Supporting Information

Total Synthesis and Structure-Activity Relationships of Odilorhabdins, a New Class of Peptides Showing Potent Antibacterial Activity.

Matthieu Sarciaux, [†] *Lucile Pantel,* [†] *Camille Midrier,* [‡] *Marine Serri,* [†] *Renata Marcia de Figueiredo,* [‡] *Jean-Marc Campagne,* [‡] *Philippe Villain-Guillot,* [†] *Maxime Gualtieri* [†] *and Emilie Racine* *[,†]

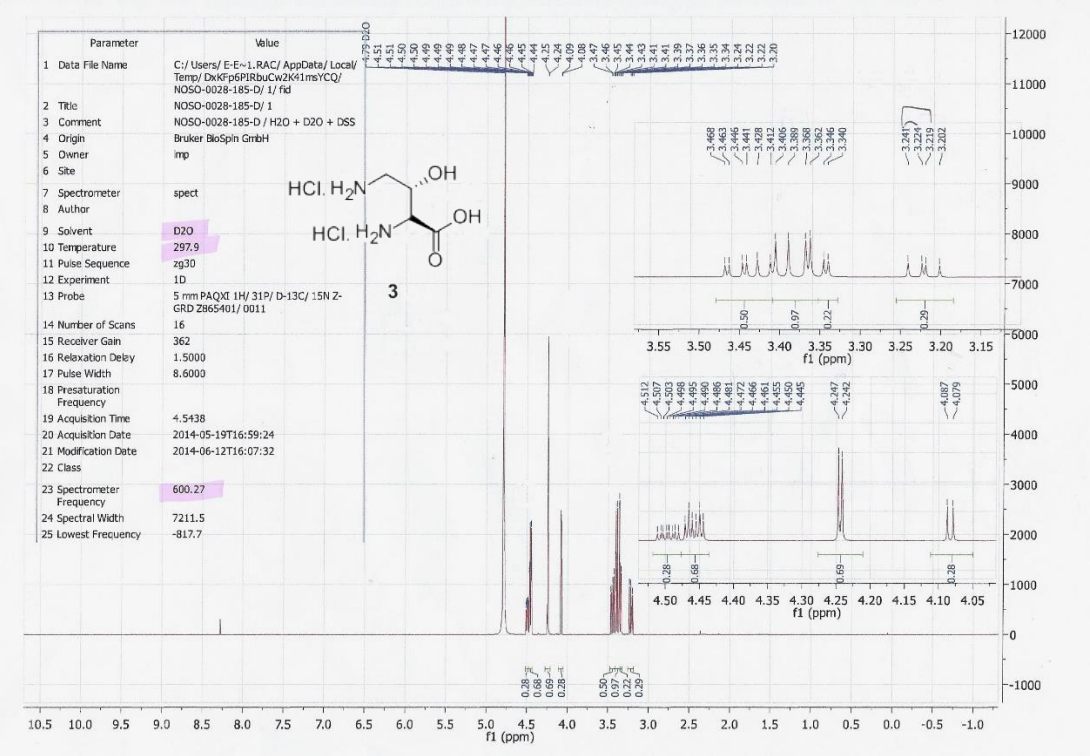
[†] Nosopharm, 110 allée Charles Babbage, Espace Innovation 2, 30000 Nîmes, France

[‡] Institut Charles Gerhardt Montpellier (ICGM), UMR 5253, Univ Montpellier, CNRS, ENSCM - Ecole Nationale Supérieure de Chimie, 8 Rue de l'Ecole Normale, Montpellier 34296 Cedex 5, France

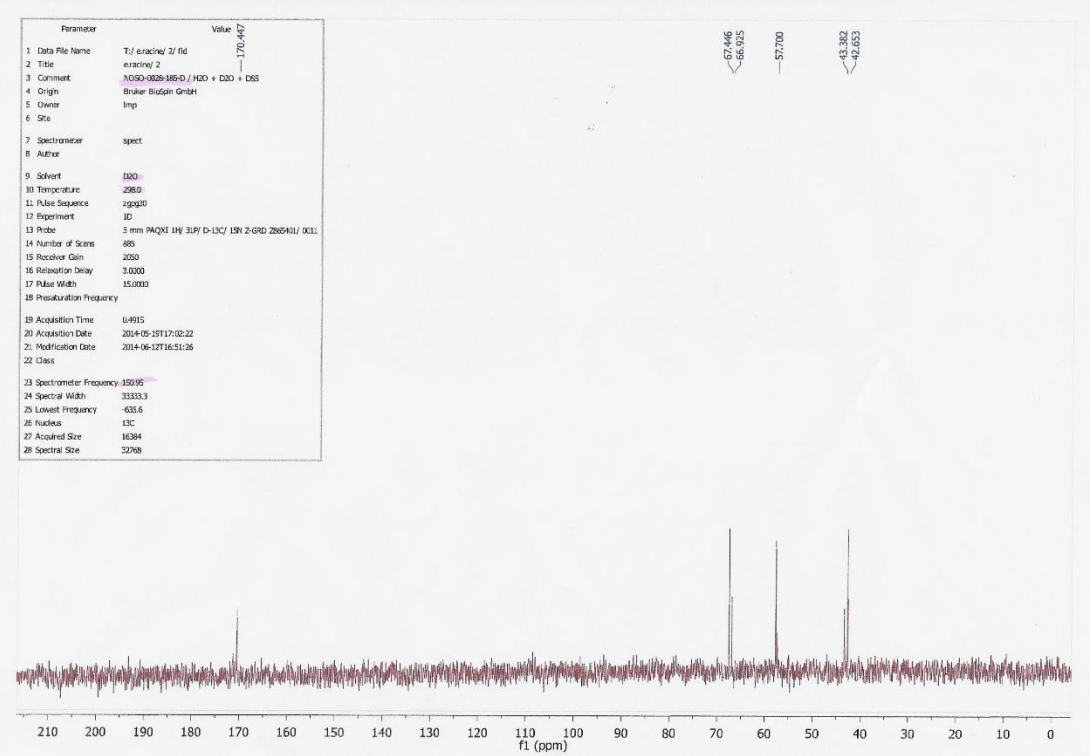
Table of contents

I- NMR spectra of the synthesis of protected Dab(βOH) (**3**, **5**, **6**)
II- NMR spectra of the synthesis of Lys-Dha (**7**-**16**)
III- NOESY of *Z* and *E* dipeptide Lys-Dha **7**
IV- Analyses of natural and synthetic NOSO-95C **1**
V- Analyses of NOSO-95179 **46**
VI- HRMS data
VII- MIC of compounds in µM
VIII- Inhibition curves of compounds **1** and **17-46**
IX- Molecular Formula String

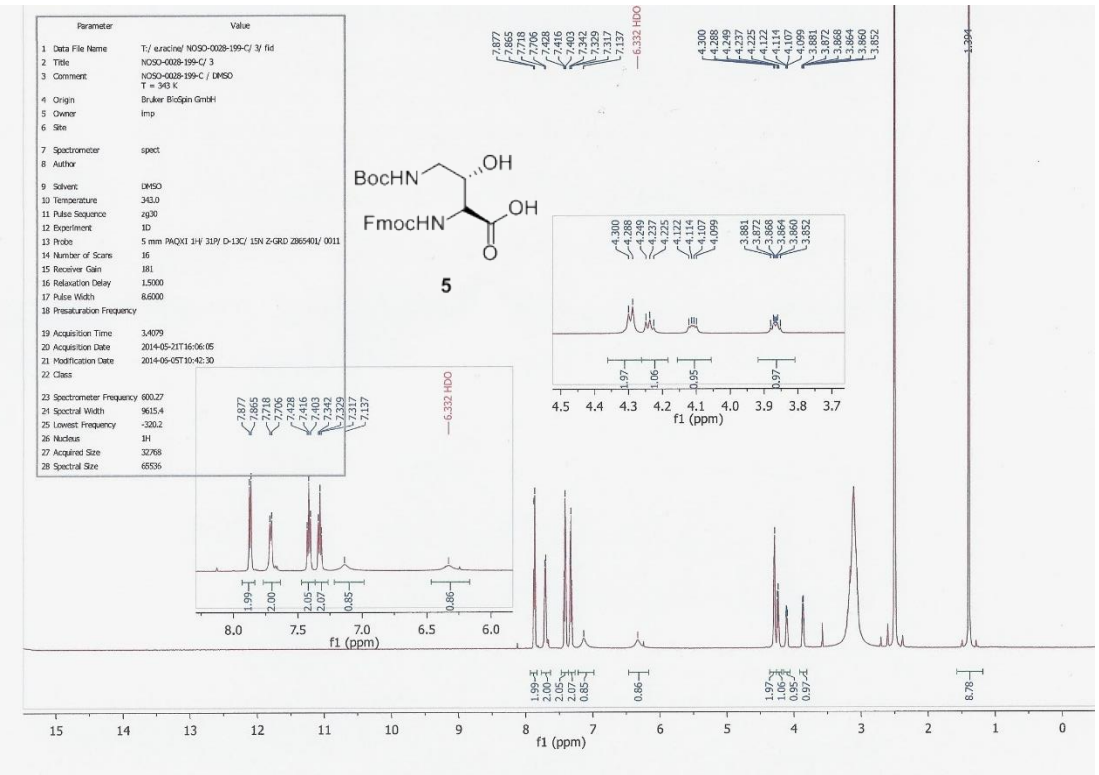
I- NMR spectra of the synthesis of protected Dab(βOH) (3, 5, 6)



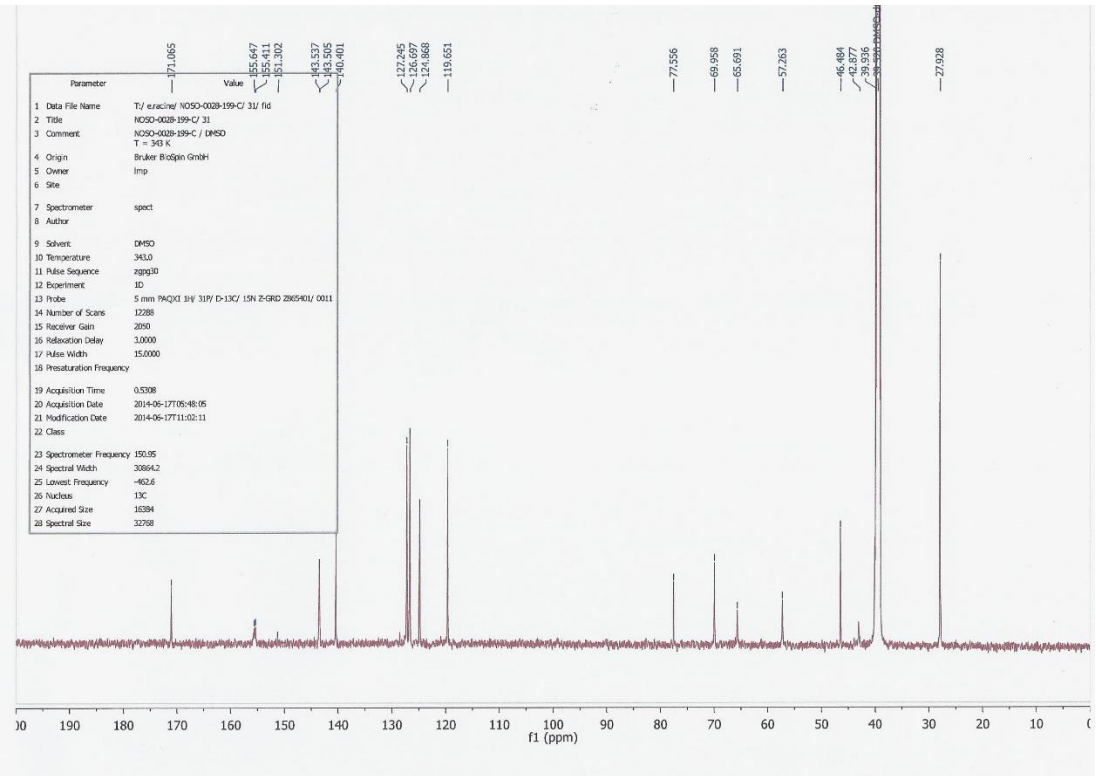
Supplementary Figure 1: ^{1}H NMR spectra of 3 (D_2O, 298 K)



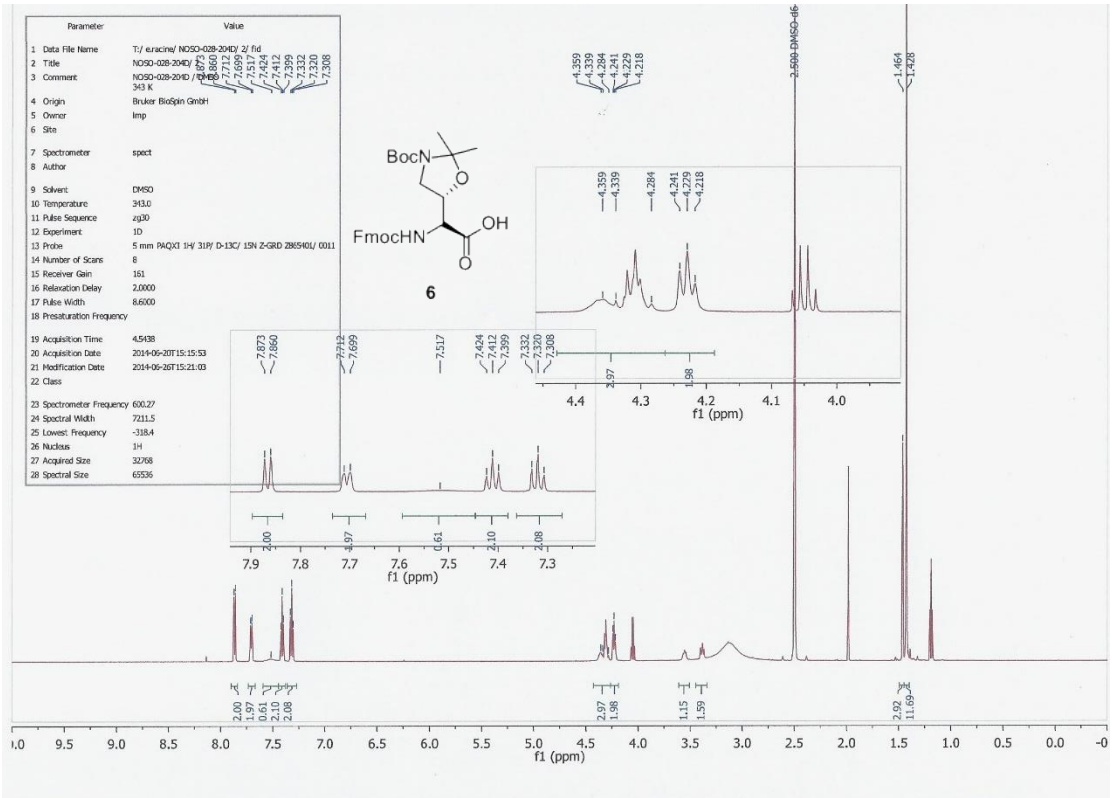
Supplementary Figure 2: ^{13}C NMR spectra of 3 (D_2O, 298 K)



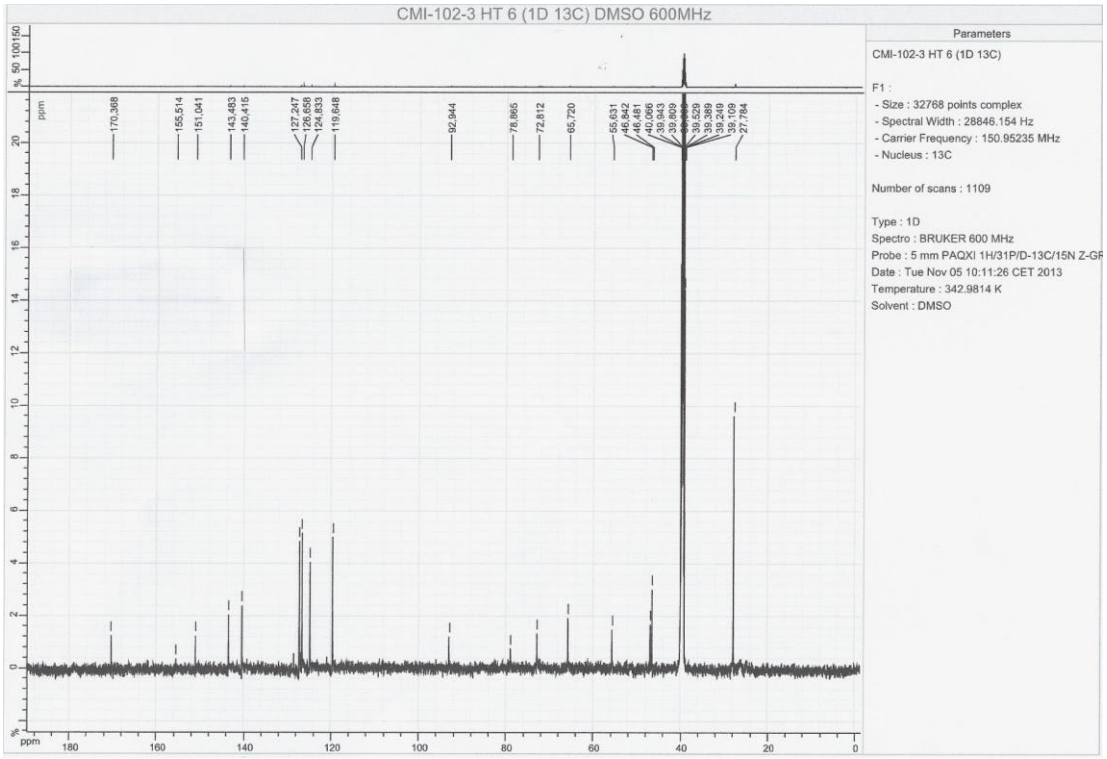
Supplementary Figure 3: ^{1}H NMR spectra of 5 (DMSO-d$_6$, 343 K)



Supplementary Figure 4: ^{13}C NMR spectra of 5 (DMSO-d$_6$, 343 K)

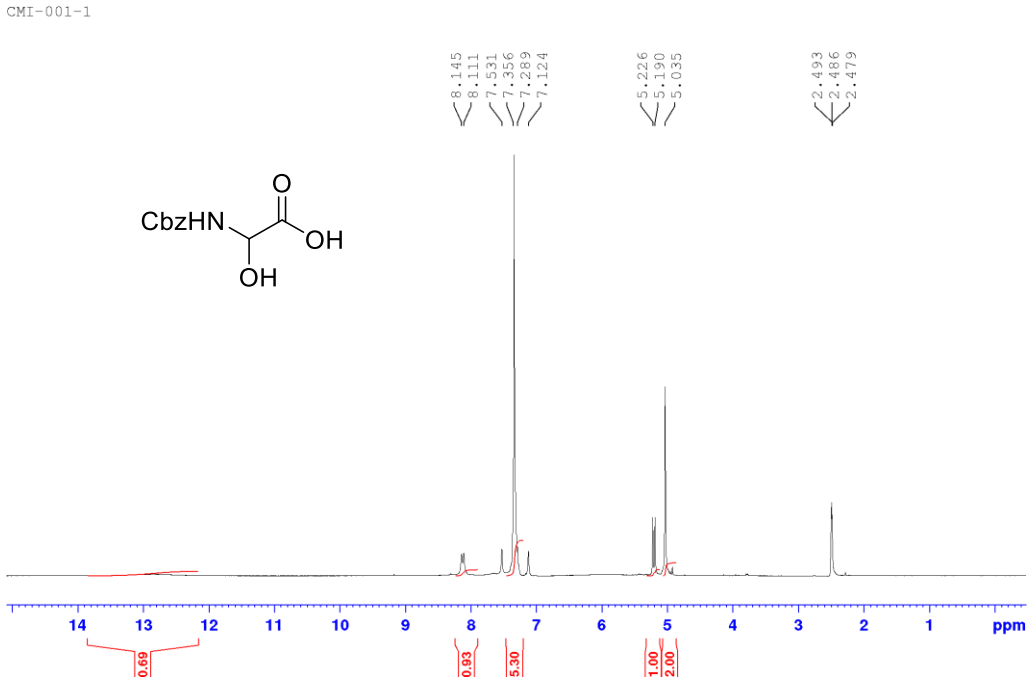


Supplementary Figure 5: ^{1}H NMR spectra of 6 (DMSO-d$_6$, 343 K)

