Electronic Supplementary Material (ESI) for New Journal of Chemistry.
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Supporting Information

Meso-tris(2-furyl/2-thienyl) substituted porphyrin-ferrocene 'click' conjugates: Synthesis, experimental and computational studies

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Contents

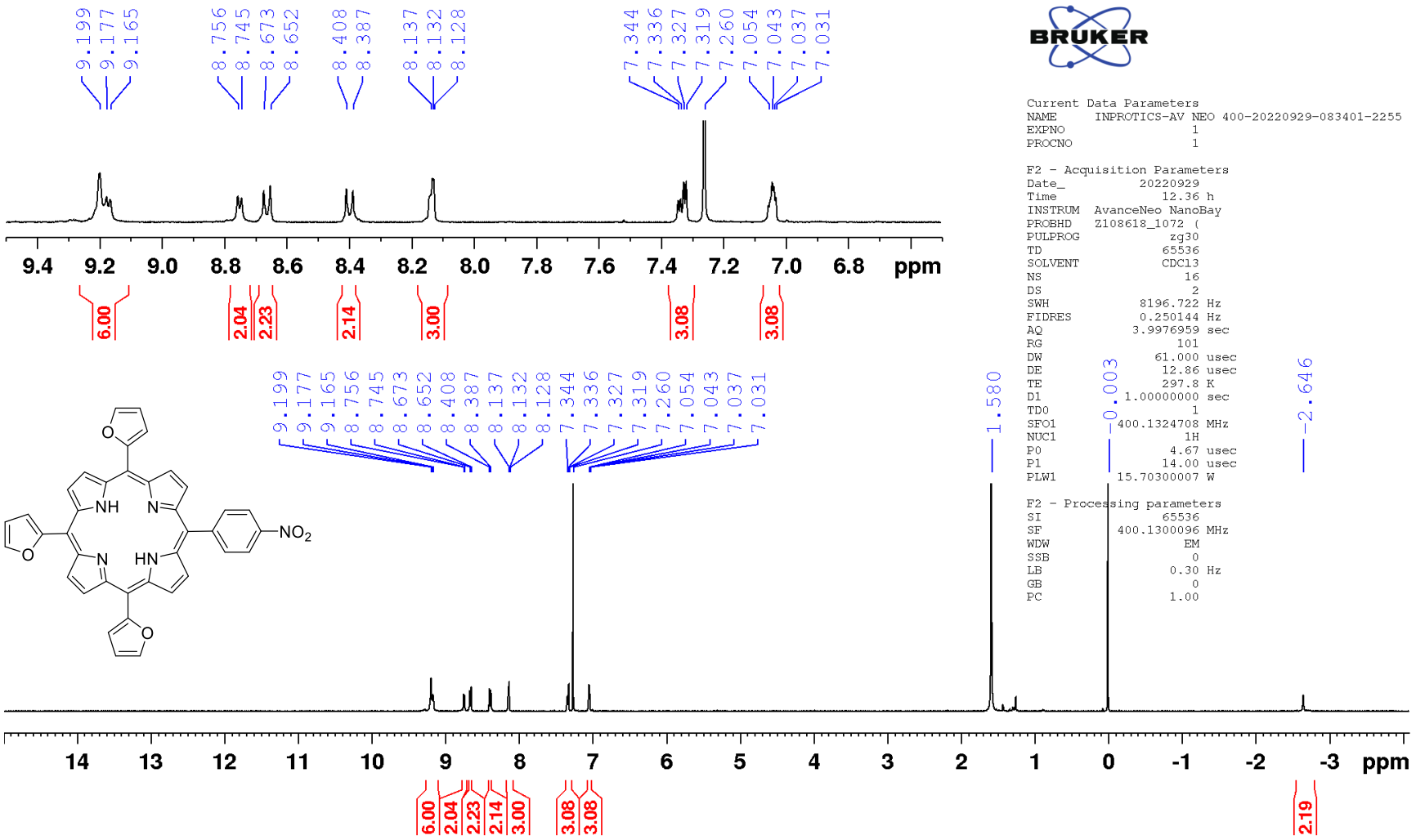


Figure S1. ^{1}H NMR spectrum of **1**

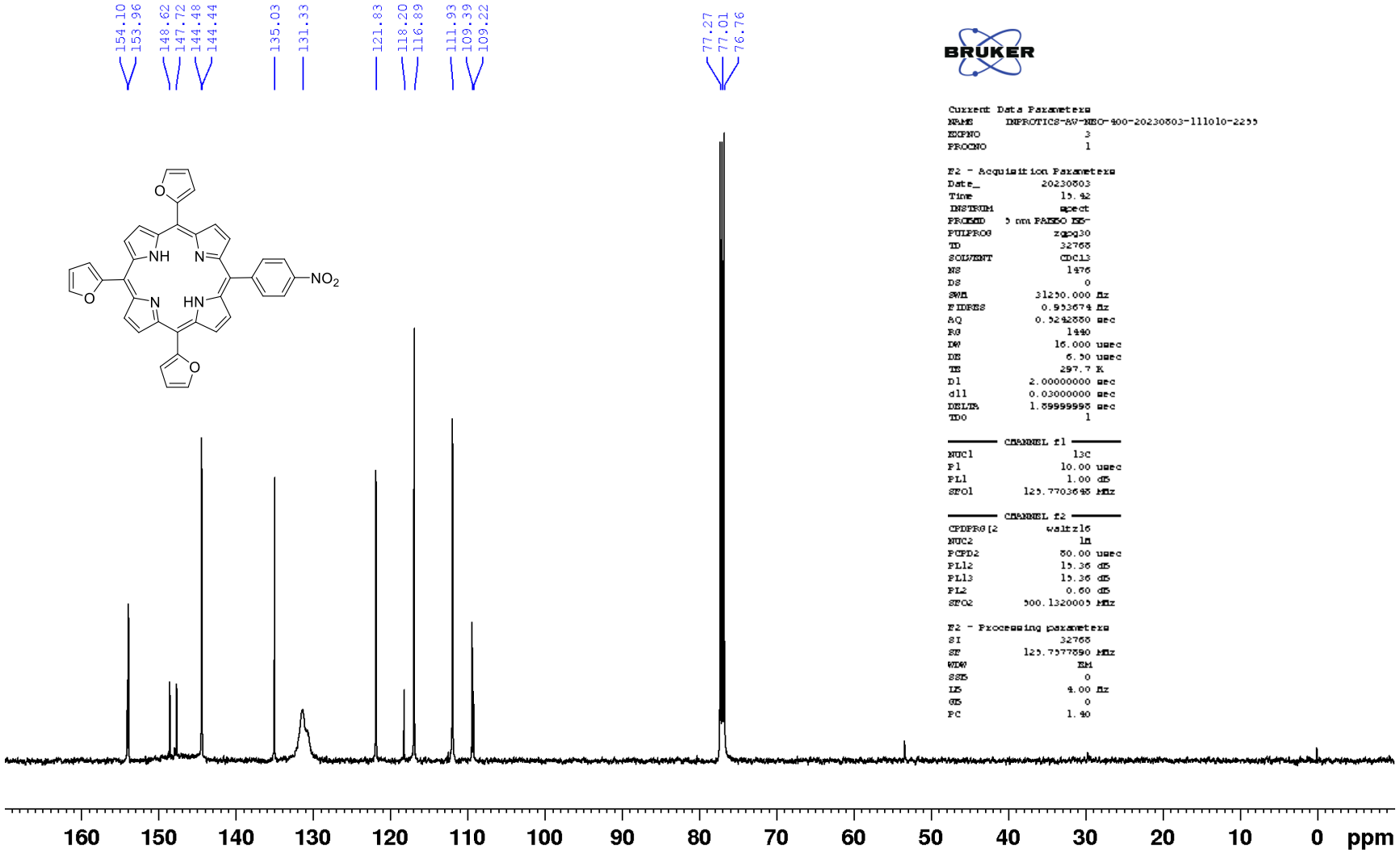
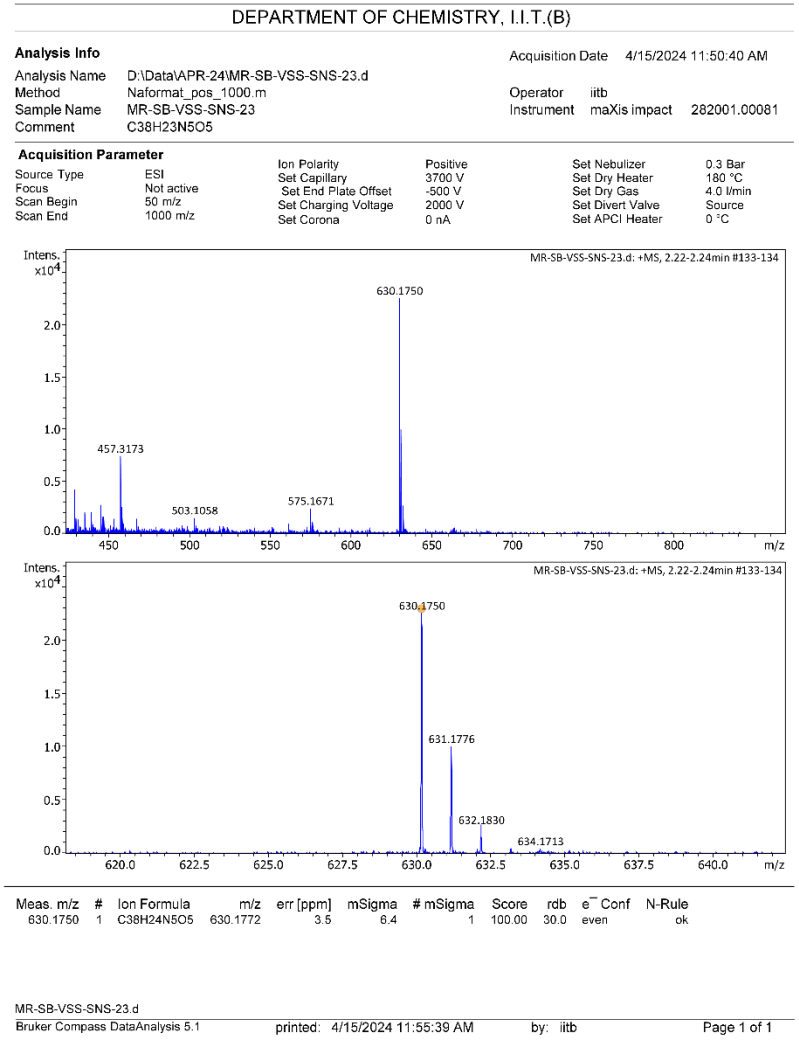
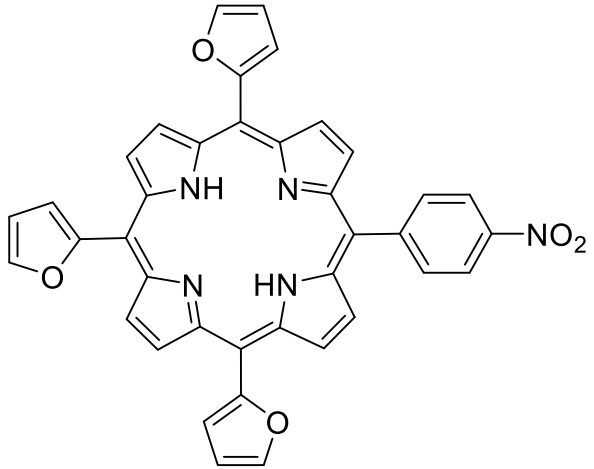


