Supporting Information

Improvement of Pharmacological Properties of Irreversible Thyroid Receptor Coactivator Binding Inhibitors

*Jong Yeon Hwang[1], Leggy A. Arnold[1], Fangyi Zhu[1], Aaron Kosinski[1], Thomas J. Mangano[2], Vincent Setola[2], Bryan L. Roth[2], and R. Kiplin Guy[1]**

R. Kiplin Guy, St Jude Children's Hospital, Department of Chemical Biology and Therapeutics, 262 Danny Thomas Place, Memphis TN, 38105-3678, USA. Tel (901) 595-5714; Fax (901) 595-5715 e-mail: kip.guy@stjude.org

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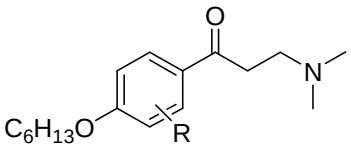
Table 1. Summary of β-Aminophenylketones Regioisomers and Ring Substitution



Compound		SRC Binding Inhibition (IC_{50}, μM)[a]		Cell viability HepG 2 (EC_{50}, μM) [b]	Solubility (μM)[c]	Permeability (10^{-6} cm/s)[d]	Synthetic Method[e]
No.	R	TRα	TRβ				
1	H	7.4±1.0	9.6±1.1	54±9	21±1	1550±340	A
9	H	16.6±1.8	16.5±1.5	65±19	180±10	1040±100	A
10	H	5.3±0.6	7.1±0.8	45±5	160±10	830±70	B
11	5-Me	>50	>50	>100	140±11	1100±10	A
12{*1*}	2-Me	3.5±0.3	10.1±1.2	38±26	130±20	1230±120	A
12{*2*}	3-Me	4.0±0.3	5.3±0.6	32±8	130±10	750±90	A
12{*3*}	2-MeO	3.8±0.3	7.0±1.1	100±37	160±2	950±70	A
12{*4*}	3-MeO	22.2±6.5	25.3±7.0	62±13	160±10	1040±260	B
12{*5*}	2-MeS	4.3±0.5	5.1±0.5	29±6	90±10	1270±160	A
12{*6*}	3-MeS	5.8±0.6	10.4±2.1	>100	110±3	1450±530	B
12{*7*}	3-Me_2N	>50	>50	>100	180±10	170±30	A
12{*8*}	2-*tert*Bu	5.4±0.5	5.0±0.7	16±2	6±1	190±60	A
12{*9*}	2-F	3.5±0.4	4.7±0.4	37±10	110±10	700±100	A
12{*10*}	2-Cl	2.6±0.2	4.3±1.9	32±13	30±10	1020±230	A
12{*11*}	3-Cl	3.2±0.4	1.8±0.2	53±9	72±7	1960±940	A
12{*12*}	2-Br	2.3±0.2	2.6±0.3	33±11	19±7	460±70	A
12{*13*}	3-Br	1.1±0.1	1.4±0.2	54±13	78±2	80±6	A
12{*14*}	2-I	1.2±0.1	2.7±0.3	31±11	14±3	540±60	A
12{*15*}	3-I	1.9±0.4	2.1±0.4	55±10	48±8	270±110	A
12{*16*}	2-$MeSO_2$	9.3±1.1	8.4±1.1	>100	130±1	730±50	A
12{*17*}	3-$MeSO_2$	4.7±0.6	2.4±0.3	45±12	40±10	850±220	B
12{*18*}	2-CF_3	3.4±0.3	2.7±0.3	34±9	6±2	930±130	B
12{*19*}	3-CF_3	1.4±0.1	1.9±0.2	10±13	20±10	500±230	B
12{*20*}	2-NO_2	3.7±0.3	3.0±0.4	43±7	54±8	1340±410	B
12{*21*}	2,6-Me_2	7.7±0.6	5.0±0.6	41±5	51±8	730±80	B
12{*22*}	3,5-Me_2	1.3±0.1	1.7±0.1	15±1	30±20	650±120	A
12{*23*}	2-Me-5-iPr	3.0±0.4	1.79±1.28	26±4	20±5	860±370	B

12{*24*}	2,3-Cl_2	0.81±0.1	1.1±0.1	31±2	10±1	600±330	B
12{*25*}	2,5-Cl_2	0.6±0.1	0.6±0.1	62±23	20±1	1040±190	B
12{*26*}	3,5-Cl_2	-[f]	0.69±0.1	18±2	2±1	700±300	B
12{*27*}	2-Ph	7.1±1.1	14.1±5.1	16±3	5±3	830±200	A
12{*28*}	2-Bn	14.8±7.2	>50	24±3	3±1	230±60	A

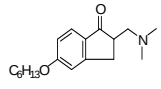
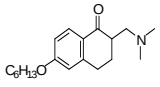
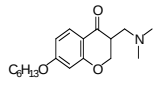
[a]Values are the mean of three independent experiments in triplicate. [b,c,d]Values are means of two independent experiments in triplicate.[e]A is Friedel-Crafts acylation and B is Mannich reaction.

Table 2. Summary of β-Aminoarylketones with Alternate Aromatic Rings

No	SRC Binding Inhibition (IC_{50}, μM)[a]		Cell viability HepG 2 (EC_{50}, μM) [b]	Solubility (μM)[c]	Permeability (10^{-6} cm/s)[d]	Synthetic Method[e]
	TRα	TRβ				
9	16.6±1.8	16.5±1.5	65±19	180±10	1040±100	A
13{*1*}	4.1±0.4	4.0±0.4	38±6	22±4	660±90	A
13{*2*}	>50	>50	>100	1.0±0.2	150±80	A
13{*3*}	13.4±10.8	>50	65±14	8±4	1420±140	B

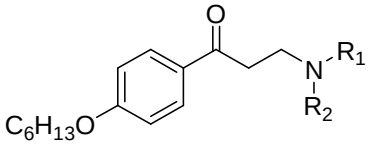
[a]Values are the mean of three independent experiments in triplicate. [b,c,d]Values are means of two independent experiments in triplicate.[e]A is Friedel-Crafts acylation and B is Mannich reaction.

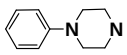
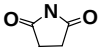
Table 3. Summary of α-Substituted β-Aminophenylketones

No.	R	SRC Binding Inhibition (IC_{50}, μM)[a]		Cell viability HepG 2 (EC_{50}, μM) [b]	Solubility (μM)[c]	Permeability (10^{-6} cm/s)[d]	Synthetic Method[e]
		TRα	TRβ				
9	H	16.6±1.8	16.5±1.5	65±19	180±10	1040±100	A
14{*1*}	Me	>50	>50	56±18	196±2	1350±630	B
14{*2*}	iPr	>50	>50	62±27	145±6	1260±170	B
14{*3*}	Ph	>50	>50	27±19	11±1	910±90	B
14{*4*}		1.9±0.2	1.7±0.3	14±2	7±2	230±40	B
14{*5*}		1.9±0.3	2.3±0.2	12±2	90±10	710±90	B
14{*6*}		1.3±0.1	1.6±0.1	12±1	13±10	700±130	B

[a]Values are the mean of three independent experiments in triplicate. [b,c,d]Values are means of two independent experiments in triplicate.[e]A is Friedel-Crafts acylation and B is Mannich reaction.

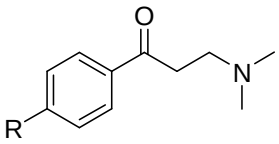
Table 4. Summary of β-Aminophenylketones Bearing Different Nitrogen Substituents

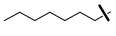
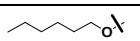
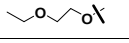
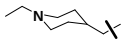
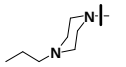
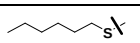
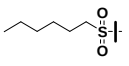
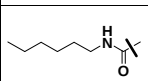
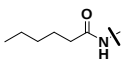
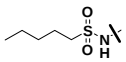
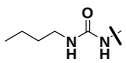


	R_1R_2NH	SRC Binding Inhibition (IC_{50}, μM)[a]		Cell viability HepG 2 (EC_{50}, μM) [b]	Solubility (μM)[c]	Permeability (10^{-6} cm/s)[d]	hERG[e]	pKa
		TRα	TRβ					
9	Me2NH	16.6±1.8	16.5±1.5	65±19	180±10	1040±100	61±9	9.12
15{*1*}	Bu_2NH	6.3±0.5	2.7±0.4	48±20	4±0.3	560±170	48±15	9.95
15{*2*}		9.2±1.0	9.1±1.2	66±34	195±2	2130±700	75±2	9.61
15{*3*}		4.8±0.5	18.9±6.8	59±17	186±4	1280±110	69±9	9.28
15{*4*}		19.8±2.0	22.0±2.4	67±22	74±3	1660±70	35±4	6.45
15{*5*}		8.4±0.6	5.6±0.9	54±13	160±20	2300±420	60±7	8.1
15{*6*}		3.0±0.3	3.8±0.3	81±32	2±0.4	undetected	29±12	6.13
15{*7*}		7.7±0.6	4.1±0.5	56±19	78±6	1790±360	32±13	6.5
15{*8*}		>50	>50	>130	1±0.1	Undetected	8±11	5.26
15{*9*}		>50	>50	>130	1±0.5	0.2±0.4	22±1	4.38
15{*10*}		>50	>50	>130	0.2±0.2	2.0±2	18±3	3.67
15{*11*}		>50	>50	54±31	48±5	1490±140	32±3	-[f]
15{*12*}		>50	>50	>130	29±3	1300±150	-11±6	-[f]

[a]Values are the mean of three independent experiments in triplicate. [b,c,d]Values are means of two independent experiments in triplicate.[e]Values are the mean of two independent experiments in quadruplicate. [f]Not available.

Table 5. Summary the Activities of Hydrophobic Side Chain Modified β-Aminophenylketones



No	R	SRC Binding Inhibition (IC_{50}, μM)[a]		Cell viability HepG 2 (EC_{50}, μM) [b]	Solubility (μM)[c]	Permeability (Pe, 10^{-6} cm/s)[d]	hERG[e]	Synthetic Route[f]
		TRα	TRβ					
1		7.5±1.0	9.6±1.1	54±9	22±1	1550±340	68±12	A
9		16.6±1.8	16.5±1.5	65±19	180±10	1040±100	61±9	A
16{*1*}		30.9±11.1	>50	>100	220±3	160±30	3±1	A
16{*2*}		>50	>50	>100	200±10	140±30	16±10	A
16{*3*}		>50	>50	>100	240±3	320±60	35±10	B
16{*4*}		6.8±0.7	5.9±0.6	34±15	83±2	1470±200	48±4	A
16{*5*}		6.2±0.7	4.9±0.7	>100	58±6	780±80	36±9	A
16{*6*}		16.8±2.8	8.1±1.4	>100	96±10	770±70	15±7	B
16{*7*}		9.8±1.5	12.4±3.2	>100	210±4	560±80	38±7	B
16{*8*}		33.3±10.2	>50	>100	170±5	50±20	15±20	B
16{*9*}		>50	>50	>100	221±1	10±3	23±15	B

[a]Values are the mean of three independent experiments in triplicate. [b,c,d]Values are means of two independent experiments in triplicate.[e]Values are the mean of two independent experiments in quadruplicate. [f]A is Friedel-Crafts acylation and B is Mannich reaction.

Table 6. Summary of the Second Generation Compounds

No	SRC Binding Inhibition, TRβ (IC_{50}, μM)[a]	Cell viability HepG 2 (EC_{50}, μM) [b]	TI[c]	Solubility (μM)[d]	Permeability (Pe, 10^{-6} cm/s)[e]	hERG[f]
17{*1,1,1*}	1.8±0.3	26±2	14	72±7	1960±940	-
17{*1,1,2*}	4.6±0.8	51±3	11	14±1	870±90	-
17{*1,1,3*}	1.8±0.2	39±2	21	10±2	Eq.[g]	-
17{*1,1,4*}	4.8±0.7	60± 13	13	36±2	Eq.[g]	-
17{*1,1,5*}	1.2±0.2	43±2	35	12±1	Eq.[g]	-
17{*1,1,6*}	2.0±0.5	28±1	14	0.6±0.1	Eq.[g]	-
17{*1,2,1*}	2.6±0.5	31±2	12	10±1	600±330	-
17{*1,2,2*}	5.0±0.9	39±2	8	1±0.1	370±90	-
17{*1,2,3*}	0.7±0.1	25±2	36	0.5±0.2	930±150	-
17{*1,2,4*}	1.2±0.2	47±5	40	6±1	Und.[h]	-
17{*1,2,5*}	0.6±0.5	17±2	27	2±0.2	Eq.[g]	-
17{*1,2,6*}	1.2±0.2	28±2	23	0.09±0.03	>1	-
17{*1,3,1*}	1.5±0.2	89±15	59	20±1	1040±190	-
17{*1,3,2*}	5.0±1.0	57±4	11	2±0.3	810±50	-
17{*1,3,3*}	1.4±0.2	28±4	20	1.4±0.1	1770±770	-
17{*1,3,4*}	2.0±0.3	54±11	27	6±1	Eq.[g]	-
17{*1,3,5*}	0.8±0.1	28±6	35	2.7±0.4	1540±760	-
17{*1,3,6*}	1.7±0.2	31±3	19	1.3±0.3	Eq.[g]	-
17{*1,4,1*}	0.7±0.1	18±2	26	2±1	700±300	-
17{*1,4,2*}	4.7±1.0	43±4	9	0.3±.1	>1	-
17{*1,4,3*}	0.8±0.1	17±1	22	1.4±0.2	>1	-
17{*1,4,4*}	1.5±0.1	23±3	15	15±1	1380±580	-

17{*1,4,5*}	0.6±0.1	15±1	25	1.8±0.7	Eq.[g]	-
17{*1,4,6*}	0.8±0.2	18±2	23	0.7±0.7	860	-
17{*1,5,1*}	0.7±0.1	17±1	25	26±19	650±120	-
17{*1,5,2*}	6.5±1.1	33±1	5	14±1	930±500	-
17{*1,5,3*}	2.0±0.3	31±1	15	6±1	Eq.[g]	-
17{*1,5,4*}	18.9±3.3	39±2	2	16±1	Eq.[g]	-
17{*1,5,5*}	1.9±0.3	34±1	18	14±2	1550±1080	-
17{*1,5,6*}	4.0±0.8	39±3	10	0.2±0.1	Eq.[g]	-
17{*2,1,1*}	1.5±0.3	36±4	24	2.4±0.3	610±100	-
17{*2,1,2*}	5.4±0.8	55±3	10	1.2±0.1	500±80	-
17{*2,1,3*}	0.8±0.1	37±2	45	0.3±0.1	2050±650	-
17{*2,1,4*}	2.0±0.3	47±8	24	6±1	1360±310	-
17{*2,1,5*}	0.6±0.1	31±2	51	1.3±0.1	1420±250	-
17{*2,1,6*}	1.7±0.2	34±2	20	0.02±0.01	740±270	-
17{*2,2,1*}	1.3±0.2	62±24	46	0.06±0.01	140±90	-
17{*2,2,2*}	3.6±0.9	62±6	17	0.05±0.01	70±50	-
17{*2,2,3*}	1.3±0.2	20±2	16	0.07±0.03	170±70	-
17{*2,2,4*}	0.8±0.2	24±4	31	0.24±0.03	1600±810	-
17{*2,2,5*}	0.9±0.2	23±2	25	0.05±0.02	2300±720	-
17{*2,2,6*}	0.7±0.1	26±3	36	0.2±0.1	30±50	-
17{*2,3,1*}	1.2±0.2	27±2	22	0.02±0.03	330±40	-
17{*2,3,2*}	4.2±0.6	78±16	19	0.14±0.01	140±20	-
17{*2,3,3*}	1.0±0.2	19±1	19	0.04±0.04	1310±500	-
17{*2,3,4*}	0.6±0.1	43±12	68	0.1±0.07	810±480	-
17{*2,3,5*}	0.8±0.1	24±3	32	0.05±0.03	1010±310	-

17{*2,3,6*}	0.7±0.1	32±3	44	0.02±0.0	20±10	-
17{*2,4,1*}	1.7±0.4	46±15	27	0.02±0.01	350±390	-
17{*2,4,2*}	2.4±0.4	29±2	12	0.05±0.02	190±320	-
17{*2,4,3*}	1.1±0.2	13±1	12	0.03±0.01	10±20	-
17{*2,4,4*}	1.7±0.2	16±3	10	1.4±0.13	Eq.[g]	-
17{*2,4,5*}	1.1±0.2	14±1	13	0.2±0.01	1060	-
17{*2,4,6*}	1.3±0.2	12±1	9	0.2±0.02	50±90	-
17{*2,5,1*}	1.5±0.3	26±1	18	2.2±0.2	Eq.[g]	-
17{*2,5,2*}	5.3±1.2	35±1	7	0.9±0.3	770±630	-
17{*2,5,3*}	1.6±0.3	35±2	22	0.8±0.1	Eq.[g]	-
17{*2,5,4*}	11.2±2.4	48±3	4	12±1	Eq.[g]	-
17{*2,5,5*}	0.9±0.1	26±2	29	2.8±0.4	Eq.[g]	-
17{*2,5,6*}	4.0±1.0	25±1	6	0.9±0.1	160±220	-
17{*3,1,1*}	3.6±1.0	66±12	18	5.5±0.6	380±30	10±18
17{*3,1,2*}	2.3±0.3	164±1	73	26±0.3	160±100	2±14
17{*3,1,3*}	0.6±0.1	98±16	177	38±2	760±70	48±18
17{*3,1,4*}	0.7±0.1	99±19	138	55±5	240±340	61±5
17{*3,1,5*}	0.5±0.1	107±25	202	44±4	360±60	45±19
17{*3,1,6*}	0.4±0.1	100±26	267	25±1	300±110	54±20
17{*3,2,1*}	2.9±0.8	66±11	23	3.4±0.4	220±90	2±12
17{*3,2,2*}	1.2±0.8	82±7	68	10±0.2	440±110	14±9
17{*3,2,3*}	0.7±0.2	56±9	79	10±1	560±80	4±12
17{*3,2,4*}	0.8±0.1	92±16	118	31±3	1100±610	6±13
17{*3,2,5*}	1.0±0.2	97±15	96	20±1	770±550	-7±5
17{*3,2,6*}	0.9±0.1	73±10	81	4.7±0.1	380±220	4±13

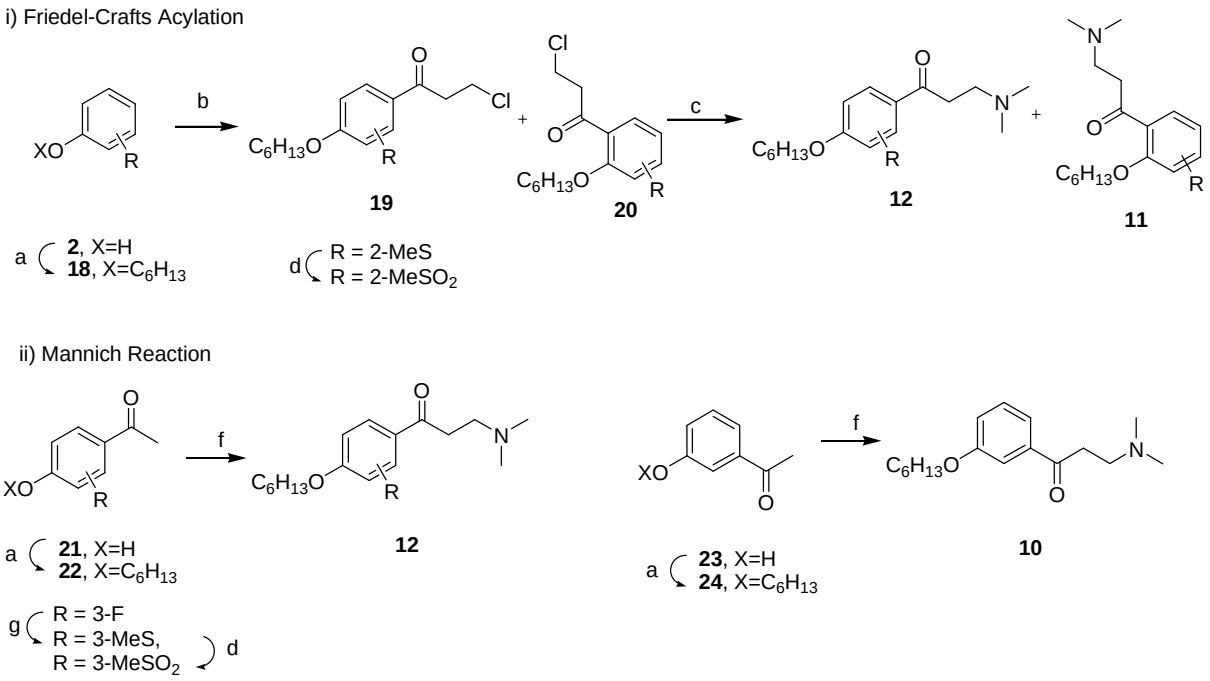
17{*3,3,1*}	2.1±0.5	63±9	30	7.2±0.5	90±30	1±6
17{*3,3,2*}	1.7±0.2	152±29	90	7.3±0.7	260±30	11±6
17{*3,3,3*}	0.9±0.2	72±22	79	13±2	680±200	15±16
17{*3,3,4*}	0.6±0.1	101±20	166	36±1	540±180	3±14
17{*3,3,5*}	0.8±0.1	87±20	104	19±2	670±80	1±6
17{*3,3,6*}	0.8±0.1	60±11	74	5.5±0.3	730±280	-7±12
17{*3,4,1*}	1.1±0.2	54±10	50	6.5±0.6	170±160	-5±17
17{*3,4,2*}	2.1±0.3	57±8	28	22±4	980±530	5±17
17{*3,4,3*}	0.8±0.2	39±3	47	4±1	470±120	9±14
17{*3,4,4*}	1.0±0.2	61±13	62	26±1	430±100	5±13
17{*3,4,5*}	0.7±0.1	43±8	62	14±1	480±50	4±10
17{*3,4,6*}	0.8±0.2	32±3	38	6±1	Und.[h]	13±12
17{*3,5,1*}	1.1±0.2	29±2	28	47±10	1880±910	26±11
17{*3,5,2*}	3.5±0.3	35±3	10	21±1	1200±370	18±10
17{*3,5,3*}	0.9±0.1	32±3	36	27±1	1140±170	36±11
17{*3,5,4*}	5.4±0.4	50±6	9	27±1	480±120	18±12
17{*3,5,5*}	1.2±0.1	28±3	24	28±1	470±80	32±8
17{*3,5,6*}	1.5±0.1	38±5	26	30±2	1010±410	20±15

[a]Values are the mean of three independent experiments in triplicate. [b]Values are means of two independent experiments in triplicate. [c]Values are EC_{50} over IC_{50}. [d,e]Values are the mean in triplicate. [f]Values are the mean of two independent experiments in quadruplicate.[g]Equilbration. [h]Undetected.

Chemistry. All materials were obtained from commercial suppliers and used without further purification. All solvents used were dried using an aluminum oxide column. Thin-layer chromatography was performed on pre-coated silica gel 60 F254 plates. Purification of compounds was carried out by normal phase column chromatography (SP1 [Biotage], Silica gel 230-400 mesh) followed by evaporation (HT-4X evaporator [Genevac]. Initiator [Biotage] was used for microwave reaction.

Chromatographic separation was performed using a UPLC-MS (BEH C18 1.7 μ, 2.1 x 50 mm column, Waters Corp.). Data were acquired using Masslynx v.4.1 and analyzed using the Openlynx software suite. The flow was then split to an evaporative light scattering detector (ELSD) and SQ mass spectrometer. The total flow rate was 1.0 mL/min and gradient program started at 90% A (0.1% formic acid in H_2O), changed to 95 % B (0.1% formic acid in ACN), then to 90% A. The mass spectrometer was operated in positive-ion mode with electrospray ionization. The conditions were as follows: capillary voltage 3.4 kV, cone voltage 30 V, source temperature 130 °C, desolvation temperature 400 °C, desolvation gas 800 L/hr, cone gas 100 L/hr. A full scan range from m/z = 110-1000 in 0.2 s was used to acquire MS data. The ELSD-drift tube temperature was set at 52 °C

NMR spectra are recorded on a Bruker 400 MHz and referenced internally to the residual resonance in $CDCl_3$ (δ 7.26 ppm) for hydrogen and (δ = 77 ppm) for carbon atoms. NMR peaks were assigned by MestRec (4.9.9.6) and MestReNova (5.2.2)



Reagent and condition. (a) Hexyl bromide, K_2CO_3, DMF, 80-90 °C, 12 h; (b)2-Chloropropyl chloride, $AlCl_3$, DCM, 0 °C; (c) 2 M dimethylamine/THF, THF, rt, 30 min; (d) *m*CPBA, DCM, 0 °C, 1 h; (e) dimethylamine hydrochloride, DMF, MW, 110 ^oC, 1 h (f) paraformaldehyde, dimethylamine hydrochloride, *c*-HCl, H_2O/MeCN (1/9, v/v), MW, 120 ^oC, 2 h; (g) NaSMe, DMF, rt, 1 h.

General procedure for 18 and **22:** To a solution the corresponding phenol **2** or **21** (5.3 mmol, 1 eq.) in DMF was added K_2CO_2 (10.6 mmol, 2 eq.) and n-hexylbromide (8.0 mmol, 1.5 eq.), and then stirred at 85 °C for overnight. The reaction mixture was poured to water and extracted with Et_2O. The combined organic layer were washed with brine and dried over $MgSO_4$ and concentrated *in vacuo* to yield crude compound **18** or **22**. The crude product **18** or **22** was used for next step without any purification. **Hexyloxybenzene 18.** ^1H NMR (400 MHz, $CDCl_3$) δ 7.28 (m, 2H), 6.92

(m, 2H), 3.96 (t, 2H, *J* = 6.6 Hz), 1.79 (m, 2H), 1.47 (m, 2H), 1.35 (m, 4H), 0.91 (t, 3H, *J* = 8.0 Hz); 159.11, 129.36, 120.41, 114.47, 67.85, 31.59, 29.26, 25.73, 22.60, 14.02.

1-(Hexyloxy)-2-methylbenzene 18{*1*}. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.14 (m, 2H), 6.83 (m, 2H), 3.96 (t, 2H, *J* = 6.4 Hz), 2.23 (s, 3H), 1.80 (m, 2H), 1.47 (m, 2H), 1.36 (m, 4H), 0.92 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.25, 130.52, 126.82, 126.65, 120.00, 110.91, 67.88, 31.58, 29.34, 25.82, 22.61, 16.20, 14.01.

1-(Hexyloxy)-3-methylbenzene 18{*2*}. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.17 (t, 1H, *J* = 7.8 Hz), 6.74 (m, 3H), 3.95 (m, 2H), 2.34 (m, 3H), 1.78 (m, 2H), 1.47 (m, 2H), 1.35 (m, 4H), 0.92 (t, 3H, *J* = 7.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.14, 139.36, 129.10, 121.24, 115.35, 111.31, 67.80, 31.59, 29.29, 25.74, 22.60, 21.50, 14.02.

1-(Hexyloxy)-3-methoxybenzene 18{*4*}. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.17 (t, 1H, *J* = 8.2 Hz), 6.49 (m, 3H), 3.94 (t, 2H, *J* = 6.6 Hz), 3.79 (s, 3H), 1.77 (m, 2H), 1.45 (m, 2H), 1.34 (m, 4H), 0.91 (t, 3H, *J* = 6.8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.81, 160.41, 129.78, 106.70, 106.08, 100.94, 68.00, 55.24, 31.58, 29.23, 25.73, 22.59, 14.02.

1-*tert*-Butyl-2-(hexyloxy)benzene 18{*8*}. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 (m, 1H), 7.18 (m, 1H), 6.89 (t, 2H, *J* = 7.7 Hz), 4.00 (t, 2H, *J* = 6.5 Hz), 1.87 (m, 2H), 1.54 (m, 2H), 1.41 (m, 13H), 0.94 (t, 3H, *J* = 7.0); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.89, 137.95, 126.90, 126.50, 119.90, 111.72, 67.67, 34.82, 31.54, 29.77, 29.44, 26.04, 22.57, 14.00.

1-Fluoro-2-(hexyloxy)benzene 18{*9*}. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.05 (m, 2H), 6.96 (m, 1H), 6.87 (m, 1H), 4.03 (t, 2H, *J* = 6.6 Hz), 1.82 (m, 2H), 1.47 (m, 2H), 1.33 (m, 4H)), 0.90 (m, 3H).

1-Chloro-2-(hexyloxy)benzene 18{*10*}. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 (m, 1H), 7.19 (m, 1H), 6.89 (m, 2H), 4.02 (t, 2H, *J* = 6.6 Hz), 1.84 (m, 2H), 1.50 (m, 2H), 1.36 (m, 4H), 0.91 (t, 3H, *J* = 8.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.62, 130.20, 127.58, 122.92, 121.05, 113.36, 69.10, 31.52, 29.07, 25.62, 22.57, 14.01.

1-Chloro-3-(hexyloxy)benzene 18{*11*}. ^{1}H NMR (400 MHz, CDCl3) δ 7.20 (t, 1H, *J* = 8.1 Hz), 6.93 (m, 2H), 6.80 (m, 1H), 3.96 (t, 2H, *J* = 6.6 Hz), 1.79 (m, 2H), 1.47 (m, 2H), 1.36 (m, 4H), 0.93 (t, 3H, *J* = 6.7); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.91, 134.78, 130.11, 120.59, 114.82, 113.06, 68.24, 31.53, 29.10, 25.66, 22.58, 14.01.

1-Bromo-2-(hexyloxy)benzene 18{*12*}. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (dd, 1H, *J* = 1.6, 7.9 Hz), 7.23 (m, 1H), 6.88 (m, 1H), 6.81 (m, 1H), 4.02 (t, 2H, *J* = 6.5), 1.84 (m, 2H), 1.51 (m, 2H), 1.35 (m, 4H), 0.91 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.47, 133.28, 128.33, 121.55, 113.19, 112.25, 77.31, 77.00, 76.68, 69.14, 31.50, 29.05, 25.65, 22.57, 14.01.

1-Bromo-3-(hexyloxy)benzene 18{*13*}. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.13 (dd, 1H, *J* = 6.9, 9.6 Hz), 7.06 (m, 2H), 6.82 (m, 1H), 3.93 (t, 2H, *J* = 6.6 Hz), 1.77 (m, 2H), 1.44 (m, 2H), 1.34 (m, 4H), 0.91 (t, 3H, *J* = 6.8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.95, 130.44, 123.51, 122.75, 117.71, 113.55, 68.25, 31.53, 29.09, 25.65, 22.57, 14.01.

1-(Hexyloxy)-2-iodobenzene 18{*14*}. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 (dd, 1H, *J* = 1.6, 7.8 Hz), 7.28 (m, 1H), 6.80 (m, 1H), 6.69 (m, 1H), 3.99 (m, 2H), 1.84 (m, 2H), 1.53 (m, 2H), 1.37 (m, 4H), 0.92 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.61, 139.36, 129.33, 122.23, 112.06, 86.71, 69.16, 31.48, 29.05, 25.74, 22.57, 14.02.

1-(Hexyloxy)-3-iodobenzene 18{*15*}. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26 (m, 2H), 6.99 (t, 1H, *J* = 7.9 Hz), 6.86 (m, 1H), 3.92 (t, 2H, *J* = 6.5 Hz), 1.77 (m, 2H), 1.46 (m, 2H), 1.34 (m, 4H), 0.92 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.72, 130.68, 129.57, 123.61, 114.21, 94.33, 68.17, 31.52, 29.10, 25.65, 22.57, 14.01.

(2-(Hexyloxy)phenyl)(methyl)sulfane 18{*16*}. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.11 (m, 2H), 6.93 (m, 1H), 6.81 (m, 1H), 4.01 (t, 2H, *J* = 6.6 Hz), 2.41 (s, 3H), 1.82 (m, 2H), 1.49 (m, 2H), 1.33 (m, 4H), 0.90 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.76, 127.26, 125.83, 125.67, 120.96, 111.10, 68.64, 31.55, 29.17, 25.72, 22.58, 14.56, 14.02.

3-Chloro-1-(4-(hexyloxy)-2,6-dimethylphenyl)propan-1-one 18{*22*}. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.54 (s, 1H), 3.93 (t, *J* = 6.6, 1H), 2.28 (t, *J* = 3.6, 3H), 1.82 – 1.70 (m, 1H), 1.53 – 1.40 (m, 1H), 1.40 – 1.28 (m, 2H), 0.92 (dd, *J* = 4.5, 9.6, 2H).

2-(Hexyloxy)biphenyl 18{*27*}. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (m, 2H), 7.40 (m, 2H), 7.31 (m, 3H), 7.01 (m, 2H), 3.96 (t, 2H, *J* = 6.5 Hz), 1.71 (m, 2H), 1.39 (m, 2H), 1.28 (m, 4H), 0.88 (t, 3H, *J* = 6.9 Hz) ; ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.03, 138.62, 130.92, 130.82, 129.59, 128.49, 127.75, 126.68, 120.69, 112.50, 68.42, 31.43, 29.12, 25.72, 22.56, 13.97.

1-Benzyl-2-(hexyloxy)benzene 18{*28*} ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26 (m, 4H), 7.19 (m, 2H), 7.11 (m, 1H), 6.88 (m, 2H), 4.00 (s, 2H), 3.96 (t, 2H, *J* = 6.4 Hz), 1.77 (m, 2H), 1.44 (m, 2H), 1.33 (m, 4H), 0.92 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.83, 141.20, 130.31, 129.79, 128.94, 128.14, 127.32, 125.66, 120.16, 111.17, 67.87, 36.13, 31.56, 29.31, 25.79, 22.59, 14.03.

General procedure for 19 and **20:** To a solution phenol **18** (0.50 g, 2.81 mmol) in DCM was added 3-chloropropanoic chloride (0.35 mL, 3.65 mmol) and $AlCl_3$ (0.49 g, 3.65 mmol) at 0 °C and stirred for 1 h. The reaction mixture was poured into ice water and extracted with DCM. The combined organic layer were washed with brine and dried over $MgSO_4$ and concentrated in vacuo to yield crude compound **19**. **3-Chloro-1-(4-(hexyloxy)phenyl)propan-1-one 19.** White solid; 82% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, 1H, *J* = 8.9 Hz), 6.95 (d, 1H, *J* = 8.9 Hz), 4.04 (t, 1H, *J* = 6.6 Hz), 3.94 (t, 1H, *J* = 6.9 Hz), 3.42 (t, 1H, *J* = 6.9 Hz), 1.82 (m, 1H), 1.49 (m, 1H), 1.37 (m, 2H), 0.93 (t, 2H, *J* = 7.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 238.90, 214.67, 182.95, 149.81, 148.72, 133.79, 87.80, 60.36, 58.47, 50.98, 48.50, 45.10, 42.03, 33.47

3-Chloro-1-(4-(hexyloxy)-3-methylphenyl)propan-1-one 19{*1*}. Yield 58%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (m, 2H), 6.83 (d, 1H, *J* = 8.5 Hz), 4.03 (t, 2H, *J* = 6.4 Hz), 3.91 (t, 2H, *J* = 7.0 Hz), 3.40 (t, 2H, *J* = 6.9 Hz), 2.25 (s, 3H), 1.82 (m, 2H), 1.49 (M, 2H), 1.35 (m, 4H), 0.91 (t, 3H, *J* = 7.1 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.47, 161.70, 130.60, 128.70, 128.17, 127.09, 110.02, 68.24, 40.85, 39.12, 31.48, 29.05, 25.70, 22.56, 16.25, 13.97.

3-Chloro-1-(4-(hexyloxy)-2-methylphenyl)propan-1-one 19{*2*}. Yield 52%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, 1H, *J* = 9.4 Hz), 6.76 (m, 2H), 4.00 (m, 2H), 3.89 (t, 2H, *J* = 6.8 Hz), 3.37 (t, 2H, *J* = 6.8 Hz), 2.56 (s, 3H), 1.79 (m, 2H), 1.55 (s, 1H), 1.46 (s, 2H), 1.35 (m, 4H), 0.91 (t, 3H, *J* = 6.9 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.83, 161.86, 142.57, 131.77, 128.89, 118.18, 111.15, 77.31, 77.00, 76.68, 68.10, 43.02, 39.39, 31.53, 31.52, 29.06, 25.64, 22.57, 22.50, 14.01,

1-(3-*tert*-Butyl-4-(hexyloxy)phenyl)prop-2-en-1-one 19{*8*}.This compound was shown enone as a major product and chloroketone as a minor product in crude NMR. The crude mixture was reacted with DBU to give eliminated product enone . Two step yield 18%, para/meta=49/51; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 (d, 1H, *J* = 2.5 Hz), 7.45 (dd, 1H, *J* = 2.6, 8.7 Hz), 7.09 (m, 1H), 6.87 (d, 1H, *J* = 8.7 Hz), 6.29 (m, 1H, *J* = 1.8, 17.2 Hz), 5.73 (dd, 1H, *J* = 1.8, 10.4 Hz), 4.00 (t, 2H, *J* = 6.4 Hz), 1.77 (m, 2H), 1.44 (s, 3H), 1.31 (m, 14H), 0.91 (d, 3H, *J* = 7.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.67, 162.09, 138.27, 132.38, 129.30, 128.93, 128.73, 127.72, 111.10, 68.23, 35.01, 31.45, 29.57, 29.18, 25.94, 22.51, 13.96,

3-Chloro-1-(4-(hexyloxy)-2-methoxyphenyl)propan-1-one 19{*4*}. Yield 16%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (d, 1H, *J* = 8.8 Hz), 6.52 (dd, 1H, *J* = 2.2, 8.8 Hz), 6.45 (d, 1H, *J* = 2.2 Hz), 4.00 (t, 2H, *J* = 6.6 Hz), 3.87 (m, 5H), 3.43 (t, 2H, *J* = 6.9 Hz), 1.79 (m, 2H), 1.46 (m, 2H), 1.34 (m, 4H), 0.91 (t, 3H, *J* = 6.9 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.07, 164.50, 161.07, 132.80, 119.88, 105.85, 98.64, 68.34, 55.43, 46.42, 39.44, 31.49, 29.04, 25.60, 22.53, 13.97,

3-Chloro-1-(4-(hexyloxy)-3-(methylthio)phenyl)propan-1-one 19{*5*}. Yield 59%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, 1H, *J* = 2.0 Hz), 7.71 (dd, 1H, *J* = 2.1, 8.5 Hz), 6.82 (d, 1H, *J* = 8.5 Hz), 4.08 (t, 2H, *J* = 6.5 Hz), 3.90 (t, 2H, *J* = 6.9 Hz), 3.40 (m, 2H), 2.45 (m, 3H), 1.85 (m, 2H), 1.50 (m, 2H), 1.33 (m, 4H), 0.89 (t, 3H, *J* = 7.1 Hz)

3-Chloro-1-(2-fluoro-4-(hexyloxy)phenyl)propan-1-one 19{*7*}. Yield 34%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (t, 1H, *J* = 8.8 Hz), 6.75 (dd, 1H, *J* = 2.4, 8.9 Hz), 6.60 (dd, 1H, *J* = 2.3, 13.4 Hz), 4.00 (t, 2H, *J* = 6.6 Hz), 3.89 (m, 2H), 3.42 (m, 2H), 1.80 (m, 2H), 1.46 (m, 2H), 1.34 (m, 4H), 0.91

(t, 3H, *J* = 7.1 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.32, 158.78, 130.38, 129.62, 128.44, 123.33, 112.14, 77.31, 77.00, 76.68, 69.42, 40.88, 38.70, 31.43, 28.82, 25.53, 22.53, 13.98.

3-Chloro-1-(3-fluoro-4-(hexyloxy)phenyl)propan-1-one 19{*9*}. Yield 91%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (m, 2H), 6.99 (t, 1H, *J* = 8.4 Hz), 4.10 (m, 2H), 3.90 (t, 2H, *J* = 6.8 Hz), 3.38 (t, 1H, *J* = 6.8 Hz), 1.84 (m, 2H), 1.47 (m, 2H), 1.33 (m, 5H), 0.90 (m, 3H)

3-Chloro-1-(3-chloro-4-(hexyloxy)phenyl)propan-1-one 19{*10*}. Yield 92%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, 1H, *J* = 2.2 Hz), 7.85 (dd, 1H, *J* = 2.2, 8.6 Hz), 6.95 (d, 1H, *J* = 8.6 Hz), 4.10 (t, 2H, *J* = 6.5 Hz), 3.91 (t, 2H, *J* = 6.8 Hz), 3.39 (t, 2H, *J* = 6.8 Hz), 1.87 (m, 2H), 1.52 (m, 2H), 1.36 (m, 4H), 0.91 (t, 3H, *J* = 7.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.32, 158.78, 130.38, 129.62, 128.44, 123.33, 112.14, 77.31, 77.00, 76.68, 69.42, 40.88, 38.70, 31.43, 28.82, 25.53, 22.53, 13.98,

3-Chloro-1-(2-chloro-4-(hexyloxy)phenyl)propan-1-one 19{*11*}. Beta-chloro/enone 1:0.7 Yield 14%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (d, 1H, *J* = 8.7 Hz), 6.93 (d, 1H, *J* = 3.2 Hz), 6.83 (m, 1H), 3.99 (t, 2H, *J* = 6.5 Hz), 3.89 (m, 2H), 3.46 (t, 2H, *J* = 6.7 Hz), 1.79 (m, 2H), 1.46 (m, 2H), 1.34 (m, 4H), 0.91 (t, 3H, *J* = 6.7 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.19, 162.22, 136.04, 133.75, 132.01, 130.28, 116.63, 113.34, 68.67, 45.13, 38.99, 31.47, 28.92, 25.57, 22.56, 14.00,

1-(3-Bromo-4-(hexyloxy)phenyl)-3-chloropropan-1-one 19{*12*}. Yield 90%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (d, 1H, *J* = 2.2 Hz), 7.89 (dd, 1H, *J* = 2.2, 8.6 Hz), 6.91 (d, 1H, *J* = 8.7 Hz), 4.10 (t, 2H, *J* = 6.5 Hz), 3.90 (t, 2H, *J* = 6.8 Hz), 3.38 (t, 2H, *J* = 6.8 Hz), 1.86 (m, 2H), 1.53 (m, 2H), 1.36 (m, 4H), 0.91 (t, 3H, *J* = 7.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.19, 159.60, 133.56, 130.08, 129.16, 112.45, 111.96, 77.31, 77.00, 76.68, 69.49, 40.87, 38.70, 31.41, 28.81, 25.55, 22.52, 13.98,

1-(2-Bromo-4-(hexyloxy)phenyl)-3-chloropropan-1-one 19{*13*}. Beta-chloro/eneone 0.8/1 Yield 9%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (d, 1H, *J* = 8.7 Hz), 7.40 (d, 1H, *J* = 8.6 Hz), 7.14 (s, 1H), 6.87 (d, 1H, *J* = 8.6 Hz), 3.98 (t, 2H, *J* = 6.5 Hz), 3.88 (t, 2H, *J* = 6.7 Hz), 3.43 (t, 2H, *J* = 6.9 Hz), 1.78 (m, 2H), 1.45 (m, 2H), 1.34 (m, 4H), 0.91 (t, 3H, *J* = 6.9 Hz).

3-Chloro-1-(4-(hexyloxy)-3-iodophenyl)propan-1-one 19{*14*}. Yield 56%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.38 (d, 1H, *J* = 2.2 Hz), 7.93 (dd, 1H, *J* = 2.2, 8.6 Hz), 6.82 (d, 1H, *J* = 8.7 Hz), 4.09 (t, 2H, *J* = 6.4 Hz), 3.90 (t, 2H, *J* = 6.8 Hz), 3.38 (t, 2H, *J* = 6.8 Hz), 1.86 (m, 2H), 1.54 (d, 2H, *J* = 5.5 Hz), 1.36 (m, 4H), 0.92 (t, 3H, *J* = 7.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.04, 161.67, 139.81, 130.77, 130.19, 110.88, 86.60, 69.60, 40.87, 38.72, 31.40, 28.83, 25.65, 22.54, 13.99,

3-Chloro-1-(4-(hexyloxy)-2-iodophenyl)propan-1-one 19{*15*}. beta-chloro/eneone 1/0.7 Yield 11%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (d, 1H, *J* = 8.7 Hz), 7.50 (d, 1H, *J* = 2.5 Hz), 6.91 (m, 1H), 3.97 (m, 2H), 3.88 (t, 2H, *J* = 6.8 Hz), 3.38 (t, 2H, *J* = 6.8 Hz), 1.78 (m, 2H), 1.45 (m, 2H), 1.33 (m, 4H), 0.90 (t, 3H, *J* = 6.9 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 204.20, 167.94, 141.77, 137.15, 134.27, 133.18, 120.45, 99.61, 75.05, 49.78, 45.47, 37.93, 35.41, 32.03, 29.01, 20.46.

General procedure for oxidation of thioether to sulfonyl compound- Synthesis of compound 21{*16*} To a solution of **19{**5**}** in DCM was added *m*CPBA (2.2 eq) at 0 ^{o}C and stirred for 1 h. The reaction mixture was poured to water and extracted with DCM. The combined organic layer was washed with $NaHCO_3$ and brine, dried over $MgSO_4$, and concentrated *in vacuo* to yield the corresponding sulfonyl compound. **3-Chloro-1-(4-(hexyloxy)-3-(methylsulfonyl)phenyl)propan-1-one 19{*16*}.** ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.51 (d, 1H, *J* = 2.3 Hz), 8.21 (dd, 1H, *J* = 2.3, 8.8

Hz), 7.11 (d, 1H, *J* = 8.8 Hz), 4.22 (t, 2H, *J* = 6.6 Hz), 3.89 (t, 2H, *J* = 6.6 Hz), 3.43 (t, 2H, *J* = 6.6 Hz), 3.23 (s, 3H), 1.90 (m, 2H), 1.50 (m, 2H), 1.34 (m, 4H), 0.89 (m, 3H).

3-Chloro-1-(4-(hexyloxy)-2,6-dimethylphenyl)propan-1-one 19{*22*}. Beta-chloro/enone 1/1 Yield 10%**;** ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.55 (s, 2H), 3.93 (m, 2H), 3.86 (m, 2H), 3.16 (t, 2H, *J* = 6.5 Hz), 2.23 (s, 6H), 2.15 (s, 6H), 1.76 (m, 2H), 1.45 (m, 2H), 1.34 (m, 4H), 0.91 (t, 3H, *J* = 7.1 Hz)

3-Chloro-1-(6-(hexyloxy)biphenyl-3-yl)propan-1-one 19{*27*}. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (m, 2H), 7.54 (m, 2H), 7.42 (dd, 2H, *J* = 6.9, 7.6 Hz), 7.36 (dd, 1H, *J* = 4.6, 11.4 Hz), 7.01 (m, 1H), 4.06 (t, 2H, *J* = 6.5 Hz), 3.93 (t, 2H, *J* = 6.9 Hz), 3.44 (t, 2H, *J* = 6.9 Hz), 1.75 (m, 2H), 1.40 (m, 2H), 1.29 (m, 4H), 0.88 (t, 3H, *J* = 6.8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.29, 160.33, 137.42, 131.17, 130.89, 129.49, 129.41, 129.23, 127.96, 127.31, 111.55, 68.64, 40.93, 39.01, 31.33, 28.83, 25.60, 22.50, 13.93.

1-(3-Benzyl-4-(hexyloxy)phenyl)-3-chloropropan-1-one 19{*28*}. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (dd, 1H, *J* = 2.3, 8.6 Hz), 7.77 (d, 1H, *J* = 2.2 Hz), 7.27 (m, 2H), 7.19 (m, 3H), 6.87 (d, 1H, *J* = 8.6 Hz), 4.01 (m, 4H), 3.89 (t, 2H, *J* = 6.9 Hz), 3.37 (t, 2H, *J* = 6.9 Hz), 1.77 (m, 2H), 1.40 (m, 2H), 1.31 (m, 4H), 0.90 (t, 3H, *J* = 6.6 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.34, 161.29, 140.23, 130.54, 130.10, 128.90, 128.77, 128.28, 126.00, 110.55, 68.33, 40.83, 39.04, 36.26, 31.48, 29.03, 25.66, 22.54, 14.00.

3-Chloro-1-(2-(hexyloxy)-4-methylphenyl)propan-1-one 20. Yield 36%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, 1H, *J* = 7.9 Hz), 6.80 (d, 1H, *J* = 7.9 Hz), 6.75 (s, 1H), 4.06 (t, 2H, *J* = 6.5 Hz),

3.86 (m, 2H), 3.49 (t, 2H, *J* = 7.0 Hz), 2.36 (s, 3H), 1.86 (m, 2H), 1.50 (m, 2H), 1.36 (m, 4H), 0.91 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 217.21, 178.24, 164.84, 150.21, 143.85, 140.93, 132.38, 88.03, 66.35, 58.85, 50.99, 48.66, 45.46, 42.04, 41.37, 33.49.

General procedure for 11 and **12:** To a solution compound **19** or **20** in THF was added 1 M dimethylamine solution (5 eq.) in THF and stirred at rt for 1 h. The reaction mixture was subjected to empty SPE cartridge to filter solid HCl salt off and washed with ether. The combined organic layer were concentrated in vacuo to yield aminoketone **11**or **12**.

3-(Dimethylamino)-1-(4-(hexyloxy)phenyl)propan-1-one 9. Yield 92% ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (d, 2H, *J* = 8.9 Hz), 6.91 (d, 2H, *J* = 8.9 Hz), 4.01 (t, 2H, *J* = 6.6 Hz), 3.11 (m, 2H), 2.76 (m, 2H), 2.29 (s, 6H), 1.79 (m, 2H), 1.45 (m, 2H), 1.34 (m, 4H), 0.91 (t, 3H, *J* = 6.9 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.58, 163.12, 130.30, 129.75, 114.17, 68.24, 54.57, 45.46, 36.46, 31.50, 29.04, 25.62, 22.55, 13.98; MS (ESI) *m/z* 278.4 $[M+H]^+$.

3-(Dimethylamino)-1-(2-(hexyloxy)-4-methylphenyl)propan-1-one 11. Yield 89% ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, 1H, *J* = 7.9 Hz), 6.76 (t, 1H, *J* = 6.3 Hz), 6.73 (m, 1H), 4.02 (t, 2H, *J* = 6.2), 3.19 (m, 2H), 2.70 (m, 2H), 2.35 (s, 3H), 2.26 (m, 6H), 1.84 (m, 2H), 1.47 (m, 2H), 1.34 (m, 4H), 0.89 (t, 3H, *J* = 7.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 220.10, 177.84, 163.94, 150.03, 144.96, 140.75, 132.35, 87.93, 73.91, 64.86, 61.53, 51.01, 48.72, 45.41, 42.05, 41.30, 33.48; MS (ESI) *m/z* 292.2 $[M+H]^+$.

3-(Dimethylamino)-1-(4-(hexyloxy)-3-methylphenyl)propan-1-one 12{*1*}. Yield 100%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (m, 2H), 6.82 (d, 1H, *J* = 8.5 Hz), 4.02 (t, 2H, *J* = 6.4 Hz), 3.11 (m, 2H), 2.76 (m, 2H), 2.30 (s, 6H), 2.24 (s, 3H), 1.82 (m, 2H), 1.46 (m, 2H), 1.36 (m, 4H), 0.90 (t, 3H, *J* = 7.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.87, 161.35, 130.64, 129.19, 128.11, 126.90, 109.93, 68.17, 54.66, 45.44, 36.41, 31.49, 29.08, 25.71, 22.55, 16.26, 13.97; MS (ESI) *m/z* 292.4 $[M+H]^+$.

3-(Dimethylamino)-1-(4-(hexyloxy)-2-methylphenyl)propan-1-one 12{*2*}. Yield 98%;^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (m, 1H), 6.74 (m, 2H), 3.99 (t, 2H, *J* = 6.6 Hz), 3.07 (t, 2H, *J* = 7.4 Hz), 2.72 (m, 2H), 2.53 (s, 3H), 2.28 (s, 6H), 1.78 (m, 2H), 1.45 (d, 2H, *J* = 7.9 Hz), 1.34 (m, 5H), 0.91 (t, 3H, *J* = 6.9 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 220.17, 180.92, 161.52, 151.02, 149.18, 137.52, 130.47, 87.50, 74.27, 64.94, 58.45, 51.00, 48.56, 45.12, 42.04, 41.86, 33.48; MS (ESI) *m/z* 292.2 $[M+H]^+$.

3-(Dimethylamino)-1-(4-(hexyloxy)-2-methoxyphenyl)propan-1-one 12{*4*}. Yield 90%;^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (t, 1H, *J* = 7.6 Hz), 6.47 (dd, 1H, *J* = 2.2, 8.8 Hz), 6.41 (d, 1H, *J* = 2.2 Hz), 3.97 (q, 2H, *J* = 6.9 Hz), 3.86 (s, 3H), 3.20 (t, 2H, *J* = 7.4 Hz), 2.79 (m, 2H), 2.33 (s, 6H), 1.75 (m, 2H), 1.42 (m, 2H), 1.30 (m, 4H), 0.87 (t, 3H, *J* = 7.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.17, 164.14, 160.81, 132.59, 120.39, 105.65, 98.60, 68.22, 55.39, 54.23, 44.94, 41.09, 31.42, 28.98, 25.54, 22.46, 13.90; MS (ESI) *m/z* 308.4 $[M+H]^+$.

3-(Dimethylamino)-1-(4-(hexyloxy)-3-(methylthio)phenyl)propan-1-one 12{*5*}. Yield 93%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (m, 2H), 6.80 (d, 1H, *J* = 8.5 Hz), 4.07 (t, 2H, *J* = 6.5 Hz), 3.09 (t, 2H, *J* = 7.4 Hz), 2.74 (m, 2H), 2.43 (d, 3H, *J* = 3.6 Hz), 2.27 (m, 6H), 1.83 (m, 2H), 1.48 (m, 2H),

1.34 (m, 4H), 0.88 (t, 3H, *J* = 7.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.46, 159.32, 130.05, 128.46, 126.78, 125.16, 109.68, 68.93, 54.58, 45.45, 36.44, 31.43, 28.89, 25.58, 22.49, 14.28, 13.95; MS (ESI) *m/z* 324.5 $[M+H]^+$.

1-(3-*tert*-Butyl-4-(hexyloxy)phenyl)-3-(dimethylamino)propan-1-one 12{*8*}. Yield 98%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (d, 1H, *J* = 2.2 Hz), 7.82 (dd, 1H, *J* = 2.3, 8.6 Hz), 6.87 (d, 1H, *J* = 8.6 Hz), 4.05 (t, 2H, *J* = 6.5 Hz), 3.74 (t, 1H, *J* = 6.7 Hz), 3.11 (m, 2H), 2.75 (m, 2H), 2.30 (s, 6H), 1.87 (m, 2H), 1.52 (m, 2H), 1.37 (m, 13H), 0.91 (t, 3H, *J* = 7.1 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.12, 161.98, 138.06, 129.10, 128.23, 127.00, 111.04, 68.20, 54.74, 45.50, 36.47, 34.98, 31.45, 29.57, 29.18, 25.94, 22.51, 13.96; MS (ESI) *m/z* 334.5 $[M+H]^+$.

1-(3-Fluoro-4-(hexyloxy)phenyl)-3-(dimethylamino)propan-1-one 12{*9*} ^{1}HNMR (400 MHz, $CDCl_3$) δ 7.75 – 7.67 (m, 2H), 6.97 (t, *J* = 8.3, 1H), 4.10 (T, *J* = 6.7, 2H), 3.10 (t, *J* = 7.4, 2H), 2.77 (t, *J* = 7.3, 2H), 2.31 (s, 6H), 1.91 – 1.75 (m, 2H), 1.47 (M, 2H), 1.34 (M, *J* = 3.6, 7.4, 6H), 0.90 (t, *J* = 7.2, 4H). NMR (101 MHz, $CDCl_3$) δ 196.63, 196.61, 153.31, 151.54, 151.43, 150.84, 129.88, 129.83, 125.26, 125.22, 115.77, 115.58, 113.21, 113.20, 69.33, 67.96, 54.29, 45.32, 36.33, 31.42, 31.41, 31.35, 28.89, 28.59, 25.47, 25.32, 22.49, 22.45, 13.94; MS (ESI) *m/z* 296.4 $[M+H]^+$.

1-(3-Chloro-4-(hexyloxy)phenyl)-3-(dimethylamino)propan-1-one 12{*10*}. Yield 99%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, 1H, *J* = 2.2 Hz), 7.84 (dd, 1H, *J* = 2.2, 8.6 Hz), 6.93 (dd, 1H, *J* = 3.1, 8.6 Hz), 4.08 (m, 2H), 3.07 (m, 2H), 2.74 (m, 2H), 2.29 (s, 6H), 1.86 (m, 2H), 1.49 (m, 2H), 1.34 (m, 4H), 0.91 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 216.15, 177.88, 149.85, 149.64, 147.86,

142.63, 131.55, 96.81, 96.49, 96.17, 88.81, 73.87, 64.94, 55.96, 50.91, 48.32, 45.01, 42.00, 33.45; MS (ESI) *m/z* 312.9 $[M+H]^+$.

1-(2-Chloro-4-(hexyloxy)phenyl)-3-(dimethylamino)propan-1-one 12{*11*}. Yield 100%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (d, 1H, *J* = 8.7 Hz), 6.92 (d, 1H, *J* = 2.4 Hz), 6.82 (dd, 1H, *J* = 2.5, 8.7 Hz), 3.98 (t, 2H, *J* = 6.5 Hz), 3.16 (t, 2H, *J* = 7.3 Hz), 2.74 (t, 2H, *J* = 7.3 Hz), 2.28 (s, 6H), 1.78 (m, 2H), 1.45 (m, 2H), 1.34 (m, 4H), 0.91 (t, 3H, *J* = 6.7 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.99, 161.73, 133.29, 131.59, 130.57, 116.46, 113.18, 68.57, 54.43, 45.32, 40.70, 31.47, 28.93, 25.57, 22.54, 13.98; MS (ESI) *m/z* 312.9 $[M+H]^+$.

1-(3-Bromo-4-(hexyloxy)phenyl)-3-(dimethylamino)propan-1-one 12{*12*}. Yield 100%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (d, 1H, *J* = 2.1 Hz), 7.86 (dd, 1H, *J* = 2.1, 8.6 Hz), 6.87 (d, 1H, *J* = 8.7 Hz), 4.05 (t, 2H, *J* = 6.5 Hz), 3.06 (t, 2H, *J* = 7.3 Hz), 2.73 (t, 2H, *J* = 7.3 Hz), 2.27 (s, 6H), 1.83 (m, 2H), 1.48 (m, 2H), 1.33 (m, 4H), 0.88 (t, 3H, *J* = 7.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.40, 159.15, 133.46, 130.52, 129.06, 112.25, 111.82, 69.33, 54.29, 45.35, 36.35, 31.35, 28.76, 25.48, 22.45, 13.91; MS (ESI) *m/z* 357.3 $[M+H]^+$.

1-(2-Bromo-4-(hexyloxy)phenyl)-3-(dimethylamino)propan-1-one 12{*13*}. Yield 97%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (d, 1H, *J* = 8.7 Hz), 7.13 (d, 1H, *J* = 2.4 Hz), 6.86 (dd, 1H, *J* = 2.5, 8.6 Hz), 3.97 (m, 2H), 3.13 (m, 2H), 2.72 (t, 2H, *J* = 7.3 Hz), 2.26 (s, 6H), 1.78 (m, 2H), 1.44 (m, 2H), 1.33 (m, 4H), 0.90 (t, 3H, *J* = 7.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 200.94, 161.32, 132.65, 131.02, 120.77, 119.88, 113.52, 68.56, 54.45, 45.36, 40.37, 31.47, 28.94, 25.57, 22.54, 13.98; MS (ESI) *m/z* 357.2 $[M+H]^+$.

3-(Dimethylamino)-1-(4-(hexyloxy)-3-iodophenyl)propan-1-one 12{*14*}. Yield 100%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.38 (d, 1H, *J* = 2.2 Hz), 7.92 (dd, 1H, *J* = 2.2, 8.6 Hz), 6.79 (d, 1H, *J* = 8.7 Hz), 4.07 (t, 2H, *J* = 6.4 Hz), 3.07 (t, 2H, *J* = 7.4 Hz), 2.73 (t, 2H, *J* = 7.3 Hz), 2.28 (s, 6H), 1.85 (m, 3H), 1.51 (m, 2H), 1.36 (m, 4H), 0.91 (t, 3H, *J* = 7.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.41, 161.26, 139.78, 131.28, 130.12, 110.78, 86.51, 69.49, 54.41, 45.47, 36.49, 31.38, 28.82, 25.63, 22.51, 13.97; MS (ESI) *m/z* 404.3 $[M+H]^+$.

3-(Dimethylamino)-1-(4-(hexyloxy)-2-iodophenyl)propan-1-one 12{*15*}. Yield 92%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (dd, 2H, *J* = 5.6, 12.5 Hz), 6.89 (dd, 1H, *J* = 2.5, 8.6 Hz), 3.96 (t, 2H, *J* = 6.5 Hz), 3.08 (t, 2H, *J* = 7.4 Hz), 2.73 (t, 2H, *J* = 7.3 Hz), 2.27 (m, 6H), 1.77 (m, 2H), 1.44 (m, 2H), 1.34 (m, 4H), 0.91 (t, 3H, *J* = 6.6 Hz) ; ^{13}C NMR (100 MHz, $CDCl_3$) δ 200.72, 161.03, 134.52, 130.21, 127.40, 113.90, 92.89, 68.50, 54.48, 45.38, 39.31, 31.46, 28.95, 25.56, 22.54, 13.98; MS (ESI) *m/z* 404.3 $[M+H]^+$.

3-(Dimethylamino)-1-(4-(hexyloxy)-3-(methylsulfonyl)phenyl)propan-1-one 12{*16*}. Yield 95%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.51 (d, 1H, *J* = 2.2 Hz), 8.18 (dd, 1H, *J* = 2.3, 8.8 Hz), 7.05 (d, 1H, *J* = 8.8 Hz), 4.17 (t, 2H, *J* = 6.6 Hz), 3.18 (s, 3H), 3.13 (t, 2H, *J* = 7.2 Hz), 2.78 (t, 2H, *J* = 7.1 Hz), 2.29 (m, 6H), 1.83 (m, 3H), 1.45 (m, 2H), 1.38 (m, 4H), 0.86 (t, 3H, *J* = 7.1 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.13, 160.19, 135.43, 130.21, 129.45, 128.41, 113.02, 69.99, 53.98, 45.21, 42.90, 36.19, 31.32, 28.77, 25.50, 22.43, 13.92; MS (ESI) *m/z* 356.4 $[M+H]^+$.

3-(Dimethylamino)-1-(4-(hexyloxy)-2,6-dimethylphenyl)propan-1-one 12{*22*}. Yield 93%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.54 (s, 2H), 3.92 (t, 2H, *J* = 6.5 Hz), 2.88 (t, 2H, *J* = 7.5 Hz), 2.71 (t, 2H, *J* = 7.0 Hz), 2.25 (s, 6H), 2.21 (s, 6H), 1.75 (m, 2H), 1.44 (m, 2H), 1.33 (m, 4H), 0.90 (t, 3H, *J* = 7.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 209.16, 159.04, 134.90, 134.66, 113.72, 67.85, 53.88, 45.42, 43.35, 31.54, 29.18, 25.68, 22.58, 19.60, 14.01; MS (ESI) *m/z* 306.5 $[M+H]^+$.

3-(Dimethylamino)-1-(6-(hexyloxy)biphenyl-3-yl)propan-1-one 12{*27*}. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (m, 2H), 7.53 (m, 2H), 7.41 (m, 2H), 7.34 (m, 1H), 6.99 (d, 1H, *J* = 8.2 Hz), 4.04 (t, 2H, *J* = 6.5 Hz), 3.15 (m, 2H), 2.78 (m, 2H), 2.28 (s, 6H), 1.74 (m, 2H), 1.40 (m, 2H), 1.29 (m, 4H), 0.89 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.61, 159.95, 137.56, 131.16, 130.69, 129.72, 129.49, 129.35, 127.89, 127.18, 111.44, 68.55, 54.51, 45.40, 36.44, 31.31, 28.83, 25.59, 22.48, 13.90; MS (ESI) *m/z* 354.5 $[M+H]^+$.

1-(3-Benzyl-4-(hexyloxy)phenyl)-3-(dimethylamino)propan-1-one 12{*28*} ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (dd, 1H, *J* = 2.2, 8.5 Hz), 7.80 (d, 1H, *J* = 2.2 Hz), 7.24 (m, 5H), 6.88 (d, 1H, *J* = 8.6 Hz), 4.02 (m, 4H), 3.09 (m, 2H), 2.75 (m, 2H), 2.30 (s, 6H), 1.79 (m, 2H), 1.43 (m, 2H), 1.33 (m, 4H), 0.92 (t, 3H, *J* = 6.7 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.81, 160.91, 140.36, 130.60, 129.89, 129.40, 128.79, 128.68, 128.25, 125.93, 110.45, 68.24, 54.65, 45.44, 36.44, 36.25, 31.48, 29.05, 25.66, 22.54, 13.99; MS (ESI) *m/z* 368.5 $[M+H]^+$.

General procedure for 22 and 24: To a solution phenol **21{*3*}** (1.0 eq.) in DMF was added K_2CO_2 (2.0 eq.) and n-hexylbromide (1.5 eq.), and then stirred at 85 °C for overnight. The reaction mixture

was poured to water and extracted with Et_2O. The combined organic layer were washed with brine and dried over $MgSO_4$ and concentrated *in vacuo* to yield crude compound **9**. Most of products were used for next step without any purification. **1-(4-(Hexyloxy)-3-methoxyphenyl)ethanone 22{*3*}.** ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (m, 2H), 6.87 (d, 1H, *J* = 8.3 Hz), 4.07 (m, 2H), 3.92 (s, 3H), 2.56 (s, 3H), 1.87 (m, 2H), 1.47 (m, 2H), 1.35 (m, 4H), 0.90 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.78, 152.97, 149.22, 130.21, 123.21, 111.02, 110.44, 69.05, 56.03, 31.52, 28.91, 26.17, 25.56, 22.54, 13.98.

Synthesis of compound 22{*6*}: To a solution of compound **21{*7*, *R=3-F*}** in DMF was added NaSMe and stirred at rt for 1 h. The reaction mixture was poured into water and extracted with Et_2O. The combined organic layer was washed with brine, dried over with $MgSO_4$. After concentration under vacuum, the crude mixture was purified on normal phase column chlromatography (SP1, Biotage) to yield the desired product. **1-(4-(Hexyloxy)-2-(methylthio)phenyl)ethanone 22{*6*}.** ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (d, 1H, *J* = 8.7 Hz), 6.77 (d, 1H, *J* = 2.4 Hz), 6.64 (dd, 1H, *J* = 2.4, 8.7 Hz), 4.02 (t, 2H, *J* = 6.6 Hz), 2.55 (s, 3H), 2.39 (s, 3H), 1.80 (m, 2H), 1.45 (m, 2H), 1.34 (m, 4H), 0.91 (t, 3H, *J* = 8.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.99, 162.27, 145.93, 133.74, 126.82, 111.08, 108.25, 68.25, 31.52, 29.07, 27.62, 25.64, 22.56, 15.78, 14.00.

1-(2-Fluoro-4-(hexyloxy)phenyl)ethanone 22{7}. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (t, 1H, *J* = 8.8 Hz), 6.72 (dd, 1H, *J* = 2.4, 8.9 Hz), 6.58 (m, 1H), 3.98 (t, 2H, *J* = 6.6 Hz), 2.57 (d, 3H, *J* = 5.2 Hz), 1.78 (m, 2H), 1.45 (m, 2H), 1.33 (m, 4H), 0.90 (t, 3H, *J* = 8.0 Hz); ^{13}C NMR (100 MHz,

$CDCl_3$) δ 194.42 (d, *J* = 2.0 Hz), 165.10, 164.44 (d, *J* = 5.9 Hz), 163.84 (d, *J* = 127.55 Hz), 131.95 (d, *J* = 2.2 Hz), 118.28 (d, *J* = 7.5 Hz), 111.04 (d, *J* = 1.2 Hz), 101.95 (d, *J* = 13.8 Hz), 68.71, 31.31 (d, *J* = 13.6 Hz), 28.87, 25.54, 22.52, 13.95.

General procedure for oxidation of thioether to sulfonyl compound- Synthesis of compound 22{17} To a solution of **22**{6} in DCM was added *m*CPBA (2.2 eq) at 0 ^{o}C and stirred for 1 h. The reaction mixture was poured to water and extracted with DCM. The combined organic layer was washed with $NaHCO_3$ and brine, dried over $MgSO_4$, and concentrated in vacuo to yield the corresponding sulfonyl compound.**1-(4-(Hexyloxy)-2-(methylsulfonyl)phenyl)ethanone 22**{17}**.** ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (d, 1H, *J* = 2.6 Hz), 7.47 (d, 1H, *J* = 8.5 Hz), 7.12 (dd, 1H, *J* = 2.6, 8.5 Hz), 4.04 (t, 2H, *J* = 6.5 Hz), 3.33 (s, 3H), 2.60 (s, 3H), 1.80 (m, 2H), 1.45 (m, 2H), 1.34 (m, 4H), 0.91 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 201.84, 160.46, 140.08, 133.41, 129.07, 118.79, 115.90, 68.86, 45.92, 31.42, 30.47, 28.88, 25.53, 22.52, 13.96.

1-(4-(Hexyloxy)-3-(trifluoromethyl)phenyl)ethanone 22{*18*}. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (d, 1H, *J* = 2.2 Hz), 8.10 (dd, 1H, *J* = 2.2, 8.7 Hz), 7.02 (d, 1H, *J* = 8.7 Hz), 4.11 (t, 2H, *J* = 6.4 Hz), 2.57 (s, 3H), 1.83 (m, 2H), 1.48 (m, 2H), 1.33 (m, 4H), 0.90 (t, 3H, *J* = 8.0 Hz).

1-(4-(Hexyloxy)-2-(trifluoromethyl)phenyl)ethanone 22{*19*}. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 (d, 1H, *J* = 8.6 Hz), 7.21 (d, 1H, *J* = 2.5 Hz), 7.03 (dd, 1H, *J* = 2.5, 8.6 Hz), 4.01 (t, 2H, *J* = 6.5 Hz), 2.55 (s, 3H), 1.79 (m, 2H), 1.45 (d, 2H), 1.34 (m, 4H), 0.91 (t, 3H, *J* = 8.0 Hz).

1-(4-(Hexyloxy)-3-nitrophenyl)ethanone 22{*20*}. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.40 (d, 1H, *J* = 2.2 Hz), 8.13 (m, 1H), 7.12 (d, 1H, *J* = 8.9 Hz), 4.17 (t, 2H, *J* = 6.5 Hz), 2.59 (s, 3H), 1.85 (m, 2H),

1.49 (m, 2H), 1.34 (m, 4H), 0.90 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.80, 155.80, 139.40, 133.77, 129.26, 126.11, 113.96, 70.15, 31.33, 28.70, 26.28, 25.39, 22.46, 13.93.

2-(Hexyloxy)-1,3-dimethylbenzene 22{*21*}. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (s, 2H), 3.79 (t, 2H, *J* = 6.6 Hz), 2.54 (s, 3H), 2.31 (s, 6H), 1.81 (m, 2H), 1.50 (m, 2H), 1.36 (m, 4H), 0.92 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.64, 160.49, 132.66, 131.20, 129.35, 72.47, 31.69, 30.35, 26.48, 25.73, 22.60, 16.45, 14.02.

1-(4-(Hexyloxy)-2-isopropyl-5-methylphenyl)ethanone 22{*23*}. ^{1}H NMR (400 MHz,) δ 7.42 (s, 1H), 6.82 (s, 1H), 4.02 (t, 2H, *J* = 6.4 Hz), 3.75 (m, 1H), 2.54 (s, 3H), 2.21 (s, 3H), 1.81 (m, 2H), 1.50 (m, 2H), 1.35 (m, 4H), 1.22 (d, 6H, *J* = 6.8 Hz), 0.92 (t, 3H, *J* = 7.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 201.27, 159.74, 149.39, 131.88, 129.52, 123.44, 108.42, 67.90, 31.53, 30.11, 29.18, 28.97, 25.76, 24.13, 22.58, 15.77, 13.99.

1-(2,5-Dichloro-4-(hexyloxy)phenyl)ethanone 22{*25*}. ^{1}H NMR (400 MHz,) δ 7.74 (s, 1H), 6.92 (s, 1H), 4.06 (t, 2H, *J* = 6.5 Hz), 2.63 (m, 3H), 1.85 (m, 2H), 1.49 (m, 2H), 1.35 (m, 4H), 0.91 (t, 3H, *J* = 7.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.99, 157.11, 131.95, 131.87, 130.54, 121.71, 114.79, 69.72, 31.38, 30.57, 28.73, 25.48, 22.51, 13.96.

General procedure for Mannich reaction: A solution of compound **24** (50 mg, 0.23 mmol, 1 equiv.), dimethylamine hydrochloride (37 mg, 0.45 mmol, 2 equiv.), paraformaldehyde (15 mg, 0.45 mmol, 2 equiv.), and conc-HCl (cat.) in H_2O/actonitrile (1/9) was heated at 120 °C in MW for 2 h. The reaction mixture was concentrated *in vacuo*, and purified on normal phase column

chlromatography (SP1, Biotage) to yield the desired product **10**. **3-(Dimethylamino)-1-(3-(hexyloxy)phenyl)propan-1-one 10.** Yield 79% ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 (d, 1H, *J* = 7.7 Hz), 7.47 (m, 1H), 7.35 (t, 1H, *J* = 7.9 Hz), 7.09 (m, 1H), 3.99 (t, 2H, *J* = 6.6 Hz), 3.15 (t, 2H, *J* = 7.4 Hz), 2.78 (t, 2H, *J* = 7.3 Hz), 2.31 (s, 6H), 1.79 (m, 2H), 1.46 (m, 2H), 1.34 (m, 4H), 0.90 (t, 3H, *J* = 7.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.86, 159.40, 138.19, 129.53, 120.45, 120.01, 113.00, 68.23, 54.36, 45.41, 36.89, 31.53, 29.13, 25.67, 22.57, 14.00; MS (ESI) *m/z* 278.3 $[M+H]^+$.

3-(Dimethylamino)-1-(4-(hexyloxy)-3-methoxyphenyl)propan-1-one 12{*3*}. Yield 83% ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (dd, 1H, *J* = 1.9, 8.4 Hz), 7.49 (d, 1H, *J* = 1.9 Hz), 6.85 (d, 1H, *J* = 8.5 Hz), 4.05 (t, 2H, *J* = 6.9 Hz), 3.89 (d, 3H, *J* = 6.9 Hz), 3.19 (t, 2H, *J* = 7.3 Hz), 2.87 (t, 2H, *J* = 7.3 Hz), 2.37 (s, 6H), 1.84 (m, 2H), 1.43 (m, 2H), 1.32 (m, 4H), 0.87 (t, 3H, *J* = 7.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.96, 153.08, 149.22, 129.50, 122.76, 111.05, 110.40, 68.99, 55.97, 54.33, 45.02, 35.72, 31.44, 28.83, 25.48, 22.46, 13.91; MS (ESI) *m/z* 308.4 $[M+H]^+$.

3-(Dimethylamino)-1-(4-(hexyloxy)-2-(methylthio)phenyl)propan-1-one 12{*6*}. Yield 65% ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, 1H, *J* = 8.8 Hz), 6.75 (d, 1H, *J* = 2.2 Hz), 6.65 (m, 1H), 4.01 (t, 2H, *J* = 6.5 Hz), 3.40 (s, 2H), 3.17 (s, 2H), 2.53 (m, 6H), 2.38 (s, 3H), 1.78 (m, 2H), 1.45 (m, 2H), 1.33 (m, 4H), 0.89 (t, 3H, *J* = 7.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.61, 162.69, 146.32, 133.37, 125.62, 111.39, 108.47, 68.33, 53.60, 44.21, 35.59, 31.48, 29.00, 25.59, 22.52, 15.75, 13.97; MS (ESI) *m/z* 324.5 $[M+H]^+$.

Synthesis of compound 12{*7*}: A solution of compound **22**{*7*} and dimethylamine hydrochloride (3eq.) in DMF was heated at 110 ^{o}C in MW for 1h. The reaction mixture was poured into water and

extracted with Et_2O. The combined organic layer was washed with brine, dried over with $MgSO_4$. After concentration under vacuum, the crude mixture was purified on normal phase column chlromatography (SP1, Biotage) to yield the desired product. **3-(Dimethylamino)-1-(2-(dimethylamino)-4-(hexyloxy)phenyl)propan-1-one 12{**7**}.** ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 (d, 1H, *J* = 8.5 Hz), 6.45 (m, 2H), 3.98 (m, 2H), 3.17 (m, 2H), 2.77 (s, 7H), 2.66 (m, 2H), 2.27 (s, 6H), 1.77 (m, 2H), 1.40 (m, 7H), 0.90 (t, 3H, *J* = 6.6 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 203.03, 162.36, 154.11, 132.01, 124.85, 105.36, 103.87, 68.01, 55.41, 45.34, 44.44, 39.03, 31.54, 29.16, 25.68, 22.56, 14.00.

3-(Dimethylamino)-1-(4-(hexyloxy)-2-(methylsulfonyl)phenyl)propan-1-one 12{*17***}.** Yield 42% ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (d, 1H, *J* = 2.5 Hz), 7.46 (d, 1H, *J* = 8.5 Hz), 7.11 (dd, 1H, *J* = 2.5, 8.5 Hz), 4.03 (t, 2H, *J* = 6.5 Hz), 3.26 (m, 3H), 3.05 (t, 2H, *J* = 7.3 Hz), 2.73 (t, 1H, *J* = 7.2 Hz), 2.25 (m, 6H), 1.79 (m, 2H), 1.45 (s, 2H), 1.33 (m, 4H), 0.89 (t, 3H, *J* = 7.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 203.54, 160.34, 139.90, 133.45, 128.86, 118.92, 115.71, 68.85, 53.80, 46.02, 45.41, 41.50, 31.42, 28.89, 25.54, 22.52, 13.96; MS (ESI) *m/z* 356.4 $[M+H]^+$.

3-(Dimethylamino)-1-(4-(hexyloxy)-3-(trifluoromethyl)phenyl)propan-1-one 12{*18***}.** Yield 8%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 (d, 1H, *J* = 8.6 Hz), 7.14 (d, 1H, *J* = 2.4 Hz), 6.97 (dd, 1H, *J* = 2.5, 8.6 Hz), 3.95 (t, 2H, *J* = 6.5 Hz), 2.95 (t, 2H, *J* = 7.3 Hz), 2.63 (t, 2H, *J* = 7.3 Hz), 2.19 (s, 6H), 1.73 (m, 2H), 1.40 (s, 2H), 1.28 (m, 5H), 0.84 (t, 3H, *J* = 6.9 Hz); MS (ESI) *m/z* 346.3 $[M+H]^+$.

3-(Dimethylamino)-1-(4-(hexyloxy)-2-(trifluoromethyl)phenyl)propan-1-one 12{*19***}.** Yield 20%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (s, 1H), 8.05 (d, 1H, *J* = 8.7 Hz), 6.97 (t, 1H, *J* = 9.5 Hz),

4.05 (t, 2H, *J* = 6.3 Hz), 3.08 (t, 2H, *J* = 7.3 Hz), 2.74 (t, 3H, *J* = 7.3 Hz), 2.26 (s, 6H), 1.77 (m, 2H), 1.43 (d, 2H, *J* = 7.1 Hz), 1.28 (m, 4H), 0.83 (t, 3H, *J* = 6.9 Hz); MS (ESI) *m/z* 346.4 $[M+H]^+$.

3-(Dimethylamino)-1-(4-(hexyloxy)-3-nitrophenyl)propan-1-one 12{*20*}. Yield 63% ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.41 (d, 1H, *J* = 2.3 Hz), 8.12 (m, 1H), 7.12 (t, 1H, *J* = 10.0 Hz), 4.16 (t, 2H, *J* = 6.4 Hz), 3.13 (t, 2H, *J* = 7.2 Hz), 2.79 (t, 2H, *J* = 7.2 Hz), 2.31 (s, 6H), 1.84 (m, 2H), 1.47 (s, 2H), 1.33 (m, 4H), 0.89 (t, 3H, *J* = 6.7 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.71, 155.81, 139.48, 133.66, 128.95, 125.82, 113.99, 70.15, 54.08, 45.35, 36.41, 31.33, 28.70, 25.40, 22.47, 13.94; MS (ESI) *m/z* 323.4 $[M+H]^+$.

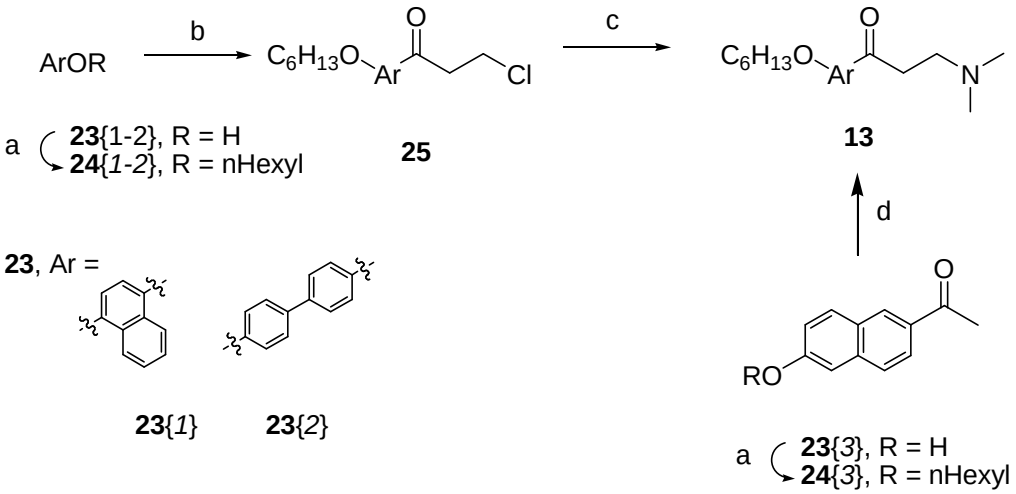
3-(Dimethylamino)-1-(4-(hexyloxy)-3,5-dimethylphenyl)propan-1-one 12{*21*}. Yield 47%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (s, 1H), 3.72 (t, 1H, *J* = 6.6 Hz), 3.02 (t, 1H, *J* = 7.4 Hz), 2.66 (m, 1H), 2.24 (s, 3H), 2.22 (s, 3H), 1.74 (m, 1H), 1.43 (m, 1H), 1.28 (m, 2H), 0.85 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.62, 161.16, 131.54, 129.66, 129.19, 72.45, 53.03, 43.64, 34.16, 31.59, 30.26, 25.63, 22.52, 16.38, 13.95; MS (ESI) *m/z* 306.5 $[M+H]^+$.

3-(Dimethylamino)-1-(4-(hexyloxy)-2-isopropyl-5-methylphenyl)propan-1-one 12{*23*}. Yield 80%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 (s, 1H), 6.79 (s, 1H), 3.99 (t, 2H, *J* = 6.4 Hz), 3.61 (m, 1H), 3.35 (t, 2H, *J* = 7.2 Hz), 3.14 (t, 2H, *J* = 7.1 Hz), 2.58 (s, 6H), 2.15 (s, 3H), 1.78 (m, 2H), 1.46 (m, 2H), 1.31 (m, 4H), 1.18 (d, 6H, *J* = 6.8 Hz), 0.88 (t, 3H, *J* = 7.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.49, 160.16, 149.88, 131.41, 128.01, 123.77, 108.45, 67.83, 53.68, 44.05, 37.69, 31.41, 31.40, 29.02, 25.63, 24.02, 22.46, 15.64, 15.63, 13.88; MS (ESI) *m/z* 334.5 $[M+H]^+$.

1-(2,3-dichloro-4-(hexyloxy)phenyl)-3-(dimethylamino)propan-1-one 12{*24***}** ^{1}H NMR (400 MHz, CDCl3) δ 7.44 (d, *J* = 8.7, 2H), 6.87 (d, *J* = 8.7, 2H), 4.08 (t, *J* = 6.5, 4H), 3.20 – 3.09 (m, 4H), 2.73 (t, *J* = 7.3, 4H), 2.27 (s, 12H), 1.93 – 1.80 (m, 4H), 1.59 – 1.42 (m, 4H), 1.43 – 1.30 (m, 8H), 0.99 – 0.82 (m, 6H); ^{13}C NMR (101 MHz, CDCl3) δ 200.65, 157.64, 136.07, 132.77, 128.00, 123.24, 110.38, 69.75, 54.41, 45.35, 41.05, 31.45, 28.87, 25.57, 22.57, 14.02; MS (ESI) *m/z* 347.3 $[M+H]^+$.

1-(2,5-Dichloro-4-(hexyloxy)phenyl)-3-(dimethylamino)propan-1-on 12{*25***}.** Yield 32%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (s, 1H), 6.84 (s, 1H), 3.98 (t, 2H, *J* = 6.5 Hz), 3.09 (t, 2H, *J* = 7.2 Hz), 2.68 (t, 2H, *J* = 7.2 Hz), 2.22 (s, 6H), 1.78 (m, 2H), 1.42 (s, 2H), 1.27 (m, 4H), 0.84 (t, 3H, *J* = 7.1 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.78, 156.92, 131.45, 131.31, 130.71, 121.75, 114.73, 69.71, 54.23, 45.24, 40.62, 31.38, 28.73, 25.48, 22.51, 13.96; MS (ESI) *m/z* 347.3 $[M+H]^+$.

1-(2,6-dichloro-4-(hexyloxy)phenyl)-3-(dimethylamino)propan-1-one12{*26***}** ^{1}H NMR (400 MHz, CDCl3) δ 6.75 (s, 2H), 3.86 (t, *J* = 6.5, 2H), 2.94 (t, *J* = 7.4, 2H), 2.68 (t, *J* = 7.4, 2H), 2.20 (s, 6H), 1.72 – 1.58 (m, 2H), 1.43 – 1.31 (m, 2H), 1.31 – 1.20 (m, 4H), 0.87 (t, *J* = 7.0, 3H); ^{13}C NMR (101 MHz, CDCl3) δ 201.28, 159.93, 131.95, 131.12, 114.56, 68.87, 53.22, 45.35, 42.36, 31.46, 28.88, 25.56, 22.57, 14.02; MS (ESI) *m/z* 346.3 $[M+H]^+$.



Reagent and condition. (a) Hexyl bromide, K_2CO_3, DMF, 80-90 °C, 12 h; (b)2-Chloropropyl chloride, $AlCl_3$, DCM, 0 °C; (c) 1 M Me2NH/THF, THF, rt, 30 min; (d) paraformaldehyde, Me_2NH•HCl, *c*-HCl, H_2O/MeCN (1/9, v/v), MW, 120 °C, 2 h

1-(Hexyloxy)naphthalene 24{*1*}. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (dd, 1H, *J* = 3.0, 6.7 Hz), 7.80 (dd, 1H, *J* = 3.1, 6.3 Hz), 7.48 (m, 2H), 7.39 (m, 2H), 6.81 (dd, 1H, *J* = 1.1, 7.3 Hz), 4.14 (t, 2H, *J* = 6.4 Hz), 1.94 (m, 2H), 1.58 (m, 2H), 1.41 (m, 4H), 0.93 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.90, 134.48, 127.38, 126.27, 125.89, 125.75, 125.00, 122.08, 119.89, 104.51, 68.13, 31.63, 29.28, 25.95, 22.63, 14.04.

4-(Hexyloxy)biphenyl 24{*2*}. ^{1}H NMR (400 MHz, CDCl3) δ 7.46 (m, 4H), 7.34 (m, 2H), 7.21 (m, 1H), 6.89 (m, 2H), 3.92 (t, 2H, *J* = 6.6 Hz), 1.73 (m, 2H), 1.41 (m, 2H), 1.28 (m, 4H), 0.84 (t, 3H, *J* = 7.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.74, 140.91, 133.54, 128.70, 128.10, 126.72, 126.59, 114.78, 68.11, 31.61, 29.28, 25.76, 22.63, 14.05.

1-(4-(hexyloxy)phenyl)ethanone 24{*3*}. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.38 (s, 1H), 7.99 (dd, 1H, *J* = 1.8, 8.6 Hz), 7.84 (d, 1H, *J* = 8.9 Hz), 7.74 (d, 1H, *J* = 8.6 Hz), 7.20 (dd, 1H, *J* = 2.5, 8.9 Hz), 7.14 (d, 1H, *J* = 2.4 Hz), 4.10 (t, 2H, *J* = 6.6 Hz), 2.70 (s, 3H), 1.86 (m, 2H), 1.50 (m, 2H), 1.38 (m, 4H), 0.92 (t, 3H, *J* = 7.1 Hz).

3-Chloro-1-(4-(hexyloxy)naphthalen-1-yl)propan-1-one 25{*1*}. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.97 (d, 1H, *J* = 8.4 Hz), 8.35 (d, 1H, *J* = 8.4 Hz), 7.98 (dd, 1H, *J* = 3.8, 8.2 Hz), 7.63 (dd, 1H, *J* = 6.9, 8.6 Hz), 7.54 (d, 1H, *J* = 8.3 Hz), 6.78 (d, 1H, *J* = 8.3 Hz), 4.20 (M, 2H), 3.99 (M, 2H), 3.52 (M, 2H), 1.96 (M, 2H), 1.58 (m, 2H), 1.40 (m, 4H), 0.94 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.29, 159.08, 132.05, 131.50, 128.84, 126.31, 125.93, 125.91, 125.84, 122.24, 102.64, 68.59, 43.28, 39.65, 31.54, 29.02, 25.85, 22.58, 14.01.

3-Chloro-1-(4'-(hexyloxy)biphenyl-4-yl)propan-1-one 25{*2*}. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, 2H, *J* = 8.5 Hz), 7.66 (d, 2H, *J* = 8.5 Hz), 7.56 (d, 2H, *J* = 8.8 Hz), 6.99 (d, 2H, *J* = 8.8 Hz), 3.97 (m, 4H), 3.48 (t, 2H, *J* = 4.8 Hz), 1.81 (m, 2H), 1.48 (m, 2H), 1.36 (m, 4H), 0.91 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.20, 159.61, 145.89, 134.39, 131.76, 128.66, 128.32, 126.67, 114.97, 68.15, 41.24, 38.80, 31.57, 29.19, 25.70, 22.59, 14.02.

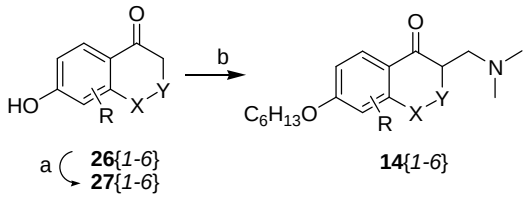
3-(Dimethylamino)-1-(4-(hexyloxy)naphthalen-1-yl)propan-1-one 13{*1*}. Yield 94%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.89 (m, 1H), 8.34 (dd, 1H, *J* = 0.6, 8.4 Hz), 7.98 (d, 1H, *J* = 8.2 Hz), 7.60 (m, 1H), 7.51 (m, 1H), 6.76 (d, 1H, *J* = 8.2 Hz), 4.18 (t, 2H, *J* = 6.4 Hz), 3.23 (t, 2H, *J* = 7.4 Hz), 2.83 (m, 2H), 2.29 (s, 6H), 1.94 (m, 2H), 1.56 (m, 2H), 1.39 (m, 4H), 0.93 (t, 3H, *J* = 7.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 201.11, 158.54, 132.01, 130.83, 128.49, 127.12, 125.98, 125.88, 125.63,

122.13, 102.63, 68.46, 55.00, 45.34, 39.25, 31.51, 29.01, 25.83, 22.55, 13.98; MS (ESI) *m/z* 328.5 $[M+H]^+$.

3-(Dimethylamino)-1-(4'-(hexyloxy)biphenyl-4-yl)propan-1-one 13{*2*}. Yield 100%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, 2H, *J* = 8.3 Hz), 7.63 (d, 2H, *J* = 8.3 Hz), 7.56 (dd, 2H, *J* = 4.9, 6.8 Hz), 6.98 (dd, 2H, *J* = 4.9, 6.8 Hz), 3.99 (t, 2H, *J* = 6.6 Hz), 3.18 (t, 2H, *J* = 7.4 Hz), 2.79 (t, 2H, *J* = 7.4 Hz), 2.31 (m, 6H), 1.80 (m, 2H), 1.45 (m, 2H), 1.33 (m, 4H), 0.91 (t, 3H, *J* = 7.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.51, 159.45, 145.35, 134.89, 131.87, 128.62, 128.23, 126.52, 114.89, 68.07, 54.41, 45.44, 36.80, 31.52, 29.16, 25.66, 22.55, 13.98; MS (ESI) *m/z* 354.5 $[M+H]^+$.

3-(Dimethylamino)-1-(6-(hexyloxy)naphthalen-2-yl)propan-1-one 13{*3*}. Yield 61%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.39 (s, 1H), 7.98 (dd, 1H, *J* = 1.7, 8.6 Hz), 7.83 (d, 1H, *J* = 9.0 Hz), 7.71 (dd, 1H, *J* = 7.2, 15.0 Hz), 7.19 (dd, 1H, *J* = 2.5, 8.9 Hz), 7.12 (d, 1H, *J* = 2.3 Hz), 4.08 (t, 2H, *J* = 6.6 Hz), 3.29 (t, 2H, *J* = 7.4 Hz), 2.86 (t, 2H, *J* = 7.3 Hz), 2.34 (d, 6H, *J* = 16.4 Hz), 1.84 (m, 2H), 1.48 (m, 2H), 1.35 (m, 4H), 0.91 (t, 3H, *J* = 7.1 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.39, 159.30, 137.33, 132.01, 131.04, 129.62, 127.64, 127.04, 124.41, 119.98, 106.37, 68.14, 54.45, 45.30, 36.47, 31.52, 29.05, 25.69, 22.54, 13.98; MS (ESI) *m/z* 328.5 $[M+H]^+$.

Scheme 4. Synthesis of α-substituted β-aminoketone [a]



[a]*Reagent and condition*. (a) *n*HexBr, K_2CO_3, DMF, 85 ^oC; (b) paraformaldehyde, Me_2NH•HCl, *c*-HCl, H_2O/MeCN (1/9, v/v), MW, 120 ^oC, 2 h;

1-(4-(Hexyloxy)phenyl)propan-1-one 27{*1*}. Yield 90%; ^1H NMR (400 MHz, $CDCl_3$) δ 7.86 (d, 2H, *J* = 8.8 Hz), 6.84 (d, 2H, *J* = 8.9 Hz), 3.94 (t, 2H, *J* = 6.6 Hz), 2.87 (t, 2H, *J* = 7.3 Hz), 1.72 (m, 2H), 1.38 (m, 2H), 1.27 (m, 4H), 1.14 (t, 3H, *J* = 7.3 Hz), 0.84 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.49, 162.94, 130.19, 129.80, 114.12, 68.23, 31.54, 31.38, 29.08, 25.66, 22.58, 14.01, 8.47.

1-(4-(Hexyloxy)phenyl)-3-methylbutan-1-one 27{*2*}. Yield 75%; ^1H NMR (400 MHz, $CDCl_3$) δ 7.83 (d, 2H, *J* = 8.9 Hz), 6.82 (d, 2H, *J* = 8.9 Hz), 3.92 (t, 2H, *J* = 6.6 Hz), 2.68 (d, 2H, *J* = 6.9 Hz), 2.18 (m, 1H), 1.70 (m, 2H), 1.36 (m, 2H), 1.25 (m, 4H), 0.89 (d, 6H, *J* = 6.6 Hz), 0.81 (t, 3H, *J* = 7.1 Hz) 218.38, 182.41, 149.83, 149.75, 133.56, 87.70, 66.65, 51.00, 48.54, 45.12, 44.88, 42.27, 42.04, 33.48.

1-(4-(Hexyloxy)phenyl)-2-phenylethanone 27{*3*}. Yield 93% ^1H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, 2H, *J* = 8.9 Hz), 7.19 (m, 5H), 6.82 (d, 2H, *J* = 8.9 Hz), 4.14 (s, 2H), 3.92 (t, 2H, *J* = 6.6 Hz), 1.71 (m, 2H), 1.36 (m, 2H), 1.26 (m, 4H), 0.83 (t, 3H, *J* = 7.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 215.72, 182.65, 154.51, 150.41, 148.86, 148.09, 146.22, 133.71, 87.74, 64.71, 51.00, 48.52, 45.12, 42.06, 33.50.

5-(Hexyloxy)-2,3-dihydro-1*H*-inden-1-one 27{*4*}. Yield 91%; ^{1}H NMR (400 MHz,) δ 7.67 (d, 1H, *J* = 9.1 Hz), 6.89 (m, 2H), 4.02 (t, 2H, *J* = 6.6 Hz), 3.07 (m, 2H), 2.66 (m, 2H), 1.81 (m, 2H), 1.47 (s, 2H), 1.35 (m, 4H), 0.91 (t, 3H, *J* = 7.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 205.25, 164.85, 158.11, 130.17, 125.29, 115.61, 110.23, 77.31, 77.00, 76.68, 68.44, 36.41, 31.49, 29.02, 25.84, 25.63, 22.56, 13.99.

6-(Hexyloxy)-3,4-dihydronaphthalen-1(2*H*)-one 27{*5*}. Yield 100%; ^{1}H NMR (400 MHz, CDCl3) δ 8.02 (d, 1H, *J* = 8.7 Hz), 6.83 (dd, 1H, *J* = 2.4, 8.7 Hz), 6.71 (d, 1H, *J* = 2.1 Hz), 4.02 (t, 2H, *J* = 6.5 Hz), 2.93 (t, 2H, *J* = 6.1 Hz), 2.62 (m, 2H), 2.13 (m, 2H), 1.81 (m, 2H), 1.48 (m, 2H), 1.37 (m, 5H), 0.93 (t, 3H, *J* = 7.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 216.69, 182.65, 166.37, 149.07, 145.57, 132.87, 132.59, 87.64, 58.37, 50.98, 49.63, 48.53, 45.11, 42.86, 42.04, 33.48.

7-(Hexyloxy)chroman-4-one 27{*6*}. Yield 89%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (d, 1H, *J* = 8.8 Hz), 6.54 (dd, 1H, *J* = 2.4, 8.8 Hz), 6.36 (d, 1H, *J* = 2.4 Hz), 4.48 (m, 2H), 3.95 (t, 2H, *J* = 6.6 Hz), 2.72 (m, 2H), 1.75 (m, 2H), 1.42 (m, 2H), 1.31 (m, 4H), 0.88 (t, 3H, *J* = 7.0 Hz).

3-(Dimethylamino)-1-(4-(hexyloxy)phenyl)-2-methylpropan-1-one 14{*1*}. Yield 72%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, 2H, *J* = 8.8 Hz), 6.85 (d, 2H, *J* = 8.8 Hz), 3.94 (t, 2H, *J* = 6.5 Hz), 3.59 (m, 1H), 2.72 (dd, 1H, *J* = 7.3, 12.3 Hz), 2.29 (m, 1H), 2.16 (m, 6H), 1.73 (m, 2H), 1.38 (dd, 2H, *J* = 7.1, 14.8 Hz), 1.27 (m, 4H), 1.12 (d, 3H, *J* = 7.0 Hz), 0.84 (t, 3H, *J* = 6.9 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 221.31, 182.56, 150.04, 148.75, 133.70, 87.70, 82.27, 65.36, 58.12, 50.98, 48.52, 45.11, 42.03, 36.26, 33.47; MS (ESI) *m/z* 292.8 $[M+H]^+$.

2-((Dimethylamino)methyl)-1-(4-(hexyloxy)phenyl)-3-methylbutan-1-one 14{*2*}. Yield 50%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, 2H, *J* = 8.9 Hz), 6.84 (d, 2H, *J* = 8.9 Hz), 3.93 (t, 2H, *J* = 6.6 Hz), 3.38 (m, 1H), 2.88 (m, 1H), 2.29 (m, 1H), 2.07 (s, 6H), 1.90 (m, 1H), 1.72 (m, 2H), 1.39 (m, 2H), 1.27 (m, 4H), 0.85 (m, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 221.28, 182.38, 150.54, 149.96, 133.60, 87.65, 78.84, 69.32, 65.46, 50.98, 49.93, 48.53, 45.11, 42.03, 40.48, 39.38, 33.46; MS (ESI) *m/z* 320.5 $[M+H]^+$.

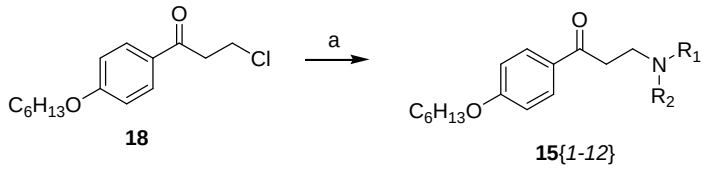
3-(Dimethylamino)-1-(4-(hexyloxy)phenyl)-2-phenylpropan-1-one 14{*3*}. Yield 74%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (m, 2H), 7.25 (m, 2H), 7.19 (t, 2H, *J* = 7.7 Hz), 7.10 (t, 1H, *J* = 7.2 Hz), 6.77 (d, 2H, *J* = 8.8 Hz), 4.72 (dd, 1H, *J* = 4.7, 8.8 Hz), 3.88 (m, 2H), 3.28 (dd, 1H, *J* = 8.9, 12.4 Hz), 2.48 (dd, 1H, *J* = 4.7, 12.4 Hz), 2.15 (s, 6H), 1.67 (m, 2H), 1.33 (m, 2H), 1.22 (m, 4H), 0.81 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 216.76, 182.50, 158.09, 150.45, 149.06, 148.36, 147.61, 146.54, 133.63, 87.66, 82.60, 70.85, 65.40, 50.97, 48.49, 45.09, 42.03, 33.48; MS (ESI) *m/z* 354.5 $[M+H]^+$.

2-((Dimethylamino)methyl)-5-(hexyloxy)-2,3-dihydro-1*H*-inden-1-one 14{*4*}. Yield 72%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (m, 1H), 6.87 (m, 2H), 4.01 (t, 2H, *J* = 6.6 Hz), 3.25 (dd, 1H, *J* = 7.7, 17.5 Hz), 3.01 (dd, 1H, *J* = 3.3, 17.5 Hz), 2.84 (m, 1H), 2.80 (s, 1H), 2.42 (dd, 1H, *J* = 10.5, 12.1 Hz), 2.28 (s, 6H), 1.79 (m, 2H), 1.47 (d, 2H, *J* = 7.0 Hz), 1.33 (m, 4H), 0.90 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 205.69, 165.03, 157.01, 129.57, 125.46, 115.65, 110.17, 68.41, 61.35, 46.57, 45.64, 32.16, 31.89, 31.46, 28.99, 25.60, 22.52, 22.51, 13.96; MS (ESI) *m/z* 290.3 $[M+H]^+$.

2-((Dimethylamino)methyl)-6-(hexyloxy)-3,4-dihydronaphthalen-1(2*H*)-one 14{*5*}. Yield 43%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, 1H, *J* = 8.8 Hz), 6.73 (dd, 1H, *J* = 2.5, 8.8 Hz), 6.61 (d, 1H, *J* = 2.3 Hz), 3.93 (t, 2H, *J* = 6.6 Hz), 2.94 (m, 3H), 2.69 (m, 1H), 2.60 (m, 1H), 2.39 (m, 7H), 1.90 (m, 1H), 1.72 (m, 2H), 1.39 (m, 2H), 1.27 (m, 4H), 0.84 (t, 3H, *J* = 7.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.50, 163.37, 146.58, 129.89, 125.58, 113.71, 112.98, 68.25, 58.95, 45.27, 31.53, 29.07, 28.74, 27.72, 25.66, 22.59, 14.03; MS (ESI) *m/z* 304.4 $[M+H]^+$.

3-((Dimethylamino)methyl)-7-(hexyloxy)chroman-4-one 14{*6*}. Yield 83%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (d, 1H, *J* = 8.8 Hz), 6.55 (dd, 1H, *J* = 2.4, 8.8 Hz), 6.38 (d, 1H, *J* = 2.3 Hz), 4.56 (dd, 1H, *J* = 4.4, 11.3 Hz), 4.36 (dd, 1H, *J* = 8.1, 11.3 Hz), 3.97 (t, 2H, *J* = 6.5 Hz), 2.79 (m, 1H), 2.65 (dd, 1H, *J* = 5.0, 12.6 Hz), 2.56 (m, 1H), 2.26 (s, 6H), 1.77 (m, 2H), 1.44 (m, 2H), 1.33 (m, 4H), 0.90 (t, 3H, *J* = 6.6 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.25, 165.52, 163.54, 128.94, 114.39, 110.32, 101.00, 69.75, 68.42, 56.12, 45.66, 44.08, 31.47, 28.92, 25.59, 22.54, 13.98; MS (ESI) *m/z* 306.4 $[M+H]^+$.

Scheme 5. Synthesis of the different amino Mannich base[a]



[a]*Reagent and condition.* (a) R_1R_2NH, DBU, THF, rt, 1-2 h

General procedure for 15: To a solution compound **18** in THF was added the corresponding amine (2 equiv.) in the presence of DBU (2 equiv.) and stirred at rt for 2 h. The reaction mixture

was concentrated in vacuuo and purified on normal phase column chlromatography (SP1, Biotage) to yield the desired product. **3-(Dibutylamino)-1-(4-(hexyloxy)phenyl)propan-1-one 15{*1*}.** Yield 45%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (t, 2H, *J* = 9.3 Hz), 6.86 (t, 2H, *J* = 9.6 Hz), 3.95 (m, 2H), 3.01 (m, 2H), 2.84 (m, 2H), 2.38 (m, 4H), 1.73 (m, 2H), 1.37 (m, 6H), 1.24 (m, 8H), 0.84 (m, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 217.88, 182.53, 149.79, 149.38, 133.62, 87.71, 73.31, 68.80, 55.35, 50.99, 48.61, 48.52, 45.11, 42.04, 40.17, 40.16, 33.52, 33.47; MS (ESI) *m/z* 362.6 $[M+H]^+$.

1-(4-(Hexyloxy)phenyl)-3-(piperidin-1-yl)propan-1-one 15{*2*}. Yield 83%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (d, 2H, *J* = 8.9 Hz), 6.86 (m, 2H), 3.95 (m, 2H), 3.09 (m, 2H), 2.72 (m, 2H), 2.40 (s, 4H), 1.72 (m, 2H), 1.54 (m, 4H), 1.39 (m, 4H), 1.27 (m, 4H), 0.83 (t, 3H, *J* = 7.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 217.30, 182.57, 149.77, 149.25, 133.63, 87.71, 74.04, 73.56, 55.34, 50.98, 48.51, 45.34, 45.10, 43.68, 42.03, 33.46; MS (ESI) *m/z* 318.5 $[M+H]^+$.

1-(4-(Hexyloxy)phenyl)-3-(pyrrolidin-1-yl)propan-1-one 15{*3*}. Yield 63%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 – 7.77 (m, 2H), 6.86 – 6.65 (m, 2H), 4.07 – 3.77 (m, 2H), 3.15 (t, *J* = 7.6, 2H), 2.98 – 2.83 (m, 2H), 2.58 (s, 4H), 1.88 – 1.67 (m, 6H), 1.47 – 1.35 (m, 2H), 1.35 – 1.09 (m, 4H), 0.98 – 0.73 (m, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.28, 163.21, 130.36, 129.60, 114.22, 68.27, 54.23, 51.10, 37.41, 31.53, 29.06, 25.65, 23.49, 22.58, 14.02; MS (ESI) *m/z* 304.4 $[M+H]^+$.

1-(4-(Hexyloxy)phenyl)-3-(2-methylaziridin-1-yl)propan-1-one 15{*4*}. Yield 69%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (m, 2H), 6.84 (m, 2H), 3.94 (t, 2H, *J* = 6.6 Hz), 3.12 (m, 2H), 2.58 (m, 2H),

1.72 (m, 2H), 1.37 (m, 4H), 1.27 (m, 4H), 1.21 (d, 1H, *J* = 6.3 Hz), 1.06 (d, 3H, *J* = 5.3 Hz), 0.84 (m, 3H) ; ^{13}C NMR (100 MHz, $CDCl_3$) δ 217.13, 182.61, 149.83, 149.33, 133.63, 87.71, 75.78, 58.04, 54.33, 50.98, 48.51, 45.09, 42.02, 37.78, 33.46; MS (ESI) *m/z* 290.4 $[M+H]^+$.

1-(4-(Hexyloxy)phenyl)-3-(4-methylpiperazin-1-yl)propan-1-one 15{*5*}. Yield 84%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, 2H, *J* = 8.9 Hz), 6.91 (d, 2H, *J* = 8.9 Hz), 4.01 (t, 2H, *J* = 6.6 Hz), 3.13 (t, 2H, *J* = 7.5 Hz), 2.84 (m, 2H), 2.53 (m, 8H), 2.29 (s, 3H), 1.79 (m, 2H), 1.46 (s, 2H), 1.34 (m, 4H), 0.91 (t, 3H, *J* = 7.0 Hz) ; ^{13}C NMR (100 MHz, $CDCl_3$) δ 217.00, 182.59, 149.73, 149.20, 133.64, 87.71, 74.47, 72.76, 72.55, 65.42, 55.22, 50.97, 48.50, 45.09, 42.02, 33.46; MS (ESI) *m/z* 3333.5 $[M+H]^+$.

1-(4-(Hexyloxy)phenyl)-3-(4-phenylpiperazin-1-yl)propan-1-one 15{*6*}. Yield 76%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (m, 2H), 7.19 (m, 2H), 6.85 (m, 4H), 6.78 (t, 1H, *J* = 7.3 Hz), 3.94 (t, 2H, *J* = 6.5 Hz), 3.14 (m, 6H), 2.84 (t, 2H, *J* = 7.4 Hz), 2.63 (m, 4H), 1.73 (m, 2H), 1.39 (m, 2H), 1.26 (m, 4H), 0.84 (t, 3H, *J* = 6.9 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.42, 163.16, 151.16, 130.28, 129.67, 129.06, 119.75, 116.06, 114.18, 68.24, 53.30, 53.21, 49.02, 35.71, 31.49, 29.01, 25.60, 22.53, 13.98; MS (ESI) *m/z* 395.6 $[M+H]^+$.

1-(4-(Hexyloxy)phenyl)-3-morpholinopropan-1-one 15{*7*}. Yield 66%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (d, 2H, *J* = 8.8 Hz), 6.86 (m, 2H), 3.96 (m, 2H), 3.64 (m, 4H), 3.08 (m, 2H), 2.74 (m, 2H), 2.44 (m, 4H), 1.72 (m, 2H), 1.32 (m, 6H), 0.83 (t, 3H, *J* = 6.9 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 216.89, 182.64, 149.74, 149.16, 133.67, 87.73, 86.36, 73.23, 73.16, 55.01, 50.98, 48.50, 45.10, 42.03, 33.47; MS (ESI) *m/z* 320.4 $[M+H]^+$.

1-(4-(Hexyloxy)phenyl)-3-(methyl(phenyl)amino)propan-1-one 15{*8*}. Yield 63%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (m, 2H), 7.18 (m, 2H), 6.82 (m, 2H), 6.66 (m, 3H), 3.93 (t, 2H, *J* = 6.6 Hz), 3.75 (m, 2H), 3.10 (m, 2H), 2.89 (s, 3H), 1.72 (m, 2H), 1.38 (m, 2H), 1.26 (m, 4H), 0.84 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.96, 163.20, 148.56, 130.28, 129.72, 129.29, 116.43, 116.41, 114.16, 112.32, 112.30, 68.24, 48.16, 38.52, 34.68, 31.49, 29.01, 25.60, 22.53, 13.98; MS (ESI) *m/z* 340.5 $[M+H]^+$.

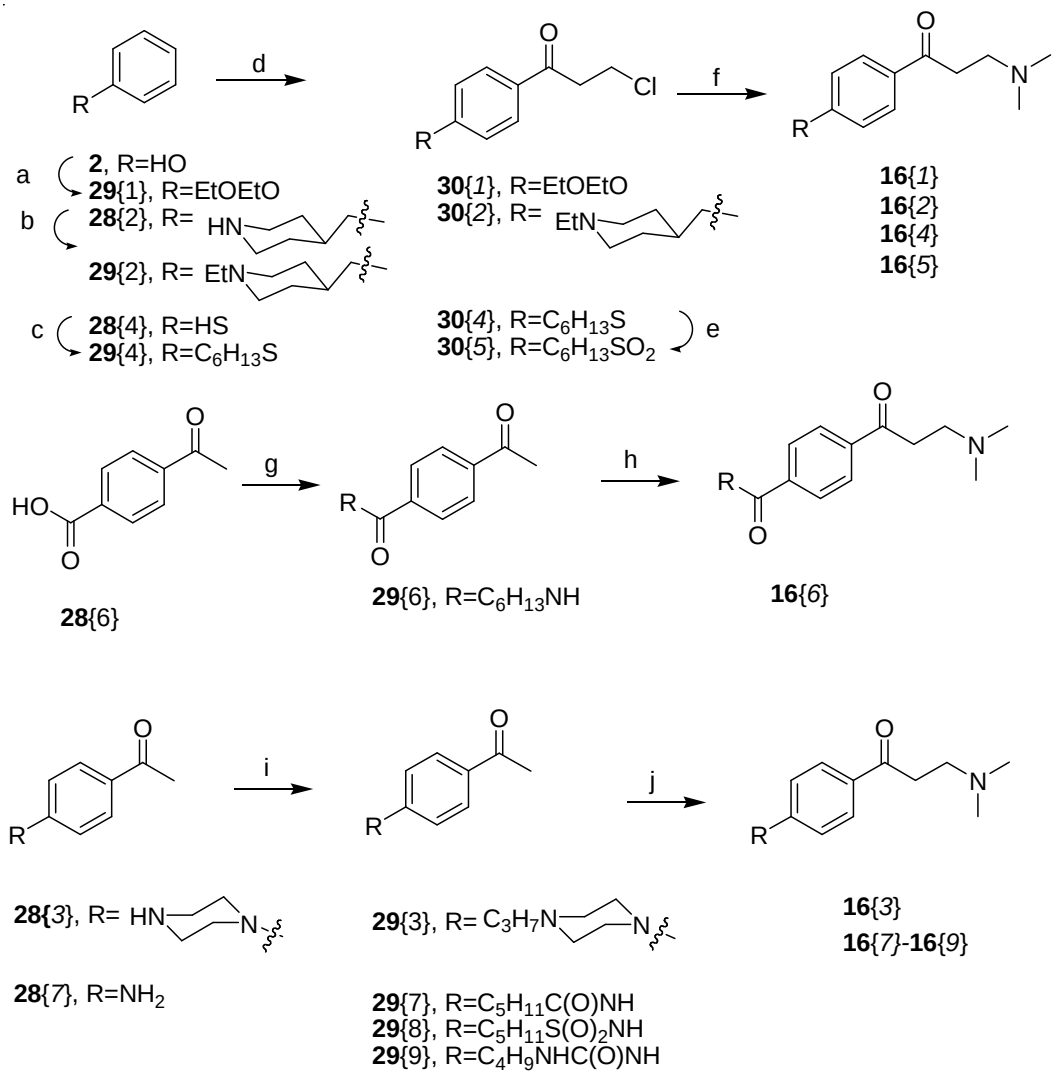
1-(4-(Hexyloxy)phenyl)-3-(phenylamino)propan-1-one 15{*9*}. Yield 41%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (m, 2H), 7.11 (t, 2H, *J* = 7.7 Hz), 6.83 (m, 2H), 6.64 (m, 1H), 6.59 (d, 2H, *J* = 8.5 Hz), 3.93 (t, 2H, *J* = 6.6 Hz), 3.52 (t, 2H, *J* = 6.1 Hz), 3.16 (t, 2H, *J* = 6.1 Hz), 1.72 (m, 2H), 1.39 (m, 2H), 1.25 (m, 4H), 0.83 (t, 3H, *J* = 6.9 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.76, 163.30, 147.45, 130.29, 129.55, 129.30, 117.79, 114.20, 113.29, 68.27, 39.15, 37.11, 31.50, 29.01, 25.61, 22.55, 13.99; MS (ESI) *m/z* 326.4 $[M+H]^+$.

3-(3-Chlorophenylamino)-1-(4-(hexyloxy)phenyl)propan-1-one 15{*10*}. Yield 34%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (d, 2H, *J* = 8.9 Hz), 6.98 (t, 1H, *J* = 8.0 Hz), 6.83 (m, 2H), 6.58 (m, 1H), 6.54 (m, 1H), 6.42 (dd, 1H, *J* = 1.9, 7.8 Hz), 4.34 (m, 1H), 3.94 (t, 2H, *J* = 6.6 Hz), 3.49 (t, 2H, *J* = 6.0 Hz), 3.14 (t, 2H, *J* = 6.0 Hz), 1.72 (m, 2H), 1.39 (m, 2H), 1.27 (m, 4H), 0.83 (t, 3H, *J* = 6.9 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 217.03, 182.88, 168.38, 154.55, 151.46, 149.84, 149.78, 149.70, 148.95, 136.80, 133.74, 133.65, 133.43, 131.97, 130.97, 87.79, 58.22, 56.41, 50.99, 48.50, 45.10, 42.04, 33.48; MS (ESI) *m/z* 360.9 $[M+H]^+$.

1-(4-(Hexyloxy)phenyl)-3-(1*H*-imidazol-1-yl)propan-1-one 15{*11*}. Yield 54%;^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (m, 2H), 7.64 (s, 1H), 7.00 (m, 2H), 6.89 (m, 2H), 4.41 (t, 2H, *J* = 6.5 Hz), 3.99 (t, 2H, *J* = 6.6 Hz), 3.37 (t, 2H, *J* = 6.6 Hz), 1.77 (m, 2H), 1.43 (m, 2H), 1.30 (m, 4H), 0.88 (t, 3H, *J* = 7.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.92, 163.59, 130.24, 128.99, 114.35, 68.33, 41.73, 39.40, 31.46, 28.97, 25.57, 22.51, 13.94; MS (ESI) *m/z* 301.4 $[M+H]^+$.

