

Supporting information

Data for ((4-(trifluoromethoxyl)benzyl)sulfanyl) acetic acid (**3a**): white solid (87%); ^1H NMR (400MHz, CDCl_3) δ 7.20-7.42 (m, 4H, ArH), 3.88 (s, 2H, SCH_2COOH), 3.12 (s, 2H, ArCH_2S).

Data for ((4-Fluorobenzyl)sulfanyl) acetic acid (**3b**): faint yellow solid (90%); ^1H NMR (400MHz, CDCl_3) δ 7.02-7.36 (m, 4H, ArH), 3.86 (s, 2H, SCH_2COOH), 3.12 (s, 2H, ArCH_2S).

Data for ((4-methylbenzyl)sulfanyl) acetic acid (**3c**): white solid (91%); ^1H NMR (400MHz, CDCl_3) δ 7.17-7.28 (m, 4H, ArH), 3.87 (s, 2H, SCH_2COOH), 3.13 (s, 2H, ArCH_2S), 2.38 (s, 3H, CH_3).

Data for ((4-tert-butylbenzyl)sulfanyl) acetic acid (**3d**): white solid (95%); ^1H NMR (400MHz, CDCl_3) δ 7.29-7.40 (m, 4H, ArH), 3.87 (s, 2H, SCH_2COOH), 3.14 (s, 2H, ArCH_2S), 1.35 (s, 9H, $\text{C}(\text{CH}_3)_3$).

Data for ((4-methoxybenzyl)sulfanyl) acetic acid (**3e**): white solid (88%); ^1H NMR (400MHz, CDCl_3) δ 6.88-7.30 (m, 4H, ArH), 3.84 (s, 2H, SCH_2COOH), 3.82 (s, 3H, CH_3O), 3.12 (s, 2H, ArCH_2S).

Data for ((4-(trifluoromethyl)benzyl)sulfanyl) acetic acid (**3f**): white solid (85%); ^1H NMR (400MHz, CDCl_3) δ 7.48-7.62 (m, 4H, ArH), 3.91 (s, 2H, SCH_2COOH), 3.11 (s, 2H, ArCH_2S).

Data for (1-phenyl-ethylsulfanyl) acetic acid (**3g**): white solid (85%); ^1H NMR (400MHz, CDCl_3) δ 7.28-7.40 (m, 5H, ArH), 4.19-4.24 (m, 1H, ArCHS), 2.93-3.12 (m, 2H, SCH_2COOH), 1.62-1.64 (d, 3H, CH_3).

Data for (benzylsulfanyl) acetic acid (**3h**): white solid (86%); ^1H NMR (400MHz, CDCl_3) δ 7.29-7.38 (m, 5H, ArH), 3.89 (s, 2H, SCH_2COOH), 3.13 (s, 2H, ArCH_2S).

Data for ((4-Chlorobenzyl)sulfanyl) acetic acid (**3i-3l**): white solid (92%); ^1H NMR (400MHz, CDCl_3) δ 8.84 (s, 1H, COOH), 7.29-7.34 (m, 4H, ArH), 3.85 (s, 2H, SCH_2COOH), 3.11 (s, 2H, ArCH_2S).

Data for ((4-(trifluoromethoxyl)benzyl)sulfonyl) acetic acid (**4a**): white solid (90%); ^1H NMR (400MHz, $\text{DMSO}-d_6$) δ 7.41-7.54 (m, 4H, ArH), 4.70 (s, 2H, $\text{SO}_2\text{CH}_2\text{COOH}$), 4.23 (s, 2H, ArCH_2SO_2).

Data for ((4-Fluorobenzyl)sulfonyl) acetic acid (**4b**): white solid (82%); ^1H NMR (400MHz, $\text{DMSO}-d_6$) δ 7.24-7.46 (m, 4H, ArH), 4.64 (s, 2H, $\text{SO}_2\text{CH}_2\text{COOH}$), 4.18 (s, 2H, ArCH_2SO_2).

Data for ((4-methylbenzyl)sulfonyl) acetic acid (**4c**): white solid (81%); ^1H NMR (400MHz, $\text{DMSO}-d_6$) δ 7.22-7.30 (m, 4H, ArH), 4.58 (s, 2H, $\text{SO}_2\text{CH}_2\text{COOH}$), 4.13 (s, 2H, ArCH_2SO_2), 2.32 (s, 3H, CH_3).

Data for ((4-tert-butylbenzyl)sulfonyl) acetic acid (**4d**): white solid (89%); ^1H NMR (400MHz, $\text{DMSO}-d_6$) δ 7.31-7.45 (m, 4H, ArH), 4.58 (s, 2H, $\text{SO}_2\text{CH}_2\text{COOH}$), 4.17 (s, 2H, ArCH_2SO_2), 1.29 (s, 9H, $\text{C}(\text{CH}_3)_3$).

Data for ((4-methoxybenzyl)sulfonyl) acetic acid (**4e**): white solid (83%); ^1H NMR (400MHz, $\text{DMSO}-d_6$) δ 6.99-7.33 (m, 4H, ArH), 4.55 (s, 2H, $\text{SO}_2\text{CH}_2\text{COOH}$), 4.12 (s, 2H, ArCH_2SO_2), 3.77 (s, 3H, CH_3O).

Data for ((4-(trifluoromethyl)benzyl)sulfonyl) acetic acid (**4f**): white solid (82%); ^1H NMR (400MHz, $\text{DMSO}-d_6$) δ 13.59 (s, 1H, COOH), 7.62-7.81 (m, 4H, ArH), 4.78 (s, 2H, $\text{SO}_2\text{CH}_2\text{COOH}$), 4.25 (s, 2H, ArCH_2SO_2).

Data for (1-phenyl-ethylsulfonyl) acetic acid (**4g**): white solid (87%); ^1H NMR (400MHz, CDCl_3) δ 7.44-7.55 (m, 5H, ArH), 4.75-4.80 (m, 1H, ArCHSO_2), 3.72-3.86 (m, 2H, $\text{SO}_2\text{CH}_2\text{COOH}$), 1.83-1.85 (d, 3H, CH_3).

