SUPPORTING INFORMATION

Synthesis and Cholinesterase Inhibitory Activity of Selected Indole-Based Compounds

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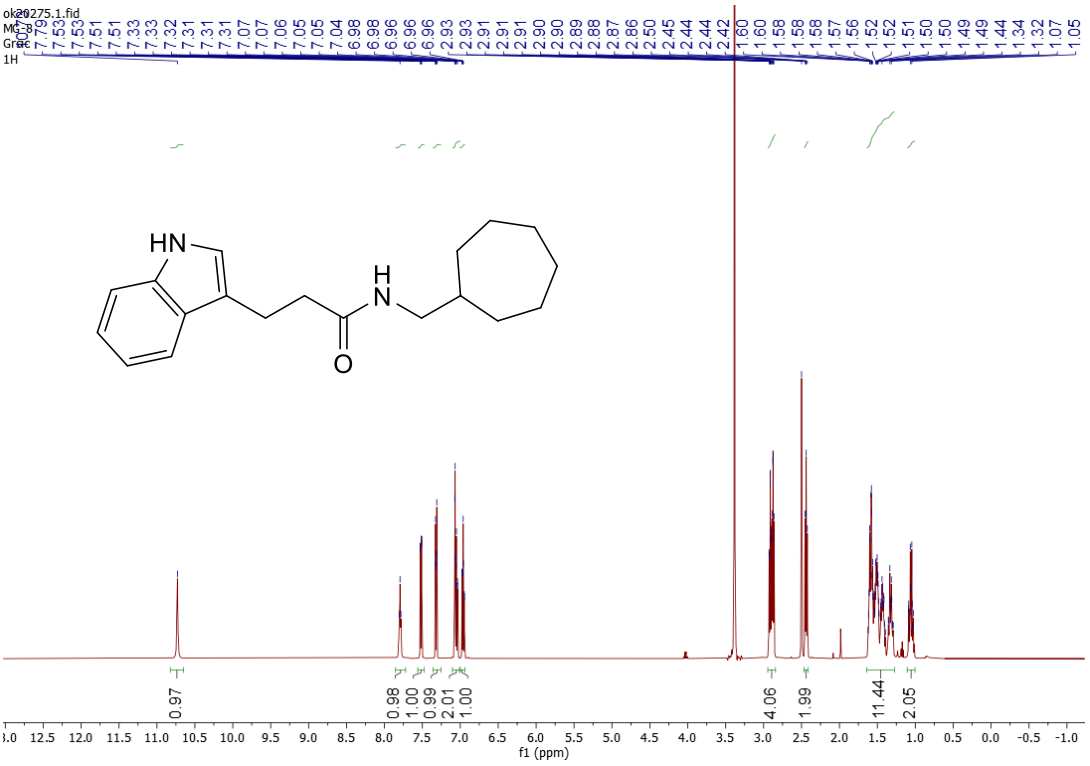
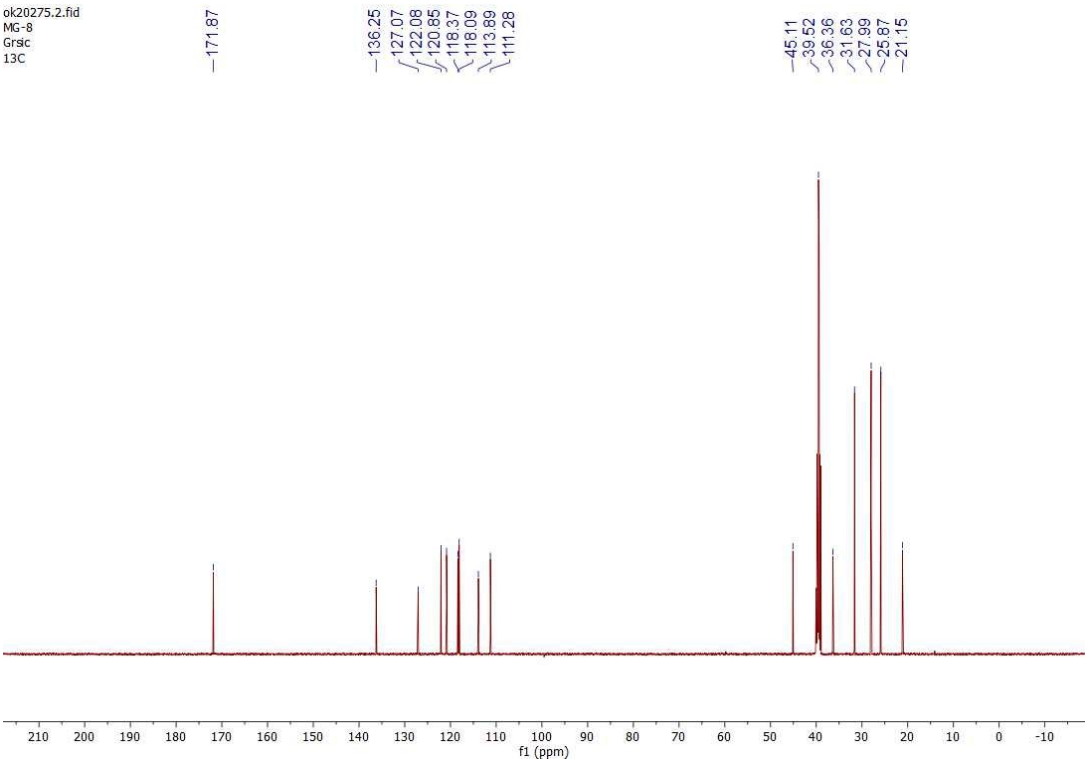
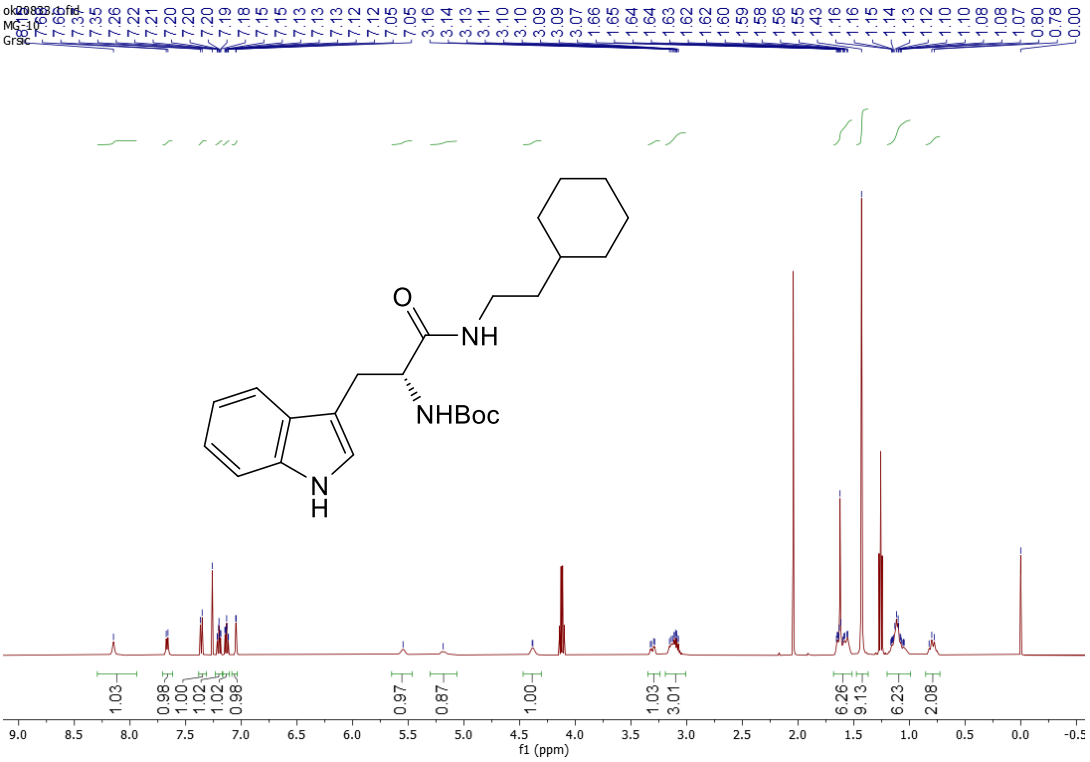
NMR spectra

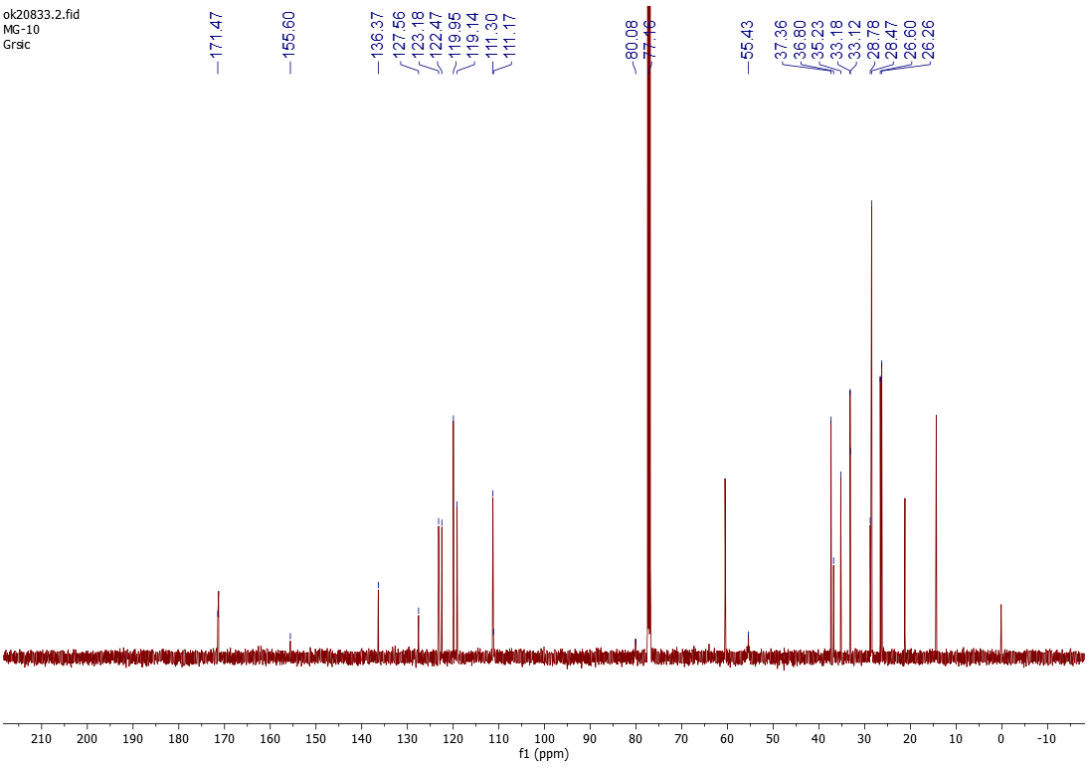
N-(Cycloheptylmethyl)-3-(1*H*-indol-3-yl)propanamide (8)



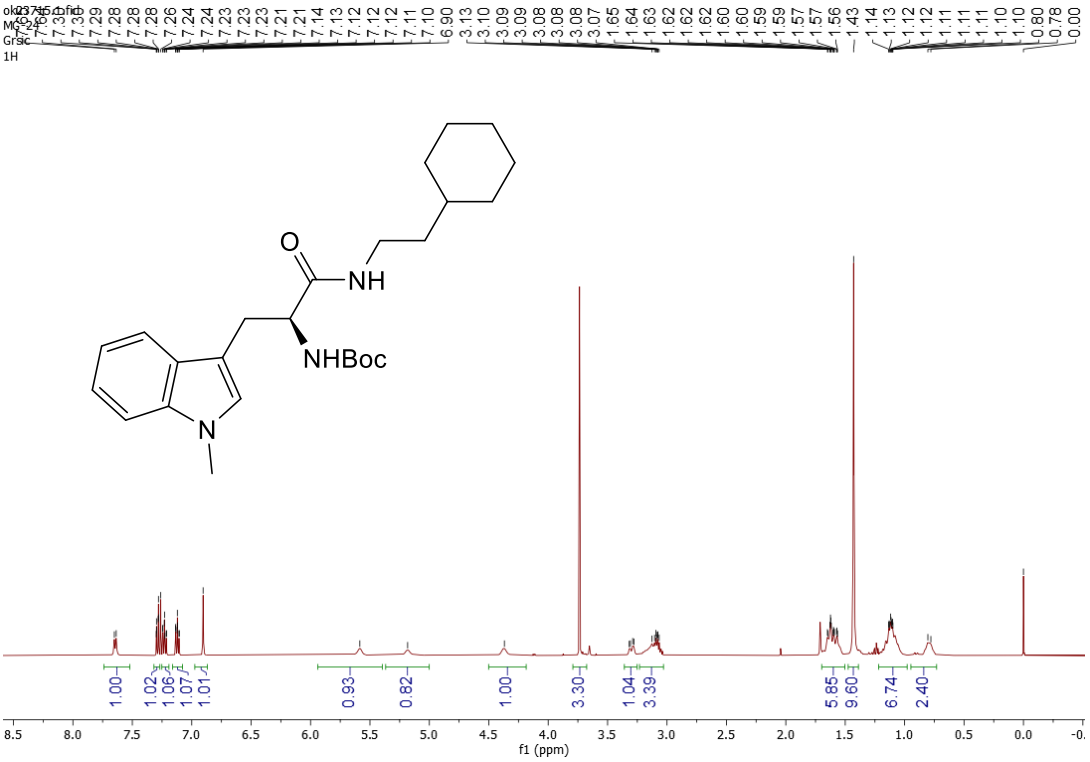


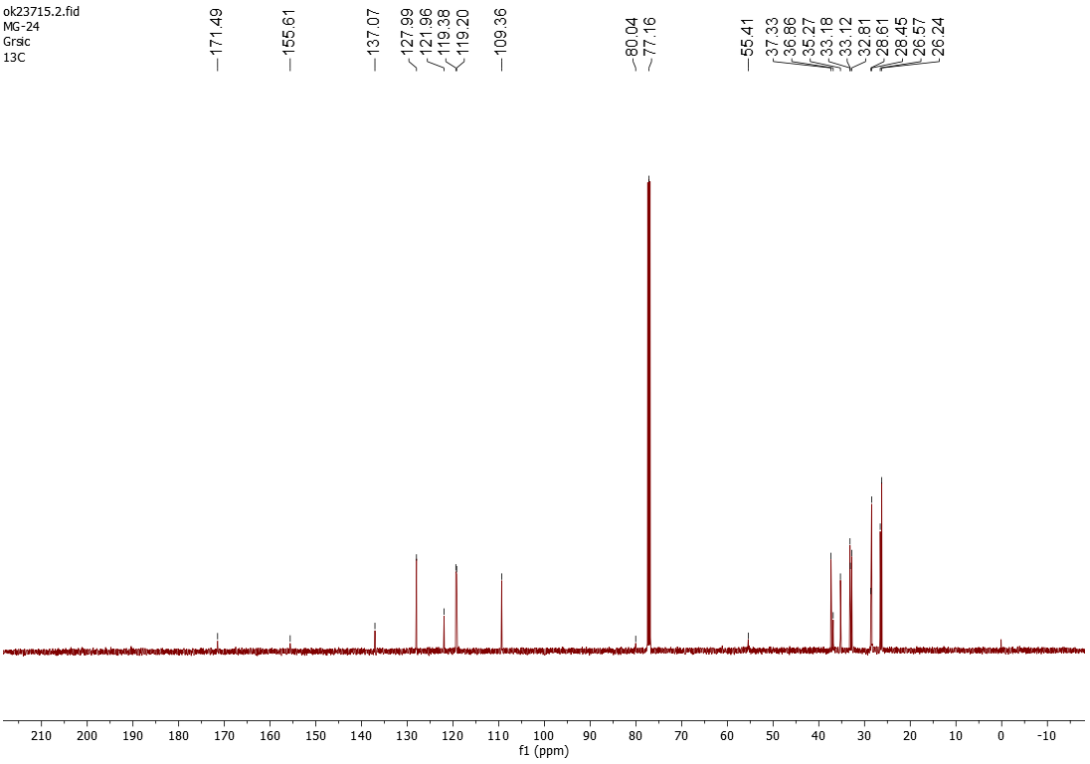
tert-Butyl (_R_)-(1-((2-cyclohexylethyl)amino)-3-(1_H_-indol-3-yl)-1-oxopropan-2-yl)carbamate (9)



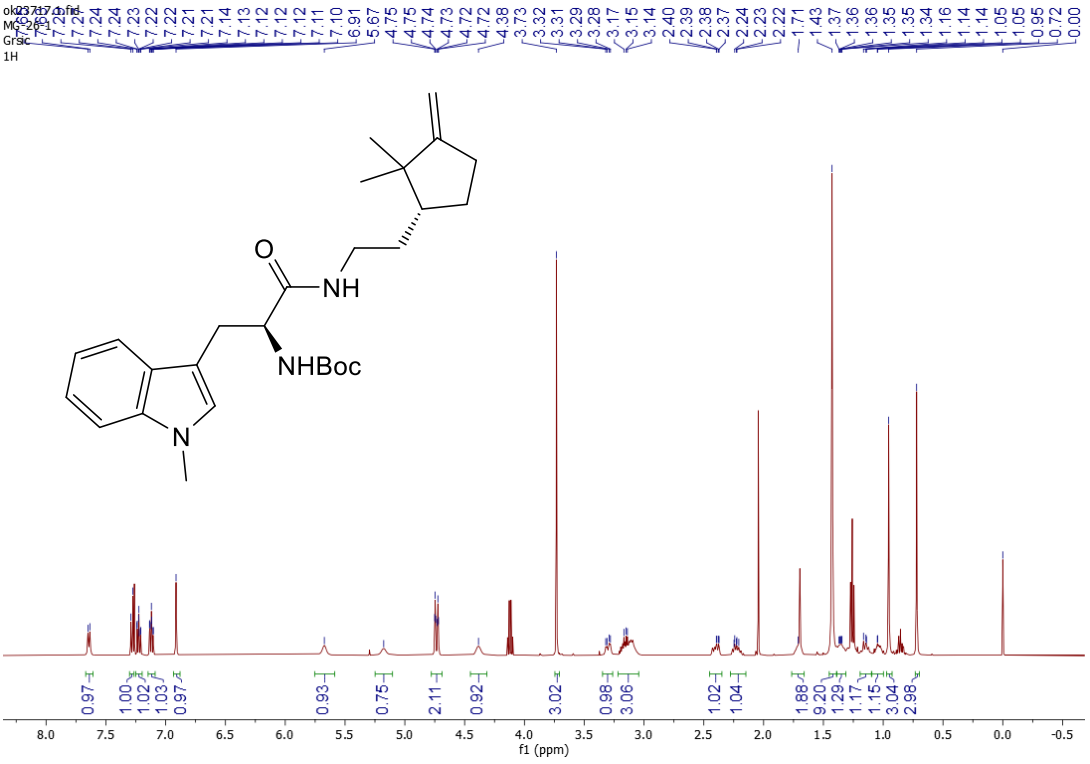


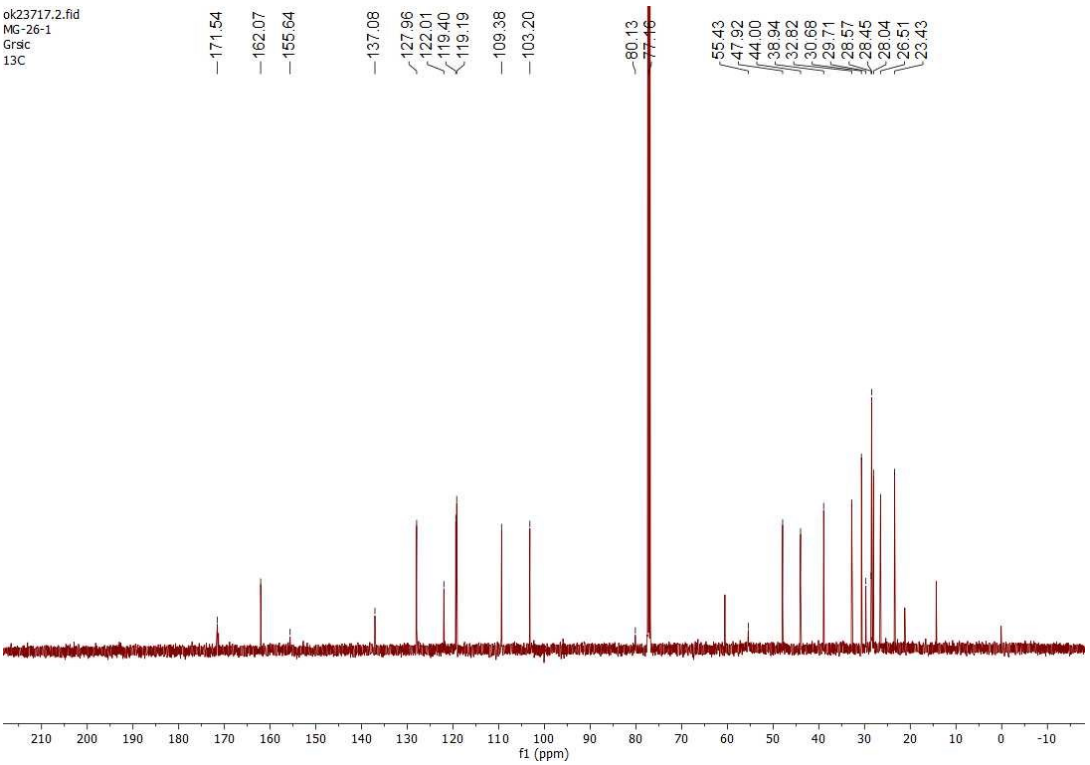
tert-Butyl (_S_)-(1-((2-cyclohexylethyl)amino)-3-(1-methyl-1_H_-indol-3-yl)-1-oxopropan-2-yl)carbamate (10)



