Science Advances
AAAS

# Supplementary Materials for

## Bioinspired large Stokes shift small molecular dyes for biomedical fluorescence imaging

Hao Chen *et al.*

Corresponding author: Zhen Cheng, zcheng@simm.ac.cn; Hong Liu, hliu@simm.ac.cn

*Sci. Adv.* **8**, eabo3289 (2022)
DOI: 10.1126/sciadv.abo3289

**The PDF file includes:**



**Other Supplementary Material for this manuscript includes the following:**

## General Information

All air and moisture-sensitive reactions were carried out in flame-dried glassware under a nitrogen atmosphere. Reactive liquid compounds were measured and transferred by gas-tight syringes and were added to the reaction flask through rubber septa. Tetrahydrofuran (THF) was freshly distilled from sodium benzophenone ketyl. Dichloromethane, toluene, and DMF were distilled from $CaH_2$. All standard synthesis reagents were purchased from Sigma-Aldrich Chemical Co. (St. Louis, MO) and used without further purification. The cell line was obtained from the American Type Tissue Culture Collection (Manassas, VA). Female athymic nude mice (nu/nu) were purchased from Shanghai Experimental Animal Center (Shanghai). Analytical thin-layer chromatography was performed on glass-backed silica gel plates with an F254 indicator. Compounds were visualized under UV lamp or by developing in iodine, vanillin, phosphomolybdic acid solution or with a potassium permanganate solution followed by heating on a hot plate to approximately 350 °C. Flash chromatography was performed on 230-400 mesh silica gel with technical grade solvents which were distilled prior to use. $^{1}H$ NMR spectra were recorded on a Bruker AV400 at 400 MHz as $CDCl_3$ solutions with tetramethylsilane ($\delta = 0$ ppm) as the internal standard. $^{13}C$ spectra were obtained on the same instruments at 100 MHz with $CDCl_3$ ($\delta = 77$ ppm) as the internal reference. Chemical shifts are reported in parts per million (ppm). Multiplicities are reported as s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet), dd (doublet of doublet), etc. High-resolution mass spectra were performed on Bruker APEX III 7.0 Tesla Ion Spec 4.7 Tesla FTMS and Thermo Scientific LTQ ORBITRAP XL. Analytical or preparative high-performance liquid chromatography (HPLC) was performed on a DIONEX ultimate 3000 instrument with PDA detection (column: Princeton SPHER-300 C18, 5 μm, 250 mm ×4.6 mm or 10.0 mm; mobile phase: water/acetonitrile with 0.1 % TFA).

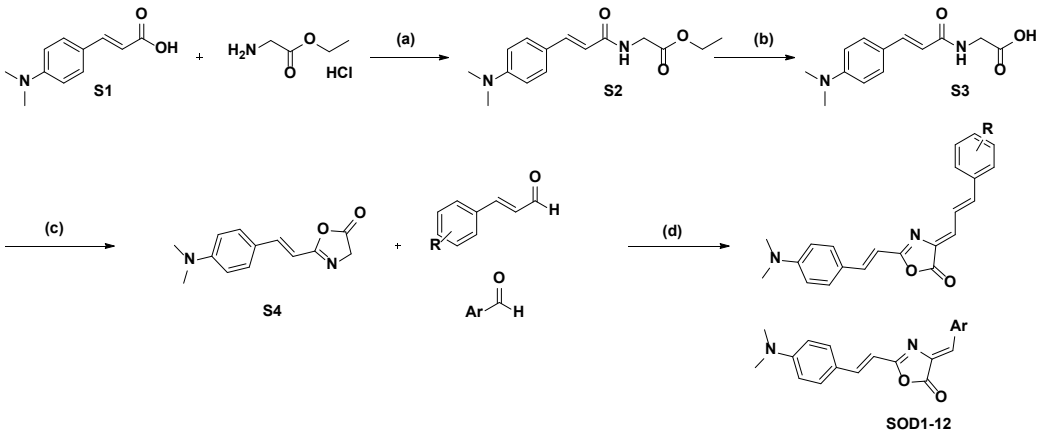



**Fig. S1. General Procedure for Preparation of Oxazolone Derivatives:**
Reagents and conditions: (a) HATU, DIPEA, DCM, r.t., 16 h; (b) LiOH, $CH_3OH/H_2O$, r.t., overnight; (c) DCC, DCM, r.t.; (d) DIPEA, DCM, r.t.

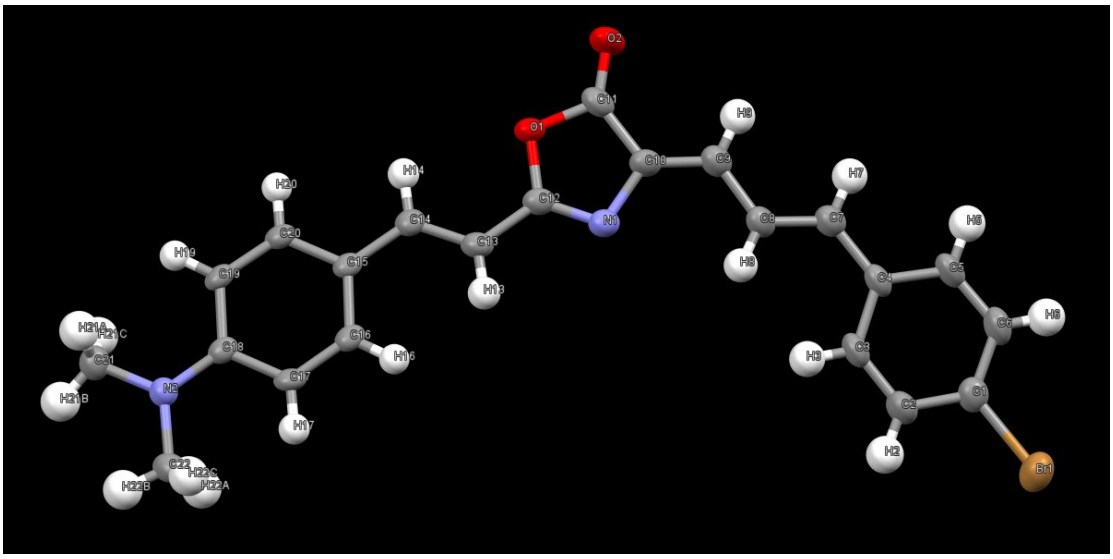



**Fig. S2. X-ray diffraction structure analysis of SOD10**

**Table S1.**
Crystal data and structure refinement data of SOD10.

| Identification code | SOD10 | |
|---|---|---|
| Empirical formula | $C_{22}$ $H_{19}$ Br $N_2$ $O_2$ | |
| Formula weight | 423.30 | |
| Temperature | 173(2) K | |
| Wavelength | 1.34138 Å | |
| Crystal system | Monoclinic | |
| Space group | $P2_1$ | |
| Unit cell dimensions | a = 4.0033(2) Å | a= 90°. |
| | b = 9.9206(5) Å | b= 93.855(3)°. |
| | c = 23.7028(14) Å | g = 90°. |
| Volume | 939.23(9) $Å^3$ | |
| Z | 2 | |
| Density (calculated) | 1.497 $Mg/m^3$ | |
| Absorption coefficient | 2.069 $mm^{-1}$ | |
| F(000) | 432 | |
| Crystal size | 0.160 x 0.070 x 0.010 $mm^3$ | |
| Theta range for data collection | 3.252 to 54.909°. | |
| Index ranges | -4<=h<=4, -12<=k<=12, -28<=l<=25 | |
| Reflections collected | 7777 | |
| Independent reflections | 3414 [R(int) = 0.0479] | |
| Completeness to theta = 53.594° | 99.5 % | |
| Absorption correction | Semi-empirical from equivalents | |
| Max. and min. transmission | 0.888 and 0.695 | |
| Refinement method | Full-matrix least-squares on $F^2$ | |
| Data / restraints / parameters | 3414 / 1 / 246 | |
| Goodness-of-fit on $F^2$ | 1.010 | |
| Final R indices [I>2sigma(I)] | R1 = 0.0409, wR2 = 0.0848 | |
| R indices (all data) | R1 = 0.0553, wR2 = 0.0906 | |
| Absolute structure parameter | -0.020(19) | |
| Extinction coefficient | n/a | |
| Largest diff. peak and hole | 0.228 and -0.575 e.$Å^{-3}$ | |

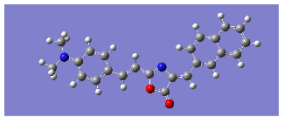
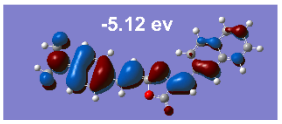
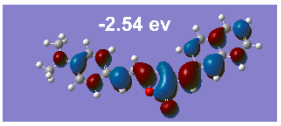
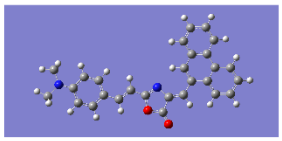
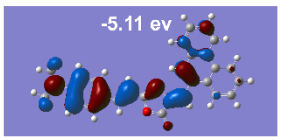
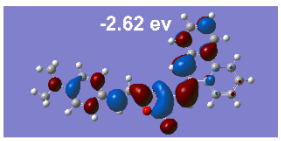
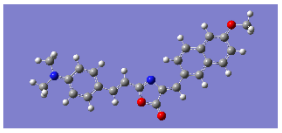
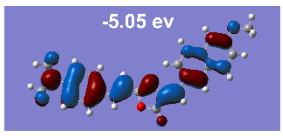
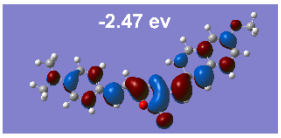
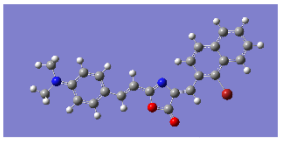
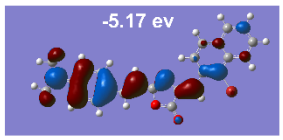
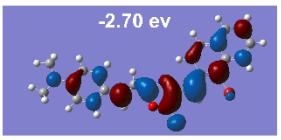
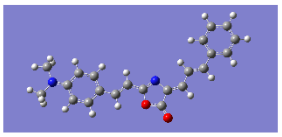
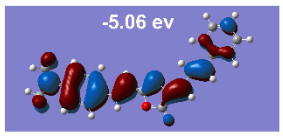
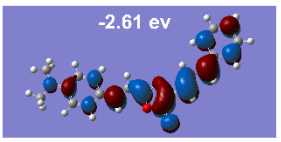
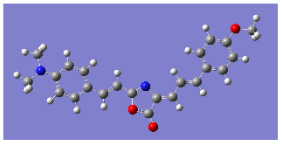
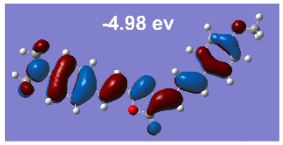
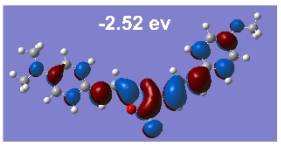
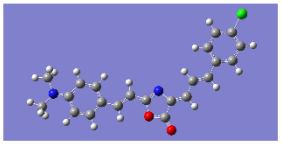
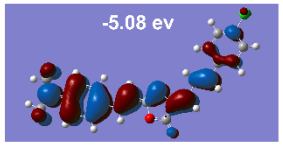
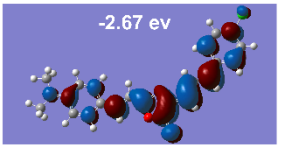
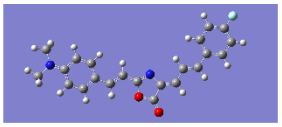
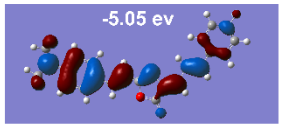
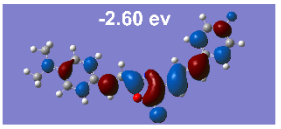
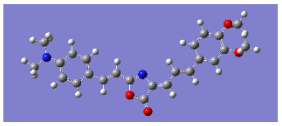
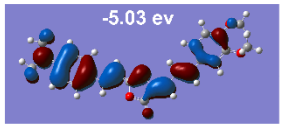
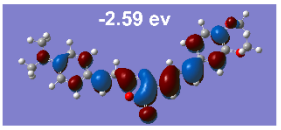
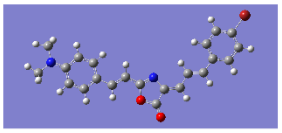
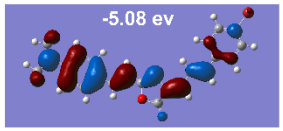
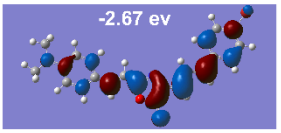
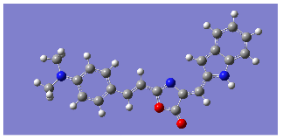
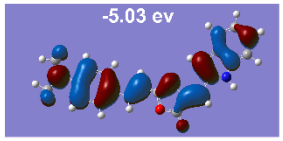
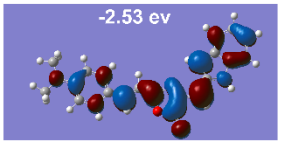
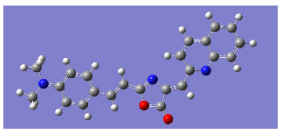
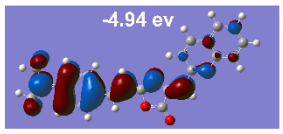
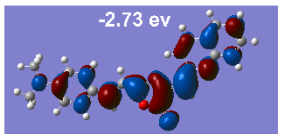
| | Optimized geometry | HOMO | LUMO | Bandgap (eV) |
|---|---|---|---|---|
| 1 |  |   |   | 2.58 (2.28) |
| 2 |  |   |   | 2.49 (2.22) |
| 3 |  |   |   | 2.58 (2.29) |
| 4 |  |   |   | 2.47 (2.20) |
| 5 |  |   |   | 2.45 (2.25) |
| 6 |  |   |   | 2.46 (2.24) |
| 7 |  |   |   | 2.41 (2.23) |
| 8 |  |   |   | 2.45 (2.25) |
| 9 |  |   |   | 2.44 (2.23) |
| 10 |  |   |   | 2.41 (2.22) |
| 11 |  |   |   | 2.50 (2.23) |
| 12 |  |   |   | 2.21 (2.20) |

**Fig. S3. Optimized ground-state ($S_0$) geometries, calculated HOMO and LUMO of SOD1~12 at the B3LYP/6-31G (d) level.** The HOMO and LUMO energy levels, as well as the energy gap are presented. The energy gap in the bracket was calculated from the onset absorption $E_g^{opt}=1240/\lambda_{a.e.\ (nm)}$ (**Fig. S4**).

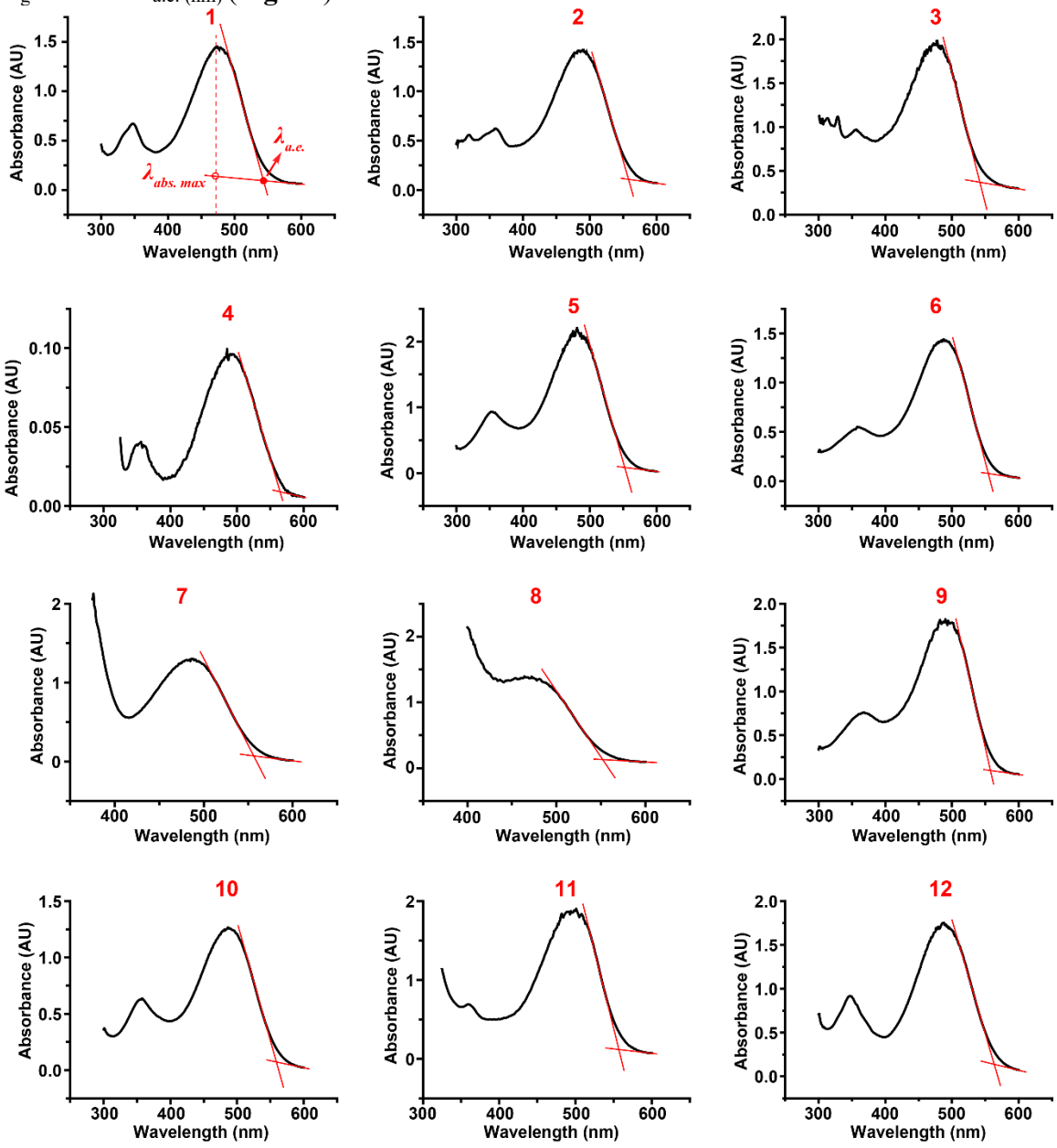



**Fig. S4. The UV-Vis Spectrum of SOD 1~12 and the respective bandgap energy estimations.**

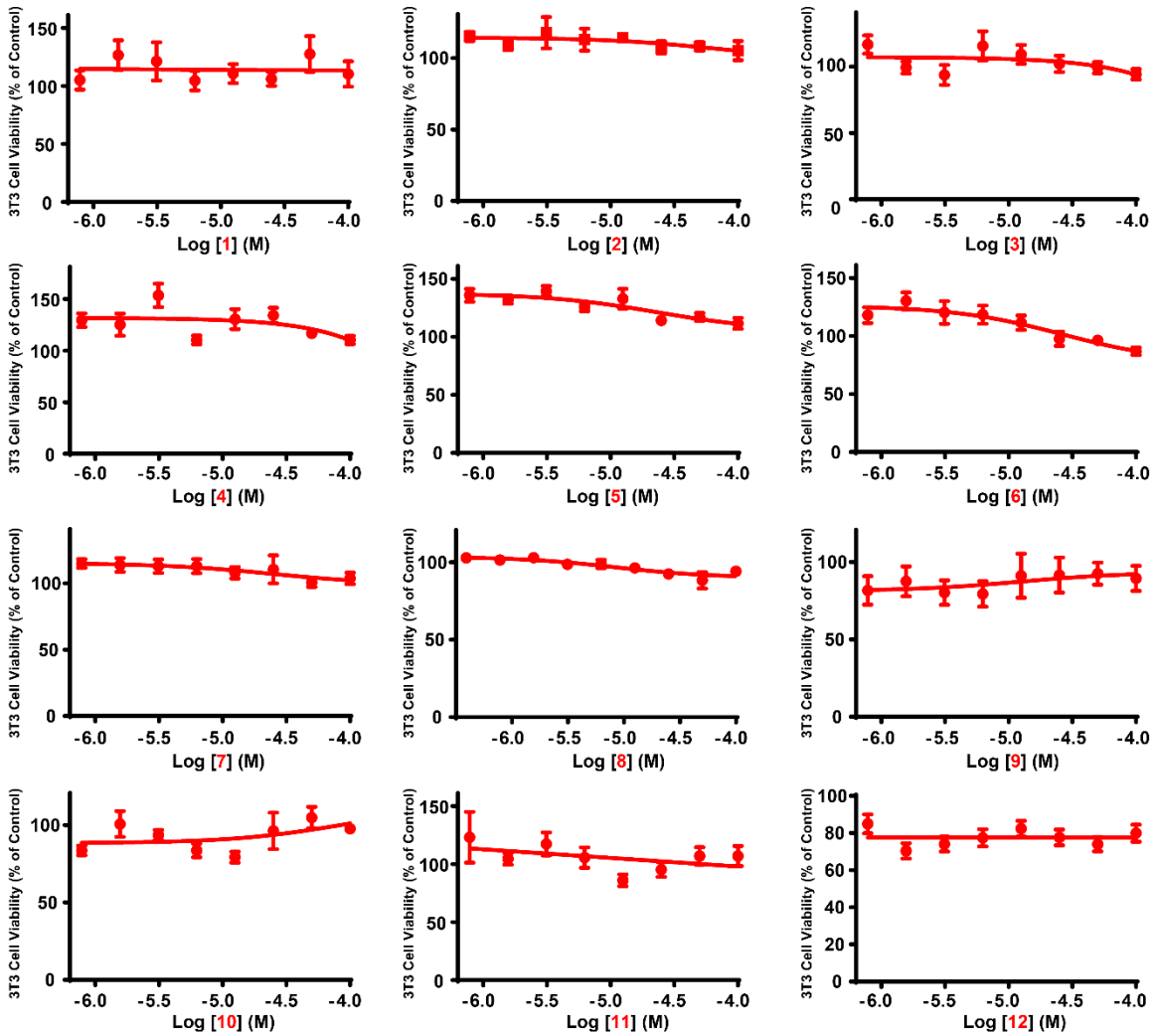
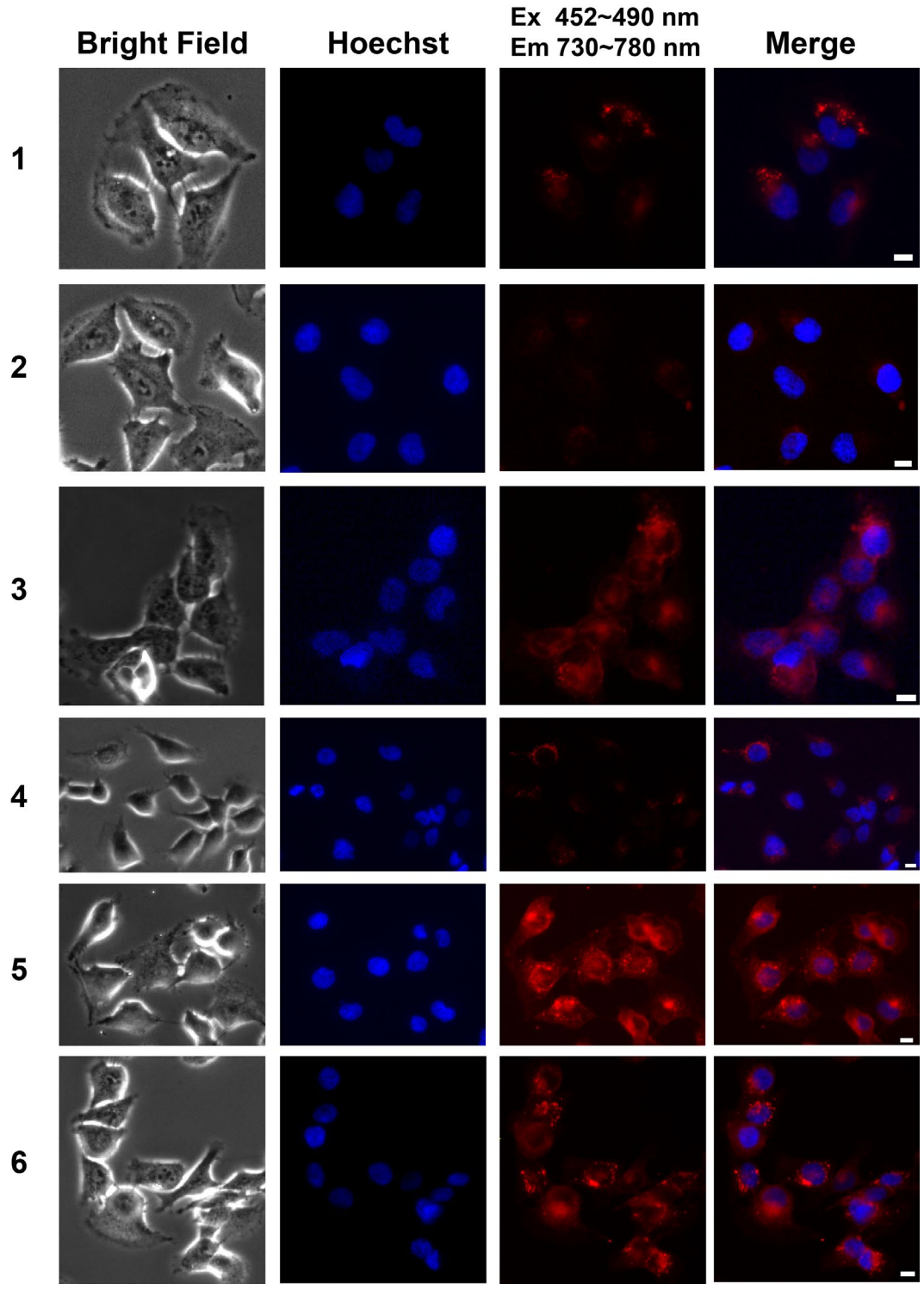



**Fig. S5. Cytotoxicity assay of SOD 1~12 towards NIH/3T3 cells.**


Bright Field
Hoechst
Ex 452~490 nm
Em 730~780 nm
Merge
1
2
3
4
5
6

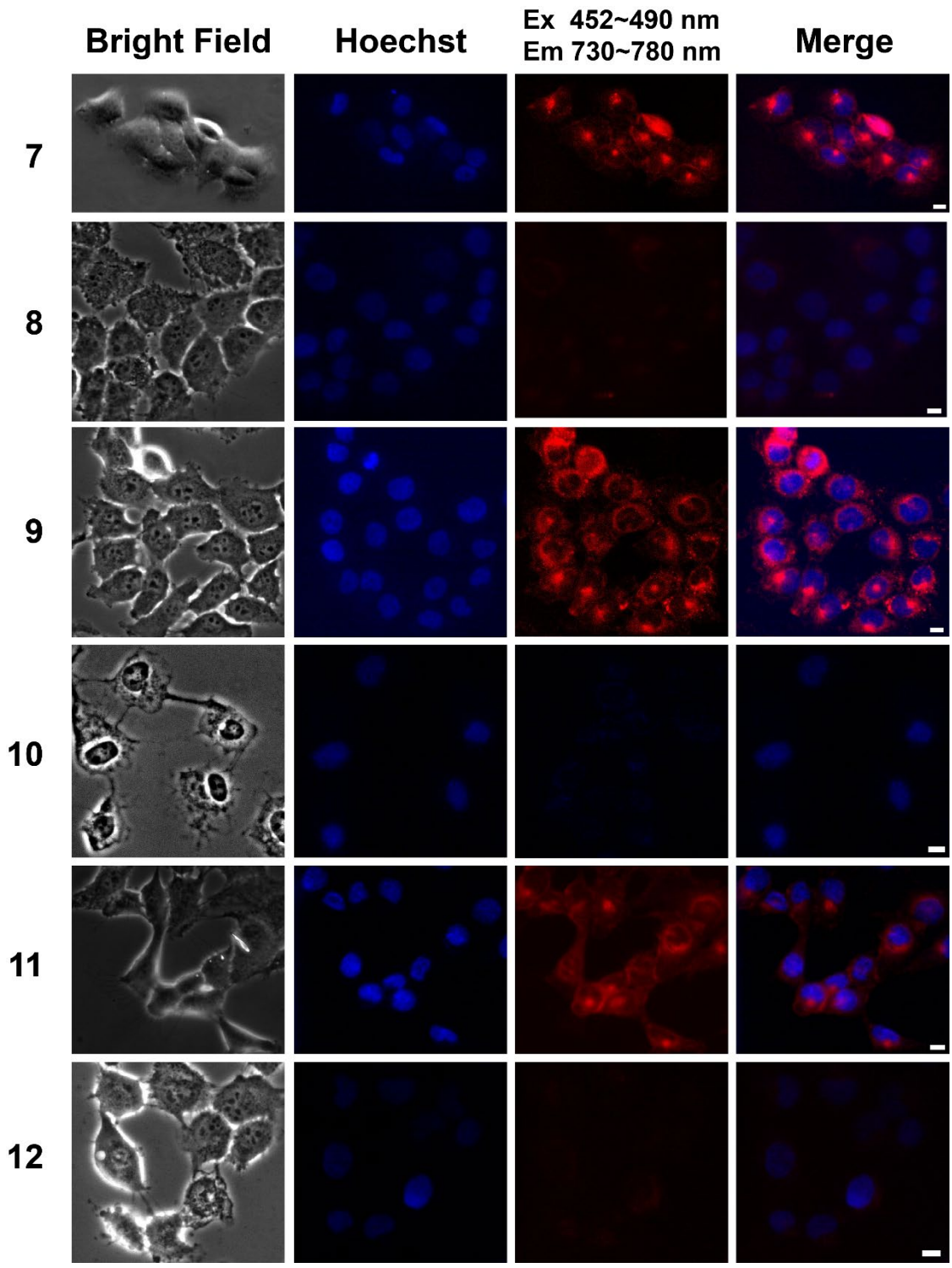



**Fig. S6. The NIH-3T3 cell staining images of the SOD derivatives.** Blue is the Hoechst in nuclei; red is SOD derivatives (excitation 453-490 nm, emission 730-780 nm). Scar bar: 10 μm.

