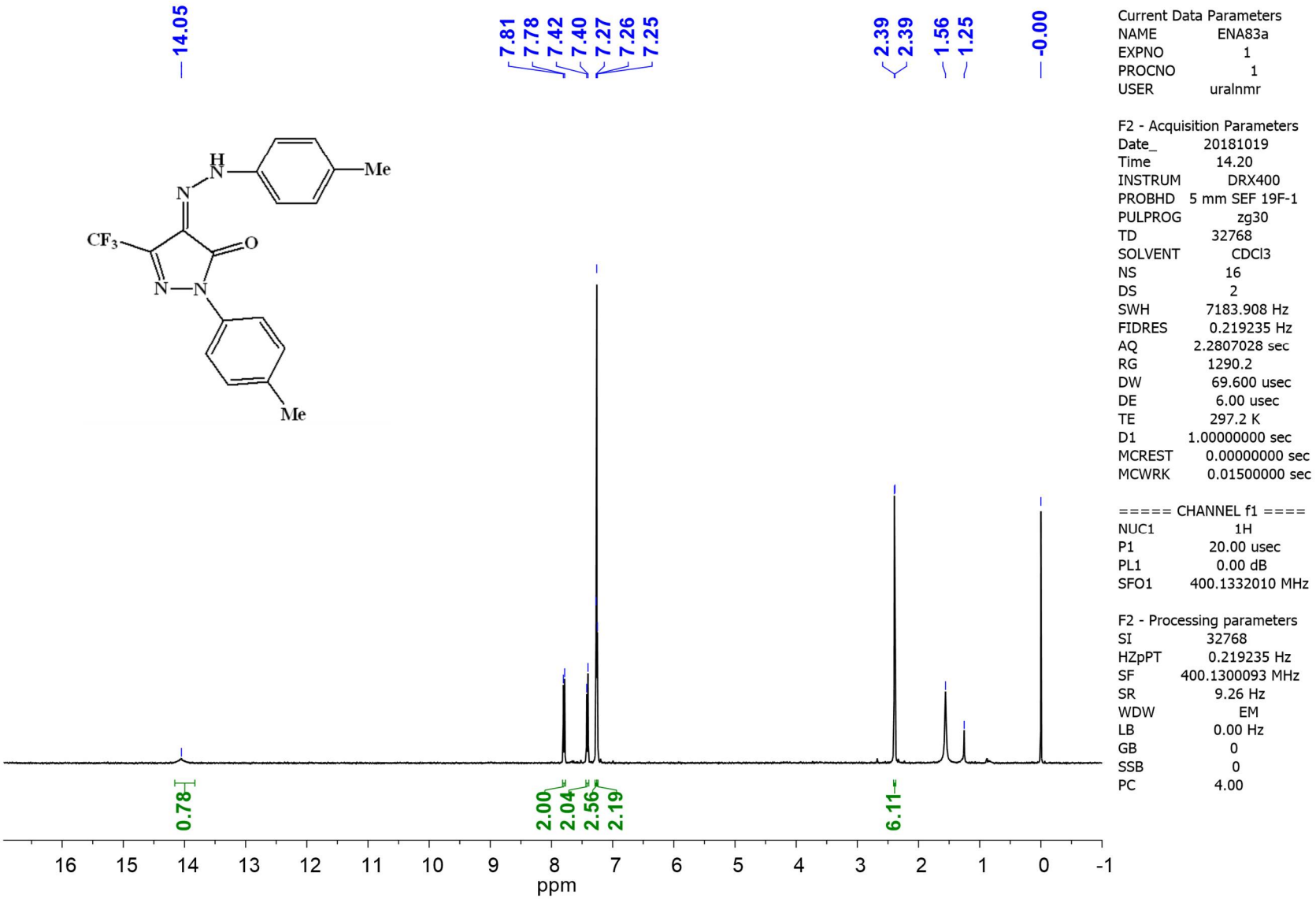
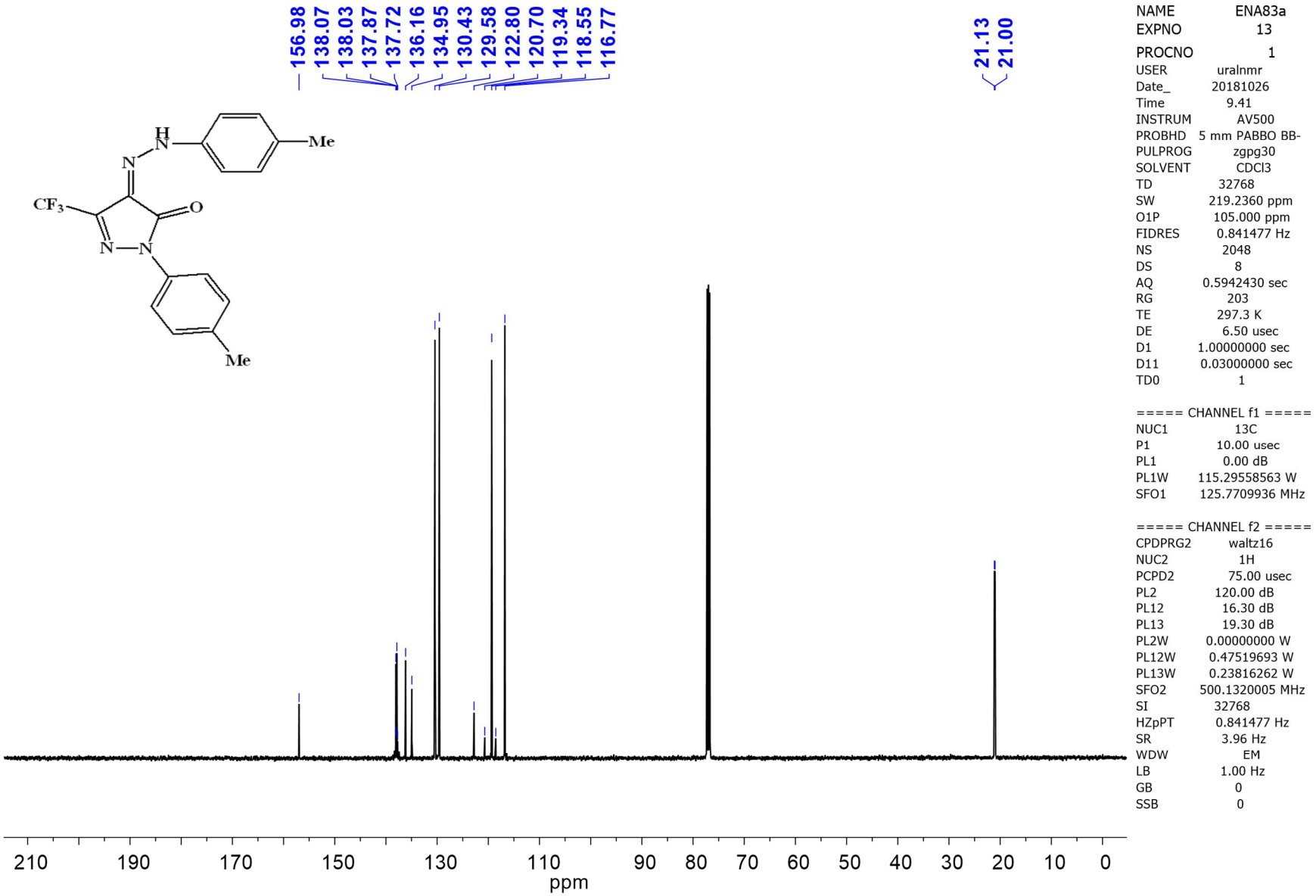
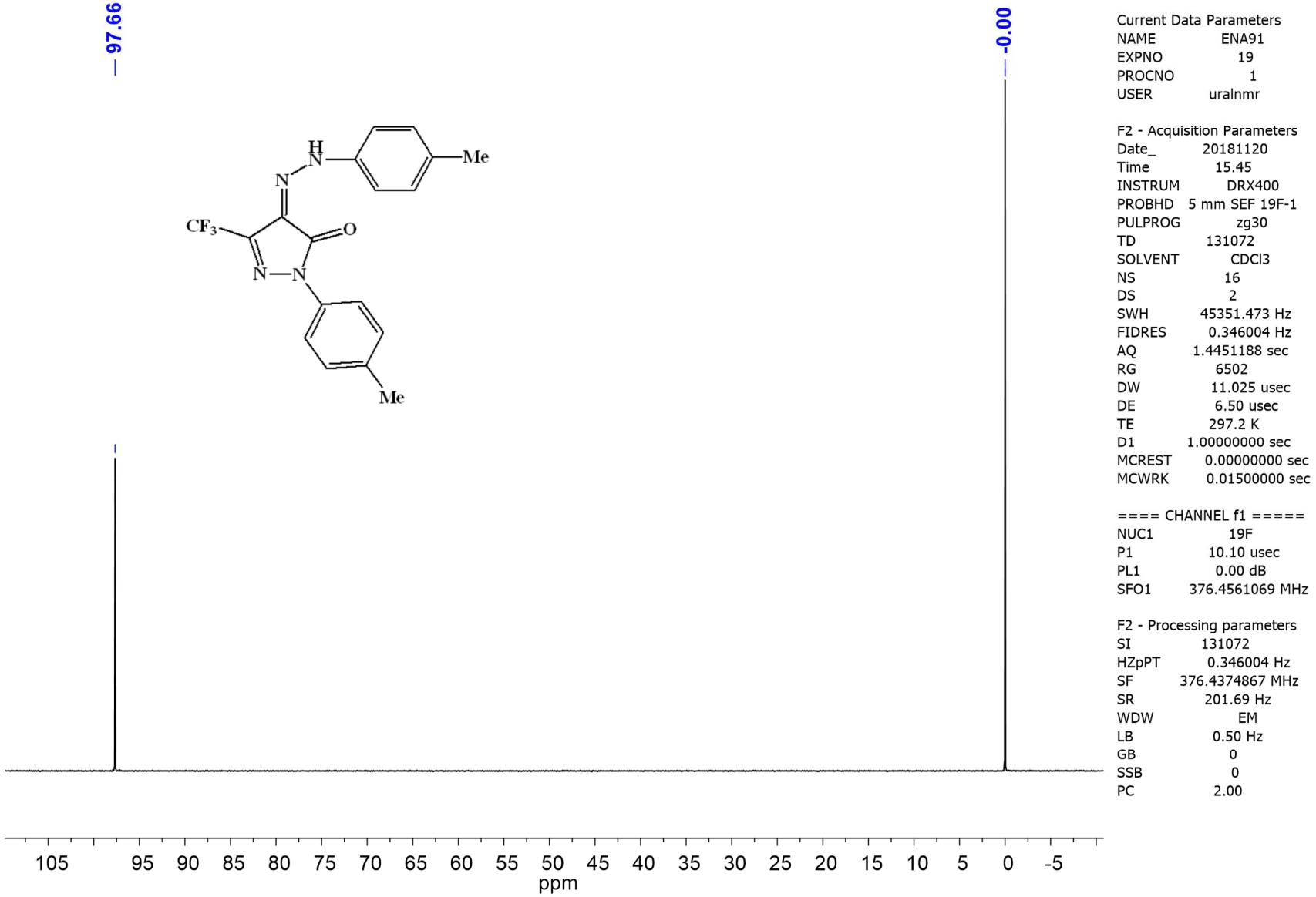


Figure S51. ^{13}C NMR spectrum of compound **5r**



NAME	ENA83a
EXPNO	13
PROCNO	1
USER	uralnmr
Date_	20181026
Time	9.41
INSTRUM	AV500
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
SOLVENT	CDCl3
TD	32768
SW	219.2360 ppm
O1P	105.000 ppm
FIDRES	0.841477 Hz
NS	2048
DS	8
AQ	0.5942430 sec
RG	203
TE	297.3 K
DE	6.50 usec
D1	1.00000000 sec
D11	0.03000000 sec
TD0	1
===== CHANNEL f1 =====	
NUC1	13C
P1	10.00 usec
PL1	0.00 dB
PL1W	115.29558563 W
SFO1	125.7709936 MHz
===== CHANNEL f2 =====	
CPDPRG2	waltz16
NUC2	1H
PCPD2	75.00 usec
PL2	120.00 dB
PL12	16.30 dB
PL13	19.30 dB
PL2W	0.00000000 W
PL12W	0.47519693 W
PL13W	0.23816262 W
SFO2	500.1320005 MHz
SI	32768
HZpPT	0.841477 Hz
SR	3.96 Hz
WDW	EM
LB	1.00 Hz
GB	0
SSB	0

Figure S52. ^{19}F NMR spectrum of compound **5r**



Current Data Parameters
NAME ENA91
EXPNO 19
PROCNO 1
USER uralnmr

F2 - Acquisition Parameters
Date_ 20181120
Time 15.45
INSTRUM DRX400
PROBHD 5 mm SEF 19F-1
PULPROG zg30
TD 131072
SOLVENT CDCl3
NS 16
DS 2
SWH 45351.473 Hz
FIDRES 0.346004 Hz
AQ 1.4451188 sec
RG 6502
DW 11.025 usec
DE 6.50 usec
TE 297.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

==== CHANNEL f1 =====
NUC1 19F
P1 10.10 usec
PL1 0.00 dB
SFO1 376.4561069 MHz

F2 - Processing parameters
SI 131072
HZpPT 0.346004 Hz
SF 376.4374867 MHz
SR 201.69 Hz
WDW EM
LB 0.50 Hz
GB 0
SSB 0
PC 2.00

Figure S53. ^{1}H NMR spectrum of compound **6a**

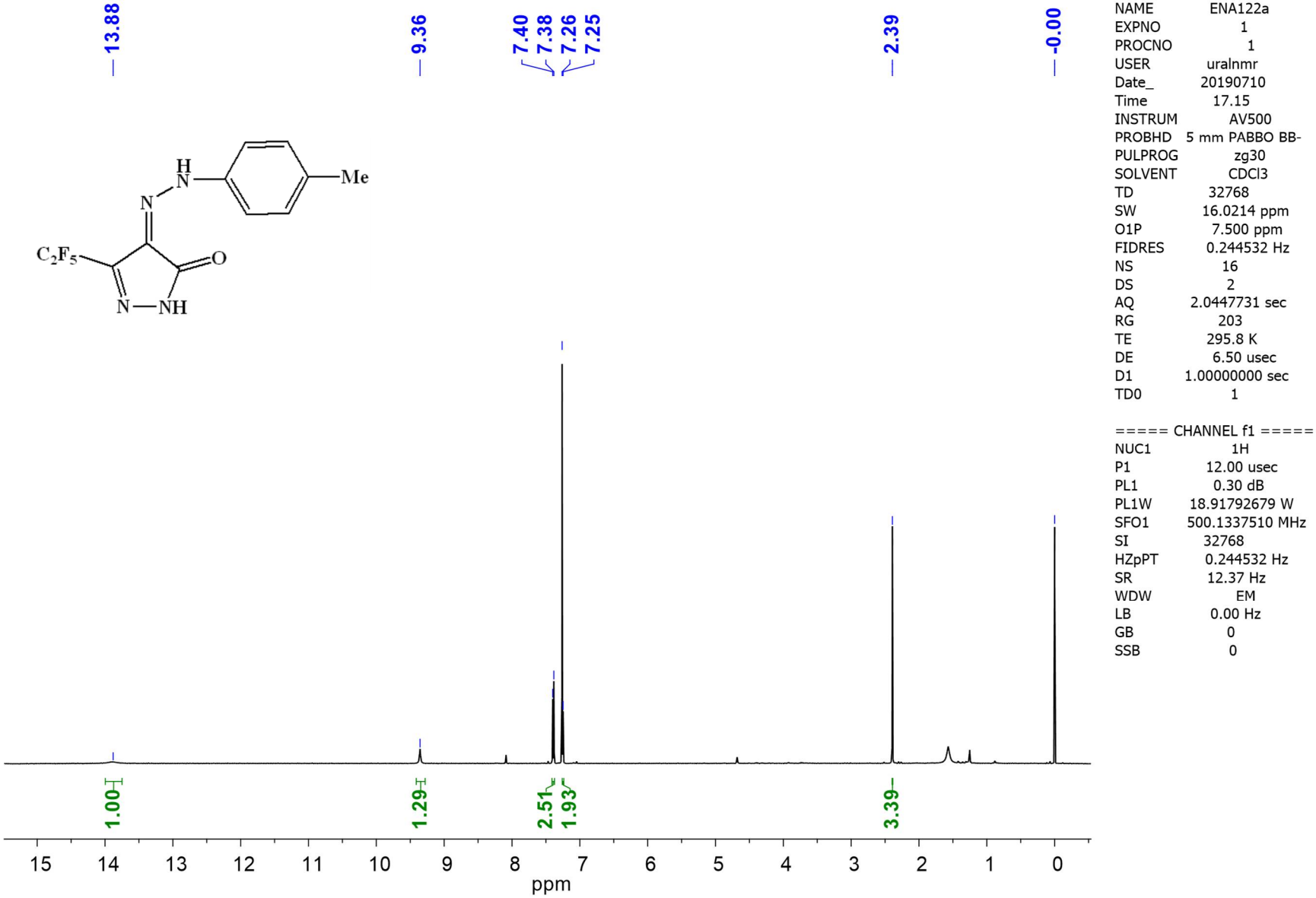
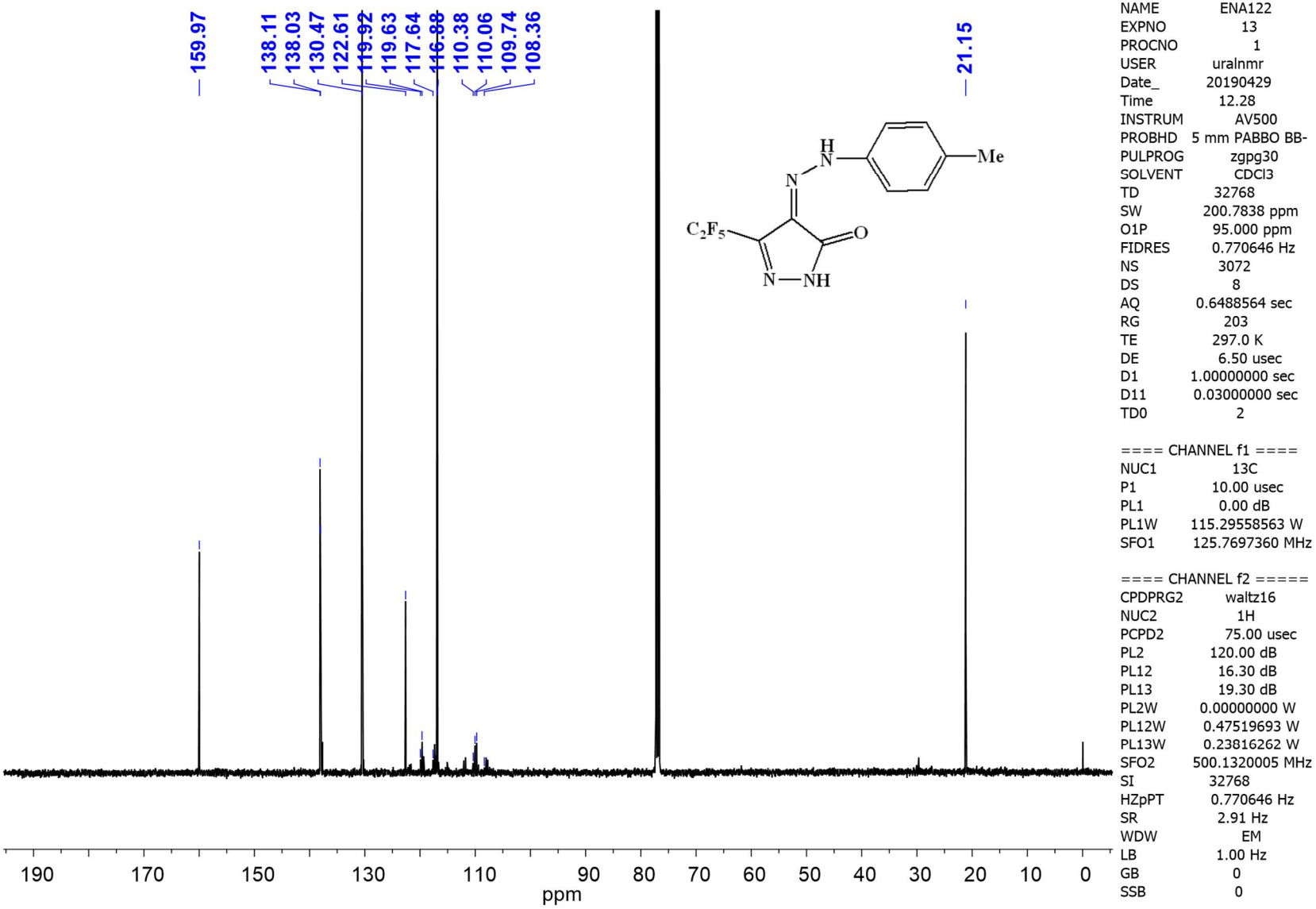
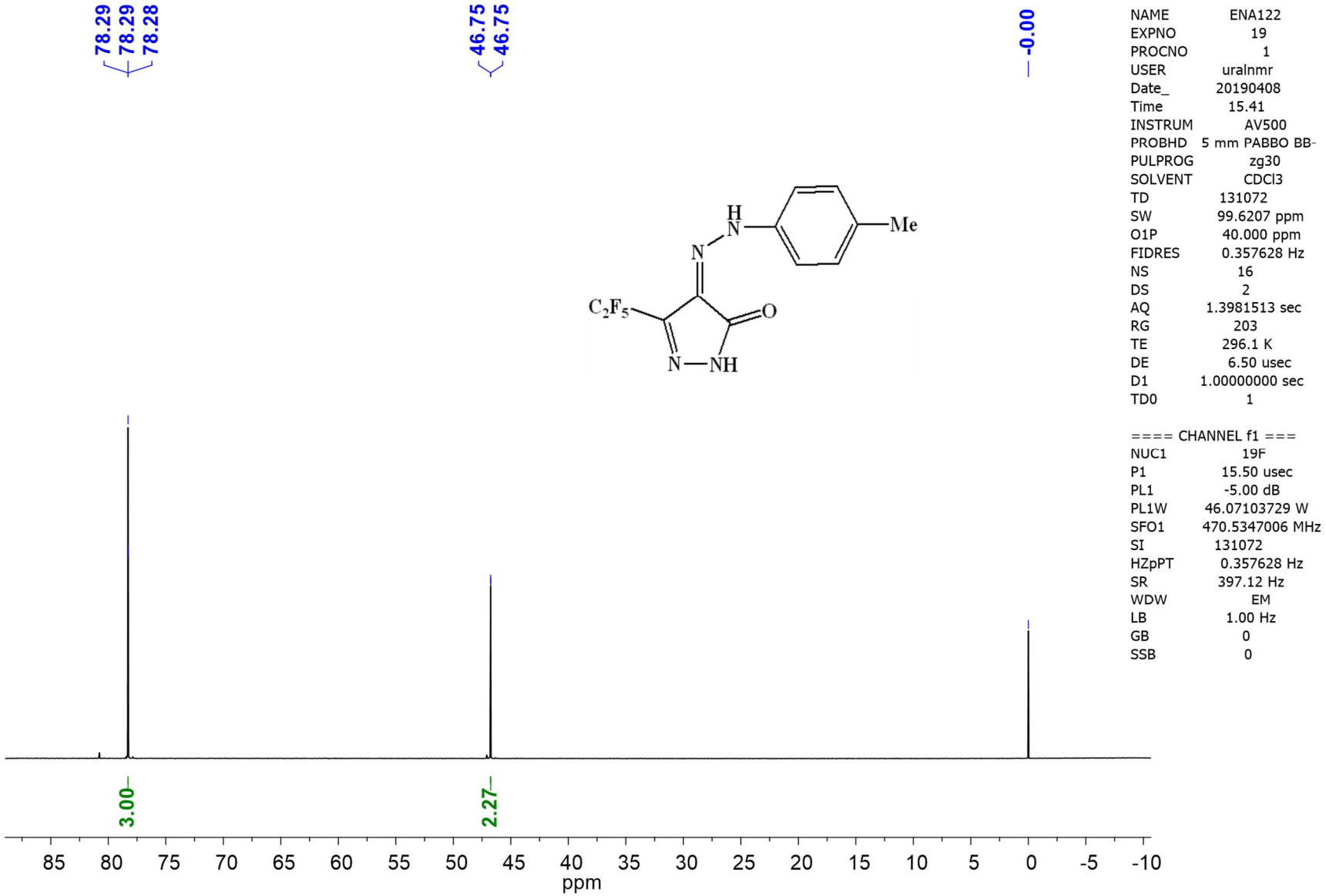


