SUPPLEMENTARY INFORMATION

Artemselenoids A–H, eight guaiane-type sesquiterpenoid dimers from *Artemisia selengensis* and their antihepatoma activities

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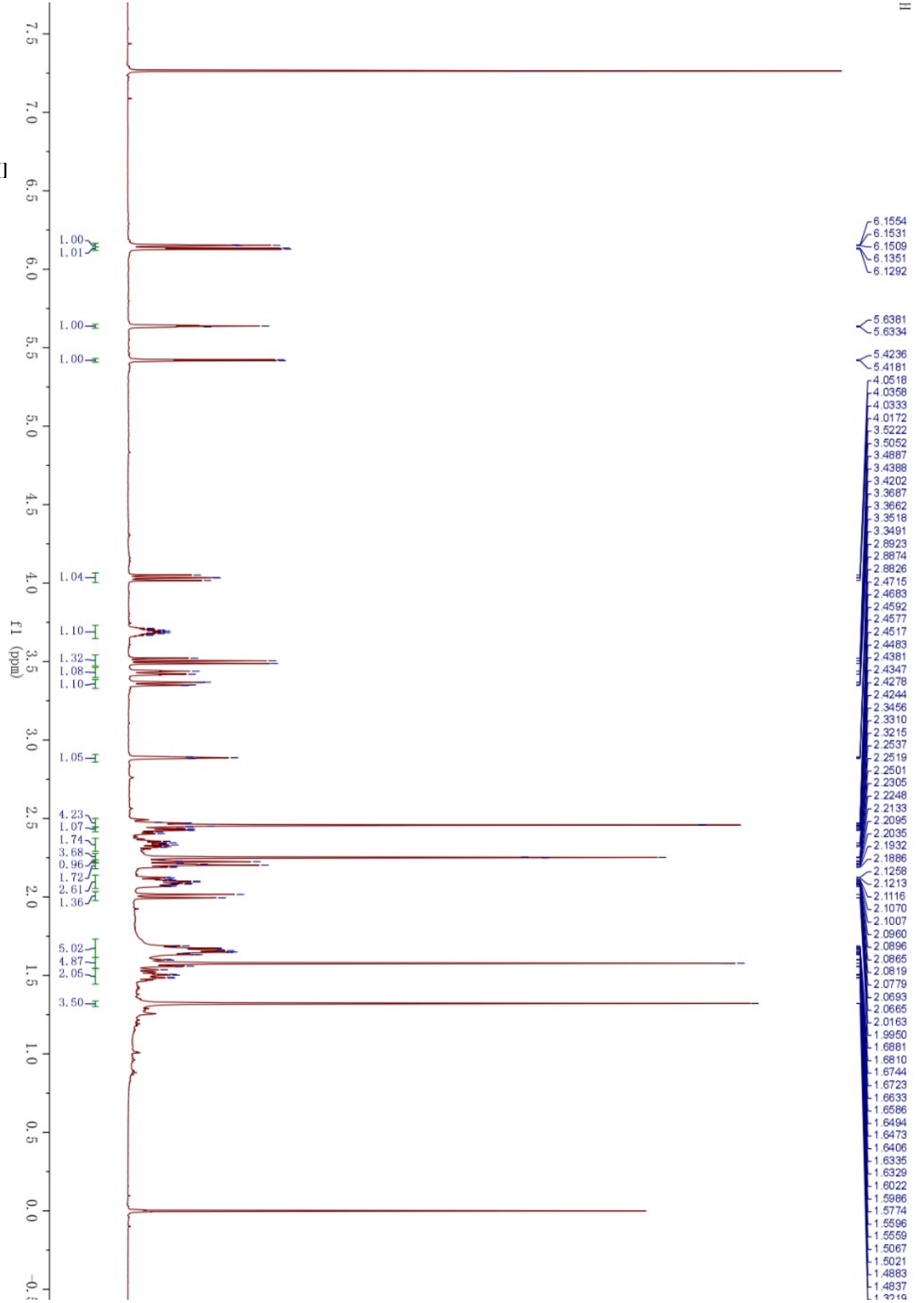
General Experimental Instruments and Procedures

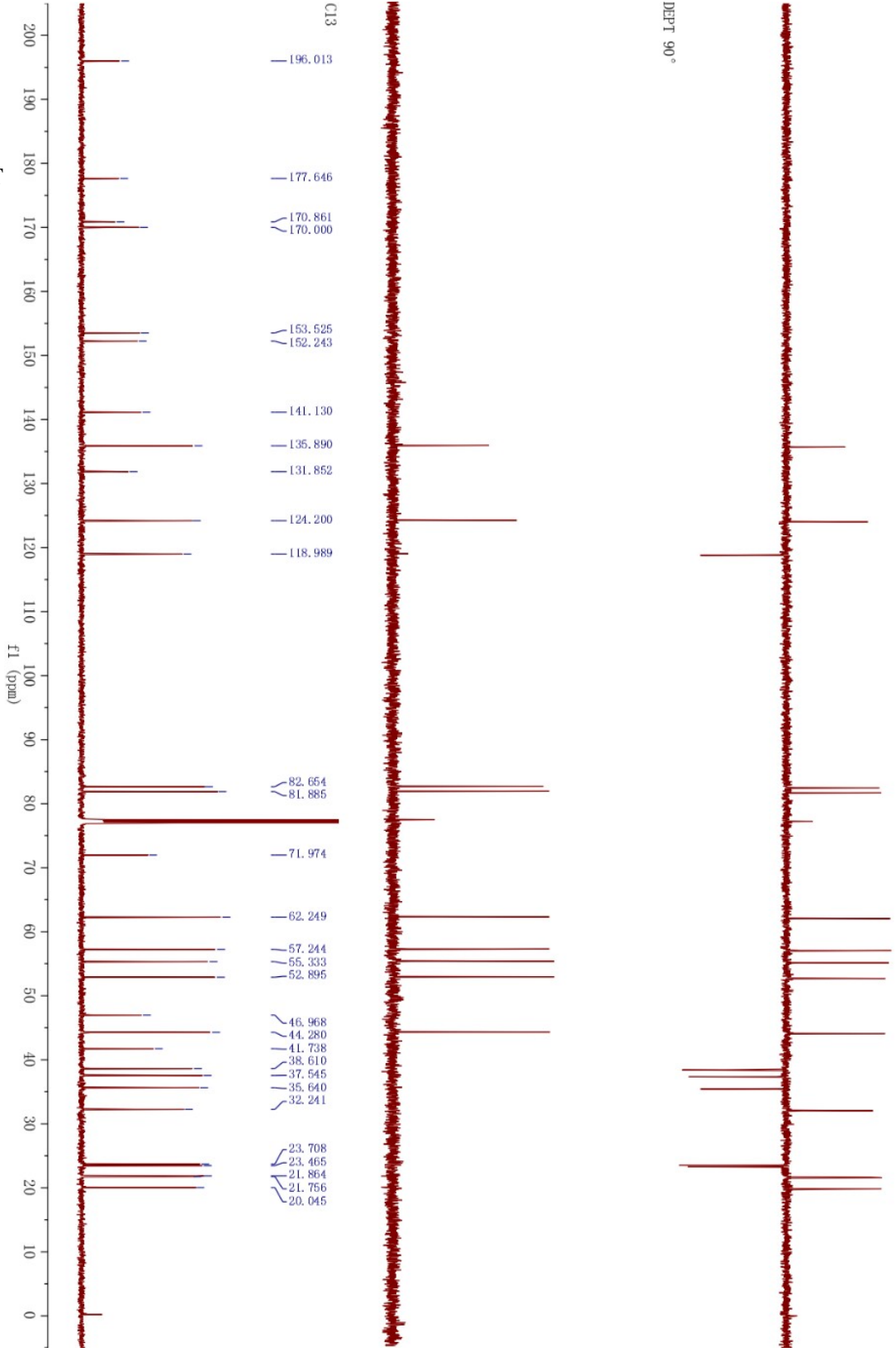
High-resolution mass spectra were acquired using a Shimadzu LC/MS-IT-TOF system (Kyoto, Japan). UV absorption profiles were recorded on a Shimadzu UV2401PC spectrophotometer (Kyoto, Japan), while IR spectra (KBr pellets) were collected via a Bio-Rad FTS-135 spectrometer (CA, USA). Nuclear magnetic resonance (NMR) data were analyzed with a Bruker Advance III-600 spectrometer (Germany, 600 MHz) using TMS as the internal standard. Optical rotations were quantified with a JASCO P-1020 polarimeter (Tokyo, Japan). Electronic circular dichroism (ECD) spectra were captured on an Applied Photophysics dichromatograph (UK). Thin-layer chromatography (TLC) was conducted using silica gel GF254 plates sourced from Yantai Jiangyou Silicon Development Company (Yantai, China). The spots were visualized under UV light or by heating after being sprayed with a 10% H_2SO_4 solution in ethanol (*v*/*v*). For column chromatography, 200–300 mesh silica gel (Linyi Haixiang, Linyi, China), and Sephadex LH-20 (GE Healthcare Bio-Sciences AB, Uppsala, Sweden) were employed. High-performance liquid chromatography (HPLC) was performed on a Shimadzu LC-20AT system equipped with Shim-pack GIST-C18 (5 μm, 9.4 × 250 mm) columns and a CXTH-LC-3000 system fitted with Agilent XDB-C18 (5 μm, 9.4 × 250 mm) columns.

The human hepatocellular carcinoma cell lines HepG2, Huh7, and SK-Hep-1 were purchased from Shanghai Jining Biotechnology Co., Ltd (Shanghai, China) and cultured in a CO_2 incubator (Model 3111, Thermo Fisher Scientific Co., Ltd., Suzhou, China) at 37°C with 5% CO_2, 95% air, and >95% humidity. HepG2 and SK-Hep-1 cells were maintained in Minimum Essential Medium (MEM, Cat# C3050-0500, VivaCell, Shanghai, China) supplemented with 10% (*v*/*v*) heat-inactivated fetal bovine serum (FBS, Gibco, Life Technologies, NY, USA), while Huh7 cells were cultured in Dulbecco's Modified Eagle Medium (DMEM, Cat# C3112-0500, VivaCell, Shanghai, China) with 10% (*v*/*v*) heat-inactivated FBS. Sorafenib (purity >99% by HPLC, Aladdin Biotechnology Co., Ltd., Shanghai, China) was used as the positive control. Cell viability was assessed using the MTT colorimetric assay (Cat# M1020, BioFROXX, Saiguo Biotech Co., Ltd., Guangzhou, China), and absorbance was measured at 490 nm using a Varioskan Lux multimode microplate reader (Thermo Fisher Scientific Co., Ltd., Suzhou, China).

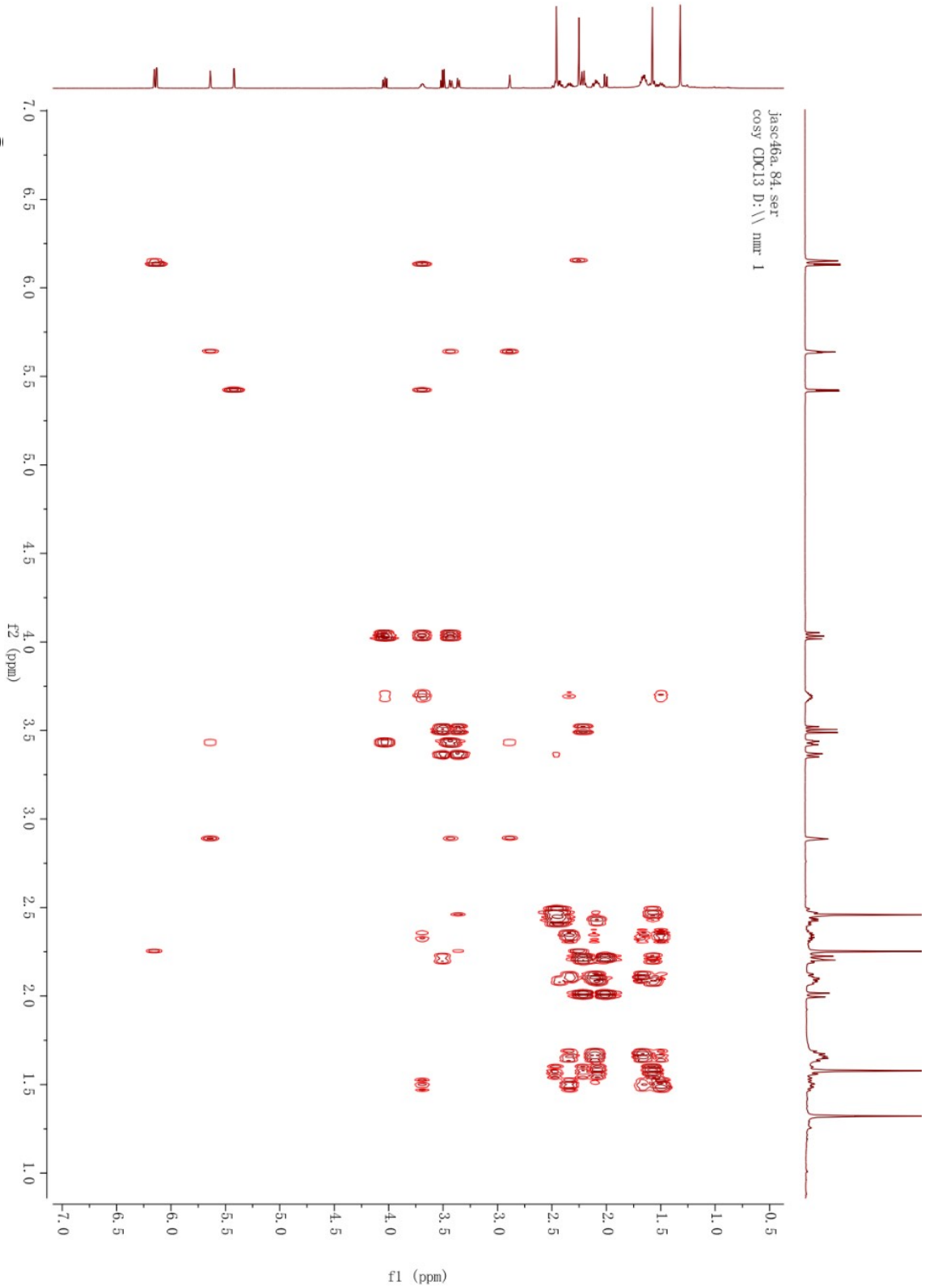
S1. ^{1}H NMR (600 M]



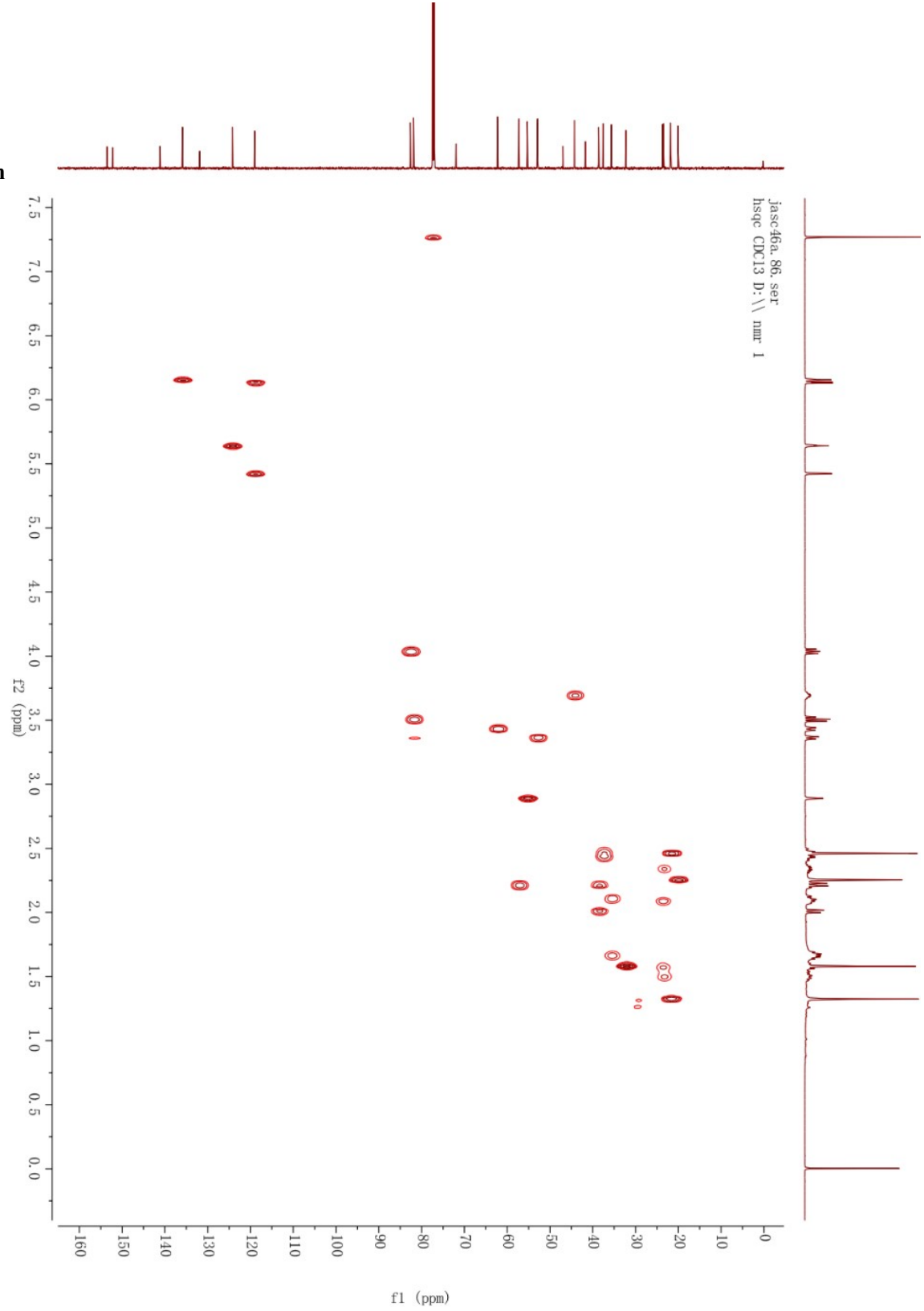
S2. ^{13}C NMR (DEPT



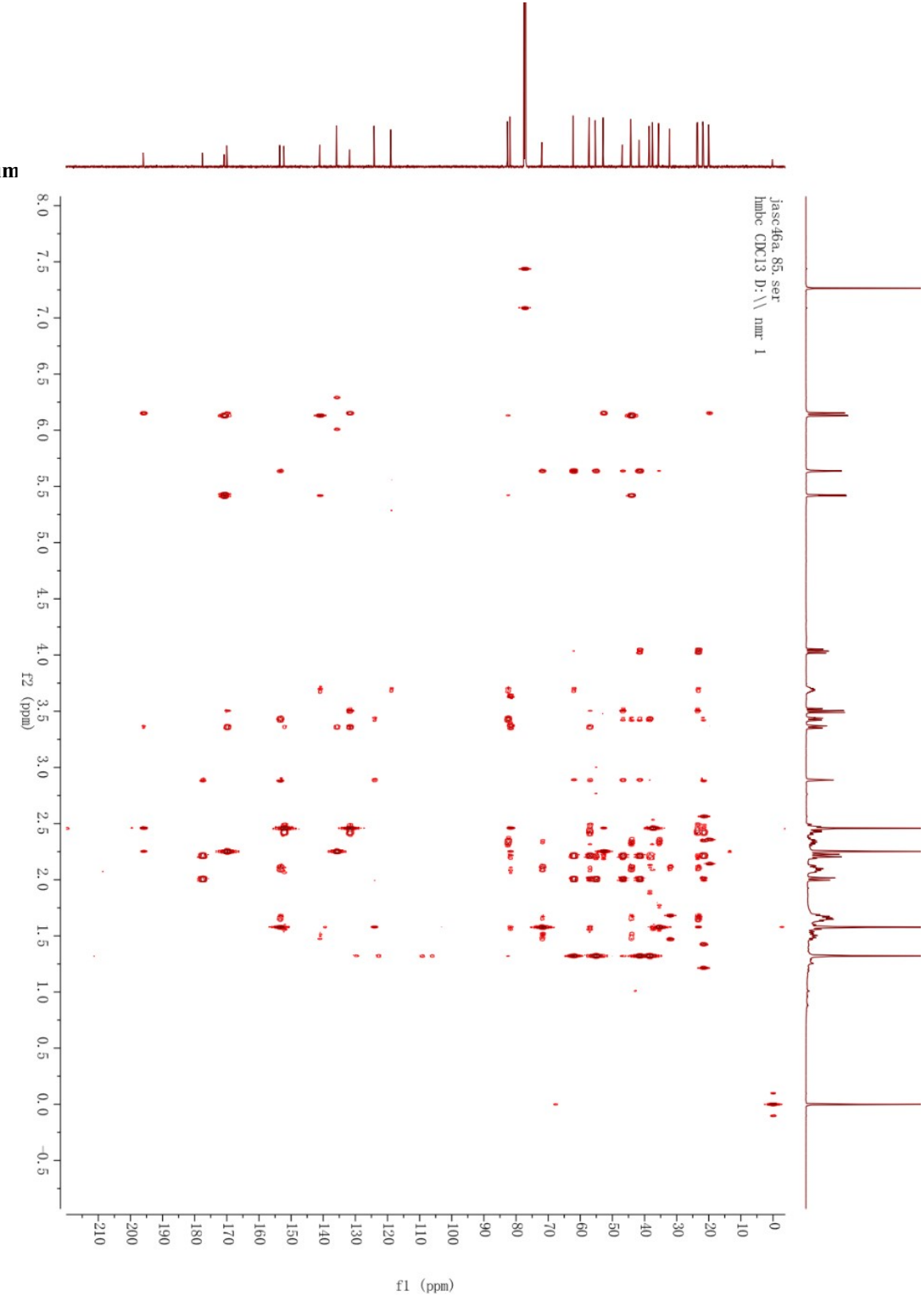
S3. ^{1}H-^{1}H COSY (60



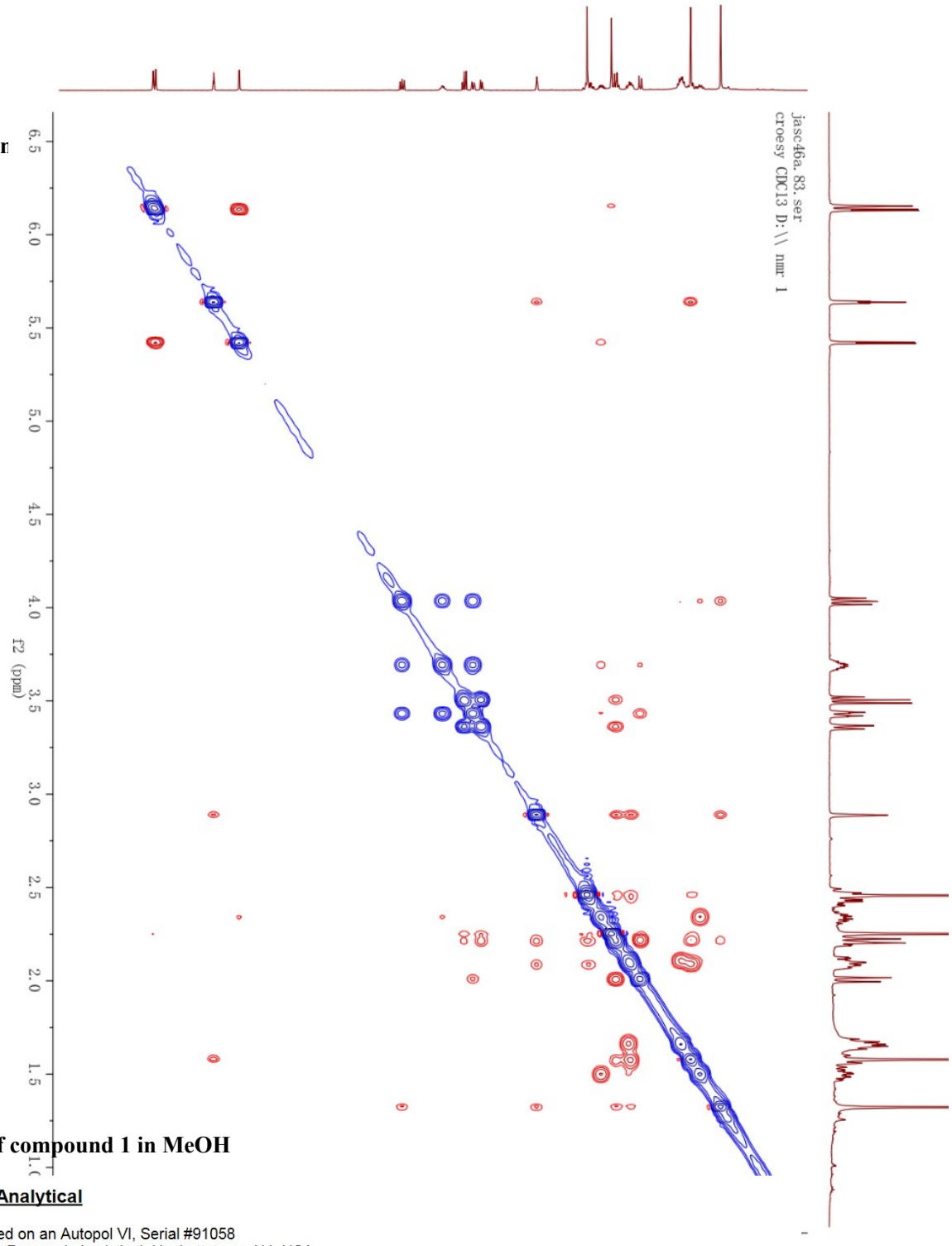
S4. HSQC spectrum



S5. HMBC spectrum



S6. ROESY spectrum



S7. $[\alpha]_D$ spectrum of compound 1 in MeOH

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Wednesday, 11-DEC-2024

Set Temperature : 20.0

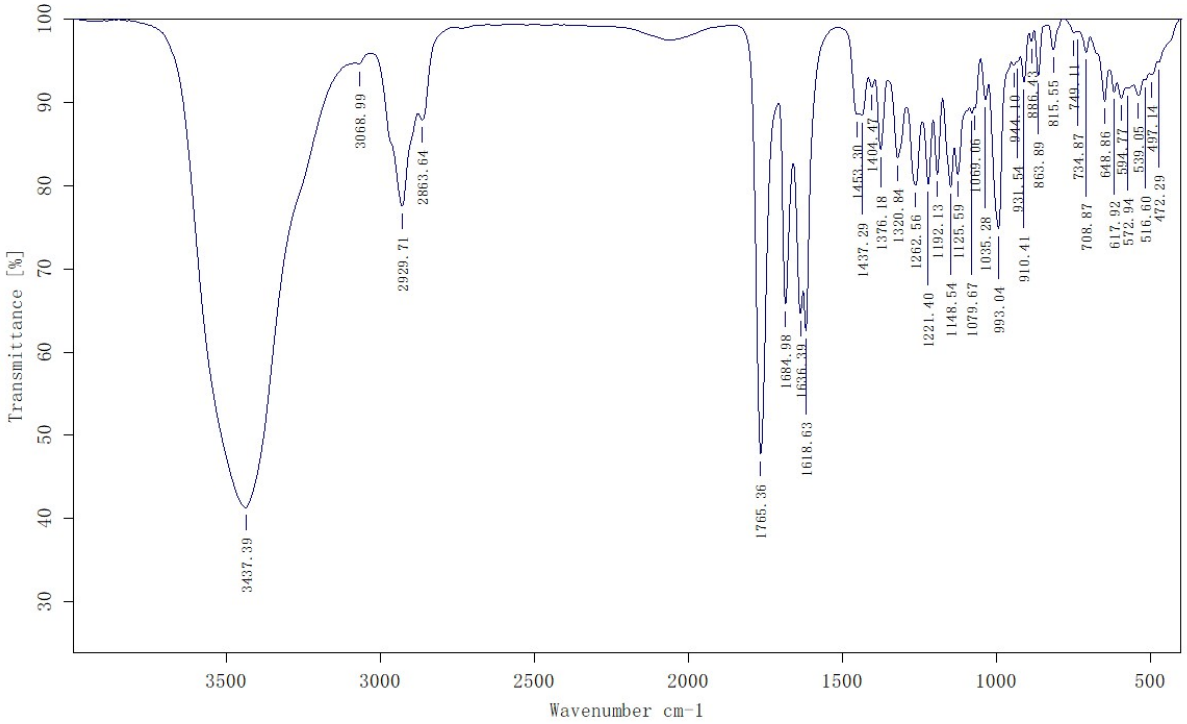
Time Delay : Disabled

Delay between Measurement : Disabled

n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	-104.86	0.42	-0.40	-104.67	-105.61

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	JASC-46	02:45:39 PM	-104.67	SR	-0.112	589	100.00	0.107	20.0
2	JASC-46	02:45:46 PM	-105.61	SR	-0.113	589	100.00	0.107	20.0
3	JASC-46	02:45:52 PM	-104.67	SR	-0.112	589	100.00	0.107	20.0
4	JASC-46	02:45:58 PM	-104.67	SR	-0.112	589	100.00	0.107	20.0
5	JASC-46	02:46:05 PM	-104.67	SR	-0.112	589	100.00	0.107	20.0

S8. IR spectrum of compound 1

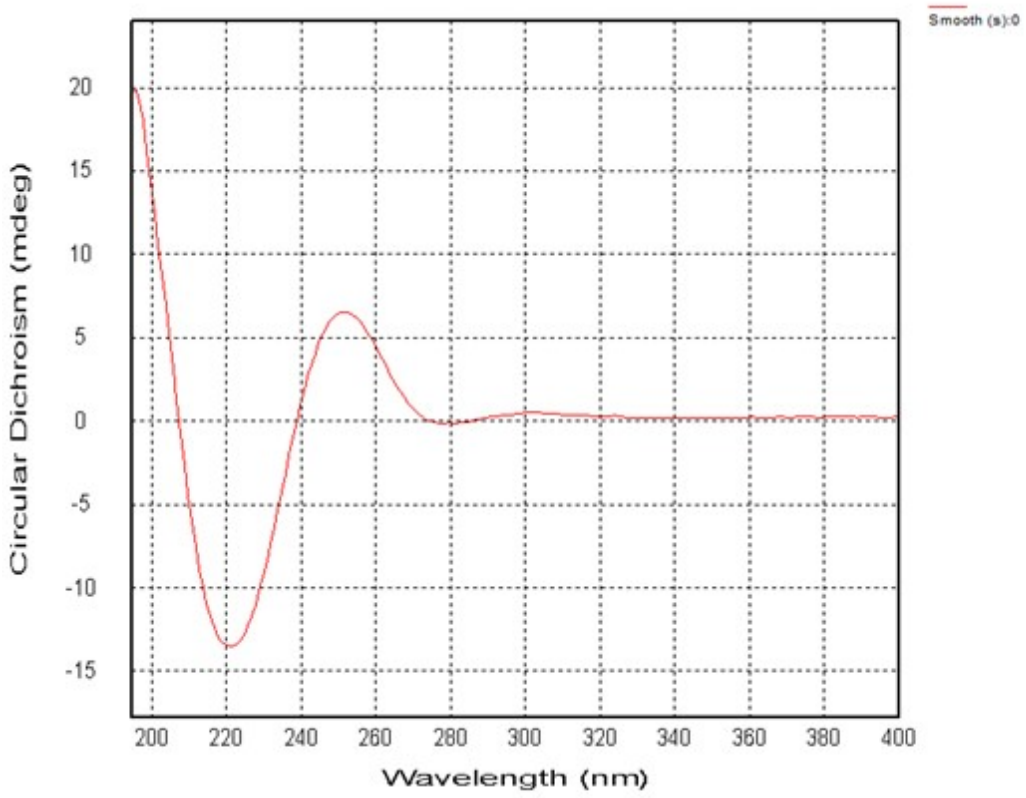


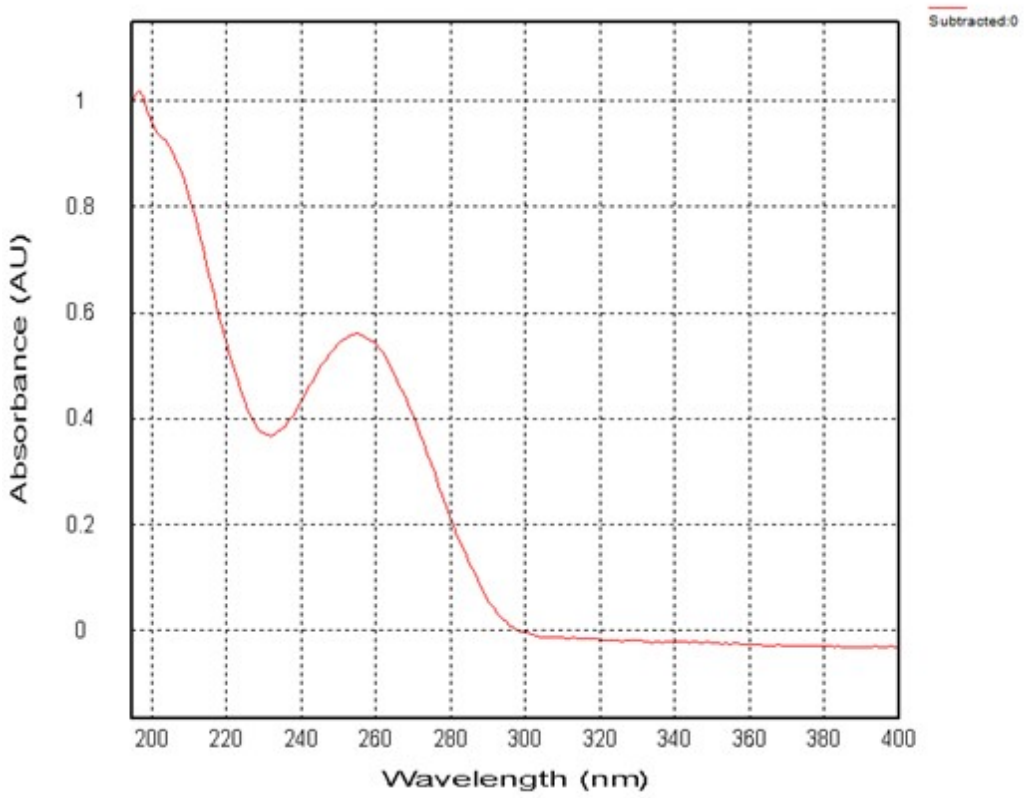
Sample Name: jasc-46I
Sample Form: KBr
Path of File: E:\data
Date of Measurement: 2025/1/2

Resolution: 4
Aperture Setting: 6 mm
Number of Background Scans: 16
Number of Sample Scans: 16

Beamsplitter Setting: KBr
Source Setting: MIR
Instrument Type: BRUKER VERTEX 70
Soft Version: OPUS8.1

S9. ECD and UV spectra of compound 1



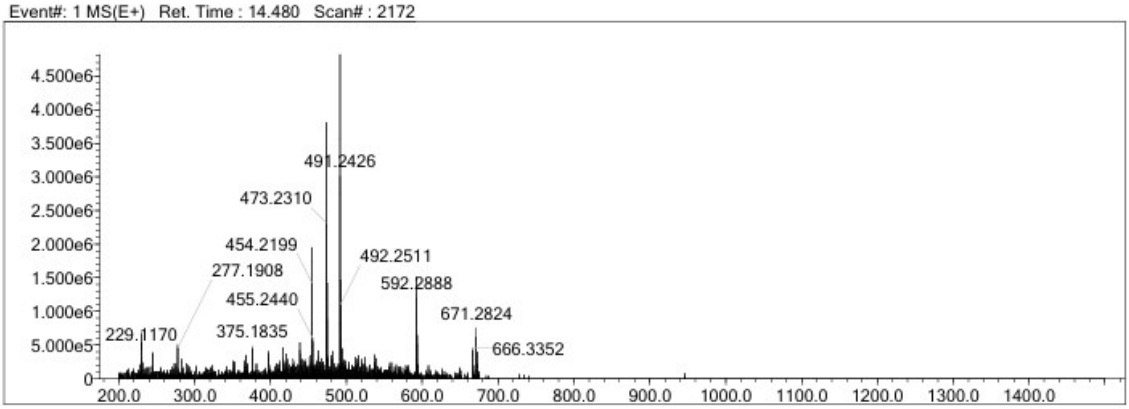


S10. HRESIMS of compound 1

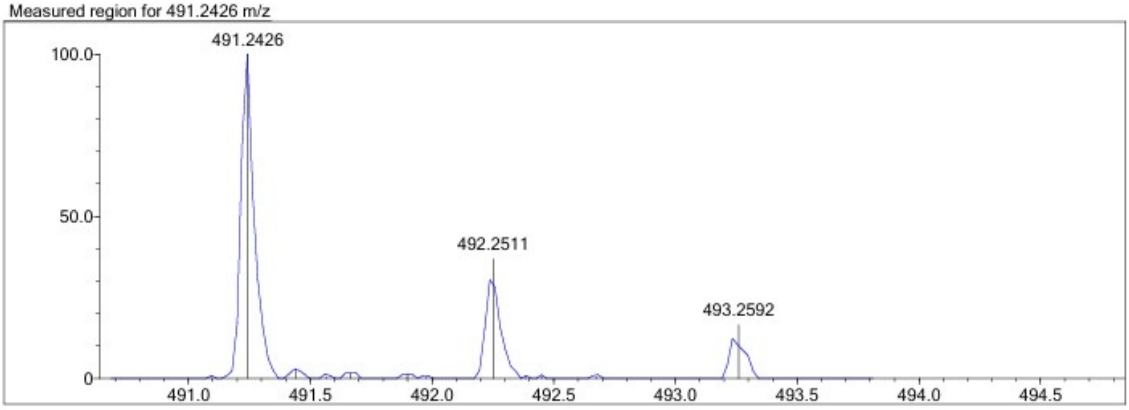
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	300	O	2	0	20	H
C	4	0	150	Cl	1	0	0	Na
N	3	0	1					

Error Margin (ppm):	100	DBE Range:	-2.0 - 1000.0	Electron Ions:	both
HC Ratio:	unlimited	Apply N Rule:	yes	Use MSn Info:	no
Max Isotopes:	all	Isotope RI (%):	1.00	Isotope Res:	10000
MSn Iso RI (%):	75.00	MSn Logic Mode:	AND	Max Results:	500

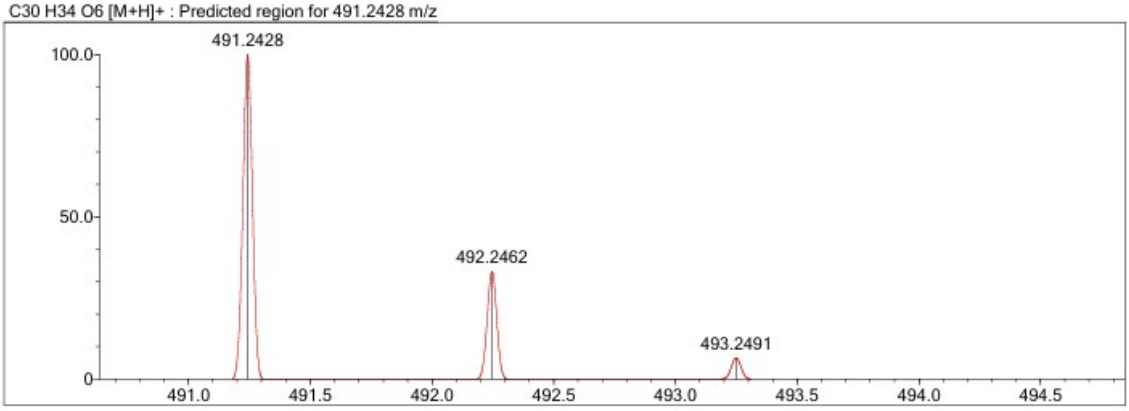
Event#: 1 MS(E+) Ret. Time : 14.480 Scan# : 2172



Measured region for 491.2426 m/z

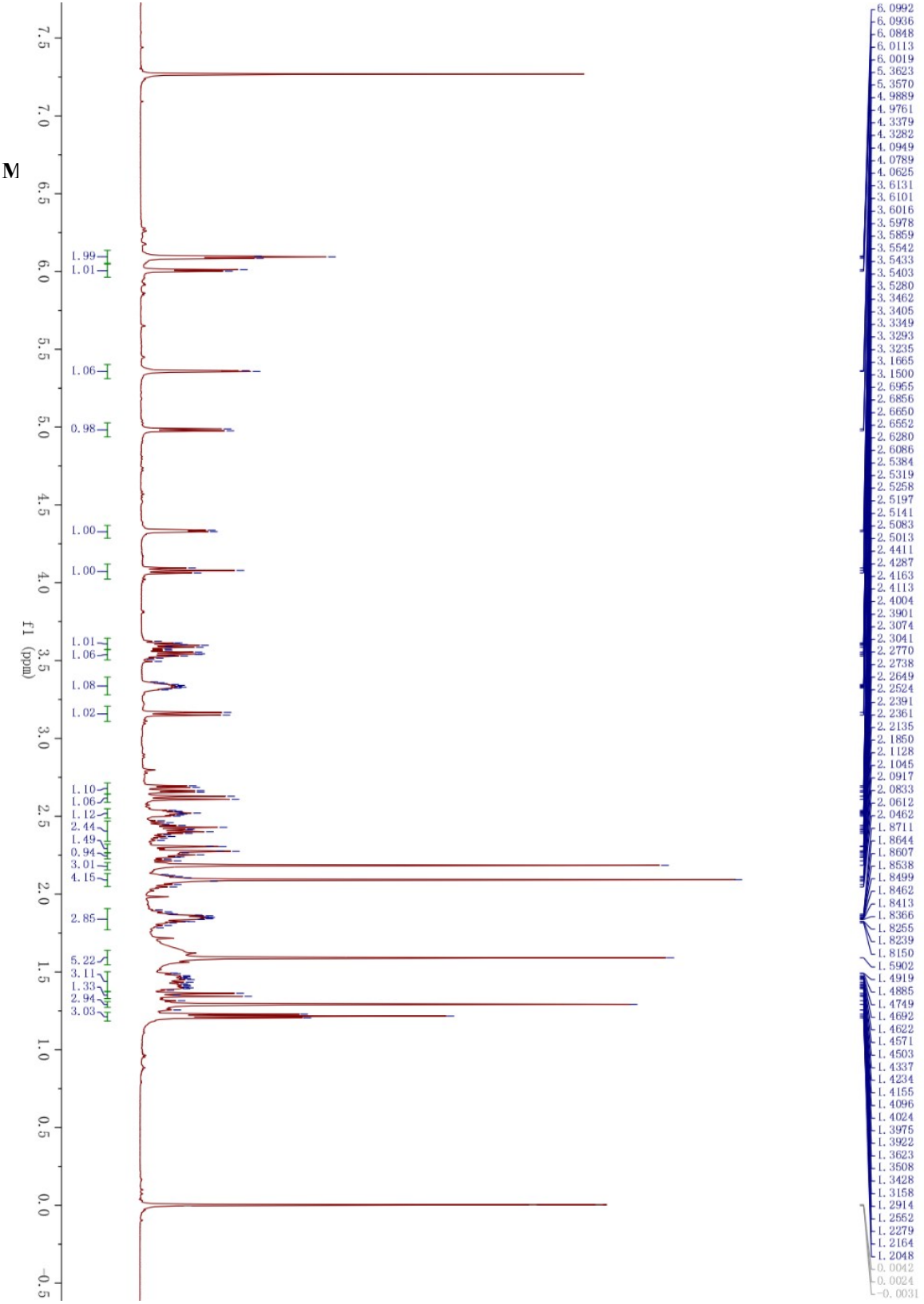


C30 H34 O6 [M+H]+ : Predicted region for 491.2428 m/z

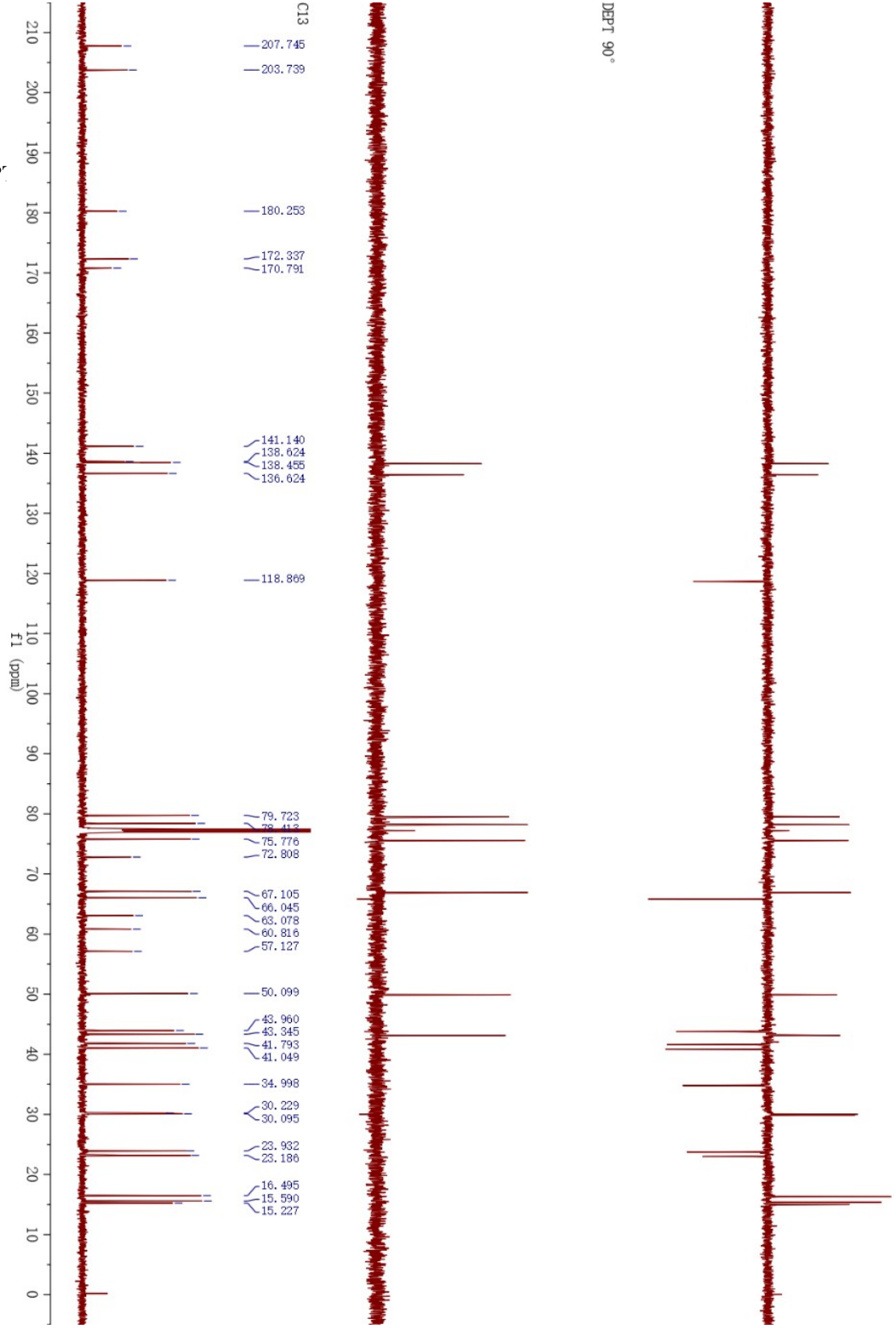


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	62.00	C30 H34 O6	[M+H]+	491.2426	491.2428	-0.2	-0.41	62.00	14.0

