

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100923\
 Data File : BF135652.D
 Acq On : 09 Oct 2023 15:03
 Operator : CG\JU
 Sample : 04656-02
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-105I

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135652.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.775	283	287	296	rVB	27599	42355	1.01%	0.170%
2	5.375	555	559	569	rBV	1440270	1627426	38.90%	6.541%
3	6.387	728	731	751	rBV	886920	999447	23.89%	4.017%
4	6.740	787	791	800	rBV	1006880	906984	21.68%	3.645%
5	7.310	883	888	891	rBV	2542743	2624583	62.73%	10.549%
6	8.016	1004	1008	1020	rBV	1334821	1185273	28.33%	4.764%
7	9.098	1187	1192	1195	rBV	4174656	4085004	97.63%	16.418%
8	9.216	1207	1212	1223	rVB	1191896	1250720	29.89%	5.027%
9	9.775	1303	1307	1311	rBV	1531862	1275647	30.49%	5.127%
10	10.575	1439	1443	1446	rBV	2569696	2467996	58.99%	9.919%
11	11.269	1558	1561	1565	rBV	1523000	1395087	33.34%	5.607%
12	11.804	1649	1652	1664	rBV2	204656	277752	6.64%	1.116%
13	12.357	1742	1746	1747	rBV2	58473	59449	1.42%	0.239%
14	12.375	1747	1749	1757	rVB	270689	238409	5.70%	0.958%
15	12.598	1784	1787	1795	rBV2	63901	93751	2.24%	0.377%
16	12.875	1829	1834	1837	rBV	3888388	4184024	100.00%	16.816%
17	13.933	2010	2014	2025	rVB	1228059	1090340	26.06%	4.382%
18	14.510	2110	2112	2118	rVB2	55659	58077	1.39%	0.233%
19	14.774	2153	2157	2161	rBV	122136	116776	2.79%	0.469%
20	15.039	2198	2202	2206	rVB2	35578	46398	1.11%	0.186%