Figure S54. ^{13}C NMR spectrum of compound **6a**



NAME	ENA122
EXPNO	13
PROCNO	1
USER	uralnmr
Date_	20190429
Time	12.28
INSTRUM	AV500
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
SOLVENT	CDCl3
TD	32768
SW	200.7838 ppm
O1P	95.000 ppm
FIDRES	0.770646 Hz
NS	3072
DS	8
AQ	0.6488564 sec
RG	203
TE	297.0 K
DE	6.50 usec
D1	1.00000000 sec
D11	0.03000000 sec
TD0	2
==== CHANNEL f1 ====	
NUC1	13C
P1	10.00 usec
PL1	0.00 dB
PL1W	115.29558563 W
SFO1	125.7697360 MHz
==== CHANNEL f2 =====	
CPDPRG2	waltz16
NUC2	1H
PCPD2	75.00 usec
PL2	120.00 dB
PL12	16.30 dB
PL13	19.30 dB
PL2W	0.00000000 W
PL12W	0.47519693 W
PL13W	0.23816262 W
SFO2	500.1320005 MHz
SI	32768
HZpPT	0.770646 Hz
SR	2.91 Hz
WDW	EM
LB	1.00 Hz
GB	0
SSB	0

Figure S55. ^{19}F NMR spectrum of compound **6a**



NAME	ENA122
EXPNO	19
PROCNO	1
USER	uralnmr
Date_	20190408
Time	15.41
INSTRUM	AV500
PROBHD	5 mm PABBO BB-
PULPROG	zg30
SOLVENT	CDCl3
TD	131072
SW	99.6207 ppm
O1P	40.000 ppm
FIDRES	0.357628 Hz
NS	16
DS	2
AQ	1.3981513 sec
RG	203
TE	296.1 K
DE	6.50 usec
D1	1.00000000 sec
TD0	1
==== CHANNEL f1 ===	
NUC1	19F
P1	15.50 usec
PL1	-5.00 dB
PL1W	46.07103729 W
SFO1	470.5347006 MHz
SI	131072
HZpPT	0.357628 Hz
SR	397.12 Hz
WDW	EM
LB	1.00 Hz
GB	0
SSB	0

Figure S56. ^{1}H NMR spectrum of compound **6b**

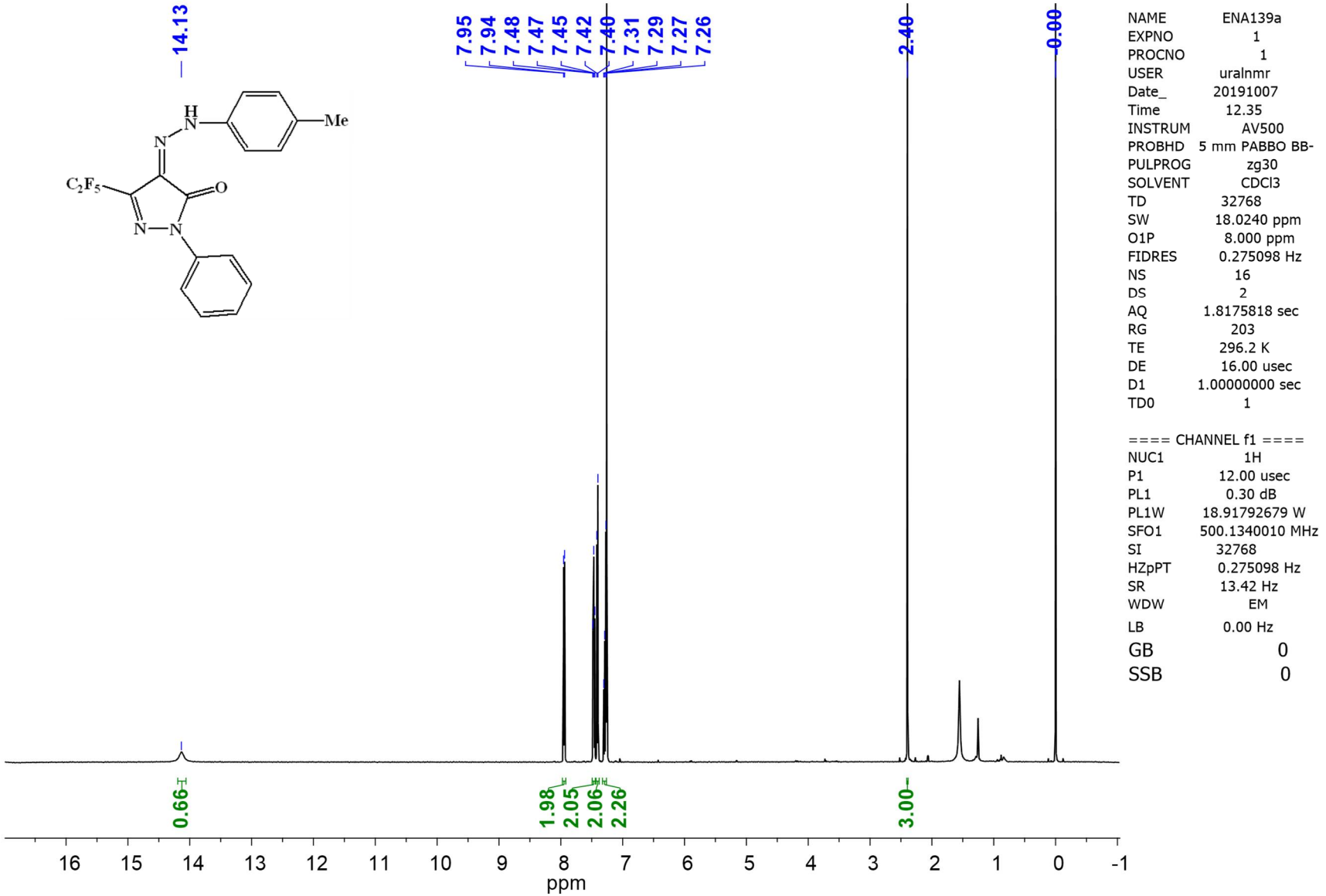
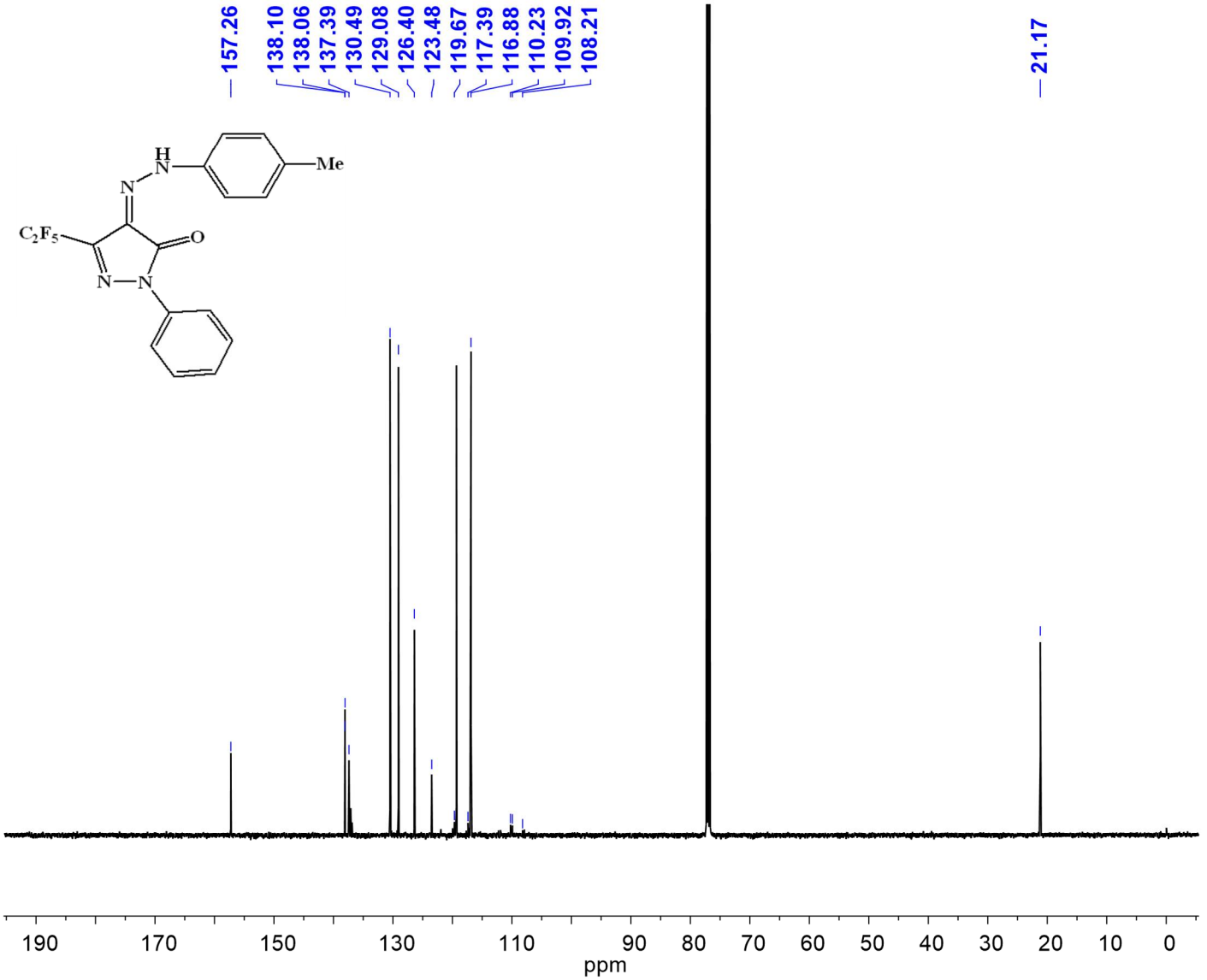
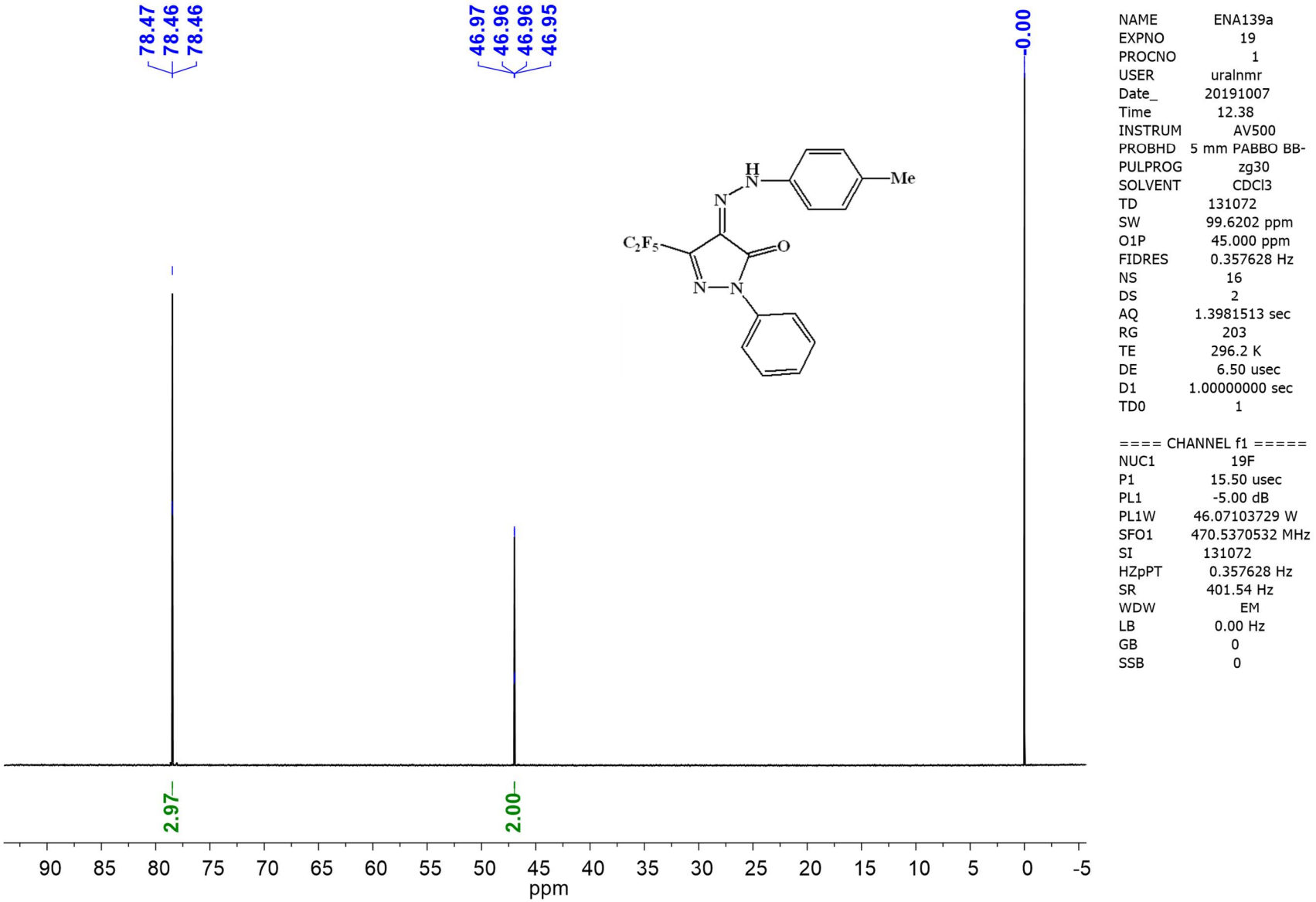


Figure S57. ^{13}C NMR spectrum of compound **6b**



NAME	ENA139a
EXPNO	13
PROCNO	1
USER	uralnmr
Date_	20191015
Time	15.43
INSTRUM	AV500
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
SOLVENT	CDCl3
TD	32768
SW	200.7838 ppm
O1P	95.000 ppm
FIDRES	0.770646 Hz
NS	2048
DS	8
AQ	0.6488564 sec
RG	203
TE	296.6 K
DE	6.50 usec
D1	1.00000000 sec
D11	0.03000000 sec
TD0	1
==== CHANNEL f1 ====	
NUC1	13C
P1	10.00 usec
PL1	0.00 dB
PL1W	115.29558563 W
SFO1	125.7697360 MHz
==== CHANNEL f2 ====	
CPDPRG2	waltz16
NUC2	1H
PCPD2	75.00 usec
PL2	120.00 dB
PL12	16.30 dB
PL13	19.30 dB
PL2W	0.00000000 W
PL12W	0.47519693 W
PL13W	0.23816262 W
SFO2	500.1320005 MHz
SI	32768
HZpPT	0.770646 Hz
SR	2.61 Hz
WDW	EM
LB	1.00 Hz
GB	0
SSB	0

Figure S58. ^{19}F NMR spectrum of compound **6b**



NAME	ENA139a
EXPNO	19
PROCNO	1
USER	uralnmr
Date_	20191007
Time	12.38
INSTRUM	AV500
PROBHD	5 mm PABBO BB-
PULPROG	zg30
SOLVENT	CDCl3
TD	131072
SW	99.6202 ppm
O1P	45.000 ppm
FIDRES	0.357628 Hz
NS	16
DS	2
AQ	1.3981513 sec
RG	203
TE	296.2 K
DE	6.50 usec
D1	1.00000000 sec
TD0	1
==== CHANNEL f1 =====	
NUC1	19F
P1	15.50 usec
PL1	-5.00 dB
PL1W	46.07103729 W
SFO1	470.5370532 MHz
SI	131072
HZpPT	0.357628 Hz
SR	401.54 Hz
WDW	EM
LB	0.00 Hz
GB	0
SSB	0

Figure S59. ^{1}H NMR spectrum of compound **6c**

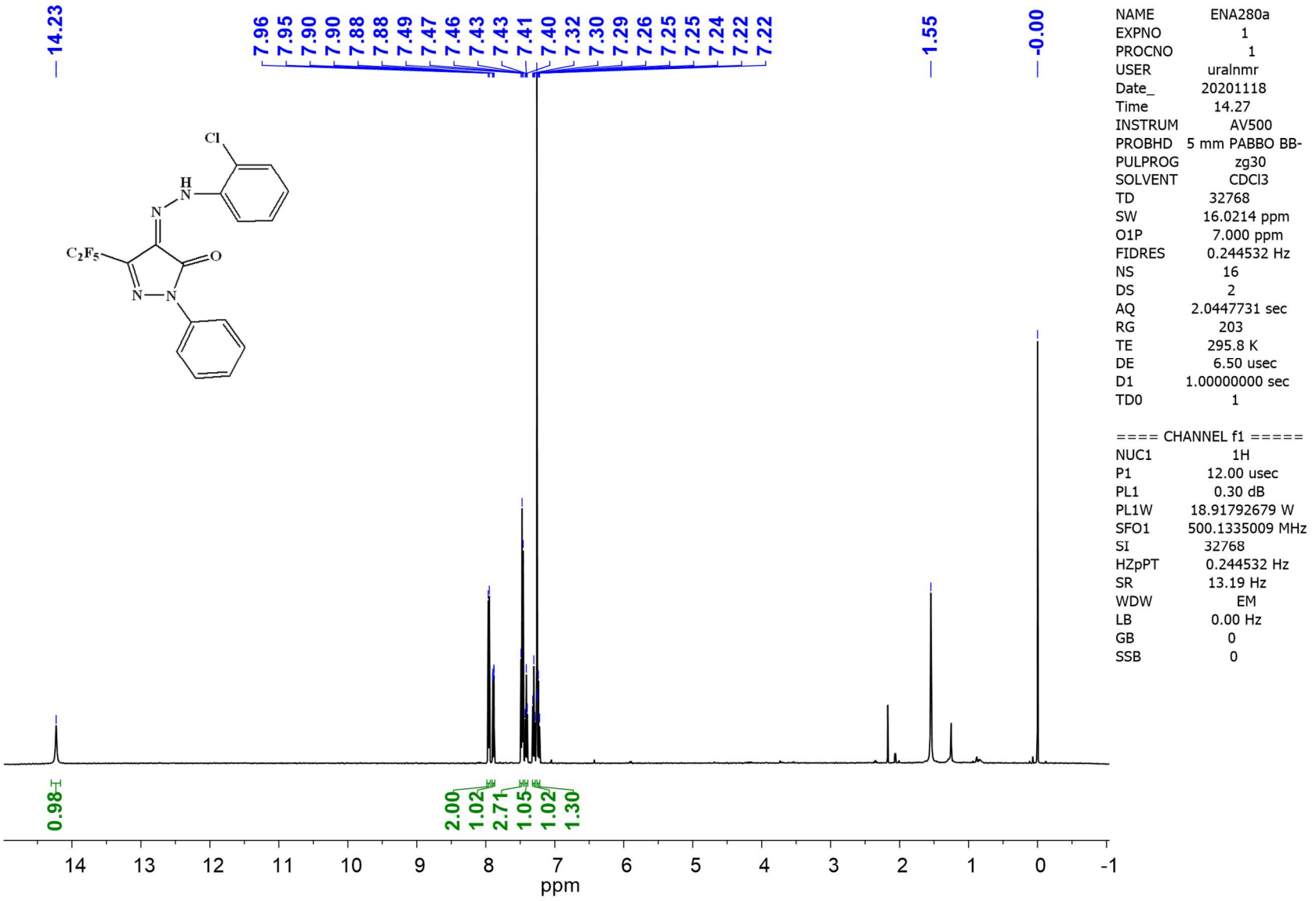
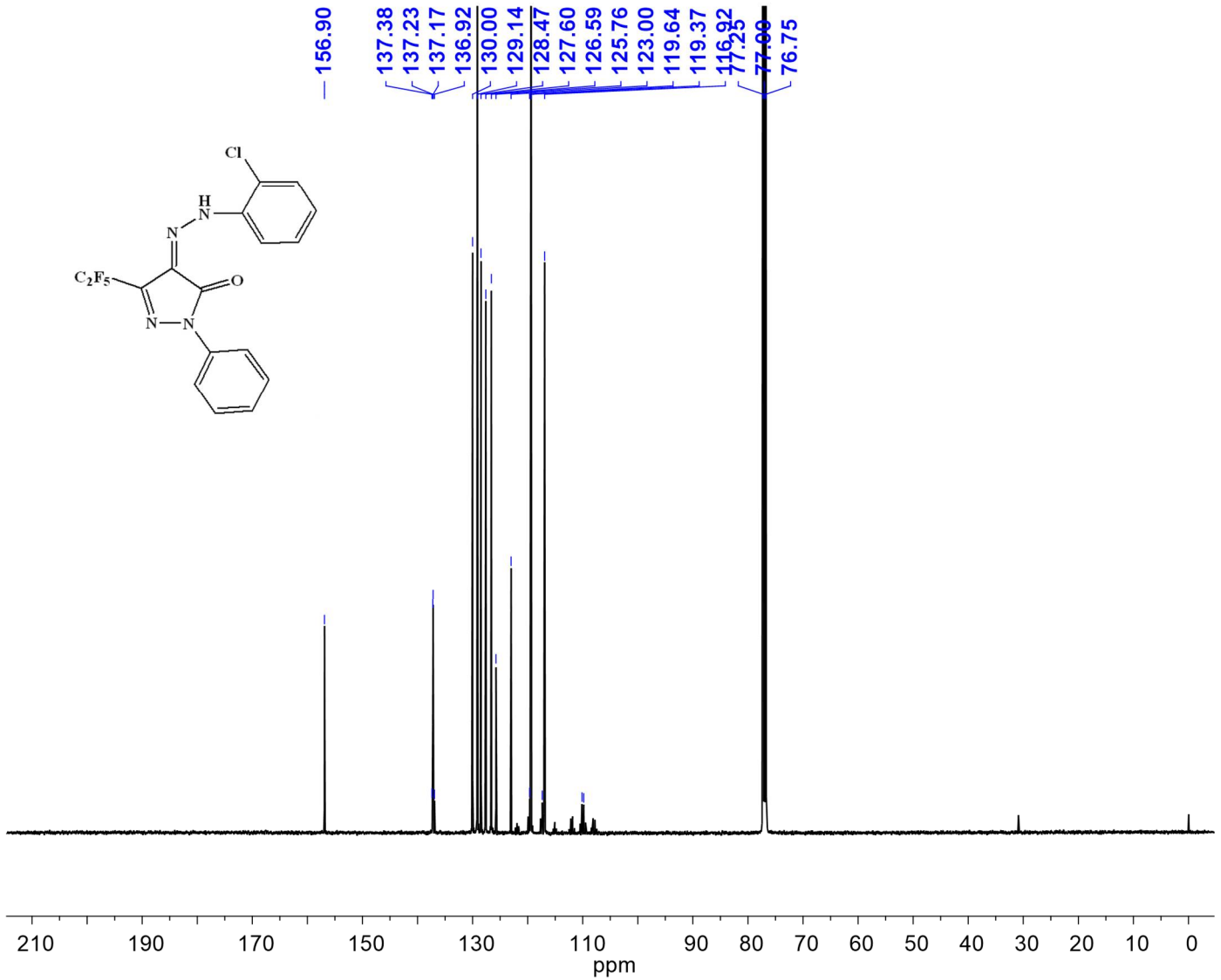
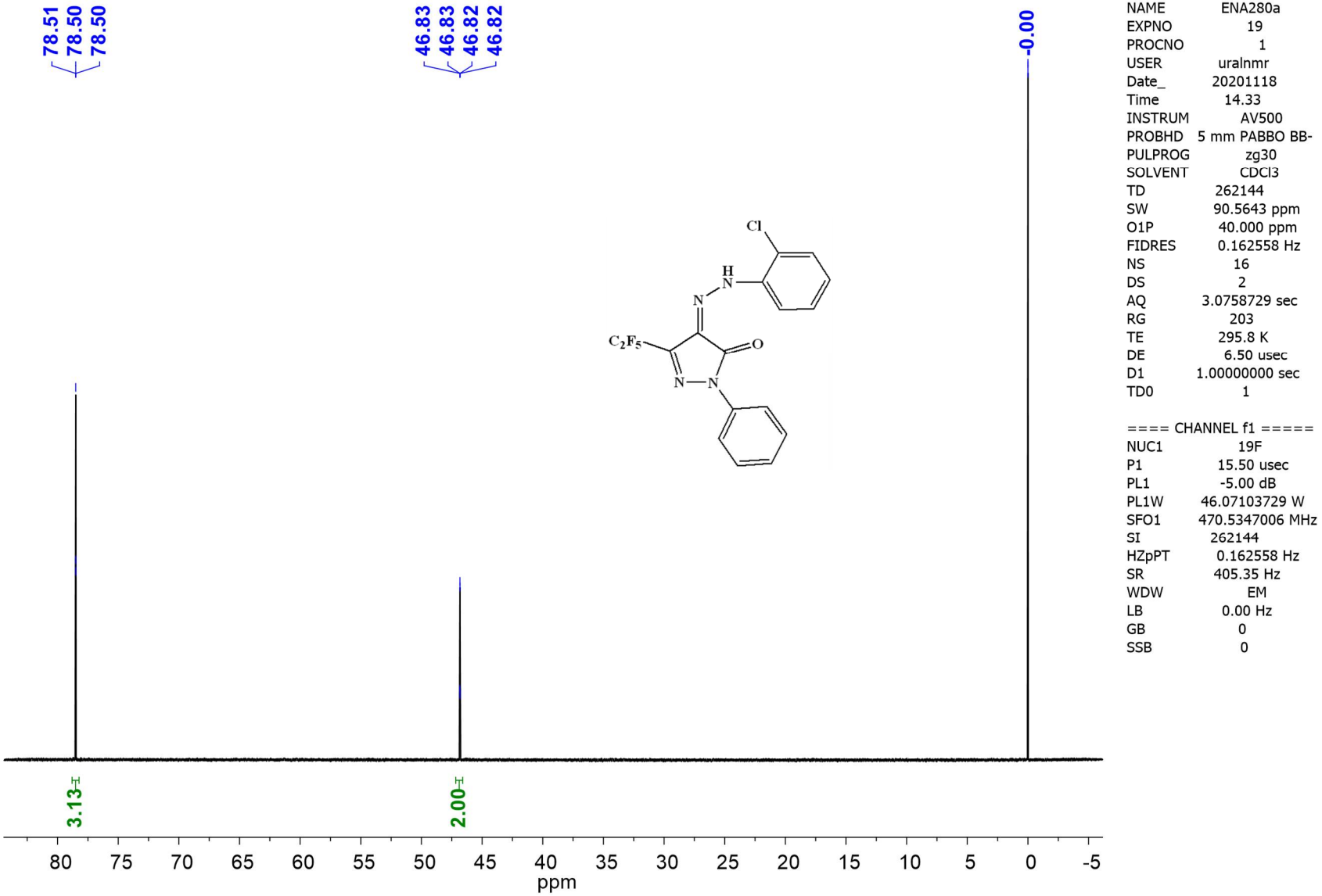


