

Potent and Selective Indole-based Inhibitors Targeting Disease-Transmitting Mosquitoes

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In silico predictions and cell viability assay

Table S1. In silico predictions of selected indole-based inhibitors against toxicity endpoints^a

Compound	Toxicity end points		
	Cytotoxicity	Mutagenicity	Carcinogenicity
8	Inactive (0.61)	Inactive (0.59)	Inactive (0.64)
9	Active (0.50)	Active (0.57)	Inactive (0.61)
10	Inactive (0.70)	Active (0.95)	Active (0.66)
15	Inactive (0.53)	Inactive (0.63)	Inactive (0.63)
16	Active (0.52)	Inactive (0.54)	Inactive (0.61)
18	Inactive (0.58)	Inactive (0.61)	Inactive (0.67)

^a The toxicity end points were predicted with ProTox 3.0 (<https://tox.charite.de/protox3/>)

Table S2. In silico assessment of selected indole-based inhibitors for physicochemical properties and lead-likeness^a

ID	MW	TPSA	iLOGP	XLOGP3	ESOL Solubility (mg/ml)	ESOL Class	PAINS #alerts	Lead likeness #violations	Lipinski #violations
8	280.36	37.05	2.81	3.34	4.29e-02	Soluble	0	0	0
9	294.39	26.19	3.55	3.30	4.13e-02	Soluble	0	0	0
10	296.34	78.22	2.38	2.54	1.22e-01	Soluble	0	0	0
15	344.84	46.28	3.27	3.94	1.19e-02	Moderately soluble	0	1	0
16	358.86	35.42	3.91	3.90	1.12e-02	Moderately soluble	0	2	0
18	314.81	37.05	2.89	3.97	1.25e-02	Moderately soluble	0	1	0

^a The in silico assessment was made with SwissADME (<https://www.swissadme.ch/>)

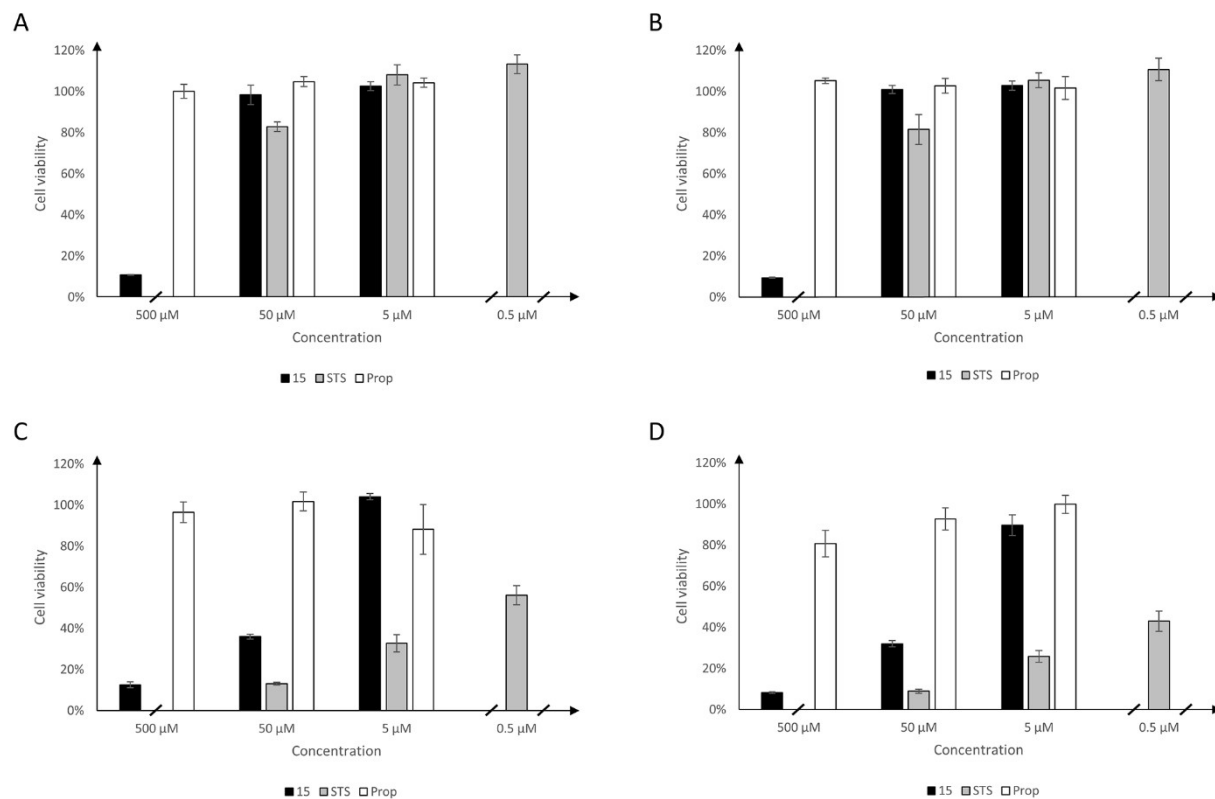


Figure S1. Assessment of cell viability after exposure to different concentrations of inhibitor **15** using the resazurin assay. (A-B) *Spodoptera frugiperda* (Sf9) insect cells. (C-D) Human embryonic kidney (HEK293) cells. Cells were exposed to three concentrations of inhibitor **15** for 24 h on two separate occasions, and viability was assessed using the resazurin reduction assay. Staurosporine (STS) and propranolol (Prop) were included as reference cytotoxic controls. Cell viability is expressed as a percentage relative to untreated controls. Data represent the mean $\pm$ SD of three independent experiments ($n = 3$).

Starting material structures

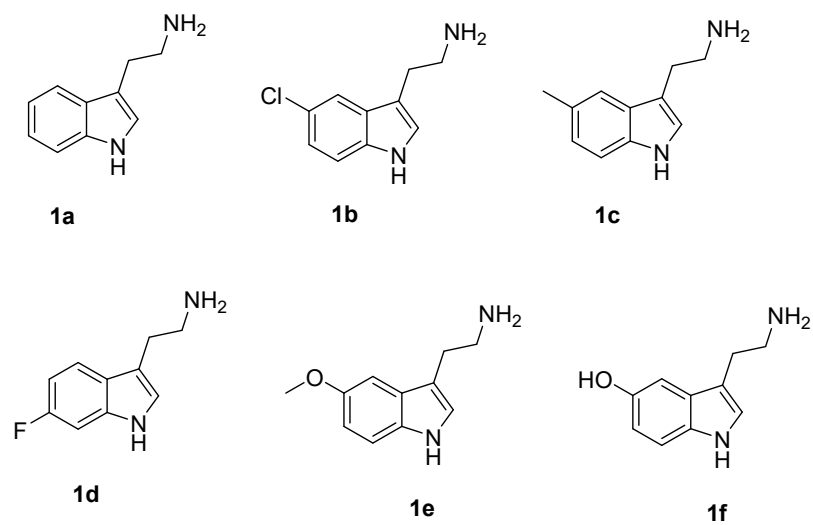


Figure S2. Indoles (**1a-f**) as starting materials.

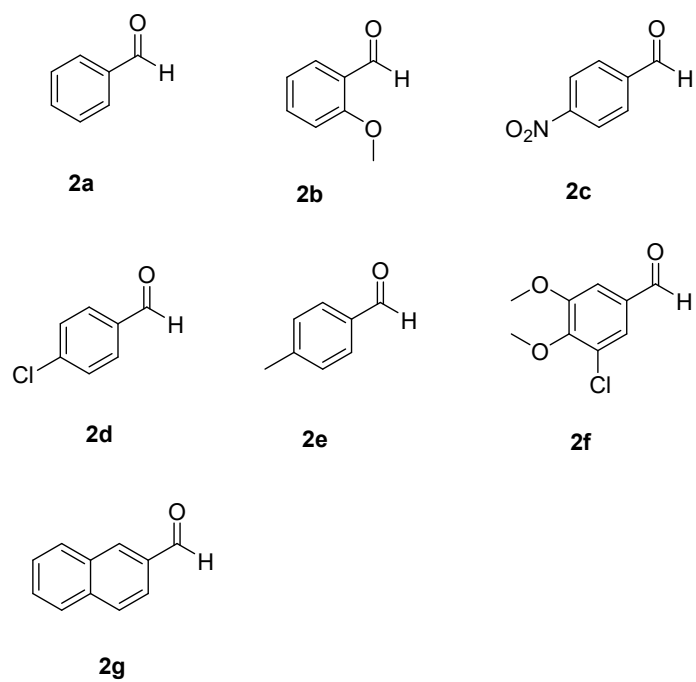
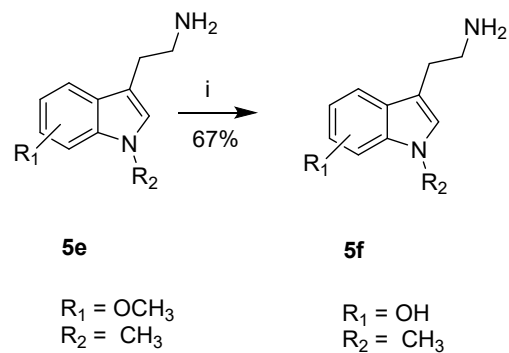
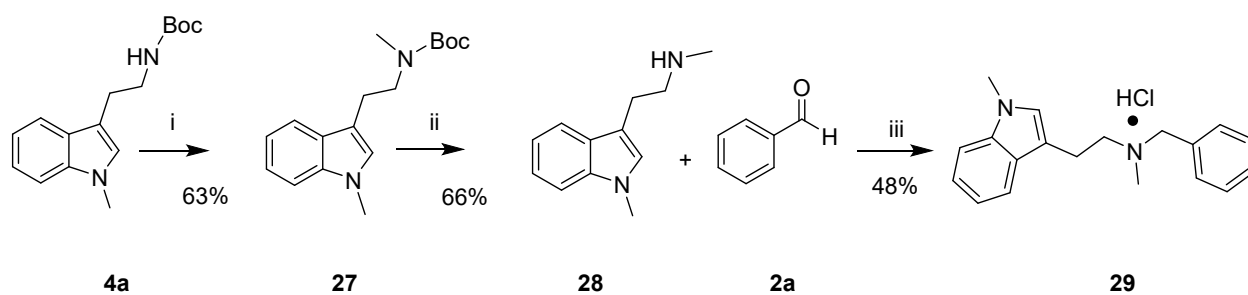


Figure S3. Aldehydes (**2a-g**) as starting materials.

Supplementary synthetic schemes



Scheme S1. Reagent and conditions: i) BBr_3 , DCM -70°C -rt, 12h.



Scheme S2. Reagent and conditions: i) NaH , DMF 0°C - 90°C ; CH_3I , 0°C -rt, 12h. ii) TFA, DCM 0°C -rt, 5h. iii) EtOH or MeOH, reflux, 12h; NaBH_4 , 0°C -rt; 12h 2M HCl in ether.

Dose-response-curves for inhibition kinetics

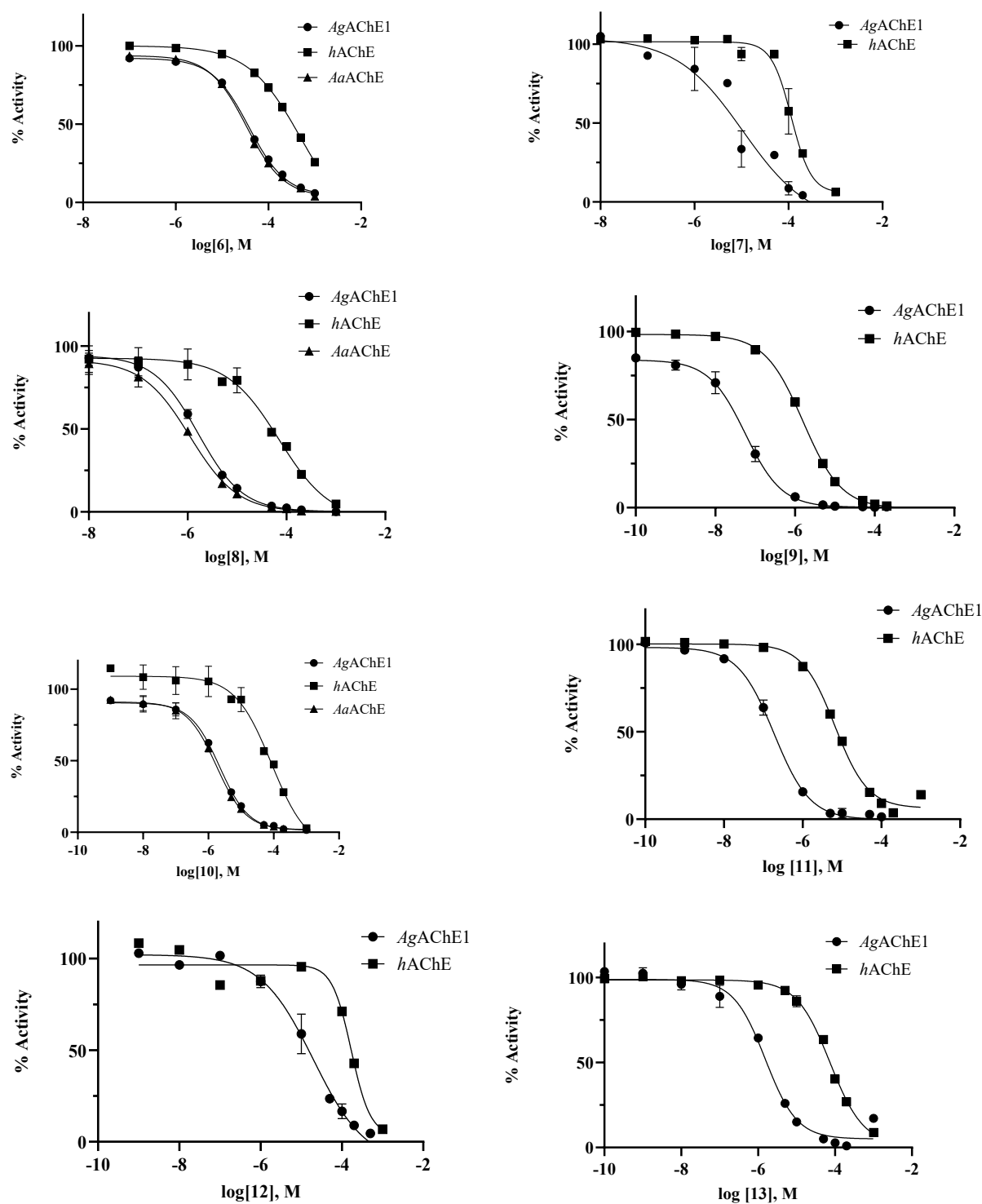


Figure S4. Dose response curves showing the inhibition of AgAChE1 (dots), AaAChE1 (triangle), and hAChE (squares) at different concentrations of inhibitors.

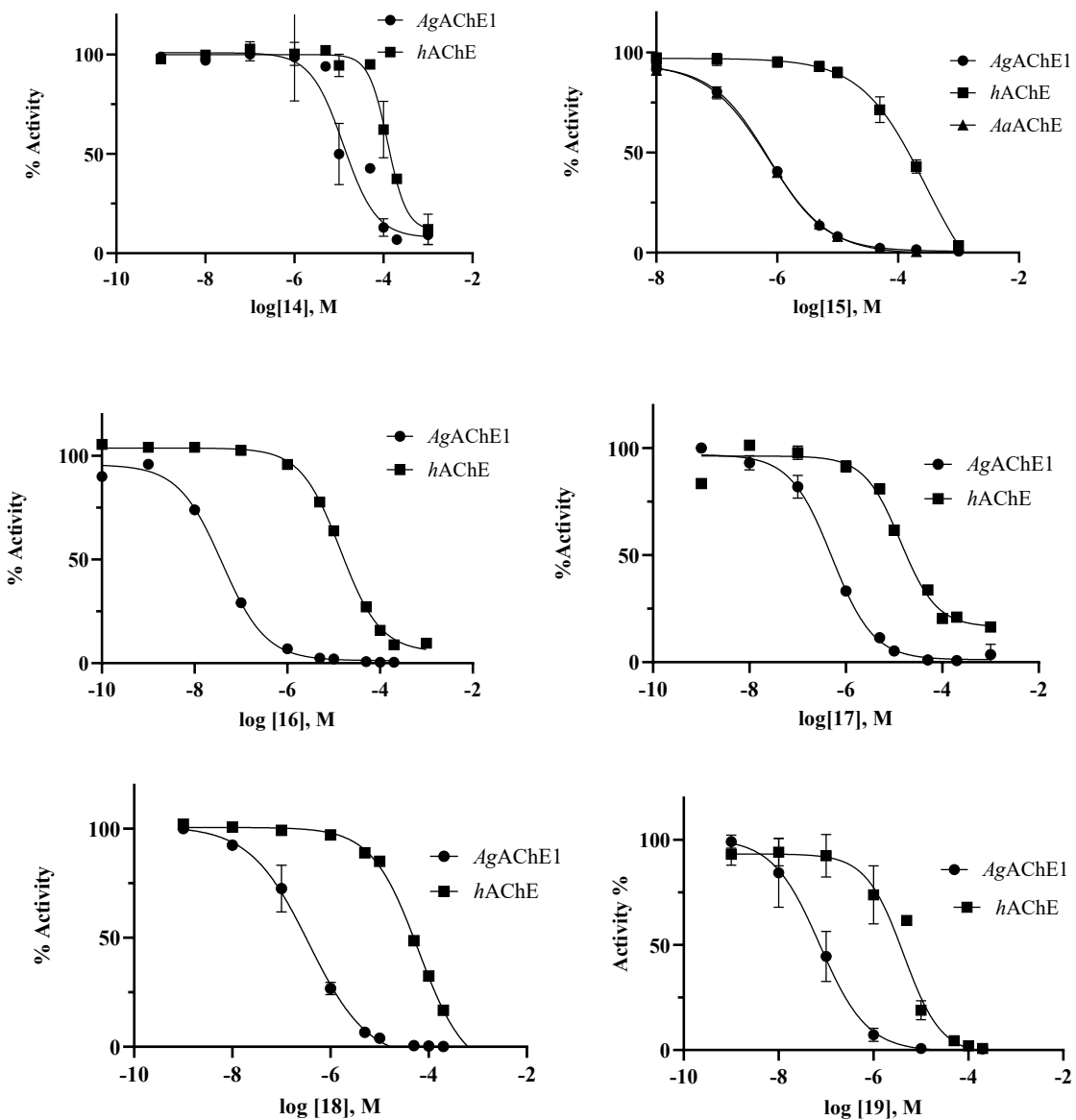


Figure S4 continued. Dose response curves showing the inhibition of *AgAChE1* (dots), *AaAChE1* (triangle), and *hAChE* (squares) at different concentrations of inhibitors.

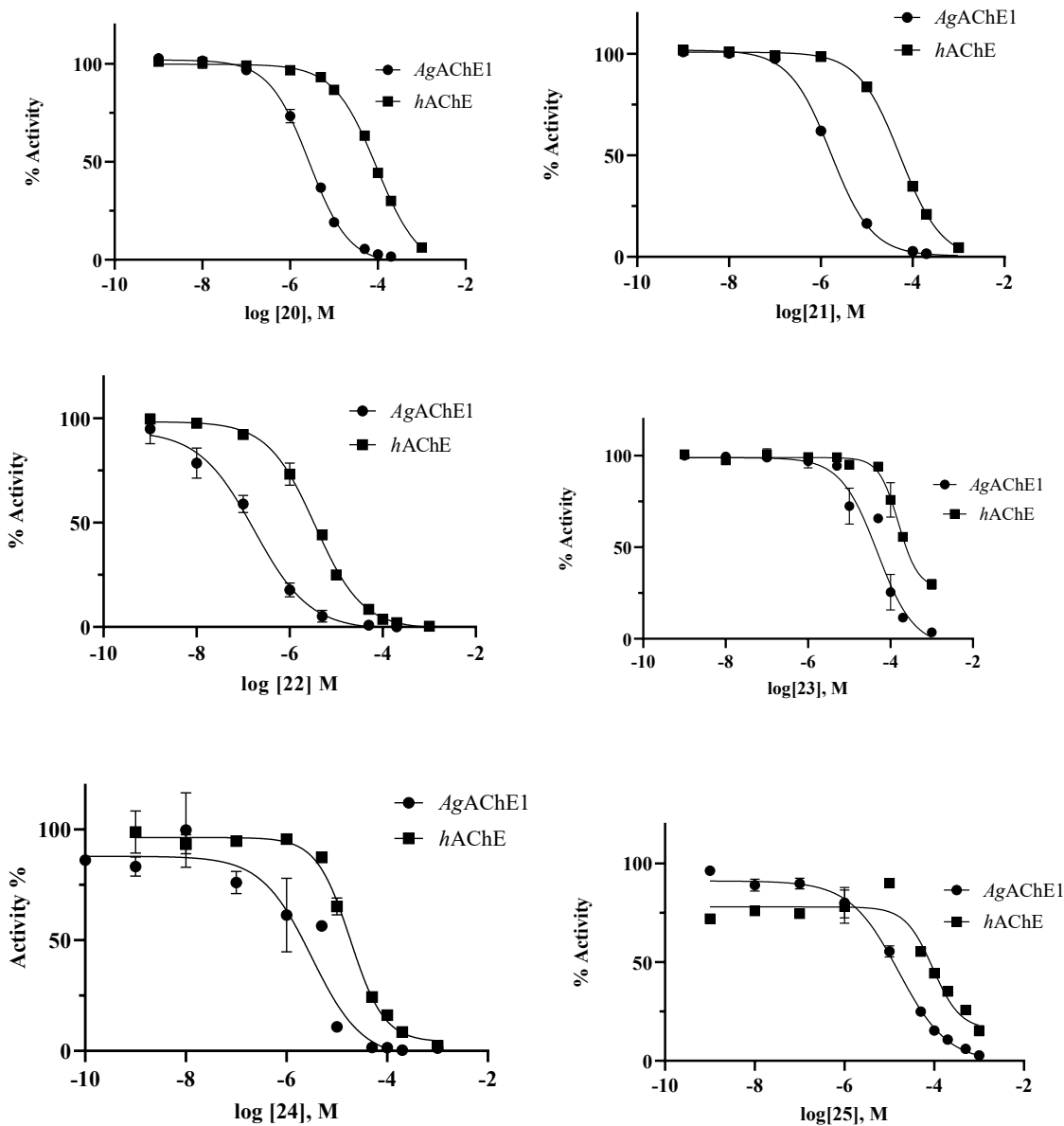


Figure S4 continued. Dose response curves showing the inhibition of *AgAChE1* (dots), *AaAChE1* (triangle), and *hAChE* (squares) at different concentrations of inhibitors.

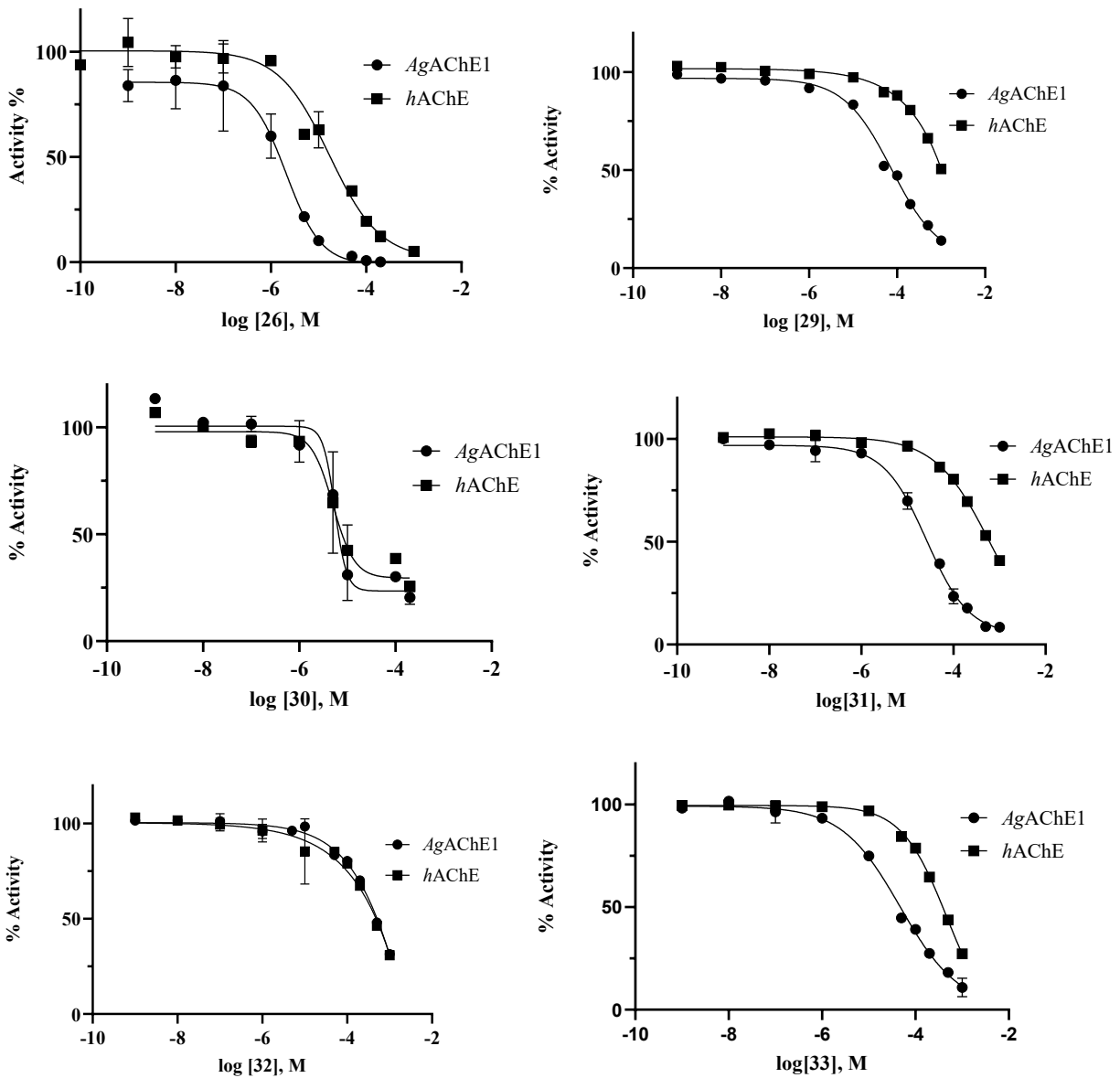


Figure S4 continued. Dose response curves showing the inhibition of AgAChE1 (dots), AaAChE1 (triangle), and hAChE (squares) at different concentrations of inhibitors.