Data for (benzylsulfonyl) acetic acid (**4h**): white solid (80%); ^1H NMR (400MHz, DMSO- d_6) δ 7.41 (s, 5H, ArH), 4.64 (s, 2H, $\text{SO}_2\text{CH}_2\text{COOH}$), 4.17 (s, 2H, ArCH_2SO_2).

Data for ((4-Chlorobenzyl)sulfonyl) acetic acid (**4i-4l**): white solid (92%); ^1H NMR (400MHz, DMSO- d_6) δ 13.55 (s, 1H, COOH), 7.41-7.51 (m, 4H, ArH), 4.66 (s, 2H, $\text{SO}_2\text{CH}_2\text{COOH}$), 4.20 (s, 2H, ArCH_2SO_2).

Data for (4-(trifluoromethoxyl)benzyl-4-carboxystyryl sulfone (**5a**): white solid (47%); ^1H NMR (400 MHz, DMSO- d_6) δ 13.22 (s, 1H, COOH), 7.36-8.05 (m, 10H, ArH, CH=CH), 4.75 (s, 2H, ArCH_2SO_2); HR-MS (ESI $^+$) m/z 387.0436 $[\text{M}+\text{H}]^+$, found 409.0340 $[\text{M}+\text{Na}]^+$.

Data for 4-Fluorobenzyl-4-carboxystyryl sulfone (**5b**): white solid (52%); ^1H NMR (400 MHz, DMSO- d_6) δ 13.18 (s, 1H, COOH), 7.19-7.99 (m, 10H, ArH, CH=CH), 4.60 (s, 2H, ArCH_2SO_2); ^{13}C NMR (100MHz, DMSO- d_6) δ 167.15, 163.90, 161.47, 142.62, 136.86, 133.67, 130.30, 129.28, 128.82, 125.46, 115.80, 59.29; HR-MS (ESI $^+$) m/z 321.0519 $[\text{M}+\text{H}]^+$, found 343.0424 $[\text{M}+\text{Na}]^+$.

Data for 4-methylbenzyl-4-carboxystyryl sulfone (**5c**): white solid (56%); ^1H NMR (400MHz, DMSO- d_6) δ 13.19 (s, 1H, COOH), 7.22-7.30 (m, 10H, ArH, CH=CH), 4.52 (s, 2H, ArCH_2SO_2), 2.28 (s, 3H, CH_3); ^{13}C NMR (100MHz, DMSO- d_6) δ 167.15, 142.27, 138.22, 136.93, 133.06, 131.47, 130.30, 129.46, 129.24, 129.10, 125.98, 60.00, 21.22; HR-MS (ESI $^-$) m/z 315.0769 $[\text{M}-\text{H}]^-$, found 315.0734 $[\text{M}-\text{H}]^-$.

Data for 4-tert-butylbenzyl-4-carboxystyryl sulfone (**5d**): white solid (45%); mp 179-180°C ; ^1H NMR (400MHz, DMSO- d_6) δ 13.13 (s, 1H, COOH), 7.29-7.99 (m, 10H, ArH, CH=CH), 4.52 (s, 2H, ArCH_2SO_2), 1.25 (s, 9H, $\text{C}(\text{CH}_3)_3$); ^{13}C NMR (100MHz, DMSO- d_6) δ 167.16, 151.31, 142.32, 136.96, 133.06, 131.35, 130.29, 129.29, 129.25, 125.82, 125.68, 59.91, 34.76, 31.49; HR-MS (ESI $^+$) m/z 359.1239 $[\text{M}+\text{H}]^+$, found 381.1140 $[\text{M}+\text{Na}]^+$.

Data for 4-methoxybenzyl-4-carboxystyryl sulfone (**5e**): white solid (55%); mp 155-156°C ; ^1H NMR (400MHz, DMSO- d_6) δ 6.90-7.99 (m, 10H, ArH, CH=CH), 4.50 (s, 2H, ArCH_2SO_2), 3.73 (s, 3H, CH_3O); ^{13}C NMR (100MHz, DMSO- d_6) δ 167.17, 159.85, 142.29, 136.94, 133.04, 132.82, 130.30, 129.23, 129.10, 120.74, 114.35, 59.63, 55.56; HR-MS (ESI $^-$) m/z 331.0718 $[\text{M}-\text{H}]^-$, found 331.0681 $[\text{M}-\text{H}]^-$.

Data for 4-(trifluoromethyl)benzyl-4-carboxystyryl sulfone (**5f**): white solid (55%); mp 158-159°C ; ^1H NMR (400MHz, DMSO- d_6) δ 13.21 (s, 1H, COOH), 7.40-8.00 (m, 10H, ArH, CH=CH), 4.75 (s, 2H, ArCH_2SO_2).

Data for 1-phenyl-ethyl-4-carboxystyryl sulfone (**5g**): faint yellow solid (46%); mp 62-63°C ; ^1H NMR (400MHz, DMSO- d_6) δ 13.16 (s, 1H, COOH), 7.35-7.98 (m, 11H, ArH, CH=CH), 4.55-4.60 (m, 1H, ArCHSO_2), 1.67-1.69 (d, 3H, CH_3); ^{13}C NMR (100MHz, DMSO- d_6) δ 167.16, 143.19, 136.93, 134.26, 133.06, 130.26, 130.09, 129.31, 129.04, 128.78, 127.64, 63.55, 14.57; HR-MS (ESI $^+$) m/z 317.0769 $[\text{M}+\text{H}]^+$, found 339.0678 $[\text{M}+\text{Na}]^+$.

Data for Benzyl-4-carboxystyryl sulfone (**5h**): white solid (86%); mp 138-139°C ; ^1H NMR (400MHz, DMSO- d_6) δ 7.35-7.99 (m, 11H, ArH, CH=CH), 4.58 (s, 2H, ArCH_2SO_2); ^{13}C NMR (100MHz, DMSO- d_6) δ 167.15, 142.42, 136.90, 133.08, 131.63, 130.30, 129.25, 129.09, 129.02, 128.86, 60.26; HR-MS (ESI $^+$) m/z 303.0613 $[\text{M}+\text{H}]^+$, found 325.0527 $[\text{M}+\text{Na}]^+$.