Figure S60. ^{13}C NMR spectrum of compound **6c**



NAME	ENA280a
EXPNO	13
PROCNO	1
USER	uralnmr
Date_	20201209
Time	17.21
INSTRUM	AV500
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
SOLVENT	CDCl3
TD	65536
SW	219.2360 ppm
O1P	105.000 ppm
FIDRES	0.420739 Hz
NS	24576
DS	8
AQ	1.1884362 sec
RG	203
TE	296.5 K
DE	6.50 usec
D1	1.00000000 sec
D11	0.03000000 sec
TD0	24
==== CHANNEL f1 =====	
NUC1	13C
P1	9.00 usec
PL1	0.00 dB
PL1W	115.29558563 W
SFO1	125.7709936 MHz
==== CHANNEL f2 =====	
CPDPRG2	waltz16
NUC2	1H
PCPD2	75.00 usec
PL2	120.00 dB
PL12	17.00 dB
PL13	20.00 dB
PL2W	0.00000000 W
PL12W	0.40445811 W
PL13W	0.20270923 W
SFO2	500.1320005 MHz
SI	32768
HZpPT	0.841477 Hz
SR	0.50 Hz
WDW	EM
LB	1.00 Hz
GB	0
SSB	0

Figure S61. ^{19}F NMR spectrum of compound **6c**



NAME	ENA280a
EXPNO	19
PROCNO	1
USER	uralnmr
Date_	20201118
Time	14.33
INSTRUM	AV500
PROBHD	5 mm PABBO BB-
PULPROG	zg30
SOLVENT	CDCl3
TD	262144
SW	90.5643 ppm
O1P	40.000 ppm
FIDRES	0.162558 Hz
NS	16
DS	2
AQ	3.0758729 sec
RG	203
TE	295.8 K
DE	6.50 usec
D1	1.00000000 sec
TD0	1
==== CHANNEL f1 =====	
NUC1	19F
P1	15.50 usec
PL1	-5.00 dB
PL1W	46.07103729 W
SFO1	470.5347006 MHz
SI	262144
HZpPT	0.162558 Hz
SR	405.35 Hz
WDW	EM
LB	0.00 Hz
GB	0
SSB	0

Figure S62. ^{1}H NMR spectrum of compound **6d**

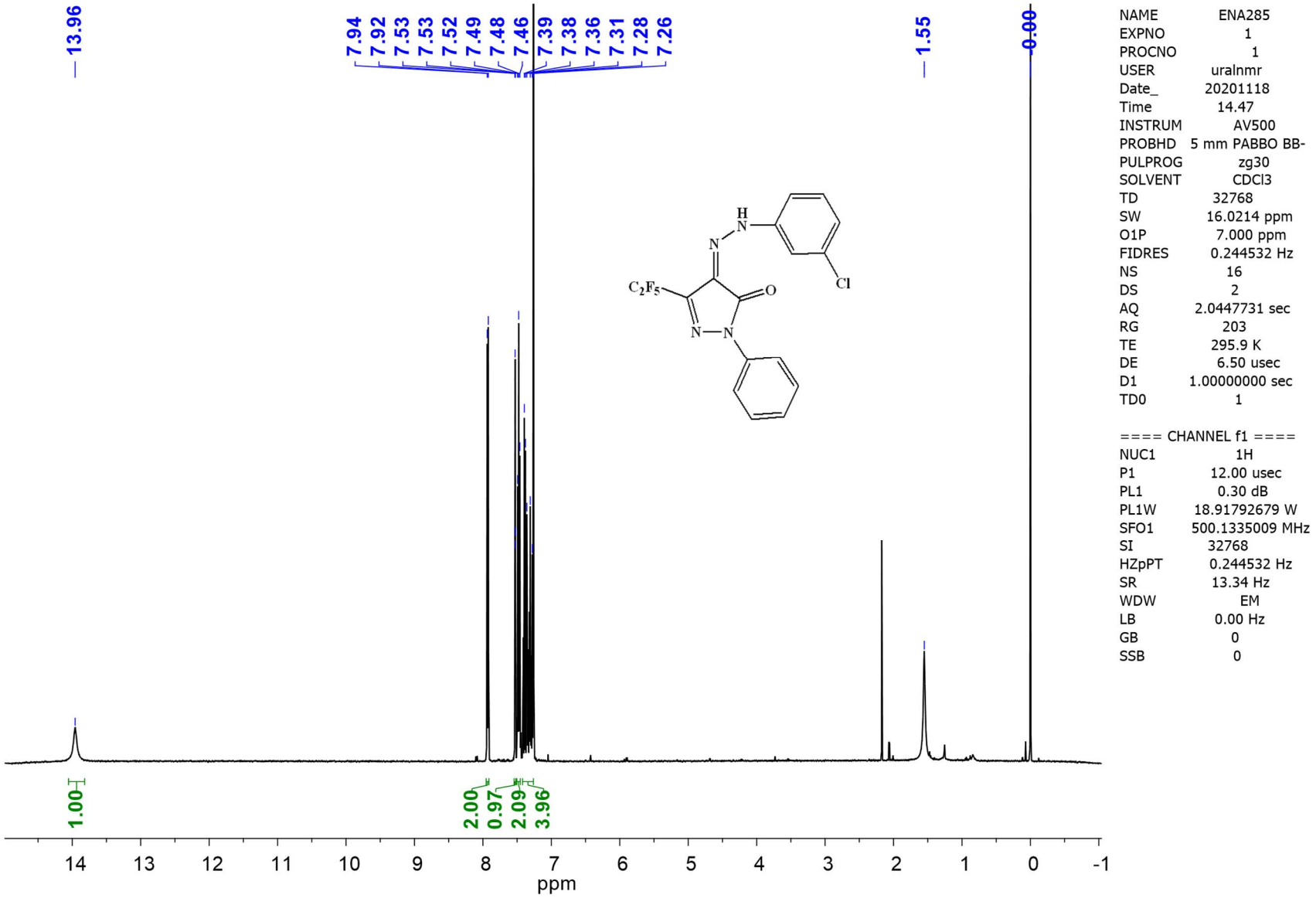


Figure S63. ^{13}C NMR spectrum of compound **6d**

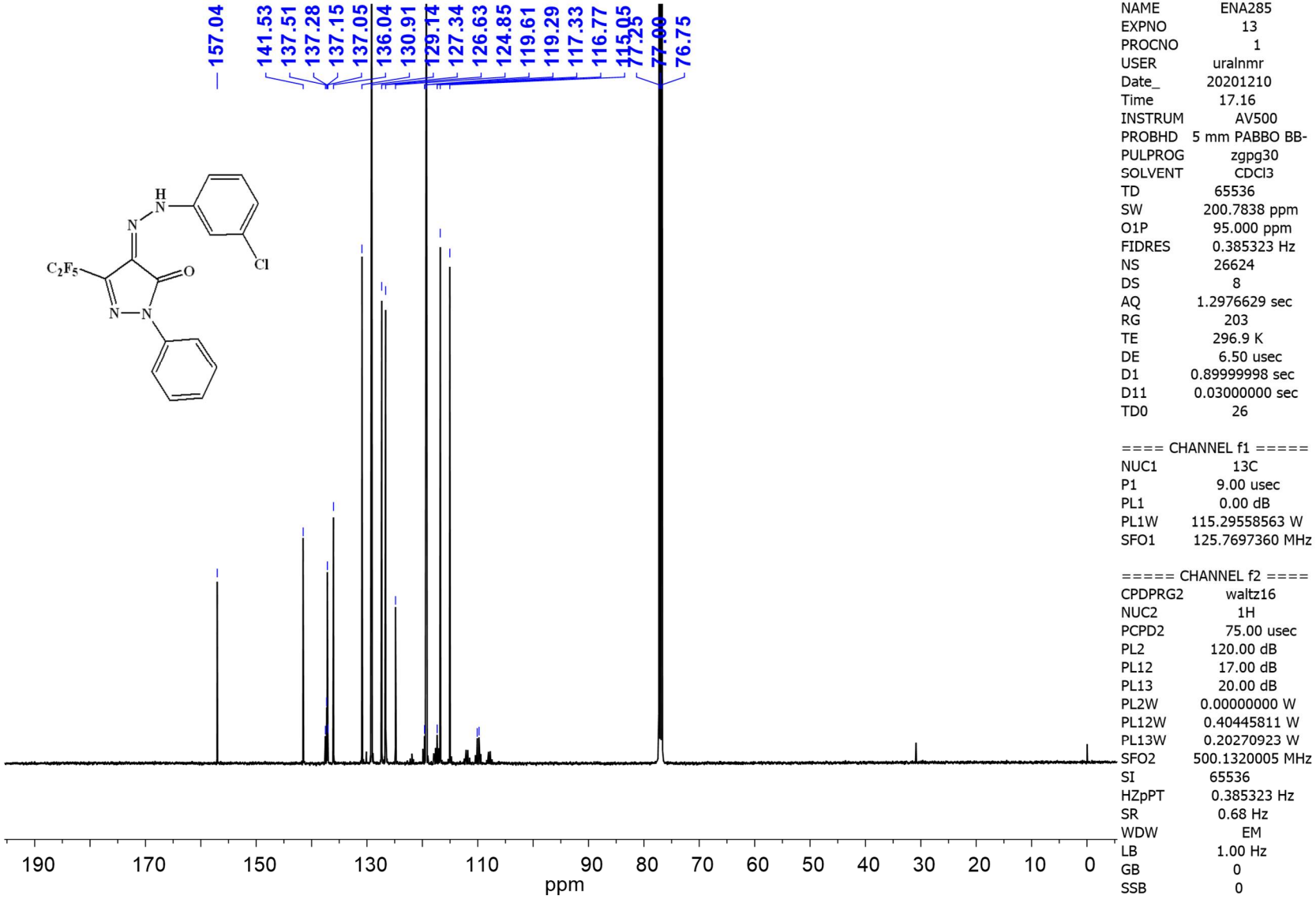
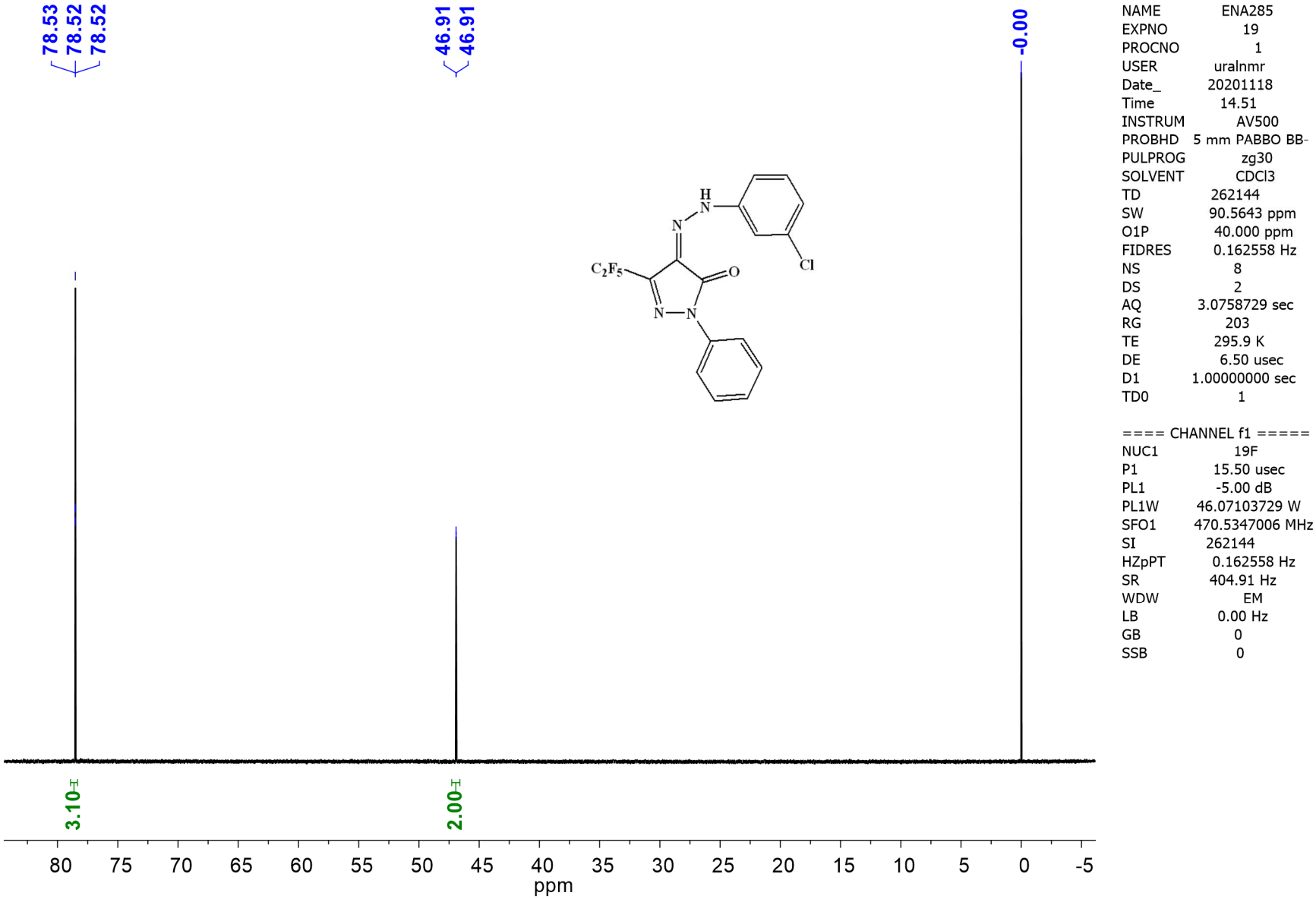


Figure S64. ^{19}F NMR spectrum of compound **6d**



NAME	ENA285
EXPNO	19
PROCNO	1
USER	uralnmr
Date_	20201118
Time	14.51
INSTRUM	AV500
PROBHD	5 mm PABBO BB-
PULPROG	zg30
SOLVENT	CDCl3
TD	262144
SW	90.5643 ppm
O1P	40.000 ppm
FIDRES	0.162558 Hz
NS	8
DS	2
AQ	3.0758729 sec
RG	203
TE	295.9 K
DE	6.50 usec
D1	1.00000000 sec
TD0	1

==== CHANNEL f1 =====

NUC1	19F
P1	15.50 usec
PL1	-5.00 dB
PL1W	46.07103729 W
SFO1	470.5347006 MHz
SI	262144
HZpPT	0.162558 Hz
SR	404.91 Hz
WDW	EM
LB	0.00 Hz
GB	0
SSB	0

Figure S65. ^{1}H NMR spectrum of compound **6e**

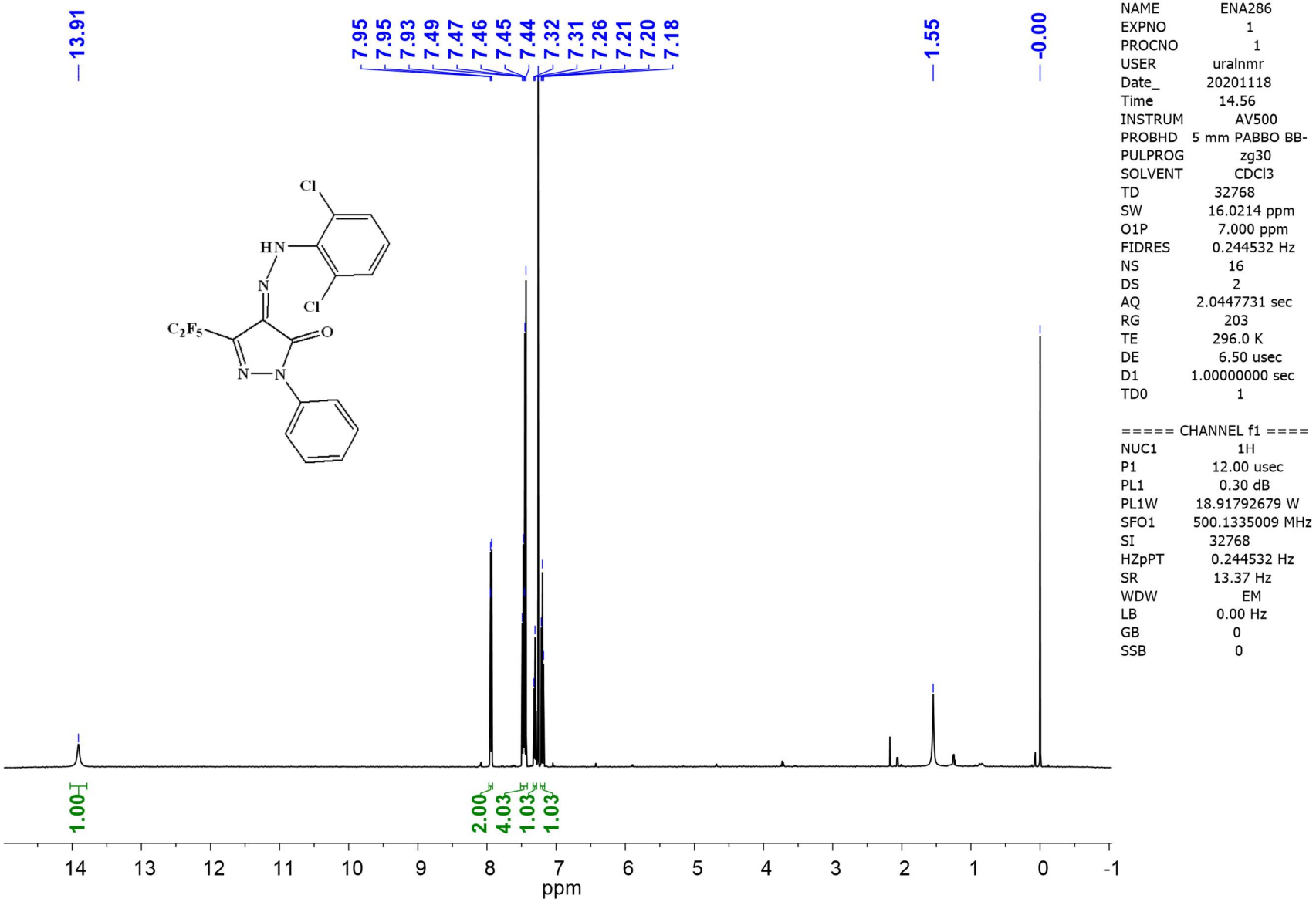
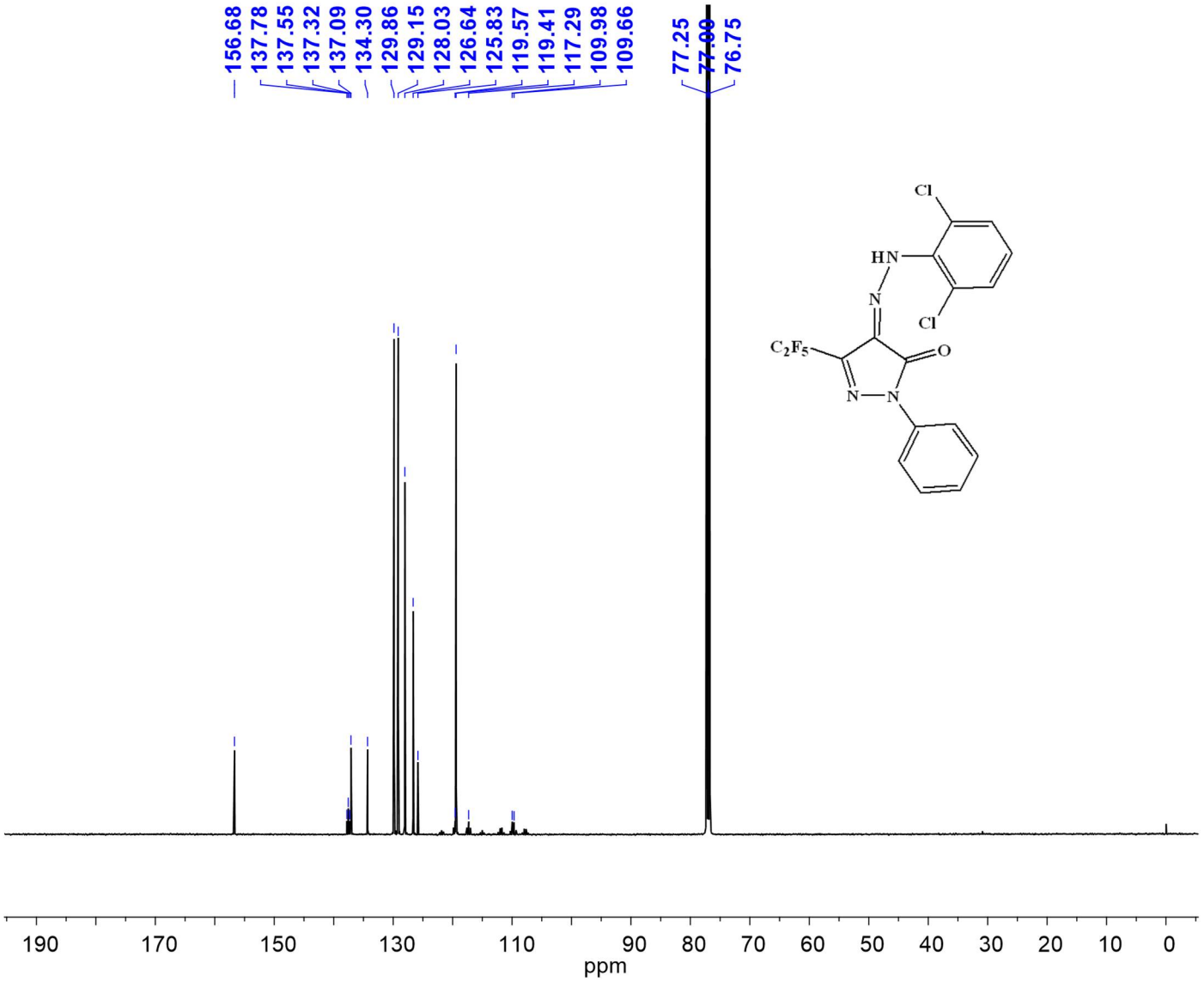


