

Supporting Information

Hybrid Peptide-Thiourea Catalyst for Asymmetric Michael Additions of Aldehydes to Heterocyclic Nitroalkenes

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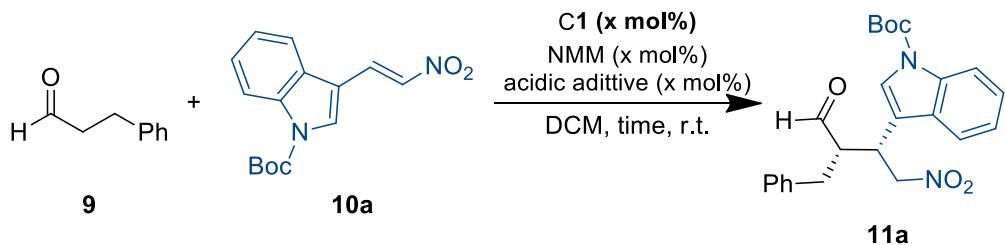
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Additional experimental results

Additional optimizations of reaction conditions

Table S1. Additive and catalyst loading screening.

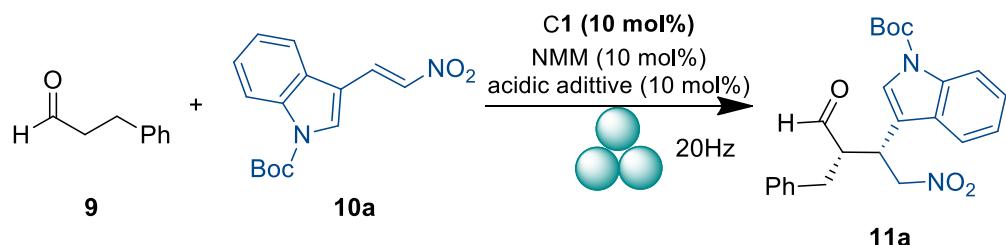


Entry	Additive/catalyst loading (mol%)	Time (h)	Yield 11a (%)	d.r. ^b	ee ^c (syn)
1	PhCO ₂ H/10	24	87	1:7	91
2	2-F-C ₆ H ₄ CO ₂ H/10	24	83	1:6	90
3	ClCH ₂ CO ₂ H/10	24	76	1:8	89
4	4-NO ₂ -C ₆ H ₄ CO ₂ H/10	24	85	1:6	89
5	PhCO ₂ H/1	96	24	1:4	85
6	PhCO ₂ H/3	48	50	1:6	87
7	PhCO ₂ H/5	36	69	1:6	88
8	PhCO ₂ H/8	28	70	1:7	88
9 ^a	PhCO ₂ H/8	60	93	1:10	94
10 ^a	PhCO ₂ H/10	48	90	1:11	92

^a Temperature -10 to 20°C; ^b Ratio of *anti/syn*-**11a** determined by ¹H NMR of the crude reaction mixture; ^c determined by chiral HPLC.

Additional optimizations of Michael additions in solvent free-conditions

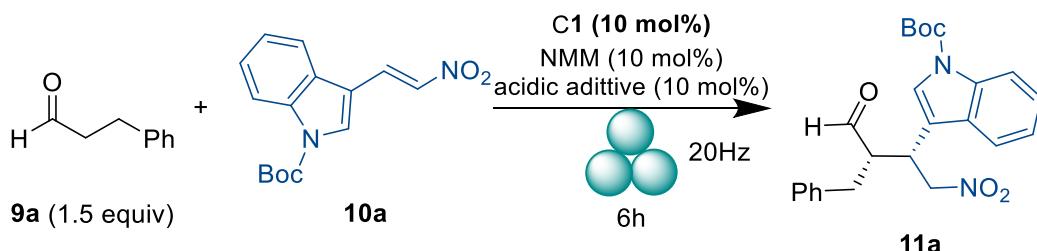
Table S2. Michael addition of 3-phenylpropanal (**9**) to *N*-Boc-indol nitroalkene **10a** with several acidic co-catalysts in solvent-free conditions of ball mill.



Entry	Additive	f [Hz/s]	Time [h]	Yield [%]	d.r. (min:maj)	ee [%]
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1	PhCOOH	25	6	70	1:7	84
2	2-F-C ₆ H ₄ -COOH	25	6	43	1:9	86
3	4-NO ₂ -C ₆ H ₄ -COOH	25	6	67	1:10	84
4	ClCH ₂ COOH	25	6	58	1:11	85
5	4-NO ₂ -C ₆ H ₄ -OH	25	6	68	1:9	85
6	PhCOOH	20	9	80	1:10	85
7	4-NO ₂ -C ₆ H ₄ -COOH	20	9	82	1:10	84

Table S3. Solvent-free Michael addition in ball mill with using of DCM, SiO₂ or NaCl.



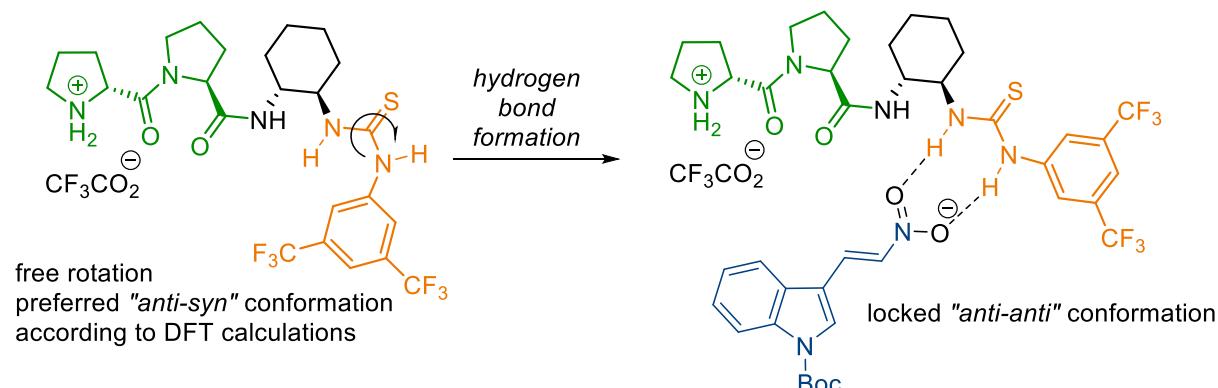
Entry	yield [%]	d.r.	ee [%]
1^a	52	1:4	86
2^b	12	1:3	85
3^c	9	1:8	83

^a with 20 µl of DCM; ^b with SiO₂; ^c with NaCl

NMR studies

Unless noted otherwise, no special precautions were used to prepare the NMR samples. An equimolar ratio of reagents was dissolved in CD_2Cl_2 and NMR spectra were recorded.

Upon addition of nitroalkene **10a** to a solution of **C1**, a slight shift of the aromatic signals of **C1** was observed, suggesting the electron density on the aromatic core changed, presumably due to hydrogen bond formation. Moreover, less signals and a clearer spectrum suggests, that the molecule has a more defined structure, with less rotamers present in solution, further confirming the formation of the double hydrogen bond.



Scheme S1.

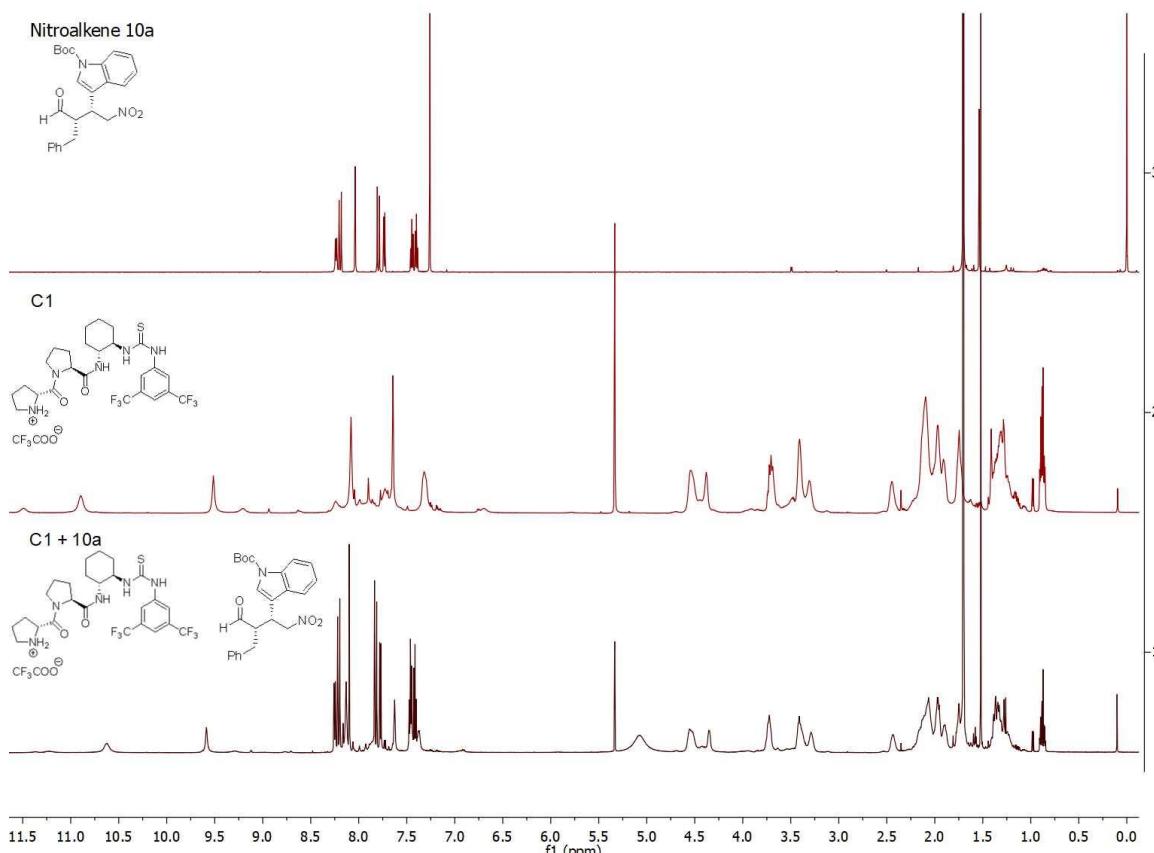


Figure S1. ^1H NMR spectra of **C1** (upper) and **C1** + nitroalkene **10a** (lower) in CD_2Cl_2 .

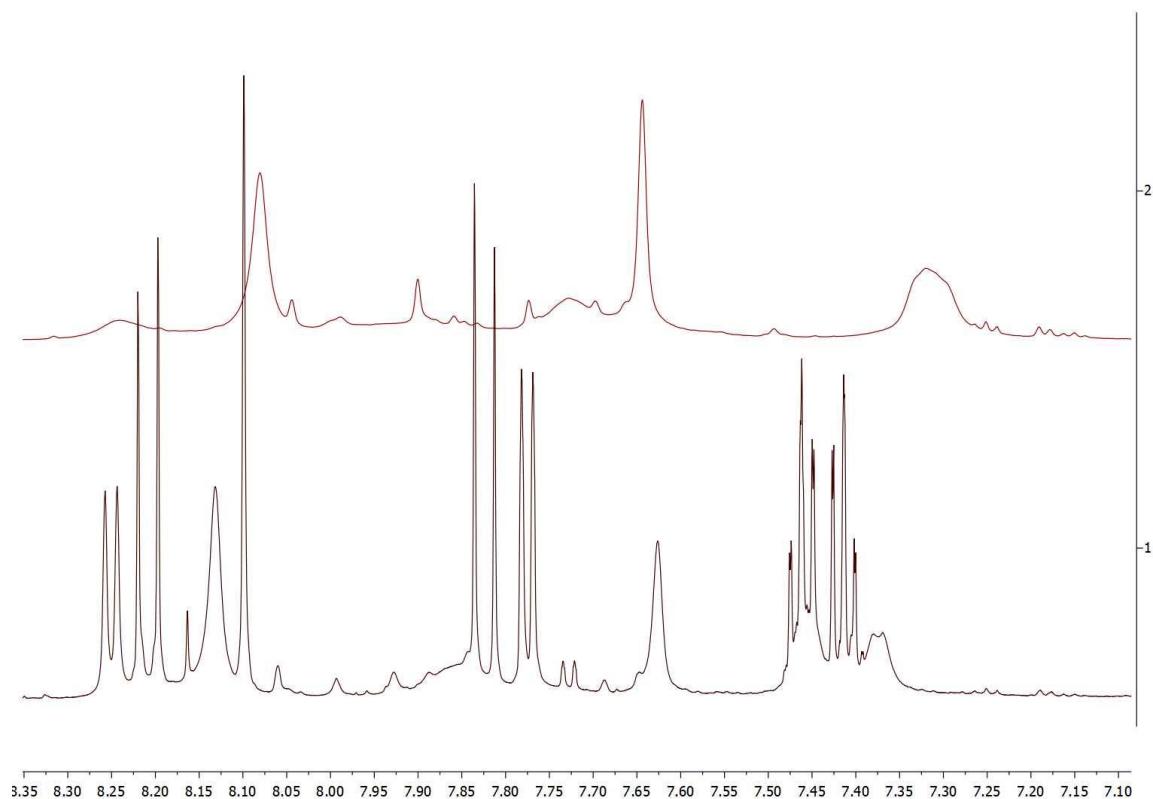


Figure S2. Zoomed in aromatic region.

In our previous studies,¹ we observed a rapid sharpening of signals of a thiourea catalyst upon addition of benzoic acid. We assigned this observation to the dissociation of thiourea dimers to monomers.² In the case of peptide catalyst **C1**, sharpening of signals was not observed (if not even more broadening). Hence, we conclude, that the catalyst does not form dimers. This observation can be attributed to steric inaccessibility of the thiourea fragment due to the adjacent peptide turn. However, a shift of aromatic signals might indicate activation of the thiourea by benzoic acid.

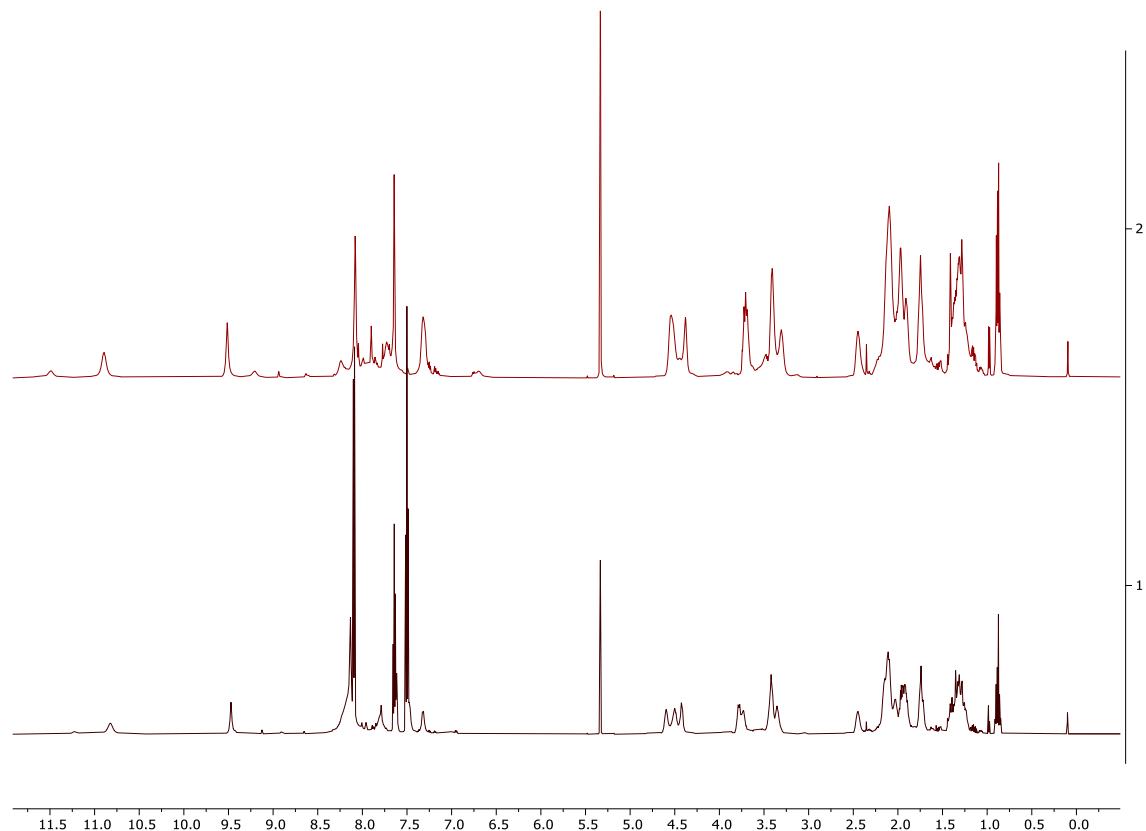


Figure S3. ¹H NMR spectra of **C1** (upper) and **C1** + benzoic acid (lower) in CD₂Cl₂.

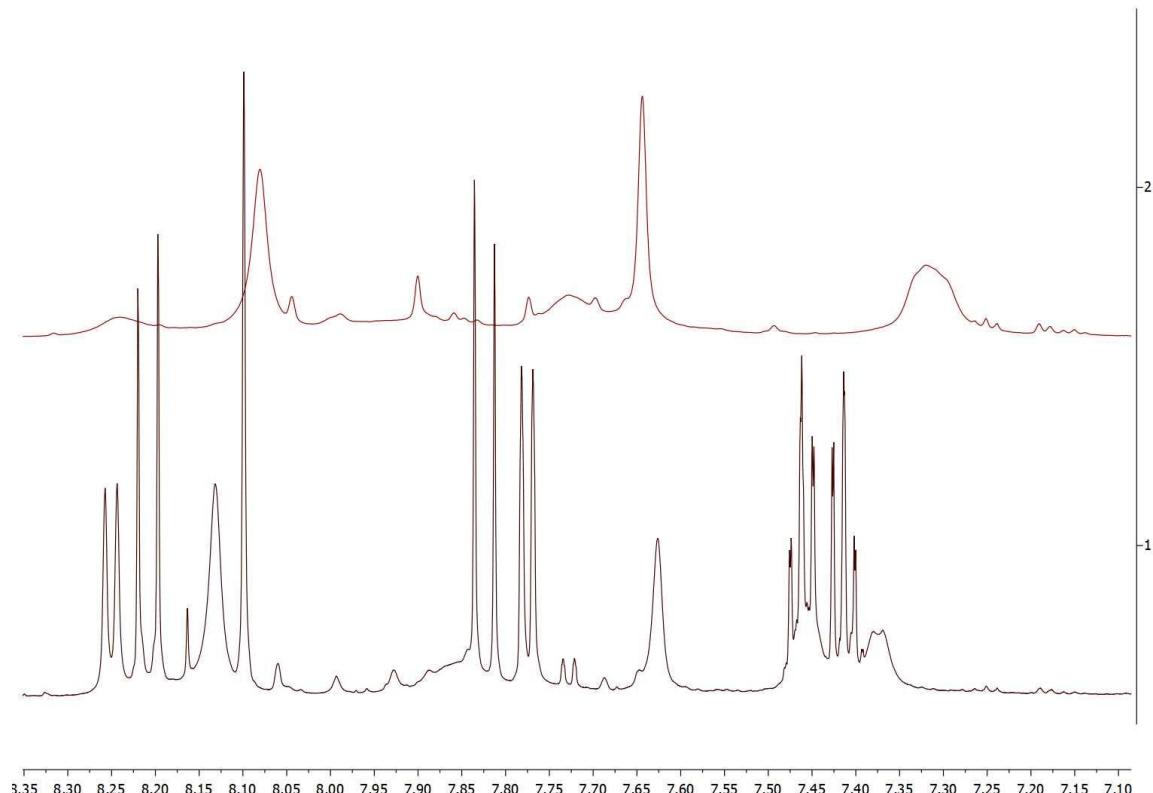
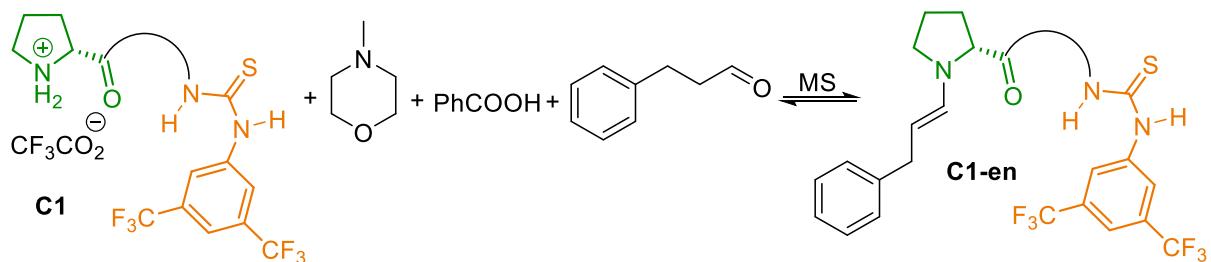


Figure S4. Zoomed in aromatic region.

Next, we attempted to detect the enamine intermediate. Molecular sieves were added to the NMR tube to shift the reaction balance towards the formation of **C1-en**. A doublet at 5.99 ppm with $J = 13.2$ Hz was detected. Wennemers reported a similar signal for a peptide-catalyst-derived enamine (5.19 ppm, $J = 13.9$ Hz).³ After some time, signals of the likely aldol self-condensation product were observed.



Scheme S2.

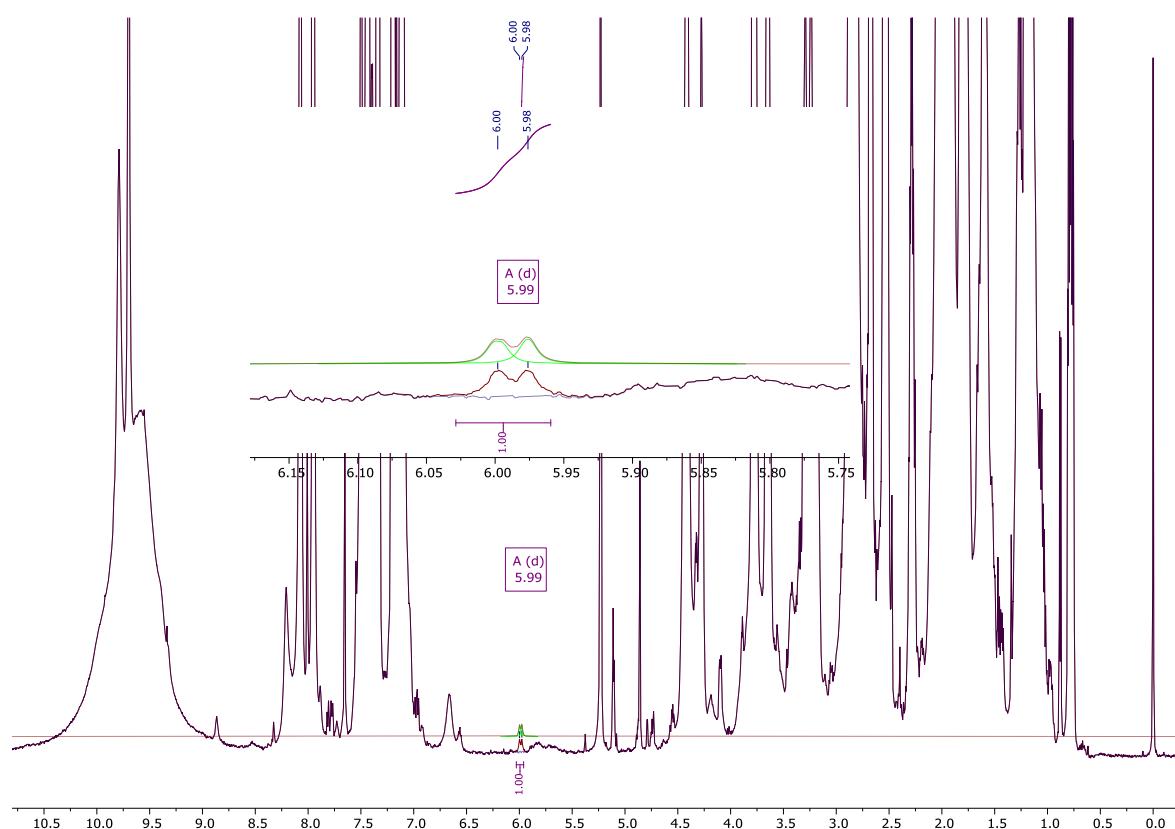


Figure S5. ^1H NMR spectra of **C1** + *N*-methylmorpholine + benzoic acid + 3-phenylpropanal + MS in CD_2Cl_2 .

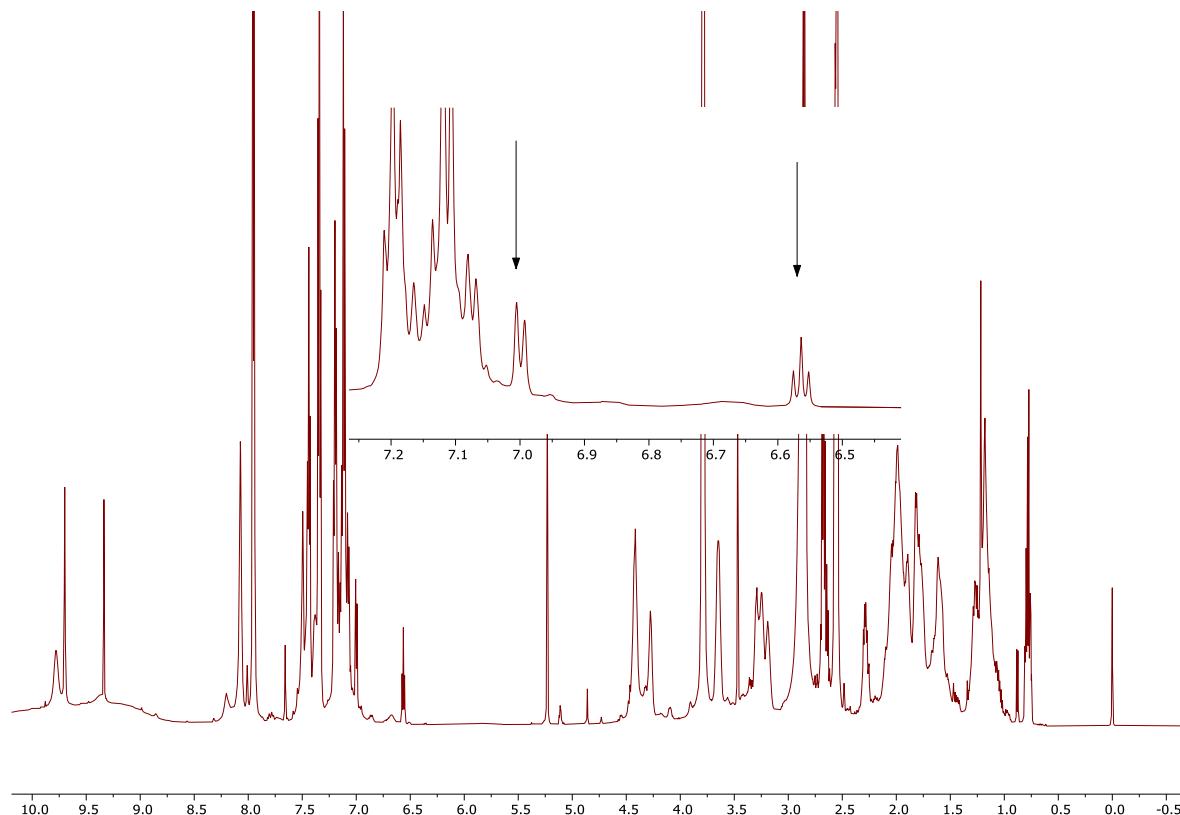
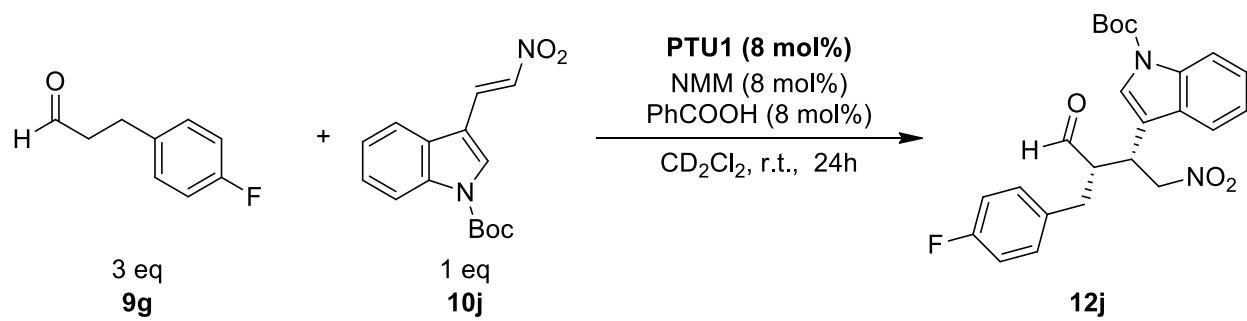


Figure S6. ^1H NMR spectra of **C1** + *N*-methylmorpholine + benzoic acid + 3-phenylpropanale + MS in CD_2Cl_2 after 22h.

The reaction progress was monitored by ^{19}F NMR



Scheme S3.

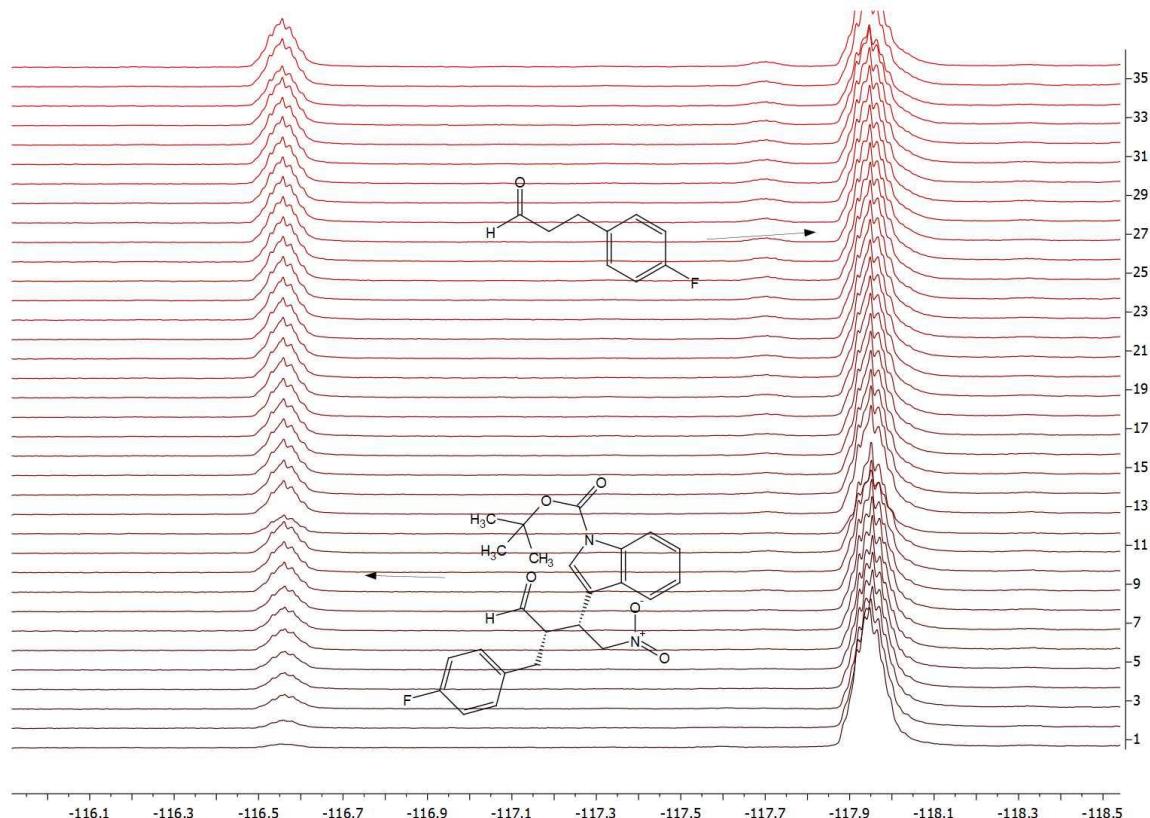


Figure S7.

Selected ^{19}F NMR spectra from monitoring of addition of **9g** to **10j**. Spectra were recorded every 30 minutes over 24 h. Relative concentration of the product was determined through integration compared with starting aldehyde.

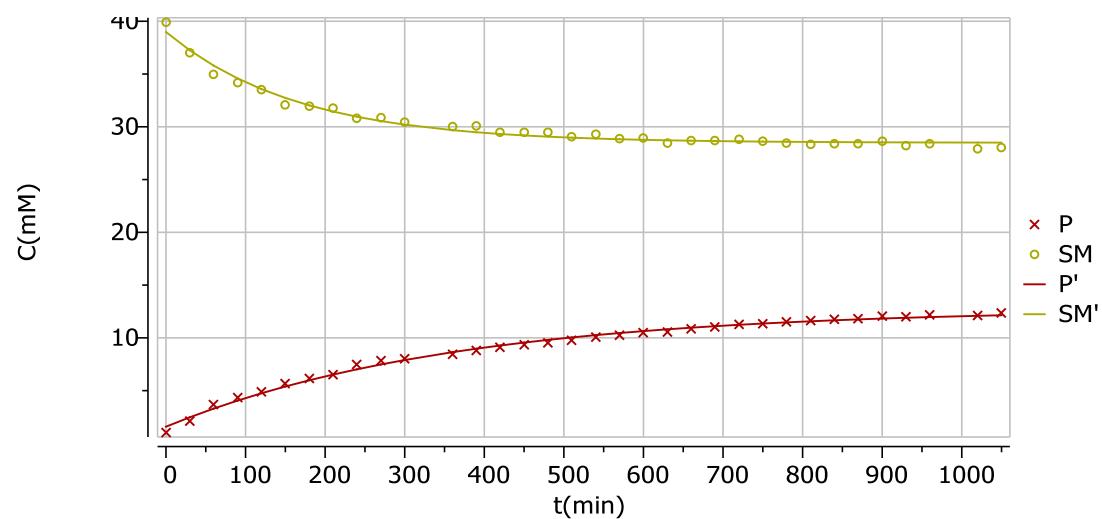


Figure S8. Reaction profile of conversion of aldehyde to product.

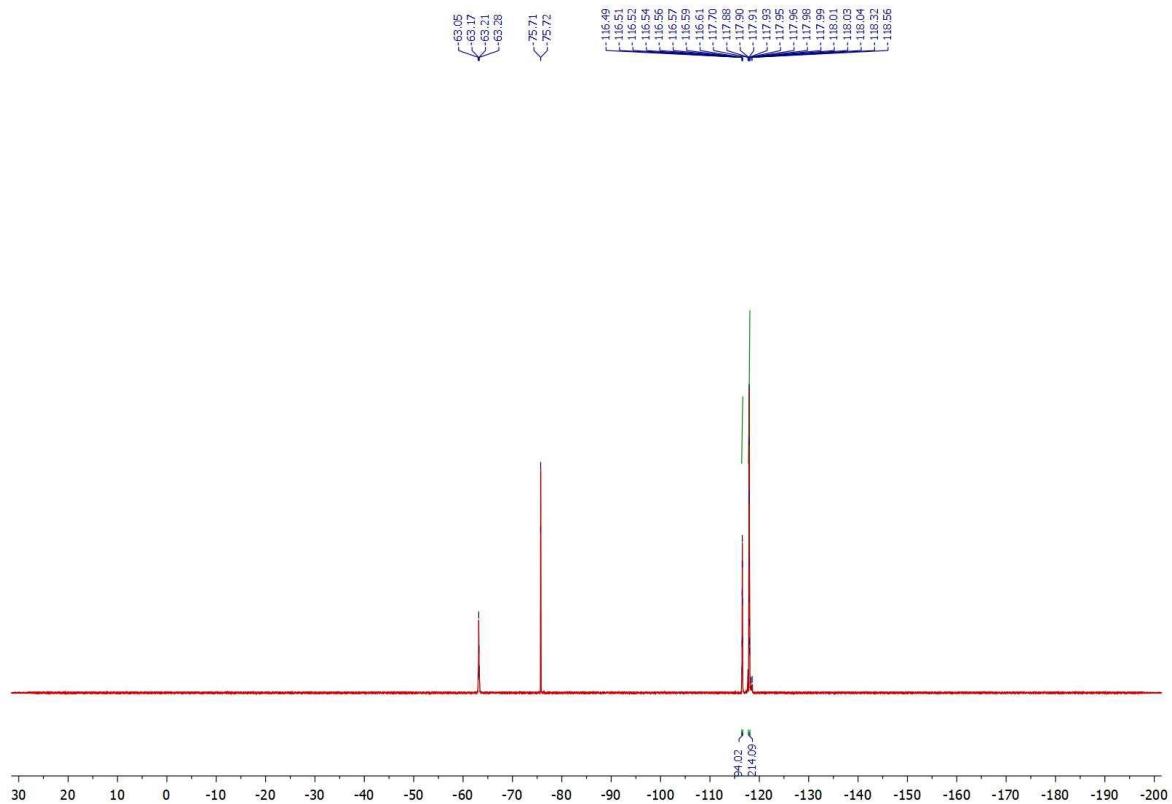


Figure S9. ^{19}F spectra at the end of the reaction. Peaks at -63 ppm and -75 ppm belong to **C1**. Small signal at -117.7 ppm can be attributed to the minor diastereomer, signals at -118.3, -118.6 ppm presumably belong to enamine **C1-en** and **C1-im** product before hydrolysis.

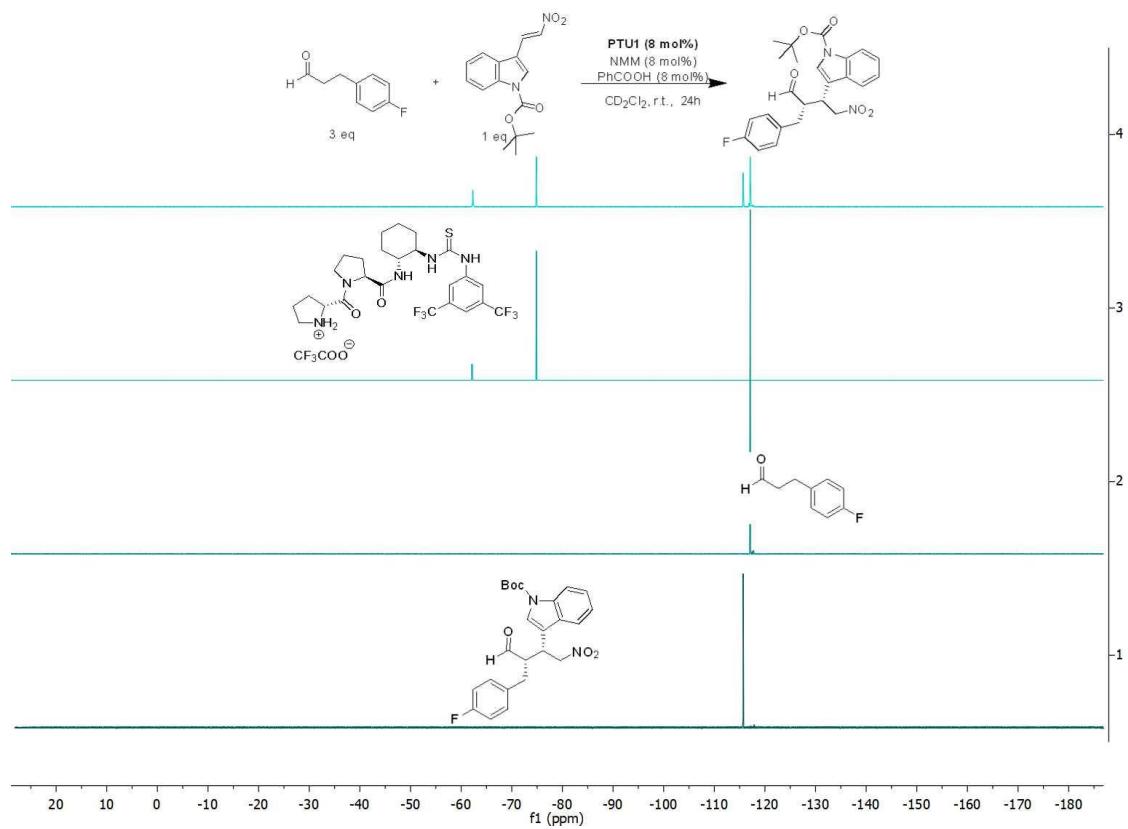
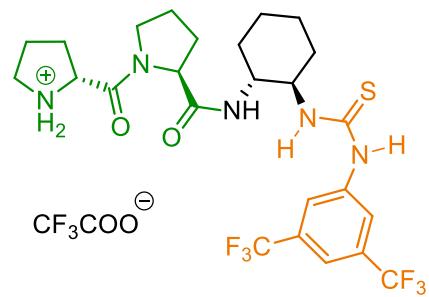


Figure S10.

DMSO titration



Two stock solution of **C1** (5.0 mM) in CD_2Cl_2 and DMSO-d₆ were prepared. Then the DMSO-d₆ solution of **C1** was slowly added into the CD_2Cl_2 solution of **C1** to yield the reported solvent mixtures. The ¹H NMR spectra were referenced to the residual CH_2Cl_2 solvent peak (δ 5.33).

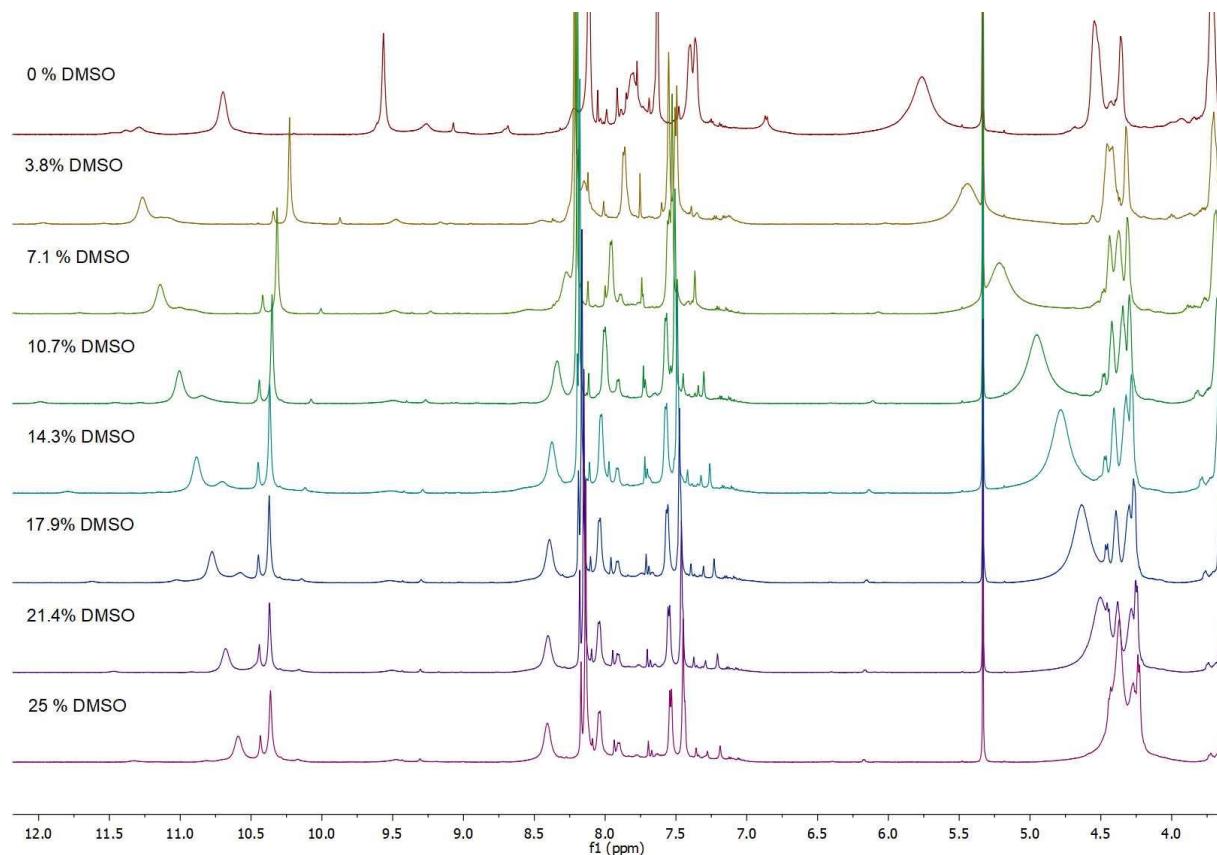


Figure S11.

¹H NMR spectra upon titration of DMSO-d₆ for **C1** (5.0 mM concentration in CD_2Cl_2 (referenced to 5.33 ppm at 25°C)

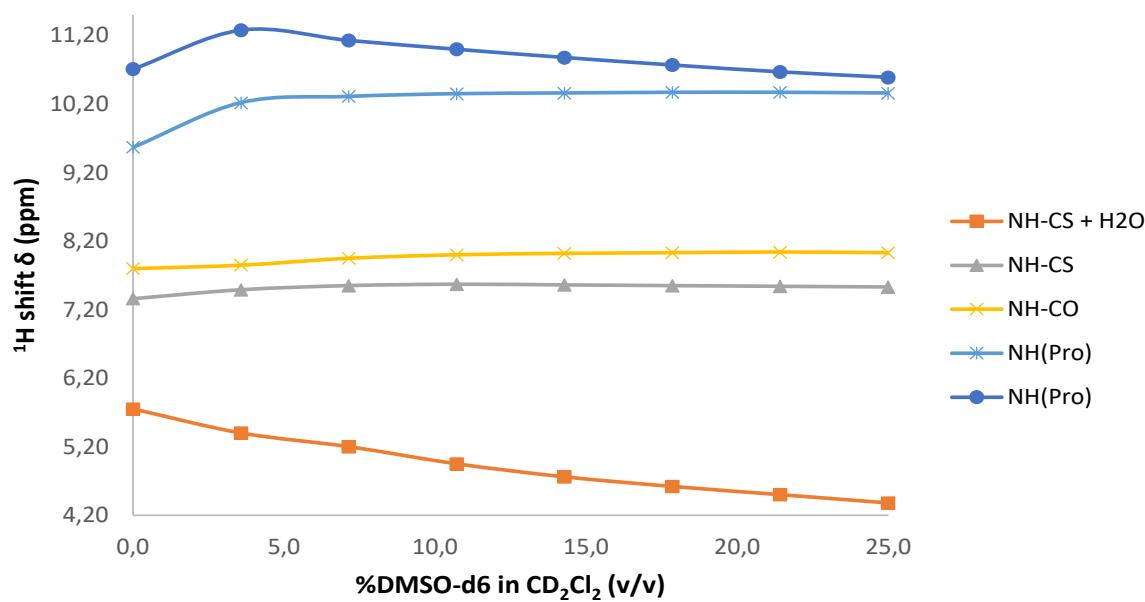


Figure S12. ^1H NMR solvent titration curve to identify solvent exposed and hydrogen-bonded NH groups for **C1** (5.0 mM concentration in CD_2Cl_2 (referenced to 5.33 ppm at 25°C).

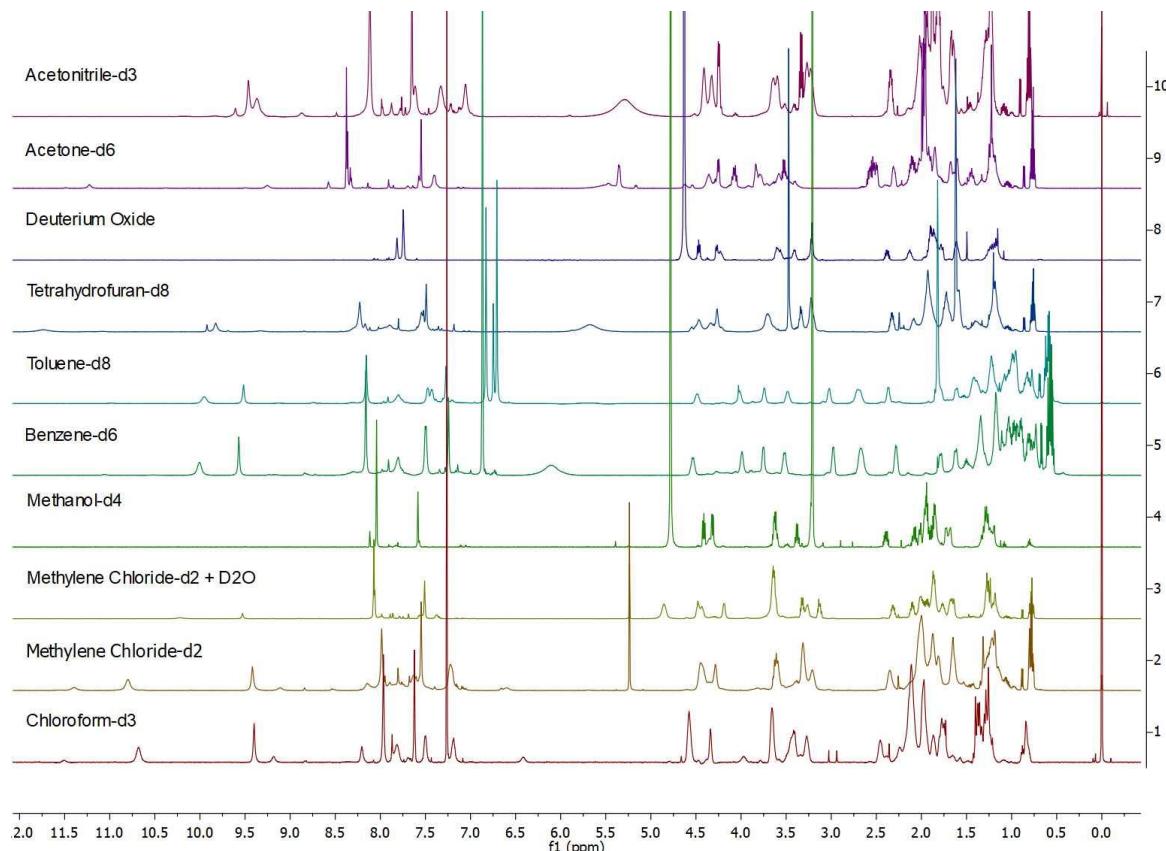


Figure S13. ^1H NMR spectra of **C1** in various NMR solvents.

CD spectroscopy

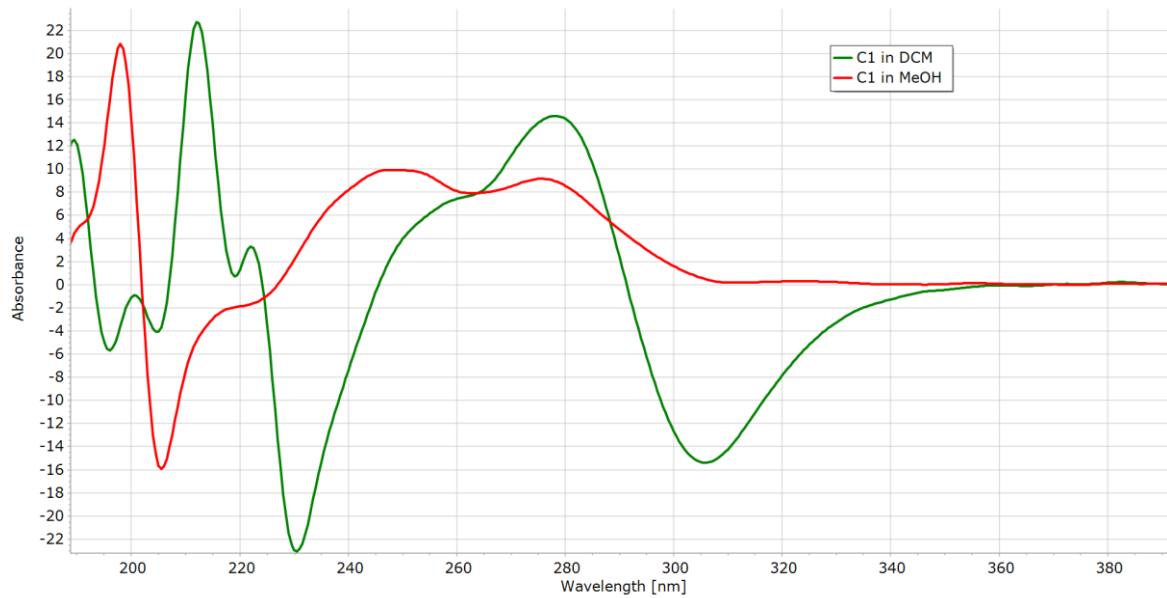


Figure S14. CD spectra of **C1** in MeOH and DCM.

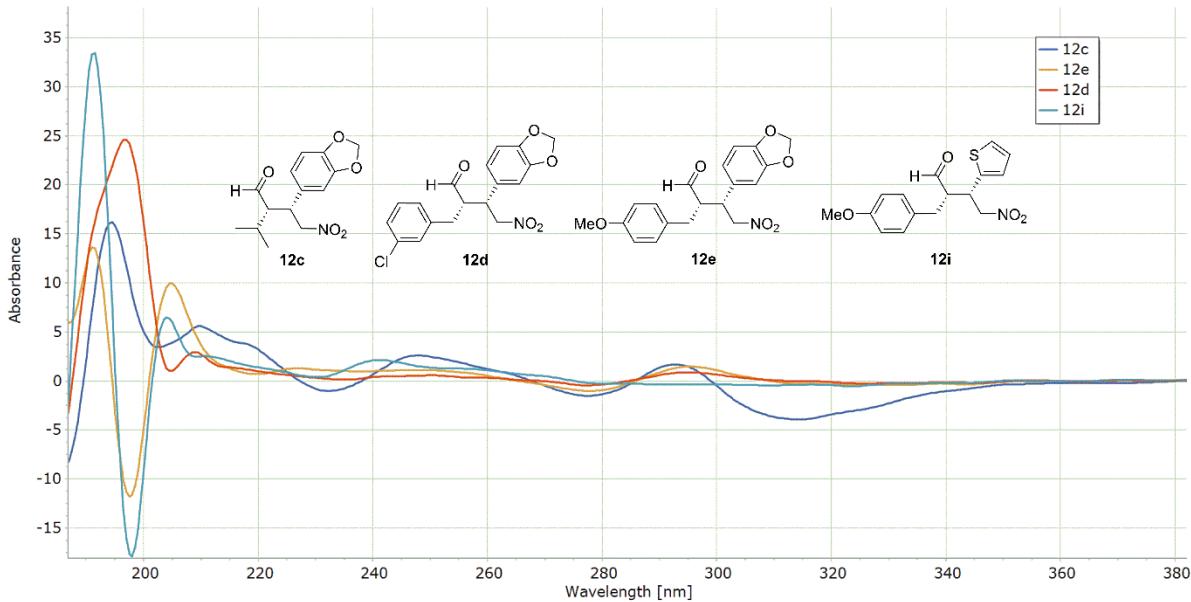
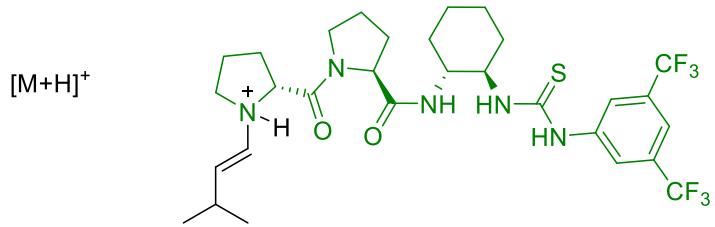


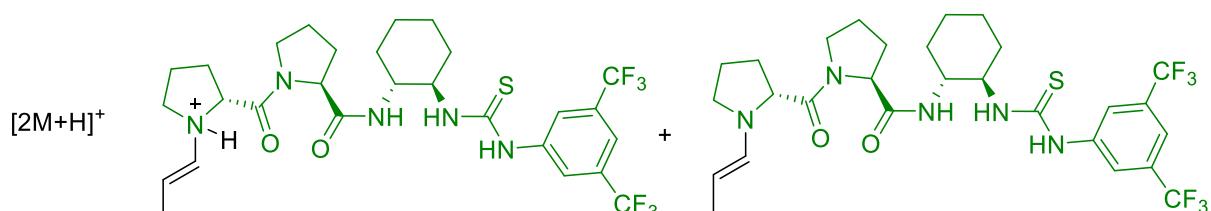
Figure S15. CD spectra of products **12c**, **12d**, **12e**, and **12i** in MeOH.

Enamide detection between C1 and isovaleraldehyde (9d) by HRMS



Chemical Formula: $C_{30}H_{40}F_6N_5O_2S^+$

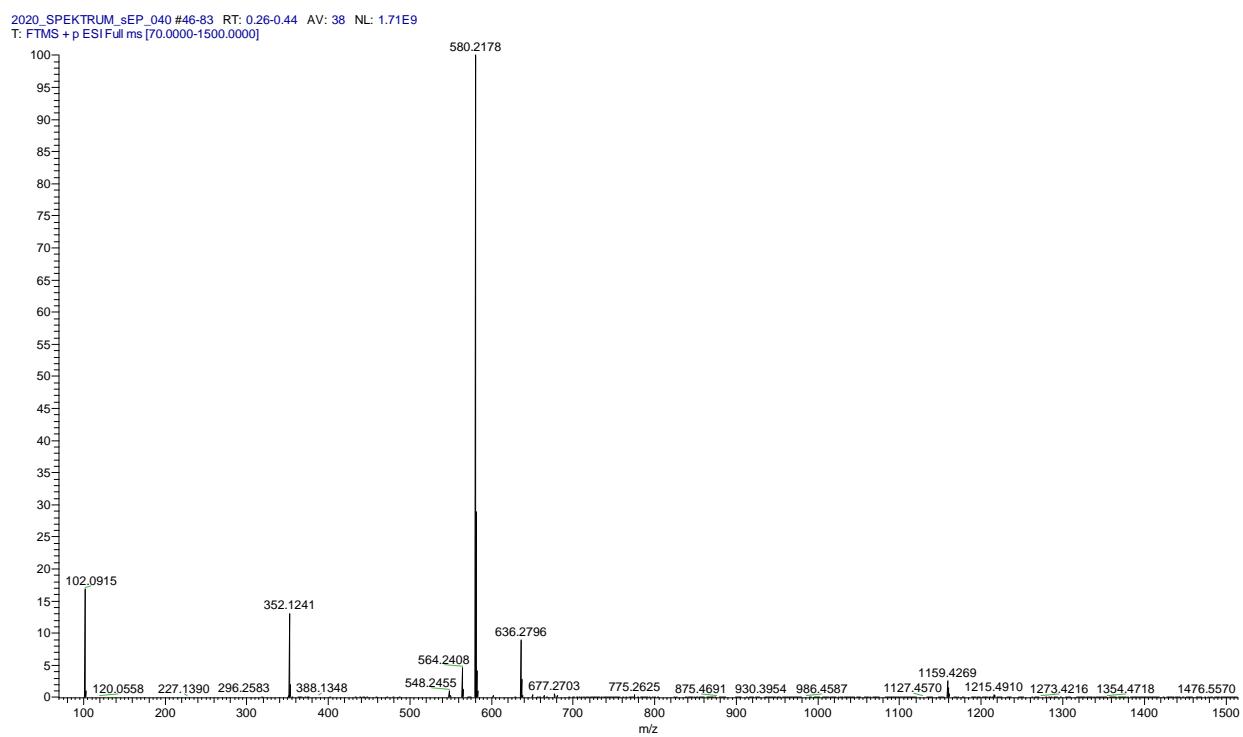
Exact Mass: 648,2801



Chemical Formula: $C_{60}H_{79}F_{12}N_{10}O_4S_2^+$

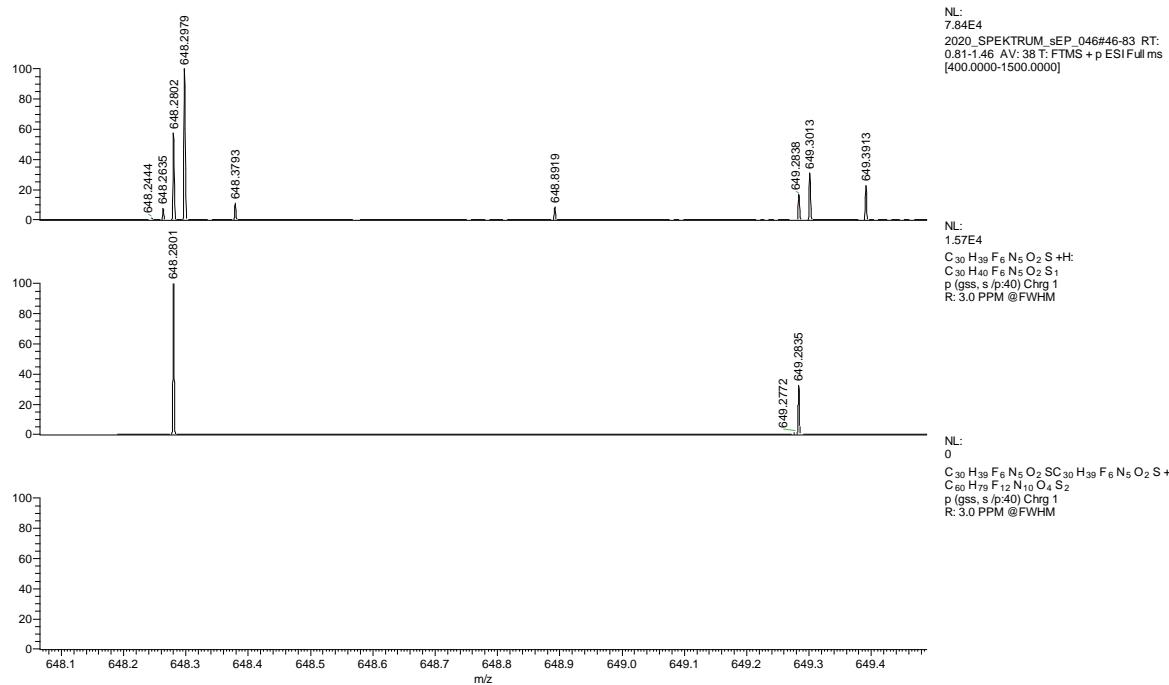
Exact Mass: 1295,5530

Whole spectrum in the range of m/z 70-1500

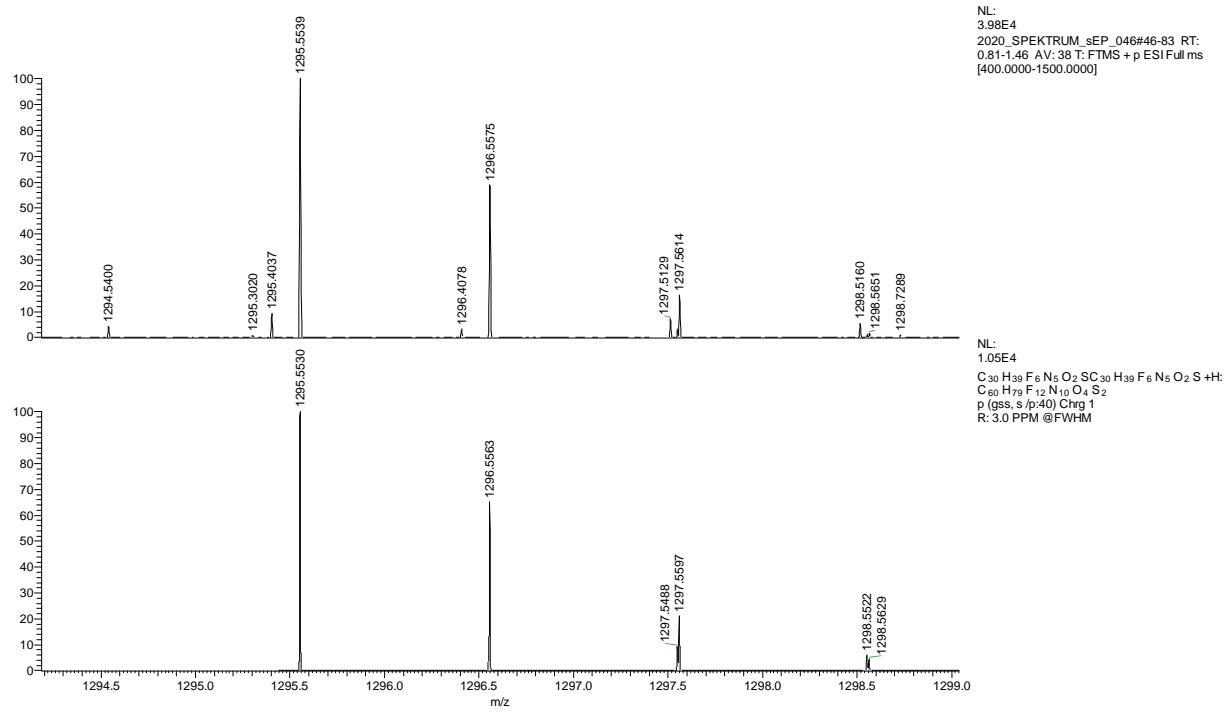


Zoomed measured spectra and theoretical prediction for expected peaks

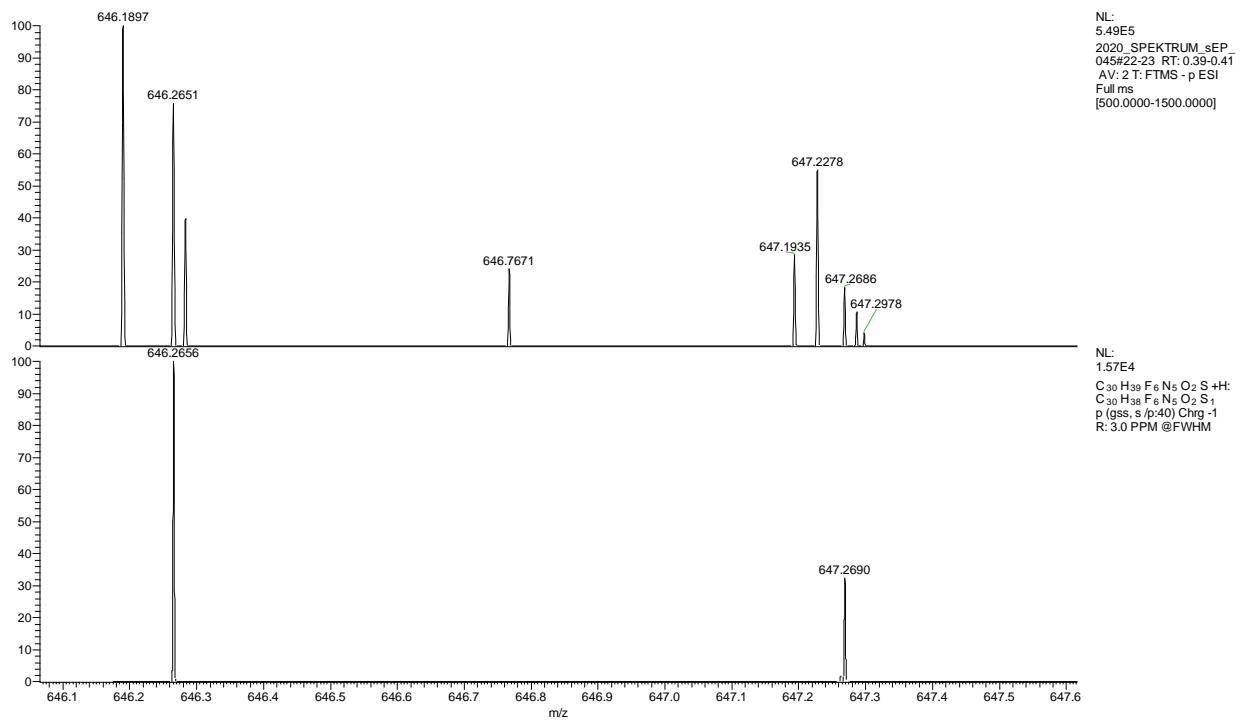
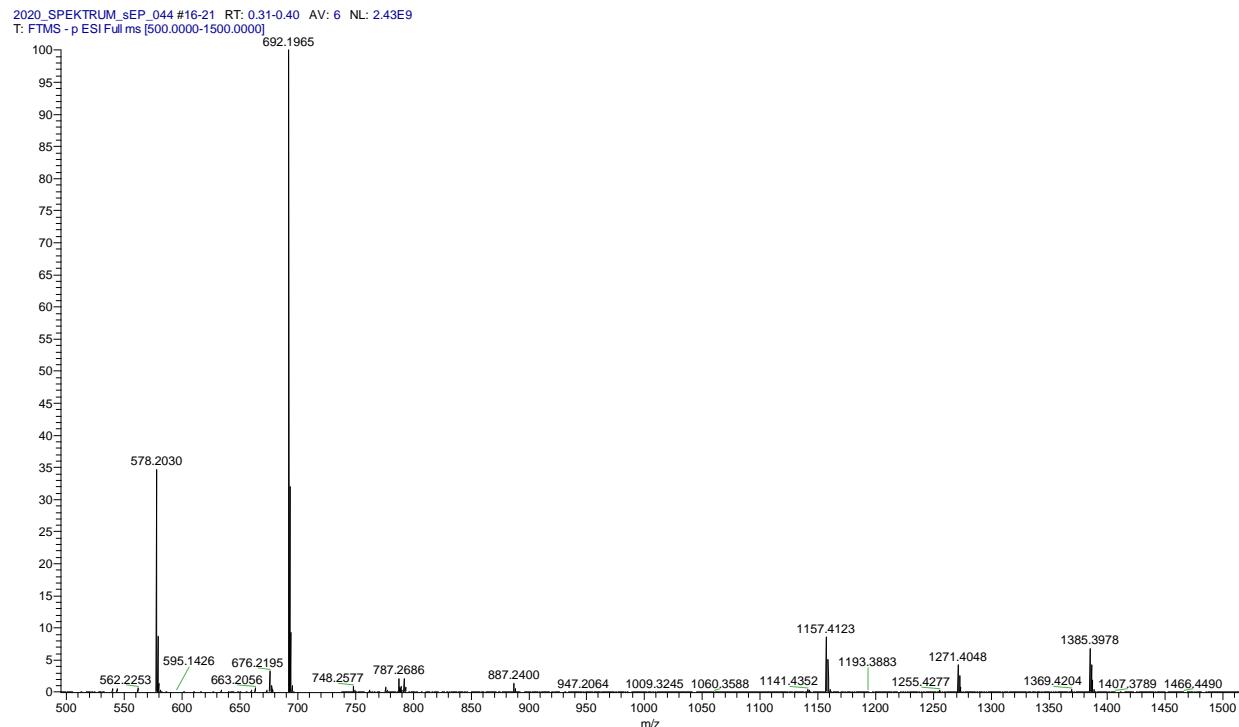
$[M+H]^+$