1-(3-(4-(Hexyloxy)phenyl)-3-oxopropyl)pyrrolidine-2,5-dione 15{*12*}. Yield 65%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (d, 2H, *J* = 8.8 Hz), 6.83 (d, 2H, *J* = 8.8 Hz), 3.94 (t, 2H, *J* = 6.6 Hz), 3.86 (t, 2H, *J* = 7.4 Hz), 3.18 (m, 2H), 2.65 (s, 6H), 1.72 (m, 2H), 1.39 (m, 2H), 1.26 (m, 4H), 0.83 (t, 3H, *J* = 7.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 215.21, 196.51, 182.80, 149.73, 148.70, 133.71, 87.75, 54.90, 54.05, 50.97, 48.49, 47.64, 45.09, 42.02, 33.47; MS (ESI) *m/z* 332.4 $[M+H]^+$.

Scheme 6. Synthesis of hydrophobic side chain modified β-aminophenylketones.



Reagent and condition. (a) EtOEtBr, K_2CO_3, DMF, 80-90 ^oC, 12 h; (b) *n*EtI, K_2CO_3, DMF; (c) *n*HexBr, K_2CO_3, DMF, 80-90 ^oC, 12 h; (d) 3-chloropropionic chloride, $AlCl_3$, DCM, 0 ^oC, 1 h; (e) *m*CPBA, DCM, 0 ^oC, 1 h; (f) 2 M Me_2NH/THF, THF, rt, 1 h; (g) $C_6H_{13}NH_2$, DIC, DMAP, DCM, rt; (h) paraformaldehyde, Me_2NH•HCl, *c*-HCl, H_2O/MeCN (1/9, v/v), MW, 120 ^oC, 2 h; (i) RX (*n*C_5H_{12}COCl, *n*$C_5H_{12}SO_2Cl$, *n*BuNCO), TEA, DCM, rt.

Synthesis of compound 29{*1*}: To a solution phenol **2** (0.5 g, 5.3 mmol) in DMF was added K_2CO_2 (1.38 g, 10.6 mmol) and ethoxyethylbromide (0.874 mL, 8.0 mmol), and then stirred at 85 °C for overnight. The reaction mixture was poured to water and extracted with Et_2O. The combined organic layer were washed with brine and dried over $MgSO_4$ and concentrated in vacuo to yield crude compound **29{*1*}**. **(2-Ethoxyethoxy)benzene 29{*1*}.** ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28 (m, 2H), 6.94 (m, 3H), 4.13 (m, 2H), 3.80 (m, 2H), 3.61 (m, 2H), 1.26 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.81, 129.37, 120.81, 114.64, 68.96, 67.34, 66.83, 15.15.

4-Benzyl-1-ethylpiperidine 29{*2*}. ^{1}H NMR (400 MHz,) δ 7.27 – 7.15 (m, 2H), 7.15 – 6.99 (m, 3H), 2.84 (d, *J* = 11.7, 2H), 2.45 (d, *J* = 7.1, 2H), 2.29 (q, *J* = 7.2, 2H), 1.74 (t, *J* = 11.7, 2H), 1.56 (d, *J* = 13.0, 2H), 1.50 – 1.34 (m, 1H), 1.33 – 1.13 (m, 2H), 1.06 – 0.87 (m, 3H); NMR (101 MHz,) δ 140.73, 129.10, 128.10, 125.71, 53.50, 52.59, 43.22, 38.00, 32.16, 12.13.

Synthesis of compound 29{*3*}**:** To a solution amine **28**{*3*} (0.50g, 2.45 mmol) in DCM were added n-propyl bromide (0.262 mL, 2.69 mmol), and TEA (0.443 mL, 3.19 mmol) and then stirred at rt for 3h. The reaction mixture was washed with water and brine, and dried over $MgSO_4$. After concentration under vacuum, the crude mixture was purified on normal phase column chlromatography (SP1, Biotage) to yield the desired product. **1-(4-(4-Propylpiperazin-1-yl)phenyl)ethanone 29**{*3*}. Yield 87%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (d, 2H, *J* = 9.0 Hz),

6.82 (d, 2H, *J* = 9.1 Hz), 3.33 (m, 4H), 2.54 (m, 4H), 2.47 (s, 3H), 2.32 (m, 2H), 1.51 (m, 2H), 0.90 (t, 3H, *J* = 7.4 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.30, 154.06, 130.23, 127.37, 113.17, 60.46, 52.75, 47.18, 25.99, 19.88, 11.82.

Synthesis of compound 29{*4*}: To a solution thiophenol **28{*4*}** (2.0 g, 18.2 mmol) in DMF was added K_2CO_2 (3.26 g, 23.6 mmol) and *n*-hexylbromide (2.95 mL, 23.6 mmol) and then stirred at 85 °C for overnight. The reaction mixture was poured to water and extracted with Et_2O. The combined organic layer were washed with brine and dried over $MgSO_4$ and concentrated in vacuo to yield crude compound **29{*4*}**. **Hexyl(phenyl)sulfane 29{*4*}** ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 (m, 4H), 7.19 (m, 1H), 2.95 (m, 2H), 1.68 (m, 2H), 1.46 (m, 2H), 1.33 (m, 4H), 0.92 (t, 3H, *J* = 7.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.04, 128.82, 128.78, 125.60, 33.58, 31.35, 29.11, 28.52, 22.52, 14.00.

Synthesis of compound 29{*6*}: To a solution phenol **28{6}** (0.5 g, 3.05 mmol) in DCM were added n-hexylamine (0.52 mL, 3.96 mmol), DIC (0.613 mL, 3.96 mmol), and DMAP (cat.) and then stirred at rt for 3h. The reaction mixture was washed with water and brine, and dried over $MgSO_4$. After concentration under vacuum, the crude mixture was purified on normal phase column chlromatography (SP1, Biotage) to yield the desired product **29{*6*}**. **4-Acetyl-*N*-hexylbenzamide 29{*6*}.** Yield 57%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (d, 2H, *J* = 8.3 Hz), 7.81 (d, 2H, *J* = 8.3 Hz), 6.48 (s, 1H), 3.42 (m, 2H), 2.59 (s, 3H), 1.58 (m, 2H), 1.29 (m, 7H), 0.85 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.43, 166.49, 138.91, 138.74, 128.38, 127.15, 40.24, 31.42, 29.48, 26.72, 26.60, 22.48, 13.94.

Synthesis of compound 29{*7*}: To a solution phenol **28{*7*}** (0.5 g, 3.70 mmol) in DCM were added n-pentanoic acid (0.60 mL, 4.81 mmol), DIC (0.745 mL, 4.81 mmol), and DMAP (cat.) and then stirred at rt for 3h. The reaction mixture was washed with water and brine, and dried over $MgSO_4$. After concentration under vacuum, the crude mixture was purified on normal phase column chlromatography (SP1, Biotage) to yield the desired product **29{*7*}**. ***N*-(4-Acetylphenyl)hexanamide 29{*7*}**. Yield 59%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (m, 2H), 7.71 (s, 1H), 7.64 (d, 2H, *J* = 8.7 Hz), 2.59 (s, 3H), 2.39 (m, 2H), 1.73 (m, 2H), 1.34 (m, 4H), 0.89 (t, 3H, *J* = 7.1 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.05, 171.84, 142.45, 132.66, 129.70, 118.81, 37.79, 31.35, 31.34, 26.41, 25.11, 22.37, 22.36, 13.87, 13.86.

Synthesis of compound 29{*8*}: To a solution phenol **28{*8*}** (0.20 g, 1.48 mmol) in DCM were added n-pentane sulfonyl chloride (0.26 mL, 1.78 mmol), and TEA (0.31 mL, 2.22 mmol) and then stirred at rt for 3h. The reaction mixture was washed with water and brine, and dried over $MgSO_4$. After concentration under vacuum, the crude mixture was purified on normal phase column chlromatography (SP1, Biotage) to yield the desired product **29{*8*}**. ***N*-(4-Acetylphenyl)pentane-1-sulfonamide 29{*8*}**. Yield 45%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (m, 2H), 7.47 (s, 1H), 7.28 (m, 2H), 3.17 (m, 2H), 2.61 (s, 3H), 1.82 (m, 2H), 1.32 (m, 4H), 0.85 (t, 3H, *J* = 7.2 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.89, 141.64, 133.03, 130.29, 117.98, 52.19, 30.09, 26.41, 23.07, 22.01, 13.59.

Synthesis of compound 29{*9*}: To a solution amine **28{*9*}** (0.50 g, 3.70 mmol) in DCM was added n-butane isocyanate (0.50 mL, 4.44 mmol) and then stirred at rt for 3h. The reaction mixture was washed with water and brine, and dried over $MgSO_4$. After concentration under vacuum, the

crude mixture was purified on normal phase column chlromatography (SP1, Biotage) to yield the desired product. **1-(4-Acetylphenyl)-3-butylurea 29{*9*}**. Yield 24%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 (s, 1H), 7.76 (d, 2H, *J* = 8.7 Hz), 7.35 (d, 2H, *J* = 8.7 Hz), 5.86 (t, 1H, *J* = 5.4 Hz), 3.15 (m, 2H), 2.46 (s, 3H), 1.40 (m, 3H), 1.24 (m, 3H), 0.81 (t, 3H, *J* = 7.3 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 217.14, 175.25, 164.06, 150.29, 149.38, 137.19, 59.35, 51.58, 45.84, 39.50, 33.20.

3-Chloro-1-(4-(2-ethoxyethoxy)phenyl)propan-1-one 30{*1*}. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (m, 2H), 6.96 (m, 2H), 4.18 (d, 2H, *J* = 5.4 Hz), 3.90 (t, 2H, *J* = 6.9 Hz), 3.81 (d, 2H, *J* = 5.4 Hz), 3.60 (m, 2H), 3.40 (t, 2H, *J* = 6.9 Hz), 1.24 (t, 3H, *J* = 7.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.19, 163.10, 130.28, 129.56, 114.45, 68.64, 67.70, 66.92, 40.89, 38.93, 15.09.

3-Chloro-1-(4-((1-ethylpiperidin-4-yl)methyl)phenyl)propan-1-one 30{*2*}. ^{1}H NMR (400 MHz,) δ 7.85 (d, *J* = 8.4, 2H), 7.28 (d, 2H), 3.87 (t, *J* = 6.7, 2H), 3.51 (d, *J* = 11.9, 2H), 3.46 – 3.30 (m, 2H), 3.10 – 2.96 (m, 2H), 2.66 (d, *J* = 6.9, 2H), 2.63 – 2.44 (m, 2H), 2.16 – 1.95 (m, 2H), 1.80 (d, *J* = 11.8, 3H), 1.41 (t, *J* = 7.3, 3H).

3-Chloro-1-(4-(hexylthio)phenyl)propan-1-one 30{*4*}. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (d, 2H, *J* = 8.5 Hz), 7.13 (d, 2H, *J* = 8.6 Hz), 3.74 (t, 2H, *J* = 6.9 Hz), 3.24 (t, 2H, *J* = 6.8 Hz), 2.82 (m, 2H), 1.53 (m, 2H), 1.29 (s, 2H), 1.14 (m, 4H), 0.72 (t, 3H, *J* = 6.8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.66, 145.81, 132.81, 128.43, 126.20, 41.03, 38.78, 31.87, 31.30, 28.65, 28.55, 22.49, 13.98.

3-Chloro-1-(4-(hexylsulfonyl)phenyl)propan-1-on 30{*5*}. Beta-chloro/enone =1:0.3 ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (d, 2H, *J* = 8.3 Hz), 8.02 (d, 2H, *J* = 8.3 Hz), 3.93 (t, 2H, *J* = 6.6 Hz),

3.50 (t, 2H, *J* = 6.6 Hz), 3.10 (m, 2H), 1.70 (m, 2H), 1.36 (m, 2H), 1.24 (m, 4H), 0.85 (t, 3H, *J* = 6.8 Hz).

3-(Dimethylamino)-1-(4-(2-ethoxyethoxy)phenyl)propan-1-one 16{*1*}. Yield 91%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 (m, 2H), 6.93 (m, 2H), 4.15 (dd, 2H, *J* = 4.2, 5.5 Hz), 3.77 (m, 2H), 3.57 (m, 2H), 3.09 (t, 2H, *J* = 7.4 Hz), 2.73 (m, 2H), 2.28 (s, 6H), 1.21 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.40, 162.71, 130.19, 130.00, 114.27, 68.61, 67.59, 66.83, 54.39, 45.29, 36.30, 15.05; MS (ESI) *m/z* 266.4 $[M+H]^+$.

3-(Dimethylamino)-1-(4-((1-ethylpiperidin-4-yl)methyl)phenyl)propan-1-one 16{*2*}**.** ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (d, 2H, *J* = 9.1 Hz), 6.85 (d, 2H, *J* = 9.0 Hz), 3.46 (s, 1H), 3.37 (m, 4H), 3.26 (t, 2H, *J* = 7.3 Hz), 3.02 (t, 2H, *J* = 7.3 Hz), 2.58 (m, 4H), 2.47 (s, 5H), 2.35 (m, 3H), 1.54 (m, 2H), 0.92 (t, 3H, *J* = 7.4 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.79, 154.31, 130.24, 126.45, 113.27, 60.47, 53.79, 52.72, 47.05, 44.34, 34.82, 19.84, 11.87; MS (ESI) *m/z* 303.4 $[M+H]^+$.

3-(Dimethylamino)-1-(4-(4-propylpiperazin-1-yl)phenyl)propan-1-one 16{*3*}. Yield 32%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (d, 2H, *J* = 9.1 Hz), 6.85 (d, 2H, *J* = 9.0 Hz), 3.37 (m, 4H), 3.26 (t, 2H, *J* = 7.3 Hz), 3.02 (t, 2H, *J* = 7.3 Hz), 2.58 (m, 4H), 2.48 (s, 6H), 2.34 (m, 2H), 1.54 (m, 2H), 0.92 (t, 3H, *J* = 7.4 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.79, 154.31, 130.24, 126.45, 113.27, 60.47, 53.79, 52.72, 47.05, 44.34, 34.82, 19.84, 11.87; MS (ESI) *m/z* 304.3 $[M+H]^+$.

3-(Dimethylamino)-1-(4-(hexylthio)phenyl)propan-1-one 16{*4*}. Yield 95%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (m, 2H), 7.22 (d, 2H, *J* = 8.3 Hz), 3.07 (m, 2H), 2.89 (m, 2H), 2.70 (t, 2H, *J* =

7.4), 2.23 (m, 6H), 1.62 (m, 2H), 1.38 (m, 2H), 1.23 (m, 4H), 0.82 (t, 3H, *J* = 6.7 Hz) ; ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.94, 144.99, 133.33, 128.42, 126.20, 54.36, 45.40, 36.55, 31.89, 31.25, 28.64, 28.50, 22.44, 13.93; MS (ESI) *m/z* 294.5 $[M+H]^+$.

3-(Dimethylamino)-1-(4-(hexylsulfonyl)phenyl)propan-1-one 16{*5*}. Yield 90%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 (d, 2H, *J* = 8.7 Hz), 7.97 (d, 2H, *J* = 8.6 Hz), 3.23 (s, 1H), 3.07 (m, 2H), 2.83 (d, 2H, *J* = 6.3 Hz), 2.34 (s, 6H), 1.66 (m, 2H), 1.33 (m, 2H), 1.22 (s, 4H), 0.82 (t, 3H, *J* = 6.9 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.44, 142.95, 140.41, 128.76, 128.47, 56.12, 53.62, 53.58, 45.06, 31.04, 27.83, 22.46, 22.18, 13.80; MS (ESI) *m/z* 326.4 $[M+H]^+$.

4-(3-(Dimethylamino)propanoyl)-*N*-hexylbenzamide 16{*6*}. Yield 27%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (d, 2H, *J* = 8.4 Hz), 7.82 (d, 2H, *J* = 8.3 Hz), 6.38 (s, 1H), 3.43 (m, 2H), 3.16 (t, 2H, *J* = 7.3 Hz), 2.76 (t, 2H, *J* = 7.2 Hz), 2.27 (s, 6H), 1.60 (m, 2H), 1.33 (m, 6H), 0.88 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.36, 166.46, 138.75, 128.18, 127.18, 54.13, 45.39, 40.23, 37.04, 31.43, 29.51, 26.61, 22.49, 13.96; MS (ESI) *m/z* 305.4 $[M+H]^+$.

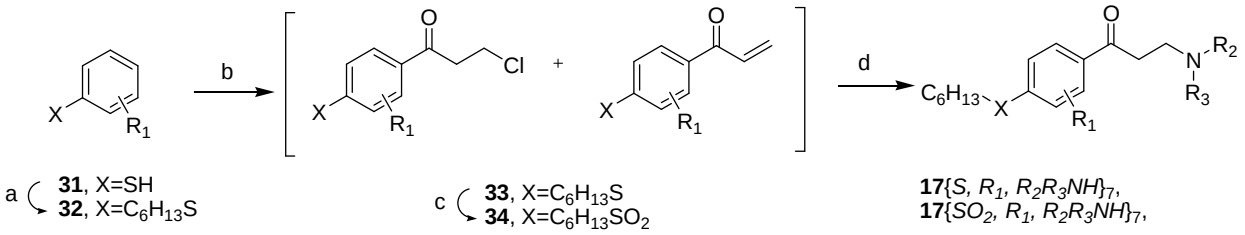
***N*-(4-(3-(Dimethylamino)propanoyl)phenyl)hexanamide 16{*7*}**. Yield 25%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.21 (s, 1H), 7.87 (d, 2H, *J* = 8.7 Hz), 7.63 (d, 2H, *J* = 8.7 Hz), 3.17 (t, 2H, *J* = 7.3 Hz), 2.85 (t, 2H, *J* = 7.3 Hz), 2.34 (m, 8H), 1.69 (m, 2H), 1.30 (m, 4H), 0.86 (t, 3H, *J* = 7.1 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.13, 172.05, 142.85, 131.94, 129.38, 118.90, 53.82, 44.74, 37.66, 35.72, 31.34, 25.09, 22.35, 13.85; MS (ESI) *m/z* 291.4 $[M+H]^+$.

***N*-(4-(3-(Dimethylamino)propanoyl)phenyl)pentane-1-sulfonamide 16{*8*}**. Yield 36%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.75 (s, 1H), 7.81 (d, 2H, *J* = 8.7 Hz), 7.20 (d, 2H, *J* = 8.6 Hz), 3.09 (m, 4H),

2.84 (t, 2H, *J* = 7.2 Hz), 2.36 (s, 6H), 1.73 (m, 2H), 1.23 (m, 4H), 0.79 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.20, 142.70, 131.69, 129.93, 118.04, 53.67, 52.23, 44.54, 35.16, 30.13, 23.03, 22.03, 13.63; MS (ESI) *m/z* 327.4 $[M+H]^+$.

1-Butyl-3-(4-(3-(dimethylamino)propanoyl)phenyl)urea 16{*9*}. Yield 18%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.49 (s, 1H), 7.70 (m, 2H), 7.43 (m, 2H), 6.15 (s, 1H), 3.20 (m, 2H), 3.11 (t, 2H, *J* = 7.1 Hz), 2.86 (m, 2H), 2.39 (s, 6H), 1.45 (m, 2H), 1.30 (m, 2H), 0.87 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.20, 155.74, 145.00, 129.85, 129.51, 117.59, 54.30, 45.04, 39.78, 35.50, 32.10, 20.03, 13.73; MS (ESI) *m/z* 292.4 $[M+H]^+$.

Scheme 7. Synthesis of the second generated compounds



[a]*Reagent and condition*. (a) nHexBr, K_2CO_3, DMF, 85 ^oC; (b) $RCH_2C(O)Cl$, $AlCl_3$, DCM, 0 ^oC, 2 h; (c) *m*CPBA, DCM, 0 ^oC, 1 h (d) R_2R_3NH, DCM, rt, 1 h

(3-Chlorophenyl)(hexyl)sulfane 32{*1*}. ^1H NMR (400 MHz, $CDCl_3$) δ 11.39 (m, 1H), 11.30 (m, 1H), 11.24 (m, 1H), 7.04 (m, 2H), 5.78 (m, 2H), 5.56 (m, 2H), 5.42 (m, 4H), 5.01 (t, 3H, *J* = 6.9 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.43, 134.60, 129.75, 127.87, 126.38, 125.55, 33.24, 31.30, 28.87, 28.47, 22.50, 13.98.

(2,3-Dichlorophenyl)(hexyl)sulfane 32{*2*}. ^1H NMR (400 MHz, $CDCl_3$) δ 7.34 (m, 1H), 7.22 (m, 2H), 3.02 (m, 2H), 1.80 (m, 2H), 1.57 (m, 2H), 1.41 (m, 4H), 0.99 (t, 3H, *J* = 6.9 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.56, 133.42, 130.41, 127.20, 126.46, 124.90, 32.61, 31.33, 28.64, 28.33, 22.49, 13.99.

(2,5-Dichlorophenyl)(hexyl)sulfane 32{3**}.** ^1H NMR (400 MHz, $CDCl_3$) δ 7.28 (d, *J* = 8.5, 1H), 7.19 (d, *J* = 2.4, 1H), 7.07 (dd, *J* = 2.4, 8.5, 1H), 2.97 – 2.92 (m, 2H), 1.78 – 1.68 (m, 2H), 1.59 – 1.42 (m, 2H), 1.42 – 1.28 (m, 4H), 0.98 – 0.84 (m, 3H).

(3,5-Dichlorophenyl)(hexyl)sulfane 32{*4*}. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.13 (s, 2H), 2.92 (m, 2H), 1.66 (m, 2H), 1.43 (m, 2H), 1.30 (m, 4H), 0.89 (t, 3H, *J* = 7.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.26, 135.08, 125.64, 125.33, 32.95, 31.25, 28.63, 28.44, 22.48, 13.97.

(3,5-Dimethylphenyl)(hexyl)sulfane 32{*5*}. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.95 (s, 2H), 6.79 (s, 1H), 2.90 (m, 2H), 2.28 (m, 6H), 1.64 (m, 2H), 1.43 (m, 2H), 1.30 (m, 4H), 0.89 (t, 3H, *J* = 6.5 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.36, 136.54, 127.51, 126.45, 33.52, 31.35, 29.14, 28.53, 22.52, 21.21, 14.00.

3-Chloro-1-(2-chloro-4-(hexylthio)phenyl)propan-1-one 33{*1*}. Yield 70%; ^{1}H NMR (400 MHz,) δ 7.53 (d, 1H, *J* = 8.3 Hz), 7.26 (d, 1H, *J* = 1.9 Hz), 7.18 (dd, 1H, *J* = 1.8, 8.3 Hz), 3.88 (t, 2H, *J* = 6.7 Hz), 3.45 (t, 2H, *J* = 6.6 Hz), 2.97 (m, 2H), 1.69 (m, 2H), 1.45 (m, 2H), 1.31 (m, 4H), 0.90 (t, 3H, *J* = 6.8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.89, 144.86, 133.84, 132.32, 130.18, 127.99, 124.96, 45.22, 38.74, 32.11, 31.25, 28.53, 28.48, 22.47, 13.96.

3-Chloro-1-(2,3-dichloro-4-(hexylthio)phenyl)propan-1-one 33{*2*}. Yield 64%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 (d, 1H, *J* = 8.3 Hz), 7.07 (d, 1H, *J* = 8.4 Hz), 3.81 (t, 2H, *J* = 6.6 Hz), 3.36 (t, 2H, *J* = 6.6 Hz), 2.90 (m, 2H), 1.68 (m, 2H), 1.42 (m, 2H), 1.26 (m, 4H), 0.84 (t, 3H, *J* = 6.9 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.18, 144.43, 135.91, 135.61, 131.78, 127.05, 123.15, 45.32, 38.66, 32.19, 31.29, 28.63, 28.04, 22.46, 13.97.

3-Chloro-1-(2,3-dichloro-4-(hexylthio)phenyl)propan-1-one 33{*3*}. Yield 63%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (s, 1H), 7.19 (s, 1H), 3.90 (t, *J* = 6.6, 2H), 3.47 (t, *J* = 6.6, 2H), 2.99 (t, *J* = 7.4, 2H), 1.83 – 1.71 (m, 2H), 1.61 – 1.46 (m, 2H), 1.42 – 1.30 (m, 4H), 0.94 (t, *J* = 7.0, 3H).

3-Chloro-1-(2,6-dichloro-4-(hexylthio)phenyl)propan-1-one 33{*4*}. Yield 55%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.17 (d, 2H, *J* = 8.9 Hz), 3.87 (t, 2H, *J* = 6.8 Hz), 3.29 (t, 2H, *J* = 6.8 Hz), 2.94 (m, 2H), 1.66 (m, 2H), 1.44 (s, 2H), 1.31 (m, 4H), 0.89 (t, 3H, *J* = 6.8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.54, 142.76, 135.01, 130.75, 126.10, 46.36, 37.23, 32.58, 31.22, 28.41, 22.46, 13.96.

3-Chloro-1-(4-(hexylthio)-2,6-dimethylphenyl)propan-1-one 33{*5*}. Yield 29%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.84 (d, 2H, *J* = 7.3 Hz), 3.76 (t, 2H, *J* = 6.4 Hz), 3.04 (t, 2H, *J* = 6.4 Hz), 2.80 (m, 2H), 2.10 (s, 6H), 1.53 (m, 2H), 1.32 (m, 2H), 1.19 (m, 4H), 0.78 (t, 3H, *J* = 6.9 Hz).

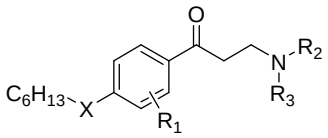
1-(2-Chloro-4-(hexylsulfonyl)phenyl)prop-2-en-1-one 34{*1*}. Yield 89%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, 1H, *J* = 1.4 Hz), 7.86 (dd, 1H, *J* = 1.7, 7.9 Hz), 7.55 (d, 1H, *J* = 8.0 Hz), 6.73 (dd, 1H, *J* = 10.6, 17.6 Hz), 6.17 (d, 1H, *J* = 10.6 Hz), 6.10 (d, 1H, *J* = 17.6 Hz), 3.11 (m, 2H), 1.71 (m, 2H), 1.38 (m, 2H), 1.25 (m, 4H), 0.87 (t, 3H, *J* = 6.9 Hz).

1-(2,3-Dichloro-4-(hexylsulfonyl)phenyl)prop-2-en-1-one 34{*2*}. Yield 70%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (d, 1H, *J* = 8.1 Hz), 7.36 (t, 1H, *J* = 7.4 Hz), 6.62 (dd, 1H, *J* = 10.6, 17.6 Hz), 6.15 (d, 1H, *J* = 10.8 Hz), 6.01 (d, 1H, *J* = 17.6 Hz), 3.36 (m, 2H), 1.63 (m, 2H), 1.34 (m, 2H), 1.21 (m, 4H), 0.80 (t, 3H, *J* = 6.9 Hz).

3-chloro-1-(2,5-dichloro-4-(hexylsulfonyl)phenyl)propan-1-one 34{*3*}. Yield 84%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (s, 1H), 7.57 (s, 1H), 3.82 (t, *J* = 6.4, 2H), 3.41 – 3.28 (m, 4H), 1.65 (dt, *J* = 7.7, 15.5, 2H), 1.39 – 1.30 (m, 2H), 1.22 (dd, 4H), 0.81 (t, *J* = 6.9, 3H).

1-(2,6-Dichloro-4-(hexylsulfonyl)phenyl)prop-2-en-1-one 34{*4*}. Yield 63%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (s, 1H), 6.60 (dd, 1H, *J* = 10.6, 17.7 Hz), 6.27 (d, 1H, *J* = 10.6 Hz), 5.98 (d, 1H, *J* = 17.7 Hz), 3.11 (m, 2H), 1.73 (m, 2H), 1.39 (m, 2H), 1.28 (m, 4H), 0.87 (t, 3H, *J* = 6.9 Hz).

1-(4-(Hexylsulfonyl)-2,6-dimethylphenyl)prop-2-en-1-one 34{*5*}. Yield 75%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (s, 2H), 6.57 (dd, 1H, *J* = 10.5, 17.7 Hz), 6.19 (d, 1H, *J* = 10.5 Hz), 5.85 (d, 1H, *J* = 17.7 Hz), 3.06 (m, 2H), 2.25 (s, 6H), 1.70 (m, 2H), 0.85 (t, 3H, *J* = 6.8 Hz).



17{*S, R_1, R_2R_3NH*}$_7$, **17**{*SO_2, R_1, R_2R_3NH*}$_7$,

17{*1,1,1*}

Same with **12**{*11*}

1-(2-Chloro-4-(hexyloxy)phenyl)-3-(2-methylaziridin-1-yl)propan-1-one 17{*1,1,2}*. Yield 87%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (d, *J* = 8.7, 1H), 6.93 (d, *J* = 2.4, 1H), 6.82 (dd, *J* = 2.4, 8.7, 1H), 3.99 (t, *J* = 6.5, 2H), 3.24 (t, *J* = 7.1, 2H), 2.71 – 2.52 (m, 2H), 1.84 – 1.71 (m, 2H), 1.52 – 1.41 (m, 4H), 1.40 – 1.30 (m, 4H), 1.15 (t, *J* = 6.3, 3H), 0.91 (t, *J* = 6.9, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.80, 161.78, 133.48, 131.70, 130.52, 116.58, 113.13, 68.59, 56.14, 42.85, 34.90, 34.87, 31.49, 28.95, 25.59, 22.57, 18.32, 14.02; MS (ESI) *m/z* 324.4 $[M+H]^+$.

1-(2-Chloro-4-(hexyloxy)phenyl)-3-morpholinopropan-1-one 17{*1,1,3}*. Yield 75%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (d, *J* = 8.7, 1H), 6.92 (d, *J* = 2.4, 1H), 6.82 (dd, *J* = 2.4, 8.7, 1H), 3.98 (t,

J = 6.5, 2H), 3.76 – 3.63 (m, 4H), 3.16 (t, *J* = 7.2, 2H), 2.79 (t, *J* = 7.2, 2H), 2.56 – 2.43 (m, 4H), 1.84 – 1.68 (m, 2H), 1.53 – 1.40 (m, 2H), 1.40 – 1.27 (m, 4H), 0.91 (t, *J* = 7.0, 3H); ^{13}C NMR (101 MHz, C $CDCl_3$) δ 200.14, 161.72, 133.20, 131.53, 130.65, 116.42, 113.18, 68.60, 66.90, 53.81, 53.53, 39.88, 31.49, 28.96, 25.60, 22.57, 14.02; MS (ESI) *m/z* 354.4 $[M+H]^+$.

4-(3-(2-Chloro-4-(hexyloxy)phenyl)-3-oxopropyl)piperazin-2-one 17{*1,1,4}*. Yield 100%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, *J* = 8.7, 1H), 6.92 (brs, 2H), 6.82 (dd, *J* = 2.3, 8.7, 1H), 3.98 (t, *J* = 6.5, 2H), 3.39 (brs, 2H), 3.22 – 3.13 (m, 4H), 2.86 (t, *J* = 7.0, 2H), 2.75 (brs, 2H), 1.85 – 1.71 (m, 2H), 1.54 – 1.40 (m, 2H), 1.40 – 1.26 (m, 4H), 0.91 (t, *J* = 6.7, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.52, 169.49, 161.88, 133.30, 131.64, 130.33, 116.51, 113.28, 68.63, 56.71, 52.45, 49.09, 41.21, 40.02, 31.48, 28.94, 25.59, 22.56, 14.02; MS (ESI) *m/z* 367.4 $[M+H]^+$.

3-(4-Acetylpiperazin-1-yl)-1-(2-chloro-4-(hexyloxy)phenyl)propan-1-one 17{*1,1,5}*. Yield 100%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (d, *J* = 8.7, 1H), 6.91 (s, 1H), 6.81 (dd, *J* = 2.3, 8.7, 1H), 3.97 (t, *J* = 6.5, 2H), 3.57 (brs, 2H), 3.47 – 3.35 (m, 2H), 3.15 (t, *J* = 7.1, 2H), 2.79 (t, *J* = 7.0, 2H), 2.51 – 2.36 (m, 4H), 2.06 (s, 3H), 1.83 – 1.69 (m, 2H), 1.51 – 1.39 (m, 2H), 1.39 – 1.25 (m, 4H), 0.90 (t, *J* = 6.3, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.99, 168.89, 161.76, 133.21, 131.52, 130.53, 116.46, 113.19, 68.61, 53.27, 53.16, 52.58, 46.21, 41.31, 39.98, 31.48, 28.94, 25.58, 22.55, 21.31, 14.01; MS (ESI) *m/z* 395.4 $[M+H]^+$.

1-(2-Chloro-4-(hexyloxy)phenyl)-3-(4-(ethylsulfonyl)piperazin-1-yl)propan-1-one 17{*1,1,6}*. Yield 85%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (d, *J* = 8.7, 1H), 6.93 (d, *J* = 2.4, 1H), 6.83 (dd, *J* = 2.4, 8.7, 1H), 3.99 (t, *J* = 6.5, 2H), 3.37 – 3.24 (m, 4H), 3.15 (t, *J* = 7.1, 2H), 2.94 (q, *J* = 7.4, 2H),

2.84 (t, *J* = 7.1, 2H), 2.60 – 2.51 (m, 4H), 1.80 (dd, *J* = 7.3, 14.3, 2H), 1.45 (dd, *J* = 6.3, 14.0, 2H), 1.35 (dt, *J* = 7.3, 10.2, 7H), 0.91 (t, *J* = 7.0, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.84, 161.80, 133.24, 131.54, 130.46, 116.49, 113.22, 68.63, 53.11, 52.64, 45.71, 43.75, 39.90, 31.49, 28.95, 25.59, 22.57, 14.02, 7.79; MS (ESI) *m/z* 345.5 $[M+H]^+$.

17{*1,2,1*} Same with **12**{24}

1-(2,3-Dichloro-4-(hexyloxy)phenyl)-3-(2-methylaziridin-1-yl)propan-1-one 17{*1,2,2}*. Yield 99%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 (d, *J* = 8.7, 1H), 6.79 (d, *J* = 8.7, 1H), 4.00 (t, *J* = 6.5, 2H), 3.13 (t, *J* = 7.0, 2H), 2.64 – 2.48 (m, 2H), 1.86 – 1.70 (m, 2H), 1.49 – 1.34 (m, 3H), 1.34 – 1.23 (m, 4H), 1.07 (t, *J* = 5.7, 3H), 0.84 (t, *J* = 7.1, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 200.23, 157.71, 132.62, 131.47, 128.13, 123.35, 110.29, 77.39, 77.07, 76.75, 69.74, 56.01, 43.10, 34.92, 34.89, 31.43, 28.85, 25.55, 22.55, 18.31, 14.00; MS (ESI) *m/z* 358.3 $[M+H]^+$.

1-(2,3-Dichloro-4-(hexyloxy)phenyl)-3-morpholinopropan-1-one 17{*1,2,3}*. Yield 100%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 (d, *J* = 8.7, 1H), 6.79 (d, *J* = 8.7, 1H), 4.00 (t, *J* = 6.5, 2H), 3.65 – 3.53 (m, 4H), 3.06 (t, *J* = 7.1, 2H), 2.69 (t, *J* = 7.1, 2H), 2.43 – 2.32 (m, 4H), 1.85 – 1.70 (m, 2H), 1.49 – 1.35 (m, 2H), 1.35 – 1.19 (m, 4H), 0.84 (t, *J* = 7.1, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 200.63, 157.63, 132.72, 131.22, 127.95, 123.20, 110.34, 69.75, 66.88, 53.78, 53.49, 40.12, 31.44, 28.86, 25.56, 22.55, 14.01; MS (ESI) *m/z* 388.3 $[M+H]^+$.

4-(3-(2,3-Dichloro-4-(hexyloxy)phenyl)-3-oxopropyl)piperazin-2-one 17{*1,2,4}*. Yield 99%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 (d, *J* = 8.7, 1H), 6.90 (s, 1H), 6.87 (d, *J* = 8.7, 1H), 4.08 (t, *J* = 6.4,

2H), 3.33 (brs, 2H), 3.19 – 3.08 (m, 4H), 2.91 – 2.82 (m, 2H), 2.72 (brs, 2H), 1.92 – 1.80 (m, 2H), 1.57 – 1.43 (m, 2H), 1.43 (brs, 4H), 0.97 – 0.82 (m, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 200.01, 169.42, 157.79, 132.39, 131.26, 128.08, 123.28, 110.42, 69.78, 56.70, 52.40, 49.01, 41.20, 40.27, 31.43, 28.84, 25.55, 22.55, 14.01; MS (ESI) *m/z* 401.3 $[M+H]^+$.

3-(4-Acetylpiperazin-1-yl)-1-(2,3-dichloro-4-(hexyloxy)phenyl)propan-1-one **17**{*1,2,5}*. Yield 100%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 (d, *J* = 8.7, 1H), 6.79 (d, *J* = 8.7, 1H), 4.00 (t, *J* = 6.5, 2H), 3.50 (brs, 2H), 3.42 – 3.30 (m, 2H), 3.06 (t, *J* = 7.0, 2H), 2.72 (t, *J* = 7.0, 2H), 2.44 – 2.28 (m, 4H), 2.00 (s, 3H), 1.85 – 1.71 (m, 2H), 1.52 – 1.37 (m, 2H), 1.35 – 1.23 (m, 4H), 0.84 (t, *J* = 6.5, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 200.43, 168.90, 157.68, 132.59, 131.24, 127.96, 123.25, 110.34, 69.77, 53.23, 53.12, 52.56, 46.19, 41.29, 40.23, 31.42, 28.84, 25.55, 22.54, 21.31, 14.00; MS (ESI) *m/z* 429.4 $[M+H]^+$.

1-(2,3-Dichloro-4-(hexyloxy)phenyl)-3-(4-(ethylsulfonyl)piperazin-1-yl)propan-1-one

17{*1,2,6}*. Yield 100%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 (d, *J* = 8.7, 1H), 6.80 (d, *J* = 8.7, 1H), 4.00 (t, *J* = 6.5, 2H), 3.27 – 3.13 (m, 4H), 3.05 (t, *J* = 7.0, 2H), 2.87 (q, *J* = 7.4, 2H), 2.74 (t, *J* = 7.0, 2H), 2.53 – 2.38 (m, 4H), 1.85 – 1.69 (m, 2H), 1.50 – 1.36 (m, 2H), 1.36 – 1.25 (m, 7H), 0.84 (t, *J* = 7.0, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 200.28, 157.71, 132.51, 131.28, 127.95, 123.29, 110.34, 69.78, 53.07, 52.61, 45.70, 43.77, 40.16, 31.43, 28.85, 25.56, 22.55, 14.01, 7.79; MS (ESI) *m/z* 479.5 $[M+H]^+$.

17{*1,3,1}*

Same with **12**{25}

1-(2,5-Dichloro-4-(hexyloxy)phenyl)-3-(2-methylaziridin-1-yl)propan-1-one **17**{*1,3,2}*. Yield 72%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (s, 1H), 6.85 (s, 1H), 3.98 (t, *J* = 6.5, 2H), 3.15 (t, *J* = 7.1, 2H), 2.63 – 2.46 (m, 2H), 1.88 – 1.72 (m, 2H), 1.51 – 1.34 (m, 3H), 1.34 – 1.24 (m, 4H), 1.07 (d, *J* = 5.3, 3H), 0.84 (dd, *J* = 4.5, 9.7, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 198.77, 156.97, 131.56, 131.52, 130.77, 121.70, 114.84, 69.74, 56.02, 42.90, 34.94, 31.42, 28.77, 25.51, 22.54, 18.31, 14.00; MS (ESI) *m/z* 358.3 $[M+H]^+$.

1-(2,5-Dichloro-4-(hexyloxy)phenyl)-3-morpholinopropan-1-one **17**{*1,3,3}*. Yield 100%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (s, 1H), 6.84 (s, 1H), 3.98 (t, *J* = 6.5, 2H), 3.69 – 3.56 (m, 4H), 3.07 (t, *J* = 7.1, 2H), 2.70 (t, *J* = 7.1, 2H), 2.40 (brs, 4H), 1.85 – 1.75 (m, 2H), 1.43 (s, 2H), 1.35 – 1.22 (m, 4H), 0.84 (t, *J* = 7.0, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.22, 168.32, 156.85, 131.38, 131.16, 130.92, 121.71, 114.70, 69.75, 66.94, 53.73, 53.54, 39.98, 31.42, 28.77, 25.51, 22.54, 14.00; MS (ESI) *m/z* 388.3 $[M+H]^+$.

4-(3-(2,5-Dichloro-4-(hexyloxy)phenyl)-3-oxopropyl)piperazin-2-one **17**{*1,3,4}*. Yield 91%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 (s, 1H), 6.93 (s, 1H), 6.72 (br, 1H), 4.07 (t, *J* = 6.5, 2H), 3.41 – 3.29 (m, 2H), 3.20 – 3.08 (m, 4H), 2.87 (t, *J* = 7.0, 2H), 2.74 – 2.65 (m, 2H), 1.94 – 1.80 (m, 2H), 1.56 – 1.45 (m, 2H), 1.43 – 1.28 (m, 4H), 0.92 (t, *J* = 7.0, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 198.41, 169.35, 157.05, 131.45, 131.38, 130.53, 121.84, 114.78, 69.78, 56.72, 52.34, 49.16, 41.26, 40.11, 31.41, 28.75, 25.51, 22.54, 14.00; MS (ESI) *m/z* 401.3 $[M+H]^+$.

3-(4-Acetylpiperazin-1-yl)-1-(2,5-dichloro-4-(hexyloxy)phenyl)propan-1-one **17**{*1,3,5*}. Yield 35%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 (s, 1H), 6.94 (s, 1H), 4.08 (t, *J* = 6.5, 2H), 3.65 – 3.53 (m, 2H), 3.53 – 3.44 (m, 2H), 3.16 (t, *J* = 7.0, 2H), 2.87 – 2.76 (m, 2H), 2.57 – 2.36 (m, 4H), 2.05 (s, 3H), 1.94 – 1.84 (m, 2H), 1.57 – 1.45 (m, 2H), 1.45 – 1.27 (m, 4H), 0.93 (t, *J* = 7.0, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.00, 168.90, 156.89, 131.35, 131.20, 130.76, 121.69, 114.73, 69.75, 53.18, 53.16, 52.58, 46.23, 41.33, 40.06, 31.40, 28.75, 25.49, 22.52, 21.31, 13.99; MS (ESI) *m/z* 429.4 $[M+H]^+$.

1-(2,5-Dichloro-4-(hexyloxy)phenyl)-3-(4-(ethylsulfonyl)piperazin-1-yl)propan-1-one

17{*1,3,6*}. Yield 100%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (s, 1H), 6.85 (s, 1H), 3.99 (t, *J* = 6.5, 2H), 3.26 – 3.18 (m, 4H), 3.06 (t, *J* = 7.0, 2H), 2.87 (q, *J* = 7.4, 2H), 2.75 (t, *J* = 7.0, 2H), 2.50 – 2.41 (m, 4H), 1.87 – 1.73 (m, 2H), 1.47 – 1.36 (m, 2H), 1.36 – 1.23 (m, 7H), 0.84 (t, *J* = 7.1, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 198.95, 156.93, 131.40, 131.21, 130.77, 121.72, 114.73, 69.78, 53.05, 52.66, 45.74, 43.71, 39.99, 31.42, 28.77, 25.52, 22.54, 14.01, 7.79; MS (ESI) *m/z* 479.5 $[M+H]^+$.

17{*1,4,1*}

Same with **12**{*26*}

1-(3,5-Dichloro-4-(hexyloxy)phenyl)-3-(2-methylaziridin-1-yl)propan-1-one **17**{*1,4,2*}. Yield 85%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.76 (s, 2H), 3.87 (t, *J* = 6.5, 2H), 3.04 (t, *J* = 7.3, 2H), 2.58 (t, *J* = 7.3, 2H), 1.74 – 1.63 (m, 2H), 1.44 – 1.32 (m, 3H), 1.32 – 1.20 (m, 4H), 1.13 – 1.03 (m, 3H),

0.84 (t, *J* = 7.0, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 201.11, 159.93, 131.93, 131.06, 114.54, 84.67, 68.86, 54.68, 44.53, 34.91, 34.86, 31.46, 28.87, 25.56, 22.57, 18.32, 14.01; MS (ESI) *m/z* 358.3 $[M+H]^+$.

1-(3,5-Dichloro-4-(hexyloxy)phenyl)-3-(morpholino)propan-1-one 17{*1,4,3}*

Yield 81%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.76 (s, 2H), 3.87 (t, *J* = 6.5, 2H), 3.67 – 3.54 (m, 4H), 2.96 (t, *J* = 7.3, 2H), 2.73 (t, *J* = 7.3, 2H), 2.48 – 2.34 (m, 4H), 1.78 – 1.62 (m, 3H), 1.44 – 1.33 (m, 2H), 1.33 – 1.21 (m, 4H), 0.90 – 0.74 (m, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 201.23, 159.93, 131.89, 131.17, 114.56, 68.88, 66.91, 53.73, 53.58, 52.63, 41.48, 31.46, 28.87, 25.55, 22.56, 14.02; MS (ESI) *m/z* 388.3 $[M+H]^+$.

4-(3-(3,5-Dichloro-4-(hexyloxy)phenyl)-3-oxopropyl)piperazin-2-one 17{*1,4,4}*. Yield 70%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.85 (s, 2H), 6.68 (s, 1H), 3.95 (t, *J* = 6.5, 2H), 3.36 (brs, 2H), 3.17 (s, 2H), 3.04 (t, *J* = 7.0, 2H), 2.89 (t, *J* = 7.0, 2H), 2.76 – 2.64 (m, 2H), 1.83 – 1.72 (m, 2H), 1.50 – 1.40 (m, 2H), 1.40 – 1.29 (m, *J* = 8.7, 4H), 0.92 (t, *J* = 7.0, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 200.75, 169.36, 160.03, 131.61, 131.16, 114.61, 68.90, 56.75, 51.27, 49.15, 41.61, 41.27, 31.45, 28.86, 25.55, 22.56, 14.02; MS (ESI) *m/z* 401.3 $[M+H]^+$.

3-(4-Acetylpiperazin-1-yl)-1-(3,5-dichloro-4-(hexyloxy)phenyl)propan-1-one 17{*1,4,5}*. Yield 52%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.85 (s, 2H), 3.95 (t, *J* = 6.5, 2H), 3.64 – 3.54 (m, 2H), 3.50 – 3.40 (m, 2H), 3.04 (t, *J* = 7.2, 2H), 2.83 (t, *J* = 7.2, 2H), 2.54 – 2.37 (m, 4H), 2.10 (s, 3H), 1.82 – 1.72 (m, 2H), 1.50 – 1.40 (m, 2H), 1.40 – 1.28 (m, 4H), 0.95 – 0.86 (m, 3H); ^{13}C NMR (101 MHz,

$CDCl_3$) δ 201.10, 168.92, 159.97, 131.78, 131.17, 114.57, 68.89, 53.25, 52.61, 52.09, 46.21, 41.62, 41.32, 31.45, 28.86, 25.55, 22.56, 21.33, 14.01; MS (ESI) *m/z* 429.4 $[M+H]^+$.

1-(3,5-Dichloro-4-(hexyloxy)phenyl)-3-(4-(ethylsulfonyl)piperazin-1-yl)propan-1-one

17{*1,4,6}*.

Yield 63%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.77 (s, 2H), 3.87 (t, *J* = 6.5, 2H), 3.30 – 3.15 (m, 4H), 2.94 (t, *J* = 7.1, 2H), 2.87 (q, *J* = 7.4, 2H), 2.78 (t, *J* = 7.1, 2H), 2.58 – 2.41 (m, 4H), 1.75 – 1.64 (m, 2H), 1.42 – 1.32 (m, 2H), 1.32 – 1.21 (m, 7H), 0.84 (t, *J* = 7.0, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 200.95, 159.99, 131.74, 131.17, 114.59, 68.91, 52.69, 51.92, 45.71, 43.78, 41.52, 31.46, 28.87, 25.55, 22.56, 14.02, 7.80; MS (ESI) *m/z* 479.5 $[M+H]^+$.

17{*1,5,1}*

Same with **12**{*22*}

1-(4-(Hexyloxy)-2,6-dimethylphenyl)-3-(2-methylaziridin-1-yl)propan-1-one **17**{*1,5,2}*. Yield 62%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.56 (s, 2H), 3.94 (t, *J* = 6.6, 2H), 3.03 – 2.93 (m, 2H), 2.70 – 2.55 (m, 2H), 2.22 (d, *J* = 13.8, 6H), 1.81 – 1.65 (m, 2H), 1.50 – 1.41 (m, 4H), 1.41 – 1.25 (m, 5H), 1.17 (d, *J* = 5.1, 3H), 0.92 (t, *J* = 7.0, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 209.00, 159.06, 134.90, 134.61, 113.73, 67.87, 55.13, 45.39, 34.94, 34.85, 31.58, 29.22, 25.72, 22.62, 19.60, 18.34, 14.05; MS (ESI) *m/z* 346.3 $[M+H]^+$.

1-(4-(Hexyloxy)-2,6-dimethylphenyl)-3-morpholinopropan-1-one **17**{*1,5,3}*. Yield 71%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.56 (s, 2H), 3.94 (t, *J* = 6.6, 2H), 3.77 – 3.66 (m, 4H), 2.91 (t, *J* = 7.0,

2H), 2.78 (t, *J* = 7.2, 2H), 2.48 (brs, 4H), 2.24 (s, 6H), 1.84 – 1.70 (m, 2H), 1.51 – 1.40 (m, 2H), 1.40 – 1.29 (m, 4H), 0.92 (t, *J* = 7.0, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 208.99, 159.11, 134.79, 113.78, 67.88, 66.85, 53.68, 53.32, 42.21, 31.58, 29.21, 25.71, 22.62, 19.75, 14.05; MS (ESI) *m/z* 348.5 $[M+H]^+$.

4-(3-(4-(Hexyloxy)-2,6-dimethylphenyl)-3-oxopropyl)piperazin-2-one **17**{*1,5,4}*. Yield 49%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.47 (s, 2H), 6.35 (brs, 1H), 3.86 (t, *J* = 6.6, 2H), 3.35 (brs, 2H), 3.10 (s, 2H), 2.88 – 2.75 (m, 4H), 2.70 – 2.59 (m, 2H), 2.15 (s, 6H), 1.75 – 1.63 (m, 2H), 1.44 – 1.31 (m, 2H), 1.31 – 1.21 (m, 4H), 0.84 (t, *J* = 7.0, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 208.39, 159.22, 134.79, 134.47, 113.86, 67.90, 56.69, 51.99, 49.28, 42.31, 41.14, 31.57, 29.20, 25.71, 22.62, 19.72, 14.05; MS (ESI) *m/z* 361.5 $[M+H]^+$.

3-(4-Acetylpiperazin-1-yl)-1-(4-(hexyloxy)-2,6-dimethylphenyl)propan-1-one **17**{*1,5,5}*. Yield 71%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.55 (s, 2H), 3.93 (t, *J* = 6.6, 2H), 3.64 – 3.54 (m, 2H), 3.50 – 3.39 (m, 2H), 2.90 (t, *J* = 6.8, 2H), 2.79 (t, *J* = 7.0, 2H), 2.52 – 2.46 (m, 2H), 2.46 – 2.40 (m, 2H), 2.23 (s, 6H), 2.08 (s, 3H), 1.81 – 1.67 (m, 2H), 1.50 – 1.39 (m, *J* = 14.0, 2H), 1.39 – 1.26 (m, 4H), 0.91 (t, *J* = 7.0, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 208.84, 168.94, 159.15, 134.78, 134.69, 113.81, 67.89, 53.39, 52.76, 52.70, 46.16, 42.39, 41.26, 31.57, 29.20, 25.70, 22.61, 21.31, 19.77, 14.05; MS (ESI) *m/z* 389.6 $[M+H]^+$.

3-(4-(Ethylsulfonyl)piperazin-1-yl)-1-(4-(hexyloxy)-2,6-dimethylphenyl)propan-1-one

17{*1,5,6}*. Yield 29%; ^{1}H NMR (400 MHz, CDCl3) δ 6.56 (s, 2H), 3.94 (t, *J* = 6.6, 2H), 3.32 (brs, 4H), 2.97 (q, *J* = 7.4, 2H), 2.93 – 2.80 (m, 4H), 2.59 (s, 4H), 2.24 (s, 6H), 1.85 – 1.70 (m, 2H),

1.53 – 1.42 (m, 2H), 1.42 – 1.31 (m, *J* = 6.9, 14.3, 7H), 0.92 (t, *J* = 7.0, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 208.58, 159.19, 134.77, 134.60, 113.83, 67.91, 52.83, 52.59, 45.60, 43.92, 42.23, 31.57, 29.21, 25.71, 22.62, 19.78, 14.05, 7.81; MS (ESI) *m/z* 439.6 $[M+H]^+$.

1-(2-Chloro-4-(hexylthio)phenyl)-3-(dimethylamino)propan-1-one 17{*2,1,1*}. Yield 89%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 (d, 1H, *J* = 8.2 Hz), 7.19 (t, 1H, *J* = 5.1 Hz), 7.10 (m, 1H), 3.06 (t, 2H, *J* = 7.3 Hz), 2.88 (t, 2H, *J* = 7.4 Hz), 2.64 (t, 2H, *J* = 7.3 Hz), 2.18 (s, 6H), 1.61 (m, 2H), 1.37 (m, 2H), 1.23 (m, 4H), 0.82 (t, 3H, *J* = 6.8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 200.81, 143.68, 134.95, 131.84, 129.80, 128.05, 125.06, 54.25, 45.29, 40.92, 32.23, 31.22, 28.55, 28.44, 22.44, 13.93; MS (ESI) *m/z* 328.8 $[M+H]^+$.

1-(2-Chloro-4-(hexylthio)phenyl)-3-(2-methylaziridin-1-yl)propan-1-one 17{*2,1,2}*. Yield 85%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 (d, *J* = 8.2, 1H), 7.26 (d, *J* = 1.8, 1H), 7.17 (dd, *J* = 1.8, 8.2, 1H), 3.26 – 3.19 (m, 2H), 2.98 – 2.92 (m, 2H), 2.68 – 2.58 (m, 2H), 1.74 – 1.63 (m, 2H), 1.52 – 1.39 (m, 4H), 1.37 – 1.25 (m, 5H), 1.15 (t, *J* = 5.4, 3H), 0.96 (t, *J* = 7.0, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 200.53, 143.94, 134.85, 132.12, 129.95, 128.16, 125.04, 55.94, 43.03, 34.92, 34.89, 32.24, 31.29, 28.60, 28.50, 22.50, 18.31, 14.00; MS (ESI) *m/z* 340.4 $[M+H]^+$.

1-(2-Chloro-4-(hexylthio)phenyl)-3-morpholinopropan-1-one 17{*2,1,3}*. Yield 82%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 (d, *J* = 8.2, 1H), 7.26 (s, 1H), 7.17 (d, *J* = 8.2, 1H), 3.69 (brs, 5H), 3.16 (t, *J* = 7.0, 2H), 2.97 (t, *J* = 7.4, 2H), 2.78 (t, *J* = 7.0, 2H), 2.50 (brs, 4H), 1.76 – 1.64 (m, 2H), 1.55 – 1.41 (m, 2H), 1.38 – 1.29 (m, 4H), 0.90 (t, *J* = 6.3, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 200.89,

143.81, 134.98, 131.87, 129.84, 128.06, 125.07, 66.87, 53.66, 53.49, 40.04, 32.27, 31.29, 28.60, 28.51, 22.51, 14.01; MS (ESI) *m/z* 370.5 $[M+H]^+$.

4-(3-(2-Chloro-4-(hexylthio)phenyl)-3-oxopropyl)piperazin-2-one **17**{*2,1,4}*. Yield 90%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 (d, *J* = 8.2, 1H), 7.25 (d, *J* = 1.6, 1H), 7.16 (dd, *J* = 1.7, 8.2, 1H), 6.97 (brs, 1H), 3.38 (brs, 2H), 3.22 – 3.09 (m, 4H), 2.96 (t, *J* = 7.4, 2H), 2.86 (t, *J* = 7.0, 2H), 2.77 – 2.64 (m, 2H), 1.75 – 1.61 (m, 2H), 1.52 – 1.40 (m, 2H), 1.40 – 1.23 (m, 4H), 0.89 (t, *J* = 6.5, 3H);^{13}C NMR (101 MHz, $CDCl_3$) δ 200.25, 169.44, 144.21, 134.58, 131.96, 129.91, 128.02, 125.05, 56.66, 52.28, 49.04, 41.18, 40.18, 32.20, 31.28, 28.57, 28.50, 22.50, 14.01; MS (ESI) *m/z* 383.5 $[M+H]^+$.

3-(4-Acetylpiperazin-1-yl)-1-(2-chloro-4-(hexylthio)phenyl)propan-1-one **17**{*2,1,5}*. Yield 85%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 (d, *J* = 8.2, 1H), 7.25 (d, *J* = 1.7, 1H), 7.16 (dd, *J* = 1.8, 8.2, 1H), 3.63 – 3.54 (m, 2H), 3.50 – 3.40 (m, 2H), 3.15 (t, *J* = 7.0, 2H), 2.96 (t, *J* = 7.4, 2H), 2.80 (t, *J* = 7.0, 2H), 2.49 – 2.37 (m, 4H), 2.07 (s, 3H), 1.74 – 1.60 (m, 2H), 1.50 – 1.39 (m, 2H), 1.37 – 1.23 (m, 4H), 0.89 (t, *J* = 6.8, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 200.71, 168.89, 143.98, 134.83, 131.90, 129.83, 128.03, 125.02, 53.14, 53.12, 52.57, 46.19, 41.29, 40.15, 32.23, 31.28, 28.57, 28.50, 22.50, 21.31, 14.01; MS (ESI) *m/z* 411.5 $[M+H]^+$.

1-(2-Chloro-4-(hexylthio)phenyl)-3-(4-(ethylsulfonyl)piperazin-1-yl)propan-1-one **17**{*2,1,6}*. Yield 86%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.19 (d, *J* = 8.2, 1H), 6.99 (d, *J* = 1.8, 1H), 6.91 (dd, *J* = 1.8, 8.2, 1H), 3.10 – 2.96 (m, 4H), 2.88 (t, *J* = 7.0, 2H), 2.77 – 2.63 (m, 4H), 2.57 (t, *J* = 7.0, 2H), 2.36 – 2.22 (m, 4H), 1.50 – 1.37 (m, 2H), 1.28 – 1.15 (m, 2H), 1.15 – 0.99 (m, 7H), 0.64 (t, *J*

= 5.8, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 200.29, 143.78, 134.48, 131.67, 129.57, 127.77, 124.76, 52.69, 52.36, 45.43, 43.52, 39.81, 31.97, 31.03, 28.31, 28.24, 22.24, 13.75, 7.53; MS (ESI) *m/z* 461.6 $[M+H]^+$.

1-(2,3-Dichloro-4-(hexylthio)phenyl)-3-(dimethylamino)propan-1-one 17{*2,2,1}*. Yield 84%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28 (d, 1H, *J* = 8.3 Hz), 7.06 (t, 1H, *J* = 7.7 Hz), 3.05 (t, 2H, *J* = 7.2 Hz), 2.88 (t, 2H, *J* = 7.4 Hz), 2.65 (t, 2H, *J* = 7.2 Hz), 2.20 (s, 6H), 1.66 (m, 2H), 1.40 (m, 2H), 1.24 (m, 4H), 0.83 (t, 3H, *J* = 6.6 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 200.88, 143.31, 136.57, 130.73, 130.02, 126.68, 123.24, 54.18, 45.22, 40.99, 32.19, 31.26, 28.60, 28.05, 22.44, 13.95; MS (ESI) *m/z* 363.3 $[M+H]^+$.

1-(2,3-Dichloro-4-(hexylthio)phenyl)-3-(2-methylaziridin-1-yl)propan-1-one 17{*2,2,2}*. Yield 97%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 (d, *J* = 8.3, 1H), 7.13 (d, *J* = 8.3, 1H), 3.20 (t, *J* = 7.0, 2H), 3.01 – 2.89 (m, 2H), 2.64 (t, *J* = 7.0, 2H), 1.81 – 1.66 (m, 2H), 1.53 – 1.39 (m, 4H), 1.39 – 1.24 (m, 5H), 1.14 (d, *J* = 5.3, 3H), 0.91 (t, *J* = 6.9, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 200.70, 143.53, 136.58, 130.87, 130.26, 126.81, 123.20, 55.85, 43.22, 34.93, 34.91, 32.24, 31.33, 28.66, 28.10, 22.50, 18.31, 14.01; MS (ESI) *m/z* 374.4 $[M+H]^+$.

1-(2,3-Dichloro-4-(hexylthio)phenyl)-3-morpholinopropan-1-one 17{*2,2,3}*. Yield 87%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 (d, *J* = 8.3, 1H), 7.13 (d, *J* = 8.3, 1H), 3.74 – 3.61 (m, 4H), 3.14 (t, *J* = 7.1, 2H), 2.96 (t, *J* = 7.4, 2H), 2.77 (t, *J* = 7.1, 2H), 2.46 (brs, 4H), 1.82 – 1.66 (m, 2H), 1.56 – 1.40 (m, 2H), 1.40 – 1.26 (m, 4H), 0.91 (t, *J* = 6.9, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 201.07,

143.38, 136.66, 130.75, 130.06, 126.73, 123.23, 66.86, 53.64, 53.46, 40.21, 32.26, 31.33, 28.66, 28.10, 22.50, 14.02; MS (ESI) *m/z* 404.4 $[M+H]^+$.

4-(3-(2,3-Dichloro-4-(hexylthio)phenyl)-3-oxopropyl)piperazin-2-one **17**{*2,2,4}*Yield 83%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26 (d, *J* = 8.3, 1H), 7.05 (d, *J* = 8.4, 1H), 6.84 (s, 1H), 3.31 – 3.19 (m, 2H), 3.11 – 3.01 (m, 4H), 2.94 – 2.84 (m, 2H), 2.77 (t, *J* = 7.0, 2H), 2.64 – 2.53 (m, 2H), 1.72 – 1.60 (m, 2H), 1.48 – 1.35 (m, 2H), 1.32 – 1.19 (m, 4H), 0.88 – 0.74 (m, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 200.50, 169.41, 143.73, 136.31, 130.73, 130.07, 126.76, 123.25, 56.74, 52.26, 48.98, 41.24, 40.42, 32.23, 31.32, 28.66, 28.08, 22.50, 14.02; MS (ESI) *m/z* 417.4 $[M+H]^+$.

3-(4-Acetylpiperazin-1-yl)-1-(2,3-dichloro-4-(hexylthio)phenyl)propan-1-one **17**{*2,2,5}.* Yield 89%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 (d, *J* = 8.3, 1H), 7.12 (d, *J* = 8.3, 1H), 3.57 (brs, 2H), 3.50 – 3.38 (m, 2H), 3.13 (t, *J* = 6.9, 2H), 2.96 (t, *J* = 7.4, 2H), 2.79 (t, *J* = 6.9, 2H), 2.52 – 2.35 (m, 4H), 2.07 (s, 3H), 1.82 – 1.62 (m, 2H), 1.57 – 1.42 (m, *J* = 7.2, 2H), 1.38 – 1.24 (m, 4H), 0.90 (t, *J* = 6.9, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 200.86, 168.89, 143.56, 136.50, 130.76, 130.09, 126.72, 123.19, 53.11, 52.56, 46.17, 41.28, 40.34, 32.24, 31.32, 28.66, 28.08, 22.50, 21.32, 14.02; MS (ESI) *m/z* 445.46 $[M+H]^+$.

1-(2,3-Dichloro-4-(hexylthio)phenyl)-3-(4-(ethylsulfonyl)piperazin-1-yl)propan-1-one

17{*2,2,6}.* Yield 86%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.07 (d, *J* = 8.3, 1H), 6.86 (d, *J* = 8.3, 1H), 3.00 (brs, 4H), 2.85 (t, *J* = 6.9, 2H), 2.74 – 2.62 (m, 4H), 2.55 (t, *J* = 6.9, 2H), 2.36 – 2.18 (m, 4H), 1.58 – 1.40 (m, 2H), 1.29 – 1.16 (m, 2H), 1.16 – 1.01 (m, 7H), 0.73 – 0.55 (m, *J* = 6.8, 3H); ^{13}C

NMR (101 MHz, $CDCl_3$) δ 200.45, 143.35, 136.15, 130.51, 129.86, 126.42, 122.92, 52.67, 52.34, 45.42, 43.53, 39.99, 31.97, 31.06, 28.40, 27.82, 22.24, 13.76, 7.53; MS (ESI) *m/z* 495.5 $[M+H]^+$.

1-(2,5-Dichloro-4-(hexylthio)phenyl)-3-(dimethylamino)propan-1-one **17**{*2,3,1}*. Yield 59%; ^1H NMR (400 MHz, $CDCl_3$) δ 7.50 (s, 1H), 7.08 (s, 1H), 3.06 (t, *J* = 7.2, 2H), 2.88 (t, *J* = 7.4, 3H), 2.65 (t, *J* = 7.2, 2H), 2.19 (s, 6H), 1.72 – 1.63 (m, 2H), 1.46 – 1.34 (m, 2H), 1.33 – 1.22 (m, 5H), 0.84 (t, *J* = 7.0, 4H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.50, 143.13, 135.01, 130.31, 130.20, 130.17, 126.97, 54.22, 45.34, 40.91, 32.01, 31.30, 28.62, 27.99, 22.50, 14.01; MS (ESI) *m/z* 362.4 $[M+H]^+$.

1-(2,5-Dichloro-4-(hexylthio)phenyl)-3-(2-methylaziridin-1-yl)propan-1-one **17**{*2,3,2}*. Yield 71%; ^1H NMR (400 MHz, $CDCl_3$) δ 7.61 (s, 1H), 7.17 (s, 1H), 3.22 (t, *J* = 7.0, 2H), 2.97 (t, *J* = 7.4, 2H), 2.73 – 2.50 (m, 2H), 1.83 – 1.66 (m, 2H), 1.56 – 1.41 (m, 4H), 1.41 – 1.31 (m, 4H), 1.29 (d, *J* = 6.3, 1H), 1.15 (d, *J* = 5.4, 3H), 0.92 (t, *J* = 7.0, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.24, 143.29, 134.91, 130.40, 130.27, 130.23, 127.04, 55.90, 43.00, 34.94, 31.99, 31.29, 28.62, 27.98, 22.49, 18.32, 14.01; MS (ESI) *m/z* 374.4 $[M+H]^+$.

1-(2,5-Dichloro-4-(hexylthio)phenyl)-3-morpholinopropan-1-one **17**{*2,3,3}*. Yield 92%; ^1H NMR (400 MHz, $CDCl_3$) δ 7.56 (s, 1H), 7.16 (s, 1H), 3.74 – 3.63 (m, 4H), 3.14 (t, *J* = 7.0, 2H), 2.96 (t, *J* = 7.4, 2H), 2.78 (q, *J* = 7.0, 2H), 2.47 (brs, 4H), 1.83 – 1.68 (m, 2H), 1.61 – 1.47 (m, 2H), 1.42 – 1.28 (m, 4H), 0.92 (t, *J* = 7.0, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.60, 143.10, 135.02, 130.23, 130.13, 130.11, 126.92, 66.86, 53.60, 53.48, 40.01, 32.00, 31.29, 28.61, 27.97, 22.49, 14.01; MS (ESI) *m/z* 404.4 $[M+H]^+$.

4-(3-(2,5-Dichloro-4-(hexylthio)phenyl)-3-oxopropyl)piperazin-2-one **17**{*2,3,4}*. Yield 89%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (s, 1H), 7.16 (s, 1H), 6.90 (brs, 1H), 3.42 (brs, 2H), 3.25 – 3.13 (m, 4H), 2.96 (t, *J* = 7.4, 2H), 2.87 (t, *J* = 6.9, 2H), 2.76 (brs, 2H), 1.81 – 1.66 (m, 2H), 1.57 – 1.43 (m, 2H), 1.43 – 1.26 (m, 4H), 0.91 (t, *J* = 7.0, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 198.80, 169.27, 143.57, 134.58, 130.28, 130.28, 130.16, 126.94, 56.62, 52.22, 49.14, 41.17, 40.15, 31.98, 31.28, 28.61, 27.95, 22.49, 14.01; MS (ESI) *m/z* 417.4 $[M+H]^+$.

3-(4-Acetylpiperazin-1-yl)-1-(2,5-dichloro-4-(hexylthio)phenyl)propan-1-one **17**{*2,3,5}*. Yield 91%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 (d, *J* = 1.7, 1H), 7.15 (d, *J* = 1.3, 1H), 3.59 (brs, 2H), 3.50 (brs, 2H), 3.14 (t, *J* = 5.9, 2H), 2.96 (t, *J* = 7.4, 2H), 2.86 – 2.72 (m, 2H), 2.44 (d, *J* = 15.8, 4H), 2.11 (s, 3H), 1.82 – 1.68 (m, 2H), 1.59 – 1.43 (m, 2H), 1.43 – 1.26 (m, 4H), 0.97 – 0.83 (m, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.39, 168.88, 143.27, 134.86, 130.20, 130.15, 130.11, 126.92, 53.16, 53.05, 52.57, 46.17, 41.27, 40.13, 31.99, 31.28, 28.61, 27.95, 22.48, 21.32, 14.01; MS (ESI) *m/z* 445.5 $[M+H]^+$.

1-(2,5-Dichloro-4-(hexylthio)phenyl)-3-(4-(ethylsulfonyl)piperazin-1-yl)propan-1-one **17**{*2,3,6}*. Yield 93%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (s, 1H), 7.15 (s, 1H), 3.28 (s, 4H), 3.13 (t, *J* = 6.8, 2H), 3.01 – 2.90 (m, 4H), 2.81 (t, *J* = 6.7, 2H), 2.59 (brs, 4H), 1.80 – 1.68 (m, 2H), 1.55 – 1.43 (m, 2H), 1.40 – 1.26 (m, 7H), 0.91 (t, *J* = 6.3, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.35, 143.29, 134.86, 130.15, 130.12, 126.90, 52.93, 52.62, 45.69, 43.71, 40.05, 31.98, 31.28, 28.61, 27.95, 22.48, 14.01, 7.79; MS (ESI) *m/z* 495.5 $[M+H]^+$.

1-(2,6-Dichloro-4-(hexylthio)phenyl)-3-(dimethylamino)propan-1-one 17{*2,4,1}*. Yield 92%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.23 (s, 2H), 3.09 (t, 2H, *J* = 7.4 Hz), 3.00 (m, 2H), 2.84 (m, 2H), 2.35 (s, 6H), 1.72 (m, 2H), 1.50 (m, 2H), 1.37 (m, 4H), 0.96 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 200.83, 142.02, 135.99, 130.62, 126.20, 53.03, 45.29, 42.04, 32.66, 31.20, 28.48, 28.39, 22.44, 13.94; MS (ESI) *m/z* 363.3 $[M+H]^+$.

1-(2,6-Dichloro-4-(hexylthio)phenyl)-3-(2-methylaziridin-1-yl)propan-1-one 17{*2,4,2}*. Yield 100%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.17 (s, 2H), 3.12 (t, *J* = 7.2, 2H), 2.94 (t, *J* = 7.3, 2H), 2.66 (t, *J* = 7.3, 2H), 1.73 – 1.61 (m, 2H), 1.52 – 1.37 (m, 4H), 1.37 – 1.26 (m, 5H), 1.17 (d, *J* = 5.1, 3H), 0.90 (t, *J* = 6.7, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 200.71, 142.07, 136.01, 130.61, 126.21, 54.51, 44.26, 34.93, 34.86, 32.69, 31.25, 28.52, 28.44, 22.50, 18.31, 14.00; MS (ESI) *m/z* 374.4 $[M+H]^+$.

1-(2,6-Dichloro-4-(hexylthio)phenyl)-3-morpholinopropan-1-one 17{*2,4,3}*. Yield 90%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.18 (s, 2H), 3.72 – 3.62 (m, 4H), 3.05 (t, *J* = 7.2, 2H), 2.94 (t, *J* = 7.4, 2H), 2.82 (t, *J* = 7.3, 2H), 2.55 (brs, 4H), 1.73 – 1.61 (m, 2H), 1.50 – 1.37 (m, 2H), 1.38 – 1.23 (m, 4H), 0.91 (t, *J* = 6.9, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 200.83, 142.15, 135.94, 130.71, 126.19, 66.84, 53.56, 52.46, 41.18, 32.67, 31.25, 28.51, 28.44, 22.50, 14.00; MS (ESI) *m/z* 404.4 $[M+H]^+$.

4-(3-(2,6-Dichloro-4-(hexylthio)phenyl)-3-oxopropyl)piperazin-2-one 17{*2,4,4}*. Yield 89%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.09 (s, 2H), 6.84 (brs, 1H), 3.33 – 3.22 (m, 2H), 3.10 (s, 2H), 2.97 (t, *J* = 7.0, 2H), 2.92 – 2.78 (m, 4H), 2.69 – 2.55 (m, 2H), 1.68 – 1.56 (m, 2H), 1.42 – 1.31 (m, 2H), 1.33 – 1.18 (m, 5H), 0.82 (t, *J* = 7.0, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 200.35, 169.31, 142.41,

135.64, 130.67, 126.16, 56.66, 51.08, 49.14, 41.32, 41.16, 32.63, 31.25, 28.49, 28.44, 22.49; MS (ESI) *m/z* 417.4 $[M+H]^+$.

3-(4-Acetylpiperazin-1-yl)-1-(2,6-dichloro-4-(hexylthio)phenyl)propan-1-one **17**{*2,4,5}*. Yield 70%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.18 (s, 2H), 3.59 (brs, 2H), 3.50 – 3.37 (m, 2H), 3.04 (t, *J* = 7.0, 2H), 2.94 (t, *J* = 7.4, 2H), 2.90 – 2.78 (m, 2H), 2.47 (d, *J* = 19.8, 4H), 2.08 (s, 3H), 1.76 – 1.62 (m, 2H), 1.51 – 1.39 (m, 2H), 1.38 – 1.25 (m, 4H), 0.90 (t, *J* = 6.8, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 200.71, 168.90, 142.27, 135.81, 130.69, 126.16, 53.23, 52.60, 51.91, 46.15, 41.33, 41.26, 32.64, 31.25, 28.49, 28.43, 22.49, 21.32, 14.00; MS (ESI) *m/z* 445.5 $[M+H]^+$.

1-(2,6-Dichloro-4-(hexylthio)phenyl)-3-(4-(ethylsulfonyl)piperazin-1-yl)propan-1-one **17**{*2,4,6}*. Yield 87%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.91 (s, 2H), 3.03 (s, 4H), 2.76 (t, *J* = 7.0, 2H), 2.68 (q, *J* = 7.4, 4H), 2.60 (t, *J* = 7.0, 2H), 2.31 (s, 4H), 1.49 – 1.35 (m, 2H), 1.25 – 1.15 (m, 2H), 1.15 – 1.00 (m, 8H), 0.64 (t, *J* = 5.4, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 200.30, 142.06, 135.52, 130.43, 125.88, 52.41, 51.48, 45.39, 43.53, 40.96, 32.37, 30.99, 28.23, 28.17, 22.23, 13.74, 7.53; MS (ESI) *m/z* 495.5 $[M+H]^+$.

3-(Dimethylamino)-1-(4-(hexylthio)-2,6-dimethylphenyl)propan-1-one **17**{*2,5,1}*. Yield 93%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.90 (s, 2H), 2.84 (m, 4H), 2.66 (t, 2H, *J* = 7.3 Hz), 2.22 (s, 6H), 2.16 (s, 6H), 1.59 (m, 2H), 1.36 (m, 2H), 1.31 (m, 4H), 0.84 (t, 3H, *J* = 6.9 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 208.86, 139.45, 137.74, 133.32, 127.34, 53.62, 45.35, 43.01, 32.97, 31.26, 28.93, 28.44, 22.46, 19.17, 13.94; MS (ESI) *m/z* 322.5 $[M+H]^+$.

1-(4-(Hexylthio)-2,6-dimethylphenyl)-3-(2-methylaziridin-1-yl)propan-1-one **17**{*2,5,2}*. Yield 82%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.87 (s, 2H), 2.89 (t, *J* = 7.0, 2H), 2.87 – 2.78 (m, 2H), 2.62 – 2.43 (m, 2H), 2.14 (s, 6H), 1.62 – 1.49 (m, 2H), 1.44 – 1.28 (m, 4H), 1.28 – 1.18 (m, 5H), 1.08 (d, *J* = 5.1, 3H), 0.82 (t, *J* = 6.9, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 208.76, 139.53, 137.78, 133.33, 127.40, 54.91, 45.12, 34.98, 34.87, 33.06, 31.35, 29.01, 28.53, 22.54, 19.22, 18.34, 14.03; MS (ESI) *m/z* 334.5 $[M+H]^+$.

1-(4-(Hexylthio)-2,6-dimethylphenyl)-3-morpholinopropan-1-one **17**{*2,5,3}*. Yield 84%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.95 (s, 2H), 3.78 – 3.64 (m, 4H), 2.98 – 2.86 (m, 4H), 2.78 (t, *J* = 6.9, 2H), 2.57 (brs, 4H), 2.29 (s, 6H), 1.74 – 1.58 (m, 2H), 1.49 – 1.38 (m, 2H), 1.38 – 1.24 (m, 4H), 0.90 (t, *J* = 6.9, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 208.78, 139.38, 137.94, 133.46, 127.37, 66.83, 53.69, 53.08, 41.99, 32.99, 31.35, 28.99, 28.53, 22.54, 19.36, 14.04; MS (ESI) *m/z* 365.6 $[M+H]^+$.

4-(3-(4-(Hexylthio)-2,6-dimethylphenyl)-3-oxopropyl)piperazin-2-one **17**{*2,5,4}*. Yield 85%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.87 (s, 2H), 6.54 (br, 1H), 3.33 (brs, 2H), 3.16 (brs, 2H), 2.87 – 2.73 (m, 6H), 2.69 (brs, 2H), 2.14 (s, 6H), 1.64 – 1.50 (m, 2H), 1.41 – 1.30 (m, 2H), 1.30 – 1.15 (m, 4H), 0.82 (t, *J* = 7.0, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 208.23, 139.09, 138.19, 133.43, 132.07, 127.35, 56.73, 51.73, 49.30, 42.14, 41.13, 32.95, 31.34, 28.98, 28.53, 22.54, 19.32, 14.04; MS (ESI) *m/z* 377.6 $[M+H]^+$.

3-(4-Acetylpiperazin-1-yl)-1-(4-(hexylthio)-2,6-dimethylphenyl)propan-1-one **17**{*2,5,5}*Yield 68%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.95 (s, 2H), 3.59 (brs, 2H), 3.50 (brs, 2H), 2.95 – 2.85 (m, 4H), 2.85 – 2.73 (m, 2H), 2.43 (t, *J* = 20.3, 4H), 2.22 (s, 6H), 2.12 (s, 3H), 1.73 – 1.57 (m, 2H), 1.50

– 1.38 (m, 2H), 1.38 – 1.24 (m, 4H), 0.90 (t, *J* = 6.9, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 208.61, 168.91, 139.28, 138.04, 133.44, 127.34, 53.41, 52.72, 52.50, 46.15, 42.18, 41.24, 32.96, 31.34, 28.98, 28.52, 22.53, 21.32, 19.37, 14.03; MS (ESI) *m/z* 405.6 $[M+H]^+$.

3-(4-(Ethylsulfonyl)piperazin-1-yl)-1-(4-(hexylthio)-2,6-dimethylphenyl)propan-1-one

17{*2,5,6}*. Yield 52%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.87 (s, 2H), 3.12 (brs, 4H), 2.93 – 2.71 (m, 8H), 2.58 (brs, 4H), 2.14 (s, 6H), 1.62 – 1.51 (m, 2H), 1.37 (d, *J* = 7.9, 2H), 1.32 (t, *J* = 7.4, 3H), 1.26 – 1.19 (m, 4H), 0.82 (t, *J* = 7.0, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 208.40, 138.14, 133.42, 132.04, 127.35, 52.86, 52.52, 52.33, 45.58, 43.97, 32.96, 31.35, 28.98, 28.53, 22.54, 19.39, 14.04, 7.81; MS (ESI) *m/z* 455.7 $[M+H]^+$.

1-(2-Chloro-4-(hexylsulfonyl)phenyl)-3-(dimethylamino)propan-1-one 17{*3,1,1*}. Yield 91%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, 1H, *J* = 8.0 Hz), 7.77 (dd, 1H, *J* = 1.6, 8.0 Hz), 7.55 (m, 1H), 3.04 (m, 4H), 2.64 (t, 1H, *J* = 7.0 Hz), 2.18 (s, 4H), 2.04 (s, 1H), 1.64 (m, 2H), 1.31 (m, 2H), 1.20 (m, 4H), 0.80 (t, 3H, *J* = 6.8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 201.62, 144.19, 141.93, 131.47, 129.76, 129.48, 126.50, 56.23, 53.84, 45.16, 41.29, 31.05, 27.84, 22.46, 22.22, 13.83; MS (ESI) *m/z* 360.0 $[M+H]^+$.

1-(2-Chloro-4-(hexylsulfonyl)phenyl)-3-(2-methylaziridin-1-yl)propan-1-one 17{*3,1,2}*. Yield 40%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (s, 1H), 7.86 (d, *J* = 8.0, 1H), 7.67 (d, *J* = 8.0, 1H), 3.21 (t, *J* = 6.8, 2H), 3.17 – 3.06 (m, 2H), 2.66 (t, *J* = 6.8, 2H), 1.80 – 1.65 (m, 2H), 1.51 – 1.45 (m, 1H), 1.45 – 1.35 (m, 2H), 1.35 – 1.22 (m, 4H), 1.15 (d, *J* = 5.3, 3H), 0.94 – 0.79 (m, 4H); ^{13}C NMR (101

MHz, $CDCl_3$) δ 201.45, 144.26, 142.08, 131.73, 129.95, 129.54, 126.58, 56.30, 55.44, 43.47, 34.99, 31.12, 27.92, 22.53, 22.29, 18.28, 13.91; MS (ESI) *m/z* 372.4 $[M+H]^+$.

1-(2-Chloro-4-(hexylsulfonyl)phenyl)-3-morpholinopropan-1-one **17**{*3,1,3}*. Yield 23%; ^1H NMR (400 MHz, $CDCl_3$) δ 7.84 (d, *J* = 1.5, 1H), 7.73 (dd, *J* = 1.7, 8.0, 1H), 7.50 (d, *J* = 8.0, 1H), 3.58 – 3.46 (m, 4H), 3.08 – 2.95 (m, 4H), 2.63 (t, *J* = 6.9, 2H), 2.36 – 2.24 (m, 4H), 1.66 – 1.48 (m, 3H), 1.31 – 1.21 (m, 2H), 1.21 – 1.06 (m, 4H), 0.75 (t, *J* = 6.9, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 201.75, 144.21, 142.05, 131.59, 129.88, 129.53, 126.51, 66.86, 56.30, 53.41, 53.26, 40.49, 31.13, 27.92, 22.54, 22.29, 13.91; MS (ESI) *m/z* 402.5 $[M+H]^+$.

4-(3-(2-Chloro-4-(hexylsulfonyl)phenyl)-3-oxopropyl)piperazin-2-one **17**{*3,1,4}*. Yield 34%; ^1H NMR (400 MHz, C $CDCl_3$) δ 7.98 (d, *J* = 1.6, 1H), 7.87 (dd, *J* = 1.6, 8.0, 1H), 7.61 (d, *J* = 8.0, 1H), 6.42 (s, 1H), 3.38 – 3.30 (m, 2H), 3.23 – 3.08 (m, 6H), 2.87 (t, *J* = 6.8, 2H), 2.80 – 2.62 (m, 2H), 1.82 – 1.67 (m, 2H), 1.39 (dd, *J* = 7.1, 14.3, 2H), 1.35 – 1.19 (m, 4H), 0.88 (t, *J* = 6.9, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 201.01, 168.94, 143.89, 142.30, 131.66, 129.99, 129.52, 126.65, 56.69, 56.29, 51.87, 49.08, 41.27, 40.67, 31.12, 27.92, 22.49, 22.29, 13.91; MS (ESI) *m/z* 415.5 $[M+H]^+$.

3-(4-Acetylpiperazin-1-yl)-1-(2-chloro-4-(hexylsulfonyl)phenyl)propan-1-one **17**{*3,1,5}*. Yield 38%; ^1H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, *J* = 1.5, 1H), 7.86 (dd, *J* = 1.6, 8.0, 1H), 7.62 (d, *J* = 8.0, 1H), 3.64 – 3.52 (m, 2H), 3.47 – 3.39 (m, 2H), 3.20 – 3.06 (m, 4H), 2.79 (t, *J* = 6.9, 2H), 2.51 – 2.35 (m, 4H), 2.09 (s, 3H), 1.73 (dt, *J* = 7.7, 15.5, 3H), 1.46 – 1.34 (m, 2H), 1.34 (d, *J* = 3.3, 4H), 0.88 (t, *J* = 6.8, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 201.47, 168.92, 144.06, 142.16, 131.65,

129.95, 129.48, 126.54, 56.28, 53.13, 52.69, 52.53, 46.18, 41.29, 40.65, 31.12, 27.91, 22.52, 22.28, 21.32, 13.91; MS (ESI) *m/z* 443.5 $[M+H]^+$.

1-(2-Chloro-4-(hexylsulfonyl)phenyl)-3-(4-(ethylsulfonyl)piperazin-1-yl)propan-1-one **17**{*3,1,6}*. Yield 21%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, *J* = 1.6, 1H), 7.87 (dd, *J* = 1.7, 8.0, 1H), 7.61 (d, *J* = 8.0, 1H), 3.35 – 3.23 (m, 4H), 3.20 – 3.06 (m, 4H), 2.96 (q, *J* = 7.4, 2H), 2.83 (t, *J* = 6.8, 2H), 2.63 – 2.50 (m, 4H), 1.81 – 1.68 (m, 2H), 1.46 – 1.35 (m, 5H), 1.35 – 1.20 (m, 4H), 0.89 (t, *J* = 6.9, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 201.32, 144.00, 142.22, 131.69, 129.99, 129.44, 126.56, 56.28, 52.63, 52.54, 45.69, 43.91, 40.54, 31.13, 27.92, 22.52, 22.29, 13.91, 7.81; MS (ESI) *m/z* 493.6 $[M+H]^+$.

1-(2,3-Dichloro-4-(hexylsulfonyl)phenyl)-3-(dimethylamino)propan-1-one **17**{*3,2,1}*. Yield 88%;^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (d, 1H, *J* = 8.1 Hz), 7.47 (d, 1H, *J* = 8.1 Hz), 3.42 (m, 2H), 3.09 (t, 2H, *J* = 6.9), 2.71 (t, 2H, *J* = 7.0 Hz), 2.25 (s, 6H), 1.69 (m, 2H), 1.41 (m), 1.27 (m, 4H), 0.86 (t, 3H, *J* = 6.9 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 201.29, 146.28, 139.57, 132.28, 131.23, 129.95, 125.89, 54.11, 53.84, 45.19, 41.38, 31.06, 27.87, 22.32, 22.22, 13.86; MS (ESI) *m/z* 395.3 $[M+H]^+$.

1-(2,3-Dichloro-4-(hexylsulfonyl)phenyl)-3-(2-methylaziridin-1-yl)propan-1-one **17**{*3,2,2}*. Yield 66%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (d, *J* = 8.1, 1H), 7.50 (d, *J* = 8.1, 1H), 3.47 – 3.37 (m, 2H), 3.15 (t, *J* = 6.8, 2H), 2.64 (t, *J* = 6.8, 2H), 1.76 – 1.59 (m, 2H), 1.45 – 1.34 (m, 2H), 1.34 – 1.21 (m, 5H), 1.14 (d, *J* = 5.3, 3H), 0.87 (t, *J* = 6.9, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 201.01,

146.34, 139.73, 132.43, 131.41, 130.02, 125.91, 55.33, 54.14, 43.44, 34.98, 34.95, 31.09, 27.90, 22.37, 22.27, 18.29, 13.90; MS (ESI) *m/z* 406.4 $[M+H]^+$.

1-(2,3-Dichloro-4-(hexylsulfonyl)phenyl)-3-morpholinopropan-1-one **17**{*3,2,3}*. Yield 44%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (d, *J* = 8.1, 1H), 7.49 (d, *J* = 8.1, 1H), 3.69 – 3.63 (m, 4H), 3.51 – 3.36 (m, 2H), 3.10 (t, *J* = 6.9, 2H), 2.74 (t, *J* = 6.9, 2H), 2.51 – 2.38 (m, 4H), 1.75 – 1.65 (m, 2H), 1.49 – 1.35 (m, 2H), 1.35 – 1.17 (m, 4H), 0.88 (t, *J* = 7.0, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 201.25, 146.21, 139.71, 132.39, 131.35, 129.93, 125.94, 66.85, 54.14, 53.39, 53.20, 40.47, 31.10, 27.91, 22.38, 22.27, 13.91; MS (ESI) *m/z* 436.4 $[M+H]^+$.

4-(3-(2,3-Dichloro-4-(hexylsulfonyl)phenyl)-3-oxopropyl)piperazin-2-one **17**{*3,2,4}*. Yield 69%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 (d, *J* = 8.1, 1H), 7.45 (d, *J* = 8.1, 1H), 6.94 (s, 1H), 3.49 – 3.37 (m, 2H), 3.32 (brs, 2H), 3.20 – 3.05 (m, 4H), 2.93 (t, *J* = 6.6, 2H), 2.75 (brs, 2H), 1.77 – 1.63 (m, 2H), 1.46 – 1.35 (m, 2H), 1.35 (brs, 4H), 0.96 – 0.79 (m, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 200.56, 169.13, 145.93, 139.92, 132.51, 131.38, 130.06, 125.86, 56.62, 54.14, 51.77, 49.03, 41.17, 40.64, 31.09, 27.90, 22.31, 22.27, 13.91; MS (ESI) *m/z* 449.4 $[M+H]^+$.

3-(4-Acetylpiperazin-1-yl)-1-(2,3-dichloro-4-(hexylsulfonyl)phenyl)propan-1-one **17**{*3,2,5}*. Yield 86%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 (d, *J* = 8.1, 1H), 7.46 (d, *J* = 8.1, 1H), 3.56 (d, *J* = 4.6, 2H), 3.47 – 3.38 (m, 4H), 3.09 (t, *J* = 6.8, 2H), 2.76 (t, *J* = 6.8, 2H), 2.46 – 2.35 (m, 4H), 2.06 (s, 3H), 1.75 – 1.62 (m, 2H), 1.45 – 1.33 (m, 2H), 1.33 – 1.20 (m, 4H), 0.86 (t, *J* = 6.8, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 200.98, 168.89, 146.06, 139.80, 132.46, 131.39, 129.94, 125.87, 54.12,

53.10, 52.61, 52.51, 46.16, 41.26, 40.62, 31.09, 27.88, 22.35, 22.25, 21.31, 13.90; MS (ESI) *m/z* 477.5 $[M+H]^+$.

1-(2,3-Dichloro-4-(hexylsulfonyl)phenyl)-3-(4-(ethylsulfonyl)piperazin-1-yl)propan-1-one **17**{*3,2,6}*. Yield 38%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (d, *J* = 8.1, 1H), 7.45 (d, *J* = 8.1, 1H), 3.48 – 3.38 (m, 2H), 3.32 – 3.21 (m, 4H), 3.10 (t, *J* = 6.7, 2H), 2.96 (q, *J* = 7.4, 2H), 2.81 (t, *J* = 6.7, 2H), 2.59 – 2.46 (m, 4H), 1.77 – 1.64 (m, 2H), 1.48 – 1.34 (m, *J* = 22.9, 5H), 1.34 – 1.23 (m, 4H), 0.88 (t, *J* = 6.8, 3H) ; MS (ESI) *m/z* 527.5 $[M+H]^+$.

1-(2,3-Dichloro-4-(hexylsulfonyl)phenyl)-3-(dimethylamino)propan-1-one **17**{*3,3,1}*. Yield 57%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (s, 1H), 7.53 (s, 1H), 3.39 – 3.28 (m, 3H), 3.05 (t, *J* = 6.9, 2H), 2.68 (t, *J* = 6.9, 2H), 2.23 (s, 6H), 1.73 – 1.55 (m, 2H), 1.41 – 1.31 (m, 2H), 1.31 – 1.16 (m, 4H), 0.80 (t, *J* = 6.9, 5H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 200.29, 144.84, 139.05, 133.16, 131.92, 131.34, 129.63, 54.31, 53.85, 45.19, 41.31, 31.08, 27.90, 22.30, 22.27, 13.90; MS (ESI) *m/z* 394.4 $[M+H]^+$.

1-(2,3-Dichloro-4-(hexylsulfonyl)phenyl)-3-(2-methylaziridin-1-yl)propan-1-one **17**{*3,3,2}*. Yield 74%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (s, 1H), 7.67 (s, 1H), 3.48 – 3.35 (m, 2H), 3.19 (t, *J* = 6.8, 2H), 2.65 (t, *J* = 6.7, 2H), 1.76 – 1.66 (m, 2H), 1.48 – 1.35 (m, 3H), 1.35 – 1.24 (m, 6H), 1.15 (d, *J* = 5.4, 3H), 0.94 (t, *J* = 6.9, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 200.11, 144.86, 139.16, 133.27, 131.97, 131.35, 129.83, 55.47, 54.31, 43.40, 35.00, 31.08, 27.91, 22.30, 22.27, 18.28, 13.90; MS (ESI) *m/z* 406.4 $[M+H]^+$.

1-(2,5-Dichloro-4-(hexylsulfonyl)phenyl)-3-morpholinopropan-1-one **17**{*3,3,3}*. Yield 73%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 (s, 1H), 7.56 (s, 1H), 3.64 – 3.55 (m, 4H), 3.38 – 3.27 (m, 2H), 3.04 (t, *J* = 6.8, 2H), 2.66 (t, *J* = 6.8, 2H), 2.42 – 2.32 (m, 4H), 1.72 – 1.55 (m, 2H), 1.41 – 1.28 (m, 2H), 1.28 – 1.14 (m, 4H), 0.80 (t, *J* = 7.0, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 200.45, 144.87, 139.08, 133.16, 131.96, 131.25, 129.60, 66.85, 54.32, 53.39, 53.26, 40.44, 31.08, 27.90, 22.30, 22.26, 13.90; MS (ESI) *m/z* 436.4 $[M+H]^+$.

4-(3-(2,3-Dichloro-4-(hexylsulfonyl)phenyl)-3-oxopropyl)piperazin-2-one **17**{*3,3,4}*. Yield 77%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 (s, 1H), 7.52 (s, 1H), 6.55 (s, 1H), 3.38 – 3.30 (m, 2H), 3.30 – 3.22 (m, 2H), 3.12 – 3.03 (m, 4H), 2.78 (t, *J* = 6.8, 2H), 2.65 – 2.56 (m, 2H), 1.70 – 1.58 (m, 2H), 1.40 – 1.29 (m, 2H), 1.26 – 1.15 (m, 4H), 0.81 (t, *J* = 6.9, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.55, 168.97, 144.45, 139.39, 133.32, 131.88, 131.46, 129.76, 56.59, 54.32, 51.82, 49.14, 41.21, 40.60, 31.08, 27.90, 22.27, 22.24, 13.91; MS (ESI) *m/z* 449.4 $[M+H]^+$.

3-(4-Acetylpiperazin-1-yl)-1-(2,3-dichloro-4-(hexylsulfonyl)phenyl)propan-1-one **17**{*3,3,5}*. Yield 60%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (s, 1H), 7.61 (s, 1H), 3.65 – 3.52 (m, 2H), 3.46 – 3.33 (m, 4H), 3.12 (t, *J* = 6.8, 2H), 2.76 (t, *J* = 6.8, 2H), 2.47 – 2.33 (m, 4H), 2.08 (s, 3H), 1.78 – 1.62 (m, 2H), 1.47 – 1.36 (m, 2H), 1.34 – 1.20 (m, 4H), 0.87 (t, *J* = 7.0, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 200.13, 168.90, 144.68, 139.19, 133.22, 131.89, 131.28, 129.67, 54.30, 53.10, 52.65, 52.51, 46.15, 41.26, 40.59, 31.07, 27.88, 22.27, 22.25, 21.32, 13.90; MS (ESI) *m/z* 477.5 $[M+H]^+$.

1-(2,3-Dichloro-4-(hexylsulfonyl)phenyl)-3-(4-(ethylsulfonyl)piperazin-1-yl)propan-1-one

17{*3,3,6}*. Yield 56%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 (s, 1H), 7.61 (s, 1H), 3.45 – 3.37 (m, 2H), 3.34 – 3.25 (m, 4H), 3.13 (t, *J* = 6.7, 2H), 2.96 (q, *J* = 7.4, 2H), 2.81 (t, *J* = 6.7, 2H), 2.59 – 2.46 (m, 4H), 1.78 – 1.68 (m, 2H), 1.48 – 1.35 (m, 5H), 1.35 – 1.21 (m, 4H), 0.89 (t, *J* = 7.0, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 200.03, 144.66, 139.27, 133.28, 131.87, 131.29, 129.73, 54.33, 52.62, 52.56, 45.69, 43.86, 40.49, 31.08, 27.90, 22.27, 13.91, 7.80; MS (ESI) *m/z* 527.5 $[M+H]^+$.

1-(2,6-Dichloro-4-(hexylsulfonyl)phenyl)-3-(dimethylamino)propan-1-one **17**{*3,4,1}*. Yield 93%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (s, 2H), 3.05 (m, 5H), 2.76 (t, 2H, *J* = 7.3 Hz), 2.24 (s, 6H), 1.68 (m, 2H), 1.34 (m, 2H), 1.24 (m, 4H), 0.84 (t, 4H, *J* = 6.8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.62, 143.94, 141.84, 131.90, 127.68, 56.31, 52.71, 45.24, 41.51, 31.05, 27.85, 22.42, 22.24, 13.84; MS (ESI) *m/z* 395.3 $[M+H]^+$.

1-(2,6-Dichloro-4-(hexylsulfonyl)phenyl)-3-(4-(ethylsulfonyl)piperazin-1-yl)propan-1-one

17{*3,4,2}*. Yield 59%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (s, 2H), 3.17 – 3.08 (m, 4H), 2.78 – 2.62 (m, 2H), 1.81 – 1.66 (m, 2H), 1.57 – 1.46 (m, 1H), 1.40 (s, 2H), 1.35 (dd, *J* = 4.9, 13.7, 6H), 1.17 (d, *J* = 5.1, 3H), 0.89 (t, *J* = 6.8, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.49, 144.01, 141.92, 131.90, 127.72, 56.35, 54.16, 43.81, 35.05, 34.92, 31.10, 27.90, 22.46, 22.30, 18.30, 13.90; MS (ESI) *m/z* 406.4 $[M+H]^+$.

3-(4-Acetylpiperazin-1-yl)-1-(2,6-dichloro-4-(hexylsulfonyl)phenyl)propan-1-one **17**{*3,4,3}*. Yield 39%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (s, 2H), 3.71 – 3.64 (m, 4H), 3.16 – 3.00 (m, 4H), 2.85 (t, *J* = 7.2, 2H), 2.53 – 2.42 (m, 4H), 1.80 – 1.64 (m, 2H), 1.48 – 1.36 (m, 2H), 1.36 – 1.17 (m, *J* = 3.3, 4H), 0.98 (t, *J* = 7.0, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.70, 144.01, 141.92, 131.97,

127.73, 66.85, 56.36, 53.58, 52.14, 40.79, 31.11, 27.90, 22.49, 22.30, 13.91; MS (ESI) *m/z* 436.4 $[M+H]^+$.

4-(3-(2,6-Dichloro-4-(hexylsulfonyl)phenyl)-3-oxopropyl)piperazin-2-one 17{*3,4,4}*. Yield 94%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (s, 2H), 7.05 – 6.66 (m, 1H), 3.34 (brs, 2H), 3.17 (brs, 2H), 3.14 – 3.08 (m, 2H), 3.08 (t, *J* = 6.8, 2H), 2.93 (t, *J* = 7.0, 2H), 2.74 – 2.64 (m, 2H), 1.73 (s, 2H), 1.39 (s, 2H), 1.28 (s, 4H), 0.88 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.15, 169.25, 143.74, 142.07, 131.91, 127.77, 56.69, 56.30, 50.72, 49.21, 43.93, 41.17, 40.95, 31.09, 27.88, 22.43, 22.29, 13.90; MS (ESI) *m/z* 449.4 $[M+H]^+$.

1-(2,6-Dichloro-4-(hexylsulfonyl)phenyl)-3-morpholinopropan-1-one 17{*3,4,5}*. Yield 63%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (s, 2H), 3.62 – 3.56 (m, 2H), 3.46 – 3.42 (m, 2H), 3.15 – 3.09 (m, 2H), 3.06 (t, *J* = 7.0, 2H), 2.86 (t, *J* = 7.0, 2H), 2.53 – 2.40 (m, *J* = 17.1, 4H), 2.08 (s, 3H), 1.78 – 1.64 (m, *J* = 7.6, 2H), 1.47 – 1.36 (m, 2H), 1.36 (d, *J* = 3.5, 4H), 0.95 (d, *J* = 7.1, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.52, 168.91, 143.91, 141.99, 131.93, 127.74, 56.32, 53.31, 52.62, 51.56, 46.17, 41.27, 40.97, 31.10, 27.89, 22.47, 22.29, 21.32, 13.90; MS (ESI) *m/z* 477.5 $[M+H]^+$.

1-(2,6-Dichloro-4-(hexylsulfonyl)phenyl)-3-(2-methylaziridin-1-yl)propan-1-one 17{*3,4,6}*. Yield 31%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (s, 2H), 3.28 (brs, 4H), 3.16 – 3.09 (m, 2H), 3.09 – 3.02 (m, 2H), 3.00 – 2.94 (m, 2H), 2.94 – 2.86 (m, 2H), 2.63 (brs, 4H), 1.79 – 1.69 (m, 2H), 1.47 – 1.35 (m, 5H), 1.35 – 1.23 (m, 4H), 0.90 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.43, 143.95, 142.03, 131.95, 127.75, 56.34, 52.73, 51.43, 45.68, 43.82, 40.84, 31.10, 27.90, 22.47, 22.30, 13.91, 7.79; MS (ESI) *m/z* 527.5 $[M+H]^+$.

3-(Dimethylamino)-1-(4-(hexylsulfonyl)-2,6-dimethylphenyl)propan-1-one **17**{*3,5,1}*. Yield 90%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (s, 2H), 3.05 (m, 2H), 2.87 (t, 2H, *J* = 7.2 Hz), 2.71 (t, 2H, *J* = 7.1 Hz), 2.29 (s, 6H), 2.24 (m, 6H), 1.68 (m, 2H), 1.34 (m, 2H), 1.24 (m, 4H), 0.84 (t, 3H, *J* = 6.9 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 207.76, 146.72, 139.05, 134.43, 127.18, 56.19, 53.28, 45.33, 42.58, 31.07, 27.87, 22.47, 22.23, 19.09, 13.83; MS (ESI) *m/z* 354.4 $[M+H]^+$.

1-(4-(Hexylsulfonyl)-2,6-dimethylphenyl)-3-(2-methylaziridin-1-yl)propan-1-one **17**{*3,5,2}*. Yield 100%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (s, 2H), 3.05 – 2.96 (m, 2H), 2.91 (t, *J* = 7.0, 2H), 2.69 – 2.49 (m, 2H), 2.26 (s, 6H), 1.69 – 1.56 (m, 2H), 1.42 (dd, *J* = 3.9, 9.3, 2H), 1.30 (dt, *J* = 7.0, 14.1, 2H), 1.26 – 1.14 (m, 5H), 1.08 (d, *J* = 5.1, 3H), 0.80 (t, *J* = 6.8, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 207.59, 146.83, 139.14, 134.43, 127.25, 56.28, 54.50, 44.68, 35.11, 34.92, 31.16, 27.96, 22.55, 22.32, 19.15, 18.30, 13.92; MS (ESI) *m/z* 366.2 $[M+H]^+$.

1-(4-(Hexylsulfonyl)-2,6-dimethylphenyl)-3-morpholinopropan-1-one **17**{*3,5,3}*. Yield 58%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 (s, 2H), 3.66 – 3.55 (m, 4H), 3.03 – 2.94 (m, 2H), 2.82 (t, *J* = 7.0, 2H), 2.71 (t, *J* = 6.8, 2H), 2.49 – 2.34 (m, 4H), 2.27 (s, 6H), 1.71 – 1.50 (m, 3H), 1.35 – 1.25 (m, 2H), 1.25 – 1.09 (m, 4H), 0.80 (t, *J* = 6.7, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 207.73, 146.74, 139.20, 134.52, 127.29, 66.87, 56.28, 53.74, 52.65, 41.72, 31.17, 27.97, 22.56, 22.32, 19.26, 13.93; MS (ESI) *m/z* 396.2 $[M+H]^+$.

4-(3-(4-(Hexylsulfonyl)-2,6-dimethylphenyl)-3-oxopropyl)piperazin-2-one **17**{*3,5,4}*. Yield 56%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (s, 2H), 6.52 (s, 1H), 3.27 (s, 2H), 3.09 (s, 2H), 3.06 – 2.93 (m, 2H), 2.82 (s, 4H), 2.64 (t, *J* = 5.4, 2H), 2.22 (d, *J* = 21.0, 6H), 1.69 – 1.56 (m, 2H), 1.34 –

1.25 (m, 2H), 1.25 – 1.10 (m, 4H), 0.80 (t, *J* = 6.8, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 207.14, 169.07, 146.53, 139.33, 134.48, 127.34, 56.86, 56.27, 51.28, 49.42, 41.91, 41.23, 31.16, 27.96, 22.53, 22.32, 19.19, 13.93; MS (ESI) *m/z* 409.2 $[M+H]^+$.

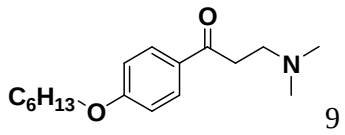
3-(4-Acetylpiperazin-1-yl)-1-(4-(hexylsulfonyl)-2,6-dimethylphenyl)propan-1-one **17**{*3,5,5}*.

Yield 100%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (s, *J* = 9.1, 2H), 3.64 (brs, 2H), 3.51 – 3.39 (m, 2H), 3.13 – 3.01 (m, 2H), 2.90 (t, *J* = 6.6, 2H), 2.81 (t, *J* = 6.5, 2H), 2.55 – 2.40 (m, 4H), 2.33 (s, 6H), 2.06 (s, 3H), 1.78 – 1.64 (m, 2H), 1.42 – 1.32 (m, 2H), 1.32 – 1.17 (m, 4H), 0.87 (t, *J* = 6.8, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 207.52, 168.93, 146.66, 139.26, 134.47, 127.30, 56.26, 53.49, 52.76, 52.03, 46.16, 41.91, 41.26, 31.16, 27.96, 22.55, 22.31, 21.32, 19.25, 13.92; MS (ESI) *m/z* 437.22 $[M+H]^+$.

3-(4-(Ethylsulfonyl)piperazin-1-yl)-1-(4-(hexylsulfonyl)-2,6-dimethylphenyl)propan-1-one

7{*3,5,6}*.