Figure S66. ^{13}C NMR spectrum of compound **6e**



NAME	ENA286
EXPNO	13
PROCNO	1
USER	uralnmr
Date_	20201211
Time	18.00
INSTRUM	AV500
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
SOLVENT	CDCl3
TD	65536
SW	200.7838 ppm
O1P	95.000 ppm
FIDRES	0.385323 Hz
NS	32768
DS	8
AQ	1.2976629 sec
RG	203
TE	298.1 K
DE	6.50 usec
D1	1.00000000 sec
D11	0.03000000 sec
TD0	32
===== CHANNEL f1 =====	
NUC1	13C
P1	9.00 usec
PL1	0.00 dB
PL1W	115.29558563 W
SFO1	125.7697360 MHz
==== CHANNEL f2 =====	
CPDPRG2	waltz16
NUC2	1H
PCPD2	75.00 usec
PL2	120.00 dB
PL12	17.00 dB
PL13	20.00 dB
PL2W	0.00000000 W
PL12W	0.40445811 W
PL13W	0.20270923 W
SFO2	500.1320005 MHz
SI	65536
HZpPT	0.385323 Hz
SR	0.60 Hz
WDW	EM
LB	1.00 Hz
GB	0
SSB	0

Figure S67. ^{19}F NMR spectrum of compound **6e**

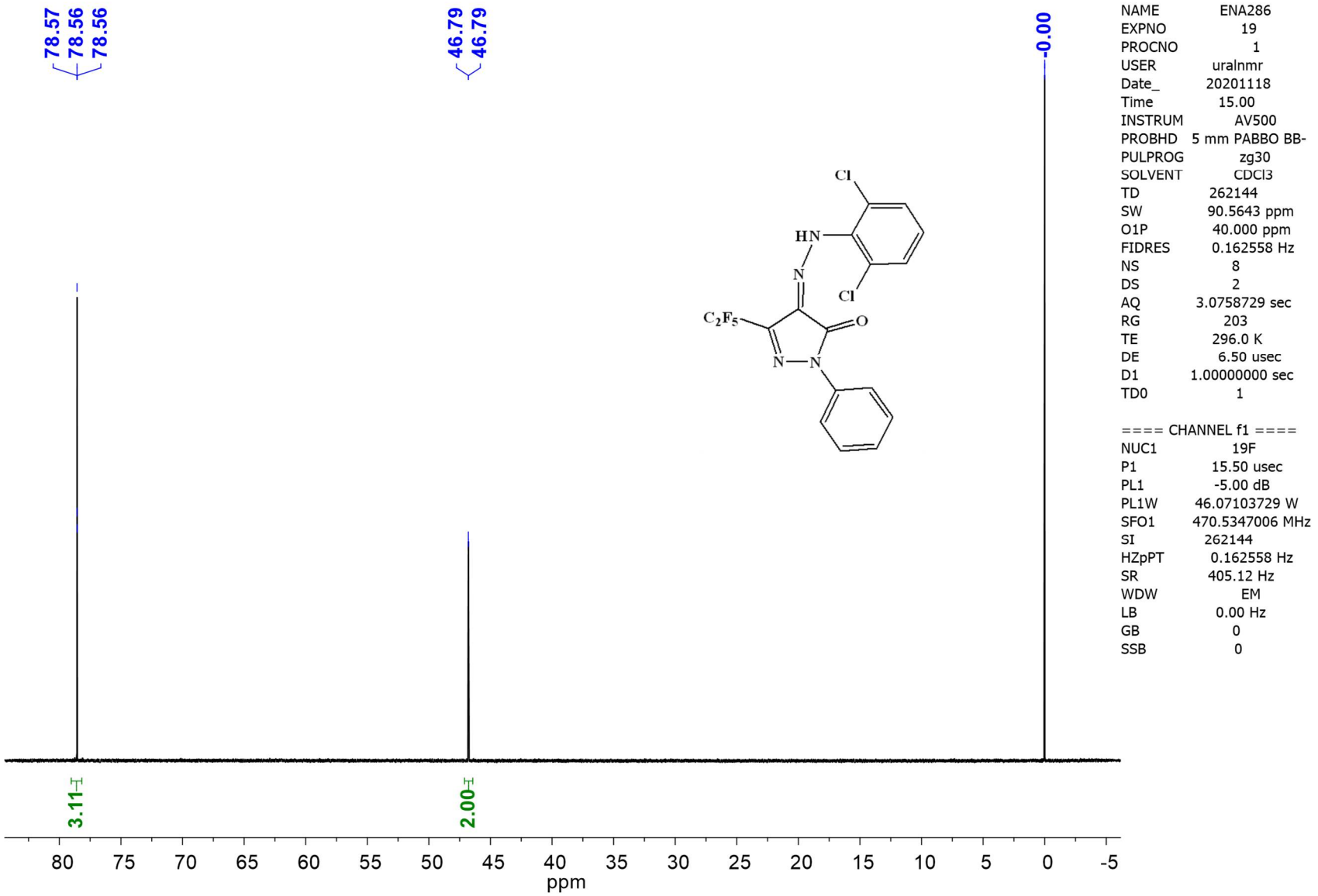
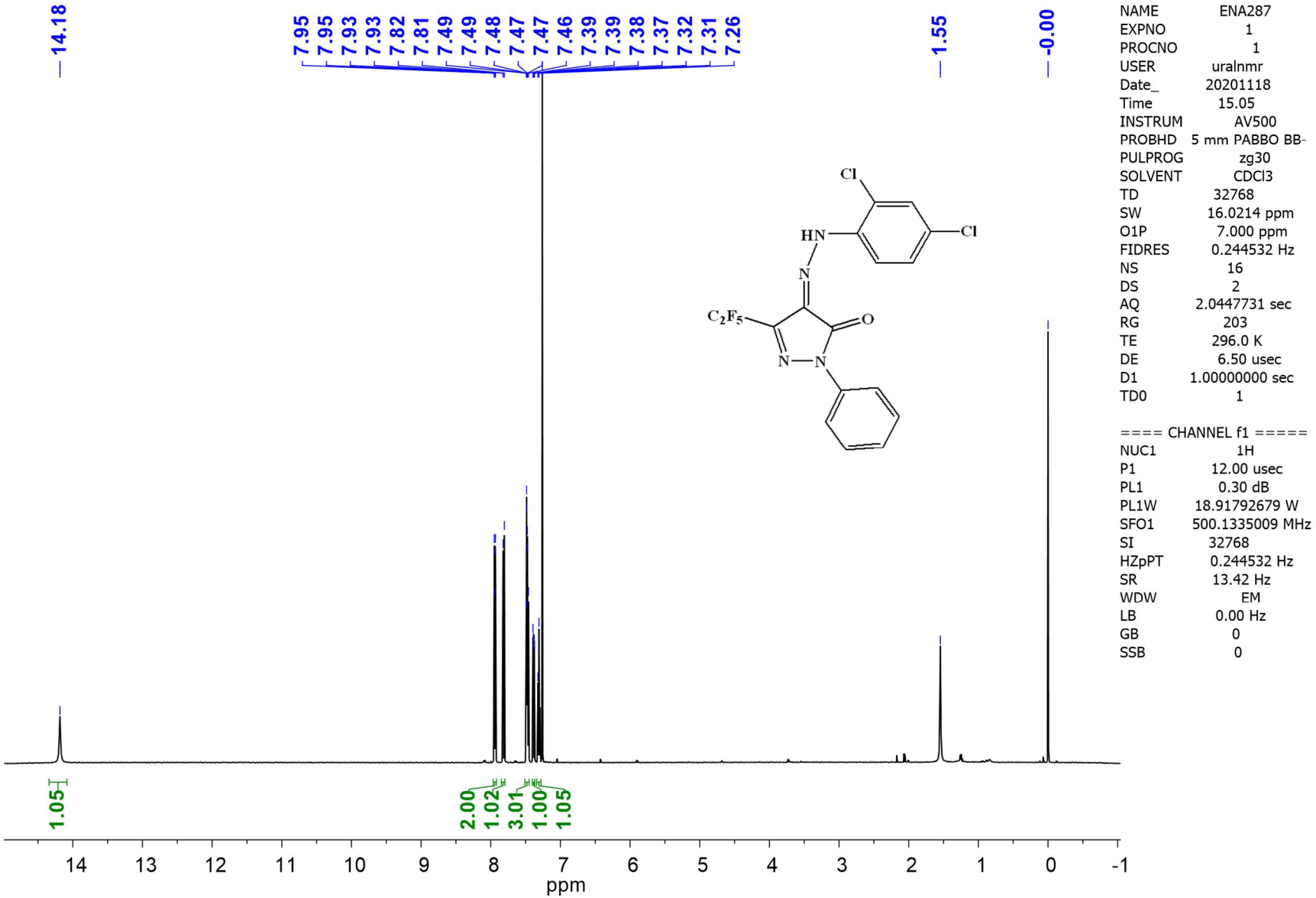
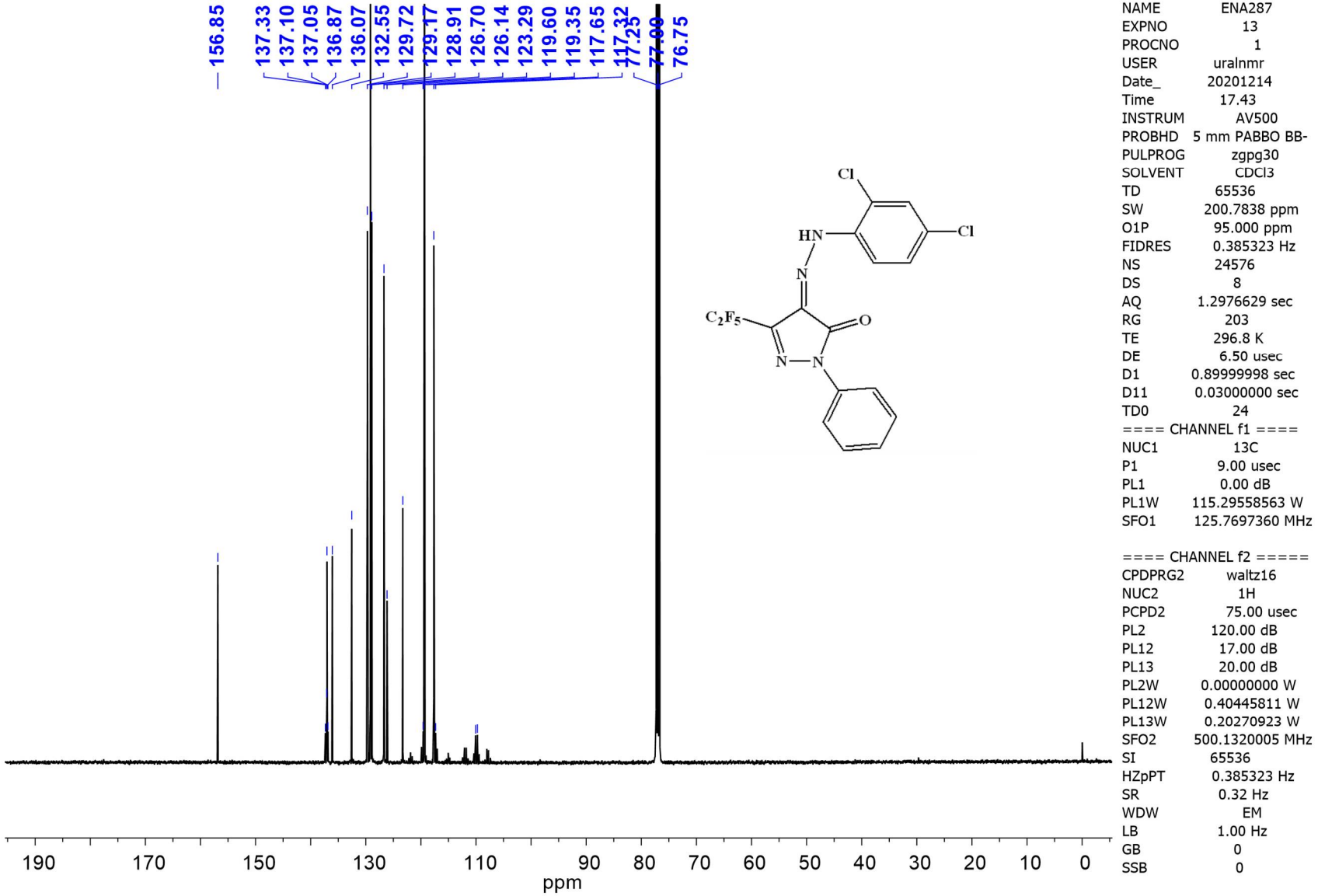


Figure S68. ^{1}H NMR spectrum of compound **6f**



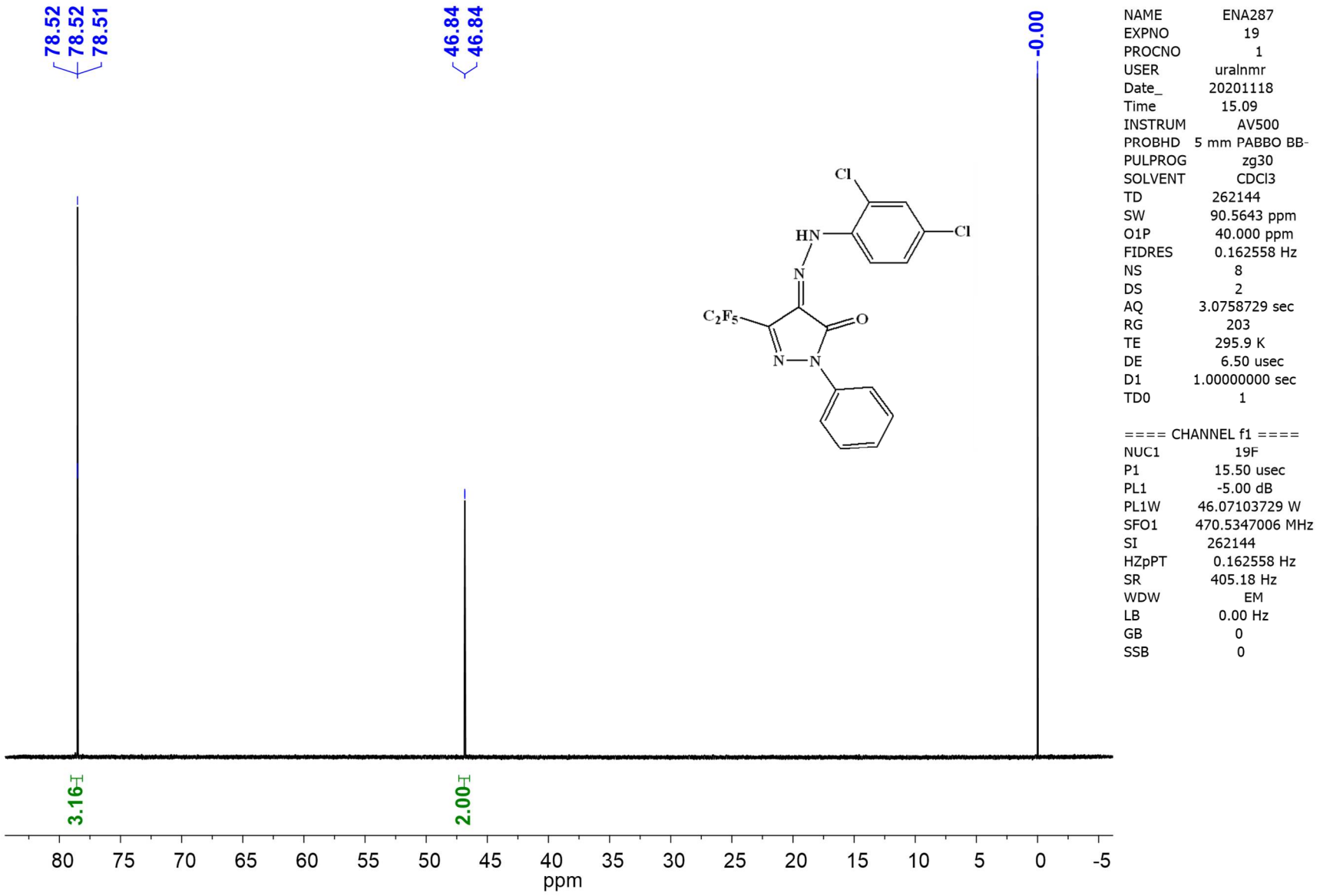
NAME	ENA287
EXPNO	1
PROCNO	1
USER	uralnmr
Date_	20201118
Time	15.05
INSTRUM	AV500
PROBHD	5 mm PABBO BB-
PULPROG	zg30
SOLVENT	CDCl3
TD	32768
SW	16.0214 ppm
O1P	7.000 ppm
FIDRES	0.244532 Hz
NS	16
DS	2
AQ	2.0447731 sec
RG	203
TE	296.0 K
DE	6.50 usec
D1	1.00000000 sec
TD0	1
==== CHANNEL f1 =====	
NUC1	1H
P1	12.00 usec
PL1	0.30 dB
PL1W	18.91792679 W
SFO1	500.1335009 MHz
SI	32768
HZpPT	0.244532 Hz
SR	13.42 Hz
WDW	EM
LB	0.00 Hz
GB	0
SSB	0

Figure S69. ^{13}C NMR spectrum of compound **6f**



NAME	ENA287
EXPNO	13
PROCNO	1
USER	uralnmr
Date_	20201214
Time	17.43
INSTRUM	AV500
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
SOLVENT	CDCl3
TD	65536
SW	200.7838 ppm
O1P	95.000 ppm
FIDRES	0.385323 Hz
NS	24576
DS	8
AQ	1.2976629 sec
RG	203
TE	296.8 K
DE	6.50 usec
D1	0.89999998 sec
D11	0.03000000 sec
TD0	24
==== CHANNEL f1 ====	
NUC1	13C
P1	9.00 usec
PL1	0.00 dB
PL1W	115.29558563 W
SFO1	125.7697360 MHz
==== CHANNEL f2 =====	
CPDPRG2	waltz16
NUC2	1H
PCPD2	75.00 usec
PL2	120.00 dB
PL12	17.00 dB
PL13	20.00 dB
PL2W	0.00000000 W
PL12W	0.40445811 W
PL13W	0.20270923 W
SFO2	500.1320005 MHz
SI	65536
HZpPT	0.385323 Hz
SR	0.32 Hz
WDW	EM
LB	1.00 Hz
GB	0
SSB	0

Figure S70. ^{19}F NMR spectrum of compound **6f**



NAME	ENA287
EXPNO	19
PROCNO	1
USER	uralnmr
Date_	20201118
Time	15.09
INSTRUM	AV500
PROBHD	5 mm PABBO BB-
PULPROG	zg30
SOLVENT	CDCl3
TD	262144
SW	90.5643 ppm
O1P	40.000 ppm
FIDRES	0.162558 Hz
NS	8
DS	2
AQ	3.0758729 sec
RG	203
TE	295.9 K
DE	6.50 usec
D1	1.00000000 sec
TD0	1
==== CHANNEL f1 ====	
NUC1	19F
P1	15.50 usec
PL1	-5.00 dB
PL1W	46.07103729 W
SFO1	470.5347006 MHz
SI	262144
HZpPT	0.162558 Hz
SR	405.18 Hz
WDW	EM
LB	0.00 Hz
GB	0
SSB	0