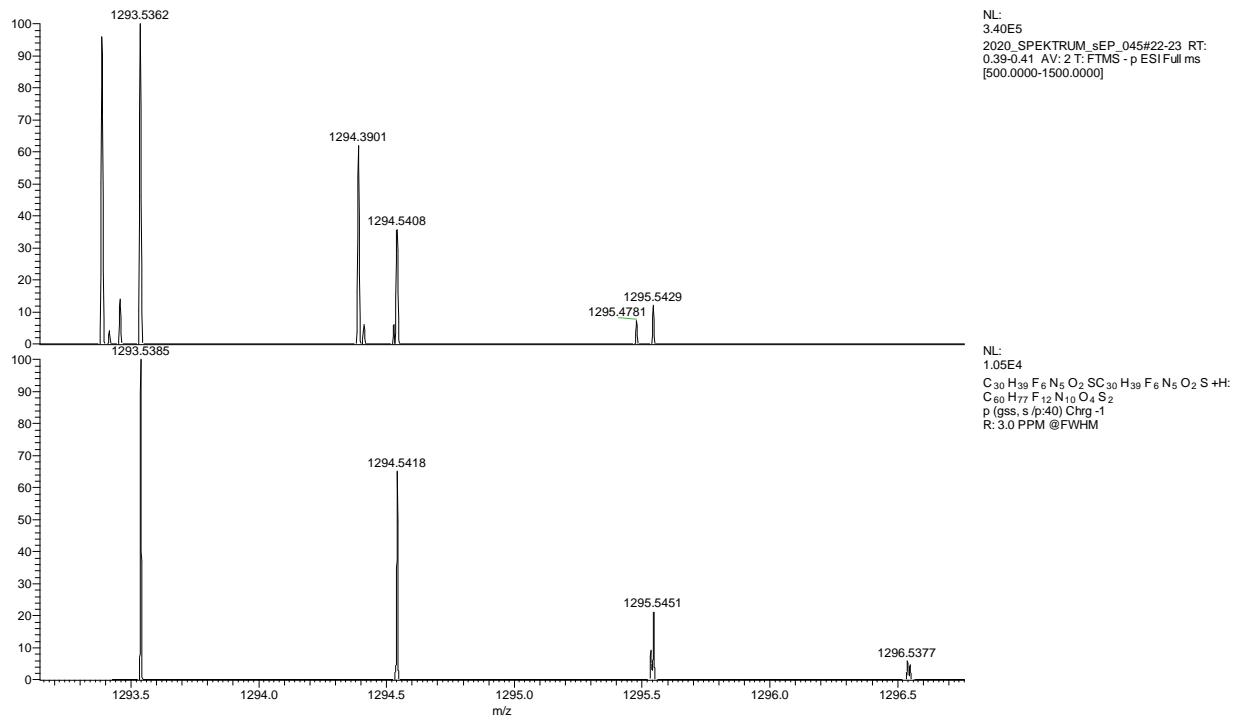


$[2M+H]^+$



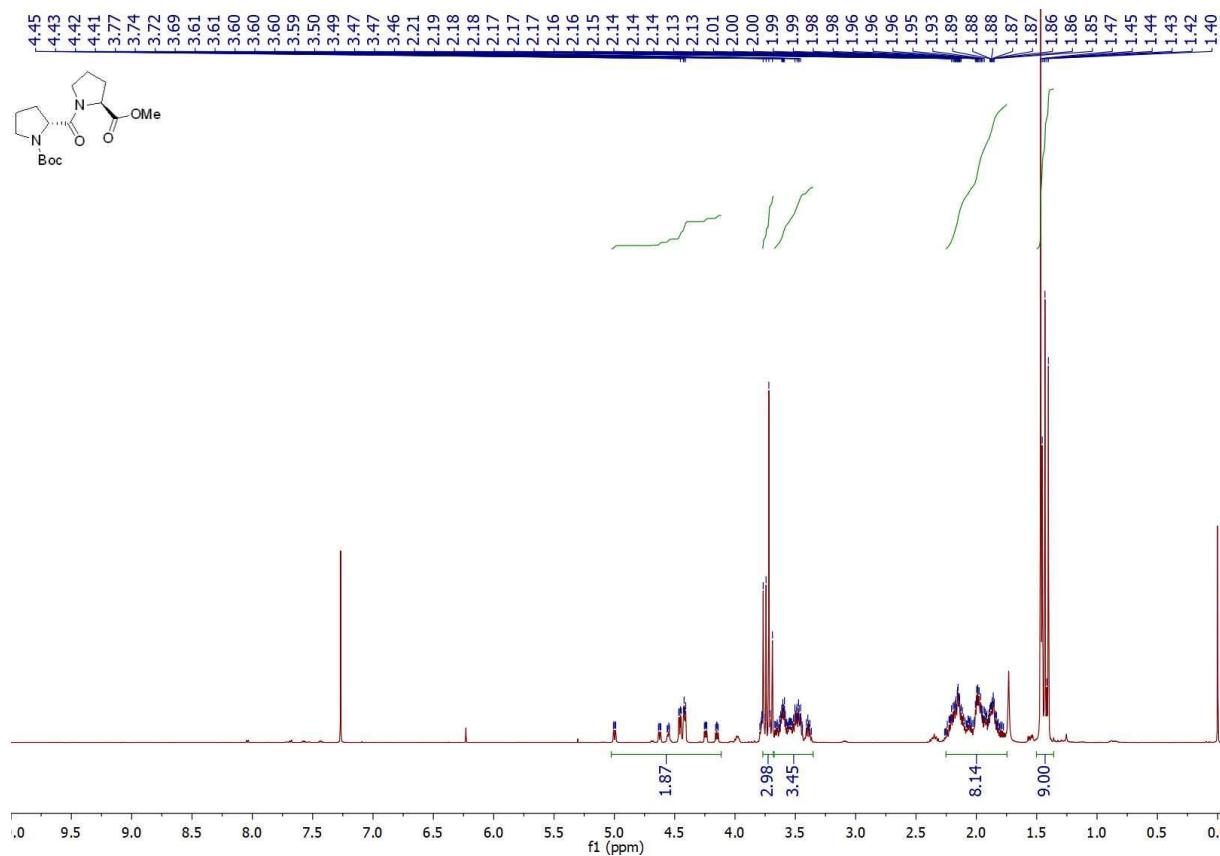
Negative mode



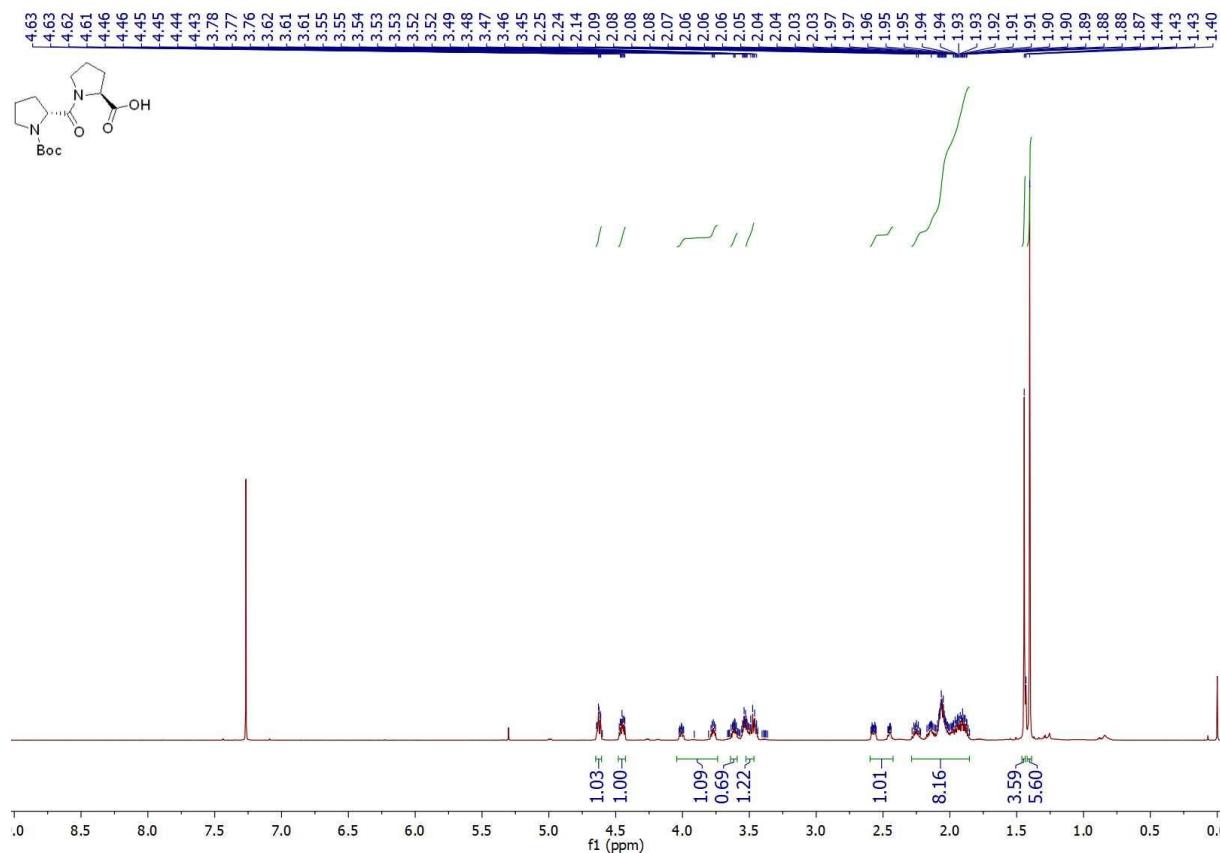


Pictures of NMR spectra

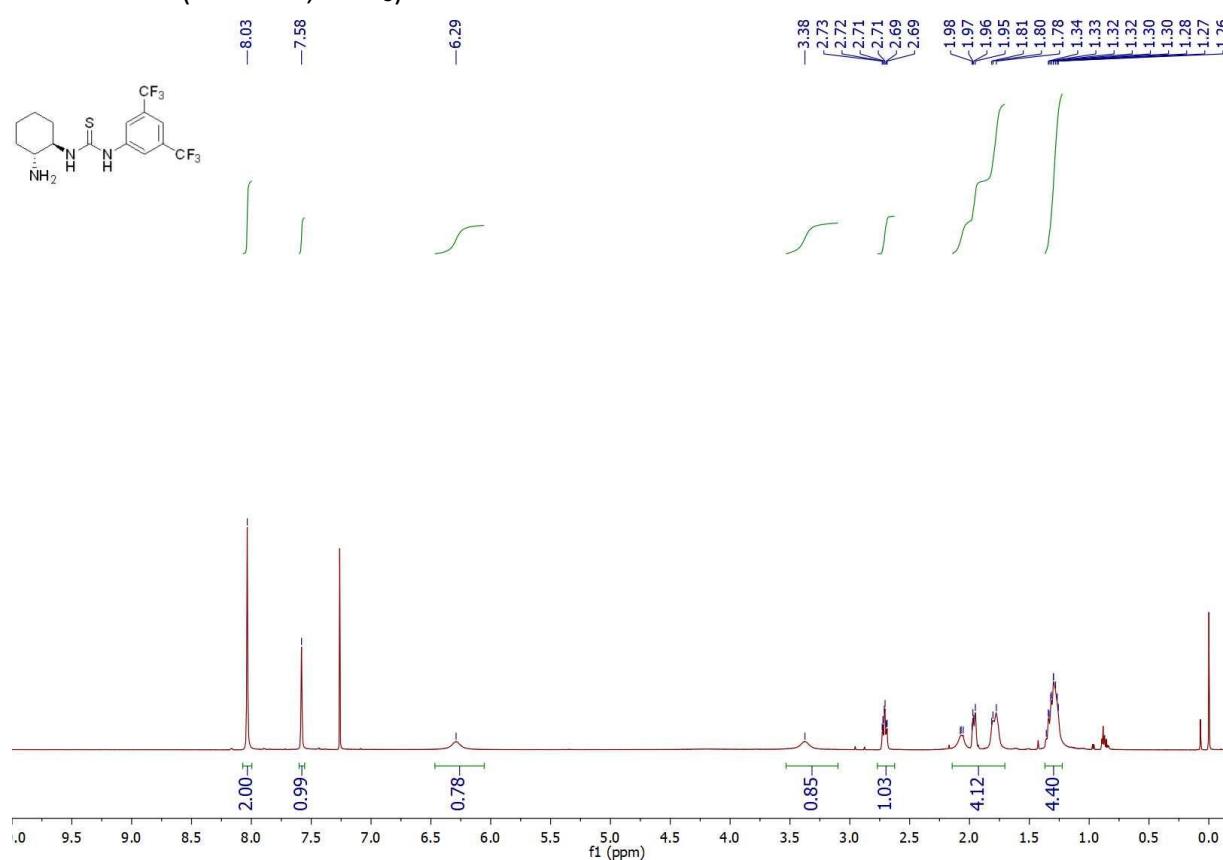
^1H NMR of 6 (600 MHz, CDCl_3)



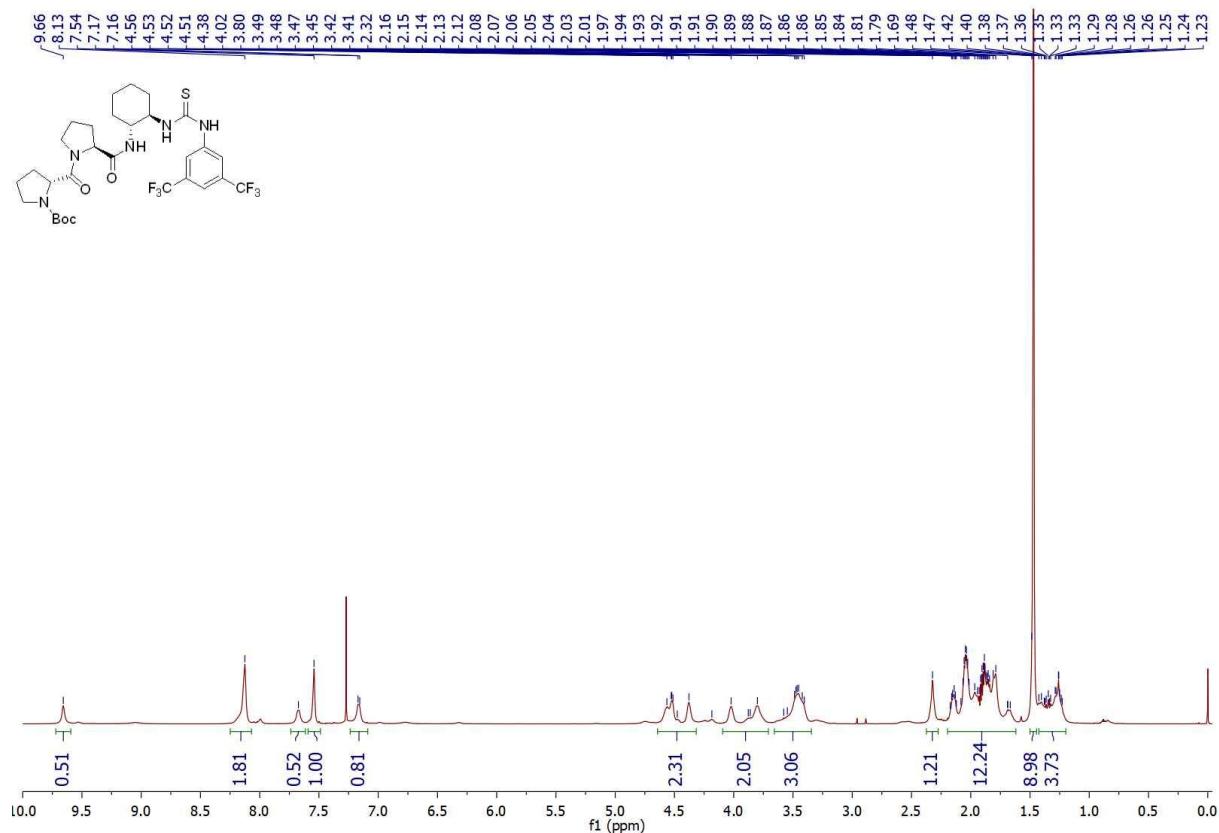
^1H NMR of 7 (600 MHz, CDCl_3)



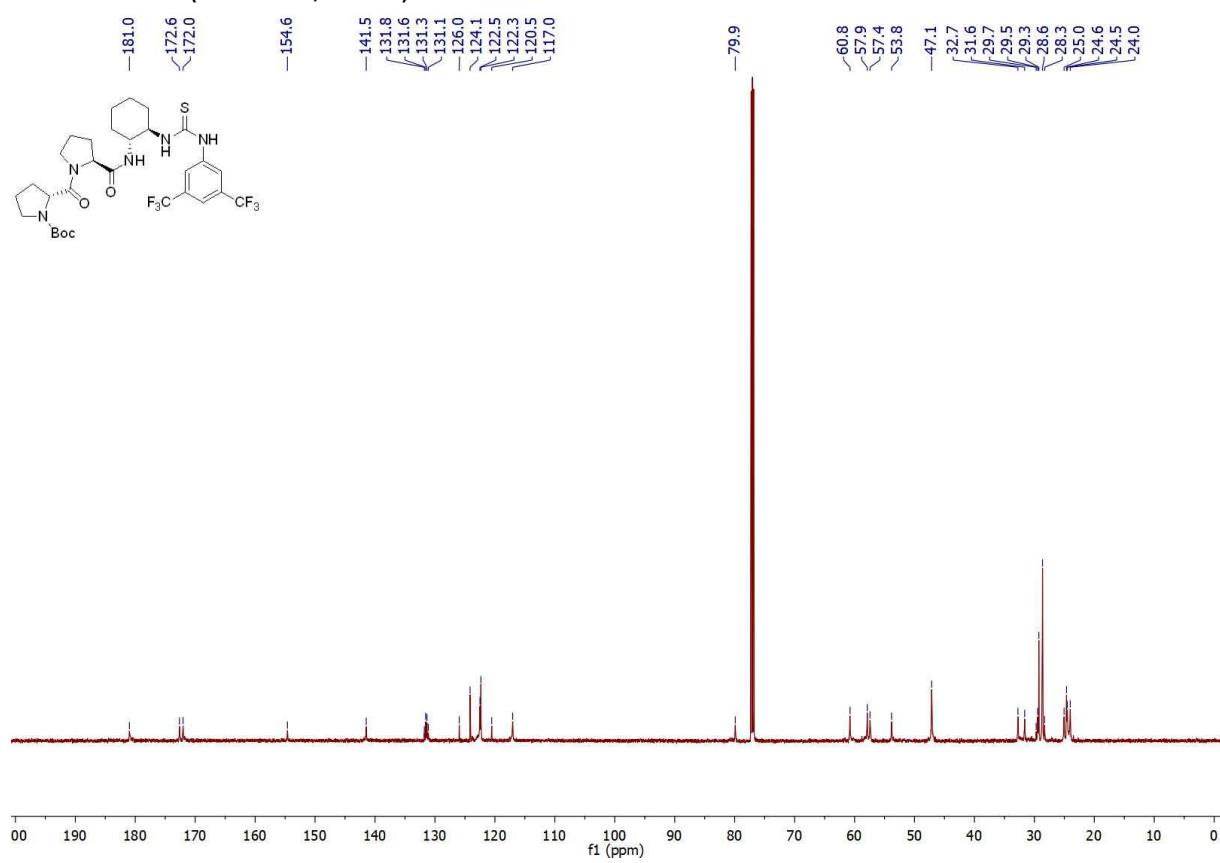
¹H NMR of **3** (600 MHz, CDCl₃)



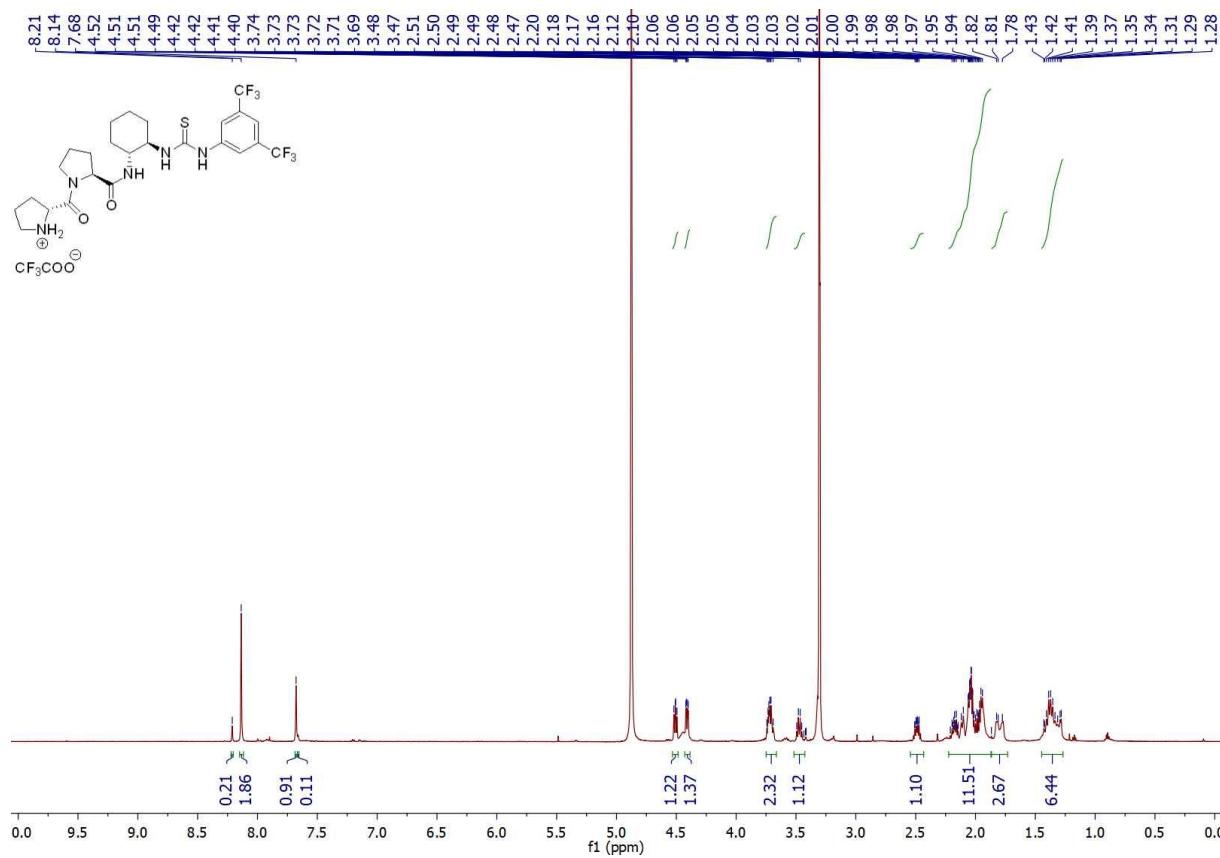
¹H NMR of **8** (600 MHz, CDCl₃)



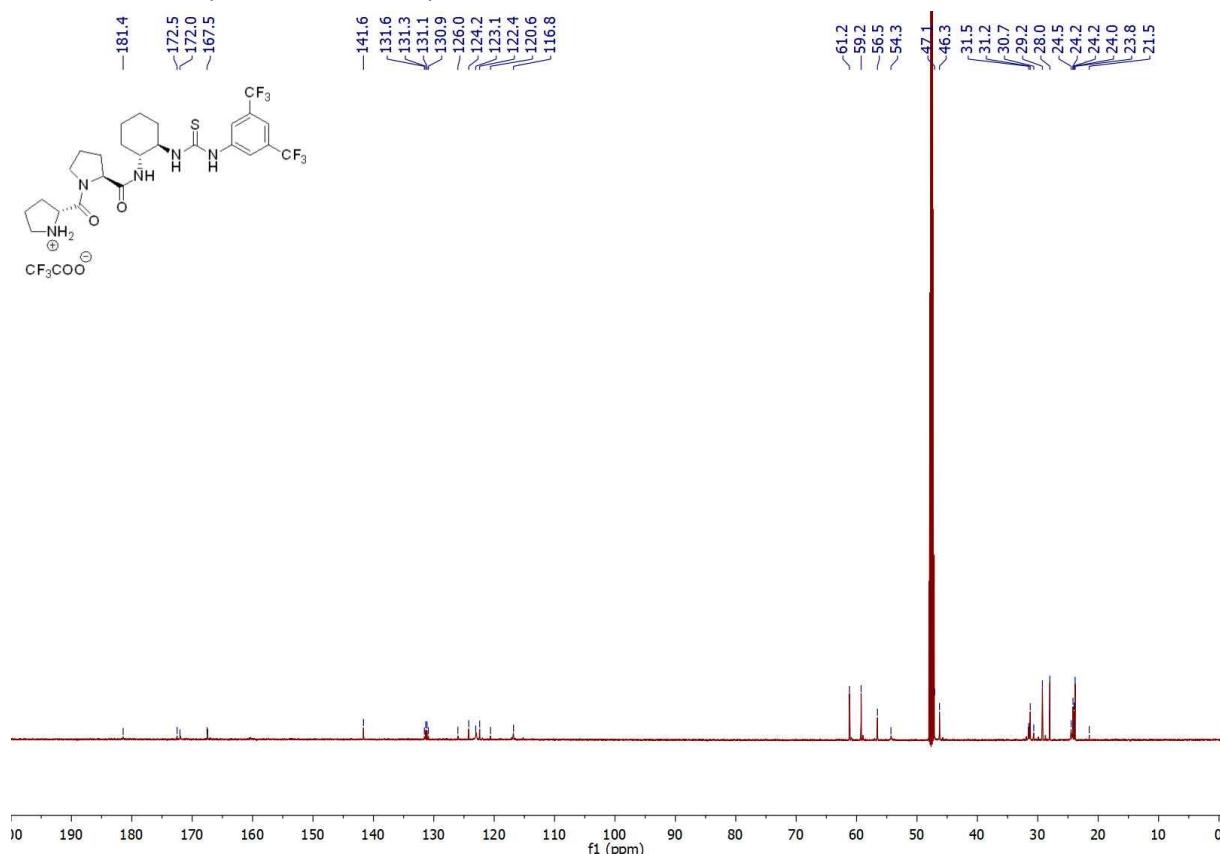
¹³C NMR of **8** (151 MHz, CDCl₃)



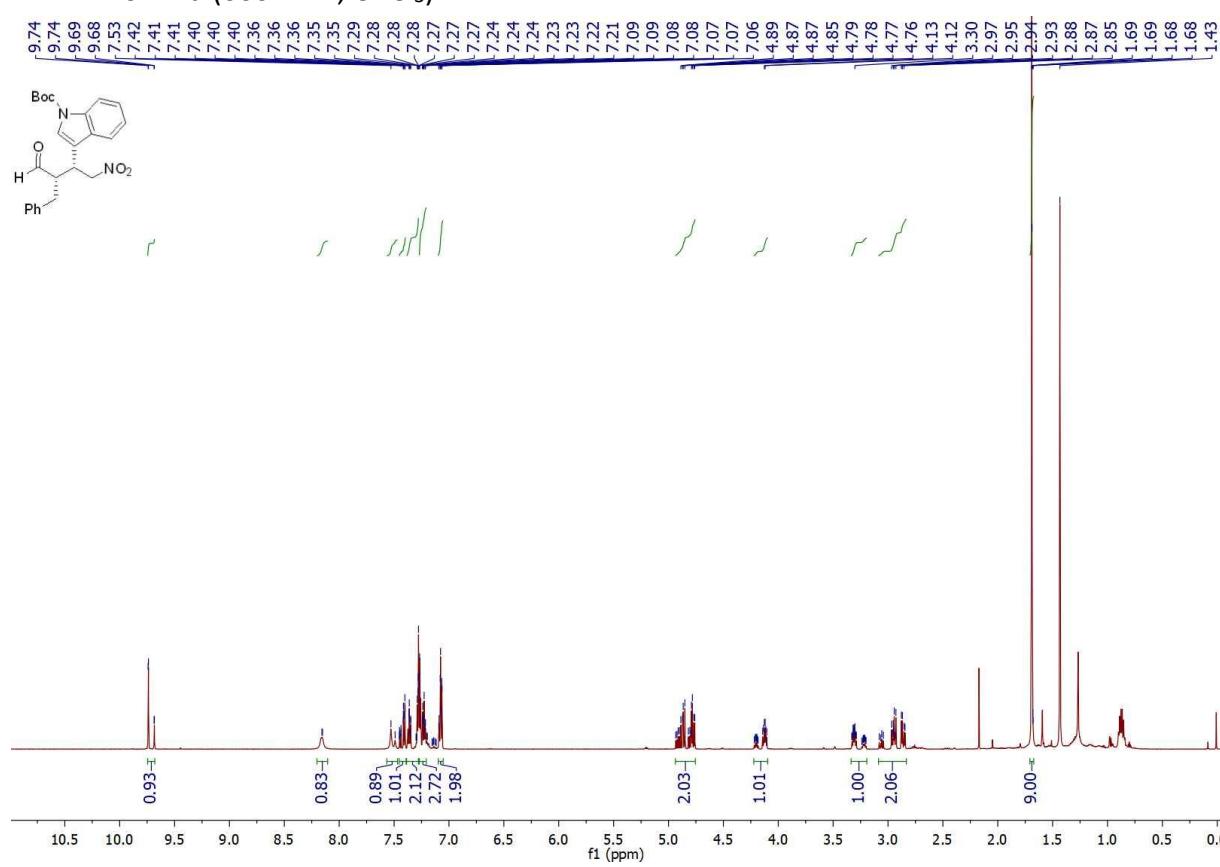
¹H NMR of **C1** (600 MHz, CD₃OD)



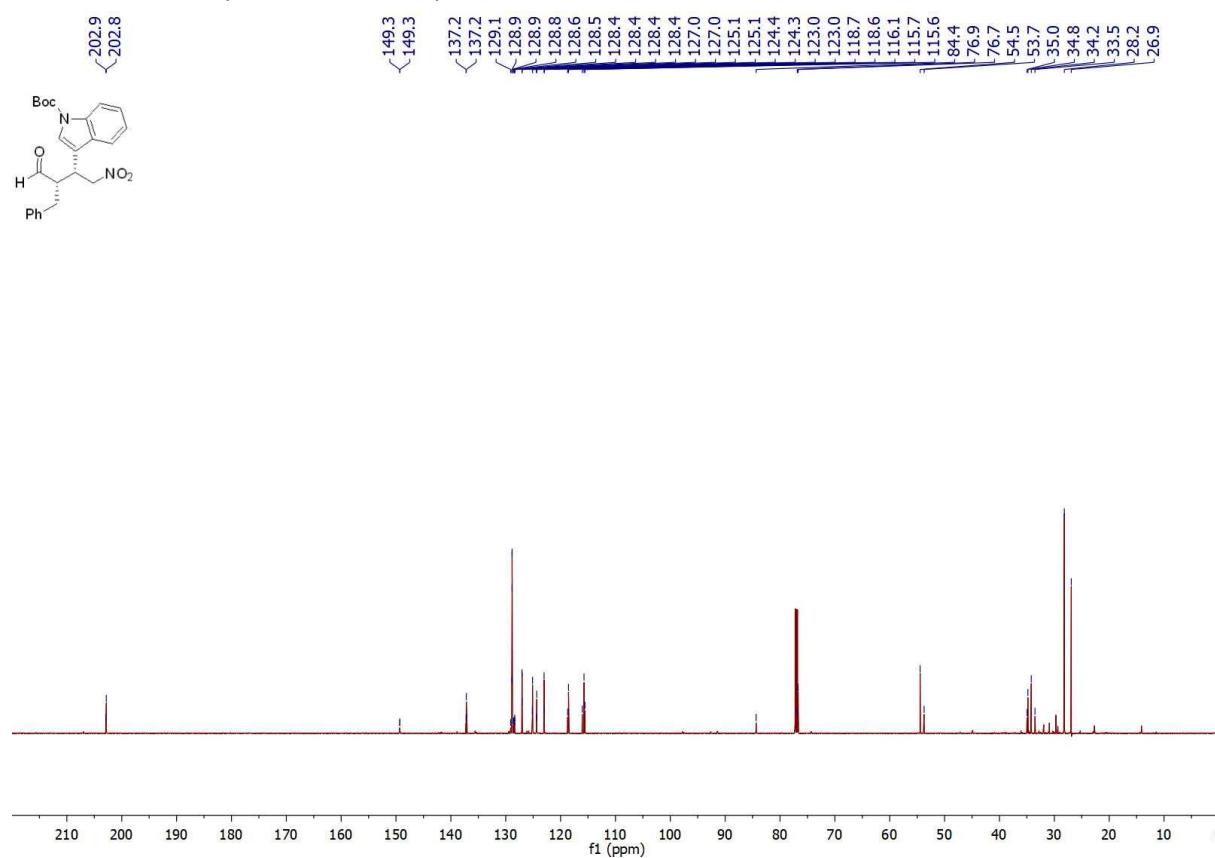
¹³C NMR of **C1** (151MHz, CD₃OD)



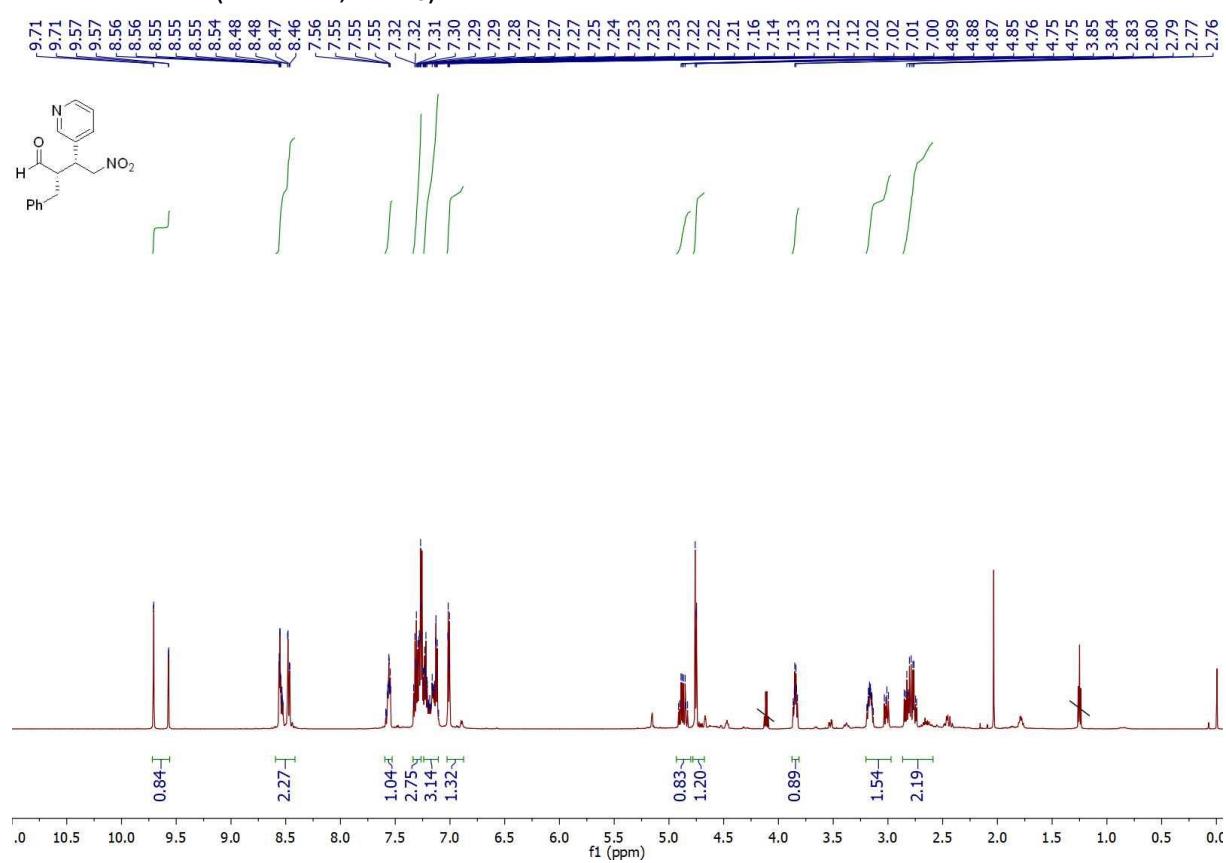
¹H NMR of **11a** (600 MHz, CDCl₃)



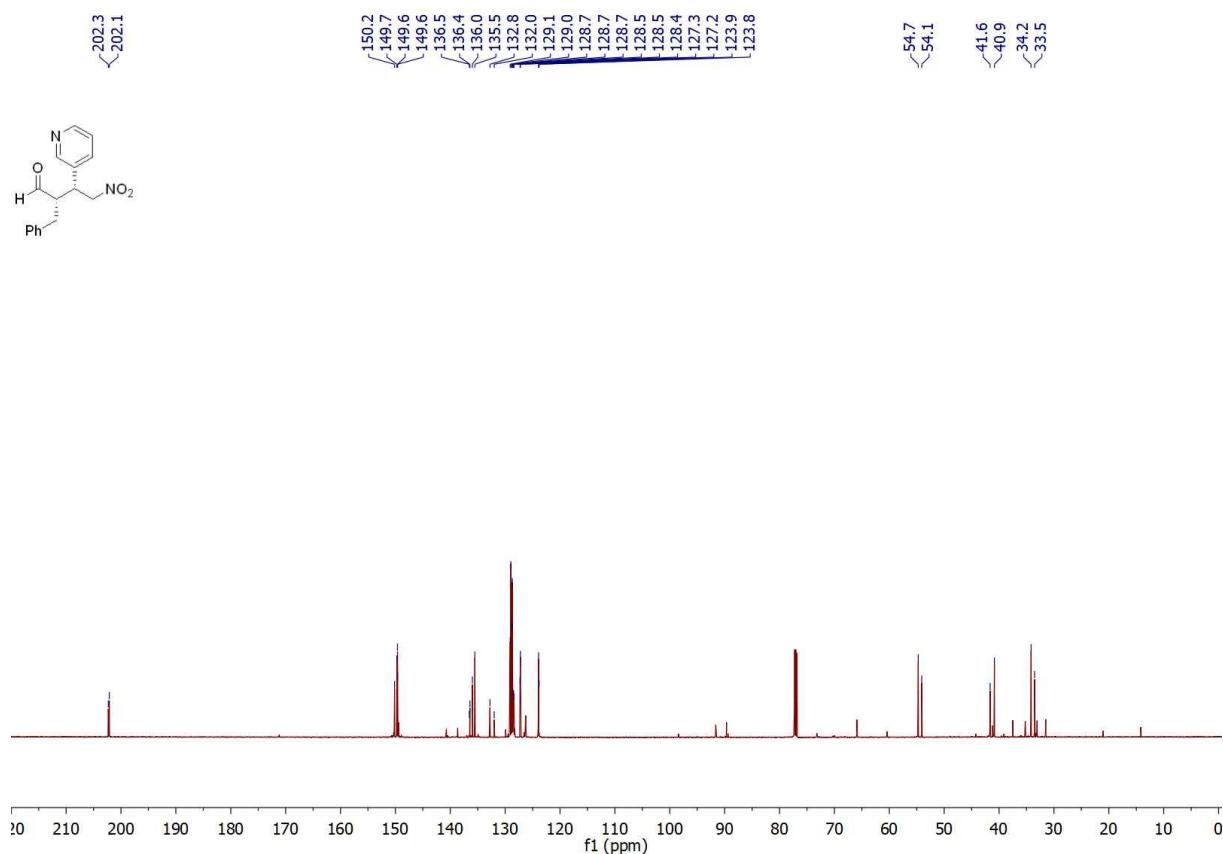
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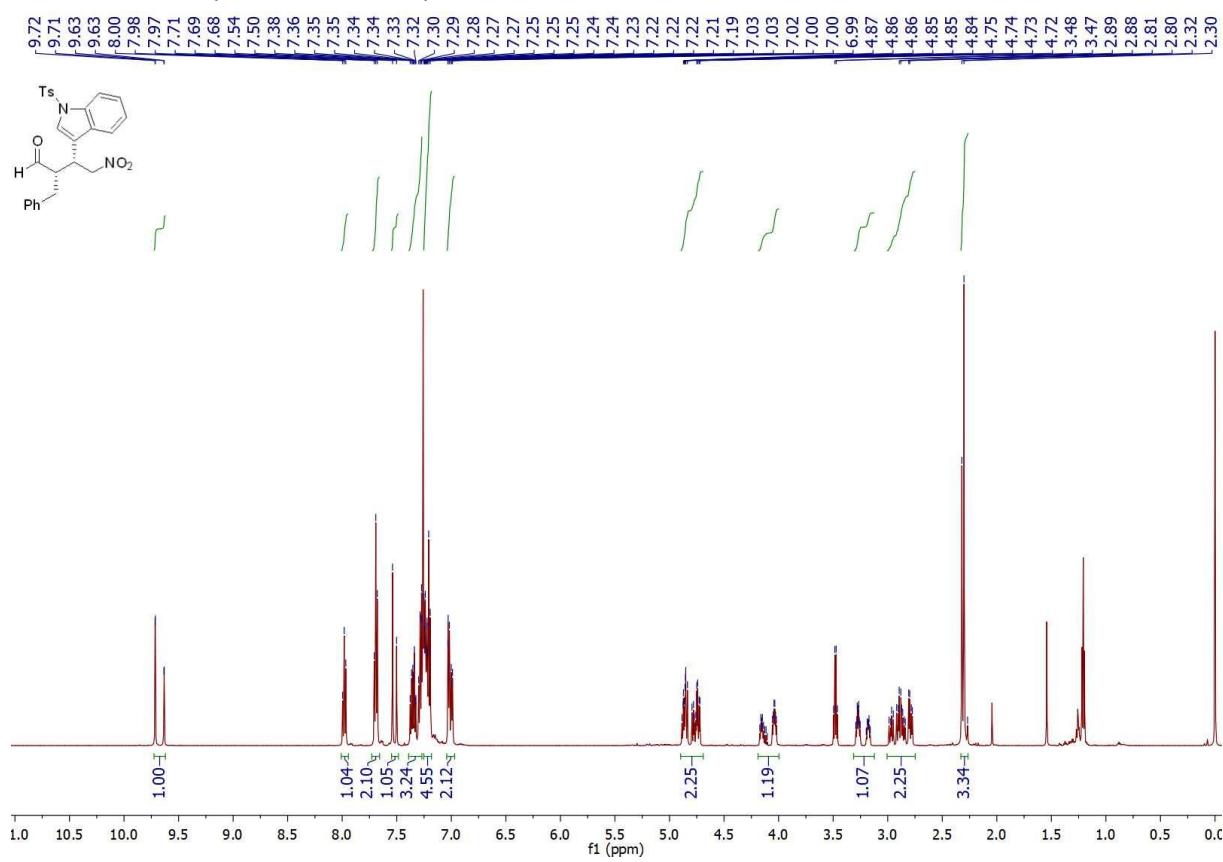
¹H NMR of **11b** (600 MHz, CDCl₃)



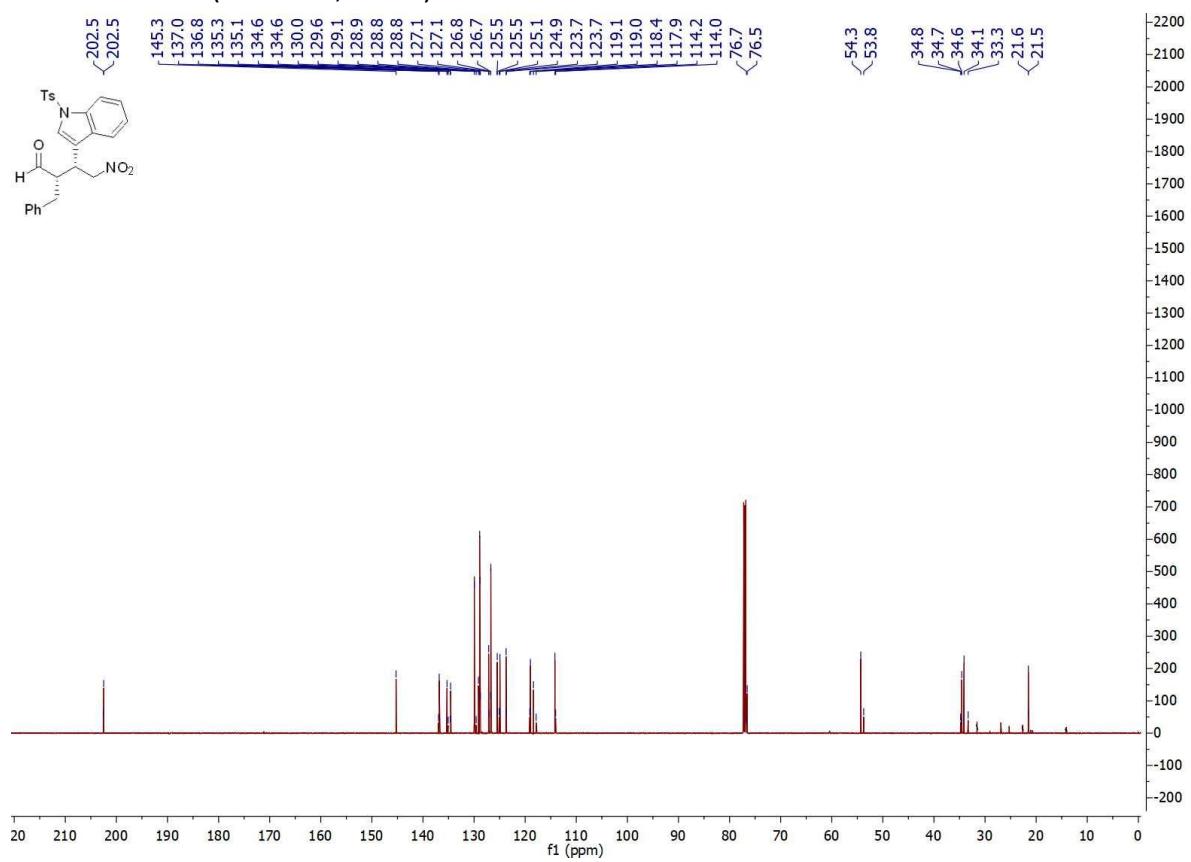
¹³C NMR of **11b** (151 MHz, CDCl₃)



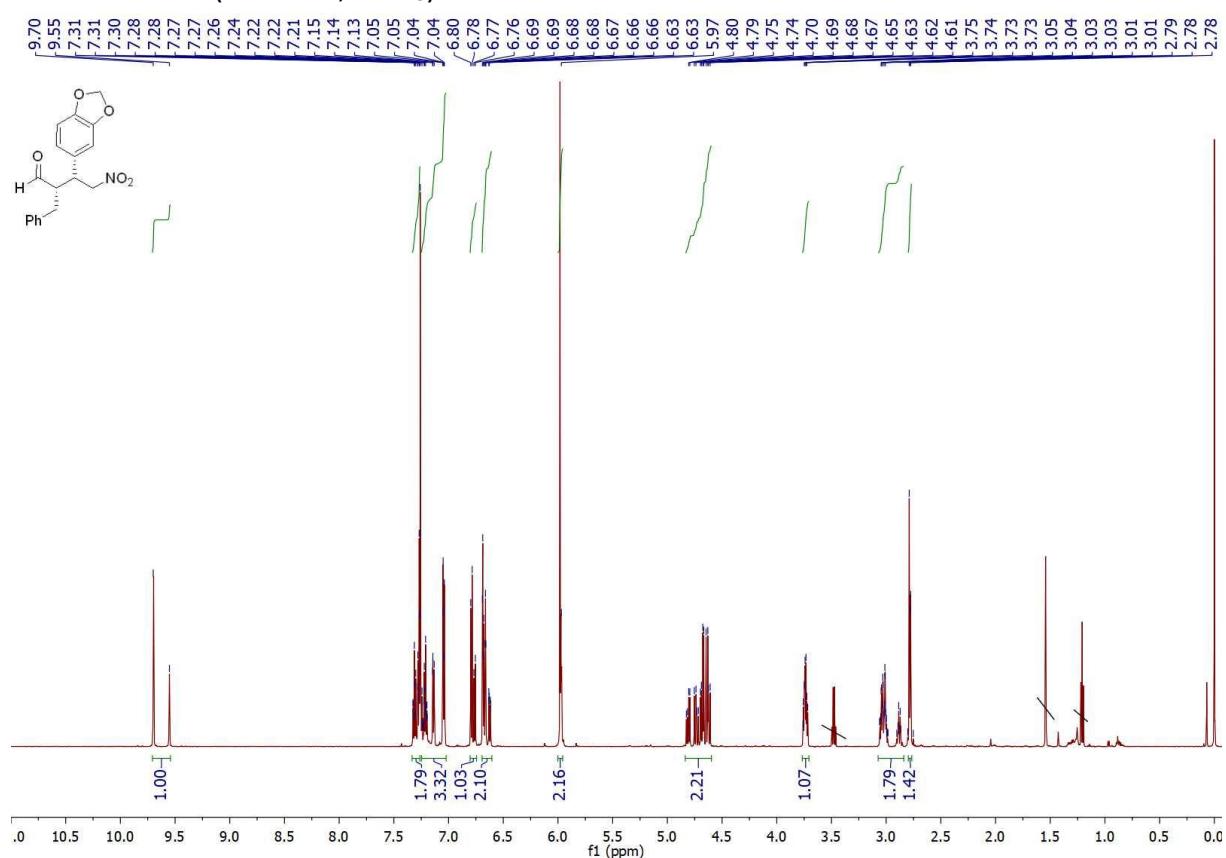
¹H NMR of **11c** (600 MHz, CDCl₃)



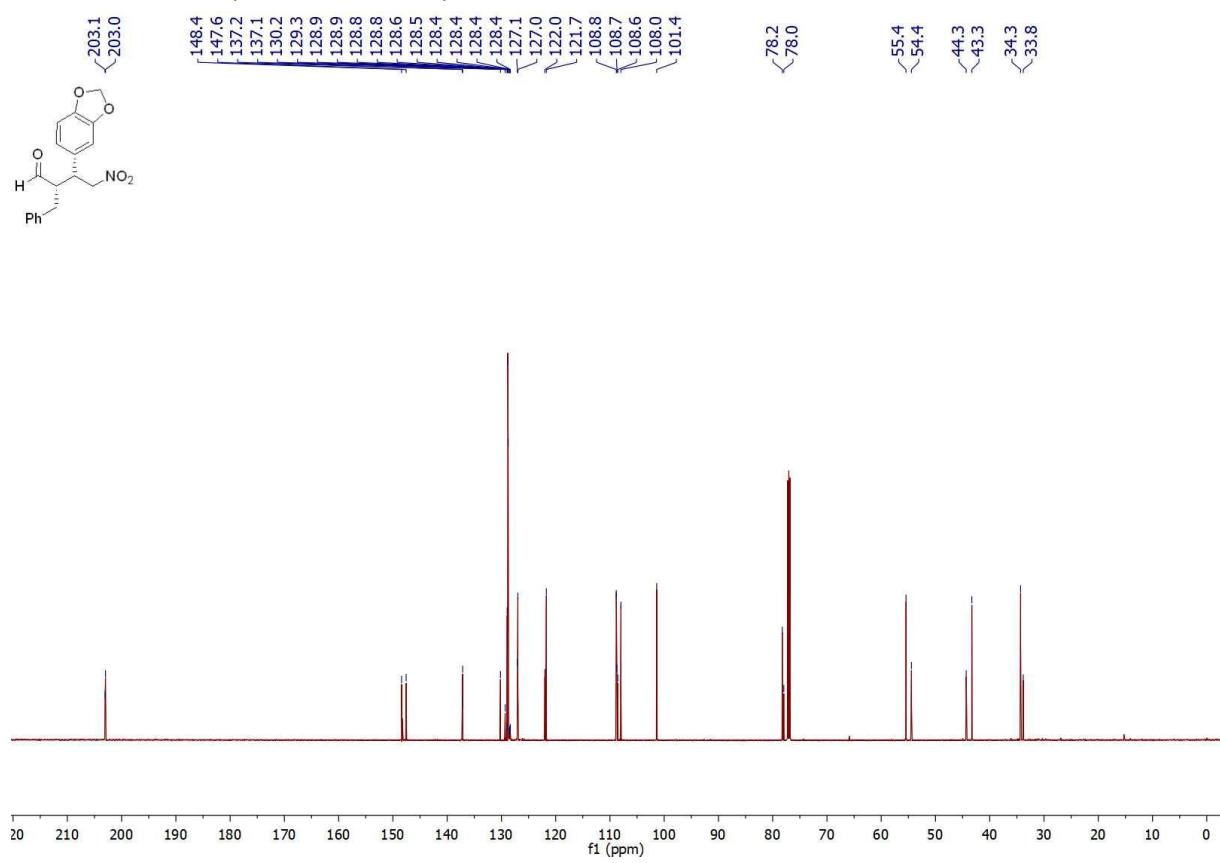
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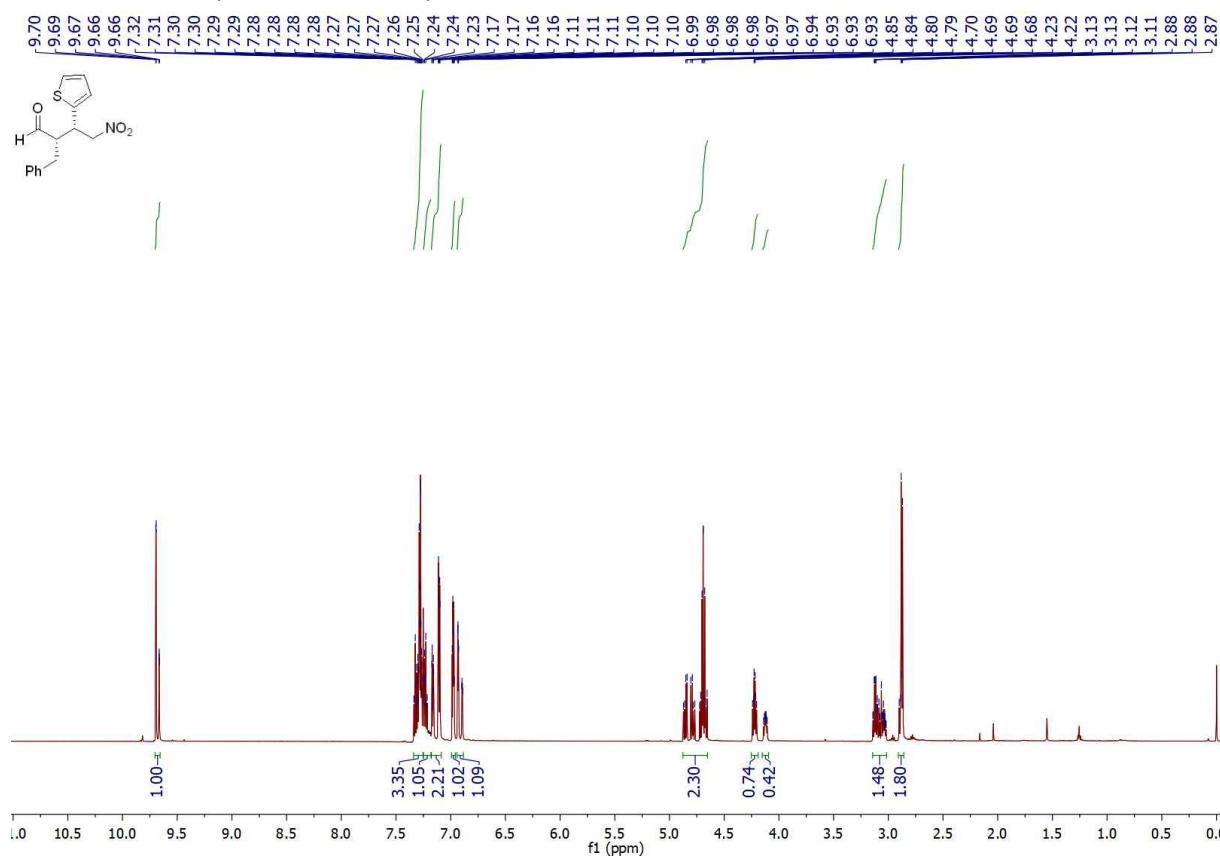
¹H NMR of **11d** (600 MHz, CDCl₃)



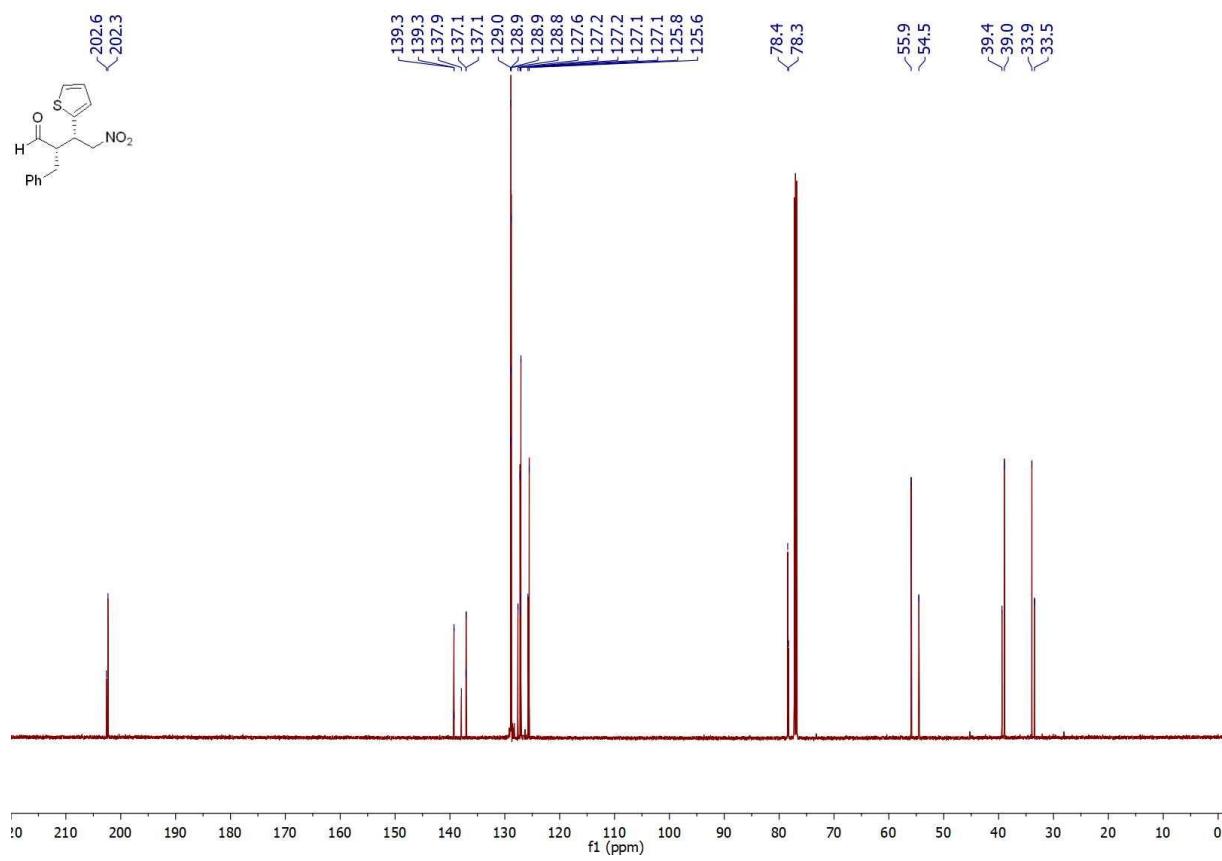
¹³C NMR of **11d** (151 MHz, CDCl₃)



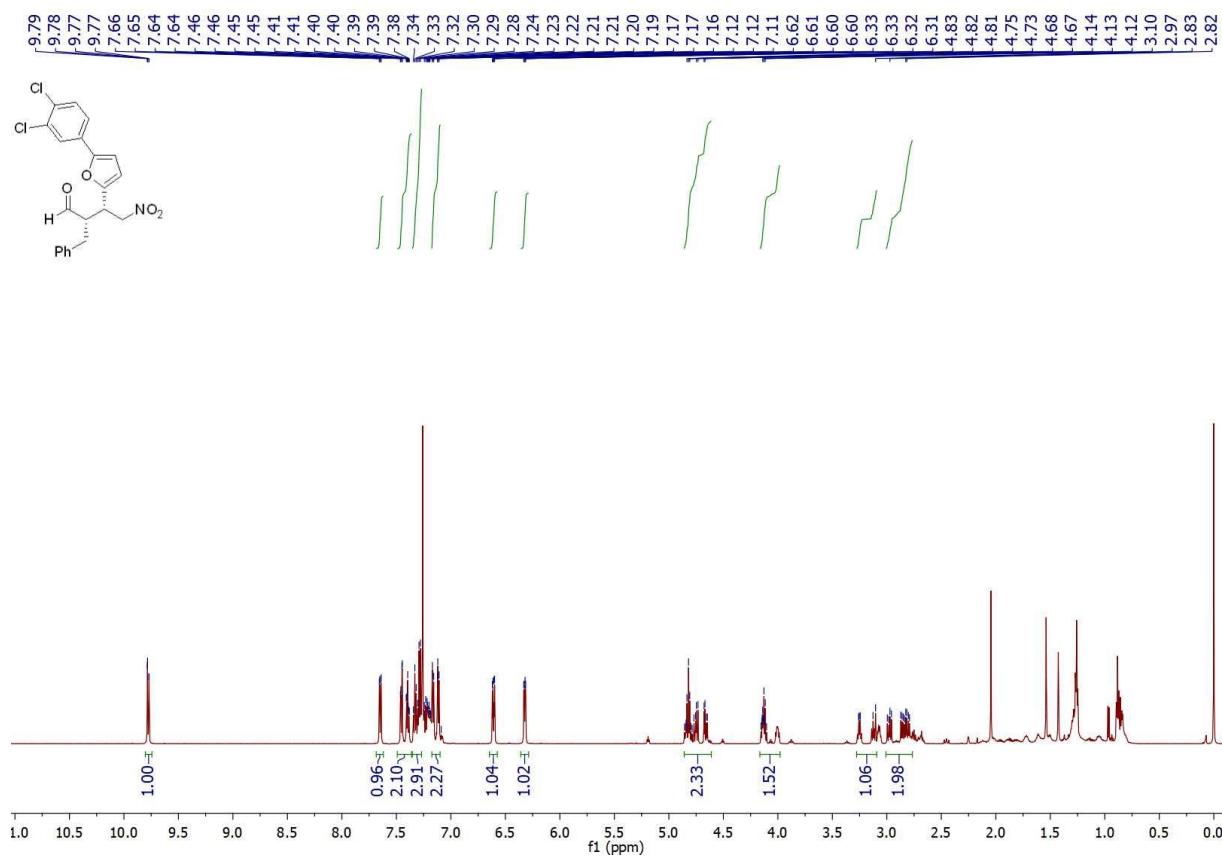
¹H NMR of **11e** (600 MHz, CDCl₃)



