Electronic Supplementary Information

Natural terpenoid glycosides with *in vitro*/*vivo* antithrombotic profiles from the leaves of *Crataegus pinnatifida*

Pin-Yi Gao,[a,b] Ling-Zhi Li,[a]* Ke-Chun Liu,[c] Chen Sun,[c] Xue Sun,[a] Ya-Nan Wu,[a] Shao-Jiang Song[a]*

[a] Key Laboratory of Structure-Based Drug Design and Discovery, Ministry of Education, School of Traditional Chinese Materia Medica, Shenyang Pharmaceutical University, Shenyang 110016, People's Republic of China

[b] College of Pharmaceutical and Biotechnology Engineering, Institute of Functional Molecules, Shenyang University of Chemical Technology, Shenyang 110142, People's Republic of China

[c] Biology Institute of Shandong Academy of Sciences, Jinan, People's Republic of China

*Corresponding author. Tel.: +86-24-23986088. Fax: +86-24-23986510. (S.-J. Song).

E-mail addresses: songsj99@163.com. (S.-J. Song).

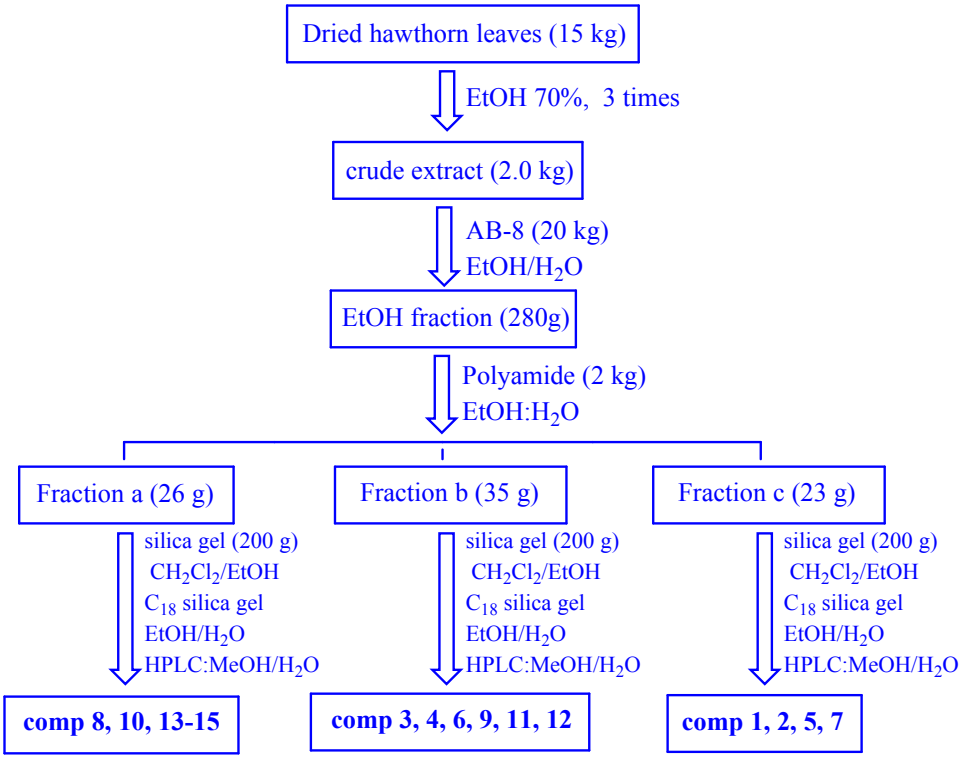
Experiment section:

Table

Spectra figure

Experiment section:

SI-E.1. *Extraction and isolation*



SI-figure-1. Extraction and isolation of **1-15**

SI-E.2. *Characteristic data of compounds* ***1-15*** *and 2D NMR correlations of* ***1-4***

Norhawthornoid A ***(1)****:* colorless oil; [α]20 D −3.5, (*c* 0.15, MeOH); UV (MeOH) λ_{max} (log ε) 208 (2.21) nm; ECD (MeOH) λ (Δε) 209 (-39.50) nm; see Table 1 for ^{1}H NMR, ^{13}C NMR; HRESIMS *m/z*: 483.2582 $[M + H]^+$ (calcd. $C_{25}H_{39}O_9$ 483.2589).

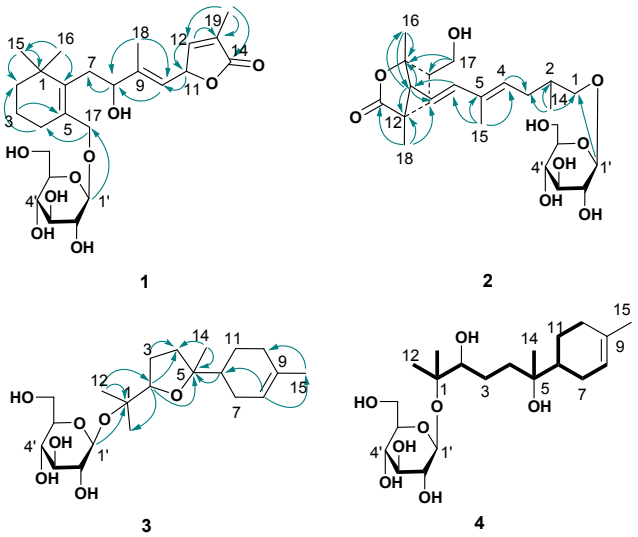
Norhawthornoid B ***(2)****:* colorless oil; [α]20 D −8.5, (*c* 0.12, MeOH); UV (MeOH) λ_{max} (log ε) 228 (2.21) nm; ECD (MeOH) λ (Δε) 230 (-9.80) nm; see Table 1 for ^{1}H NMR, ^{13}C NMR; HRESIMS *m/z*: 471.2588 $[M + H]^+$ (calcd. $C_{24}H_{38}O_9$ 471.2589).

Pinnatifidanoside F ***(3)****:* colorless oil; [α]20 D −2.8, (*c* 0.4, MeOH); see Table 2 for ^{1}H NMR, ^{13}C NMR; HRESIMS *m/z*: 401.2536 $[M + H]^+$ (calcd. $C_{21}H_{37}O_7$ 401.2534).

*Pinnatifidanoside G (**4**):* colorless oil; [α]20 D −7.5, (*c* 0.2, MeOH); see Table 2 for ^{1}H NMR, ^{13}C NMR; HRESIMS *m/z*: 419.2636 $[M + H]^+$ (calcd. $C_{21}H_{39}O_8$ 419.2639).

*Shnyegenin B (**5**)*: Colourless oil; ESI-MS m/z: 277 $[M+Na]^+$; ^{1}H NMR (DMSO-d_6, 300 MHz) δ_H 5.19 (1H, *J* = 17.1, 1.8 Hz, H-1a), 5.04 (1H, *J* = 10.8, 1.8 Hz, H-1b), 5.91 (1H, *J* = 17.1, 10.8 Hz, H-2), 2.20 (1H, m, H-4a), 2.21 (1H, m, H-4b) 5.57 (1H, *J* = 7.2, 3.9 Hz, H-5), 5.58 (1H, *J* = 7.2 Hz, H-6),1.69 (1H, m, H-8a), 1.89 (1H, m, H-8b), 1.82 (1H, m, H-9a), 1.82 (1H, m, H-9b), 3.76 (1H, *J* = 6.6 Hz, H-10), 1.26 (3H, s, H-12), 1.31 (3H, s, H-13), 1.21 (3H, s, H-14) and 1.12 (3H, s, H-15). ^{13}C-NMR (DMSO-d_6, 75 MHz): δ_C 111.9 (C-1), 144.7 (C-2), 72.6 (C-3), 45.5 (C-4), 122.1 (C-5), 139.5 (C-6), 82.6 (C-7), 37.8 (C-8), 26.3 (C-9), 85.4 (C-10), 71.1 (C-11), 27.1 (C-12), 27.1 (C-13), 27.1 (C-14), 24.1 (C-15).

*Shnyeside B (**6**):* Colourless oil; ESI-MS m/z: 439 $[M+Na]^+$; ^{1}H NMR (DMSO-d_6, 300 MHz) δ_H 5.10 (1H, *J* = 17.1, 1.8 Hz, H-1a), 4.91 (1H, *J* = 10.8, 1.8 Hz, H-1b), 5.84 (1H, *J* = 17.1, 10.8 Hz, H-2), 2.10 (1H, *J* = 3.9 Hz, H-4a), 2.10 (1H, *J* = 3.9 Hz, H-4b) 5.54 (1H, *J* = 7.2, 3.9 Hz, H-5), 5.53 (1H, *J* = 7.2 Hz, H-6),1.67 (1H, m, H-8a), 1.67 (1H, m, H-8b), 1.81 (1H, m, H-9a), 1.91 (1H, m, H-9b), 3.86 (1H, *J* = 6.6 Hz, H-10), 1.09 (3H, s, H-12), 1.16 (3H, s, H-13), 1.16 (3H, s, H-14), 1.07 (3H, s, H-15), 4.35 (1H, *J* = 7.8 Hz, H-1′), 2.84 (1H, *J* = 7.8 Hz, H-2′), 3.10 (1H, *J* = 7.8 Hz, H-3′), 3.00 (1H, m, H-4′), 3.02 (1H, m, H-5′), 3.35 (1H, *J* = 10.8 Hz, H-6′a), 3.62 (1H, *J* = 10.8 Hz, H-6′b). ^{13}C-NMR (DMSO-d_6, 75 MHz): δ_C 111.3 (C-1), 146.4 (C-2), 71.9 (C-3), 45.5 (C-4), 123.0 (C-5), 139.4 (C-6), 82.5 (C-7), 38.1 (C-8), 26.7 (C-9), 83.9 (C-10), 78.3 (C-11), 27.3 (C-12), 26.4 (C-13), 24.0 (C-14), 22.2 (C-15), 97.6 (C-1′), 74.0 (C-2′), 77.5 (C-3′), 70.6 (C-4′), 77.0 (C-5′), 61.6 (C-6′).



SI-figure-2. HMBC correlations (arrows) of **1-3**, and $^{1}H-^{1}H$ COSY (bold lines) of **4**

(3S,5R,6R,7E,9S)-megastiman-7-ene-3,5,6,9-tetrol (7): Colourless oil; ^{1}H NMR (DMSO-d_6, 300 MHz) δ_H 5.90 (1H, d, J = 15.9 Hz), 5.66 (1H, d, J = 15.9 Hz), 1.08 (3H, s), 0.99 (3H, s), 0.71 (3H, s), 1.13 (3H, d, J=6.3 Hz), 4.15 (1H, m), 3.84 (1H, m). ^{13}C-NMR (DMSO-d_6, 75 MHz): δ_C 41.2 (C-1), 46.7 (C-2), 63.6 (C-3), 46.2 (C-4), 76.7 (C-5), 77.8 (C-6), 129.9 (C-7), 135.7 (C-8), 67.8 (C-9), 25.5 (C-10), 28.0 (C-11), 26.6 (C-12), 27.8 (C-13).

*Euodionosides D (**8**)*: Colourless oil; ^{1}H NMR (DMSO-d_6, 300 MHz) δ_H 5.97 (1H, d, J = 15.9 Hz), 5.72 (1H, d, J = 15.9 Hz), 1.05 (3H, s), 1.00 (3H, s), 0.72 (3H, s), 1.20 (3H, d, J=6.0 Hz), 4.14 (1H, d, J = 7.8 Hz). ^{13}C-NMR (DMSO-d_6, 75 MHz): δ_C 41.3 (C-1), 46.6 (C-2), 63.5 (C-3), 46.0 (C-4), 77.0 (C-5), 77.5 (C-6), 133.5 (C-7), 132.6 (C-8), 76.6 (C-9), 22.3 (C-10), 28.0 (C-11), 26.6 (C-12), 27.9 (C-13), 101.7 (C-1′), 74.5 (C-2′), 77.7 (C-3′), 71.0 (C-4′), 77.7 (C-5′), 61.9 (C-6′).

*(6R,9R)-3-oxo-α-ionol-9-O-β-D-glucopyranoside (**9**)*: Colourless oil; ^{1}H NMR (DMSO-d_6, 300 MHz) δ_H 5.79 (1H, s), 5.66 (1H, dd, J = 15.0、6.6 Hz), 5.56 (1H, dd, J = 15.0、9.6 Hz), 1.83 (3H, s), 0.93 (3H, s), 0.89 (3H, s), 1.17 (3H, d, J=6.6 Hz), 4.16 (1H, d, J = 7.8 Hz).

*(6S,7E,9R)-6,9-Dihydroxy-4,7-megastiymadien-3-one-9-O-[β-D-xylopyranosy-(1-6)β-D-glucopyranoside] (**10**)*: Colourless oil; ^{1}H NMR (DMSO-d_6, 300 MHz) δ_H 5.79 (1H, s), 5.68 (1H, dd, J = 15.3, 6.0 Hz), 5.56 (1H, dd, J = 15.3, 9.0 Hz), 1.84 (3H, s), 0.94 (3H, s), 0.90 (3H, s), 1.18

(3H, d, *J*=6.3 Hz), 4.18 (1H, d, *J* = 7.2 Hz), 4.17 (1H, d, *J* = 7.2 Hz). ^{13}C-NMR (DMSO-d_6, 75 MHz): δ_C 36.5 (C-1), 48.0 (C-2), 199.5 (C-3), 125.7 (C-4), 163.0 (C-5), 55.3 (C-6), 128.1 (C-7), 137.4 (C-8), 76.5 (C-9), 21.5 (C-10), 27.6 (C-11), 28.3 (C-12), 23.8 (C-13), 101.6 (C-1′), 74.4 (C-2′), 77.5 (C-3′), 70.6 (C-4′), 75.3 (C-5′), 69.0 (C-6′), 104.8 (C-1″), 74.2 (C-2″), 77.5 (C-3″), 70.4 (C-4″), 66.5 (C-5″).

Linarionoside A ***(11)***: Colourless oil; ^{1}H NMR (DMSO-d_6, 300 MHz) δ_H 1.54 (3H, s), 0.97 (3H, s), 0.96 (3H, s), 1.08 (3H, d, *J*=6.0 Hz), 4.17 (1H, d, *J* = 7.5 Hz). ^{13}C-NMR (DMSO-d_6, 75 MHz): δ_C 37.6 (C-1), 48.6 (C-2), 62.9 (C-3), 37.3 (C-4), 124.0 (C-5), 136.6 (C-6), 23.7 (C-7), 42.8 (C-8), 73.7 (C-9), 19.5 (C-10), 28.3 (C-11), 29.6 (C-12), 19.3 (C-13), 100.8 (C-1′), 73.7 (C-2′), 76.9 (C-3′), 70.2 (C-4′), 76.7 (C-5′), 61.2 (C-6′).

Linarionoside B ***(12)***: Colourless oil; ^{1}H NMR (DMSO-d_6, 300 MHz) δ_H 1.57 (3H, s), 0.99 (3H, s), 0.98 (3H, s), 1.04 (3H, d, *J*=6.0 Hz), 4.25 (1H, d, *J* = 7.8 Hz). ^{13}C-NMR (DMSO-d_6, 75 MHz): δ_C 39.3 (C-1), 46.8 (C-2), 70.9 (C-3), 38.1 (C-4), 124.0 (C-5), 138.0 (C-6), 24.9 (C-7), 40.9 (C-8), 67.1 (C-9), 20.3 (C-10), 29.0 (C-11), 30.4 (C-12), 24.2 (C-13), 101.4 (C-1′), 74.3 (C-2′), 77.5 (C-3′), 71.0 (C-4′), 77.5 (C-5′), 61.9 (C-6′).

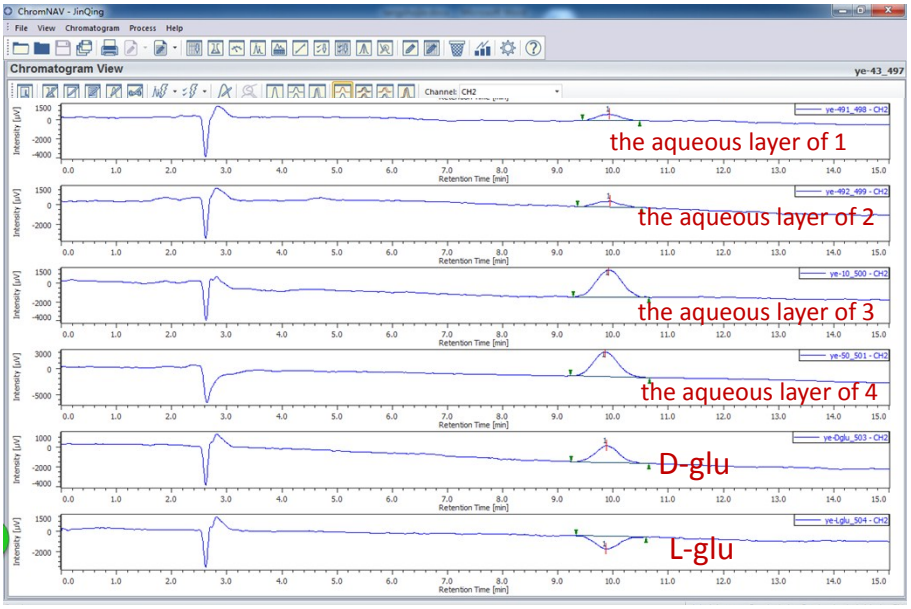
Linarionoside C ***(13)***: Colourless oil; ^{1}H NMR (DMSO-d_6, 300 MHz) δ_H 1.57 (3H, s), 1.06 (3H, s), 1.03 (3H, s), 1.11 (3H, d, *J*=6.0 Hz), 4.26 (1H, d, *J* = 7.8 Hz), 4.17 (1H, d, *J* = 7.5 Hz). ^{13}C-NMR (DMSO-d_6, 75 MHz): δ_C 38.1 (C-1), 47.2 (C-2), 71.1 (C-3), 39.5 (C-4), 124.5 (C-5), 138.2 (C-6), 24.5 (C-7), 39.0 (C-8), 74.4 (C-9), 20.2 (C-10), 29.1 (C-11), 30.4 (C-12), 20.4 (C-13), 101.6 (C-1′), 74.4 (C-2′), 77.6 (C-3′), 71.1 (C-4′), 77.6 (C-5′), 62.1 (C-6′), 101.6 (C-1″), 74.4 (C-2″), 77.6 (C-3″), 71.0 (C-4″), 77.6 (C-5″), 62.1 (C-6″).