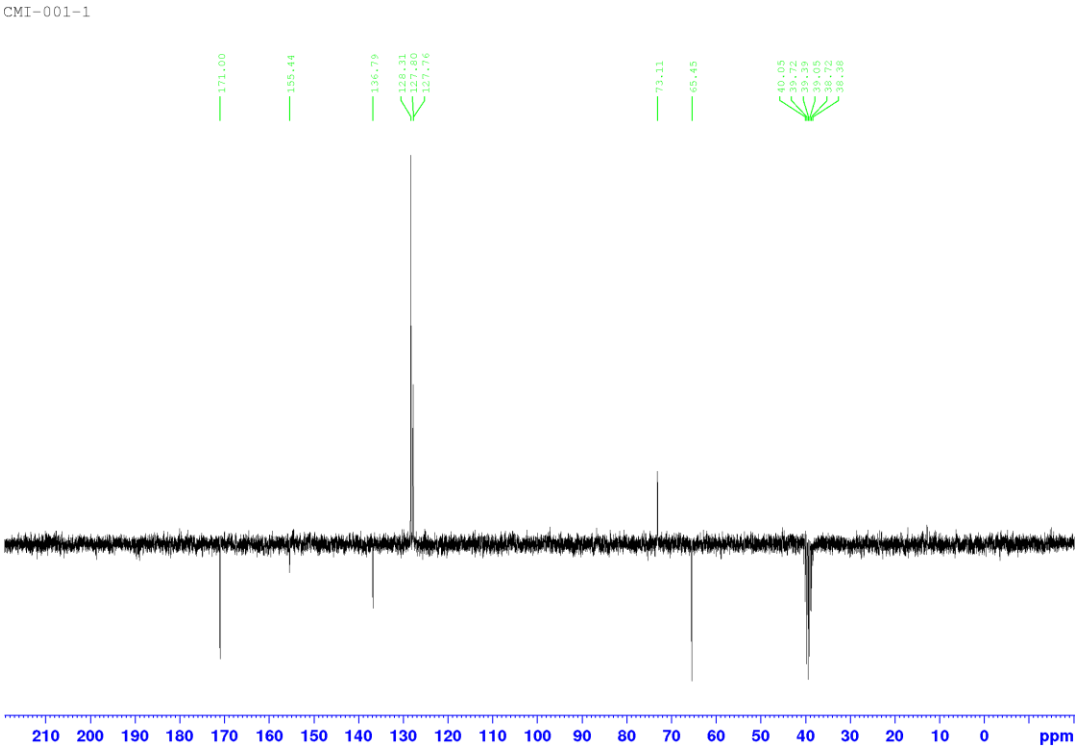


Supplementary Figure 6: ^{13}C NMR spectra of 6 (DMSO-d$_6$, 343 K)

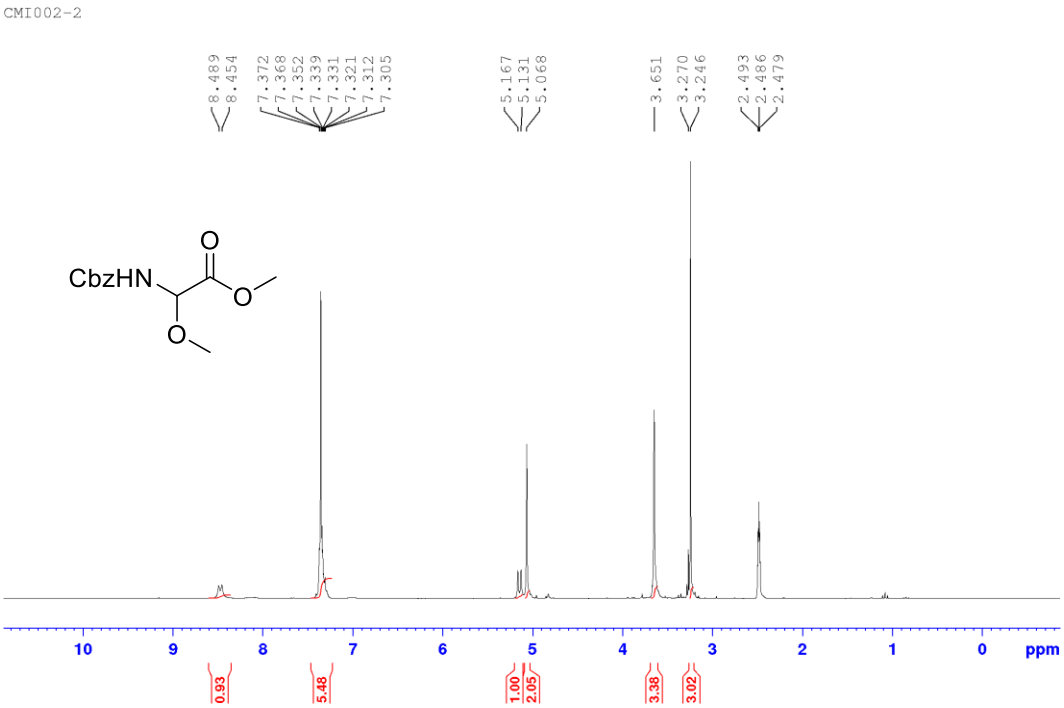
II- NMR spectra of the synthesis of Lys-Dha (7, 9-16)



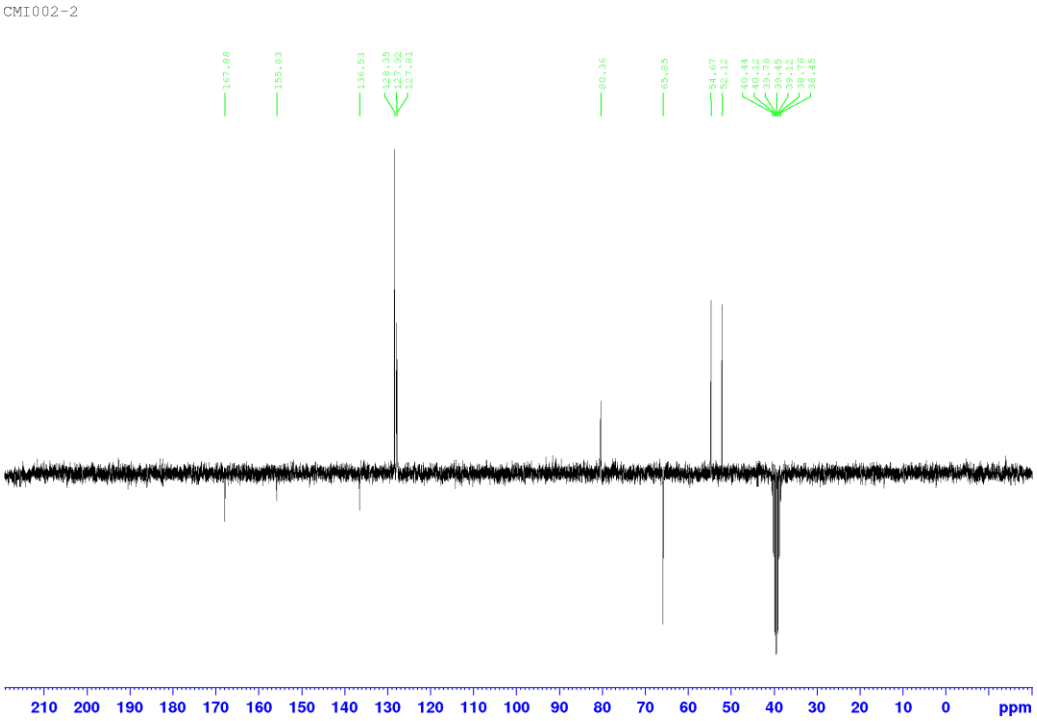
Supplementary Figure 7: ^{1}H NMR spectra of 9 (DMSO-d$_6$)



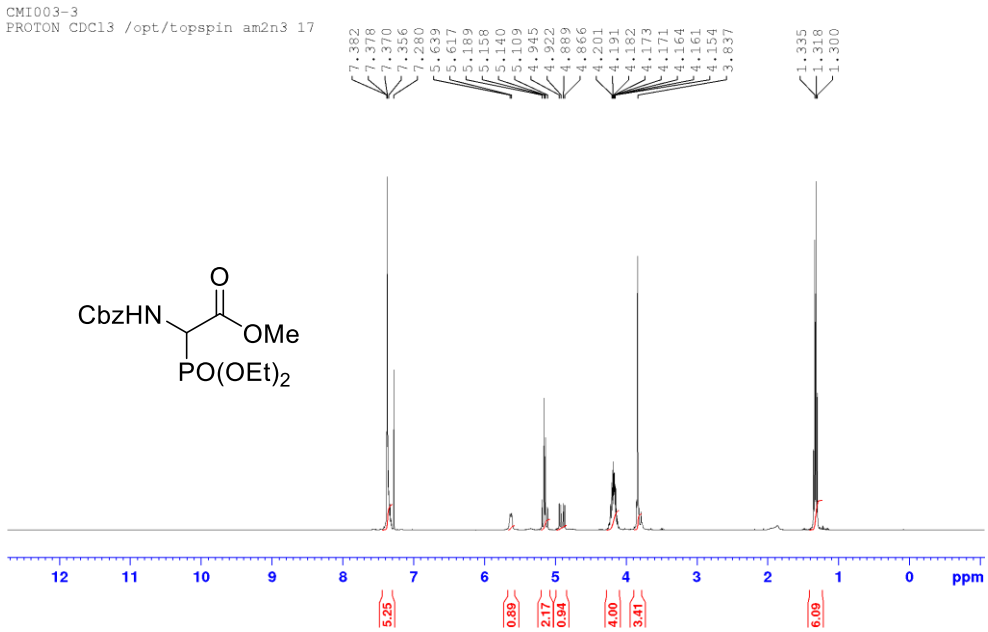
Supplementary Figure 8: ^{13}C NMR spectra of 9 (DMSO-d$_6$)



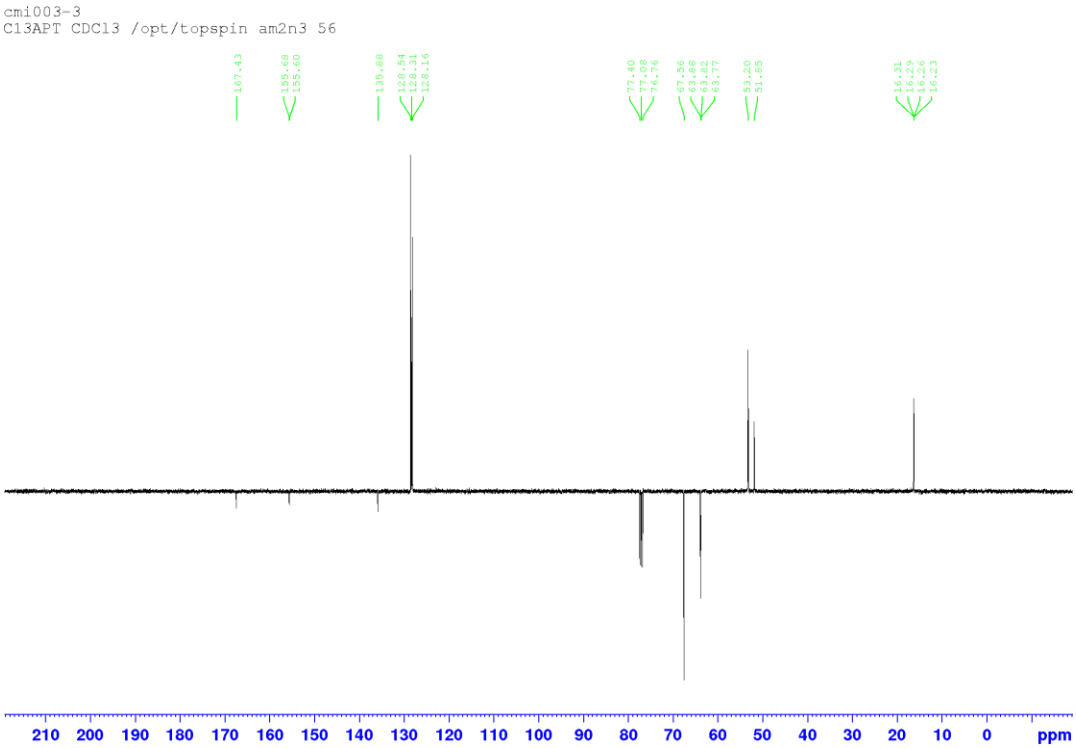
Supplementary Figure 9: ^{1}H NMR spectra of 10 (DMSO-d$_6$)



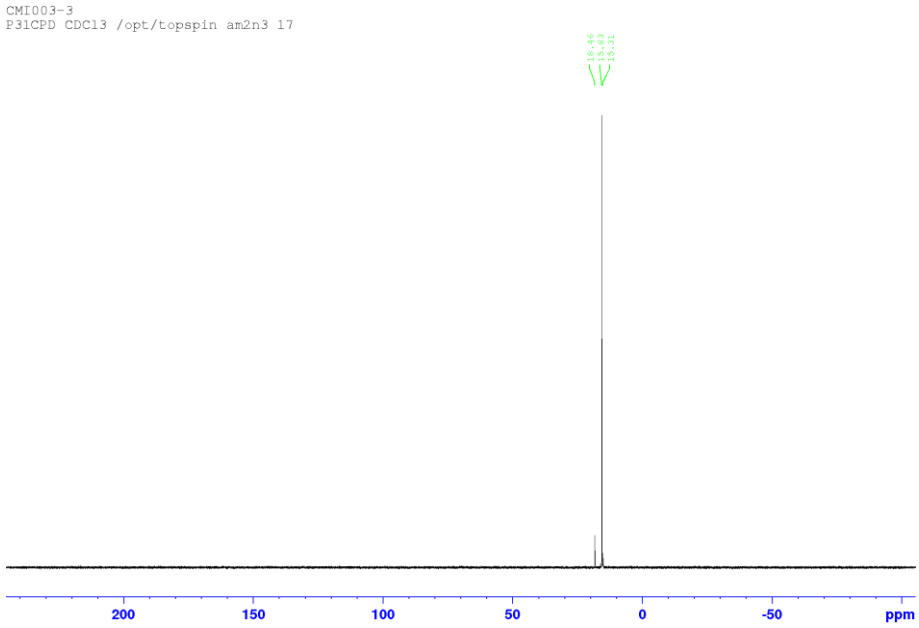
Supplementary Figure 10: ^{13}C NMR spectra of 10 (DMSO-d$_6$)



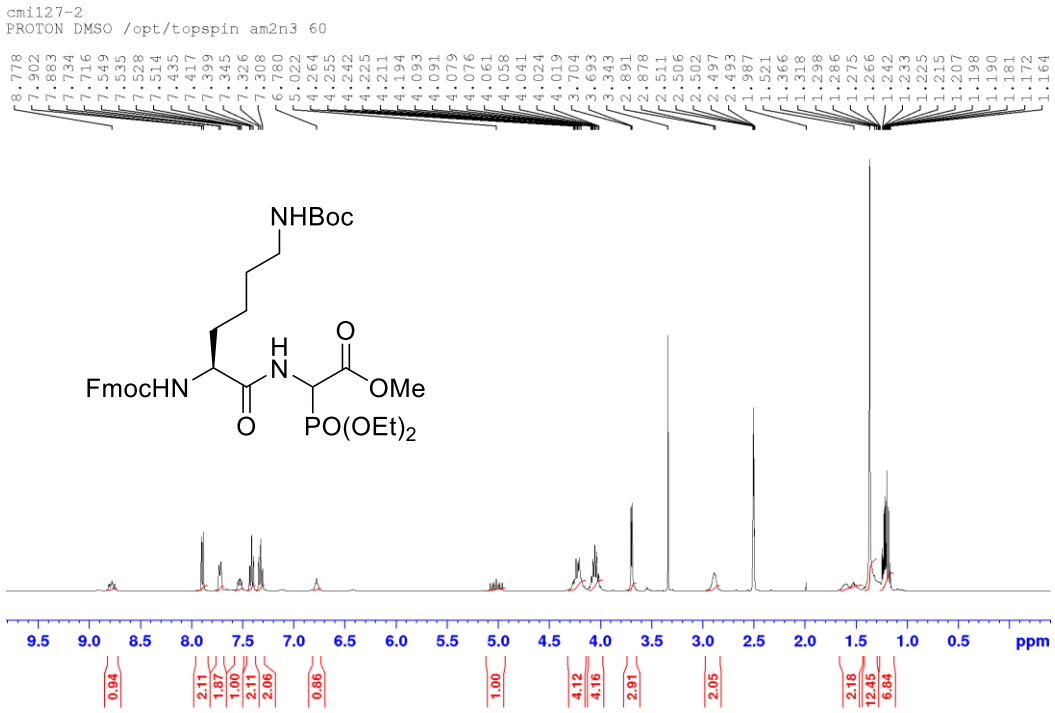
Supplementary Figure 11: ^{1}H NMR spectra of 11 ($CDCl_3$)



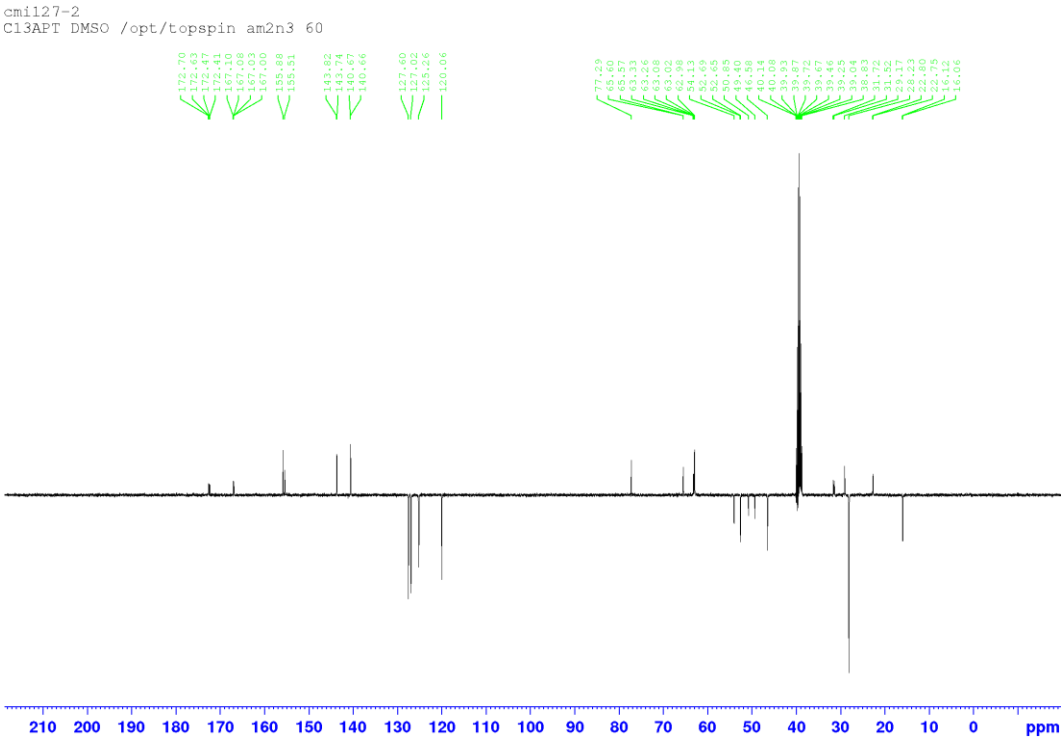
Supplementary Figure 12: ^{13}C NMR spectra of 11 ($CDCl_3$)



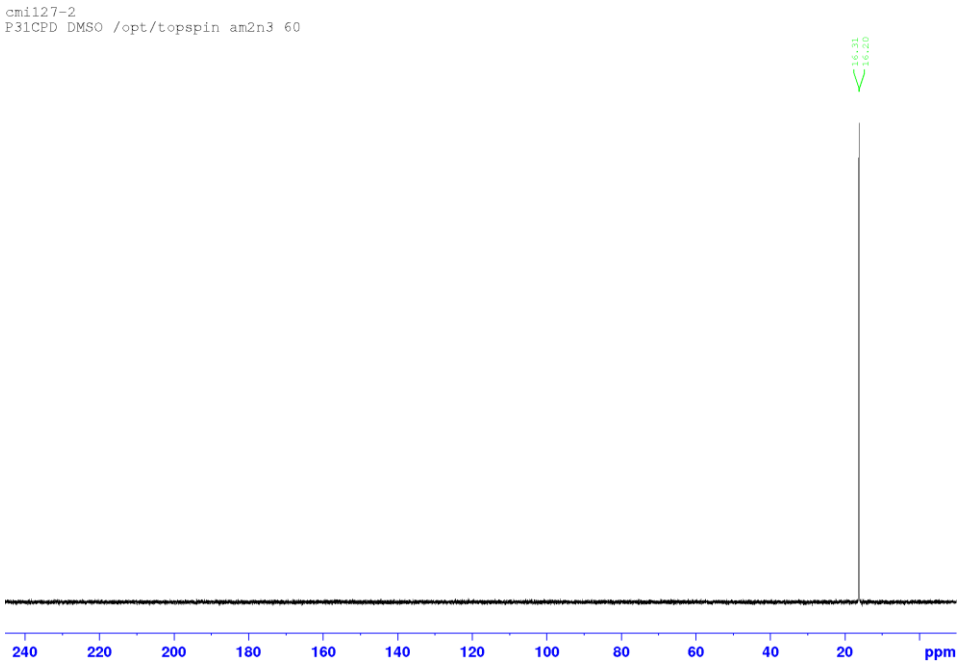
Supplementary Figure 13: ^{31}P NMR spectra of 11 ($CDCl_3$)