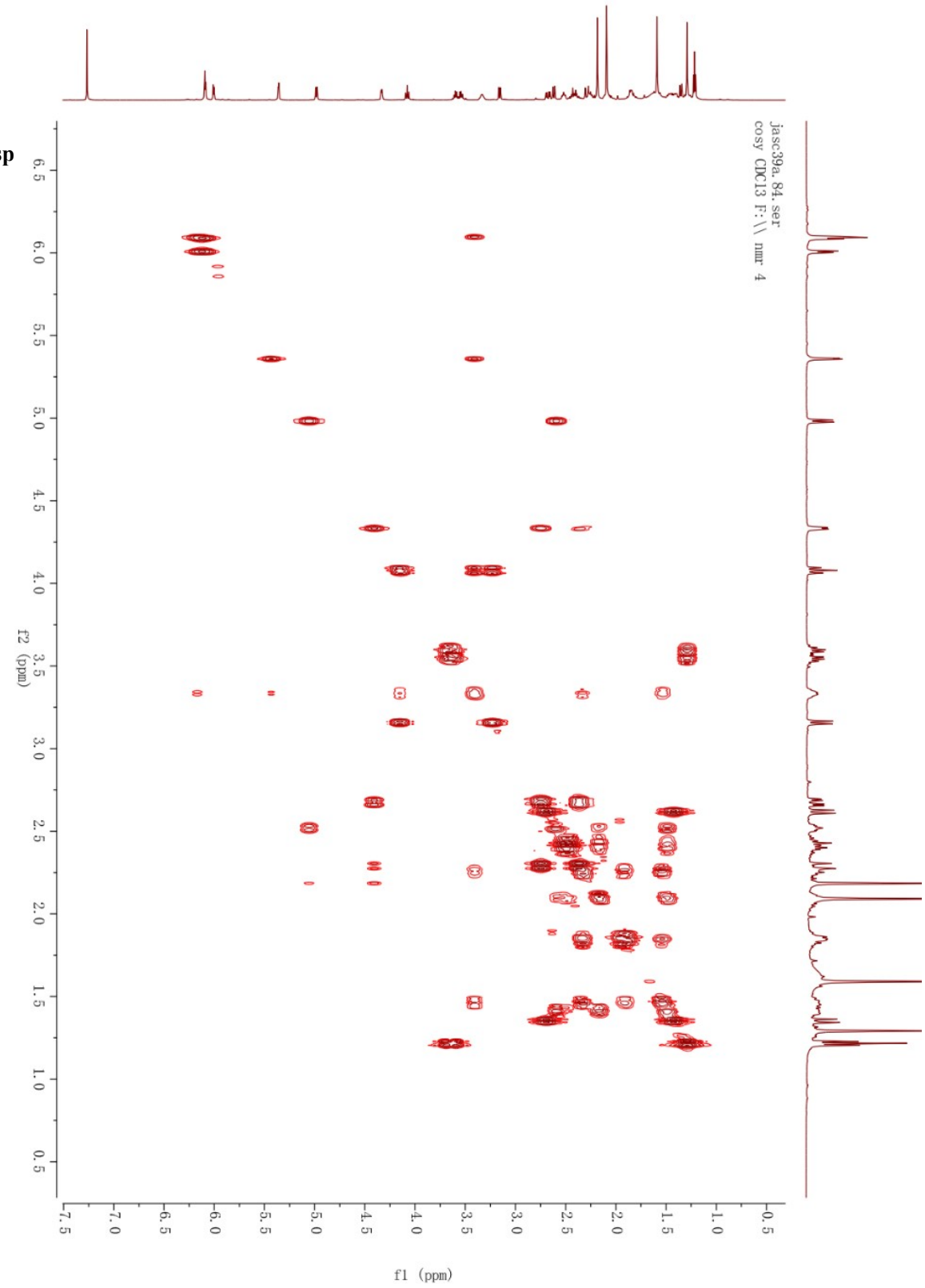
S11. ^{1}H NMR (600 M



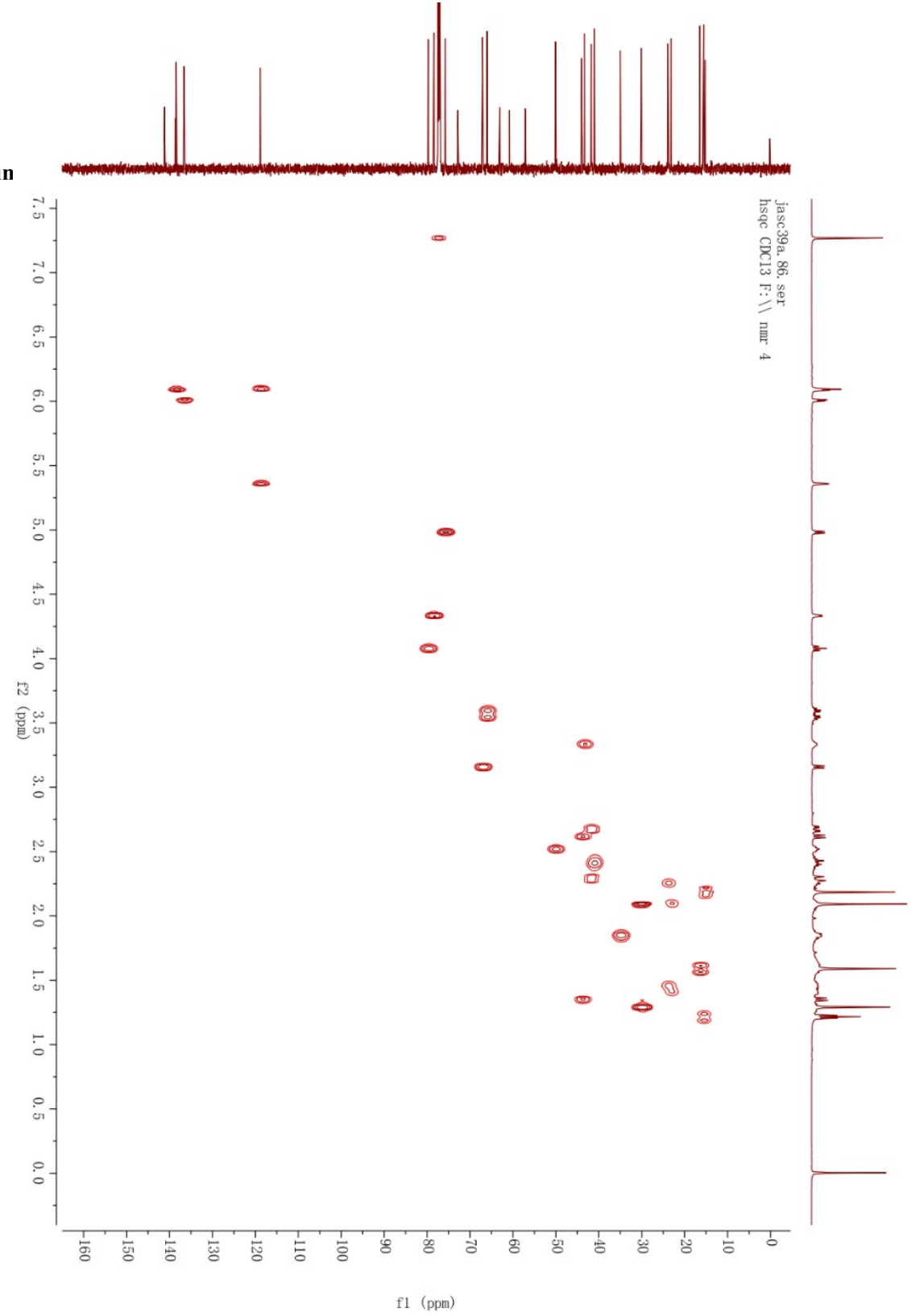
S12. ^{13}C NMR (DEP



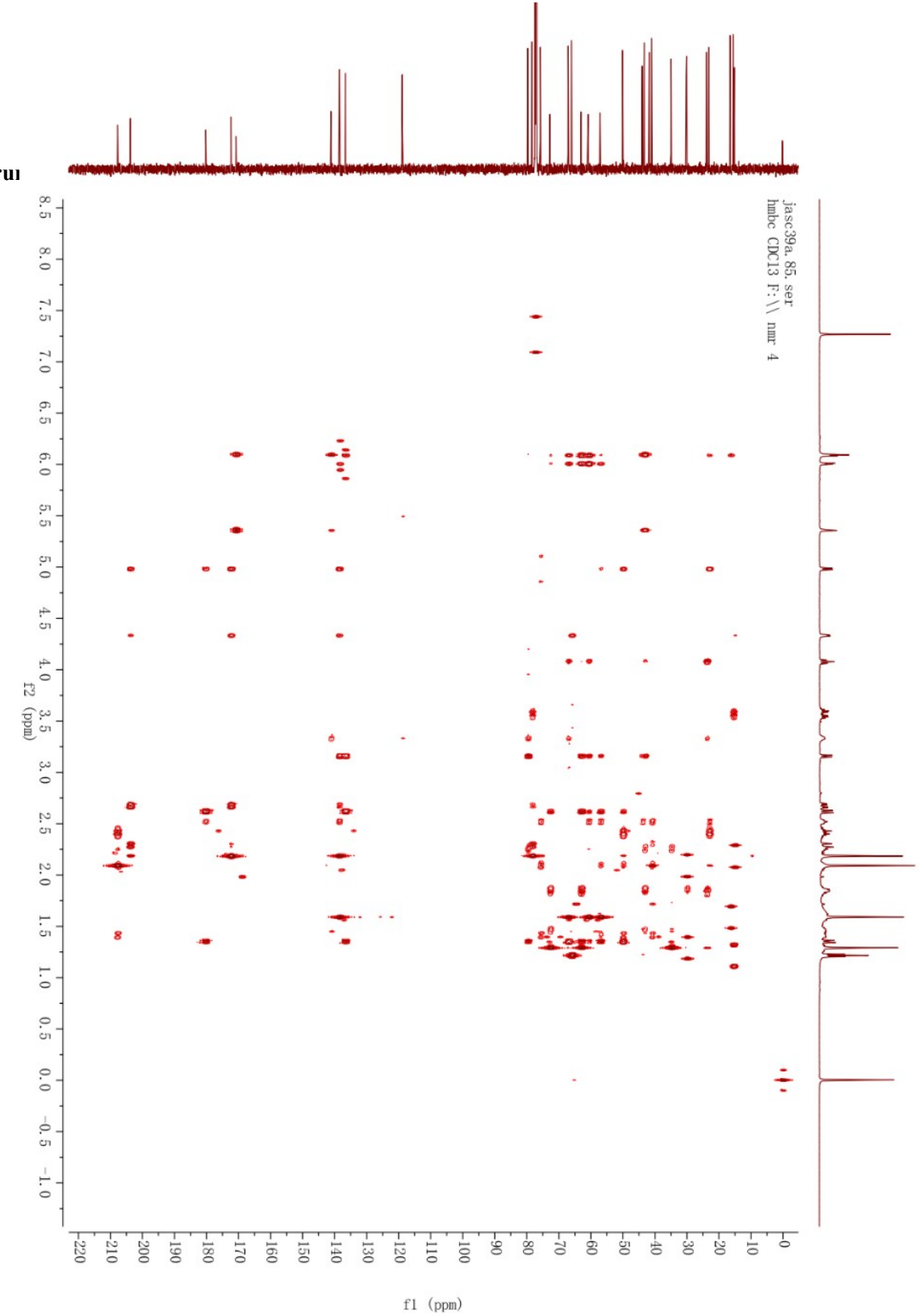
S13. ^{1}H-^{1}H COSY sp



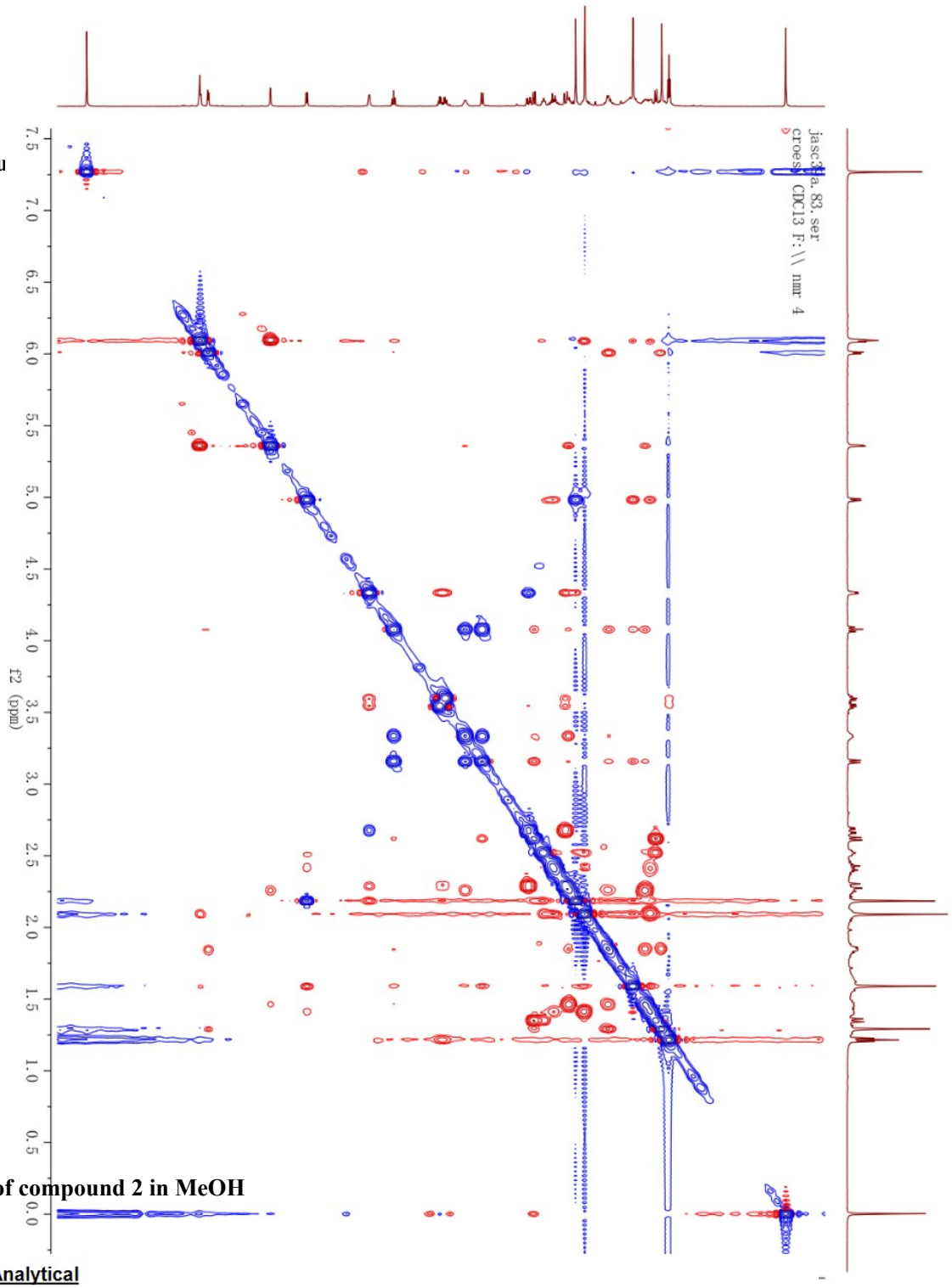
S14. HSQC spectrun



S15. HMBC spectrum



S16. ROESY spectru



S17. $[\alpha]_D$ spectrum of compound 2 in MeOH

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Wednesday, 11-DEC-2024

Set Temperature : 20.0

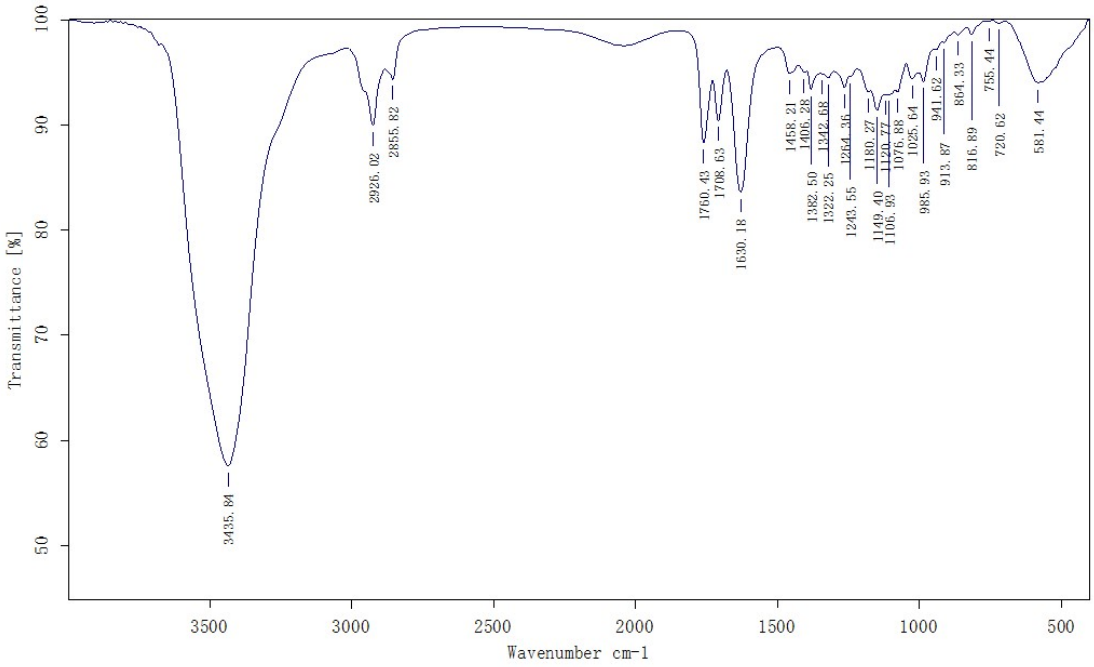
Time Delay : Disabled

Delay between Measurement : Disabled

n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	-23.36	0.42	-1.79	-22.90	-23.66

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	JASC-39	03:35:24 PM	-23.66	SR	-0.031	589	100.00	0.131	20.0
2	JASC-39	03:35:30 PM	-22.90	SR	-0.030	589	100.00	0.131	20.0
3	JASC-39	03:35:37 PM	-23.66	SR	-0.031	589	100.00	0.131	20.0
4	JASC-39	03:35:43 PM	-22.90	SR	-0.030	589	100.00	0.131	20.0
5	JASC-39	03:35:50 PM	-23.66	SR	-0.031	589	100.00	0.131	20.0

S18. IR spectrum of compound 2

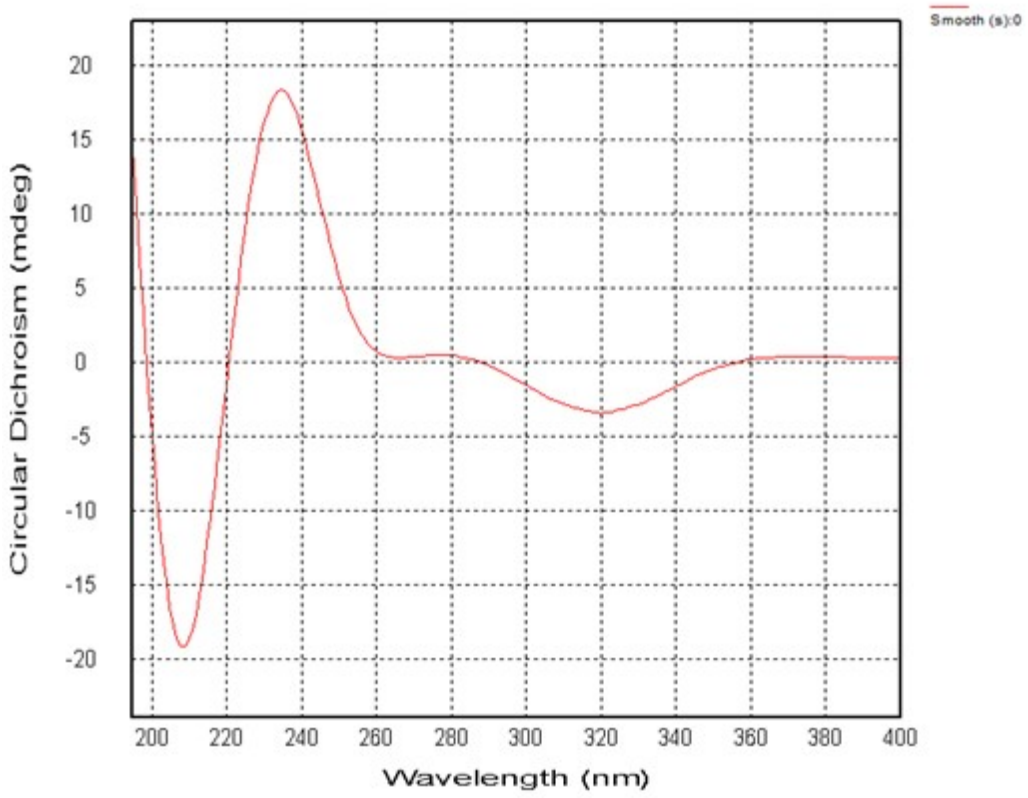


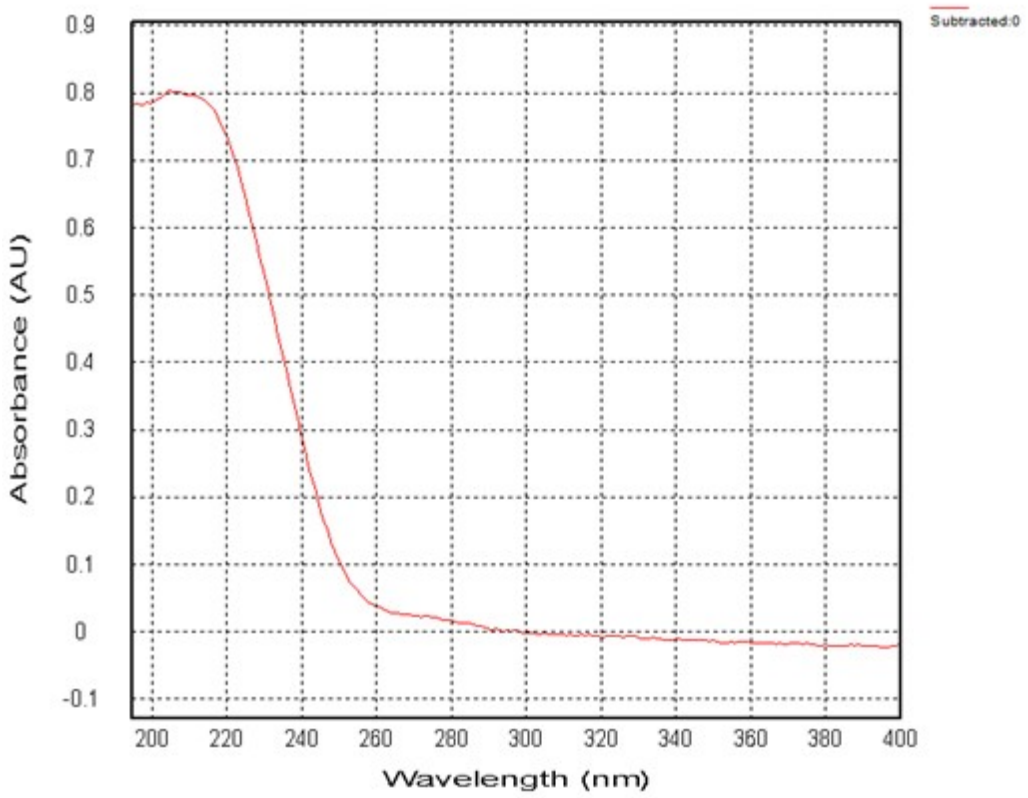
Sample Name: jasc-39
Sample Form: KBr
Path of File: E:\data
Date of Measurement: 2024/12/31

Resolution: 4
Aperture Setting: 6 mm
Number of Background Scans: 16
Number of Sample Scans: 16

Beamsplitter Setting: KBr
Source Setting: MIR
Instrument Type: BRUKER VERTEX 70
Soft Version: OPUS8.1

S19. ECD and UV spectra of compound 2





S20. HRESIMS of compound 2

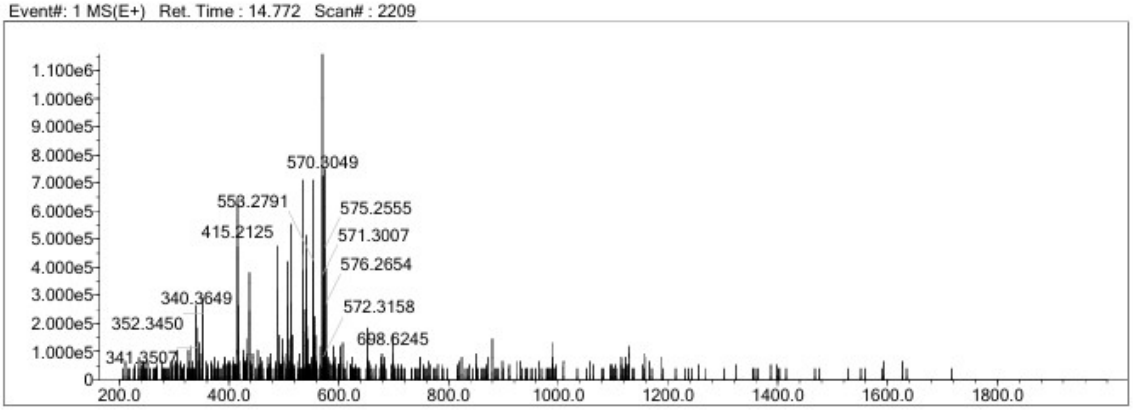
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	300	O	2	0	20	H
C	4	0	150	Cl	1	0	0	Na
N	3	0	1					

Error Margin (ppm): 100
HC Ratio: unlimited
Max Isotopes: all
MSn Iso RI (%): 75.00

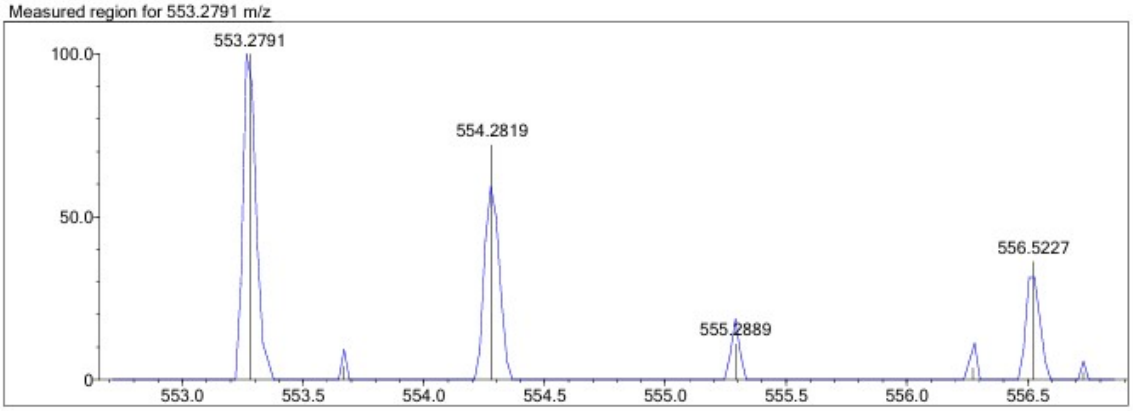
DBE Range: -2.0 - 1000.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

Electron Ions: both
Use MSn Info: no
Isotope Res: 10000
Max Results: 500

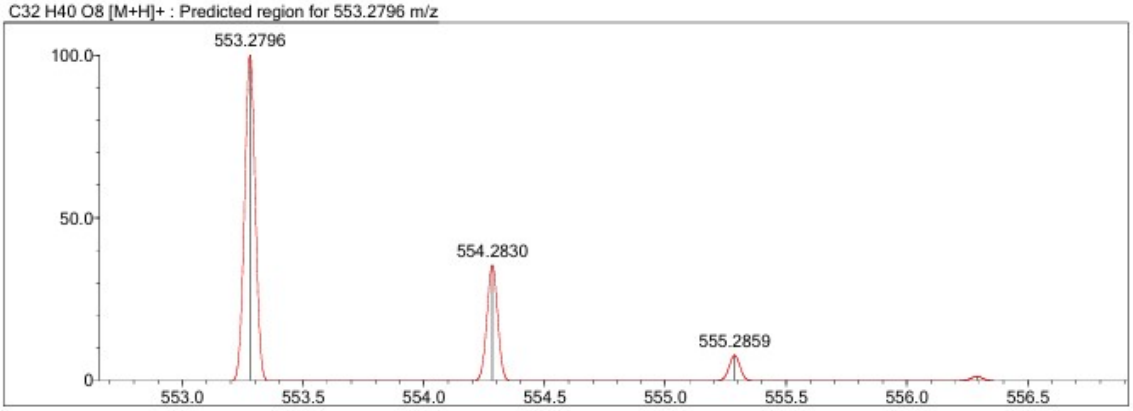
Event#: 1 MS(E+) Ret. Time : 14.772 Scan# : 2209



Measured region for 553.2791 m/z

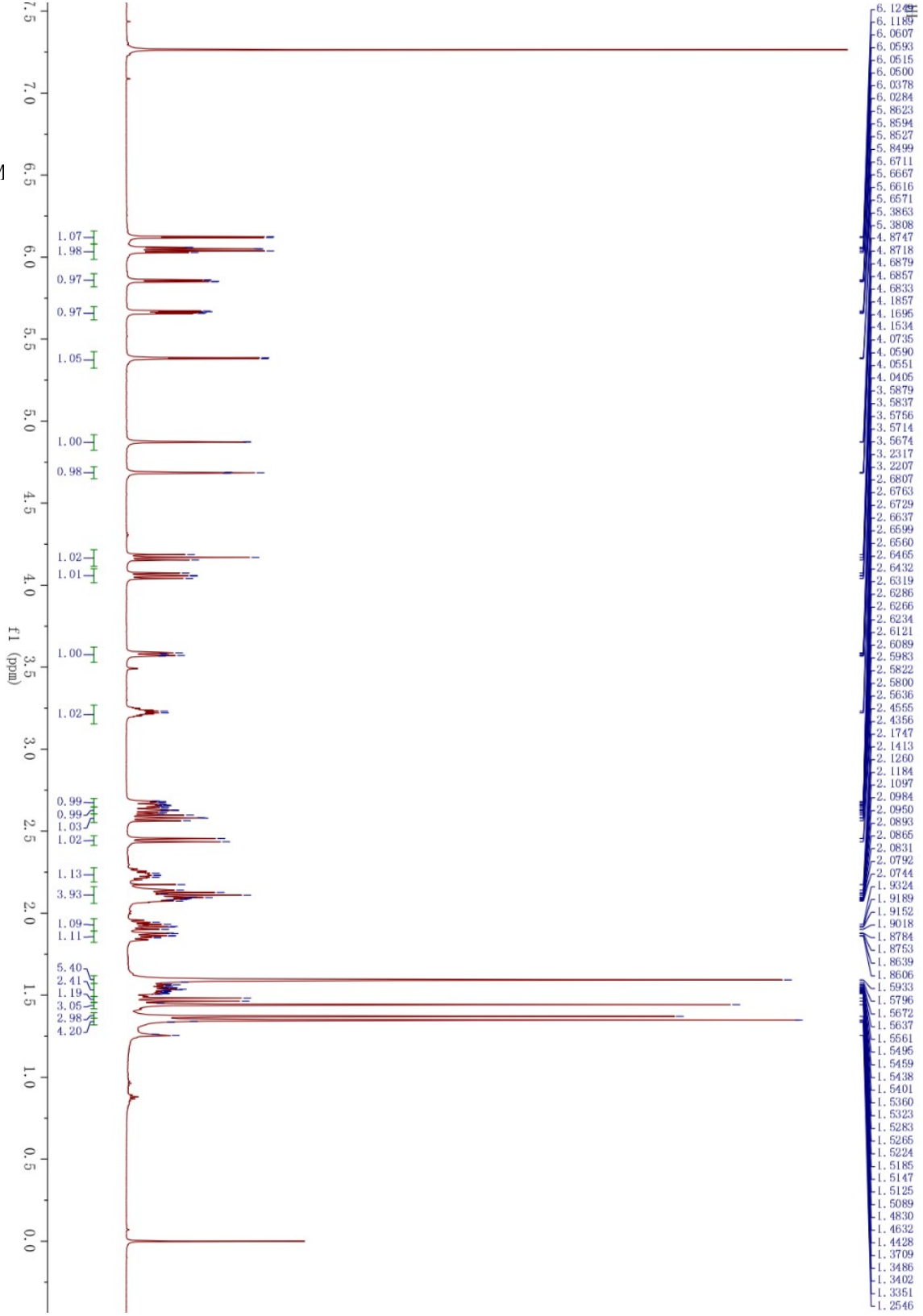


C32 H40 O8 [M+H]+ : Predicted region for 553.2796 m/z

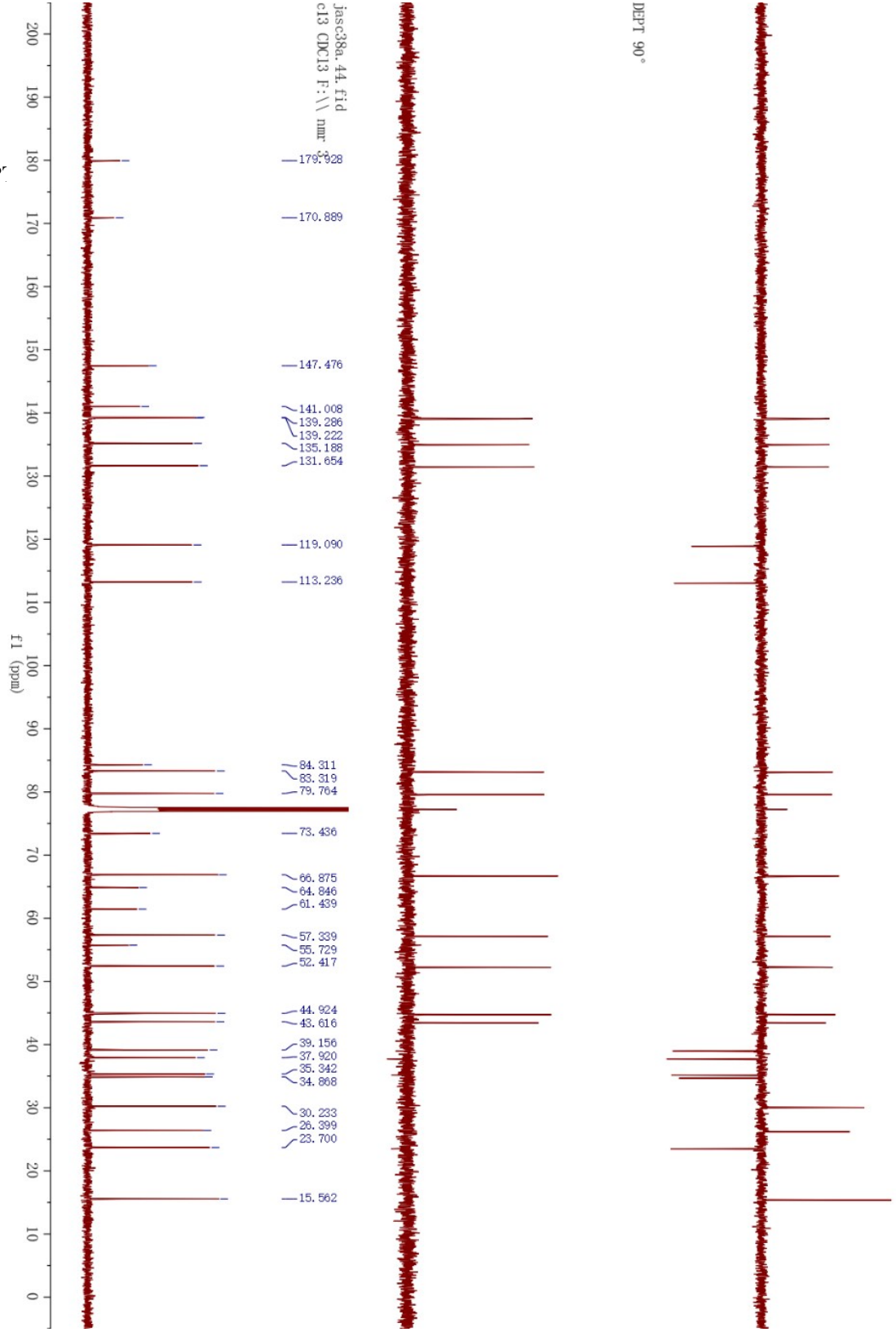


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	35.94	C32 H40 O8	[M+H]+	553.2791	553.2796	-0.5	-0.90	35.94	13.0