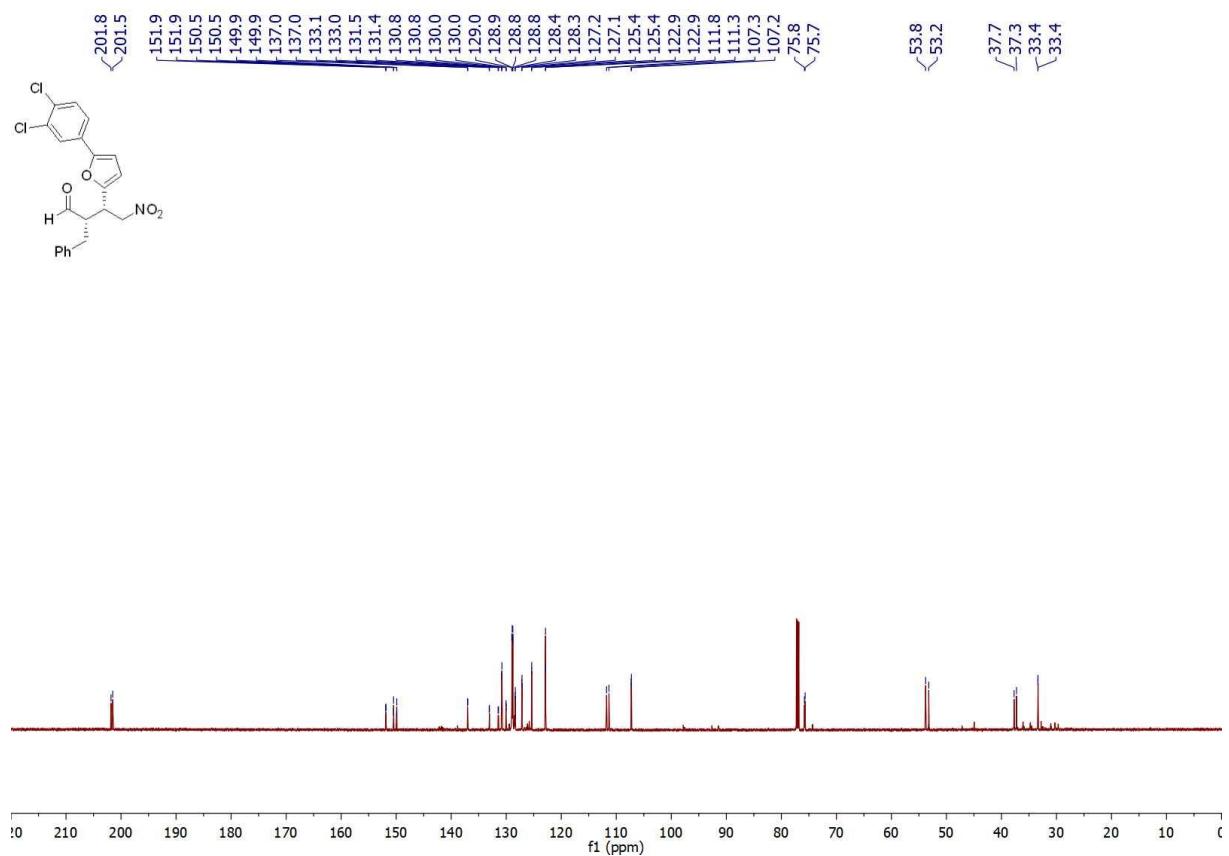
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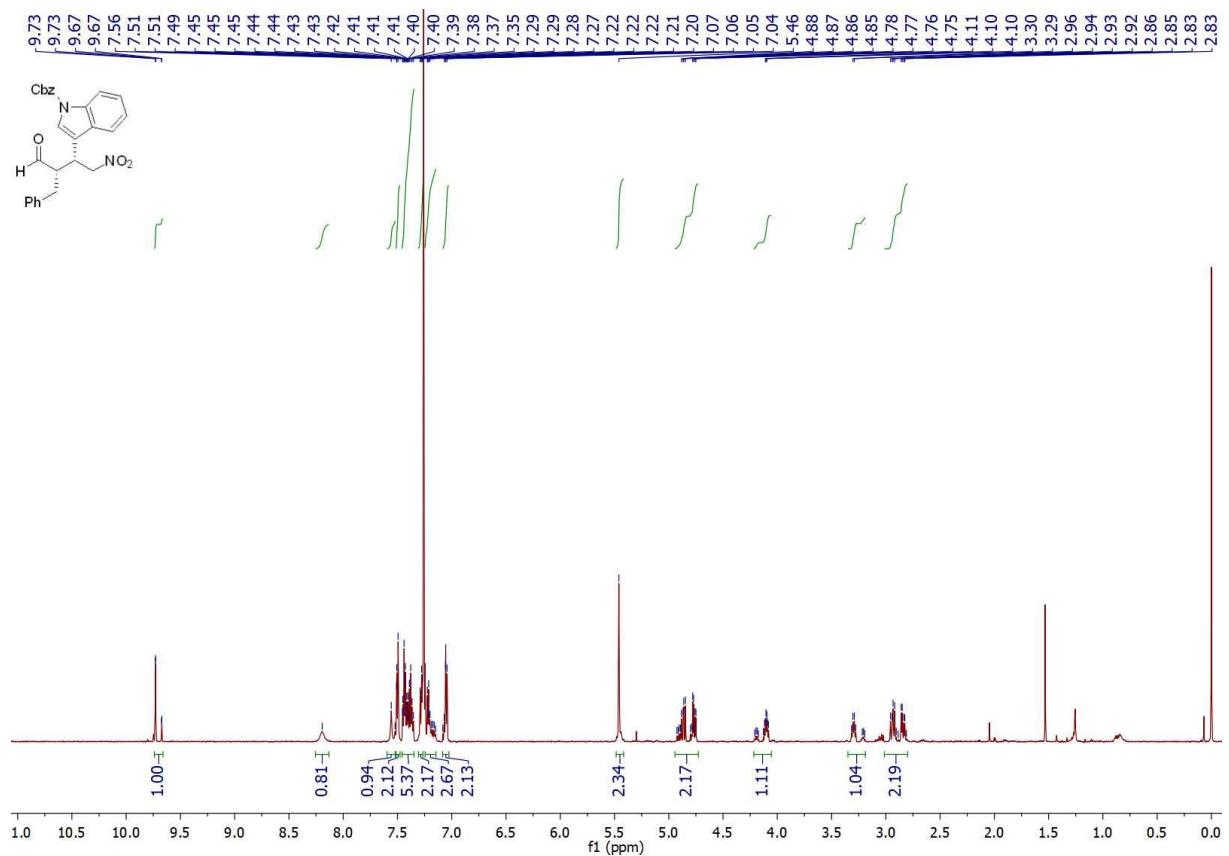
¹H NMR of **11f** (600 MHz, CDCl₃)



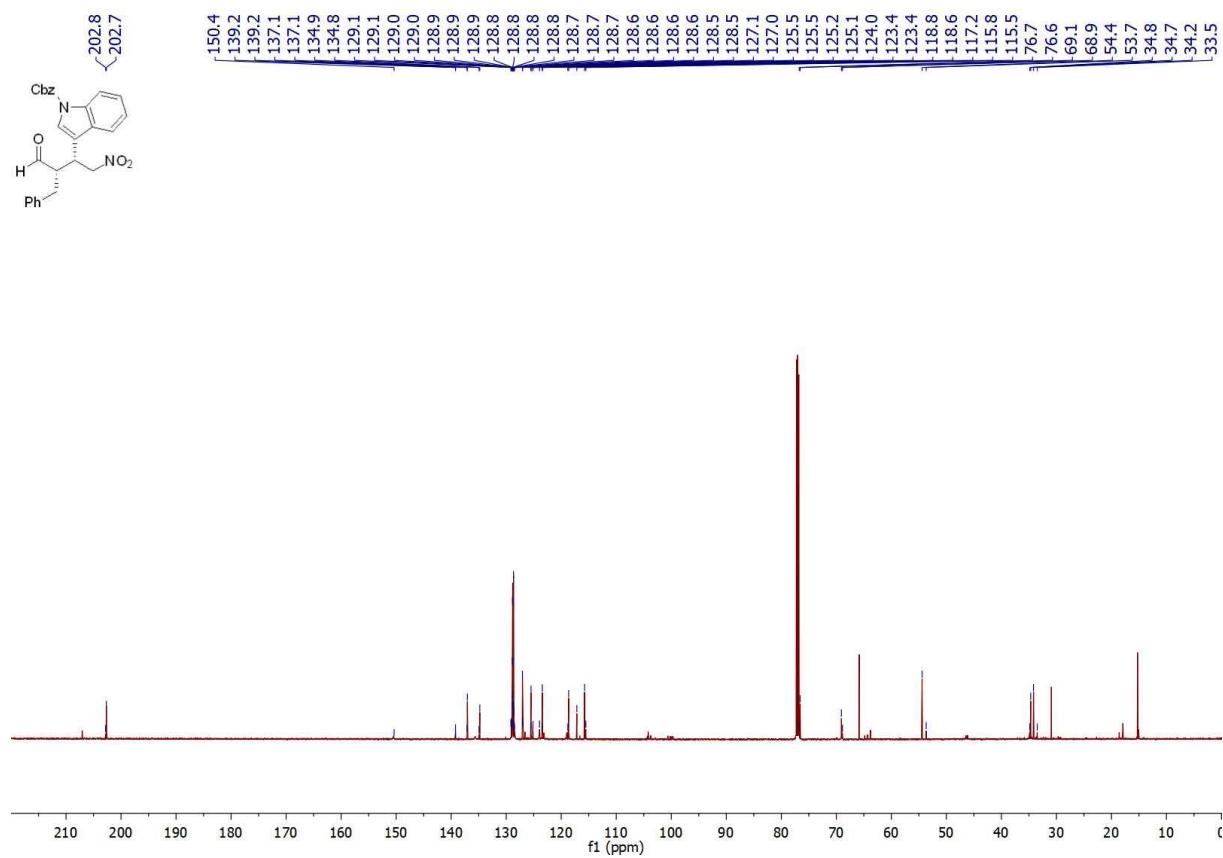
¹³C NMR of **11f** (151 MHz, CDCl₃)



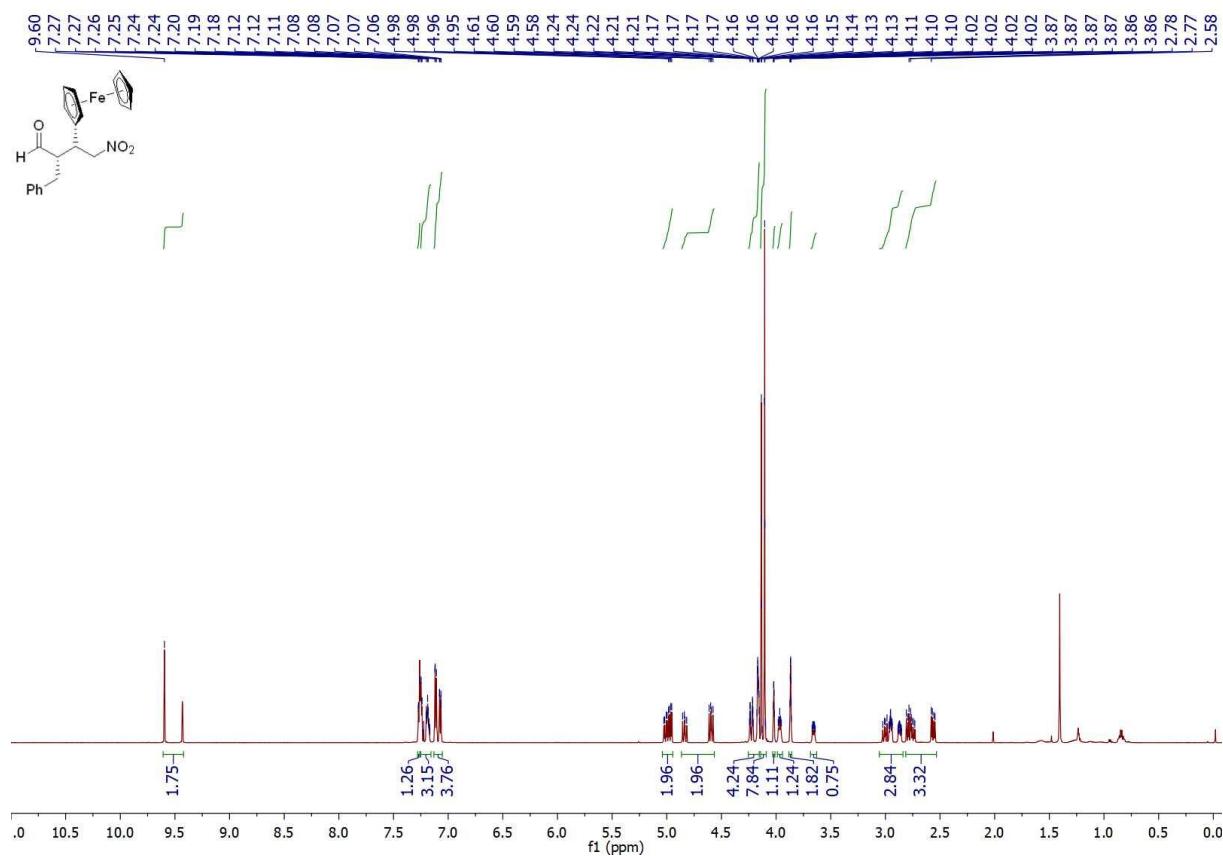
¹H NMR of **11g** (600 MHz, CDCl₃)



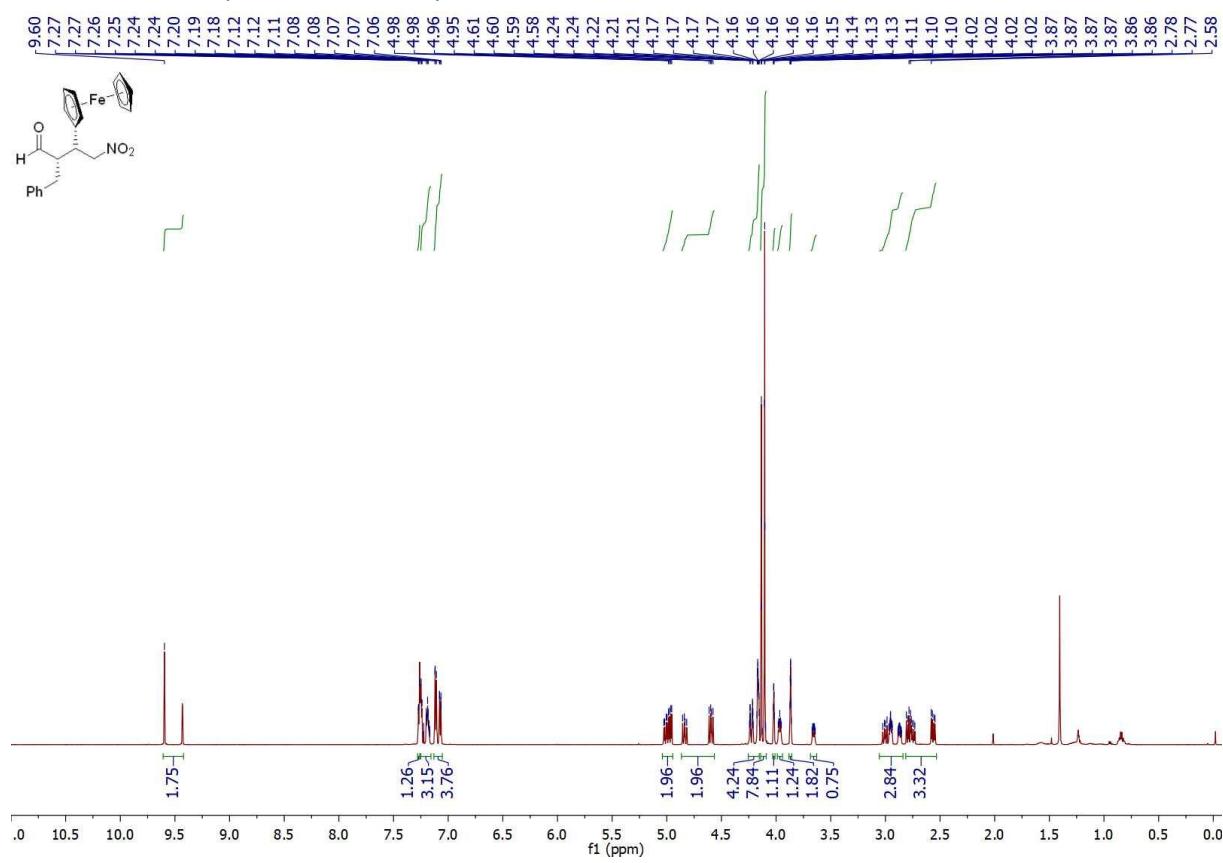
¹³C NMR of **11g** (151 MHz, CDCl₃)



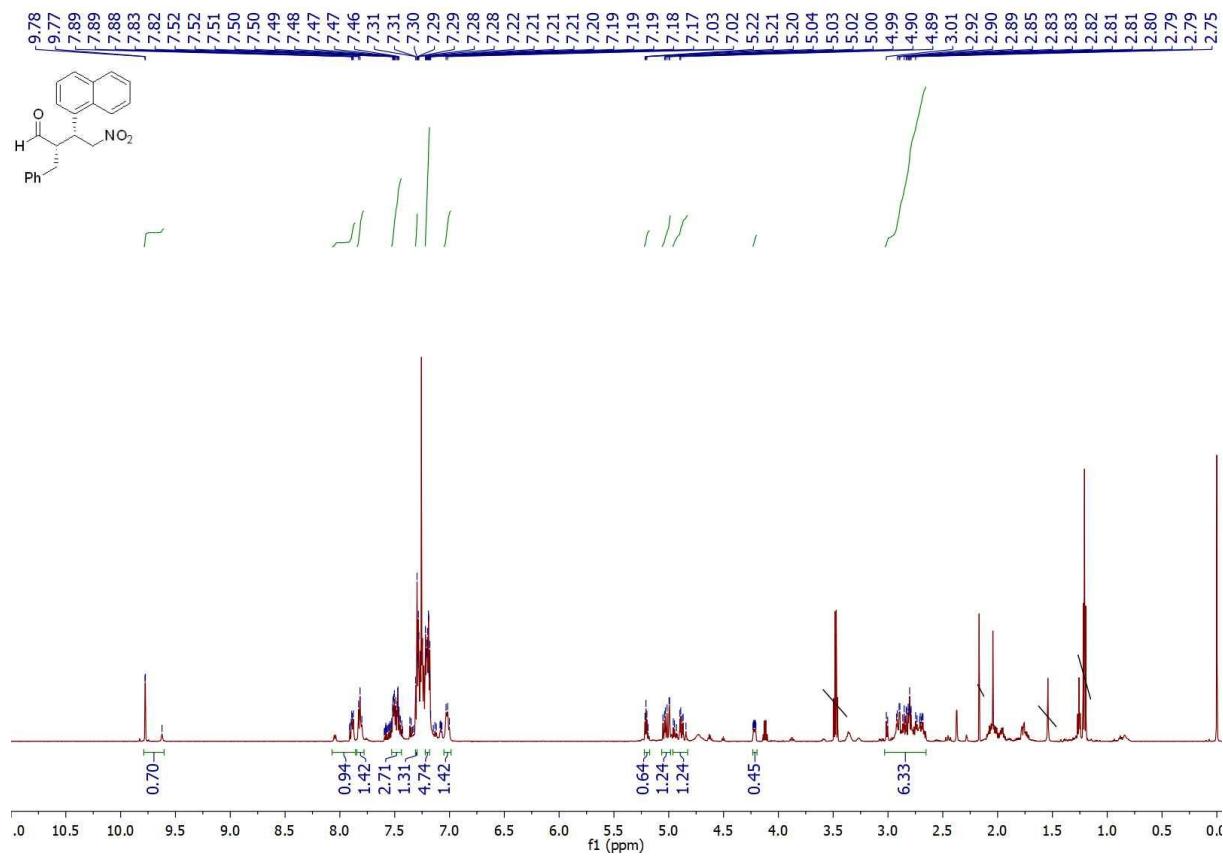
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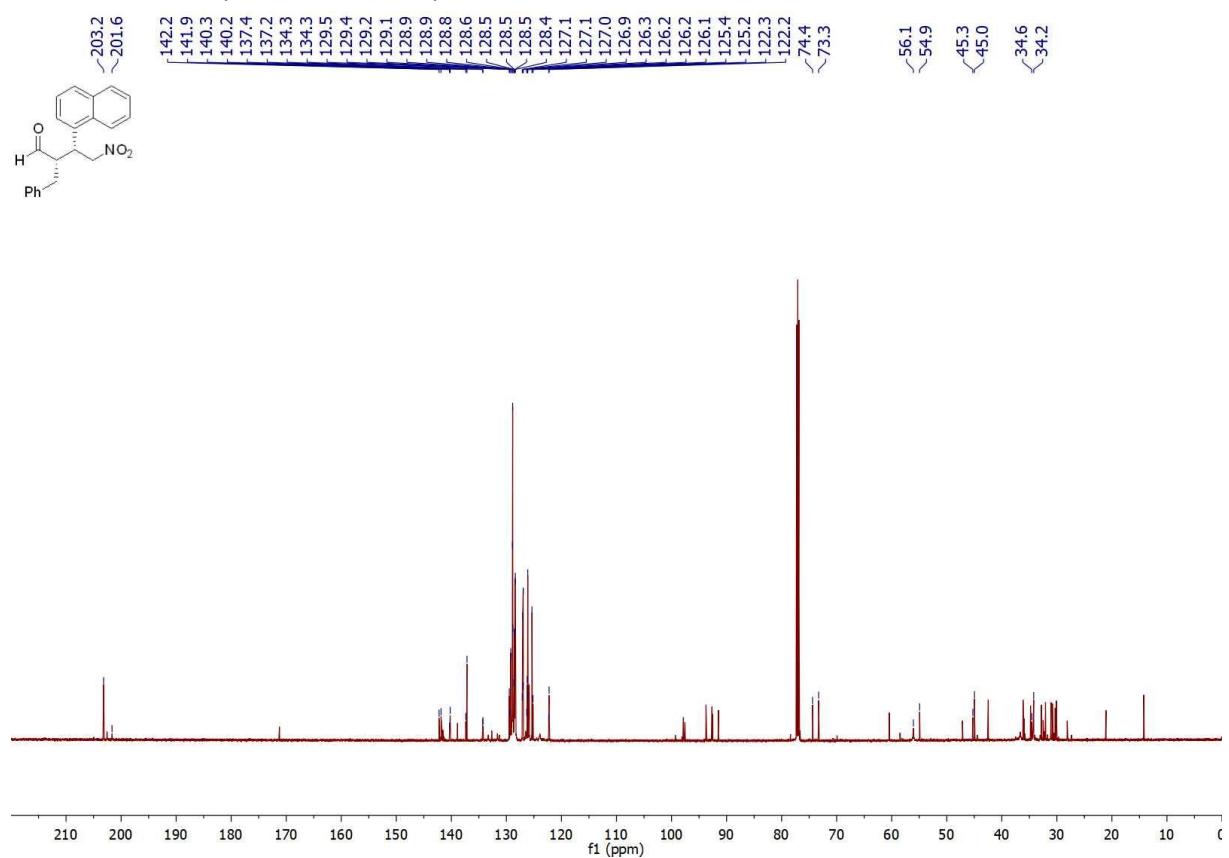
¹³C NMR of **11h** (151 MHz, CDCl₃)



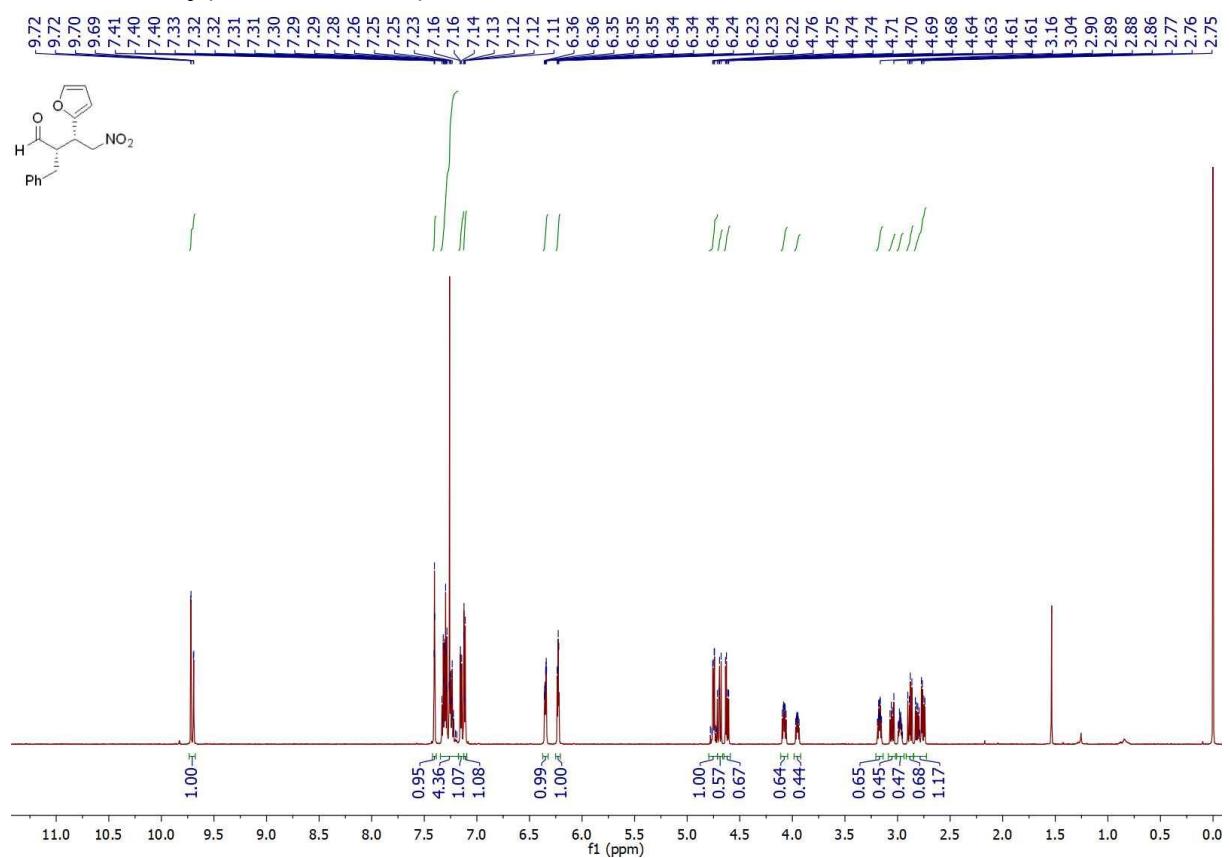
¹H NMR of **11i** (600 MHz, CDCl₃)



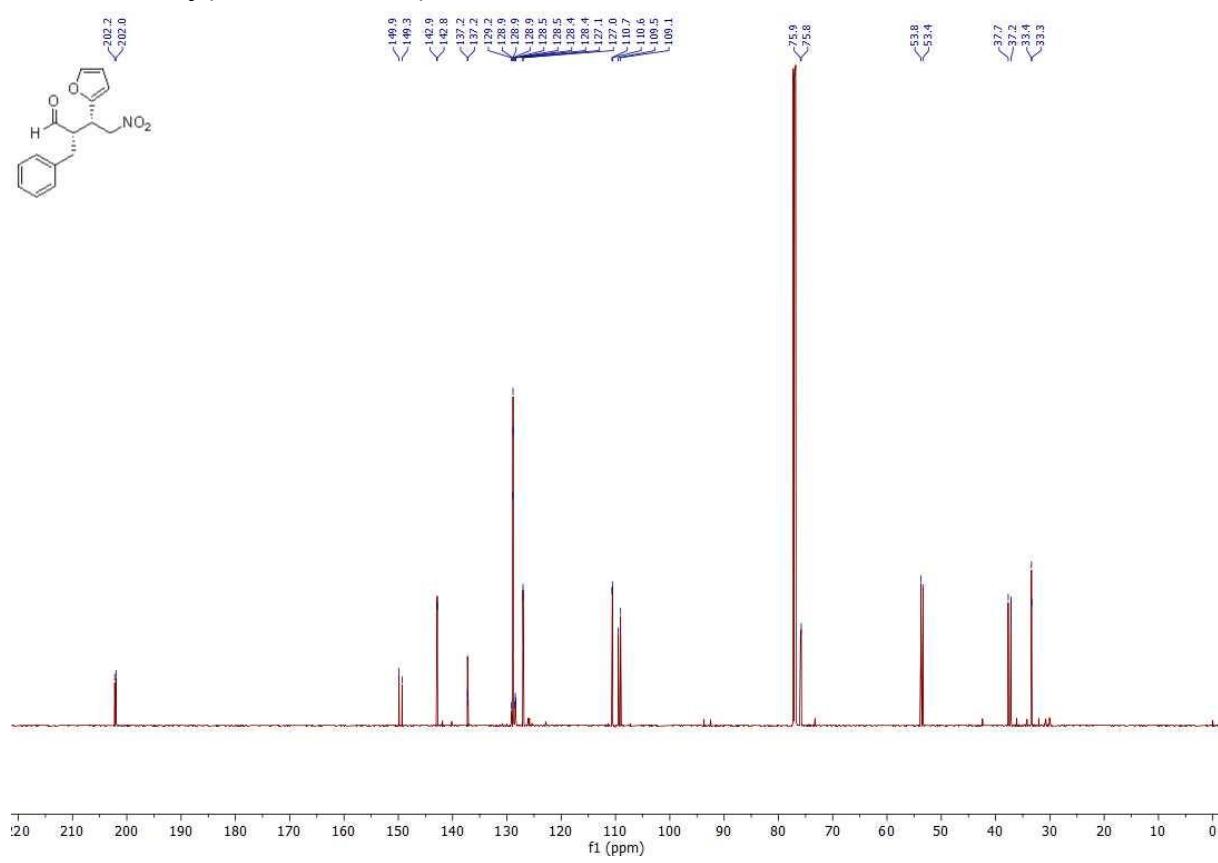
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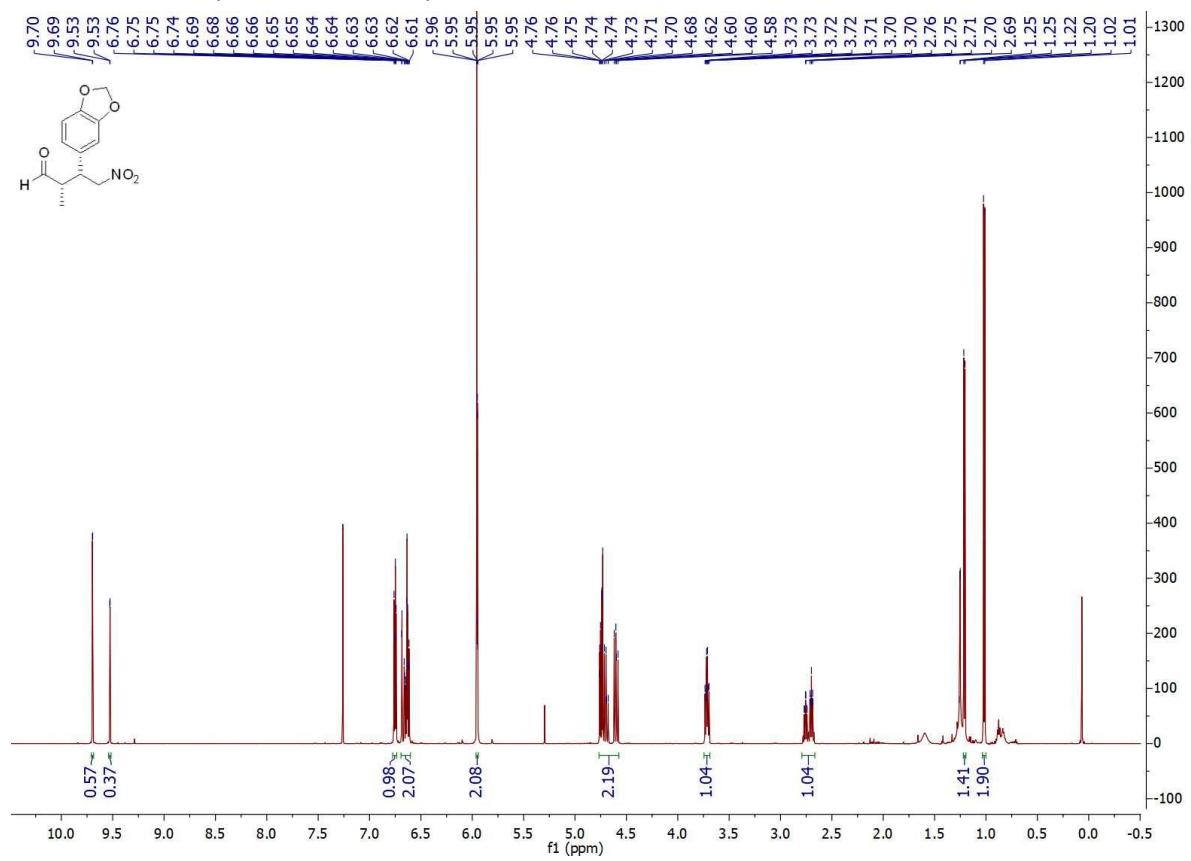
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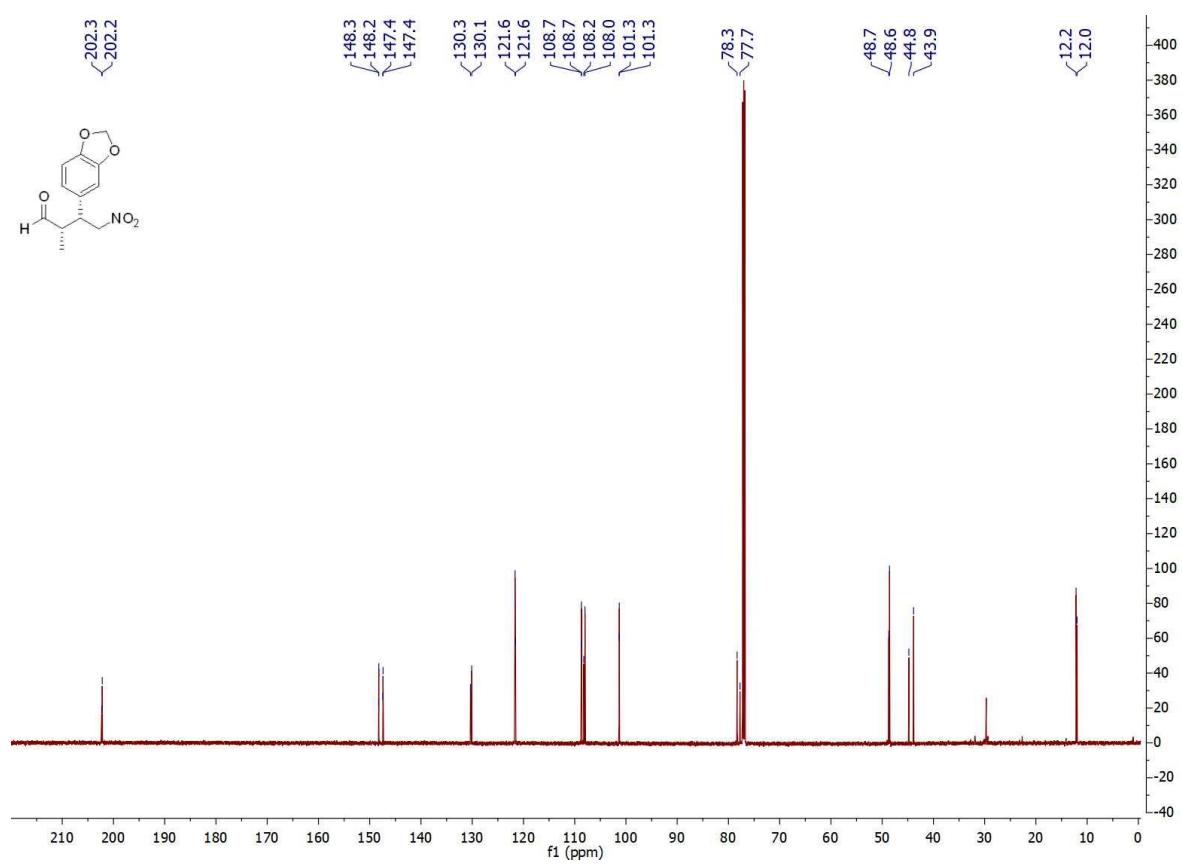
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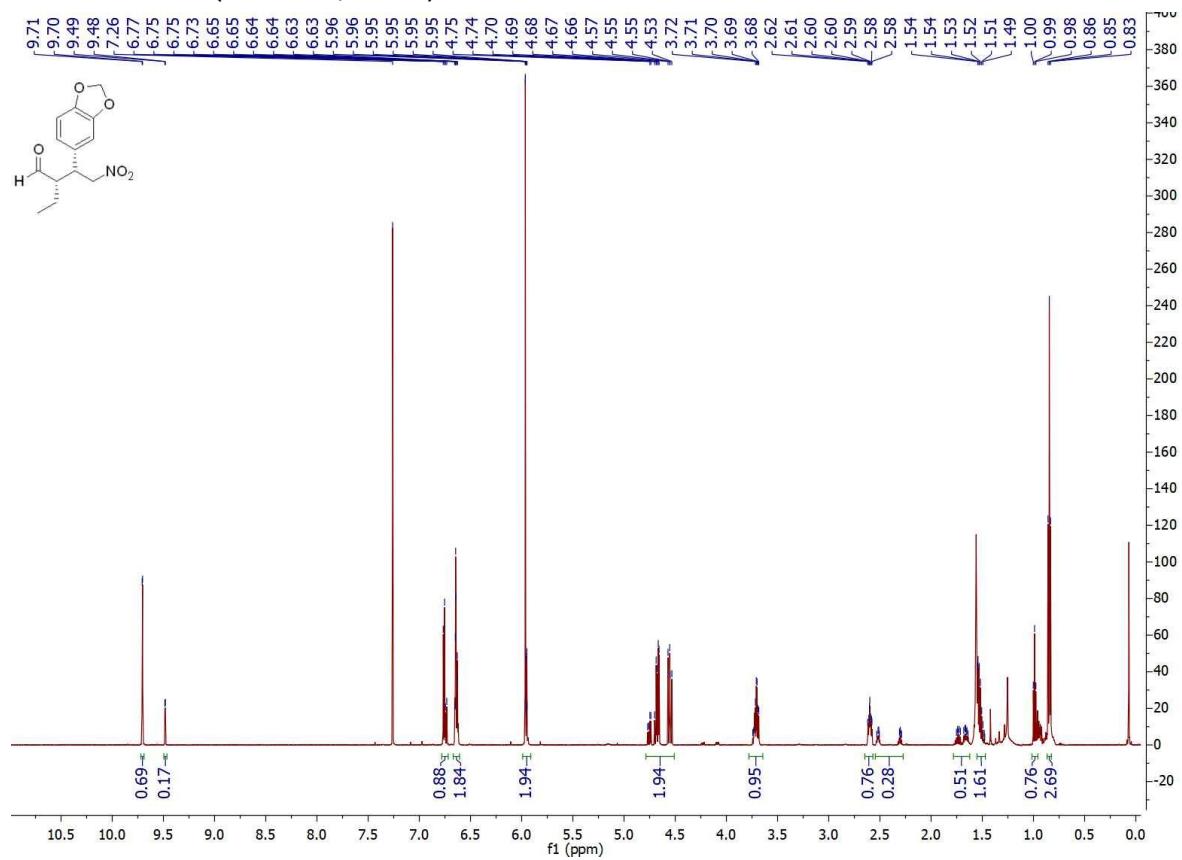
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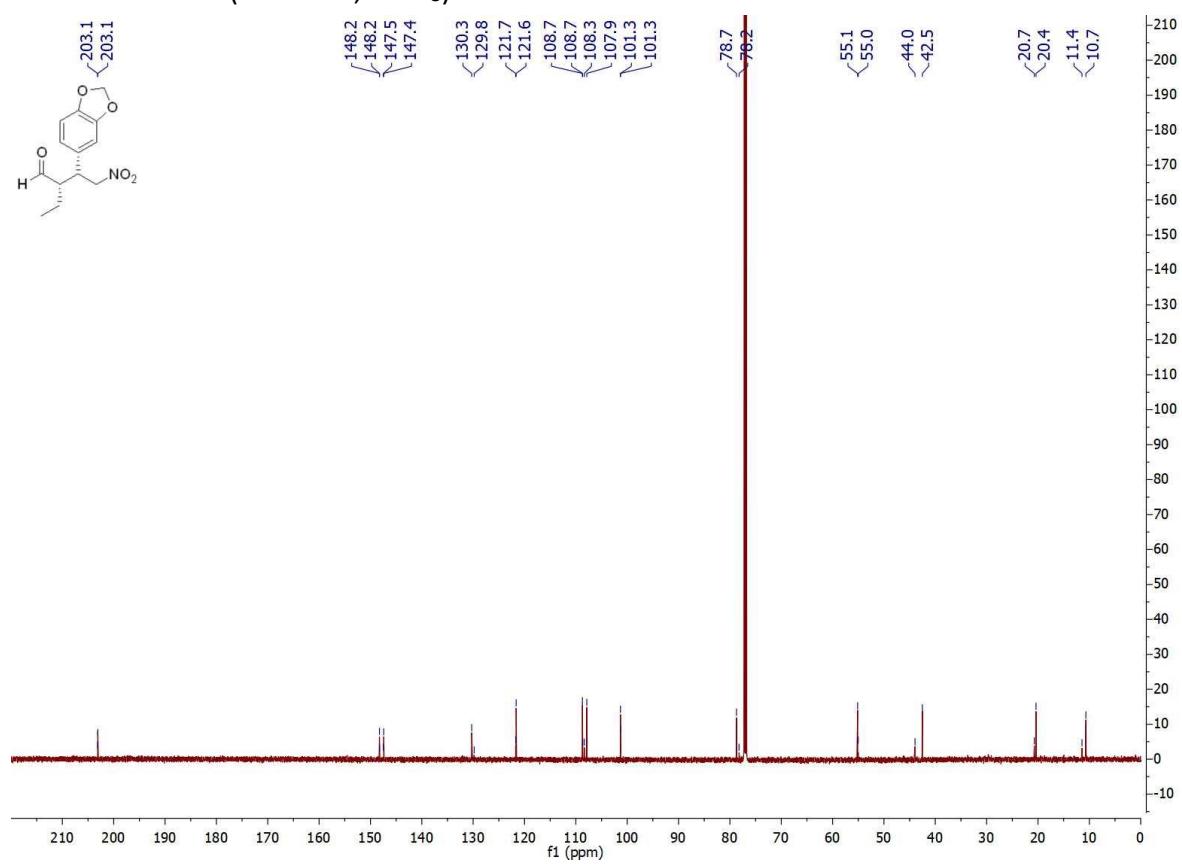
¹³C NMR of **12a** (151 MHz, CDCl₃)



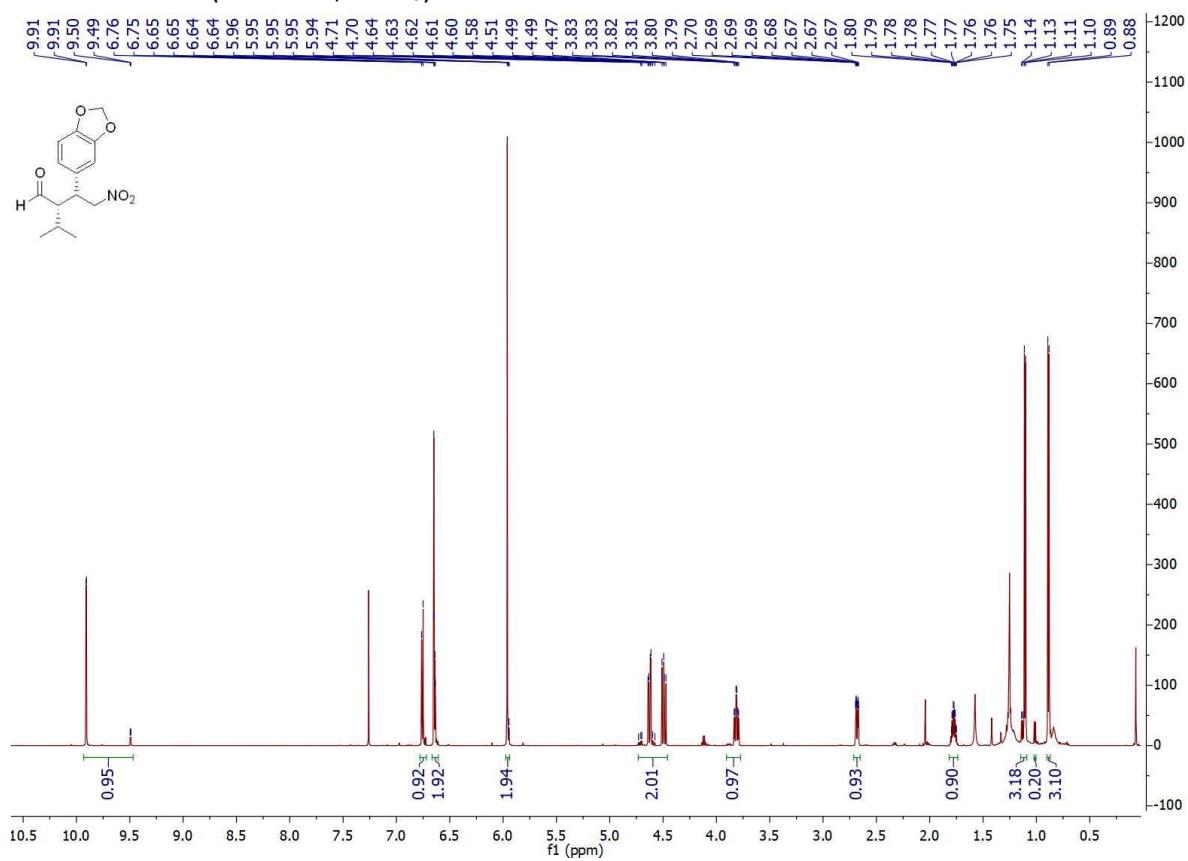
¹H NMR of **12b** (600 MHz, CDCl₃)



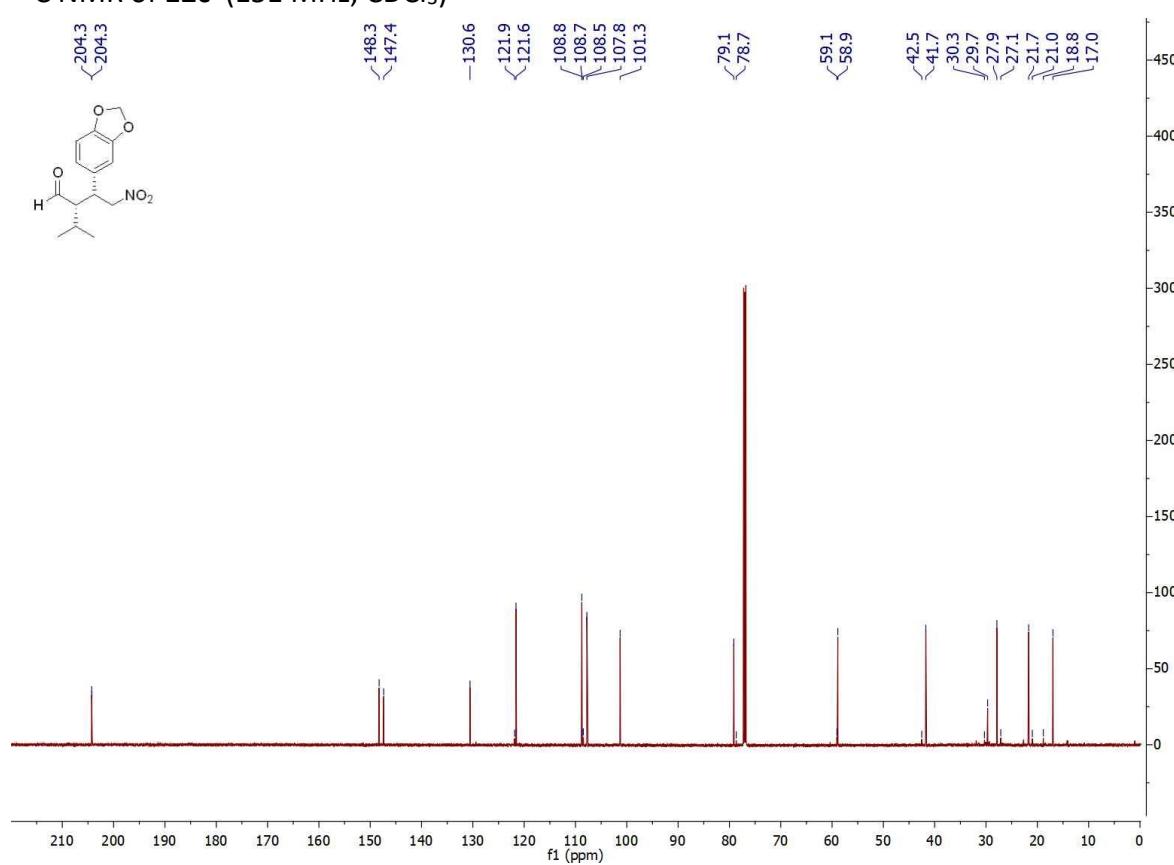
¹³C NMR of **12b** (151 MHz, CDCl₃)



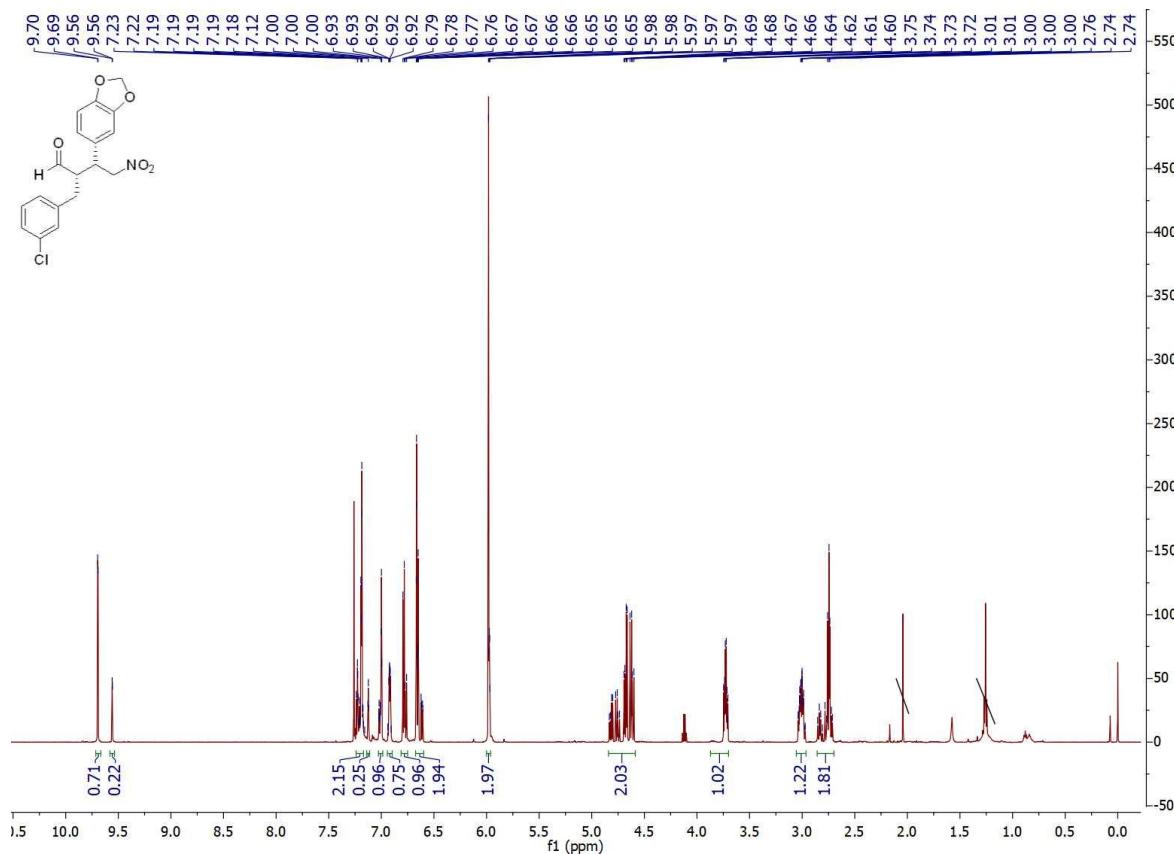
¹H NMR of **12c** (600 MHz, CDCl₃)



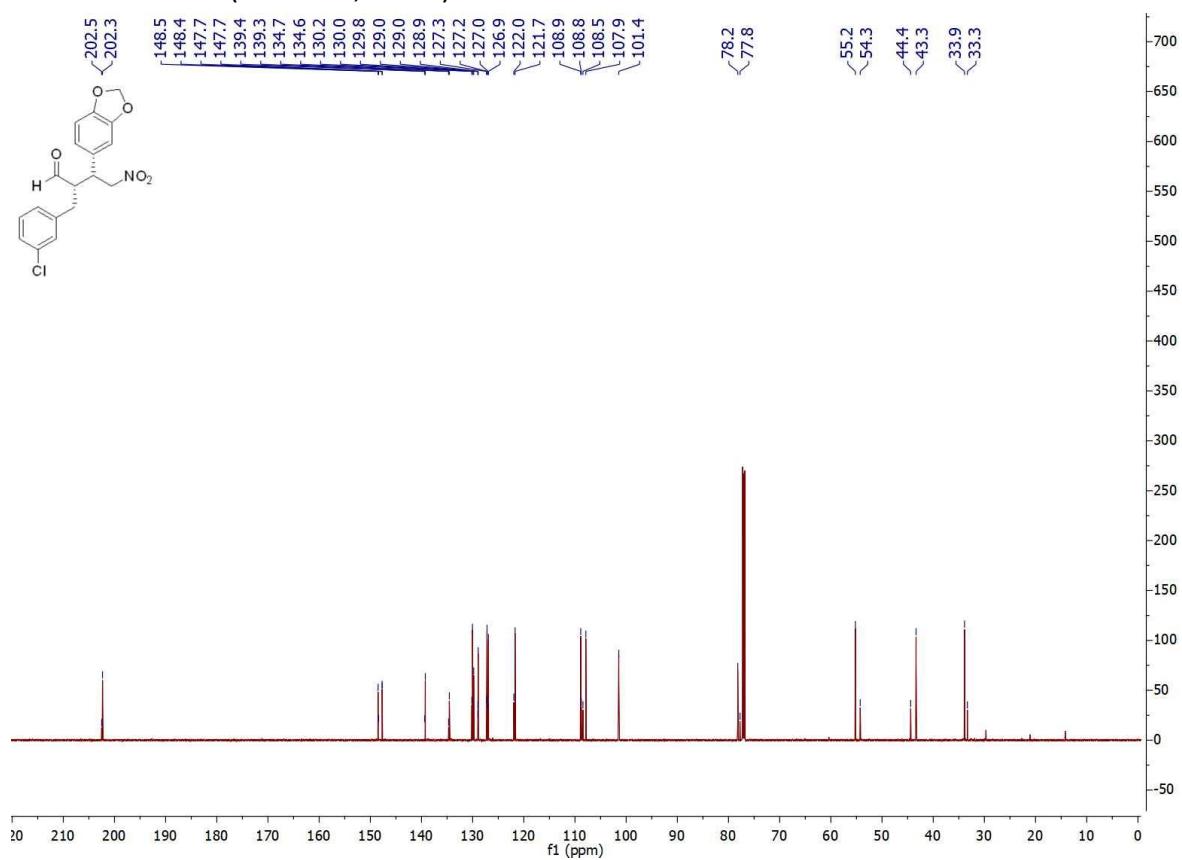
¹³C NMR of **12c** (151 MHz, CDCl₃)



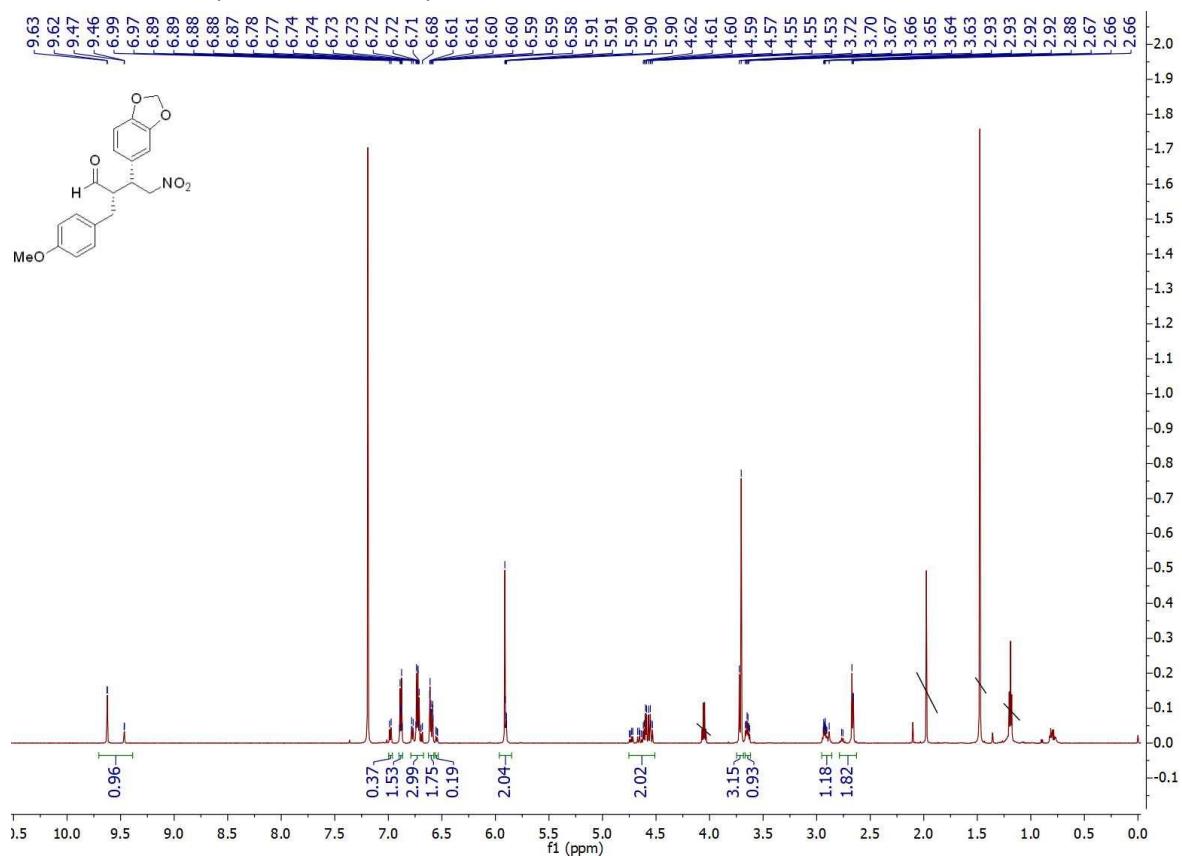
¹H NMR of **12d** (600 MHz, CDCl₃)



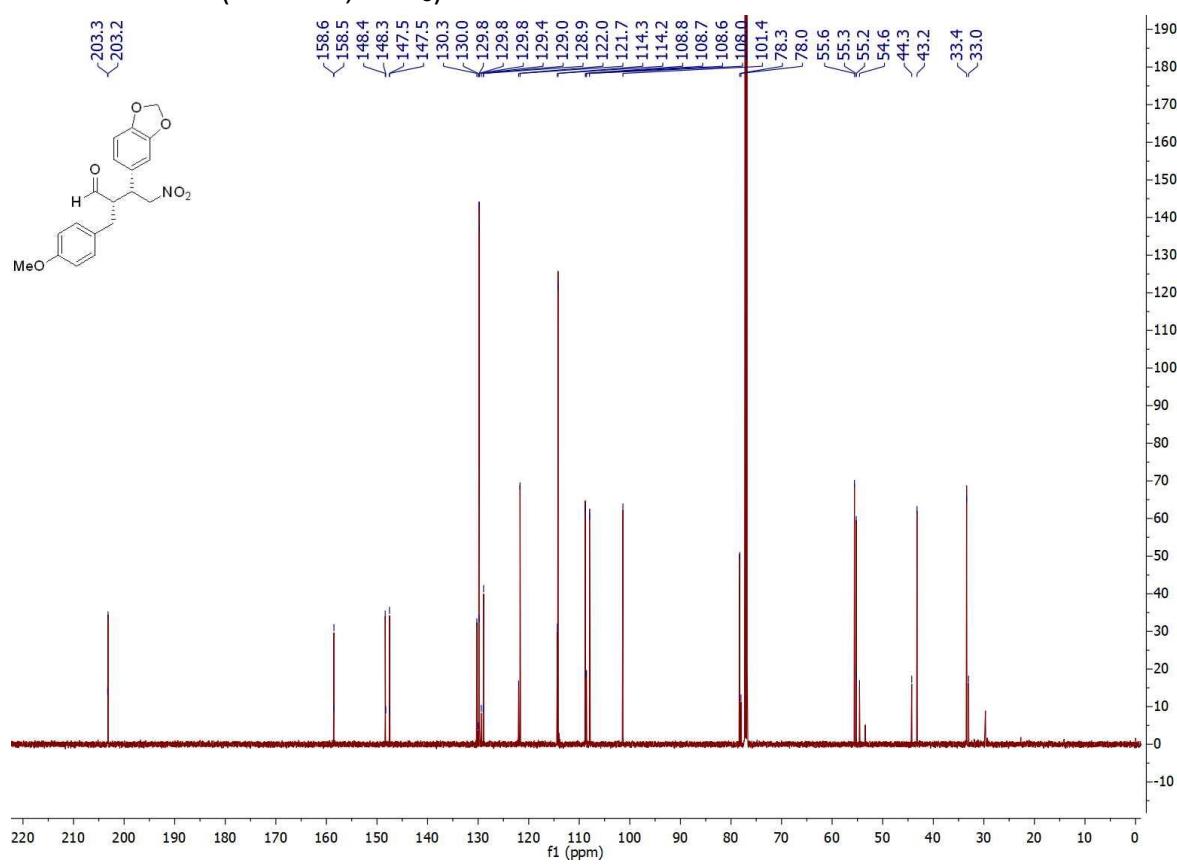
¹³C NMR of **12d** (151 MHz, CDCl₃)



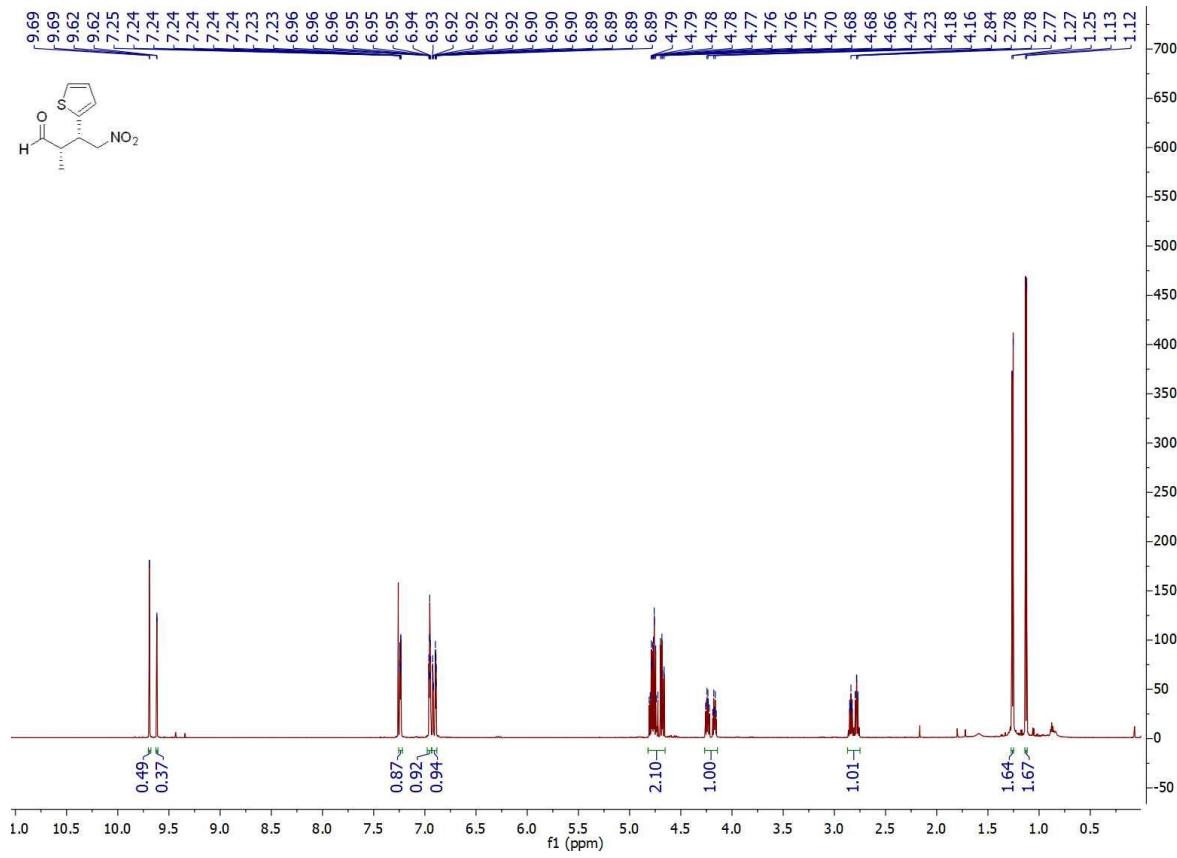
¹H NMR of **12e** (600 MHz, CDCl₃)



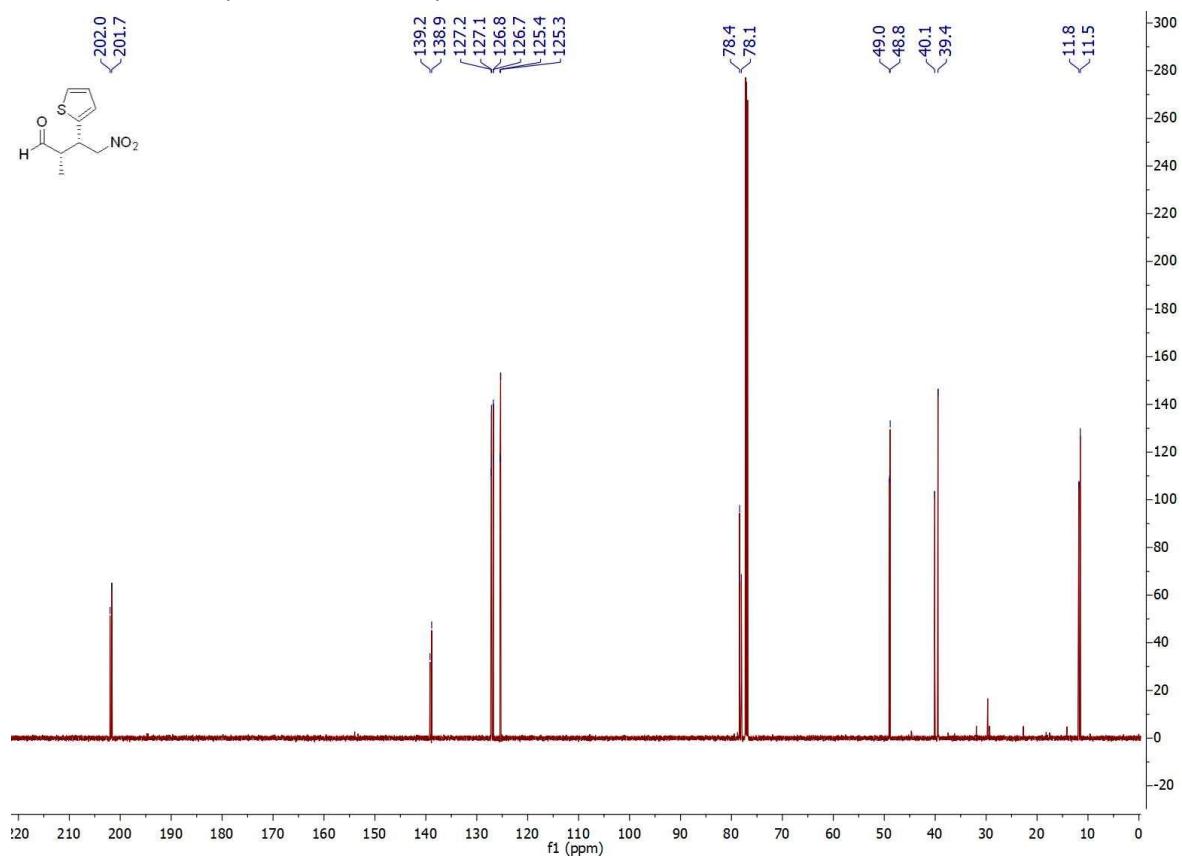
¹³C NMR of **12e** (151 MHz, CDCl₃)



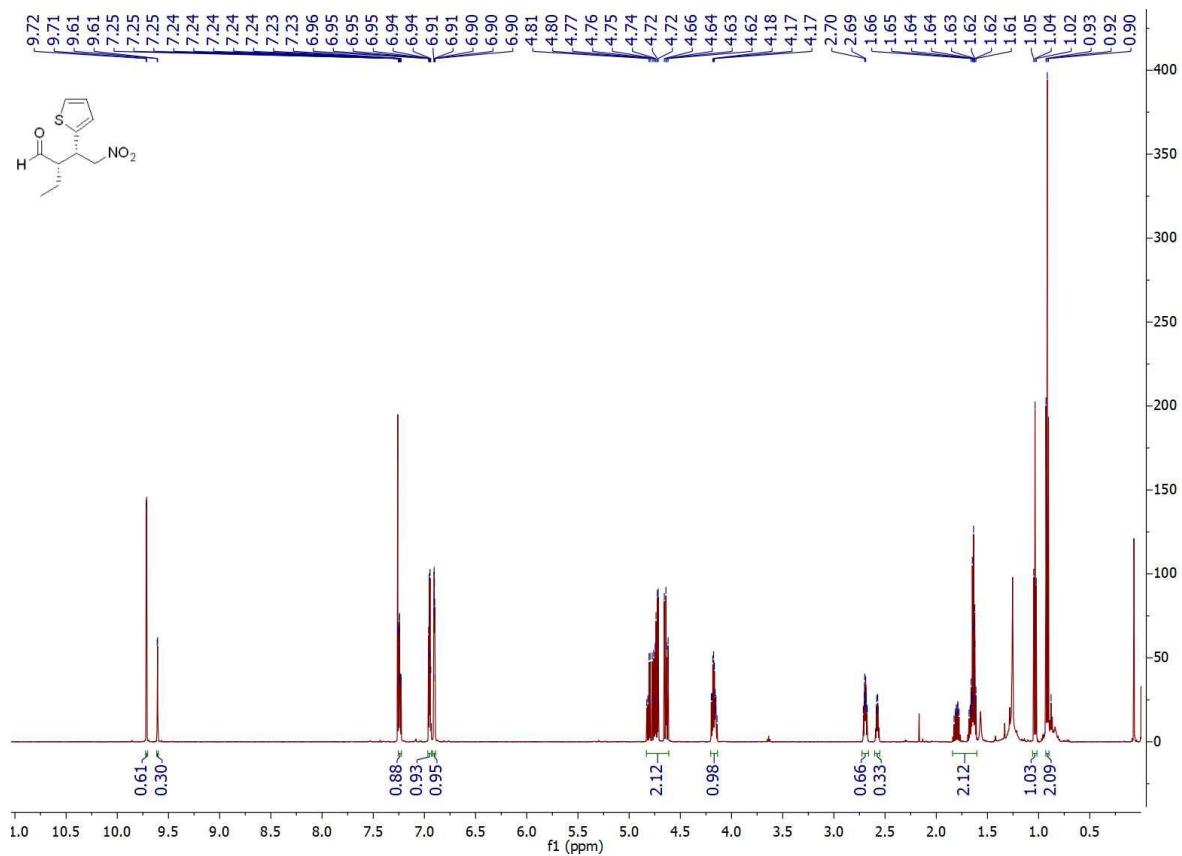
¹H NMR of **12f** (600 MHz, CDCl₃)



