

Supporting Information

α -Hydroxy- β -azidotetrazoles: A Versatile Platform for the synthesis of a Multichromophoric Array by Sequential CuAAC Reactions

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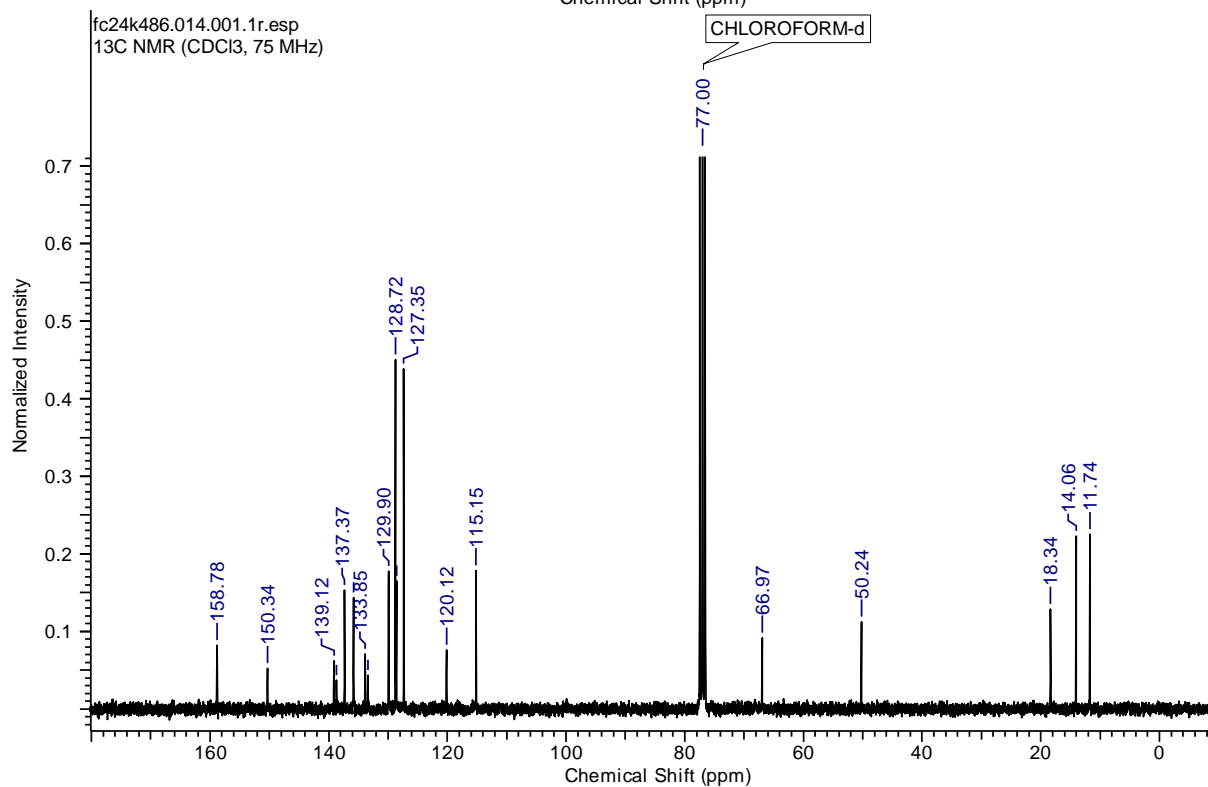
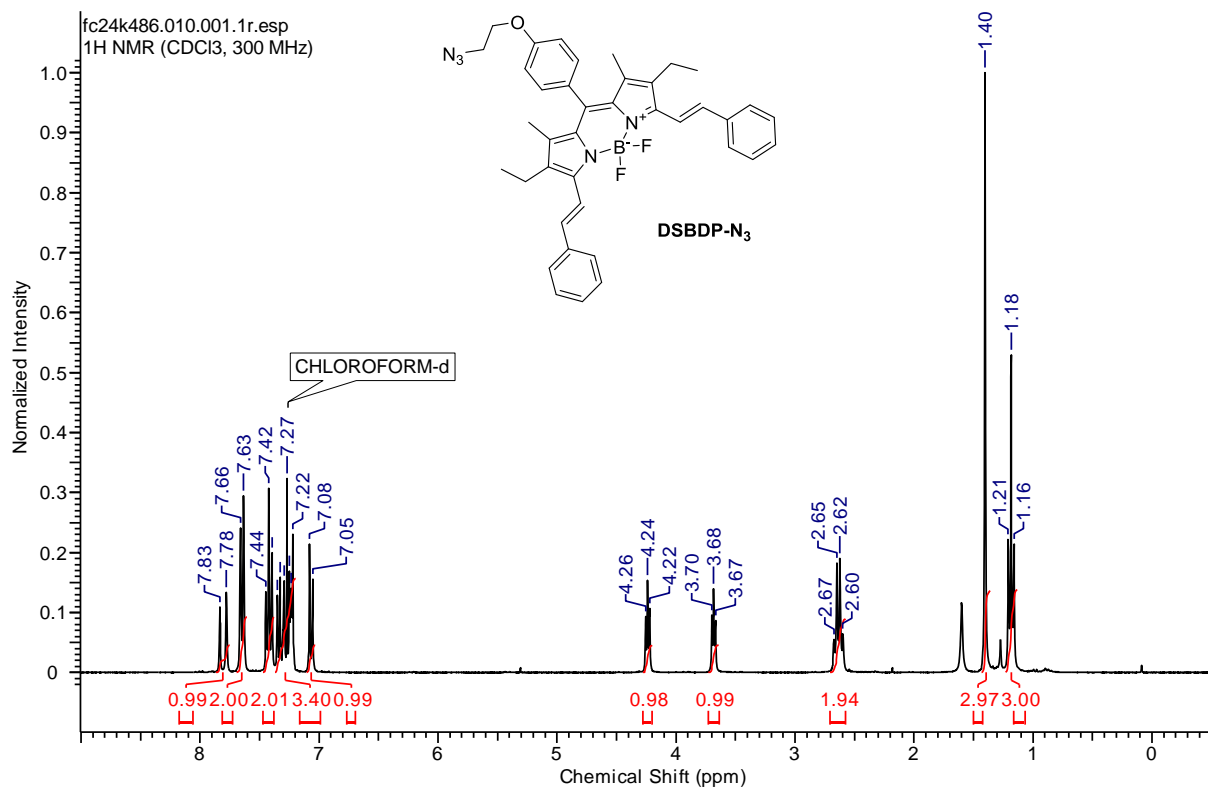
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Contents

¹H, ¹³C NMR and HRMS spectra	3
Computational studies	33
Figure S1. Structures of the three fragments studied	33
Figure S2. Calculated relative energies as a function of the dihedral angle defined by the C(8), O, C(7) and C(6) in the phenyl-triazole fragment	33
Figure S3. Calculated relative energies) as a function of the dihedral angle defined by O, C(7), C(6) and N(1) in the phenyl-triazole fragment	34
Figure S4. Calculated relative energies as a function of the dihedral angle defined by C(7), C(6), N(1) and N(2) in the phenyl-triazole fragment	34
Figure S5. Calculated relative energies as a function of the dihedral angle defined by C(7), C(6), O, C(5) in the di(phenyl-triazole)fragment	35
Figure S6. Calculated relative energies as a function of the dihedral angle defined by C(6), O, C(5) and C(4) in the di(phenyl-triazole)fragment	35
Figure S7. Calculated relative energies as a function of the dihedral angle defined by O, C(5), C(4) and N(3) in the di(phenyl-triazole) fragment	36
Figure S8. Calculated relative energies as a function of the dihedral angle defined by C(1), N, C(2) and C(3) in the di(phenyl-triazole)-coumarin fragment	36
Figure S9. Calculated relative energies as a function of the dihedral angle defined by N, C(2), C(3) and C(4) in the di(phenyl-triazole)-coumarin fragment	37
Figure S10. Alternative conformers of the dyads BDP-DSBDP 7 and Coum-DSBDP 11	38

Figure S11	Representation of the three most stable conformers of the triad Coum-BDP-DSBDP 14 with their relative energies	38
Figure S12.	Plot of the frontier molecular orbitals of the dyad Coum-DSBDP 11-extended conformer (isovalue 0.02).	39
Figure S13.	Plot of the frontier molecular orbitals of the triad- conformer II Coum-BDP-DSBDP 14 (isovalue 0.02) with their energies in eV	40
Emission and absorption spectra		41
Figure S14.	Normalized absorption spectra of Coum-BDP (13) in different solvents	41
Figure S15.	Normalized fluorescence emission spectra of Coum-BDP (13) in different solvents – ($\lambda_{exc} = 400$ nm)	41
Figure S16.	Normalized absorption spectra of BDP-DSBDP (7) in different solvents	42
Figure S17.	Normalized fluorescence emission spectra of BDP-DSBDP (7) in different solvents – ($\lambda_{exc} = 495$ nm)	42
Figure S18.	Normalized absorption spectra of Coum-DSBDP (11) in different solvents	43
Figure S19.	Normalized fluorescence emission spectra of Coum-DSBDP (11) in different solvents – ($\lambda_{exc} = 400$ nm)	43
Figure S20.	Normalized absorption spectra of Coum-BDP-DSBDP (14) in different solvents	44
Figure S21.	Normalized fluorescence emission spectra of Coum-BDP-DSBDP (14) in different solvents – ($\lambda_{exc} = 400$ nm)	44
Table S1.	Spectroscopic data of 7, 11, 13 and 14 in different solvents	45
Figure S22.	Fluorescence spectrum of Coumarin 10	46
Figure S23.	Fluorescence spectrum of Bodipy BDP-alkyne	46
Figure S24.	Fluorescence spectrum of distyrylBodipy DSBDP-N₃	47
Figure S25.	Overlap of the emission and absorption spectra of Coumarin 10 and Bodipy BDP-alkyne	47
Figure S26.	Overlap of the emission and absorption spectra of Coumarin 10 and distyrylBodipy DSBDP-N₃	48
Figure S27.	Overlap of the emission and absorption spectra of Bodipy BDP-alkyne and distyrylBodipy DSBDP-N₃	48
Energy transfer efficiency and calculation of the Förster distance (R_0)		49
Cartesian coordinates of all minima		50



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 150.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 9

Monoisotopic Mass, Odd and Even Electron Ions

7028 formula(e) evaluated with 67 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-110 H: 0-150 B: 0-1 N: 0-15 O: 0-10 F: 0-2

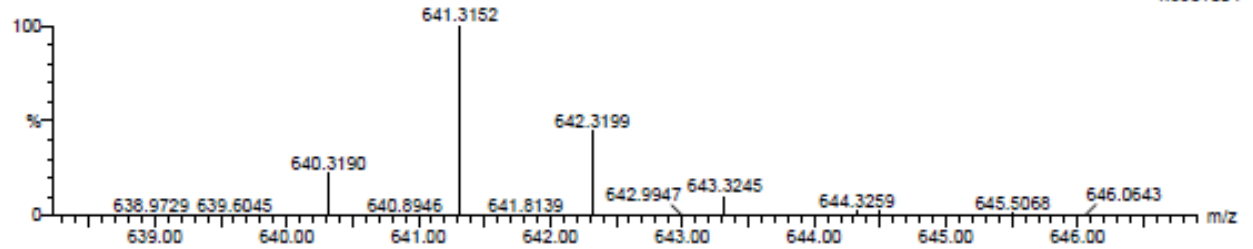
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Infusion - dilution 1000

HN17-(01) 16 (0.625) Cm (12:16)

17-Jun-2019

1: TOF MS ES+
4.88e+004

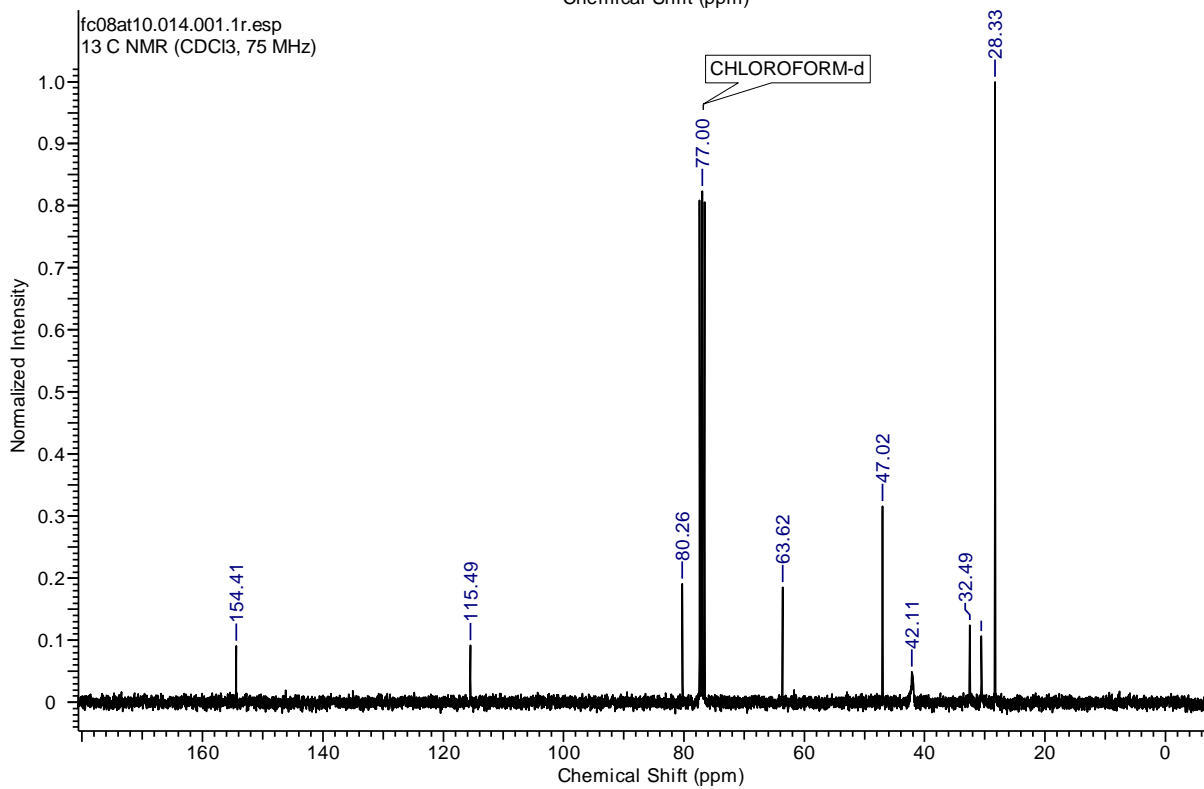
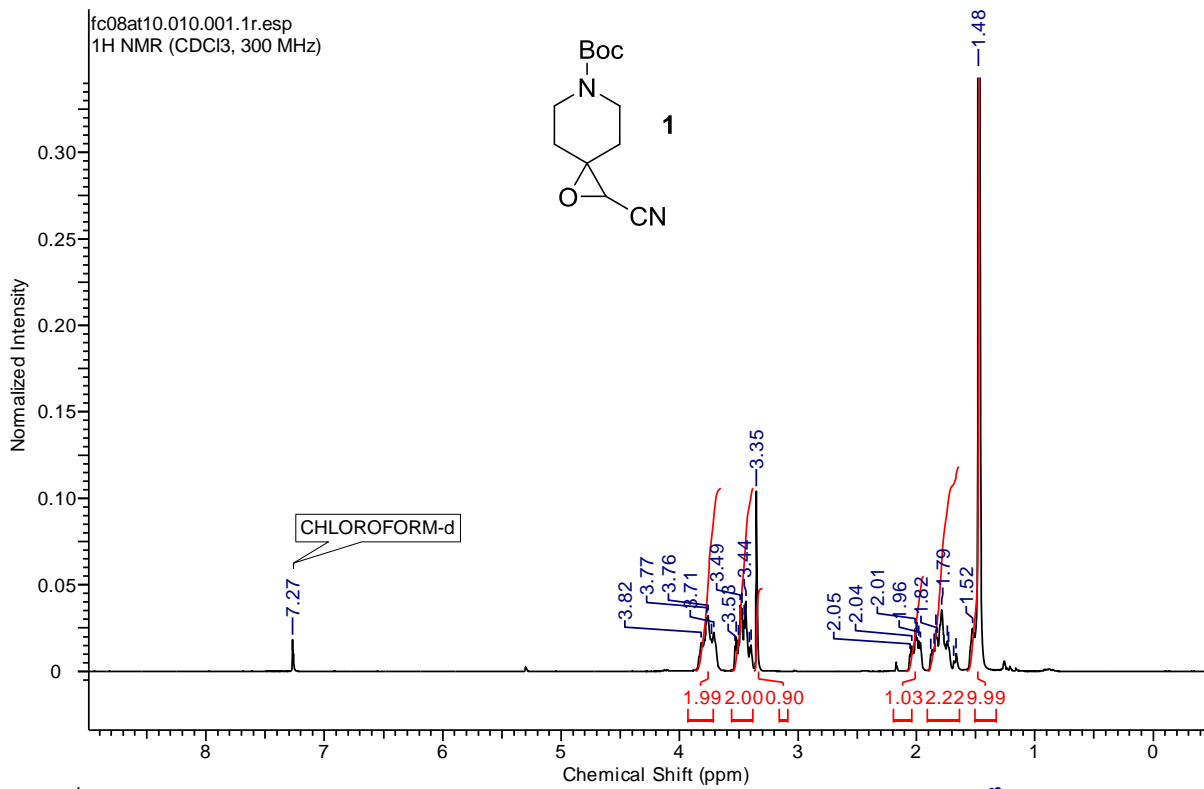


Minimum:

Maximum:

5.0 5.0 -1.5

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
							F2
641.3160		-0.8	-1.2	14.5	474.0	13.1	C29 H41 N10 O7
641.3124		2.8	4.4	15.5	474.4	13.5	C30 H39 N10 O4 F2
641.3156		-0.4	-0.6	10.0	474.6	13.7	C27 H42 B N7 O8 F2
641.3156		-0.4	-0.6	15.5	475.2	14.3	C26 H36 B N14 O3
							F2
641.3178		-2.6	-4.1	9.5	475.8	14.9	C24 H42 B N10 O10
641.3143		0.9	1.4	10.5	475.8	14.9	C25 H40 B N10 O7
							F2
641.3146		0.6	0.9	15.0	476.0	15.2	C27 H39 N13 O6
641.3165		-1.3	-2.0	10.0	476.8	15.9	C22 H40 B N13 O9
641.3129		2.3	3.6	11.0	477.0	16.1	C23 H38 B N13 O6
							F2
641.3133		1.9	3.0	10.0	477.3	16.5	C26 H43 N9 O10
641.3171		-1.9	-3.0	10.5	477.5	16.6	C26 H42 N10 O8 F
641.3176		-2.4	-3.7	6.0	478.5	17.6	C19 H41 B N13 O10
							F
641.3158		-0.6	-0.9	11.0	478.9	18.1	C24 H40 N13 O7 F
641.3183		-3.1	-4.8	6.5	480.2	19.3	C23 H43 N10 O9 F2
641.3169		-1.7	-2.7	7.0	481.2	20.4	C21 H41 N13 O8 F2
641.3131		2.1	3.3	6.5	481.3	20.4	C21 H42 N12 O10 F
641.3129		2.3	3.6	3.0	484.2	23.3	C16 H41 N15 O10 F2



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 150.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

384 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-100 H: 0-150 N: 0-10 O: 0-10 F: 0-3 S: 0-2

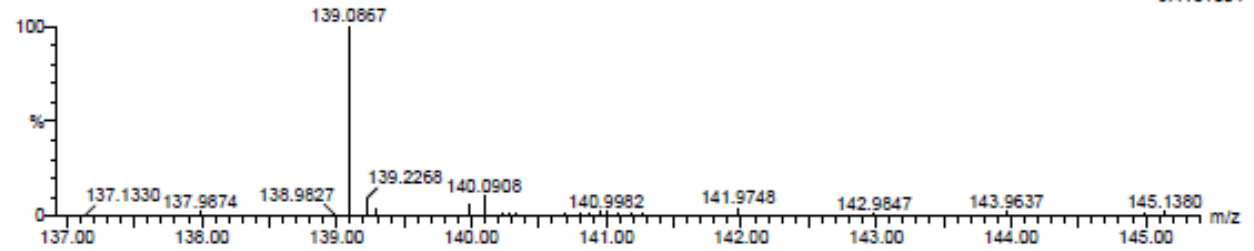
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LCMS - dilution 100

AT10-(01) 537 (3.763) Cm (536:540)

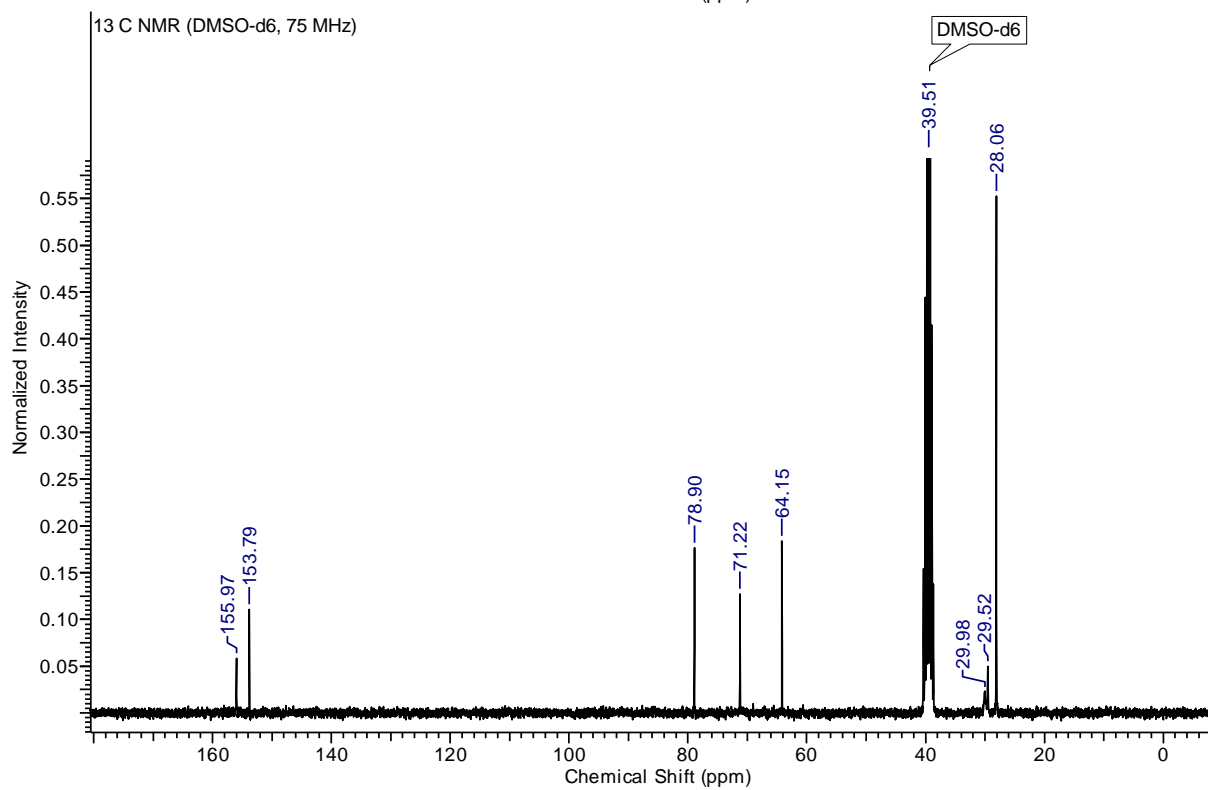
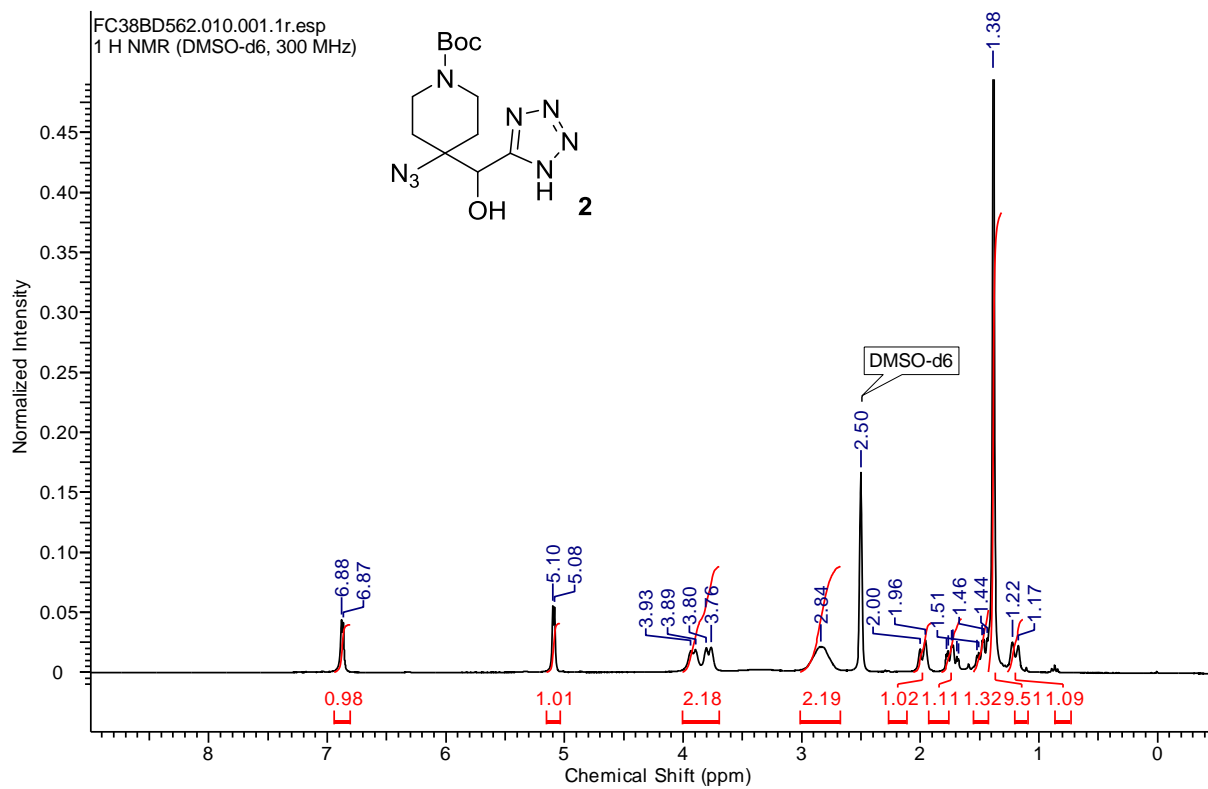
30-Mar-2016

1: TOF MS ES+
6.41e+004



Minimum: 5.0 5.0 -1.5
Maximum: 5.0 5.0 150.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
139.0867	139.0871	-0.4	-2.9	3.5	566.2	0.0	C7 H11 N2 O



Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 150.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

850 formula(e) evaluated with 3 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-100 H: 0-150 N: 0-10 O: 0-10 Na: 0-1

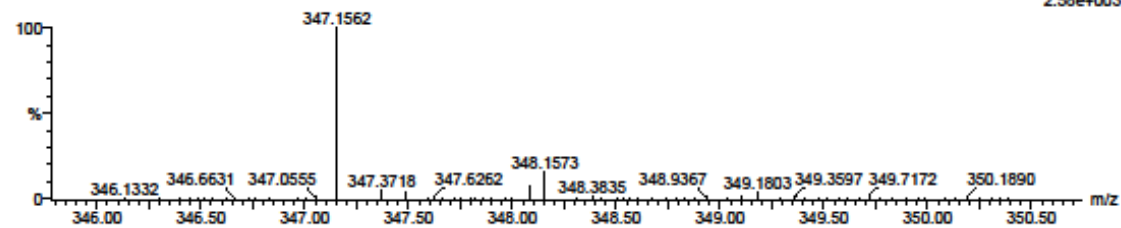
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04-Apr-2016

LCMS - dilution 100

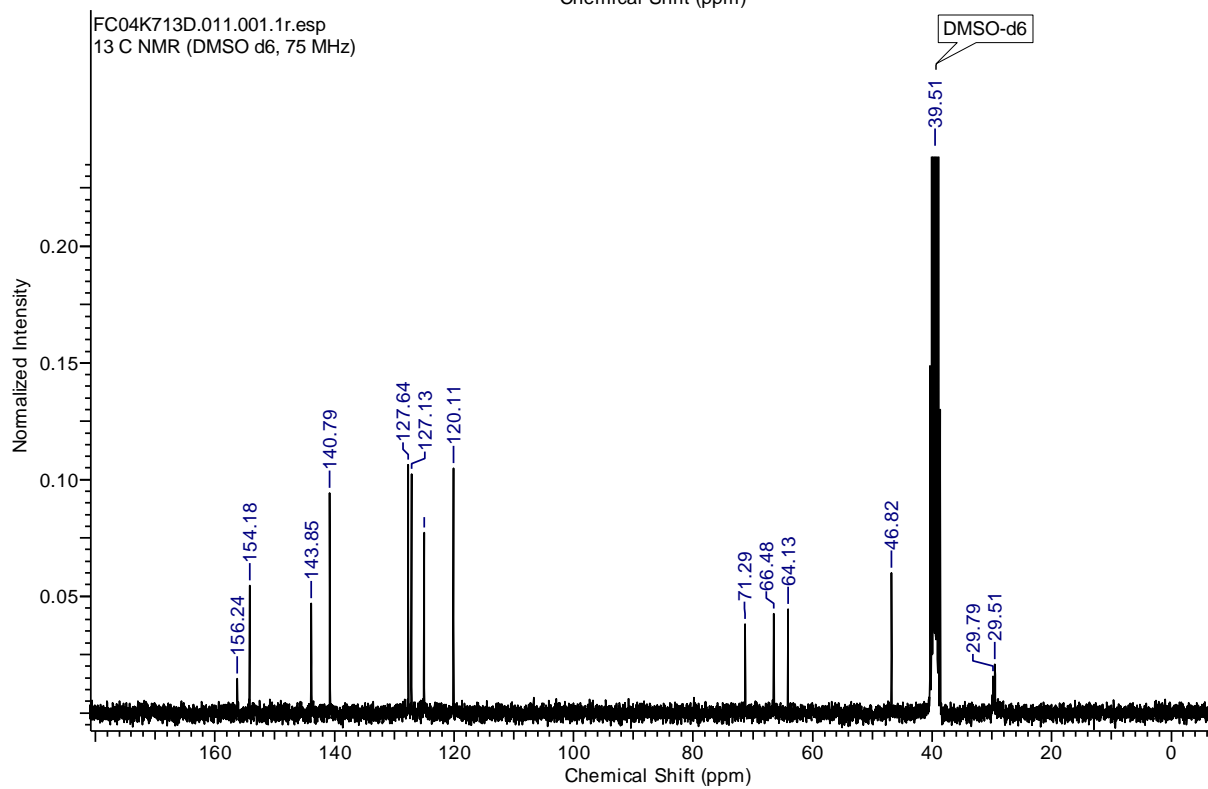
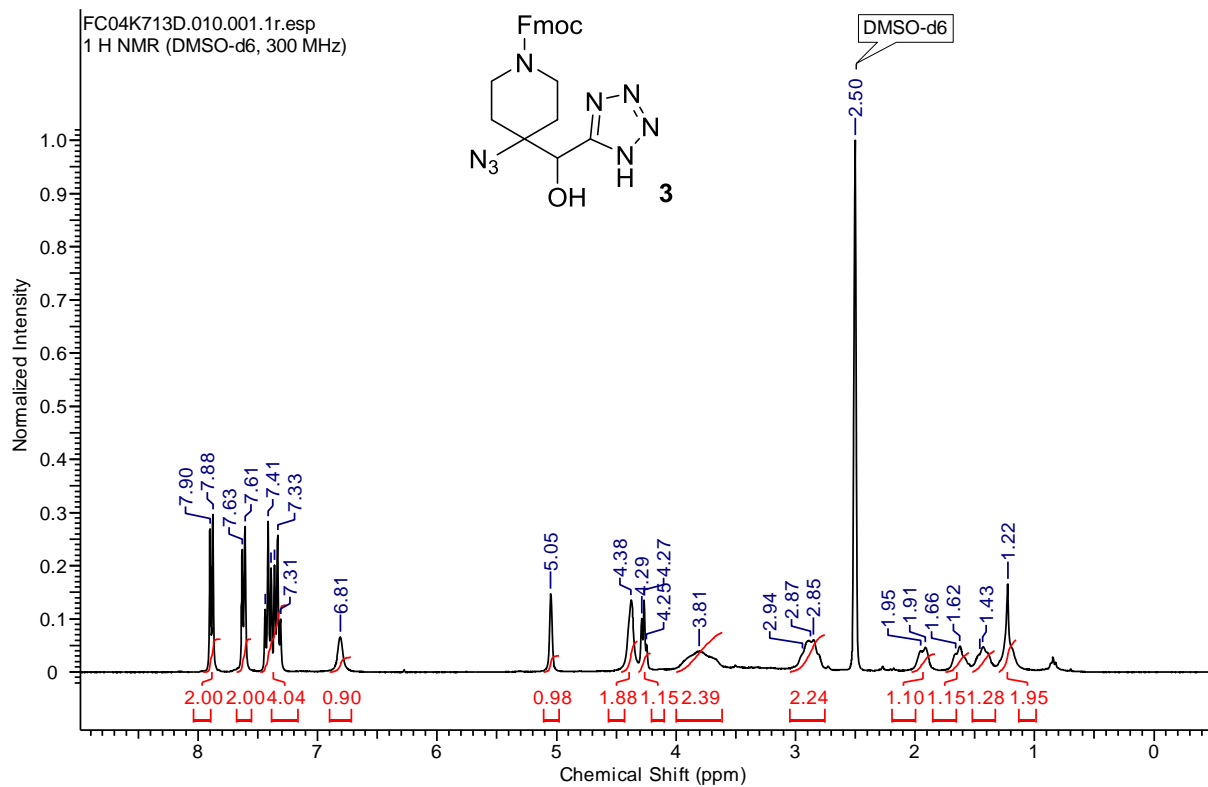
AT14C-(01) 474 (3.321) Cm (474:478)

1: TOF MS ES+
2.58e+003



Minimum: -1.5
Maximum: 5.0 5.0 150.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
347.1562	347.1567	-0.5	-1.4	4.5	181.8	0.1	C13 H23 N4 O7
	347.1556	0.6	1.7	6.5	184.2	2.5	C12 H20 N8 O3 Na
	347.1548	1.4	4.0	17.5	188.6	6.9	C25 H19 N2



Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 150.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

599 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-100 H: 0-150 N: 0-10 O: 0-10

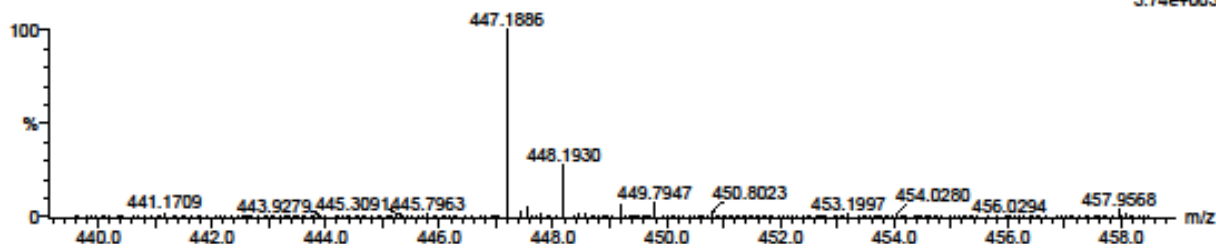
Karen WRIGHT

LCMS - dilution 100

AT30-(01) 610 (4.273) Cm (610:614)

14-Apr-2016

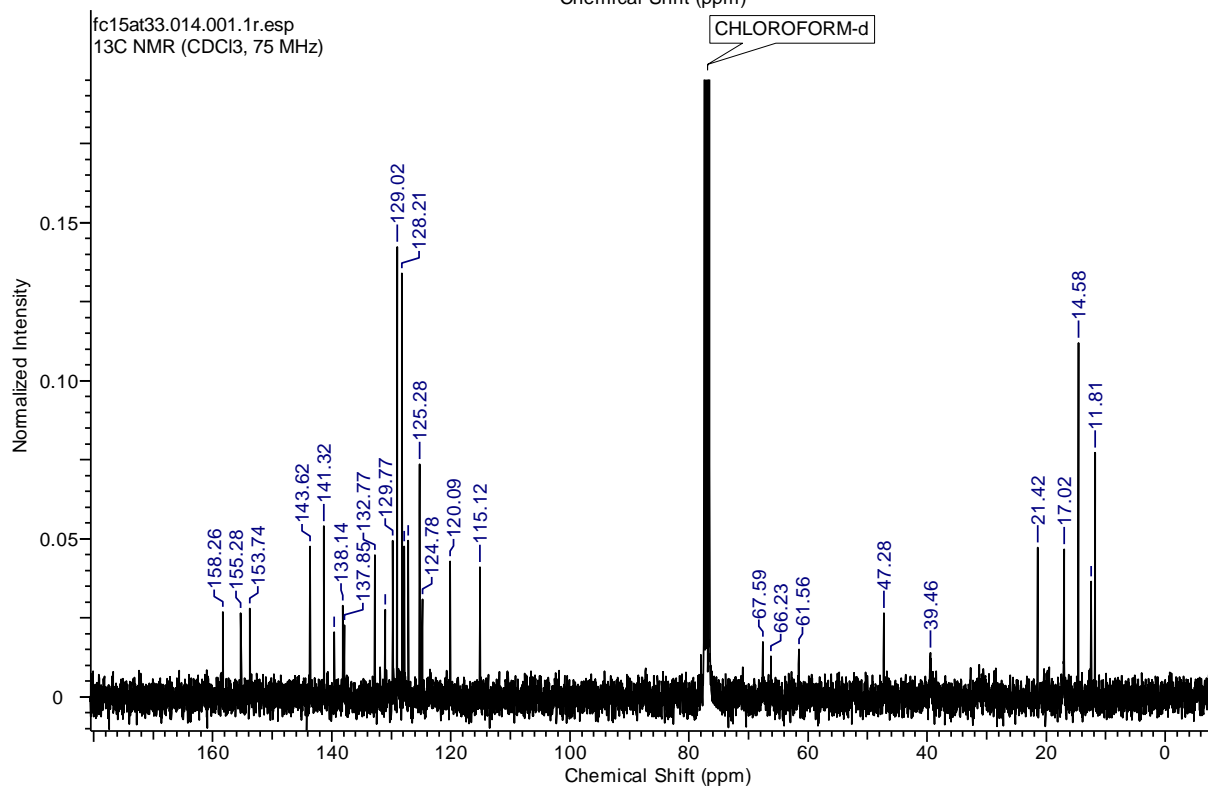
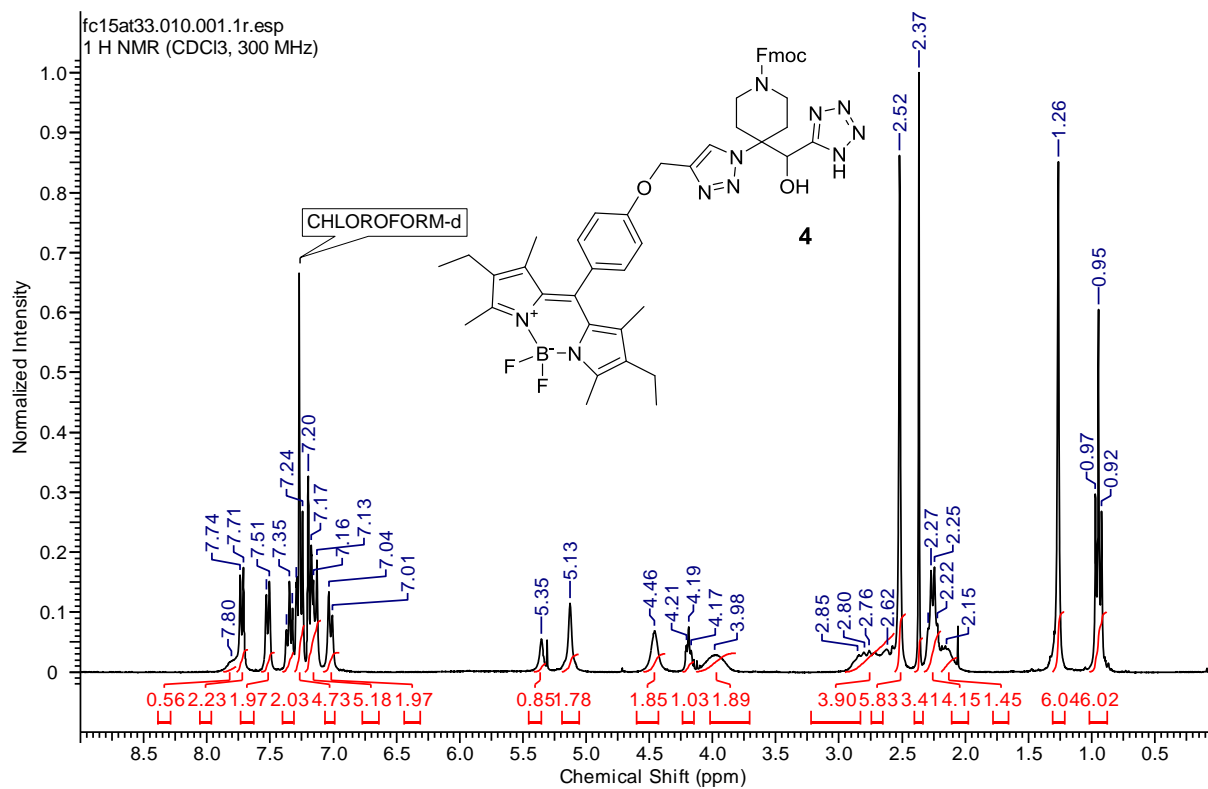
1: TOF MS ES+
5.74e+003