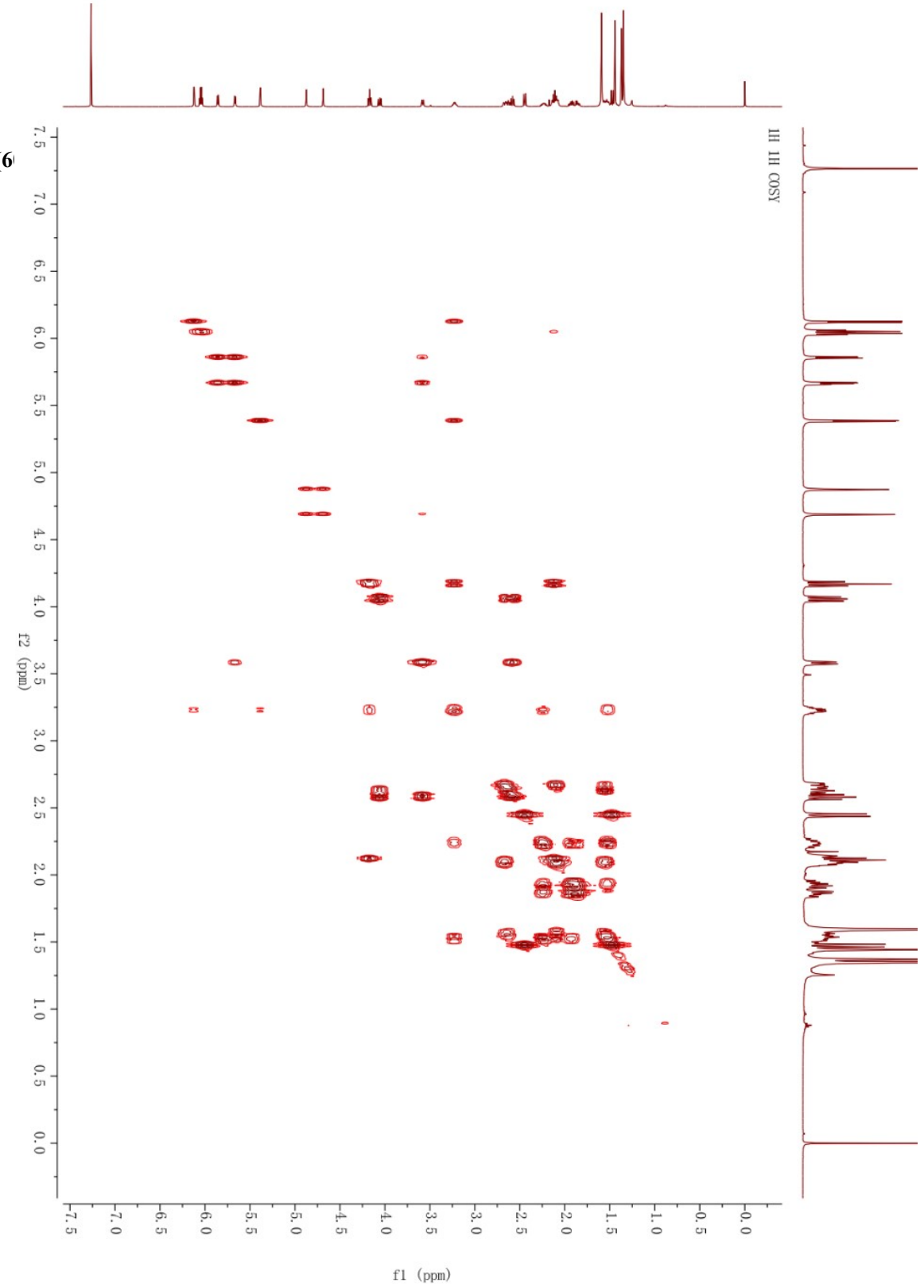
S21. ^{1}H NMR (600 M



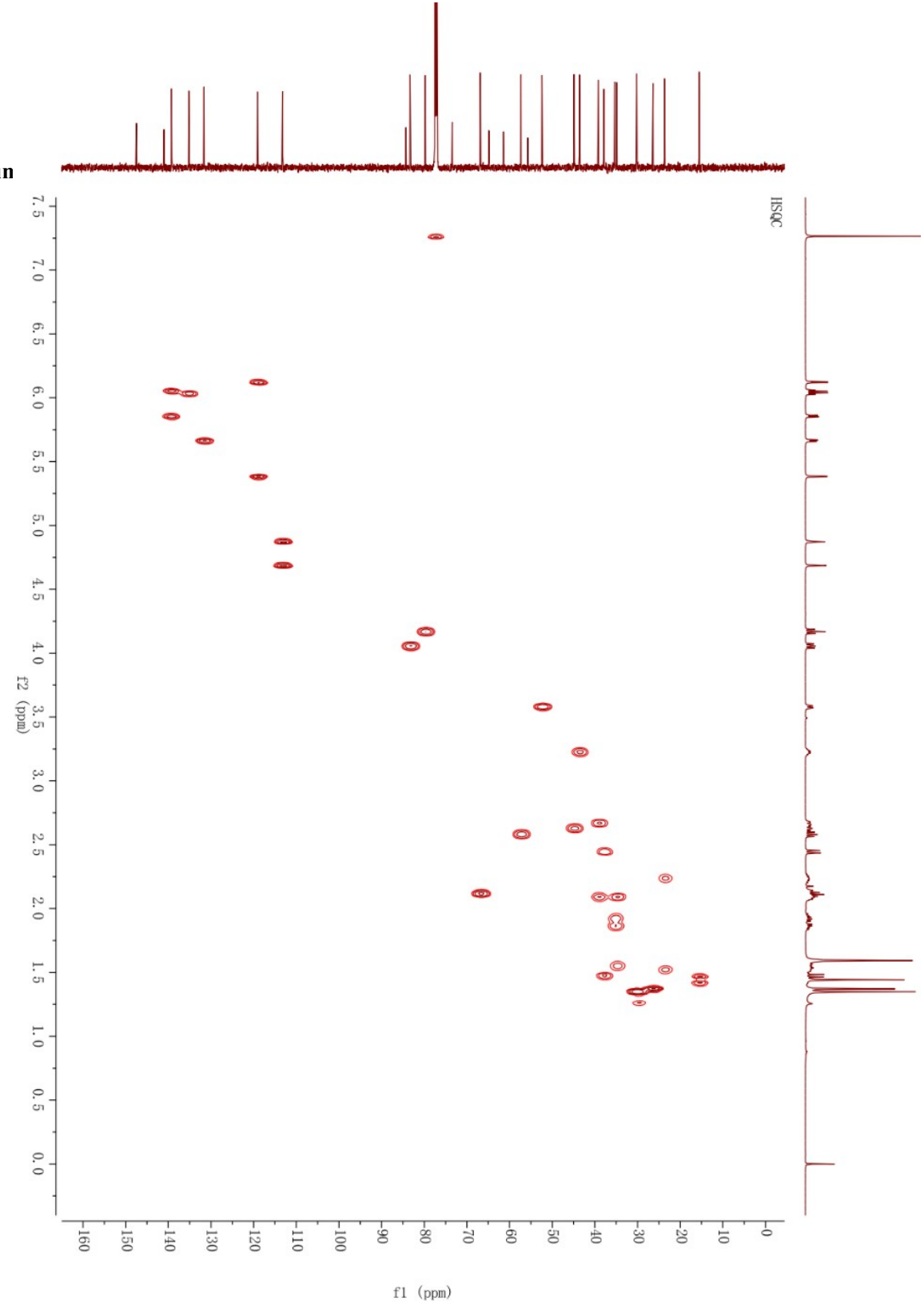
S22. ^{13}C NMR (DEP



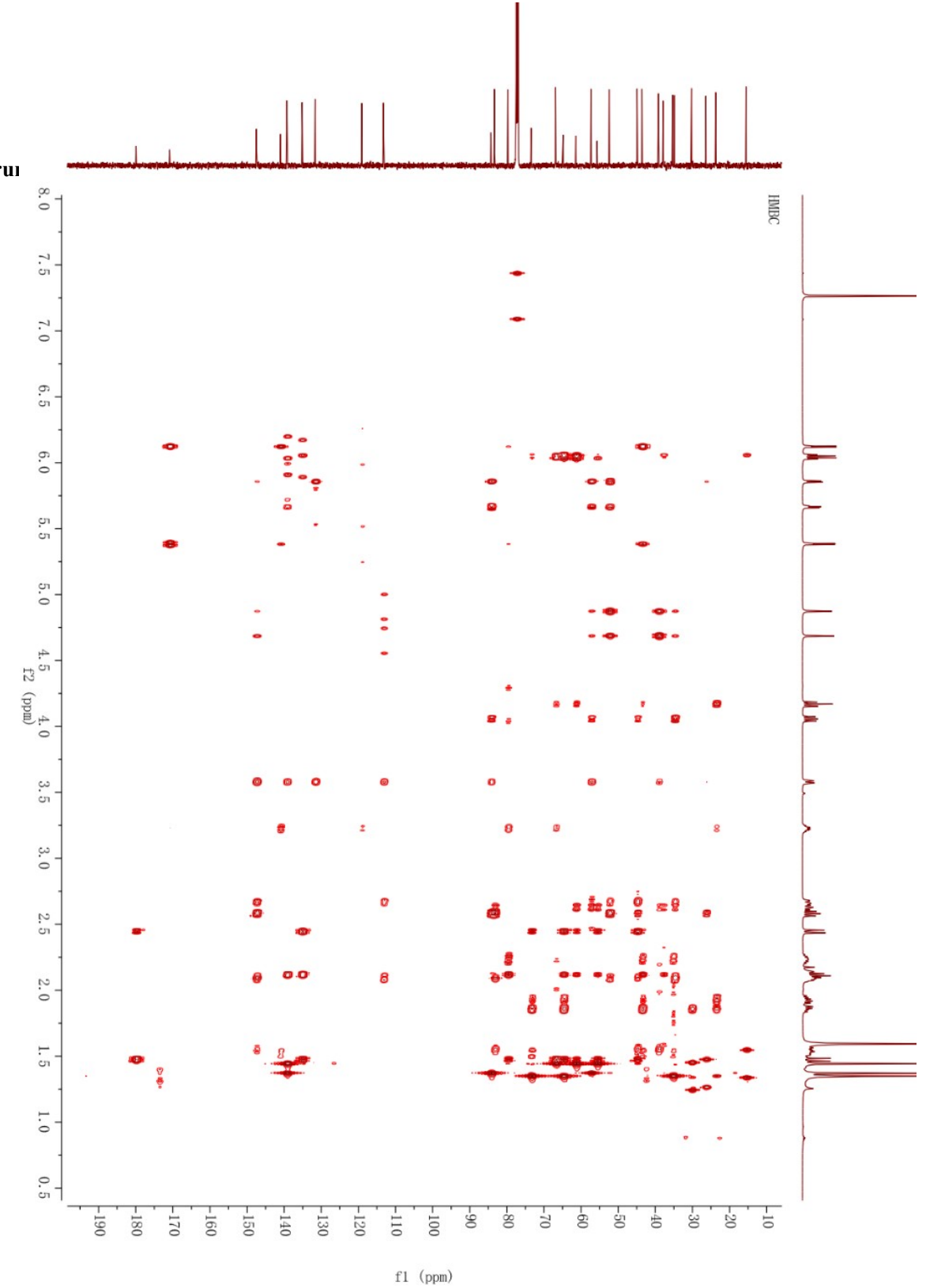
S23. ^{1}H-^{1}H COSY (6



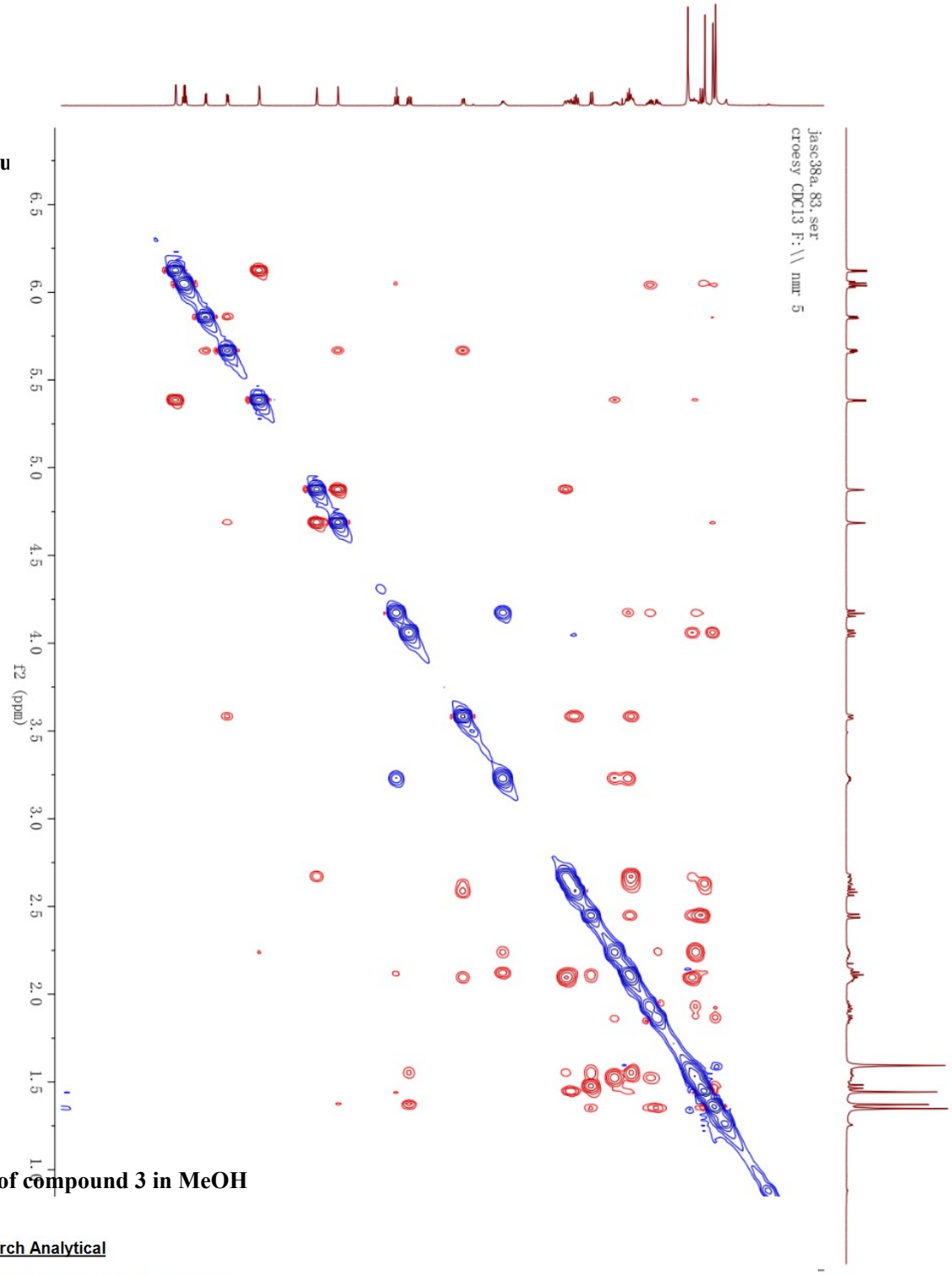
S24. HSQC spectrun



S25. HMBC spectrum



S26. ROESY spectru



S27. $[\alpha]_D$ spectrum of compound 3 in MeOH

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Wednesday, 11-DEC-2024

Set Temperature : 20.0

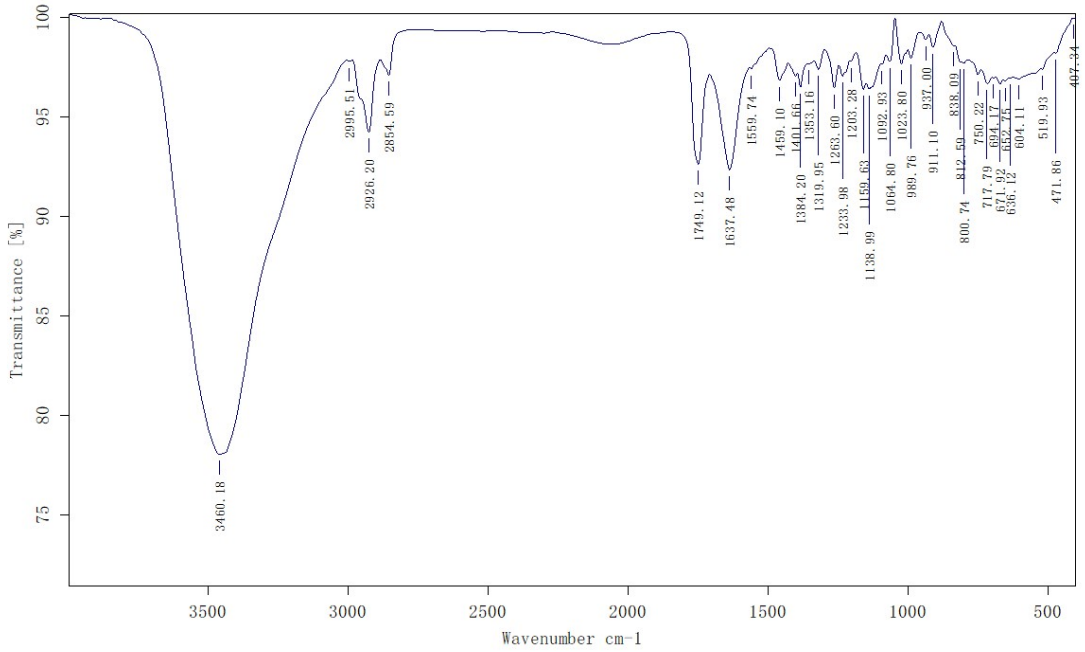
Time Delay : Disabled

Delay between Measurement : Disabled

n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	-84.16	0.76	-0.90	-83.33	-84.72

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	JASC-38	03:29:31 PM	-83.33	SR	-0.060	589	100.00	0.072	20.0
2	JASC-38	03:29:38 PM	-83.33	SR	-0.060	589	100.00	0.072	20.0
3	JASC-38	03:29:44 PM	-84.72	SR	-0.061	589	100.00	0.072	20.0
4	JASC-38	03:29:50 PM	-84.72	SR	-0.061	589	100.00	0.072	20.0
5	JASC-38	03:29:57 PM	-84.72	SR	-0.061	589	100.00	0.072	20.0

S28. IR spectrum of compound 3

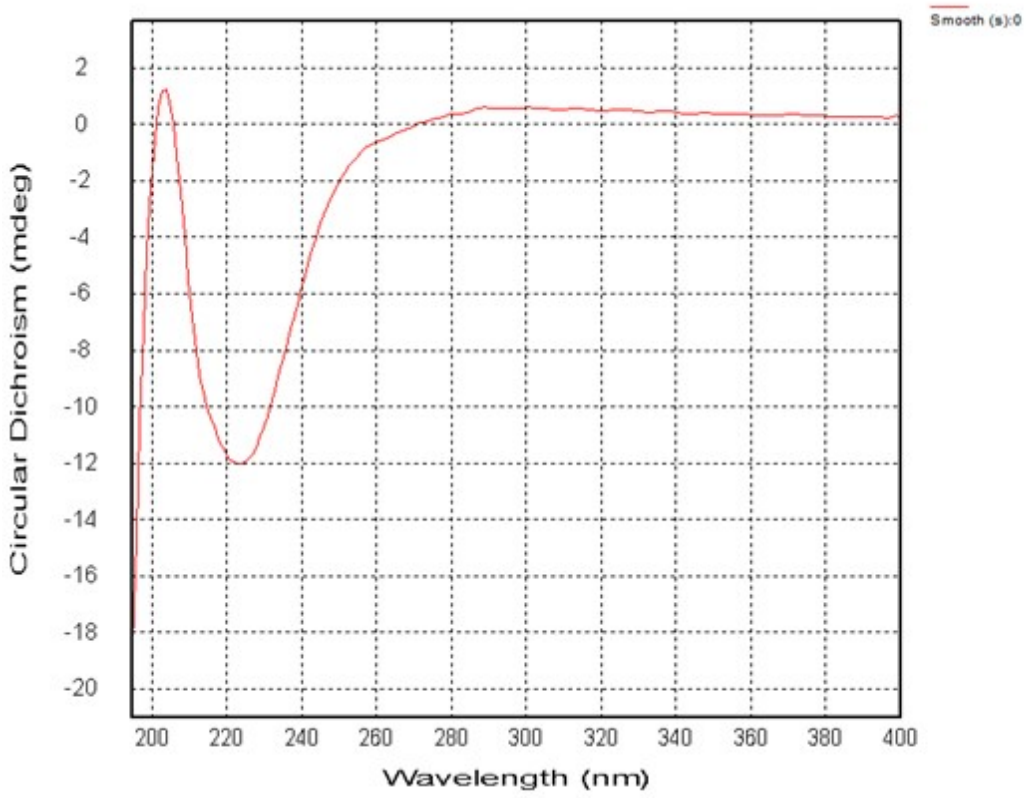


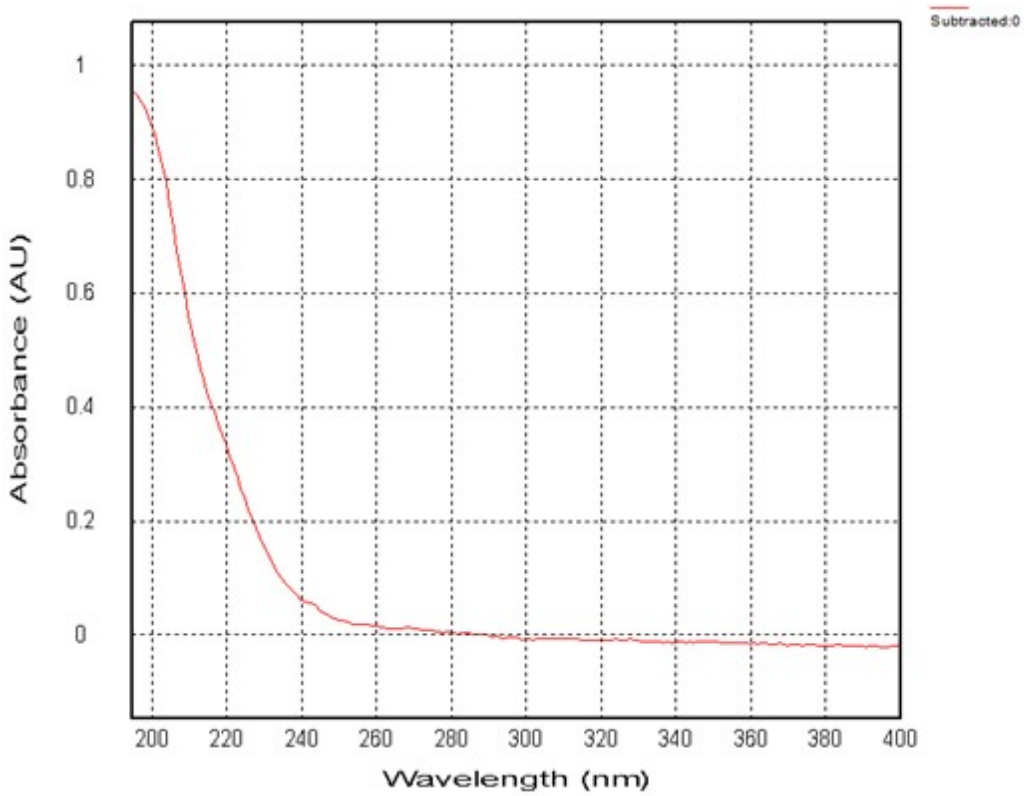
Sample Name: jasc-38
Sample Form: KBr
Path of File: E:\data
Date of Measurement: 2024/12/31

Resolution: 4
Aperture Setting: 6 mm
Number of Background Scans: 16
Number of Sample Scans: 16

Beamsplitter Setting: KBr
Source Setting: MIR
Instrument Type: BRUKER VERTEX 70
Soft Version: OPUS8.1

S29. ECD and UV spectra of compound 3



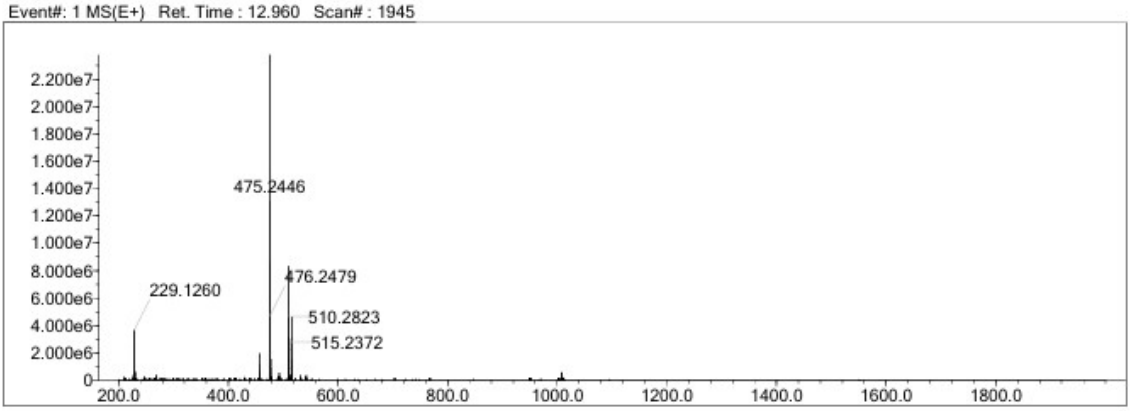


S30. HRESIMS of compound 3

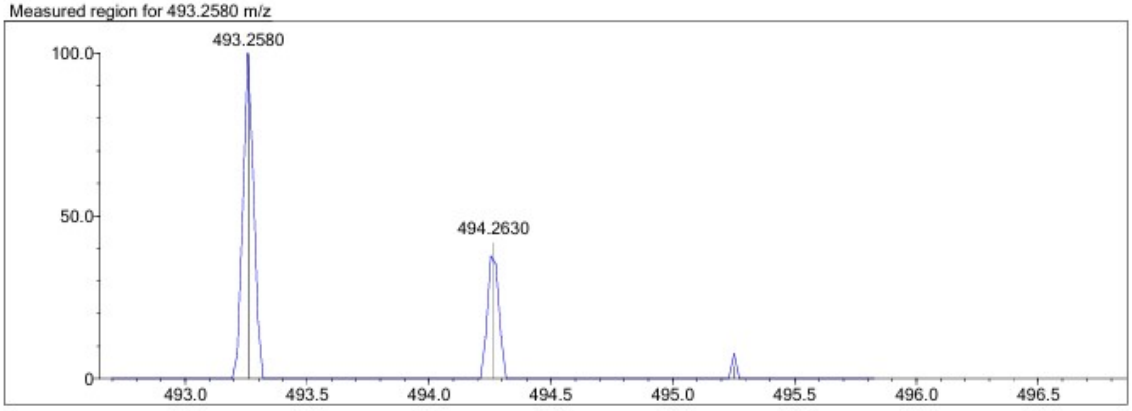
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	300	O	2	0	20	H
C	4	0	150	Cl	1	0	0	Na
N	3	0	1					

Error Margin (ppm): 100 | DBE Range: -2.0 - 1000.0 | Electron Ions: both
HC Ratio: unlimited | Apply N Rule: yes | Use MSn Info: no
Max Isotopes: all | Isotope RI (%): 1.00 | Isotope Res: 10000
MSn Iso RI (%): 75.00 | MSn Logic Mode: AND | Max Results: 500

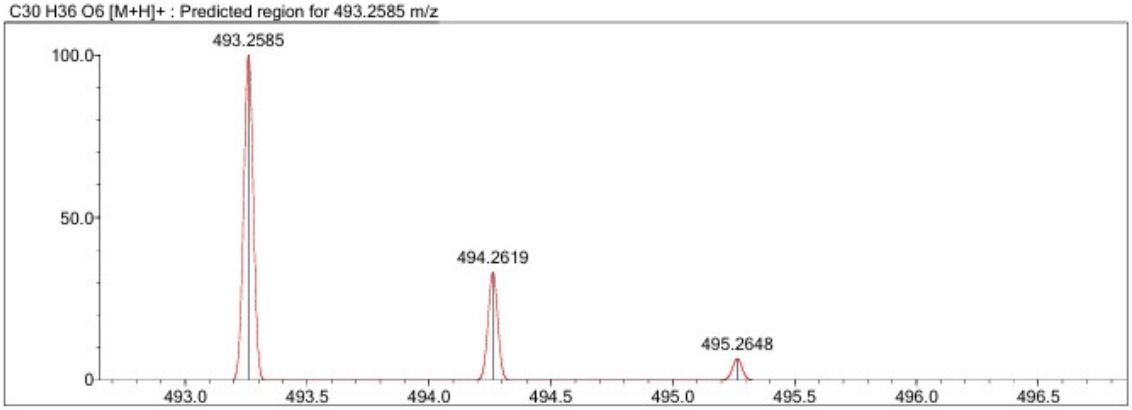
Event#: 1 MS(E+) Ret. Time : 12.960 Scan# : 1945



Measured region for 493.2580 m/z

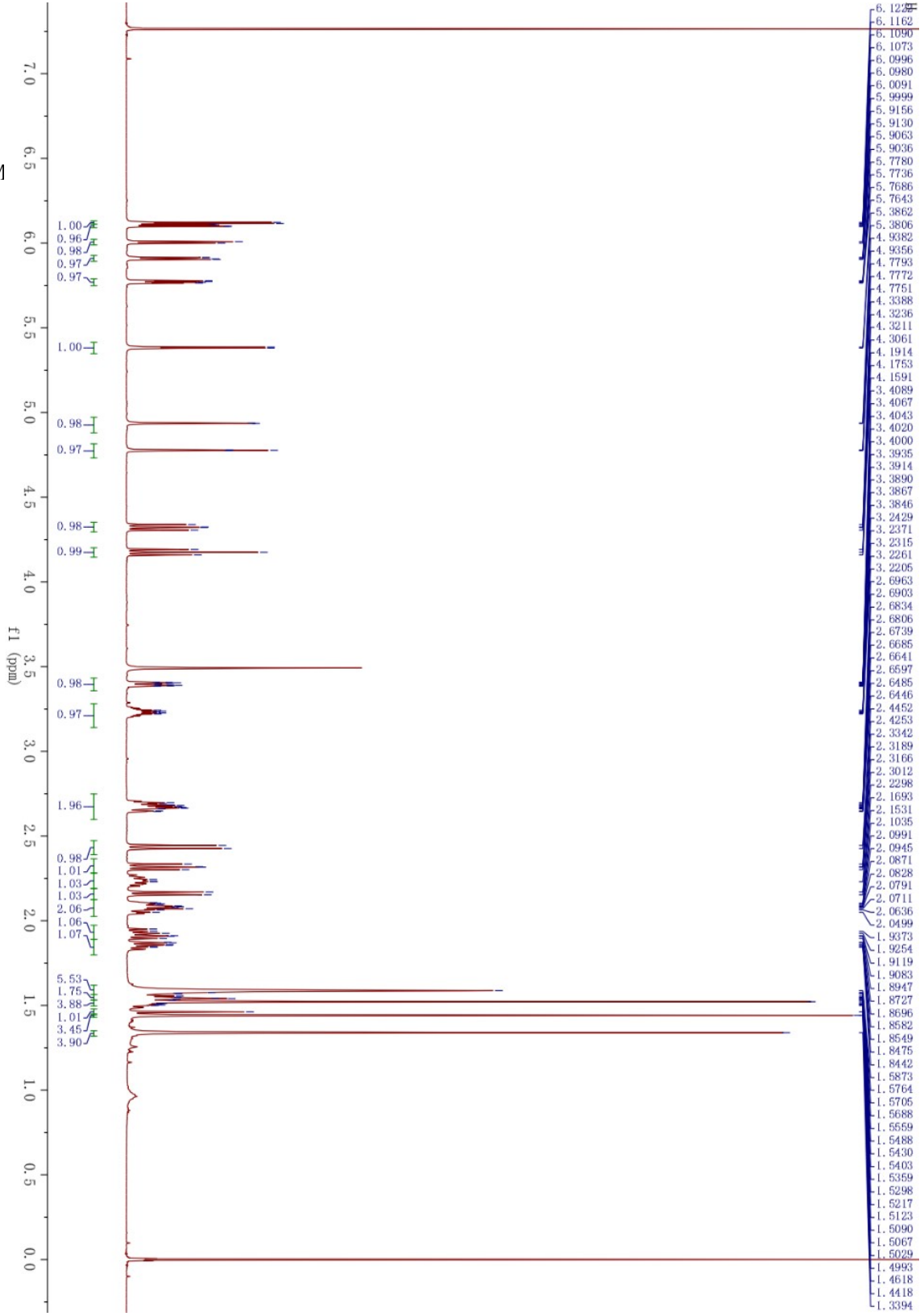


C30 H36 O6 [M+H]+ : Predicted region for 493.2585 m/z

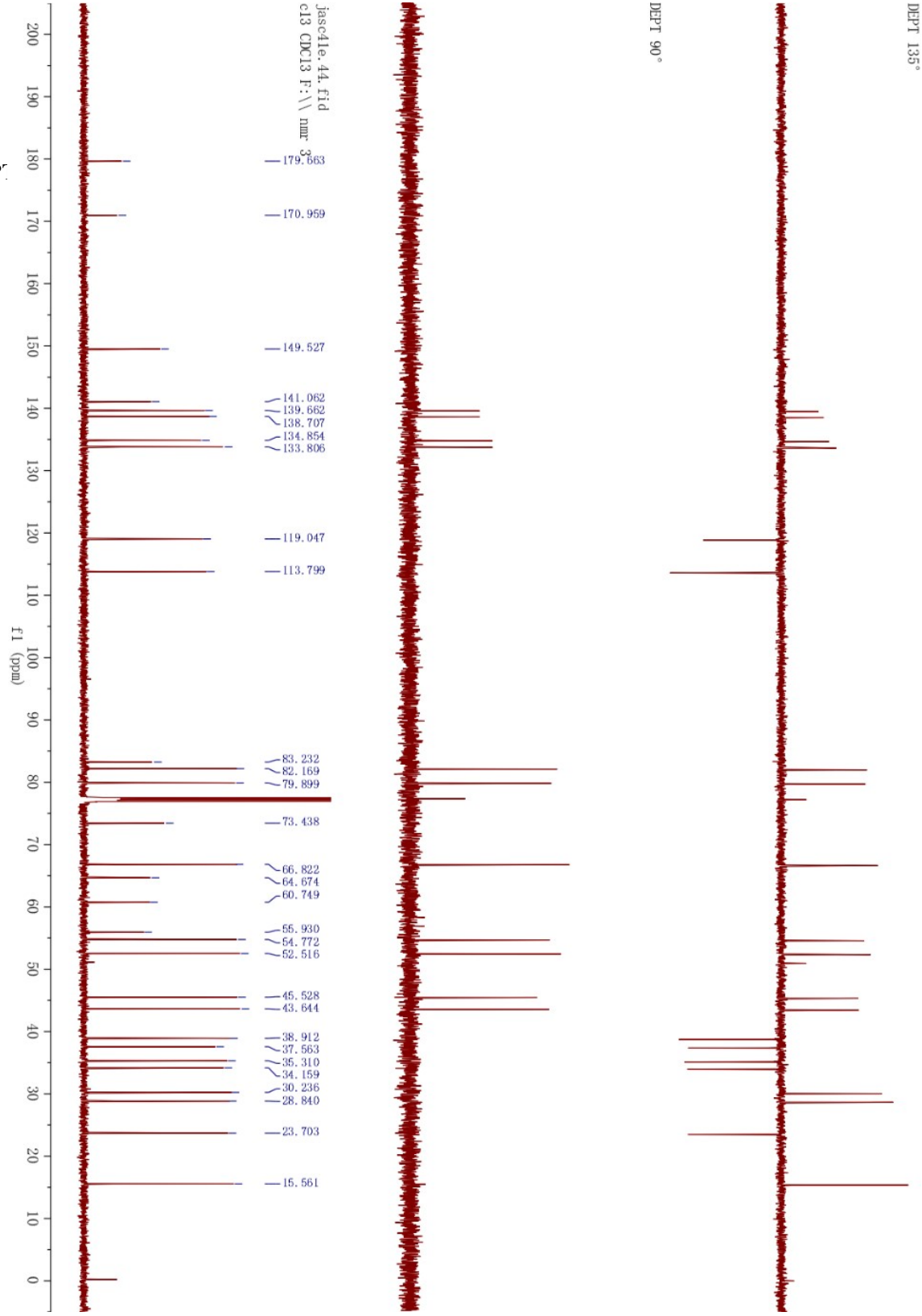


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
2	52.52	C30 H36 O6	[M+H]+	493.2580	493.2585	-0.5	-1.01	52.53	13.0

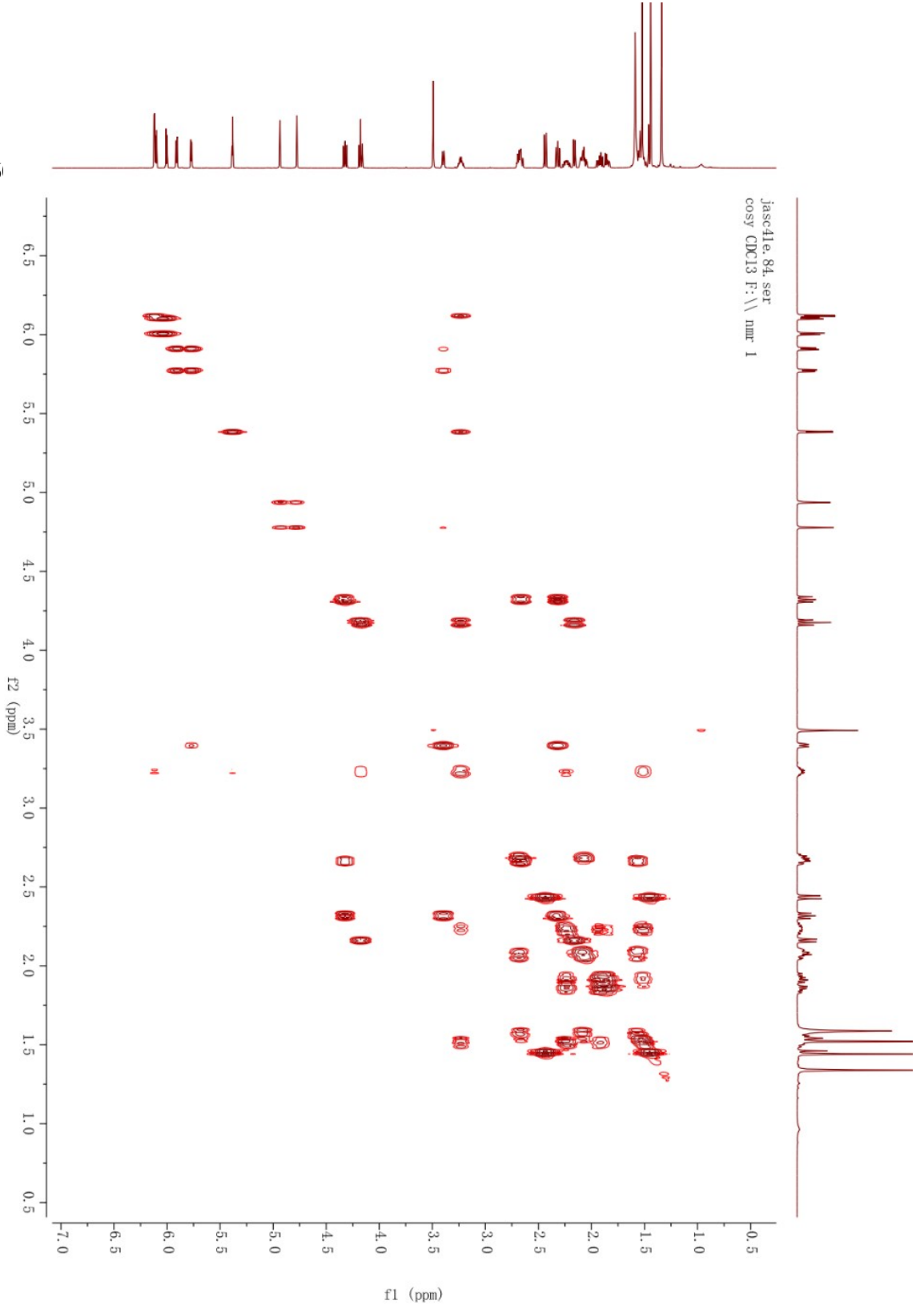
S31. ^{1}H NMR (600 M



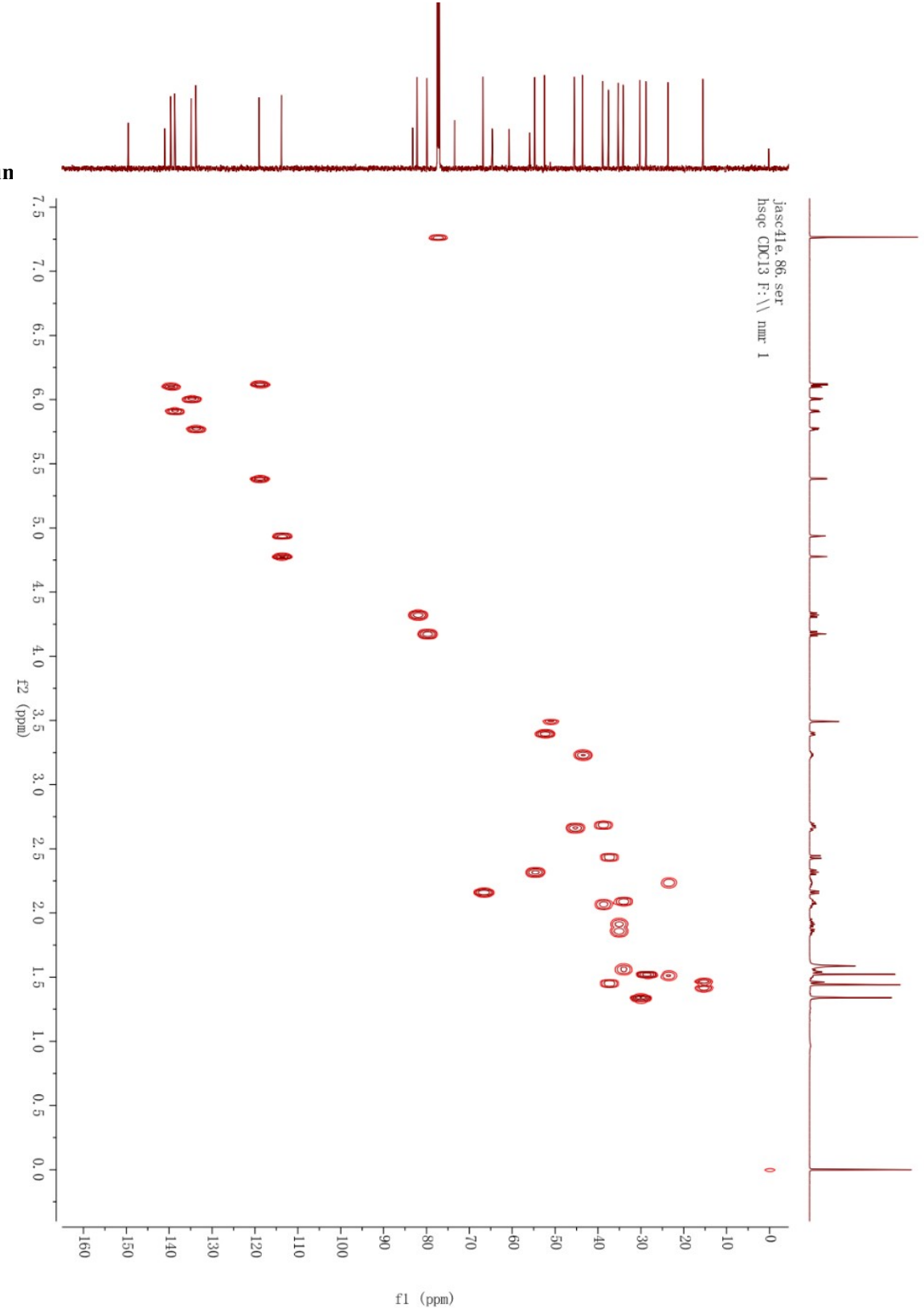
S32. ^{13}C NMR (DEP



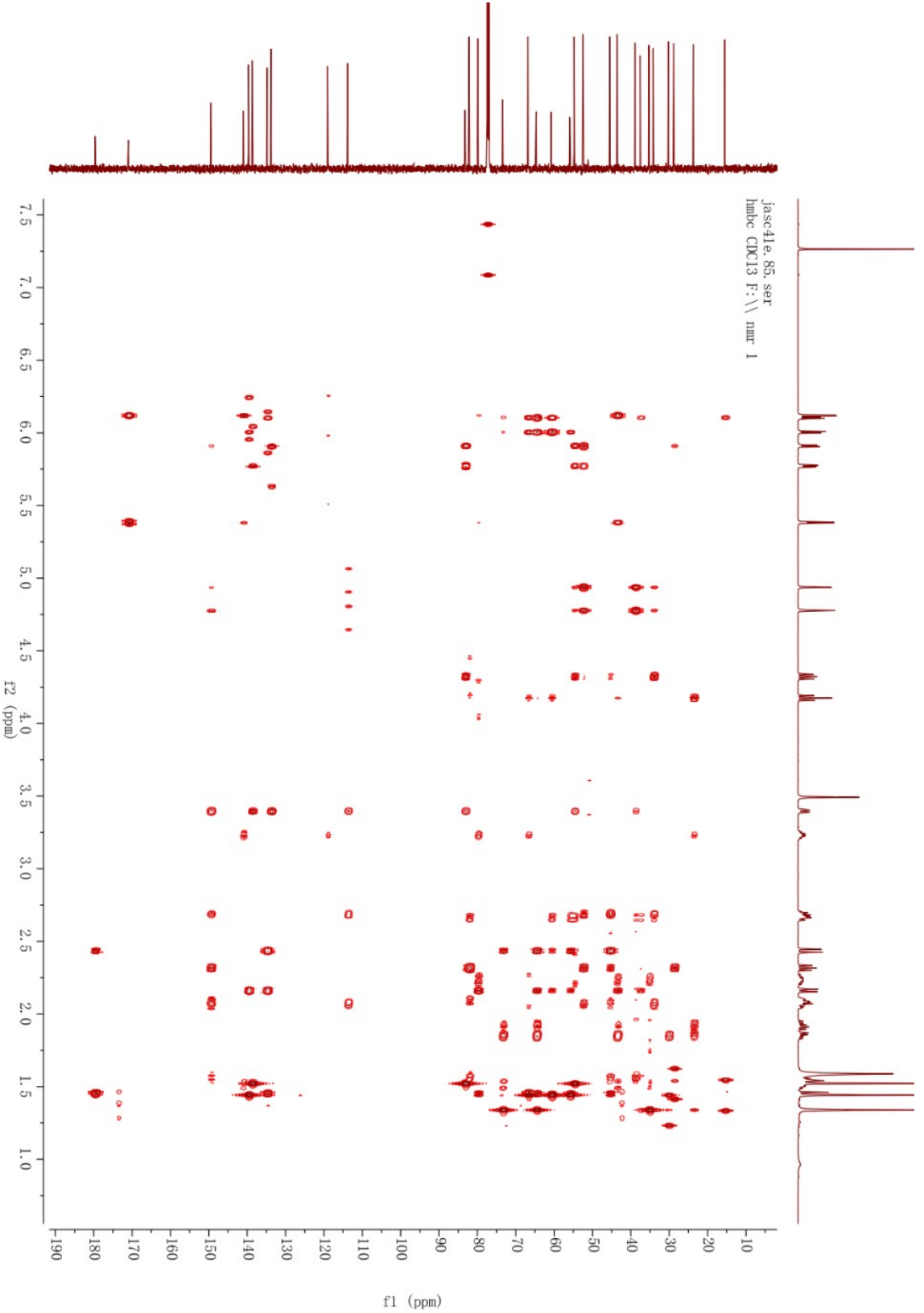
S33. ^{1}H-^{1}H COSY (6



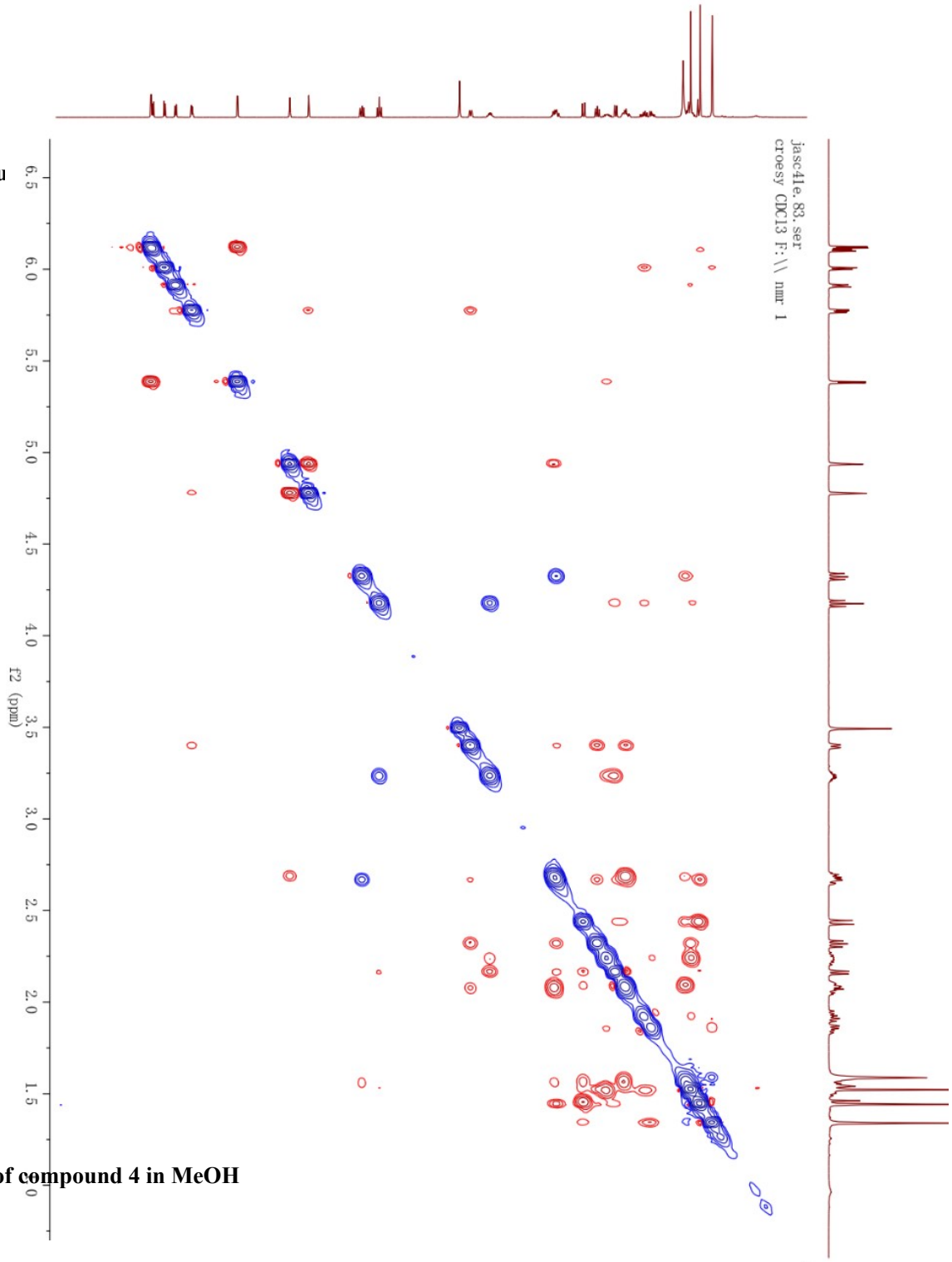
S34. HSQC spectrun



S35. HMBC spectrum



S36. ROESY spectru



S37. $[\alpha]_D$ spectrum of compound 4 in MeOH

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Wednesday, 11-DEC-2024

Set Temperature : 20.0

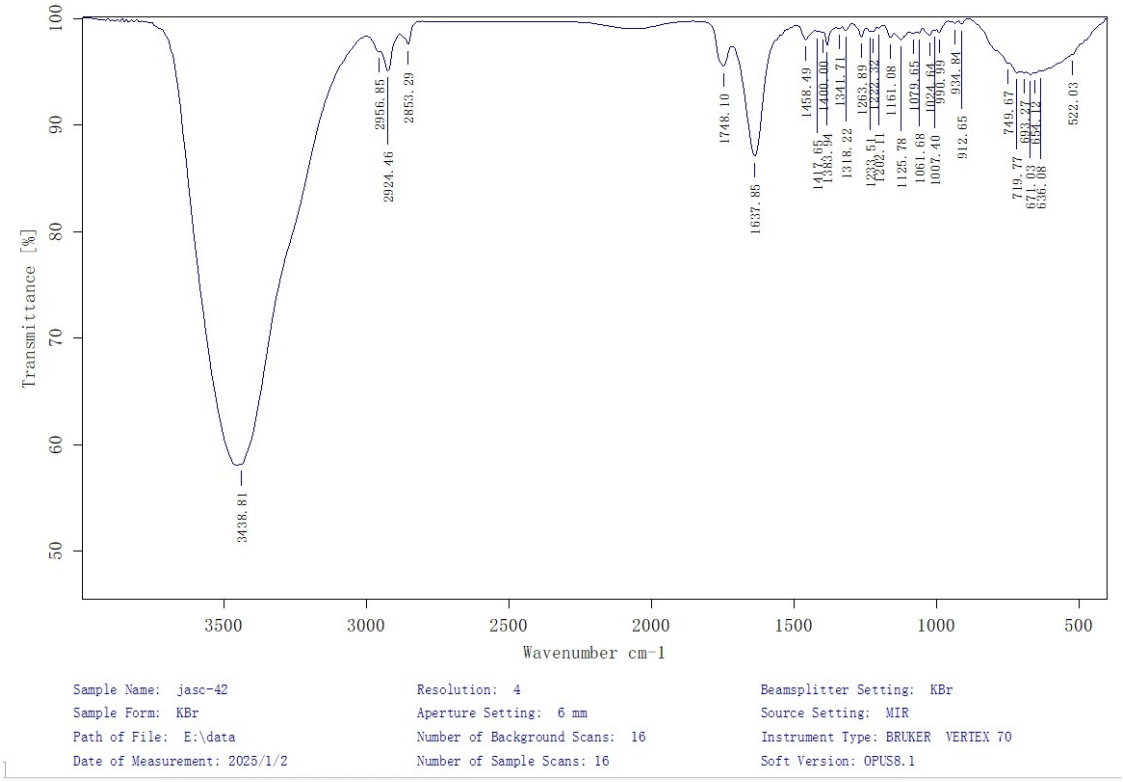
Time Delay : Disabled

Delay between Measurement : Disabled

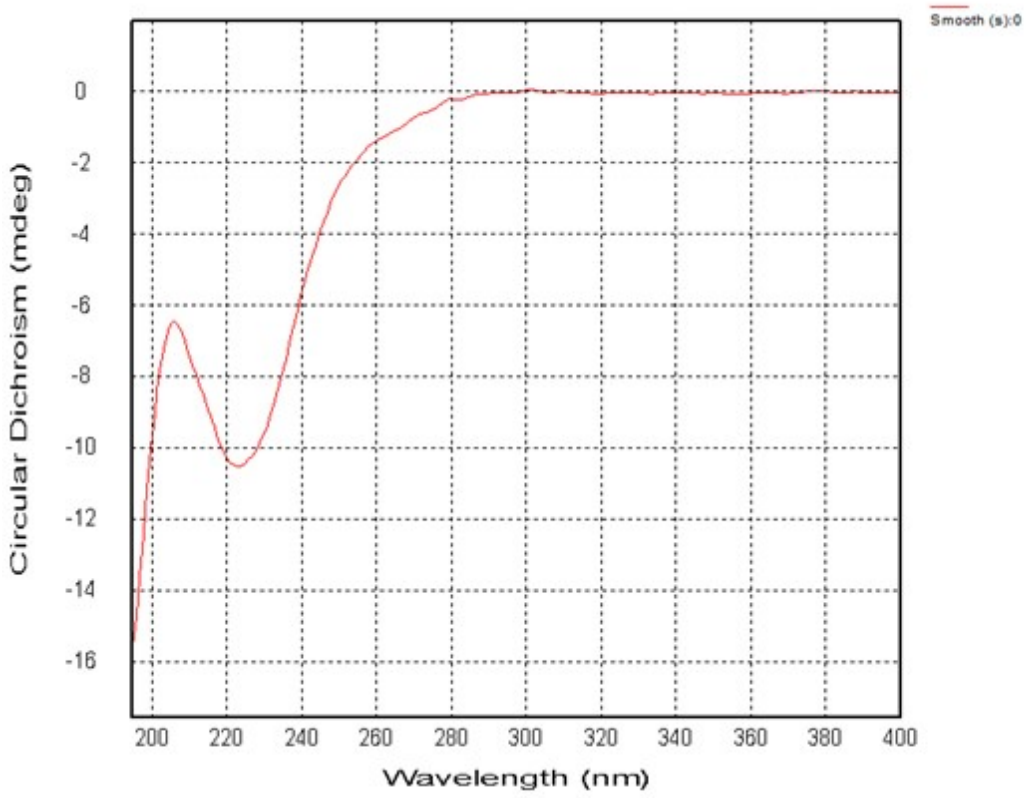
n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	-39.53	0.00	0.00	-39.53	-39.53