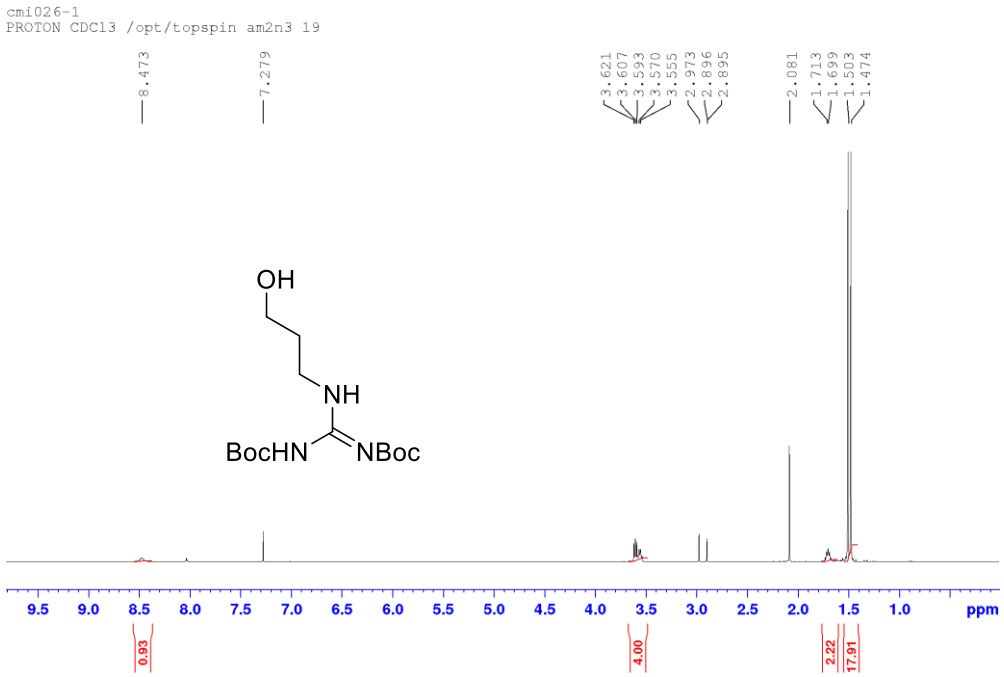
Supplementary Figure 14: ^{1}H NMR spectra of 12 (DMSO-d$_6$)



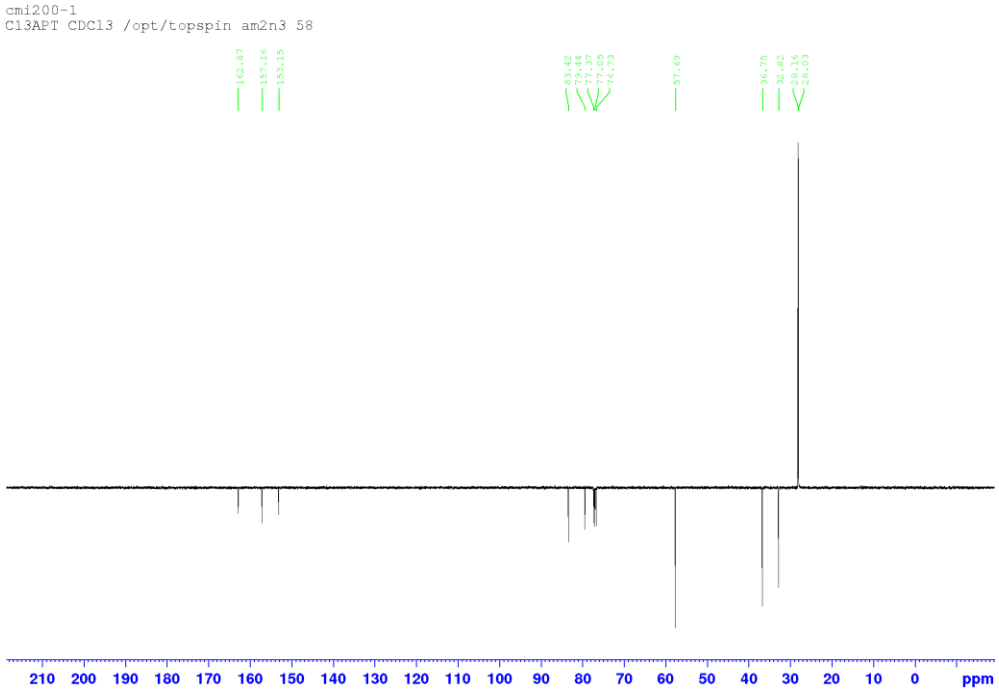
Supplementary Figure 15: ^{13}C NMR spectra of 12 (DMSO-d$_6$)



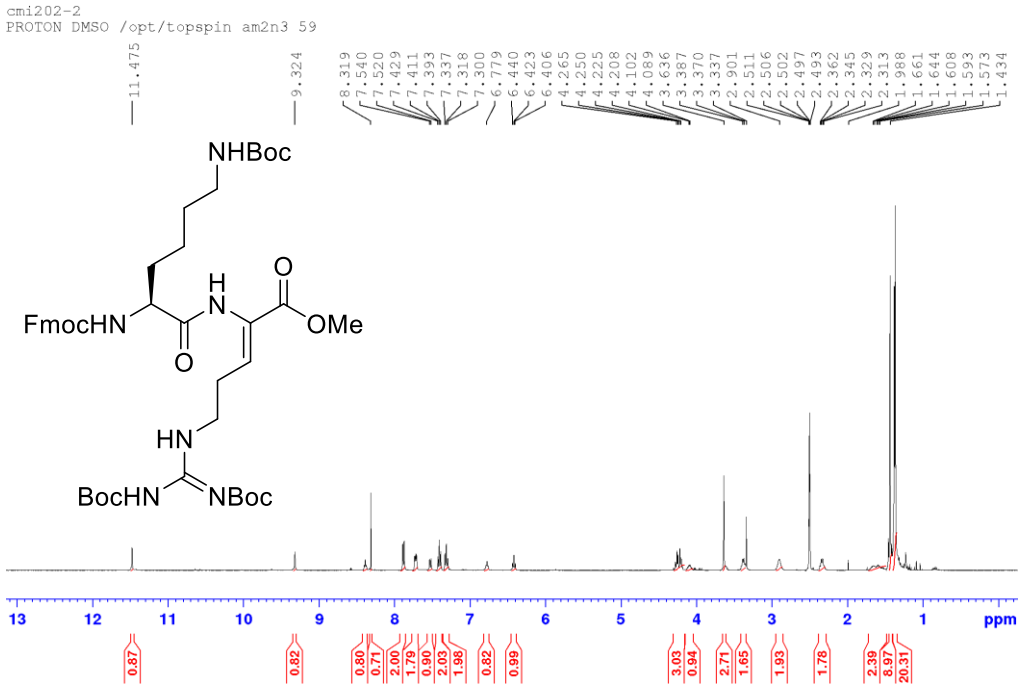
Supplementary Figure 16: ^{31}P NMR spectra of 12 (DMSO-d$_6$)



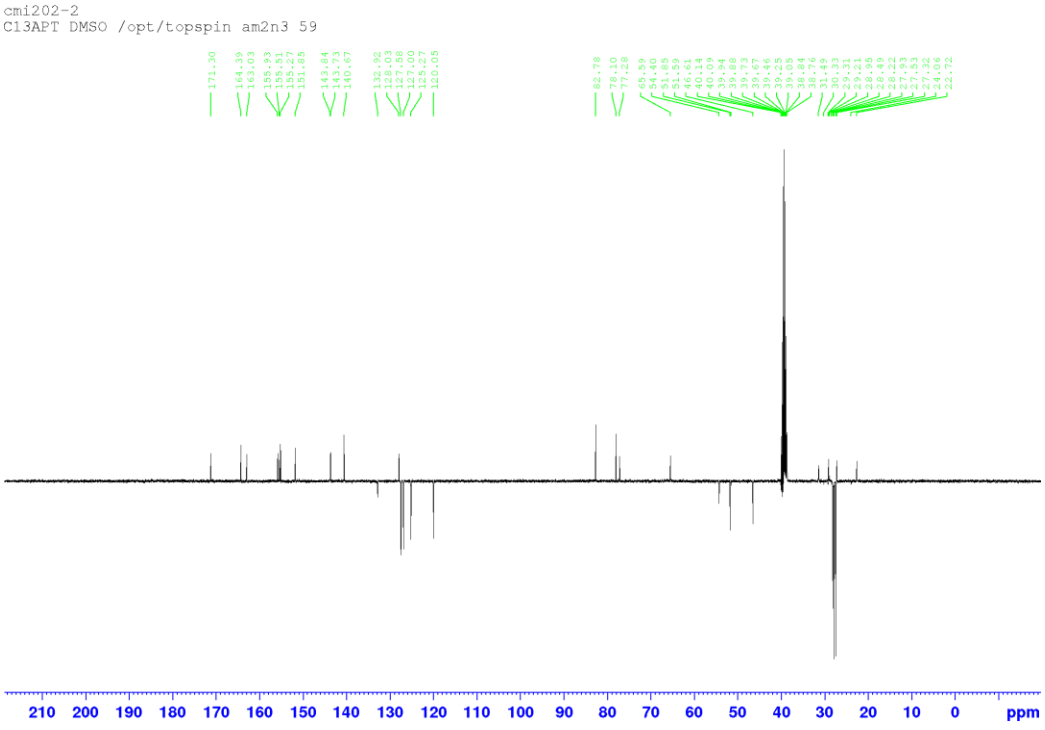
Supplementary Figure 17: ^{1}H NMR spectra of 14 ($CDCl_3$)



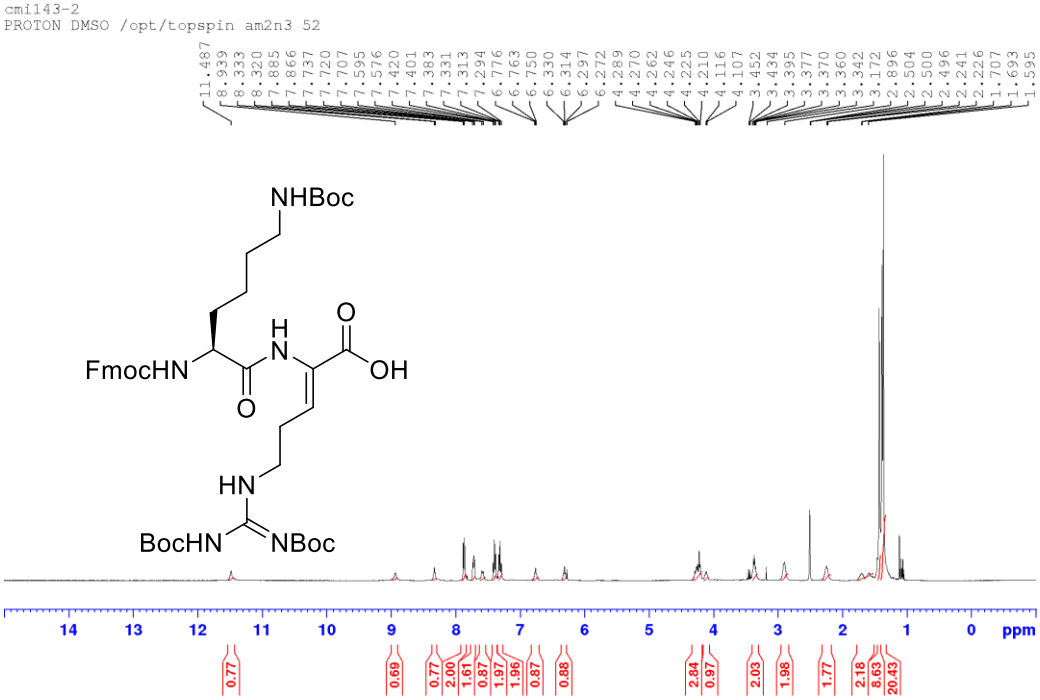
Supplementary Figure 18: ^{13}C NMR spectra of 14 ($CDCl_3$)



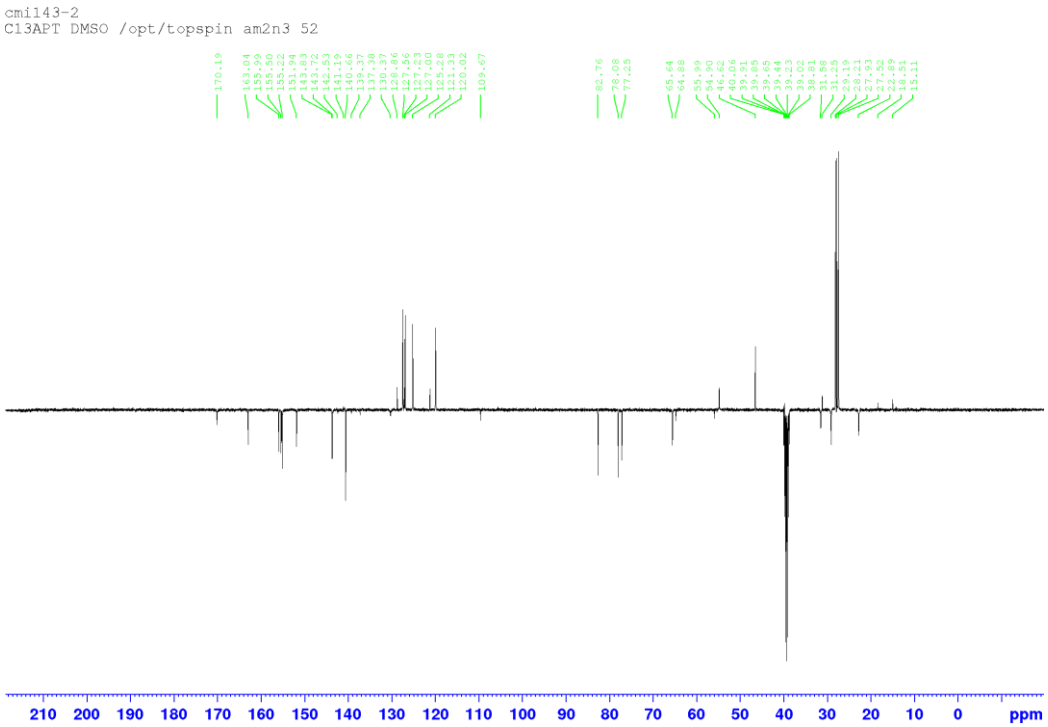
Supplementary Figure 19: ^{1}H NMR spectra of 16 (DMSO-d$_6$)



Supplementary Figure 20: ^{13}C NMR spectra of 16 (DMSO-d$_6$)

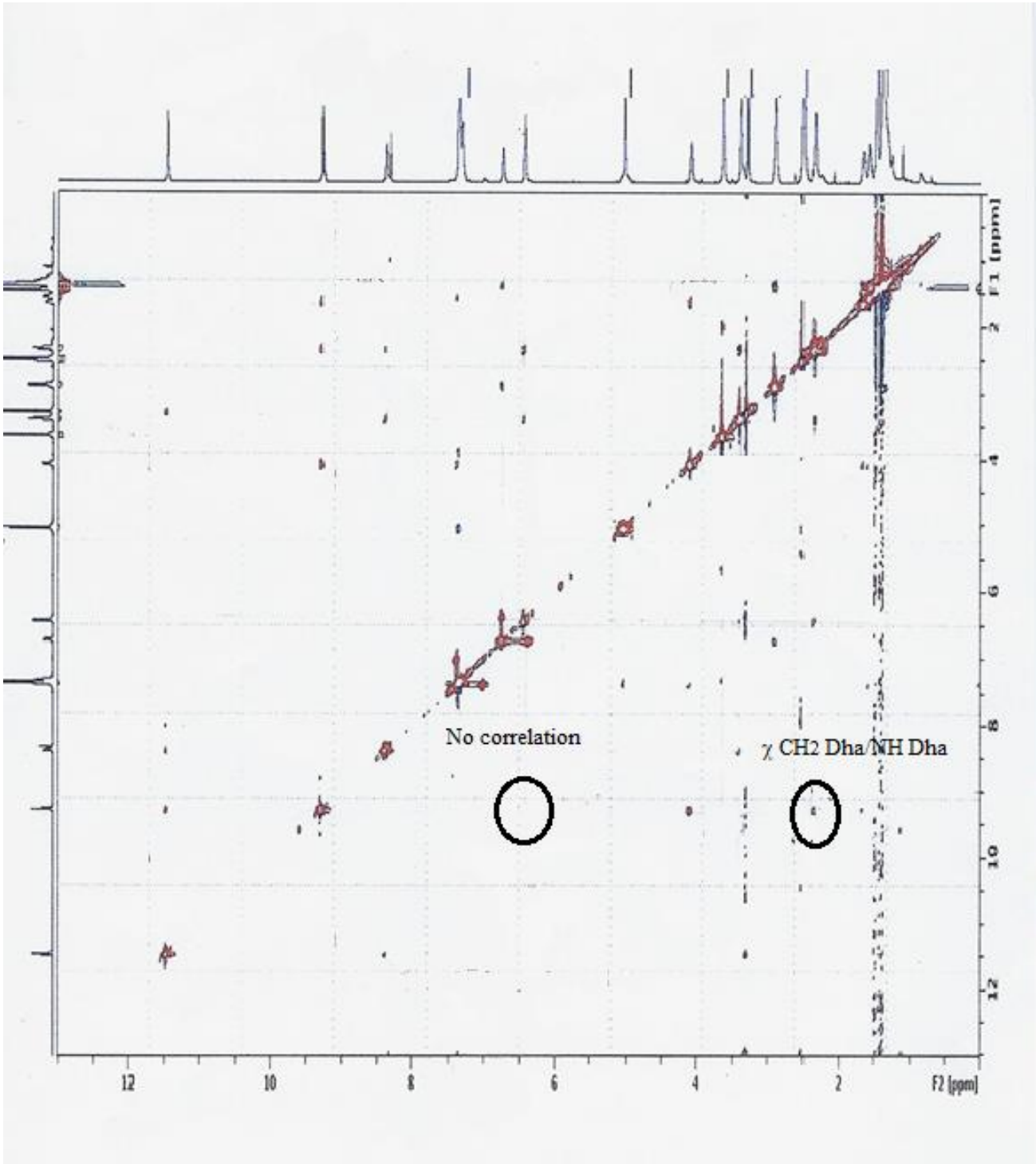


Supplementary Figure 21: ^{1}H NMR spectra of 7 (DMSO-d$_6$)

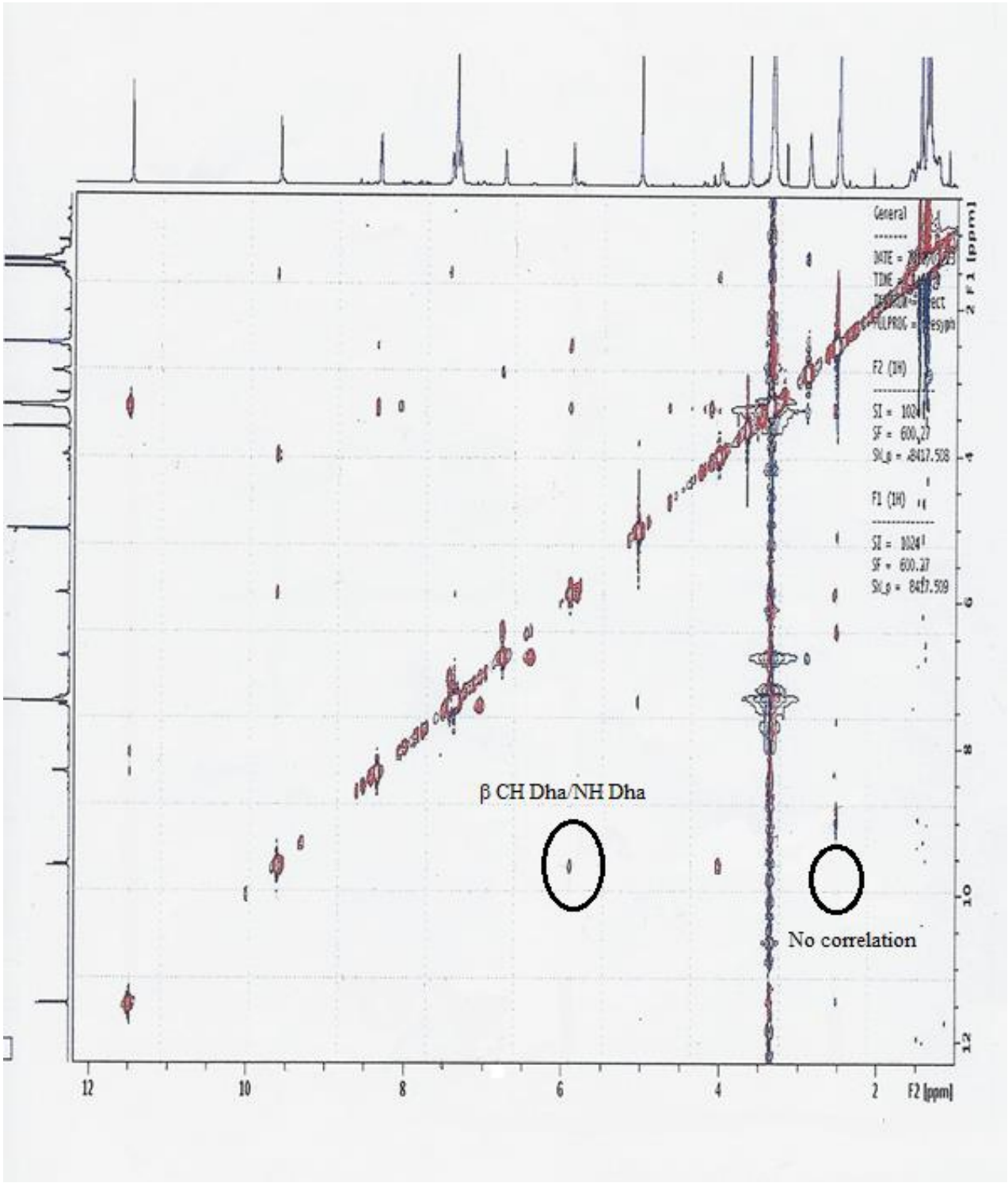


Supplementary Figure 22: ^{13}C NMR spectra of 7 (DMSO-d$_6$)