Minimum:

Maximum: 5.0 5.0 -1.5 150.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
447.1886	447.1893	-0.7	-1.6	15.5	161.8	0.6	C22 H23 N8 O3
	447.1880	0.6	1.3	10.5	162.1	0.8	C21 H27 N4 O7



Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 150.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions

18753 formula(e) evaluated with 101 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-100 H: 0-150 B: 0-1 N: 0-10 O: 0-10 F: 0-3 Na: 0-1

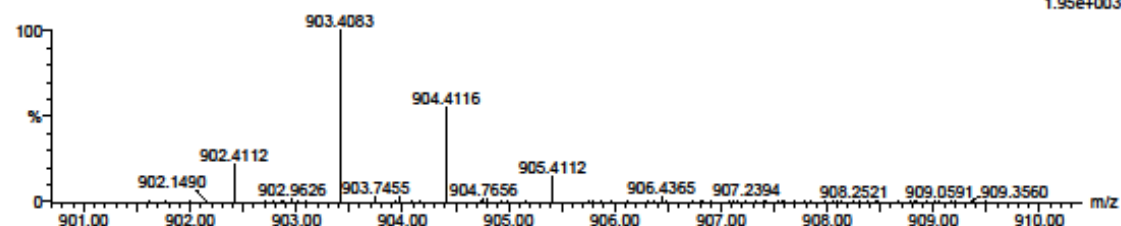
Karen WRIGHT

LCMS - dilution 100

AT33-(01) 790 (5.517) Cm (790:793)

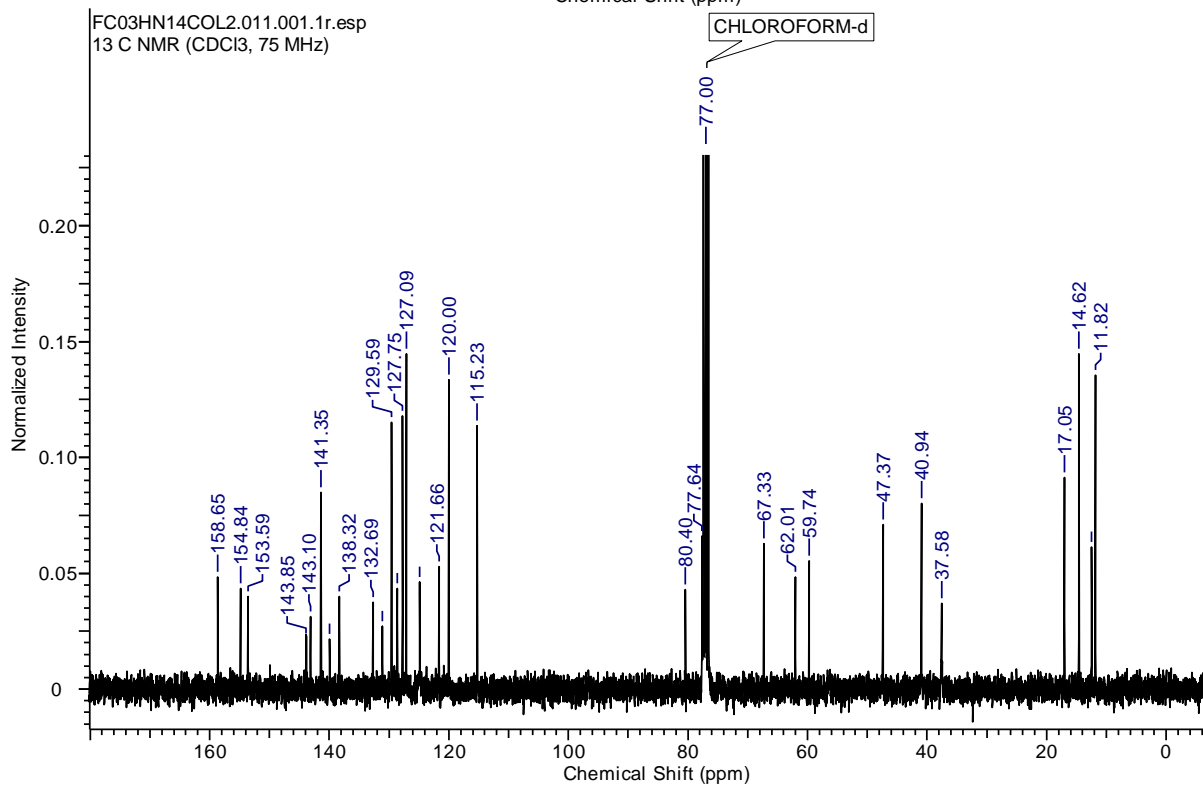
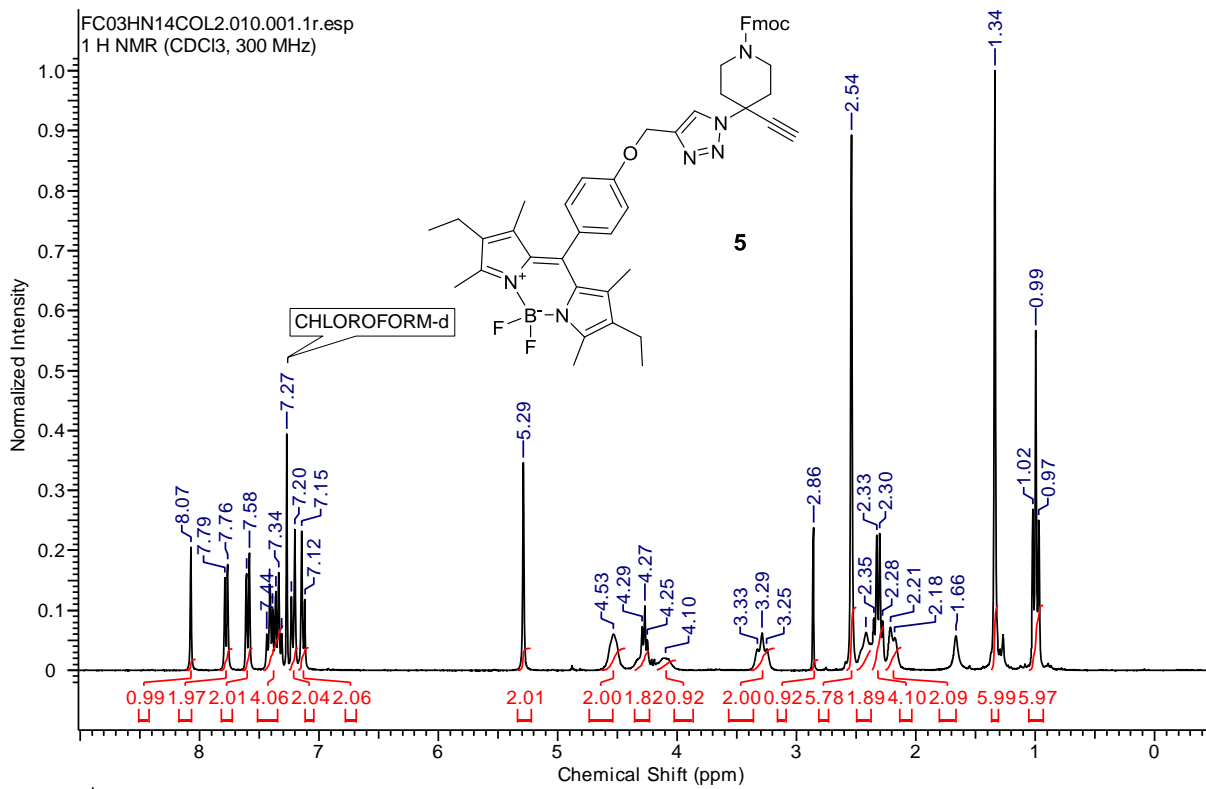
21-Apr-2016

1: TOF MS ES+
1.95e+003



Minimum: -1.5
Maximum: 5.0 5.0 150.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
903.4083	903.4105	-2.2	-2.4	19.5	151.5	0.4	C43 H55 N10 O7 F3
							Na
	903.4094	-1.1	-1.2	23.5	153.1	2.0	C46 H54 N10 O6 F2
							Na
	903.4080	0.3	0.3	18.5	153.1	2.0	C45 H58 N6 O10 F2
							Na
	903.4104	-2.1	-2.3	21.5	155.5	4.4	C47 H57 N6 O10 F2
	903.4069	1.4	1.5	22.5	155.8	4.7	C48 H57 N6 O9 F Na
	903.4065	1.8	2.0	23.5	155.9	4.8	C45 H52 B N10 O5
							F3 Na
	903.4082	0.1	0.1	27.5	156.0	4.9	C49 H53 N10 O5 F
							Na
	903.4089	-0.6	-0.7	26.5	156.2	5.1	C47 H51 B N10 O5
							F3
	903.4118	-3.5	-3.9	26.5	156.3	5.2	C48 H53 N10 O6 F2
	903.4076	0.7	0.8	21.5	156.7	5.6	C46 H55 B N6 O9 F3
	903.4054	2.9	3.2	27.5	156.9	5.8	C48 H51 B N10 O4
							F2 Na
	903.4101	-1.8	-2.0	22.5	156.9	5.8	C44 H54 B N10 O8 F
							Na
	903.4046	3.7	4.1	28.5	156.9	5.8	C50 H51 N10 O2 F3
							Na
	903.4089	-0.6	-0.7	26.5	157.1	6.1	C47 H53 B N10 O7
							Na
	903.4092	-0.9	-1.0	22.5	157.2	6.1	C49 H56 B N4 O7 F3
							Na
	903.4093	-1.0	-1.1	25.5	157.4	6.3	C50 H56 N6 O9 F
	903.4052	3.1	3.4	18.5	157.5	6.4	C44 H56 B N6 O9 F3
							Na
	903.4120	-3.7	-4.1	22.5	157.6	6.5	C50 H58 N4 O8 F2
							Na
	903.4057	2.6	2.9	26.5	157.6	6.5	C51 H54 N6 O6 F3
	903.4105	-2.2	-2.4	27.5	157.6	6.6	C50 H52 B N8 O3 F3
							Na
	903.4070	1.3	1.4	31.5	157.7	6.6	C52 H50 N10 O2 F3
	903.4040	4.3	4.8	22.5	157.8	6.7	C47 H55 B N6 O8 F2
							Na
	903.4044	3.9	4.3	21.5	157.9	6.8	C50 H58 N2 O10 F3
	903.4041	4.2	4.6	25.5	158.1	7.0	C48 H55 N8 O10
	903.4078	0.5	0.6	30.5	158.1	7.0	C50 H50 B N10 O4
							F2
	903.4106	-2.3	-2.5	30.5	158.2	7.1	C51 H52 N10 O5 F
	903.4073	1.0	1.1	27.5	158.2	7.1	C54 H55 N4 O4 F3
							Na
	903.4064	1.9	2.1	25.5	158.2	7.1	C49 H54 B N6 O8 F2
	903.4060	2.3	2.5	22.5	158.2	7.1	C53 H59 O8 F3 Na
	903.4071	1.2	1.3	31.5	158.3	7.2	C52 H52 N10 O4 Na
	903.4057	2.6	2.9	26.5	158.3	7.2	C51 H56 N6 O8 Na
	903.4125	-4.2	-4.6	25.5	158.4	7.3	C46 H53 B N10 O8 F
	903.4086	-0.3	-0.3	32.5	158.6	7.5	C55 H51 N8 F3 Na



Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 150.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 9

Monoisotopic Mass, Odd and Even Electron Ions

8431 formula(e) evaluated with 83 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-100 H: 0-150 B: 0-1 N: 0-10 O: 0-10 F: 0-3

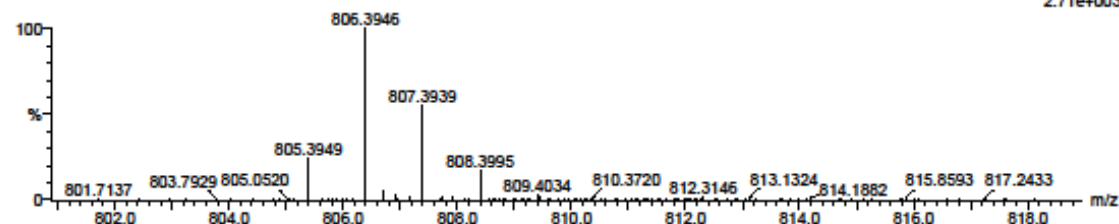
Karen WRIGHT

LCMS - dilution 100

AT36-(01) 832 (5.809) Cm (832:836-800:814)

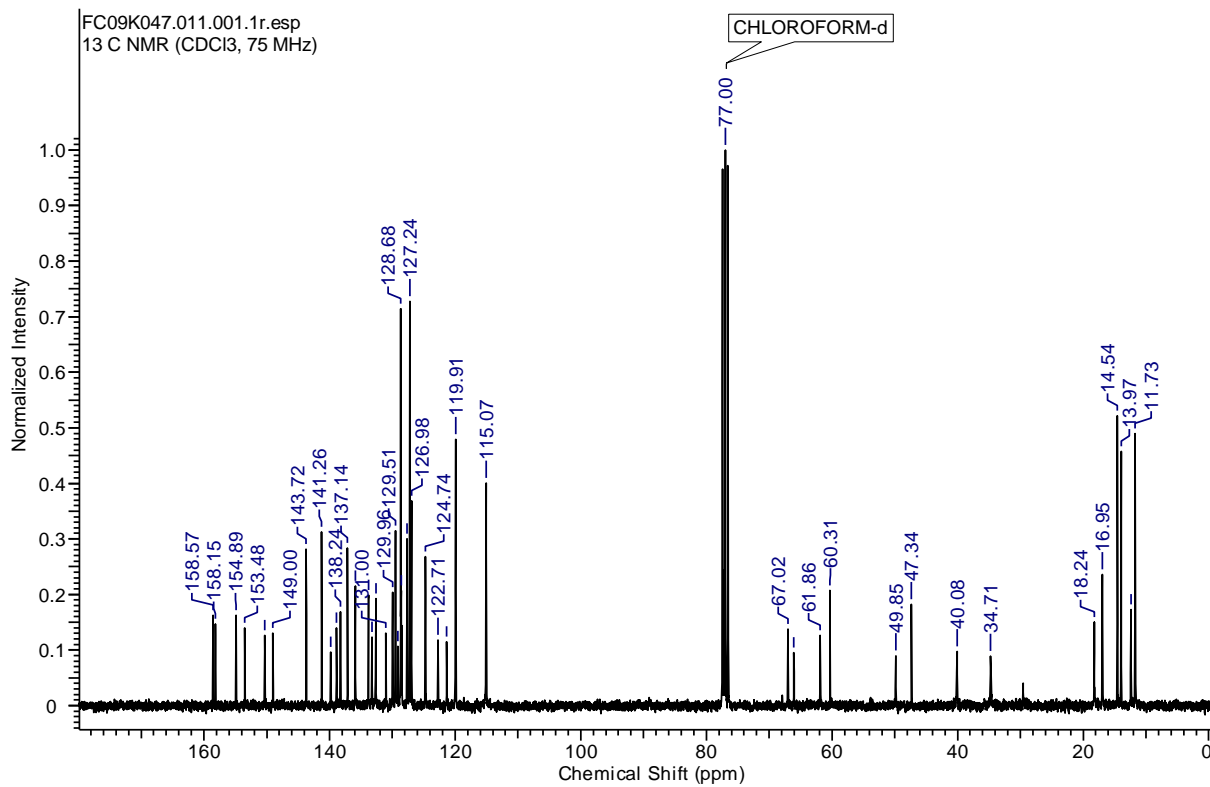
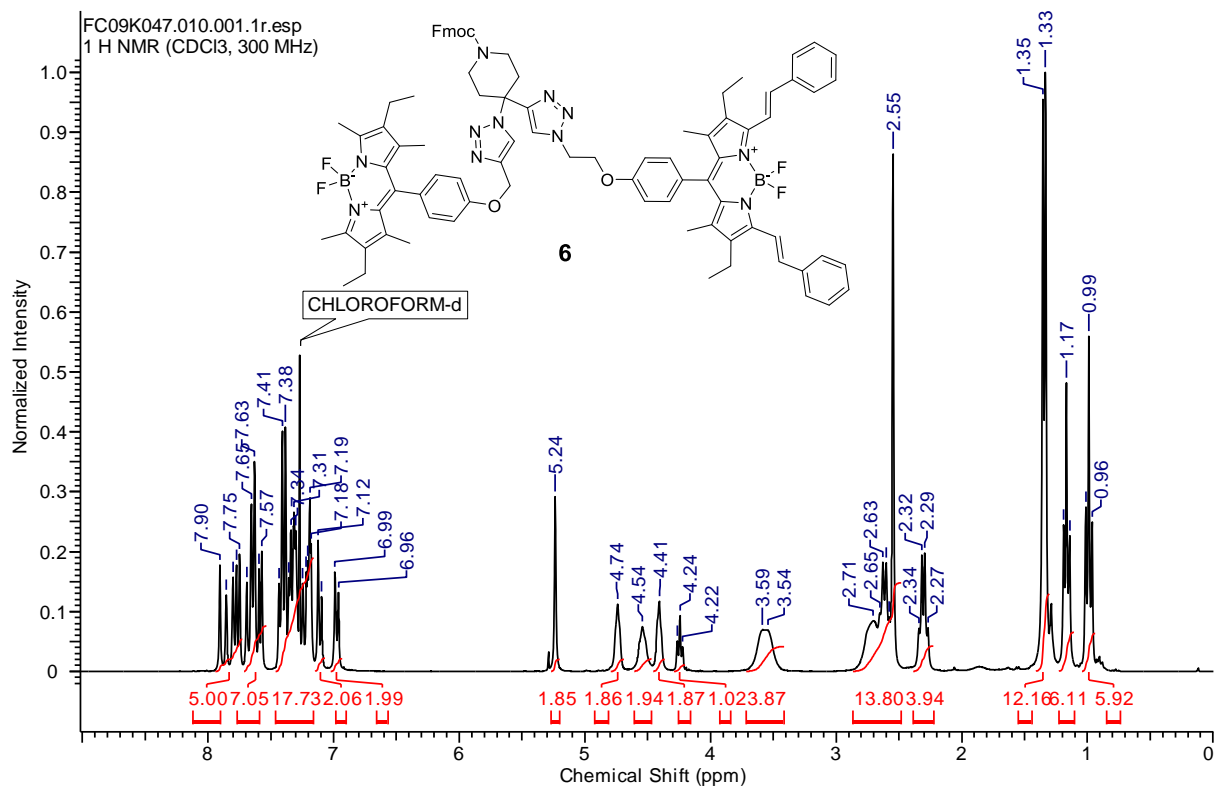
21-Apr-2016

1: TOF MS ES+
2.71e+003



Minimum: -1.5
Maximum: 5.0 5.0 150.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
806.3979	-3.3	-4.1	19.0	304.7	7.2	C43 H53 N6 O6 F3	
806.3981	-3.5	-4.3	30.5	304.9	7.4	C55 H51 B N O2 F2	
806.3969	-2.3	-2.9	32.0	304.9	7.4	C50 H47 N10 F	
806.3934	1.2	1.5	18.0	305.1	7.6	C39 H52 B N8 O9 F	
806.3965	-1.9	-2.4	19.5	305.1	7.6	C41 H51 N9 O5 F3	
806.3963	-1.7	-2.1	18.0	305.3	7.8	C40 H54 N8 O10	
806.3931	1.5	1.9	34.0	305.4	7.9	C58 H51 B O3	
806.3931	1.5	1.9	26.0	305.6	8.1	C51 H54 N2 O7	
806.3965	-1.9	-2.4	14.0	305.7	8.2	C42 H57 N2 O10 F3	
806.3952	-0.6	-0.7	14.5	306.1	8.6	C40 H55 N5 O9 F3	
806.3909	3.7	4.6	32.0	306.2	8.7	C53 H48 N6 F2	
806.3944	0.2	0.2	31.0	306.2	8.7	C52 H50 N6 O3	
806.3969	-2.3	-2.9	26.5	306.3	8.8	C51 H53 N3 O5 F	
806.3947	-0.1	-0.1	27.0	306.6	9.1	C54 H53 O3 F3	
806.3969	-2.3	-2.9	34.5	306.8	9.3	C58 H50 B N O F	
806.3938	0.8	1.0	15.0	306.8	9.3	C38 H53 N8 O8 F3	
806.3986	-4.0	-5.0	18.0	307.2	9.7	C41 H53 B N6 O8 F2	
806.3973	-2.7	-3.3	18.5	307.3	9.8	C39 H51 B N9 O7 F2	
806.3922	2.4	3.0	31.5	307.5	10.0	C55 H50 N3 O F2	
806.3946	0.0	0.0	14.0	307.6	10.1	C36 H53 B N8 O10 F2	
806.3983	-3.7	-4.6	31.5	307.7	10.2	C52 H49 N7 O F	
806.3958	-1.2	-1.5	38.5	308.3	10.8	C61 H49 B N	
806.3958	-1.2	-1.5	30.5	308.6	11.1	C54 H52 N3 O4	
806.3983	-3.7	-4.6	26.0	309.0	11.5	C53 H55 O6 F	
806.3935	1.1	1.4	31.0	309.1	11.6	C57 H52 O2 F2	
806.3984	-3.8	-4.7	14.5	309.2	11.7	C36 H52 B N9 O8 F3	
806.3971	-2.5	-3.1	35.5	309.9	12.4	C55 H48 N7	
806.3974	-2.8	-3.5	31.5	310.3	12.8	C57 H51 N F3	
806.3911	3.5	4.3	35.5	310.4	12.9	C58 H49 N3 F	
806.3971	-2.5	-3.1	30.0	311.0	13.4	C56 H54 O5	
806.3924	2.2	2.7	35.0	311.4	13.9	C60 H51 O F	
806.3985	-3.9	-4.8	35.0	312.2	14.7	C57 H50 N4 O	
806.3913	3.3	4.1	39.0	313.6	16.0	C63 H50	



Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 150.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions

10190 formula(e) evaluated with 134 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 80-100 H: 0-150 B: 0-2 N: 5-15 O: 0-8 F: 3-5

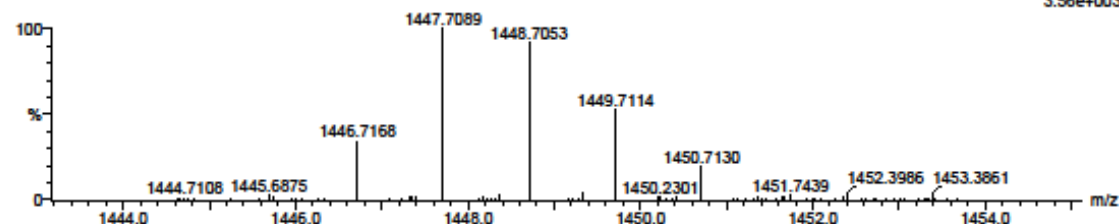
Karen WRIGHT

Infusion - dilution 100

AT38-(03) 1 (0.054) Cm (1:9)

28-Apr-2016

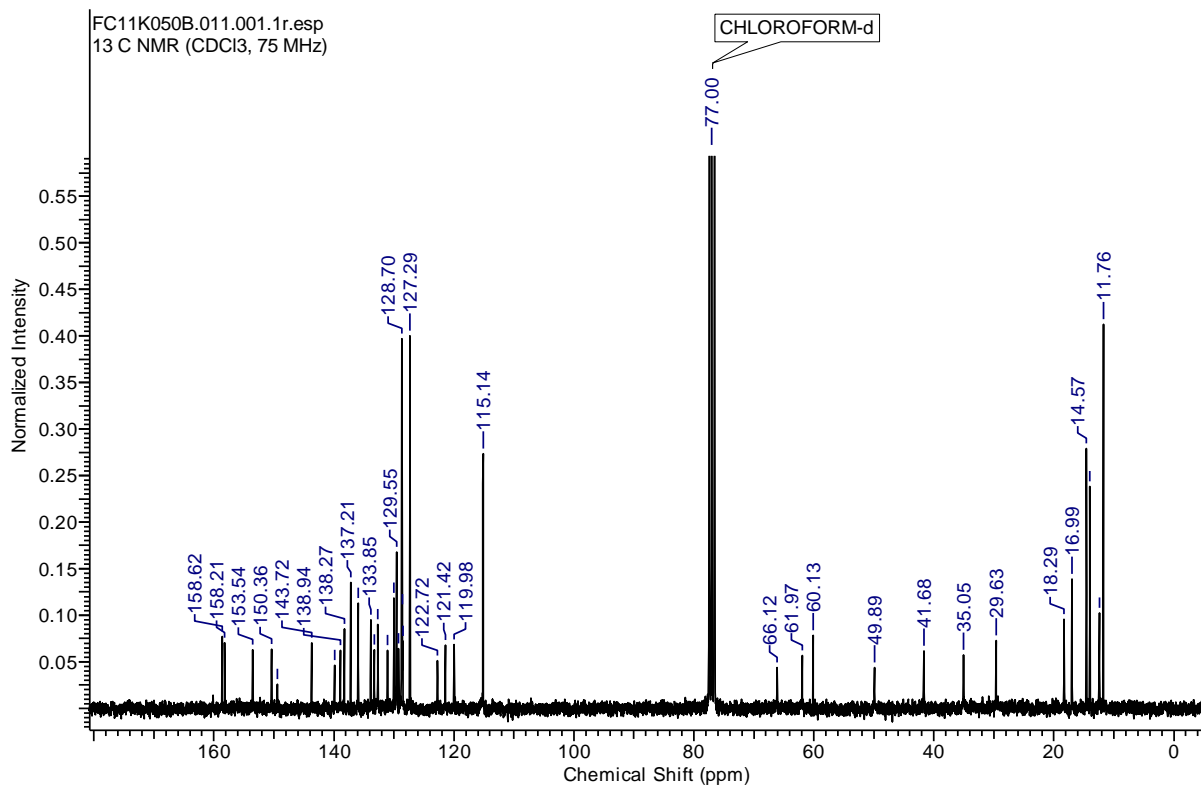
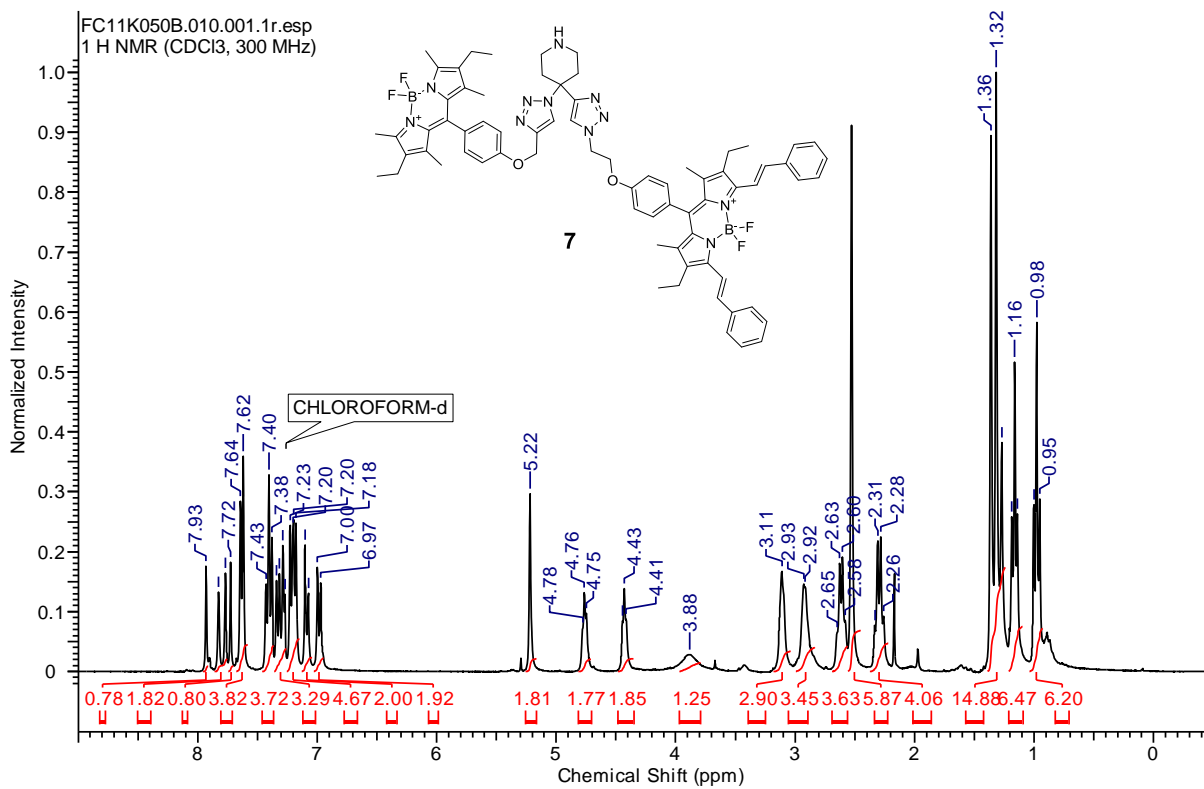
1: TOF MS ES+
3.56e+003



Minimum:

Maximum: 5.0 5.0 -1.5

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
1447.7051	3.8	2.6	49.5	114.0	27.0	C85 H85 B2 N14 O3	
1447.7067	2.2	1.5	44.5	100.4	13.3	P4 C85 H91 B N10 O8	
1447.7139	-5.0	-3.5	48.5	115.6	28.6	P3 C86 H88 B2 N12 O5	
1447.7090	-0.1	-0.1	44.5	114.2	27.2	P3 C86 H90 B2 N8 O6	
1447.7031	5.8	4.0	45.5	100.2	13.1	P5 C86 H89 B N10 O5	
1447.7051	3.8	2.6	44.0	114.0	27.0	P5 C86 H91 B2 N7 O8	
1447.7084	0.5	0.3	41.0	89.7	2.7	P4 C86 H94 N7 O8 P5	
1447.7133	-4.4	-3.0	45.0	91.2	4.2	C86 H92 N11 O7 P3	
1447.7118	-2.9	-2.0	50.0	101.3	14.2	C86 H86 B N15 O2	
1447.7080	0.9	0.6	49.5	100.3	13.3	P4 C86 H87 B N14 O4	
1447.7103	-1.4	-1.0	49.5	114.6	27.5	P3 C87 H86 B2 N12 O2	
1447.7147	-5.8	-4.0	50.0	92.2	5.2	P5 C87 H88 N15 O3 P3	
1447.7156	-6.7	-4.6	45.0	102.2	15.2	C87 H91 B N9 O5 P5	
1447.7059	3.0	2.1	45.5	89.6	2.6	C87 H91 N10 O6 P4	
1447.7118	-2.9	-2.0	44.5	101.4	14.3	C87 H92 B N8 O7 P4	
1447.7027	6.2	4.3	48.5	114.5	27.5	C87 H88 B2 N10 O6	
1447.7044	4.5	3.1	50.5	100.0	12.9	P3 C87 H85 B N14 O P5	
1447.7097	-0.8	-0.6	46.0	90.5	3.4	C87 H90 N11 O4 P5	
1447.7065	2.4	1.7	49.0	114.0	26.9	C87 H87 B2 N11 O4	
1447.7021	6.8	4.7	45.0	90.0	2.9	P4 C87 H92 N9 O8 P3	
1447.7152	-6.3	-4.4	48.0	115.9	28.9	C88 H90 B2 N9 O6	
1447.7034	5.5	3.8	50.0	90.2	3.2	P3 C88 H88 N13 O4 P3	
1447.7103	-1.4	-1.0	44.0	114.6	27.6	C88 H92 B2 N5 O7	
1447.7093	-0.4	-0.3	49.0	100.8	13.7	P5 C88 H89 B N11 O5	
1447.7040	4.9	3.4	53.5	114.2	27.2	P3 C88 H84 B2 N14 O2	
1447.7073	1.6	1.1	50.5	90.3	3.2	P3 C88 H87 N14 O2 P4	
1447.7132	-4.3	-3.0	49.5	101.7	14.7	C88 H88 B N12 O3	
1447.7111	-2.2	-1.5	51.0	91.3	4.3	P4 C88 H86 N15 P5	
1447.7044	4.5	3.1	45.0	100.0	13.0	C88 H91 B N7 O6 P5	
1447.7147	-5.8	-4.0	44.5	91.9	4.8	C88 H94 N8 O8 P3	
1447.7078	1.1	0.8	54.0	114.1	27.0	C88 H83 B2 N15 P4	
1447.7040	4.9	3.4	48.0	114.2	27.2	C89 H90 B2 N7 O7	
1447.7116	-2.7	-1.9	49.0	115.0	28.0	P3 C89 H88 B2 N9 O3	
						P5	



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 150.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 9

Monoisotopic Mass, Even Electron Ions

7228 formula(e) evaluated with 40 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 70-100 H: 0-150 B: 0-2 N: 5-15 O: 0-8 F: 3-5

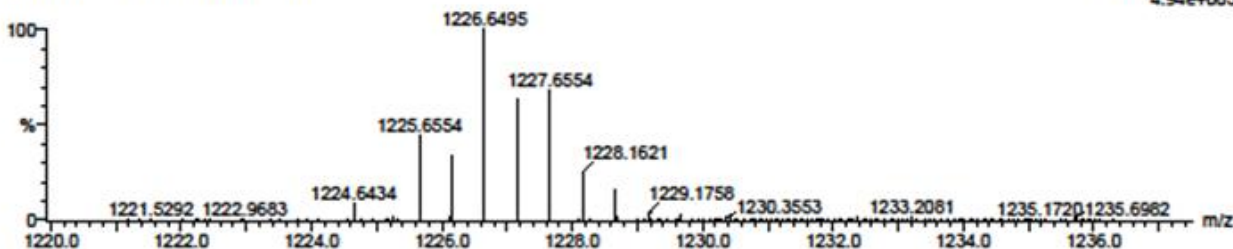
Karen WRIGHT

LCMS - dilution 100

AT41-(01) 732 (5.120) Cm (732:738)