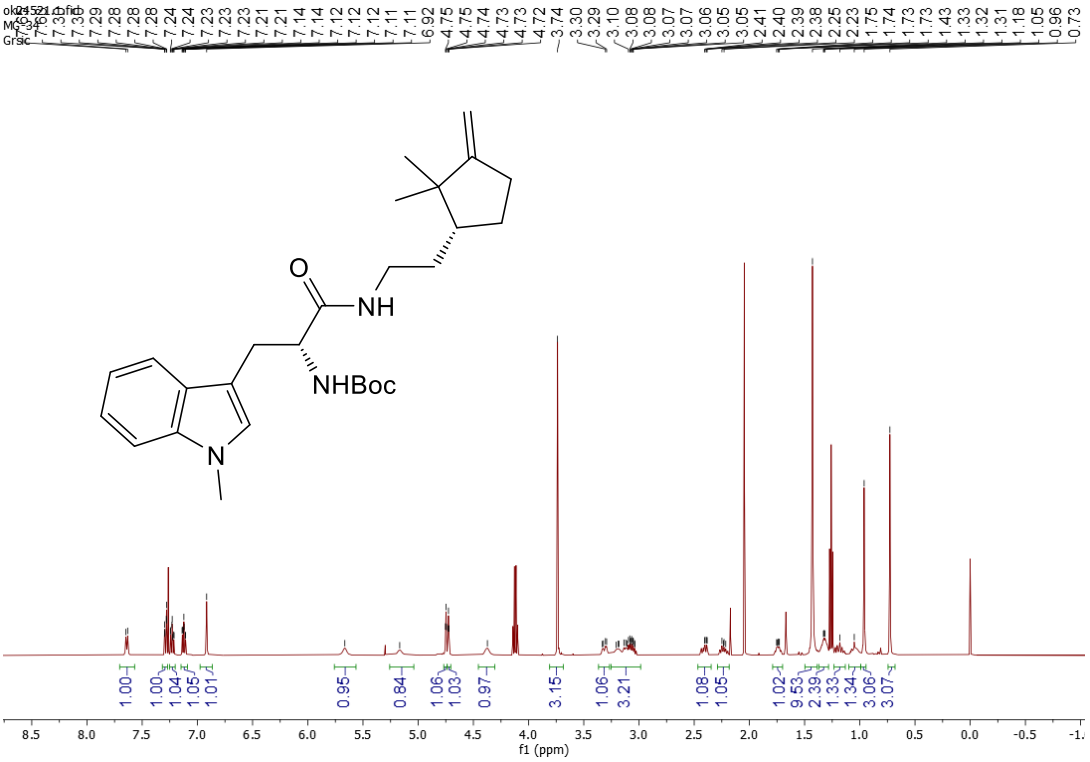


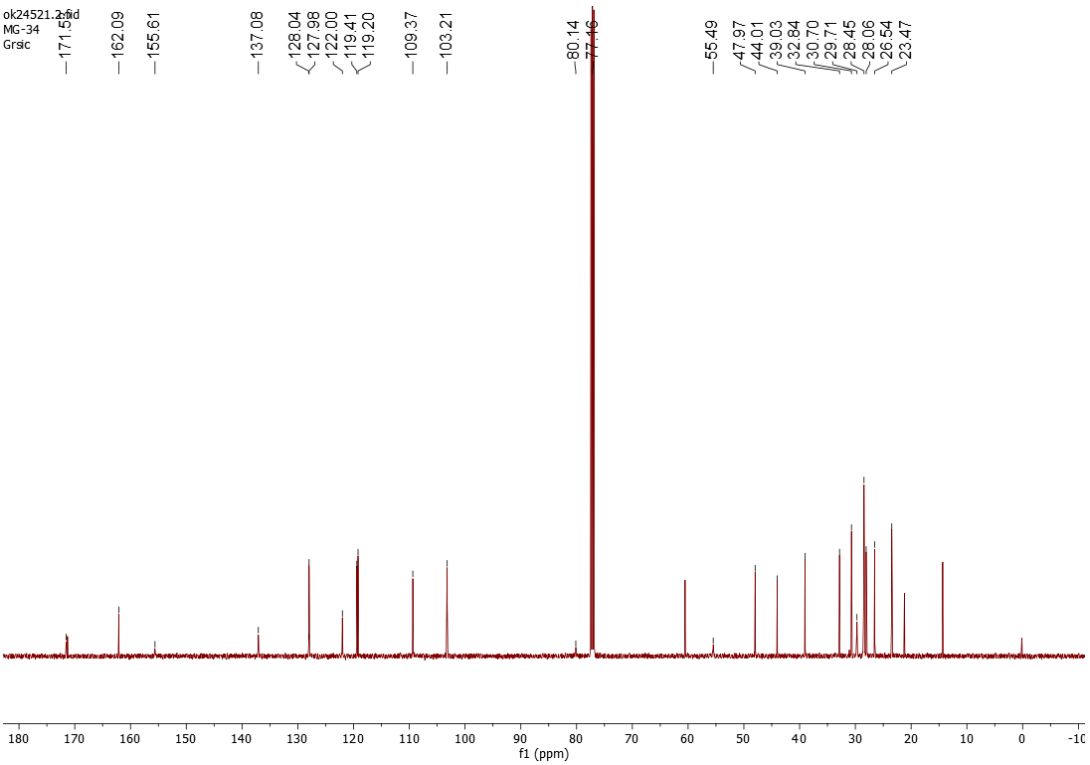
tert-Butyl ((S)-1-((2-((*R*)-2,2-dimethyl-3-methylenecyclopentyl)ethyl)amino)-3-(1-methyl-1*H*-indol-3-yl)-1-oxopropan-2-yl)carbamate (11)



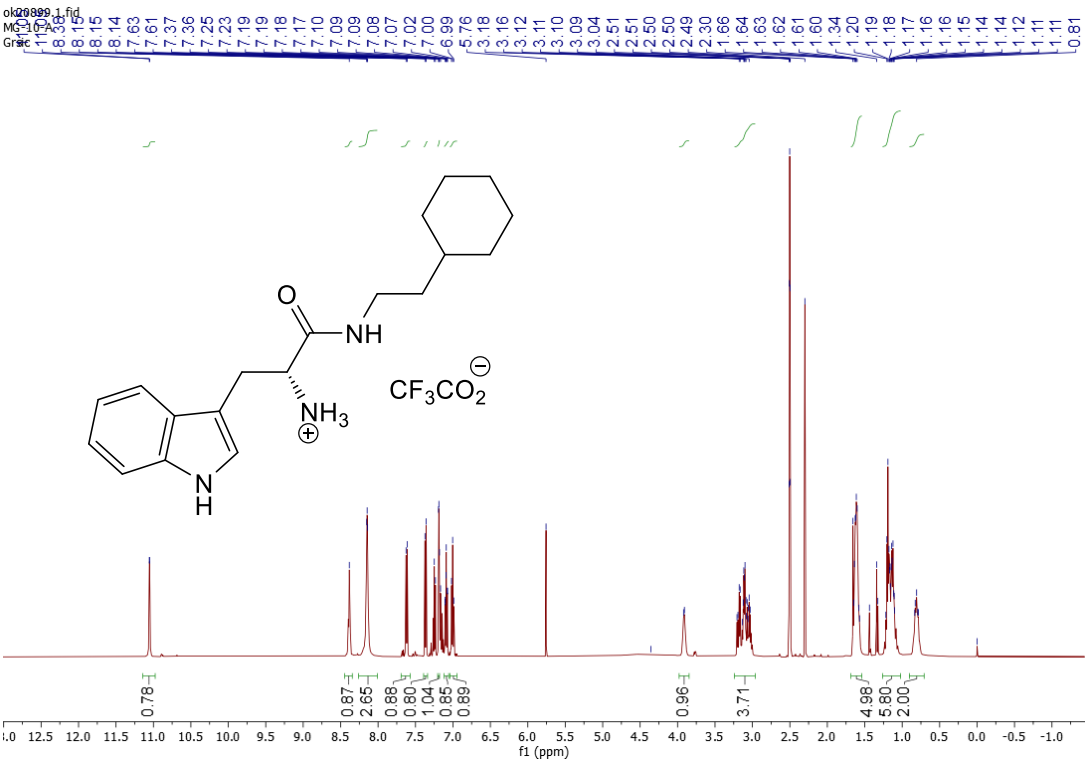


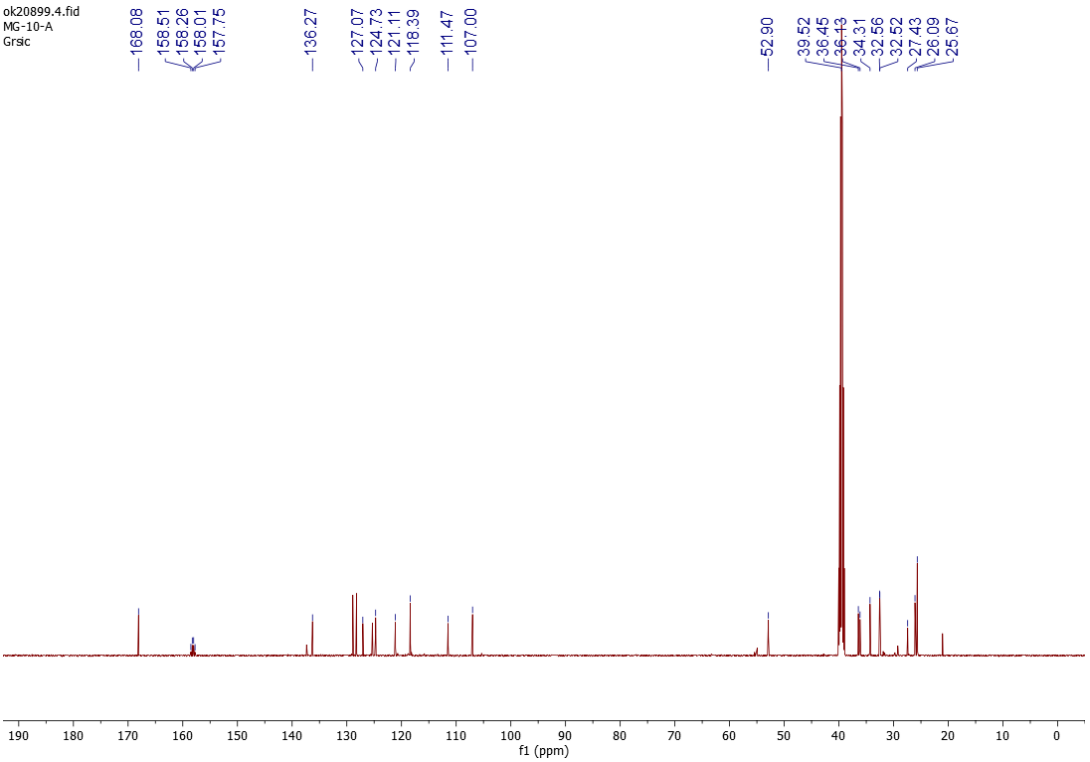
tert-Butyl ((_R_)-1-((2-((_R_)-2,2-dimethyl-3-methylenecyclopentyl)ethyl)amino)-3-(1-methyl-1_H_-indol-3-yl)-1-oxopropan-2-yl)carbamate (12)





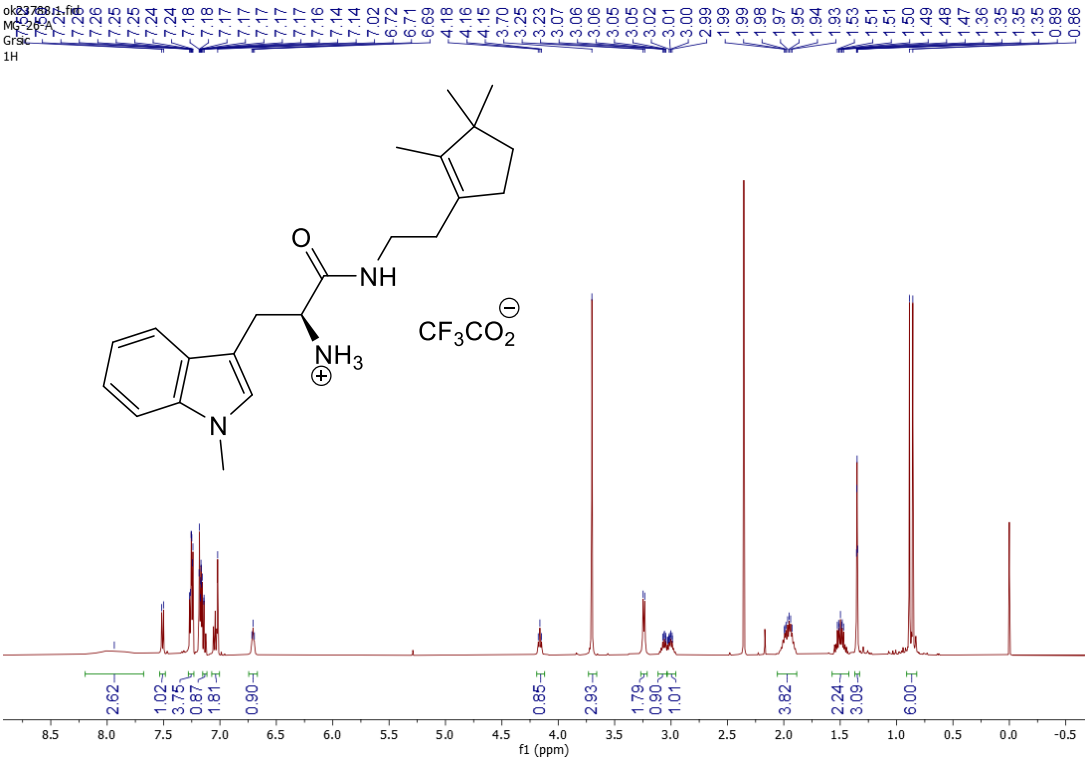
(*R*)-1-((2-Cyclohexylethyl)amino)-3-(1*H*-indol-3-yl)-1-oxopropan-2-aminium 2,2,2-trifluoroacetate (13)

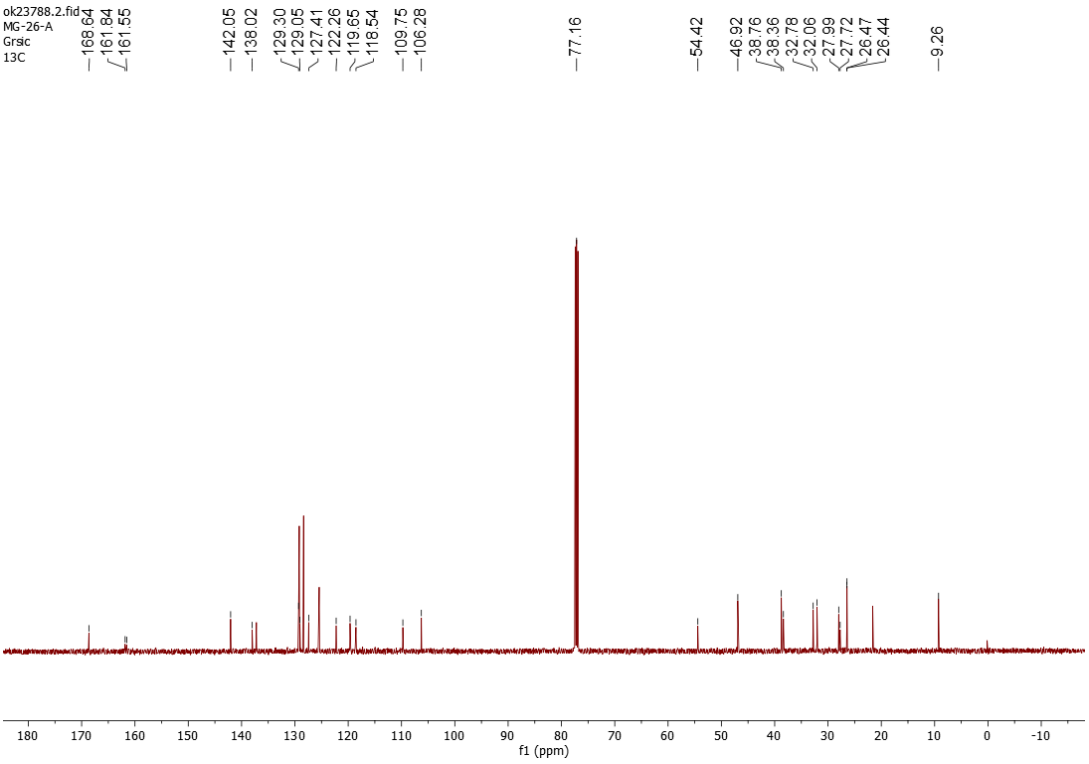




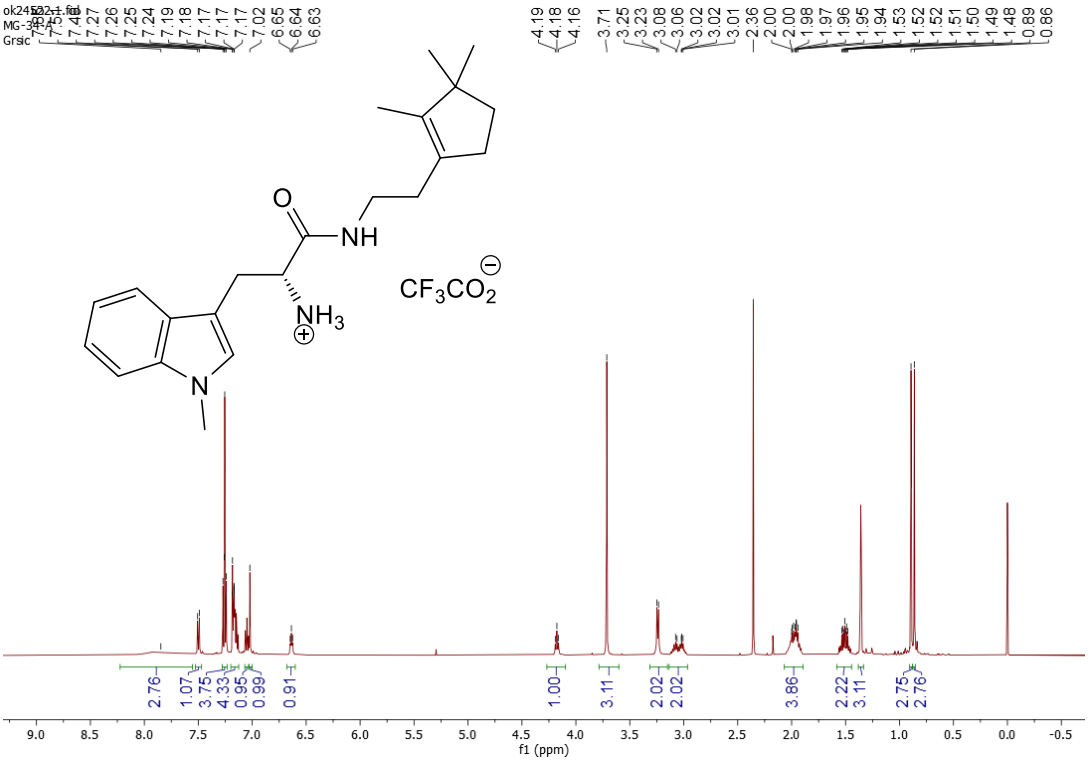
Toluene is present in the sample.