Yield 54%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (s, 2H), 3.22 (brs, 4H), 3.03 – 2.95 (m, 2H), 2.94 – 2.84 (m, 2H), 2.84 – 2.71 (m, 4H), 2.49 (s, 4H), 2.26 (s, 6H), 1.71 – 1.56 (m, 3H), 1.30 (t, *J* = 7.4, 5H), 1.26 – 1.10 (m, 4H), 0.80 (t, *J* = 6.8, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 207.53, 146.63, 139.31, 134.45, 127.32, 56.27, 52.94, 51.87, 45.69, 43.97, 41.84, 31.17, 27.97, 22.55, 22.32, 19.26, 13.93, 7.81; MS (ESI) *m/z* 487.2 $[M+H]^+$.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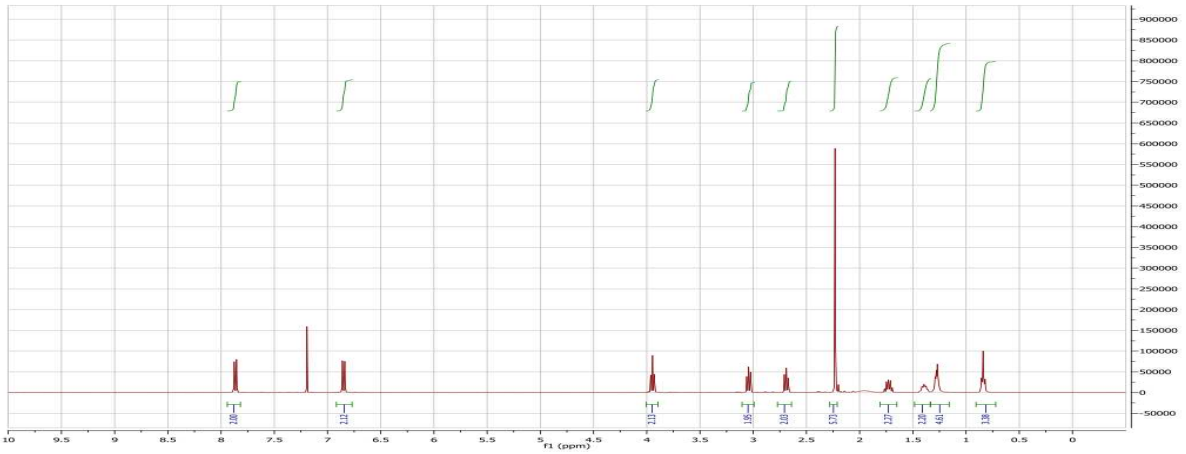
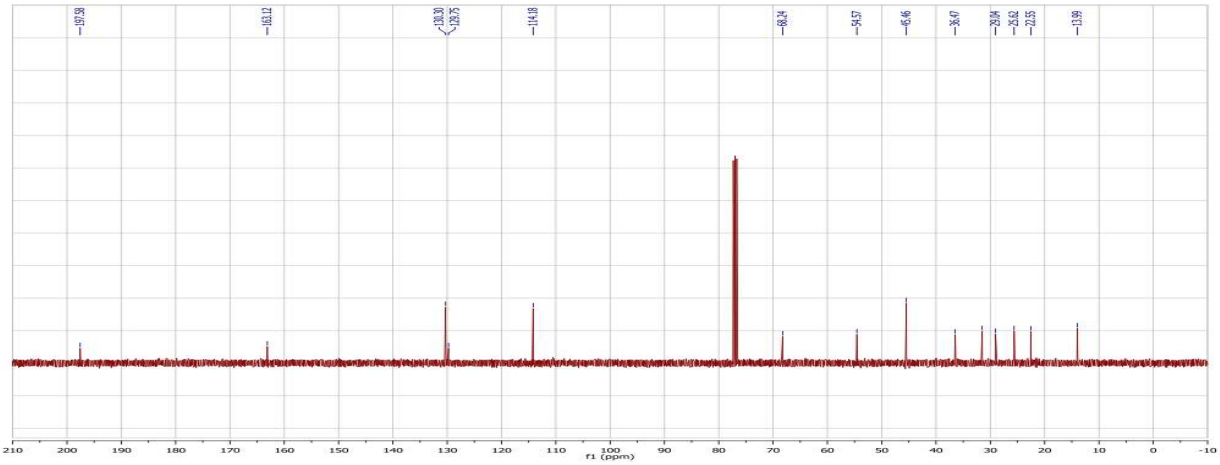
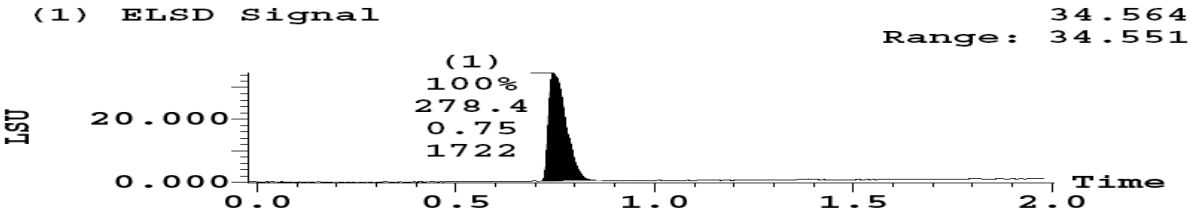
O

9



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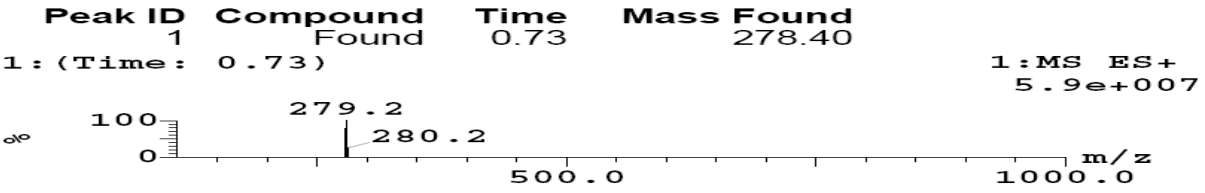
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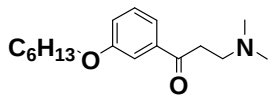

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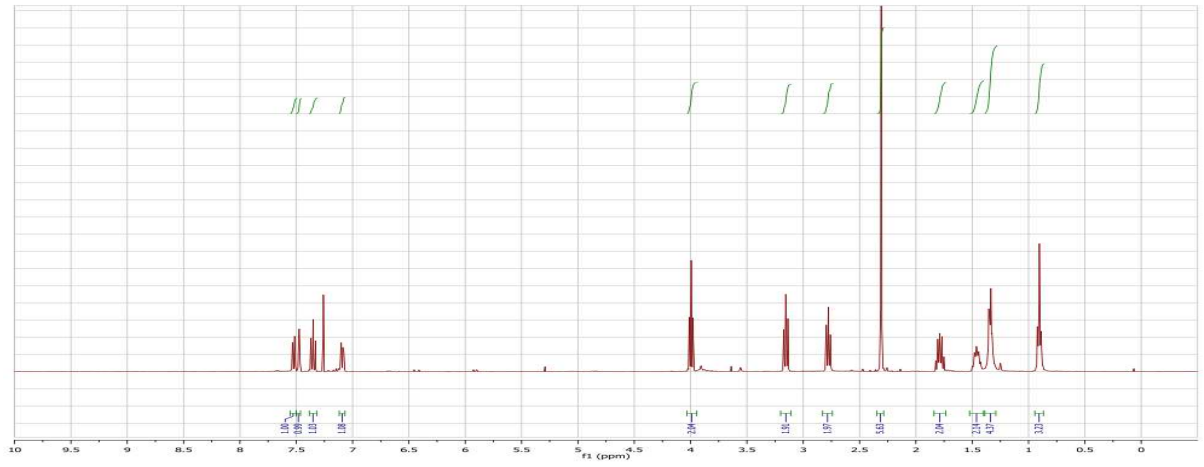

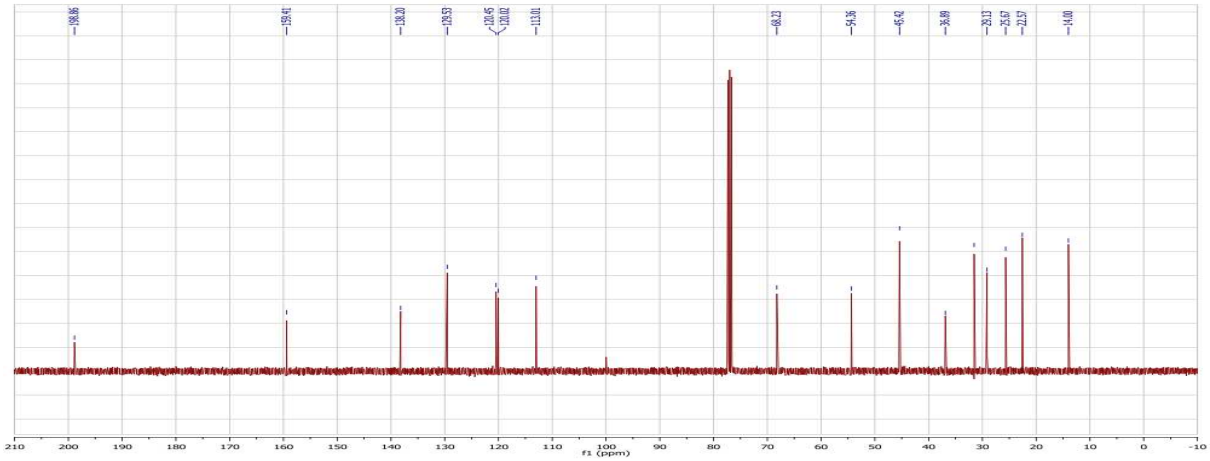

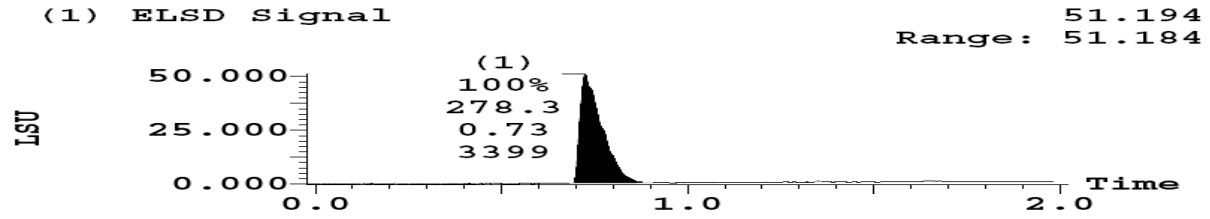

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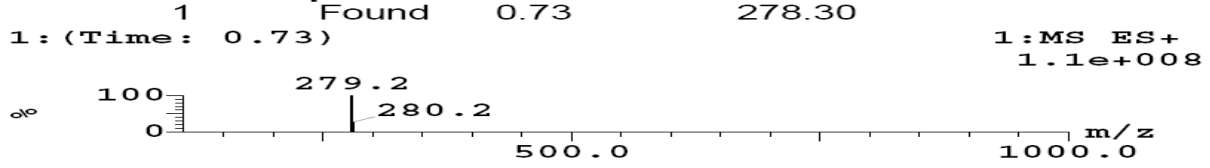

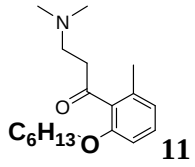

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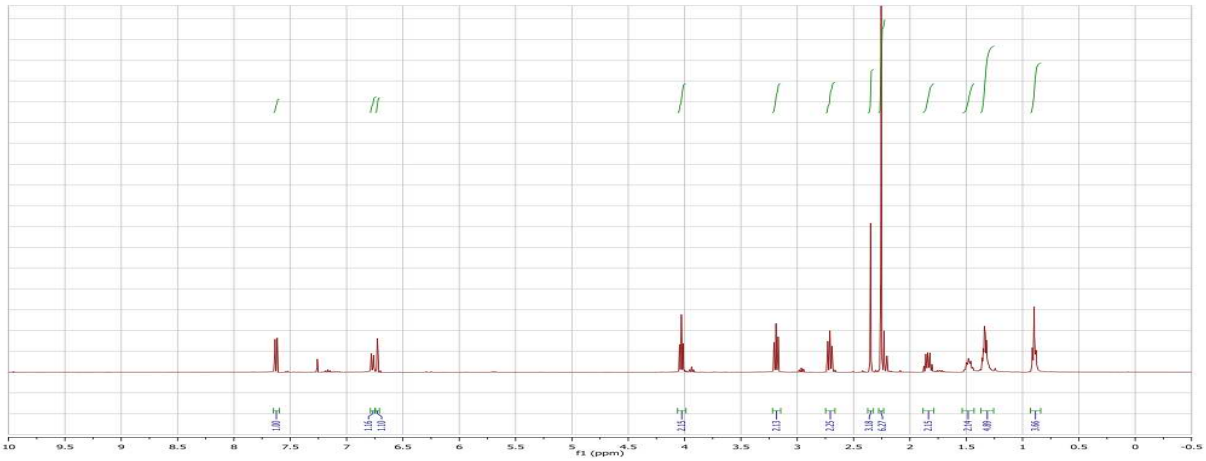

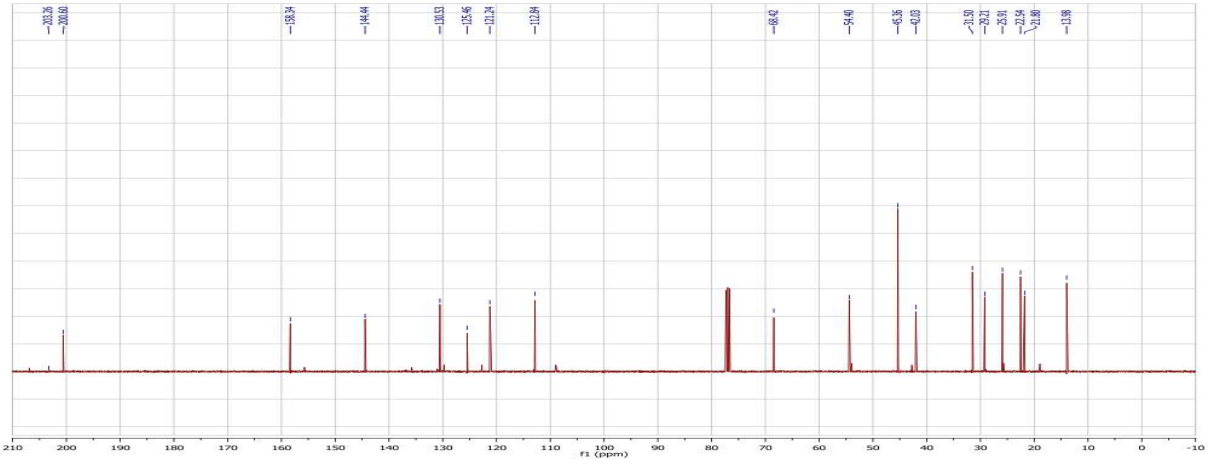

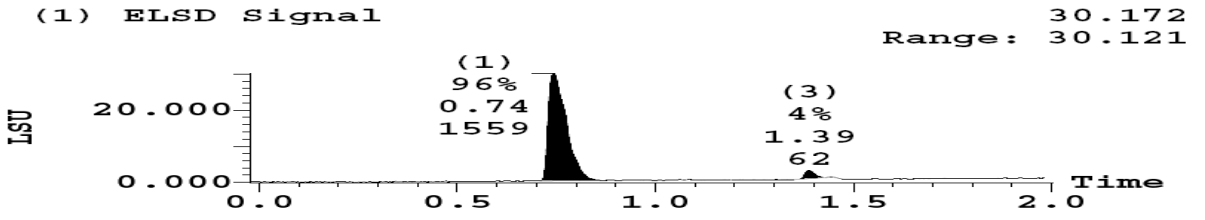

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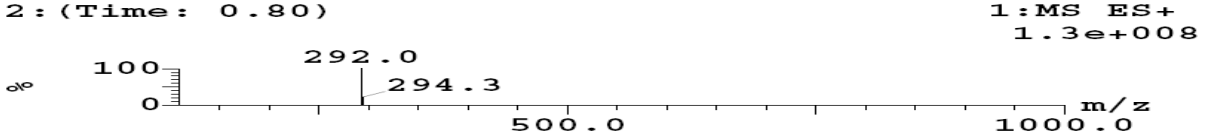
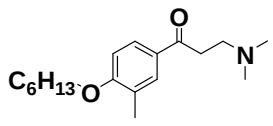
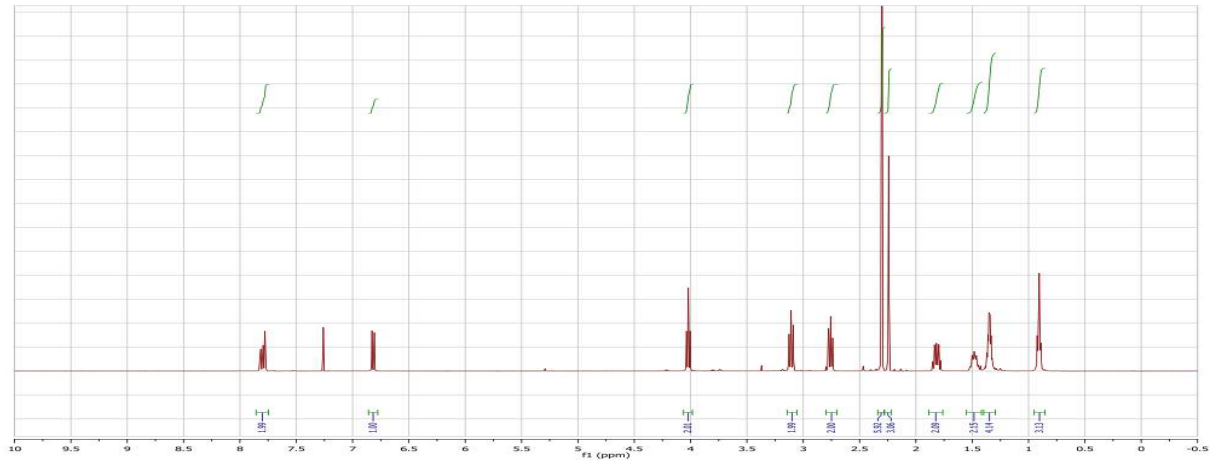
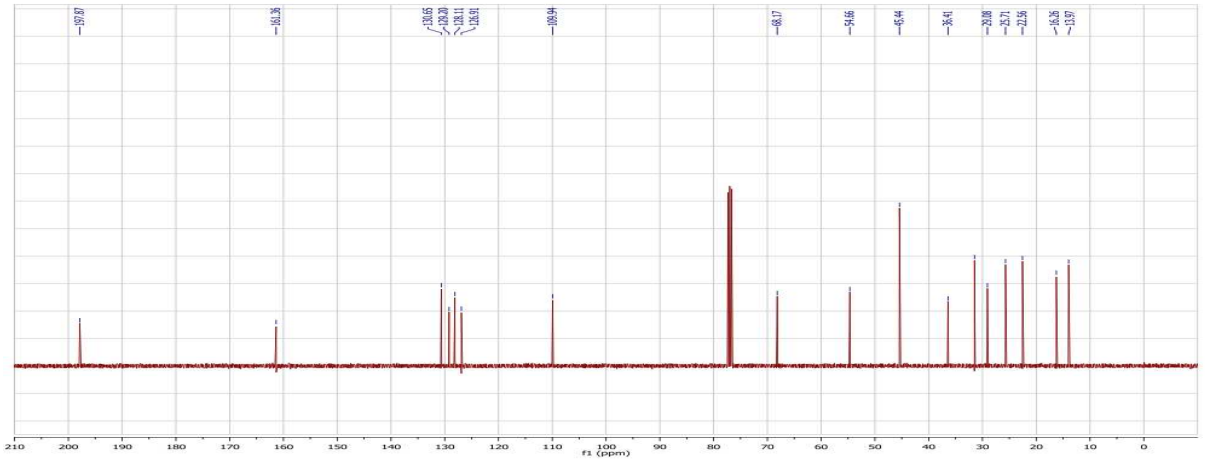
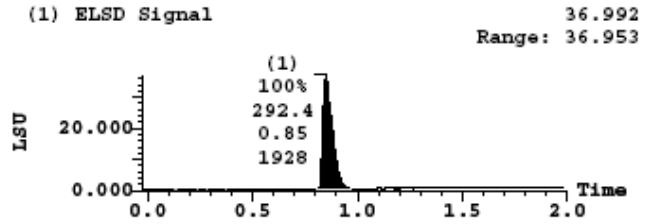




12{*1*}







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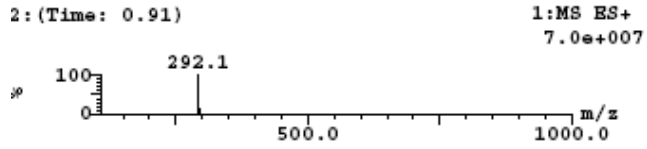

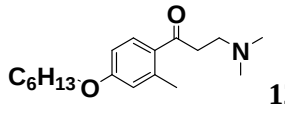
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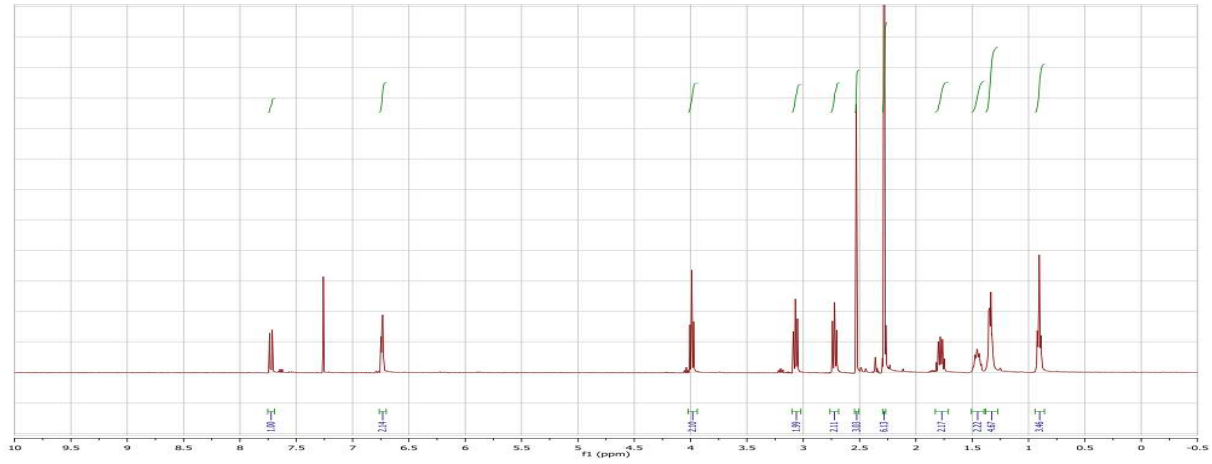
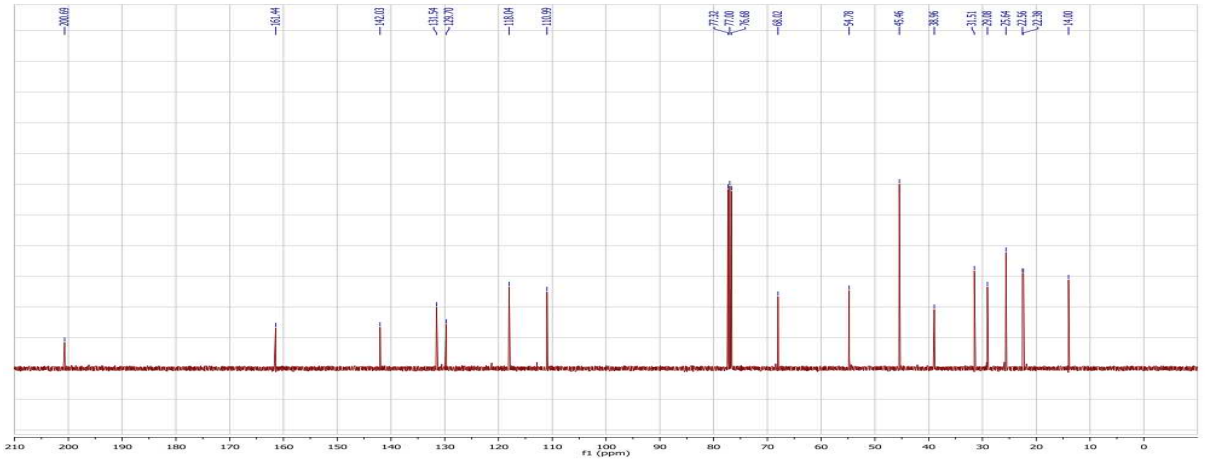
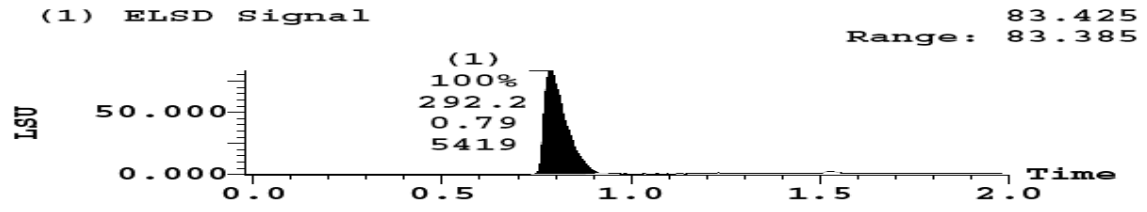
12{*2*}



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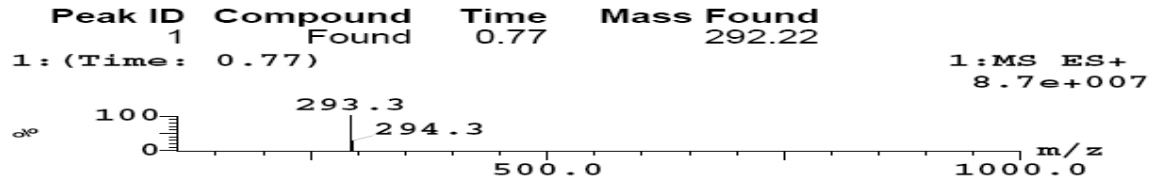
Time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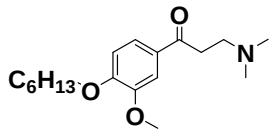
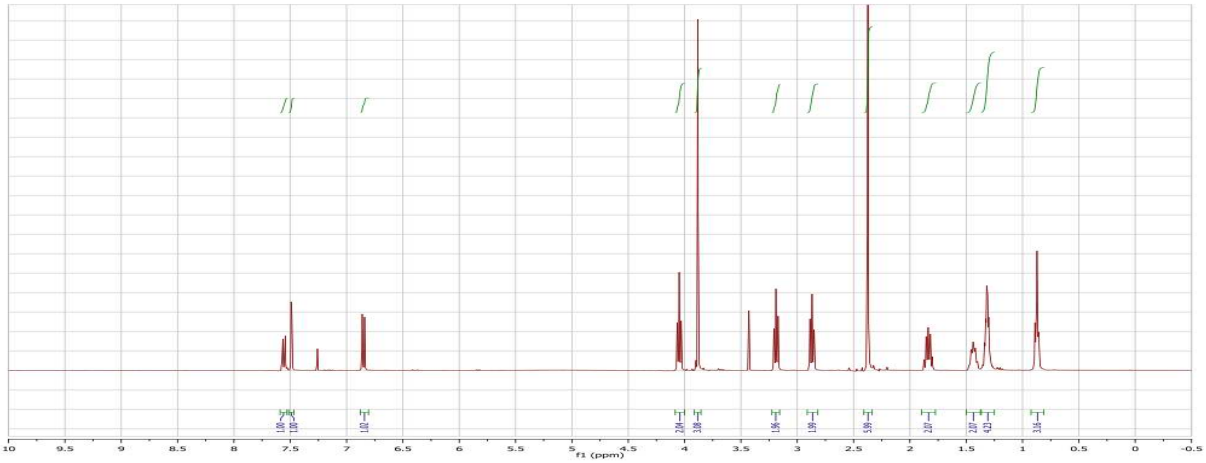
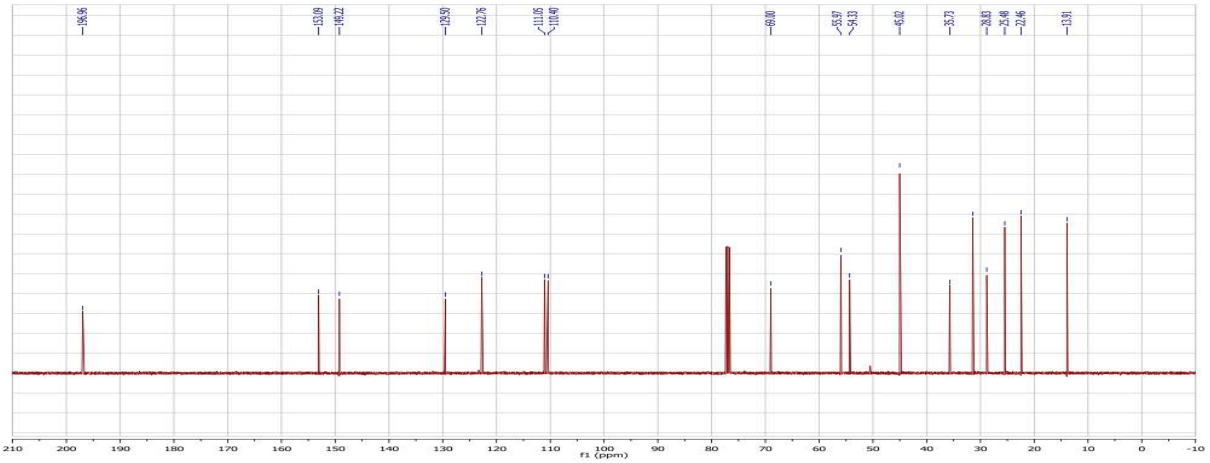
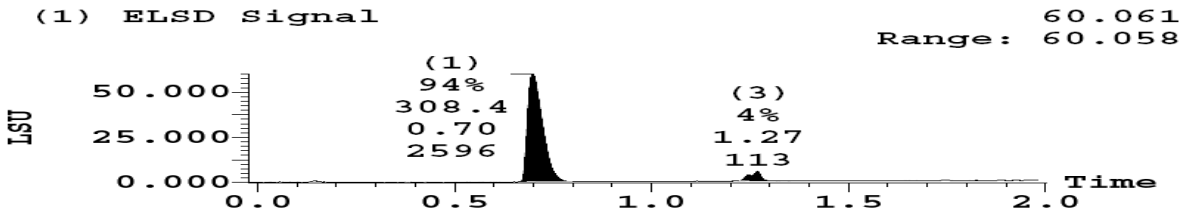


12{*3*}







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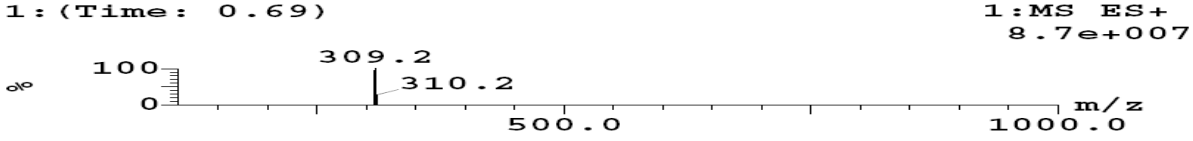
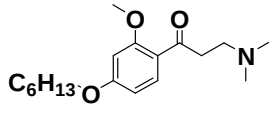
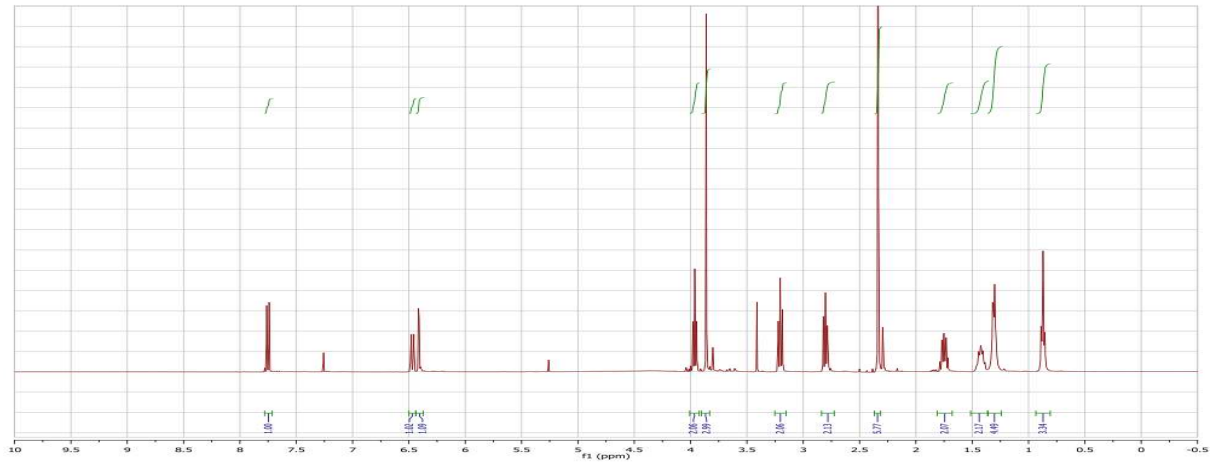
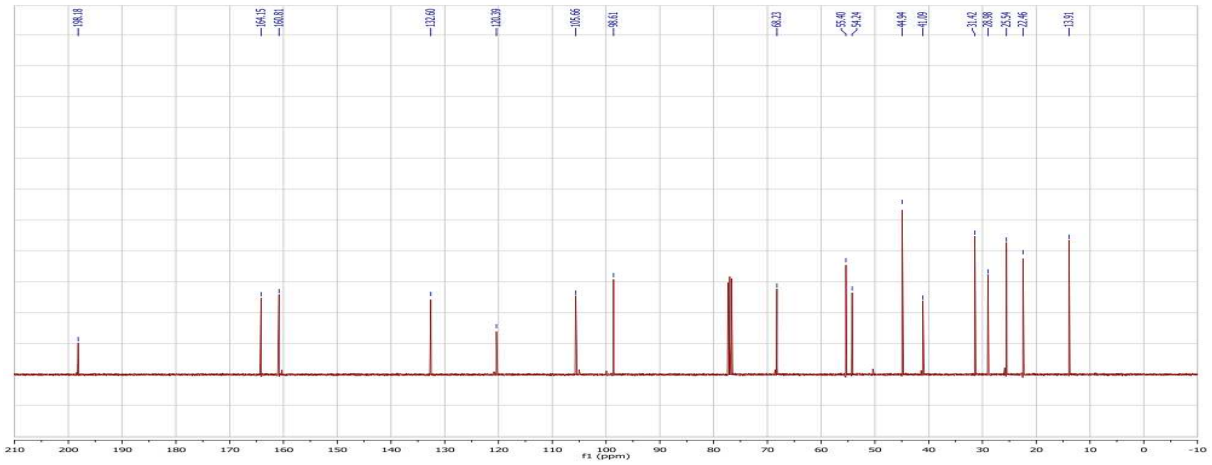
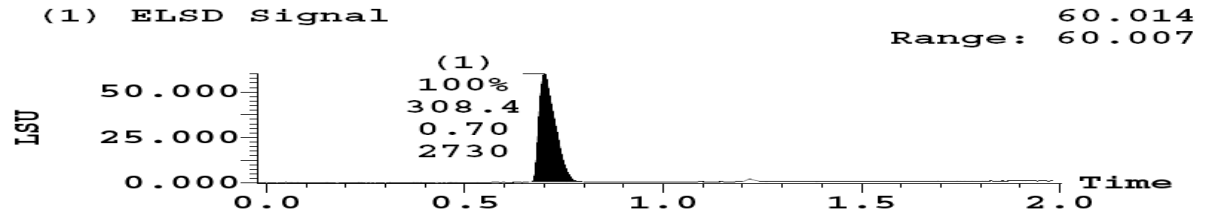




12{*4*}







Peak ID	Compound	Time	Mass Found
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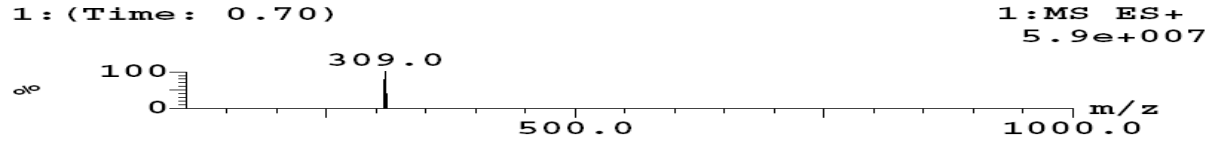

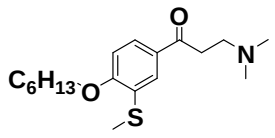

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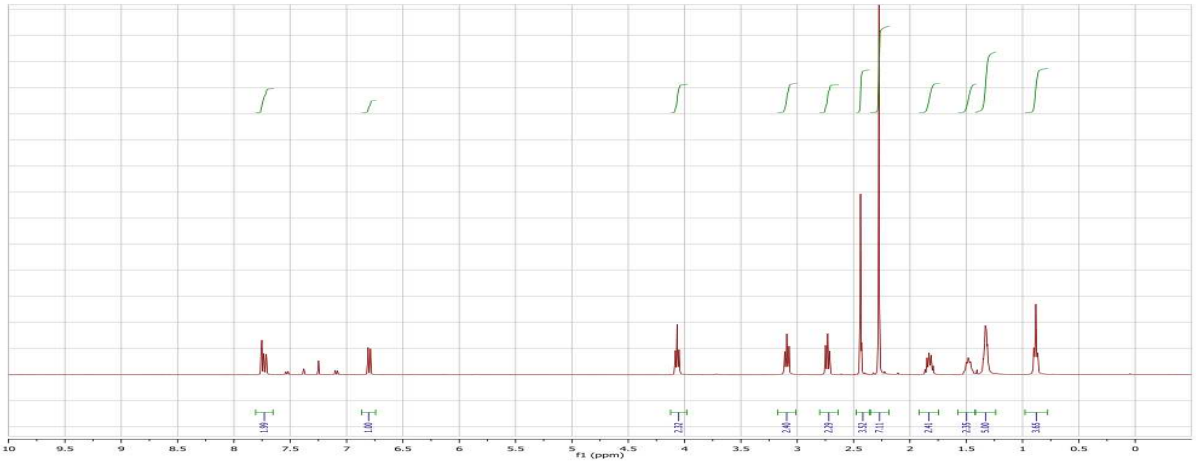

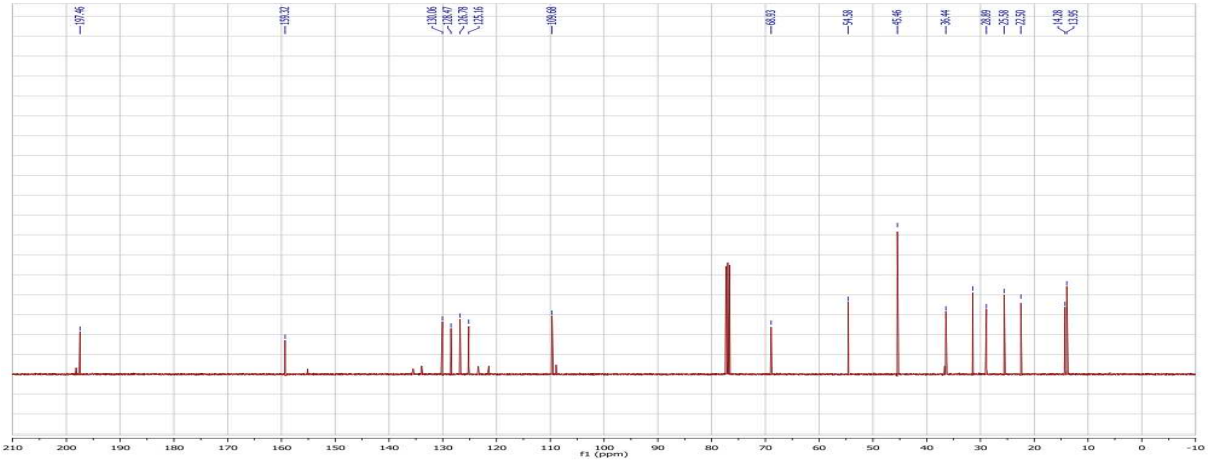

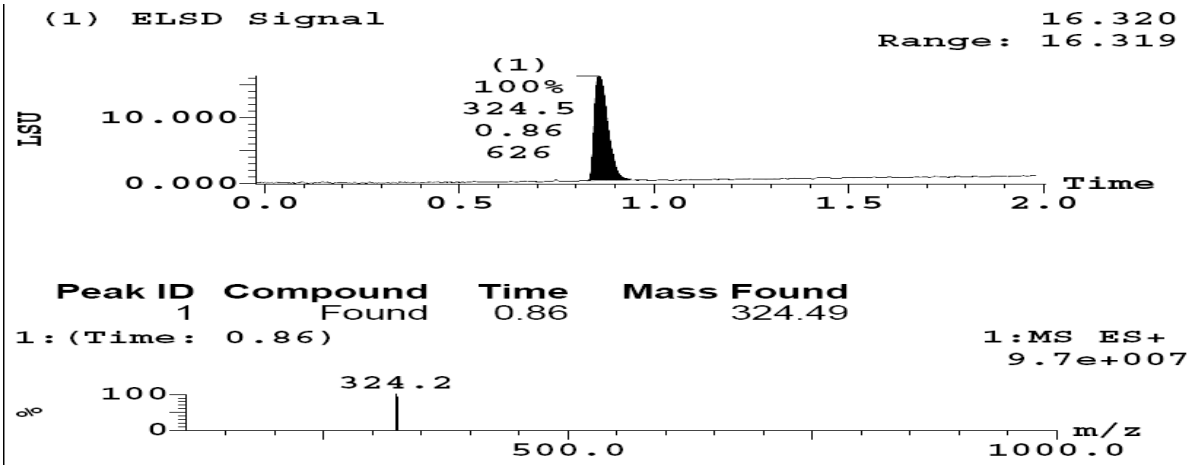
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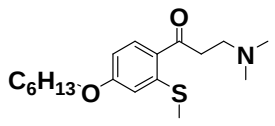
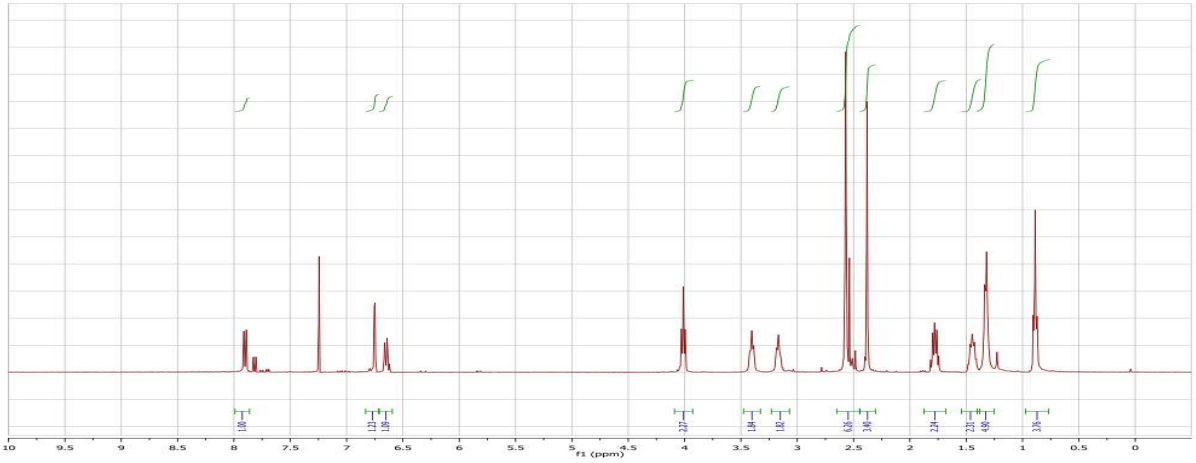
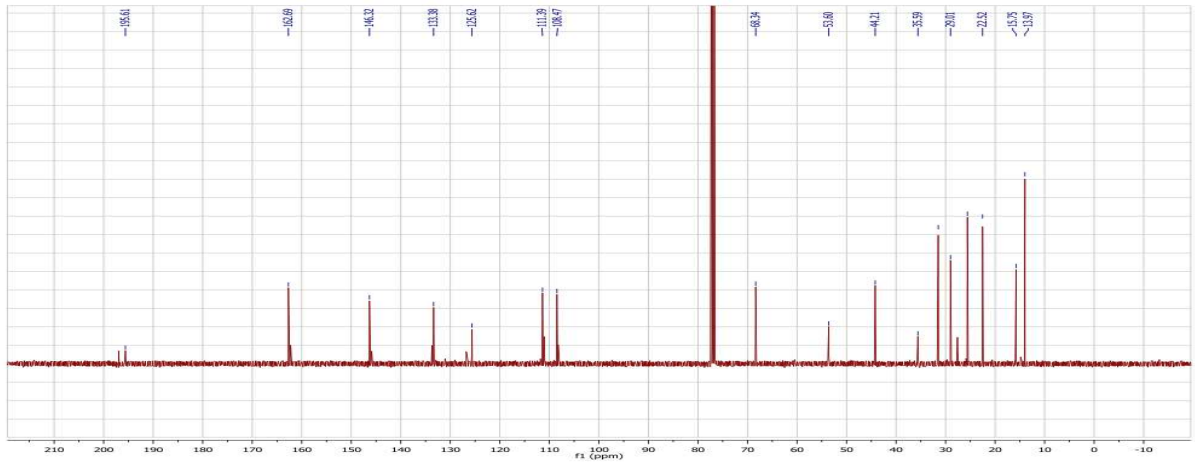
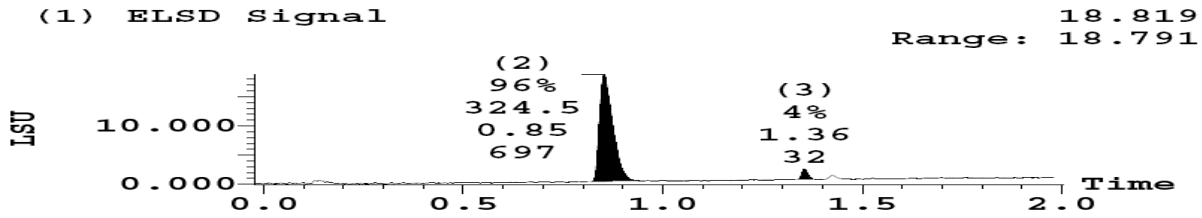
100%
324.5
0.86
626
LSU
10.000
0.000
Time
0.0
0.5
1.0
1.5
2.0
Peak ID Compound Time Mass Found
1 Found 0.86 324.49
1:(Time: 0.86)
1:MS ES+
9.7e+007
324.2
%
100
0
m/z
500.0
1000.0



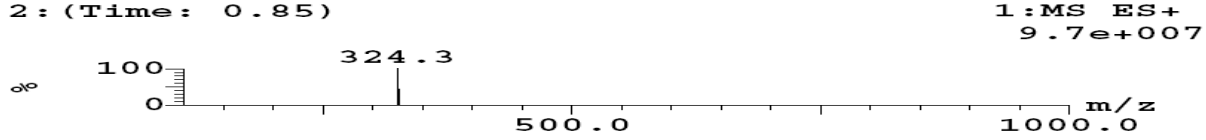
12{*6*}

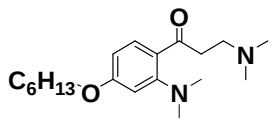




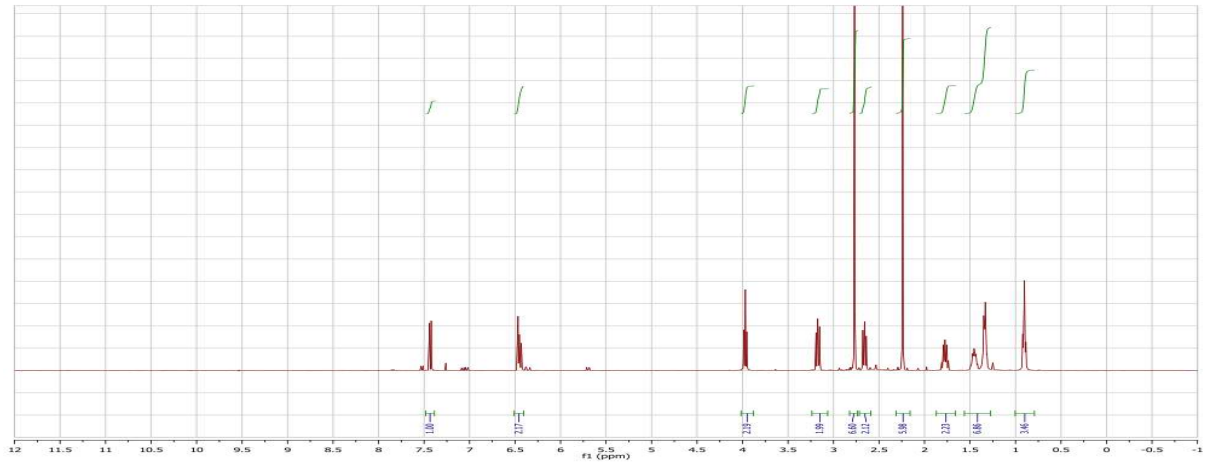


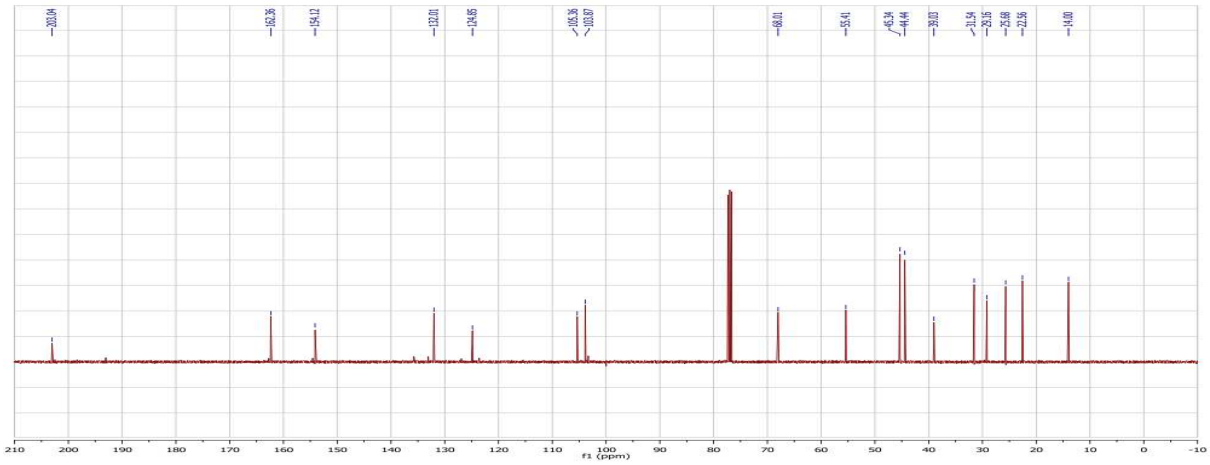
Peak ID	Compound	Time	Mass Found
2	Found	0.85	324.49

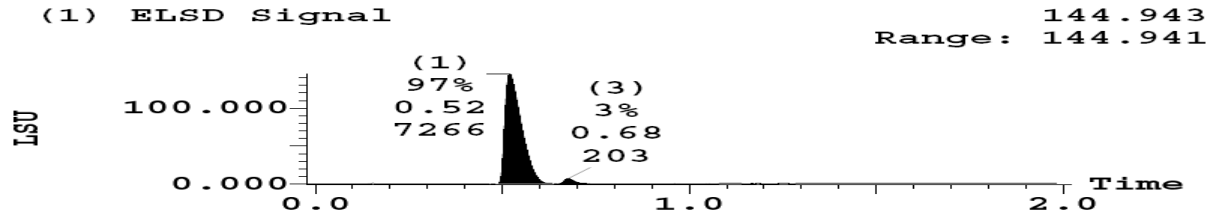




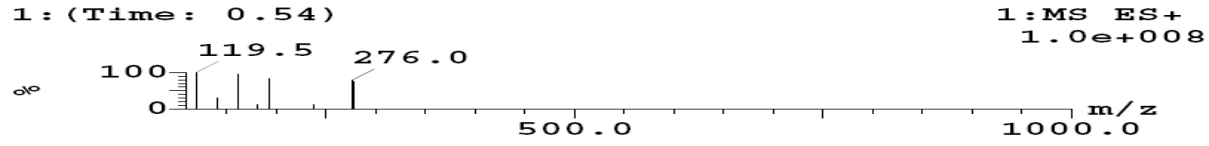
12{*7*}

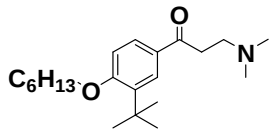




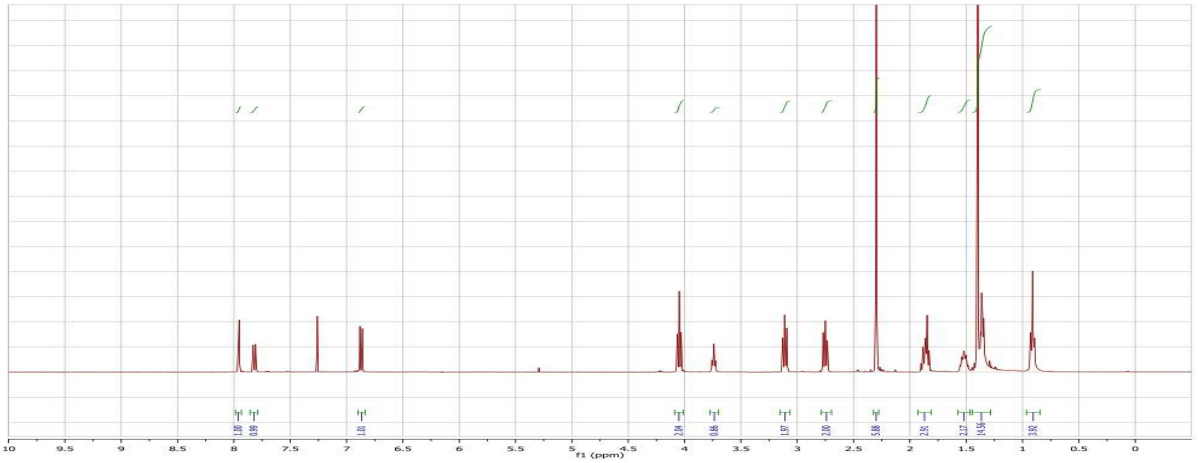


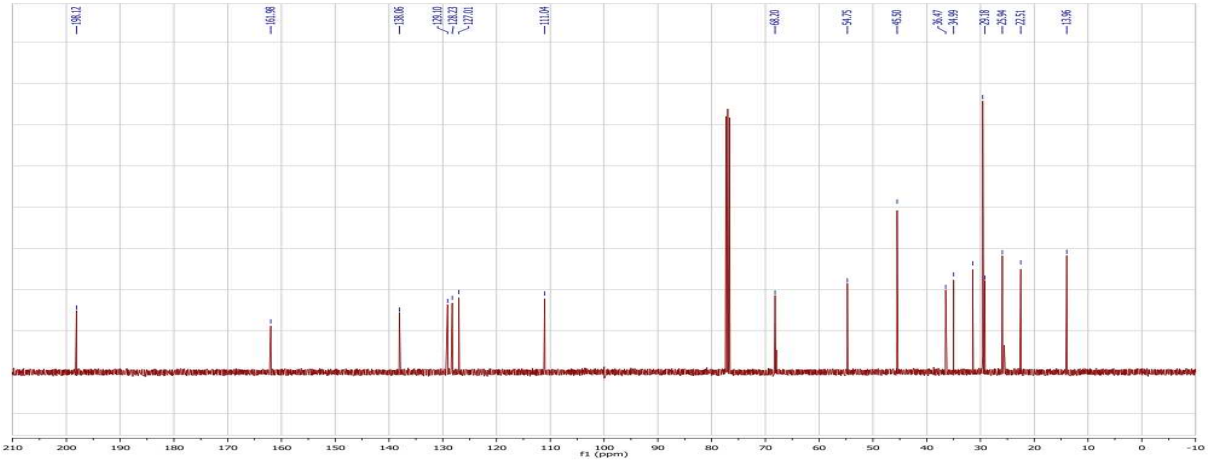
Peak ID	Compound	Time	Mass Found
1		0.54	

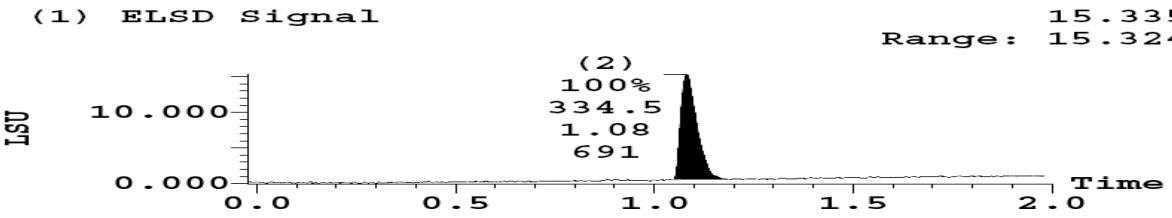


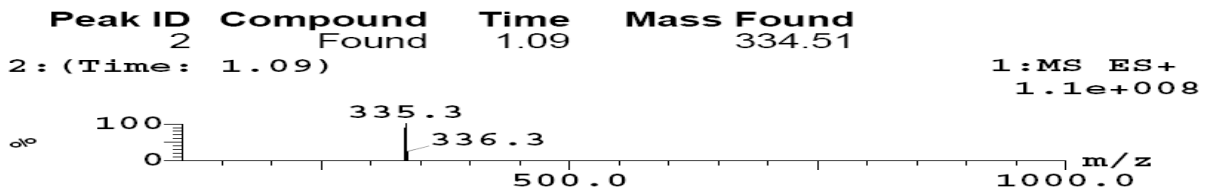

O
N
C6H13O

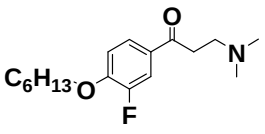
12{*8*}



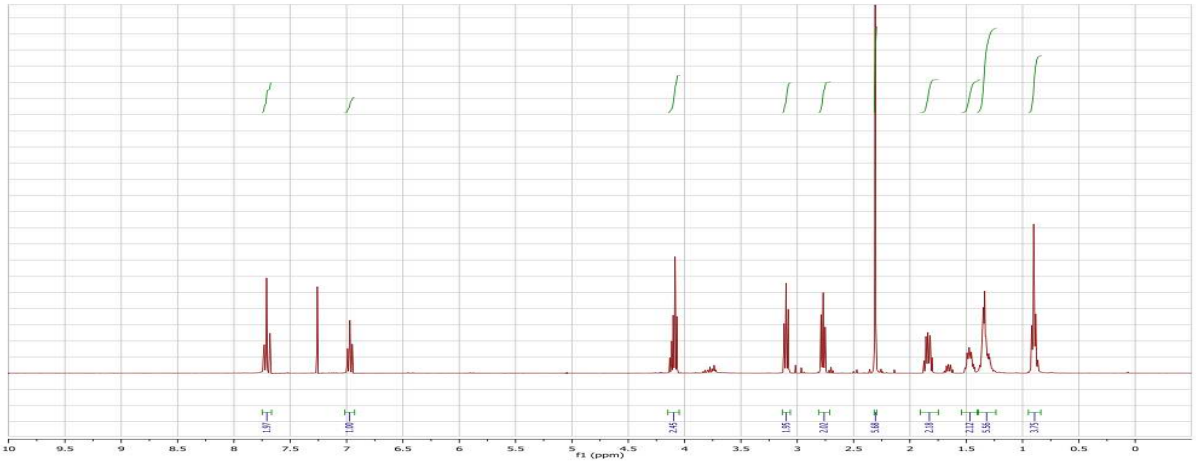


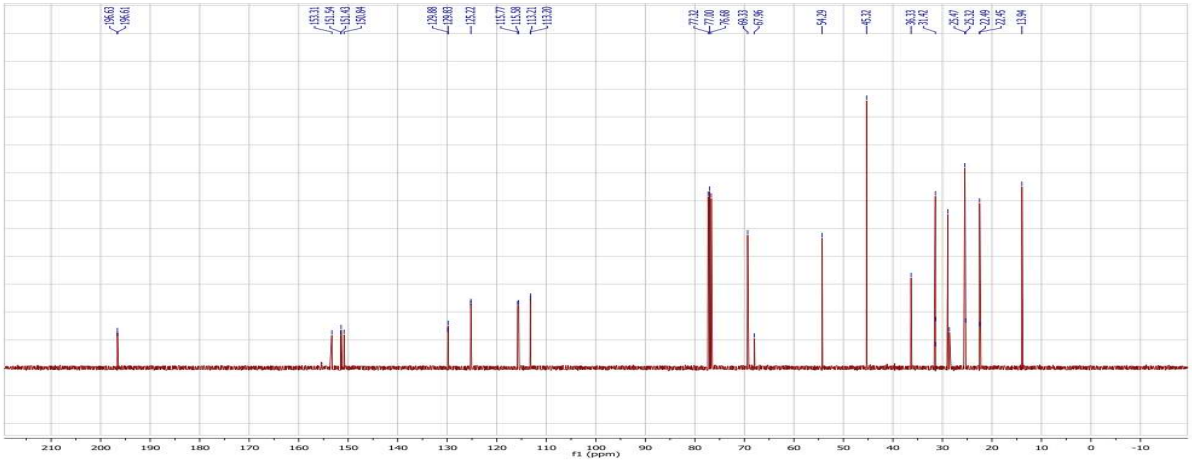

(1) ELSD Signal
15.335
Range: 15.324
(2)
100%
334.5
1.08
691
LSU
10.000
0.000
Time
0.0
0.5
1.0
1.5
2.0

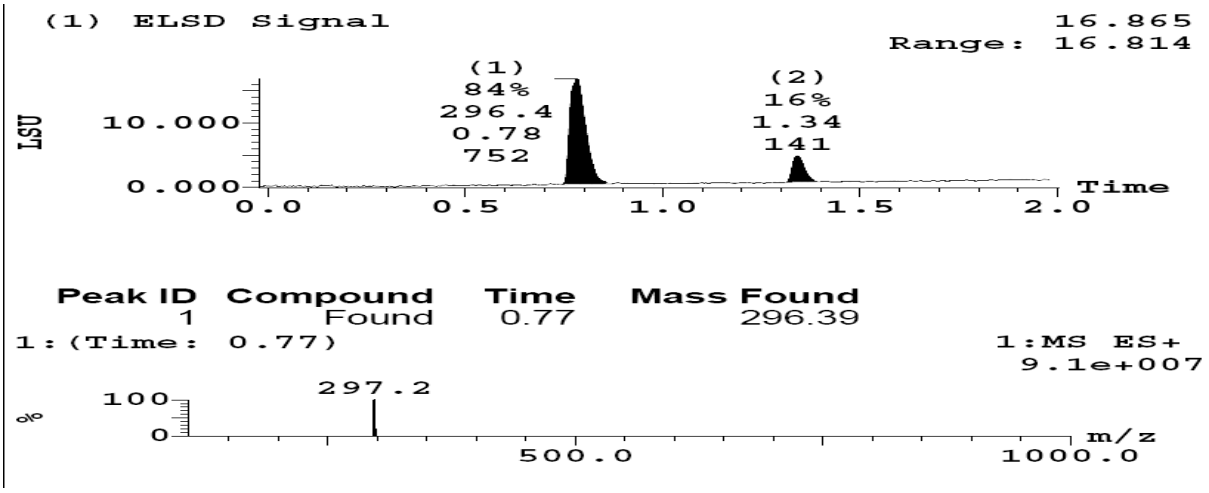

Peak ID Compound Time Mass Found
2 Found 1.09 334.51
2:(Time: 1.09)
1:MS ES+
1.1e+008
335.3
336.3
100
0
%
500.0
1000.0
m/z


O
N
C6H13O
F

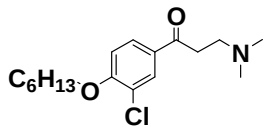
12{*9*}


f1 (ppm)

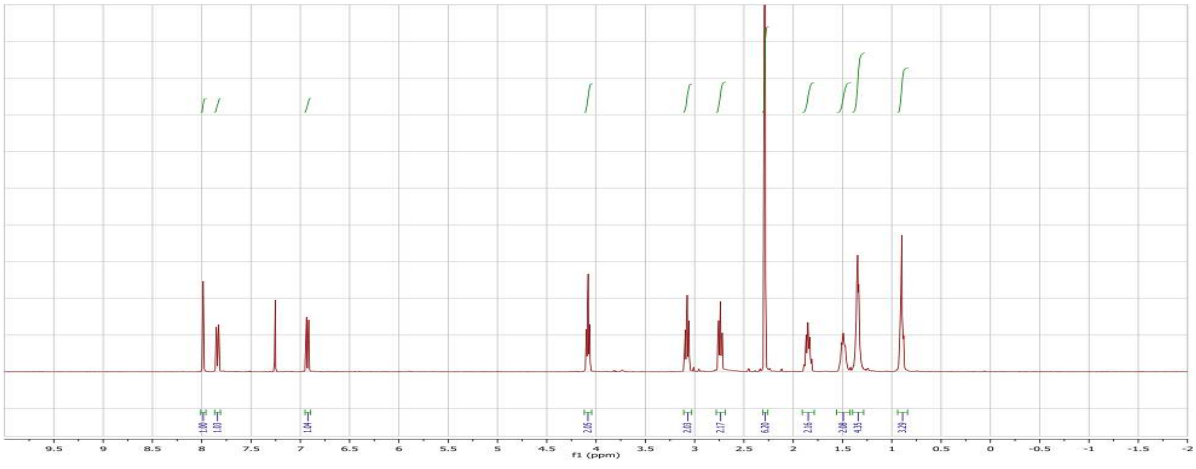

f1 (ppm)

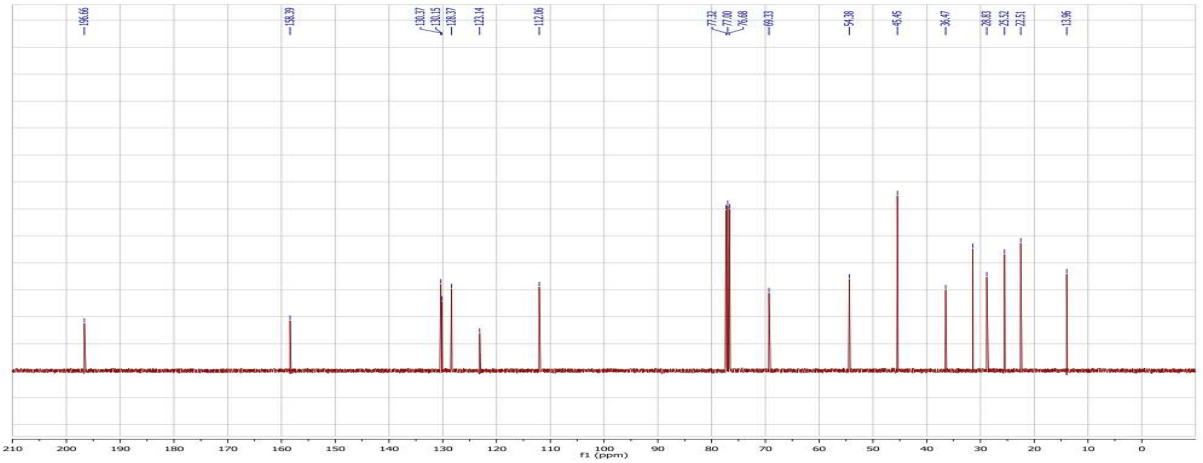


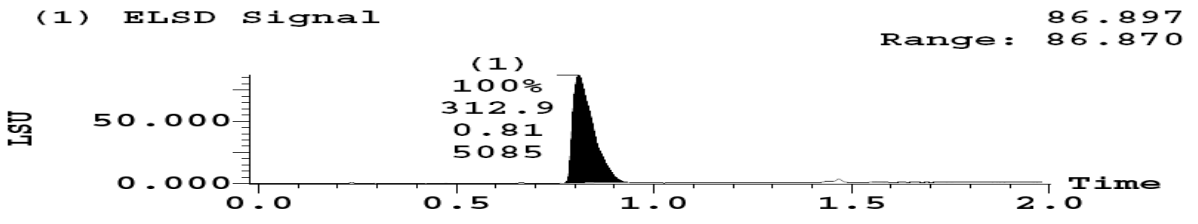
Peak ID	Compound	Time	Mass Found
1	Found	0.77	296.39



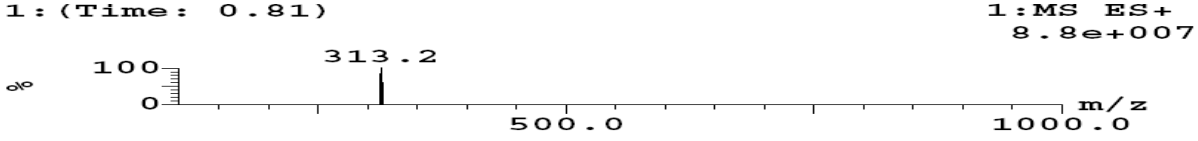
12{*10*}

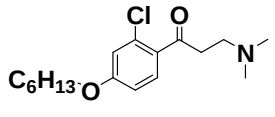




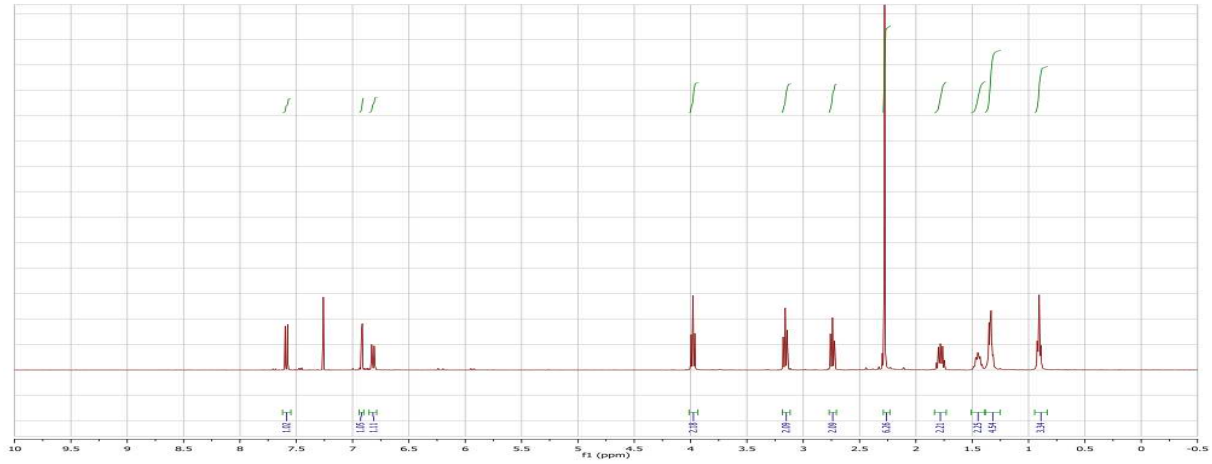


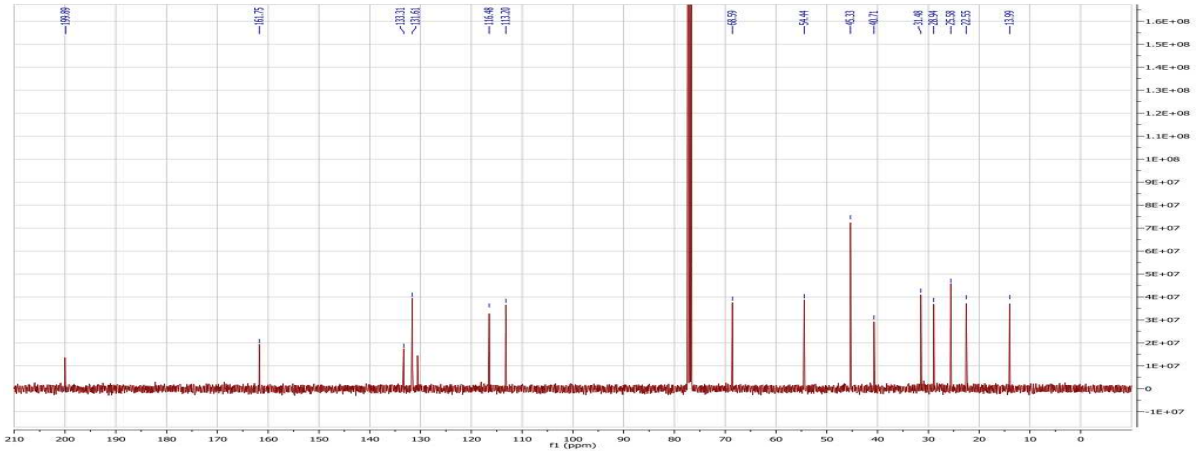
Peak ID	Compound	Time	Mass Found
1	Found	0.81	312.85

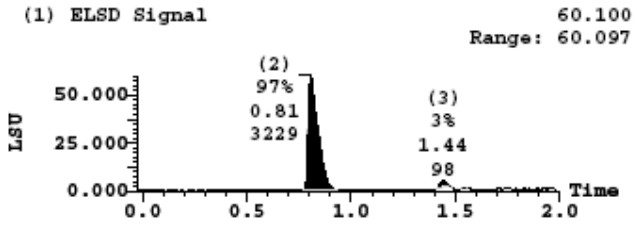




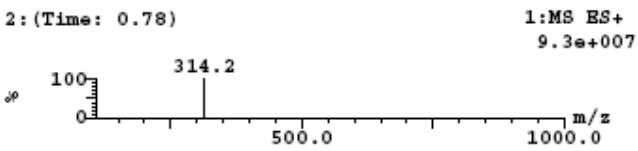
12{*11*}

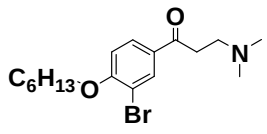




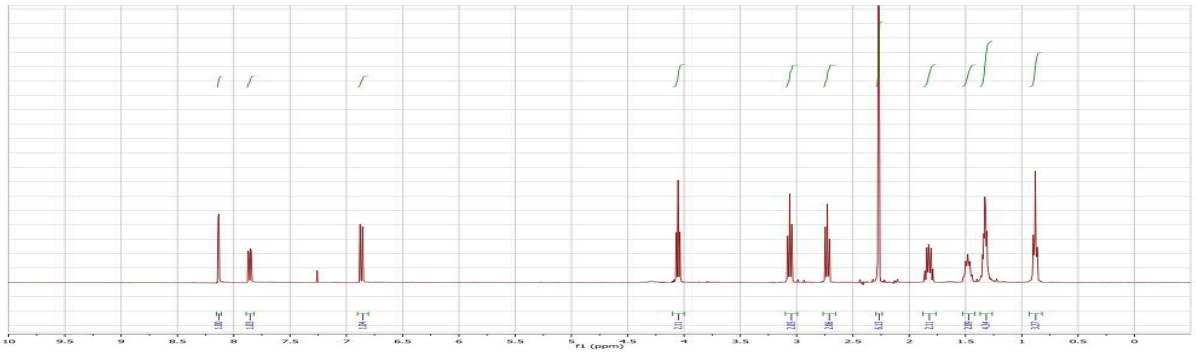


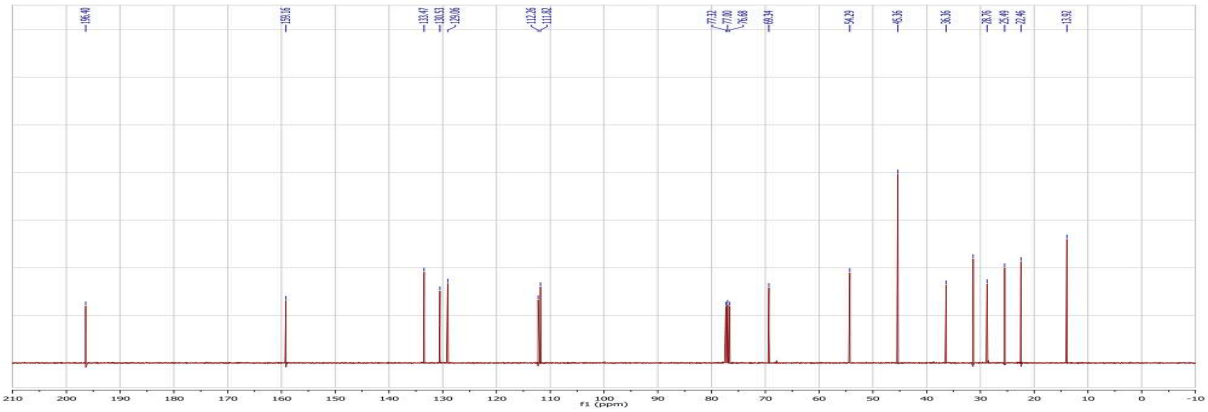
Peak ID	Compound	Time	Mass Found
2	Found	0.78	312.85

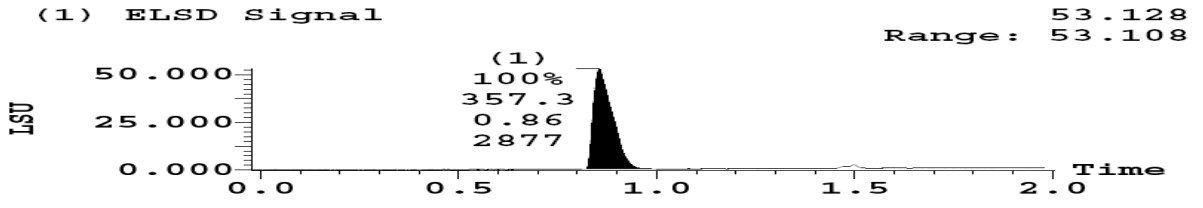




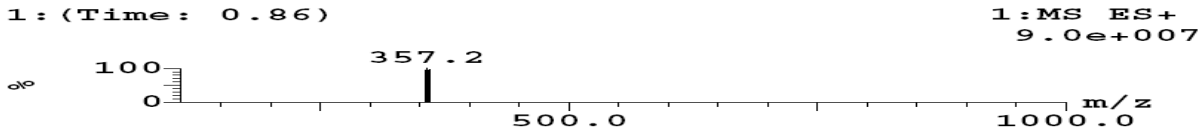
12{*12*}



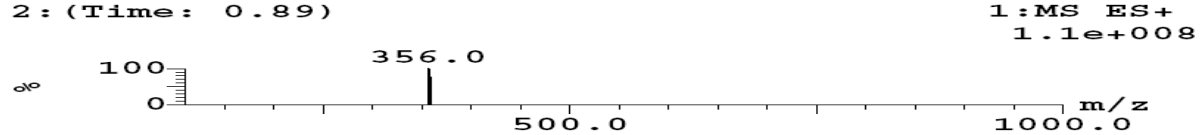


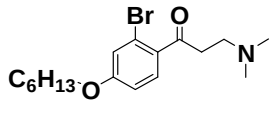


Peak ID	Compound	Time	Mass Found
1	Found	0.86	357.30

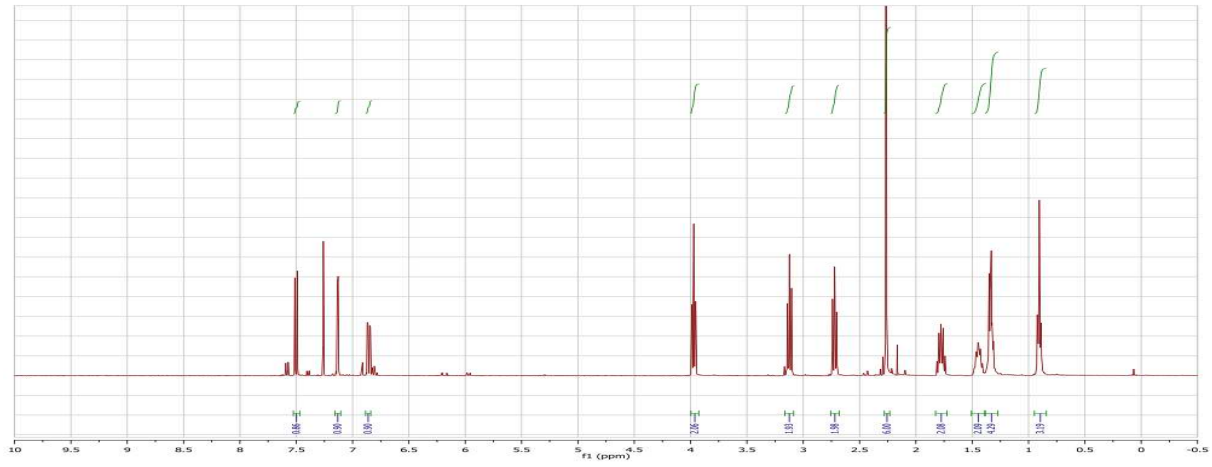


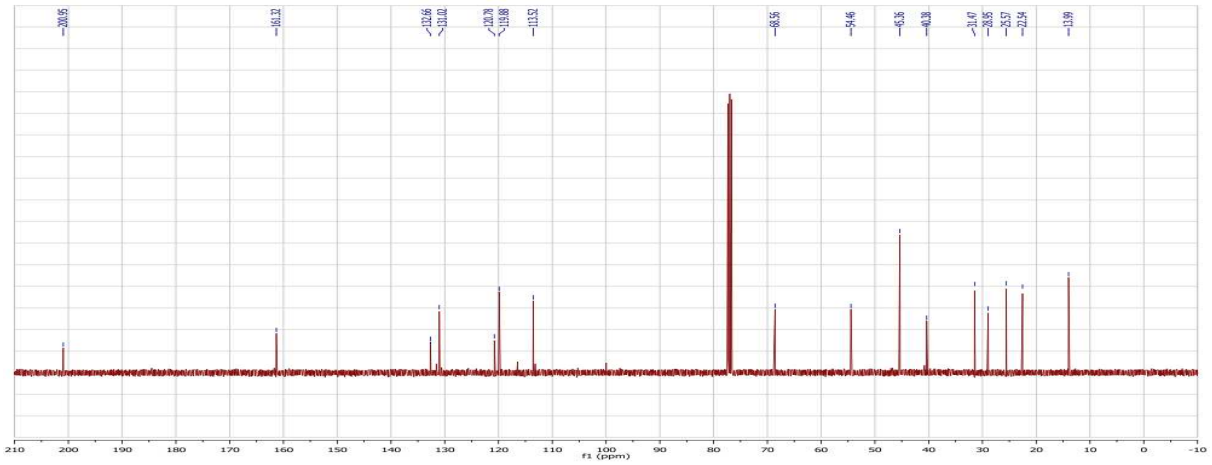
Peak ID	Compound	Time	Mass Found
2	Found	0.89	357.30

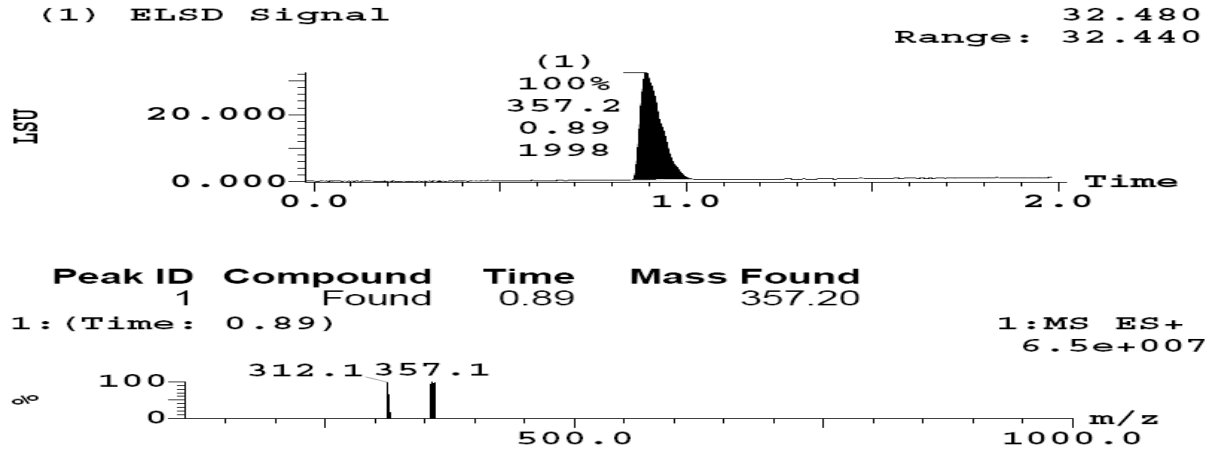




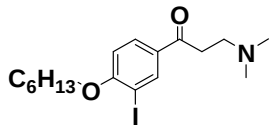
12{*13*}



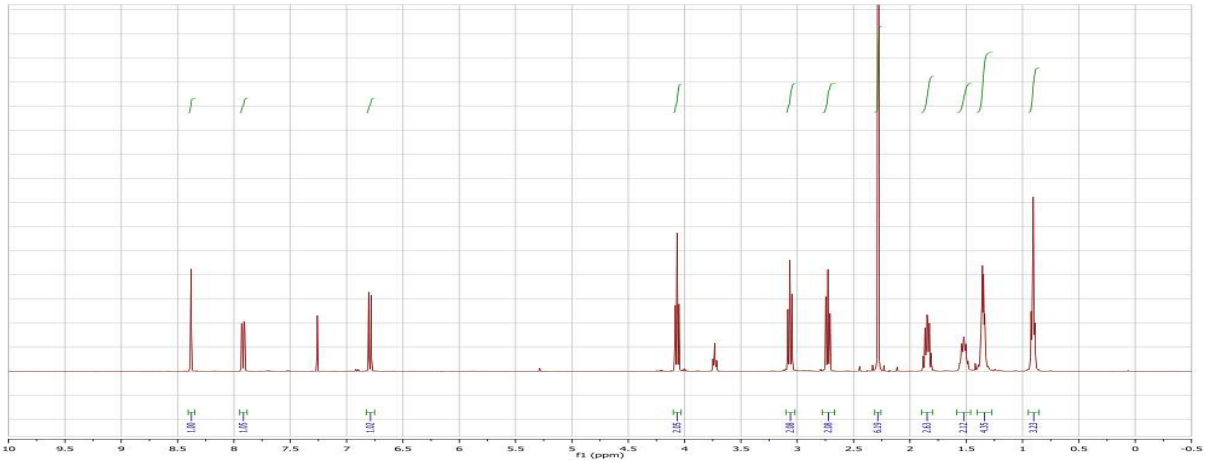


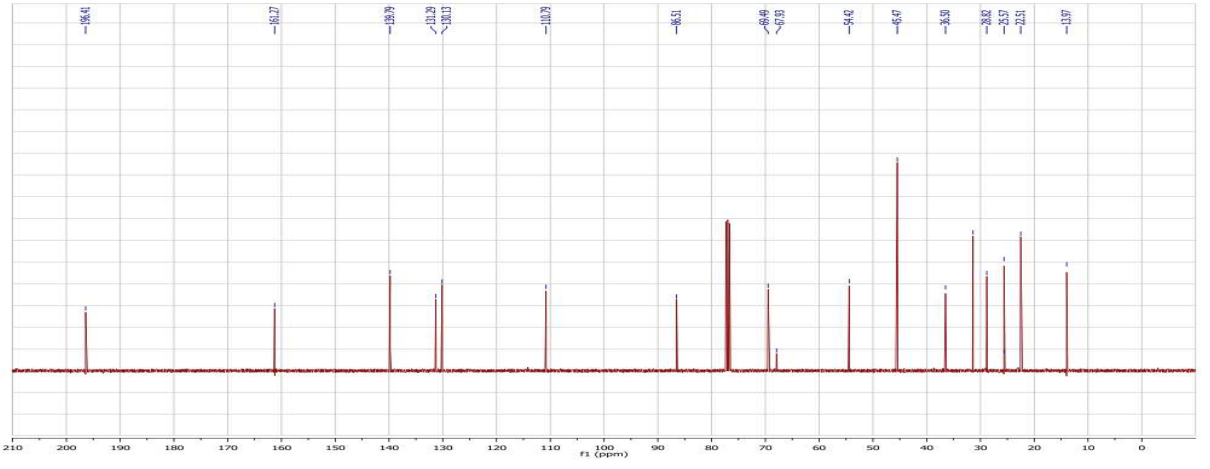


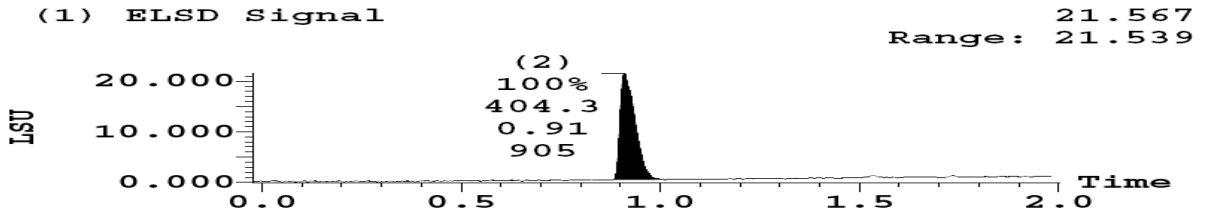
Peak ID	Compound	Time	Mass Found
1	Found	0.89	357.20

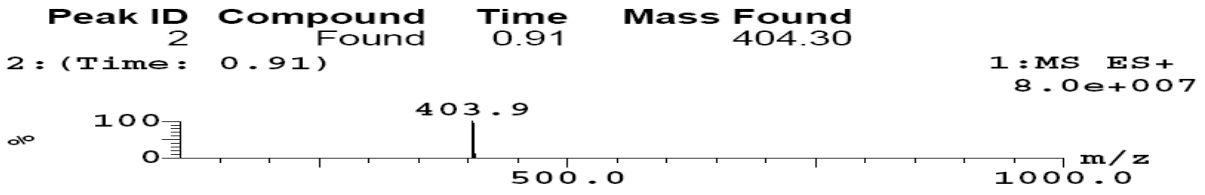


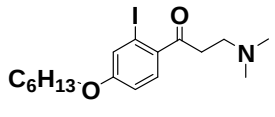
12{*14*}



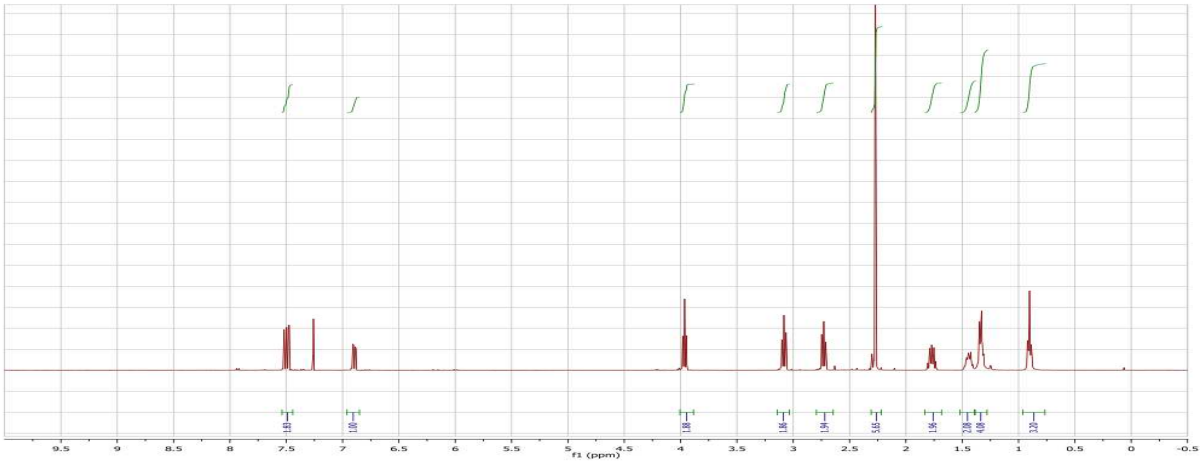


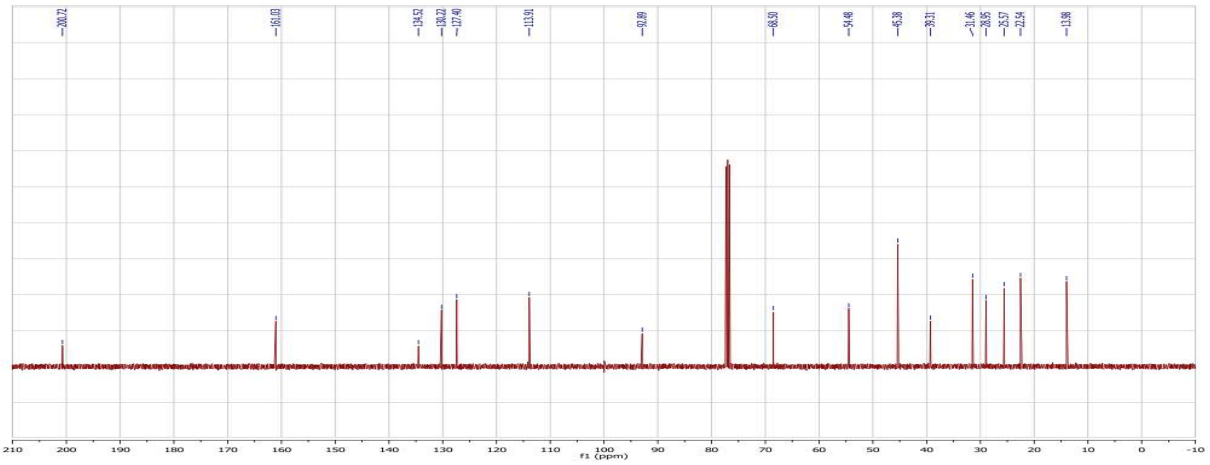

(1) ELSD Signal
21.567
Range: 21.539
(2)
100%
404.3
0.91
905
LSU
20.000
10.000
0.000
Time
0.0
0.5
1.0
1.5
2.0

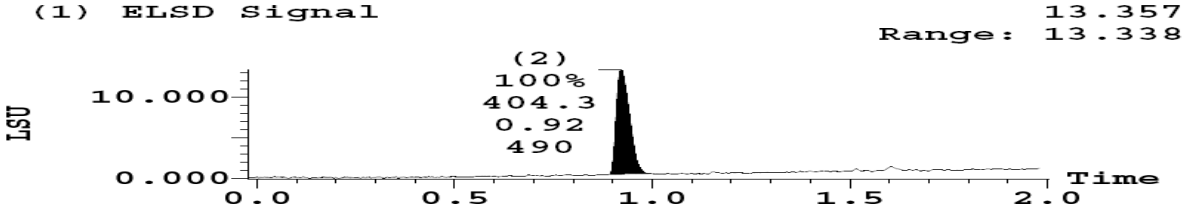

Peak ID Compound Time Mass Found
2 Found 0.91 404.30
2:(Time: 0.91)
1:MS ES+
8.0e+007
403.9
%
100
0
500.0
1000.0
m/z

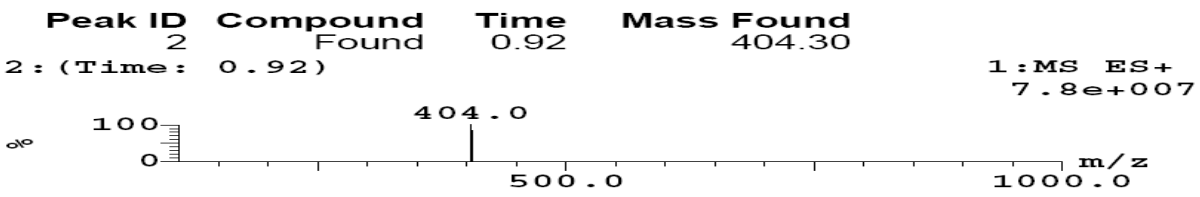

I
O
N
C6H13O

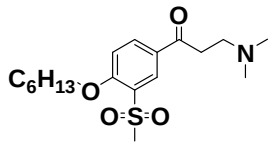
12{*15*}



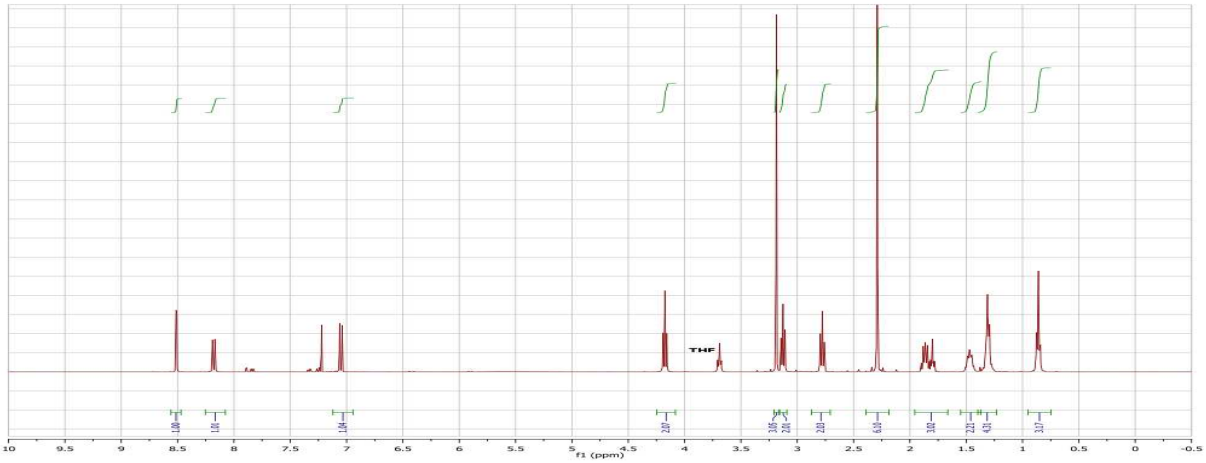


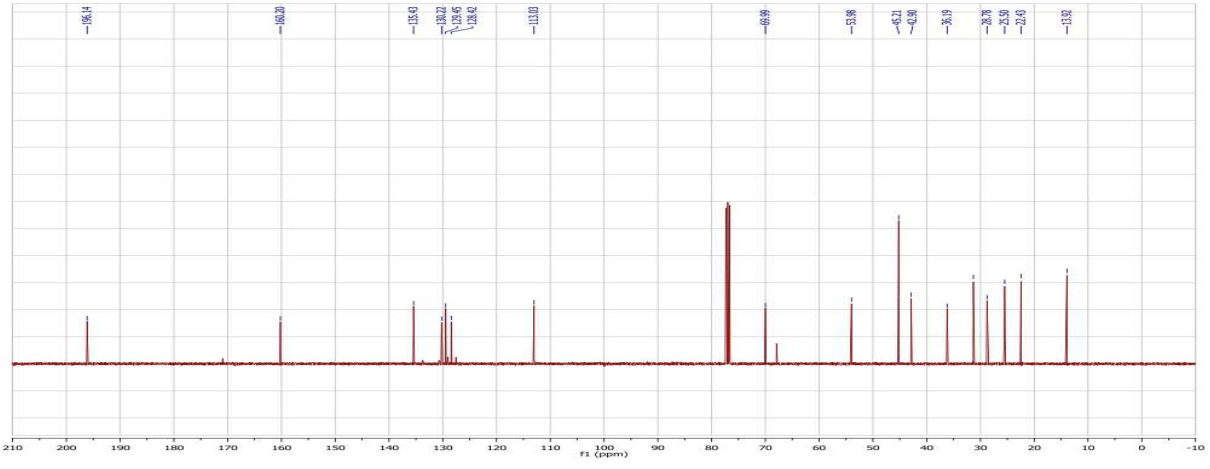

(1) ELSD Signal
13.357
Range: 13.338
(2)
100%
404.3
0.92
490
10.000
0.000
LSU
Time
0.0
0.5
1.0
1.5
2.0

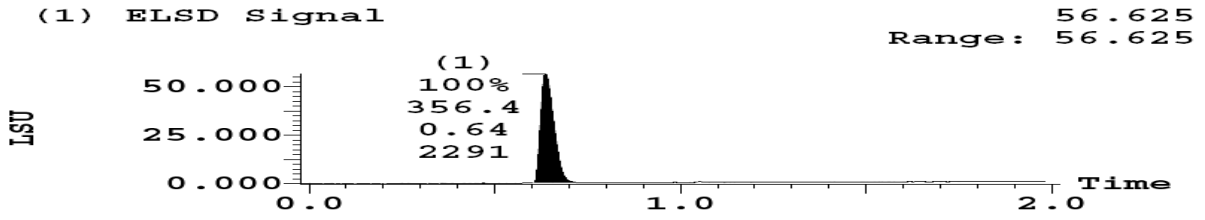

Peak ID Compound Time Mass Found
2 Found 0.92 404.30
2:(Time: 0.92)
1:MS ES+
7.8e+007
404.0
100
%
0
500.0
1000.0
m/z



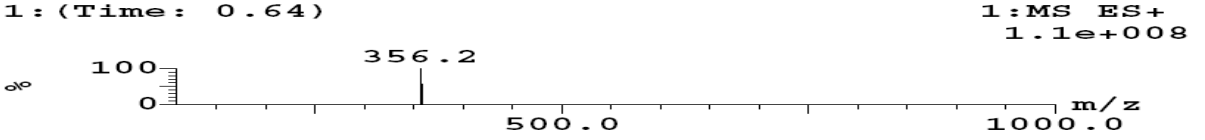
12{*16*}

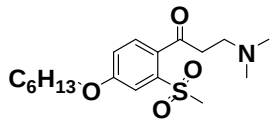




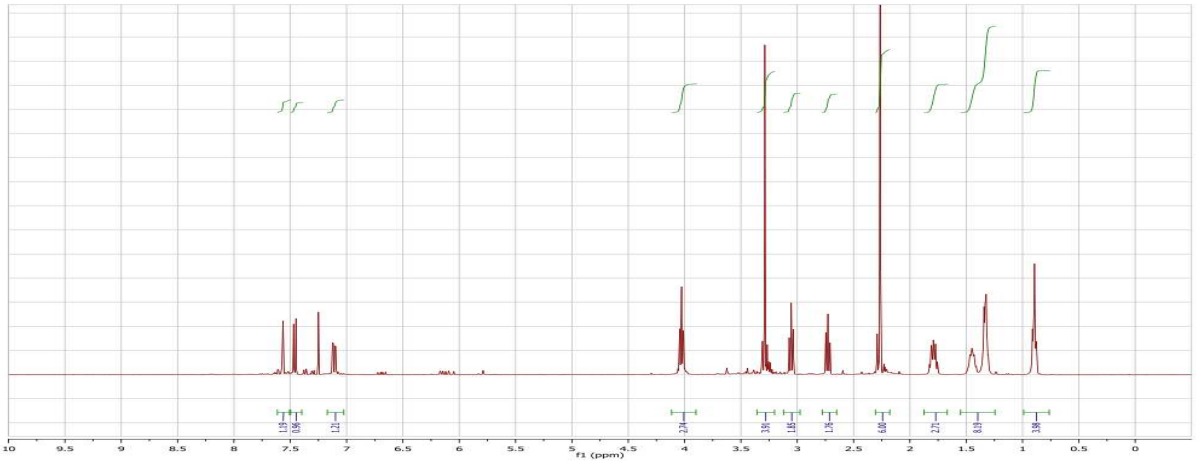


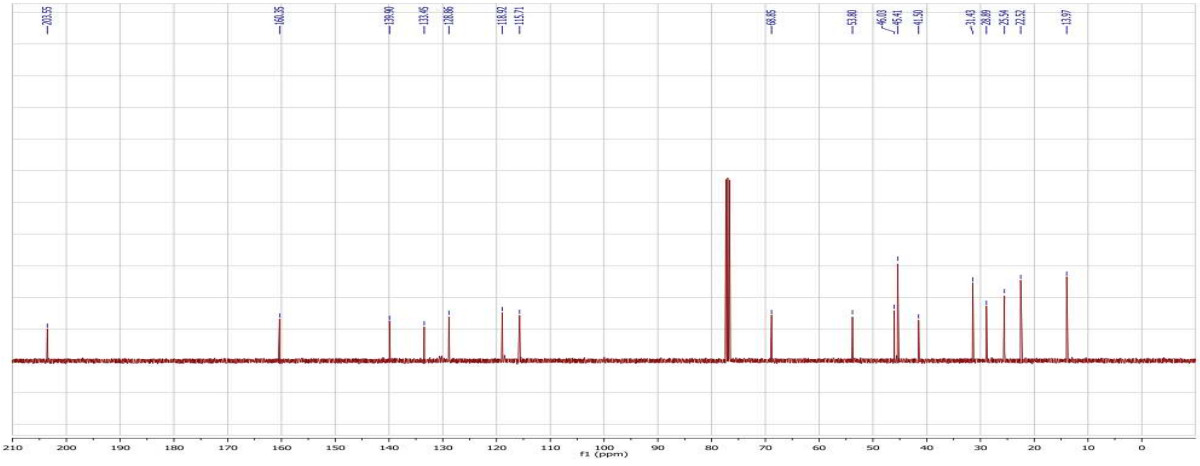
Peak ID	Compound	Time	Mass Found
1	Found	0.64	356.39

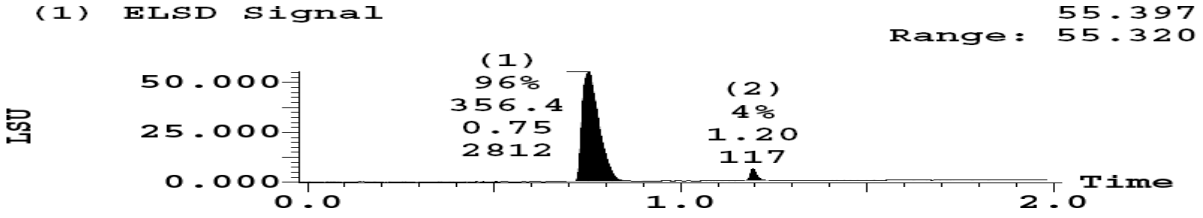




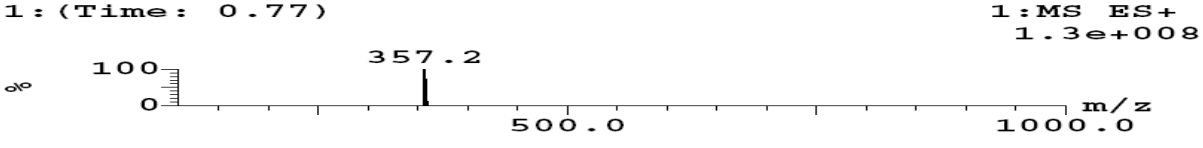
12{*17*}

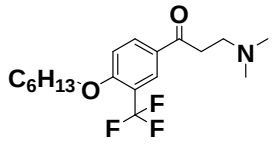




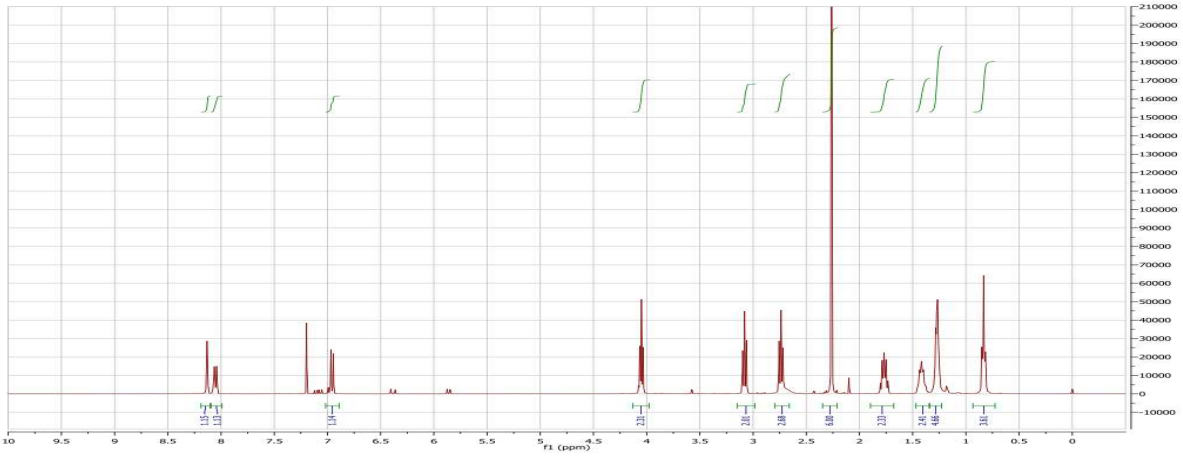


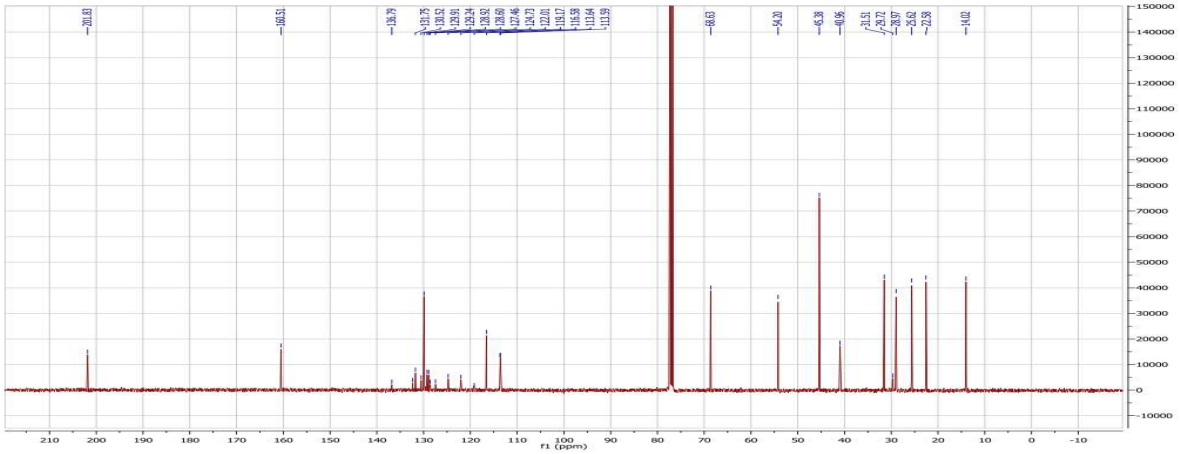
Peak ID	Compound	Time	Mass Found
1	Found	0.76	356.39

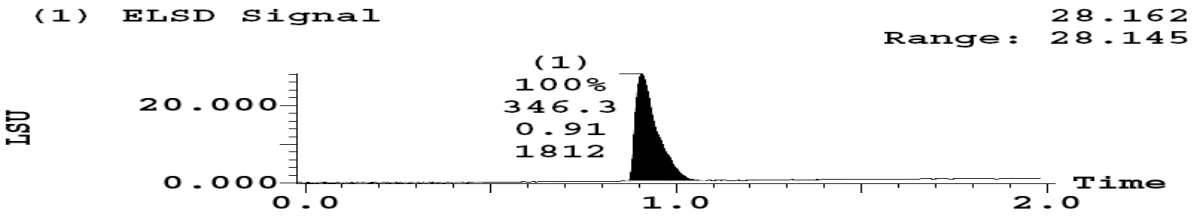


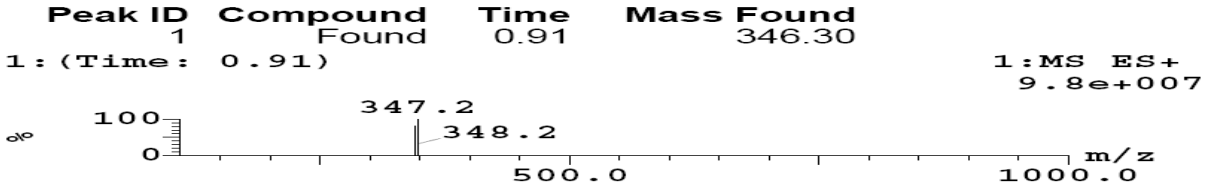

O
N
C6H13O
F
F
F

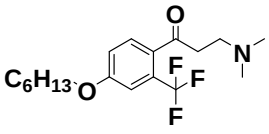
12{*18*}



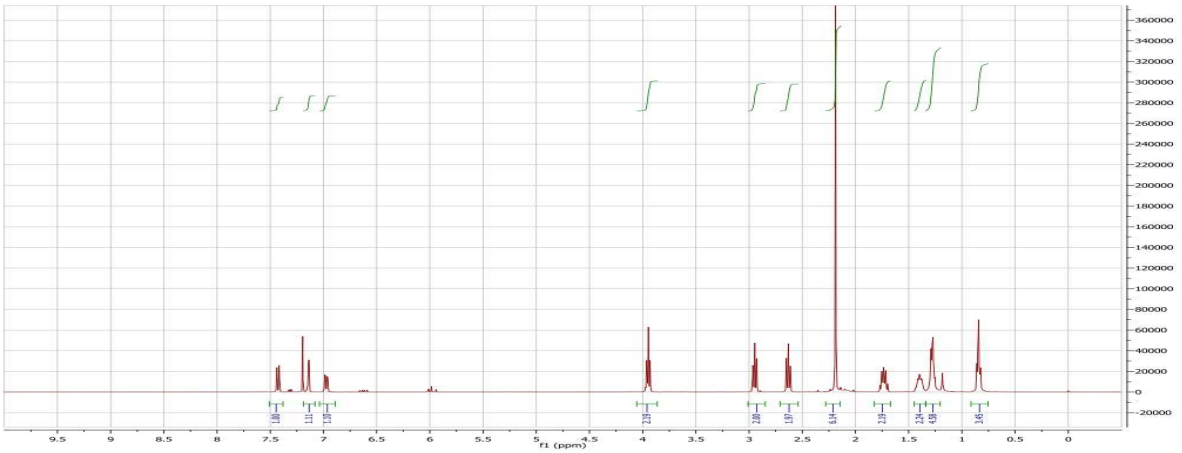


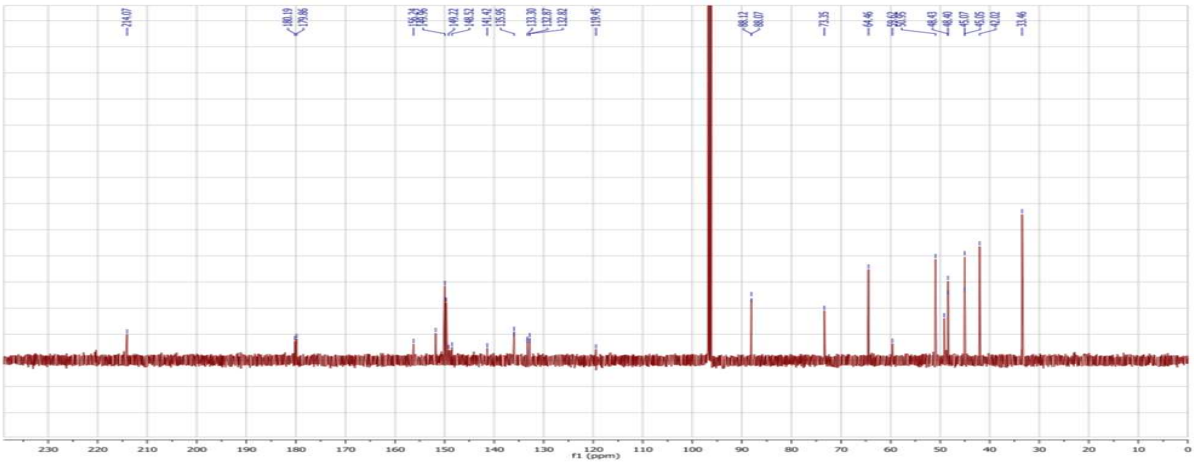

(1) ELSD Signal
28.162
Range: 28.145
(1)
100%
346.3
0.91
1812
20.000
0.000
LSU
0.0
1.0
2.0
Time

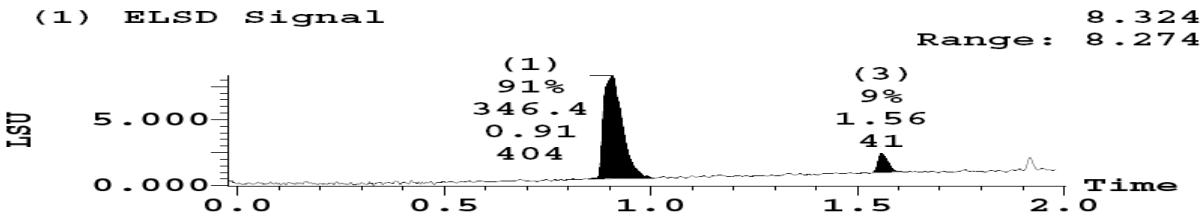

Peak ID Compound Time Mass Found
1 Found 0.91 346.30
1:(Time: 0.91)
1:MS ES+
9.8e+007
100
0
347.2
348.2
m/z
500.0
1000.0


O
N
F
F
F
C6H13O

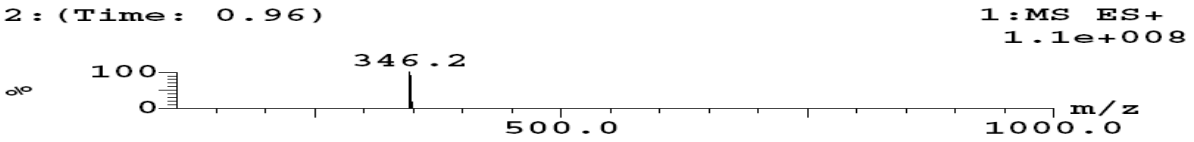
12{*19*}

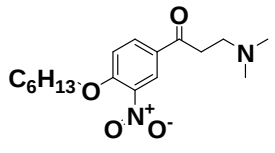




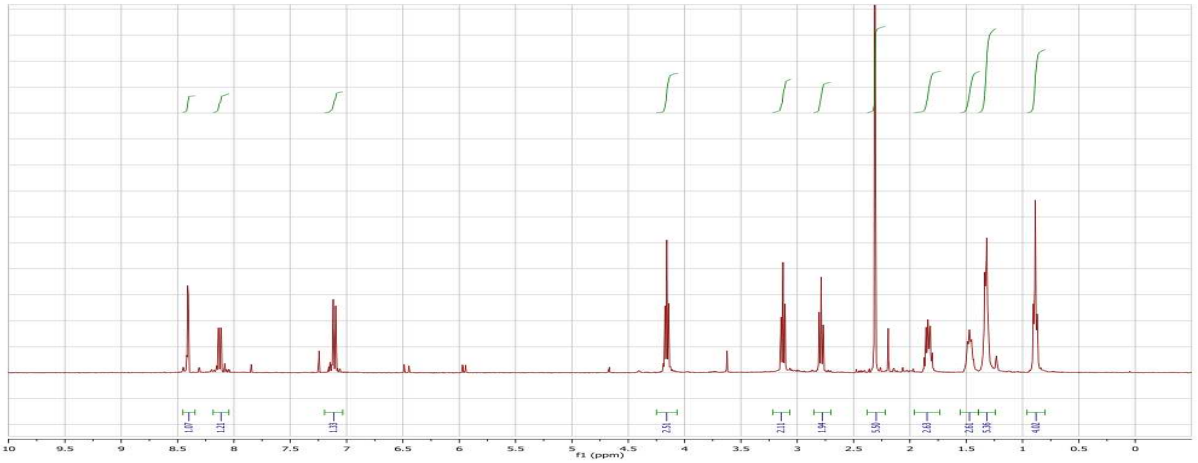

(1) ELSD Signal
8.324
Range: 8.274
(1)
91%
346.4
0.91
404
(3)
9%
1.56
41
LSU
5.000
0.000
Time
0.0
0.5
1.0
1.5
2.0

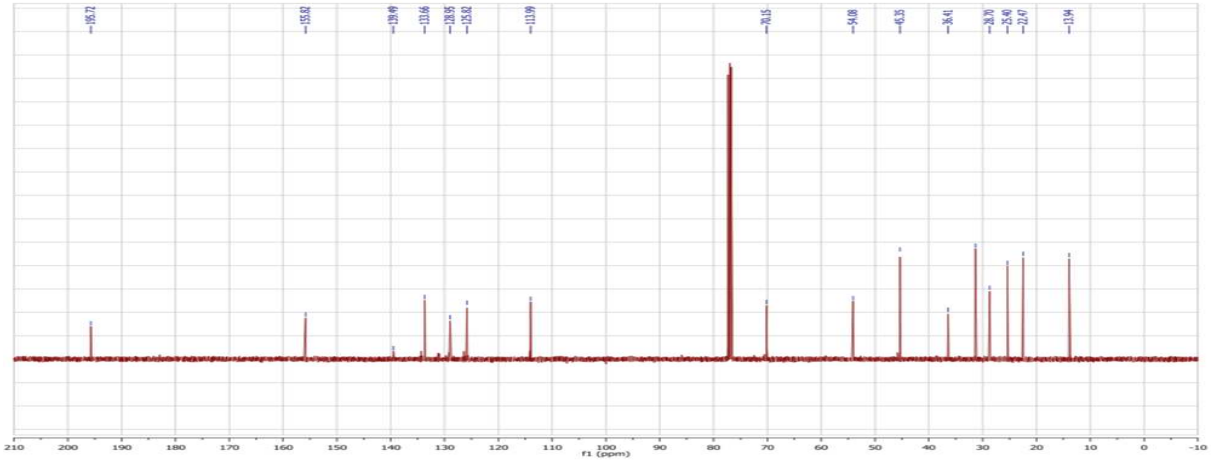
Peak ID	Compound	Time	Mass Found
2	Found	0.96	346.40

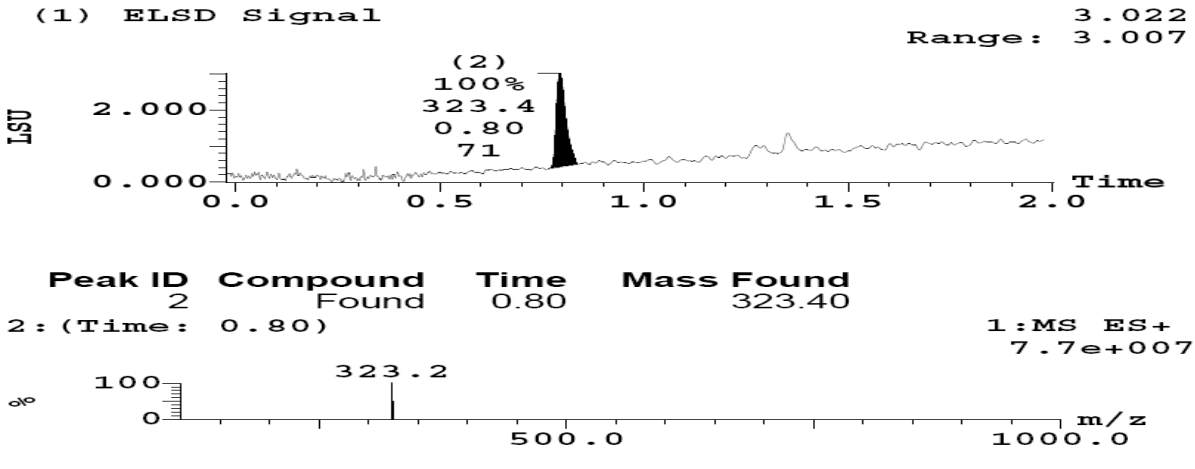




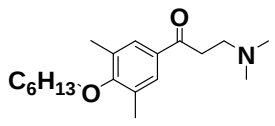
12{*20*}



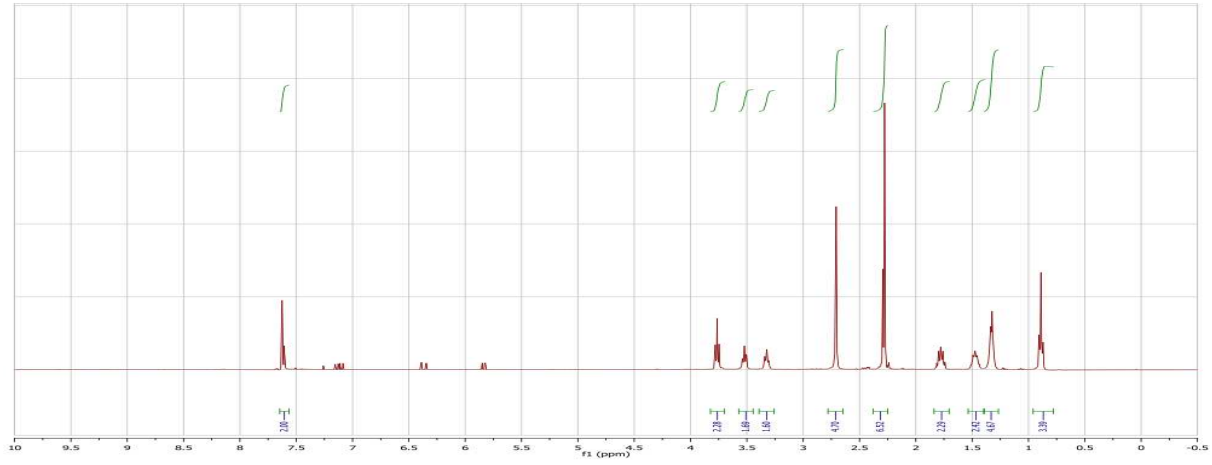


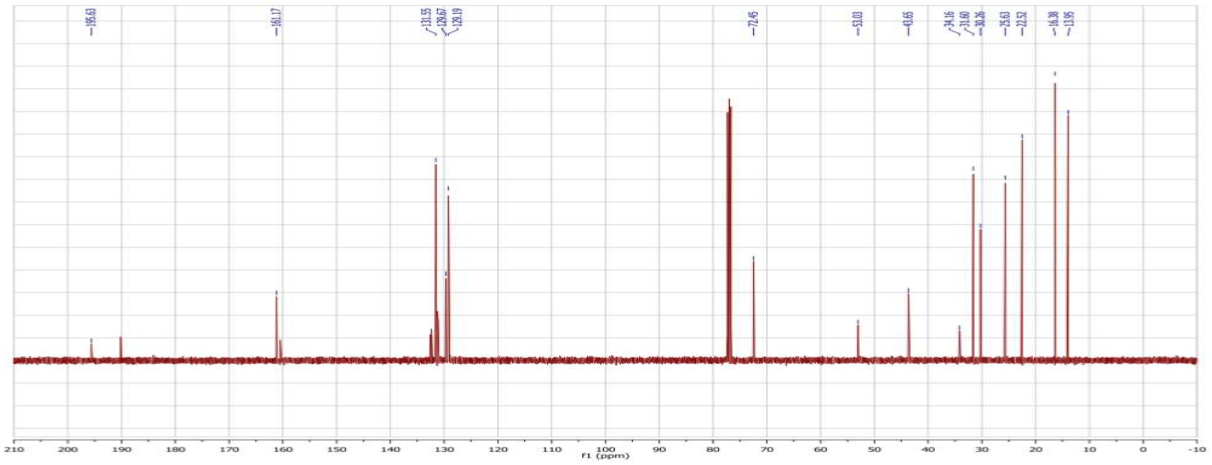


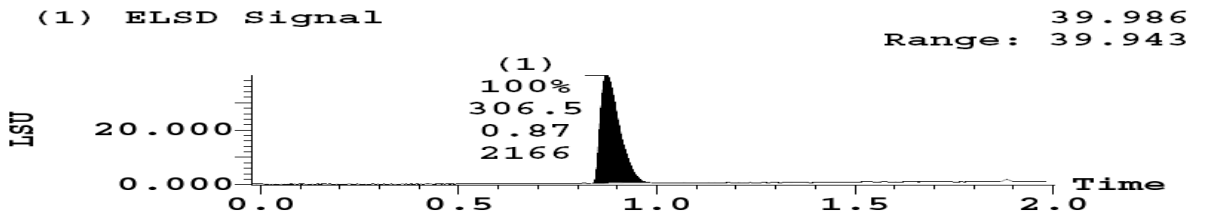
Peak ID	Compound	Time	Mass Found
2	Found	0.80	323.40