21	15.404	2259	2264	2274	rBV	636862	855465	20.45%	3.438%

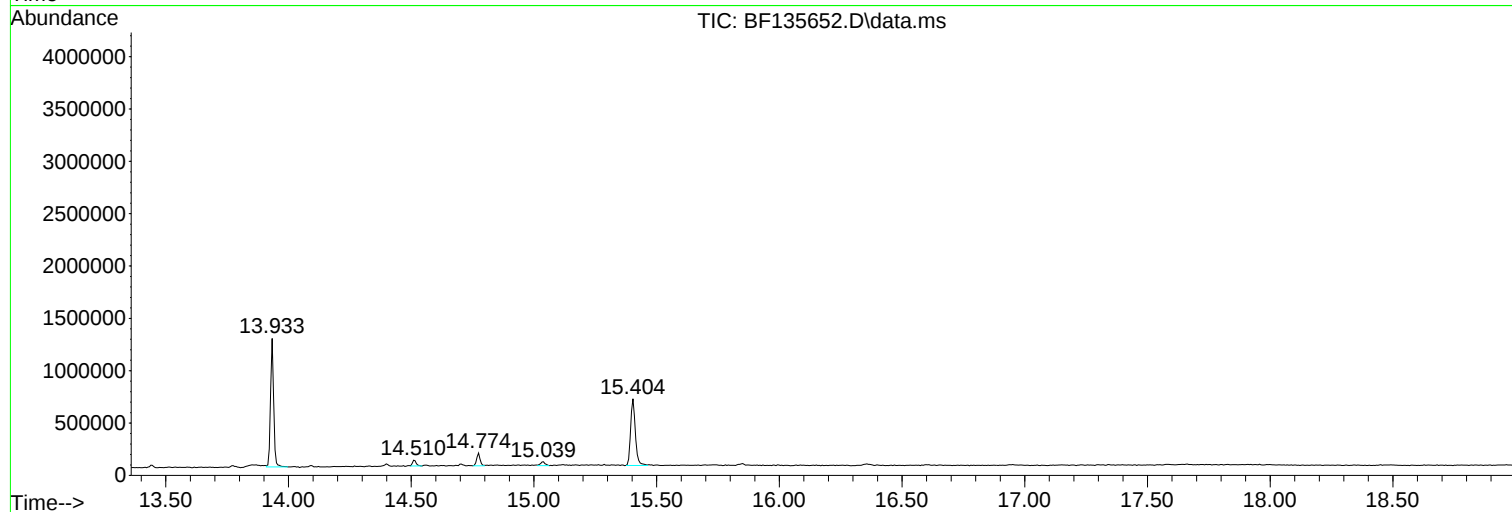
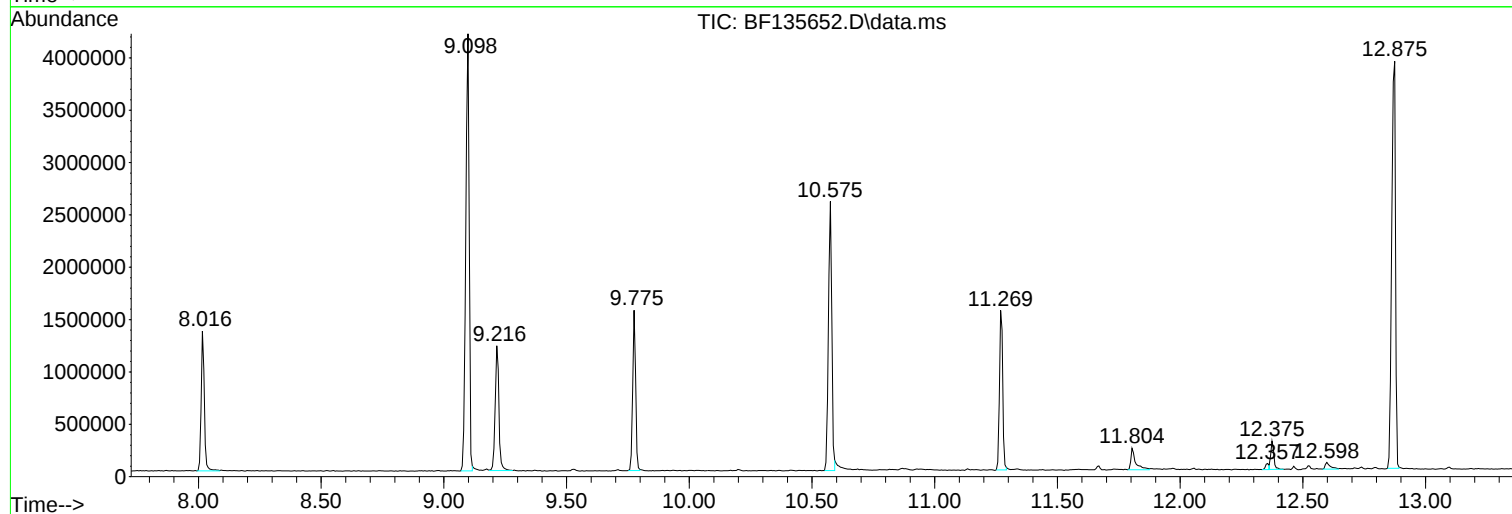
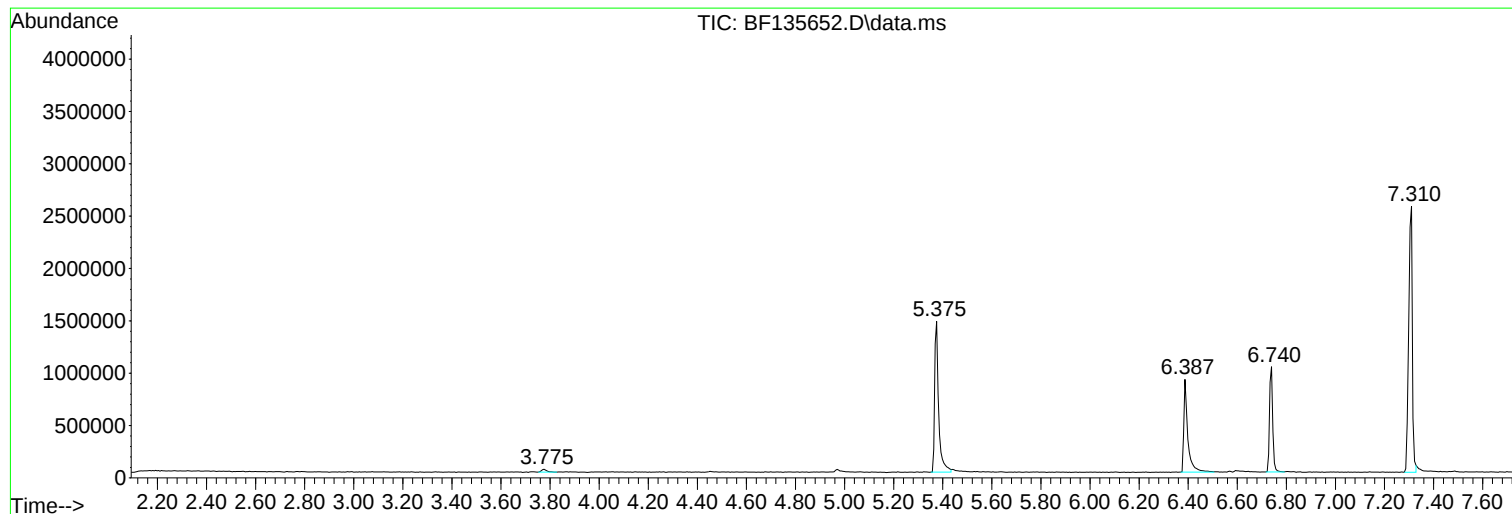
Sum of corrected areas: 24880963

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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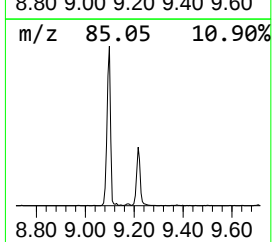
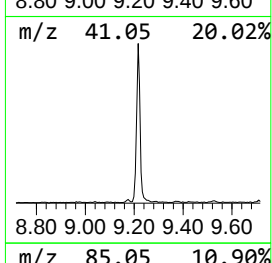
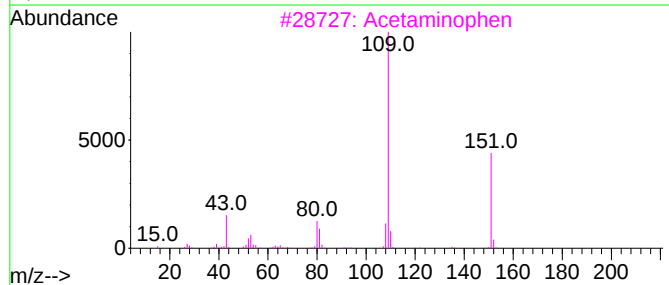
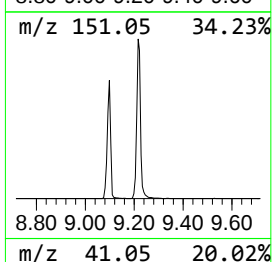
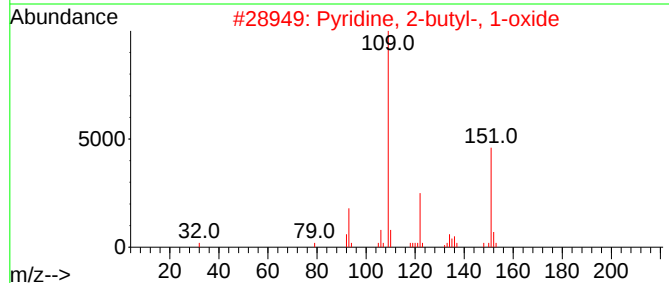
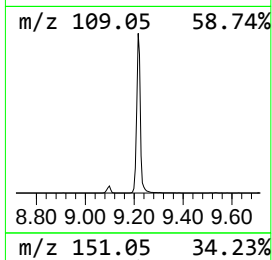
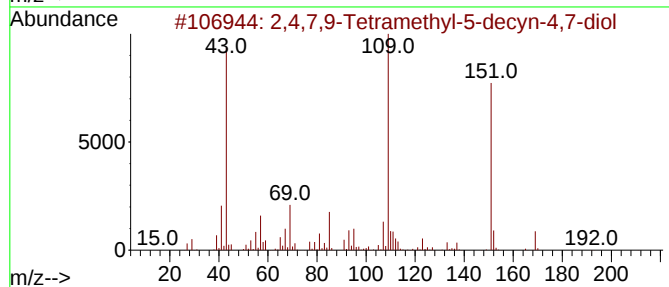
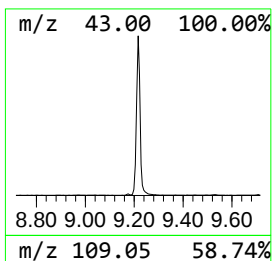
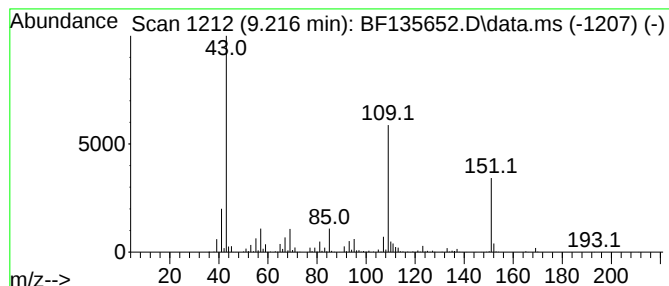