III- NOESY of dipeptide 7



Supplementary Figure 23: NOESY of (*Z*)-7



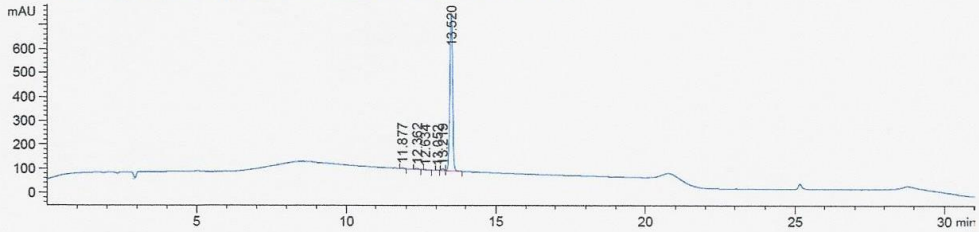
Supplementary Figure 24: NOESY of (*E*)-7

IV- Analyses of NOSO-95C **1**

Data File D:\DATA\OOPERA\MS131009 2013-10-23 16-25-07\012-0301.D
Sample Name: NOSO-0056-010-B

```
==================================================================
Acq. Operator   : SYSTEM                        Seq. Line :   3
Acq. Instrument : LCMS                           Location : Vial 12
Injection Date  : 10/23/2013 5:16:24 PM               Inj :   1
                                               Inj Volume : 10.000 µl
Acq. Method     : D:\DATA\OOPERA\MS131009 2013-10-23 16-25-07\ANALYSE-HFBA.M
Last changed    : 10/23/2013 4:25:07 PM by SYSTEM
Analysis Method : D:\METHODS\ANALYSE-HFBA.M
Last changed    : 4/12/2018 9:06:13 AM by SYSTEM
Method Info     : 20 à 50% pendant 15 min puis 80% 7 min et 20% 7 min (hfba)
```

DAD1 D, Sig=230,4 Ref=off (OOPERA\MS131009 2013-10-23 16-25-07\012-0301.D)



Signal 5: DAD1 D, Sig=230,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.877	BB	0.0790	18.54815	3.54499	0.4290
2	12.362	BB	0.0857	30.40491	5.39553	0.7033
3	12.634	VB	0.1002	8.65815	1.22912	0.2003
4	13.052	BB	0.0751	7.14569	1.63034	0.1653

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
5	13.219	BV	0.0902	47.56071	8.13798	1.1001
6	13.520	VB	0.1006	4211.02686	658.53625	97.4021

Totals : 4323.34447 678.47422

Supplementary Figure 25: UV trace of LC-MS analysis of natural NOSO-95C 1

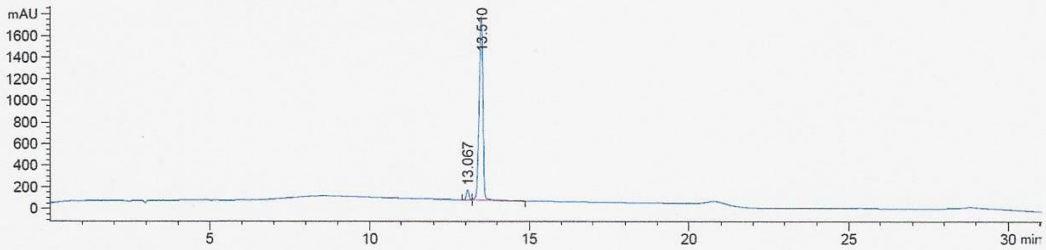
Supplementary Figure 26: mass spectrum of LC-MS analysis of natural NOSO-95C 1

Supplementary Figure 27: mass spectrum of LC-MS analysis of natural NOSO-95C 1 (zoom)

Data File D:\DATA\OOPERA\MS131009 2014-02-05 11-42-13\015-1401.D
Sample Name: NOSO-0068-021-B

```
==================================================================
Acq. Operator   : SYSTEM                        Seq. Line :  14
Acq. Instrument : LCMS                           Location : Vial 15
Injection Date  : 2/5/2014 6:17:59 PM                 Inj :   1
                                               Inj Volume : 10.000 µl
Acq. Method     : D:\DATA\OOPERA\MS131009 2014-02-05 11-42-13\ANALYSE-HFBA.M
Last changed    : 2/5/2014 11:42:14 AM by SYSTEM
Analysis Method : D:\METHODS\ANALYSE-HFBA.M
Last changed    : 4/25/2018 3:12:12 PM by SYSTEM
                  (modified after loading)
Method Info     : 20 à 50% pendant 15 min puis 80% 7 min et 20% 7 min (hfba)
```

DAD1 D, Sig=230,4 Ref=off (OOPERA\MS131009 2014-02-05 11-42-13\015-1401.D)

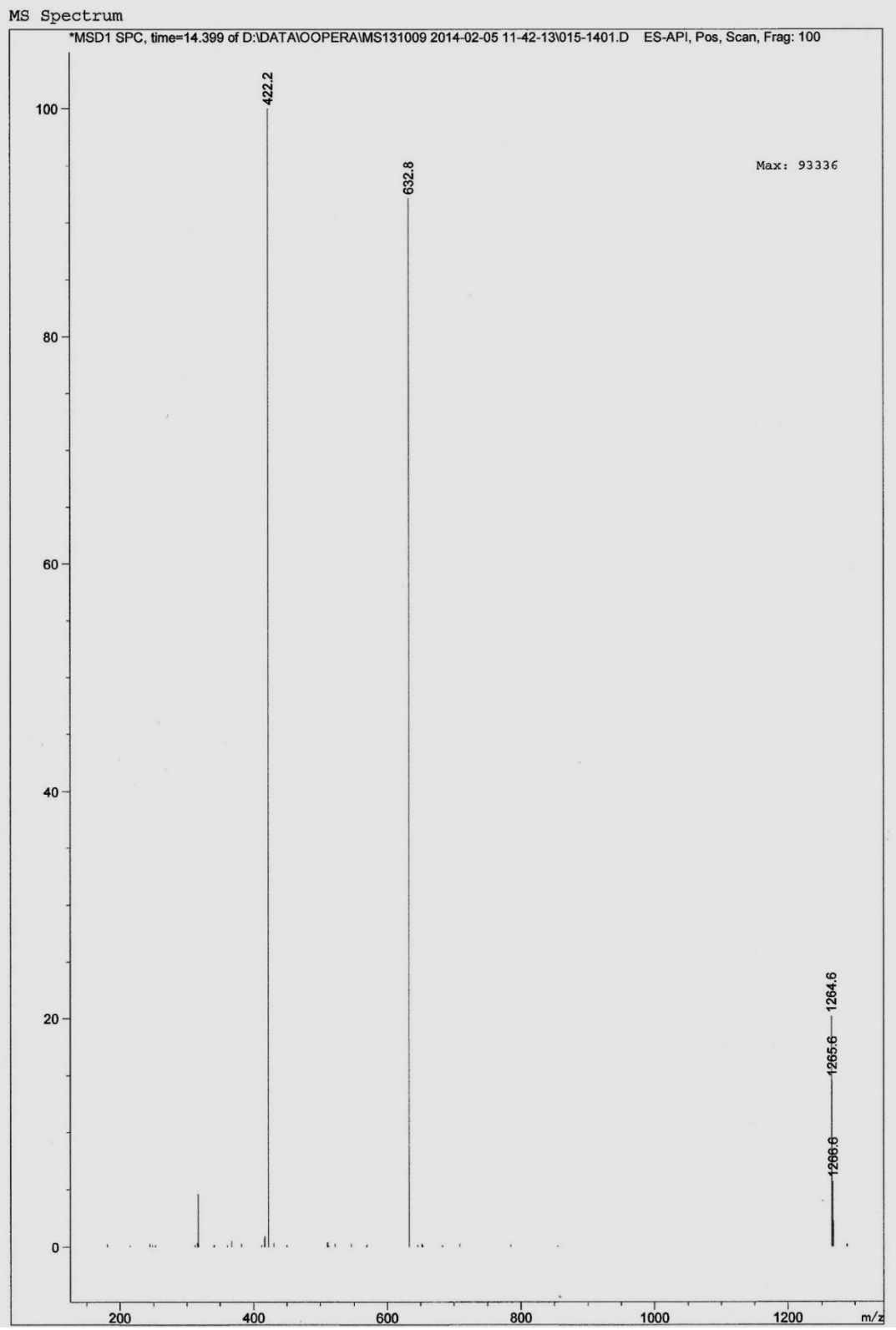


Signal 5: DAD1 D, Sig=230,4 Ref=off

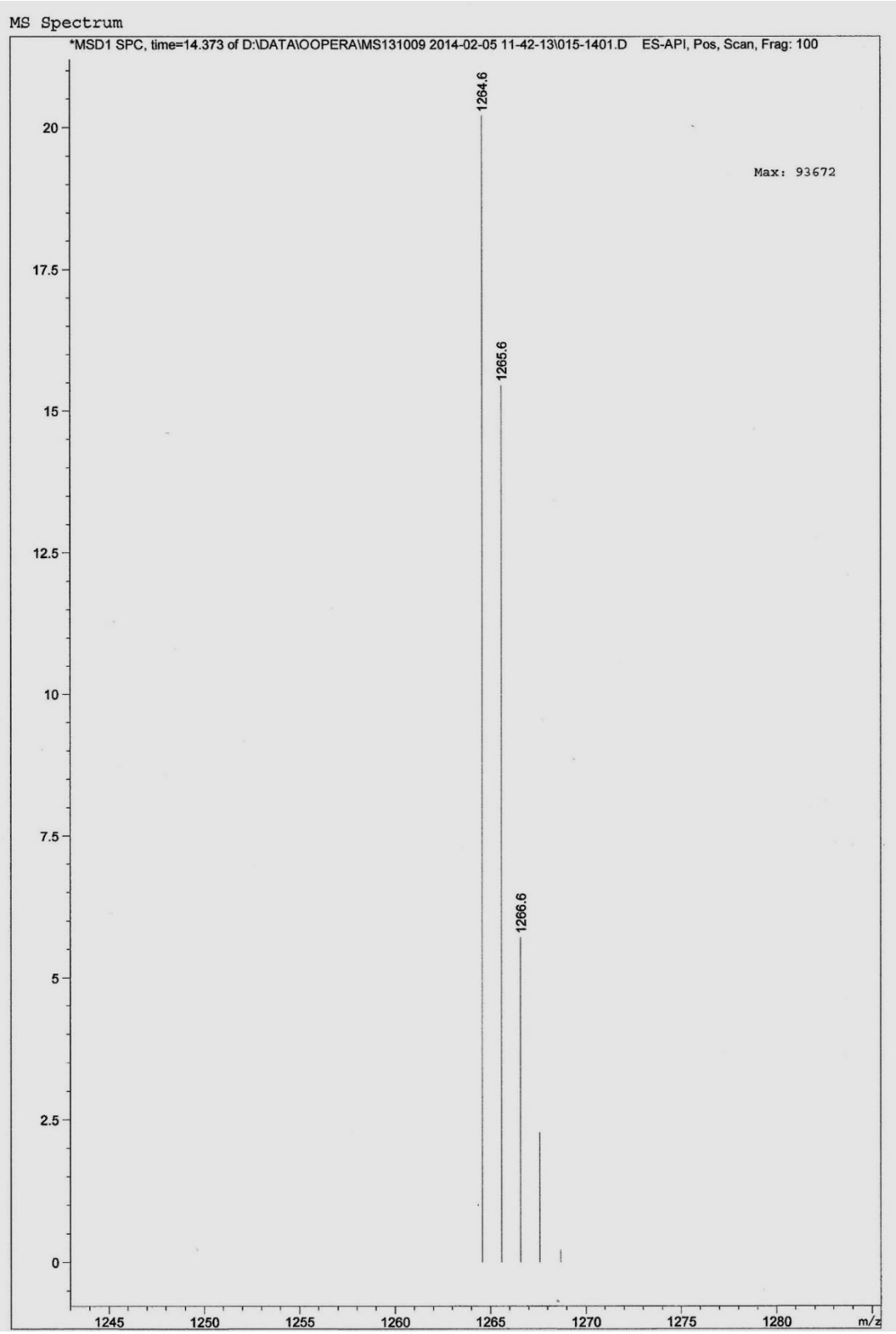
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.067	BV	0.0879	525.90576	93.09110	3.4508
2	13.510	VB	0.1369	1.47140e4	1700.82166	96.5492

Totals : 1.52399e4 1793.91276

Supplementary Figure 28: UV trace of LC-MS analysis of synthetic NOSO-95C 1



Supplementary Figure 29: mass spectrum of LC-MS analysis of synthetic NOSO-95C 1



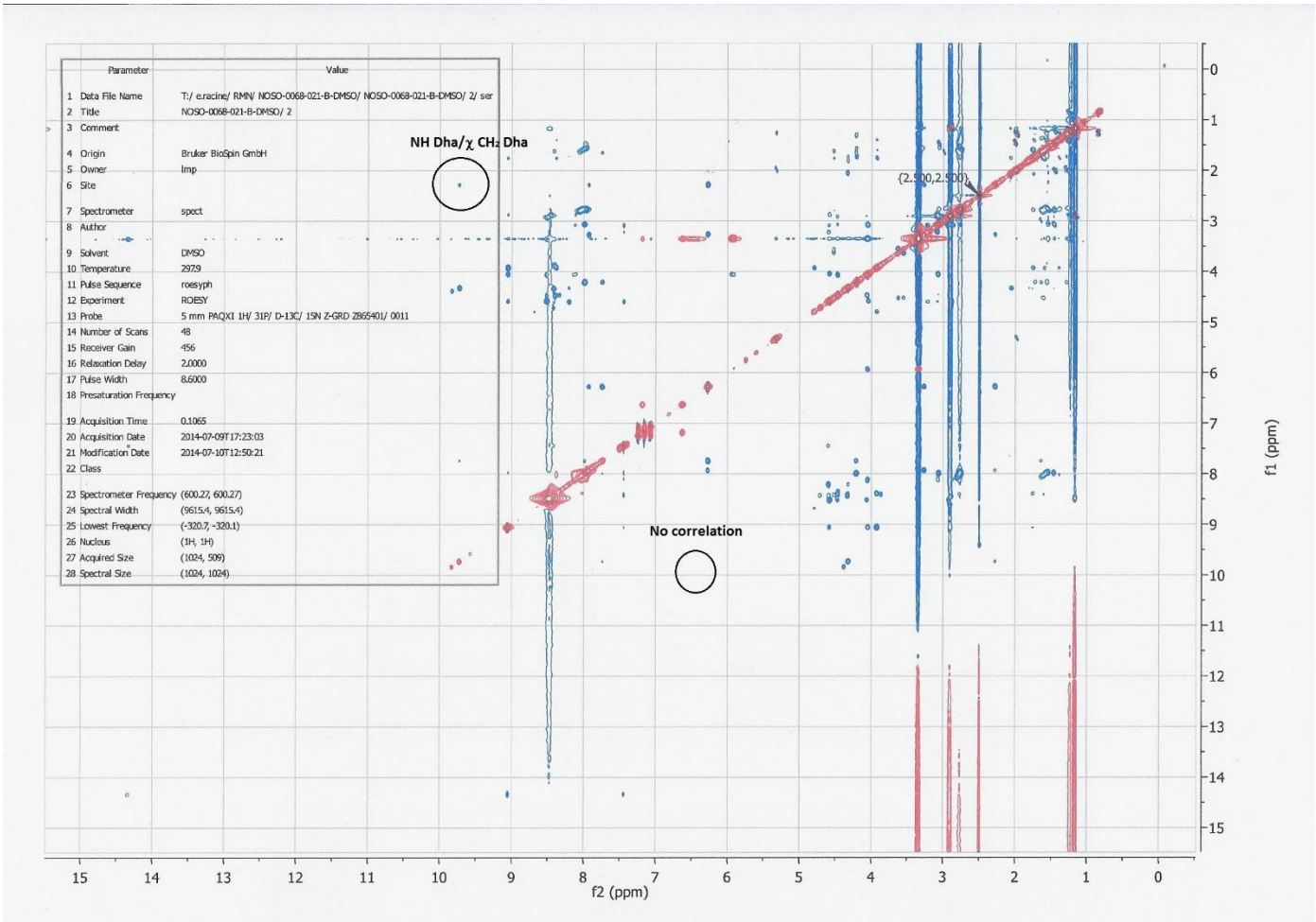
Supplementary Figure 30: mass spectrum of LC-MS analysis of synthetic NOSO-95C 1 (zoom)

Supplementary Table S1: Comparison of chemical shifts of natural and synthetic NOSO-95C 1 (water, 280 K)

Spin system	Group	^{1}H (ppm) natural **1**[1]	^{1}H (ppm) synthetic **1**	^{13}C (ppm) natural **1**1	^{13}C (ppm) synthetic **1**
Lys1	H_2N	–	–	–	–
	CαH	3.80	3.83	53.0	53.2
	$C\beta H_2$	1.66/1.62	1.64/1.60	30.4	30.4
	$C\chi H_2$	1.20	1.20	21.1	21.0
	$C\delta H_2$	1.45	1.46	26.3	26.2
	$C\varepsilon H_2$	2.78	2.74	39.0	39.0
	NH_2	–	–	–	–
Dab(βOH)2	HN	8.83	8.87	–	–
	CαH	4.28	4.28	56.3	56.3
	CβH-OH	3.89	3.84	67.4	67.3
	$C\chi H_2$	2.99/2.79	3.01/2.81	41.9	42.0
	NH_2	–	–	–	–
Dab(βOH)3	HN	8.63	8.58	–	–
	CαH	4.33	4.33	56.3	56.2
	CβH-OH	3.93	3.97	67.7	67.7
	$C\chi H_2$	2.98/2.80	2.97/2.79	41.5	41.4
	NH_2	–	–	–	–
Gly4	HN	8.37	8.40	–	–
	CαH	3.80	3.80	42.1	42.1
Orn5	HN	8.15	8.19	–	–
	CαH	4.46	4.44	51.2	51.5
	$C\beta H_2$	1.58/1.42	1.58/1.42	27.5	27.3
	$C\chi H_2$	1.49/1.40	1.50/1.41	23.2	23.2
	$C\delta H_2$	2.74	2.71	39.0	39.1

	NH_2	–	–	–	–
Pro6	CαH	4.10	4.12	60.4	60.2
	$C\beta H_2$	1.98/1.60	1.98/1.60	29.5	29.5
	$C\chi H_2$	1.72	1.71	24.3	24.3
	$C\delta H_2$	3.48/3.38	3.50/3.40	47.7	47.7
His7	HN	8.49	8.45	–	–
	CαH	4.46	4.48	52.0	52.2
	$C\beta H_2$	2.98/2.91	2.98/2.91	26.3	26.2
	$C\delta_2H$	7.03	6.98	118.0	118.2
	$C\varepsilon_1H$	8.33	8.28	134.0	133.8
Lys8	HN	8.41	8.43	–	–
	CαH	4.12	4.13	53.8	53.7
	$C\beta H_2$	1.70	1.70	27.0	27.0
	$C\chi H_2$	1.36/1.26	1.35/1.25	30.0	30.1
	$C\delta H_2$	1.53	1.51	26.4	26.4
	$C\varepsilon H_2$	2.86/2.63	2.89/2.66	44.5	44.7
	NH_2	–	–	–	–
Dha9	HN	9.60	9.64	–	–
	Cα	–	–	–	–
	CβH	6.17	6.14	132.0	132.3
	$C\chi H_2$	2.20	2.22	26.5	26.4
	$C\delta H_2$	3.10	3.13	39.5	39.5
	HNε	7.00	6.97	–	–
	$C(NH_2)=NH$	–	–	–	–
Lys10	HN	8.05	8.07	–	–
	CαH	4.06	4.07	54.0	54.2

	$C\beta H_2$	1.65	1.65	27.0	26.9
	$C\chi H_2$	1.27	1.27	30.0	30.1
	$C\delta H_2$	1.58	1.59	26.3	26.3
	$C\varepsilon H_2$	2.86/2.63	2.84/2.61	44.5	44.3
	NH_2	–	–	–	–
Dbt11	HN	8.05	8.08	–	–
	$C\alpha H_2$	2.95	2.96	39.5	39.5
	$C\beta H_2$	1.30	1.30	25.3	25.2
	$C\chi H_2$	1.40	1.40	24.0	24.0
	$C\delta H_2$	2.78	2.76	39.0	38.8
	NH_2	–	–	–	–



Supplementary Figure 31: ROESY of synthetic NOSO-95C 1 (DMSO-d_6, 298 K)

Supplementary Table S2: Marfey's analysis of DL-FDAA and D- or L-FDAA amino acids

Amino acid	*m/z (Da)*	*Rt DL-FDAA (min)*	*Rt L-FDAA (min)*
Lys	652	100.76/104.23	100.76
DL-(3*R*)-Dab(βOH) + DL-(3*S*)-Dab(βOH)	639	92.34; 93.08; 95.24 and 95.63	93.12 L-(3*S*)-Dab(βOH)
Gly	637	68.26	N/A
Orn	368	92.08 and 96.32	92.28 (D-Orn)
Pro	660	74.25 and 76.87	74.19
His	408	49.47 and 55.36	55.39
Lys-*Z*-Dha	805	84.32 and 90.73	84.25
1,4-diaminobutane	652	106.06	N/A