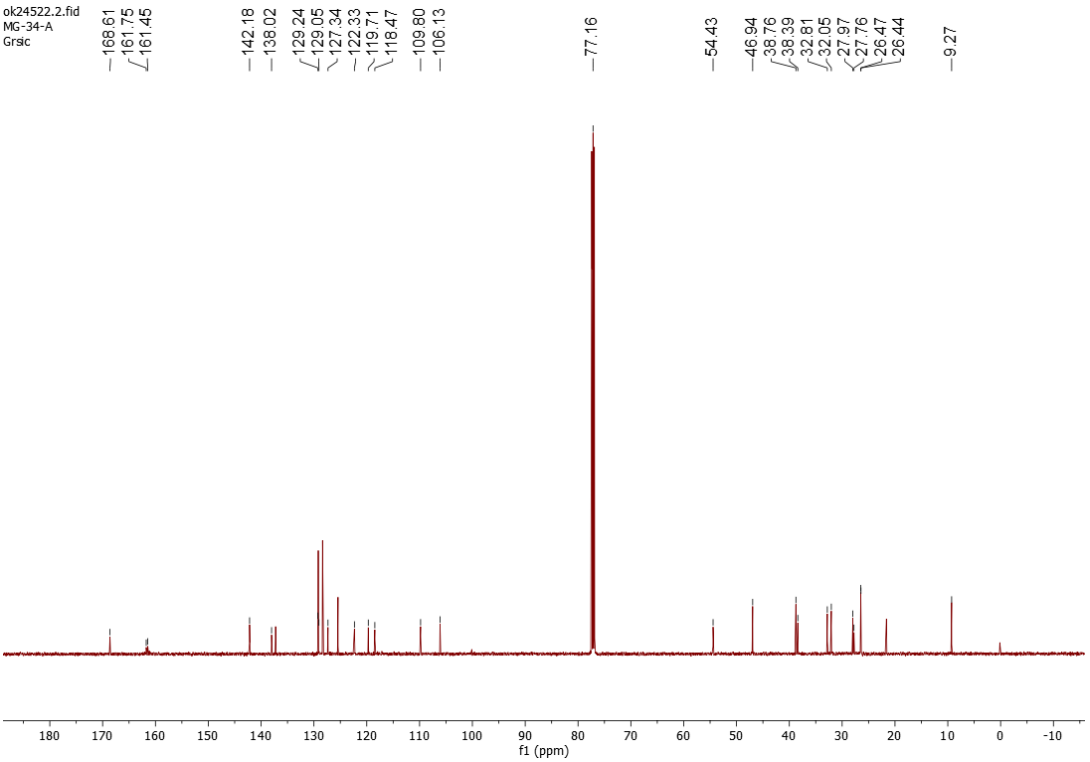
(*S*)-3-(1-Methyl-1*H*-indol-3-yl)-1-oxo-1-((2-(2,3,3-trimethylcyclopent-1-en-1-yl)ethyl)amino)propan-2-aminium 2,2,2-trifluoroacetate (14)



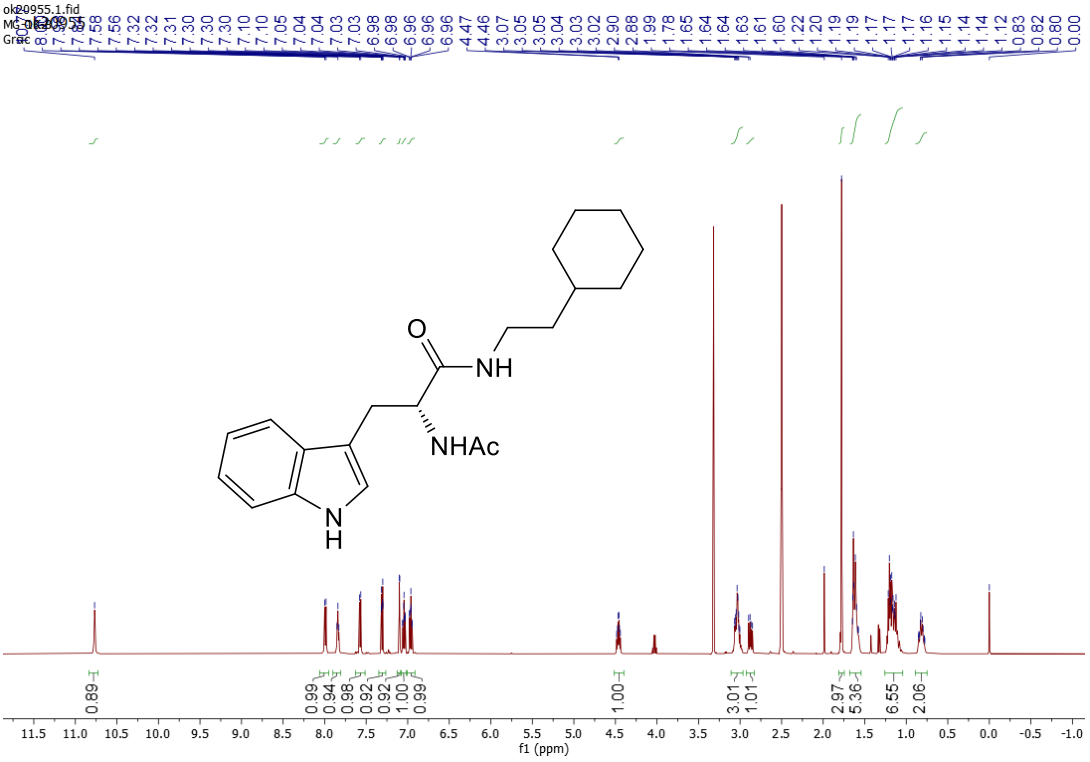


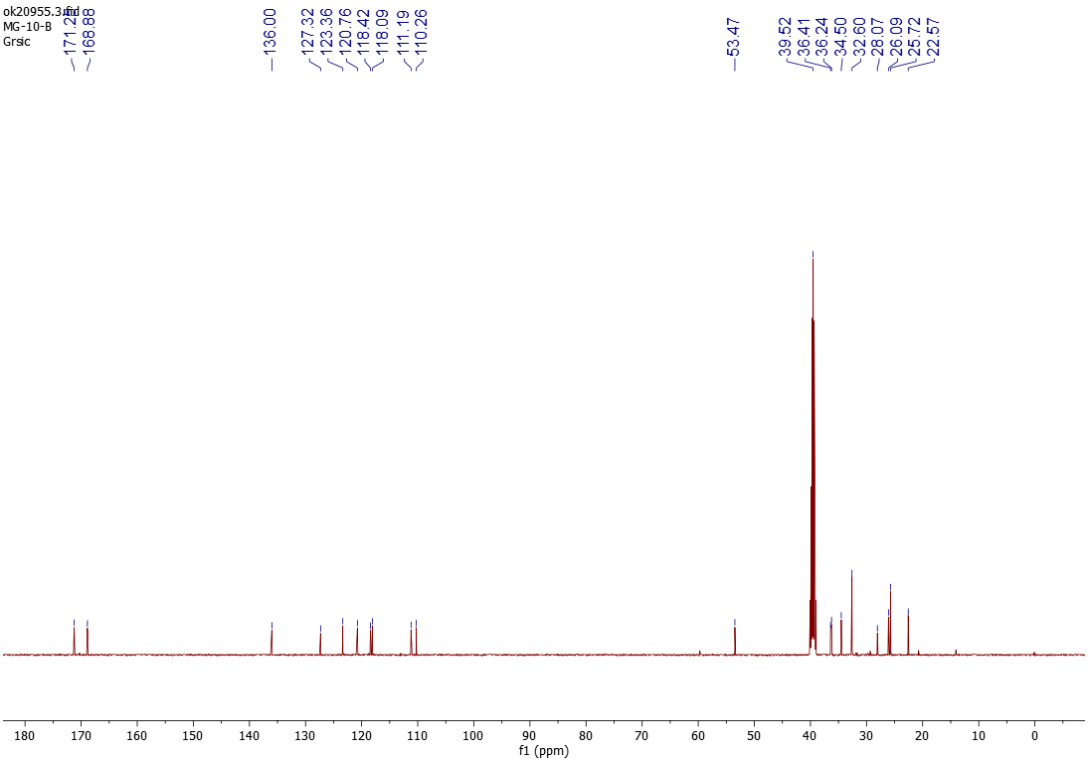
(*R*)-3-(1-Methyl-1*H*-indol-3-yl)-1-oxo-1-((2-(2,3,3-trimethylcyclopent-1-en-1-yl)ethyl)amino)propan-2-aminium 2,2,2-trifluoroacetate (15)



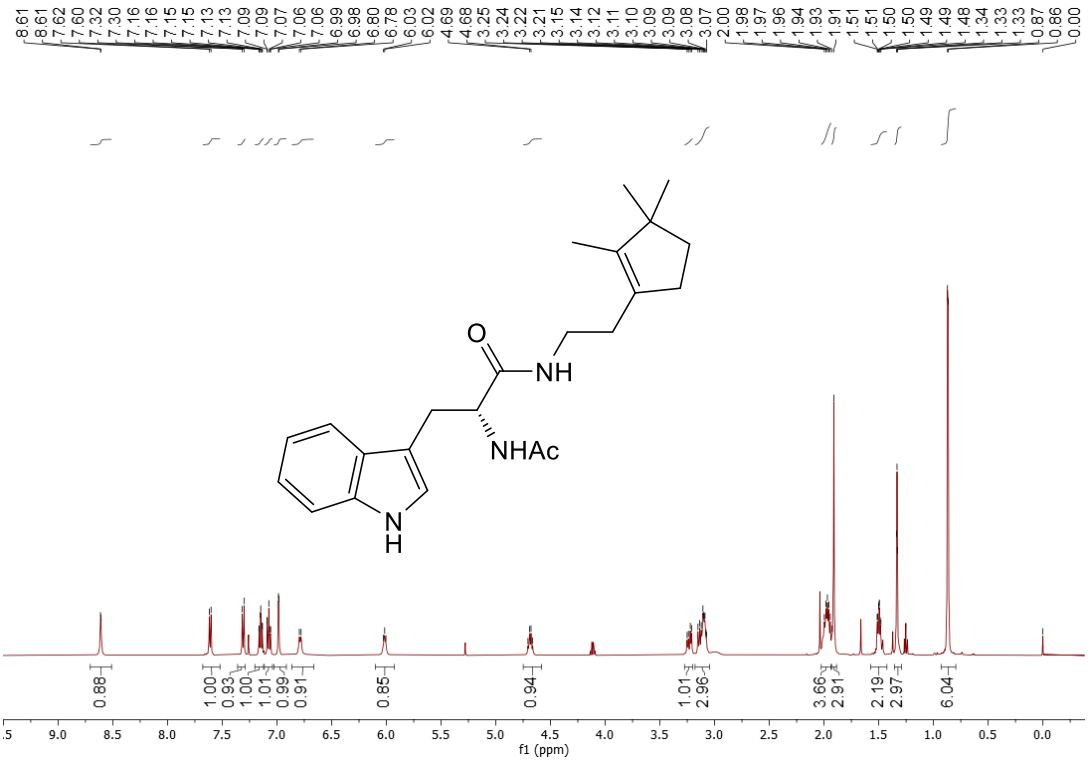


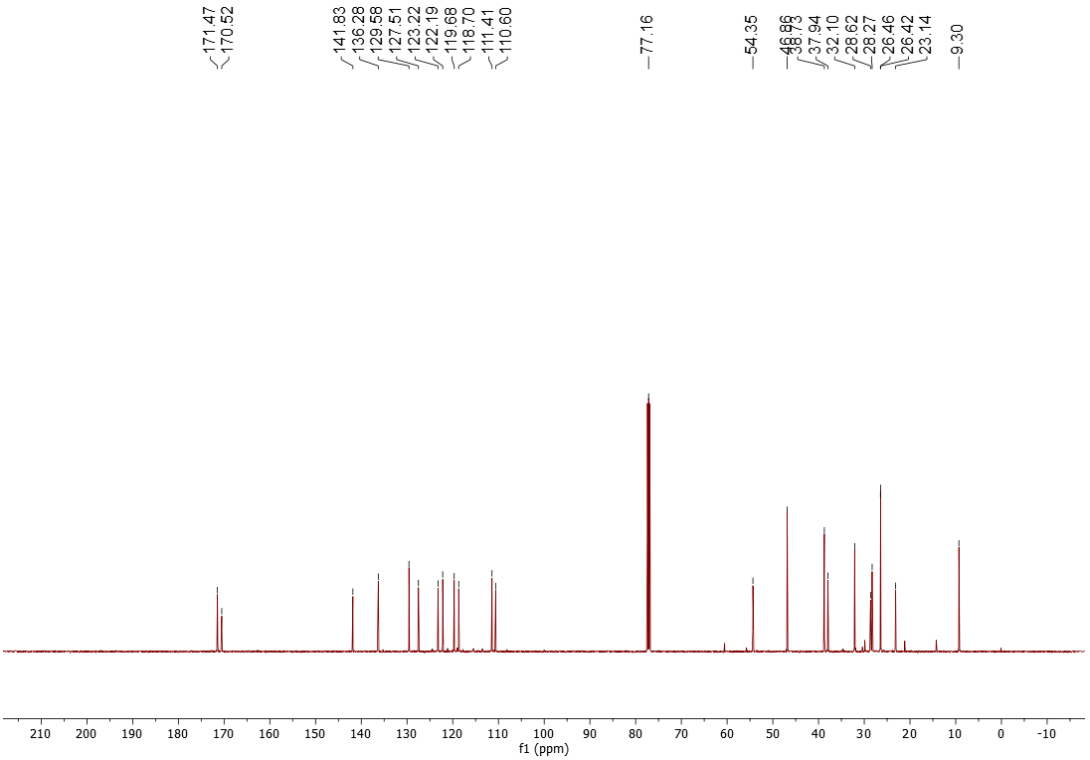
(*R*)-2-Acetamido-*N*-(2-cyclohexylethyl)-3-(1*H*-indol-3-yl)propanamide (19)



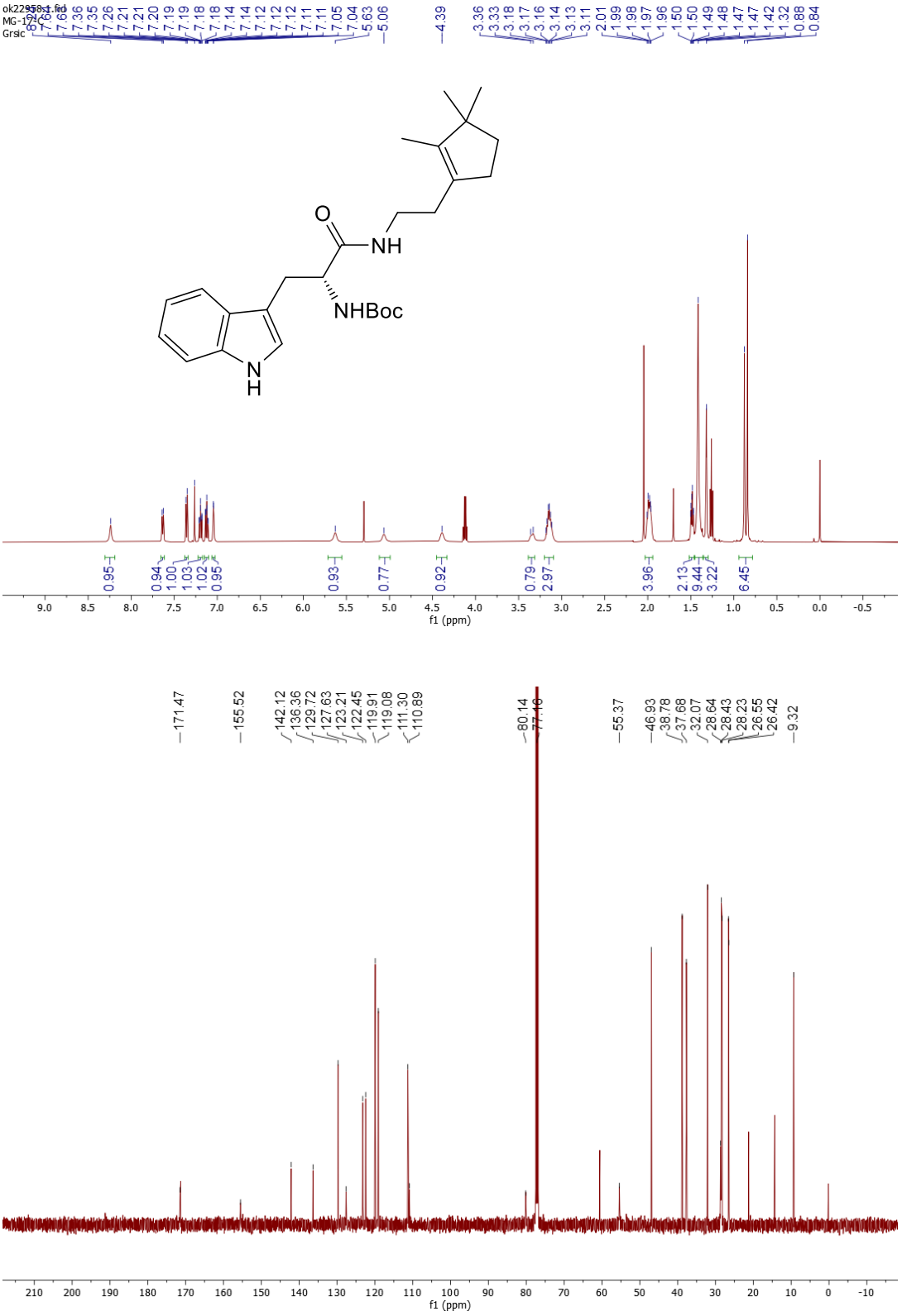


(*R*)-2-Acetamido-3-(1*H*-indol-3-yl)-*N*-(2-(2,3,3-trimethylcyclopent-1-en-1-yl)ethyl)propanamide (20)

