Additional Spectra and Data

1a

C:\Xcalibur\data\Wang\89362ESIPN1 02/09/23 16:15:55 PNP-5040-34
Sarah

89362ESIPN1 #9-18 RT: 0.13-0.24 AV: 5 SB: 22 0.01-0.08 , 1.17-1.70 NL: 1.62E7
T: FTMS + p ESI Full ms [120.0000-1500.0000]

89362ESIPN1#9-17 RT: 0.13-0.24 AV: 5
SB: 22 0.01-0.08 , 1.17-1.70
T: FTMS + p ESI Full ms [120.0000-1500.0000]
m/z= 372.25837-379.37535

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
373.94477	16365587.0	100.00	373.94607	-3.46	$C_{12}H_{15}O_2Fe$ I

%T
cm-1
2913.21cm-1
2976.15cm-1
1824.54cm-1
1948.30cm-1
2001.99cm-1
1452.05cm-1
1432.66cm-1
1481.81cm-1
1376.96cm-1
1073.77cm-1
1017.80cm-1
612.78cm-1
549.28cm-1
569.54cm-1

BF4
Fe
OC
CO
O
Br

1c

C:\Xcalibur\data\Wang\89459ESIPN1 03/01/23 11:39:28 pnp_5040-4B
Megan

89459ESIPN1 #7-25 RT: 0.10-0.35 AV: 10 SB: 32 0.01-0.05 , 1.40-2.23 NL: 8.53E8
T: FTMS + p ESI Full ms [120.0000-1500.0000]

89459ESIPN1#7-25 RT: 0.10-0.35 AV: 10
SB: 32 0.01-0.05 , 1.40-2.23
T: FTMS + p ESI Full ms [120.0000-1500.0000]
m/z= 484.58149-485.37441

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
485.04100	871063680.0	100.00	485.04093	0.16	$C_{23}H_{26}O_3BrFe$

%T
cm-1
3406.79cm-1, 89.55%T
2924.55cm-1, 91.87%T
2103.91cm-1, 92.81%T
1587.79cm-1, 89.38%T
1172.18cm-1, 85.15%T
1271.81cm-1, 80.33%T
1240.84cm-1, 75.61%T
1428.88cm-1, 76.28%T
1384.93cm-1, 70.55%T
1488.09cm-1, 66.15%T
761.81cm-1, 77.24%T
827.88cm-1, 68.79%T
435.71cm-1, 60.79%T
2051.5cm-1
1983.67cm-1, 47.04%T
2026.67cm-1, 38.23%T
599.86cm-1, 52.57%T
536.38cm-1, 43.90%T
522.24cm-1, 44.70%T
995.82cm-1, 38.23%T
561.53cm-1, 39.72%T
1053.12cm-1, 32.51%T
1025.40cm-1, 34.24%T

BF4
Fe
OC
CO
Cy

1d

C:\Xcalibur\data\Wang\88153ESIPN1 08/01/22 10:55:28 PNP-5039-49-0
Megan

88153ESIPN1 #13-37 RT: 0.18-0.52 AV: 13 NL: 2.35E9
T: FTMS + p ESI Full ms [120.0000-1500.0000]

88153ESIPN1#13-37 RT: 0.18-0.52 AV: 13
T: FTMS + p ESI Full ms [120.0000-1500.0000]
m/z= 349.27865-390.29111

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
369.15094	2351929856.0	100.00	369.15115	-0.57	$C_{21}H_{29}O_2Fe$

%T
cm-1
2874.46cm-1, 79.76%T
2962.94cm-1, 76.42%T
2931.17cm-1, 72.14%T
1469.36cm-1, 71.56%T
2014.03cm-1, 47.52%T
2049.19cm-1, 47.54%T
1085.62cm-1, 50.86%T
540.16cm-1, 46.63%T
564.00cm-1, 51.30%T
1048.27cm-1, 34.64%T

BF4
Fe
OC
CO

1e

C:\Xcalibur\data\Wang\88154ESIPN1 08/01/22 11:02:28 PNP-5040-7
Megan

88154ESIPN1 #7-27 RT: 0.09-0.37 AV: 11 NL: 4.35E9
T: FTMS + p ESI Full ms [120.0000-1500.0000]

88154ESIPN1#7-27 RT: 0.09-0.37 AV: 11
T: FTMS + p ESI Full ms [120.0000-1500.0000]
m/z= 299.97695-335.03040

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
315.10345	4442536960.0	100.00	315.10420	-2.36	$C_{17}H_{23}O_2Fe$