3,9-dihydroxy-5-megastigmen-3-O-[β-D-xylopyranosy-(1-6)β-D-glucopyranoside] ***(14)***: Colourless oil; ^{1}H NMR (DMSO-d_6, 300 MHz) δ_H 1.57 (3H, s), 0.98 (6H, s), 1.04 (3H, d, *J*=6.0 Hz), 4.24 (1H, d, *J* = 7.8 Hz), 4.20 (1H, d, *J* = 7.5 Hz). ^{13}C-NMR (DMSO-d_6, 75 MHz): δ_C 37.8 (C-1), 46.5 (C-2), 71.0 (C-3), 39.6 (C-4), 123.7 (C-5), 137.6 (C-6), 24.6 (C-7), 40.1 (C-8), 66.8 (C-9), 23.9

(C-10), 28.8 (C-11), 30.1 (C-12), 20.0 (C-13), 101.1 (C-1′), 73.9 (C-2′), 77.1 (C-3′), 70.5 (C-4′), 76.1 (C-5′), 68.8 (C-6′), 104.4 (C-1″), 73.9 (C-2″), 77.0 (C-3″), 70.1 (C-4″), 66.1 (C-5″).

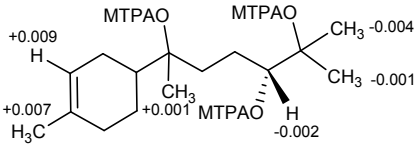
*Pinnatifidanoside C (**15**)*: Colourless oil; ^{1}H NMR (DMSO-d_6, 300 MHz) δ_H 2.07 (3H, s), 1.54 (3H, s), 0.98 (6H, s), 4.24 (1H, d, J = 8.1 Hz), 4.20 (1H, d, J = 7.5 Hz). ^{13}C-NMR (DMSO-d_6, 75 MHz): δ_C 37.3 (C-1), 45.9 (C-2), 70.0 (C-3), 38.0 (C-4), 124.3 (C-5), 136.2 (C-6), 21.4 (C-7), 43.6 (C-8), 208.2 (C-9), 29.7 (C-10), 28.4 (C-11), 29.4 (C-12), 19.5 (C-13), 103.9 (C-1′), 73.4 (C-2′), 76.7 (C-3′), 69.6 (C-4′), 75.8 (C-5′), 68.3 (C-6′), 100.5 (C-1″), 73.4 (C-2″), 76.6 (C-3″), 70.3 (C-4″), 65.7 (C-5″).

SI-E.3. *Acid Hydrolysis of **1-4**.*



SI-figure-3. Retention times for authentic samples after acid hydrolysis of **1-4**

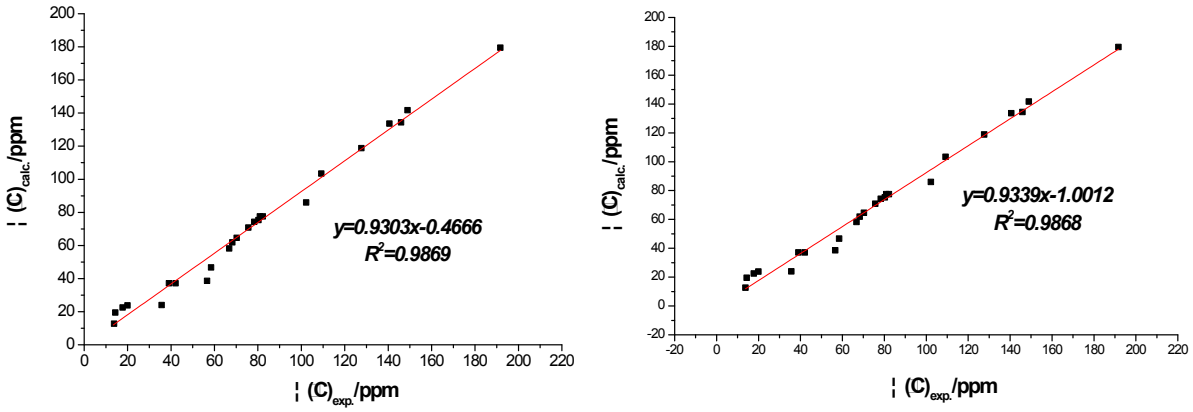
SI-E.4. *Preparation of the (R)- and (S)-MTPA Esters of **4a***



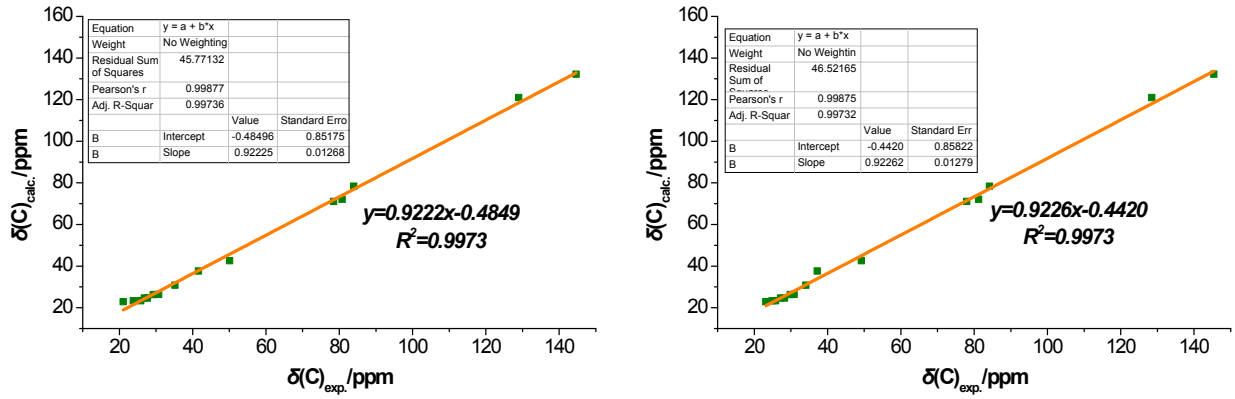
SI-figure-4. $\Delta\delta_H$ values for the MTPA esters of **4a**

SI-E.5. *^{13}C NMR calculation section (SI-table 3 and 4.)*

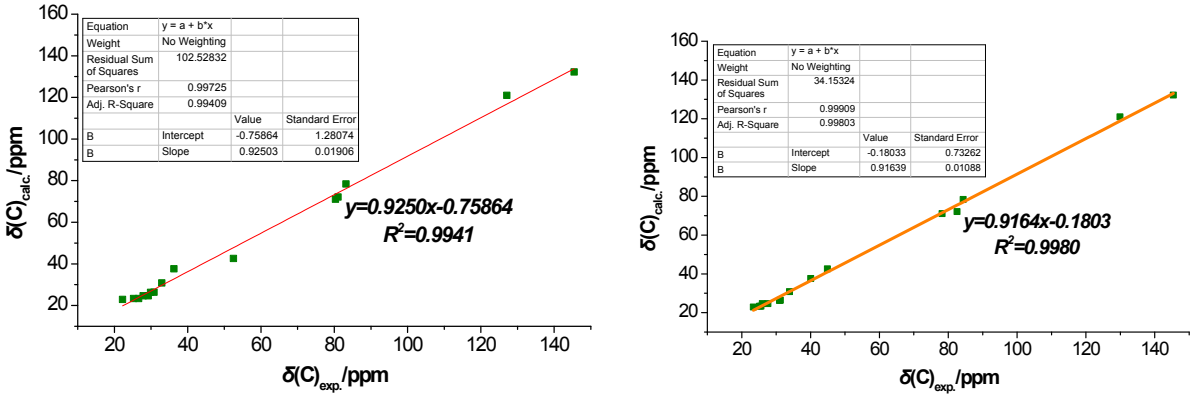
After optimization of the major conformers (>98%) was performed using the Gaussian 09 program at B3LYP/6-31G(d) level. Computed chemical shifts reported in this study were determined using the GIAO method in Gaussian 09 at the B3LYP/6-311+G(d) level of theory. The scaled calculated ^{13}C NMR chemical shifts were obtained from the following: $\delta_{scal.calc.} = (\delta_{calc.} - \text{intercept})/\text{slope}$.[1-3] The results were evaluated in terms of R^2, MaxDev and AveDev. Among them, R^2 is its coefficient of determination. MaxDev is the maximum absolute deviation with respect to the experimental chemical shifts δ_{exp}. AveDev is the average absolute deviation, computed as $(1/n)\ \Sigma^{n}_{i=1}\ |\delta_{scale.calc.} - \delta_{exp.}|$.



SI-figure-5. Correlation between experimental and calculated ^{13}C chemical shifts of stereoisomers (2*S* left, 2*R right*) of **2**



SI-figure-6. Correlation between experimental and calculated ^{13}C chemical shifts of stereoisomers (2*R/5R/6R* left, 2*R/5R/6S* right) of **4a**



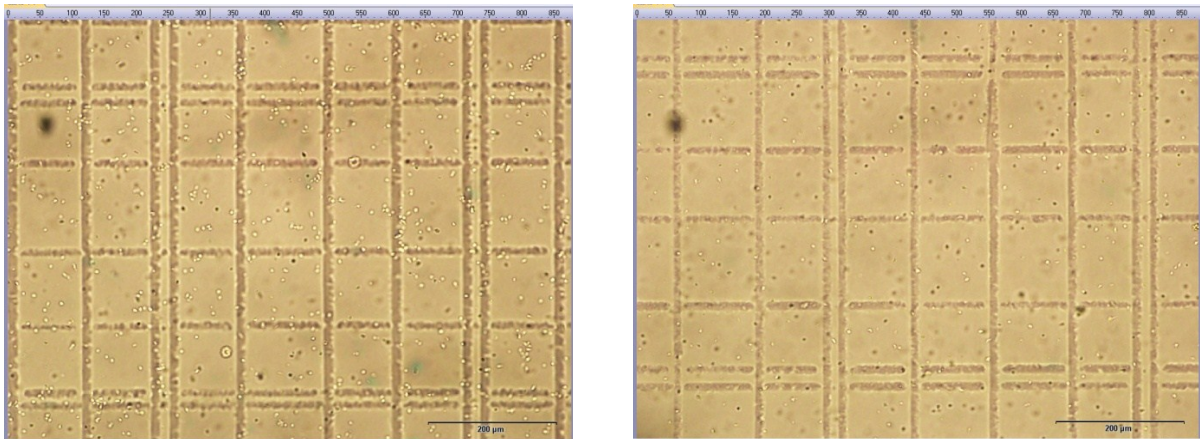
SI-figure-7. Correlation between experimental and calculated ^{13}C chemical shifts of stereoisomers (2*R/5S/6R* left, 2*R/5S/6S* right) of **4a**

(1) Barone, G.; Gomez-Paloma, L.; Duca, D.; Silvestri, A.; Riccio, R.; Bifulco, G. *Chem. Eur. J.* **2002**, *8*, 3233–3239.

(2) Tang, Y.; Xue, Y. B.; Du, G.; Wang, J. P.; Liu, J. J.; Sun, B.; Li, X. N.; Yao, G. M.; Luo, Z. W.; Zhang, Y. H. *Angew. Chem. Int. Ed.* **2016**, *55*, 4069 –4073.

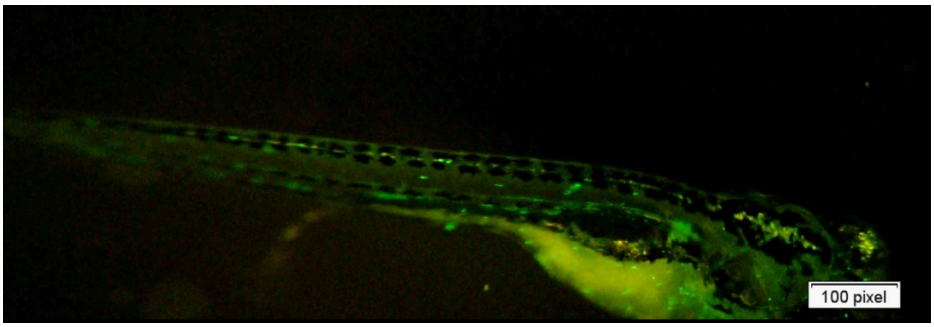
(3) Barone, G.; Duca, D.; Silvestri, A.; Gomez-Paloma, L.; Riccio, R.; Bifulco, G. *Chem. Eur. J.* **2002**, *8*, 3240-3245.

SI-E.6. *Evaluation of Antiplatelet Activity in Rat PRP.*



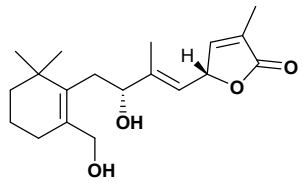
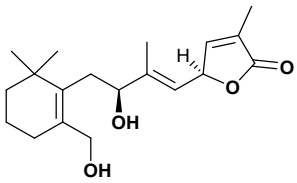
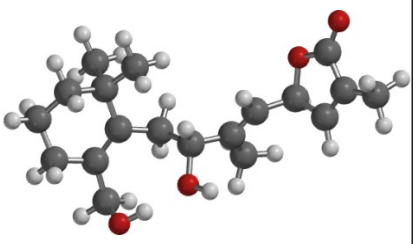
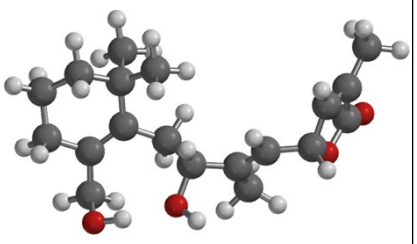
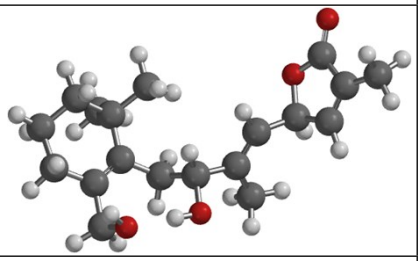
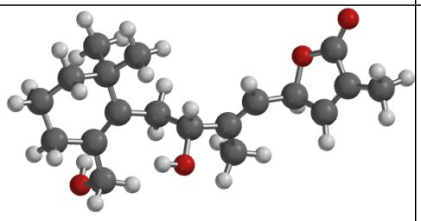
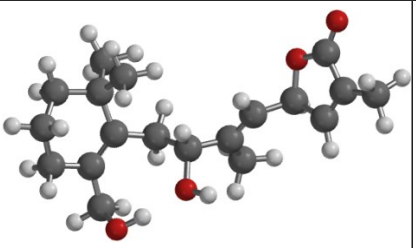
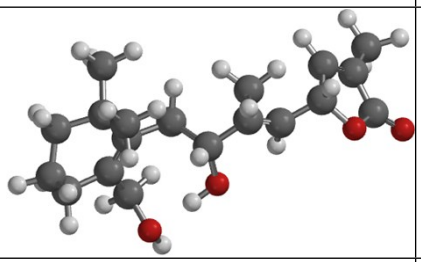
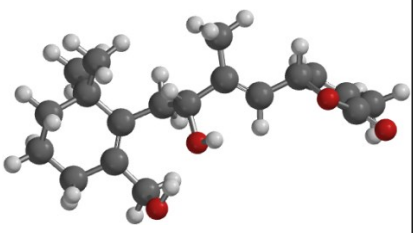
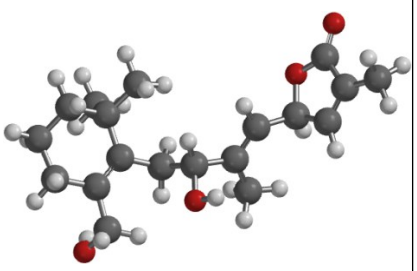
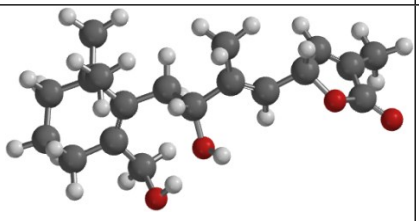
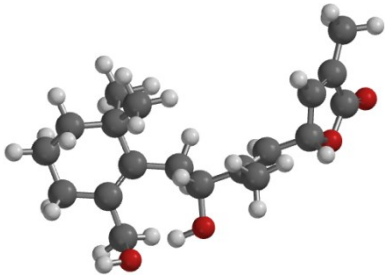
SI-figure-8. The platelet the aggregation model induced by adenosine diphosphate (ADP)

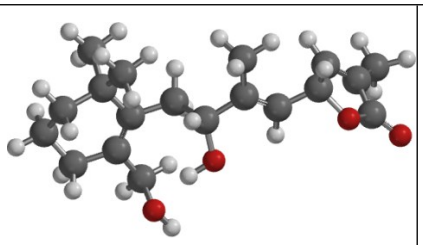
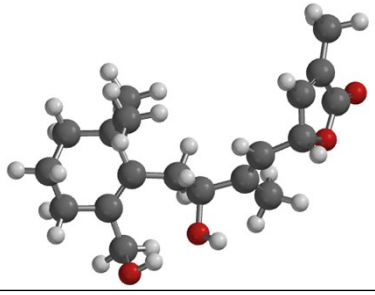
SI-E.7. *Antithrombotic assay using a transgenic zebrafish system*



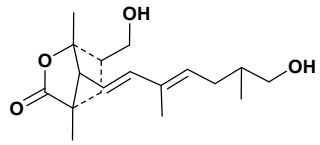
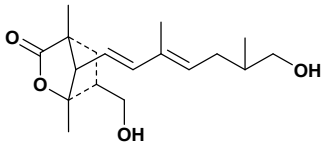
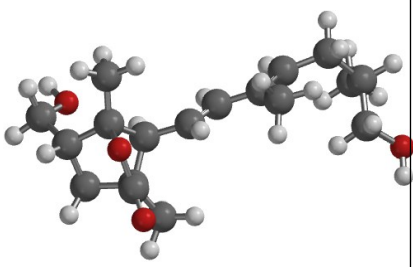
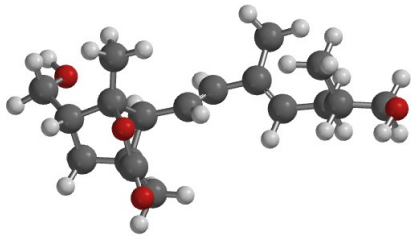
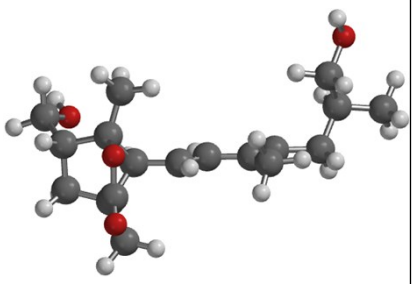
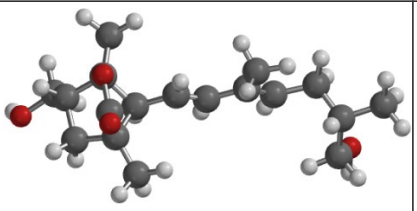
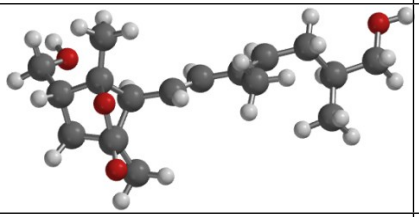
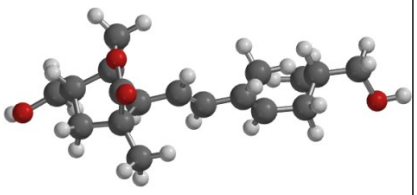
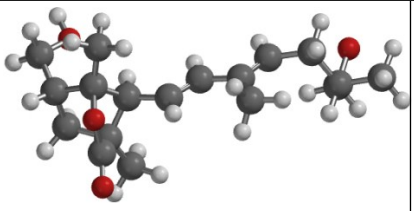
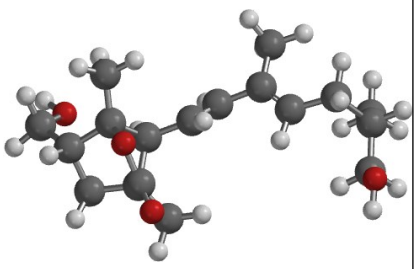
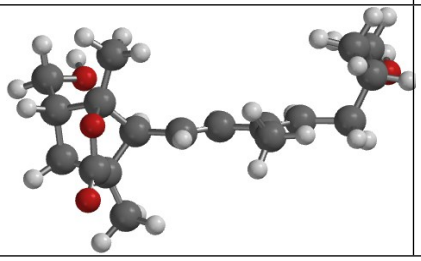
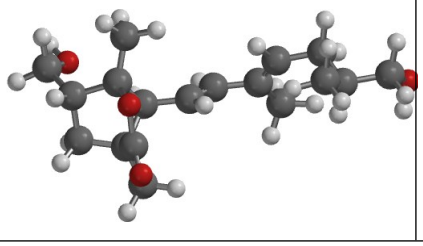
SI-figure-9. The $FeCl_3$-induced thrombosis model in the transgenic zebrafish system