11-May-2016

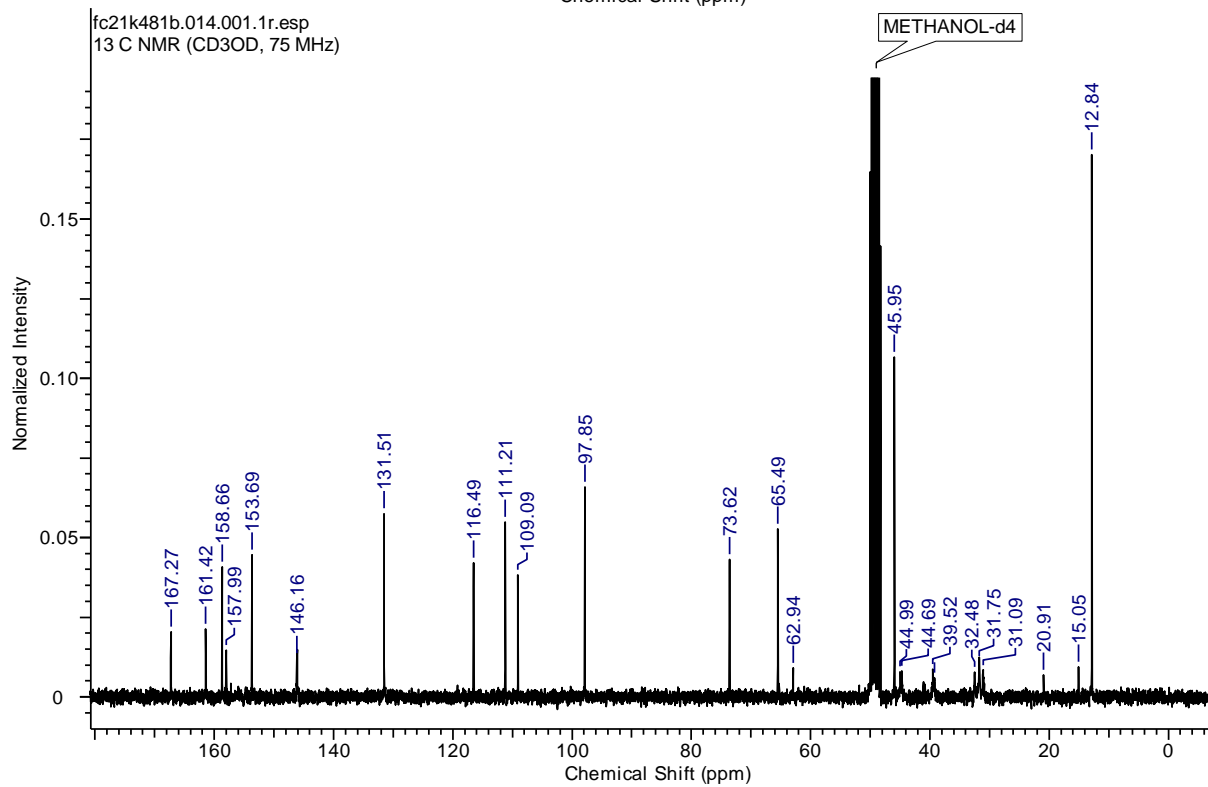
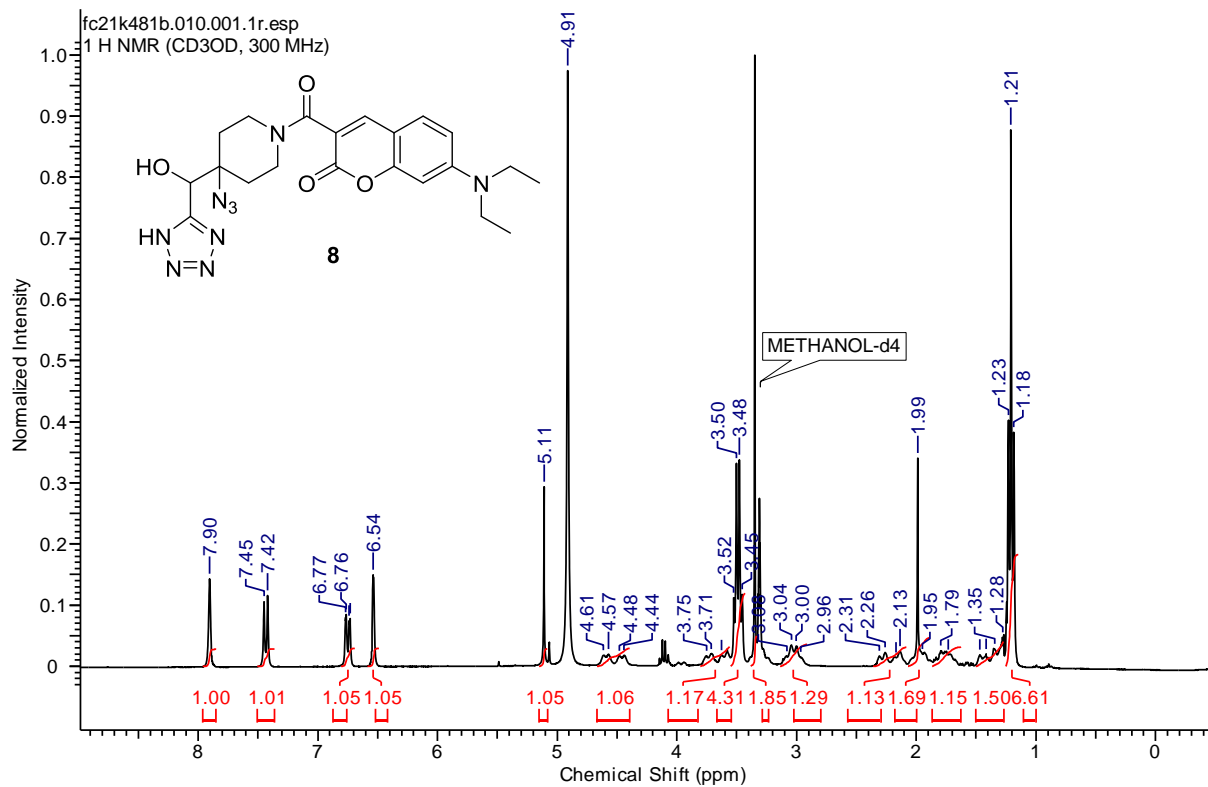
1: TOF MS ES+
4.94e+003



Minimum:

Maximum: 5.0 5.0 -1.5 150.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
1226.6495	1226.6443	5.2	4.2	35.5	490.3	3.3	C70 H80 N13 O3 F4
	1226.6502	-0.7	-0.6	34.5	490.1	3.1	C70 H81 B N11 O4 F4
	1226.6482	1.3	1.1	30.5	489.7	2.6	C71 H85 N7 O6 F5
	1226.6449	4.6	3.8	33.5	491.0	3.9	C71 H82 B2 N7 O6 F4
	1226.6540	-4.5	-3.7	29.5	490.3	3.2	C71 H86 B N5 O7 F5
	1226.6516	-2.1	-1.7	39.5	490.2	3.2	C71 H77 B N15 F4
	1226.6531	-3.6	-2.9	34.5	489.8	2.7	C71 H83 N11 O5 F3
	1226.6462	3.3	2.7	38.5	490.8	3.8	C72 H78 B2 N11 O2 F4
	1226.6544	-4.9	-4.0	39.5	490.0	2.9	C72 H79 N15 O F3
	1226.6495	0.0	0.0	35.5	489.7	2.7	C72 H81 N11 O2 F5
	1226.6536	-4.1	-3.3	32.5	490.9	3.8	C72 H85 B2 N5 O8 F3
	1226.6477	1.8	1.5	33.5	491.0	3.9	C72 H84 B N7 O7 F3
	1226.6554	-5.9	-4.8	34.5	490.5	3.4	C72 H82 B N9 O3 F5
	1226.6491	0.4	0.3	38.5	491.0	3.9	C73 H80 B N11 O3 F3
	1226.6550	-5.5	-4.5	37.5	491.2	4.1	C73 H81 B2 N9 O4 F3
	1226.6442	5.3	4.3	34.5	491.2	4.2	C73 H82 B N7 O4 F5
	1226.6500	-0.5	-0.4	33.5	490.4	3.4	C73 H83 B2 N5 O5 F5
	1226.6470	2.5	2.0	34.5	490.6	3.6	C74 H84 N7 O5 F4
	1226.6437	5.8	4.7	37.5	492.0	4.9	C74 H81 B2 N7 O5 F3
	1226.6514	-1.9	-1.5	38.5	490.5	3.4	C74 H79 B2 N9 O F5
	1226.6455	4.0	3.3	39.5	491.2	4.1	C74 H78 B N11 F5
	1226.6529	-3.4	-2.8	33.5	491.0	3.9	C74 H85 B N5 O6 F4
	1226.6483	1.2	1.0	39.5	490.6	3.5	C75 H80 N11 O F4
	1226.6451	4.4	3.6	42.5	491.8	4.7	C75 H77 B2 N11 O F3
	1226.6542	-4.7	-3.8	38.5	491.1	4.1	C75 H81 B N9 O2 F4
	1226.6489	0.6	0.5	37.5	491.2	4.2	C76 H82 B2 N5 O4 F4
	1226.6522	-2.7	-2.2	34.5	490.3	3.2	C76 H85 N5 O4 F5
	1226.6502	-0.7	-0.6	42.5	491.3	4.2	C77 H78 B2 N9 F4
	1226.6518	-2.3	-1.9	37.5	491.6	4.5	C77 H84 B N5 O5 F3
	1226.6459	3.6	2.9	38.5	491.6	4.5	C77 H83 N7 O4 F3
	1226.6535	-4.0	-3.3	39.5	490.5	3.5	C77 H81 N9 F5
	1226.6531	-3.6	-2.9	42.5	491.7	4.7	C78 H80 B N9 O F3
	1226.6482	1.3	1.1	38.5	491.6	4.5	C78 H82 B N5 O2 F5
	1226.6472	2.3	1.9	43.5	491.5	4.4	C78 H79 N11 F3
	1226.6478	1.7	1.4	41.5	492.0	4.9	C79 H81 B2 N5 O3 F3
	1226.6510	-1.5	-1.2	38.5	491.0	3.9	C79 H84 N5 O3 F4
	1226.6442	5.3	4.3	42.5	492.5	5.4	C80 H79 B2 N5 F5
	1226.6470	2.5	2.0	42.5	492.4	5.3	C81 H81 B N5 O F4
	1226.6499	-0.4	-0.3	42.5	491.8	4.7	C82 H83 N5 O2 F3



Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 150.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

526 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-100 H: 0-100 N: 0-10 O: 0-8

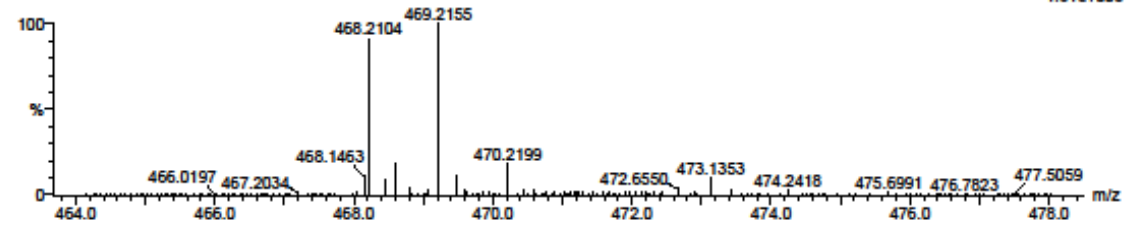
Karen WRIGHT

LCMS - dilution 100

K481B-(01)493 (3.447) Cm (489:494)

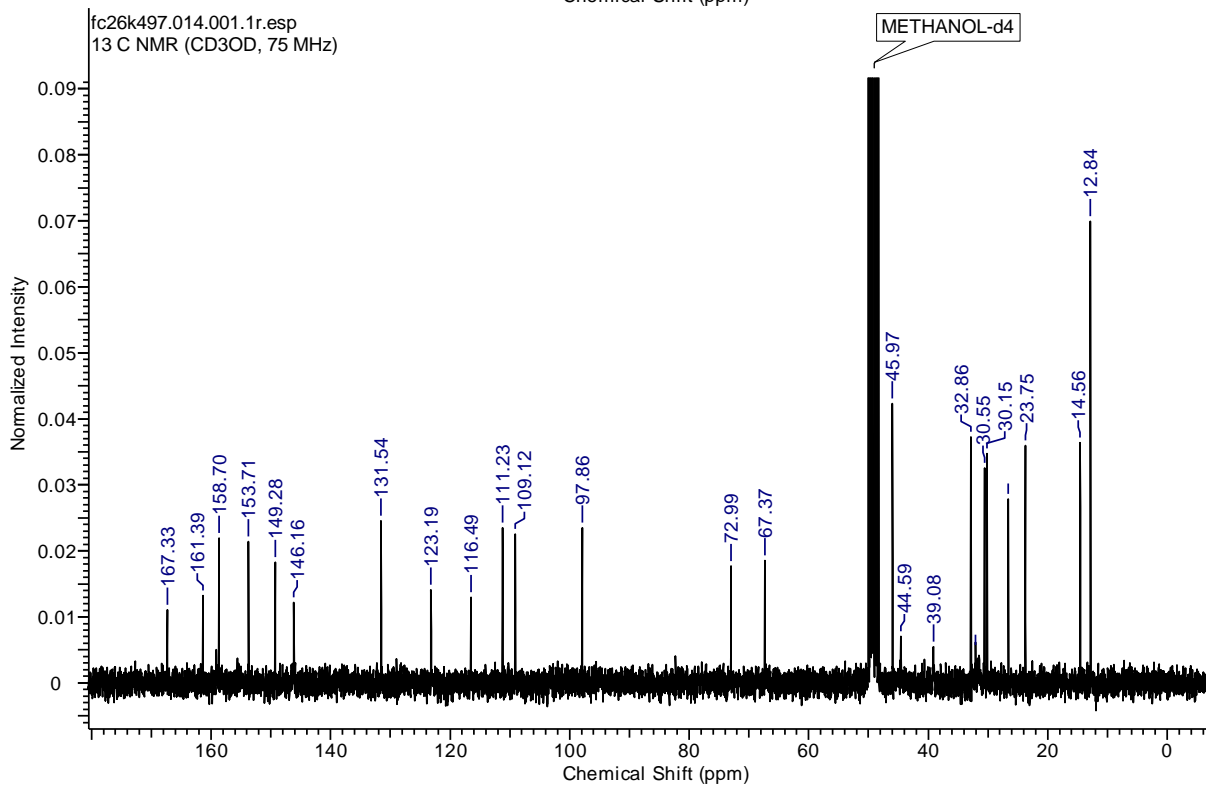
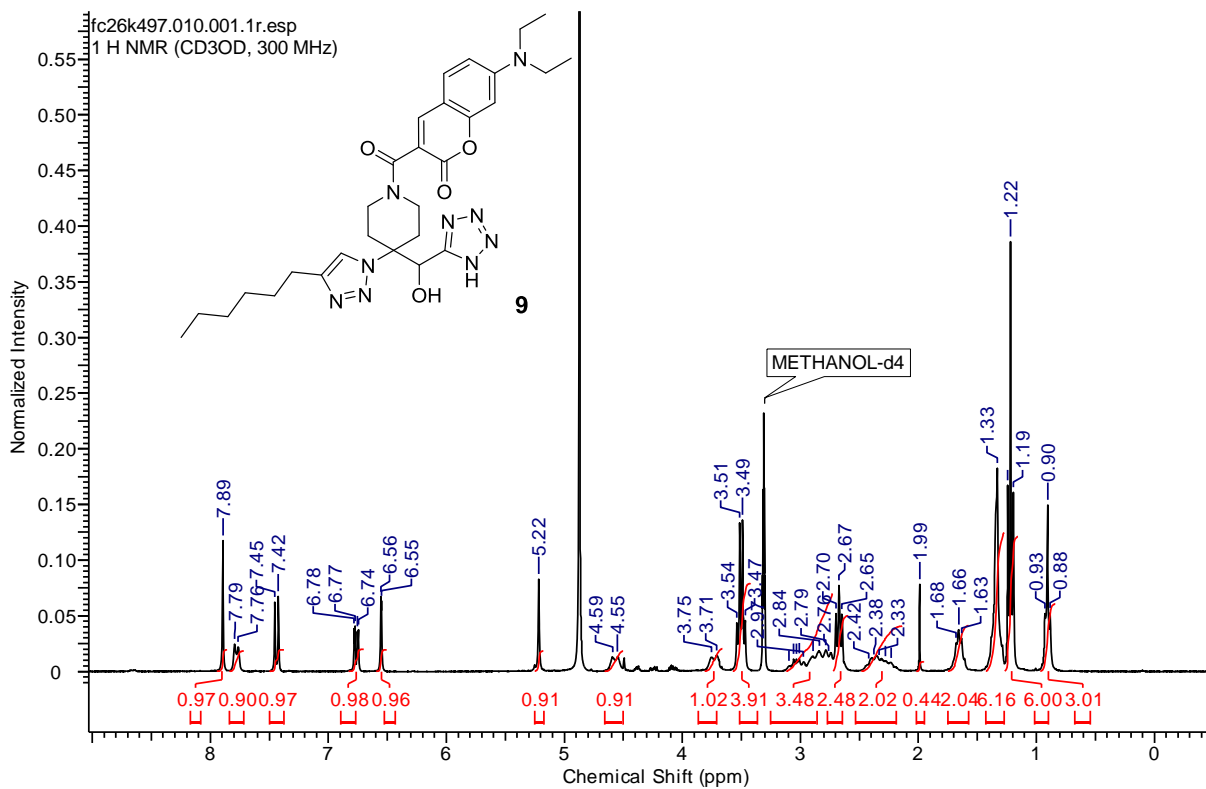
26-May-2016

1: TOF MS ES+
1.61e+005



Minimum: -1.5
Maximum: 5.0 5.0 150.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
468.2104	468.2108	-0.4	-0.9	13.5	410.2	0.6	C21 H26 N9 O4
	468.2094	1.0	2.1	8.5	410.3	0.8	C20 H30 N5 O8



Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 150.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

655 formula(e) evaluated with 3 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-100 H: 0-100 N: 0-10 O: 0-8

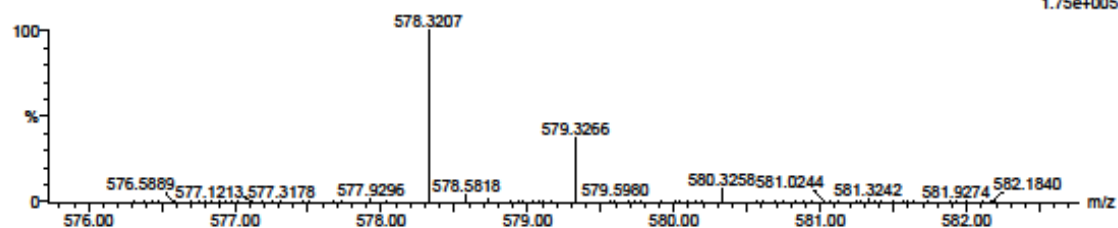
Karen WRIGHT

LCMS - dilution 100

K497-(01) 634 (4.432) Cm (631:635)

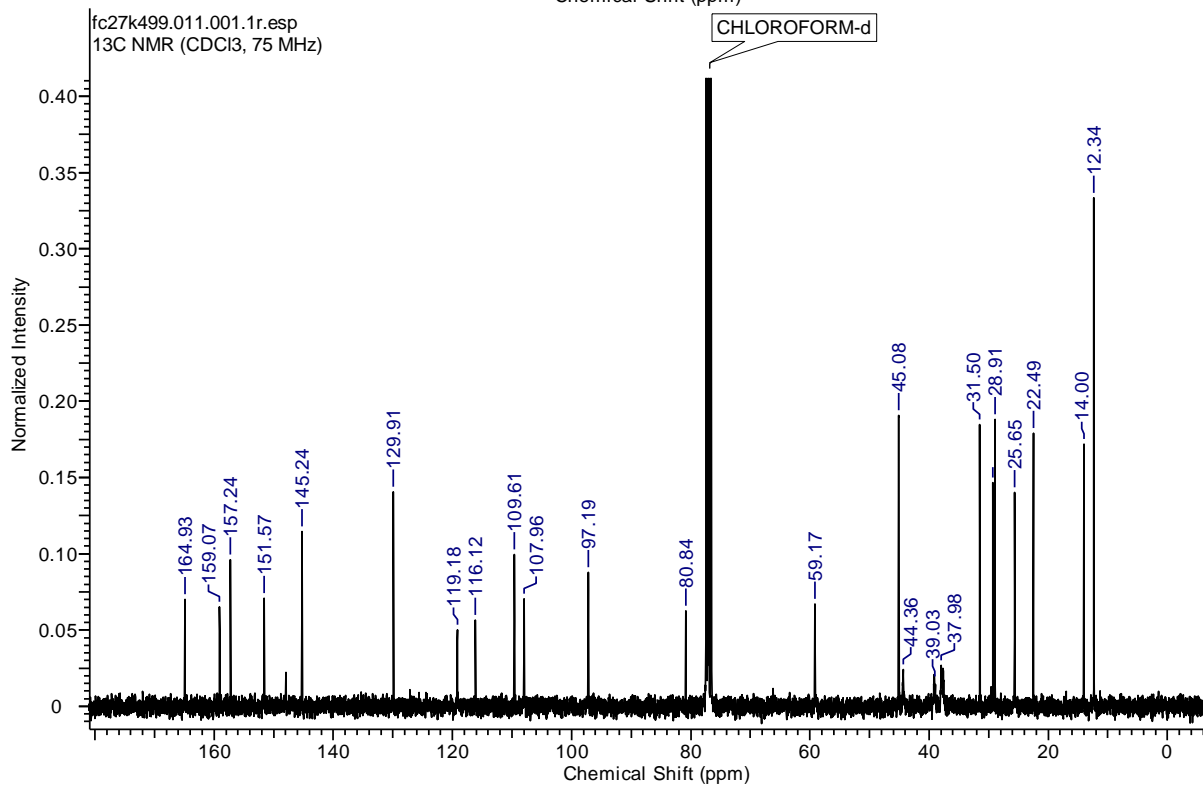
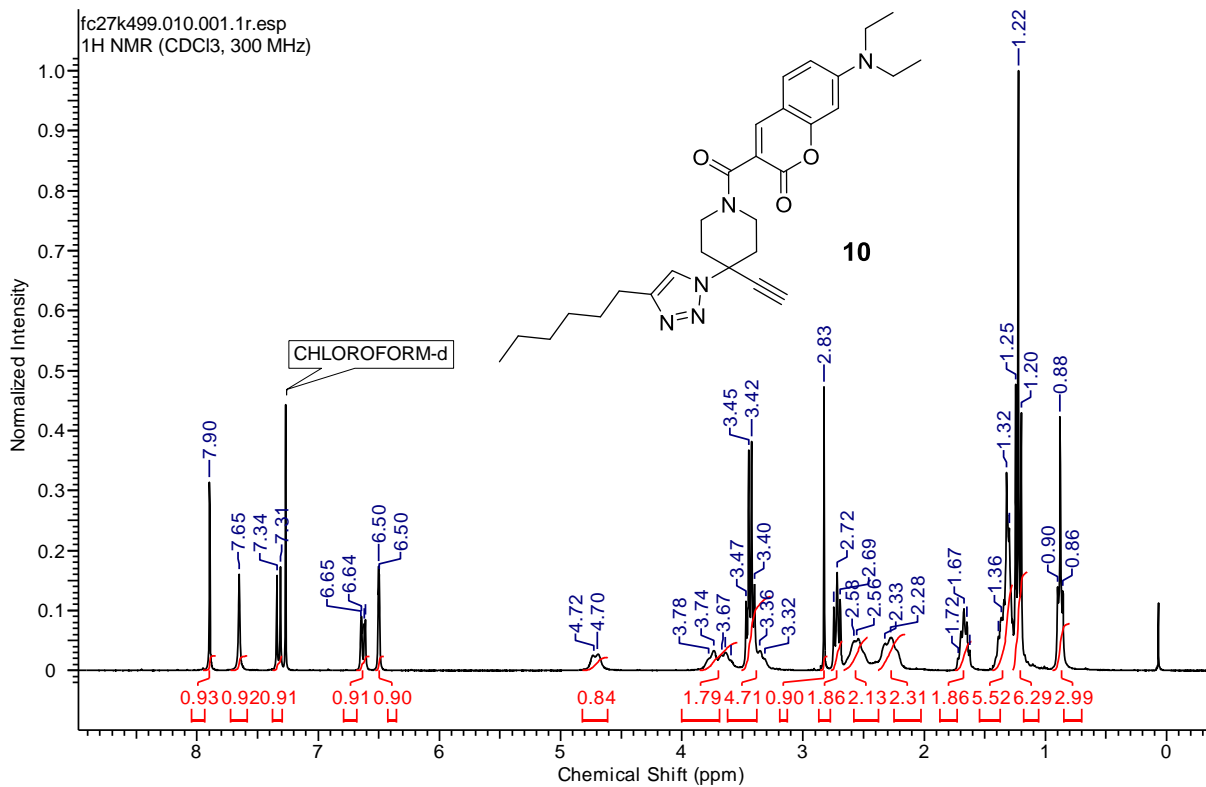
08-Jul-2016

1: TOF MS ES+
1.75e+005



Minimum: -1.5
Maximum: 5.0 5.0 150.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
578.3207	578.3203	0.4	0.7	14.5	313.7	0.0	C29 H40 N9 O4
	578.3190	1.7	2.9	9.5	318.7	5.0	C28 H44 N5 O8
	578.3230	-2.3	-4.0	13.5	317.9	4.2	C33 H44 N3 O6



Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 150.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

571 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-100 H: 0-100 N: 0-10 O: 0-8

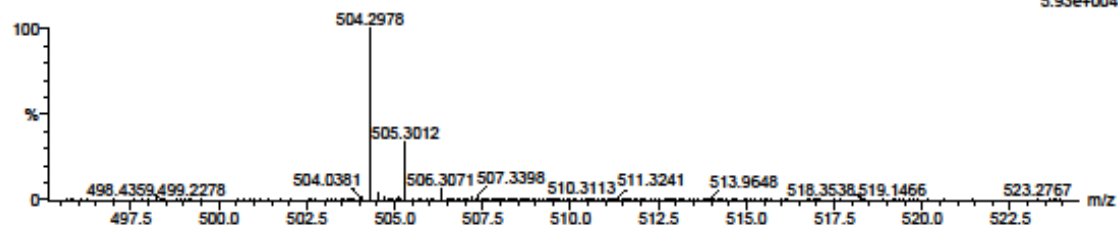
Karen WRIGHT

LCMS - dilution 100

K499-(01) 727 (5.087) Cm (727:729-706:710)

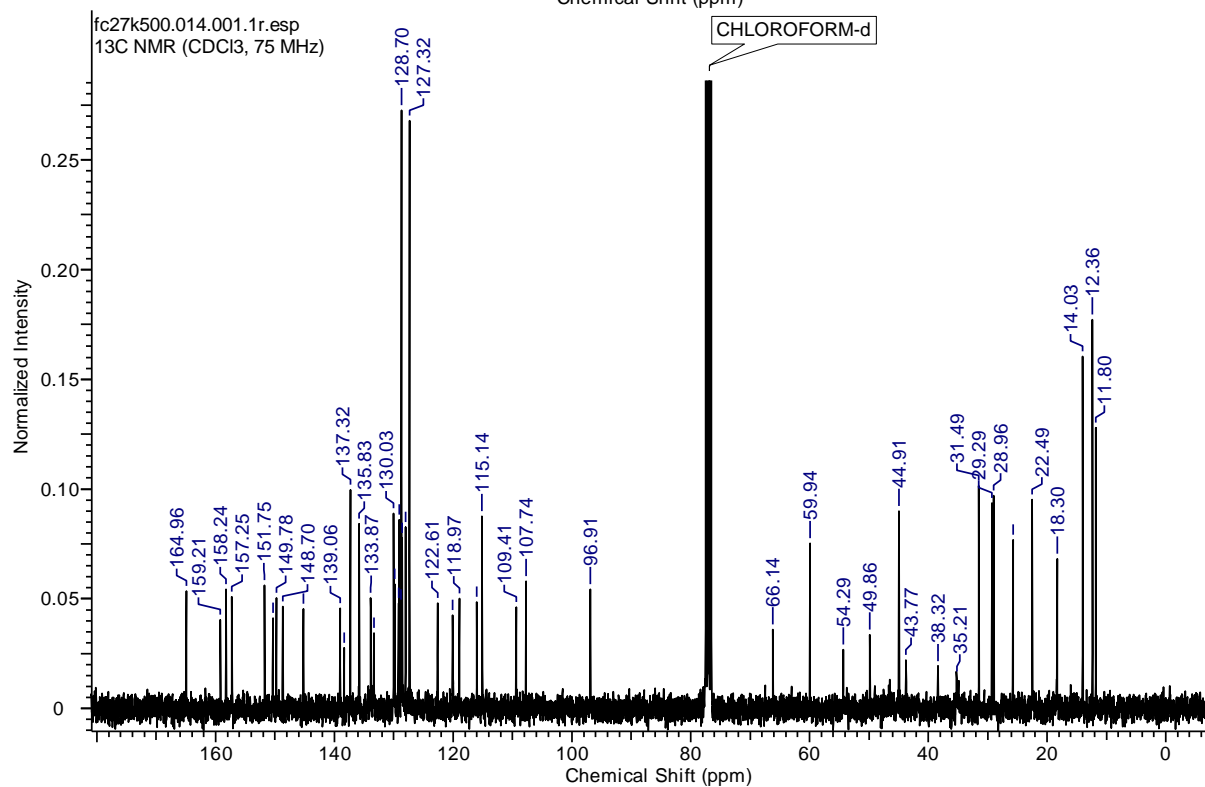
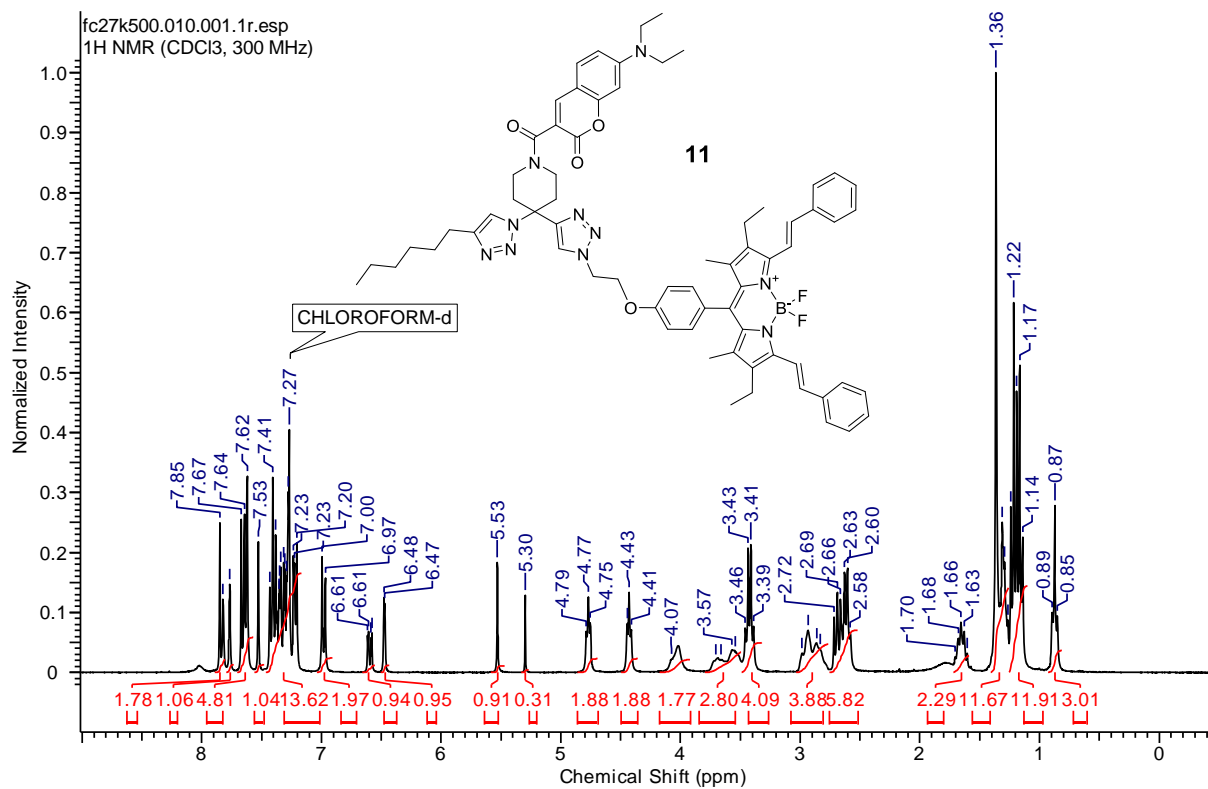
08-Jul-2016

1: TOF MS ES+
5.93e+004



Minimum: -1.5
Maximum: 5.0 5.0 150.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
504.2978	504.2975	0.3	0.6	13.5	215.8	0.2	C29 H38 N5 O3
	504.2961	1.7	3.4	8.5	217.3	1.7	C28 H42 N O7



Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 150.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 9

Monoisotopic Mass, Odd and Even Electron Ions

6798 formula(e) evaluated with 99 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-100 H: 0-100 B: 0-1 N: 0-10 O: 0-8 F: 0-3

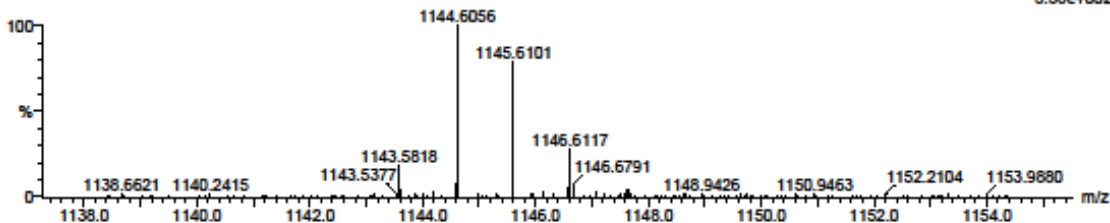
Karen WRIGHT

LCMS - dilution 100

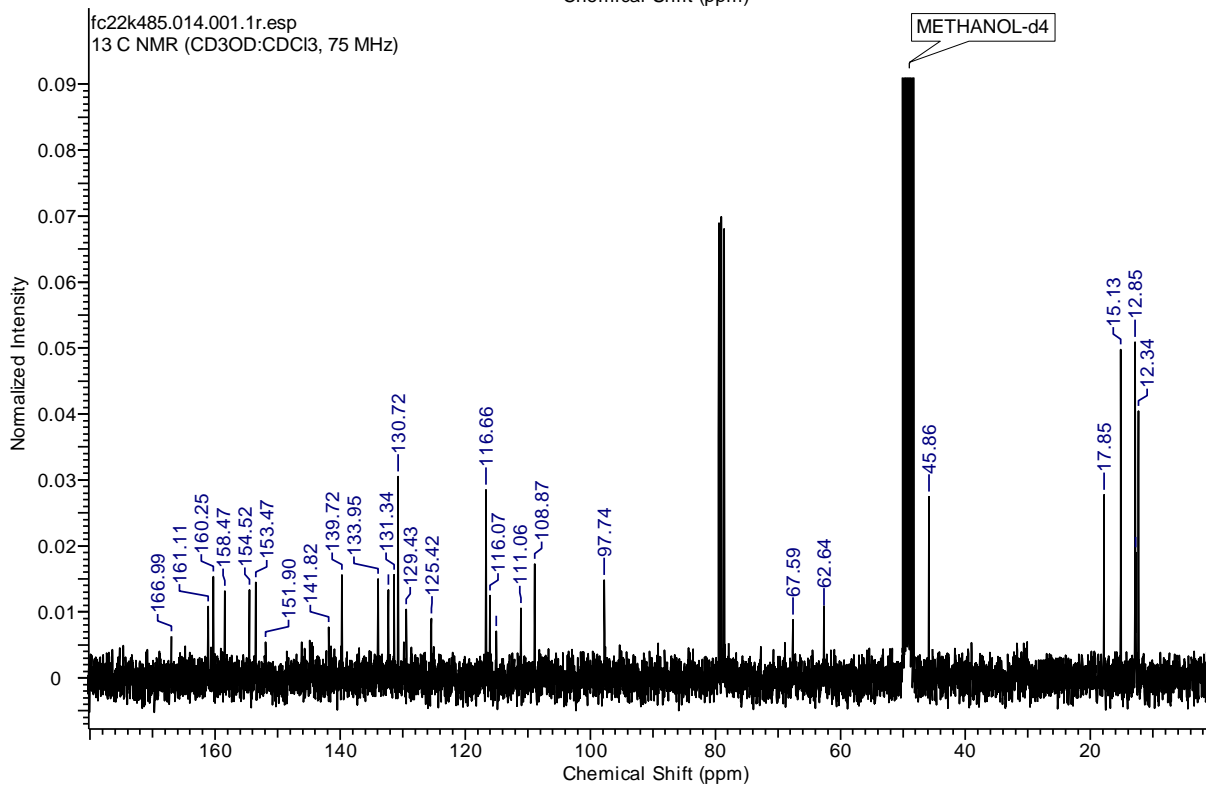
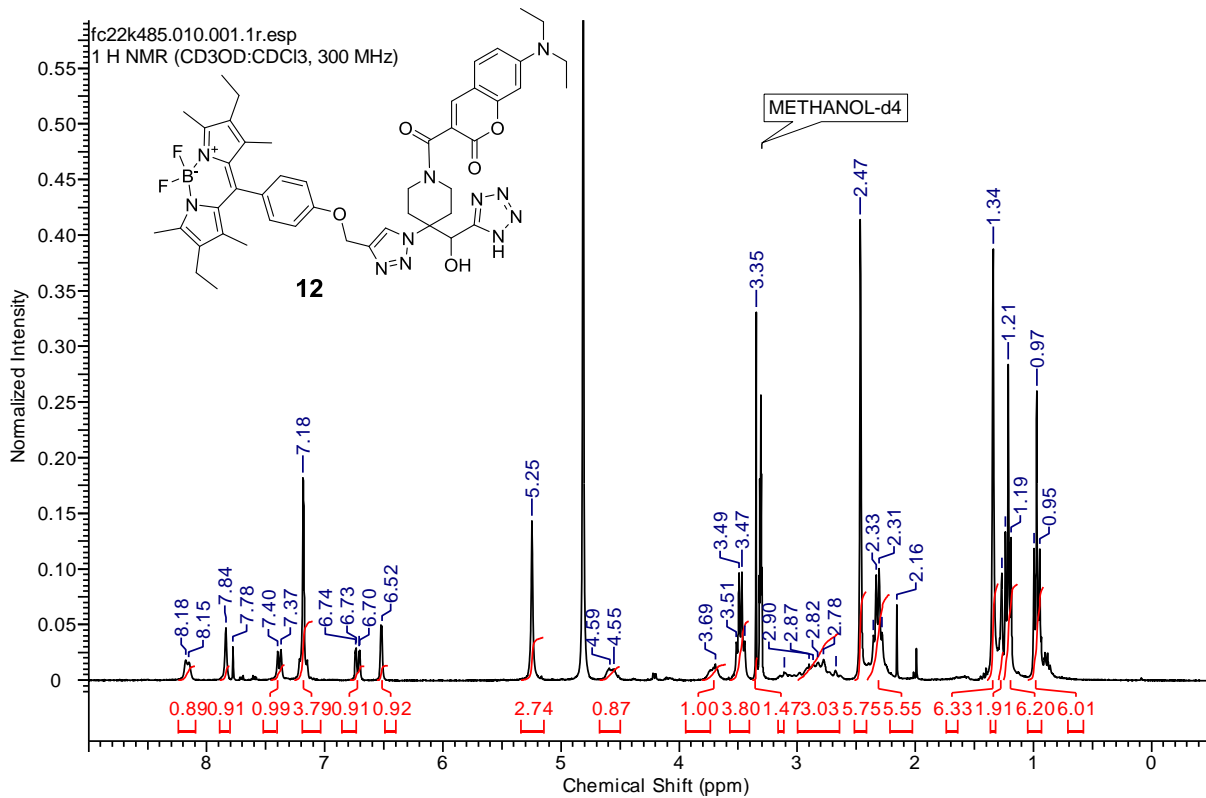
K500-(01) 917 (6.410) Cm (913:918-890:897)