Data for 4-Chlorobenzyl-styryl sulfone (**5i**): white solid (55%); mp 144-145°C ; ^1H NMR (400MHz, DMSO- d_6) δ 7.30-7.70 (m, 11H, ArH, CH=CH), 4.59 (s, 2H, ArCH_2SO_2); ^{13}C NMR (100MHz, DMSO- d_6) δ 144.01, 133.76, 133.36, 132.82, 131.61, 129.54, 129.21, 128.89, 128.42, 126.42, 59.51; HR-MS (ESI $^+$) m/z 293.0325 $[\text{M}+\text{H}]^+$, found 315.0217 $[\text{M}+\text{Na}]^+$.

Data for 4-Chlorobenzyl-4-methylstyryl sulfone (**5j**): white solid (45%); mp 144-145°C; ^1H NMR (400MHz, DMSO- d_6) δ 7.24-7.58 (m, 10H, ArH, CH=CH), 4.57 (s, 2H, ArCH₂SO₂), 2.34 (s, 3H, CH₃), HR-MS (ESI⁺) m/z 307.0481 [M+H]⁺, found 328.9213 [M+Na]⁺.

Data for 4-Chlorobenzyl-4-methoxystyryl sulfone (**5k**): white solid (43%); mp 144-145°C ; ^1H NMR (400MHz, DMSO- d_6) δ 6.99-7.66 (m, 10H, ArH, CH=CH), 4.54 (s, 2H, ArCH₂SO₂), 3.81 (s, 3H, OCH₃); ^{13}C NMR (100MHz, DMSO- d_6) δ 162.09, 143.88, 133.69, 133.33, 131.11, 128.84, 128.59, 125.32, 123.38, 114.99, 59.70, 55.86; HR-MS (ESI⁺) m/z 323.0430 [M+H]⁺, found 344.9188 [M+Na]⁺.

Data for 4-Chlorobenzyl-4-phenylstyryl sulfone (**5l**): white solid (64%); mp 144-145°C ; ^1H NMR (400MHz, DMSO- d_6) δ 7.34-7.80 (m, 15H, ArH, CH=CH), 4.60 (s, 2H, ArCH₂SO₂); ^{13}C NMR (100MHz, DMSO- d_6) δ 143.51, 143.07, 139.49, 133.75, 133.37, 131.91, 129.89, 129.52, 128.90, 128.60, 128.48, 127.70, 127.26, 126.26, 59.56; HR-MS (ESI⁺) m/z 369.0638 [M+H]⁺, found 391.0529 [M+Na]⁺.

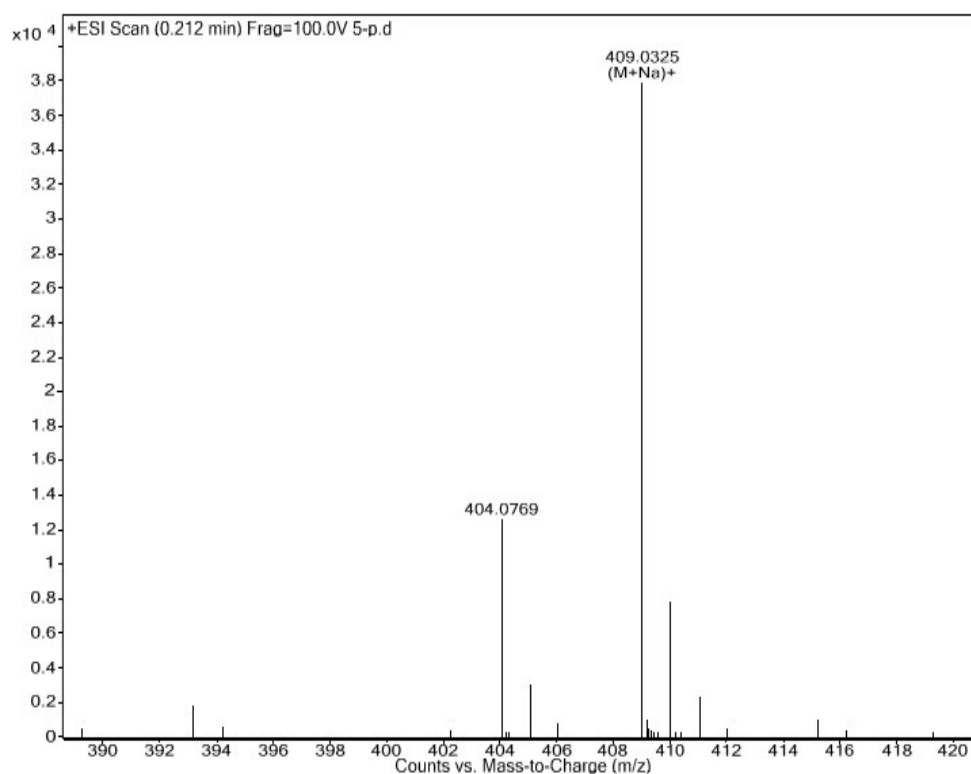
Data for **6a**: orange solid (65%); HR-MS (ESI⁺) m/z 491.1455 [M+H]⁺, found 513.1348 [M+Na]⁺.

Data for **6b**: orange solid (45%); HR-MS (ESI⁺) m/z 542.1626 [M+H]⁺, found 542.1759 [M+H]⁺.