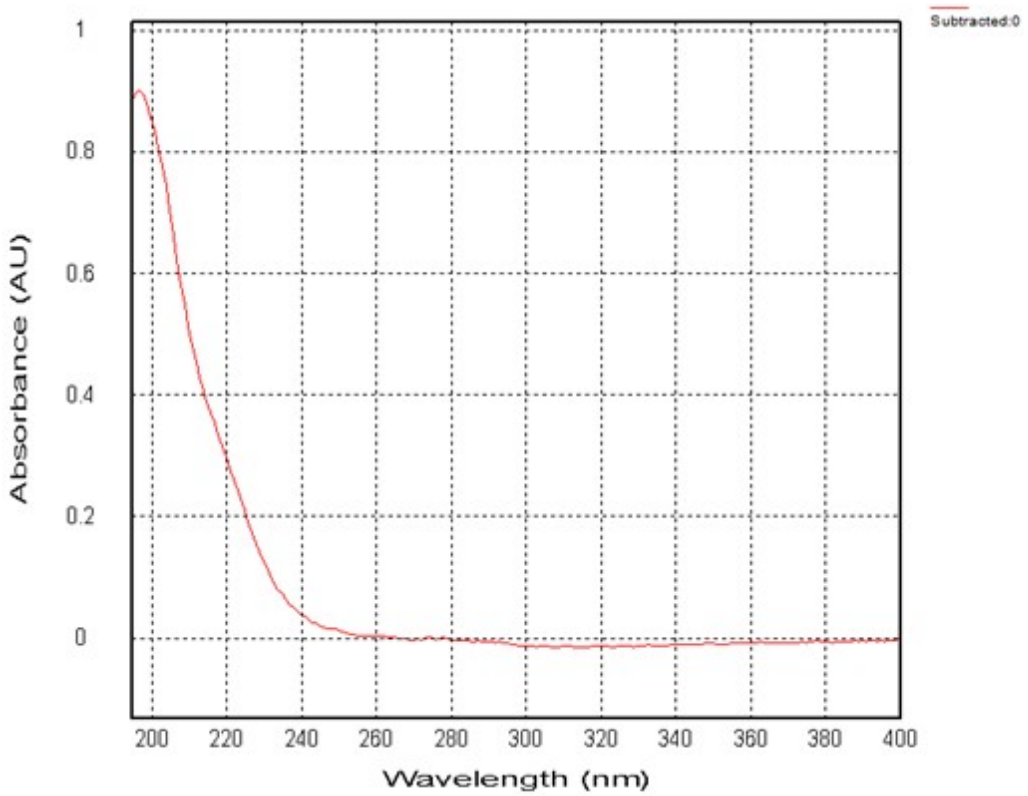
S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	JASC-42	04:08:44 PM	-39.53	SR	-0.017	589	100.00	0.043	20.0
2	JASC-42	04:08:51 PM	-39.53	SR	-0.017	589	100.00	0.043	20.0
3	JASC-42	04:08:57 PM	-39.53	SR	-0.017	589	100.00	0.043	20.0
4	JASC-42	04:09:03 PM	-39.53	SR	-0.017	589	100.00	0.043	20.0
5	JASC-42	04:09:10 PM	-39.53	SR	-0.017	589	100.00	0.043	20.0

S38. IR spectrum of compound 4



S39. ECD and UV spectra of compound 4





S40. HRESIMS of compound 4

Elmt	Val.	Min	Max
H	1	0	300
C	4	0	150
N	3	0	1

Elmt	Val.	Min	Max
O	2	0	20
Cl	1	0	0

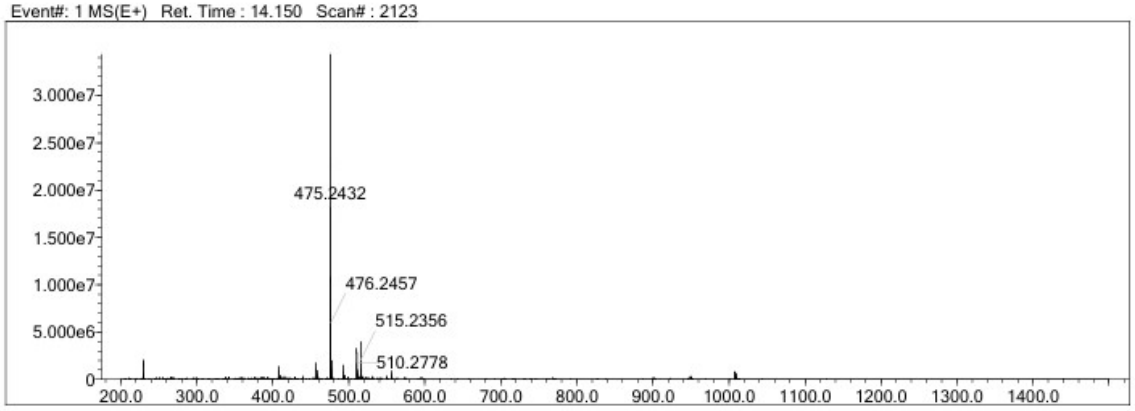
Use Adduct
H
Na

Error Margin (ppm): 100
HC Ratio: unlimited
Max Isotopes: all
MSn Iso RI (%): 75.00

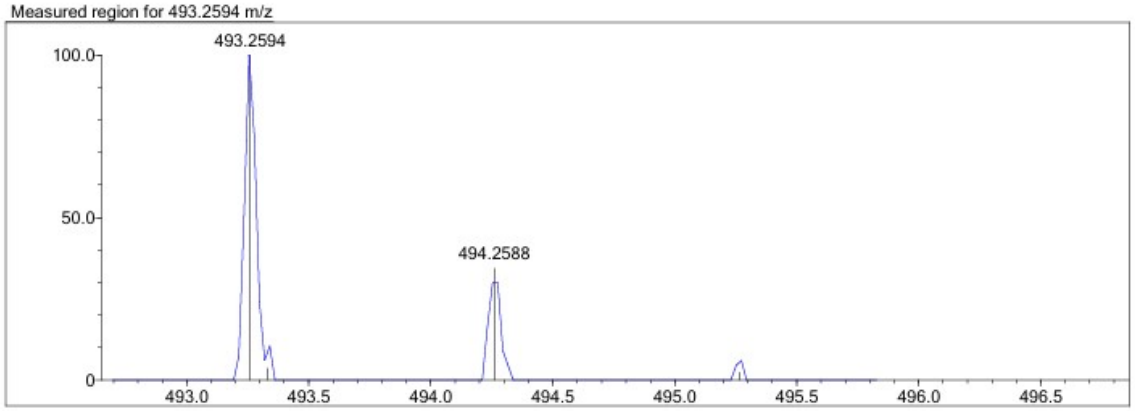
DBE Range: -2.0 - 1000.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

Electron Ions: both
Use MSn Info: no
Isotope Res: 10000
Max Results: 500

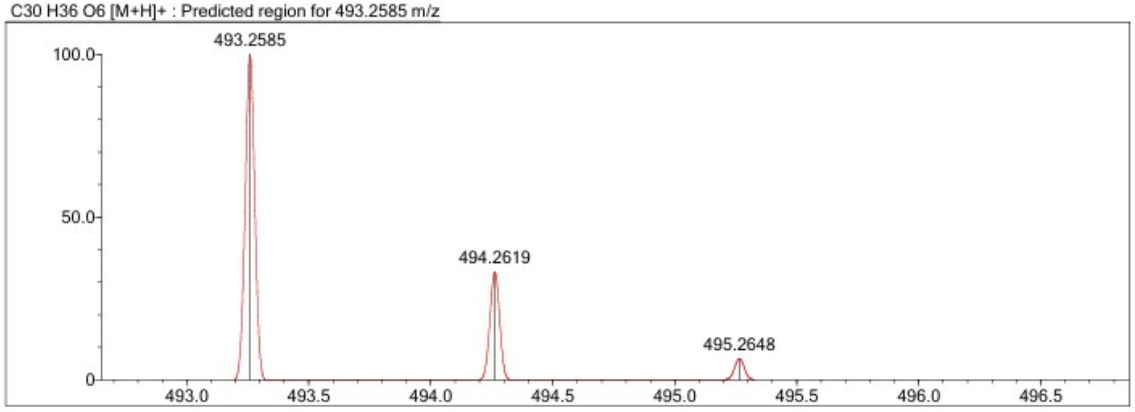
Event#: 1 MS(E+) Ret. Time : 14.150 Scan# : 2123



Measured region for 493.2594 m/z

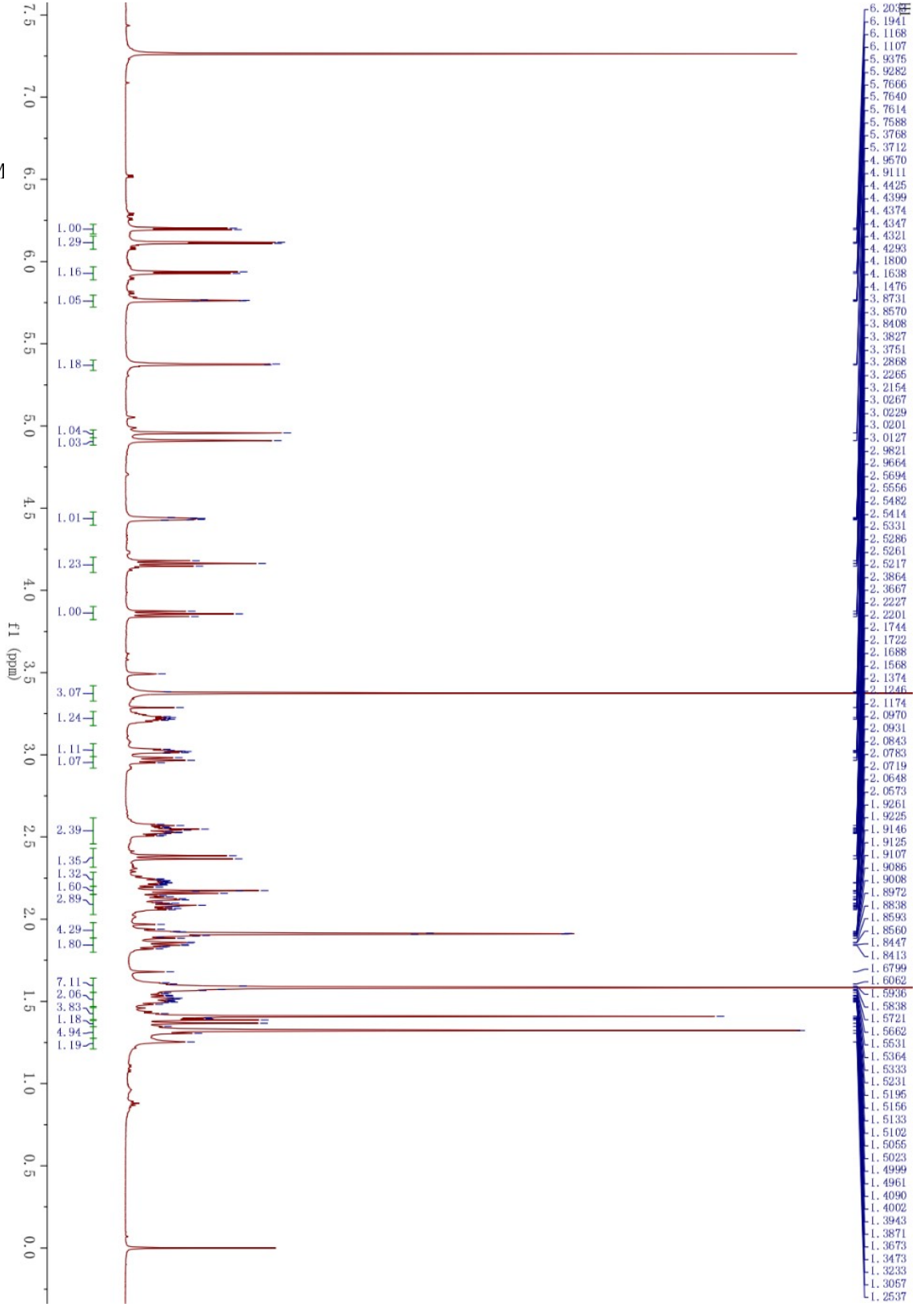


C30 H36 O6 [M+H]+ : Predicted region for 493.2585 m/z

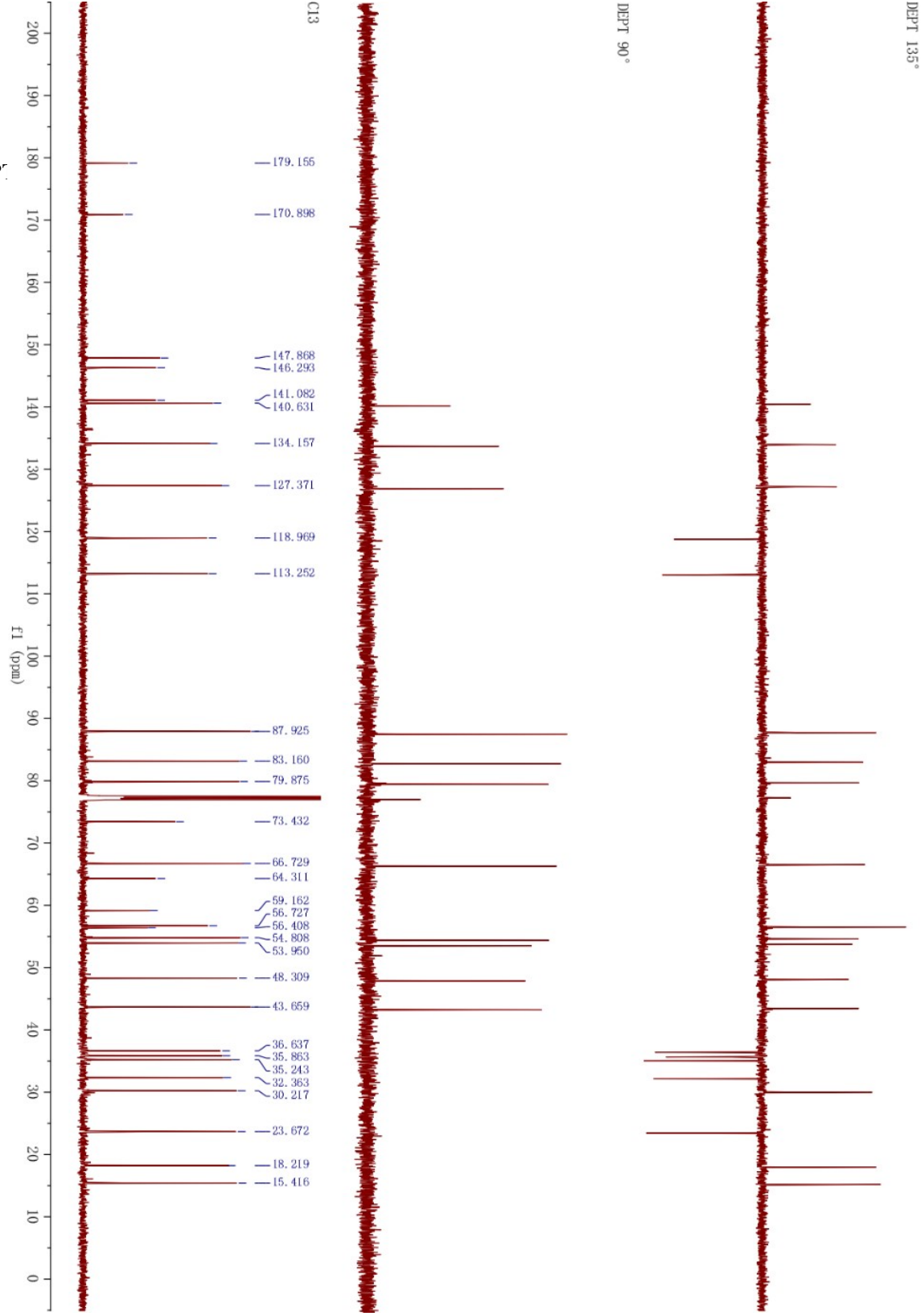


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	85.34	C30 H36 O6	[M+H]+	493.2594	493.2585	0.9	1.82	87.13	13.0

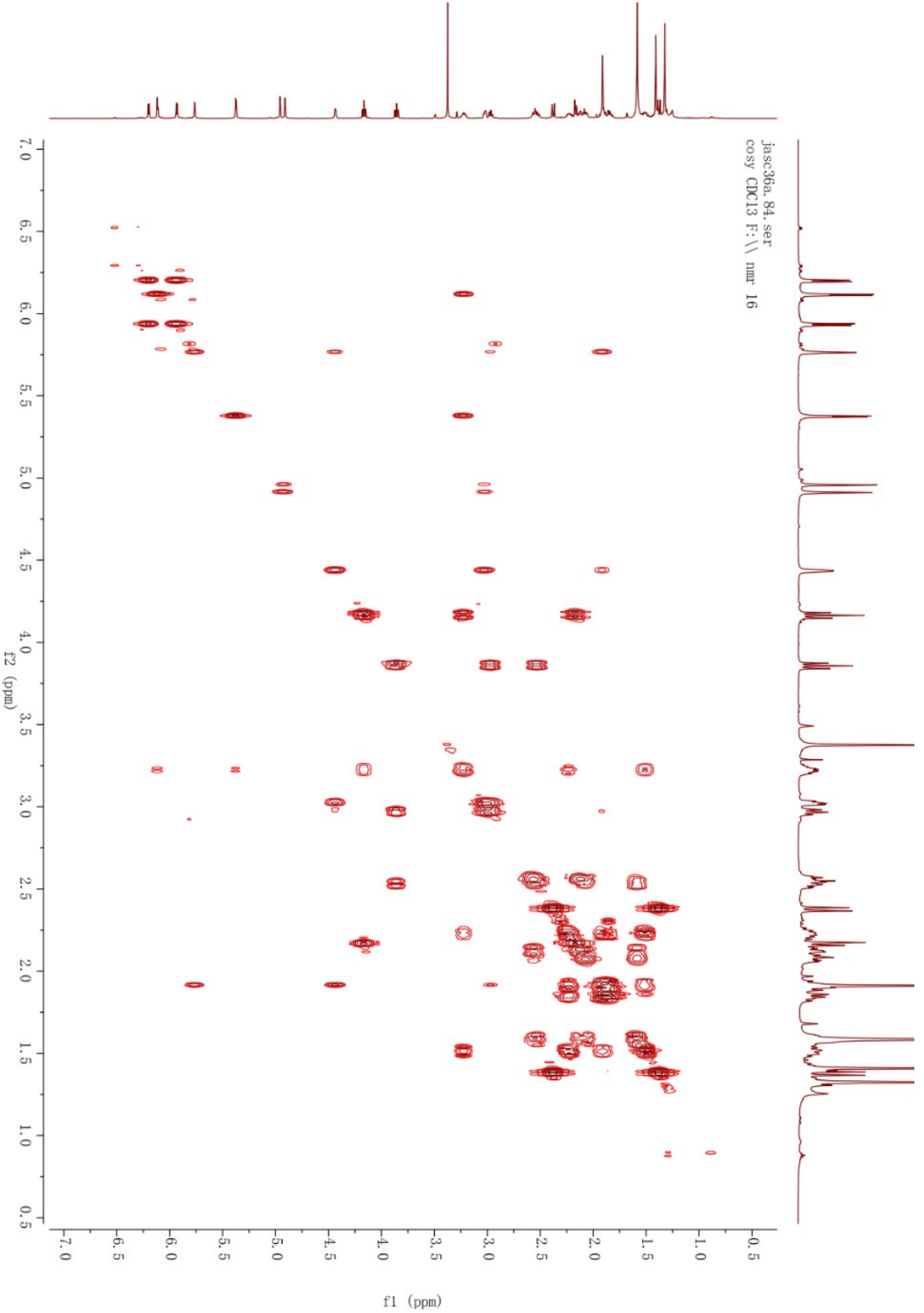
S41. ^{1}H NMR (600 M



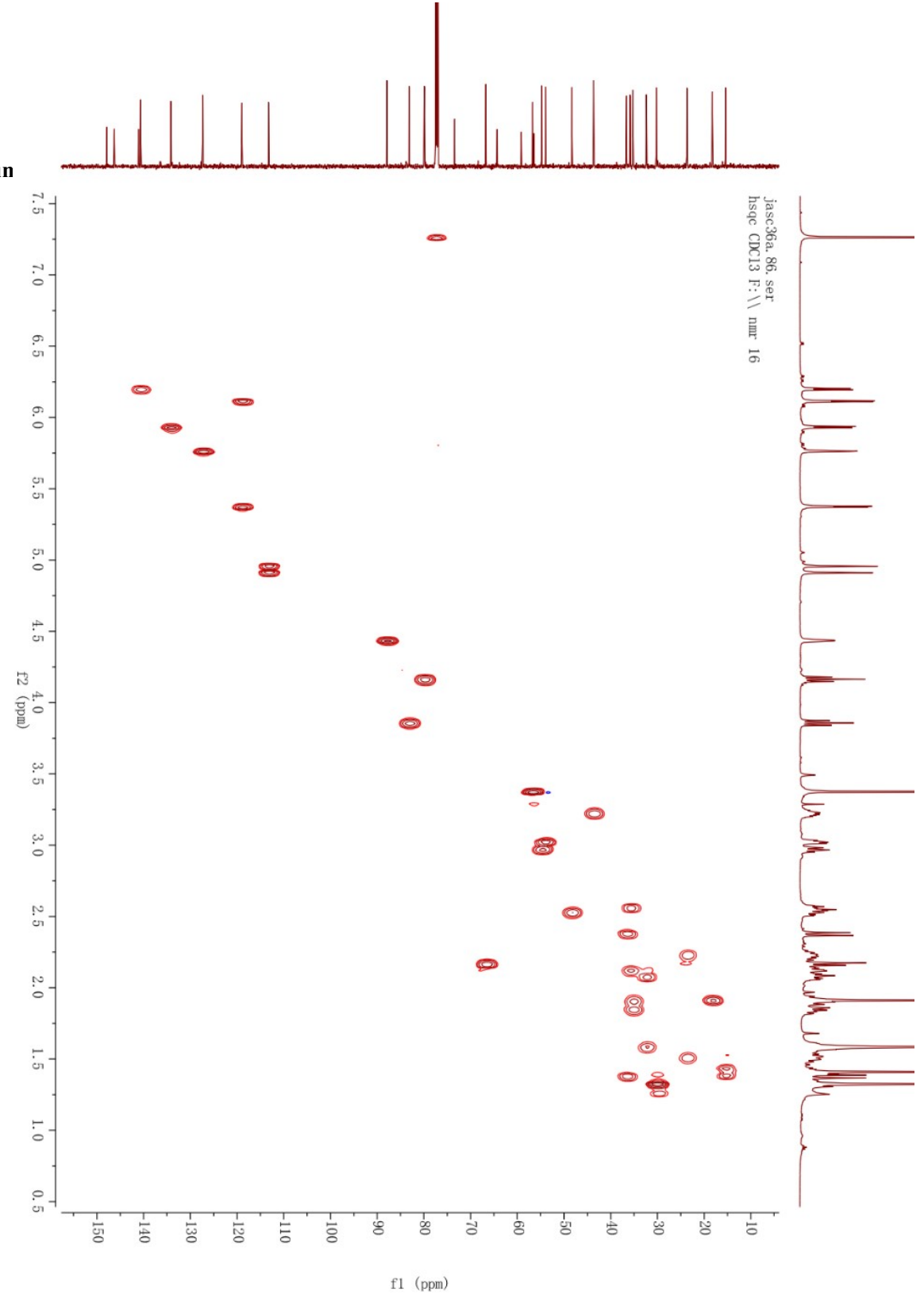
S42. ^{13}C NMR (DEP



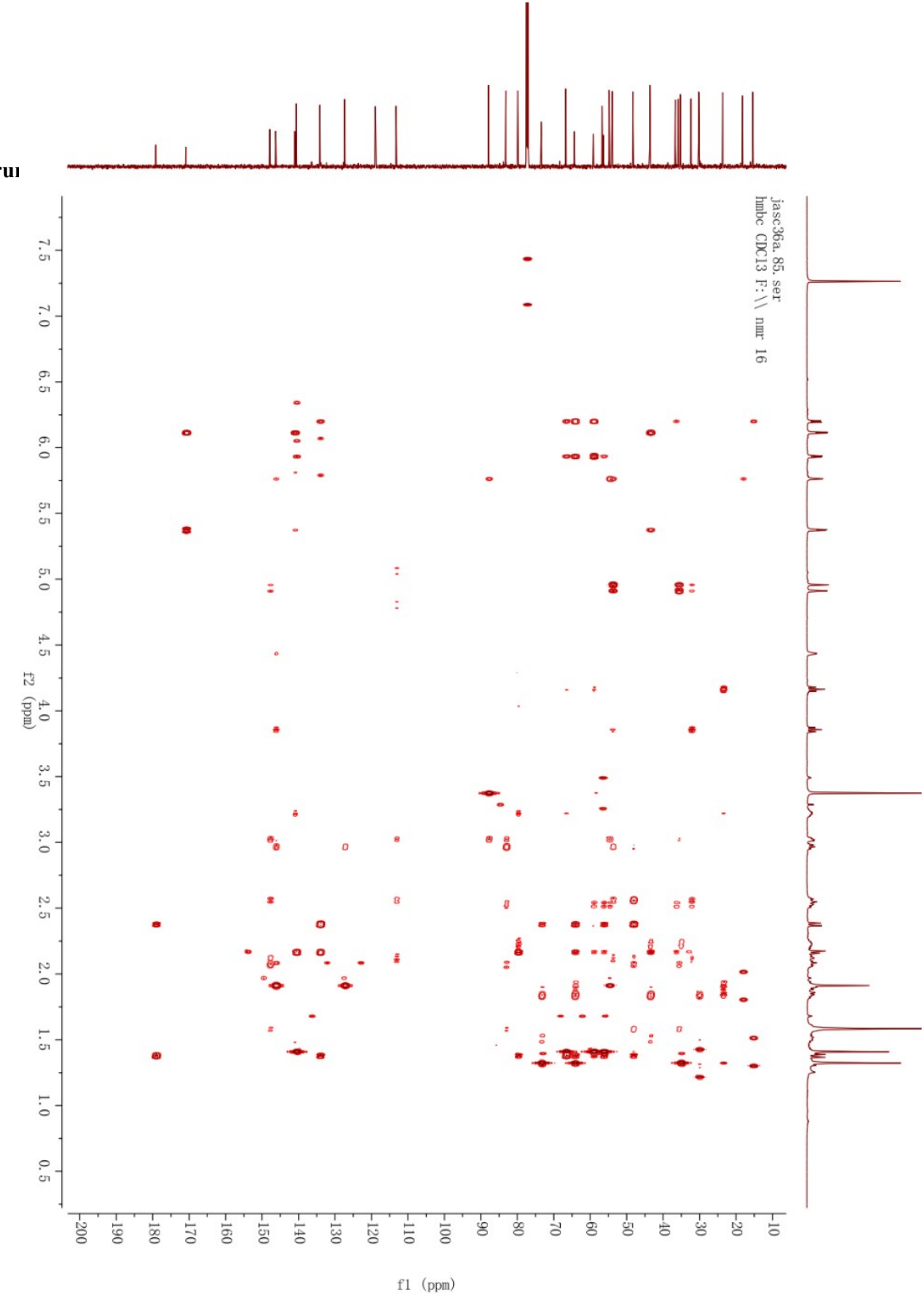
S43. ^{1}H-^{1}H COSY (6



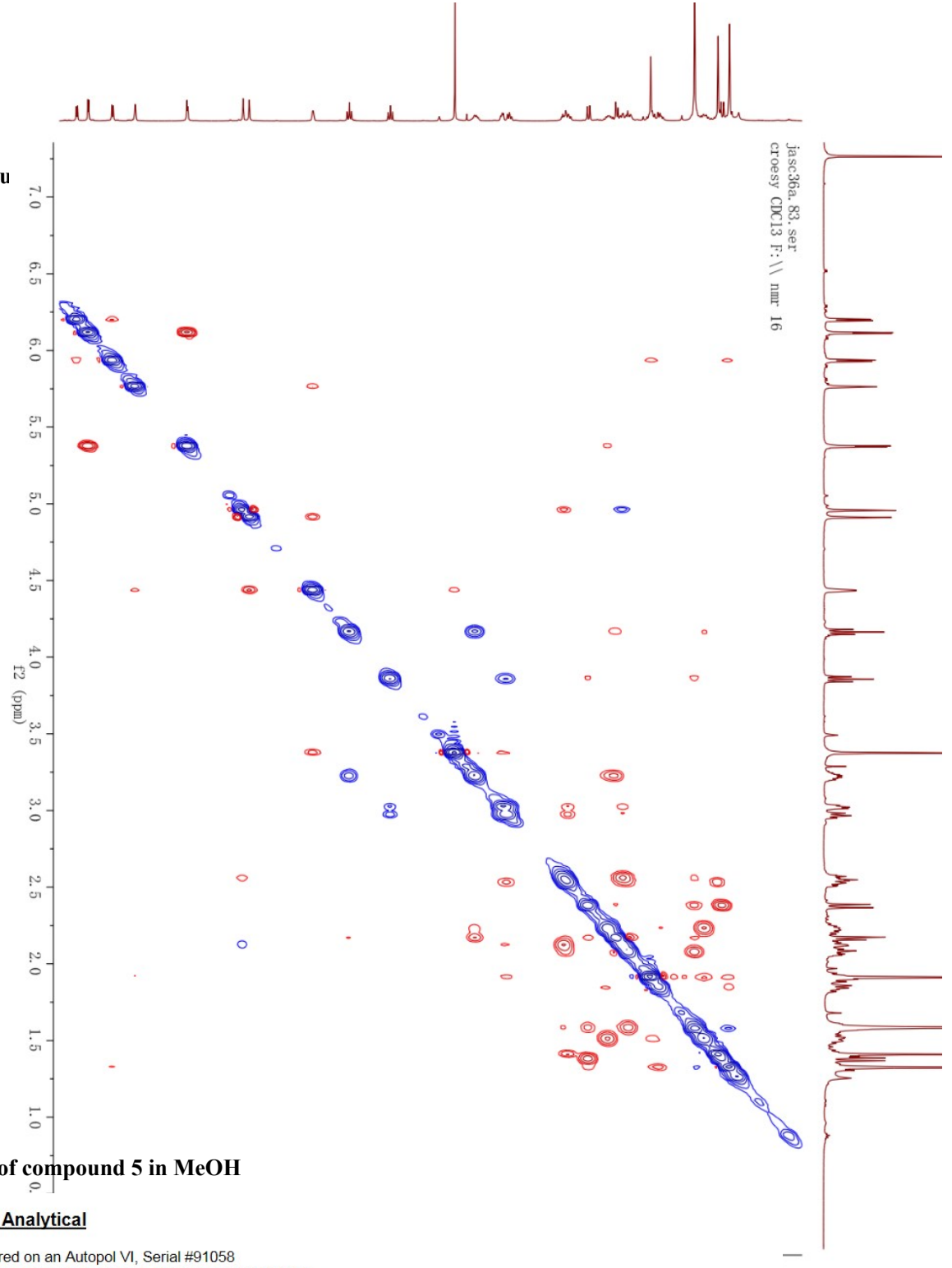
S44. HSQC spectrun



S45. HMBC spectrum



S46. ROESY spectru



S47. $[\alpha]_D$ spectrum of compound 5 in MeOH

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Wednesday, 11-DEC-2024

Set Temperature : 20.0

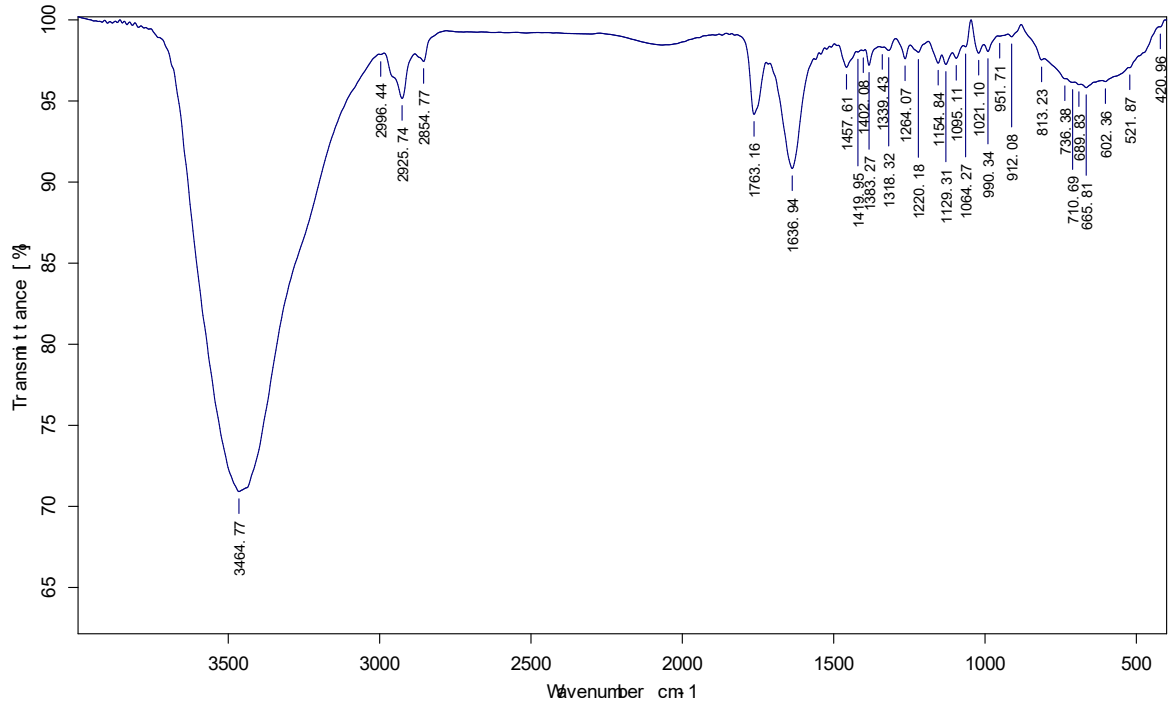
Time Delay : Disabled

Delay between Measurement : Disabled

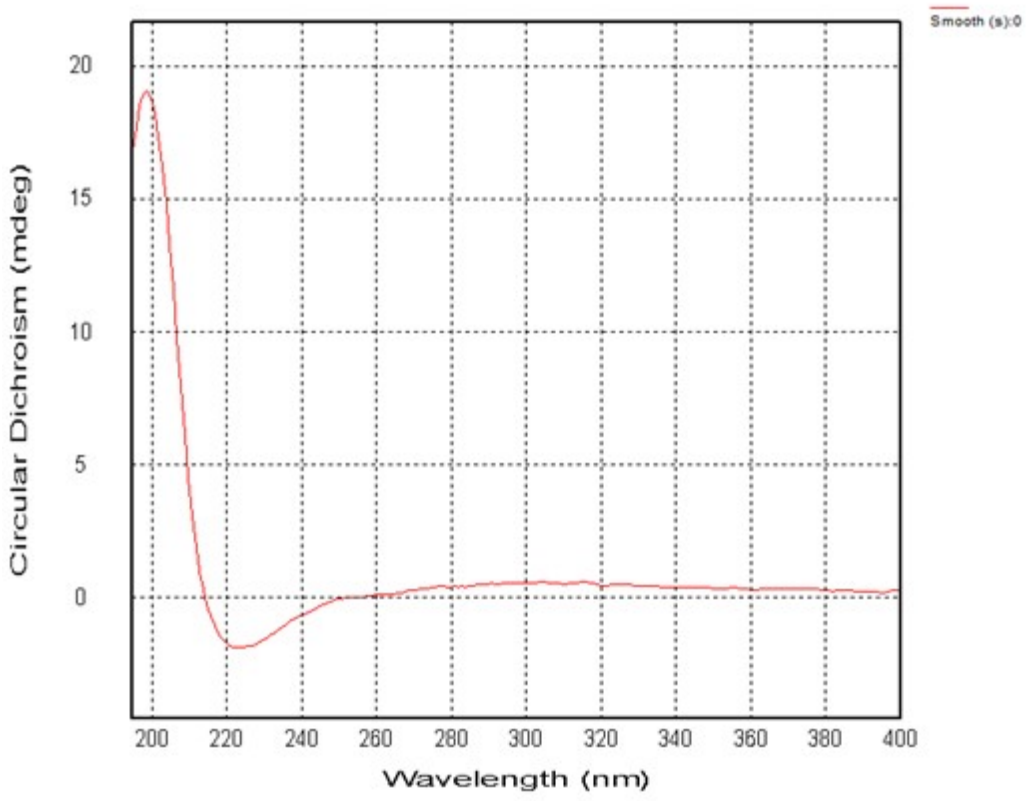
n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	12.47	0.96	7.69	12.90	10.75

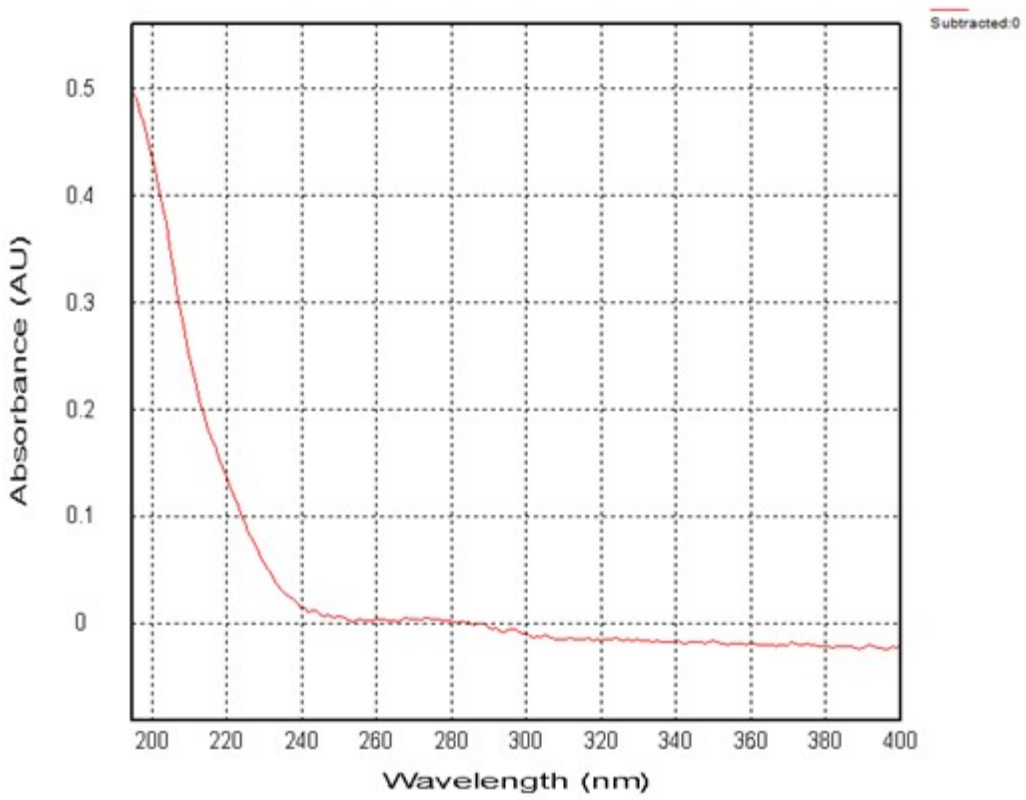
S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	JASC-36	03:14:58 PM	12.90	SR	0.012	589	100.00	0.093	20.0
2	JASC-36	03:15:04 PM	12.90	SR	0.012	589	100.00	0.093	20.0
3	JASC-36	03:15:11 PM	12.90	SR	0.012	589	100.00	0.093	20.0
4	JASC-36	03:15:17 PM	12.90	SR	0.012	589	100.00	0.093	20.0
5	JASC-36	03:15:23 PM	10.75	SR	0.010	589	100.00	0.093	20.0

S48. IR spectrum of compound 5



S49. ECD and UV spectra of compound 5




Subtracted:0
Absorbance (AU)
0.5
0.4
0.3
0.2
0.1
0
200
220
240
260
280
300
320
340
360
380
400
Wavelength (nm)

S50. HRESIMS of compound 5

Elmt	Val.	Min	Max
H	1	0	300
C	4	0	150
N	3	0	1

Elmt	Val.	Min	Max
O	2	0	20
Cl	1	0	0

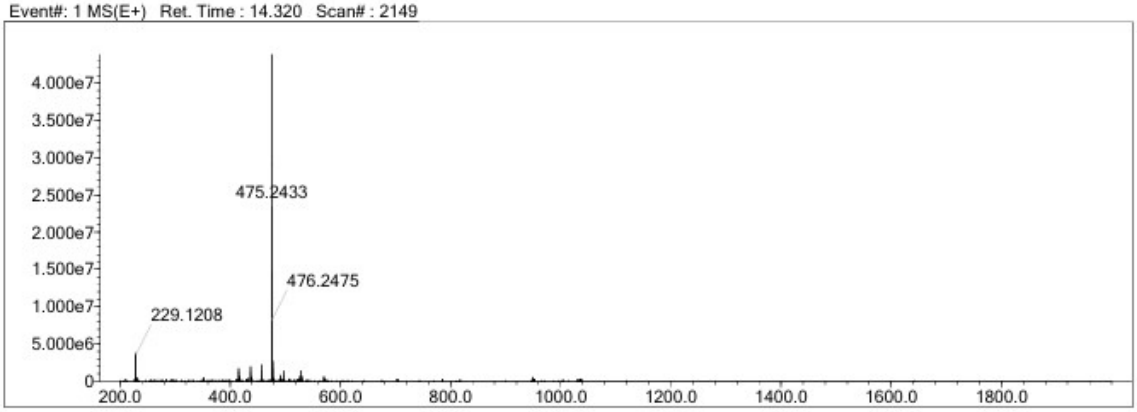
Use Adduct
H
Na

Error Margin (ppm): 100
HC Ratio: unlimited
Max Isotopes: all
MSn Iso RI (%): 75.00