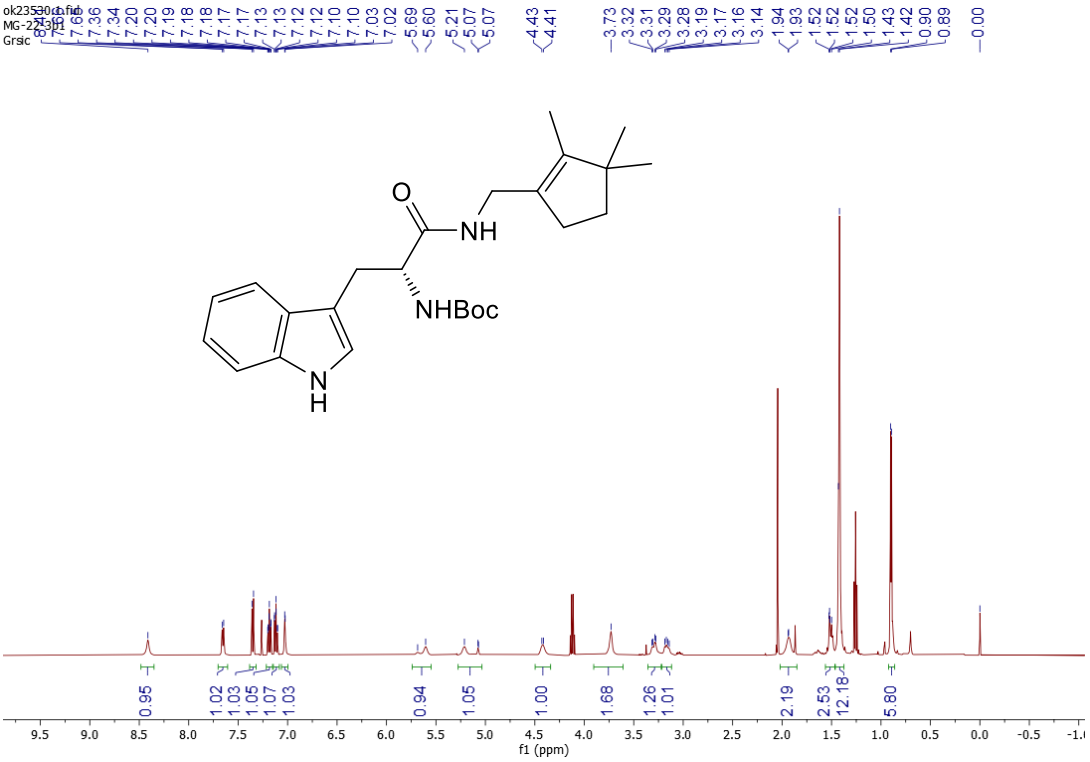


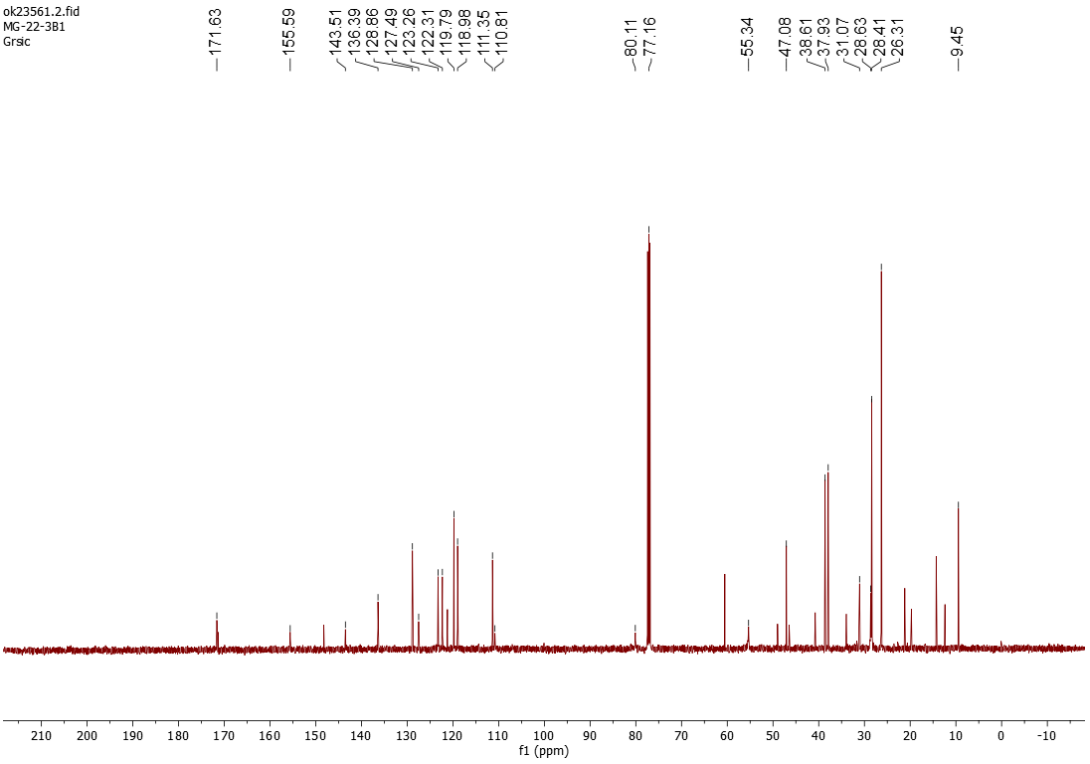


tert-Butyl (_R_)-(3-(1_H_-indol-3-yl)-1-oxo-1-((2-(2,3,3-trimethylcyclopent-1-en-1-yl)ethyl)amino)propan-2-yl)carbamate (21)

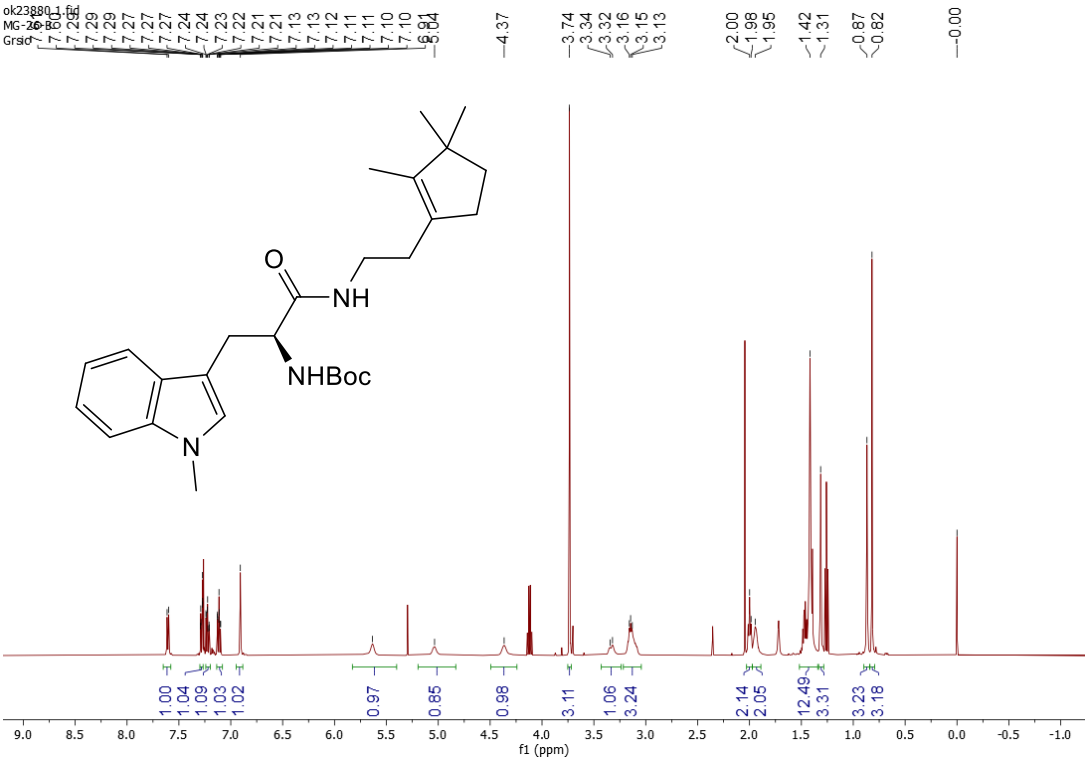


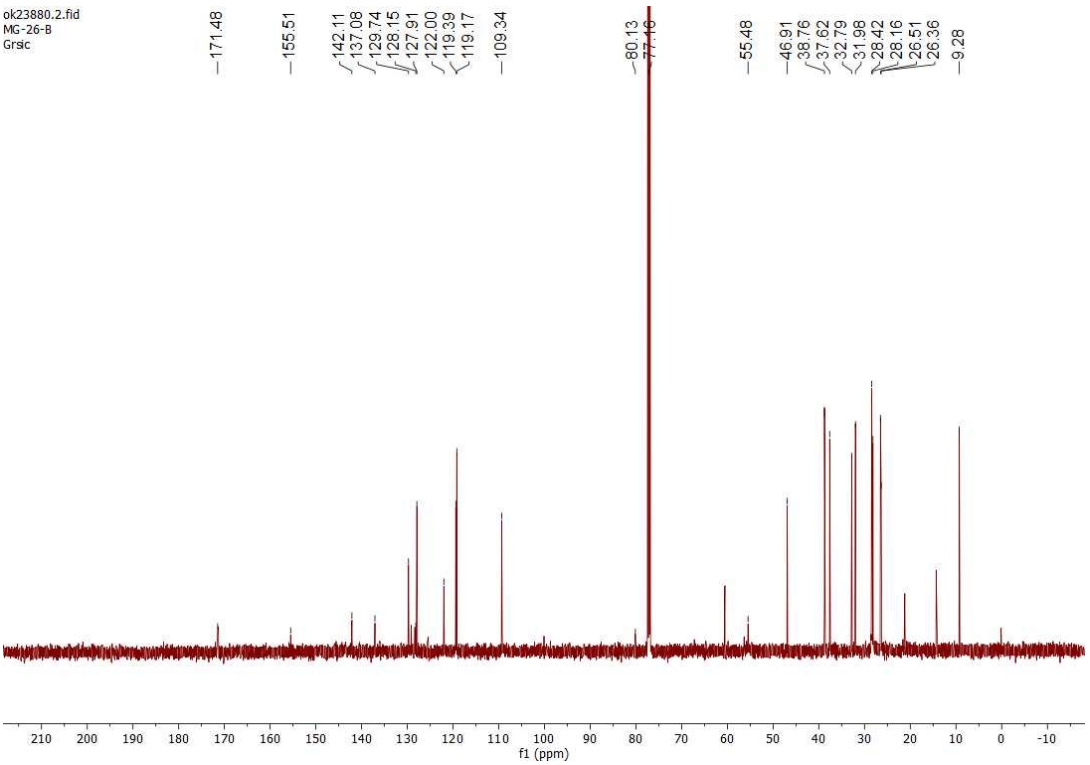
***tert*-Butyl (*R*)-(3-(1*H*-indol-3-yl)-1-oxo-1-(((2,3,3-trimethylcyclopent-1-en-1-yl)methyl)amino)propan-2-yl)carbamate (22)**



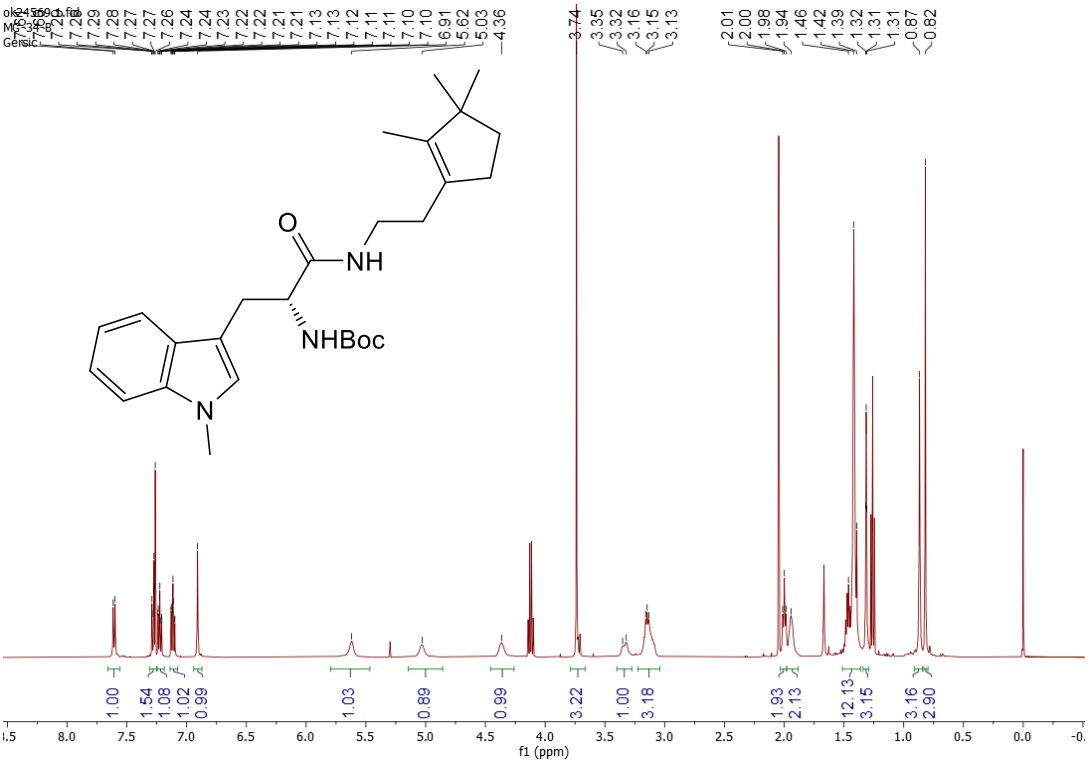


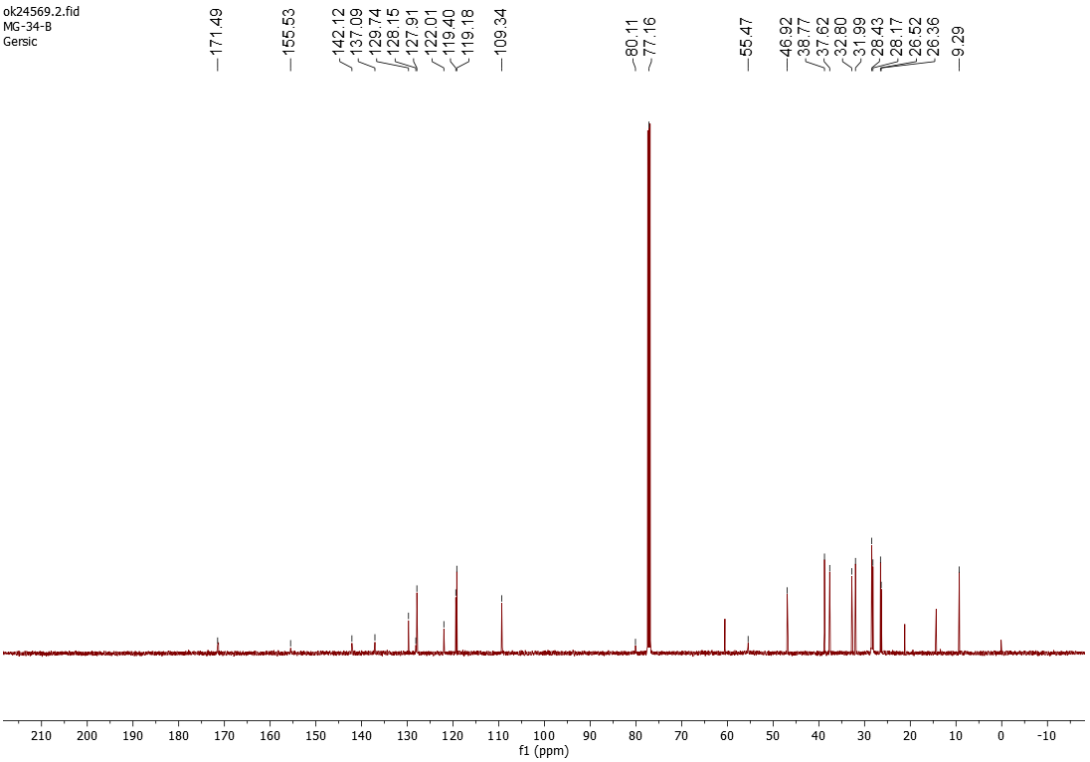
tert-Butyl (_S_)-(3-(1-methyl-1_H_-indol-3-yl)-1-oxo-1-((2-(2,3,3-trimethylcyclopent-1-en-1-yl)ethyl)amino)propan-2-yl)carbamate (23)



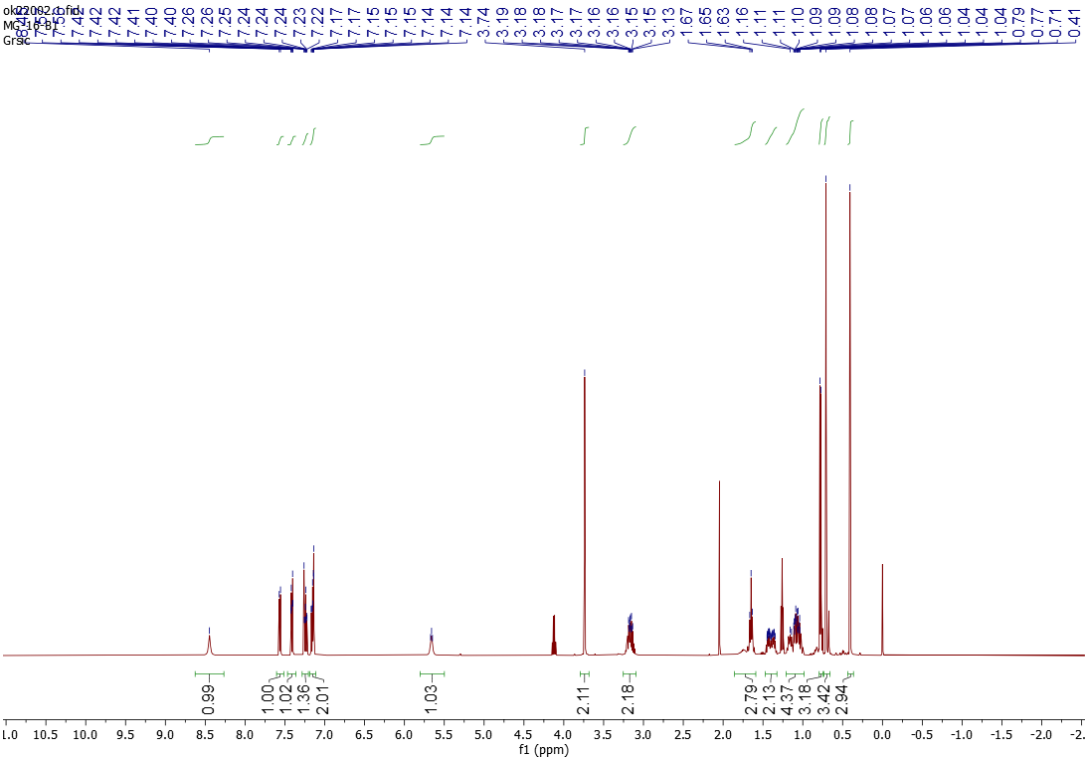


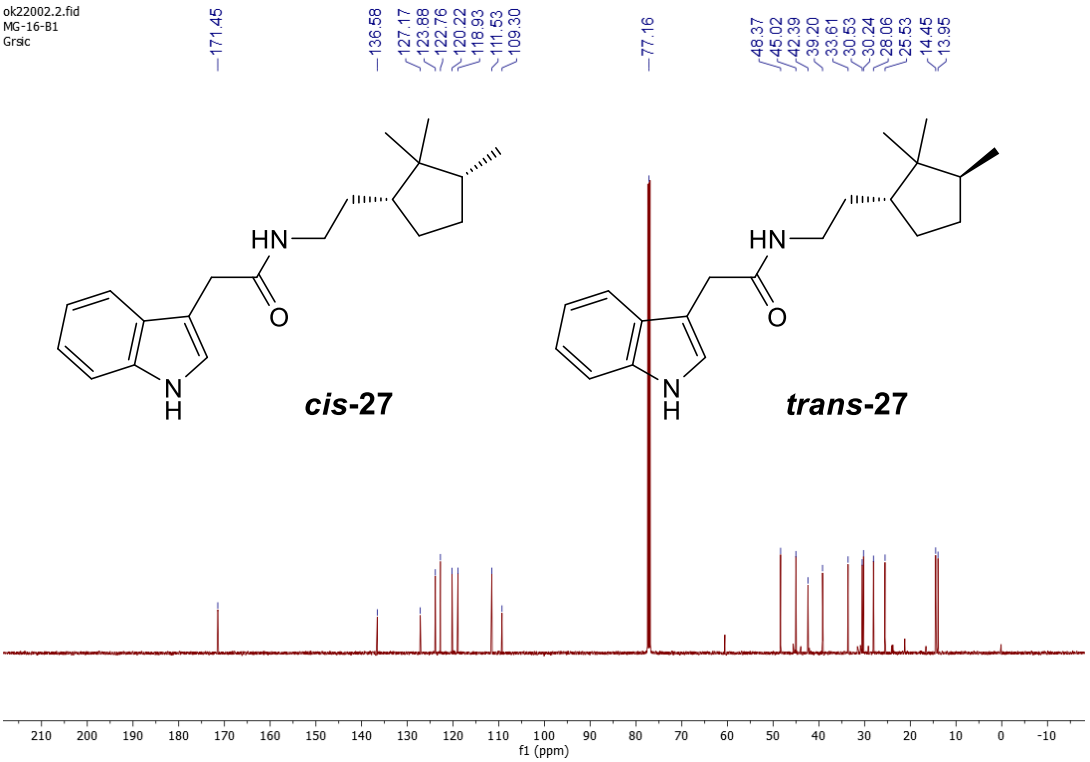
tert-Butyl (_R_)-(3-(1-methyl-1_H_-indol-3-yl)-1-oxo-1-((2-(2,3,3-trimethylcyclopent-1-en-1-yl)ethyl)amino)propan-2-yl)carbamate (24)