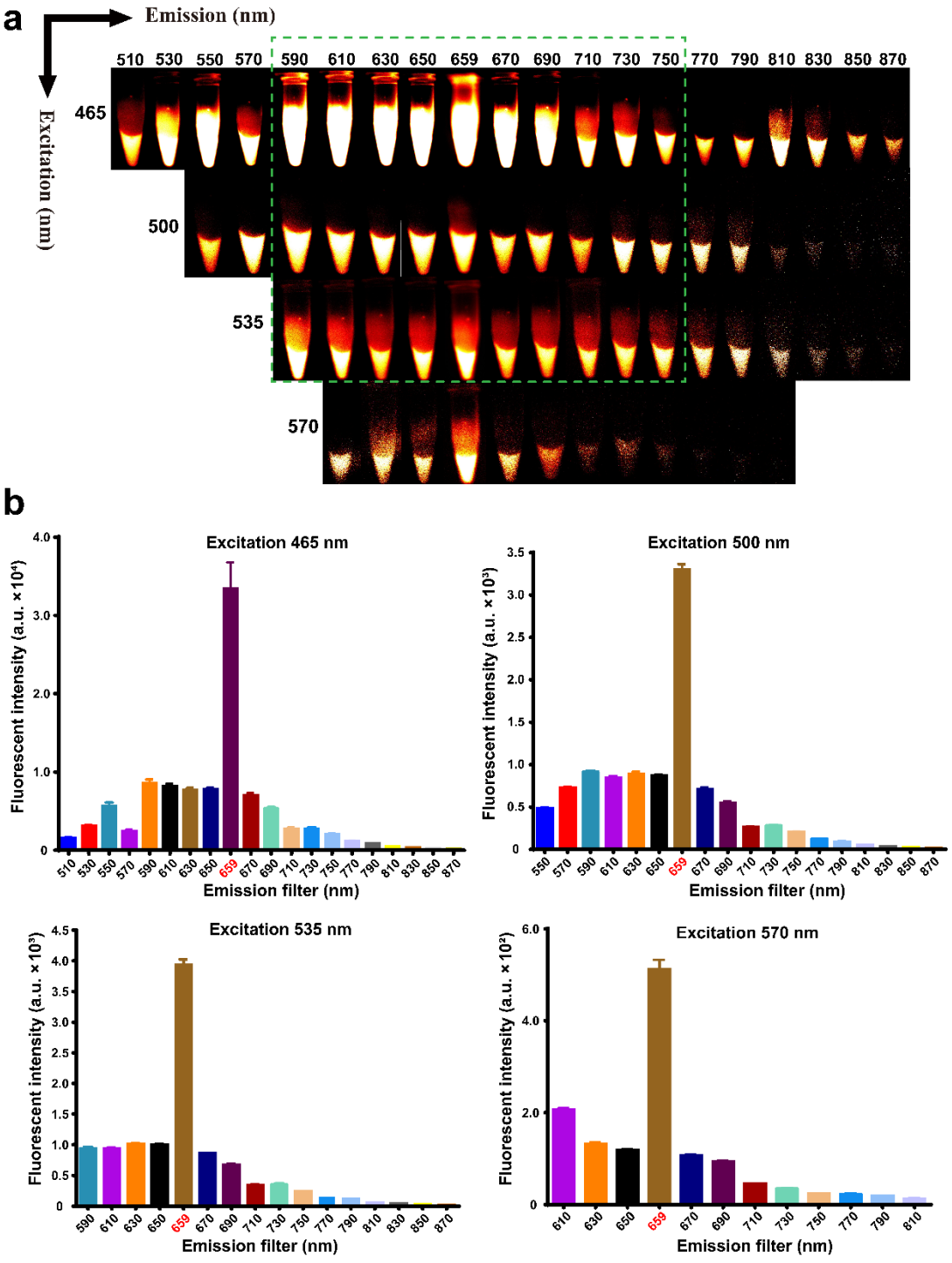



**Fig. S7. The best *in vivo* fluorescent imaging filter set selection of SOD9. a.** The same SOD9 in 1.5 mL Eppendorf tube was imaged under different excitation wavelengths (vertical axis), and the emission light was collected under different cut-off filters (bandwidth ~10 nm, abscissa axis). **b.** The quantifications of (**a**) under the same excitation wavelength. The best excitation was chosen as 535 nm. The best emission filter was selected as 659 nm (bandwidth ~10 nm).

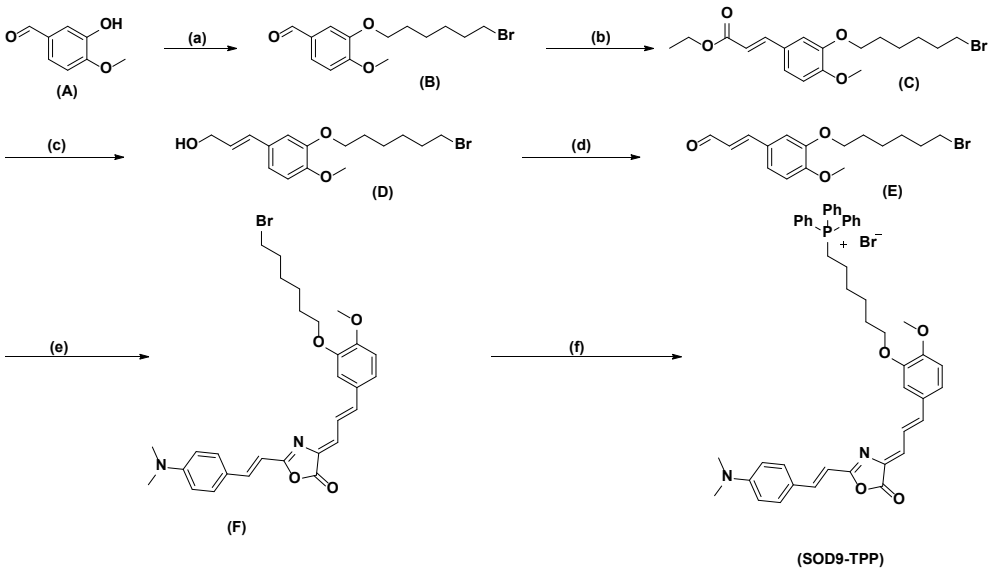



**Fig. S8. Synthesis of (6-(5-((1*E*,3*Z*)-3-(2-((*E*)-4-(dimethylamino)styryl)-5-oxooxazol-4(5*H*)-ylidene)prop-1-en-1-yl)-2-methoxyphenoxy)hexyl)triphenylphosphonium bromide (SOD9-TPP).** Reagents and conditions: (a) 1,6-Dibromohexane, $K_2CO_3$, Acetonitrile, 80°C; (b) Ethyl (triphenylphosphoranylidene)acetate, $Et_3N$, Acetonitrile, r.t.; (c) $LiAlH_4$, THF, -20°C; (d) $MnO_2$, DCM, r.t.; (e) S4, DIPEA, DCM, r.t.; (f) Triphenylphosphine, Toluene, 110°C.

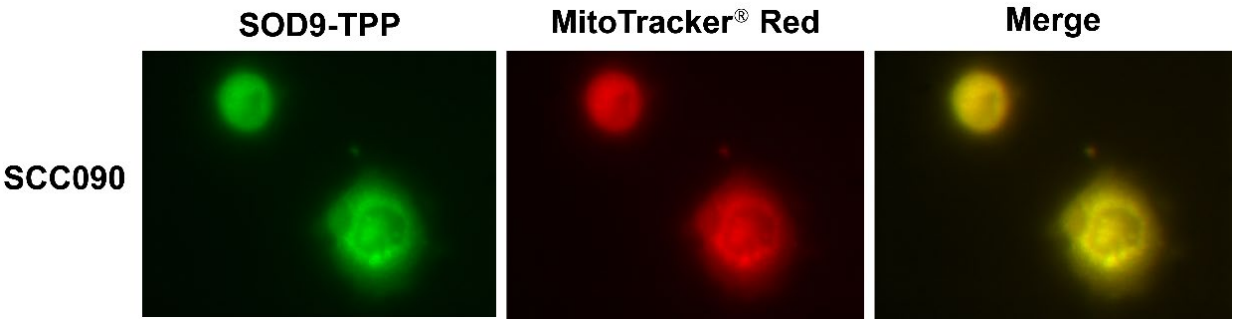



**Fig. S9. Fluorescence colocalization images of SOD9-TPP and MitoTracker Red in SCC090.** Colocalization of SOD-TPP, mitochondrial specific probe (Mitotracker Red) in SCC090 cell lines.

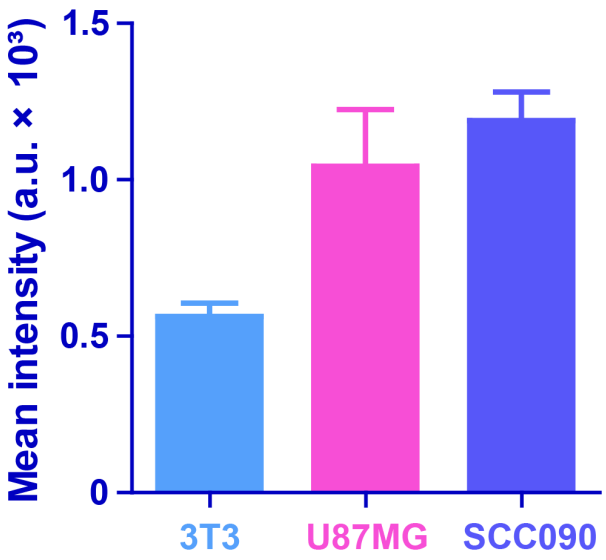
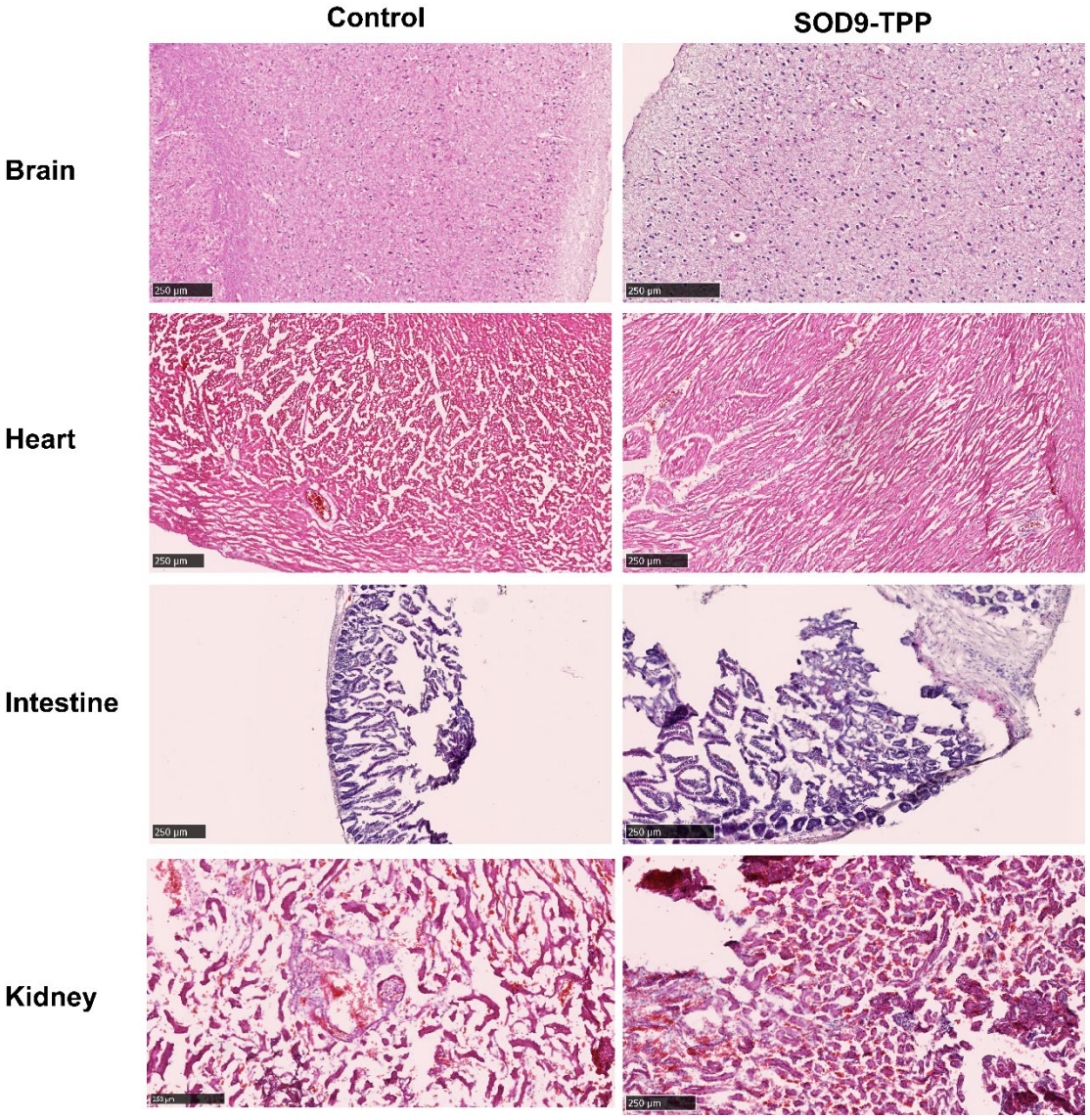



**Fig. S10. The SOD9-TPP cell uptake quantification by fluorescent imaging.** The mean fluorescent intensities of SOD9-TPP in 3T3, U87MG, and SCC090 cell lines were compared with the same incubation concentration (3 μM) and time (1 h) (n=6).


Control
SOD9-TPP
Brain
Heart
Intestine
Kidney
250 µm

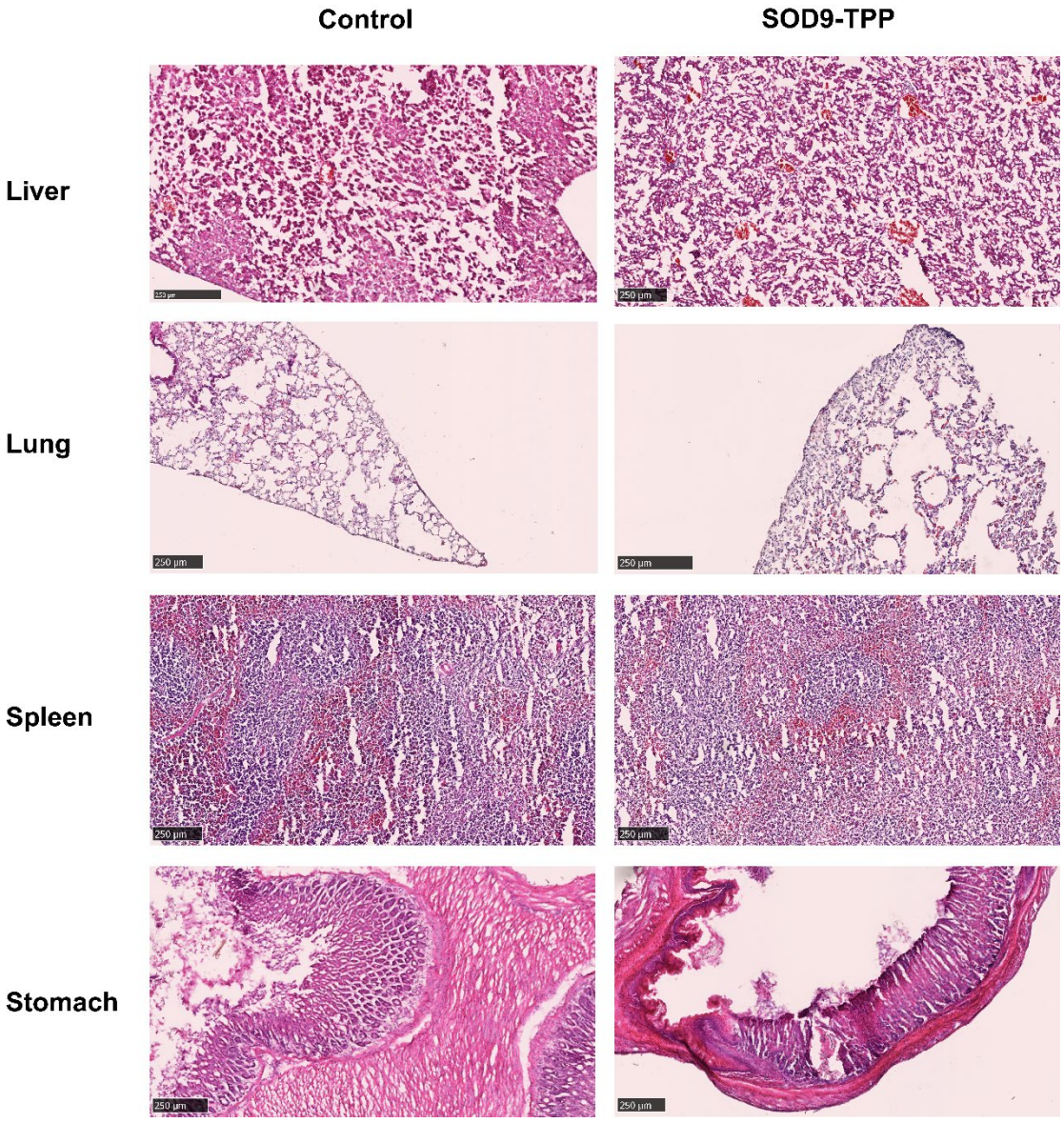



**Fig. S11. Histological analysis of the major organs injected with SOD9-TPP.** Representative H&E images of major organs including brain, heart, intestine, kidney, liver, lung, spleen, and stomach were collected from the mice treated with pH 7.4 PBS (Control group) or SOD9-TPP (SOD9-TPP group, 24 h post-injection, 5.0 mg/kg). No obvious organ damage or lesion was observed for SOD9-TPP injected mice. Scale bar: 250 μm.

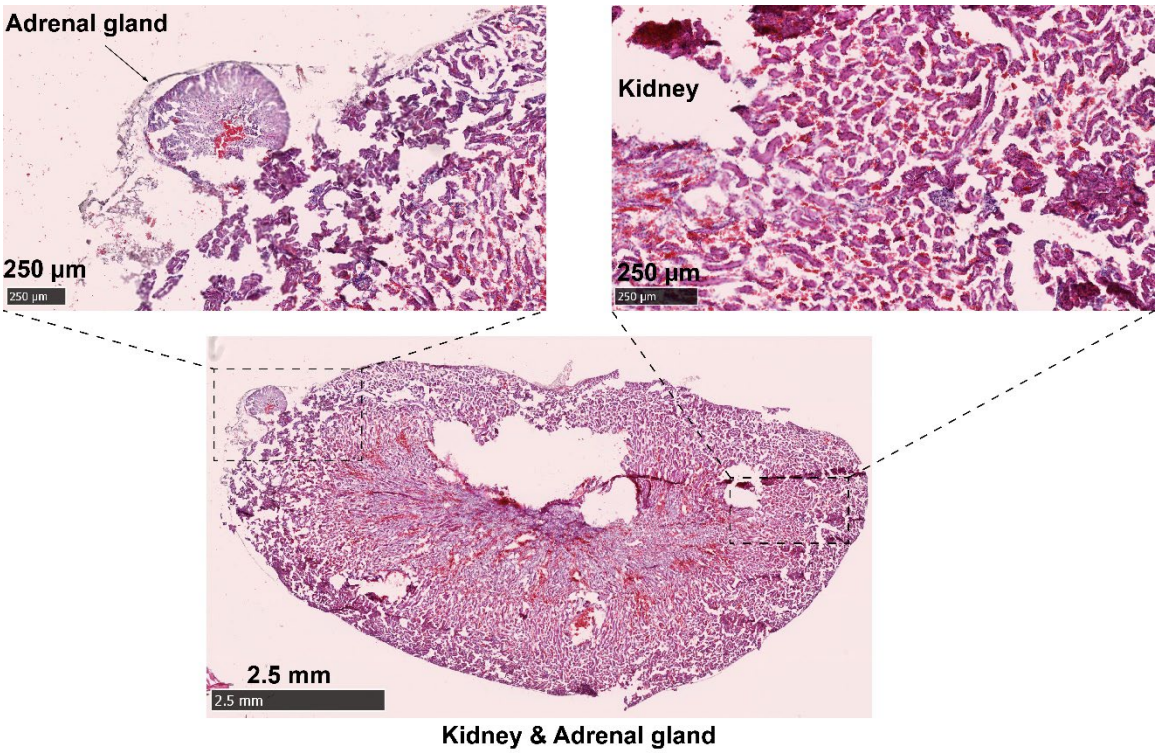



**Fig. S12. Histological analysis of kidney and adrenal gland at the main paper Fig. 4g.** The histological analysis identified the adrenal gland.

**Movie S1.** Real-time imaging of SOD9-TPP in the NIH/3T3 cells' mitochondria (100×objective lens, excitation 453-490 nm, emission 730-780 nm).

**Movie S2.** Real-time monitoring of SOD9-TPP in the orthotopic HNSCC (SCC090) mouse with confocal fluorescent endomicroscopy after 2h i.v. injection (excitation 488 nm laser, emission 540 nm long-pass filter). SOD9-TPP was found in the tumor tissues.

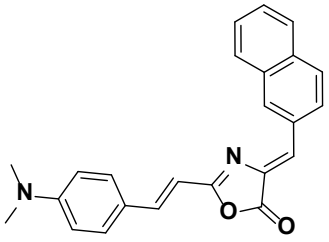
**Movie S3.** Real-time monitoring of SOD9-TPP in the skull-opened mouse brain with confocal fluorescent endomicroscopy after i.v. injection (excitation 488 nm laser, emission 540 nm long-pass filter). SOD9-TPP was found in the blood vessel and the brain tissues.

**General synthesis procedure and the chemical characterization of oxazolone derivatives (Fig. S1):**

**Ethyl (*E*)-(3-(4-(dimethylamino)phenyl)acryloyl)glycinate (S2).**
To a solution of **S1** (10.00 g, 52.29 mmol) in 50 mL dichloromethane was added ethyl glycinate hydrochloride (7.30 g, 52.29 mmol), HATU (18.91 g, 78.44 mmol), and DIPEA (21.61 mL, 130.73 mmol). The resulting mixture was stirred at room temperature for 16 h. After this period, saturated aqueous $NH_4Cl$ solution was added and extracted twice with dichloromethane. The combined organic layer was washed with brine, dried over anhydrous $Na_2SO_4$, and concentrated under vacuum. The residue was purified by silica gel column using 30% ethyl acetate in petroleum ether as eluent to afford the title compound as a primrose yellow solid.