08-Jul-2016

1: TOF MS ES+
3.36e+002



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
1144.6056	1144.6085	-2.9	-2.5	28.0	145.2	2.0	C63 H79 N10 O7 F3
	1144.6045	1.1	1.0	32.0	145.7	2.5	C65 H76 B N10 O5 F3
	1144.6074	-1.8	-1.6	32.0	145.9	2.7	C66 H78 N10 O6 F2
	1144.6019	3.7	3.2	27.5	146.2	3.0	C62 H78 B N9 O8 F3
	1144.6059	-0.3	-0.3	31.5	146.2	3.0	C67 H78 B N7 O6 F3
	1144.6099	-4.3	-3.8	27.5	146.4	3.2	C65 H81 N7 O8 F3
	1144.6036	2.0	1.7	31.5	146.5	3.3	C66 H79 N9 O8 F
	1144.6081	-2.5	-2.2	31.0	146.5	3.3	C64 H78 B N10 O8 F
	1144.6034	2.2	1.9	36.0	146.6	3.4	C68 H75 B N10 O4 F2
	1144.6062	-0.6	-0.5	36.0	146.8	3.6	C69 H77 N10 O5 F
	1144.6070	-1.4	-1.2	35.0	146.9	3.7	C67 H77 B N10 O7
	1144.6087	-3.1	-2.7	31.5	147.0	3.8	C68 H80 N7 O7 F2
	1144.6047	0.9	0.8	35.5	147.0	3.8	C70 H77 B N7 O5 F2
	1144.6072	-1.6	-1.4	31.0	147.0	3.8	C69 H80 B N4 O7 F3
	1144.6021	3.5	3.1	31.0	147.1	3.9	C67 H79 B N6 O8 F2
	1144.6007	4.9	4.3	31.5	147.2	4.0	C65 H77 B N9 O7 F2
	1144.6027	2.9	2.5	37.0	147.3	4.1	C70 H75 N10 O2 F3
	1144.6086	-3.0	-2.6	36.0	147.4	4.2	C70 H76 B N8 O3 F3
	1144.6040	1.6	1.4	36.5	147.5	4.3	C72 H77 N7 O3 F3
	1144.6061	-0.5	-0.4	35.0	147.6	4.4	C72 H79 B N4 O6 F2
	1144.6076	-2.0	-1.7	35.5	147.7	4.5	C71 H79 N7 O6 F
	1144.6022	3.4	3.0	40.0	147.8	4.6	C71 H74 B N10 O3 F
	1144.6027	2.9	2.5	31.5	147.8	4.6	C71 H81 N3 O7 F3
	1144.6013	4.3	3.8	32.0	147.8	4.7	C69 H79 N6 O6 F3
	1144.6074	-1.8	-1.6	40.0	147.9	4.7	C73 H75 B N8 O2 F2
	1144.6083	-2.7	-2.4	34.5	147.9	4.7	C69 H79 B N7 O8
	1144.6051	0.5	0.4	40.0	147.9	4.7	C72 H76 N10 O4
	1144.6053	0.3	0.3	36.0	147.9	4.7	C74 H79 N4 O4 F3
	1144.6024	3.2	2.8	35.5	147.9	4.7	C69 H78 N9 O7
	1144.6036	2.0	1.7	39.5	148.0	4.8	C73 H76 B N7 O4 F
	1144.6040	1.6	1.4	31.0	148.0	4.8	C73 H83 O8 F3
	1144.6000	5.6	4.9	32.5	148.0	4.8	C67 H77 N9 O5 F3
	1144.6038	1.8	1.6	35.0	148.1	4.9	C71 H80 N6 O8
	1144.6086	-3.0	-2.6	30.5	148.1	4.9	C71 H82 B N O8 F3
	1144.6067	-1.1	-1.0	41.0	148.1	4.9	C75 H75 N8 F3
	1144.6101	-4.5	-3.9	31.0	148.2	5.1	C70 H82 N4 O8 F2
	1144.6023	3.3	2.9	34.5	148.3	5.1	C72 H80 B N3 O8 F
	1144.6009	4.7	4.1	35.0	148.4	5.2	C70 H78 B N6 O7 F
	1144.6049	0.7	0.6	39.0	148.4	5.2	C75 H78 B N4 O5 F
	1144.6074	-1.8	-1.6	34.5	148.5	5.3	C74 H81 B N O7 F2
	1144.6064	-0.8	-0.7	39.5	148.5	5.3	C74 H78 N7 O5
	1144.6063	-0.7	-0.6	44.0	148.5	5.3	C76 H74 B N8 O F
	1144.6067	-1.1	-1.0	35.5	148.6	5.4	C76 H81 N O5 F3
	1144.6099	-4.3	-3.8	35.5	148.7	5.5	C72 H78 B N5 O4 F3
	1144.6089	-3.3	-2.9	35.0	148.7	5.5	C73 H81 N4 O7 F
	1144.6029	2.7	2.4	40.5	148.9	5.7	C75 H76 N7 O2 F2
	1144.6015	4.1	3.6	41.0	148.9	5.7	C73 H74 N10 O F2
	1144.6080	-2.4	-2.1	40.5	149.0	5.8	C77 H77 N5 O F3



Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 150.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 9

Monoisotopic Mass, Odd and Even Electron Ions

6727 formula(e) evaluated with 82 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-100 H: 0-100 B: 0-1 N: 5-15 O: 0-8 F: 0-3

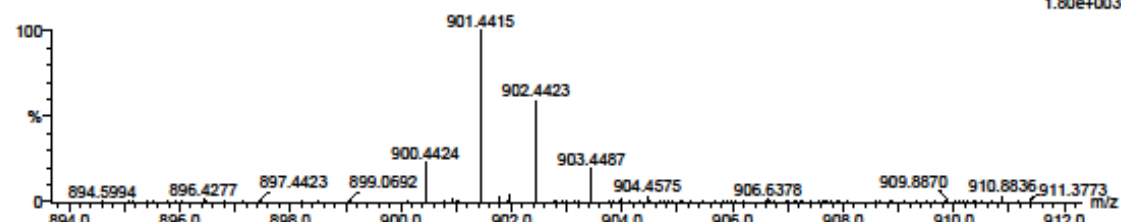
Karen WRIGHT

LCMS - dilution 100

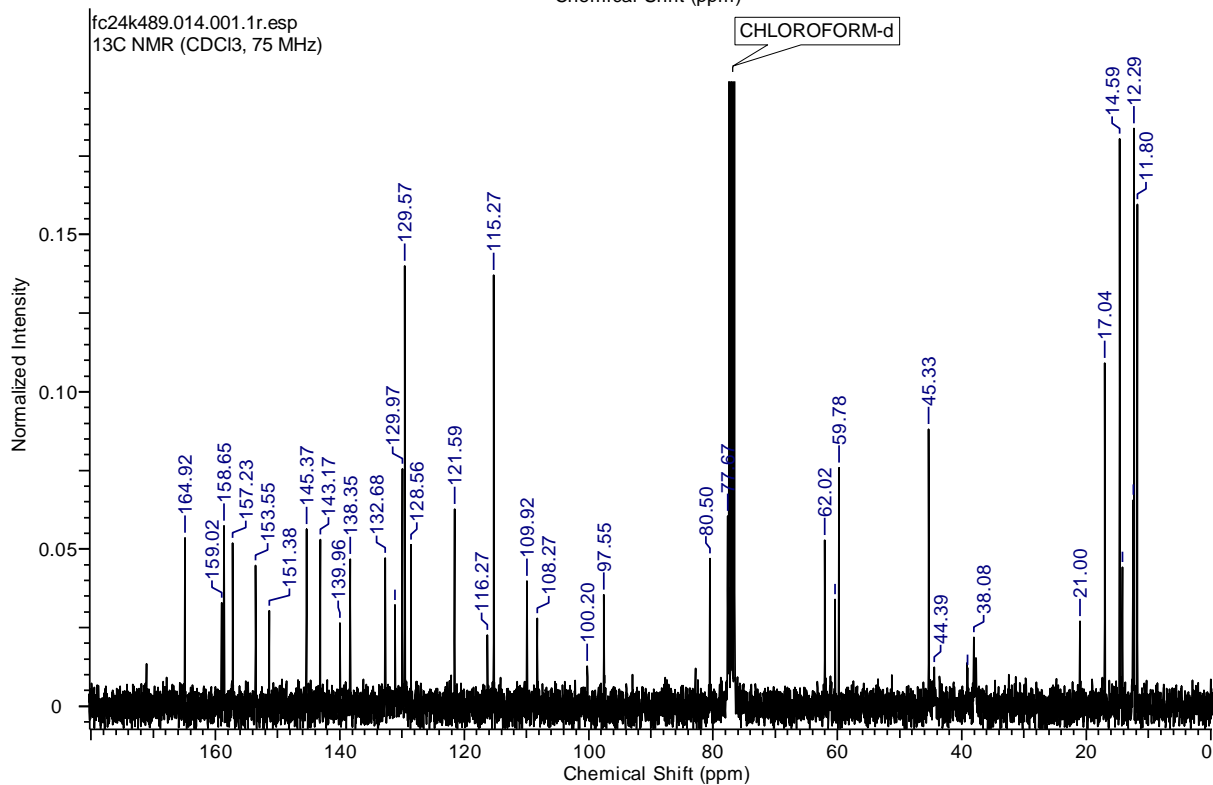
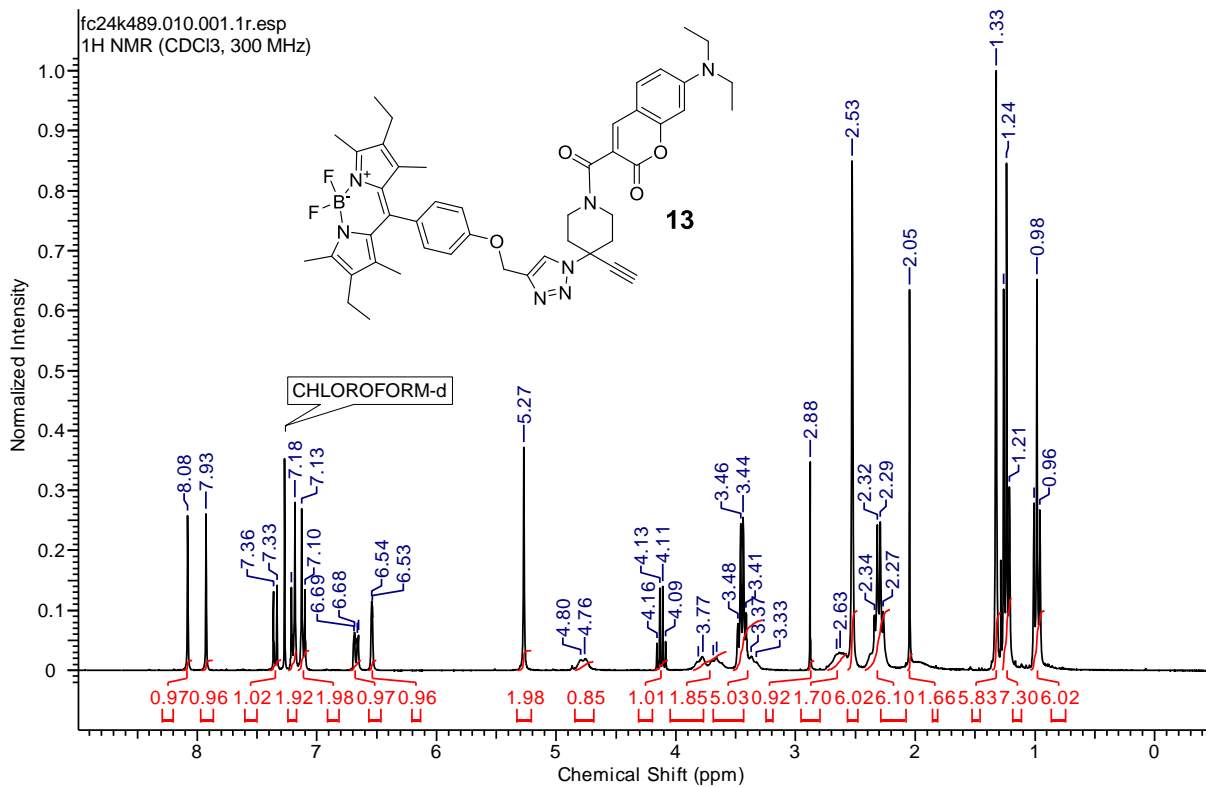
K485-(01) 729 (5.100) Cm (729:731)

02-Jun-2016

1: TOF MS ES+
1.80e+003



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901.4415	901.4454	-3.9	-4.3	18.0	227.5	15.4	C38 H55 B N15 O7
	901.4409	0.6	0.7	18.5	220.2	8.1	F3
	901.4404	1.1	1.2	21.5	222.6	10.5	C40 H56 N14 O7 F3
	901.4443	-2.8	-3.1	22.0	224.5	12.4	C41 H55 B N14 O8 F
	901.4422	-0.7	-0.8	18.0	218.8	6.7	C41 H54 B N15 O6
	901.4397	1.8	2.0	22.5	217.3	5.2	F2
	901.4456	-4.1	-4.5	21.5	224.3	12.2	C42 H58 N11 O8 F3
	901.4435	-2.0	-2.2	23.0	217.9	5.8	C43 H55 N14 O6 F2
	901.4431	-1.6	-1.8	26.0	221.0	8.9	C43 H56 B N12 O7
	901.4382	3.3	3.7	22.0	222.0	9.9	F2
	901.4393	2.2	2.4	25.5	220.2	8.1	C43 H54 N15 O4 F3
	901.4411	0.4	0.4	22.0	215.7	3.6	C44 H53 B N15 O5 F
	901.4449	-3.4	-3.8	22.5	217.3	5.2	C44 H55 B N11 O6
	901.4460	-4.5	-5.0	26.0	217.1	5.0	C44 H54 B N14 O7
	901.4395	2.0	2.2	27.0	220.4	8.3	C45 H57 N11 O7 F2
	901.4406	0.9	1.0	25.0	218.7	6.6	C45 H56 N12 O5 F3
	901.4386	2.9	3.2	26.5	215.3	3.2	C45 H55 N15 O6
	901.4424	-0.9	-1.0	27.0	214.6	2.5	C45 H51 B N15 O2
	901.4445	-3.0	-3.3	25.5	220.6	8.5	F3
	901.4395	2.0	2.2	21.5	220.0	7.9	C46 H56 B N11 O8
	901.4420	-0.5	-0.6	30.0	217.6	5.4	C46 H54 N14 O5 F
	901.4371	4.4	4.9	26.0	219.8	7.7	C46 H53 N15 O3 F2
	901.4409	0.6	0.7	26.5	218.6	6.5	C46 H55 B N12 O6 F
	901.4424	-0.9	-1.0	21.5	215.3	3.1	C46 H56 B N11 O8
	901.4384	3.1	3.4	31.0	217.8	5.7	C46 H54 N14 O5 F
	901.4437	-2.2	-2.4	26.5	214.8	2.7	C46 H53 N15 O3 F2
	901.4399	1.6	1.8	26.0	214.5	2.4	C46 H55 B N12 O6 F
	901.4458	-4.3	-4.8	25.0	220.6	8.5	C46 H57 B N9 O7 F
	901.4409	0.6	0.7	21.0	218.7	6.6	C46 H55 B N12 O6 F
	901.4422	-0.7	-0.8	26.0	217.6	5.5	C48 H59 B N5 O8 F3
	901.4374	4.1	4.5	30.5	216.0	3.9	C49 H55 B N9 O4 F3
	901.4412	0.3	0.3	31.0	214.0	1.9	C49 H53 N14 O4
	901.4384	3.1	3.4	25.5	217.7	5.6	C49 H52 N15 O2 F
	901.4433	-1.8	-2.0	29.5	217.5	5.3	C49 H56 B N8 O6 F2
	901.4413	0.2	0.2	25.5	215.2	3.0	C49 H54 B N12 O5
	901.4397	1.8	2.0	30.5	216.0	3.9	C50 H58 N8 O7 F
	901.4436	-2.1	-2.3	31.0	217.4	5.2	C50 H52 B N12 O2
	901.4451	-3.6	-4.0	26.0	216.2	4.1	F2
	901.4372	4.3	4.8	35.0	216.5	4.4	C50 H51 B N13 F3
	901.4426	-1.1	-1.2	30.5	215.3	3.2	C50 H57 N9 O5 F2
	901.4388	2.7	3.0	30.0	216.4	4.3	C51 H49 B N15 F
	901.4377	3.8	4.2	26.5	215.7	3.6	C51 H54 N12 O3 F
							C51 H55 N11 O5
							C51 H56 N8 O4 F3



Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 150.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions

2732 formula(e) evaluated with 29 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-100 H: 0-100 B: 0-1 N: 5-10 O: 0-8 F: 0-2

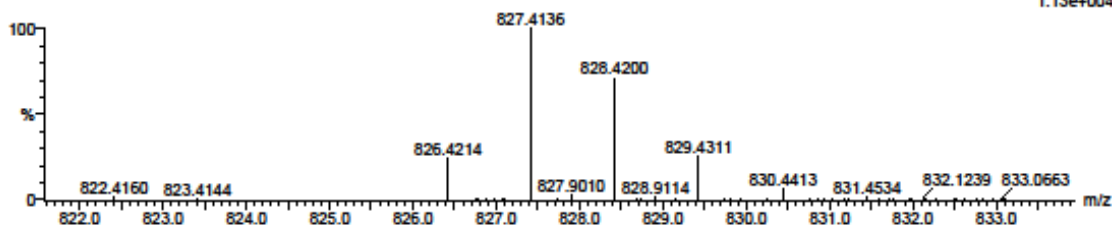
Karen WRIGHT

LCMS - dilution 100

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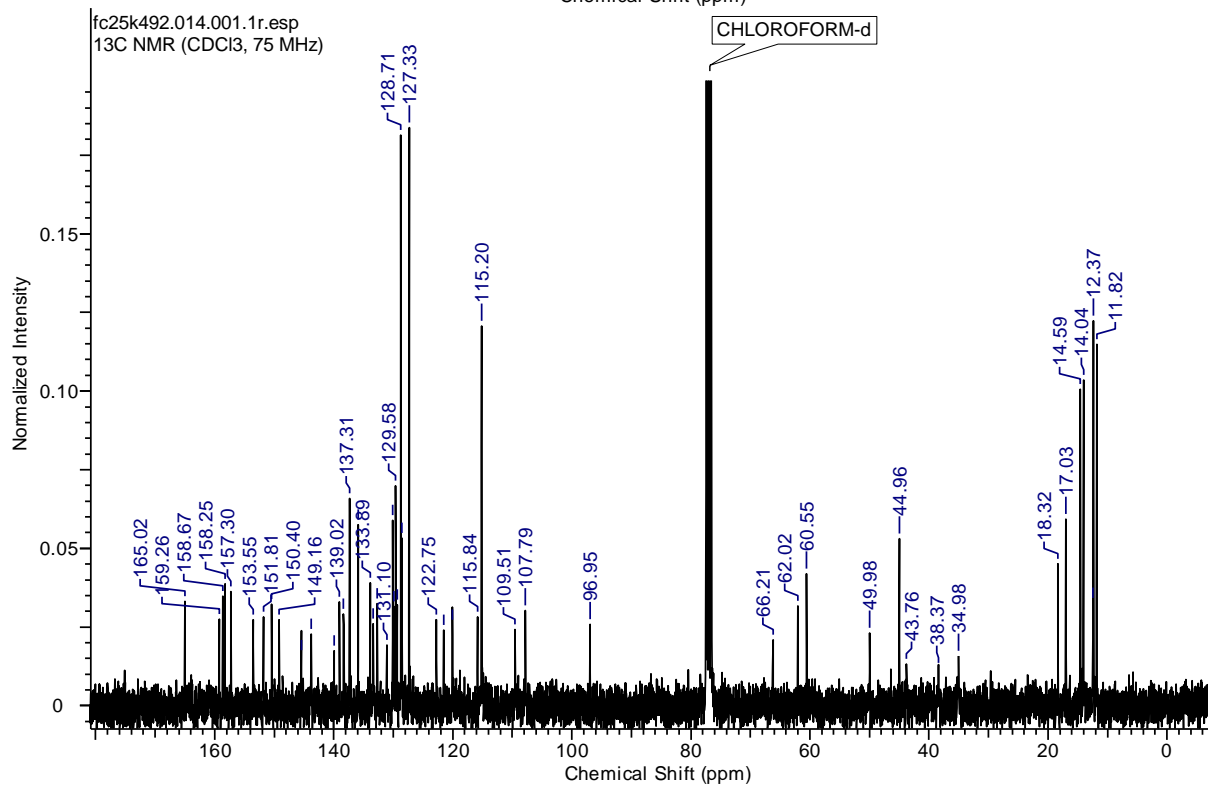
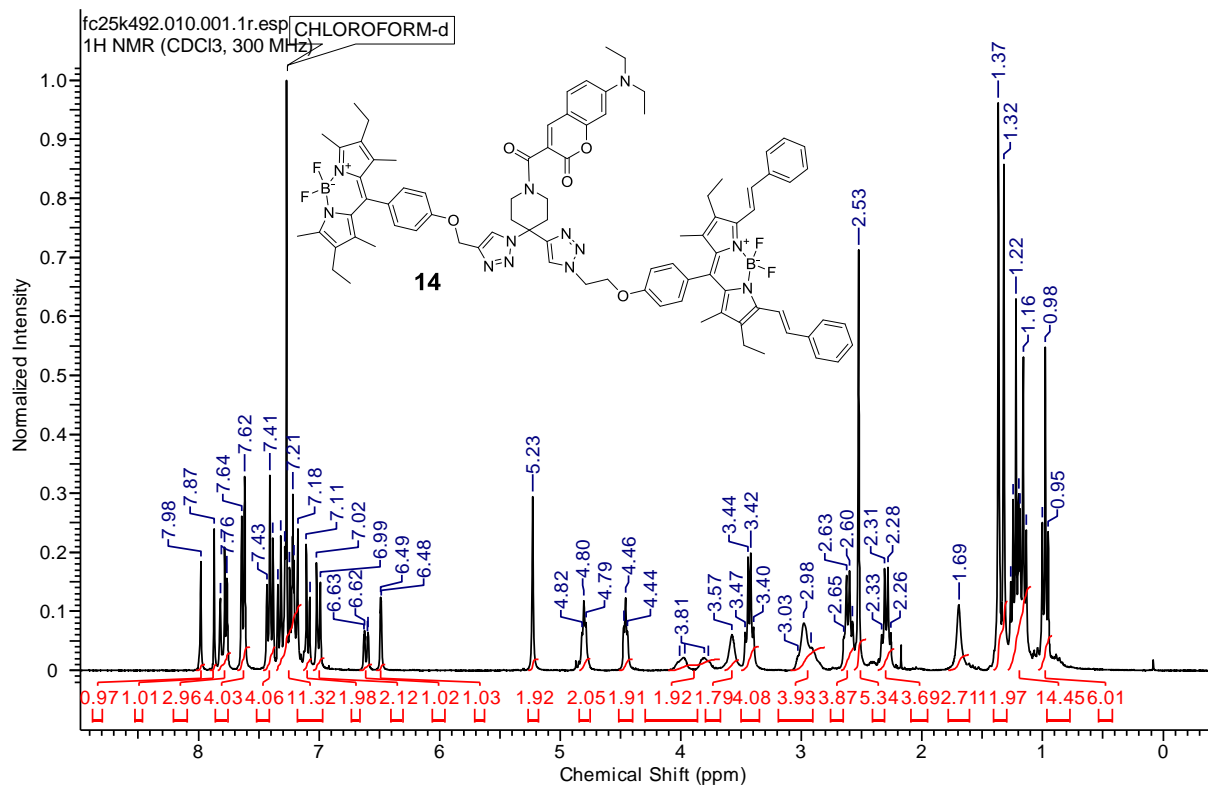
27-Jun-2016

1: TOF MS ES+
1.13e+004



Minimum: -1.5
Maximum: 5.0 5.0 150.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
827.4136	827.4112	2.4	2.9	34.0	77.7	0.9	C55 H50 N7 F
	827.4159	-2.3	-2.8	29.0	78.8	2.0	C51 H53 N7 O4
	827.4123	1.3	1.6	30.0	79.0	2.2	C52 H51 N7 O F2
	827.4146	-1.0	-1.2	29.5	79.5	2.7	C49 H51 N10 O3
	827.4110	2.6	3.1	30.5	79.8	3.0	C50 H49 N10 F2
	827.4170	-3.4	-4.1	25.0	79.9	3.1	C48 H54 N7 O5 F
	827.4132	0.4	0.5	24.5	80.0	3.2	C48 H55 N6 O7
	827.4157	-2.1	-2.5	25.5	80.4	3.6	C46 H52 N10 O4 F
	827.4096	4.0	4.8	25.5	80.4	3.6	C49 H53 N6 O4 F2
	827.4119	1.7	2.1	25.0	80.7	3.9	C46 H53 N9 O6
	827.4144	-0.8	-1.0	20.5	80.8	4.0	C45 H56 N6 O8 F
	827.4168	-3.2	-3.9	21.5	81.2	4.4	C43 H53 N10 O5 F2
	827.4130	0.6	0.7	21.0	81.4	4.6	C43 H54 N9 O7 F
	827.4142	-0.6	-0.7	17.0	81.9	5.1	C40 H55 N9 O8 F2
	827.4159	-2.3	-2.8	37.0	87.1	10.3	C58 H50 B N5
	827.4157	-2.1	-2.5	33.5	88.3	11.5	C53 H49 B N8 F
	827.4171	-3.5	-4.2	33.0	88.3	11.5	C55 H51 B N5 O F
	827.4119	1.7	2.1	33.0	88.6	11.8	C53 H50 B N7 O2
	827.4130	0.6	0.7	29.0	89.0	12.2	C50 H51 B N7 O3 F
	827.4169	-3.3	-4.0	29.5	89.2	12.4	C50 H50 B N8 O F2
	827.4106	3.0	3.6	33.5	89.3	12.5	C51 H48 B N10 O
	827.4142	-0.6	-0.7	25.0	89.4	12.6	C47 H52 B N7 O4 F2
	827.4117	1.9	2.3	29.5	89.6	12.8	C48 H49 B N10 O2 F
	827.4128	0.8	1.0	25.5	89.8	13.0	C45 H50 B N10 O3 F2
	827.4164	-2.8	-3.4	24.5	90.0	13.2	C44 H52 B N10 O6
	827.4104	3.2	3.9	24.5	90.3	13.5	C47 H53 B N6 O6 F
	827.4115	2.1	2.5	20.5	90.4	13.6	C44 H54 B N6 O7 F2
	827.4176	-4.0	-4.8	20.5	90.7	13.9	C41 H53 B N10 O7 F
	827.4102	3.4	4.1	21.0	91.1	14.3	C42 H52 B N9 O6 F2



Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 150.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 9

Monoisotopic Mass, Odd and Even Electron Ions

12508 formula(e) evaluated with 263 results within limits (all results (up to 1000) for each mass)

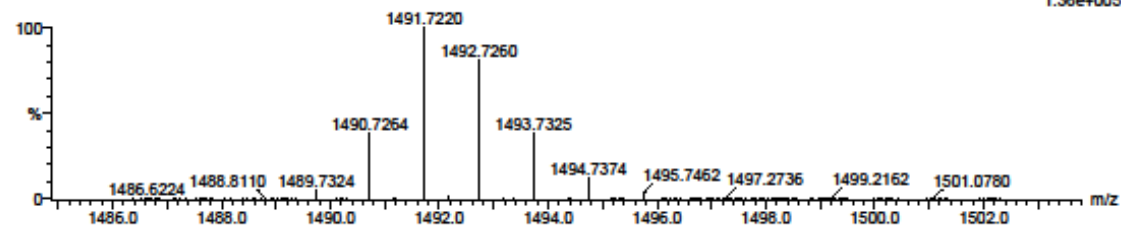
Elements Used:

C: 70-100 H: 0-100 B: 0-2 N: 5-15 O: 0-8 F: 3-5 Na: 0-1

Karen WRIGHT
 Infusion - dilution 100
 AT42-(03) 20 (0.762) Cm (20:38)

30-May-2016

1: TOF MS ES+
 1.36e+005



Minimum: -1.5
 Maximum: 5.0 5.0 150.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
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	1491.7215	0.5	0.3	39.0	659.1	2.6	F5 Na C79 H92 B N15 O7
	1491.7274	-5.4	-3.6	38.0	659.1	2.6	F5 Na C79 H93 B2 N13 O8
	1491.7263	-4.3	-2.9	42.0	659.5	3.0	C82 H92 B2 N13 O7
	1491.7189	3.1	2.1	42.5	659.5	3.0	F4 Na C83 H91 B2 N12 O6
	1491.7199	2.1	1.4	46.0	659.5	3.0	F5 Na C83 H88 B2 N15 O5
	1491.7211	0.9	0.6	42.0	659.6	3.1	F5 C80 H91 B2 N15 O8
	1491.7215	0.5	0.3	47.0	659.8	3.3	F3 Na C86 H89 B2 N13 O3
	1491.7172	4.8	3.2	41.5	659.8	3.3	F5 Na C80 H90 B2 N14 O8
	1491.7148	7.2	4.8	38.5	659.9	3.4	F5 C78 H91 B2 N14 O8
	1491.7164	5.6	3.8	47.0	659.9	3.5	F5 Na C84 H88 B2 N15 O4
	1491.7289	-6.9	-4.6	46.5	660.0	3.5	F4 Na C85 H90 B2 N14 O4
	1491.7229	-0.9	-0.6	38.5	660.4	3.9	F4 Na C81 H94 B N12 O8
	1491.7235	-1.5	-1.0	45.0	660.4	3.9	F5 Na C82 H90 B2 N15 O8
	1491.7202	1.8	1.2	42.0	660.4	3.9	F3 C85 H93 B2 N9 O7
	1491.7213	0.7	0.5	45.5	660.5	4.0	F5 Na C85 H90 B2 N12 O6
	1491.7276	-5.6	-3.8	41.5	660.5	4.0	F5 C84 H94 B2 N10 O8
	1491.7242	-2.2	-1.5	51.5	660.6	4.1	F4 Na C89 H87 B2 N14 F5
	1491.7251	-3.1	-2.1	46.0	660.7	4.2	Na C85 H91 B2 N13 O6
	1491.7239	-1.9	-1.3	42.0	660.7	4.2	F3 Na C81 H91 B N15 O7
	1491.7287	-6.7	-4.5	45.0	660.7	4.2	F5 C84 H91 B2 N13 O7
	1491.7150	7.0	4.7	42.0	660.7	4.2	F4 C83 H92 B2 N11 O8
	1491.7161	5.9	4.0	45.5	660.8	4.3	F4 Na C83 H89 B2 N14 O7
	1491.7177	4.3	2.9	46.5	660.9	4.4	F4 C86 H90 B2 N12 O5
	1491.7229	-0.9	-0.6	46.5	661.0	4.5	F4 Na C88 H91 B2 N10 O4

Computational studies

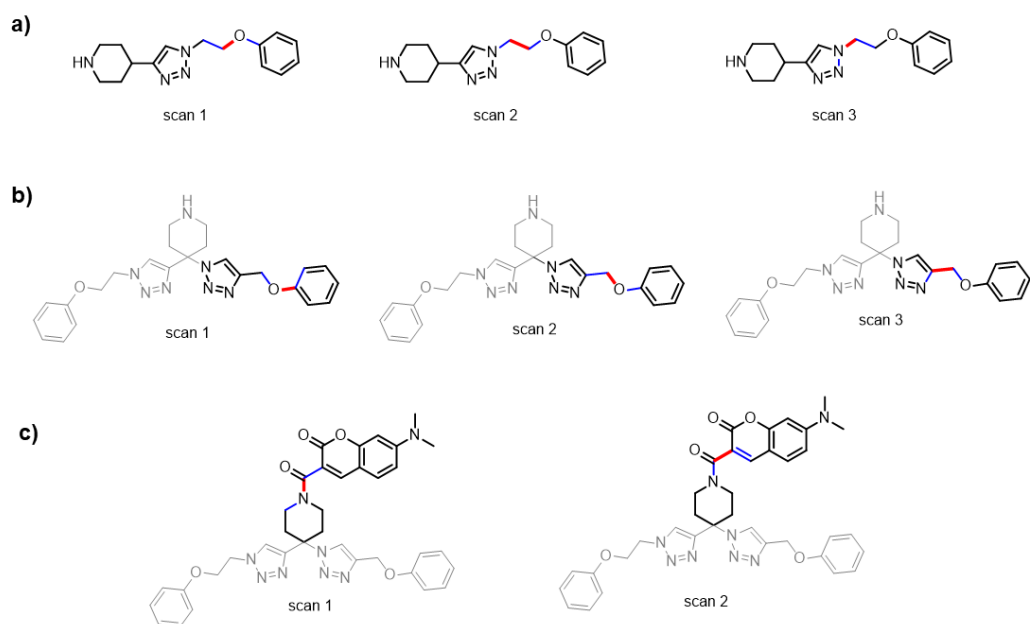


Figure S1. Structures of the three fragments studied with their relevant degrees of freedom: a) phenyl-triazole (1st fragment), b) di(phenyl-triazole) (2nd fragment) and c) di(phenyl-triazole)-coumarin (3rd fragment).

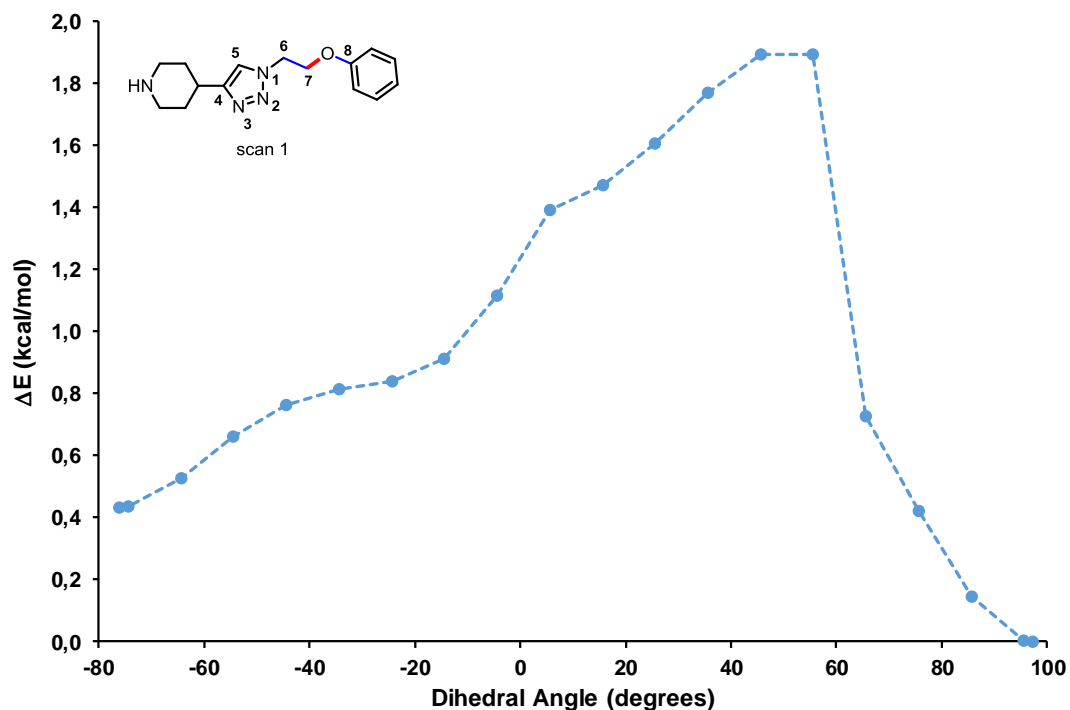


Figure S2. Calculated relative energies in (kcal/mol) as a function of the dihedral angle defined by the C(8), O, C(7) and C(6) atoms in the phenyl-triazole fragment.

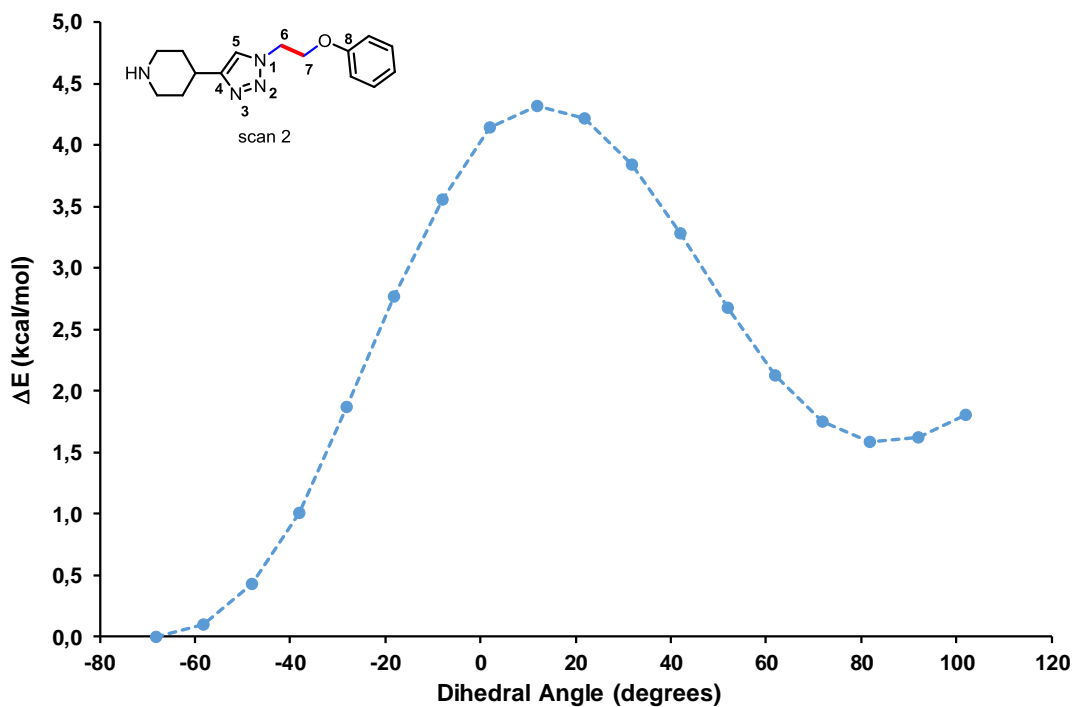


Figure S3. Calculated relative energies in (kcal/mol) as a function of the dihedral angle defined by the O, C(7), C(6) and N(1) atoms in the phenyl-triazole fragment.

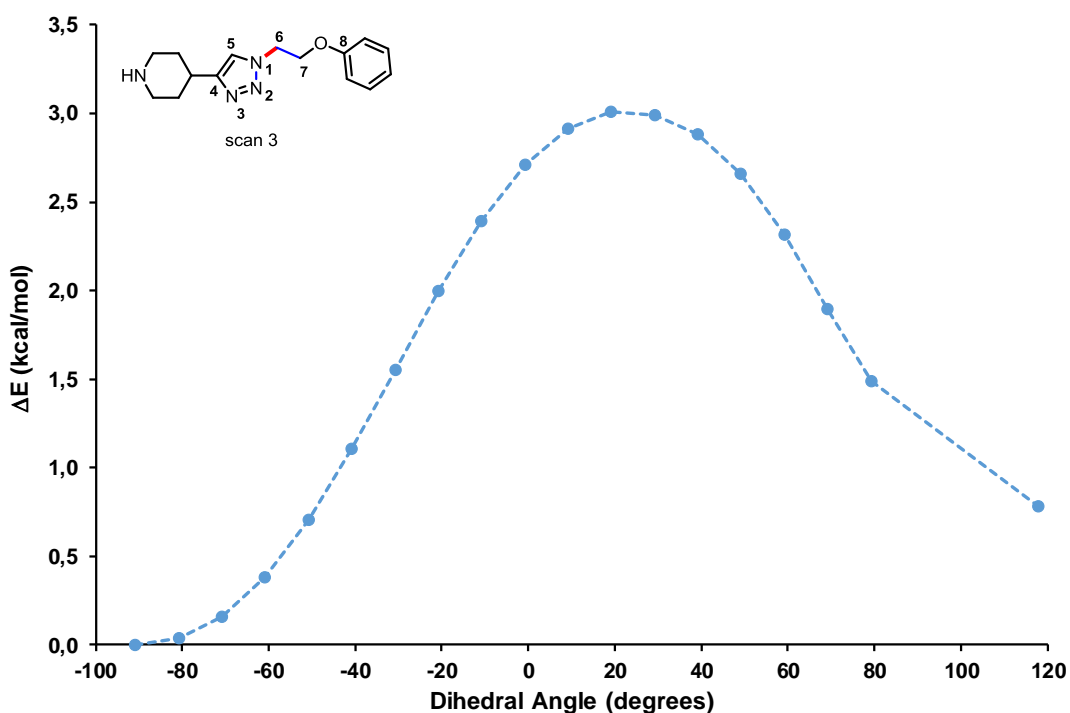


Figure S4. Calculated relative energies in (kcal/mol) as a function of the dihedral angle defined by the C(7), C(6), N(1) and N(2) atoms in the phenyl-triazole fragment.