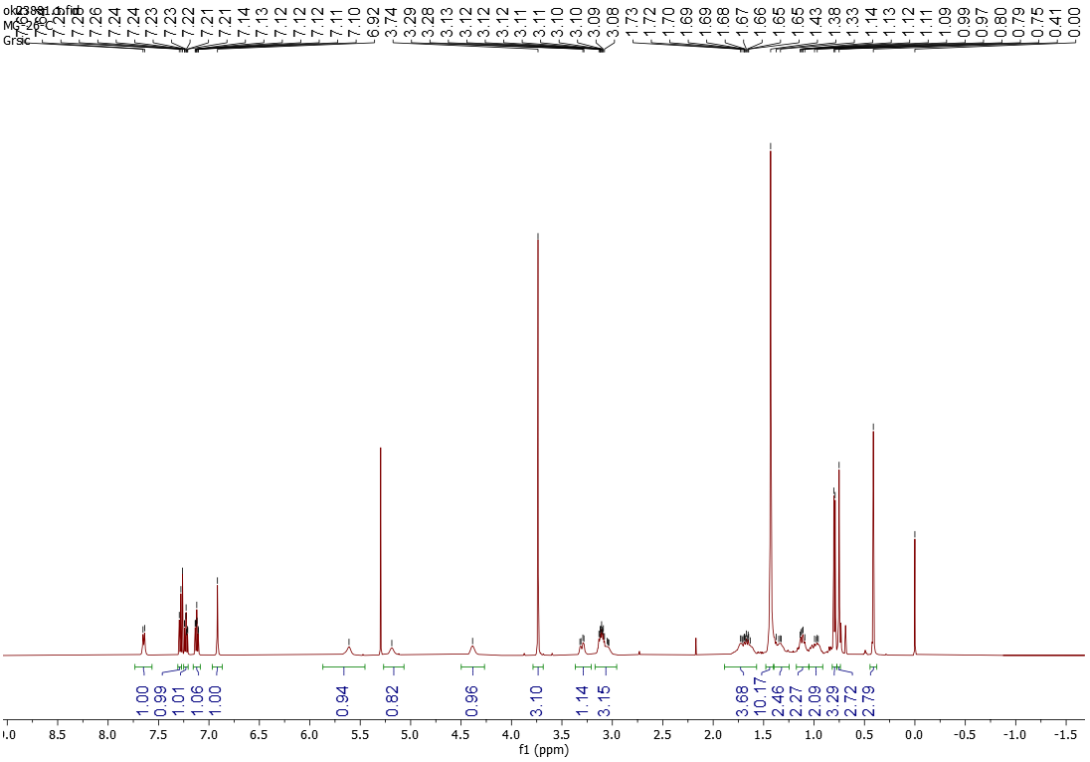


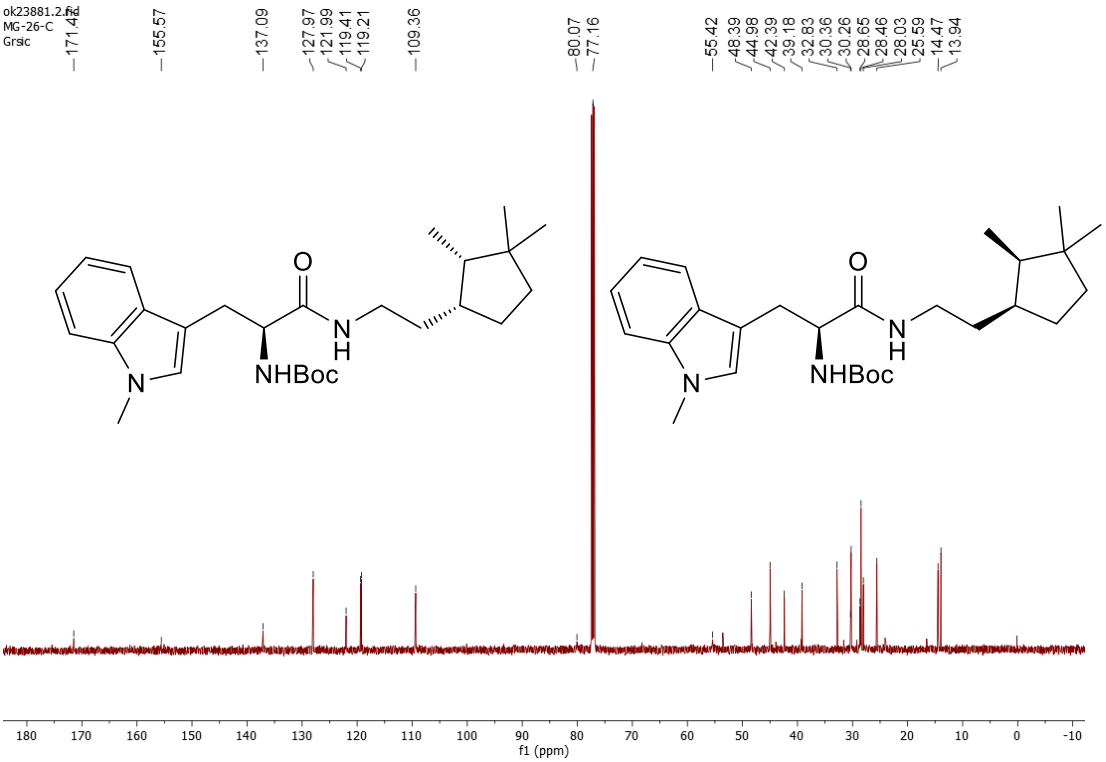
2-(1*H*-Indol-3-yl)-*N*-(2-((1*R*,3*R*)-2,2,3-trimethylcyclopentyl)ethyl)acetamide (*cis*-27) and 2-(1*H*-indol-3-yl)-*N*-(2-((1*R*,3*S*)-2,2,3-trimethylcyclopentyl)ethyl)acetamide (*trans*-27)



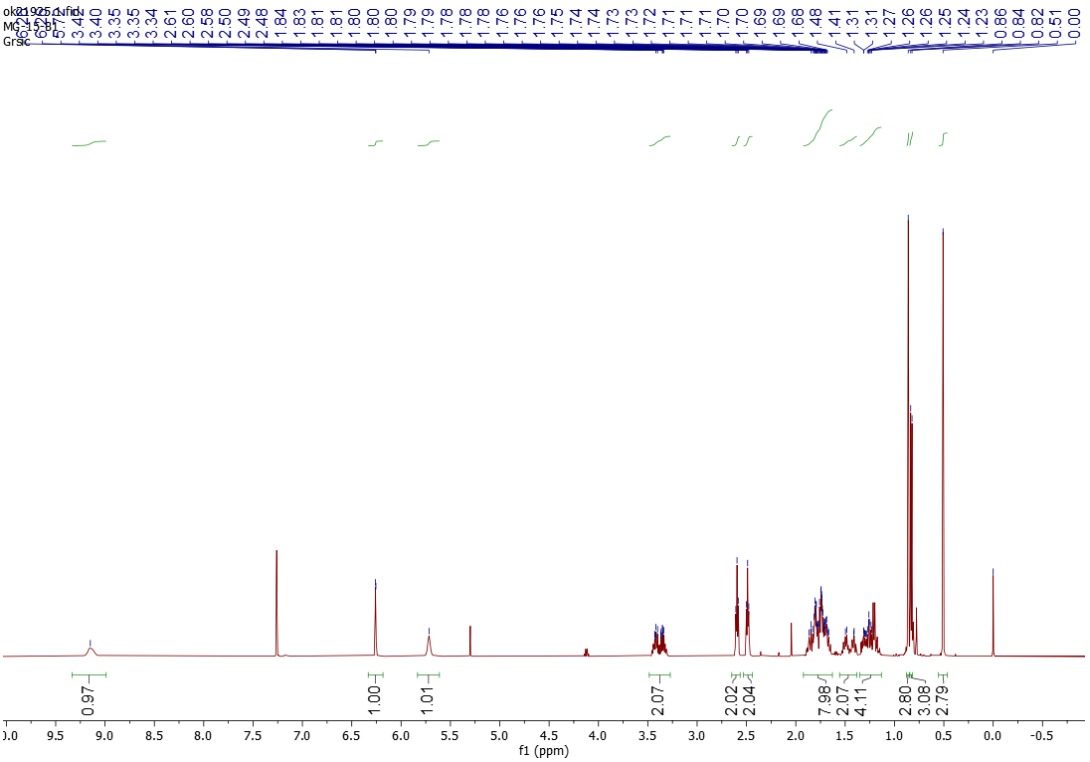


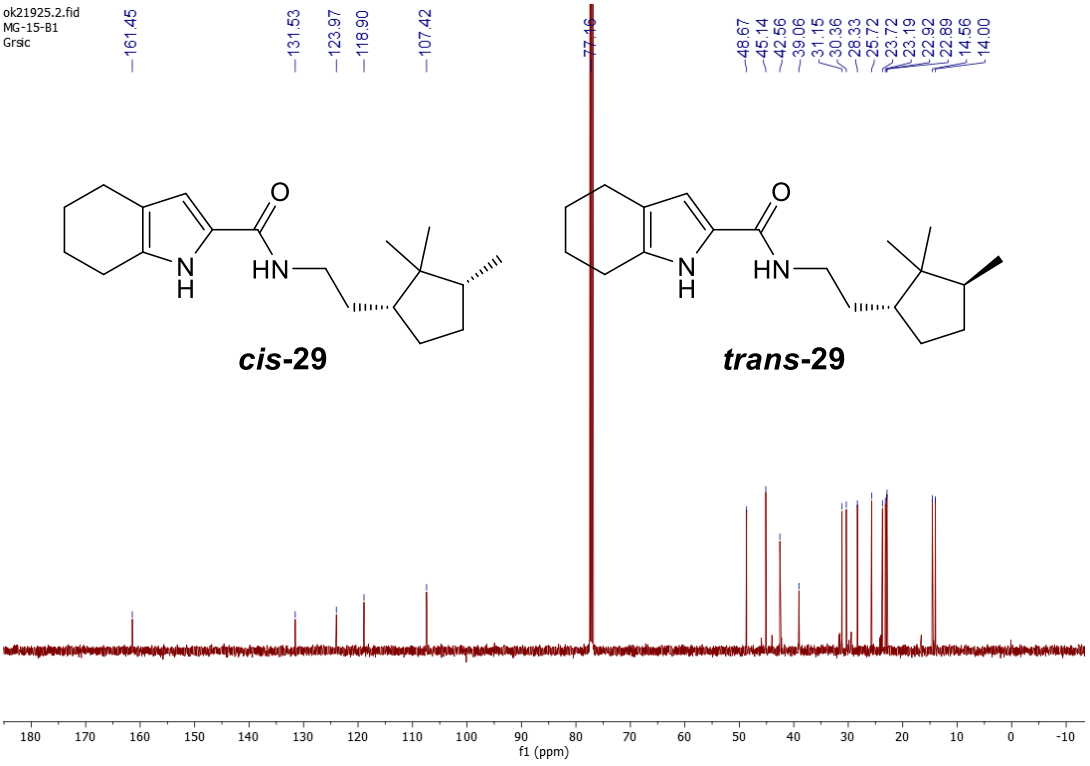
tert-Butyl ((*S*)-3-(1-methyl-1*H*-indol-3-yl)-1-oxo-1-((2-(2,3,3-trimethylcyclopentyl)ethyl)-amino)propan-2-yl)carbamate (28)



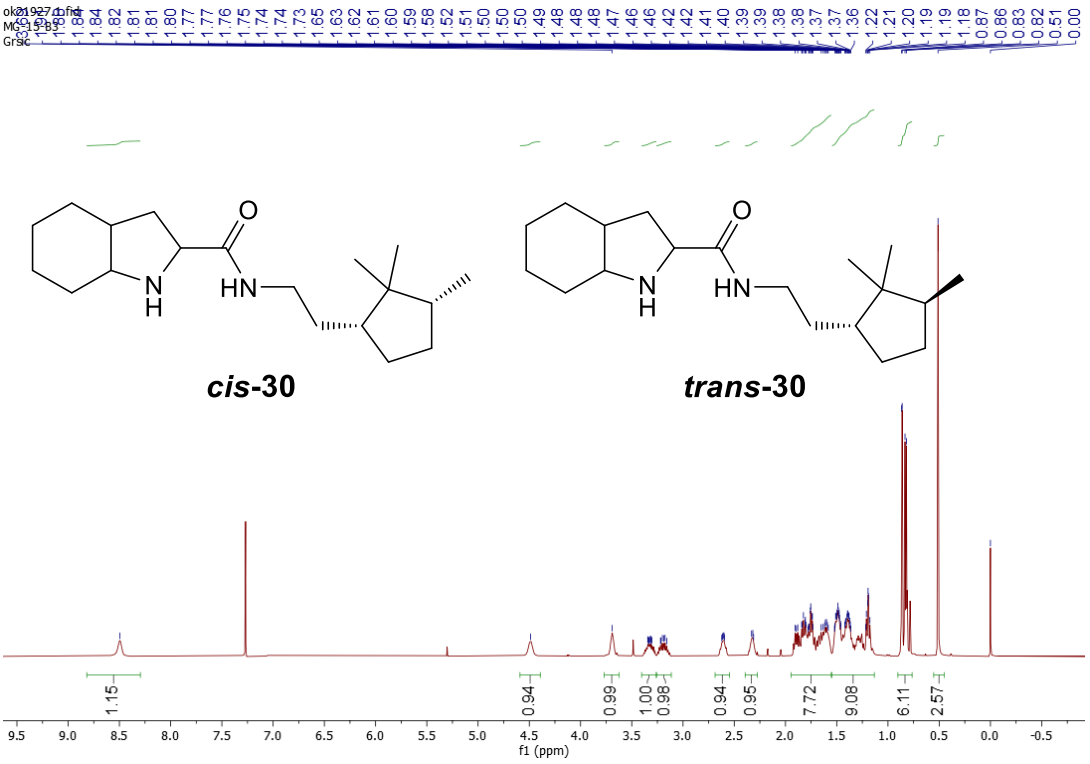


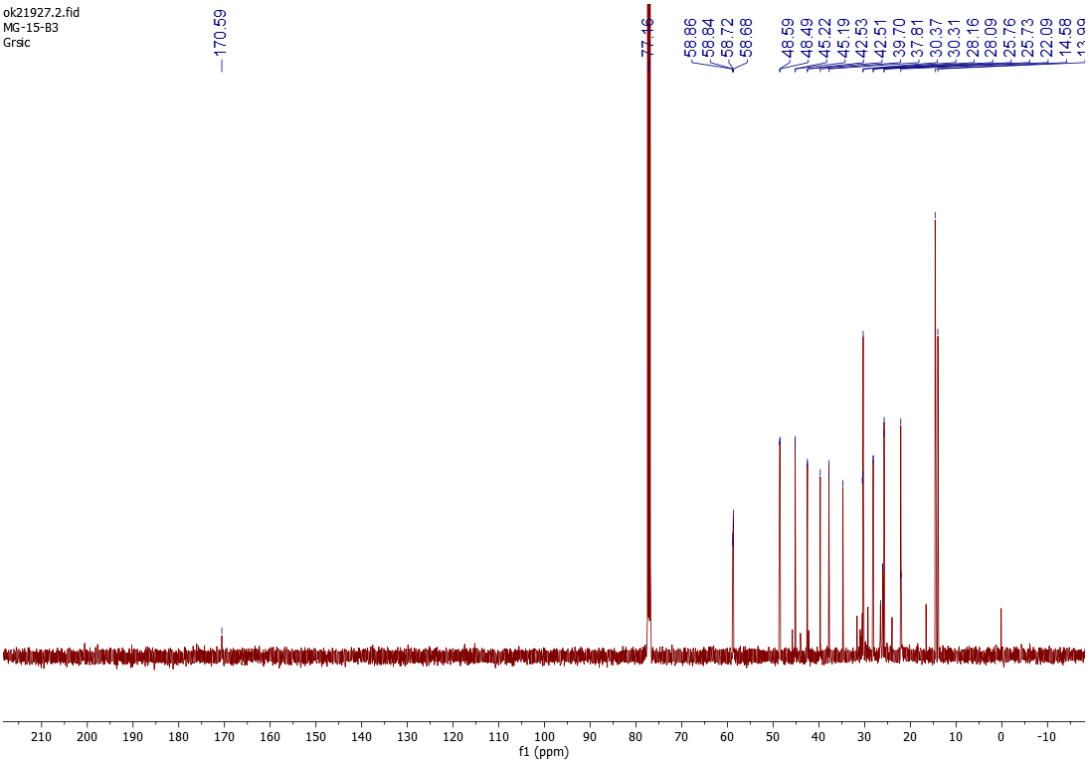
***N*-(2-((1*R*,3*R*)-2,2,3-Trimethylcyclopentyl)ethyl)-4,5,6,7-tetrahydro-1*H*-indole-2-carboxamide (*cis*-29) and *N*-(2-((1*R*,3*S*)-2,2,3-trimethylcyclopentyl)ethyl)-4,5,6,7-tetrahydro-1*H*-indole-2-carboxamide (*trans*-29)**





***N*-(2-((1*R*,3*R*)-2,2,3-Trimethylcyclopentyl)ethyl)octahydro-1*H*-indole-2-carboxamide (*cis*-30) and *N*-(2-((1*R*,3*S*)-2,2,3-trimethylcyclopentyl)ethyl)octahydro-1*H*-indole-2-carboxamide (*trans*-30)**





MS spectra

N-(Cycloheptylmethyl)-3-(1*H*-indol-3-yl)propanamide (8)

Qualitative Compound Report

Data File	MG-8_001.d	**Sample Name**	MG-8
Sample Type	Sample	**Position**	Vial 2
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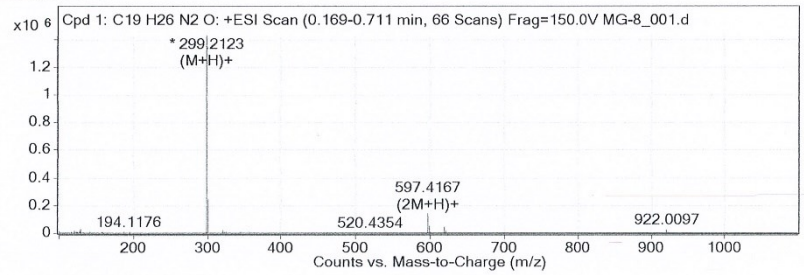
Acq Method	Bypass.m	**Acquired Time**	5/27/2016 9:57:17 AM
IRM Calibration Status	Success	**DA Method**	Damijana.m
Comment			

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C19 H26 N2 O	299.2119	0.237	Find by Molecular Feature	298.2044

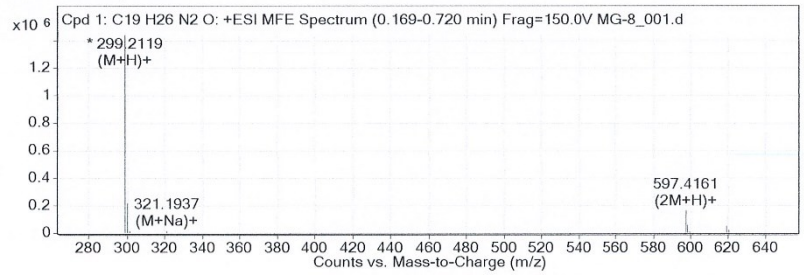
Compound Identification Results

Ion Mass	Calc Ion Mass	Difference	IonFormula	IonSpecies	Best
299.2119	299.2118	-0.1	C19 H27 N2 O	(M+H)+	✓
321.1937	321.1924	-1.3	C17 H24 N5 Na	(M+Na)+	

MS Spectrum



MFE MS Zoomed Spectrum



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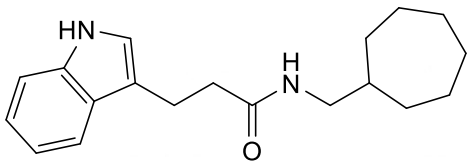

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***tert*-Butyl (*R*)-(1-((2-cyclohexylethyl)amino)-3-(1*H*-indol-3-yl)-1-oxopropan-2-yl)carbamate (9)**