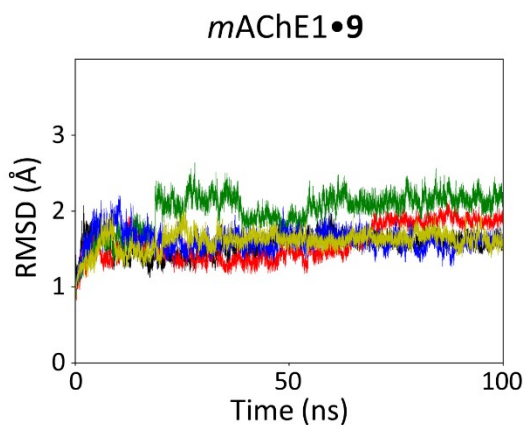
X-ray crystallography

Table S3. Data collection and refinement statistics

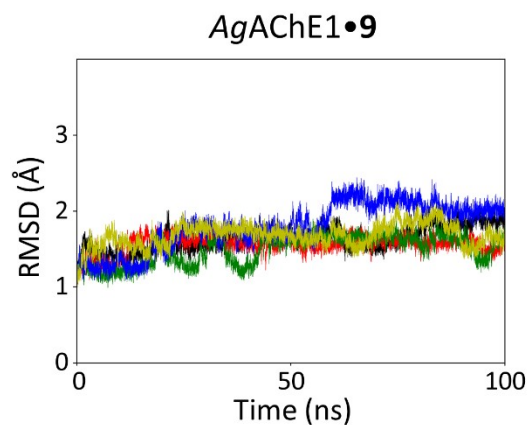
	<i>m</i>AChE•8	<i>m</i>AChE•9
PDB entry code	9SND	9SNJ
Resolution range (Å)	29.68 - 2.4 (2.48 - 2.4)	29.27 - 2.3 (2.36 - 2.3)
Space group	P 21 21 21	P 21 21 21
Unit cell	78.353 111.104 227.383 90 90 90	79.493 112.581 227.811 90 90 90
Total reflections	596475 (40287)	678925 (49391)
Unique reflections	168071 (11817)	190385 (14316)
Multiplicity	3.5 (3.4)	3.6 (3.5)
Completeness (%)	99.34 (99.08)	99.68 (99.29)
Mean I/sigma (I)	7.78 (0.96)	8.40 (1.49)
Wilson B-factor	48.62	47.39
R-merge	0.08845 (0.8472)	0.07242 (0.6556)
R-meas	0.1043 (1.002)	0.08531 (0.7763)
R-pim	0.05486 (0.5298)	0.04464 (0.4103)
CC1/2	0.996 (0.823)	0.996 (0.894)
CC*	0.999 (0.95)	0.999 (0.972)
Reflections used in refinement	77905 (6982)	91241 (6880)
Reflections used for R-free	1533 (115)	1798 (142)
R-work	0.2088 (0.3090)	0.1795 (0.2382)
R-free	0.2232 (0.2973)	0.2033 (0.2826)
Number of non-hydrogen atoms	8772	8866
macromolecules	8356	8373
Ligands	163	135
Solvent	253	358
Protein residues	1068	1068
RMS (bonds)	0.002	0.002
RMS (angles)	0.57	0.60
Ramachandran favored (%)	95.85	96.42
Ramachandran allowed (%)	3.49	2.92
Ramachandran outliers (%)	0.66	0.66
Rotamer outliers (%)	0.23	0.34
Clashscore	2.20	1.55
Average B-factor	64.44	64.96
Macromolecules	64.41	65.06
Ligands	79.14	70.23
Solvent	56.45	60.64

MD simulations data

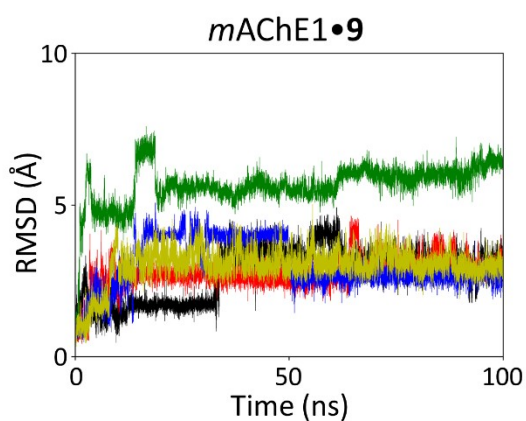
A



B



C



D

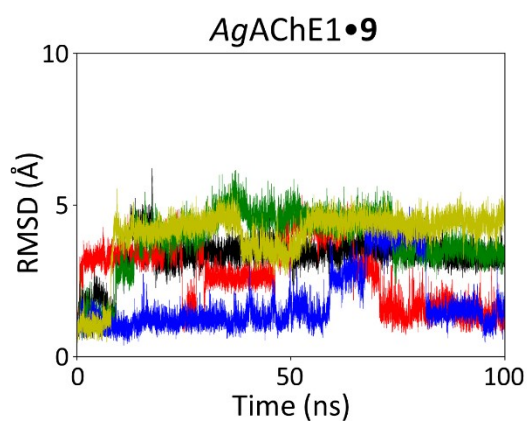


Figure S5. Root mean square deviation (RMSD) values vs simulation time for each MD simulation. (A) RMSD for protein mainchain atoms, for *m*AChE•**9**. (B) RMSD for protein mainchain atoms, for *Ag*AChE1•**9**. (C) RMSD for inhibitor **9** heavy atoms, for *m*AChE•**9**. (D) RMSD for inhibitor **9** heavy atoms, for *Ag*AChE1•**9**.

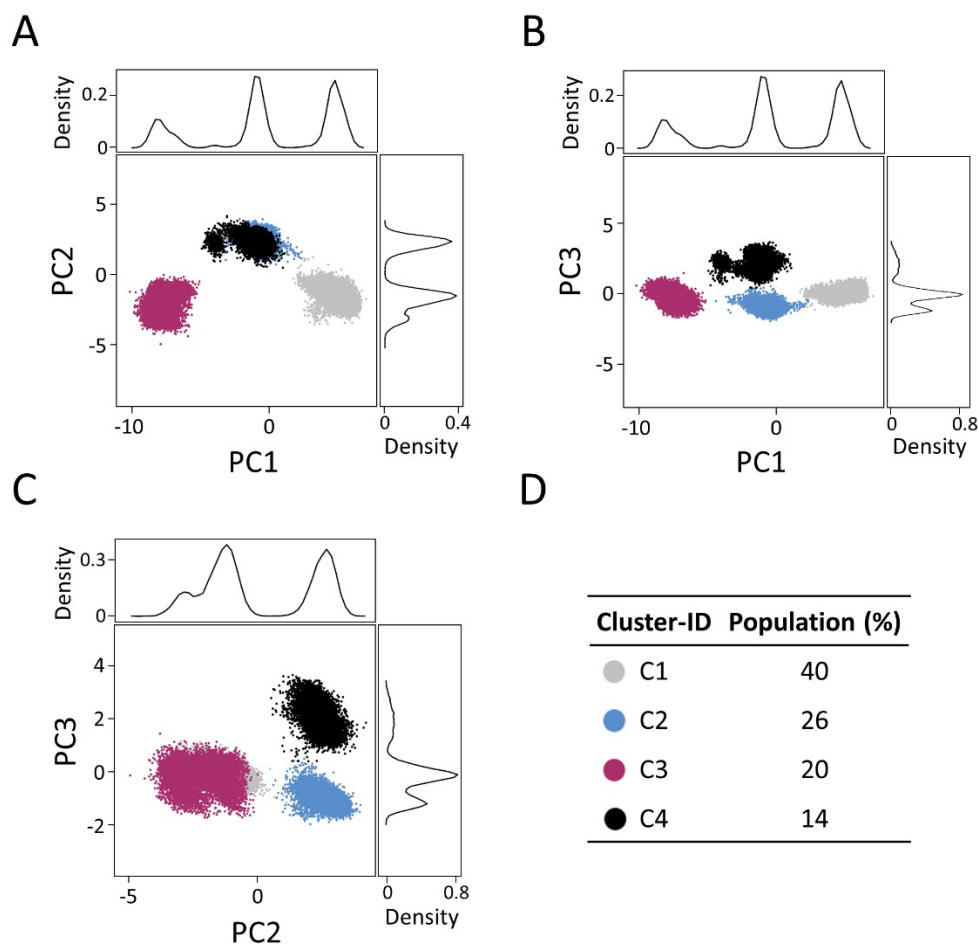


Figure S6. Projections of the first three PCs of the concatenated 50-100ns trajectories for *mAChE*•**9**, displaying the largest collective motion of the inhibitor **9** along the PCs. The different clusters in the PCA subspace, representing different binding conformations of the inhibitor **9**, are color coded. The density visualizes the relative population of conformations. **(A)** PC1 vs PC2. **(B)** PC1 vs PC3. **(C)** PC2 vs PC3. **(D)** Color code and population for the different clusters.

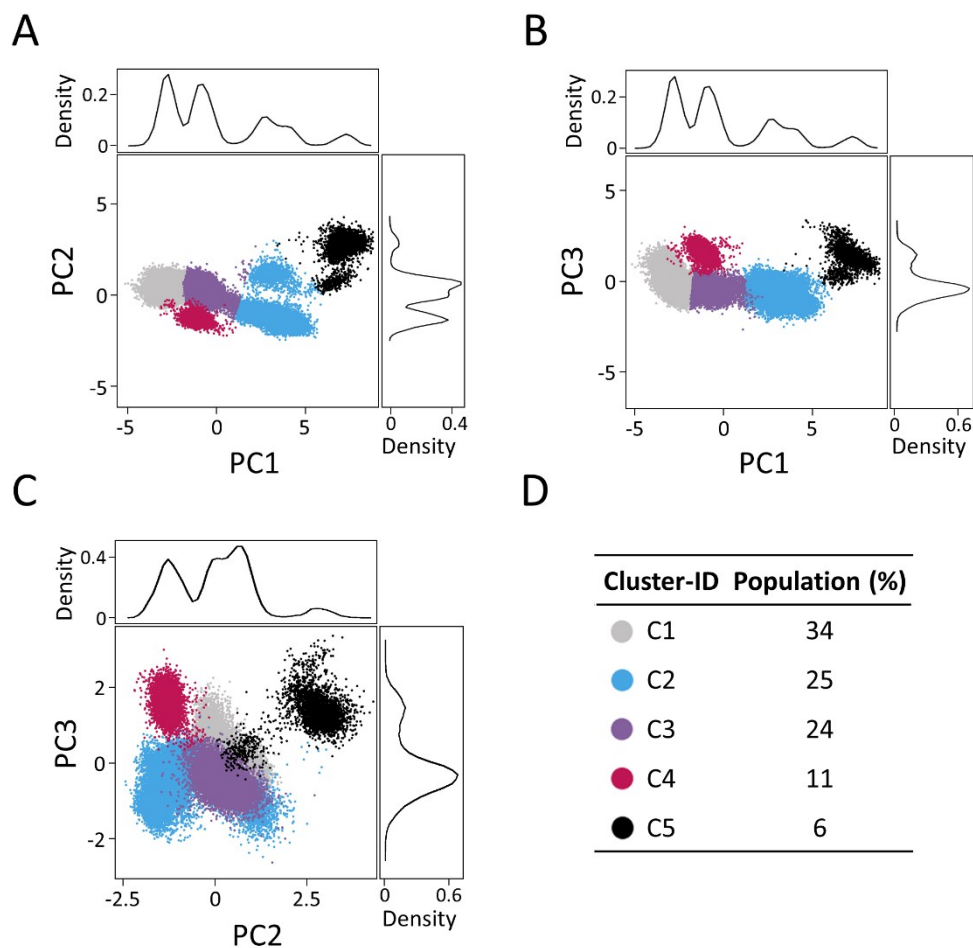


Figure S7. Projections of the first three PCs of the concatenated 50-100ns trajectories for *AgAChE1*•**9**, displaying the largest collective motion of the inhibitor **9** along the PCs. The different clusters in the PCA subspace, representing different binding conformations of the inhibitor **9**, are color coded. The density visualizes the relative population of conformations. (A) PC1 vs PC2. (B) PC1 vs PC3. (C) PC2 vs PC3. (D) Color code and population for the different clusters.

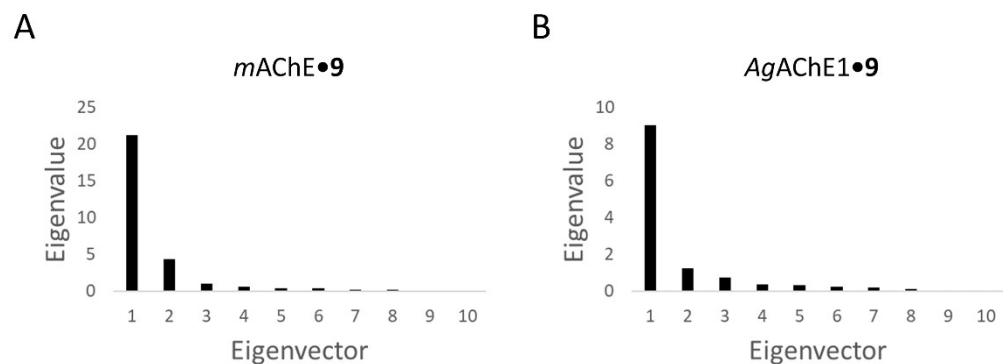


Figure S8. Eigenvalues for the first ten PCs (eigenvectors) for the PCA of heavy atoms of inhibitor **9**, over the concatenated 50-100 ns MD simulations for **A)** *mAChE*•**9**. **B)** *AgAChE1*•**9**.

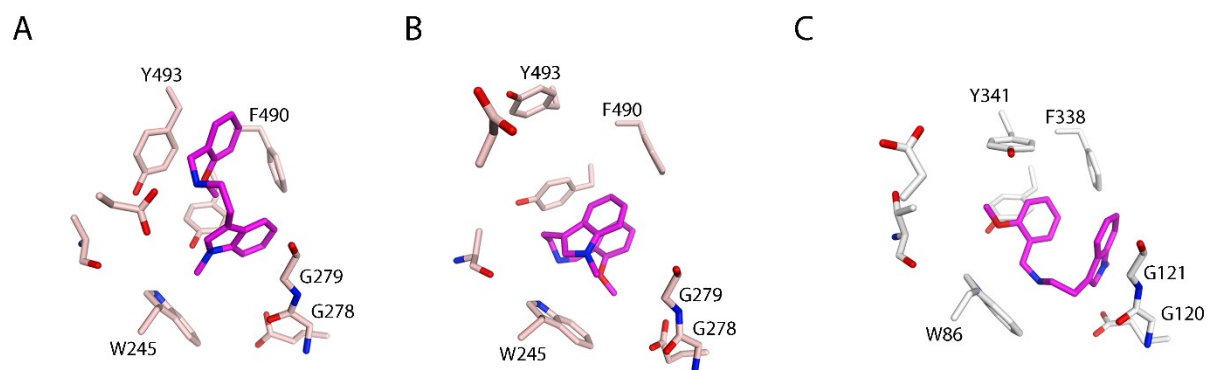


Figure S9. Representative binding poses of **9** in complex with *AgAChE1* and *mAChE*, selected based on cluster analysis of the inhibitors' conformations during the MD-simulations. **(A-B)** The centroid of clusters 4 and 5 of *AgAChE*•**9** with populations of 11% and 6% of the full trajectory. **(C)** The centroid of cluster 4 of *mAChE*•**9** with a population of 14%. Amino acid residues identified as important for interactions with **9** are highlighted. The tyrosine residue in the center of the residues is Y489/Y337. The centroid inhibitor conformations of the three largest clusters are shown in Figure 6.

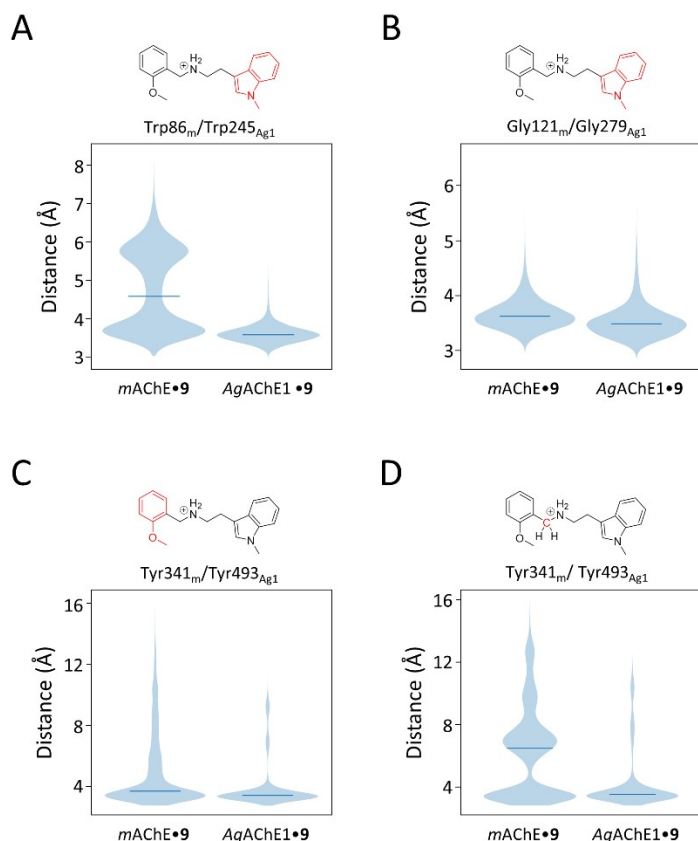


Figure S10. Pairwise minimum distances measured between the indicated atoms of inhibitor **9** (marked in red) and heavy atoms of the side chain of selected amino acids. Distances were calculated for the concatenated 50-100 ns MD simulations. The dark blue line indicates the mean value of the minimum distance, and the width of the light blue shape represents the fraction of frames at each distance. **(A)** Distance between the indole moiety of **9** and Trp86_m/Trp245_{Ag1}. **(B)** Distance between the indole moiety of **9** and Gly121_m/Gly279_{Ag1}. **(C)** Distance between the methoxy benzyl moiety of **9** and Tyr341_m/Tyr493_{Ag1}. **(D)** Distance between one α -carbon to the secondary amine in the linker of **9** and Tyr341_m/Tyr493_{Ag1}.

Table S4. Water occupancy at hydrogen bonding distances ($< 3 \text{ \AA}$) to selected heavy atoms of inhibitor **9**, for concatenated 50-100 ns MD simulations of *mAChE•9* and *AgAChE1•9*. The average number of water molecules are reported.

	Water occupancy		
	Methoxy benzyl (any atom)	Indole (any atom)	Linker (nitrogen)
<i>mAChE•9</i>	0.07	0.18	0.89
<i>AgAChE1•9</i>	0.06	0.11	0.41

In vivo raw data

Table S5. In vivo raw data for compound **8** as insecticide towards *Ae. aegypti* at a dose of 2, 1, 0.5, 0.2 and 0.02 nmol/mosquito.

Compound	Dose (nmol)	No. Mosquitoes (Aa)	24h Mortality ^a	% 24 Mortality ^b	48h Mortality ^a	% 48 Mortality ^b
Acetone	Control	50	1	2.00	1	2.00
8	2	100	58	58.00	63	63.00
8	1	100	31	31.00	39	39.00
8	0.5	100	9	9.00	12	12.00
8	0.2	100	2	2.00	4	4.00

^{a,b} Average value from of three different experiments (triplicate).

Table S6. In vivo raw data for compound **9** as insecticide towards *Ae. aegypti* at a dose of 2, 1, 0.5, 0.2 and 0.02 nmol/mosquito.

Compound	Dose (nmol)	No. Mosquitoes (Aa)	24h Mortality ^a	% 24 Mortality ^b	48h Mortality ^a	% 48 Mortality ^b
Acetone	Control	50	1	2.00	1	2.00
9	2	100	100	100.00	100	100.00
9	1	100	100	100.00	100	100.00
9	0.5	100	90	90.00	90	90.00
9	0.2	100	45	45.00	54	54.00
9	0.02	100	2	2.00	3	3.00

^{a,b} Average value from of three different experiments (triplicate).

Table S7. In vivo raw data for compounds **16** and **18** as insecticide towards *An. gambiae* at a dose of 2 and 0.2 nmol/mosquito.

Compound	Dose (nmol)	No. Mosquitoes (Ag)	24h Mortality ^a	% 24 Mortality ^b	48h Mortality ^a	% 48 Mortality ^b
Acetone	Control	50	2	4.00	2	4.00
16	2	98	98	100.00	98	100.00
16	0.2	100	50	50.00	53	53.00
18	2	100	100	100.00	100	100.00
18	0.2	90	41	45.56	43	47.78

^{a,b} Average value from of three different experiments (triplicate).

Table S8. In vivo raw data for compounds **16** and **18** as insecticide towards *Ae. aegypti* at a dose of 2 and 0.2 nmol/mosquito.

Compound	Dose (nmol)	No. Mosquitoes (Aa)	24h Mortality ^a	% 24 Mortality ^b	48h Mortality ^a	% 48 Mortality ^b
Acetone	Control	50	2	4.00	2	4.00
16	2	98	98	100.00	98	100.00
16	0.2	100	6	12.00	6	12.00
18	2	100	100	100.00	100	100.00
18	0.2	50	2	4.00	2	4.00

^{a,b} Average value from of three different experiments (triplicate).

Table S9. In vivo raw data for propoxur insecticide (positive control) towards *An. gambiae* at a dose of 0.02-0.00002 nmol/mosquito.

Compound	Dose (nmol)	No. Mosquitoes (Ag)	24 Mortality ^a	% 24 Mortality ^b	48 Mortality ^a	% 48 Mortality ^b
Propoxur	0.02	115	115	100.00	115	100.00
Propoxur	0.002	129	100	77.52	108	83.72
Propoxur	0.0002	88	4	4.55	6	6.82
Propoxur	0.00002	150	1	0.67	1	0.67

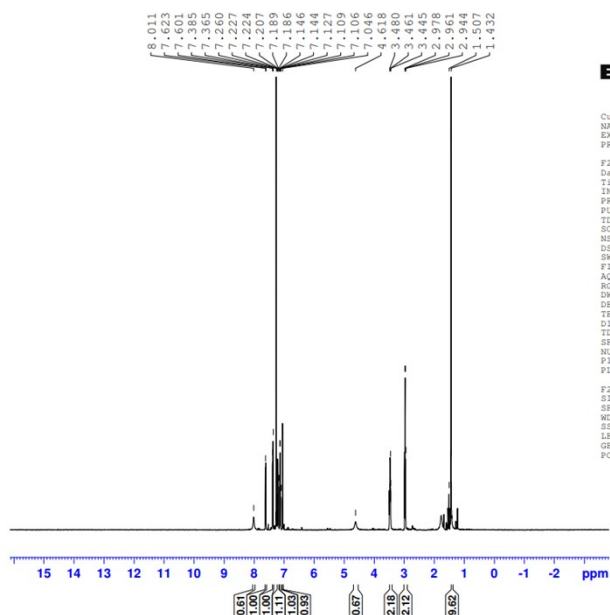
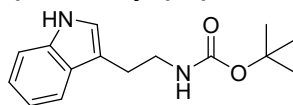
^{a,b} Average value from of three different experiments (triplicate).

Table S10. In vivo raw data for propoxur insecticide (positive control) towards *Ae. aegypti* at a dose of 0.02-0.00002 nmol/mosquito.

Compound	Dose (nmol)	No. Mosquitoes (Aa)	24 Mortality ^a	% 24 Mortality ^b	48 Mortality ^a	% 48 Mortality ^b
Propoxur	0.02	115	115	99.00	115	99.00
Propoxur	0.002	129	100	73.52	108	83.72
Propoxur	0.0002	88	4	1.69	6	1.7
Propoxur	0.00002	150	1	0.67	1	0.67

^{a,b} Average value from of three different experiments (triplicate).