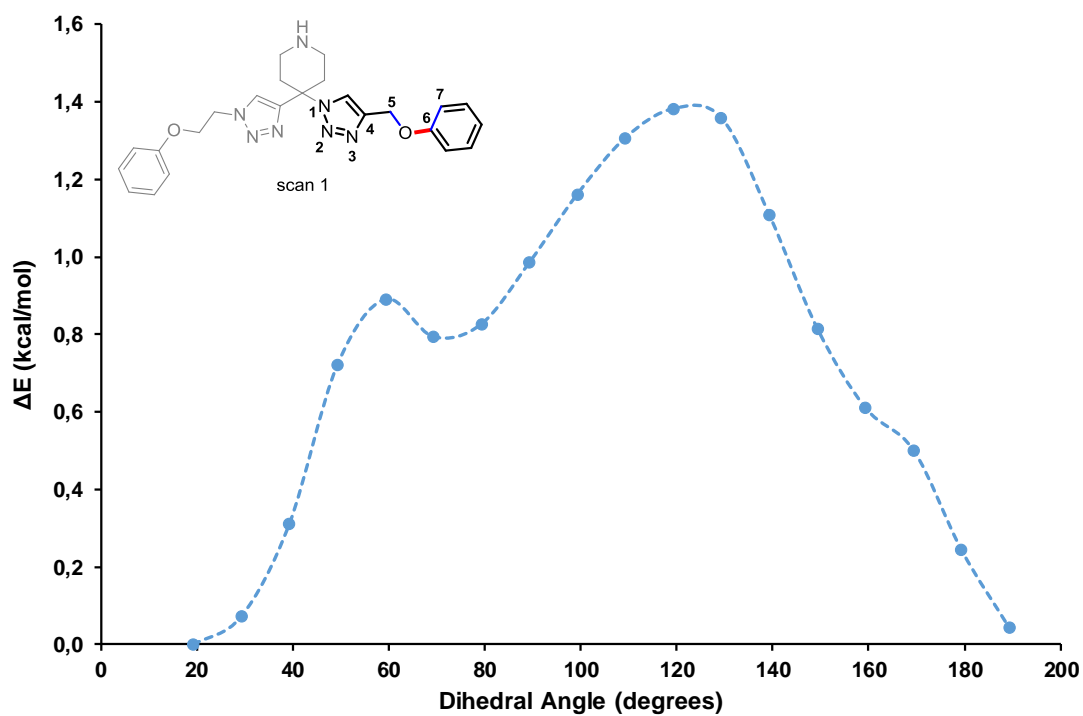


Figure S5. Calculated relative energies in (kcal/mol) as a function of the dihedral angle defined by the C(7), C(6), O, C(5) atoms in the di(phenyl-triazole) fragment.

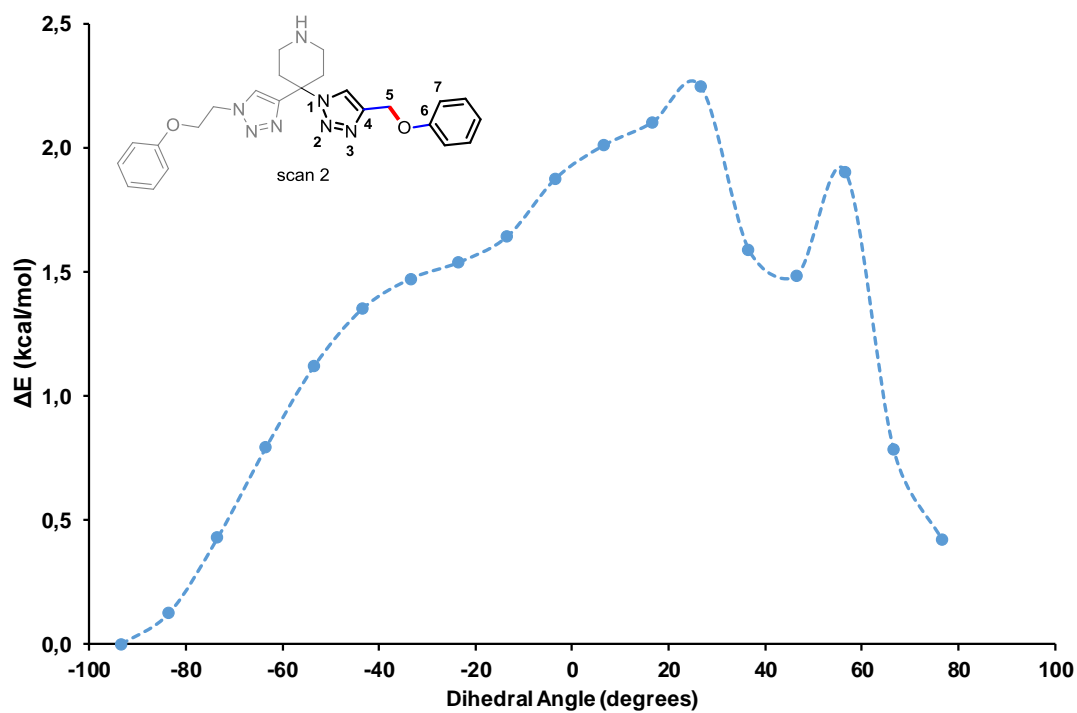


Figure S6. Calculated relative energies in (kcal/mol) as a function of the dihedral angle defined by the C(6), O, C(5) and C(4) atoms in the di(phenyl-triazole) fragment.

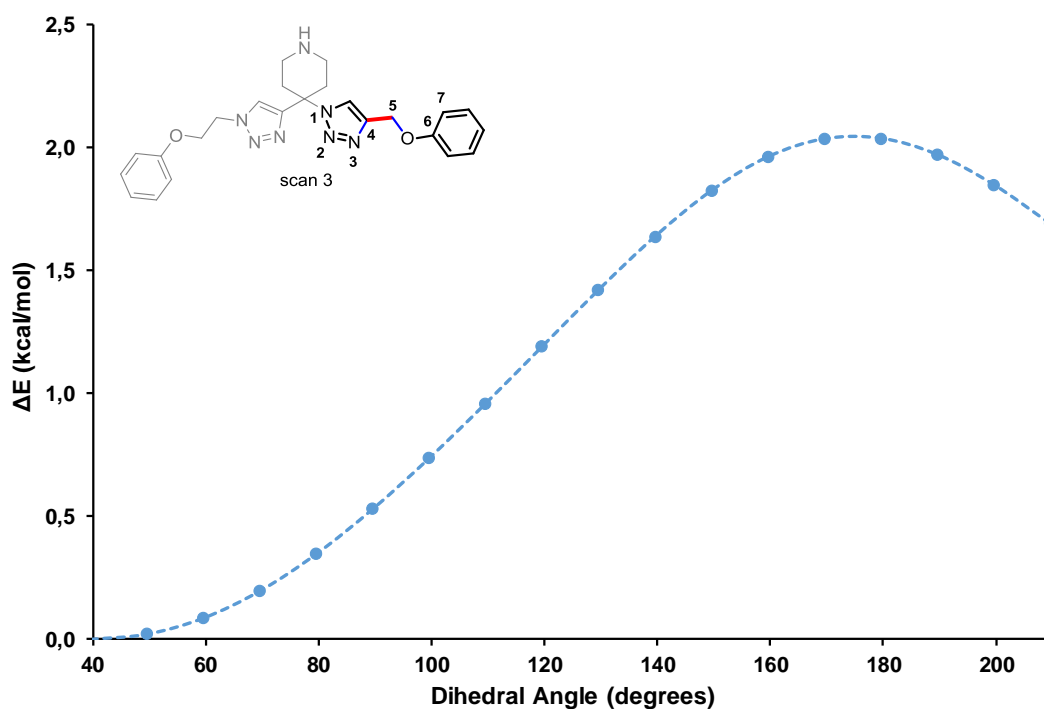


Figure S7. Calculated relative energies in (kcal/mol) as a function of the dihedral angle defined by the O, C(5), C(4) and N(3) atoms in the di(phenyl-triazole) fragment.

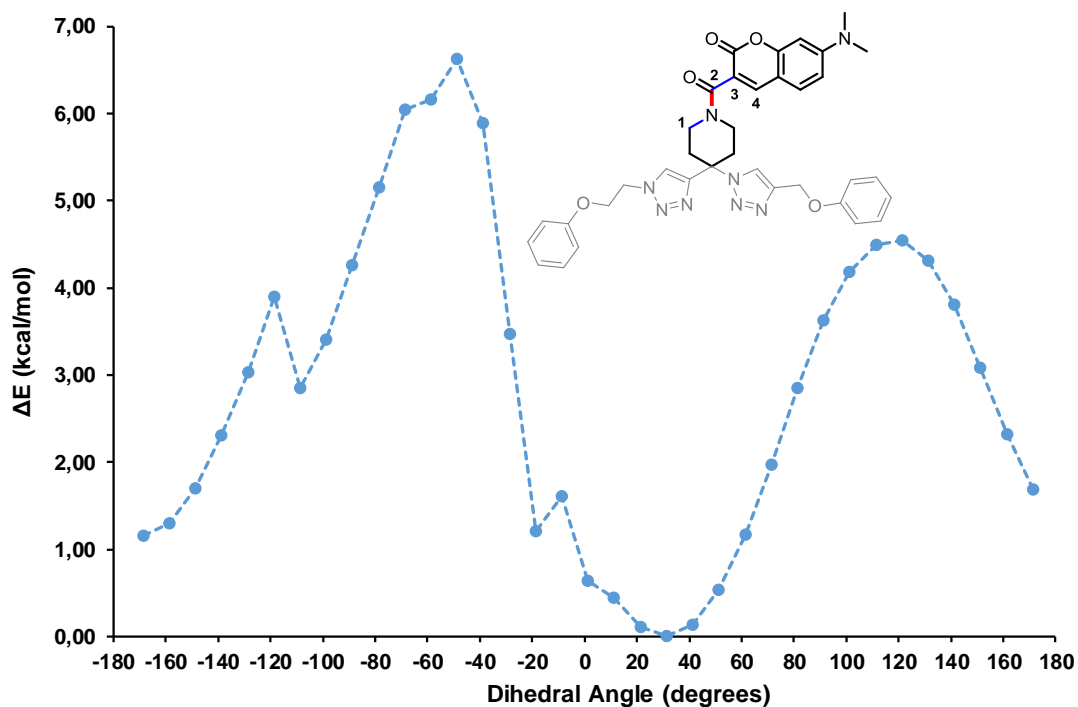


Figure S8. Calculated relative energies in (kcal/mol) as a function of the dihedral angle defined by the C(1), N, C(2) and C(3) atoms in the di(phenyl-triazole)-coumarin fragment.

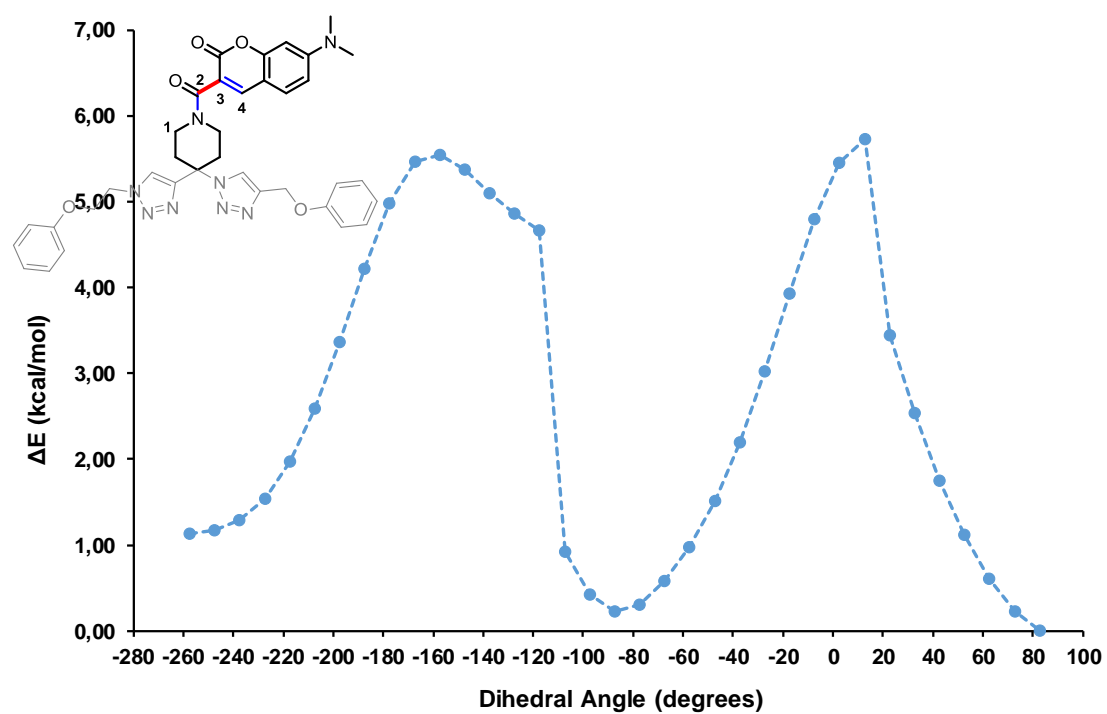


Figure S9. Calculated relative energies in (kcal/mol) as a function of the dihedral angle defined by the N, C(2), C(3) and C(4) atoms in the di(phenyl-triazole)-coumarin fragment.

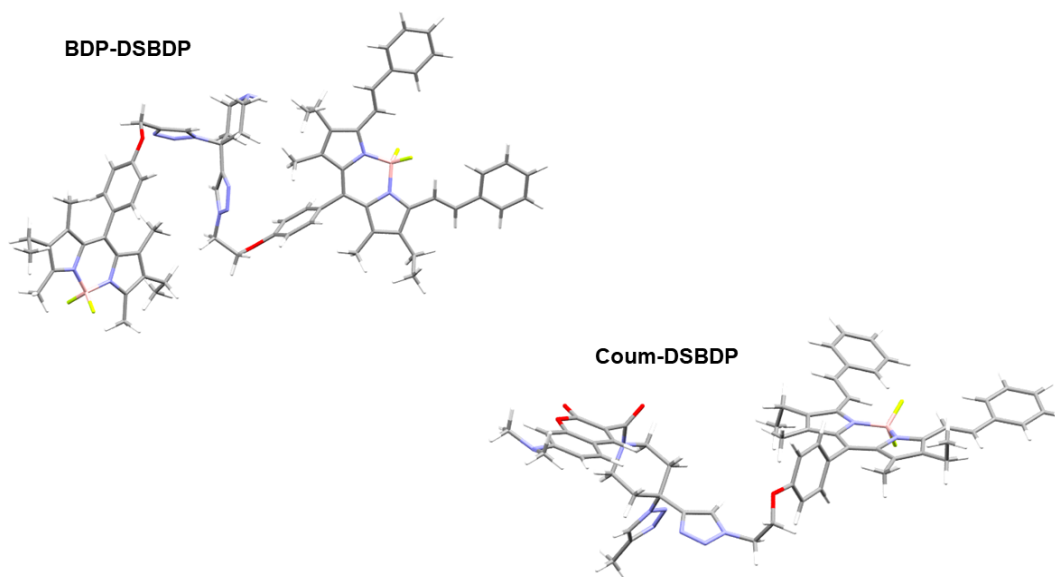


Figure S10. Alternative conformers of the dyads **BDP-DSBDP 7** and **Coum-DSBDP 11** obtained after geometrical optimizations starting from the remarkable conformers of the di(phenyl-triazole) and di(phenyl-triazole)-coumarin fragments. For the computational study, the methoxyphenyl group was substituted for a methyl group in the **Coum-DSBDP** dyad.

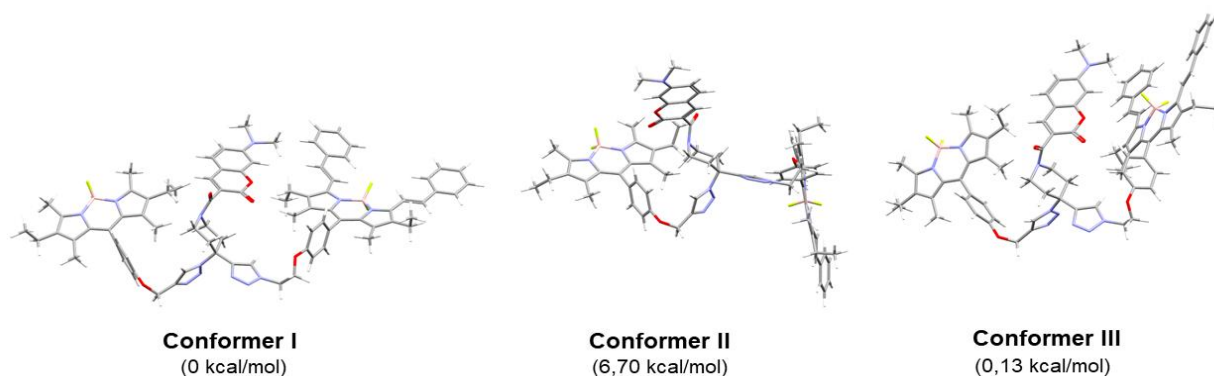
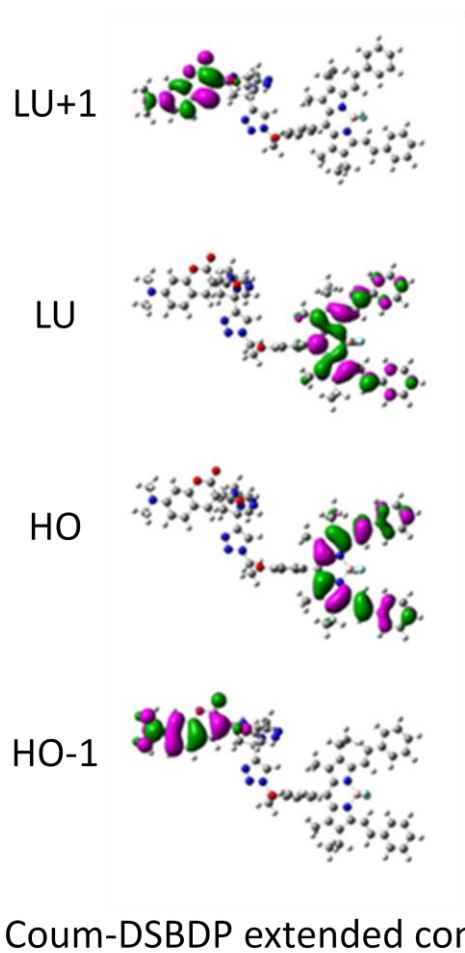


Figure S11 Representation of the three most stable conformers of the triad **Coum-BDP-DSBDP 14** with their relative energies



Coum-DSBDP extended conformer

Figure S12. Plot of the frontier molecular orbitals of the dyad **Coum-DSBDP 11-extended conformer** (isovalue 0.02).

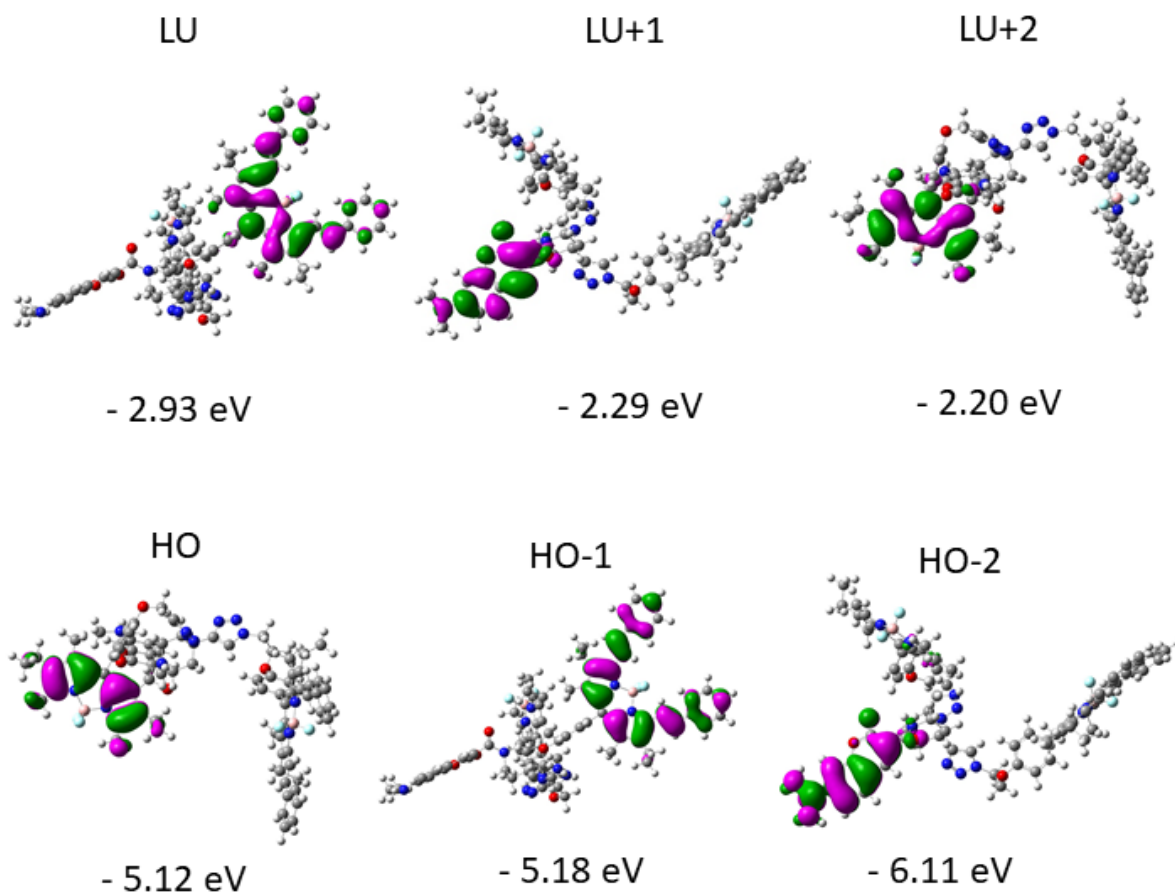


Figure S13. Plot of the frontier molecular orbitals of the triad-conformer II Coum-BDP-DSBDP 14 (isovalue 0.02) with their energies in eV

Emission and absorption spectra

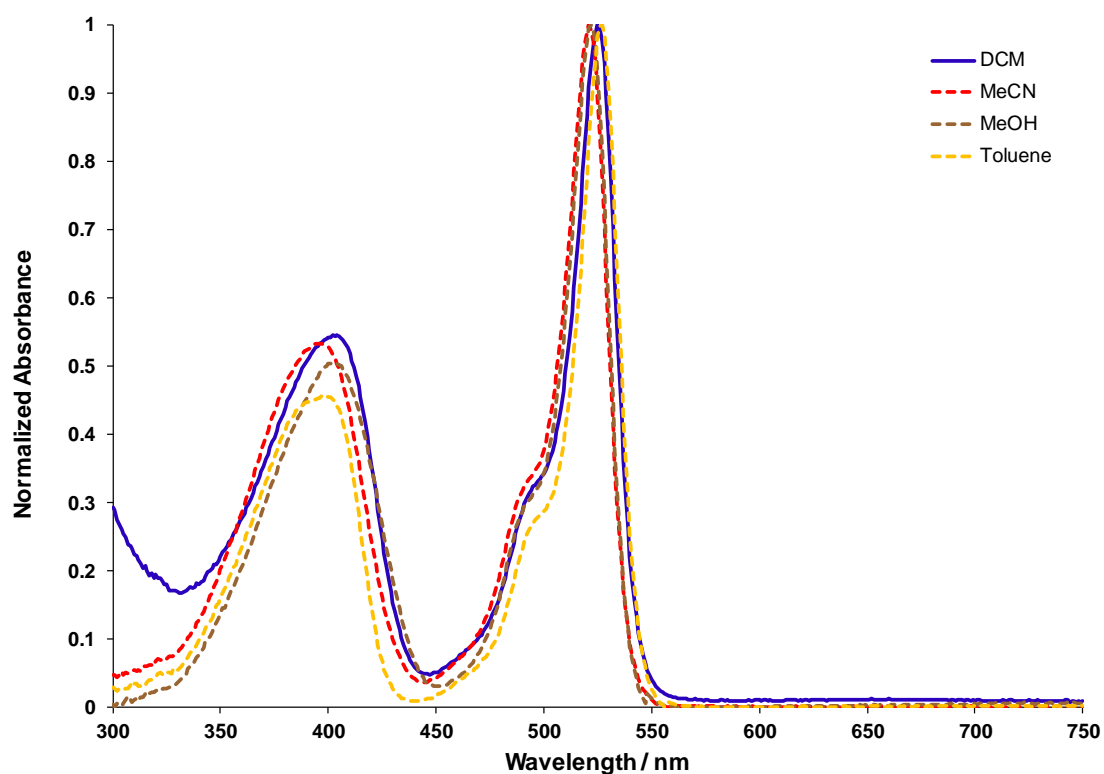


Figure S14. Normalized absorption spectra of **Coum-BDP (13)** in different solvents.

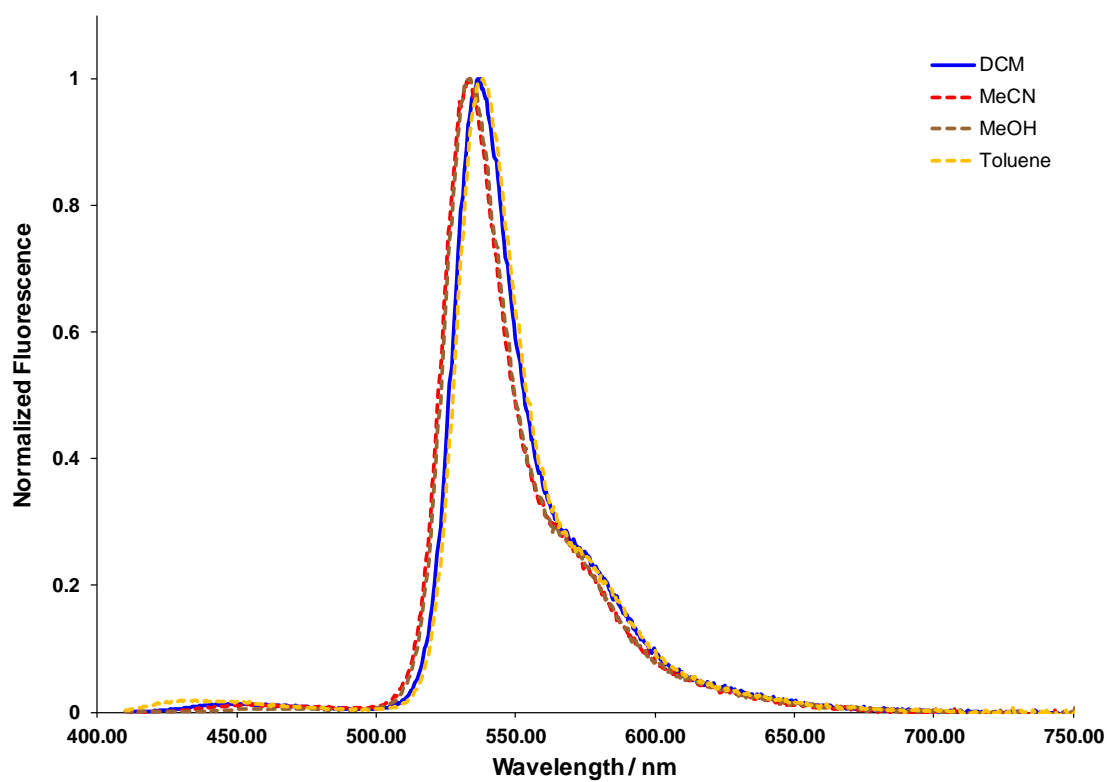


Figure S15. Normalized fluorescence emission spectra of **Coum-BDP (13)** in different solvents – ($\lambda_{exc} = 400 \text{ nm}$).

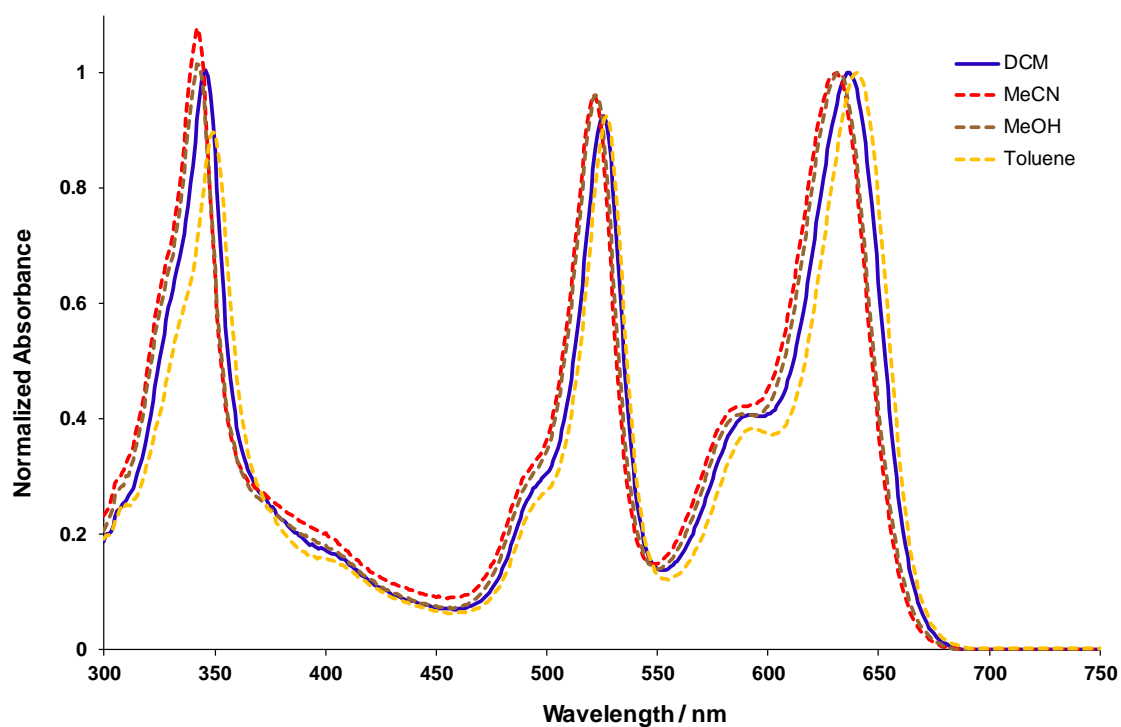


Figure S16. Normalized absorption spectra of **BDP-DSBDP (7)** in different solvents.

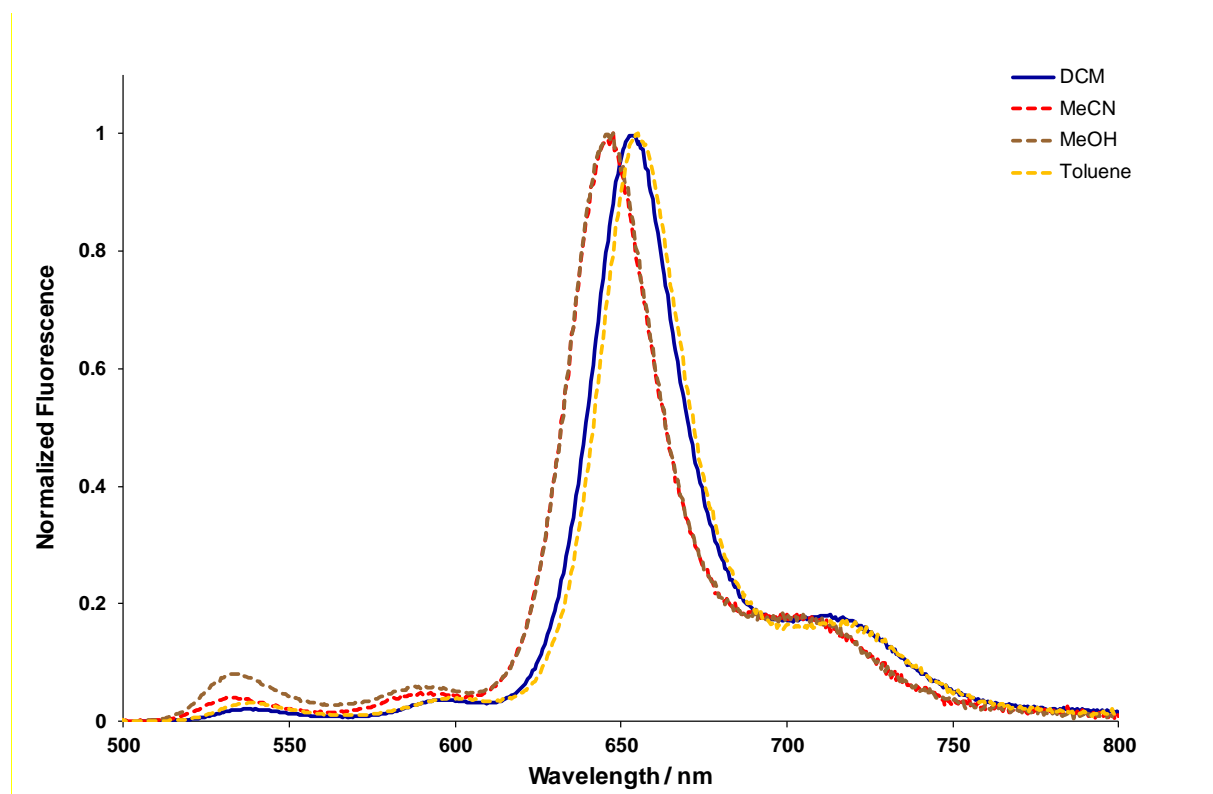


Figure S17. Normalized fluorescence emission spectra of **BDP-DSBDP (7)** in different solvents – ($\lambda_{exc} = 495$ nm).

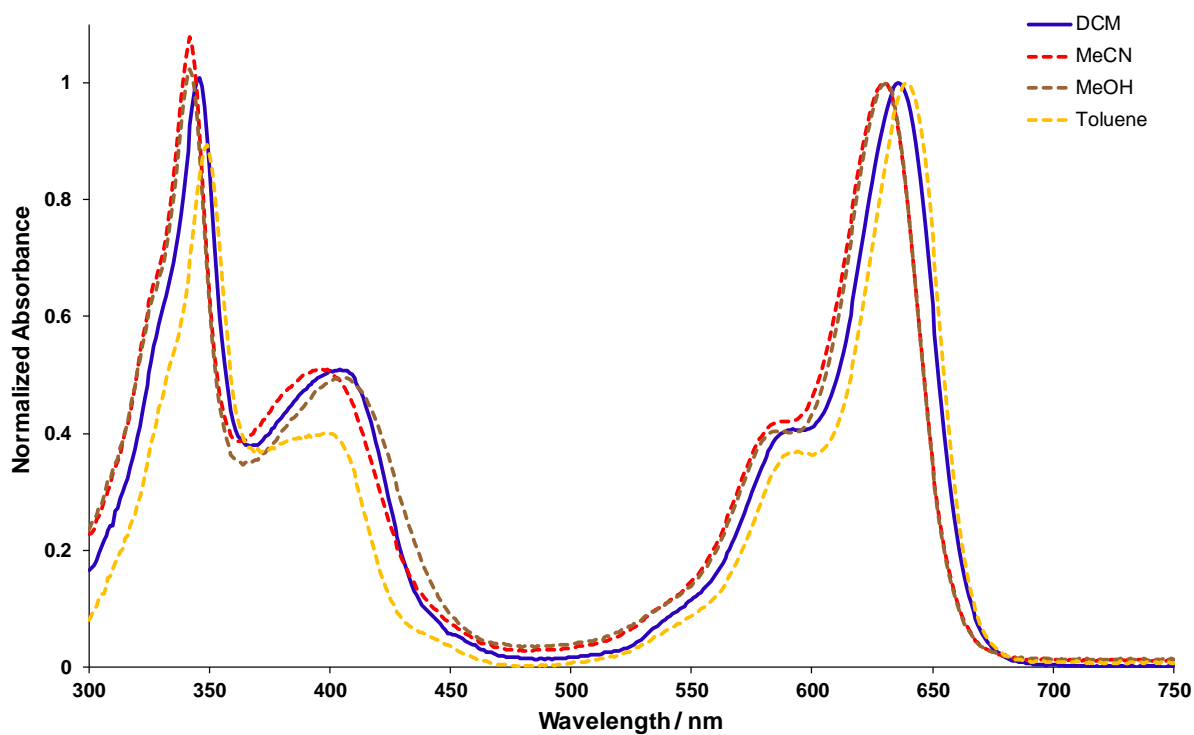


Figure S18. Normalized absorption spectra of **Coum-DSBDP (11)** in different solvents.

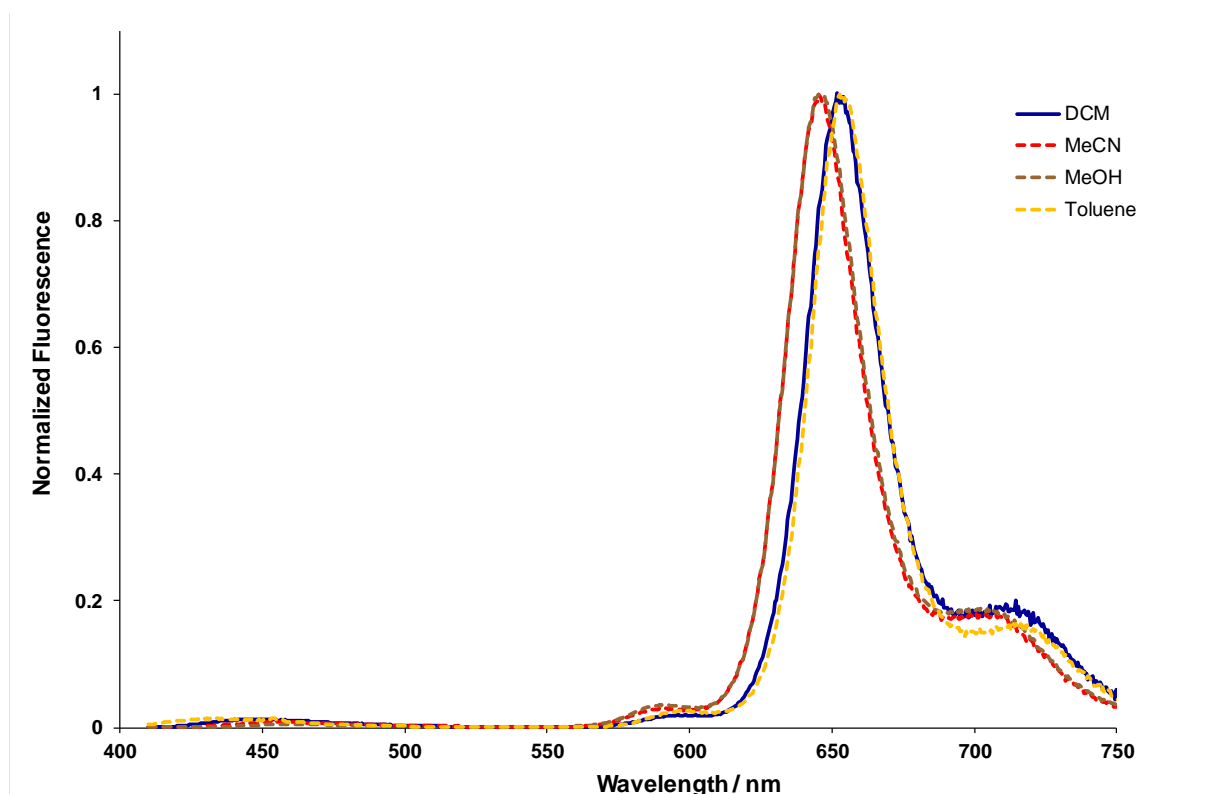


Figure S19. Normalized fluorescence emission spectra of **Coum-DSBDP (11)** in different solvents – ($\lambda_{exc} = 400$ nm).