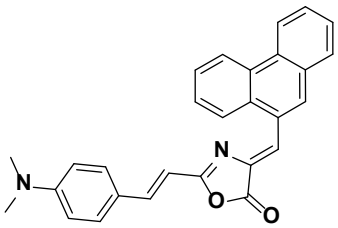
**(*E*)-(3-(4-(dimethylamino)phenyl)acryloyl)glycine (S3).**
To a solution of **S2** (11.00 g, 39.81 mmol) in 20 mL methanol and 10 mL $H_2O$ was added lithium hydrate (7.96 g, 199.03 mmol), and the reaction was stirred at room temperature overnight. After the reaction was completed, the mixture was concentrated under a vacuum and diluted with water. The diluted solution was adjusted to neutral with 1N hydrochloric acid. The precipitate was filtered using a Buchner funnel and washed with diethyl ether to afford the title compound as a yellow solid.

**(*E*)-2-(4-(dimethylamino)styryl)oxazol-5(4*H*)-one (S4).**
A solution of **S3** (5.00 g, 20.14 mmol) in 30 mL dichloromethane was added DCC (6.23 g, 30.21 mmol). The reaction was stirred at room temperature overnight. The resulting suspension was filtered, and the precipitate was washed with cold ethanol to afford the title compound as an orange solid.

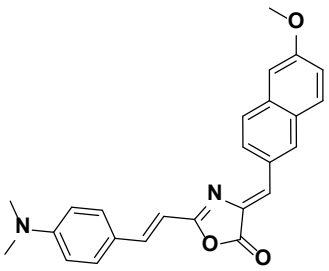



**(*Z*)-2-((*E*)-4-(dimethylamino)styryl)-4-(naphthalen-2-ylmethylene)oxazol-5(4*H*)-one (SOD1).**
To a solution of **S4** in 30 mL dichloromethane was added 2-naphthaldehyde (339.14 mg, 2.17 mmol) and DIPEA (538.32 μL, 3.26 mmol). The resulting mixture was stirred at room temperature overnight. Then the solvent was removed and the residue was

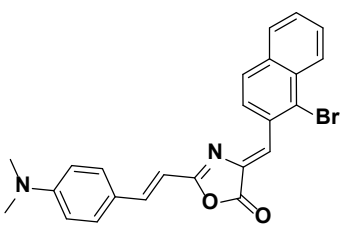
purified by flash column chromatography using dichloromethane/methanol (100:1) as an eluent to afford the title compound as a red solid. **$^1$H NMR** (400 MHz, Chloroform-*d*) $\delta$ 8.45 (s, 1H), 8.41 (dd, *J* = 8.7, 1.7 Hz, 1H), 7.95 – 7.91 (m, 1H), 7.89 (d, *J* = 8.7 Hz, 1H), 7.87 – 7.83 (m, 1H), 7.67 (d, *J* = 15.9 Hz, 1H), 7.55 – 7.53 (m, 1H), 7.53 – 7.49 (m, 3H), 7.25 (s, 1H), 6.72 (d, *J* = 8.7 Hz, 2H), 6.64 (d, *J* = 16.0 Hz, 1H), 3.07 (s, 6H). **$^{13}$C NMR** (126 MHz, Chloroform-*d*) δ 168.1, 164.4, 152.2, 144.7, 134.5, 134.3, 133.4, 133.3, 132.0, 130.3, 129.2, 128.9, 128.7, 127.9, 127.9, 127.8, 126.7, 122.8, 112.1, 107.5, 40.3. **HRMS** (ESI) m/z $[M + H]^+$ calcd for $C_{24}H_{21}N_2O_2$ 369.1598, found 369.1608.



**(*Z*)-2-((*E*)-4-(dimethylamino)styryl)-4-(phenanthren-9-ylmethylene)oxazol-5(4*H*)-one (SOD2).**
Compound **SOD2** was prepared in a similar manner as described for compound **SOD1** as a red solid. **$^1$H NMR** (400 MHz, Chloroform-*d*) δ 9.13 (s, 1H), 8.76 (d, *J* = 9.7 Hz, 1H), 8.68 (d, *J* = 8.2 Hz, 1H), 8.34 (d, *J* = 9.8 Hz, 1H), 8.09 – 8.05 (m, 1H), 7.96 (s, 1H), 7.74 – 7.67 (m, 4H), 7.67 – 7.60 (m, 1H), 7.56 – 7.48 (m, 2H), 6.73 (d, *J* = 8.9 Hz, 2H), 6.67 (d, *J* = 15.9 Hz, 1H), 3.07 (s, 6H). **$^{13}$C NMR** (126 MHz, Chloroform-*d*) δ 167.9, 165.1, 152.1, 144.9, 135.5, 133.3, 131.5, 131.4, 130.7, 130.7, 130.4, 128.5, 128.4, 127.4, 127.1, 127.0, 124.6, 123.9, 123.4, 122.7, 112.4, 107.7, 40.5. **HRMS** (EI) m/z $[M]^+$ calcd for $C_{28}H_{22}O_2N_2$ 418.1676, found 418.1668.

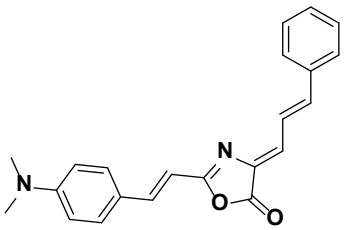


**(*Z*)-2-((*E*)-4-(dimethylamino)styryl)-4-((6-methoxynaphthalen-2-yl)methylene)oxazol-5(4*H*)-one (SOD3).**
Compound **SOD3** was prepared in a similar manner as described for compound **SOD1** as a red solid. **$^1$H NMR** (400 MHz, Chloroform-*d*) δ 8.45 – 8.33 (m, 2H), 7.80 (dd, *J* = 22.7, 8.7 Hz, 2H), 7.65 (d, *J* = 16.0 Hz, 1H), 7.50 (d, *J* = 8.4 Hz, 2H), 7.23 (s, 1H), 7.20 – 7.09 (m, 2H), 6.73 (d, *J* = 8.2 Hz, 2H), 6.63 (d, *J* = 15.9 Hz, 1H), 3.95 (s, 3H), 3.07 (s, 6H). **$^{13}$C NMR** (126 MHz, Chloroform-*d*) δ 168.2, 163.9, 159.5, 159.5, 151.9, 144.2, 135.9, 133.5, 133.3, 130.9, 130.2, 129.8, 129.5, 128.9, 128.7, 127.5, 119.5, 112.3, 107.8, 106.1, 55.6, 40.5. **HRMS** (EI) m/z $[M]^+$ calcd for $C_{25}H_{22}O_3N_2$ 398.1625, found 398.1629.

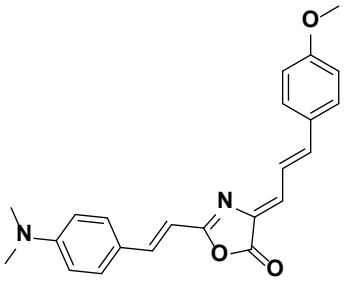


**(*Z*)-2-((*E*)-4-(dimethylamino)styryl)4-((1-bromonaphthalen-2-yl)methylene)-oxazol-5(4*H*)-one (SOD4).**
Compound **SOD4** was prepared in a similar manner as described for compound **SOD1** as a black solid. **$^1$H NMR** (400 MHz, Chloroform-*d*) $\delta$ 8.85 (d, *J* = 8.7 Hz, 1H), 8.41 (d, *J* = 8.2 Hz, 1H), 7.93 (s, 1H), 7.85 (t, *J* = 7.8 Hz, 2H), 7.71 (d, *J* = 16.0 Hz, 1H), 7.60 (d, *J* = 8.0 Hz, 4H), 7.19 (s, 2H), 6.73 (d, *J* = 16.0 Hz, 1H), 3.13 (s,

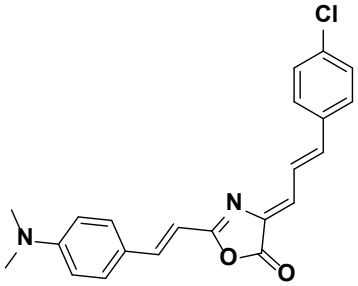
6H). **$^{13}$C NMR** (126 MHz, Chloroform-*d*) δ 167.7, 145.5, 136.0, 135.8, 135.3, 135.0, 134.7, 134.1, 134.0, 132.7, 132.2, 130.5, 128.7, 128.3, 128.2, 127.9, 127.8, 127.3, 112.1, 107.2, 40.3. **HRMS** (EI) m/z [M]+ calcd for $C_{24}H_{19}O_2N_2Br$ 446.0624, found 446.0631.



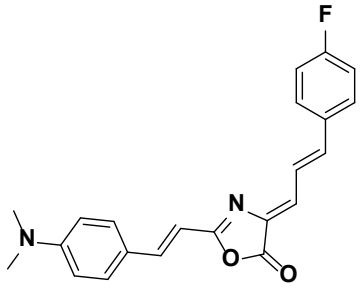
**(*Z*)-2-((*E*)-4-(dimethylamino)styryl)-4-((*E*)-3-phenylallylidene)oxazol-5(4*H*)-one (SOD5).**
Compound **SOD5** was prepared in a similar manner as described for compound **SOD1** as a red solid. **$^1$H NMR** (400 MHz, Chloroform-*d*) *δ* 7.65 – 7.54 (m, 4H), 7.50 – 7.45 (m, 2H), 7.42 – 7.31 (m, 3H), 7.06 (d, *J* = 15.7 Hz, 1H), 6.99 (dd, *J* = 11.7, 1.0 Hz, 1H), 6.72 (d, *J* = 8.5 Hz, 2H), 6.54 (d, *J* = 15.9 Hz, 1H), 3.06 (s, 6H). **$^{13}$C NMR** (126 MHz, Chloroform-*d*) δ 167.0, 163.2, 152.1, 144.3, 142.7, 136.4, 134.9, 130.2, 130.1, 129.7, 129.0, 127.9, 123.6, 122.9, 112.2, 107.3, 40.3. **HRMS** (ESI) m/z [M + H]$^+$ calcd for $C_{22}H_{21}N_2O_2$ 345.1598, found 345.1603.



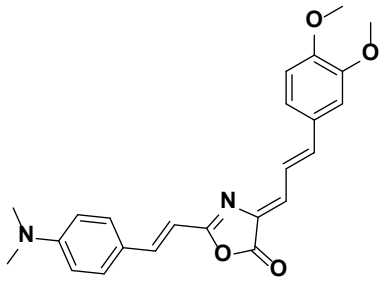
**(*Z*)-2-((*E*)-4-(dimethylamino)styryl)-4-((*E*)-3-(4-methoxyphenyl)allylidene)oxazol-5(4*H*)-one (SOD6).**
Compound **SOD6** was prepared in a similar manner as described for compound **SOD1** as a red solid. **$^1$H NMR** (400 MHz, Chloroform-*d*) *δ* 7.59 (d, *J* = 15.9 Hz, 1H), 7.54 (d, *J* = 8.6 Hz, 2H), 7.52 – 7.42 (m, 3H), 7.05 (s, 1H), 7.00 (d, *J* = 11.0 Hz, 1H), 6.91 (d, *J* = 8.6 Hz, 2H), 6.74 (d, *J* = 8.3 Hz, 2H), 6.55 (d, *J* = 15.9 Hz, 1H), 3.85 (s, 3H), 3.06 (s, 6H). **$^{13}$C NMR** (126 MHz, Chloroform-*d*) δ 167.1, 162.7, 161.2, 152.1, 143.8, 142.7, 133.8, 130.9, 130.1, 129.6, 129.3, 122.9, 121.6, 114.6, 112.1, 107.4, 55.6, 40.3. **HRMS** (EI) m/z [M]$^+$ calcd for $C_{23}H_{22}O_3N_2$ 374.1625, found 374.1624.



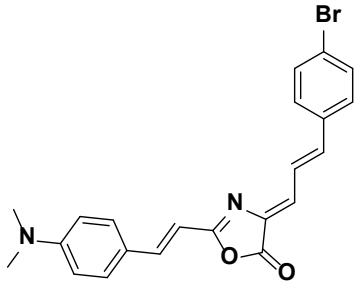
**(*Z*)-4-((*E*)-3-(4-chlorophenyl)allylidene)-2-((*E*)-4-(dimethylamino)styryl)oxazol-5(4*H*)-one (SOD7).**
Compound **SOD7** was prepared in a similar manner as described for compound **SOD1** as a red solid. **$^1$H NMR** (400 MHz, Chloroform-*d*) *δ* 7.63 (d, *J* = 16.0 Hz, 1H), 7.50 (t, *J* = 9.1 Hz, 5H), 7.35 (d, *J* = 8.4 Hz, 2H), 6.98 (t, *J* = 13.4 Hz, 2H), 6.77 (d, *J* = 8.2 Hz, 2H), 6.54 (d, *J* = 15.9 Hz, 1H), 3.07 (s, 6H). **$^{13}$C NMR** (126 MHz, Chloroform-*d*) δ 166.8, 163.4, 144.6, 141.0, 135.5, 135.1, 134.9, 130.3, 129.8, 129.6, 129.5, 129.3, 129.0, 124.1, 112.5, 107.2, 40.5. **HRMS** (EI) m/z [M]$^+$ calcd for $C_{22}H_{19}O_2N_2Cl$ 378.1130, found 378.1137.



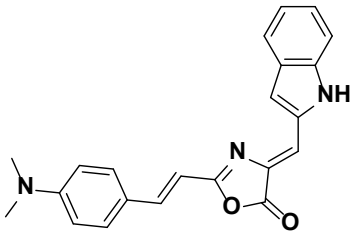
**(*Z*)-2-((*E*)-4-(dimethylamino)styryl)-4-((*E*)-3-(4-fluorophenyl)allylidene)oxazol-5(4*H*)-one (SOD8).**
Compound **SOD8** was prepared in a similar manner as described for compound **SOD1** as a red solid. **$^{1}$H NMR** (400 MHz, Chloroform-*d*) $\delta$ 7.61 (d, $J$ = 16.0 Hz, 1H), 7.58 – 7.54 (m, 2H), 7.54 – 7.48 (m, 1H), 7.48 – 7.45 (m, 2H), 7.07 (t, $J$ = 8.6 Hz, 2H), 7.01 (d, $J$ = 15.6 Hz, 1H), 6.96 (dd, $J$ = 11.6, 1.1 Hz, 1H), 6.72 – 6.67 (m, 2H), 6.52 (d, $J$ = 15.9 Hz, 1H), 3.06 (s, 6H). **$^{13}$C NMR** (126 MHz, Chloroform-*d*) δ 166.7, 163.5 (d, $J$ = 254.5 Hz), 163.1, 162.4, 151.9, 144.3, 141.1, 134.7, 132.5 (d, $J$ = 3.8 Hz), 130.1, 129.7, 129.5 (d, $J$ = 7.6 Hz), 123.2, 116.0 (d, $J$ = 21.4 Hz), 112.2, 107.1, 40.3. **HRMS** (ESI) m/z $[M + H]^+$ calcd for $C_{22}H_{20}FN_2O_2$ 363.1503, found 363.1505.



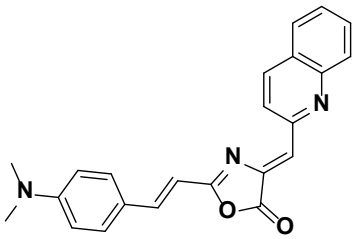
**(*Z*)-2-((*E*)-4-(dimethylamino)styryl)-4-((*E*)-3-(3,4-dimethoxyphenyl)allylidene)-oxazol-5(4*H*)-one (SOD9).**
Compound **SOD9** was prepared in a similar manner as described for compound **SOD1** as a red solid.**$^{1}$H NMR** (400 MHz, Chloroform-*d*) δ 7.60 (d, $J$ = 15.9 Hz, 1H), 7.46 (d, $J$ = 9.0 Hz, 2H), 7.43 (d, $J$ = 11.9 Hz, 1H), 7.15 (d, $J$ = 2.0 Hz, 1H), 7.12 (dd, $J$ = 8.3, 1.9 Hz, 1H), 7.04 – 7.00 (m, 1H), 6.99 (d, $J$ = 5.6 Hz, 1H), 6.87 (d, $J$ = 8.3 Hz, 1H), 6.71 (d, $J$ = 8.7 Hz, 2H), 6.54 (d, $J$ = 15.9 Hz, 1H), 3.96 (s, 3H), 3.93 (s, 3H), 3.06 (s, 6H). **$^{13}$C NMR** (126 MHz, Chloroform-*d*) δ 167.1, 162.8, 152.1, 151.0, 149.5, 144.0, 143.1, 133.7, 130.8, 130.1, 129.5, 122.8, 122.8, 121.6, 112.1, 111.3, 109.3, 107.2, 56.2, 56.1, 40.3. **HRMS** (EI) m/z $[M]^+$ calcd for $C_{24}H_{25}N_2O_4$ 405.1809, found 405.18097.



**(*Z*)-2-((*E*)-4-(dimethylamino)styryl)-4-((*E*)-3-(4-bromophenyl)allylidene)-oxazol-5(4*H*)-one (SOD10).**
Compound **SOD10** was prepared in a similar manner as described for compound **SOD1** as a red solid. **$^{1}$H NMR** (400 MHz, Chloroform-*d*) $\delta$ 7.63 (d, $J$ = 15.5 Hz, 1H), 7.59 – 7.53 (m, 1H), 7.50 (t, $J$ = 9.1 Hz, 4H), 7.44 (d, $J$ = 8.3 Hz, 2H), 6.98 (d, $J$ = 10.3 Hz, 1H), 6.95 (d, $J$ = 6.4 Hz, 1H), 6.76 (d, $J$ = 8.3 Hz, 2H), 6.54 (d, $J$ = 15.9 Hz, 1H), 3.07 (s, 6H). **$^{13}$C NMR** (126 MHz, Chloroform-*d*) δ 166.8, 163.5, 152.2, 144.6, 140.9, 135.3, 132.6, 132.2, 130.3, 129.4, 129.2, 124.2, 123.8, 122.9, 112.2, 107.1, 40.4. **HRMS** (EI) m/z $[M]^+$ calcd for $C_{22}H_{19}O_2N_2Br$ 422.0624, found 422.0618.



**(*Z*)-2-((*E*)-4-(dimethylamino)styryl)-4-((1H-indol-2-yl)methylene)- oxazol-5(4*H*)-one (SOD11).**
Compound **SOD11** was prepared in a similar manner as described for compound **SOD1** as a black solid. **$^{1}$H NMR** (400 MHz, Chloroform-*d*) $\delta$ 10.51 (s, 1H), 7.65 (s, 1H), 7.62 (d, $J$ = 8.5 Hz, 1H), 7.53 – 7.48 (m, 2H), 7.46 (dd, $J$ = 8.3, 1.1 Hz, 1H), 7.30 (ddd, $J$ = 8.1, 6.9, 1.1 Hz, 1H), 7.15 (s, 1H), 7.12 (ddd, $J$ = 8.0, 7.0, 1.0 Hz, 1H), 6.95 (d, $J$ = 1.6 Hz, 1H), 6.71 (d, $J$ = 8.9 Hz, 2H), 6.60 (d, $J$ = 15.9 Hz, 1H), 3.07 (s, 6H). **$^{13}$C NMR** (126 MHz, Chloroform-*d*) δ 166.8, 163.0, 152.2, 144.4, 139.2, 134.2, 131.8, 130.3, 128.3, 125.7, 122.8, 122.1, 120.7, 118.3, 112.5, 112.2, 111.7, 107.1, 40.3 **HRMS** (ESI) m/z $[M + H]^+$ calcd for $C_{22}H_{20}N_3O_2$ 358.155, found 358.1553.



**(*Z*)-2-((*E*)-4-(dimethylamino)styryl)-4-(quinolin-2-ylmethylene)oxazol-5(4*H*)-one (SOD12).**
Compound **SOD12** was prepared in a similar manner as described for compound **SOD11** as a black solid. **$^{1}$H NMR** (400 MHz, Chloroform-*d*) $\delta$ 8.86 (d, $J$ = 8.6 Hz, 1H), 8.23 (d, $J$ = 8.7 Hz, 1H), 8.14 – 8.10 (m, 1H), 7.82 (s, 1H), 7.77 – 7.70 (m, 2H), 7.58 (s, 1H), 7.52 (d, $J$ = 8.8 Hz, 2H), 7.43 (s, 1H), 6.71 (d, $J$ = 8.9 Hz, 2H), 6.61 (d, $J$ = 15.8 Hz, 1H), 3.08 (s, 6H). **$^{13}$C NMR** (126 MHz, Chloroform-*d*) δ 167.4, 165.9, 153.9, 152.5, 148.7, 146.2, 137.9, 136.3, 130.7, 130.0, 130.0, 128.2, 127.8, 127.6, 123.8, 122.5, 112.1, 106.8, 40.2. **HRMS** (EI) m/z $[M]^+$ calcd for $C_{23}H_{19}O_2N_3$ 369.1472, found 369.1472.

**Synthesis procedure and the chemical characterization of SOD9-TPP (Fig. S8):**

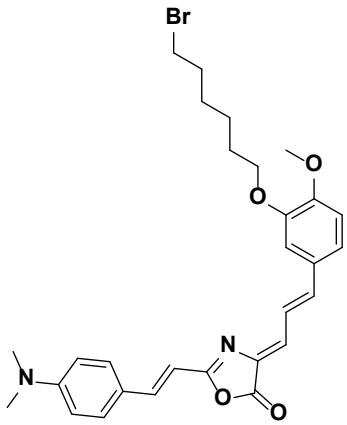
To a solution of Isovanillin (5.00 g, 32.86 mmol) and $K_2CO_3$ (9.08 g, 65.73 mmol) in 100 mL acetonitrile was added 1,6-dibromohexane (10.08 mL, 65.73 mmol). The mixture was refluxed at 80°C for 3 h. After this period, the mixture was concentrated under vacuum and dissolved in $CH_2Cl_2$. The organic layer was washed with water, brine, dried over anhydrous $Na_2SO_4$, and concentrated under vacuum. The residue was purified by silica gel column using 33% ethyl acetate in petroleum ether as eluent to afford compound **B**.

To a solution of ethyl (triphenylphosphoranylidene)acetate (7.18 g, 20.62 mmol) and trimethylamine (3.31 mL, 23.79 mmol) in 100 mL acetonitrile was added compound **B** (5.00 g, 15.86 mmol) portion-wise. The reaction was stirred at room temperature overnight. After the reaction was completed, the mixture was concentrated under vacuum and purified by silica gel column using 15% ethyl acetate in petroleum ether as eluent to afford compound **C** as a white solid.

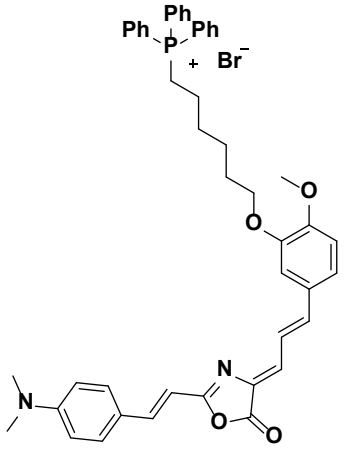
To a solution of $LiAlH_4$ (591.03 mg, 15.57 mmol) in 20 mL THF was added dropwise the solution of C (5.00 g, 12.98 mmol) in 30 mL THF at -20 °C. The resulting mixture was stirred at 0 °C for 1 hour. After the reaction was completed (monitored by TLC), the reaction was quenched by water and filtered through a Celite pad. The residue was concentrated under

vacuum and purified by silica gel column using 20% ethyl acetate in petroleum ether as eluent to afford compound **D**.

To a solution of **D** (3.17 g, 9.24 mmol) in 30 mL $CH_2Cl_2$ was added $MnO_2$ (8.03 g, 92.41 mmol). The reaction was stirred at room temperature overnight. The mixture was filtered through a Celite pad and concentrated under a vacuum. The residue was purified by silica gel column using 20% ethyl acetate in petroleum ether as eluent to afford compound **E**.



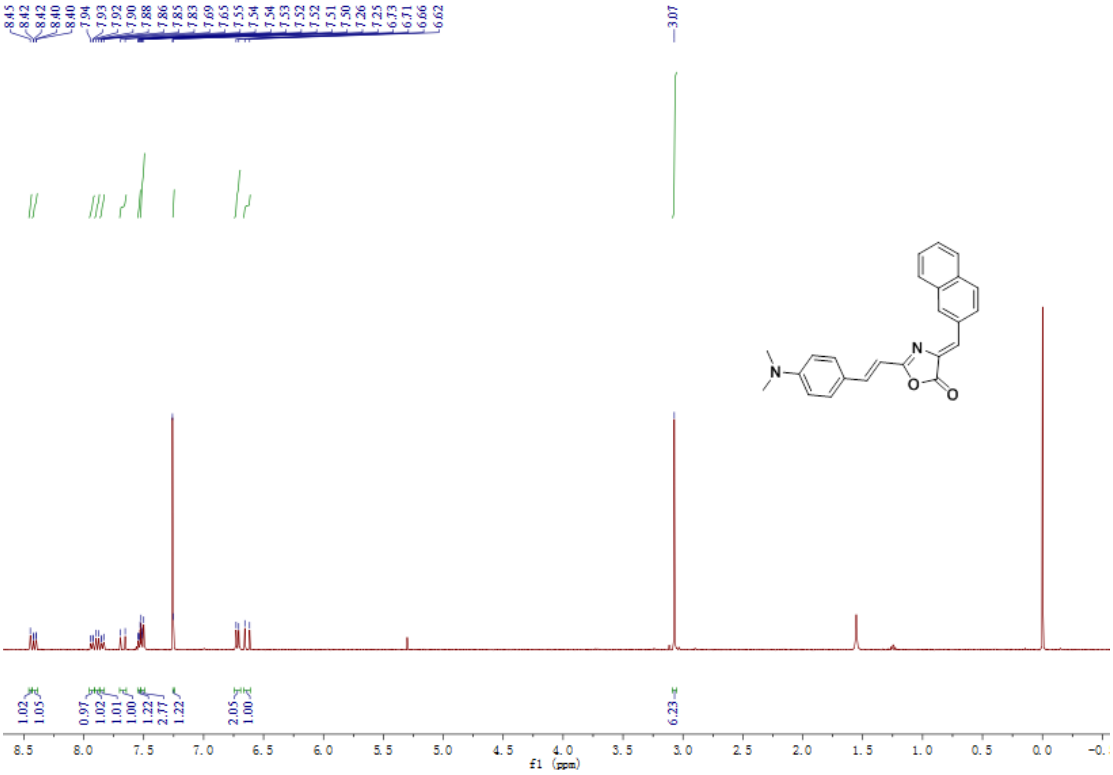

**(*Z*)-4-((*E*)-3-(3-((6-bromohexyl)oxy)-4-methoxyphenyl)allylidene)-2-((*E*)-4-(dimethylamino)styryl)oxazol-5(4*H*)-one (F).**
Compound **F**（**SOD9-Br**） was prepared in a similar manner as described for compound **SOD1**. **$^1$H NMR** (500 MHz, Chloroform-*d*) δ 7.59 (d, *J* = 15.9 Hz, 1H), 7.48-7.38 (m, 3H), 7.14 (d, *J* = 2.1 Hz, 1H), 7.10 (dd, *J* = 8.3, 1.9 Hz, 1H), 7.00 (d, *J* = 8.3 Hz, 1H), 6.97 (d, *J* = 4.4 Hz, 1H), 6.86 (d, *J* = 8.3 Hz, 1H), 6.70 (d, *J* = 8.4 Hz, 2H), 6.53 (d, *J* = 15.9 Hz, 1H), 4.07 (t, *J* = 6.7 Hz, 2H), 3.90 (s, 3H), 3.45 (t, *J* = 6.8 Hz, 2H), 3.05 (s, 6H), 1.96 – 1.87 (m, 4H), 1.58-1.50 (m, 4H). **$^{13}$C NMR** (126 MHz, Chloroform-*d*) δ 167.1, 162.8, 152.1, 151.4, 149.0, 144.0, 143.3, 133.6, 130.9, 130.2, 129.4, 122.9, 122.8, 121.5, 112.1, 111.6, 110.9, 107.2, 69.1, 56.2, 40.3, 33.9, 32.9, 29.2, 28.1, 25.4. **HRMS** (ESI) m/z $[M + H]^+$ calcd for $C_{29}H_{34}BrN_2O_4$ 553.1696, found 553.1698.