Figure S2. ^{13}C NMR spectrum of **1**



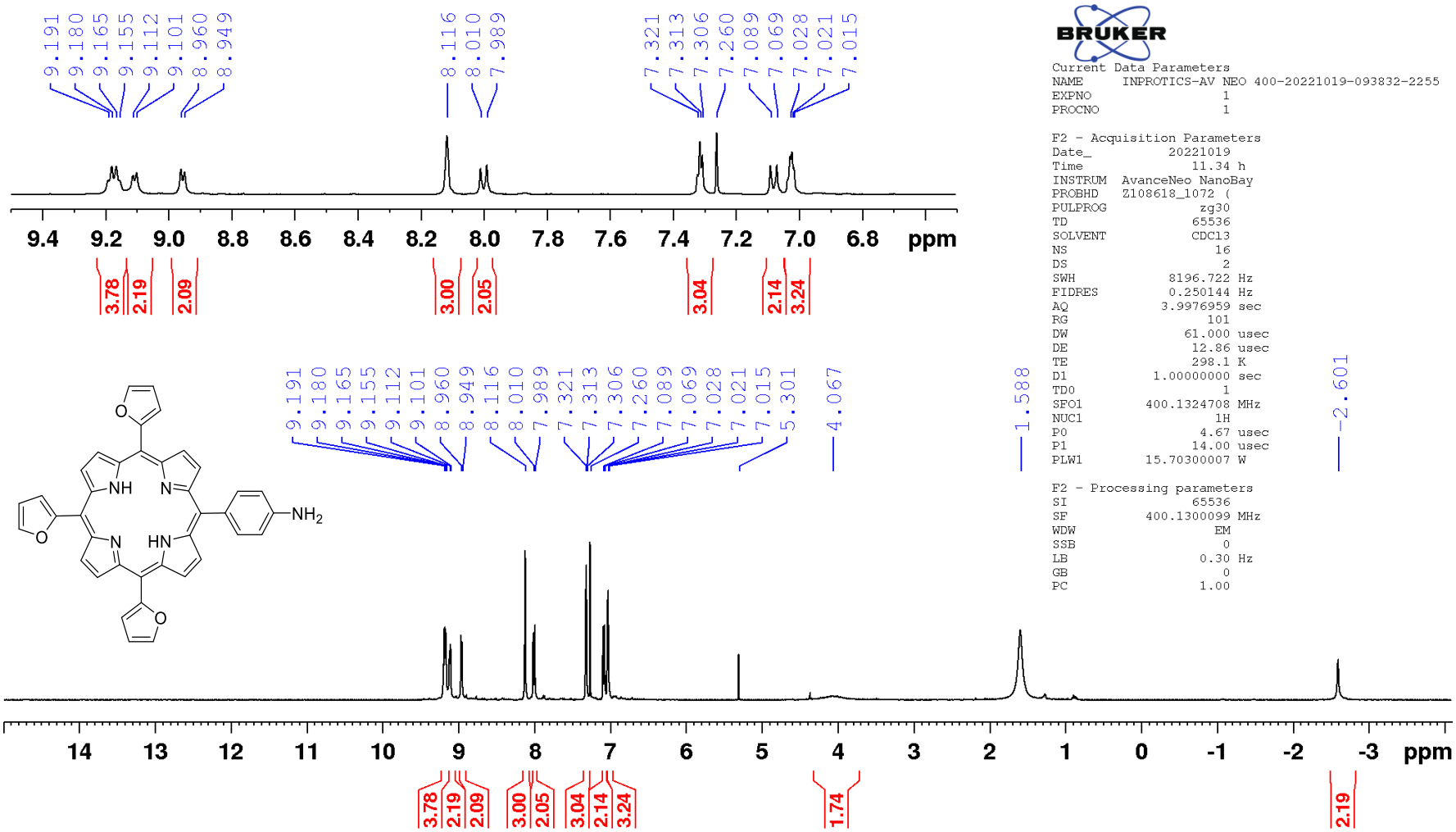


Chemical Formula: $C_{38}H_{23}N_5O_5$

Expected Mol. Wt.= 630.1772 $[M+H]^+$

Observed Mol. Wt.= 630.1750 $[M+H]^+$

Figure S3. ES MS spectrum of **1**



BRUKER

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PROCNO                1

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DE                12.86 usec
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D1             1.00000000 sec
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P0                 4.67 usec
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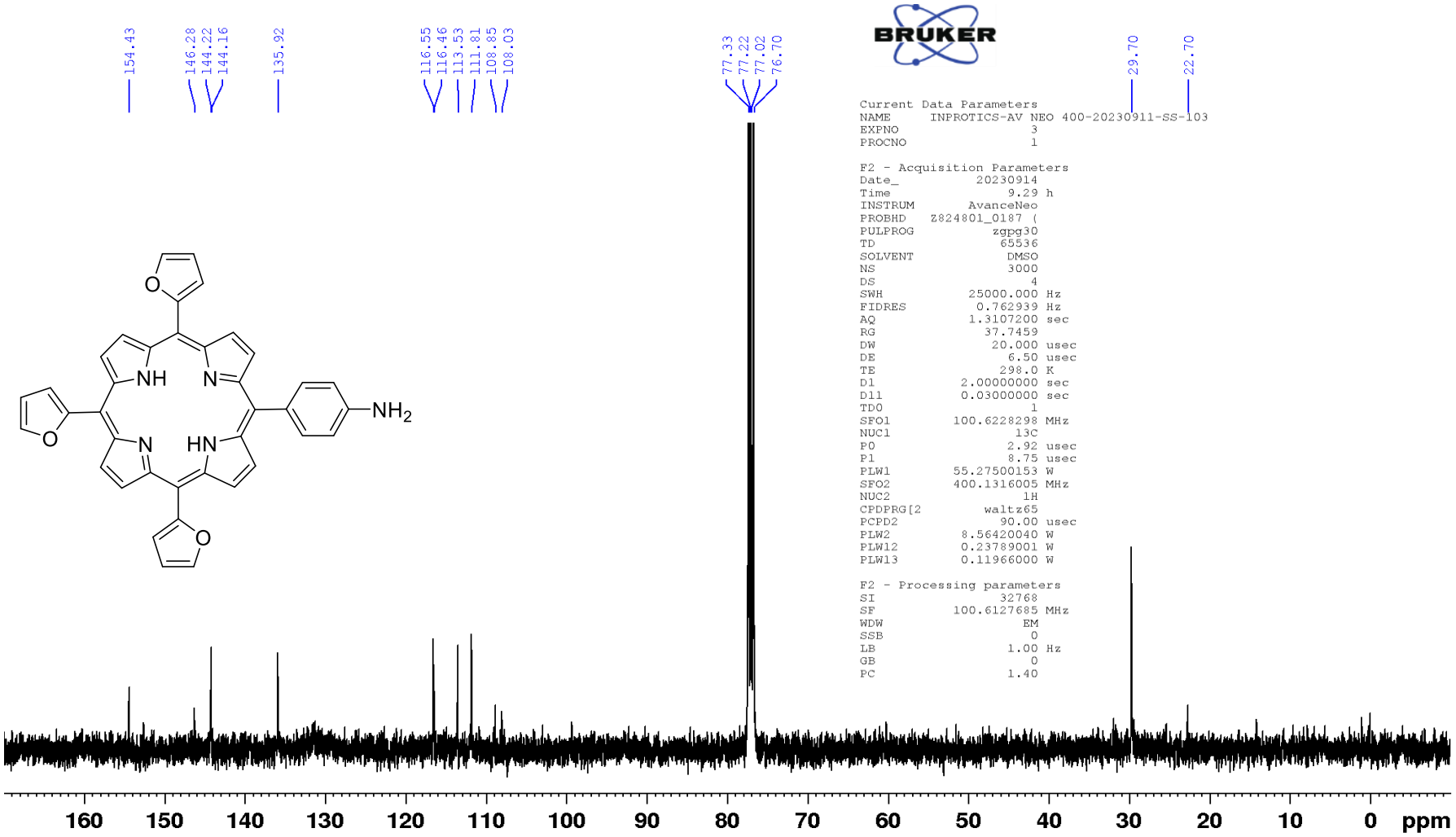
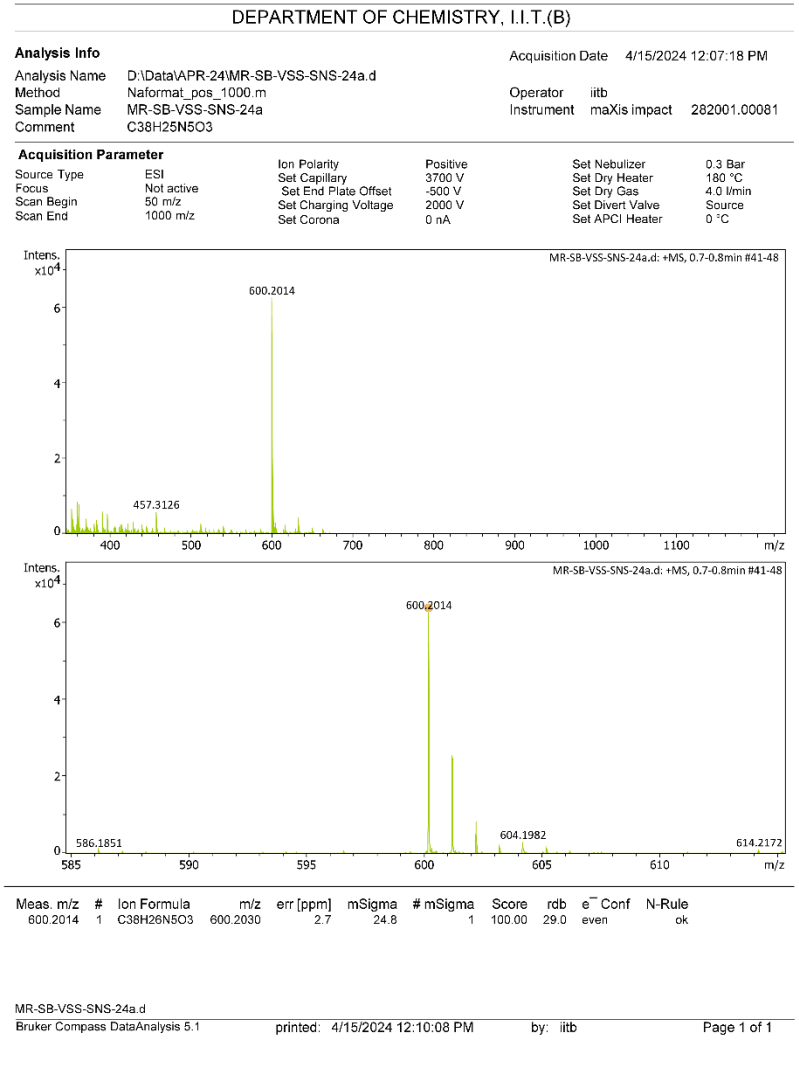
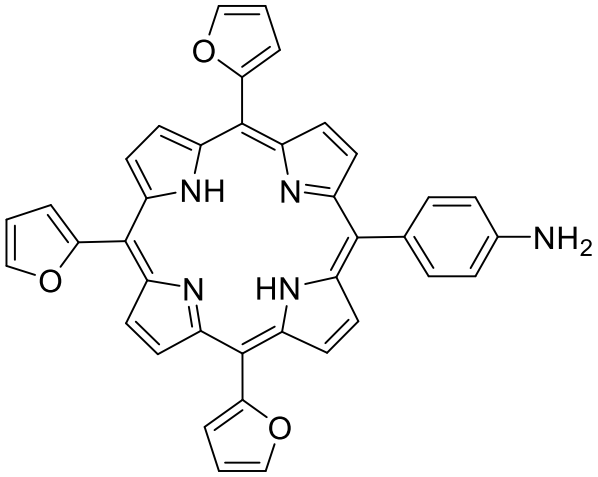


Figure S5. ^{13}C NMR spectrum of **3**





Chemical Formula: $C_{38}H_{25}N_5O_3$

Expected Mol. Wt.= 600.2030 $[M+H]^+$

Observed Mol. Wt.= 600.2014 $[M+H]^+$

Figure S6. ES MS spectrum of **3**

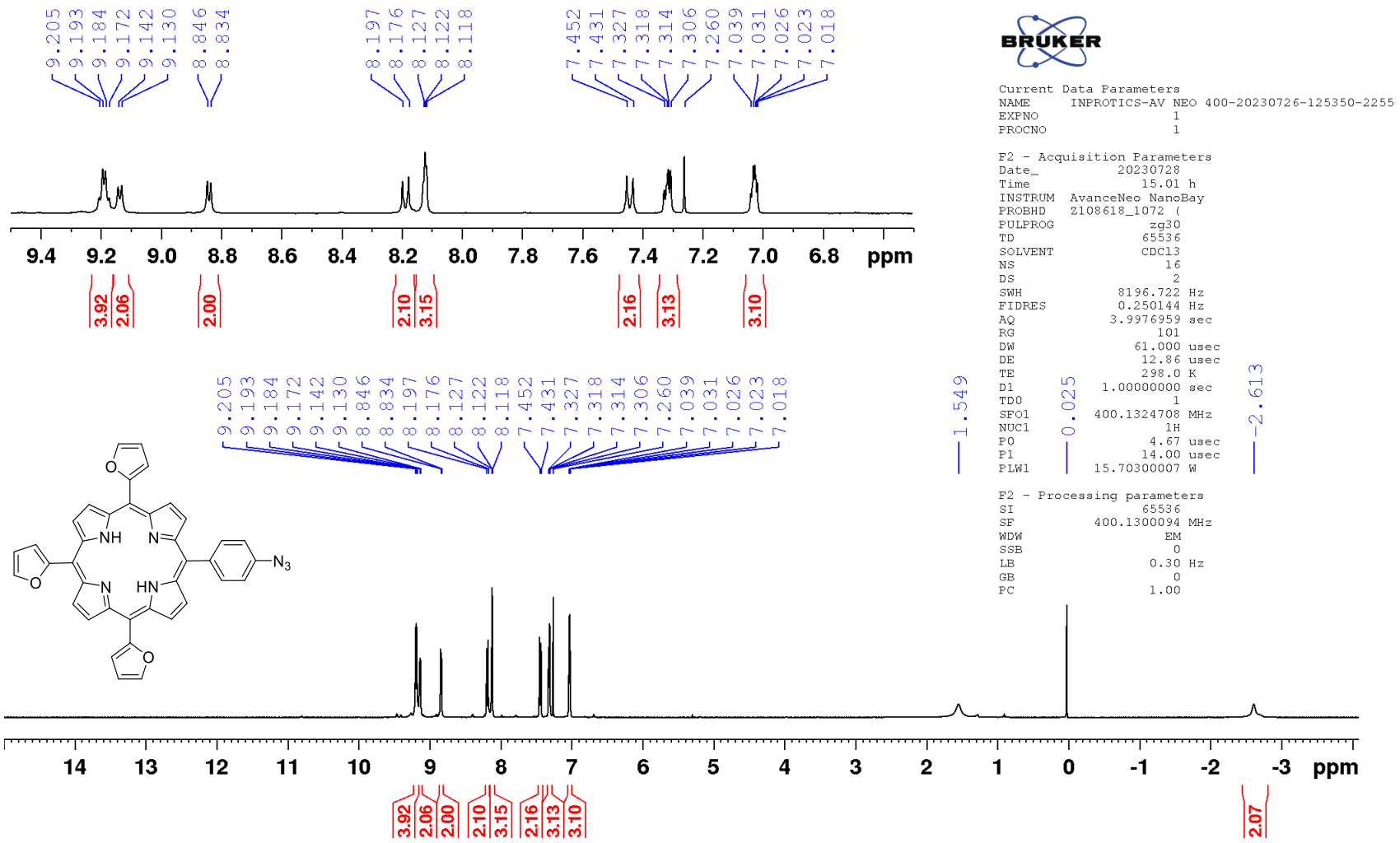


Figure S7. ^{1}H NMR spectrum of **5**

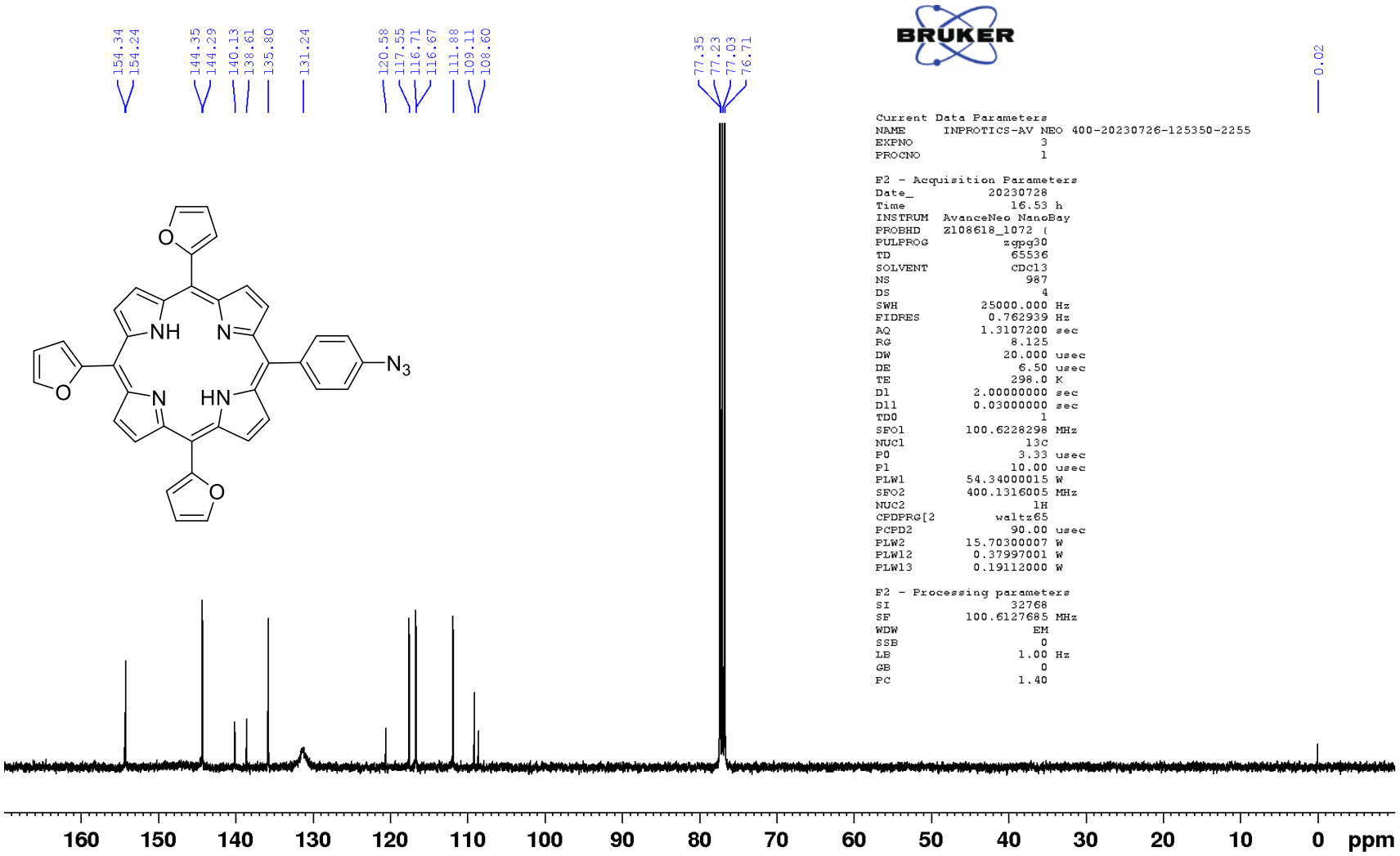
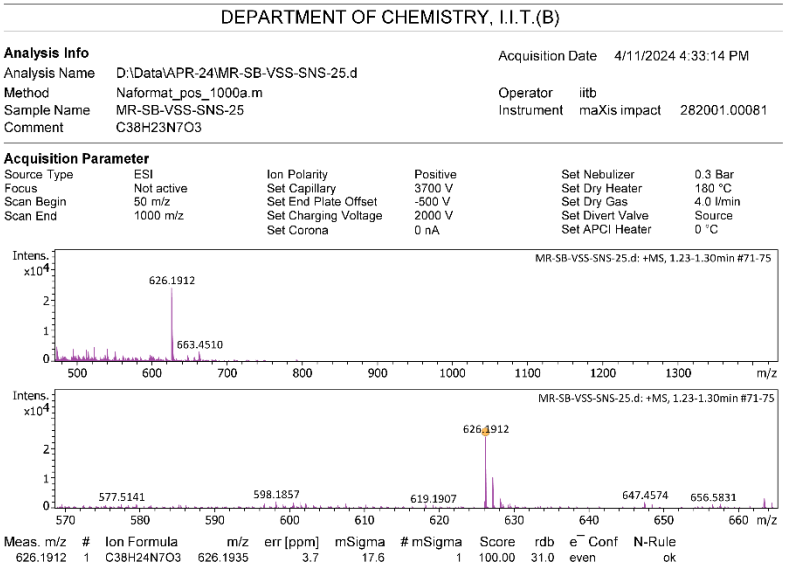