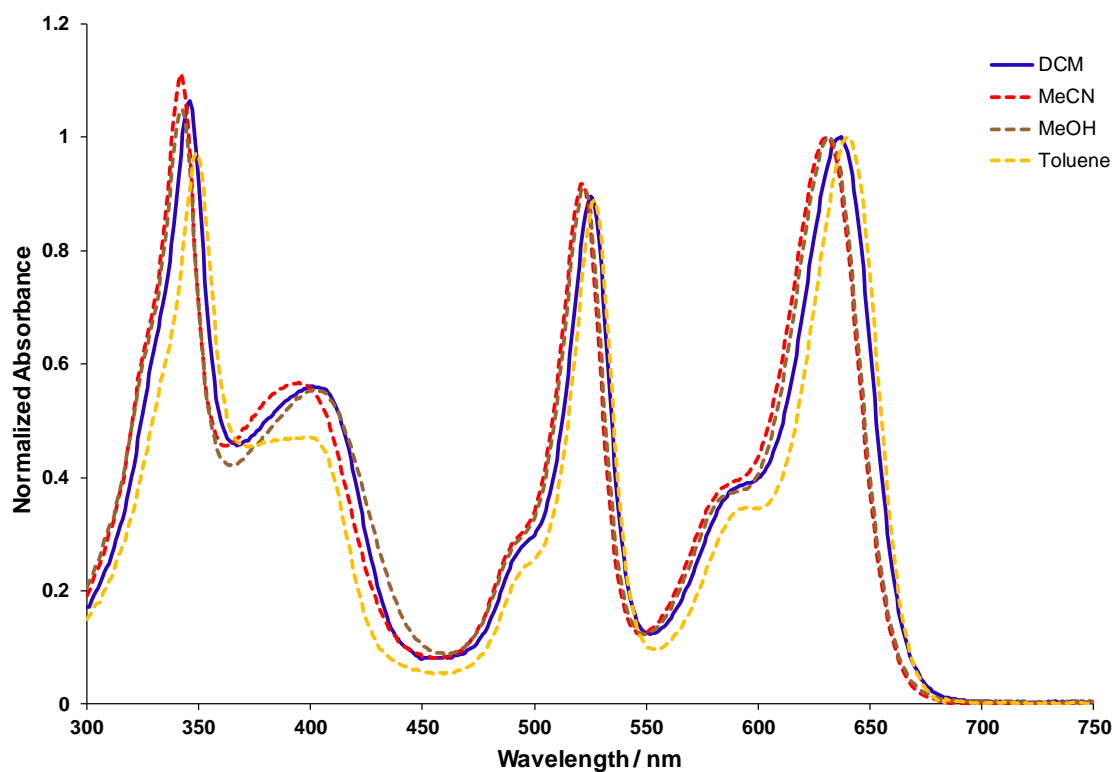


Figure S20. Normalized absorption spectra of **Coum-BDP-DSBDP (14)** in different solvents.

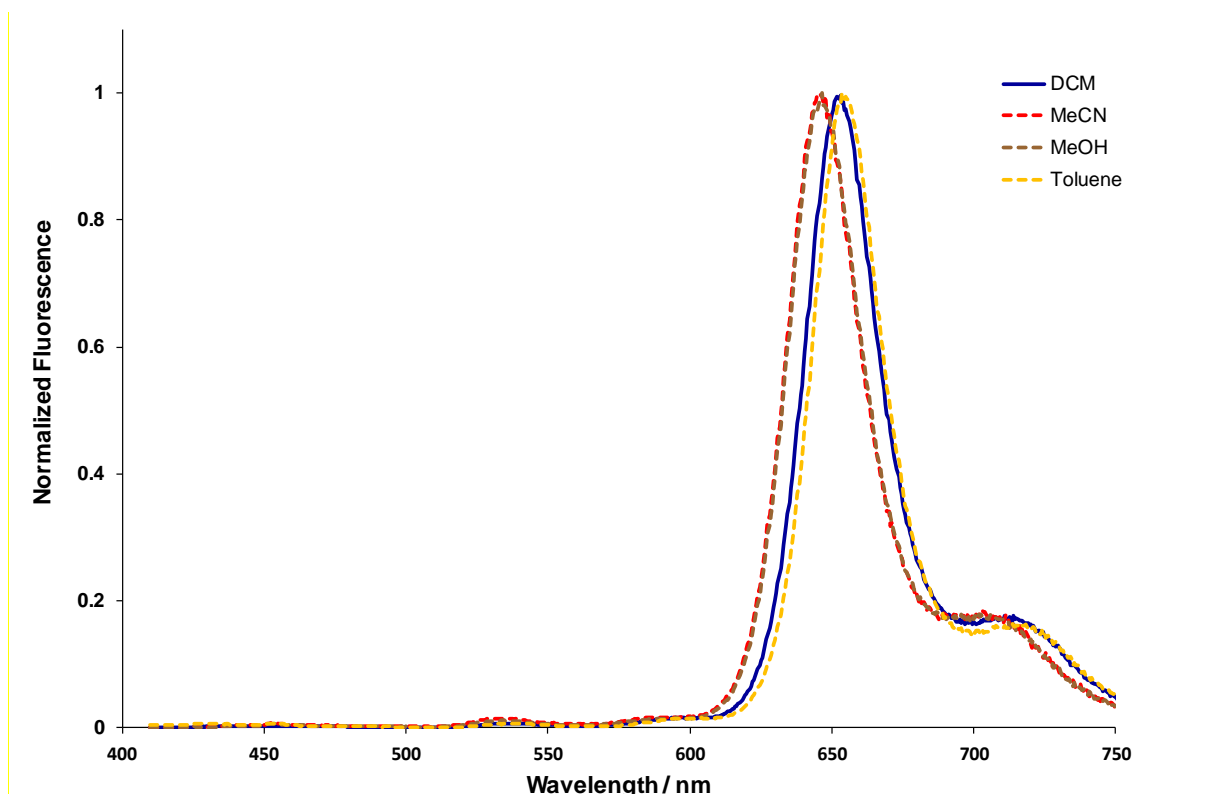


Figure S21. Normalized fluorescence emission spectra of **Coum-BDP-DSBDP (14)** in different solvents – ($\lambda_{exc} = 400$ nm).

Table S1. Spectroscopic data of **7**, **11**, **13** and **14** in different solvents.

Compd	Solvent	DCM		MeCN		MeOH		Toluene	
		λ abs [nm]	λ em [nm]	λ abs [nm]	λ em [nm]	λ abs [nm]	λ em [nm]	λ abs [nm]	λ em [nm]
BDP-DSBDP (7)		346	654 ^a	342	648 ^a	342	648 ^a	349	655 ^a
		526		521		522		527	
		637		631		632		640	
COUM-DSBDP (11)		346	654 ^b	342	646 ^b	342	646 ^b	349	654 ^b
		404		395		402		398	
		636		629		631		639	
COUM-BDP (13)		404	537 ^b	397	534 ^b	403	533 ^b	397	539 ^b
		525		521		522		527	
COUM-BDP-DSBDP (14)		346	653 ^b	342	646 ^b	342	647 ^b	349	654 ^b
		401		395		402		397	
		525		521		522		527	
		637		631		632		640	

^a Excited at 495 nm. ^b Excited at 400 nm.

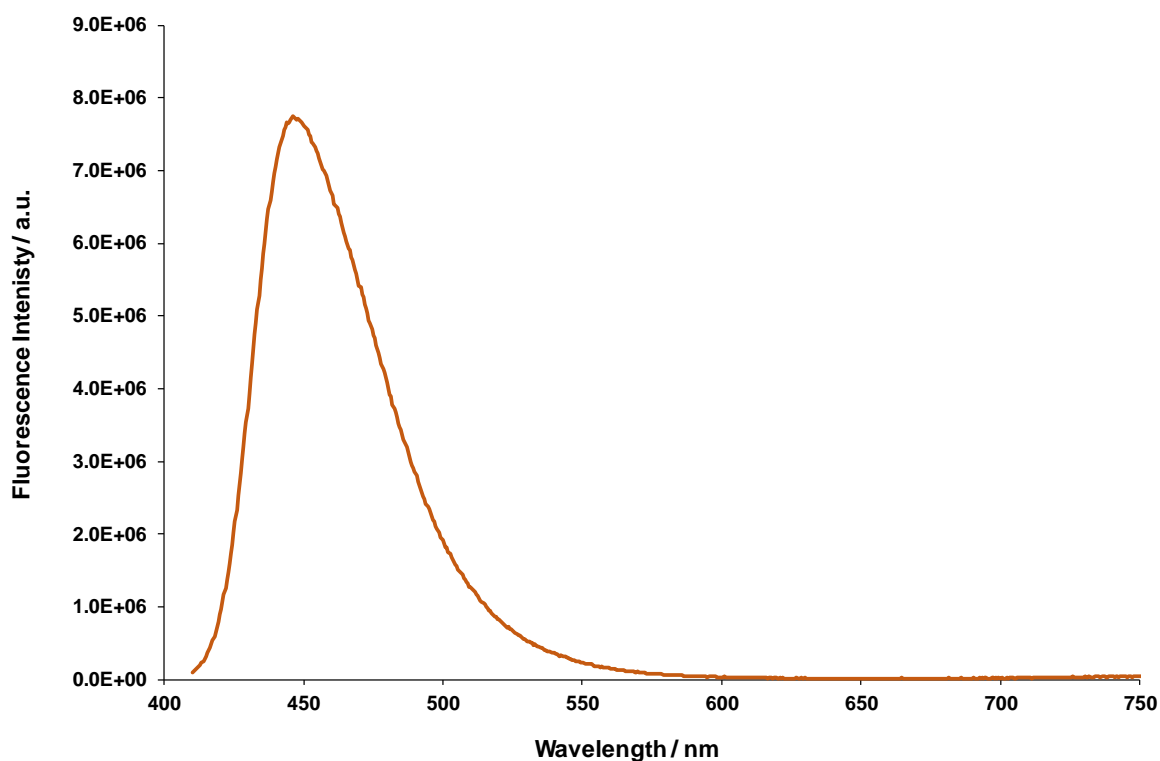


Figure S22. Fluorescence spectrum of coumarin **10** ($[C] = 4.95 \mu\text{M}$) in dichloromethane, $\lambda_{\text{exc}} = 400 \text{ nm}$, (slits 0.9 nm/0.9 nm). The emission spectrum was corrected for absorption at 400 nm.

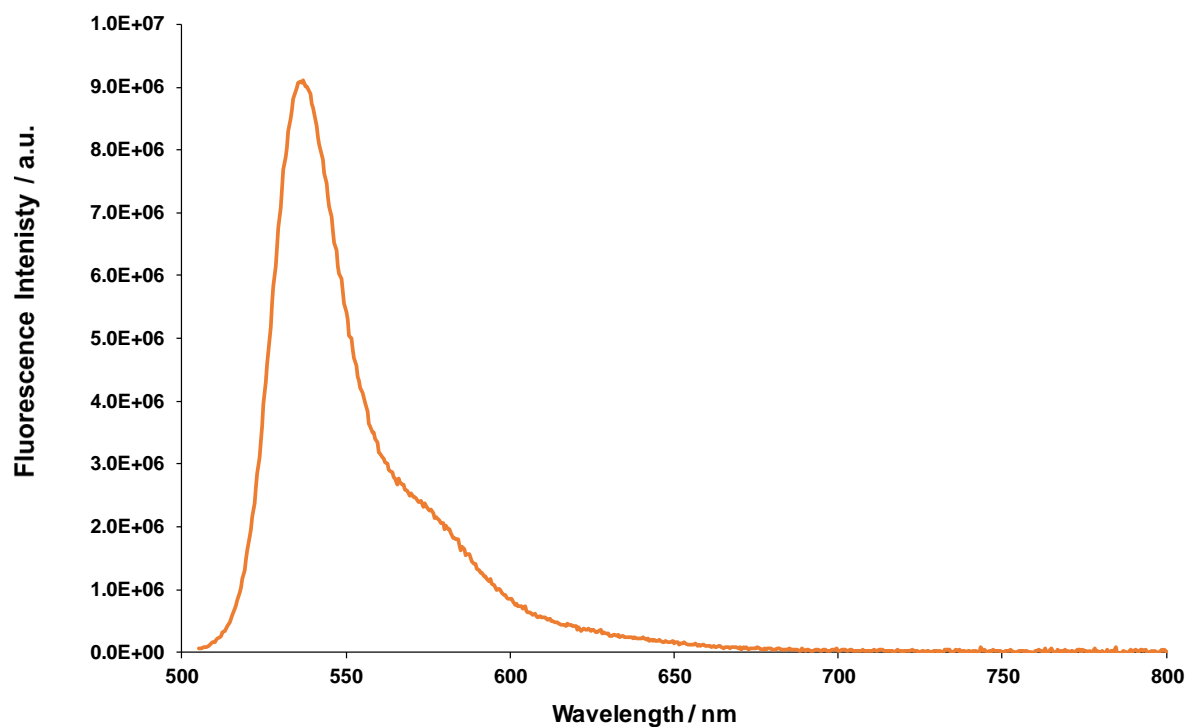


Figure S23. Fluorescence spectrum of Bodipy **BDP-alkyne** ($[C] = 1.84 \mu\text{M}$) in dichloromethane, $\lambda_{\text{exc}} = 495 \text{ nm}$, (slits 0.9 nm/0.9 nm). The emission spectrum was corrected for absorption at 495 nm.

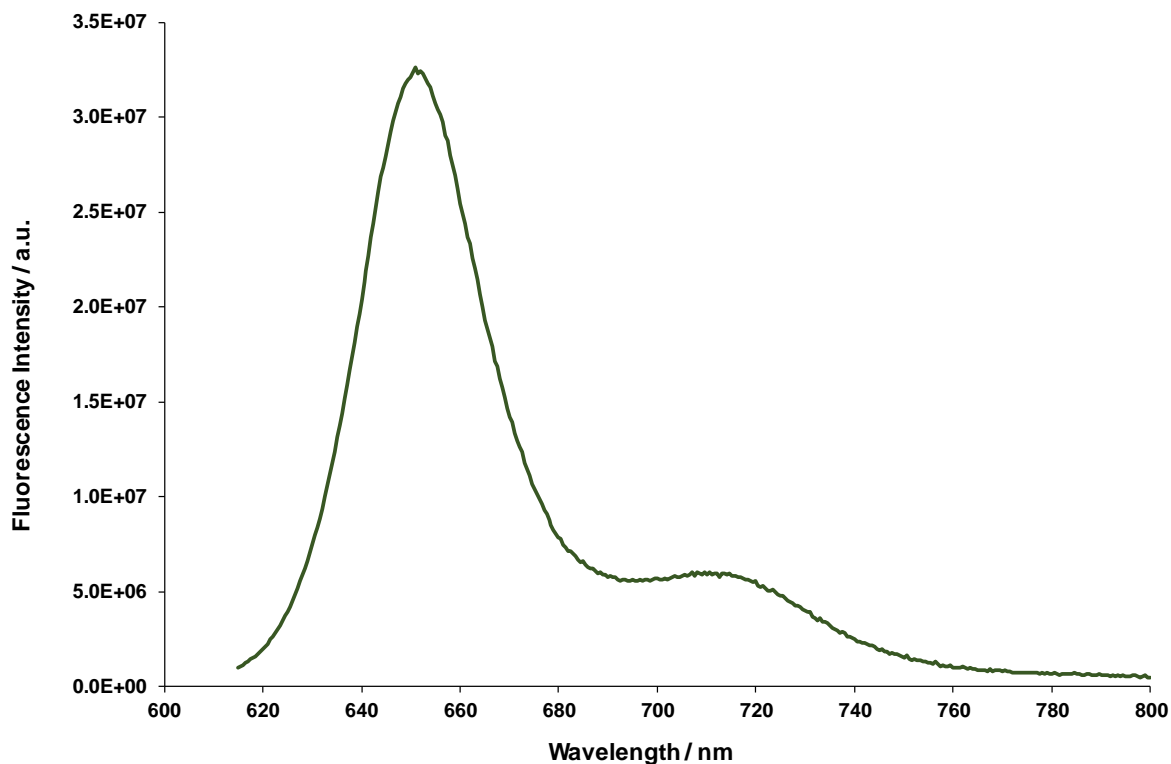


Figure S24. Fluorescence spectrum of distyrylBodipy **DSBDP-N₃** ([C] = 1.36 μ M) in dichloromethane, λ_{exc} = 605 nm, (slits 2.0 nm/2.0 nm). The emission spectrum was corrected for absorption at 605 nm.

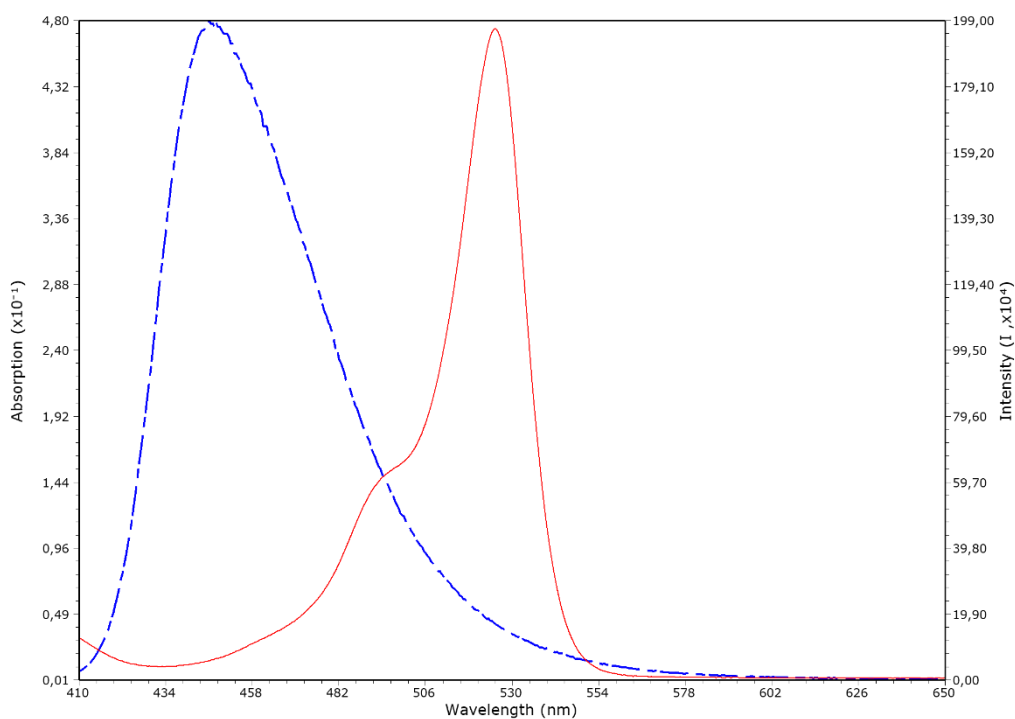


Figure S25. Overlap of the emission and absorption spectra of the donor (Coumarin **10**) and acceptor (Bodipy **BDP-alkyne**).

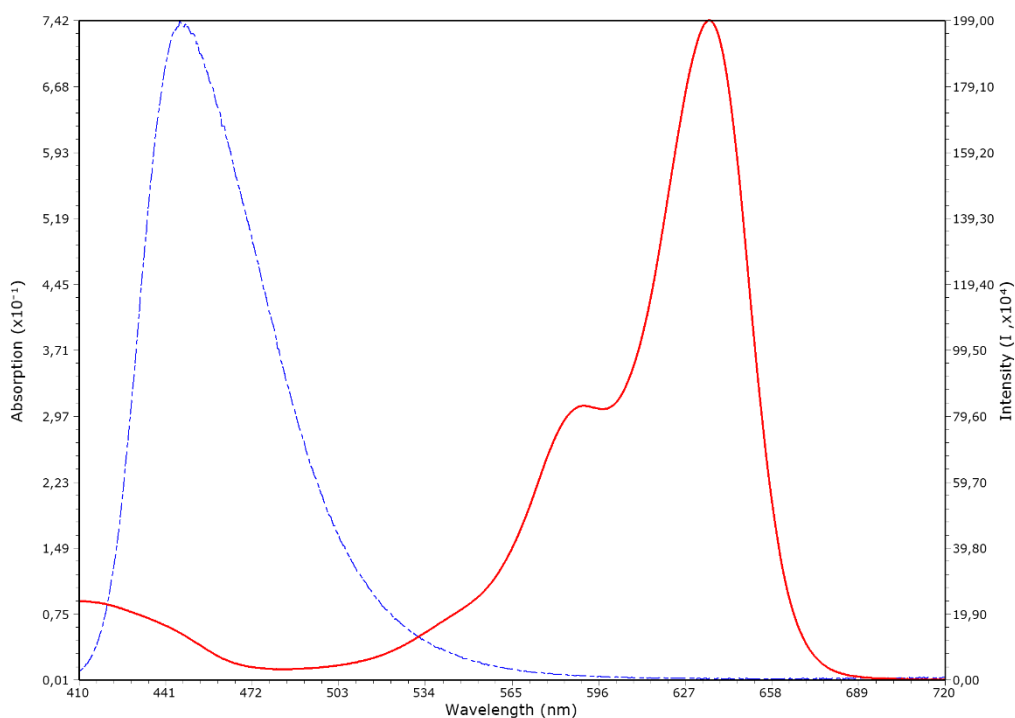


Figure S26. Overlap of the emission and absorption spectra of the donor (Coumarin **10**) and acceptor (distyrylBodipy **DSBDP-N₃**).

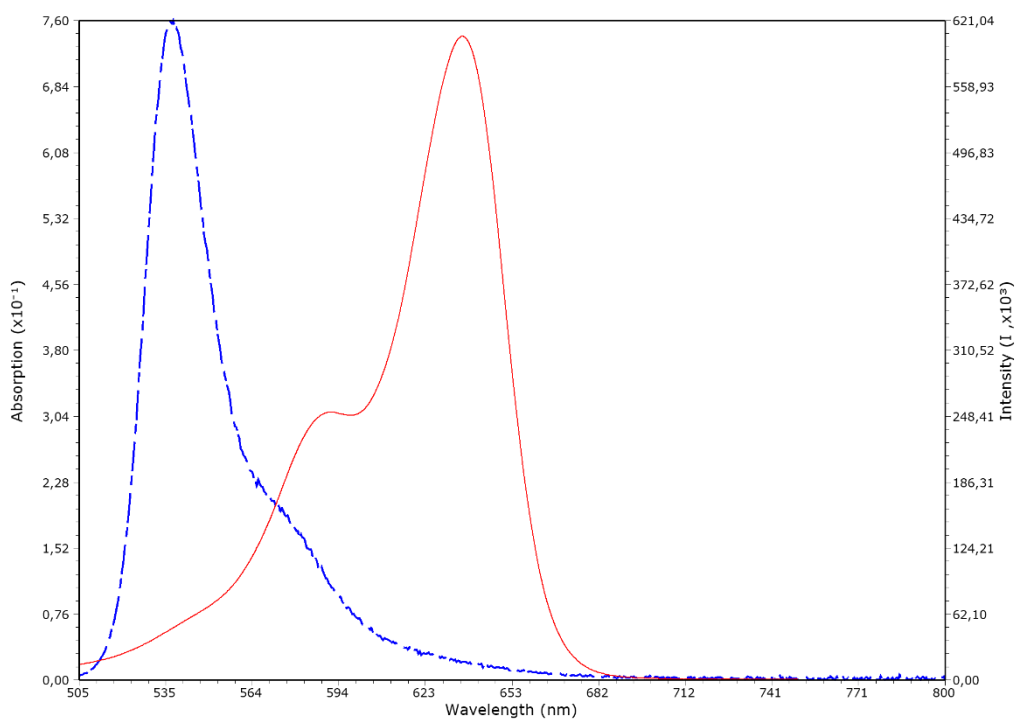


Figure S27. Overlap of the emission and absorption spectra of the donor (Bodipy **BDP-alkyne**) and acceptor (distyrylBodipy **DSBDP-N₃**).

Energy transfer efficiency and calculation of the Förster distance (R_0)

According to the Förster resonance energy-transfer theory, the energy transfer efficiency was estimated using the equation (eq 1).

$$E = \frac{R_0^6}{R_0^6 + R^6} \quad (1)$$

(R) is the distance between the donor and the acceptor and (R_0) is the Förster distance or critical distance, at which the efficiency of the transfer is 50%.

The Förster distance (R_0), which is dependent on the spectral properties of the donor and acceptor molecules, is expressed as follows (eq 2):

$$R_0 = 0.2108 [\kappa^2 \times \Phi_D \times n^{-4} \times J(\lambda)]^{1/6} \text{ in } \text{Å} \quad (2)$$

κ^2 is the relative orientation of the donor and acceptor transition dipole moments. n is the solvent refractive index. Φ_D is the donor fluorescence quantum yield in the absence of acceptor. $J(\lambda)$ is the spectral overlap term which measures the overlap of the donor fluorescence band and the acceptor absorption band and is expressed as follows (eq 3):

$$J(\lambda) = \int_0^\infty I_D(\lambda) \times \varepsilon_A(\lambda) \times \lambda^4 \times d\lambda \quad (3)$$

$I_D(\lambda)$ is the fluorescence intensity of the donor in the absence of acceptor, $\varepsilon_A(\lambda)$ is the molar absorption coefficient of the acceptor.

The values of R_0 were calculated with *PhotoChemCAD* [1]

For Coumarin (donor) and Bodipy (acceptor): The Förster distance (R_0) has been estimated assuming a random orientation of the donor and acceptor molecules taking $\kappa^2 = 2/3$, $n = 1.424$, $\Phi_D = 0.84$, $\varepsilon_A = 60\,255 \text{ mol}^{-1} \cdot \text{L} \cdot \text{cm}^{-1}$ at 525 nm.

$$R_0 (\text{Coumarin-Bodipy}) = 41.7 \text{ Å}$$
$$J(\lambda) = 4.4 \times 10^{-14} \text{ cm}^6 \text{ mmol}^{-1}$$

For Coumarin (donor) and distyrylBodipy (acceptor): The Förster distance (R_0) has been estimated assuming a random orientation of the donor and acceptor molecules taking $\kappa^2 = 2/3$, $n = 1.424$, $\Phi_D = 0.84$, $\varepsilon_A = 75\,860 \text{ mol}^{-1} \cdot \text{L} \cdot \text{cm}^{-1}$ at 636 nm.

$$R_0 (\text{Coumarin-distyrylBodipy}) = 36.6 \text{ Å}$$
$$J(\lambda) = 2.0 \times 10^{-14} \text{ cm}^6 \text{ mmol}^{-1}$$

For Bodipy (donor) and distyrylBodipy (acceptor): The Förster distance (R_0) has been estimated assuming a random orientation of the donor and acceptor molecules taking $\kappa^2 = 2/3$, $n = 1.424$, $\Phi_D = 0.91$, $\varepsilon_A = 75\,860 \text{ mol}^{-1} \cdot \text{L} \cdot \text{cm}^{-1}$ at 636 nm.

$$R_0 (\text{Bodipy-distyrylBodipy}) = 51.5 \text{ Å}$$
$$J(\lambda) = 1.4 \times 10^{-13} \text{ cm}^6 \text{ mmol}^{-1}$$

Cartesian coordinates of all minima

Phenyl triazole

Conformer 1 (most stable)

Total Energy (PM3) : 0.070350 Hartree

Imaginary frequency: 0

Atom#	Symbol	X	Y	Z
1	N	4.609608	-2.265752	-0.083423
2	C	4.252351	-1.6569	1.21978
3	C	4.751557	-1.24883	-1.152186
4	C	3.02402	-0.754482	1.146558
5	H	5.134451	-1.083153	1.567886
6	H	4.096535	-2.472654	1.951618
7	C	3.535005	-0.33671	-1.281367
8	H	5.658561	-0.654565	-0.922715
9	H	4.950527	-1.774548	-2.105786
10	C	3.204371	0.316173	0.065041
11	H	2.852694	-0.274887	2.129109
12	H	2.112006	-1.351762	0.941148
13	H	3.730797	0.442663	-2.042247
14	H	2.658166	-0.905687	-1.652879
15	C	1.971441	1.140203	-0.051884
16	C	0.678824	0.768065	-0.388802
17	N	-0.04928	1.962241	-0.342575
18	H	0.261062	-0.209196	-0.634186
19	N	1.95046	2.527484	0.183877
20	N	0.777206	2.995887	0.01958
21	H	3.907075	-2.925953	-0.344897
22	C	-1.494053	2.124329	-0.591573
23	C	-2.357664	1.907128	0.65946
24	H	-1.784972	1.414022	-1.392754
25	H	-1.672949	3.147284	-0.981394
26	O	-2.350262	0.564055	1.101313
27	H	-3.391203	2.264216	0.455851
28	H	-1.972596	2.439625	1.546951
29	C	-3.223563	-0.307729	0.469724
30	C	-4.387099	0.091093	-0.195733
31	C	-2.898201	-1.664911	0.598049
32	C	-5.224405	-0.876522	-0.737618
33	H	-4.631503	1.160336	-0.277772
34	C	-3.751657	-2.615181	0.052261
35	H	-1.990446	-1.971687	1.130081
36	C	-4.909253	-2.225466	-0.615973
37	H	-6.13767	-0.571441	-1.259139
38	H	-3.510159	-3.67901	0.149576
39	H	4.059553	0.97623	0.358533
40	H	-5.573829	-2.982841	-1.044107

Conformer 2 (+0.43 kcal/mol vs Conformer 1)

Total Energy (PM3) : 0.071040 Hartree

Imaginary frequency: 0

Atom#	Symbol	X	Y	Z
1	N	-4.499559	1.45319	-0.701106
2	C	-3.525389	1.940468	0.303973
3	C	-4.771378	0.003588	-0.555282
4	C	-2.230677	1.133265	0.328714
5	H	-4.025146	1.901765	1.29251
6	H	-3.31803	3.007674	0.095703
7	C	-3.505996	-0.849358	-0.550376
8	H	-5.333707	-0.132383	0.390113
9	H	-5.449292	-0.305416	-1.373986
10	C	-2.528048	-0.357627	0.522046
11	H	-1.577359	1.498003	1.144177
12	H	-1.655937	1.287596	-0.607537
13	H	-3.76925	-1.90833	-0.366061
14	H	-3.018271	-0.829985	-1.546545
15	C	-1.266173	-1.14349	0.467143
16	C	-0.346517	-1.282708	-0.561482
17	N	0.630428	-2.138575	-0.040474
18	H	-0.329049	-0.848903	-1.562126
19	N	-0.794999	-1.915082	1.54535
20	N	0.303723	-2.486534	1.24582
21	H	-4.148497	1.634341	-1.618554
22	C	1.845195	-2.611716	-0.731643
23	C	3.116525	-1.836491	-0.35387
24	H	1.65718	-2.553217	-1.823463
25	H	1.995032	-3.683118	-0.48547
26	O	3.217404	-0.626952	-1.082162
27	H	4.003129	-2.394926	-0.705385
28	H	3.213963	-1.694975	0.74487
29	C	2.916958	0.553595	-0.423616
30	C	2.902611	0.710301	0.965627
31	C	2.682653	1.645387	-1.2718
32	C	2.644781	1.965394	1.504071
33	H	3.089537	-0.152149	1.622454
34	C	2.432058	2.891233	-0.711771
35	H	2.705847	1.520478	-2.36022
36	C	2.409942	3.053408	0.670737
37	H	2.628223	2.093469	2.591608
38	H	2.250481	3.751399	-1.364807
39	H	-3.003116	-0.497431	1.525996
40	H	2.208601	4.039238	1.102053

Conformer 3 (+0.78 kcal/mol vs Conformer 1)

Total Energy (PM3) : 0.071597 Hartree

Imaginary frequency: 0

Atom#	Symbol	X	Y	Z
1	N	-5.858126	0.573836	0.929591
2	C	-5.734606	-0.439406	-0.144914
3	C	-4.92422	1.708077	0.734764
4	C	-4.303737	-0.928366	-0.350481
5	H	-6.124742	0.018704	-1.075723
6	H	-6.406843	-1.28474	0.097634
7	C	-3.474286	1.269662	0.550176
8	H	-5.273786	2.273741	-0.151972
9	H	-5.020672	2.388623	1.60245
10	C	-3.358794	0.253753	-0.591322
11	H	-4.266031	-1.624551	-1.209904
12	H	-3.961939	-1.515168	0.526689
13	H	-2.840547	2.151675	0.337523
14	H	-3.075777	0.833068	1.488887
15	C	-1.95572	-0.225203	-0.71239
16	C	-1.162298	-0.903205	0.200438
17	N	0.054019	-1.089476	-0.468017
18	H	-1.378445	-1.237633	1.215321
19	N	-1.178688	-0.03872	-1.870887
20	N	-0.015705	-0.537069	-1.719308
21	H	-5.678448	0.14404	1.813202
22	C	1.257831	-1.750163	0.072193
23	C	1.827174	-1.053075	1.315659
24	H	2.026474	-1.80549	-0.727281
25	H	0.988248	-2.793735	0.334347
26	O	2.320448	0.24282	1.047869
27	H	2.607611	-1.701272	1.771787
28	H	1.052995	-0.84675	2.076589
29	C	3.604877	0.325723	0.529908
30	C	4.593368	-0.641579	0.736056
31	C	3.886664	1.505794	-0.170923
32	C	5.870635	-0.423531	0.233785
33	H	4.354099	-1.559693	1.291885
34	C	5.171152	1.704125	-0.661068
35	H	3.106925	2.259758	-0.329008
36	C	6.160501	0.744677	-0.462355
37	H	6.649857	-1.176565	0.390492
38	H	5.404364	2.622043	-1.211112
39	H	-3.65716	0.757348	-1.545582
40	H	7.168494	0.910351	-0.855987

di(phenyl-triazole

Conformer 1 (+0.09 kcal/mol vs Conformer 2)

Total Energy (PM3) : 0.183063 Hartree

Imaginary frequency: 0

Atom#	Symbol	X	Y	Z
1	N	-0.196749	5.001444	0.308888
2	C	-1.207572	4.255681	1.090262
3	C	0.318439	4.206252	-0.828038
4	C	-0.731325	2.878246	1.54453
5	H	-2.118483	4.172613	0.462781
6	H	-1.489441	4.869442	1.968061
7	C	0.834444	2.829668	-0.420271
8	H	-0.498718	4.124028	-1.572027
9	H	1.125748	4.785257	-1.317865
10	C	-0.204045	2.01002	0.380839
11	H	-1.551534	2.36304	2.087071
12	H	0.085825	2.988005	2.28732
13	H	1.169512	2.278645	-1.32251
14	H	1.740685	2.936034	0.21195
15	N	-1.337723	1.554446	-0.510637
16	C	-2.695951	1.483738	-0.187324
17	C	-3.288117	0.902845	-1.298249
18	H	-3.134164	1.818133	0.755937
19	N	-1.135646	1.0145	-1.756659
20	N	-2.262346	0.642067	-2.222006
21	C	0.451277	0.76576	0.910165
22	C	1.449497	-0.015016	0.341921
23	N	1.626606	-1.062576	1.246064
24	H	1.999001	0.103397	-0.594934
25	N	0.088492	0.147073	2.121045
26	N	0.776265	-0.905781	2.313759
27	H	0.55956	5.266774	0.904837
28	C	-4.717425	0.594771	-1.575329
29	O	-5.38086	0.059955	-0.441966
30	H	-4.820721	-0.064905	-2.464802
31	H	-5.291198	1.522749	-1.74915
32	C	-5.300586	-1.308526	-0.252443
33	C	-5.62321	-1.744276	1.040712
34	C	-4.990871	-2.227173	-1.260806
35	C	-5.631067	-3.106605	1.309503
36	H	-5.868839	-1.021352	1.82648
37	C	-5.001494	-3.585328	-0.967941
38	H	-4.739511	-1.867638	-2.269845
39	C	-5.32037	-4.026326	0.311619
40	H	-5.881717	-3.458081	2.315779
41	H	-4.758109	-4.30911	-1.752517
42	C	2.585376	-2.177557	1.127155

43	C	3.943064	-1.894858	1.788256
44	H	2.727251	-2.404384	0.044781
45	H	2.139529	-3.080162	1.5931
46	O	4.633744	-0.800692	1.21884
47	H	4.552768	-2.818778	1.774644
48	H	3.837022	-1.565554	2.838019
49	C	5.443775	-1.06505	0.124032
50	C	5.161016	-2.021738	-0.855781
51	C	6.569455	-0.236929	0.014445
52	C	6.018714	-2.153612	-1.942248
53	H	4.267119	-2.657666	-0.778166
54	C	7.40808	-0.380515	-1.0832
55	H	6.782172	0.516218	0.781888
56	C	7.138237	-1.337654	-2.057724
57	H	5.805002	-2.902751	-2.711994
58	H	8.289293	0.262757	-1.179482
59	H	-5.327291	-5.097673	0.535104
60	H	7.807837	-1.446256	-2.917146

Conformer 2 (most stable)

Total Energy (PM3) : 0.182916 Hartree

Imaginary frequency: 0

Atom#	Symbol	X	Y	Z
1	N	1.218608	3.237059	-1.565402
2	C	1.698689	2.042631	-2.294247
3	C	0.750088	2.899065	-0.202953
4	C	0.68673	0.899944	-2.321644
5	H	2.647501	1.721208	-1.817697
6	H	1.956978	2.34706	-3.327333
7	C	-0.289369	1.782473	-0.179924
8	H	1.641996	2.629101	0.396867
9	H	0.33334	3.816279	0.257403
10	C	0.182261	0.506185	-0.915486
11	H	1.125912	0.027044	-2.847912
12	H	-0.194886	1.1922	-2.929135
13	H	-0.567746	1.559437	0.870175
14	H	-1.226671	2.126553	-0.66534
15	N	1.25835	-0.200752	-0.123336
16	C	2.419308	-0.808152	-0.610863
17	C	2.99828	-1.395952	0.503305
18	H	2.752162	-0.787755	-1.650986
19	N	1.142325	-0.450795	1.22225
20	N	2.153658	-1.131042	1.594371
21	C	-0.966171	-0.455379	-1.036194
22	C	-2.114709	-0.568911	-0.264733
23	N	-2.78857	-1.664725	-0.80562
24	H	-2.462777	0.022863	0.584845

25	N	-1.015047	-1.484438	-1.995688
26	N	-2.074365	-2.176264	-1.861653
27	H	0.478982	3.669399	-2.078829
28	C	4.24854	-2.193104	0.629304
29	O	5.306052	-1.66106	-0.151406
30	H	4.122423	-3.193072	0.176835
31	H	4.541714	-2.313244	1.695378
32	C	6.080939	-0.671265	0.426979
33	C	6.861197	0.066988	-0.474391
34	C	6.158955	-0.432757	1.803089
35	C	7.715764	1.044269	0.018533
36	H	6.801881	-0.127753	-1.550873
37	C	7.017903	0.55293	2.273248
38	H	5.540407	-1.022282	2.496293
39	C	7.794741	1.290335	1.386452
40	H	8.330291	1.626151	-0.676221
41	H	7.080825	0.746563	3.34904
42	C	-4.084375	-2.211206	-0.359756
43	C	-5.293611	-1.586916	-1.072765
44	H	-4.169607	-2.058654	0.741414
45	H	-4.087873	-3.306156	-0.537676
46	O	-5.427037	-0.197222	-0.850127
47	H	-6.209082	-2.13956	-0.786305
48	H	-5.196437	-1.624995	-2.173114
49	C	-6.136565	0.197349	0.274848
50	C	-6.132222	-0.489243	1.492968
51	C	-6.827975	1.408863	0.13661
52	C	-6.834546	0.037988	2.571032
53	H	-5.573868	-1.43007	1.605134
54	C	-7.516043	1.921132	1.228806
55	H	-6.822053	1.946292	-0.818693
56	C	-7.524352	1.237977	2.442014
57	H	-6.838216	-0.496023	3.527179
58	H	-8.05814	2.867916	1.132059
59	H	8.469009	2.065409	1.763917
60	H	-8.073656	1.647594	3.295989