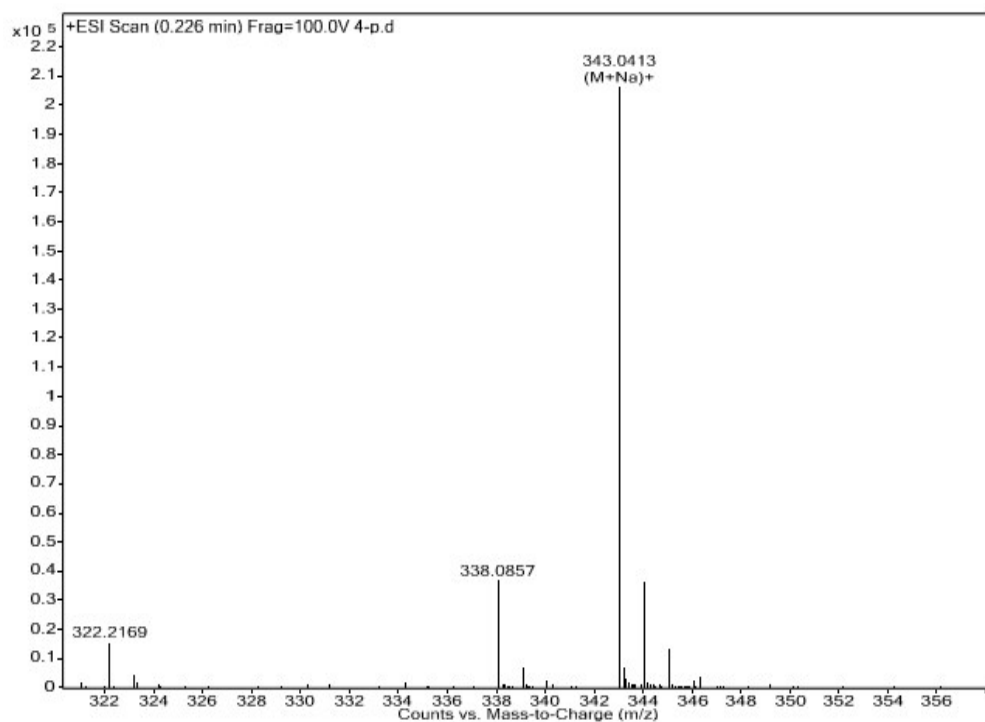
Data for **6c**: orange solid (56%); HR-MS (ESI⁺) m/z 476.1784 [M+H]⁺, found 476.1884 [M+H]⁺.

Data for **6d**: orange solid (87%); HR-MS (ESI⁺) m/z 513.2471 [M+H]⁺, found 513.2518 [M+H]⁺.

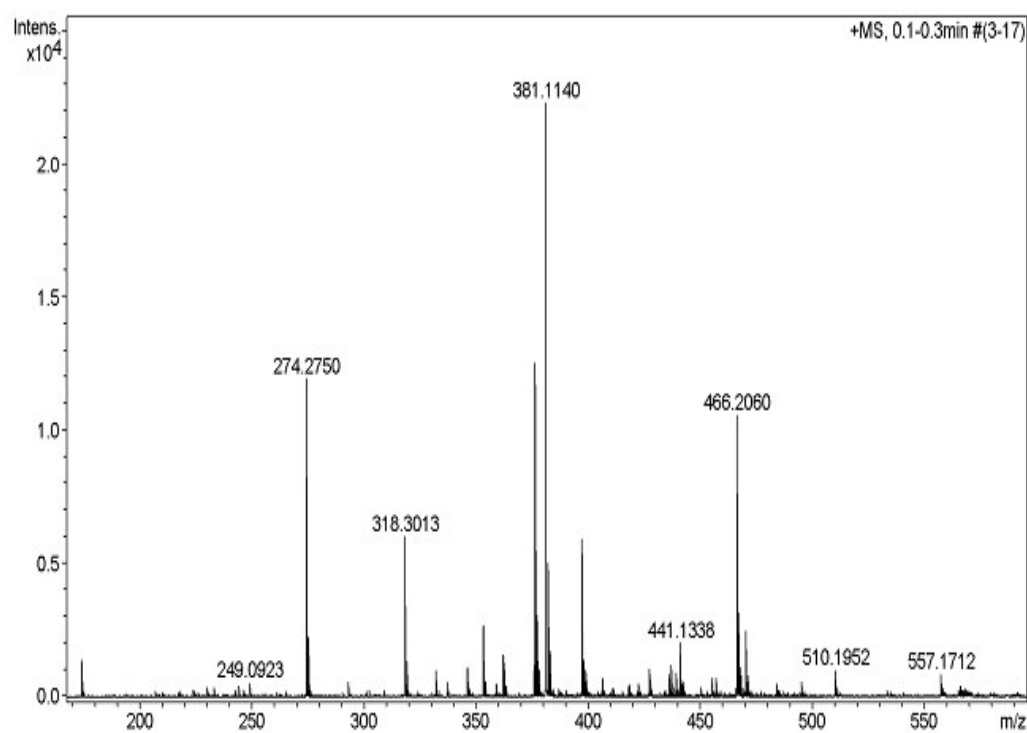
Data for **6e**: orange solid (67%); HR-MS (ESI⁺) m/z 472.2035 [M+H]⁺, found 472.2118 [M+H]⁺.