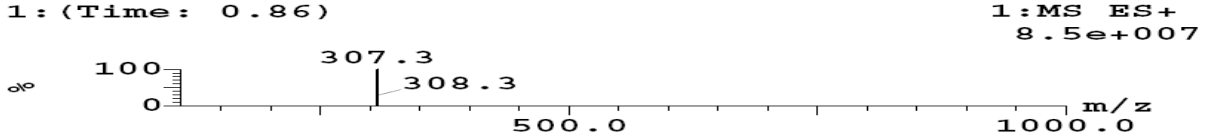
12{*21*}

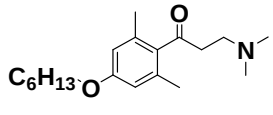




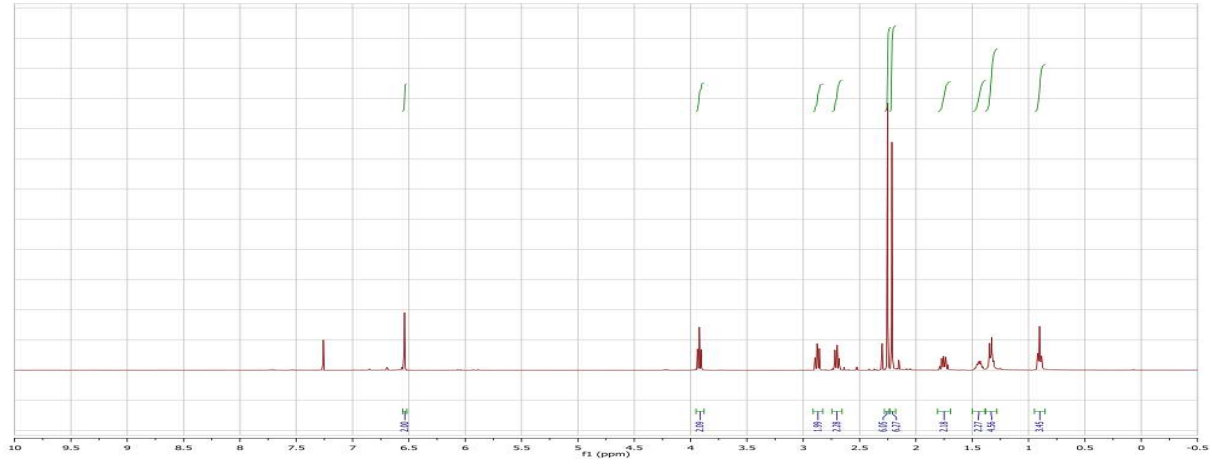


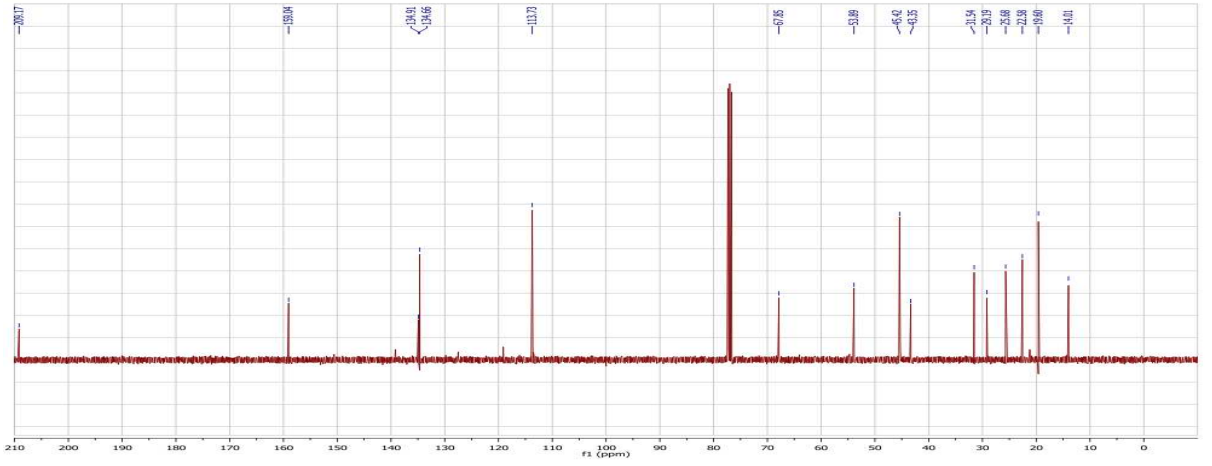
Peak ID	Compound	Time	Mass Found
1	Found	0.86	306.45

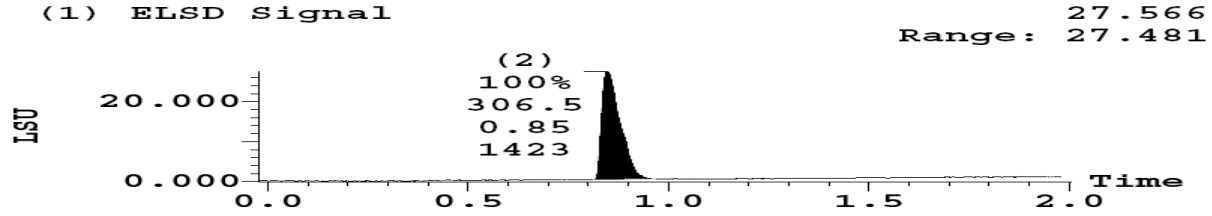


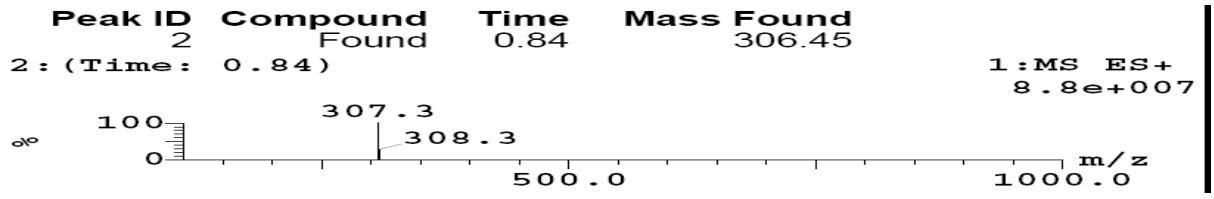

O
N
C6H13O

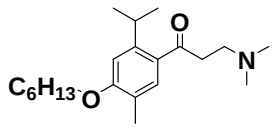
12{*22*}



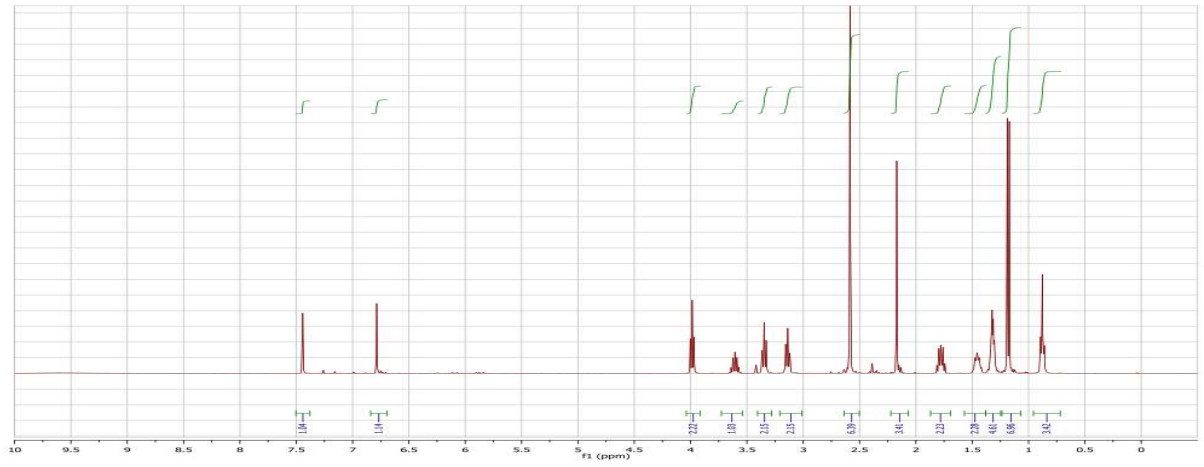


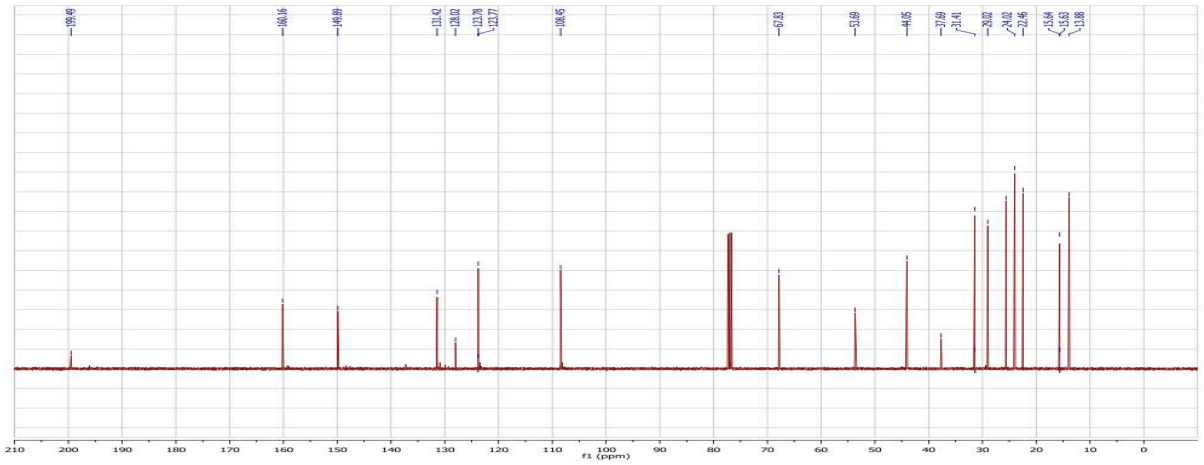

(1) ELSD Signal
27.566
Range: 27.481
(2)
100%
306.5
0.85
1423
20.000
0.000
LSU
Time
0.0
0.5
1.0
1.5
2.0

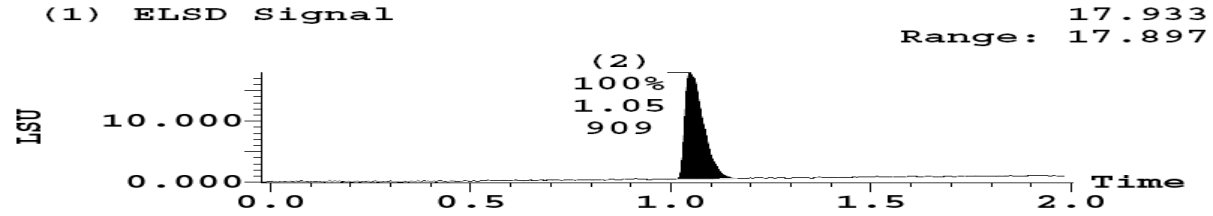

Peak ID Compound Time Mass Found
2 Found 0.84 306.45
2:(Time: 0.84)
1:MS ES+
8.8e+007
307.3
308.3
100
0
m/z
500.0
1000.0

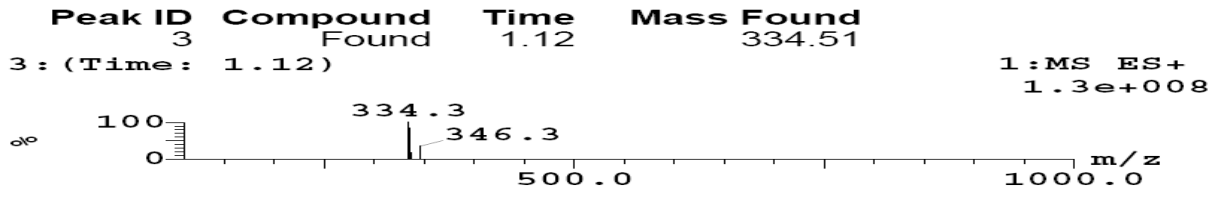

O
N
C6H13O

12{*23*}

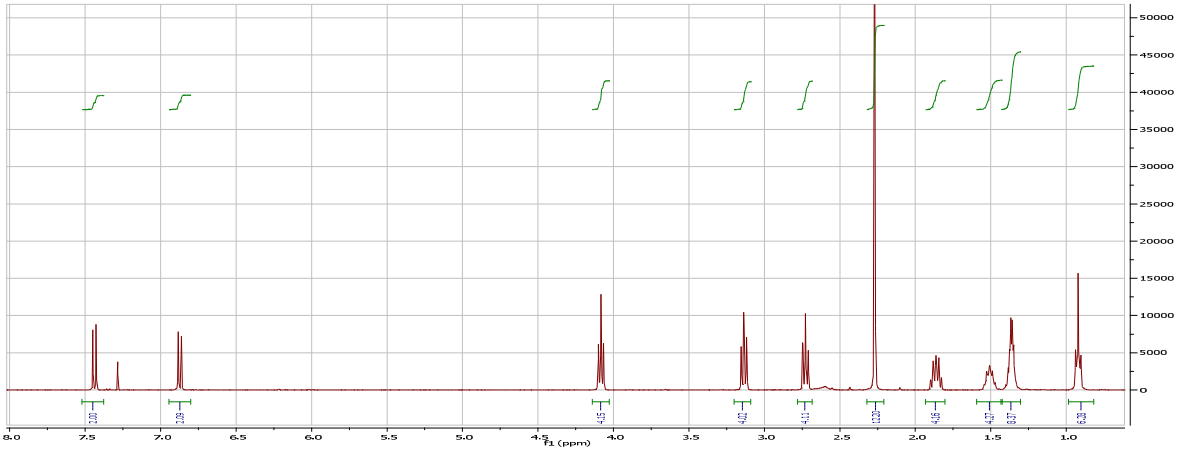


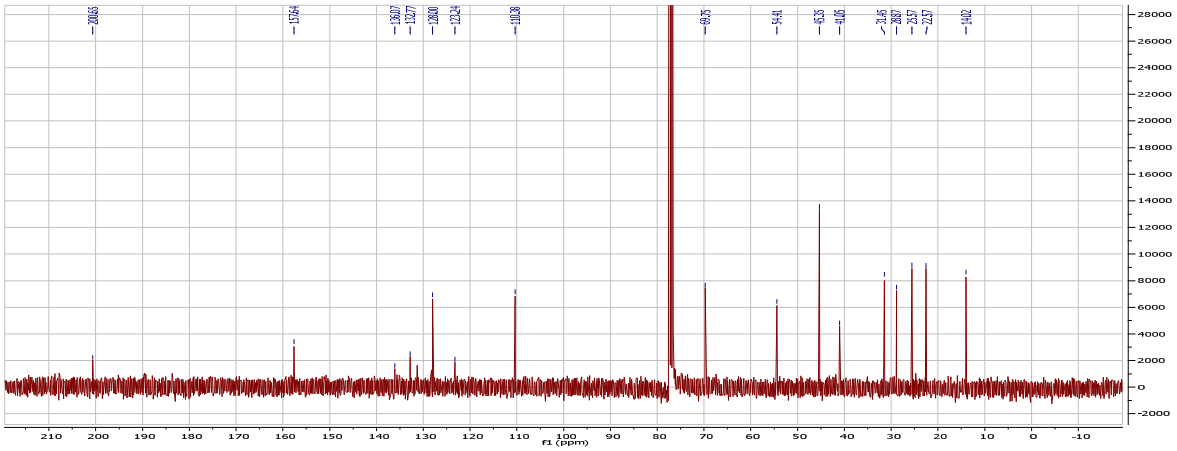


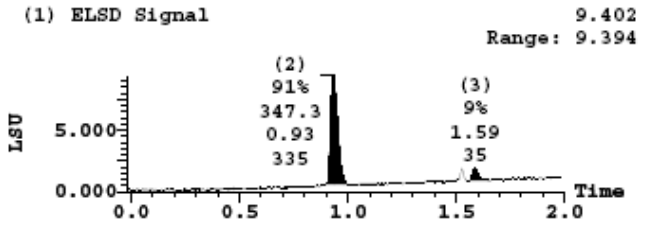

(1) ELSD Signal
17.933
Range: 17.897
(2)
100%
1.05
909
LSU
10.000
0.000
Time
0.0
0.5
1.0
1.5
2.0


Peak ID Compound Time Mass Found
3 Found 1.12 334.51
3:(Time: 1.12)
1:MS ES+
1.3e+008
100
0
%
334.3
346.3
m/z
500.0
1000.0

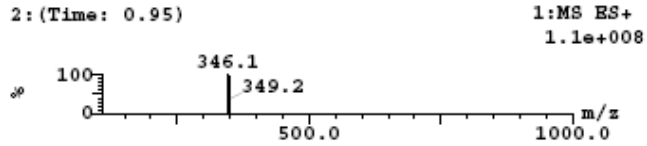
12{*24*}

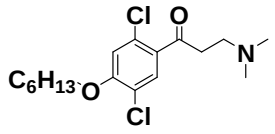




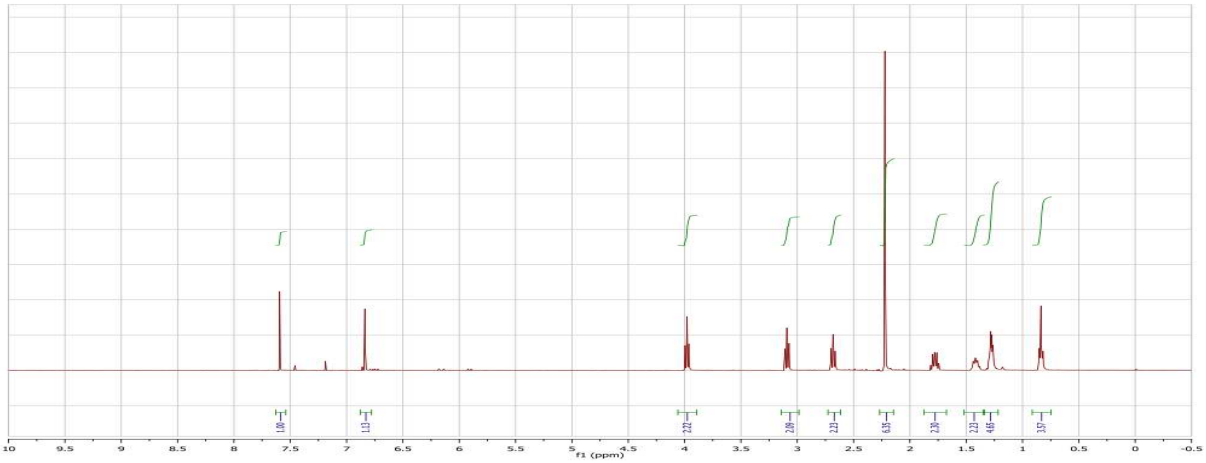


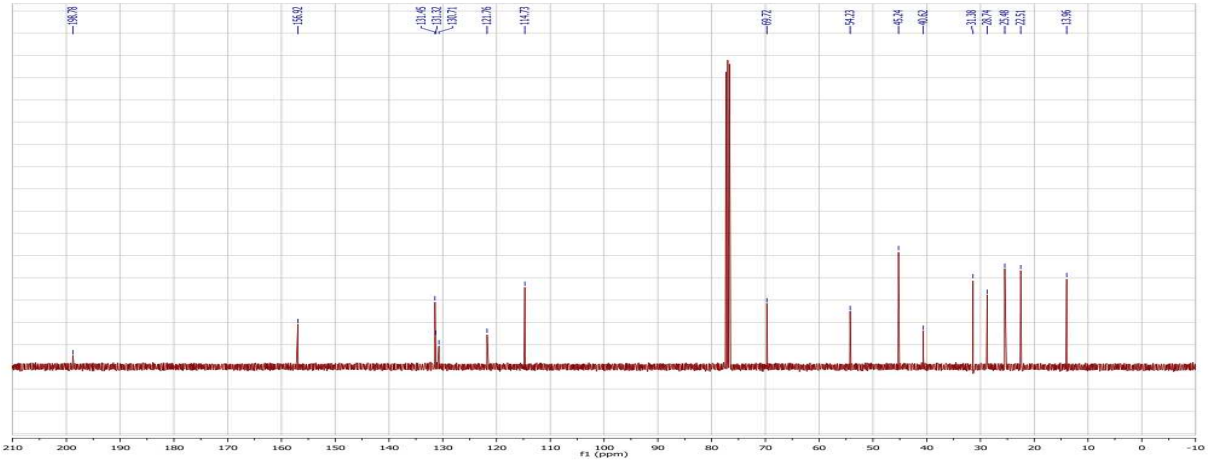
Peak ID	Compound	Time	Mass Found
2	Found	0.95	347.29

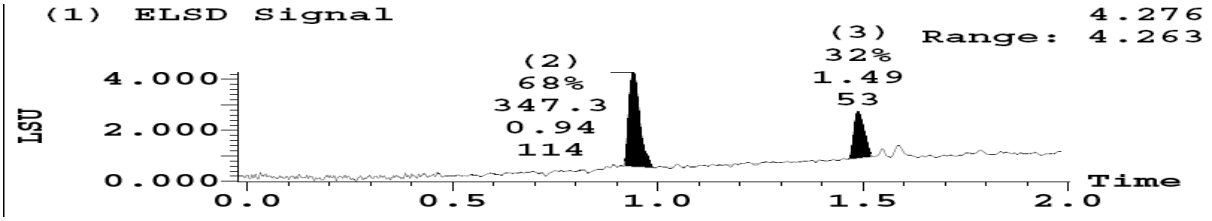


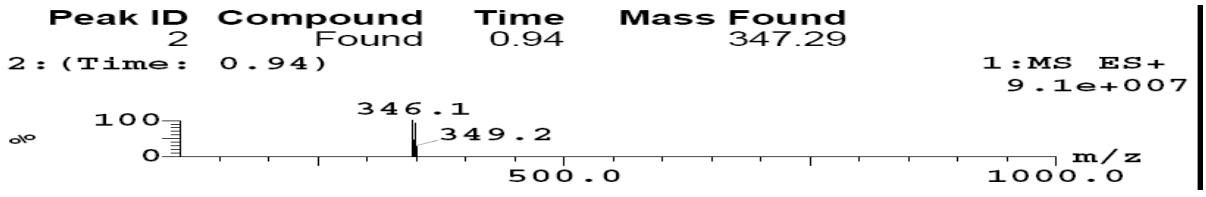

Cl
O
N
C6H13O
Cl

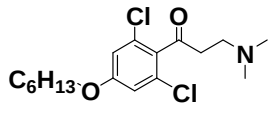
12{*25*}



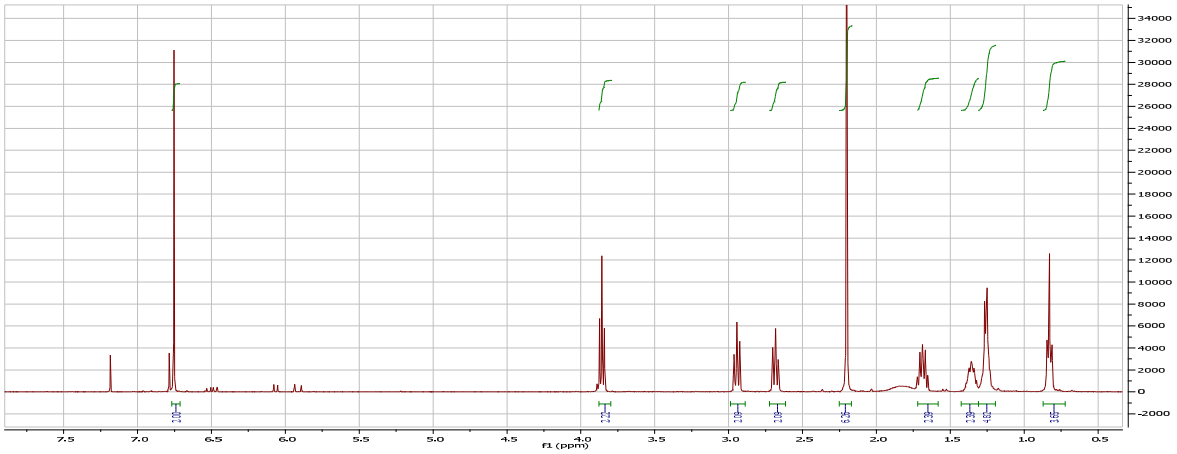


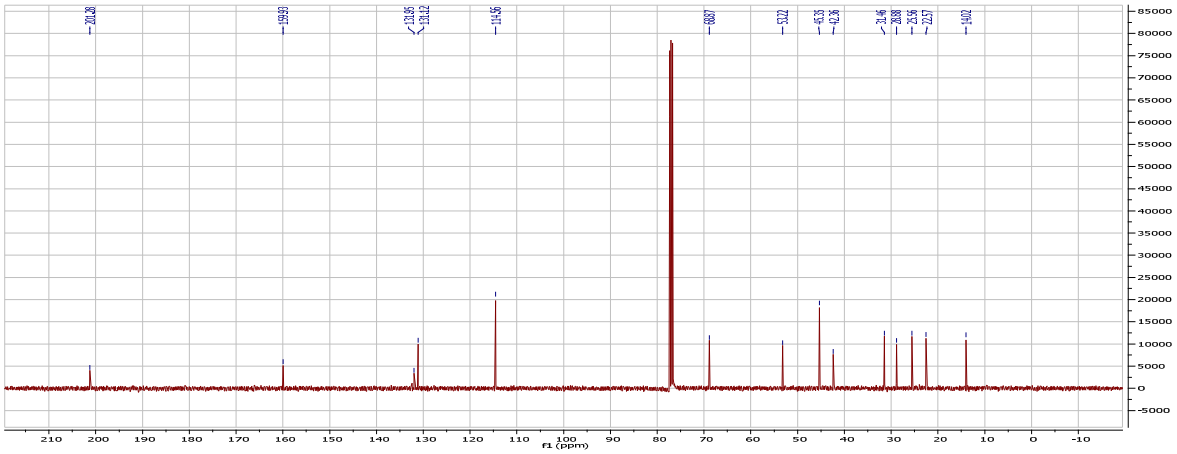

(1) ELSD Signal
4.276
Range: 4.263
(2)
68%
347.3
0.94
114
(3)
32%
1.49
53
LSU
4.000
2.000
0.000
0.0
0.5
1.0
1.5
2.0
Time

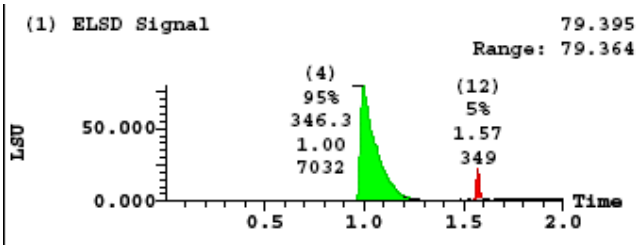

Peak ID Compound Time Mass Found
2 Found 0.94 347.29
2:(Time: 0.94)
1:MS ES+
9.1e+007
346.1
349.2
100
%
0
500.0
1000.0
m/z



12{*26*}

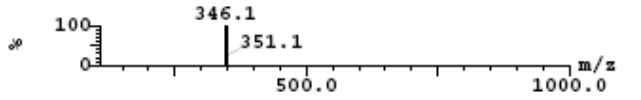


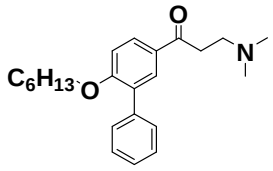




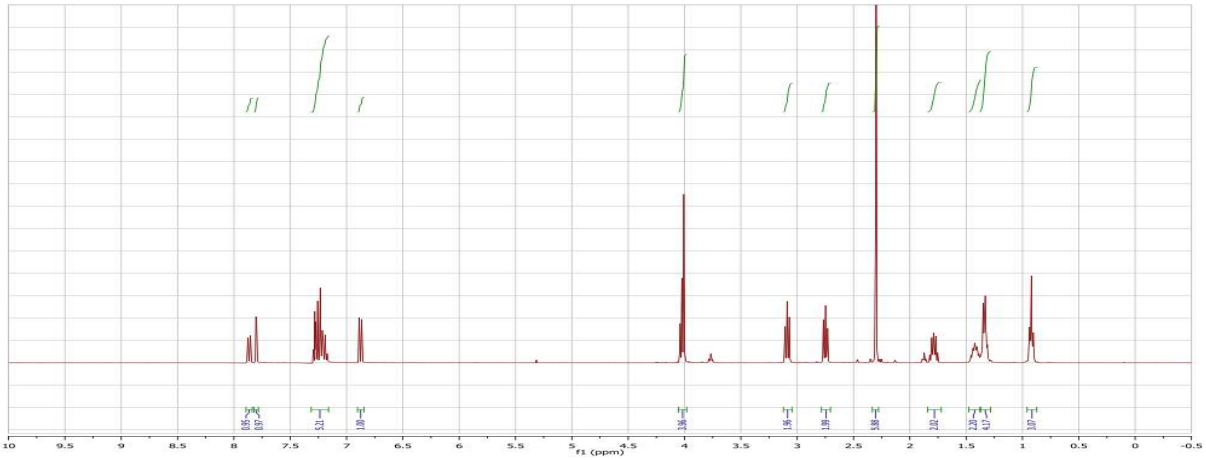
Peak ID	Compound	Time	Mass Found
4	Found	0.97	346.30

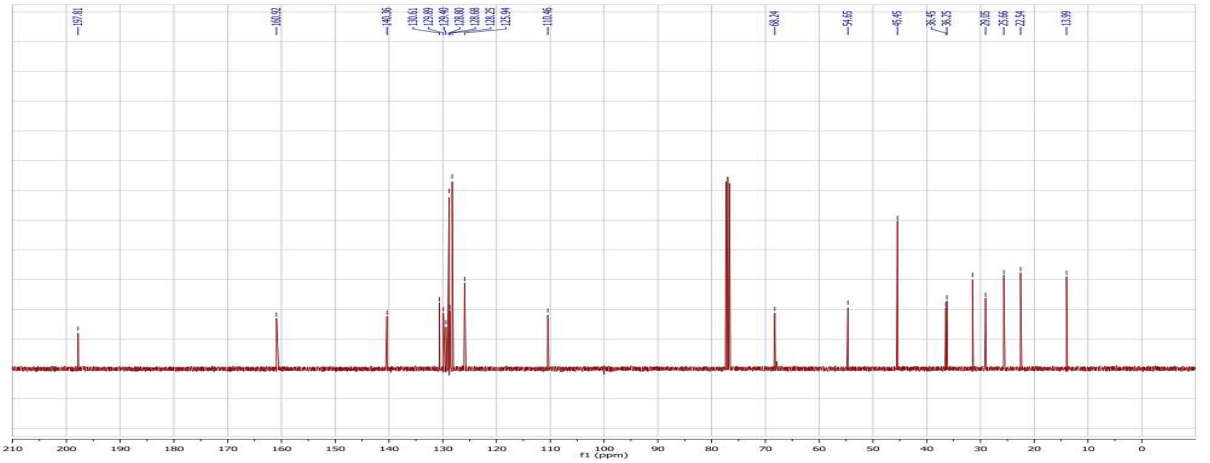
4:(Time: 0.97) 1:MS ES+ 3.5e+007

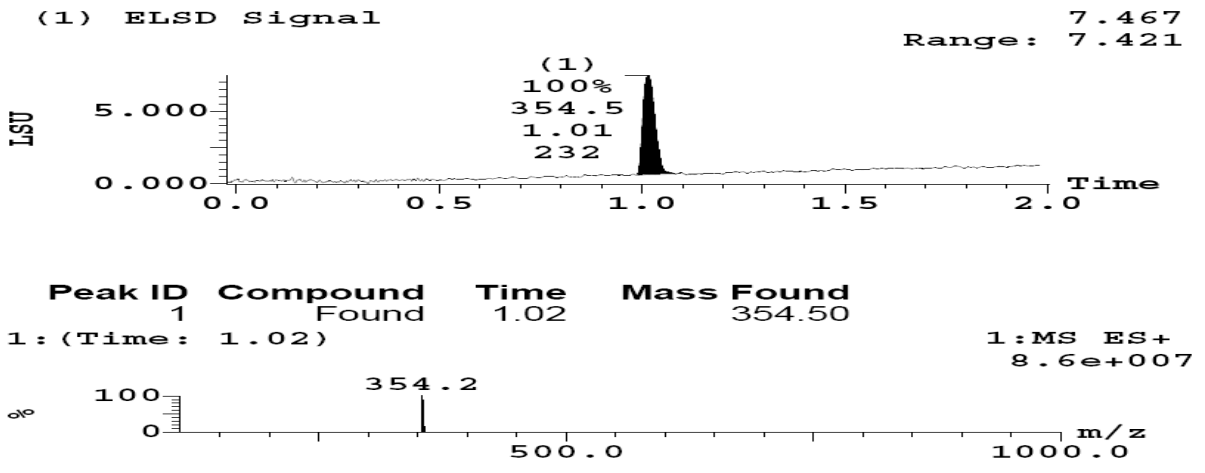




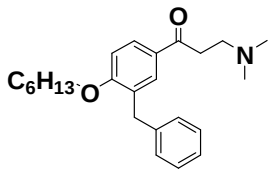
12{*27*}



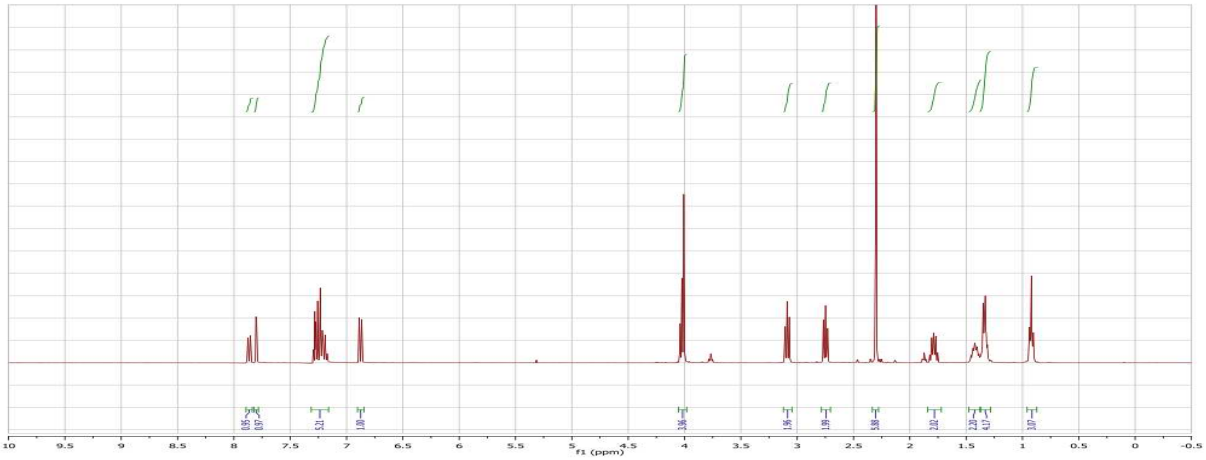


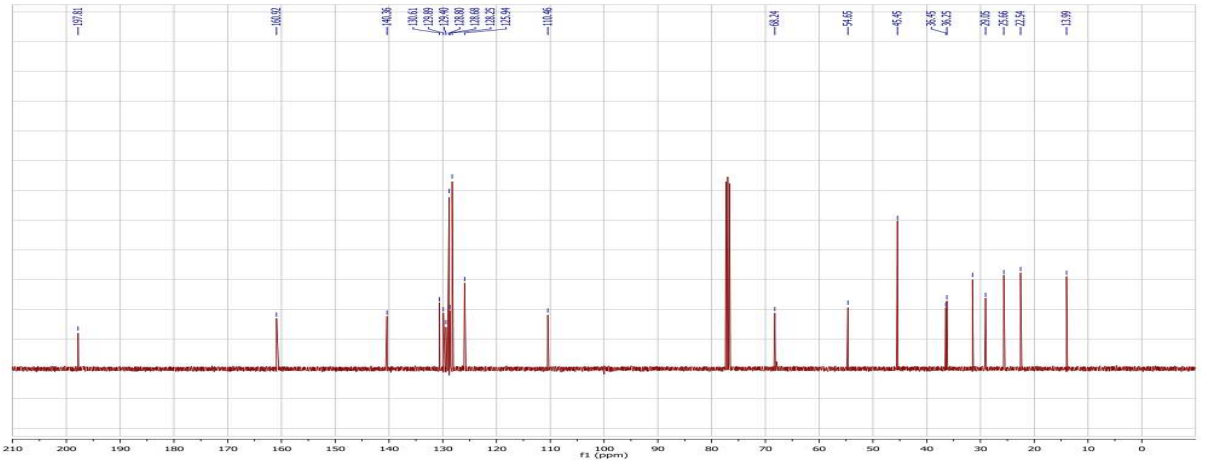


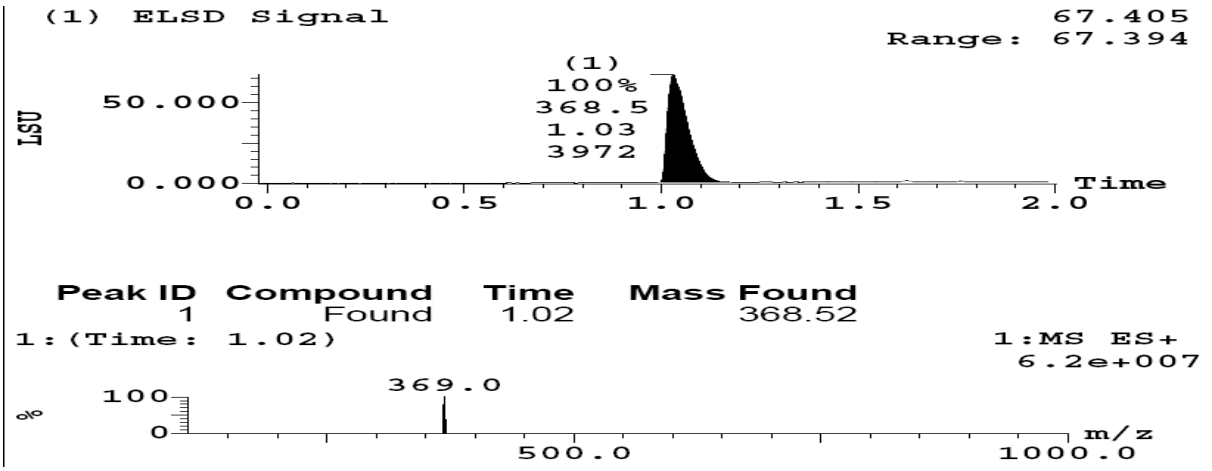
Peak ID	Compound	Time	Mass Found
1	Found	1.02	354.50

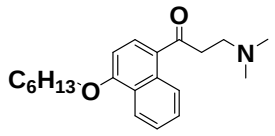


12{*28*}

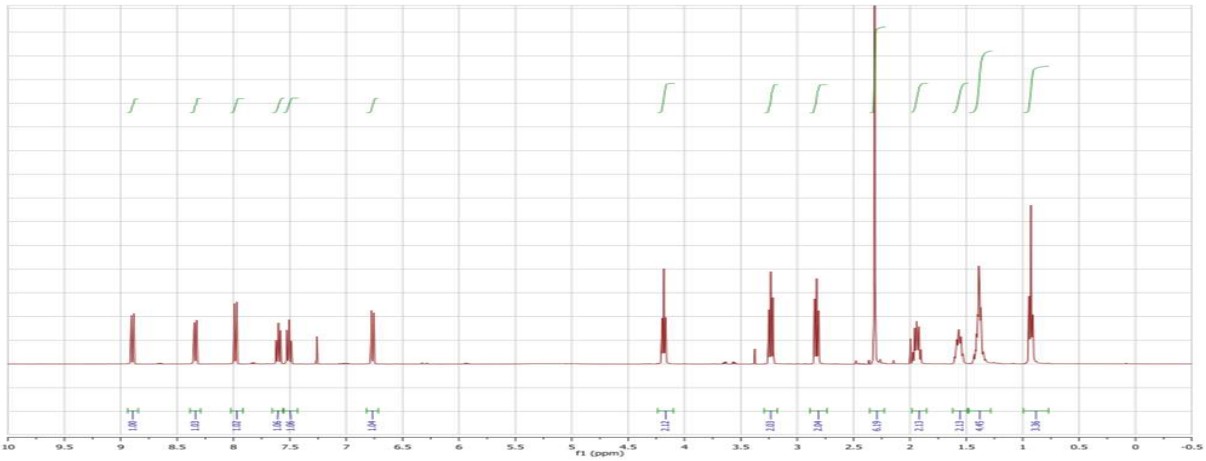


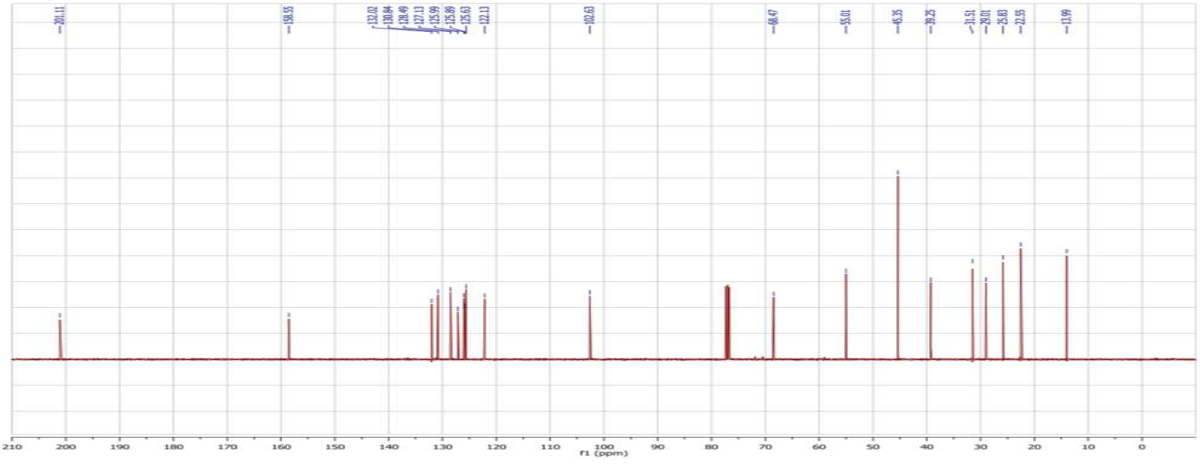


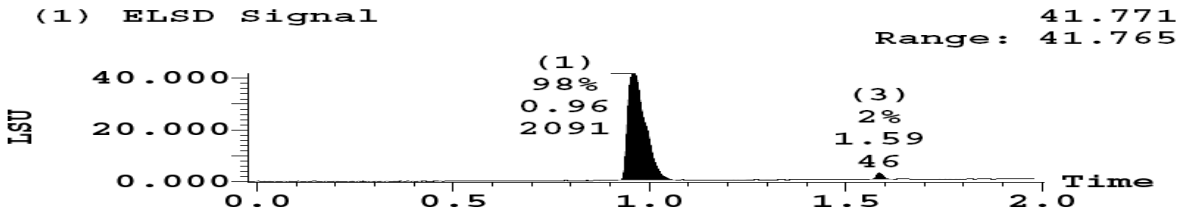

(1) ELSD Signal
67.405
Range: 67.394
(1)
100%
368.5
1.03
3972
50.000
0.000
LSU
0.0
0.5
1.0
1.5
2.0
Time
Peak ID Compound Time Mass Found
1 Found 1.02 368.52
1:(Time: 1.02)
1:MS ES+
6.2e+007
369.0
100
0
%
500.0
1000.0
m/z



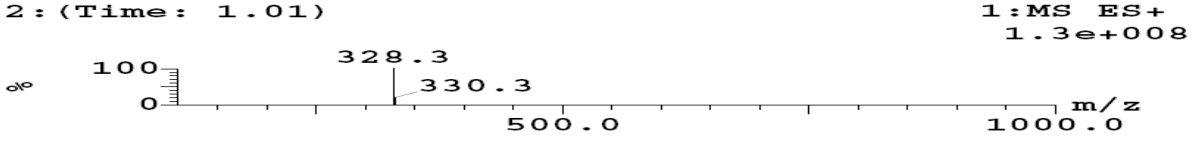
13{*1*}

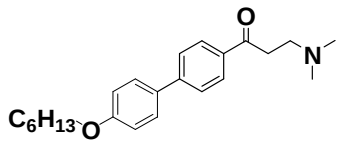




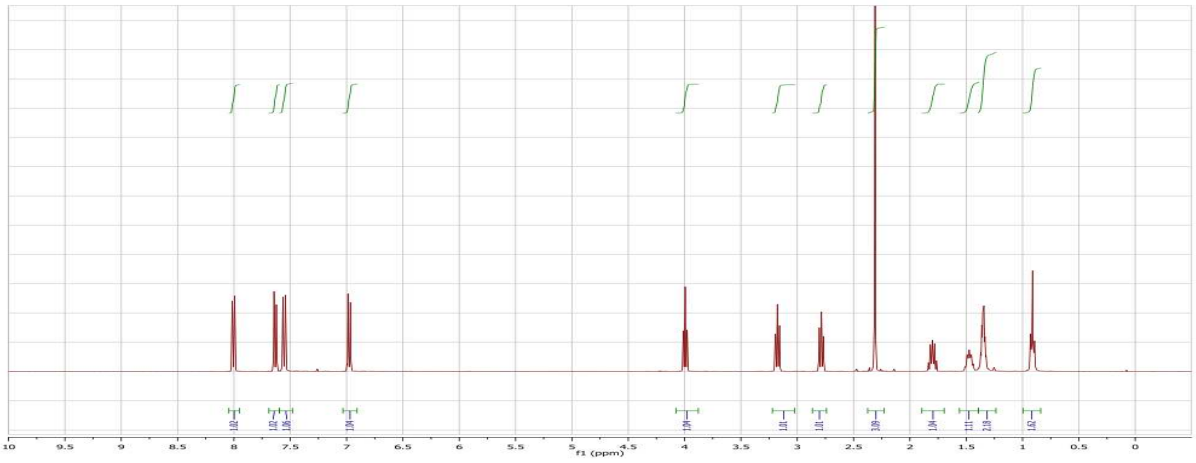


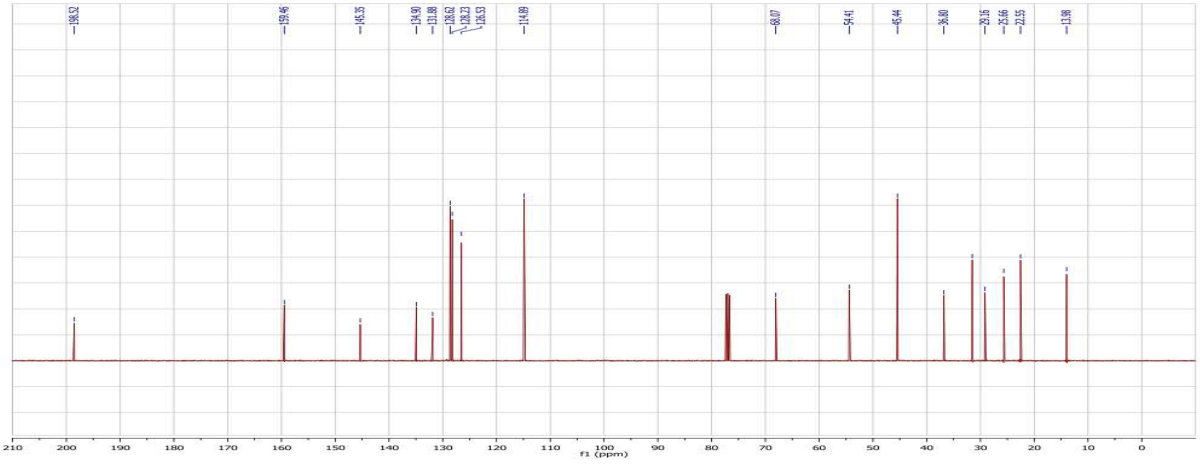
Peak ID	Compound	Time	Mass Found
2	Found	1.01	328.46

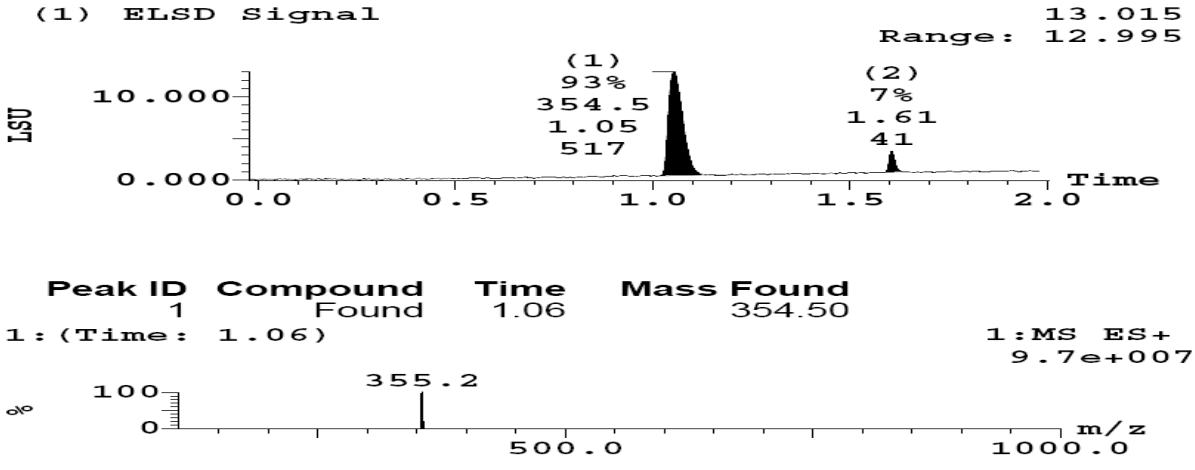




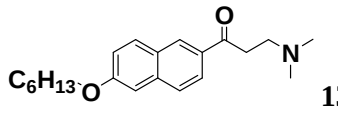
13{*2*}



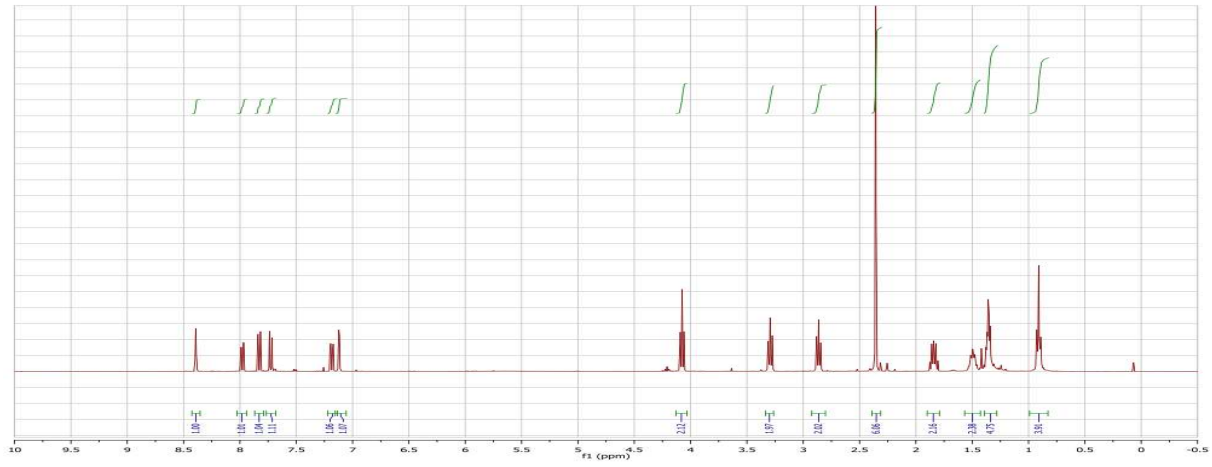


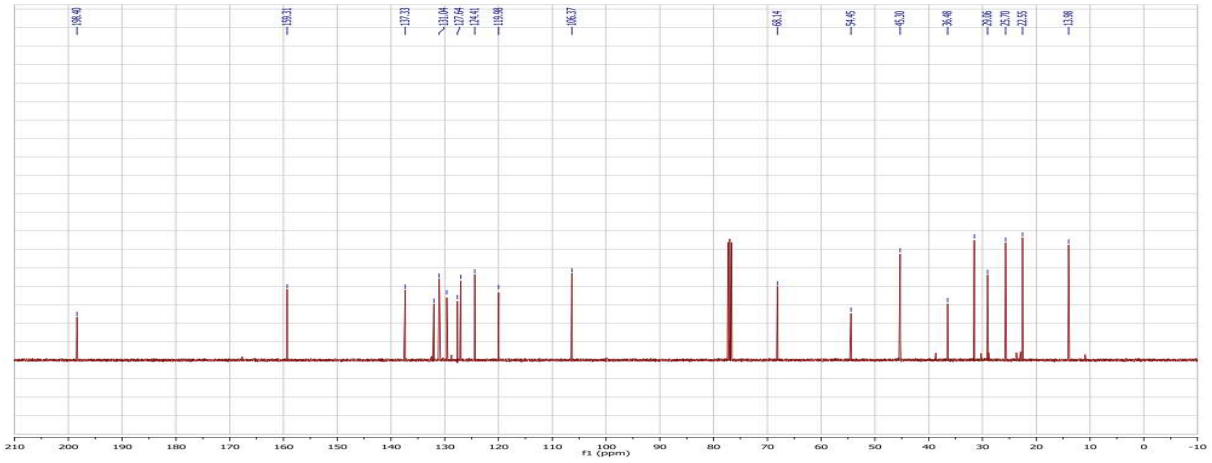


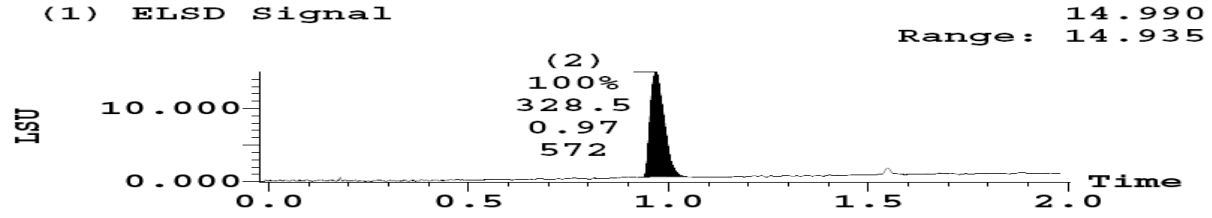
Peak ID	Compound	Time	Mass Found
1	Found	1.06	354.50

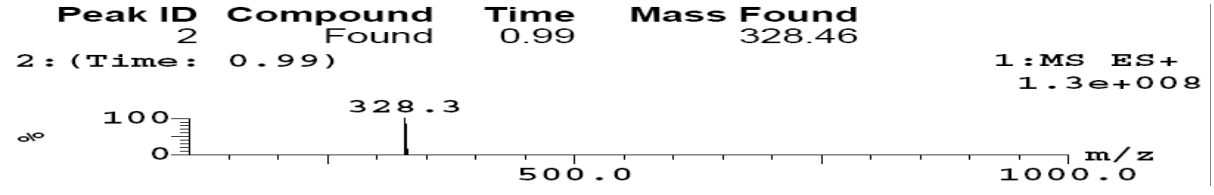

O
N
C6H13O

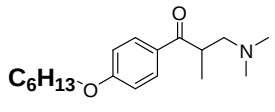
13{*3*}



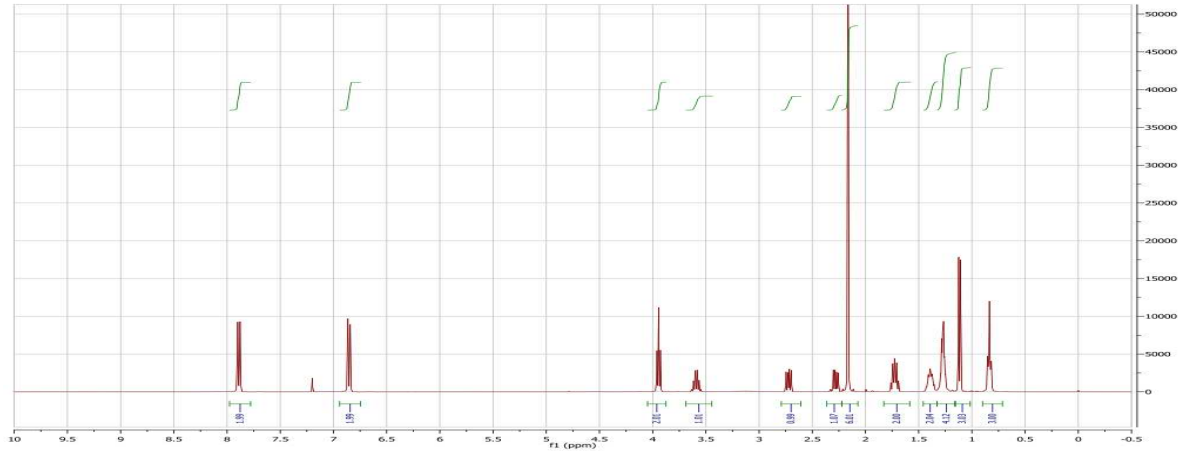


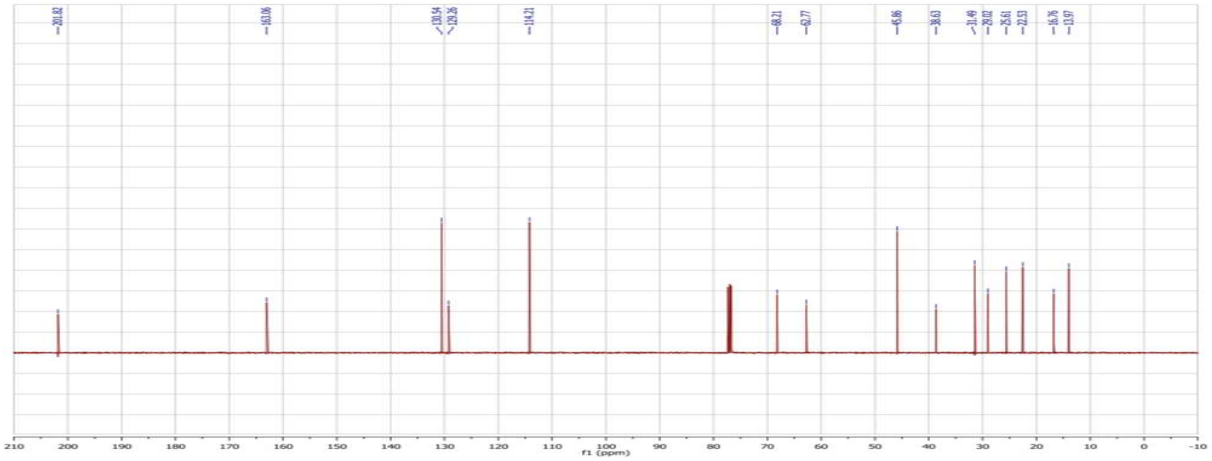

(1) ELSD Signal
14.990
Range: 14.935
(2)
100%
328.5
0.97
572
10.000
0.000
LSU
0.0
0.5
1.0
1.5
2.0
Time

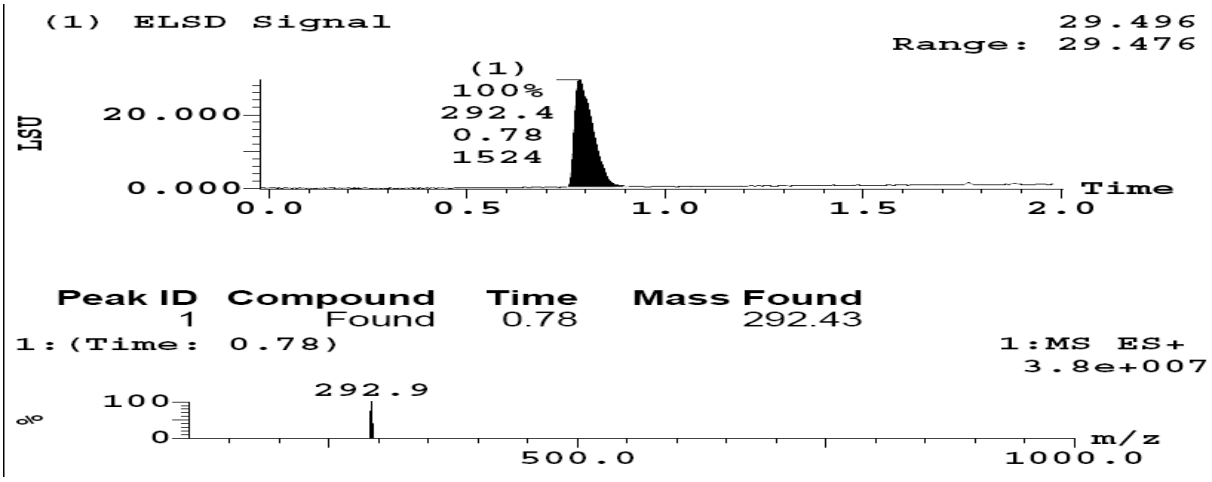

Peak ID Compound Time Mass Found
2 Found 0.99 328.46
2:(Time: 0.99)
1:MS ES+
1.3e+008
328.3
100
%
0
500.0
1000.0
m/z

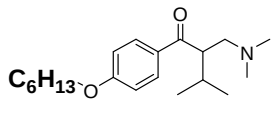


14{*1*}

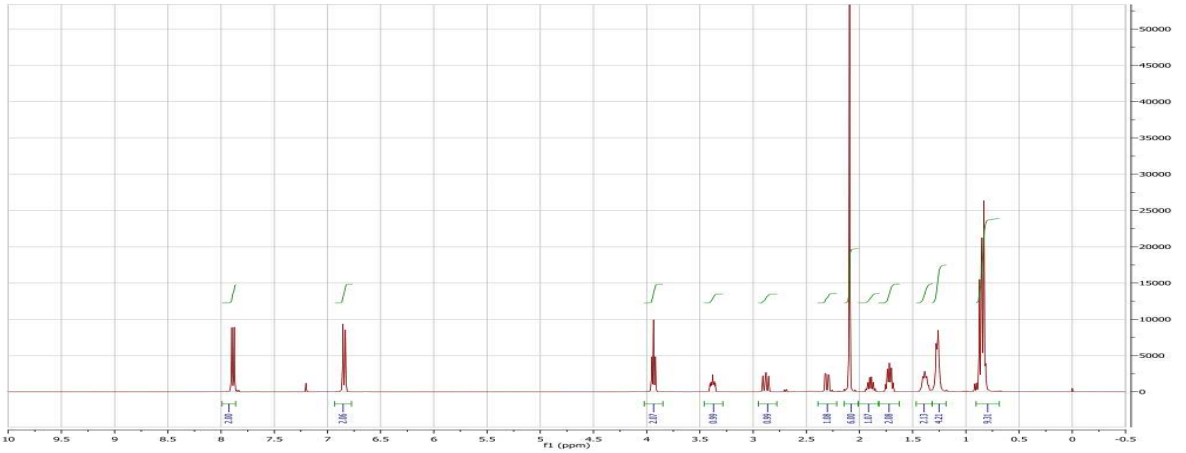


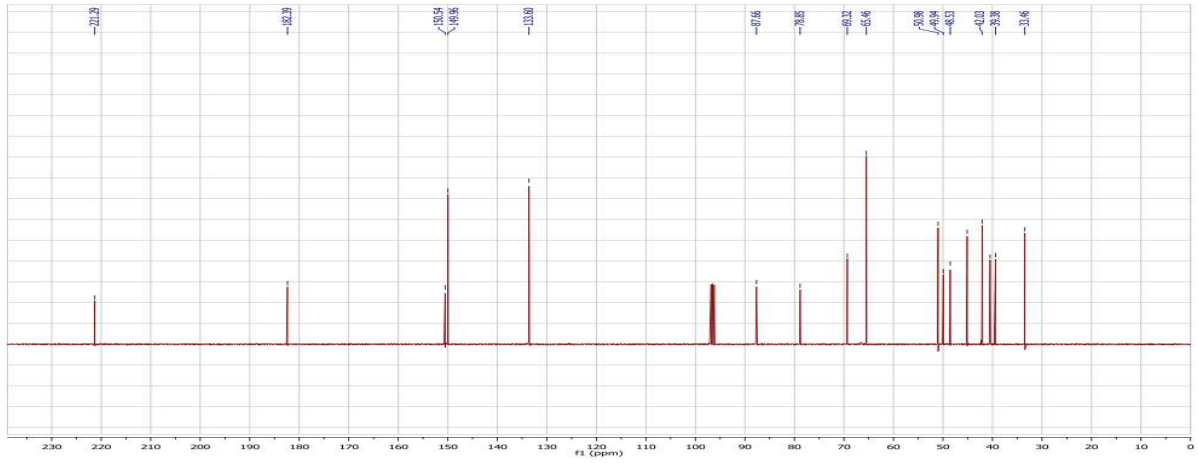


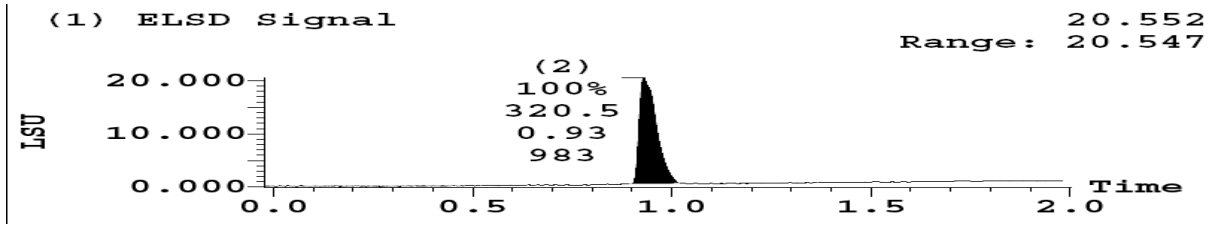

(1) ELSD Signal
29.496
Range: 29.476
(1)
100%
292.4
0.78
1524
20.000
0.000
LSU
Time
0.0
0.5
1.0
1.5
2.0
Peak ID
Compound
Time
Mass Found
1
Found
0.78
292.43
1:(Time: 0.78)
1:MS ES+
3.8e+007
292.9
100
0
%
500.0
1000.0
m/z



14{*2*}



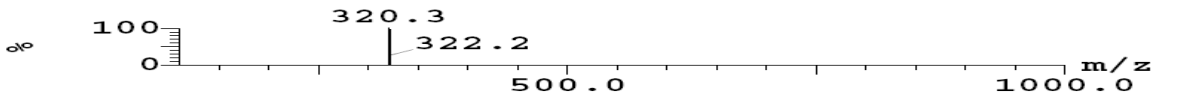


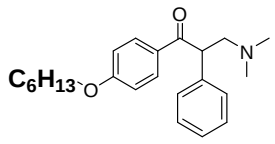


Peak ID	Compound	Time	Mass Found
2	Found	0.93	320.48

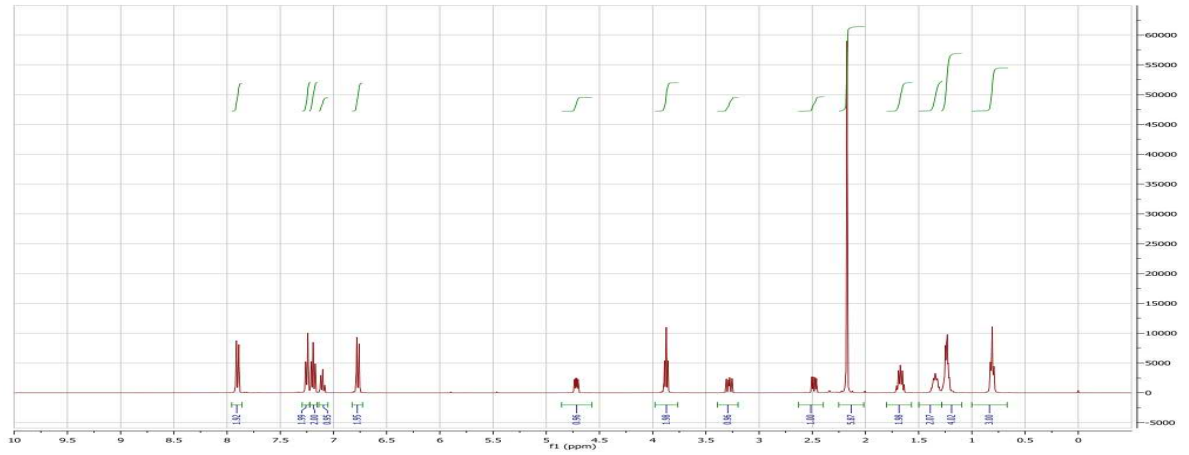
2:(Time: 0.93)

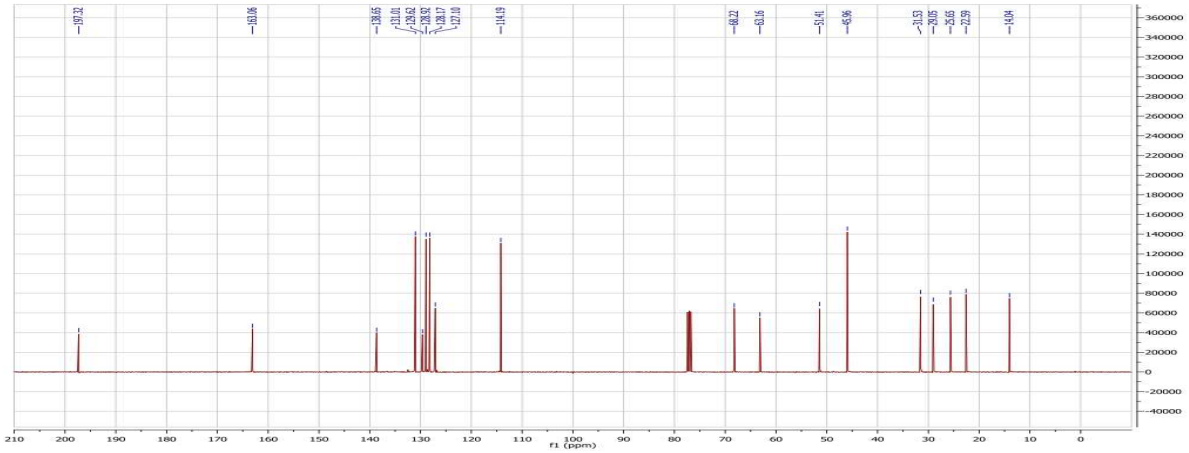
1:MS ES+
9.1e+007

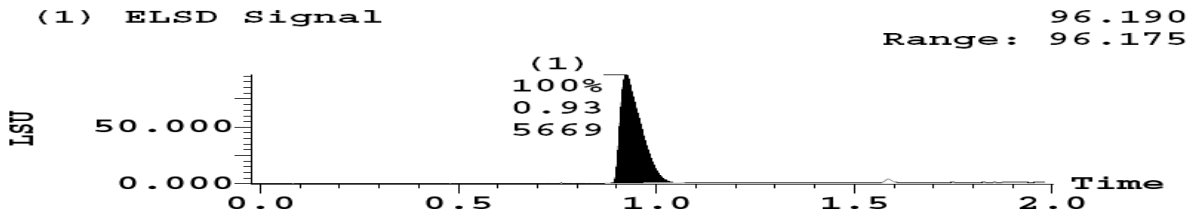


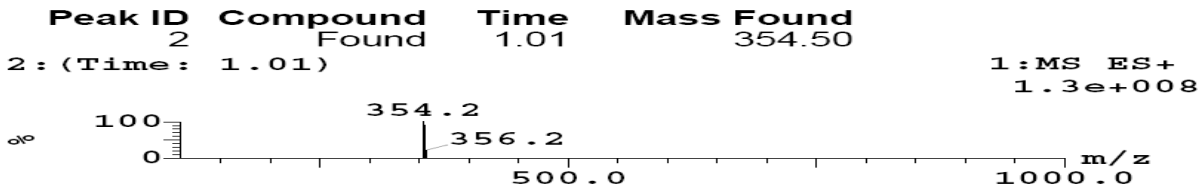


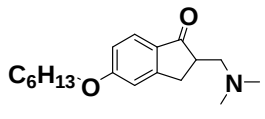
14{*3*}



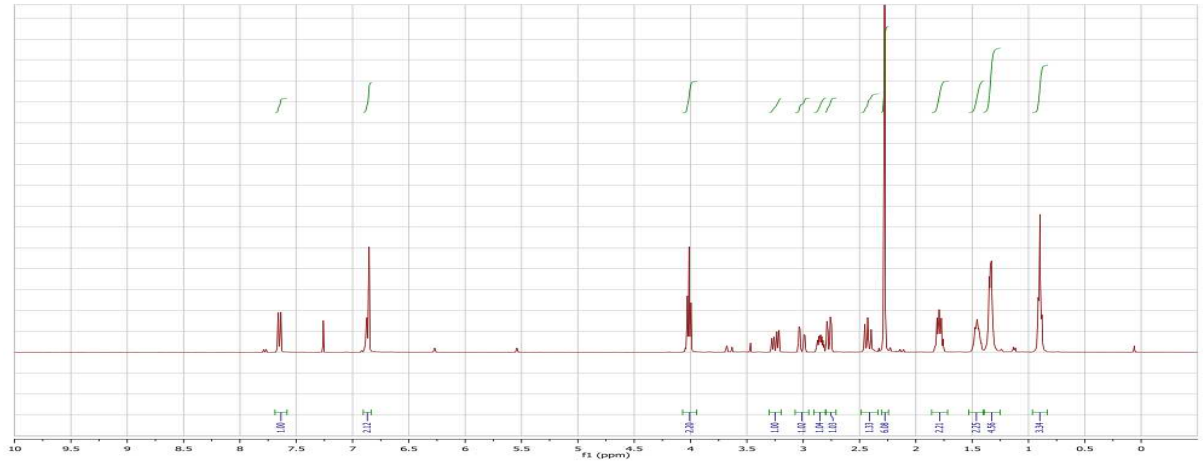


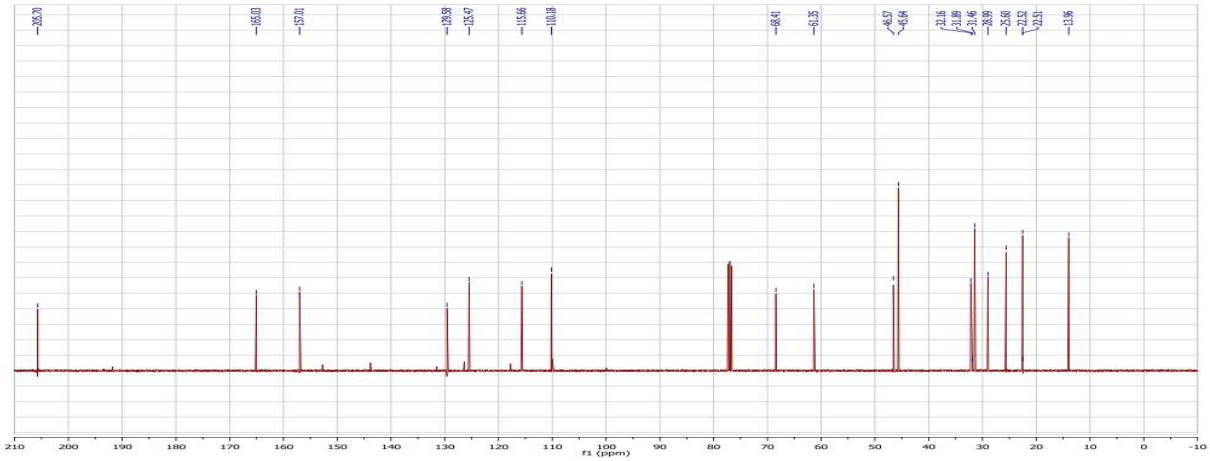

(1) ELSD Signal
96.190
Range: 96.175
(1)
100%
0.93
5669
LSU
50.000
0.000
0.0
0.5
1.0
1.5
2.0
Time

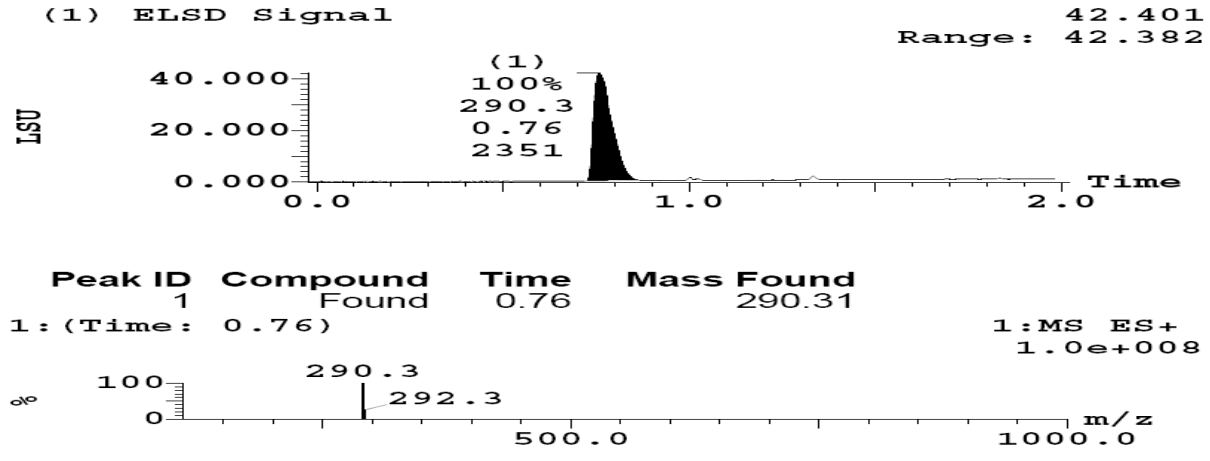

Peak ID Compound Time Mass Found
2 Found 1.01 354.50
2:(Time: 1.01)
1:MS ES+
1.3e+008
100
%
0
354.2
356.2
500.0
1000.0
m/z



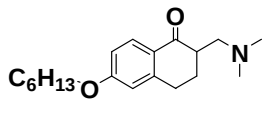
14{*4*}



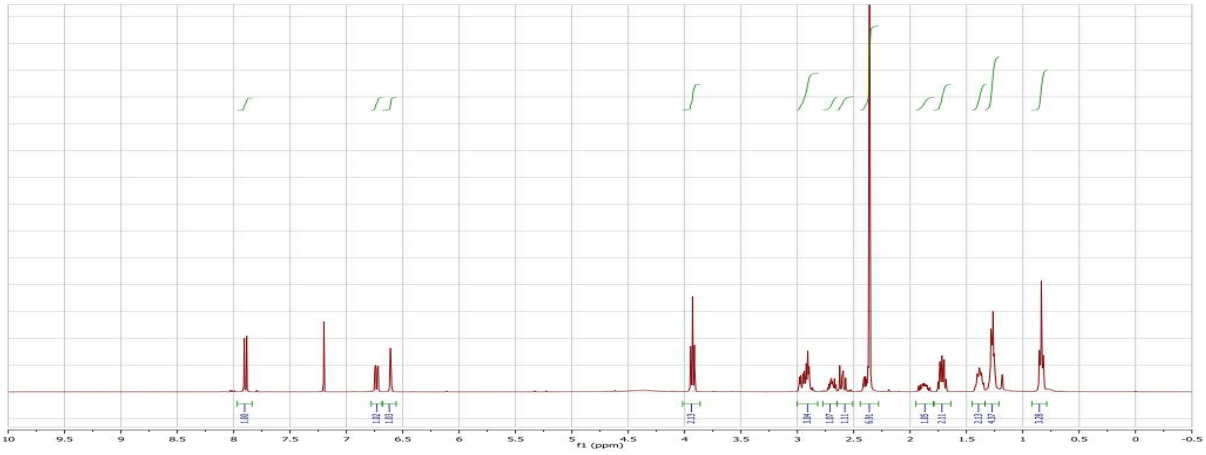


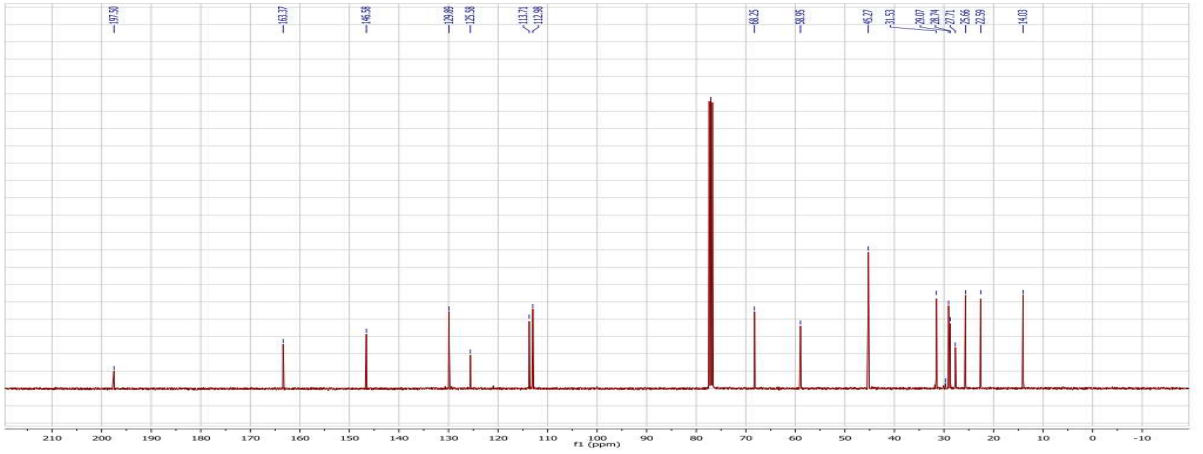


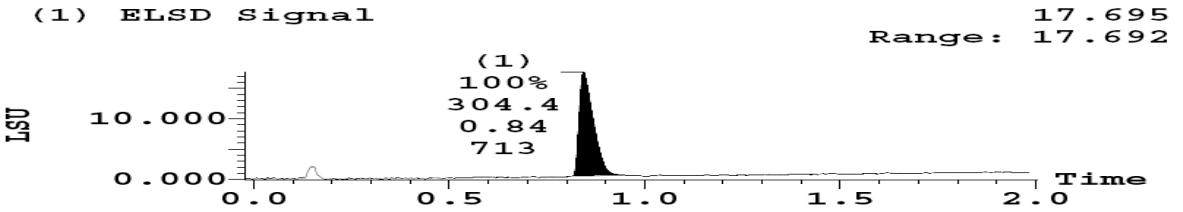
Peak ID	Compound	Time	Mass Found
1	Found	0.76	290.31

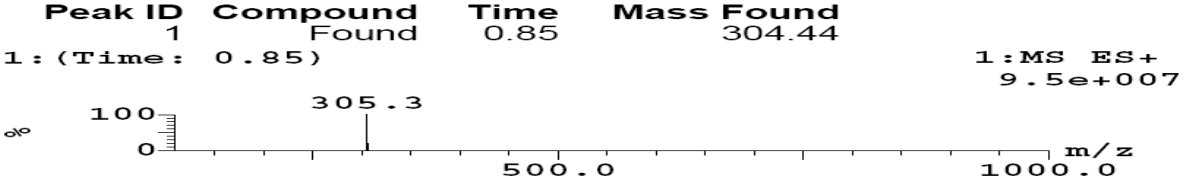

O
N
C6H13O

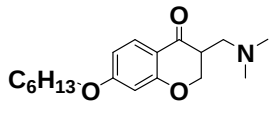
14{*5*}



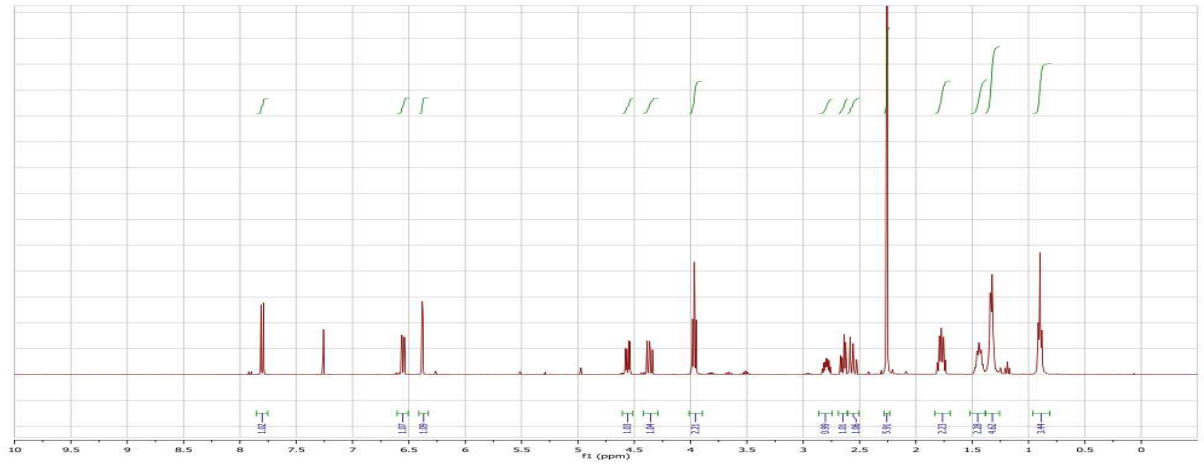


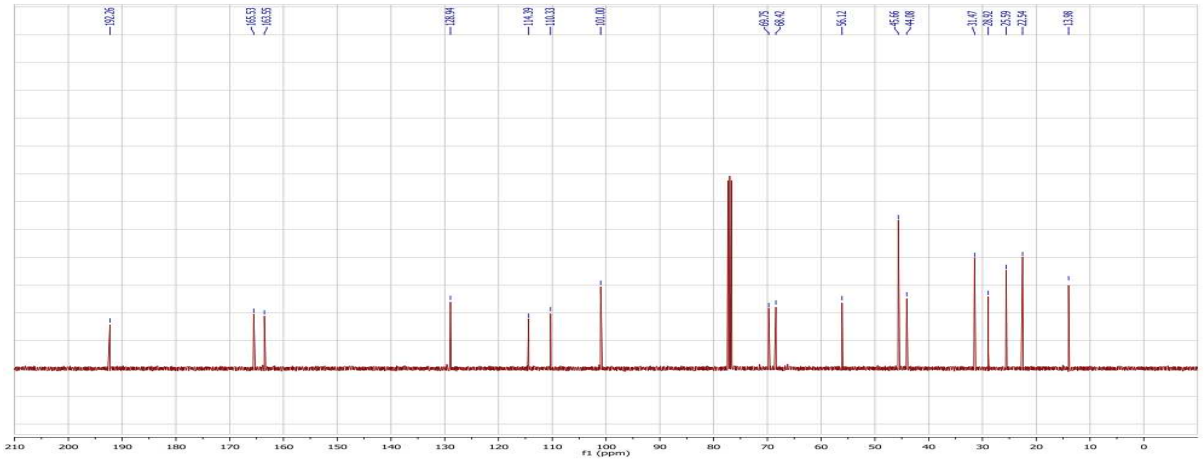

(1) ELSD Signal
17.695
Range: 17.692
(1)
100%
304.4
0.84
713
LSU
10.000
0.000
Time
0.0
0.5
1.0
1.5
2.0

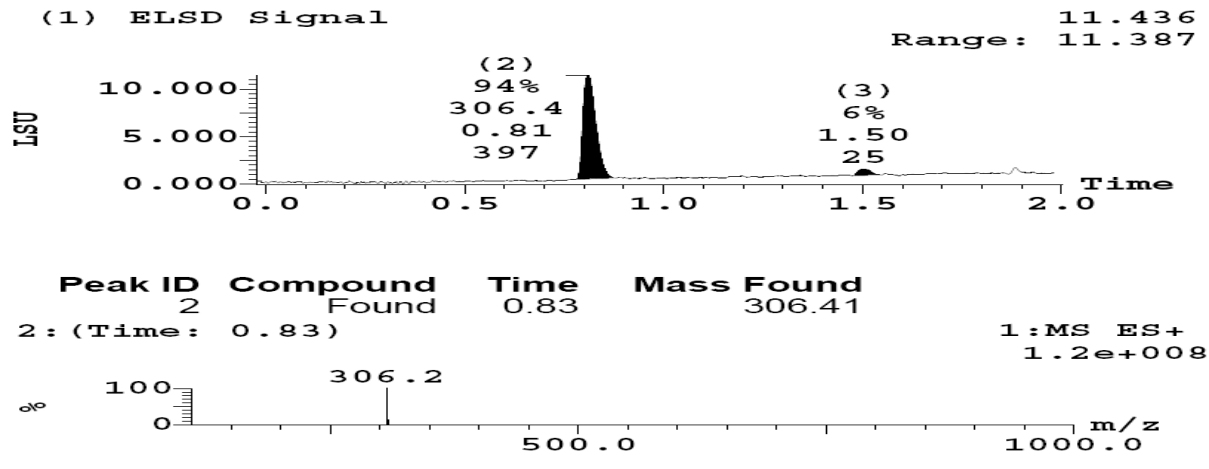

Peak ID Compound Time Mass Found
1 Found 0.85 304.44
1:(Time: 0.85)
1:MS ES+
9.5e+007
305.3
100
%
0
m/z
500.0
1000.0



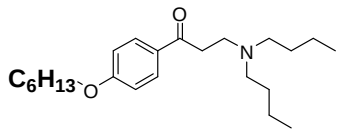
14{*6*}



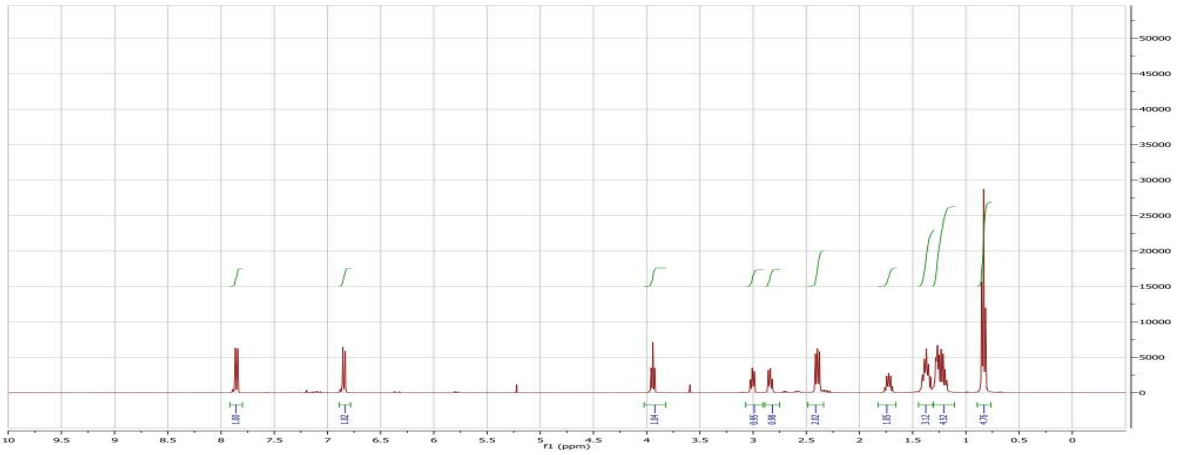


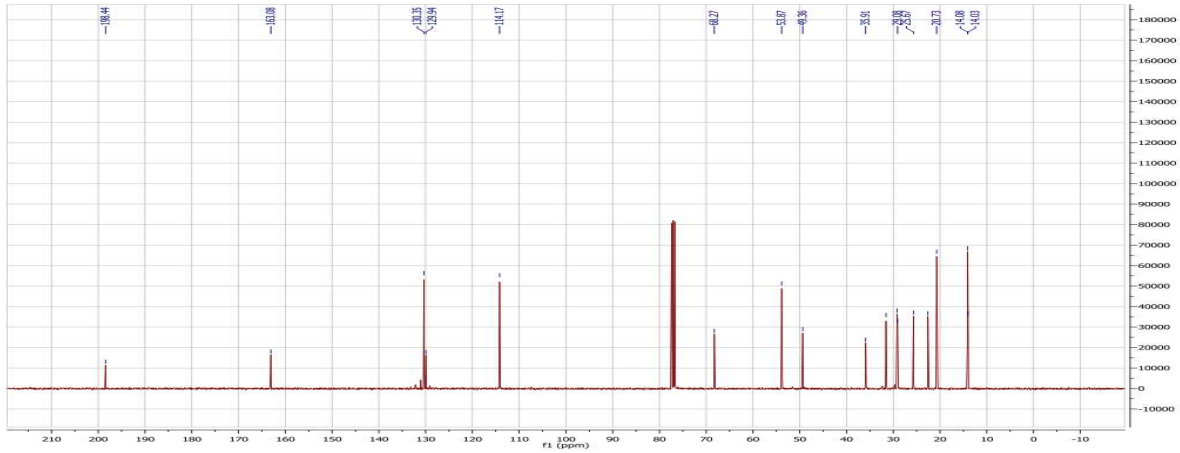


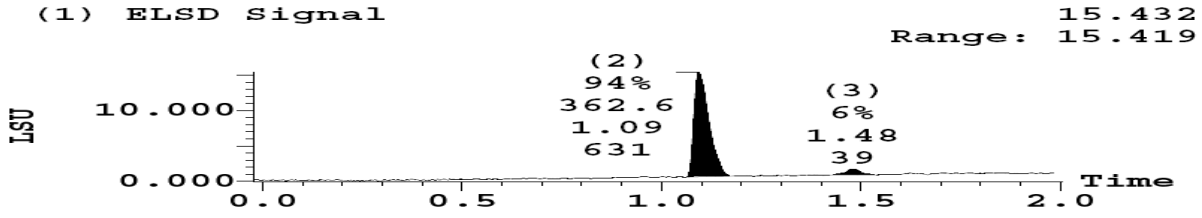
Peak ID	Compound	Time	Mass Found
2	Found	0.83	306.41

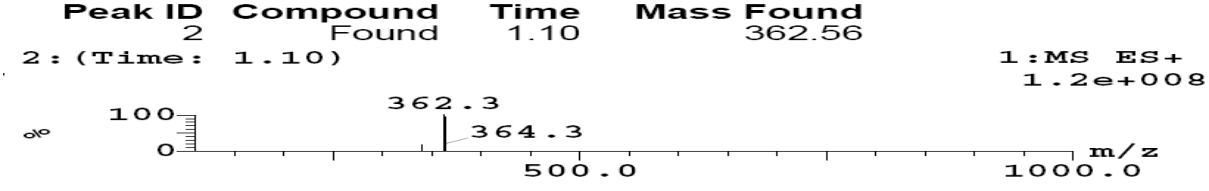

O
N
C6H13O

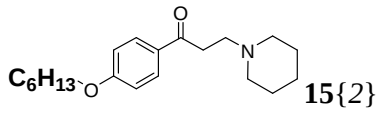
15{*1*}



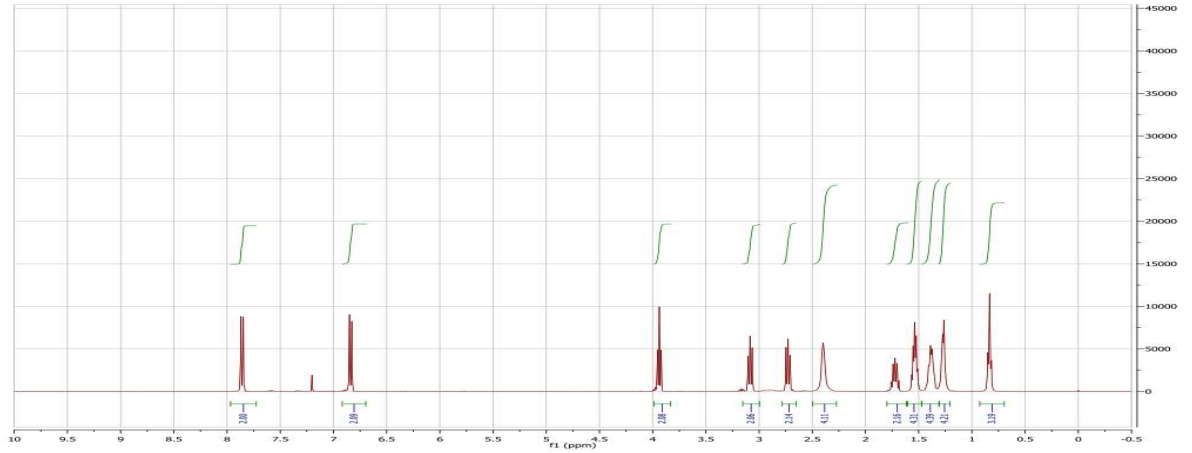


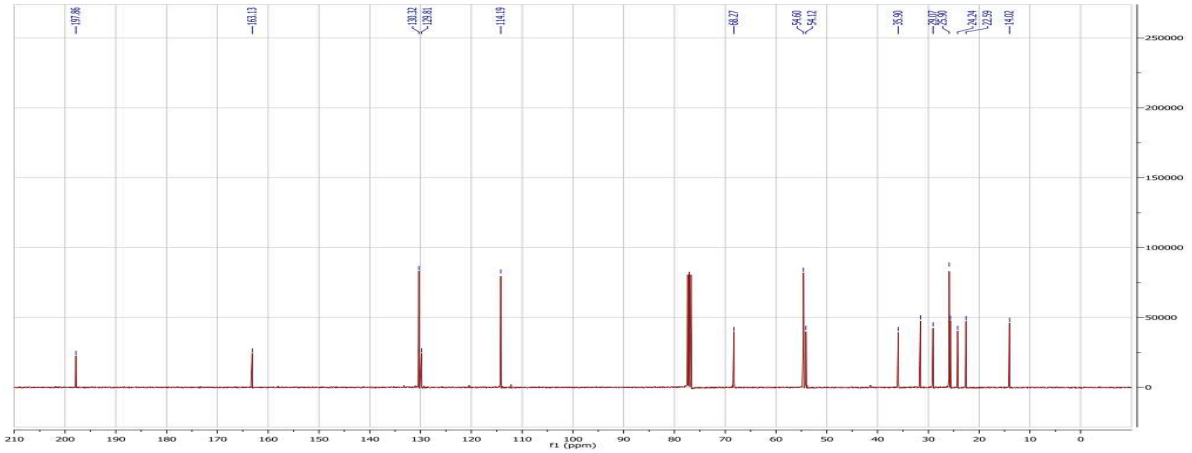

(1) ELSD Signal
15.432
Range: 15.419
(2)
94%
362.6
1.09
631
(3)
6%
1.48
39
LSU
10.000
0.000
Time
0.0
0.5
1.0
1.5
2.0

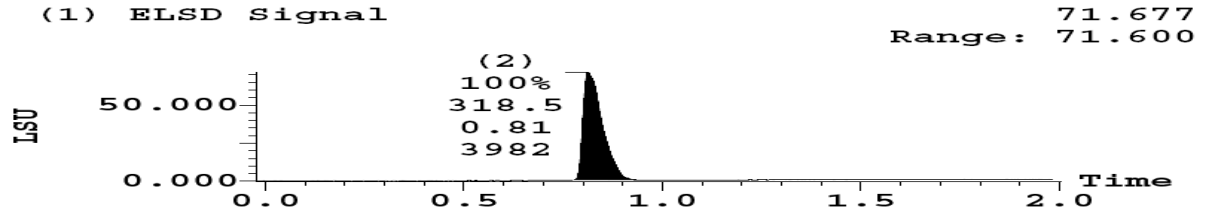

Peak ID Compound Time Mass Found
2 Found 1.10 362.56
2:(Time: 1.10)
1:MS ES+
1.2e+008
362.3
364.3
100
%
0
500.0
m/z
1000.0

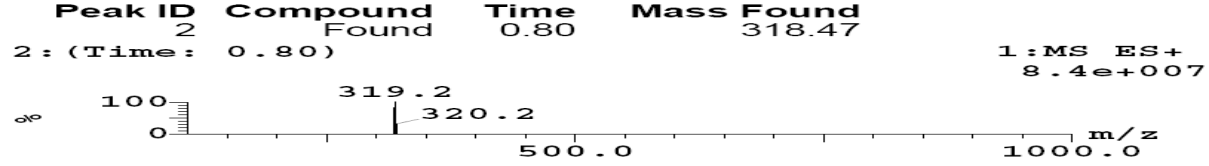


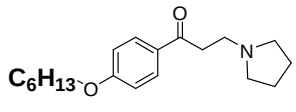
15{*2*}






(1) ELSD Signal
71.677
Range: 71.600
(2)
100%
318.5
0.81
3982
LSU
50.000
0.000
Time
0.0
0.5
1.0
1.5
2.0


Peak ID Compound Time Mass Found
2 Found 0.80 318.47
2:(Time: 0.80)
1:MS ES+
8.4e+007
%
100
0
319.2
320.2
500.0
m/z
1000.0



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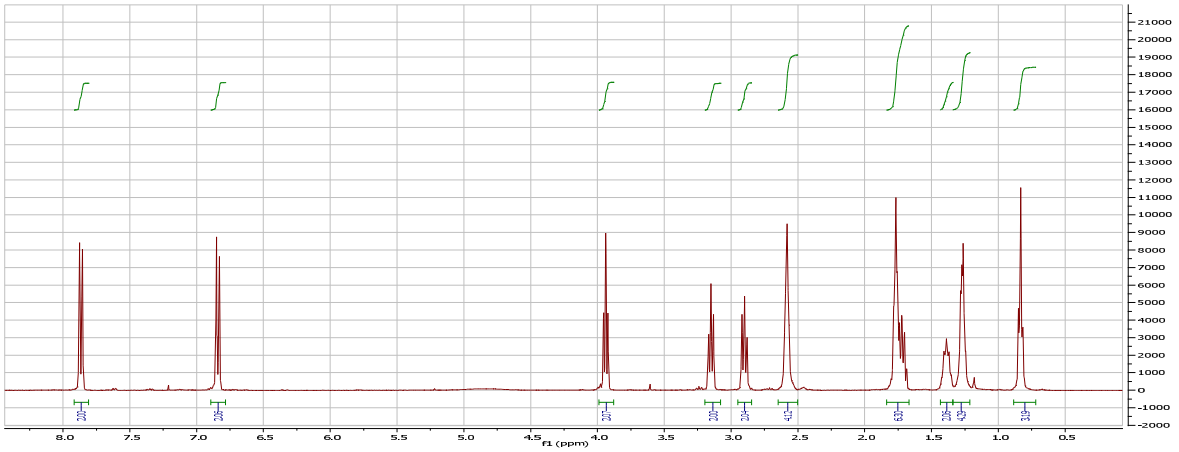
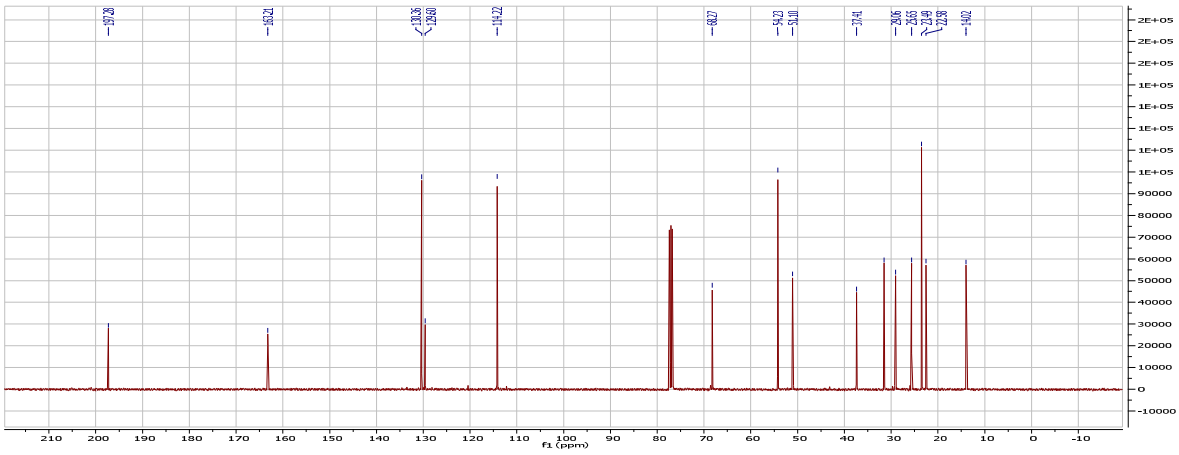
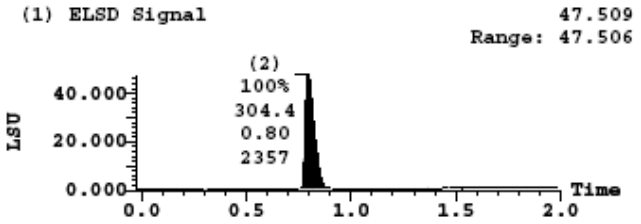
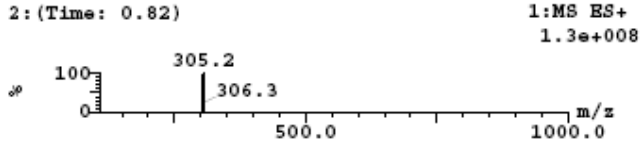
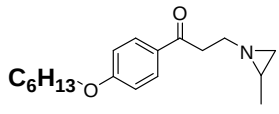






Peak ID	Compound	Time	Mass Found
2	Found	0.82	304.44





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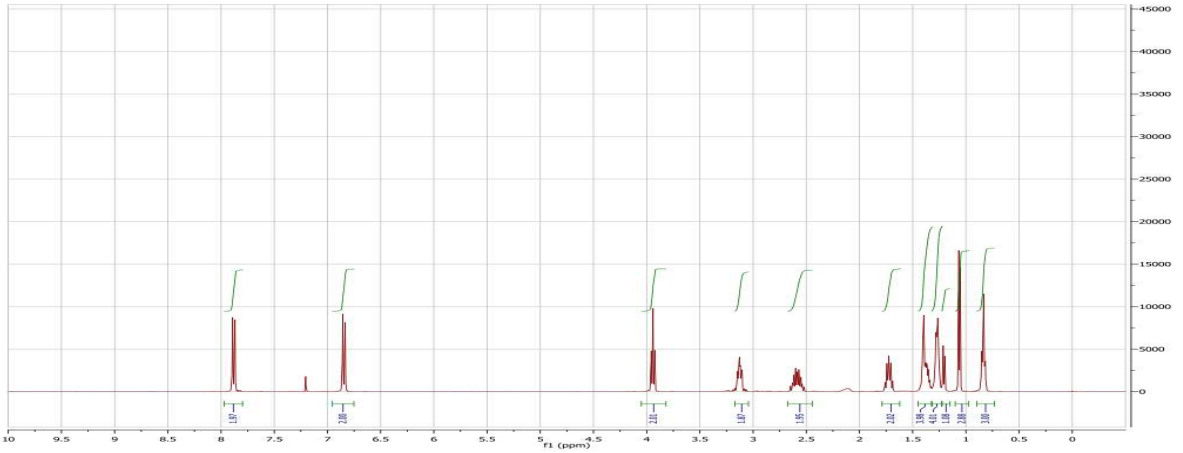
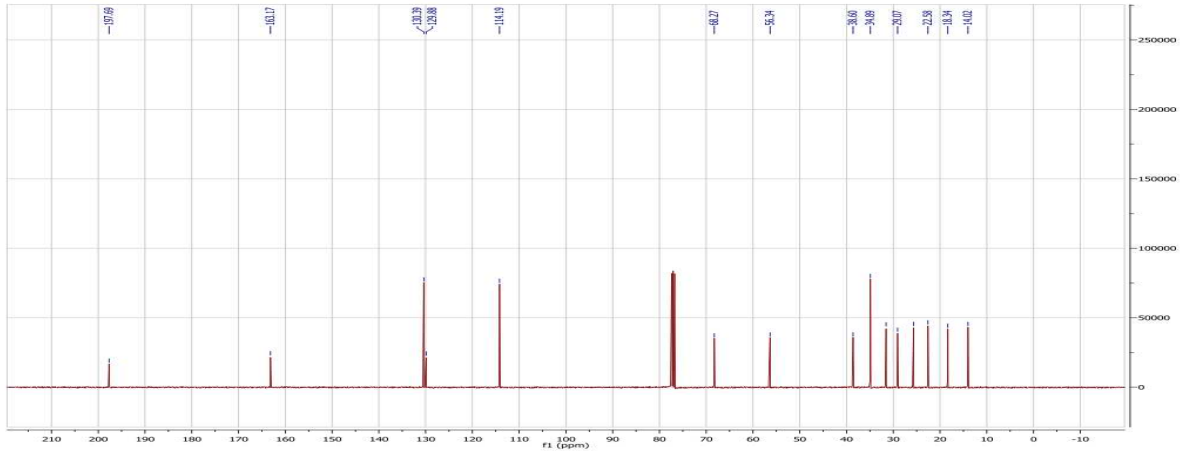
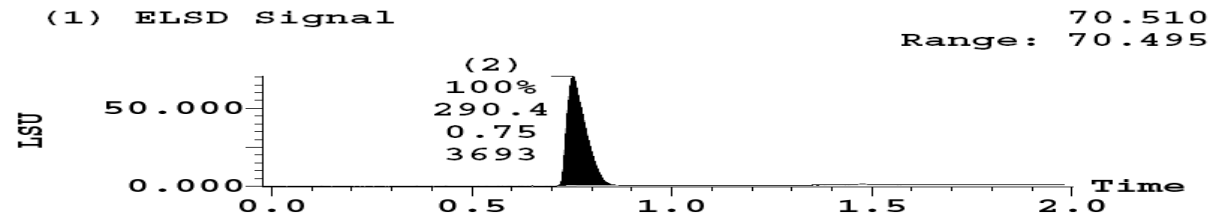
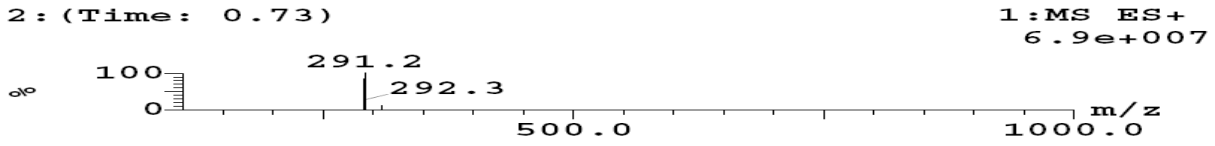
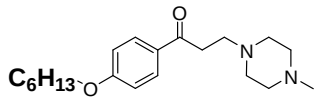




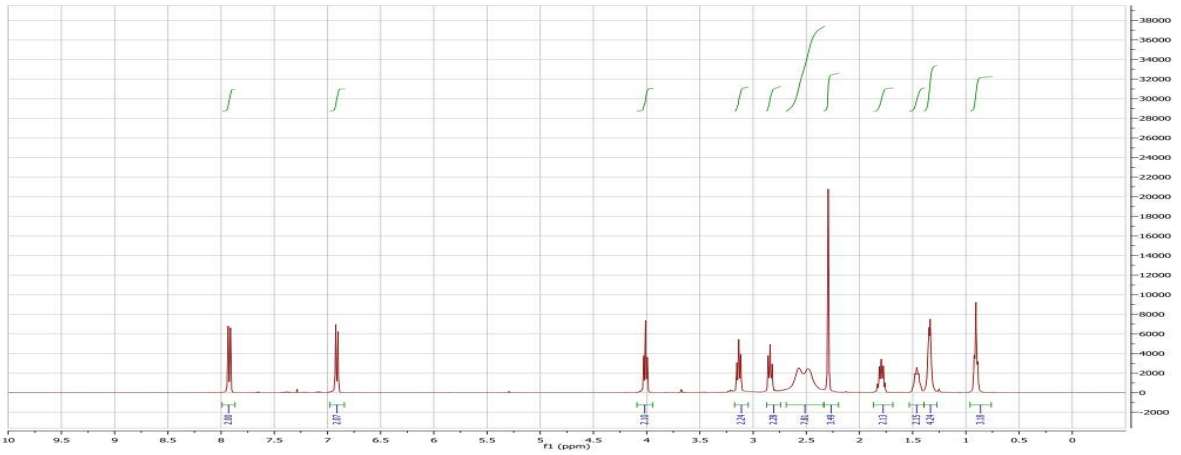


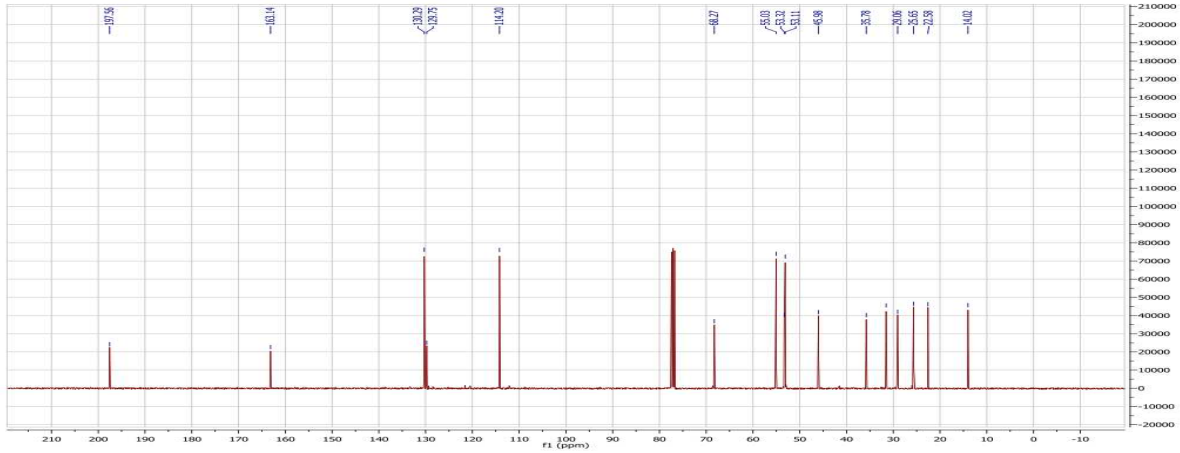
Peak ID	Compound	Time	Mass Found
2	Found	0.73	290.41

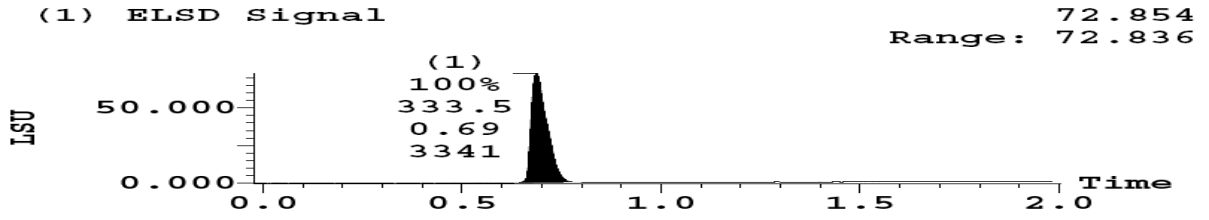




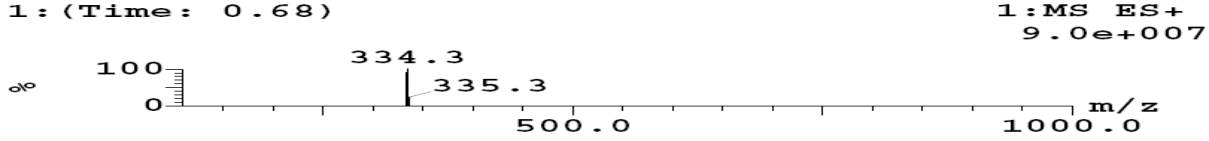
15{*5*}

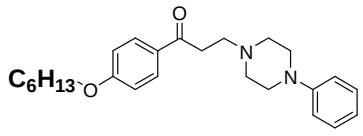




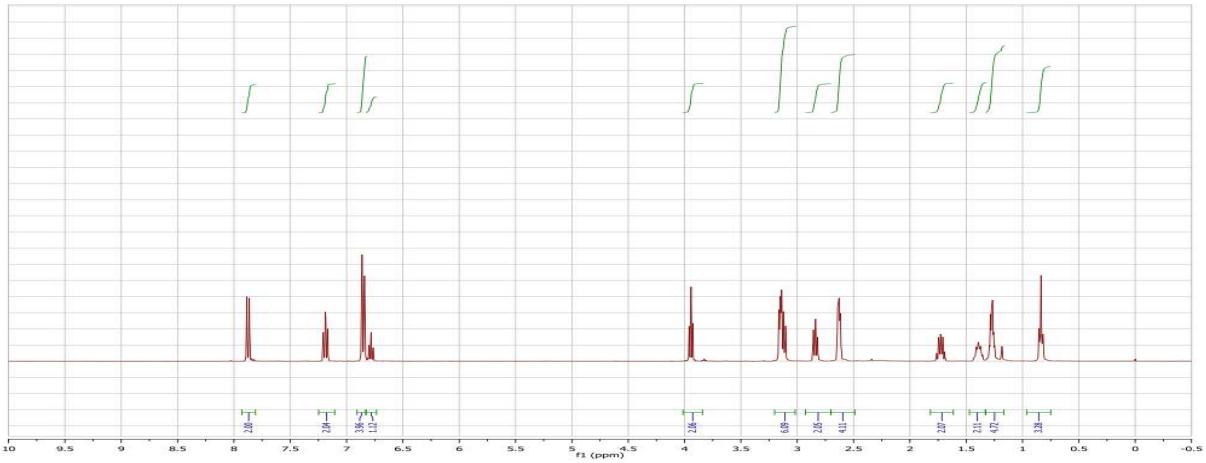


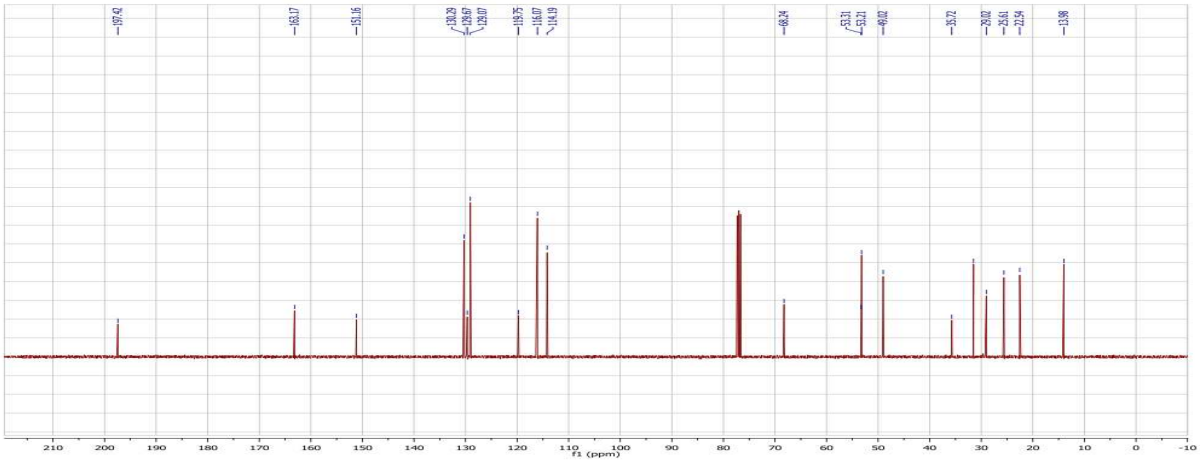
Peak ID	Compound	Time	Mass Found
1	Found	0.68	333.48