Figure S71. ^{1}H NMR spectrum of compound **6g**

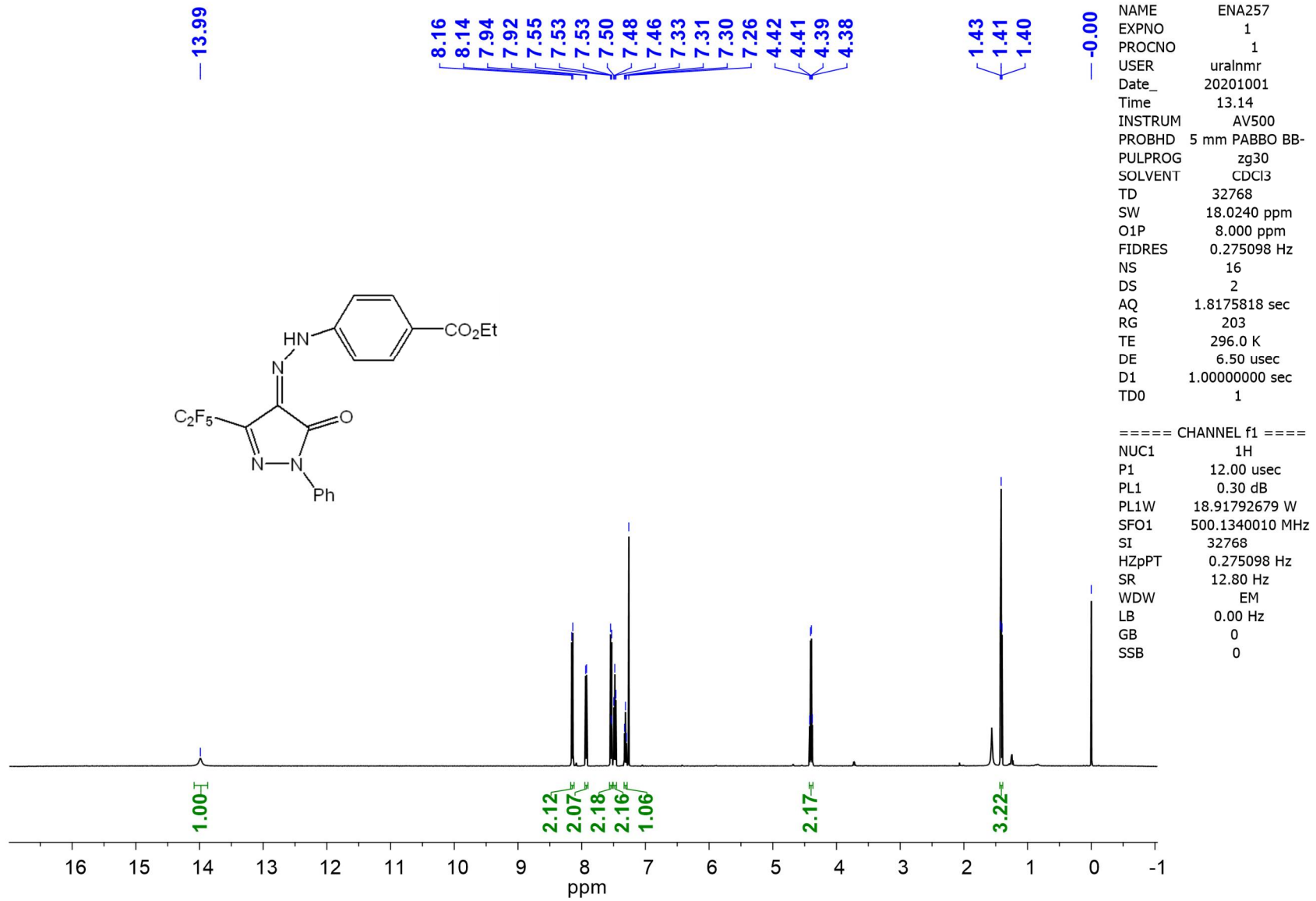
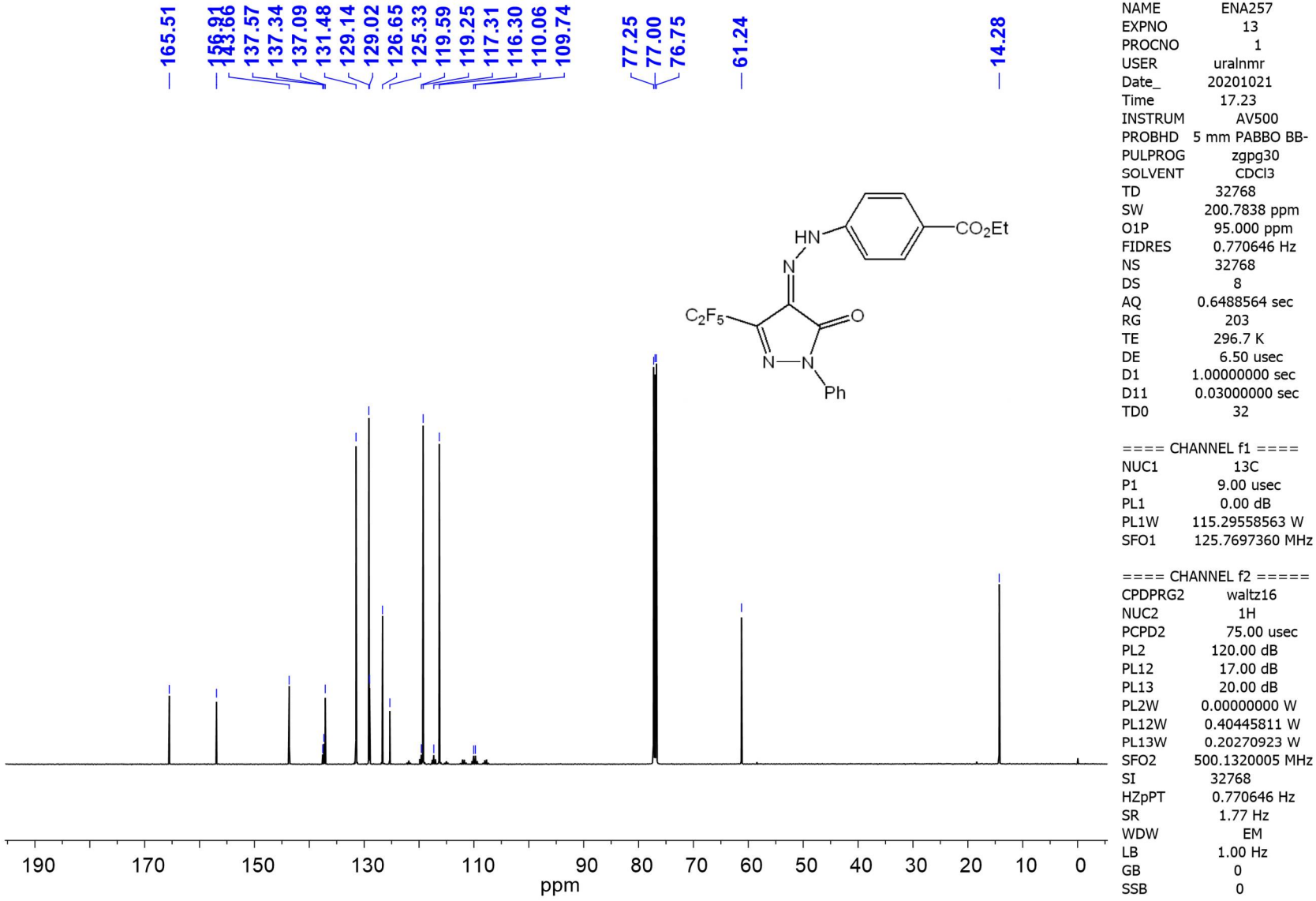
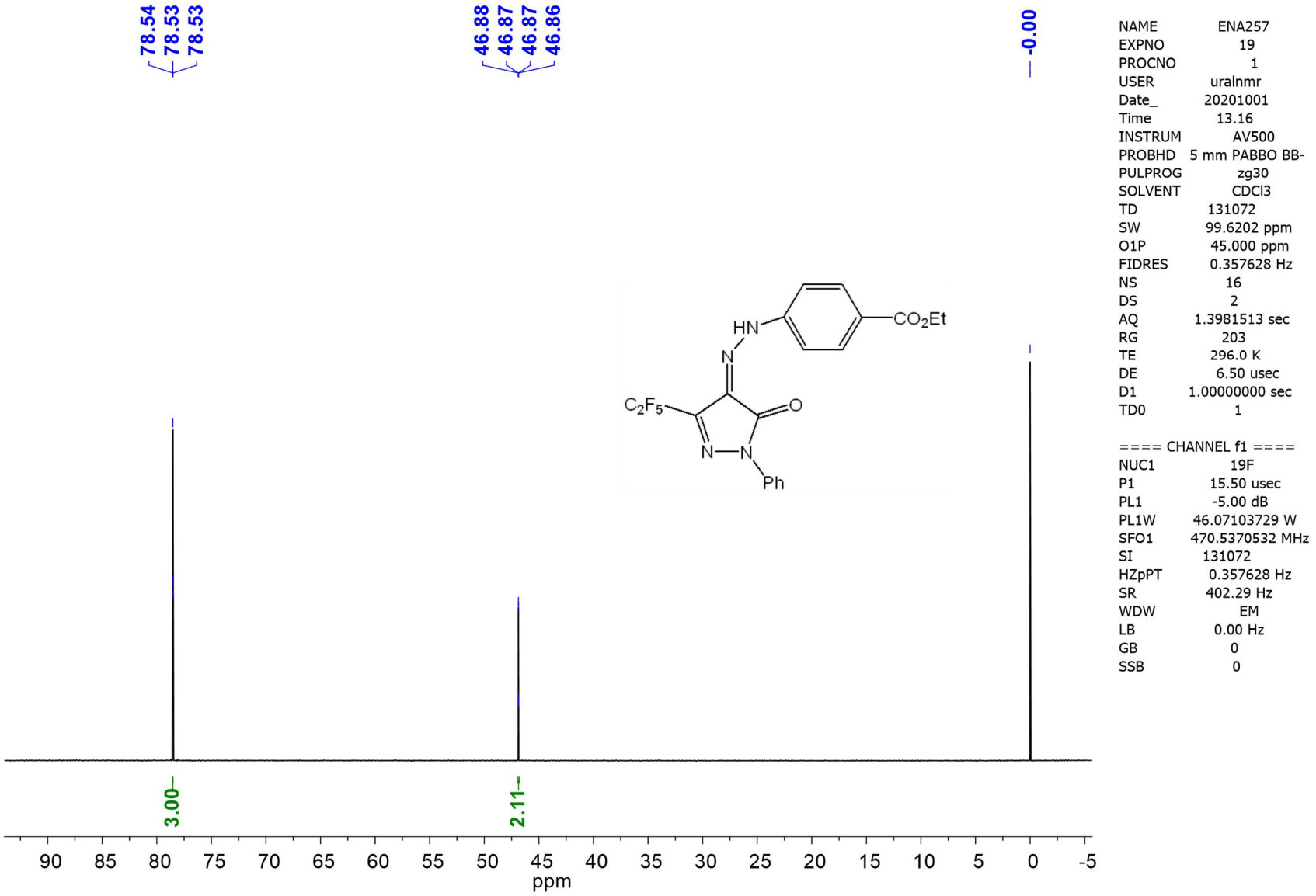


Figure S72. ^{13}C NMR spectrum of compound **6g**



NAME	ENA257
EXPNO	13
PROCNO	1
USER	uralnmr
Date_	20201021
Time	17.23
INSTRUM	AV500
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
SOLVENT	CDCl3
TD	32768
SW	200.7838 ppm
O1P	95.000 ppm
FIDRES	0.770646 Hz
NS	32768
DS	8
AQ	0.6488564 sec
RG	203
TE	296.7 K
DE	6.50 usec
D1	1.00000000 sec
D11	0.03000000 sec
TD0	32
==== CHANNEL f1 ====	
NUC1	13C
P1	9.00 usec
PL1	0.00 dB
PL1W	115.29558563 W
SFO1	125.7697360 MHz
==== CHANNEL f2 =====	
CPDPRG2	waltz16
NUC2	1H
PCPD2	75.00 usec
PL2	120.00 dB
PL12	17.00 dB
PL13	20.00 dB
PL2W	0.00000000 W
PL12W	0.40445811 W
PL13W	0.20270923 W
SFO2	500.1320005 MHz
SI	32768
HZpPT	0.770646 Hz
SR	1.77 Hz
WDW	EM
LB	1.00 Hz
GB	0
SSB	0

Figure S73. ^{19}F NMR spectrum of compound **6g**



NAME	ENA257
EXPNO	19
PROCNO	1
USER	uralnmr
Date_	20201001
Time	13.16
INSTRUM	AV500
PROBHD	5 mm PABBO BB-
PULPROG	zg30
SOLVENT	CDCl3
TD	131072
SW	99.6202 ppm
O1P	45.000 ppm
FIDRES	0.357628 Hz
NS	16
DS	2
AQ	1.3981513 sec
RG	203
TE	296.0 K
DE	6.50 usec
D1	1.00000000 sec
TD0	1
==== CHANNEL f1 ====	
NUC1	19F
P1	15.50 usec
PL1	-5.00 dB
PL1W	46.07103729 W
SFO1	470.5370532 MHz
SI	131072
HZpPT	0.357628 Hz
SR	402.29 Hz
WDW	EM
LB	0.00 Hz
GB	0
SSB	0

Figure S74. ^{1}H NMR spectrum of compound **6h**

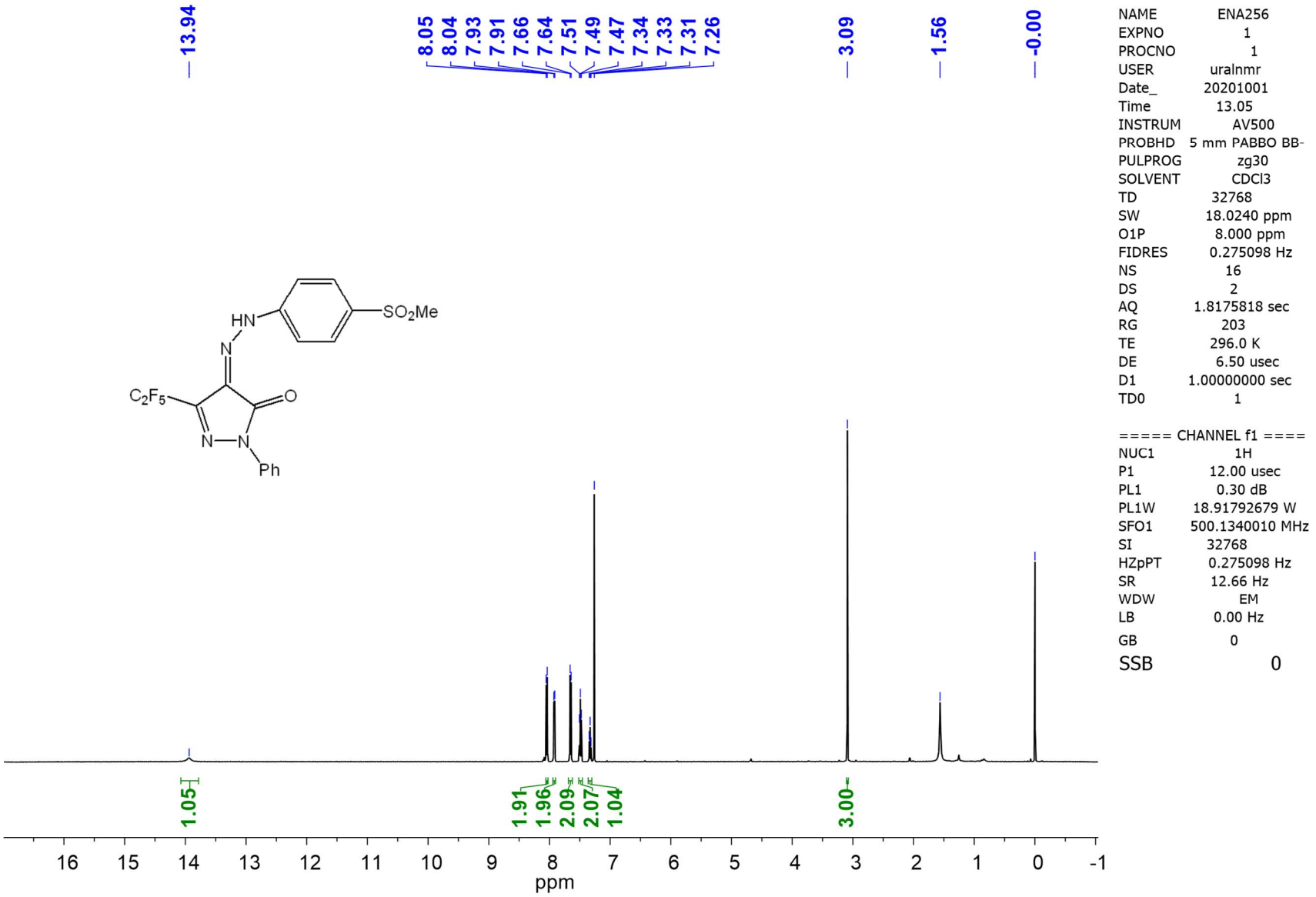
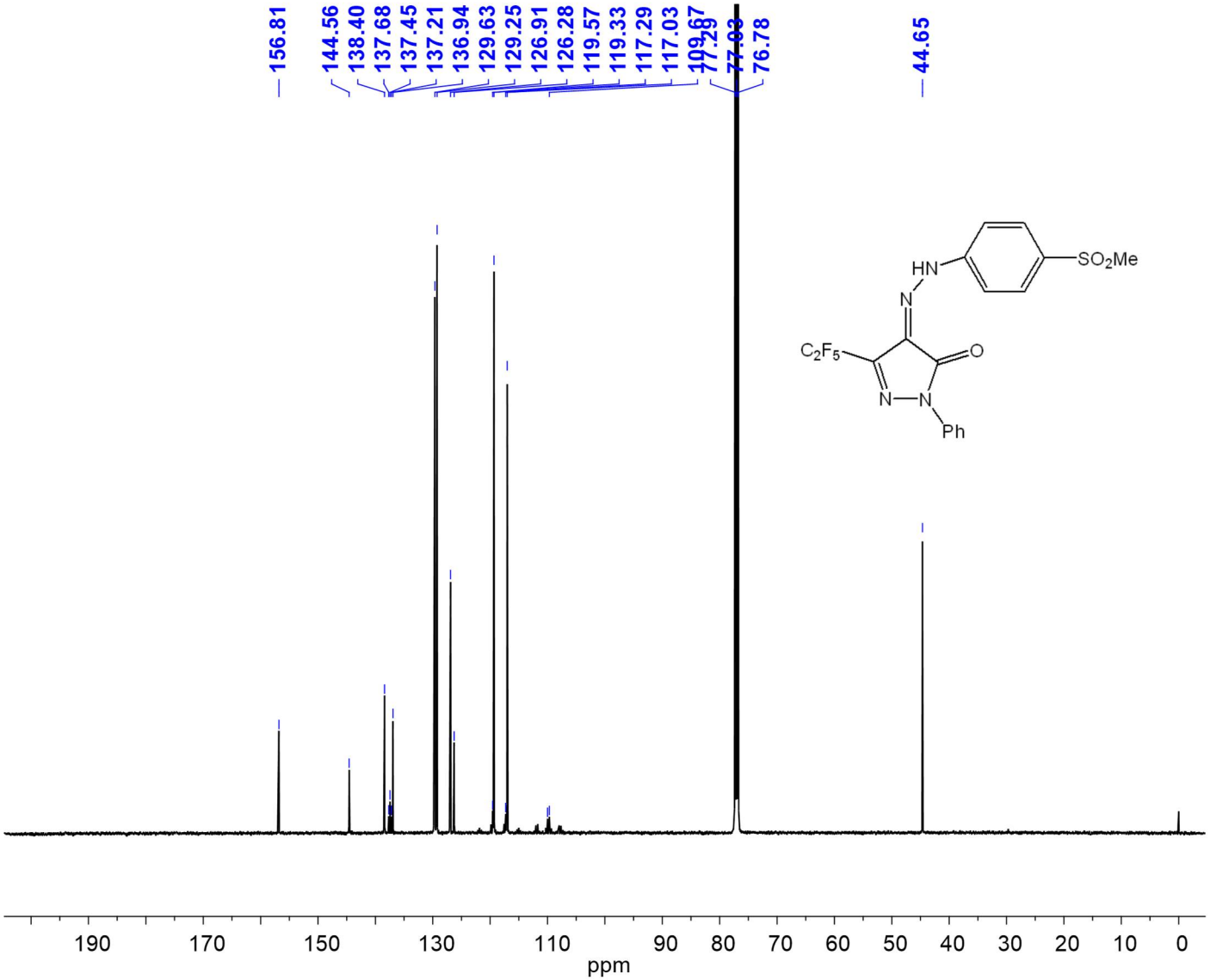


Figure S75. ^{13}C NMR spectrum of compound **6h**



NAME	ENA256
EXPNO	13
PROCNO	1
USER	uralnmr
Date_	20201020
Time	17.37
INSTRUM	AV500
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
SOLVENT	CDCl3
TD	65536
SW	209.2368 ppm
O1P	100.000 ppm
FIDRES	0.401547 Hz
NS	24576
DS	8
AQ	1.2452340 sec
RG	203
TE	296.9 K
DE	6.50 usec
D1	1.00000000 sec
D11	0.03000000 sec
TD0	24
==== CHANNEL f1 ====	
NUC1	13C
P1	9.00 usec
PL1	0.00 dB
PL1W	115.29558563 W
SFO1	125.7703648 MHz
==== CHANNEL f2 =====	
CPDPRG2	waltz16
NUC2	1H
PCPD2	75.00 usec
PL2	120.00 dB
PL12	17.00 dB
PL13	20.00 dB
PL2W	0.00000000 W
PL12W	0.40445811 W
PL13W	0.20270923 W
SFO2	500.1320005 MHz
SI	32768
HZpPT	0.803094 Hz
SR	-2.93 Hz
WDW	EM
LB	1.00 Hz
GB	0
SSB	0