Figure S8. ^{13}C NMR spectrum of **5**



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Analysis Info

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Comment	C38H23N7O3		

Acquisition Parameter

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Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
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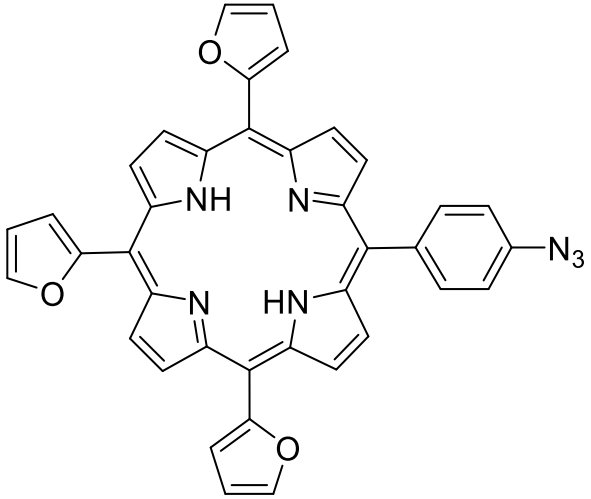
MR-SB-VSS-SNS-25.d

Bruker Compass DataAnalysis 5.1 printed: 4/11/2024 4:35:58 PM by: iitb Page 1 of 1



Chemical Formula: $C_{38}H_{23}N_7O_3$

Expected Mol. Wt.= 626.1935 $[M+H]^+$

Observed Mol. Wt.= 626.1912 $[M+H]^+$

Figure S9. ES MS spectrum of **5**

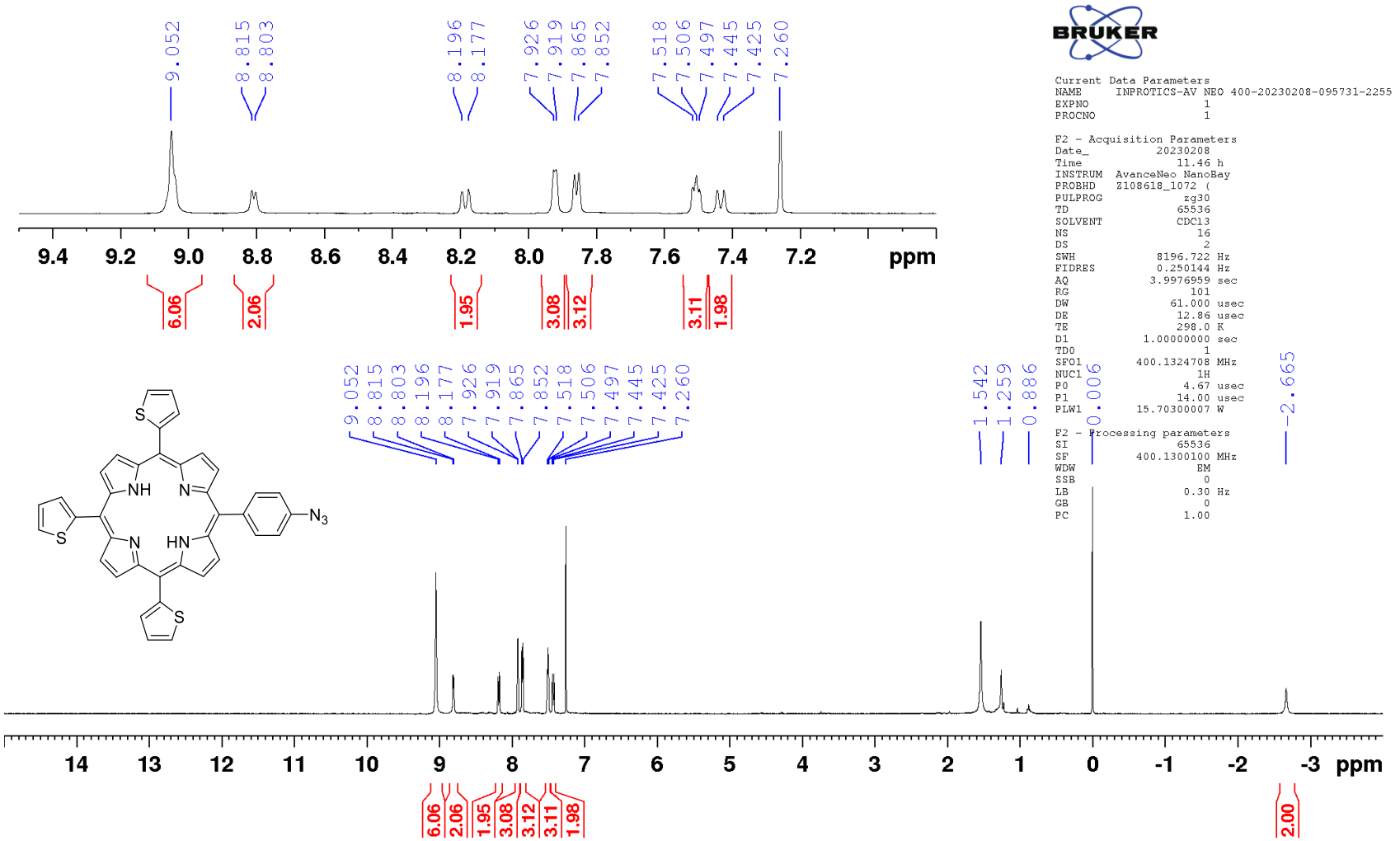


Figure S10. ^{1}H NMR spectrum of **6**

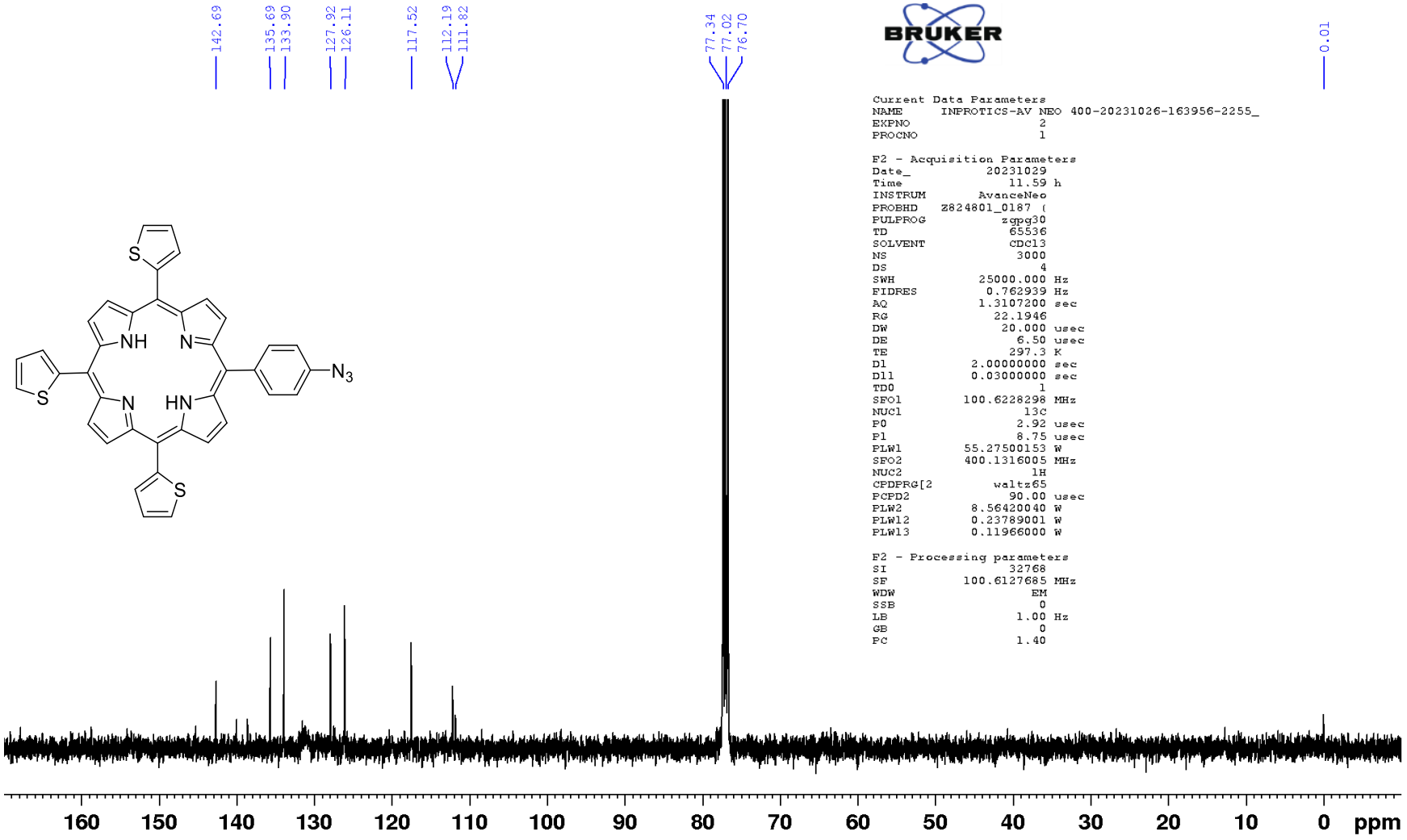
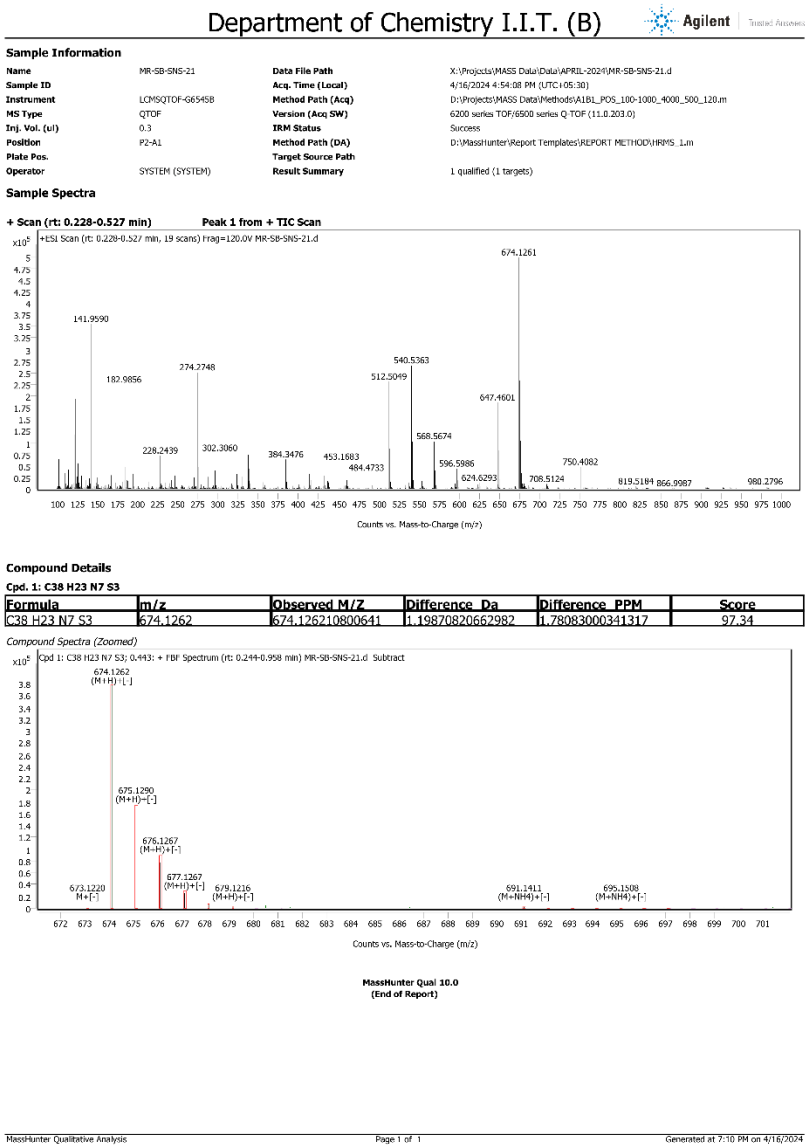


Figure S11. ^{13}C NMR spectrum of **6**



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Sample Information

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Instrument	LCMSQTOF-G6545B	**Method Path (Acq)**	D:\Projects\MASS Data\Methods\A1B1_POS_100-1000_4000_500_120.m
MS Type	QTOF	**Version (Acq SW)**	6200 series TOF/6500 series Q-TOF (11.0.203.0)
Inj. Vol. (ul)	0.3	**IRM Status**	Success
Position	P2-A1	**Method Path (DA)**	D:\MassHunter\Report Templates\REPORT METHOD\HRMS_1.m
Plate Pos.		**Target Source Path**	
Operator	SYSTEM (SYSTEM)	**Result Summary**	1 qualified (1 targets)

Sample Spectra

+ Scan (rt: 0.228-0.527 min) **Peak 1 from + TIC Scan**

Compound Details

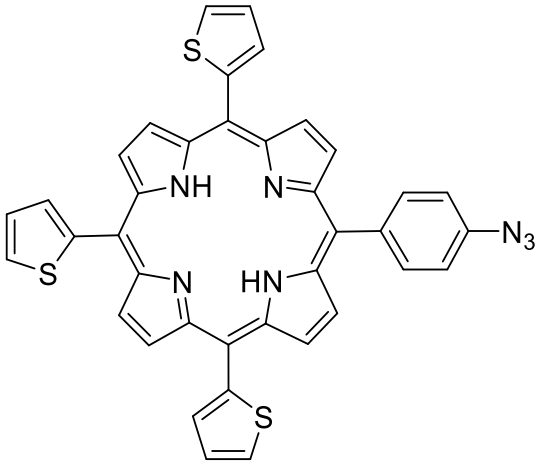
Cpd. 1: C38 H23 N7 S3

Formula	m/z	Observed M/Z	Difference_Da	Difference_PPM	Score
C38 H23 N7 S3	674.1262	674.126210800641	1.19870820662982	1.78083000341317	97.34