Qualitative Compound Report

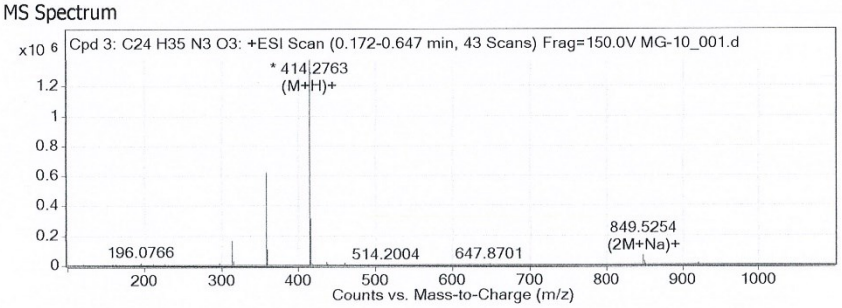
Data File	MG-10_001.d	**Sample Name**	MG-10
Sample Type	Sample	**Position**	Vial 16
Instrument Name	US10310002	**User Name**	TOF-PC\admin
Acq Method	Bypass.m	**Acquired Time**	8/9/2016 2:47:47 PM
IRM Calibration Status	Success	**DA Method**	Damijana.m
Comment			

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 3: C24 H35 N3 O3	414.2762	0.234	Find by Molecular Feature	413.2694

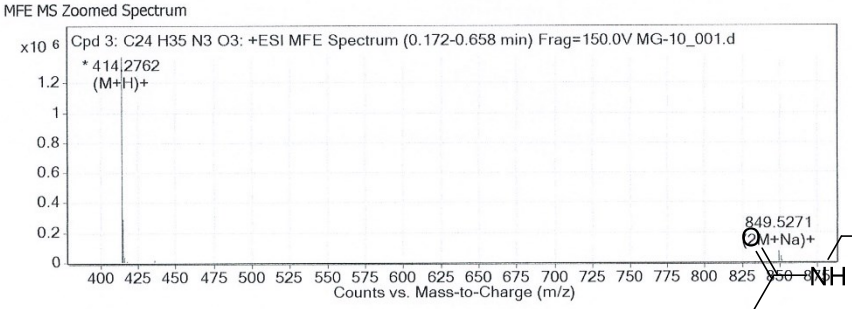
Compound Identification Results

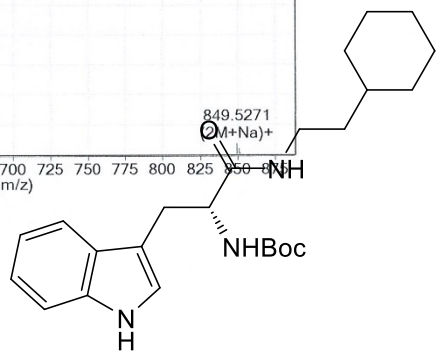
Ion Mass	Calc Ion Mass	Difference	IonFormula	IonSpecies	Best
414.2762	414.2765	0.2	C26 H38 O4	(M+H)+	
414.2762	414.277	0.8	C11 H34 N12 O5	(M+H)+	
414.2762	414.2751	-1.1	C24 H36 N3 O3	(M+H)+	✓
414.2762	414.2778	1.6	C27 H34 N4	(M+H)+	
452.2316	452.2297	-1.9	C22 H33 K N6 O2	(M+K)+	
414.2762	414.2783	2.1	C12 H30 N16 O	(M+H)+	
414.2762	414.2783	2.1	C13 H36 N9 O6	(M+H)+	

MS Spectrum



MFE MS Zoomed Spectrum





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***tert*-Butyl (*S*)-(1-((2-cyclohexylethyl)amino)-3-(1-methyl-1*H*-indol-3-yl)-1-oxopropan-2-yl)carbamate (10)**

Qualitative Compound Report

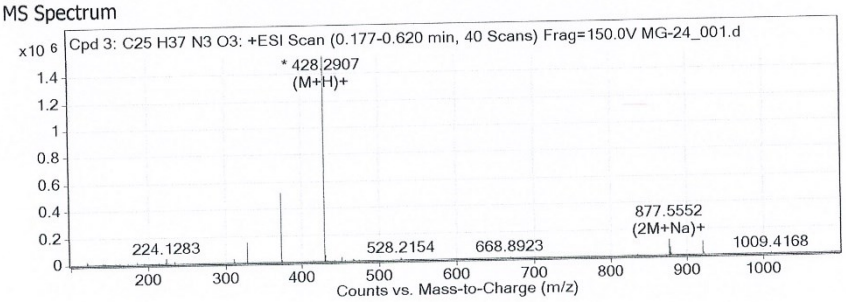
Data File	MG-24_001.d	**Sample Name**	MG-24
Sample Type	Sample	**Position**	Vial 12
Instrument Name	US10310002	**User Name**	TOF-PC\admin
Acq Method	Bypass.m	**Acquired Time**	5/25/2017 10:27:50 AM
IRM Calibration Status	Success	**DA Method**	Damijana.m
Comment			

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 3: C25 H37 N3 O3	428.291	0.237	Find by Molecular Feature	427.2836

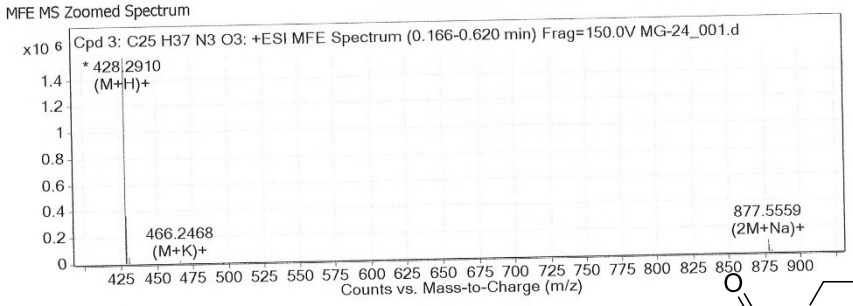
Compound Identification Results

Ion Mass	Calc Ion Mass	Difference	IonFormula	IonSpecies	Best
428.291	428.2908	-0.2	C25 H38 N3 O3	(M+H)+	✓
893.5358	893.5355	-0.3	C56 H70 K N8	(2M+K)+	
893.5358	893.5365	0.7	C26 H62 K N32 O2	(2M+K)+	
893.5358	893.5365	0.7	C28 H74 K N18 O12	(2M+K)+	
428.291	428.2921	1.1	C27 H40 O4	(M+H)+	
428.291	428.2894	-1.6	C23 H36 N6 O2	(M+H)+	
428.291	428.2926	1.6	C12 H36 N12 O5	(M+H)+	

MS Spectrum



MFE MS Zoomed Spectrum



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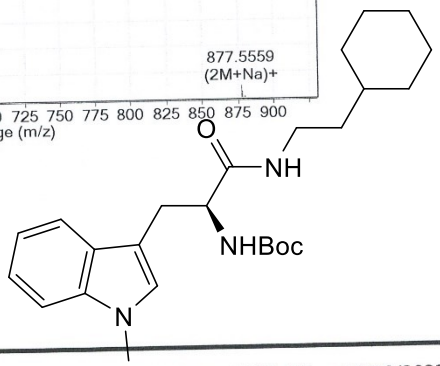


***tert*-Butyl ((S)-1-((2-((*R*)-2,2-dimethyl-3-methylenecyclopentyl)ethyl)amino)-3-(1-methyl-1*H*-indol-3-yl)-1-oxopropan-2-yl)carbamate (11)**

Qualitative Compound Report

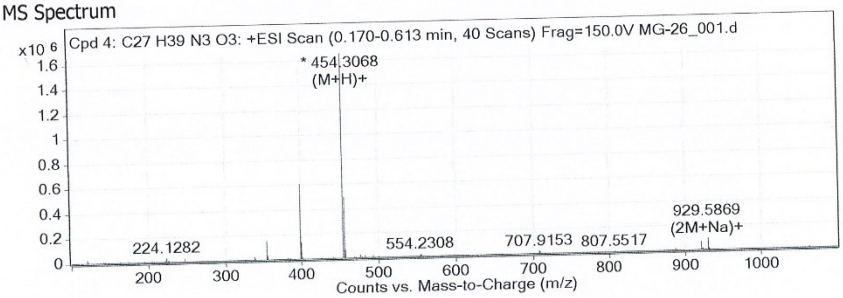
Data File	MG-26_001.d	**Sample Name**	MG-26
Sample Type	Sample	**Position**	Vial 12
Instrument Name	US10310002	**User Name**	TOF-PC\admin
Acq Method	Bypass.m	**Acquired Time**	5/30/2017 2:01:11 PM
IRM Calibration Status	Success	**DA Method**	Damijana.m
Comment			

Compound Label	m/z	RT	Algorithm	Mass
Cpd 4: C27 H39 N3 O3	454.3068	0.237	Find by Molecular Feature	453.2997

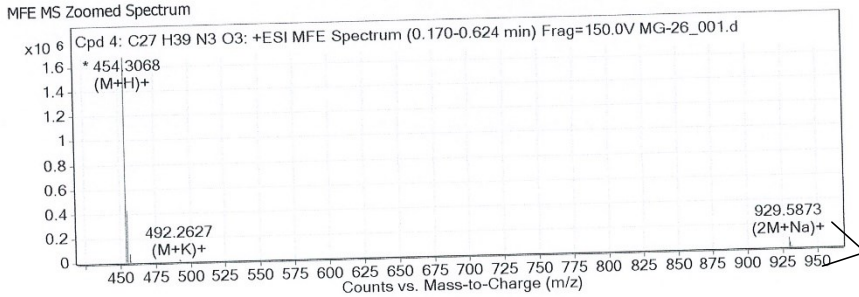
Compound Identification Results

Ion Mass	Calc Ion Mass	Difference	IonFormula	IonSpecies	Best
454.3068	454.3064		-0.4 C27 H40 N3 O3	(M+H)+	✓
454.3068	454.3078		1 C29 H42 O4	(M+H)+	
454.3068	454.3083		1.5 C13 H32 N19	(M+H)+	
454.3068	454.3083		1.5 C14 H38 N12 O5	(M+H)+	
454.3068	454.3051		-1.7 C25 H38 N6 O2	(M+H)+	
492.2627	492.265		2.2 C30 H37 K N4	(M+K)+	
492.2627	492.2655		2.7 C15 H33 K N16 O	(M+K)+	

MS Spectrum



MFE MS Zoomed Spectrum



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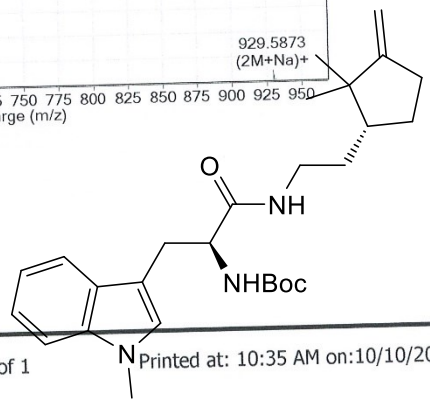


***tert*-Butyl ((*R*)-1-((2-((*R*)-2,2-dimethyl-3-methylenecyclopentyl)ethyl)amino)-3-(1-methyl-1*H*-indol-3-yl)-1-oxopropan-2-yl)carbamate (12)**

Qualitative Compound Report

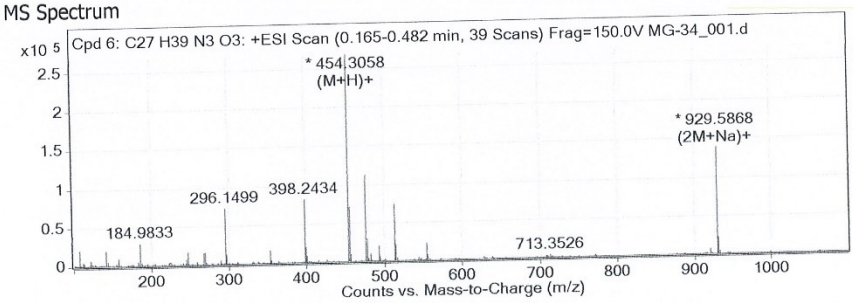
Data File	MG-34_001.d	**Sample Name**	MG-34
Sample Type	Sample	**Position**	Vial 4
Instrument Name	US10310002	**User Name**	TOF-PC\admin
Acq Method	Bypass.m	**Acquired Time**	8/3/2017 10:28:19 AM
IRM Calibration Status	Success	**DA Method**	Damijana.m
Comment			

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 6: C27 H39 N3 O3	454.3048	0.234	Find by Molecular Feature	453.3007

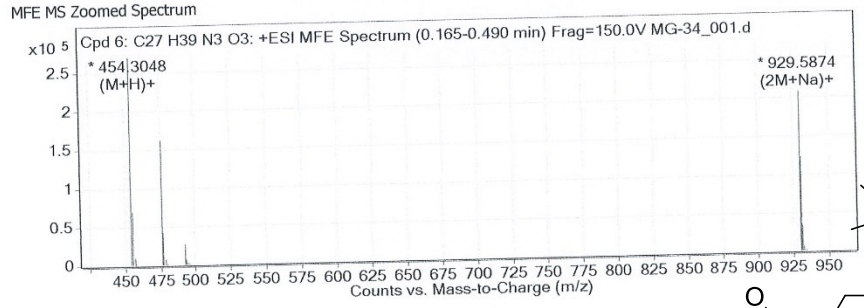
Compound Identification Results

Ion Mass	Calc Ion Mass	Difference	IonFormula	IonSpecies	Best
454.3048	454.3051	0.3	C25 H38 N6 O2	(M+H)+	
492.2639	492.265	1.1	C30 H37 K N4	(M+K)+	
454.3048	454.3037	-1.1	C24 H42 N2 O6	(M+H)+	
454.3048	454.3037	-1.1	C23 H36 N9 O	(M+H)+	
454.3048	454.3064	1.6	C27 H40 N3 O3	(M+H)+	✓
492.2639	492.2655	1.6	C15 H33 K N16 O	(M+K)+	
492.2639	492.2655	1.6	C16 H39 K N9 O6	(M+K)+	
476.2877	476.2897	2	C29 H41 Na O4	(M+Na)+	
476.2877	476.2902	2.5	C13 H31 N19 Na	(M+Na)+	
476.2877	476.2902	2.5	C14 H37 N12 Na O5	(M+Na)+	

MS Spectrum



MFE MS Zoomed Spectrum



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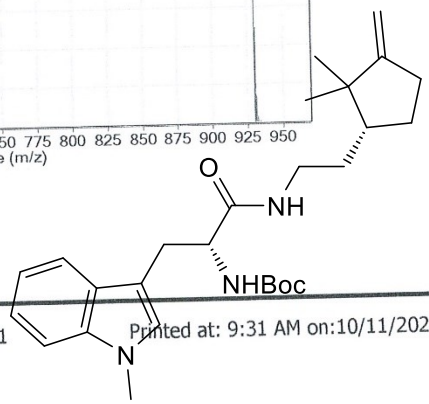

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(*R*)-1-((2-Cyclohexylethyl)amino)-3-(1*H*-indol-3-yl)-1-oxopropan-2-aminium 2,2,2-trifluoroacetate (13)

Qualitative Compound Report

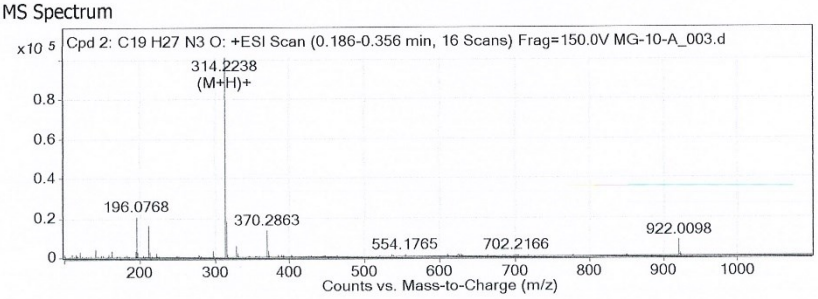
Data File	MG-10-A_003.d	**Sample Name**	MG-10-A
Sample Type	Sample	**Position**	13
Instrument Name	US10310002	**User Name**	TOF-PC\admin
Acq Method	Bypass.m	**Acquired Time**	8/9/2016 2:45:25 PM
IRM Calibration Status	Success	**DA Method**	Damijana.m
Comment			

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 2: C19 H27 N3 O	314.2242	0.234	Find by Molecular Feature	313.2169

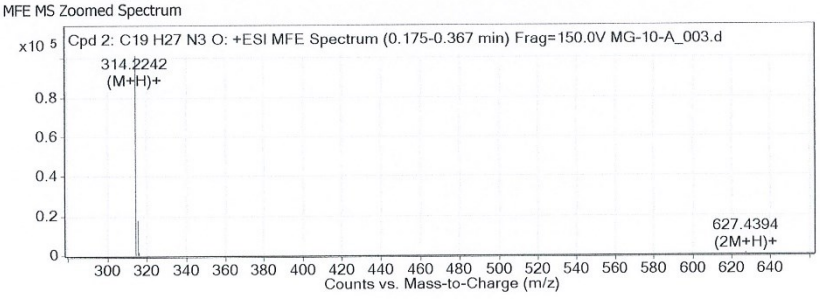
Compound Identification Results

Ion Mass	Calc Ion Mass	Difference	IonFormula	IonSpecies	Best
314.2242	314.224	-0.1	C21 H30 O2	(M+H)+	
314.2242	314.2227	-1.5	C19 H28 N3 O	(M+H)+	✓
314.2242	314.2259	1.7	C8 H28 N9 O4	(M+H)+	

MS Spectrum



MFE MS Zoomed Spectrum



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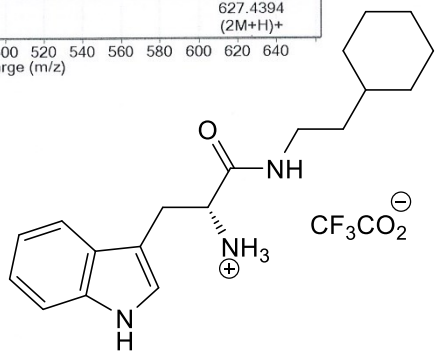

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(*S*)-3-(1-Methyl-1*H*-indol-3-yl)-1-oxo-1-((2-(2,3,3-trimethylcyclopent-1-en-1-yl)ethyl)amino)propan-2-aminium 2,2,2-trifluoroacetate (14)

Qualitative Compound Report

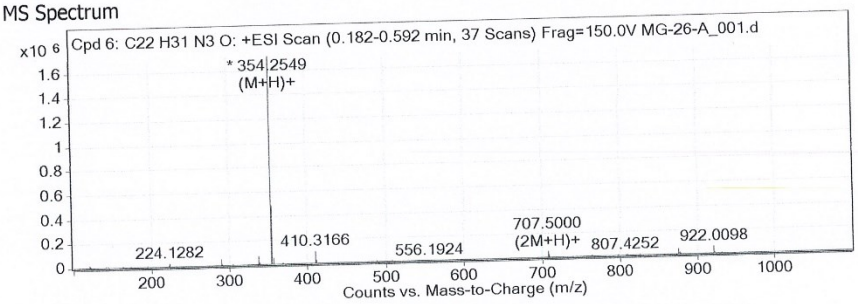
Data File	MG-26-A_001.d	**Sample Name**	MG-26-A
Sample Type	Sample	**Position**	Vial 11
Instrument Name	US10310002	**User Name**	TOF-PC\admin
Acq Method	Bypass.m	**Acquired Time**	5/30/2017 1:58:56 PM
IRM Calibration Status	Success	**DA Method**	Damijana.m
Comment			

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 6: C22 H31 N3 O	354.2541	0.236	Find by Molecular Feature	353.246

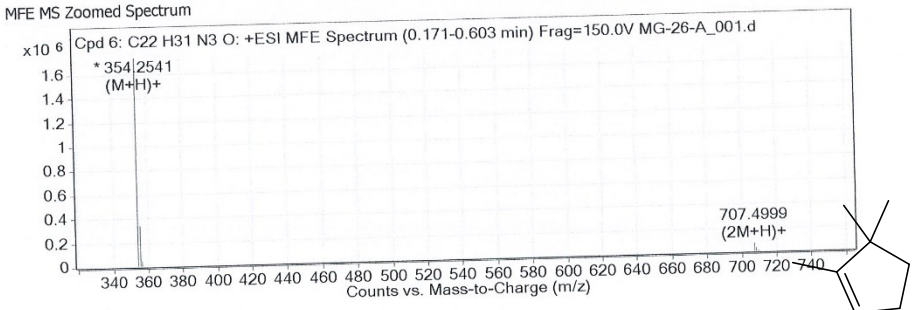
Compound Identification Results

Ion Mass	Calc Ion Mass	Difference	IonFormula	IonSpecies	Best
354.2541	354.254	-0.2	C22 H32 N3 O	(M+H)+	✓
354.2541	354.2553	1.2	C24 H34 O2	(M+H)+	
354.2541	354.2526	-1.5	C20 H30 N6	(M+H)+	