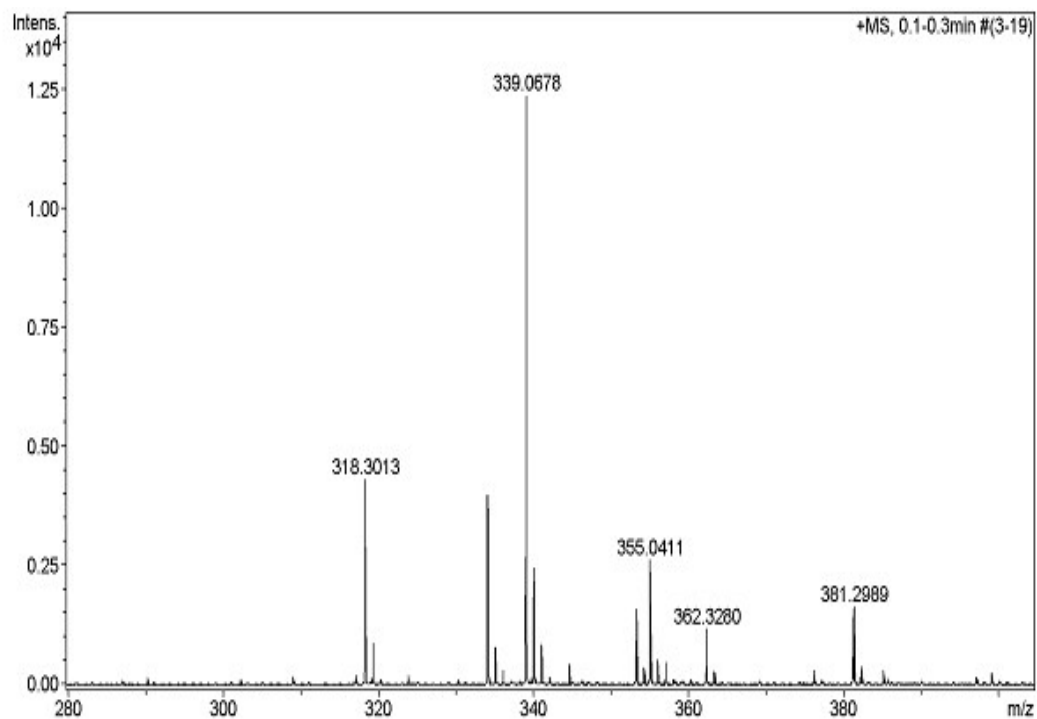
5a HRMS



5b HRMS



5d HRMS



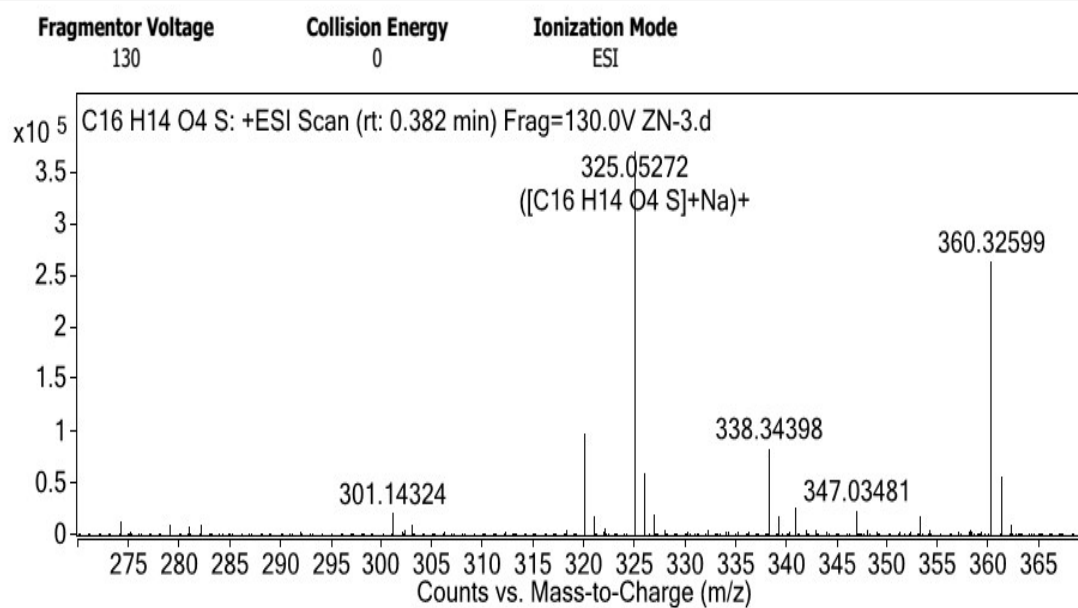
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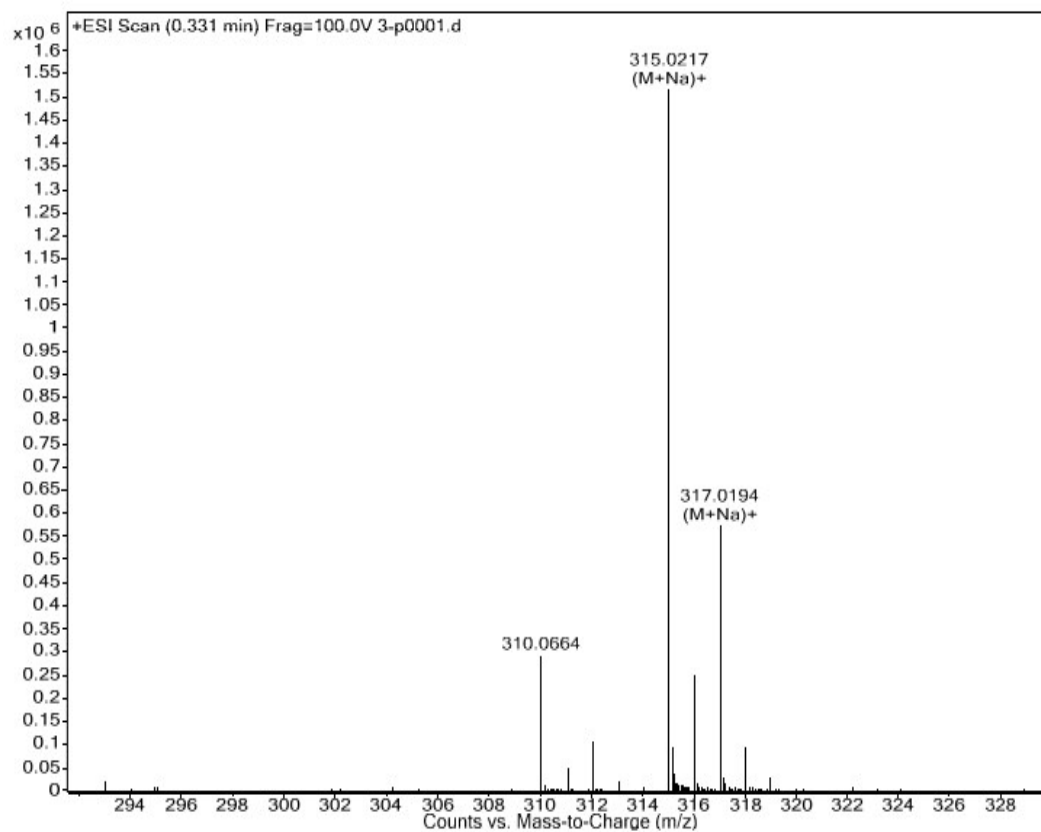
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5g HRMS