Compound Spectra (Zoomed)

MassHunter Qual 10.0
(End of Report)

MassHunter Qualitative Analysis Page 1 of 1 Generated at 7:10 PM on 4/16/2024



Chemical Formula: $C_{38}H_{23}N_7S_3$

Expected Mol. Wt.= 674.1262 $[M+H]^+$

Observed Mol. Wt.= 674.1262 $[M+H]^+$

Figure S12. LCMS QTOF spectrum of **6**

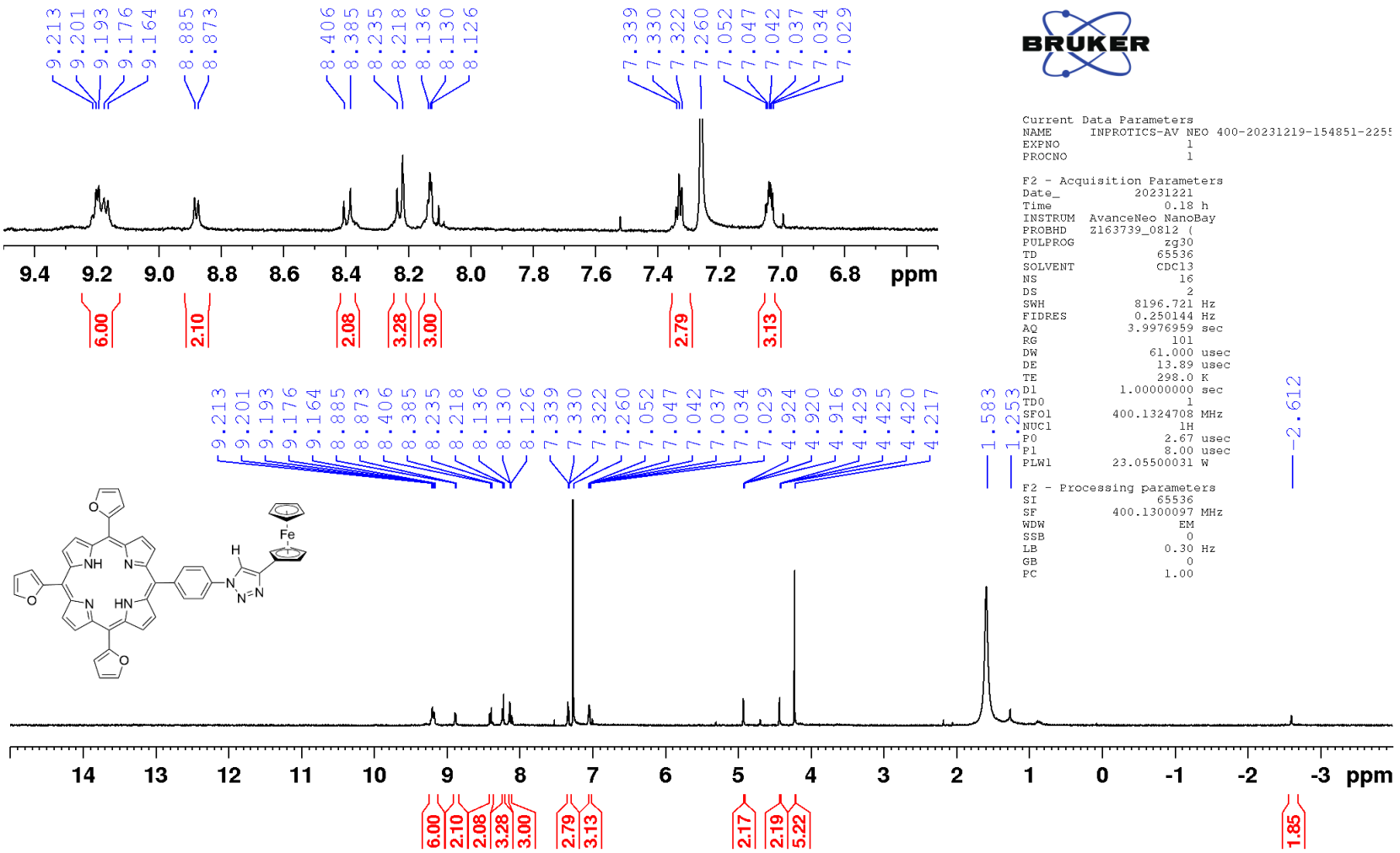


Figure S13. ^{1}H NMR spectrum of **8**

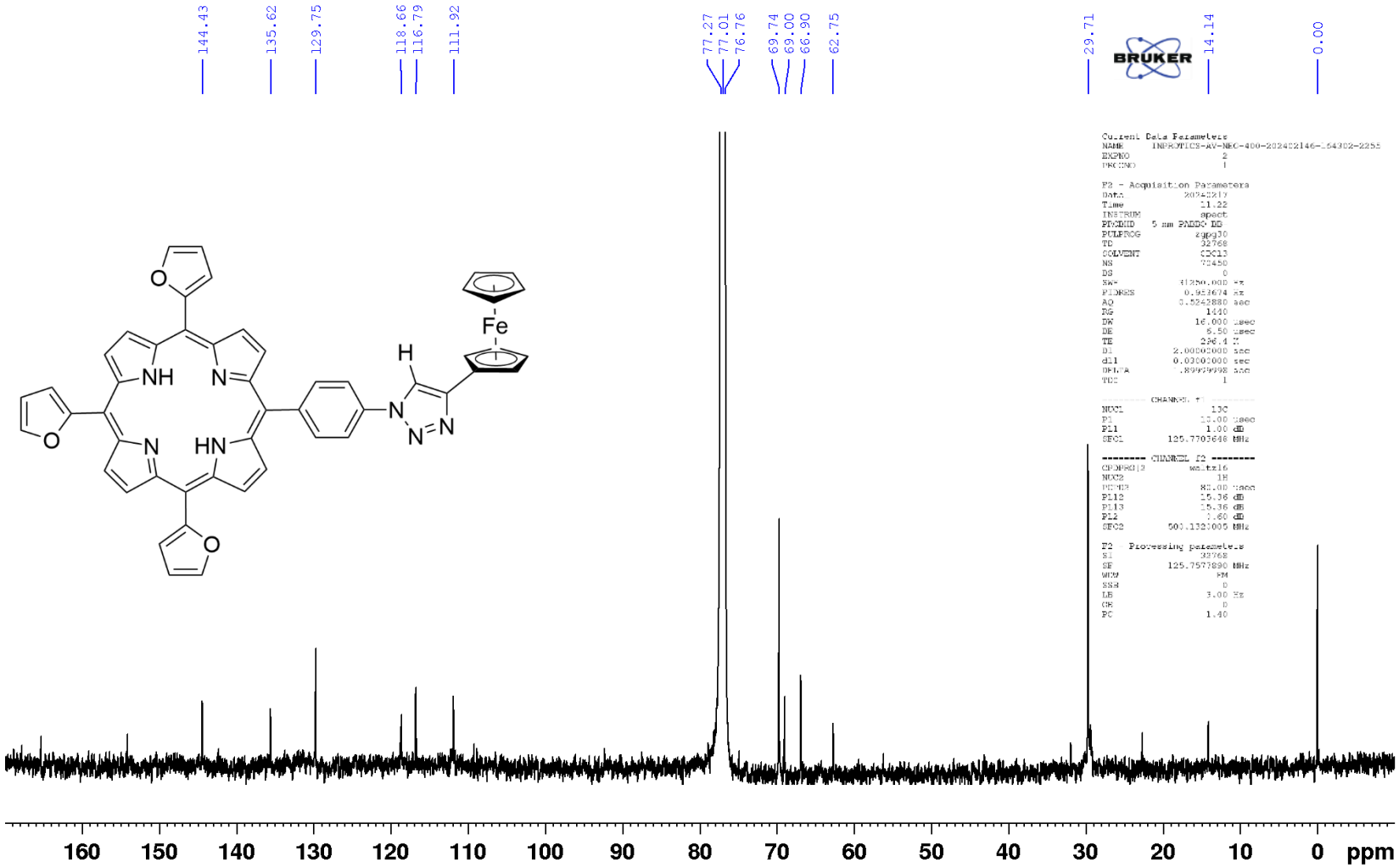
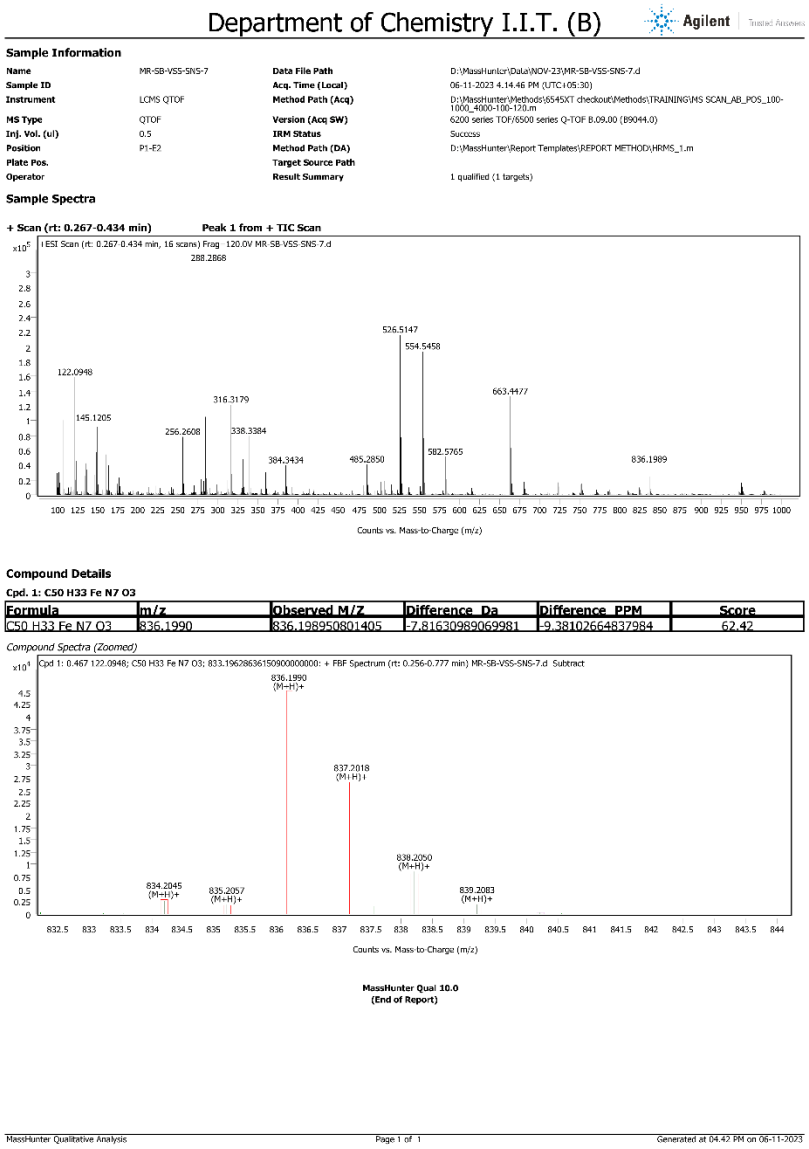


Figure S14. ^{13}C NMR spectrum of **8**



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Sample Information

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MS Type	QTOF	**Version (Acq SW)**	6200 series TOF/6500 series Q-TOF B.09.00 (B9044.0)
Inj. Vol. (ul)	0.5	**IRM Status**	Success
Position	P1-E2	**Method Path (DA)**	D:\MassHunter\Report Templates\REPORT METHOD\HRMS_1.m
Plate Pos.		**Target Source Path**	
Operator		**Result Summary**	1 qualified (1 targets)

Sample Spectra

+ Scan (rt: 0.267-0.434 min) **Peak 1 from + TIC Scan**

Compound Details

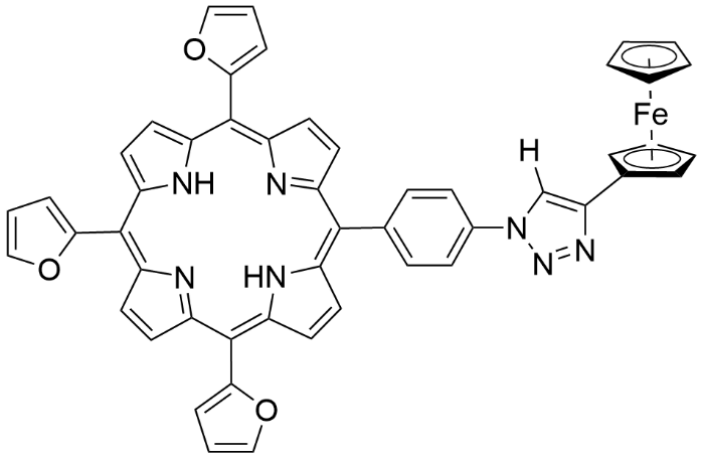
Cpd. 1: C50 H33 Fe N7 O3

Formula	m/z	Observed M/Z	Difference_Da	Difference_PPM	Score
C50 H33 Fe N7 O3	836.1990	836.198950801405	-7.81630989069981	-9.38102664837984	62.42

Compound Spectra (Zoomed)

MassHunter Qual 10.0
(End of Report)