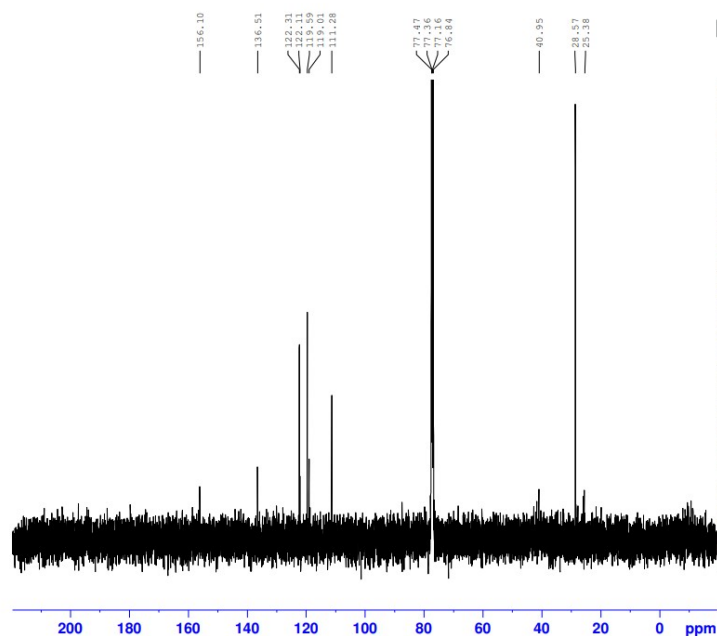
NMR spectra of intermediates (Tert-butyl (2-(1H-indol-3-yl)ethyl)carbamate) (3a)



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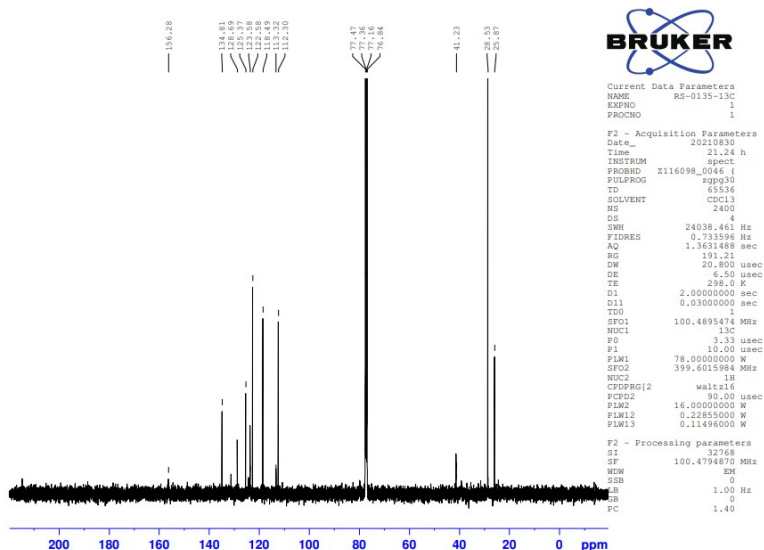
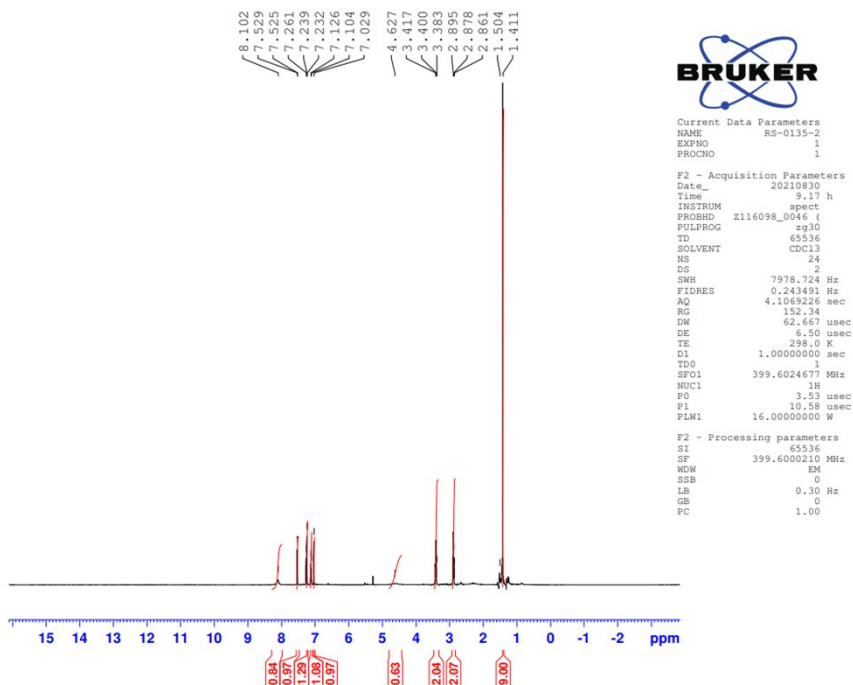
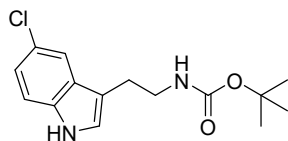


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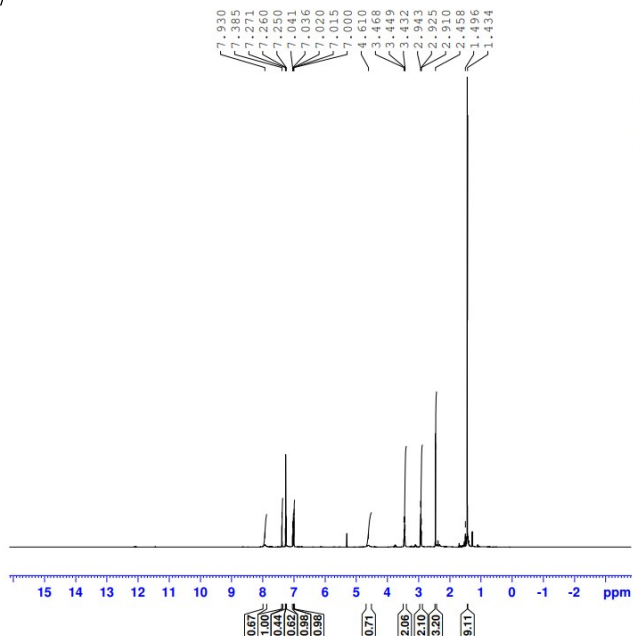
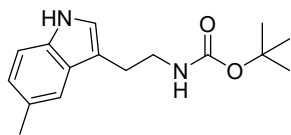
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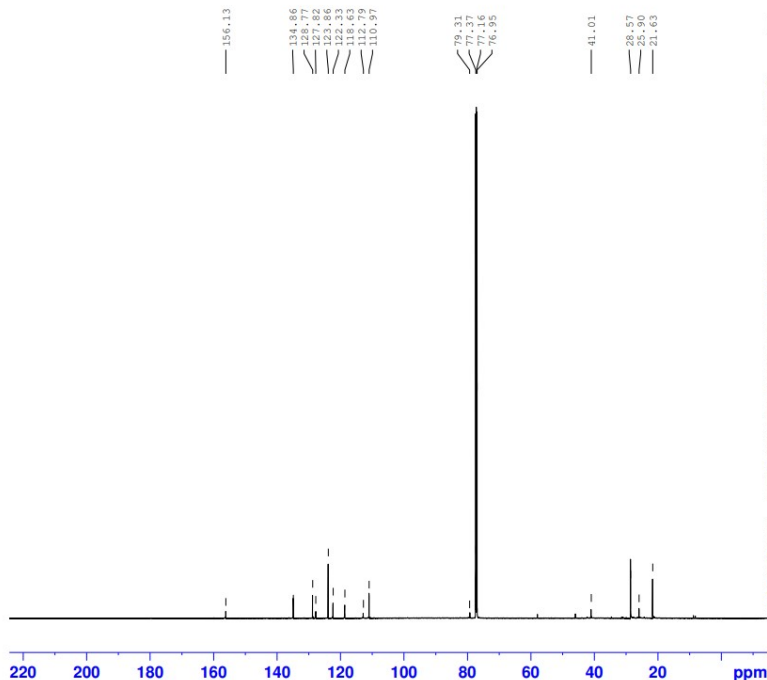
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TDO 1
SFO1 399.6024677 MHz
NUC1 1H
P1 10.34 usec
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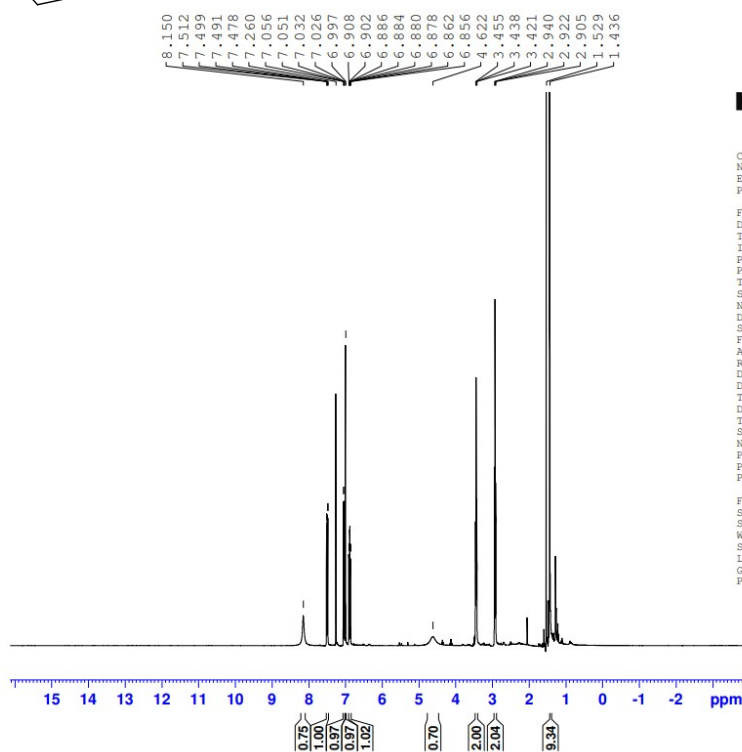
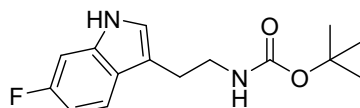


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PC 1.40

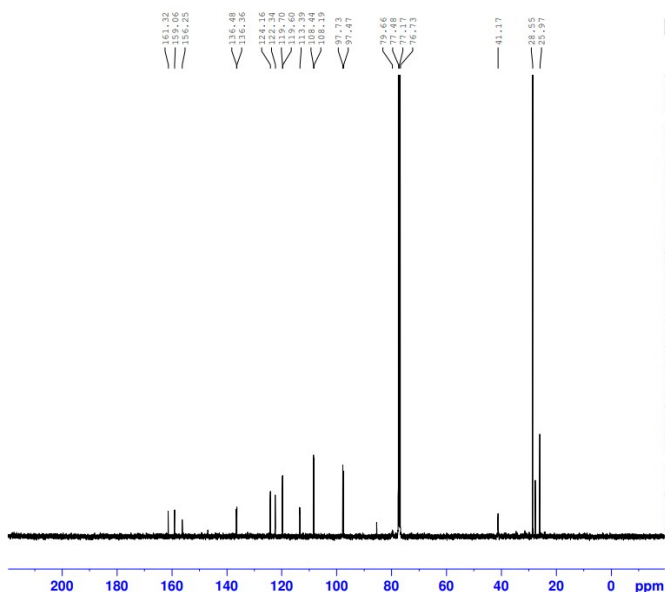
Tert-butyl (2-(6-fluoro-1H-indol-3-yl)ethyl)carbamate (3d).



Current Data Parameters
NAME rs-0092-1_new
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20211213
Time 17.33 h
INSTRUM spect
PROBHD z116098_0046 (zpg30)
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 7978.724 Hz
FIDRES 0.243491 Hz
AQ 4.1069226 sec
RG 123.45
DW 62.667 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TDO 1
SFO1 399.6024677 MHz
NUC1 1H
P0 3.49 usec
P1 10.48 usec
PLW1 16.00000000 W

F2 - Processing parameters
SI 65536
SF 399.6000097 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

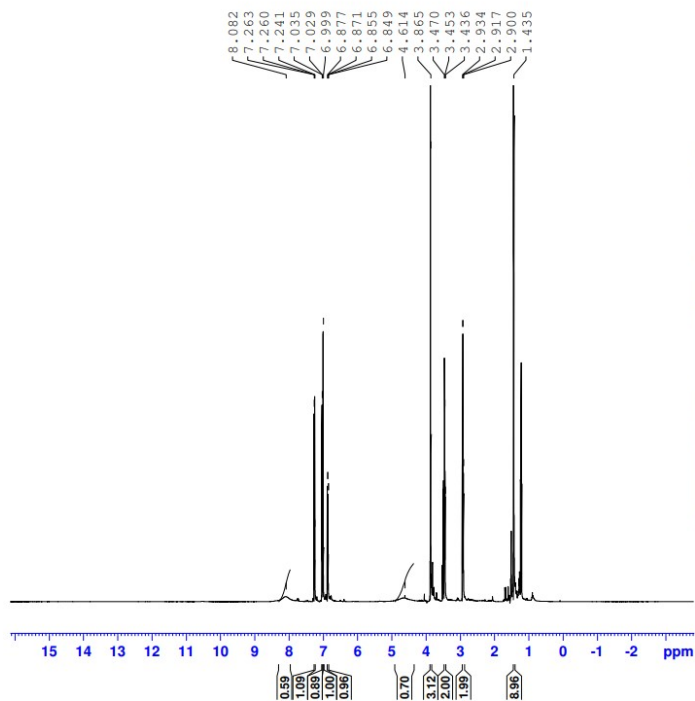
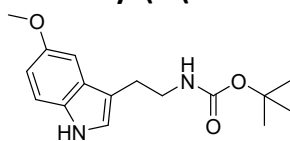


Current Data Parameters
NAME rs-0092-1_new
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20211214
Time 4.18 h
INSTRUM spect
PROBHD z116098_0046 (zpg30)
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2400
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 191.21
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1
SFO1 100.4895474 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 78.00000000 W
SFO2 399.6019984 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 50.00 usec
PLW2 16.00000000 W
PLW12 0.22200000 W
PLW13 0.11166000 W

F2 - Processing parameters
SI 32768
SF 100.4794873 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

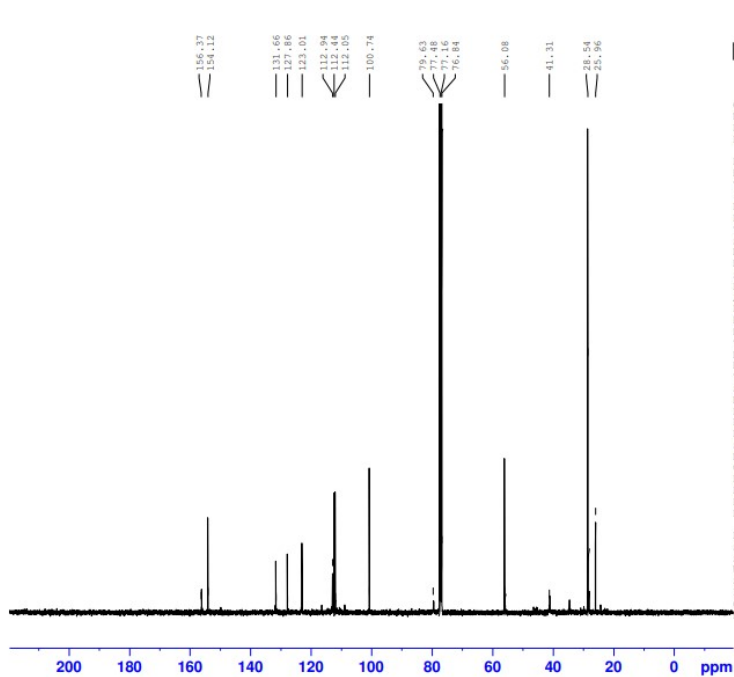
Tert-butyl (2-(5-methoxy-1H-indol-3-yl)ethyl)carbamate (3e).



Current Data Parameters
NAME RS-0125-REP
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210810
Time 10.46 h
INSTRUM spect
PROBHD Z116098_0046 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 24
DS 2
SWH 7978.724 Hz
FIDRES 0.243491 Hz
AQ 4.1063226 sec
RG 69.1
DW 62.667 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 399.6024677 MHz
NUC1 1H
PQ 3.56 usec
PI 10.68 usec
PLW1 16.00000000 W

F2 - Processing parameters
SI 65536
SF 399.6000098 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME RS-0125-REP-2
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210816
Time 23.41 h
INSTRUM spect
PROBHD Z116098_0046 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2400
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 191.21
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.4895474 MHz
NUC1 13C
PQ 3.33 usec
PI 10.00 usec
PLW1 78.00000000 W
SFO2 399.6015984 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 16.00000000 W
PLW12 0.22471000 W
PLW13 0.11303000 W

F2 - Processing parameters
SI 32768
SF 100.4794894 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

CC(C)(C)OC(=O)NCCCc1c[nH]c2ccccc12

```

Current Data
NAME          RS-0063-1-P
EXPNO         1
PROCNO        1

F2 - Acquisition Parameters
Date_         20111222
Time          17.31 h
INSTRUM       spect
PROBHD        T16098_0046
PULPROG       zg30
GAMMA         63.336
SOLVENT       CDCl3
NS            32
DS            2
SWH           7977.724 Hz
AQ            0.214391 s
AQ2            0.1409226 sec
RG            137.88
DE            62.467 usec
RG2            6.50 usec
RG3            2.986 K
TD            1.000000000 sec
TE           300.2
SFO1          399.624647 MHz
NUC1           1H
FID1           10.46 usec
PL11          16.00000000 W

F2 - Processing parameters
SI            65536
SF            399.600098 MHz
WDW           EM
SS            0
GB            0.30 Hz
LB            1.00

```



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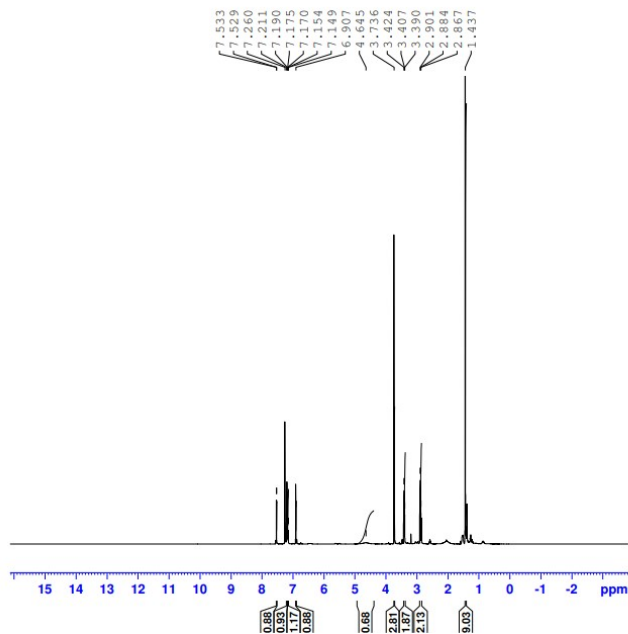
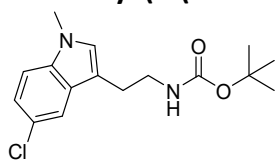
Current Data Parameters
NAME      RS-0065-1P_CARBON
PROCNO    1

F2 - Acquisition Parameters
Date_     20181124
Time      8.42 h
INSTRUM   spect
PROBHD    T126908_0046
PULPROG   zgpg30
SOLVENT   CDCl3
NS         4068
DS         4
SWH        24038.461 Hz
FIDRES     0.731596 Hz
AQ         1.363488 sec
RG          191.21
WDW         20.800 usec
SSB         0.50 usec
TE         298.0 K
D1          2.0000000 sec
DE          0.0300000 sec
TDO         1
SF01        100.4895474 MHz
PC          3.00
P1          10.00 usec
PL1         78.0000000 W
PCPD2       399.6015984 MHz
NUC2        1H
CPDPRG2    wait16
PCPD2       90.00 usec
PLM2        16.0000000 W
PLM22       0.21437000 W
PLM23       0.1071000 W
W           1.00 Hz