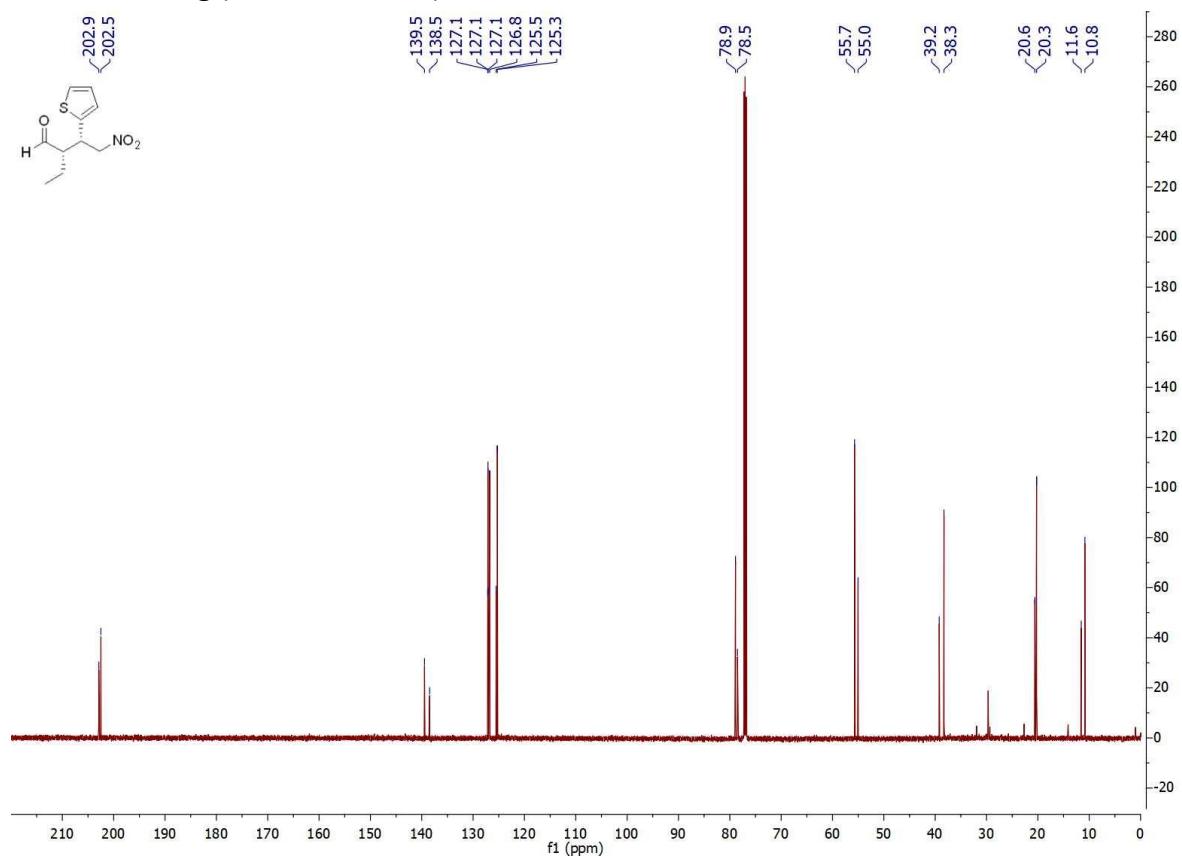
¹³C NMR of **12f** (151 MHz, CDCl₃)



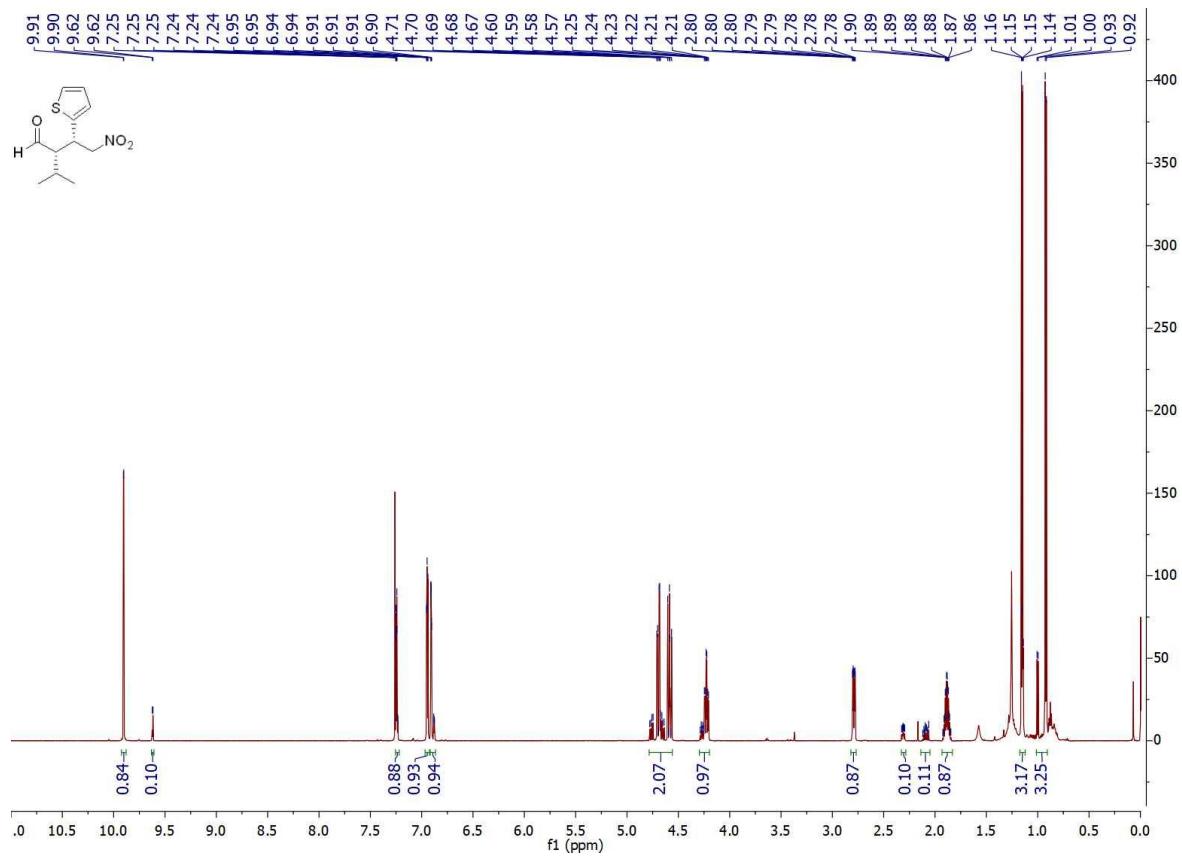
¹H NMR of **12g** (600 MHz, CDCl₃)



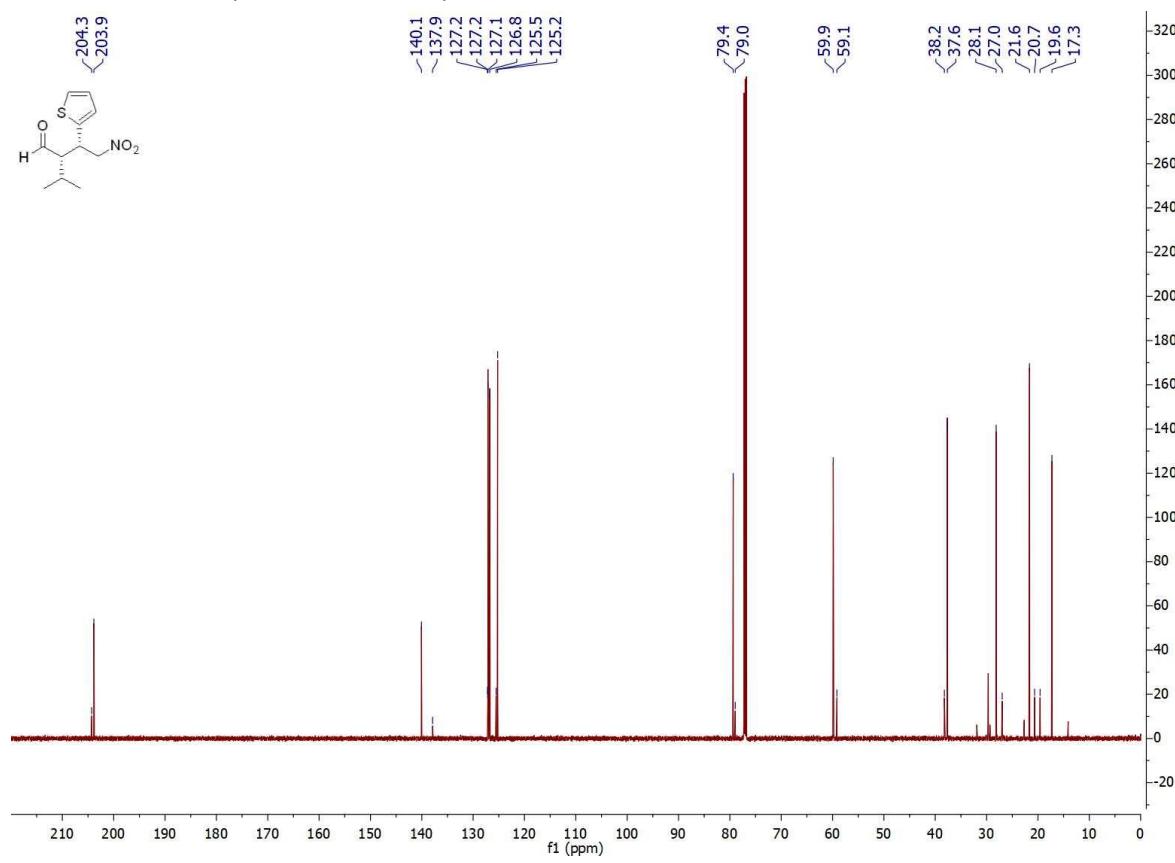
¹³C NMR of **12g** (151 MHz, CDCl₃)



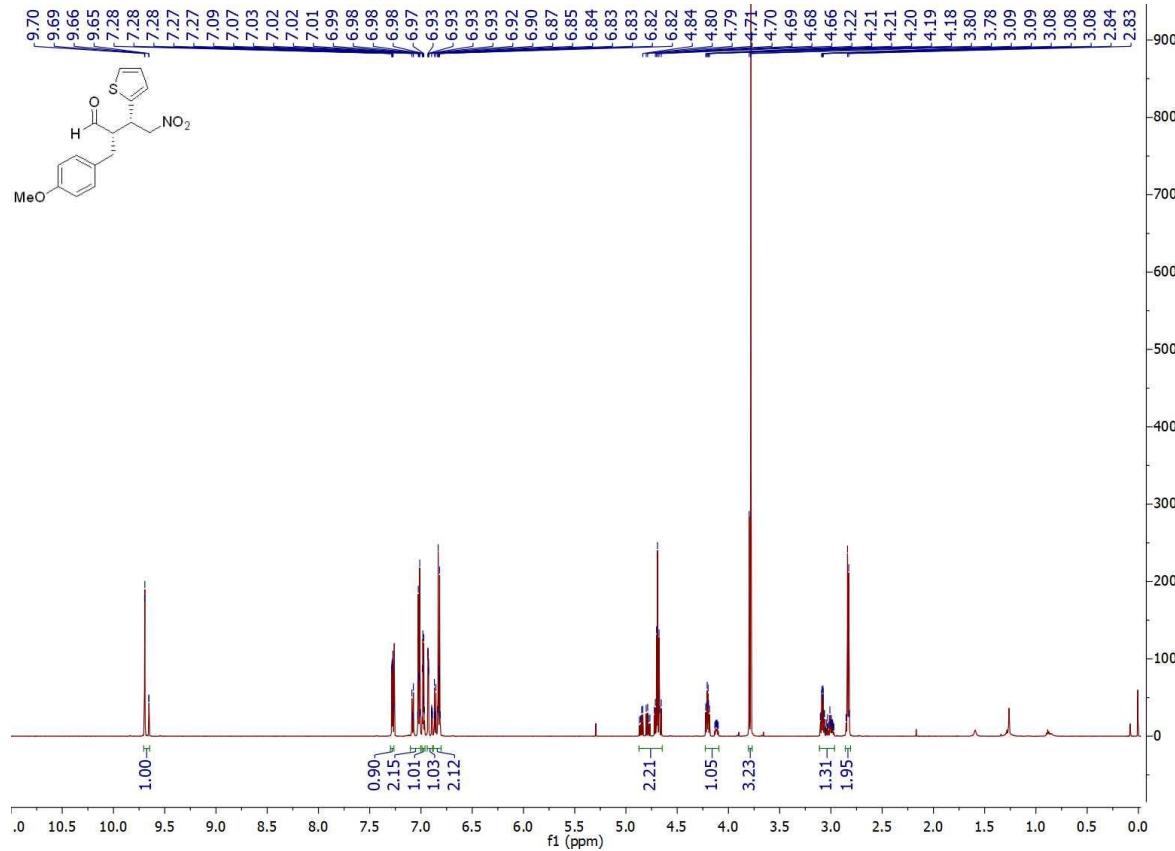
¹H NMR of **12h** (600 MHz, CDCl₃)



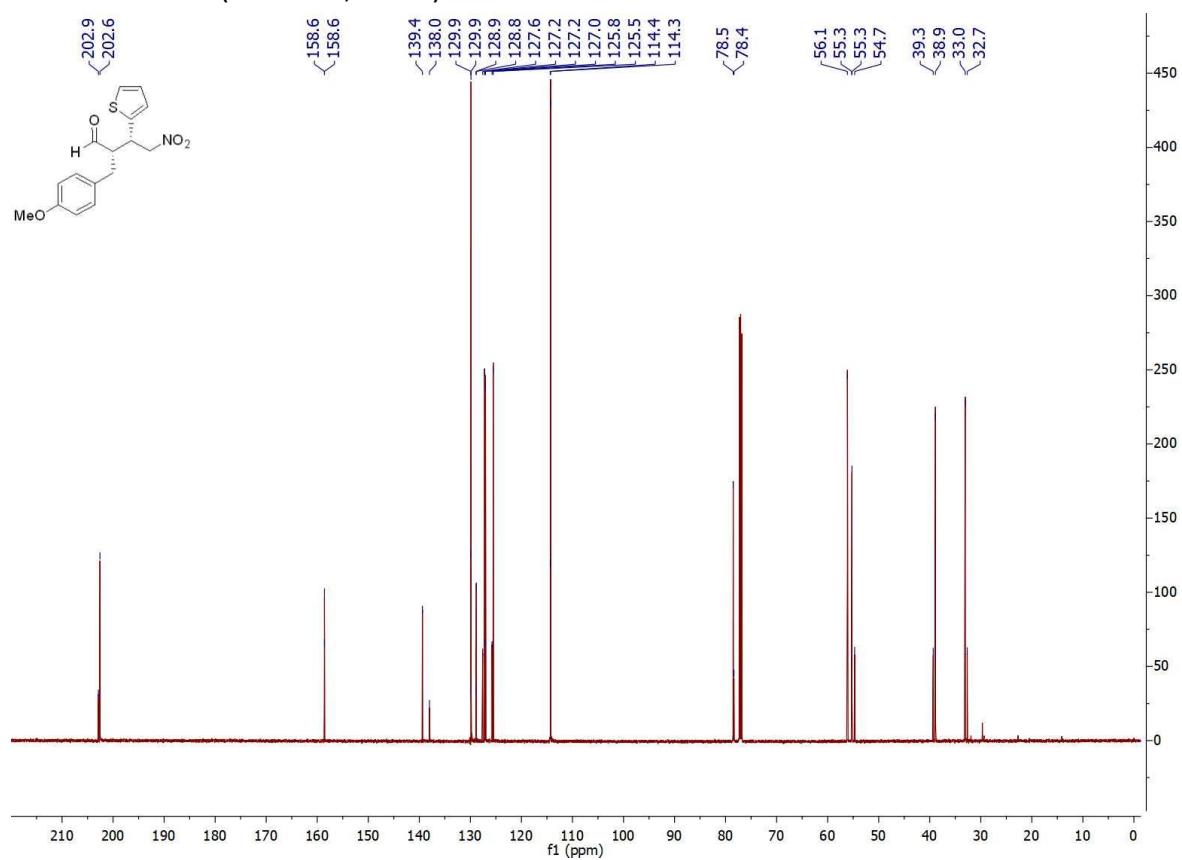
¹³C NMR of **12h** (151 MHz, CDCl₃)



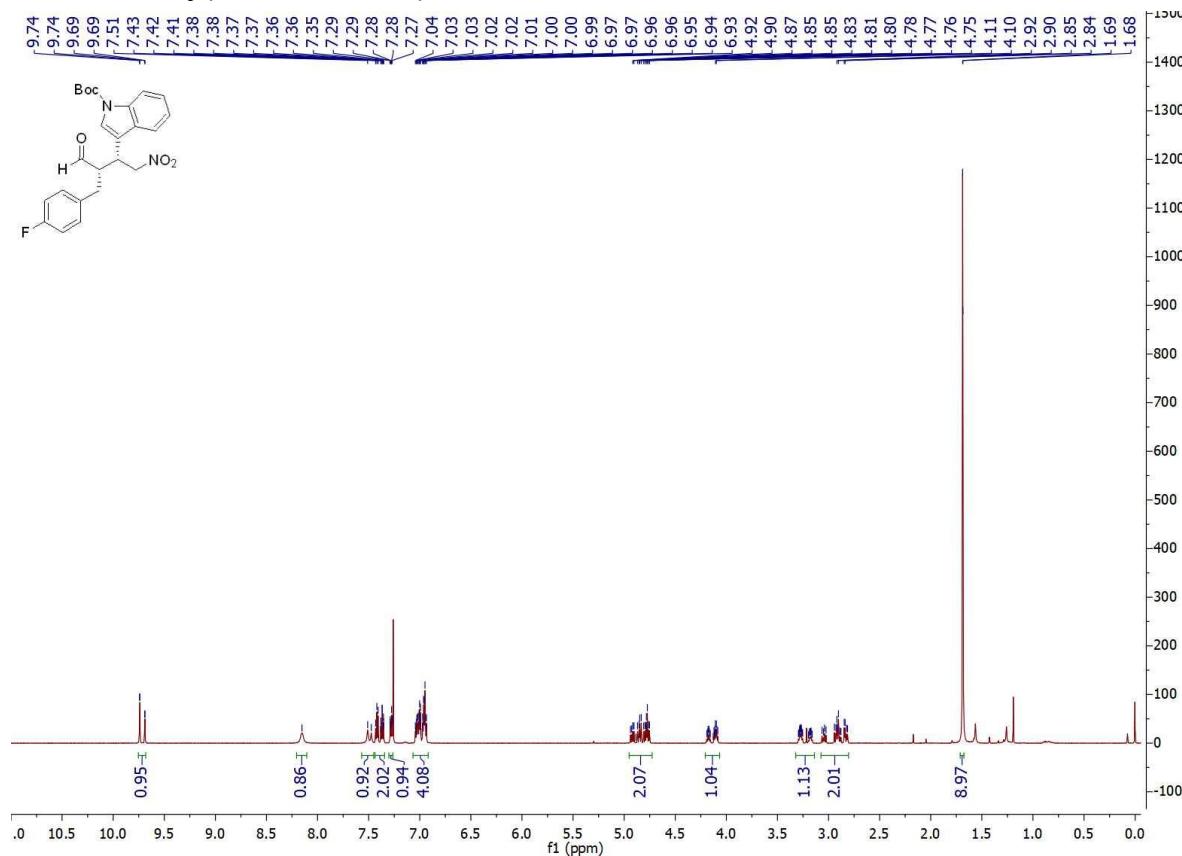
¹H NMR of **12i** (600 MHz, CDCl₃)



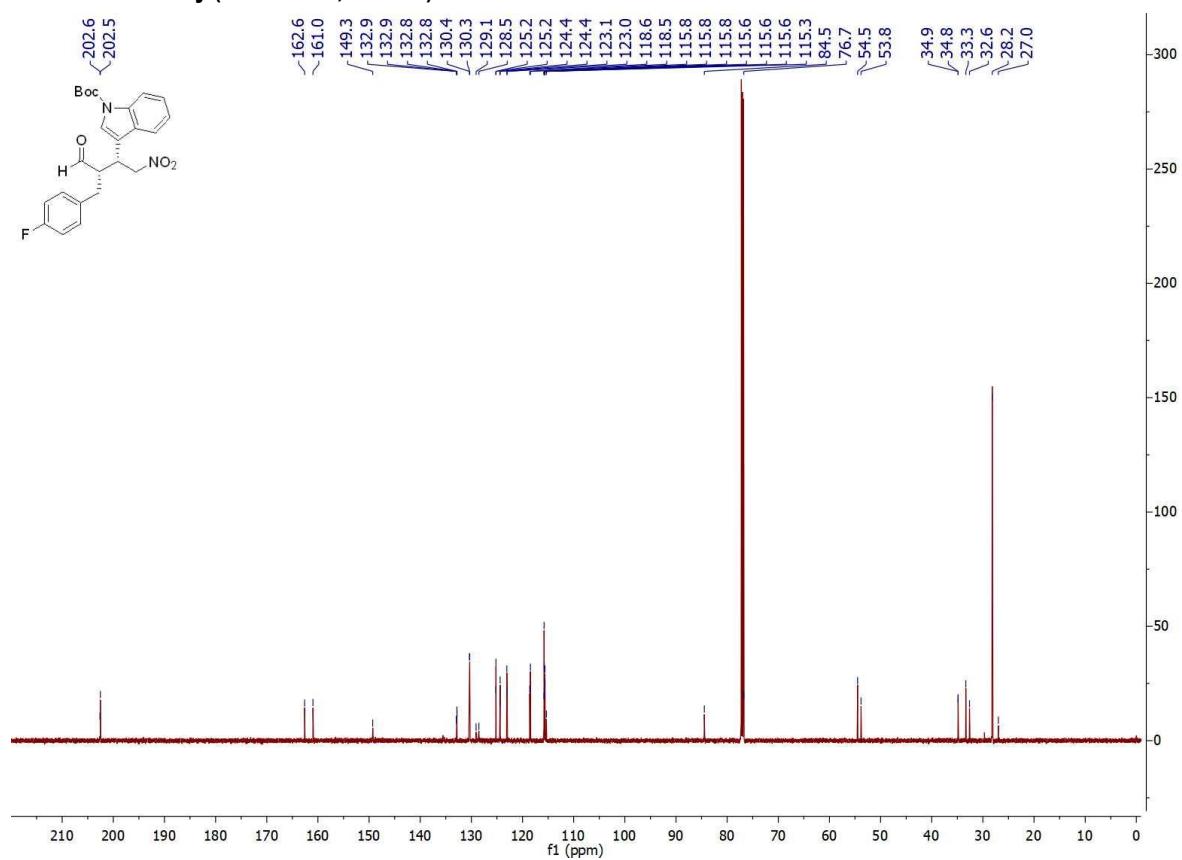
¹³C NMR of **12i** (151 MHz, CDCl₃)



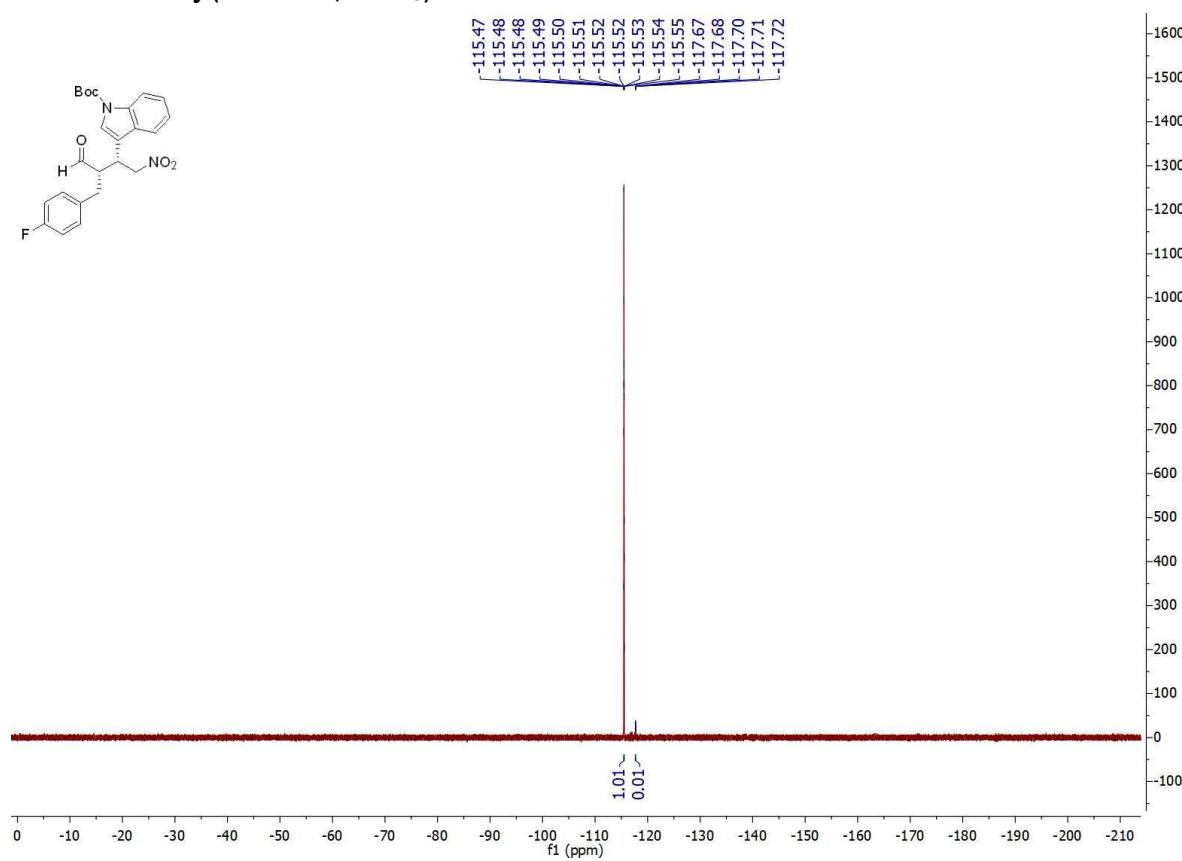
¹H NMR of **12j** (600 MHz, CDCl₃)



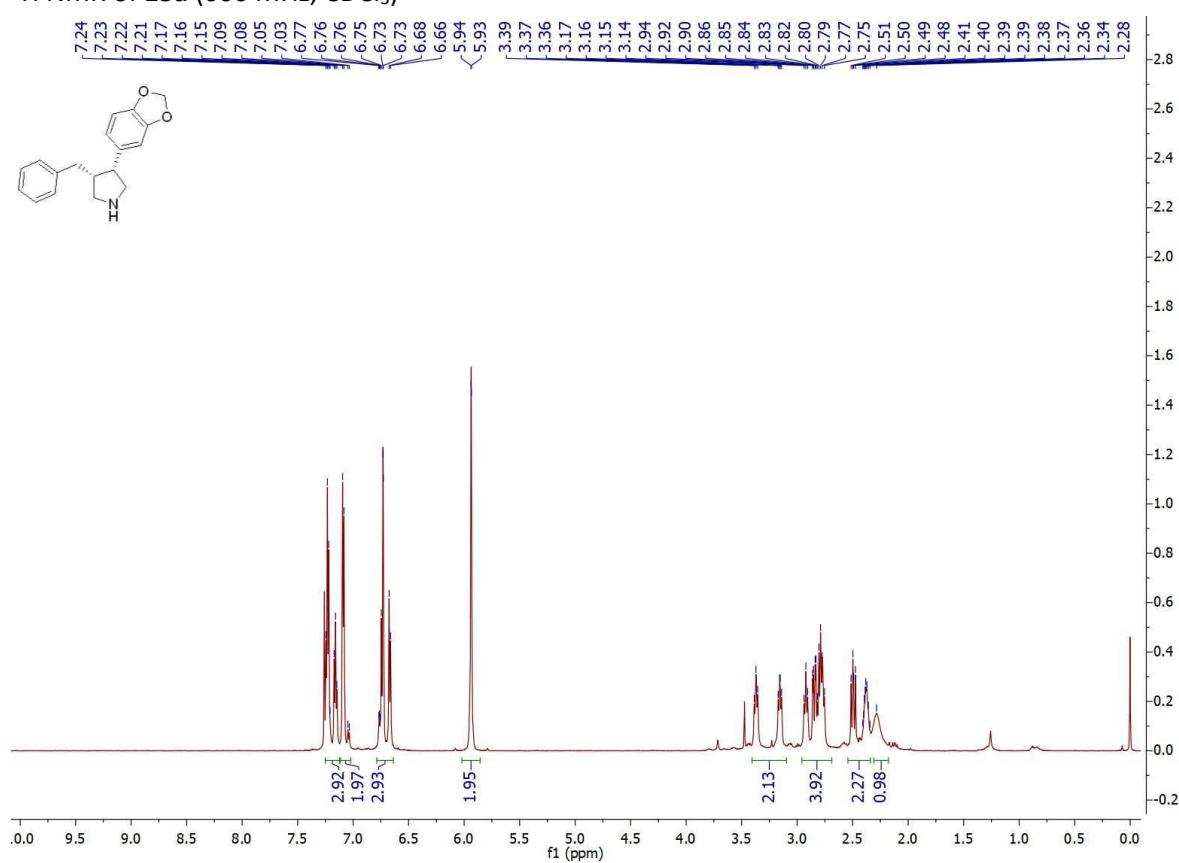
¹³C NMR of **12j** (151 MHz, CDCl₃)



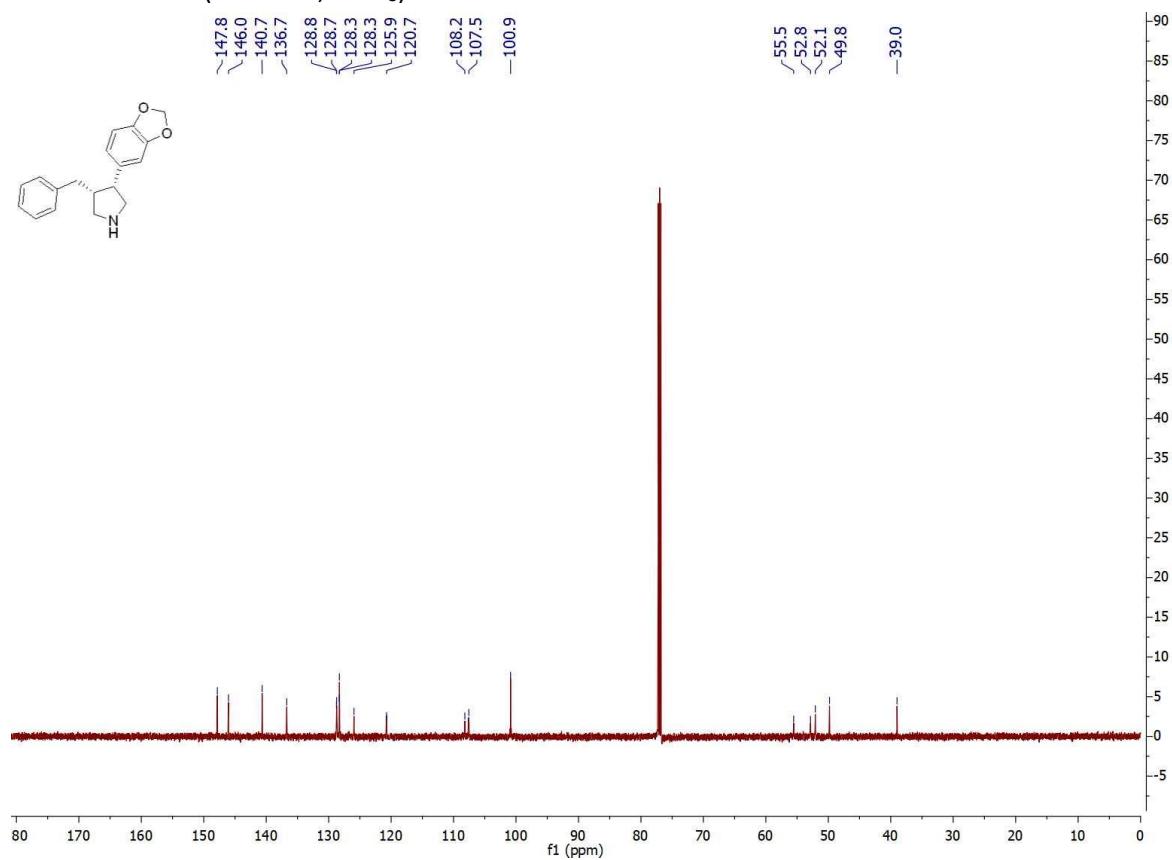
¹⁹F NMR of **12j** (564 MHz, CDCl₃)



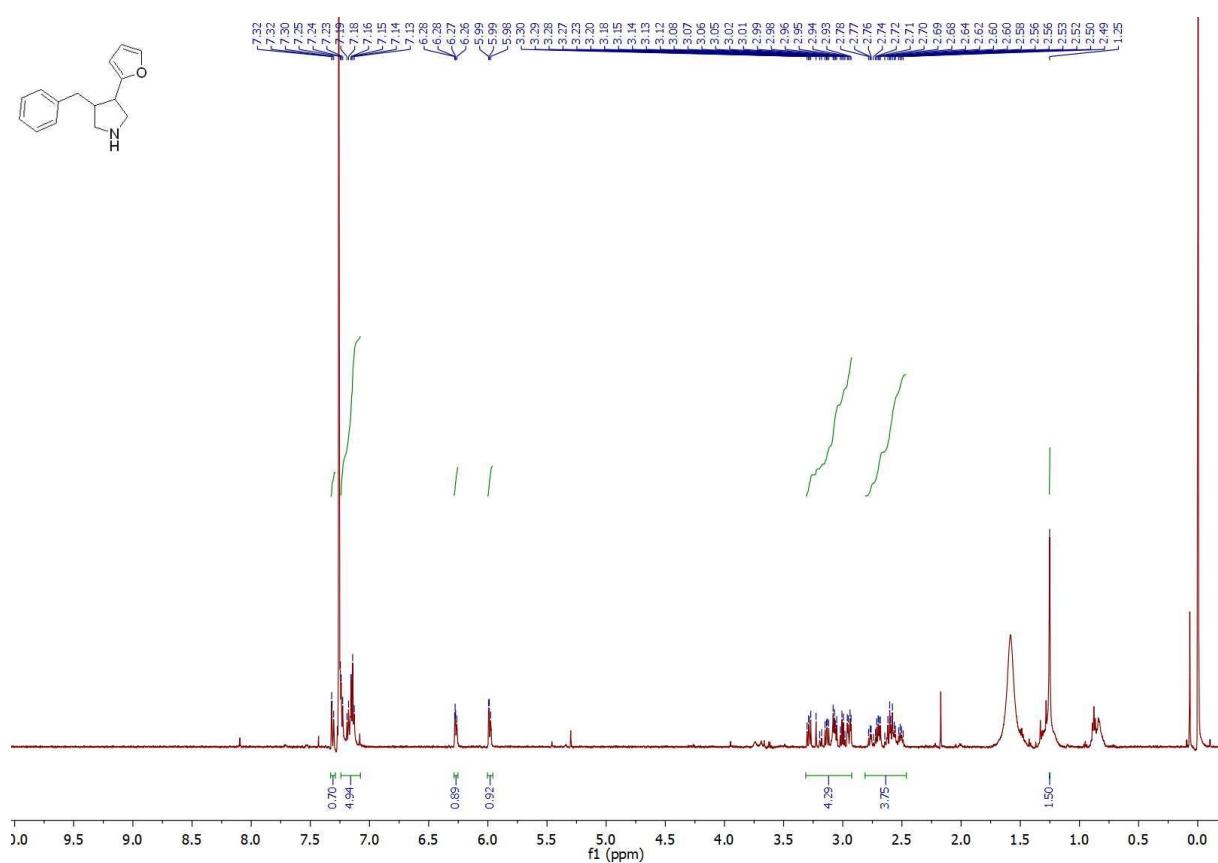
¹H NMR of **13a** (600 MHz, CDCl₃)



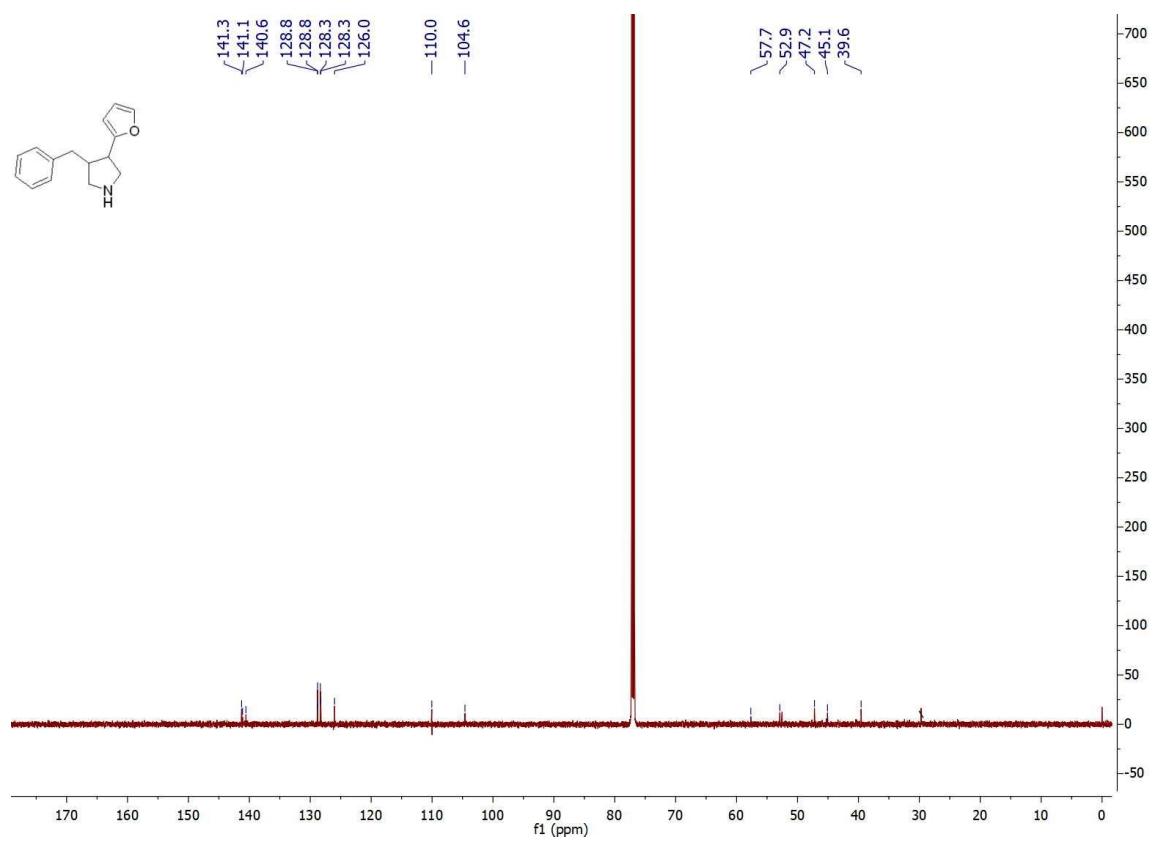
¹³C NMR of **13b** (151 MHz, CDCl₃)



¹H NMR of **13b** (600 MHz, CDCl₃)

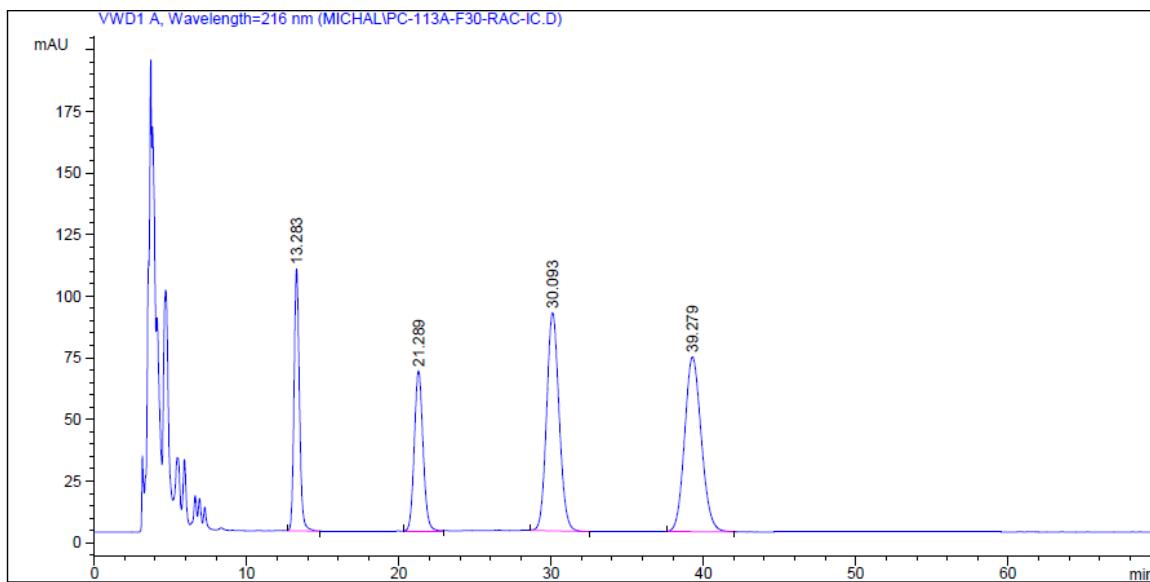


¹³C NMR of **13b** (151 MHz, CDCl₃)



Pictures of HPLC Chromatograms

11a (HPLC: Chiralcel IC, hexane:iPrOH 80:20, 1 ml/min, $\lambda = 216$ nm.)

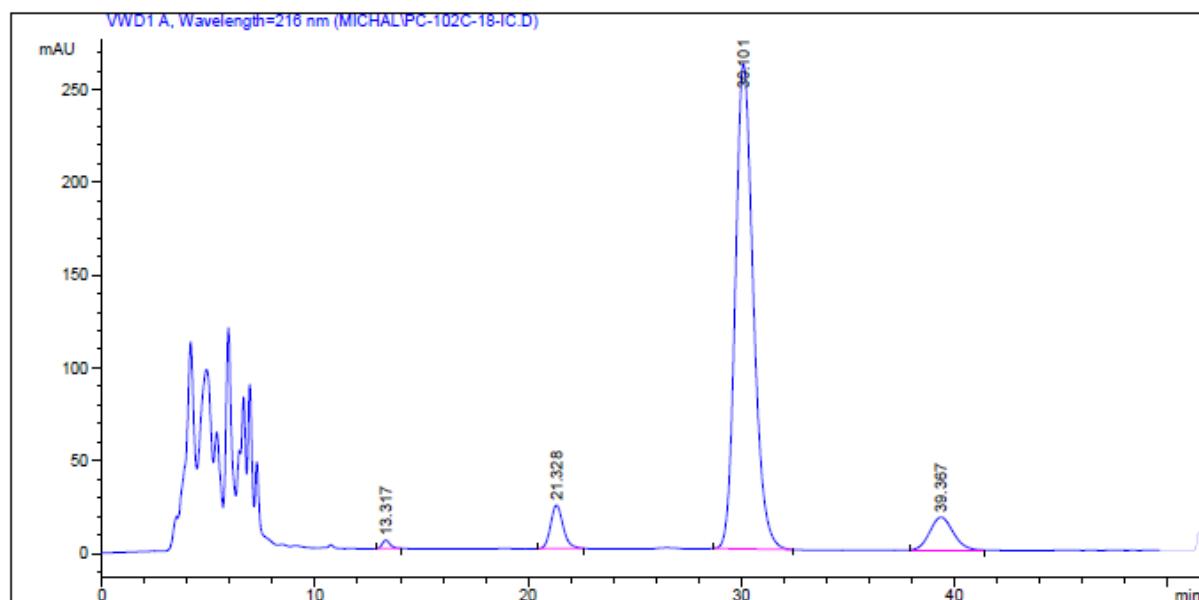


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Area Percent Report
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Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=216 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height *s [mAU]	Area %
1	13.283	BB	0.3785	2596.47290	106.17657	16.6090
2	21.289	BB	0.6153	2580.76416	64.90897	16.5085
3	30.093	BB	0.8815	5051.90039	88.49815	32.3157
4	39.279	BB	1.1803	5403.83691	70.91242	34.5669



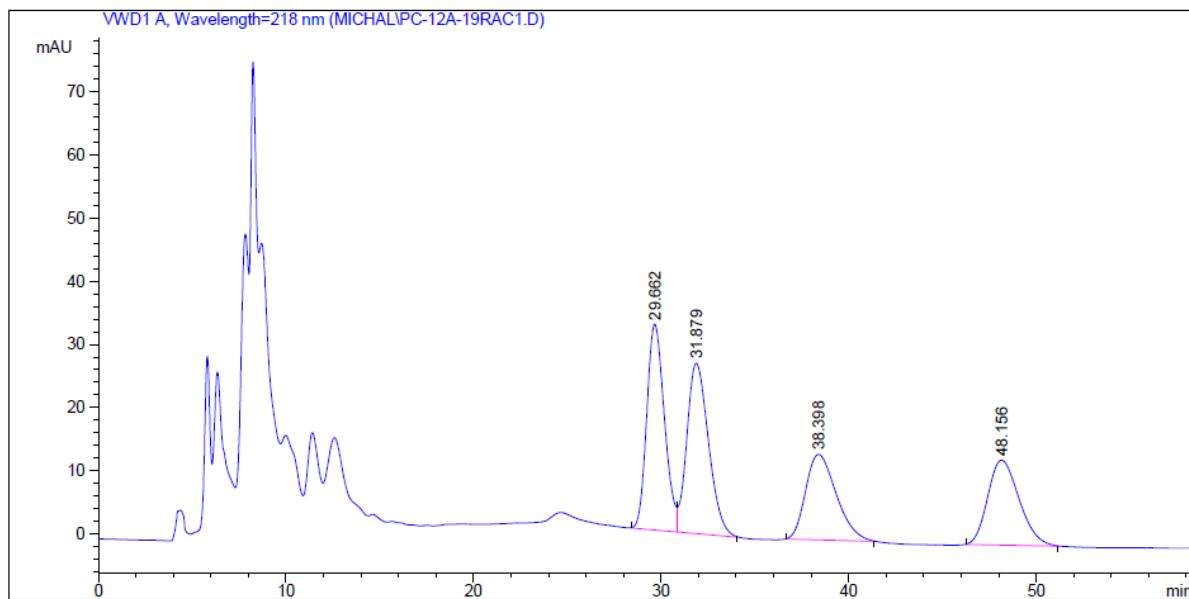
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Area Percent Report
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Sorted By : Signal
 Multiplier: : 1.0000
 Dilution: : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=216 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height *s	Area [mAU]	Area %
1	13.317	BB	0.3892	114.25976	4.50370	0.6436	
2	21.328	BB	0.6286	954.89642	23.42157	5.3785	
3	30.101	BB	0.9003	1.58224e4	261.57767	86.3044	
4	39.367	BB	1.1564	1362.35425	17.77286	7.6735	

11b (HPLC: Chiralcel AS-H, hexane:*i*PrOH 70:30, 0.75 mL/min, λ = 218nm.)

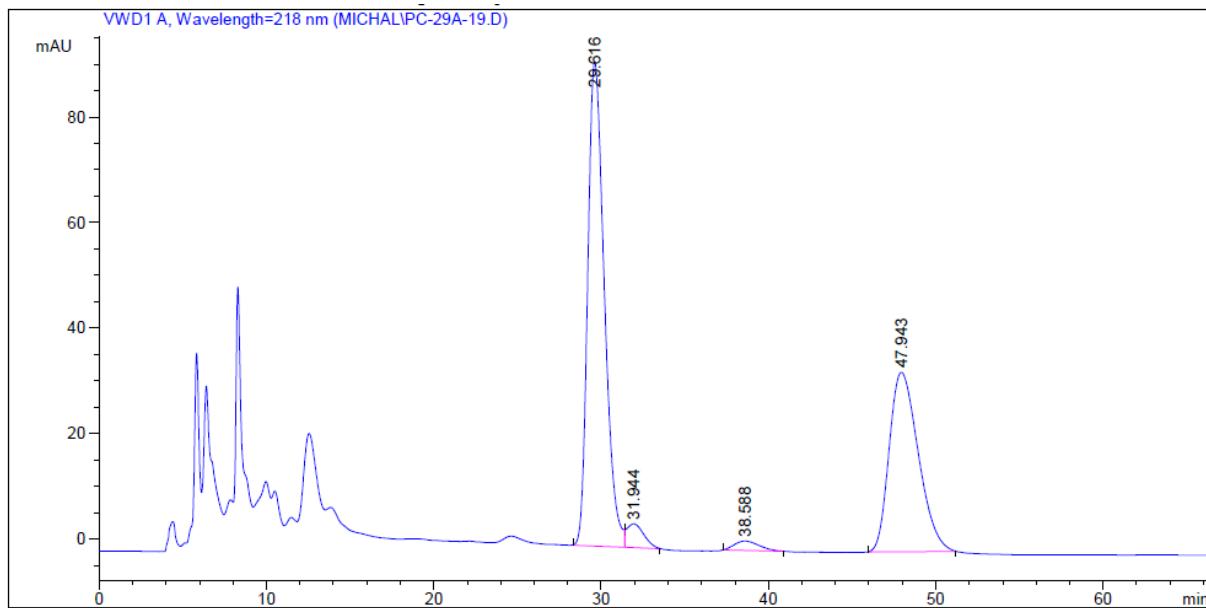


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Area Percent Report
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Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=218 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height *s	Area [mAU]	Area %
1	29.662	BV	1.0044	2129.78882	32.57758	28.8187	
2	31.879	VB	1.2195	2165.70410	26.96570	29.3047	
3	38.398	BB	1.6063	1537.77490	13.53716	20.8080	
4	48.156	BB	1.6541	1557.02344	13.44305	21.0685	



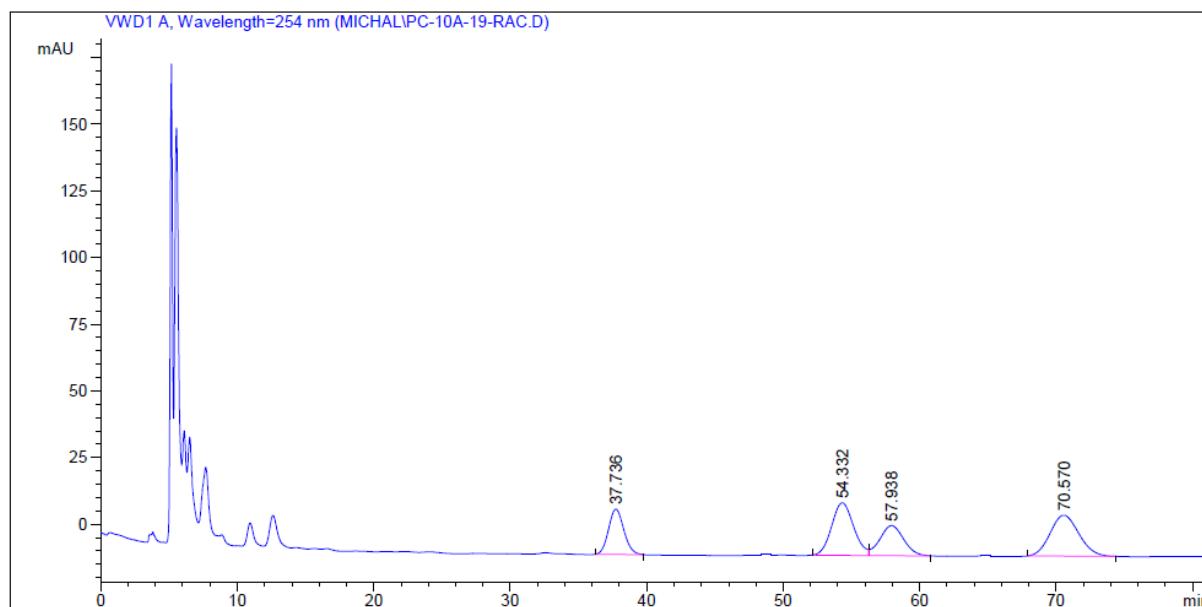
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Area Percent Report
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Sorted By : Signal
 Multiplier: : 1.0000
 Dilution: : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=218 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height *s	Area [mAU]	Area %
1	29.616	BB	1.0625	6311.06006	91.81905	57.7402	
2	31.944	BB	0.8779	318.79883	4.50557	2.9167	
3	38.588	BB	1.2097	181.20999	1.76899	1.6579	
4	47.943	BB	1.8305	4119.02002	34.01846	37.6851	

11c (HPLC: Chiralcel IC, hexane:iPrOH 70:30, 0.9 ml/min, λ = 254 nm.)

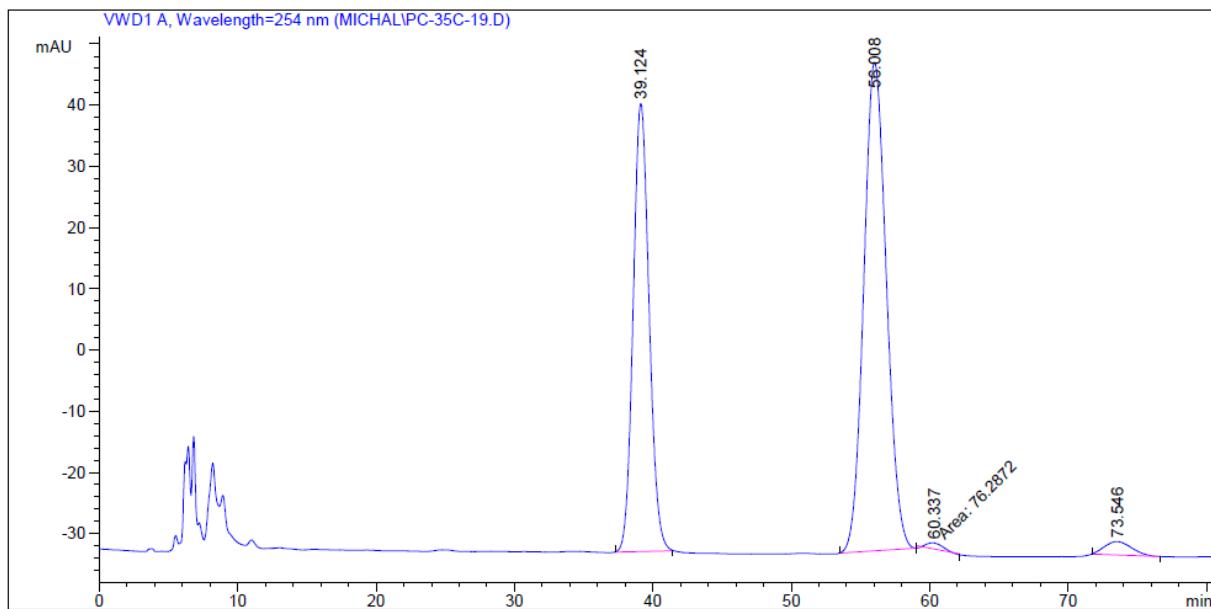


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Area Percent Report
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Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height *s	Area [mAU]	Area %
1	37.736	BB	1.1803	1329.17200	17.02256	18.5975	
2	54.332	BV	1.6316	2207.19336	19.68071	30.8826	
3	57.938	VB	1.4702	1355.96545	11.23905	18.9724	
4	70.570	BB	1.8405	2254.71875	15.36189	31.5475	



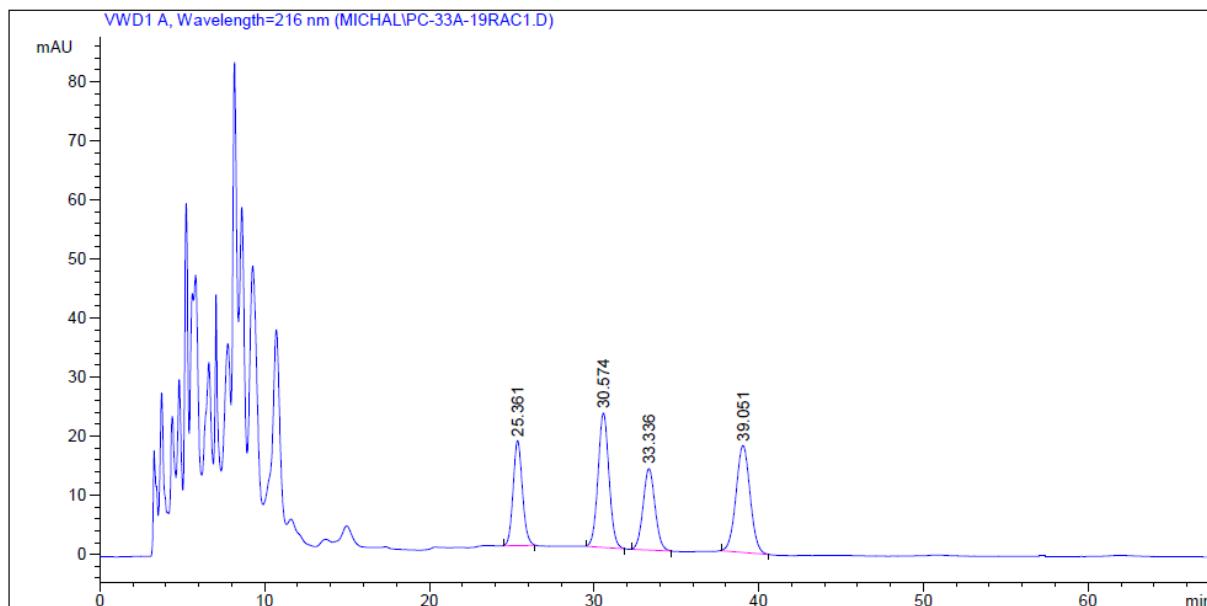
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Area Percent Report
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Sorted By : Signal
 Multiplier: : 1.0000
 Dilution: : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height *s	Area [mAU]	Area %
1	39.124	BB	1.2420	5861.13379	73.15380	38.3304	
2	56.008	BB	1.7506	9058.49023	79.81829	59.2404	
3	60.337	MM	1.2861	76.28722	9.88641e-1	0.4989	
4	73.546	BB	1.5934	295.16974	2.17711	1.9303	

11d (HPLC: Chiralcel IC, hexane:iPrOH 85:15, 1 ml/min, $\lambda = 216$ nm.)

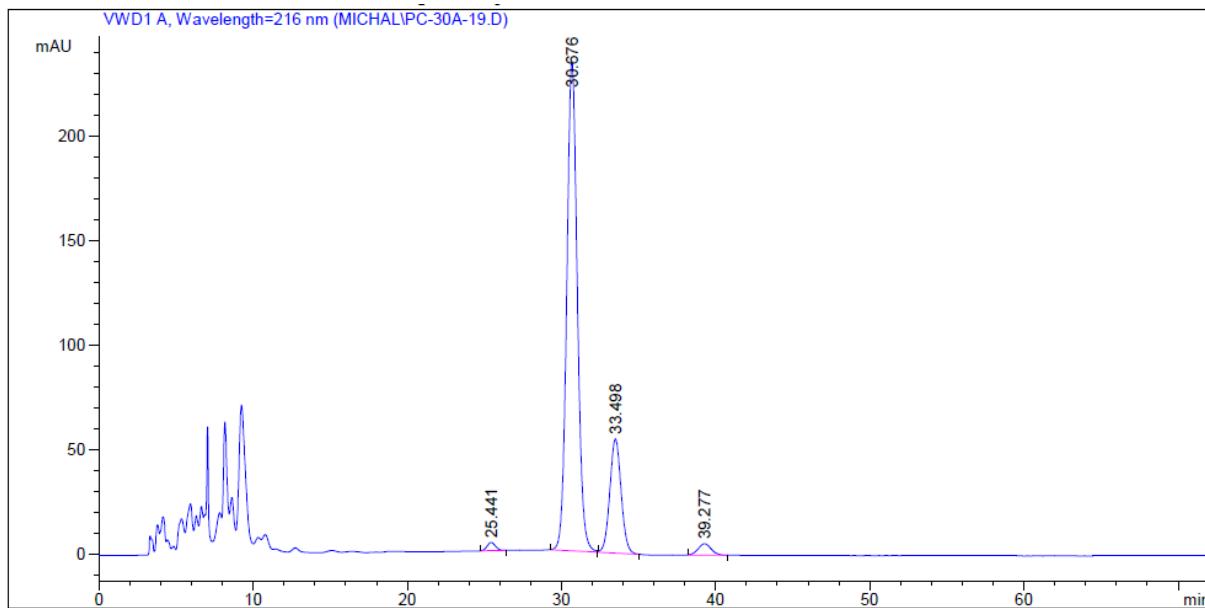


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Area Percent Report
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Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=216 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height *s	Area [mAU]	Area %
1	25.361	BB	0.6018	694.84918	17.77041	19.7196	
2	30.574	BB	0.7181	1054.23633	22.75504	29.9189	
3	33.336	BB	0.7709	696.17719	13.79111	19.7573	
4	39.051	BB	0.9135	1078.38232	18.09880	30.6042	



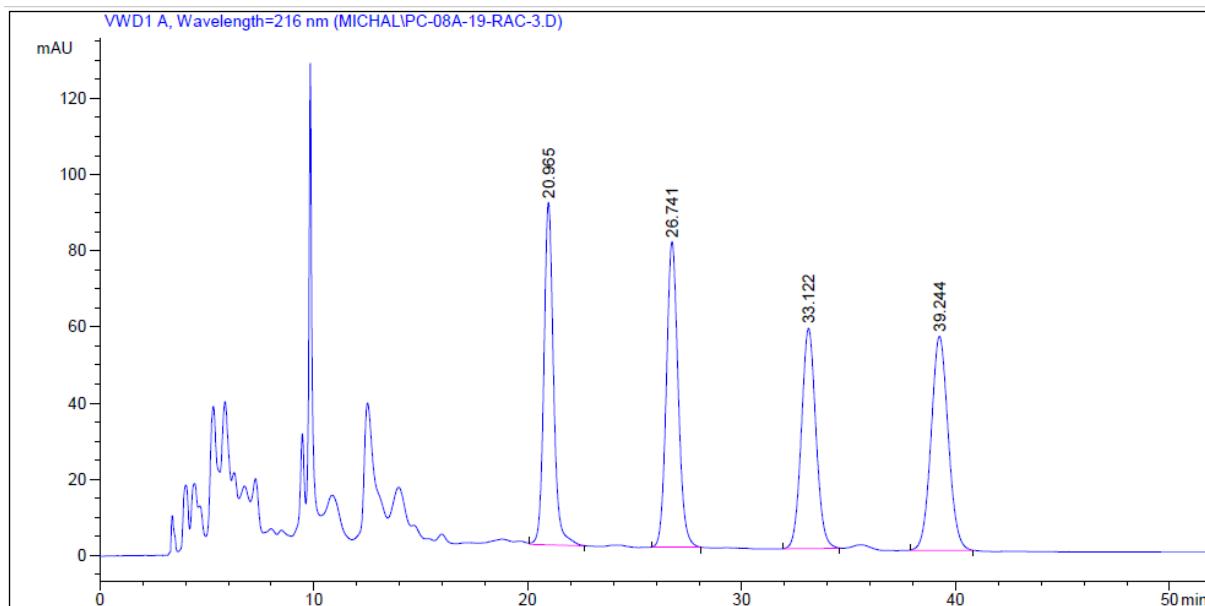
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Area Percent Report
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Sorted By : Signal
 Multiplier: : 1.0000
 Dilution: : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=216 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height *s	Area [mAU]	Area %
1	25.441	BB	0.5615	148.19505	3.93668	1.0307	
2	30.676	BB	0.7315	1.11226e4	234.27180	77.3578	
3	33.498	BB	0.7929	2789.59351	54.71293	19.4016	
4	39.277	BB	0.8821	317.74774	5.40730	2.2099	

11e (HPLC: Chiralcel IC, hexane:iPrOH 90:10, 1 ml/min, $\lambda = 216$ nm.)

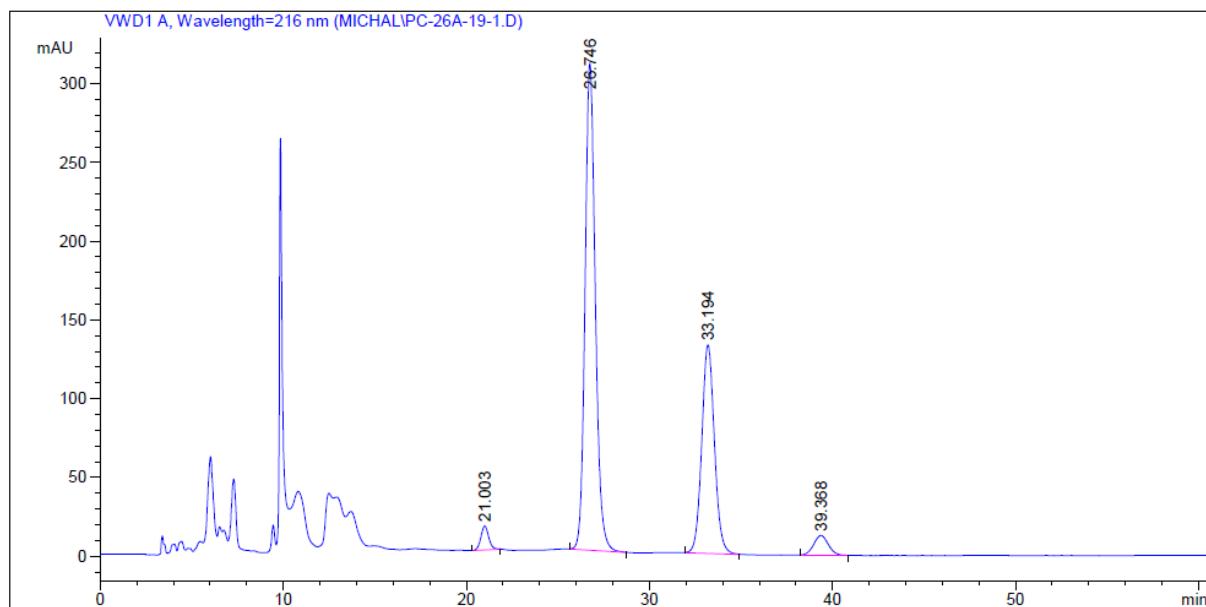


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Area Percent Report
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Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=216 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height *s	Area [mAU]	Area %
1	20.965	VB	0.4755	2800.93237	89.92025	23.8957	
2	26.741	BB	0.5866	3064.42139	80.28000	26.1436	
3	33.122	BB	0.7263	2725.66919	57.80637	23.2536	
4	39.244	BB	0.8606	3130.47363	56.22982	26.7071	



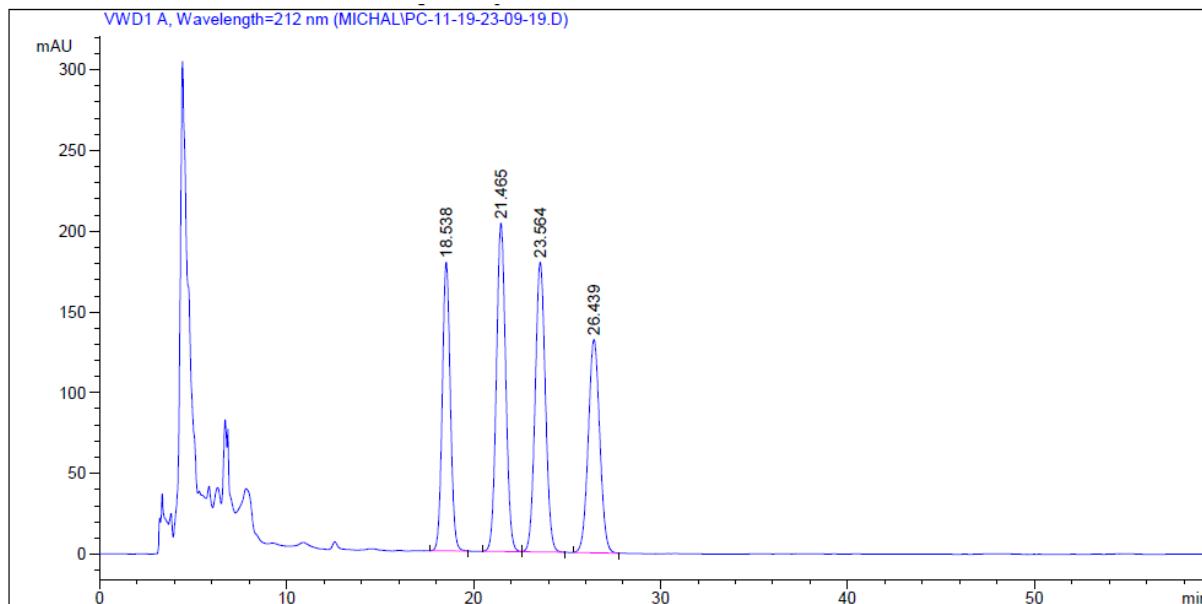
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Area Percent Report
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Sorted By : Signal
 Multiplier: : 1.0000
 Dilution: : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=216 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height *s	Area [mAU]	Area %
1	21.003	BB	0.4558	447.51834	15.12592	2.2917	
2	26.746	BB	0.5980	1.20314e4	309.28647	61.6113	
3	33.194	BB	0.7385	6347.80322	132.37378	32.5064	
4	39.368	BB	0.8604	701.16449	12.54262	3.5906	

11f (HPLC: Chiralcel IC, hexane:iPrOH 85:15, 1 ml/min, $\lambda = 212$ nm.)