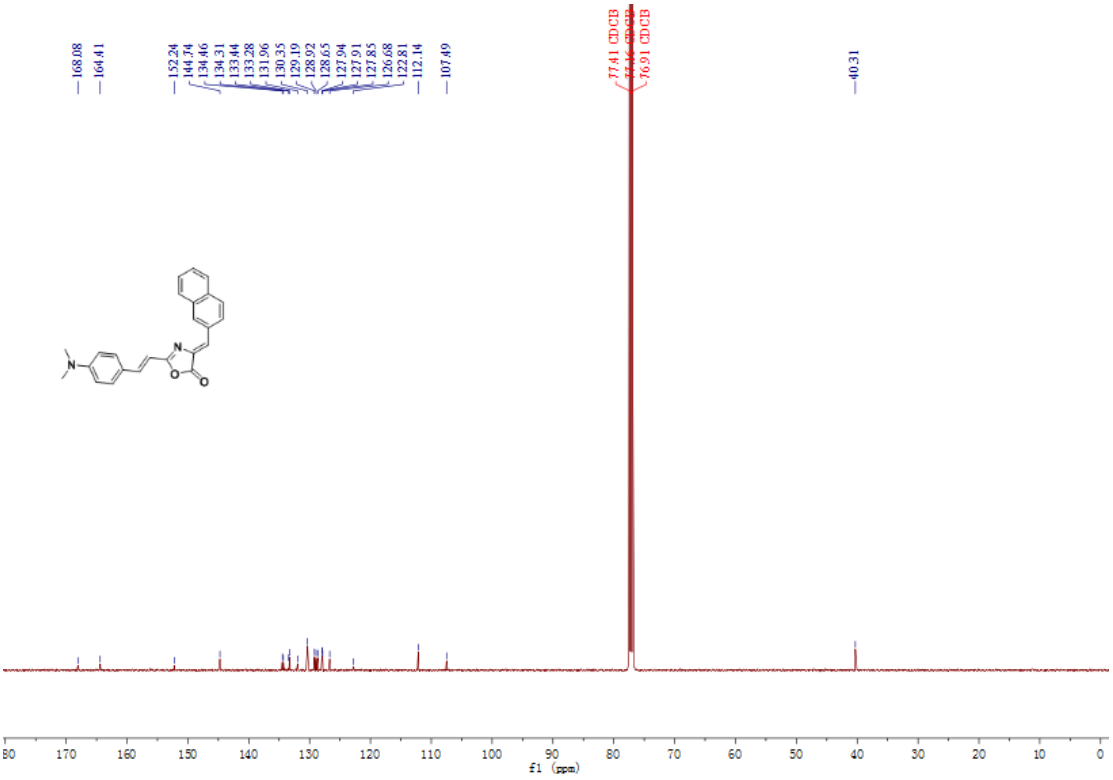



**(6-(5-((1*E*,3*Z*)-3-(2-((*E*)-4-(dimethylamino)styryl)-5-oxooxazol-4(5*H*)-ylidene)prop-1-en-1-yl)-2-methoxyphenoxy)hexyl)triphenylphosphonium bromide(SOD9-TPP).**
(*Z*)-4-((*E*)-3-(3-((6-bromohexyl)oxy)-4-methoxyphenyl)allylidene)-2-((*E*)-4-(dimethylamino)styryl)oxazol-5(4*H*)-one was prepared in a similar manner as described for compound **SOD1** as a black solid. Then the black solid was dissolved in toluene and stirred with triphenylphosphine for 12h. After the reaction completed, the solvent was removed and the residue was purified by thin layer chromatography using dichloromethane/methanol (20:1) as an eluent to afford the title compound as a black solid.**$^1$H NMR** (400 MHz, Methanol-$d_4$) δ 7.90 – 7.71 (m, 15H), 7.60 (d, *J* = 15.9 Hz, 1H), 7.53 – 7.42 (m, 3H), 7.24 – 7.06 (m, 3H), 7.04 – 6.91 (m, 2H), 6.77 – 6.71 (m, 2H), 6.49 (d, *J* = 15.9 Hz, 1H), 4.05 (t, *J* = 6.2 Hz, 2H), 3.82 (s, 3H), 3.49 – 3.35 (m, 2H), 3.05 (s, 6H), 1.85 – 1.51 (m, 8H). **HRMS** (ESI) m/z $[M]^+$ calcd for $C_{47}H_{48}N_2O_4P$ 735.3346, found 735.3333.

## NMR and MS spectrum data

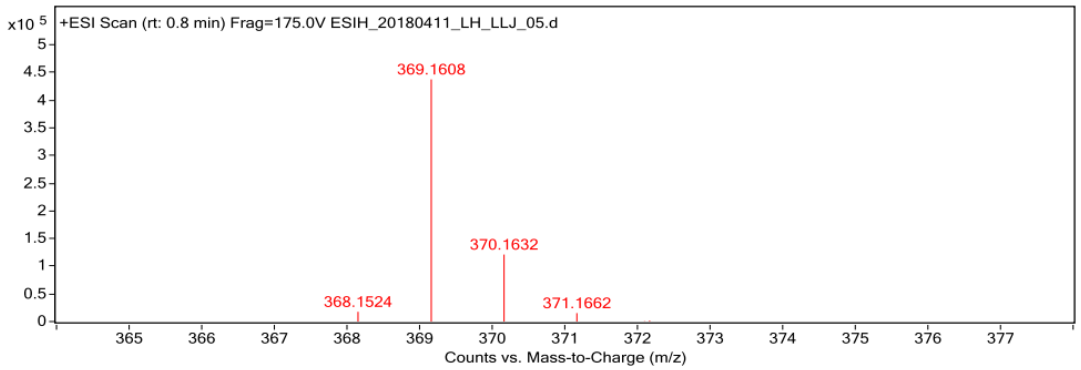
**(*Z*)-2-((*E*)-4-(dimethylamino)styryl)-4-(naphthalen-2-ylmethylene)oxazol-5(4*H*)-one (SOD1)**



**User Spectra**

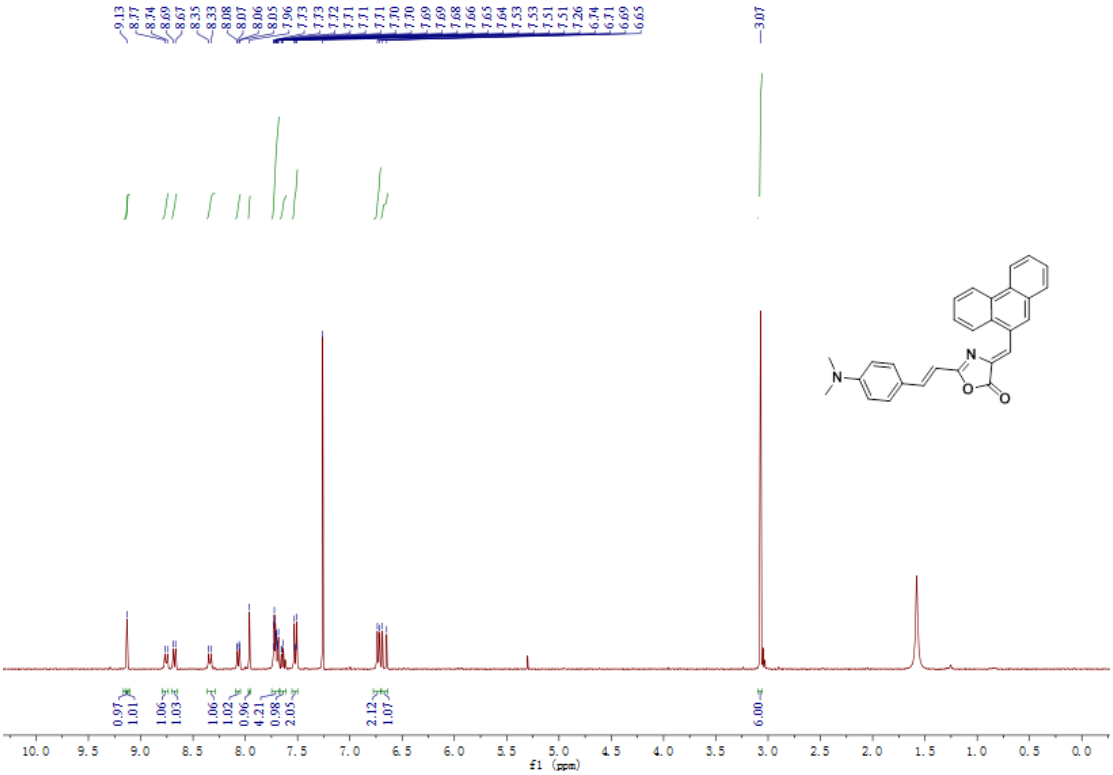
| Fragmentor Voltage | Collision Energy | Ionization Mode |
|---|---|---|
| 175 | 0 | ESI |

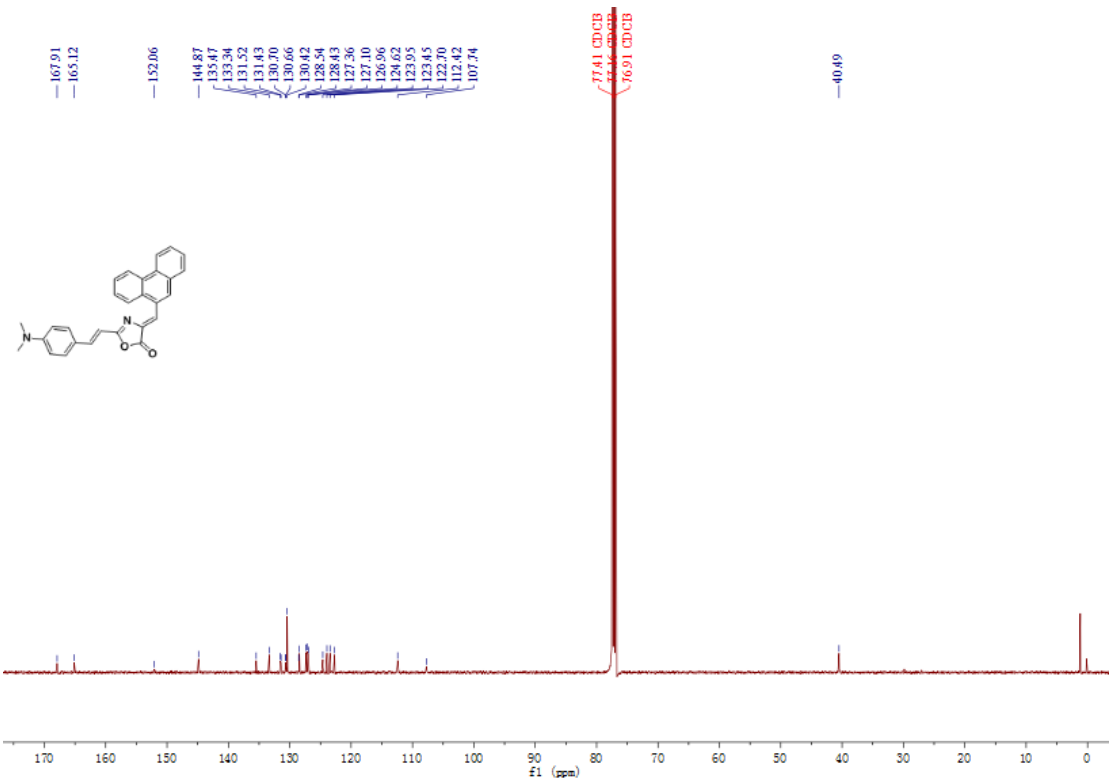



**Formula Calculator Results**

| m/z | Calc m/z | Diff (mDa) | Diff (ppm) | Ion Formula | Ion |
|---|---|---|---|---|---|
| 369.1608 | 369.1598 | -1.06 | -2.86 | C24 H21 N2 O2 | (M+H)+ |

**(*Z*)-2-((*E*)-4-(dimethylamino)styryl)-4-(phenanthren-9-ylmethylene)oxazol-5(4*H*)-one (SOD2)**

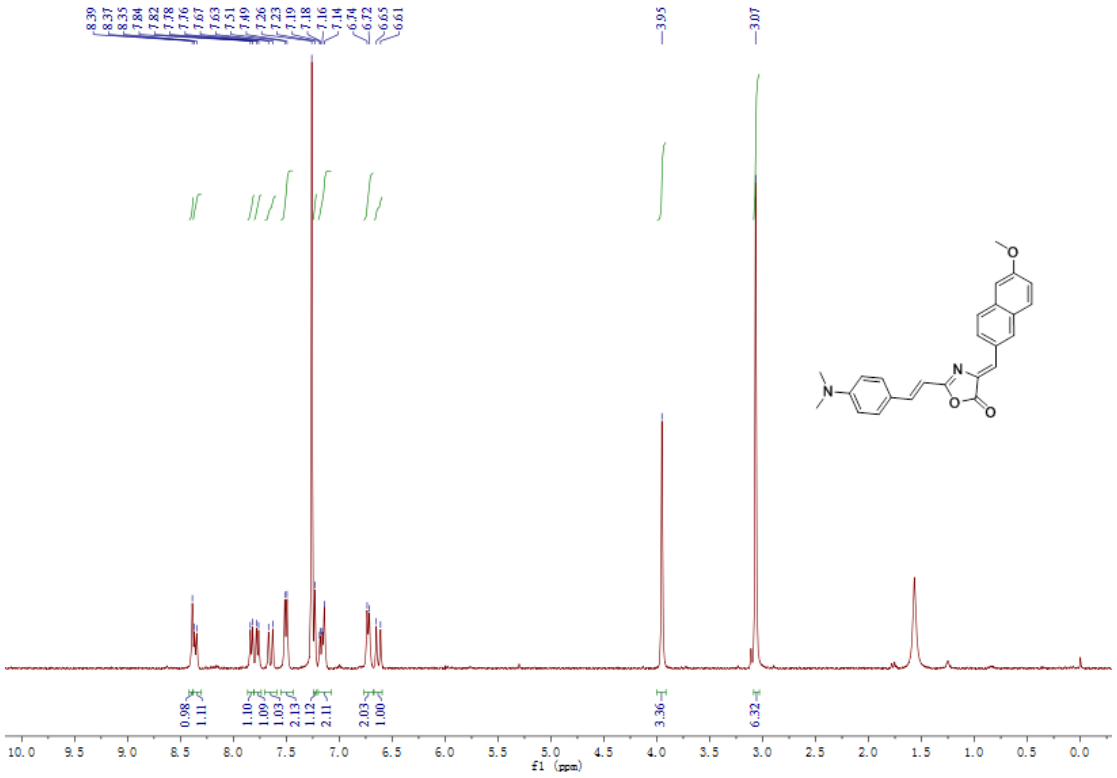


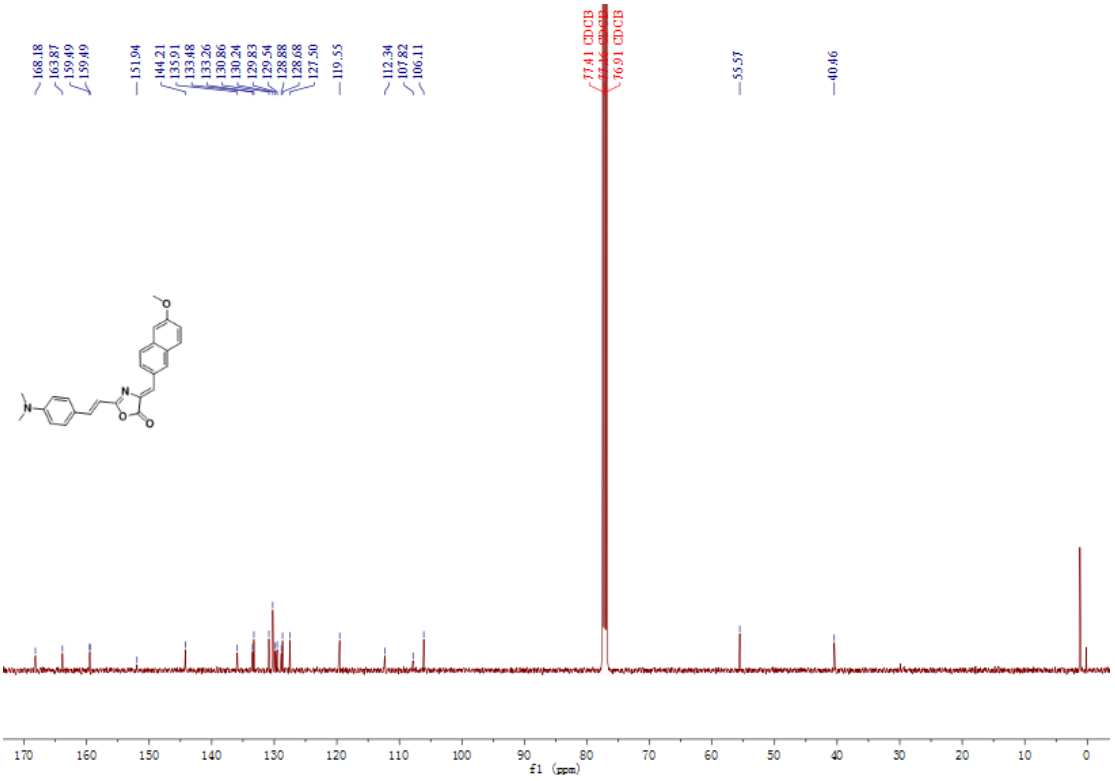



T: + c EI Full ms [ 49.50-800.50]
m/z= 48-803

| m/z | Intensity | Relative | Theo. Mass | Delta (mmu) | RDB equiv. | Composition |
|---|---|---|---|---|---|---|
| 51.0227 | 657629.0 | 1.53 | 51.0229 | -0.18 | 3.5 | $C_4H_3$ |
| 77.0159 | 1562204.0 | 3.63 | 77.0134 | 2.48 | 5.5 | $C_4H_1N_2$ |
| 91.0504 | 461415.0 | 1.07 | 91.0502 | 0.20 | 0.5 | $C_2H_7O_2N_2$ |
| 101.0388 | 579640.0 | 1.35 | 101.0386 | 0.19 | 6.5 | $C_8H_5$ |
| 102.0464 | 1025248.0 | 2.38 | 102.0464 | 0.01 | 6.0 | $C_8H_6$ |
| 103.0543 | 1851834.0 | 4.31 | 103.0542 | 0.06 | 5.5 | $C_8H_7$ |
| 115.0543 | 520544.0 | 1.21 | 115.0542 | 0.04 | 6.5 | $C_9H_7$ |
| 116.0492 | 703367.0 | 1.64 | 116.0495 | -0.25 | 6.5 | $C_8H_6N_1$ |
| 118.0654 | 334889.0 | 0.78 | 118.0651 | 0.30 | 5.5 | $C_8H_8N_1$ |
| 119.0726 | 356709.0 | 0.83 | 119.0730 | -0.37 | 5.0 | $C_8H_9N_1$ |
| 128.0490 | 479450.0 | 1.11 | 128.0495 | -0.43 | 7.5 | $C_9H_6N_1$ |
| 129.0561 | 367714.0 | 0.86 | 129.0573 | -1.24 | 7.0 | $C_9H_7N_1$ |
| 130.0650 | 2545723.0 | 5.92 | 130.0651 | -0.14 | 6.5 | $C_9H_8N_1$ |
| 131.0727 | 2850142.0 | 6.63 | 131.0730 | -0.26 | 6.0 | $C_9H_9N_1$ |
| 132.0781 | 449902.0 | 1.05 | 132.0781 | -0.04 | 1.0 | $C_6H_{12}O_3$ |
| 134.0968 | 1238033.0 | 2.88 | 134.0964 | 0.40 | 4.5 | $C_9H_{12}N_1$ |
| 144.0811 | 2222347.0 | 5.17 | 144.0808 | 0.36 | 6.5 | $C_{10}H_{10}N_1$ |
| 145.0884 | 1426804.0 | 3.32 | 145.0886 | -0.21 | 6.0 | $C_{10}H_{11}N_1$ |
| 146.0962 | 9949440.0 | 23.14 | 146.0964 | -0.27 | 5.5 | $C_{10}H_{12}N_1$ |
| 147.1001 | 1230304.0 | 2.86 | 147.1016 | -1.50 | 0.5 | $C_7H_{15}O_3$ |
| 158.0593 | 393541.0 | 0.92 | 158.0600 | -0.72 | 7.5 | $C_{10}H_8O_1N_1$ |
| 158.0962 | 464755.0 | 1.08 | 158.0964 | -0.23 | 6.5 | $C_{11}H_{12}N_1$ |
| 160.0744 | 839181.0 | 1.95 | 160.0757 | -1.33 | 6.5 | $C_{10}H_{10}O_1N_1$ |
| 165.0692 | 362752.0 | 0.84 | 165.0699 | -0.68 | 9.5 | $C_{13}H_9$ |
| 171.0919 | 807470.0 | 1.88 | 171.0917 | 0.19 | 7.5 | $C_{11}H_{11}N_2$ |
| 172.0994 | 550633.0 | 1.28 | 172.0995 | -0.06 | 7.0 | $C_{11}H_{12}N_2$ |
| 174.0919 | 43004672.0 | 100.00 | 174.0913 | 0.56 | 6.5 | $C_{11}H_{12}O_1N_1$ |
| 176.0617 | 342014.0 | 0.80 | 176.0621 | -0.35 | 11.0 | $C_{14}H_8$ |
| 187.0532 | 375474.0 | 0.87 | 187.0542 | -1.03 | 12.5 | $C_{15}H_7$ |
| 188.0938 | 1152124.0 | 2.68 | 188.0944 | -0.64 | 7.0 | $C_{11}H_{12}O_1N_2$ |
| 189.0701 | 986158.0 | 2.29 | 189.0699 | 0.20 | 11.5 | $C_{15}H_9$ |
| 190.0669 | 698246.0 | 1.62 | 190.0651 | 1.79 | 11.5 | $C_{14}H_8N_1$ |
| 191.0861 | 353464.0 | 0.82 | 191.0855 | 0.61 | 10.5 | $C_{15}H_{11}$ |
| 200.0620 | 353369.0 | 0.82 | 200.0621 | -0.09 | 13.0 | $C_{16}H_8$ |
| 202.0770 | 671688.0 | 1.56 | 202.0777 | -0.69 | 12.0 | $C_{16}H_{10}$ |
| 214.0642 | 519844.0 | 1.21 | 214.0651 | -0.91 | 13.5 | $C_{16}H_8N_1$ |
| 215.0711 | 324584.0 | 0.75 | 215.0703 | 0.80 | 8.5 | $C_{13}H_{11}O_3$ |
| 216.0797 | 1206354.0 | 2.81 | 216.0808 | -1.08 | 12.5 | $C_{16}H_{10}N_1$ |
| 217.0873 | 913067.0 | 2.12 | 217.0886 | -1.30 | 12.0 | $C_{16}H_{11}N_1$ |
| 229.0973 | 447325.0 | 1.04 | 229.0972 | 0.19 | 8.5 | $C_{13}H_{13}O_2N_2$ |
| 373.1645 | 425601.0 | 0.99 | 373.1672 | -2.78 | 14.0 | $C_{24}H_{23}O_3N_1$ |
| 376.1910 | 490518.0 | 1.14 | 376.1907 | 0.28 | 12.5 | $C_{24}H_{26}O_3N_1$ |
| 417.1594 | 753462.0 | 1.75 | 417.1598 | -0.33 | 19.5 | $C_{28}H_{21}O_2N_2$ |
| 418.1668 | 11111680.0 | 25.84 | 418.1676 | -0.74 | 19.0 | $C_{28}H_{22}O_2N_2$ |