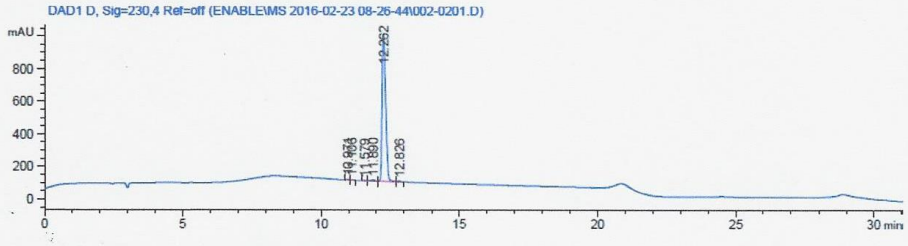
Supplementary Table S3: Marfey's analysis of FDAA-derivatized synthetic NOSO-95C 1

Amino acid	*m/z (Da)*	*Rt FDAA derivative (min)*	*Configuration*
Lys	652	101.15	*S*
Dab(βOH)	639	93.58	*S*,*S*
Gly	637	68.48	N/A
Orn	368	92.29	*R*
Pro	660	74.53	*S*
His	408	55.86	*S*
Lys-*Z*-Dha	805	84.32	*S*
1,4-diaminobutane	652	106.47	N/A

V- Analyses of NOSO-95179 **46**

```
Data File D:\DATA\ENABLE\MS 2016-02-23 08-26-44\002-0201.D
Sample Name: NOSO-95179-B

    ==================================================================
    Acq. Operator   : SYSTEM                          Seq. Line :   2
    Acq. Instrument : LCMS                             Location : Vial 2
    Injection Date  : 2/23/2016 9:00:51 AM                  Inj :   1
                                                     Inj Volume : 10.000 µl
    Acq. Method     : D:\DATA\ENABLE\MS 2016-02-23 08-26-44\ANALYSE-HFBA.M
    Last changed    : 2/23/2016 8:26:45 AM by SYSTEM
    Analysis Method : D:\METHODS\ANALYSE-HFBA.M
    Last changed    : 4/25/2018 3:12:12 PM by SYSTEM
                      (modified after loading)
    Method Info     : 20 à 50% pendant 15 min puis 80% 7 min et 20% 7 min (hfba)
```

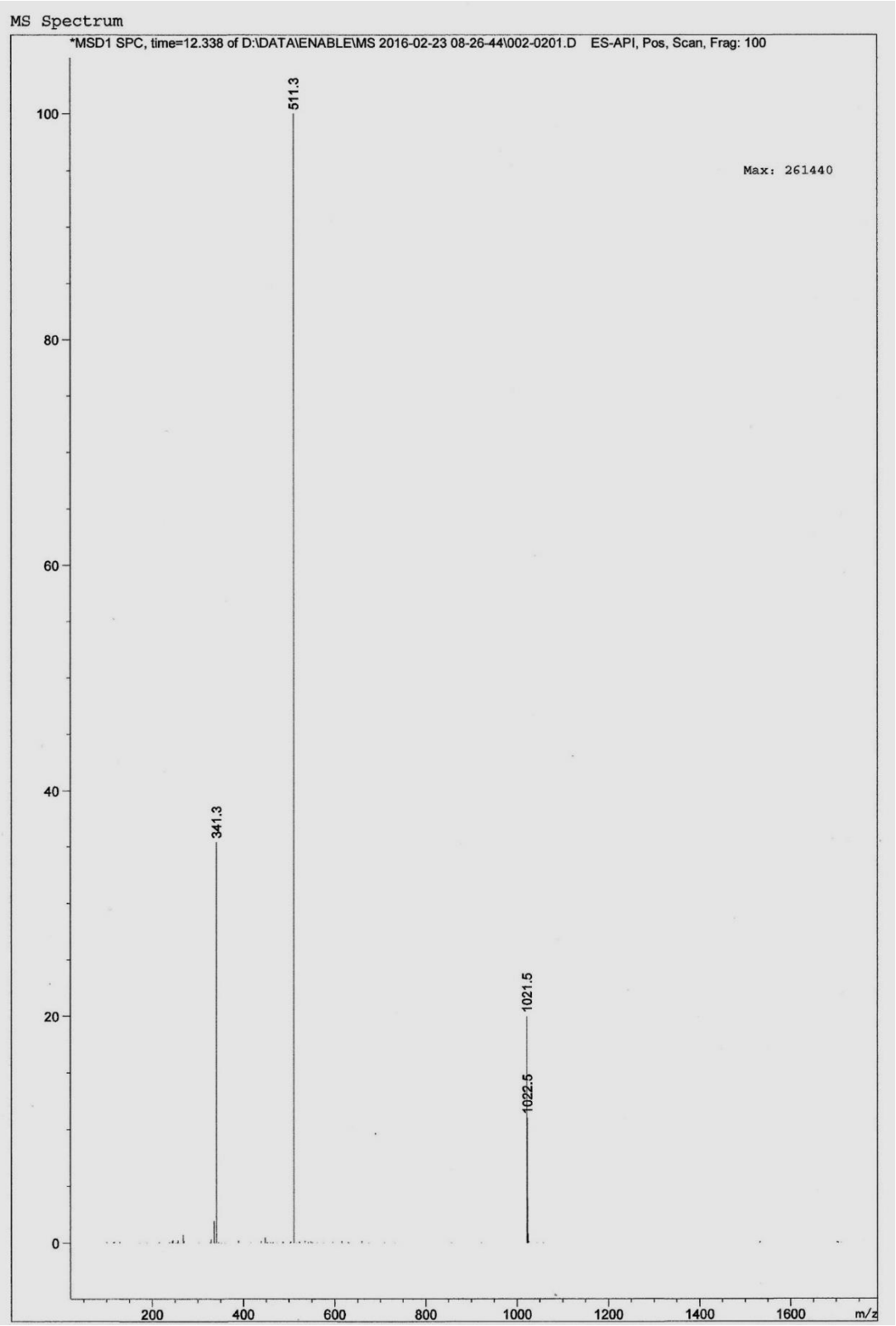



```
    Signal 3: DAD1 D, Sig=230,4 Ref=off

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  10.971 BV    0.0872   18.99574    3.29910   0.2294
       2  11.106 VB    0.0900   12.42229    2.13080   0.1500
       3  11.579 BV    0.0939   12.32771    2.00046   0.1489
       4  11.890 VB    0.1369   74.63856    7.71597   0.9015
       5  12.262 BV    0.1421 8095.35742  907.13776  97.7796
       6  12.826 VB    0.1152   65.44447    8.36988   0.7905

    Totals :                  8279.18620  930.65396
```

Supplementary Figure 32: UV trace of LC-MS analysis of NOSO-95179 46 (TFA salt)

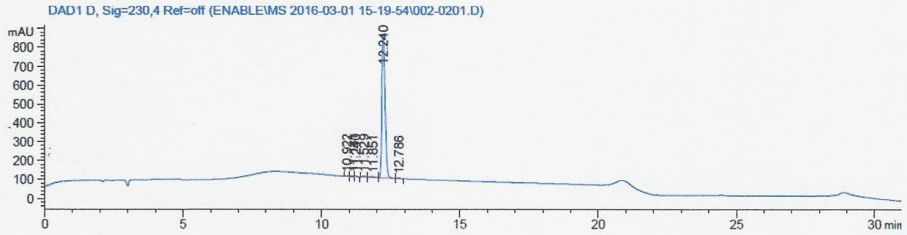


Supplementary Figure 33: mass spectrum of LC-MS analysis of NOSO-95179 46 (TFA salt)

Supplementary Figure 34: mass spectrum of LC-MS analysis of NOSO-95179 46 (TFA salt, zoom)

Data File D:\DATA\ENABLE\MS 2016-03-01 15-19-54\002-0201.D
Sample Name: NOSO-0074-161-C

```
==================================================================
Acq. Operator   : SYSTEM                        Seq. Line :   2
Acq. Instrument : LCMS                           Location : Vial 2
Injection Date  : 3/1/2016 3:54:27 PM                 Inj :   1
                                               Inj Volume : 10.000 µl
Acq. Method     : D:\DATA\ENABLE\MS 2016-03-01 15-19-54\ANALYSE-HFBA.M
Last changed    : 3/1/2016 3:19:54 PM by SYSTEM
Analysis Method : D:\METHODS\ANALYSE-HFBA.M
Last changed    : 4/25/2018 3:17:55 PM by SYSTEM
                  (modified after loading)
Method Info     : 20 à 50% pendant 15 min puis 80% 7 min et 20% 7 min (hfba)
```

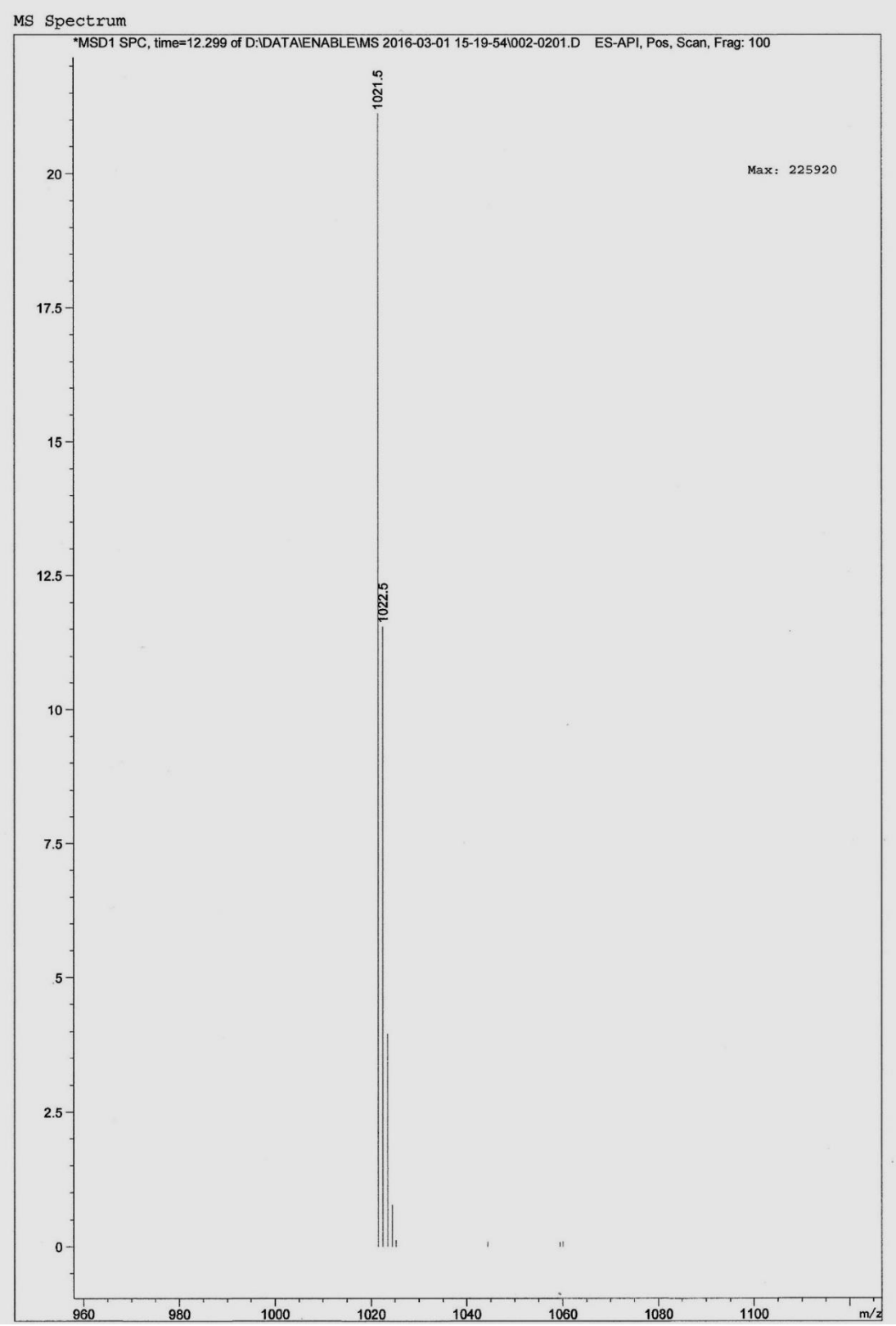


Signal 3: DAD1 D, Sig=230,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.922	BV	0.0828	13.87575	2.57865	0.2182
2	11.141	VV	0.1078	29.50630	3.75158	0.4640
3	11.240	VB	0.0765	15.34874	3.05990	0.2413
4	11.529	BV	0.1047	38.60001	5.44766	0.6069
5	11.851	VV	0.1646	74.16328	6.06764	1.1661
6	12.240	VV	0.1257	6144.33789	764.73407	96.6129
7	12.786	VB	0.1094	43.91577	6.00263	0.6905
Totals :				6359.74775	791.64212	

Supplementary Figure 35: UV trace of LC-MS analysis of NOSO-95179 46 (HCl salt)

Supplementary Figure 36: mass spectrum of LC-MS analysis of NOSO-95179 46 (HCl salt)



Supplementary Figure 37: mass spectrum of LC-MS analysis of NOSO-95179 46 (HCl salt, zoom)

VI – HRMS data

Supplementary Table S4: HRMS data of new compounds

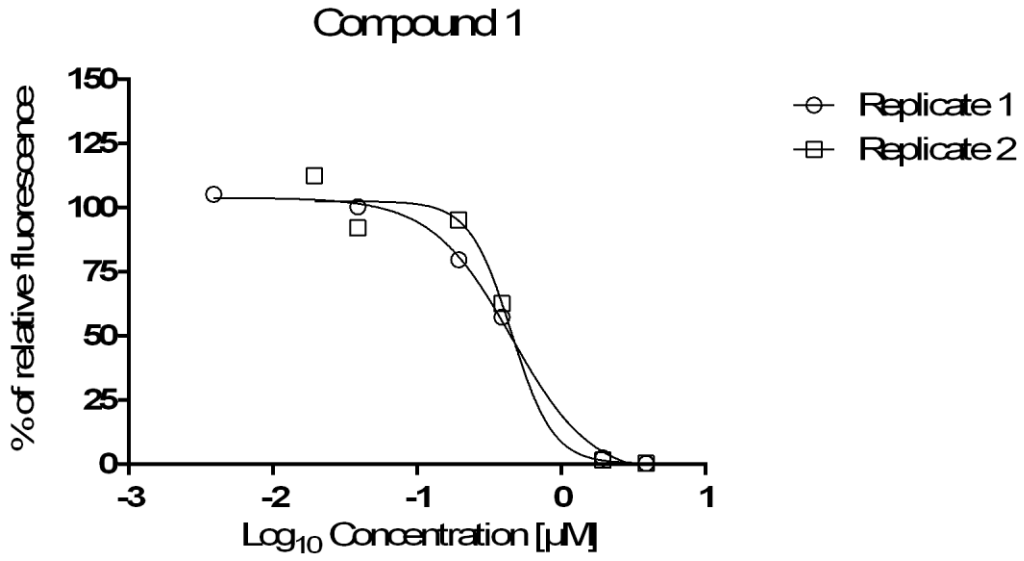
Cmpd	Observed mass	Calculated mass
1	1264.8066	1264.8065
17	1207.7500	1207.7500
18	1219.7871	1219.7877
19	1219.7848	1219.7864
20	1278.8220	1278.8221
21	1221.7649	1221.7656
22	1238.7913	1238.7908
23	1198.7848	1198.7847
24	1207.7526	1207.7513
25	1181.7567	1181.7595
26	1207.7490	1207.7500
27	1194.9197	1194.9201
28	1248.8124	1248.8129
29	1249.7943	1249.7911
30	1235.7814	1235.7813
31	1248.8104	1248.8129
32	1249.7952	1249.7969
33	1235.7795	1235.7813
34	1205.7687	1205.7707
35	1247.8153	1247.8177
36	1233.8019	1233.8020
37	1193.7609	1193.7613
38	1266.8239	1266.8235
39	1266.8232	1266.8235
40	1194.9197	1194.9201
41	1066.8081	1066.8085
42	912.5375	912.5379
43	784.4432	784.4430
44	1136.7098	1136.7088
45	1020.6542	1020.6543
46	1021.6026	1021.6019

VII – MIC of compounds in µM

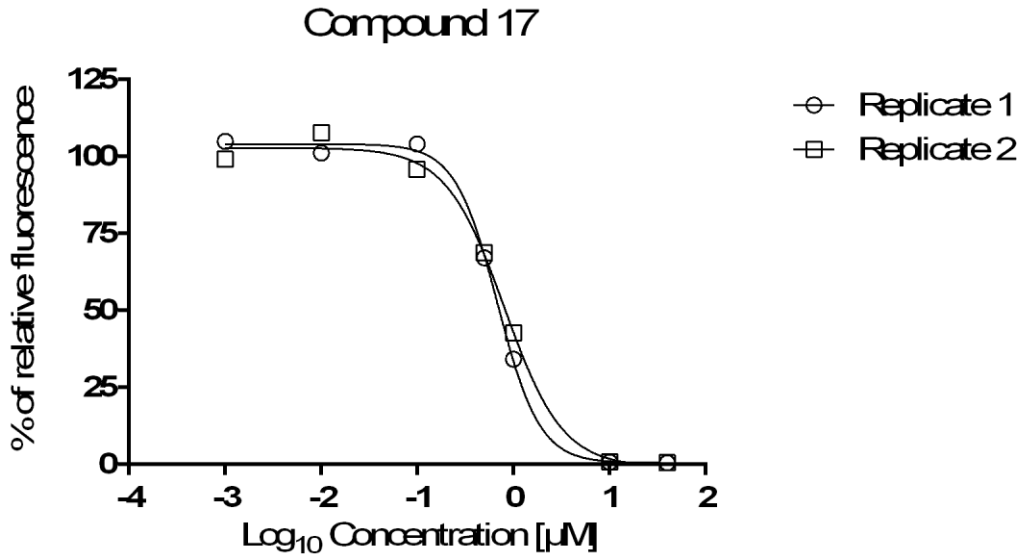
Supplementary Table S5: comparison of MIC in µg/mL and µM

Compound	MIC *E.coli* ATCC 25922		MIC *K. pneumoniae* ATCC 43816	
	µg/mL	µM	µg/mL	µM
1	8	3,33	4	1,66
17	16	7,17	8	3,58
18	>64	>28,51	>64	>28,51
19	2	0,89	1	0,45
20	>64	>26,47	>64	>26,47
21	>64	>28,48	>64	>28,48
22	16	6,73	32	13,46
23	8	3,33	8	3,33
24	16	7,17	4	1,79
25	>64	>29,00	64	29,00
26	8	3,58	8	3,58
27	16	7,21	4	1,80
28	>64	>26,80	64	26,80
29	>64	>28,13	>64	>28,13
30	>64	>28,31	>64	>28,31
31	4	1,68	4	1,68
32	8	3,52	8	3,52
33	4	1,77	4	1,77
34	8	3,41	8	3,41
35	4	1,76	2	0,88
36	4	1,77	4	1,77
37	16	7,21	8	3,61
38	32	13,96	8	3,49
39	16	6,65	16	6,65
40	16	7,21	4	1,80
41	16	8,13	4	2,03
42	>64	>37,43	>64	>37,43
43	>64	>43,63	>64	>43,63
44	>64	>29,60	>64	>29,60
45	>64	>29,82	>64	>29,82
46	16	12,54	4	3,13

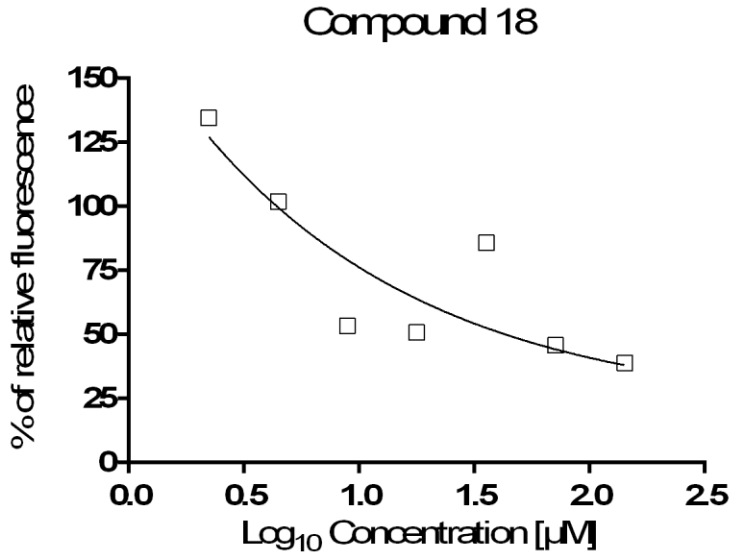
VIII – Inhibition curves of compounds 1, 17-46