MassHunter Qualitative Analysis Page 1 of 1 Generated at 04:42 PM on 06-11-2023



Chemical Formula: $C_{50}H_{33}FeN_7O_3$

Expected Mol. Wt.= 836.1990 $[M+H]^+$

Observed Mol. Wt.= 836.1989 $[M+H]^+$

Figure S15. LCMS QTOF spectrum of

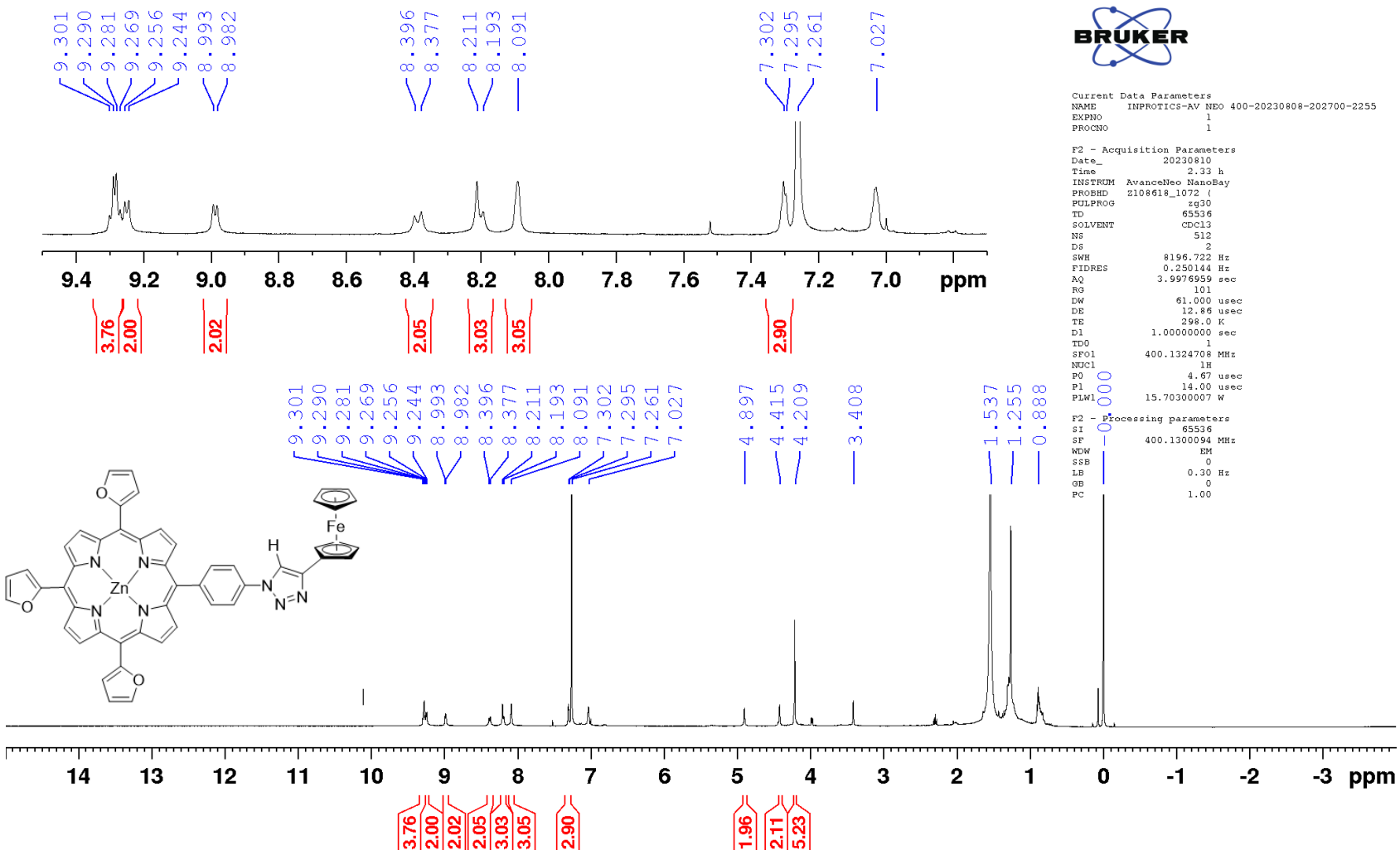


Figure S16. ^{1}H NMR spectrum of **Zn-8**

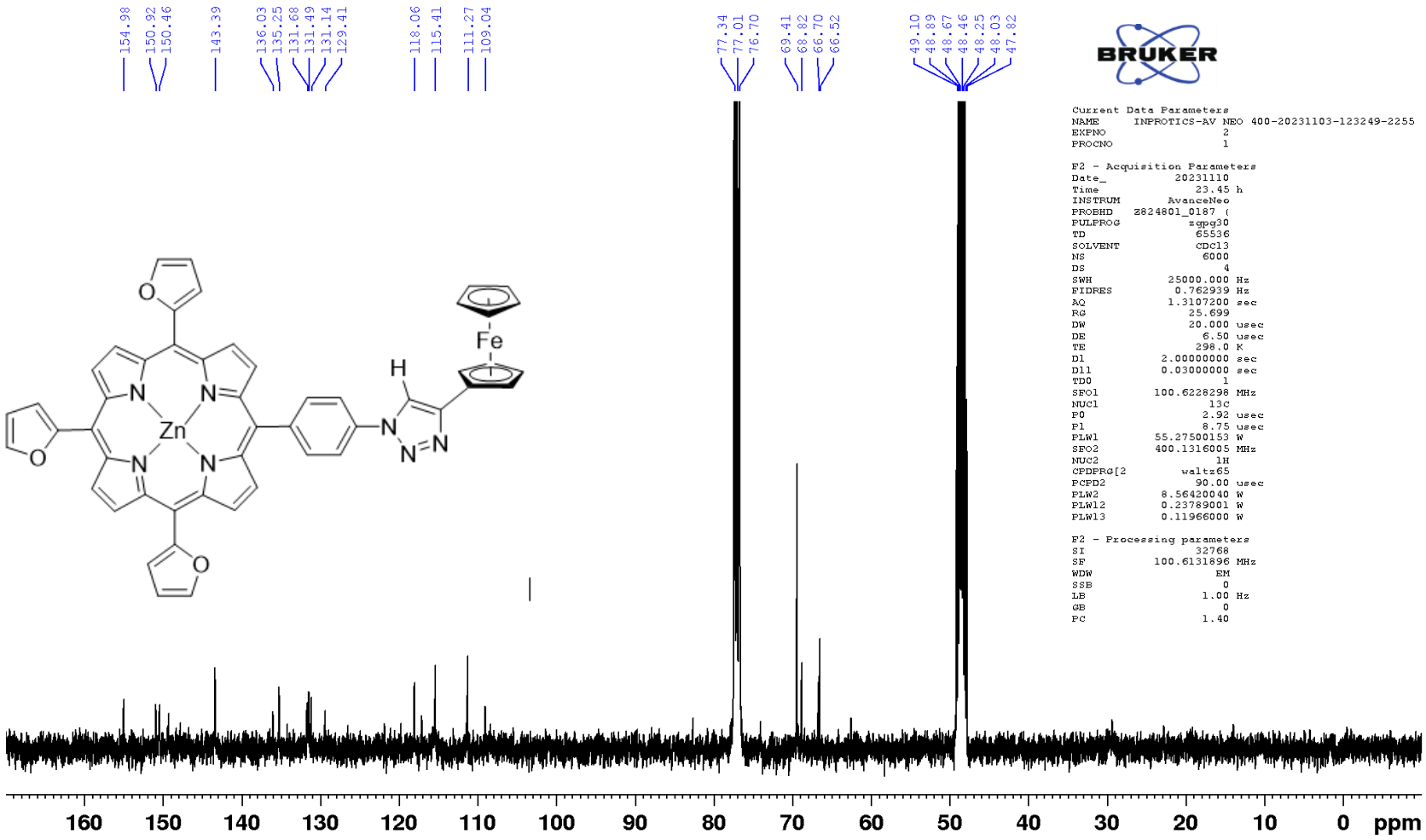
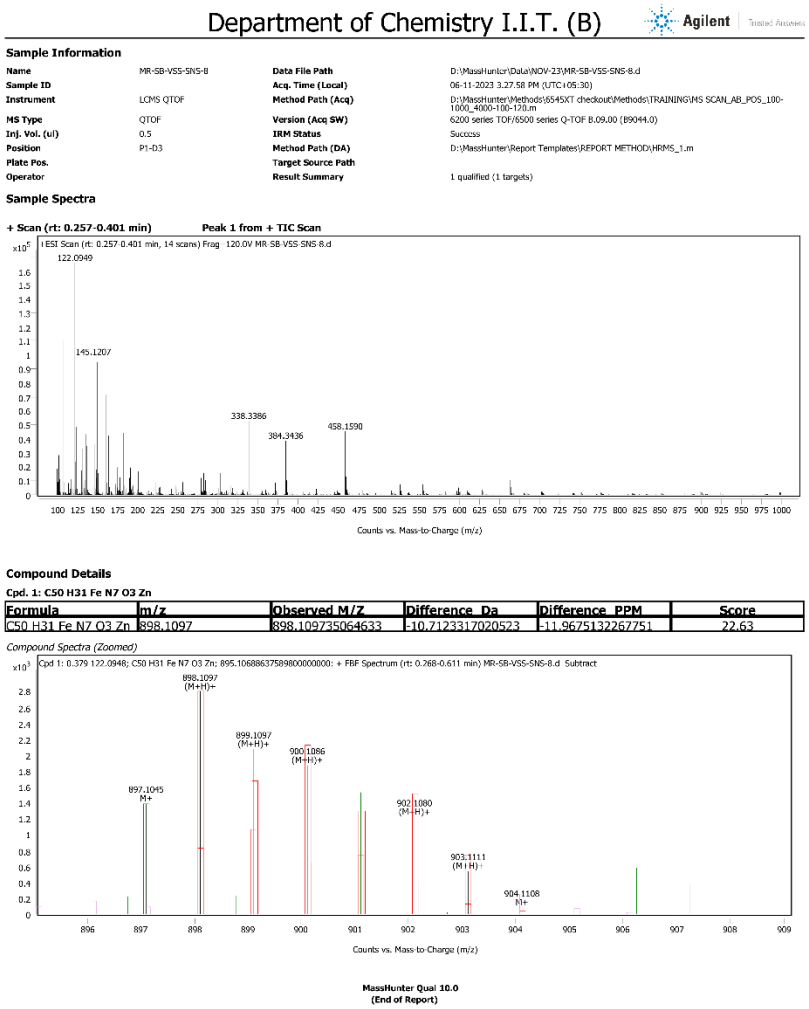


Figure S17. ^{13}C NMR spectrum of **Zn-8**



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Sample Information

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Sample ID		**Acq. Time (Local)**	06-11-2023 3.27.58 PM (UTC+05:30)
Instrument	LCMS QTOF	**Method Path (Acq)**	D:\MassHunter\Methods\6545XT checkout\Methods\TRAINING\MS SCAN_AB_POS_100-1000_4000-100-120.m
MS Type	QTOF	**Version (Acq SW)**	6200 series TOF/6500 series Q-TOF B.09.00 (B9044.0)
Inj. Vol. (ul)	0.5	**IRM Status**	Success
Position	P1-D3	**Method Path (DA)**	D:\MassHunter\Report Templates\REPORT METHOD\HRMS_1.m
Plate Pos.		**Target Source Path**	
Operator		**Result Summary**	1 qualified (1 targets)

Sample Spectra

+ Scan (rt: 0.257-0.401 min) **Peak 1 from + TIC Scan**

Compound Details

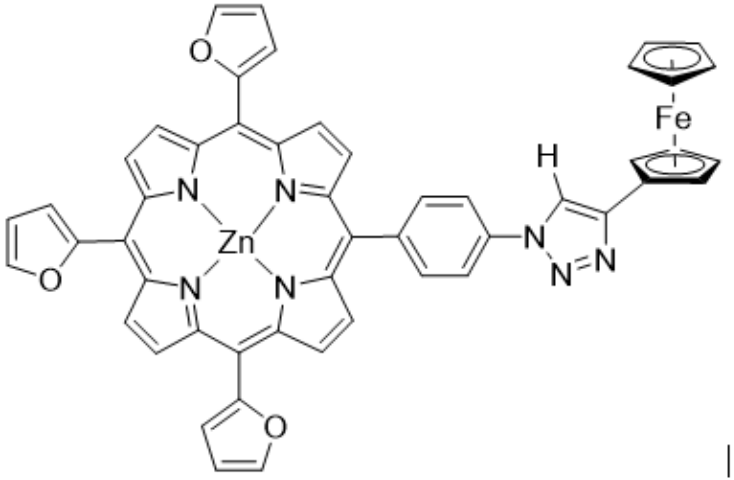
Cpd. 1: C50 H31 Fe N7 O3 Zn

Formula	m/z	Observed M/Z	Difference_Da	Difference_PPM	Score
C50 H31 Fe N7 O3 Zn	898.1097	898.109735064633	-10.7123317020523	-11.9675132267751	22.63

Compound Spectra (Zoomed)

MassHunter Qual 10.0
(End of Report)