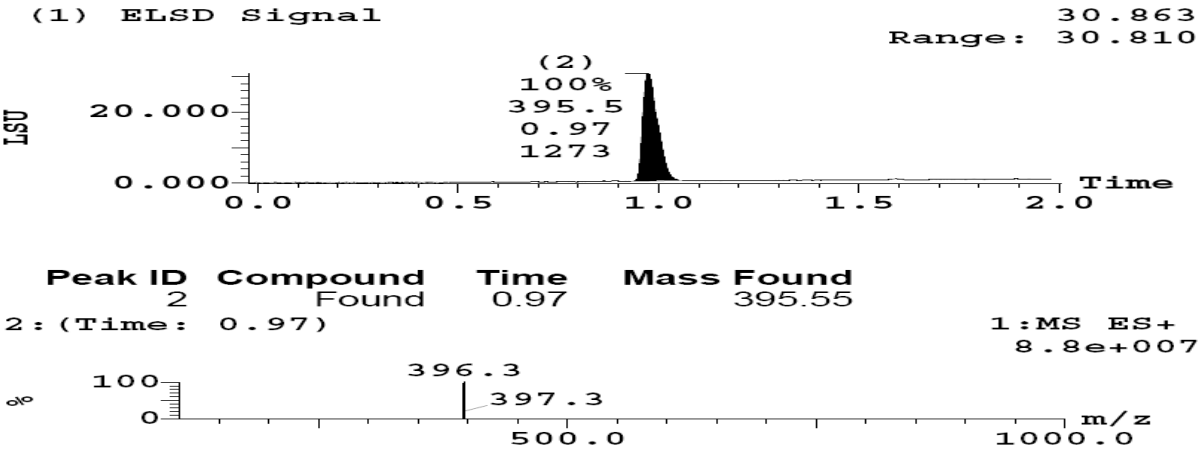




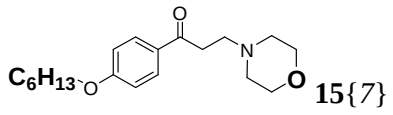
15{*6*}



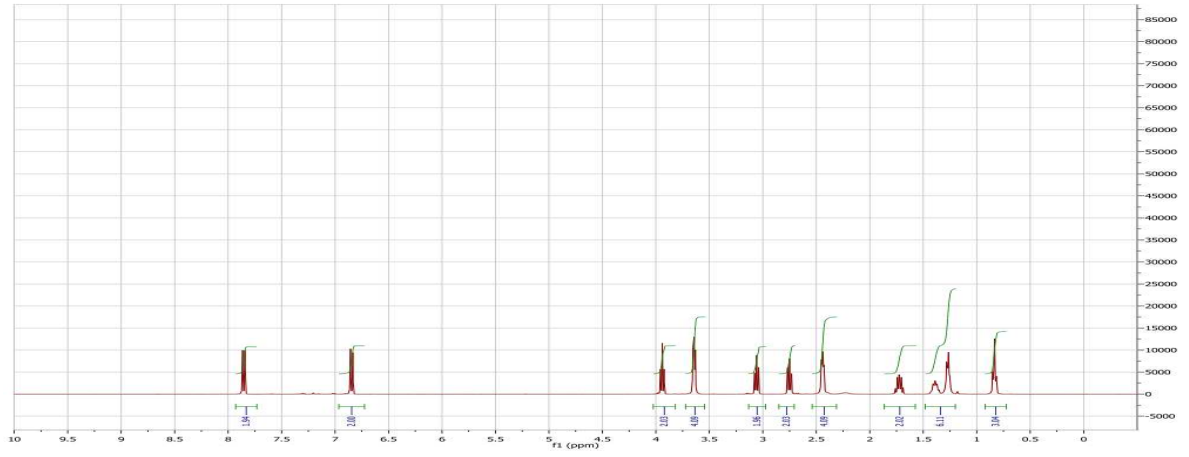


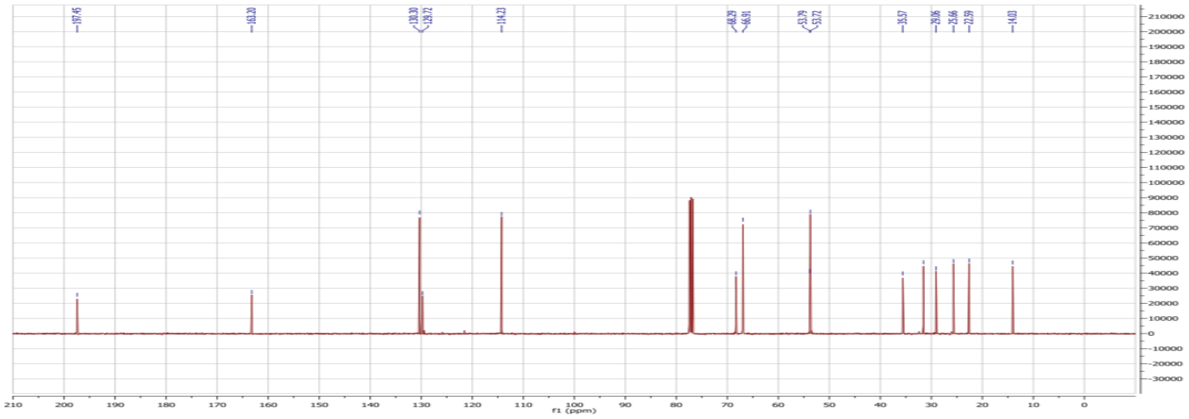


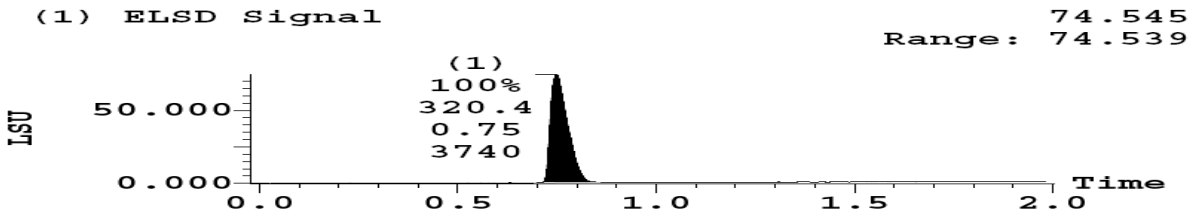
Peak ID	Compound	Time	Mass Found
2	Found	0.97	395.55



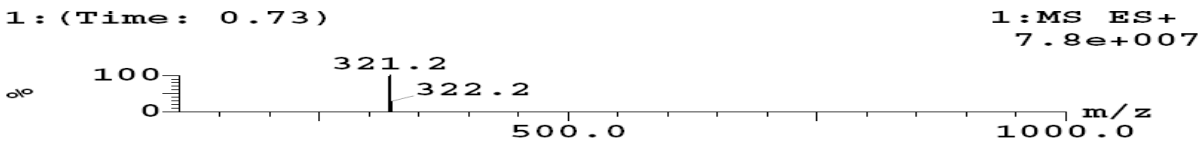
15{*7*}

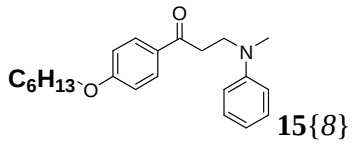




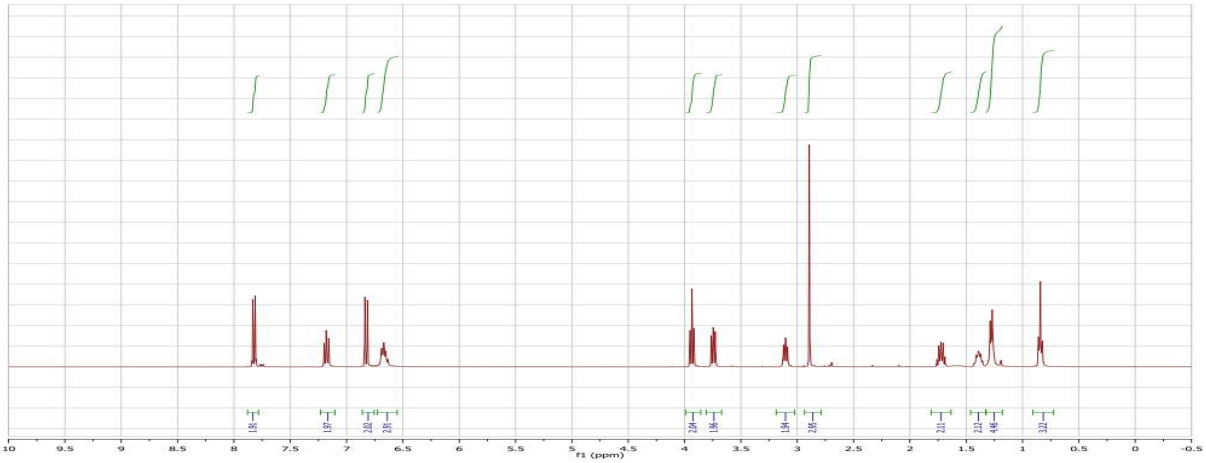


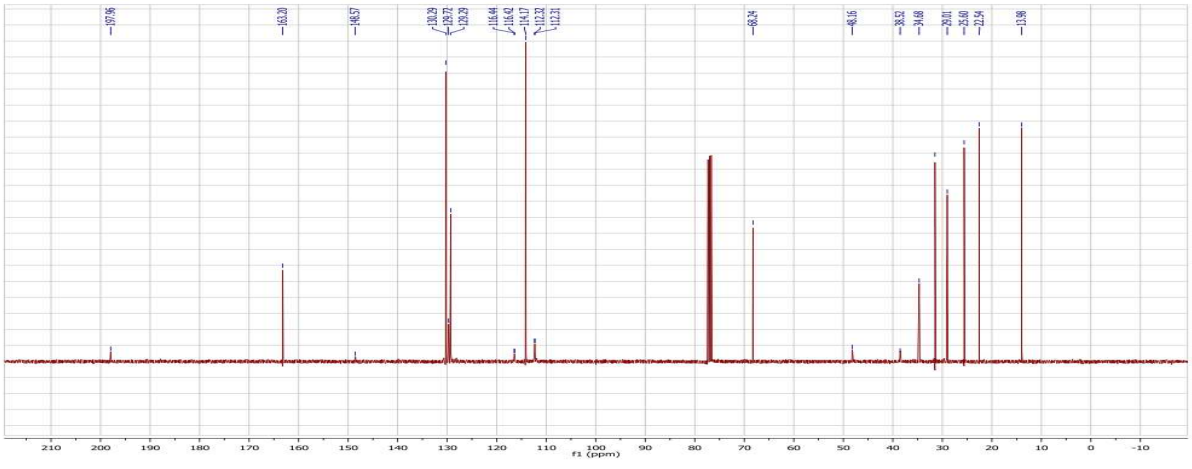
Peak ID	Compound	Time	Mass Found
1	Found	0.73	320.44

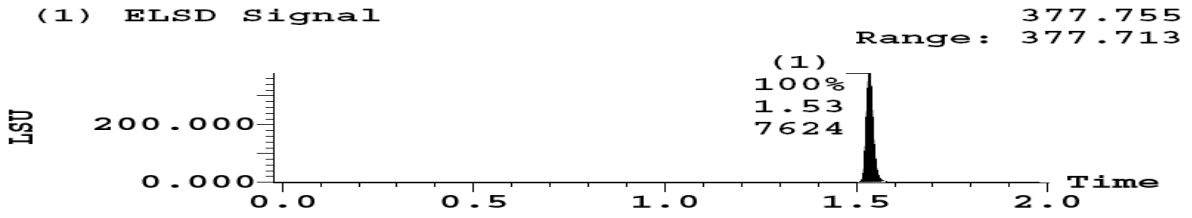




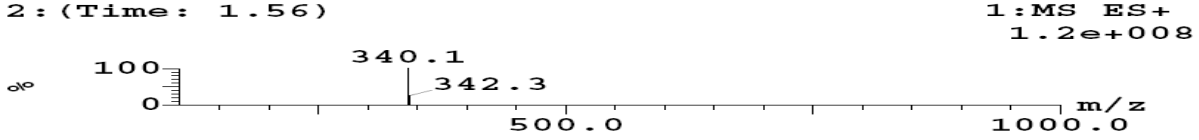
15{*8*}

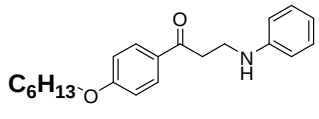




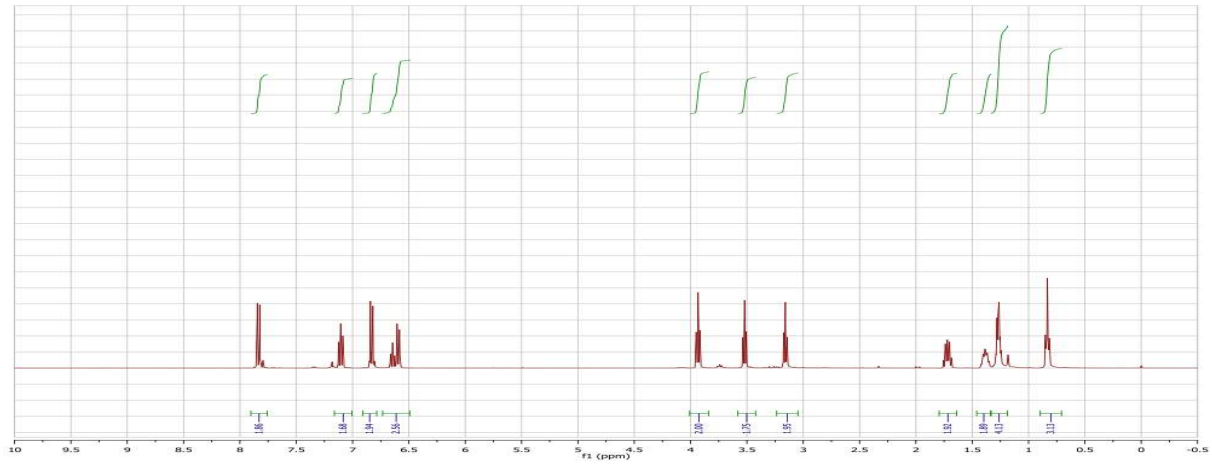


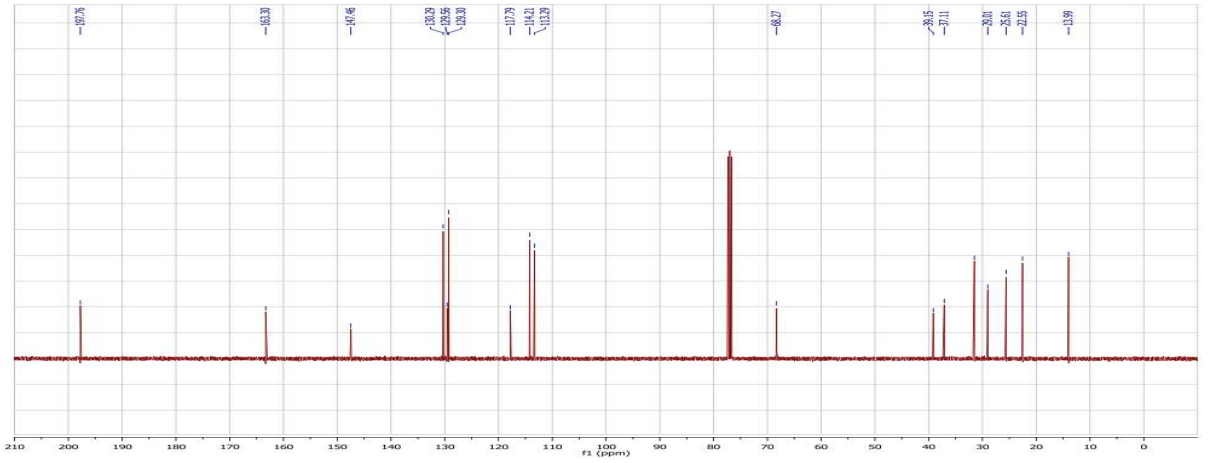
Peak ID	Compound	Time	Mass Found
2	Found	1.56	340.47

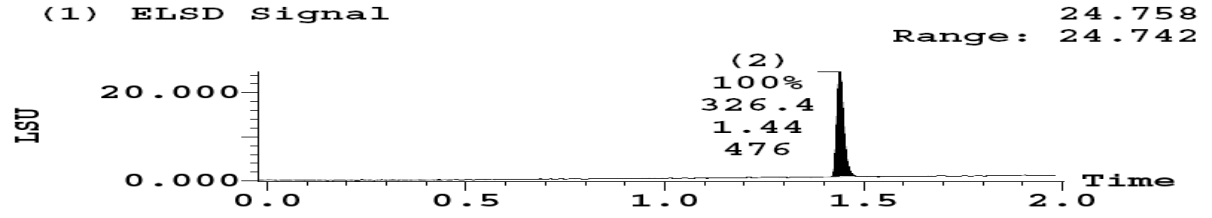




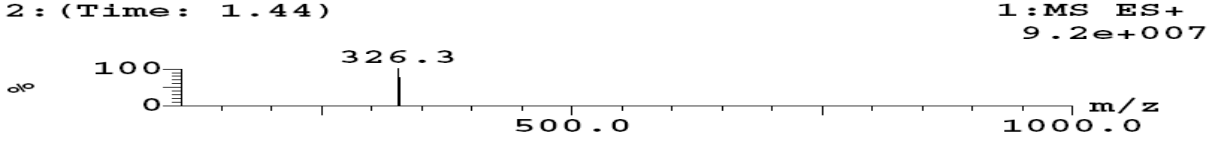
15{9}

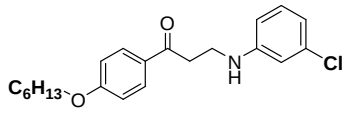




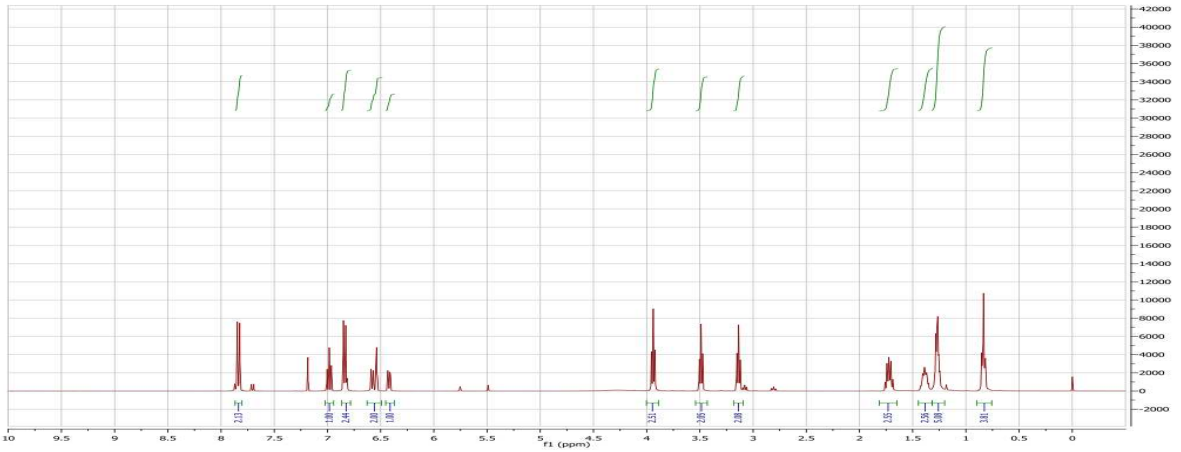


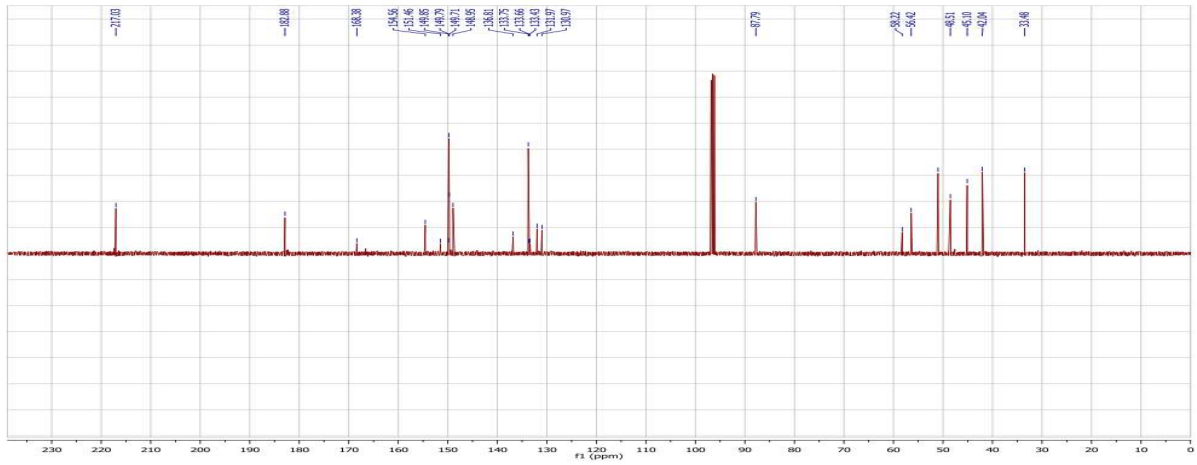
Peak ID	Compound	Time	Mass Found
2	Found	1.44	326.44

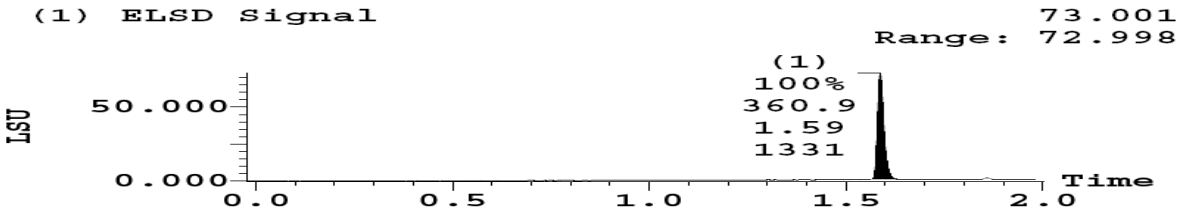




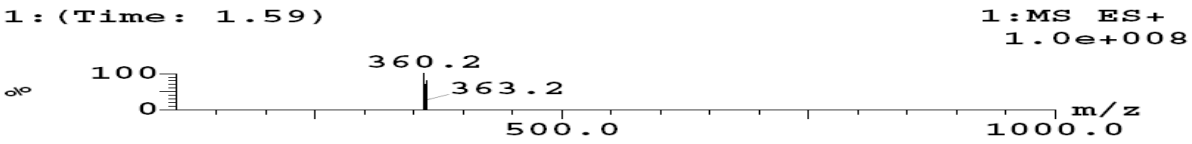
15{*10*}

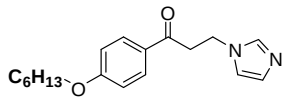




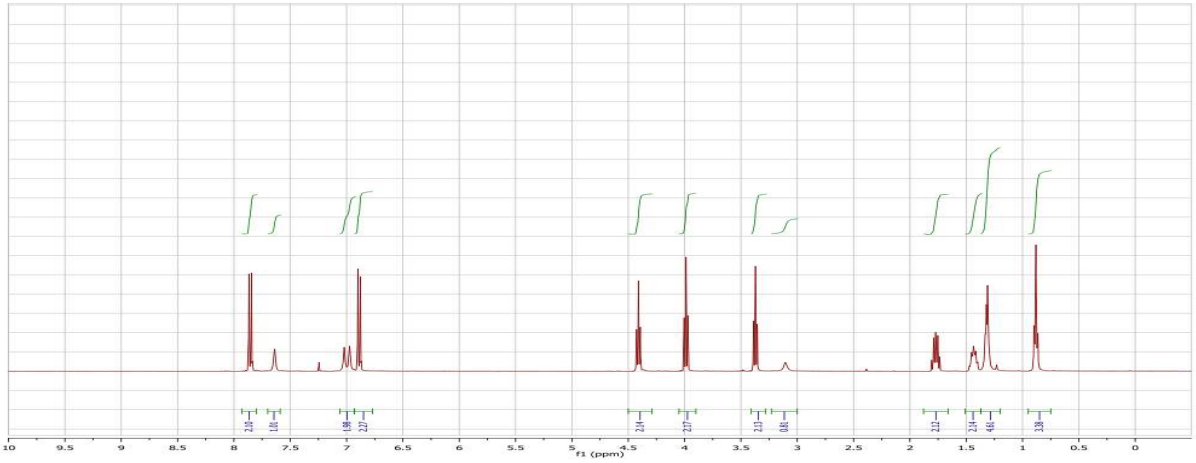


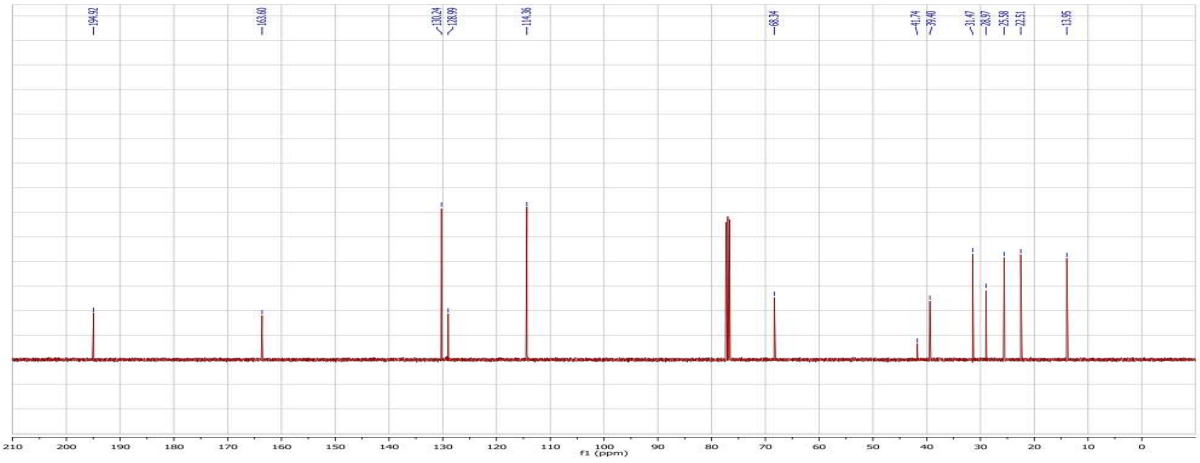
Peak ID	Compound	Time	Mass Found
1	Found	1.59	360.89

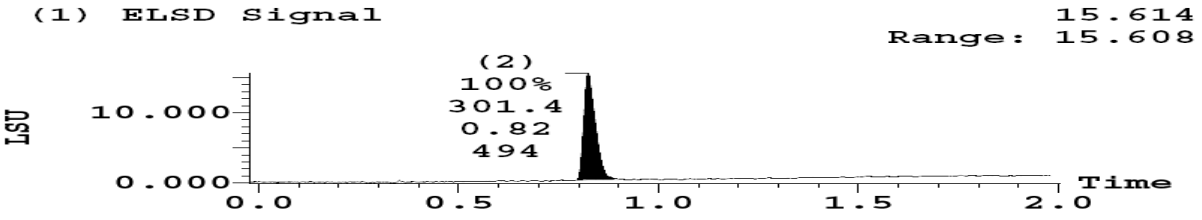




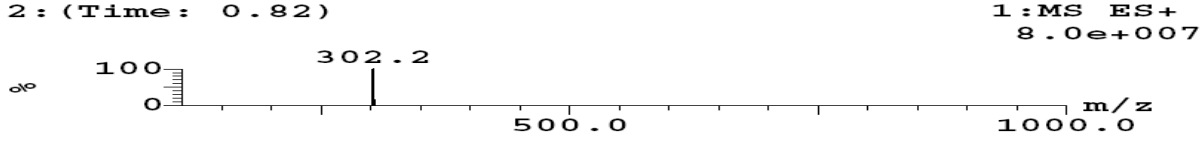
15{*11*}

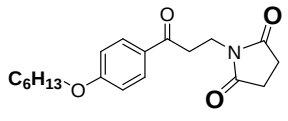




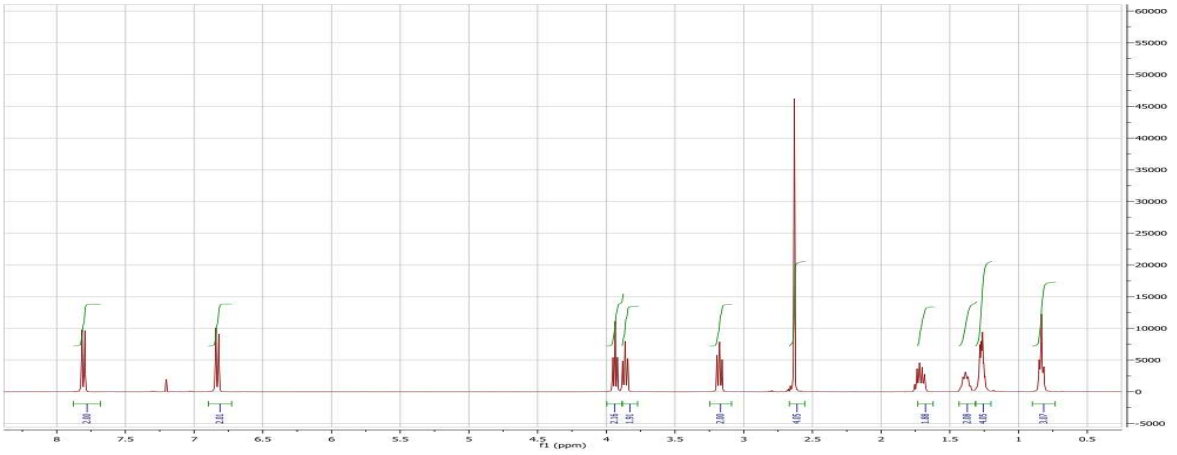


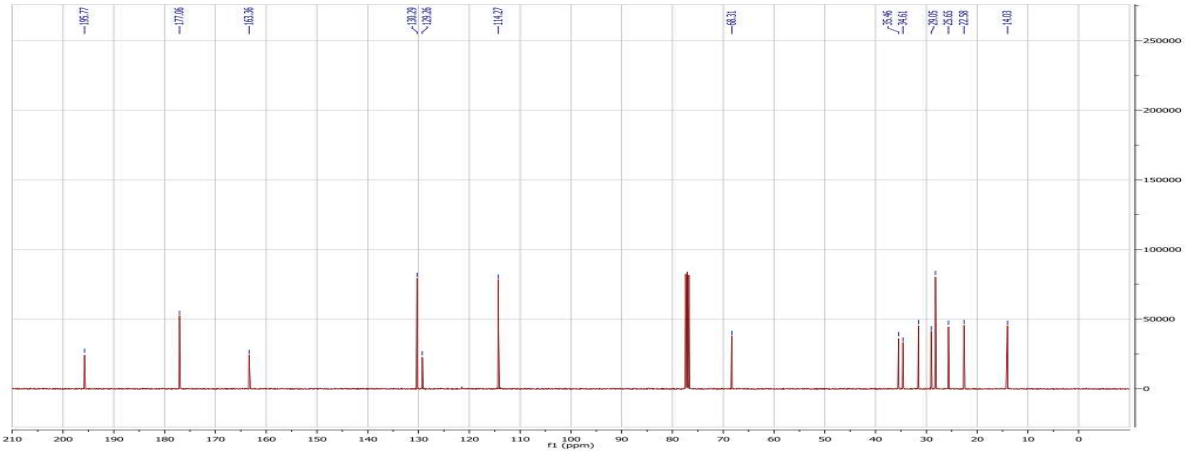
Peak ID	Compound	Time	Mass Found
2	Found	0.82	301.40

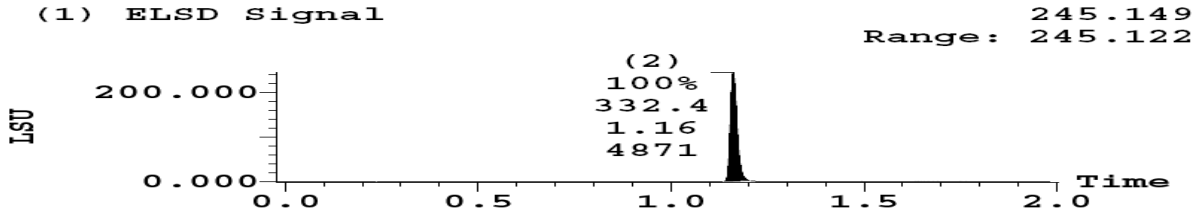




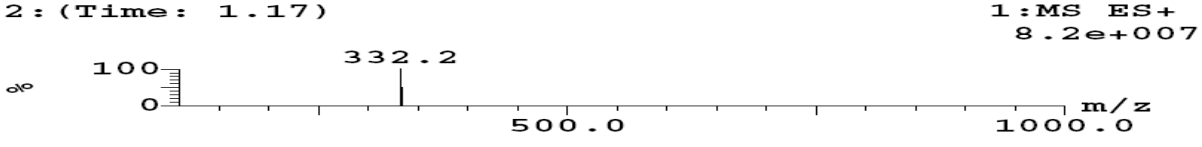
15{*12*}

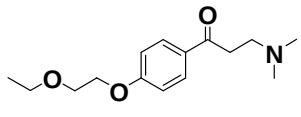




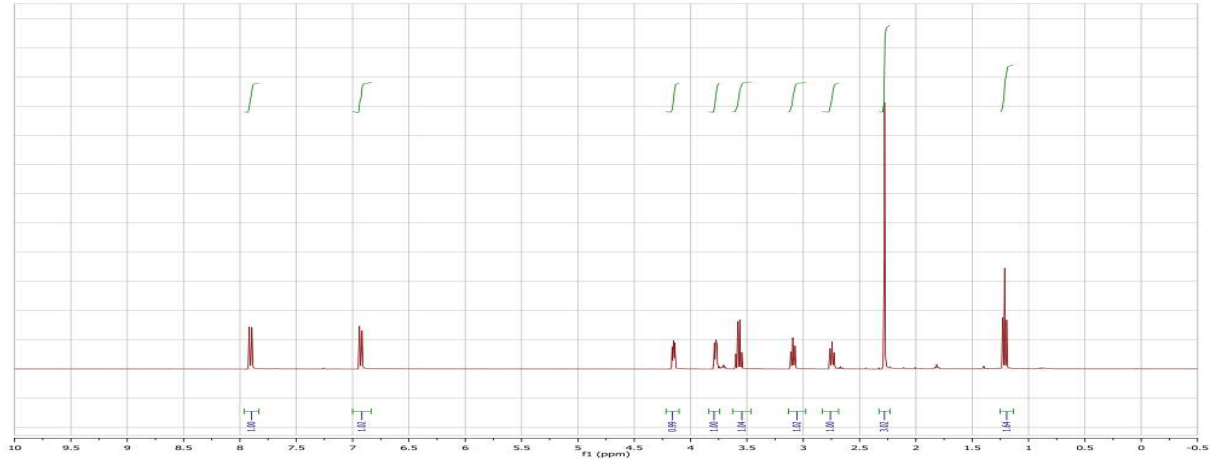


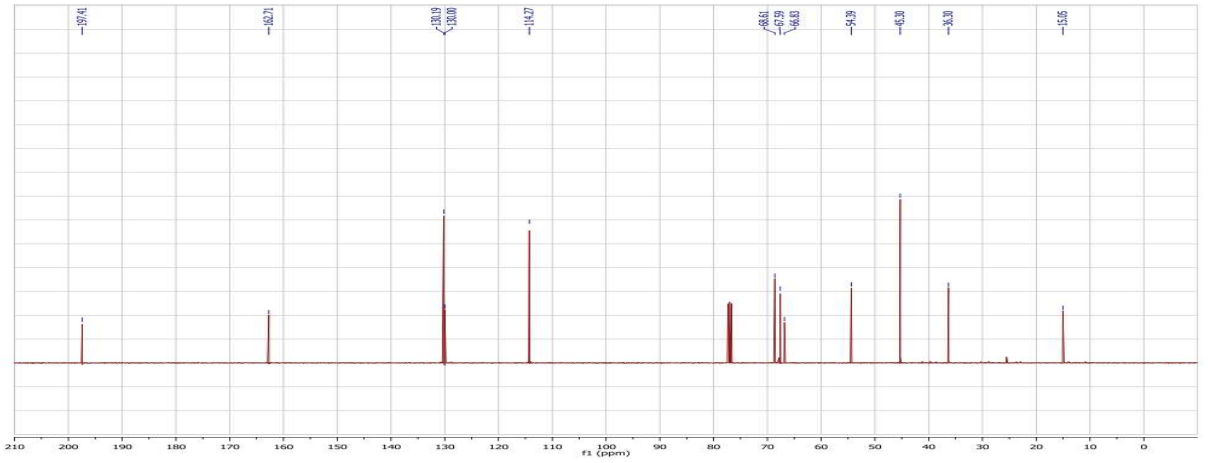
Peak ID	Compound	Time	Mass Found
2	Found	1.17	332.41

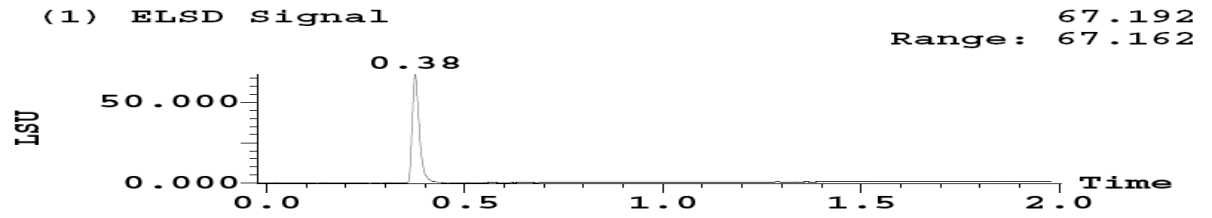




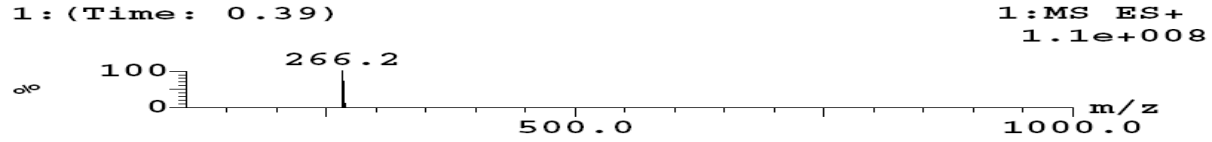
16{*1*}

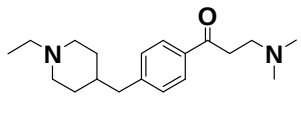




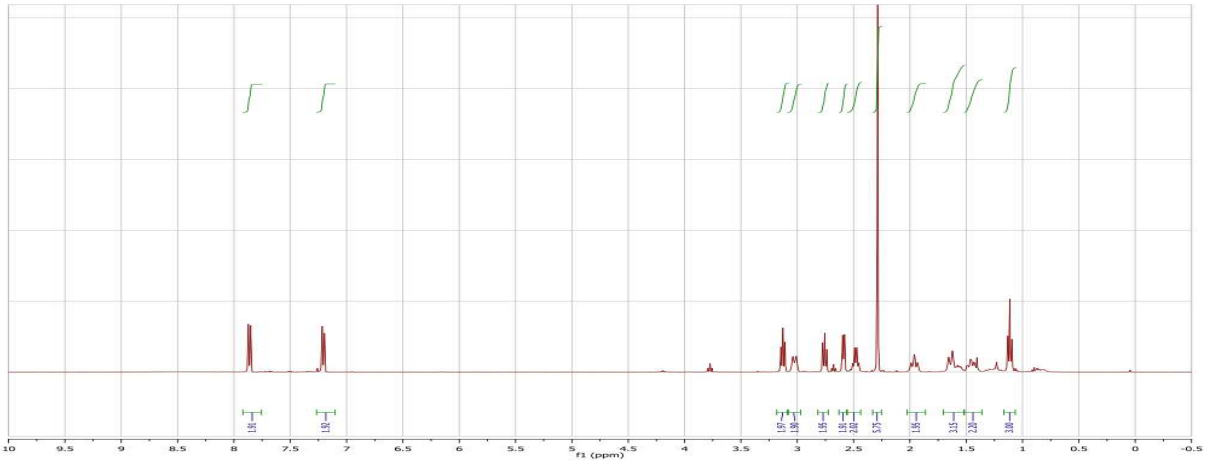


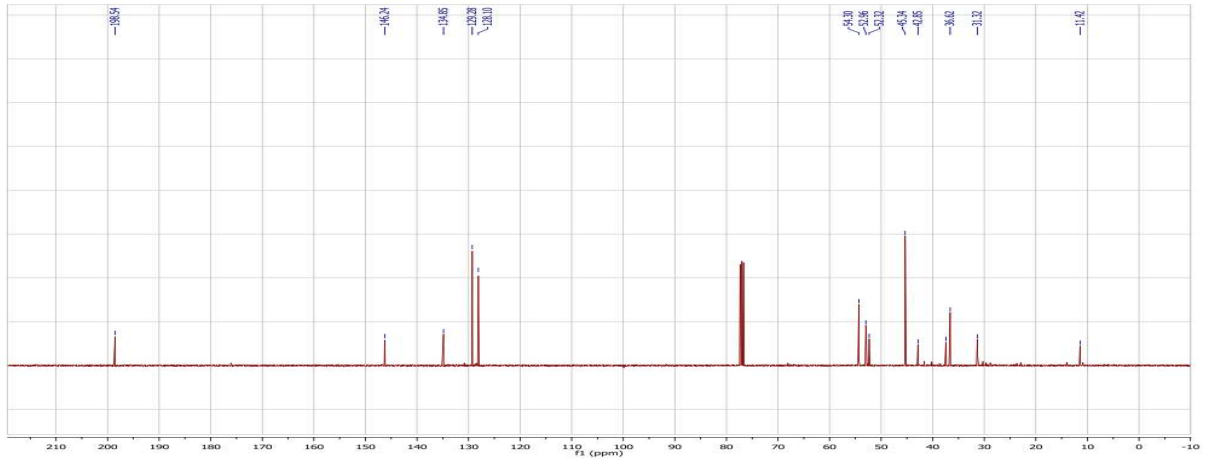
Peak ID	Compound	Time	Mass Found
1	Found	0.39	266.35

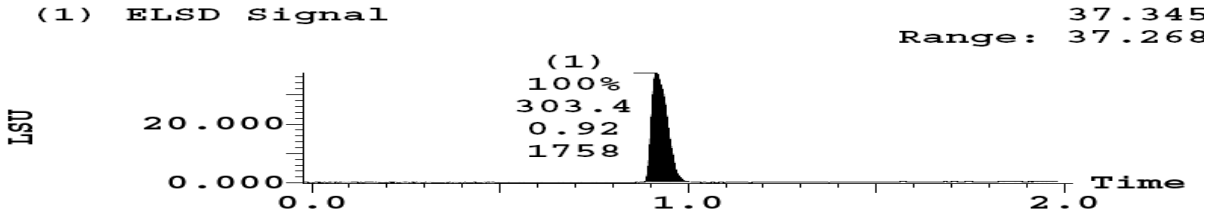




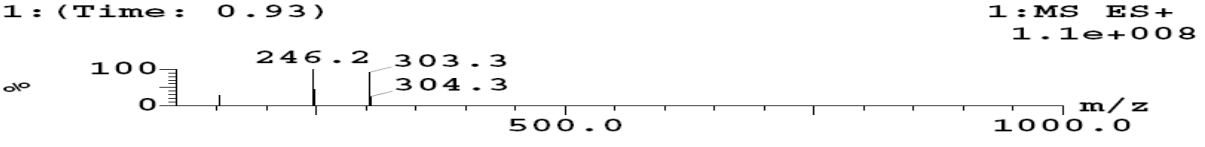
16{*2*}

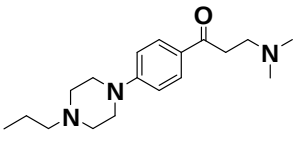




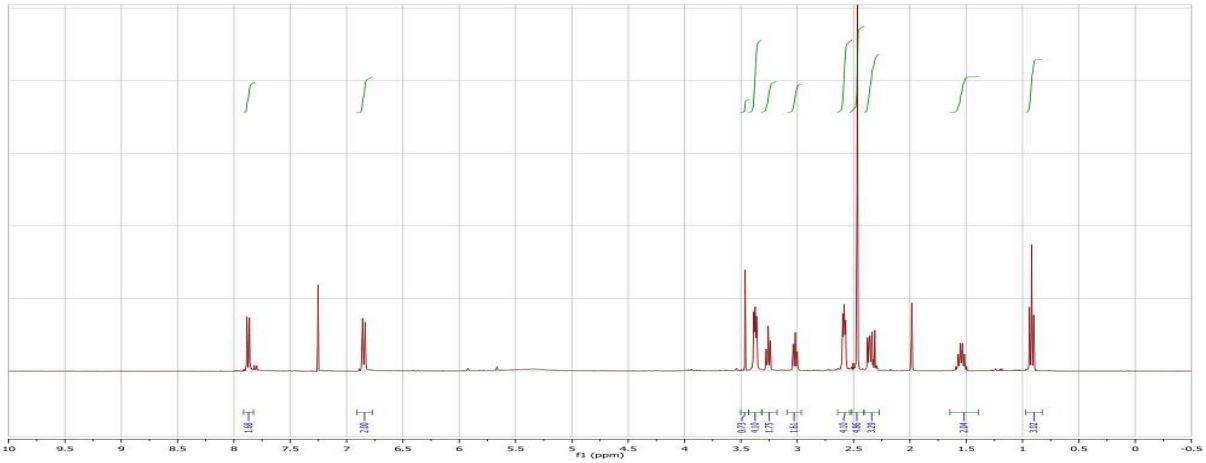


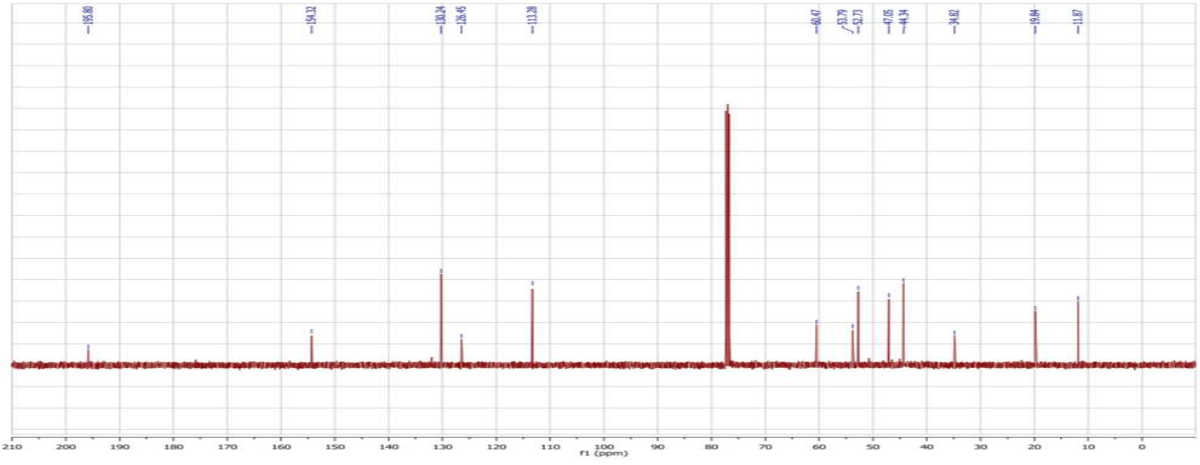
Peak ID	Compound	Time	Mass Found
1	Tentative	0.93	303.35

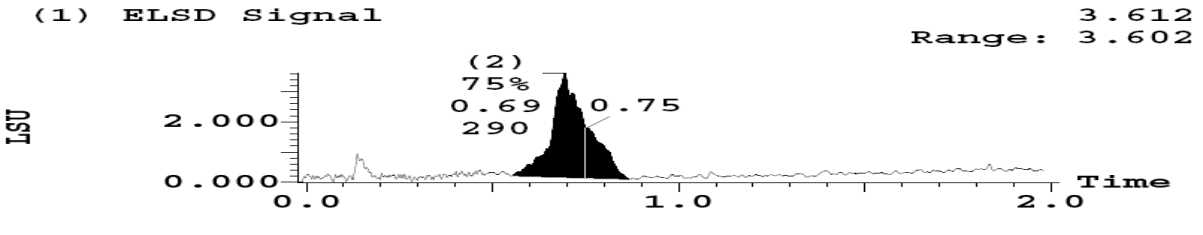


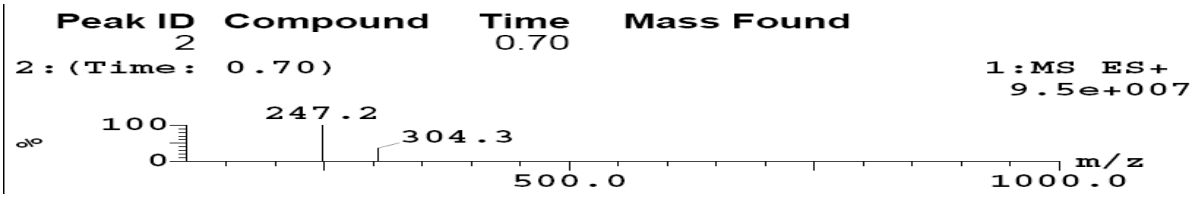


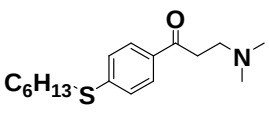
16{*3*}



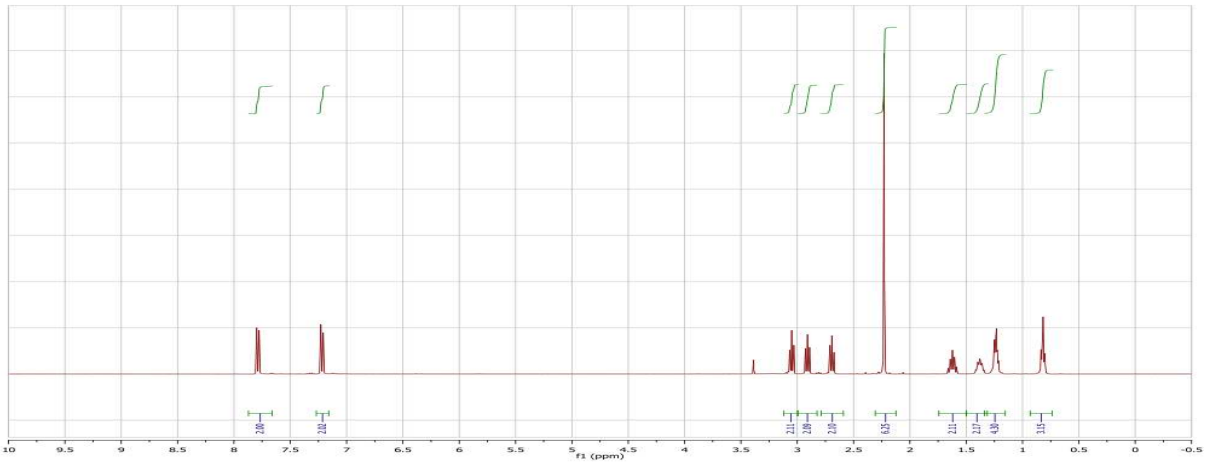


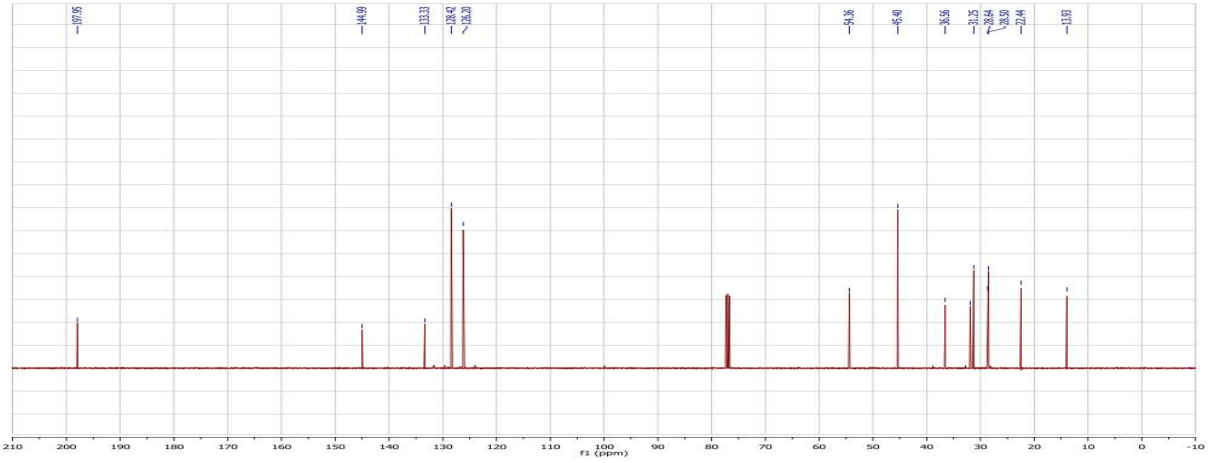

(1) ELSD Signal
3.612
Range: 3.602
(2)
75%
0.69
290
0.75
LSU
2.000
0.000
0.0
1.0
2.0
Time

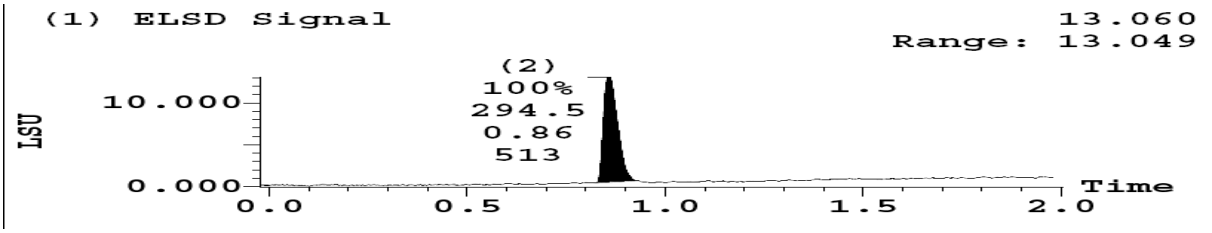

Peak ID Compound Time Mass Found
2 0.70
2:(Time: 0.70)
1:MS ES+
9.5e+007
100
%
0
247.2
304.3
500.0
1000.0
m/z



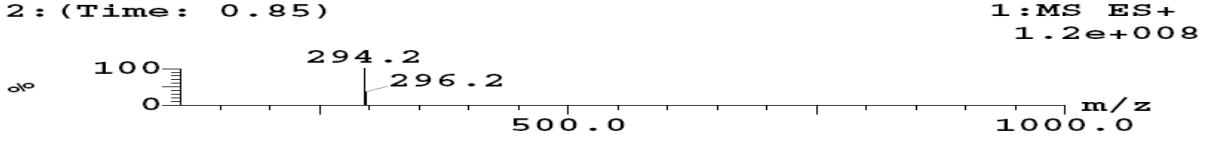
16{*4*}

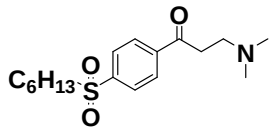




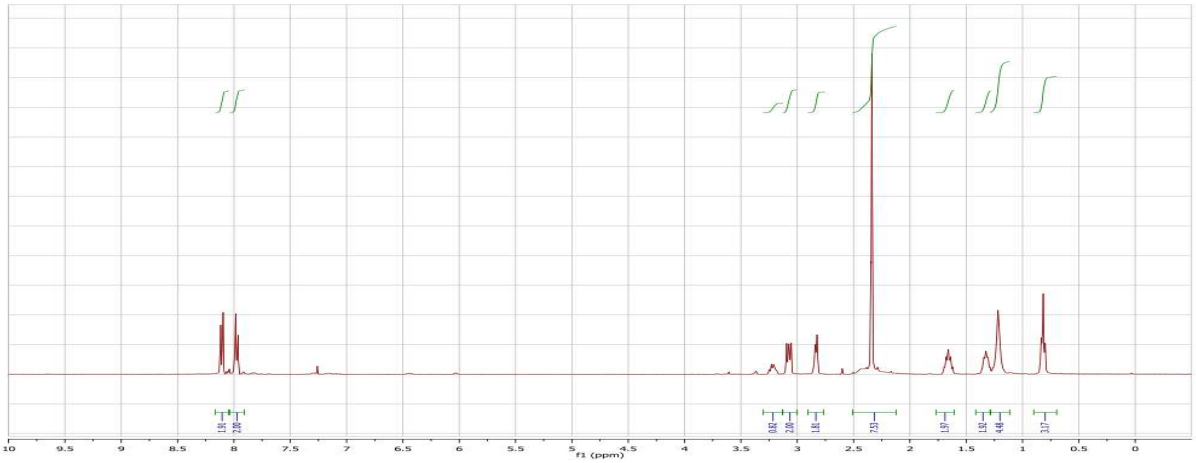


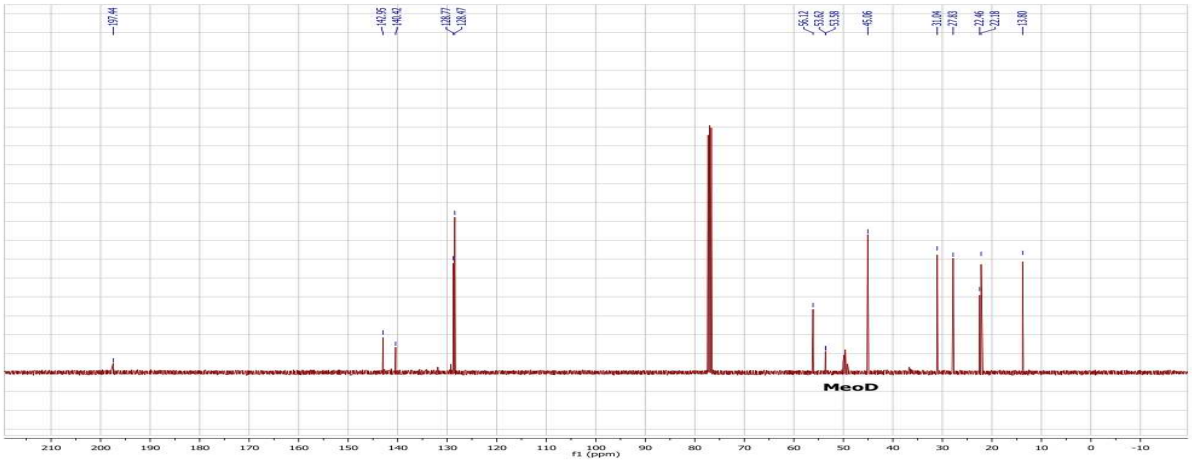
Peak ID	Compound	Time	Mass Found
2	Found	0.85	294.47

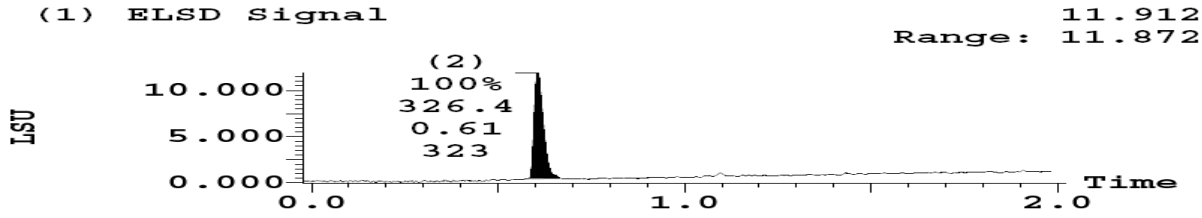




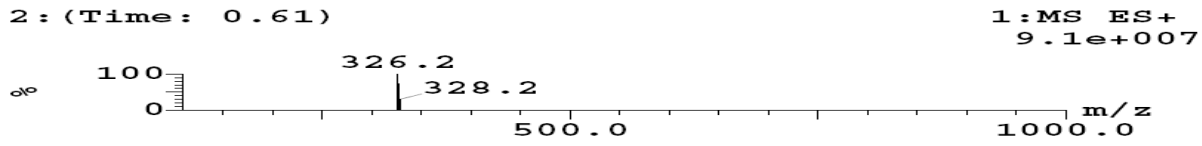
16{*5*}

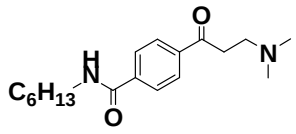




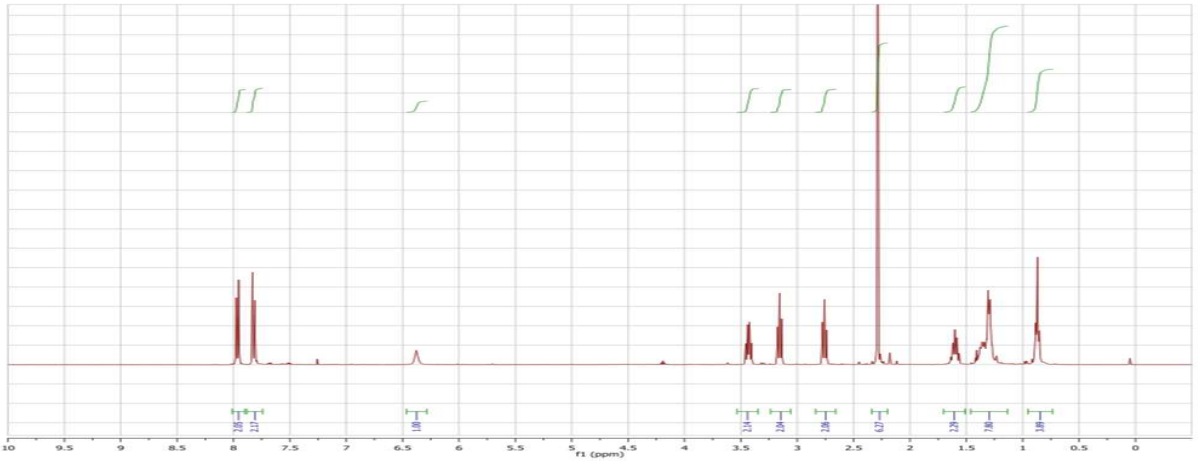


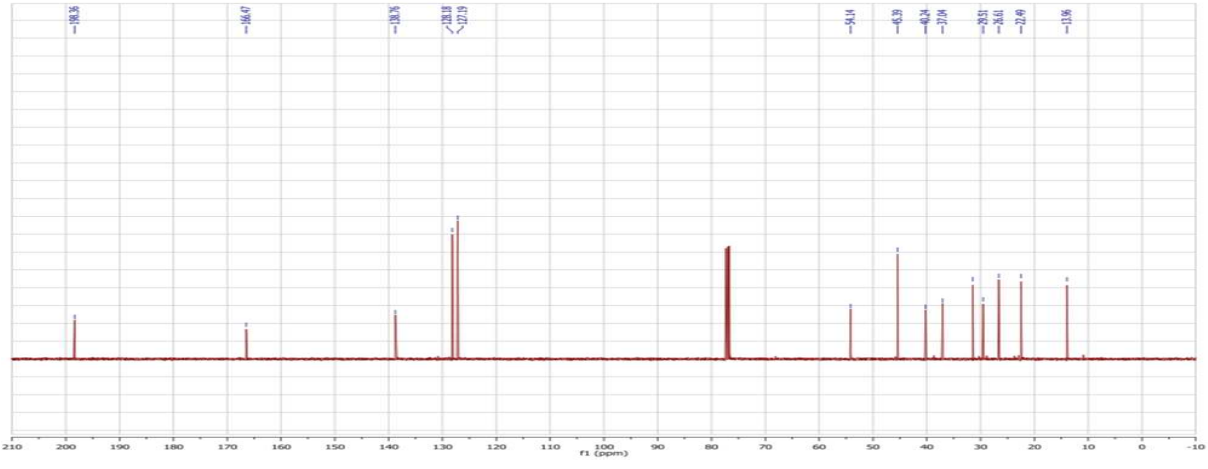
Peak ID	Compound	Time	Mass Found
2	Found	0.61	326.37

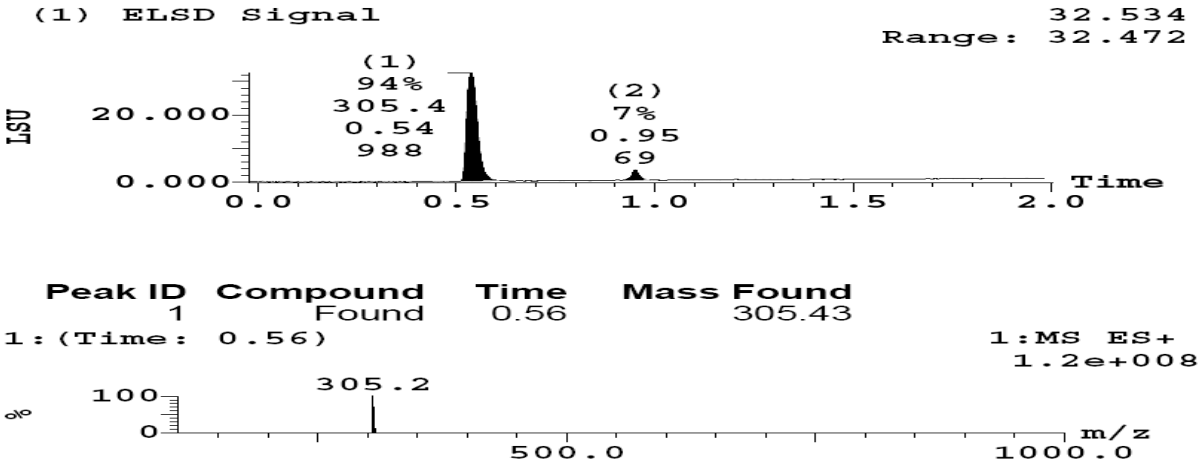




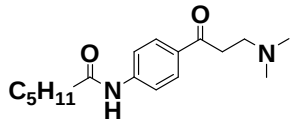
16{*6*}



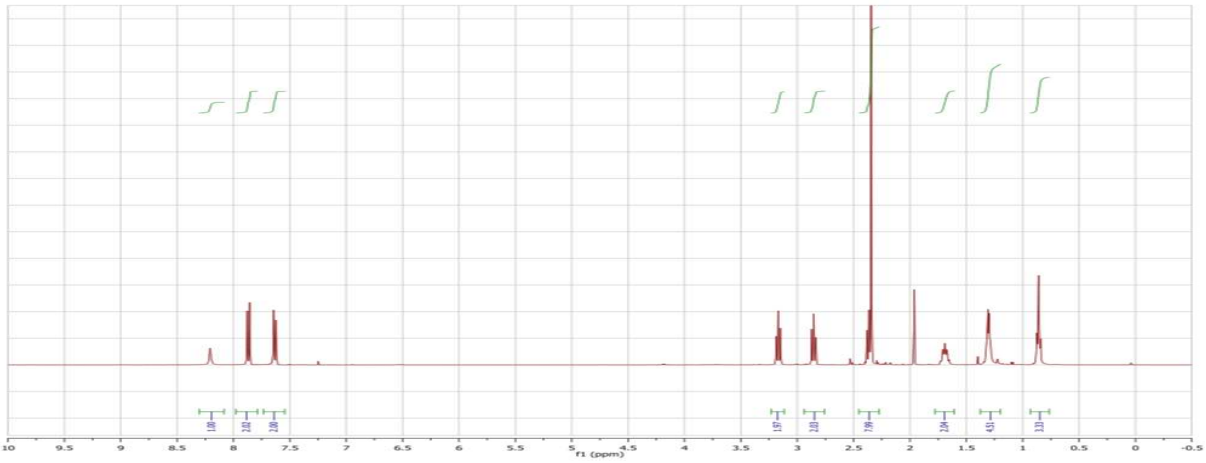


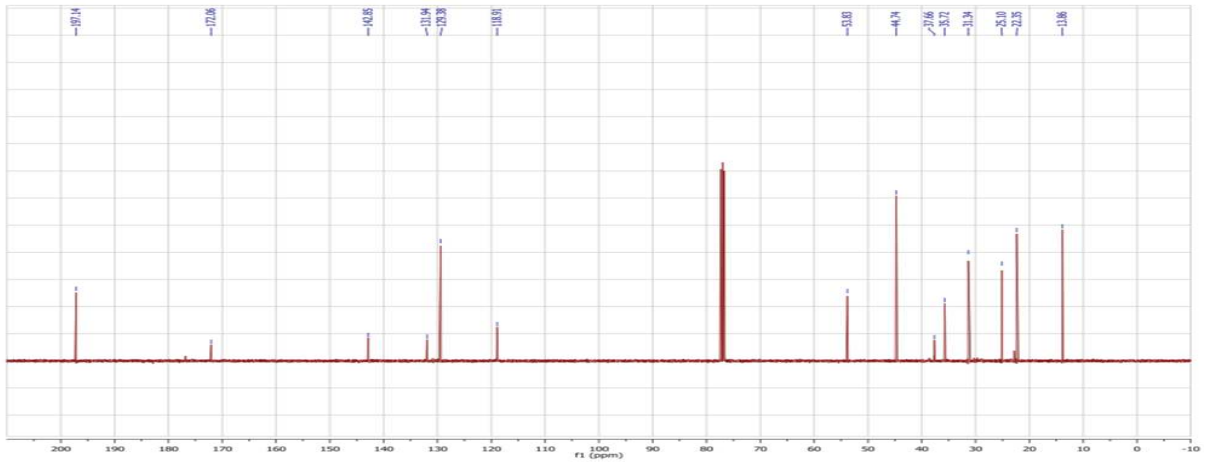


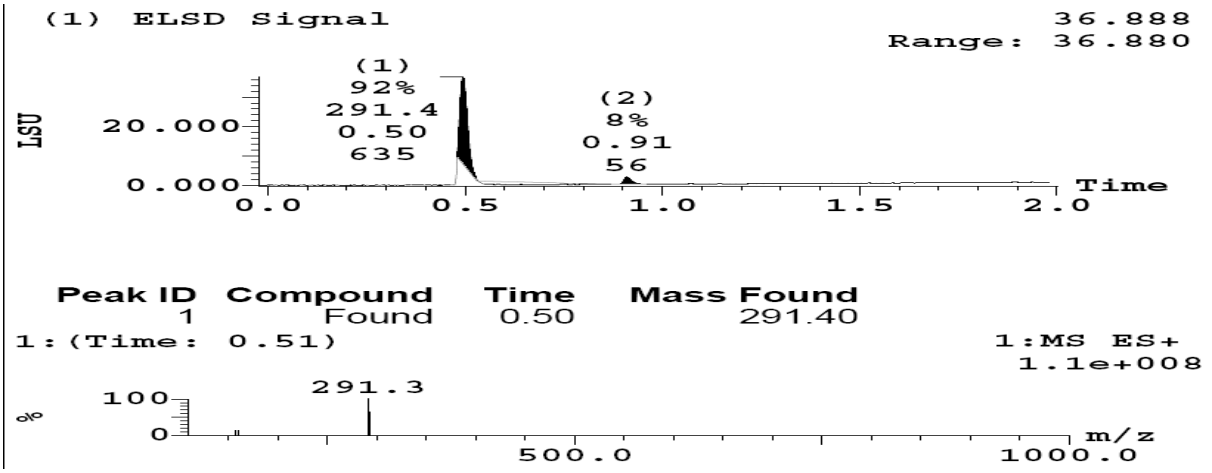
Peak ID	Compound	Time	Mass Found
1	Found	0.56	305.43

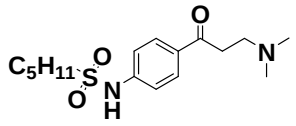


16{*7*}

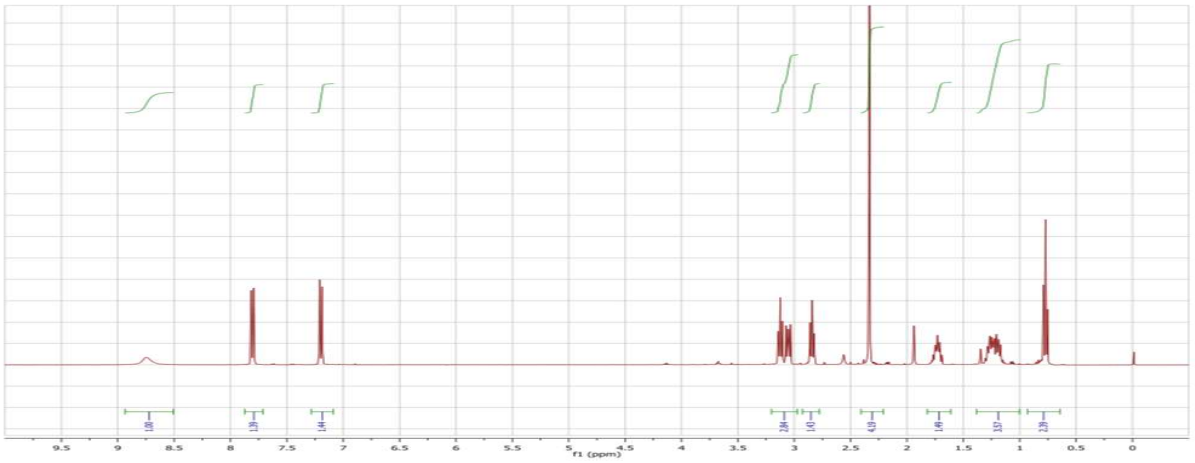


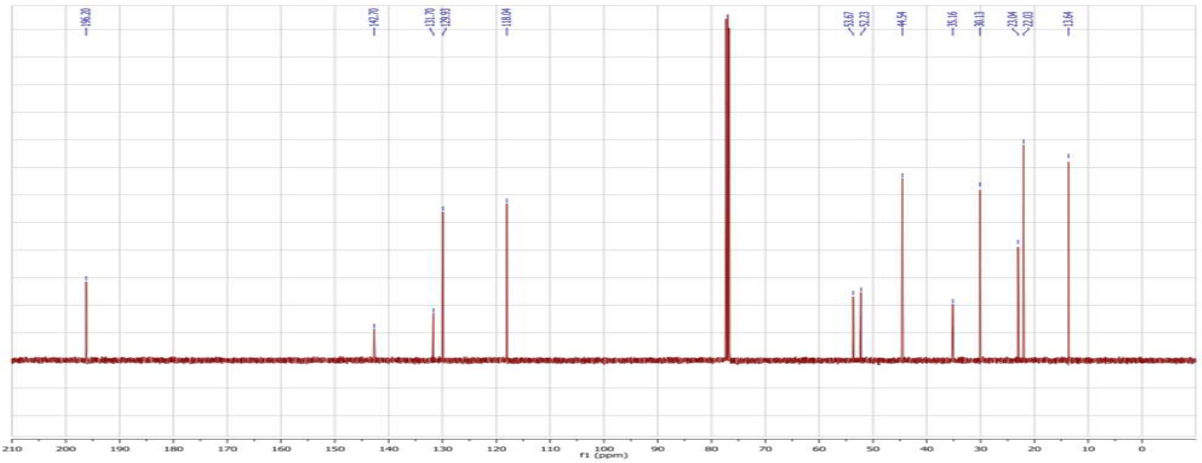


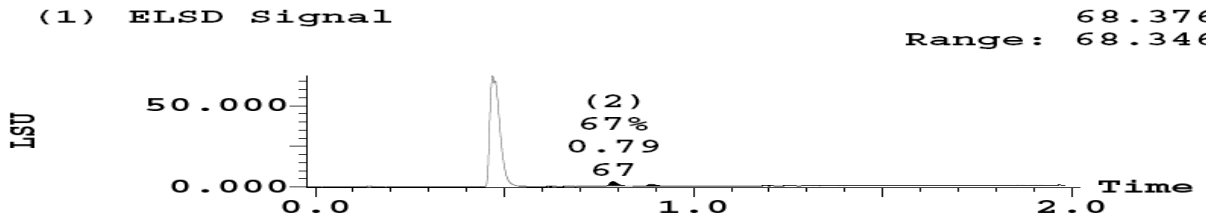

(1) ELSD Signal
36.888
Range: 36.880
(1)
92%
291.4
0.50
635
(2)
8%
0.91
56
LSU
20.000
0.000
Time
0.0
0.5
1.0
1.5
2.0
Peak ID Compound Time Mass Found
1 Found 0.50 291.40
1:(Time: 0.51)
1:MS ES+
1.1e+008
291.3
100
%
0
m/z
500.0
1000.0



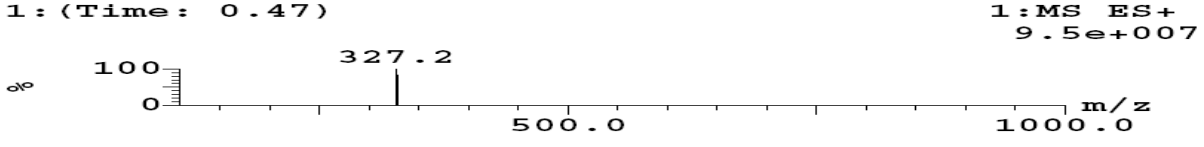
16{*8*}

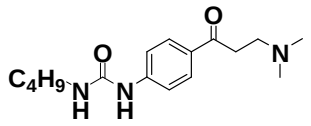




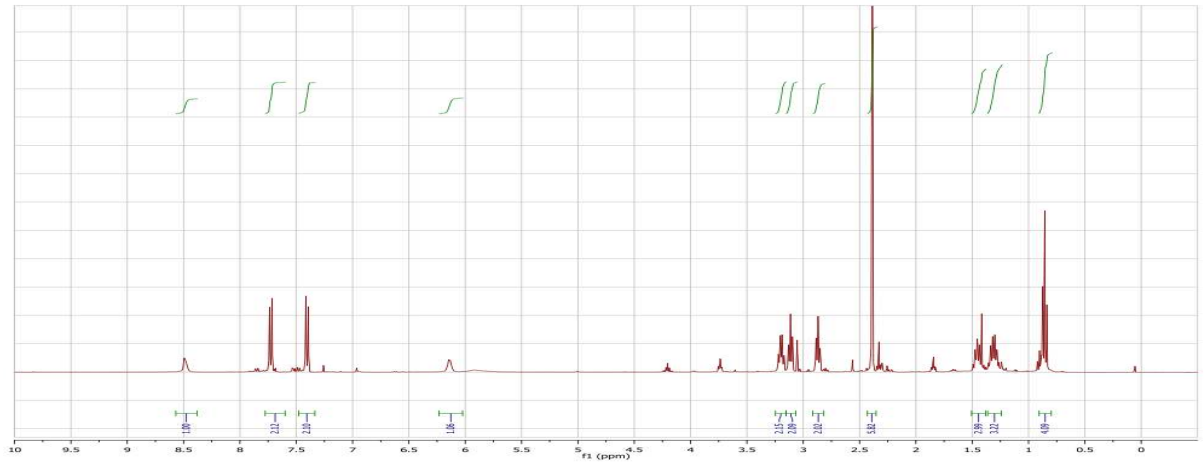


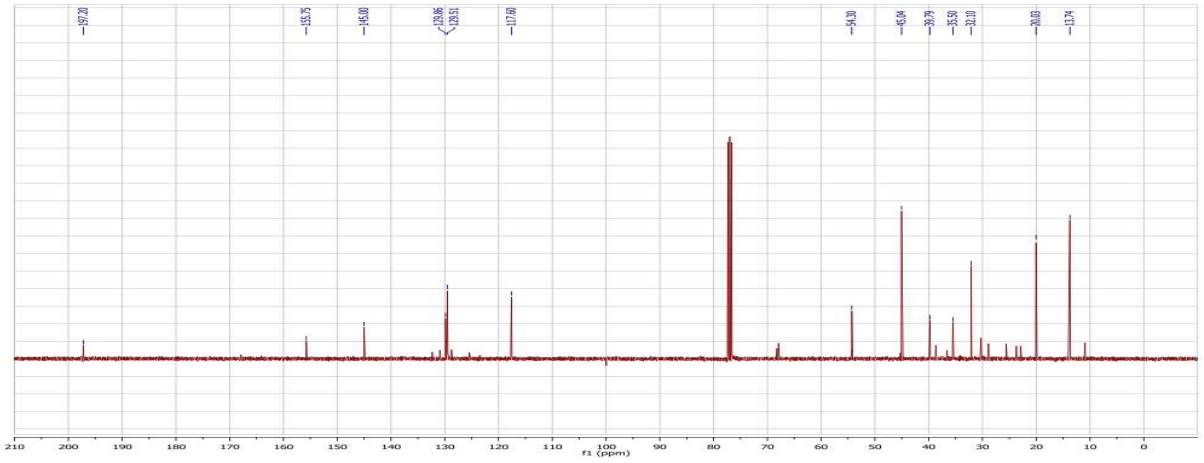
Peak ID	Compound	Time	Mass Found
1	Found	0.47	327.35

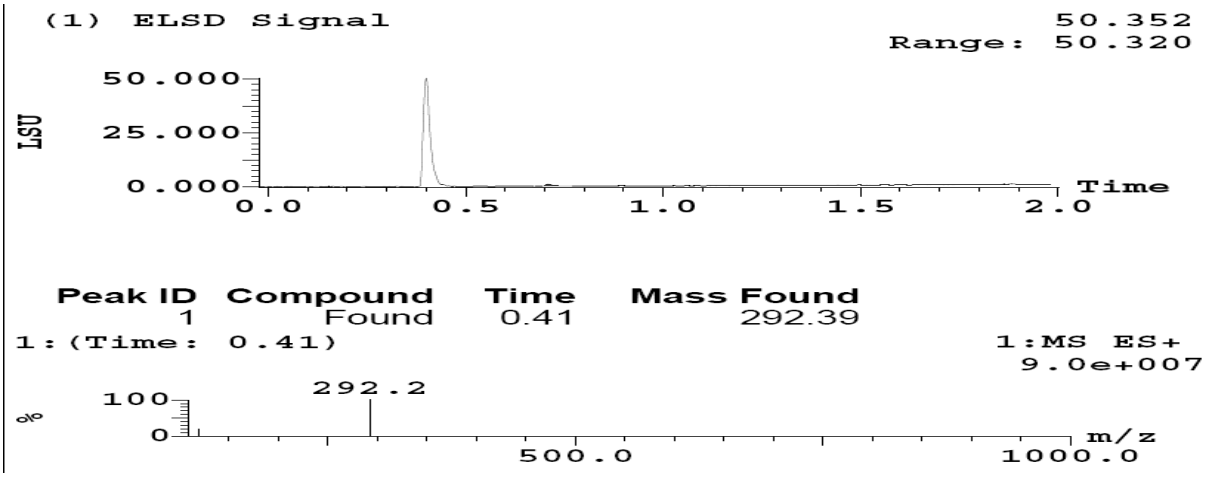




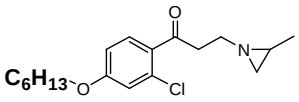
16{*9*}



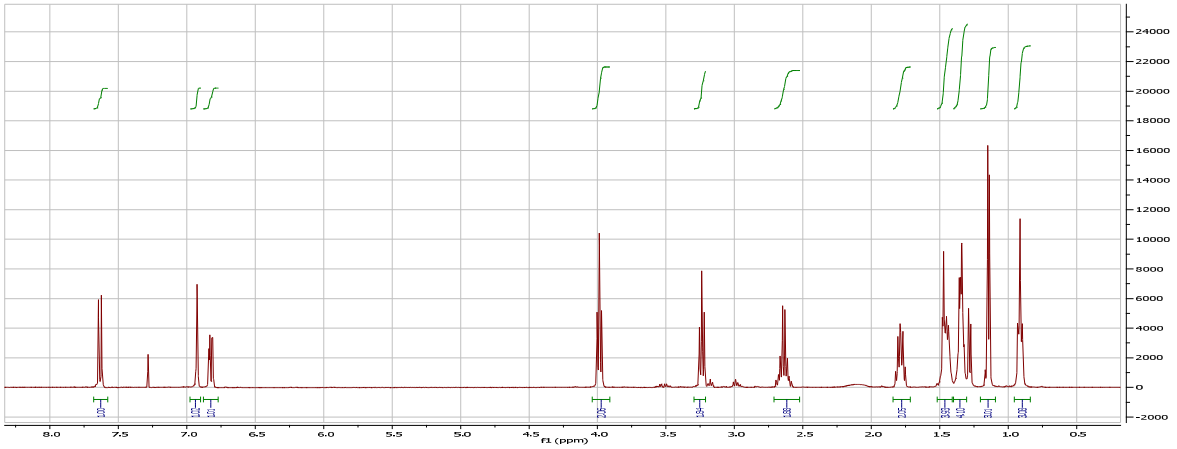


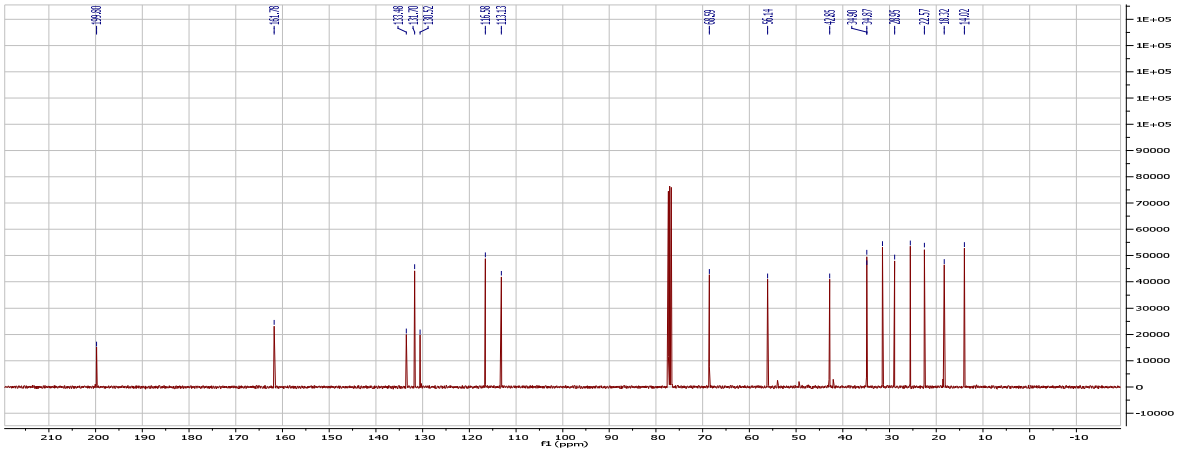

(1) ELSD Signal
50.352
Range: 50.320
50.000
25.000
0.000
LSU
0.0
0.5
1.0
1.5
2.0
Time
Peak ID Compound Time Mass Found
1 Found 0.41 292.39
1:(Time: 0.41)
1:MS ES+
9.0e+007
292.2
100
0
%
500.0
1000.0
m/z

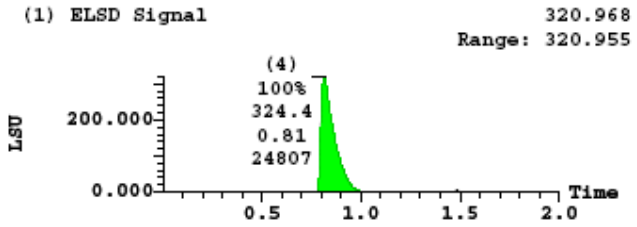
17{*1,1,1*} Same with **12**{*11*}

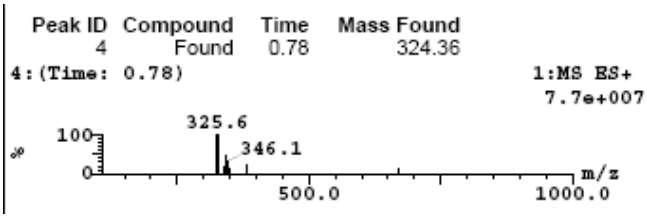


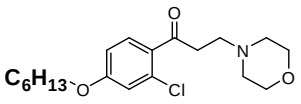
17{*1,1,2*}



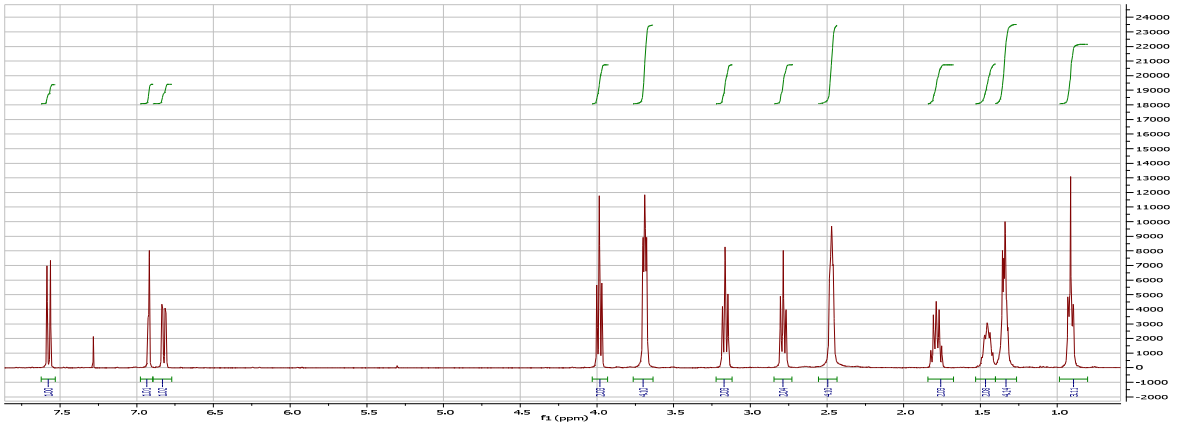


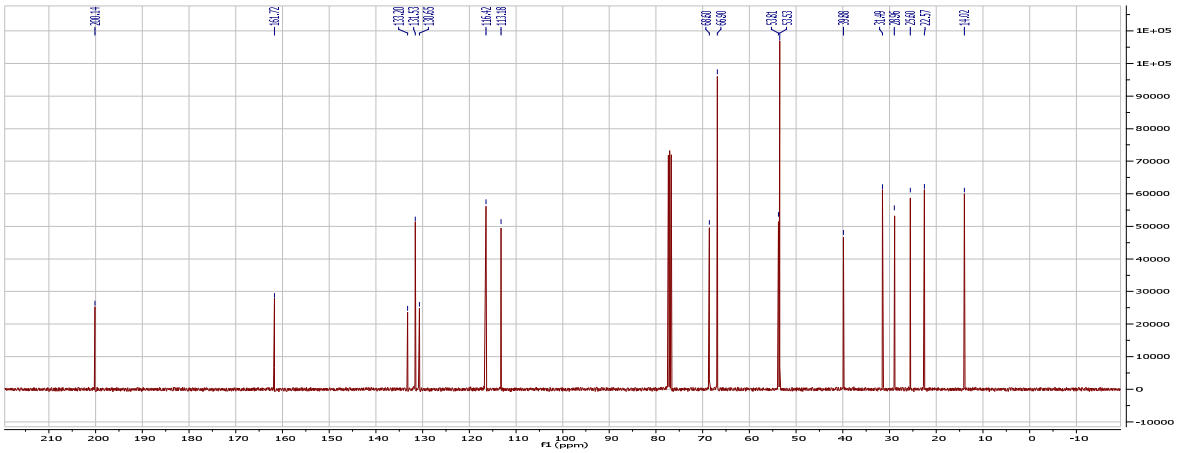


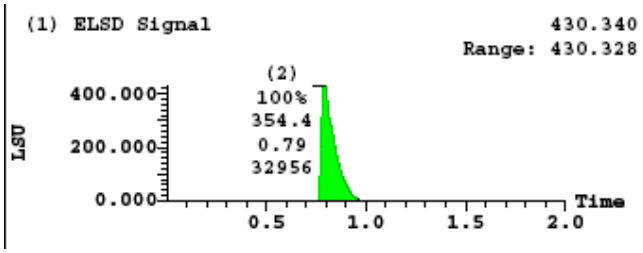




17{*1,1,3*}

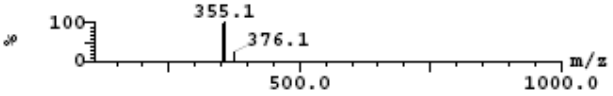


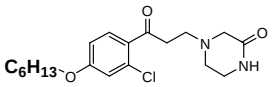




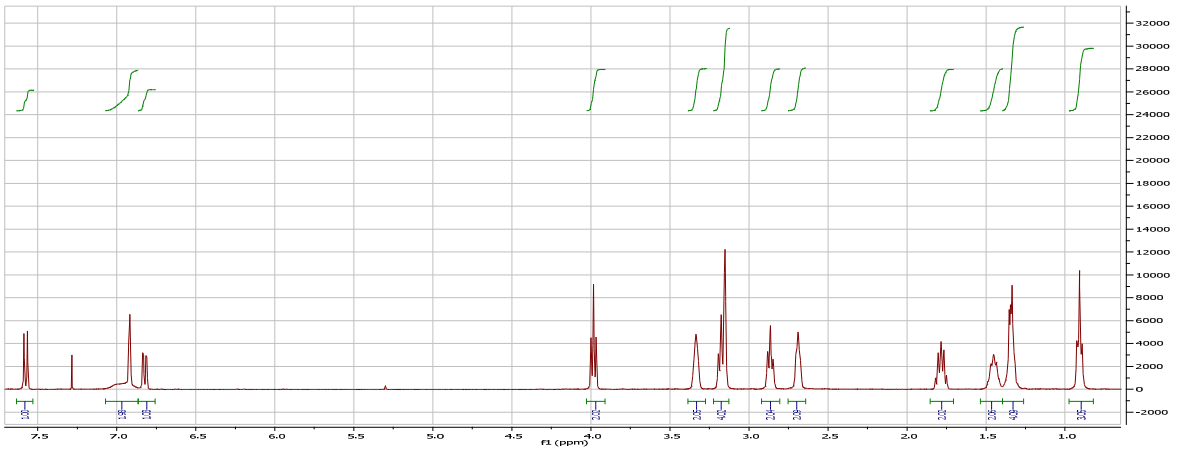
Peak ID	Compound	Time	Mass Found
2	Found	0.77	354.39

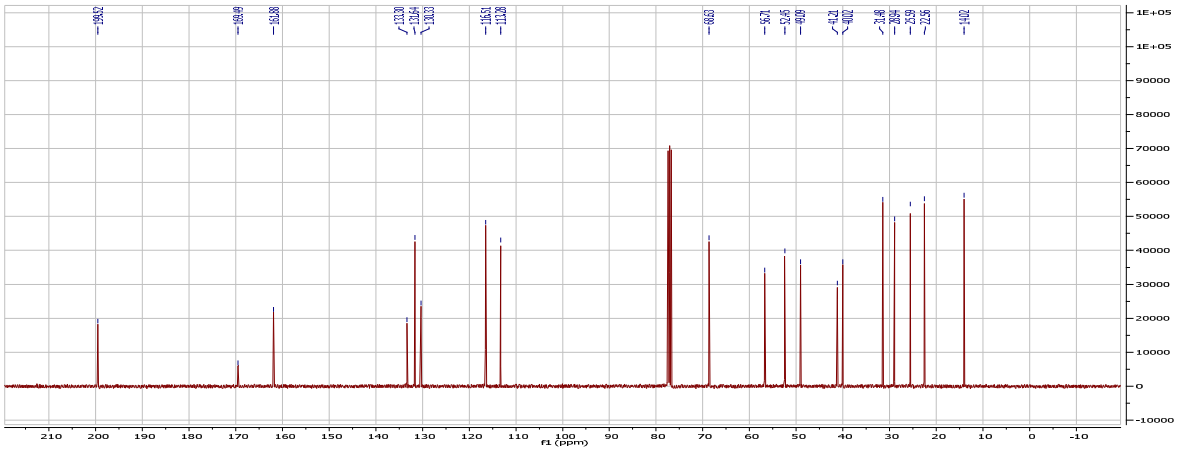
2:(Time: 0.77) 1:MS ES+ 1.0e+008

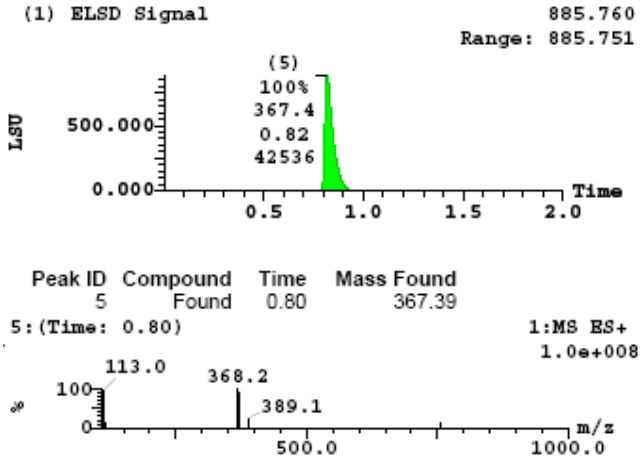




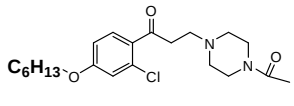
17{*1,1,4*}



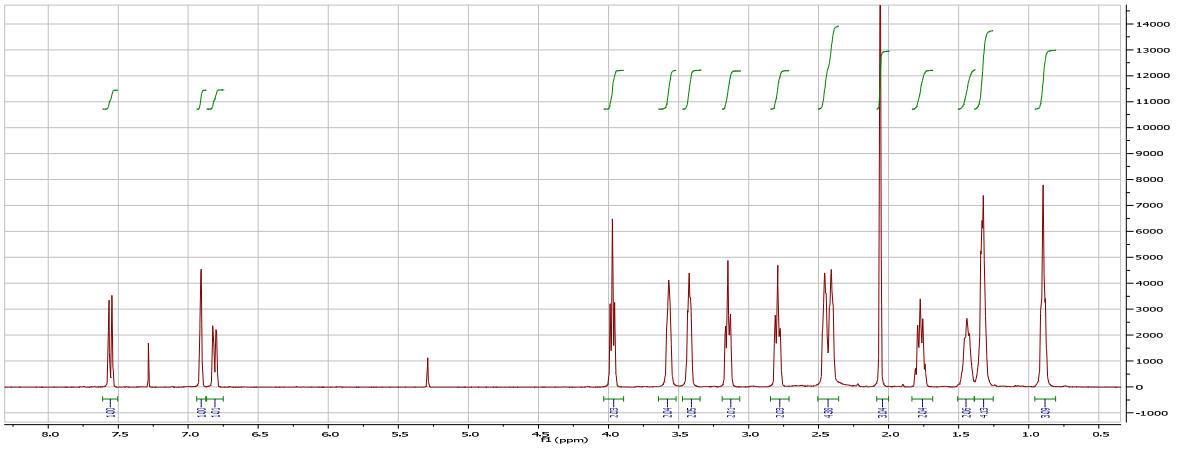


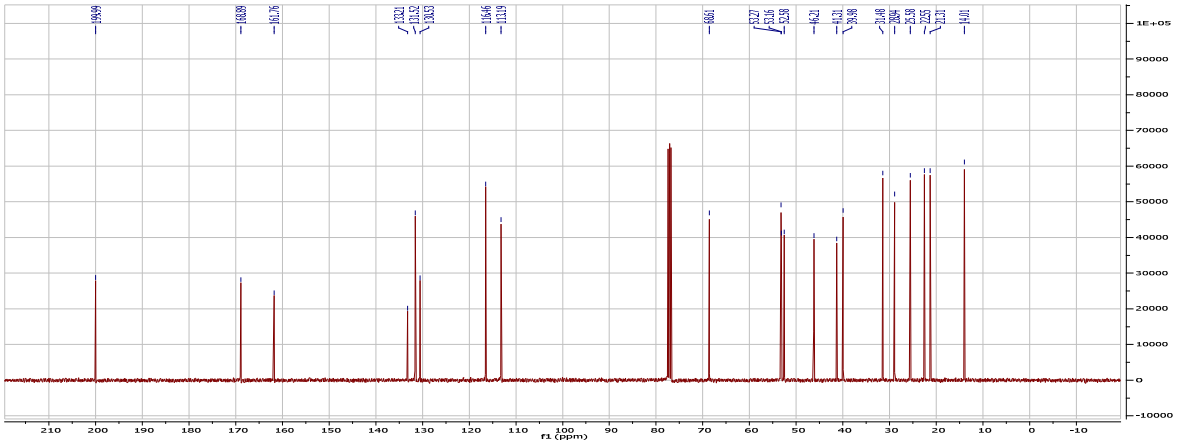


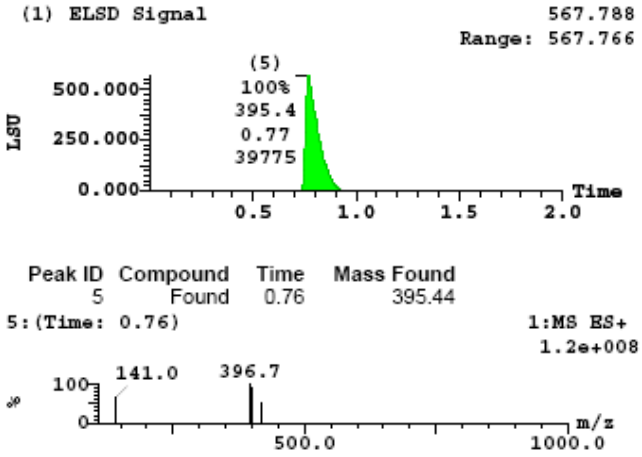
Peak ID	Compound	Time	Mass Found
5	Found	0.80	367.39



17{*1,1,5*}

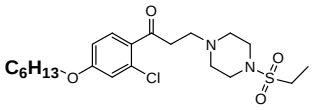




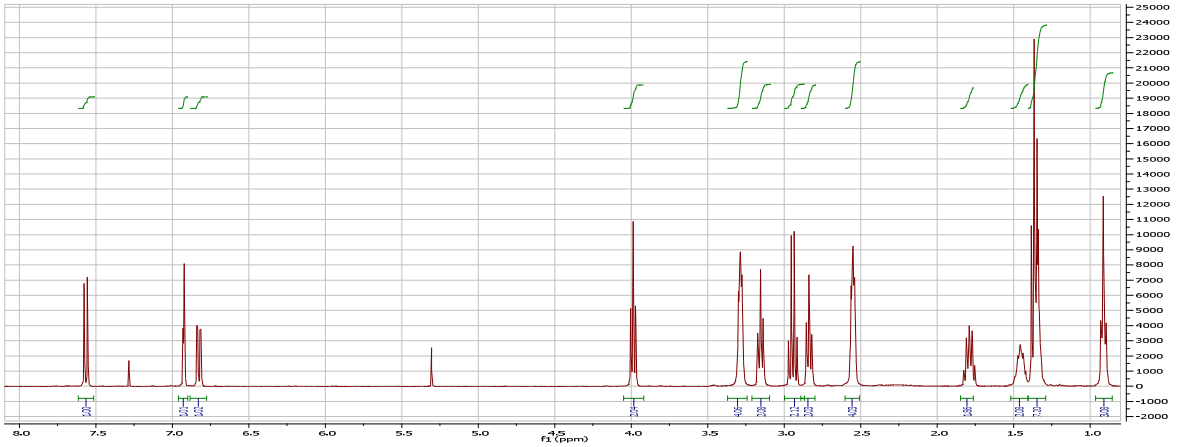


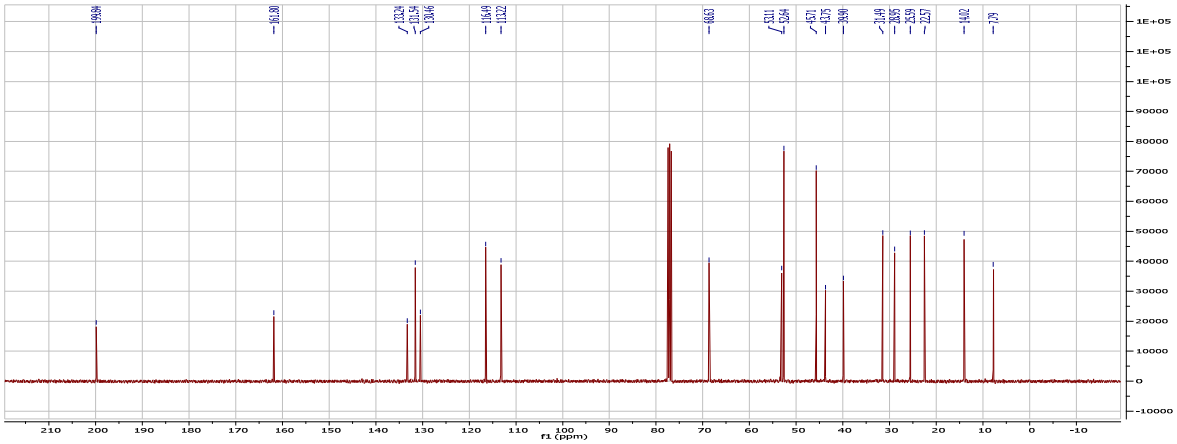
Peak ID	Compound	Time	Mass Found
5	Found	0.76	395.44

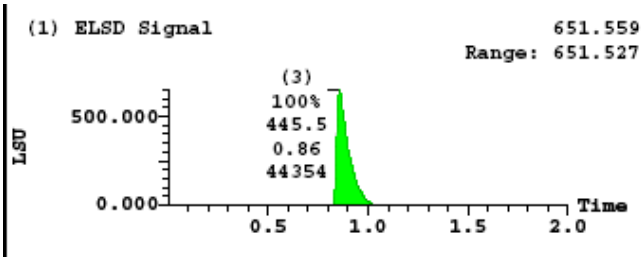
5:(Time: 0.76)



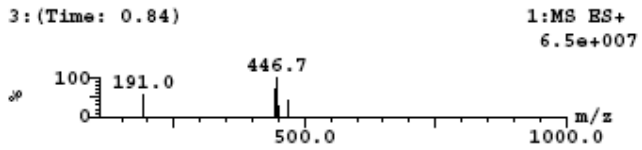
17{*1,1,6*}



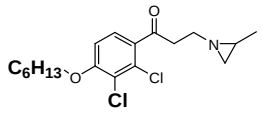




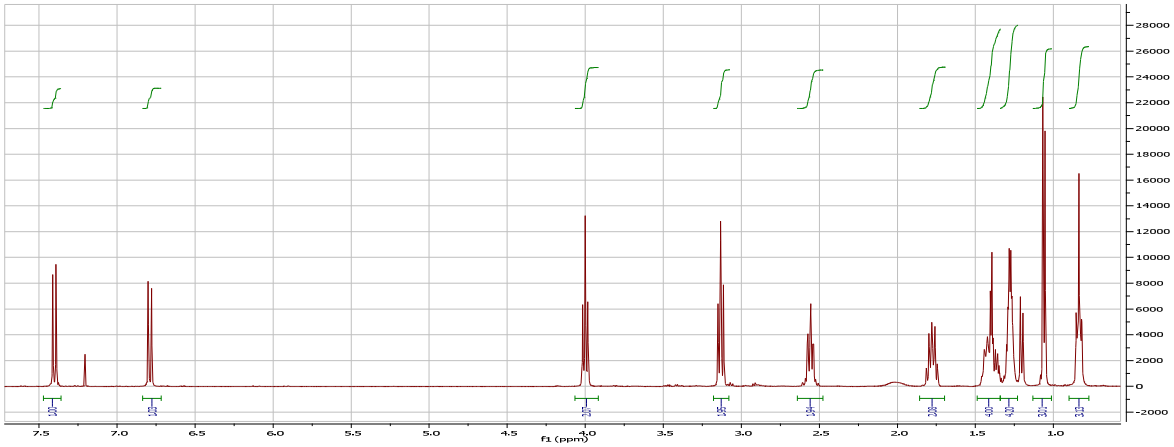
Peak ID	Compound	Time	Mass Found
3	Found	0.84	445.52

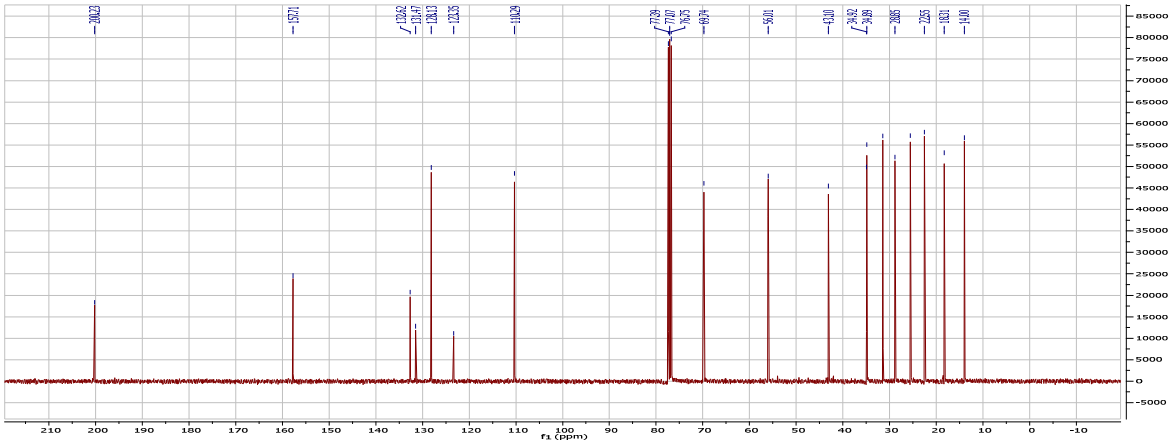


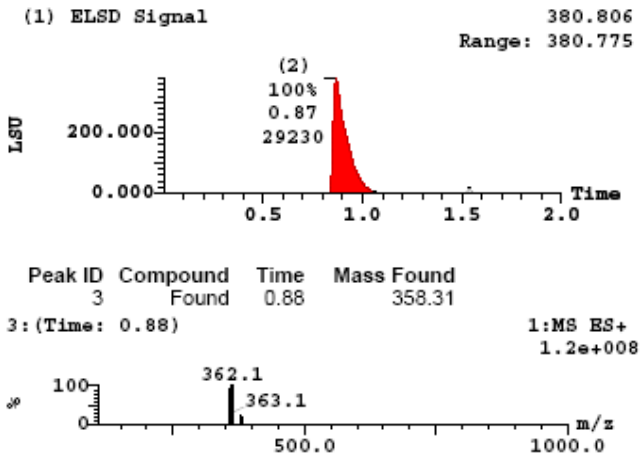
17{*1,2,1}* Same with **12**{*24*}



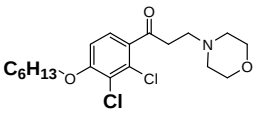
17{*1,2,2}*



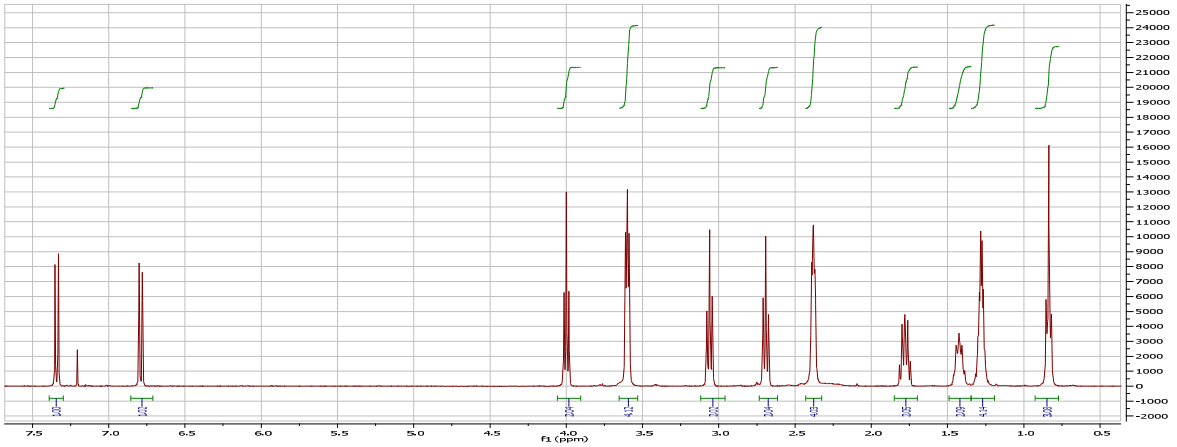


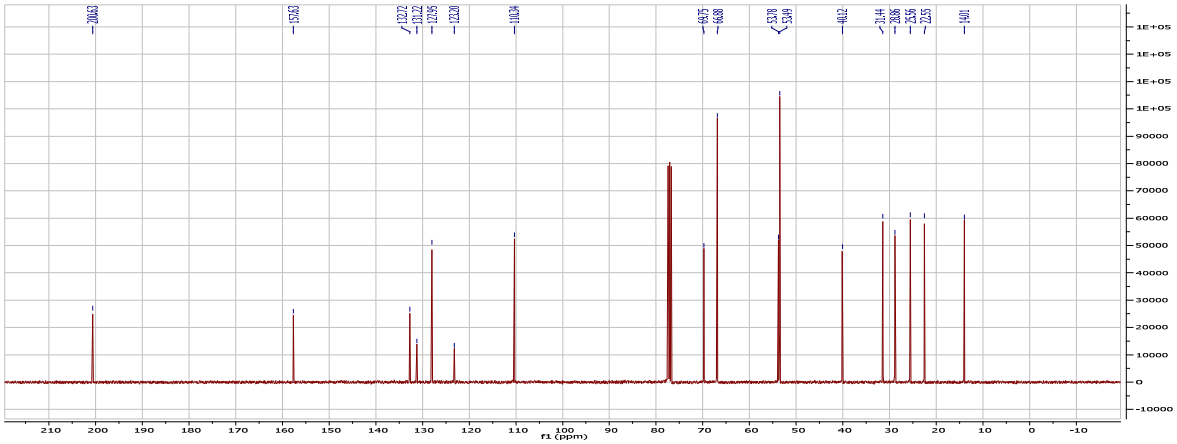


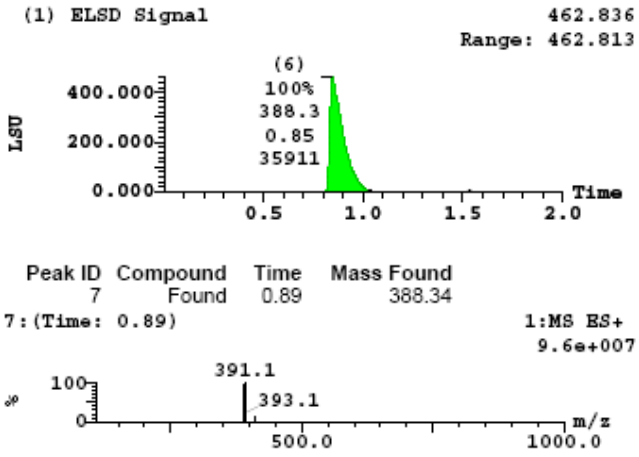
Peak ID	Compound	Time	Mass Found
3	Found	0.88	358.31



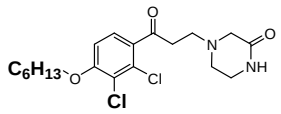
17{*1,2,3*}



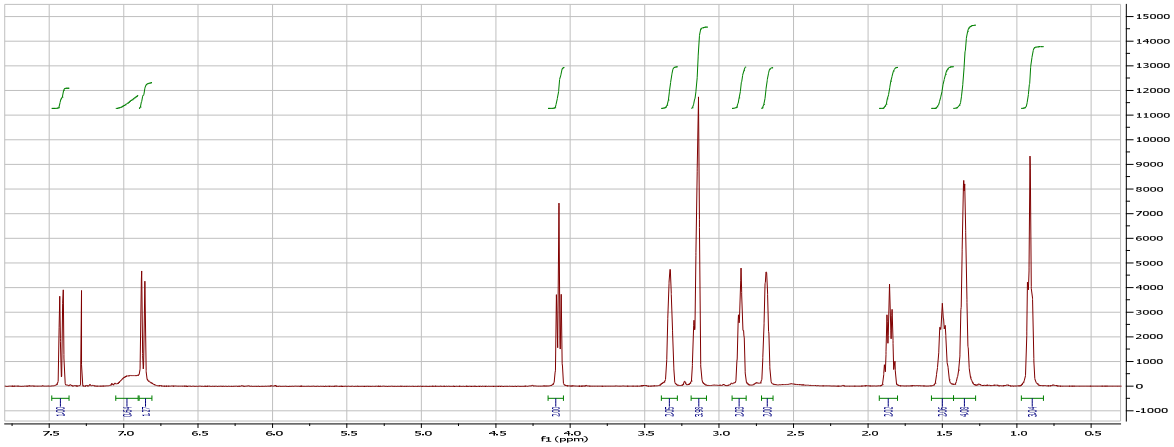


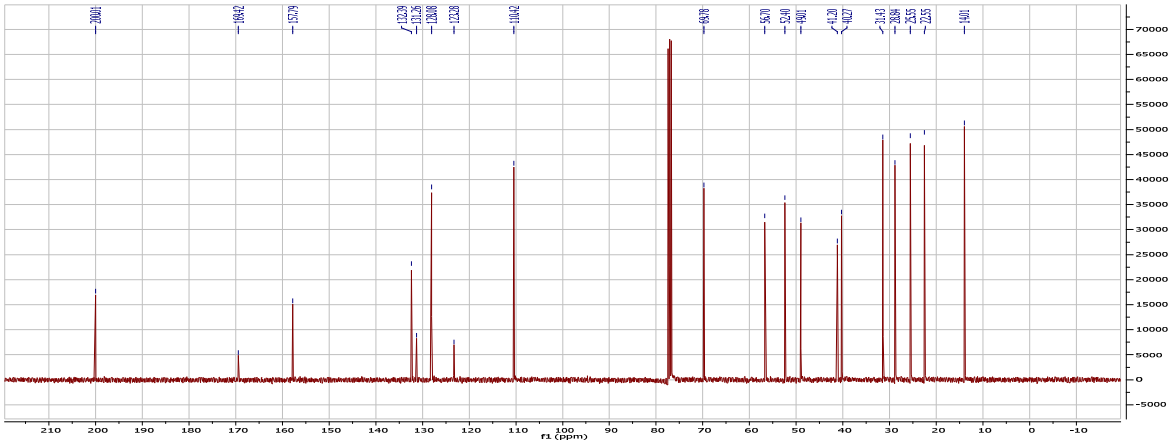


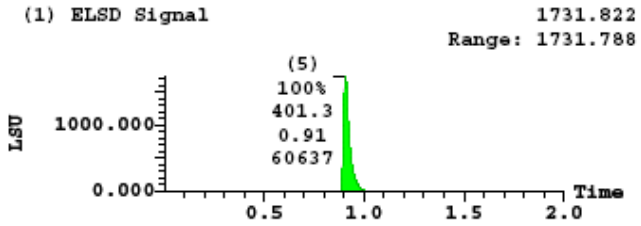
Peak ID	Compound	Time	Mass Found
7	Found	0.89	388.34