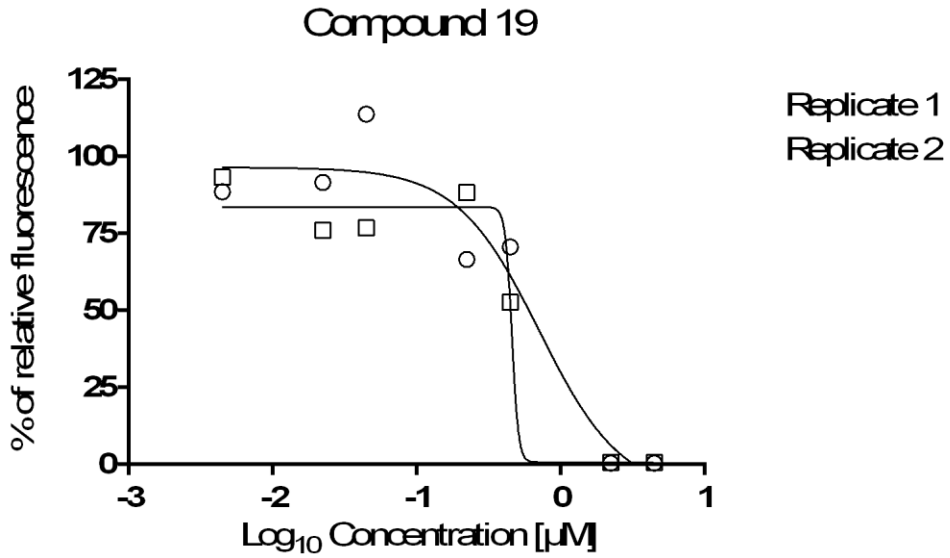
Supplementary Figure 36: Inhibition curve of compound 1



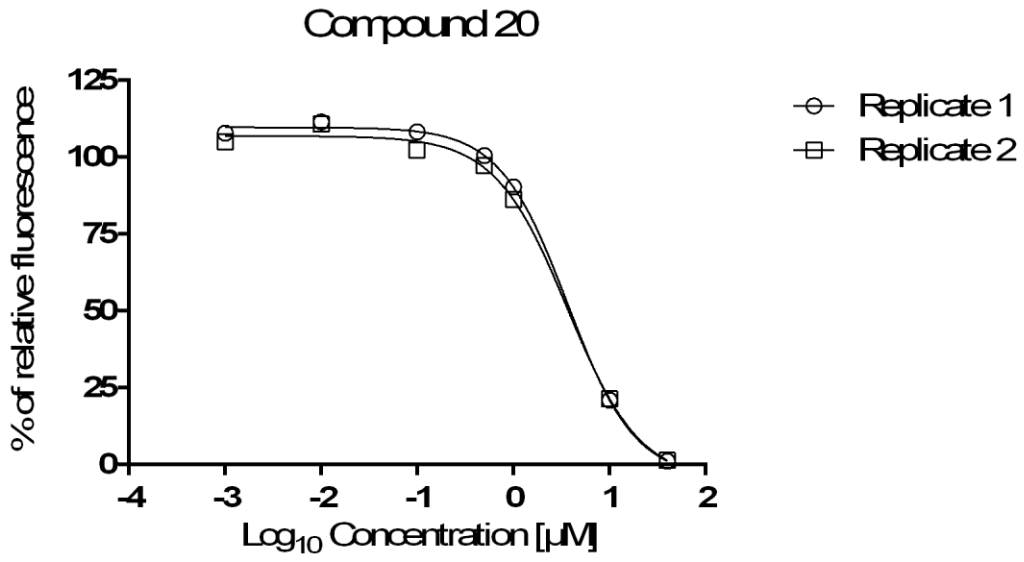
Supplementary Figure 37: Inhibition curve of compound 17



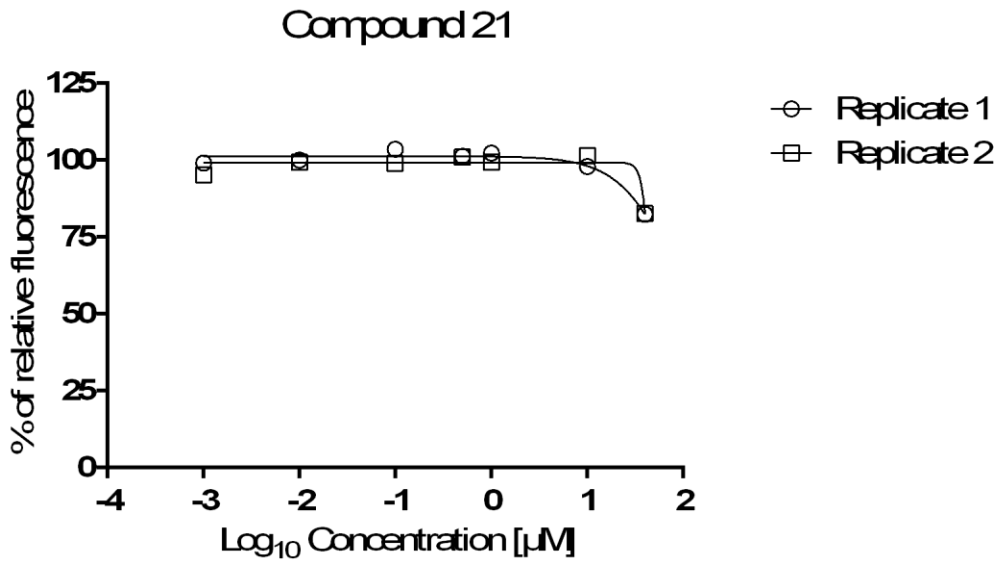
Supplementary Figure 38: Inhibition curve of compound 18



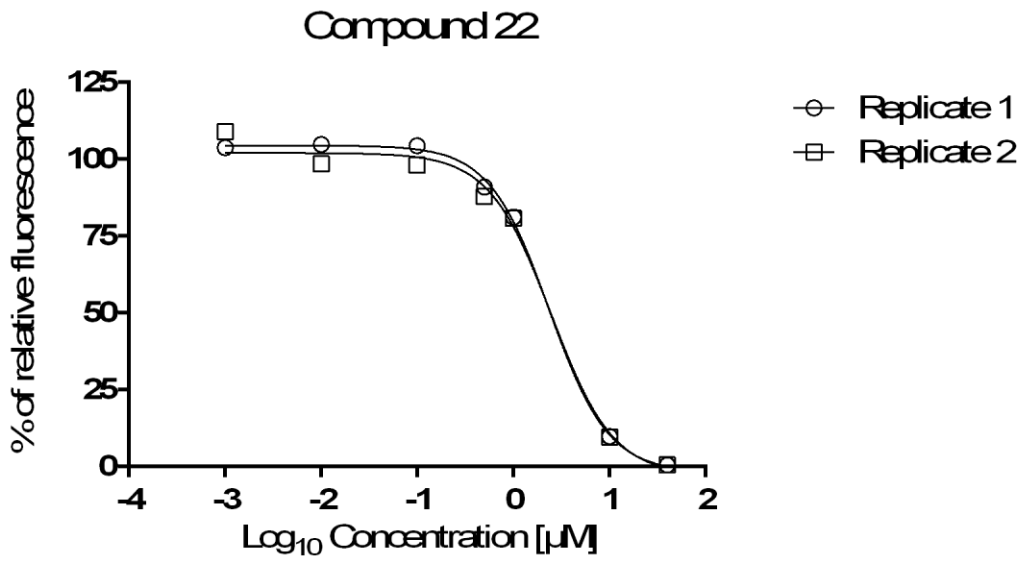
Supplementary Figure 39: Inhibition curve of compound 19



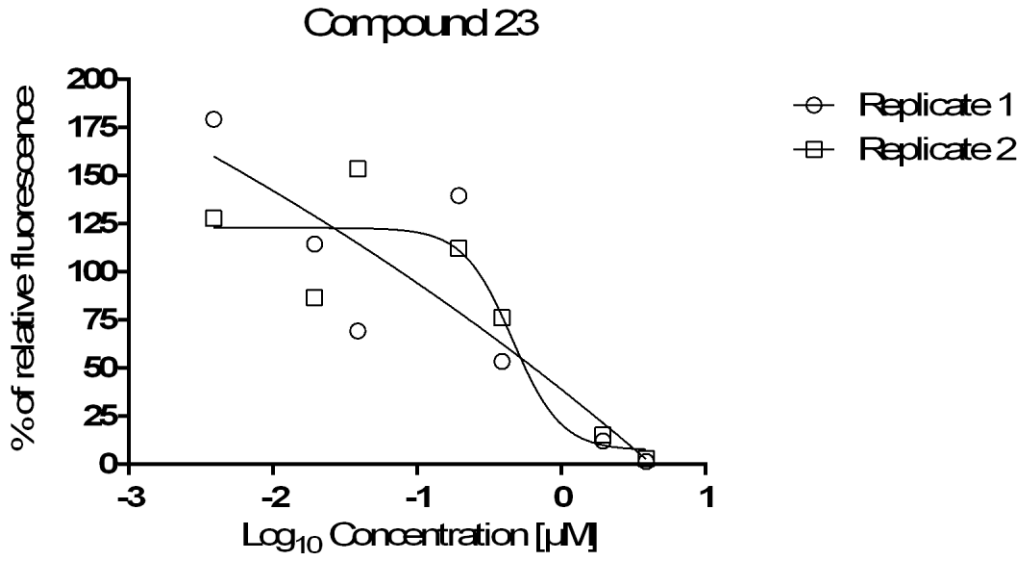
Supplementary Figure 40: Inhibition curve of compound 20



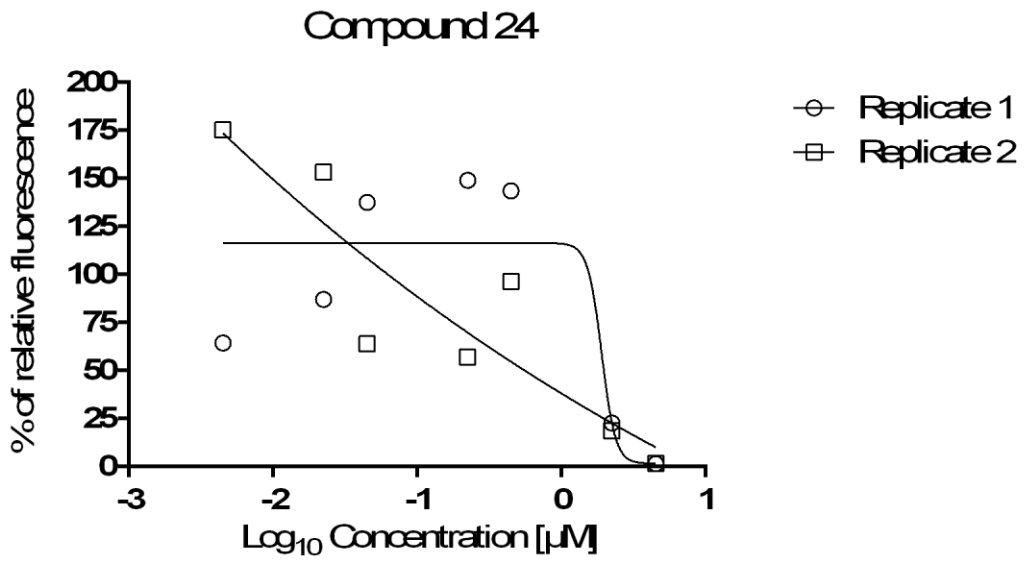
Supplementary Figure 41: Inhibition curve of compound 21



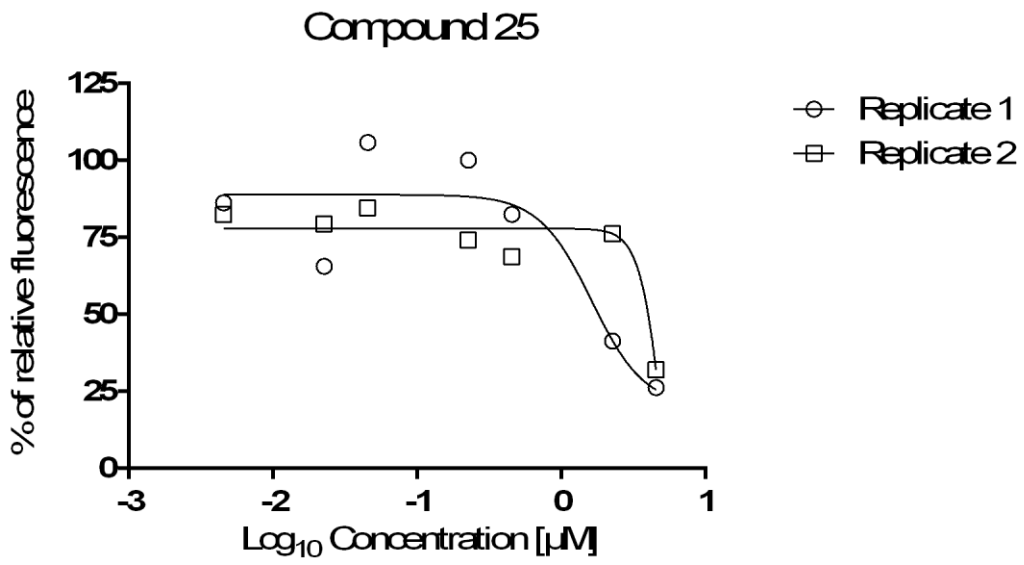
Supplementary Figure 42: Inhibition curve of compound 22



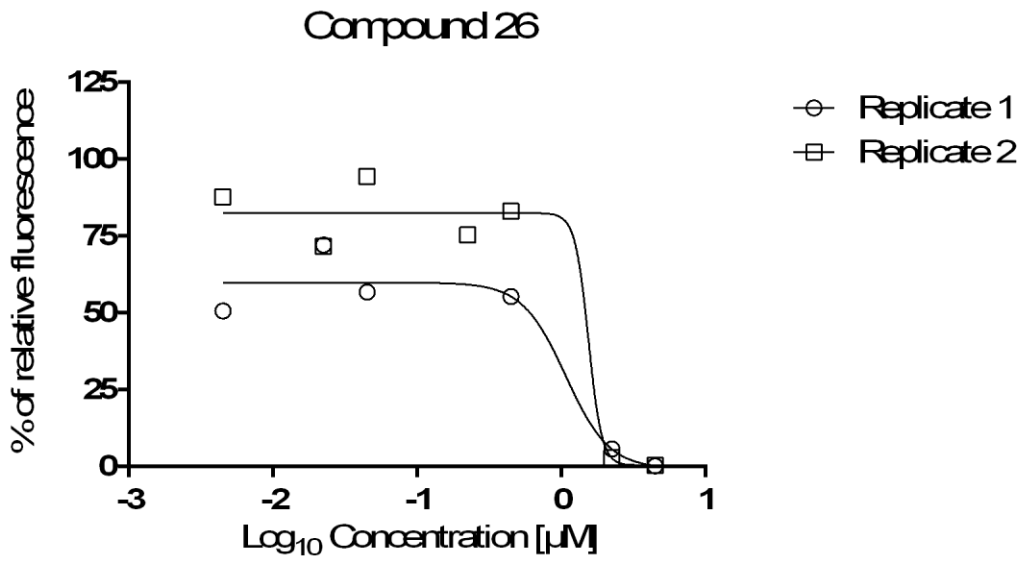
Supplementary Figure 43: Inhibition curve of compound 23



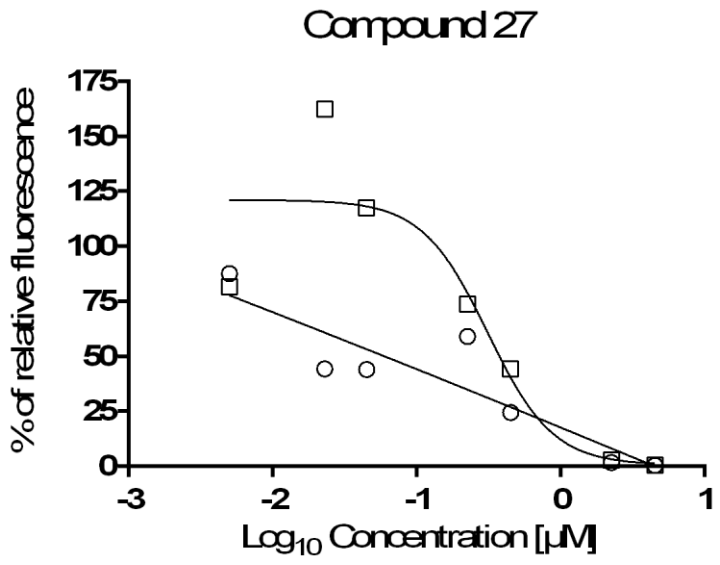
Supplementary Figure 44: Inhibition curve of compound 24



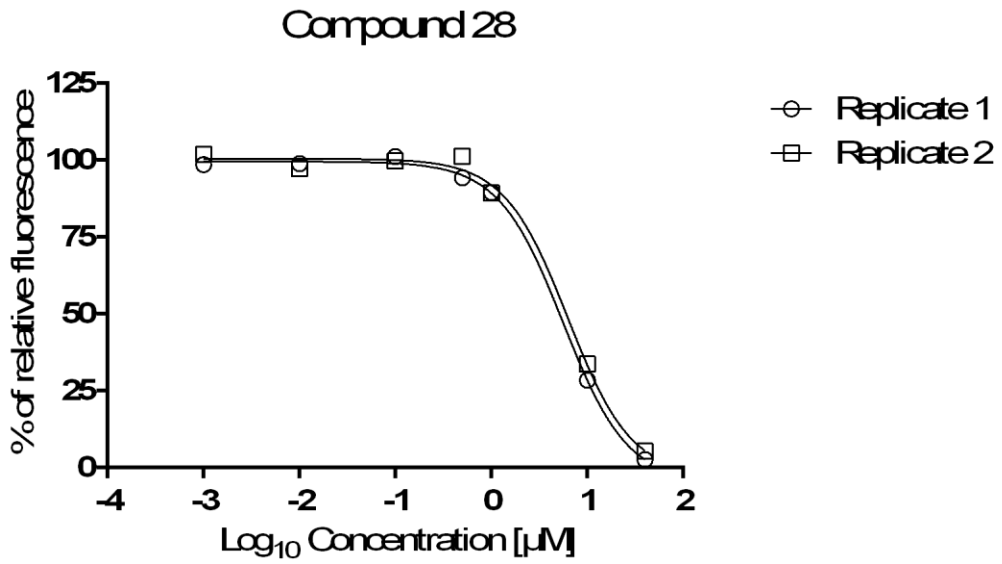
Supplementary Figure 45: Inhibition curve of compound 25



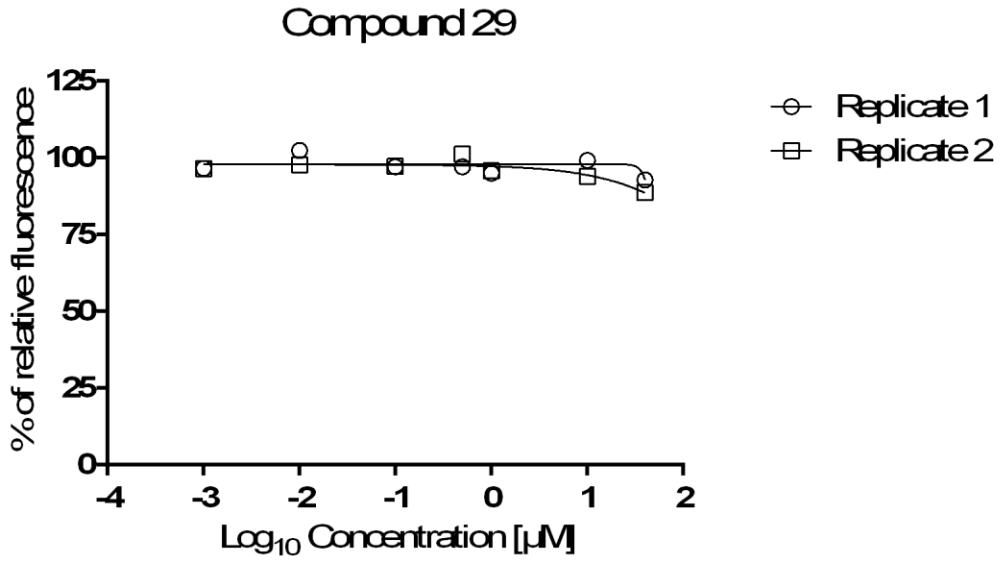
Supplementary Figure 46: Inhibition curve of compound 26



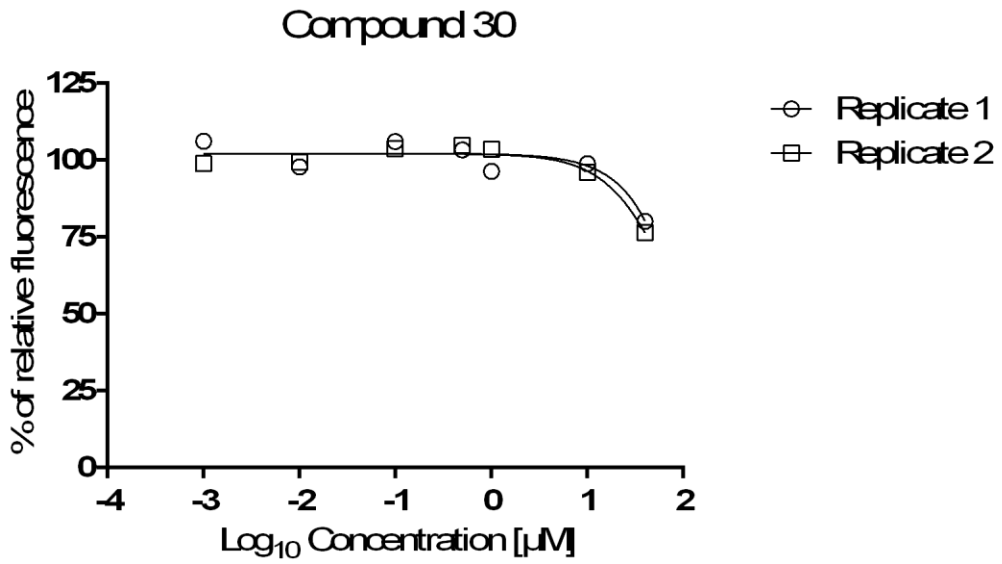
Supplementary Figure 47: Inhibition curve of compound 27