3391.09cm-1
2919.55cm-1
2058.33cm-1
2016.90cm-1
1985.25cm-1
1482.33cm-1
1456.43cm-1
1428.14cm-1
1386.77cm-1
1078.91cm-1
1048.03cm-1
1031.74cm-1
761.49cm-1
605.22cm-1
563.14cm-1
532.24cm-1
501.17cm-1
454.81cm-1
409.91cm-1
cm-1

nPr
nPr
nPr
nPr
nPr
Fe
OC
CO

2a

C:\Xcalibur\data\Wang\89223ESIPN1 01/26/23 10:28:45 PNP-31-0
Sarah

89223ESIPN1 #9-18 RT: 0.12-0.23 AV: 5 SB: 33 0.01-0.12 , 0.59-1.39 NL: 7.31E6
T: FTMS + p ESI Full ms [120.0000-1500.0000]

89223ESIPN1#9-17 RT: 0.12-0.23 AV: 5
SB: 33 0.01-0.12 , 0.59-1.39
T: FTMS + p ESI Full ms [120.0000-1500.0000]
m/z= 513.90169-516.02289

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
514.10278	7338012.0	100.00	514.10257	0.42	$C_{22}H_{35}O_2Fe$ I

2c

C:\Xcalibur\data\Wang\89457ESIPN2 02/27/23 16:19:54 pnp_5040-23
Megan

89457ESIPN2 #10-13 RT: 0.15-0.18 AV: 2 SB: 18 0.01-0.10 , 1.04-1.43 NL: 3.27E7
T: FTMS + p ESI Full ms [120.0000-1500.0000]

89457ESIPN2#11-13 RT: 0.15-0.18 AV: 2
SB: 18 0.01-0.10 , 1.04-1.43
T: FTMS + p ESI Full ms [120.0000-1500.0000]
m/z= 624.60951-625.51301

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
625.19726	33061986.0	100.00	625.19743	-0.27	$C_{33}H_{46}O_3BrFe$

FTIR User 674 (3716.3 cm-1, 99.188 %T)
2874.89cm-1, 82.16%T
2931.45cm-1, 77.42%T
2963.18cm-1, 77.28%T
2064.33cm-1, 54.98%T
2010.03cm-1, 49.69%T
1707.81cm-1, 82.63%T
1592.34cm-1, 84.57%T
1489.49cm-1, 69.25%T
1469.52cm-1, 64.23%T
1384.48cm-1, 80.65%T
1238.84cm-1, 54.20%T
1174.75cm-1, 80.52%T
1255.69cm-1, 77.02%T
912.40cm-1, 78.53%T
1031.96cm-1, 36.71%T
822.73cm-1, 63.67%T
743.79cm-1, 77.60%T
694.27cm-1, 85.42%T
645.50cm-1, 76.78%T
603.72cm-1, 66.80%T
468.50cm-1, 68.85%T
506.39cm-1, 54.02%T
540.44cm-1, 48.84%T
565.53cm-1, 50.30%T
%T
cm-1

nPr
nPr
nPr
nPr
nPr
Fe
OC
CO
Cy
BF4

C:\Xcalibur\data\Wang\88165ESIPN1 08/02/22 10:48:48 PNP-5040-15
Megan

88165ESIPN1 #9-16 RT: 0.12-0.21 AV: 4 NL: 3.69E9
T: FTMS + p ESI Full ms [120.0000-1500.0000]

88165ESIPN1#9-15 RT: 0.12-0.21 AV: 4
T: FTMS + p ESI Full ms [120.0000-1500.0000]
m/z= 489.68829-530.07596

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
509.30601	3697650432.0	100.00	509.30765	-3.21	$C_{31}H_{49}O_2Fe$

%T
cm-1
2851.61cm-1, 91.19%T
2924.84cm-1, 88.04%T
2053.51cm-1, 68.65%T
2018.56cm-1, 61.10%T
1450.97cm-1, 88.87%T
1484.24cm-1, 88.44%T
1382.02cm-1, 88.57%T
1428.84cm-1, 89.05%T
1021.67cm-1, 56.75%T
1047.75cm-1, 53.97%T
603.82cm-1, 73.72%T
541.83cm-1, 67.40%T
565.46cm-1, 64.83%T
497.11cm-1, 79.29%T
441.98cm-1, 80.82%T
410.45cm-1, 88.03%T

nPr
nPr
nPr
nPr
nPr
Fe
OC
CO
BF4

2e

C:\Xcalibur\data\Wang\88190ESIPN1 08/04/22 12:23:47 PNP-5040-16.39TI
Sarah

88190ESIPN1 #11 RT: 0.15 AV: 1 SB: 172 0.01-0.11 , 0.22-4.93 NL: 4.30E8
T: FTMS + p ESI Full ms [120.0000-1500.0000]