Figure S76. ^{19}F NMR spectrum of compound **6h**

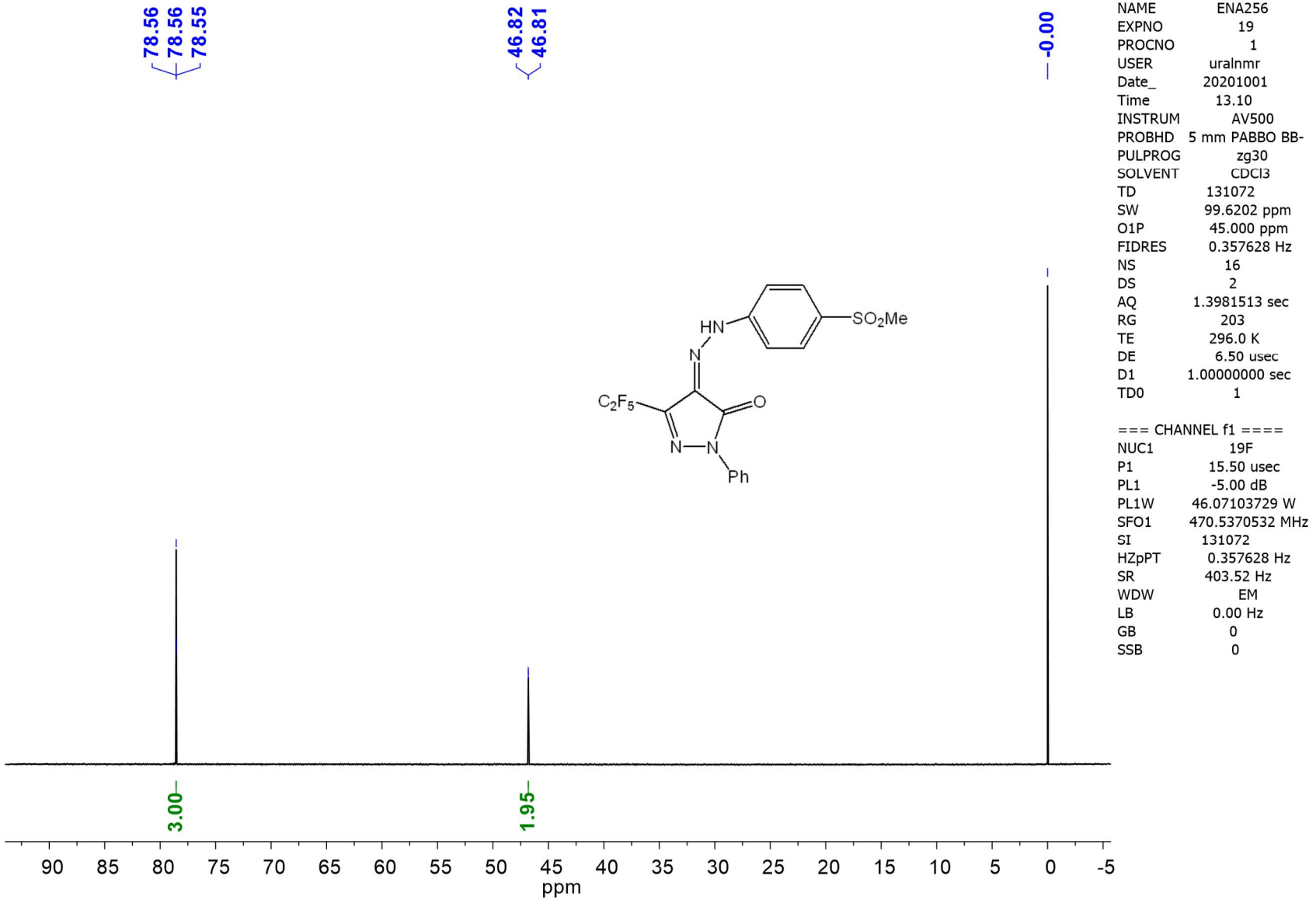


Figure S77. ^{1}H NMR spectrum of compound **6i**

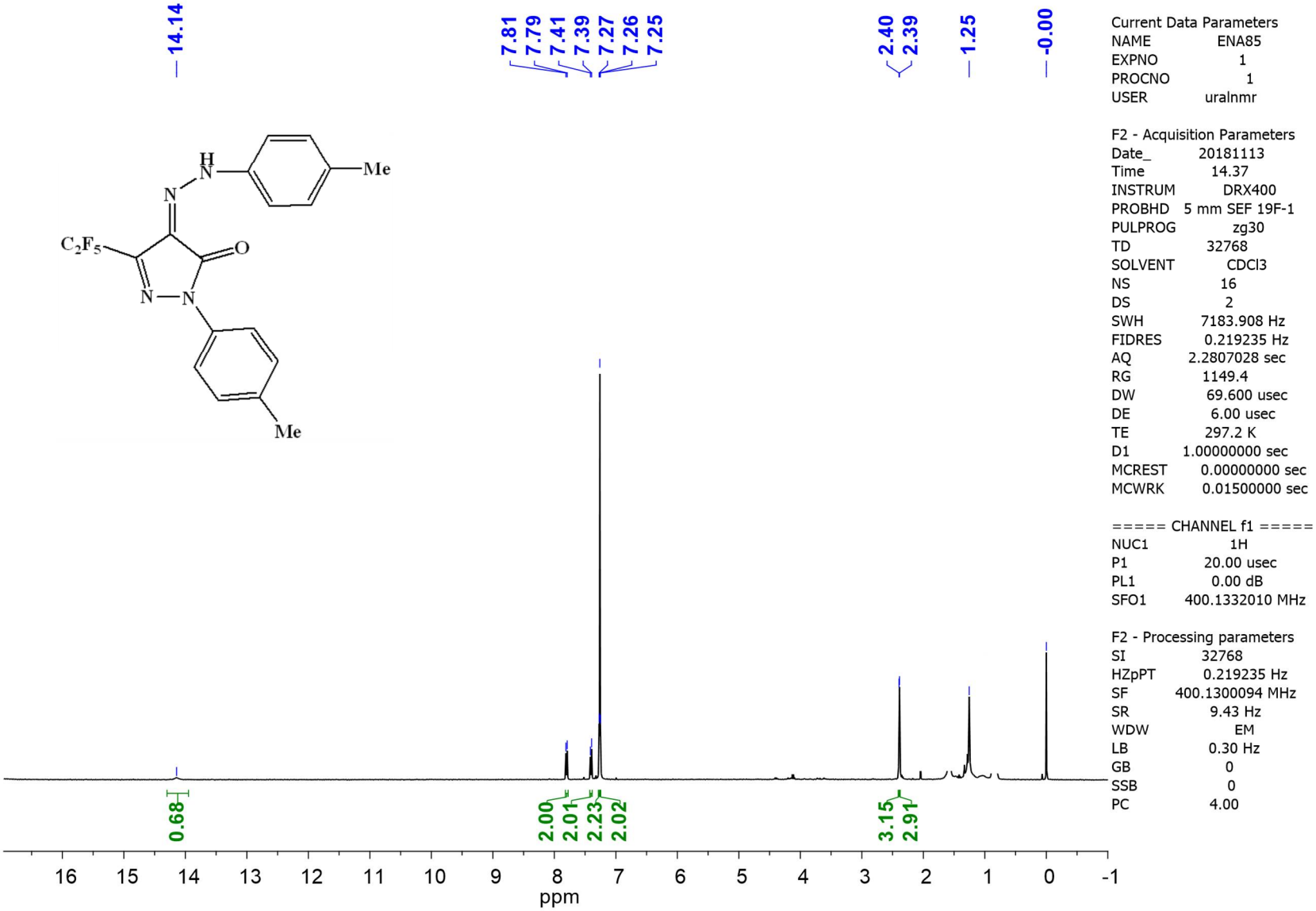
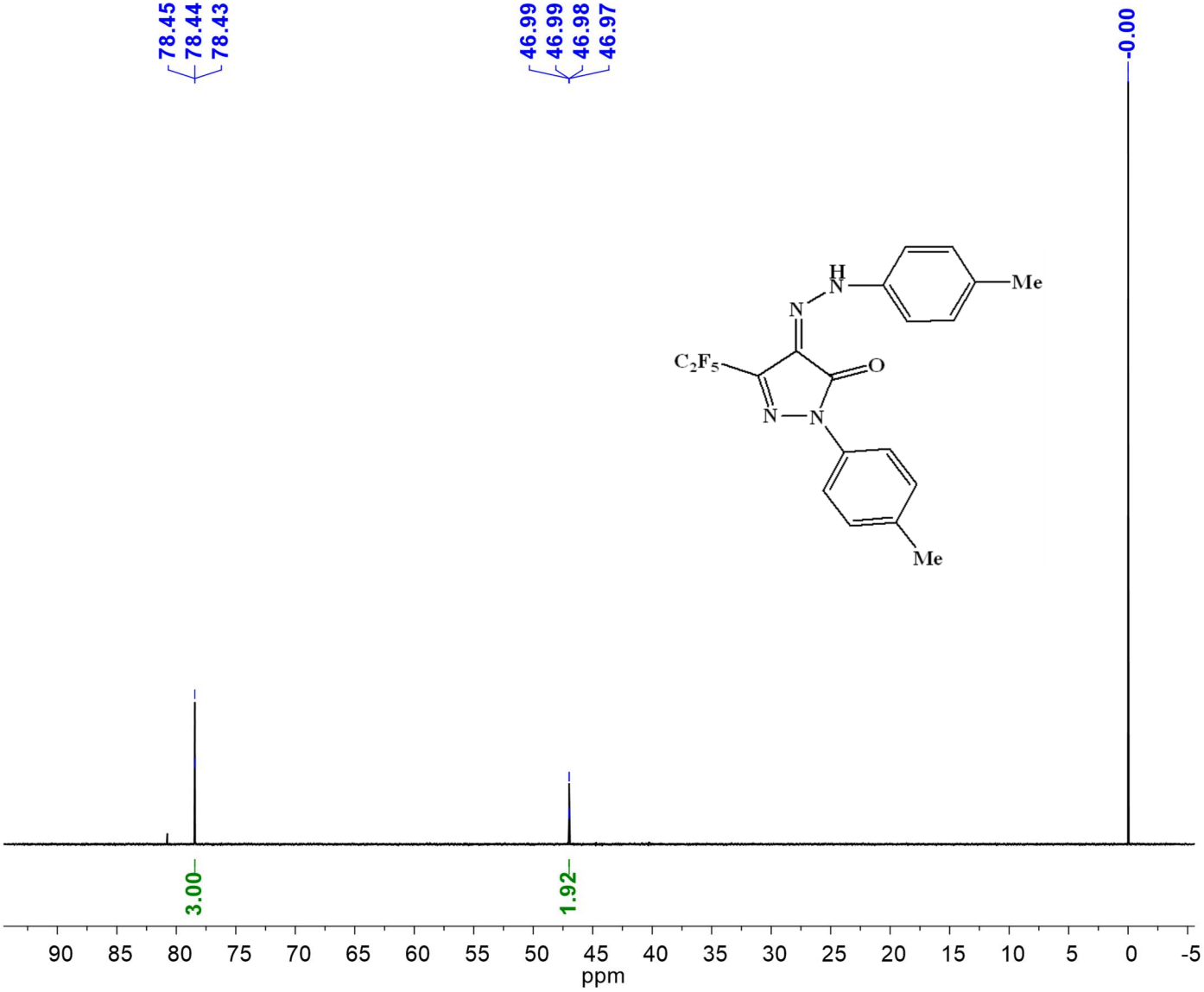


Figure S78. ^{19}F NMR spectrum of compound **6i**



Current Data Parameters
NAME ENA85
EXPNO 19
PROCNO 1
USER uralnmr

F2 - Acquisition Parameters
Date_ 20181113
Time 14.43
INSTRUM DRX400
PROBHD 5 mm SEF 19F-1
PULPROG zg30
TD 131072
SOLVENT CDCl3
NS 16
DS 2
SWH 37664.785 Hz
FIDRES 0.287360 Hz
AQ 1.7400308 sec
RG 6502
DW 13.275 usec
DE 6.50 usec
TE 297.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 ====
NUC1 19F
P1 10.10 usec
PL1 0.00 dB
SFO1 376.4542247 MHz

F2 - Processing parameters
SI 131072
HZpPT 0.287360 Hz
SF 376.4374871 MHz
SR 202.09 Hz
WDW EM
LB 0.00 Hz
GB 0
SSB 0
PC 2.00

Figure S79. ^{1}H NMR spectrum of compound **7a**

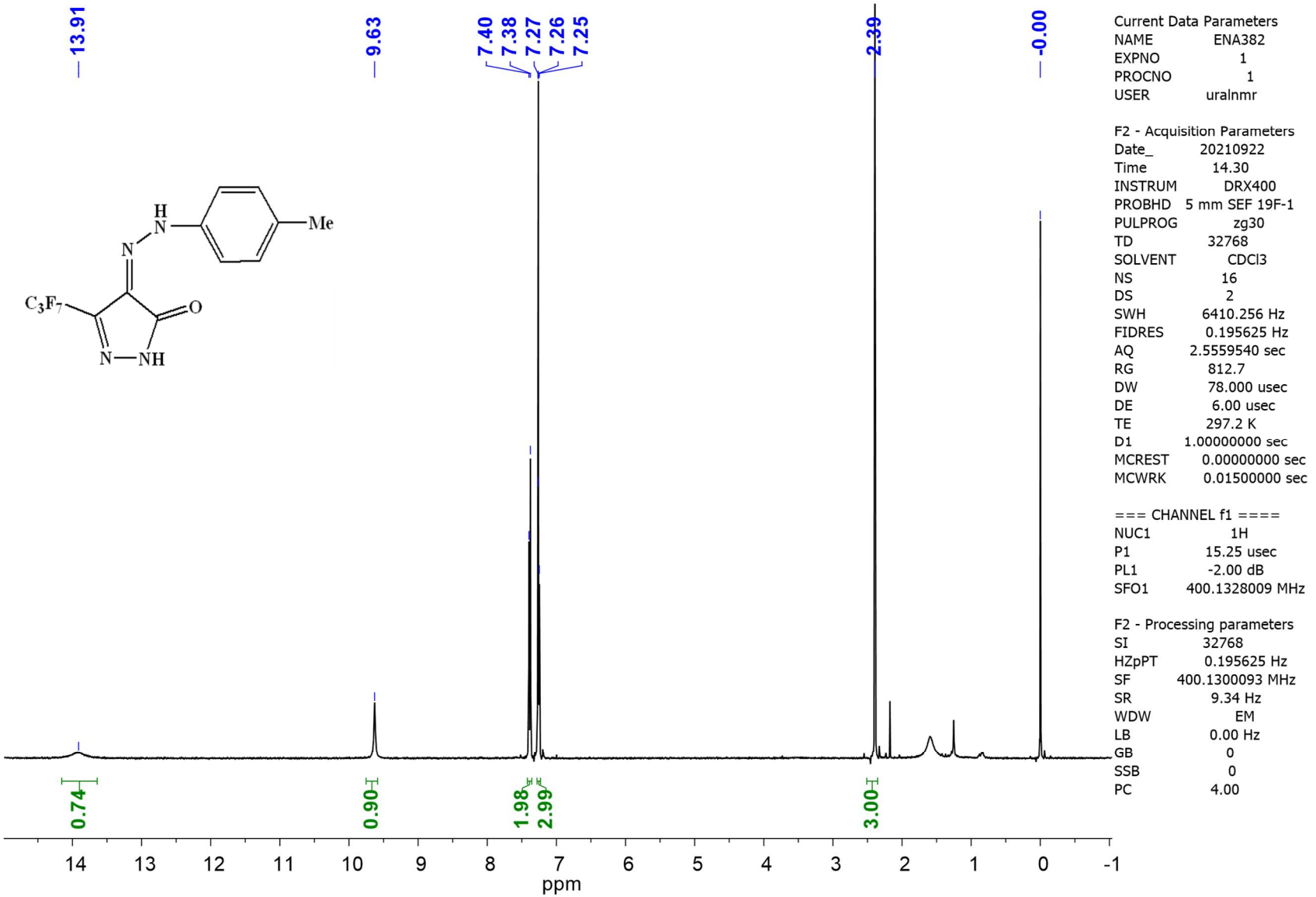
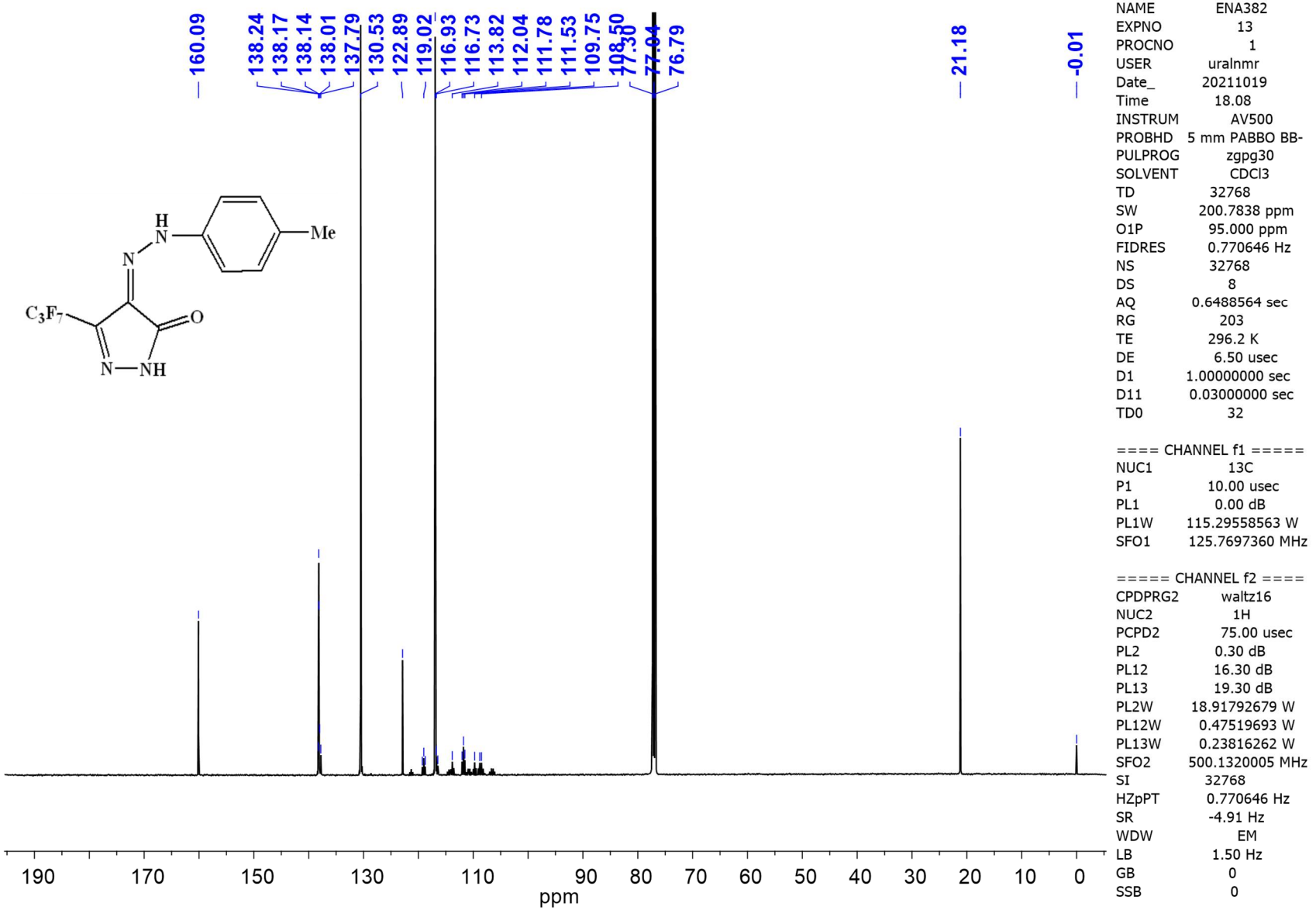


Figure S80. ^{13}C NMR spectrum of compound **7a**



NAME	ENA382
EXPNO	13
PROCNO	1
USER	uralnmr
Date_	20211019
Time	18.08
INSTRUM	AV500
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
SOLVENT	CDCl3
TD	32768
SW	200.7838 ppm
O1P	95.000 ppm
FIDRES	0.770646 Hz
NS	32768
DS	8
AQ	0.6488564 sec
RG	203
TE	296.2 K
DE	6.50 usec
D1	1.00000000 sec
D11	0.03000000 sec
TD0	32
==== CHANNEL f1 =====	
NUC1	13C
P1	10.00 usec
PL1	0.00 dB
PL1W	115.29558563 W
SFO1	125.7697360 MHz
===== CHANNEL f2 ====	
CPDPRG2	waltz16
NUC2	1H
PCPD2	75.00 usec
PL2	0.30 dB
PL12	16.30 dB
PL13	19.30 dB
PL2W	18.91792679 W
PL12W	0.47519693 W
PL13W	0.23816262 W
SFO2	500.1320005 MHz
SI	32768
HZpPT	0.770646 Hz
SR	-4.91 Hz
WDW	EM
LB	1.50 Hz
GB	0
SSB	0

Figure S81. ^{19}F NMR spectrum of compound **7a**

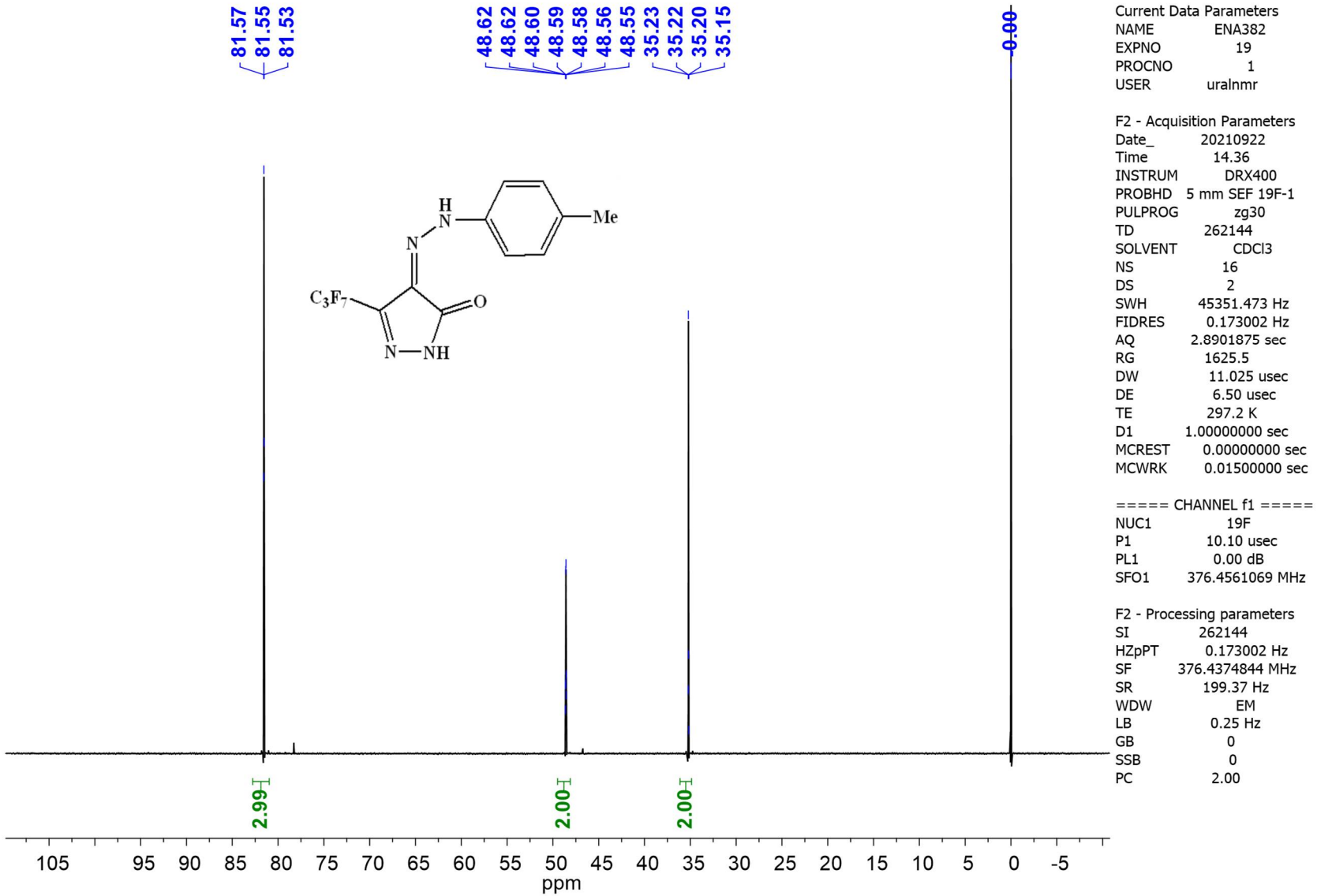
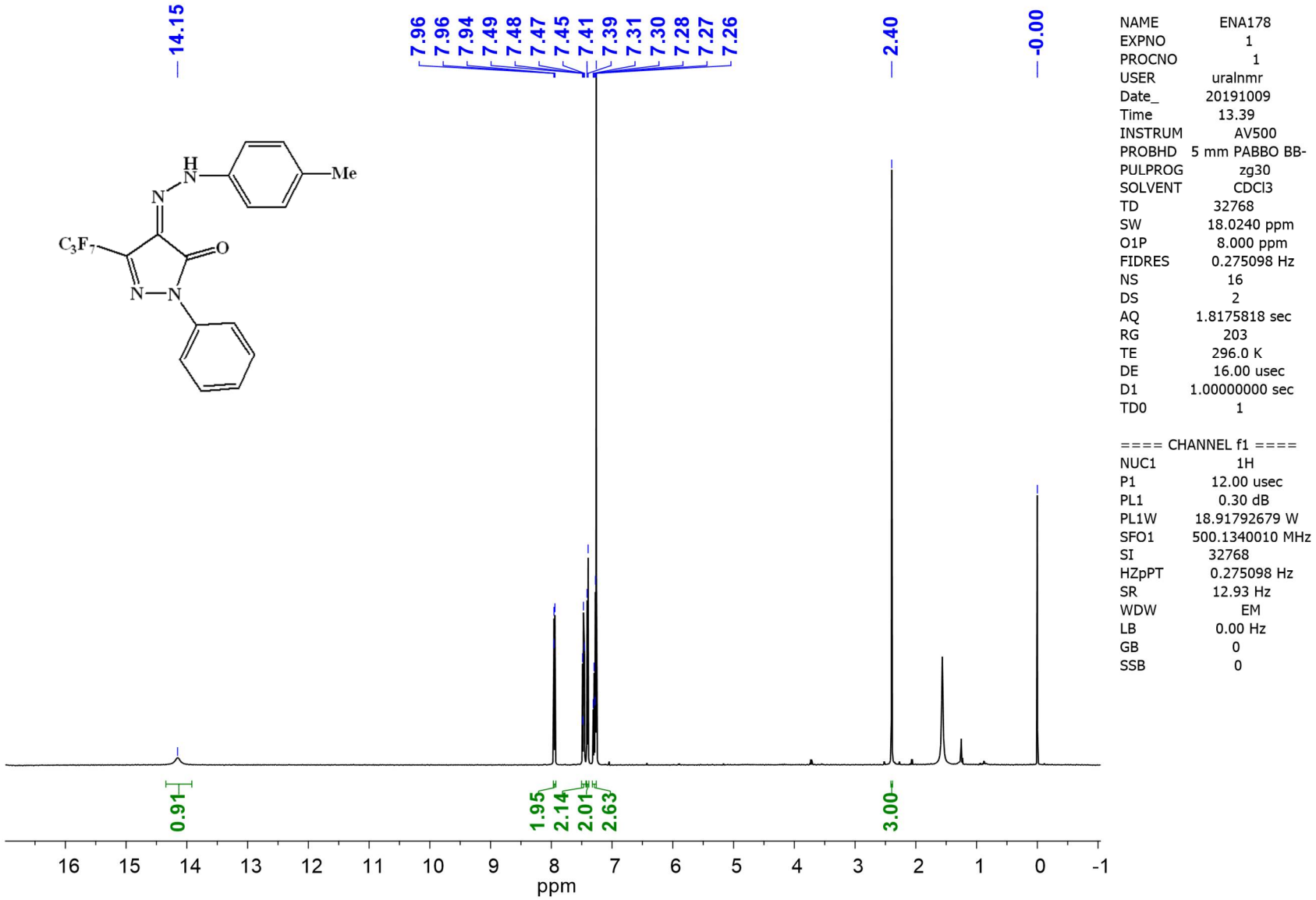
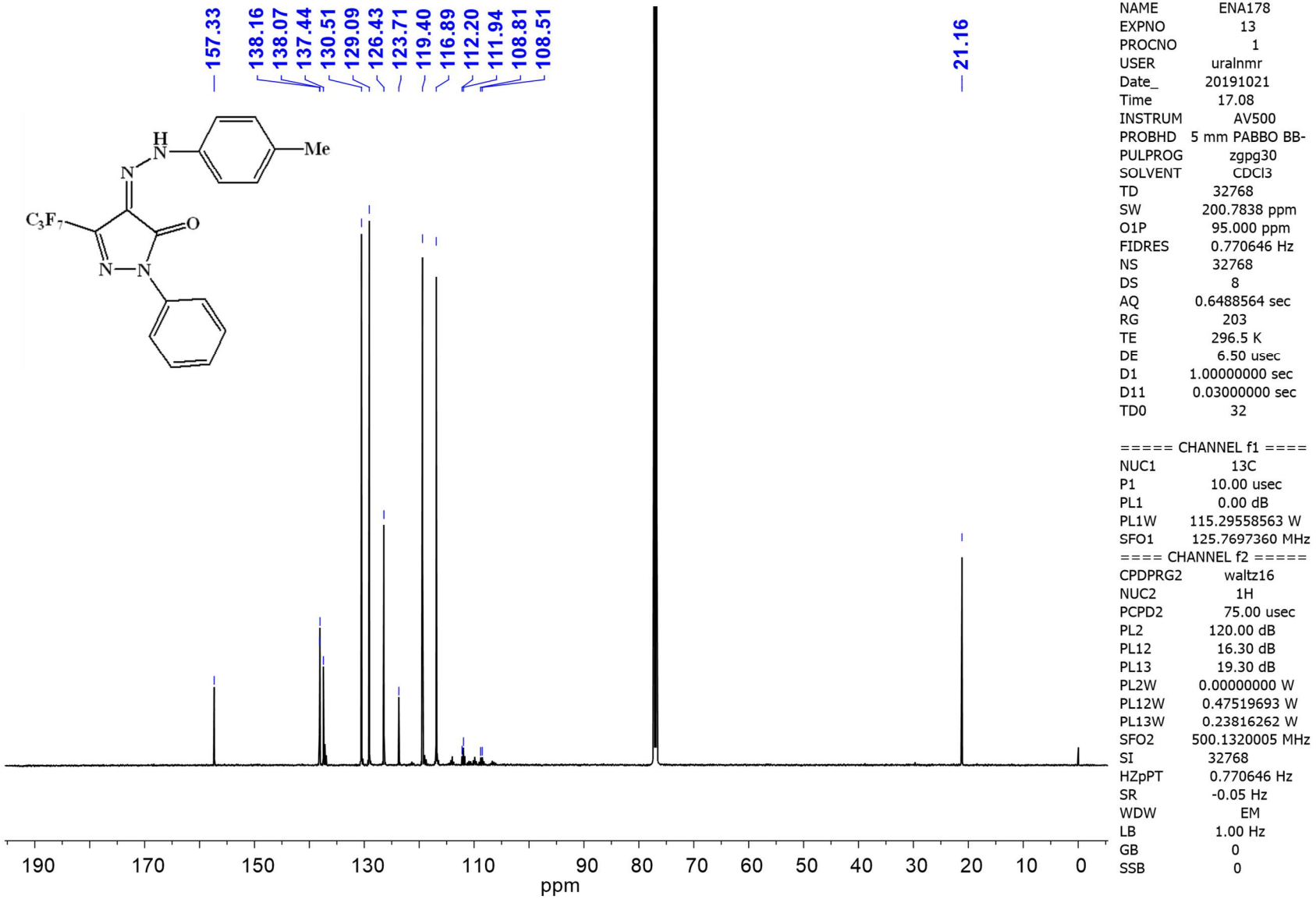