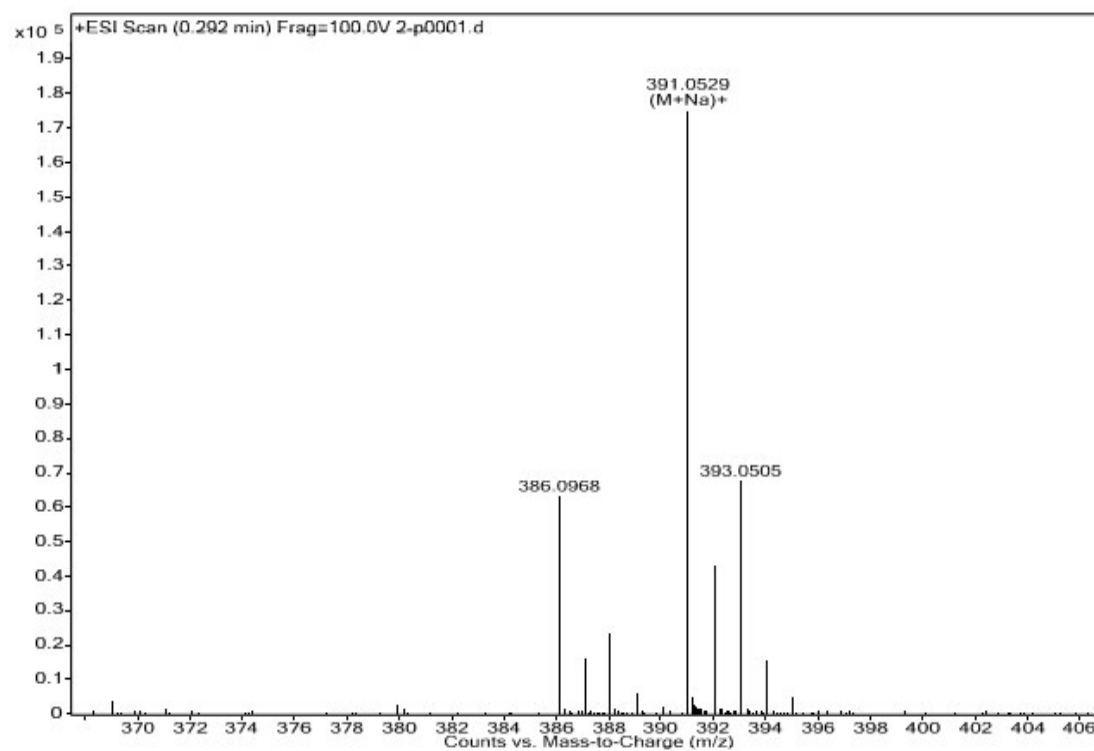
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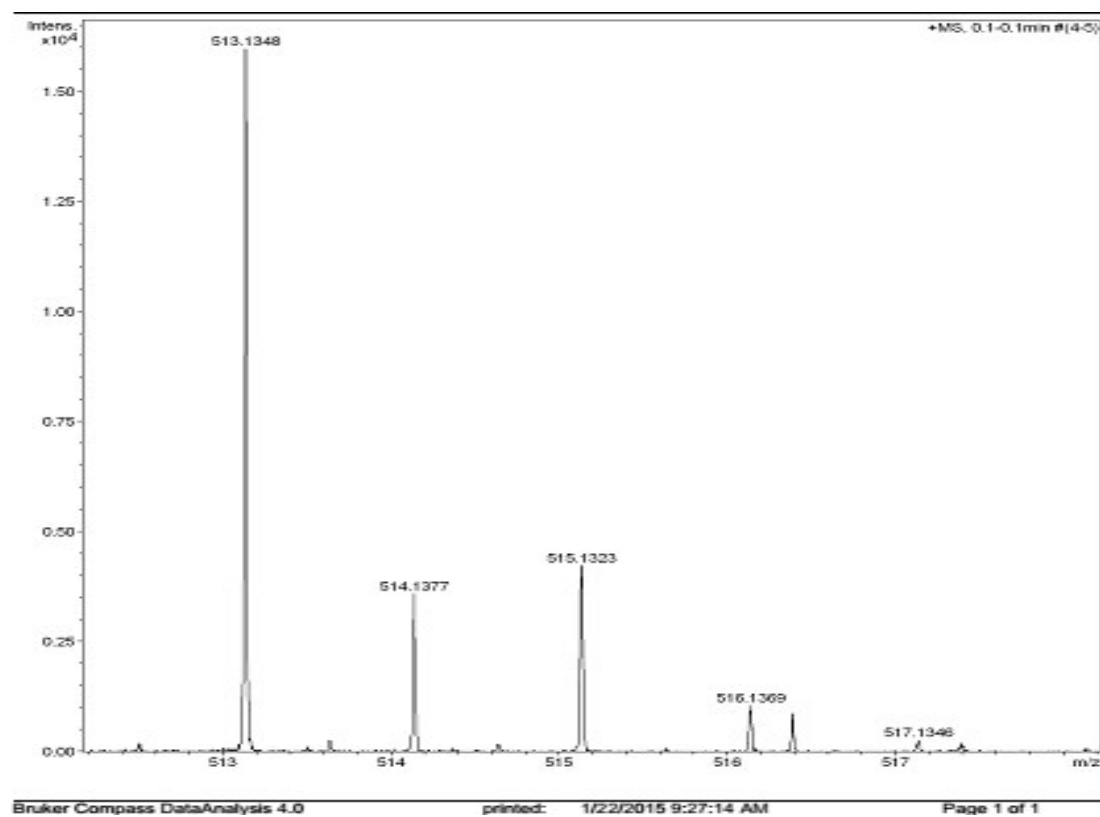
5h HRMS