MS Spectrum



MFE MS Zoomed Spectrum



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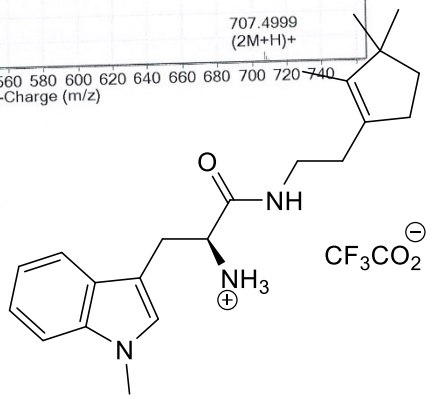

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(*R*)-3-(1-Methyl-1*H*-indol-3-yl)-1-oxo-1-((2-(2,3,3-trimethylcyclopent-1-en-1-yl)ethyl)amino)propan-2-aminium 2,2,2-trifluoroacetate (15)

Qualitative Compound Report

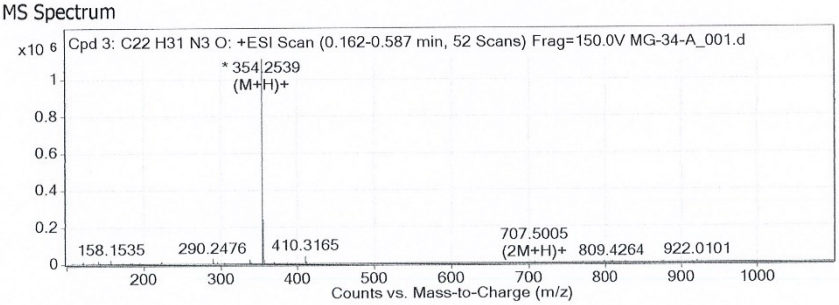
Data File	MG-34-A_001.d	**Sample Name**	MG-34-A
Sample Type	Sample	**Position**	Vial 5
Instrument Name	US10310002	**User Name**	TOF-PC\admin
Acq Method	Bypass.m	**Acquired Time**	8/3/2017 10:41:44 AM
IRM Calibration Status	Success	**DA Method**	Damijana.m
Comment			

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 3: C22 H31 N3 O	354.2535	0.233	Find by Molecular Feature	353.2463

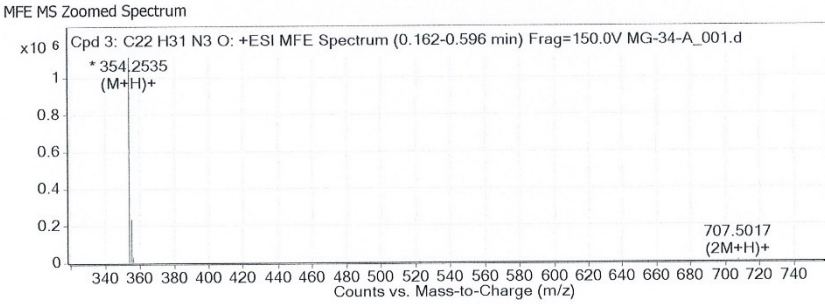
Compound Identification Results

Ion Mass	Calc Ion Mass	Difference	IonFormula	IonSpecies	Best
354.2535	354.254	0.5	C22 H32 N3 O	(M+H)+	✓
354.2535	354.2526	-0.9	C20 H30 N6	(M+H)+	
376.2358	376.2373	1.5	C24 H33 Na O2	(M+Na)+	

MS Spectrum



MFE MS Zoomed Spectrum



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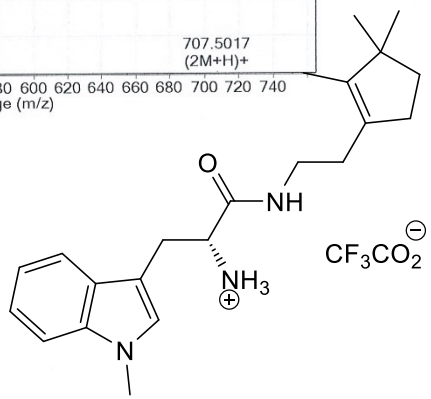

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(*R*)-2-Acetamido-*N*-(2-cyclohexylethyl)-3-(1*H*-indol-3-yl)propanamide (19)

Qualitative Compound Report

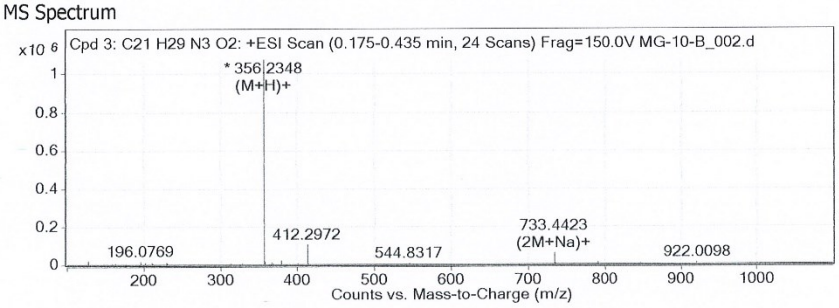
Data File	MG-10-B_002.d	**Sample Name**	MG-10-B
Sample Type	Sample	**Position**	Vial 15
Instrument Name	US10310002	**User Name**	TOF-PC\admin
Acq Method	Bypass.m	**Acquired Time**	8/9/2016 2:40:08 PM
IRM Calibration Status	Success	**DA Method**	Damijana.m
Comment			

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 3: C21 H29 N3 O2	356.2347	0.234	Find by Molecular Feature	355.2262

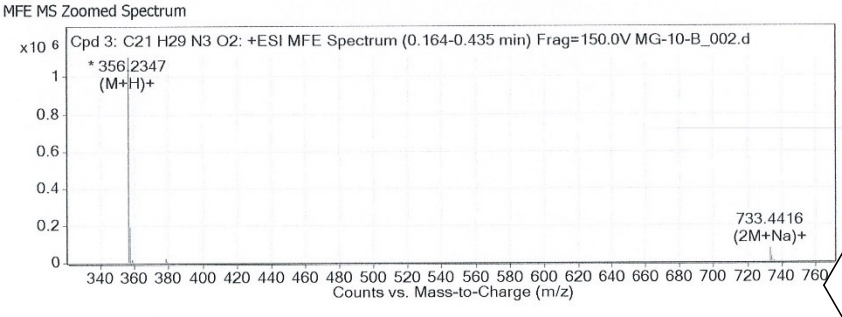
Compound Identification Results

Ion Mass	Calc Ion Mass	Difference	IonFormula	IonSpecies	Best
356.2347	356.2346	-0.1	C23 H32 O3	(M+H)+	
356.2347	356.2333	-1.5	C21 H30 N3 O2	(M+H)+	✓
356.2347	356.2364	1.7	C10 H30 N9 O5	(M+H)+	

MS Spectrum



MFE MS Zoomed Spectrum



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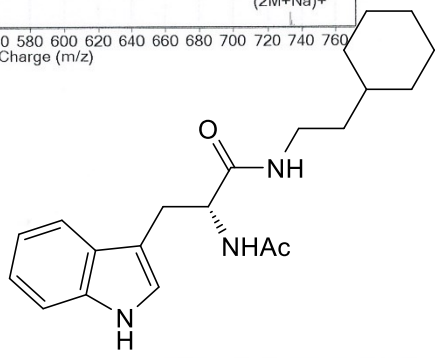

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(*R*)-2-Acetamido-3-(1*H*-indol-3-yl)-*N*-(2-(2,3,3-trimethylcyclopent-1-en-1-yl)ethyl)propanamide (20)

Qualitative Compound Report

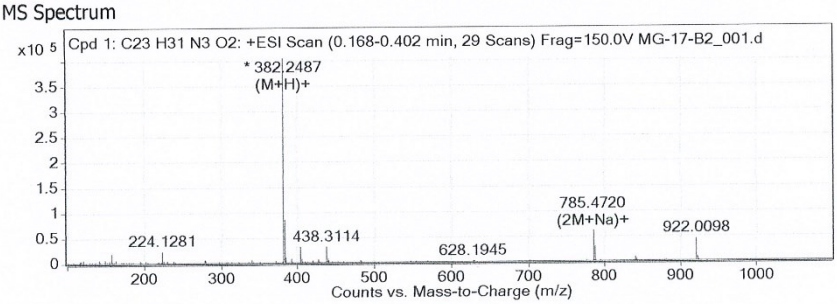
Data File	MG-17-B2_001.d	**Sample Name**	MG-17-B2
Sample Type	Sample	**Position**	Vial 36
Instrument Name	US10310002	**User Name**	TOF-PC\admin
Acq Method	Bypass.m	**Acquired Time**	3/21/2017 9:56:33 AM
IRM Calibration Status	Success	**DA Method**	Damijana.m
Comment			

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C23 H31 N3 O2	382.2489	0.234	Find by Molecular Feature	381.2412

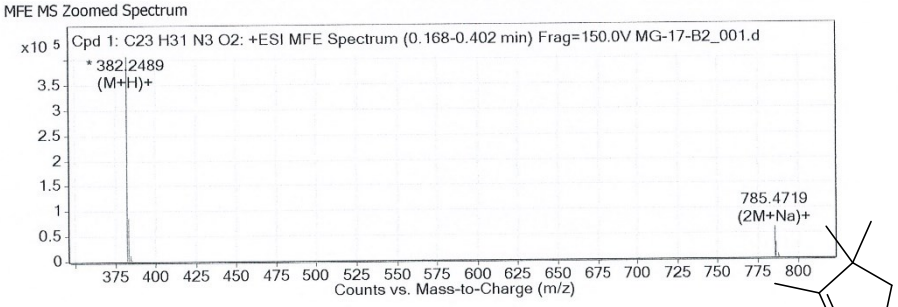
Compound Identification Results

Ion Mass	Calc Ion Mass	Difference	IonFormula	IonSpecies	Best
382.2489	382.2489	0	C23 H32 N3 O2	(M+H)+	✓
382.2489	382.2476	-1.3	C21 H30 N6 O	(M+H)+	
382.2489	382.2502	1.4	C25 H34 O3	(M+H)+	
382.2489	382.2507	1.9	C10 H30 N12 O4	(M+H)+	

MS Spectrum



MFE MS Zoomed Spectrum



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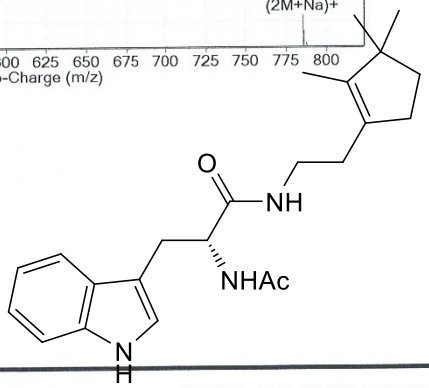


***tert*-Butyl (*R*)-(3-(1*H*-indol-3-yl)-1-oxo-1-((2-(2,3,3-trimethylcyclopent-1-en-1-yl)ethyl)amino)propan-2-yl)carbamate (21)**

Qualitative Compound Report

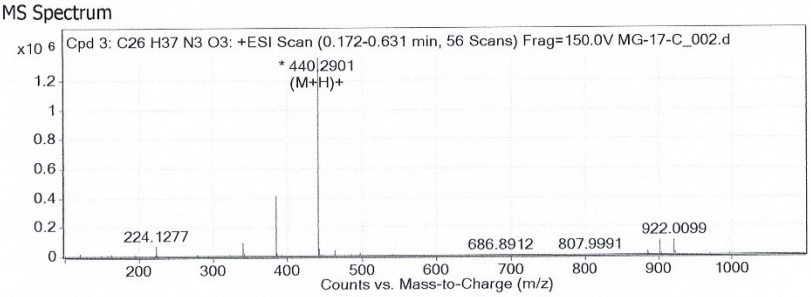
Data File	MG-17-C_002.d	**Sample Name**	MG-17-C
Sample Type	Sample	**Position**	Vial 3
Instrument Name	US10310002	**User Name**	TOF-PC\admin
Acq Method	Bypass.m	**Acquired Time**	3/23/2017 11:43:52 AM
IRM Calibration Status	Success	**DA Method**	Damijana.m
Comment			

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 3: C26 H37 N3 O3	440.2903	0.236	Find by Molecular Feature	439.2834

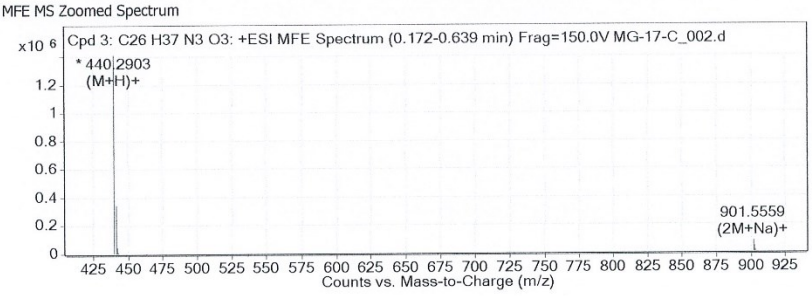
Compound Identification Results

Ion Mass	Calc Ion Mass	Difference	IonFormula	IonSpecies	Best
440.2903	440.2908	0.4	C26 H38 N3 O3	(M+H)+	✓
440.2903	440.2894	-0.9	C24 H36 N6 O2	(M+H)+	
440.2903	440.2921	1.8	C28 H40 O4	(M+H)+	
440.2903	440.2926	2.3	C13 H36 N12 O5	(M+H)+	

MS Spectrum



MFE MS Zoomed Spectrum



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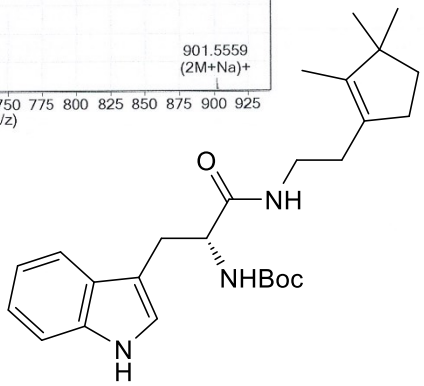


***tert*-Butyl (*R*)-(3-(1*H*-indol-3-yl)-1-oxo-1-(((2,3,3-trimethylcyclopent-1-en-1-yl)methyl)amino)propan-2-yl)carbamate (22)**

Qualitative Compound Report

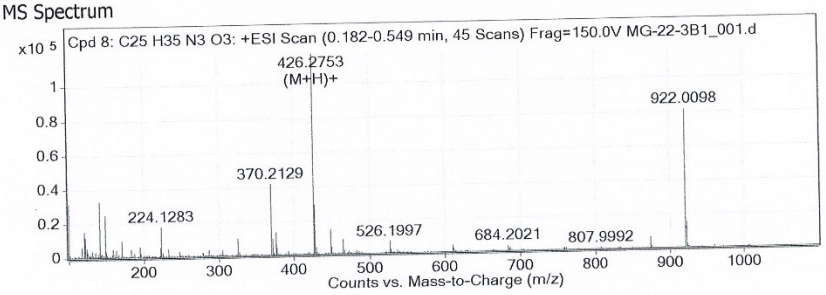
Data File	MG-22-3B1_001.d	**Sample Name**	MG-22-3B1
Sample Type	Sample	**Position**	Vial 31
Instrument Name	US10310002	**User Name**	TOF-PC\admin
Acq Method	Bypass.m	**Acquired Time**	5/18/2017 11:22:59 AM
IRM Calibration Status	Success	**DA Method**	Damijana.m
Comment			

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 8: C25 H35 N3 O3	426.2751	0.237	Find by Molecular Feature	425.2681

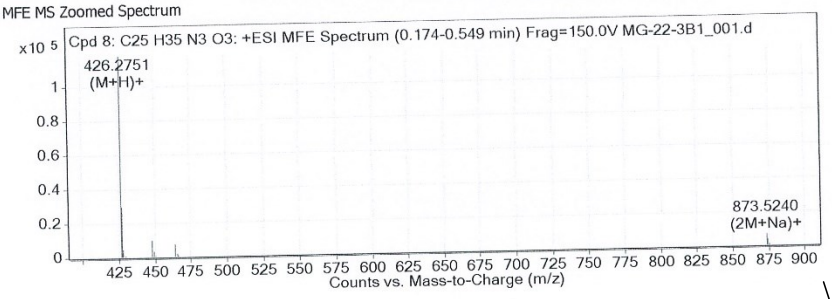
Compound Identification Results

Ion Mass	Calc Ion Mass	Difference	IonFormula	IonSpecies	Best
426.2751	426.2751		0 C25 H36 N3 O3	(M+H)+	✓
426.2751	426.2738		-1.3 C23 H34 N6 O2	(M+H)+	
426.2751	426.2765		1.4 C27 H38 O4	(M+H)+	
426.2751	426.277		1.9 C12 H34 N12 O5	(M+H)+	

MS Spectrum



MFE MS Zoomed Spectrum



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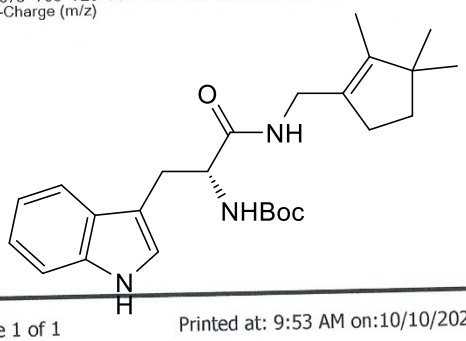


***tert*-Butyl (*S*)-(3-(1-methyl-1*H*-indol-3-yl)-1-oxo-1-((2-(2,3,3-trimethylcyclopent-1-en-1-yl)ethyl)amino)propan-2-yl)carbamate (23)**

Qualitative Compound Report

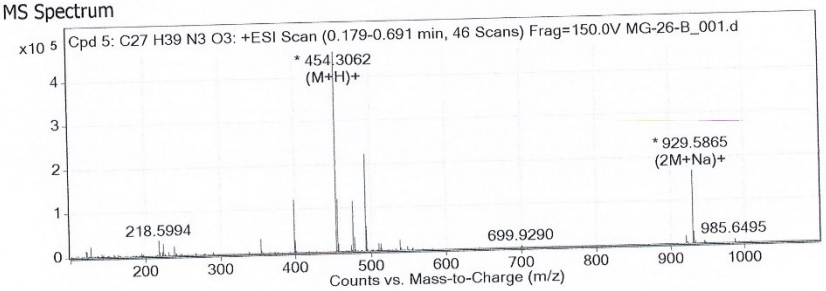
Data File	MG-26-B_001.d	**Sample Name**	MG-26-B
Sample Type	Sample	**Position**	Vial 15
Instrument Name	US10310002	**User Name**	TOF-PC\admin
Acq Method	Bypass.m	**Acquired Time**	6/1/2017 10:33:06 AM
IRM Calibration Status	Success	**DA Method**	Damijana.m
Comment			

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 5: C27 H39 N3 O3	454.3068	0.234	Find by Molecular Feature	453.2985