Figure S82. ^{1}H NMR spectrum of compound **7b**



NAME	ENA178
EXPNO	1
PROCNO	1
USER	uralnmr
Date_	20191009
Time	13.39
INSTRUM	AV500
PROBHD	5 mm PABBO BB-
PULPROG	zg30
SOLVENT	CDCl3
TD	32768
SW	18.0240 ppm
O1P	8.000 ppm
FIDRES	0.275098 Hz
NS	16
DS	2
AQ	1.8175818 sec
RG	203
TE	296.0 K
DE	16.00 usec
D1	1.00000000 sec
TD0	1
==== CHANNEL f1 ====	
NUC1	1H
P1	12.00 usec
PL1	0.30 dB
PL1W	18.91792679 W
SFO1	500.1340010 MHz
SI	32768
HZpPT	0.275098 Hz
SR	12.93 Hz
WDW	EM
LB	0.00 Hz
GB	0
SSB	0

Figure S83. ^{13}C NMR spectrum of compound **7b**



NAME	ENA178
EXPNO	13
PROCNO	1
USER	uralnmr
Date_	20191021
Time	17.08
INSTRUM	AV500
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
SOLVENT	CDCl3
TD	32768
SW	200.7838 ppm
O1P	95.000 ppm
FIDRES	0.770646 Hz
NS	32768
DS	8
AQ	0.6488564 sec
RG	203
TE	296.5 K
DE	6.50 usec
D1	1.00000000 sec
D11	0.03000000 sec
TD0	32
===== CHANNEL f1 ====	
NUC1	13C
P1	10.00 usec
PL1	0.00 dB
PL1W	115.29558563 W
SFO1	125.7697360 MHz
==== CHANNEL f2 =====	
CPDPRG2	waltz16
NUC2	1H
PCPD2	75.00 usec
PL2	120.00 dB
PL12	16.30 dB
PL13	19.30 dB
PL2W	0.00000000 W
PL12W	0.47519693 W
PL13W	0.23816262 W
SFO2	500.1320005 MHz
SI	32768
HZpPT	0.770646 Hz
SR	-0.05 Hz
WDW	EM
LB	1.00 Hz
GB	0
SSB	0

Figure S84. ^{19}F NMR spectrum of compound **7b**

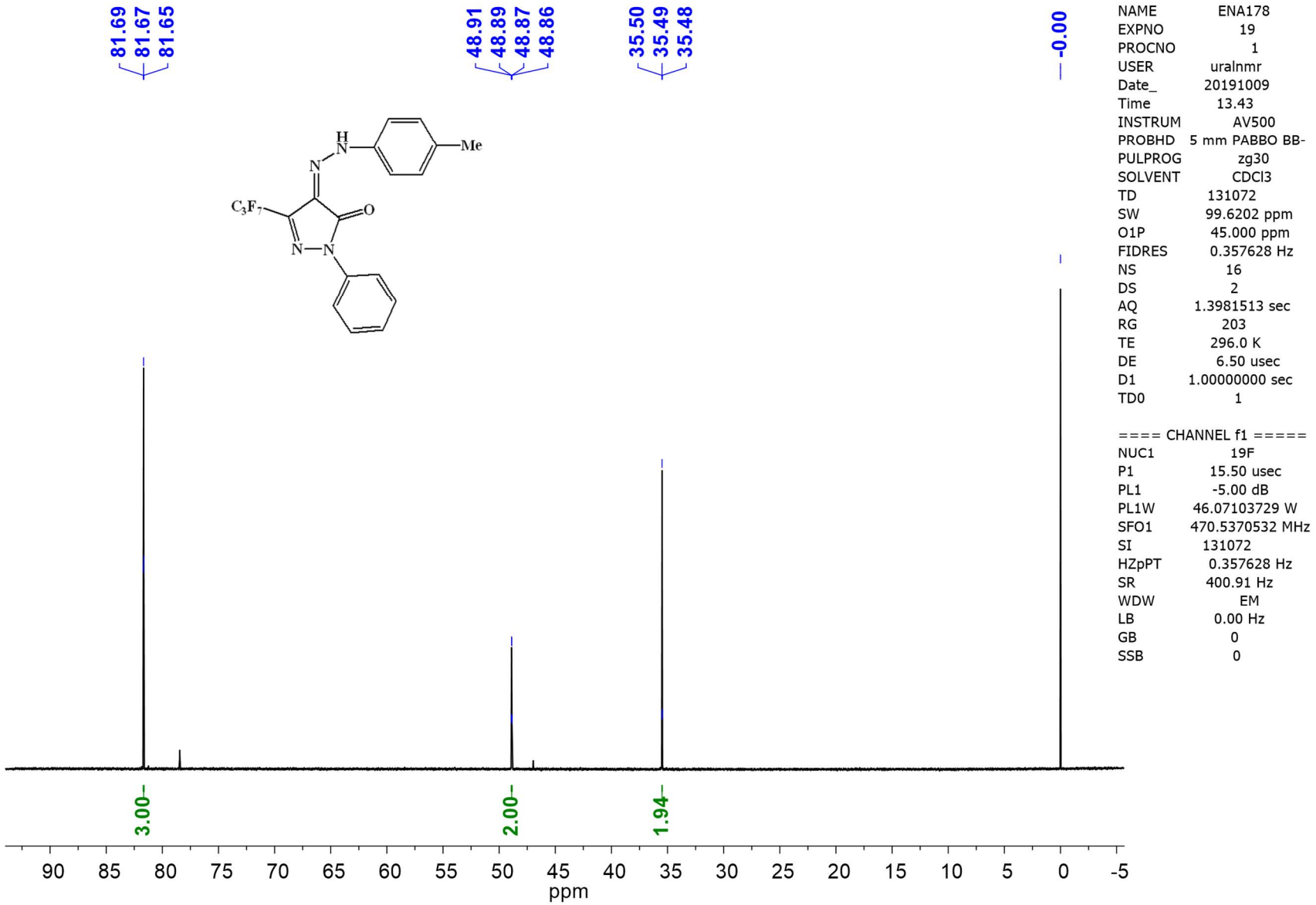


Figure S85. ^{1}H NMR spectrum of compound **8a**

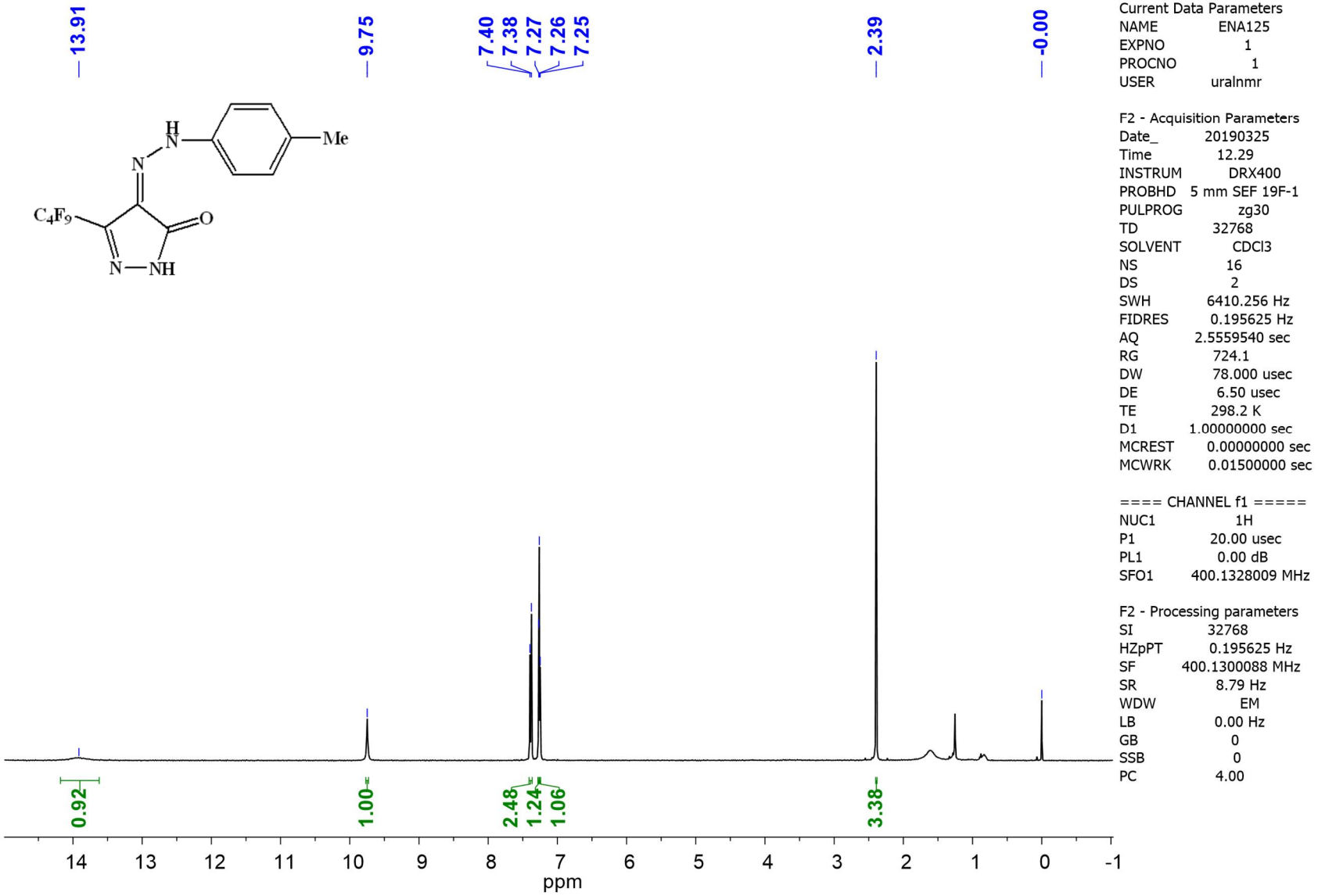
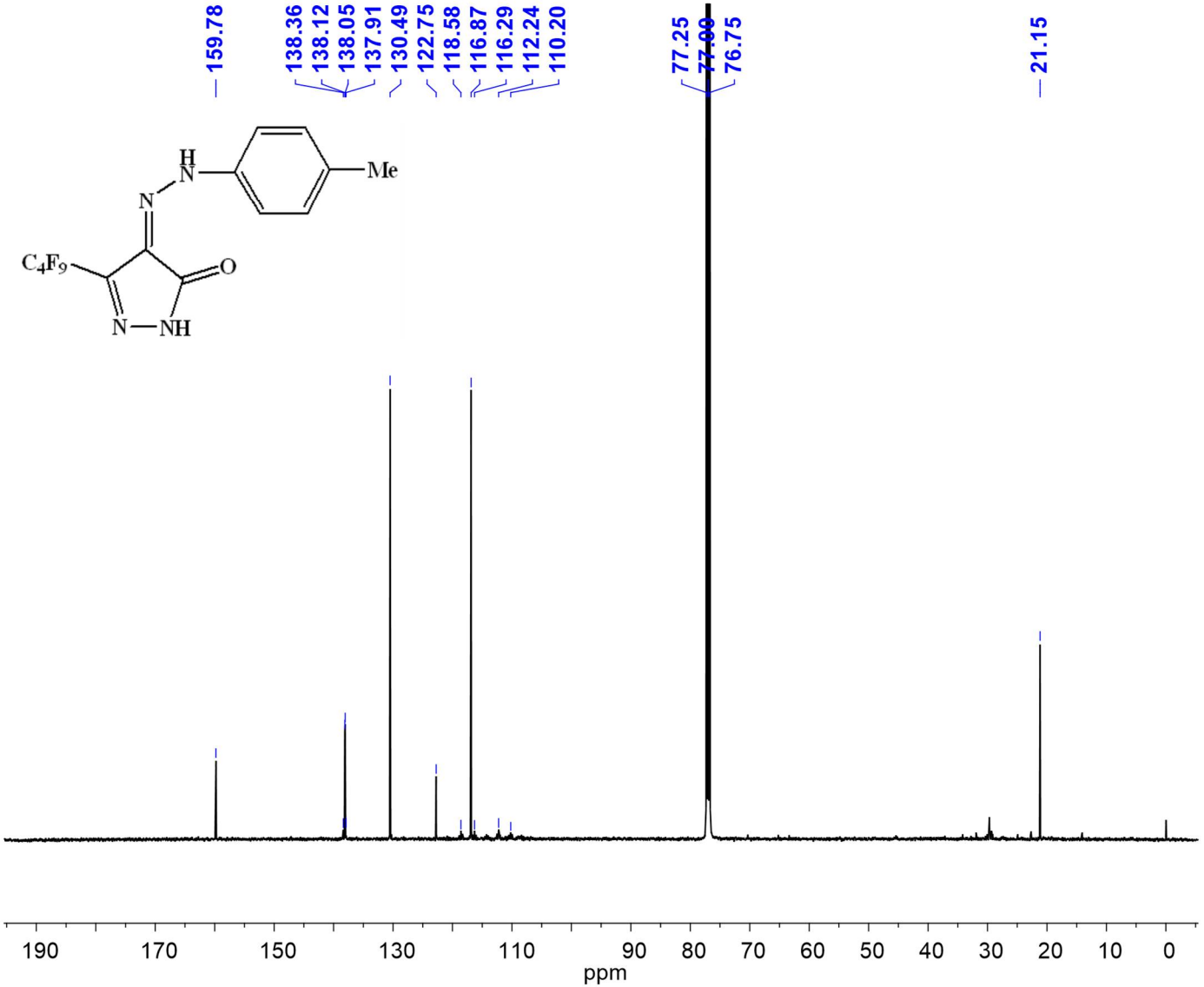


Figure S86. ^{13}C NMR spectrum of compound **8a**



NAME	ENA125
EXPNO	13
PROCNO	1
USER	uralnmr
Date_	20190531
Time	17.57
INSTRUM	AV500
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
SOLVENT	CDCl3
TD	65536
SW	200.7838 ppm
O1P	95.000 ppm
FIDRES	0.385323 Hz
NS	49152
DS	8
AQ	1.2976629 sec
RG	203
TE	296.7 K
DE	6.50 usec
D1	1.00000000 sec
D11	0.03000000 sec
TD0	48
==== CHANNEL f1 ======	
NUC1	13C
P1	10.00 usec
PL1	0.00 dB
PL1W	115.29558563 W
SFO1	125.7697360 MHz
===== CHANNEL f2 ======	
CPDPRG2	waltz16
NUC2	1H
PCPD2	75.00 usec
PL2	120.00 dB
PL12	16.30 dB
PL13	19.30 dB
PL2W	0.00000000 W
PL12W	0.47519693 W
PL13W	0.23816262 W
SFO2	500.1320005 MHz
SI	65536
HZpPT	0.385323 Hz
SR	-0.58 Hz
WDW	EM
LB	1.00 Hz
GB	0
SSB	0