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.216	19.61 ng	1250720	Acenaphthene-d10	9.775

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	87	
2	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	53	
3	Acetaminophen	151	C8H9NO2	000103-90-2	49	
4	Metacetamol	151	C8H9NO2	000621-42-1	47	
5	Butanamide, N-acetyl-N-(4-hydrox...	221	C12H15NO3	1000107-08-7	47	



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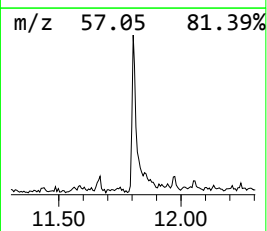
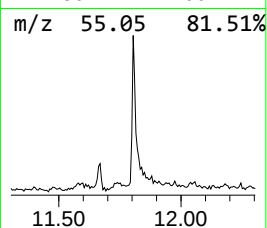
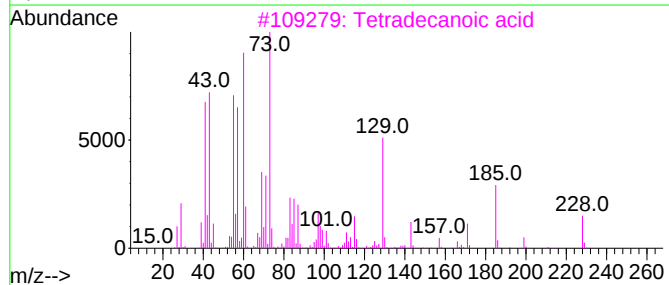
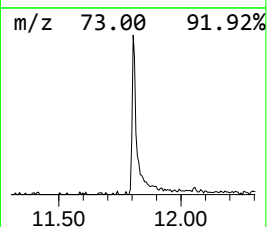
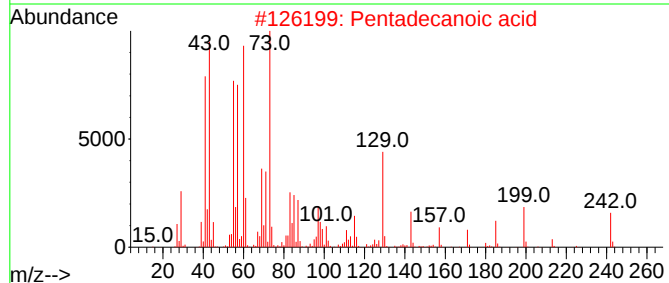
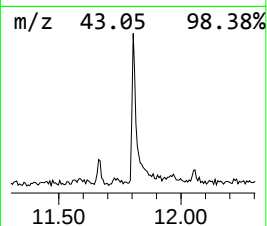
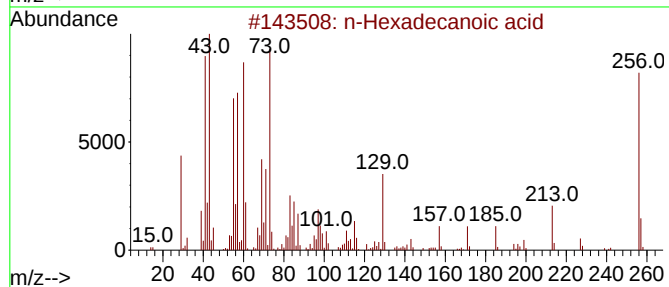
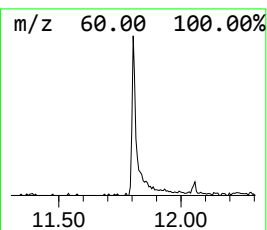