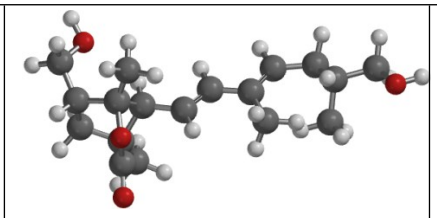
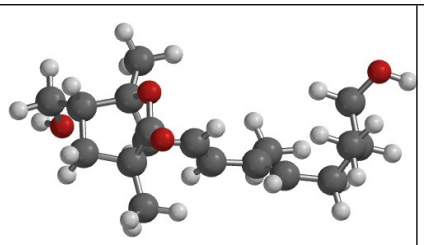
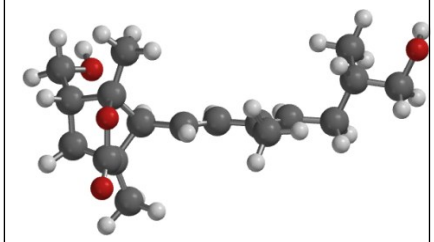
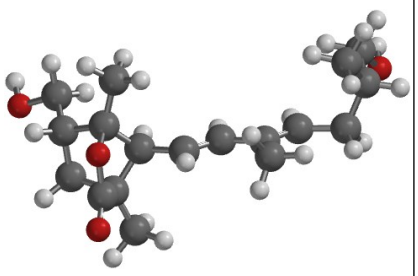
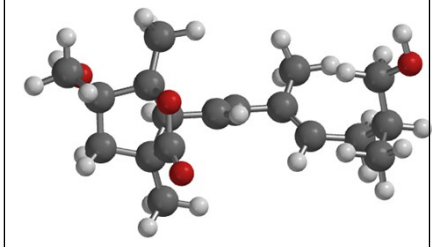
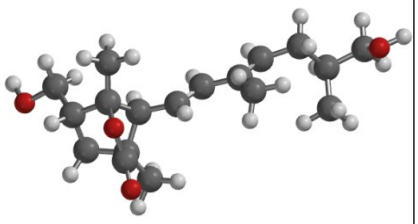
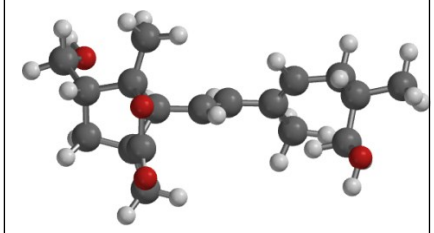
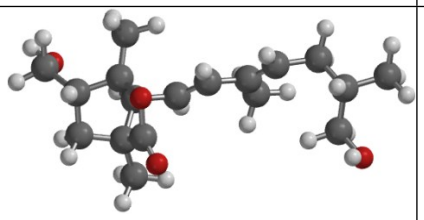
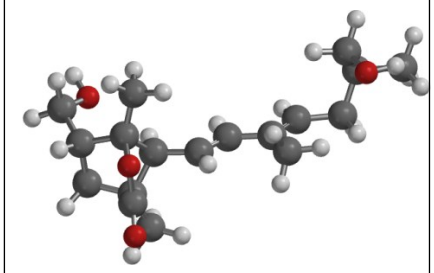
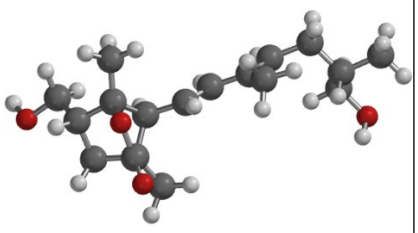
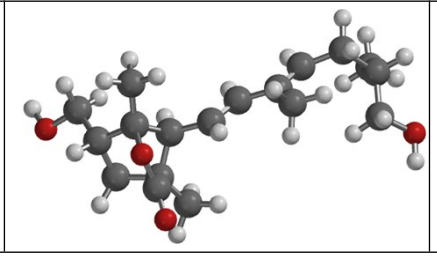
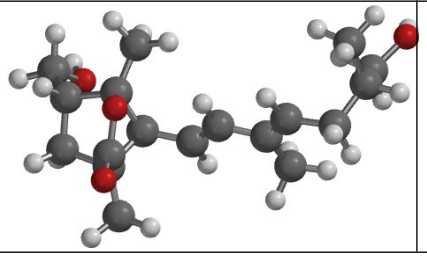
SI-table 1. Conformations of 1a were Obtained after the Optimization.

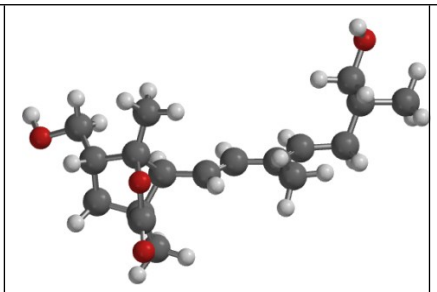
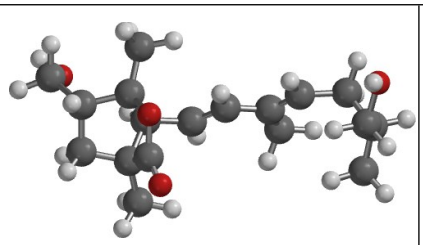
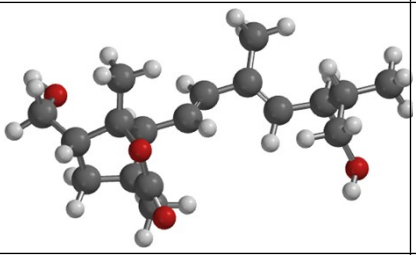
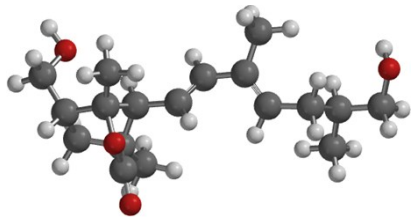
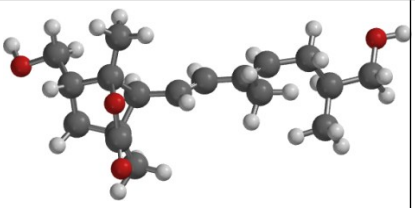
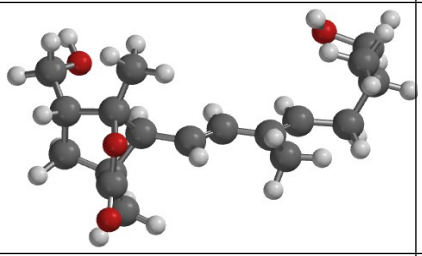
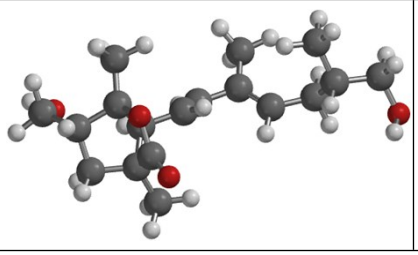
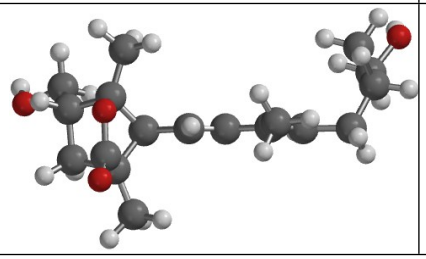
1a			1b		
no.	conformer	population (%)	no.	conformer	population (%)
1a-1		40.8	1a-7		0.8
1a-2		28.1	1a-8		0.6
1a-3		12.9	1a-9		0.4
1a-4		9.8	1a-10		0.3
1a-5		3.3	1a-11		0.3

1a-6		1.0	1a-12		0.3

SI-table 2. Conformations of 2a were obtained after the optimization.

2a			2b		
no.	conformer	population (%)	no.	conformer	population (%)
2a-1		20.9	2a-16		0.9
2a-2		18.4	2a-17		0.7
2a-3		12.0	2a-18		0.7
2a-4		8.7	2a-19		0.6
2a-5		7.8	2a-20		0.6

2a-6		6.7	2a-21		0.6
2a-7		1.8	2a-22		0.6
2a-8		1.6	2a-23		0.5
2a-9		1.6	2a-24		0.5
2a-10		1.4	2a-25		0.5
2a-11		1.4	2a-26		0.4

2a-12		1.2	2a-27		0.4
2a-13		1.1	2a-28		0.4
2a-14		1.1	2a-29		0.4
2a-15		0.9	2a-30		0.3

SI-table 3 Deviations between the calculated and experimental ^{13}C NMR chemical shifts for stereoisomers (2*S,* 2*R*) of **2**

EXL		2S				2R		
	calc.	scal.calc.	Δδ	|Δδ|	calc.	scal.calc.	Δδ	|Δδ|
12.7	13.4	12.0	0.7	0.7	13.8	11.9	0.8	0.8
19.5	14.2	12.8	6.7	6.7	14.4	12.4	7.1	7.1
22.5	16.2	14.6	7.9	7.9	17.7	15.5	7.0	7.0
23.8	18.3	16.6	7.2	7.2	19.9	17.6	6.2	6.2
24	36.3	33.3	-9.3	9.3	35.7	32.3	-8.3	8.3
37.1	39.0	35.8	1.3	1.3	39.0	35.5	1.6	1.6
37.1	41.3	37.9	-0.8	0.8	42.1	38.3	-1.2	1.2
38.6	54.7	50.4	-11.8	11.8	56.6	51.9	-13.3	13.3
46.7	58.0	53.5	-6.8	6.8	58.5	53.6	-6.9	6.9
58.2	67.4	62.2	-4.0	4.0	66.8	61.4	-3.2	3.2
61.9	68.4	63.2	-1.3	1.3	68.3	62.7	-0.8	0.8
64.6	69.3	64.0	0.6	0.6	70.3	64.6	0.0	0.0
70.8	76.1	70.3	0.5	0.5	75.7	69.7	1.1	1.1
74.3	79.7	73.7	0.6	0.6	78.3	72.2	2.1	2.1
75.3	80.1	74.1	1.2	1.2	80.3	74.0	1.3	1.3
77.5	80.9	74.8	2.7	2.7	80.9	74.6	2.9	2.9
77.5	82.1	75.9	1.6	1.6	82.3	75.8	1.7	1.7
86	101.8	94.3	-8.3	8.3	102.3	94.5	-8.5	8.5
103.4	109.3	101.2	2.2	2.2	109.2	101.0	2.4	2.4
118.8	128.2	118.8	0.0	0.0	127.7	118.3	0.5	0.5
133.6	141.0	130.7	2.9	2.9	140.6	130.3	3.3	3.3
134.4	145.0	134.4	0.0	0.0	145.9	135.3	-0.9	0.9
141.7	148.0	137.3	4.4	4.4	148.9	138.1	3.6	3.6
179.5	191.7	177.9	1.6	1.6	191.7	178.0	1.5	1.5
			AveDev	3.5			AveDev	3.6
			MaxDev	11.8			MaxDev	13.3
			R^2	0.9875			R^2	0.9875

SI-table 4 Deviations between the calculated and experimental ^{13}C NMR chemical shifts for stereoisomers (2*R/5R/6R,* 2*R/5R/6S*) of **4a**

EXL		2*R/5R/6R*				2*R/5R/6S*		
	calc.	scal.calc.	Δδ	|Δδ|	calc.	scal.calc.	Δδ	|Δδ|
22.9	21.1	18.9	-4.0	4.0	23.2	21.0	-1.9	1.9
23.3	23.8	21.5	-1.8	1.8	24.9	22.5	-0.8	0.8
23.3	25.9	23.4	0.1	0.1	25.9	23.4	0.1	0.1
24.6	26.8	24.3	-0.3	0.3	27.2	24.6	0.0	0.0
24.6	27.7	25.1	0.5	0.5	28.3	25.6	1.0	1.0
26.3	29.3	26.5	0.2	0.2	29.8	27.1	0.8	0.8
26.4	30.7	27.9	1.5	1.5	30.9	28.1	1.7	1.7
30.8	35.2	32.0	1.2	1.2	34.1	31.0	0.2	0.2
37.6	41.6	37.9	0.3	0.3	37.2	33.9	-3.7	3.7
42.6	50.1	45.7	3.1	3.1	49.2	45.0	2.4	2.4
71.1	78.5	71.9	0.8	0.8	78.0	71.5	0.4	0.4
72.1	80.8	74.0	1.9	1.9	81.2	74.5	2.4	2.4
78.4	83.9	76.9	-1.5	1.5	84.2	77.2	-1.2	1.2
121.0	129.0	118.5	-2.5	2.5	128.5	118.1	-2.9	2.9
132.2	144.6	132.9	0.7	0.7	145.4	133.7	1.5	1.5
			AveDev	1.3			AveDev	1.4
			MaxDev	4.0			MaxDev	3.7
			R^2	0.9973			R^2	0.9973

SI-table 5. Deviations between the calculated and experimental ^{13}C NMR chemical shifts for stereoisomers (2*R/5S/6R,* 2*R/5S/6S*) of **4a**

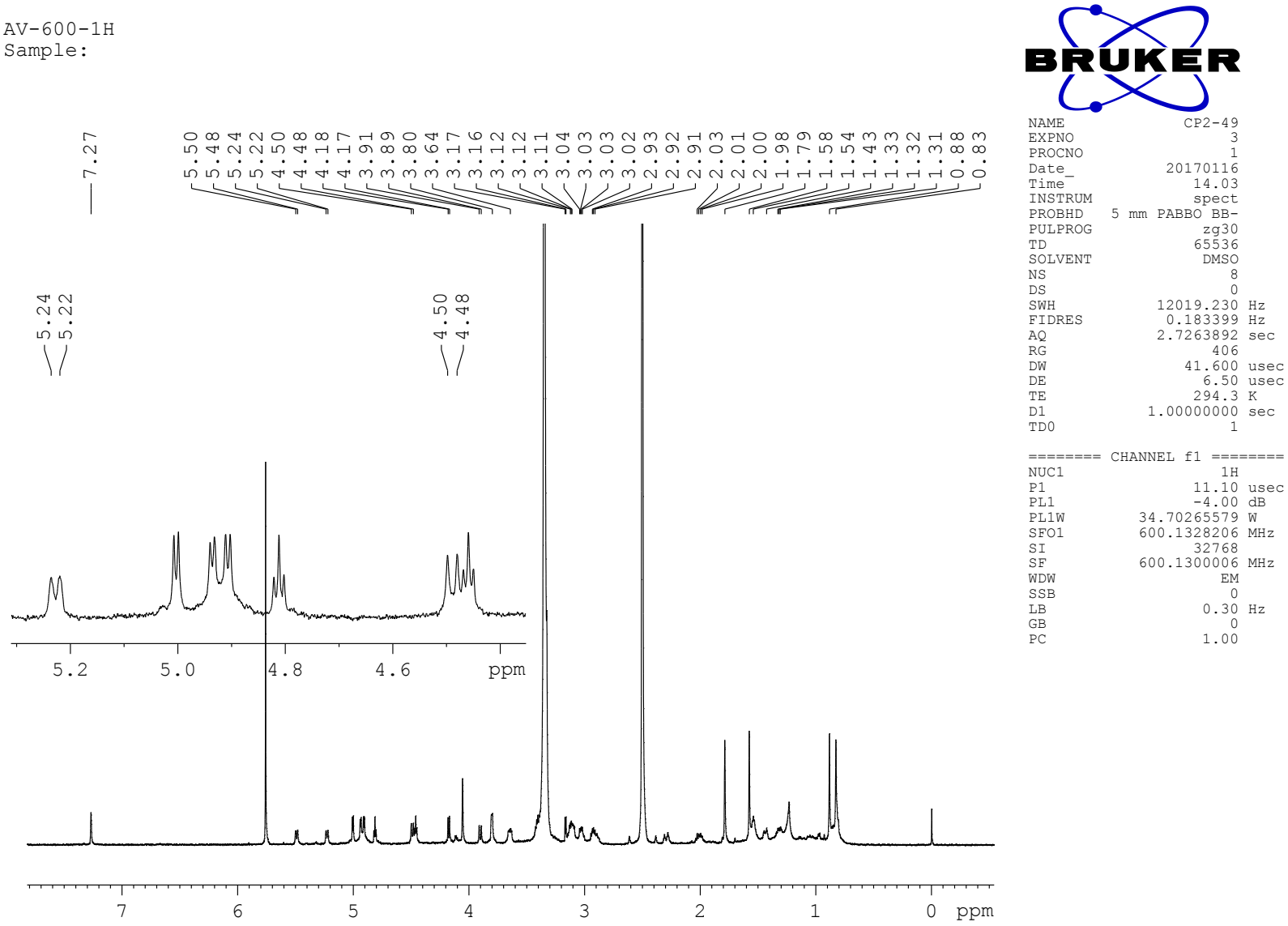
EXL		2*R/5S/6R*				2*R/5S/6S*		
	calc.	scal.calc.	Δδ	|Δδ|	calc.	scal.calc.	Δδ	|Δδ|
22.9	22.3	19.8	-3.1	3.1	23.4	21.2	-1.7	1.7
23.3	25.3	22.6	-0.7	0.7	25.2	22.9	-0.4	0.4
23.3	26.6	23.9	0.6	0.6	25.6	23.3	0.0	0.0
24.6	27.9	25.0	0.4	0.4	26.0	23.6	-1.0	1.0
24.6	29.3	26.3	1.7	1.7	27.6	25.1	0.5	0.5
26.3	29.9	26.9	0.6	0.6	31.0	28.2	1.9	1.9
26.4	30.8	27.8	1.4	1.4	31.2	28.4	2.0	2.0
30.8	32.9	29.7	-1.1	1.1	33.9	30.9	0.1	0.1
37.6	36.3	32.8	-4.8	4.8	40.1	36.5	-1.1	1.1
42.6	52.5	47.8	5.2	5.2	44.9	41.0	-1.6	1.6
71.1	80.3	73.6	2.5	2.5	78.2	71.5	0.4	0.4
72.1	81.1	74.2	2.1	2.1	82.6	75.5	3.4	3.4
78.4	83.2	76.2	-2.2	2.2	84.4	77.1	-1.3	1.3
121.0	127.1	116.8	-4.2	4.2	129.9	118.9	-2.1	2.1
132.2	145.5	133.8	1.6	1.6	145.4	133.1	0.9	0.9
			AveDev	2.1			AveDev	1.2
			MaxDev	5.2			MaxDev	3.4
			R^2	0.9941			R^2	0.9980