MassHunter Qualitative Analysis Page 1 of 1 Generated at 04.58 PM on 06-11-2023



Chemical Formula: $C_{50}H_{31}FeN_7O_3Zn$

Expected Mol. Wt.= 898.1097 $[M+H]^+$

Observed Mol. Wt.= 898.1097 $[M+H]^+$

Figure S18. LCMS QTOF spectrum of **Zn-8**

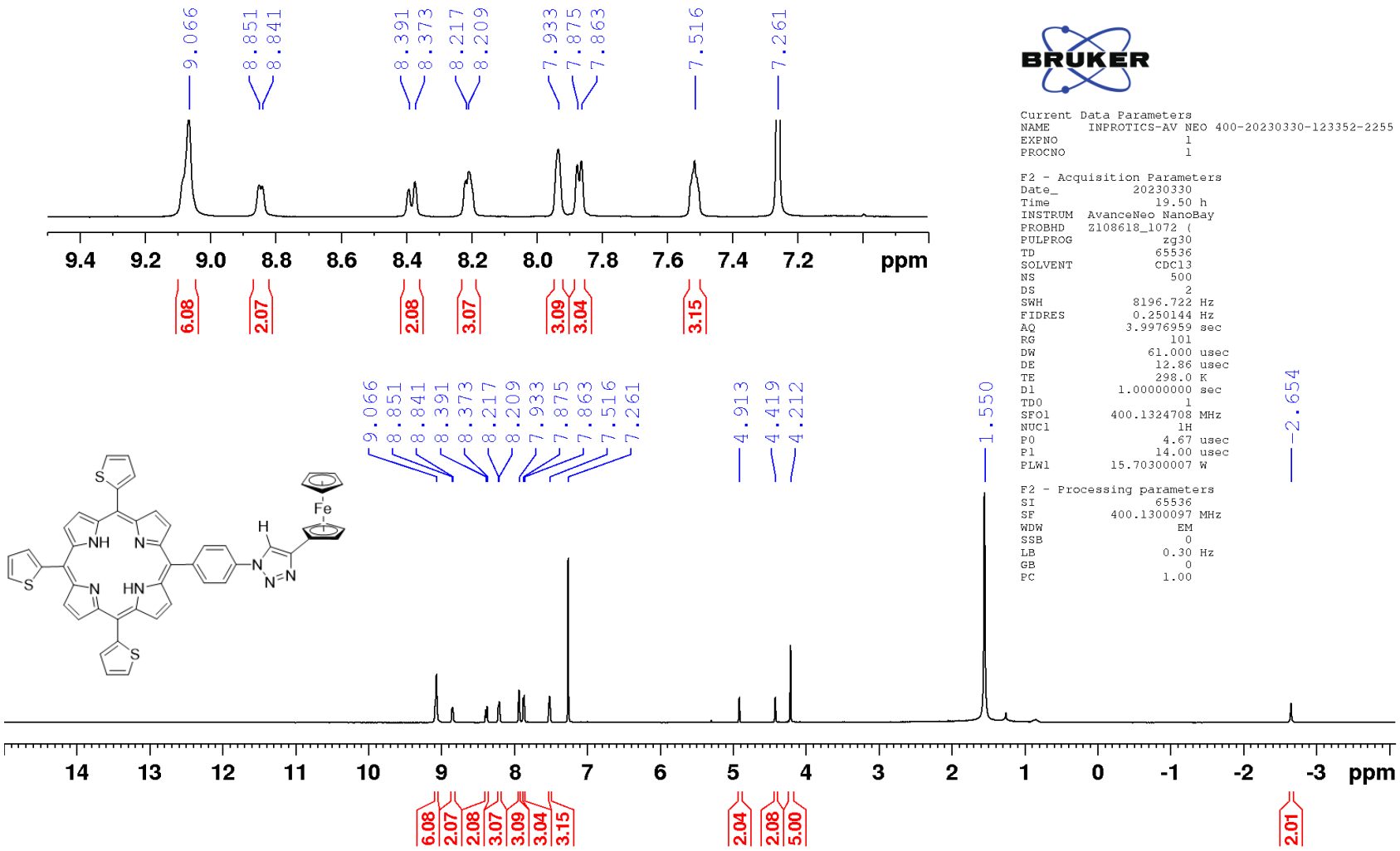


Figure S19. ^{1}H NMR spectrum of **9**

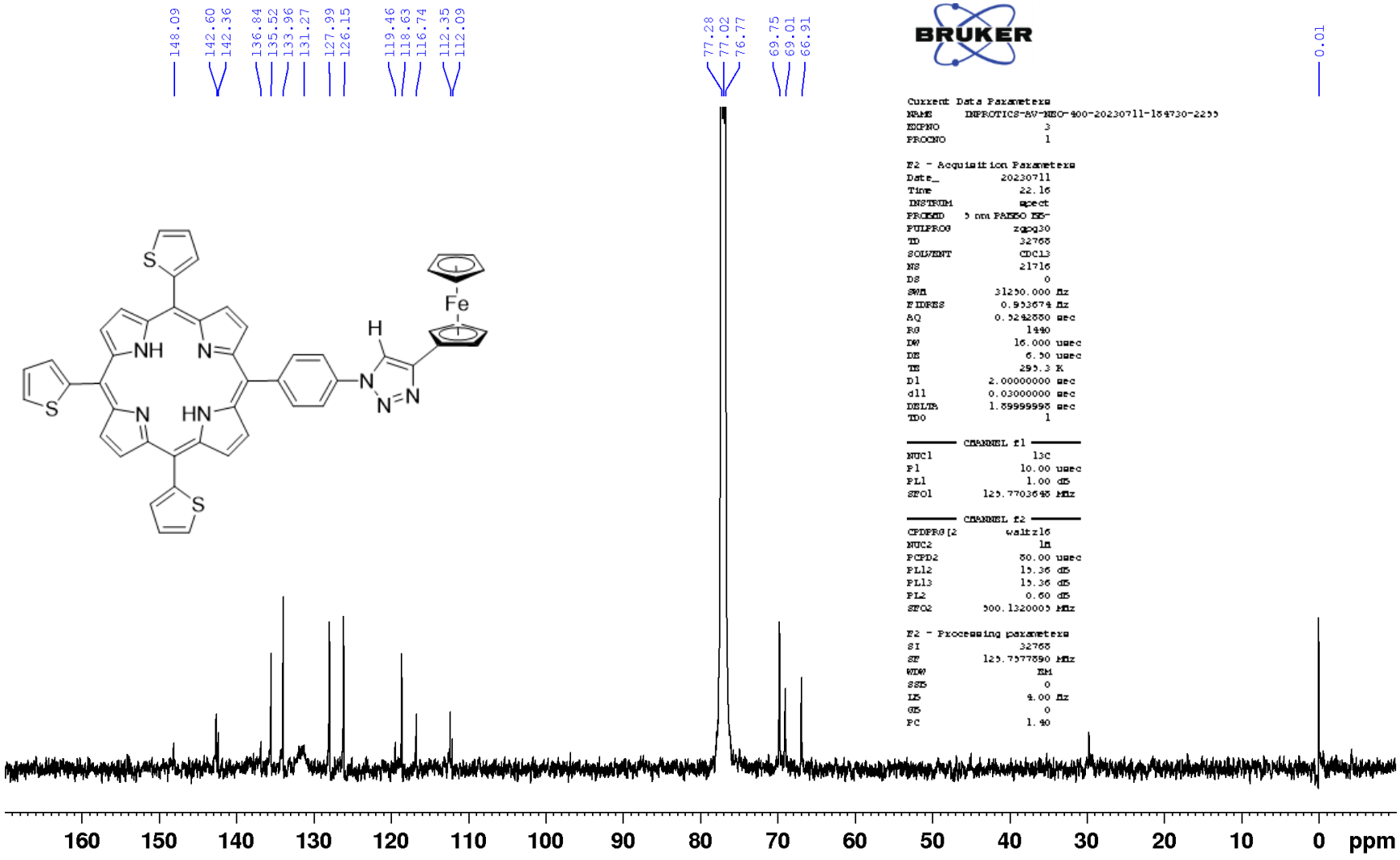
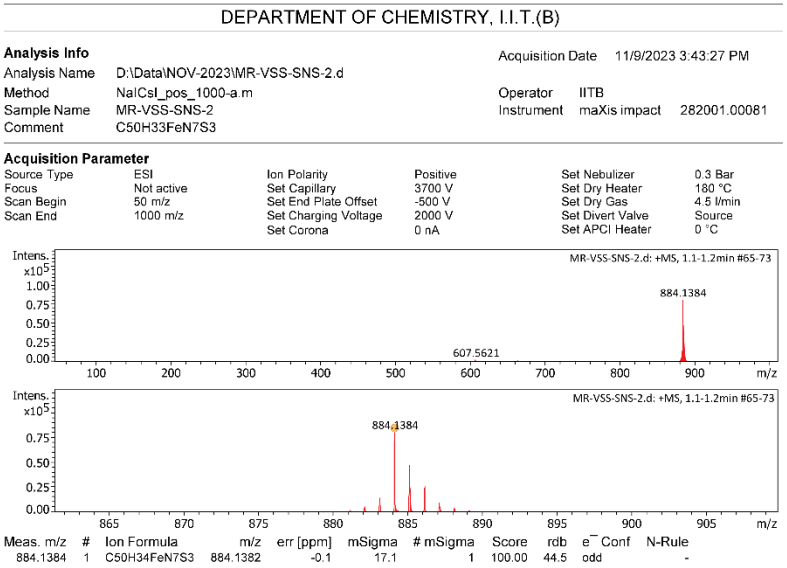


Figure S20. ^{13}C NMR spectrum of **9**



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Analysis Info

Analysis Name	D:\Data\NOV-2023\MR-VSS-SNS-2.d	Acquisition Date	11/9/2023 3:43:27 PM
Method	NaICsI_pos_1000-a.m	Operator	IITB
Sample Name	MR-VSS-SNS-2	Instrument	maXis impact 282001.00081
Comment	C50H33FeN7S3		

Acquisition Parameter

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Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.5 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
884.1384	1	C50H34FeN7S3	884.1382	-0.1	17.1	1	100.00	44.5	odd	-

MR-VSS-SNS-2.d

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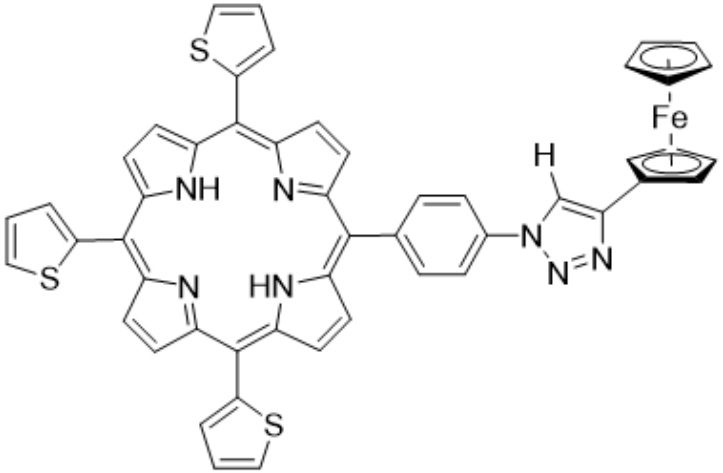


Chemical Formula: $C_{50}H_{33}FeN_7S_3$

Expected Mol. Wt.= 884.1382 $[M+H]^+$

Observed Mol. Wt.= 884.1384 $[M+H]^+$

Figure S21. ES MS spectrum of **9**

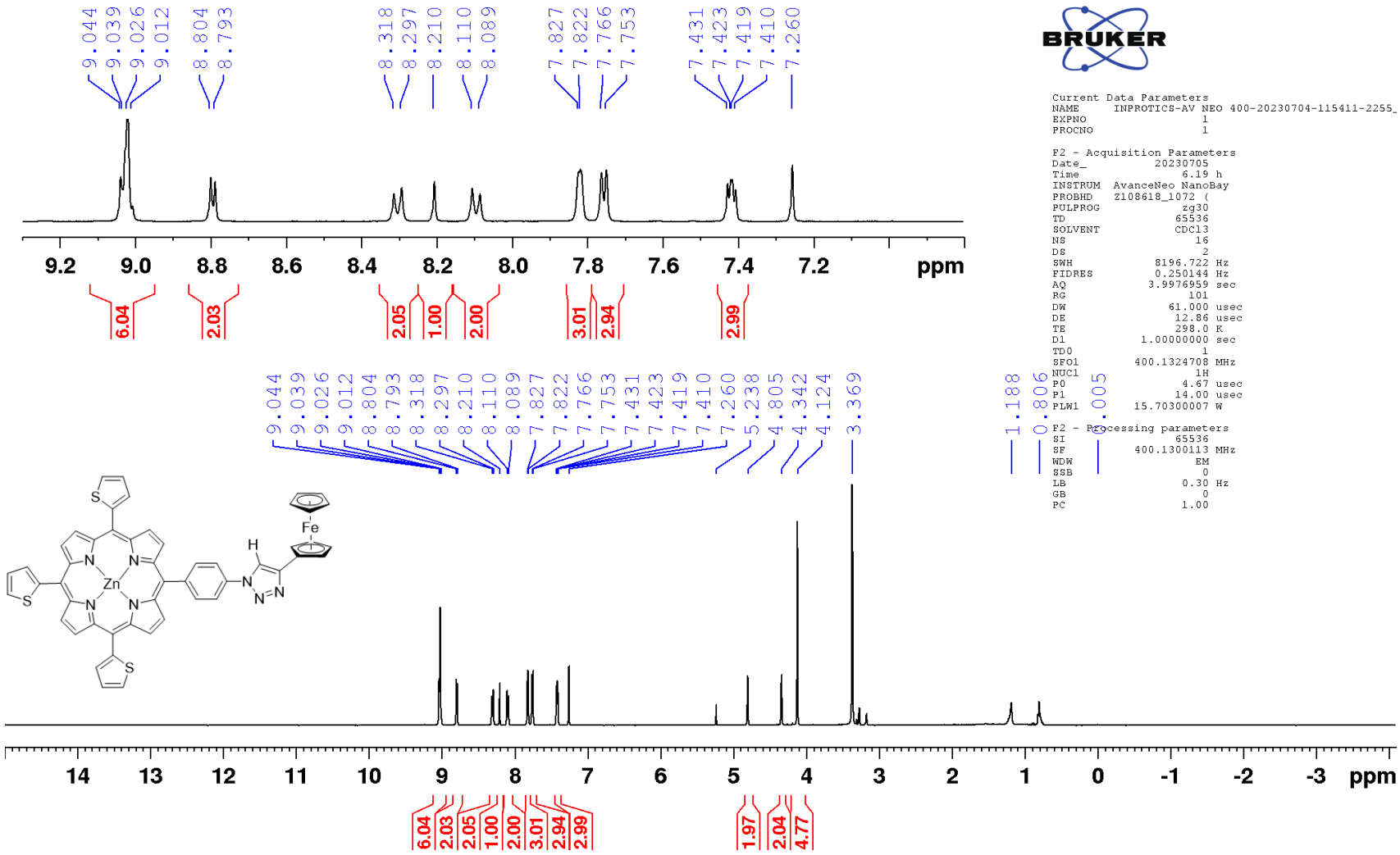


Figure S22. ^{1}H NMR spectrum of **Zn-9**

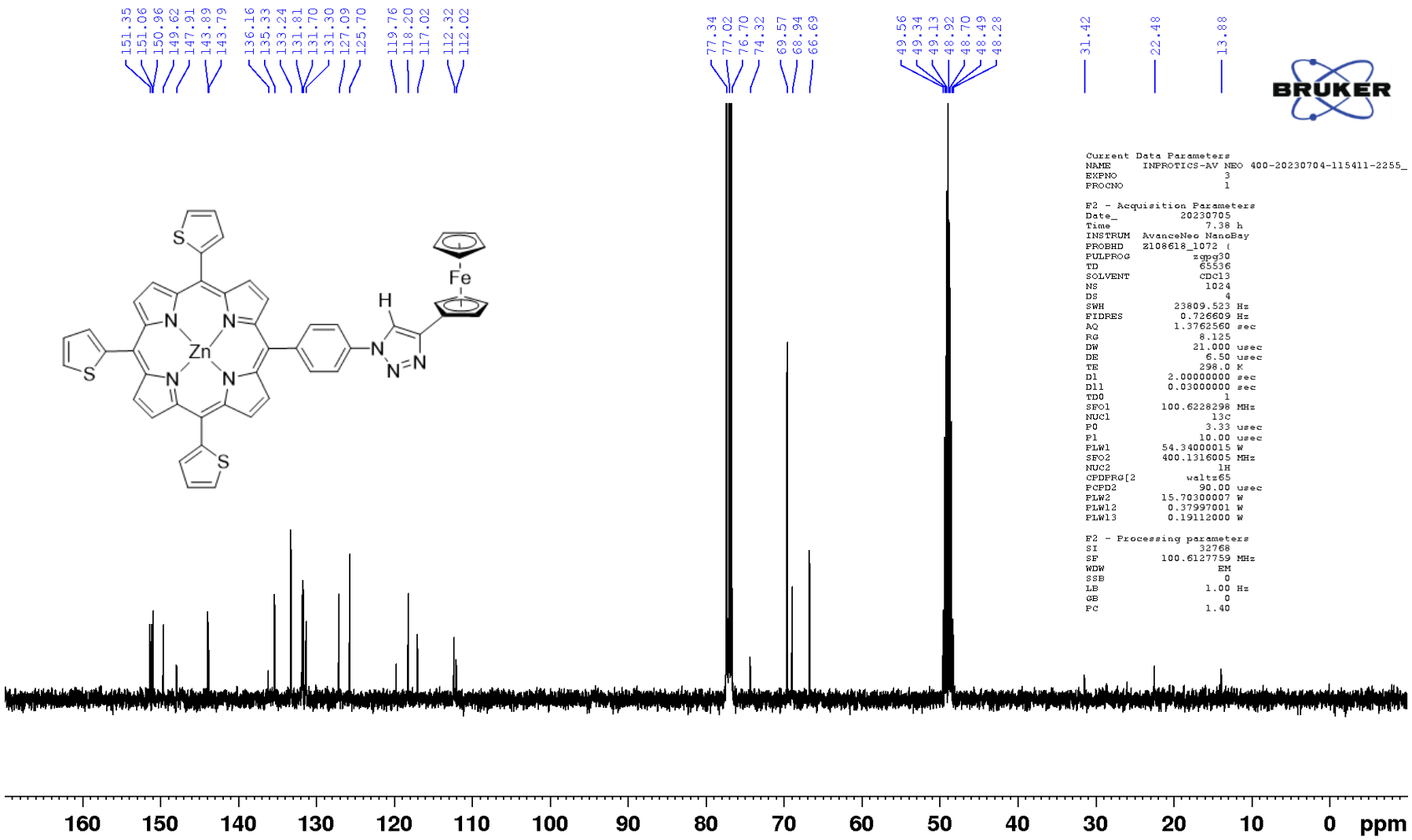
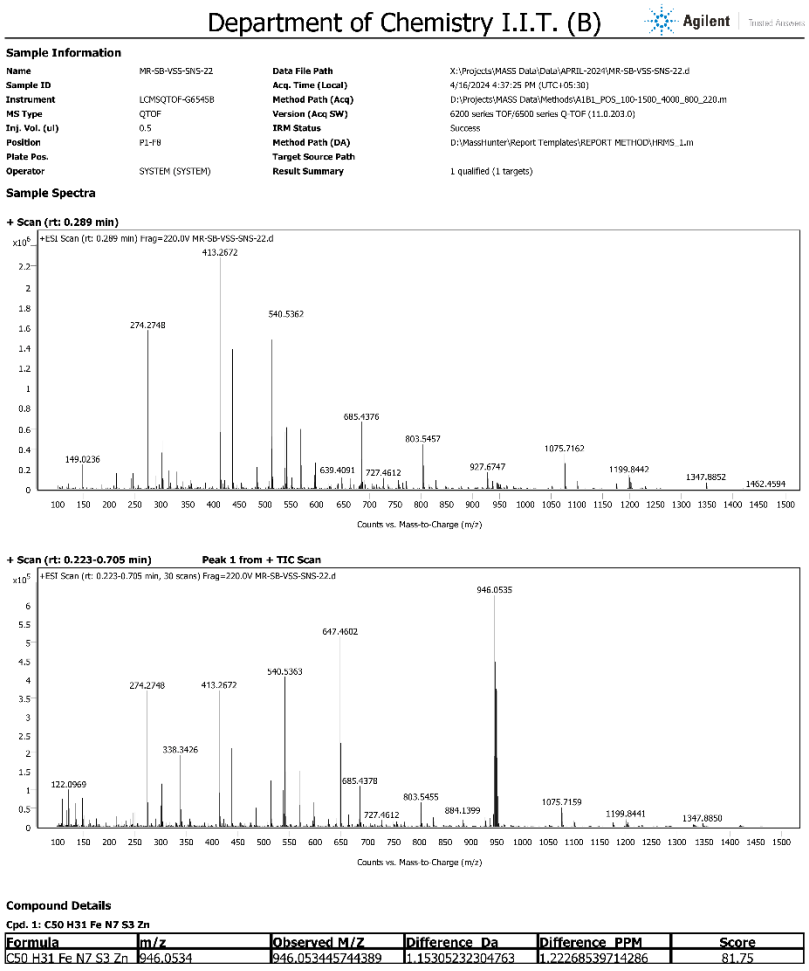