Conformer 3 (+0.46 kcal/mol vs Conformer 2)

Total Energy (PM3) : 0.183643 Hartree Imaginary frequency: 0

Atom#	Symbol	X	Y	Z
1	N	-2.496068	3.846949	0.111457
2	C	-2.500638	2.887489	1.237271
3	C	-2.09123	3.204159	-1.158416
4	C	-1.185912	2.127189	1.393201
5	H	-3.346565	2.188309	1.075256
6	H	-2.730776	3.444056	2.166769

7	C	-0.764606	2.456504	-1.062575
8	H	-2.912647	2.525426	-1.463072
9	H	-2.030975	3.987295	-1.939437
10	C	-0.73626	1.426963	0.091618
11	H	-1.27361	1.401239	2.228185
12	H	-0.38065	2.826735	1.699412
13	H	-0.542937	1.973158	-2.035797
14	H	0.064522	3.17541	-0.895586
15	N	-1.618043	0.241391	-0.22594
16	C	-2.468776	-0.448629	0.643296
17	C	-2.955443	-1.504145	-0.111993
18	H	-2.673509	-0.168377	1.679022
19	N	-1.580775	-0.405032	-1.437875
20	N	-2.363408	-1.408731	-1.38292
21	C	0.660278	0.893557	0.24941
22	C	1.672185	0.764895	-0.692339
23	N	2.7196	0.159609	0.004543
24	H	1.69444	1.029821	-1.751833
25	N	1.155875	0.363479	1.455702
26	N	2.34922	-0.05292	1.309322
27	H	-1.87946	4.605056	0.317814
28	C	-3.899614	-2.594521	0.254855
29	O	-4.965413	-2.131405	1.067253
30	H	-3.412272	-3.324755	0.925579
31	H	-4.269487	-3.125577	-0.649654
32	C	-6.076139	-1.619992	0.419242
33	C	-6.929943	-0.857126	1.228697
34	C	-6.394379	-1.871279	-0.919449
35	C	-8.101044	-0.349858	0.681358
36	H	-6.680248	-0.668895	2.278687
37	C	-7.569416	-1.350097	-1.446837
38	H	-5.713838	-2.473494	-1.539825
39	C	-8.421534	-0.591712	-0.651605
40	H	-8.775691	0.246306	1.304556
41	H	-7.822428	-1.540656	-2.494926
42	C	4.046642	-0.185668	-0.539336
43	C	5.091657	0.899514	-0.223573
44	H	3.94276	-0.328141	-1.634718
45	H	4.370097	-1.162018	-0.120845
46	O	6.286291	0.663653	-0.939416
47	H	5.274411	0.977872	0.870737
48	H	4.795139	1.891951	-0.605819
49	C	7.198596	-0.210943	-0.367211
50	C	7.219676	-0.550997	0.988826
51	C	8.169742	-0.703879	-1.248977
52	C	8.218444	-1.394691	1.459985
53	H	6.453829	-0.148828	1.668667
54	C	9.160671	-1.542646	-0.755057

55	H	8.152273	-0.427528	-2.309264
56	C	9.186057	-1.890254	0.592846
57	H	8.240596	-1.666722	2.520529
58	H	9.926482	-1.933283	-1.433558
59	H	-9.345436	-0.184196	-1.073786
60	H	9.970058	-2.55437	0.970784

di(phenyl-triazole)-coumarin

Conformer 1 (+1.16 kcal/mol vs Conformer 2)

Total Energy (PM3) : 0.068795 Hartree

Imaginary frequency: 0

Atom#	Symbol	X	Y	Z
1	N	-0.822207	0.529879	1.784939
2	C	-1.070462	0.981917	0.393387
3	C	0.568935	0.830156	2.214457
4	C	-0.068548	0.397822	-0.599178
5	H	-1.026708	2.09111	0.398673
6	H	-2.103986	0.715349	0.092455
7	C	1.612629	0.249065	1.266541
8	H	0.648665	1.934581	2.275997
9	H	0.736738	0.451737	3.243172
10	C	1.401007	0.666991	-0.207289
11	H	-0.28907	0.789936	-1.614469
12	H	-0.210463	-0.701161	-0.672546
13	H	2.623472	0.536188	1.622408
14	H	1.590987	-0.859939	1.313
15	N	1.757207	2.122191	-0.410856
16	C	1.089981	3.057876	-1.208686
17	C	1.876696	4.19654	-1.140631
18	H	0.153485	2.875566	-1.740778
19	N	2.912768	2.680678	0.078516
20	N	2.981098	3.885862	-0.328239
21	C	2.322572	-0.130343	-1.086135
22	C	3.56436	-0.680634	-0.796777
23	N	3.975066	-1.258936	-1.99801
24	H	4.141137	-0.685921	0.13126
25	N	2.056423	-0.410987	-2.43927
26	N	3.012749	-1.070232	-2.959523
27	C	1.699409	5.529867	-1.7779
28	O	0.3388	5.924264	-1.830377
29	H	1.958905	5.488311	-2.851032
30	H	2.333525	6.297678	-1.282482
31	C	-0.173221	6.56868	-0.717222
32	C	-1.57315	6.603465	-0.649082
33	C	0.606984	7.20393	0.254417

34	C	-2.179238	7.27832	0.402525
35	H	-2.180271	6.110987	-1.416603
36	C	-0.021002	7.869793	1.299781
37	H	1.704417	7.167931	0.184233
38	C	-1.408961	7.908214	1.376116
39	H	-3.2719	7.311767	0.466019
40	H	0.584154	8.365893	2.065621
41	C	5.230632	-1.99625	-2.237056
42	C	5.106529	-3.511324	-2.01418
43	H	6.017007	-1.575493	-1.567836
44	H	5.558122	-1.811563	-3.280664
45	O	4.74108	-3.862172	-0.694884
46	H	6.048819	-4.00215	-2.325368
47	H	4.27751	-3.953261	-2.596471
48	C	5.764742	-3.999431	0.231466
49	C	6.942165	-3.245363	0.228161
50	C	5.509021	-4.926431	1.25146
51	C	7.870269	-3.433005	1.246559
52	H	7.132652	-2.503892	-0.561329
53	C	6.446049	-5.091473	2.26306
54	H	4.580165	-5.508465	1.253852
55	C	7.625658	-4.351611	2.260718
56	H	8.796073	-2.847974	1.248772
57	H	6.254753	-5.810919	3.066503
58	H	-1.896959	8.433362	2.203223
59	H	8.360165	-4.491915	3.060487
60	C	-1.444399	-0.684177	2.234515
61	O	-0.950495	-1.314912	3.153984
62	C	-2.730594	-1.094594	1.594872
63	C	-2.773702	-2.072949	0.66348
64	C	-3.980993	-0.473182	2.056242
65	C	-4.044451	-2.478925	0.119996
66	H	-1.864192	-2.570269	0.302756
67	C	-5.218439	-1.859652	0.585256
68	C	-4.158423	-3.479345	-0.85758
69	C	-6.479693	-2.222115	0.099443
70	C	-5.394906	-3.845486	-1.344416
71	H	-3.251443	-3.968997	-1.231252
72	C	-6.574828	-3.223584	-0.872977
73	H	-7.381322	-1.7139	0.478655
74	H	-5.463135	-4.628182	-2.115632
75	O	-5.199791	-0.86967	1.537157
76	O	-4.183816	0.40007	2.869081
77	N	-7.842207	-3.539412	-1.467507
78	C	-9.059583	-3.169135	-0.709833
79	H	-9.903273	-3.11419	-1.410163
80	H	-9.310224	-3.893778	0.079541
81	H	-8.937485	-2.17987	-0.239983

82	C	-7.975003	-4.862805	-2.118424
83	H	-8.149123	-5.678592	-1.400677
84	H	-8.824004	-4.826867	-2.813646
85	H	-7.06795	-5.101971	-2.696248

Conformer 2 (most stable)

Total Energy (PM3) : 0.066945 Hartree

Imaginary frequency: 0

Atom#	Symbol	X	Y	Z
1	N	0.56831	-1.500694	1.449964
2	C	1.787883	-0.981115	2.124056
3	C	0.48791	-1.052524	0.035057
4	C	1.938717	0.531678	2.005714
5	H	2.648955	-1.50376	1.657385
6	H	1.786706	-1.278436	3.192159
7	C	0.606526	0.460171	-0.116992
8	H	1.29755	-1.57798	-0.510825
9	H	-0.464356	-1.403161	-0.411924
10	C	1.877472	1.034342	0.546366
11	H	2.885127	0.842749	2.496052
12	H	1.13362	1.039362	2.576824
13	H	0.563436	0.72197	-1.194063
14	H	-0.275584	0.95711	0.342412
15	N	3.113442	0.630973	-0.224847
16	C	4.366819	0.295974	0.295953
17	C	5.16908	0.113411	-0.819782
18	H	4.602451	0.213462	1.359401
19	N	3.185043	0.676988	-1.595735
20	N	4.369281	0.364579	-1.947461
21	C	1.823527	2.535068	0.539424
22	C	0.954977	3.398779	-0.112534
23	N	1.411763	4.672638	0.230233
24	H	0.093529	3.194576	-0.752713
25	N	2.748855	3.3347	1.237943
26	N	2.50221	4.569872	1.059049
27	C	6.60785	-0.253007	-0.916773
28	O	6.946071	-1.328219	-0.055304
29	H	7.245887	0.556246	-0.518847
30	H	6.899818	-0.459697	-1.969739
31	C	6.76343	-2.609569	-0.542945
32	C	6.769497	-3.616726	0.432958
33	C	6.641309	-2.928815	-1.899464
34	C	6.650846	-4.941492	0.034128
35	H	6.872751	-3.362814	1.49372
36	C	6.519529	-4.260933	-2.274854
37	H	6.639832	-2.126021	-2.652045
38	C	6.523977	-5.265844	-1.313715

39	H	6.656588	-5.735908	0.787611
40	H	6.420897	-4.516603	-3.334889
41	C	0.82831	5.962372	-0.185546
42	C	-0.290872	6.459226	0.742547
43	H	0.439849	5.855911	-1.225254
44	H	1.634882	6.723256	-0.21628
45	O	-1.40611	5.594413	0.802198
46	H	-0.581401	7.485208	0.444646
47	H	0.022644	6.482556	1.802219
48	C	-2.374587	5.730342	-0.180443
49	C	-2.131988	6.178968	-1.482193
50	C	-3.656173	5.313401	0.207686
51	C	-3.183873	6.224822	-2.390883
52	H	-1.121504	6.480002	-1.794395
53	C	-4.689132	5.359406	-0.718747
54	H	-3.837065	4.94682	1.225116
55	C	-4.457967	5.818577	-2.013146
56	H	-3.001511	6.579264	-3.410792
57	H	-5.692811	5.032278	-0.426932
58	H	6.428667	-6.313115	-1.616849
59	H	-5.280476	5.855895	-2.734614
60	C	-0.646731	-1.622299	2.208719
61	O	-0.614526	-1.543227	3.424756
62	C	-1.896676	-1.988571	1.476038
63	C	-2.227927	-3.279556	1.250052
64	C	-2.824983	-0.921003	1.079965
65	C	-3.483445	-3.585778	0.612803
66	H	-1.570783	-4.108077	1.542448
67	C	-4.350027	-2.535444	0.261441
68	C	-3.883774	-4.902378	0.337039
69	C	-5.58858	-2.776933	-0.342574
70	C	-5.100741	-5.154305	-0.259369
71	H	-3.21712	-5.731443	0.602386
72	C	-5.97299	-4.096285	-0.606852
73	H	-6.243753	-1.93224	-0.611057
74	H	-5.393891	-6.193767	-0.473273
75	O	-4.035621	-1.216155	0.487451
76	O	-2.727336	0.284783	1.163686
77	N	-7.186292	-4.368357	-1.322986
78	C	-8.227248	-3.315018	-1.32141
79	H	-8.895625	-3.483513	-2.175923
80	H	-8.832659	-3.311978	-0.40244
81	H	-7.770137	-2.318647	-1.43344
82	C	-7.767572	-5.723147	-1.183573
83	H	-8.334358	-5.852806	-0.249272
84	H	-8.446888	-5.900617	-2.027652
85	H	-6.975624	-6.4885	-1.213464

BDP-DSBDP 7

Conformer 1 (from figure 3)

Total Energy (PM3) : -0.311252 Hartree Imaginary frequency: 0

Total Energy (B3LYP/6-31+G(d,p)) : -3992.313442 Hartree

Atom#	Symbol	X	Y	Z
1	N	-4.128064	-2.784805	3.139191
2	C	-4.717643	-4.014419	2.566307
3	C	-3.338268	-2.035025	2.13721
4	C	-3.696378	-4.915033	1.875831
5	H	-5.514865	-3.700883	1.861235
6	H	-5.22371	-4.568657	3.38089
7	C	-2.277292	-2.884752	1.444347
8	H	-4.054946	-1.60414	1.407302
9	H	-2.863631	-1.172754	2.645757
10	C	-2.853002	-4.175343	0.813993
11	H	-4.211587	-5.794394	1.436866
12	H	-2.998241	-5.335422	2.629531
13	H	-1.749399	-2.270345	0.686864
14	H	-1.496727	-3.184372	2.174731
15	N	-3.671206	-3.846672	-0.414496
16	C	-4.92718	-4.342745	-0.773022
17	C	-5.191457	-3.761963	-2.004524
18	H	-5.530045	-5.030853	-0.176267
19	N	-3.198955	-3.031877	-1.414698
20	N	-4.078948	-2.970339	-2.334005
21	C	-1.724269	-5.053843	0.353831
22	C	-0.434571	-4.713885	-0.030905
23	N	0.145828	-5.92631	-0.406734
24	H	0.064505	-3.743037	-0.066499
25	N	-1.845991	-6.447064	0.189799
26	N	-0.759752	-6.946907	-0.24325
27	H	-3.550072	-3.019224	3.919194
28	C	-6.387651	-3.872953	-2.882702
29	O	-7.602496	-3.795836	-2.151478
30	H	-6.467646	-4.8792	-3.330077
31	H	-6.361029	-3.11186	-3.692894
32	C	-7.986175	-2.535282	-1.731482
33	C	-8.860899	-2.508578	-0.636146
34	C	-7.588518	-1.350453	-2.361857
35	C	-9.307877	-1.284588	-0.157359
36	H	-9.187006	-3.44075	-0.160972
37	C	-8.038817	-0.132316	-1.871327
38	H	-6.911999	-1.396343	-3.229138
39	C	-8.886274	-0.096808	-0.761621
40	H	-9.986068	-1.248	0.702883

41	H	-7.723072	0.80129	-2.350847
42	C	1.524452	-6.133782	-0.888961
43	C	2.532859	-6.41748	0.234422
44	H	1.837407	-5.231367	-1.464227
45	H	1.527535	-6.987431	-1.597716
46	O	2.671982	-5.354494	1.156813
47	H	3.505055	-6.702958	-0.21181
48	H	2.203077	-7.237604	0.898249
49	C	3.570591	-4.349314	0.840219
50	C	3.872648	-3.933838	-0.460342
51	C	4.134354	-3.701229	1.949469
52	C	4.755561	-2.877304	-0.652383
53	H	3.410527	-4.426052	-1.329093
54	C	5.006438	-2.641074	1.745657
55	H	3.887426	-4.0254	2.967531
56	C	5.325098	-2.232231	0.446132
57	H	5.000979	-2.548186	-1.668964
58	H	5.45122	-2.124513	2.604456
59	C	6.258742	-1.111716	0.229561
60	C	7.627793	-1.367694	0.102333
61	C	5.747473	0.191049	0.164741
62	C	8.429508	-2.558088	0.229748
63	N	8.55126	-0.310844	-0.138253
64	C	4.41141	0.700304	0.325069
65	N	6.571235	1.331484	-0.083754
66	C	9.772562	-2.200182	0.090496
67	C	7.957265	-3.930073	0.474311
68	C	9.832738	-0.784442	-0.129076
69	B	8.125901	1.200898	-0.469195
70	C	4.449867	2.084937	0.167619
71	C	3.191743	-0.066755	0.621145
72	C	5.808258	2.46524	-0.09078
73	C	10.919348	-3.137147	0.157945
74	H	7.002499	-3.953479	1.016393
75	H	7.818845	-4.461724	-0.477384
76	H	8.696743	-4.493005	1.070749
77	C	10.919934	0.159976	-0.275735
78	F	8.94939	2.080482	0.210193
79	F	8.313427	1.489739	-1.802567
80	C	3.266643	2.973854	0.241898
81	H	2.924238	-0.719326	-0.221508
82	H	3.326379	-0.70415	1.506683
83	H	2.345976	0.615955	0.811066
84	C	6.385846	3.769988	-0.33771
85	H	10.740824	-3.969268	-0.553436
86	H	11.846104	-2.636198	-0.193564
87	C	11.12568	-3.684689	1.5558
88	C	12.193035	-0.136934	-0.572169

89	H	10.606022	1.231028	-0.130015
90	H	3.505562	3.859737	0.870211
91	H	2.44839	2.426451	0.762823
92	C	2.80388	3.415254	-1.131282
93	H	7.365076	3.794514	-0.856209
94	C	5.81752	4.925506	0.041506
95	H	11.303311	-2.88437	2.284706
96	H	10.239788	-4.249146	1.89242
97	H	11.985718	-4.364766	1.592091
98	H	12.520668	-1.175933	-0.733626
99	C	13.21707	0.89398	-0.701227
100	H	1.909762	4.047676	-1.061432
101	H	3.58048	3.994787	-1.64864
102	H	2.554097	2.557988	-1.769345
103	H	4.846777	4.933836	0.566135
104	C	6.436027	6.221714	-0.209774
105	C	14.535282	0.524594	-0.991631
106	C	12.903946	2.24822	-0.540286
107	C	5.779573	7.388751	0.197435
108	C	7.675475	6.32074	-0.85103
109	C	15.519904	1.496536	-1.11653
110	H	14.791594	-0.533068	-1.121199
111	C	13.892579	3.215382	-0.666401
112	H	11.861571	2.528364	-0.31423
113	C	6.356705	8.630534	-0.036348
114	H	4.808486	7.323127	0.70136
115	C	8.247766	7.564812	-1.082137
116	H	8.184539	5.395505	-1.165397
117	C	15.20127	2.841411	-0.95429
118	H	16.549892	1.202878	-1.343886
119	H	13.639352	4.272997	-0.539316
120	C	7.58954	8.721033	-0.67556
121	H	5.839291	9.540915	0.28367
122	H	9.218055	7.633495	-1.584822
123	H	15.980059	3.604383	-1.053866
124	H	8.040954	9.701638	-0.858
125	C	-9.322447	1.199817	-0.213229
126	C	-10.510808	1.775256	-0.671604
127	C	-8.53639	1.821053	0.761575
128	C	-11.480374	1.328167	-1.635105
129	N	-10.991268	3.030681	-0.182743
130	C	-7.307453	1.425374	1.397824
131	N	-8.89174	3.079988	1.340132
132	C	-12.495013	2.281393	-1.698814
133	C	-11.438734	0.099206	-2.441024
134	C	-12.169502	3.337793	-0.78897
135	B	-10.189115	3.919499	0.892282
136	C	-6.960772	2.414418	2.315852

137	C	-6.530775	0.200415	1.156577
138	C	-7.96279	3.436653	2.266354
139	C	-13.686696	2.213913	-2.574084
140	H	-10.483078	0.006785	-2.97623
141	H	-11.550046	-0.791188	-1.806458
142	H	-12.256184	0.10166	-3.181982
143	C	-12.956539	4.560061	-0.53556
144	F	-10.981684	4.215889	1.978772
145	F	-9.821758	5.130708	0.347591
146	C	-5.771366	2.399208	3.197491
147	H	-7.140358	-0.697036	1.335423
148	H	-6.175359	0.156331	0.117167
149	H	-5.652975	0.161256	1.825401
150	C	-8.002943	4.66925	3.07665
151	H	-13.5076	1.427372	-3.342873
152	H	-13.796372	3.17074	-3.122073
153	C	-14.950027	1.902745	-1.798867
154	H	-13.855752	4.315816	0.049057
155	H	-12.393299	5.325439	0.018321
156	H	-13.289124	4.999935	-1.4862
157	H	-5.248704	1.423955	3.064299
158	H	-6.10248	2.431732	4.254443
159	C	-4.826878	3.547173	2.908199
160	H	-8.684819	5.42926	2.668992
161	H	-8.329173	4.437106	4.100347
162	H	-6.990521	5.104712	3.139938
163	H	-15.819377	1.849425	-2.466438
164	H	-14.876362	0.941597	-1.274151
165	H	-15.160313	2.671864	-1.042989
166	H	-3.96749	3.535263	3.5898
167	H	-4.438601	3.505811	1.882886
168	H	-5.335338	4.519194	3.027388

Conformer 2 (from figure S11)

Total Energy (PM3) : -0.321138 Hartree Imaginary frequency: 0

Total Energy (B3LYP/6-31+G(d,p)) : -3992.296562 Hartree

Atom#	Symbol	X	Y	Z
1	N	1.182038	4.679153	-1.976083
2	C	0.443096	4.607476	-0.696403
3	C	0.414716	4.107645	-3.103546
4	C	-0.100698	3.216983	-0.378129
5	H	-0.37193	5.356838	-0.734926
6	H	1.140968	4.927045	0.113568
7	C	-0.098681	2.696799	-2.832927
8	H	-0.419523	4.803285	-3.322676

9	H	1.064707	4.110753	-4.000467
10	C	-0.924345	2.602235	-1.529878
11	H	-0.692681	3.257511	0.559892
12	H	0.751401	2.528086	-0.160676
13	H	-0.682638	2.341616	-3.705944
14	H	0.756277	1.991363	-2.741003
15	N	-2.256269	3.303256	-1.675082
16	C	-2.962164	3.987999	-0.681342
17	C	-4.180995	4.292261	-1.267875
18	H	-2.582141	4.196889	0.32157
19	N	-3.04076	3.188674	-2.797121
20	N	-4.151684	3.76914	-2.572107
21	C	-1.23549	1.159363	-1.240862
22	C	-1.454963	0.106994	-2.121016
23	N	-1.755339	-0.97861	-1.297273
24	H	-1.427986	0.077316	-3.213069
25	N	-1.417943	0.648892	0.057398
26	N	-1.71999	-0.586818	0.01856
27	H	2.060318	4.19886	-1.875412
28	C	-5.358469	5.018643	-0.72017
29	O	-5.788128	4.48667	0.524489
30	H	-6.191295	5.045064	-1.456579
31	H	-5.093432	6.051535	-0.433795
32	C	-6.569454	3.348018	0.477859
33	C	-6.617972	2.610159	1.66985
34	C	-7.315537	2.954504	-0.639163
35	C	-7.394853	1.461311	1.723704
36	H	-6.046386	2.932465	2.547863
37	C	-8.08545	1.800846	-0.574407
38	H	-7.273867	3.554779	-1.561194
39	C	-8.116208	1.046145	0.600253
40	H	-7.435374	0.871263	2.646516
41	H	-8.663335	1.479681	-1.448505
42	C	-8.892559	-0.205716	0.650056
43	C	-10.226074	-0.175016	1.054468
44	C	-8.264321	-1.406105	0.288834
45	C	-11.078775	0.912232	1.463783
46	N	-11.034982	-1.355435	1.119079
47	C	-6.926286	-1.685333	-0.150065
48	N	-8.939454	-2.664036	0.323924
49	C	-12.335704	0.388271	1.74947
50	C	-10.719418	2.334041	1.565472
51	C	-12.289452	-1.027301	1.522247
52	B	-10.481289	-2.822992	0.75335
53	C	-6.818199	-3.061003	-0.356432
54	C	-5.836557	-0.719846	-0.350667
55	C	-8.083113	-3.654005	-0.049823
56	C	-13.516697	1.161346	2.196457

57	H	-9.923823	2.486877	2.308275
58	H	-10.351163	2.718346	0.60358
59	H	-11.597125	2.930429	1.867027
60	C	-13.407152	-1.976752	1.684449
61	F	-10.597978	-3.680115	1.825037
62	F	-11.227963	-3.378748	-0.261791
63	C	-5.602214	-3.781065	-0.796856
64	H	-6.102016	0.022953	-1.116435
65	H	-5.615789	-0.173518	0.577804
66	H	-4.919625	-1.240798	-0.672982
67	C	-8.419919	-5.089517	-0.110821
68	H	-13.251646	2.243609	2.183538
69	H	-14.334429	1.032999	1.459724
70	C	-13.984256	0.748965	3.576605
71	H	-14.122091	-1.859586	0.85759
72	H	-13.082489	-3.026816	1.703892
73	H	-13.94566	-1.757437	2.623032
74	H	-4.756094	-3.050126	-0.861758
75	H	-5.313507	-4.515631	-0.019083
76	C	-5.794771	-4.475131	-2.129141
77	H	-7.969088	-5.618584	0.740762
78	H	-9.502603	-5.278935	-0.090373
79	H	-8.004466	-5.529625	-1.033995
80	H	-14.237016	-0.32479	3.605916
81	H	-13.212312	0.923343	4.3365
82	H	-14.878034	1.309844	3.876326
83	H	-6.627196	-5.19799	-2.081523
84	H	-6.02852	-3.762044	-2.929583
85	H	-4.892225	-5.024239	-2.425286
86	C	-2.158138	-2.3305	-1.738318
87	C	-1.175027	-3.437716	-1.335605
88	H	-2.288427	-2.299133	-2.840008
89	H	-3.163179	-2.566539	-1.304175
90	O	-0.04758	-3.45811	-2.192996
91	H	-1.639777	-4.421837	-1.530563
92	H	-0.905911	-3.393325	-0.257221
93	C	1.148323	-2.967197	-1.701988
94	C	1.459949	-2.840671	-0.344056
95	C	2.094593	-2.651308	-2.687956
96	C	2.714716	-2.375522	0.028338
97	H	0.712347	-3.097137	0.42197
98	C	3.34586	-2.188739	-2.303687
99	H	1.853855	-2.771634	-3.750808
100	C	3.655535	-2.039907	-0.948587
101	H	2.963505	-2.2661	1.09051
102	H	4.092343	-1.934052	-3.065167
103	C	4.972001	-1.503701	-0.556953
104	C	6.042627	-2.374026	-0.350837

105	C	5.111592	-0.115146	-0.389155
106	C	6.165765	-3.811607	-0.345557
107	N	7.332051	-1.880443	0.002902
108	C	4.153202	0.951463	-0.480997
109	N	6.351225	0.501313	-0.050246
110	C	7.471805	-4.138464	0.021478
111	C	5.116783	-4.79485	-0.657483
112	C	8.188181	-2.914945	0.247659
113	B	7.728778	-0.324352	0.015889
114	C	4.807816	2.153981	-0.206656
115	C	2.726566	0.805262	-0.806462
116	C	6.186814	1.857195	0.048995
117	C	8.006892	-5.515288	0.14671
118	H	4.108999	-4.410553	-0.450343
119	H	5.159599	-5.074763	-1.719355
120	H	5.257131	-5.71319	-0.060567
121	C	9.52791	-2.610904	0.703679
122	F	8.498339	-0.050348	1.132462
123	F	8.529364	-0.00973	-1.059522
124	C	4.174502	3.493765	-0.209187
125	H	2.595594	0.416928	-1.827608
126	H	2.238406	0.09934	-0.117643
127	H	2.181033	1.762119	-0.737102
128	C	7.30752	2.729297	0.332434
129	H	7.80126	-6.063306	-0.795508
130	H	9.112936	-5.490647	0.243749
131	C	7.400888	-6.25677	1.32115
132	C	10.571429	-3.452283	0.714454
133	H	9.650394	-1.549445	1.057895
134	H	3.516282	3.586191	-1.103444
135	H	4.951006	4.280497	-0.328333
136	C	3.374092	3.751389	1.053672
137	H	8.319803	2.294816	0.206743
138	C	7.20354	4.00464	0.738006
139	H	7.586509	-5.738472	2.269982
140	H	6.308297	-6.353676	1.204378
141	H	7.816163	-7.268461	1.407809
142	H	10.479142	-4.49056	0.358731
143	C	11.887715	-3.044656	1.193203
144	H	2.682919	4.601548	0.917015
145	H	2.7605	2.882756	1.331684
146	H	4.023748	3.97891	1.908328
147	H	6.218495	4.481007	0.873327
148	C	8.369362	4.836252	1.013661
149	C	12.936374	-3.97134	1.201279
150	C	12.120961	-1.740913	1.644623
151	C	8.187096	6.163151	1.420066
152	C	9.667921	4.333033	0.880725

153	C	14.194415	-3.59598	1.655345
154	H	12.765364	-4.994827	0.84857
155	C	13.380837	-1.37152	2.097362
156	H	11.288224	-1.018062	1.631452
157	C	9.287438	6.968063	1.686486
158	H	7.174504	6.568319	1.528438
159	C	10.764404	5.142243	1.148384
160	H	9.800922	3.286782	0.561787
161	C	14.418793	-2.297816	2.103678
162	H	15.011933	-4.324311	1.659838
163	H	13.555329	-0.349315	2.448766
164	C	10.576088	6.460362	1.551321
165	H	9.139679	8.005508	2.003907
166	H	11.777278	4.740328	1.041502
167	H	15.411791	-2.005862	2.460468
168	H	11.440717	7.097991	1.762144

Coum-BDP 13

Total Energy (PM3) : -0.271302 Hartree Imaginary frequency: 0

Total Energy (B3LYP/6-31+G(d,p)) : -2652.606677 Hartree

Atom#	Symbol	X	Y	Z
1	N	-3.549344	1.644311	1.229518
2	C	-2.703547	2.728442	1.794137
3	C	-3.59106	1.692994	-0.255613
4	C	-3.10784	4.116508	1.309734
5	H	-1.659333	2.494441	1.500574
6	H	-2.729565	2.69194	2.902046
7	C	-4.01739	3.052601	-0.797707
8	H	-2.577344	1.417277	-0.610687
9	H	-4.275407	0.905813	-0.631982
10	C	-3.177572	4.21771	-0.232668
11	H	-2.39082	4.865298	1.713717
12	H	-4.098221	4.395327	1.724316
13	H	-3.978961	3.034871	-1.905848
14	H	-5.082386	3.246801	-0.545168
15	N	-1.781415	4.246876	-0.811161
16	C	-0.657937	4.800288	-0.185663
17	C	0.346907	4.707287	-1.133397
18	H	-0.661591	5.18395	0.838616
19	N	-1.458031	3.874579	-2.090887
20	N	-0.224153	4.123893	-2.280045
21	C	1.773373	5.123324	-1.065351
22	O	2.427657	4.593928	0.078179
23	H	1.858543	6.20933	-0.882984

24	H	2.312454	4.869906	-2.004494
25	C	2.978301	3.332656	-0.036104
26	C	3.297356	2.71738	1.183816
27	C	3.268842	2.703904	-1.252183
28	C	3.904312	1.46939	1.175053
29	H	3.075728	3.216756	2.133963
30	C	3.872398	1.453297	-1.247748
31	H	3.012824	3.201512	-2.200346
32	C	4.190029	0.834104	-0.037068
33	H	4.159761	0.978682	2.121222
34	H	4.098831	0.952569	-2.196092
35	C	-4.728623	1.240511	1.948005
36	O	-4.874764	1.58505	3.107967
37	C	-5.669693	0.293606	1.278848
38	C	-5.49453	-1.045309	1.346236
39	C	-6.863336	0.837517	0.616838
40	C	-6.476301	-1.916267	0.752694
41	H	-4.626723	-1.493934	1.845551
42	C	-7.609866	-1.356001	0.136721
43	C	-6.350725	-3.314234	0.774401
44	C	-8.601812	-2.155487	-0.440845
45	C	-7.319954	-4.113639	0.207867
46	H	-5.471377	-3.765496	1.249018
47	C	-8.461337	-3.547586	-0.407641
48	H	-9.475949	-1.686393	-0.921403
49	H	-7.200109	-5.207909	0.229673
50	O	-7.811565	0.002139	0.064248
51	O	-7.208676	1.984679	0.429567
52	N	-9.404565	-4.387682	-1.086556
53	C	-10.741141	-3.818249	-1.373613
54	H	-11.195607	-4.390316	-2.193093
55	H	-11.417925	-3.856053	-0.506696
56	H	-10.654151	-2.767642	-1.694493
57	C	-9.483266	-5.804007	-0.661701
58	H	-10.078446	-5.944684	0.253135
59	H	-9.947122	-6.385901	-1.468989
60	H	-8.475217	-6.210332	-0.48119
61	C	-3.822384	5.47502	-0.590085
62	C	-4.363949	6.494268	-0.883258
63	H	-4.850195	7.404785	-1.147858
64	C	4.826986	-0.495168	-0.036019
65	C	6.221436	-0.58516	-0.025782
66	C	4.020435	-1.637602	-0.037267
67	C	7.245771	0.424994	-0.005049
68	N	6.907521	-1.840743	-0.023408
69	C	2.591363	-1.80074	-0.027184
70	N	4.567635	-2.958746	-0.038256
71	C	8.482475	-0.216253	0.020162

72	C	7.063762	1.883802	-0.021839
73	C	8.250528	-1.629268	0.003616
74	B	6.147407	-3.25755	-0.087785
75	C	2.314182	-3.166489	-0.018755
76	C	1.572666	-0.740611	-0.019461
77	C	3.560232	-3.871808	-0.023699
78	C	9.80139	0.455306	0.039028
79	H	6.417159	2.194267	-0.854817
80	H	6.594539	2.232423	0.908891
81	H	8.039042	2.388358	-0.129124
82	C	9.273528	-2.692747	0.011287
83	F	6.52679	-4.070153	0.957317
84	F	6.479528	-3.937901	-1.238974
85	C	0.965565	-3.776906	0.004192
86	H	1.705306	-0.07043	0.84177
87	H	1.636744	-0.126471	-0.928938
88	H	0.562237	-1.180084	0.03297
89	C	3.742639	-5.336085	-0.009623
90	H	9.64898	1.525739	-0.230587
91	H	10.447589	0.020947	-0.749394
92	C	10.477299	0.352552	1.390464
93	H	9.734022	-2.766493	1.007559
94	H	8.865898	-3.681817	-0.244472
95	H	10.071889	-2.455049	-0.705625
96	H	0.213553	-2.960684	0.103355
97	H	0.865756	-4.403224	0.912823
98	C	0.687236	-4.602125	-1.234816
99	H	4.754093	-5.645868	-0.309197
100	H	3.553637	-5.730191	0.99893
101	H	3.015173	-5.80693	-0.693551
102	H	11.448717	0.86303	1.385363
103	H	9.868863	0.807067	2.182792
104	H	10.655117	-0.693611	1.675141
105	H	-0.30418	-5.069029	-1.186342
106	H	0.723155	-3.992162	-2.146081
107	H	1.431872	-5.408248	-1.350002

Coum-DSBDP 11

Conformer 1 (from figure 3)

Total Energy (PM3) : -0.106621 Hartree Imaginary frequency: 0

Total Energy (B3LYP/6-31+G(d,p)) : -3434.433533 Hartree

Atom#	Symbol	X	Y	Z
1	N	7.059804	1.351142	-1.104188

2	C	8.098522	0.313517	-1.342521
3	C	6.468825	1.234542	0.25439
4	C	7.601612	-1.10234	-1.067928
5	H	8.953471	0.568247	-0.682101
6	H	8.476929	0.38621	-2.382179
7	C	5.937552	-0.162056	0.556423
8	H	7.263299	1.526775	0.970807
9	H	5.657413	1.981044	0.372254
10	C	6.991884	-1.269691	0.341905
11	H	8.437061	-1.81671	-1.226178
12	H	6.828739	-1.385061	-1.812536
13	H	5.539491	-0.183513	1.591576
14	H	5.068427	-0.385333	-0.099512
15	N	8.058452	-1.207994	1.408349
16	C	9.421263	-1.498218	1.260183
17	C	9.93676	-1.417293	2.543572
18	H	9.905257	-1.740565	0.312089
19	N	7.779264	-0.995781	2.734582
20	N	8.863005	-1.101564	3.396783
21	C	6.336162	-2.618514	0.440499
22	C	5.045986	-2.963114	0.816329
23	N	5.025344	-4.358001	0.746521
24	H	4.199024	-2.339149	1.109925
25	N	7.015285	-3.820722	0.161111
26	N	6.251151	-4.822302	0.336747
27	C	11.318981	-1.609541	3.012302
28	H	11.3816	-2.4287	3.741544
29	H	11.705862	-0.703302	3.497786
30	C	3.874042	-5.23524	1.031877
31	C	3.155669	-5.742912	-0.226986
32	H	3.157125	-4.677371	1.678414
33	H	4.229179	-6.10813	1.617244
34	O	2.647782	-4.718315	-1.05575
35	H	2.364784	-6.459403	0.068328
36	H	3.843385	-6.255181	-0.925101
37	C	1.435625	-4.145843	-0.717291
38	C	0.874178	-4.142501	0.563132
39	C	0.797732	-3.488144	-1.781594
40	C	-0.334904	-3.489191	0.778174
41	H	1.387685	-4.631849	1.404016
42	C	-0.401045	-2.830279	-1.552024
43	H	1.248644	-3.482107	-2.781582
44	C	-0.972379	-2.832061	-0.273767
45	H	-0.781517	-3.483629	1.779143
46	H	-0.902208	-2.303743	-2.372827
47	C	6.227856	1.766663	-2.199225
48	O	6.587874	1.552494	-3.344152
49	C	5.003723	2.56888	-1.895727

50	C	5.032407	3.919222	-1.827906
51	C	3.723454	1.862806	-1.757253
52	C	3.80937	4.64073	-1.58114
53	H	5.962798	4.487408	-1.951537
54	C	2.608954	3.924224	-1.432823
55	C	3.765031	6.040398	-1.476738
56	C	1.394725	4.567609	-1.173553
57	C	2.574253	6.688172	-1.224895
58	H	4.691157	6.615161	-1.5958
59	C	1.371205	5.961618	-1.060684
60	H	0.475454	3.970945	-1.044772
61	H	2.559091	7.786171	-1.142585
62	O	2.553058	2.553463	-1.526238
63	O	3.460567	0.678678	-1.793619
64	N	0.169058	6.639871	-0.668915
65	C	-1.102469	5.891885	-0.794904
66	H	-1.870386	6.364129	-0.156139
67	H	-1.484807	5.861993	-1.826089
68	H	-0.973882	4.847546	-0.444698
69	C	0.029838	8.056642	-1.075121
70	H	-0.294319	8.172954	-2.120161
71	H	-0.715462	8.53519	-0.426337
72	H	0.986963	8.588129	-0.950215
73	H	11.98359	-1.853417	2.17359
74	C	-2.236983	-2.112203	-0.03737
75	C	-3.457942	-2.771436	-0.203693
76	C	-2.180415	-0.759077	0.328346
77	C	-3.816127	-4.092117	-0.655535
78	N	-4.692922	-2.096976	0.019132
79	C	-1.064397	0.127696	0.514345
80	N	-3.348704	0.025471	0.569205
81	C	-5.209205	-4.172928	-0.715219
82	C	-2.903259	-5.189988	-1.010594
83	C	-5.744005	-2.908352	-0.301064
84	B	-4.818579	-0.617589	0.629775
85	C	-1.561521	1.386083	0.856395
86	C	0.36369	-0.188912	0.363125
87	C	-2.991307	1.307664	0.880648
88	C	-5.979681	-5.36798	-1.134333
89	H	-1.923056	-4.826637	-1.347299
90	H	-2.741126	-5.846765	-0.144589
91	H	-3.333302	-5.802734	-1.822413
92	C	-7.084443	-2.366954	-0.223549
93	F	-5.775584	0.100866	-0.064548
94	F	-5.270982	-0.65031	1.930289
95	C	-0.721382	2.566961	1.161263
96	H	0.684126	-0.929881	1.108776
97	H	0.575935	-0.605809	-0.632476