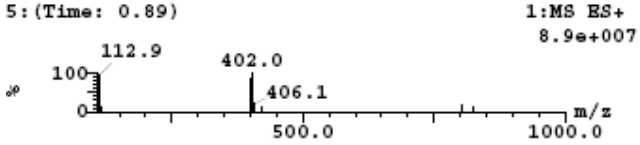
17{*1,2,4*}

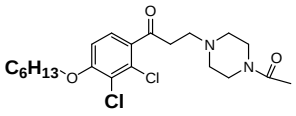




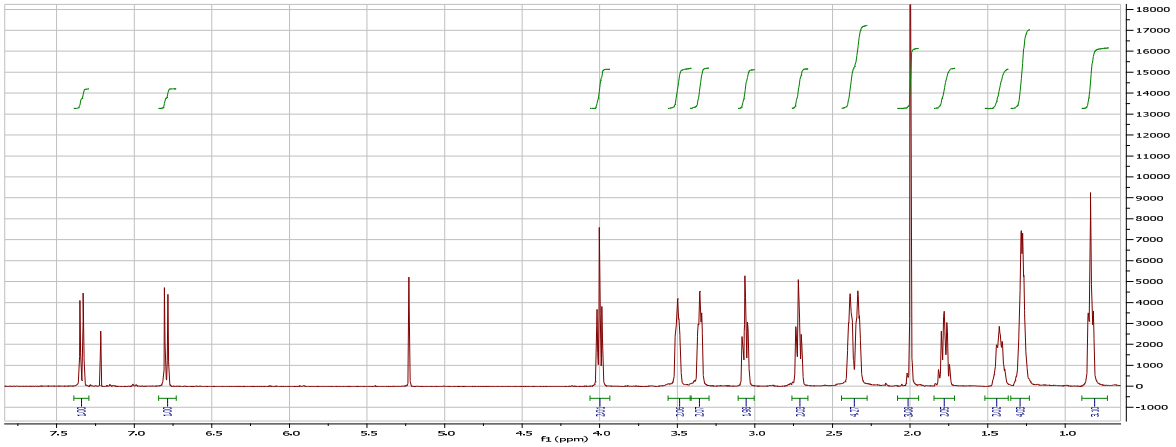


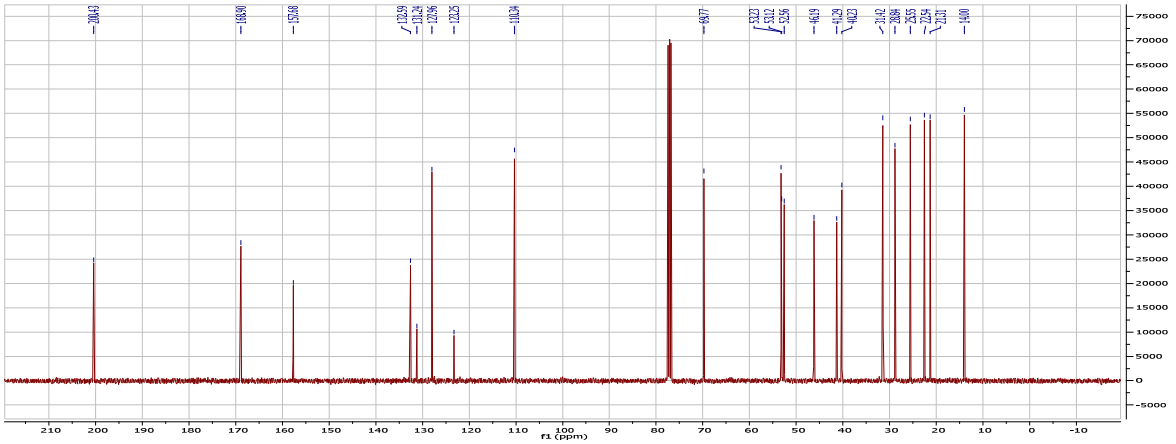
Peak ID	Compound	Time	Mass Found
5	Found	0.89	401.33

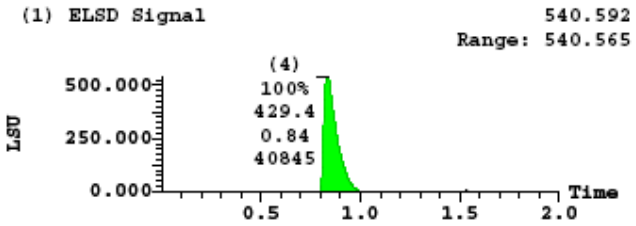


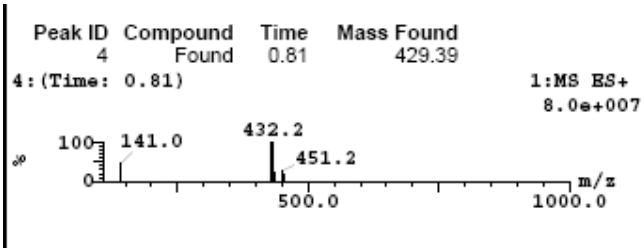

C6H13
O
Cl
Cl
O
N
N
O

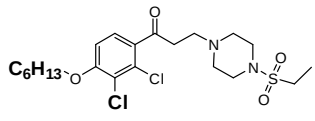
17{*1,2,5*}


f1 (ppm)

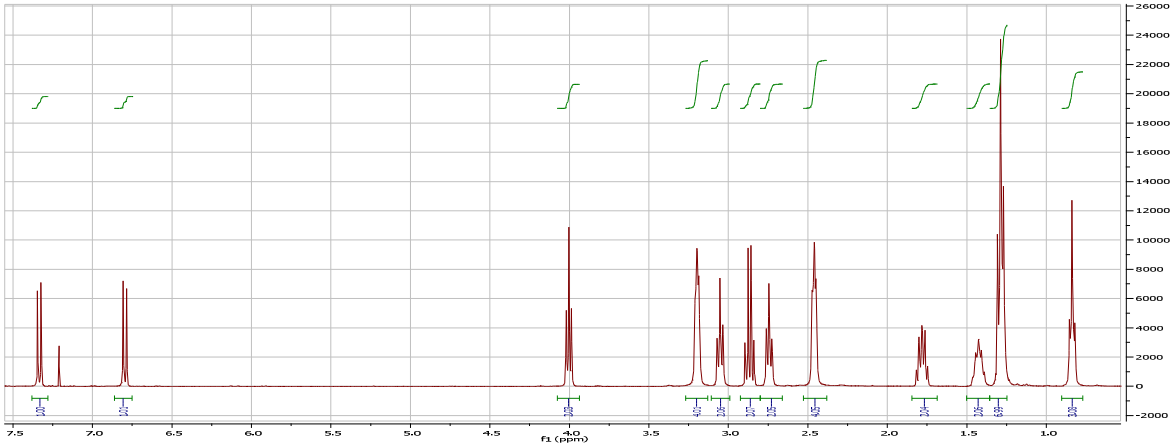

f1 (ppm)

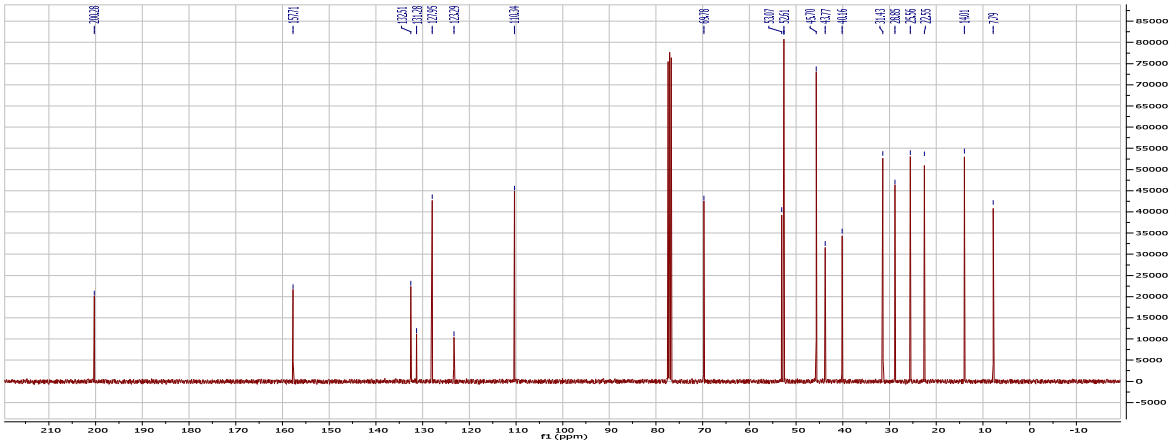

(1) ELSD Signal
540.592
Range: 540.565
(4)
100%
429.4
0.84
40845
500.000
250.000
0.000
LSU
0.5
1.0
1.5
2.0
Time

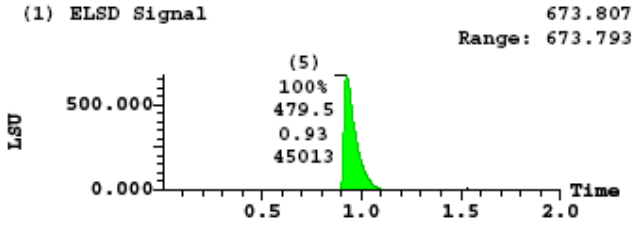

Peak ID Compound Time Mass Found
4 Found 0.81 429.39
4:(Time: 0.81)
1:MS ES+
8.0e+007
100
%
0
141.0
432.2
451.2
500.0
1000.0
m/z



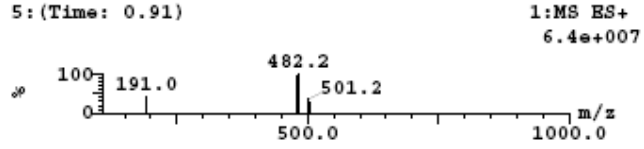
17{*1,2,6*}



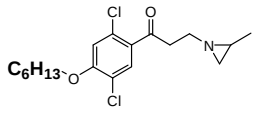




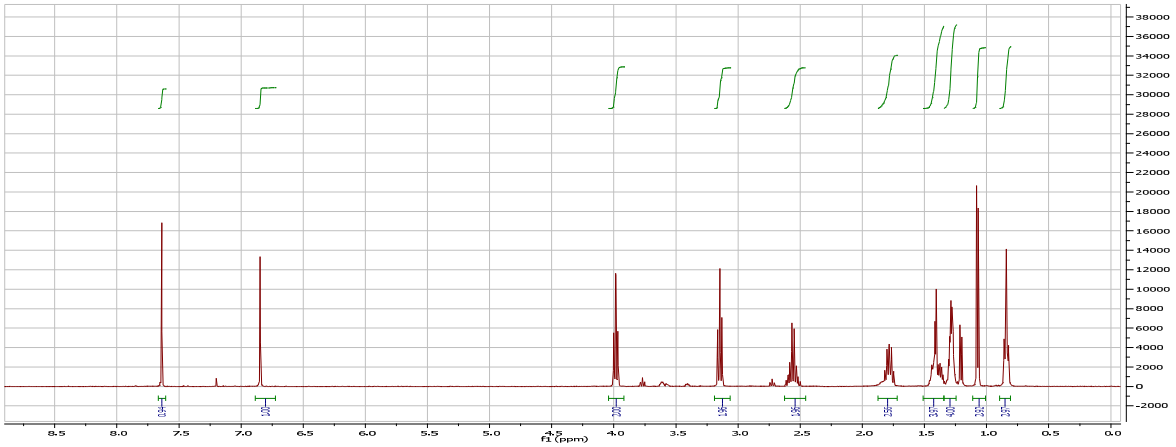
Peak ID	Compound	Time	Mass Found
5	Found	0.91	479.47

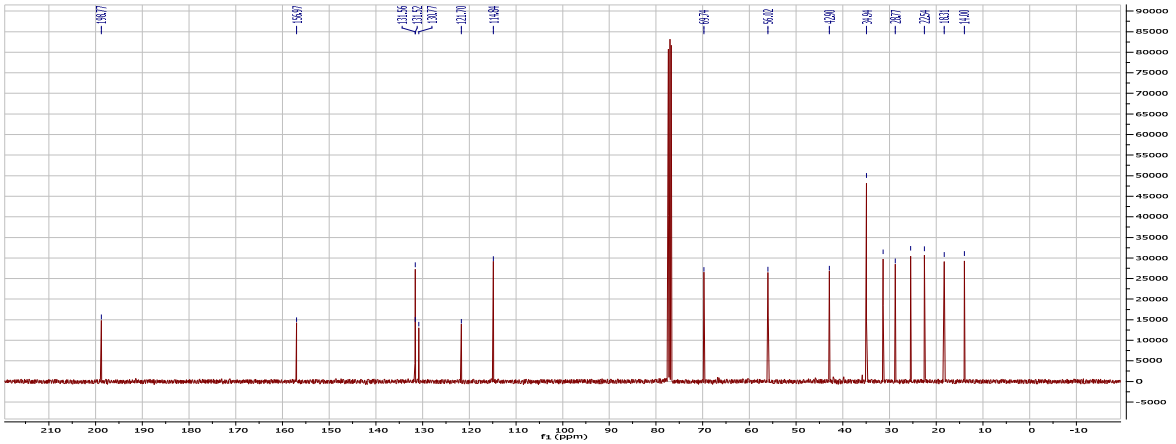


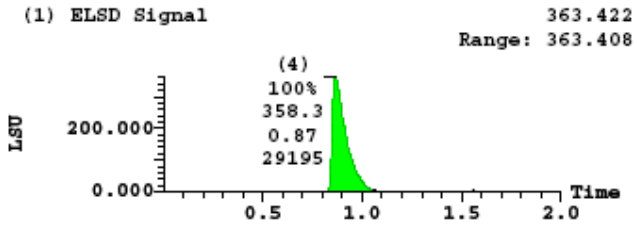
17{*1,3,1}* Same with **12**{25}

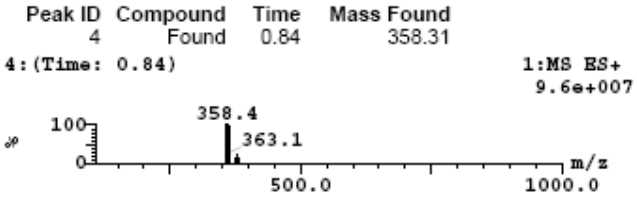


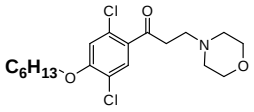
17{*1,3,2}*



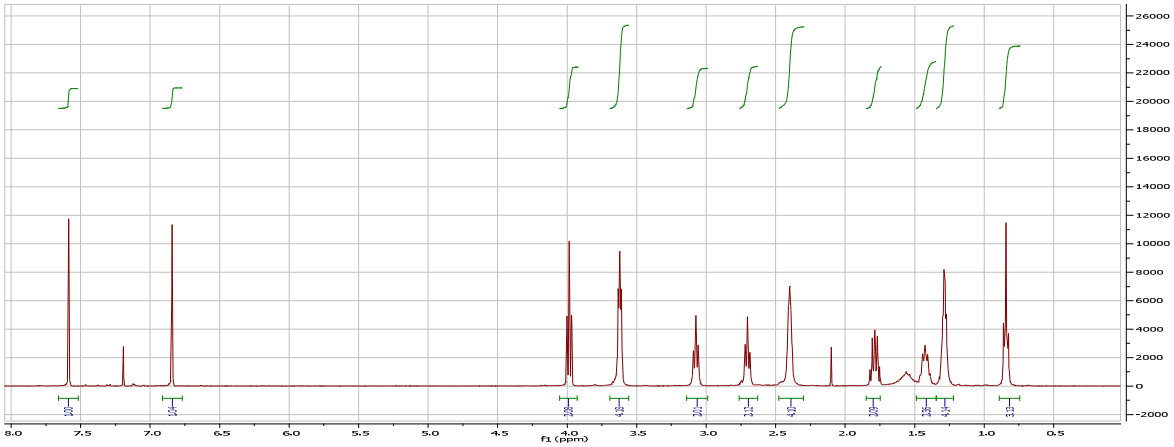


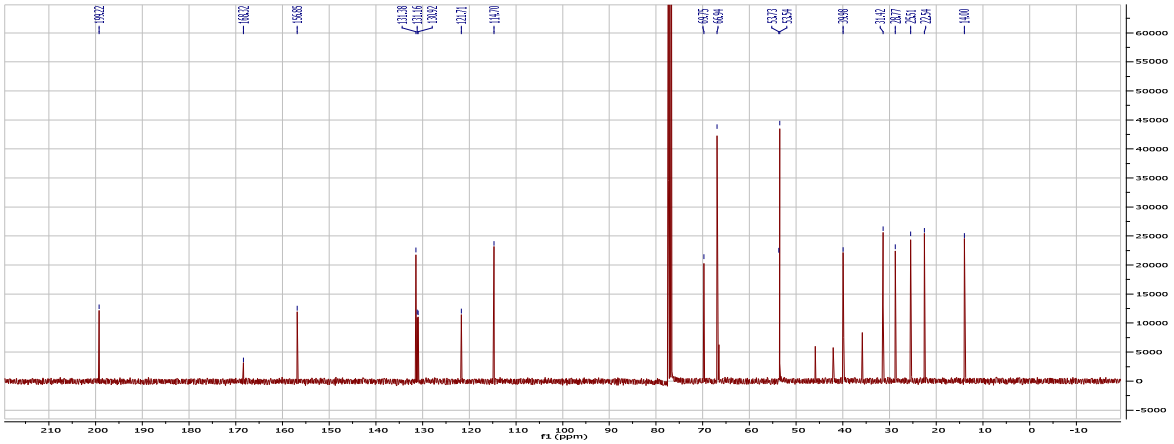


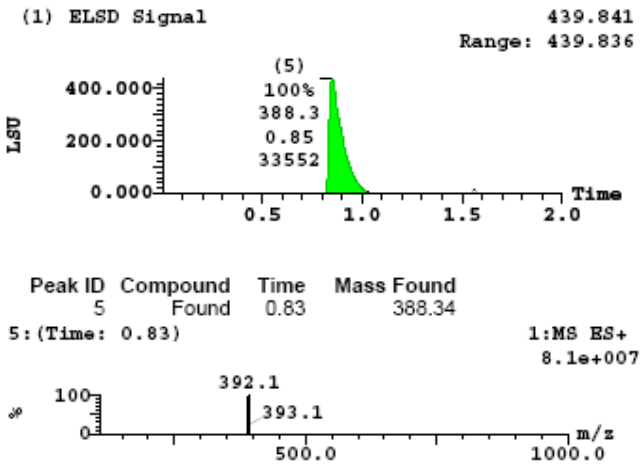




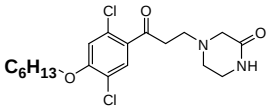
17{*1,3,3*}



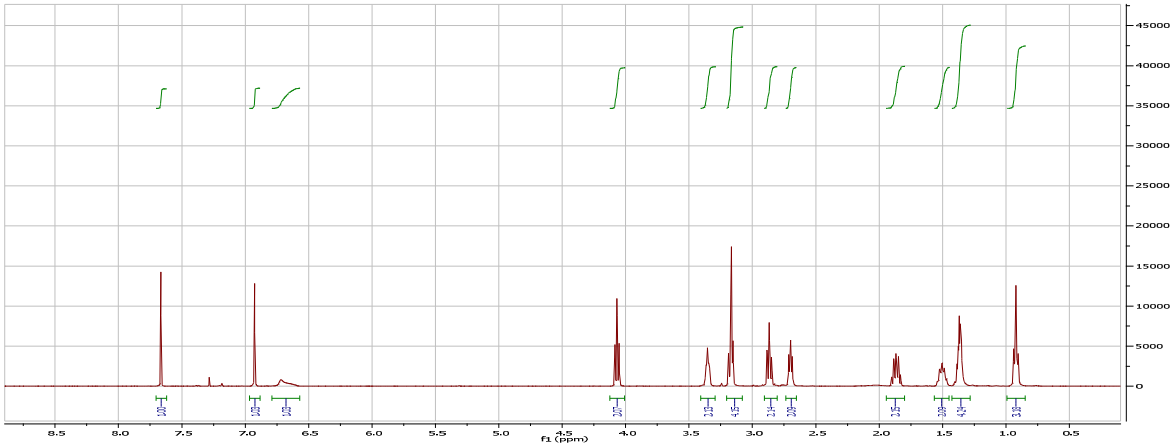


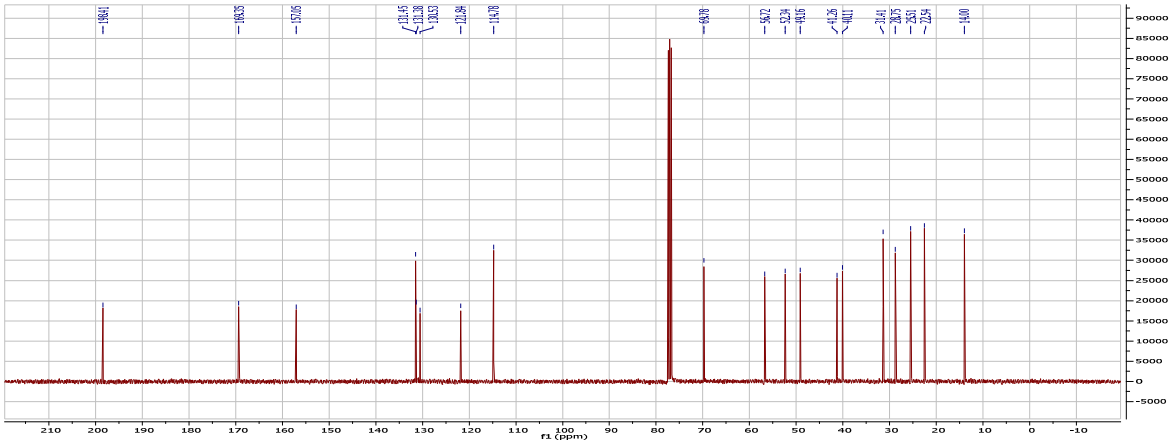


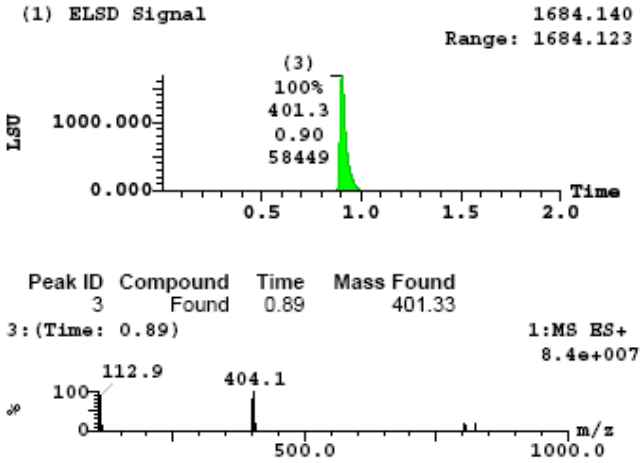
Peak ID	Compound	Time	Mass Found
5	Found	0.83	388.34



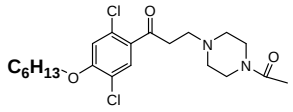
17{*1,3,4*}



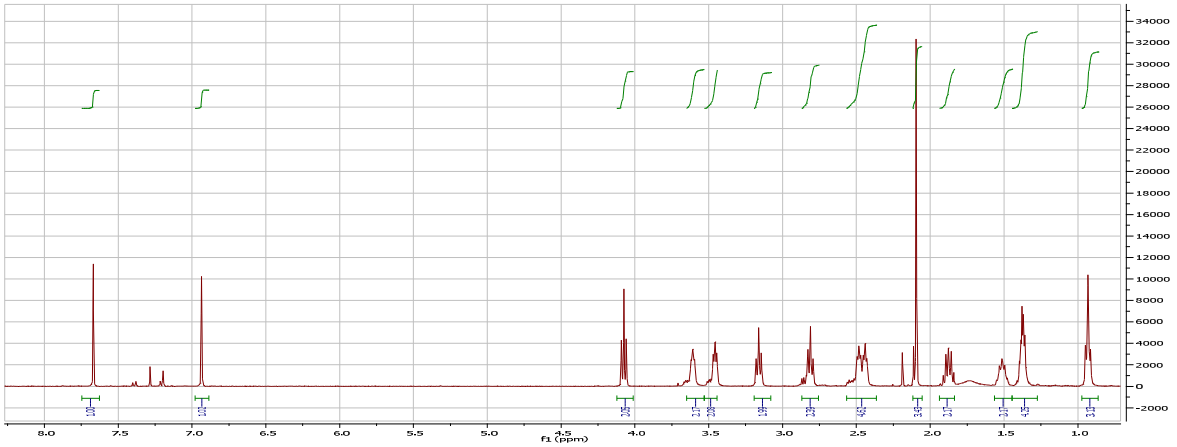


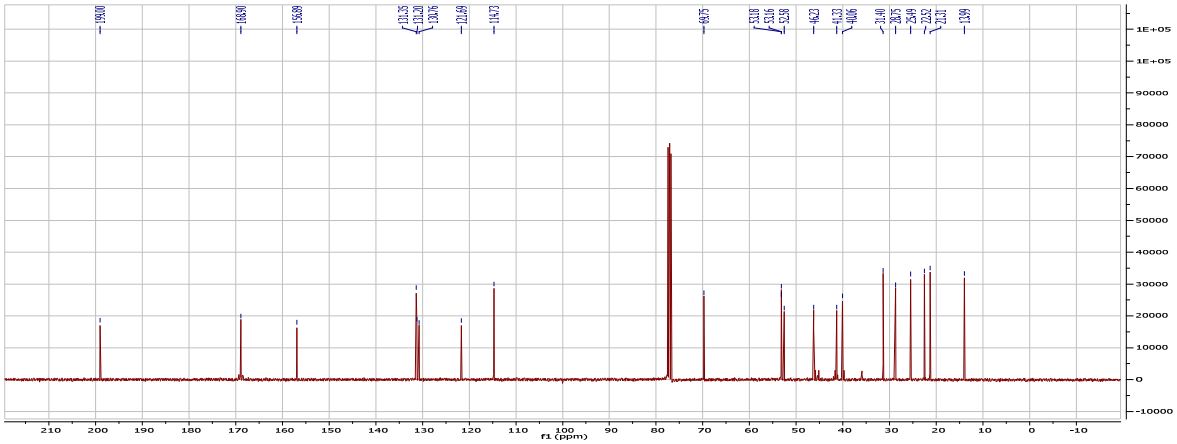


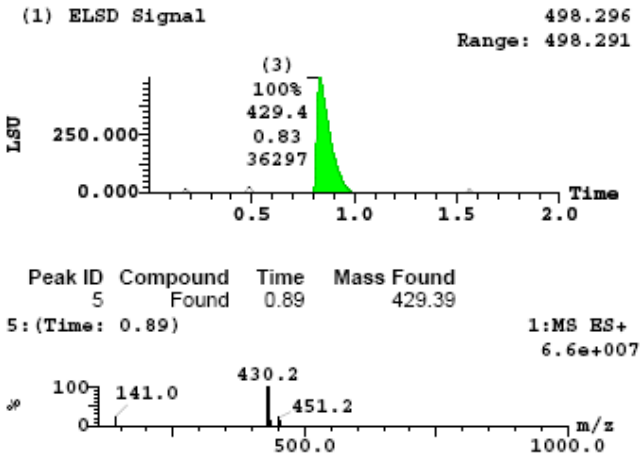
Peak ID	Compound	Time	Mass Found
3	Found	0.89	401.33



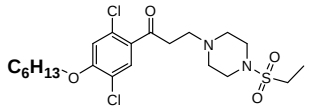
17{*1,3,5*}



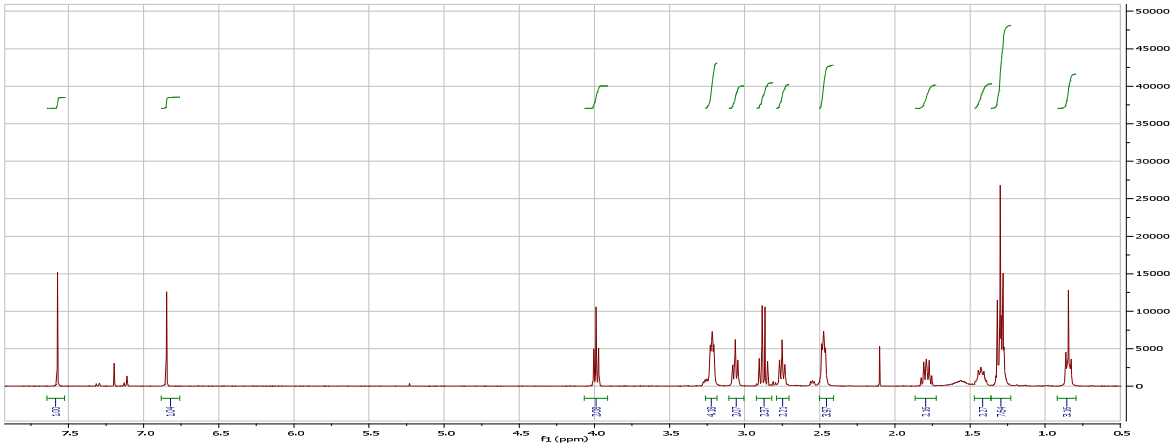


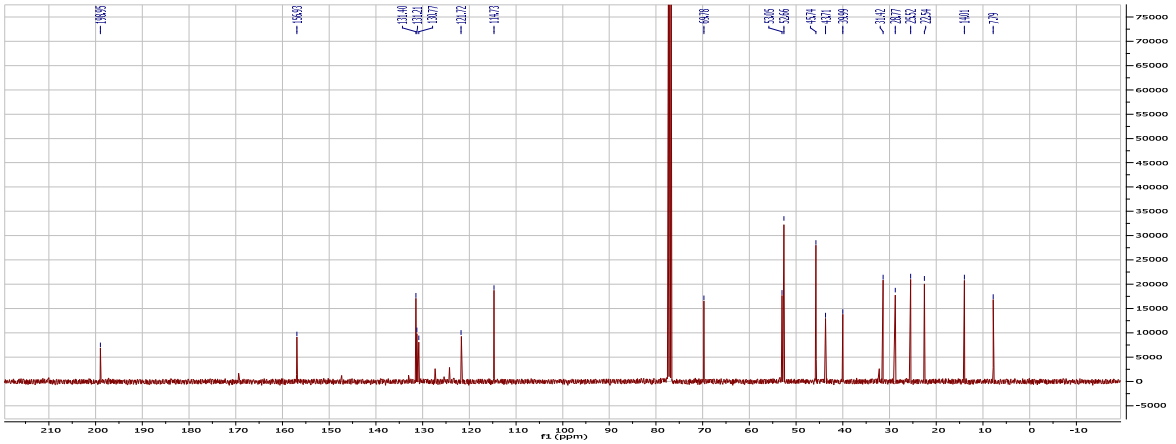


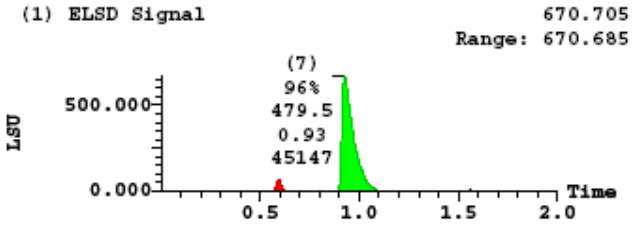
Peak ID	Compound	Time	Mass Found
5	Found	0.89	429.39



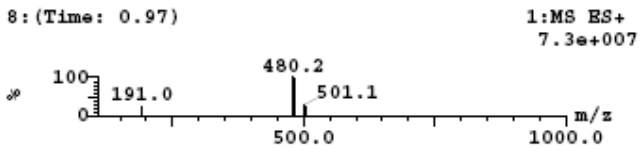
17{*1,3,6*}



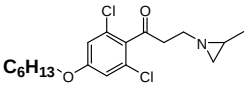




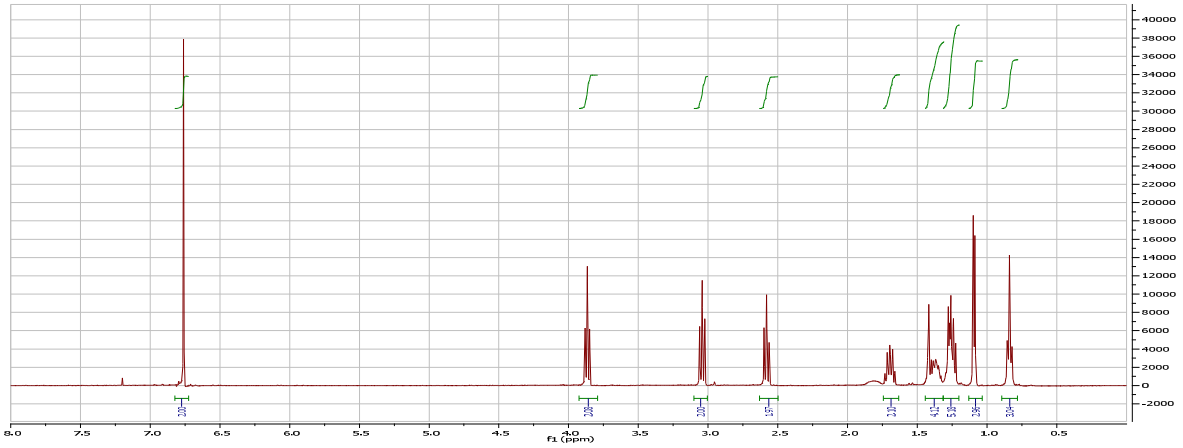
Peak ID	Compound	Time	Mass Found
8	Found	0.97	479.47

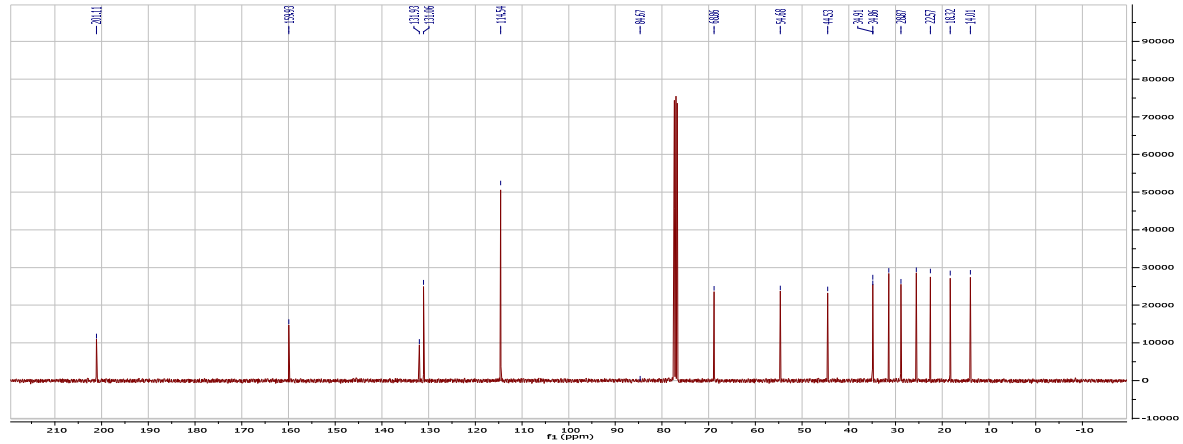


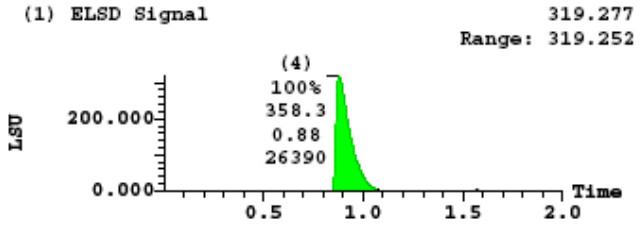
17{*1,4,1}* Same with 12{26}

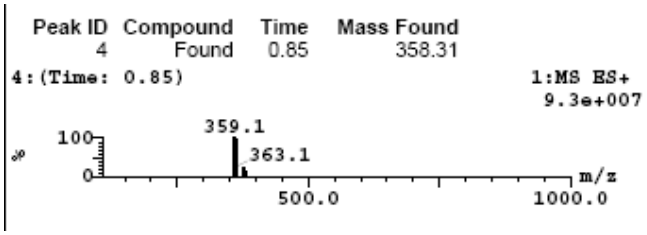


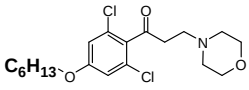
17{*1,4,2}*



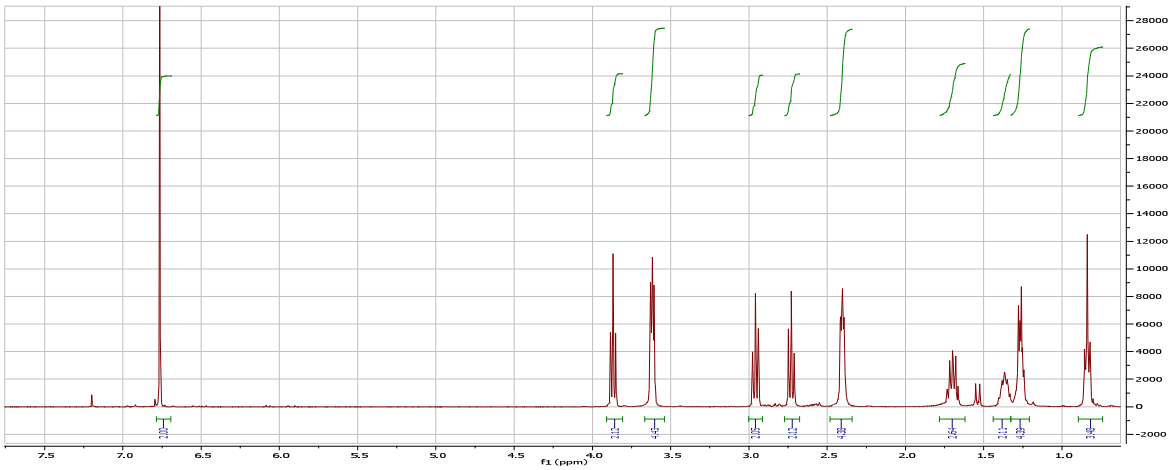


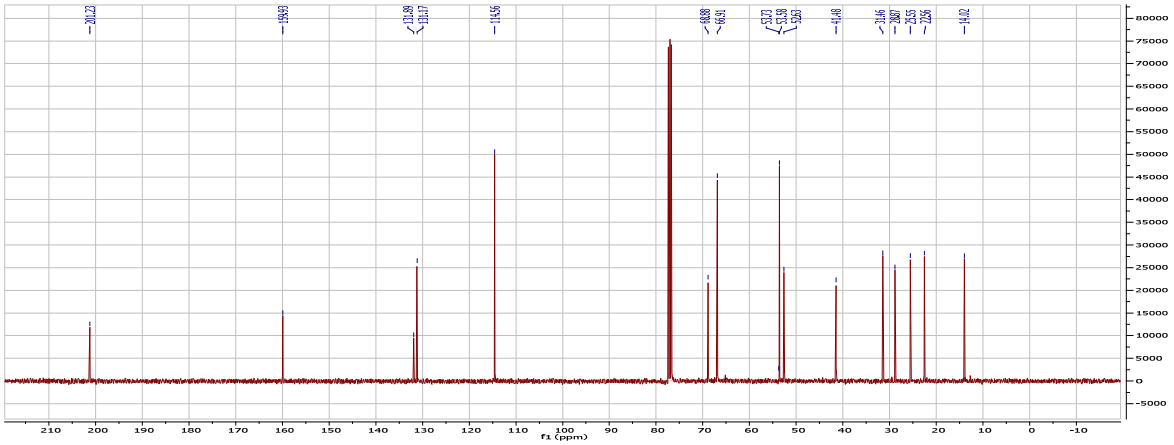


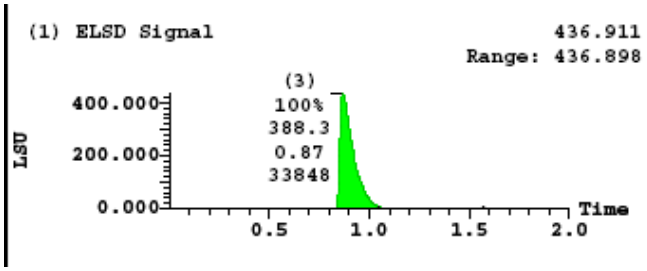




17{*1,4,3*}



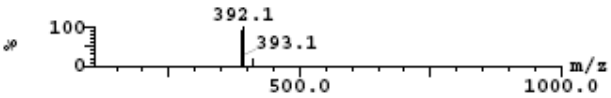


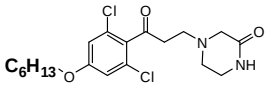


Peak ID	Compound	Time	Mass Found
3	Found	0.84	388.34

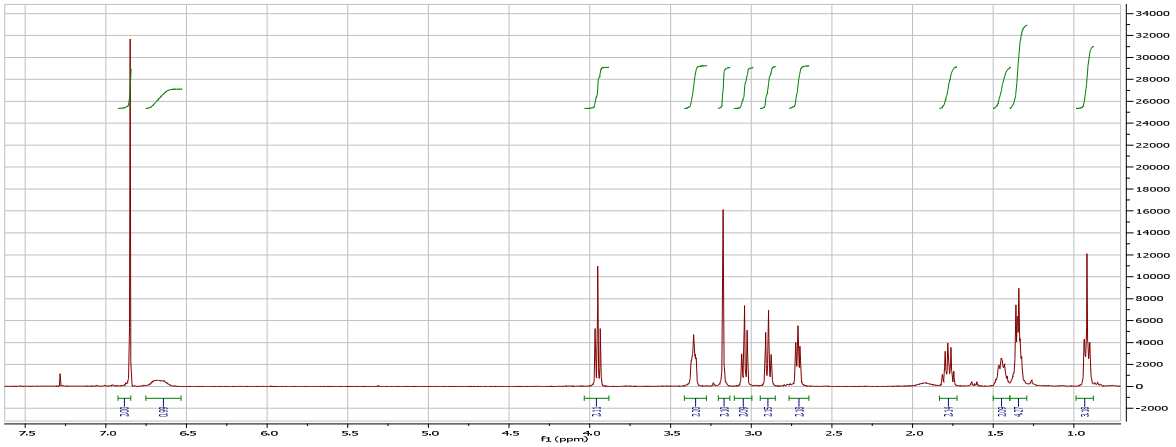
3:(Time: 0.84)

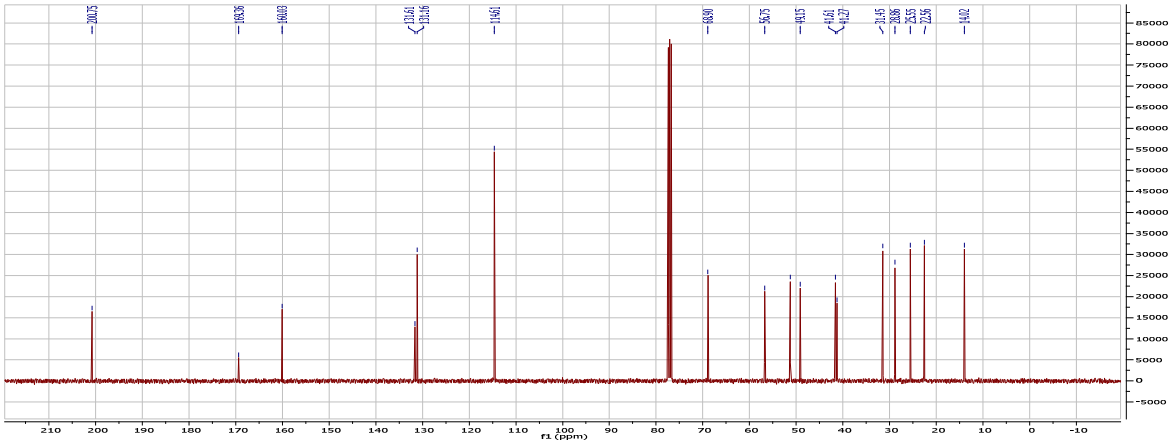
1:MS ES+
7.3e+007

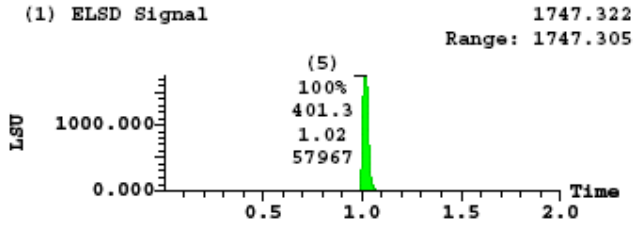


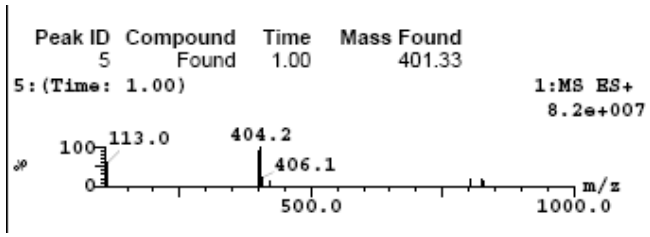

Cl
O
N
O
NH
Cl
C6H13
O

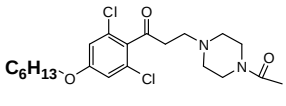
17{*1,4,4*}



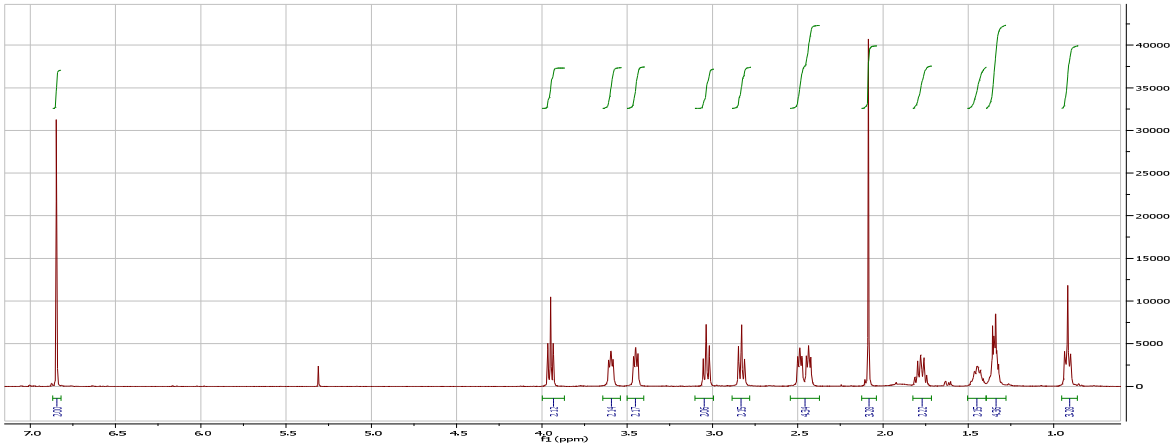


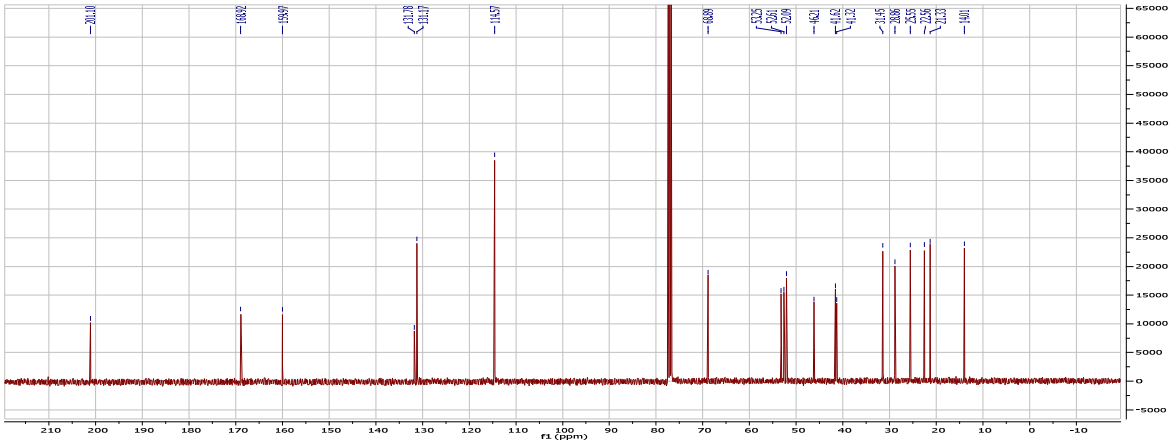

(1) ELSD Signal
1747.322
Range: 1747.305
(5)
100%
401.3
1.02
57967
LSU
1000.000
0.000
0.5
1.0
1.5
2.0
Time

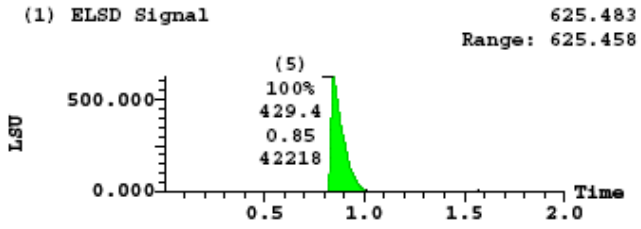

Peak ID Compound Time Mass Found
5 Found 1.00 401.33
5:(Time: 1.00)
1:MS ES+
8.2e+007
100
%
0
113.0
404.2
406.1
500.0
1000.0
m/z



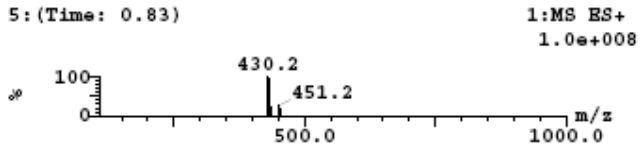
17{*1,4,5*}

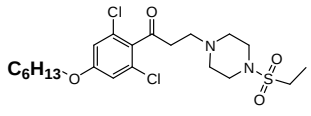




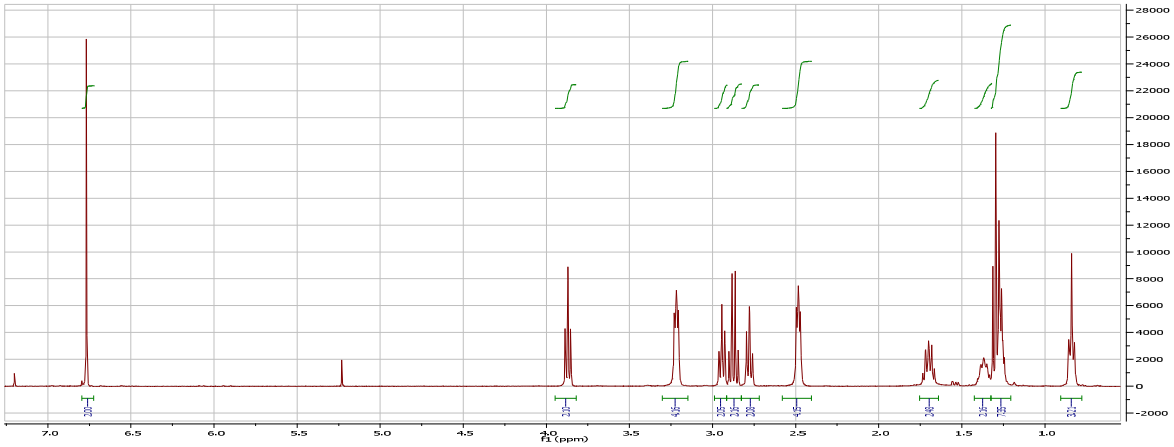


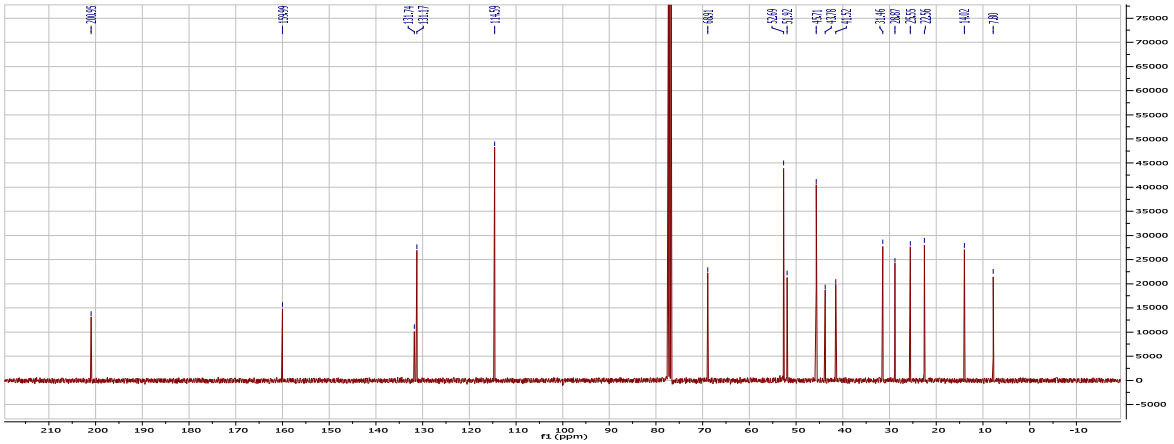
Peak ID	Compound	Time	Mass Found
5	Found	0.83	429.39

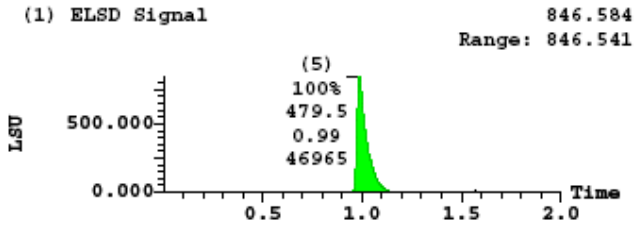


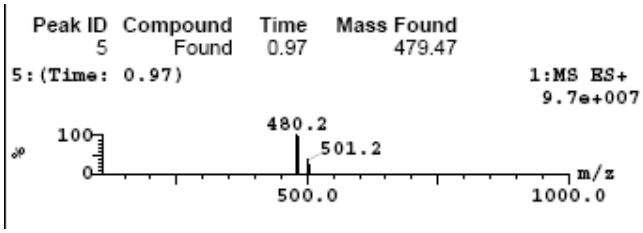

Cl
O
N
N
O
S
O
Cl
C6H13O

17{*1,4,6*}

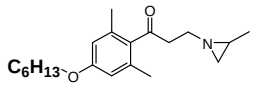




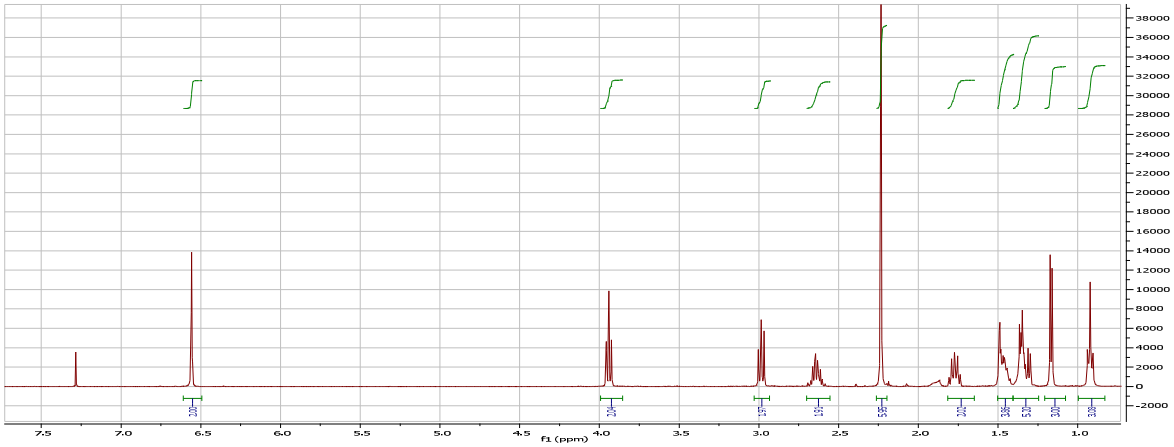

(1) ELSD Signal
846.584
Range: 846.541
(5)
100%
479.5
0.99
46965
LSU
500.000
0.000
Time
0.5
1.0
1.5
2.0

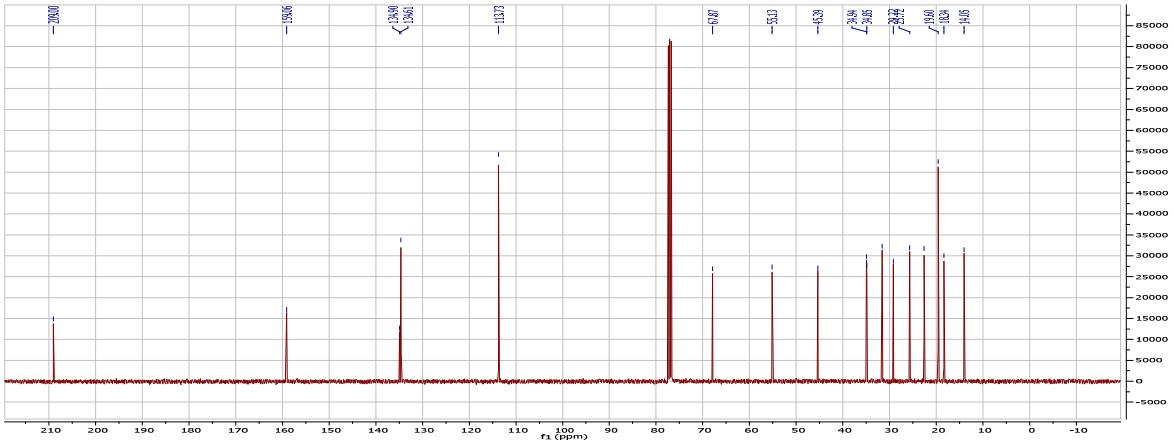

Peak ID Compound Time Mass Found
5 Found 0.97 479.47
5:(Time: 0.97)
1:MS ES+
9.7e+007
480.2
501.2
100
%
0
m/z
500.0
1000.0

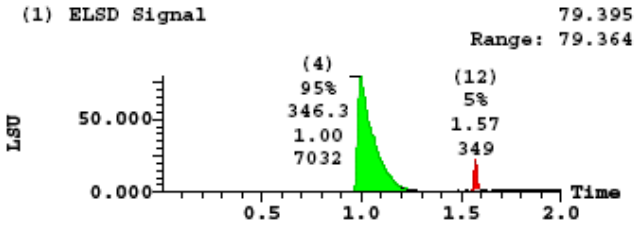
17{*1,5,1}* Same with **12**{*22*}



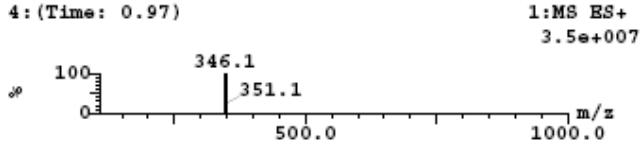
17{*1,5,2}*

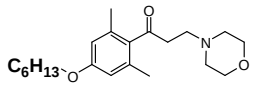




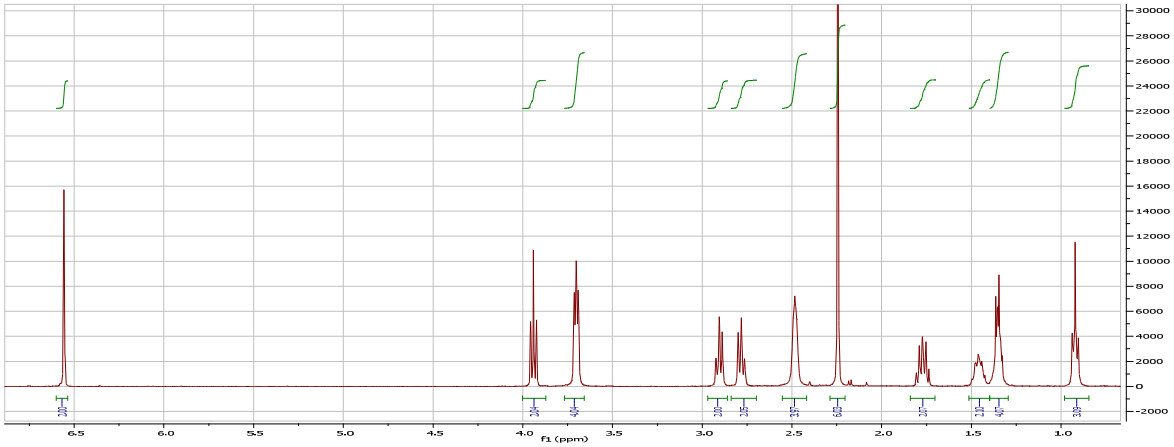


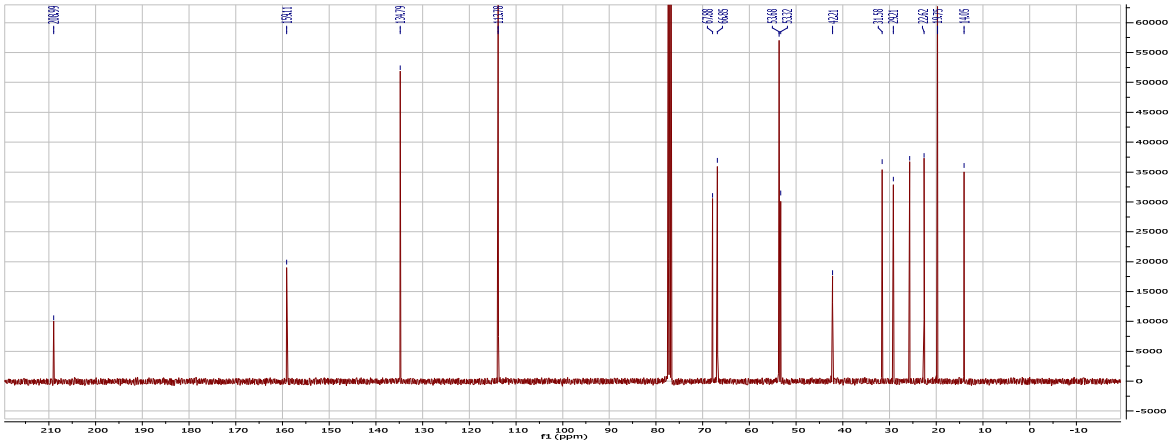
Peak ID	Compound	Time	Mass Found
4	Found	0.97	346.30

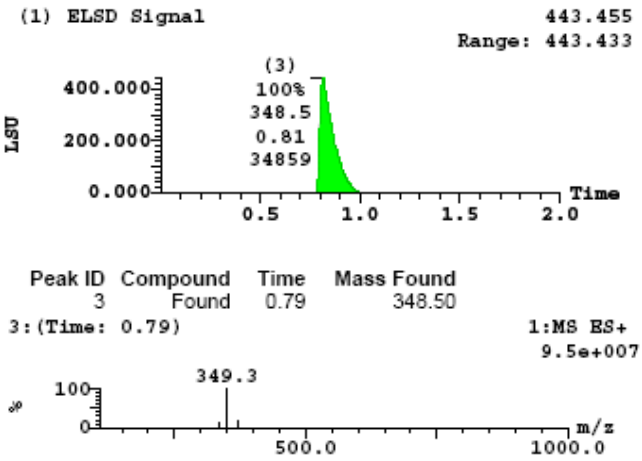




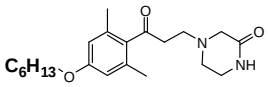
17{*1,5,3*}



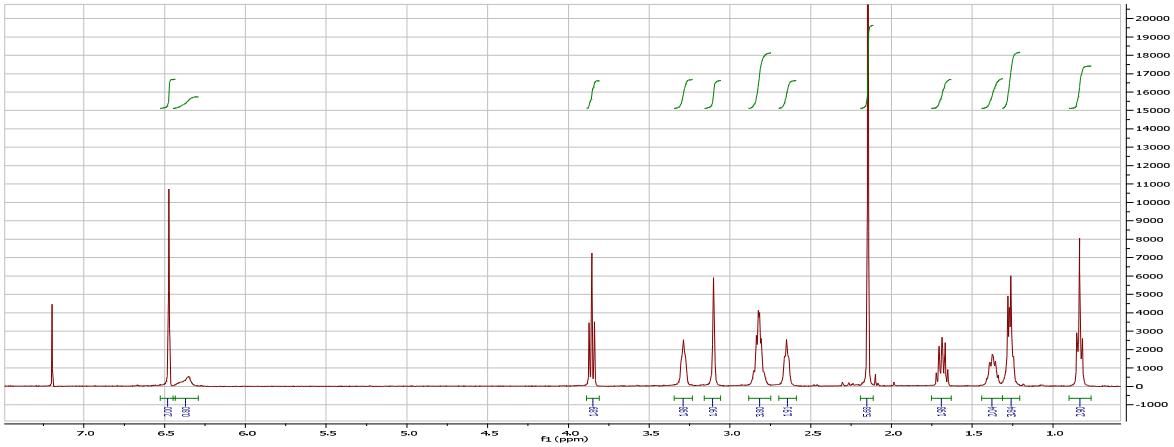


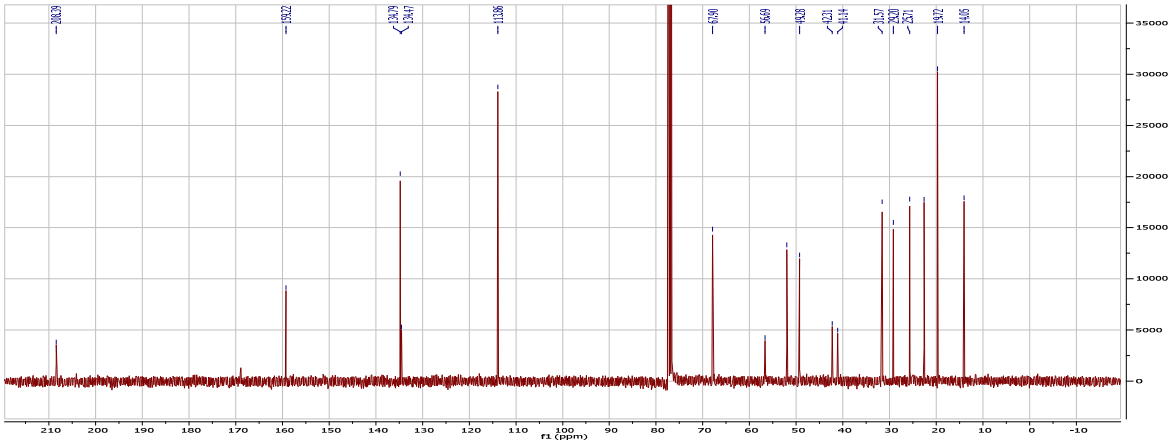


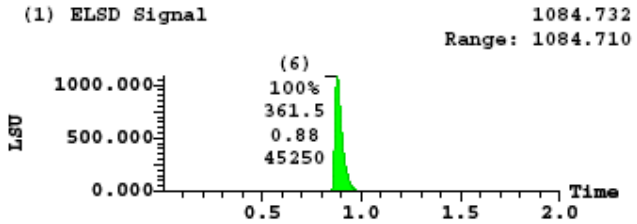
Peak ID	Compound	Time	Mass Found
3	Found	0.79	348.50

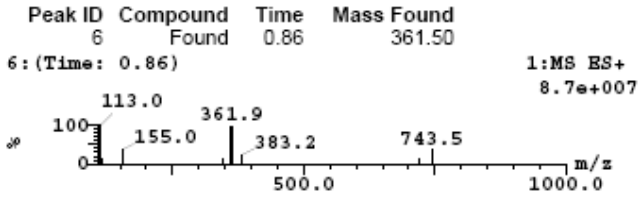


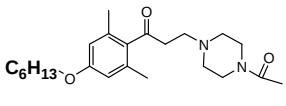
17{*1,5,4*}



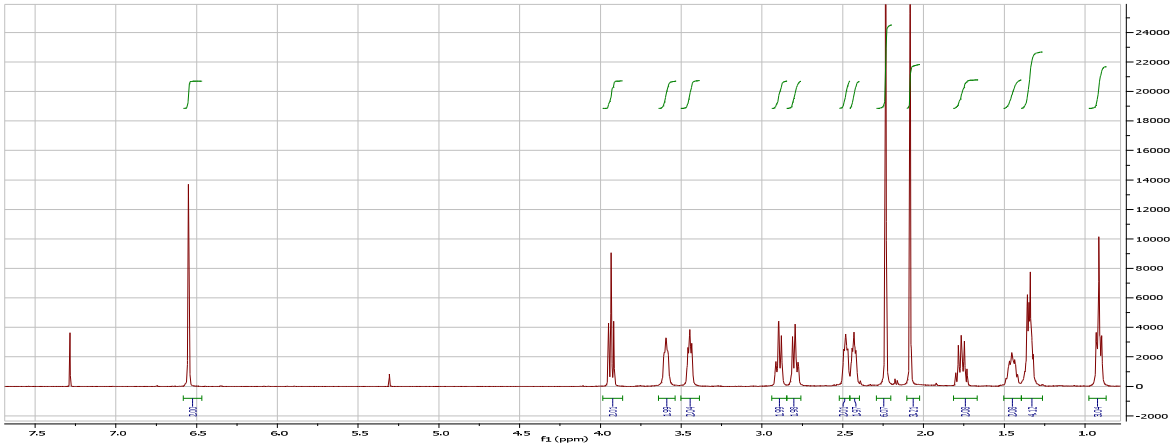


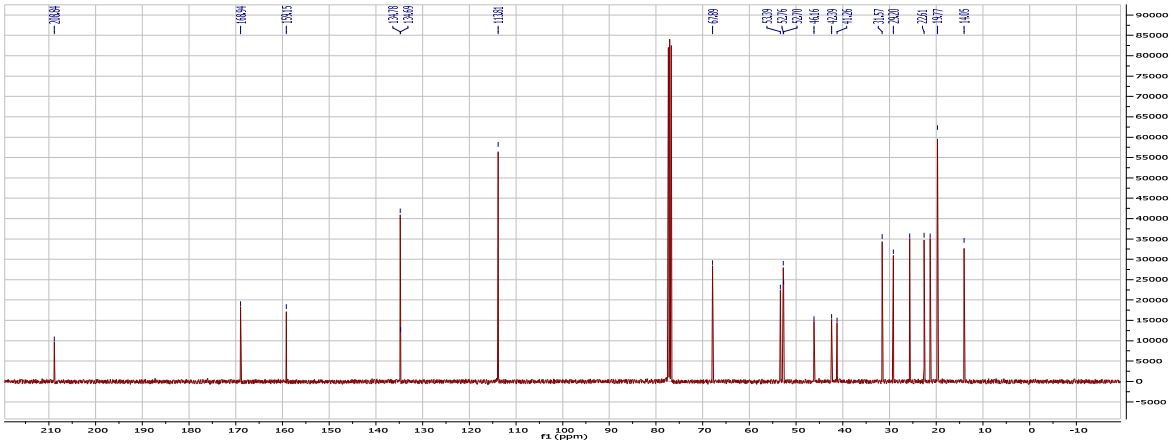

(1) ELSD Signal
1084.732
Range: 1084.710
(6)
100%
361.5
0.88
45250
1000.000
500.000
0.000
LSU
0.5
1.0
1.5
2.0
Time

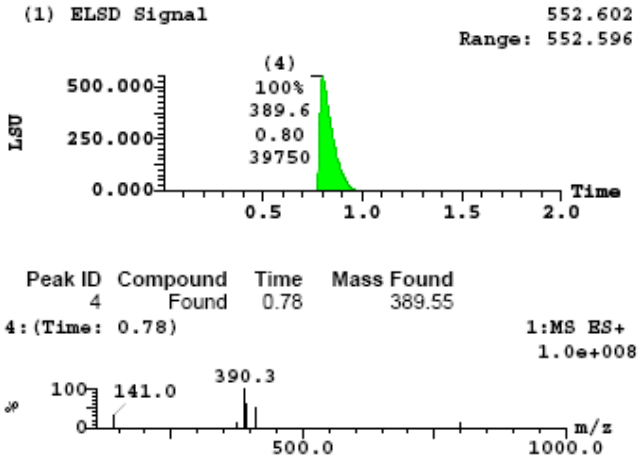

Peak ID Compound Time Mass Found
6 Found 0.86 361.50
6:(Time: 0.86)
1:MS ES+
8.7e+007
113.0
361.9
155.0
383.2
743.5
100
%
0
500.0
1000.0
m/z



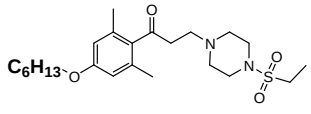
17{*1,5,5*}



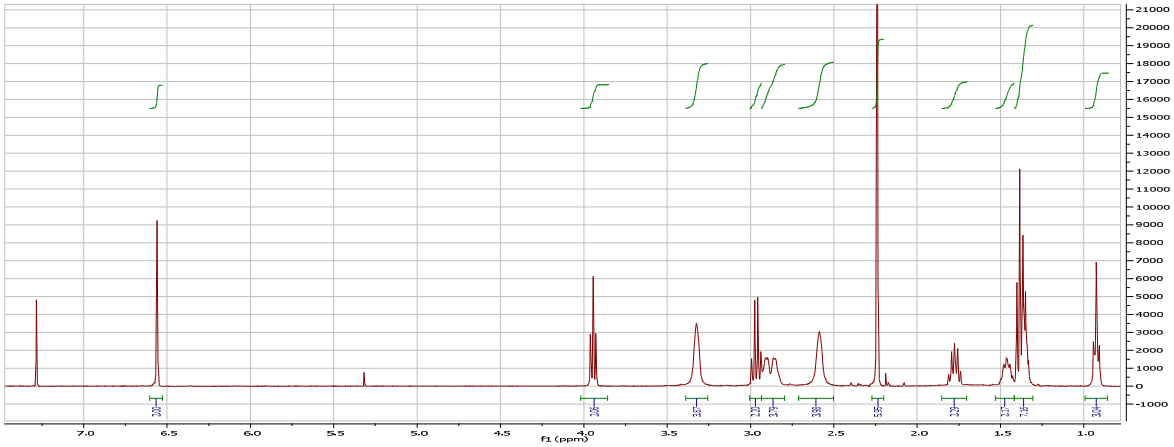


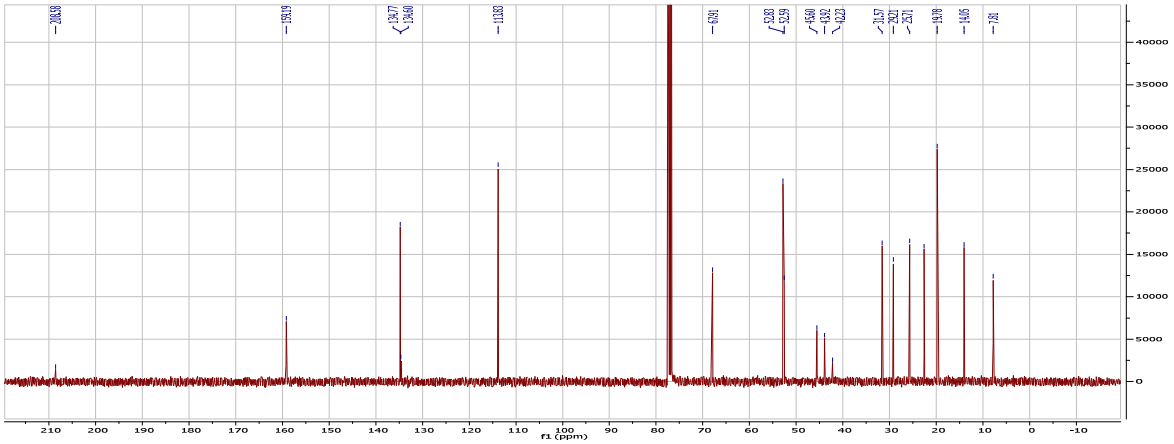


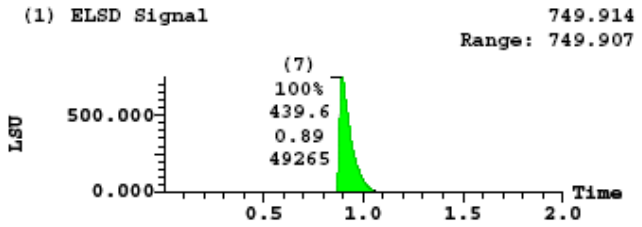
Peak ID	Compound	Time	Mass Found
4	Found	0.78	389.55



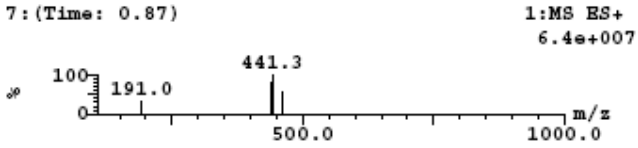
17{*1,5,6*}

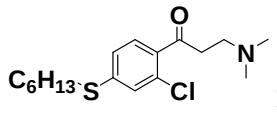




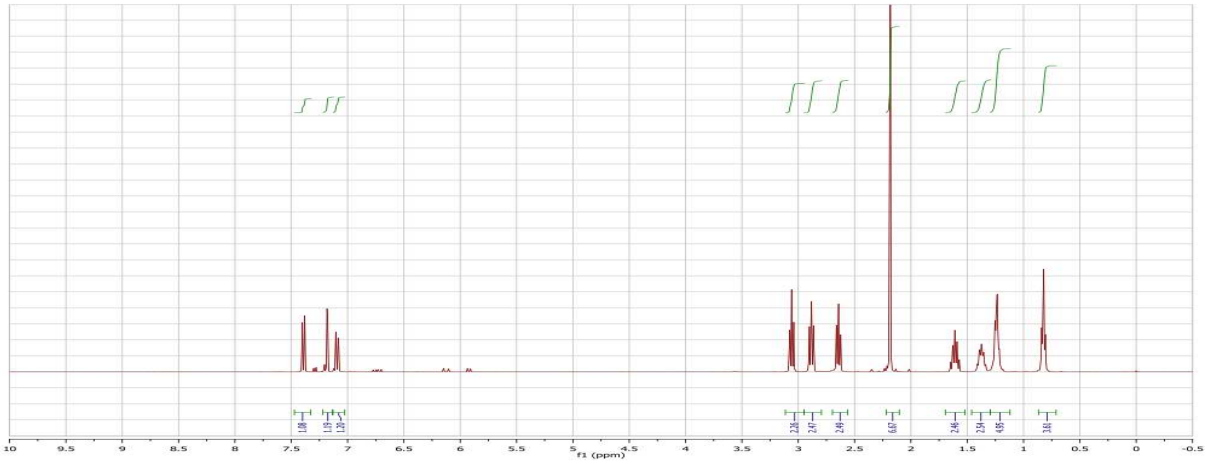


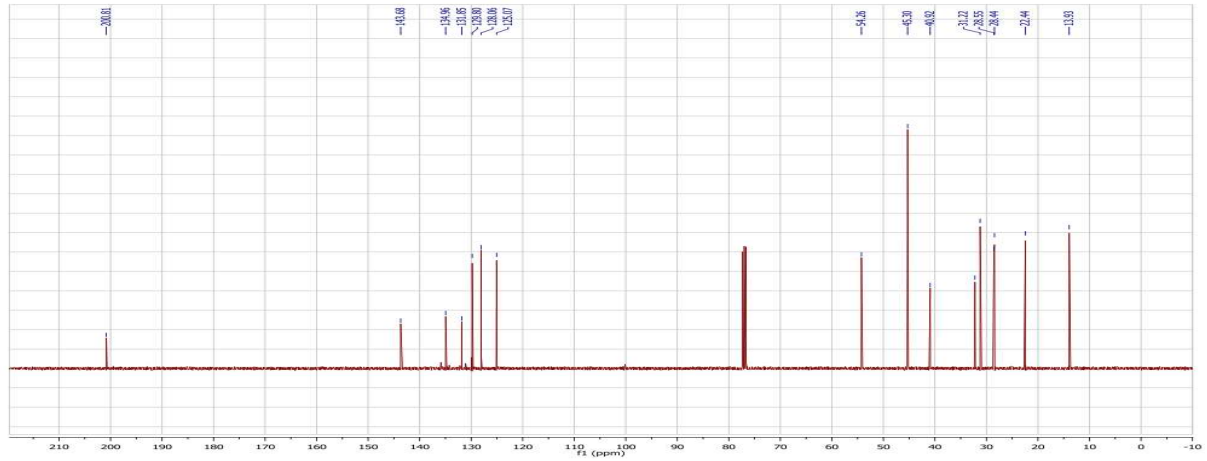
Peak ID	Compound	Time	Mass Found
7	Found	0.87	439.63

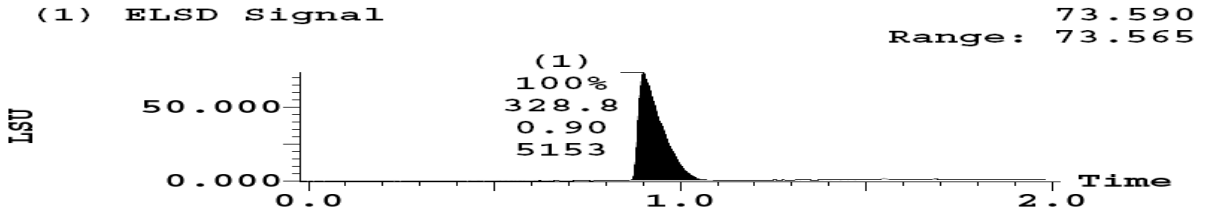




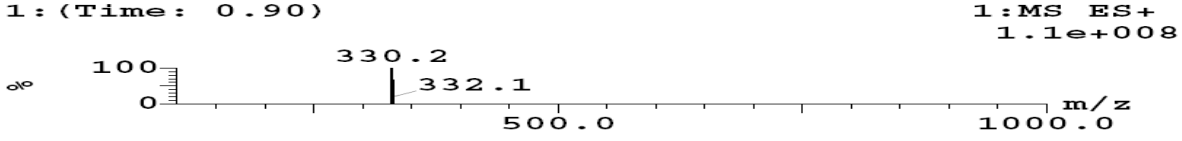
17{*2,1,1*}

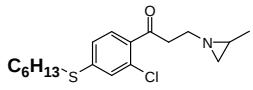




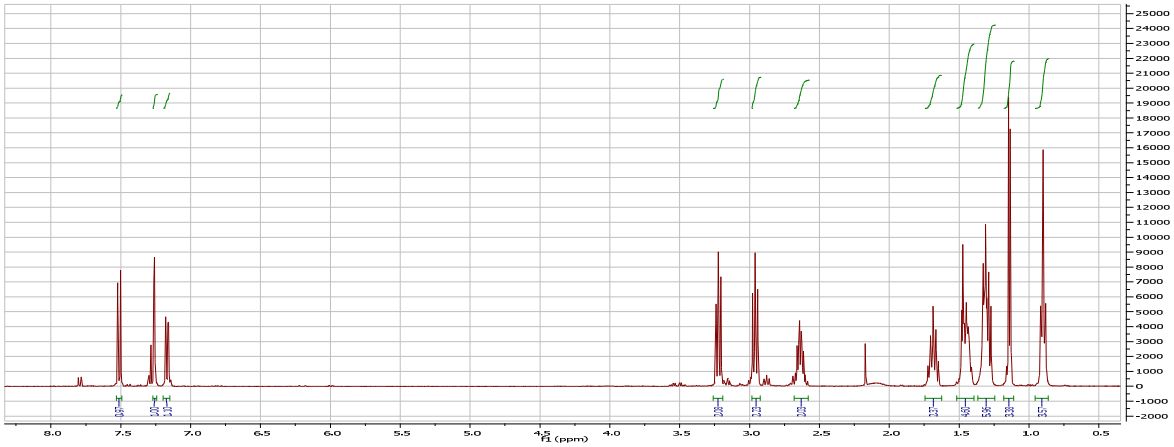


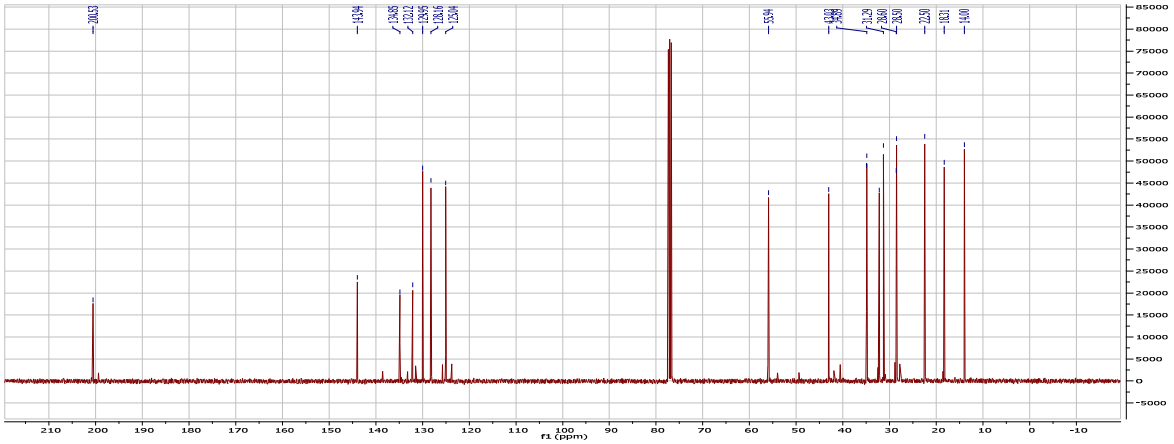
Peak ID	Compound	Time	Mass Found
1	Found	0.90	328.81

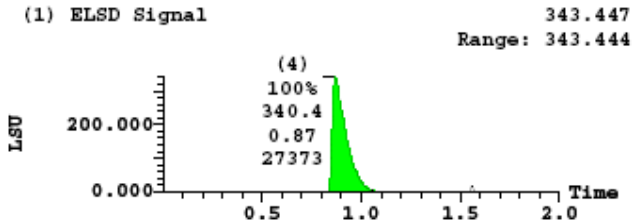




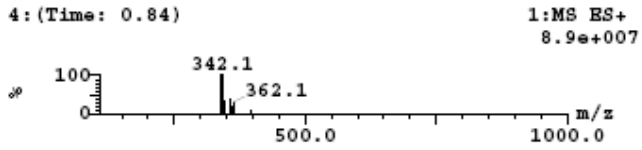
17{*2,1,2*}

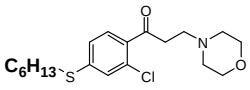




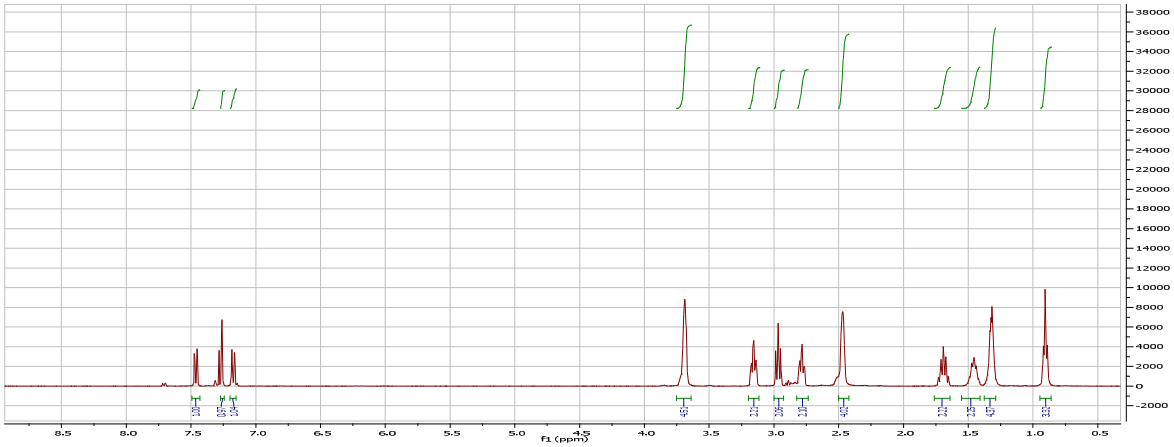


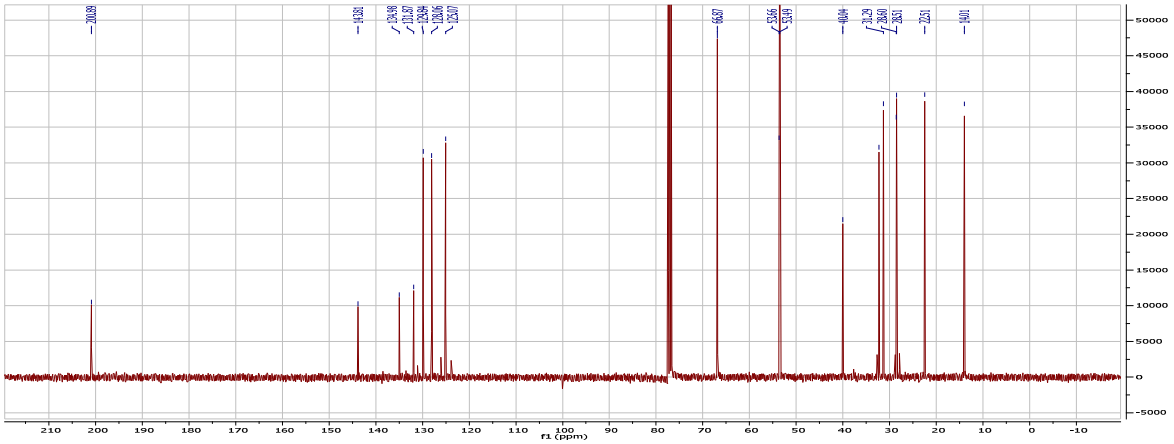
Peak ID	Compound	Time	Mass Found
4	Found	0.84	340.43

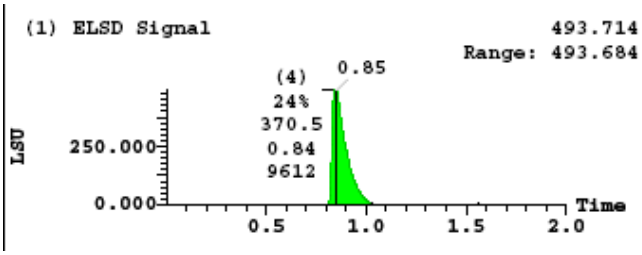




17{*2,1,3*}

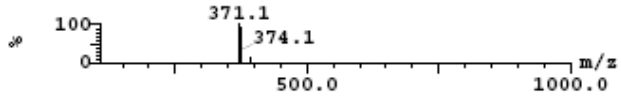


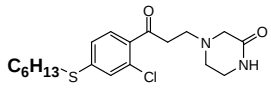




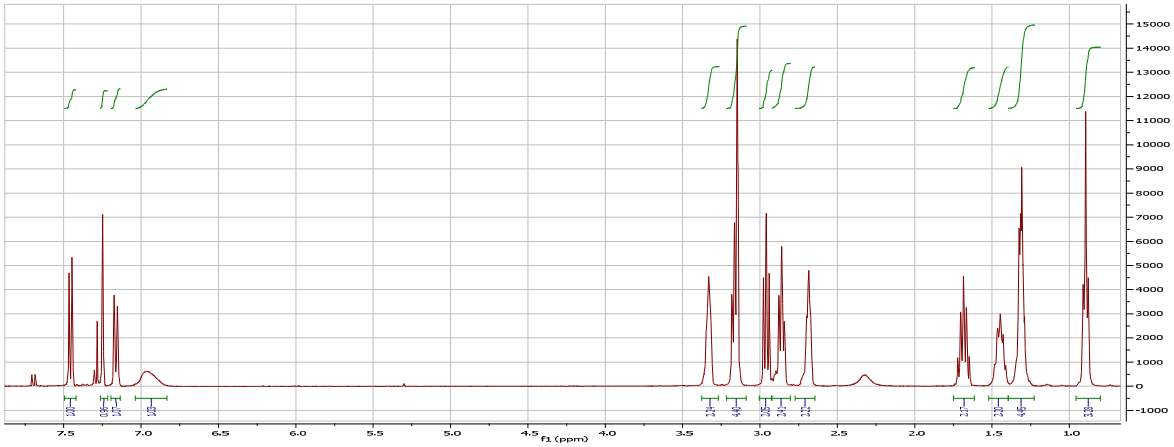
Peak ID	Compound	Time	Mass Found
4	Found	0.82	370.46

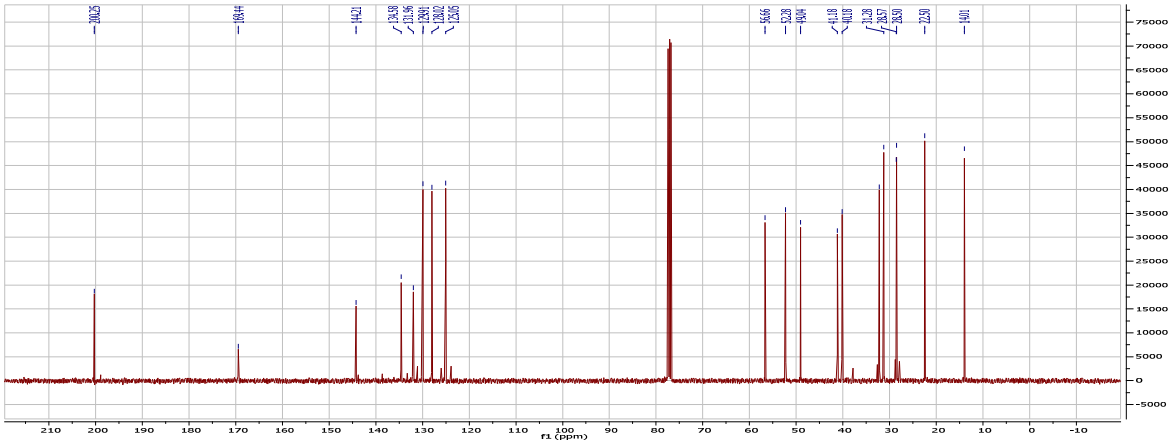
4:(Time: 0.82) 1:MS ES+ 1.0e+008

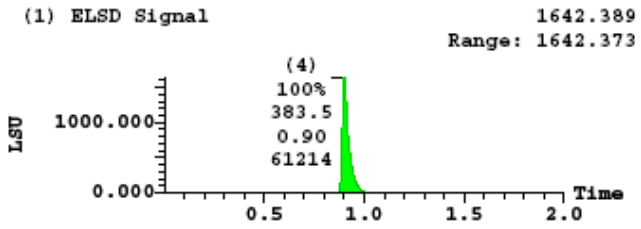




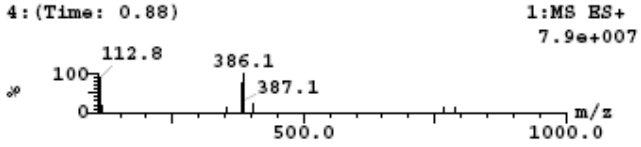
17{*2,1,4*}

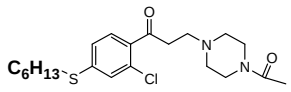




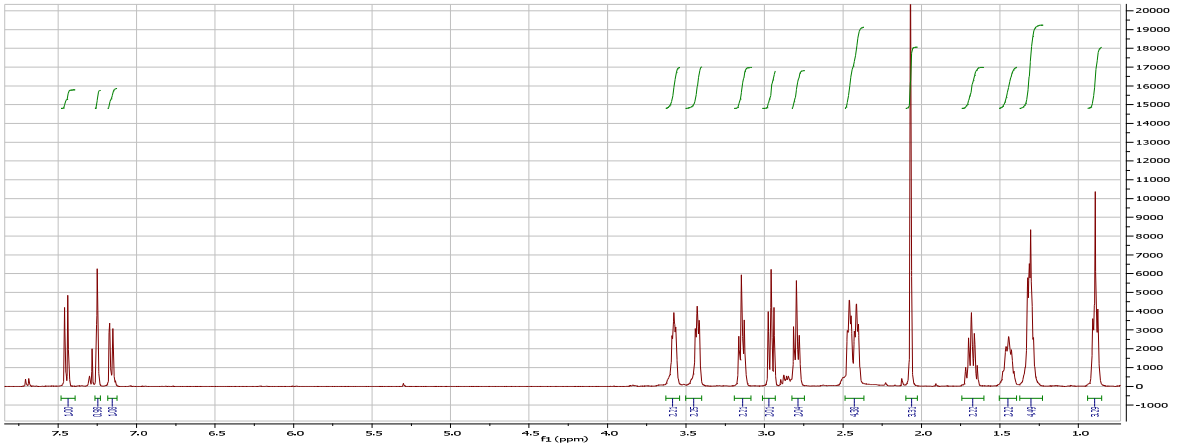


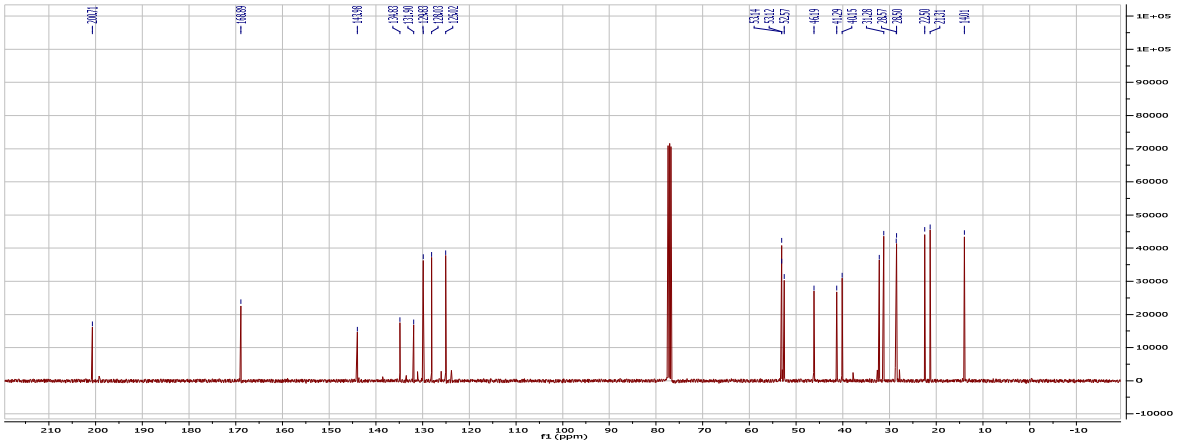
Peak ID	Compound	Time	Mass Found
4	Found	0.88	383.46

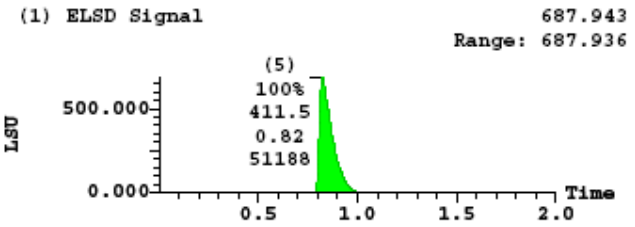




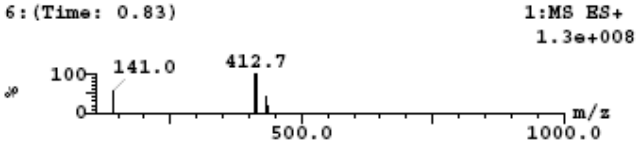
17{*2,1,5*}

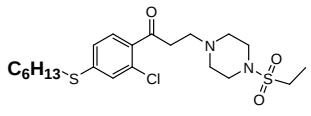




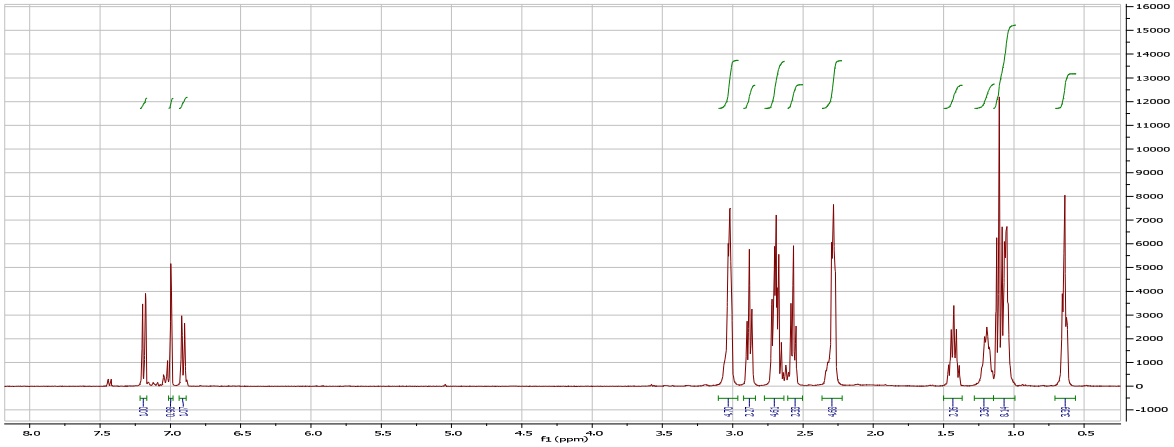


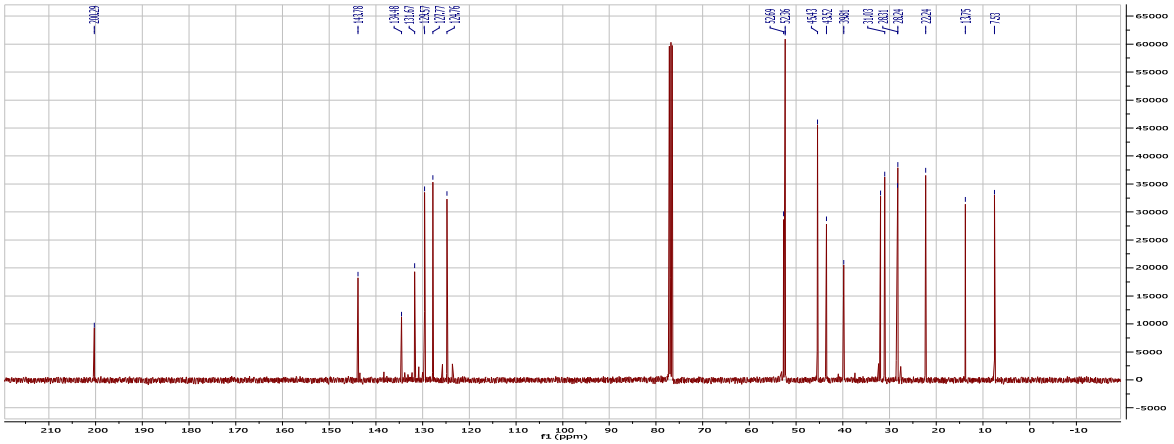
Peak ID	Compound	Time	Mass Found
6	Found	0.83	411.51

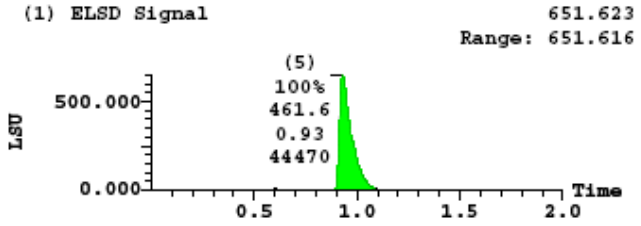




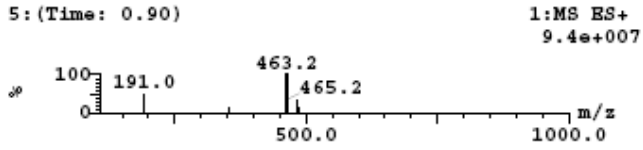
17{*2,1,6*}

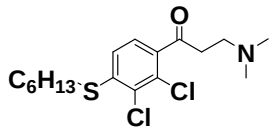




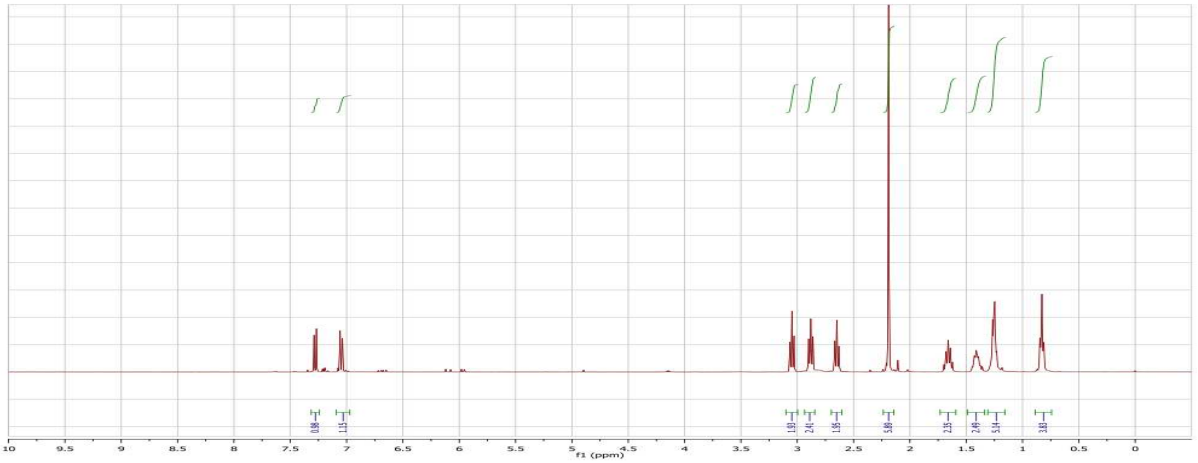


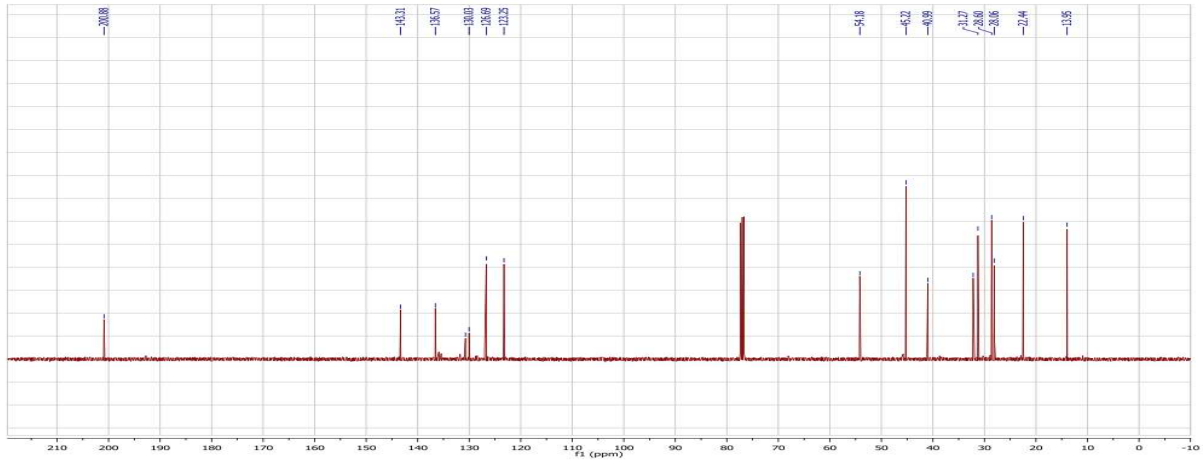
Peak ID	Compound	Time	Mass Found
5	Found	0.90	461.59

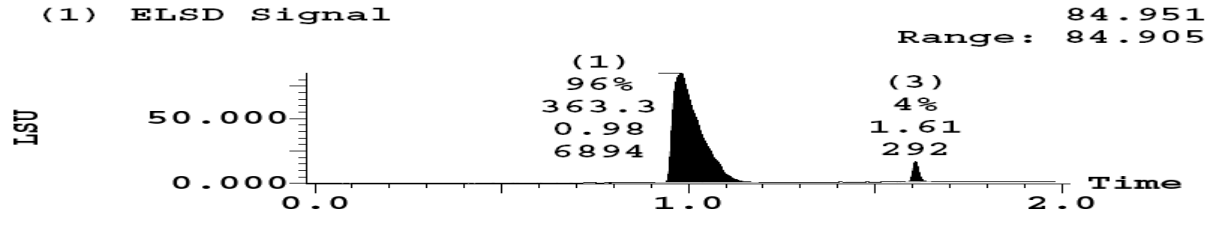




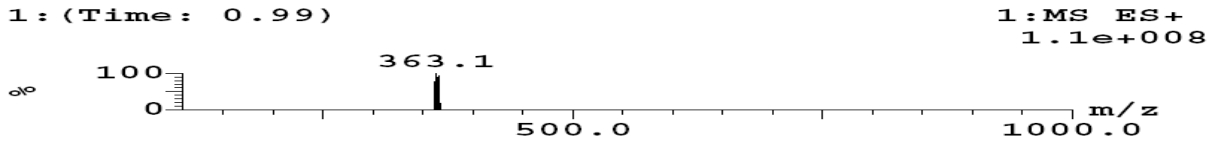
17{*2,2,1*}

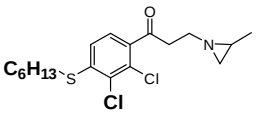




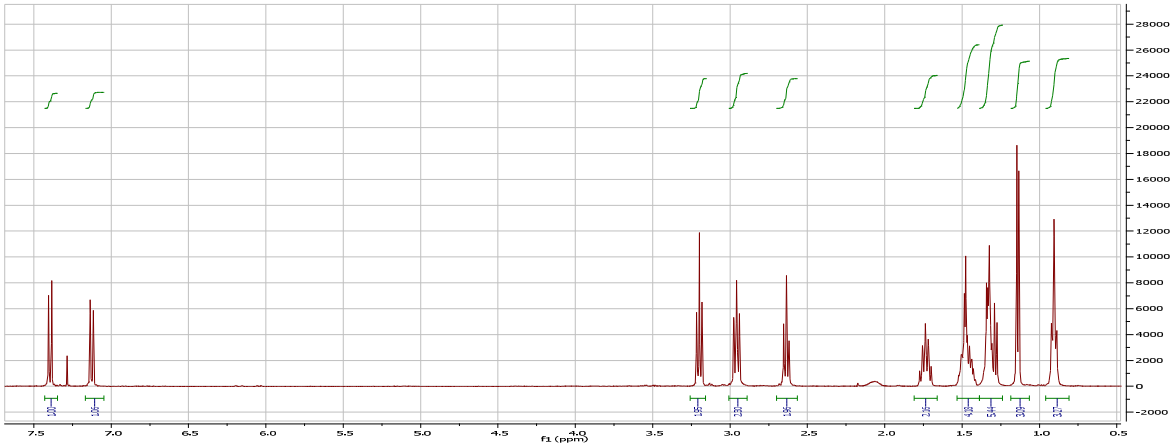


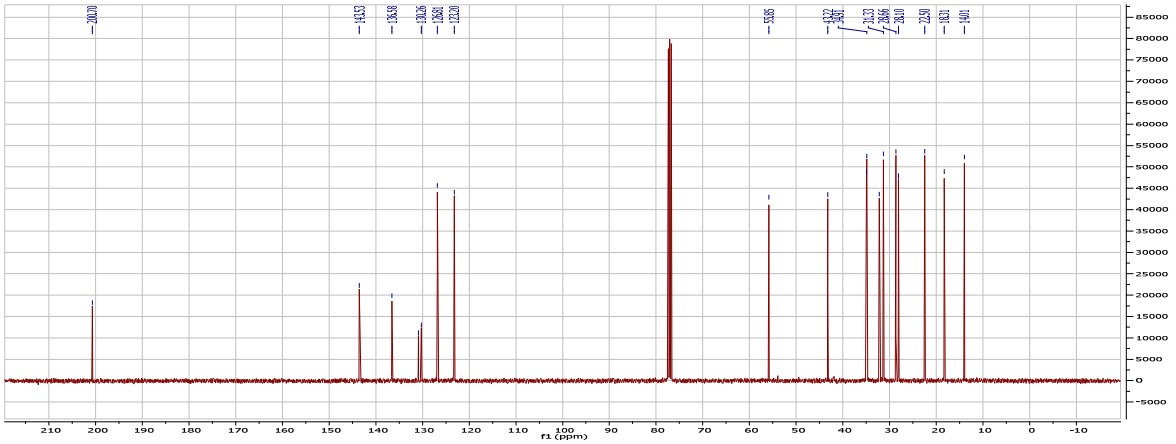
Peak ID	Compound	Time	Mass Found
1	Found	0.99	363.26

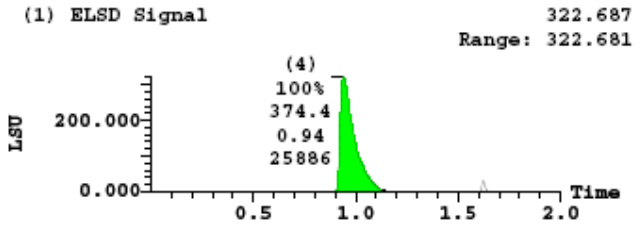




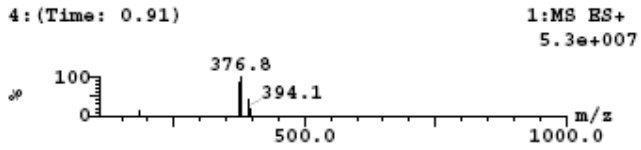
17{*2,2,2*}

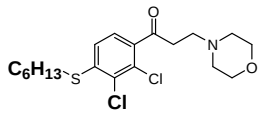




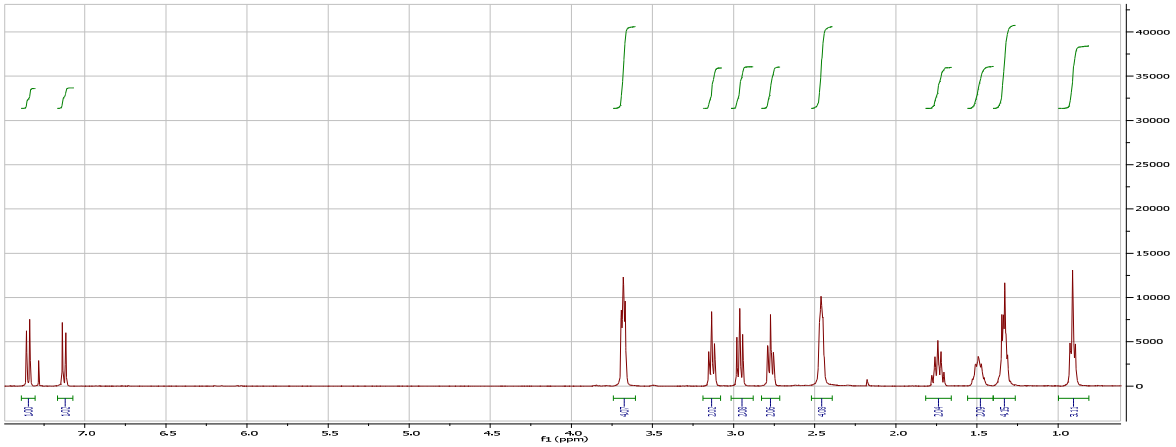


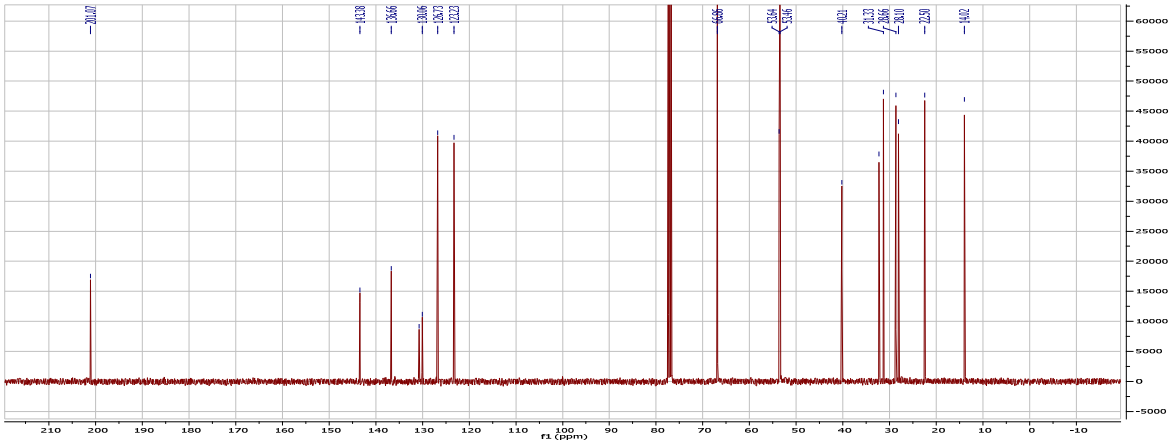
Peak ID	Compound	Time	Mass Found
4	Found	0.91	374.38