Figure S23. ^{13}C NMR spectrum of **Zn-9**



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Sample Information

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Sample ID		**Acq. Time (Local)**	4/16/2024 4:37:25 PM (UTC+05:30)
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MS Type	QTOF	**Version (Acq SW)**	6200 series TOF/6500 series Q-TOF (11.0.203.0)
Inj. Vol. (ul)	0.5	**IRM Status**	Success
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Plate Pos.		**Target Source Path**	
Operator	SYSTEM (SYSTEM)	**Result Summary**	1 qualified (1 targets)

Sample Spectra

+ Scan (rt: 0.289 min)

+ Scan (rt: 0.223-0.705 min) **Peak 1 from + TIC Scan**

Compound Details

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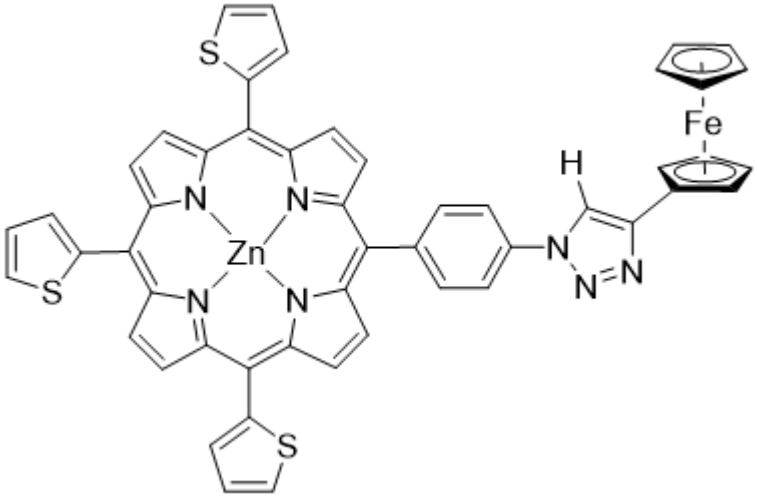
Formula	m/z	Observed M/Z	Difference_Da	Difference_PPM	Score
C50 H31 Fe N7 S3 Zn	946.0534	946.053445744389	1.15305232304763	1.22268539714286	81.75

MassHunter Qualitative Analysis Page 1 of 2 Generated at 3:17 PM on 4/17/2024



Chemical Formula: $C_{50}H_{31}FeN_7S_3Zn$

Expected Mol. Wt.= 946.0534 $[M+H]^+$

Observed Mol. Wt.= 946.0534 $[M+H]^+$

Figure S24. LCMS QTOF spectrum of **Zn-9**

Table S1. The selected dihedral angles (in °) in the lowest energy conformers of **8, 9, 10,** Zn-8, Zn-9 and Zn-10.

'Click' conjugates	**α**	**B**	**γ**
8	65	31	5
9	66	30	3
10	66	31	-8
Zn-8	65	31	5
Zn-9	66	30	3
Zn-10	66	31	-8

Table S2. Optimized Geometries (Cartesian coordinates) of 'click' conjugates.
Optimized geometries ($PCM_{(dichlromethane)}$/B3LYP-D3, Cartesian coordinates in Å) and energies of 'click' conjugates (in a.u.). Notation: E = total electronic energy, Tc = thermal correction at 298K to obtain the Gibbs free energy, Nimag = number of imaginary frequencies.

8 E = -2658.1750444 Nimag = 0 Tc = 0.626130	**9** E = -3627.1289074 Nimag = 0 Tc = 0.611517
N 5.53916400 -1.20485700 0.06697000	N -5.23727900 -1.19855300 -0.03218500
N 2.66000100 -1.62010200 -0.14151300	N -2.33608800 -1.62255700 0.10573600
N 5.21423200 1.73838300 0.09699400	N -4.91170700 1.70660500 -0.03141900
N 2.33962700 1.31961600 -0.18059800	N -2.01454400 1.28282700 0.16879100
C 6.82139100 -0.83633600 0.35480300	C -6.54680500 -0.84187300 -0.16514600
C 7.61999100 -1.99493400 0.73220600	C -7.38880000 -2.01726600 -0.36421200
C 6.80347100 -3.06914400 0.63599500	C -6.56187700 -3.08706500 -0.33552400
C 5.50752200 -2.56293400 0.19952500	C -5.21819700 -2.56141000 -0.11560500
H 8.65118800 -1.97883200 1.04387000	H -8.45508700 -2.00657000 -0.52349800
H 7.03498900 -4.09580400 0.86647800	H -6.81499700 -4.12752600 -0.46054600
C 4.38651700 -3.39141800 -0.03941500	C -4.07996700 -3.38269500 -0.00440000
C 7.34158000 0.47646300 0.29542600	C -7.05662700 0.47217000 -0.13400000
C 1.90550700 -3.70451300 -0.52346500	C -1.59270200 -3.73390100 0.33433700
C 0.83260300 -2.85747300 -0.57459500	C -0.51017000 -2.90126400 0.41595600
C 1.30078700 -1.52735800 -0.32728700	C -0.97209800 -1.55344500 0.26381700
C 3.07221000 -2.92710100 -0.23356700	C -2.75905800 -2.92823800 0.13271100
H 1.89705700 -4.77110000 -0.66443800	H -1.60065900 -4.80751400 0.42143000
H -0.19292500 -3.11880100 -0.77543300	H 0.51680700 -3.18226700 0.57941900
C 0.52580900 -0.36057500 -0.27571300	C -0.19442600 -0.38732800 0.27690100
C 4.81679700 3.03897500 -0.10438300	C -4.49583800 3.01395300 0.04325700
C 6.01112300 3.80818100 -0.27440700	C -5.68081900 3.81929700 0.09115100
C 7.08103100 2.96427900 -0.15786500	C -6.76338200 2.98603000 0.03916000
C 6.58480000 1.64413900 0.08887200	C -6.28343200 1.63791800 -0.04551100
H 6.03799800 4.86648500 -0.46738500	H -5.68400300 4.89365700 0.16997000
H 8.12262900 3.21810000 -0.25468700	H -7.80503200 3.25941900 0.06252400
C 0.16618200 2.11287500 0.03744700	C 0.16023000 2.10504400 0.11268600
C 0.98606000 3.18861400 0.08581100	C -0.66702900 3.17380000 0.05152100

C 2.34285400 2.67837100 -0.07596200	C -2.02510400 2.64431600 0.09751200
C 1.02412100 0.94934400 -0.14520400	C -0.69570200 0.92573500 0.19528900
H -0.90701300 2.09715400 0.14019500	H 1.23812100 2.10268300 0.08819100
H 0.71335700 4.21886200 0.24380100	H -0.40273800 4.21595400 -0.02841900
C 3.49012800 3.50519500 -0.13008300	C -3.17092200 3.46706100 0.07379900
C -0.95415600 -0.53908600 -0.37688200	C 1.28438400 -0.57118900 0.38684900
C -1.66589500 -1.20493200 0.62757900	C 2.01004400 -1.17077500 -0.64854600
C -3.04334100 -1.37204900 0.53835800	C 3.38608600 -1.34482300 -0.55066300
C -3.72608400 -0.85957200 -0.56443700	C 4.05368400 -0.90337100 0.59135900
C -3.03679200 -0.19351100 -1.57826000	C 3.34995800 -0.30308900 1.63598900
C -1.65934000 -0.04242900 -1.48042400	C 1.97362000 -0.14722700 1.52987600
H -1.13551700 -1.59854700 1.48605900	H 1.49204200 -1.50805500 -1.53802300
H -3.57591400 -1.90796500 1.31371000	H 3.92865400 -1.83175900 -1.35087600
H -3.57992600 0.19566000 -2.42839200	H 3.88108500 0.03137400 2.51638500
H -1.12181100 0.47280400 -2.26700300	H 1.42505800 0.31592200 2.34089600
C -8.93612800 1.98245900 -0.23715200	C 9.25372500 1.95439200 0.35106000
C -10.12479300 1.75793900 -0.99331800	C 10.43607900 1.72448600 1.11549200
C -9.30808200 2.15474100 1.12940300	C 9.63796200 2.14679200 -1.00941600
C -10.72799400 2.03737800 1.21803900	C 11.05911700 2.03635100 -1.08602800
C -11.23250500 1.79260800 -0.09389100	C 11.55211300 1.77574800 0.22722900
Fe -9.91011100 0.29579600 0.45218700	Fe 10.24107600 0.28122700 -0.35173400
C -8.61167000 -1.29869400 0.24440800	C 8.94756800 -1.32179000 -0.17888900
C -8.98945700 -1.13870700 1.61739900	C 9.33816300 -1.14079300 -1.54566100
C -9.80676100 -1.52962600 -0.51019000	C 10.13619900 -1.55817100 0.58417100
C -10.40452300 -1.27849100 1.70499700	C 10.75460000 -1.27320800 -1.62121500
C -10.90806500 -1.51874500 0.39212000	C 11.24623300 -1.52989300 -0.30695600
H -7.92854600 1.97064300 -0.62405500	H 8.24250000 1.93358800 0.72800800
H -10.17304400 1.55854200 -2.05259700	H 10.47519000 1.51114600 2.17243300
H -11.31329400 2.08840700 2.12311800	H 11.65279000 2.10187800 -1.98469800
H -12.26603400 1.62440200 -0.35436500	H 12.58379900 1.60814300 0.49528800
H -9.84945700 -1.66025700 -1.57924000	H 10.16908400 -1.70369400 1.65164200
H -11.94606500 -1.63654000 0.12262100	H 12.28205000 -1.64688600 -0.02884900
H -8.32152700 -0.92324200 2.43694700	H 8.67734700 -0.91760700 -2.36889000
H -8.63189800 2.31099300 1.95571100	H 8.96901400 2.31144800 -1.83996800
H -10.99390300 -1.18097600 2.60336700	H 11.35227500 -1.16083300 -2.51234300
C 4.61100700 -4.83756500 -0.10412600	C -4.28359200 -4.85033300 -0.02404600
C 5.53444800 -5.59930200 -0.76644000	C -4.85145200 -5.63841300 0.94087400
O 3.75613800 -5.66637800 0.58546300	C -4.91553200 -7.01808100 0.58511100
C 5.23881100 -6.96553400 -0.46896500	H -5.20771100 -5.23551300 1.87969700
H 6.31673100 -5.22145600 -1.40418500	C -4.40118700 -7.26834600 -0.65455100
C 4.15525400 -6.94807100 0.35197200	H -5.32419800 -7.78797300 1.22595600
H 5.75957900 -7.84031700 -0.82440100	H -4.32196900 -8.21267900 -1.17164800
H 3.57667600 -7.71635600 0.83687200	C -2.96541500 4.93488800 0.08878200
C 3.28847500 4.95082500 -0.25273100	C -2.54101800 5.71928800 1.12738800
C 2.49822200 5.71123100 -1.07067800	C -2.42558000 7.10004100 0.78858800
O 4.02443700 5.78217100 0.56039800	H -2.32281000 5.31336600 2.10632300
C 2.75435300 7.07890500 -0.74452600	C -2.75721200 7.35452100 -0.51106500
H 1.83161200 5.33179200 -1.82770500	H -2.11221100 7.86756500 1.48368200
C 3.68416300 7.06362400 0.24731400	H -2.76144700 8.30049700 -1.03121200
H 2.31037100 7.95303600 -1.19350000	C -8.52423000 0.66359500 -0.20254900

H 4.18084500 7.83375000 0.81333100	C -9.26624300 1.17374300 -1.23424500
C 8.78488200 0.66272000 0.47218600	C -10.66270800 1.24257700 -0.95232300
C 9.52446300 1.49544900 1.26657600	H -8.81944700 1.48224400 -2.17020100
O 9.63487400 -0.13605100 -0.25653200	C -10.97158700 0.79133800 0.29869800
C 10.89972200 1.19775800 1.01579600	H -11.40213100 1.60861400 -1.65211800
H 9.12629700 2.21672800 1.96160100	H -11.94050400 0.72882700 0.77066800
C 10.90792000 0.20463800 0.08699800	N 5.46365900 -1.06129100 0.69623400
H 11.76265000 1.65687200 1.47119100	C 6.39635600 -1.06856600 -0.29441000
H 11.69160100 -0.33998500 -0.41240000	C 7.59714700 -1.25013400 0.35750900
N -5.13747000 -1.01116900 -0.65989800	H 6.14808000 -0.92236700 -1.33011000
C -6.05824200 -1.06161600 0.34053000	N 6.05609600 -1.23550500 1.90193600
C -7.26731300 -1.20940500 -0.30450400	N 7.33455500 -1.34774000 1.69815700
H -5.79646900 -0.96446200 1.37866400	H -4.29563500 0.90312700 -0.03468800
N -5.74463600 -1.12876300 -1.86511800	H -2.94524600 -0.81885100 0.01604400
N -7.02095700 -1.24689100 -1.65127200	S -3.22072400 5.90629100 -1.34554800
H 4.57825700 0.95470300 0.17398300	S -9.55672000 0.26993400 1.15563000
H 3.28472000 -0.83201300 -0.02393200	S -3.82482100 -5.81748500 -1.41013000
10 E =-2782.8385439 Nimag = 0 Tc = 0.784537	**Zn-8** E = -2722.6714224 Nimag = 0 Tc = 0.603060
N -4.92492700 -1.25258100 0.05997000	N -5.32651800 -1.26365600 -0.03334600
N -2.02885500 -1.60986900 -0.19442300	N -2.40512500 -1.57744100 0.10793900
N -4.67086700 1.66743300 -0.00468900	N -5.00383900 1.66945300 -0.11897700
N -1.76942900 1.31089900 -0.19229100	N -2.09806100 1.35355800 0.22168400
C -6.25027700 -0.92220000 0.08845400	C -6.62864300 -0.90356000 -0.26722500
C -7.08165300 -2.11767200 0.00120100	C -7.40316800 -2.08978900 -0.55545800
C -6.23321300 -3.16990800 -0.06182500	C -6.55435500 -3.15022700 -0.48172000
C -4.88476600 -2.61572100 -0.01286200	C -5.24759000 -2.62853100 -0.14355900
H -8.15930400 -2.13458600 -0.02591000	H -8.45214700 -2.11077700 -0.79950500
H -6.48140400 -4.21534900 -0.15023300	H -6.78591800 -4.18570800 -0.66775100
C -3.72415800 -3.41501200 -0.04634700	C -4.07606400 -3.40425800 0.02018000
C -6.78328700 0.37891900 0.18021500	C -7.13765800 0.41698500 -0.25799500
C -1.20485800 -3.69961100 -0.06248300	C -1.58527200 -3.69552900 0.43823400
C -0.14491300 -2.83930700 -0.14624400	C -0.52984500 -2.83979000 0.50854800
C -0.65909100 -1.50445400 -0.23741100	C -1.04787200 -1.50574900 0.29562200
C -2.41155700 -2.92754100 -0.09903600	C -2.76342500 -2.89753500 0.17504700
H -1.16904300 -4.77238400 0.02755300	H -1.56543900 -4.76569800 0.55831300
H 0.90198300 -3.09302400 -0.13526400	H 0.50032500 -3.08876300 0.70583300
C 0.08315900 -0.32091100 -0.34544800	C -0.27573800 -0.32625100 0.30262800
C -4.27888200 2.98480800 0.02555000	C -4.65641300 2.98752100 0.03652400
C -5.46510200 3.75738800 0.24677800	C -5.85909200 3.78201800 0.15458200
C -6.52488600 2.89669000 0.33253500	C -6.91431700 2.92911600 0.05975800
C -6.03106000 1.56186700 0.16698300	C -6.37321300 1.59919000 -0.12092600
H -5.48633600 4.83044100 0.33809700	H -5.89502400 4.84792900 0.30563600
H -7.55781500 3.14819100 0.50586300	H -7.96063300 3.17449900 0.13381400
C 0.35277800 2.17535500 -0.58223500	C 0.04103700 2.17890600 0.10458700
C -0.49610100 3.22740400 -0.52285200	C -0.80676100 3.24181800 0.03974300
C -1.82136500 2.67433000 -0.26638400	C -2.15340100 2.71856000 0.12547600
C -0.45579300 0.98081600 -0.36267400	C -0.77347600 0.99036100 0.22370300