98	H	0.977596	0.71902	0.490526
99	C	-3.975276	2.334786	1.159319
100	H	-5.640305	-6.237563	-0.535163
101	H	-7.055164	-5.237065	-0.89014
102	C	-5.816213	-5.660678	-2.612166
103	C	-8.223737	-3.073033	-0.211861
104	H	-7.111135	-1.243961	-0.155027
105	H	-1.08918	3.449175	0.580263
106	H	0.313677	2.366238	0.799012
107	C	-0.703701	2.885519	2.641482
108	H	-4.971023	2.001958	1.512402
109	C	-3.738655	3.643445	0.979737
110	H	-6.14438	-4.817993	-3.233095
111	H	-4.760323	-5.862986	-2.859111
112	H	-6.400744	-6.540263	-2.909017
113	H	-8.220794	-4.173189	-0.263767
114	C	-9.530592	-2.430227	-0.127563
115	H	-0.056863	3.74677	2.851617
116	H	-1.709616	3.127138	3.011049
117	H	-0.331323	2.039118	3.232433
118	H	-2.754833	3.993735	0.621044
119	C	-4.736169	4.673653	1.237491
120	C	-10.688382	-3.216207	-0.140444
121	C	-9.647158	-1.03905	-0.033052
122	C	-4.412728	6.016064	1.007487
123	C	-6.010645	4.344504	1.709825
124	C	-11.938828	-2.616273	-0.061328
125	H	-10.60884	-4.306898	-0.212695
126	C	-10.899984	-0.445017	0.045839
127	H	-8.728177	-0.429597	-0.021079
128	C	-5.351962	7.009309	1.252423
129	H	-3.411943	6.282807	0.629631
130	C	-6.945766	5.342414	1.952665
131	H	-6.252214	3.283053	1.880169
132	C	-12.047069	-1.232027	0.031608
133	H	-12.841916	-3.235231	-0.071702
134	H	-10.982686	0.644213	0.119931
135	C	-6.617639	6.675125	1.725466
136	H	-5.095792	8.058544	1.073082
137	H	-7.941637	5.07777	2.323036
138	H	-13.034344	-0.763106	0.094122
139	H	-7.354855	7.461341	1.917953

Conformer 2 (from figure S11)

Total Energy (PM3) : -0.097397 Hartree Imaginary frequency: 0

Total Energy (B3LYP/6-31+G(d,p)) : -3434.437383 Hartree

Atom#	Symbol	X	Y	Z
1	N	-6.481034	2.120618	0.419036
2	C	-7.248549	1.776228	-0.803129
3	C	-5.05709	2.407241	0.102925
4	C	-6.635623	0.610376	-1.575095
5	H	-7.288229	2.691331	-1.429799
6	H	-8.297922	1.542212	-0.531312
7	C	-4.383902	1.260903	-0.643426
8	H	-5.047402	3.340992	-0.495289
9	H	-4.501359	2.633251	1.035447
10	C	-5.14455	0.826214	-1.917084
11	H	-7.227895	0.443791	-2.502135
12	H	-6.732184	-0.324337	-0.984541
13	H	-3.339128	1.547157	-0.882455
14	H	-4.299856	0.375589	0.021036
15	N	-5.013722	1.855134	-3.015464
16	C	-5.988685	2.171898	-3.971679
17	C	-5.357428	3.050516	-4.83591
18	H	-7.002985	1.764434	-3.962074
19	N	-3.842449	2.494513	-3.328471
20	N	-4.036351	3.200132	-4.371893
21	C	-4.526046	-0.442118	-2.435787
22	C	-3.1824	-0.778805	-2.540274
23	N	-3.187479	-2.047013	-3.12186
24	H	-2.286125	-0.219579	-2.260391
25	N	-5.259799	-1.524594	-2.954327
26	N	-4.480911	-2.453246	-3.342695
27	C	-5.884917	3.74058	-6.024422
28	H	-5.288726	3.510343	-6.917805
29	H	-5.871789	4.830786	-5.889283
30	C	-2.00882	-2.875788	-3.438409
31	C	-1.601551	-3.826715	-2.302902
32	H	-1.159832	-2.198498	-3.691117
33	H	-2.228263	-3.474534	-4.346232
34	O	-1.2577	-3.16842	-1.100288
35	H	-0.78656	-4.487797	-2.655935
36	H	-2.44109	-4.4623	-1.966313
37	C	0.039244	-2.700918	-0.971814
38	C	0.854009	-2.303632	-2.036352
39	C	0.484468	-2.586251	0.353992
40	C	2.12543	-1.805546	-1.774735
41	H	0.495389	-2.367782	-3.074426
42	C	1.751375	-2.078017	0.603239
43	H	-0.162309	-2.889712	1.186049
44	C	2.576972	-1.694215	-0.45929
45	H	2.771753	-1.495195	-2.604117
46	H	2.108931	-1.979452	1.63508
47	C	-6.800384	1.442385	1.644576

48	O	-5.958927	1.347187	2.522081
49	C	-8.193695	0.934977	1.825324
50	C	-8.490044	-0.376003	1.682826
51	C	-9.24112	1.876186	2.248741
52	C	-9.834881	-0.829452	1.928883
53	H	-7.733779	-1.111762	1.380448
54	C	-10.809338	0.101189	2.332129
55	C	-10.212012	-2.173893	1.787842
56	C	-12.127893	-0.28636	2.595247
57	C	-11.507657	-2.568509	2.043713
58	H	-9.463423	-2.9099	1.471662
59	C	-12.485546	-1.631519	2.452525
60	H	-12.870908	0.467189	2.903687
61	H	-11.785488	-3.626797	1.921615
62	O	-10.529371	1.436487	2.491227
63	O	-9.207948	3.070541	2.441227
64	N	-13.852388	-2.03921	2.609523
65	C	-14.742346	-1.148238	3.388879
66	H	-15.782581	-1.367377	3.114689
67	H	-14.634856	-1.279484	4.476193
68	H	-14.538785	-0.091943	3.149906
69	C	-14.104628	-3.468827	2.901622
70	H	-13.94497	-3.725276	3.959792
71	H	-15.146381	-3.699926	2.643213
72	H	-13.449036	-4.109664	2.290597
73	H	-6.921069	3.43766	-6.222418
74	C	3.925964	-1.161038	-0.194925
75	C	5.015909	-2.037655	-0.134413
76	C	4.082538	0.216371	-0.002011
77	C	5.13709	-3.471428	-0.184526
78	N	6.334891	-1.551129	0.086762
79	C	3.123334	1.289187	0.042989
80	N	5.357129	0.825152	0.216885
81	C	6.478139	-3.806522	0.022466
82	C	4.06159	-4.451744	-0.402679
83	C	7.214968	-2.590709	0.20188
84	B	6.73309	0.003082	0.098368
85	C	3.810571	2.47998	0.270369
86	C	1.663109	1.189326	-0.102587
87	C	5.208441	2.174009	0.373992
88	C	7.021379	-5.185583	0.045358
89	H	3.082795	-4.079642	-0.071822
90	H	3.984619	-4.703385	-1.469568
91	H	4.271126	-5.384719	0.149663
92	C	8.597845	-2.294824	0.511442
93	F	7.626975	0.252501	1.124245
94	F	7.401425	0.354502	-1.05348
95	C	3.173695	3.814762	0.363413

96	H	1.390156	0.885943	-1.122871
97	H	1.242933	0.446029	0.589937
98	H	1.188999	2.163711	0.105877
99	C	6.344553	3.04469	0.593497
100	H	6.705542	-5.707552	-0.880999
101	H	8.131217	-5.16203	0.012421
102	C	6.556276	-5.960429	1.261784
103	C	9.635333	-3.133904	0.384223
104	H	8.760147	-1.242559	0.876438
105	H	3.585691	4.363518	1.238486
106	H	2.086843	3.672096	0.561122
107	C	3.369193	4.624027	-0.902054
108	H	7.337478	2.659984	0.286236
109	C	6.259833	4.259192	1.159047
110	H	6.852439	-5.467902	2.196167
111	H	5.457406	-6.056	1.271247
112	H	6.977424	-6.973354	1.271492
113	H	9.503037	-4.163264	0.015775
114	C	10.99743	-2.735455	0.722137
115	H	2.866324	5.596699	-0.829126
116	H	4.433519	4.814469	-1.09575
117	H	2.962837	4.106465	-1.780375
118	H	5.286571	4.666732	1.482277
119	C	7.428179	5.103004	1.380104
120	C	12.039894	-3.659561	0.589067
121	C	11.280799	-1.442947	1.177148
122	C	7.265563	6.366585	1.959457
123	C	8.710667	4.672305	1.023769
124	C	13.341245	-3.292865	0.908109
125	H	11.829703	-4.674249	0.232238
126	C	12.583795	-1.082143	1.494515
127	H	10.452192	-0.721961	1.27587
128	C	8.369735	7.181486	2.175148
129	H	6.265542	6.71396	2.243354
130	C	9.81093	5.491175	1.241726
131	H	8.827411	3.674814	0.57052
132	C	13.61541	-2.005878	1.360845
133	H	14.153626	-4.019226	0.802367
134	H	12.797217	-0.068667	1.849641
135	C	9.642248	6.746444	1.817261
136	H	8.237673	8.16939	2.628467
137	H	10.811212	5.146494	0.959827
138	H	14.64235	-1.720692	1.610955
139	H	10.509852	7.391723	1.988939

Coum-BDP-DSBDP 14

Conformer I

Total Energy (PM3) : -0.437265 Hartree Imaginary frequency: 0

Total Energy (B3LYP/6-31+G(d,p)) : -4735.457893 Hartree

Atom#	Symbol	X	Y	Z
1	N	-3.369518	-1.305921	1.968933
2	C	-4.025055	-2.61726	2.212894
3	C	-2.977122	-1.149423	0.544234
4	C	-3.182697	-3.799502	1.744664
5	H	-4.998779	-2.582166	1.679191
6	H	-4.26419	-2.726002	3.290068
7	C	-2.108757	-2.295787	0.039392
8	H	-3.928673	-1.04545	-0.030345
9	H	-2.445472	-0.184601	0.40905
10	C	-2.734941	-3.688865	0.269618
11	H	-3.748472	-4.73944	1.917977
12	H	-2.271719	-3.886208	2.373019
13	H	-1.876587	-2.133477	-1.032906
14	H	-1.127204	-2.272254	0.561484
15	N	-3.894746	-3.914994	-0.672482
16	C	-5.090261	-4.586658	-0.400231
17	C	-5.761955	-4.60548	-1.612898
18	H	-5.37278	-4.986784	0.576511
19	N	-3.846725	-3.58817	-2.006004
20	N	-4.930658	-3.972336	-2.55325
21	C	-1.719213	-4.760043	-0.012666
22	C	-0.417945	-4.669659	-0.485064
23	N	0.014039	-5.995571	-0.566024
24	H	0.186257	-3.79911	-0.749807
25	N	-1.993951	-6.1301	0.168735
26	N	-0.986905	-6.838289	-0.15029
27	C	-7.104273	-5.143681	-1.964543
28	O	-8.092092	-4.816963	-0.996501
29	H	-7.122335	-6.246829	-1.927348
30	H	-7.419933	-4.803687	-2.974777
31	C	-8.485346	-3.490793	-0.966068
32	C	-8.926007	-3.016211	0.276883
33	C	-8.49126	-2.663055	-2.095371
34	C	-9.31017	-1.68741	0.394104
35	H	-8.956993	-3.680905	1.14774
36	C	-8.876971	-1.335902	-1.96588
37	H	-8.162153	-3.067011	-3.06504
38	C	-9.255455	-0.839769	-0.716044
39	H	-9.640166	-1.296479	1.36343
40	H	-8.866217	-0.673937	-2.839325

41	C	1.344711	-6.464717	-0.998186
42	C	2.283148	-6.817883	0.165286
43	H	1.809748	-5.675377	-1.633743
44	H	1.2138	-7.361952	-1.637439
45	O	2.55091	-5.739531	1.036958
46	H	3.215231	-7.258508	-0.238738
47	H	1.831385	-7.546124	0.864021
48	C	3.518476	-4.824721	0.663602
49	C	3.947145	-4.594118	-0.647041
50	C	4.029854	-4.066761	1.729349
51	C	4.89909	-3.610001	-0.892107
52	H	3.524869	-5.166198	-1.486389
53	C	4.96868	-3.079554	1.47064
54	H	3.680873	-4.242364	2.754425
55	C	5.408131	-2.8508	0.161142
56	H	5.24114	-3.424857	-1.916891
57	H	5.365663	-2.472919	2.293198
58	C	6.38762	-1.781924	-0.106192
59	C	7.756227	-2.059074	-0.06139
60	C	5.911189	-0.490779	-0.378912
61	C	8.517899	-3.234216	0.279307
62	N	8.720035	-1.041426	-0.317783
63	C	4.574463	0.034641	-0.434376
64	N	6.777404	0.612609	-0.643831
65	C	9.874222	-2.903314	0.245426
66	C	7.994773	-4.566995	0.618025
67	C	9.983483	-1.520193	-0.118485
68	B	8.360953	0.433989	-0.839553
69	C	4.65471	1.396777	-0.72706
70	C	3.317273	-0.694462	-0.209631
71	C	6.038691	1.744476	-0.849011
72	C	10.989773	-3.835225	0.536196
73	H	6.980932	-4.52412	1.038067
74	H	7.963213	-5.203444	-0.277262
75	H	8.646965	-5.060922	1.359744
76	C	11.097952	-0.605028	-0.245814
77	F	9.1204	1.372355	-0.16384
78	F	8.697456	0.590489	-2.165926
79	C	3.485371	2.28884	-0.900198
80	H	3.167335	-1.467245	-0.976498
81	H	3.316469	-1.19373	0.770619
82	H	2.457833	-0.003309	-0.240963
83	C	6.655355	3.026832	-1.124903
84	H	10.871841	-4.738782	-0.096287
85	H	11.957782	-3.382212	0.234265
86	C	11.036038	-4.228257	1.998992
87	C	12.38868	-0.942688	-0.37519
88	H	10.791415	0.477851	-0.243536

89	H	3.626375	3.214671	-0.288771
90	H	2.586395	1.777527	-0.484005
91	C	3.255383	2.649796	-2.352634
92	H	7.673956	3.017932	-1.559959
93	C	6.061775	4.198569	-0.85007
94	H	11.152917	-3.354631	2.652053
95	H	10.107728	-4.743737	2.297884
96	H	11.872792	-4.908545	2.200287
97	H	12.71006	-1.995973	-0.394161
98	C	13.440997	0.059811	-0.500663
99	H	2.371078	3.289945	-2.464496
100	H	4.113928	3.192737	-2.770912
101	H	3.098784	1.756803	-2.970947
102	H	5.050091	4.227442	-0.408666
103	C	6.690475	5.487605	-1.106273
104	C	14.774575	-0.349721	-0.611475
105	C	13.139912	1.426225	-0.512987
106	C	6.004902	6.663213	-0.778267
107	C	7.966093	5.570532	-1.673328
108	C	15.786012	0.595005	-0.730945
109	H	15.02178	-1.417427	-0.604354
110	C	14.155358	2.366012	-0.632771
111	H	12.085473	1.737628	-0.42761
112	C	6.589713	7.899421	-1.020009
113	H	5.000943	6.605342	-0.326223
114	C	8.545742	6.809927	-1.912466
115	H	8.495088	4.636196	-1.920722
116	C	15.479134	1.952289	-0.741636
117	H	16.827965	0.269957	-0.817399
118	H	13.91147	3.433345	-0.641941
119	C	7.858558	7.975023	-1.587262
120	H	6.05083	8.817386	-0.76379
121	H	9.54465	6.867827	-2.357219
122	H	16.279092	2.693662	-0.836295
123	H	8.315663	8.951672	-1.776769
124	C	-9.550853	0.594019	-0.54855
125	C	-10.862376	1.051709	-0.664221
126	C	-8.492346	1.464283	-0.25313
127	C	-12.094306	0.363487	-0.951512
128	N	-11.212606	2.428817	-0.486693
129	C	-7.084313	1.232676	-0.083642
130	N	-8.692679	2.861033	-0.033471
131	C	-13.124119	1.299872	-0.932226
132	C	-12.269676	-1.067847	-1.236996
133	C	-12.553523	2.582996	-0.643193
134	B	-10.126775	3.576656	-0.174197
135	C	-6.484153	2.449999	0.239378
136	C	-6.370852	-0.045201	-0.222824

137	C	-7.504471	3.452357	0.268122
138	C	-14.553503	1.013599	-1.188633
139	H	-11.584015	-1.402875	-2.028066
140	H	-12.065248	-1.674158	-0.343396
141	H	-13.305054	-1.267016	-1.561974
142	C	-13.276112	3.864716	-0.532043
143	F	-10.450859	4.260831	0.976035
144	F	-10.106176	4.515198	-1.182514
145	C	-5.045523	2.654725	0.519546
146	H	-6.731727	-0.783116	0.509258
147	H	-6.522237	-0.473076	-1.224656
148	H	-5.28139	0.084269	-0.065906
149	C	-7.328394	4.8849	0.576369
150	H	-14.625419	0.003541	-1.653903
151	H	-14.945619	1.732988	-1.934622
152	C	-15.38345	1.061435	0.077321
153	H	-13.871736	3.882993	0.392631
154	H	-12.605051	4.736097	-0.516954
155	H	-13.970967	3.981322	-1.375568
156	H	-4.536754	1.661715	0.493519
157	H	-4.925863	3.034842	1.555666
158	C	-4.388189	3.604803	-0.459386
159	H	-8.184932	5.499523	0.263994
160	H	-7.190109	5.024081	1.657852
161	H	-6.423762	5.266234	0.072167
162	H	-16.436919	0.837694	-0.133436
163	H	-15.032459	0.332613	0.819085
164	H	-15.344252	2.052575	0.549753
165	H	-3.343644	3.797372	-0.178384
166	H	-4.39245	3.204748	-1.480715
167	H	-4.911263	4.575845	-0.485213
168	C	-2.526546	-0.742338	2.989569
169	O	-2.624181	-1.136671	4.137803
170	C	-1.646347	0.403335	2.609848
171	C	-2.108686	1.672147	2.541621
172	C	-0.223301	0.134744	2.365492
173	C	-1.196924	2.738845	2.215508
174	H	-3.166093	1.918091	2.713682
175	O	0.656295	1.161142	2.093995
176	O	0.390057	-0.911346	2.325888
177	C	0.161952	2.441976	2.011381
178	C	-1.614673	4.073565	2.08697
179	C	1.091983	3.437468	1.695521
180	C	-0.708138	5.064982	1.778021
181	H	-2.676528	4.315603	2.226351
182	C	0.659318	4.762448	1.574373
183	H	2.148488	3.16726	1.527391
184	H	-1.052784	6.106341	1.680325

185	N	1.561723	5.785855	1.131649
186	C	3.010354	5.488985	1.202916
187	C	1.252115	7.178005	1.528795
188	H	3.559396	6.177822	0.535839
189	H	3.422593	5.591976	2.217677
190	H	3.20917	4.455943	0.852448
191	H	1.561505	7.408215	2.559293
192	H	1.777643	7.861253	0.84877
193	H	0.170652	7.370852	1.442384

Conformer II

Total Energy (PM3) : -0.426646 Hartree Imaginary frequency: 0

Total Energy (B3LYP/6-31+G(d,p)) : -4735.460011 Hartree

Atom#	Symbol	X	Y	Z
5	H	5.242561	1.267065	-1.540811
6	H	6.151387	2.552222	-0.722299
7	C	2.318478	2.041101	-0.088023
8	H	3.34826	0.106271	-0.250731
9	H	3.014772	0.629294	1.409754
10	C	2.711233	2.672843	-1.445271
11	H	4.52989	3.5417	-2.33405
12	H	4.184724	4.056208	-0.684509
13	H	1.312544	1.576094	-0.140162
14	H	2.222358	2.861781	0.653237
15	N	2.538892	1.676564	-2.570921
16	C	3.456182	1.332954	-3.566697
17	C	2.811276	0.358355	-4.314459
18	H	4.4561	1.75643	-3.687135
19	N	1.381742	0.958249	-2.75022
20	N	1.535177	0.1885	-3.754799
21	C	1.783425	3.816176	-1.741808
22	C	0.421384	3.926966	-1.495706
23	N	0.075264	5.174575	-2.015507
24	H	-0.283615	3.236286	-1.011941
25	N	2.177926	4.999706	-2.392841
26	N	1.187137	5.784534	-2.542193
27	C	3.308738	-0.443946	-5.464933
28	O	4.644398	-0.898017	-5.286466
29	H	3.415857	0.175368	-6.373219
30	H	2.632146	-1.291479	-5.688965
31	C	-1.271752	5.780382	-2.021048
32	C	-1.690552	6.347952	-0.657688
33	H	-1.992408	5.00452	-2.355013
34	H	-1.294924	6.592766	-2.776193
35	O	-1.812207	5.361404	0.349804

36	H	-2.629657	6.923385	-0.774853
37	H	-0.927702	7.01531	-0.218521
38	C	5.202288	2.100075	1.686806
39	O	4.536082	2.01165	2.706146
40	C	6.556453	2.728188	1.684447
41	C	6.721477	4.019276	2.054846
42	C	7.737465	1.910601	1.368927
43	C	8.045398	4.582488	2.100684
44	H	5.869937	4.655744	2.327134
45	C	9.148478	3.768799	1.785696
46	C	8.28171	5.91909	2.45917
47	C	10.45777	4.260414	1.825917
48	C	9.566381	6.415922	2.502639
49	H	7.431326	6.565434	2.706488
50	C	10.674865	5.594563	2.187915
51	H	11.301364	3.599327	1.568184
52	H	9.730888	7.468407	2.780758
53	O	9.008239	2.451609	1.423392
54	O	7.840211	0.751293	1.034094
55	N	11.993841	6.155197	2.133195
56	C	13.136376	5.214015	2.179586
57	H	14.017727	5.71396	1.75698
58	H	13.379835	4.885965	3.20141
59	H	12.925503	4.318108	1.573617
60	C	12.247182	7.375957	2.932167
61	H	12.424733	7.16234	3.996971
62	H	13.134688	7.880357	2.527979
63	H	11.394655	8.069969	2.858917
64	C	4.821673	-1.771211	-4.217089
65	C	4.250066	-3.048177	-4.206468
66	C	5.665125	-1.351823	-3.181325
67	C	4.498103	-3.894004	-3.131764
68	H	3.604013	-3.378033	-5.028313
69	C	5.908988	-2.205134	-2.112803
70	H	6.121636	-0.354679	-3.206508
71	C	5.309577	-3.466974	-2.078035
72	H	4.049208	-4.893602	-3.105438
73	H	6.558868	-1.882844	-1.289681
74	C	5.522956	-4.331381	-0.902614
75	C	6.602887	-5.217593	-0.887804
76	C	4.647084	-4.22423	0.181409
77	C	7.615306	-5.508365	-1.867806
78	N	6.893961	-6.048918	0.239231
79	C	3.471093	-3.420515	0.388844
80	N	4.829184	-4.974601	1.386513
81	C	8.467476	-6.471634	-1.332562
82	C	7.760031	-4.910536	-3.203199
83	C	8.005722	-6.788971	-0.014187

84	B	6.019323	-6.038355	1.590186
85	C	2.990693	-3.685471	1.668566
86	C	2.839167	-2.482756	-0.550343
87	C	3.851723	-4.65569	2.275075
88	C	9.652049	-7.051193	-2.005422
89	H	6.880794	-5.121572	-3.827963
90	H	7.864307	-3.818172	-3.137106
91	H	8.652474	-5.315605	-3.709553
92	C	8.624803	-7.743111	0.925834
93	F	5.502864	-7.286695	1.860655
94	F	6.807121	-5.712335	2.671519
95	C	1.797224	-3.074379	2.295691
96	H	3.446798	-1.56743	-0.66439
97	H	2.71402	-2.928439	-1.546795
98	H	1.846909	-2.179034	-0.173741
99	C	3.709163	-5.210157	3.634618
100	H	9.79188	-6.528904	-2.97974
101	H	10.555538	-6.831093	-1.402758
102	C	9.516737	-8.544017	-2.221617
103	H	9.546099	-7.313631	1.344415
104	H	7.966445	-8.011393	1.764213
105	H	8.902664	-8.665951	0.387372
106	H	1.254382	-2.485289	1.521426
107	H	1.10408	-3.876031	2.619237
108	C	2.170821	-2.195071	3.471269
109	H	2.863787	-5.911777	3.669842
110	H	4.60589	-5.742735	3.980834
111	H	3.490013	-4.387942	4.339144
112	H	9.363119	-9.071234	-1.264451
113	H	8.663512	-8.785619	-2.867648
114	H	10.416779	-8.960216	-2.690599
115	H	2.747301	-2.76688	4.219183
116	H	2.787587	-1.341308	3.159988
117	H	1.27918	-1.796094	3.969982
118	C	-2.942105	4.552421	0.250846
119	C	-4.223345	5.062927	0.484314
120	C	-2.738697	3.185907	0.028251
121	C	-5.307171	4.193364	0.493932
122	H	-4.374944	6.132934	0.668668
123	C	-3.828744	2.323987	0.043556
124	H	-1.723499	2.797477	-0.151202
125	C	-5.112111	2.826984	0.271966
126	H	-6.316826	4.577507	0.681232
127	H	-3.682597	1.250494	-0.126162
128	C	-6.266199	1.908404	0.285098
129	C	-6.933524	1.624207	-0.910362
130	C	-6.675047	1.354498	1.504316
131	C	-6.794634	2.105903	-2.261133

132	N	-8.04673	0.737703	-0.934037
133	C	-6.177573	1.534171	2.842417
134	N	-7.762689	0.43457	1.612835
135	C	-7.807635	1.537103	-3.036277
136	C	-5.779777	3.039653	-2.774342
137	C	-8.594064	0.692623	-2.184803
138	B	-8.55116	-0.120726	0.32491
139	C	-6.943403	0.748731	3.702217
140	C	-5.05198	2.379977	3.268408
141	C	-7.914462	0.043413	2.915043
142	C	-8.014601	1.773191	-4.485011
143	H	-5.415417	3.726825	-1.999027
144	H	-4.916152	2.486294	-3.168901
145	H	-6.195219	3.648682	-3.596391
146	C	-9.799114	-0.083496	-2.387983
147	F	-9.928362	-0.020739	0.419949
148	F	-8.298233	-1.461792	0.150009
149	C	-6.756852	0.697579	5.171408
150	H	-4.145115	2.15543	2.689014
151	H	-5.282766	3.445066	3.124925
152	H	-4.829315	2.216022	4.33647
153	C	-8.901919	-0.943646	3.297331
154	H	-7.06409	1.566936	-5.01822
155	H	-8.749708	1.046026	-4.890745
156	C	-8.474512	3.188247	-4.77192
157	C	-10.282771	-0.496113	-3.568112
158	H	-10.329303	-0.348676	-1.432861
159	H	-5.73747	1.078599	5.409469
160	H	-6.786433	-0.358233	5.518168
161	C	-7.799615	1.519153	5.901622
162	H	-9.651473	-1.227234	2.532078
163	C	-8.943898	-1.558035	4.490533
164	H	-9.413631	3.423906	-4.256272
165	H	-7.720981	3.922324	-4.440261
166	H	-8.636901	3.342036	-5.84592
167	H	-9.770721	-0.260437	-4.514408
168	C	-11.508375	-1.280555	-3.670262
169	H	-7.631072	1.495951	6.985786
170	H	-7.780135	2.570153	5.586175
171	H	-8.813535	1.139621	5.715902
172	H	-8.206973	-1.327295	5.278024
173	C	-9.946811	-2.564918	4.817384
174	C	-11.979856	-1.663144	-4.931111
175	C	-12.221505	-1.659176	-2.527505
176	C	-9.949163	-3.14444	6.091513
177	C	-10.90675	-2.96485	3.881535
178	C	-13.145863	-2.410117	-5.041792
179	H	-11.428102	-1.373975	-5.832833

180	C	-13.386454	-2.406095	-2.64443
181	H	-11.838897	-1.355121	-1.539068
182	C	-10.897626	-4.105129	6.418703
183	H	-9.200995	-2.840411	6.832536
184	C	-11.852367	-3.926137	4.21389
185	H	-10.8949	-2.505045	2.880324
186	C	-13.850382	-2.782275	-3.900881
187	H	-13.510797	-2.707553	-6.030304
188	H	-13.938246	-2.699223	-1.745339
189	C	-11.84954	-4.497316	5.482355
190	H	-10.895153	-4.555737	7.416622
191	H	-12.599054	-4.23445	3.474796
192	H	-14.768444	-3.371629	-3.992331
193	H	-12.594725	-5.255597	5.743754

Conformer III

Total Energy (PM3) : -0.437066 Hartree Imaginary frequency: 0

Total Energy (B3LYP/6-31+G(d,p)) : -4735.474030 Hartree

Atom#	Symbol	X	Y	Z
1	N	2.143117	-1.618838	-1.94707
2	C	2.941626	-2.84347	-2.216809
3	C	1.726343	-1.533102	-0.523628
4	C	2.25627	-4.123722	-1.748998
5	H	3.914253	-2.699201	-1.700062
6	H	3.173462	-2.914452	-3.298835
7	C	1.009621	-2.787702	-0.035818
8	H	2.648451	-1.333784	0.061581
9	H	1.07413	-0.647529	-0.379237
10	C	1.828424	-4.077268	-0.265534
11	H	2.924856	-4.988076	-1.94527
12	H	1.349027	-4.312848	-2.359988
13	H	0.744728	-2.663313	1.035137
14	H	0.038058	-2.89629	-0.567118
15	N	3.026388	-4.11967	0.654994
16	C	4.312666	-4.575974	0.3556
17	C	5.008711	-4.458569	1.54914
18	H	4.640153	-4.9366	-0.622333
19	N	2.957628	-3.782279	1.984343
20	N	4.106099	-3.964738	2.505764
21	C	0.990624	-5.282883	0.050928
22	C	-0.264334	-5.373681	0.633925
23	N	-0.513553	-6.746598	0.708366
24	H	-0.950126	-4.591518	0.977258
25	N	1.423075	-6.601256	-0.194717
26	N	0.547297	-7.441975	0.186248

27	C	6.431393	-4.757606	1.865487
28	O	7.304672	-4.411546	0.800434
29	H	6.607462	-5.844848	1.944967
30	H	6.743159	-4.265121	2.812435
31	C	-1.730452	-7.375373	1.257933
32	C	-2.706548	-7.901294	0.196012
33	H	-2.231016	-6.619716	1.900238
34	H	-1.433748	-8.217651	1.9162
35	O	-3.041535	-6.981117	-0.820012
36	H	-3.615542	-8.283124	0.702033
37	H	-2.276583	-8.720409	-0.409184
38	C	1.253577	-1.124368	-2.964707
39	O	1.3663	-1.526028	-4.109398
40	C	0.306163	-0.031875	-2.593345
41	C	0.673408	1.270051	-2.611155
42	C	-1.084204	-0.385691	-2.284841
43	C	-0.306627	2.281108	-2.314671
44	H	1.70244	1.584782	-2.840785
45	C	-1.629704	1.899799	-2.02399
46	C	0.009399	3.649437	-2.309472
47	C	-2.619868	2.841599	-1.72778
48	C	-0.956077	4.589356	-2.027059
49	H	1.043426	3.959563	-2.533376
50	C	-2.285717	4.202285	-1.729311
51	H	-3.64577	2.51138	-1.483608
52	H	-0.687111	5.656987	-2.024889
53	O	-2.024348	0.581052	-2.011043
54	O	-1.615267	-1.47492	-2.196016
55	N	-3.242146	5.18599	-1.325976
56	C	-4.673969	4.811548	-1.357763
57	H	-5.220196	5.463361	-0.663324
58	H	-5.119613	4.918643	-2.358088
59	H	-4.812903	3.768023	-1.029028
60	C	-3.018825	6.580964	-1.768671
61	H	-3.342849	6.757422	-2.80543
62	H	-3.58667	7.251772	-1.110516
63	H	-1.952537	6.847353	-1.692266
64	C	-3.681204	-5.81173	-0.444685
65	C	-4.5017	-5.67396	0.679448
66	C	-3.476268	-4.737113	-1.323023
67	C	-5.076633	-4.437454	0.953434
68	H	-4.697705	-6.524531	1.343352
69	C	-4.054157	-3.508555	-1.039507
70	H	-2.856174	-4.858217	-2.2202
71	C	-4.831211	-3.350635	0.113162
72	H	-5.71601	-4.315557	1.835265
73	H	-3.877756	-2.653811	-1.70673
74	C	-5.366237	-2.015755	0.43347

75	C	-4.590685	-1.1329	1.195104
76	C	-6.636443	-1.657312	-0.034547
77	C	-3.326343	-1.25516	1.871558
78	N	-5.051461	0.181588	1.48183
79	C	-7.621047	-2.408006	-0.76512
80	N	-7.199423	-0.359178	0.161605
81	C	-3.072805	-0.058377	2.549137
82	C	-2.423309	-2.416972	1.878779
83	C	-4.169342	0.829175	2.302733
84	B	-6.361133	0.837621	0.831044
85	C	-8.720457	-1.580359	-0.992243
86	C	-7.517282	-3.80291	-1.219698
87	C	-8.430293	-0.291764	-0.433766
88	C	-1.869078	0.222009	3.36783
89	H	-2.959098	-3.364777	1.730182
90	H	-1.674389	-2.322929	1.076119
91	H	-1.88181	-2.481562	2.839276
92	C	-4.506876	2.156751	2.770954
93	F	-7.052032	1.542537	1.801886
94	F	-6.024946	1.776591	-0.121558
95	C	-9.958391	-2.010699	-1.683829
96	H	-6.600554	-3.960028	-1.806083
97	H	-7.487392	-4.494604	-0.365972
98	H	-8.382436	-4.068779	-1.850366
99	C	-9.197927	0.935711	-0.454595
100	H	-0.967115	0.0099	2.75775
101	H	-1.815798	1.303348	3.615195
102	C	-1.83961	-0.601299	4.639651
103	C	-3.665793	3.037594	3.330671
104	H	-5.588116	2.425317	2.613731
105	H	-9.73608	-2.941126	-2.254736
106	H	-10.254884	-1.245632	-2.434062
107	C	-11.092718	-2.258441	-0.710693
108	H	-8.869388	1.747414	0.223356
109	C	-10.247738	1.161097	-1.260649
110	H	-2.721928	-0.416923	5.264823
111	H	-1.815136	-1.679917	4.410216
112	H	-0.951268	-0.370462	5.240588
113	H	-2.600785	2.801821	3.482744
114	C	-4.107518	4.357545	3.767787
115	H	-11.992172	-2.606651	-1.234208
116	H	-10.827854	-3.019662	0.034162
117	H	-11.360548	-1.343865	-0.164406
118	H	-10.600158	0.390364	-1.96671
119	C	-10.976506	2.424279	-1.262233
120	C	-3.188183	5.232709	4.357117
121	C	-5.436474	4.765169	3.607828
122	C	-12.066301	2.588283	-2.125114

123	C	-10.607866	3.476787	-0.417532
124	C	-3.596286	6.491932	4.778714
125	H	-2.14441	4.924394	4.4865
126	C	-5.838652	6.025071	4.031437
127	H	-6.151999	4.06808	3.14096
128	C	-12.771637	3.784972	-2.137855
129	H	-12.36398	1.771096	-2.792176
130	C	-11.316651	4.670916	-0.434209
131	H	-9.747538	3.338504	0.25663
132	C	-4.919916	6.889928	4.617409
133	H	-2.873554	7.172916	5.240005
134	H	-6.880714	6.335852	3.904095
135	C	-12.399256	4.826872	-1.293825
136	H	-13.623559	3.90826	-2.8146
137	H	-11.021707	5.489227	0.230732
138	H	-5.237785	7.882669	4.951986
139	H	-12.957965	5.768308	-1.306581
140	C	7.582703	-3.065703	0.649565
141	C	7.979919	-2.674821	-0.63704
142	C	7.532178	-2.139408	1.697931
143	C	8.299851	-1.344544	-0.871131
144	H	8.037052	-3.408825	-1.449032
145	C	7.852829	-0.811438	1.451164
146	H	7.226482	-2.471942	2.701942
147	C	8.224635	-0.410349	0.165959
148	H	8.605532	-1.023347	-1.873532
149	H	7.808696	-0.077524	2.263943
150	C	8.528667	1.006249	-0.103476
151	C	7.486549	1.866823	-0.471777
152	C	9.843787	1.457869	0.011054
153	C	6.076888	1.644759	-0.643634
154	N	7.705141	3.251387	-0.750136
155	C	11.062279	0.778869	0.371183
156	N	10.21327	2.816056	-0.250904
157	C	5.49185	2.858151	-1.005249
158	C	5.341136	0.383854	-0.466308
159	C	6.522933	3.848497	-1.060674
160	B	9.153606	3.9477	-0.682548
161	C	12.101905	1.702763	0.315214
162	C	11.219207	-0.637233	0.73358
163	C	11.552589	2.966298	-0.081358
164	C	4.052175	3.085748	-1.261856
165	H	5.673605	-0.374774	-1.189387
166	H	5.498716	-0.028802	0.540762
167	H	4.258201	0.544574	-0.609187
168	C	6.352789	5.278076	-1.385112
169	F	9.502334	4.49504	-1.897411
170	F	9.145664	4.990901	0.21688

171	C	13.527324	1.42357	0.602356
172	H	10.644266	-0.878399	1.638692
173	H	10.858724	-1.293629	-0.071362
174	H	12.280966	-0.868883	0.923375
175	C	12.301009	4.221491	-0.284928
176	H	3.500547	2.140835	-1.046346
177	H	3.671632	3.838435	-0.542848
178	C	3.782505	3.536887	-2.682391
179	H	5.868672	5.79892	-0.546854
180	H	7.302986	5.788894	-1.596456
181	H	5.695759	5.382656	-2.265898
182	H	13.639483	0.330675	0.78852
183	H	14.129947	1.648368	-0.300002
184	C	14.04037	2.215803	1.786704
185	H	12.876341	4.168014	-1.220162
186	H	11.652377	5.107408	-0.337697
187	H	13.020801	4.361054	0.540554
188	H	4.3771	4.430479	-2.93709
189	H	4.031492	2.756612	-3.412591
190	H	2.719514	3.795217	-2.821231
191	H	13.922149	3.300253	1.620288
192	H	13.499412	1.966201	2.708008
193	H	15.105137	2.020027	1.963335

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