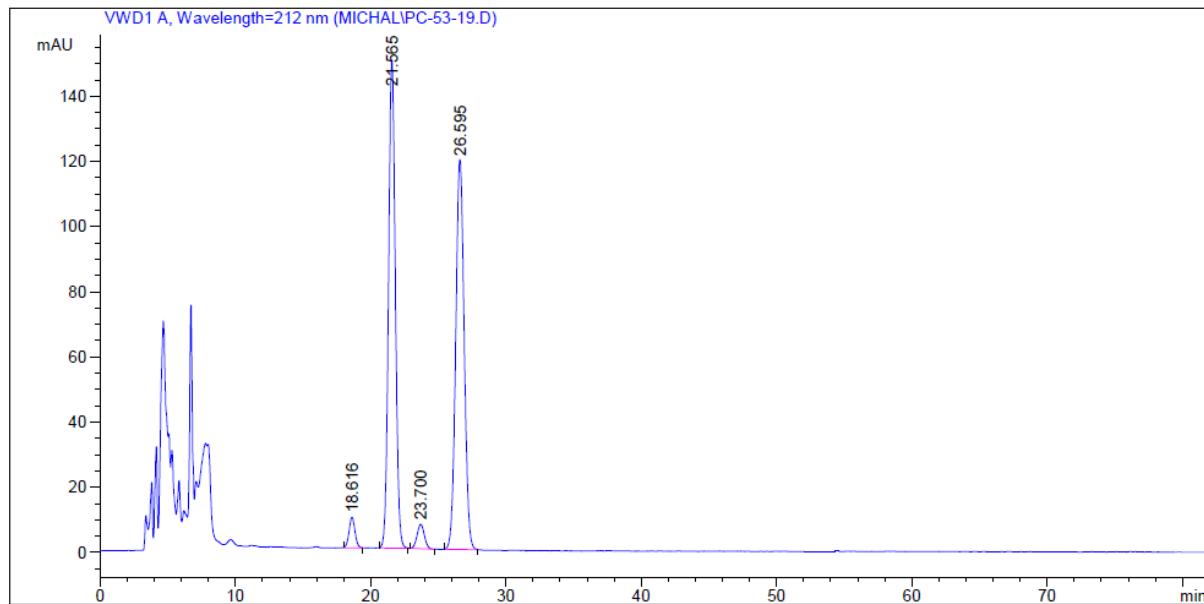


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Area Percent Report
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Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=212 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height *s	Area [mAU]	Area %
1	18.538	BB	0.4614	5331.98047	178.84648	21.5050	
2	21.465	BB	0.5351	7019.46680	203.41415	28.3110	
3	23.564	BB	0.5876	6802.26318	179.54926	27.4349	
4	26.439	BB	0.6612	5640.44238	132.10074	22.7491	



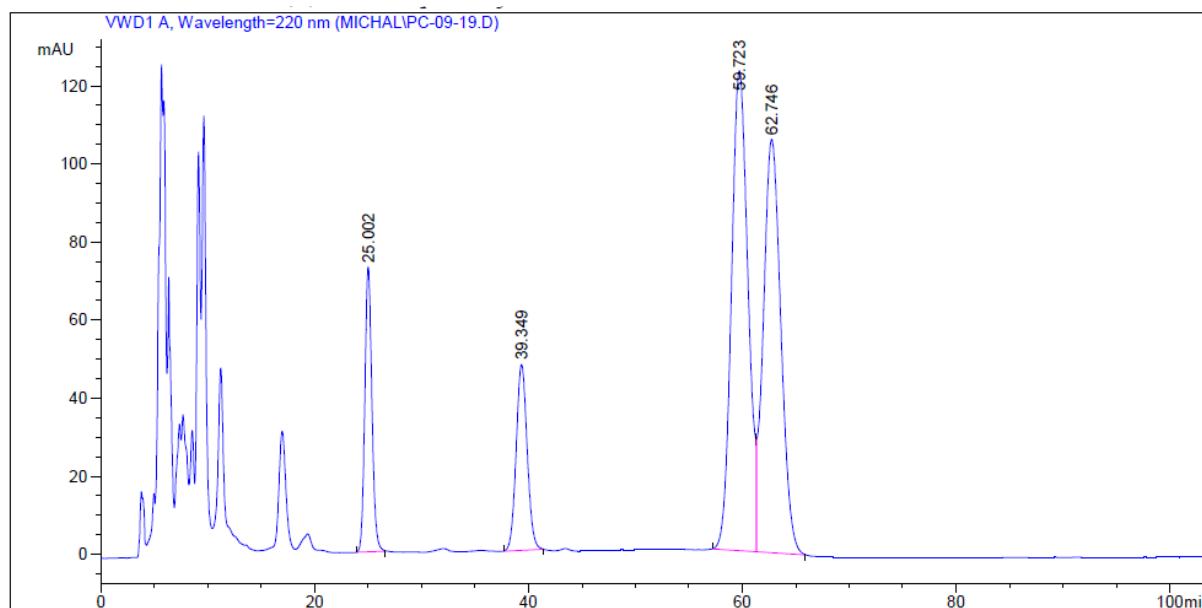
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          Area Percent Report
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Sorted By : Signal
 Multiplier: : 1.0000
 Dilution: : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=212 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height *s	Area [mAU]	Area %
1	18.616	BB	0.4622	282.45081	9.37424	2.5738	
2	21.565	BB	0.5397	5226.68555	149.75716	47.6269	
3	23.700	BB	0.5773	281.34131	7.47760	2.5637	
4	26.595	BB	0.6715	5183.74658	119.63189	47.2357	

11g (HPLC: Chiralcel IC, hexane:iPrOH 80:20, 0.95 ml/min, λ = 220 nm.)

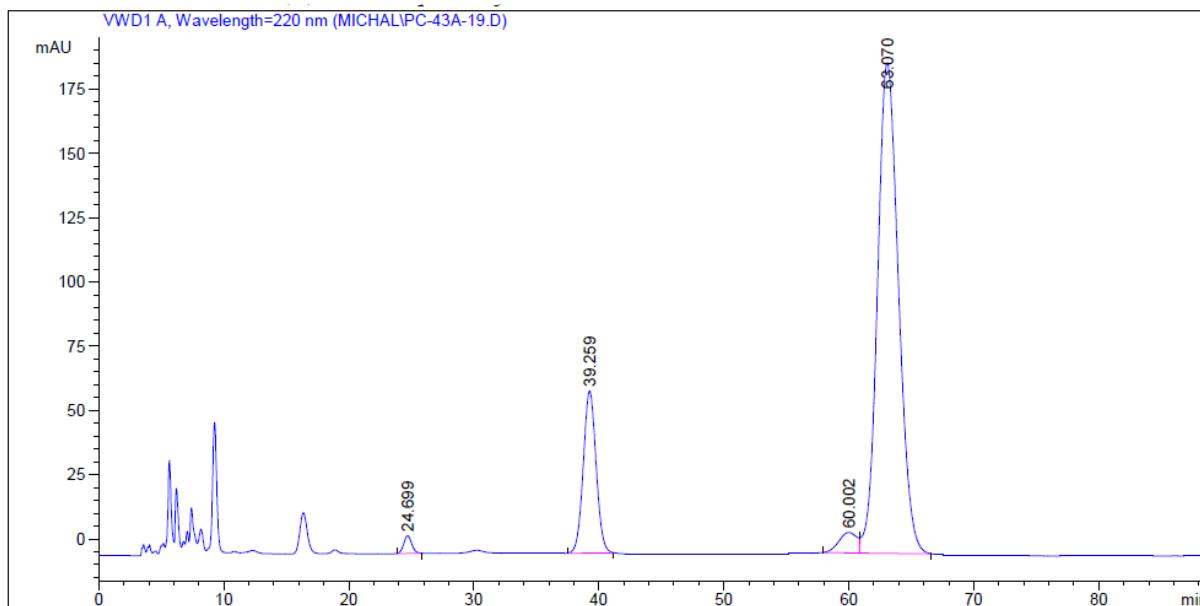


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Area Percent Report
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Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=220 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height *s	Area [mAU]	Area %
1	25.002	BB	0.7067	3353.71924	72.94981	10.4383	
2	39.349	BB	1.1103	3412.42041	47.58894	10.6210	
3	59.723	BV	1.6459	1.32201e4	122.96600	41.1470	
4	62.746	VB	1.7289	1.21427e4	105.93920	37.7937	



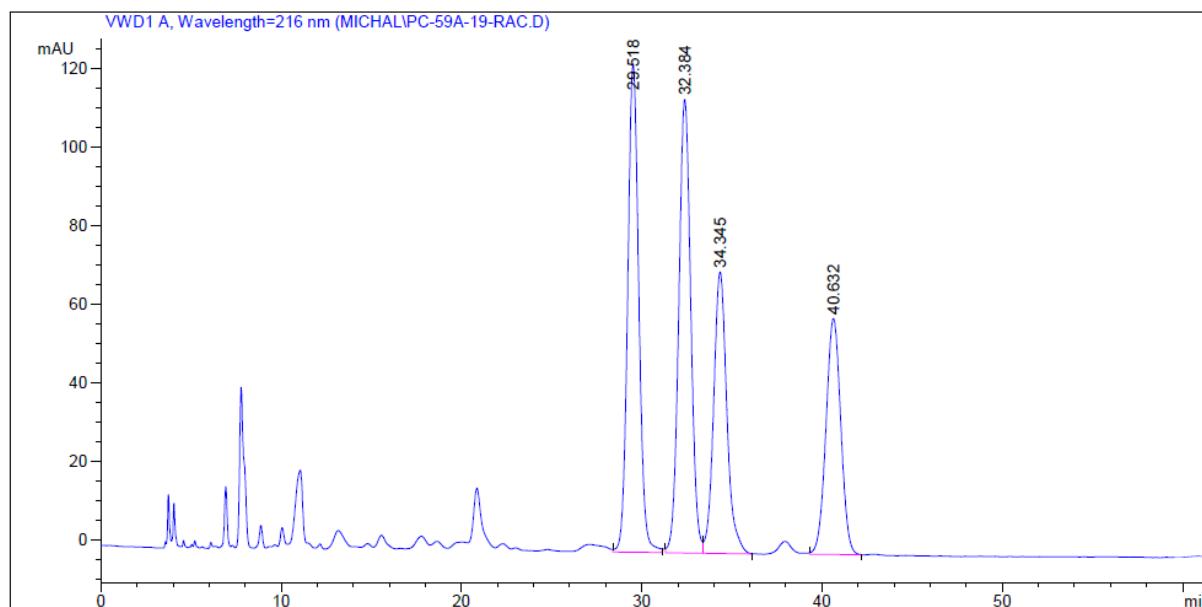
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          Area Percent Report
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Sorted By           :      Signal
Multiplier:        :      1.0000
Dilution:         :      1.0000
Use Multiplier & Dilution Factor with ISTDs
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Signal 1: VWD1 A, Wavelength=220 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height *s	Area [mAU]	Area %
1	24.699	BB	0.6821	306.94781	6.89938	1.0997	
2	39.259	BB	1.1091	4499.16260	63.05508	16.1197	
3	60.002	BV	1.2419	796.33228	7.94703	2.8531	
4	63.070	VB	1.8071	2.23085e4	190.94662	79.9274	

11h (HPLC: Chiralcel IC, hexane:iPrOH 91:9, 0.9 ml/min, $\lambda = 216$ nm.)

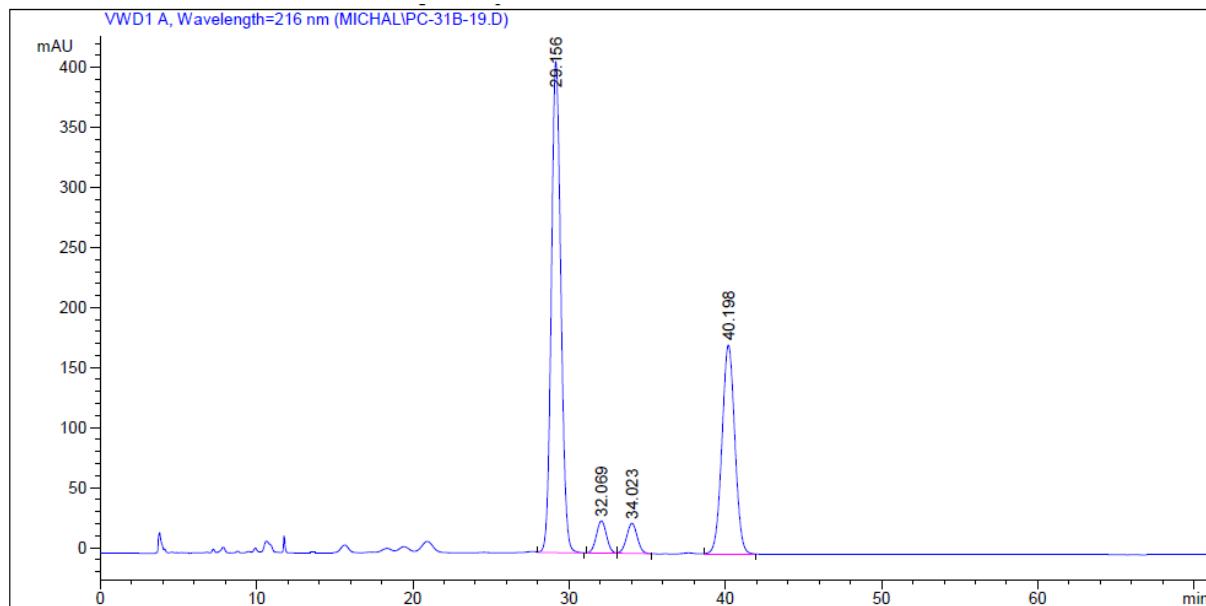


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Area Percent Report
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Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=216 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height *s	Area [mAU]	Area %
1	29.518	VB	0.6619	5314.45605	124.29707	29.9878	
2	32.384	BV	0.7186	5327.38721	115.50718	30.0608	
3	34.345	VB	0.7770	3644.51099	71.64185	20.5649	
4	40.632	BB	0.8879	3435.67676	60.12780	19.3865	



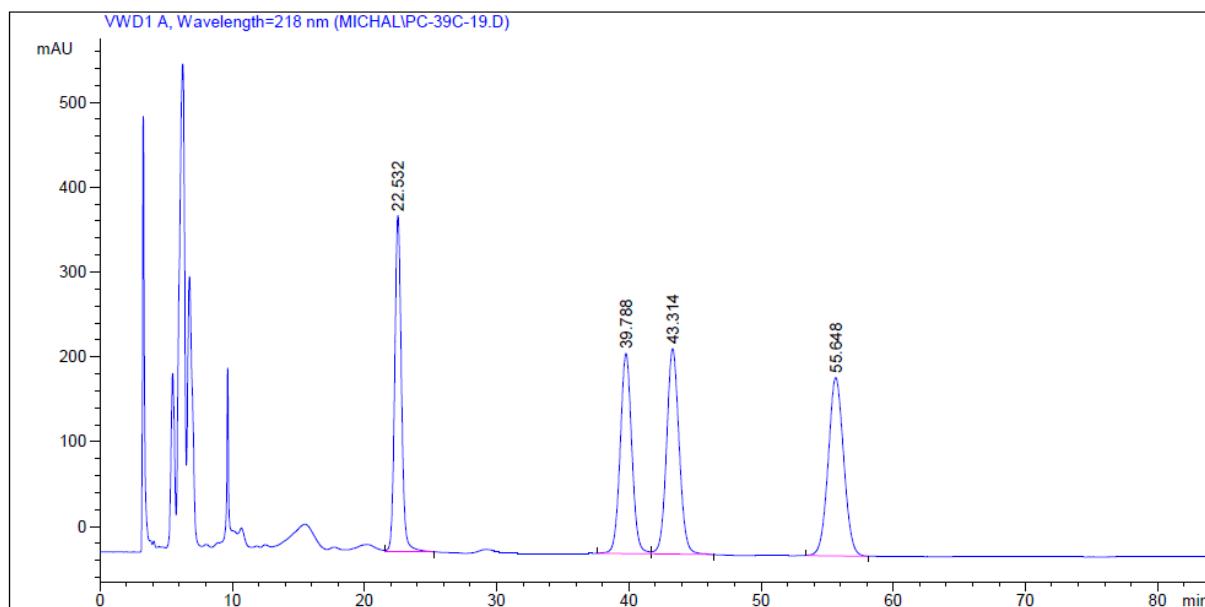
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          Area Percent Report
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Sorted By      :      Signal
Multiplier:    :      1.0000
Dilution:     :      1.0000
Use Multiplier & Dilution Factor with ISTDs
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Signal 1: VWD1 A, Wavelength=216 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height *s	Area [mAU]	Area %
1	29.156	VB	0.6572	1.73226e4	408.95953	58.3895	
2	32.069	BV	0.7031	1208.98865	26.84185	4.0752	
3	34.023	VB	0.7379	1192.29956	25.15563	4.0189	
4	40.198	BB	0.8910	9943.40332	173.97682	33.5164	

11i (HPLC: Chiralcel IC, hexane:iPrOH 90:10, 1 ml/min, $\lambda = 218 \text{ nm}.$)

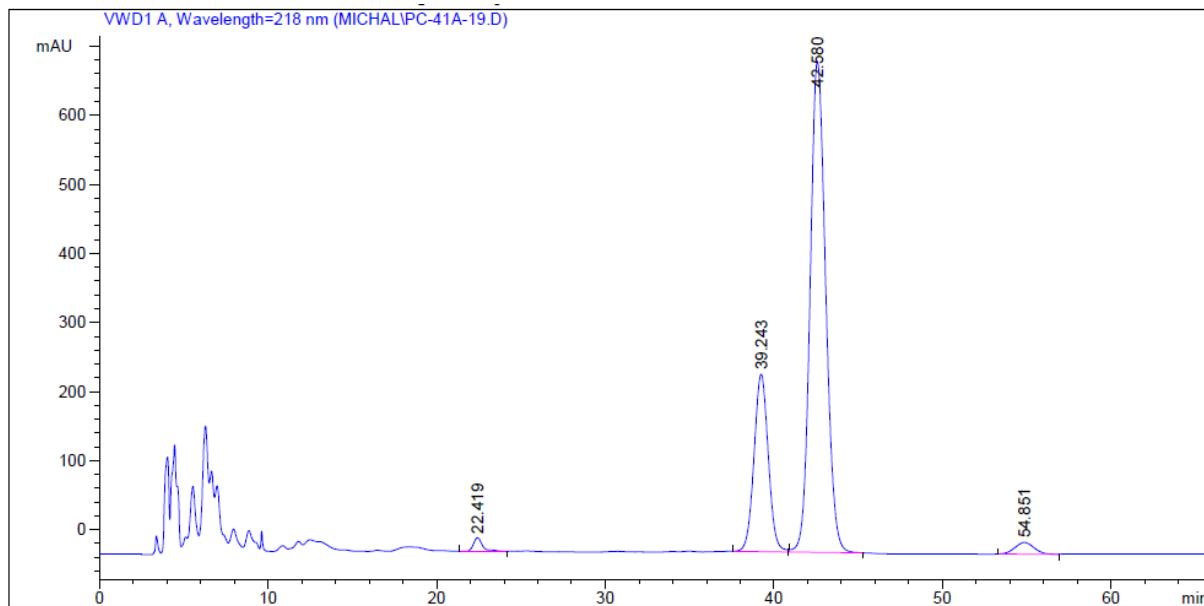


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Area Percent Report
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Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=218 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height *s	Area [mAU]	Area %
1	22.532	VB	0.5442	1.40404e4	396.47687	22.8383	
2	39.788	BB	0.9374	1.43587e4	235.83685	23.3561	
3	43.314	BB	1.0115	1.59789e4	242.15331	25.9916	
4	55.648	BB	1.2484	1.70992e4	209.99814	27.8139	



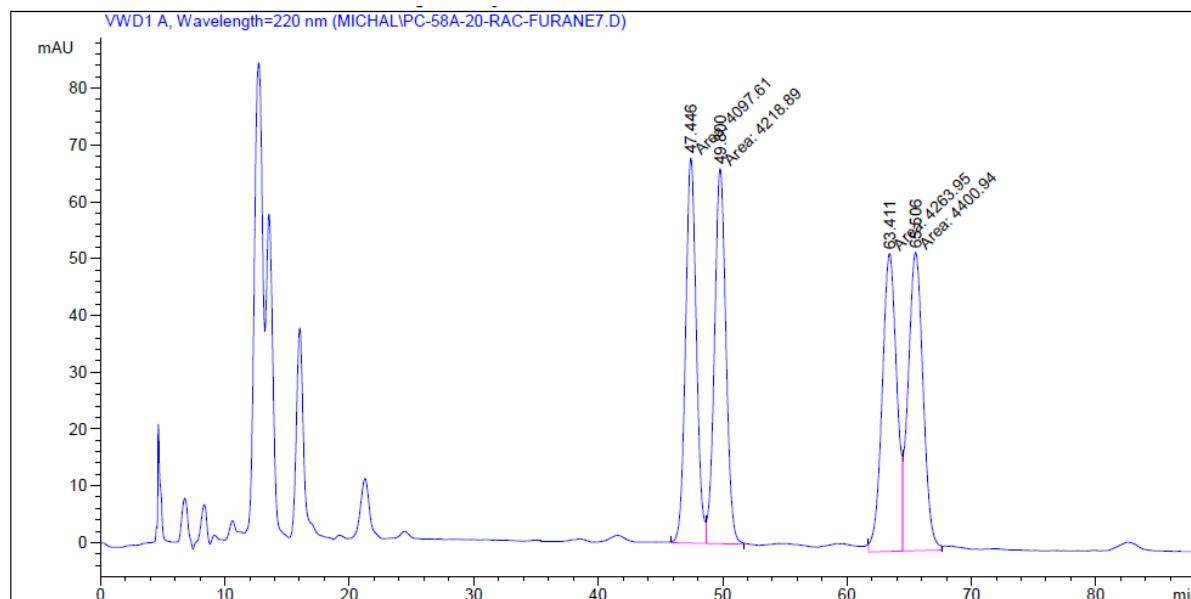
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Area Percent Report
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Sorted By : Signal
 Multiplier: : 1.0000
 Dilution: : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=218 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height *s	Area [mAU]	Area %
1	22.419	VB	0.5783	762.43298	19.69760	1.2139	
2	39.243	BB	0.9060	1.50859e4	257.05795	24.0195	
3	42.580	BB	0.9933	4.56143e4	710.78998	72.6262	
4	54.851	BB	1.1978	1344.32703	16.91994	2.1404	

11j (HPLC: IC, hexane/iPrOH 96:6, 0.75 mL/min, $\lambda = 216$ nm)

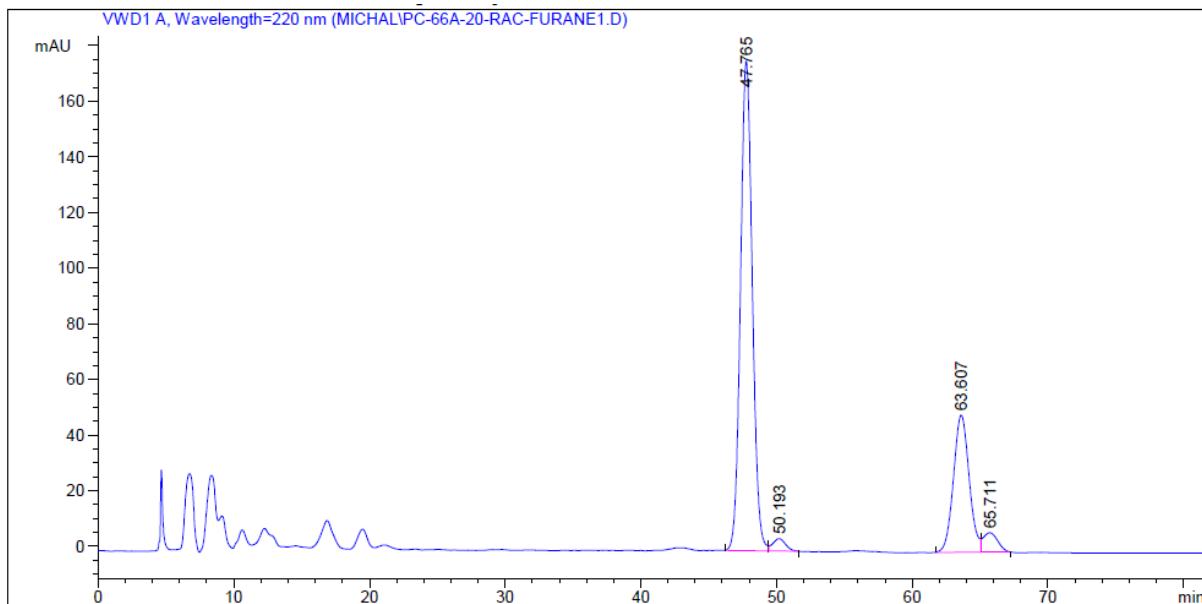


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Area Percent Report
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Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=220 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height *s	Area [mAU]	Area %
1	47.446	FM	1.0077	4097.61230	67.76893	24.1300	
2	49.800	FM	1.0650	4218.88965	66.02110	24.8442	
3	63.411	MF	1.3553	4263.95117	52.43453	25.1095	
4	65.506	FM	1.3967	4400.94092	52.51561	25.9163	



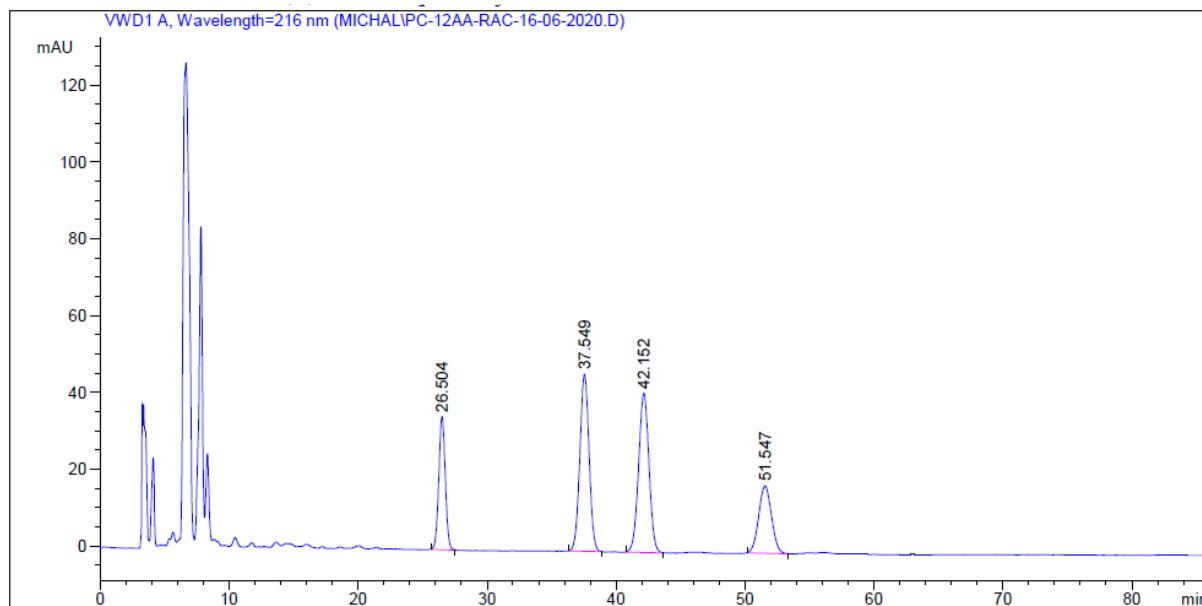
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Area Percent Report
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Sorted By : Signal
 Multiplier: : 1.0000
 Dilution: : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=220 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height *s	Area [mAU]	Area %
1	47.765	BB	0.9373	1.06399e4	175.88651	68.9821	
2	50.193	BB	0.9072	292.29660	4.45176	1.8951	
3	63.607	BV	1.2335	3961.23096	49.34758	25.6820	
4	65.711	VB	1.0449	530.72394	6.99872	3.4409	

12a (HPLC: IC, hexane/*i*PrOH 85:15, 1 mL/min, $\lambda = 216$ nm)

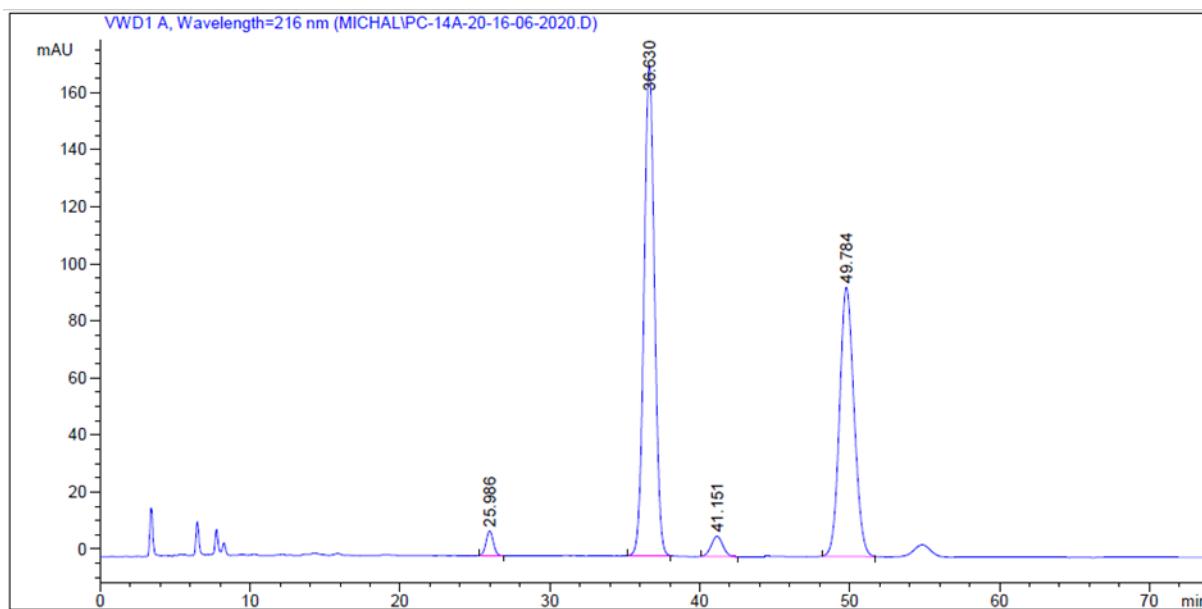


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Area Percent Report
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Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=216 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height *s	Area [mAU]	Area %
1	26.504	BB	0.5445	1218.14233	34.73084	17.2682	
2	37.549	BB	0.7783	2300.11426	46.12481	32.6060	
3	42.152	BB	0.8681	2324.16138	41.45860	32.9469	
4	51.547	BB	1.0530	1211.84680	17.58374	17.1789	



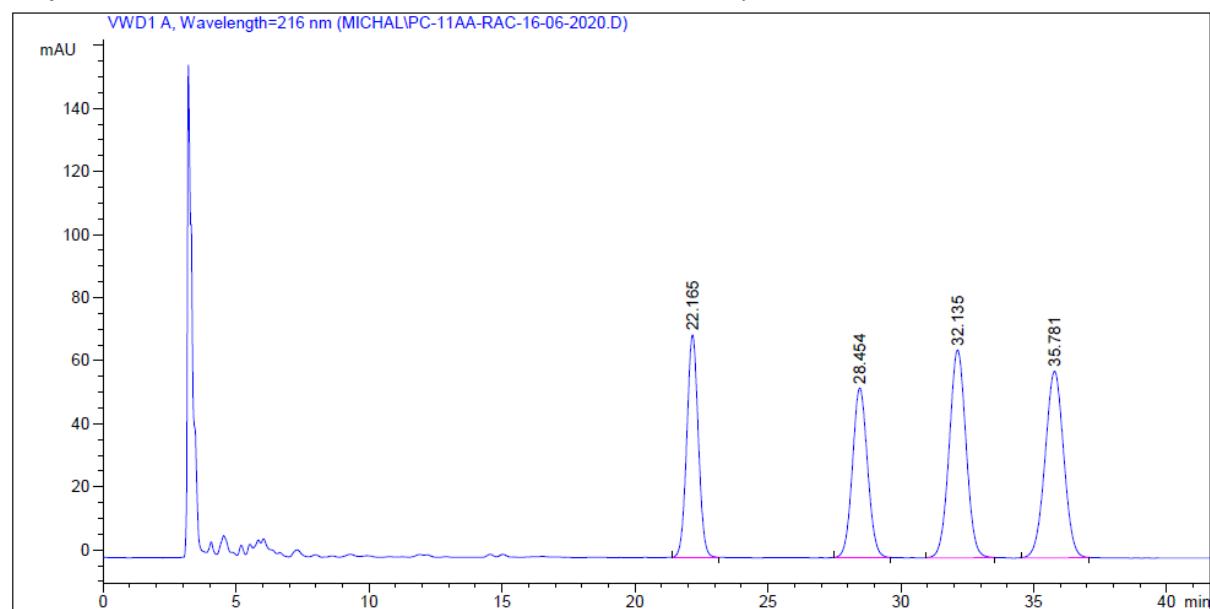
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Area Percent Report
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Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=216 nm

#	RetTime	Type	Width	Area	Height	Area	
	[min]		[min]	mAU	*s	[mAU]	%
1	25.986	BB	0.5300	296.04974	8.72120	1.9179	
2	36.630	BB	0.7604	8397.25195	171.98152	54.4010	
3	41.151	BB	0.8099	380.14072	7.08006	2.4627	
4	49.784	BB	1.0531	6362.39160	94.35485	41.2183	

12b (HPLC: IC, hexane/iPrOH 85:15, 1 mL/min, $\lambda = 216$ nm)

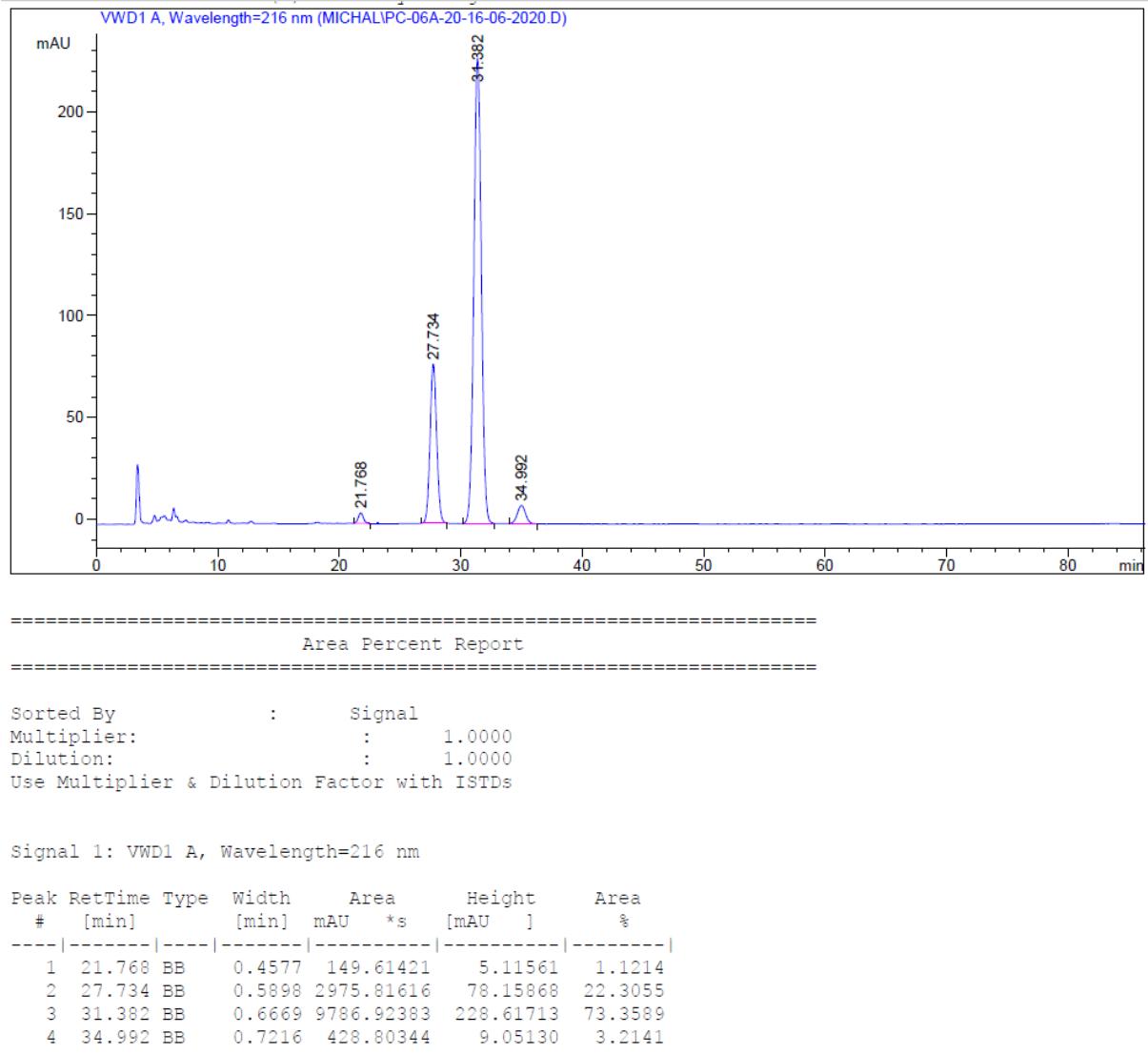


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Area Percent Report
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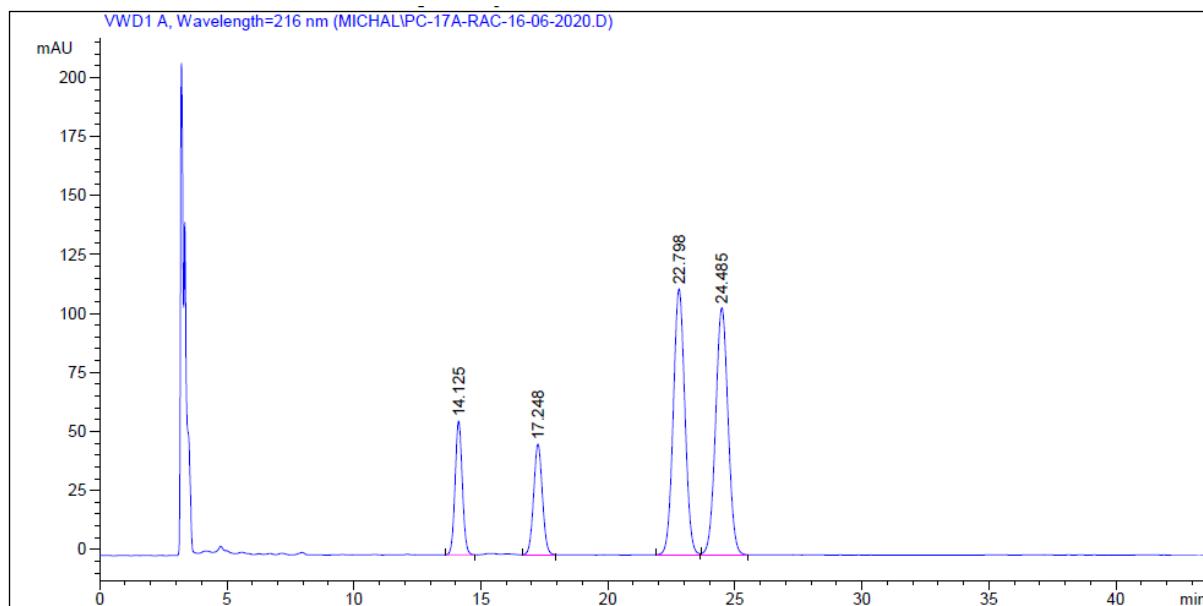
Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=216 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height *s	Area [mAU]	Area %
1	22.165	BB	0.4651	2119.31909	70.62737	21.1343	
2	28.454	BB	0.6121	2124.46069	53.80249	21.1856	
3	32.135	BB	0.6842	2901.33325	65.86937	28.9328	
4	35.781	BB	0.7551	2882.73242	59.13799	28.7473	



12c (HPLC: IC, hexane/*i*PrOH 85:15, 1 mL/min, λ = 216 nm)

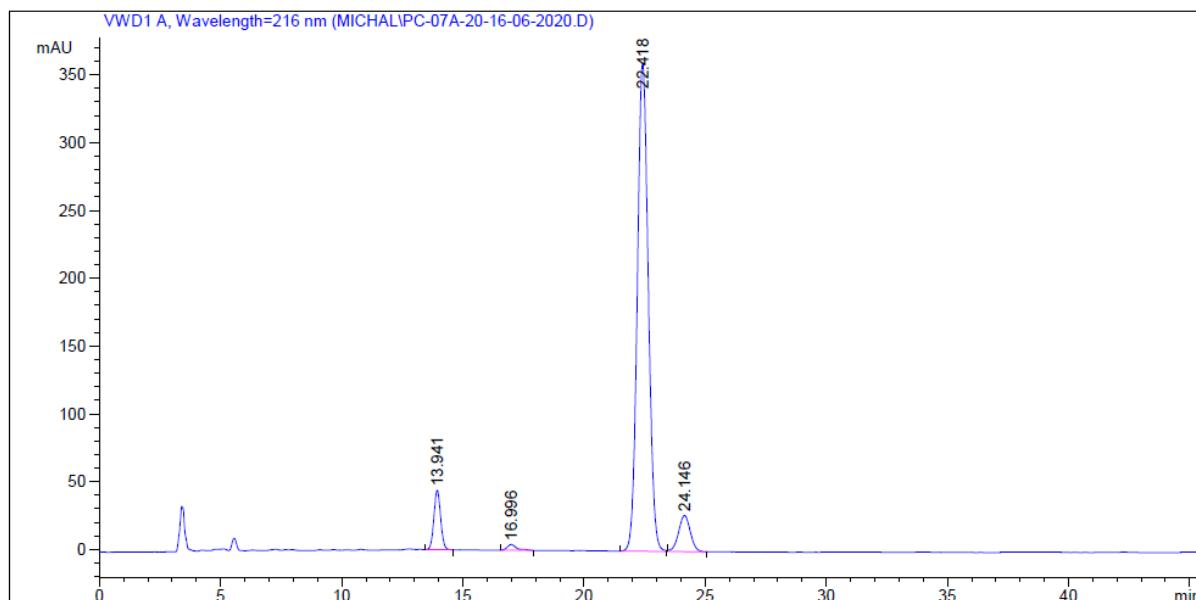


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Area Percent Report
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Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=216 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height *s	Area [mAU]	Area %
1	14.125	BB	0.3060	1118.26355	56.66345	11.9274	
2	17.248	BB	0.3712	1116.65479	46.85920	11.9102	
3	22.798	BB	0.4917	3569.45630	112.73074	38.0718	
4	24.485	BB	0.5304	3571.21826	104.71623	38.0906	



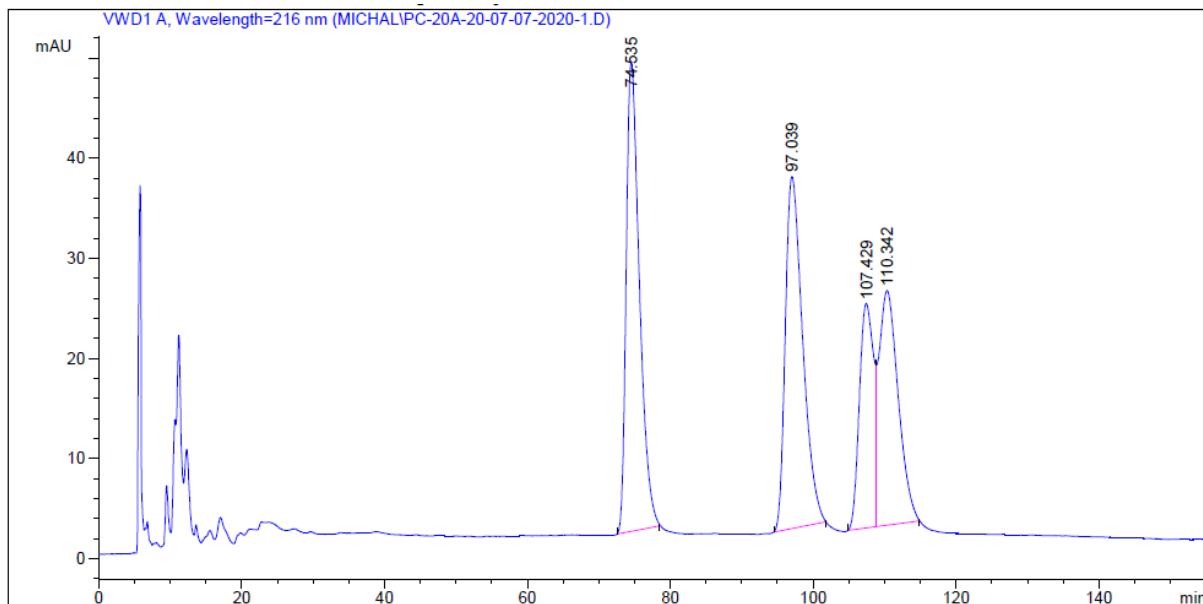
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          Area Percent Report
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Sorted By : Signal
 Multiplier: : 1.0000
 Dilution: : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=216 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height *s	Area [mAU]	Area %
1	13.941	VB	0.2993	855.40991	44.06462	6.4908	
2	16.996	BB	0.4071	115.54956	4.21620	0.8768	
3	22.418	BB	0.4871	1.13079e4	360.17386	85.8037	
4	24.146	BB	0.5234	899.93457	26.66271	6.8287	

12d (HPLC: OJ-H, hexane/iPrOH 63:37, 0.63 mL/min, $\lambda = 216$ nm)

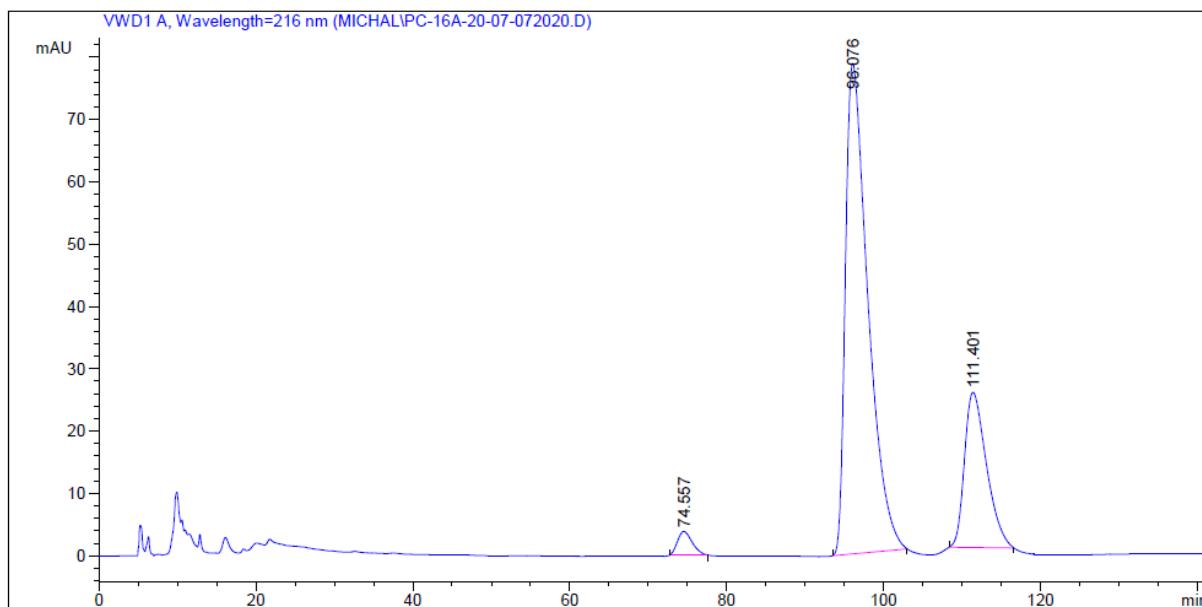


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Area Percent Report
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Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=216 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height *s	Area [mAU]	Area %
1	74.535	BB	1.8374	6020.59521	46.92868	30.9928	
2	97.039	BB	2.3580	5929.91211	35.15653	30.5260	
3	107.429	BV	1.8226	3105.11987	22.41953	15.9845	
4	110.342	VB	2.2004	4370.13281	23.43453	22.4966	



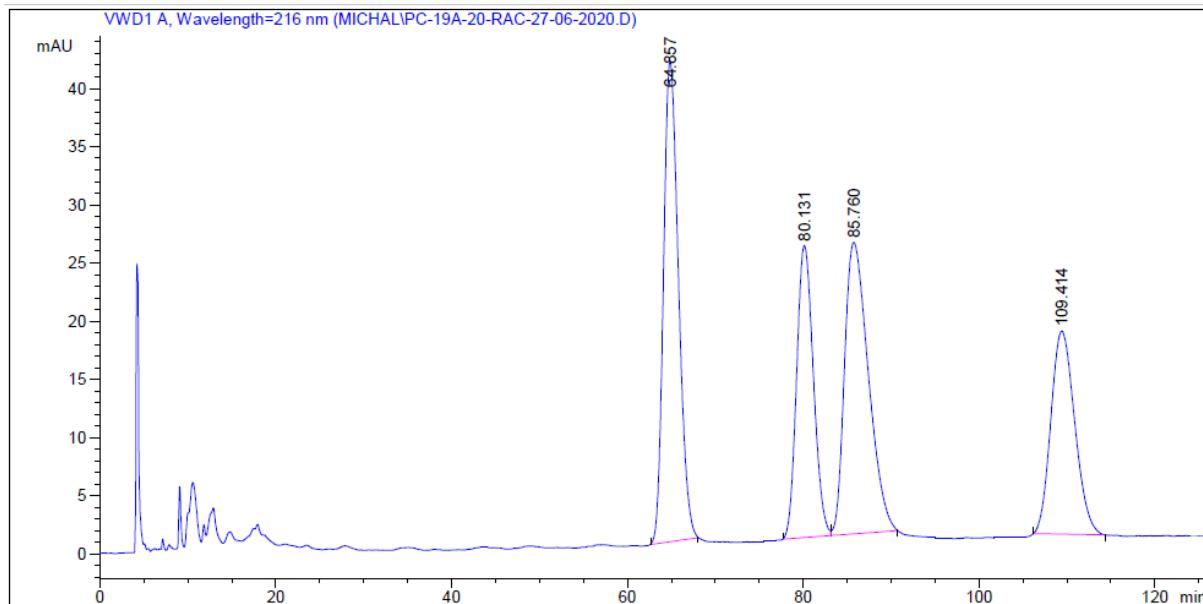
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Area Percent Report
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Sorted By : Signal
 Multiplier: : 1.0000
 Dilution: : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=216 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height *s	Area [mAU]	Area %
1	74.557	BB	1.5331	501.06918	3.82042	2.3843	
2	96.076	BB	2.7949	1.56523e4	78.70187	74.4818	
3	111.401	BB	2.3618	4861.57471	24.90583	23.1339	

12e (HPLC: AS-H, hexane/iPrOH 80:20, 0.75 mL/min, $\lambda = 216$ nm)

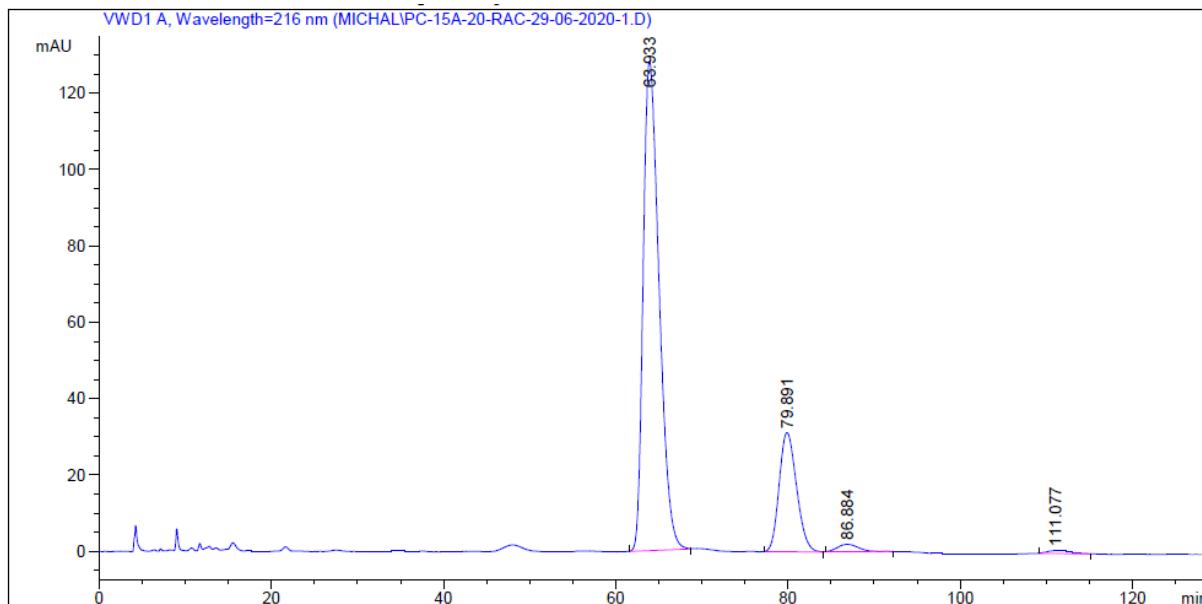


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Area Percent Report
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Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=216 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height *s	Area [mAU]	Area %
1	64.857	BB	1.8014	4878.97217	41.27309	30.1181	
2	80.131	BV	1.8742	3316.86548	25.09081	20.4752	
3	85.760	VB	2.2611	4709.45166	25.05838	29.0717	
4	109.414	BB	2.2445	3294.15771	17.46213	20.3350	



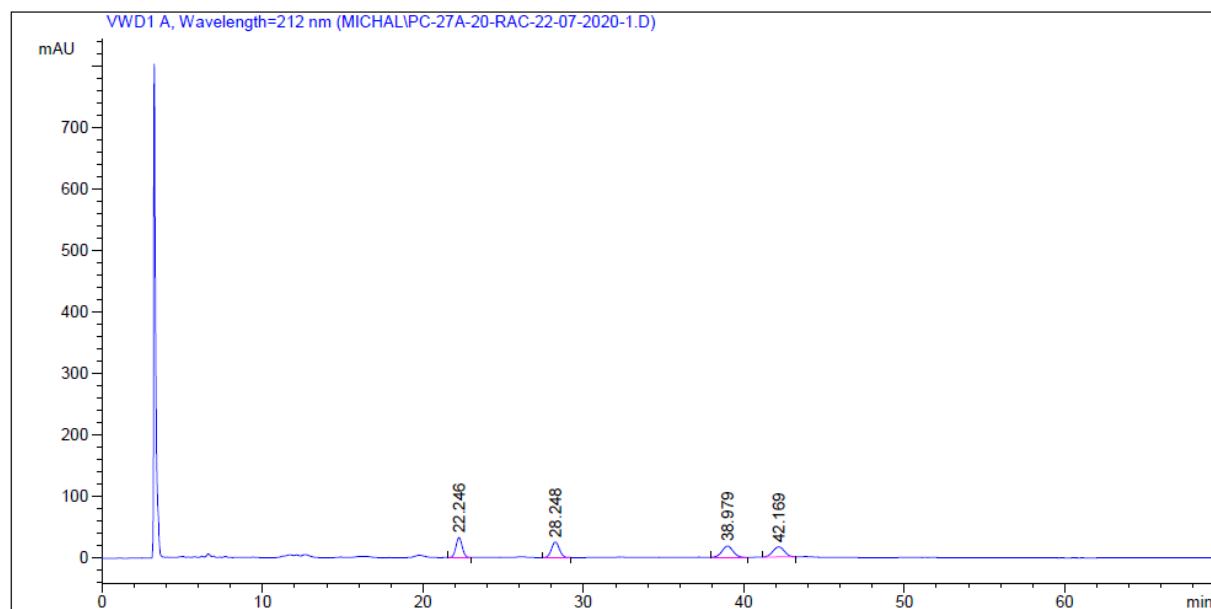
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Area Percent Report
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Sorted By : Signal
 Multiplier: : 1.0000
 Dilution: : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=216 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height *s	Area [mAU]	Area %
1	63.933	BB	2.0096	1.64385e4	128.10201	77.2029	
2	79.891	BB	2.1914	4381.96143	31.20850	20.5797	
3	86.884	BB	2.0405	317.42117	1.94830	1.4908	
4	111.077	BB	2.2264	154.71976	8.43856e-1	0.7266	

12f (HPLC: IC, hexane/iPrOH 90:10, 1 mL/min, $\lambda = 216$ nm)

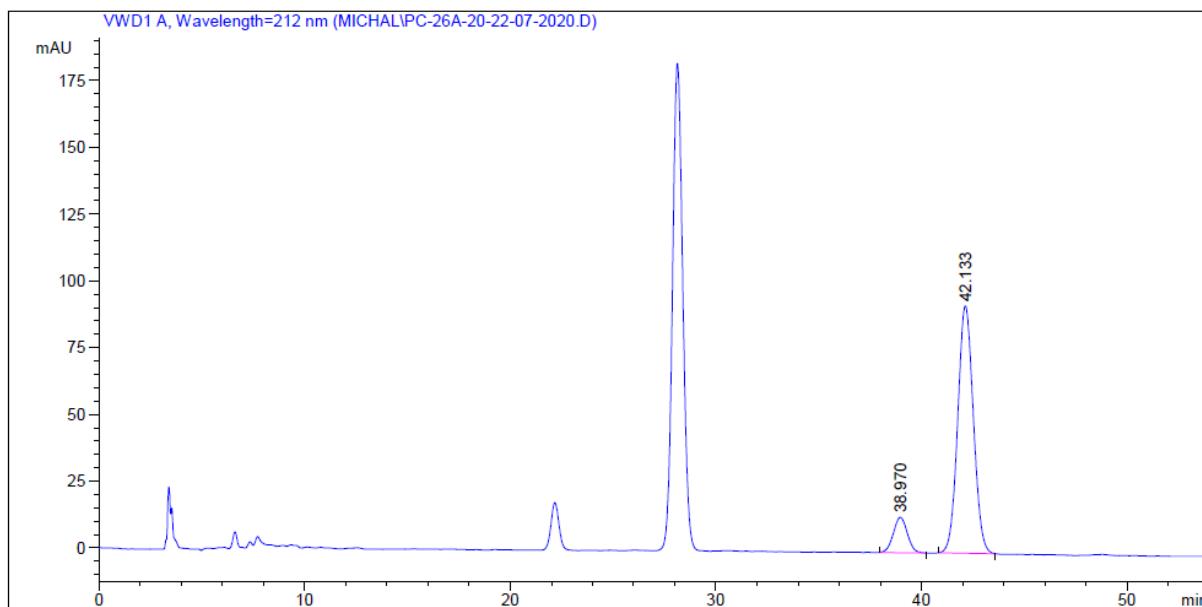


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Area Percent Report
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Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=212 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height *s	Area [mAU]	Area %
1	22.246	BB	0.4248	898.66571	32.61378	25.9616	
2	28.248	BB	0.5387	887.90607	25.59263	25.5520	
3	38.979	BB	0.7347	856.66040	18.12992	24.6528	
4	42.169	BV	0.7732	831.67224	16.61622	23.9337	



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Area Percent Report
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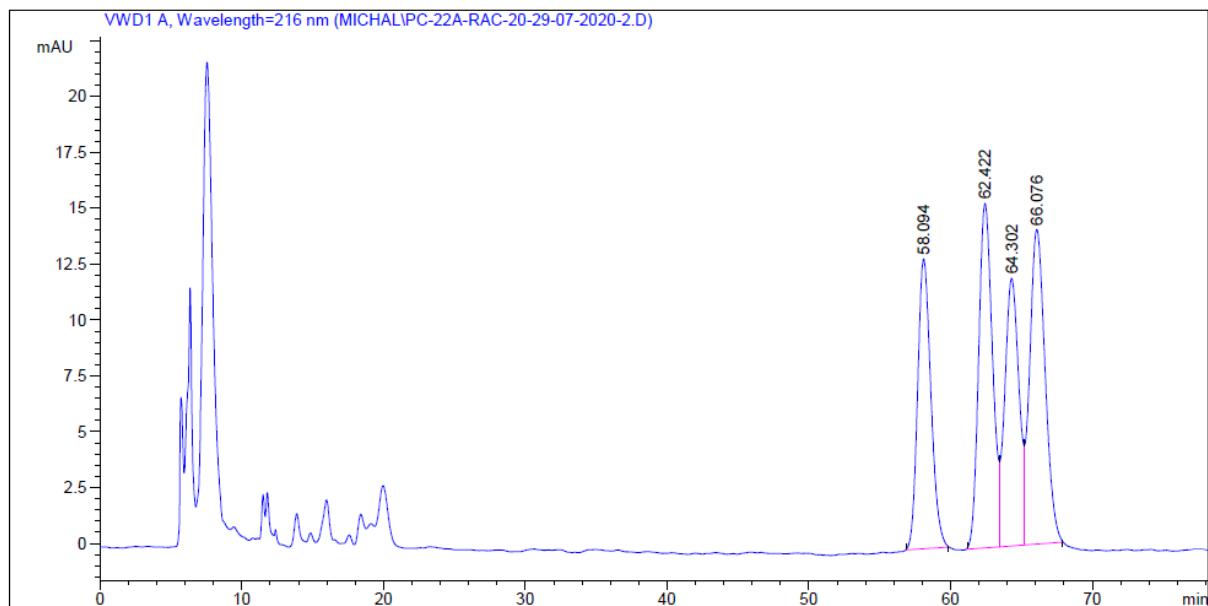
Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=212 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height *s	Area [mAU]	Area %
1	38.970	BB	0.7335	628.67230	13.22931	11.3876	
2	42.133	BB	0.8212	4891.97949	92.67209	88.6124	

Totals : 5520.65179 105.90140

12g (HPLC: OJ-H, hexane/iPrOH 90:10, 0.57 mL/min, λ = 216 nm)

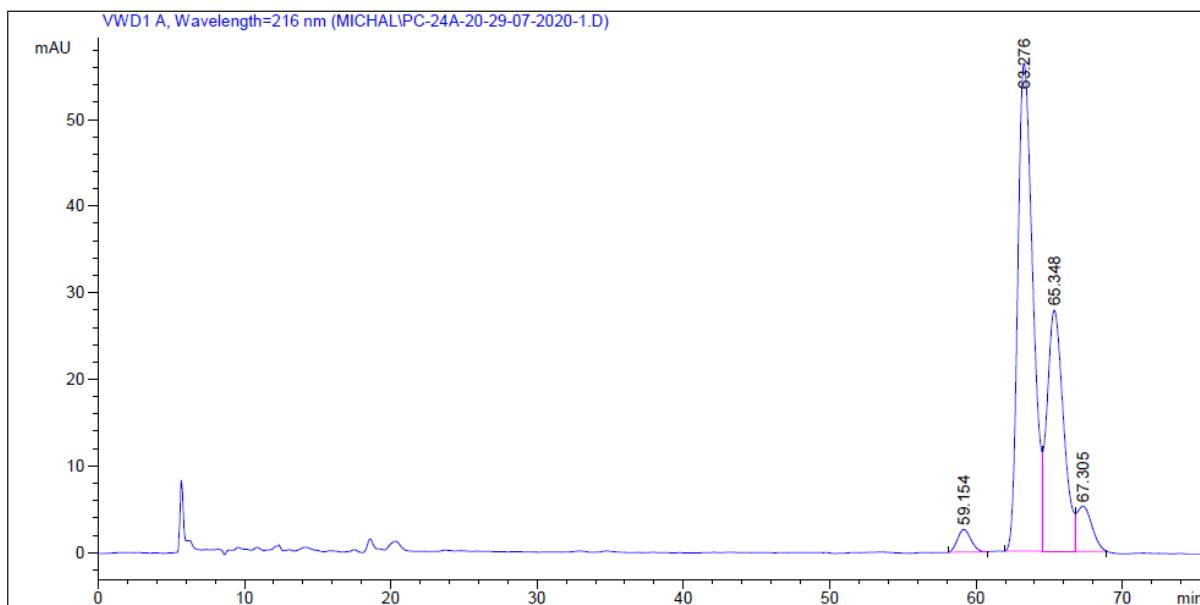


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Area Percent Report
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Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=216 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height *s	Area [mAU]	Area %
1	58.094	BB	0.9992	840.64044	12.97252	22.1657	
2	62.422	BV	1.0326	1041.30920	15.41756	27.4569	
3	64.302	VV	1.0162	837.42957	11.98346	22.0811	
4	66.076	VB	1.1263	1073.14429	14.08339	28.2963	



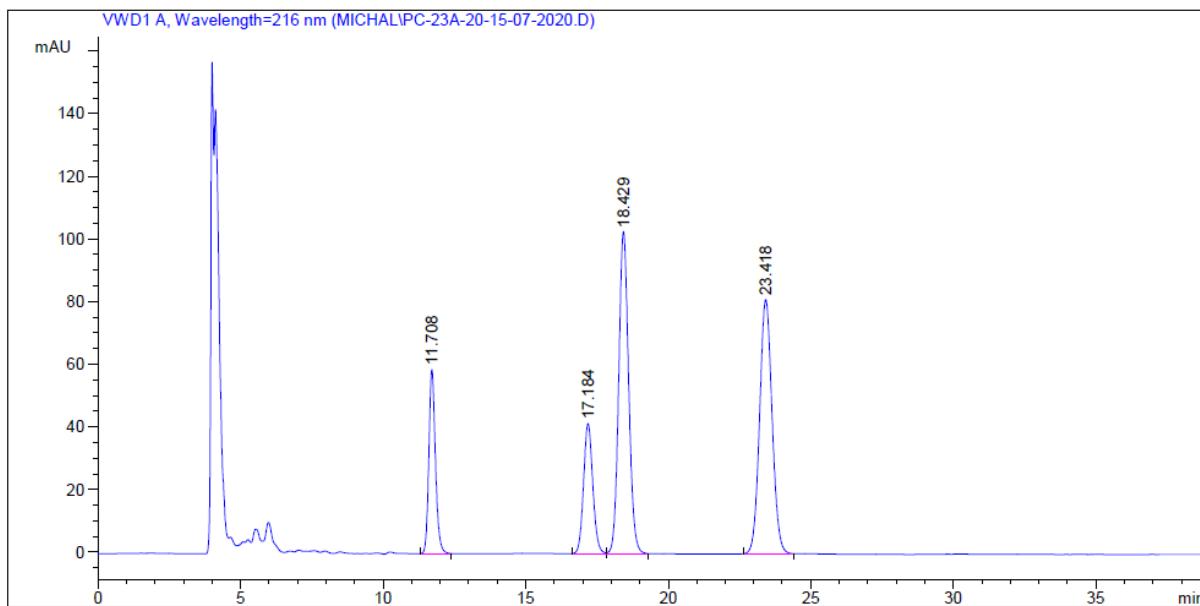
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Area Percent Report
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Sorted By : Signal
 Multiplier: : 1.0000
 Dilution: : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=216 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height *s	Area [mAU]	Area %
1	59.154	BB	0.7510	166.10590	2.61584	2.4482	
2	63.276	BV	1.1004	4034.66431	56.34627	59.4669	
3	65.348	VV	1.1933	2211.13989	27.83177	32.5900	
4	67.305	VB	0.8437	372.81638	5.22743	5.4949	