H 1.41366900 2.19387600 -0.77420000	H 1.11754600 2.19839800 0.04974200
H -0.26450100 4.27200100 -0.65511300	H -0.54488800 4.27956500 -0.08258700
C -2.97323000 3.47297500 -0.12659200	C -3.33767800 3.49443400 0.10316500
C 1.56673300 -0.46984700 -0.44617800	C 1.20636200 -0.48970500 0.39732100
C 2.15464800 -1.06267800 -1.57060900	C 1.92105600 -1.12115500 -0.62763900
C 3.53281300 -1.21179600 -1.66574800	C 3.29853800 -1.28887500 -0.54410800
C 4.34399600 -0.75161100 -0.62830800	C 3.98124000 -0.80913600 0.57335900
C 3.78166200 -0.14754400 0.49596300	C 3.29107800 -0.17292700 1.60555700
C 2.40014800 -0.01770600 0.58334100	C 1.91284000 -0.02278600 1.51316000
H 1.52361400 -1.41434400 -2.37780200	H 1.39073300 -1.49194200 -1.49619600
H 3.98385500 -1.67520500 -2.53234900	H 3.83085300 -1.80213000 -1.33481600
H 4.41289800 0.23137600 1.28972300	H 3.83364300 0.19136300 2.46703000
H 1.96197200 0.44794500 1.45756500	H 1.37505300 0.46589100 2.31645900
C 9.72284900 1.92766800 -0.08585000	C 9.21637300 2.00144200 0.25951300
C 10.06433000 1.98984500 1.29800300	C 10.40458000 1.76112800 1.01155100
C 10.91927400 1.68988200 -0.82543900	C 9.58710800 2.18106200 -1.10643700
C 12.00139700 1.60631600 0.10148000	C 11.00579900 2.05243800 -1.19882500
C 11.47322300 1.79116200 1.41390200	C 11.51078500 1.79334100 0.11017800
Fe 10.58860200 0.14981600 0.51341100	Fe 10.17472400 0.31197700 -0.44466100
C 9.21105500 -1.35572700 0.18570400	C 8.86307000 -1.27288400 -0.24652700
C 10.40199000 -1.59832500 -0.57179800	C 9.23962800 -1.10551300 -1.61897100
C 9.57898300 -1.30928900 1.56983200	C 10.05759300 -1.52007700 0.50380100
C 11.49078200 -1.70632900 0.33932800	C 10.65327800 -1.25673500 -1.71049800
C 10.98347200 -1.52961200 1.66088200	C 11.15724400 -1.51154100 -0.40055100
H 8.72754600 1.99484400 -0.49793200	H 8.20945800 1.99513500 0.64829200
H 9.37398900 2.12769600 2.11585900	H 10.45322400 1.55315700 2.06916600
H 13.03178900 1.40031500 -0.14386800	H 11.58974600 2.10542400 -2.10466600
H 12.03441000 1.75089700 2.33468200	H 12.54336000 1.61438700 0.36726400
H 8.91268300 -1.11200400 2.39527500	H 10.10119500 -1.65963400 1.57168100
H 11.56554000 -1.52410400 2.56923600	H 12.19470700 -1.64039200 -0.13404800
H 10.45152000 -1.65883000 -1.64682400	H 8.57196700 -0.87823900 -2.43555400
H 10.98714400 1.55824100 -1.89417600	H 8.91062100 2.34918300 -1.93016100
H 12.52465200 -1.86027100 0.07211800	H 11.24168700 -1.15740000 -2.60930900
N 5.75572300 -0.90184700 -0.72252600	C -4.24690900 -4.86156700 0.04517000
C 6.66146600 -1.08631000 0.27608300	C -5.07732900 -5.68697900 0.75153500
C 7.87856400 -1.16466100 -0.36599100	O -3.43215200 -5.62517900 -0.75885200
H 6.37980100 -1.17257200 1.31004000	C -4.76266400 -7.02714500 0.36429500
N 6.37992600 -0.87161300 -1.92425000	H -5.81073600 -5.36851600 1.47433400
N 7.65174900 -1.03114700 -1.71014100	C -3.76182600 -6.93110600 -0.55053100
C -3.88800800 -4.90035600 -0.02196800	H -5.21683500 -7.93655600 0.72439300
C -4.39963300 -5.54610400 1.10978300	H -3.20410200 -7.65399500 -1.12196100
C -3.53042200 -5.68256100 -1.12617500	C -3.17694600 4.95081800 0.18389400
C -4.54803700 -6.92980300 1.13378400	C -2.47735400 5.76377100 1.03231500
H -4.67428000 -4.95752700 1.97774100	O -3.85393500 5.72889900 -0.72703800
C -3.68476200 -7.06590200 -1.09908600	C -2.73188600 7.11079900 0.62516800
H -3.13360400 -5.20056300 -2.01252600	H -1.87092100 5.43293500 1.85968900
C -4.19701200 -7.71456700 0.02967600	C -3.56983700 7.03106800 -0.44223400
H -4.93852200 -7.40776300 2.02641300	H -2.34758200 8.01372200 1.07242900
H -3.40360400 -7.64996100 -1.96943500	H -4.03091300 7.76416700 -1.08264200
C -8.26508600 0.52880900 0.30423600	C -8.58596900 0.58145000 -0.42716000

C -9.01680700 1.11990900 -0.71800100 C -8.93817000 0.07696300 1.44530100 C -10.39767400 1.25163600 -0.60159700 H -8.51458900 1.46689600 -1.61397100 C -10.31859800 0.21494300 1.55907300 H -8.37280500 -0.38400200 2.24719500 C -11.07333400 0.80508300 0.53937400 H -10.95955500 1.70348600 -1.41266700 H -10.81698500 -0.14179200 2.45462000 C -2.81008100 4.95856100 -0.13555200 C -3.33154800 5.73344400 -1.17802700 C -2.12773400 5.61111900 0.89790700 C -3.17244300 7.11641100 -1.18588900 H -3.85454200 5.24514600 -1.99254200 C -1.97508000 6.99458100 0.88798500 H -1.71661000 5.02739400 1.71365500 C -2.49495900 7.77251400 -0.15244600 H -3.57650100 7.69391300 -2.01104200 H -1.44354200 7.47724100 1.70176200 C -4.39278200 -9.21077800 0.04558300 H -4.29019200 -9.61536100 1.05503900 H -5.39386600 -9.47428200 -0.31260600 H -3.67102300 -9.71435200 -0.60136100 C -12.56575000 0.98075400 0.67748800 H -12.80152100 1.94880500 1.13270000 H -13.06232100 0.94760600 -0.29490900 H -13.00159100 0.20608800 1.31230500 C -2.35435100 9.27498900 -0.14518200 H -2.33619700 9.67850900 -1.16003600 H -3.19689900 9.74048200 0.37766100 H -1.44046400 9.58744600 0.36505300 H -4.04029400 0.88153400 -0.10244900 H -2.66720000 -0.82405000 -0.19430800	C -9.34312400 1.35164400 -1.26583900 O -9.42028100 -0.17356900 0.36506000 C -10.71320000 1.06091100 -0.97718800 H -8.95977500 2.02899800 -2.01148700 C -10.70144800 0.13320300 0.01641400 H -11.58579700 1.48193000 -1.45080000 H -11.47387200 -0.38268600 0.56176600 N 5.39237600 -0.96733400 0.66569600 C 6.31222800 -1.00757100 -0.33594300 C 7.52029200 -1.17836700 0.30542700 H 6.05129400 -0.88960600 -1.37211100 N 5.99906200 -1.11237900 1.86799500 N 7.27445800 -1.23764600 1.65134800 Zn -3.71250300 0.04902200 0.06988300
Zn-9 E = -3691.6254379 Nimag = 0 Tc = 0.587715	**Zn-10** E = -2847.3341725 Nimag = 0 Tc = 0.760208
N -5.03856400 -1.27024900 -0.01260900 N -2.11653400 -1.58409800 0.09294600 N -4.72348700 1.64937800 -0.05563200 N -1.80978400 1.33565100 0.19002000 C -6.35531600 -0.91529800 -0.14417100 C -7.15420300 -2.11167600 -0.31179900 C -6.30124900 -3.17107200 -0.27424700 C -4.96863100 -2.63788400 -0.08043500 H -8.22190500 -2.13260000 -0.45960000 H -6.54331500 -4.21617300 -0.38038600 C -3.79113600 -3.40857900 0.01065400 C -6.86049500 0.40285000 -0.14447500	N -4.74510400 -1.31760200 0.09919300 N -1.83478300 -1.57110800 -0.21952900 N -4.49988900 1.60835000 0.00468400 N -1.57675400 1.35566900 -0.16223600 C -6.07652000 -0.98813200 0.14662800 C -6.86316800 -2.20209300 0.09217100 C -5.99019800 -3.24417000 0.02089600 C -4.65512000 -2.68470900 0.03008100 H -7.94021400 -2.24870700 0.09028900 H -6.22713600 -4.29347700 -0.04966100 C -3.46188600 -3.43474200 -0.04511000 C -6.60637900 0.31791200 0.21185100

C -1.29191400 -3.71409800 0.31741000	C -0.93927900 -3.68205000 -0.11371400
C -0.23339700 -2.86169500 0.39467200	C 0.09956200 -2.80663000 -0.19833600
C -0.75510300 -1.51863800 0.24610400	C -0.46753200 -1.47614400 -0.26900100
C -2.47590100 -2.90522900 0.12413100	C -2.15872000 -2.90215100 -0.13113100
H -1.27725900 -4.78845500 0.40540500	H -0.88541200 -4.75546800 -0.03000200
H 0.80108100 -3.11858300 0.55591300	H 1.15205400 -3.04036900 -0.19496600
C 0.01570200 -0.33732200 0.27808100	C 0.27530700 -0.27954300 -0.34831700
C -4.37136100 2.97231000 0.01884100	C -4.16754000 2.93898600 0.02912100
C -5.57298400 3.78016600 0.05661200	C -5.36876100 3.72000600 0.23634000
C -6.63110100 2.92668500 0.00009700	C -6.40722000 2.84428500 0.32496200
C -6.09187900 1.58437500 -0.07509800	C -5.85814400 1.51338100 0.17257000
H -5.59911000 4.85499300 0.13652300	H -5.40867800 4.79411100 0.31955500
H -7.67998300 3.17484200 0.01999200	H -7.44653700 3.07570900 0.49363300
C 0.32503900 2.17977200 0.16838000	C 0.51213400 2.24114600 -0.51137100
C -0.52861300 3.23846700 0.10920400	C -0.36187800 3.28258100 -0.44573400
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C -0.48462800 0.98021100 0.22386900	C -0.25565000 1.02717800 -0.32863600
H 1.40274900 2.20819200 0.15884700	H 1.57469400 2.29003900 -0.68778300
H -0.27713800 4.28488100 0.04644400	H -0.13971700 4.33156000 -0.55717800
C -3.05490700 3.47439200 0.07590100	C -2.86753900 3.47213500 -0.10386800
C 1.49791600 -0.50056600 0.37887000	C 1.76010700 -0.40974400 -0.45882400
C 2.22480800 -1.08983600 -0.66212500	C 2.34926500 -0.97904300 -1.59516100
C 3.60115200 -1.26262400 -0.56795600	C 3.72778900 -1.12091700 -1.69621700
C 4.27027400 -0.82854000 0.57606400	C 4.53959200 -0.67621700 -0.65259000
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C 2.19061700 -0.07842200 1.52069700	C 2.59555300 0.03065100 0.57447700
H 1.70519600 -1.42574700 -1.55113900	H 1.71746600 -1.32188000 -2.40551900
H 4.14240400 -1.74579200 -1.37138700	H 4.17862900 -1.56888800 -2.57110400
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H 1.64304700 0.37762300 2.33650600	H 2.15788100 0.47861900 1.45824100
C 9.51063400 1.97276300 0.35653500	C 9.93020000 1.96742700 -0.02920900
C 10.68849900 1.72312100 1.12170000	C 10.26388100 1.99171700 1.35770900
C 9.89974300 2.16713200 -1.00228300	C 11.13001700 1.74461100 -0.76799800
C 11.31943800 2.03821900 -1.07711800	C 12.20646000 1.63257700 0.16253700
C 11.80665500 1.76417400 0.23557000	C 11.67135200 1.78473400 1.47634900
Fe 10.47683600 0.29032600 -0.35345900	Fe 10.78586900 0.17111900 0.52751700
C 9.16109400 -1.29523500 -0.19082200	C 9.40271200 -1.31837000 0.15413900
C 9.55623400 -1.11279100 -1.55607500	C 10.59486000 -1.54522800 -0.60631500
C 10.34518400 -1.55230600 0.57264300	C 9.76665100 -1.31229400 1.54009600
C 10.97083100 -1.26456300 -1.63029600	C 11.68041800 -1.68350000 0.30463300
C 11.45687600 -1.53483600 -0.31669100	C 11.16987500 -1.54137000 1.62911200
H 8.49857800 1.96322400 0.73169800	H 8.93752900 2.04912100 -0.44501200
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H 10.37423200 -1.70397100 1.63935900	H 9.09877500 -1.13518300 2.36883400
H 12.49053300 -1.66784300 -0.03773100	H 11.74917000 -1.56378900 2.53898300
H 8.89982500 -0.87601300 -2.37904100	H 10.64742100 -1.57571300 -1.68247100
H 9.23444600 2.34481700 -1.83307900	H 11.20355800 1.64072100 -1.83941600
H 11.57134300 -1.15594500 -2.51998200	H 12.71442600 -1.83455700 0.03629600

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