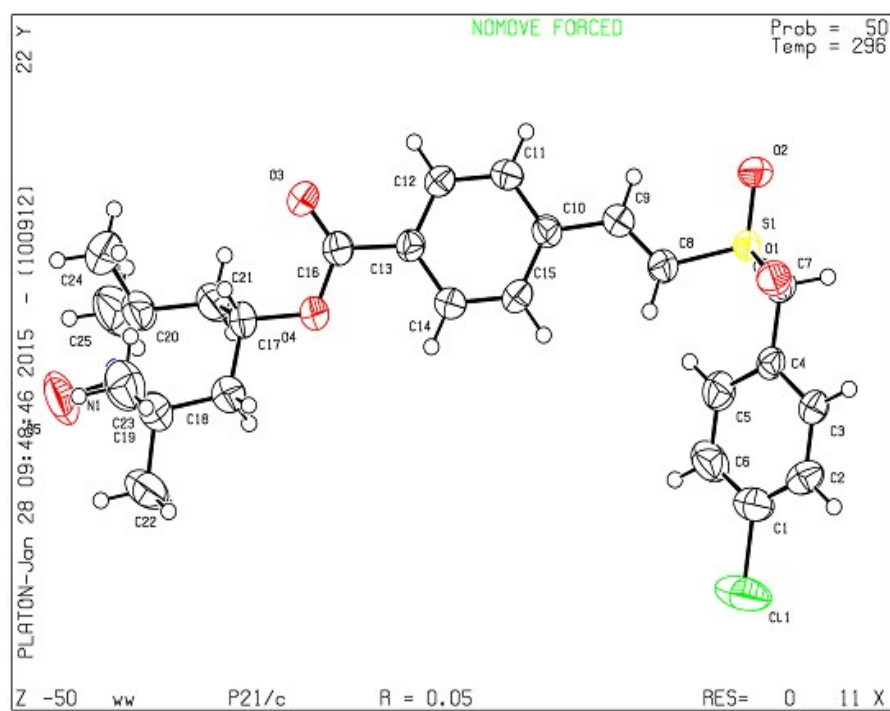
5i HRMS



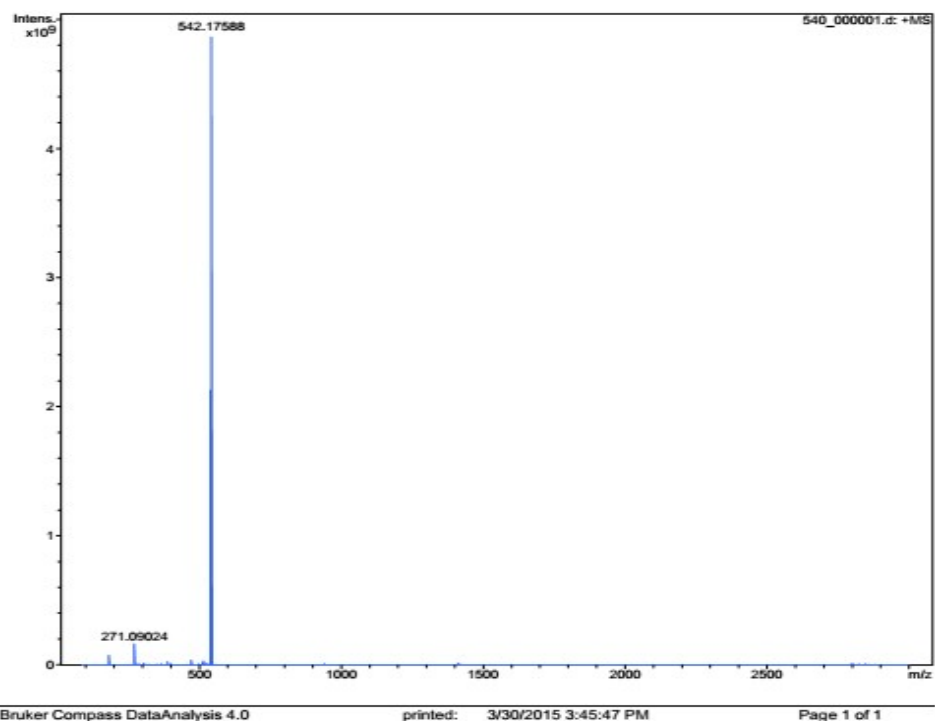
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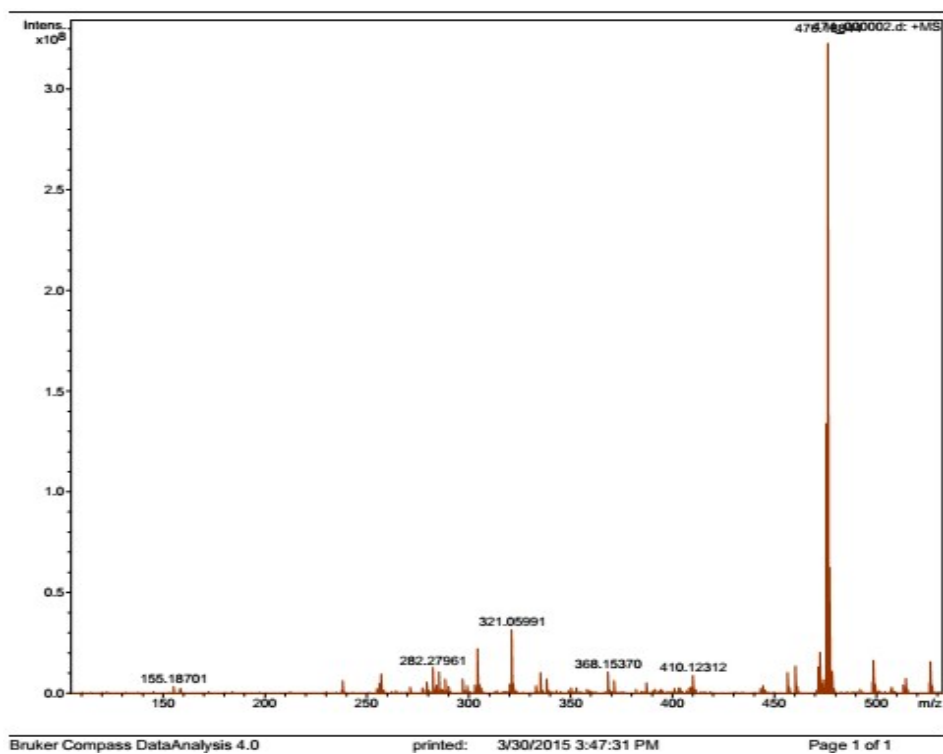
6a HRMS