F2 - Processing parameters
SI          32768
SF          100.4794864 MHz
NF          EM
SSB         0
GB          1.00 Hz
LB          0
GC          1.40

```

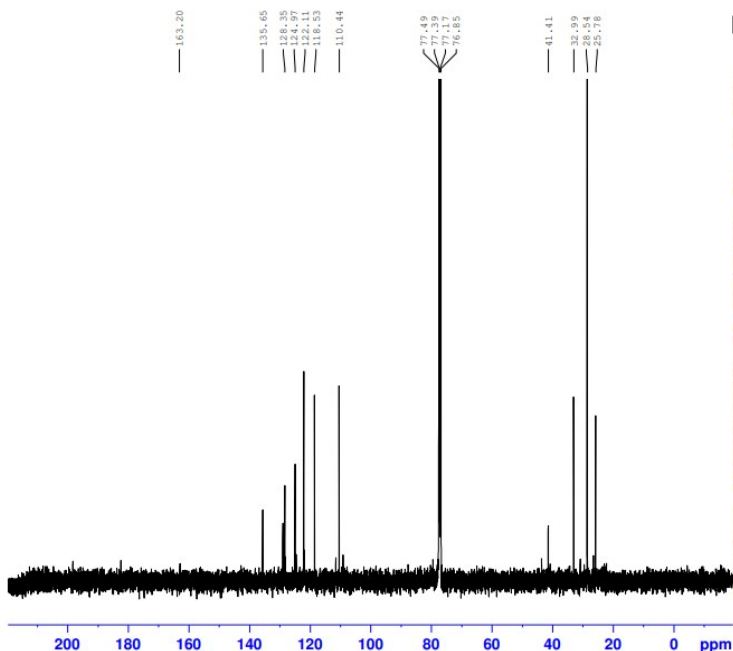
Tert-butyl (2-(5-chloro-1-methyl-1H-indol-3-yl)ethyl)carbamate (4b)



Current Data Parameters
NAME RS-0136-2
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210831
Time 11.11 h
INSTRUM spect
PROBHD Z116098_0046 ()
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 24
DS 2
SWH 7978.724 Hz
FIDRES 0.243491 Hz
AQ 4.1069226 sec
RG 171.52
DW 62.667 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 399.6024677 MHz
NUC1 1H
PQ 3.33 usec
P1 10.58 usec
PLW1 16.00000000 W

F2 - Processing parameters
SI 65536
SF 399.600101 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

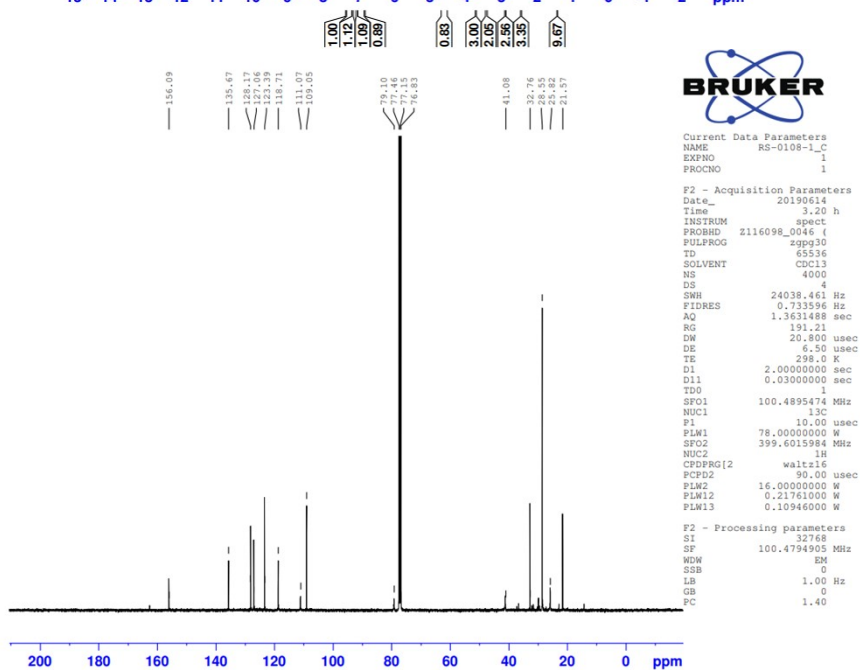
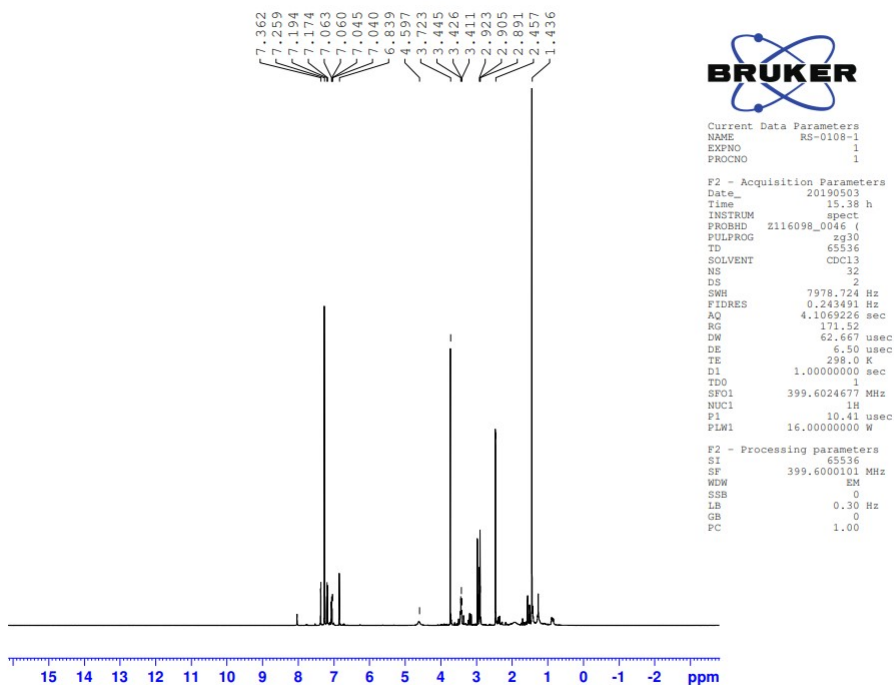
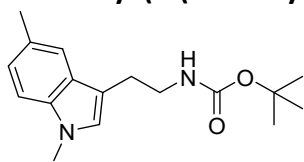


Current Data Parameters
NAME RS-0136-2
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210831
Time 23.29 h
INSTRUM spect
PROBHD Z116098_0046 ()
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2400
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 191.21
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.4895474 MHz
NUC1 13C
PQ 3.33 usec
P1 10.00 usec
PLW1 78.00000000 W
SFO2 399.6015984 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLM2 16.00000000 W
PLW2 0.22654000 W
PLW13 0.11395000 W

F2 - Processing parameters
SI 32768
SF 100.4794855 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Tert-butyl (2-(5-methyl-1H-indol-3-yl)ethyl)carbamate (4c)



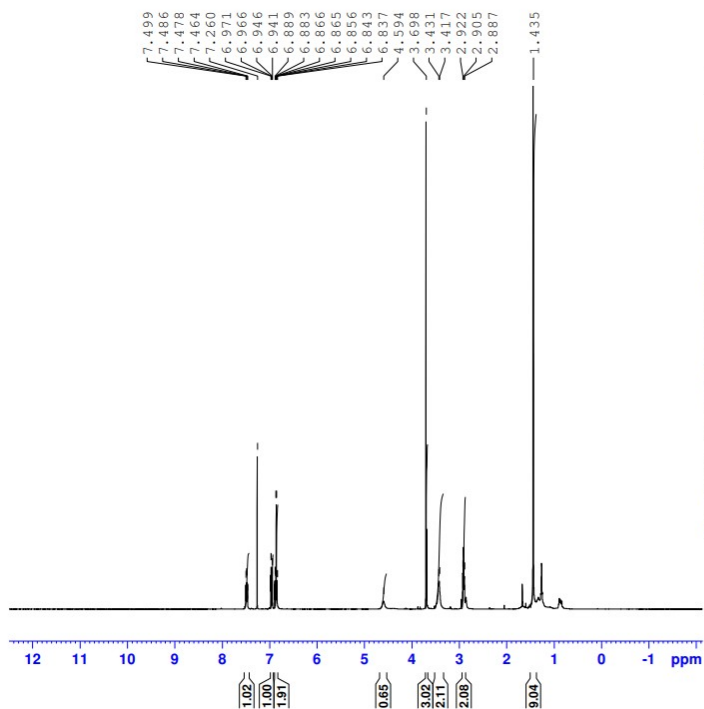
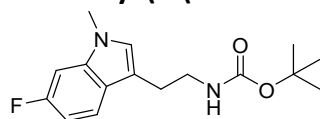
BRUKER

Current Data Parameters
NAME RS-0108-1_C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190614
Time 3.20 h
INSTRUM spect
PROBHD Z116098_0046 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 4000
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 191.21
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.4895474 MHz
NUC1 13C
P1 10.00 usec
PLW1 78.00000000 W
SFO2 399.6015984 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 16.00000000 W
PLW12 0.21761000 W
PLW13 0.10946000 W

F2 - Processing parameters
SI 32768
SF 100.4794905 MHz
WDW RM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

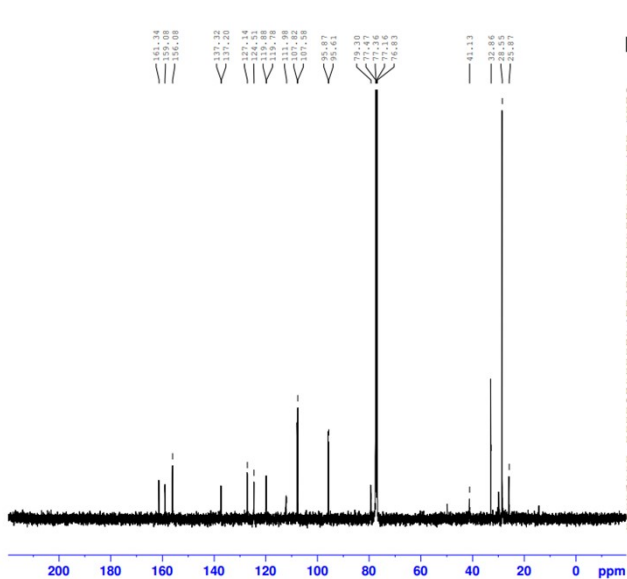
Tert-butyl (2-(6-fluoro-1-methyl-1H-indol-3-yl)ethyl)carbamate (4d).



Current Data Parameters
NAME rs-0093_2nd_211222
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20211222
Time 9.53 h
INSTRUM spect
PROBHD Z116098_0046 ()
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 7978.724 Hz
FIDRES 0.243491 Hz
AQ 4.1069226 sec
RG 123.45
DM 62.667 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 399.6024677 MHz
NUC1 1H
PC 3.51 usec
P1 10.52 usec
PLW1 16.00000000 W

F2 - Processing parameters
SI 65536
SF 399.6000098 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

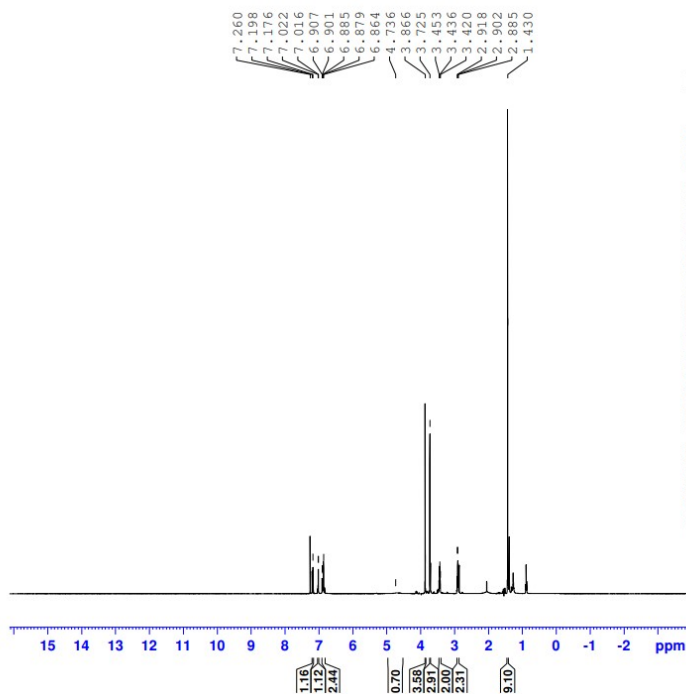
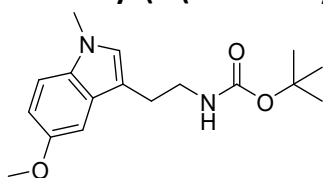


Current Data Parameters
NAME rs-009-13-211222
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20211222
Time 21.26 h
INSTRUM spect
PROBHD Z116098_0046 ()
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2400
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 191.21
DM 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.4895474 MHz
NUC1 13C
PC 3.33 usec
P1 10.00 usec
PLW1 78.00000000 W
SFO2 399.6015984 MHz
NUC2 1H
PCPD2 waltz16
PCPD2 90.00 usec
PLW2 16.00000000 W
PLW12 0.22547001 W
PLW13 0.11341000 W

F2 - Processing parameters
SI 32768
SF 100.4794873 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

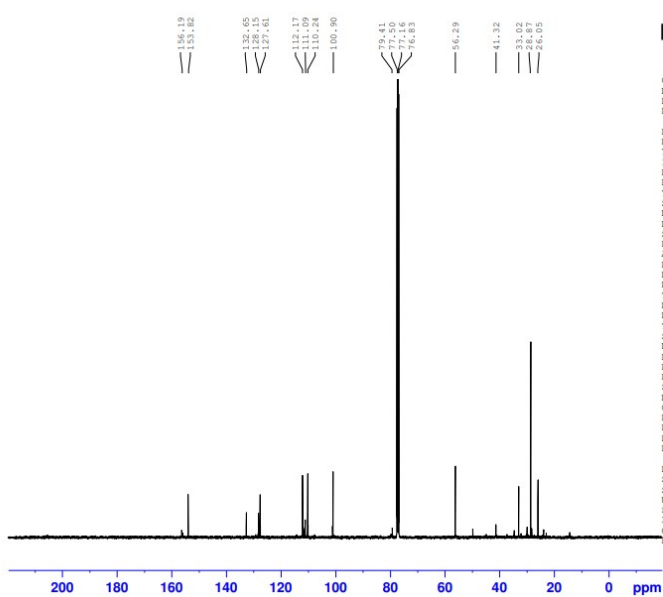
Tert-butyl (2-(5-methoxy-1-methyl-1H-indol-3-yl)ethyl)carbamate (4e)



Current Data Parameters
NAME RS-0128-P
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210816
Time 11.12 h
INSTRUM spect
PROBHD Z116098_0046 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 24
DS 2
SWH 7978.724 Hz
FIDRES 0.243491 Hz
AQ 4.1063226 sec
RG 137.88
DW 62.667 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 399.6024677 MHz
NUC1 1H
P0 3.51 usec
P1 10.53 usec
PLW1 16.00000000 W

F2 - Processing parameters
SI 65536
SF 399.6000099 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

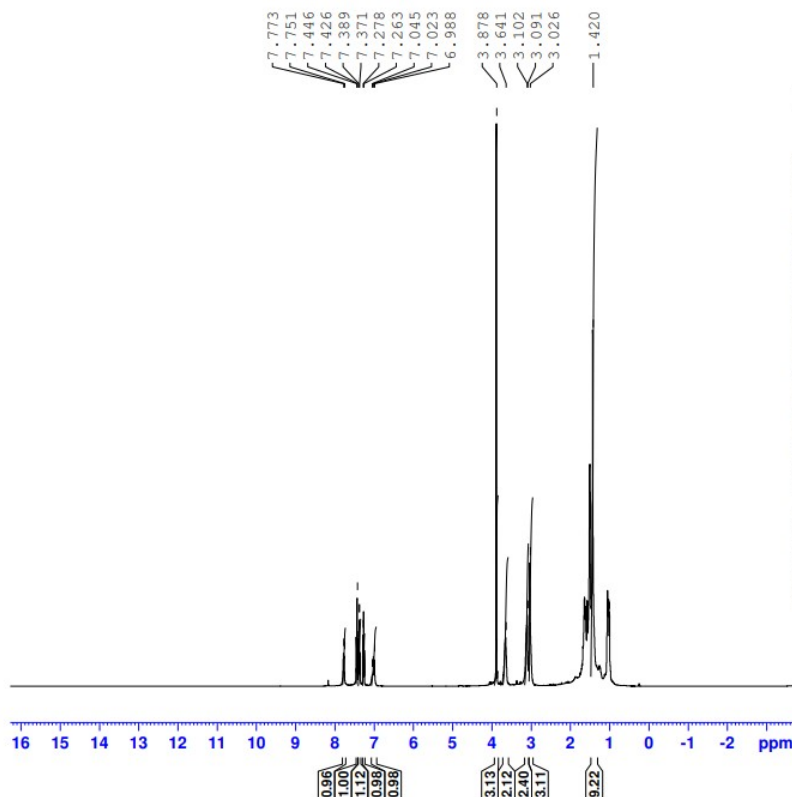
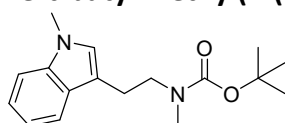


Current Data Parameters
NAME RS-0128-13C-2
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210813
Time 21.26 h
INSTRUM spect
PROBHD Z116098_0046 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2400
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 191.21
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.4895474 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 78.00000000 W
SFO2 399.6015984 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 16.00000000 W
PLW12 0.22724999 W
PLW13 0.11431000 W

F2 - Processing parameters
SI 32768
SF 100.4794889 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

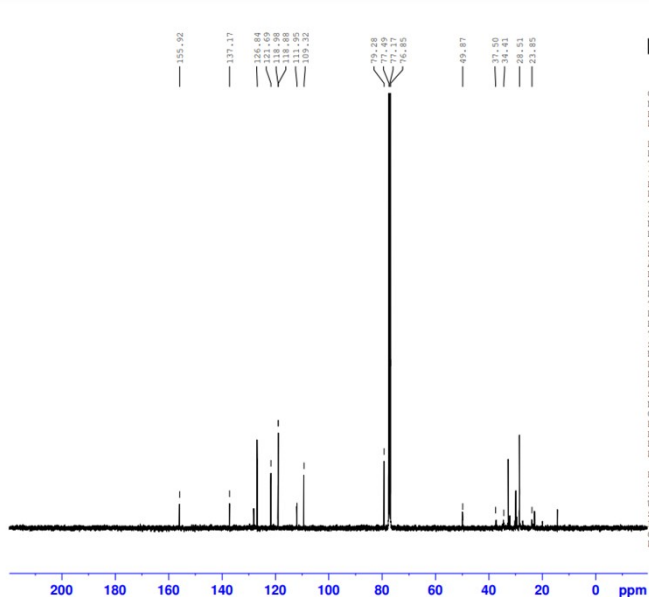
Tert-butyl methyl(2-(1-methyl-1H-indol-3-yl)ethyl)carbamate (27)



Current Data Parameters
NAME RS-0117-1-200519
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190520
Time 17.47 h
INSTRUM spect
PROBHD Z116098_0046 {
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 7978.724 Hz
FIDRES 0.243491 Hz
AQ 4.1069226 sec
RG 33.09
DW 62.667 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 399.6024677 MHz
NUC1 1H
P1 10.52 usec
PLW1 16.00000000 W

F2 - Processing parameters
SI 65536
SF 399.599555 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

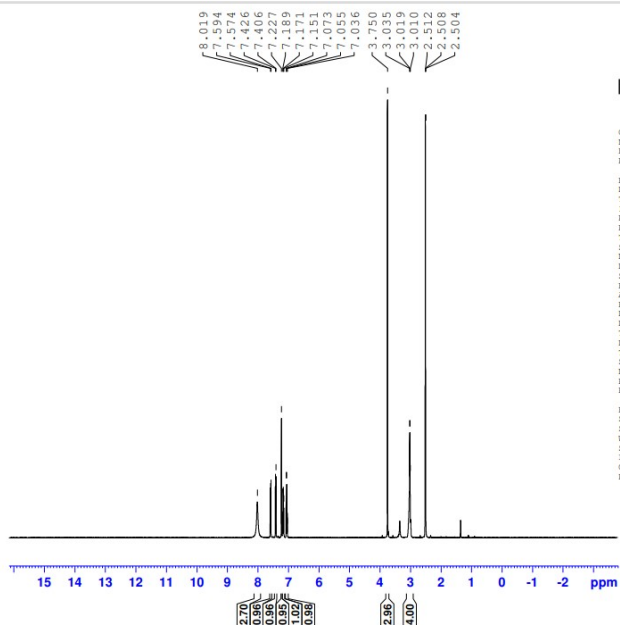
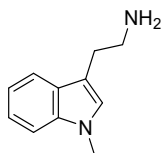


Current Data Parameters
NAME rs-0117-13c_211222
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20111222
Time 23.49 h
INSTRUM spect
PROBHD Z116098_0046 {
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2400
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 191.21
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.4895474 MHz
NUC1 13C
P1 3.33 usec
P1 10.00 usec
PLW1 78.00000000 W
SFO2 399.6015984 MHz
NUC2 1H
PCPD2 waltz16
PLW2 16.00000000 W
PLW12 0.22442595 W
PLW13 0.11289000 W

F2 - Processing parameters
SI 32768
SF 100.4794861 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

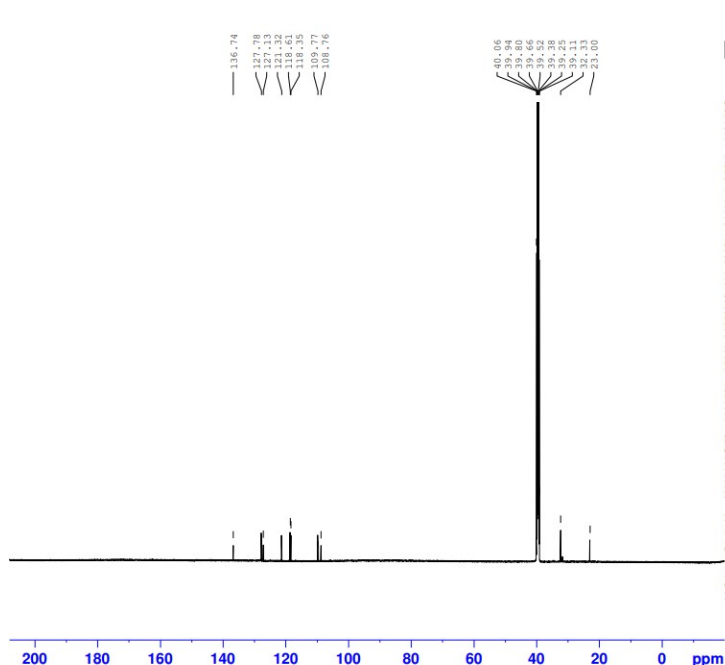
2-(1-methyl-1H-indol-3-yl)ethan-1-amine (5a)



Current Data Parameters
 NAME RS-0067-1-0281118
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20181128
 Time 12.06 h
 INSTRUM spect
 PROBRD Z116098_0046 (
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 32
 DS 2
 SWH 7978.724 Hz
 FIDRES 0.243491 Hz
 AQ 4.1069226 sec
 RG 191.21
 DW 62.667 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.00000000 sec
 TD0 1
 SFO1 399.6024677 MHz
 NUC1 1H
 P1 26.60 usec
 PLW1 16.00000000 W

F2 - Processing parameters
 SI 65536
 SF 399.6000000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

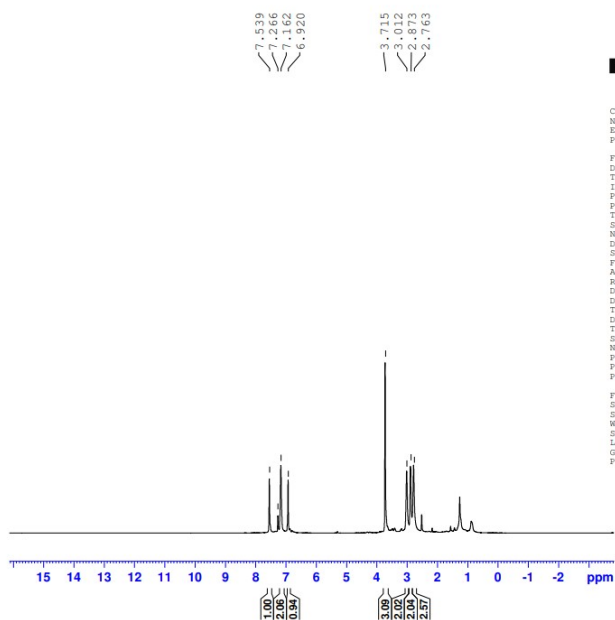
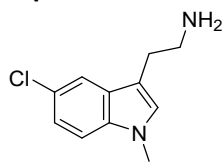


Current Data Parameters
 NAME RS-0067-1_C
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190129
 Time 23.04 h
 INSTRUM spect
 PROBRD Z132572_0007 (
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 1024
 DS 4
 SWH 36057.691 Hz
 FIDRES 1.100393 Hz
 AQ 0.9087659 sec
 RG 182.66
 DW 13.867 usec
 DE 18.00 usec
 TE 298.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1
 SFO1 150.9279571 MHz
 NUC1 13C
 P1 9.70 usec
 PLW1 35.09999847 W
 SFO2 600.1724007 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 70.00 usec
 PLW2 21.00000000 W
 PLW12 0.59069002 W
 PLW13 0.28944001 W

F2 - Processing parameters
 SI 65536
 SF 150.9129371 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

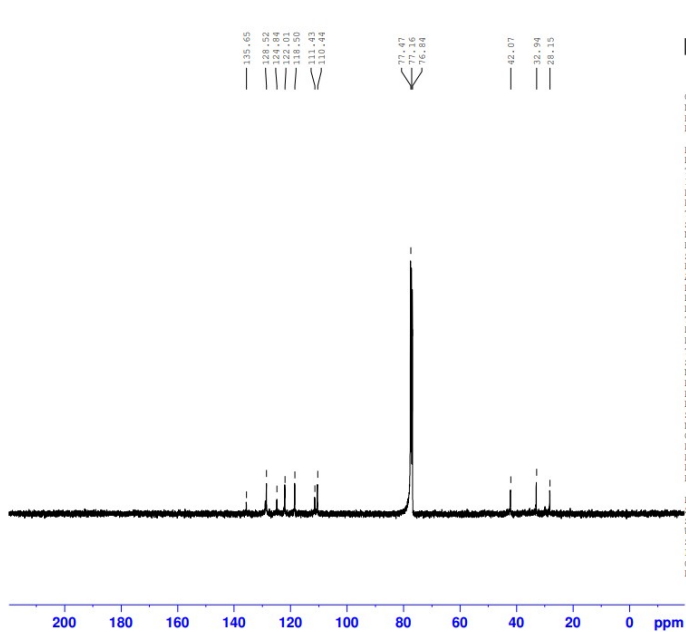
2-(5-chloro-1-methyl-1H-indol-3-yl)ethan-1-amine (5b).



Current Data Parameters
NAME RS-0138-1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210831
Time 16.43 h
INSTRUM spect
PROBHD z116098_0046 (z116098_0046)
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 24
DS 2
SWH 7978.724 Hz
FIDRES 0.243491 Hz
AQ 4.1869226 sec
RG 137.88
DW 62.667 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 399.6024677 MHz
NUC1 1H
P0 3.52 usec
P1 10.57 usec
PLW1 16.00000000 W

F2 - Processing parameters
SI 65536
SF 399.6051119 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

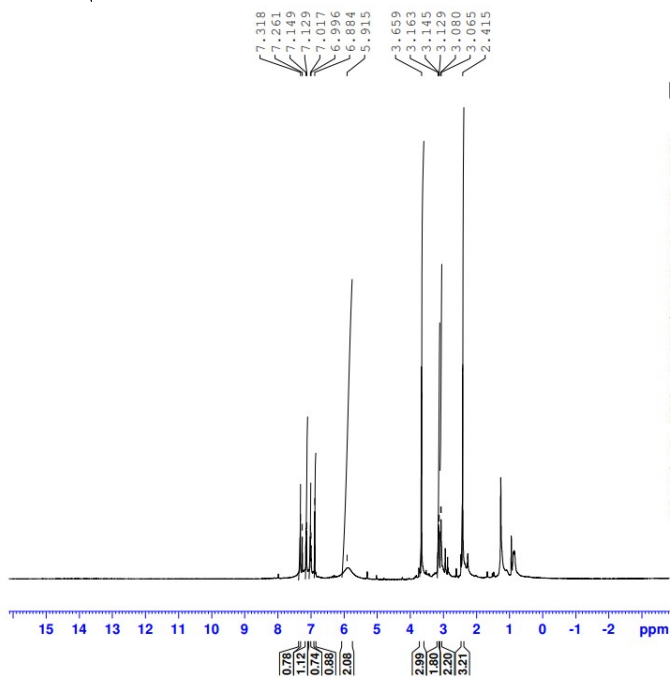
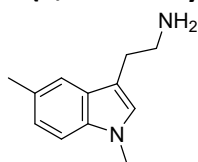


Current Data Parameters
NAME RS-0138-13C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210901