**(*Z*)-2-((*E*)-4-(dimethylamino)styryl)-4-((6-methoxynaphthalen-2-yl)methylene)oxazol-5(4*H*)-one (SOD3)**

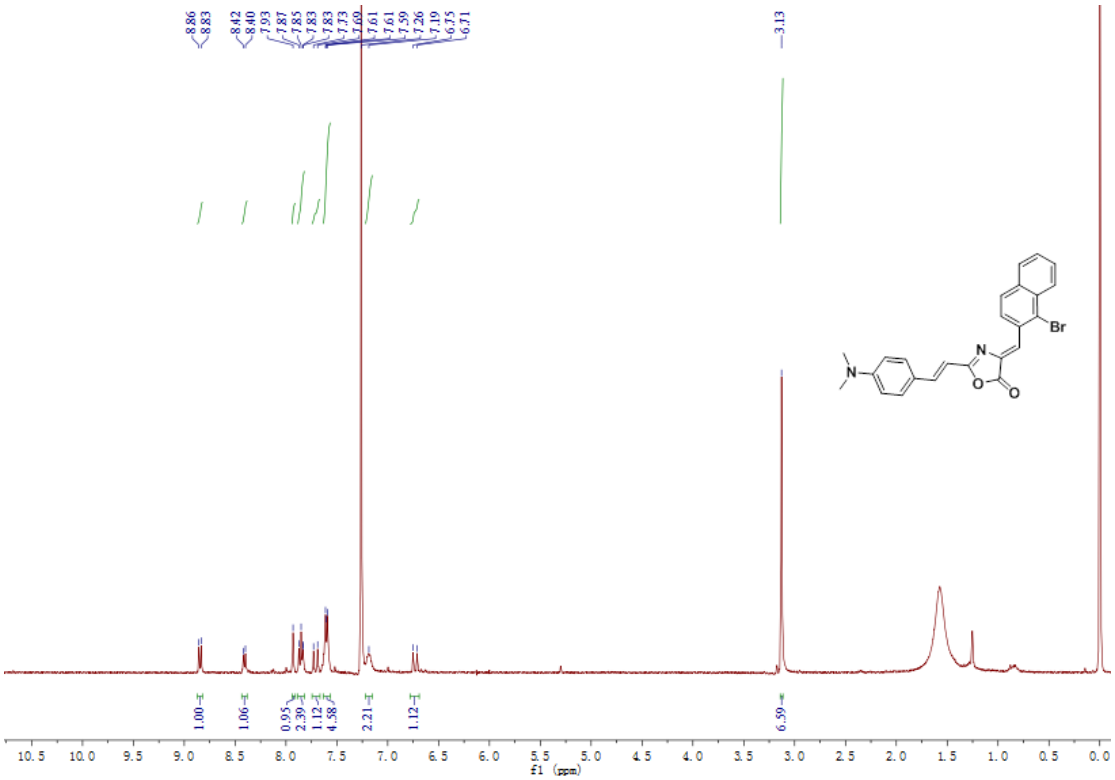


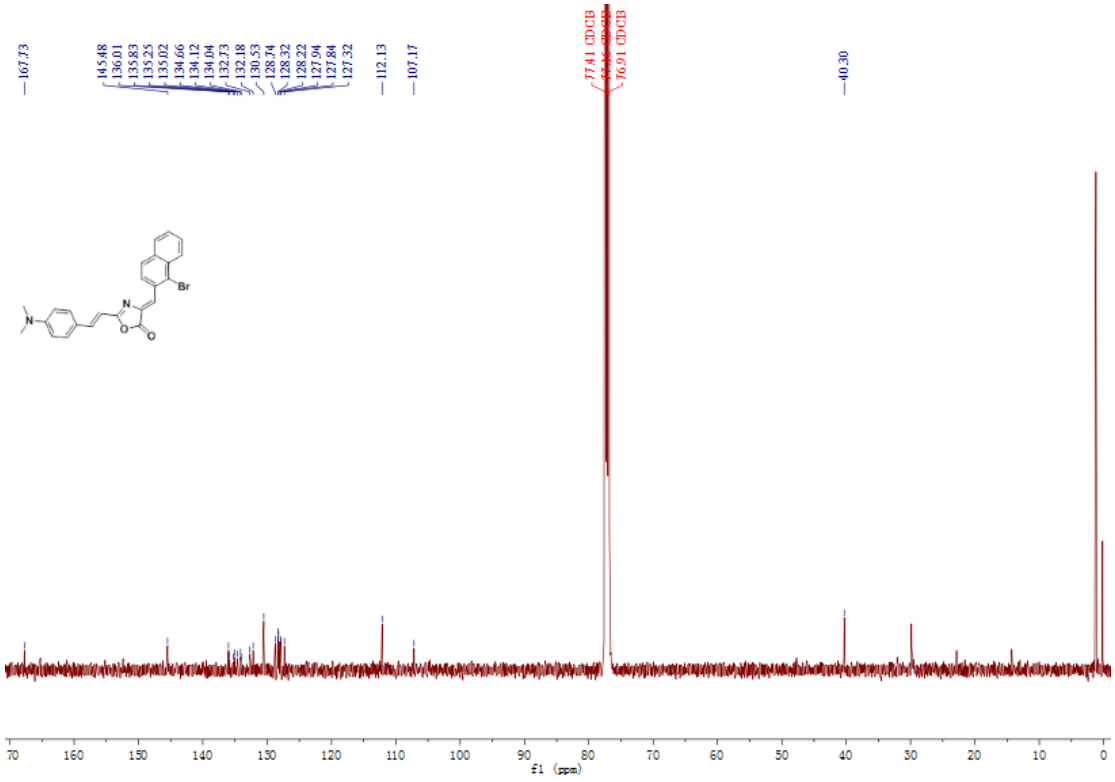



T: + c EI Full ms [ 49.50-800.50]
m/z= 48-803

| m/z | Intensity | Relative | Theo. Mass | Delta (mmu) | RDB equiv. | Composition |
|---|---|---|---|---|---|---|
| 51.0087 | 532121.0 | 2.41 | 51.0077 | 1.07 | -0.5 | $H_3O_3$ |
| 55.0515 | 399775.0 | 1.81 | 55.0542 | -2.75 | 1.5 | $C_4H_7$ |
| 56.0600 | 211258.0 | 0.96 | 56.0621 | -2.01 | 1.0 | $C_4H_8$ |
| 57.0684 | 473693.0 | 2.15 | 57.0699 | -1.45 | 0.5 | $C_4H_9$ |
| 60.0202 | 326970.0 | 1.48 | 60.0206 | -0.40 | 1.0 | $C_2H_4O_2$ |
| 63.0229 | 430054.0 | 1.95 | 63.0229 | 0.00 | 4.5 | $C_5H_3$ |
| 65.0385 | 192683.0 | 0.87 | 65.0386 | -0.05 | 3.5 | $C_5H_5$ |
| 69.0702 | 278051.0 | 1.26 | 69.0699 | 0.28 | 1.5 | $C_5H_9$ |
| 71.0845 | 175635.0 | 0.80 | 71.0855 | -1.02 | 0.5 | $C_5H_{11}$ |
| 73.0278 | 259572.0 | 1.18 | 73.0284 | -0.59 | 1.5 | $C_3H_5O_2$ |
| 74.0141 | 256582.0 | 1.16 | 74.0151 | -1.00 | 6.0 | $C_6H_2$ |
| 75.0218 | 324934.0 | 1.47 | 75.0229 | -1.14 | 5.5 | $C_6H_3$ |
| 76.0300 | 322708.0 | 1.46 | 76.0308 | -0.75 | 5.0 | $C_6H_4$ |
| 77.0377 | 1079351.0 | 4.90 | 77.0386 | -0.86 | 4.5 | $C_6H_5$ |
| 79.0538 | 199330.0 | 0.90 | 79.0542 | -0.44 | 3.5 | $C_6H_7$ |
| 87.0445 | 182727.0 | 0.83 | 87.0441 | 0.40 | 1.5 | $C_4H_7O_2$ |
| 89.0386 | 403210.0 | 1.83 | 89.0386 | 0.05 | 5.5 | $C_7H_5$ |
| 91.0542 | 303624.0 | 1.38 | 91.0542 | -0.07 | 4.5 | $C_7H_7$ |
| 101.0390 | 299998.0 | 1.36 | 101.0386 | 0.44 | 6.5 | $C_8H_5$ |
| 102.0467 | 662432.0 | 3.00 | 102.0464 | 0.35 | 6.0 | $C_8H_6$ |
| 103.0547 | 1136952.0 | 5.16 | 103.0542 | 0.42 | 5.5 | $C_8H_7$ |
| 115.0547 | 426015.0 | 1.93 | 115.0542 | 0.49 | 6.5 | $C_9H_7$ |
| 116.0503 | 387275.0 | 1.76 | 116.0495 | 0.84 | 6.5 | $C_8H_6N_1$ |
| 126.0461 | 346658.0 | 1.57 | 126.0464 | -0.34 | 8.0 | $C_{10}H_6$ |
| 127.0538 | 223790.0 | 1.02 | 127.0542 | -0.47 | 7.5 | $C_{10}H_7$ |
| 128.0500 | 264597.0 | 1.20 | 128.0495 | 0.53 | 7.5 | $C_9H_6N_1$ |
| 129.0565 | 233999.0 | 1.06 | 129.0573 | -0.85 | 7.0 | $C_9H_7N_1$ |
| 130.0652 | 1502567.0 | 6.82 | 130.0651 | 0.03 | 6.5 | $C_9H_8N_1$ |
| 131.0728 | 1571301.0 | 7.13 | 131.0730 | -0.16 | 6.0 | $C_9H_9N_1$ |
| 132.0792 | 265870.0 | 1.21 | 132.0781 | 1.07 | 1.0 | $C_6H_{12}O_3$ |
| 134.0967 | 305914.0 | 1.39 | 134.0964 | 0.23 | 4.5 | $C_9H_{12}N_1$ |
| 139.0542 | 216983.0 | 0.98 | 139.0542 | -0.02 | 8.5 | $C_{11}H_7$ |
| 144.0811 | 1235139.0 | 5.60 | 144.0808 | 0.28 | 6.5 | $C_{10}H_{10}N_1$ |
| 145.0880 | 733042.0 | 3.33 | 145.0886 | -0.62 | 6.0 | $C_{10}H_{11}N_1$ |
| 146.0962 | 5376846.0 | 24.39 | 146.0964 | -0.22 | 5.5 | $C_{10}H_{12}N_1$ |
| 147.0996 | 628113.0 | 2.85 | 147.1016 | -1.97 | 0.5 | $C_7H_{15}O_3$ |
| 149.0233 | 1054446.0 | 4.78 | 149.0233 | 0.02 | 6.5 | $C_8H_5O_3$ |
| 153.0573 | 798818.0 | 3.62 | 153.0573 | -0.05 | 9.0 | $C_{11}H_7N_1$ |
| 154.0636 | 223058.0 | 1.01 | 154.0624 | 1.18 | 4.0 | $C_8H_{10}O_3$ |
| 158.0593 | 196150.0 | 0.89 | 158.0600 | -0.76 | 7.5 | $C_{10}H_8O_1N_1$ |
| 158.0956 | 402001.0 | 1.82 | 158.0964 | -0.88 | 6.5 | $C_{11}H_{12}N_1$ |
| 160.0746 | 585206.0 | 2.65 | 160.0757 | -1.14 | 6.5 | $C_{10}H_{10}O_1N_1$ |
| 171.0914 | 370544.0 | 1.68 | 171.0917 | -0.31 | 7.5 | $C_{11}H_{11}N_2$ |
| 172.0988 | 236830.0 | 1.07 | 172.0995 | -0.67 | 7.0 | $C_{11}H_{12}N_2$ |
| 174.0913 | 22044672.0 | 100.00 | 174.0913 | -0.08 | 6.5 | $C_{11}H_{12}O_1N_1$ |
| 196.0757 | 472420.0 | 2.14 | 196.0757 | -0.03 | 9.5 | $C_{13}H_{10}O_1N_1$ |
| 197.0818 | 212657.0 | 0.96 | 197.0835 | -1.76 | 9.0 | $C_{13}H_{11}O_1N_1$ |
| 398.1629 | 5496406.0 | 24.93 | 398.1625 | 0.41 | 16.0 | $C_{25}H_{22}O_3N_2$ |

**(*Z*)-2-((*E*)-4-(dimethylamino)styryl)4-((1-bromonaphthalen-2-yl)methylene)-oxazol-5(4*H*)-one (SOD4)**

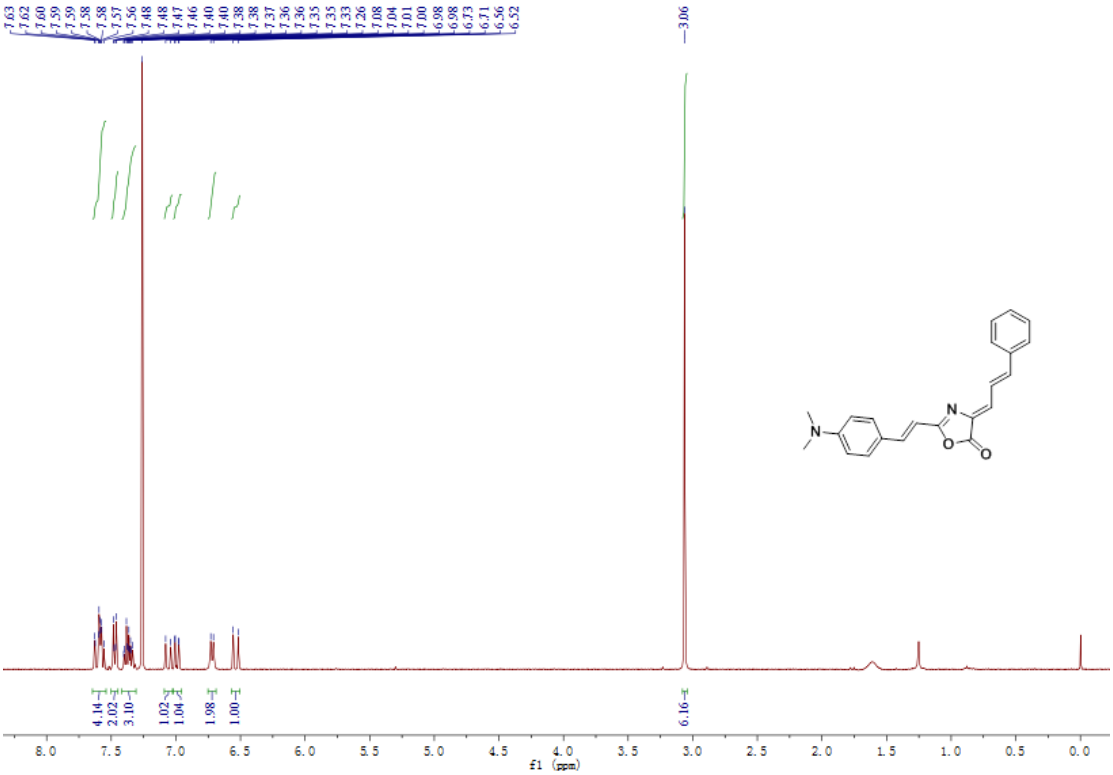


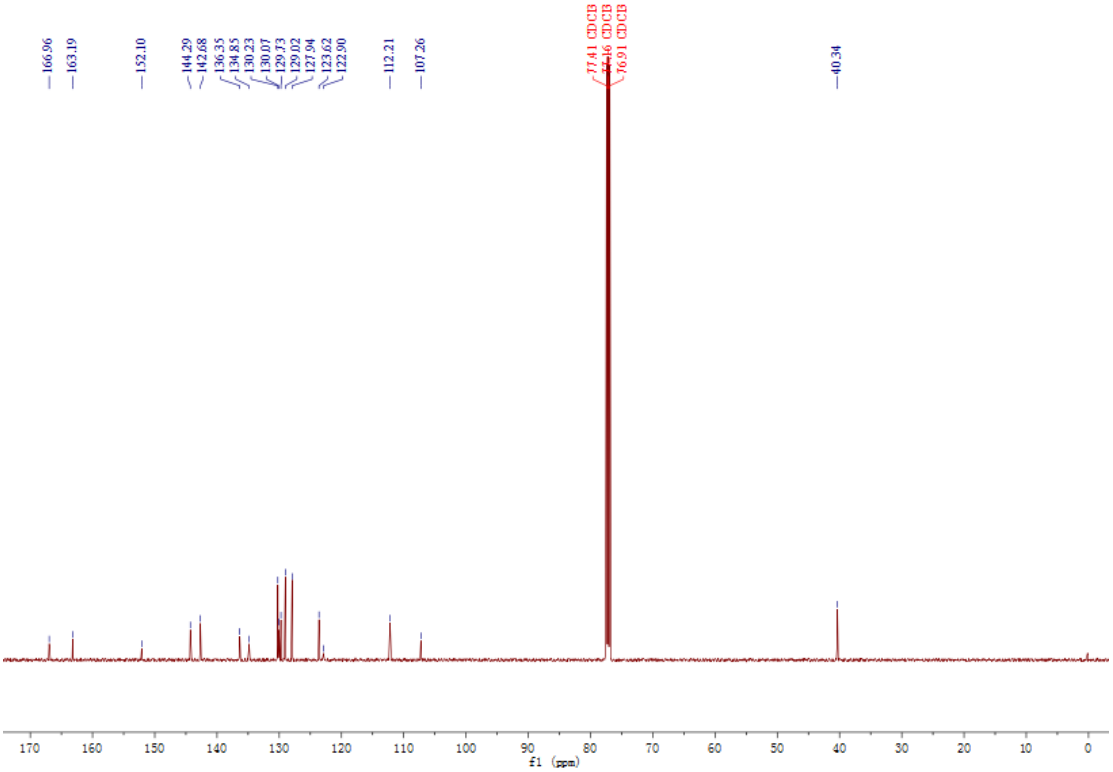



T: + c EI Full ms [ 49.50-800.50]
m/z= 48-803

| m/z | Intensity | Relative | Theo. Mass | Delta (mmu) | RDB equiv. | Composition |
|---|---|---|---|---|---|---|
| 51.0090 | 718475.0 | 0.92 | 51.0104 | -1.32 | 4.0 | $C_3H_1N_1$ |
| 60.0656 | 489501.0 | 0.62 | 60.0682 | -2.64 | 0.0 | $C_2H_8N_2$ |
| 63.0581 | 717203.0 | 0.91 | 63.0553 | 2.83 | -0.5 | $C_1H_7O_1N_2$ |
| 101.0388 | 648724.0 | 0.83 | 101.0386 | 0.20 | 6.5 | $C_8H_5$ |
| 102.0467 | 1479317.0 | 1.89 | 102.0464 | 0.32 | 6.0 | $C_8H_6$ |
| 103.0550 | 2575239.0 | 3.29 | 103.0542 | 0.77 | 5.5 | $C_8H_7$ |
| 105.0588 | 531740.0 | 0.68 | 105.0573 | 1.49 | 5.0 | $C_7H_7N_1$ |
| 115.0551 | 929066.0 | 1.19 | 115.0542 | 0.86 | 6.5 | $C_9H_7$ |
| 116.0503 | 954415.0 | 1.22 | 116.0495 | 0.82 | 6.5 | $C_8H_6N_1$ |
| 119.0728 | 663100.0 | 0.85 | 119.0730 | -0.15 | 5.0 | $C_8H_9N_1$ |
| 128.0491 | 644016.0 | 0.82 | 128.0495 | -0.35 | 7.5 | $C_9H_6N_1$ |
| 129.0567 | 654830.0 | 0.84 | 129.0573 | -0.62 | 7.0 | $C_9H_7N_1$ |
| 130.0654 | 3680354.0 | 4.70 | 130.0651 | 0.27 | 6.5 | $C_9H_8N_1$ |
| 131.0726 | 4372621.0 | 5.58 | 131.0730 | -0.37 | 6.0 | $C_9H_9N_1$ |
| 134.0968 | 782279.0 | 1.00 | 134.0964 | 0.41 | 4.5 | $C_9H_{12}N_1$ |
| 138.0461 | 918029.0 | 1.17 | 138.0464 | -0.26 | 9.0 | $C_{11}H_6$ |
| 139.0539 | 1053015.0 | 1.34 | 139.0542 | -0.35 | 8.5 | $C_{11}H_7$ |
| 144.0816 | 4056402.0 | 5.17 | 144.0808 | 0.83 | 6.5 | $C_{10}H_{10}N_1$ |
| 145.0883 | 2679628.0 | 3.42 | 145.0886 | -0.30 | 6.0 | $C_{10}H_{11}N_1$ |
| 146.0965 | 17638144.0 | 22.50 | 146.0964 | 0.08 | 5.5 | $C_{10}H_{12}N_1$ |
| 149.0237 | 2287010.0 | 2.92 | 149.0260 | -2.31 | 11.0 | $C_{11}H_3N_1$ |
| 158.0964 | 2048207.0 | 2.61 | 158.0964 | -0.04 | 6.5 | $C_{11}H_{12}N_1$ |
| 160.0748 | 813417.0 | 1.04 | 160.0757 | -0.92 | 6.5 | $C_{10}H_{10}O_1N_1$ |
| 164.0493 | 1951420.0 | 2.49 | 164.0495 | -0.17 | 10.5 | $C_{12}H_6N_1$ |
| 165.0569 | 1650181.0 | 2.11 | 165.0573 | -0.40 | 10.0 | $C_{12}H_7N_1$ |
| 166.0643 | 893824.0 | 1.14 | 166.0651 | -0.81 | 9.5 | $C_{12}H_8N_1$ |
| 171.0917 | 1181481.0 | 1.51 | 171.0917 | 0.02 | 7.5 | $C_{11}H_{11}N_2$ |
| 172.0986 | 695765.0 | 0.89 | 172.0995 | -0.87 | 7.0 | $C_{11}H_{12}N_2$ |
| 174.0912 | 78385152.0 | 100.00 | 174.0913 | -0.11 | 6.5 | $C_{11}H_{12}O_1N_1$ |
| 176.0973 | 577255.0 | 0.74 | 176.0944 | 2.84 | 6.0 | $C_{10}H_{12}O_1N_2$ |
| 183.0676 | 1419934.0 | 1.81 | 183.0679 | -0.26 | 9.0 | $C_{12}H_9O_1N_1$ |
| 184.0731 | 1730747.0 | 2.21 | 184.0757 | -2.64 | 8.5 | $C_{12}H_{10}O_1N_1$ |
| 229.0971 | 856610.0 | 1.09 | 229.0972 | -0.09 | 8.5 | $C_{13}H_{13}O_2N_2$ |
| 339.1485 | 1558419.0 | 1.99 | 339.1492 | -0.68 | 15.5 | $C_{23}H_{19}O_1N_2$ |
| 367.1429 | 36165120.0 | 46.14 | 367.1441 | -1.18 | 16.5 | $C_{24}H_{19}O_2N_2$ |
| 368.1459 | 10220800.0 | 13.04 | 368.1458 | 0.08 | 5.0 | $C_{18}H_{29}O_1N_2{}^{79}Br_1$ |
| 446.0631 | 9491456.0 | 12.11 | 446.0624 | 0.67 | 16.0 | $C_{24}H_{19}O_2N_2{}^{79}Br_1$ |

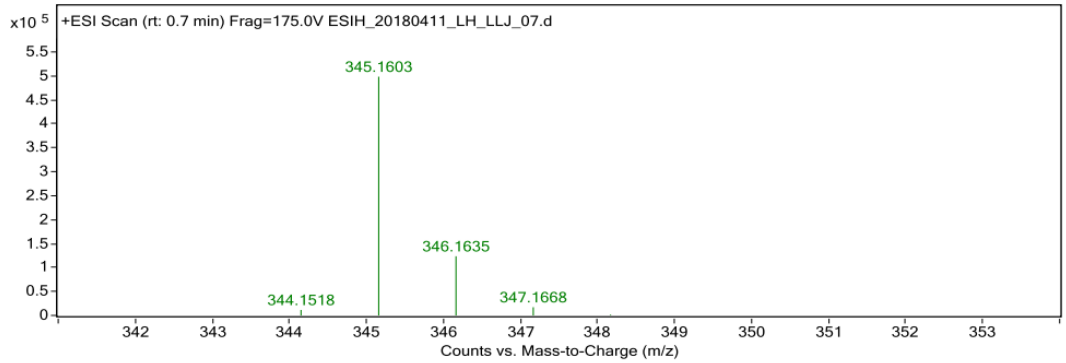
**(*Z*)-2-((*E*)-4-(dimethylamino)styryl)-4-((*E*)-3-phenylallylidene)oxazol-5(4*H*)-one (SOD5)**



**User Spectra**

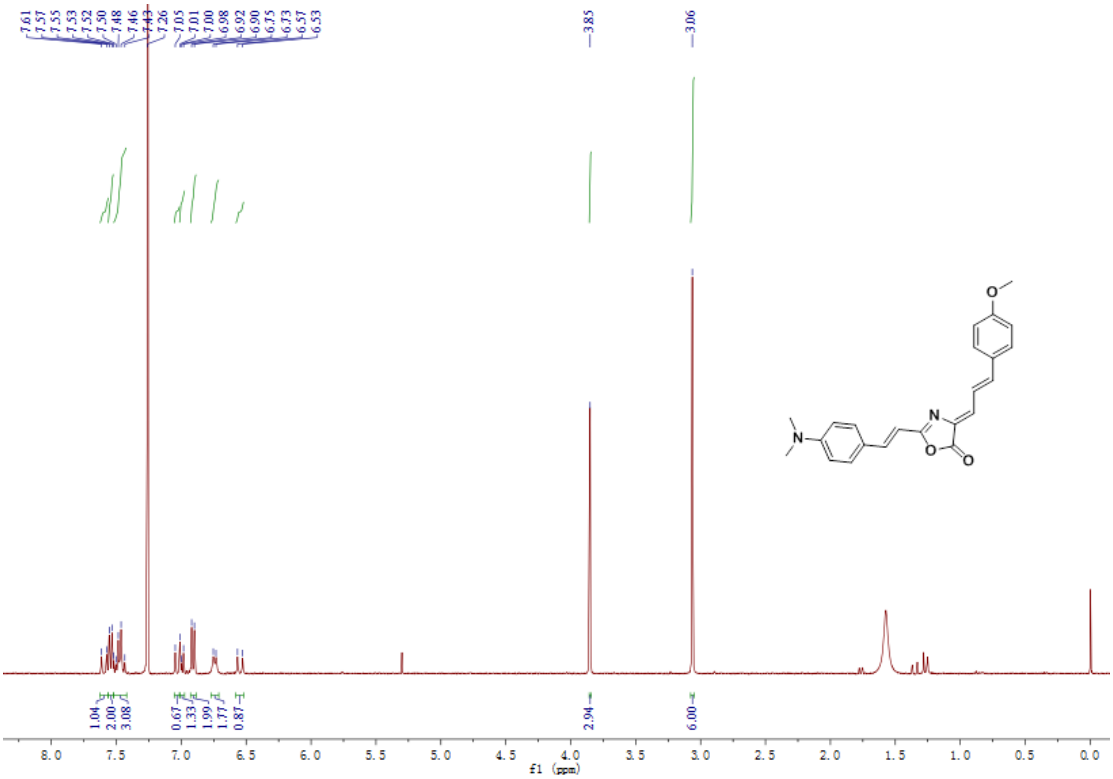
| Fragmentor Voltage | Collision Energy | Ionization Mode |
|---|---|---|
| 175 | 0 | ESI |