12h (HPLC: IC, hexane/iPrOH 85:15, 0.8 mL/min, $\lambda = 216$ nm)

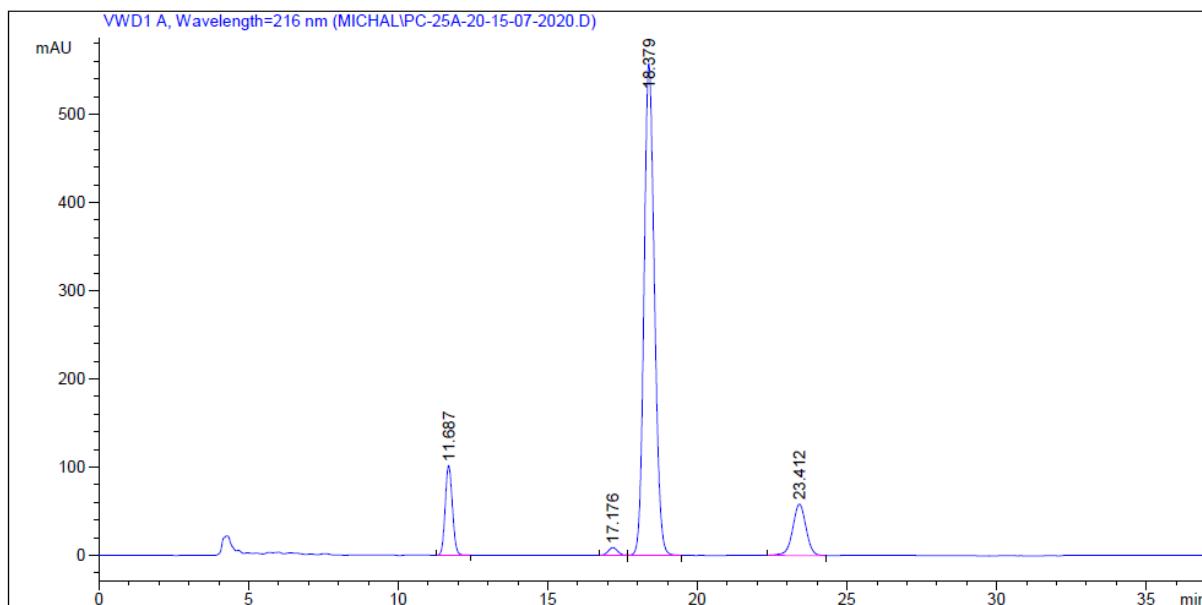


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Area Percent Report
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Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=216 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area *s	Height [mAU]	Area %
1	11.708	BB	0.2439	943.01947		58.79366	13.8030
2	17.184	BB	0.3470	935.19525		41.56036	13.6885
3	18.429	BB	0.3736	2484.77954		102.82776	36.3697
4	23.418	BB	0.4697	2469.00342		81.21720	36.1388



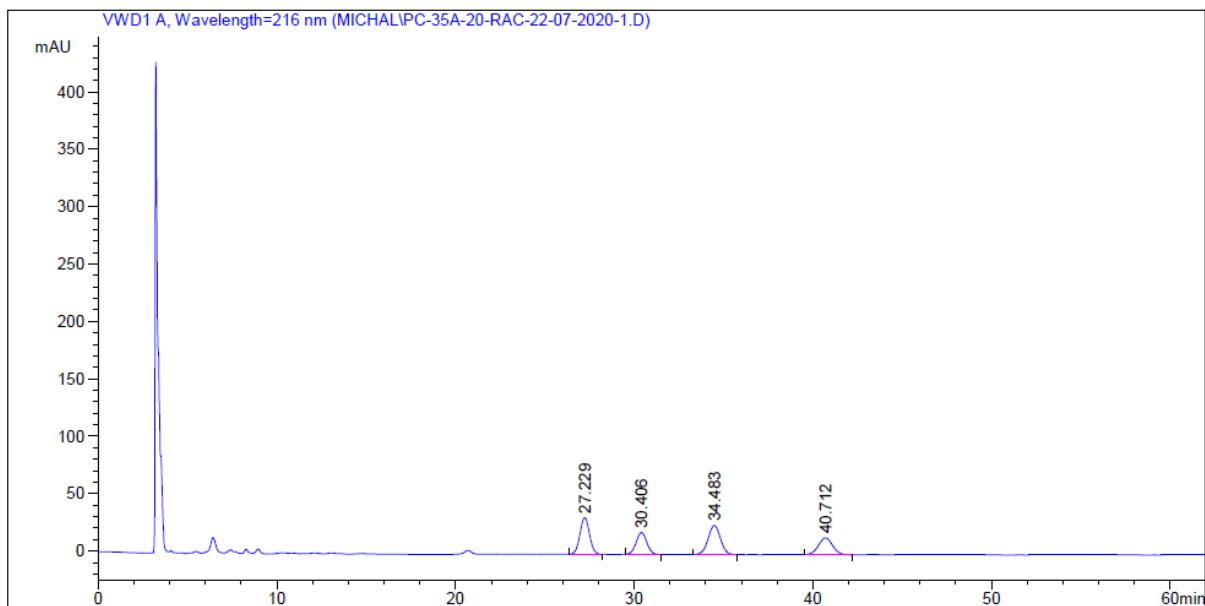
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Area Percent Report
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Sorted By : Signal
 Multiplier: : 1.0000
 Dilution: : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=216 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height *s	Area [mAU]	Area %
1	11.687	BB	0.2615	1695.98926	101.72340	9.8826	
2	17.176	BV	0.3414	189.06337	8.68262	1.1017	
3	18.379	VB	0.3736	1.34733e4	557.69965	78.5098	
4	23.412	BB	0.4781	1802.95898	58.17044	10.5059	

12i (HPLC: IC, hexane/iPrOH 87:13, 1 mL/min, λ = 216 nm)

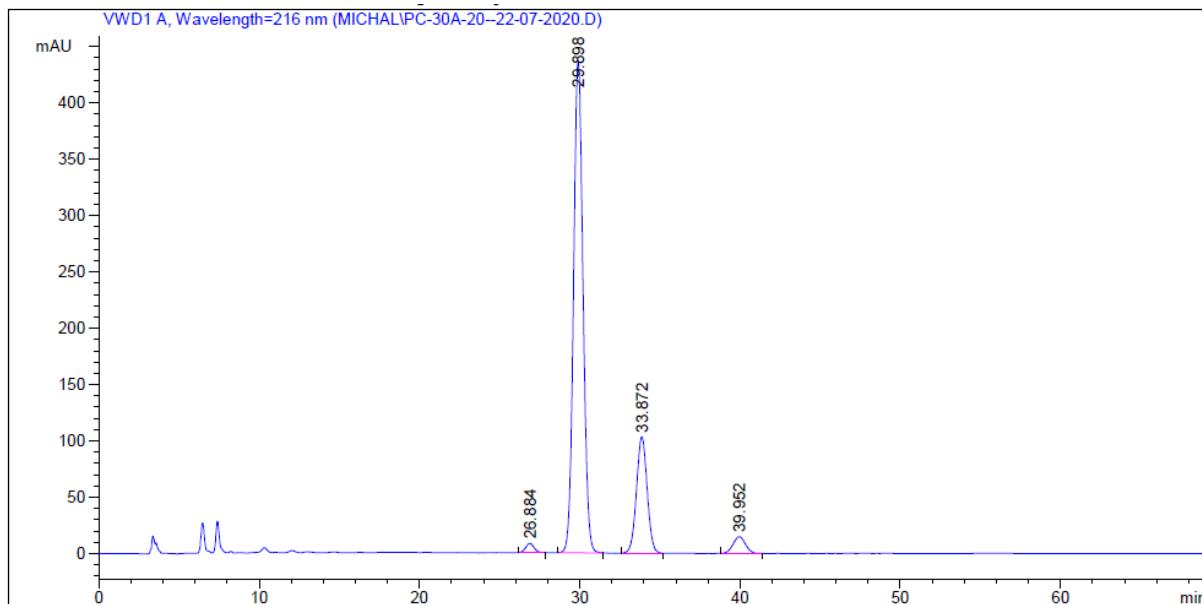


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Area Percent Report
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Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=216 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area *s	Height [mAU]	Area %
1	27.229	BB	0.5803	1200.15430		31.99292	29.7061
2	30.406	BB	0.6484	799.83221		19.16825	19.7973
3	34.483	BB	0.7454	1228.16565		25.43390	30.3994
4	40.712	BB	0.8407	811.94604		14.67316	20.0972



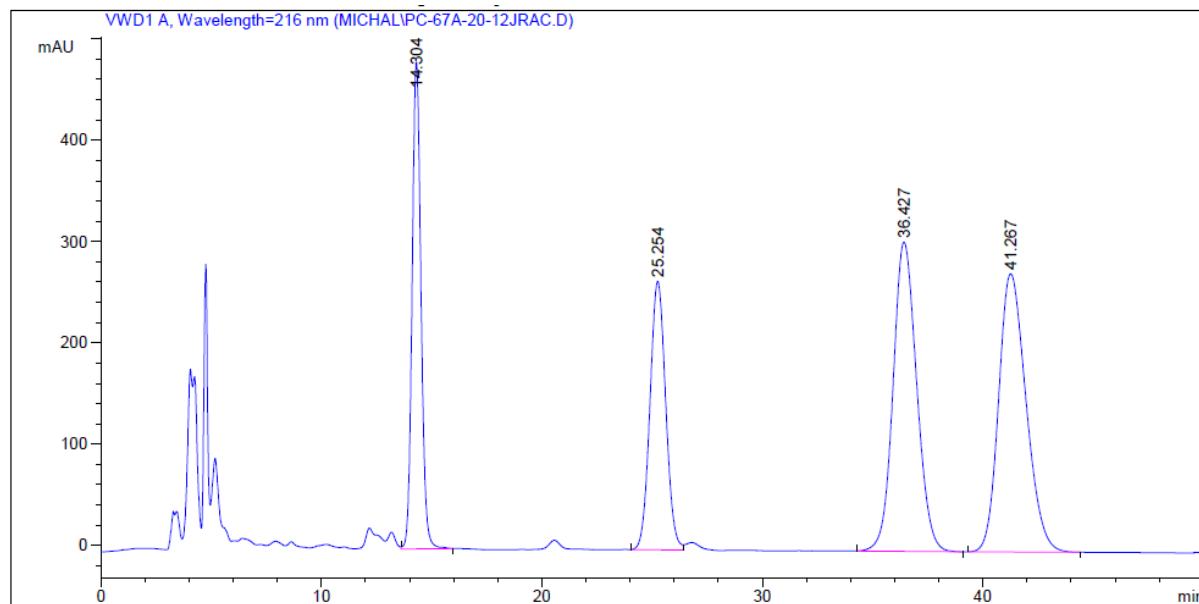
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Area Percent Report
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Sorted By : Signal
 Multiplier: : 1.0000
 Dilution: : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=216 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height *s	Area [mAU]	Area %
1	26.884	BB	0.5635	302.24506	8.20895	1.2707	
2	29.898	BB	0.6374	1.78841e4	435.87268	75.1875	
3	33.872	BB	0.7219	4791.63672	103.26453	20.1448	
4	39.952	BB	0.8395	808.00519	14.89784	3.3970	

12j (HPLC: IC, hexane/iPrOH 80:20, 1 mL/min, $\lambda = 216$ nm)

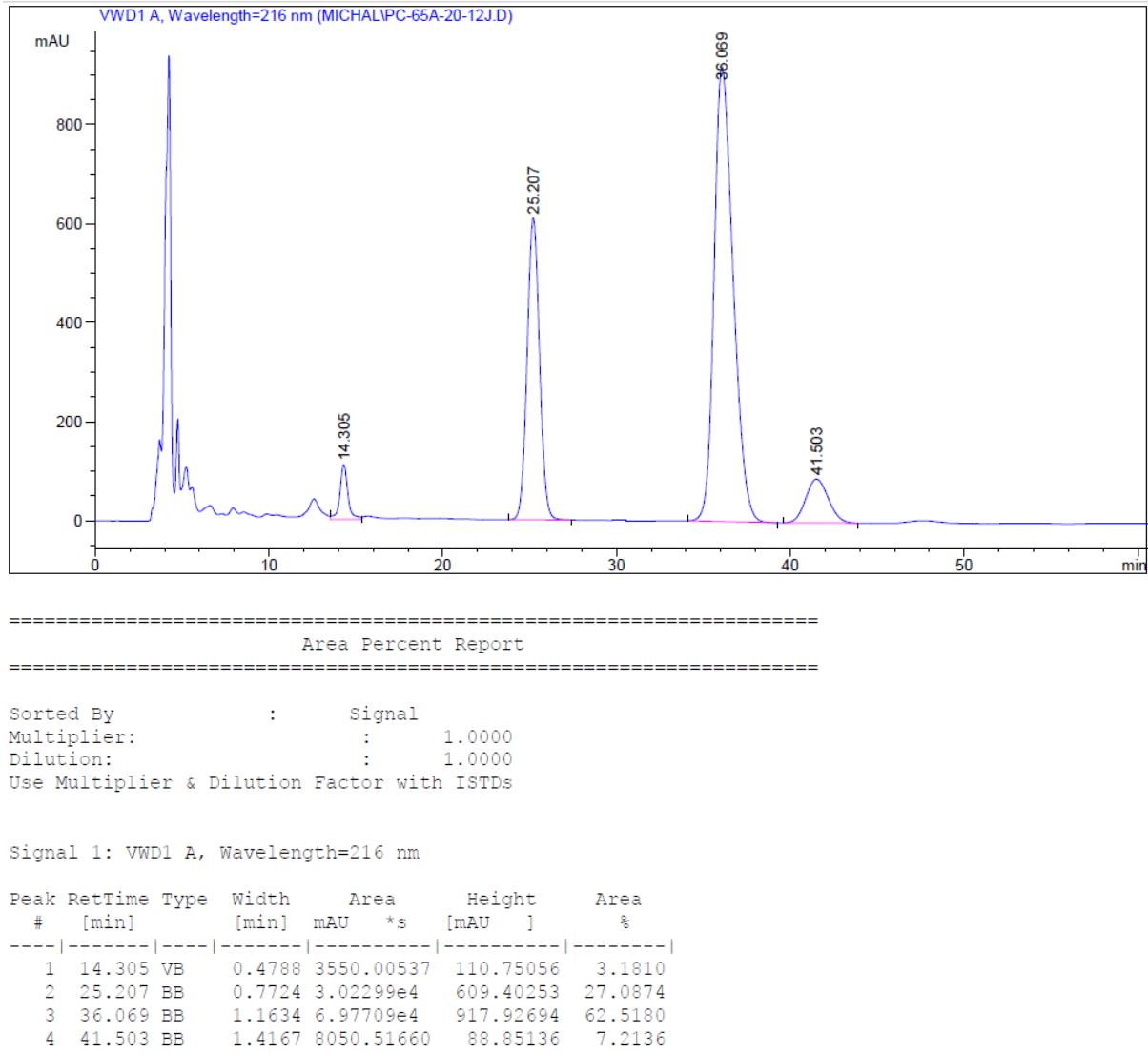


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Area Percent Report
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Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

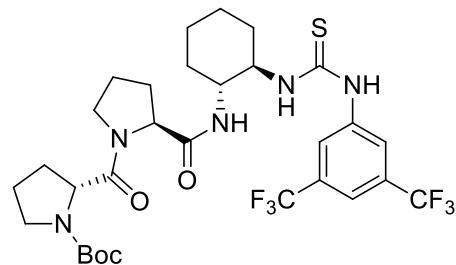
Signal 1: VWD1 A, Wavelength=216 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height *s	[mAU]	Area %
1	14.304	VB	0.4310	1.34343e4	480.53134	18.3998	
2	25.254	BV	0.7707	1.31406e4	265.02625	17.9974	
3	36.427	BB	1.1458	2.27128e4	305.36743	31.1077	
4	41.267	BB	1.3352	2.37258e4	274.72635	32.4950	

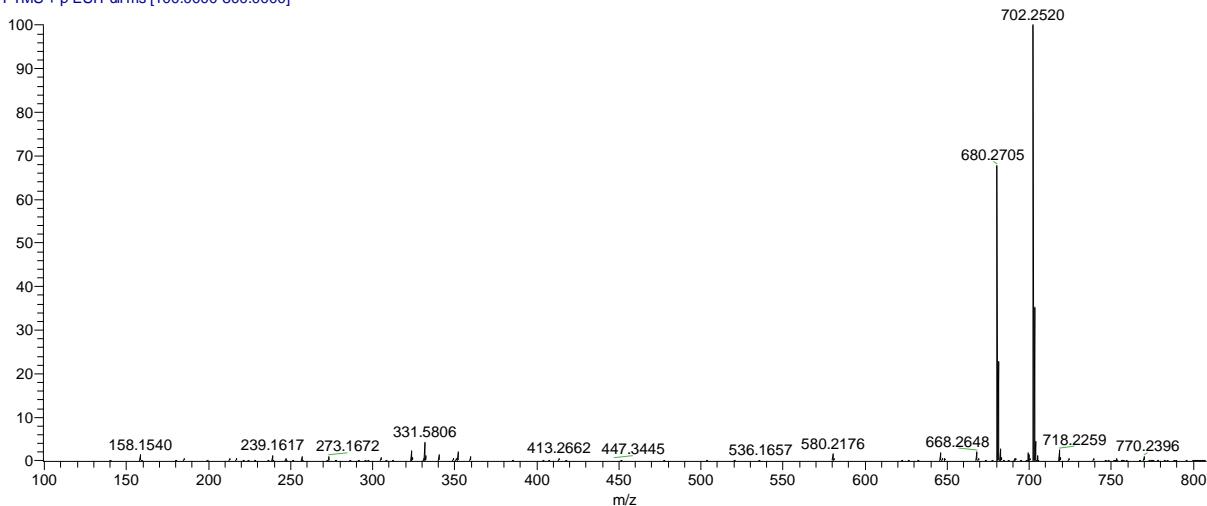


Pictures of HRMS spectra

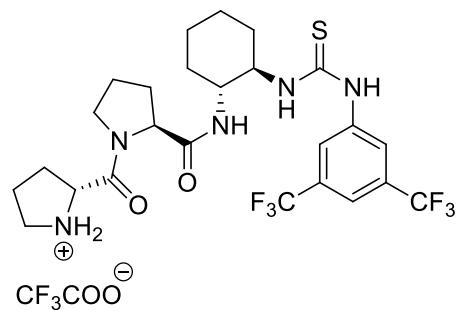
(R)-*tert*-butyl-2-((S)-2-(((1*R*,2*R*)-2-(3-(3,5-bis(trifluoromethyl)phenyl)thioureido)cyclohexyl carbamoyl)pyrrolidine-1-carbonyl)pyrrolidine-1-carboxylate (**8**)



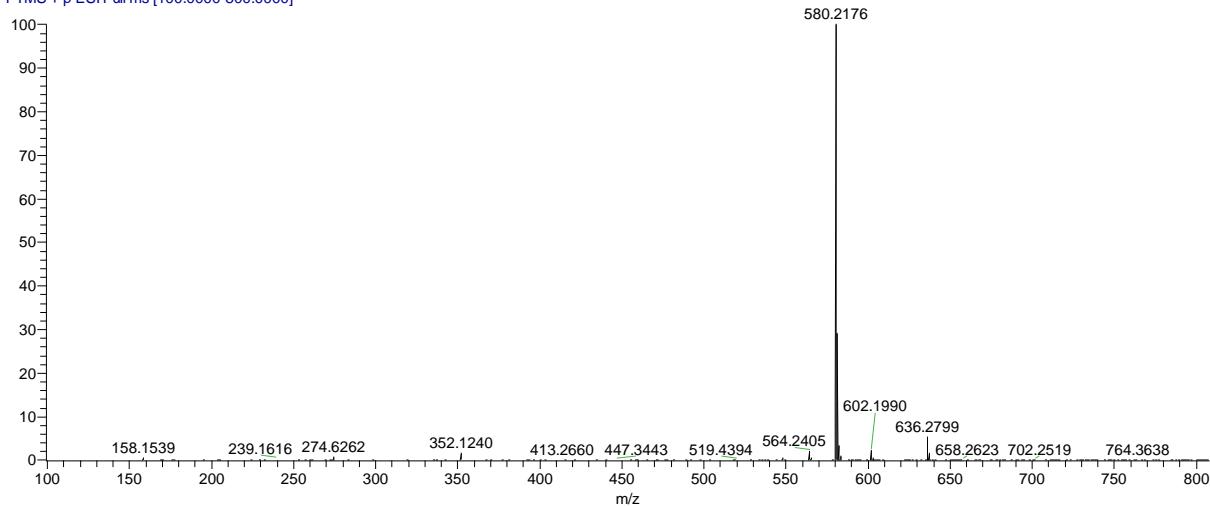
Mar_22_006 #74-92 RT: 0.35-0.43 AV: 19 NL: 3.51E8
T: FTMS + p ESI Full ms [100.0000-800.0000]



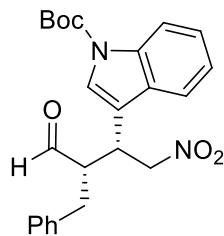
(R)-2-((S)-2-(((1*R*,2*R*)-2-(3-(3,5-bis(trifluoromethyl)phenyl)thioureido)cyclohexyl carbamoyl)pyrrolidine-1-carbonyl)pyrrolidin-1-ium (C1)



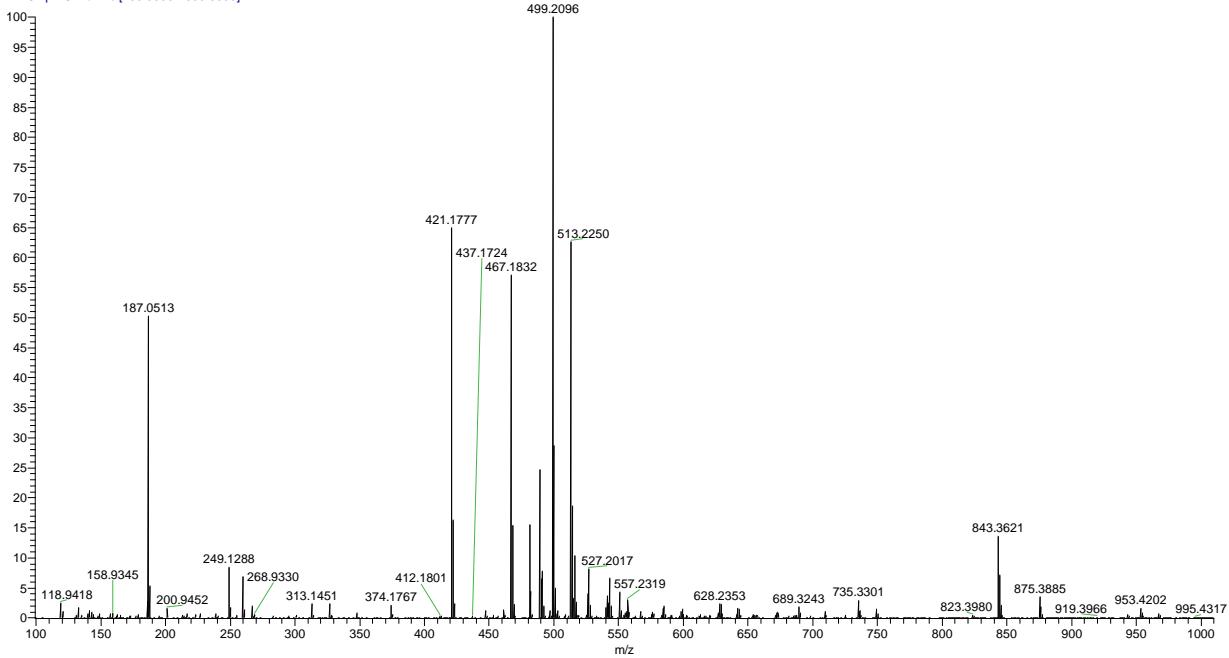
Mar_22_007 #81-95 RT: 0.38-0.44 AV: 15 NL: 1.08E9
T: FTMS + p ESI Full ms [100.0000-800.0000]

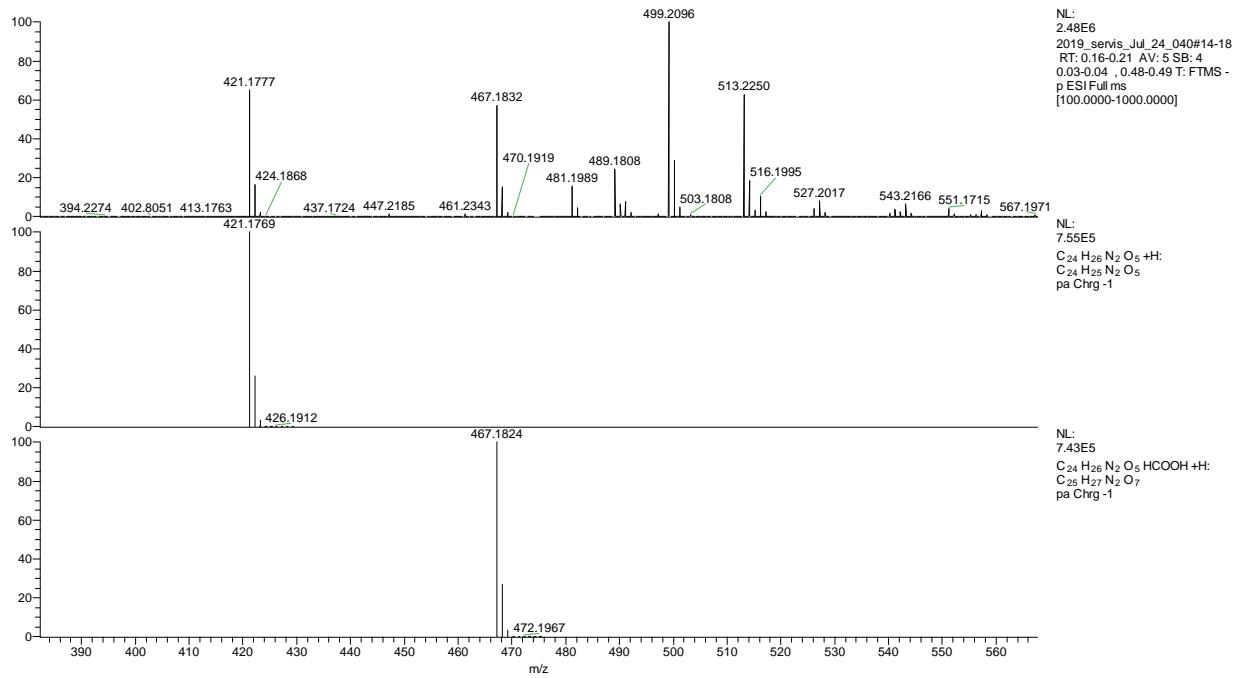


Tert-butyl 3-((2*R*,3*S*)-3-benzyl-1-nitro-4-oxobutan-2-yl)-1*H*-indole-1-carboxylate (**11a**)

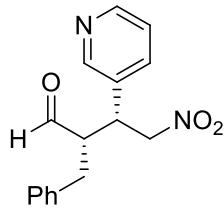


2019_servis_Jul_24_040 #14-18 RT: 0.16-0.21 AV: 5 SB: 4 0.03-0.04 , 0.48-0.49 NL: 2.48E6
T: FTMS - p ESI Full ms [100.0000-1000.0000]

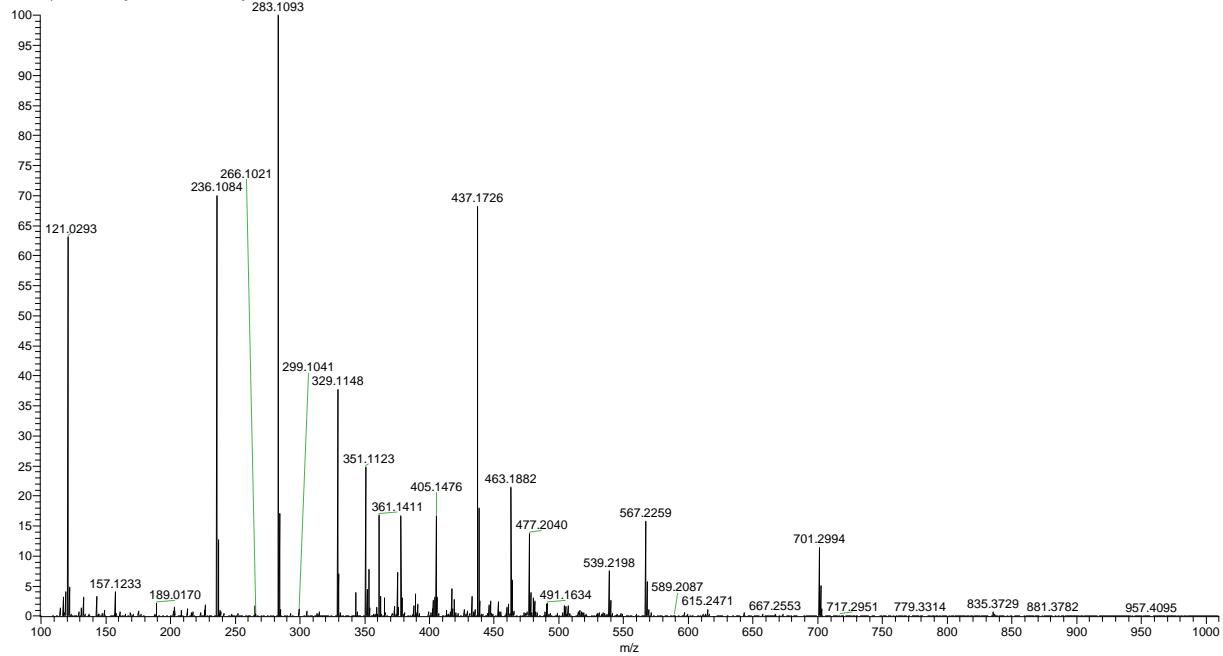


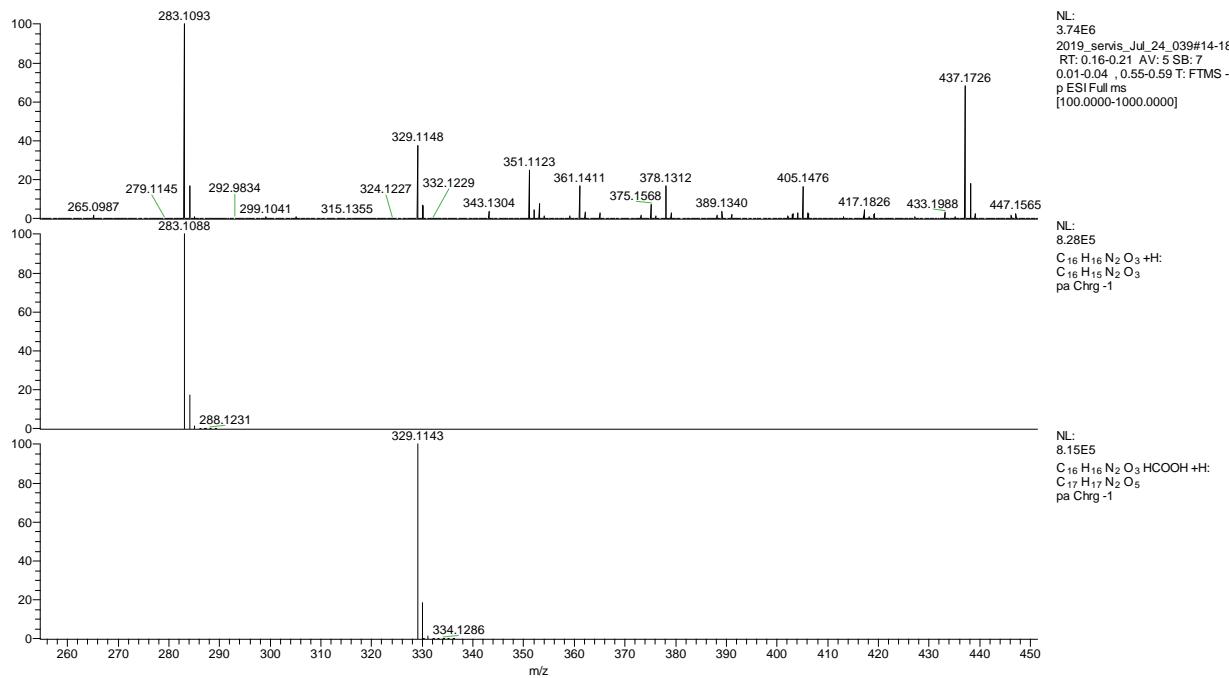


(2S,3R)-2-benzyl-4-nitro-3-(pyridin-3-yl)butanal (**11b**)

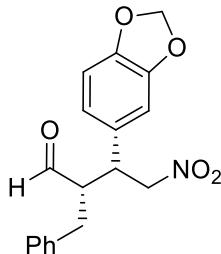


2019_servis_Jul_24_039 #14-18 RT: 0.16-0.21 AV: 5 SB: 7 0.01-0.04 , 0.55-0.59 NL: 3.74E6
T: FTMS - p ESI Full ms [100.0000-1000.0000]

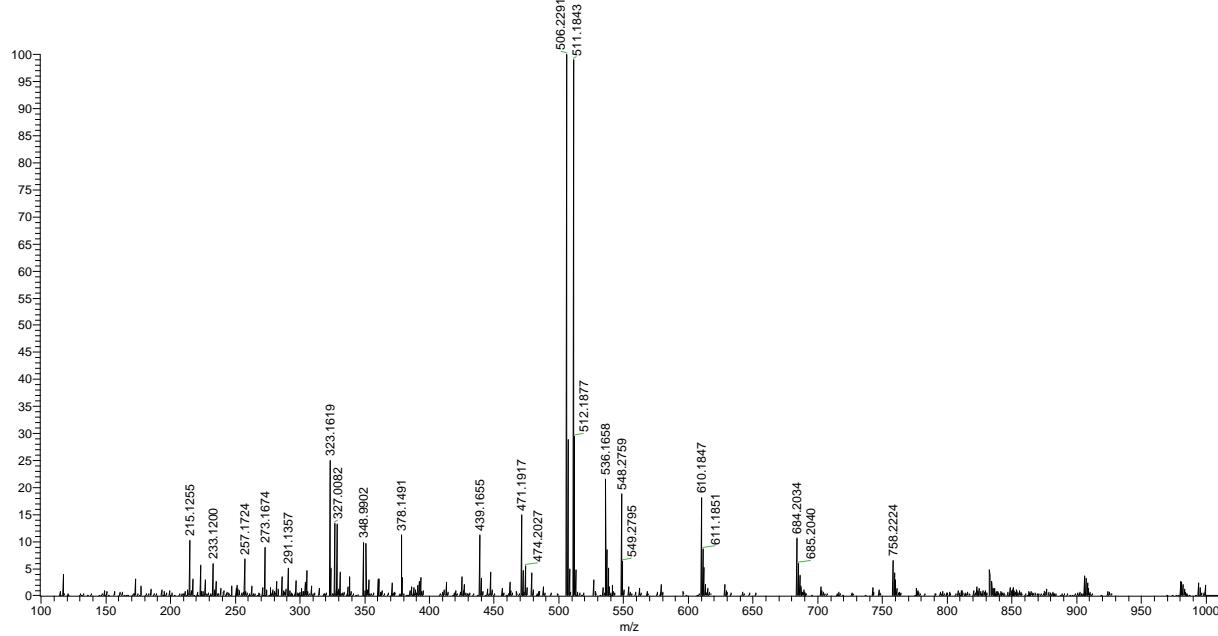




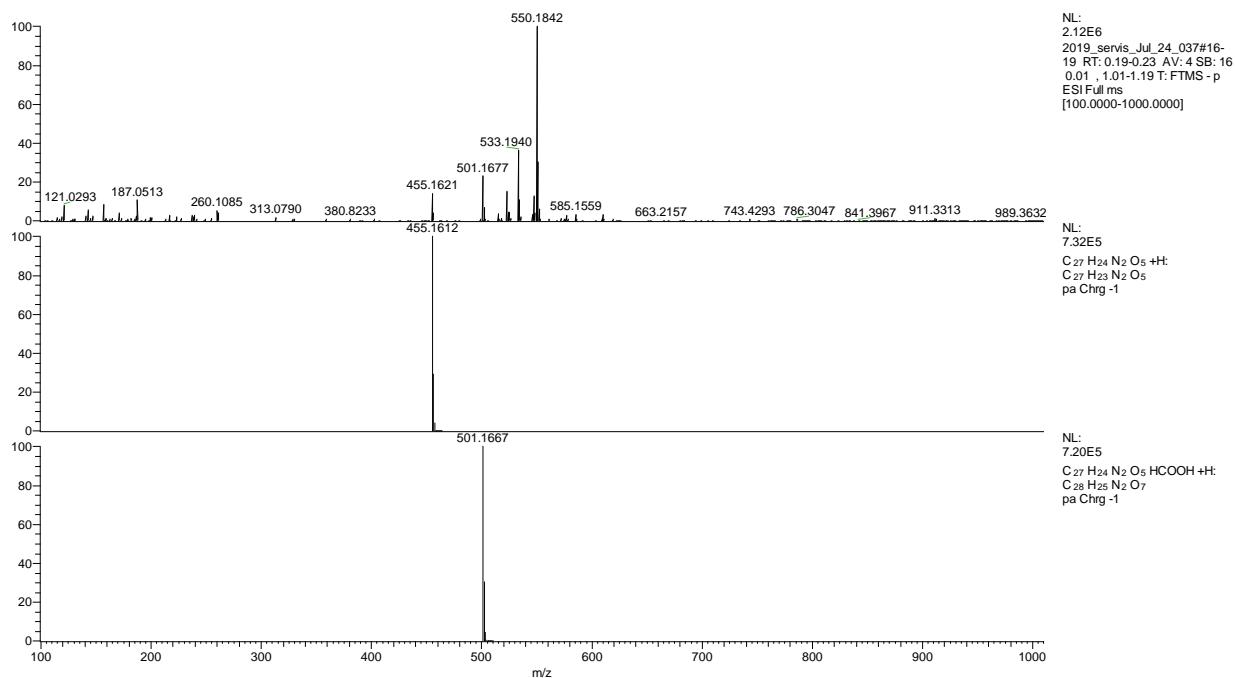
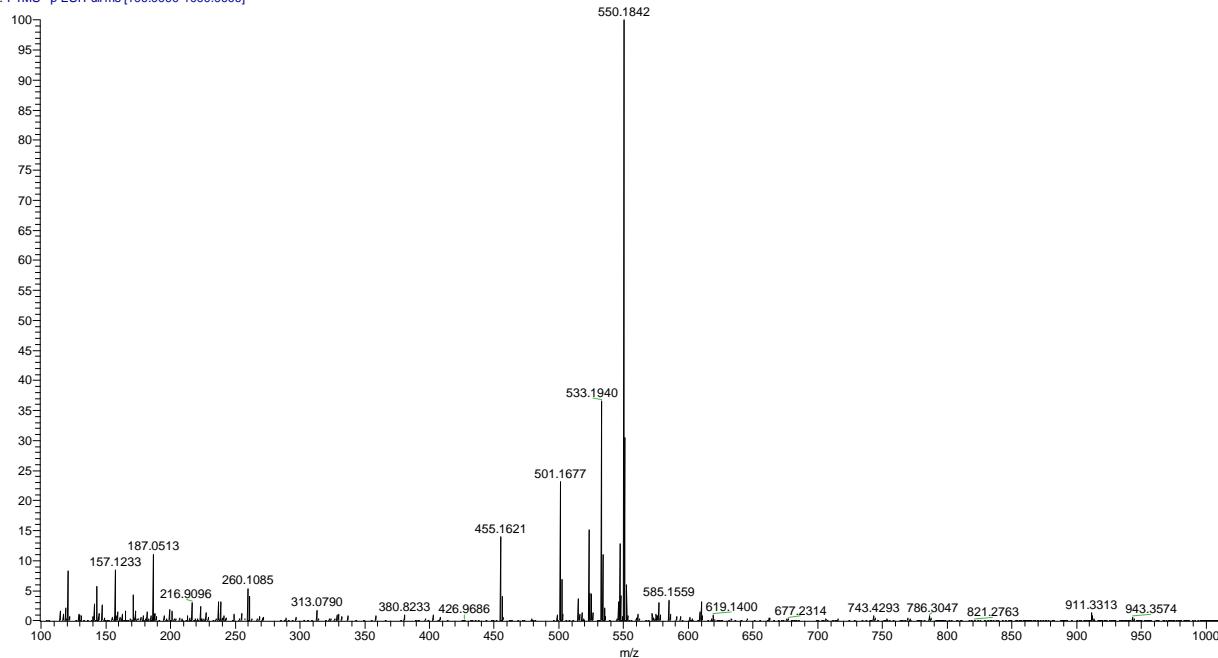
(2S,3R)-3-(benzo[d][1,3]dioxol-5-yl)-2-benzyl-4-nitrobutanal (**11d**)



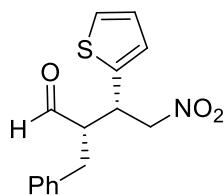
2019_servis_Jul_24_055 #17-24 RT: 0.16-0.22 AV: 8 SB: 9 0.02-0.05 , 0.49-0.53 NL: 1.56E7
T: FTMS + p ESI Full ms [100.0000-1000.0000]



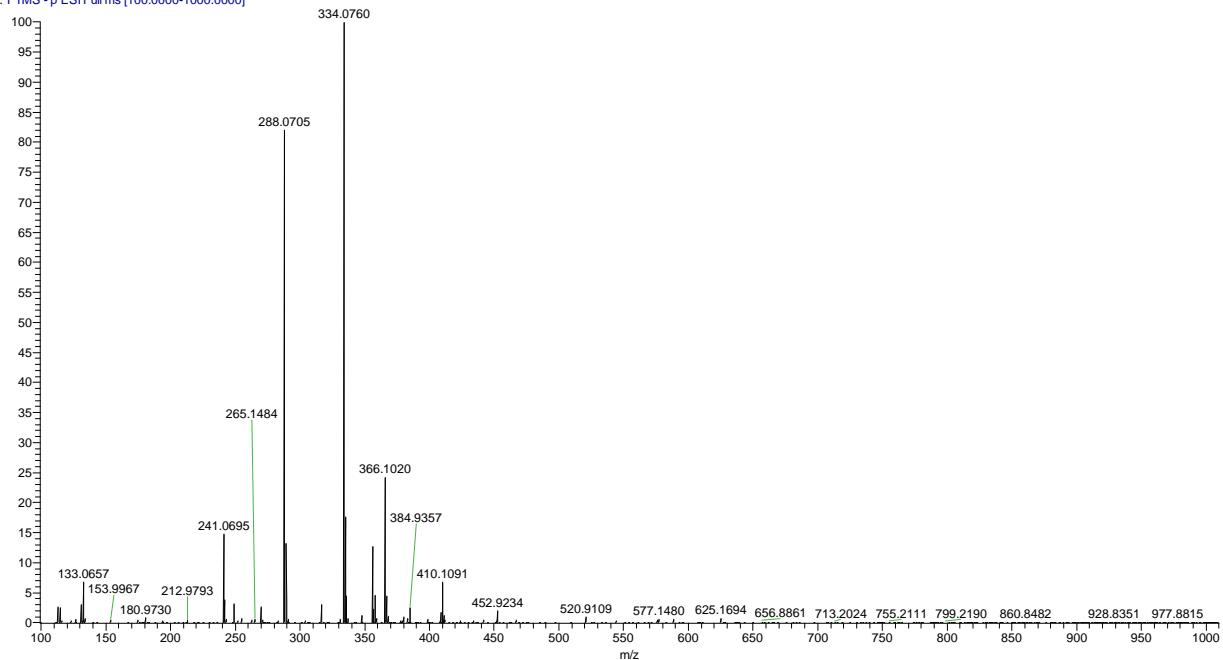
2019_servis_Jul_24_037 #16-19 RT: 0.19-0.23 AV: 4 SB: 16 0.01 , 1.01-1.19 NL: 2.12E6
T: FTMS - p ESI Full ms [100.0000-1000.0000]



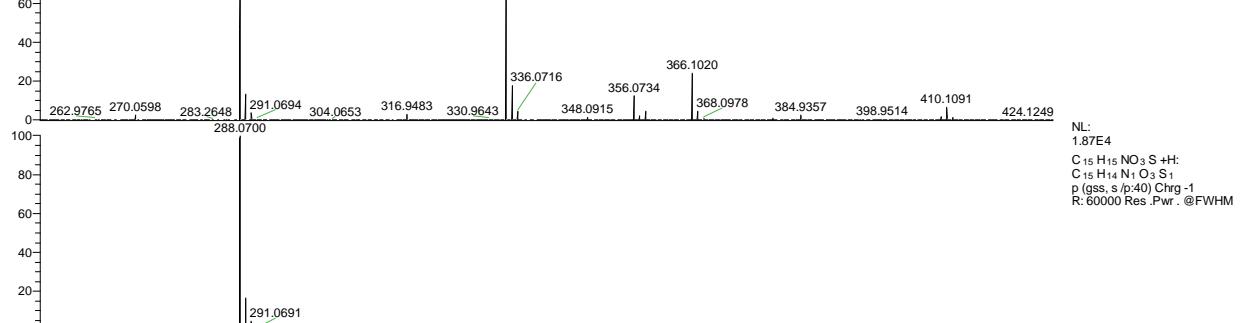
(2S,3S)-2-benzyl-4-nitro-3-(thiophen-2-yl)butanal (**11e**)



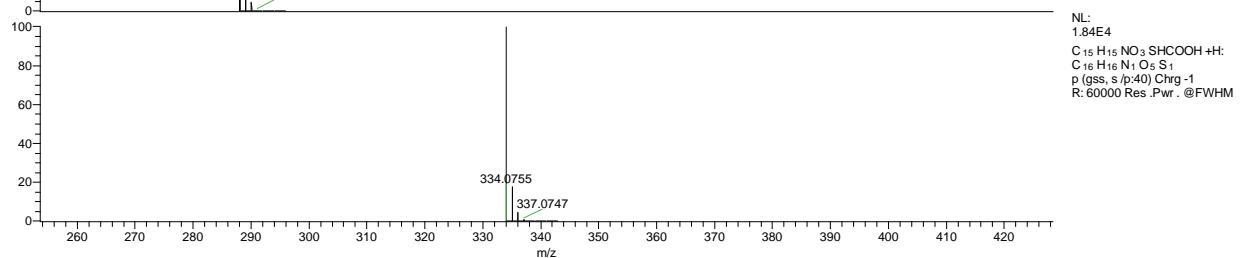
2019_servis_Jul_24_035 #15-22 RT: 0.17-0.25 AV: 8 NL: 1.55E7
T: FTMS - p ESI Full ms [100.0000-1000.0000]



NL:
1.55E7
2019_servis_Jul_24_035#15-
22 RT: 0.17-0.25 AV: 8 T:
FTMS - p ESI Full ms
[100.0000-1000.0000]

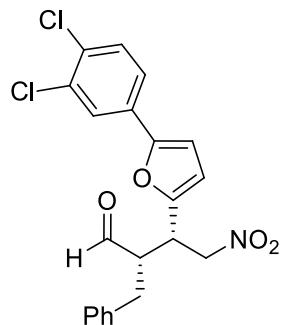


NL:
1.87E4
C₁₅H₁₅NO₃S +H:
C₁₅H₁₄N₁O₃S₁
p (gss, s /b40) Chrg -1
R: 60000 Res.Pwr. @FWHM

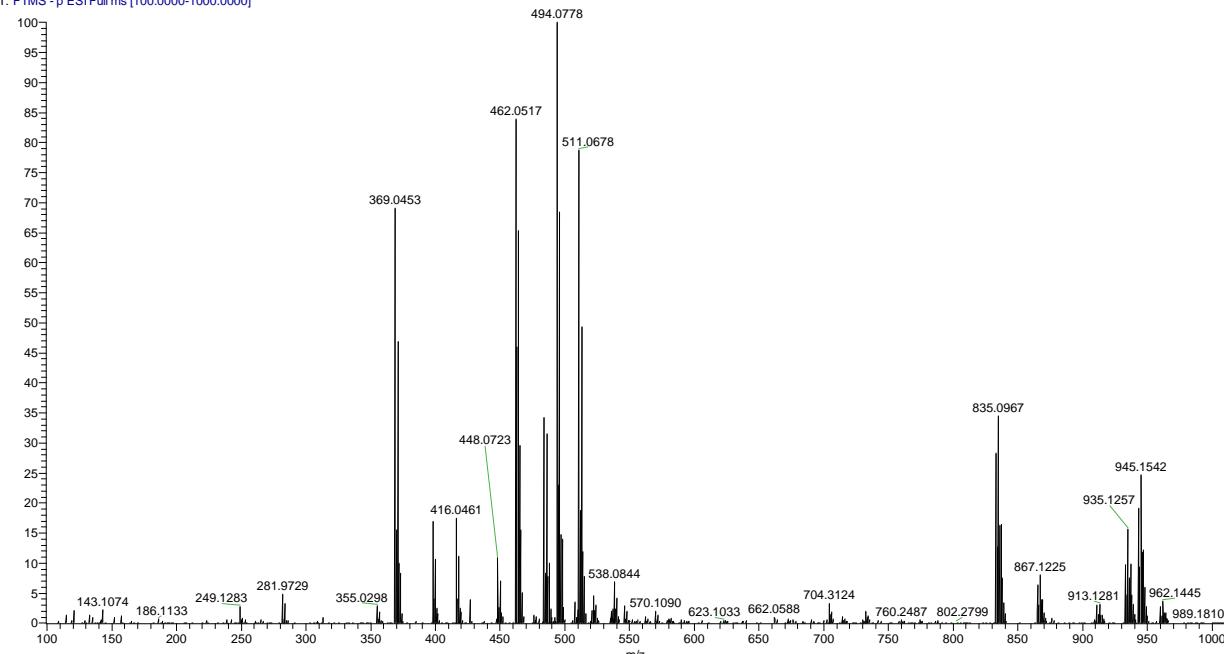


NL:
1.84E4
C₁₅H₁₅NO₃SHCOOH +H:
C₁₆H₁₆N₁O₅S₁
p (gss, s /b40) Chrg -1
R: 60000 Res.Pwr. @FWHM

(2S,3S)-2-benzyl-3-(5-(3,4-dichlorophenyl)furan-2-yl)-4-nitrobutanal (11f**)**



2019_servis_Jul_24_110 #20-26 RT: 0.24-0.32 AV: 7 SB: 37 0.04-0.12 , 0.56-0.92 NL: 9.44E5
T: FTMS - p ESI Full ms [100.0000-1000.0000]

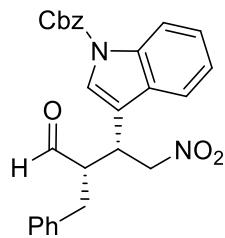


NL: 9.44E5
2019_servis_Jul_24_110#20-26
RT: 0.24-0.32 AV: 7 SB: 37
0.04-0.12 , 0.56-0.92 T: FTMS -
p ESI Full ms
[100.0000-1000.0000]

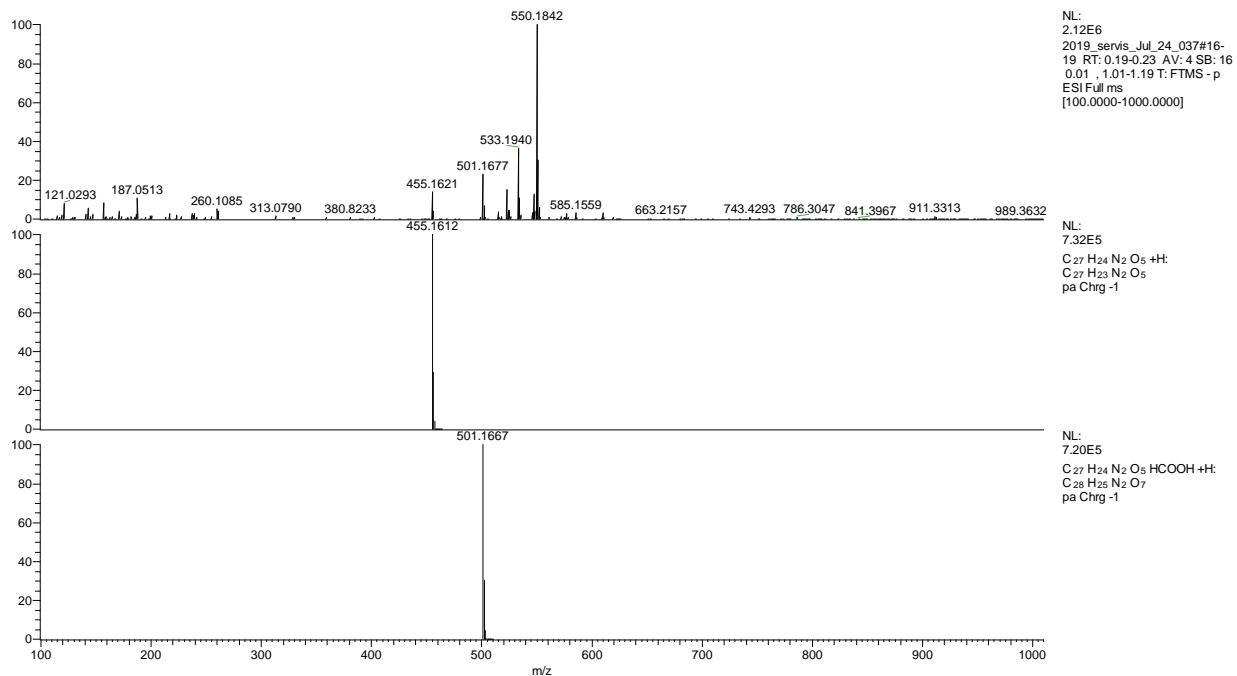
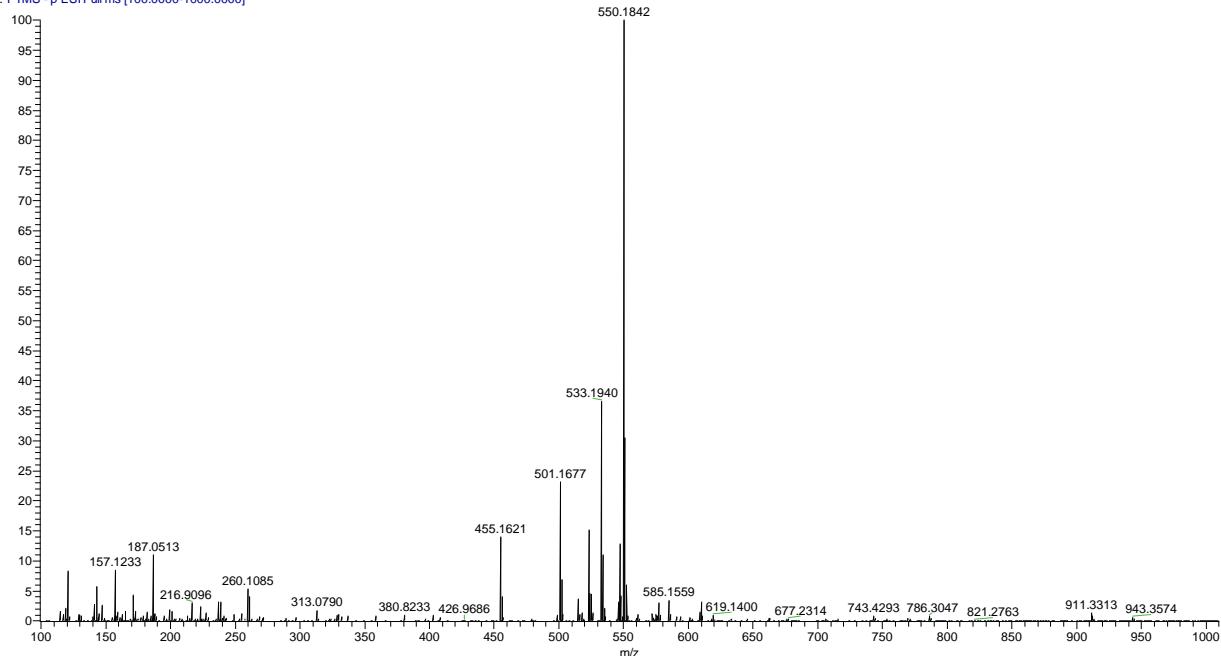
NL:
4.51E5
 $C_{21}H_{17}Cl_2NO_4+H^+$:
 $C_{21}H_{16}Cl_2N_1O_4$
c (gss, s/p/40)(Val) Chrg -1
R: 20000 Res.Pwr. @FWHM

NL:
4.44E5
 $C_{21}H_{17}Cl_2NO_4HCOOH +H^+$:
 $C_{22}H_{18}Cl_2N_1O_6$
c (gss, s/p/40)(Val) Chrg -1
R: 20000 Res.Pwr. @FWHM

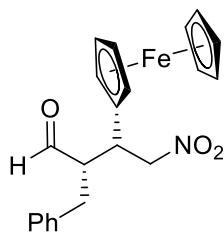
Benzyl 3-((2R,3S)-3-benzyl-1-nitro-4-oxobutan-2-yl)-1H-indole-1-carboxylate (11g)



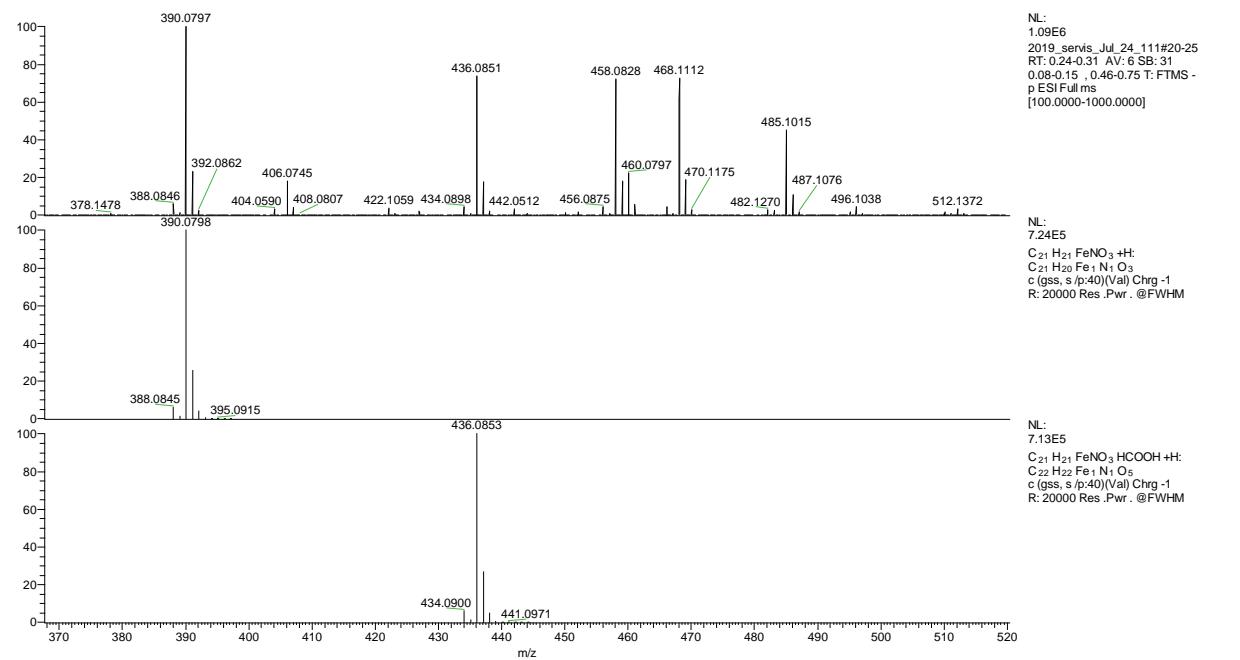
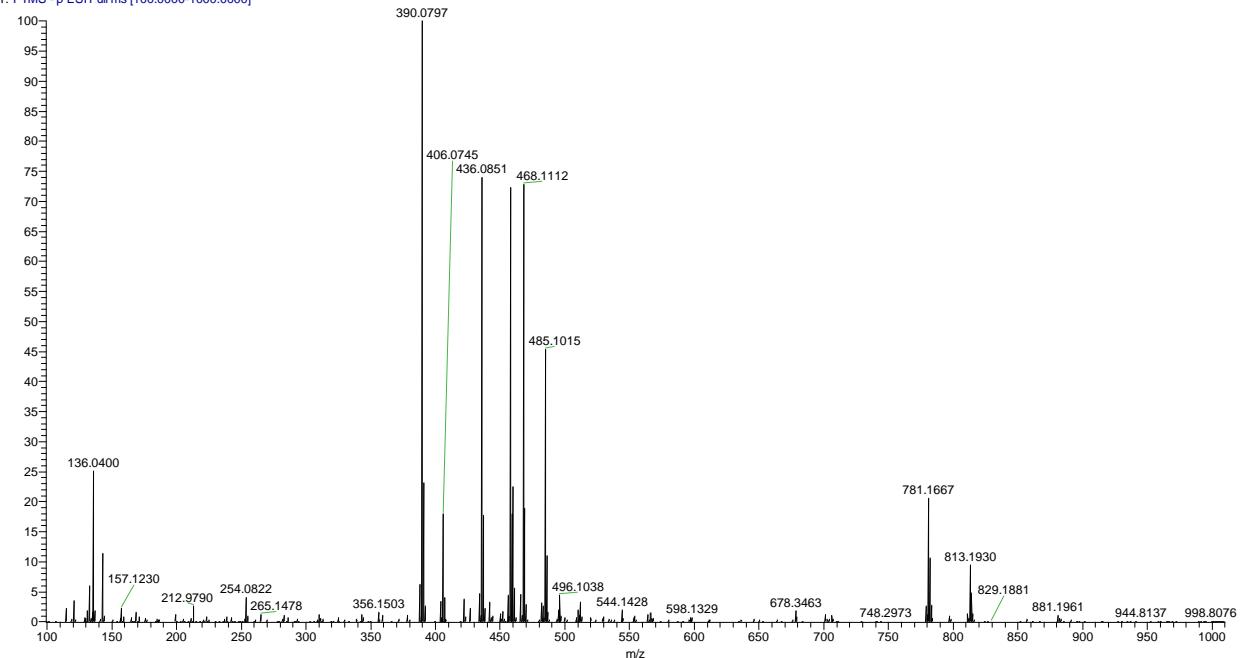
2019_servis_Jul_24_037 #16-19 RT: 0.19-0.23 AV: 4 SB: 16 0.01 , 1.01-1.19 NL: 2.12E6
T: FTMS - p ESI Full ms [100.0000-1000.0000]



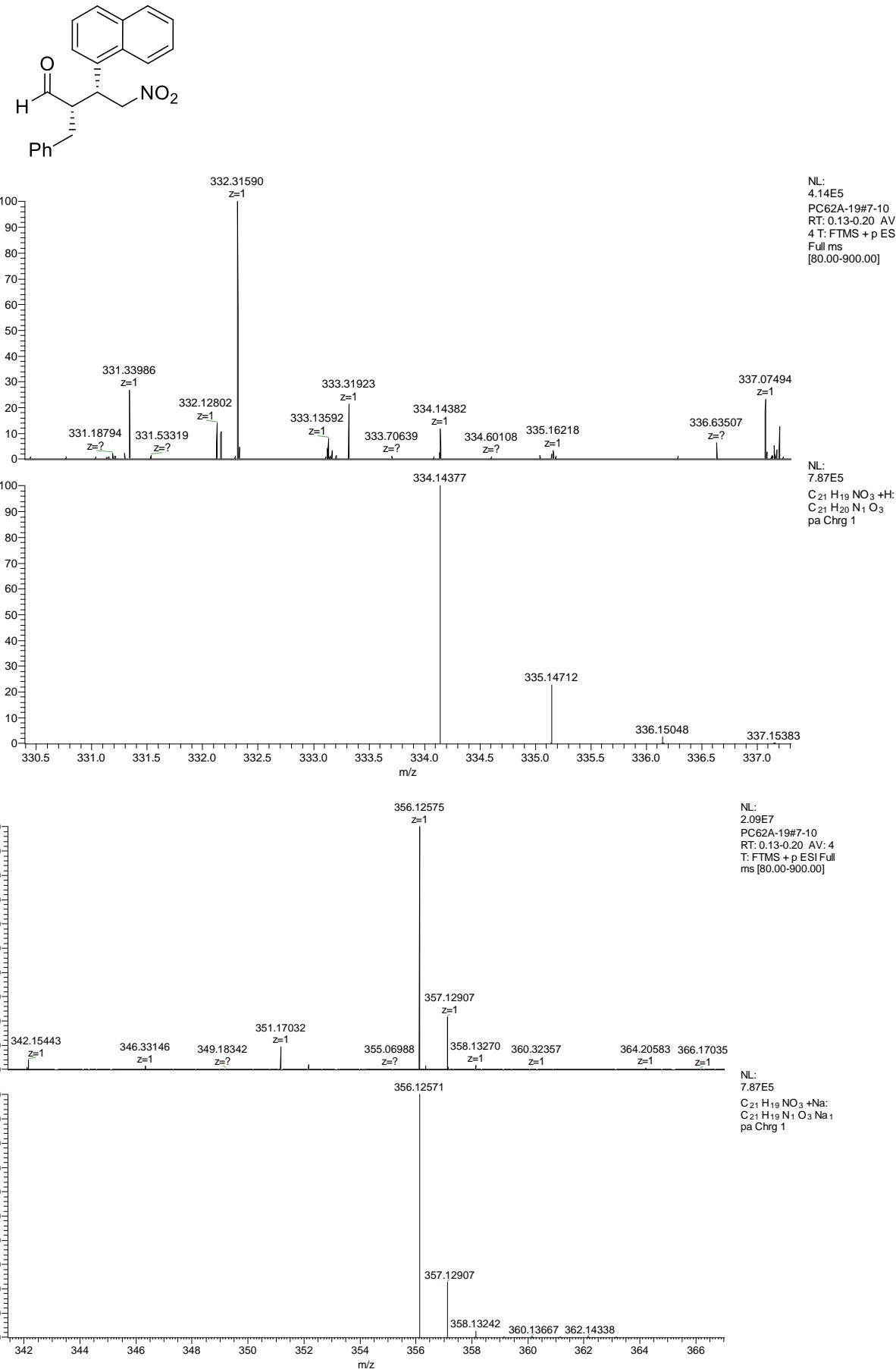
(2S,3S)-2-benzyl-3-ferrocenyl-4nitrobutanal (11h**)**