Time 22.57 h
INSTRUM spect
PROBHD z116098_0046 (z116098_0046)
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 4000
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 191.21
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.4895474 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 78.00000000 W
SFO2 399.6015984 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 16.00000000 W
PLW12 0.22026999 W
PLW13 0.11080000 W

F2 - Processing parameters
SI 32768
SF 100.4754876 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

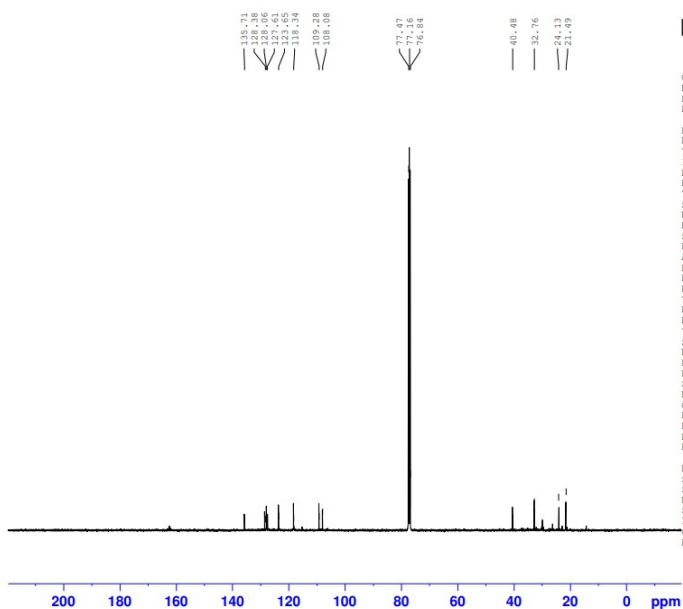
2-(1,5-dimethyl-1H-indol-3-yl)ethan-1-amine (5c).



Current Data Parameters
NAME RS-0110-1-H
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190617
Time 10.18 h
INSTRUM spect
PROBHD Z116098_0046 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 7978.724 Hz
FIDRES 0.243491 Hz
AQ 4.1063226 sec
RG 107.6
DM 62.667 usec
DE 5.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 399.6024677 MHz
NUC1 1H
P1 10.36 usec
PLW1 16.00000000 W

F2 - Processing parameters
SI 65536
SF 399.6001013 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

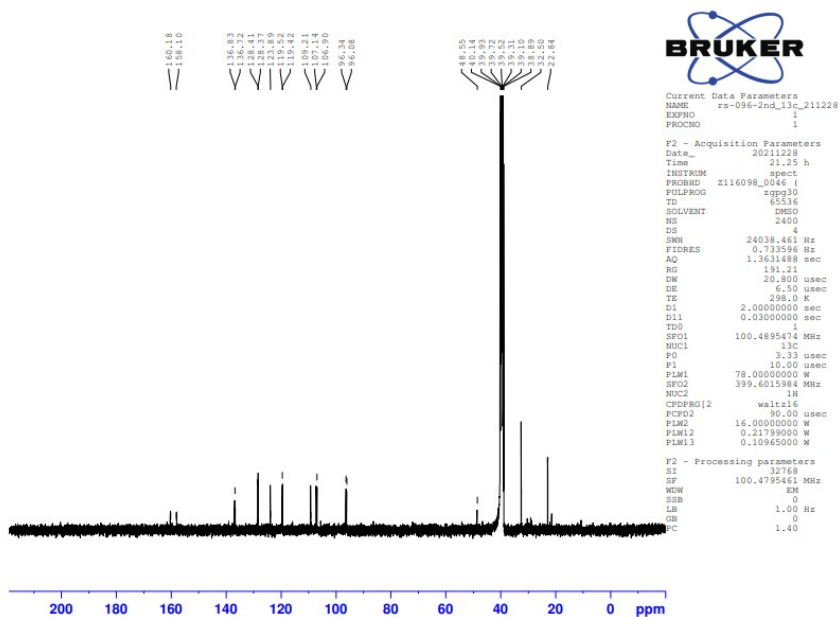
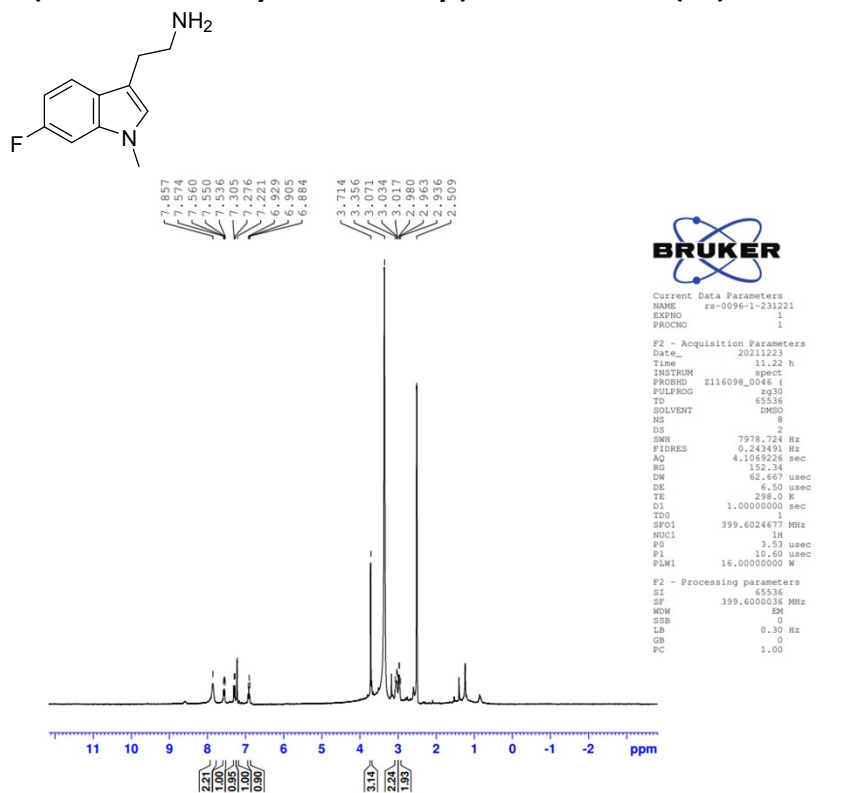


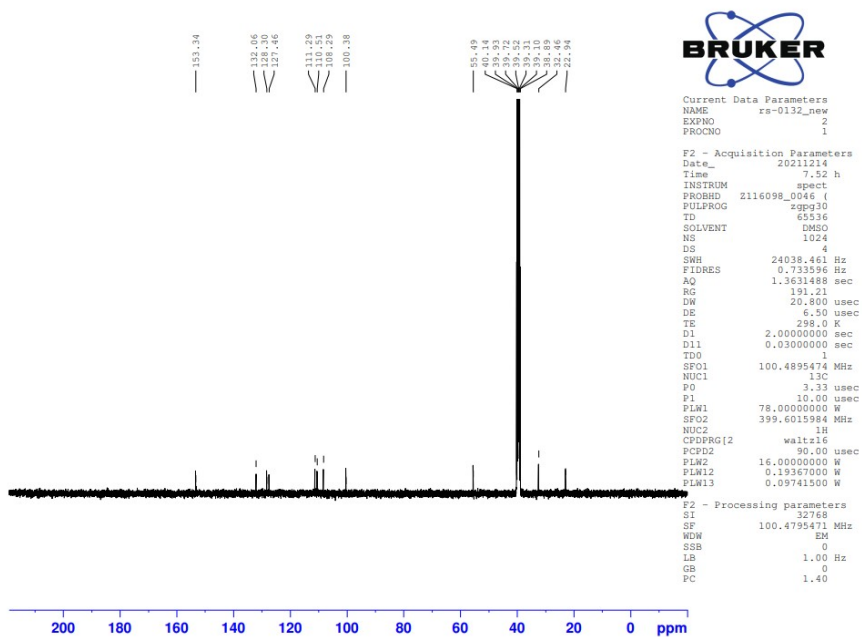
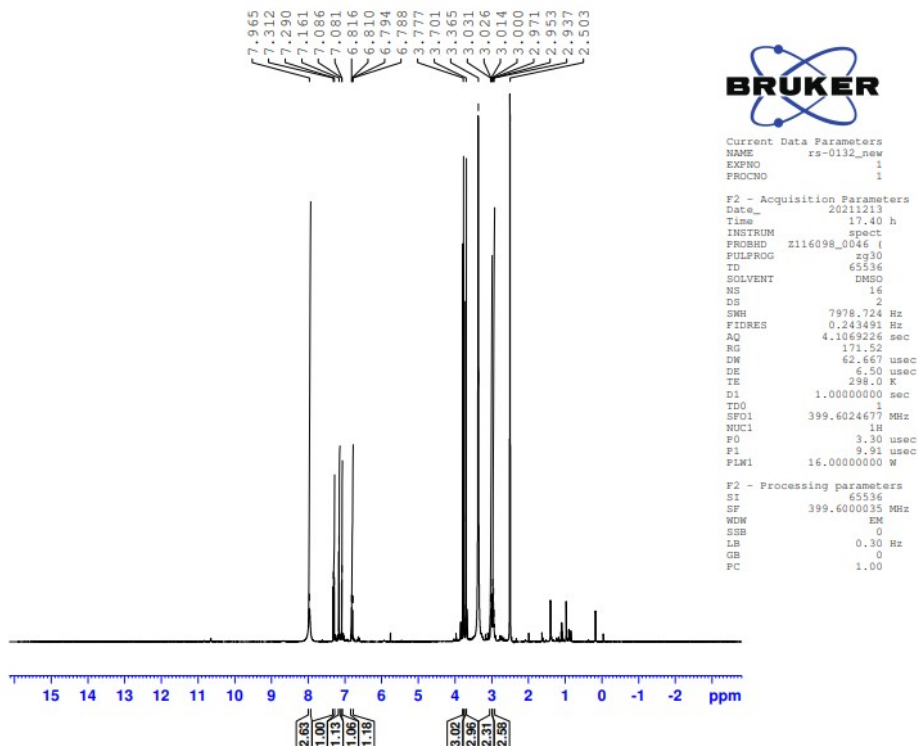
Current Data Parameters
NAME RS-0110-1-C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190614
Time 7.17 h
INSTRUM spect
PROBHD Z116098_0046 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 4000
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 191.21
DM 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.4895474 MHz
NUC1 13C
P1 10.00 usec
PLW1 78.00000000 W
SFO2 399.6015984 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 16.00000000 W
PLW12 0.20250000 W
PLW13 0.10185000 W

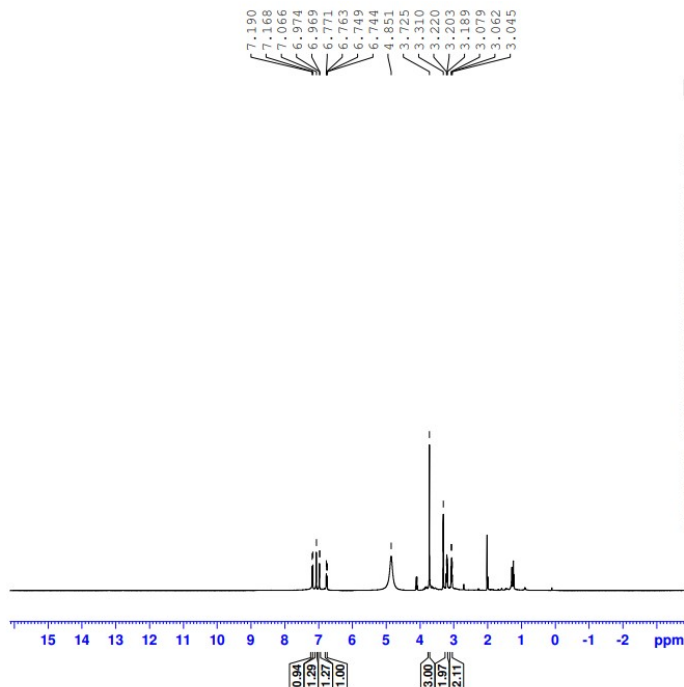
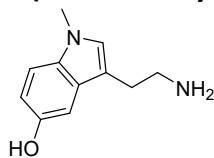
F2 - Processing parameters
SI 32768
SF 100.4794880 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

2-(6-fluoro-1-methyl-1H-indol-3-yl)ethan-1-amine (5d).



CNCCc1c[nH]c2cc(OC)ccc12

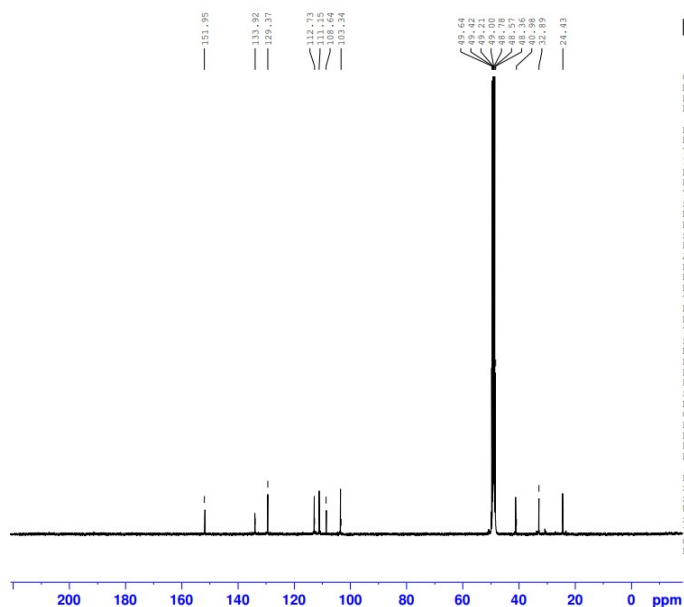
3-(2-aminoethyl)-1-methyl-1H-indol-5-ol (5f)



Current Data Parameters
NAME rs-0154-1-220112
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220111
Time 17.14 h
INSTRUM spect
PROBHD Z116098_0046 (4
PULPROG zgpg30
TD 65536
SOLVENT MeOD
NS 64
DS 2
SWH 7978.724 Hz
FIDRES 0.243491 Hz
AQ 4.1069226 sec
RG 152.34
SW 62.667 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 399.6024677 MHz
NUC1 1H
P0 3.80 usec
P1 11.39 usec
PLW1 16.00000000 W

F2 - Processing parameters
SI 65536
SF 399.6000079 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

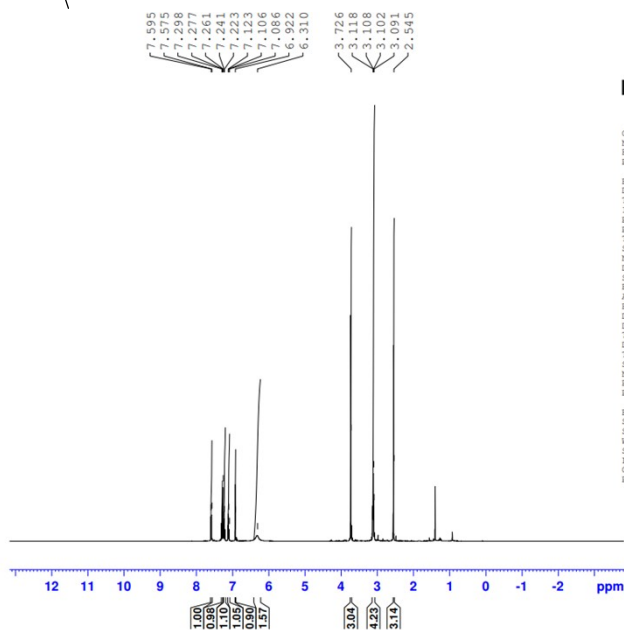
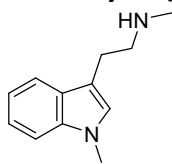


Current Data Parameters
NAME RS-0154-13c-231030
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20231031
Time 1.02 h
INSTRUM spect
PROBHD Z116098_0046 (4
PULPROG zgpg30
TD 65536
SOLVENT MeOD
NS 2400
DS 4
SWH 24038.461 Hz
FIDRES 0.723596 Hz
AQ 1.3631488 sec
RG 191.21
SW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.4895474 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 78.00000000 W
SFO2 399.6015984 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 16.00000000 W
PLW12 0.24358000 W
PLW13 0.12252000 W

F2 - Processing parameters
SI 32768
SF 100.4793611 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

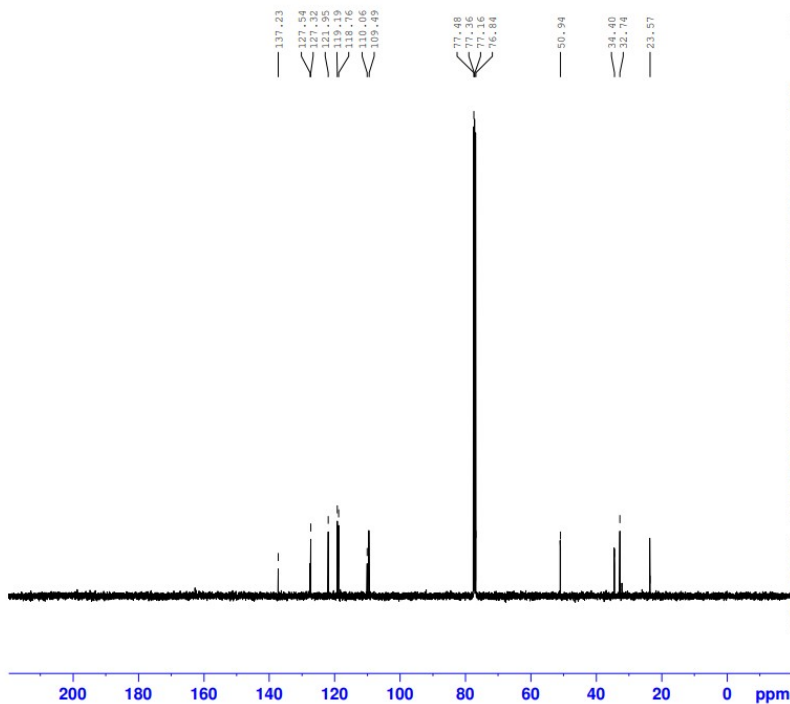
N-methyl-2-(1-methyl-1H-indol-3-yl)ethan-1-amine (28)



Current Data Parameters
NAME RS-0120-1-270519
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190527
Time 10.15 h
INSTRUM spect
PROBHD Z116098_0046 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 7978.724 Hz
FIDRES 0.243491 Hz
AQ 4.1069226 sec
RG 123.45
DW 62.667 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TDO 1
SFO1 399.6024677 MHz
NUC1 1H
P1 10.09 usec
PLW1 16.00000000 W

F2 - Processing parameters
SI 65536
SF 399.6000098 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

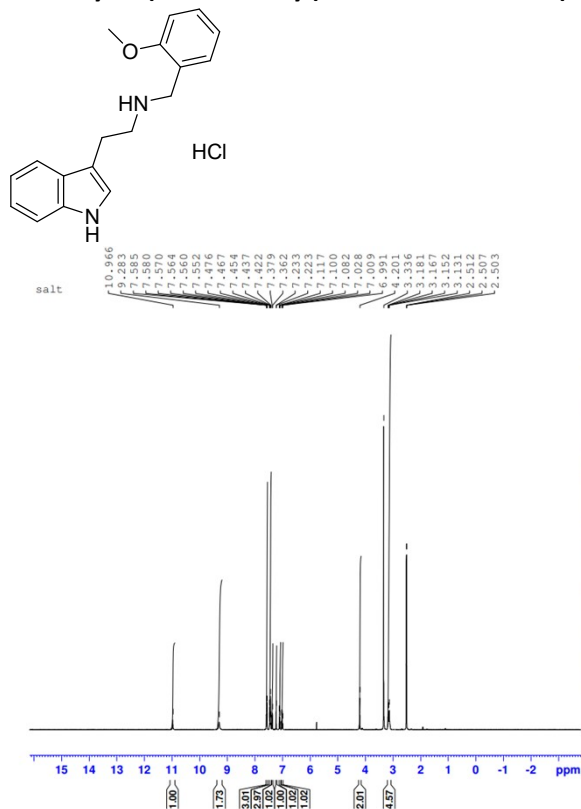


Current Data Parameters
NAME RS-0120-1-270519
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190527
Time 10.32 h
INSTRUM spect
PROBHD Z116098_0046 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 191.21
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1
SFO1 100.4895474 MHz
NUC1 13C
P1 10.00 usec
PLW1 78.00000000 W
SFO2 399.6015984 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 16.00000000 W
PLW12 0.20407000 W
PLW13 0.10265000 W

F2 - Processing parameters
SI 32768
SF 100.4794880 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

NMR spectra of final compounds N-benzyl-2-(1H-indol-3-yl)ethan-1-amine HCl (6)

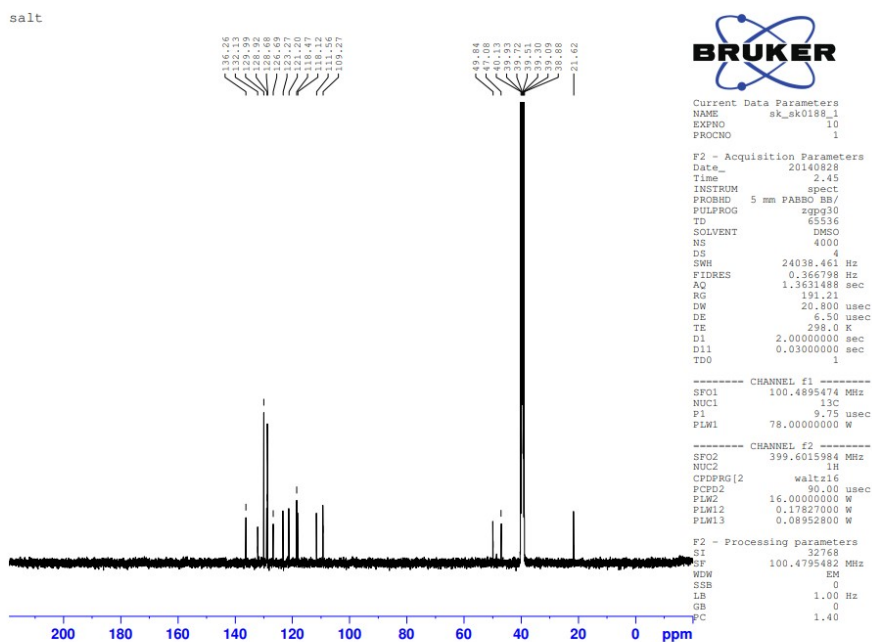


Current Data Parameters
NAME sk_ak0188_1
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140826
Time 10.35
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 8
DS 2
SWH 7910.724 Hz
FIDRES 0.121744 Hz
AQ 4.1059226 sec
RG 137.68
DW 62.687 usec
DE 8.50 usec
TE 298.0 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
SF01 399.6024677 MHz
NUC1 1H
P1 10.25 usec
PLW1 16.0000000 W

F2 - Processing parameters
SI 65536
SF 399.6000000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME sk_ak0188_1
EXPNO 10
PROCNO 1

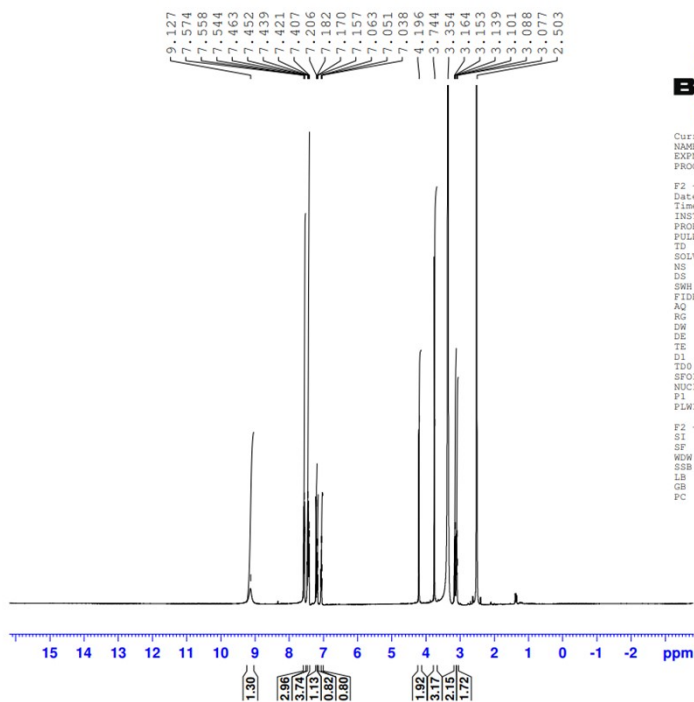
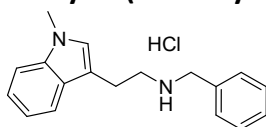
F2 - Acquisition Parameters
Date_ 20140828
Time 2.45
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 4000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 191.21
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

===== CHANNEL f1 =====
SF01 100.4895474 MHz
NUC1 13C
P1 9.75 usec
PLW1 78.0000000 W

===== CHANNEL f2 =====
SF02 399.6015984 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 16.0000000 W
PLW12 0.17827000 W
PLW13 0.08952800 W

F2 - Processing parameters
SI 32768
SF 100.4795482 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

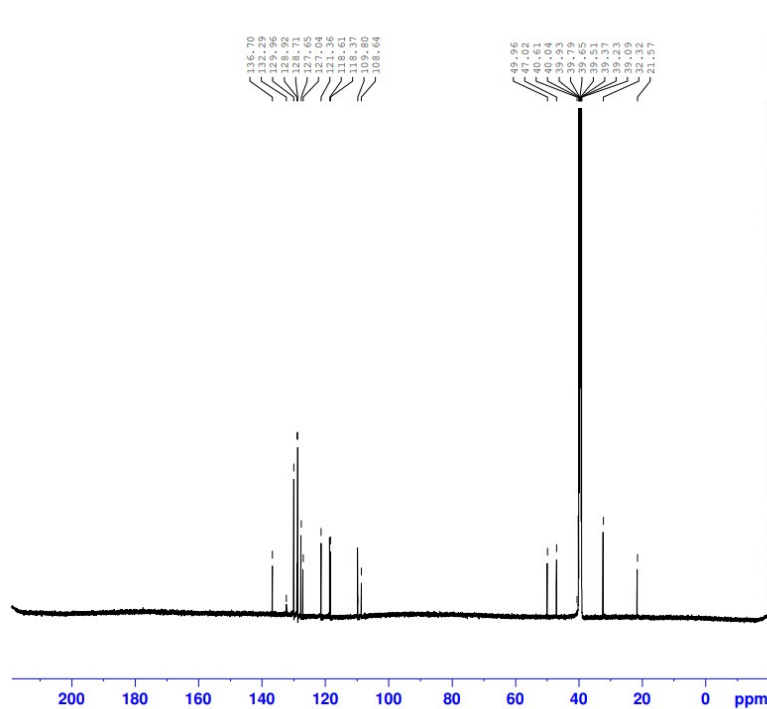
benzyl-2-(1-methyl-1H-indol-3-yl)ethan-1-amine HCl (7).



Current Data Parameters
NAME RS-0068-1_FINAL061218
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181206
Time 17.45 h
INSTRUM spect
PROBHD Z132572_0007 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 2.7262976 sec
RG 145.45
DW 41.600 usec
DE 40.00 usec
TE 298.9 K
D1 1.00000000 sec
TDO 1
SFO1 600.1737063 MHz
NUC1 1H
P1 11.43 usec
PLW1 21.00000000 W

F2 - Processing parameters
SI 65536
SF 600.1700009 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

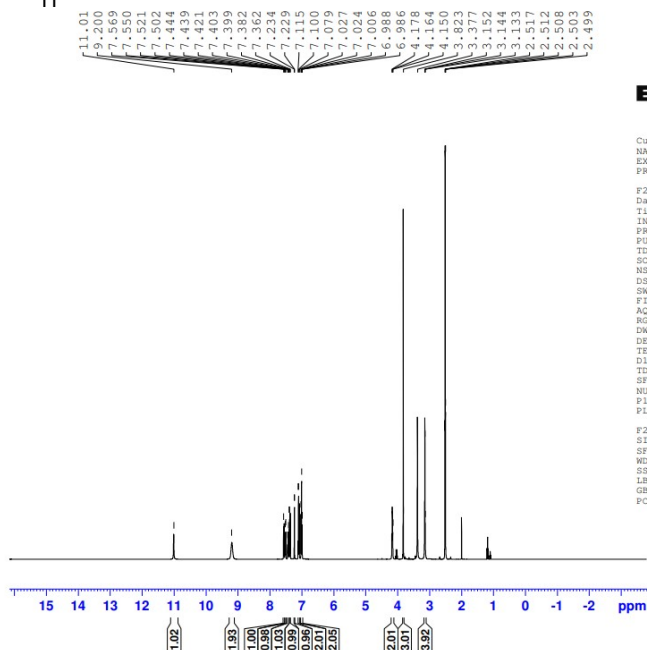
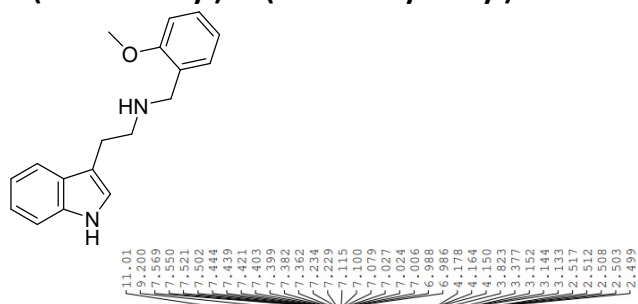


Current Data Parameters
NAME RS-0068-1_FINAL061218
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181207
Time 2.06 h
INSTRUM spect
PROBHD Z132572_0007 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 36057.691 Hz
FIDRES 1.100393 Hz
AQ 0.9087659 sec
RG 182.66
DW 13.867 usec
DE 18.00 usec
TE 298.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1
SFO1 150.9279571 MHz
NUC1 13C
P1 9.70 usec
PLW1 35.09999847 W
SFO2 600.1724007 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 70.00 usec
PLW2 21.00000000 W
PLW12 0.59069002 W
PLW13 0.28944001 W

F2 - Processing parameters
SI 65536
SF 150.9129371 MHz
WDW EM
SSB 0
LB 1.60 Hz
GB 0
PC 1.40

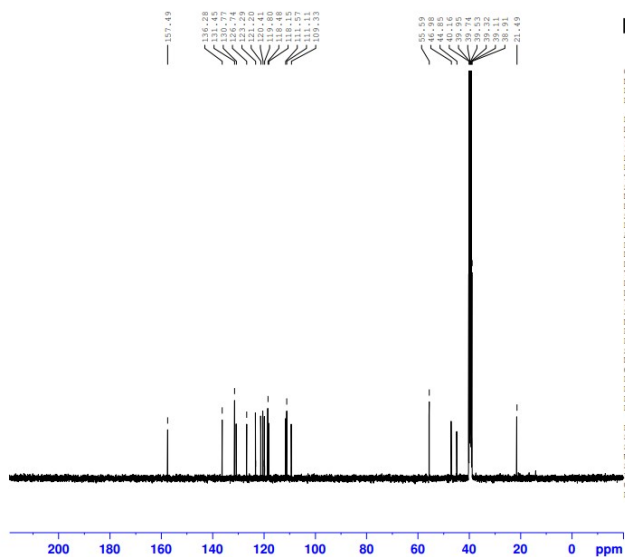
2-(1H-indol-3-yl)-N-(2-methoxybenzyl)ethan-1-amine HCl (8).



Current Data Parameters
NAME altk370
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171026
Time 17.01 h
INSTRUM spect
PROBHD Z116098_0046 (4
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 2
SWH 7978.724 Hz
FIDRES 0.243491 Hz
AQ 4.106226 sec
RG 157.6
DW 62.667 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 399.6024677 MHz
NUC1 1H
P1 10.61 usec
PLW1 16.00000000 W

F2 - Processing parameters
SI 65536
SF 399.6000000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME altk370
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171026
Time 21.57 h
INSTRUM spect
PROBHD Z116098_0046 (4
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 4
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 181.21
DW 25.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.4895474 MHz
NUC1 13C
P1 10.00 usec
PLW1 78.00000000 W
SFO2 399.6015984 MHz
NUC2 1H
CPCPG2 waltz16
PCPD2 90.00 usec
PLW2 16.00000000 W
PLW12 0.22070000 W
PLW13 0.11115000 W

F2 - Processing parameters
SI 32768
SF 100.4795458 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

C1=CC=C2C(=C1)N(C2)CCNCCc3ccc4ccccc4c3

HCl