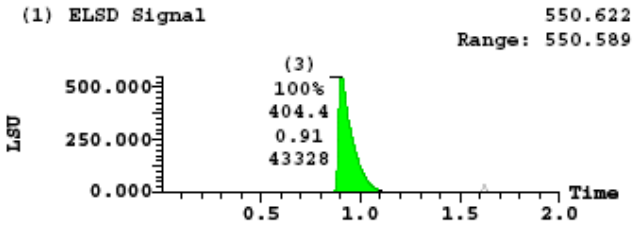




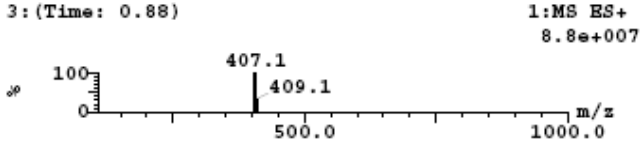
17{*2,2,3*}

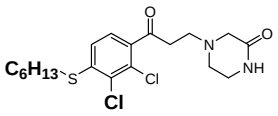




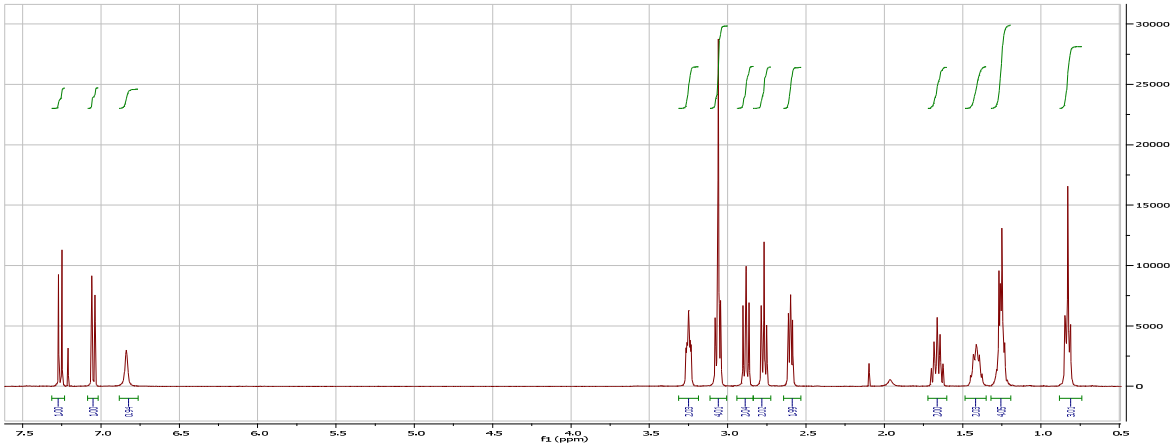


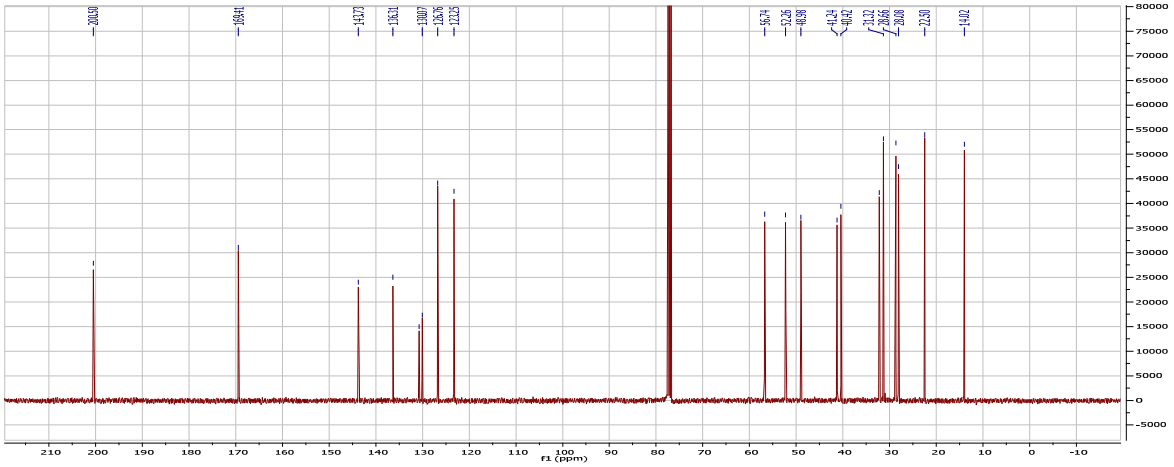
Peak ID	Compound	Time	Mass Found
3	Found	0.88	404.40

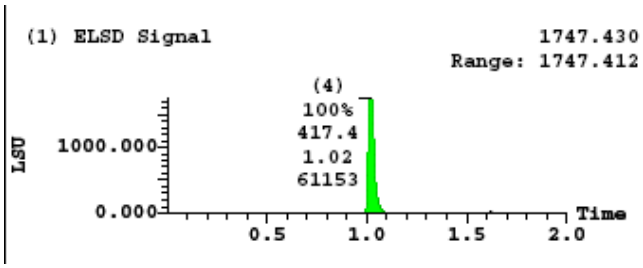




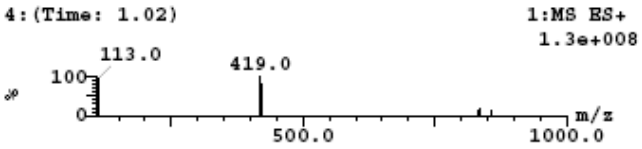
17{*2,2,4*}

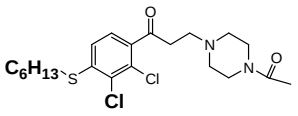




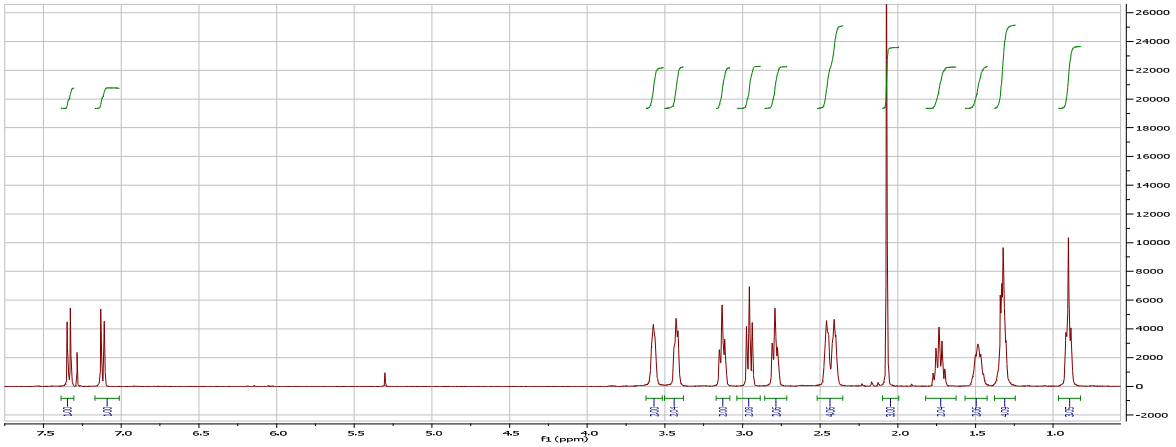


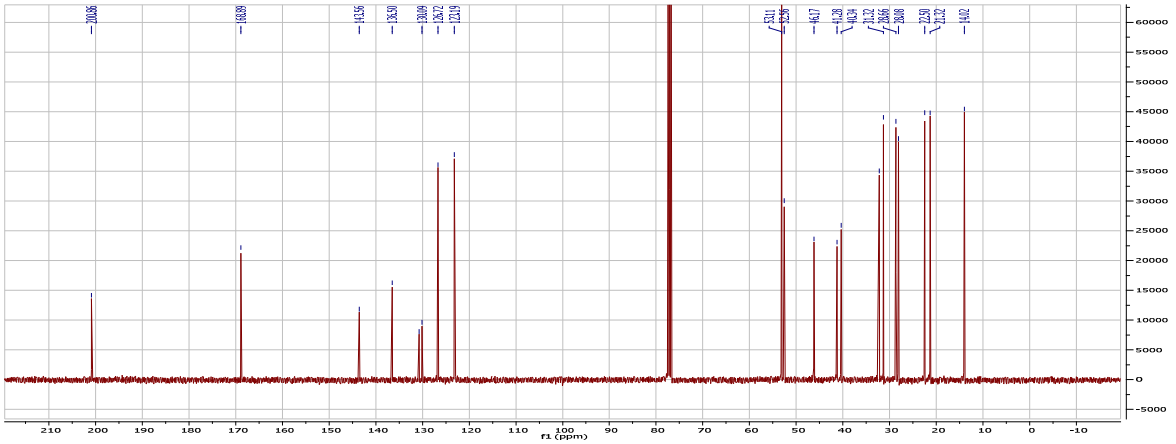
Peak ID	Compound	Time	Mass Found
4	Found	1.00	417.40

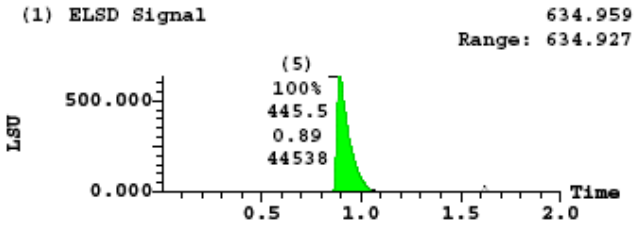


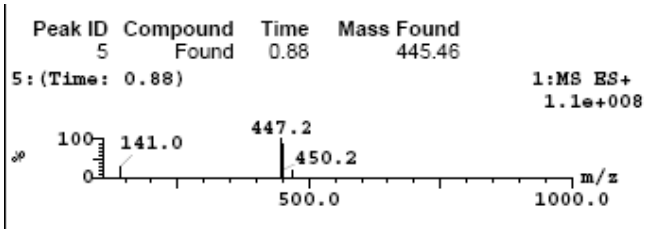

C6H13
S
Cl
Cl
O
N
N
O

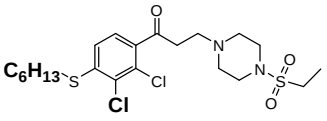
17{*2,2,5*}



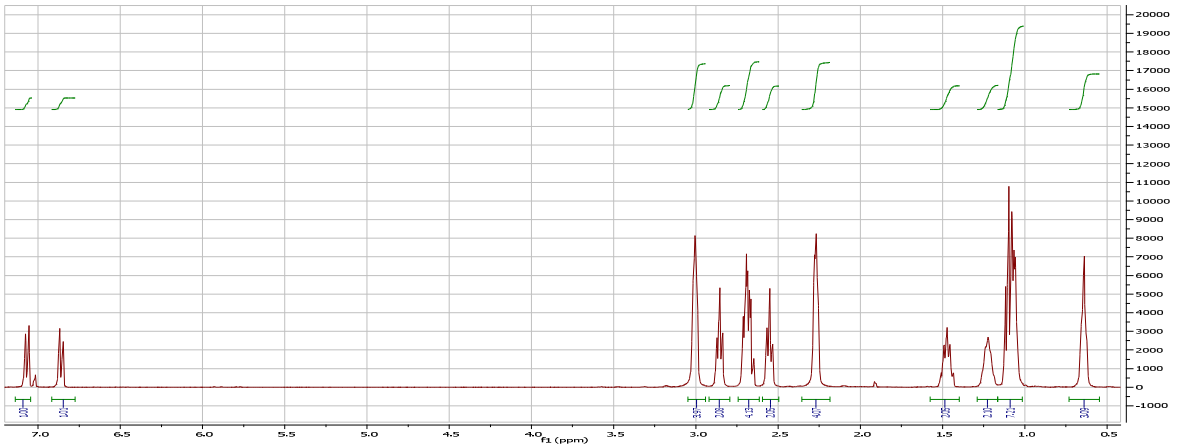


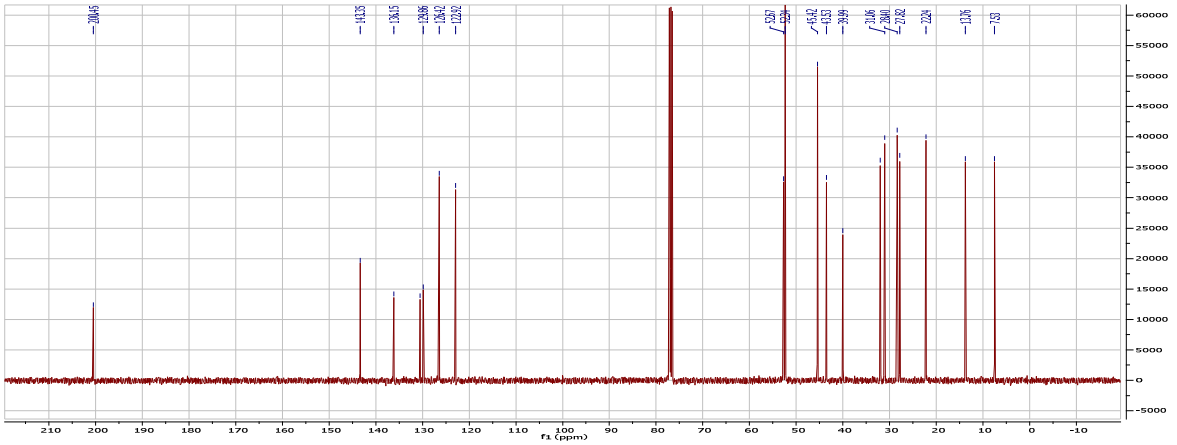

(1) ELSD Signal
634.959
Range: 634.927
(5)
100%
445.5
0.89
44538
500.000
0.000
LSU
Time
0.5
1.0
1.5
2.0

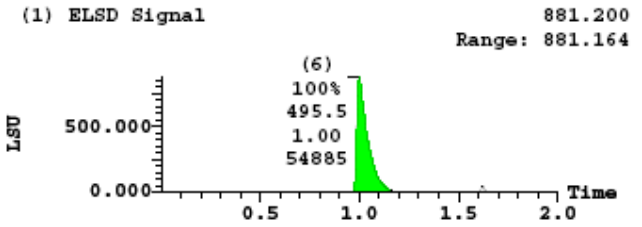

Peak ID Compound Time Mass Found
5 Found 0.88 445.46
5:(Time: 0.88)
1:MS ES+
1.1e+008
%
100
0
141.0
447.2
450.2
m/z
500.0
1000.0



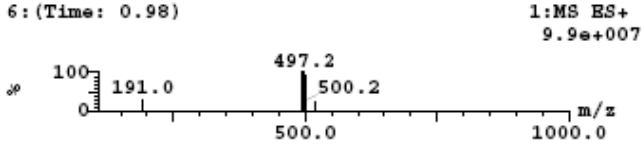
17{*2,2,6*}

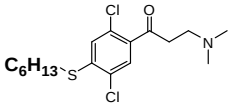




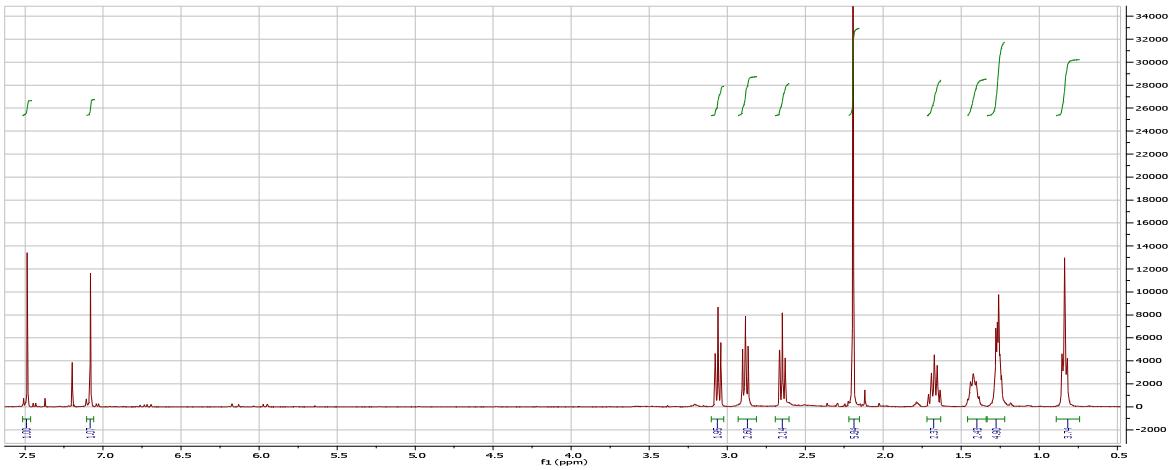


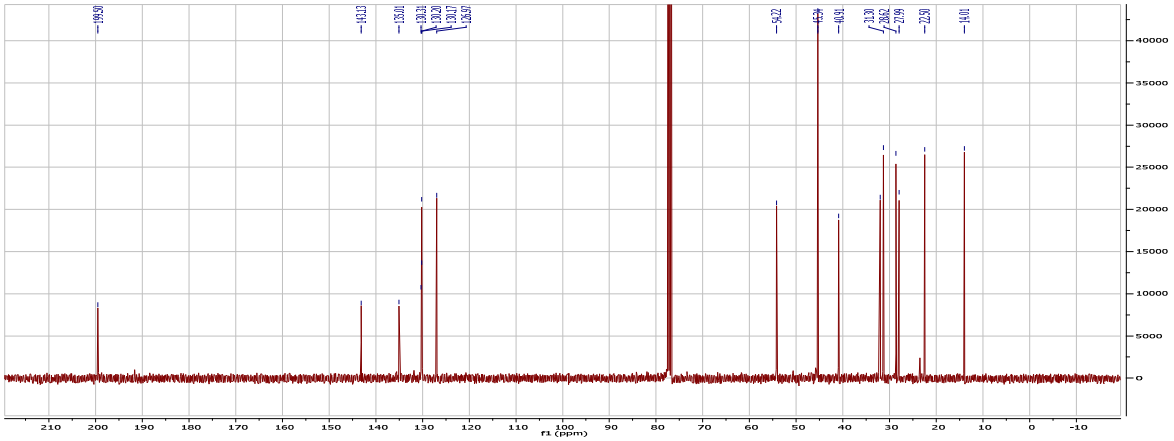
Peak ID	Compound	Time	Mass Found
6	Found	0.98	495.54

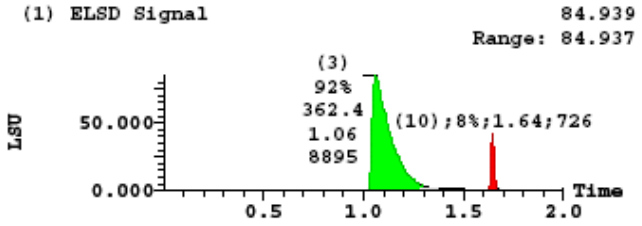




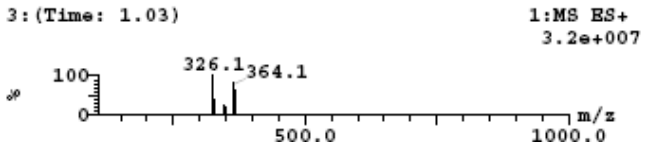
17{*2,3,1*}

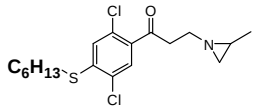




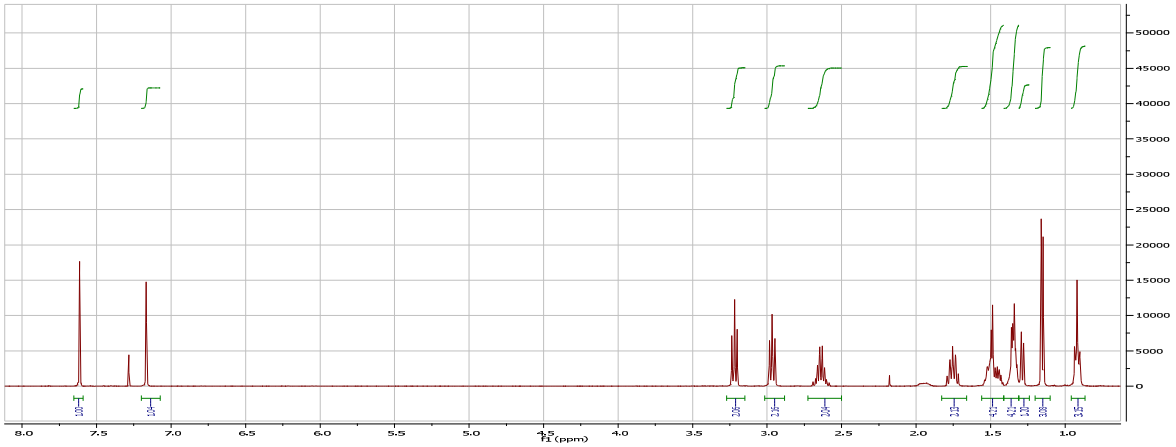


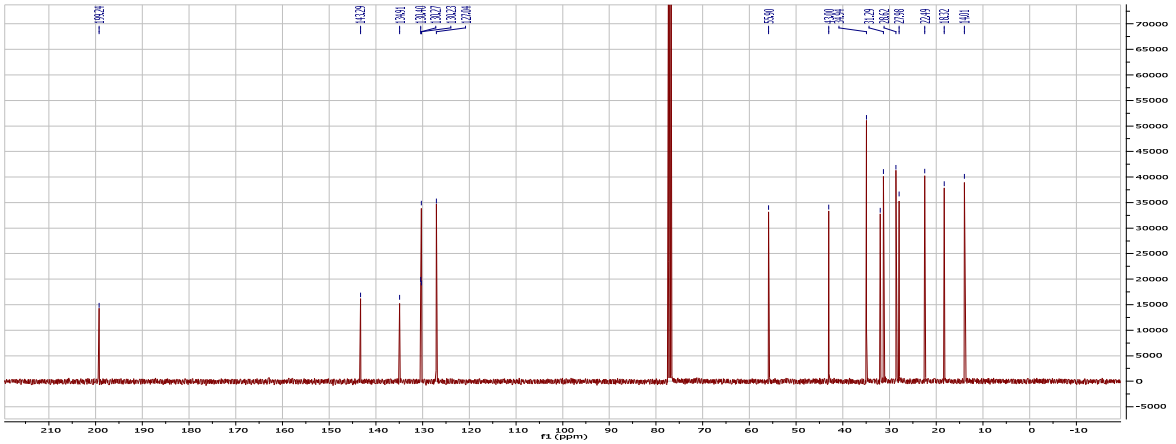
Peak ID	Compound	Time	Mass Found
3	Found	1.03	362.37

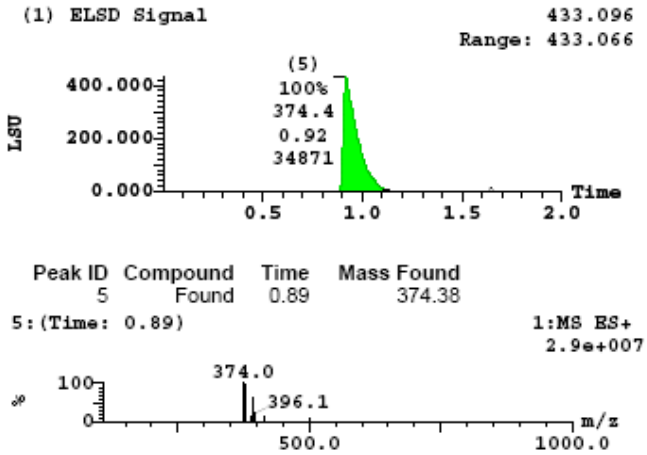




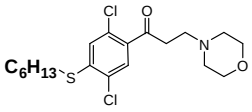
17{*2,3,2*}



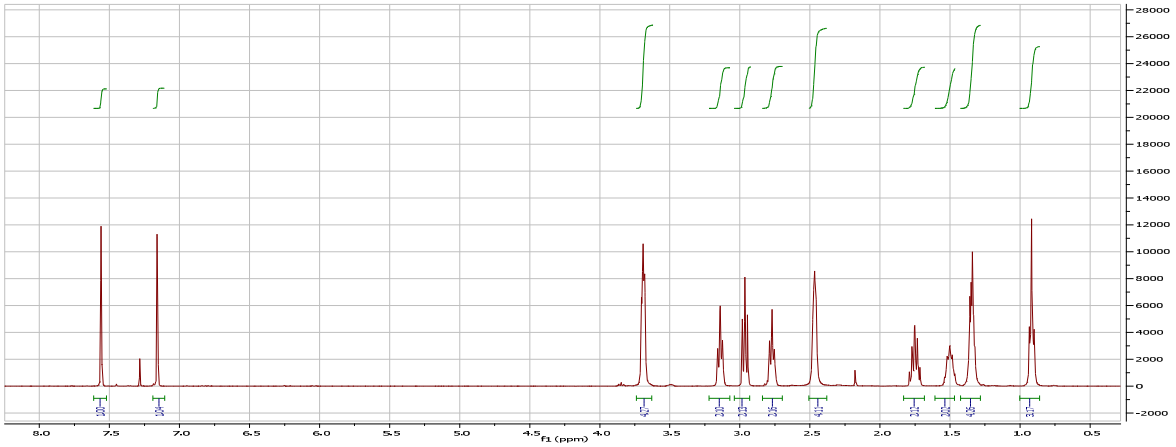


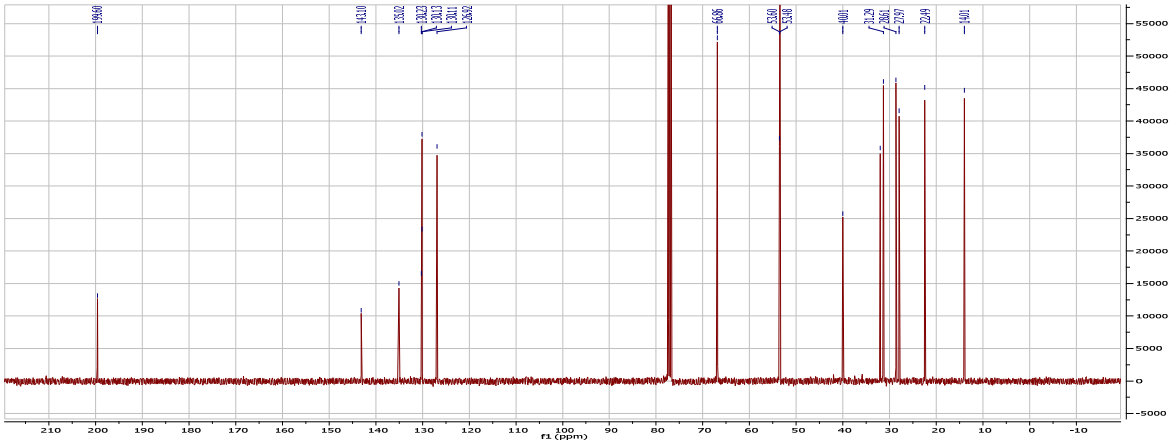


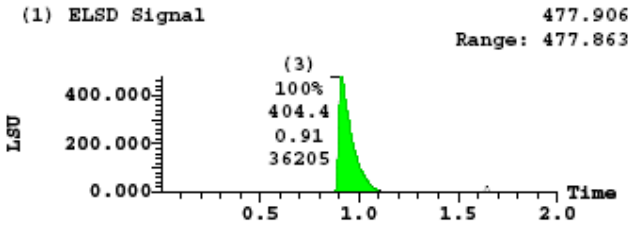
Peak ID	Compound	Time	Mass Found
5	Found	0.89	374.38



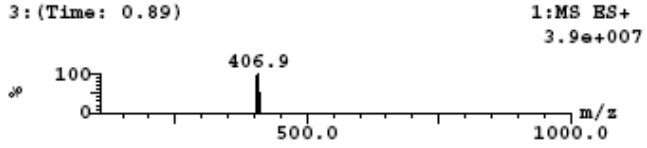
17{*2,3,3*}

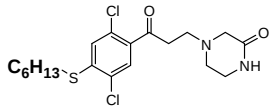




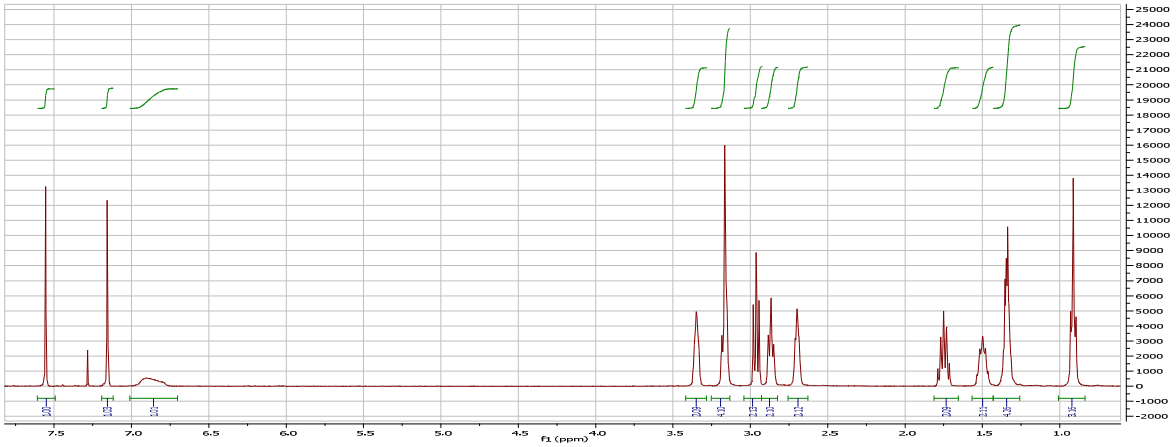


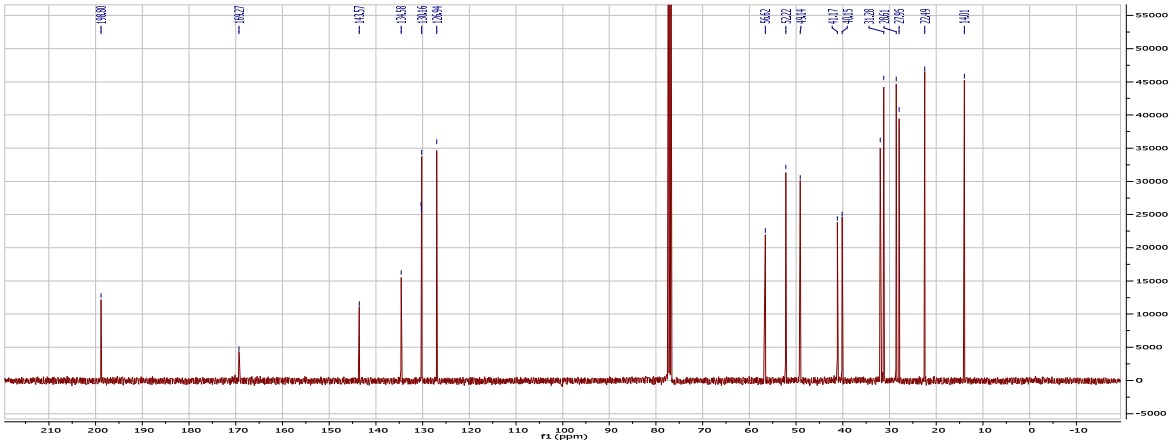
Peak ID	Compound	Time	Mass Found
3	Found	0.89	404.40

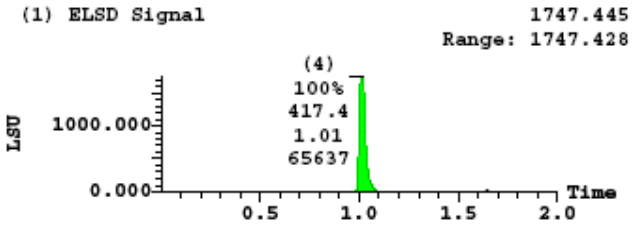




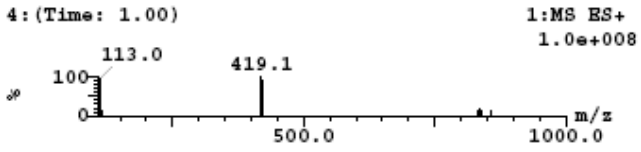
17{*2,3,4*}

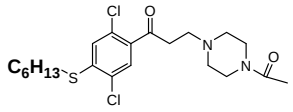




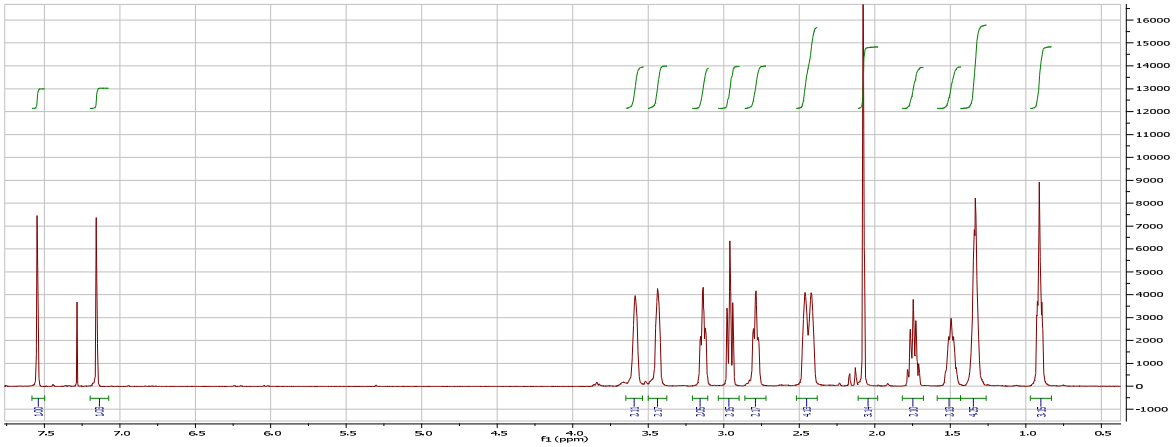


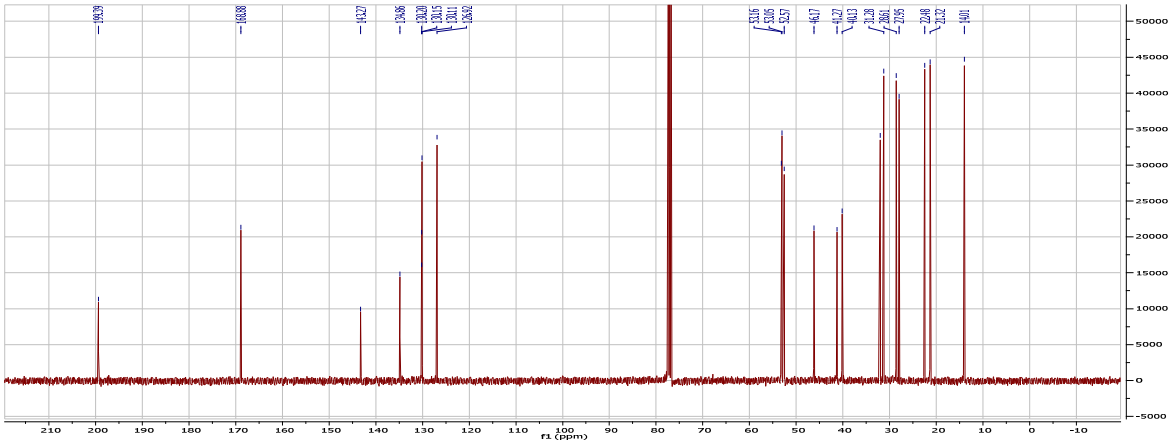
Peak ID	Compound	Time	Mass Found
4	Found	1.00	417.40

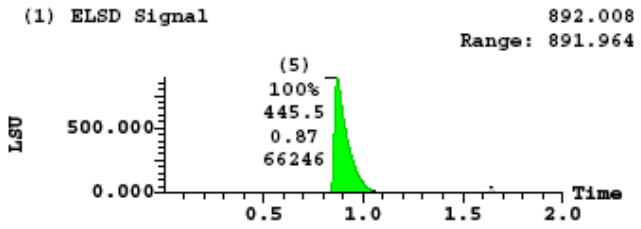




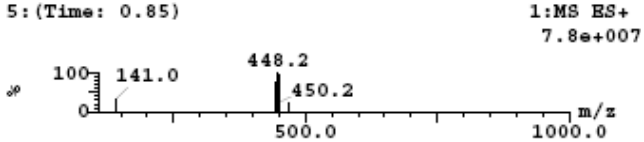
17{*2,3,5*}

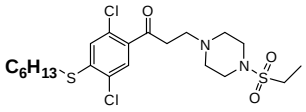




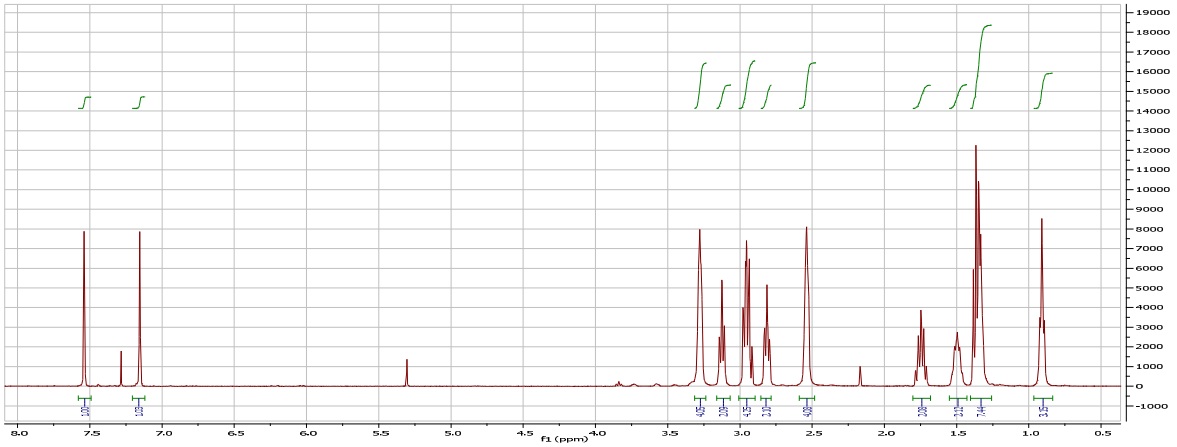


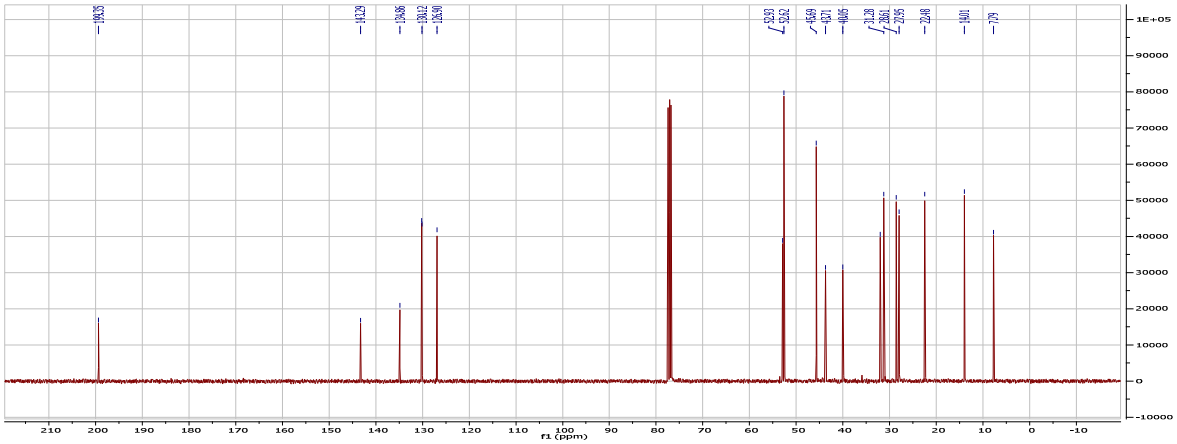
Peak ID	Compound	Time	Mass Found
5	Found	0.85	445.46

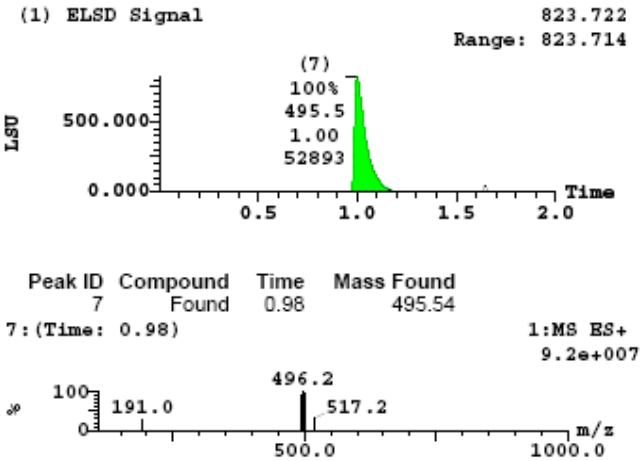




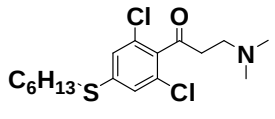
17{*2,3,6*}



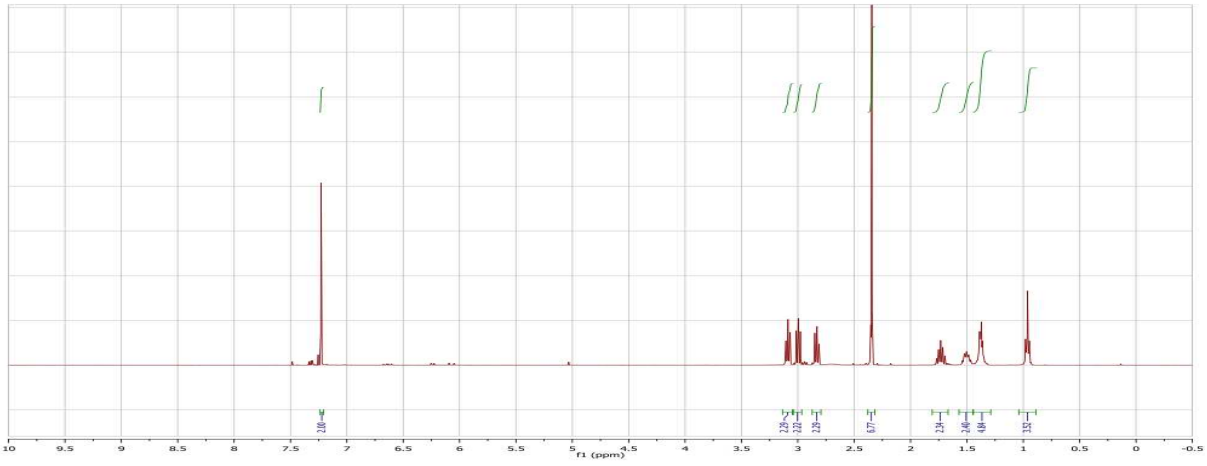


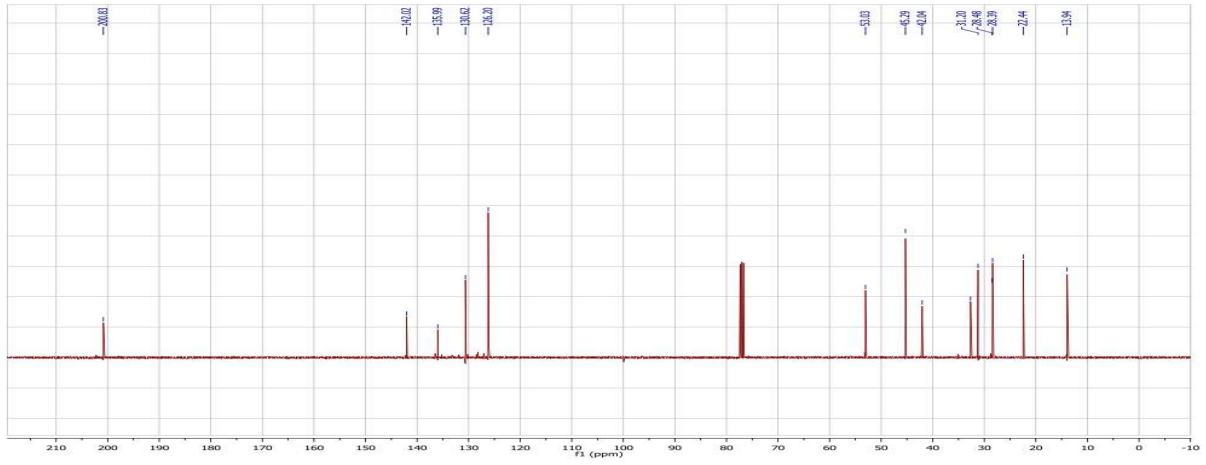


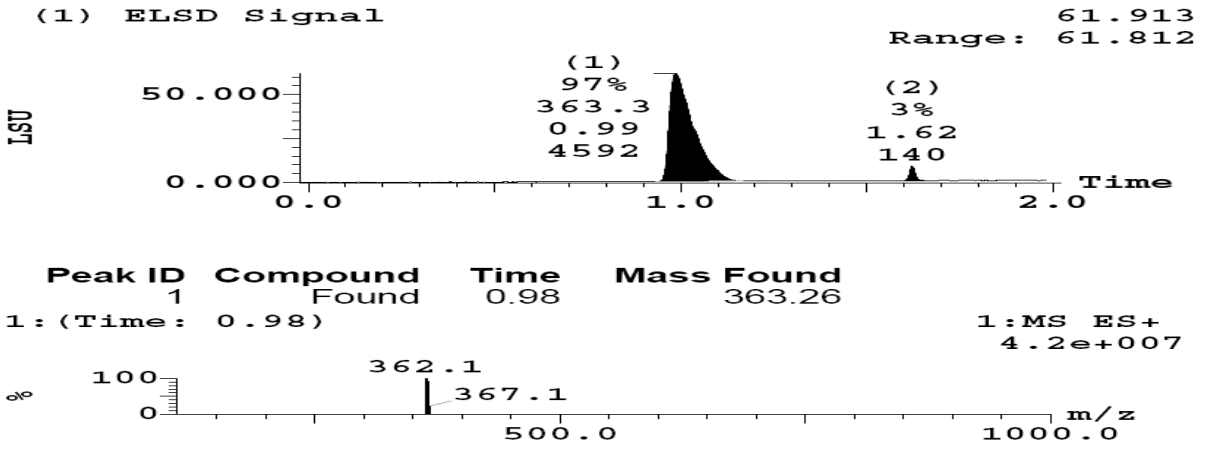
Peak ID	Compound	Time	Mass Found
7	Found	0.98	495.54



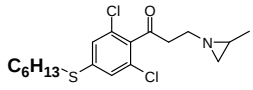
17{*2,4,1*}



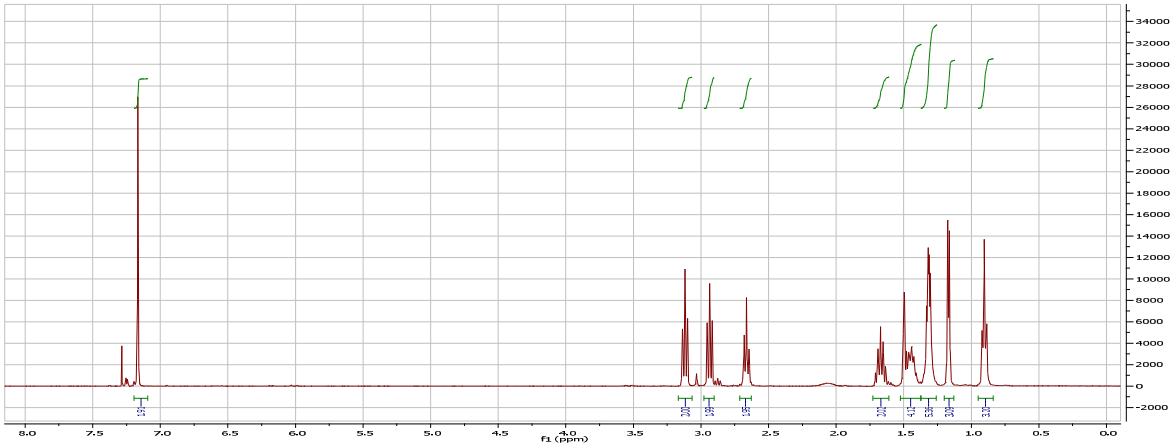


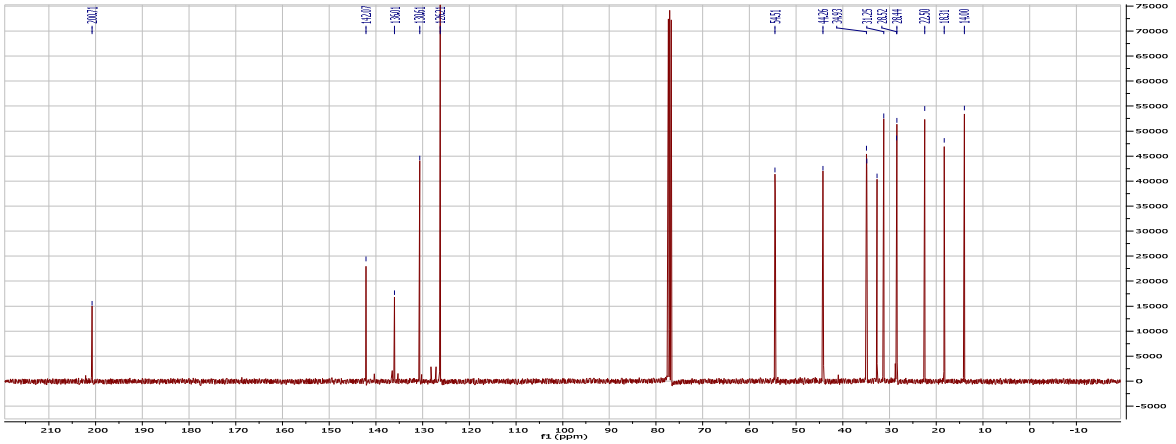


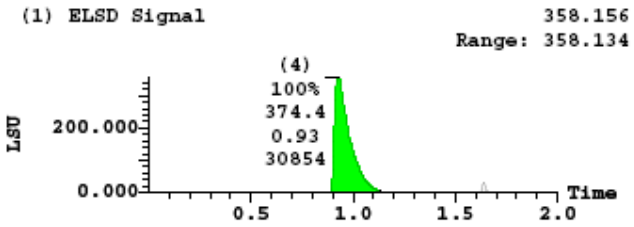
Peak ID	Compound	Time	Mass Found
1	Found	0.98	363.26



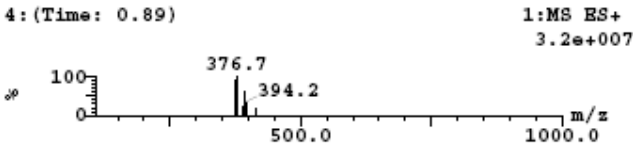
17{*2,4,2*}

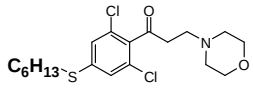




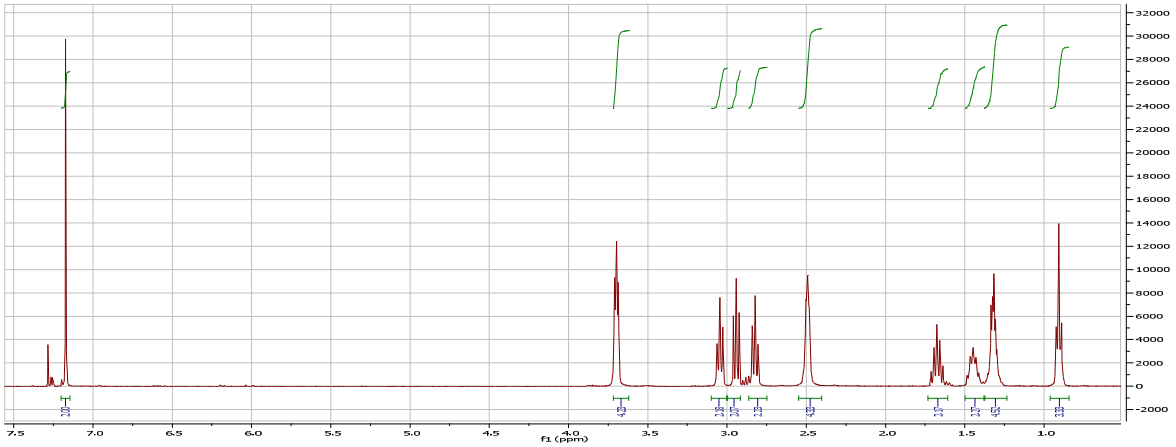


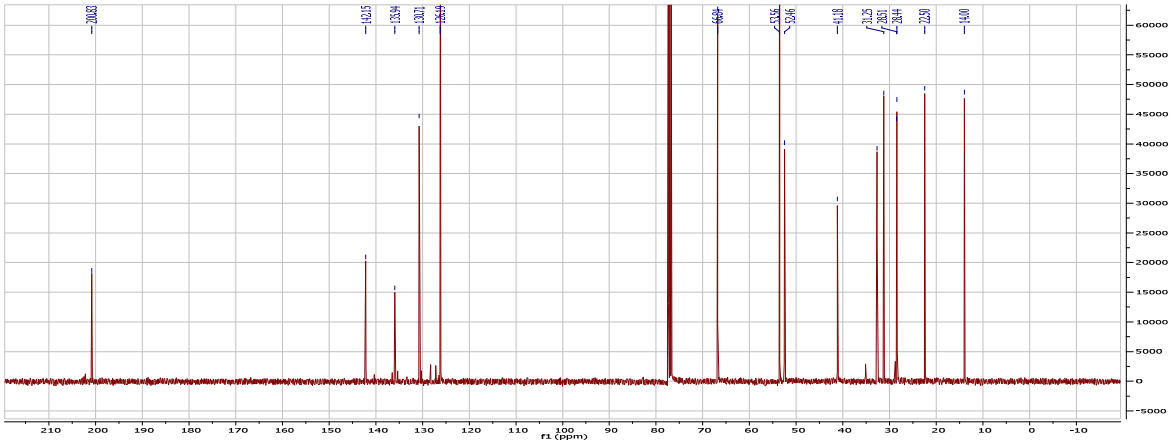
Peak ID	Compound	Time	Mass Found
4	Found	0.89	374.38

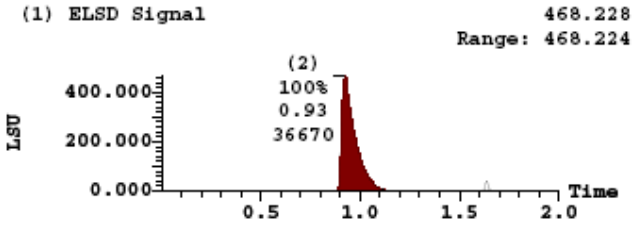




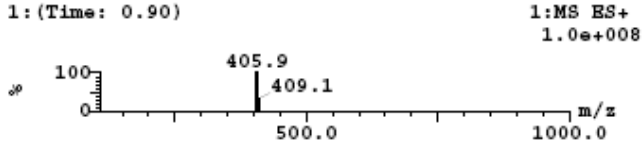
17{*2,4,3*}

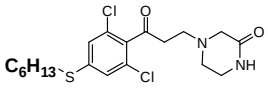




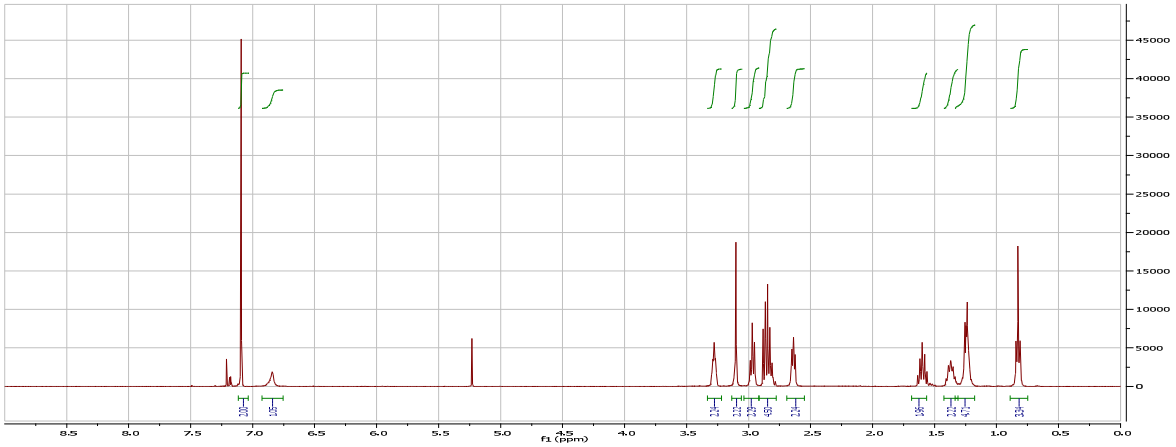


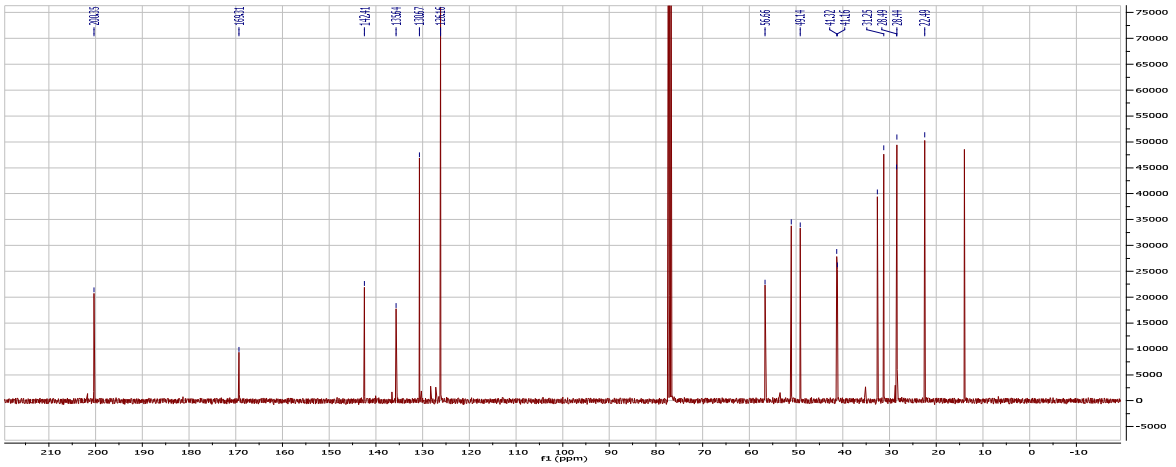
Peak ID	Compound	Time	Mass Found
1	Found	0.90	404.40

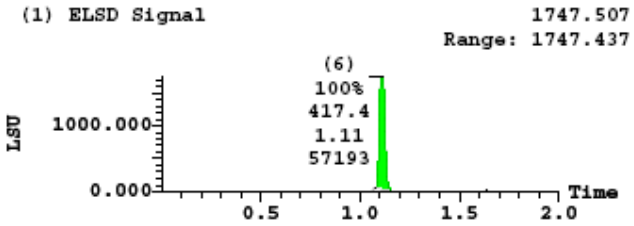




17{*2,4,4*}

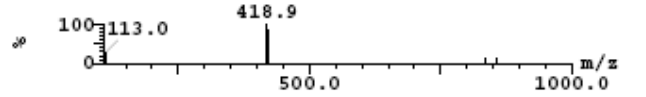


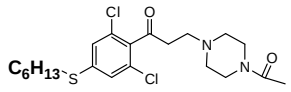




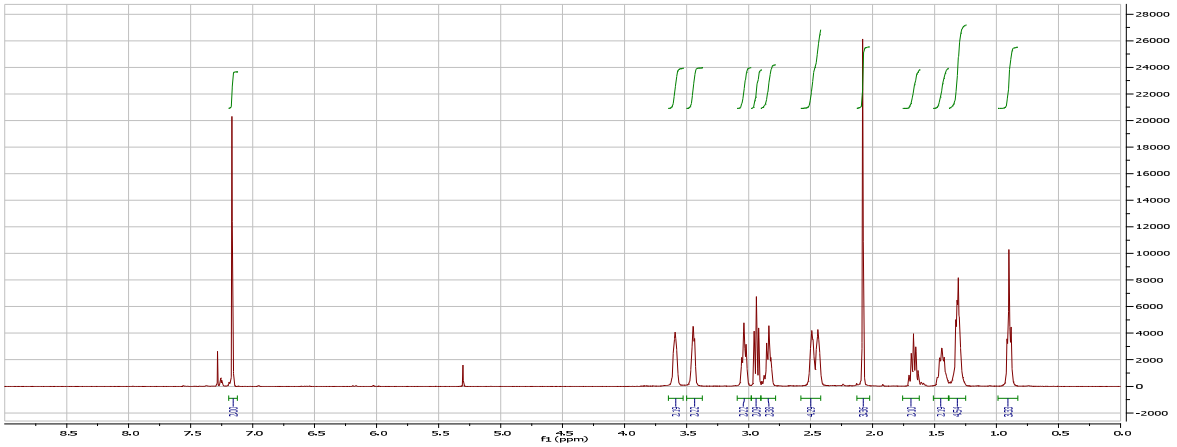
Peak ID	Compound	Time	Mass Found
6	Found	1.09	417.40

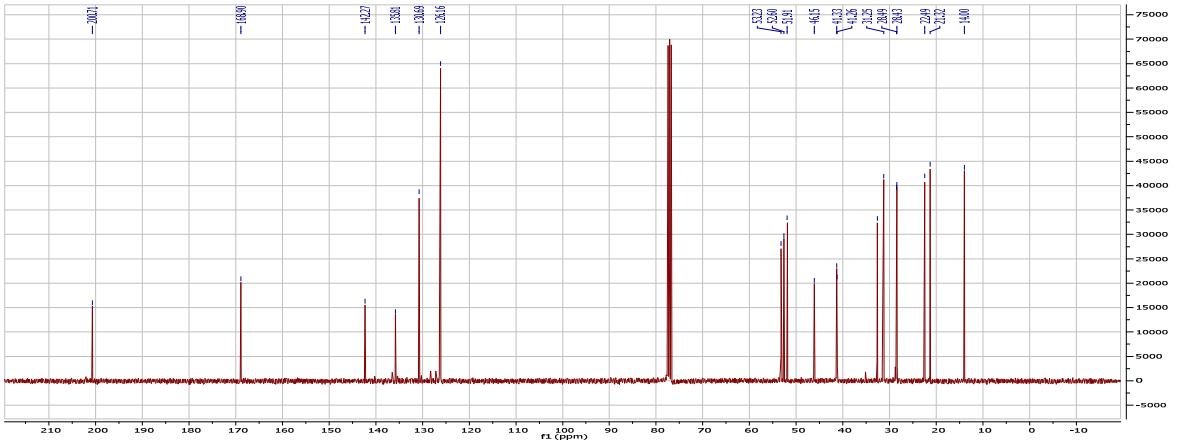
6:(Time: 1.09) 1:MS ES+ 1.3e+008

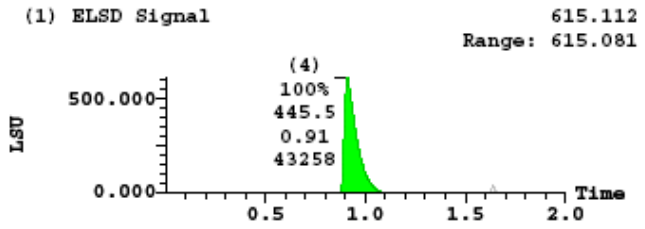




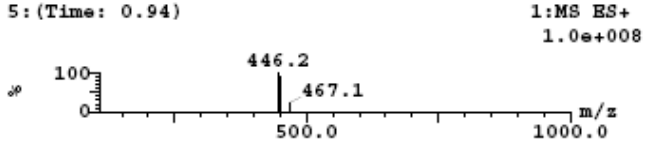
17{*2,4,5*}

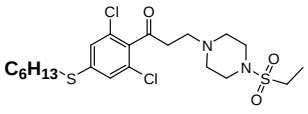




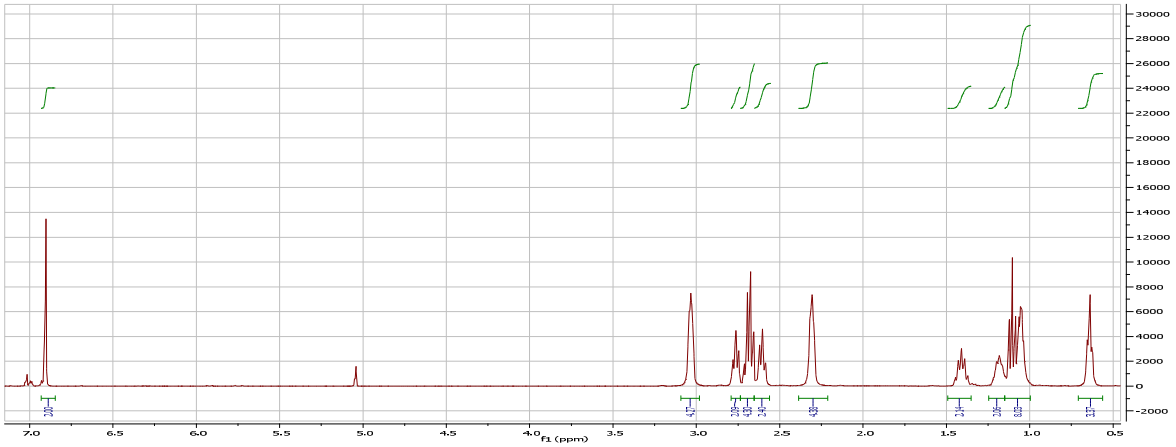


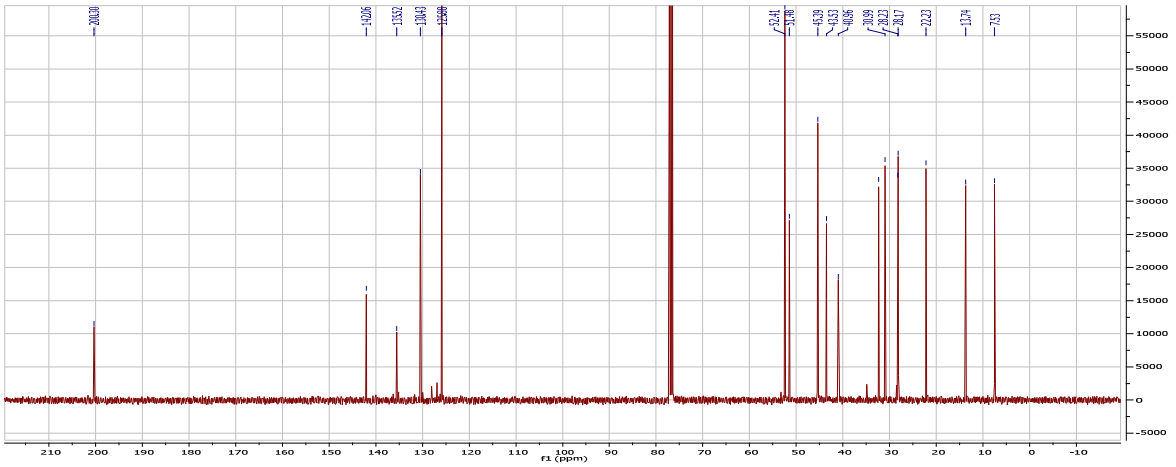
Peak ID	Compound	Time	Mass Found
5	Found	0.94	445.46

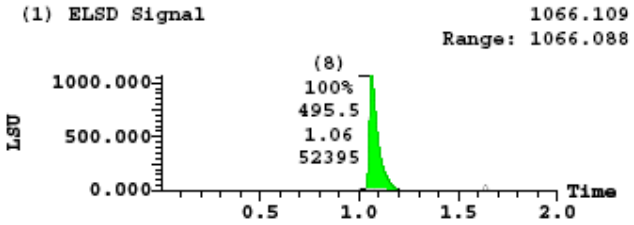




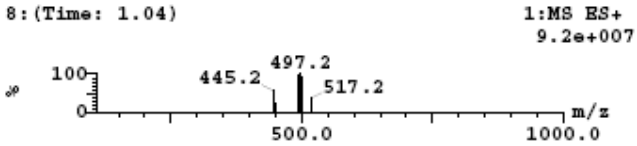
17{*2,4,6*}

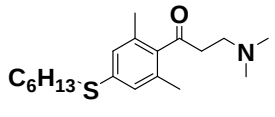




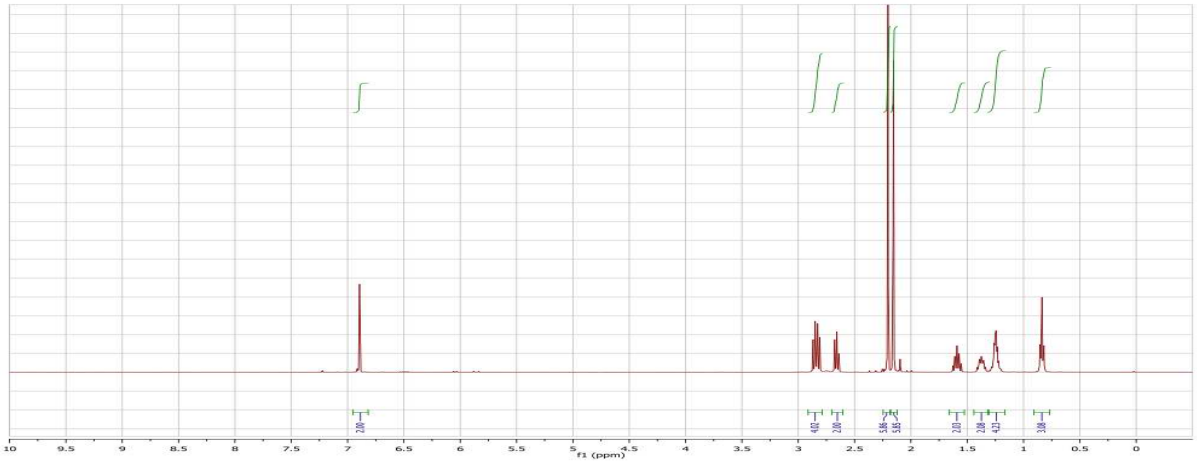


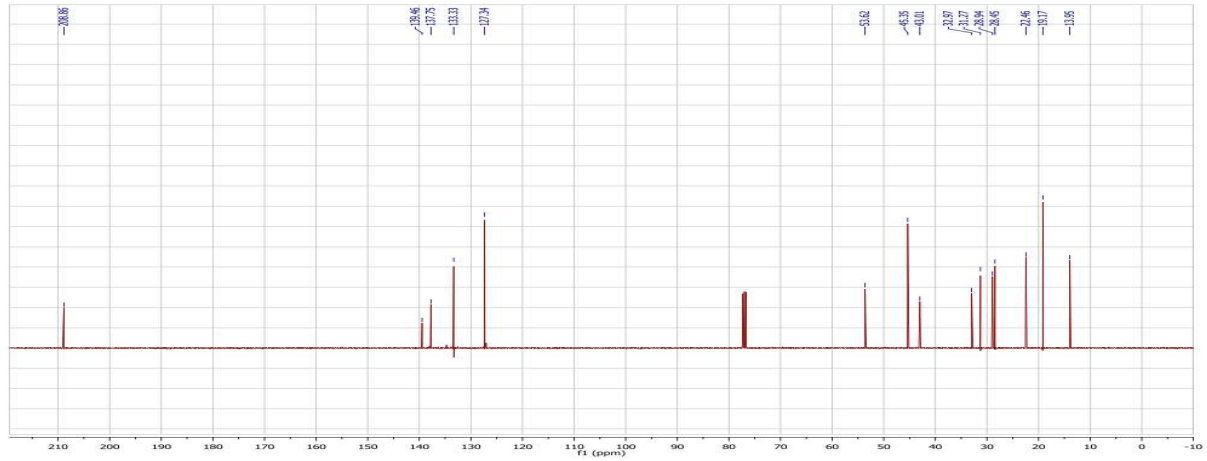
Peak ID	Compound	Time	Mass Found
8	Found	1.04	495.54

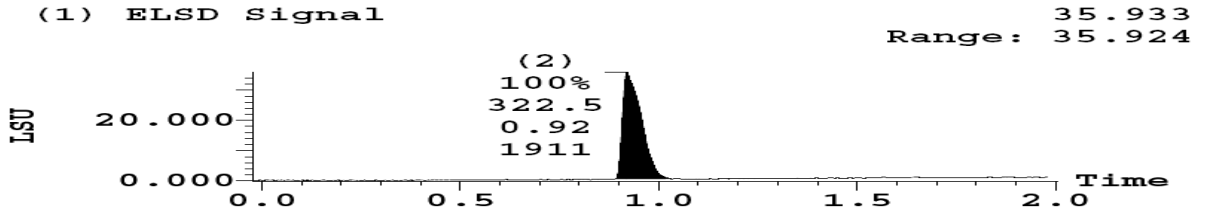




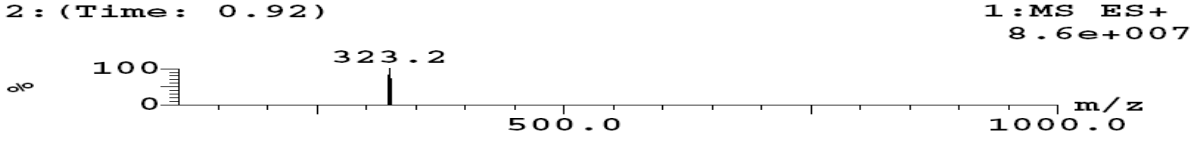
17{*2,5,1*}

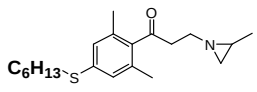




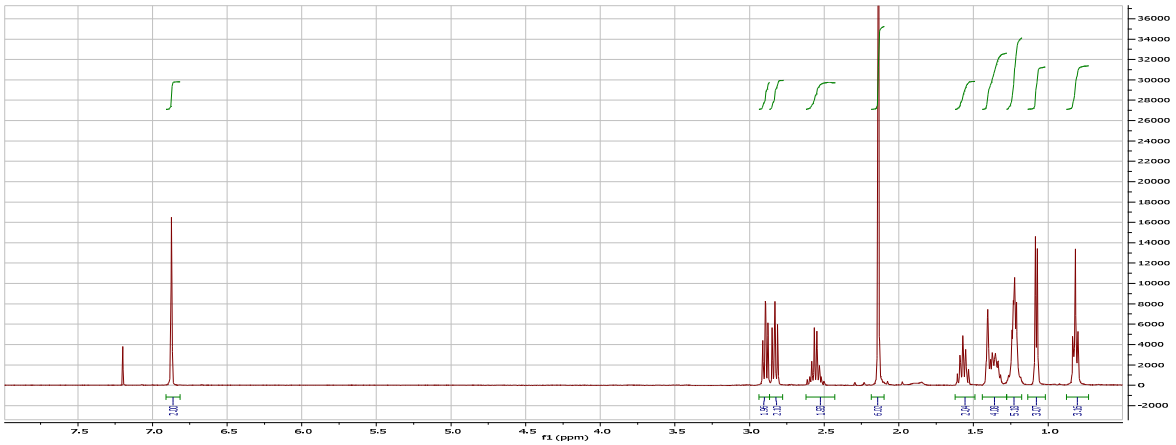


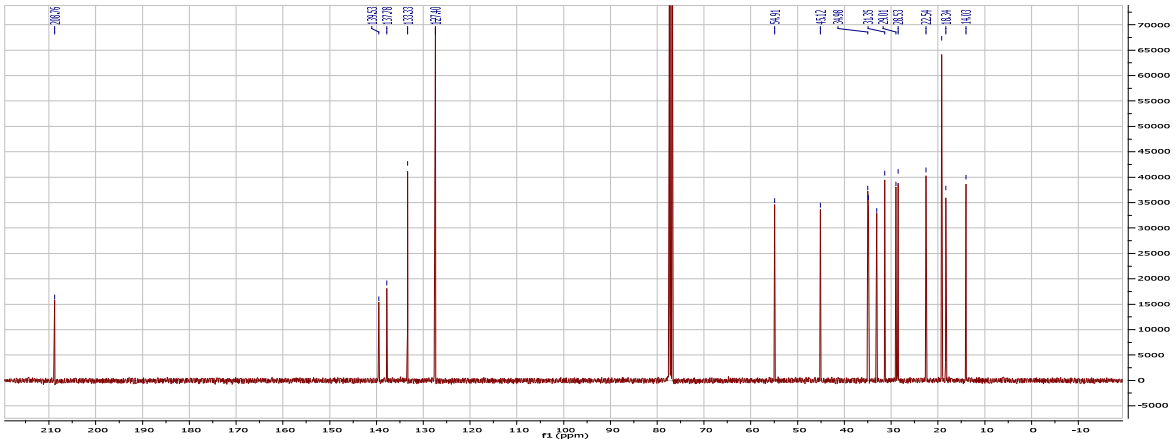
Peak ID	Compound	Time	Mass Found
2	Found	0.92	322.52

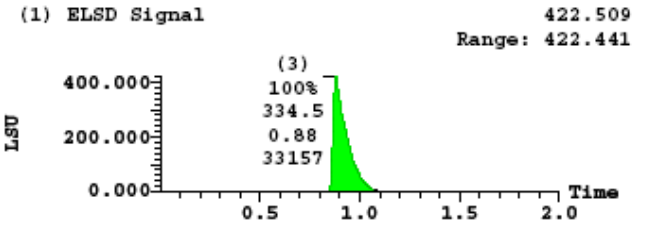




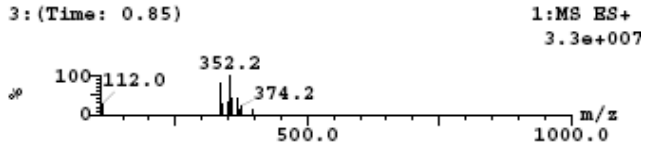
17{*2,5,2*}

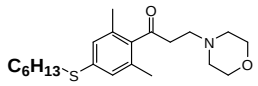




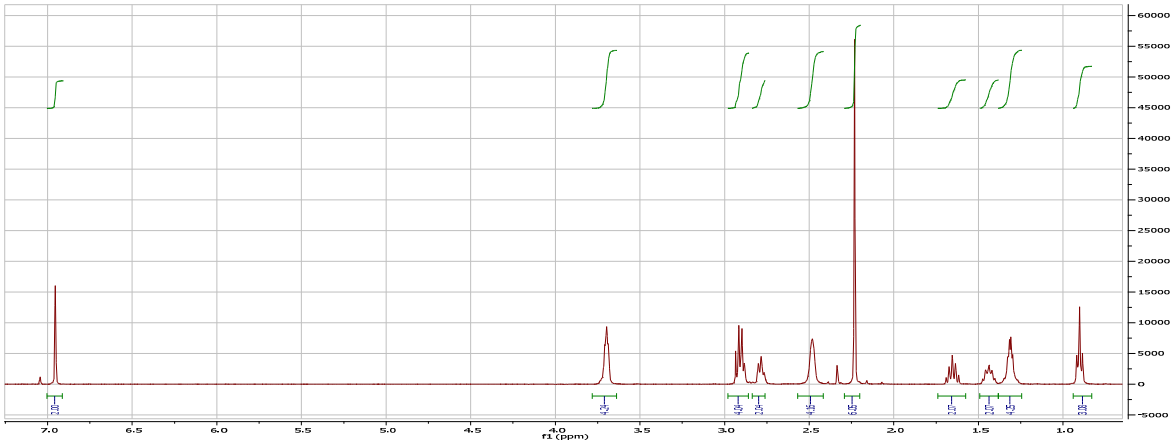


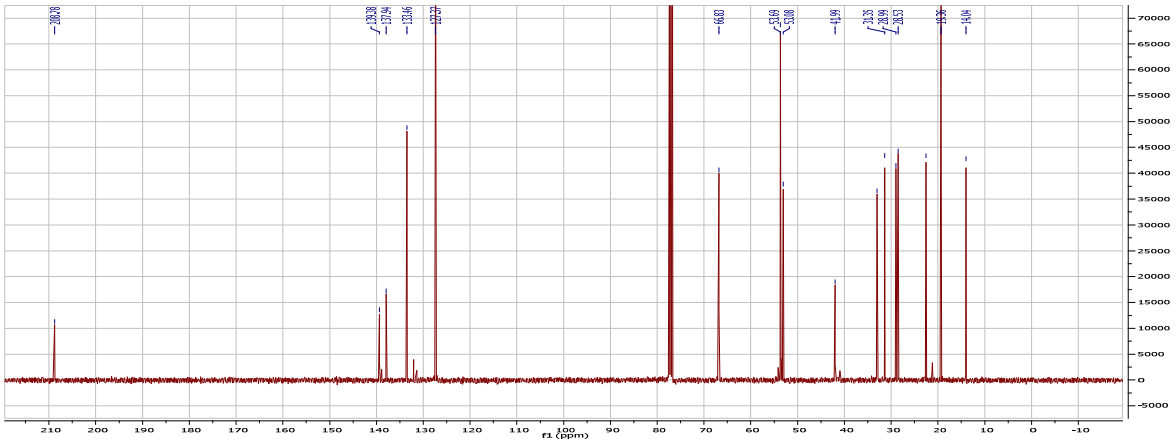
Peak ID	Compound	Time	Mass Found
3	Found	0.85	334.54

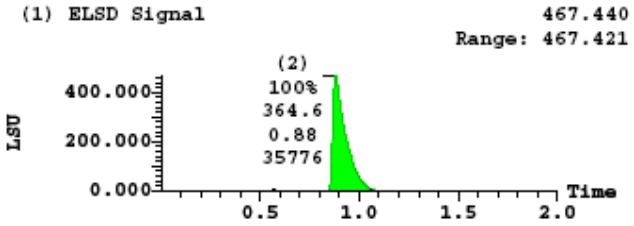




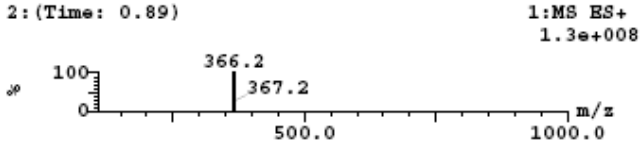
17{*2,5,3*}

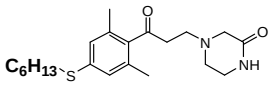




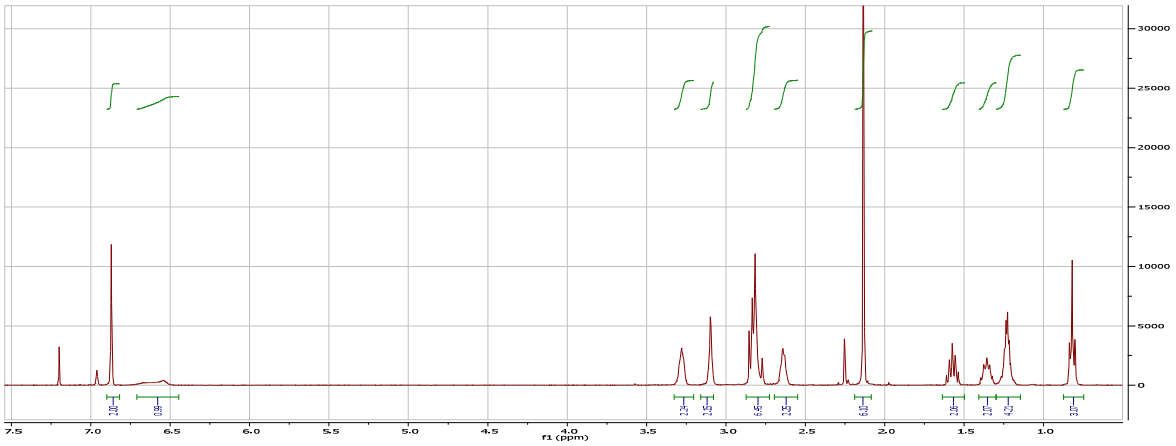


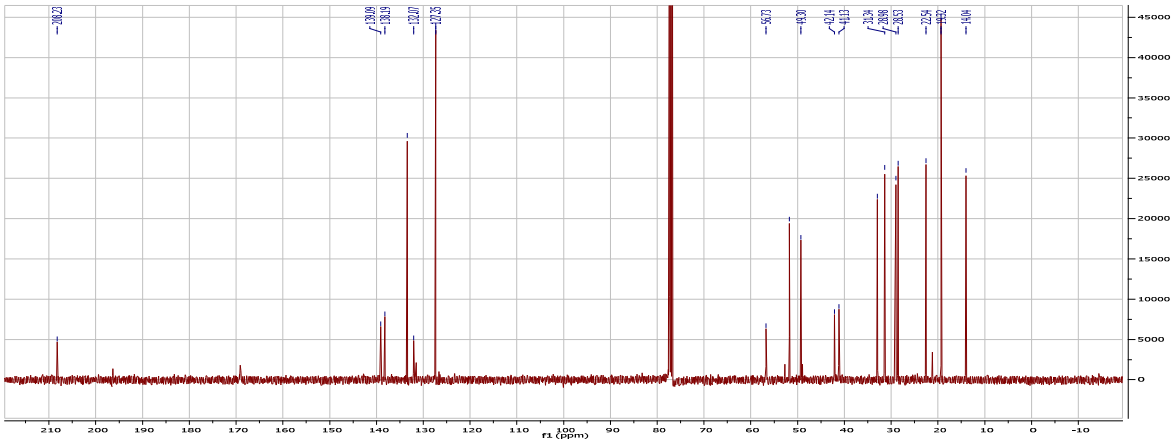
Peak ID	Compound	Time	Mass Found
2	Found	0.89	364.57

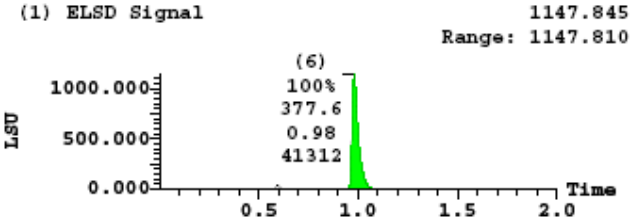




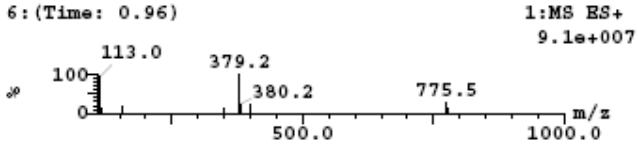
17{*2,5,4*}

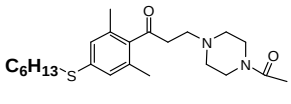




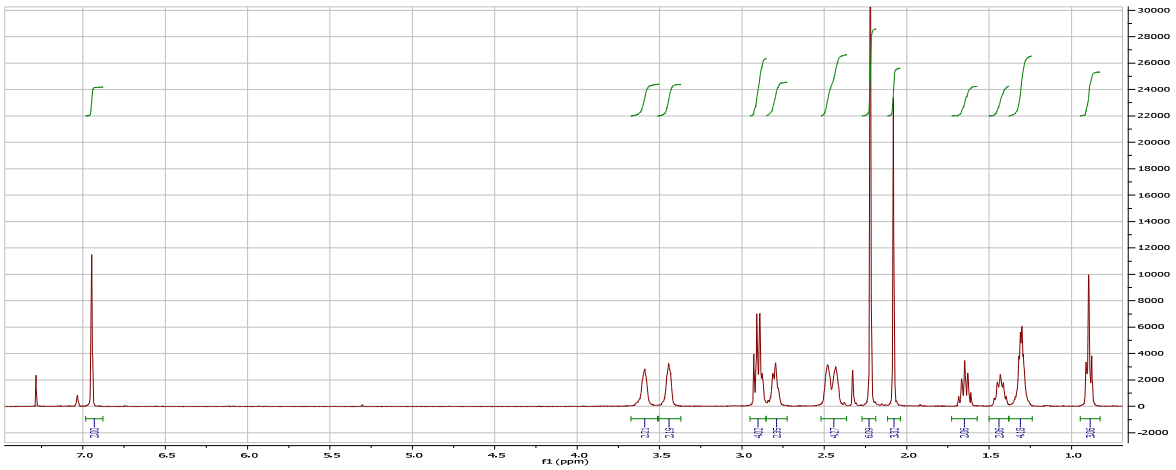


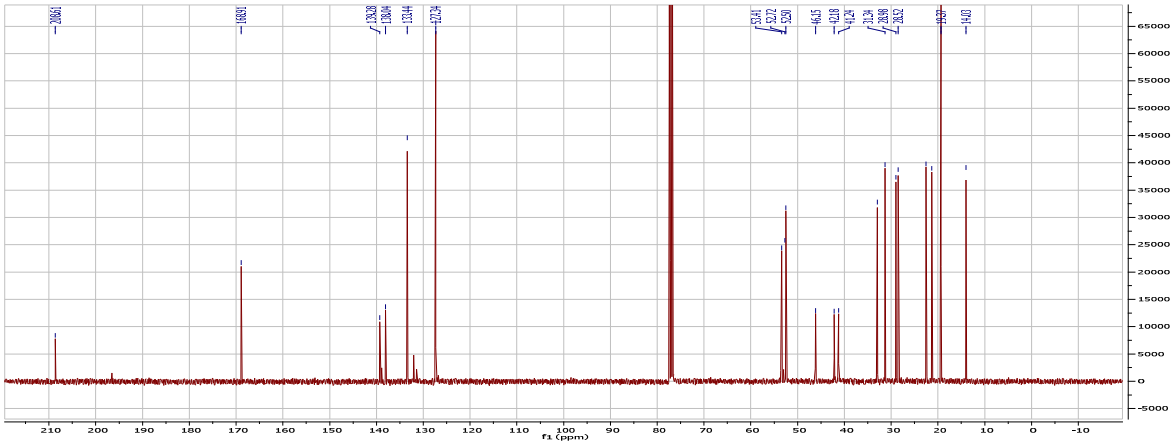
Peak ID	Compound	Time	Mass Found
6	Found	0.96	377.57

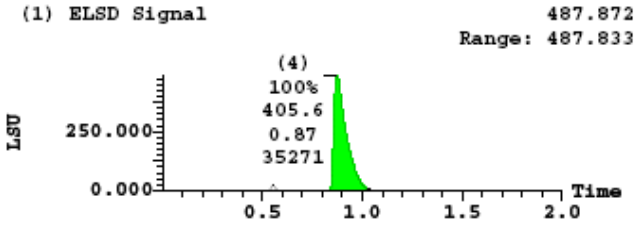




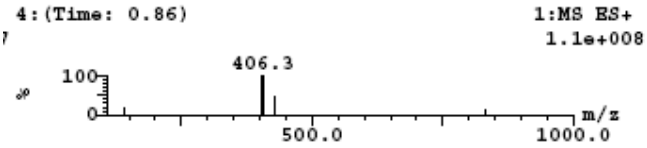
17{*2,5,5*}

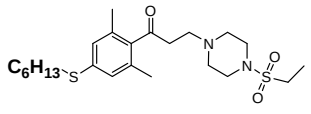




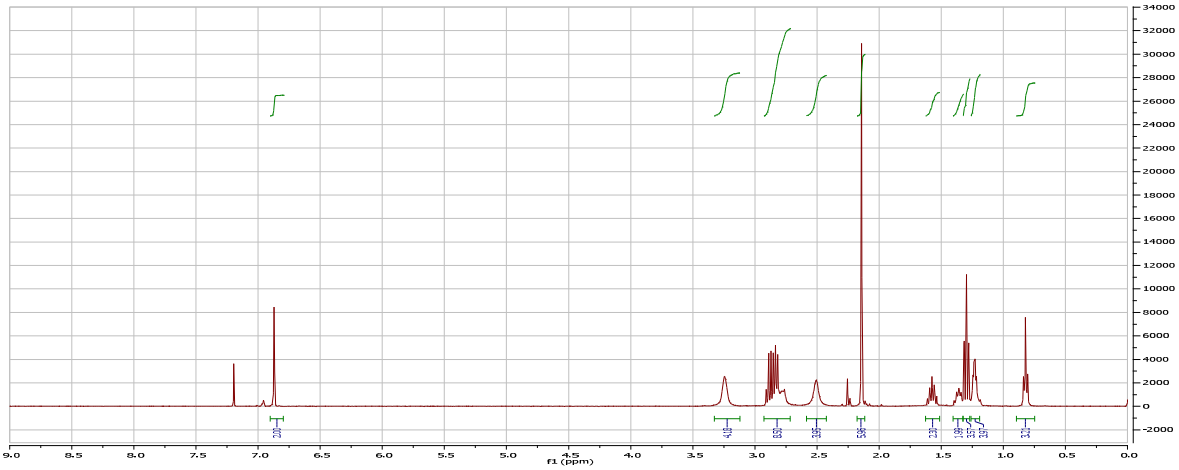


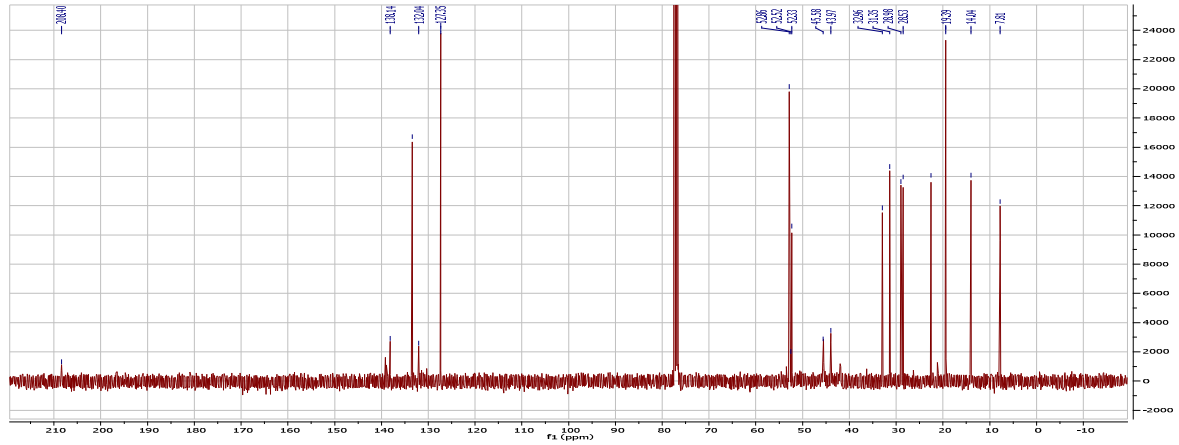
Peak ID	Compound	Time	Mass Found
4	Found	0.86	405.62

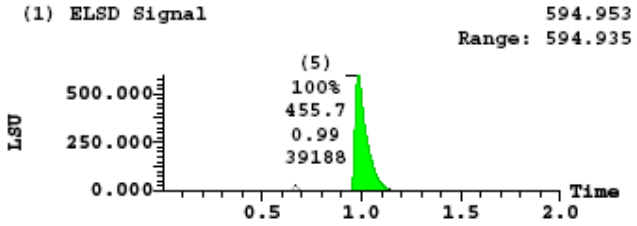




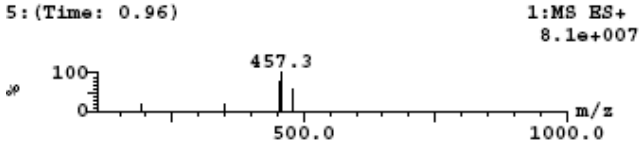
17{*2,5,6*}

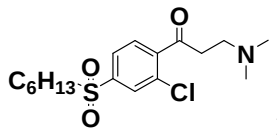




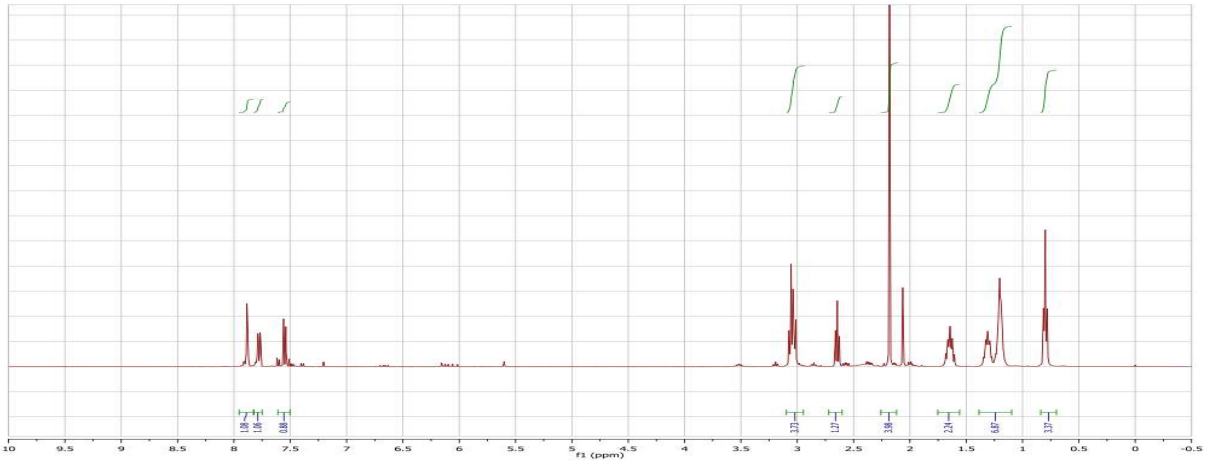


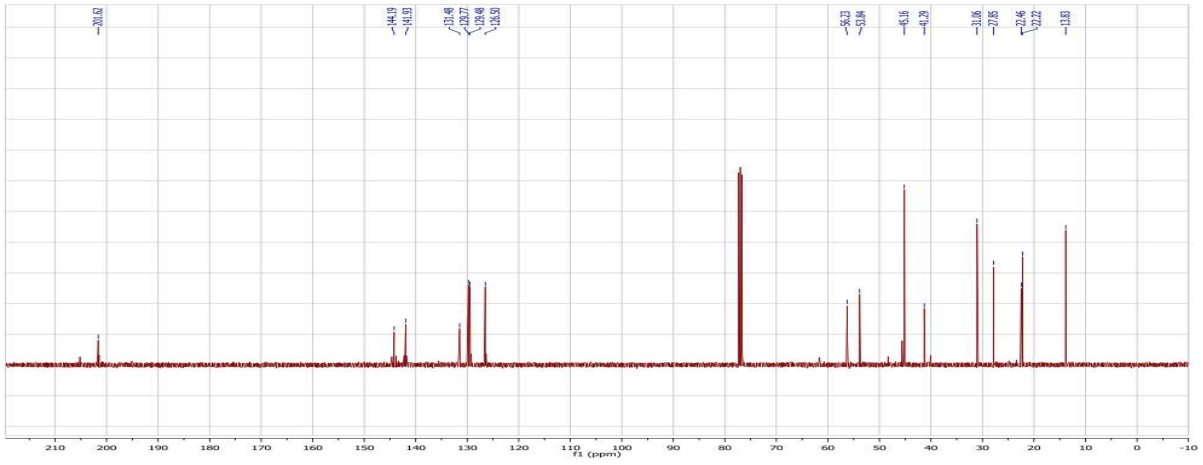
Peak ID	Compound	Time	Mass Found
5	Found	0.96	455.70

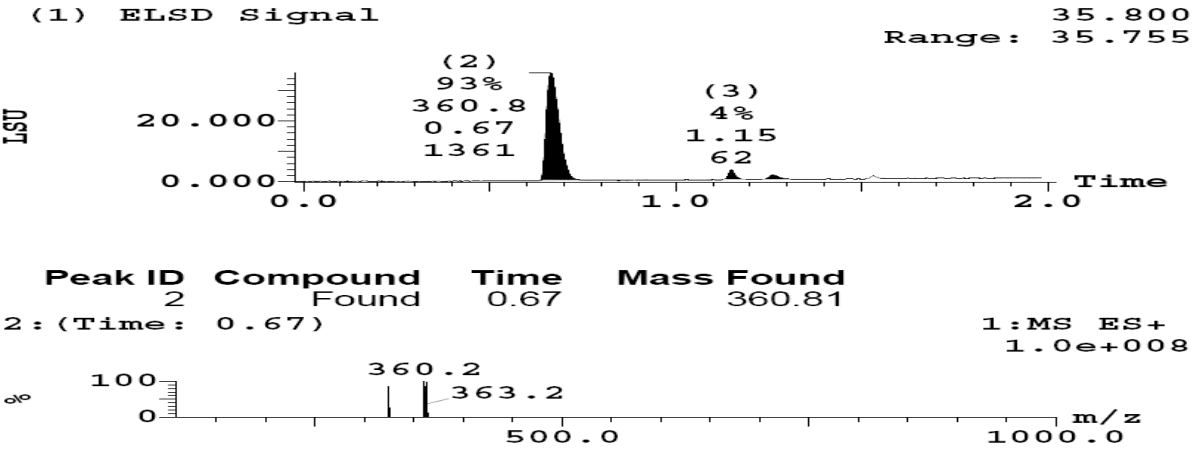




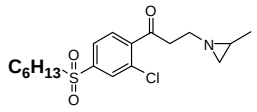
17{*3,1,1*}



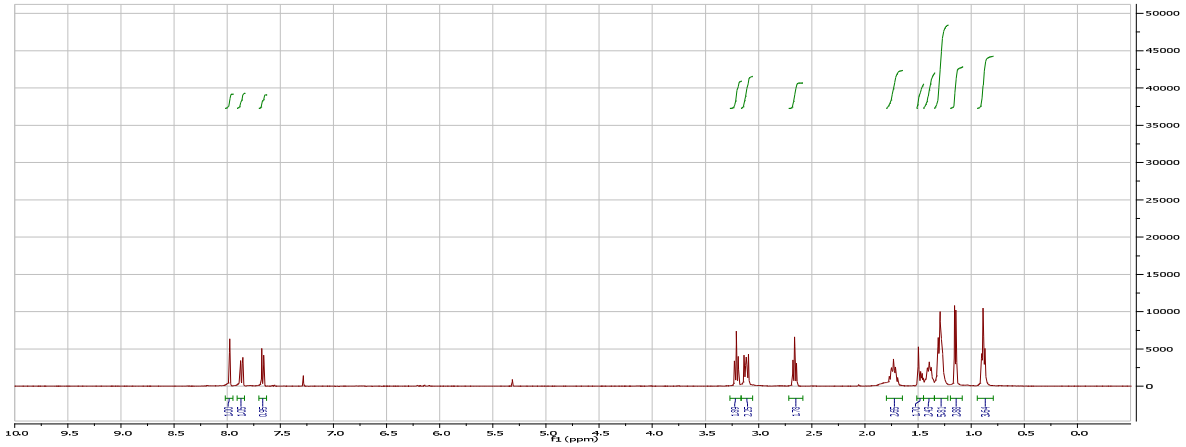


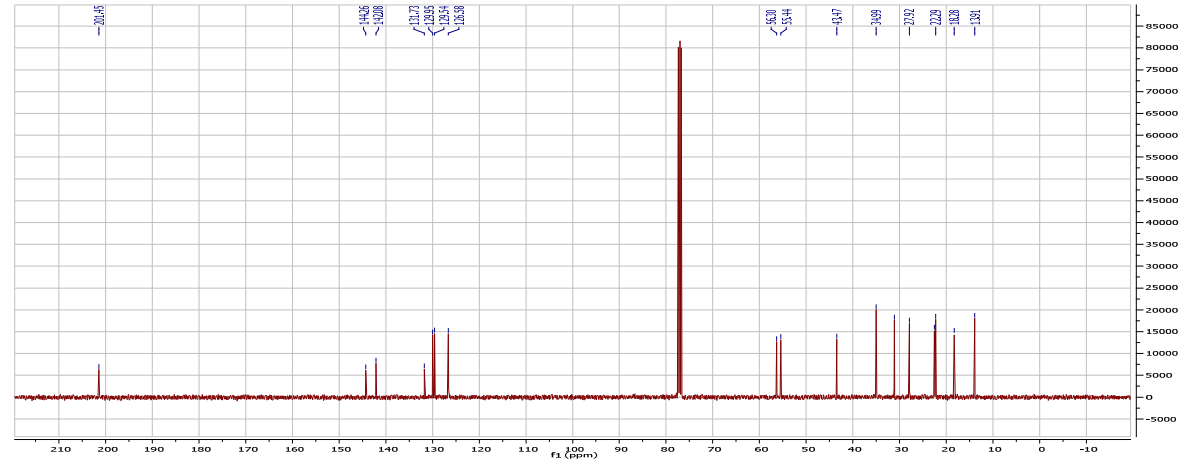


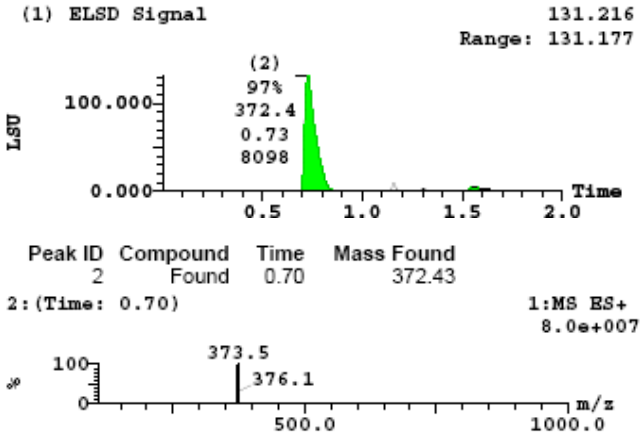
Peak ID	Compound	Time	Mass Found
2	Found	0.67	360.81

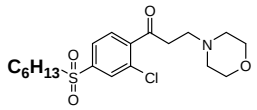

C6H13
O
S
O
O
Cl
N

17{*3,1,2*}

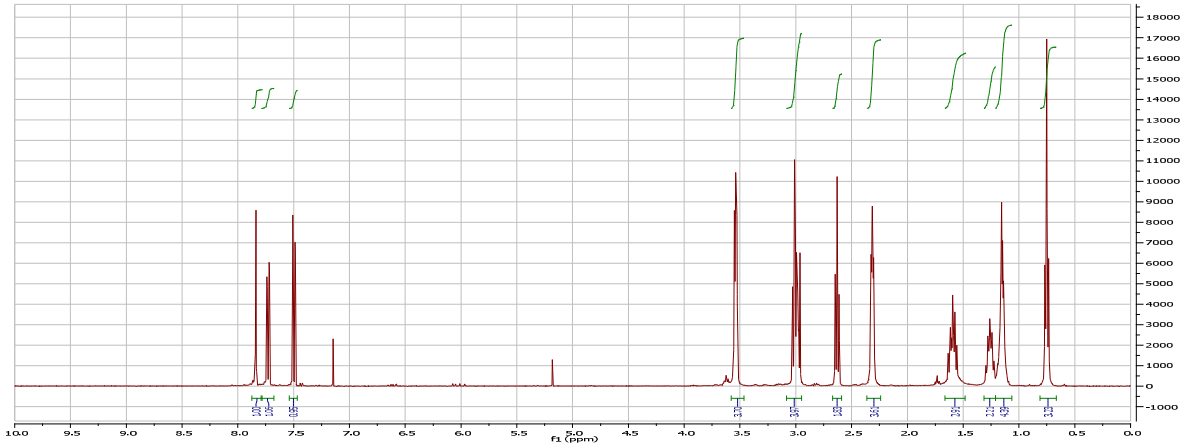


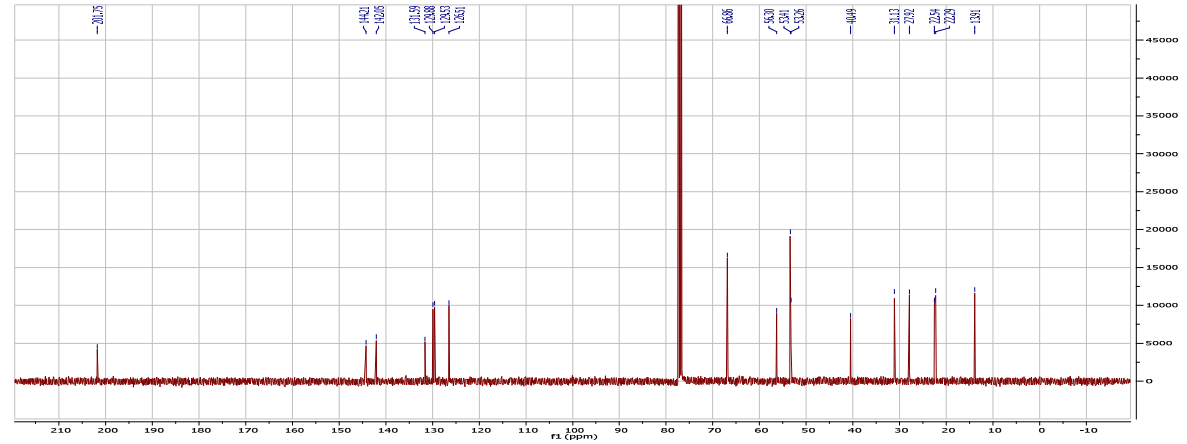


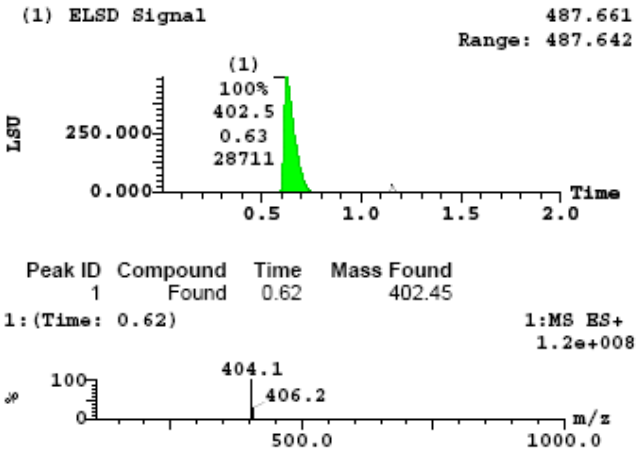

(1) ELSD Signal
131.216
Range: 131.177
(2)
97%
372.4
0.73
8098
100.000
0.000
LSU
0.5
1.0
1.5
2.0
Time
Peak ID Compound Time Mass Found
2 Found 0.70 372.43
2:(Time: 0.70)
1:MS ES+
8.0e+007
373.5
376.1
100
0
%
500.0
1000.0
m/z

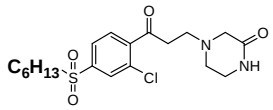

C6H13
O
S
O
O
Cl
N
O

17{*3,1,3*}

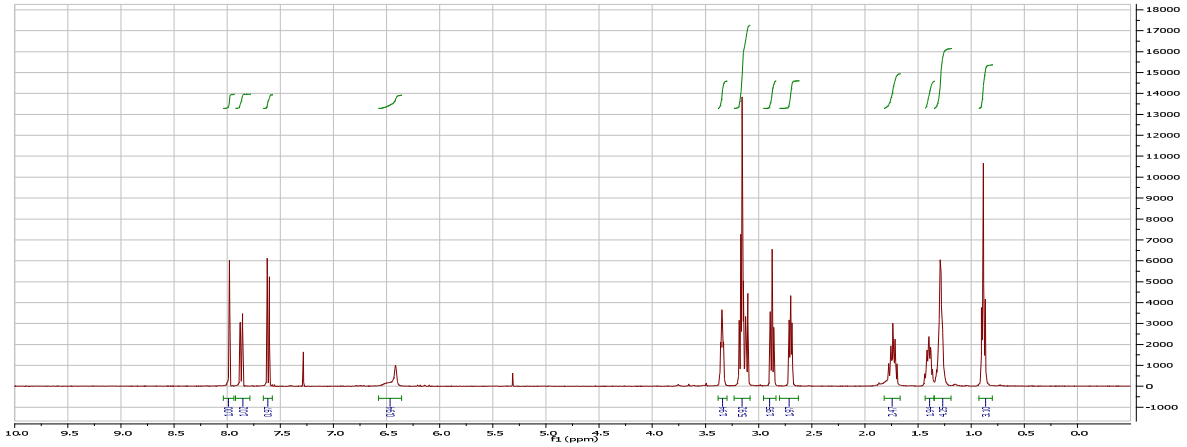


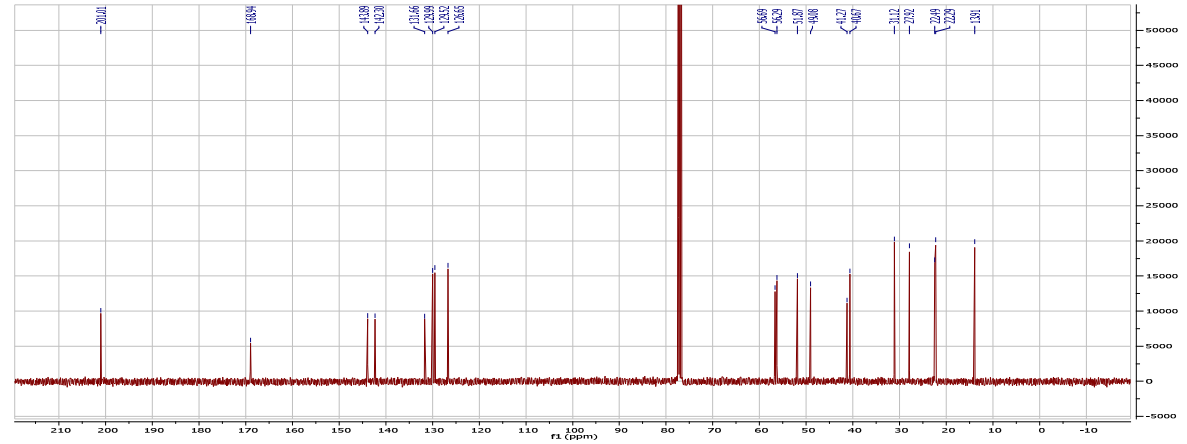


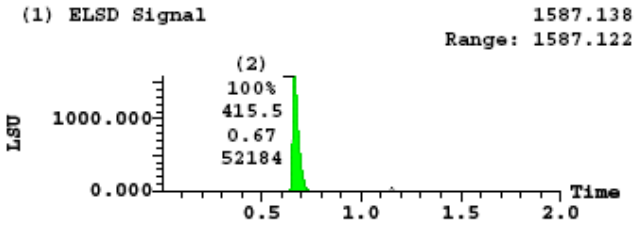

(1) ELSD Signal
487.661
Range: 487.642
(1)
100%
402.5
0.63
28711
LSU
250.000
0.000
Time
0.5
1.0
1.5
2.0
Peak ID Compound Time Mass Found
1 Found 0.62 402.45
1:(Time: 0.62)
1:MS ES+
1.2e+008
404.1
406.2
100
%
0
m/z
500.0
1000.0



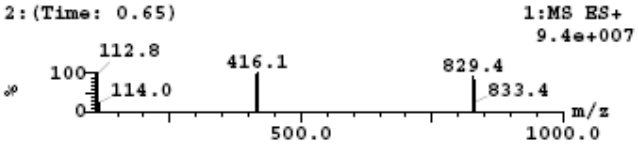
17{*3,1,4*}

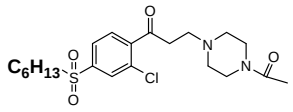




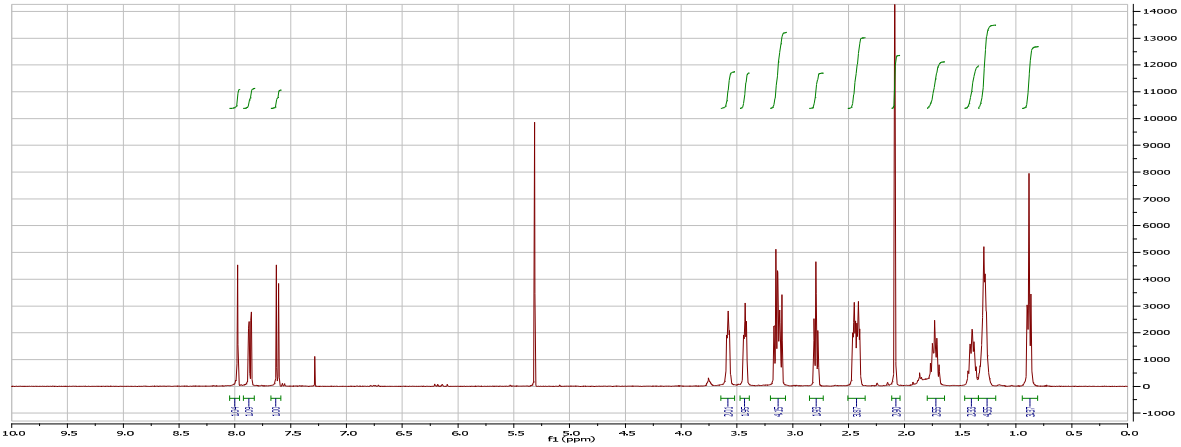


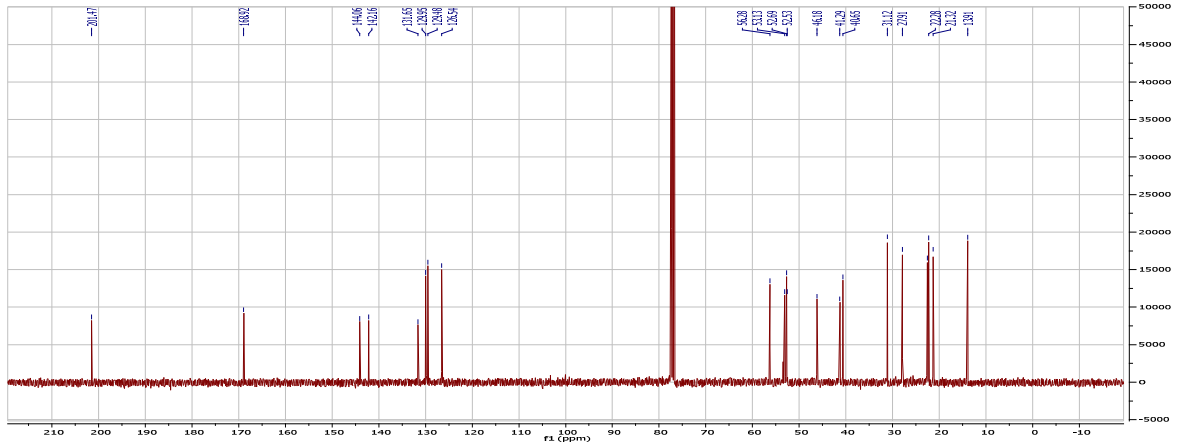
Peak ID	Compound	Time	Mass Found
2	Found	0.65	415.45