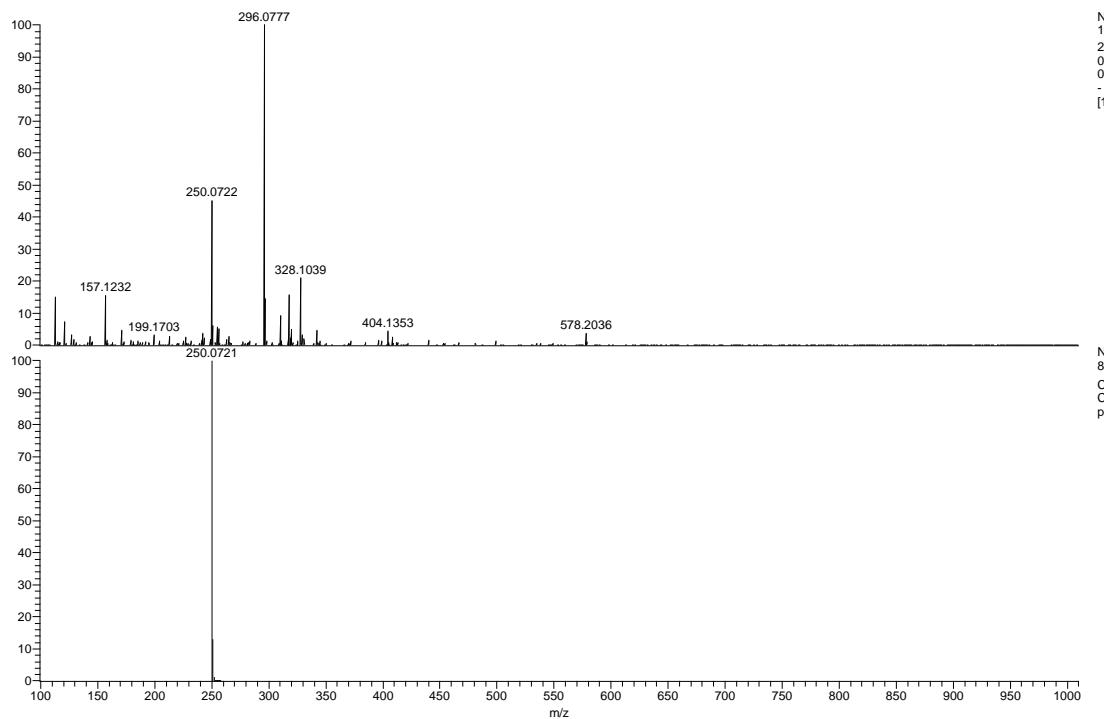
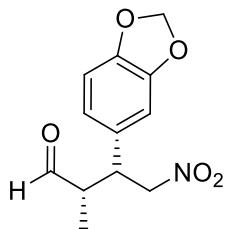
2019_servis_Jul_24_111 #20-25 RT: 0.24-0.31 AV: 6 SB: 31 0.08-0.15 , 0.46-0.75 NL: 1.09E6
 T: FTMS - p ESI Full ms [100.0000-1000.0000]



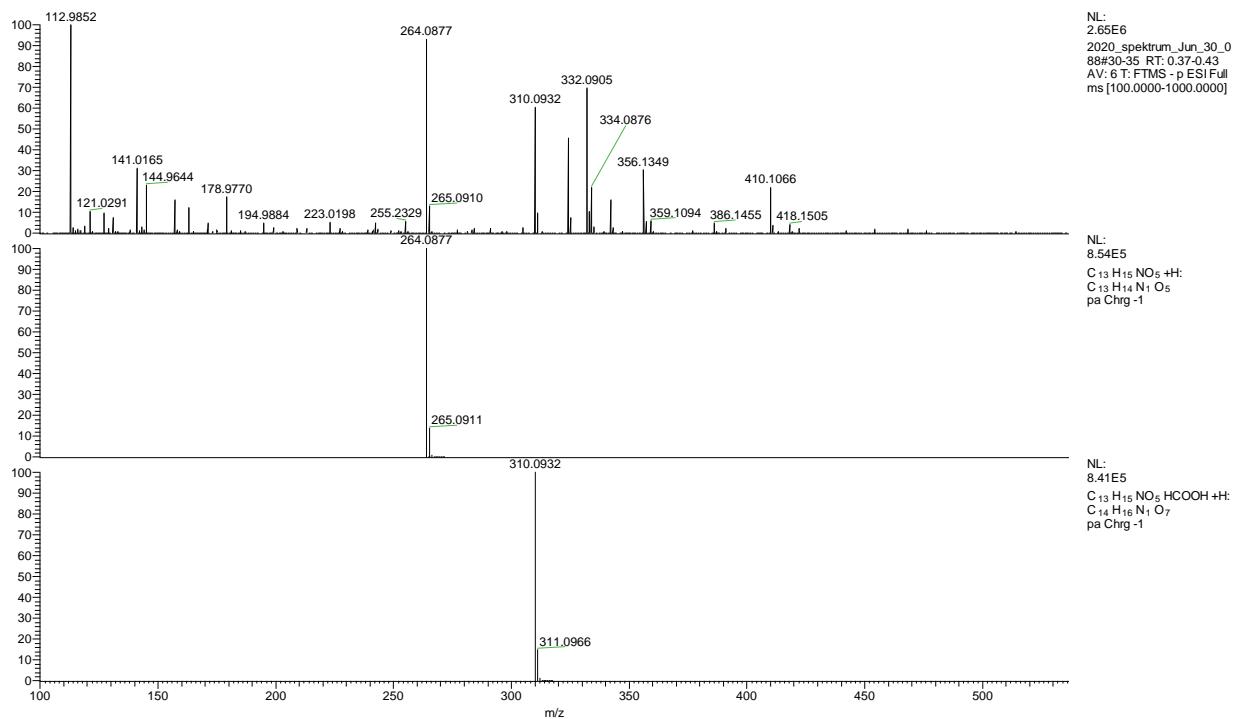
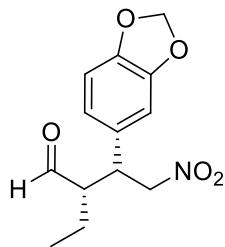
(2S,3R)-2-benzyl-3-(naphthalen-1-yl)-4-nitrobutanal (11i**)**



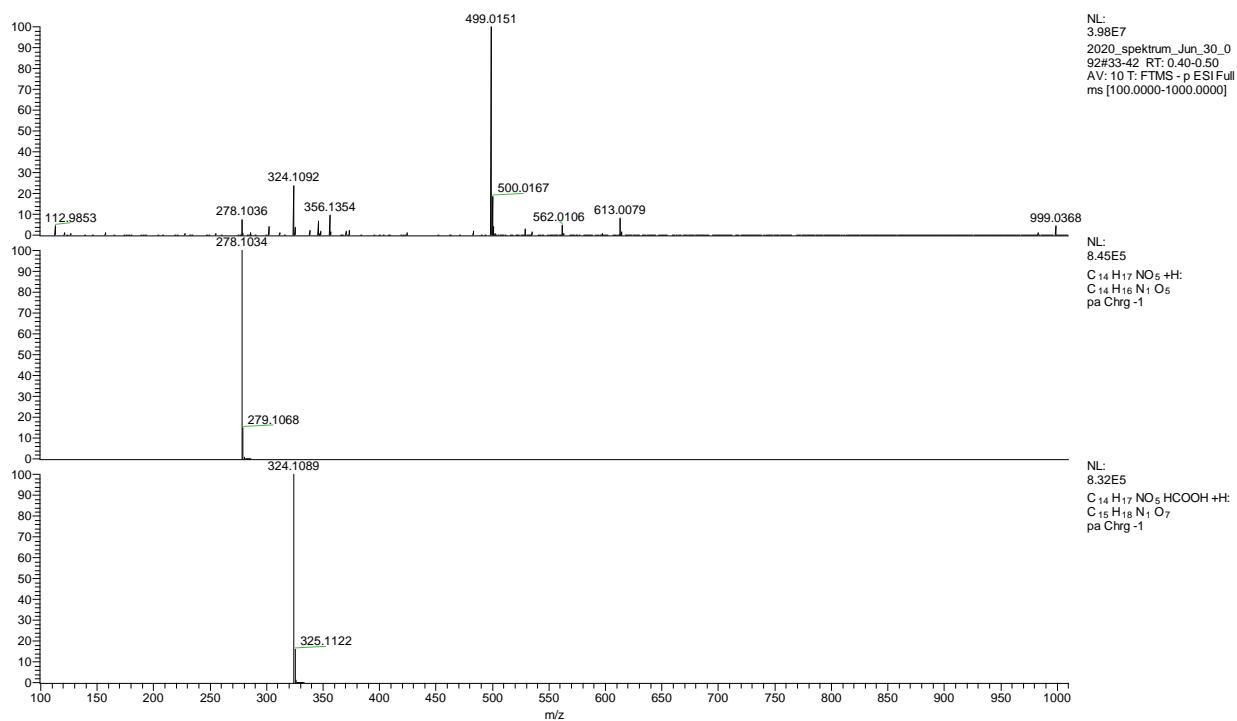
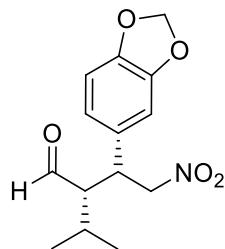
(2S,3R)-3-(benzo[d][1,3]dioxol-5-yl)-2-methyl-4-nitrobutanal (12a**)**



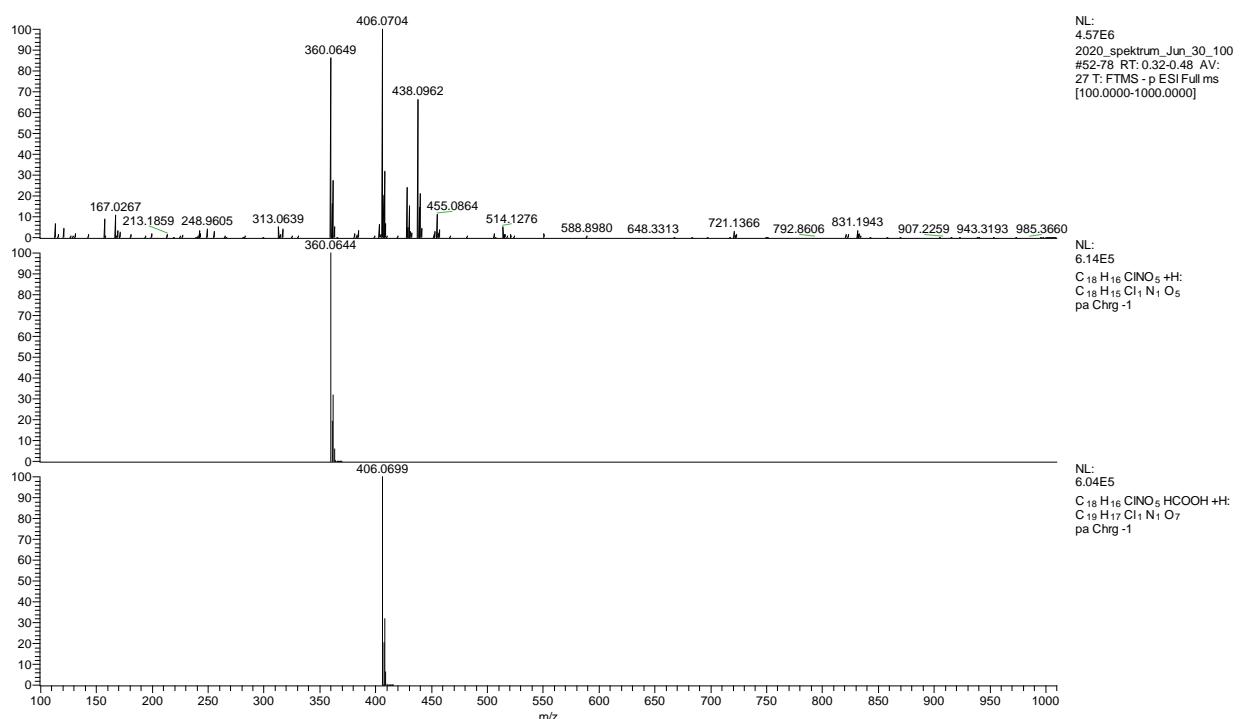
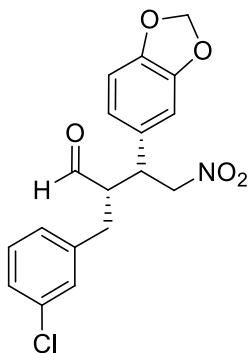
(2S,3R)-3-(benzo[d][1,3]dioxol-5-yl)-2-ethyl-4-nitrobutanal (12b**)**



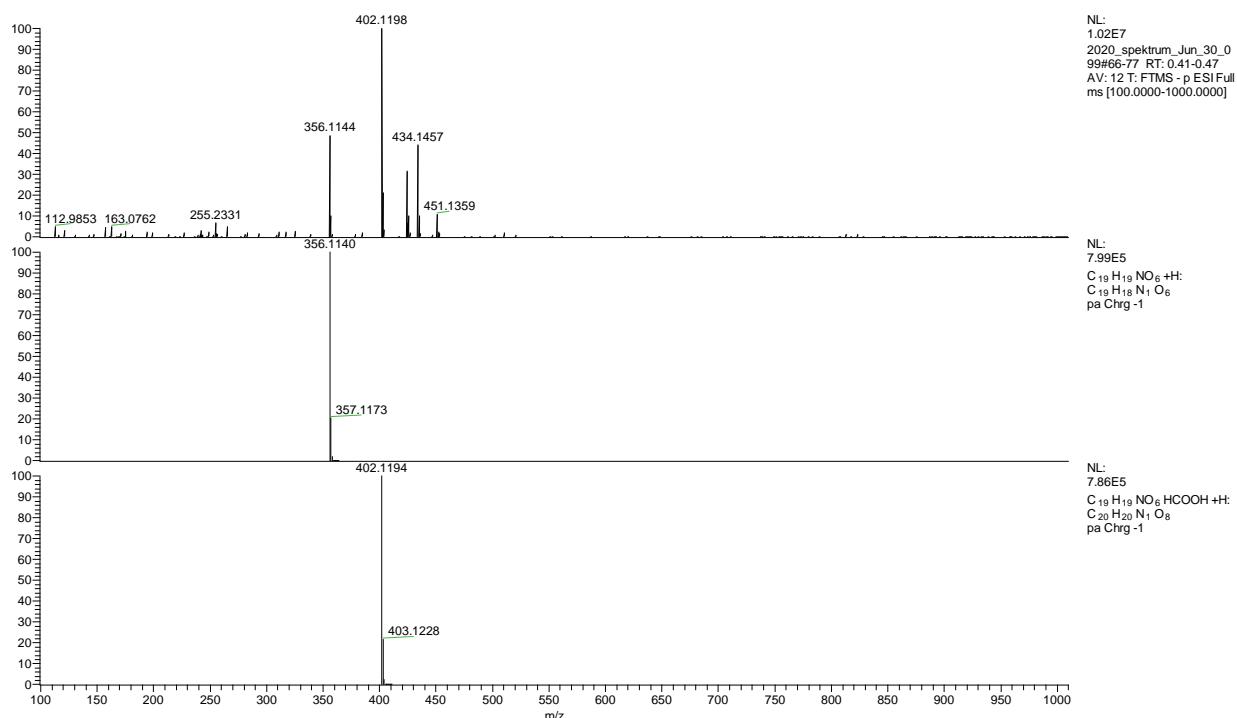
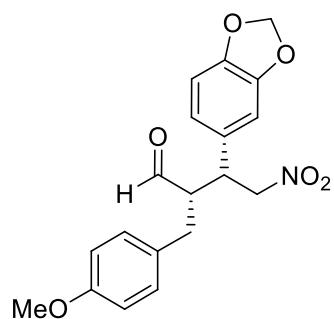
(2S,3R)-3-(benzo[d][1,3]dioxol-5-yl)-2-isopropyl-4-nitrobutanal (12c**)**



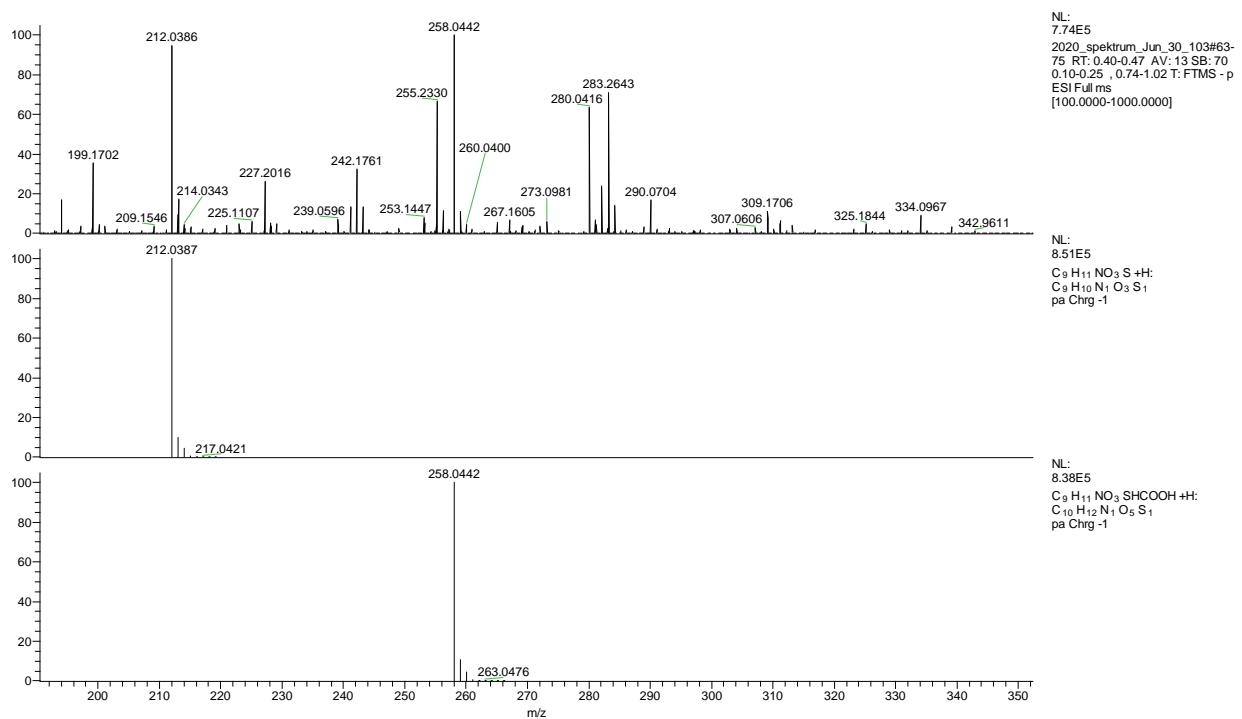
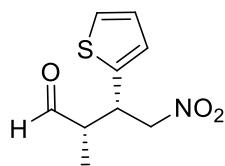
(2S,3R)-3-(benzo[d][1,3]dioxol-5-yl)-2-(3-chlorobenzyl)-4-nitrobutanal (12d**)**



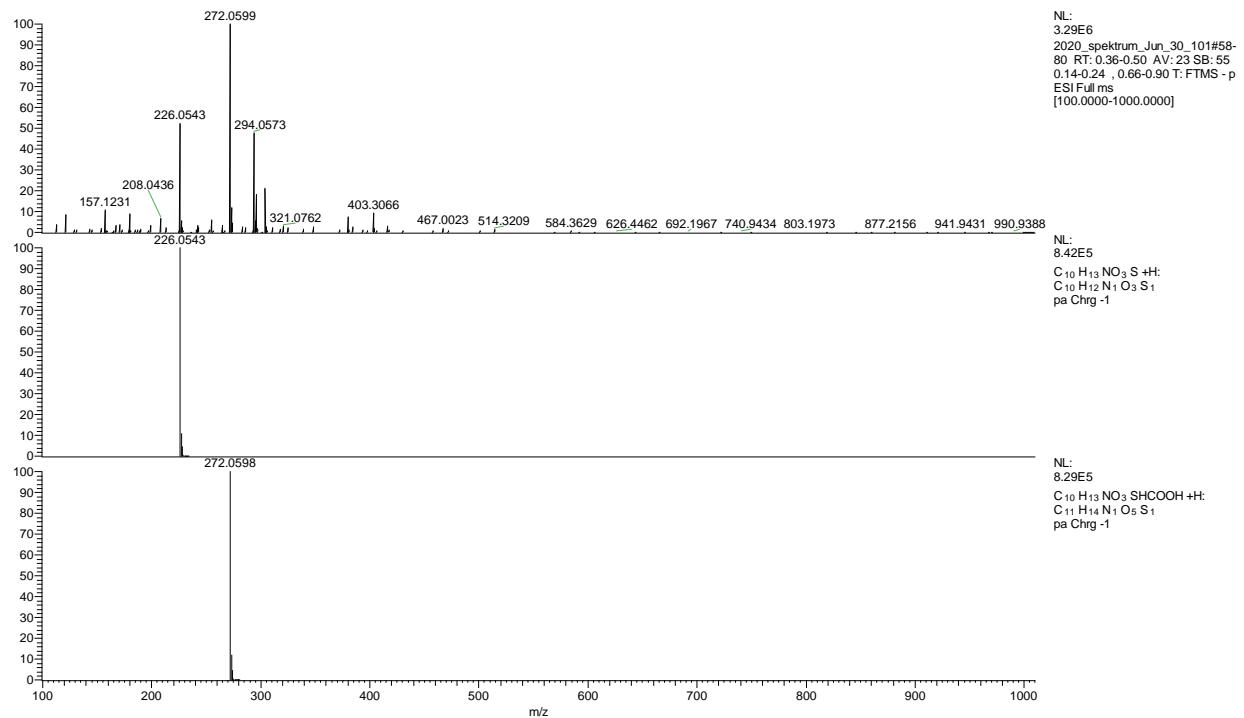
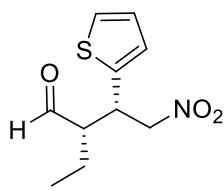
(2*S*,3*R*)-3-(benzo[d][1,3]dioxol-5-yl)-2-(4-methoxybenzyl)-4-nitrobutanal (**12e**)



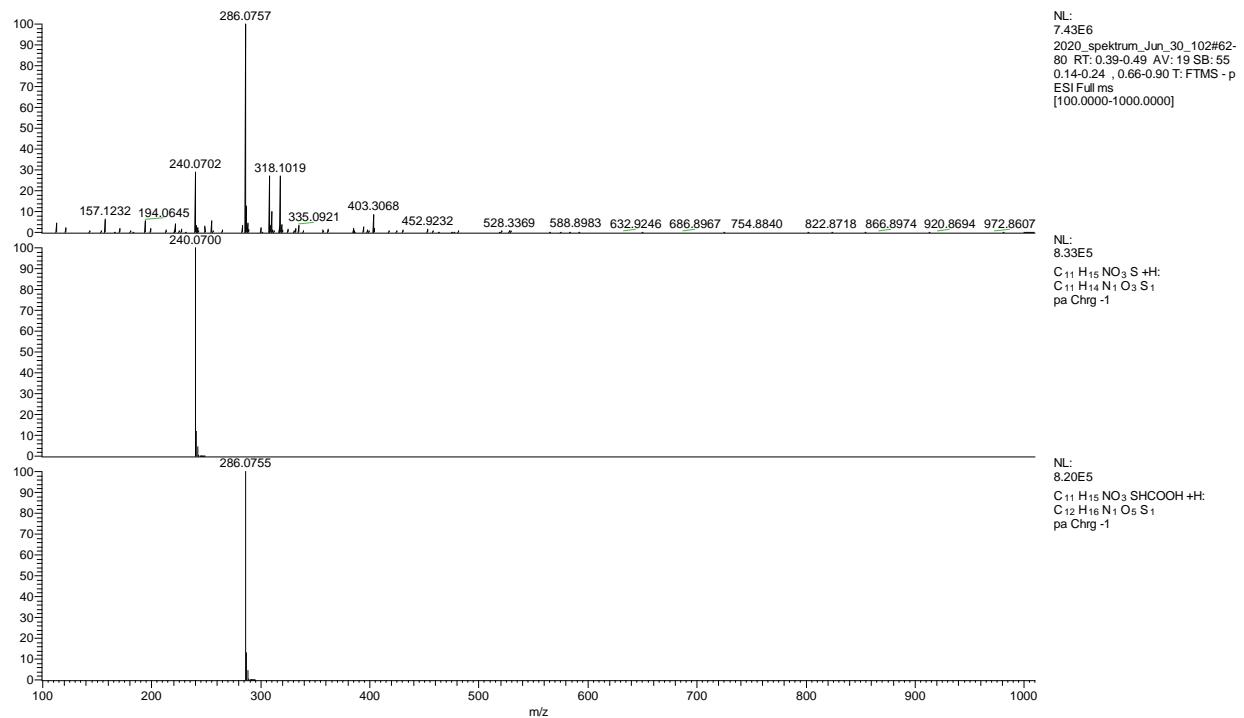
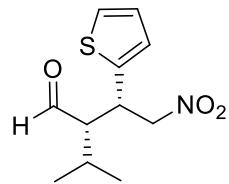
(*2S,3S*)-2-methyl-4-nitro-3-(thiophen-2-yl)butanal (**12f**)



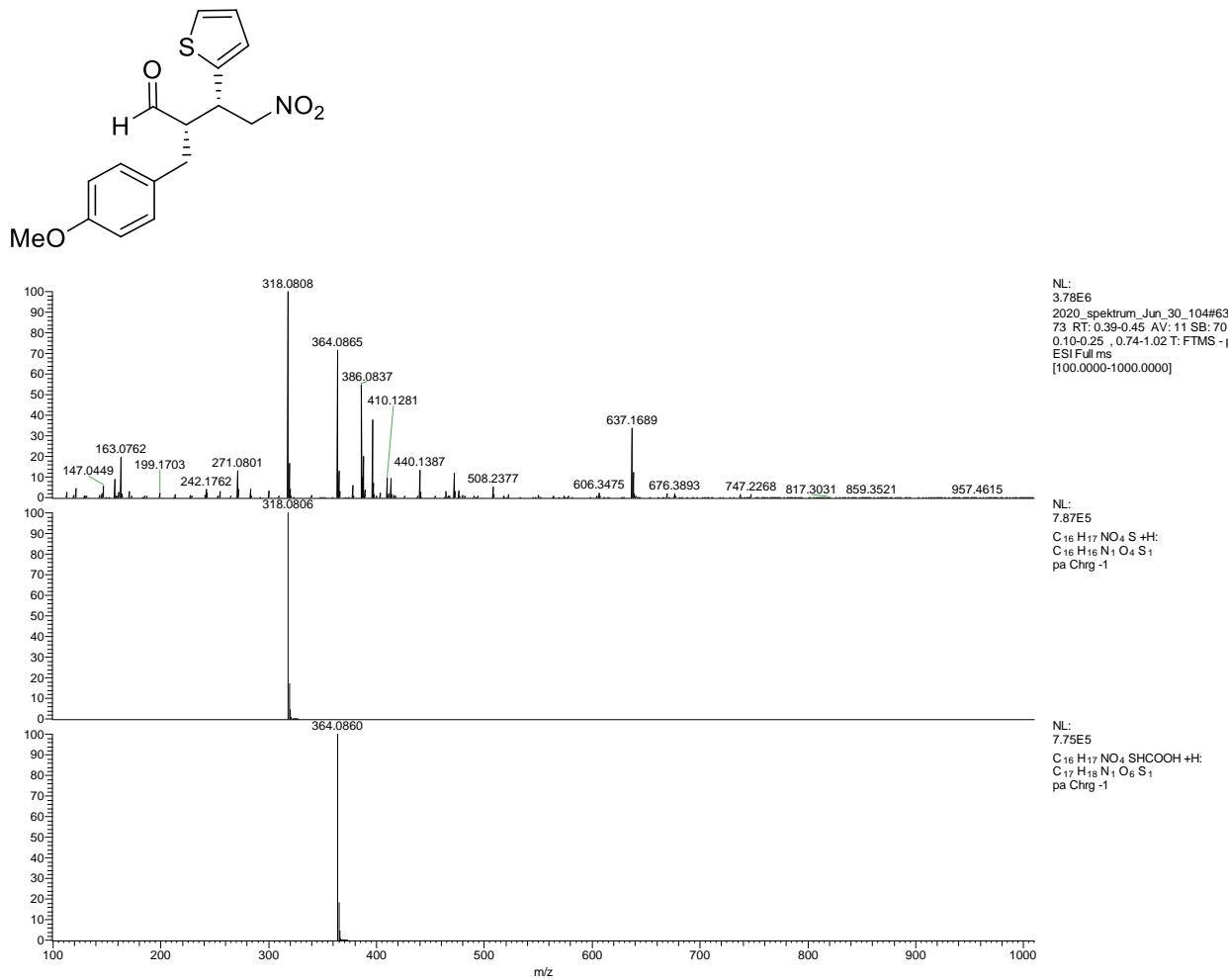
(2S,3S)-2-ethyl-4-nitro-3-(thiophen-2-yl)butanal (**12g**)



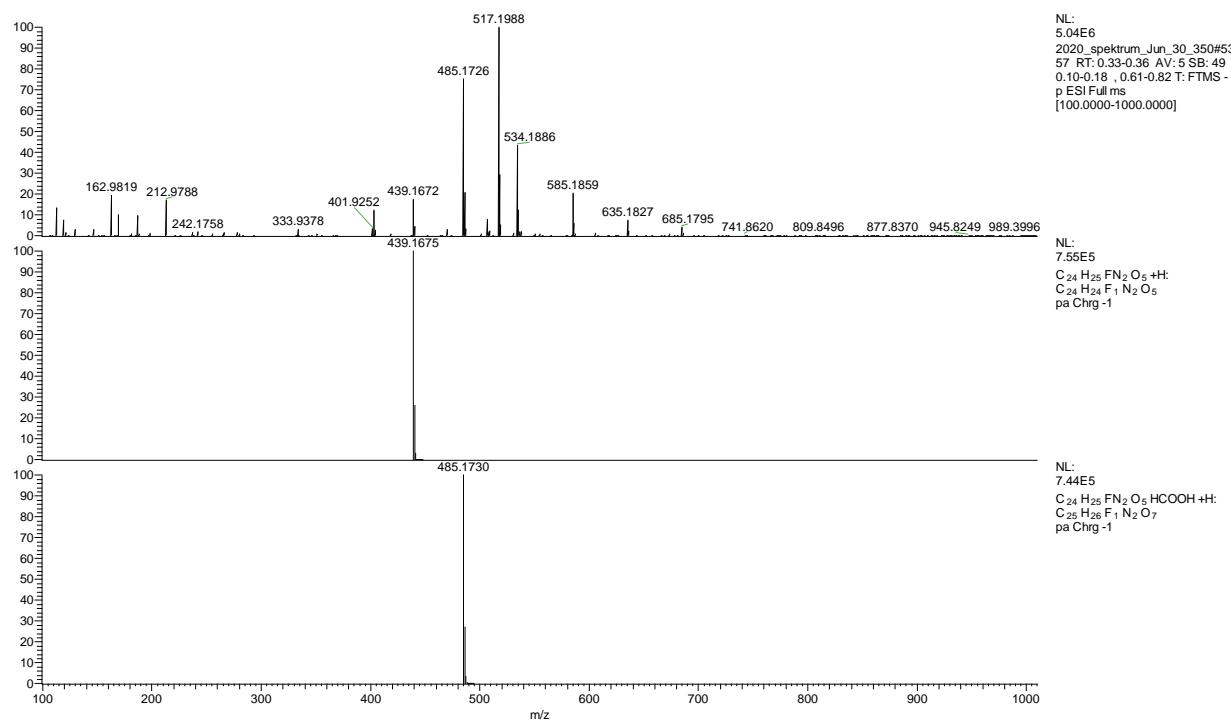
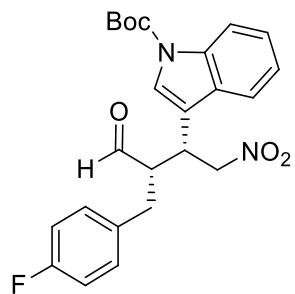
(2S,3S)-2-isopropyl-4-nitro-3-(thiophen-2-yl)butanal (**12h**)



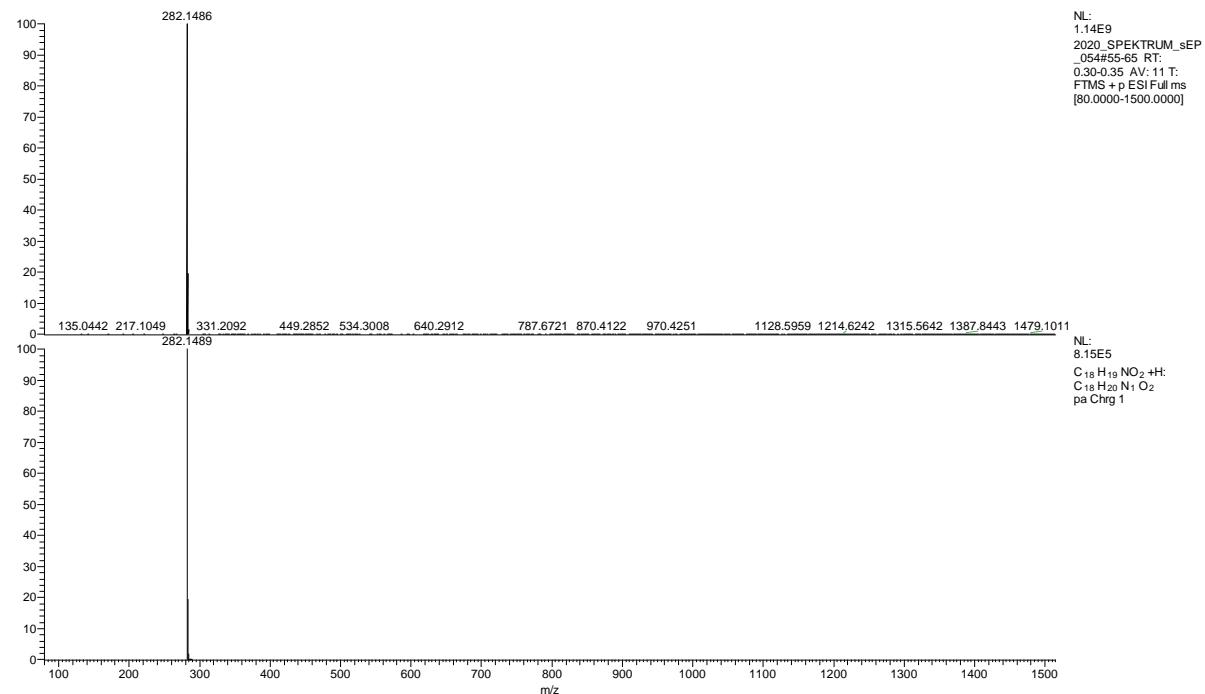
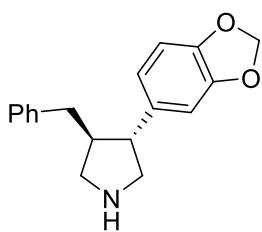
(2S,3S)-2-(4-methoxybenzyl)-4-nitro-3-(thiophen-2-yl)butanal (**12i**)



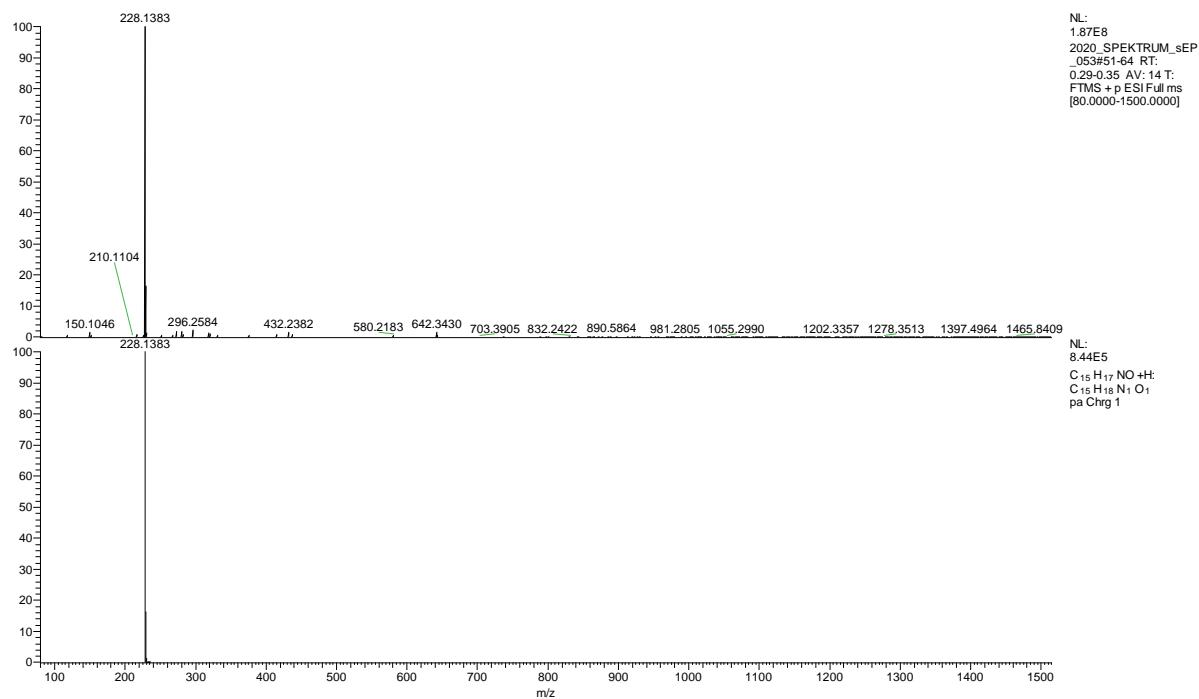
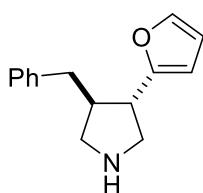
Tert-butyl 3-((2*R*,3*S*)-3-(4-fluorobenzyl)-1-nitro-4-oxobutan-2-yl)-1*H*-indole-1-carboxyl-ate
(12j)



(3R,4S)-3-(benzo[d][1,3]dioxol-5-yl)-4-benzylpyrrolidine (13a**)**



3-benzyl-4-(furan-2-yl)pyrrolidine (**13b**)



Computational details

The molecular models were built and preoptimized by semiempirical AM1 method in Spartan 18 program package.⁴ From the conformer distribution performed by MM (250 lowest conformers), 70 most stable conformers were selected and single point energy calculated at HF/3-21G level, then 50 lowest conformers were geometrically optimized at HF/3-21G level and finally 31 lowest ones were geometrically optimized at B3LYP-D3/6-31G* level and for 16 lowest ones energy refined at M06-2X/Def2-TZVP (IEFPCM=DCM) level.⁵⁻⁶

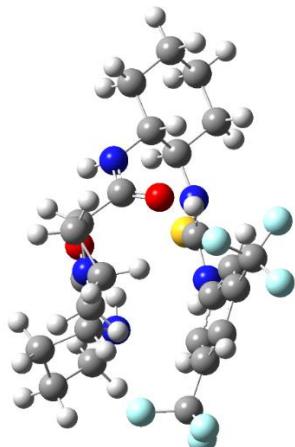
Transition states were located at semiempirical AM1 level, preoptimized at HF/3-21G and then fully geometrically optimized at B3LYP-D3/6-31G* level. Energies were refined by single point calculations at M06-2X/Def2-TZVP level (IEFPCM=DCM). Transition states were verified by visualization of the imaginary vibration, which corresponds to the bond formation between enamine and nitroalkene in the Michael addition.

Frequency calculations at M06-2X/Def2-TZVP (IEFPCM=DCM) level were performed using Gaussian 16, rev. C.01.⁷

Catalyst conformers

Note: Conformers are numbered conformer1-16 according to energies from geometrical optimization at B3LYP-D3/6-31G*; in parentheses order is given according to M06-2X/Def2-TZVP (DCM) Gibbs free energies.

Conformer1 (C1-conf3)



Imaginary Freq	0	
Temperature	298.15	Kelvin
Pressure	1	atm
Frequencies scaled by	1	
Electronic Energy (EE)	-2392.931	Hartree
Zero-point Energy Correction	0.564056	Hartree
Thermal Correction to Energy	0.59841	Hartree
Thermal Correction to Enthalpy	0.599355	Hartree
Thermal Correction to Free Energy	0.501032	Hartree
EE + Zero-point Energy	-2392.367	Hartree

EE + Thermal Energy Correction	-2392.3326	Hartree
EE + Thermal Enthalpy Correction	-2392.3317	Hartree
EE + Thermal Free Energy Correction	-2392.43	Hartree
E (Thermal)	375.508	kcal/mol
Heat Capacity (Cv)	136.362	cal/mol-kelvin
Entropy (S)	206.936	cal/mol-kelvin

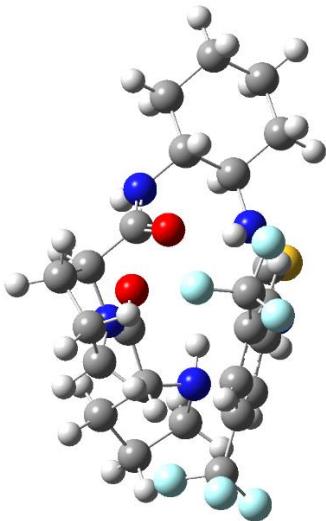
Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

N	0.2574	1.9052	-2.6342
C	0.5631	2.9254	-3.6711
C	0.3126	4.2916	-3.0043
C	0.63	4.0162	-1.5291
C	0.0351	2.6	-1.3496
C	0.7099	1.8448	-0.2068
N	0.0886	1.803	0.9987
C	-1.1802	2.4374	1.3949
C	-1.493	1.7778	2.7406
C	-0.1014	1.5406	3.3495
C	0.7767	1.1687	2.1384
O	1.8108	1.3065	-0.3806
C	0.8393	-0.3531	1.9264
O	-0.1678	-1.0566	2.0509
N	2.0657	-0.8426	1.6133
C	2.3078	-4.0197	-0.5222
C	2.276	-2.2529	1.2913
C	3.9075	-4.1907	1.4324
C	3.6674	-2.7075	1.7515
C	3.6962	-4.4801	-0.0609
C	2.1032	-2.5291	-0.216
N	0.7911	-2.0518	-0.655
C	0.5698	-1.5357	-1.8805
S	1.6982	-1.5419	-3.1367
N	-0.6639	-0.9553	-2.1246
C	-1.7468	-0.6715	-1.2844
C	-3.9814	0.0514	0.2823
C	-2.1523	-1.4743	-0.2072
C	-2.5128	0.4616	-1.6028
C	-3.6159	0.8069	-0.8308
C	-3.2372	-1.0897	0.5757
C	-4.3538	2.068	-1.1816
C	-3.5945	-1.8932	1.7976
F	-4.9361	-1.9801	1.9538
F	-3.1077	-3.1494	1.7478
F	-3.1083	-1.3173	2.9221
F	-3.6464	3.17	-0.7959
F	-4.5425	2.1858	-2.512
F	-5.5575	2.1451	-0.5822
H	-0.7403	4.5815	-3.1109
H	0.2025	4.7515	-0.8393
H	1.6076	2.8389	-3.9977
H	-0.069	2.7794	-4.5543

H	1.0602	1.2866	-2.5227
H	-1.0406	2.693	-1.1703
H	0.9233	5.0899	-3.4374
H	1.7144	3.9741	-1.3698
H	-2.1328	2.4065	3.3668
H	-1.9898	0.8183	2.5815
H	-0.1024	0.7552	4.1087
H	-1.9589	2.2627	0.6554
H	-1.0431	3.5226	1.5011
H	1.7915	1.5718	2.2168
H	0.285	2.4604	3.8033
H	2.6981	-0.1751	1.1836
H	1.5116	-2.8072	1.8473
H	2.8573	-1.9512	-0.7646
H	-0.6133	-0.3519	-2.9392
H	-1.6554	-2.4058	0.0225
H	-4.8366	0.3283	0.8863
H	-2.2147	1.0757	-2.446
H	0.1437	-1.8308	0.0939
H	3.8246	-5.5496	-0.2649
H	4.4623	-3.9528	-0.647
H	3.2097	-4.8021	2.0227
H	4.919	-4.4785	1.7435
H	4.427	-2.0954	1.2428
H	3.7675	-2.5146	2.8257
H	1.5262	-4.5972	-0.0081
H	2.1787	-4.174	-1.5979

Conformer2 (C1-conf2)



Imaginary Freq	0
Temperature	298.15 Kelvin
Pressure	1 atm
Frequencies scaled by	1
Electronic Energy (EE)	-2392.9315 Hartree
Zero-point Energy Correction	0.564035 Hartree

Thermal Correction to Energy	0.598427	Hartree
Thermal Correction to Enthalpy	0.599371	Hartree
Thermal Correction to Free Energy	0.500773	Hartree
EE + Zero-point Energy	-2392.3675	Hartree
EE + Thermal Energy Correction	-2392.3331	Hartree
EE + Thermal Enthalpy Correction	-2392.3322	Hartree
EE + Thermal Free Energy Correction	-2392.4308	Hartree
E (Thermal)	375.519	kcal/mol
Heat Capacity (Cv)	136.37	cal/mol-kelvin
Entropy (S)	207.517	cal/mol-kelvin

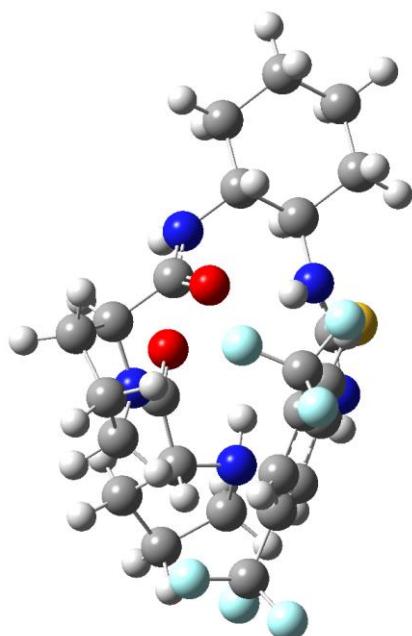
Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

N	0.3055	1.8706	-2.6567
C	0.6604	2.8762	-3.6917
C	0.3764	4.2466	-3.0517
C	0.6705	3.9933	-1.5677
C	0.0779	2.5773	-1.3788
C	0.7447	1.8334	-0.2244
N	0.1227	1.8187	0.9816
C	-1.1407	2.4701	1.3681
C	-1.4631	1.8268	2.7194
C	-0.0753	1.5831	3.3337
C	0.798	1.1837	2.1282
O	1.8377	1.2766	-0.3891
C	0.8284	-0.3408	1.9314
O	-0.1951	-1.0209	2.0557
N	2.0455	-0.8619	1.6341
C	2.238	-4.061	-0.4732
C	2.2258	-2.2795	1.3257
C	3.8109	-4.2527	1.5007
C	3.6014	-2.7619	1.8053
C	3.6104	-4.5486	0.0075
C	2.0614	-2.5639	-0.1811
N	0.7621	-2.0655	-0.6349
C	0.5537	-1.5692	-1.8709
S	1.6867	-1.6142	-3.1215
N	-0.6699	-0.9734	-2.1299
C	-1.7504	-0.6589	-1.2976
C	-3.9593	0.1337	0.2715
C	-2.4989	0.4803	-1.6329
C	-2.1656	-1.437	-0.2049
C	-3.234	-1.0164	0.5797
C	-3.5908	0.8594	-0.8593
C	-3.6261	-1.7958	1.8063
C	-4.3076	2.1274	-1.2284
F	-4.521	2.215	-2.5572
F	-5.4961	2.2485	-0.6066
F	-3.567	3.2223	-0.8864
F	-4.9461	-2.0985	1.7912
F	-2.9452	-2.9496	1.9312
F	-3.4124	-1.0697	2.9306

H	-0.6793	4.5167	-3.1805
H	0.2289	4.7351	-0.894
H	1.7207	2.7921	-3.9648
H	0.073	2.7167	-4.603
H	1.0874	1.2289	-2.529
H	-0.9984	2.6711	-1.2059
H	0.9822	5.0485	-3.4849
H	1.7528	3.9589	-1.3922
H	-2.099	2.4672	3.3377
H	-1.9676	0.8701	2.5688
H	-0.0855	0.8087	4.1042
H	-1.9193	2.297	0.628
H	-0.9925	3.5547	1.4644
H	1.8203	1.5676	2.2043
H	0.3215	2.5047	3.775
H	2.6988	-0.2138	1.2063
H	1.4427	-2.8109	1.8778
H	2.8322	-2.0061	-0.7273
H	-0.6087	-0.3884	-2.9568
H	-2.1954	1.0761	-2.487
H	-4.8001	0.4423	0.8808
H	-1.6819	-2.3712	0.04
H	0.1153	-1.8209	0.1072
H	3.7168	-5.6223	-0.1869
H	4.3955	-4.0439	-0.5735
H	3.0916	-4.8427	2.087
H	4.8115	-4.5616	1.8264
H	4.3807	-2.1713	1.3008
H	3.6936	-2.5623	2.879
H	1.4382	-4.6176	0.0362
H	2.1178	-4.2214	-1.549

Conformer3 (C1-conf1)



Imaginary Freq	0	
Temperature	298.15	Kelvin
Pressure	1	atm
Frequencies scaled by	1	
Electronic Energy (EE)	-2392.9308	Hartree
Zero-point Energy Correction	0.563711	Hartree
Thermal Correction to Energy	0.598184	Hartree
Thermal Correction to Enthalpy	0.599128	Hartree
Thermal Correction to Free Energy	0.49999	Hartree
EE + Zero-point Energy	-2392.367	Hartree
EE + Thermal Energy Correction	-2392.3326	Hartree
EE + Thermal Enthalpy Correction	-2392.3316	Hartree
EE + Thermal Free Energy Correction	-2392.4308	Hartree
E (Thermal)	375.366	kcal/mol
Heat Capacity (Cv)	136.471	cal/mol-kelvin
Entropy (S)	208.654	cal/mol-kelvin

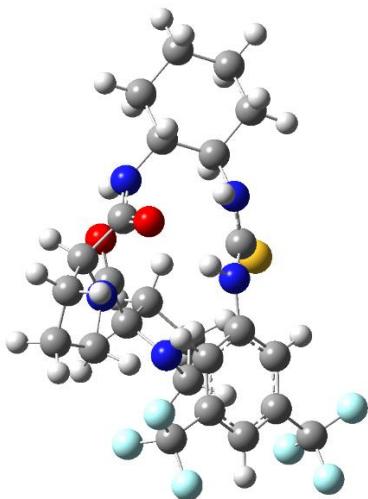
Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

N	1.1989	2.2336	-2.0838
C	1.7986	3.3861	-2.808
C	1.1795	4.6494	-2.1772
C	0.899	4.2099	-0.7343
C	0.409	2.7612	-0.9526
C	0.6104	1.8945	0.2872
N	-0.4444	1.6982	1.1189
C	-1.8128	2.234	1.0121
C	-2.5929	1.3997	2.0333
C	-1.556	1.1415	3.1387
C	-0.2374	0.9396	2.3659
O	1.7209	1.4061	0.5315
C	0.0027	-0.5438	2.0413
O	-0.9215	-1.2711	1.6645
N	1.2757	-0.9776	2.2184
C	2.5726	-3.8899	0.0858
C	1.6806	-2.3404	1.8793
C	3.209	-4.2667	2.5068
C	2.7723	-2.8325	2.8406
C	3.6637	-4.3836	1.0446
C	2.1702	-2.4468	0.4211
N	1.1349	-1.9443	-0.4849
C	1.4153	-1.2911	-1.631
S	2.9652	-1.1181	-2.2792
N	0.3606	-0.7155	-2.3217
C	-0.9908	-0.5658	-1.9909
C	-3.7005	-0.0784	-1.3844
C	-1.7491	-1.5247	-1.3065
C	-1.6255	0.6101	-2.4303
C	-2.9571	0.8457	-2.1219
C	-3.0808	-1.2597	-0.9916
C	-3.614	2.1352	-2.5278
C	-3.8502	-2.2308	-0.1358

F	-3.3261	-3.4732	-0.1695
F	-3.8648	-1.8325	1.1571
F	-5.142	-2.3188	-0.5311
F	-4.2142	2.7204	-1.4588
F	-2.7272	3.0294	-3.0214
F	-4.5707	1.9526	-3.4605
H	0.2362	4.9011	-2.6778
H	0.1662	4.8374	-0.2157
H	2.8895	3.3878	-2.6871
H	1.5875	3.3197	-3.881
H	1.9409	1.6484	-1.7
H	-0.6477	2.7899	-1.2356
H	1.839	5.5199	-2.2457
H	1.8241	4.194	-0.1456
H	-3.4853	1.9209	2.3914
H	-2.8942	0.4486	1.5877
H	-1.8014	0.2734	3.7551
H	-2.2047	2.1237	0.0031
H	-1.8236	3.3017	1.2717
H	0.6276	1.3485	2.8974
H	-1.4595	2.0158	3.7932
H	1.9888	-0.2572	2.1708
H	0.7847	-2.9597	2.0015
H	3.0467	-1.7992	0.2996
H	0.7053	-0.0085	-2.9632
H	-1.3267	-2.4791	-1.0235
H	-4.7335	0.1179	-1.1222
H	-1.0461	1.3465	-2.9732
H	0.2165	-1.83	-0.0675
H	3.9323	-5.4203	0.8102
H	4.5714	-3.7814	0.8951
H	2.3652	-4.9496	2.6825
H	4.0111	-4.5767	3.1875
H	3.64	-2.1601	2.7663
H	2.3991	-2.7624	3.8688
H	1.6829	-4.5311	0.1625
H	2.9136	-3.9229	-0.9536

Conformer4 (C1-conf16)



Imaginary Freq	0	
Temperature	298.15	Kelvin
Pressure	1	atm
Frequencies scaled by	1	
Electronic Energy (EE)	-2392.9248	Hartree
Zero-point Energy Correction	0.563528	Hartree
Thermal Correction to Energy	0.597744	Hartree
Thermal Correction to Enthalpy	0.598688	Hartree
Thermal Correction to Free Energy	0.499974	Hartree
EE + Zero-point Energy	-2392.3613	Hartree
EE + Thermal Energy Correction	-2392.3271	Hartree
EE + Thermal Enthalpy Correction	-2392.3262	Hartree
EE + Thermal Free Energy Correction	-2392.4249	Hartree
E (Thermal)	375.09	kcal/mol
Heat Capacity (Cv)	136.1	cal/mol-kelvin
Entropy (S)	207.761	cal/mol-kelvin

Symbolic Z-matrix:

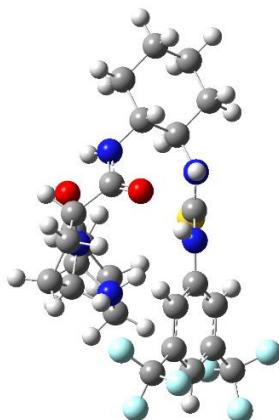
Charge = 0 Multiplicity = 1

N	-1.3064	1.9014	-1.3129
C	-1.7723	2.3032	-2.6506
C	-0.5153	2.3555	-3.5575
C	0.6591	2.6007	-2.5728
C	-0.0212	2.6102	-1.1771
C	0.8592	2.051	-0.0628
N	0.2474	1.7211	1.1108
C	-1.0628	2.2544	1.5564
C	-0.8793	2.4344	3.0667
C	0.0883	1.3062	3.4456
C	1.0489	1.2177	2.2519
O	2.0789	1.9083	-0.2272
C	1.56	-0.2285	2.0159
O	0.9767	-1.2149	2.4971
N	2.6832	-0.2989	1.2739
C	3.3937	-3.3854	-0.9086
C	3.3357	-1.5335	0.8422

C	5.5564	-2.4902	0.0446
C	4.8179	-1.2455	0.557
C	4.8667	-3.0722	-1.1966
C	2.6492	-2.1411	-0.4062
N	1.2603	-2.4521	-0.0729
C	0.1788	-1.8327	-0.6168
S	0.1669	-1.2059	-2.1791
N	-0.8664	-1.789	0.2881
C	-2.1621	-1.2815	0.1325
C	-4.7477	-0.179	-0.0077
C	-2.765	-0.7272	1.2684
C	-2.8847	-1.3345	-1.0672
C	-4.1586	-0.7747	-1.1227
C	-4.0398	-0.1737	1.1907
C	-4.8944	-0.75	-2.4367
C	-4.591	0.5443	2.3899
F	-5.9375	0.5977	2.381
F	-4.2043	-0.0337	3.5495
F	-4.1435	1.8289	2.4319
F	-6.2293	-0.8697	-2.2636
F	-4.691	0.4218	-3.0911
F	-4.4969	-1.7372	-3.2647
H	-0.591	3.1317	-4.3264
H	1.1931	3.5363	-2.7661
H	-2.5439	1.6125	-2.9991
H	-2.2289	3.2994	-2.5703
H	-1.0929	0.902	-1.3636
H	-0.2563	3.6527	-0.9029
H	-0.3841	1.3971	-4.0705
H	1.3927	1.7921	-2.6116
H	-0.4289	3.4114	3.2791
H	-1.8339	2.3759	3.5966
H	-0.4396	0.353	3.5442
H	-1.8599	1.5553	1.3119
H	-1.2893	3.1872	1.0394
H	1.9216	1.8718	2.379
H	0.6231	1.4824	4.3827
H	2.8904	0.554	0.7463
H	3.2566	-2.2506	1.6703
H	2.6283	-1.3836	-1.1968
H	-0.5443	-1.7828	1.256
H	-2.2253	-0.7079	2.2101
H	-5.7376	0.2568	-0.0699
H	-2.4558	-1.7945	-1.9453
H	1.1415	-2.7475	0.8918
H	5.3852	-3.9771	-1.5339
H	4.9288	-2.3481	-2.021
H	5.5833	-3.251	0.8382
H	6.5988	-2.2336	-0.1782
H	4.879	-0.4482	-0.1988
H	5.2855	-0.8552	1.4683
H	3.3245	-4.176	-0.1467

H 2.8818 -3.7573 -1.8026

Conformer5 (C1-conf15)



Imaginary Freq	0	
Temperature	298.15	Kelvin
Pressure	1	atm
Frequencies scaled by	1	
Electronic Energy (EE)	-2392.9255	Hartree
Zero-point Energy Correction	0.563536	Hartree
Thermal Correction to Energy	0.597781	Hartree
Thermal Correction to Enthalpy	0.598725	Hartree
Thermal Correction to Free Energy	0.499888	Hartree
EE + Zero-point Energy	-2392.362	Hartree
EE + Thermal Energy Correction	-2392.3277	Hartree
EE + Thermal Enthalpy Correction	-2392.3268	Hartree
EE + Thermal Free Energy Correction	-2392.4256	Hartree
E (Thermal)	375.113	kcal/mol
Heat Capacity (Cv)	136.113	cal/mol-kelvin
Entropy (S)	208.02	cal/mol-kelvin

Symbolic Z-matrix:

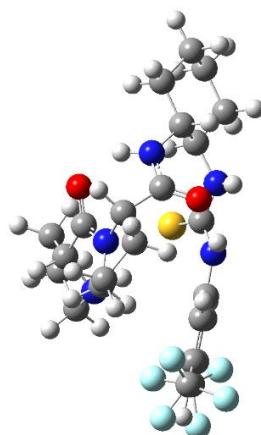
Charge = 0 Multiplicity = 1

N	-1.2951	1.9573	-1.2683
C	-1.7771	2.3787	-2.5953
C	-0.5345	2.4351	-3.5215
C	0.6613	2.6371	-2.5531
C	0.0032	2.6459	-1.1472
C	0.8889	2.0619	-0.0512
N	0.2923	1.7302	1.1304
C	-1.0004	2.2754	1.6099
C	-0.7668	2.4727	3.1108
C	0.1953	1.3338	3.4732
C	1.115	1.2152	2.2505
O	2.1025	1.898	-0.2376
C	1.5862	-0.2411	1.9983
O	0.982	-1.2187	2.4714
N	2.7011	-0.329	1.2445
C	3.3417	-3.4035	-0.9803
C	3.324	-1.5743	0.8025

C	5.5179	-2.5882	0.0187
C	4.8146	-1.3238	0.5306
C	4.8283	-3.1293	-1.2417
C	2.6258	-2.1513	-0.4548
N	1.2329	-2.4399	-0.1179
C	0.1576	-1.8033	-0.6526
S	0.1461	-1.1702	-2.2113
N	-0.8806	-1.7479	0.2593
C	-2.1777	-1.2424	0.1125
C	-4.7663	-0.1453	-0.0035
C	-2.7743	-0.6951	1.2572
C	-2.9073	-1.2885	-1.0814
C	-4.1847	-0.7306	-1.1254
C	-4.0489	-0.1446	1.1911
C	-4.918	-0.7259	-2.4413
C	-4.6686	0.4398	2.4292
F	-3.7227	0.9262	3.2755
F	-5.5106	1.4524	2.1366
F	-5.3762	-0.4784	3.1236
F	-6.2498	-0.5724	-2.2785
F	-4.5005	0.2867	-3.2423
F	-4.7159	-1.8715	-3.1262
H	-0.6122	3.2317	-4.2687
H	1.2175	3.5605	-2.7413
H	-2.5561	1.6948	-2.9395
H	-2.2282	3.3757	-2.4976
H	-1.0948	0.9557	-1.3333
H	-0.2125	3.6895	-0.8612
H	-0.4265	1.4881	-4.0595
H	1.3734	1.8107	-2.616
H	-0.2972	3.4463	3.2954
H	-1.7009	2.4308	3.6762
H	-0.345	0.3913	3.6044
H	-1.8068	1.5726	1.405
H	-1.239	3.1999	1.0844
H	2.0054	1.8503	2.3458
H	0.7657	1.5163	4.3878
H	2.9198	0.5217	0.7184
H	3.2226	-2.2969	1.623
H	2.617	-1.3806	-1.2328
H	-0.5561	-1.7528	1.2262
H	-2.2219	-0.6701	2.1909
H	-5.753	0.2975	-0.0552
H	-2.4824	-1.7414	-1.9659
H	1.1135	-2.74	0.845
H	5.323	-4.0452	-1.5859
H	4.924	-2.3936	-2.0534
H	5.5002	-3.3583	0.8044
H	6.5733	-2.3689	-0.1829
H	4.9033	-0.5256	-0.2215
H	5.2868	-0.9506	1.4468
H	3.2375	-4.2117	-0.2412

H 2.8305 -3.7355 -1.8907

Conformer6 (C1-conf14)



Imaginary Freq	0	
Temperature	298.15	Kelvin
Pressure	1	atm
Frequencies scaled by	1	
Electronic Energy (EE)	-2392.9256	Hartree
Zero-point Energy Correction	0.563441	Hartree
Thermal Correction to Energy	0.597721	Hartree
Thermal Correction to Enthalpy	0.598665	Hartree
Thermal Correction to Free Energy	0.499634	Hartree
EE + Zero-point Energy	-2392.3621	Hartree
EE + Thermal Energy Correction	-2392.3278	Hartree
EE + Thermal Enthalpy Correction	-2392.3269	Hartree
EE + Thermal Free Energy Correction	-2392.4259	Hartree
E (Thermal)	375.075	kcal/mol
Heat Capacity (Cv)	136.156	cal/mol-kelvin
Entropy (S)	208.429	cal/mol-kelvin

Symbolic Z-matrix:

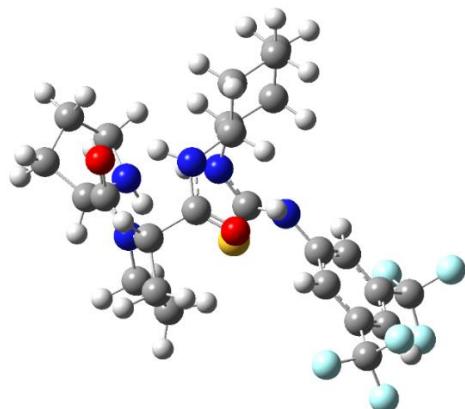
Charge = 0 Multiplicity = 1

N	-1.2467	1.9499	-1.3184
C	-1.6714	2.3653	-2.666
C	-0.388	2.441	-3.5337
C	0.7579	2.6596	-2.5107
C	0.0363	2.6532	-1.1364
C	0.8829	2.0726	-0.0078
N	0.2393	1.7278	1.1446
C	-1.0769	2.2612	1.5714
C	-0.9074	2.4494	3.0819
C	0.038	1.307	3.4764
C	1.0152	1.209	2.2969
O	2.1055	1.9236	-0.1422
C	1.5127	-0.2398	2.054
O	0.9053	-1.2252	2.5057
N	2.6535	-0.3126	1.3389
C	3.3916	-3.3711	-0.8739
C	3.3033	-1.5488	0.9093

C	5.5303	-2.5323	0.1772
C	4.7974	-1.2794	0.6762
C	4.8794	-3.0779	-1.1006
C	2.6475	-2.1275	-0.3688
N	1.2485	-2.4311	-0.0763
C	0.1859	-1.8012	-0.6428
S	0.22	-1.156	-2.1972
N	-0.8842	-1.764	0.2323
C	-2.1786	-1.2644	0.044
C	-4.7662	-0.1785	-0.1579
C	-2.8632	-1.3026	-1.1768
C	-2.8203	-0.7328	1.1713
C	-4.0947	-0.1867	1.0632
C	-4.1405	-0.7508	-1.2629
C	-4.7613	0.3768	2.2869
C	-4.8251	-0.7337	-2.6052
F	-4.3879	0.295	-3.3747
F	-4.5896	-1.8668	-3.3002
F	-6.1633	-0.5934	-2.4886
F	-5.623	1.3667	1.9771
F	-5.4595	-0.5645	2.9598
F	-3.8508	0.8847	3.1587
H	-0.4435	3.2364	-4.2846
H	1.3094	3.5908	-2.6735
H	-2.4214	1.6695	-3.0484
H	-2.1418	3.3549	-2.5881
H	-1.0343	0.9506	-1.3737
H	-0.2031	3.6924	-0.8528
H	-0.2415	1.4963	-4.0672
H	1.4825	1.8425	-2.5404
H	-0.4429	3.4209	3.291
H	-1.8662	2.4091	3.6046
H	-0.505	0.3611	3.5662
H	-1.8699	1.5548	1.3278
H	-1.3008	3.1887	1.0445
H	1.8929	1.8524	2.4419
H	0.5626	1.4772	4.4206
H	2.8824	0.5452	0.8286
H	3.1877	-2.2761	1.7238
H	2.6542	-1.3553	-1.1452
H	-0.5928	-1.7729	1.2095
H	-2.4025	-1.7434	-2.0491
H	-5.7532	0.2578	-0.2465
H	-2.303	-0.7169	2.1253
H	1.1028	-2.7395	0.8803
H	5.3936	-3.9856	-1.4371
H	4.9852	-2.3385	-1.9072
H	5.5069	-3.3052	0.9593
H	6.5861	-2.2961	0.0022
H	4.8933	-0.4796	-0.0729
H	5.2418	-0.9018	1.6043
H	3.2818	-4.1773	-0.1337

H 2.9075 -3.7144 -1.7942

Conformer7 (C1-conf11)



Imaginary Freq	0	
Temperature	298.15	Kelvin
Pressure	1	atm
Frequencies scaled by	1	
Electronic Energy (EE)	-2392.9275	Hartree
Zero-point Energy Correction	0.563657	Hartree
Thermal Correction to Energy	0.597633	Hartree
Thermal Correction to Enthalpy	0.598578	Hartree
Thermal Correction to Free Energy	0.499886	Hartree
EE + Zero-point Energy	-2392.3639	Hartree
EE + Thermal Energy Correction	-2392.3299	Hartree
EE + Thermal Enthalpy Correction	-2392.329	Hartree
EE + Thermal Free Energy Correction	-2392.4276	Hartree
E (Thermal)	375.021	kcal/mol
Heat Capacity (Cv)	135.299	cal/mol-kelvin
Entropy (S)	207.713	cal/mol-kelvin

Symbolic Z-matrix:

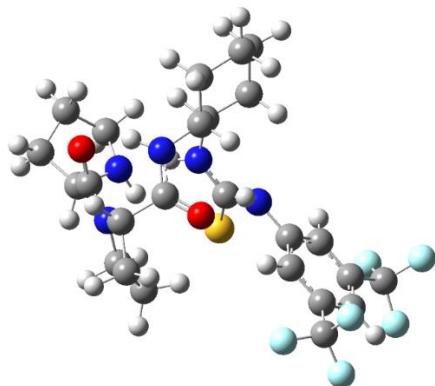
Charge = 0 Multiplicity = 1

N	1.8673	1.3777	-2.5728
C	3.2422	1.2808	-3.0989
C	3.8991	2.5611	-2.58
C	2.7831	3.5985	-2.7812
C	1.4925	2.8146	-2.453
C	1.053	3.038	-0.9976
N	-0.2518	2.8416	-0.6982
C	-1.3292	2.4912	-1.6531
C	-2.5518	2.256	-0.7535
C	-2.2778	3.1302	0.4815
C	-0.7668	2.9888	0.6852
O	1.8948	3.3257	-0.1305
C	-0.4129	1.72	1.4915
O	-1.2683	0.8687	1.7671
N	0.8945	1.601	1.8218
C	2.4738	-1.8113	1.1551
C	1.4582	0.2952	2.1249