```

F2 - Acquisition Parameters
Date_      20171103
Time       17.51 h
INSTRUM    spect
PROBHD     Z116098_0046
PULPROG    zg30
TD          65536
SOLVENT    DMSO
NS          8
DS          2
SWH         7978.724 Hz
FIDRES     0.243491 Hz
AQ          4.1069226 sec
RG          107.6
WDW         62.667 used
DE          6.50 use
TE          298.0 K
D1          1.00000000 sec
TD0         1
SFO1       399.6024671 MHz
NUC1       13H
P1          10.45 use
PL1        16.00000000 W

```

```
F2 - Processing parameters
SI                65536
SF                399.6000000 MHz
WDW               EM
SSB               0
LB                0.30 Hz
GB                0
PC                1.00
```



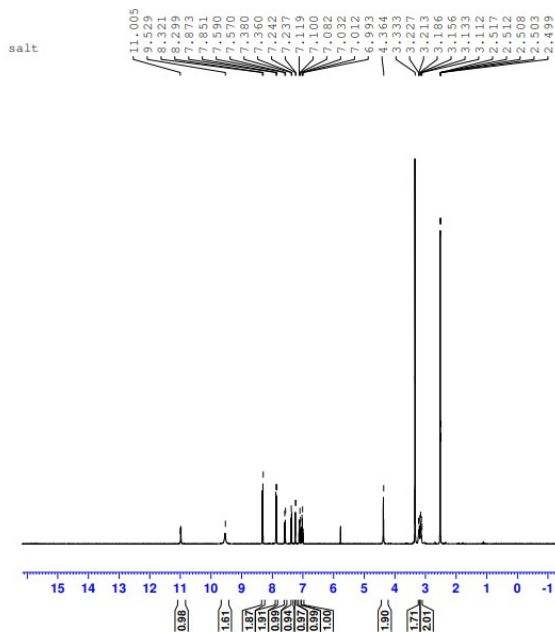
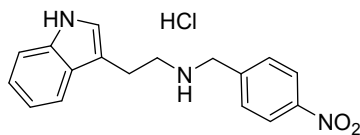
```

P2 - Acquisition Parameters
Date_          20171103
TIME           21:02.1 h
INST           SHSD
FREQ           Z116098.00 spect
PULPROG        zgpg30
PRG            65536
SOLVENT        DMSO
NS              2048
DS              5
SWH             24038.461 Hz
FIDRES          0.733396 Hz
AQ              1.3631488 sec
RG              191.21
DE              20.800 usec
DM              6.50 usec
TE              298.0 K
D1              2.0000000 sec
D11             0.03000000 sec
TDC1            1
NUC1            100.4895474 MHz
NUC2            13C
P1              10.00 usec
PL1             78.0000000 W
SFO2            399.6015984 MHz
PCPD2           1H
PCPD2[2]       16.00 usec
PLM2            0.2170000 W
PLM3            0.10933000 W
FLM13           0.10933000 W

```

```
F2 - Processing parameters
SI                32768
SF                100.4795482 MHz
WDW               EM
SSB               0
LB                1.00 Hz
GB                0
PC                1.40
```

2-(1H-indol-3-yl)-N-(4-nitrobenzyl)ethan-1-amine HCl (10)

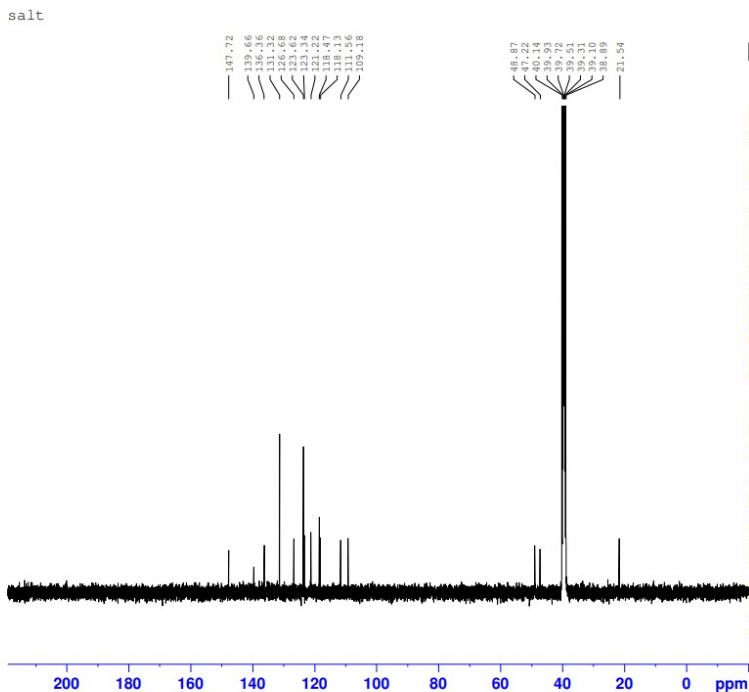


Current Data Parameters
NAME sk_sk0190_1
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140826
Time 10.44
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 8
DS 2
SWH 7978.724 Hz
FIDRES 0.121746 Hz
AQ 4.1069226 sec
RG 137.88
DW 62.667 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 399.6024677 MHz
NUC1 1H
P1 10.25 usec
PLW1 16.00000000 W

F2 - Processing parameters
SI 65536
SF 399.6000000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME sk_sk0190_1
EXPNO 4
PROCNO 1

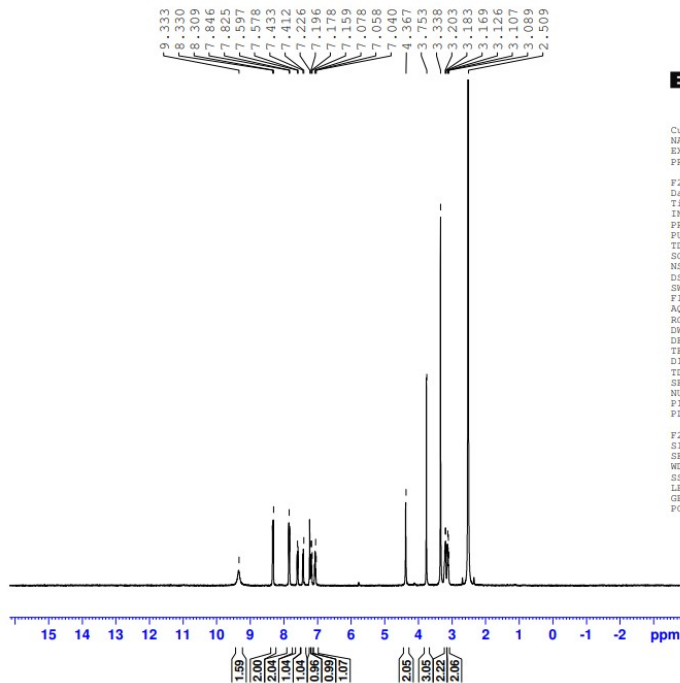
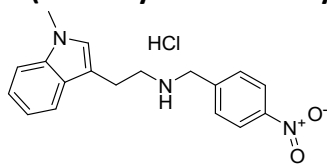
F2 - Acquisition Parameters
Date_ 20140827
Time 0.56
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 191.21
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.4895474 MHz
NUC1 13C
P1 9.75 usec
PLW1 78.00000000 W

===== CHANNEL f2 =====
SFO2 399.6015984 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 16.00000000 W
PLW12 0.17821000 W
PLW13 0.08952800 W

F2 - Processing parameters
SI 32768
SF 100.4795479 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

2-(1-methyl-1H-indol-3-yl)-N-(4-nitrobenzyl)ethan-1-amine HCl (11).

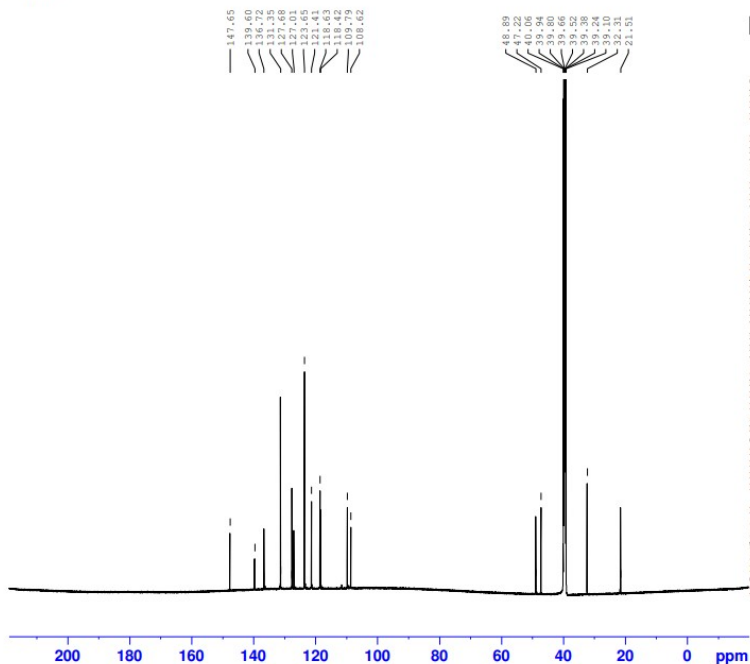


Current Data Parameters
 NAME RS-0038-1-241018
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20181024
 Time 22.29 h
 INSTRUM spect
 PROBHD Z116098_0046 (
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 32
 DS 2
 SWH 7978.724 Hz
 FIDRES 0.243491 Hz
 AQ 4.1069226 sec
 RG 191.21
 DW 62.667 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.00000000 sec
 TDO 1
 SFO1 399.6024677 MHz
 NUC1 1H
 P1 16.35 usec
 PLW1 16.00000000 W

F2 - Processing parameters
 SI 65536
 SF 399.5999993 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

FINAL

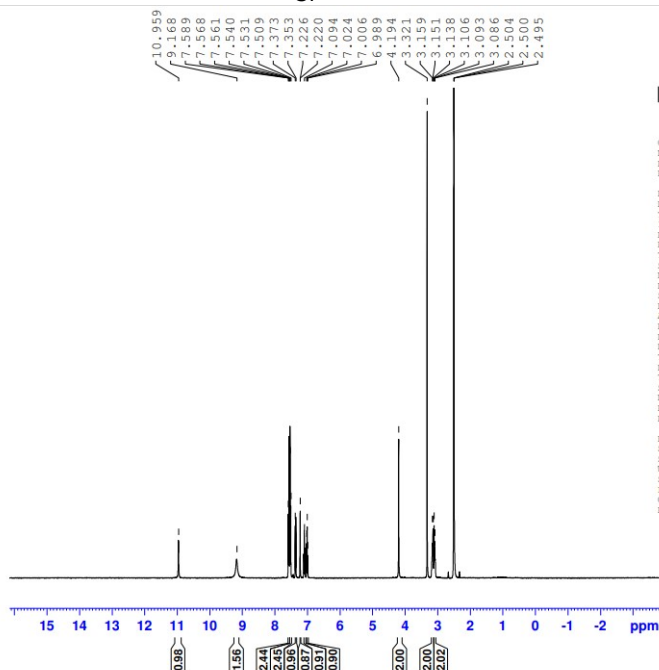
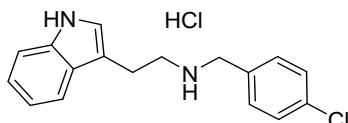


Current Data Parameters
 NAME RS-0038-1_FINAL
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20181024
 Time 20.47 h
 INSTRUM spect
 PROBHD Z132572_0007 (
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 2048
 DS 4
 SWH 36057.691 Hz
 FIDRES 1.100393 Hz
 AQ 0.9087659 sec
 RG 182.66
 DW 13.867 usec
 DE 18.00 usec
 TE 298.9 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1
 SFO1 150.9279571 MHz
 NUC1 13C
 P1 9.70 usec
 PLW1 35.09999847 W
 SFO2 600.1724007 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 70.00 usec
 PLW2 21.00000000 W
 PLW12 0.59069002 W
 PLW13 0.28944001 W

F2 - Processing parameters
 SI 65536
 SF 150.9129383 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

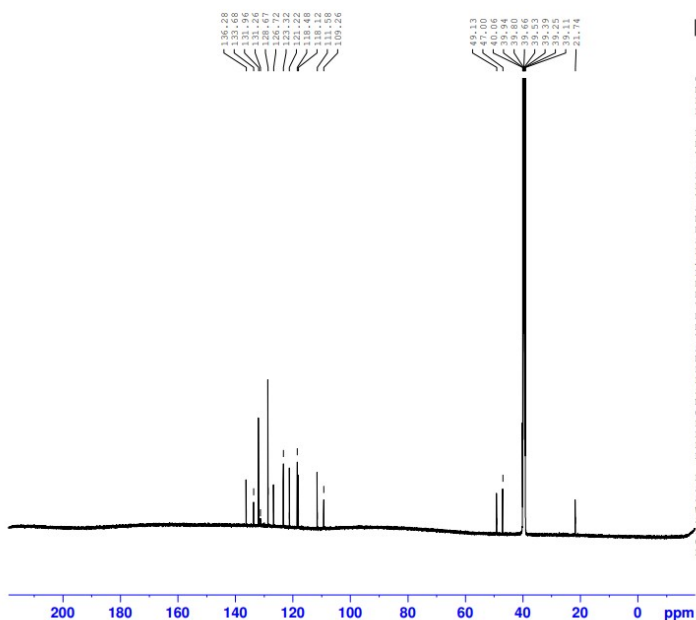
N-(4-chlorobenzyl)-2-(1H-indol-3-yl)ethan-1-amine HCl (12).



Current Data Parameters
NAME RS-0079-1
EXPRO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190117
Time 11.54 h
INSTRUM spect
PROBHD Z116098_0046 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 7978.724 Hz
FIDRES 0.243491 Hz
AQ 4.1069226 sec
RG 171.52
DW 62.667 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 399.6024677 MHz
NUC1 1H
P1 10.51 usec
PLM1 16.00000000 W

F2 - Processing parameters
SI 65536
SF 399.6000034 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

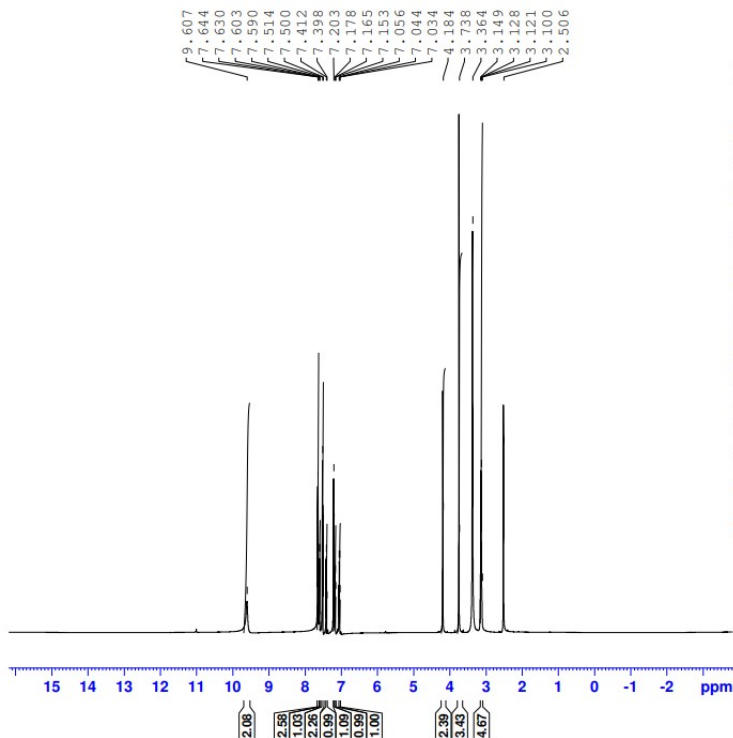
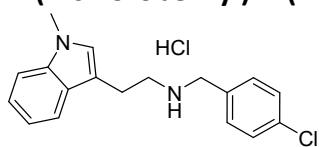


Current Data Parameters
NAME RS-0079-1-220119
EXPRO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190123
Time 3.11 h
INSTRUM spect
PROBHD Z132572_0007 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 3012
DS 4
SWH 36057.691 Hz
FIDRES 1.100393 Hz
AQ 0.3087659 sec
RG 182.66
DW 13.867 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.9279571 MHz
NUC1 13C
P1 9.70 usec
PLM1 35.09999847 W
SFO2 600.1724007 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 70.00 usec
PLM2 21.00000000 W
PLM12 0.59069002 W
PLM13 0.28944001 W

F2 - Processing parameters
SI 65536
SF 150.9129367 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

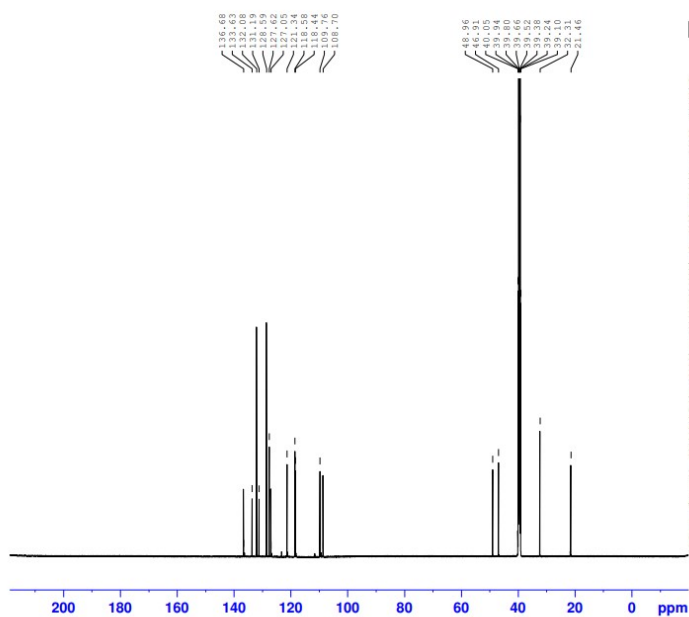
N-(4-chlorobenzyl)-2-(1-methyl-1H-indol-3-yl)ethan-1-amine HCl (13).



Current Data Parameters
NAME RS-0041-1-FINAL
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181029
Time 18.39 h
INSTRUM spect
PROBHD Z132572_0007 (4
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 2
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 2.7262976 sec
RG 91.61
DW 41.600 usec
DE 40.00 usec
TE 298.9 K
D1 1.00000000 sec
TD0 1
SFO1 600.1737063 MHz
NUC1 1H
P1 11.43 usec
PLW1 21.00000000 W

F2 - Processing parameters
SI 65536
SF 600.1700000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



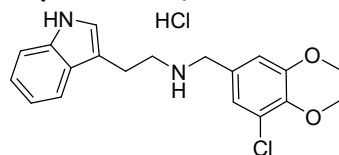
Current Data Parameters
NAME RS-0041-1-FINAL
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181101
Time 19.56 h
INSTRUM spect
PROBHD Z132572_0007 (4
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 36057.691 Hz
FIDRES 1.100393 Hz
AQ 0.9087659 sec
RG 182.66
DW 13.867 usec
DE 18.00 usec
TE 298.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.9279571 MHz
NUC1 13C
P1 9.70 usec
PLW1 35.09999847 W
SFO2 600.1724007 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 70.00 usec
PLW2 21.00000000 W
PLW12 0.59069002 W
PLW13 0.28944001 W

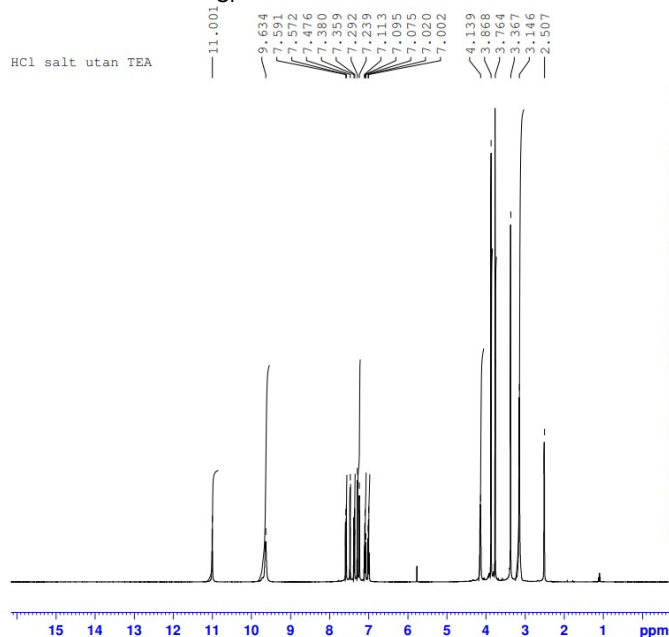
F2 - Processing parameters
SI 65536
SF 150.9129370 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

[illegible]

N-(3-chloro-4,5-dimethoxybenzyl)-2-(1H-indol-3-yl)ethan-1-amine (15).



HCl salt utan TEA



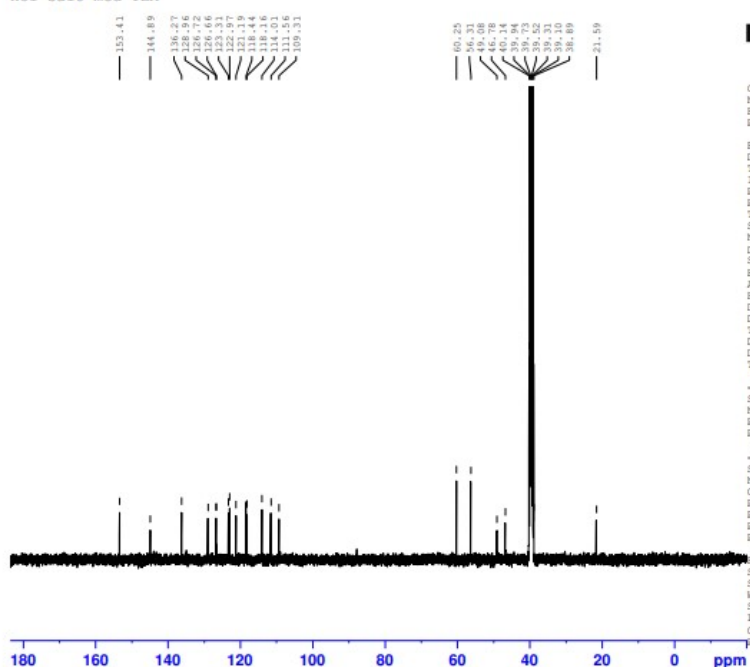
Current Data Parameters
NAME sk_sk0185_1
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140703
Time 9.59
INSTRUM spect
PROBHD 5 mm PARBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 2
SWH 7978.724 Hz
FIDRES 0.121746 Hz
AQ 4.1069226 sec
RG 84.69
DW 62.667 usec
DE 6.50 usec
TE 298.0 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 399.6024677 MHz
NUC1 1H
P1 10.25 usec
PLW1 16.0000000 W

F2 - Processing parameters
SI 65536
SF 399.6000000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

HCl salt med TEA



Current Data Parameters
NAME sk_sk0185_1
EXPNO 8
PROCNO 1

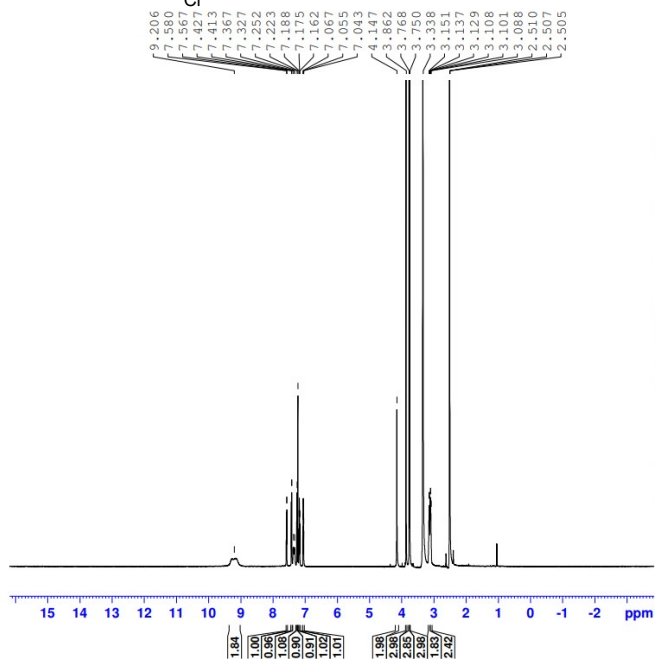
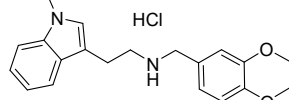
F2 - Acquisition Parameters
Date_ 20140703
Time 11.22
INSTRUM spect
PROBHD 5 mm PARBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 191.21
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.4895474 MHz
NUC1 13C
P1 9.75 usec
PLW1 78.0000000 W

===== CHANNEL f2 =====
SFO2 399.6015984 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 16.0000000 W
PLW12 0.1782100 W
PLW13 0.0895280 W

F2 - Processing parameters
SI 32768
SF 100.4795473 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

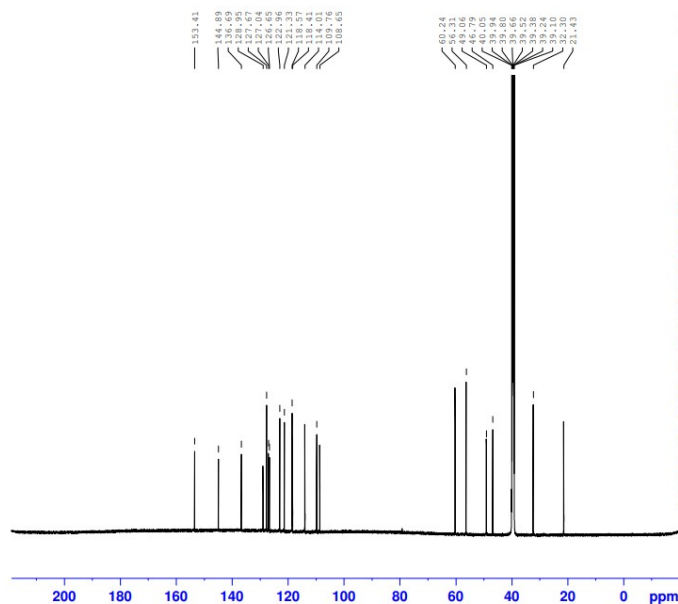
N-(3-chloro-4,5-dimethoxybenzyl)-2-(1-methyl-1H-indol-3-yl)ethan-1-amine HCl (16).



Current Data Parameters
NAME RS-0048-1-061118
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181106
Time 9.39 h
INSTRUM spect
PROBHD Z132572_0007 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 8
DS 2
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 2.7262976 sec
RG 83.49
DW 41.600 usec
DE 40.00 usec
TE 298.2 K
D1 1.00000000 sec
TDO
SFO1 600.1737063 MHz
NUC1 1H
P1 11.43 usec
PLW1 21.00000000 W

F2 - Processing parameters
SI 65536
SF 600.1700000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME RS-0048-1_FINAL061218
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181207
Time 0.20 h
INSTRUM spect
PROBHD Z132572_0007 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 36057.691 Hz
FIDRES 1.100393 Hz
AQ 0.9087659 sec
RG 192.66
DW 13.867 usec
DE 18.00 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO
SFO1 150.9279571 MHz
NUC1 13C
P1 9.70 usec
PLW1 35.09999847 W
SFO2 400.1724007 MHz
NUC2 1H
PCPD2 waltz16
PCPD2 70.00 usec
PLW2 21.00000000 W
PLW12 0.59069002 W
PLW13 0.28944001 W

F2 - Processing parameters
SI 65536
SF 150.9129388 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Cc1c[nH]c2ccccc12CCNCCc3ccc4ccccc4c3