SI-table 6. Calculated Boltzmann distributions and optical rotations for each conformer of **4** and **3**

Compound 4 (2R,5S,6S)			**Compound 3 (2R,5R,6S)**		
Conformer	Optical rotation	Boltzmann distribution	Conformer	Optical rotation	Boltzmann distribution
1	-18.13	0.602	1	-18.13	0.602
2	-25	0.329	2	-25	0.329
3	10.07	0.011	3	10.07	0.011
4	-37.48	0.01	4	-37.48	0.01
5	-52.23	0.008	5	-52.23	0.008
6	-8.89	0.006	6	-8.89	0.006
7	-55.86	0.006	7	-55.86	0.006
8	-6.5	0.005	8	-6.5	0.005
9	-45.14	0.004	9	-45.14	0.004
10	-73.72	0.004	10	-73.72	0.004
11	-123.89	0.003	11	-123.89	0.003
12	-102.1	0.002			
13	-81.32	0.002			
14	-20.78	0.002			
15	-46.69	0.001			
16	-3.19	0.001			
17	-52.75	0.001			
18	-31.32	0.001			
19	-88.4	0.001			
20	-0.42	0.001			
21	-51.66	0.001			
Weighted optical rotation	**-21.77**		Weighted optical rotation	**-8.68**	

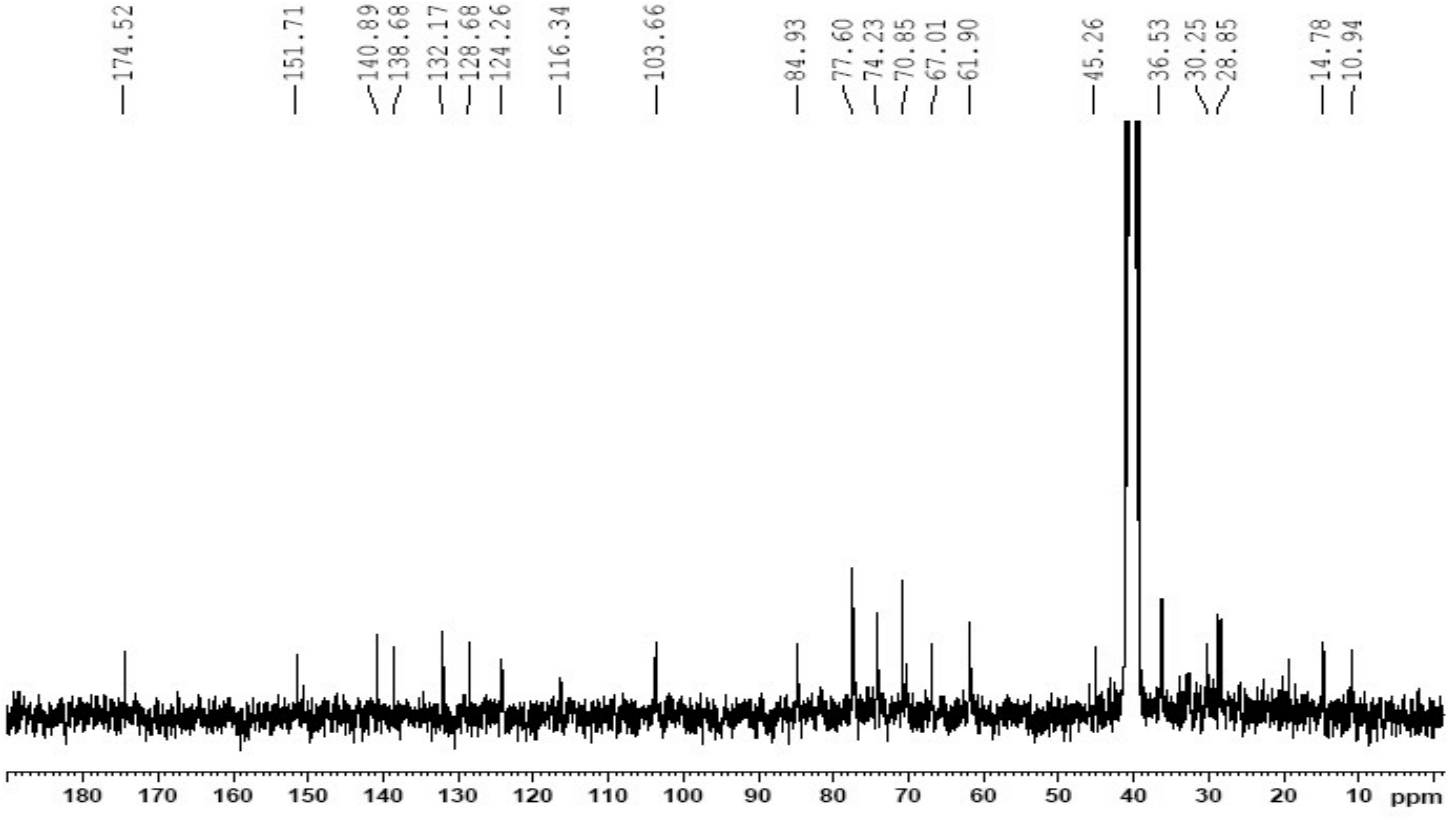
Spectra figure

S1. ^{1}H NMR spectrum (600MHz, DMSO-*d6*) of compound 1

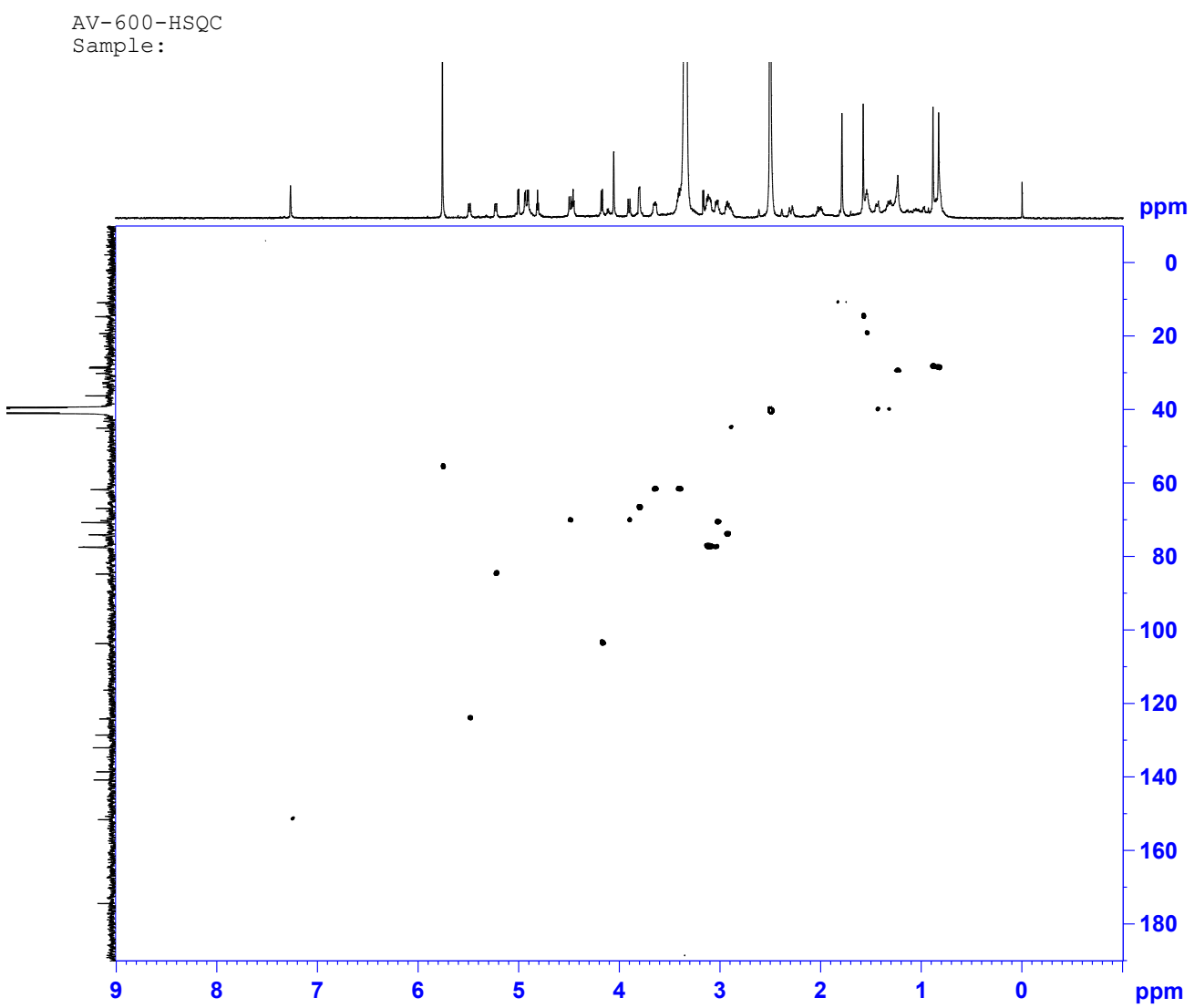


NAME	CP2-49
EXPNO	3
PROCNO	1
Date_	20170116
Time	14.03
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	8
DS	0
SWH	12019.230 Hz
FIDRES	0.183399 Hz
AQ	2.7263892 sec
RG	406
DW	41.600 usec
DE	6.50 usec
TE	294.3 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	11.10 usec
PL1	-4.00 dB
PL1W	34.70265579 W
SFO1	600.1328206 MHz
SI	32768
SF	600.1300006 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

S2. ^{13}C NMR spectrum (150MHz, DMSO-*d6*) of compound 1

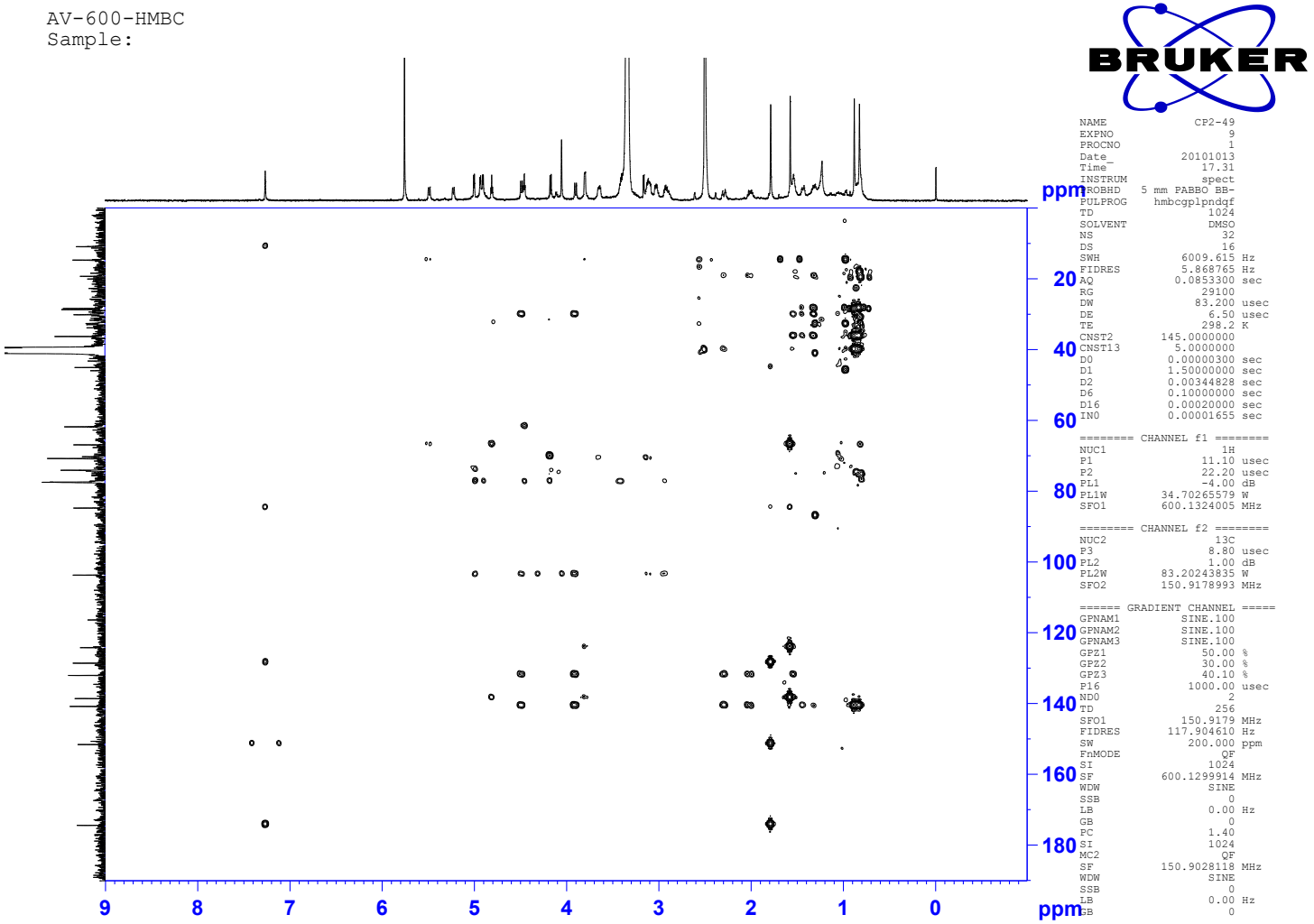


S3. HSQC spectrum (600MHz, DMSO-*d6*) of compound 1

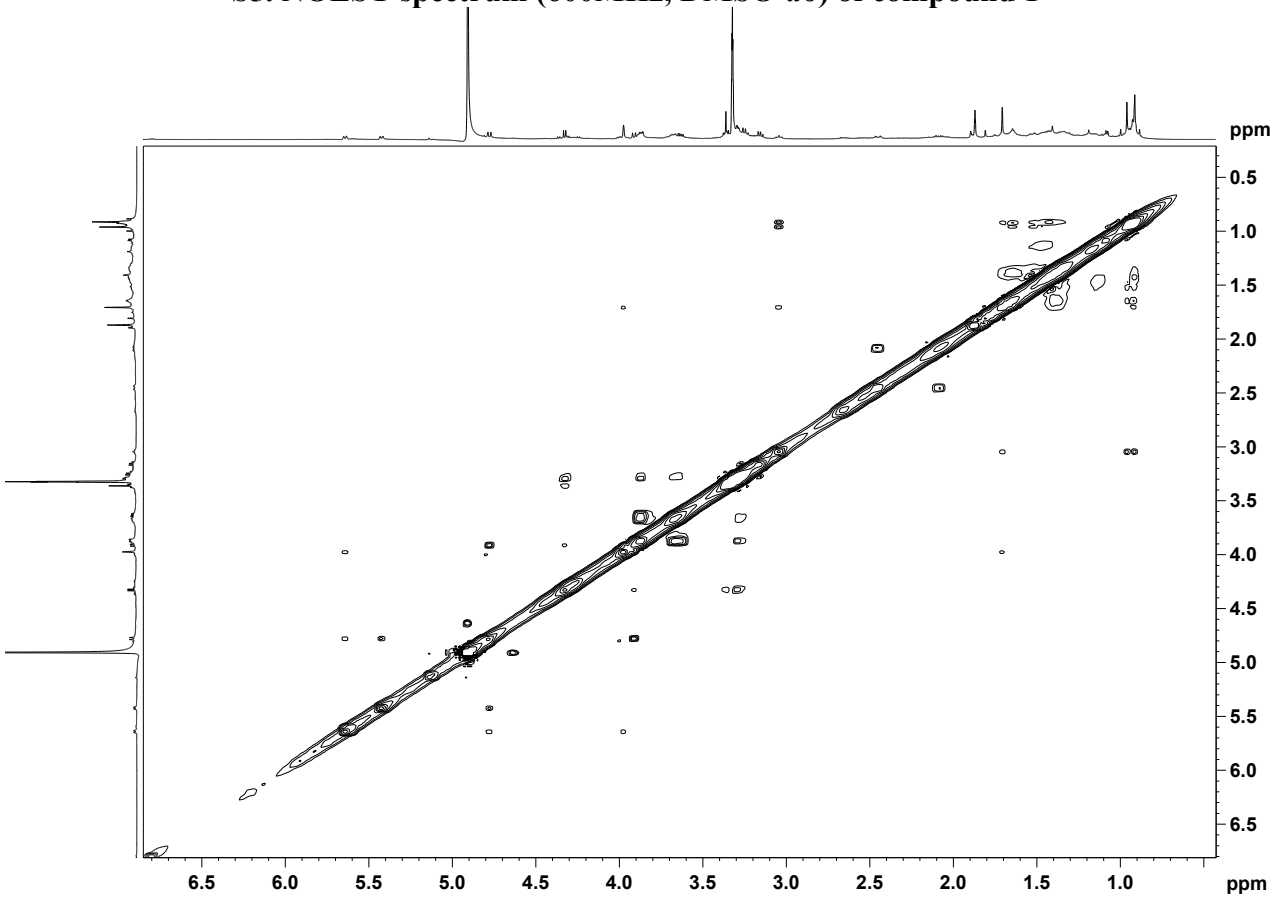



```
NAME                CP2-49
EXPNO                    8
PROCNO                   1
Date_             20170116
Time                 14.05
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG         hsqcetgpsi
TD                    1024
SOLVENT                DMSO
NS                       8
DS                      16
SWH                6009.615 Hz
FIDRES             5.868765 Hz
AQ                 0.0853300 sec
RG                     29100
DW                  83.200 usec
DE                   6.50 usec
TE                  294.3 K
CNST2             145.0000000
D0                 0.00000300 sec
D1                 1.50000000 sec
D4                 0.00172414 sec
D11                0.03000000 sec
D13                0.00000400 sec
D16                0.00020000 sec
D24                0.00110000 sec
IN0                0.00001655 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                     1H
P1                   11.10 usec
P2                   22.20 usec
P28                2500.00 usec
PL1                  -4.00 dB
PL1W             34.70265579 W
SFO1             600.1324005 MHz

======== CHANNEL f2 ========
CPDPRG2                garp
NUC2                    13C
P3                    9.53 usec
P4                   19.06 usec
PCPD2                80.00 usec
PL2                   1.00 dB
PL12                 19.48 dB
PL2W             83.20243835 W
PL12W             1.18069065 W
SFO2             150.9163903 MHz

====== GRADIENT CHANNEL =====
GPNAM1               SINE.100
GPNAM2               SINE.100
GPZ1                    80.00 %
GPZ2                    20.10 %
P16                   1000.00 usec
ND0                        2
TD                       225
SFO1              150.9164 MHz
FIDRES            134.147903 Hz
SW                200.000 ppm
FnMODE      Echo-Antiecho
SI                      1024
SF             600.1300000 MHz
WDW                   QSINE
SSB                        2
LB                    0.00 Hz
GB                         0
PC                    1.40
SI                      1024
MC2           echo-antiecho
SF             150.9027963 MHz
WDW                   QSINE
SSB                        2
LB                    0.00 Hz
GB                         0
```