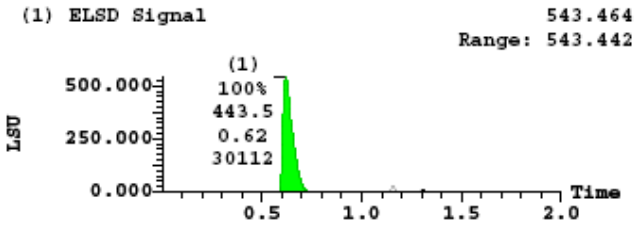




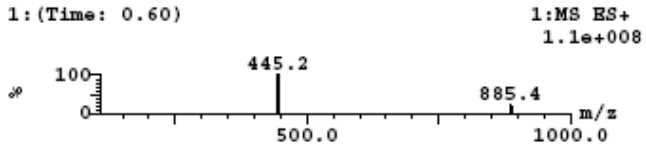
17{*3,1,5*}

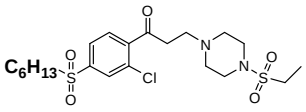




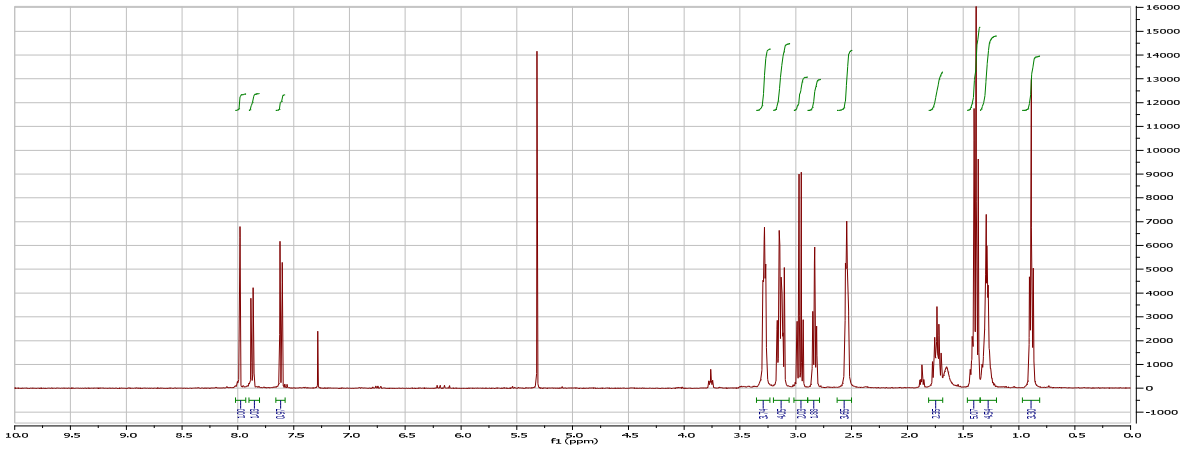


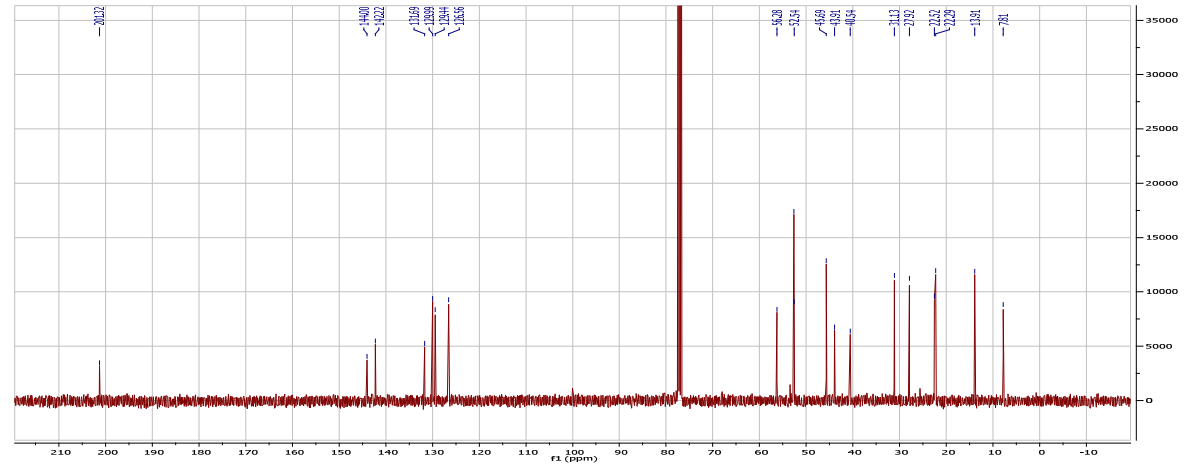
Peak ID	Compound	Time	Mass Found
1	Found	0.60	443.51

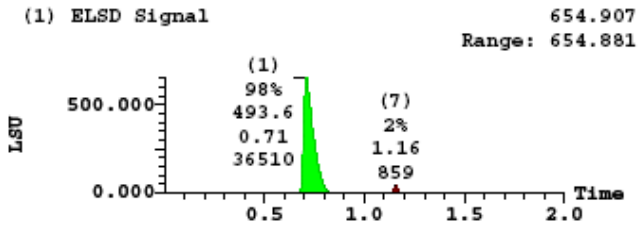




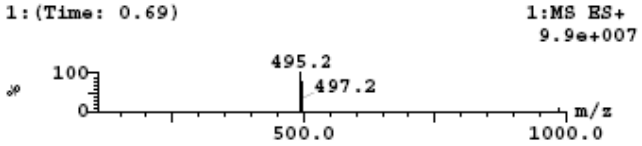
17{*3,1,6*}

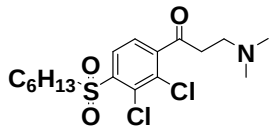




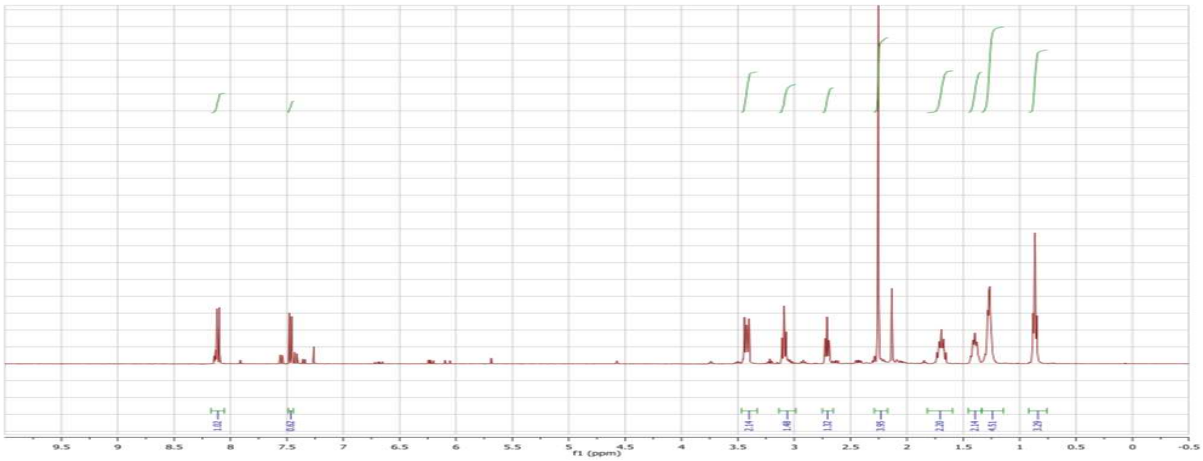


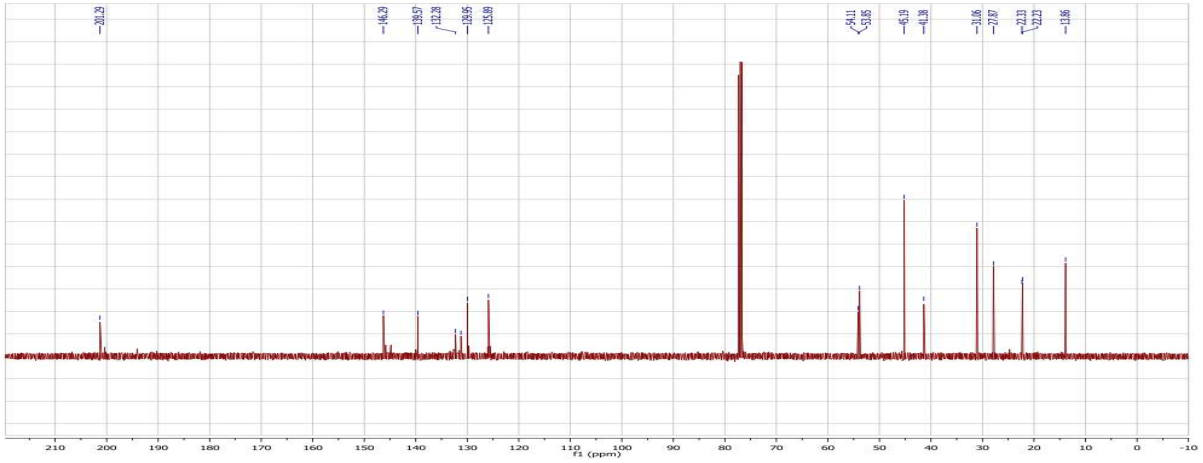
Peak ID	Compound	Time	Mass Found
1	Found	0.69	493.59

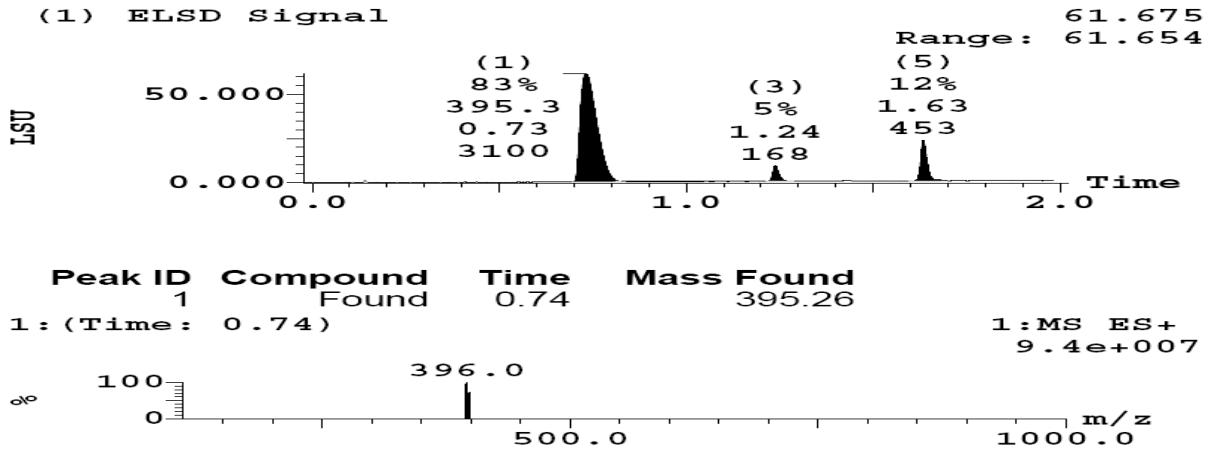




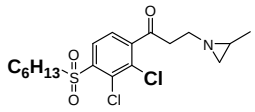
17{*3,2,1*}



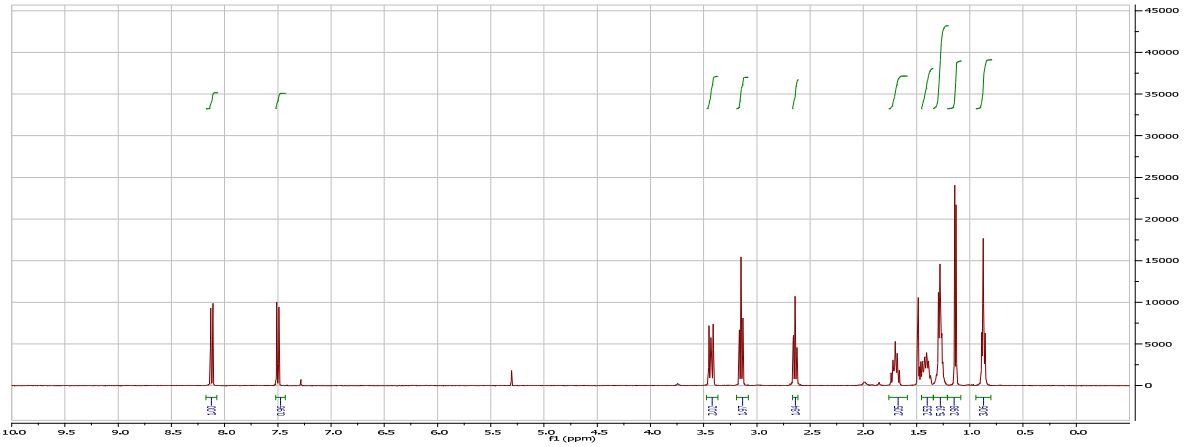


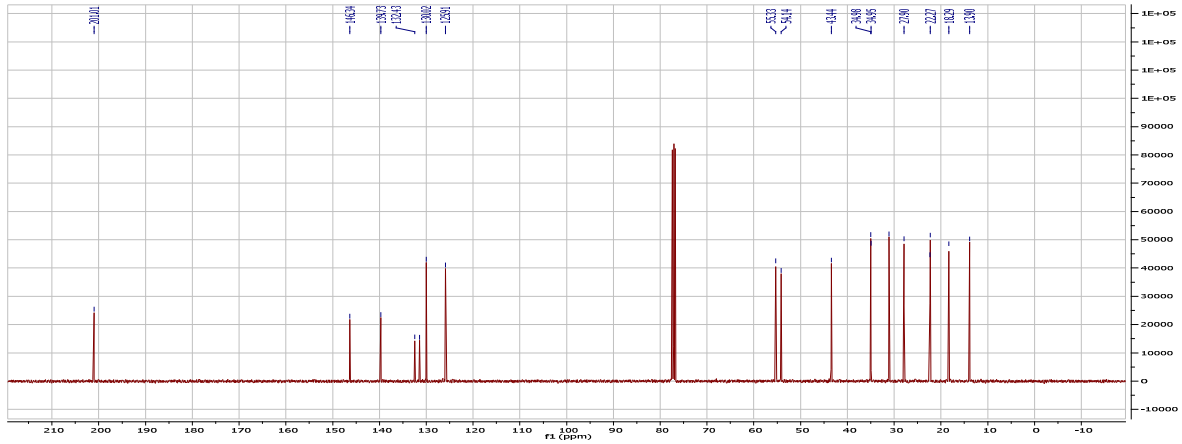


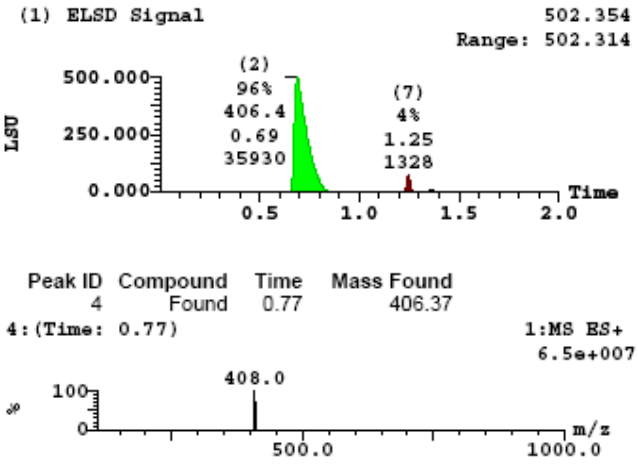
Peak ID	Compound	Time	Mass Found
1	Found	0.74	395.26



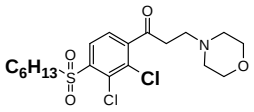
17{*3,2,2*}



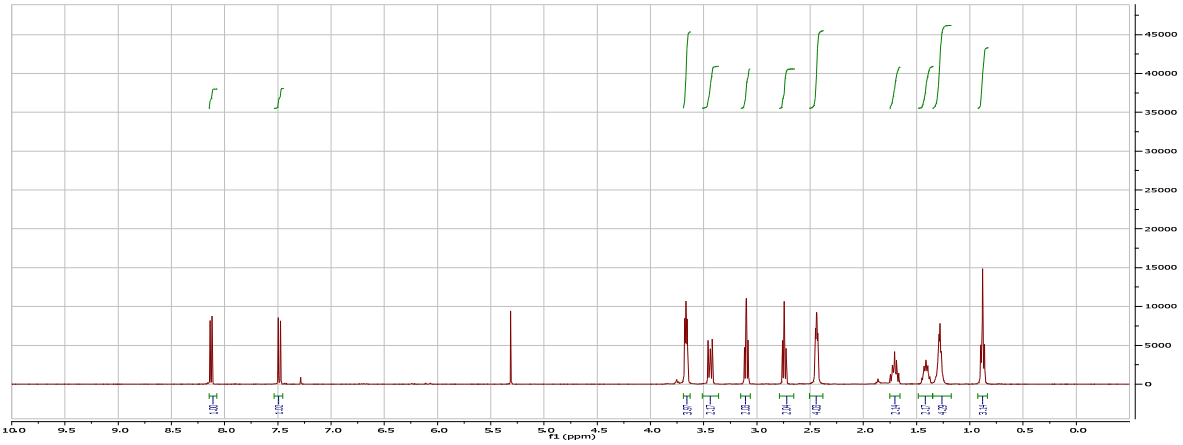


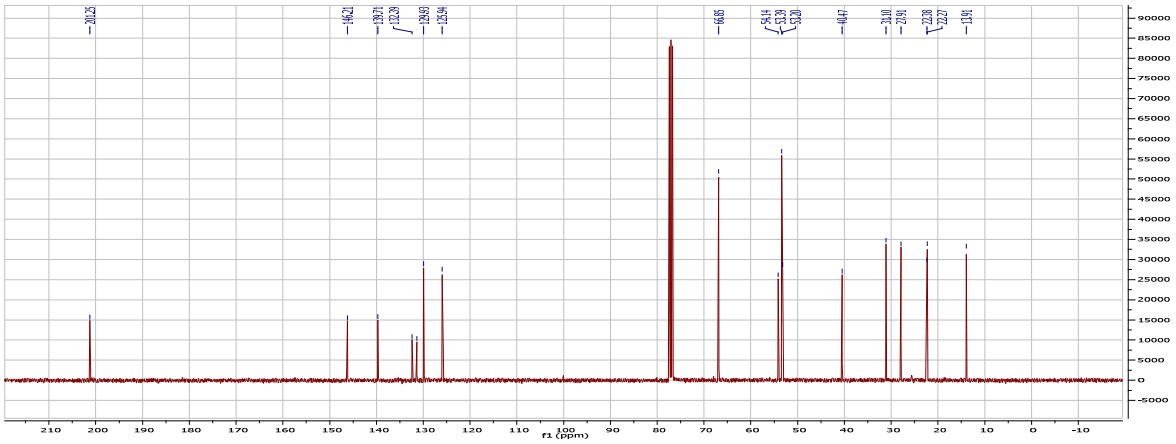


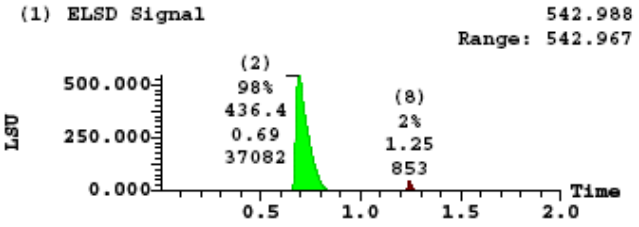
Peak ID	Compound	Time	Mass Found
4	Found	0.77	406.37



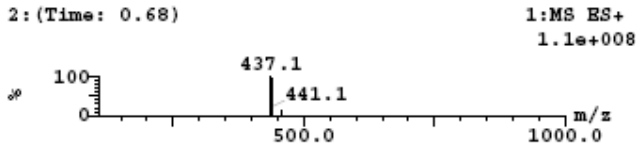
17{*3,2,3*}

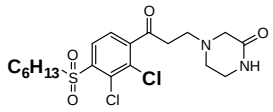




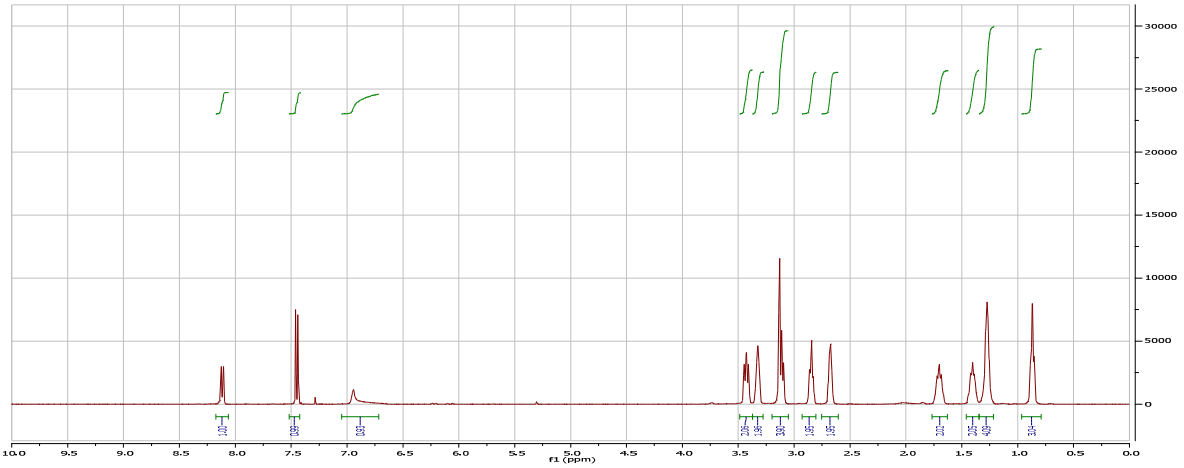


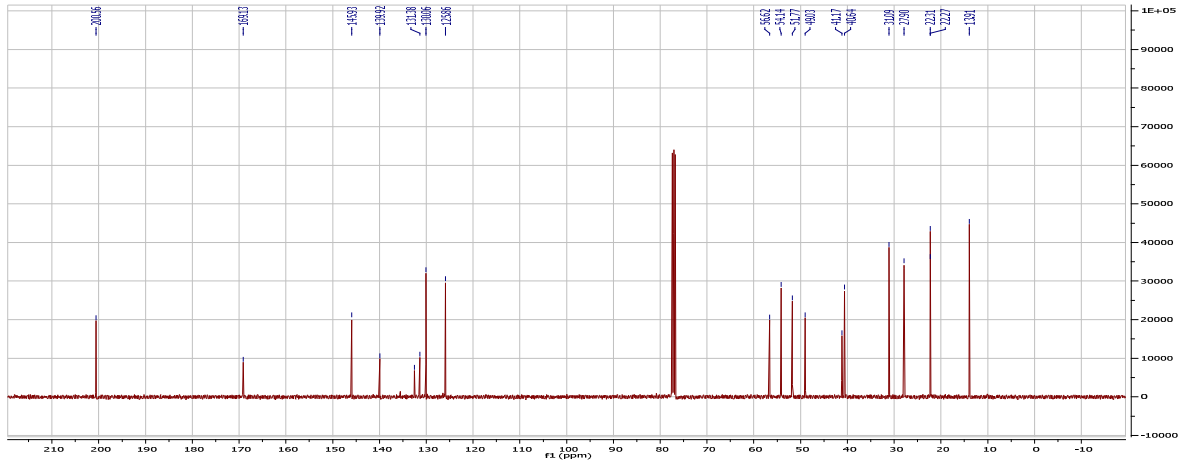
Peak ID	Compound	Time	Mass Found
2	Found	0.68	436.40

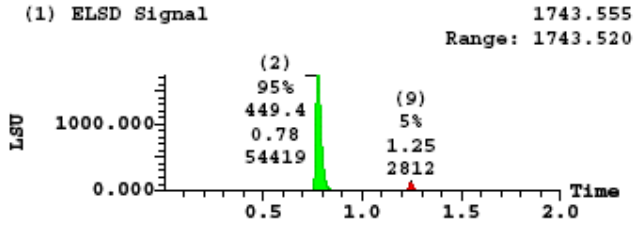




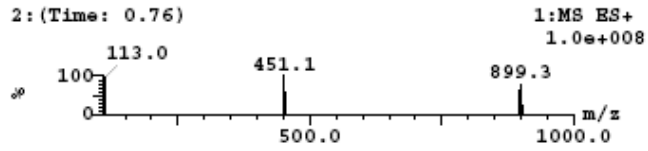
17{*3,2,4*}

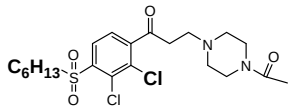




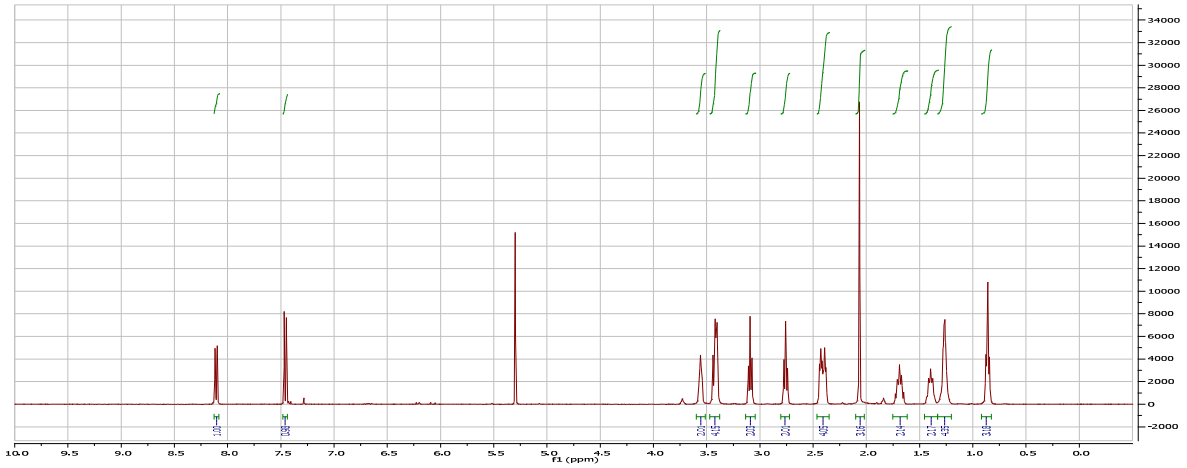


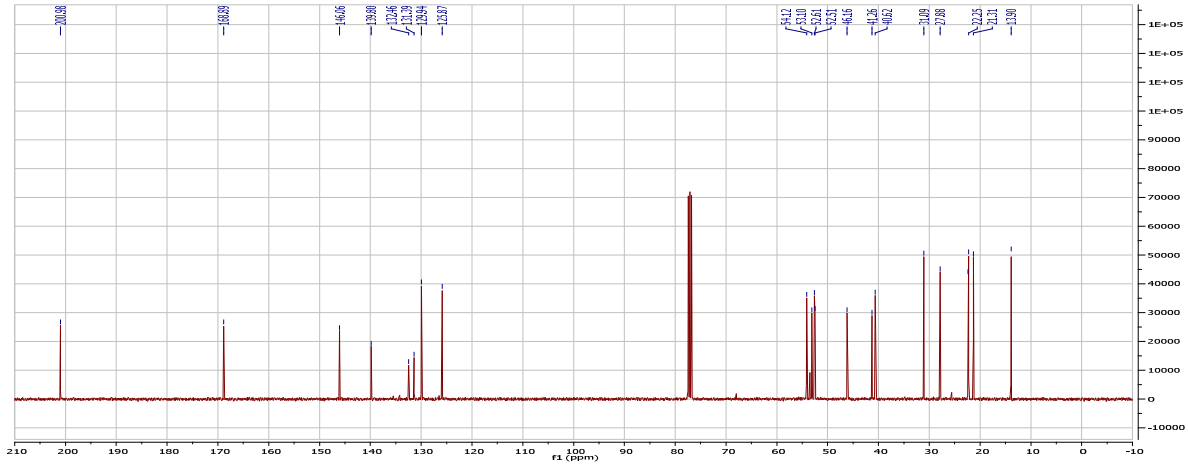
Peak ID	Compound	Time	Mass Found
2	Found	0.76	449.40

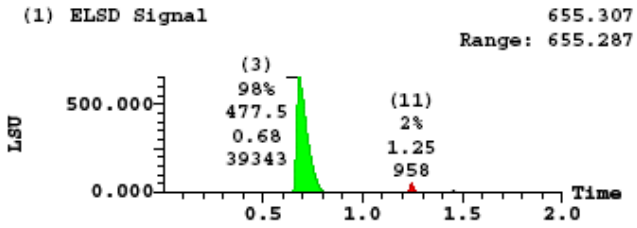




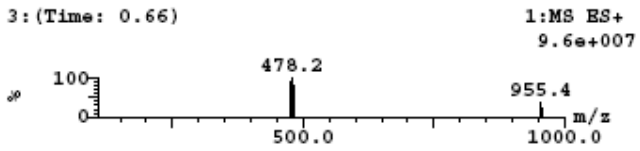
17{*3,2,5*}

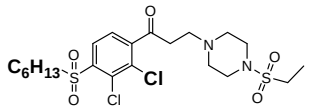




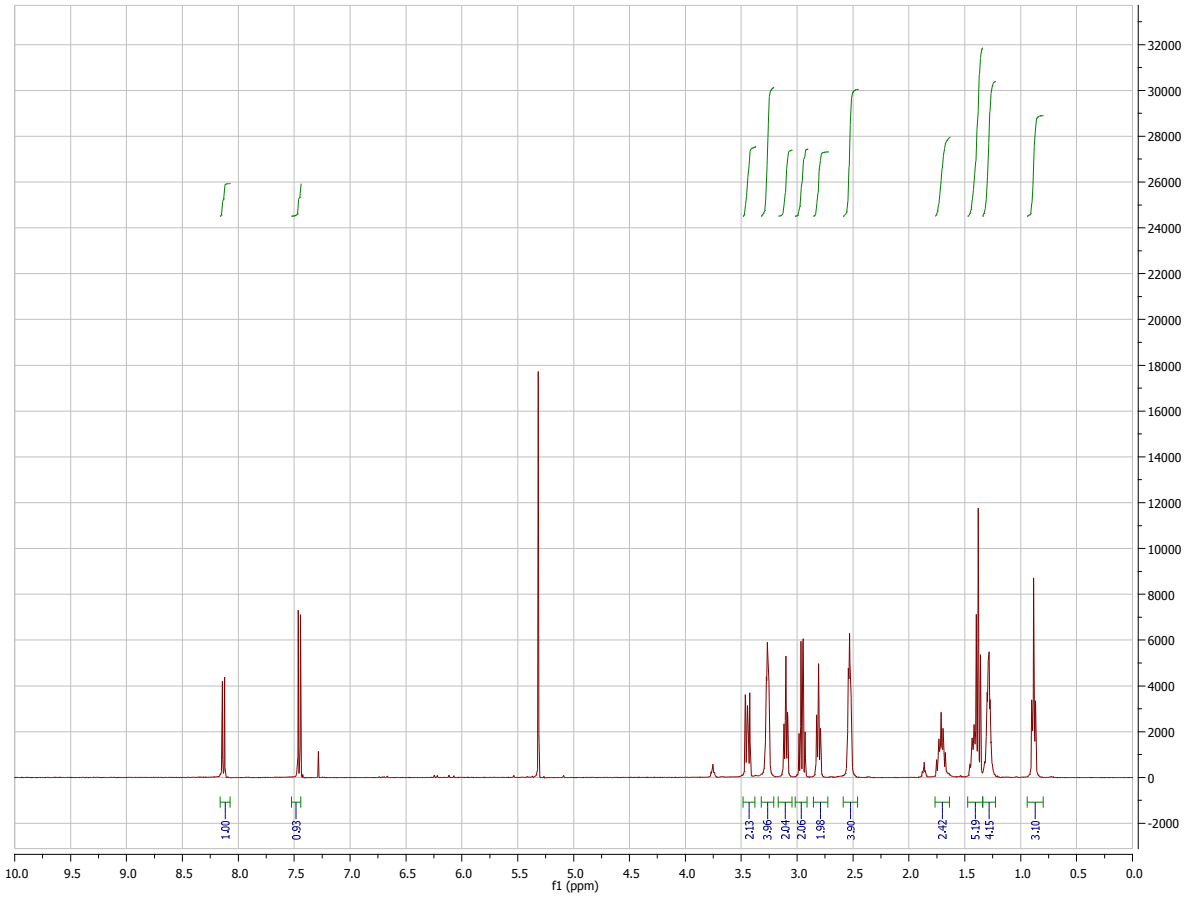


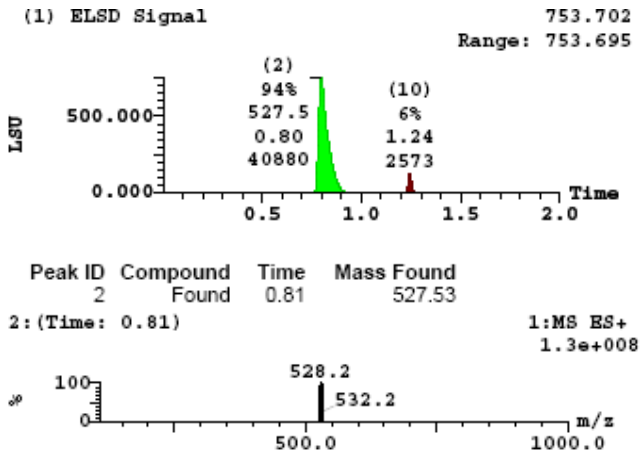
Peak ID	Compound	Time	Mass Found
3	Found	0.66	477.45



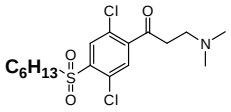


17{*3,2,6*}

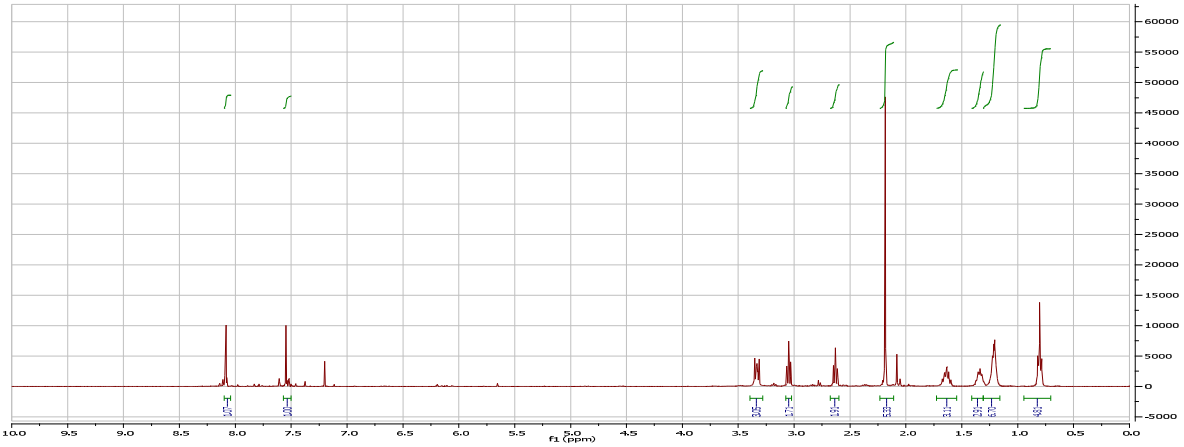


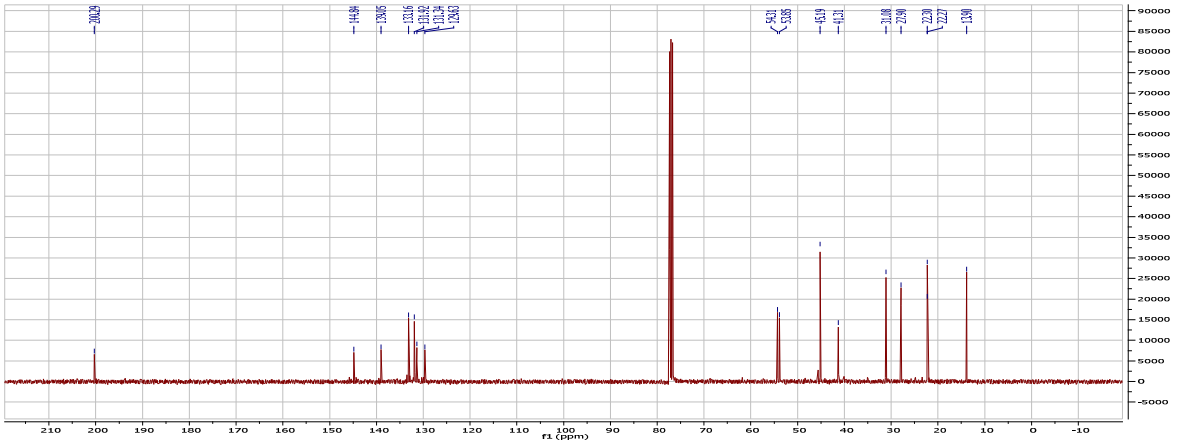


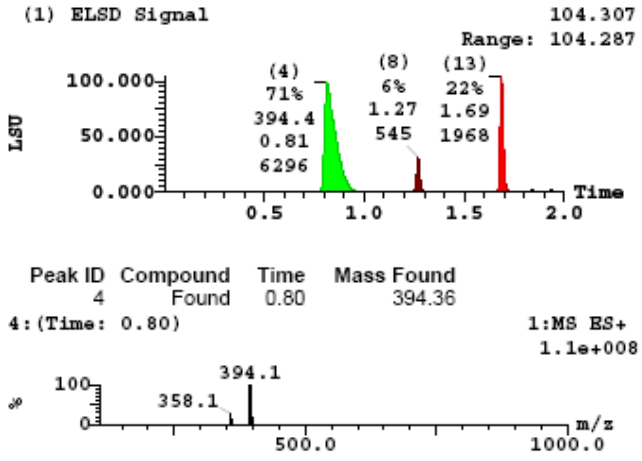
Peak ID	Compound	Time	Mass Found
2	Found	0.81	527.53



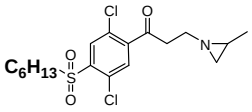
17{*3,3,1*}



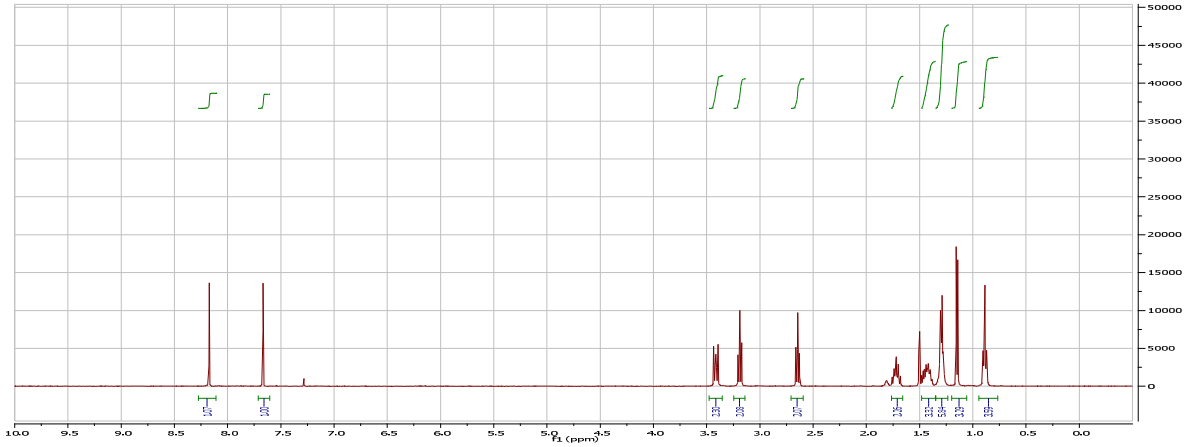


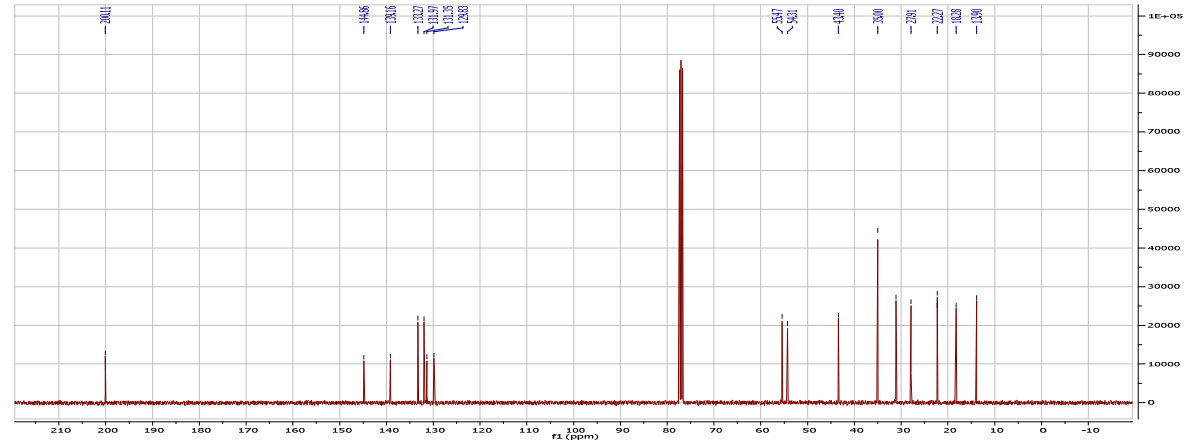


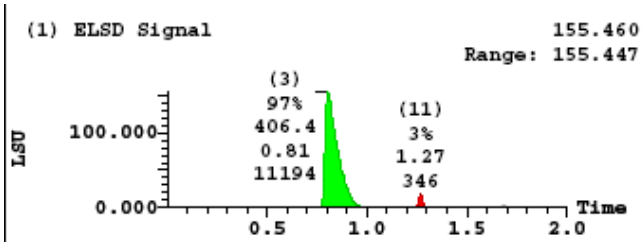
Peak ID	Compound	Time	Mass Found
4	Found	0.80	394.36



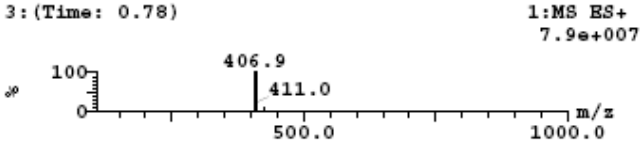
17{*3,3,2*}

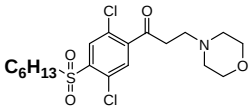




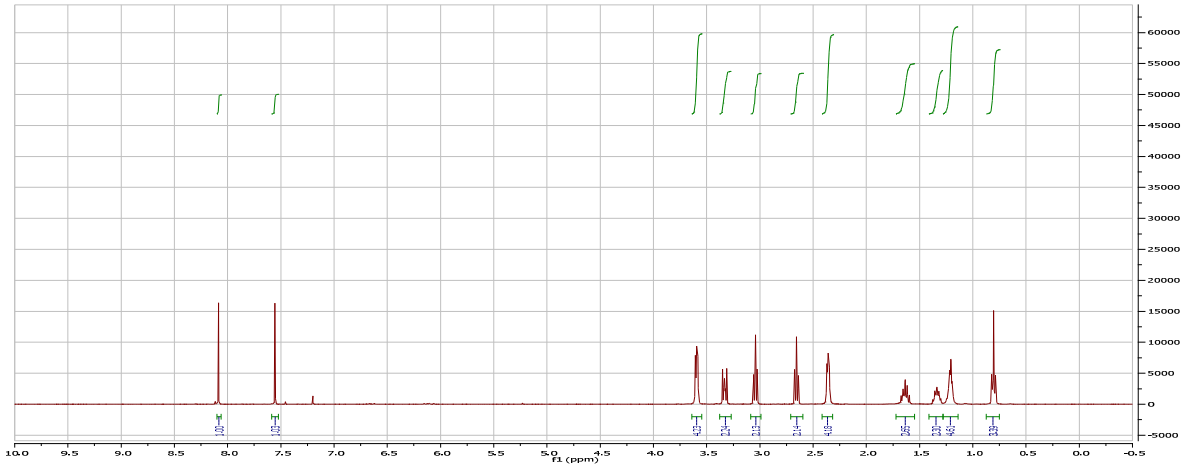


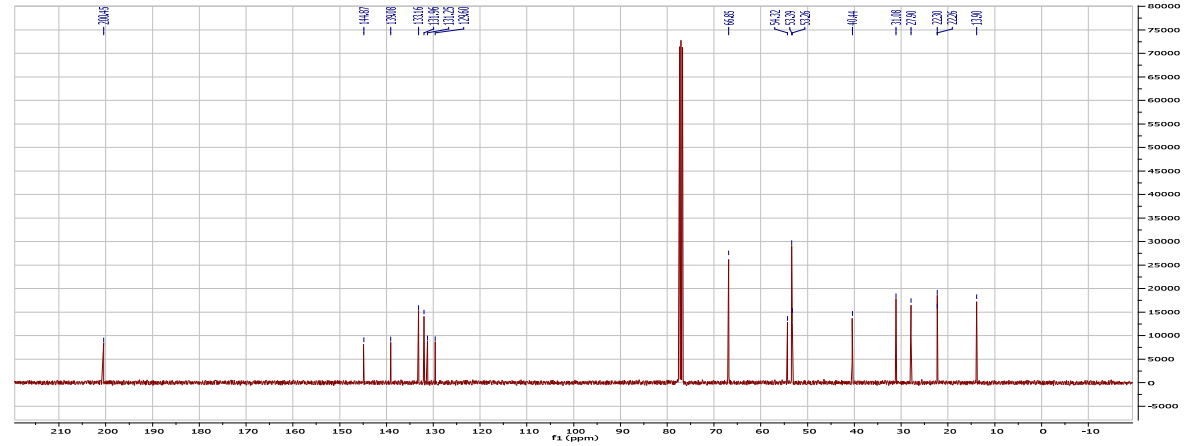
Peak ID	Compound	Time	Mass Found
3	Found	0.78	406.37

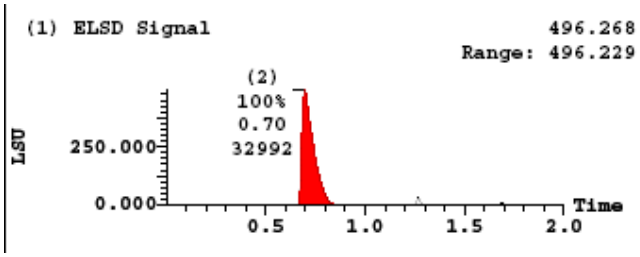




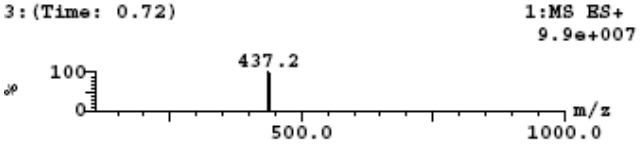
17{*3,3,3*}

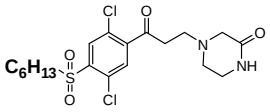




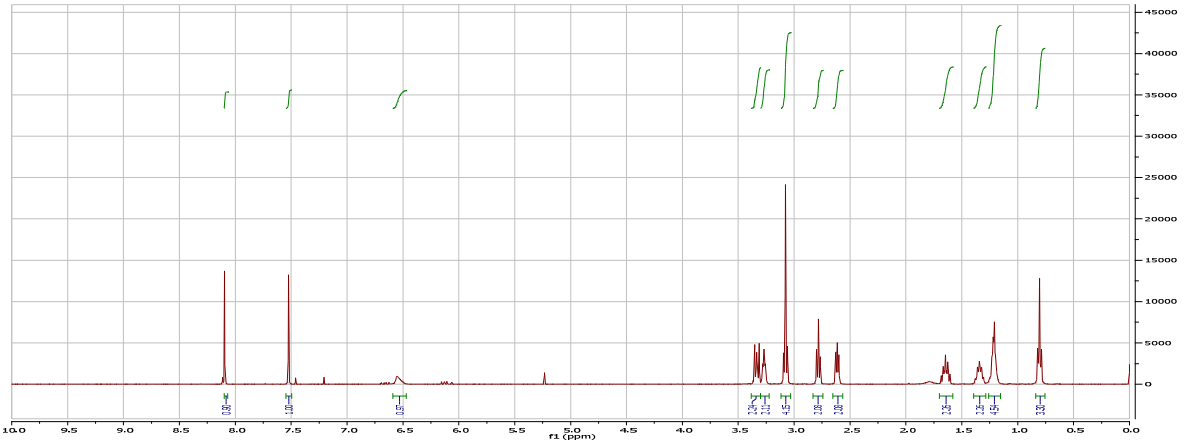


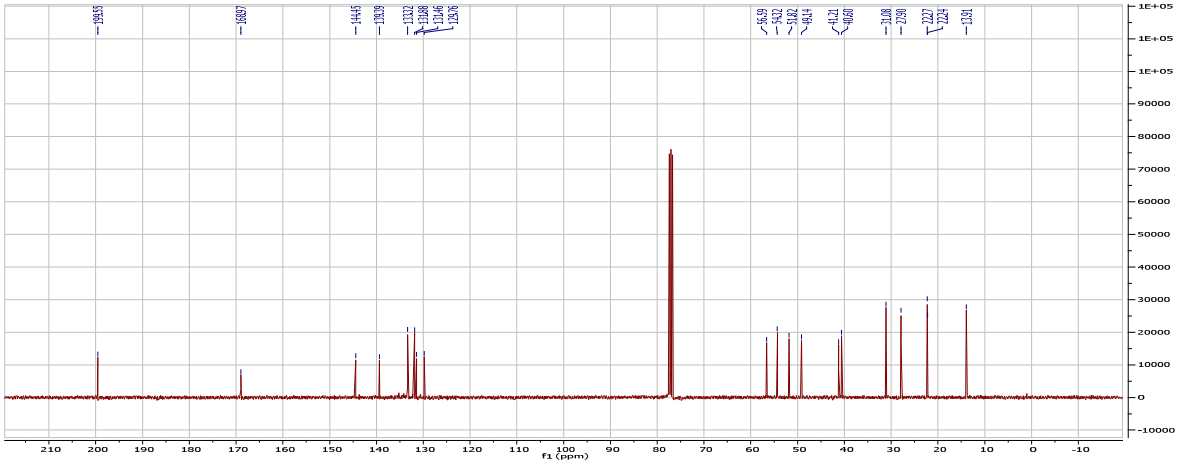
Peak ID	Compound	Time	Mass Found
3	Found	0.72	436.40

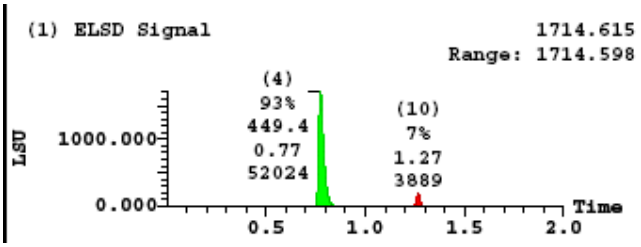


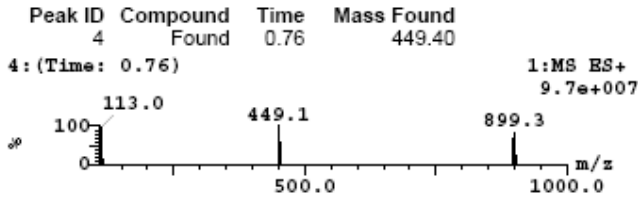

Cl
O
N
O
NH
C_6H_{13}
O
S
O
Cl

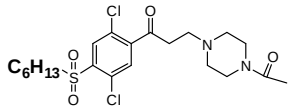
17{*3,3,4*}



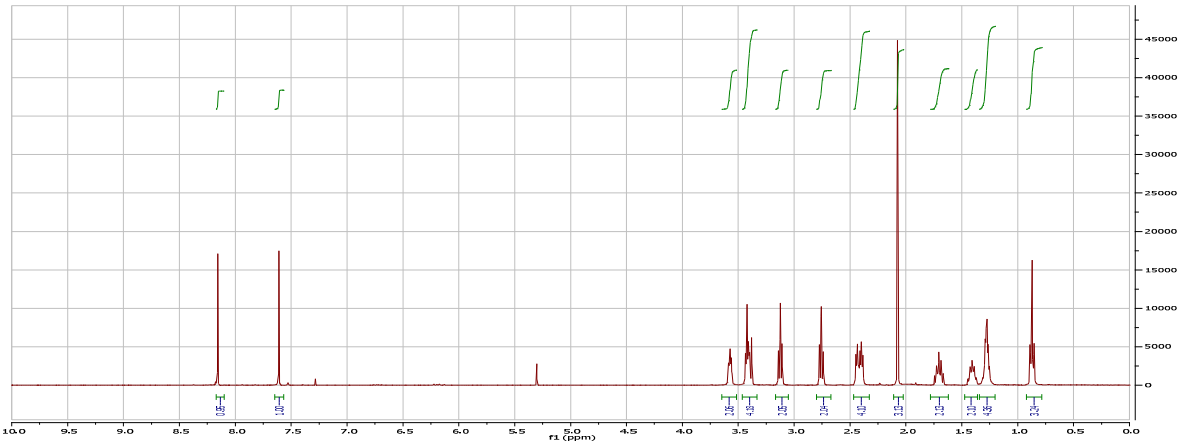


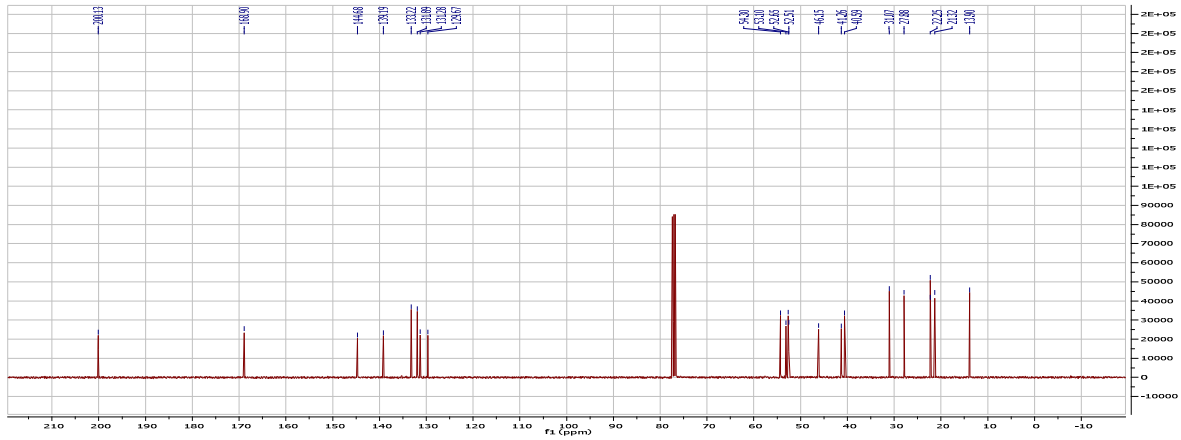

(1) ELSD Signal
1714.615
Range: 1714.598
(4)
93%
449.4
0.77
52024
(10)
7%
1.27
3889
LSU
1000.000
0.000
Time
0.5
1.0
1.5
2.0

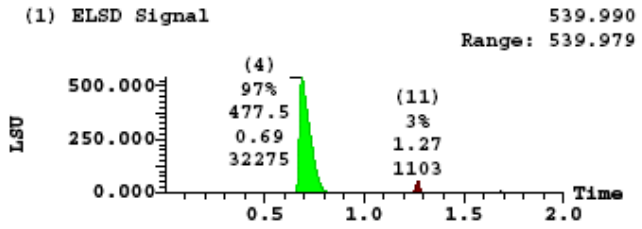

Peak ID Compound Time Mass Found
4 Found 0.76 449.40
4:(Time: 0.76)
1:MS ES+
9.7e+007
113.0
449.1
899.3
100
%
0
m/z
500.0
1000.0



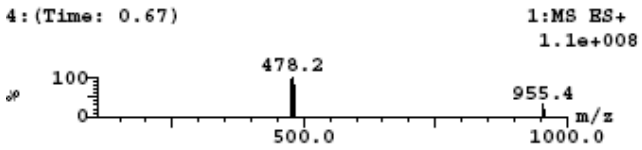
17{*3,3,5*}

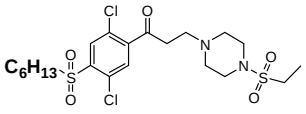




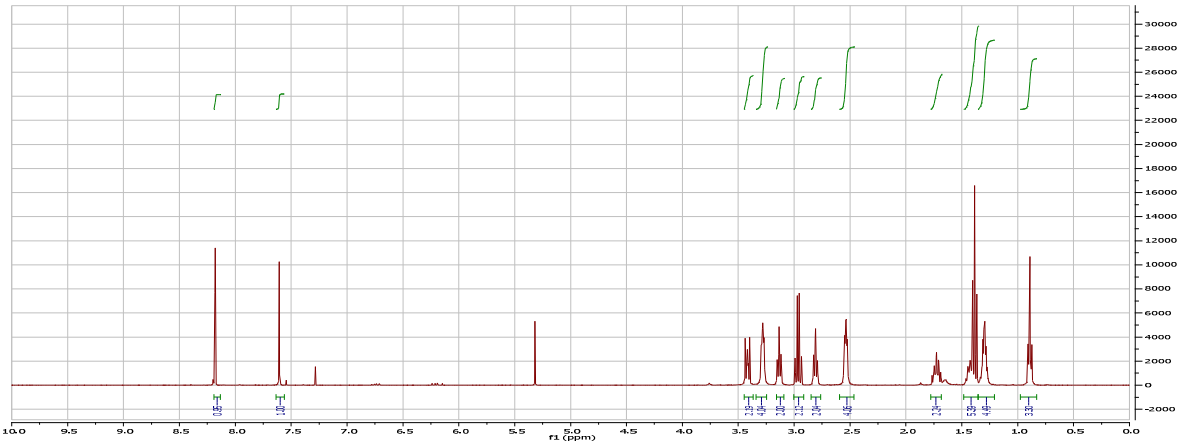


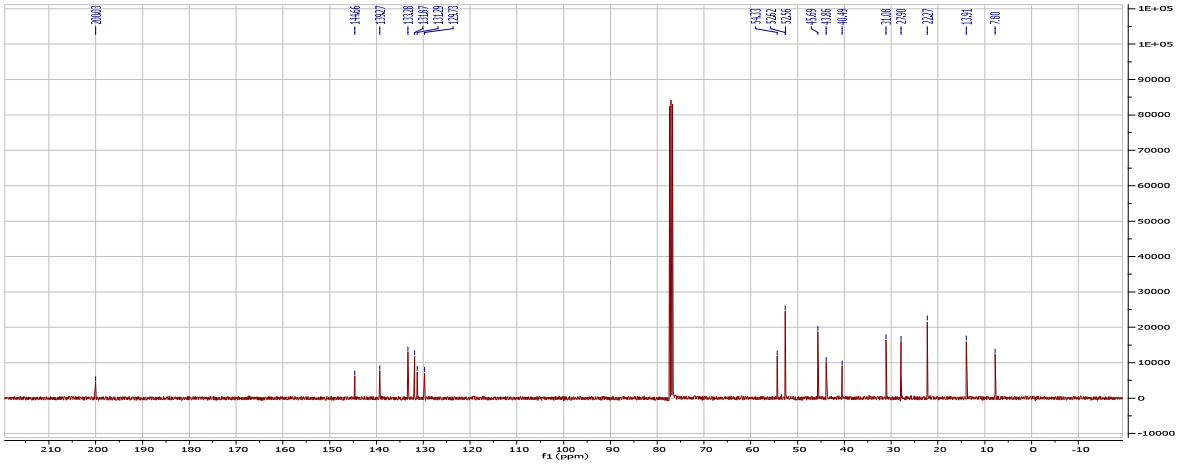
Peak ID	Compound	Time	Mass Found
4	Found	0.67	477.45

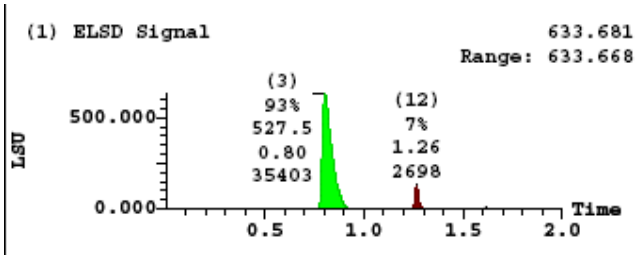




17{*3,3,6*}

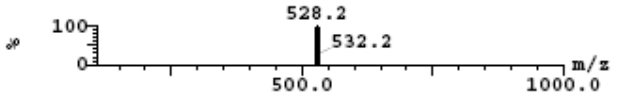


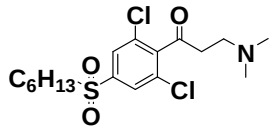




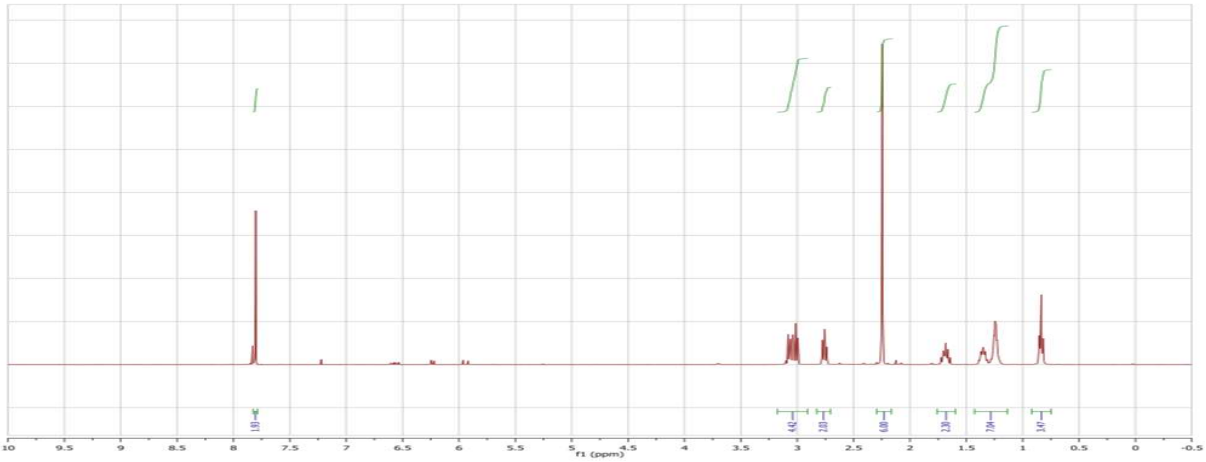
Peak ID	Compound	Time	Mass Found
3	Found	0.78	527.53

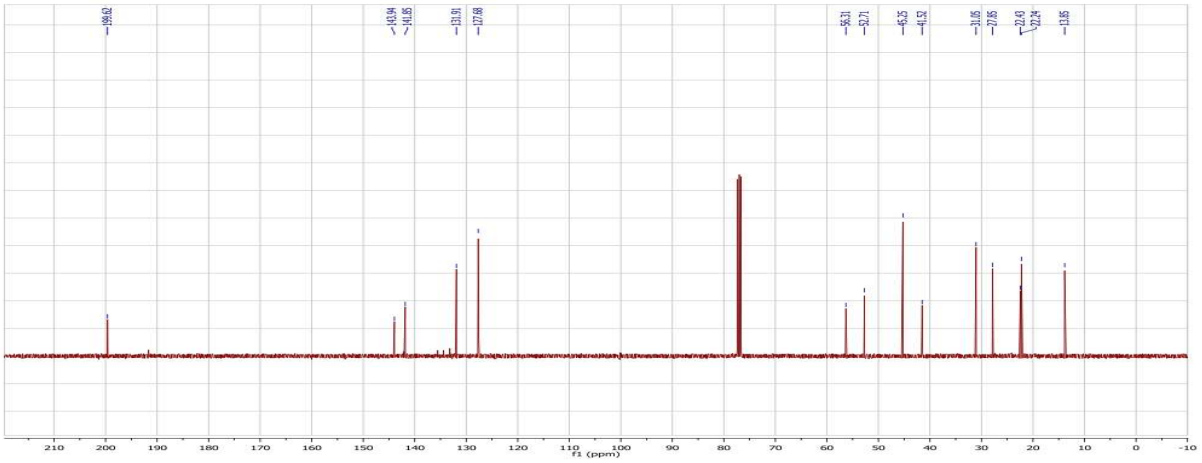
3:(Time: 0.78) 1:MS ES+ 8.7e+007

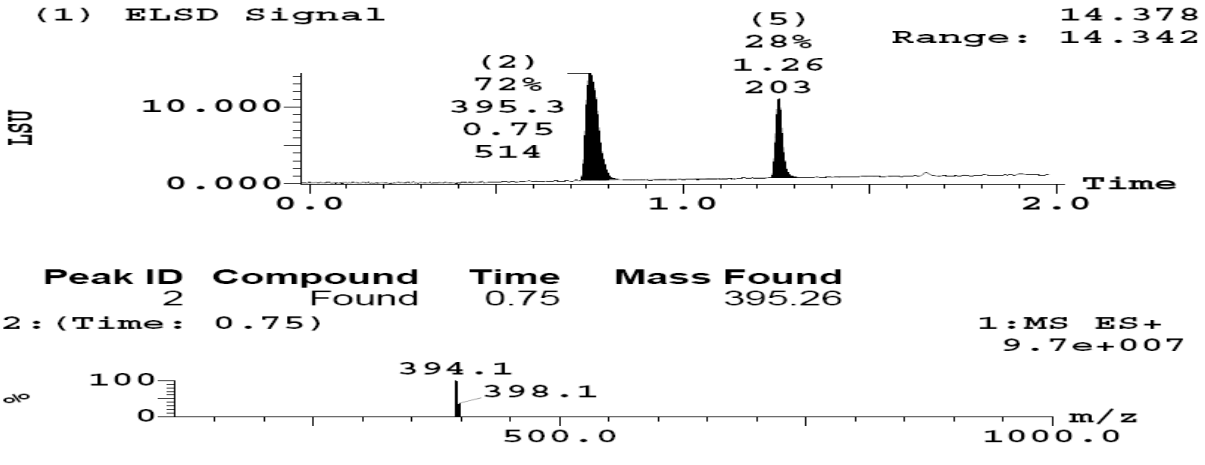




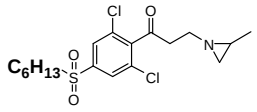
17{*3,4,1*}



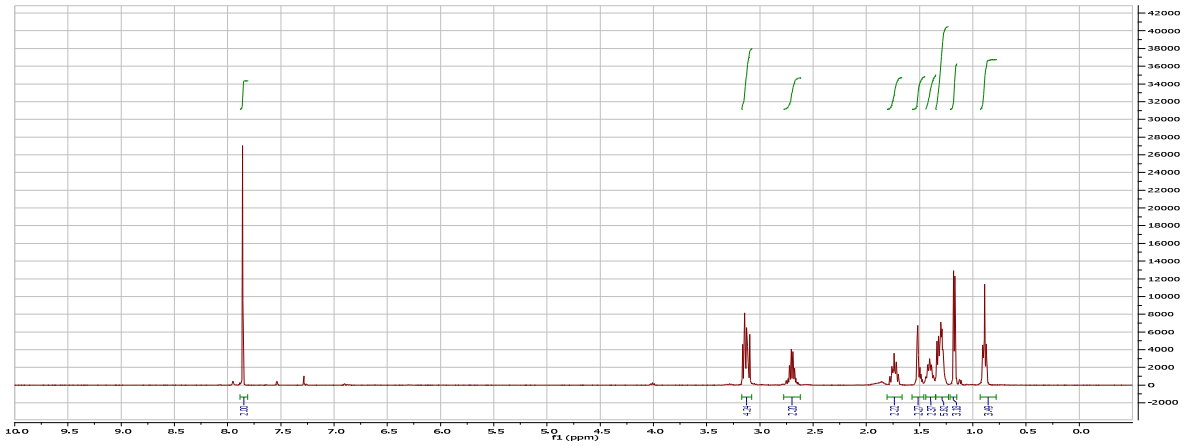


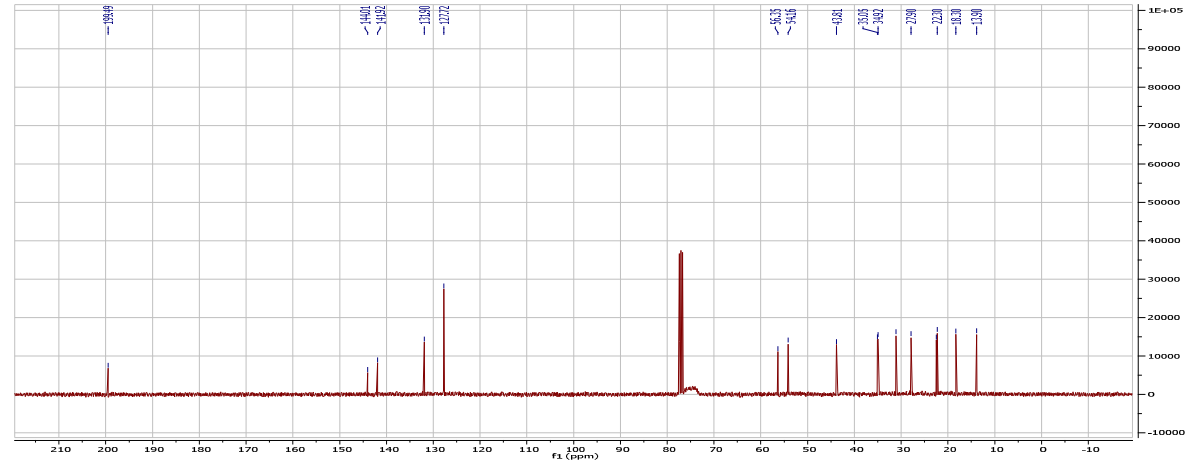


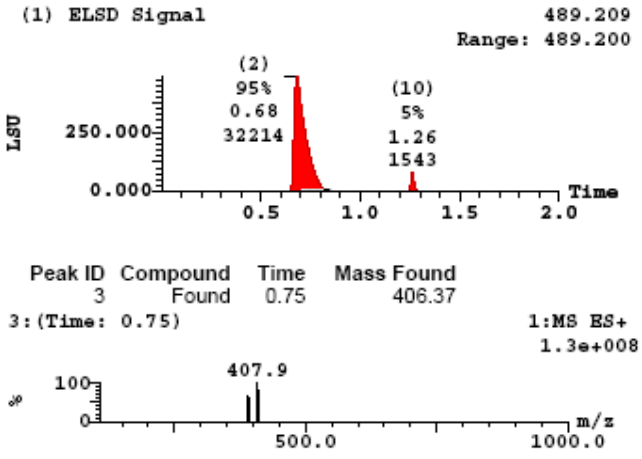
Peak ID	Compound	Time	Mass Found
2	Found	0.75	395.26



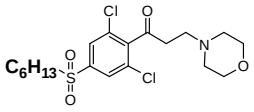
17{*3,4,2*}



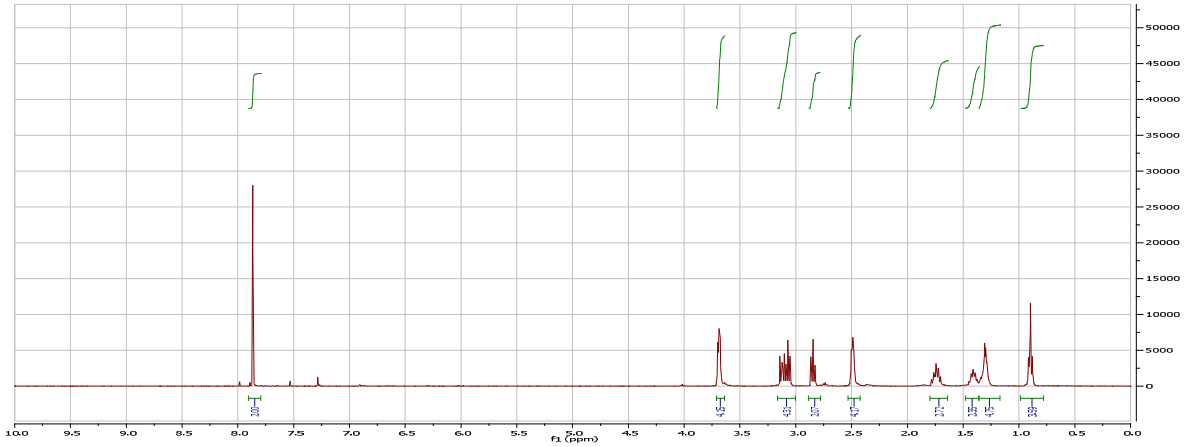


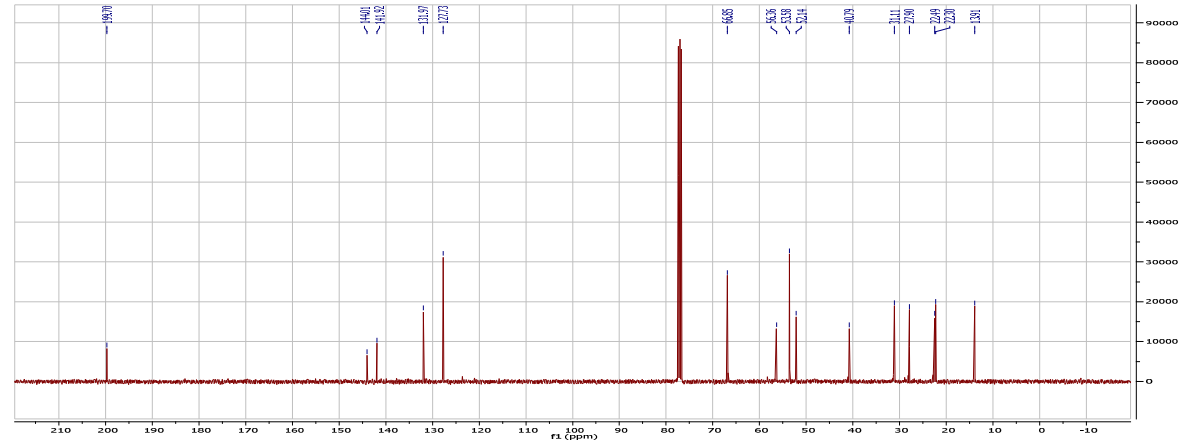


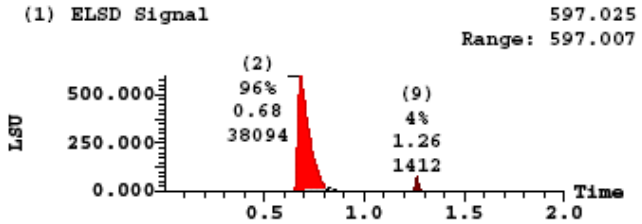
Peak ID	Compound	Time	Mass Found
3	Found	0.75	406.37

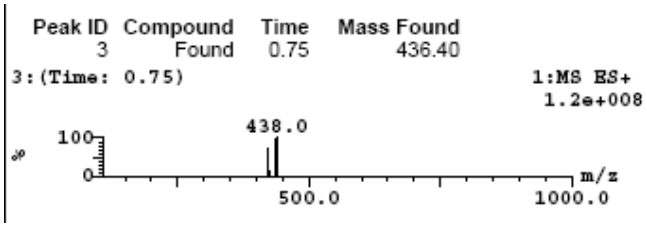

Cl
O
N
O
C_6H_{13}
O
S
O
Cl

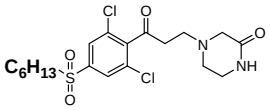
17{*3,4,3*}



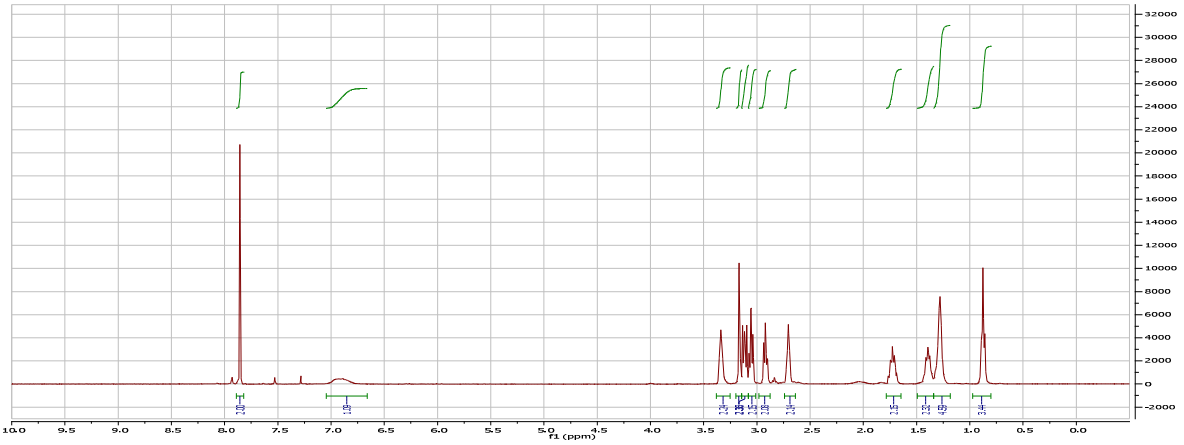


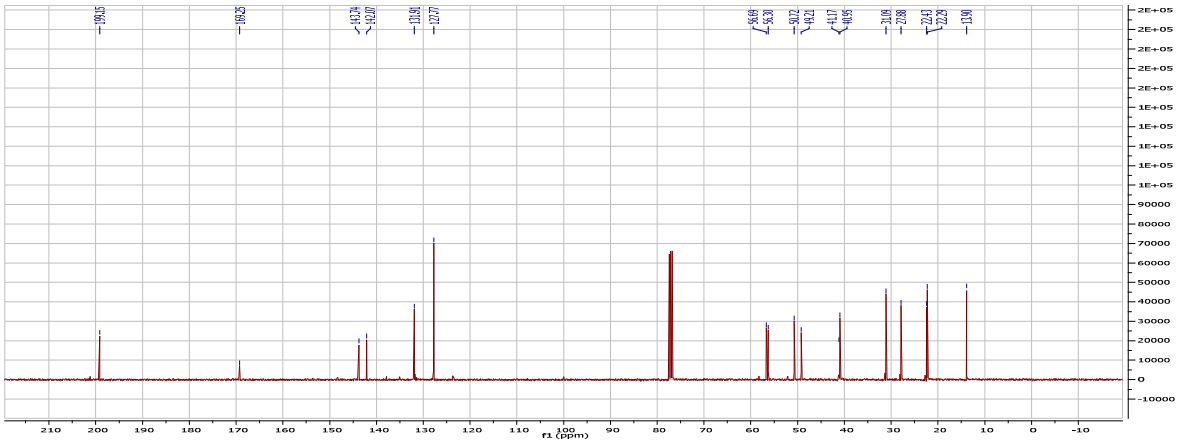

(1) ELSD Signal
597.025
Range: 597.007
(2)
96%
0.68
38094
(9)
4%
1.26
1412
LSU
500.000
250.000
0.000
0.5
1.0
1.5
2.0
Time

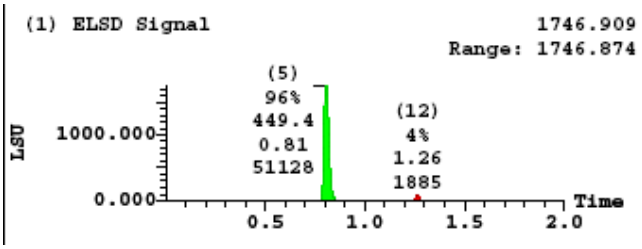

Peak ID Compound Time Mass Found
3 Found 0.75 436.40
3:(Time: 0.75)
1:MS ES+
1.2e+008
438.0
100
%
0
500.0
1000.0
m/z



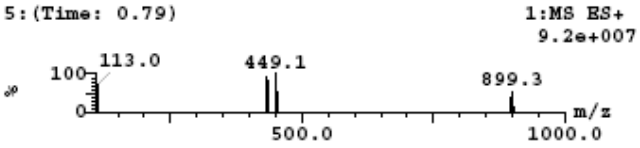
17{*3,4,4*}

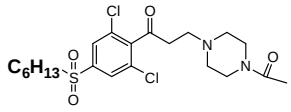




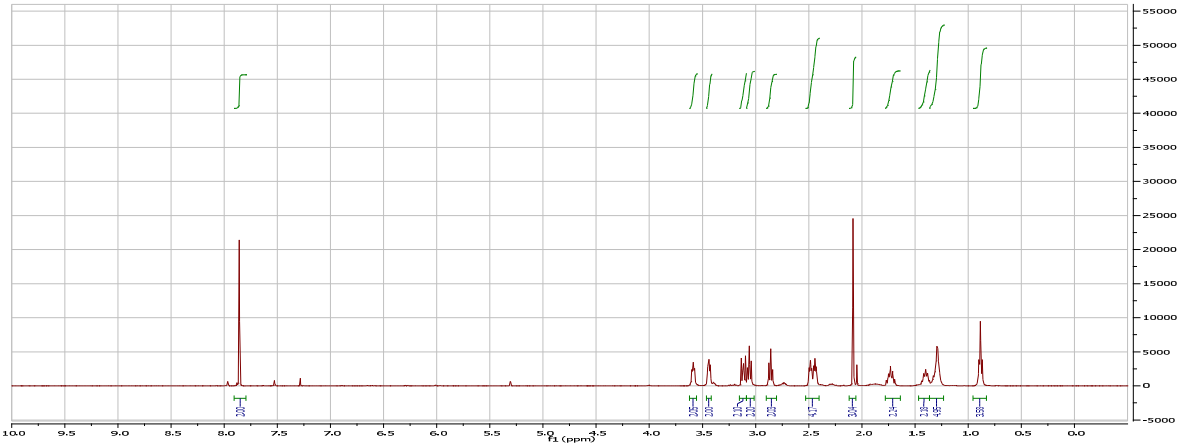


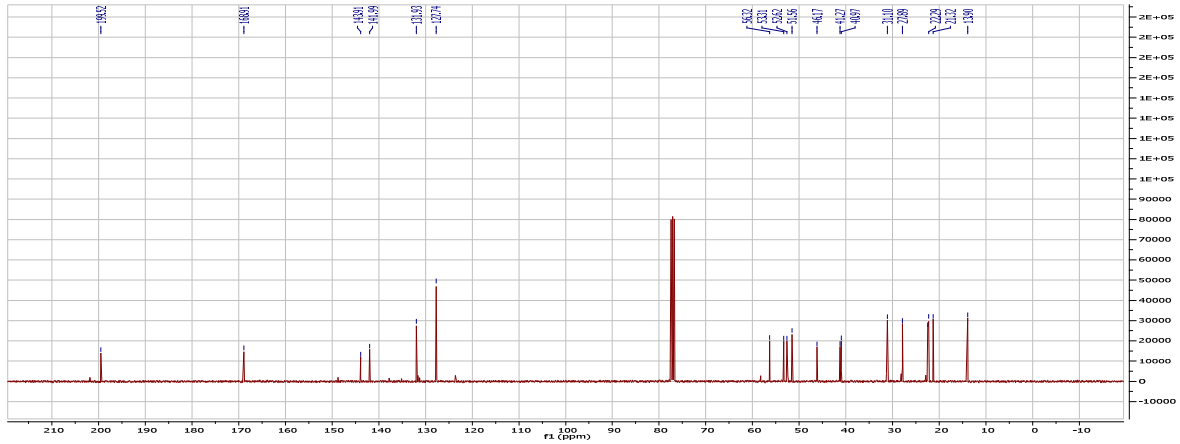
Peak ID	Compound	Time	Mass Found
5	Found	0.79	449.40

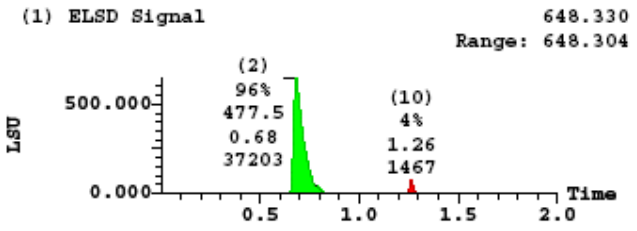




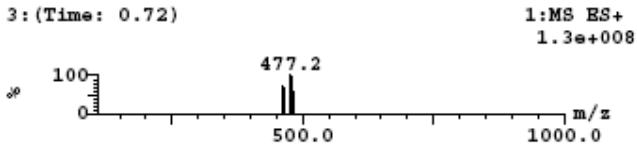
17{*3,4,5*}

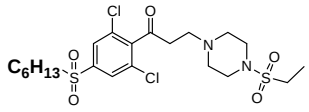




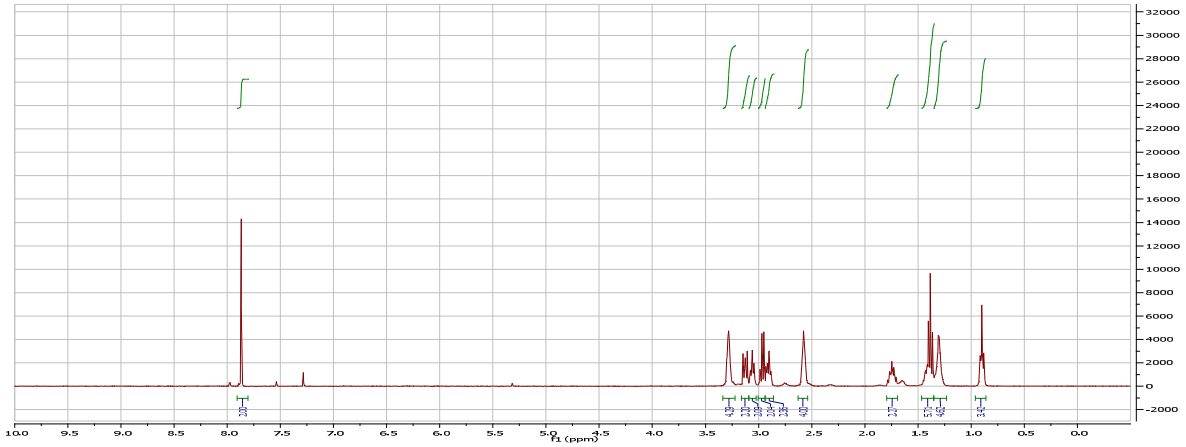


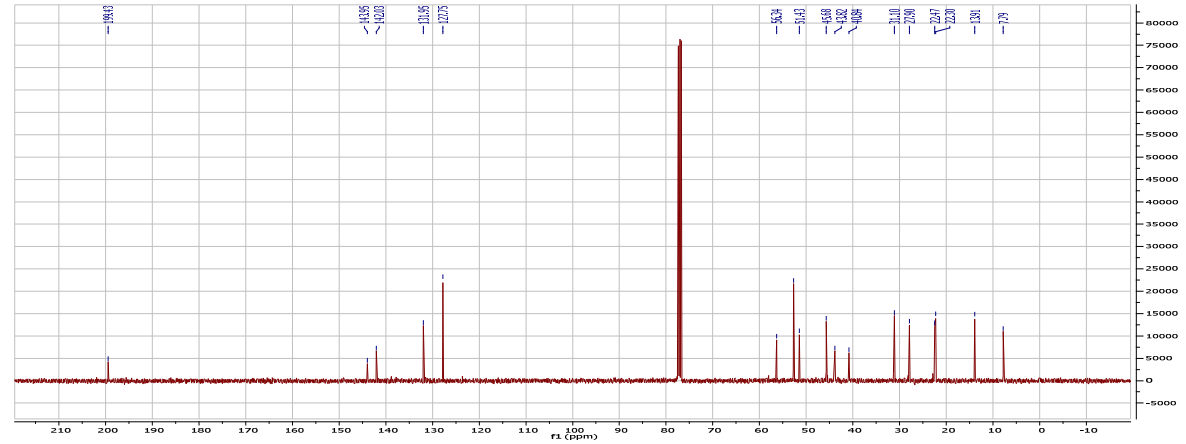
Peak ID	Compound	Time	Mass Found
3	Found	0.72	477.45

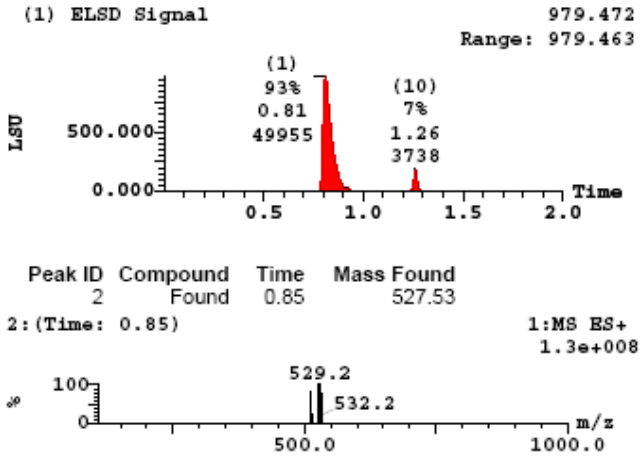




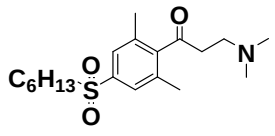
17{*3,4,6*}



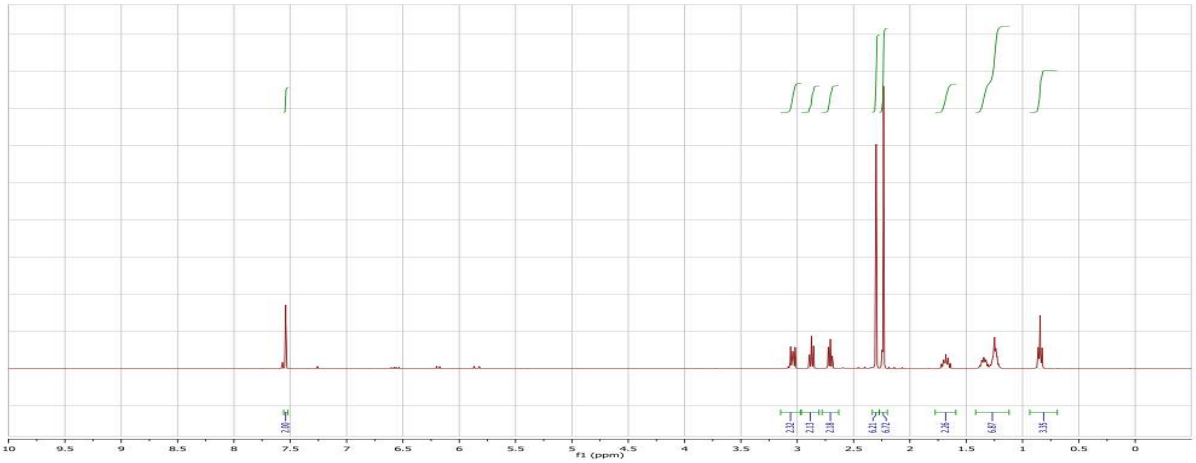


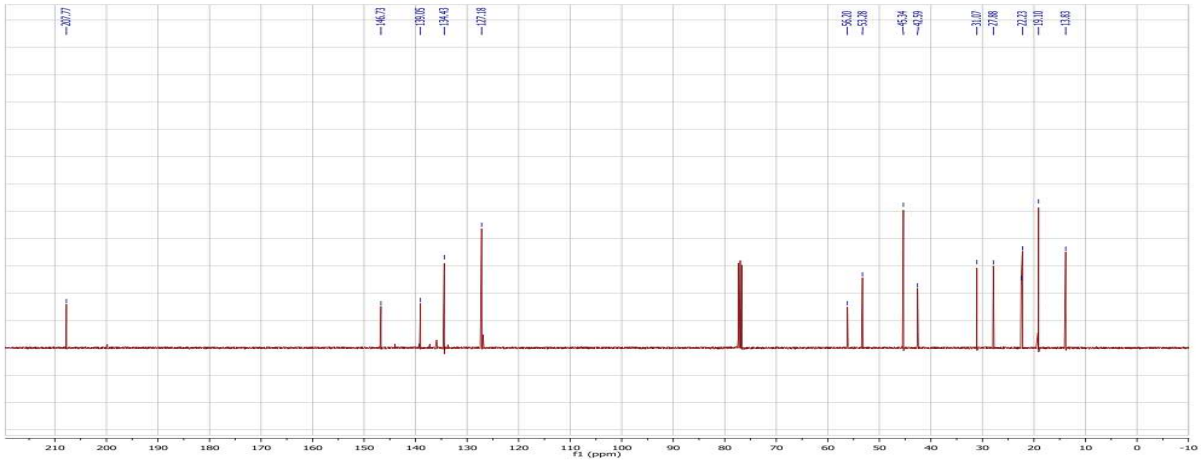


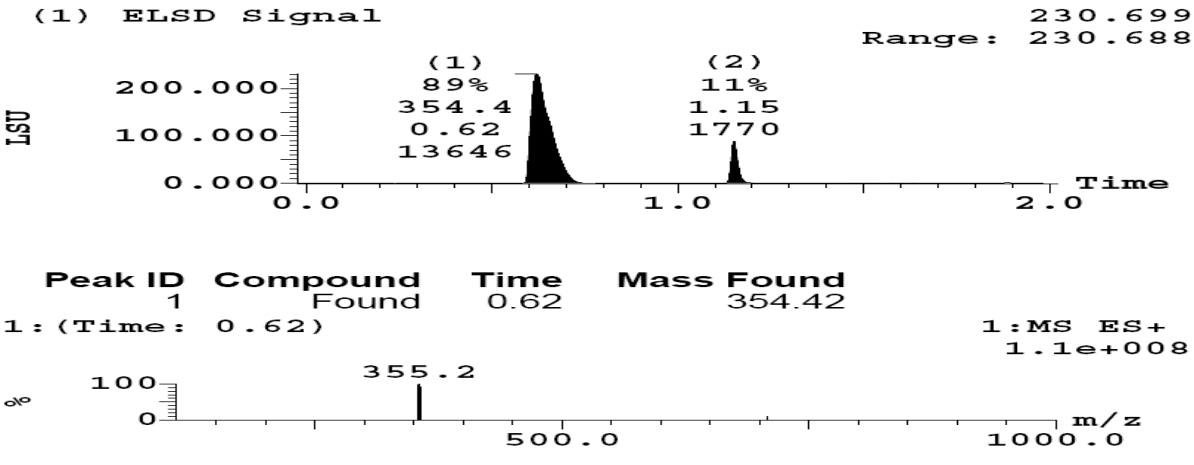
Peak ID	Compound	Time	Mass Found
2	Found	0.85	527.53



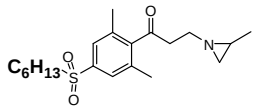
17{*3,5,1*}



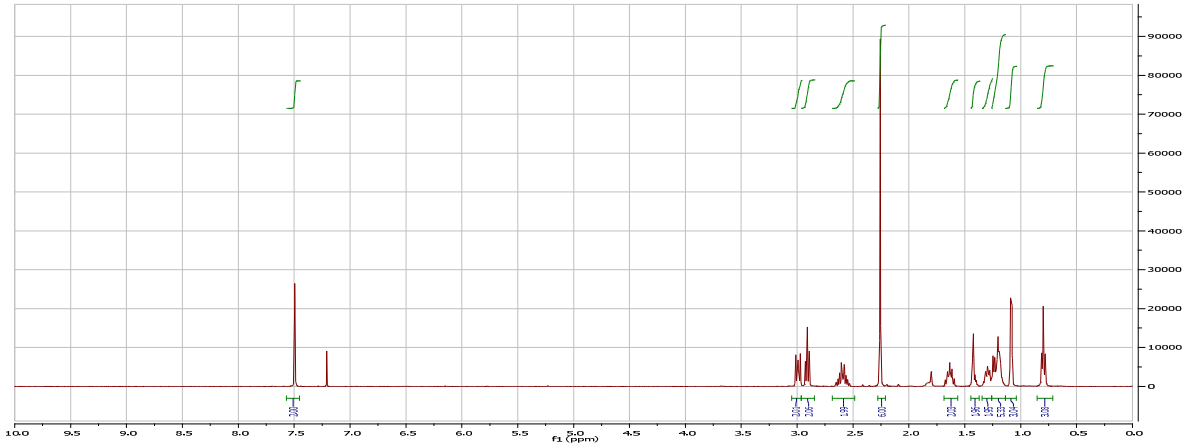


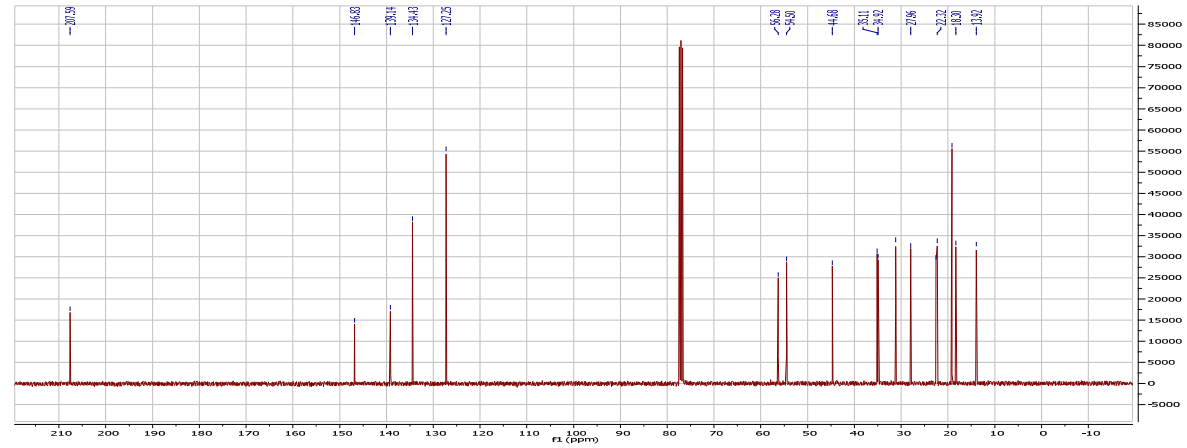


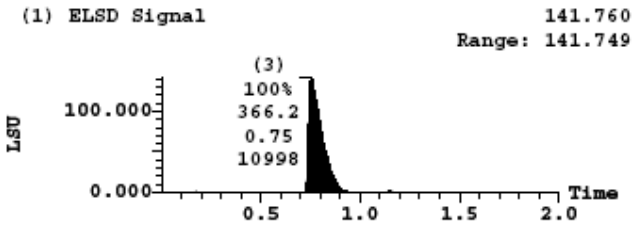
Peak ID	Compound	Time	Mass Found
1	Found	0.62	354.42



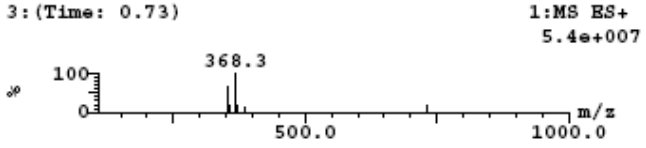
17{*3,5,2*}

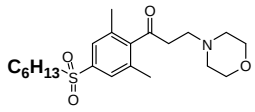




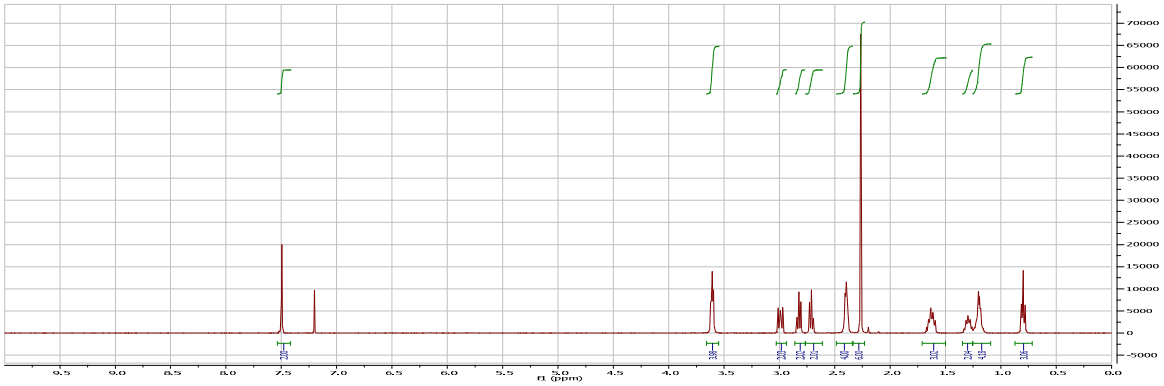


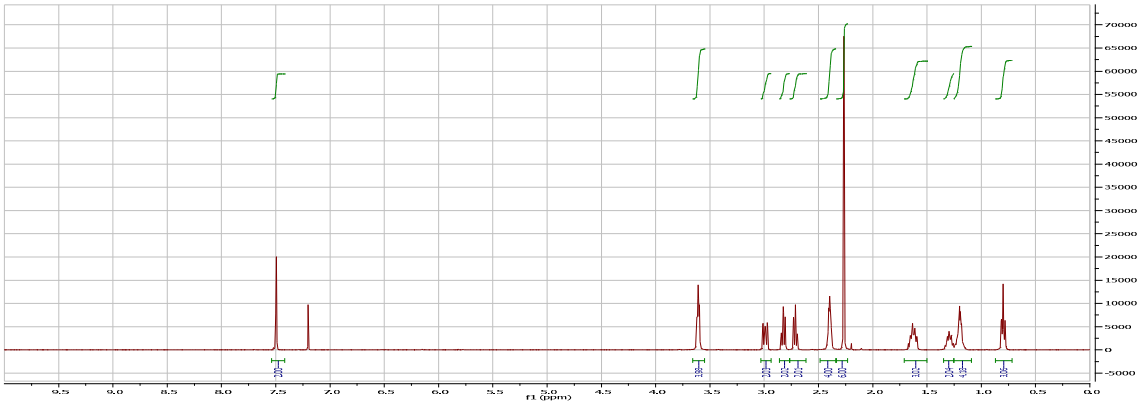
Peak ID	Compound	Time	Mass Found
3	Found	0.73	366.20

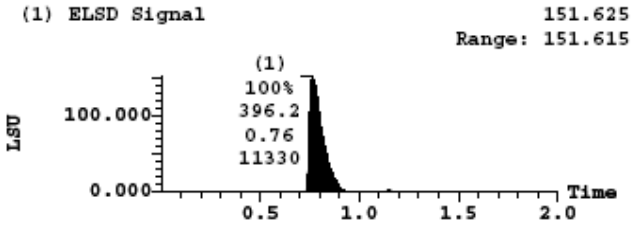




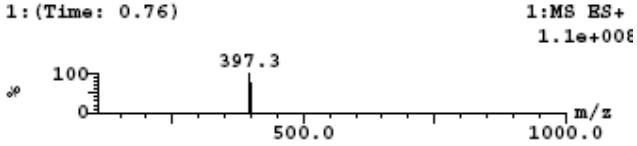
17{*3,5,3*}

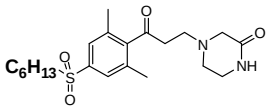




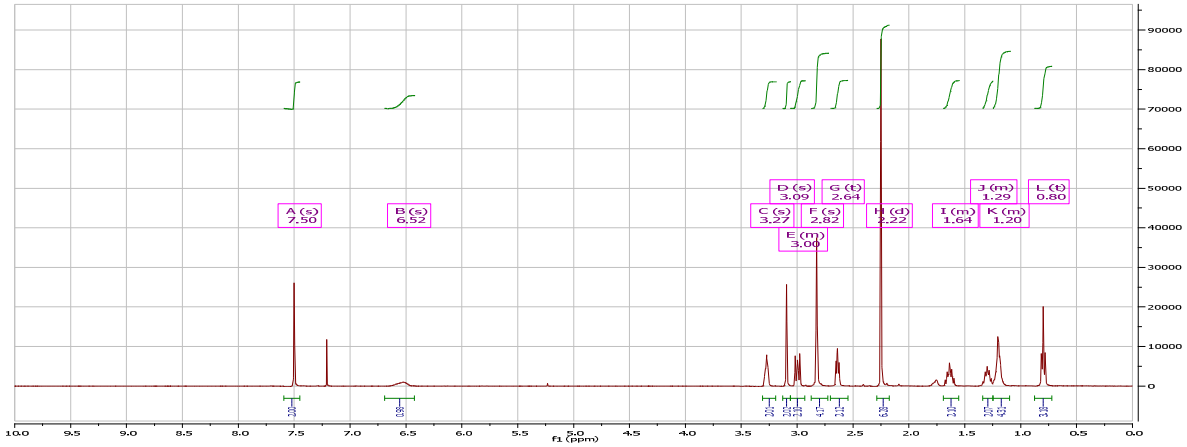


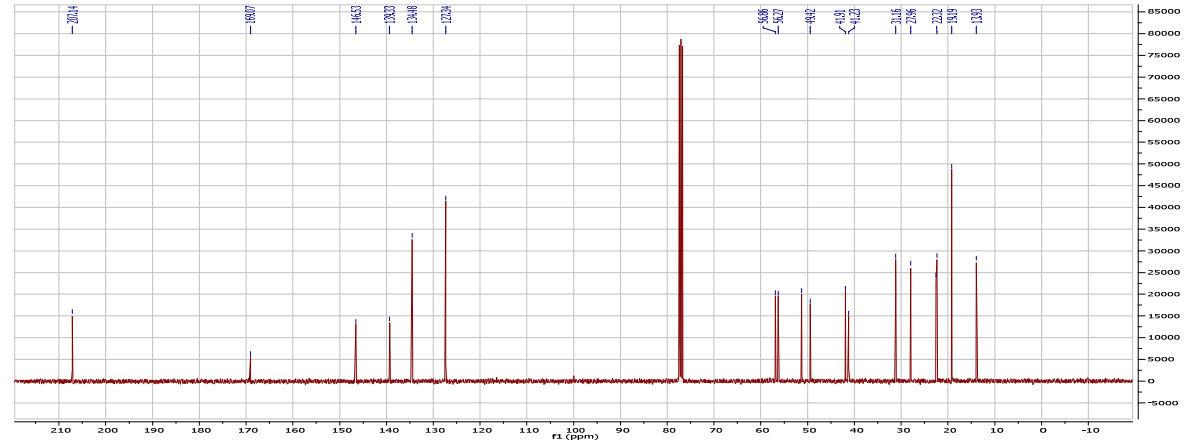
Peak ID	Compound	Time	Mass Found
1	Found	0.76	396.21

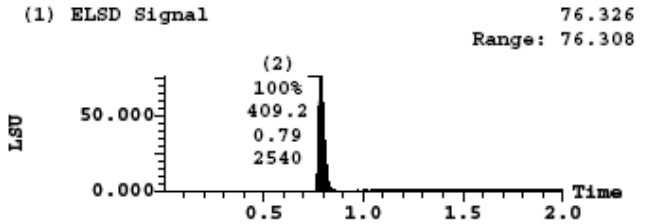




17{*3,5,4*}



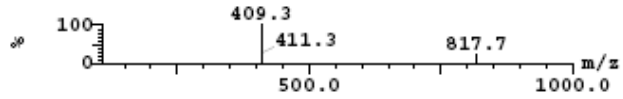


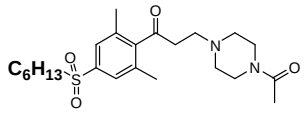


Peak ID	Compound	Time	Mass Found
2	Found	0.77	409.21

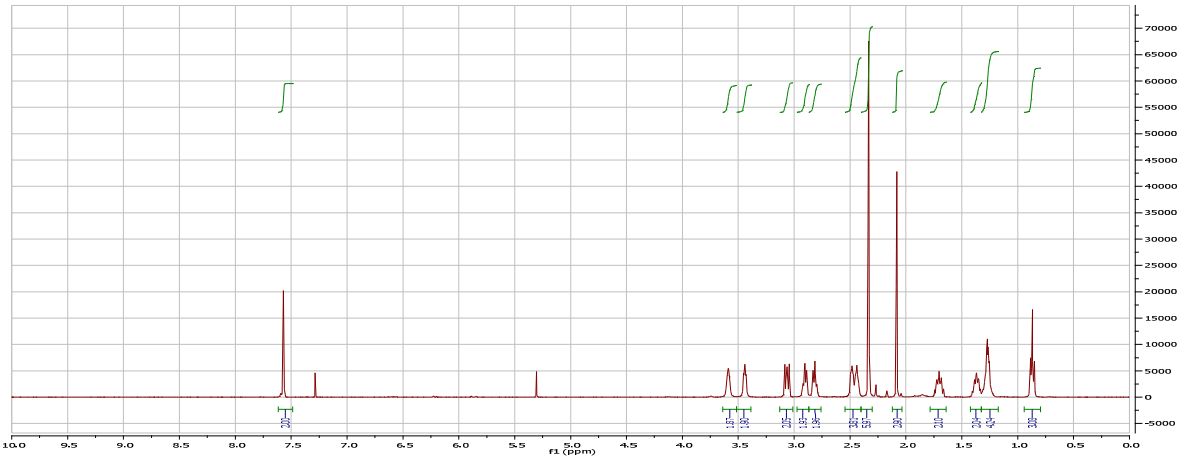
2:(Time: 0.77)

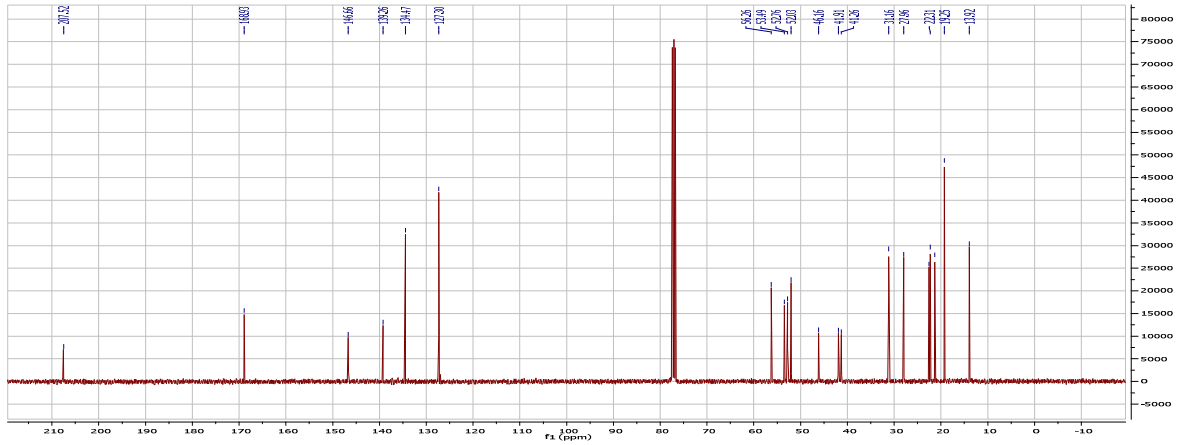
1:MS ES+
1.0e+008

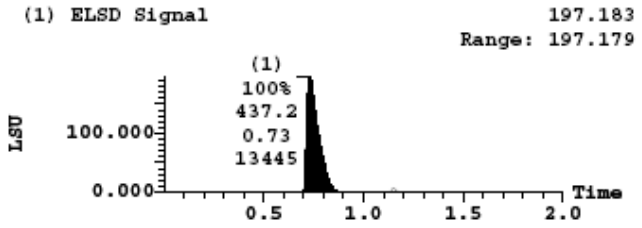


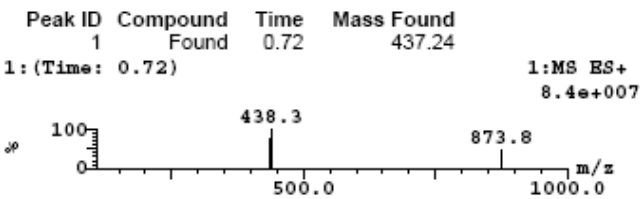


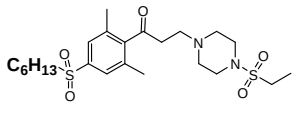
17{*3,5,5*}



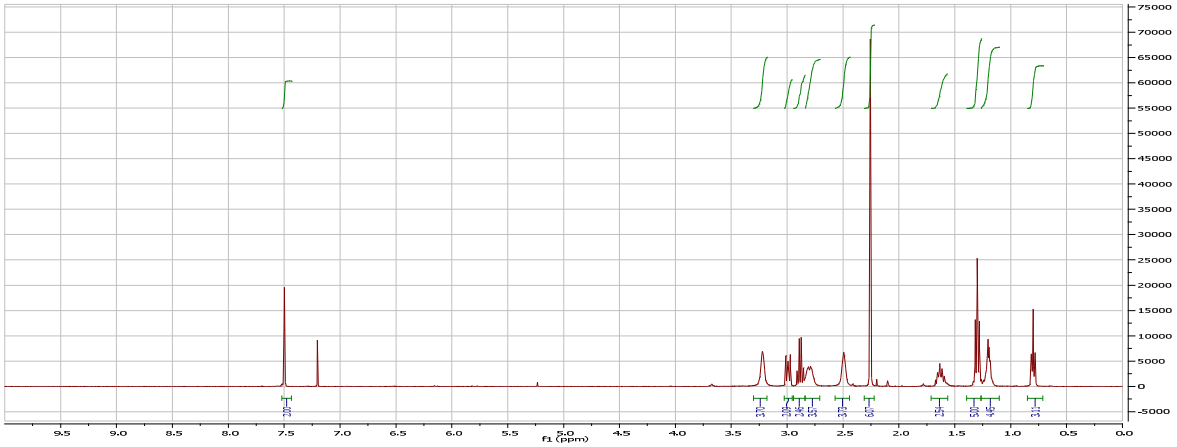


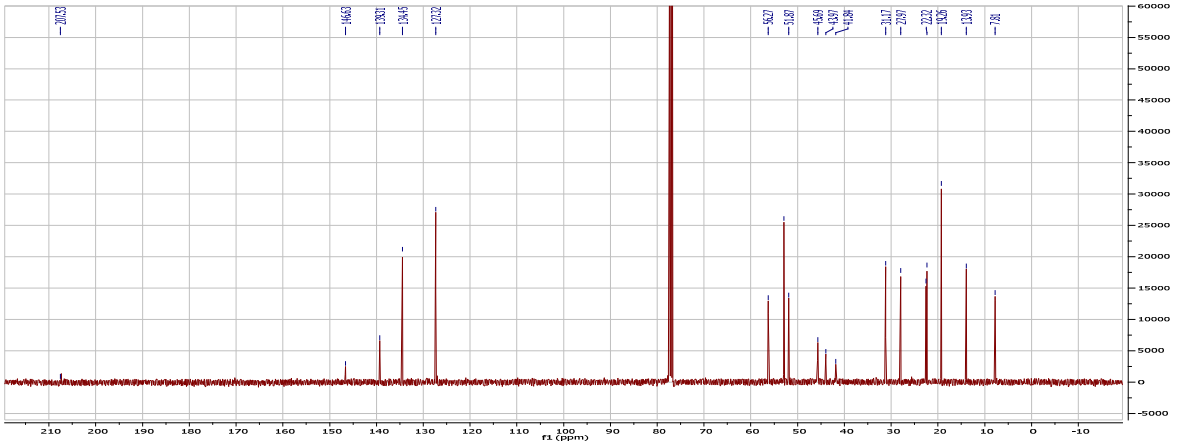

(1) ELSD Signal
197.183
Range: 197.179
(1)
100%
437.2
0.73
13445
LSU
100.000
0.000
Time
0.5
1.0
1.5
2.0

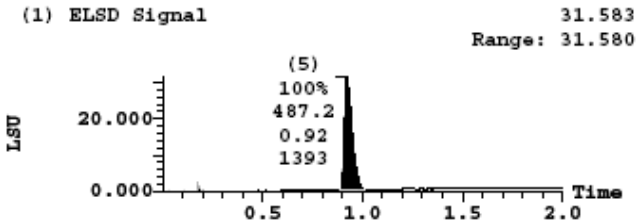

Peak ID Compound Time Mass Found
1 Found 0.72 437.24
1:(Time: 0.72)
1:MS ES+
8.4e+007
438.3
873.8
%
100
0
m/z
500.0
1000.0



17{*3,5,6*}







Peak ID	Compound	Time	Mass Found
5	Found	0.91	487.22