Figure S87. ^{19}F NMR spectrum of compound **8a**

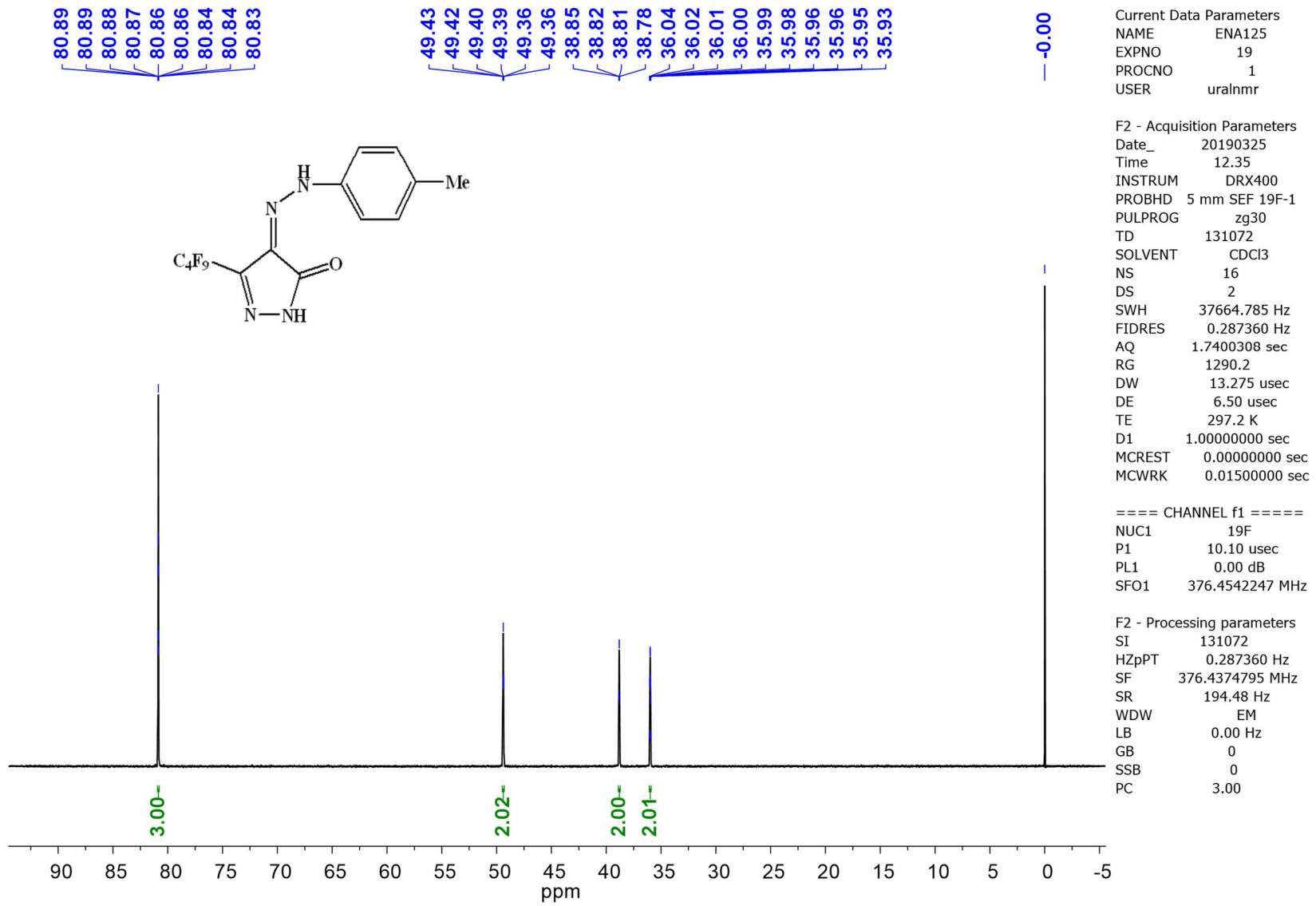


Figure S88. ^{1}H NMR spectrum of compound **8b**

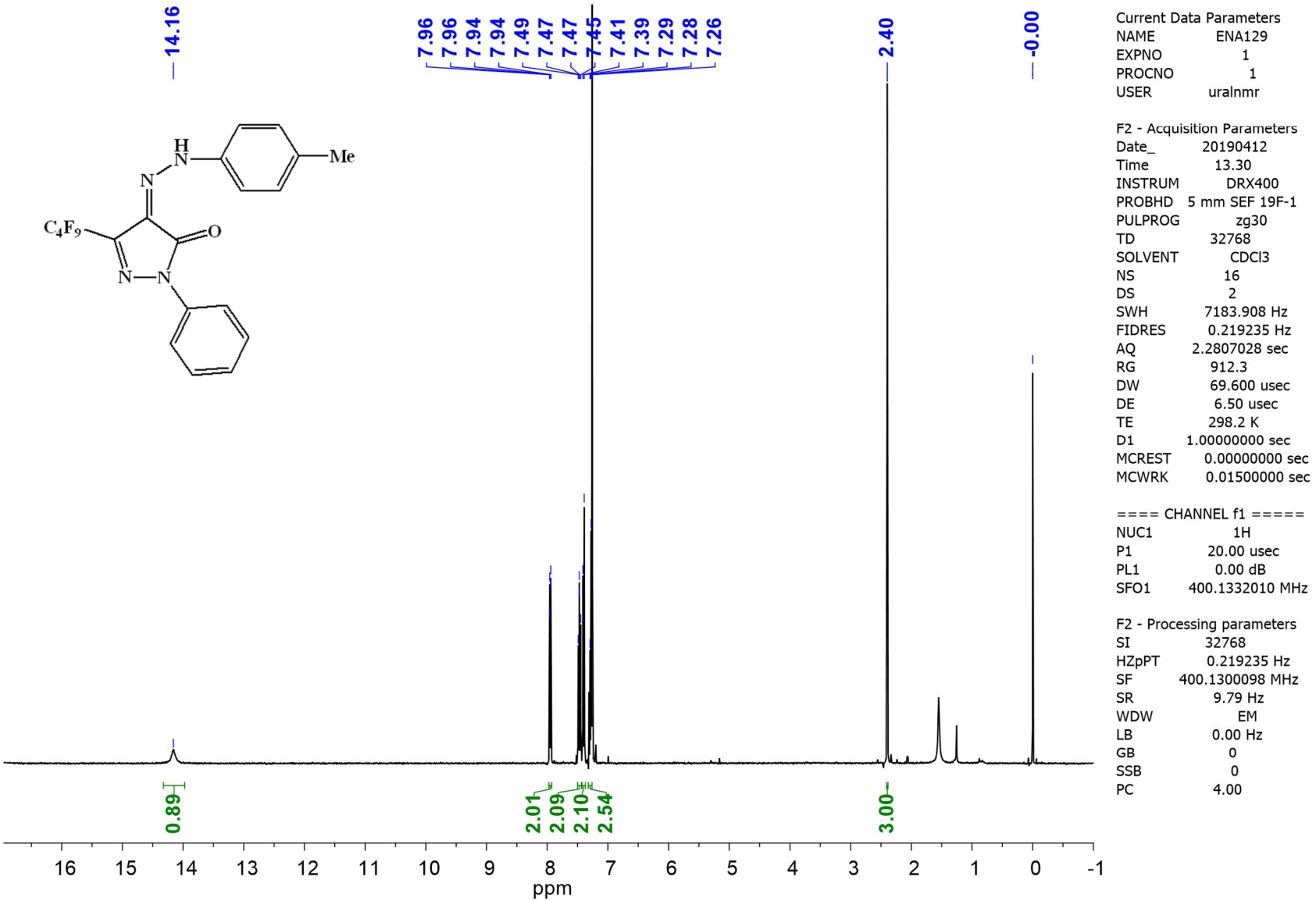
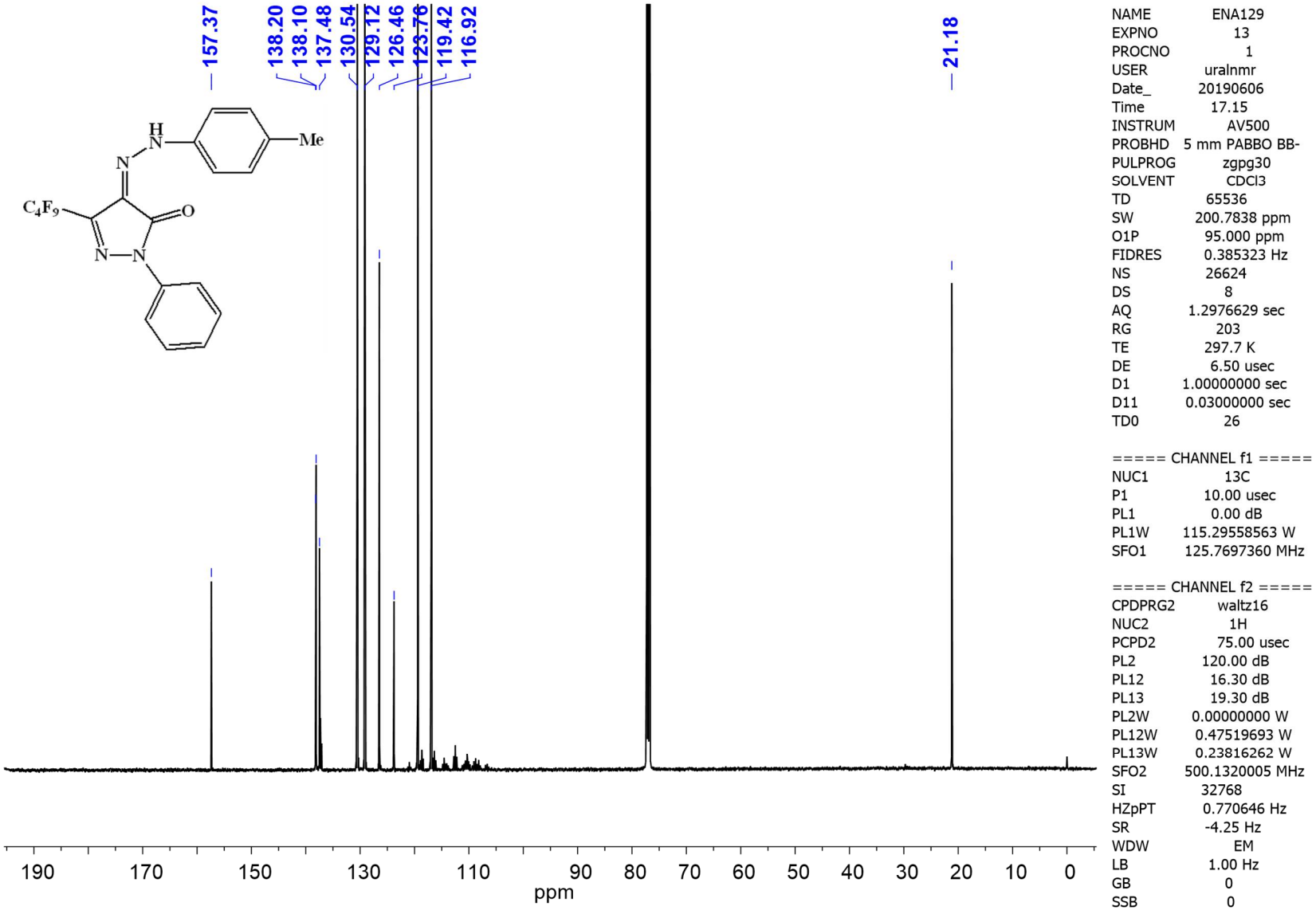


Figure S89. ^{13}C NMR spectrum of compound **8b**



NAME	ENA129
EXPNO	13
PROCNO	1
USER	uralnmr
Date_	20190606
Time	17.15
INSTRUM	AV500
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
SOLVENT	CDCl3
TD	65536
SW	200.7838 ppm
O1P	95.000 ppm
FIDRES	0.385323 Hz
NS	26624
DS	8
AQ	1.2976629 sec
RG	203
TE	297.7 K
DE	6.50 usec
D1	1.00000000 sec
D11	0.03000000 sec
TD0	26
===== CHANNEL f1 =====	
NUC1	13C
P1	10.00 usec
PL1	0.00 dB
PL1W	115.29558563 W
SFO1	125.7697360 MHz
===== CHANNEL f2 =====	
CPDPRG2	waltz16
NUC2	1H
PCPD2	75.00 usec
PL2	120.00 dB
PL12	16.30 dB
PL13	19.30 dB
PL2W	0.00000000 W
PL12W	0.47519693 W
PL13W	0.23816262 W
SFO2	500.1320005 MHz
SI	32768
HZpPT	0.770646 Hz
SR	-4.25 Hz
WDW	EM
LB	1.00 Hz
GB	0
SSB	0

Figure S90. ^{19}F NMR spectrum of compound **8b**

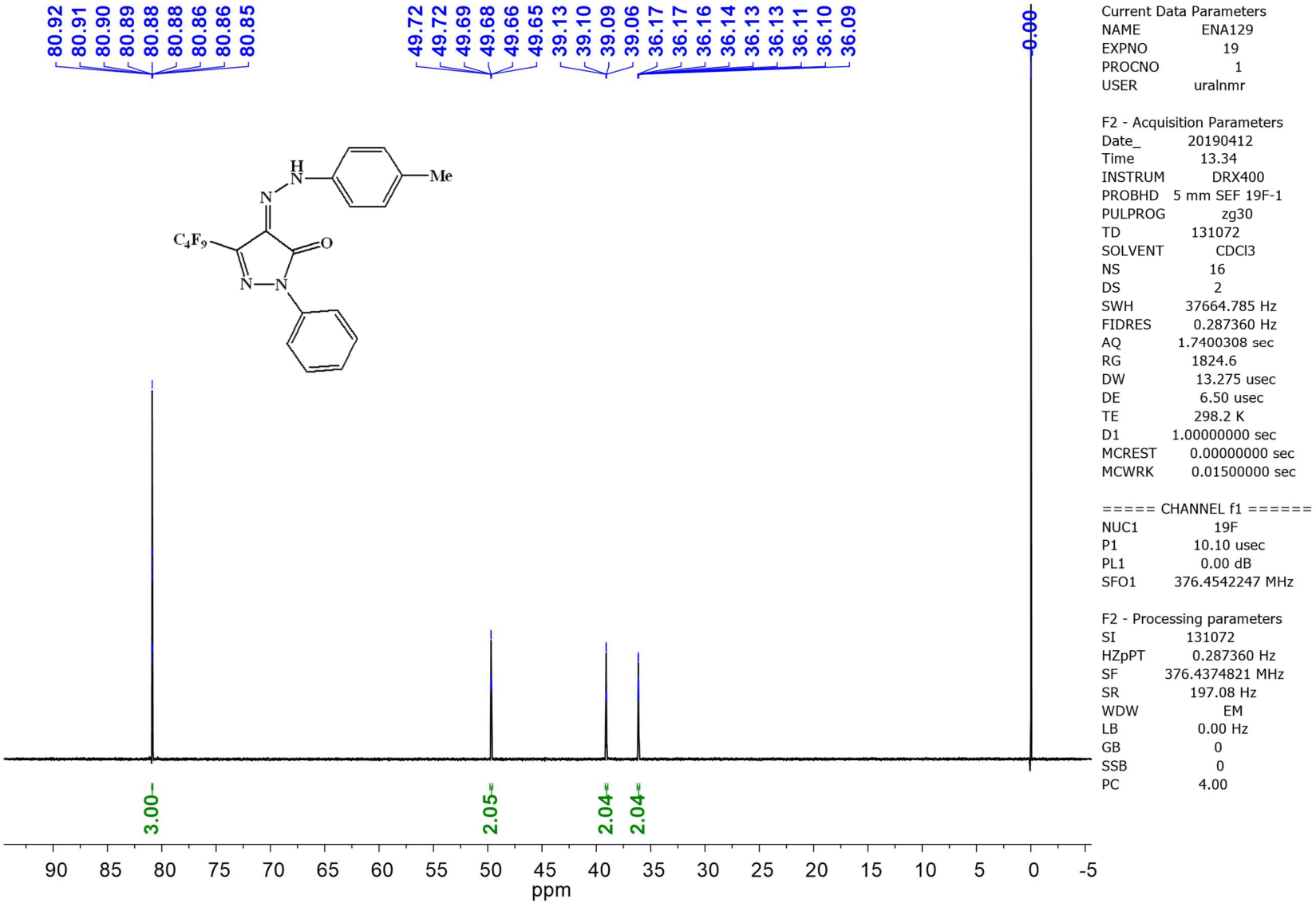
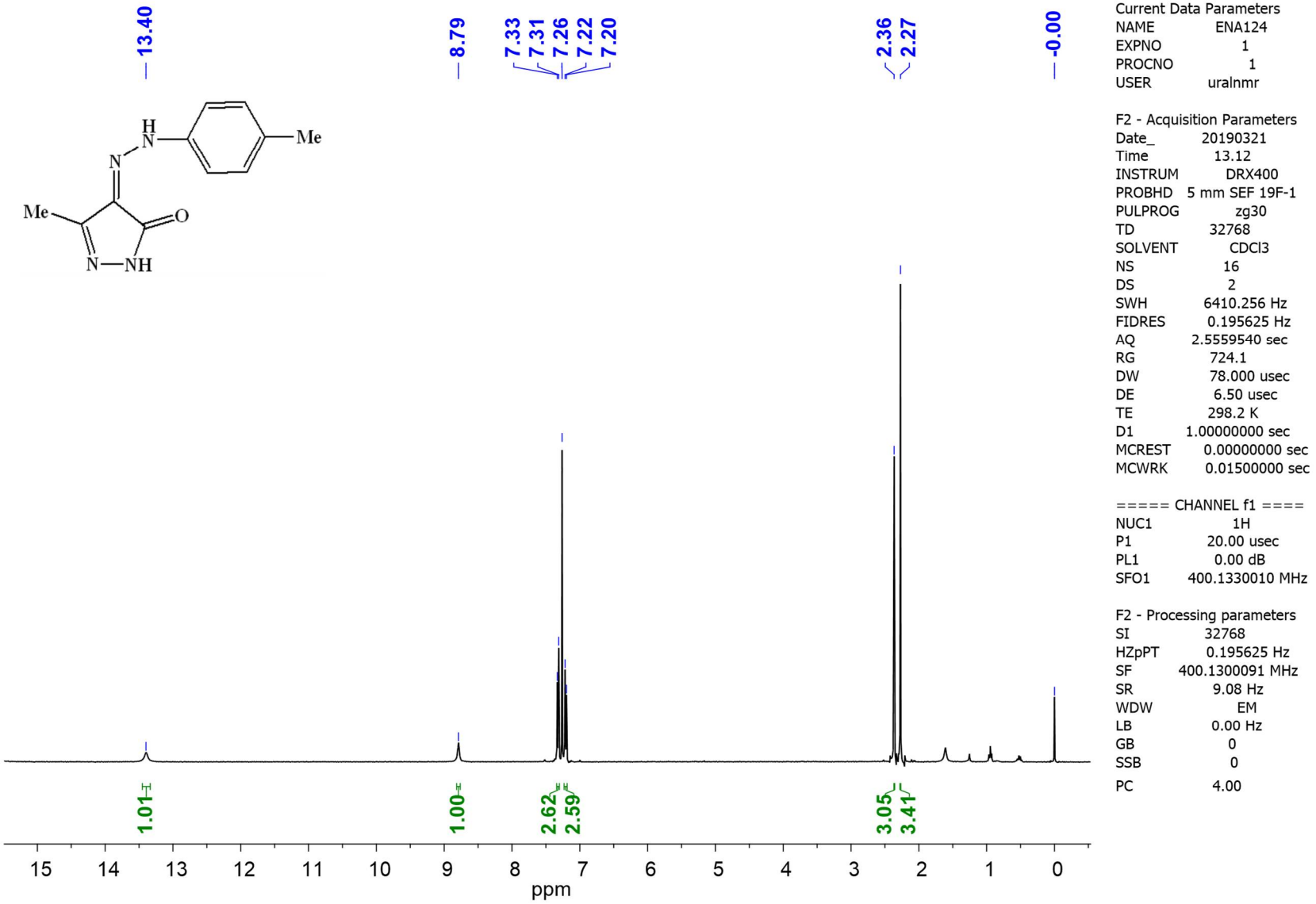


Figure S91. ^{1}H NMR spectrum of compound **9a**



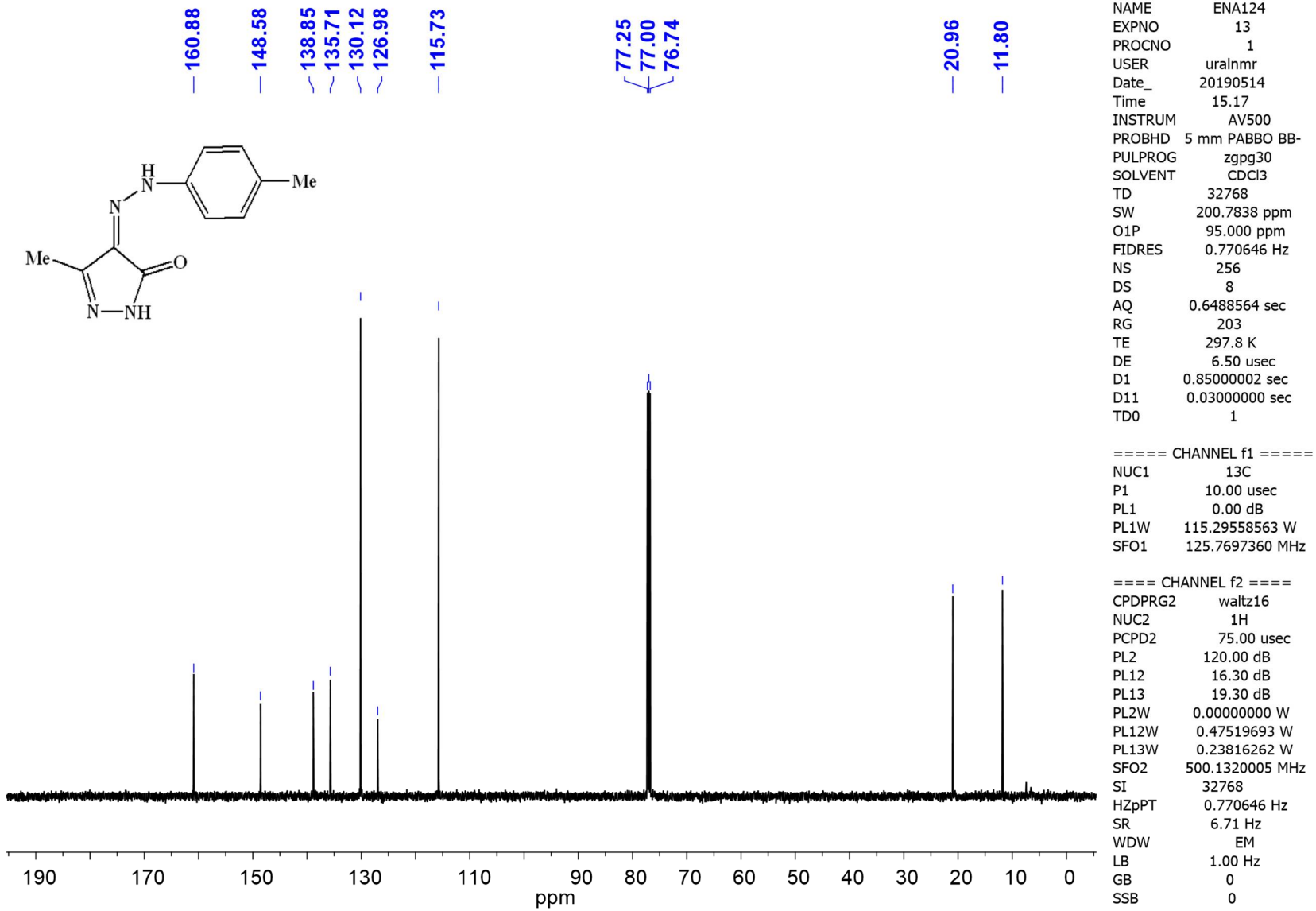
Current Data Parameters
NAME ENA124
EXPNO 1
PROCNO 1
USER uralnmr

F2 - Acquisition Parameters
Date_ 20190321
Time 13.12
INSTRUM DRX400
PROBHD 5 mm SEF 19F-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 724.1
DW 78.000 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 ====
NUC1 1H
P1 20.00 usec
PL1 0.00 dB
SFO1 400.1330010 MHz

F2 - Processing parameters
SI 32768
HZpPT 0.195625 Hz
SF 400.1300091 MHz
SR 9.08 Hz
WDW EM
LB 0.00 Hz
GB 0
SSB 0
PC 4.00

Figure S92. ^{13}C NMR spectrum of compound **9a**



NAME	ENA124
EXPNO	13
PROCNO	1
USER	uralnmr
Date_	20190514
Time	15.17
INSTRUM	AV500
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
SOLVENT	CDCl3
TD	32768
SW	200.7838 ppm
O1P	95.000 ppm
FIDRES	0.770646 Hz
NS	256
DS	8
AQ	0.6488564 sec
RG	203
TE	297.8 K
DE	6.50 usec
D1	0.85000002 sec
D11	0.03000000 sec
TD0	1
===== CHANNEL f1 =====	
NUC1	13C
P1	10.00 usec
PL1	0.00 dB
PL1W	115.29558563 W
SFO1	125.7697360 MHz
==== CHANNEL f2 ====	
CPDPRG2	waltz16
NUC2	1H
PCPD2	75.00 usec
PL2	120.00 dB
PL12	16.30 dB
PL13	19.30 dB
PL2W	0.00000000 W
PL12W	0.47519693 W
PL13W	0.23816262 W
SFO2	500.1320005 MHz
SI	32768
HZpPT	0.770646 Hz
SR	6.71 Hz
WDW	EM
LB	1.00 Hz
GB	0
SSB	0

Figure S93. ^{1}H NMR spectrum of compound **9b**

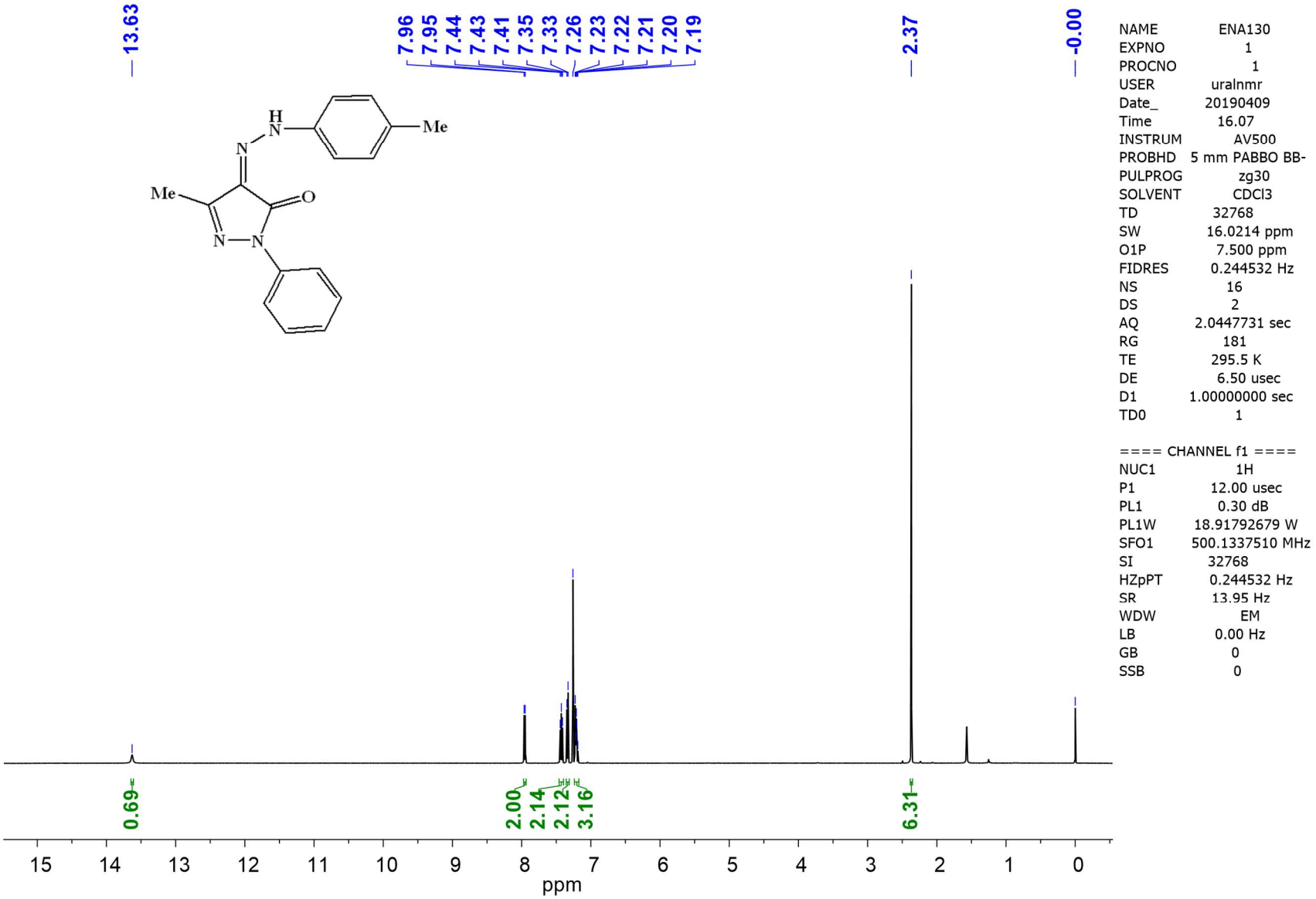


Figure S94. ^{13}C NMR spectrum of compound **9b**