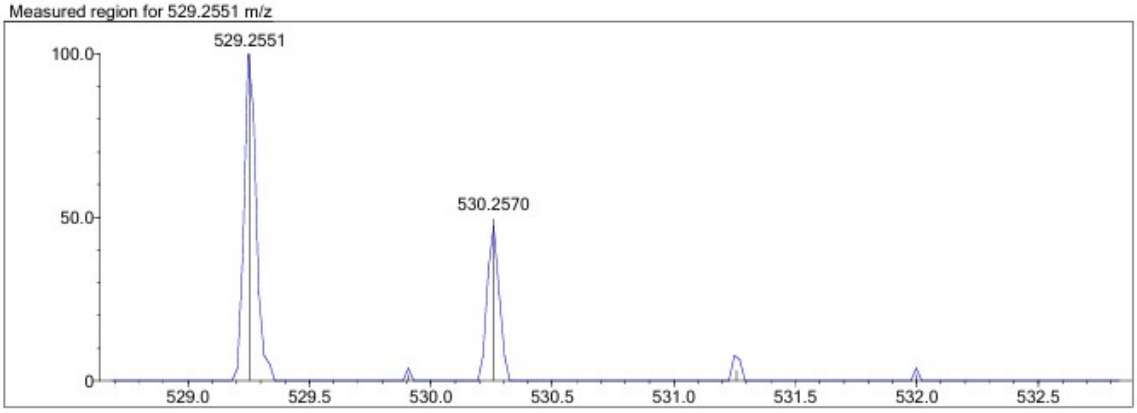
DBE Range: -2.0 - 1000.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

Electron Ions: both
Use MSn Info: no
Isotope Res: 10000
Max Results: 500

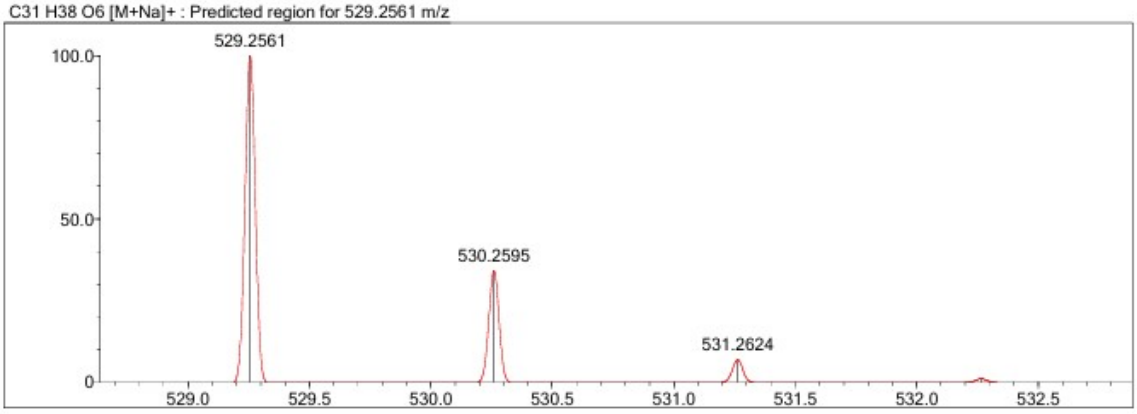
Event#: 1 MS(E+) Ret. Time : 14.320 Scan# : 2149



Measured region for 529.2551 m/z

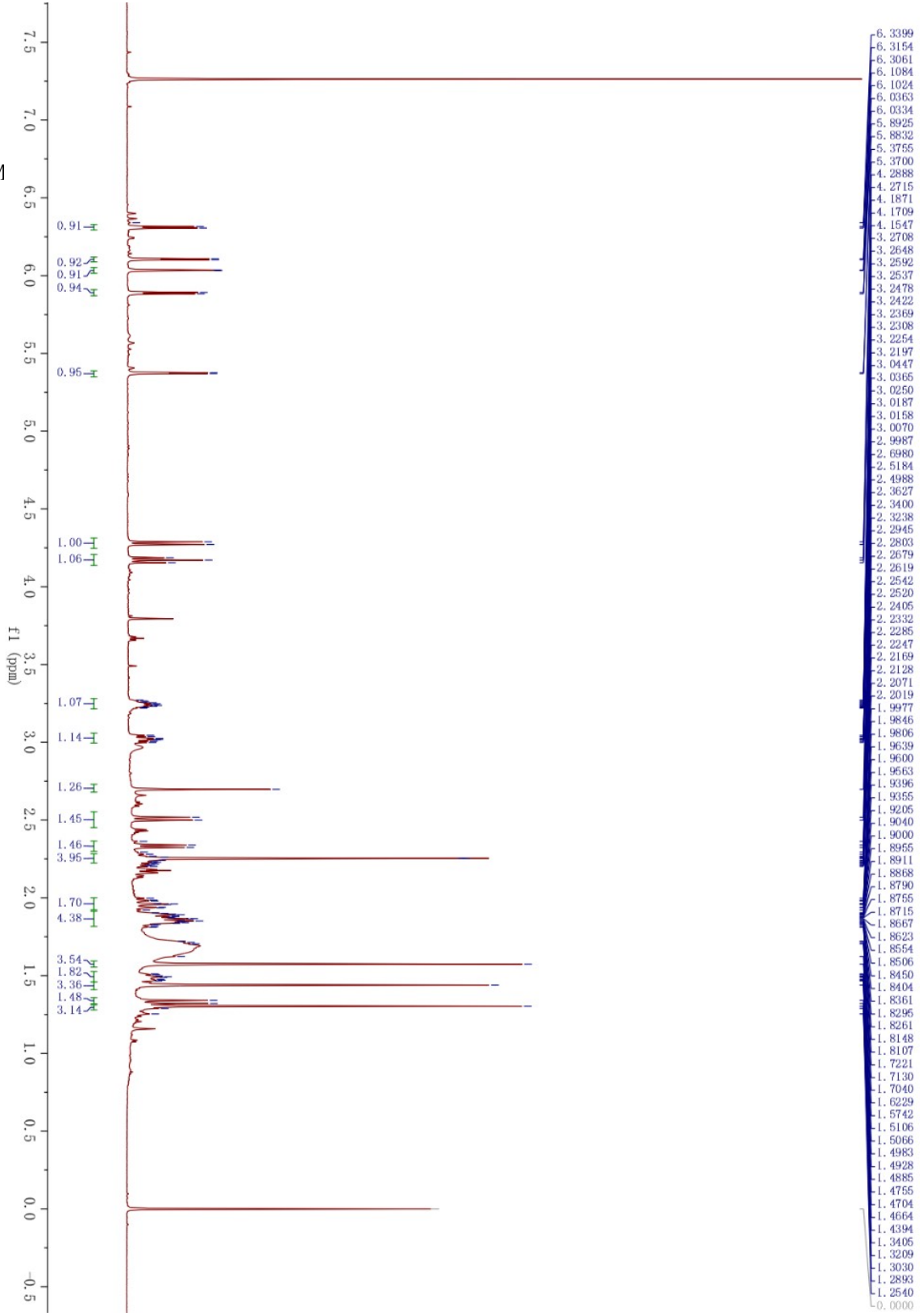


C31 H38 O6 [M+Na]+ : Predicted region for 529.2561 m/z

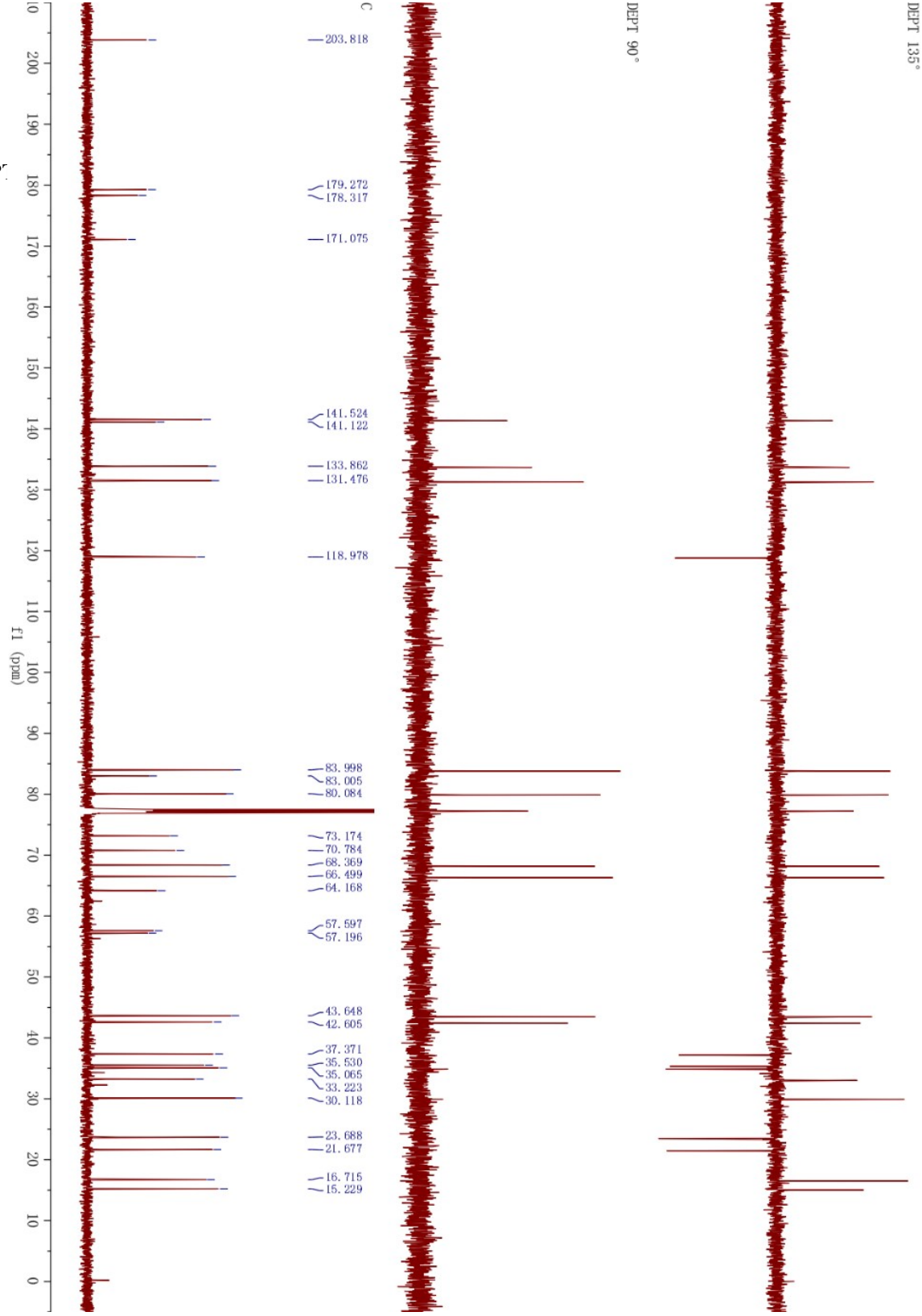


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
2	56.29	C31 H38 O6	[M+Na]+	529.2551	529.2561	-1.0	-1.89	57.57	13.0

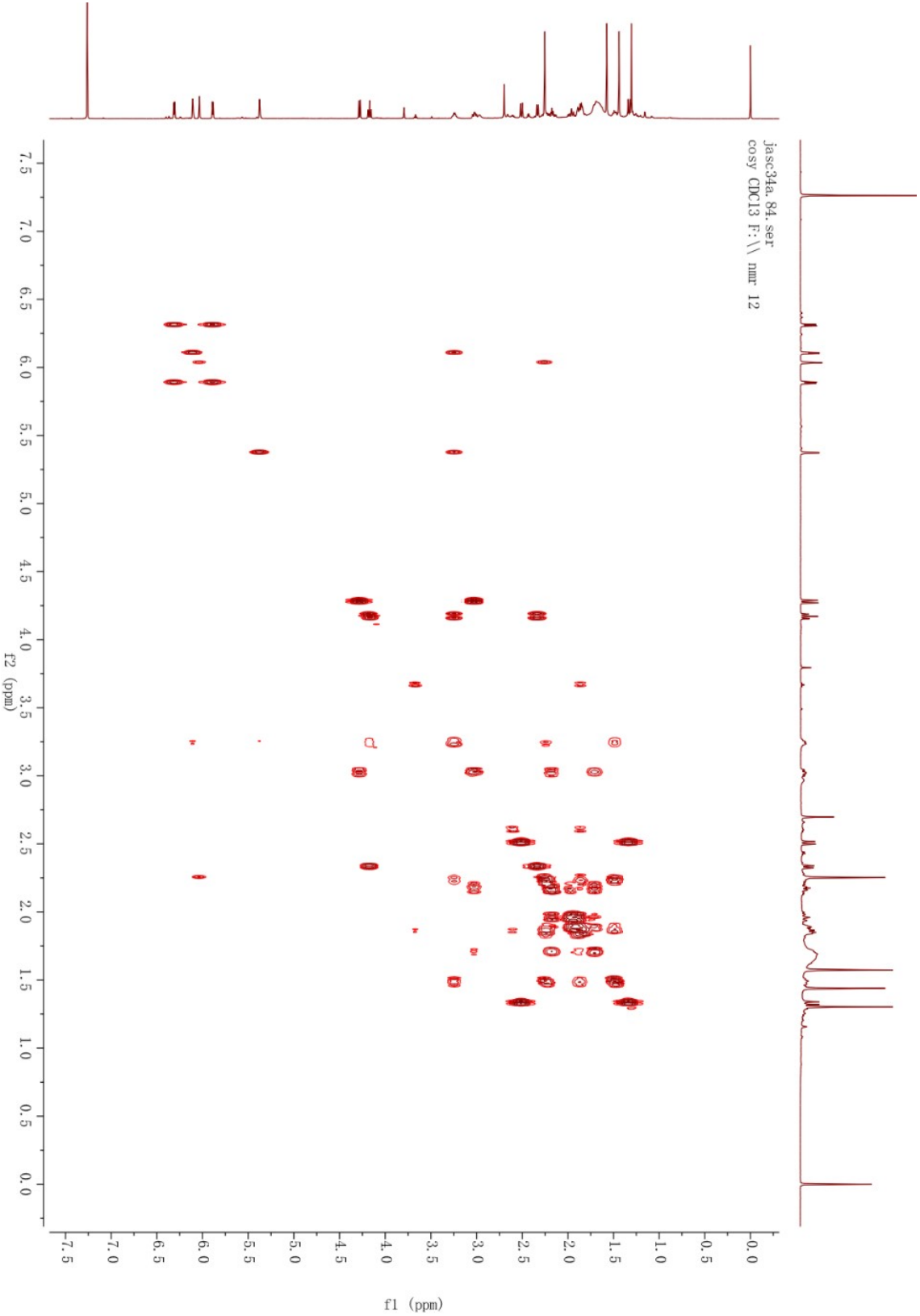
S51. ^{1}H NMR (600 M



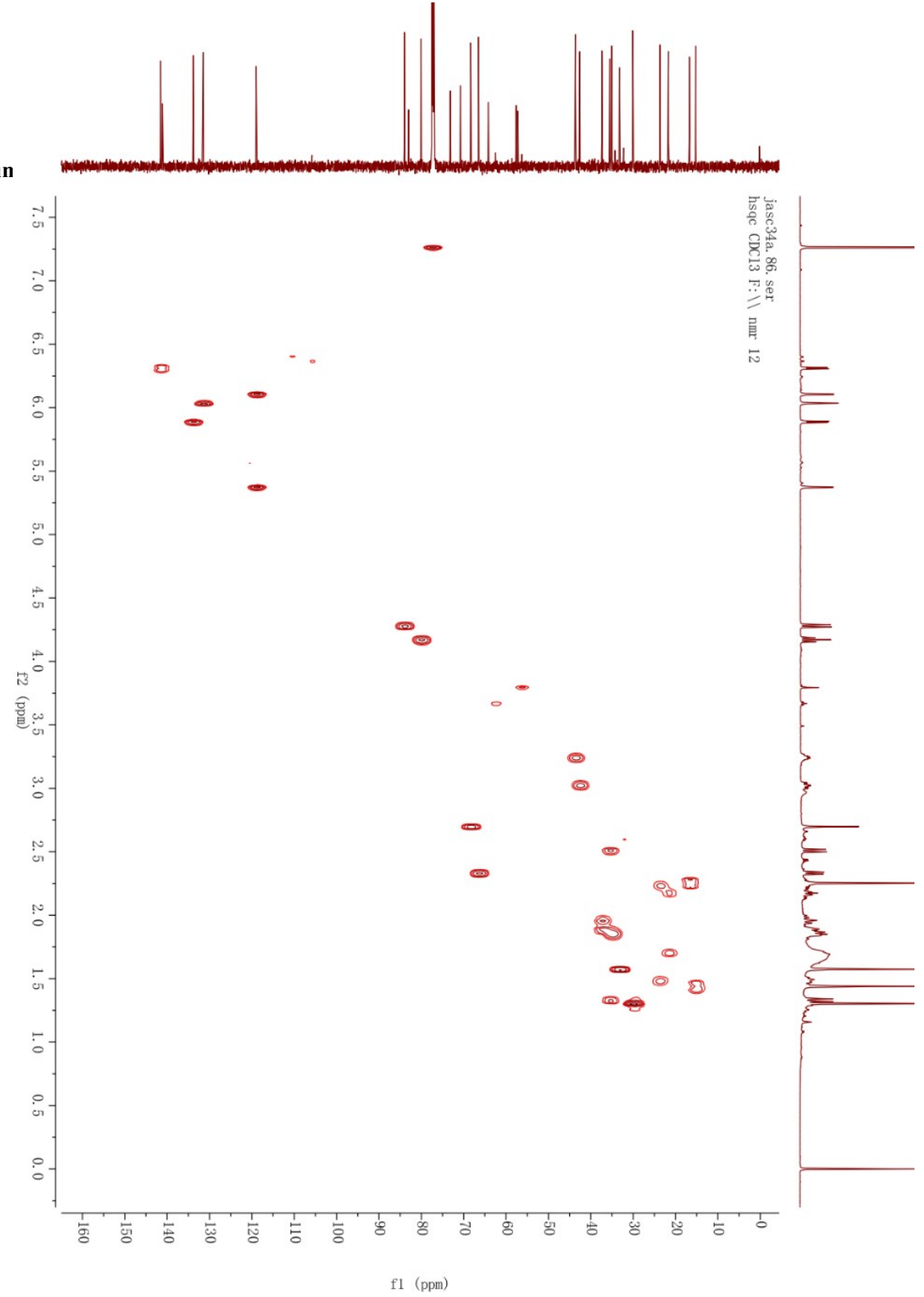
S52. ^{13}C NMR (DEP



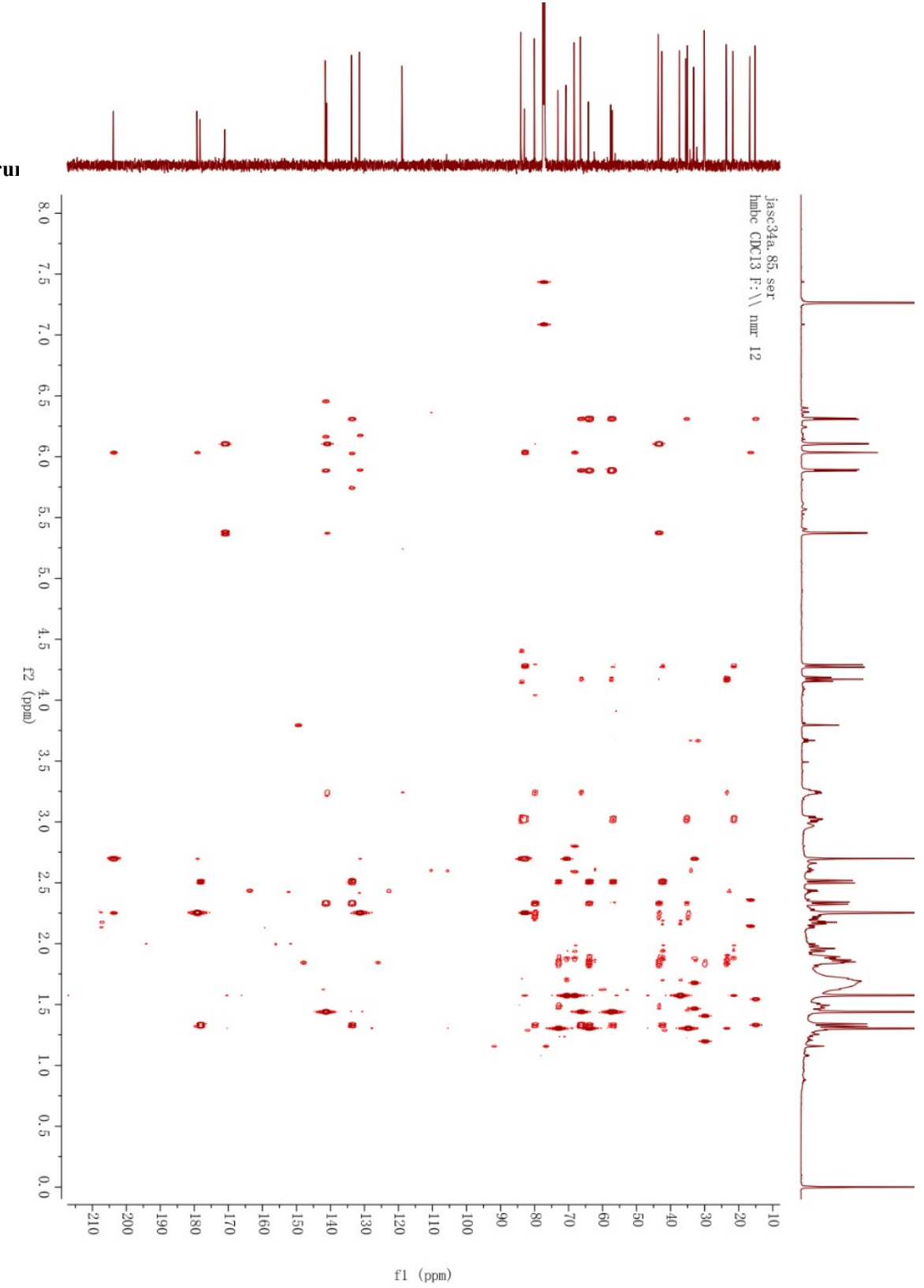
S53. ^{1}H-^{1}H COSY (6



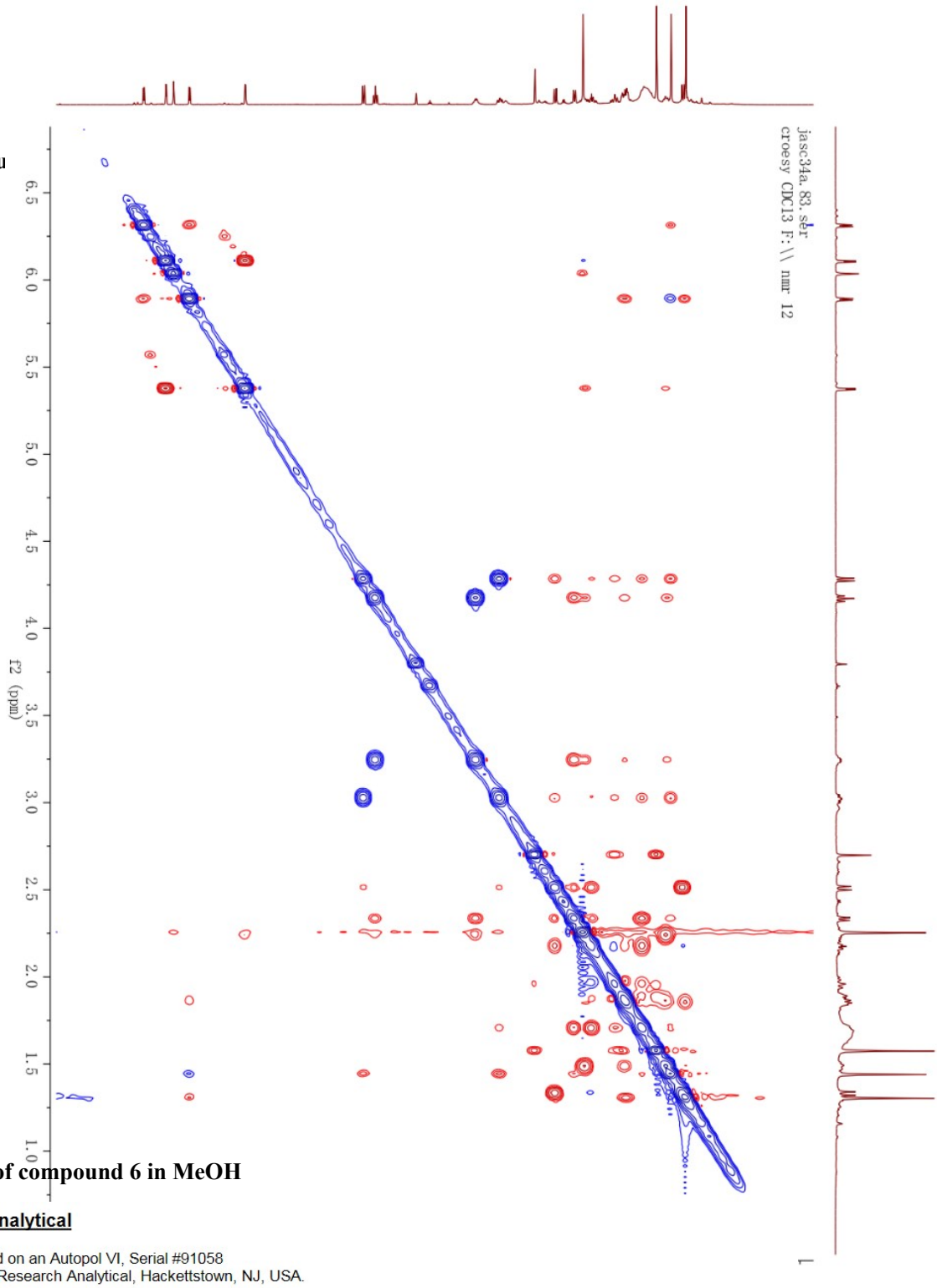
S54. HSQC spectrun



S55. HMBC spectrum



S56. ROESY spectru



S57. $[\alpha]_D$ spectrum of compound 6 in MeOH

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Wednesday, 11-DEC-2024

Set Temperature : 20.0

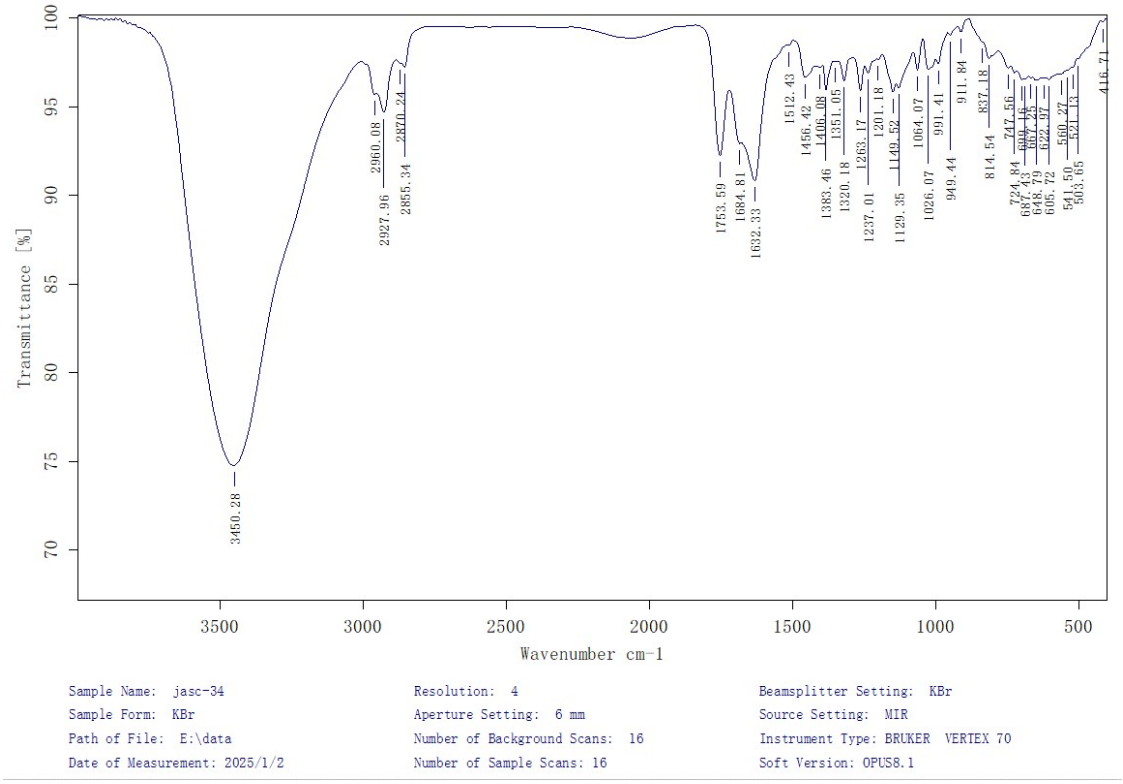
Time Delay : Disabled

Delay between Measurement : Disabled

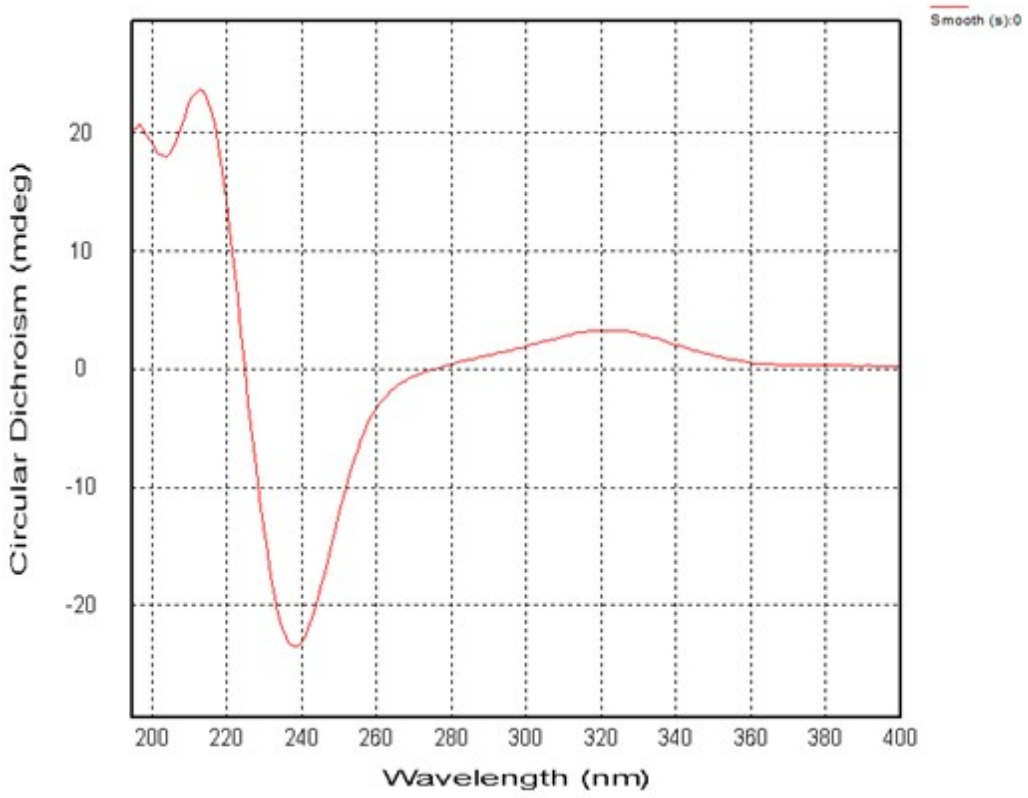
n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	-22.04	2.23	-10.11	-20.41	-24.49

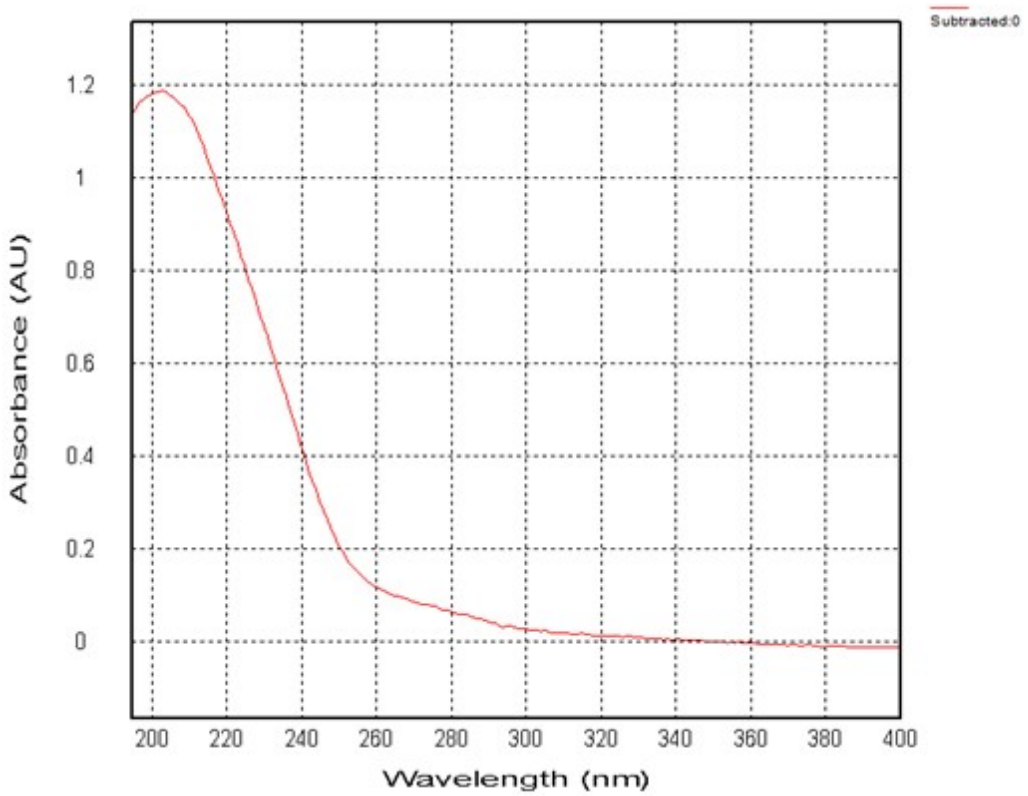
S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	JASC-34	03:08:36 PM	-20.41	SR	-0.010	589	100.00	0.049	20.0
2	JASC-34	03:08:43 PM	-24.49	SR	-0.012	589	100.00	0.049	20.0
3	JASC-34	03:08:49 PM	-20.41	SR	-0.010	589	100.00	0.049	20.0
4	JASC-34	03:08:55 PM	-24.49	SR	-0.012	589	100.00	0.049	20.0
5	JASC-34	03:09:02 PM	-20.41	SR	-0.010	589	100.00	0.049	20.0

S58. IR spectrum of compound 6



S59. ECD and UV spectra of compound 6



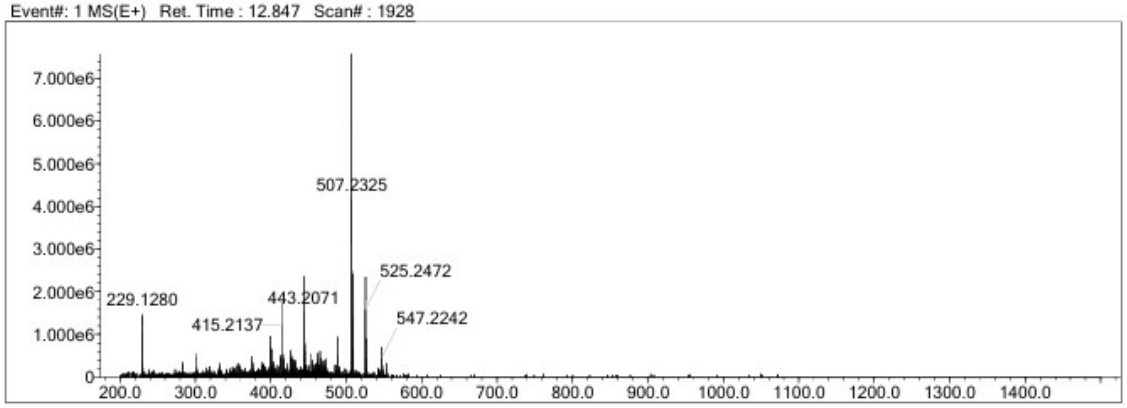


S60. HRESIMS of compound 6

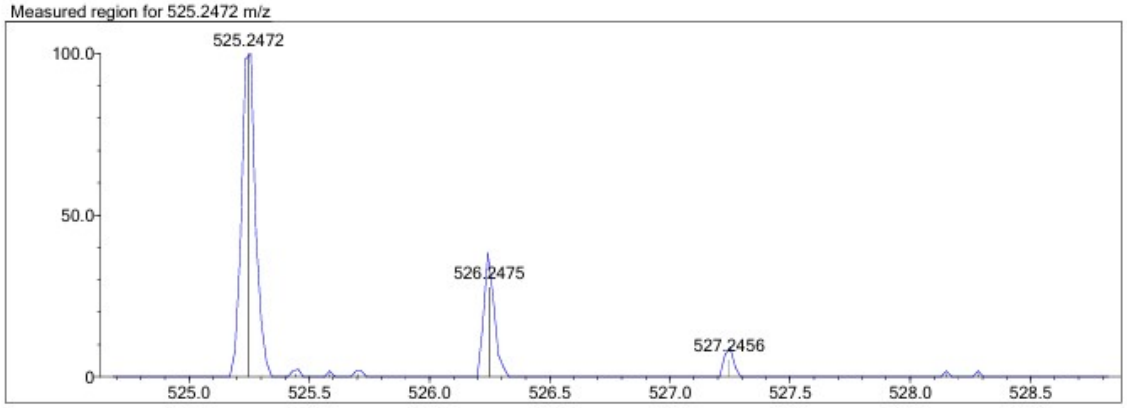
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	300	O	2	0	20	H
C	4	0	150	Cl	1	0	0	Na
N	3	0	1					

Error Margin (ppm):	100	DBE Range:	-2.0 - 1000.0	Electron Ions:	both
HC Ratio:	unlimited	Apply N Rule:	yes	Use MSn Info:	no
Max Isotopes:	all	Isotope RI (%):	1.00	Isotope Res:	10000
MSn Iso RI (%):	75.00	MSn Logic Mode:	AND	Max Results:	500

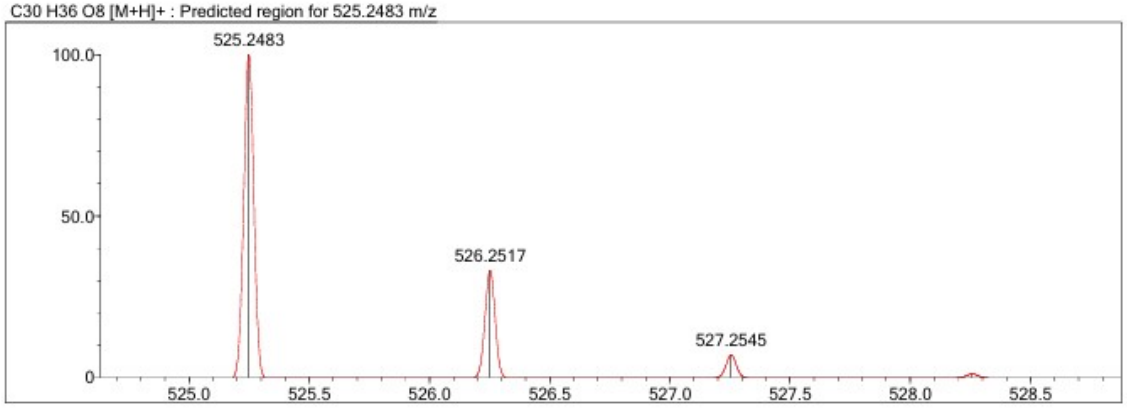
Event#: 1 MS(E+) Ret. Time : 12.847 Scan# : 1928



Measured region for 525.2472 m/z

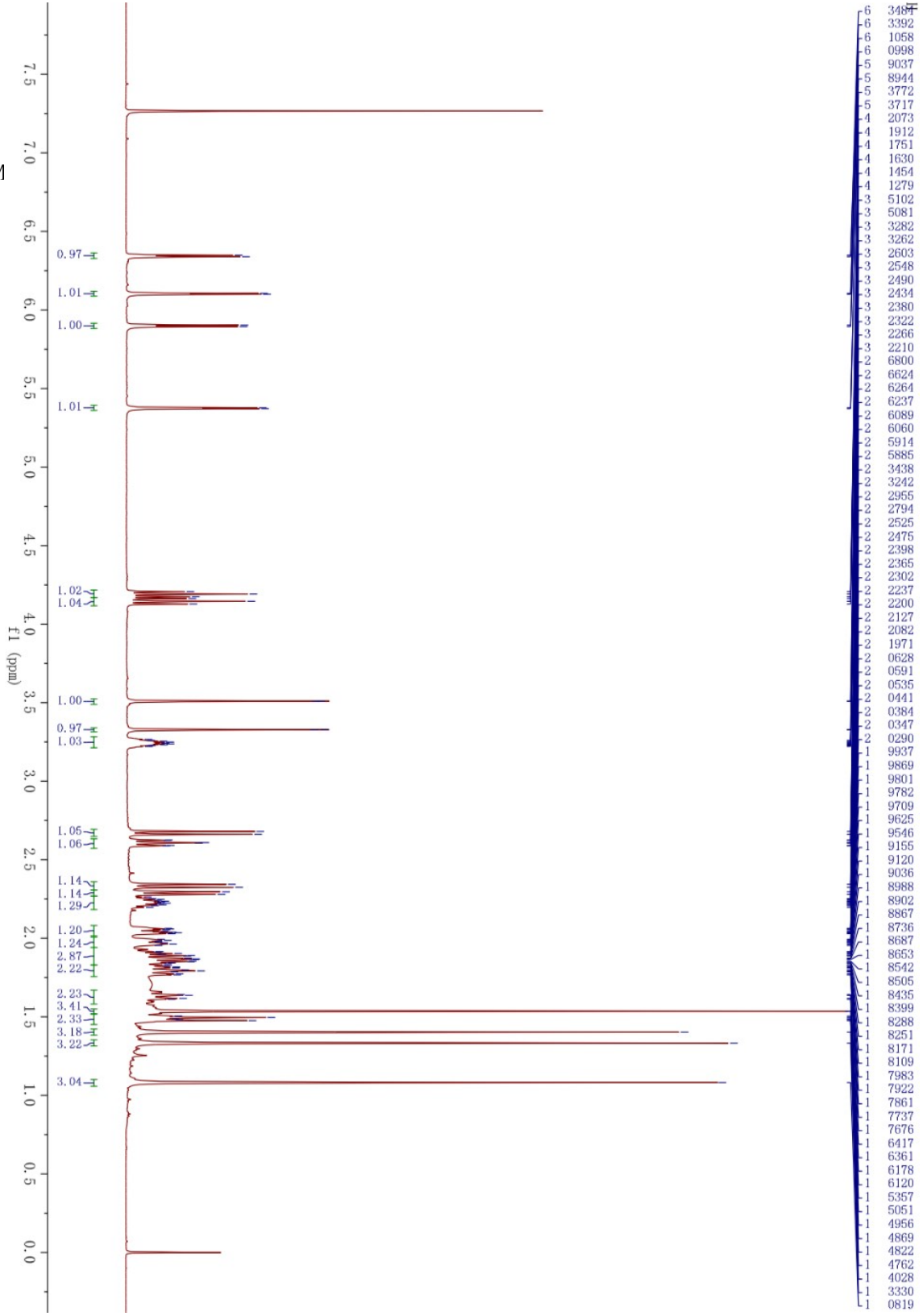


C30 H36 O8 [M+H]+ : Predicted region for 525.2483 m/z

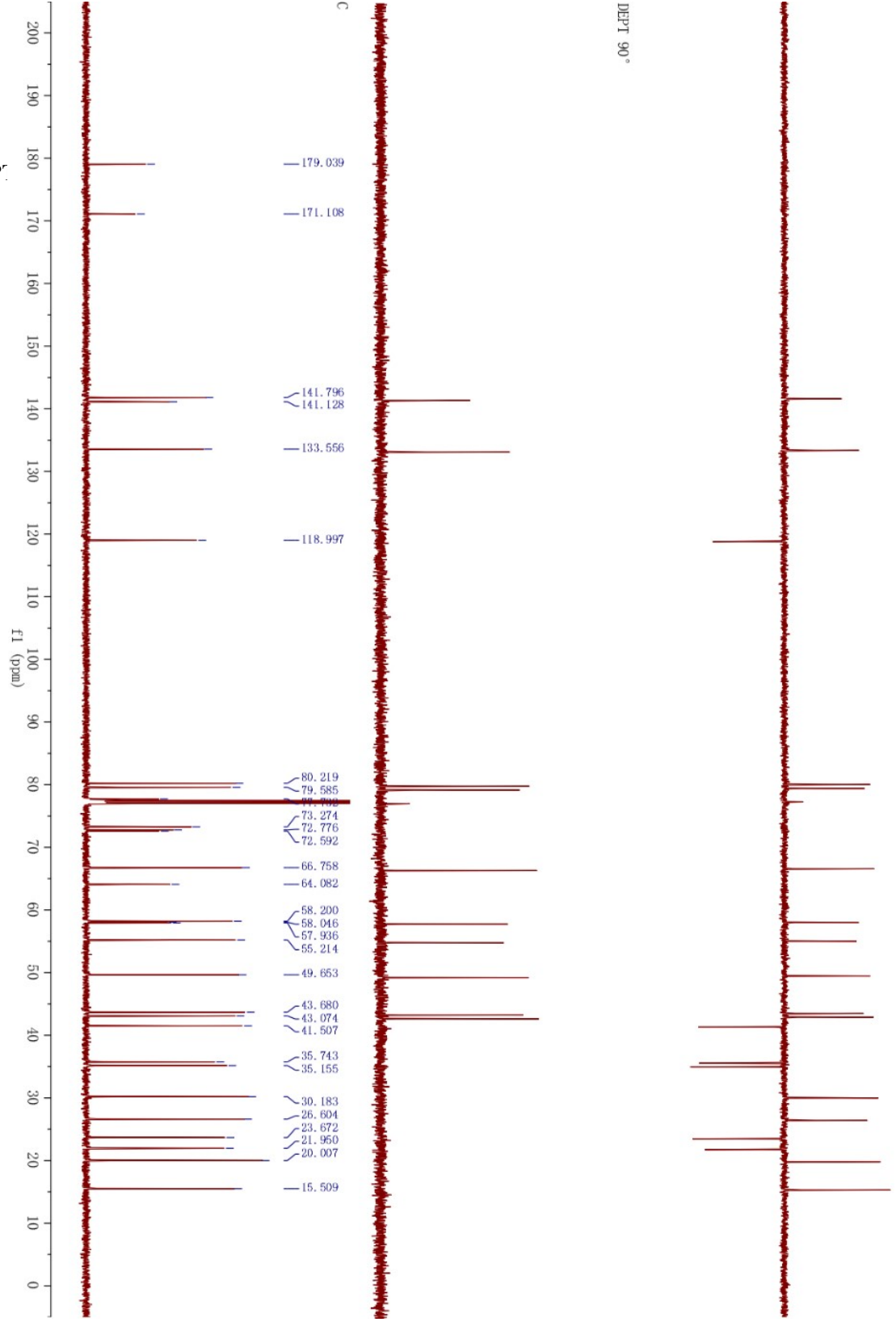


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	80.29	C30 H36 O8	[M+H]+	525.2472	525.2483	-1.1	-2.09	82.54	13.0