S4.HMBC spectrum (600MHz, DMSO-*d6*) of compound 1



S5. NOESY spectrum (600MHz, DMSO-*d6*) of compound 1



Mass Spectrum Molecular Formula Report

Analysis Info

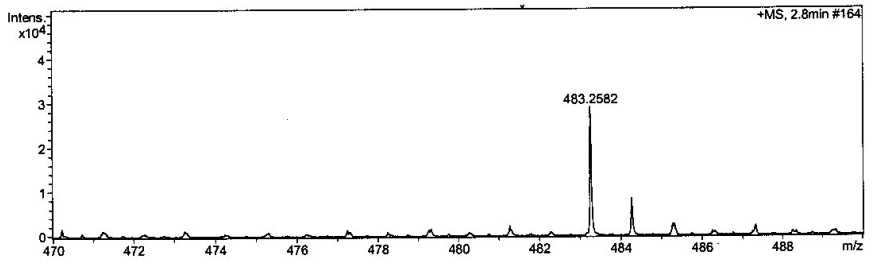
Analysis Name	D:\Data\20110107\YE-49.d	Acquisition Date	1/7/2011 5:12:44 PM
Method	tune low 100-500.m	Operator	Bruker Customer
Sample Name	YE-49	Instrument / Ser#	micrOTOF-Q 125
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	90.0 Vpp	Set Divert Valve	Source

Generate Molecular Formula Parameter

Formula, min.	C25H38O9				
Formula, max.					
Measured m/z	483.258	Tolerance	3 ppm	Charge	1
Check Valence	no	Minimum	0	Maximum	0
Nirogen Rule	no	Electron Configuration	both		
Filter H/C Ratio	no	Minimum	0	Maximum	3
Estimate Carbon	yes				

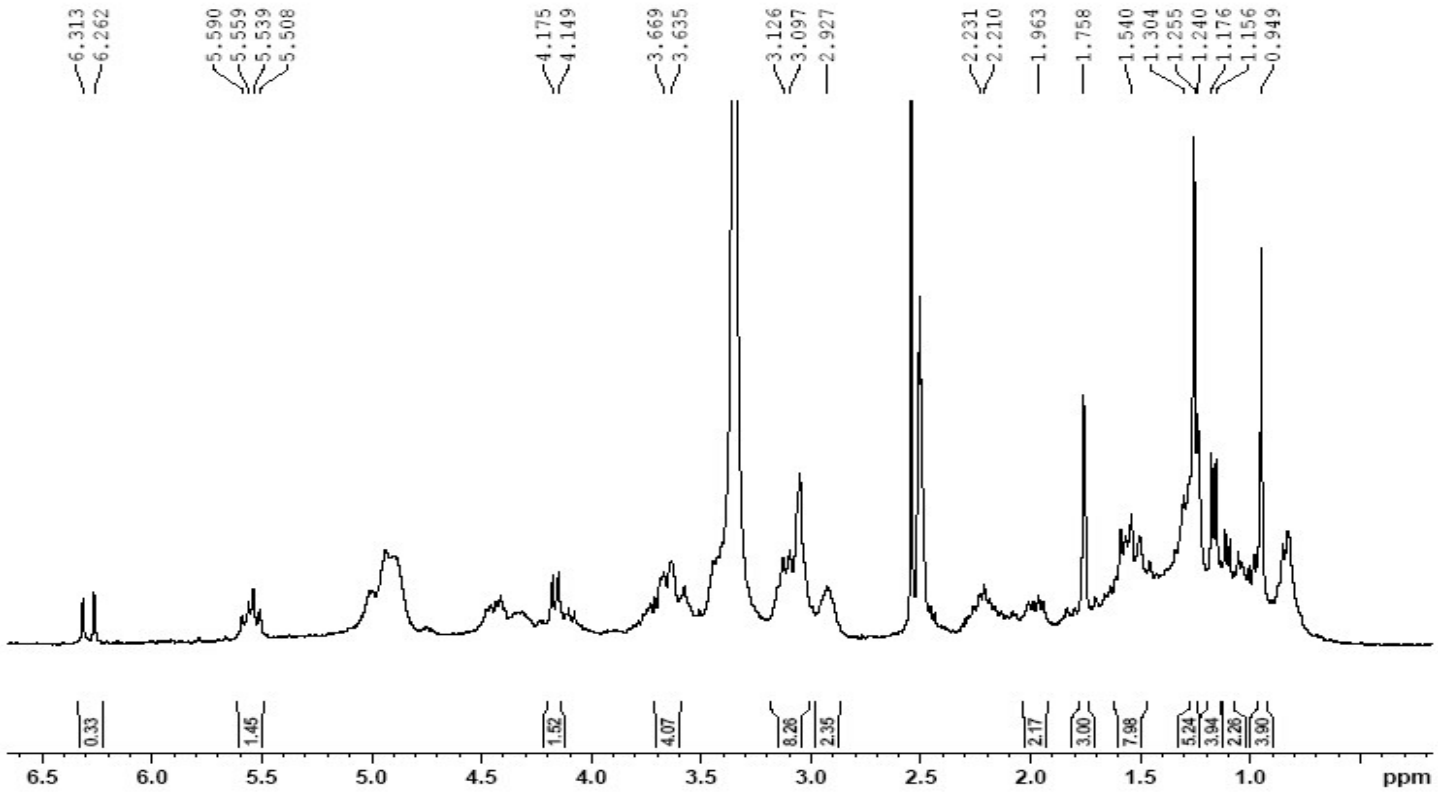


#	m/z	I
1	483.2582	28825

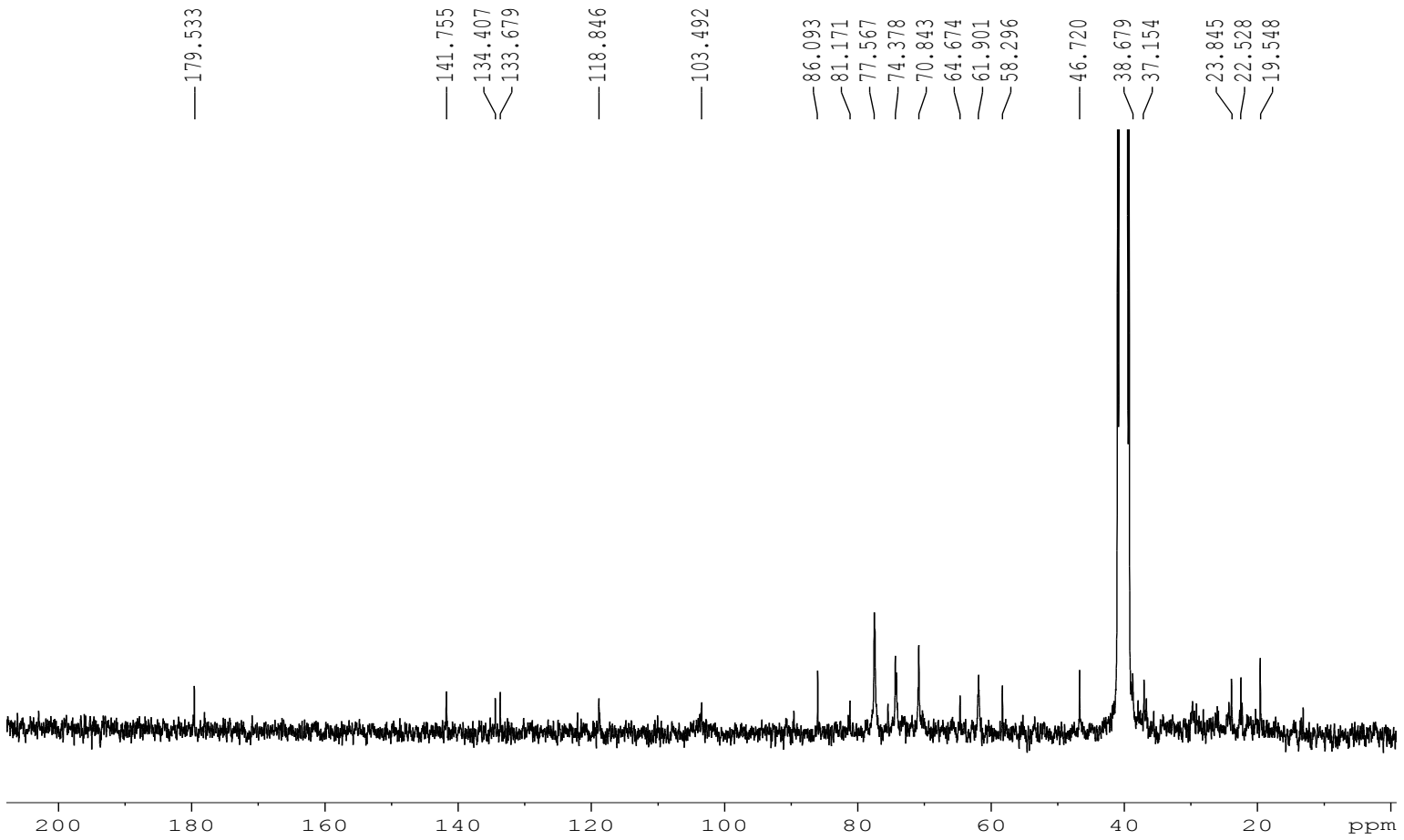
Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	Err [mDa]	rdb	N Rule	e⁻
C 25 H 39 O 9	0.019	483.2589	1.39	-0.02	0.67	6.50	ok	even

S6. The HREIMS spectrum of compound 1

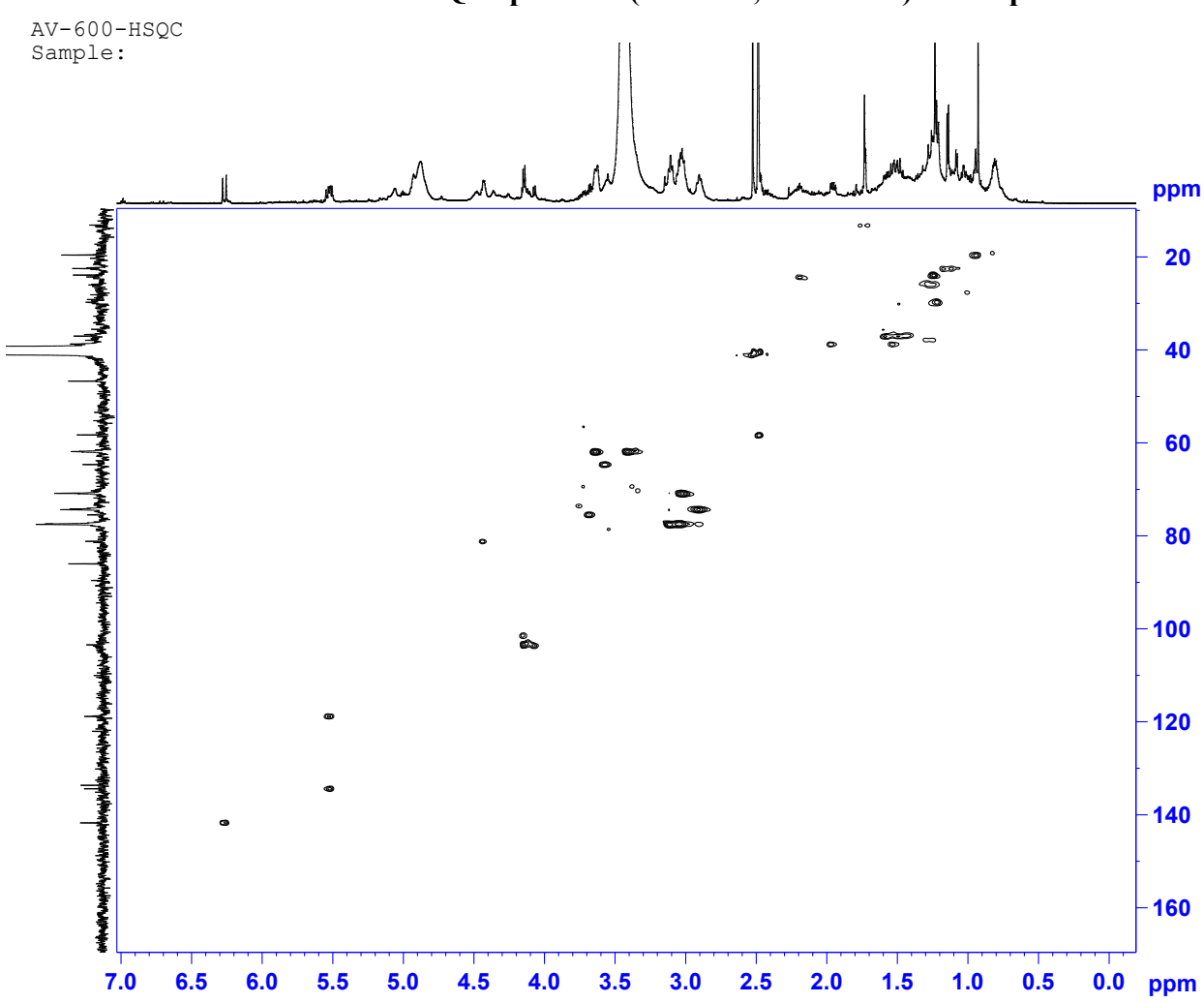
S7. ^{1}H NMR spectrum (600MHz, DMSO-*d6*) of compound 2