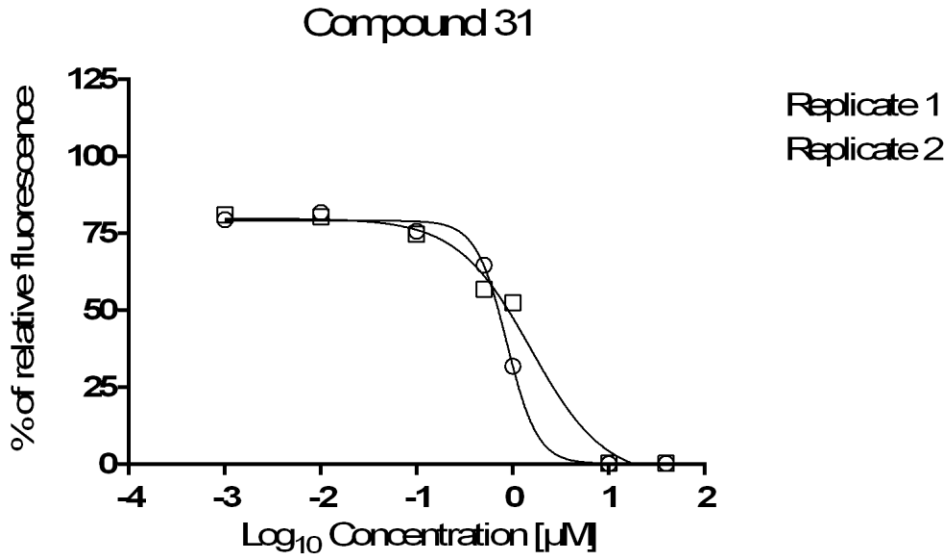
Supplementary Figure 48: Inhibition curve of compound 28



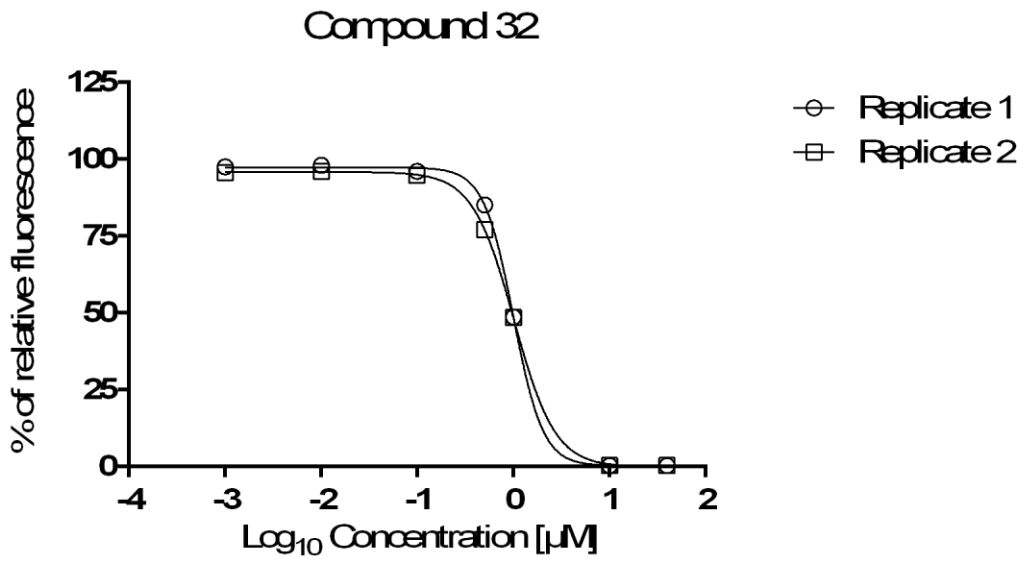
Supplementary Figure 49: Inhibition curve of compound 29



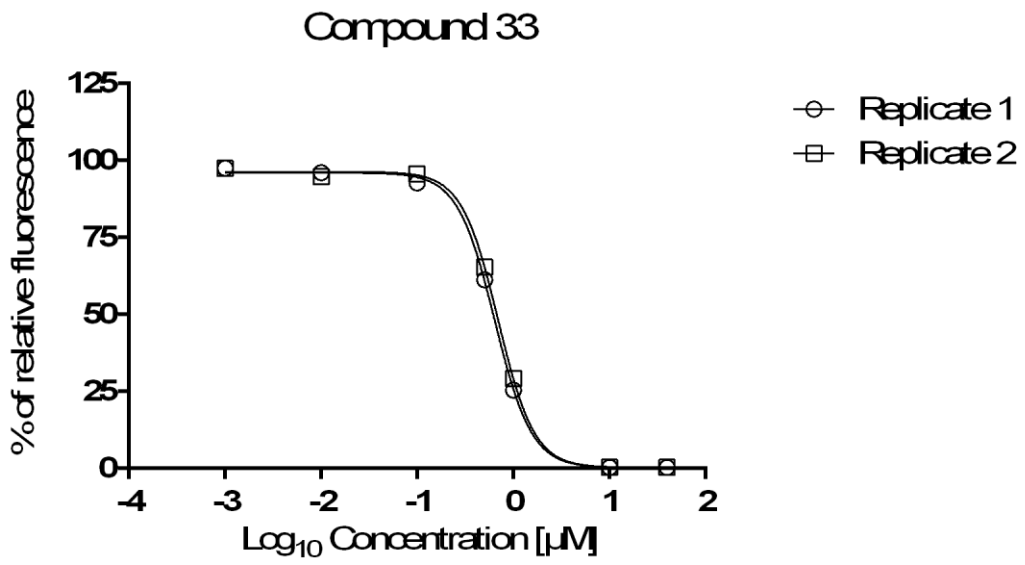
Supplementary Figure 50: Inhibition curve of compound 30



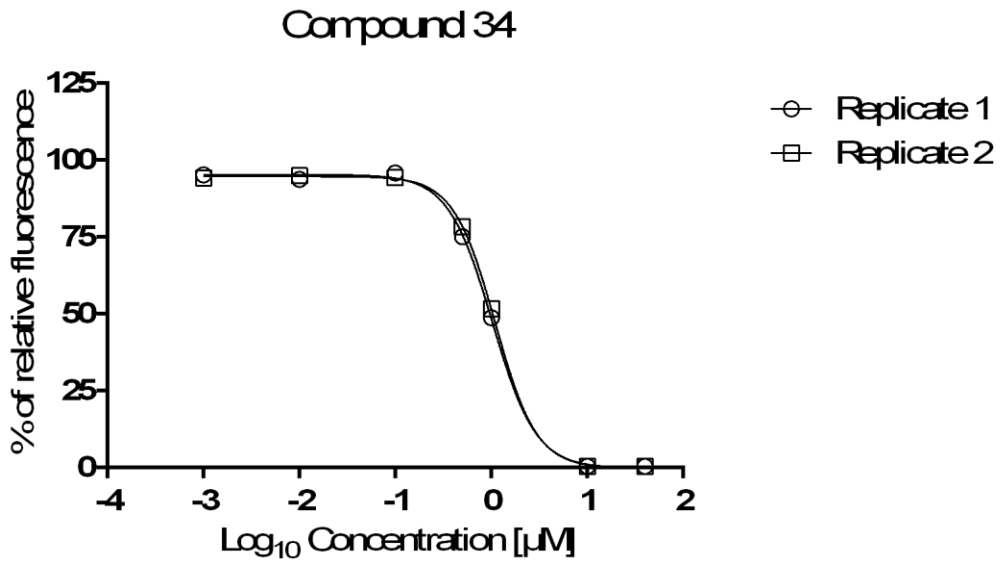
Supplementary Figure 51: Inhibition curve of compound 31



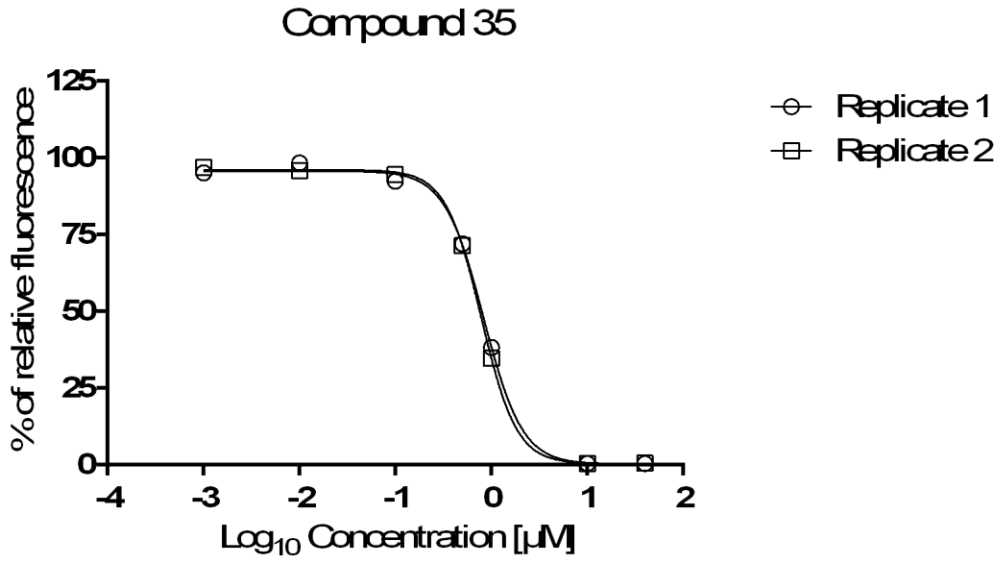
Supplementary Figure 52: Inhibition curve of compound 32



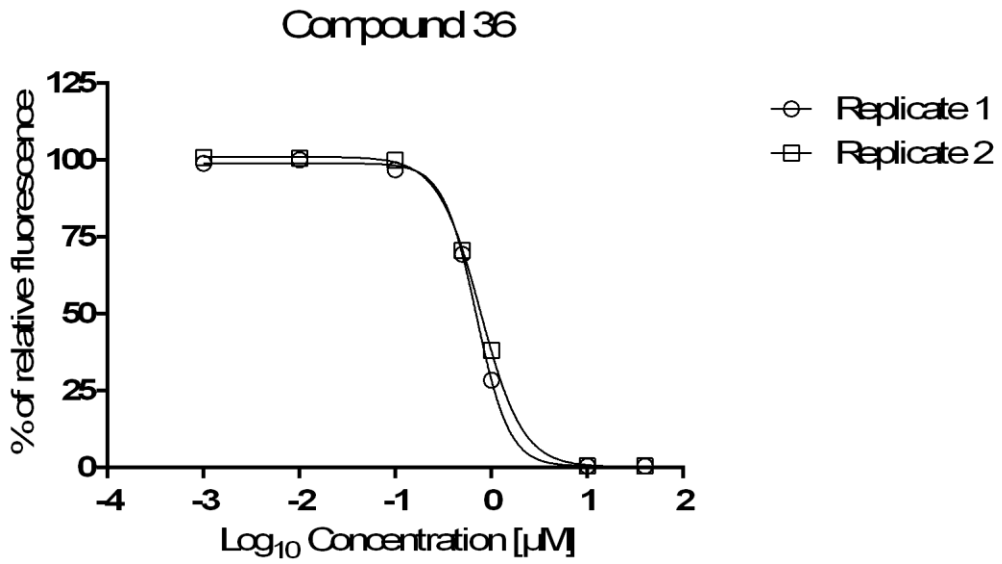
Supplementary Figure 53: Inhibition curve of compound 33



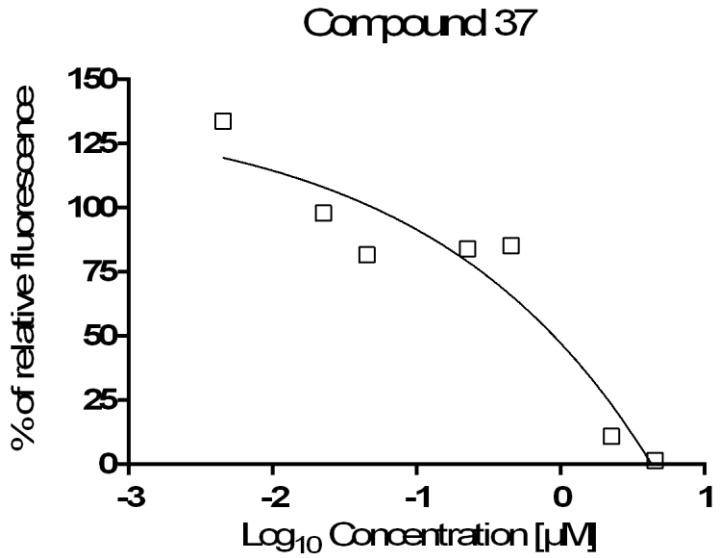
Supplementary Figure 54: Inhibition curve of compound 34



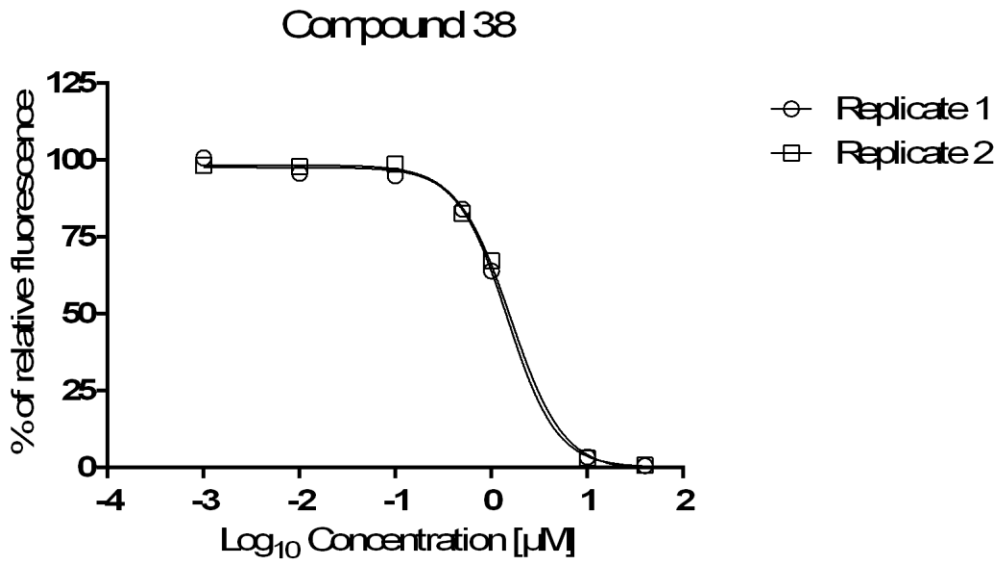
Supplementary Figure 55: Inhibition curve of compound 35



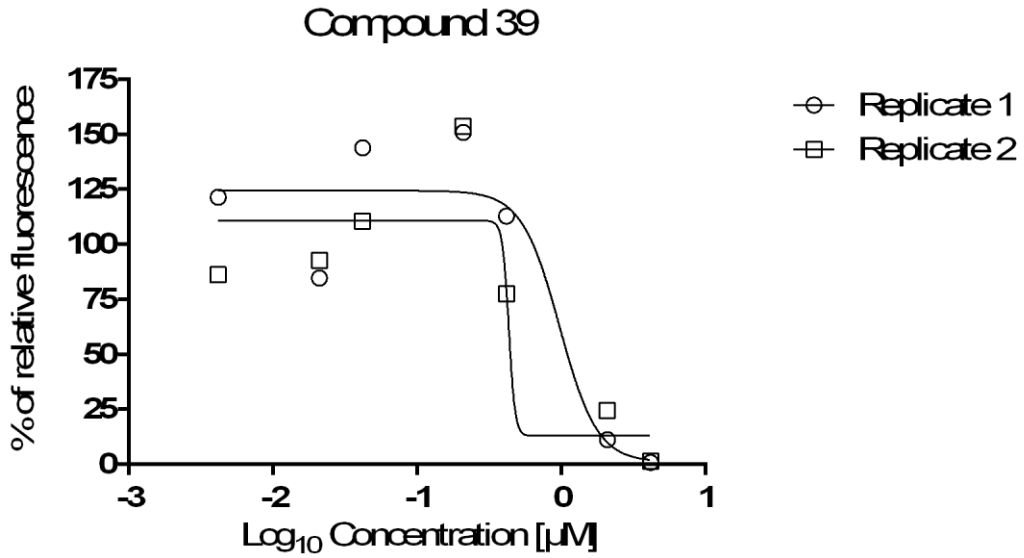
Supplementary Figure 56: Inhibition curve of compound 36



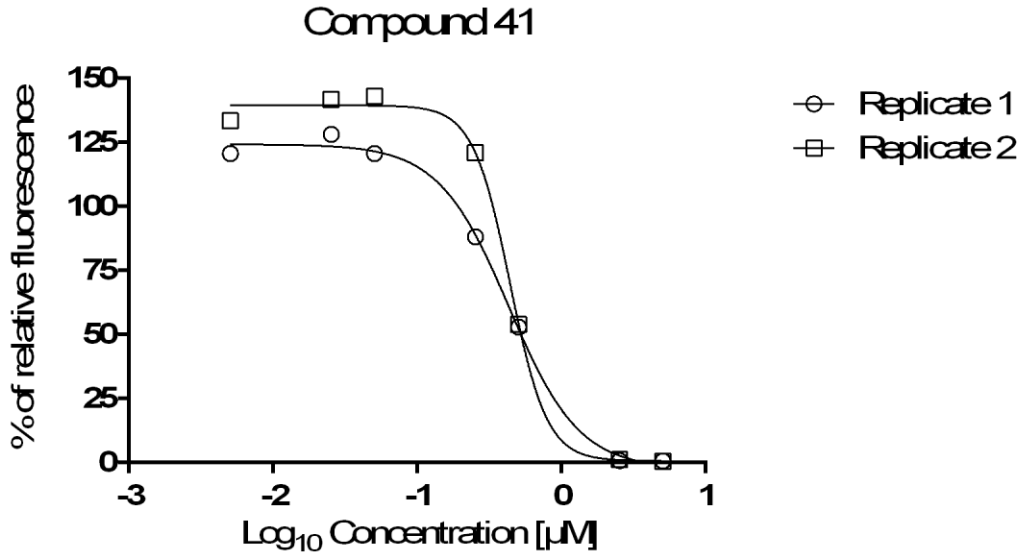
Supplementary Figure 57: Inhibition curve of compound 37



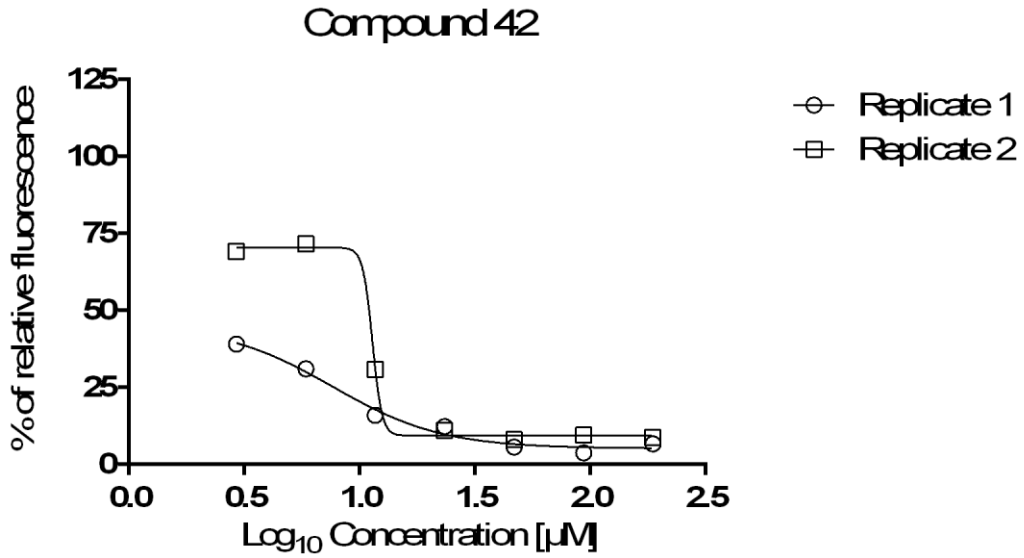
Supplementary Figure 58: Inhibition curve of compound 38



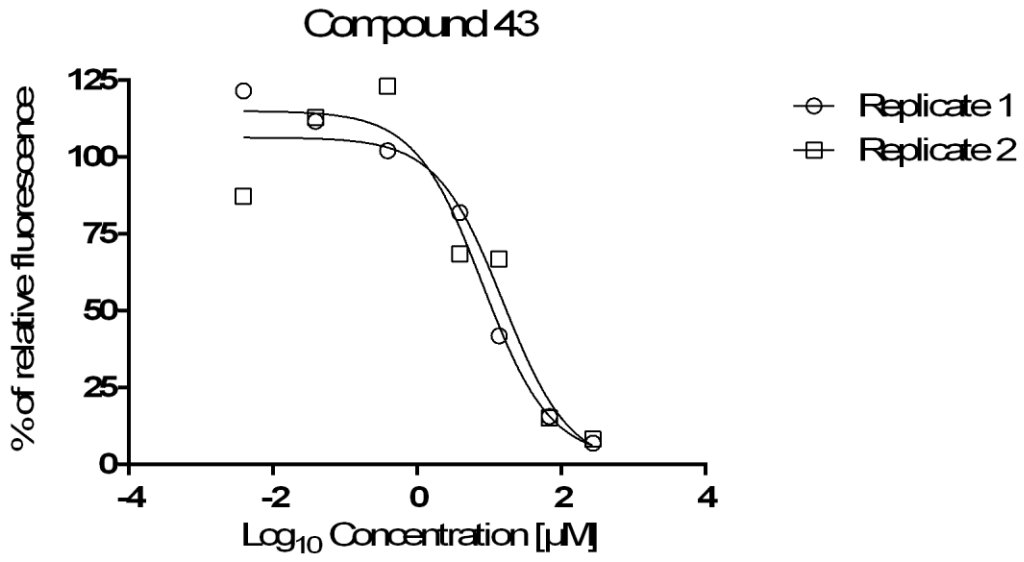
Supplementary Figure 59: Inhibition curve of compound 39