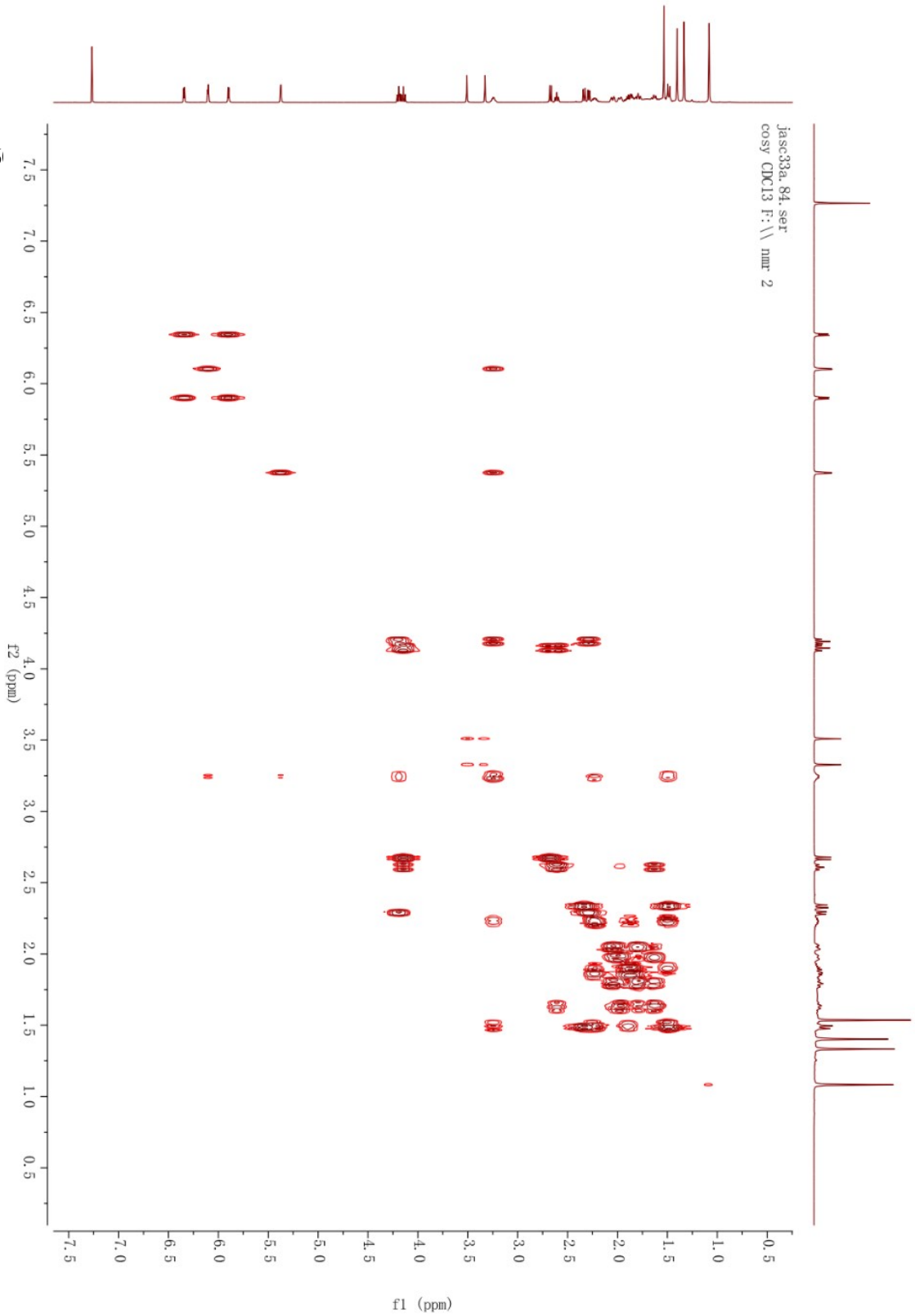
S61. ^{1}H NMR (600 M



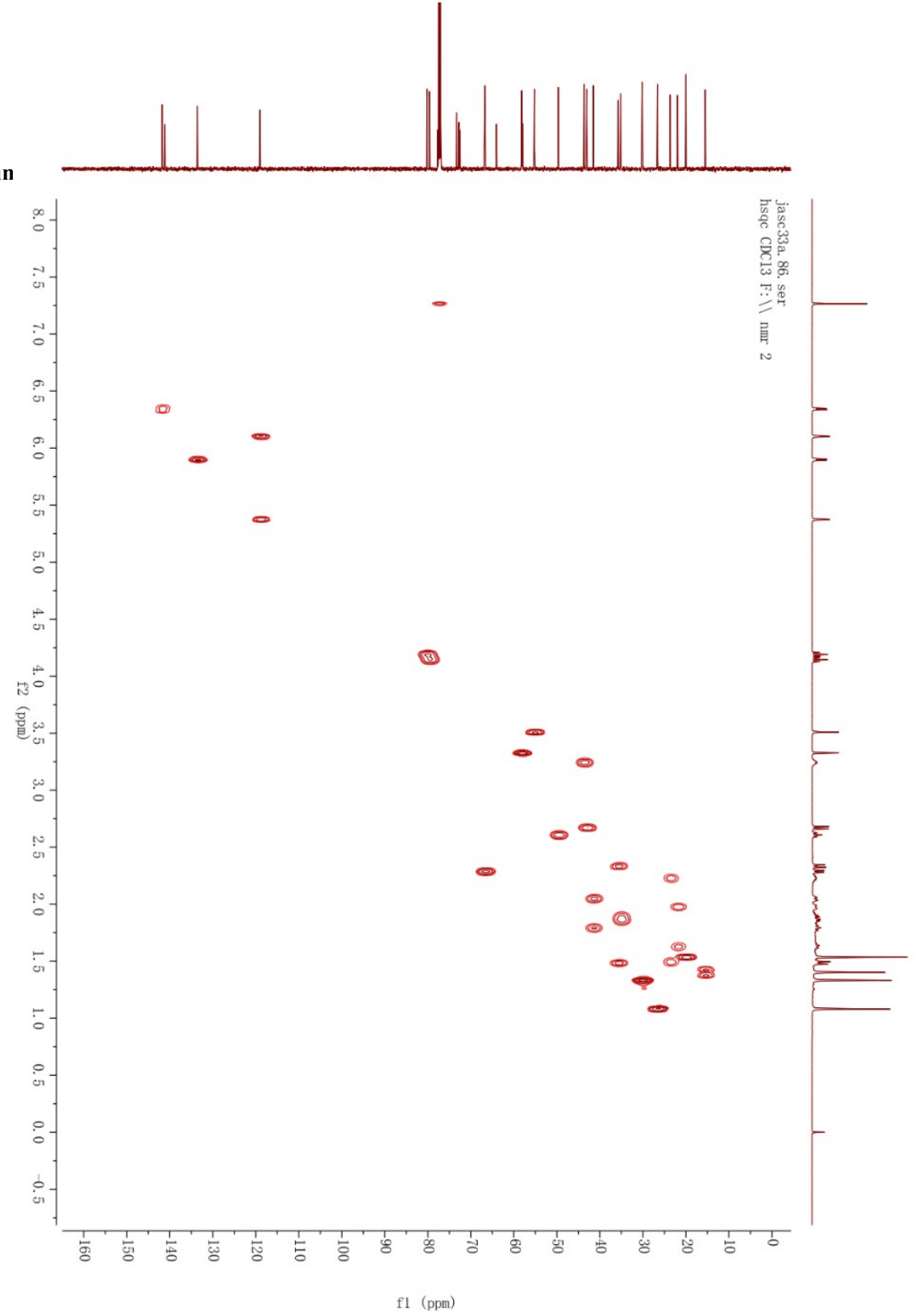
S62. ^{13}C NMR (DEP



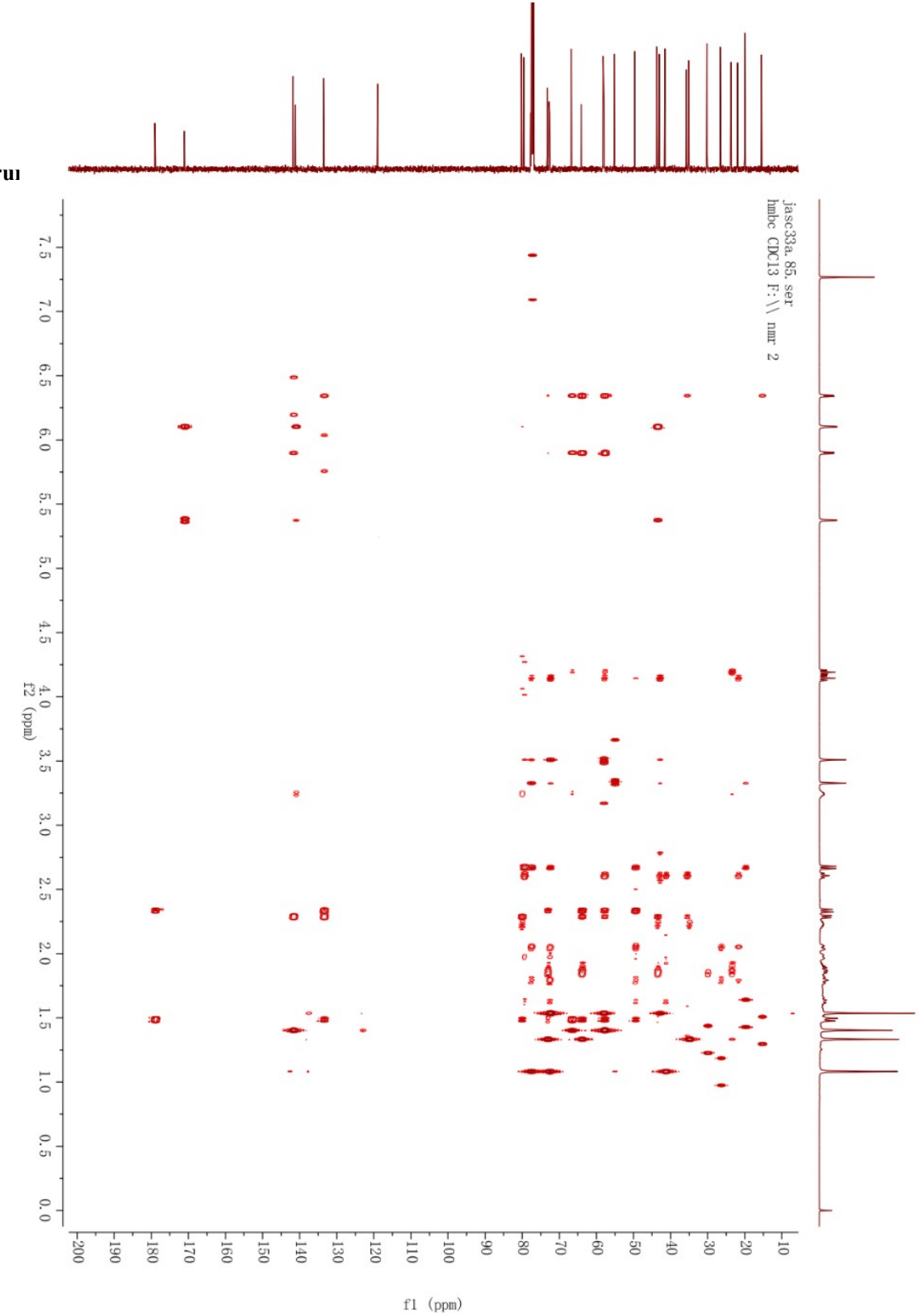
S63. ^{1}H-^{1}H COSY (6



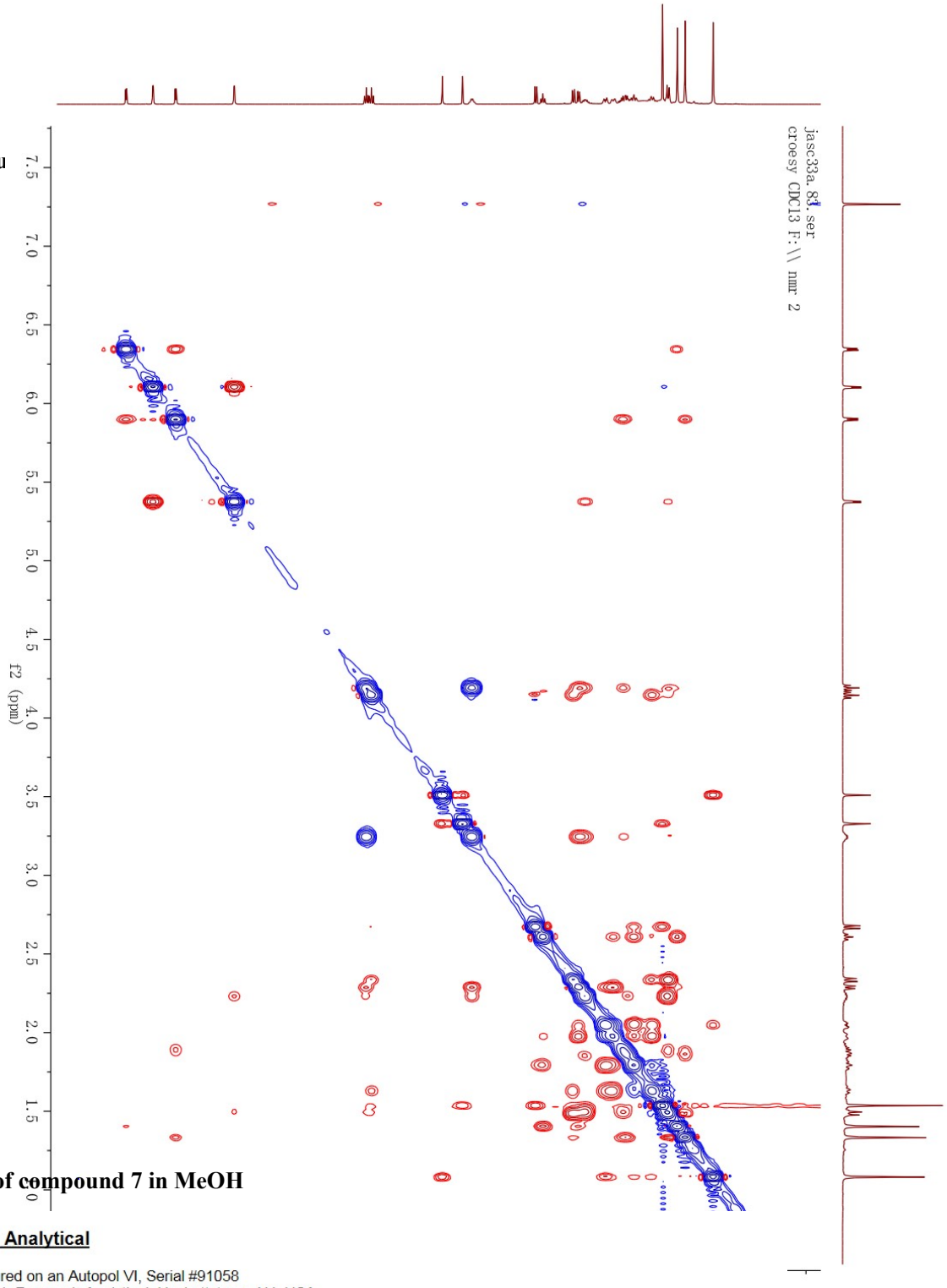
S64. HSQC spectrun



S65. HMBC spectrum



S66. ROESY spectru



S67. $[\alpha]_D$ spectrum of compound 7 in MeOH

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Wednesday, 11-DEC-2024

Set Temperature : 20.0

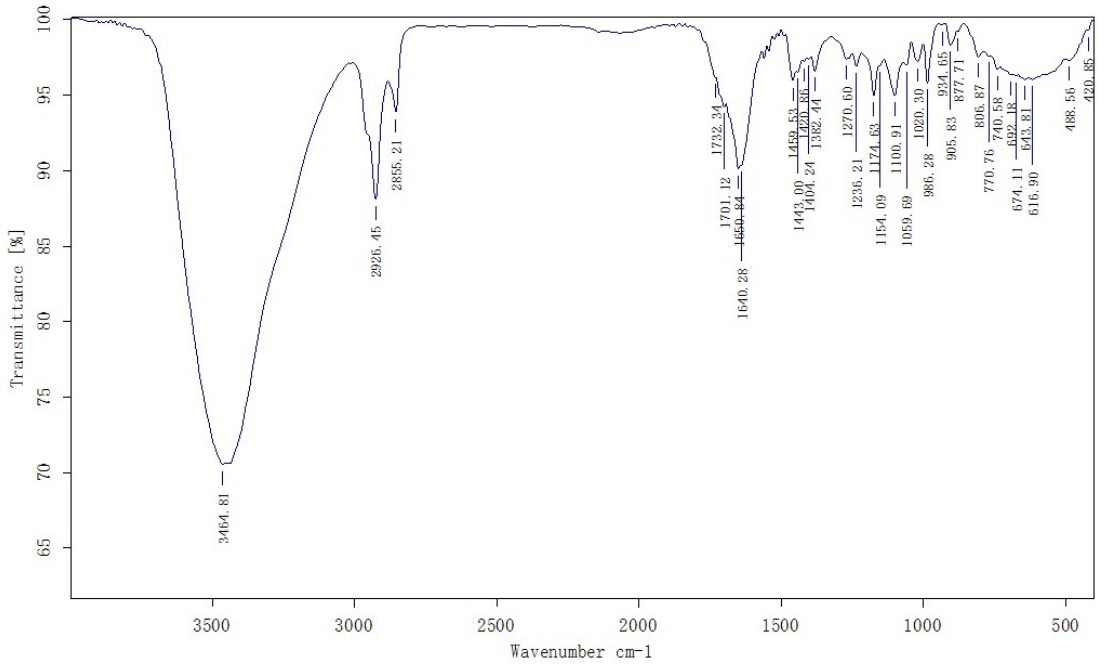
Time Delay : Disabled

Delay between Measurement : Disabled

n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	123.64	1.09	0.88	124.68	122.08

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	JASC-33	02:58:32 PM	123.38	SR	0.095	589	100.00	0.077	20.0
2	JASC-33	02:58:39 PM	123.38	SR	0.095	589	100.00	0.077	20.0
3	JASC-33	02:58:45 PM	124.68	SR	0.096	589	100.00	0.077	20.0
4	JASC-33	02:58:51 PM	122.08	SR	0.094	589	100.00	0.077	20.0
5	JASC-33	02:58:58 PM	124.68	SR	0.096	589	100.00	0.077	20.0

S68. IR spectrum of compound 7

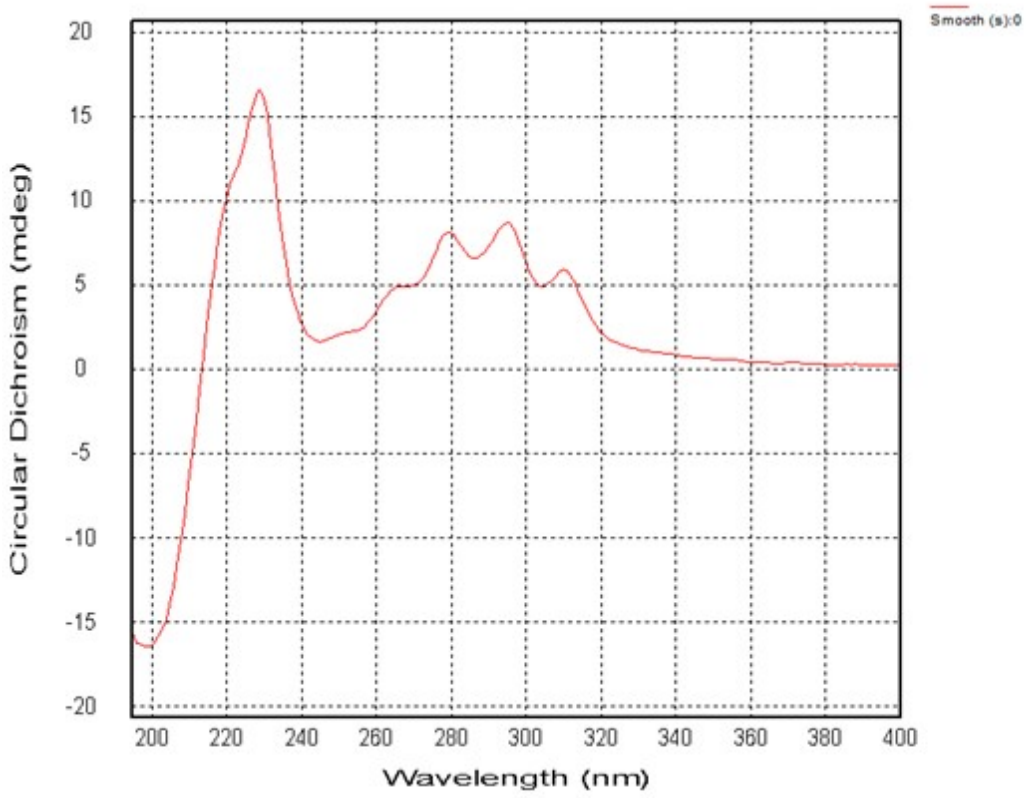


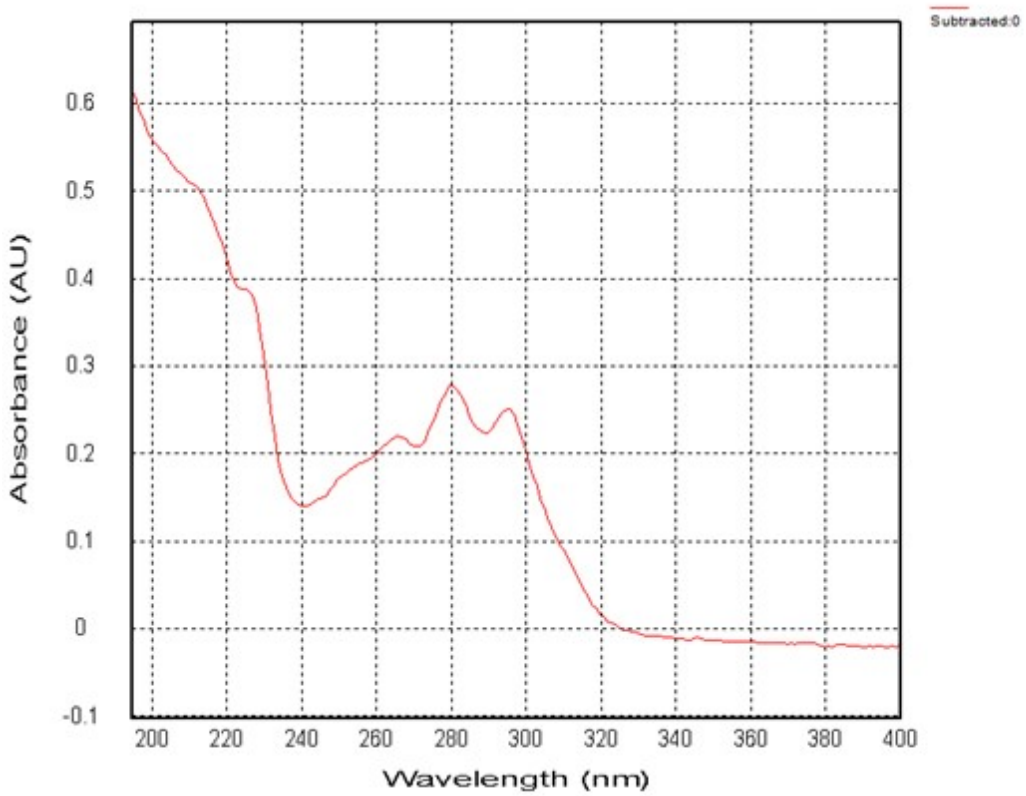
Sample Name: jasc-33
Sample Form: KBr
Path of File: E:\data
Date of Measurement: 2024/12/31

Resolution: 4
Aperture Setting: 6 mm
Number of Background Scans: 16
Number of Sample Scans: 16

Beamsplitter Setting: KBr
Source Setting: MIR
Instrument Type: BRUKER VERTEX 70
Soft Version: OPUS8.1

S69. ECD and UV spectra of compound 7



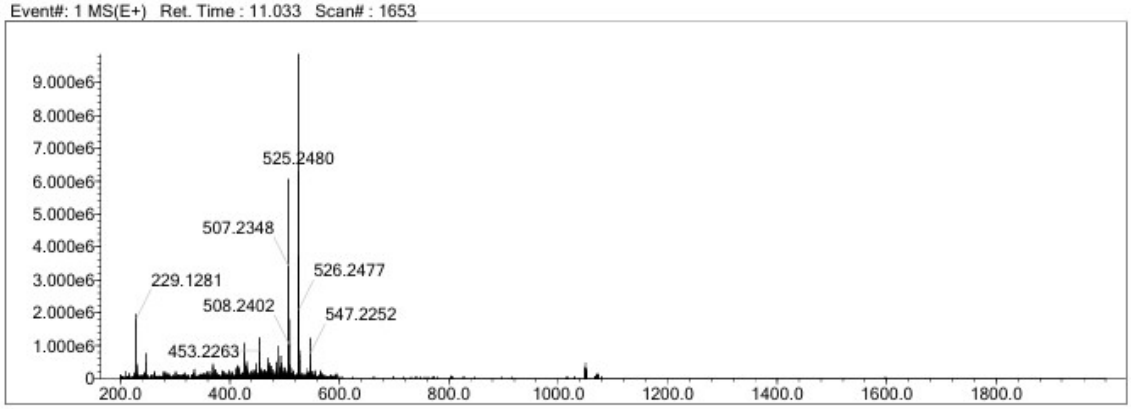


S70. HRESIMS of compound 7

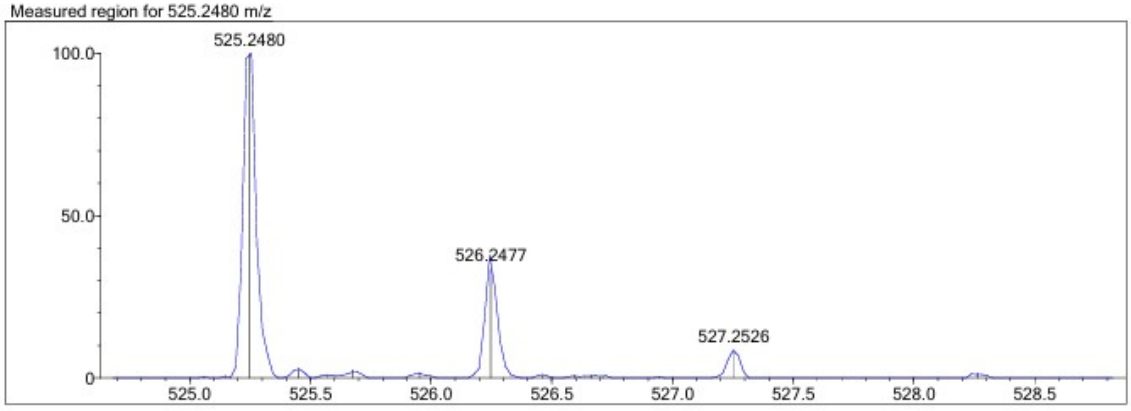
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	300	O	2	0	20	H
C	4	0	150	Cl	1	0	0	Na
N	3	0	1					

Error Margin (ppm):	100	DBE Range:	-2.0 - 1000.0	Electron Ions:	both
HC Ratio:	unlimited	Apply N Rule:	yes	Use MSn Info:	no
Max Isotopes:	all	Isotope RI (%):	1.00	Isotope Res:	10000
MSn Iso RI (%):	75.00	MSn Logic Mode:	AND	Max Results:	500

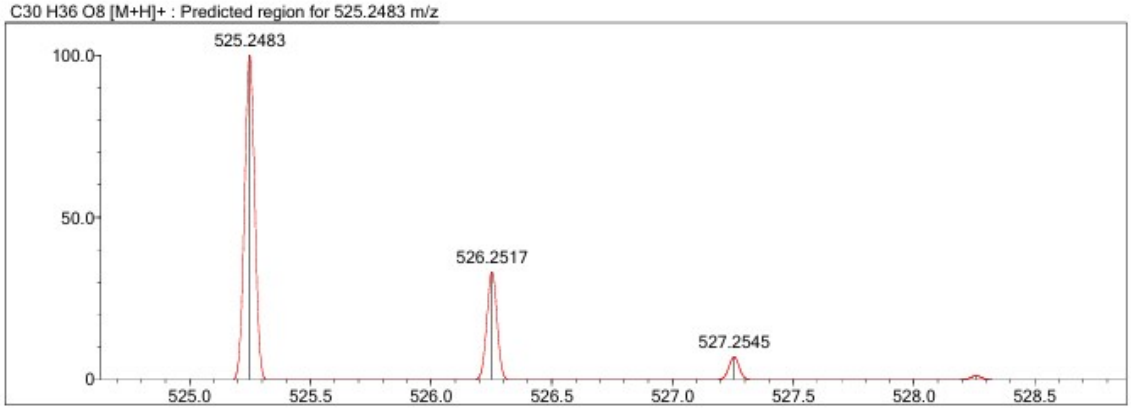
Event#: 1 MS(E+) Ret. Time : 11.033 Scan# : 1653



Measured region for 525.2480 m/z

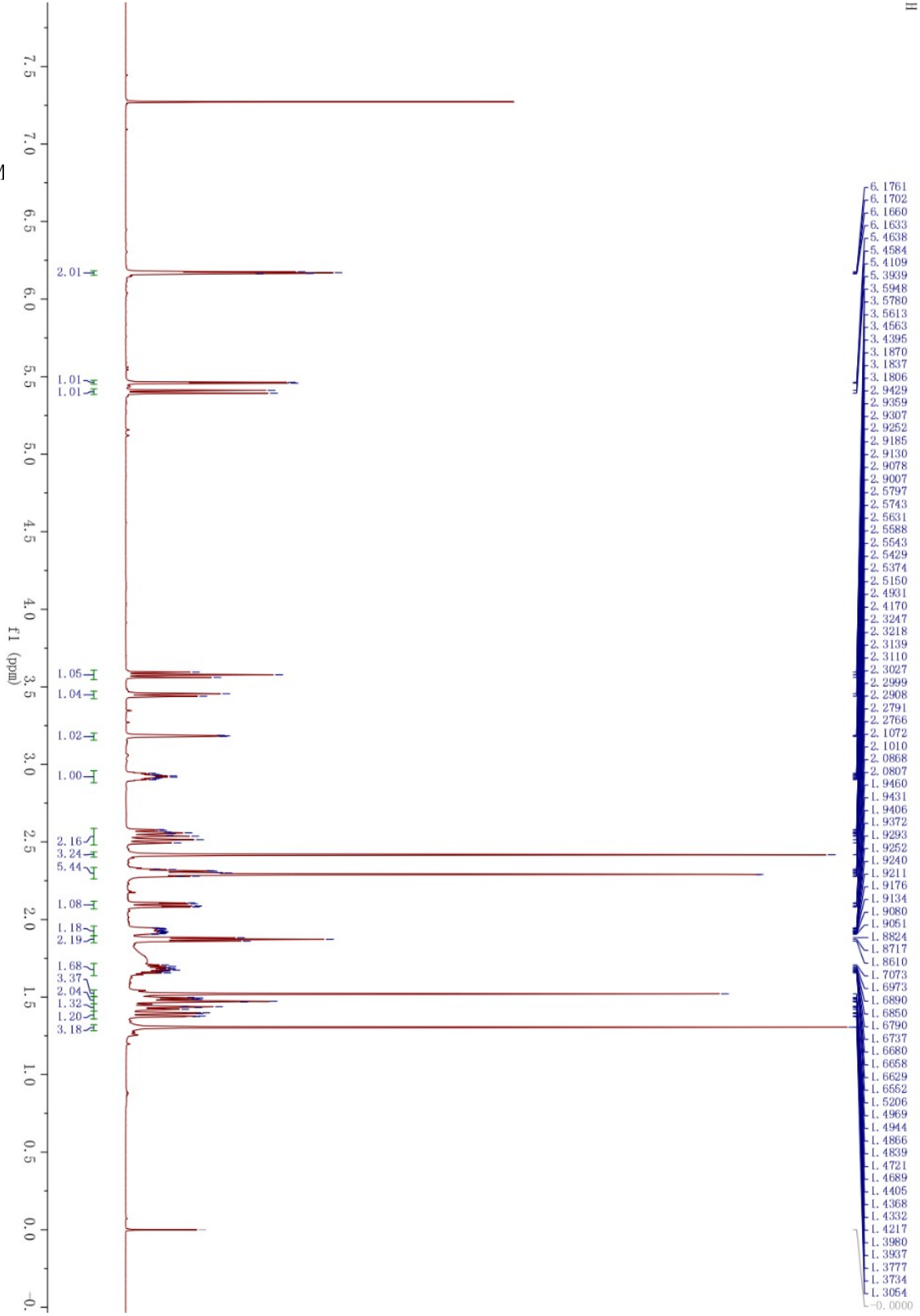


C30 H36 O8 [M+H]+ : Predicted region for 525.2483 m/z

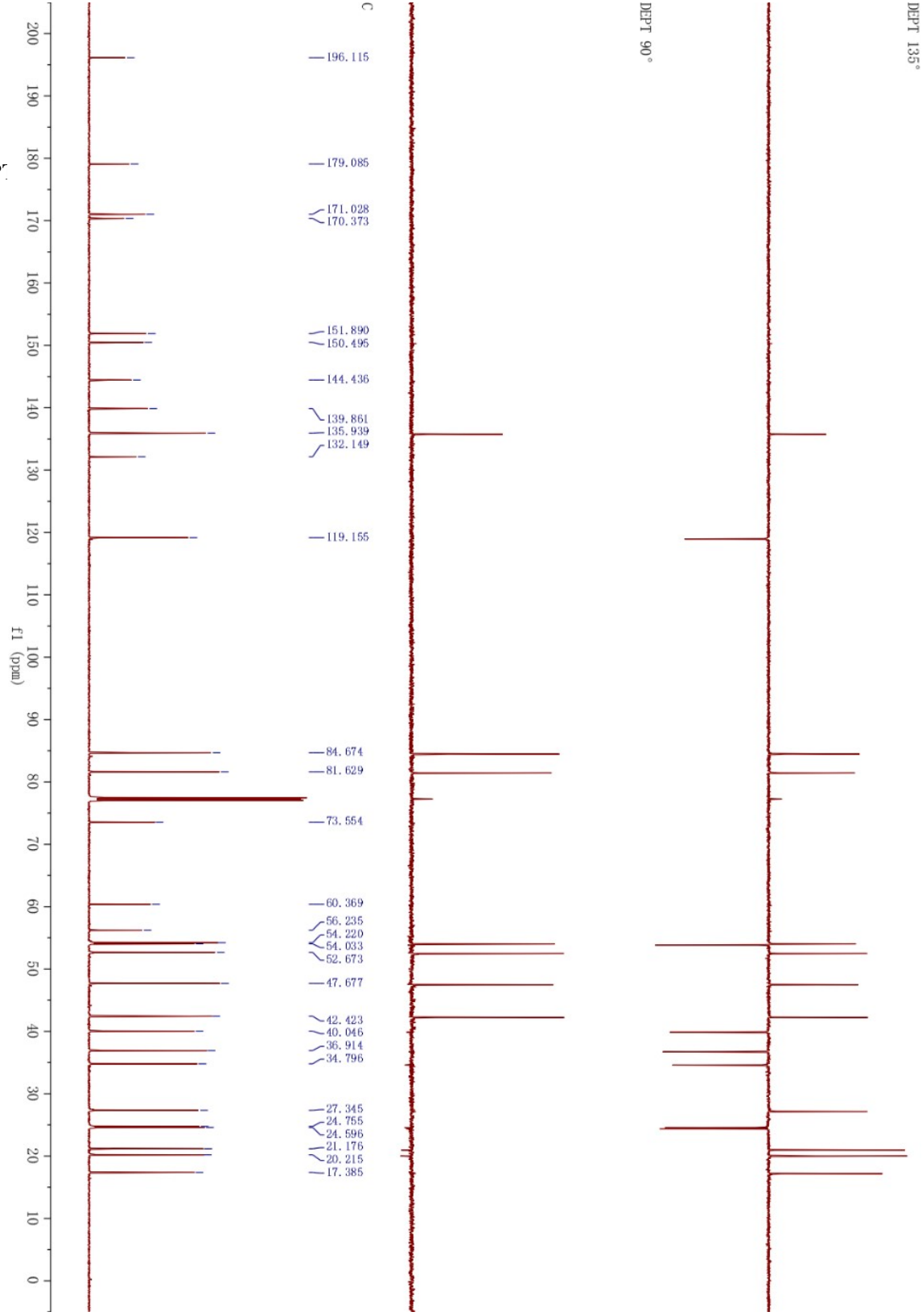


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	86.27	C30 H36 O8	[M+H]+	525.2480	525.2483	-0.3	-0.57	86.27	13.0