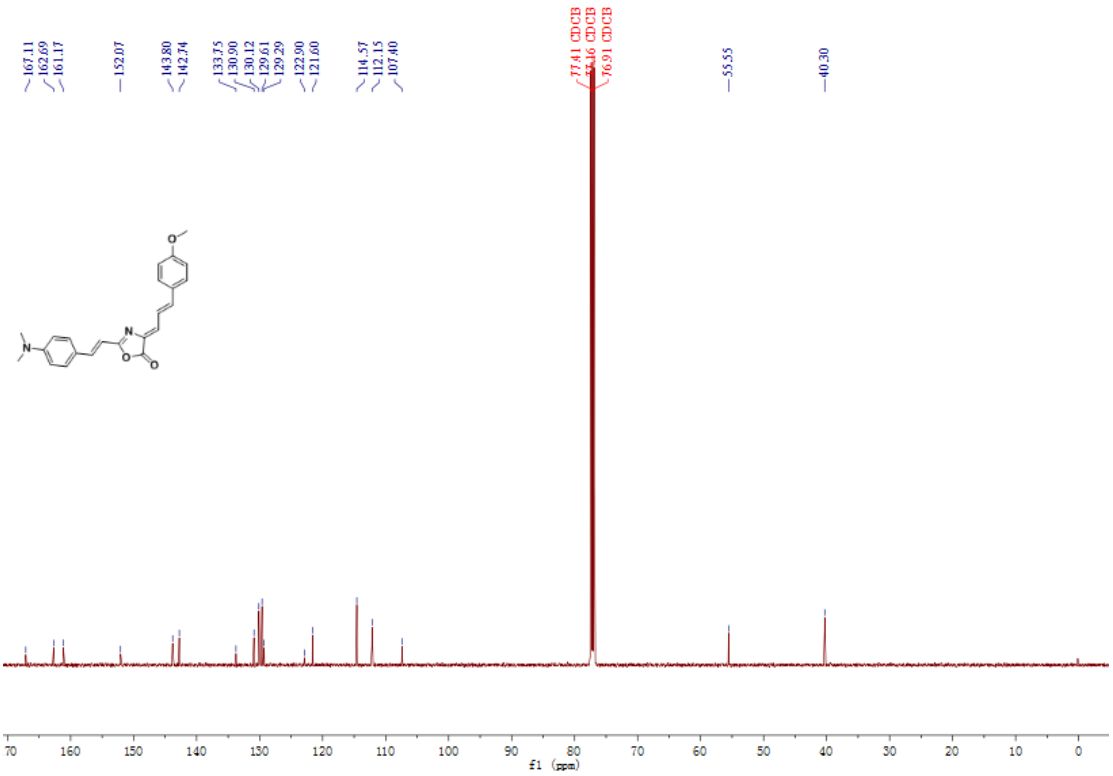



**Formula Calculator Results**

| m/z | Calc m/z | Diff (mDa) | Diff (ppm) | Ion Formula | Ion |
|---|---|---|---|---|---|
| 345.1603 | 345.1598 | -0.53 | -1.55 | C22 H21 N2 O2 | (M+H)+ |

**(*Z*)-2-((*E*)-4-(dimethylamino)styryl)-4-((*E*)-3-(4-methoxyphenyl)allylidene)oxazol-5(4*H*)-one (SOD6)**

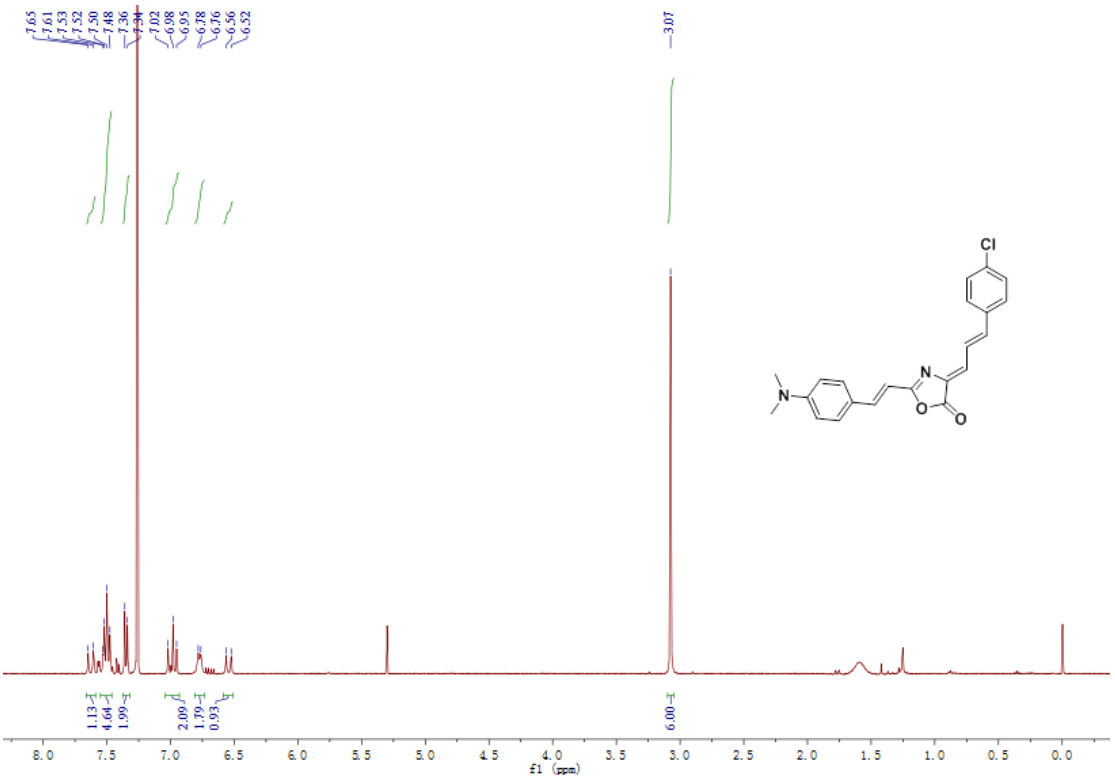


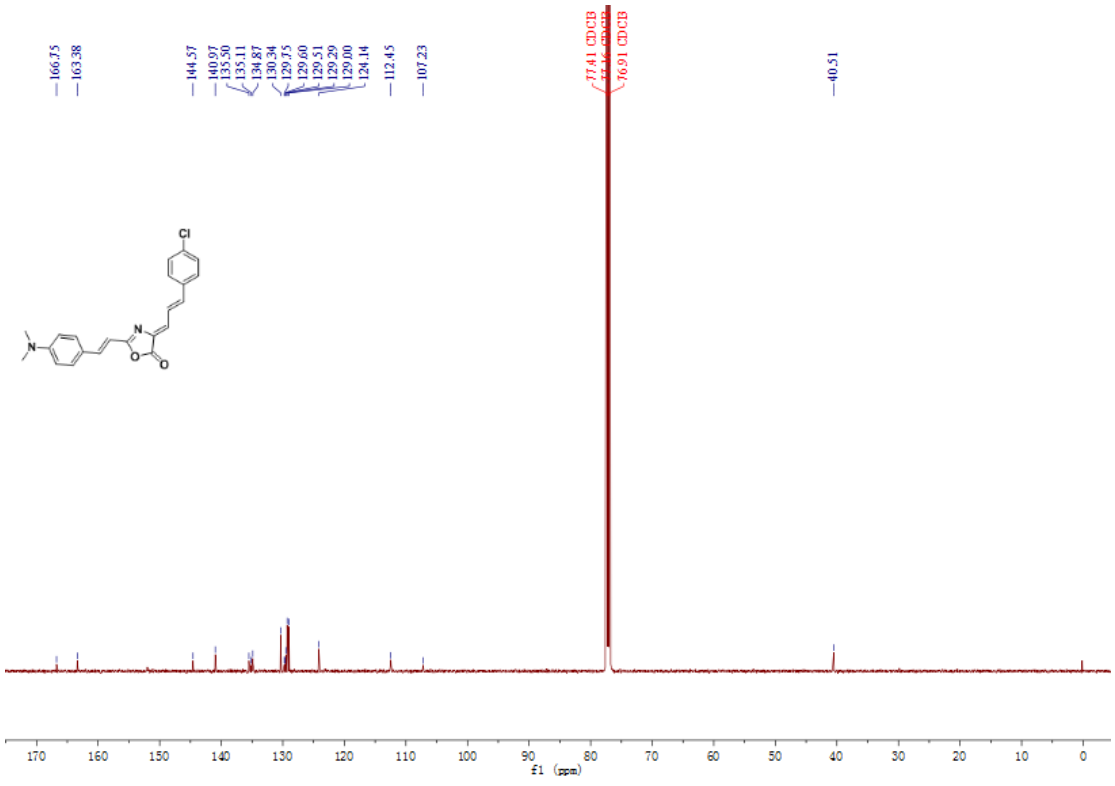



T: + c EI Full ms [ 49.50-800.50]
m/z= 48-803

| m/z | Intensity | Relative | Theo. Mass | Delta (mmu) | RDB equiv. | Composition |
|---|---|---|---|---|---|---|
| 51.0239 | 868633.0 | 2.32 | 51.0229 | 0.98 | 3.5 | $C_4H_3$ |
| 60.0232 | 275857.0 | 0.74 | 60.0206 | 2.59 | 1.0 | $C_2H_4O_2$ |
| 63.0238 | 705498.0 | 1.88 | 63.0229 | 0.86 | 4.5 | $C_5H_3$ |
| 65.0389 | 348534.0 | 0.93 | 65.0386 | 0.35 | 3.5 | $C_5H_5$ |
| 74.0138 | 355214.0 | 0.95 | 74.0151 | -1.30 | 6.0 | $C_6H_2$ |
| 75.0219 | 502668.0 | 1.34 | 75.0229 | -1.07 | 5.5 | $C_6H_3$ |
| 76.0301 | 577700.0 | 1.54 | 76.0308 | -0.64 | 5.0 | $C_6H_4$ |
| 77.0380 | 1876484.0 | 5.01 | 77.0386 | -0.57 | 4.5 | $C_6H_5$ |
| 78.0457 | 379737.0 | 1.01 | 78.0464 | -0.67 | 4.0 | $C_6H_6$ |
| 79.0540 | 324075.0 | 0.86 | 79.0542 | -0.26 | 3.5 | $C_6H_7$ |
| 89.0384 | 712336.0 | 1.90 | 89.0386 | -0.16 | 5.5 | $C_7H_5$ |
| 91.0539 | 665263.0 | 1.78 | 91.0542 | -0.37 | 4.5 | $C_7H_7$ |
| 101.0392 | 586765.0 | 1.57 | 101.0386 | 0.57 | 6.5 | $C_8H_5$ |
| 102.0469 | 1398878.0 | 3.73 | 102.0464 | 0.48 | 6.0 | $C_8H_6$ |
| 103.0554 | 2037138.0 | 5.44 | 103.0542 | 1.16 | 5.5 | $C_8H_7$ |
| 104.0508 | 277002.0 | 0.74 | 104.0495 | 1.33 | 5.5 | $C_7H_6N_1$ |
| 115.0546 | 1046940.0 | 2.79 | 115.0542 | 0.38 | 6.5 | $C_9H_7$ |
| 116.0498 | 780879.0 | 2.08 | 116.0495 | 0.35 | 6.5 | $C_8H_6N_1$ |
| 118.0654 | 290233.0 | 0.77 | 118.0651 | 0.31 | 5.5 | $C_8H_8N_1$ |
| 119.0725 | 382822.0 | 1.02 | 119.0730 | -0.43 | 5.0 | $C_8H_9N_1$ |
| 128.0495 | 687050.0 | 1.83 | 128.0495 | 0.03 | 7.5 | $C_9H_6N_1$ |
| 129.0573 | 570066.0 | 1.52 | 129.0573 | 0.02 | 7.0 | $C_9H_7N_1$ |
| 130.0656 | 2489330.0 | 6.64 | 130.0651 | 0.51 | 6.5 | $C_9H_8N_1$ |
| 131.0491 | 268382.0 | 0.72 | 131.0491 | -0.01 | 6.5 | $C_9H_7O_1$ |
| 131.0726 | 2533255.0 | 6.76 | 131.0730 | -0.33 | 6.0 | $C_9H_9N_1$ |
| 132.0786 | 393222.0 | 1.05 | 132.0781 | 0.54 | 1.0 | $C_6H_{12}O_3$ |
| 134.0967 | 789149.0 | 2.11 | 134.0964 | 0.30 | 4.5 | $C_9H_{12}N_1$ |
| 144.0811 | 2161247.0 | 5.77 | 144.0808 | 0.29 | 6.5 | $C_{10}H_{10}N_1$ |
| 145.0883 | 1265069.0 | 3.38 | 145.0886 | -0.32 | 6.0 | $C_{10}H_{11}N_1$ |
| 146.0967 | 9352960.0 | 24.96 | 146.0964 | 0.32 | 5.5 | $C_{10}H_{12}N_1$ |
| 147.1003 | 1252791.0 | 3.34 | 147.1016 | -1.31 | 0.5 | $C_7H_{15}O_3$ |
| 149.0237 | 1382912.0 | 3.69 | 149.0233 | 0.36 | 6.5 | $C_8H_5O_3$ |
| 158.0595 | 336512.0 | 0.90 | 158.0600 | -0.53 | 7.5 | $C_{10}H_8O_1N_1$ |
| 158.0958 | 361098.0 | 0.96 | 158.0964 | -0.66 | 6.5 | $C_{11}H_{12}N_1$ |
| 159.0662 | 255214.0 | 0.68 | 159.0679 | -1.63 | 7.0 | $C_{10}H_9O_1N_1$ |
| 160.0748 | 637687.0 | 1.70 | 160.0757 | -0.85 | 6.5 | $C_{10}H_{10}O_1N_1$ |
| 171.0915 | 421085.0 | 1.12 | 171.0917 | -0.14 | 7.5 | $C_{11}H_{11}N_2$ |
| 172.0746 | 468413.0 | 1.25 | 172.0757 | -1.09 | 7.5 | $C_{11}H_{10}O_1N_1$ |
| 172.0988 | 903620.0 | 2.41 | 172.0995 | -0.68 | 7.0 | $C_{11}H_{12}N_2$ |
| 173.0830 | 372326.0 | 0.99 | 173.0835 | -0.49 | 7.0 | $C_{11}H_{11}O_1N_1$ |
| 174.0913 | 37478912.0 | 100.00 | 174.0913 | -0.03 | 6.5 | $C_{11}H_{12}O_1N_1$ |
| 253.1463 | 1375437.0 | 3.67 | 253.1461 | 0.15 | 9.0 | $C_{17}H_{19}O_1N_1$ |
| 330.1712 | 296849.0 | 0.79 | 330.1727 | -1.47 | 13.0 | $C_{22}H_{22}O_1N_2$ |
| 374.1624 | 8271454.0 | 22.07 | 374.1625 | -0.13 | 14.0 | $C_{23}H_{22}O_3N_2$ |

**(*Z*)-4-((*E*)-3-(4-chlorophenyl)allylidene)-2-((*E*)-4-(dimethylamino)styryl)oxazol-5(4*H*)-one (SOD7)**

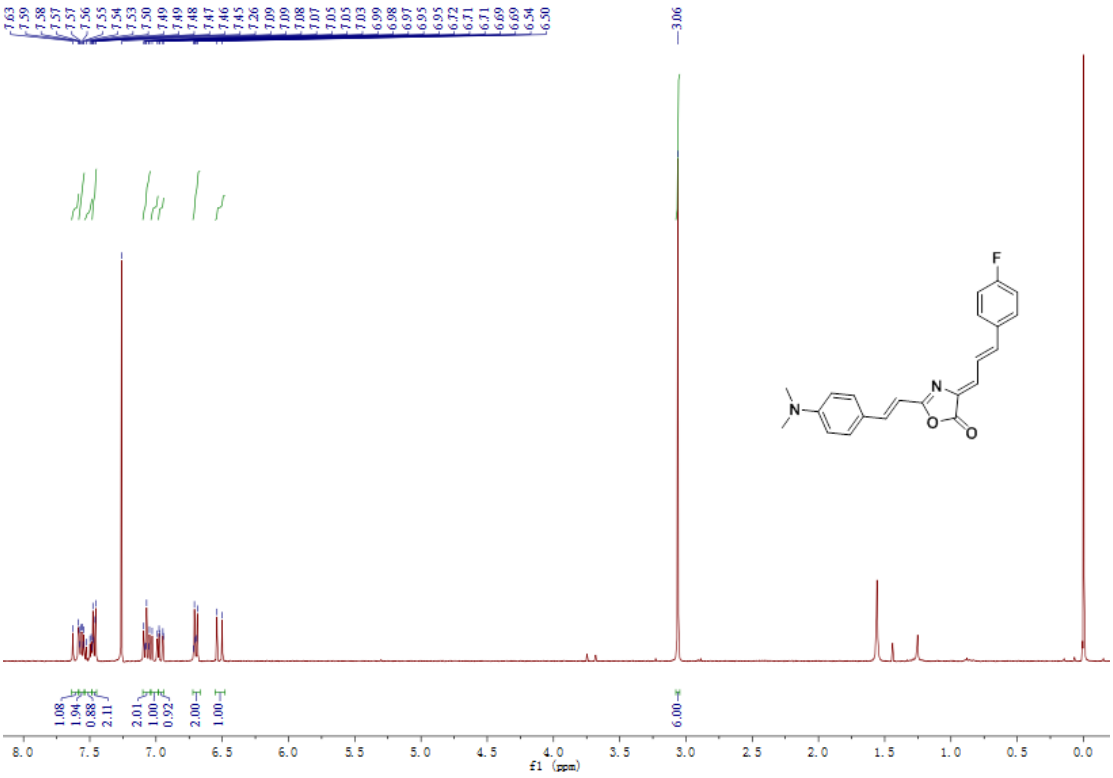


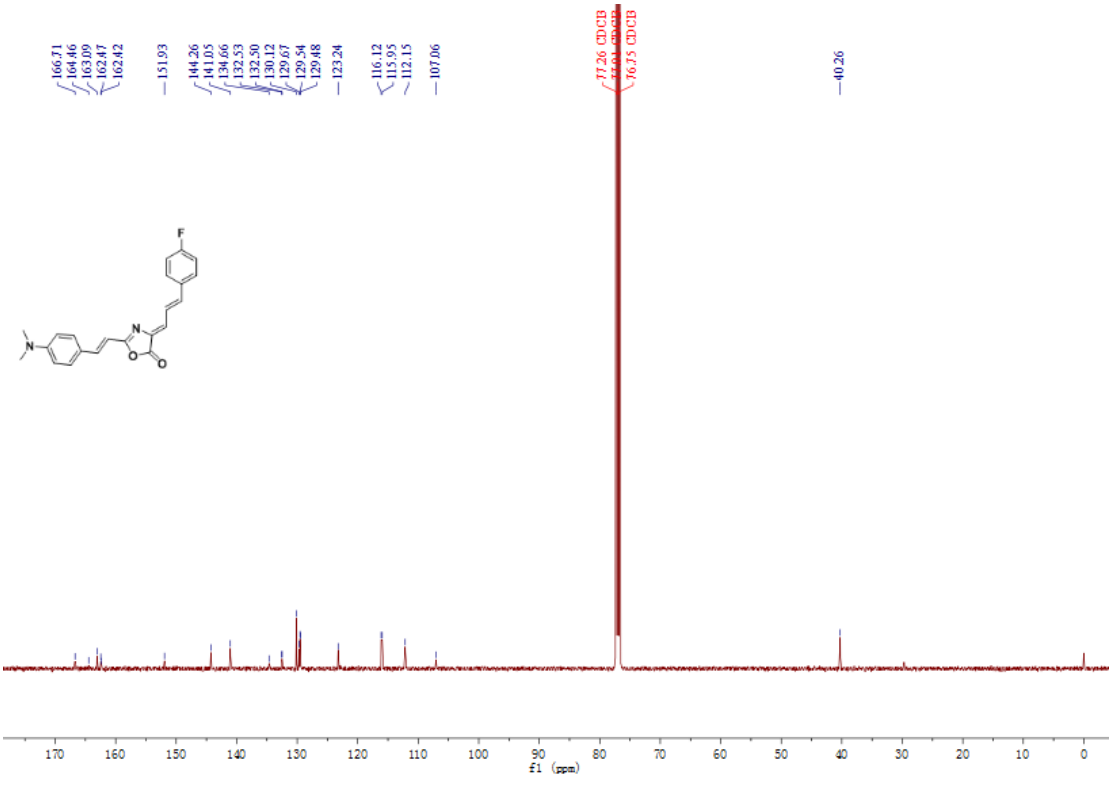



T: + c EI Full ms [ 49.50-800.50]
m/z= 48-803

| m/z | Intensity | Relative | Theo. Mass | Delta (mmu) | RDB equiv. | Composition |
|---|---|---|---|---|---|---|
| 55.0150 | 1081037.0 | 1.75 | 55.0178 | -2.85 | 2.5 | $C_3H_3O_1$ |
| 55.0514 | 3487798.0 | 5.64 | 55.0542 | -2.84 | 1.5 | $C_4H_7$ |
| 56.0598 | 1148753.0 | 1.86 | 56.0621 | -2.23 | 1.0 | $C_4H_8$ |
| 57.0681 | 4231560.0 | 6.84 | 57.0699 | -1.77 | 0.5 | $C_4H_9$ |
| 60.0195 | 1429317.0 | 2.31 | 60.0206 | -1.07 | 1.0 | $C_2H_4O_2$ |
| 67.0543 | 1460869.0 | 2.36 | 67.0542 | 0.03 | 2.5 | $C_5H_7$ |
| 68.0621 | 726967.0 | 1.18 | 68.0621 | 0.03 | 2.0 | $C_5H_8$ |
| 69.0700 | 3105325.0 | 5.02 | 69.0699 | 0.14 | 1.5 | $C_5H_9$ |
| 70.0764 | 916502.0 | 1.48 | 70.0777 | -1.31 | 1.0 | $C_5H_{10}$ |
| 71.0842 | 2614743.0 | 4.23 | 71.0855 | -1.38 | 0.5 | $C_5H_{11}$ |
| 73.0276 | 1823240.0 | 2.95 | 73.0284 | -0.85 | 1.5 | $C_3H_5O_2$ |
| 77.0383 | 1422924.0 | 2.30 | 77.0386 | -0.27 | 4.5 | $C_6H_5$ |
| 79.0539 | 783297.0 | 1.27 | 79.0542 | -0.37 | 3.5 | $C_6H_7$ |
| 81.0699 | 1634437.0 | 2.64 | 81.0699 | 0.05 | 2.5 | $C_6H_9$ |
| 82.0775 | 985077.0 | 1.59 | 82.0777 | -0.16 | 2.0 | $C_6H_{10}$ |
| 83.0492 | 546180.0 | 0.88 | 83.0491 | 0.05 | 2.5 | $C_5H_7O_1$ |
| 83.0855 | 2475463.0 | 4.00 | 83.0855 | -0.02 | 1.5 | $C_6H_{11}$ |
| 84.0570 | 886031.0 | 1.43 | 84.0570 | 0.07 | 2.0 | $C_5H_8O_1$ |
| 85.1012 | 1609564.0 | 2.60 | 85.1012 | 0.03 | 0.5 | $C_6H_{13}$ |
| 87.0440 | 714690.0 | 1.16 | 87.0441 | -0.05 | 1.5 | $C_4H_7O_2$ |
| 91.0539 | 908773.0 | 1.47 | 91.0542 | -0.37 | 4.5 | $C_7H_7$ |
| 93.0697 | 563164.0 | 0.91 | 93.0699 | -0.18 | 3.5 | $C_7H_9$ |
| 95.0857 | 1508738.0 | 2.44 | 95.0855 | 0.13 | 2.5 | $C_7H_{11}$ |
| 96.0934 | 707438.0 | 1.14 | 96.0934 | 0.00 | 2.0 | $C_7H_{12}$ |
| 97.0649 | 681484.0 | 1.10 | 97.0648 | 0.08 | 2.5 | $C_6H_9O_1$ |
| 97.1012 | 1911630.0 | 3.09 | 97.1012 | 0.03 | 1.5 | $C_7H_{13}$ |
| 98.0726 | 1153460.0 | 1.86 | 98.0726 | 0.00 | 2.0 | $C_6H_{10}O_1$ |
| 102.0413 | 869747.0 | 1.41 | 102.0424 | -1.09 | 2.0 | $C_3H_6O_2N_2$ |
| 111.0943 | 972799.0 | 1.57 | 111.0917 | 2.62 | 2.5 | $C_6H_{11}N_2$ |
| 116.0371 | 823023.0 | 1.33 | 116.0369 | 0.16 | 7.0 | $C_7H_4N_2$ |
| 129.0568 | 932246.0 | 1.51 | 129.0573 | -0.45 | 7.0 | $C_9H_7N_1$ |
| 129.0925 | 775218.0 | 1.25 | 129.0910 | 1.50 | 1.5 | $C_7H_{13}O_2$ |
| 130.0656 | 2478198.0 | 4.01 | 130.0651 | 0.47 | 6.5 | $C_9H_8N_1$ |
| 131.0724 | 2756536.0 | 4.46 | 131.0730 | -0.58 | 6.0 | $C_9H_9N_1$ |
| 134.0964 | 843156.0 | 1.36 | 134.0964 | 0.01 | 4.5 | $C_9H_{12}N_1$ |
| 140.0496 | 1078015.0 | 1.74 | 140.0495 | 0.16 | 8.5 | $C_{10}H_6N_1$ |
| 144.0817 | 2393784.0 | 3.87 | 144.0808 | 0.97 | 6.5 | $C_{10}H_{10}N_1$ |
| 145.0890 | 1666148.0 | 2.69 | 145.0886 | 0.38 | 6.0 | $C_{10}H_{11}N_1$ |
| 146.0969 | 10940928.0 | 17.69 | 146.0964 | 0.49 | 5.5 | $C_{10}H_{12}N_1$ |
| 149.0229 | 797578.0 | 1.29 | 149.0238 | -0.96 | 2.0 | $C_5H_8O_2N_1{}^{35}Cl_1$ |
| 172.0995 | 722260.0 | 1.17 | 172.0995 | -0.02 | 7.0 | $C_{11}H_{12}N_2$ |
| 174.0920 | 61854208.0 | 100.00 | 174.0918 | 0.17 | 2.0 | $C_8H_{15}N_2{}^{35}Cl_1$ |
| 189.0559 | 630689.0 | 1.02 | 189.0551 | 0.83 | 3.0 | $C_8H_{12}O_2N_1{}^{35}Cl_1$ |
| 255.1124 | 843729.0 | 1.36 | 255.1128 | -0.43 | 9.5 | $C_{15}H_{15}O_2N_2$ |
| 257.0969 | 1730301.0 | 2.80 | 257.0966 | 0.31 | 9.0 | $C_{16}H_{16}N_1{}^{35}Cl_1$ |
| 378.1137 | 17430016.0 | 28.18 | 378.1130 | 0.79 | 14.0 | $C_{22}H_{19}O_2N_2{}^{35}Cl_1$ |