```

Current Data Parameters
NAME          KS_006_DMSSO
EXPNO         1
PROCNO        1

F2 - Acquisition Parameters
Date_         20190411
TIME          16:46 h
INSTRUM       spect
PROBHD        Z116980_0046 f
PULPROG       zgpg30
TD            65536
SOLVENT       DMSO
NS            32
DSR           2
SWH           7978.724 Hz
AQ           0.243436 Hz
RG            4.1089226 sec
AQ            171.52
DM            62.467 usec
DE            6.50 usec
TE            298.0 K
D1            1.00000000 sec
SFO           400.141 MHz
SF1           399.6024677 MHz
NUC1           1H
NUC2           15N
FLN1          16.0000000 W

F2 - Processing parameters
SI            65536
SF            399.6000000 MHz
MW            EM
GB            0.30 Hz
LB            0
GC            1.00

```



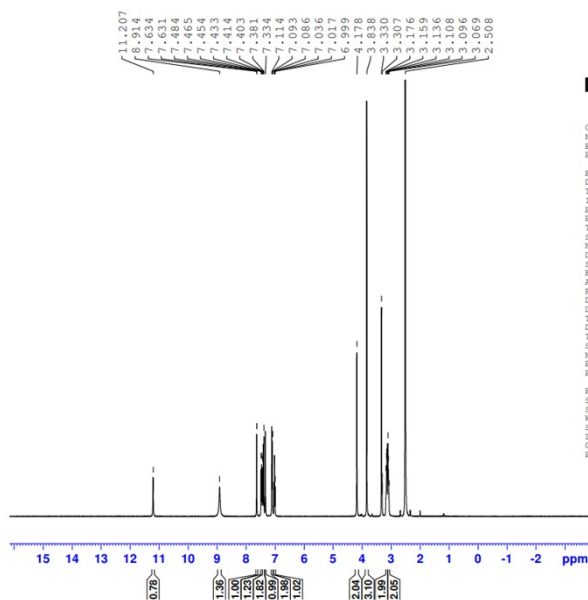
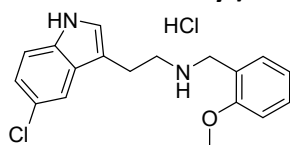
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Current Data Parameters
NAME      KS_006_DM500_1_190418
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
-----
Date_     20190418
Time      20.14 h
INSTRUM    spect
PROBHD     12132572.0
PULPROG    zgpg30
TD          65536
SFO         400
AQ          0.0000000
NS          1024
DS          4
SWH          36057.691 Hz
FIDRES      1.100393 Hz
AQ          0.9087659 sec
DE          182.66
DQ          13.867 usec
DI          18.00 usec
D2          298.0 K
D3          2.0000000 sec
D4          0.0300000 sec
D5          1
D6          1
D7          150.9279571 MHz
D8          1
D9          1
D10         1
D11         1
D12         1
D13         1
D14         1
D15         1
D16         1
D17         1
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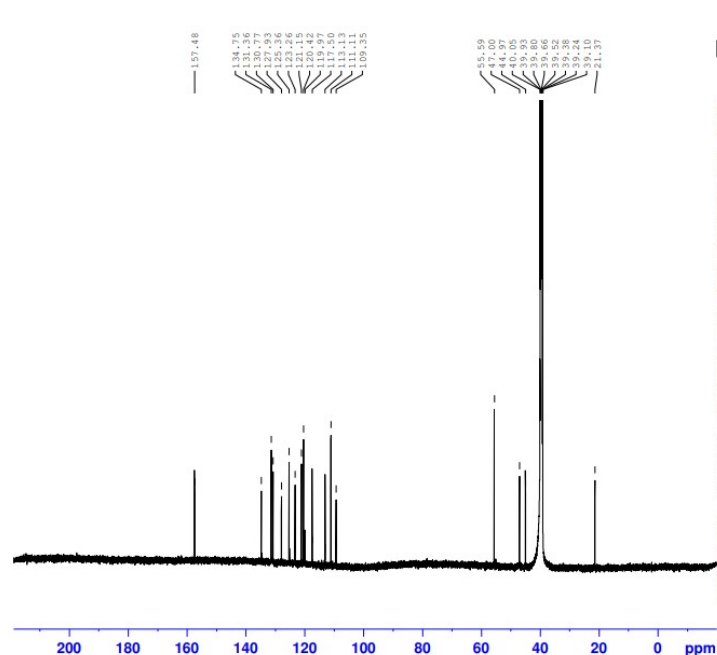
2-(5-chloro-1H-indol-3-yl)-N-(2-methoxybenzyl)ethan-1-amine HCl (18).



Current Data Parameters
NAME RS-0984-1-070119
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190207
Time 11:27 h
INSTRUM spect
PROBHD z116098_0046 f
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 7978.724 Hz
FIDRES 0.243491 Hz
AQ 4.1069226 sec
RG 371.52
DM 62.467 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
D11 1
SFO1 399.6024677 MHz
NUC1 1H
P1 10.47 usec
PLW1 16.00000000 W

F2 - Processing parameters
SI 65536
SF 399.6000000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

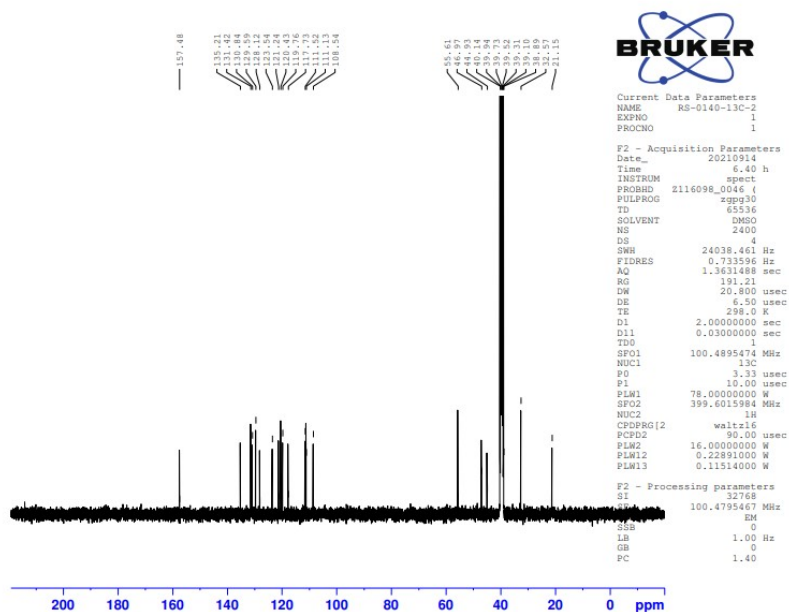
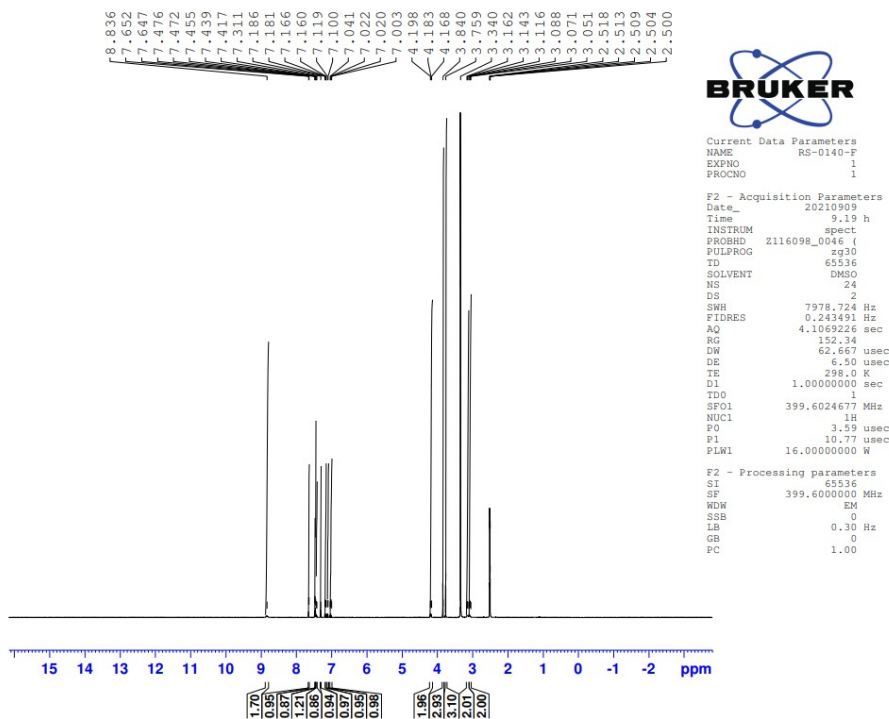
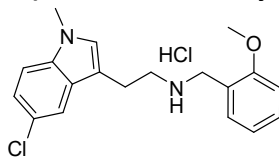


Current Data Parameters
NAME RS_098-13c-240614
EXPNO 1
PROCNO 1

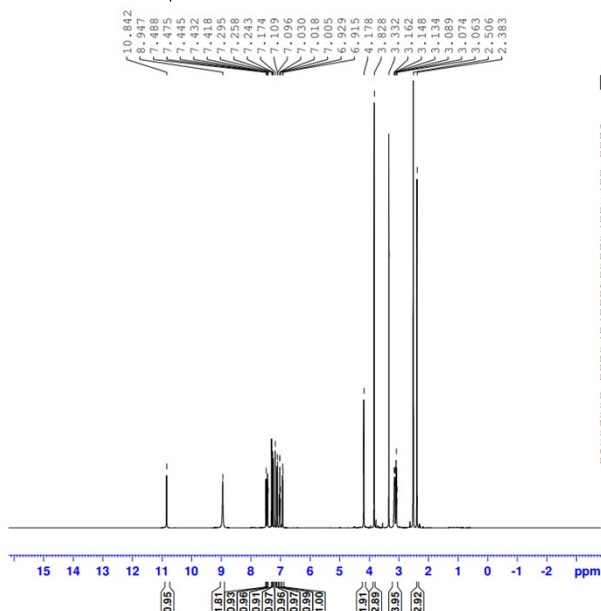
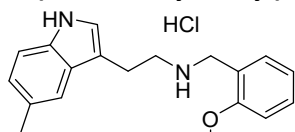
F2 - Acquisition Parameters
Date_ 20240614
Time 20:57 h
INSTRUM spect
PROBHD Z132572_0007 f
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 36057.691 Hz
FIDRES 1.100393 Hz
AQ 0.9087659 sec
RG 182.66
DM 13.867 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
D12 1
SFO1 150.9279571 MHz
NUC1 13C
P1 3.23 usec
P2 9.70 usec
PLW1 35.09999847 W
SFO2 600.1724007 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 70.00 usec
PLW2 21.00000000 W
PLW12 0.59069002 W
PLW13 0.28944001 W

F2 - Processing parameters
SI 65536
SF 150.9129383 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

2-(5-chloro-1-methyl-1H-indol-3-yl)-N-(2-methoxybenzyl) ethan-1-amine HCl (19).



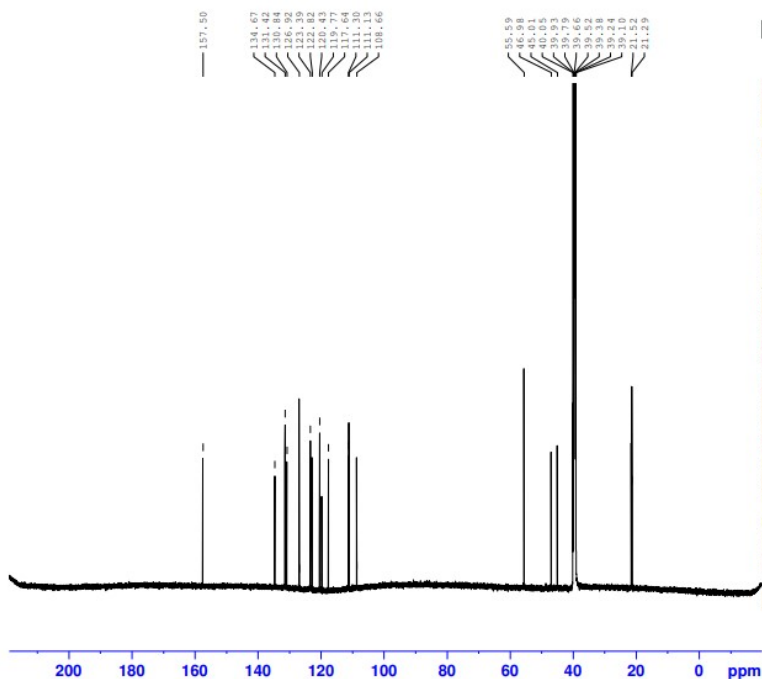
N-(2-methoxybenzyl)-2-(5-methyl-1H-indol-3-yl)ethan-1-amine HCl (20).



Current Data Parameters
 NAME RS-0087-1_FINAL
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190207
 Time 15.58 h
 INSTRUM spect
 PROBHD Z132572_0007 (
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 32
 DS 2
 SWH 12019.230 Hz
 FIDRES 0.368758 Hz
 AQ 2.7262976 sec
 RG 182.66
 DW 41.600 usec
 DE 40.00 usec
 TE 298.0 K
 D1 1.00000000 sec
 TDO 1
 SFO1 600.137063 MHz
 NUC1 1H
 P1 11.43 usec
 PLW1 21.00000000 W

F2 - Processing parameters
 SI 65536
 SF 600.1700000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

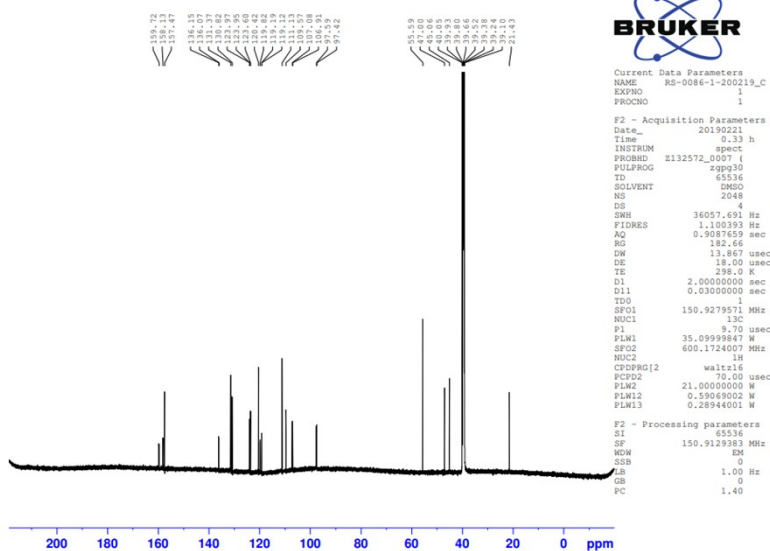
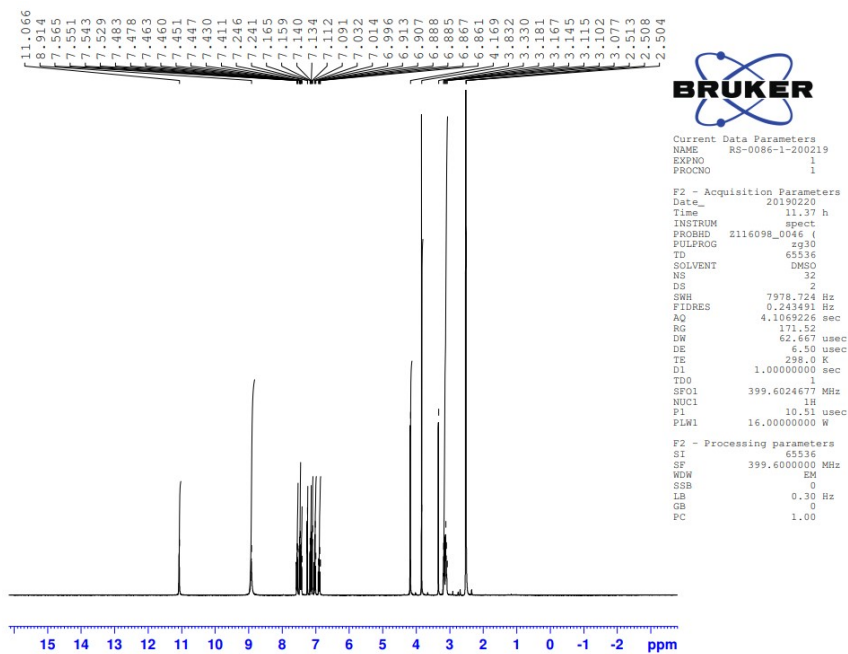
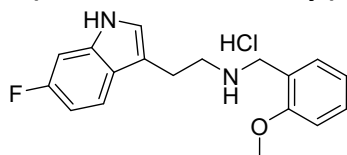


Current Data Parameters
 NAME RS-0087-1_FINAL_
 EXPNO 1
 PROCNO 1

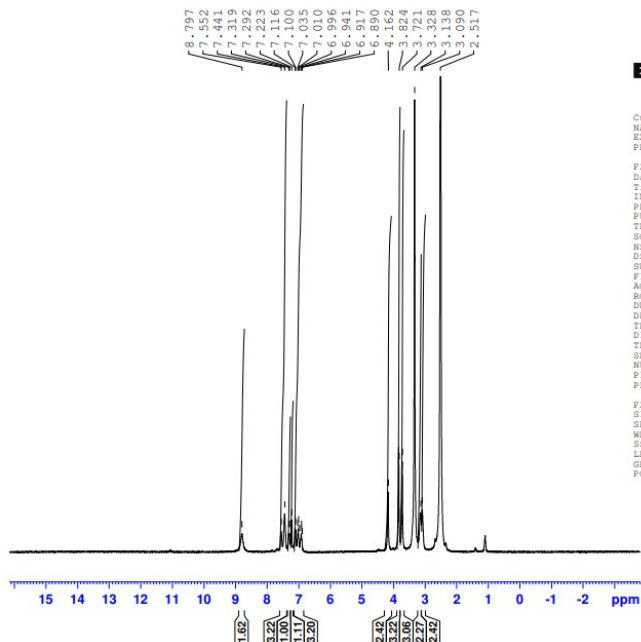
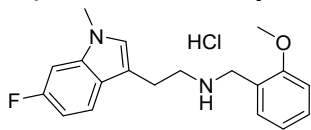
F2 - Acquisition Parameters
 Date_ 20190219
 Time 0.36 h
 INSTRUM spect
 PROBHD Z132572_0007 (
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 2048
 DS 4
 SWH 36057.691 Hz
 FIDRES 1.100393 Hz
 AQ 0.5907659 sec
 RG 182.66
 DW 13.867 usec
 DE 18.00 usec
 TE 298.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1
 SFO1 150.9279571 MHz
 NUC1 13C
 P1 9.70 usec
 PLW1 35.09999847 W
 SFO2 600.1724007 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 70.00 usec
 PLW2 21.00000000 W
 PLW12 0.59069002 W
 PLW13 0.28944001 W

F2 - Processing parameters
 SI 65536
 SF 150.9129373 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

2-(6-fluoro-1H-indol-3-yl)-N-(2-methoxybenzyl)ethan-1-amine HCl (21).



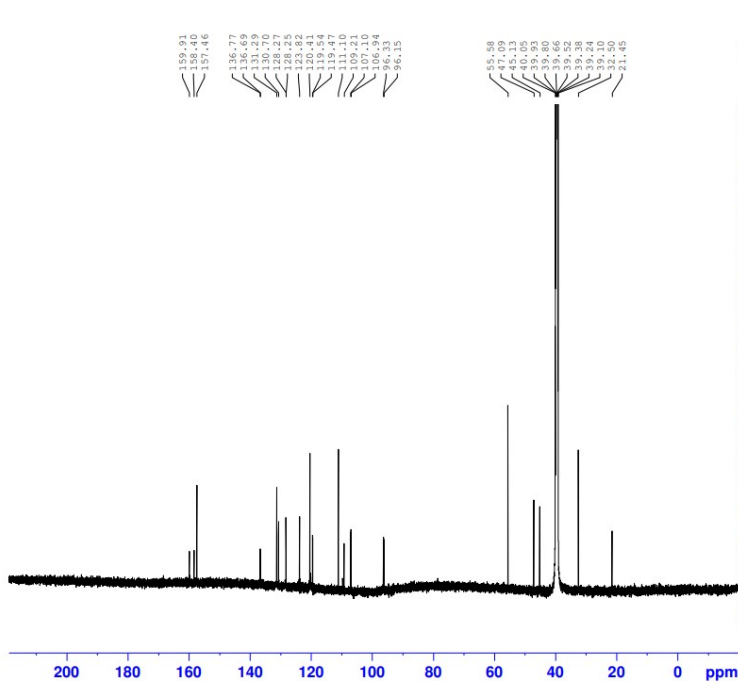
2-(6-fluoro-1-methyl-1H-indol-3-yl)-N-(2-methoxybenzyl) ethan-1-amine HCl (22).



Current Data Parameters
NAME RS-0098-1_FINAL
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190410
Time 9.42 h
INSTRUM spect
PROBHD Z116098_0046 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 7978.724 Hz
FIDRES 0.243491 Hz
AQ 4.1063226 sec
RG 171.52
DW 62.667 usec
DE 4.50 usec
TE 298.0 K
D1 1.00000000 sec
TDO
SFO1 399.6024677 MHz
NUC1 1H
P1 10.37 usec
PLW1 16.00000000 W

F2 - Processing parameters
SI 65536
SF 399.6000000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

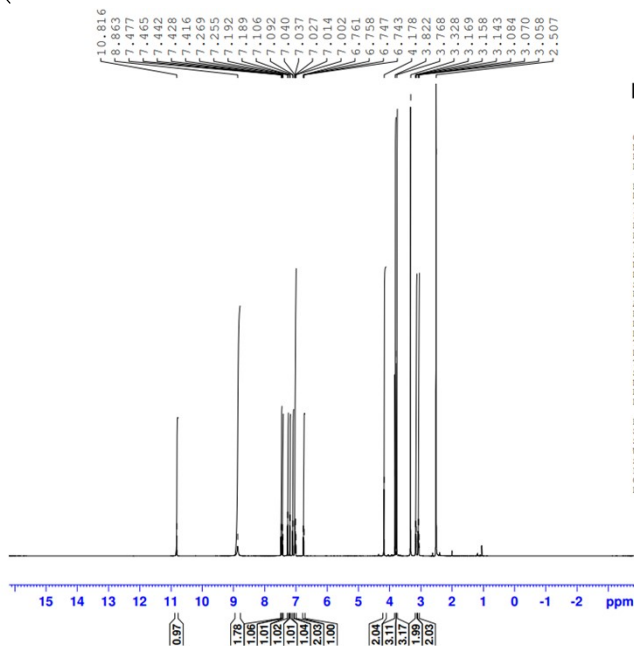
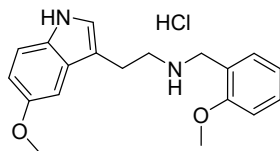


Current Data Parameters
NAME RS-098-13C-240614
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240614
Time 19.59 h
INSTRUM spect
PROBHD Z132572_0007 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 36057.691 Hz
FIDRES 1.100393 Hz
AQ 0.9087659 sec
RG 182.66
DW 13.867 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1
SFO1 150.9279571 MHz
NUC1 13C
P0 3.23 usec
P1 9.70 usec
PLW1 35.09999847 W
SFO2 600.1724007 MHz
NUC2 1H
CPCPDG[2] waltz16
PCPD2 70.00 usec
PLW2 21.00000000 W
PLW12 0.59069002 W
PLW13 0.28944001 W

F2 - Processing parameters
SI 65536
SF 150.9129379 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

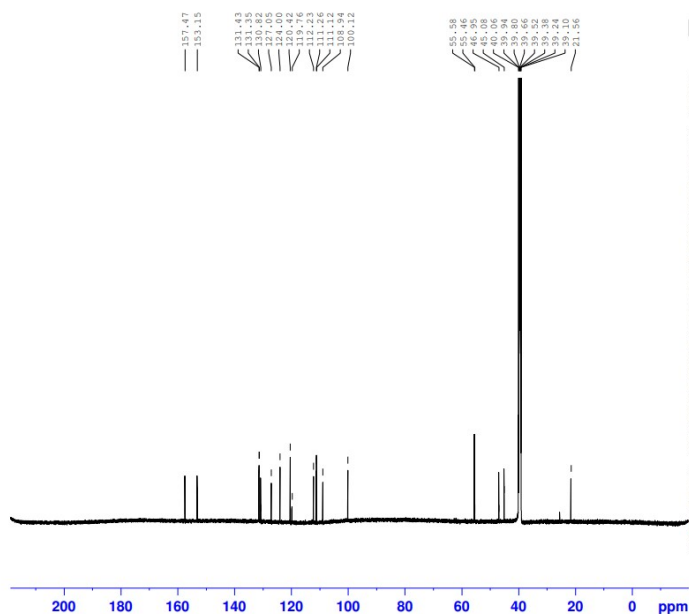
2-(5-methoxy-1H-indol-3-yl)-N-(2-methoxybenzyl)ethan-1-amine HCl (23).



Current Data Parameters
NAME RS-0069-1_-FINAL
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181206
Time 9:10 h
INSTRUM spect
PROBHD Z132572_0007 (4
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 2
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 2.7262976 sec
RG 104.42
DW 41.600 usec
DE 45.00 usec
TE 298.9 K
D1 1.00000000 sec
TD0 1
SFO1 600.1737063 MHz
NUC1 1H
P1 11.43 usec
PLW1 21.00000000 W

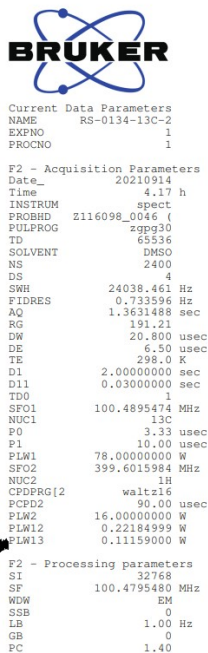
F2 - Processing parameters
SI 65536
SF 600.1700000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



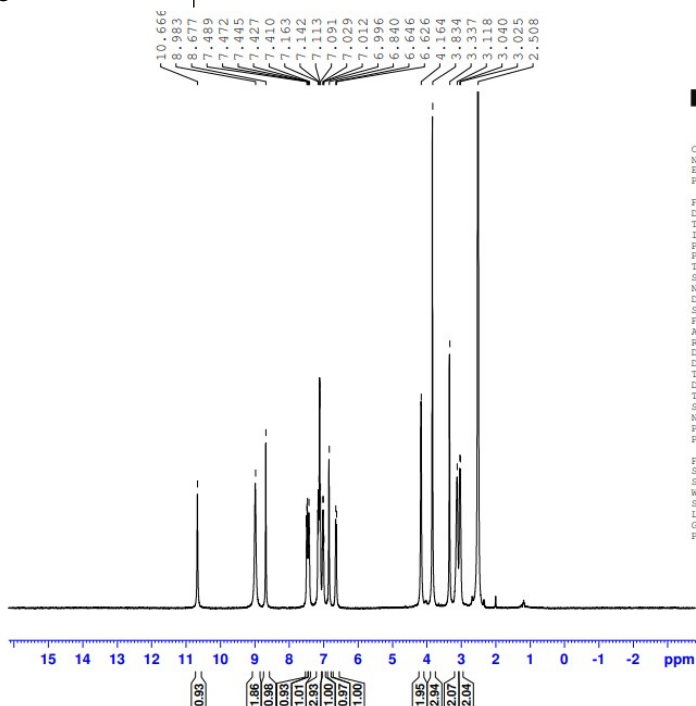
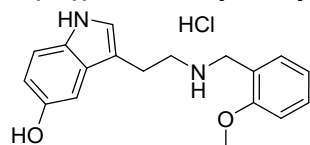
Current Data Parameters
NAME RS-0069-1_-FINAL
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181206
Time 20:46 h
INSTRUM spect
PROBHD Z132572_0007 (4
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2040
DS 4
SWH 36057.691 Hz
FIDRES 1.100393 Hz
AQ 0.9087659 sec
RG 182.66
DW 13.867 usec
DE 18.00 usec
TE 298.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.9279571 MHz
NUC1 13C
P1 9.70 usec
PLW1 35.09999847 W
SFO2 600.1724007 MHz
NUC2 1H
CPCPD2 waltz16
PCPD2 70.00 usec
PLW2 21.00000000 W
PLW12 0.59069002 W
PLW13 0.28944001 W

F2 - Processing parameters
SI 65536
SF 150.9129387 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

CN1C=CC2=C(C=C1)C(=C(C=C2)OC)CCNCCc3ccccc3OC

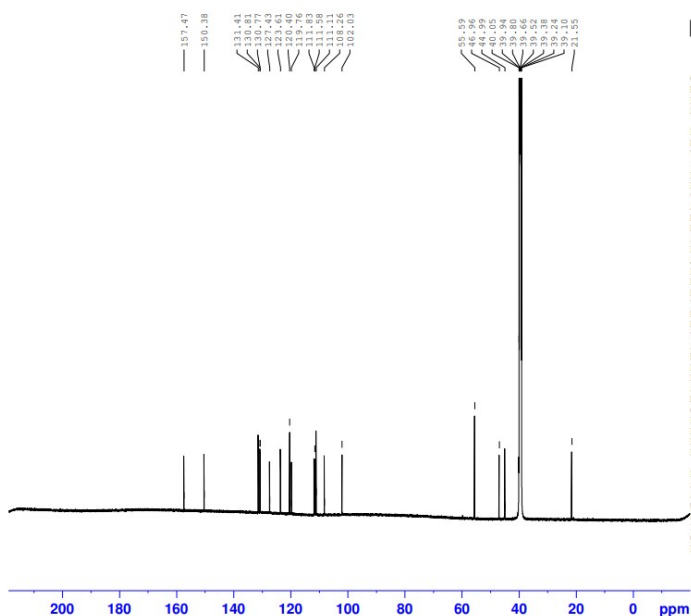
3-((2-methoxybenzyl)amino)ethyl)-1H-indol-5-ol HCl (25).



Current Data Parameters
NAME RS-0080-1-220119
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190122
Time 12.35 h
INSTRUM spect
PROBHD Z116098_0046 ()
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 7978.724 Hz
FIDRES 0.243491 Hz
AQ 4.1069226 sec
RG 152.34
DW 62.667 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 399.6024677 MHz
NUC1 1H
PL1 10.40 usec
PLW1 16.00000000 W

F2 - Processing parameters
SI 65536
SF 399.6000000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

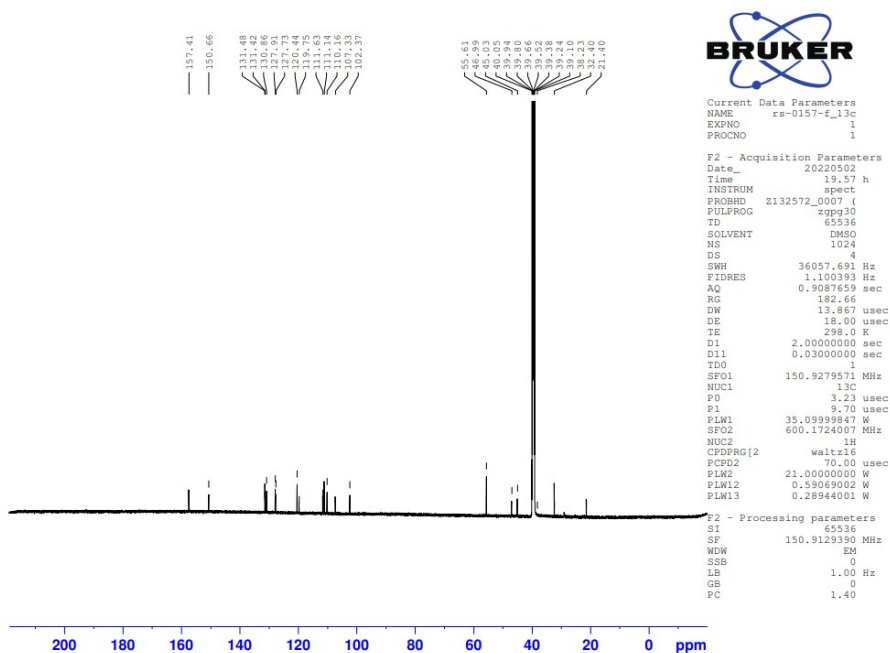
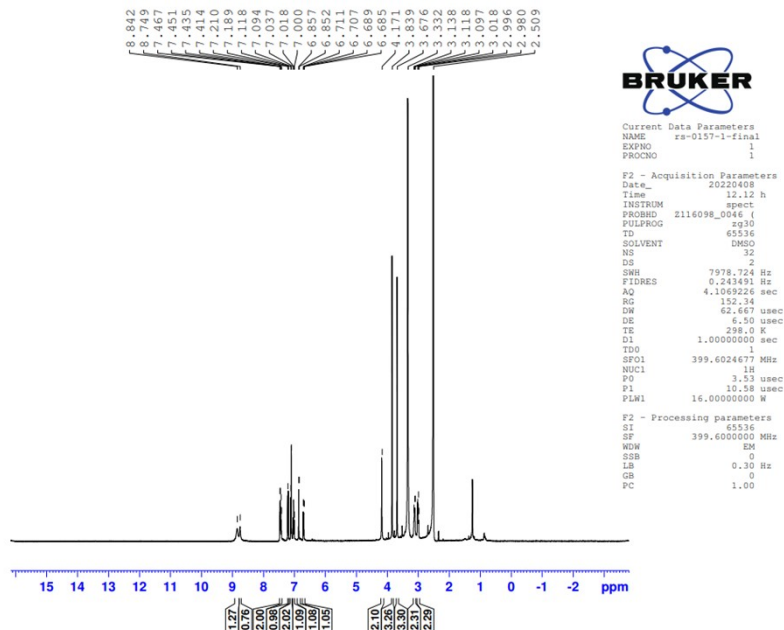
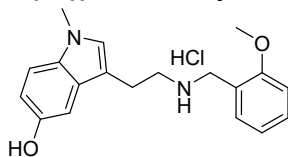


Current Data Parameters
NAME RS-0080-1-220119
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190123
Time 0.38 h
INSTRUM spect
PROBHD Z132572_0007 ()
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 36057.691 Hz
FIDRES 1.100393 Hz
AQ 0.9087659 sec
RG 182.66
SM 13.867 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.9279571 MHz
NUC1 13C
PL1 35.09999847 W
PLW1 0.28944001 W
SFO2 600.1724007 MHz
NUC2 1H
PCPD2 70.00 usec
PLM2 21.00000000 W
PLM12 0.59060002 W
PLM13 0.28944001 W

F2 - Processing parameters
SI 65536
SF 150.9129409 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

3-((2-methoxybenzyl)amino)ethyl)-1-methyl-1H-indol-5-ol HCl (26).



CN(C)CCc1c[nH]c2ccccc12.[Cl-]