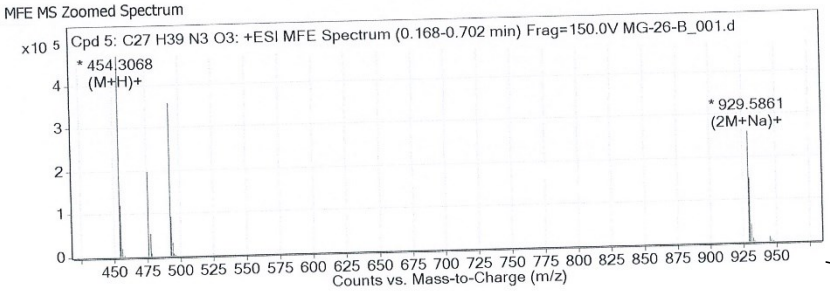
Compound Identification Results

Ion Mass	Calc Ion Mass	Difference	IonFormula	IonSpecies	Best
454.3068	454.3064		-0.4 C27 H40 N3 O3	(M+H)+	✓
454.3068	454.3078		0.9 C29 H42 O4	(M+H)+	
454.3068	454.3083		1.4 C13 H32 N19	(M+H)+	
454.3068	454.3083		1.4 C14 H38 N12 O5	(M+H)+	
454.3068	454.3051		-1.7 C25 H38 N6 O2	(M+H)+	
454.3068	454.3091		2.3 C30 H38 N4	(M+H)+	

MS Spectrum



MFE MS Zoomed Spectrum



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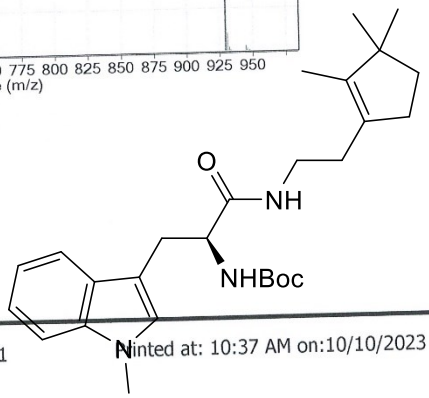


***tert*-Butyl (*R*)-(3-(1-methyl-1*H*-indol-3-yl)-1-oxo-1-((2-(2,3,3-trimethylcyclopent-1-en-1-yl)ethyl)amino)propan-2-yl)carbamate (24)**

Qualitative Compound Report

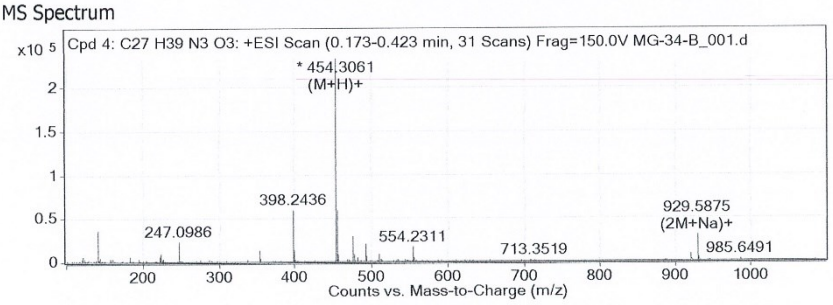
Data File	MG-34-B_001.d	**Sample Name**	MG-34-B
Sample Type	Sample	**Position**	Vial 7
Instrument Name	US10310002	**User Name**	TOF-PC\admin
Acq Method	Bypass.m	**Acquired Time**	8/8/2017 10:50:47 AM
IRM Calibration Status	Success	**DA Method**	Damijana.m
Comment			

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 4: C27 H39 N3 O3	454.3067	0.234	Find by Molecular Feature	453.2996

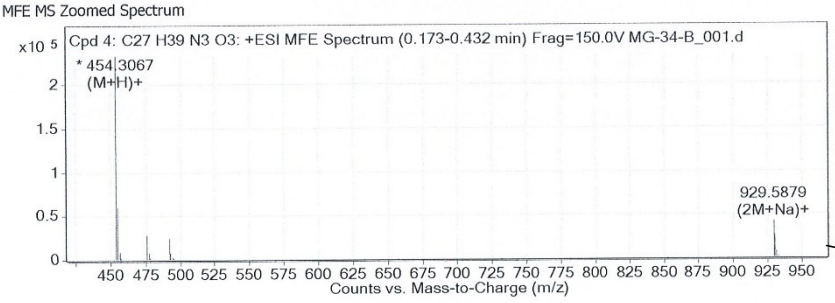
Compound Identification Results

Ion Mass	Calc Ion Mass	Difference	IonFormula	IonSpecies	Best
454.3067	454.3064	-0.3	C27 H40 N3 O3	(M+H)+	✓
454.3067	454.3078	1	C29 H42 O4	(M+H)+	
454.3067	454.3083	1.5	C13 H32 N19	(M+H)+	
454.3067	454.3083	1.5	C14 H38 N12 O5	(M+H)+	
454.3067	454.3051	-1.7	C25 H38 N6 O2	(M+H)+	
492.2631	492.265	1.9	C30 H37 K N4	(M+K)+	
492.2631	492.2655	2.4	C15 H33 K N16 O	(M+K)+	
492.2631	492.2655	2.4	C16 H39 K N9 O6	(M+K)+	

MS Spectrum



MFE MS Zoomed Spectrum



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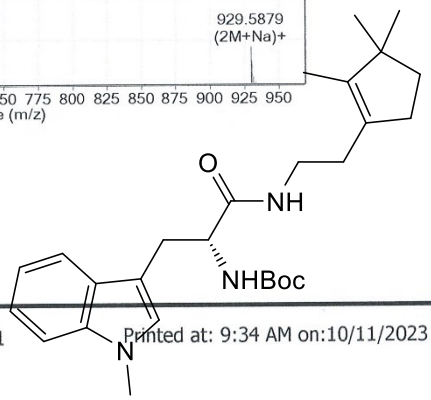


2-(1*H*-Indol-3-yl)-*N*-(2-((1*R*,3*R*)-2,2,3-trimethylcyclopentyl)ethyl)acetamide (*cis*-27) and 2-(1*H*-indol-3-yl)-*N*-(2-((1*R*,3*S*)-2,2,3-trimethylcyclopentyl)ethyl)acetamide (*trans*-27)

Qualitative Compound Report

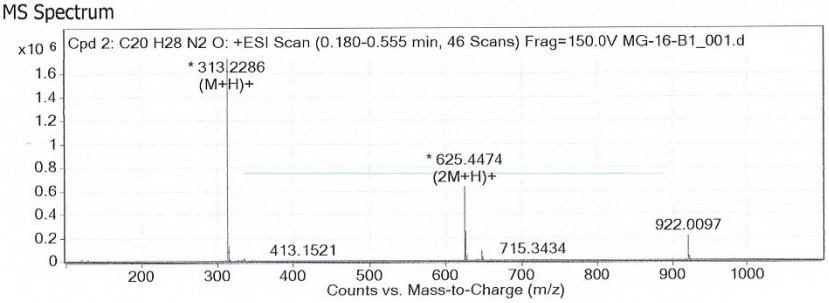
Data File	MG-16-B1_001.d	**Sample Name**	MG-16-B1
Sample Type	Sample	**Position**	Vial 25
Instrument Name	US10310002	**User Name**	TOF-PC\admin
Acq Method	Bypass.m	**Acquired Time**	11/23/2016 10:48:01 AM
IRM Calibration Status	Success	**DA Method**	Damijana.m
Comment			

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 2: C20 H28 N2 O	313.2277	0.232	Find by Molecular Feature	312.2201

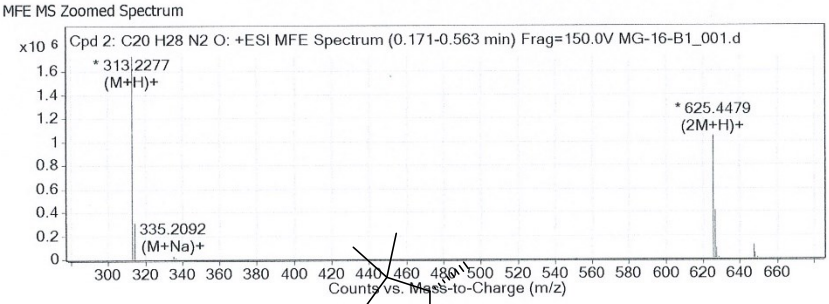
Compound Identification Results

Ion Mass	Calc Ion Mass	Difference	IonFormula	IonSpecies	Best
313.2277	313.2274	-0.3	C20 H29 N2 O	(M+H)+	✓
351.1861	351.1865	0.4	C9 H28 K N8 O4	(M+K)+	
335.2092	335.208	-1.1	C18 H26 N5 Na	(M+Na)+	
351.1861	351.1878	1.8	C10 H24 K N12	(M+K)+	
351.1861	351.1879	1.8	C11 H30 K N5 O5	(M+K)+	

MS Spectrum



MFE MS Zoomed Spectrum



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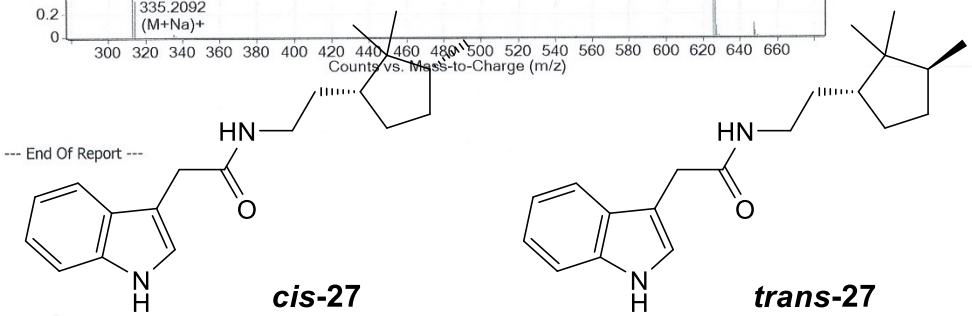


***cis*-27** ***trans*-27**

***tert*-Butyl ((*S*)-3-(1-methyl-1*H*-indol-3-yl)-1-oxo-1-((2-(2,3,3-trimethylcyclopentyl)ethyl)-amino)propan-2-yl)carbamate (28)**

Qualitative Compound Report

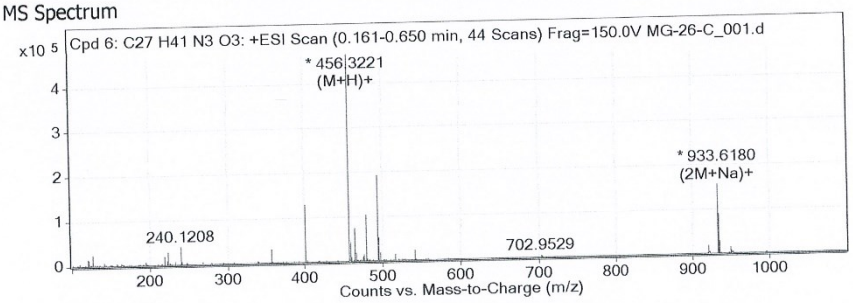
Data File	MG-26-C_001.d	**Sample Name**	MG-26-C
Sample Type	Sample	**Position**	Vial 14
Instrument Name	US10310002	**User Name**	TOF-PC\admin
Acq Method	Bypass.m	**Acquired Time**	6/1/2017 10:29:17 AM
IRM Calibration Status	Success	**DA Method**	Damijana.m
Comment			

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 6: C27 H41 N3 O3	456.3222	0.233	Find by Molecular Feature	455.3165

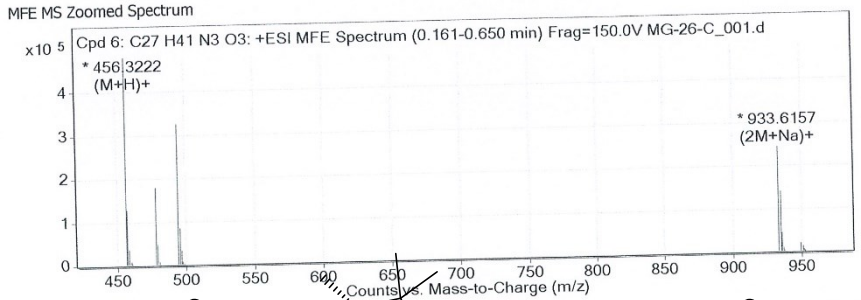
Compound Identification Results

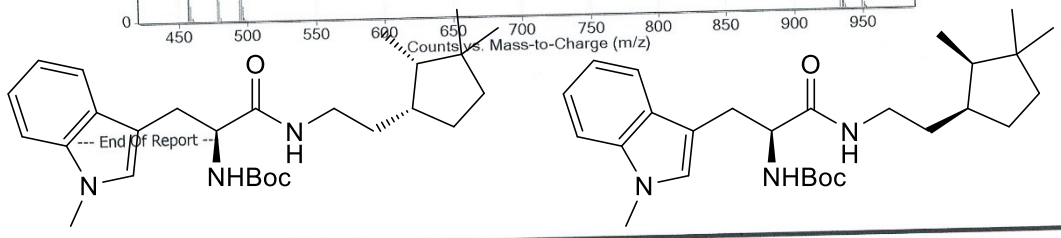
Ion Mass	Calc Ion Mass	Difference	IonFormula	IonSpecies	Best
456.3222	456.3221		-0.1 C27 H42 N3 O3	(M+H)+	✓
456.3222	456.3234		1.2 C29 H44 O4	(M+H)+	
456.3222	456.3207		-1.5 C25 H40 N6 O2	(M+H)+	
456.3222	456.3239		1.7 C13 H34 N19	(M+H)+	
456.3222	456.3239		1.7 C14 H40 N12 O5	(M+H)+	
456.3222	456.3247		2.6 C30 H40 N4	(M+H)+	
456.3222	456.3253		3.1 C16 H42 N9 O6	(M+H)+	
456.3222	456.3253		3.1 C15 H36 N16 O	(M+H)+	

MS Spectrum



MFE MS Zoomed Spectrum





_N_-(2-((1_R_,3_R_)-2,2,3-Trimethylcyclopentyl)ethyl)-4,5,6,7-tetrahydro-1_H_-indole-2-carboxamide (_cis_-29) and _N_-(2-((1_R_,3_S_)-2,2,3-trimethylcyclopentyl)ethyl)-4,5,6,7-tetrahydro-1_H_-indole-2-carboxamide (_trans_-29)

Qualitative Compound Report

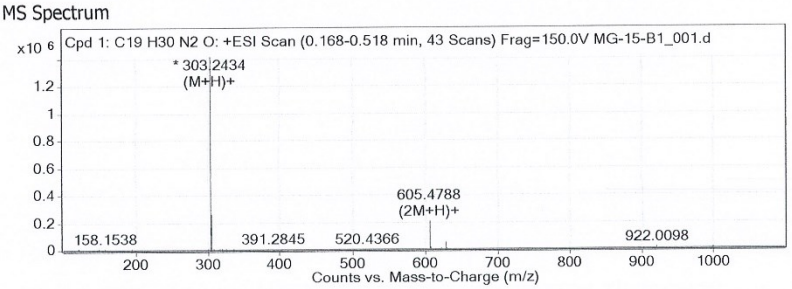
Data File	MG-15-B1_001.d	**Sample Name**	MG-15-B1
Sample Type	Sample	**Position**	Vial 12
Instrument Name	US10310002	**User Name**	TOF-PC\admin
Acq Method	Bypass.m	**Acquired Time**	11/10/2016 10:28:54 AM
IRM Calibration Status	Success	**DA Method**	Damijana.m
Comment			

Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C19 H30 N2 O	303.2429	0.234	Find by Molecular Feature	302.2358

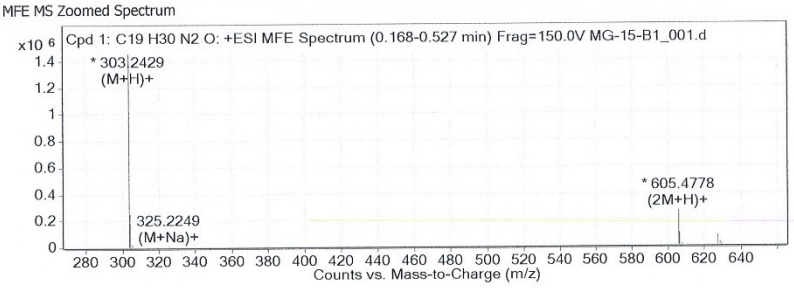
Compound Identification Results

Ion Mass	Calc Ion Mass	Difference	IonFormula	IonSpecies	Best
303.2429	303.2431	0.2	C19 H31 N2 O	(M+H)+	✓
303.2429	303.2417	-1.2	C17 H29 N5	(M+H)+	

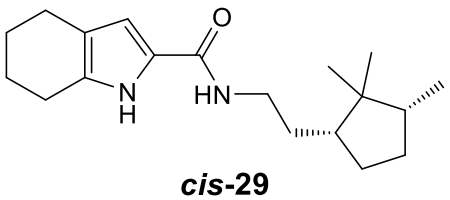
MS Spectrum



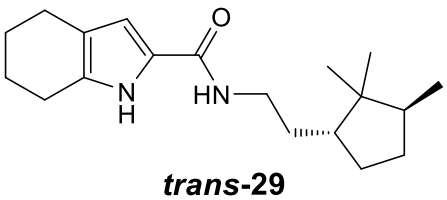
MFE MS Zoomed Spectrum



--- End Of Report ---



***cis*-29**



***trans*-29**

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***N*-(2-((1*R*,3*R*)-2,2,3-Trimethylcyclopentyl)ethyl)octahydro-1*H*-indole-2-carboxamide (*cis*-30) and *N*-(2-((1*R*,3*S*)-2,2,3-trimethylcyclopentyl)ethyl)octahydro-1*H*-indole-2-carboxamide (*trans*-30)**

Qualitative Compound Report

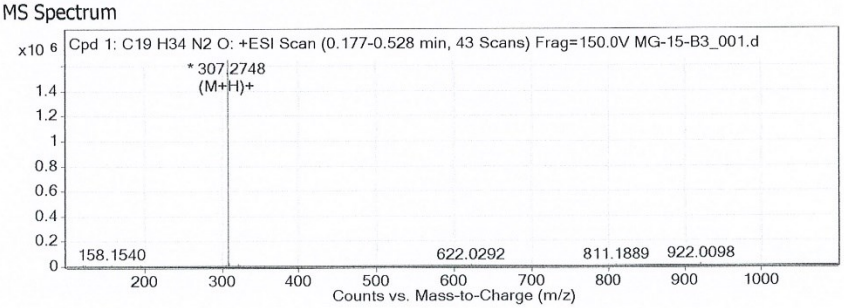
Data File	MG-15-B3_001.d	**Sample Name**	MG-15-B3
Sample Type	Sample	**Position**	Vial 11
Instrument Name	US10310002	**User Name**	TOF-PC\admin
Acq Method	Bypass.m	**Acquired Time**	11/10/2016 10:24:33 AM
IRM Calibration Status	Success	**DA Method**	Damijana.m
Comment			

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C19 H34 N2 O	307.2751	0.234	Find by Molecular Feature	306.2677

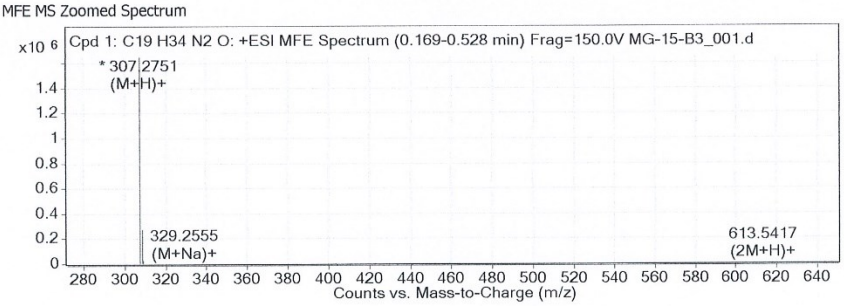
Compound Identification Results

Ion Mass	Calc Ion Mass	Difference	IonFormula	IonSpecies	Best
329.2555	329.255	-0.6	C17 H32 N5 Na	(M+Na)+	
307.2751	307.2744	-0.7	C19 H35 N2 O	(M+H)+	✓

MS Spectrum



MFE MS Zoomed Spectrum



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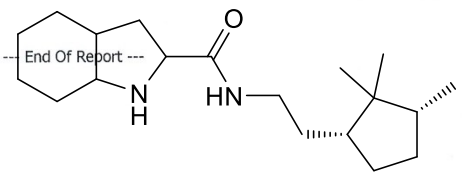
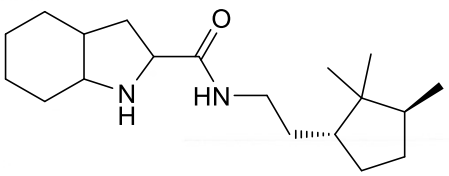


***cis*-30**



***trans*-30**

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