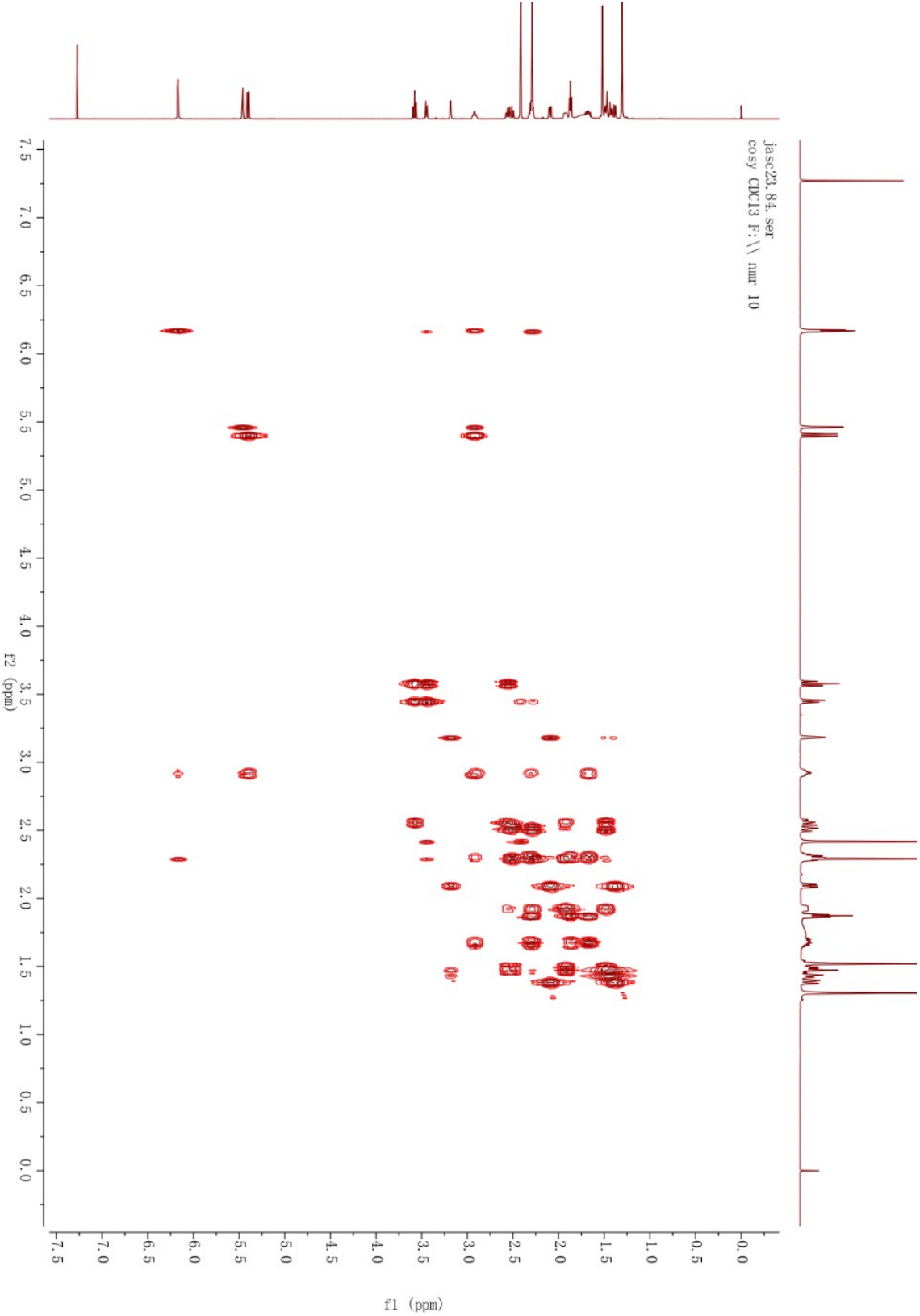
S71. ^{1}H NMR (600 M



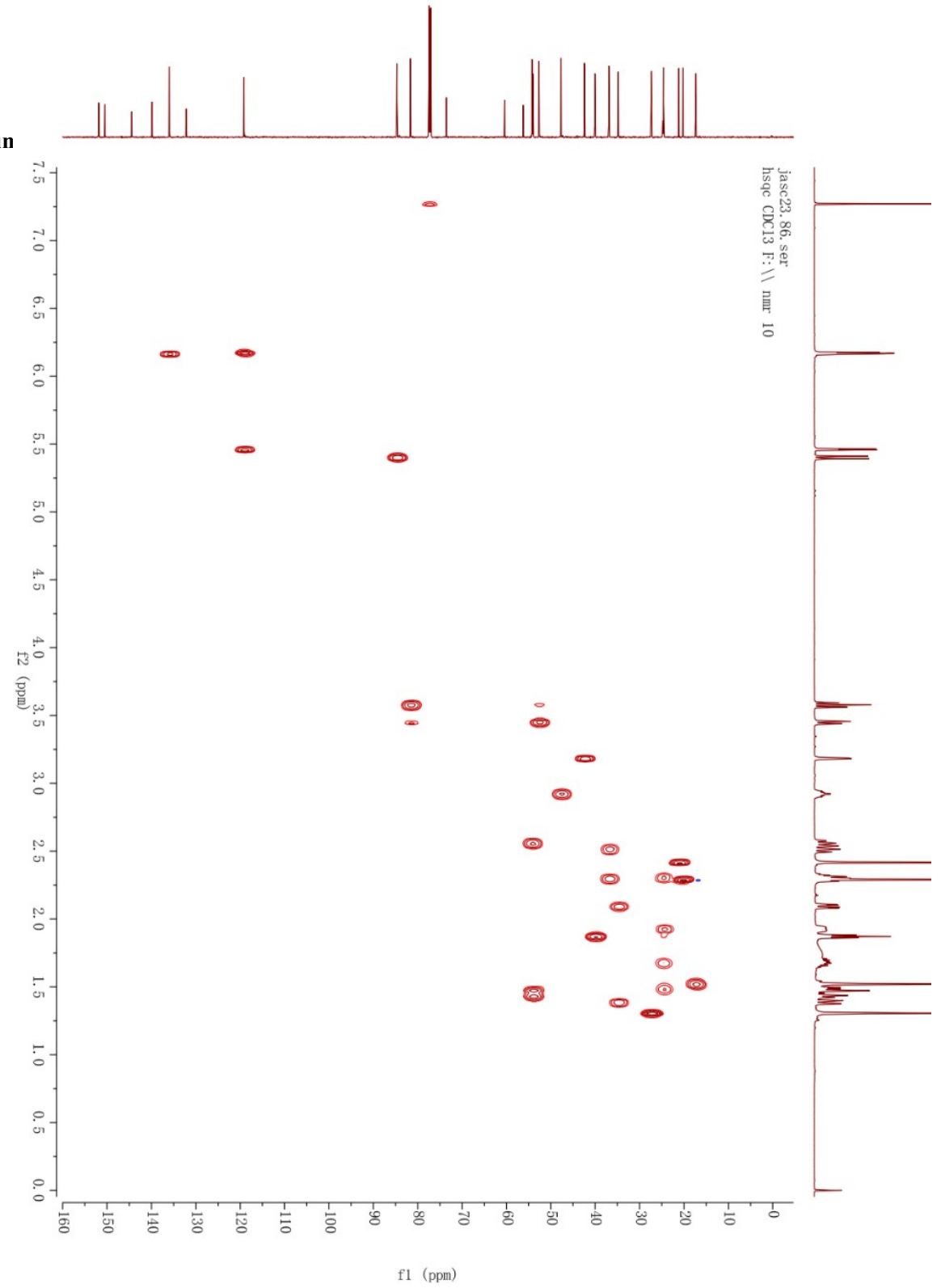
S72. ^{13}C NMR (DEP



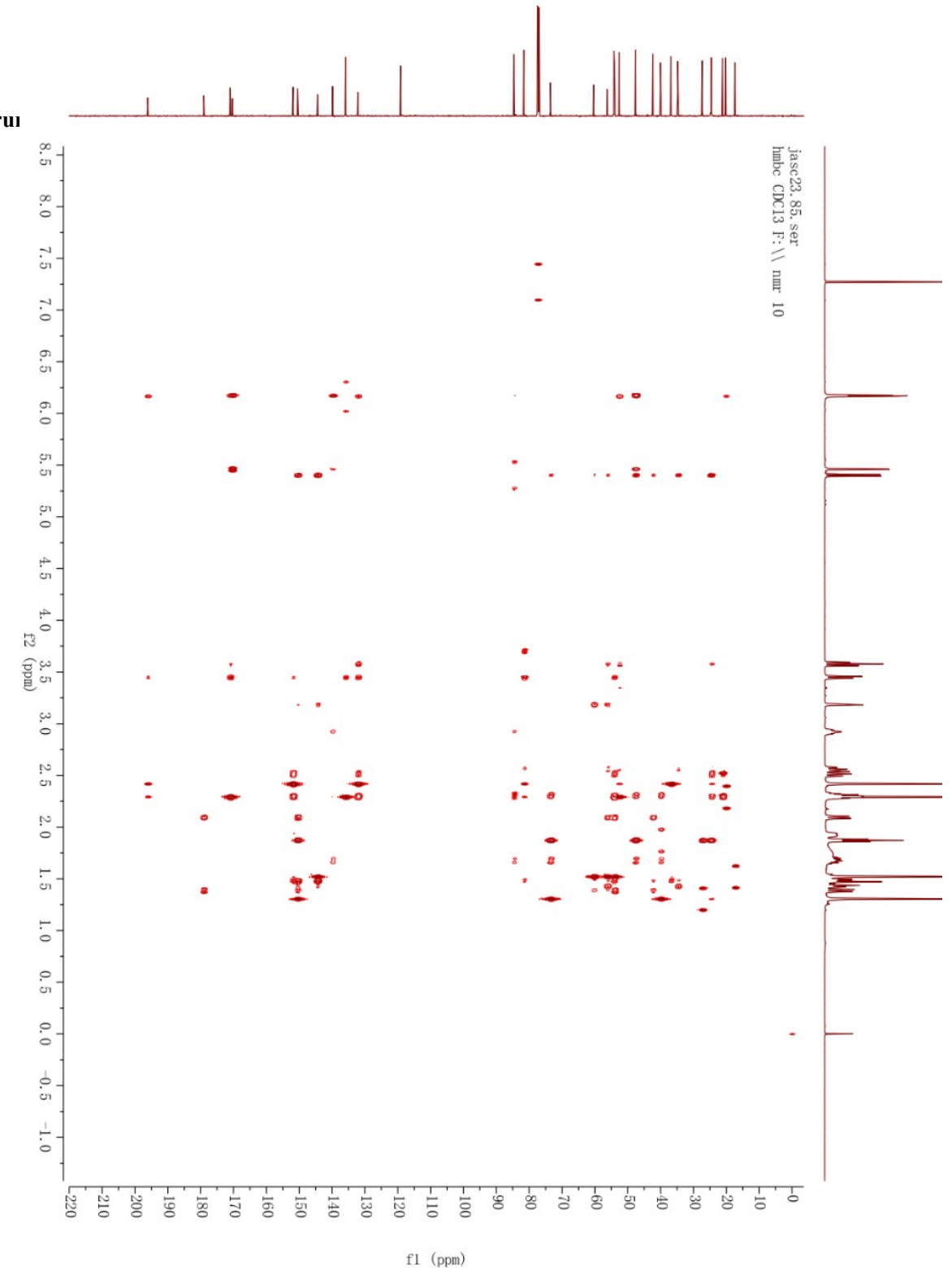
S73. ^{1}H-^{1}H COSY (6



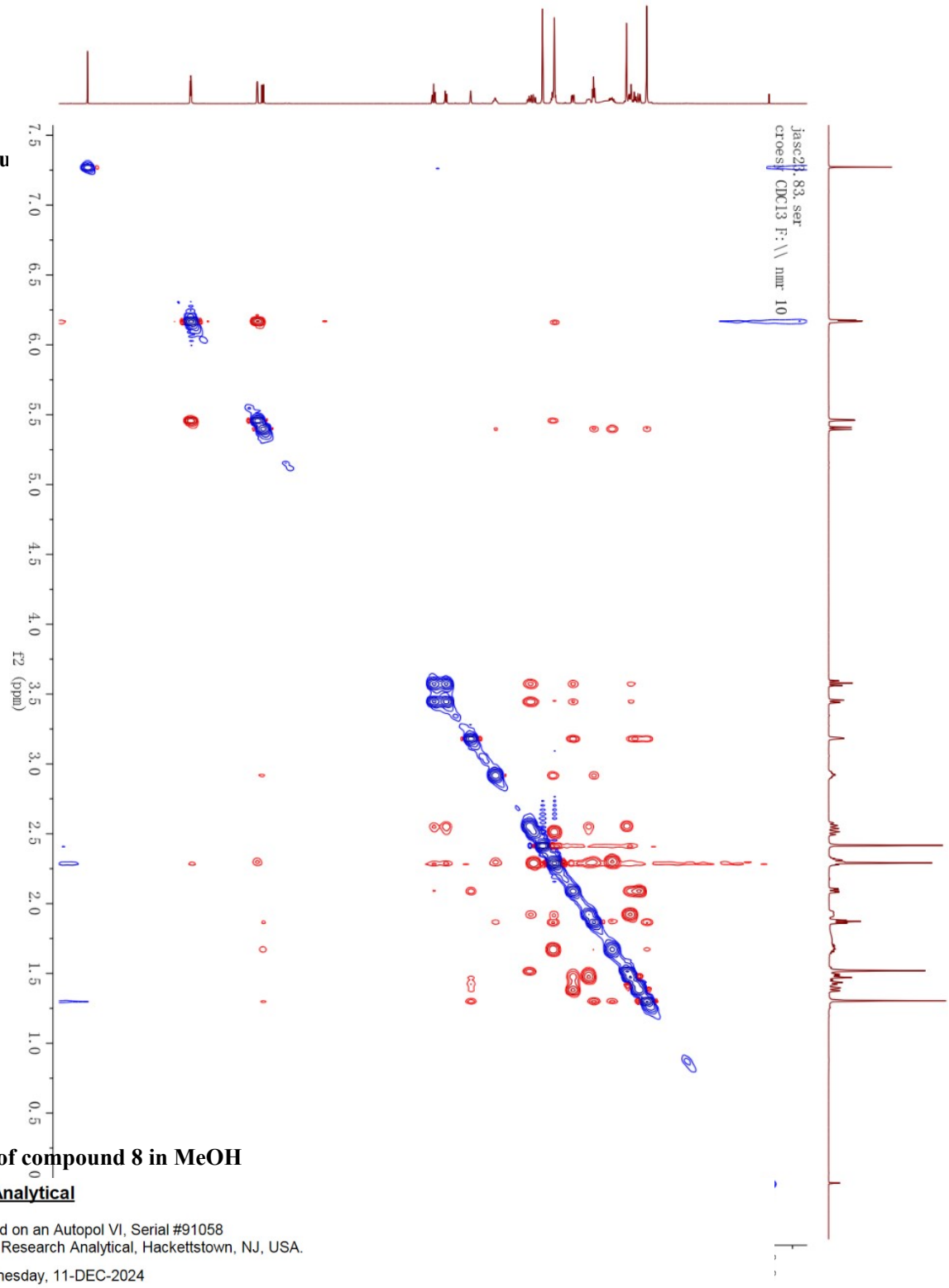
S74. HSQC spectrun



S75. HMBC spectrum



S76. ROESY spectru



S77. $[\alpha]_D$ spectrum of compound 8 in MeOH

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Wednesday, 11-DEC-2024

Set Temperature : 20.0

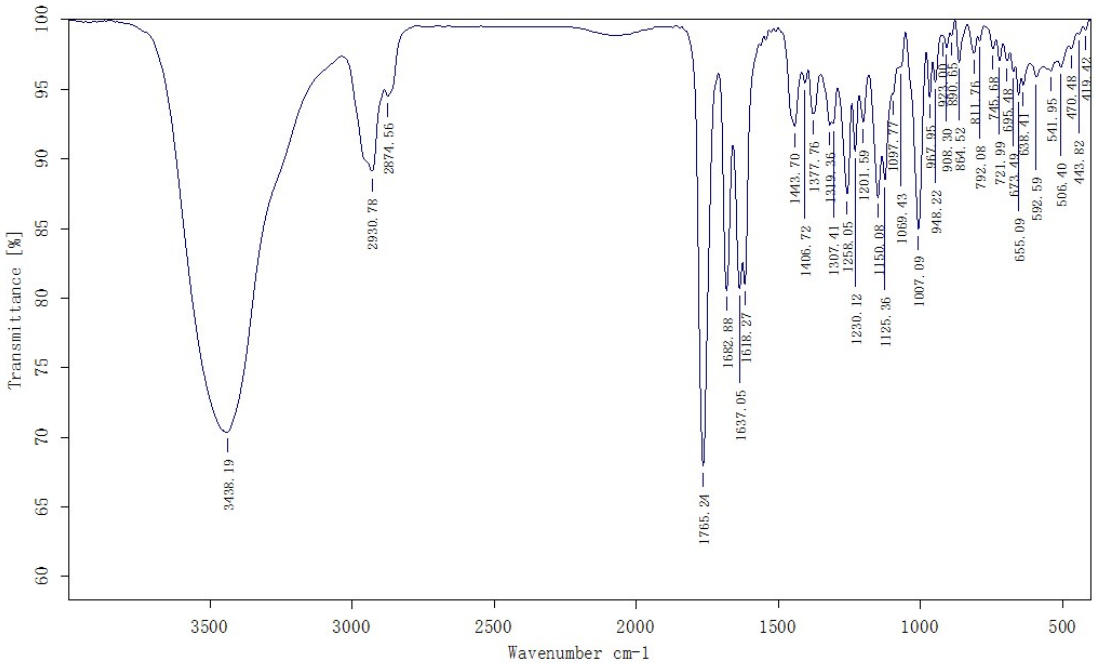
Time Delay : Disabled

Delay between Measurement : Disabled

n	Average	Std.Dev.	% RSD	Maximum	Minimum
5	139.85	0.34	0.24	140.00	139.23

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG.nm	Lg.mm	Conc.g/100ml	Temp.
1	JASC-23	02:30:07 PM	140.00	SR	0.182	589	100.00	0.130	20.0
2	JASC-23	02:30:13 PM	140.00	SR	0.182	589	100.00	0.130	20.0
3	JASC-23	02:30:19 PM	140.00	SR	0.182	589	100.00	0.130	20.0
4	JASC-23	02:30:26 PM	139.23	SR	0.181	589	100.00	0.130	20.0
5	JASC-23	02:30:32 PM	140.00	SR	0.182	589	100.00	0.130	20.0

S78. IR spectrum of compound 8

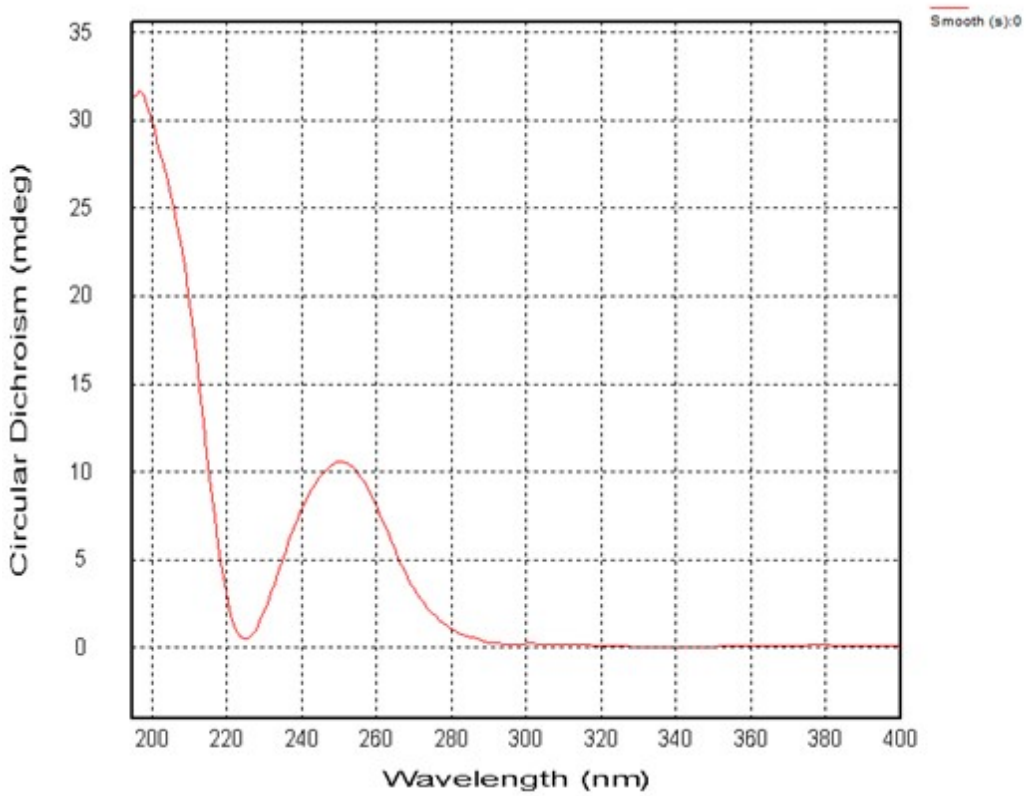


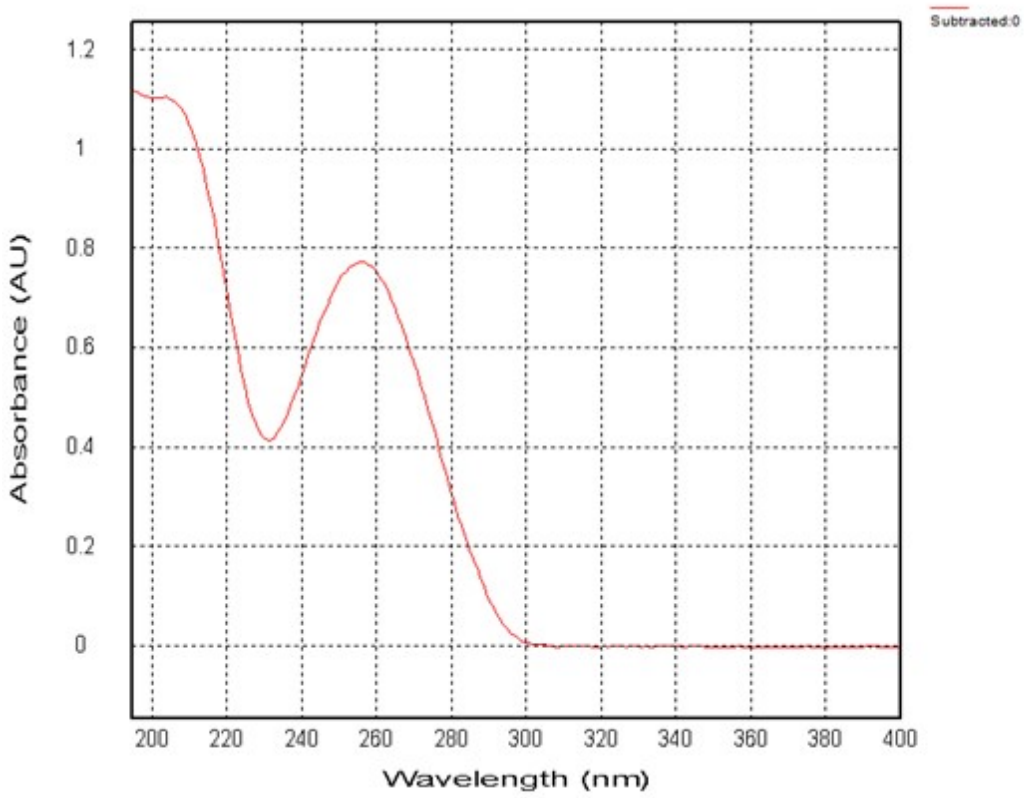
Sample Name: jasc-23
Sample Form: KBr
Path of File: E:\data
Date of Measurement: 2024/12/31

Resolution: 4
Aperture Setting: 6 mm
Number of Background Scans: 16
Number of Sample Scans: 16

Beamsplitter Setting: KBr
Source Setting: MIR
Instrument Type: BRUKER VERTEX 70
Soft Version: OPUS8.1

S79. ECD and UV spectra of compound 8



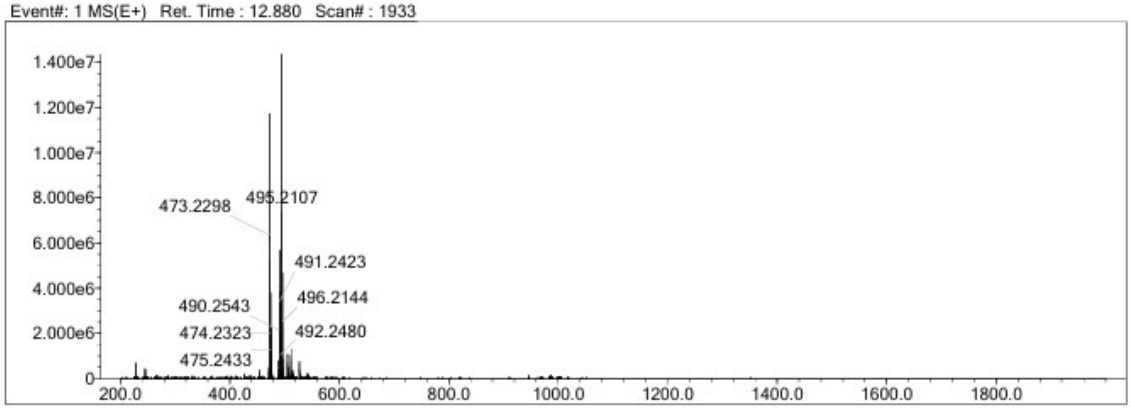

Subtracted:0
Absorbance (AU)
1.2
1
0.8
0.6
0.4
0.2
0
200
220
240
260
280
300
320
340
360
380
400
Wavelength (nm)

S80. HRESIMS of compound 8

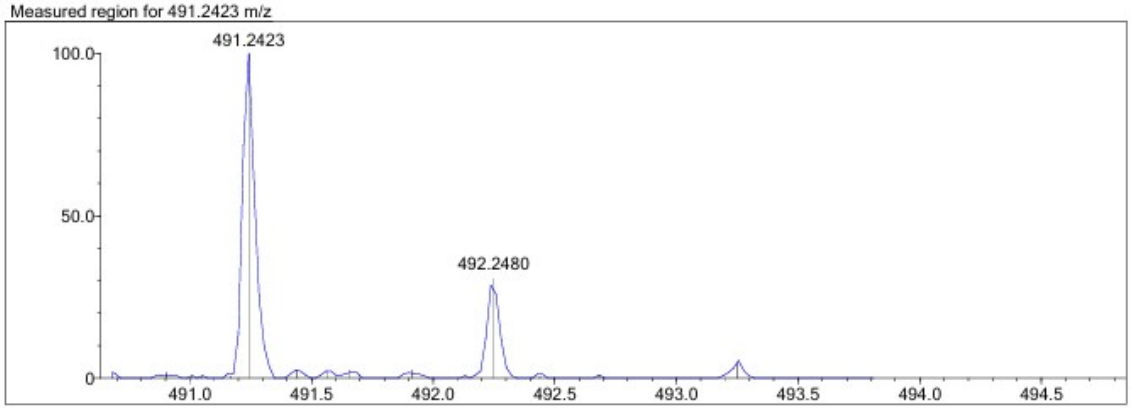
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	300	O	2	0	20	H
C	4	0	150	Cl	1	0	0	Na
N	3	0	1					

Error Margin (ppm):	100	DBE Range:	-2.0 - 1000.0	Electron Ions:	both
HC Ratio:	unlimited	Apply N Rule:	yes	Use MSn Info:	no
Max Isotopes:	all	Isotope RI (%):	1.00	Isotope Res:	10000
MSn Iso RI (%):	75.00	MSn Logic Mode:	AND	Max Results:	500

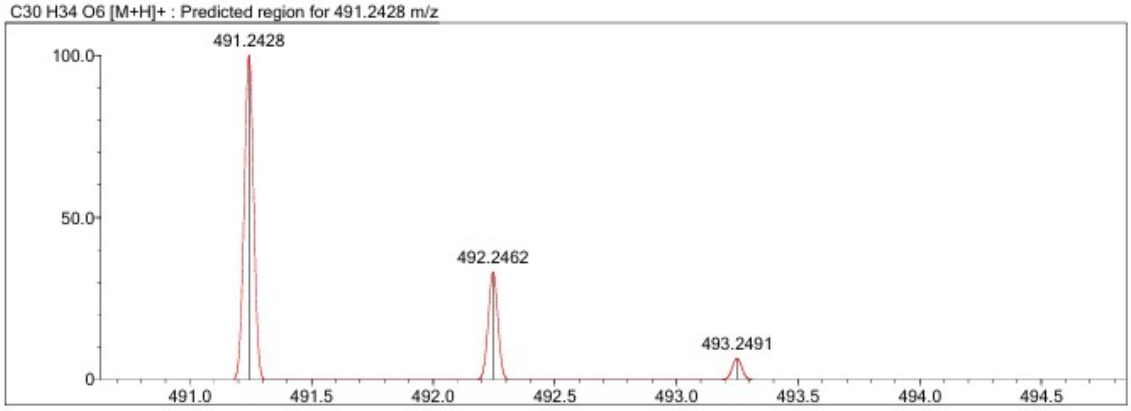
Event#: 1 MS(E+) Ret. Time : 12.880 Scan# : 1933



Measured region for 491.2423 m/z



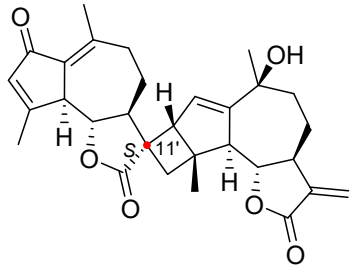
C30 H34 O6 [M+H]+ : Predicted region for 491.2428 m/z



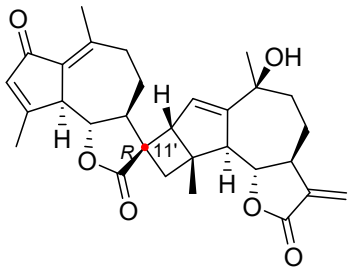
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	83.10	C30 H34 O6	[M+H]+	491.2423	491.2428	-0.5	-1.02	83.14	14.0

General results for NMR calculation

S81. Structures of two possible diastereoisomers of 1 (1a–1b).



(11'*S**)-**1a**



(11'*R**)-**1b**

S82. Conformational analysis of the B3LYP-D3BJ/6-31G(d) optimized conformers of 1a in the gas phase (T=298.15 K)

Conformer	E (Hartree)[a]	G (kcal/mol)[b]	⊿G (kcal/mol)[c]	Population[d]
1a-1	-1614.810243	-1013309.575817	0.00	88.70%
1a-2	-1614.808306	-1013308.360161	-1.215656	11.30%

[a]Electronic energy obtained at M06-2X-D3/6-311+G(2d,p) level of theory;

[b]Gibbs free energy (E*627.51);

[c]The relative Gibbs free energy;

[d]The Boltzmann distribution of each conformer.

S83. Cartesian coordinates for the low-energy Conf. of Compound 1a at B3LYP/6311+G(d,p) level of theory in methanol

Conformer 1a-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.524297	-2.486033	-1.373018
2	6	0	5.448369	-1.313779	-1.414938
3	8	0	3.468448	-2.169596	-0.562116
4	6	0	4.738747	-0.170952	-0.742626
5	6	0	5.612836	0.844116	0.000813
6	6	0	0.368089	0.176424	1.584187
7	6	0	1.218561	-0.957223	0.946568
8	6	0	3.702934	-0.909290	0.124976
9	6	0	4.918386	1.612973	1.138781
10	6	0	1.267563	1.363744	1.653586
11	8	0	3.293839	3.214776	1.895188
12	6	0	2.379361	-0.171452	0.246767
13	6	0	3.511331	2.212913	0.886932
14	6	0	2.413363	1.165727	0.986319
15	8	0	4.620047	-3.551647	-1.927704
16	6	0	6.663383	-1.383439	-1.956657
17	6	0	1.667759	-2.053679	1.901652
18	6	0	3.422105	2.984223	-0.434237
19	6	0	-0.739010	1.051153	-0.661165

20	6	0	-0.706962	0.005916	0.444636
21	8	0	-2.030189	1.252252	-1.063947
22	6	0	-2.177237	-0.044723	0.871890
23	6	0	-2.685781	-1.275228	1.610358
24	6	0	-6.002362	0.802805	-1.918716
25	6	0	-4.918687	1.477325	-1.495163
26	6	0	-2.907203	0.286144	-0.430325
27	6	0	-4.116311	-1.072688	2.150623
28	6	0	-6.314237	-0.337711	-1.039486
29	6	0	-4.327647	0.833359	-0.245983
30	6	0	-5.206721	-1.170512	1.098031
31	6	0	-5.287366	-0.314498	0.058504
32	8	0	0.177351	1.631301	-1.188207
33	6	0	-4.358632	2.723641	-2.098987
34	6	0	-6.177281	-2.300362	1.311480
35	8	0	-7.243130	-1.121985	-1.194573
36	6	0	0.038853	-1.300511	-0.002661
37	1	0	4.164969	0.354306	-1.519214
38	1	0	6.012103	1.556315	-0.729939
39	1	0	6.478898	0.322693	0.425955
40	1	0	-0.088441	-0.086153	2.546959
41	1	0	4.124537	-1.155417	1.106753
42	1	0	4.848618	0.967320	2.025687
43	1	0	5.558465	2.455368	1.421483
44	1	0	1.014698	2.290346	2.156566
45	1	0	3.266070	2.750621	2.748319
46	1	0	2.067186	0.050007	-0.783487
47	1	0	7.339480	-0.533762	-1.975100
48	1	0	7.003691	-2.314166	-2.401086
49	1	0	2.340897	-1.651226	2.668840
50	1	0	0.799139	-2.479451	2.417355
51	1	0	2.183249	-2.862286	1.376647
52	1	0	4.216441	3.736742	-0.478896
53	1	0	3.509746	2.324455	-1.299906
54	1	0	2.451791	3.482027	-0.490927
55	1	0	-2.324478	0.821942	1.537220
56	1	0	-2.016459	-1.483470	2.454730
57	1	0	-2.660859	-2.158169	0.960848
58	1	0	-6.616868	1.051419	-2.776767
59	1	0	-2.952909	-0.589714	-1.090200
60	1	0	-4.312431	-1.823110	2.923239
61	1	0	-4.167237	-0.095058	2.651380
62	1	0	-4.299380	1.576808	0.565484
63	1	0	-5.016442	3.109127	-2.883023

64	1	0	-4.231883	3.499474	-1.333019
65	1	0	-3.364292	2.544276	-2.518187
66	1	0	-6.666946	-2.185689	2.288635
67	1	0	-6.932435	-2.351222	0.530222
68	1	0	-5.628080	-3.251687	1.353944
69	1	0	-0.495600	-2.203641	0.303089
70	1	0	0.280847	-1.380159	-1.065599

Conformer 1a-2

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	5.092211	-2.532742	-0.807457
2	6	0	5.954634	-1.324260	-0.676818
3	8	0	3.822664	-2.188727	-0.435382
4	6	0	5.034969	-0.158184	-0.432385
5	6	0	5.655693	1.015868	0.336058
6	6	0	0.447645	0.072820	1.267758
7	6	0	1.133629	-0.873335	0.223471
8	6	0	3.788936	-0.861595	0.156161
9	6	0	4.707938	2.026742	1.011482
10	6	0	1.358438	1.244384	1.368045
11	8	0	2.874659	3.483563	1.030933
12	6	0	2.469225	-0.164176	-0.192236
13	6	0	3.361553	2.333670	0.325030
14	6	0	2.392782	1.180988	0.523324
15	8	0	5.382132	-3.643632	-1.174775
16	6	0	7.282641	-1.380862	-0.765063
17	6	0	1.224525	-2.337746	0.632994
18	6	0	3.492277	2.727067	-1.156272
19	6	0	-1.117090	1.676336	-0.177478
20	6	0	-0.781281	0.269462	0.316324
21	8	0	-2.456371	1.754355	-0.429186
22	6	0	-2.157831	-0.199655	0.808712
23	6	0	-2.400464	-1.682117	1.061630
24	6	0	-6.357495	0.916881	-1.257928
25	6	0	-5.364900	1.571578	-0.629064
26	6	0	-3.087030	0.465439	-0.209227
27	6	0	-3.785370	-1.948442	1.687505
28	6	0	-6.380646	-0.513196	-0.901611
29	6	0	-4.545924	0.620113	0.237271
30	6	0	-4.942695	-1.865899	0.709880
31	6	0	-5.269529	-0.714680	0.088987
32	8	0	-0.392912	2.619669	-0.384450
33	6	0	-5.090870	3.038699	-0.695322

34	6	0	-5.677335	-3.160040	0.491718
35	8	0	-7.171585	-1.343235	-1.334259
36	6	0	-0.032534	-0.577119	-0.769776
37	1	0	4.722544	0.197737	-1.423877
38	1	0	6.304402	1.545993	-0.371324
39	1	0	6.321664	0.612322	1.107840
40	1	0	0.167901	-0.369491	2.232341
41	1	0	3.882846	-0.984117	1.242910
42	1	0	4.464731	1.691120	2.025262
43	1	0	5.236220	2.980229	1.120895
44	1	0	1.143996	2.102898	1.992078
45	1	0	1.986636	3.663663	0.675530
46	1	0	2.474751	-0.039595	-1.284813
47	1	0	7.910119	-0.501114	-0.659087
48	1	0	7.769882	-2.333497	-0.951052
49	1	0	1.930516	-2.481827	1.457585
50	1	0	0.246023	-2.694112	0.969527
51	1	0	1.552966	-2.968524	-0.195226
52	1	0	4.144246	3.602214	-1.237304
53	1	0	3.895871	1.933485	-1.788683
54	1	0	2.503477	2.991692	-1.548266
55	1	0	-2.327043	0.322134	1.765379
56	1	0	-1.634976	-2.046120	1.755726
57	1	0	-2.295734	-2.263310	0.138069
58	1	0	-7.090510	1.354698	-1.926294
59	1	0	-3.070303	-0.071740	-1.166092
60	1	0	-3.780581	-2.945598	2.139375
61	1	0	-3.940133	-1.237307	2.511627
62	1	0	-4.545709	0.981990	1.276836
63	1	0	-5.883536	3.561049	-1.238317
64	1	0	-5.018394	3.462575	0.314527
65	1	0	-4.130459	3.238205	-1.179363
66	1	0	-6.087554	-3.517166	1.446629
67	1	0	-6.481163	-3.061483	-0.234741
68	1	0	-4.969903	-3.931107	0.154989
69	1	0	-0.575027	-1.460101	-1.119081
70	1	0	0.266926	0.012268	-1.640933

S84. Conformational analysis of the B3LYP-D3BJ/6-31G(d) optimized conformers of 1b in the gas phase (T=298.15 K)

Conformer	E (Hartree)[a]	G (kcal/mol)[b]	ΔG (kcal/mol)[c]	Population[d]
1b-1	-1615.068114	-1013471.392015	0	46.29%
1b-2	-1615.067516	-1013471.016670	0.375345	24.37%
1b-3	-1615.067372	-1013470.926415	0.465600	20.93%
1b-4	-1615.066503	-1013470.381254	1.010762	8.41%

[a]Electronic energy obtained at M06-2X-D3/6-311+G(2d,p) level of theory;

[b]Gibbs free energy (E*627.51);

[c]The relative Gibbs free energy;

[d]The Boltzmann distribution of each conformer.

S85. Cartesian coordinates for the low-energy Conf. of Compound 1b at B3LYP/6311+G(d,p) level of theory in methanol

Conformer 1b-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.205640	-1.281121	1.113988
2	6	0	-5.526329	0.161206	0.902786
3	8	0	-4.009374	-1.545520	0.504218
4	6	0	-4.297911	0.799837	0.315771
5	6	0	-4.524638	1.985712	-0.625277
6	6	0	0.018331	-1.046273	-1.353085
7	6	0	-1.253175	-1.602973	-0.644336
8	6	0	-3.571504	-0.413949	-0.296087
9	6	0	-3.397799	2.259640	-1.635483
10	6	0	-0.240915	0.406558	-1.549889
11	8	0	-1.142212	2.934585	-2.117543
12	6	0	-2.052489	-0.323864	-0.212655
13	6	0	-1.928244	2.230651	-1.143339
14	6	0	-1.404271	0.806135	-1.015260
15	8	0	-5.831966	-2.121731	1.707747
16	6	0	-6.717451	0.679232	1.198175
17	6	0	-2.022617	-2.623472	-1.473528
18	6	0	-1.715854	3.032606	0.145801
19	6	0	1.875158	-2.637989	-0.720523
20	6	0	0.911575	-1.609491	-0.154487
21	8	0	3.134695	-2.109971	-0.759325
22	6	0	1.852582	-0.721426	0.677320
23	6	0	1.320129	0.671657	1.128833
24	6	0	5.238610	1.570209	-0.734964
25	6	0	5.353763	0.228301	-0.765369
26	6	0	3.114764	-0.761585	-0.232187
27	6	0	2.085439	1.370498	2.330047

28	6	0	4.366614	2.003178	0.390713
29	6	0	4.527871	-0.389896	0.355403
30	6	0	3.403304	0.652860	2.333806
31	6	0	4.179867	0.786054	1.231762
32	8	0	1.626667	-3.742294	-1.133937
33	6	0	6.029958	-0.624801	-1.784465
34	6	0	3.578796	-0.471448	3.315793
35	8	0	3.945763	3.138170	0.591574
36	6	0	-0.365327	-2.201170	0.484103
37	1	0	-3.675337	1.129965	1.159841
38	1	0	-4.694216	2.880385	-0.015530
39	1	0	-5.450313	1.819683	-1.189055
40	1	0	0.272974	-1.552376	-2.290741
41	1	0	-3.909256	-0.594344	-1.323431
42	1	0	-3.477138	1.550366	-2.471216
43	1	0	-3.553747	3.257032	-2.060103
44	1	0	0.430166	1.069082	-2.085588
45	1	0	-1.232397	2.452497	-2.956342
46	1	0	-1.850051	-0.139056	0.854787
47	1	0	-6.952378	1.726428	1.032183
48	1	0	-7.491132	0.045480	1.621634
49	1	0	-2.431856	-2.163505	-2.382043
50	1	0	-1.339042	-3.420806	-1.783226
51	1	0	-2.845284	-3.069142	-0.909590
52	1	0	-2.185650	2.557071	1.009778
53	1	0	-0.643370	3.120060	0.338751
54	1	0	-2.129179	4.039677	0.030878
55	1	0	2.071302	-1.327117	1.564204
56	1	0	0.261897	0.571622	1.390972
57	1	0	1.369033	1.351658	0.275597
58	1	0	5.646313	2.269789	-1.456321
59	1	0	2.931504	-0.080242	-1.073881
60	1	0	2.193021	2.432656	2.106567
61	1	0	1.542733	1.252409	3.272990
62	1	0	4.982757	-1.270490	0.816369
63	1	0	6.474694	-0.030176	-2.587220
64	1	0	6.820136	-1.228526	-1.318233
65	1	0	5.316371	-1.336981	-2.218613
66	1	0	3.951636	-0.038666	4.256548
67	1	0	2.637439	-0.973491	3.565205
68	1	0	4.310674	-1.214657	2.988721
69	1	0	-0.581170	-1.827662	1.490217
70	1	0	-0.355310	-3.293783	0.503811

Conformer 1b-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.142276	-1.338636	1.070795
2	6	0	-5.389457	0.133953	1.121867
3	8	0	-3.952550	-1.545084	0.424560
4	6	0	-4.101155	0.788007	0.703952
5	6	0	-4.170417	2.185765	0.110482
6	6	0	0.058402	-1.023321	-1.396677
7	6	0	-1.236849	-1.574994	-0.731357
8	6	0	-3.499849	-0.308288	-0.197743
9	6	0	-2.796672	2.791791	-0.206431
10	6	0	-0.194382	0.430132	-1.613995
11	8	0	-3.045885	1.926267	-2.407844
12	6	0	-1.979449	-0.283858	-0.248645
13	6	0	-2.036212	2.169267	-1.399002
14	6	0	-1.370586	0.831867	-1.103464
15	8	0	-5.810585	-2.241561	1.507020
16	6	0	-6.565938	0.654915	1.464727
17	6	0	-2.043752	-2.504284	-1.627740
18	6	0	-1.034167	3.201040	-1.933822
19	6	0	1.905297	-2.624892	-0.763188
20	6	0	0.915087	-1.624876	-0.189716
21	8	0	3.158684	-2.080113	-0.757238
22	6	0	1.826226	-0.752990	0.693549
23	6	0	1.269102	0.622014	1.170284
24	6	0	5.181883	1.632138	-0.630660
25	6	0	5.330044	0.293914	-0.683037
26	6	0	3.105014	-0.748054	-0.195946
27	6	0	2.004424	1.304318	2.398527
28	6	0	4.282805	2.022826	0.488969
29	6	0	4.504187	-0.362765	0.415704
30	6	0	3.336924	0.614879	2.400190
31	6	0	4.120996	0.788315	1.309448
32	8	0	1.681297	-3.718760	-1.215130
33	6	0	6.039545	-0.524461	-1.707748
34	6	0	3.525926	-0.527037	3.358762
35	8	0	3.820683	3.141128	0.695785
36	6	0	-0.380199	-2.255070	0.375322
37	1	0	-3.457195	0.828251	1.599427
38	1	0	-4.668520	2.842431	0.834730
39	1	0	-4.784472	2.180437	-0.794077
40	1	0	0.328034	-1.525806	-2.332174
41	1	0	-3.933848	-0.260592	-1.201557

42	1	0	-2.947273	3.851907	-0.436901
43	1	0	-2.147859	2.754839	0.678644
44	1	0	0.478938	1.056246	-2.189692
45	1	0	-2.593152	1.497666	-3.152068
46	1	0	-1.667062	-0.100338	0.790884
47	1	0	-6.742458	1.726218	1.483763
48	1	0	-7.388419	-0.000178	1.736792
49	1	0	-2.447514	-1.957108	-2.489409
50	1	0	-1.390137	-3.296152	-2.009068
51	1	0	-2.876185	-2.963956	-1.092003
52	1	0	-0.277575	3.451716	-1.182465
53	1	0	-0.518686	2.836323	-2.827971
54	1	0	-1.572095	4.112222	-2.209176
55	1	0	2.035632	-1.380472	1.567536
56	1	0	0.209873	0.501291	1.416913
57	1	0	1.321535	1.321593	0.333158
58	1	0	5.581305	2.353978	-1.334546
59	1	0	2.918926	-0.048019	-1.021814
60	1	0	2.091394	2.374136	2.204714
61	1	0	1.453497	1.149114	3.331266
62	1	0	4.970815	-1.243077	0.865006
63	1	0	6.481280	0.094687	-2.493425
64	1	0	6.837064	-1.118227	-1.241280
65	1	0	5.348496	-1.244859	-2.164177
66	1	0	3.870573	-0.107164	4.315941
67	1	0	2.594007	-1.059193	3.579507
68	1	0	4.282563	-1.242929	3.027488
69	1	0	-0.625056	-1.964093	1.401629
70	1	0	-0.366594	-3.345581	0.306720

Conformer 1b-3

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	-5.559352	-1.290585	0.622358
2	6	0	-5.829854	0.154656	0.374520
3	8	0	-4.249071	-1.534375	0.317643
4	6	0	-4.497215	0.808862	0.131405
5	6	0	-4.515021	2.052080	-0.763548
6	6	0	-0.046956	-1.028124	-1.027733
7	6	0	-1.275015	-1.563150	-0.220962
8	6	0	-3.638663	-0.387499	-0.333409
9	6	0	-3.195455	2.425551	-1.458258
10	6	0	-0.297509	0.427162	-1.195389
11	8	0	-0.956799	3.079036	-1.412097
12	6	0	-2.167487	-0.304166	0.082308

13	6	0	-1.886631	2.296604	-0.648041
14	6	0	-1.424610	0.845258	-0.605314
15	8	0	-6.303233	-2.148359	1.026140
16	6	0	-7.060532	0.664210	0.377585
17	6	0	-1.947364	-2.768352	-0.870400
18	6	0	-1.975368	2.917852	0.756008
19	6	0	1.751945	-2.682142	-0.405069
20	6	0	0.917132	-1.534207	0.136352
21	8	0	3.019901	-2.234211	-0.659729
22	6	0	2.001672	-0.645137	0.770390
23	6	0	1.607931	0.806016	1.178535
24	6	0	5.209898	1.363084	-1.269350
25	6	0	5.292843	0.019528	-1.206443
26	6	0	3.127801	-0.840621	-0.285540
27	6	0	2.550334	1.518530	2.233158
28	6	0	4.511121	1.905747	-0.073484
29	6	0	4.622572	-0.483044	0.065773
30	6	0	3.831604	0.746548	2.098270
31	6	0	4.436359	0.766911	0.886762
32	8	0	1.414186	-3.814308	-0.640565
33	6	0	5.794921	-0.931506	-2.238933
34	6	0	4.117935	-0.311020	3.126759
35	8	0	4.119657	3.059211	0.081440
36	6	0	-0.324122	-1.948662	0.952154
37	1	0	-4.104427	1.086626	1.119689
38	1	0	-4.858315	2.895011	-0.152300
39	1	0	-5.274714	1.913923	-1.541804
40	1	0	0.151955	-1.532566	-1.979939
41	1	0	-3.731162	-0.537279	-1.416203
42	1	0	-3.065272	1.827324	-2.366773
43	1	0	-3.257353	3.469219	-1.783658
44	1	0	0.357769	1.076664	-1.764470
45	1	0	-0.119001	3.099038	-0.921369
46	1	0	-2.187937	-0.145214	1.171575
47	1	0	-7.254813	1.715256	0.185875
48	1	0	-7.910417	0.018508	0.578297
49	1	0	-2.444083	-2.490855	-1.807769
50	1	0	-1.182676	-3.515815	-1.102786
51	1	0	-2.692436	-3.220418	-0.214028
52	1	0	-2.648804	2.380370	1.426624
53	1	0	-0.982537	2.915987	1.222457
54	1	0	-2.313874	3.955595	0.676863
55	1	0	2.302600	-1.194531	1.670376
56	1	0	0.580201	0.796889	1.556108

57	1	0	1.606097	1.427675	0.280048
58	1	0	5.520894	1.991366	-2.096661
59	1	0	2.856326	-0.239224	-1.163556
60	1	0	2.663381	2.566233	1.951113
61	1	0	2.136810	1.459873	3.244647
62	1	0	5.114161	-1.344189	0.525277
63	1	0	6.631199	-1.523147	-1.842991
64	1	0	5.010219	-1.651213	-2.506272
65	1	0	6.130226	-0.416553	-3.143361
66	1	0	4.618880	0.174227	3.978103
67	1	0	3.209658	-0.770866	3.532086
68	1	0	4.786727	-1.093505	2.759204
69	1	0	-0.461780	-1.345447	1.855768
70	1	0	-0.342114	-3.007217	1.224394

Conformer 1b-4

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	-5.302369	-1.255189	1.000985
2	6	0	-5.601498	0.187832	0.765462
3	8	0	-4.072246	-1.526595	0.468851
4	6	0	-4.332274	0.816892	0.260384
5	6	0	-4.493052	2.014275	-0.679451
6	6	0	0.006854	-1.077087	-1.285884
7	6	0	-1.259983	-1.613883	-0.553535
8	6	0	-3.580623	-0.401543	-0.310814
9	6	0	-3.303513	2.304887	-1.611419
10	6	0	-0.234595	0.376072	-1.490052
11	8	0	-0.993926	2.854804	-1.987182
12	6	0	-2.065060	-0.325811	-0.151398
13	6	0	-1.867364	2.228815	-1.033236
14	6	0	-1.380887	0.794004	-0.937513
15	8	0	-5.969357	-2.090165	1.557650
16	6	0	-6.806625	0.713299	0.979232
17	6	0	-2.020420	-2.668434	-1.348965
18	6	0	-1.718863	2.967335	0.308241
19	6	0	1.855859	-2.672905	-0.642344
20	6	0	0.910457	-1.622859	-0.087534
21	8	0	3.115484	-2.147720	-0.730703
22	6	0	1.875160	-0.723257	0.703969
23	6	0	1.357957	0.677235	1.149667
24	6	0	5.199941	1.551588	-0.852786
25	6	0	5.322151	0.209911	-0.865535
26	6	0	3.109677	-0.785048	-0.241174
27	6	0	2.156551	1.387661	2.321417

28	6	0	4.364167	1.997494	0.294599
29	6	0	4.539487	-0.394780	0.292754
30	6	0	3.476670	0.674353	2.291137
31	6	0	4.214737	0.793561	1.161507
32	8	0	1.597389	-3.790257	-1.011983
33	6	0	5.965927	-0.656042	-1.894622
34	6	0	3.689575	-0.434953	3.282714
35	8	0	3.941015	3.133020	0.490180
36	6	0	-0.363321	-2.178192	0.586520
37	1	0	-3.762353	1.132188	1.146218
38	1	0	-4.706220	2.898700	-0.067651
39	1	0	-5.379632	1.856423	-1.304983
40	1	0	0.246874	-1.594917	-2.220884
41	1	0	-3.864452	-0.580562	-1.354573
42	1	0	-3.329728	1.638111	-2.480427
43	1	0	-3.436102	3.320047	-2.007906
44	1	0	0.428152	1.025174	-2.048770
45	1	0	-1.197971	3.802995	-1.980036
46	1	0	-1.911136	-0.146245	0.925241
47	1	0	-7.024284	1.761163	0.794853
48	1	0	-7.610377	0.084970	1.351668
49	1	0	-2.437366	-2.241647	-2.269811
50	1	0	-1.326276	-3.464802	-1.636908
51	1	0	-2.835851	-3.107972	-0.770719
52	1	0	-2.103393	3.992292	0.223671
53	1	0	-2.256201	2.480659	1.125733
54	1	0	-0.659430	3.015582	0.574248
55	1	0	2.117778	-1.314840	1.594375
56	1	0	0.306333	0.582882	1.439656
57	1	0	1.386161	1.346270	0.287064
58	1	0	5.577113	2.241261	-1.599833
59	1	0	2.898598	-0.127201	-1.094787
60	1	0	2.253483	2.448495	2.086708
61	1	0	1.644045	1.275071	3.281840
62	1	0	5.015736	-1.264828	0.752092
63	1	0	6.377281	-0.072512	-2.722895
64	1	0	6.776101	-1.247820	-1.447785
65	1	0	5.241042	-1.379029	-2.290572
66	1	0	4.414496	-1.179049	2.942522
67	1	0	4.089686	0.012561	4.205213
68	1	0	2.759345	-0.938296	3.568525
69	1	0	-0.561878	-1.761970	1.579570
70	1	0	-0.364776	-3.269233	0.650872

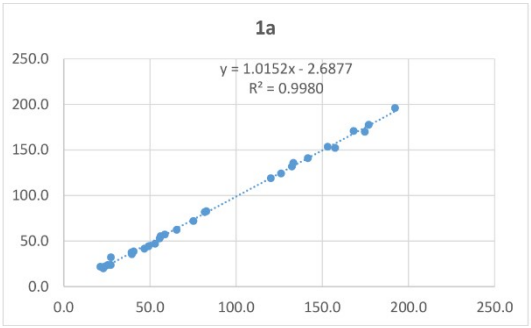
S86. Experimental and calculated ^{13}C NMR chemical shifts of 1a and 1b

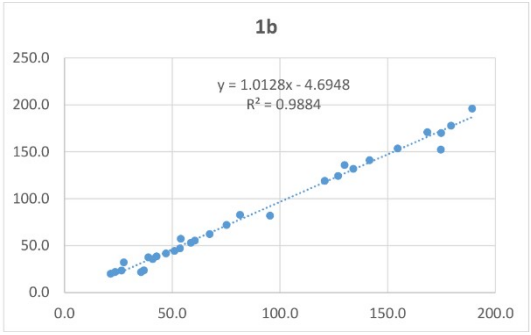
NO.	$\delta_{exptl.}$	$\delta_{calcd.}$ (ppm)		NO.	$\delta_{exptl.}$	$\delta_{calcd.}$ (ppm)	
		1a	**1b**			**1a**	**1b**
1	153.5	153.1	154.6	1′	131.9	132.3	134.0
2	124.2	126.0	126.9	2′	196	192.1	189.2
3	55.3	56.1	60.5	3′	135.9	133.2	129.9
4	41.7	46.7	47.1	4′	170	174.6	174.8
5	62.2	65.5	67.4	5′	52.9	55.5	58.6
6	82.7	82.7	81.5	6′	81.9	81.7	95.3
7	44.3	49.2	51.0	7′	57.2	58.6	53.9
8	23.5	25.3	26.4	8′	23.7	27.2	36.8
9	35.6	39.4	40.9	9′	37.5	39.2	38.8
10	72	75.2	75.2	10′	152.2	157.3	174.6
11	141.1	141.6	141.6	11′	47	52.9	53.5
12	170.9	168.1	168.4	12′	177.6	176.9	179.4
13	119	120.1	120.7	13′	38.6	40.5	42.7
14	32.2	27.3	27.5	14′	21.8	21.2	35.5
15	21.9	23.7	23.5	15′	20	22.8	21.4
				R^2		0.9980	0.9884
				MAE		2.5	5.2
				CMAE		1.9	4.6

S87. Experimental and calculated ^{1}H NMR chemical shifts of 1a and 1b

NO.	$\delta_{exptl.}$	$\delta_{calcd.}$ (ppm)		NO.	$\delta_{exptl.}$	$\delta_{calcd.}$ (ppm)	
		1a	**1b**			**1a**	**1b**
2	5.64	6.16	6.18	3′	6.16	6.21	6.32
3	2.89	2.76	2.98	5′	3.37	4.07	3.41
5	3.43	3.13	2.81	6′	3.51	3.51	3.41
6	4.04	4.36	3.99	7′	2.21	2.33	2.10
7	3.69	3.06	3.18	8′a	2.09	2.18	1.54
8a	2.34	2.28	2.24	8′b	1.57	2.05	2.04
8b	1.5	1.77	1.50	9′a	2.44	4.71	2.29
9a	2.11	1.87	1.91	9′b	2.44	2.65	2.38
9b	1.67	1.80	1.65	13′a	2.21	2.63	1.70
13a	6.14	6.68	6.51	13′b	2.01	1.97	2.29
13b	5.42	6.04	5.90	14′a	2.46	2.42	1.52
14a	1.58	1.53	1.33	14′b	2.46	2.32	4.51
14b	1.58	1.41	1.69	14′c	2.46	2.59	1.65
14c	1.58	1.45	1.26	15′a	2.26	2.49	2.26
15a	1.33	1.18	1.05	15′b	2.26	2.51	2.04
15b	1.33	1.32	1.26	15′c	2.26	2.55	2.82
15c	1.33	1.77	1.53				

S88. Linear regression analysis between the experimental and calculated 13C NMR chemical shifts of 1a/1b.