S8. ^{13}C NMR spectrum (150MHz, DMSO-*d6*) of compound 2

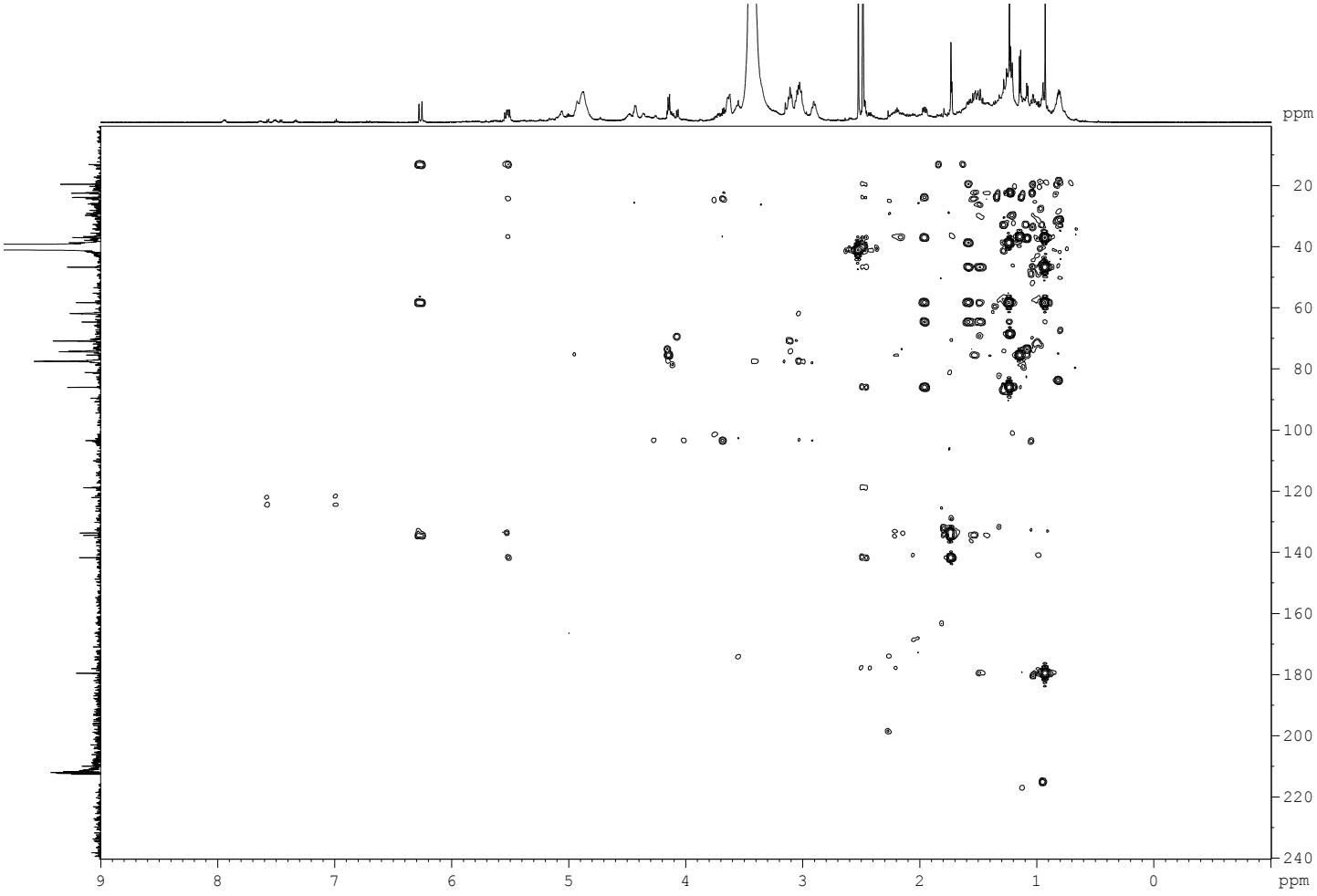


S9. HSQC spectrum (600MHz, DMSO-*d6*) of compound 2

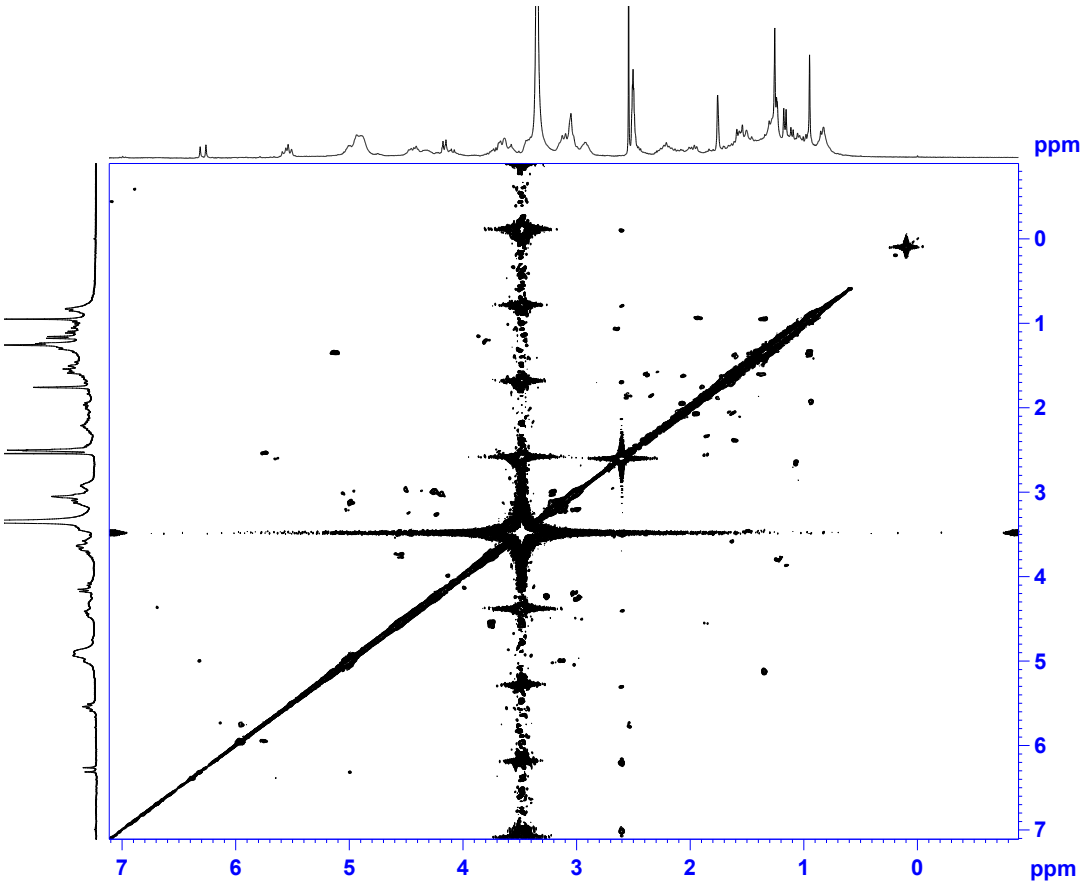



```
NAME                YE-50-1
EXPNO                     8
PROCNO                    1
Date_              20110107
Time                  8.12
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG       hsqcetgpsi
TD                     1024
SOLVENT                DMSO
NS                        8
DS                       16
SWH                6009.615 Hz
FIDRES             5.868765 Hz
AQ                 0.0853300 sec
RG                     11500
DW                  83.200 usec
DE                    6.50 usec
TE                  298.2 K
CNST2            145.0000000
D0                 0.00000300 sec
D1                 1.50000000 sec
D4                 0.00172414 sec
D11                0.03000000 sec
D13                0.00000400 sec
D16                0.00020000 sec
D24                0.00110000 sec
IN0                0.00001655 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                      1H
P1                     11.10 usec
P2                     22.20 usec
P28                  1000.00 usec
PL1                    -4.00 dB
PL1W            34.70265579 W
SFO1            600.1324005 MHz

======== CHANNEL f2 ========
CPDPRG2                garp
NUC2                    13C
P3                      8.80 usec
P4                     17.60 usec
PCPD2                  80.00 usec
PL2                     1.00 dB
PL12                   20.17 dB
PL2W            83.20243835 W
PL12W            1.00724721 W
SFO2            150.9178993 MHz

====== GRADIENT CHANNEL =====
GPNAM1               SINE.100
GPNAM2               SINE.100
GPZ1                    80.00 %
GPZ2                    20.10 %
P16                   1000.00 usec
ND0                        2
TD                       256
SFO1              150.9179 MHz
FIDRES         117.904610 Hz
SW                 200.000 ppm
FnMODE     Echo-Antiecho
SI                      1024
SF             600.1300000 MHz
WDW                    QSINE
SSB                        2
LB                      0.00 Hz
GB                         0
PC                      1.40
SI                      1024
MC2            echo-antiecho
SF              150.9027474 MHz
WDW                    QSINE
SSB                        2
LB                      0.00 Hz
GB                         0
```

S10. HMBC spectrum (600MHz, DMSO-*d6*) of compound 2



S11. NOESY spectrum (600MHz, DMSO-*d6*) of compound 2




```
NAME                YE-50-1
EXPNO                     5
PROCNO                    1
Date_              20161010
Time                  14.26
INSTRUM               spect
PROBHD   5 mm PABBO BB-
PULPROG           cosygpqf
TD                     1024
SOLVENT                DMSO
NS                       50
DS                        8
SWH                4807.692 Hz
FIDRES             4.695012 Hz
AQ                0.1066500 sec
RG                     1150
DW                 104.000 usec
DE                   6.50 usec
TE                   294.3 K
D0                0.00000300 sec
D1                2.00000000 sec
D13               0.00000400 sec
D16               0.00020000 sec
IN0               0.00020800 sec

======== CHANNEL f1 ========
NUC1                     1H
P0                    11.10 usec
P1                    11.10 usec
PL1                   -4.00 dB
PL1W             34.70265579 W
SFO1             600.1318004 MHz

====== GRADIENT CHANNEL =====
GPNAM1              SINE.100
GPZ1                  16.00 %
P16                 1000.00 usec
ND0                       1
TD                      256
SFO1              600.1318 MHz
FIDRES            18.779905 Hz
SW                    8.011 ppm
FnMODE                   QF
SI                     1024
SF               600.1299352 MHz
WDW                    SINE
SSB                       0
LB                     0.00 Hz
GB                        0
PC                     1.40
SI                     1024
MC2                      QF
SF               600.1299371 MHz
WDW                    SINE
SSB                       0
LB                     0.00 Hz
GB                        0
```

Mass Spectrum Molecular Formula Report

Analysis Info

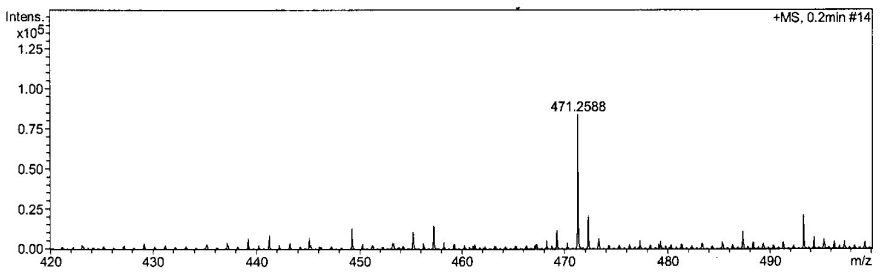
Analysis Name	D:\Data\20110517\YE-50.d	Acquisition Date	5/17/2011 11:48:42 AM
Method	tune_50-1000_POS_20110328.m	Operator	YP
Sample Name	YE-50	Instrument / Ser#	micrOTOF-Q 125
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.5 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Source

Generate Molecular Formula Parameter

Formula, min.	C24H38H1O9						
Formula, max.							
Measured m/z	471.259	Tolerance	4	mDa	Charge	1	
Check Valence	no	Minimum	0		Maximum	0	
Nirogen Rule	no	Electron Configuration		both			
Filter H/C Ratio	no	Minimum	0		Maximum	3	
Estimate Carbon	yes						



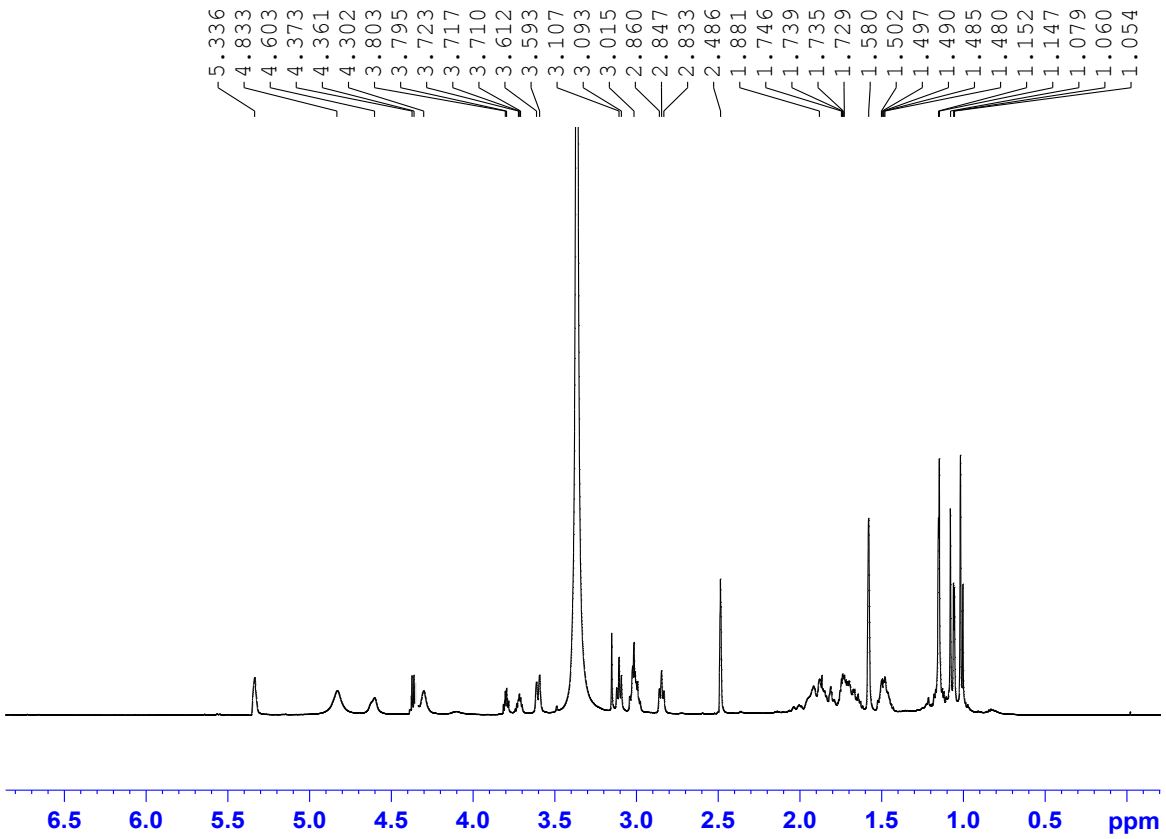
#	m/z	I
1	471.2588	83549

Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	Err [mDa]	rdb	N Rule	e⁻
C 24 H 39 O 9	0.018	471.2589	0.17	-0.46	0.08	5.50	ok	even

S12. The HREIMS spectrum of compound 2

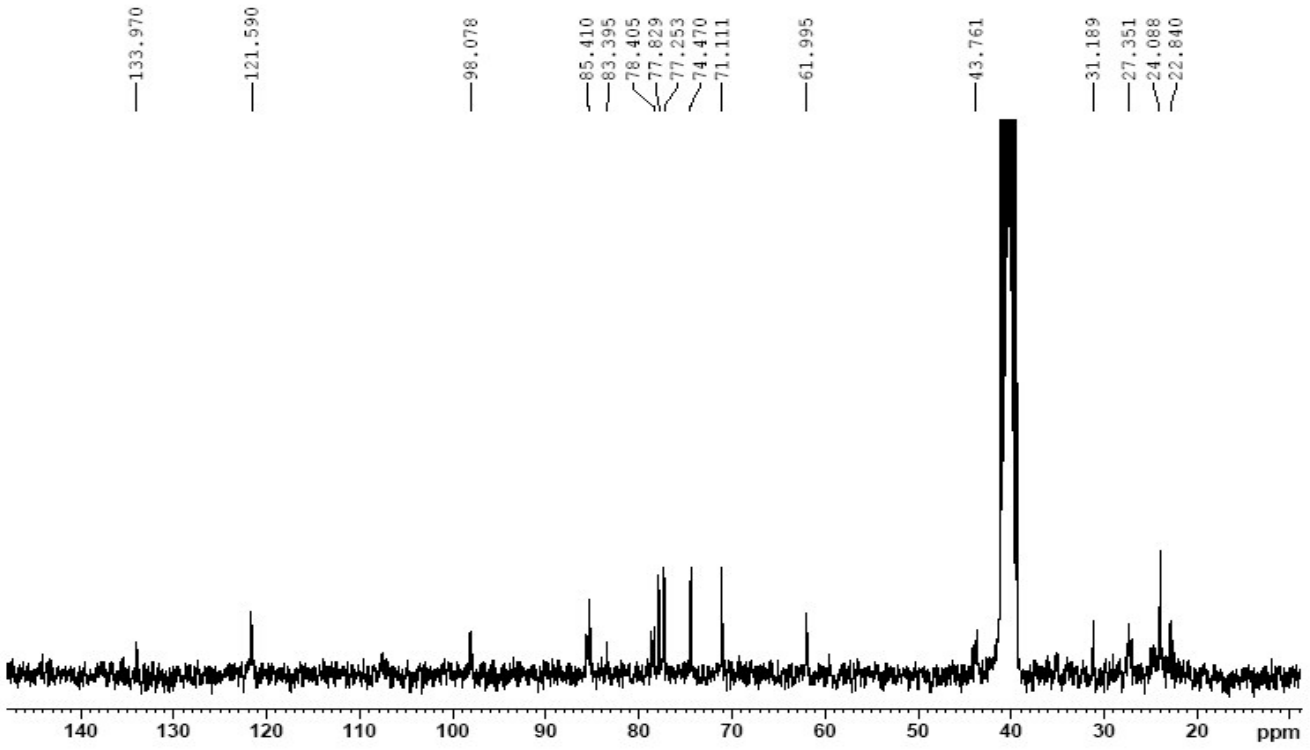
S13. ^{1}H NMR spectrum (600MHz, DMSO-*d6*) of compound 3

AV-600-1H
Sample:

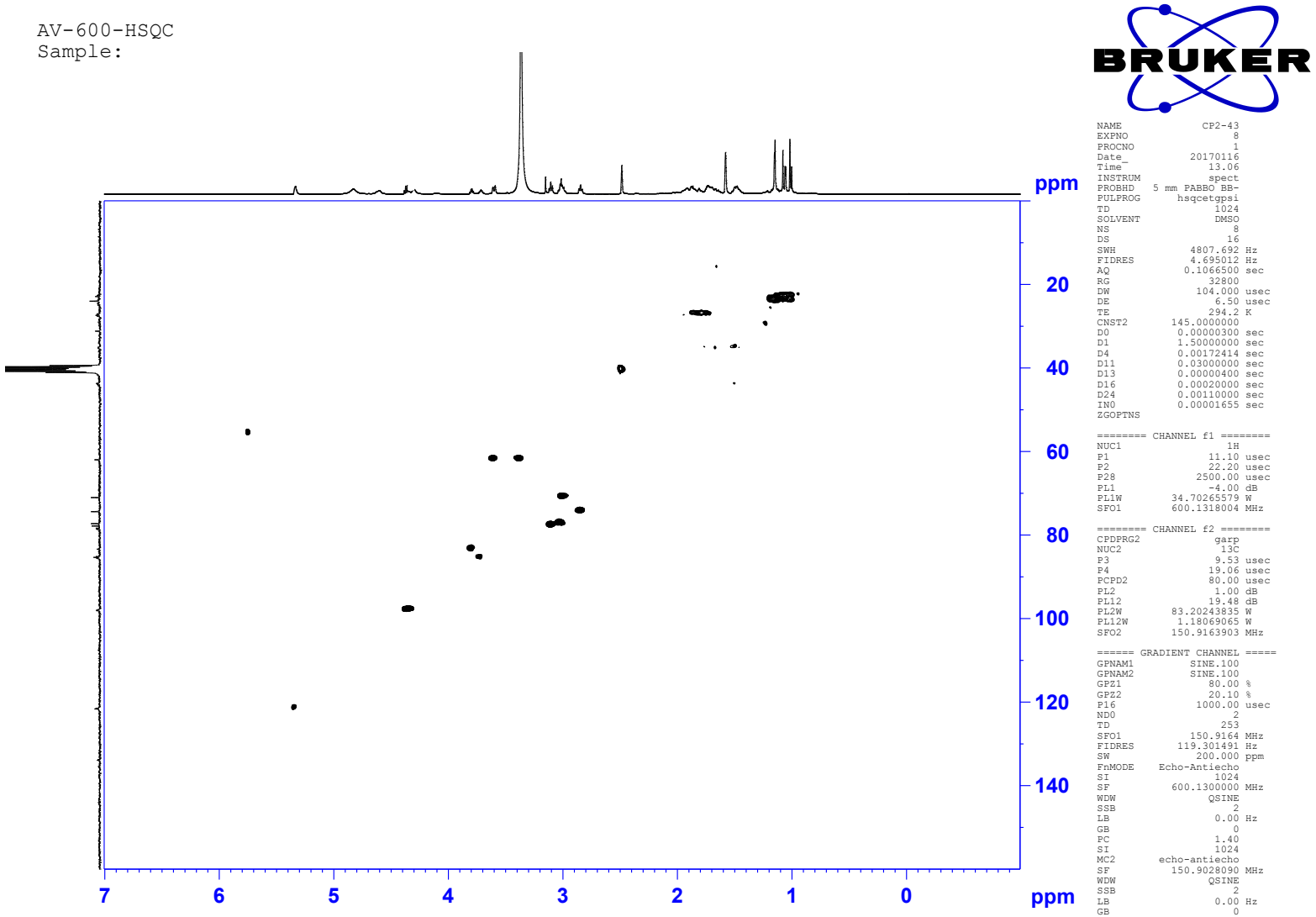


NAME	YE-43	
EXPNO	1	
PROCNO	1	
Date_	20101108	
Time	12.37	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zg30	
TD	65536	
SOLVENT	DMSO	
NS	8	
DS	2	
SWH	13227.514	Hz
FIDRES	0.201836	Hz
AQ	2.4773486	sec
RG	90.5	
DW	37.800	usec
DE	6.50	usec
TE	298.2	K
D1	1.00000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	1H	
P1	11.10	usec
PL1	-4.00	dB
PL1W	34.70265579	W
SFO1	600.1333017	MHz
SI	32768	
SF	600.1300086	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	