```
Current Data Parameters
NAME          RS-0123-1-180619
EXPNO         1
PROCNO        1
```

```

F2 - Acquisition Parameters
Date_      20190618
Time       13.37 h
INSTRUM    spect
PROGNAME   Z116098_0046
PULPROG    zg30
TD         835336
CT         2
SOLVENT    DMF0
NS         8
DS         2
SWH         7978.724 Hz
FIDRES     0.243491
AQ         4.1069928 sec
RG         5.5.79
CW         62.647 usec
DE         6.50 usec
TE         298.0 K
D1         1.0000000 sec
TDC         1
SFO1       399.602467 MHz
MDEL1      18
P1         10.67 usec
FL1        18.0000000 W

```

F2 - Processing parameters	
SI	85536
SF	399.59999996 MHz
MDW	EM
SGR	0
LR	0.30 Hz
GR	0
PC	1.00



```
Current Data Parameters
NAME          RS-0123-1_C
EXPNO         1
PROCNO        1
```

F2 - Acquisition Parameters	
Date_	20190617
Time	16.10 h
INSTRUM	UNITY
PROBHD	2312572-0007
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	128
DS	4
DW	36057.591 Hz
FIDRES	1.000393
AQ	0.9087659 sec
RG	182.66
DE	13.867 usec
DW	18.067 usec
TE	298.0 K
D1	2.0000000 sec
D11	0.03000000 sec
TD0	1
SFO1	150.9279571 MHz
NUC1	13C
PL1	1.970 usec
PF1	650.1999847 MHz
SFO2	300.1724007 MHz
NUC2	1H
PCPDUG2	waltz16
PCPD2	70.00 usec
PLW2	21.0000000 W
PLW1	20.9999002 W
PLW13	0.28944001 W

```
F2 - Processing parameters
SI                65536
SF                150.9129285 MHz
WDW              EM
SSB              0
LB              1.00 Hz
GB              0
PC              1.40
```

CN(C)CCc1c[nH]c2ccccc12

```

Current Data Parameters
NAME      RS-0099-1-070619
EXPNO     1
PROCNO    1
PROCNAME   1
Date_     20150907
Time      16.25 h
INSTRUM    spect
PROBHD     2116098_046
PULPROG    zg30
PCPDPRG1   gssi36
SOLVENT     DMSO
NS          32
DS          2
SWH         7987.724 Hz
AQ          0.21433 s
AQ2         0.106922 sec
RG          191.21
DE          62.467 usec
RG2         6.50 usec
TE          298.0 K
TD          1.00000000 sec
SF01        399.6024467 MHz
SF          18
FIDRES      26.44 usec
F1W1        16.00000000 W

```



```

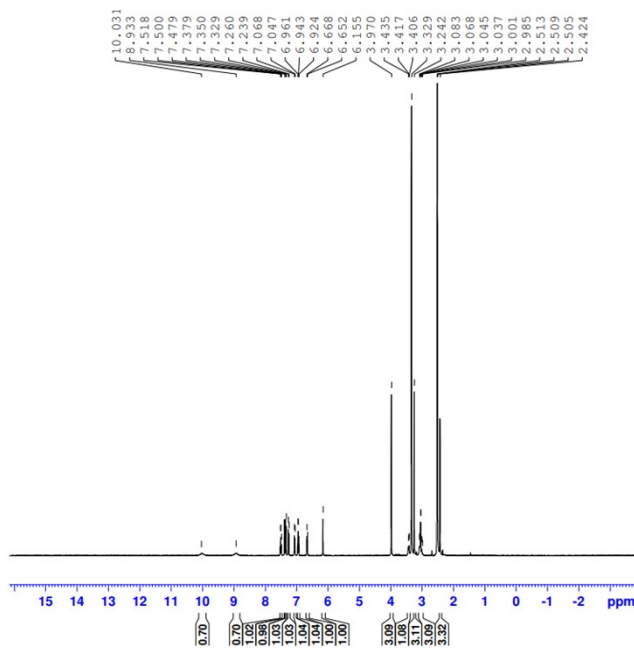
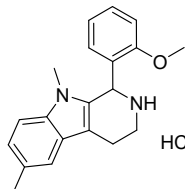
Current Data Parameters
NAME      RS-099-L_F_C
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_      20190521
Time       22.32 h
INSTRUM    spect
PROBHD      1232572_0007
PULPROG     zgpg30
PCPD2       6.336
SOLVENT      DMSO
NS           2048
DS           4
SWH          36057.691 Hz
FIDRES      1.100393 Hz
AQ           0.9087659 sec
RG           182.66
DE           13.867 Hz/sec
TE           18.00 usec
TD           298.000 K
N1           2.0000000 sec
N2           0.03000000 sec
SFO          270
TFO          150.927951 MHz
NUC1          13C
NUC2          13C
P1           9.70 usec
PLW1         35.0999847 W
SFO2          600.1427047 MHz
NUC2          1H
PCPD2         12H
PCPD22       wait1s
PLW2         21.00000000 W
PLW12        0.90649002 W
PLW13        0.2894400 W

F2 - Processing parameters
SI          5536
CF          150.9129386 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB          0
PC           1.40

```

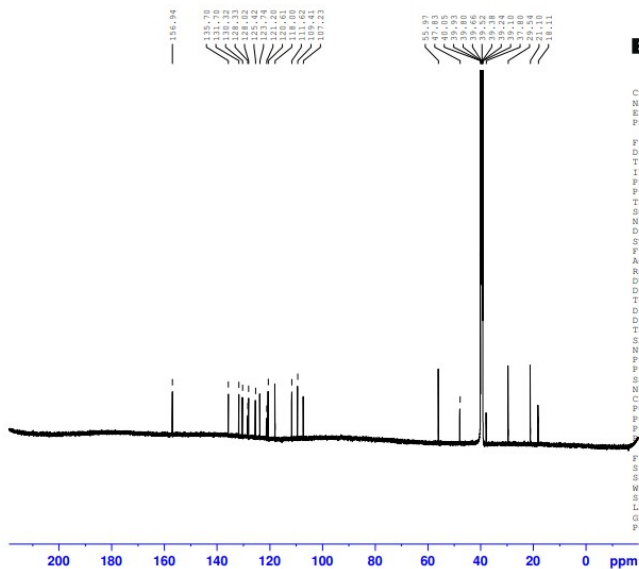
1-(2-methoxyphenyl)-6-methyl-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole (31).



Current Data Parameters
NAME RS-0112-1_F
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190521
Time 11:59 h
INSTRUM spect
PROBHD Z116098_0046 (i
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 7978.724 Hz
FIDRES 0.243491 Hz
AQ 4.1069226 sec
RG 171.52
DW 62.667 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TDO 1
SFO1 399.6024677 MHz
NUC1 1H
P1 10.45 usec
PLW1 16.00000000 W

F2 - Processing Parameters
SI 65536
SF 399.6000000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

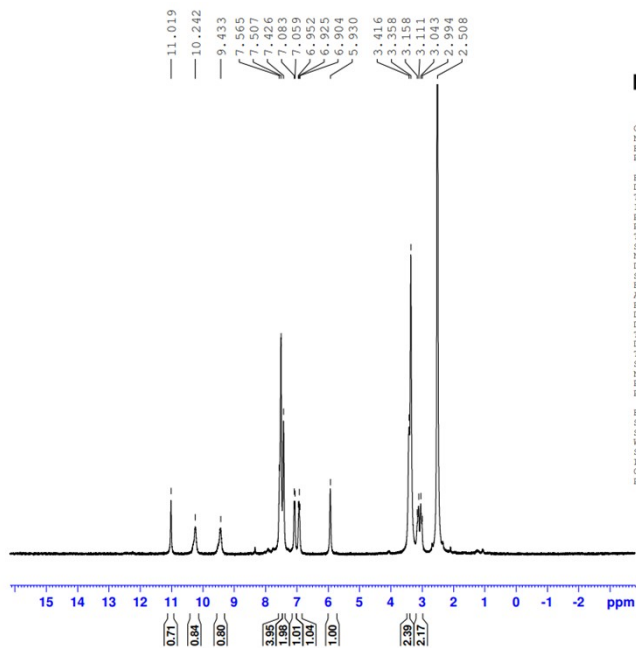
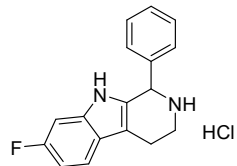


Current Data Parameters
NAME RS-0112-1_F_C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190522
Time 1:57 h
INSTRUM spect
PROBHD Z132572_0007 (i
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 4048
DS 4
SWH 36057.691 Hz
FIDRES 1.100393 Hz
AQ 0.9087659 sec
RG 182.66
DW 13.867 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1
SFO1 150.9279571 MHz
NUC1 13C
P1 9.70 usec
PLW1 35.09999847 W
SFO2 600.1724007 MHz
NUC2 1H
CPCPD2 waltz16
PCPD2 70.00 usec
PLW2 21.00000000 W
PLW12 0.59059002 W
PLW13 0.28944001 W

F2 - Processing parameters
SI 65536
SF 150.9193900 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

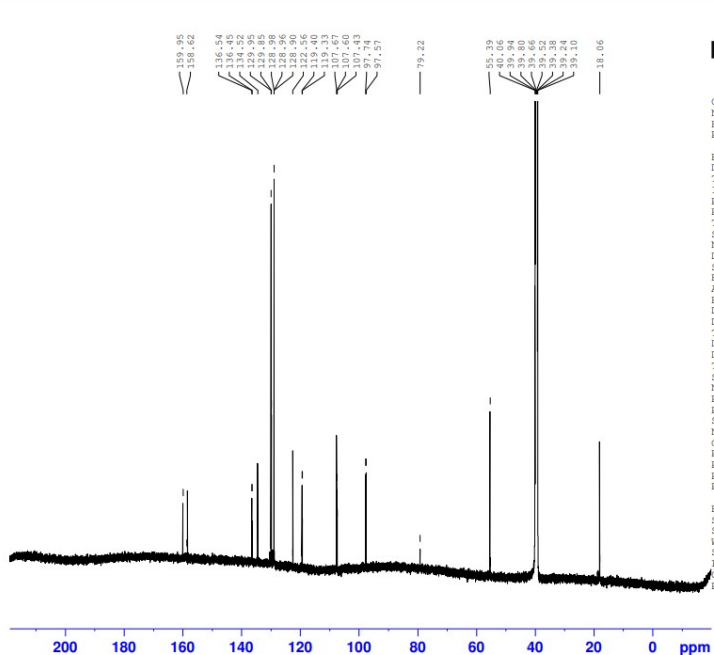
7-fluoro-1-phenyl-2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indole HCl (32).



Current Data Parameters
NAME RS-0089-1_FINAL
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190315
Time 14.25 h
INSTRUM spect
PROBHD Z116098_0046 f
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 7978.724 Hz
FIDRES 0.243491 Hz
AQ 4.1069226 sec
RG 191.21
DW 62.687 usec
DE 6.50 usec
TE 298.0 K
D1 1.0000000 sec
TDO 1
SFO1 399.6024677 MHz
NUC1 1H
P1 26.11 usec
PLW1 16.0000000 W

F2 - Processing parameters
SI 65536
SF 399.6000000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME RS-0089-1-150419
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190416
Time 6.29 h
INSTRUM spect
PROBHD Z132572_0007 f
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 36057.691 Hz
FIDRES 1.100393 Hz
AQ 0.9087659 sec
RG 182.66
DW 13.867 usec
DE 18.00 usec
TE 298.0 K
D1 2.0000000 sec
D11 0.0300000 sec
TDO 1
SFO1 150.9279571 MHz
NUC1 13C
P1 9.70 usec
PLW1 35.09999847 W
SFO2 600.1724007 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 70.00 usec
PLW2 21.00000000 W
PLW12 0.59069002 W
PLW13 0.28944001 W

F2 - Processing parameters
SI 65536
SF 150.9129383 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

COc1ccccc1C2CNCCc3c2[nH]c4cc(F)ccc43.Cl