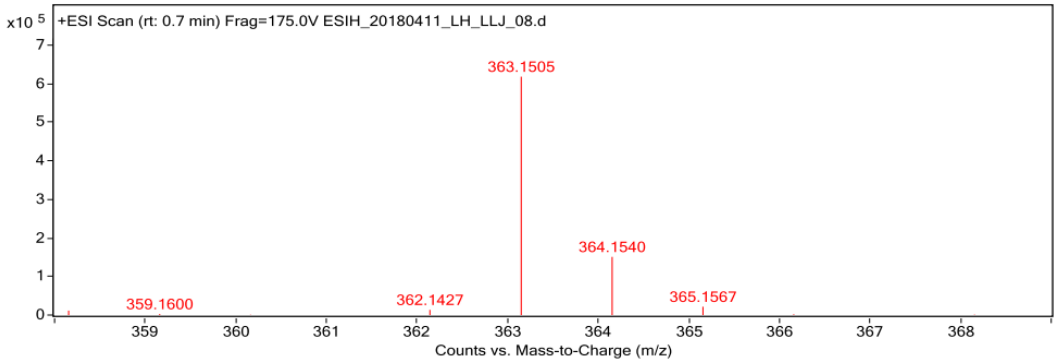
**(*Z*)-2-((*E*)-4-(dimethylamino)styryl)-4-((*E*)-3-(4-fluorophenyl)allylidene)oxazol-5(4*H*)-one (SOD8)**



**User Spectra**

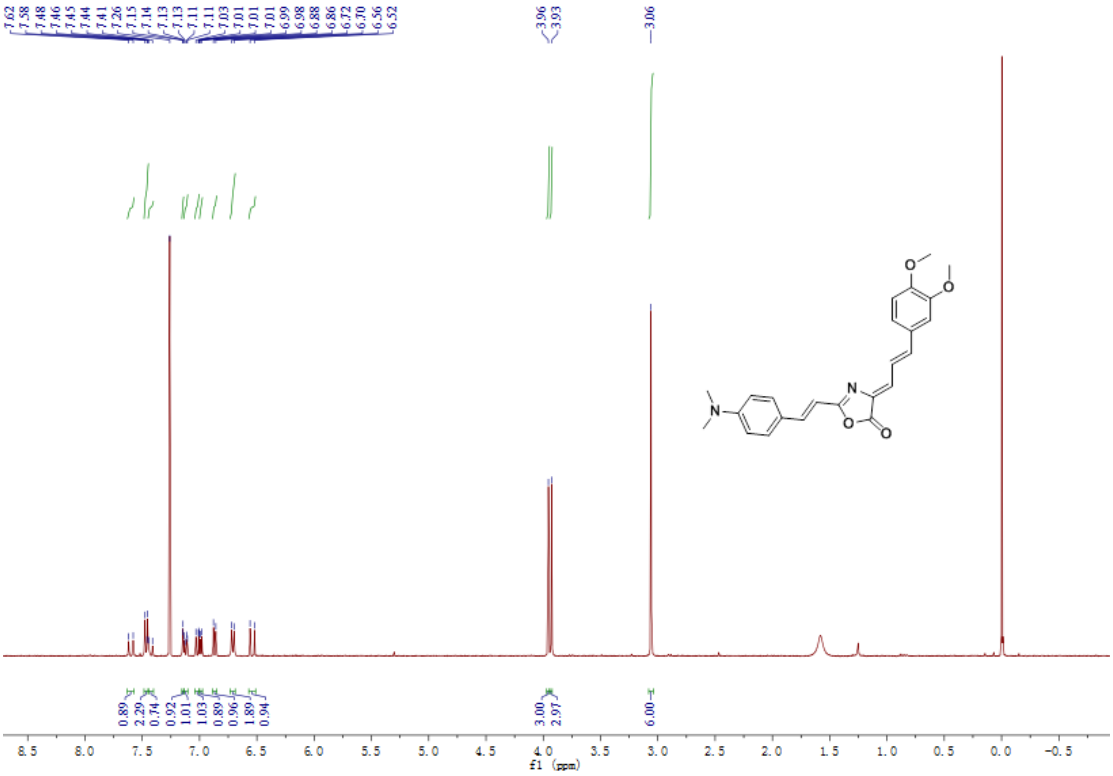
| Fragmentor Voltage | Collision Energy | Ionization Mode |
|---|---|---|
| 175 | 0 | ESI |

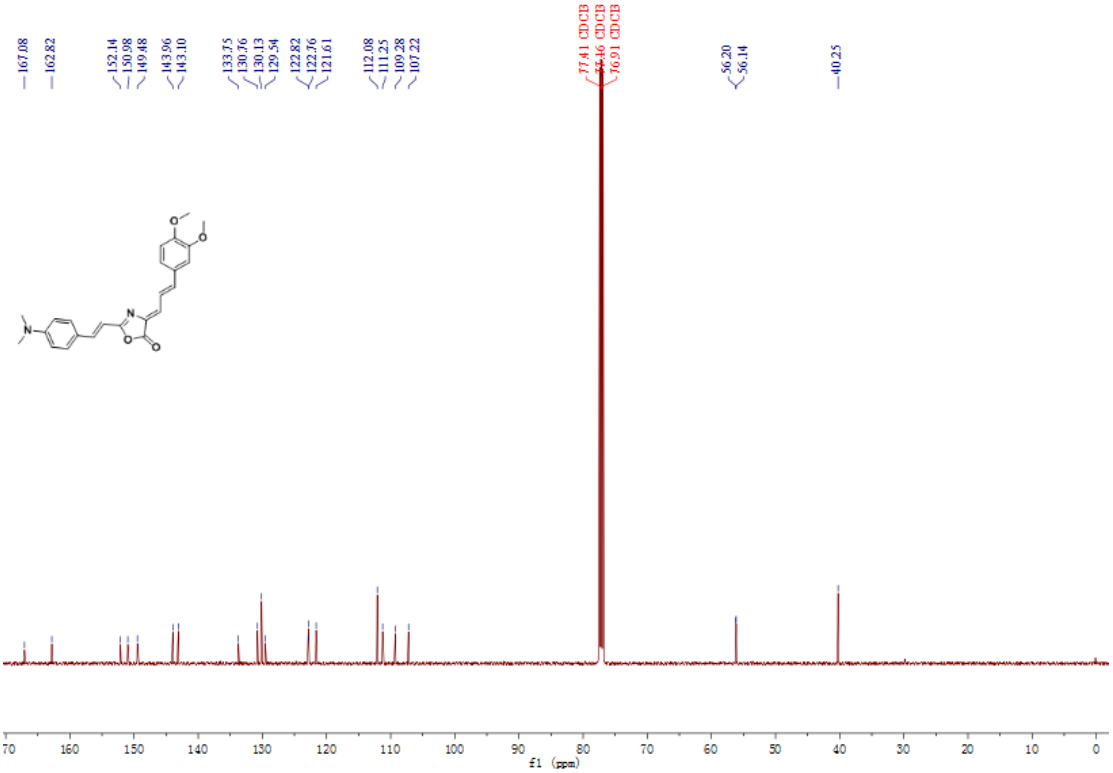



**Formula Calculator Results**

| m/z | Calc m/z | Diff (mDa) | Diff (ppm) | Ion Formula | Ion |
|---|---|---|---|---|---|
| 363.1505 | 363.1503 | -0.14 | -0.4 | C22 H20 F N2 O2 | (M+H)+ |

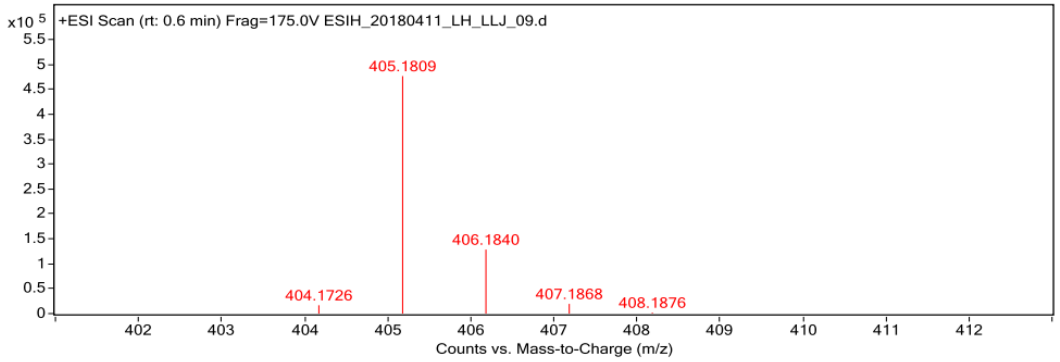
**(*Z*)-2-((*E*)-4-(dimethylamino)styryl)-4-((*E*)-3-(3,4-dimethoxyphenyl)allylidene)-oxazol-5(4*H*)-one (SOD9)**



**User Spectra**

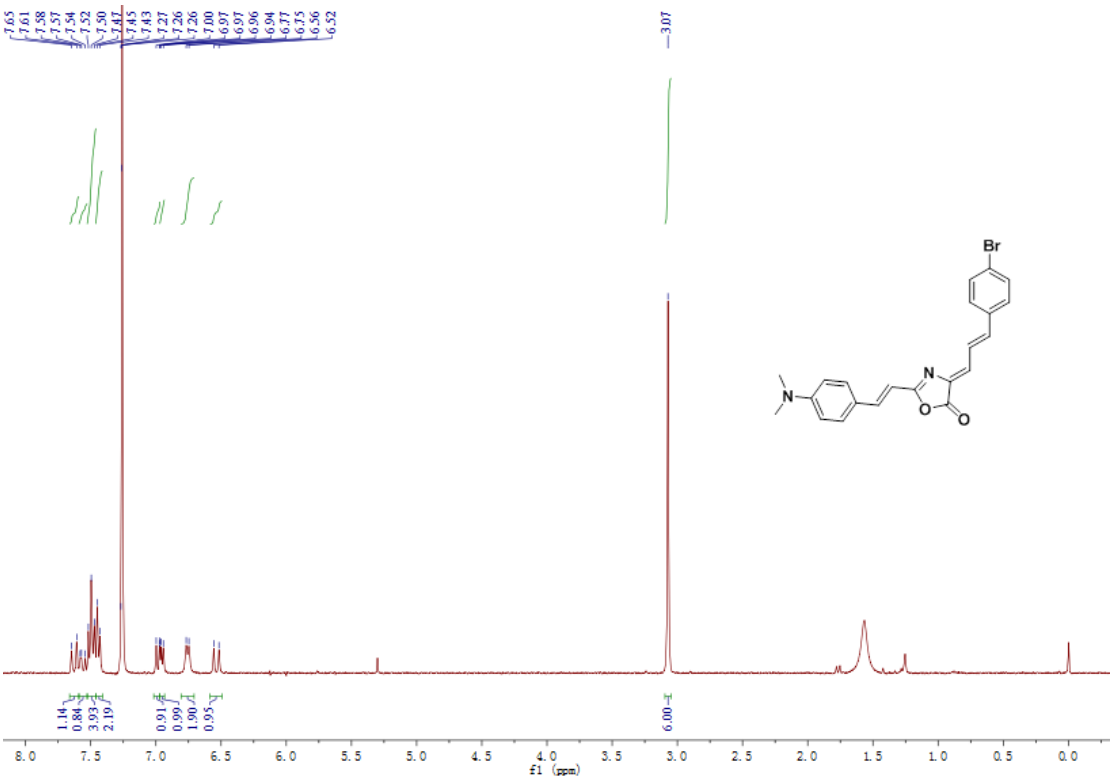
| Fragmentor Voltage | Collision Energy | Ionization Mode |
|---|---|---|
| 175 | 0 | ESI |

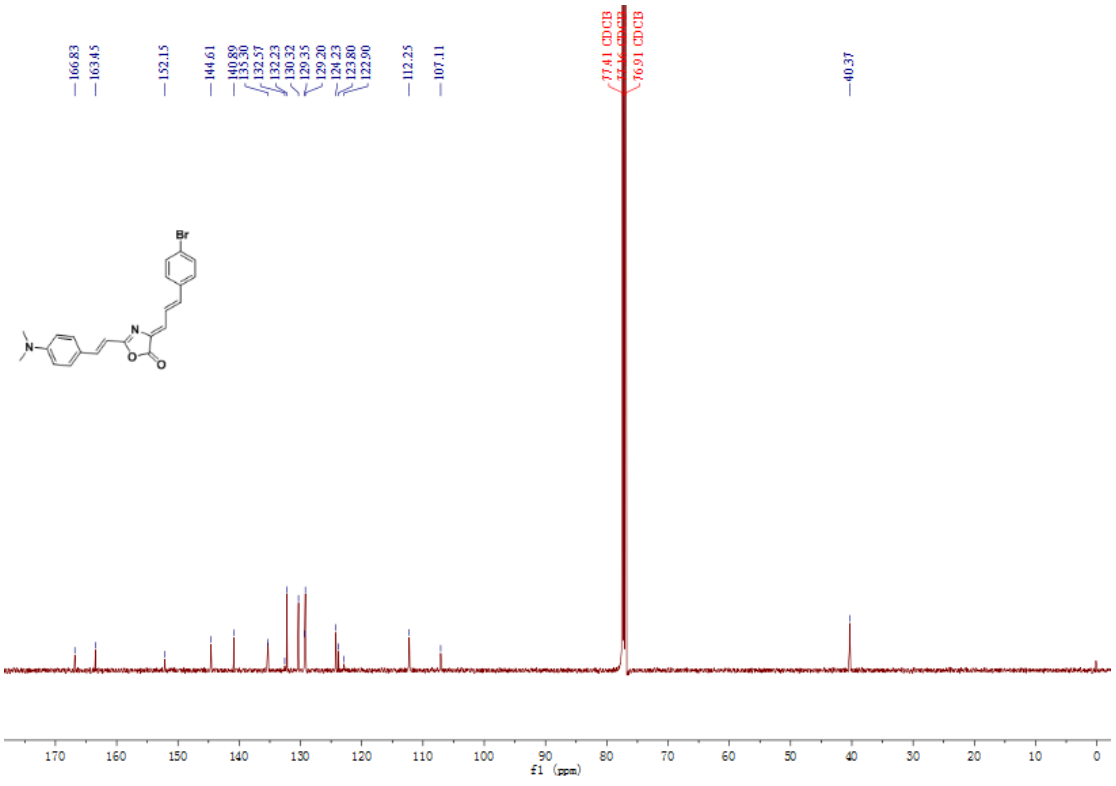



**Formula Calculator Results**

| m/z | Calc m/z | Diff (mDa) | Diff (ppm) | Ion Formula | Ion |
|---|---|---|---|---|---|
| 405.1809 | 405.1809 | 0.01 | 0.03 | C24 H25 N2 O4 | (M+H)+ |

**(*Z*)-2-((*E*)-4-(dimethylamino)styryl)-4-((*E*)-3-(4-bromophenyl)allylidene)-oxazol-5(4*H*)-one (SOD10)**

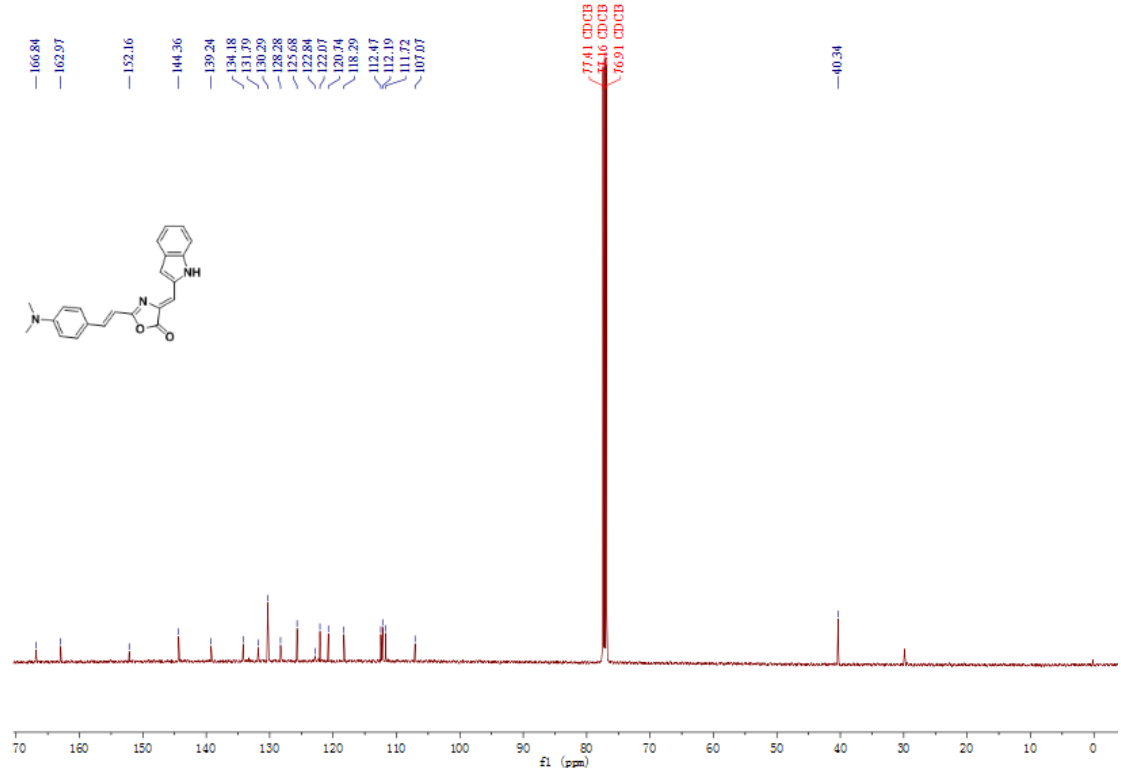


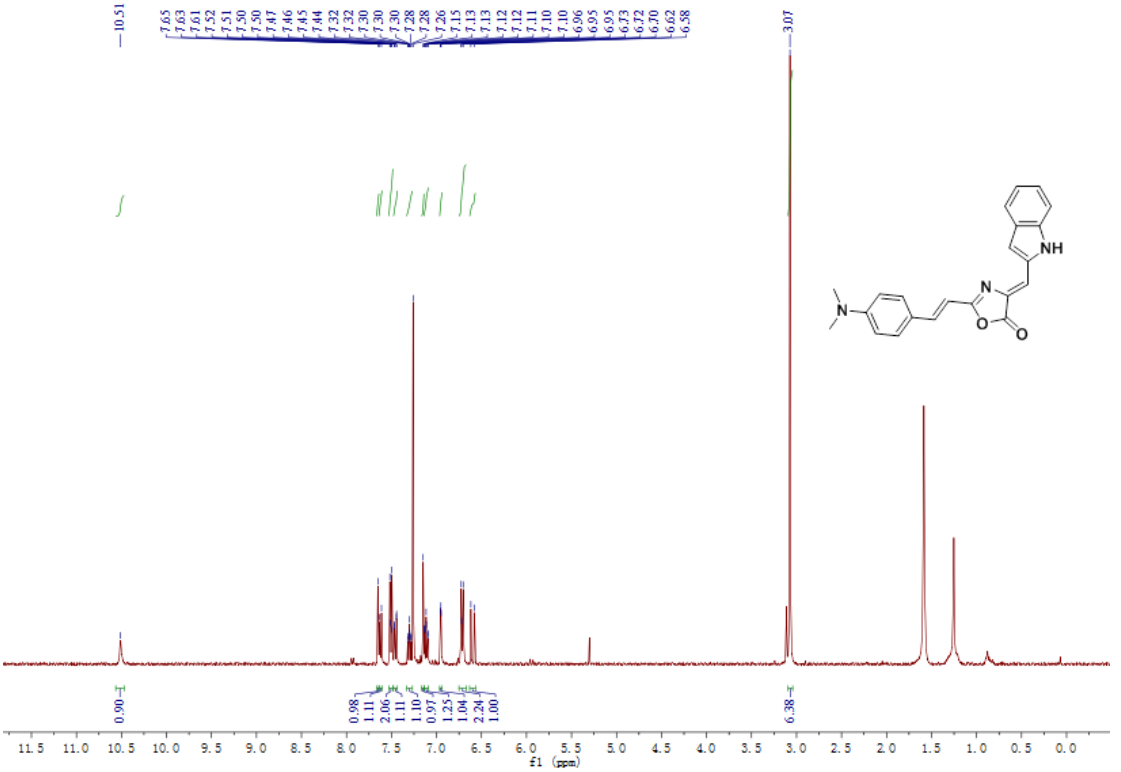



T: + c EI Full ms [ 49.50-800.50]
m/z= 48-803

| m/z | Intensity | Relative | Theo. Mass | Delta (mmu) | RDB equiv. | Composition |
|---|---|---|---|---|---|---|
| 57.0718 | 224521.0 | 1.72 | 57.0699 | 1.88 | 0.5 | $C_4H_9$ |
| 61.0081 | 157314.0 | 1.20 | 61.0073 | 0.80 | 5.5 | $C_5H_1$ |
| 62.0158 | 229101.0 | 1.75 | 62.0151 | 0.74 | 5.0 | $C_5H_2$ |
| 63.0232 | 537337.0 | 4.12 | 63.0229 | 0.30 | 4.5 | $C_5H_3$ |
| 65.0387 | 191601.0 | 1.47 | 65.0386 | 0.11 | 3.5 | $C_5H_5$ |
| 74.0138 | 311893.0 | 2.39 | 74.0151 | -1.32 | 6.0 | $C_6H_2$ |
| 75.0217 | 425442.0 | 3.26 | 75.0229 | -1.22 | 5.5 | $C_6H_3$ |
| 76.0294 | 325920.0 | 2.50 | 76.0308 | -1.39 | 5.0 | $C_6H_4$ |
| 77.0378 | 1087366.0 | 8.33 | 77.0386 | -0.80 | 4.5 | $C_6H_5$ |
| 78.0450 | 154706.0 | 1.18 | 78.0464 | -1.40 | 4.0 | $C_6H_6$ |
| 79.0537 | 172200.0 | 1.32 | 79.0542 | -0.55 | 3.5 | $C_6H_7$ |
| 89.0387 | 426238.0 | 3.26 | 89.0386 | 0.08 | 5.5 | $C_7H_5$ |
| 91.0542 | 278465.0 | 2.13 | 91.0542 | 0.00 | 4.5 | $C_7H_7$ |
| 101.0385 | 338038.0 | 2.59 | 101.0386 | -0.09 | 6.5 | $C_8H_5$ |
| 102.0462 | 631294.0 | 4.84 | 102.0464 | -0.15 | 6.0 | $C_8H_6$ |
| 103.0547 | 949072.0 | 7.27 | 103.0542 | 0.47 | 5.5 | $C_8H_7$ |
| 104.0508 | 190520.0 | 1.46 | 104.0495 | 1.29 | 5.5 | $C_7H_6N_1$ |
| 105.0586 | 168828.0 | 1.29 | 105.0573 | 1.29 | 5.0 | $C_7H_7N_1$ |
| 113.0398 | 255978.0 | 1.96 | 113.0386 | 1.25 | 7.5 | $C_9H_5$ |
| 114.0473 | 461256.0 | 3.53 | 114.0464 | 0.92 | 7.0 | $C_9H_6$ |
| 115.0549 | 437847.0 | 3.35 | 115.0542 | 0.63 | 6.5 | $C_9H_7$ |
| 116.0498 | 372103.0 | 2.85 | 116.0495 | 0.36 | 6.5 | $C_8H_6N_1$ |
| 118.0640 | 168319.0 | 1.29 | 118.0651 | -1.15 | 5.5 | $C_8H_8N_1$ |
| 119.0724 | 188739.0 | 1.45 | 119.0730 | -0.56 | 5.0 | $C_8H_9N_1$ |
| 128.0494 | 236608.0 | 1.81 | 128.0495 | -0.11 | 7.5 | $C_9H_6N_1$ |
| 129.0569 | 219973.0 | 1.68 | 129.0573 | -0.36 | 7.0 | $C_9H_7N_1$ |
| 130.0648 | 1291309.0 | 9.89 | 130.0651 | -0.29 | 6.5 | $C_9H_8N_1$ |
| 131.0729 | 1318663.0 | 10.10 | 131.0730 | -0.10 | 6.0 | $C_9H_9N_1$ |
| 134.0959 | 280087.0 | 2.15 | 134.0964 | -0.54 | 4.5 | $C_9H_{12}N_1$ |
| 140.0497 | 637941.0 | 4.89 | 140.0495 | 0.21 | 8.5 | $C_{10}H_6N_1$ |
| 141.0570 | 1051011.0 | 8.05 | 141.0573 | -0.29 | 8.0 | $C_{10}H_7N_1$ |
| 142.0632 | 223980.0 | 1.72 | 142.0651 | -1.91 | 7.5 | $C_{10}H_8N_1$ |
| 144.0804 | 1164242.0 | 8.92 | 144.0808 | -0.41 | 6.5 | $C_{10}H_{10}N_1$ |
| 145.0882 | 652986.0 | 5.00 | 145.0886 | -0.40 | 6.0 | $C_{10}H_{11}N_1$ |
| 146.0962 | 4123450.0 | 31.58 | 146.0964 | -0.18 | 5.5 | $C_{10}H_{12}N_1$ |
| 149.0236 | 440614.0 | 3.37 | 149.0260 | -2.39 | 11.0 | $C_{11}H_3N_1$ |
| 160.0749 | 198917.0 | 1.52 | 160.0757 | -0.80 | 6.5 | $C_{10}H_{10}O_1N_1$ |
| 171.0911 | 169210.0 | 1.30 | 171.0917 | -0.55 | 7.5 | $C_{11}H_{11}N_2$ |
| 172.0747 | 144592.0 | 1.11 | 172.0757 | -0.95 | 7.5 | $C_{11}H_{10}O_1N_1$ |
| 172.0981 | 317173.0 | 2.43 | 172.0995 | -1.38 | 7.0 | $C_{11}H_{12}N_2$ |
| 174.0914 | 13056512.0 | 100.00 | 174.0913 | 0.02 | 6.5 | $C_{11}H_{12}O_1N_1$ |
| 301.0472 | 248122.0 | 1.90 | 301.0461 | 1.10 | 9.0 | $C_{16}H_{16}N_1{}^{79}Br_1$ |
| 303.0449 | 252002.0 | 1.93 | 303.0441 | 0.82 | 19.5 | $C_{22}H_7O_2$ |
| 422.0618 | 1453713.0 | 11.13 | 422.0624 | -0.68 | 14.0 | $C_{22}H_{19}O_2N_2{}^{79}Br_1$ |