S14. ^{13}C NMR spectrum (150MHz, DMSO-*d6*) of compound 3

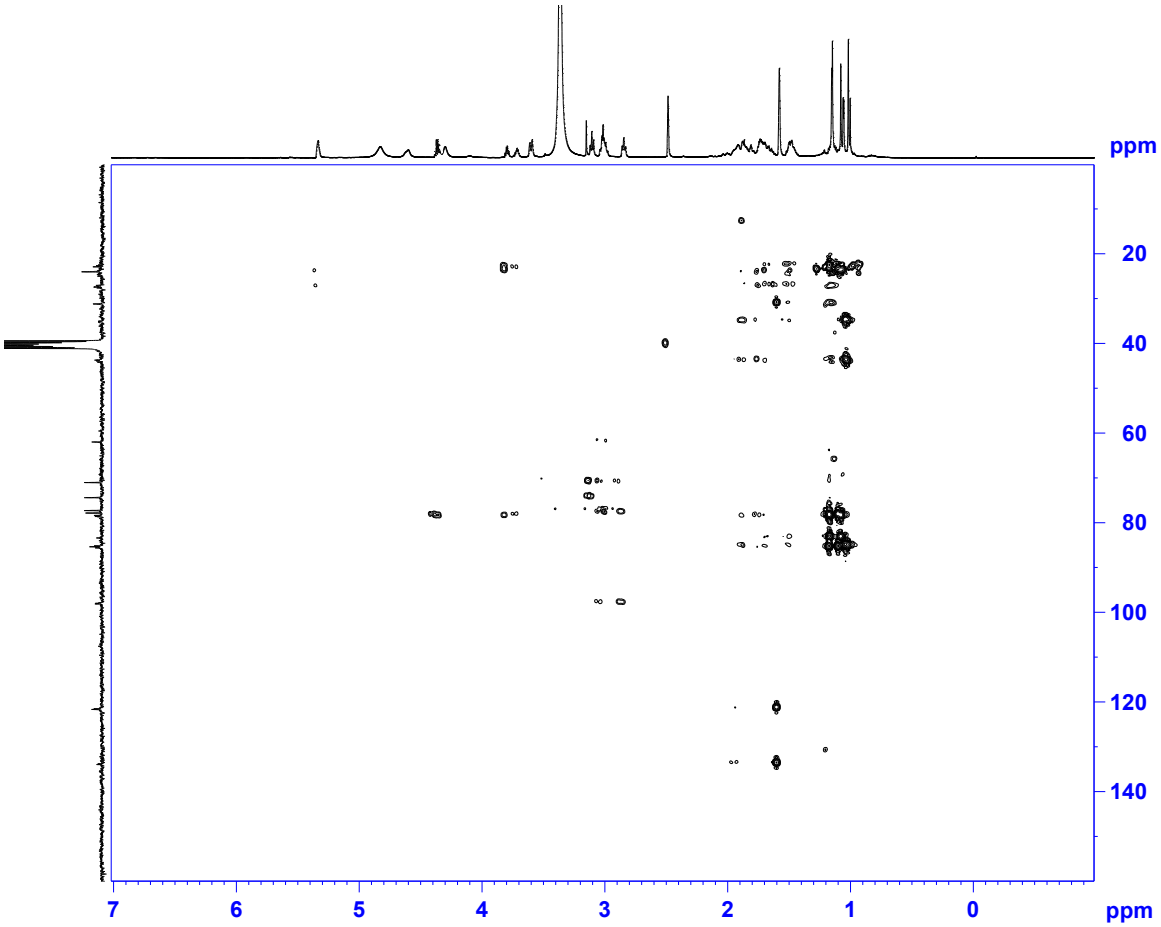


S15. HSQC spectrum (600MHz, DMSO-*d6*) of compound 3



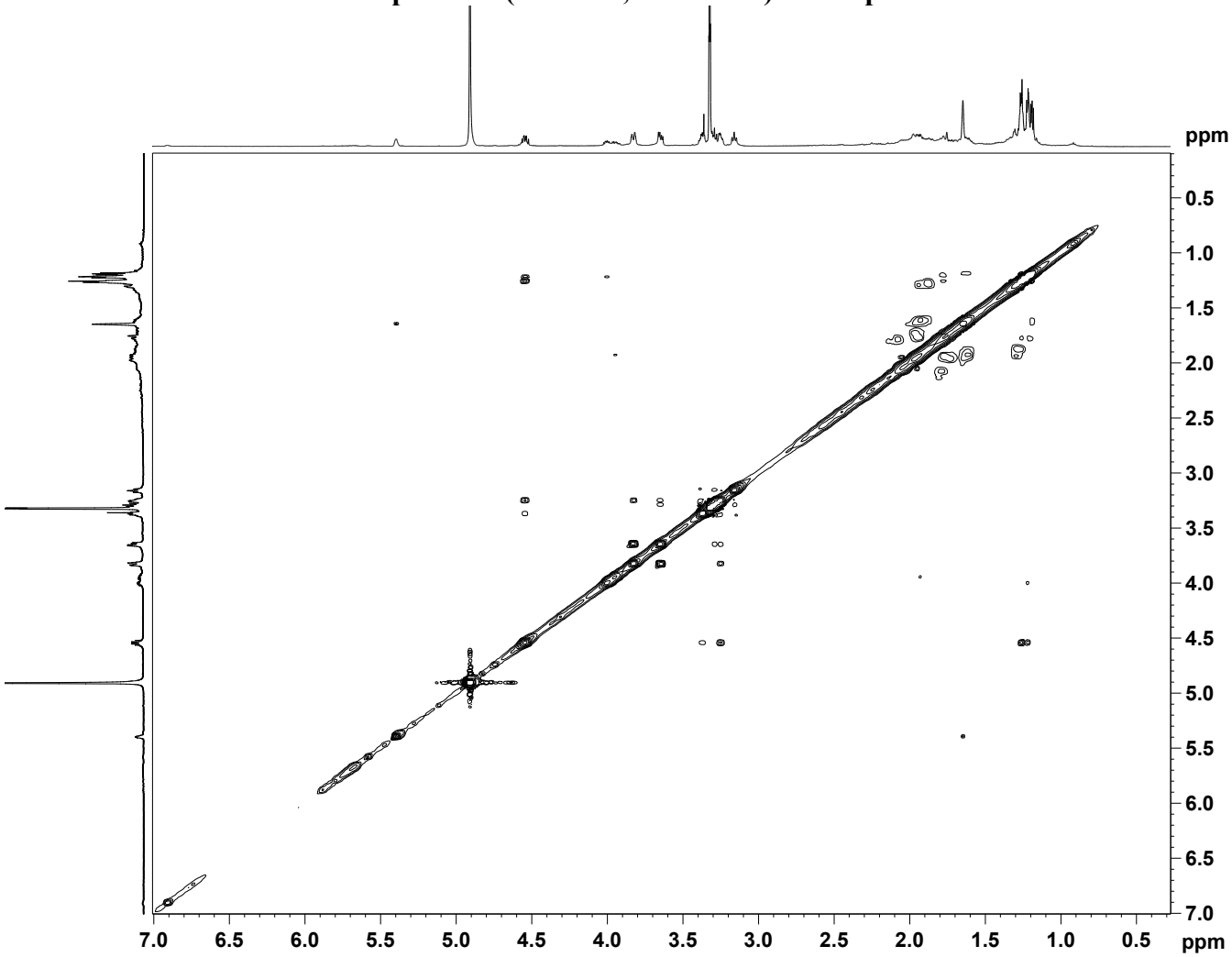

```
NAME                CP2-43
EXPNO                    8
PROCNO                   1
Date_             20170116
Time                 13.06
INSTRUM                  spect
PROBHD   5 mm PABBO BB-
PULPROG          hsqcetgpsi
TD                    1024
SOLVENT                DMSO
NS                        8
DS                       16
SWH                4807.692 Hz
FIDRES             4.695012 Hz
AQ                 0.1066500 sec
RG                     32800
DW                  104.000 usec
DE                    6.50 usec
TE                     294.2 K
CNST2             145.0000000
D0                 0.00000300 sec
D1                 1.50000000 sec
D4                 0.00172414 sec
D11                0.03000000 sec
D13                0.00000400 sec
D16                0.00020000 sec
D24                0.00110000 sec
IN0                0.00001655 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                     1H
P1                    11.10 usec
P2                    22.20 usec
P28                 2500.00 usec
PL1                   -4.00 dB
PL1W              34.70265579 W
SFO1              600.1318004 MHz

======== CHANNEL f2 ========
CPDPRG2                garp
NUC2                    13C
P3                     9.53 usec
P4                    19.06 usec
PCPD2                 80.00 usec
PL2                    1.00 dB
PL12                  19.48 dB
PL2W              83.20243835 W
PL12W              1.18069065 W
SFO2              150.9163903 MHz

====== GRADIENT CHANNEL =====
GPNAM1               SINE.100
GPNAM2               SINE.100
GPZ1                    80.00 %
GPZ2                    20.10 %
P16                   1000.00 usec
ND0                        2
TD                       253
SFO1              150.9164 MHz
FIDRES            119.301491 Hz
SW                   200.000 ppm
FnMODE          Echo-Antiecho
SI                      1024
SF                600.1300000 MHz
WDW                    QSINE
SSB                        2
LB                      0.00 Hz
GB                         0
PC                      1.40
SI                      1024
MC2             echo-antiecho
SF                150.9028090 MHz
WDW                    QSINE
SSB                        2
LB                      0.00 Hz
GB                         0
```

S16. HMBC spectrum (600MHz, DMSO-*d6*) of compound 3




```
NAME                YE-43
EXPNO                   9
PROCNO                  1
Date_            20101108
Time                12.48
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG    hmbcgplpndqf
TD                   1024
SOLVENT              DMSO
NS                     32
DS                     16
SWH              4807.692 Hz
FIDRES           4.695012 Hz
AQ               0.1066500 sec
RG                   29100
DW                 104.000 usec
DE                   6.50 usec
TE                  298.2 K
CNST2          145.0000000
CNST13           5.0000000
D0              0.00000300 sec
D1              1.50000000 sec
D2              0.00344828 sec
D6              0.10000000 sec
D16             0.00020000 sec
IN0             0.00002070 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                  11.10 usec
P2                  22.20 usec
PL1                 -4.00 dB
PL1W           34.70265579 W
SFO1           600.1318004 MHz

======== CHANNEL f2 ========
NUC2                  13C
P3                   8.80 usec
PL2                  1.00 dB
PL2W           83.20243835 W
SFO2           150.9148812 MHz

====== GRADIENT CHANNEL =====
GPNAM1            SINE.100
GPNAM2            SINE.100
GPNAM3            SINE.100
GPZ1                50.00 %
GPZ2                30.00 %
GPZ3                40.10 %
P16               1000.00 usec
ND0                     2
TD                    256
SFO1             150.9149 MHz
FIDRES          94.321800 Hz
SW                160.000 ppm
FnMODE                 QF
SI                   1024
SF             600.1299914 MHz
WDW                  SINE
SSB                     0
LB                   0.00 Hz
GB                      0
PC                   1.40
SI                   1024
MC2                    QF
SF             150.9028118 MHz
WDW                  SINE
SSB                     0
LB                   0.00 Hz
GB                      0
```

S17. NOESY spectrum (600MHz, DMSO-*d6*) of compound 3



Mass Spectrum Molecular Formula Report

Analysis Info

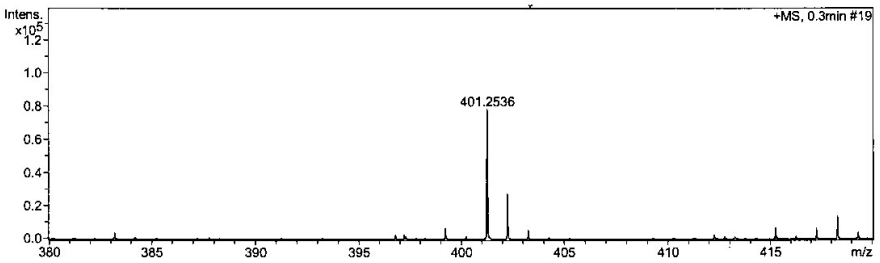
Analysis Name	D:\Data\20110113\YE-43.d	Acquisition Date	1/13/2011 2:01:31 PM
Method	tune low 100-500.m	Operator	Bruker Customer
Sample Name	YE-43	Instrument / Ser#	micrOTOF-Q 125
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Source

Generate Molecular Formula Parameter

Formula, min.	C21H36O7						
Formula, max.							
Measured m/z	401.254	Tolerance	3	ppm	Charge	1	
Check Valence	no	Minimum	0		Maximum	0	
Nitrogen Rule	no	Electron Configuration		both			
Filter H/C Ratio	no	Minimum	0		Maximum	3	
Estimate Carbon	yes						

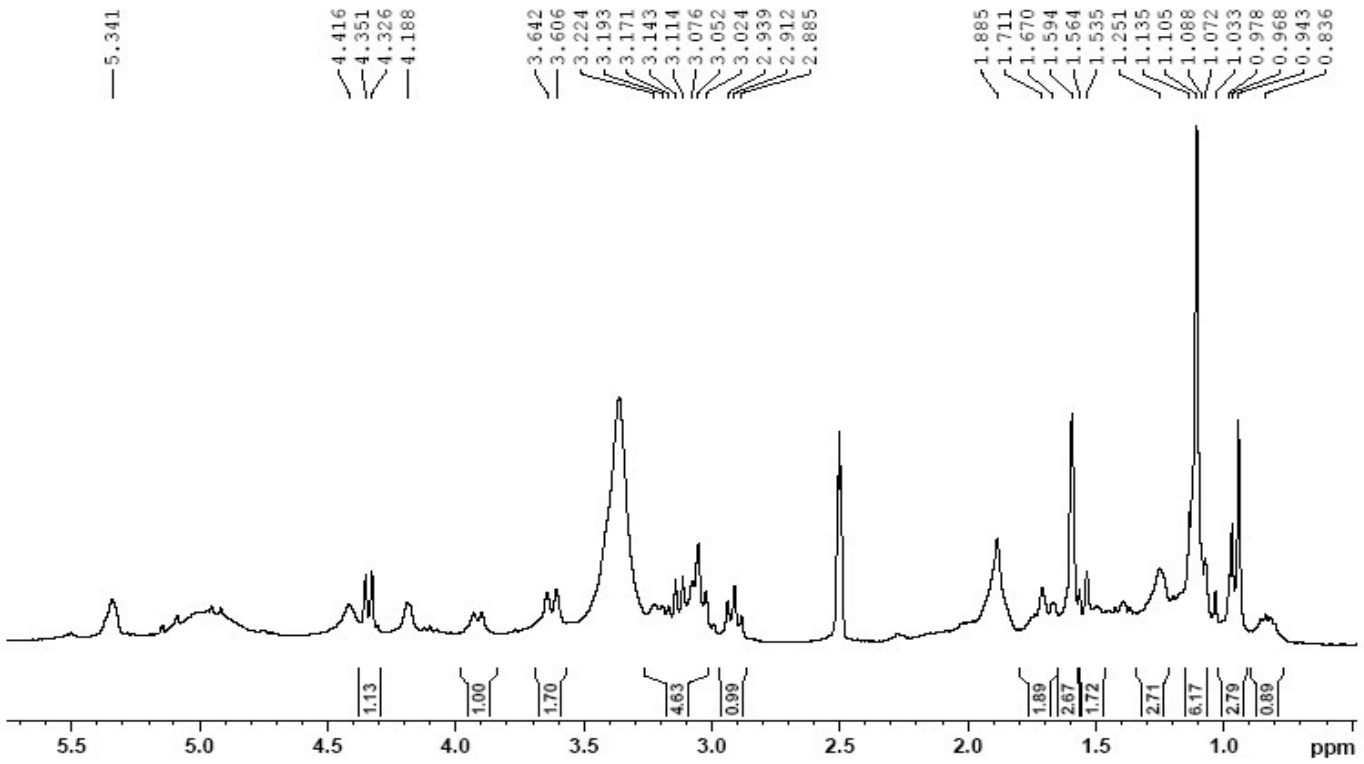


#	m/z	I
1	401.2536	78153

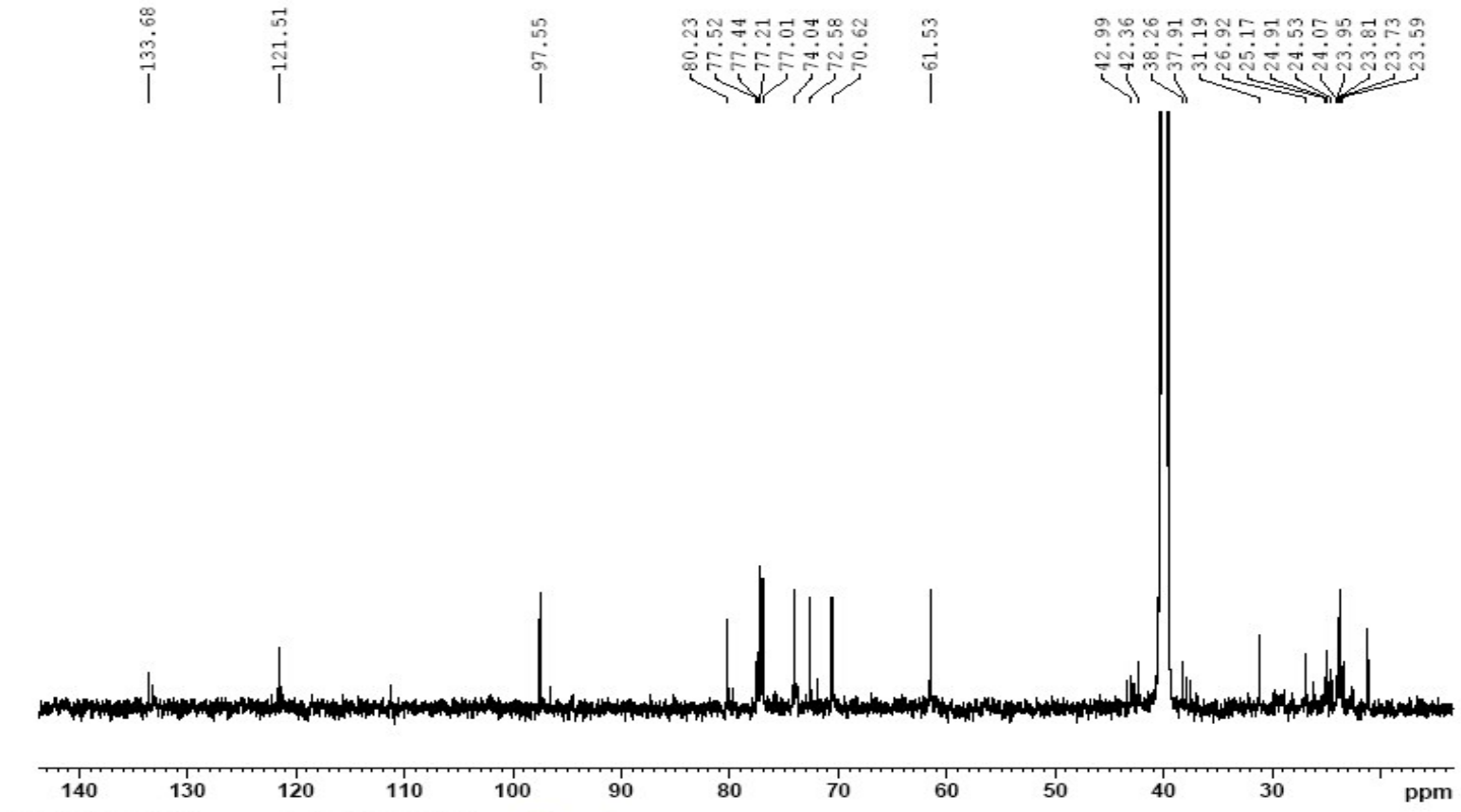
Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	Err [mDa]	rdb	N Rule	e⁻
C 21 H 37 O 7	0.137	401.2534	-0.46	-0.46	-0.18	3.50	ok	even