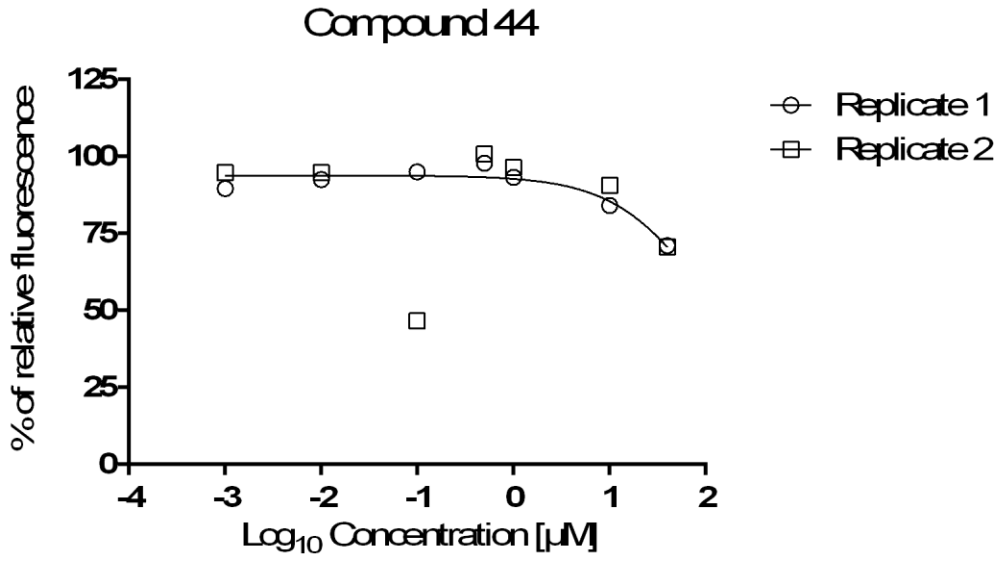
Supplementary Figure 61: Inhibition curve of compound 41



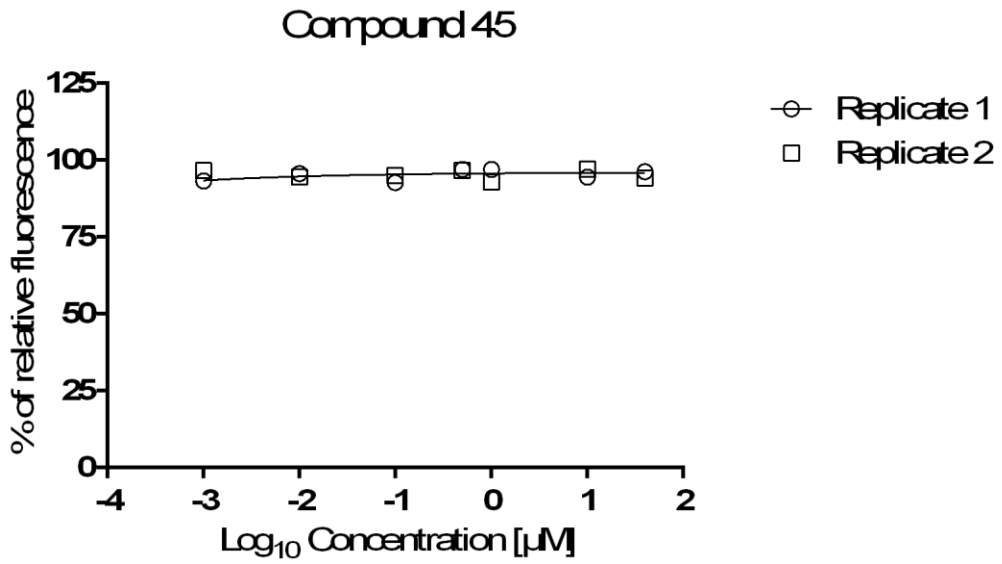
Supplementary Figure 62: Inhibition curve of compound 42



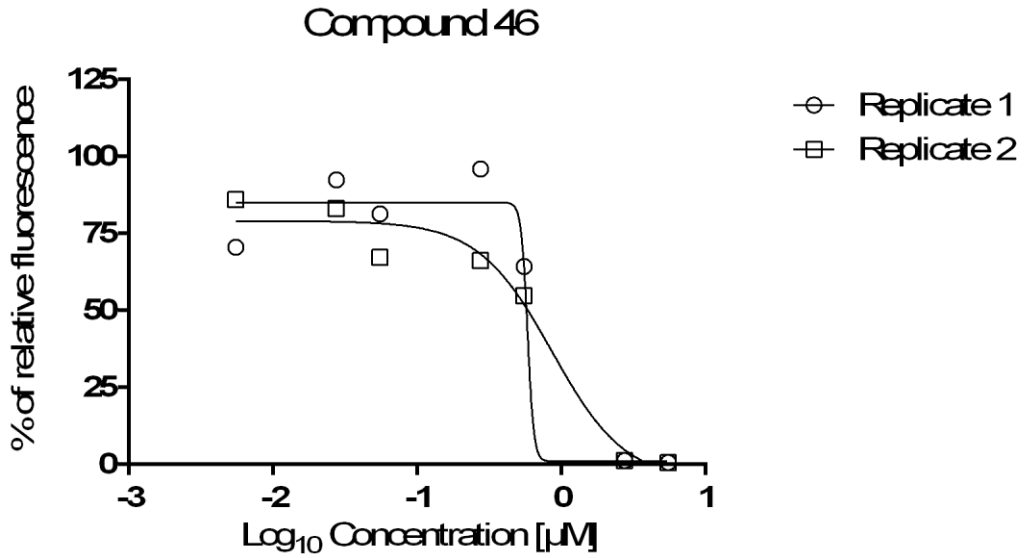
Supplementary Figure 63: Inhibition curve of compound 43



Supplementary Figure 64: Inhibition curve of compound 44



Supplementary Figure 65: Inhibition curve of compound 45



Supplementary Figure 66: Inhibition curve of compound 46

IX – Molecular Formula String

Supplementary Table S6: Molecular formula string with associated biological data

Compound ID	SMILES	MIC E. coli ATCC 25922 (µg/mL)	MIC K. pneumoniae ATCC 43816 (µg/mL)	IC50 IVTT (µM)
1	c1c([nH]cn1)C[C@@H](C(=O)N[C@@H](CCCCN)C(=O)N/C(=C\CCNC(=N)N)/C(=O)N[C@@H](CCCCN)C(=O)NCCCCN)NC(=O)[C@@H]2CCCN2C(=O)[C@@H](CCCN)NC(=O)CNC(=O)[C@H]([C@H](CN)O)NC(=O)[C@H]([C@H](CN)O)NC(=O)[C@H](CCCCN)N	8	4	0.63
17	C[C@@H](C(=O)N[C@@H]([C@H](CN)O)C(=O)N[C@@H]([C@H](CN)O)C(=O)NCC(=O)N[C@H](CCCN)C(=O)N1CCC[C@H]1C(=O)N[C@@H](Cc2cnc[nH]2)C(=O)N[C@@H](CCCCN)C(=O)N/C(=C\CCNC(=N)N)/C(=O)N[C@@H](CCCCN)C(=O)NCCCCN)N	16	8	0.73
18	C[C@@H](C(=O)N[C@@H]([C@H](CN)O)C(=O)NCC(=O)N[C@H](CCCN)C(=O)N1CCC[C@H]1C(=O)N[C@@H](Cc2cnc[nH]2)C(=O)N[C@@H](CCCCN)C(=O)N/C(=C\CCNC(=N)N)/C(=O)N[C@@H](CCCCN)C(=O)NCCCCN)NC(=O)[C@H](CCCCN)N	>64	>64	4.50
19	C[C@H]([C@@H](C(=O)N[C@@H]([C@@H](C)O)C(=O)NCC(=O)N[C@H](CCCN)C(=O)N1CCC[C@H]1C(=O)N[C@@H](Cc2cnc[nH]2)C(=O)N[C@@H](CCCCN)C(=O)N[C@@H](CCCNC(=N)N)C(=O)N[C@@H](CCCCN)C(=O)NCCCCN)NC(=O)CCCCCN)O	2	1	0.63
20	C[C@H]([C@@H](C(=O)NCC(=O)N[C@H](CCCN)C(=O)N1CCC[C@H]1C(=O)N[C@@H](Cc2cnc[nH]2)C(=O)N[C@@H](CCCCN)C(=O)N[C@@H](CCCNC(=N)N)C(=O)N[C@@H](CCCCN)C(=O)NCCCCN)NC(=O)[C@H](CCN)NC(=O)[C@H](CCCCN)N)O	>64	>64	3.64
21	C[C@H](C(=O)N1CCC[C@H]1C(=O)N[C@@H](Cc2cnc[nH]2)C(=O)N[C@@H](CCCCN)C(=O)N/C(=C\CCNC(=N)N)/C(=O)N[C@@H](CCCCN)C(=O)NCCCCN)NC(=O)CNC(=O)[C@H]([C@H](CN)O)NC(=O)[C@H]([C@H](CN)O)NC(=O)[C@H](CCCCN)N	>64	>64	>40
22	C[C@@H](C(=O)N[C@@H](Cc1cnc[nH]1)C(=O)N[C@@H](CCCCN)C(=O)N/C(=C\CCNC(=N)N)/C(=O)N[C@@H](CCCCN)C(=O)NCCCCN)NC(=O)[C@@H](CCCN)NC(=O)CNC(=O)[C@H]([C@H](CN)O)NC(=O)[C@H]([C@H](CN)O)NC(=O)[C@H](CCCCN)N	16	32	2.41
23	C[C@@H](C(=O)N[C@@H](CCCCN)C(=O)N/C(=C\CCNC(=N)N)/C(=O)N[C@@H](CCCCN)C(=O)NCCCCN)NC(=O)[C@@H]1CCCN1C(=O)[C@@H](CCCN)NC(=O)CNC(=O)[C@H]([C@H](CN)O)NC(=O)[C@H]([C@H](CN)O)NC(=O)[C@H](CCCCN)N	8	8	0.39
24	C[C@@H](C(=O)N/C(=C\CCNC(=N)N)/C(=O)N[C@@H](CCCCN)C(=O)NCCCCN)NC(=O)[C@H](Cc1cnc[nH]1)NC(=O)[C@@H]2CCCN2C(=O)[C@@H](CCCN)NC(=O)CNC(=O)[C@H]([C@H](CN)O)NC(=O)[C@H]([C@H](CN)O)NC(=O)[C@H](CCCCN)N	16	4	1.85
25	C[C@@H](C(=O)N[C@@H](CCCCN)C(=O)NCCCCN)NC(=O)[C@H](CCCCN)NC(=O)[C@H](Cc1cnc[nH]1)NC(=O)[C@@H]2CCCN2C(=O)[C@@H](CCCN)NC(=O)CNC(=O)[C@H]([C@H](CN)O)NC(=O)[C@H]([C@H](CN)O)NC(=O)[C@H](CCCCN)N	>64	64	2.40
26	C[C@@H](C(=O)NCCCCN)NC(=O)/C(=C/CCNC(=N)N)/NC(=O)[C@H](CCCCN)NC(=O)[C@H](Cc1cnc[nH]1)NC(=O)[C@@H]2CCCN2C(=O)[C@@H](CCCN)NC(=O)CNC(=O)[C@H]([C@H](CN)O)NC(=O)[C@H]([C@H](CN)O)NC(=O)[C@H](CCCCN)N	8	8	1.04
27	c1c([nH]cn1)C[C@@H](C(=O)N[C@@H](CCCCN)C(=O)N/C(=C\CCNC(=N)N)/C(=O)N[C@@H](CCCCN)C(=O)NCCO)NC(=O)[C@@H]2CCCN2C(=O)[C@@H](CCCN)NC(=O)CNC(=O)[C@H]([C@H](CN)O)NC(=O)[C@H]([C@H](CN)O)NC(=O)[C@H](CCCCN)N	16	4	0.36
28	c1c(nc[nH]1)C[C@@H](C(=O)N[C@@H](CCCCN)C(=O)N/C(=C\CCNC(=N)N)/C(=O)N[C@@H](CCCCN)C(=O)NCCCCN)NC(=O)[C@@H]2CCCN2C(=O)[C@@H](CCCN)NC(=O)CNC(=O)[C@H]([C@H](CN)O)NC(=O)[C@H](CCN)NC(=O)[C@H](CCCCN)N	>64	64	5.91
29	C[C@@H]([C@@H](C(=O)N[C@@H]([C@H](CN)O)C(=O)NCC(=O)N[C@H](CCCN)C(=O)N1CCC[C@H]1C(=O)N[C@@H](Cc2c[nH]cn2)C(=O)N[C@@H](CCCCN)C(=O)N/C(=C\CCNC(=N)N)/C(=O)N[C@@H](CCCCN)C(=O)NCCCCN)NC(=O)[C@H](CCCCN)N)O	>64	>64	>40
30	c1c([nH]cn1)C[C@@H](C(=O)N[C@@H](CCCCN)C(=O)N/C(=C\CCNC(=N)N)/C(=O)N[C@@H](CCCCN)C(=O)NCCCCN)NC(=O)[C@@H]2CCCN2C(=O)[C@@H](CCCN)NC(=O)CNC(=O)[C@H]([C@H](CN)O)NC(=O)[C@H](CO)NC(=O)[C@H](CCCCN)N	>64	>64	>40

31	c1c([nH]cn1)C[C@@H](C(=O)N[C@@H](CCCCN)C(=O)N/C(=C\CCNC(=N)N)/C(=O)N[C@@H](CCCCN)C(=O)NCCCCN)NC(=O)[C@@H]2CCCN2C(=O)[C@@H](CCCN)NC(=O)CNC(=O)[C@H](CCN)NC(=O)[C@H]([C@H](CN)O)NC(=O)[C@H](CCCCN)N	4	4	1.10
32	C[C@@H]([C@@H](C(=O)NCC(=O)N[C@H](CCCN)C(=O)N1CCC[C@H]1C(=O)N[C@@H](Cc2cnc[nH]2)C(=O)N[C@@H](CCCCN)C(=O)N/C(=C\CCNC(=N)N)/C(=O)N[C@@H](CCCCN)C(=O)NCCCCN)NC(=O)[C@H]([C@H](CN)O)NC(=O)[C@H](CCCCN)N)O	8	8	1.00
33	c1c([nH]cn1)C[C@@H](C(=O)N[C@@H](CCCCN)C(=O)N/C(=C\CCNC(=N)N)/C(=O)N[C@@H](CCCCN)C(=O)NCCCCN)NC(=O)[C@@H]2CCCN2C(=O)[C@@H](CCCN)NC(=O)CNC(=O)[C@H](CO)NC(=O)[C@H]([C@H](CN)O)NC(=O)[C@H](CCCCN)N	4	4	0.66
34	c1c(nc[nH]1)C[C@@H](C(=O)N[C@@H](CCCCN)C(=O)N/C(=C\CCNC(=N)N)/C(=O)N[C@@H](CCCCN)C(=O)NCCCCN)NC(=O)[C@@H]2CCCN2C(=O)[C@@H](CCCN)NC(=O)CNC(=O)CNC(=O)[C@H]([C@H](CN)O)NC(=O)[C@H](CCCCN)N	8	8	1.06
35	CC(C)[C@@H](C(=O)NCC(=O)N[C@H](CCCN)C(=O)N1CCC[C@H]1C(=O)N[C@@H](Cc2c[nH]cn2)C(=O)N[C@@H](CCCCN)C(=O)N/C(=C\CCNC(=N)N)/C(=O)N[C@@H](CCCCN)C(=O)NCCCCN)NC(=O)[C@H]([C@H](CN)O)NC(=O)[C@H](CCCCN)N	4	2	0.80
36	CC[C@@H](C(=O)NCC(=O)N[C@H](CCCN)C(=O)N1CCC[C@H]1C(=O)N[C@@H](Cc2c[nH]cn2)C(=O)N[C@@H](CCCCN)C(=O)N/C(=C\CCNC(=N)N)/C(=O)N[C@@H](CCCCN)C(=O)NCCCCN)NC(=O)[C@H]([C@H](CN)O)NC(=O)[C@H](CCCCN)N	4	4	0.73
37	C/C=C(/C(=O)N[C@@H](CCCCN)C(=O)NCCCCN)\NC(=O)[C@H](CCCCN)NC(=O)[C@H](Cc1cnc[nH]1)NC(=O)[C@@H]2CCCN2C(=O)[C@@H](CCCN)NC(=O)CNC(=O)[C@H]([C@H](CN)O)NC(=O)[C@H]([C@H](CN)O)NC(=O)[C@H](CCCCN)N	16	8	0.83
38	c1c([nH]cn1)C[C@@H](C(=O)N[C@@H](CCCCN)C(=O)N[C@@H](CCCNC(=N)N)C(=O)N[C@@H](CCCCN)C(=O)NCCCCN)NC(=O)[C@@H]2CCCN2C(=O)[C@@H](CCCN)NC(=O)CNC(=O)[C@H]([C@H](CN)O)NC(=O)[C@H]([C@H](CN)O)NC(=O)[C@H](CCCCN)N	32	8	1.53
39	c1c([nH]cn1)C[C@@H](C(=O)N[C@@H](CCCCN)C(=O)N[C@H](CCCNC(=N)N)C(=O)N[C@@H](CCCCN)C(=O)NCCCCN)NC(=O)[C@@H]2CCCN2C(=O)[C@@H](CCCN)NC(=O)CNC(=O)[C@H]([C@H](CN)O)NC(=O)[C@H]([C@H](CN)O)NC(=O)[C@H](CCCCN)N	16	16	0.98
40	c1c([nH]cn1)C[C@@H](C(=O)N[C@@H](CCCCN)C(=O)N/C(=C\CCNC(=N)N)/C(=O)N[C@@H](CCCCN)C(=O)NCCO)NC(=O)[C@@H]2CCCN2C(=O)[C@@H](CCCN)NC(=O)CNC(=O)[C@H]([C@H](CN)O)NC(=O)[C@H]([C@H](CN)O)NC(=O)[C@H](CCCCN)N	16	4	0.36
41	c1c([nH]cn1)C[C@@H](C(=O)N[C@@H](CCCCN)C(=O)N/C(=C\CCNC(=N)N)/C(=O)O)NC(=O)[C@@H]2CCCN2C(=O)[C@@H](CCCN)NC(=O)CNC(=O)[C@H]([C@H](CN)O)NC(=O)[C@H]([C@H](CN)O)NC(=O	16	4	0.43
42	c1c([nH]cn1)C[C@@H](C(=O)N[C@@H](CCCCN)C(=O)O)NC(=O)[C@@H]2CCCN2C(=O)[C@@H](CCCN)NC(=O)CNC(=O)[C@H]([C@H](CN)O)NC(=O)[C@H]([C@H](CN)O)NC(=O)[C@H](CCCCN)N	>64	>64	10.01
43	c1c([nH]cn1)C[C@@H](C(=O)O)NC(=O)[C@@H]2CCCN2C(=O)[C@@H](CCCN)NC(=O)CNC(=O)[C@H]([C@H](CN)O)NC(=O)[C@H]([C@H](CN)O)NC(=O)[C@H](CCCCN)N	>64	>64	9.60
44	c1c([nH]cn1)C[C@@H](C(=O)N[C@@H](CCCCN)C(=O)N/C(=C\CCNC(=N)N)/C(=O)N[C@@H](CCCCN)C(=O)NCCCCN)NC(=O)[C@@H]2CCCN2C(=O)[C@@H](CCCN)NC(=O)CNC(=O)[C@H]([C@H](CN)O)NC(	>64	>64	>40
45	c1c([nH]cn1)C[C@@H](C(=O)N[C@@H](CCCCN)C(=O)N/C(=C\CCNC(=N)N)/C(=O)N[C@@H](CCCCN)C(=O)NCCCCN)NC(=O)[C@@H]2CCCN2C(=O)[C@@H](CCCN)NC(=O)CNC(=O)[C@H]([C@H](CN)O)N	>64	>64	>40
46	C[C@@H](C(=O)NCC(=O)N[C@H](CCCN)C(=O)N1CCC[C@H]1C(=O)N[C@@H](Cc2cnc[nH]2)C(=O)N[C@@H](CCCCN)C(=O)N/C(=C\CCNC(=N)N)/C(=O)O)NC(=O)[C@H]([C@H](CN)O)NC(=O)[C@H](CCCCN	16	4	0.55

Supplementary references

1. Gualtieri, M.; Villain-Guillot, P.; Givaudan, A.; Pages, S. Novel peptide derivatives as antibiotics. PCT Int. Appl. **2012**, WO 2013045600A1.