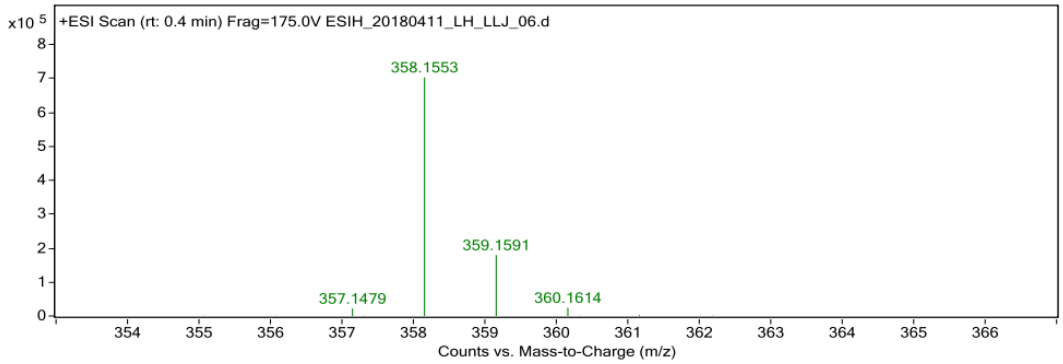
**(*Z*)-2-((*E*)-4-(dimethylamino)styryl)-4-((1H-indol-2-yl)methylene)- oxazol-5(4*H*)-one (SOD11)**



**User Spectra**

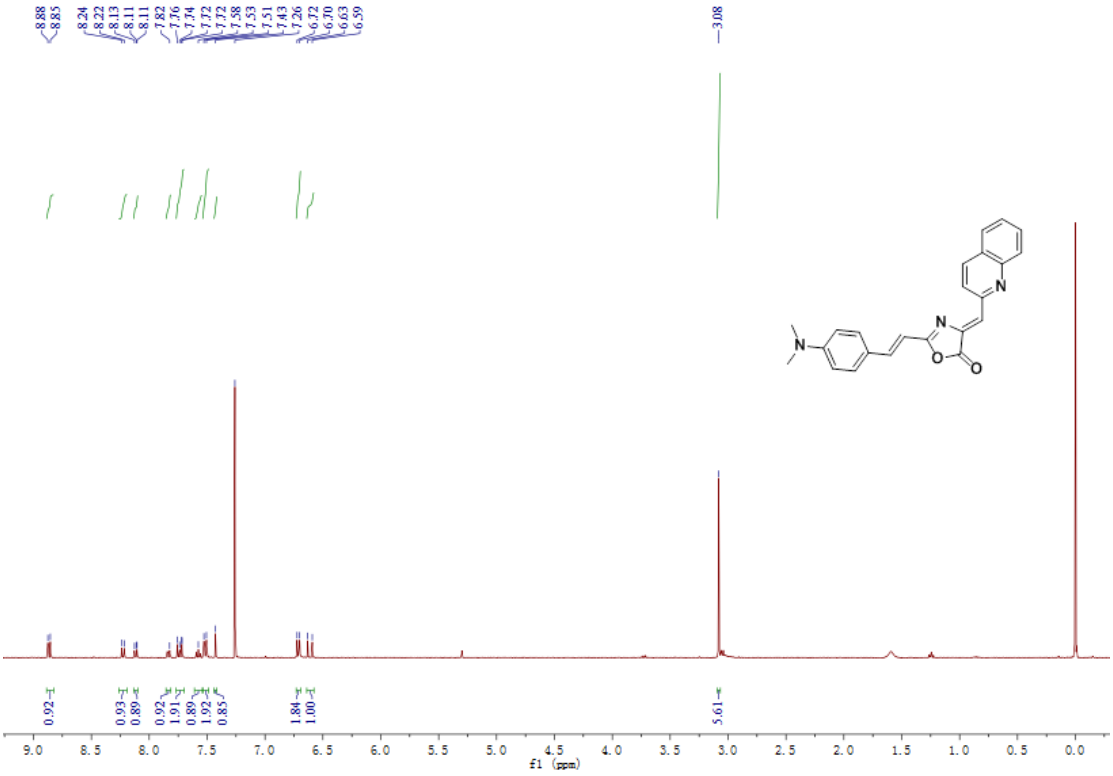
| Fragmentor Voltage | Collision Energy | Ionization Mode |
|---|---|---|
| 175 | 0 | ESI |

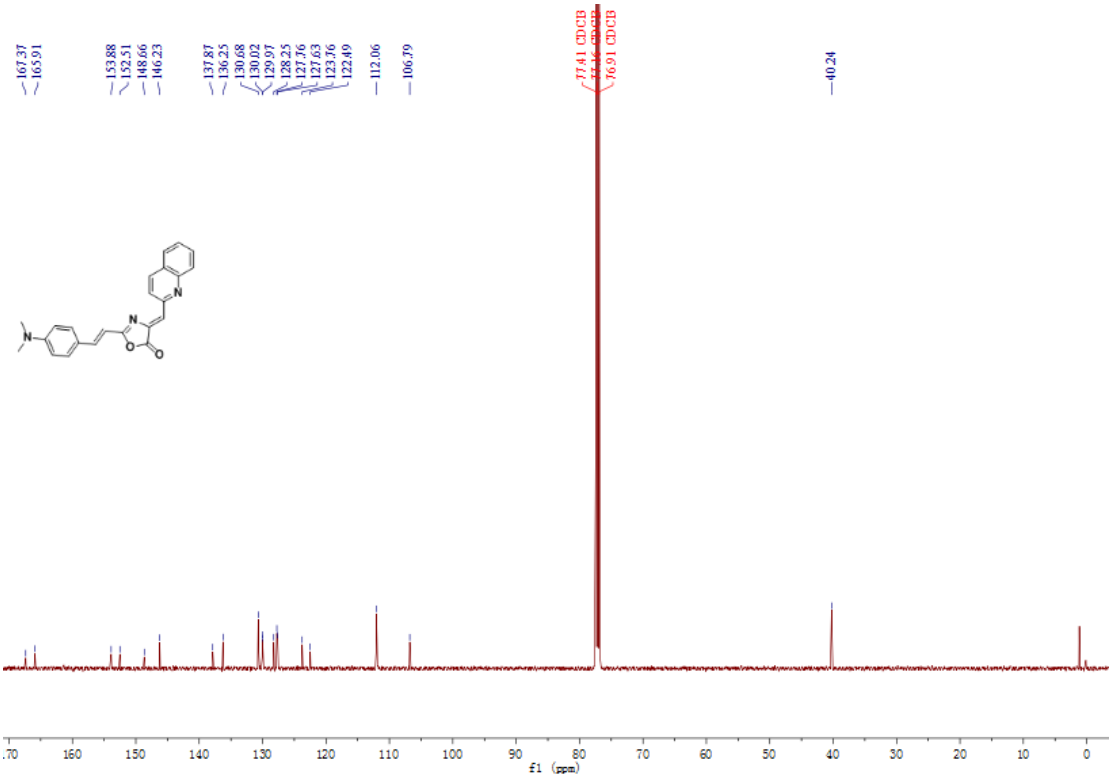



**Formula Calculator Results**

| m/z | Calc m/z | Diff (mDa) | Diff (ppm) | Ion Formula | Ion |
|---|---|---|---|---|---|
| 358.1553 | 358.155 | -0.31 | -0.87 | C22 H20 N3 O2 | (M+H)+ |

**(*Z*)-2-((*E*)-4-(dimethylamino)styryl)-4-((1H-indol-2-yl)methylene)- oxazol-5(4*H*)-one (SOD12)**

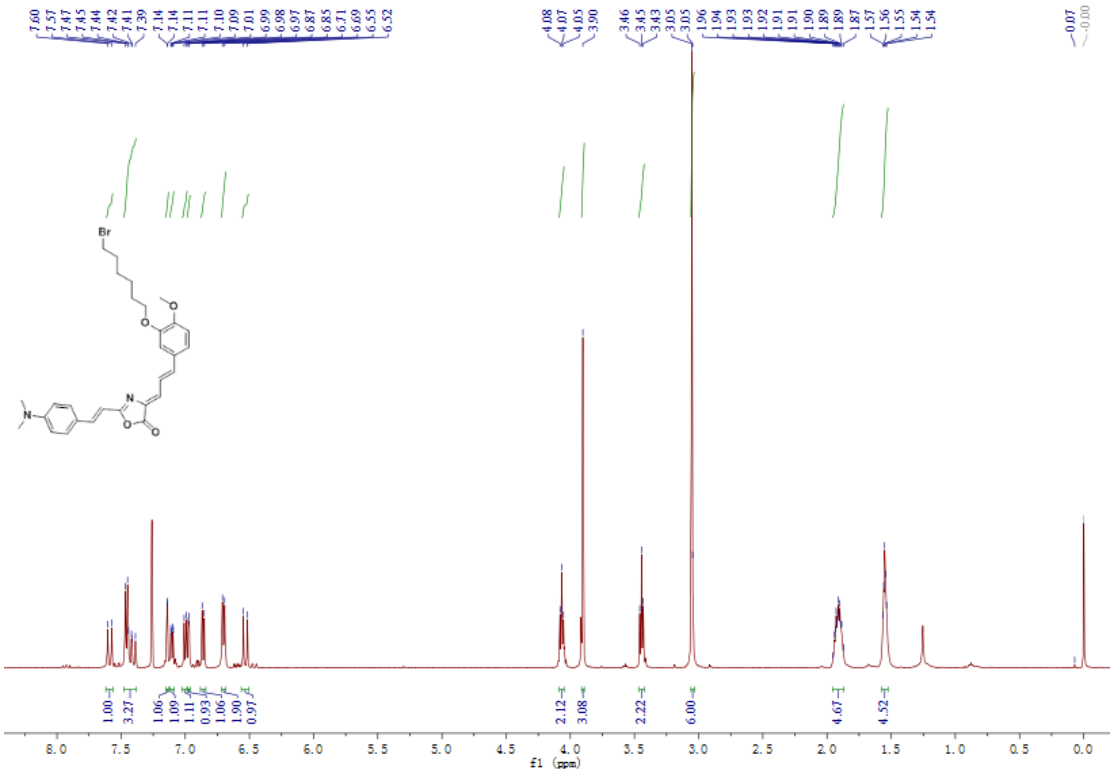


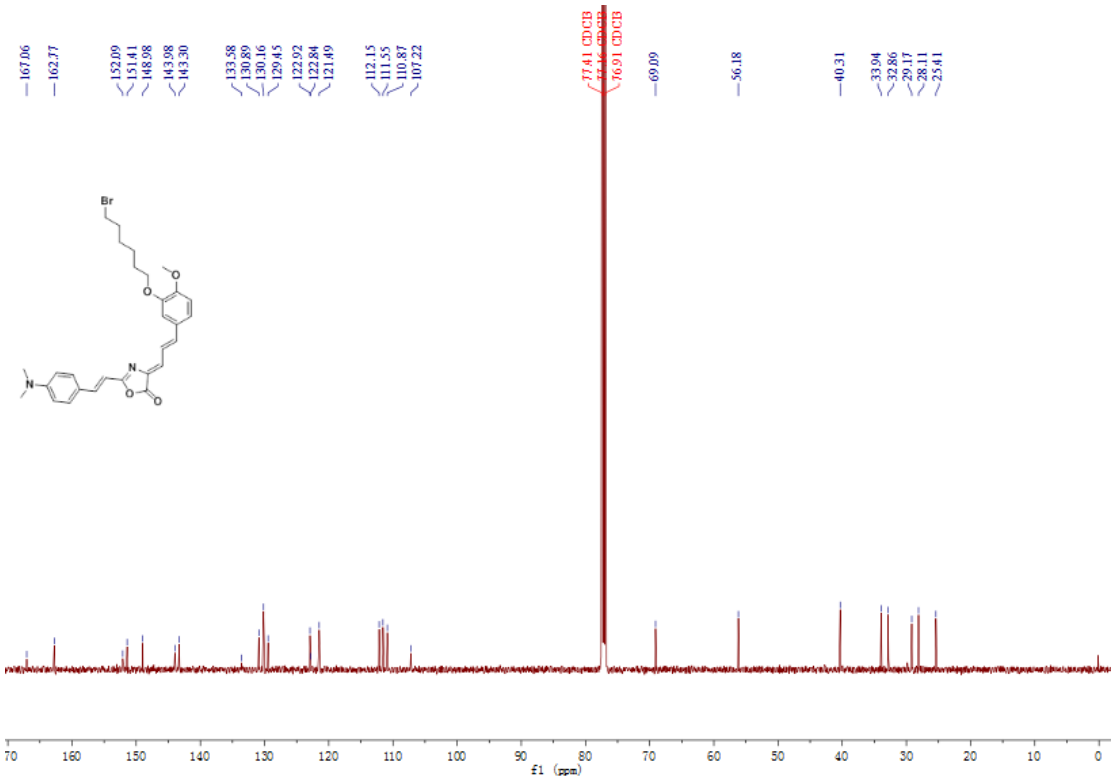



T: + c EI Full ms [ 49.50-800.50]
m/z= 48-803

| m/z | Intensity | Relative | Theo. Mass | Delta (mmu) | RDB equiv. | Composition |
|---|---|---|---|---|---|---|
| 51.0236 | 830688.0 | 5.10 | 51.0229 | 0.71 | 3.5 | $C_4H_3$ |
| 63.0464 | 675409.0 | 4.15 | 63.0441 | 2.32 | -0.5 | $C_2H_7O_2$ |
| 69.0695 | 279355.0 | 1.72 | 69.0699 | -0.35 | 1.5 | $C_5H_9$ |
| 73.0099 | 318255.0 | 1.95 | 73.0073 | 2.64 | 6.5 | $C_6H_1$ |
| 89.0268 | 588991.0 | 3.62 | 89.0260 | 0.81 | 6.0 | $C_6H_3N_1$ |
| 91.0489 | 433871.0 | 2.66 | 91.0502 | -1.26 | 0.5 | $C_2H_7O_2N_2$ |
| 101.0383 | 828144.0 | 5.09 | 101.0386 | -0.28 | 6.5 | $C_8H_5$ |
| 102.0465 | 1001648.0 | 6.15 | 102.0464 | 0.06 | 6.0 | $C_8H_6$ |
| 103.0541 | 1498910.0 | 9.21 | 103.0542 | -0.17 | 5.5 | $C_8H_7$ |
| 115.0534 | 594335.0 | 3.65 | 115.0542 | -0.83 | 6.5 | $C_9H_7$ |
| 116.0489 | 602604.0 | 3.70 | 116.0495 | -0.58 | 6.5 | $C_8H_6N_1$ |
| 119.0726 | 279833.0 | 1.72 | 119.0730 | -0.36 | 5.0 | $C_8H_9N_1$ |
| 128.0499 | 1439082.0 | 8.84 | 128.0495 | 0.46 | 7.5 | $C_9H_6N_1$ |
| 129.0570 | 878271.0 | 5.39 | 129.0573 | -0.27 | 7.0 | $C_9H_7N_1$ |
| 130.0654 | 2082844.0 | 12.79 | 130.0651 | 0.29 | 6.5 | $C_9H_8N_1$ |
| 131.0730 | 1891719.0 | 11.62 | 131.0730 | 0.02 | 6.0 | $C_9H_9N_1$ |
| 132.0784 | 279992.0 | 1.72 | 132.0768 | 1.62 | 1.5 | $C_4H_{10}O_2N_3$ |
| 134.0969 | 534825.0 | 3.28 | 134.0964 | 0.52 | 4.5 | $C_9H_{12}N_1$ |
| 140.0500 | 760873.0 | 4.67 | 140.0495 | 0.48 | 8.5 | $C_{10}H_6N_1$ |
| 142.0654 | 333299.0 | 2.05 | 142.0651 | 0.32 | 7.5 | $C_{10}H_8N_1$ |
| 143.0731 | 456613.0 | 2.80 | 143.0730 | 0.18 | 7.0 | $C_{10}H_9N_1$ |
| 144.0815 | 1702280.0 | 10.46 | 144.0808 | 0.72 | 6.5 | $C_{10}H_{10}N_1$ |
| 145.0882 | 1124389.0 | 6.91 | 145.0886 | -0.40 | 6.0 | $C_{10}H_{11}N_1$ |
| 146.0963 | 6062561.0 | 37.24 | 146.0964 | -0.13 | 5.5 | $C_{10}H_{12}N_1$ |
| 147.1004 | 850853.0 | 5.23 | 147.1002 | 0.21 | 1.0 | $C_5H_{13}O_2N_3$ |
| 149.0233 | 770797.0 | 4.73 | 149.0220 | 1.30 | 7.0 | $C_6H_3O_2N_3$ |
| 154.0650 | 466091.0 | 2.86 | 154.0651 | -0.10 | 8.5 | $C_{11}H_8N_1$ |
| 168.0680 | 604703.0 | 3.71 | 168.0682 | -0.19 | 9.0 | $C_{11}H_8N_2$ |
| 171.0918 | 489501.0 | 3.01 | 171.0917 | 0.14 | 7.5 | $C_{11}H_{11}N_2$ |
| 172.0755 | 300698.0 | 1.85 | 172.0757 | -0.24 | 7.5 | $C_{11}H_{10}O_1N_1$ |
| 172.0985 | 353051.0 | 2.17 | 172.0995 | -1.04 | 7.0 | $C_{11}H_{12}N_2$ |
| 174.0916 | 16281856.0 | 100.00 | 174.0913 | 0.28 | 6.5 | $C_{11}H_{12}O_1N_1$ |
| 182.0599 | 2288632.0 | 14.06 | 182.0600 | -0.11 | 9.5 | $C_{12}H_8O_1N_1$ |
| 189.1026 | 285049.0 | 1.75 | 189.1022 | 0.37 | 6.5 | $C_{11}H_{13}O_1N_2$ |
| 190.1097 | 321944.0 | 1.98 | 190.1101 | -0.35 | 6.0 | $C_{11}H_{14}O_1N_2$ |
| 213.1018 | 434444.0 | 2.67 | 213.1022 | -0.43 | 8.5 | $C_{13}H_{13}O_1N_2$ |
| 312.1511 | 819461.0 | 5.03 | 312.1509 | 0.20 | 14.0 | $C_{23}H_{20}O_1$ |
| 313.1564 | 378623.0 | 2.33 | 313.1573 | -0.99 | 14.0 | $C_{21}H_{19}N_3$ |
| 327.1493 | 336607.0 | 2.07 | 327.1492 | 0.08 | 14.5 | $C_{22}H_{19}O_1N_2$ |
| 340.1446 | 946686.0 | 5.81 | 340.1444 | 0.13 | 15.5 | $C_{22}H_{18}O_1N_3$ |
| 341.1517 | 939466.0 | 5.77 | 341.1523 | -0.60 | 15.0 | $C_{22}H_{19}O_1N_3$ |
| 369.1472 | 2281316.0 | 14.01 | 369.1472 | 0.03 | 16.0 | $C_{23}H_{19}O_2N_3$ |
| 371.1617 | 314247.0 | 1.93 | 371.1628 | -1.08 | 15.0 | $C_{23}H_{21}O_2N_3$ |

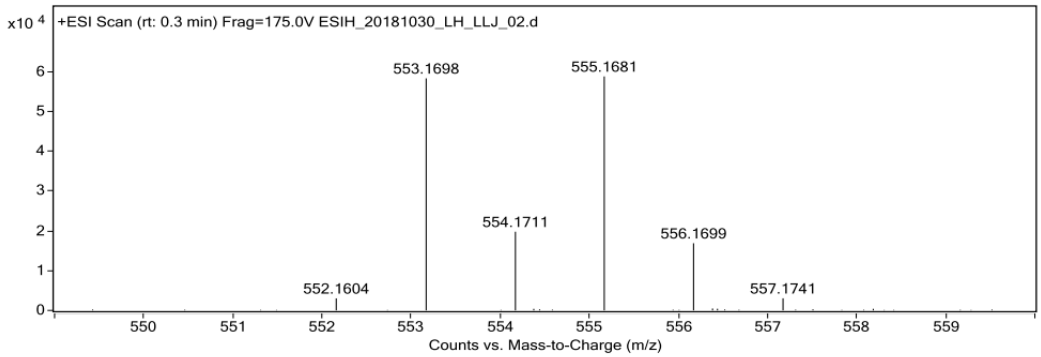
**(*Z*)-4-((*E*)-3-(3-((6-bromohexyl)oxy)-4-methoxyphenyl)allylidene)-2-((*E*)-4-(dimethylamino)styryl)oxazol-5(4*H*)-one (SOD9-Br).**



**User Spectra**

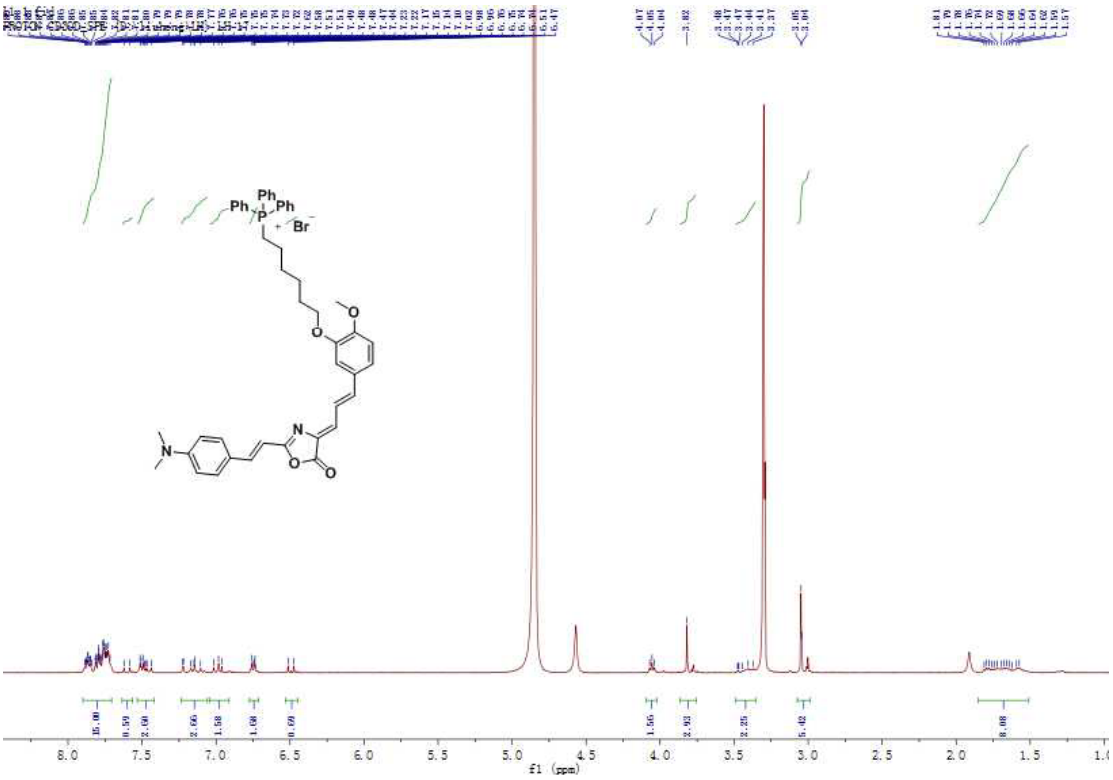
| Fragmentor Voltage | Collision Energy | Ionization Mode |
|---|---|---|
| 175 | 0 | ESI |




**Formula Calculator Results**

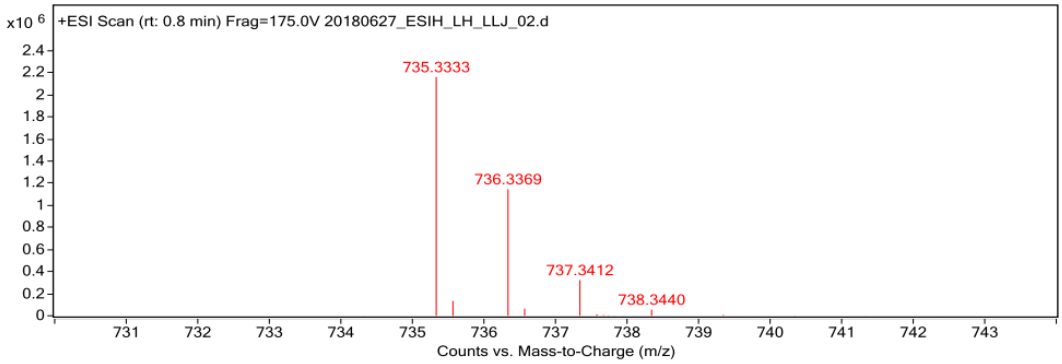
| m/z | Calc m/z | Diff (mDa) | Diff (ppm) | Ion Formula | Ion |
|---|---|---|---|---|---|
| 553.1698 | 553.1696 | -0.13 | -0.23 | C29 H34 Br N2 O4 | (M+H)+ |

**(6-(5-((1*E*,3*Z*)-3-(2-((*E*)-4-(dimethylamino)styryl)-5-oxooxazol-4(5*H*)-ylidene)prop-1-en-1-yl)-2-methoxyphenoxy)hexyl)triphenylphosphonium bromide(SOD9-TPP)**




**User Spectra**

| Fragmentor Voltage | Collision Energy | Ionization Mode |
|---|---|---|
| 175 | 0 | ESI |




**Formula Calculator Results**

| m/z | Calc m/z | Diff (mDa) | Diff (ppm) | Ion Formula | Ion |
|---|---|---|---|---|---|
| 735.3333 | 735.3346 | 1.37 | 1.86 | C47 H48 N2 O4 P | M+ |