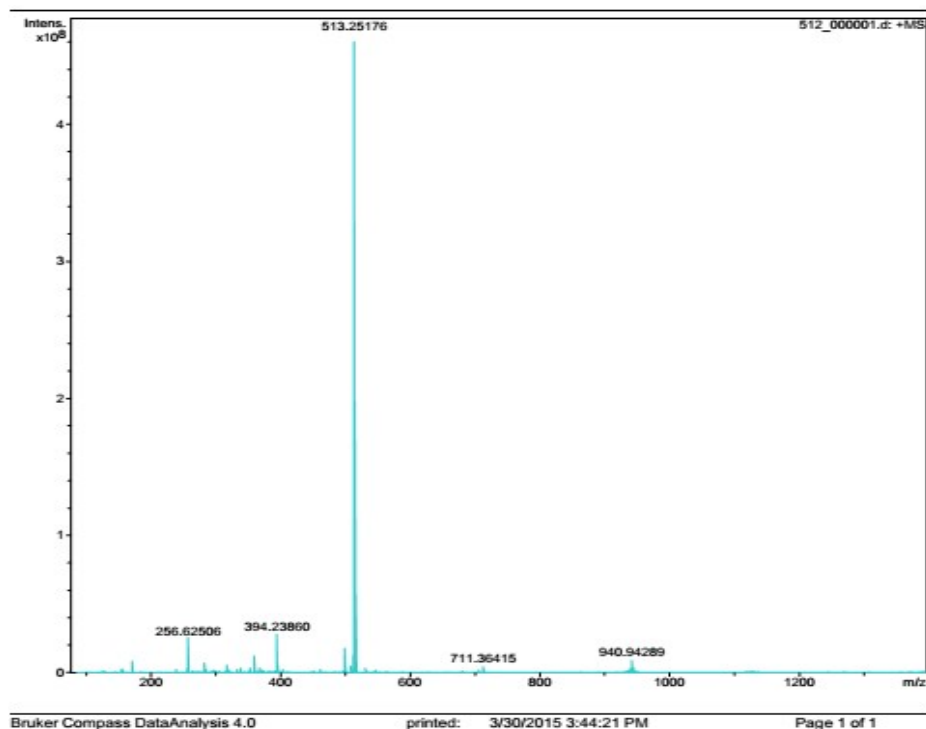
6a X-ray structure



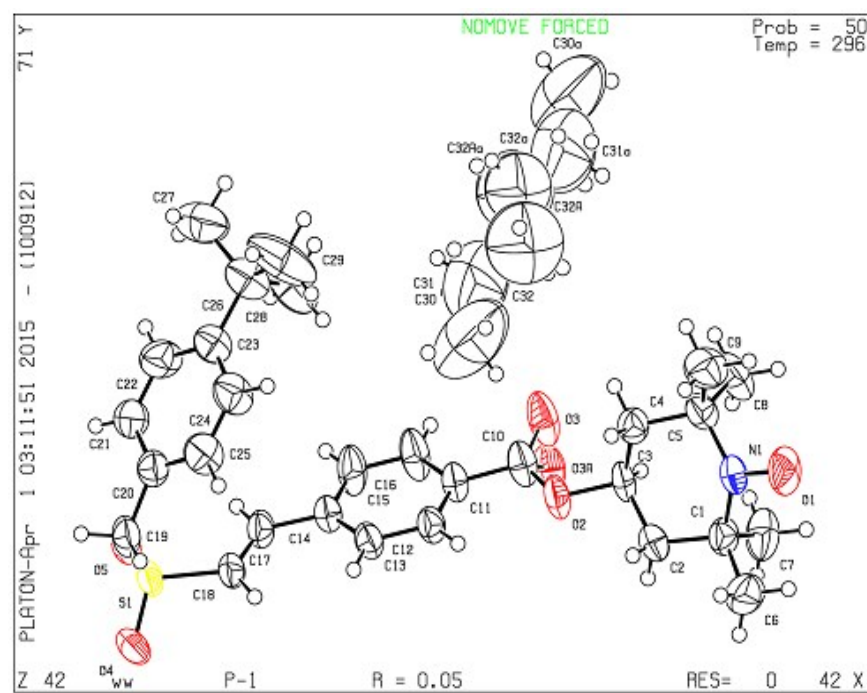
6b-HRMS



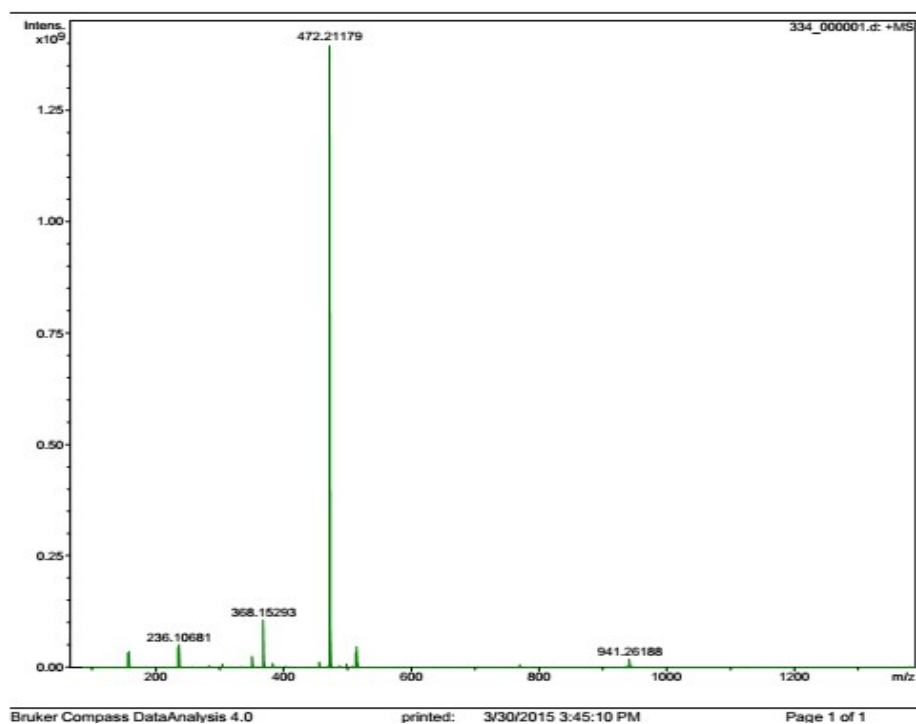
6c-HRMS



6d HRMS



6d-X-ray structure



6e-HRMS