S18. The HREIMS spectrum of compound 3

S19. ^{1}H NMR spectrum (600MHz, DMSO-*d6*) of compound 4

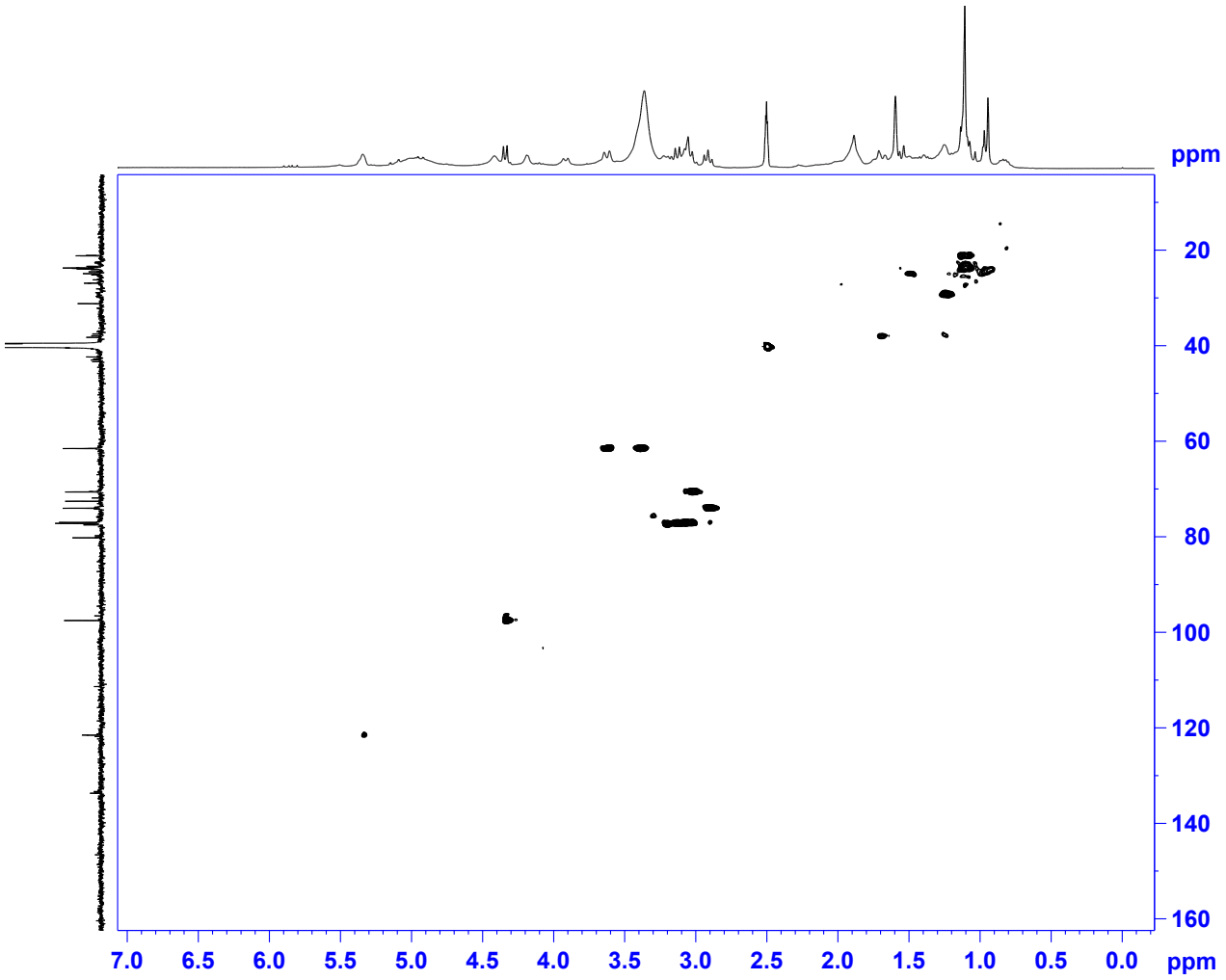


S20. ^{13}C NMR spectrum (150MHz, DMSO-*d6*) of compound 4



S21. HSQC spectrum (600MHz, DMSO-*d6*) of compound 4

AV-600-HSQC
Sample:

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EXPNO                     8
PROCNO                    1
Date_              20170116
Time                  14.59
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG        hsqcetgpsi
TD                     1024
SOLVENT                DMSO
NS                        8
DS                       16
SWH                6009.615 Hz
FIDRES             5.868765 Hz
AQ                 0.0853300 sec
RG                     29100
DW                    83.200 usec
DE                     6.50 usec
TE                    293.9 K
CNST2             145.0000000
D0                 0.00000300 sec
D1                 1.50000000 sec
D4                 0.00172414 sec
D11                0.03000000 sec
D13                0.00000400 sec
D16                0.00020000 sec
D24                0.00110000 sec
IN0                0.00001655 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                      1H
P1                     11.10 usec
P2                     22.20 usec
P28                  2500.00 usec
PL1                    -4.00 dB
PL1W              34.70265579 W
SFO1             600.1324005 MHz

======== CHANNEL f2 ========
CPDPRG2                 garp
NUC2                     13C
P3                      9.53 usec
P4                     19.06 usec
PCPD2                  80.00 usec
PL2                     1.00 dB
PL12                   19.48 dB
PL2W              83.20243835 W
PL12W              1.18069065 W
SFO2             150.9163903 MHz

====== GRADIENT CHANNEL =====
GPNAM1               SINE.100
GPNAM2               SINE.100
GPZ1                    80.00 %
GPZ2                    20.10 %
P16                   1000.00 usec
ND0                        2
TD                       256
SFO1              150.9164 MHz
FIDRES            117.903427 Hz
SW                   200.000 ppm
FnMODE         Echo-Antiecho
SI                      1024
SF               600.1300000 MHz
WDW                    QSINE
SSB                        2
LB                      0.00 Hz
GB                         0
PC                      1.40
SI                      1024
MC2            echo-antiecho
SF                150.9028090 MHz
WDW                    QSINE
SSB                        2
LB                      0.00 Hz
GB                         0
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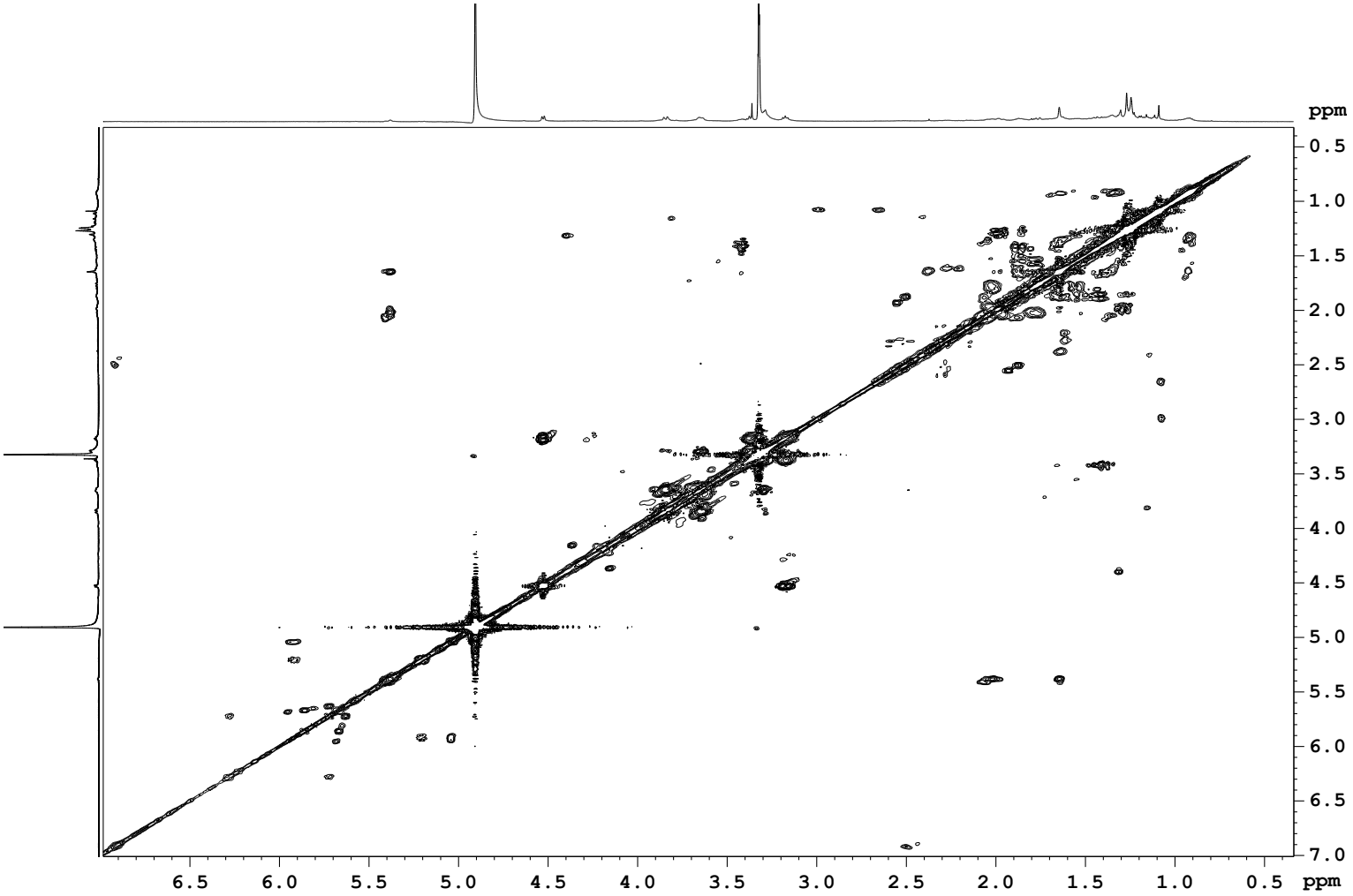
S22. H-H COSY spectrum (600MHz, DMSO-*d6*) of compound 4



Mass Spectrum Molecular Formula Report

Analysis Info

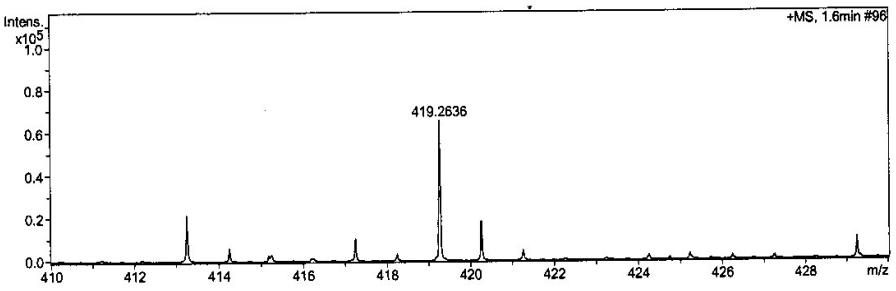
Analysis Name	D:\Data\20110107\YE-10-1.d	Acquisition Date	1/7/2011 3:56:17 PM
Method	tune low 100-500.m	Operator	Bruker Customer
Sample Name	YE-10	Instrument / Ser#	micrOTOF-Q 125
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source

Generate Molecular Formula Parameter

Formula, min.	C21H38O8						
Formula, max.							
Measured m/z	419.264	Tolerance	3	ppm	Charge	1	
Check Valence	no	Minimum	0		Maximum	0	
Nitrogen Rule	no	Electron Configuration		both			
Filter H/C Ratio	no	Minimum	0		Maximum	3	
Estimate Carbon	yes						

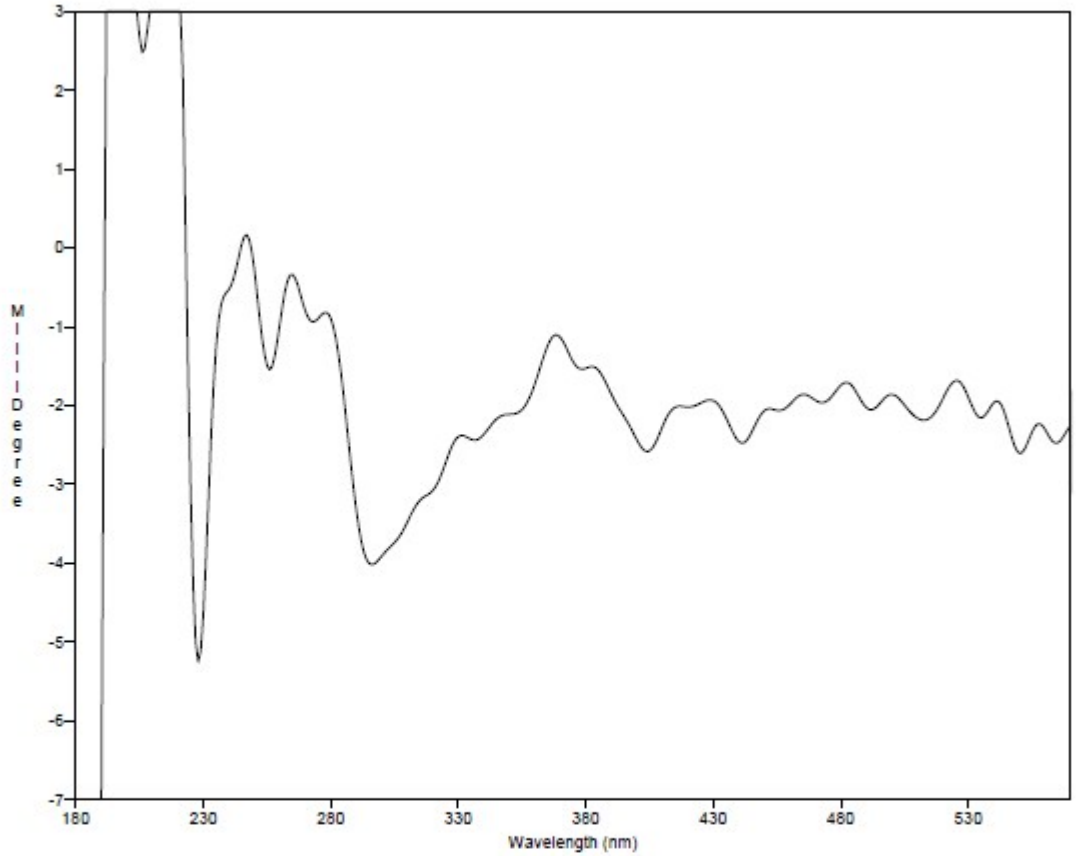


#	m/z	I
1	419.2636	65358

Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	Err [mDa]	rdb	N Rule	e⁻
C 21 H 39 O 8	0.032	419.2639	0.78	3.18	0.33	2.50	ok	even

S23.The HREIMS spectrum of compound 4

S24. $Rh_2(OCOCF_3)_4$-induced CD spectrum of 1a



Bio-Kine Software V4.74 Date : 2016-9-4 Time : 19:11:50

COMMENTS :
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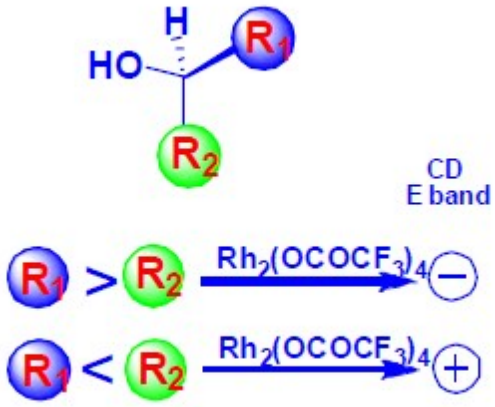
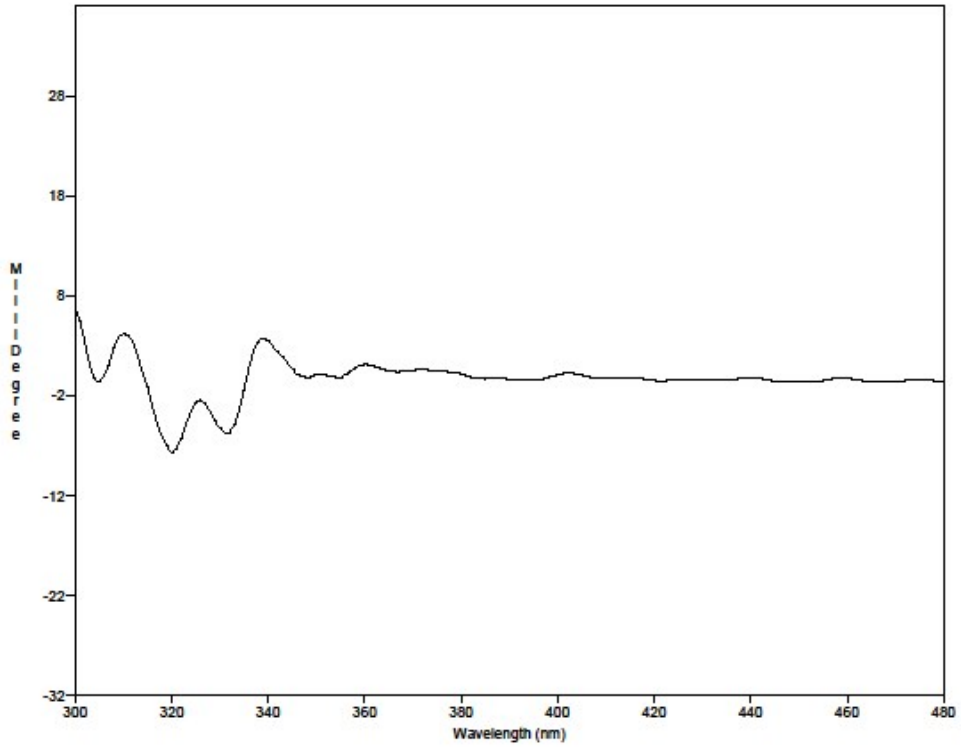


S25. $Rh_2(OCOCF_3)_4$-induced CD spectrum of 5



Bio-Kine Software V4.74 Date : 2016-6-23 Time : 20:18:08

COMMENTS :
File name : d:\高品一\ye5yuan5.bka
MOS-450 Spectrometer
Spectrum measurement
Acq duration = .5 s
Biokine V4.74