88190ESIPN1#11 RT: 0.15
SB: 172 0.01-0.11 , 0.22-4.93
T: FTMS + p ESI Full ms [120.0000-1500.0000]
m/z= 451.33114-458.50037

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
455.25995	439164224.0	100.00	455.26070	-1.63	$C_{27}H_{43}O_2Fe$

C:\Xcalibur\data\Wang\89053ESIPN1 01/04/23 11:23:49 PNP-5040-29
Megan

89053ESIPN1 #11 RT: 0.15 AV: 1 NL: 1.69E7
T: FTMS + p ESI Full ms [120.0000-1500.0000]

89053ESIPN1#11 RT: 0.15
T: FTMS + p ESI Full ms [120.0000-1500.0000]
m/z= 223.98332-226.94978

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
224.99086	17658996.0	100.00	224.99095	-0.42	$C_{10}H_{10}OBr$

3c

C:\Xcalibur\data\Wang\89087ESIPN1 01/05/23 12:13:09 PNP-5040-25.2
Sarah

89087ESIPN1 #9-18 RT: 0.12-0.23 AV: 5 SB: 78 0.01-0.12 , 1.00-3.04 NL: 9.01E6
T: FTMS + p ESI Full ms [120.0000-1500.0000]

89087ESIPN1#9-17 RT: 0.12-0.23 AV: 5
SB: 78 0.01-0.12 , 1.00-3.04
T: FTMS + p ESI Full ms [120.0000-1500.0000]
m/z= 238.78679-239.07796

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
239.00706	7957454.0	100.00	239.00660	1.93	$C_{11}H_{12}OBr$

3c-*d*

C:\Xcalibur\data\Wang\89117ESIPN1 01/10/23 15:53:26 PNP-2040-24.2
Megan

89117ESIPN1 #15 RT: 0.21 AV: 1 NL: 9.74E7
T: FTMS + p ESI Full ms [120.0000-1500.0000]

89117ESIPN1#15 RT: 0.21
T: FTMS + p ESI Full ms [120.0000-1500.0000]
m/z= 239.56987-251.02740

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
241.01973	100103448.0	100.00	241.01916	2.37	$C_{11}H_{10}{}^{2}H_{2}OBr$

5c

C:\Xcalibur\data\Wang\89550ESIPN3 03/10/23 12:24:25 PNP-5040-39
Sarah

89550ESIPN3 #10-18 RT: 0.15-0.24 AV: 4 SB: 12 0.01-0.08 , 0.71-0.95 NL: 7.39E7
T: FTMS + p ESI Full ms [120.0000-1500.0000]

89550ESIPN3#11-17 RT: 0.15-0.24 AV: 4
SB: 12 0.01-0.08 , 0.71-0.95
T: FTMS + p ESI Full ms [120.0000-1500.0000]
m/z= 578.99821-579.12405

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
579.09184	5134446.5	100.00	579.09241	-0.99	$C_{27}H_{37}O_2Br_2Si$

4c

C:\Xcalibur\data\Wang\89510ESIPN1 03/06/23 14:54:57 PNP-30.4W
Megan

89510ESIPN1 #7-23 RT: 0.10-0.32 AV: 9 NL: 1.16E9
T: FTMS + p ESI Full ms [120.0000-1500.0000]

89510ESIPN1#7-23 RT: 0.10-0.32 AV: 9
T: FTMS + p ESI Full ms [120.0000-1500.0000]
m/z= 419.68486-449.43716

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
428.08559	1164521088.0	100.00	428.08558	0.03	$C_{22}H_{23}O_3NBr$

4c-*d*

C:\Xcalibur\data\Wang\89578ESIPN1 03/16/23 10:48:39 PNP-30.7
Sarah

89578ESIPN1 #9-24 RT: 0.13-0.32 AV: 8 SB: 4 0.01-0.05 , 0.56-0.62 NL: 2.61E9
T: FTMS + p ESI Full ms [120.0000-1500.0000]

89578ESIPN1#9 RT: 0.13
T: FTMS + p ESI Full ms [120.0000-1500.0000]

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
430.09784	1529589888.0	100.00	430.09868	-1.97	$C_{22}H_{21}{}^{2}H_{2}O_{3}NBr$