C	3.1232	-1.0227	3.4876
C	2.5889	0.3799	3.1575
C	3.5764	-1.7705	2.2246
C	1.9898	-0.3881	0.8315
N	1.117	-0.3129	-0.3455
C	0.0102	-1.0195	-0.6643
S	-0.4971	-1.1741	-2.2771
N	-0.6816	-1.5431	0.4141
C	-1.8768	-2.2866	0.2908
C	-4.2615	-3.7464	0.1103
C	-3.0244	-1.8351	0.9468
C	-1.9142	-3.478	-0.4405
C	-3.1054	-4.1908	-0.5336
C	-4.207	-2.5709	0.8532
C	-3.133	-5.4935	-1.2875
C	-5.4242	-2.0996	1.6006
F	-5.4216	-2.5462	2.8789
F	-5.4871	-0.7498	1.6575
F	-6.5704	-2.536	1.0325
F	-2.8578	-6.5418	-0.4733
F	-4.347	-5.7316	-1.834
F	-2.2227	-5.5189	-2.2836
H	4.8222	2.8071	-3.1125
H	2.7516	3.9225	-3.828
H	3.7187	0.3646	-2.7344
H	3.2637	1.2592	-4.2001
H	1.1914	0.833	-3.1056
H	0.686	3.0751	-3.146
H	4.1205	2.4661	-1.5121
H	2.8984	4.4794	-2.1472
H	-3.4855	2.5111	-1.2622
H	-2.5965	1.2041	-0.4588
H	-2.833	2.7988	1.3607
H	-1.071	1.5958	-2.2238
H	-1.4953	3.3282	-2.3431
H	-0.296	3.8626	1.1462
H	-2.5235	4.1792	0.2816
H	1.5144	2.2842	1.3789
H	0.6554	-0.3062	2.5581
H	2.8602	0.2066	0.5235
H	-0.7211	-0.8852	1.1942
H	-3.0021	-0.8996	1.4956
H	-5.1885	-4.2997	0.0195
H	-1.0251	-3.8282	-0.9484
H	1.488	0.2602	-1.1209
H	3.8851	-2.7913	2.4792
H	4.4624	-1.2707	1.8067
H	2.3261	-1.5964	3.982
H	3.9503	-0.9505	4.2038
H	3.3991	1.0079	2.7582
H	2.2123	0.8779	4.0576
H	1.6241	-2.4101	1.5054

H 2.8407 -2.2824 0.2362

Conformer8 (C1-conf10)



Imaginary Freq	0	
Temperature	298.15	Kelvin
Pressure	1	atm
Frequencies scaled by	1	
Electronic Energy (EE)	-2392.9275	Hartree
Zero-point Energy Correction	0.563651	Hartree
Thermal Correction to Energy	0.597625	Hartree
Thermal Correction to Enthalpy	0.598569	Hartree
Thermal Correction to Free Energy	0.499876	Hartree
EE + Zero-point Energy	-2392.3639	Hartree
EE + Thermal Energy Correction	-2392.3299	Hartree
EE + Thermal Enthalpy Correction	-2392.329	Hartree
EE + Thermal Free Energy Correction	-2392.4277	Hartree
E (Thermal)	375.015	kcal/mol
Heat Capacity (Cv)	135.296	cal/mol-kelvin
Entropy (S)	207.717	cal/mol-kelvin

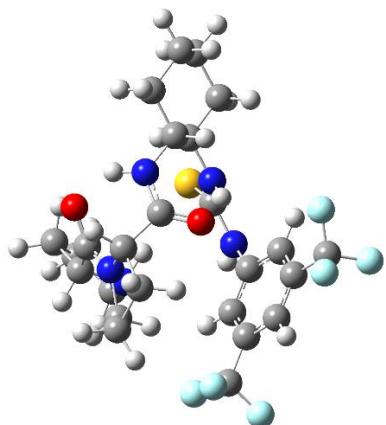
Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

N	1.8869	1.373	-2.5644
C	3.2671	1.2813	-3.0767
C	3.9115	2.5675	-2.5567
C	2.7924	3.598	-2.7753
C	1.5023	2.8086	-2.4586
C	1.0428	3.0385	-1.0103
N	-0.264	2.8332	-0.726
C	-1.3255	2.4661	-1.6925
C	-2.5557	2.2213	-0.8064
C	-2.3087	3.1094	0.4242
C	-0.7987	2.9863	0.6493
O	1.8713	3.3396	-0.1348
C	-0.4432	1.7284	1.4724
O	-1.2954	0.874	1.7485
N	0.8616	1.6211	1.8168
C	2.474	-1.7842	1.1947
C	1.4308	0.3216	2.1374
C	3.0863	-0.9763	3.53

C	2.547	0.4209	3.1846
C	3.5622	-1.7284	2.2782
C	1.984	-0.3666	0.8559
N	1.1249	-0.3059	-0.332
C	0.0263	-1.0222	-0.6576
S	-0.4619	-1.1934	-2.2747
N	-0.674	-1.5416	0.4172
C	-1.8629	-2.2942	0.2881
C	-4.236	-3.7719	0.0987
C	-3.0189	-1.8464	0.9319
C	-1.8862	-3.4906	-0.4355
C	-3.0717	-4.2122	-0.5331
C	-4.1955	-2.5911	0.8341
C	-3.0841	-5.5203	-1.2781
C	-5.4213	-2.1242	1.5702
F	-5.4237	-2.5629	2.8512
F	-5.4949	-0.7746	1.6183
F	-6.5603	-2.573	0.9973
F	-4.2929	-5.772	-1.8299
F	-2.1678	-5.5449	-2.2686
F	-2.8051	-6.5606	-0.4548
H	4.8394	2.8157	-3.0798
H	2.7714	3.9178	-3.8236
H	3.7449	0.3691	-2.7039
H	3.2996	1.2554	-4.1776
H	1.2194	0.8204	-3.0996
H	0.703	3.06	-3.1634
H	4.1212	2.4785	-1.4858
H	2.8952	4.4818	-2.1434
H	-3.4867	2.4581	-1.3288
H	-2.5888	1.1713	-0.5032
H	-2.8721	2.7794	1.2985
H	-1.0506	1.5709	-2.2555
H	-1.4928	3.2981	-2.3884
H	-0.3435	3.869	1.109
H	-2.563	4.1538	0.2114
H	1.4817	2.3046	1.3746
H	0.6265	-0.2824	2.564
H	2.8538	0.2323	0.5544
H	-0.726	-0.8782	1.1919
H	-3.0074	-0.9071	1.4744
H	-5.1581	-4.3326	0.0047
H	-0.9907	-3.8385	-0.9335
H	1.501	0.2643	-1.1071
H	3.8752	-2.7451	2.5434
H	4.4499	-1.2244	1.8688
H	2.2862	-1.5525	4.0166
H	3.9028	-0.8946	4.2573
H	3.3581	1.052	2.7924
H	2.155	0.9217	4.0767
H	1.6241	-2.3865	1.5385
H	2.8555	-2.2586	0.2835

Conformer9 (C1-conf9)



Imaginary Freq	0	
Temperature	298.15	Kelvin
Pressure	1	atm
Frequencies scaled by	1	
Electronic Energy (EE)	-2392.927	Hartree
Zero-point Energy Correction	0.563383	Hartree
Thermal Correction to Energy	0.597868	Hartree
Thermal Correction to Enthalpy	0.598812	Hartree
Thermal Correction to Free Energy	0.498693	Hartree
EE + Zero-point Energy	-2392.3636	Hartree
EE + Thermal Energy Correction	-2392.3291	Hartree
EE + Thermal Enthalpy Correction	-2392.3282	Hartree
EE + Thermal Free Energy Correction	-2392.4283	Hartree
E (Thermal)	375.168	kcal/mol
Heat Capacity (Cv)	136.247	cal/mol-kelvin
Entropy (S)	210.719	cal/mol-kelvin

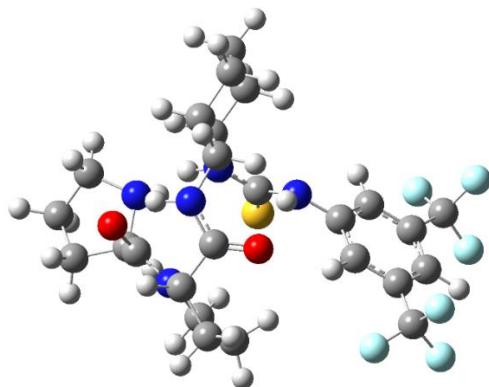
Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

N	-0.3424	-0.4195	-2.9923
C	-0.807	-1.2047	-4.1525
C	0.2894	-2.2609	-4.4488
C	1.5756	-1.6768	-3.8018
C	1.1206	-0.3188	-3.2204
C	1.8285	0.0862	-1.9252
N	1.4427	1.2625	-1.3647
C	0.7186	2.3551	-2.0372
C	1.3053	3.6096	-1.3851
C	1.524	3.163	0.0671
C	1.964	1.6935	-0.0455
O	2.6626	-0.6553	-1.3872
C	1.3629	0.8144	1.0781
O	0.3692	1.1624	1.7266
N	2.0047	-0.3598	1.2676
C	0.0544	-3.413	2.542
C	1.5404	-1.3796	2.2015
C	2.3071	-3.2973	3.682

C	2.7399	-2.1909	2.7127
C	1.261	-4.2188	3.0395
C	0.4927	-2.3171	1.5608
N	-0.6454	-1.5116	1.1093
C	-1.446	-1.8362	0.0806
S	-1.3236	-3.2587	-0.8308
N	-2.4209	-0.9153	-0.2614
C	-2.5605	0.403	0.2306
C	-2.742	3.034	1.1772
C	-2.7134	0.6496	1.5965
C	-2.5422	1.4737	-0.6708
C	-2.642	2.7763	-0.1922
C	-2.7739	1.9615	2.0614
C	-2.6152	3.9449	-1.1393
C	-2.9164	2.1988	3.5406
F	-4.2078	2.0906	3.9324
F	-2.2099	1.2965	4.2544
F	-2.494	3.4299	3.8949
F	-1.7118	4.8752	-0.7367
F	-2.2826	3.5831	-2.3984
F	-3.8122	4.5644	-1.201
H	0.4016	-2.4405	-5.5234
H	2.397	-1.5549	-4.5147
H	-1.7831	-1.6473	-3.9315
H	-0.9286	-0.5186	-5.0009
H	-0.4622	-1.0277	-2.1785
H	1.2731	0.465	-3.9759
H	0.0278	-3.214	-3.9794
H	1.9394	-2.3108	-2.9902
H	2.2572	3.8701	-1.8627
H	0.6295	4.4638	-1.466
H	0.5819	3.2016	0.6224
H	-0.3503	2.2689	-1.8546
H	0.8743	2.3177	-3.1163
H	3.0542	1.5807	-0.0468
H	2.2605	3.765	0.6061
H	2.6106	-0.6545	0.5004
H	1.0737	-0.8508	3.0417
H	0.9397	-2.7852	0.6745
H	-2.8451	-1.1213	-1.1568
H	-2.7547	-0.1779	2.2953
H	-2.7746	4.0524	1.5457
H	-2.3956	1.2755	-1.7276
H	-0.6675	-0.5588	1.4711
H	0.9321	-4.984	3.7528
H	1.7147	-4.7523	2.192
H	1.8801	-2.8389	4.5858
H	3.1831	-3.8728	4.0032
H	3.2561	-2.639	1.8504
H	3.4516	-1.5068	3.1885
H	-0.4581	-2.9408	3.3929
H	-0.6721	-4.0578	2.0379

Conformer10 (C1-conf12)



Imaginary Freq	0	
Temperature	298.15	Kelvin
Pressure	1	atm
Frequencies scaled by	1	
Electronic Energy (EE)	-2392.9271	Hartree
Zero-point Energy Correction	0.563839	Hartree
Thermal Correction to Energy	0.597883	Hartree
Thermal Correction to Enthalpy	0.598827	Hartree
Thermal Correction to Free Energy	0.500194	Hartree
EE + Zero-point Energy	-2392.3632	Hartree
EE + Thermal Energy Correction	-2392.3292	Hartree
EE + Thermal Enthalpy Correction	-2392.3282	Hartree
EE + Thermal Free Energy Correction	-2392.4269	Hartree
E (Thermal)	375.177	kcal/mol
Heat Capacity (Cv)	135.446	cal/mol-kelvin
Entropy (S)	207.591	cal/mol-kelvin

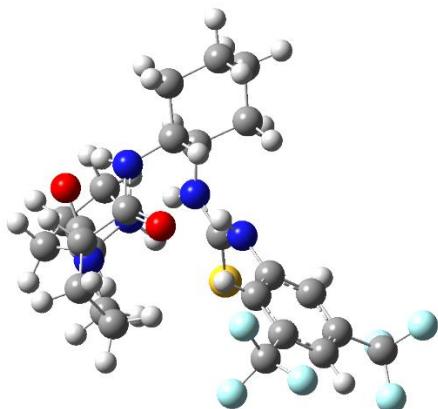
Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

N	-0.4064	0.2868	-3.5183
C	0.0415	0.1376	-4.9165
C	-0.3174	1.4678	-5.5929
C	0.0346	2.4873	-4.4944
C	-0.263	1.7299	-3.165
C	0.9092	1.854	-2.1904
N	0.6925	2.3873	-0.9659
C	-0.5695	2.9713	-0.4536
C	-0.2499	3.3153	1.0092
C	1.2765	3.5112	1.0301
C	1.7892	2.4739	0.0269
O	2.0253	1.4321	-2.5382
C	1.9605	1.0773	0.6595
O	1.4736	0.8021	1.7634
N	2.6124	0.1763	-0.1151
C	1.1454	-3.3329	-0.4914
C	2.4537	-1.252	0.1142
C	3.5625	-3.5105	0.29
C	3.7718	-2.0235	-0.0368

C	2.4552	-4.1326	-0.5754
C	1.3923	-1.8574	-0.8485
N	0.157	-1.0862	-1.0284
C	-0.8934	-0.8818	-0.2054
S	-2.3926	-0.3729	-0.8235
N	-0.6474	-1.0738	1.1432
C	-1.6058	-0.8425	2.159
C	-3.4663	-0.3507	4.1983
C	-2.8198	-1.5348	2.1793
C	-1.3107	0.0739	3.171
C	-2.2447	0.3159	4.1791
C	-3.7396	-1.279	3.1917
C	-1.9003	1.298	5.2635
C	-5.0192	-2.0705	3.2375
F	-5.4285	-2.4423	2.0063
F	-4.8658	-3.2055	3.9619
F	-6.024	-1.3717	3.8121
F	-3.0019	1.867	5.8004
F	-1.2268	0.7067	6.2778
F	-1.111	2.295	4.7974
H	-1.3918	1.4951	-5.8156
H	-0.5349	3.4185	-4.5686
H	1.1272	-0.0105	-4.9191
H	-0.4288	-0.7411	-5.369
H	-1.3918	0.0426	-3.426
H	-1.1955	2.0672	-2.713
H	0.226	1.6465	-6.5269
H	1.0999	2.7319	-4.5438
H	-0.7981	4.1989	1.3467
H	-0.5236	2.4793	1.657
H	1.7033	3.3563	2.0229
H	-1.3905	2.2547	-0.5354
H	-0.8167	3.8678	-1.0352
H	2.7105	2.7676	-0.4852
H	1.5451	4.5141	0.6796
H	2.7722	0.4783	-1.0791
H	2.1258	-1.3679	1.1505
H	1.8437	-1.8194	-1.8489
H	0.2831	-0.7721	1.4277
H	-3.0485	-2.2473	1.3975
H	-4.1986	-0.1453	4.9692
H	-0.3732	0.6175	3.1486
H	0.0018	-0.7479	-1.9921
H	2.2782	-5.1721	-0.2752
H	2.7903	-4.161	-1.6225
H	3.2906	-3.6061	1.3512
H	4.5026	-4.0595	0.1582
H	4.1437	-1.9124	-1.0658
H	4.5233	-1.5785	0.6246
H	0.7256	-3.3918	0.5207
H	0.3938	-3.7446	-1.174

Conformer11 (C1-conf13)



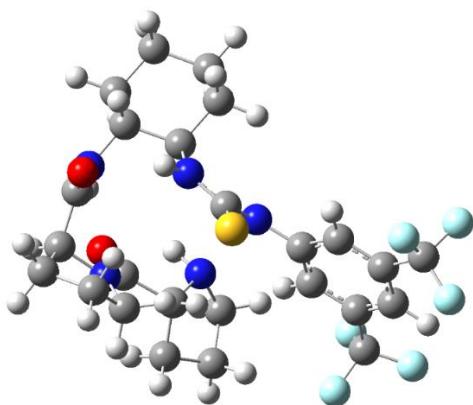
Imaginary Freq	0	
Temperature	298.15	Kelvin
Pressure	1	atm
Frequencies scaled by	1	
Electronic Energy (EE)	-2392.9267	Hartree
Zero-point Energy Correction	0.563956	Hartree
Thermal Correction to Energy	0.597962	Hartree
Thermal Correction to Enthalpy	0.598907	Hartree
Thermal Correction to Free Energy	0.500273	Hartree
EE + Zero-point Energy	-2392.3628	Hartree
EE + Thermal Energy Correction	-2392.3288	Hartree
EE + Thermal Enthalpy Correction	-2392.3278	Hartree
EE + Thermal Free Energy Correction	-2392.4265	Hartree
E (Thermal)	375.227	kcal/mol
Heat Capacity (Cv)	135.329	cal/mol-kelvin
Entropy (S)	207.593	cal/mol-kelvin

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

N	2.0952	2.1755	-1.8515
C	3.3331	2.9612	-2.0135
C	2.8813	4.2947	-2.6214
C	1.5717	4.5674	-1.8578
C	0.9977	3.1465	-1.5678
C	0.6252	2.9908	-0.0921
N	-0.6333	2.6113	0.2311
C	-1.7719	2.4026	-0.6949
C	-2.8845	1.8515	0.2094
C	-2.5454	2.4022	1.6056
C	-1.0139	2.3655	1.6415
O	1.5003	3.1763	0.7701
C	-0.476	0.9765	2.0455
O	-1.2145	-0.0162	2.0809
N	0.8541	0.9217	2.2969
C	2.8149	-1.9865	0.7795
C	1.5515	-0.3545	2.2402
C	3.2236	-1.9164	3.2924
C	2.6009	-0.5126	3.3479

C	3.8297	-2.2127	1.9121
C	2.2314	-0.5647	0.8576
N	1.4433	-0.1871	-0.3198
C	0.3915	-0.7866	-0.9182
S	-0.0093	-0.4263	-2.5309
N	-0.3342	-1.6542	-0.1217
C	-1.4937	-2.3446	-0.5424
C	-3.8187	-3.7229	-1.2895
C	-1.4825	-3.1784	-1.6655
C	-2.6599	-2.2187	0.2184
C	-3.8119	-2.9076	-0.1618
C	-2.6445	-3.851	-2.0327
C	-5.0894	-2.6777	0.5978
C	-2.6126	-4.7847	-3.2133
F	-1.7291	-4.3807	-4.1502
F	-2.2517	-6.0375	-2.8434
F	-3.824	-4.8844	-3.8061
F	-4.8641	-2.4525	1.911
F	-5.7535	-1.5958	0.1232
F	-5.9326	-3.7301	0.5009
H	2.6854	4.1665	-3.6935
H	0.8651	5.1846	-2.4199
H	3.7716	3.1241	-1.0229
H	4.0523	2.4075	-2.625
H	1.8605	1.6828	-2.7124
H	0.1556	2.9112	-2.2184
H	3.6146	5.0993	-2.5048
H	1.7913	5.0707	-0.9116
H	-3.8773	2.1478	-0.1406
H	-2.8408	0.7597	0.2246
H	-2.981	1.8045	2.4084
H	-1.5022	1.6986	-1.4859
H	-2.0555	3.3618	-1.1457
H	-0.5638	3.139	2.2704
H	-2.8846	3.4388	1.7107
H	1.376	1.7614	2.0359
H	0.7942	-1.1258	2.4
H	3.066	0.1478	0.8239
H	-0.4107	-1.34	0.8452
H	-0.5809	-3.2839	-2.2541
H	-4.7189	-4.2468	-1.5877
H	-2.6706	-1.5737	1.0902
H	1.8367	0.6022	-0.8591
H	4.207	-3.2413	1.8749
H	4.696	-1.5542	1.7506
H	2.4431	-2.6586	3.5135
H	3.9858	-2.0202	4.0733
H	3.3832	0.2511	3.2264
H	2.126	-0.3321	4.3183
H	1.9963	-2.7148	0.8482
H	3.2857	-2.1269	-0.2002

Conformer12 (C1-conf6)

Imaginary Freq	0	
Temperature	298.15	Kelvin
Pressure	1	atm
Frequencies scaled by	1	
Electronic Energy (EE)	-2392.9289	Hartree
Zero-point Energy Correction	0.563766	Hartree
Thermal Correction to Energy	0.597978	Hartree
Thermal Correction to Enthalpy	0.598922	Hartree
Thermal Correction to Free Energy	0.499677	Hartree
EE + Zero-point Energy	-2392.3652	Hartree
EE + Thermal Energy Correction	-2392.331	Hartree
EE + Thermal Enthalpy Correction	-2392.33	Hartree
EE + Thermal Free Energy Correction	-2392.4293	Hartree
E (Thermal)	375.237	kcal/mol
Heat Capacity (Cv)	135.945	cal/mol-kelvin
Entropy (S)	208.879	cal/mol-kelvin

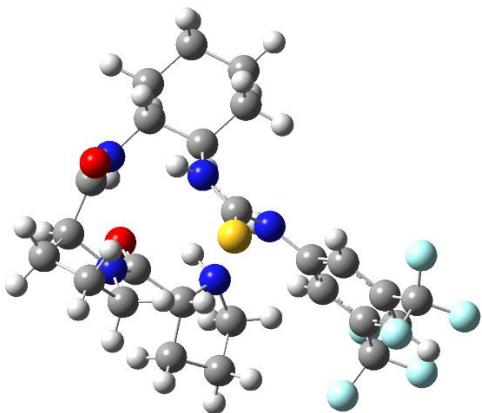
Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

N	1.9399	0.1789	-1.1488
C	2.7115	0.0387	-2.4218
C	2.1291	1.0933	-3.3796
C	1.7002	2.2197	-2.4294
C	1.1374	1.4234	-1.2321
C	1.2605	2.1669	0.0962
N	0.208	2.876	0.5443
C	-1.0336	3.1792	-0.2052
C	-1.9237	3.8668	0.8369
C	-0.9252	4.5323	1.7991
C	0.2164	3.5171	1.8866
O	2.3203	2.0626	0.7445
C	-0.0673	2.4064	2.9325
O	-1.1596	2.2915	3.4851
N	0.9643	1.534	3.1008
C	0.1356	-2.2026	2.8299
C	0.7542	0.1634	3.5587
C	1.9051	-1.8542	4.5997
C	2.0508	-0.3901	4.1645
C	1.4425	-2.7349	3.4308

C	0.2782	-0.7358	2.3889
N	-0.9813	-0.2016	1.8639
C	-1.5925	-0.4723	0.6881
S	-3.155	0.0974	0.3955
N	-0.8275	-1.1902	-0.2153
C	-1.2773	-1.7505	-1.4262
C	-2.0307	-2.9192	-3.8722
C	-2.508	-2.4133	-1.5405
C	-0.4221	-1.7056	-2.5285
C	-0.8021	-2.2836	-3.7395
C	-2.8712	-2.9799	-2.7579
C	0.1126	-2.1307	-4.9209
C	-4.1694	-3.7366	-2.8656
F	-3.9844	-5.0617	-2.652
F	-5.0809	-3.3125	-1.9678
F	-4.7158	-3.6135	-4.0968
F	-0.2129	-2.9526	-5.9371
F	0.0814	-0.8617	-5.4081
F	1.4052	-2.3785	-4.5919
H	1.2611	0.6876	-3.9106
H	0.9691	2.9091	-2.8627
H	3.7776	0.2263	-2.2413
H	2.6182	-0.9741	-2.8272
H	2.5968	0.3238	-0.3838
H	0.0922	1.1599	-1.4265
H	2.8545	1.4173	-4.1326
H	2.5732	2.7977	-2.1029
H	-2.6134	4.5769	0.3737
H	-2.508	3.1119	1.37
H	-1.3578	4.7268	2.782
H	-1.4943	2.2689	-0.5965
H	-0.7931	3.8457	-1.0433
H	1.1996	3.9623	2.0633
H	-0.546	5.4726	1.3825
H	1.7594	1.6748	2.4769
H	-0.0302	0.1886	4.3241
H	1.0475	-0.6658	1.6056
H	0.1797	-1.0135	-0.2084
H	-3.1761	-2.4739	-0.693
H	-2.3319	-3.3548	-4.817
H	0.5365	-1.2174	-2.4293
H	-1.5298	0.3786	2.4909
H	1.3059	-3.7715	3.7605
H	2.2229	-2.7536	2.6553
H	1.1709	-1.9189	5.4156
H	2.8572	-2.2183	5.0036
H	2.8509	-0.3102	3.4128
H	2.3449	0.2463	5.0065
H	-0.6716	-2.2638	3.5728
H	-0.1785	-2.8052	1.9707

Conformer13 (C1-conf5)



Imaginary Freq	0	
Temperature	298.15	Kelvin
Pressure	1	atm
Frequencies scaled by	1	
Electronic Energy (EE)	-2392.9285	Hartree
Zero-point Energy Correction	0.563455	Hartree
Thermal Correction to Energy	0.597749	Hartree
Thermal Correction to Enthalpy	0.598693	Hartree
Thermal Correction to Free Energy	0.49917	Hartree
EE + Zero-point Energy	-2392.365	Hartree
EE + Thermal Energy Correction	-2392.3308	Hartree
EE + Thermal Enthalpy Correction	-2392.3298	Hartree
EE + Thermal Free Energy Correction	-2392.4293	Hartree
E (Thermal)	375.093	kcal/mol
Heat Capacity (Cv)	136.13	cal/mol-kelvin
Entropy (S)	209.465	cal/mol-kelvin

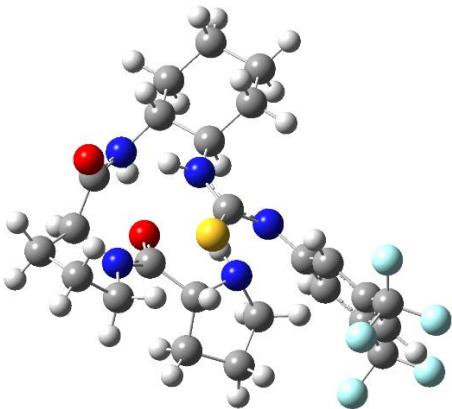
Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

N	2.2081	0.6973	-0.1582
C	3.3725	1.178	-0.9566
C	2.8608	2.4172	-1.7041
C	1.8812	3.038	-0.6996
C	1.1992	1.7809	-0.1105
C	0.7269	1.9529	1.3317
N	-0.5076	2.445	1.5508
C	-1.4309	3.0036	0.5365
C	-2.7311	3.2323	1.3197
C	-2.2592	3.4732	2.7647
C	-1.0837	2.5052	2.9202
O	1.4746	1.5958	2.2631
C	-1.5568	1.0742	3.2883
O	-2.7441	0.7532	3.2571
N	-0.5448	0.2018	3.5533
C	-0.634	-3.138	1.659
C	-0.7084	-1.2389	3.3678
C	0.2142	-3.5212	4.0051
C	0.3086	-2.0046	4.2243
C	0.3907	-3.8806	2.5244

C	-0.552	-1.6162	1.8732
N	-1.5747	-0.9085	1.0959
C	-1.6431	-0.7264	-0.244
S	-3.0341	-0.0697	-0.9388
N	-0.4957	-1.0782	-0.9305
C	-0.2908	-1.1188	-2.3232
C	0.2995	-1.2552	-5.0703
C	-1.2776	-1.517	-3.2347
C	0.9946	-0.8232	-2.7898
C	1.2798	-0.8915	-4.1517
C	-0.9728	-1.5705	-4.5929
C	2.6492	-0.4887	-4.6198
C	-2.0658	-1.9225	-5.5683
F	-2.9225	-2.8334	-5.0581
F	-2.7959	-0.8339	-5.8989
F	-1.5677	-2.431	-6.7185
F	2.9348	-0.9606	-5.8495
F	2.775	0.8638	-4.6765
F	3.6155	-0.9279	-3.7763
H	2.3335	2.1146	-2.615
H	1.1676	3.73	-1.157
H	4.21	1.4451	-0.2969
H	3.7247	0.4018	-1.6439
H	2.5039	0.5353	0.803
H	0.3488	1.5038	-0.7444
H	3.6714	3.0922	-1.9949
H	2.4268	3.5735	0.0875
H	-3.3081	4.0658	0.9102
H	-3.3447	2.3284	1.2777
H	-3.0408	3.2664	3.4983
H	-1.5761	2.3105	-0.2957
H	-1.017	3.9432	0.1496
H	-0.3125	2.8429	3.6185
H	-1.9052	4.502	2.8984
H	0.394	0.5677	3.3922
H	-1.7241	-1.4942	3.6894
H	0.4455	-1.2618	1.5669
H	0.3748	-0.9954	-0.4096
H	-2.2676	-1.7804	-2.8912
H	0.522	-1.3091	-6.1285
H	1.7567	-0.5391	-2.0748
H	-2.3945	-0.5877	1.603
H	0.2862	-4.9616	2.3771
H	1.4082	-3.616	2.1994
H	-0.769	-3.8747	4.348
H	0.9651	-4.0321	4.6186
H	1.321	-1.6587	3.9656
H	0.1464	-1.746	5.2764
H	-1.6514	-3.4658	1.9127
H	-0.4873	-3.3563	0.5952

Conformer14 (C1-conf7)



Imaginary Freq	0	
Temperature	298.15	Kelvin
Pressure	1	atm
Frequencies scaled by	1	
Electronic Energy (EE)	-2392.9286	Hartree
Zero-point Energy Correction	0.563557	Hartree
Thermal Correction to Energy	0.597831	Hartree
Thermal Correction to Enthalpy	0.598776	Hartree
Thermal Correction to Free Energy	0.499421	Hartree
EE + Zero-point Energy	-2392.3651	Hartree
EE + Thermal Energy Correction	-2392.3308	Hartree
EE + Thermal Enthalpy Correction	-2392.3299	Hartree
EE + Thermal Free Energy Correction	-2392.4292	Hartree
E (Thermal)	375.145	kcal/mol
Heat Capacity (Cv)	136.113	cal/mol-kelvin
Entropy (S)	209.109	cal/mol-kelvin

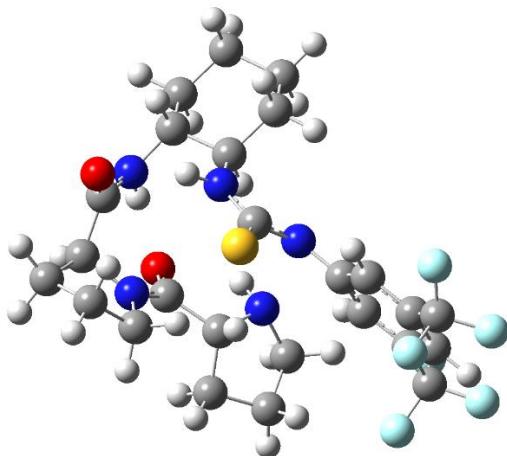
Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

N	0.649	1.6292	-1.5638
C	0.3363	2.5767	-2.6734
C	-0.8178	3.4453	-2.1512
C	-0.5127	3.5484	-0.6519
C	-0.0113	2.121	-0.3335
C	0.9885	2.0726	0.8222
N	0.5169	1.9649	2.0789
C	-0.9032	2.0405	2.4956
C	-0.8603	1.6762	3.9842
C	0.5353	2.1346	4.4404
C	1.4289	1.8019	3.2425
O	2.209	2.1061	0.5697
C	1.8992	0.3234	3.2607
O	1.4374	-0.4986	4.0506
N	2.7849	0.0112	2.2747
C	1.9654	-3.0666	0.1296
C	2.9212	-1.3504	1.7654
C	4.4598	-2.9286	0.4938
C	4.2965	-1.5323	1.1089
C	3.3462	-3.2212	-0.5203

C	1.7921	-1.6694	0.7517
N	0.4975	-1.5317	1.4275
C	-0.7379	-1.4324	0.8837
S	-2.1045	-1.4907	1.8744
N	-0.7542	-1.2445	-0.485
C	-1.871	-1.1979	-1.3431
C	-3.9738	-1.0768	-3.2029
C	-1.792	-0.3429	-2.4473
C	-2.9941	-2.0206	-1.186
C	-4.0335	-1.9409	-2.1097
C	-2.838	-0.2886	-3.3667
C	-5.2686	-2.7755	-1.8921
C	-2.7467	0.6742	-4.5171
F	-1.4902	0.7361	-5.0227
F	-3.5747	0.342	-5.5276
F	-3.0714	1.9382	-4.1395
F	-5.9094	-3.0351	-3.0546
F	-4.9789	-3.9601	-1.3124
F	-6.1527	-2.1447	-1.0868
H	-1.7744	2.9383	-2.316
H	-1.3764	3.8391	-0.0467
H	1.2114	3.1983	-2.9073
H	0.0597	2.0352	-3.5836
H	1.6505	1.6473	-1.3786
H	-0.8699	1.4781	-0.1052
H	-0.8692	4.418	-2.6503
H	0.2937	4.2711	-0.4745
H	-1.6727	2.1508	4.5414
H	-0.9489	0.5921	4.0945
H	0.8696	1.6149	5.3401
H	-1.5216	1.3436	1.9248
H	-1.2712	3.0611	2.3331
H	2.2845	2.473	3.123
H	0.5547	3.2153	4.6224
H	2.9574	0.7581	1.6007
H	2.8285	-2.0312	2.6189
H	1.865	-0.9073	-0.0409
H	0.0661	-0.7948	-0.8845
H	-0.9051	0.2694	-2.567
H	-4.7849	-1.0388	-3.9195
H	-3.0546	-2.7123	-0.3584
H	0.4955	-1.6052	2.4404
H	3.4539	-4.2317	-0.9313
H	3.431	-2.5243	-1.3671
H	4.4285	-3.6816	1.2944
H	5.4446	-3.0131	0.0199
H	4.4178	-0.7688	0.326
H	5.0707	-1.339	1.8593
H	1.8348	-3.8136	0.924
H	1.1639	-3.2352	-0.5988

Conformer15 (C1-conf8)



Imaginary Freq	0	
Temperature	298.15	Kelvin
Pressure	1	atm
Frequencies scaled by	1	
Electronic Energy (EE)	-2392.9286	Hartree
Zero-point Energy Correction	0.563662	Hartree
Thermal Correction to Energy	0.597922	Hartree
Thermal Correction to Enthalpy	0.598867	Hartree
Thermal Correction to Free Energy	0.499552	Hartree
EE + Zero-point Energy	-2392.3649	Hartree
EE + Thermal Energy Correction	-2392.3307	Hartree
EE + Thermal Enthalpy Correction	-2392.3297	Hartree
EE + Thermal Free Energy Correction	-2392.429	Hartree
E (Thermal)	375.202	kcal/mol
Heat Capacity (Cv)	136.081	cal/mol-kelvin
Entropy (S)	209.025	cal/mol-kelvin

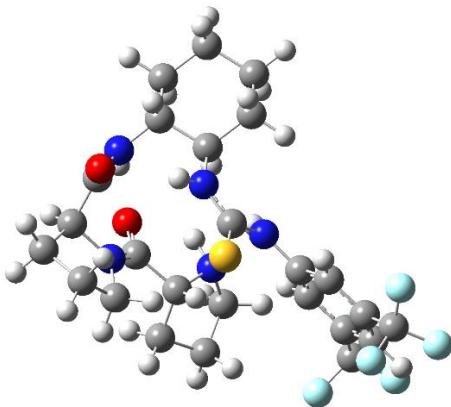
Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

N	0.6216	1.585	-1.6122
C	0.2782	2.5058	-2.7351
C	-0.8493	3.4003	-2.1973
C	-0.4988	3.5339	-0.7103
C	0.0002	2.1095	-0.3752
C	1.0325	2.0765	0.7517
N	0.5972	1.9936	2.0232
C	-0.8092	2.0857	2.4812
C	-0.7219	1.7537	3.9756
C	0.6893	2.2146	4.3782
C	1.5433	1.8494	3.1614
O	2.2454	2.0983	0.4638
C	2.0035	0.3679	3.1969
O	1.5605	-0.4335	4.0179
N	2.8567	0.0284	2.1911
C	1.9377	-3.0719	0.1182
C	2.9621	-1.3438	1.702
C	4.4424	-2.9568	0.4049
C	4.3142	-1.5507	1.0055
C	3.296	-3.2474	-0.5723

C	1.7967	-1.6669	0.7311
N	0.527	-1.513	1.4501
C	-0.7253	-1.4116	0.9464
S	-2.0588	-1.4408	1.9823
N	-0.7847	-1.2469	-0.424
C	-1.9253	-1.2046	-1.2502
C	-4.0754	-1.0975	-3.0575
C	-3.0608	-1.9973	-1.0372
C	-1.8603	-0.3858	-2.3826
C	-2.9293	-0.3381	-3.2754
C	-4.1228	-1.9244	-1.9353
C	-2.8502	0.5872	-4.4574
C	-5.3719	-2.7194	-1.6576
F	-5.1006	-3.8797	-1.0235
F	-6.2282	-2.0274	-0.8728
F	-6.0372	-3.021	-2.7962
F	-3.145	1.8677	-4.112
F	-1.6053	0.6128	-4.9938
F	-3.7073	0.2375	-5.4372
H	-1.816	2.9012	-2.3218
H	-1.3422	3.8445	-0.0867
H	1.1503	3.1108	-3.0178
H	-0.0357	1.9429	-3.6198
H	1.6283	1.6047	-1.4574
H	-0.857	1.4799	-0.1093
H	-0.9048	4.362	-2.7168
H	0.3171	4.2544	-0.5714
H	-1.5145	2.2443	4.5473
H	-0.811	0.6726	4.1119
H	1.0493	1.7144	5.2791
H	-1.4475	1.3797	1.945
H	-1.1779	3.1042	2.3077
H	2.3997	2.5109	3.
H	0.7199	3.2992	4.5341
H	3.0138	0.7604	1.497
H	2.8905	-2.0093	2.5694
H	1.8471	-0.9131	-0.0714
H	0.0289	-0.8174	-0.8581
H	-3.1138	-2.6597	-0.1857
H	-4.9047	-1.0665	-3.7533
H	-0.9658	0.2048	-2.5457
H	0.5602	-1.5664	2.4637
H	3.3803	-4.263	-0.9761
H	3.3626	-2.5598	-1.4281
H	4.4242	-3.6995	1.2153
H	5.4118	-3.0603	-0.096
H	4.4199	-0.7993	0.2088
H	5.1131	-1.3564	1.7292
H	1.8247	-3.8097	0.9238
H	1.1125	-3.2402	-0.5832

Conformer16 (C1-conf4)



Imaginary Freq	0	
Temperature	298.15	Kelvin
Pressure	1	atm
Frequencies scaled by	1	
Electronic Energy (EE)	-2392.9288	Hartree
Zero-point Energy Correction	0.56334	Hartree
Thermal Correction to Energy	0.59771	Hartree
Thermal Correction to Enthalpy	0.598654	Hartree
Thermal Correction to Free Energy	0.498833	Hartree
EE + Zero-point Energy	-2392.3654	Hartree
EE + Thermal Energy Correction	-2392.3311	Hartree
EE + Thermal Enthalpy Correction	-2392.3301	Hartree
EE + Thermal Free Energy Correction	-2392.4299	Hartree
E (Thermal)	375.069	kcal/mol
Heat Capacity (Cv)	136.264	cal/mol-kelvin
Entropy (S)	210.092	cal/mol-kelvin

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

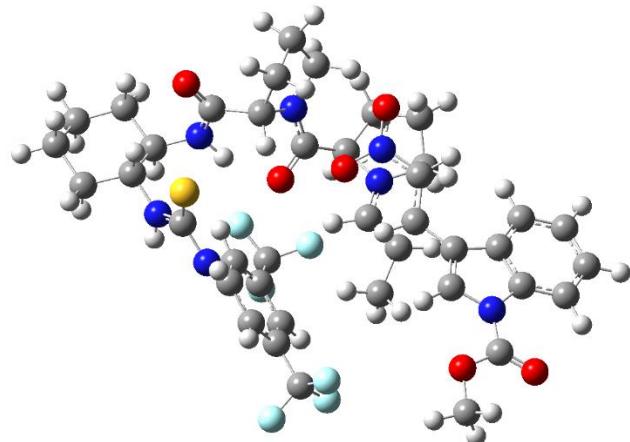
N	2.3343	0.4587	-0.1832
C	3.572	0.718	-0.9723
C	3.2119	1.8702	-1.9228
C	2.2318	2.7041	-1.0886
C	1.4161	1.6034	-0.3696
C	0.8816	2.0413	0.9934
N	-0.29	2.7039	1.0432
C	-1.0828	3.184	-0.1114
C	-2.3739	3.7077	0.5305
C	-1.94	4.1411	1.9421
C	-0.9137	3.0769	2.3396
O	1.5272	1.7543	2.0207
C	-1.5864	1.8049	2.9151
O	-2.8009	1.6219	2.8464
N	-0.7103	0.8875	3.4112
C	-1.1149	-2.7265	2.1818
C	-1.0503	-0.5308	3.4848
C	-0.4903	-2.7308	4.628
C	-0.2045	-1.2242	4.5611
C	-0.2608	-3.3966	3.2641

C	-0.8427	-1.2139	2.1078
N	-1.7033	-0.5584	1.1181
C	-1.6539	-0.6294	-0.2322
S	-2.9041	0.0282	-1.1588
N	-0.5158	-1.2266	-0.7436
C	-0.2526	-1.5335	-2.0943
C	0.41	-2.1921	-4.7458
C	1.0582	-1.3821	-2.5546
C	-1.2292	-2.0522	-2.9546
C	-0.8902	-2.3624	-4.269
C	1.3787	-1.7088	-3.8716
C	-1.9677	-2.8407	-5.2077
C	2.7786	-1.4599	-4.3555
F	2.978	-0.146	-4.6386
F	3.7014	-1.7935	-3.4198
F	3.0665	-2.1516	-5.4758
F	-1.4619	-3.6052	-6.2034
F	-2.9046	-3.5729	-4.5664
F	-2.6062	-1.8029	-5.7928
H	2.7155	1.4788	-2.8171
H	1.605	3.3739	-1.6846
H	4.3993	1.009	-0.3103
H	3.8831	-0.1785	-1.5177
H	2.5633	0.4339	0.8091
H	0.5819	1.2959	-1.0113
H	4.0912	2.4339	-2.249
H	2.7725	3.3061	-0.3476
H	-2.8174	4.5197	-0.0522
H	-3.0993	2.8936	0.6039
H	-2.7745	4.1698	2.645
H	-1.2805	2.3746	-0.8181
H	-0.5301	3.9804	-0.6246
H	-0.1345	3.4358	3.0182
H	-1.4575	5.1249	1.9212
H	0.2751	1.1008	3.2519
H	-2.1103	-0.5981	3.7532
H	0.21	-1.0441	1.8352
H	0.3301	-1.1335	-0.186
H	1.8114	-1.0037	-1.874
H	0.6597	-2.4458	-5.7685
H	-2.2393	-2.208	-2.6036
H	-2.5174	-0.0648	1.4713
H	-0.4934	-4.4669	3.3133
H	0.8025	-3.3184	2.9946
H	-1.5333	-2.8892	4.9375
H	0.1404	-3.1955	5.3948
H	0.8605	-1.0662	4.3334
H	-0.3975	-0.7413	5.5253
H	-2.181	-2.8694	2.403
H	-0.9315	-3.1725	1.1982

Transition states

Four transition states correspond to different arrangements of reactants, which would all lead to major enantiomer of the Michael adduct. Lowest energy transition state (TS-major_conf4) is discussed in the manuscript.

TS-major_conf1



Imaginary Freq	-482.78	cm ⁻¹
Temperature	298.15	Kelvin
Pressure	1	atm
Frequencies scaled by	1	
Electronic Energy (EE)	-3383.21	Hartree
Zero-point Energy Correction	0.836987	Hartree
Thermal Correction to Energy	0.889507	Hartree
Thermal Correction to Enthalpy	0.890451	Hartree
Thermal Correction to Free Energy	0.753758	Hartree
EE + Zero-point Energy	-3382.373	Hartree
EE + Thermal Energy Correction	-3382.3205	Hartree
EE + Thermal Enthalpy Correction	-3382.3196	Hartree
EE + Thermal Free Energy Correction	-3382.4562	Hartree
E (Thermal)	558.174	kcal/mol
Heat Capacity (Cv)	208.879	cal/mol-kelvin
Entropy (S)	287.695	cal/mol-kelvin

Symbolic Z-matrix:

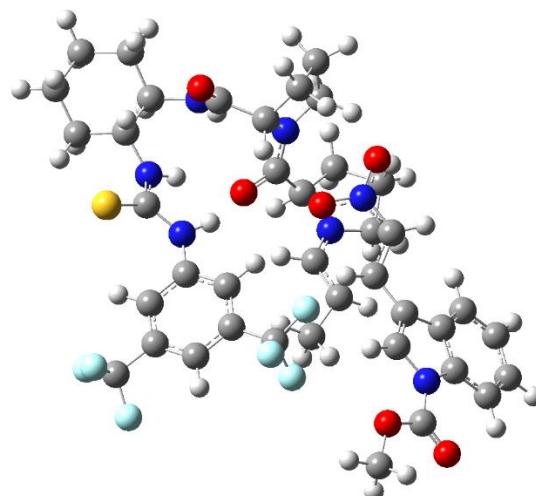
Charge = 0 Multiplicity = 1

N	-0.4873	-1.1798	2.1643
C	-1.0592	-1.3156	3.5122
C	0.1838	-1.3052	4.3973
C	1.1579	-2.1764	3.5883
C	0.8502	-1.86	2.1042
C	1.7932	-1.0794	1.1582
O	1.4956	-1.2193	-0.0476
C	-1.1166	-0.6787	1.1046
C	-2.3942	-0.0819	1.1038
C	-3.0639	0.0088	-0.2522
H	-0.0068	-1.7013	5.3985

H	0.5495	-0.2762	4.4798
H	2.2001	-2.0282	3.8616
H	-1.6046	-2.2703	3.5863
H	0.9322	-3.2351	3.7592
H	0.7075	-2.7959	1.5583
H	-0.5428	-0.7119	0.1878
H	-3.0559	-0.3708	1.918
H	-3.4475	-0.9637	-0.5851
H	-2.3617	0.3612	-1.0151
H	-3.9148	0.6954	-0.2309
H	-1.7509	-0.5025	3.7116
C	-4.3903	1.8185	3.1208
C	-5.7141	2.2228	2.8227
C	-3.5551	2.1978	1.9894
C	-4.3784	2.7973	1.0806
N	-5.6911	2.8361	1.5552
C	-6.8116	3.2312	0.8245
O	-6.4512	3.6311	-0.411
O	-7.9504	3.2047	1.2398
C	-7.5471	4.0251	-1.2577
C	-2.1543	1.8671	1.7126
C	-1.1864	1.948	2.7321
N	0.131	1.777	2.4109
O	0.4369	1.5645	1.1974
O	1.004	1.8225	3.328
H	-1.3953	2.0592	3.7844
H	-1.7994	2.1626	0.7277
H	-4.153	3.1864	0.1006
H	-7.0902	4.2935	-2.2103
H	-8.0758	4.879	-0.8262
H	-8.2473	3.1951	-1.3846
C	-4.1539	1.1173	4.3112
C	-6.7928	1.9621	3.6668
C	-6.5242	1.266	4.8432
C	-5.2223	0.8465	5.1614
H	-3.1532	0.7923	4.5719
H	-5.0473	0.3011	6.0845
H	-7.3421	1.0408	5.5218
H	-7.7928	2.277	3.4005
N	2.8329	-0.3168	1.5202
C	3.3873	-0.0738	2.8715
C	4.4114	1.0499	2.6529
C	3.8546	1.8075	1.4426
C	3.3465	0.6862	0.5421
C	4.4321	0.1435	-0.4205
O	5.4858	0.7439	-0.6084
H	5.3953	0.6323	2.4098
H	4.6026	2.4131	0.9299
H	4.5115	1.6735	3.5454
H	2.5895	0.2616	3.5326
H	3.8541	-0.9852	3.2579
H	2.5004	1.0049	-0.0719

H	2.9993	2.4173	1.7423
N	4.0741	-1.0017	-1.0728
H	3.1159	-1.2989	-0.9009
C	4.7184	-1.4728	-2.2952
C	5.2304	-0.9002	-4.7377
C	4.5295	-0.4504	-3.4478
N	3.1012	-0.246	-3.7026
H	5.1201	-0.1147	-5.4942
H	2.6203	-1.0129	-4.1577
H	4.9334	0.509	-3.1173
C	2.3935	0.8866	-3.4917
S	3.0309	2.3761	-3.0681
N	1.0175	0.777	-3.705
C	0.1364	-0.276	-3.4164
C	-1.7706	-2.257	-2.7677
C	-1.214	-0.1154	-3.7631
C	0.5183	-1.4447	-2.7387
C	-0.4287	-2.4081	-2.4193
C	-2.149	-1.0942	-3.4303
C	-3.5933	-0.8446	-3.7732
C	-0.038	-3.6085	-1.6001
F	-3.7858	-0.7717	-5.1089
F	-4.408	-1.8076	-3.2949
F	-4.0169	0.3357	-3.2555
F	1.2955	-3.7693	-1.505
F	-0.5515	-4.7464	-2.1231
F	-0.5302	-3.5199	-0.3346
H	-2.5021	-3.0124	-2.5099
H	1.5271	-1.5654	-2.386
H	-1.5397	0.7866	-4.2734
H	0.586	1.6925	-3.7393
C	6.7082	-1.2302	-4.4908
C	6.2013	-1.8261	-2.0911
H	4.1863	-2.3947	-2.5763
C	6.8534	-2.2964	-3.3966
H	6.2683	-2.5967	-1.3139
H	6.3823	-3.2317	-3.7365
H	7.912	-2.5237	-3.2226
H	7.1737	-1.5656	-5.4254
H	4.7246	-1.797	-5.1319
H	7.2353	-0.3177	-4.1803
H	6.7144	-0.9386	-1.7116

TS-major_conf2



Imaginary Freq	-487.35	cm ⁻¹
Temperature	298.15	Kelvin
Pressure	1	atm
Frequencies scaled by	1	
Electronic Energy (EE)	-3383.2154	Hartree
Zero-point Energy Correction	0.83717	Hartree
Thermal Correction to Energy	0.889672	Hartree
Thermal Correction to Enthalpy	0.890616	Hartree
Thermal Correction to Free Energy	0.754201	Hartree
EE + Zero-point Energy	-3382.3782	Hartree
EE + Thermal Energy Correction	-3382.3257	Hartree
EE + Thermal Enthalpy Correction	-3382.3247	Hartree
EE + Thermal Free Energy Correction	-3382.4612	Hartree
E (Thermal)	558.278	kcal/mol
Heat Capacity (Cv)	209.026	cal/mol-kelvin
Entropy (S)	287.11	cal/mol-kelvin

Symbolic Z-matrix:

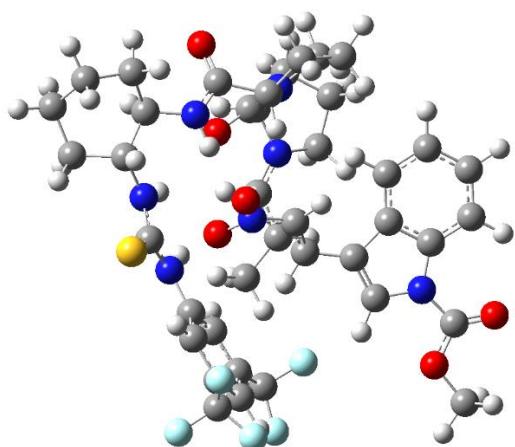
Charge = 0 Multiplicity = 1

N	-0.4847	-1.746	1.9959
C	-0.9939	-2.0507	3.3442
C	0.2883	-2.2958	4.1331
C	1.1326	-3.0859	3.1225
C	0.813	-2.4493	1.75
C	1.7914	-1.5189	0.9844
O	1.5227	-1.4067	-0.2295
C	-1.1526	-1.0905	1.0484
C	-2.3982	-0.448	1.2137
C	-3.187	-0.2297	-0.0638
H	0.1139	-2.8449	5.0622
H	0.7452	-1.3284	4.3657
H	2.1941	-3.1065	3.3562
H	-1.6243	-2.953	3.3011
H	0.7912	-4.1273	3.0975
H	0.6269	-3.2381	1.0139
H	-0.648	-1.0509	0.0911

H	-2.9999	-0.8104	2.0451
H	-3.7597	-1.1277	-0.328
H	-2.5277	0.0022	-0.9057
H	-3.8994	0.5914	0.0398
H	-1.5878	-1.2247	3.7215
C	-4.25	1.2299	3.4606
C	-5.5517	1.7497	3.255
C	-3.4055	1.7457	2.3948
C	-4.1977	2.5385	1.616
N	-5.4998	2.5693	2.1117
C	-6.6053	3.0801	1.4255
O	-6.2154	3.6113	0.253
O	-7.748	3.0282	1.826
C	-7.2783	4.1189	-0.5733
C	-2.0428	1.3692	2.0067
C	-1.0183	1.2844	2.9773
N	0.2621	1.095	2.5597
O	0.4901	1.0233	1.3049
O	1.1917	0.9722	3.4134
H	-1.1695	1.2739	4.0458
H	-1.7254	1.7902	1.0587
H	-3.9583	3.0547	0.7031
H	-6.7885	4.4575	-1.4863
H	-7.7895	4.9467	-0.0747
H	-8.0004	3.3274	-0.791
C	-4.0479	0.3124	4.5006
C	-6.6407	1.3899	4.0478
C	-6.4073	0.4749	5.0726
C	-5.128	-0.0597	5.2964
H	-3.0635	-0.1044	4.6851
H	-4.9805	-0.7757	6.1001
H	-7.2359	0.1662	5.7036
H	-7.625	1.7936	3.8514
N	2.8587	-0.8979	1.516
C	3.4264	-0.9823	2.8824
C	4.5451	0.0727	2.8844
C	4.0645	1.1071	1.86
C	3.4551	0.2332	0.7597
C	4.4789	-0.1684	-0.3143
O	5.0757	0.6996	-0.9379
H	5.4906	-0.3768	2.5576
H	4.8593	1.7387	1.4589
H	4.6938	0.49	3.8838
H	2.6579	-0.7332	3.6111
H	3.8208	-1.9854	3.0685
H	2.6468	0.7482	0.2377
H	3.2726	1.7209	2.2942
N	4.6269	-1.5063	-0.5397
H	4.0267	-2.1074	0.0035
C	5.1343	-2.0593	-1.8
C	4.905	-2.2259	-4.2861
C	4.4997	-1.405	-3.0517

N	3.0526	-1.2795	-2.8652
H	4.4201	-1.8016	-5.1679
H	2.6763	-1.6428	-1.9942
H	4.9024	-0.3929	-3.1603
C	2.2907	-0.339	-3.4826
S	2.7565	0.4814	-4.8725
N	1.0977	-0.1167	-2.8073
C	-0.0311	0.5543	-3.2917
C	-2.3673	1.8318	-4.1988
C	-0.7595	1.3869	-2.4292
C	-0.4888	0.3543	-4.6024
C	-1.6413	0.9948	-5.0438
C	-1.9205	2.0118	-2.8918
C	-2.7365	2.9067	-2.0056
C	-2.0951	0.8066	-6.4679
F	-2.9648	4.1085	-2.5752
F	-3.9618	2.3765	-1.7384
F	-2.1438	3.1346	-0.8061
F	-1.5934	1.7599	-7.2826
F	-3.4443	0.8723	-6.5706
F	-1.708	-0.3883	-6.9644
H	-3.2665	2.3255	-4.549
H	0.0506	-0.3077	-5.2654
H	-0.412	1.55	-1.4129
H	1.1037	-0.3352	-1.8127
C	6.4335	-2.2058	-4.4395
C	6.6647	-2.0038	-1.9132
H	4.8288	-3.1151	-1.7854
C	7.1379	-2.7344	-3.1801
H	7.1057	-2.4536	-1.0156
H	6.9244	-3.8088	-3.0728
H	8.2262	-2.6408	-3.2801
H	6.7319	-2.794	-5.3156
H	4.5436	-3.2587	-4.1715
H	6.7549	-1.1723	-4.6292
H	6.9669	-0.9508	-1.9302

TS-maor_conf3



Imaginary Freq	-467.86	cm ⁻¹
Temperature	298.15	Kelvin
Pressure	1	atm
Frequencies scaled by	1	
Electronic Energy (EE)	-3383.2096	Hartree
Zero-point Energy Correction	0.836835	Hartree
Thermal Correction to Energy	0.88973	Hartree
Thermal Correction to Enthalpy	0.890674	Hartree
Thermal Correction to Free Energy	0.752579	Hartree
EE + Zero-point Energy	-3382.3728	Hartree
EE + Thermal Energy Correction	-3382.3199	Hartree
EE + Thermal Enthalpy Correction	-3382.3189	Hartree
EE + Thermal Free Energy Correction	-3382.457	Hartree
E (Thermal)	558.314	kcal/mol
Heat Capacity (Cv)	209.012	cal/mol-kelvin
Entropy (S)	290.644	cal/mol-kelvin

Symbolic Z-matrix:

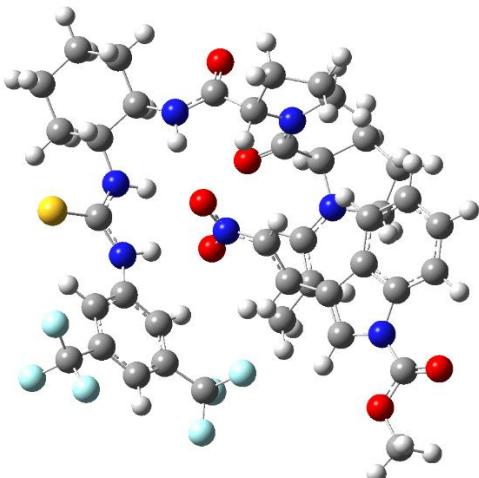
Charge = 0 Multiplicity = 1

N	-1.0665	0.7595	3.2273
C	-0.3867	1.5039	4.3065
C	0.0787	0.422	5.2816
C	-0.9284	-0.7253	5.0853
C	-1.3736	-0.6498	3.612
C	-0.8578	-1.5836	2.4832
O	-1.5756	-1.5987	1.48
C	-1.5089	1.3122	2.1083
C	-1.1208	2.5709	1.6042
C	-2.11	3.2804	0.6953
H	0.1035	0.7853	6.3121
H	1.0952	0.1179	5.0174
H	-0.5332	-1.7043	5.3584
H	-1.1124	2.1911	4.759
H	-1.8093	-0.5531	5.7131
H	-2.4549	-0.7939	3.5425
H	-2.0982	0.6575	1.4713
H	-0.5906	3.2263	2.2904
H	-2.9299	3.7283	1.2697
H	-2.5329	2.5784	-0.0296
H	-1.621	4.0854	0.1347
H	0.4446	2.0838	3.9048
C	2.3932	2.4344	1.9189
C	3.2879	3.5013	2.1665
C	1.4841	2.8591	0.8731
C	1.8369	4.1306	0.5277
N	2.9304	4.5443	1.2921
C	3.58	5.7739	1.1838
O	2.9954	6.5248	0.2346
O	4.5309	6.1041	1.8582
C	3.593	7.8189	0.031
C	0.3624	2.0978	0.3147
C	0.6295	0.7234	0.0307

N	-0.2569	-0.0414	-0.6404
O	-1.471	0.3621	-0.7741
O	0.1054	-1.1493	-1.1301
H	1.5788	0.2482	0.2204
H	-0.1774	2.6024	-0.4826
H	1.4248	4.7692	-0.237
H	3.0105	8.2793	-0.7666
H	4.6395	7.7117	-0.265
H	3.5349	8.4125	0.947
C	2.5126	1.2415	2.6476
C	4.3006	3.4087	3.1217
C	4.4003	2.2128	3.8325
C	3.5197	1.1413	3.6017
H	1.8287	0.4173	2.4652
H	3.6349	0.22	4.1674
H	5.1819	2.1084	4.5791
H	4.9779	4.2341	3.2928
N	0.3013	-2.2787	2.5305
C	1.2578	-2.4762	3.6294
C	2.4916	-3.0436	2.92
C	1.87	-3.9136	1.8232
C	0.675	-3.0828	1.3345
C	-0.4911	-3.9839	0.8885
O	-1.0276	-4.7475	1.6865
H	3.1405	-3.5975	3.6048
H	1.495	-4.8501	2.2507
H	3.0763	-2.225	2.4816
H	1.4794	-1.5425	4.1449
H	0.8618	-3.1993	4.3547
H	0.955	-2.3946	0.533
H	2.5573	-4.1505	1.0072
N	-0.7941	-3.8941	-0.4296
H	-0.4789	-3.0484	-0.8996
C	-2.0033	-4.5349	-0.9494
C	-2.7845	-6.7374	-2.0317
C	-3.7605	-4.5124	-2.7482
C	-4.075	-5.9247	-2.2013
C	-2.3406	-4.0375	-2.365
C	-1.856	-6.0782	-0.9871
N	-2.2105	-2.5878	-2.4887
H	-2.0563	-6.4579	0.0181
H	-3.0081	-7.7685	-1.7338
H	-4.574	-5.8486	-1.2259
H	-4.7754	-6.44	-2.8686
H	-4.4824	-3.7837	-2.3605
H	-2.2232	-2.042	-1.6318
H	-0.8085	-6.3096	-1.2122
H	-1.6158	-4.4677	-3.0638
H	-3.8324	-4.4817	-3.8399
H	-2.2762	-6.7993	-3.0028
C	-1.8626	-1.9436	-3.6385
S	-1.6448	-2.7472	-5.1048

N	-1.7614	-0.5859	-3.4376
C	-1.1792	0.4425	-4.1813
C	0.0376	2.6897	-5.4086
C	-0.6211	0.3373	-5.4644
C	-1.14	1.6946	-3.5392
C	-0.5297	2.7875	-4.1377
C	-0.0294	1.456	-6.0534
C	0.5029	1.3144	-7.4558
C	-0.4244	4.0499	-3.337
F	-0.486	1.4263	-8.3738
F	1.4213	2.2658	-7.7487
F	1.0876	0.1135	-7.6534
F	-1.5472	4.297	-2.6176
F	-0.1745	5.1355	-4.0931
F	0.5874	3.9733	-2.4161
H	0.5132	3.5407	-5.8794
H	-1.5685	1.7946	-2.5496
H	-0.6383	-0.6116	-5.9819
H	-1.8784	-0.3037	-2.4598
H	-2.8313	-4.2721	-0.2742

TS-major_conf4



Imaginary Freq	-466.92 cm ⁻¹	
Temperature	298.15 Kelvin	
Pressure	1 atm	
Frequencies scaled by	1	
Electronic Energy (EE)	-3383.2194	Hartree
Zero-point Energy Correction	0.836845	Hartree
Thermal Correction to Energy	0.888632	Hartree
Thermal Correction to Enthalpy	0.889576	Hartree
Thermal Correction to Free Energy	0.754955	Hartree
EE + Zero-point Energy	-3382.3826	Hartree
EE + Thermal Energy Correction	-3382.3308	Hartree
EE + Thermal Enthalpy Correction	-3382.3299	Hartree
EE + Thermal Free Energy Correction	-3382.4645	Hartree
E (Thermal)	557.625	kcal/mol
Heat Capacity (Cv)	206.795	cal/mol-kelvin

Entropy (S) 283.333 cal/mol-kelvin

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

N	-1.0819	0.7333	3.2412
C	-0.399	1.4731	4.3216
C	0.0791	0.3864	5.2854
C	-0.9204	-0.7664	5.0839
C	-1.369	-0.6834	3.6124
C	-0.8404	-1.5962	2.473
O	-1.5556	-1.6059	1.4682
C	-1.532	1.2909	2.1279
C	-1.1517	2.5551	1.6313
C	-2.1487	3.2665	0.7321
H	0.106	0.7412	6.3188
H	1.0963	0.092	5.0137
H	-0.5186	-1.7446	5.3499
H	-1.1253	2.1528	4.7842
H	-1.8015	-0.6043	5.7144
H	-2.4481	-0.8428	3.5427
H	-2.119	0.6371	1.4877
H	-0.6235	3.2082	2.3213
H	-2.9687	3.7044	1.3141
H	-2.5703	2.5679	0.0031
H	-1.6668	4.079	0.1763
H	0.4265	2.0603	3.9184
C	2.3666	2.4189	1.9374
C	3.2575	3.4858	2.1981
C	1.4505	2.8558	0.9027
C	1.7959	4.1343	0.5762
N	2.8909	4.5409	1.3424
C	3.5324	5.7762	1.2529
O	2.9385	6.5403	0.3201
O	4.4845	6.1004	1.9285
C	3.527	7.8416	0.1375
C	0.3279	2.0989	0.3379
C	0.5984	0.7286	0.0358
N	-0.2862	-0.0323	-0.6423
O	-1.5021	0.3671	-0.7699
O	0.0798	-1.1339	-1.1437
H	1.5499	0.2549	0.2177
H	-0.213	2.6127	-0.4524
H	1.3765	4.7839	-0.175
H	2.9374	8.313	-0.6485
H	4.5725	7.7466	-0.166
H	3.4702	8.4179	1.0646
C	2.4946	1.2155	2.6473
C	4.2749	3.3831	3.1474
C	4.3832	2.1769	3.8393
C	3.5063	1.1052	3.5955
H	1.8137	0.3909	2.4561
H	3.6278	0.1758	4.1465

H	5.1683	2.0644	4.5809
H	4.9491	4.2089	3.3287
N	0.3275	-2.2775	2.5121
C	1.2747	-2.496	3.6146
C	2.512	-3.0533	2.9035
C	1.8956	-3.9088	1.7923
C	0.7002	-3.0729	1.3109
C	-0.4715	-3.9691	0.8691
O	-1.0267	-4.7014	1.6832
H	3.1581	-3.6164	3.5836
H	1.5215	-4.8515	2.2066
H	3.098	-2.2286	2.4789
H	1.4938	-1.5717	4.1478
H	0.8717	-3.2311	4.3239
H	0.9777	-2.3807	0.512
H	2.5861	-4.1337	0.9758
N	-0.7521	-3.909	-0.4573
H	-0.4172	-3.0737	-0.9313
C	-1.9751	-4.5151	-0.9925
C	-3.1973	-6.6793	-1.5159
C	-3.5434	-4.6335	-2.9607
C	-2.2221	-4.0462	-2.4387
C	-1.9087	-6.0527	-0.9673
N	-2.1947	-2.5856	-2.5423
H	-1.7253	-6.3753	0.06
H	-3.1093	-7.7728	-1.511
H	-3.7025	-4.2673	-3.9786
H	-2.2058	-2.0577	-1.6742
H	-1.0478	-6.3676	-1.5732
H	-1.4062	-4.424	-3.0673
C	-1.8117	-1.9147	-3.6677
S	-1.4899	-2.696	-5.1275
N	-1.7657	-0.5558	-3.4516
C	-1.1922	0.4964	-4.1705
C	-0.0076	2.7842	-5.3553
C	-0.6285	0.4237	-5.4538
C	-1.1761	1.738	-3.5072
C	-0.5821	2.851	-4.0858
C	-0.052	1.561	-6.0212
C	0.4869	1.4528	-7.424
C	-0.5009	4.1031	-3.2665
F	-0.4996	1.576	-8.3435
F	1.3983	2.4182	-7.6927
F	1.0826	0.2616	-7.6447
F	-1.6292	4.3213	-2.5468
F	-0.2673	5.2033	-4.0065
F	0.5105	4.0308	-2.3446
H	0.456	3.6508	-5.8093
H	-1.6092	1.8145	-2.5177
H	-0.6281	-0.5158	-5.9877
H	-1.913	-0.2889	-2.4737
H	-2.8176	-4.1943	-0.3587

H	-4.3681	-4.2573	-2.3389
H	-4.0328	-6.4293	-0.8454
C	-3.5106	-6.1667	-2.9282
H	-4.4659	-6.5711	-3.2855
H	-2.7382	-6.521	-3.6261

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