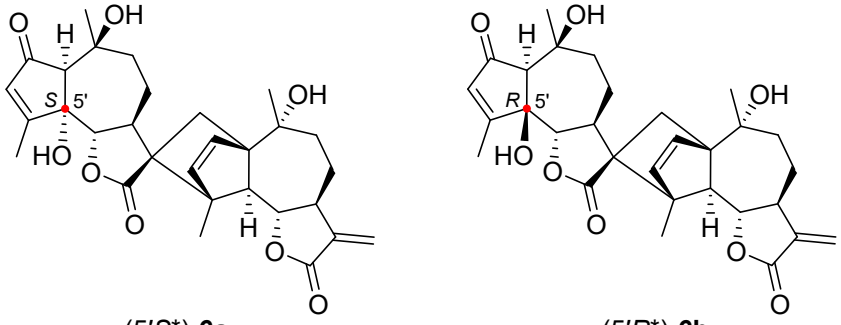




S89. DP4+ probability analysis of 1a/1b.

Functional	Solvent?	Basis Set	Type of Data			
mPW1PW91	PCM	6-311G(d,p)	Unscaled Shifts			
	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6
sDP4+ (H data)	77.46%	22.54%				
sDP4+ (C data)	100.00%	0.00%				
sDP4+ (all data)	100.00%	0.00%				
uDP4+ (H data)	93.86%	6.14%				
uDP4+ (C data)	100.00%	0.00%				
uDP4+ (all data)	100.00%	0.00%				
DP4+ (H data)	98.13%	1.87%				
DP4+ (C data)	100.00%	0.00%				
DP4+ (all data)	100.00%	0.00%				

S90. Structures of two possible diastereoisomers of 6 (6a–6b).



(5′*S**)-**6a** (5′*R**)-**6b**

S91. Conformational analysis of the B3LYP-D3BJ/6-31G(d) optimized conformers of 6a in the gas phase (T=298.15 K)

Conformer	E (Hartree)[a]	G (kcal/mol)[b]	⊿G (kcal/mol)[c]	Population[d]
6a-1	-1766.49643	-1108494.174971	0.00	56.19%
6a-2	-1766.496092	-1108493.962440	0.212531	39.41%
6a-3	-1766.493678	-1108492.447631	1.727341	3.03%
6a-4	-1766.492919	-1108491.971759	2.203213	1.37%

[a]Electronic energy obtained at M06-2X-D3/6-311+G(2d,p) level of theory;

[b]Gibbs free energy (E*627.51);

[c]The relative Gibbs free energy;

[d]The Boltzmann distribution of each conformer.

S92 Cartesian coordinates for the low-energy Conf. of Compound 6a at B3LYP/6311+G(d,p) level of theory in methanol

Conformer 6a-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.507505	1.606385	-1.896800
2	6	0	5.073275	1.697994	-0.518148
3	8	0	3.529252	0.651481	-1.897132
4	6	0	4.186375	0.881265	0.378588
5	6	0	4.859718	0.198047	1.570607
6	6	0	1.821412	-2.608204	-0.899367
7	6	0	1.213374	-1.242647	-1.212623
8	6	0	3.497584	-0.061868	-0.628685
9	6	0	4.108260	-1.007752	2.166420
10	6	0	2.201085	-2.618190	0.381040
11	8	0	2.297019	0.470961	2.667273
12	6	0	2.056674	-0.344436	-0.255637
13	6	0	2.573095	-0.893569	2.306974
14	6	0	1.854495	-1.261188	0.986872
15	8	0	4.803328	2.231089	-2.885037
16	6	0	6.178026	2.392923	-0.249972

17	6	0	1.120507	-0.891277	-2.689300
18	6	0	2.107177	-1.814835	3.444055
19	8	0	-3.692017	0.159914	-2.149821
20	6	0	-1.084772	-2.370733	-0.744819
21	6	0	-0.162675	-1.195573	-0.437546
22	8	0	-2.380677	-1.982253	-0.532214
23	6	0	-1.131529	-0.023070	-0.769874
24	6	0	-0.743473	1.399870	-0.380996
25	6	0	-5.616049	-0.371486	0.705668
26	6	0	-4.944846	-0.898719	-0.334838
27	6	0	-2.437051	-0.572547	-0.177477
28	6	0	-1.842379	2.444324	-0.600066
29	6	0	-5.056106	0.931446	1.066659
30	6	0	-3.757049	-0.003966	-0.736269
31	6	0	-3.031841	2.363028	0.373738
32	6	0	-4.117487	1.352782	-0.076703
33	8	0	-0.829989	-3.484908	-1.122446
34	6	0	0.286532	-1.242349	1.065569
35	6	0	-5.283022	-2.153874	-1.067936
36	6	0	-3.681852	3.752539	0.482178
37	8	0	-5.270170	1.572290	2.088258
38	8	0	-2.500998	1.977648	1.650958
39	1	0	3.402176	1.537888	0.775892
40	1	0	5.001551	0.950870	2.352112
41	1	0	5.860027	-0.142219	1.275217
42	1	0	1.830548	-3.436731	-1.595722
43	1	0	4.066975	-0.986105	-0.768455
44	1	0	4.317294	-1.902560	1.570400
45	1	0	4.532720	-1.198437	3.158472
46	1	0	2.573050	-3.467646	0.943492
47	1	0	1.370010	0.524407	2.946926
48	1	0	1.581656	0.623519	-0.095322
49	1	0	6.597969	2.449617	0.749944
50	1	0	6.686406	2.928215	-1.046639
51	1	0	0.797089	0.141538	-2.846586
52	1	0	2.092246	-0.998852	-3.175078
53	1	0	0.409615	-1.560109	-3.189749
54	1	0	2.354914	-2.862362	3.243656
55	1	0	2.595673	-1.517459	4.376732
56	1	0	1.023012	-1.752988	3.591548
57	1	0	-3.384790	-0.683249	-2.523841
58	1	0	-1.275428	-0.029939	-1.857135
59	1	0	0.113740	1.693712	-0.995360
60	1	0	-0.424913	1.454811	0.662328

61	1	0	-6.455042	-0.819141	1.227164
62	1	0	-2.452991	-0.487436	0.912551
63	1	0	-1.381203	3.430990	-0.477704
64	1	0	-2.221815	2.395031	-1.627052
65	1	0	-4.750285	1.847489	-0.825349
66	1	0	-0.081461	-0.361841	1.601761
67	1	0	-0.093505	-2.125865	1.582996
68	1	0	-6.215425	-2.586835	-0.696472
69	1	0	-5.408183	-1.933920	-2.135759
70	1	0	-4.479852	-2.890607	-0.979364
71	1	0	-2.962073	4.451907	0.918534
72	1	0	-3.971799	4.125481	-0.506895
73	1	0	-4.571080	3.720525	1.117053
74	1	0	-3.252609	2.032628	2.269127

Conformer 6a-2

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	4.499172	1.686765	-1.852827
2	6	0	5.078175	1.726072	-0.476669
3	8	0	3.521378	0.733042	-1.880227
4	6	0	4.198737	0.875880	0.395816
5	6	0	4.884803	0.148407	1.554353
6	6	0	1.828758	-2.565437	-0.986150
7	6	0	1.212347	-1.191712	-1.241824
8	6	0	3.500384	-0.028827	-0.639879
9	6	0	4.142452	-1.080931	2.112836
10	6	0	2.225616	-2.620550	0.287922
11	8	0	2.204780	0.364707	2.617007
12	6	0	2.063671	-0.326009	-0.262609
13	6	0	2.601937	-0.973787	2.267299
14	6	0	1.875804	-1.290262	0.945992
15	8	0	4.787762	2.349002	-2.818463
16	6	0	6.186631	2.408935	-0.193448
17	6	0	1.104004	-0.786459	-2.703554
18	6	0	2.143204	-1.935445	3.373191
19	8	0	-3.679856	0.177127	-2.138769
20	6	0	-1.072235	-2.347371	-0.785550
21	6	0	-0.155679	-1.176767	-0.448910
22	8	0	-2.368946	-1.974691	-0.553951
23	6	0	-1.132457	0.000423	-0.737954
24	6	0	-0.757628	1.410348	-0.294072
25	6	0	-5.635919	-0.404432	0.680352
26	6	0	-4.942108	-0.915455	-0.353157
27	6	0	-2.436643	-0.573768	-0.166708

28	6	0	-1.855979	2.456261	-0.513084
29	6	0	-5.096551	0.900885	1.062648
30	6	0	-3.756726	-0.005469	-0.727473
31	6	0	-3.068148	2.352170	0.429991
32	6	0	-4.137269	1.340378	-0.056744
33	8	0	-0.813734	-3.449481	-1.196228
34	6	0	0.310464	-1.271005	1.046681
35	6	0	-5.259289	-2.166141	-1.103486
36	6	0	-3.731144	3.735960	0.539392
37	8	0	-5.342044	1.532276	2.083054
38	8	0	-2.563753	1.954895	1.712284
39	1	0	3.416684	1.515698	0.823428
40	1	0	5.040054	0.875645	2.359480
41	1	0	5.883732	-0.176196	1.238094
42	1	0	1.829207	-3.369124	-1.710908
43	1	0	4.068642	-0.946637	-0.820590
44	1	0	4.354174	-1.953697	1.485176
45	1	0	4.579184	-1.311105	3.093234
46	1	0	2.604266	-3.489879	0.814658
47	1	0	2.504692	0.534338	3.523817
48	1	0	1.587311	0.633221	-0.060560
49	1	0	6.617744	2.427451	0.803229
50	1	0	6.687646	2.973281	-0.974555
51	1	0	0.779153	0.251320	-2.819281
52	1	0	2.070232	-0.876700	-3.203927
53	1	0	0.387266	-1.436284	-3.220474
54	1	0	2.398736	-2.973589	3.137087
55	1	0	2.641114	-1.684161	4.318322
56	1	0	1.063680	-1.869626	3.529067
57	1	0	-3.357020	-0.657523	-2.518752
58	1	0	-1.275575	0.032740	-1.824910
59	1	0	0.111533	1.727043	-0.879909
60	1	0	-0.463651	1.431713	0.757667
61	1	0	-6.480367	-0.864303	1.182121
62	1	0	-2.460597	-0.512840	0.924862
63	1	0	-1.401719	3.441367	-0.356579
64	1	0	-2.211317	2.430676	-1.549807
65	1	0	-4.758392	1.840796	-0.811434
66	1	0	-0.023401	-0.408956	1.627392
67	1	0	-0.063197	-2.173935	1.534972
68	1	0	-6.196685	-2.606595	-0.753864
69	1	0	-5.364761	-1.937614	-2.171608
70	1	0	-4.454232	-2.899527	-1.006192
71	1	0	-3.026978	4.434697	1.001522

72	1	0	-4.000246	4.119243	-0.451698
73	1	0	-4.634877	3.689771	1.152519
74	1	0	-3.327020	1.998318	2.316471

Conformer 6a-3

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	4.490495	1.655175	-1.902078
2	6	0	5.081298	1.713958	-0.531464
3	8	0	3.511653	0.703349	-1.907451
4	6	0	4.207133	0.879235	0.360783
5	6	0	4.901202	0.168809	1.524984
6	6	0	1.815903	-2.578141	-0.943057
7	6	0	1.201734	-1.207498	-1.218429
8	6	0	3.497886	-0.039640	-0.654986
9	6	0	4.159171	-1.047652	2.111242
10	6	0	2.225143	-2.611327	0.327842
11	8	0	2.231088	0.413407	2.606903
12	6	0	2.063453	-0.326854	-0.261841
13	6	0	2.620338	-0.932431	2.275351
14	6	0	1.882951	-1.268887	0.965426
15	8	0	4.772441	2.303510	-2.879389
16	6	0	6.193918	2.397960	-0.268025
17	6	0	1.085150	-0.827803	-2.686392
18	6	0	2.166868	-1.873694	3.400801
19	8	0	-3.518855	0.173828	-2.166309
20	6	0	-1.085446	-2.347699	-0.713716
21	6	0	-0.159717	-1.171821	-0.415409
22	8	0	-2.373369	-1.969989	-0.469215
23	6	0	-1.128826	0.005816	-0.723313
24	6	0	-0.763284	1.413985	-0.257922
25	6	0	-5.661373	-0.437219	0.554045
26	6	0	-4.927902	-0.906965	-0.474160
27	6	0	-2.442842	-0.557074	-0.164123
28	6	0	-1.864504	2.465923	-0.442138
29	6	0	-5.130421	0.845345	1.021991
30	6	0	-3.737587	0.019458	-0.768303
31	6	0	-3.085482	2.335058	0.489201
32	6	0	-4.145441	1.340273	-0.048843
33	8	0	-0.827409	-3.464434	-1.084929
34	6	0	0.318271	-1.246794	1.077770
35	6	0	-5.176035	-2.147579	-1.264774
36	6	0	-3.749882	3.714249	0.639589
37	8	0	-5.393428	1.419233	2.071523
38	8	0	-2.598908	1.896912	1.763533

39	1	0	3.429883	1.527231	0.784898
40	1	0	5.066829	0.909175	2.316052
41	1	0	5.895935	-0.165010	1.204981
42	1	0	1.806113	-3.395170	-1.652623
43	1	0	4.062016	-0.961753	-0.826298
44	1	0	4.362745	-1.932096	1.497464
45	1	0	4.602880	-1.261827	3.092214
46	1	0	2.604270	-3.472703	0.867231
47	1	0	2.539500	0.595421	3.508452
48	1	0	1.590648	0.637279	-0.074181
49	1	0	6.633682	2.430222	0.724529
50	1	0	6.689705	2.948980	-1.061894
51	1	0	0.774936	0.212560	-2.817679
52	1	0	2.045380	-0.941932	-3.193830
53	1	0	0.352329	-1.474373	-3.183683
54	1	0	2.417235	-2.916485	3.180241
55	1	0	2.672537	-1.608152	4.337984
56	1	0	1.088690	-1.801750	3.562951
57	1	0	-4.339350	0.509438	-2.560609
58	1	0	-1.258666	0.034301	-1.809812
59	1	0	0.099310	1.749773	-0.843035
60	1	0	-0.460111	1.417991	0.791513
61	1	0	-6.514596	-0.924730	1.013214
62	1	0	-2.497109	-0.442483	0.922088
63	1	0	-1.410639	3.445316	-0.251583
64	1	0	-2.214072	2.475325	-1.481226
65	1	0	-4.758247	1.882688	-0.783626
66	1	0	-0.011917	-0.379649	1.652744
67	1	0	-0.050838	-2.144592	1.578778
68	1	0	-6.187899	-2.527464	-1.099568
69	1	0	-5.028344	-1.954320	-2.332573
70	1	0	-4.448008	-2.917596	-0.992920
71	1	0	-3.051270	4.396621	1.133210
72	1	0	-4.009962	4.134019	-0.339342
73	1	0	-4.659699	3.645346	1.242245
74	1	0	-3.372617	1.906875	2.356061

Conformer 6a-4

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	4.558528	1.629550	-1.874809
2	6	0	5.125690	1.701729	-0.495146
3	8	0	3.546104	0.710365	-1.873818
4	6	0	4.203345	0.917818	0.397532
5	6	0	4.831619	0.240351	1.622231

6	6	0	1.838759	-2.541776	-0.981029
7	6	0	1.216554	-1.169593	-1.231642
8	6	0	3.505910	-0.015227	-0.613452
9	6	0	4.124442	-1.024425	2.142489
10	6	0	2.227709	-2.602792	0.294896
11	8	0	2.155385	0.291800	2.829408
12	6	0	2.064931	-0.308488	-0.244096
13	6	0	2.581833	-0.973860	2.300686
14	6	0	1.867895	-1.279694	0.964090
15	8	0	4.877772	2.244399	-2.860925
16	6	0	6.253507	2.354047	-0.218333
17	6	0	1.111040	-0.757063	-2.691671
18	6	0	2.166493	-1.985565	3.373455
19	8	0	-3.676463	0.174099	-2.148413
20	6	0	-1.064386	-2.336015	-0.795285
21	6	0	-0.155140	-1.163269	-0.445039
22	8	0	-2.363325	-1.971683	-0.565488
23	6	0	-1.136662	0.009852	-0.734349
24	6	0	-0.772723	1.420194	-0.283888
25	6	0	-5.644782	-0.417701	0.661070
26	6	0	-4.943826	-0.925221	-0.369251
27	6	0	-2.440750	-0.573188	-0.171509
28	6	0	-1.873149	2.462011	-0.512431
29	6	0	-5.113560	0.890183	1.046214
30	6	0	-3.760670	-0.009732	-0.737584
31	6	0	-3.090044	2.351544	0.423911
32	6	0	-4.150849	1.334168	-0.068680
33	8	0	-0.797669	-3.432404	-1.215337
34	6	0	0.302811	-1.265924	1.051793
35	6	0	-5.252193	-2.177213	-1.121249
36	6	0	-3.760583	3.731827	0.530172
37	8	0	-5.367032	1.521068	2.064638
38	8	0	-2.587814	1.956561	1.707277
39	1	0	3.431379	1.627924	0.737955
40	1	0	4.886942	0.977018	2.430421
41	1	0	5.865189	-0.032912	1.379644
42	1	0	1.848502	-3.339337	-1.712408
43	1	0	4.075341	-0.938112	-0.755816
44	1	0	4.370417	-1.873771	1.494609
45	1	0	4.561342	-1.252403	3.121137
46	1	0	2.610568	-3.471551	0.818605
47	1	0	2.233860	0.956726	2.129480
48	1	0	1.582577	0.654719	-0.059128
49	1	0	6.668047	2.395836	0.784508

50	1	0	6.788091	2.867736	-1.011988
51	1	0	0.787561	0.281638	-2.803884
52	1	0	2.076475	-0.848443	-3.192748
53	1	0	0.392374	-1.403507	-3.209841
54	1	0	2.503330	-2.995258	3.119755
55	1	0	2.618832	-1.700187	4.327743
56	1	0	1.081968	-1.998368	3.504411
57	1	0	-3.359169	-0.662825	-2.528120
58	1	0	-1.275003	0.046189	-1.821671
59	1	0	0.102016	1.742154	-0.858990
60	1	0	-0.496556	1.439524	0.773133
61	1	0	-6.489371	-0.881674	1.158731
62	1	0	-2.470258	-0.517493	0.920163
63	1	0	-1.424826	3.449504	-0.353713
64	1	0	-2.220577	2.433015	-1.551599
65	1	0	-4.770661	1.831443	-0.826460
66	1	0	-0.038949	-0.412806	1.642075
67	1	0	-0.068544	-2.173065	1.532912
68	1	0	-6.188140	-2.622655	-0.774204
69	1	0	-5.356621	-1.948906	-2.189573
70	1	0	-4.443933	-2.906807	-1.022366
71	1	0	-3.062682	4.434222	0.996269
72	1	0	-4.026960	4.113926	-0.462119
73	1	0	-4.666895	3.680418	1.138906
74	1	0	-3.351815	1.995263	2.310868

S93. Conformational analysis of the B3LYP-D3BJ/6-31G(d) optimized conformers of 6b in the gas phase (T=298.15 K)

Conformer	E (Hartree)[a]	G (kcal/mol)[b]	ΔG (kcal/mol)[c]	Population[d]
6b-1	-1766.484564	-1108486.729019	0.00	67.45%
6b-2	-1766.483782	-1108486.238269	0.490750	29.48%
6b-3	-1766.481114	-1108484.563921	2.165098	1.73%
6b-4	-1766.480862	-1108484.405463	2.323557	1.34%

[a]Electronic energy obtained at M06-2X-D3/6-311+G(2d,p) level of theory;

[b]Gibbs free energy (E*627.51);

[c]The relative Gibbs free energy;

[d]The Boltzmann distribution of each conformer.

S94 Cartesian coordinates for the low-energy Conf. of Compound 6b at B3LYP/6311+G(d,p) level of theory in methanol

Conformer 6b-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.985394	2.713632	-1.086965

2	6	0	4.830639	2.195181	0.029844
3	8	0	3.088897	1.742230	-1.433504
4	6	0	4.205994	0.910026	0.494511
5	6	0	5.159841	-0.156543	1.037354
6	6	0	1.829607	-1.809094	-2.028903
7	6	0	1.090233	-0.590257	-1.482927
8	6	0	3.373406	0.496745	-0.736375
9	6	0	4.631388	-1.603779	1.024305
10	6	0	2.489029	-2.389690	-1.022822
11	8	0	2.740096	-0.893661	2.447868
12	6	0	2.066717	-0.163482	-0.346360
13	6	0	3.151178	-1.828686	1.431803
14	6	0	2.194802	-1.598541	0.247196
15	8	0	4.023453	3.787089	-1.634770
16	6	0	5.926605	2.830140	0.443151
17	6	0	0.660008	0.431979	-2.523502
18	6	0	2.996075	-3.256171	1.976349
19	8	0	-4.037894	-0.543390	1.799966
20	6	0	-1.006062	-2.118936	-1.334928
21	6	0	-0.083303	-1.155643	-0.582501
22	8	0	-2.272803	-2.028490	-0.829017
23	6	0	-1.142280	-0.130305	-0.093833
24	6	0	-0.778640	0.944655	0.942468
25	6	0	-5.705376	-0.099108	-0.820709
26	6	0	-4.880495	-1.058618	-0.352315
27	6	0	-2.305457	-1.073697	0.258883
28	6	0	-1.957991	1.545165	1.731184
29	6	0	-5.192219	1.234636	-0.489203
30	6	0	-3.702593	-0.424656	0.406489
31	6	0	-3.174491	2.072074	0.940311
32	6	0	-3.730425	1.043241	-0.065903
33	8	0	-0.752774	-2.867837	-2.243146
34	6	0	0.684993	-1.887191	0.567451
35	6	0	-5.135882	-2.526075	-0.327530
36	6	0	-2.857258	3.393670	0.238012
37	8	0	-5.802288	2.295899	-0.490987
38	8	0	-4.190153	2.276497	1.953480
39	1	0	3.486031	1.145567	1.288392
40	1	0	5.426045	0.124431	2.062816
41	1	0	6.093611	-0.134340	0.462295
42	1	0	1.729207	-2.168647	-3.044625
43	1	0	3.952890	-0.128133	-1.423028
44	1	0	4.769705	-2.035508	0.026845
45	1	0	5.273300	-2.193791	1.691172

46	1	0	3.023197	-3.333244	-1.052935
47	1	0	3.225861	-1.109655	3.259427
48	1	0	1.579375	0.506993	0.361886
49	1	0	6.551044	2.447662	1.245250
50	1	0	6.218959	3.764534	-0.026995
51	1	0	0.272583	1.346776	-2.065500
52	1	0	1.504590	0.725029	-3.150329
53	1	0	-0.117123	0.007282	-3.170390
54	1	0	3.273082	-4.005484	1.227667
55	1	0	3.655244	-3.400737	2.841669
56	1	0	1.968608	-3.447197	2.295491
57	1	0	-4.416560	0.313567	2.086376
58	1	0	-1.458155	0.390179	-1.003109
59	1	0	-0.232094	1.740253	0.423283
60	1	0	-0.085612	0.539060	1.687229
61	1	0	-6.679579	-0.257108	-1.270272
62	1	0	-2.112264	-1.614516	1.191012
63	1	0	-2.324630	0.793421	2.431376
64	1	0	-1.581343	2.377796	2.335887
65	1	0	-3.172129	1.113794	-1.004882
66	1	0	0.418934	-1.487143	1.548549
67	1	0	0.485439	-2.960836	0.574980
68	1	0	-6.138749	-2.762995	-0.693193
69	1	0	-4.393943	-3.057655	-0.930172
70	1	0	-5.038347	-2.890565	0.702374
71	1	0	-3.728787	3.755406	-0.314981
72	1	0	-2.567921	4.145241	0.979111
73	1	0	-2.029815	3.270633	-0.470261
74	1	0	-4.943538	2.689207	1.491246

Conformer 6b-2

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	3.972054	2.726849	-1.068493
2	6	0	4.822927	2.203620	0.041147
3	8	0	3.079185	1.753052	-1.420960
4	6	0	4.207884	0.910596	0.497102
5	6	0	5.167823	-0.156637	1.026758
6	6	0	1.824741	-1.798620	-2.038339
7	6	0	1.089163	-0.582316	-1.482424
8	6	0	3.372877	0.504044	-0.734354
9	6	0	4.641746	-1.604079	1.000858
10	6	0	2.482826	-2.388248	-1.036941
11	8	0	2.895234	-0.914196	2.488443
12	6	0	2.069632	-0.163843	-0.345761

13	6	0	3.172492	-1.838653	1.420080
14	6	0	2.201462	-1.601597	0.239870
15	8	0	4.000963	3.804808	-1.608052
16	6	0	5.915684	2.841708	0.458245
17	6	0	0.655764	0.446197	-2.515560
18	6	0	3.030836	-3.272306	1.951229
19	8	0	-4.027530	-0.538363	1.809595
20	6	0	-1.006285	-2.116818	-1.335332
21	6	0	-0.082367	-1.152761	-0.583320
22	8	0	-2.272050	-2.028482	-0.825815
23	6	0	-1.142891	-0.130449	-0.091544
24	6	0	-0.780312	0.950150	0.938697
25	6	0	-5.710134	-0.115052	-0.807238
26	6	0	-4.881242	-1.069528	-0.335863
27	6	0	-2.304291	-1.075387	0.262934
28	6	0	-1.959539	1.556331	1.723181
29	6	0	-5.198188	1.222197	-0.487815
30	6	0	-3.701518	-0.427783	0.413223
31	6	0	-3.178280	2.074063	0.929228
32	6	0	-3.734127	1.036800	-0.068613
33	8	0	-0.754289	-2.863736	-2.244926
34	6	0	0.690262	-1.888681	0.561845
35	6	0	-5.132417	-2.537500	-0.300390
36	6	0	-2.864873	3.391082	0.216757
37	8	0	-5.809836	2.282284	-0.495371
38	8	0	-4.191840	2.282903	1.943130
39	1	0	3.491614	1.135824	1.297487
40	1	0	5.430755	0.108794	2.055367
41	1	0	6.097975	-0.127341	0.445858
42	1	0	1.723905	-2.149071	-3.057314
43	1	0	3.952397	-0.113276	-1.427836
44	1	0	4.766100	-2.022658	-0.003609
45	1	0	5.287255	-2.196977	1.658507
46	1	0	3.017344	-3.331162	-1.074908
47	1	0	2.096551	-1.220605	2.944305
48	1	0	1.584199	0.501841	0.368951
49	1	0	6.542885	2.455283	1.256176
50	1	0	6.201658	3.782138	-0.003759
51	1	0	0.270108	1.358724	-2.051637
52	1	0	1.499079	0.742696	-3.142299
53	1	0	-0.122836	0.025494	-3.163389
54	1	0	3.296363	-4.013161	1.190373
55	1	0	3.693461	-3.409997	2.810998
56	1	0	2.004103	-3.482442	2.272490

57	1	0	-4.413945	0.316843	2.090865
58	1	0	-1.460791	0.387697	-1.001218
59	1	0	-0.230525	1.741065	0.416297
60	1	0	-0.087830	0.549693	1.687375
61	1	0	-6.685589	-0.278136	-1.252178
62	1	0	-2.110002	-1.617335	1.194409
63	1	0	-2.324834	0.810492	2.430215
64	1	0	-1.583320	2.395157	2.319410
65	1	0	-3.179620	1.102760	-1.010218
66	1	0	0.405007	-1.484983	1.539529
67	1	0	0.486427	-2.961268	0.575453
68	1	0	-6.135588	-2.779724	-0.661557
69	1	0	-4.391026	-3.071082	-0.902008
70	1	0	-5.031073	-2.894990	0.731614
71	1	0	-3.738007	3.746634	-0.337653
72	1	0	-2.576297	4.148906	0.951711
73	1	0	-2.038198	3.264832	-0.491892
74	1	0	-4.946628	2.692897	1.480736

Conformer 6b-3

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	4.052114	2.691324	-1.105931
2	6	0	4.885389	2.176883	0.021747
3	8	0	3.118065	1.741493	-1.415582
4	6	0	4.211728	0.930603	0.527302
5	6	0	5.115103	-0.145622	1.144219
6	6	0	1.834303	-1.756050	-2.041904
7	6	0	1.091435	-0.550459	-1.470918
8	6	0	3.381603	0.502762	-0.700064
9	6	0	4.609213	-1.598170	1.062356
10	6	0	2.486548	-2.361349	-1.045972
11	8	0	2.729468	-1.098326	2.582310
12	6	0	2.067331	-0.152663	-0.322010
13	6	0	3.129722	-1.871336	1.438478
14	6	0	2.185211	-1.604566	0.244381
15	8	0	4.124083	3.745784	-1.684576
16	6	0	6.006402	2.778255	0.416312
17	6	0	0.664571	0.495710	-2.489126
18	6	0	3.002319	-3.324003	1.906965
19	8	0	-4.055705	-0.572492	1.777568
20	6	0	-1.005643	-2.077725	-1.374612
21	6	0	-0.087240	-1.135566	-0.589846
22	8	0	-2.275518	-1.999853	-0.875318
23	6	0	-1.149835	-0.122557	-0.083423

24	6	0	-0.795310	0.925382	0.982460
25	6	0	-5.709033	-0.077419	-0.843996
26	6	0	-4.887109	-1.046075	-0.389217
27	6	0	-2.316189	-1.073908	0.236651
28	6	0	-1.981764	1.516576	1.767934
29	6	0	-5.197166	1.249598	-0.485125
30	6	0	-3.713705	-0.427023	0.388518
31	6	0	-3.189145	2.059303	0.973223
32	6	0	-3.738044	1.049378	-0.055999
33	8	0	-0.745962	-2.800552	-2.301669
34	6	0	0.673363	-1.896612	0.544770
35	6	0	-5.142050	-2.513731	-0.394300
36	6	0	-2.862337	3.391936	0.296429
37	8	0	-5.805461	2.311741	-0.472159
38	8	0	-4.212678	2.248624	1.980423
39	1	0	3.481629	1.266708	1.283349
40	1	0	5.291243	0.114434	2.193478
41	1	0	6.092234	-0.107119	0.649061
42	1	0	1.740819	-2.088366	-3.067483
43	1	0	3.966724	-0.136289	-1.367444
44	1	0	4.775739	-1.985416	0.050626
45	1	0	5.247033	-2.193654	1.724936
46	1	0	3.023152	-3.302292	-1.095493
47	1	0	2.731003	-0.163060	2.330574
48	1	0	1.573357	0.515934	0.387981
49	1	0	6.614842	2.395434	1.230278
50	1	0	6.336532	3.684394	-0.083126
51	1	0	0.280499	1.402260	-2.011952
52	1	0	1.508143	0.797860	-3.112518
53	1	0	-0.115770	0.086451	-3.141872
54	1	0	3.333848	-4.021201	1.131641
55	1	0	3.625187	-3.470990	2.794063
56	1	0	1.970402	-3.562380	2.175245
57	1	0	-4.444114	0.275463	2.076779
58	1	0	-1.458352	0.422200	-0.980745
59	1	0	-0.234745	1.728806	0.490550
60	1	0	-0.119725	0.494112	1.729564
61	1	0	-6.680441	-0.226447	-1.302517
62	1	0	-2.130411	-1.638289	1.156178
63	1	0	-2.357185	0.753970	2.451206
64	1	0	-1.610142	2.338248	2.390495
65	1	0	-3.174325	1.137660	-0.990269
66	1	0	0.403924	-1.526593	1.537098
67	1	0	0.474467	-2.969813	0.524316

68	1	0	-6.142397	-2.743911	-0.770877
69	1	0	-4.396220	-3.033371	-1.002606
70	1	0	-5.050796	-2.898195	0.628885
71	1	0	-3.728142	3.764904	-0.258081
72	1	0	-2.578405	4.130354	1.052711
73	1	0	-2.029053	3.279201	-0.406865
74	1	0	-4.961608	2.670395	1.519038

Conformer 6b-4

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	-4.065460	2.793940	0.747647
2	6	0	-4.898694	2.142165	-0.306547
3	8	0	-3.154320	1.881851	1.199908
4	6	0	-4.253671	0.823136	-0.625445
5	6	0	-5.191285	-0.312657	-1.041841
6	6	0	-1.841124	-1.560427	2.178096
7	6	0	-1.115559	-0.399044	1.503125
8	6	0	-3.414221	0.562937	0.642290
9	6	0	-4.638223	-1.740166	-0.868611
10	6	0	-2.481393	-2.260579	1.237925
11	8	0	-2.768495	-1.159631	-2.373942
12	6	0	-2.095916	-0.114055	0.326333
13	6	0	-3.155527	-1.982402	-1.257573
14	6	0	-2.198858	-1.606102	-0.109995
15	8	0	-4.123267	3.920283	1.174412
16	6	0	-6.002594	2.710539	-0.789793
17	6	0	-0.702378	0.741419	2.419837
18	6	0	-2.975889	-3.458566	-1.641292
19	8	0	3.612008	-0.427561	-1.918260
20	6	0	0.989586	-1.921661	1.561712
21	6	0	0.069949	-1.050805	0.678050
22	8	0	2.277868	-1.864793	1.092588
23	6	0	1.146645	-0.097125	0.101546
24	6	0	0.973695	0.852407	-1.092072
25	6	0	5.848207	-0.476653	0.331490
26	6	0	4.851605	-1.284732	-0.071926
27	6	0	2.274766	-1.091474	-0.127994
28	6	0	1.758315	2.154871	-0.843601
29	6	0	5.429861	0.927272	0.257855
30	6	0	3.623981	-0.466203	-0.484150
31	6	0	3.292593	2.162940	-0.588398
32	6	0	3.886054	0.930791	0.141692
33	8	0	0.715473	-2.566768	2.539886
34	6	0	-0.683883	-1.889355	-0.406705

35	6	0	4.894976	-2.756899	-0.289240
36	6	0	3.602998	3.454394	0.184216
37	8	0	6.165321	1.903153	0.220362
38	8	0	3.929306	2.237062	-1.896738
39	1	0	-3.538446	0.978116	-1.442976
40	1	0	-5.463639	-0.152869	-2.091431
41	1	0	-6.124215	-0.241032	-0.469433
42	1	0	-1.743540	-1.804088	3.227776
43	1	0	-3.982373	0.005807	1.393596
44	1	0	-4.765695	-2.059155	0.171720
45	1	0	-5.271799	-2.412256	-1.461748
46	1	0	-3.000907	-3.203488	1.369698
47	1	0	-3.252890	-1.475761	-3.152804
48	1	0	-1.616254	0.482867	-0.450895
49	1	0	-6.617925	2.231791	-1.545919
50	1	0	-6.310888	3.686607	-0.426683
51	1	0	-0.330282	1.602862	1.857291
52	1	0	-1.551023	1.090351	3.011603
53	1	0	0.083038	0.407597	3.108762
54	1	0	-3.234067	-4.125711	-0.812470
55	1	0	-3.636792	-3.710272	-2.480396
56	1	0	-1.946631	-3.663830	-1.945290
57	1	0	3.857442	0.484044	-2.192449
58	1	0	1.455434	0.515196	0.957450
59	1	0	-0.070240	1.142254	-1.233537
60	1	0	1.294333	0.365154	-2.016111
61	1	0	6.866400	-0.769354	0.563076
62	1	0	2.029774	-1.768194	-0.954254
63	1	0	1.606807	2.840199	-1.684503
64	1	0	1.295697	2.632466	0.028706
65	1	0	3.515518	0.909025	1.174750
66	1	0	-0.429563	-1.547846	-1.413753
67	1	0	-0.460387	-2.956251	-0.338867
68	1	0	5.891483	-3.165126	-0.101135
69	1	0	4.173002	-3.257866	0.365159
70	1	0	4.609148	-2.980043	-1.324697
71	1	0	4.678307	3.605904	0.282749
72	1	0	3.160169	4.306750	-0.341185
73	1	0	3.171245	3.409743	1.189967
74	1	0	4.857288	2.480216	-1.727284

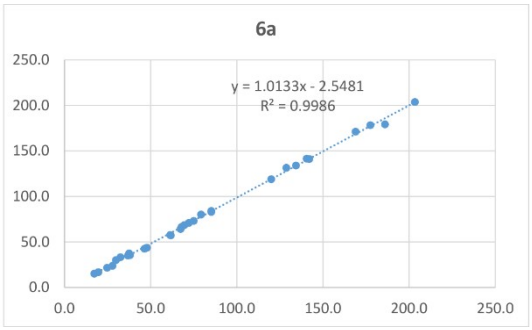
S95. Experimental and calculated ^{13}C NMR chemical shifts of 6a and 6b

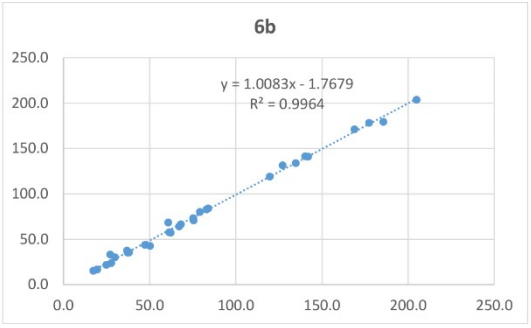
NO.	$\delta_{exptl.}$	$\delta_{calcd.}$ (ppm)		NO.	$\delta_{exptl.}$	$\delta_{calcd.}$ (ppm)	
		6a	**6b**			**6a**	**6b**
1	64.2	67.3	67.1	1′	68.4	69.4	60.8
2	133.9	134.3	134.7	2′	203.8	203.3	204.8
3	141.5	140.5	140.2	3′	131.5	128.7	127.1
4	57.6	61.2	61.3	4′	179.3	185.9	185.5
5	66.5	67.9	68.1	5′	83	85.1	83.0
6	80.1	79.2	79.1	6′	84	85.1	83.9
7	43.7	47.8	47.2	7′	42.6	46.4	50.2
8	23.7	27.8	27.6	8′	21.7	24.7	24.8
9	35.1	36.8	37.3	9′	37.4	37.4	36.8
10	73.2	74.9	75.3	10′	70.8	72.0	75.4
11	141.1	142.0	141.9	11′	57.2	61.7	62.2
12	171.1	168.9	168.8	12′	178.3	177.4	177.3
13	119	119.9	119.7	13′	35.5	38.0	38.0
14	30.1	29.8	29.8	14′	33.2	32.4	27.1
15	15.2	17.3	17.3	15′	16.7	19.6	19.5
				R^2		0.9986	0.9964
				MAE		2.1	2.7
				CMAE		1.4	2.3

S96. Experimental and calculated ^{1}H NMR chemical shifts of 6a and 6b

NO.	$\delta_{exptl.}$	$\delta_{calcd.}$ (ppm)		NO.	$\delta_{exptl.}$	$\delta_{calcd.}$ (ppm)	
		6a	**6b**			**6a**	**6b**
2	5.89	6.29	6.33	1'	2.75	6.21	2.93
3	6.31	6.72	6.62	3'	6.25	4.07	6.04
5	2.34	2.34	2.19	6'	4.51	3.51	4.54
6	4.18	4.18	4.18	7'	2.89	2.33	2.44
7	3.25	3.37	3.42	8'a	2.29	2.18	1.91
8a	2.23	2.26	2.24	8'b	1.56	2.05	1.71
8b	1.49	1.36	1.37	9'a	1.90	4.71	1.59
9a	186	1.81	1.85	9'b	1.64	2.65	2.57
9b	1.86	1.66	1.63	13'a	2.55	2.63	2.56
13b	5.38	5.85	5.84	13'b	1.26	1.97	1.34
13a	6.11	6.46	6.44	14'a	0.88	2.42	0.96
14a	1.31	1.34	1.37	14'b	1.02	2.32	1.42
14b	1.31	0.95	0.92	14'c	2.18	2.59	2.15
w14c	1.31	1.13	1.22	15'a	2.26	2.49	2.20
15a	1.44	1.15	1.11	15'b	2.27	2.51	2.76
15b	1.44	1.60	1.59	15'c	2.71	2.55	2.41
15c	1.44	1.18	1.05				

S97. Linear regression analysis between the experimental and calculated ^{13}C NMR chemical shifts of 6a/6b.





S98. DP4+ probability analysis of 6a/6b.

Functional	Solvent?	Basis Set	Type of Data
mPW1PW91	PCM	6-311G(d,p)	Unscaled Shifts

	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6
sDP4+ (H data)	99.83%	0.17%				
sDP4+ (C data)	100.00%	0.00%				
sDP4+ (all data)	100.00%	0.00%				
uDP4+ (H data)	99.92%	0.08%				
uDP4+ (C data)	100.00%	0.00%				
uDP4+ (all data)	100.00%	0.00%				
DP4+ (H data)	100.00%	0.00%				
DP4+ (C data)	100.00%	0.00%				
DP4+ (all data)	100.00%	0.00%				