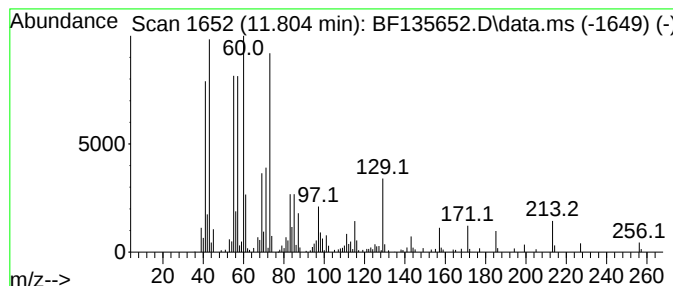
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.804	3.98 ng	277752	Phenanthrene-d10	11.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	86
4			Tridecanoic acid	214	C13H26O2	000638-53-9	70
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	60



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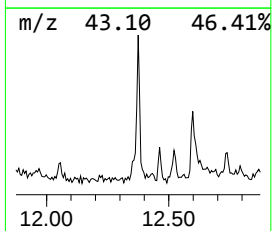
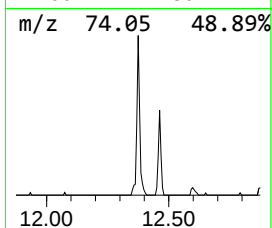
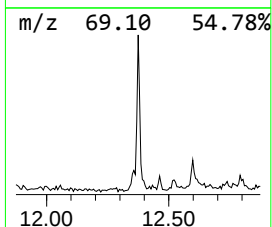
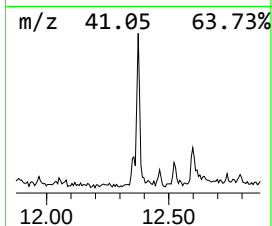
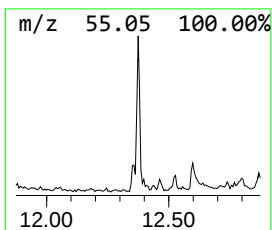
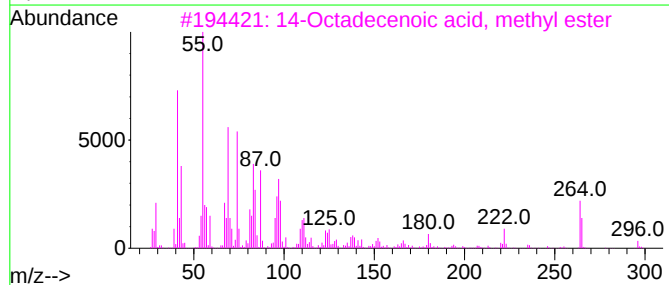
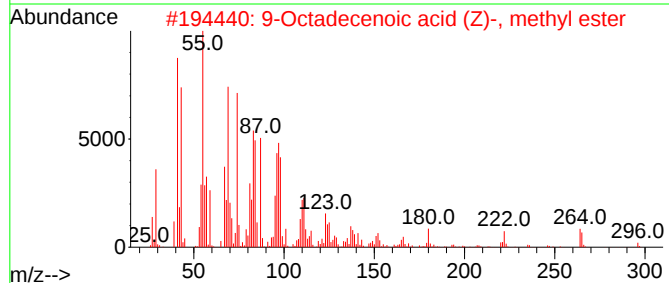
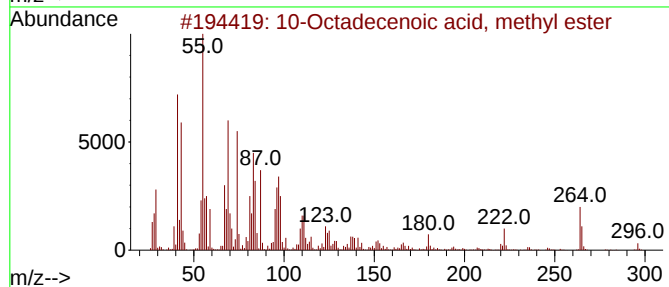
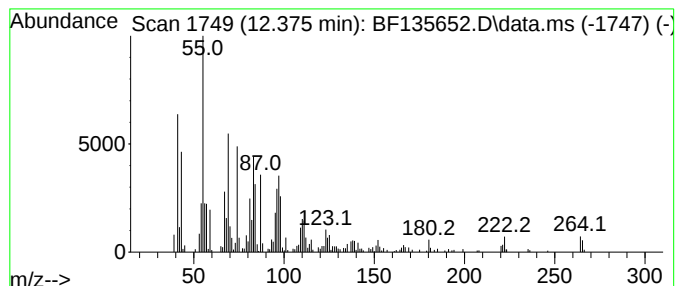
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Peak Number 3 10-Octadecenoic acid, methyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.375	3.42 ng	238409	Phenanthrene-d10	11.269	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	94
2	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	93
3	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	91
4	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	91
5	Cyclopropaneoctanoic acid, 2-hex...	282	C18H34O2	010152-61-1	87



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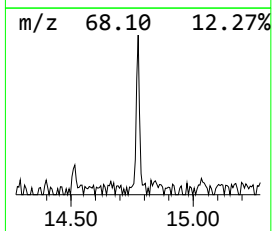
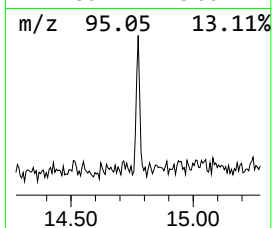
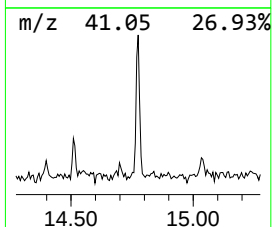
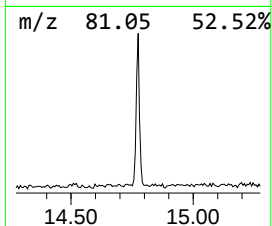
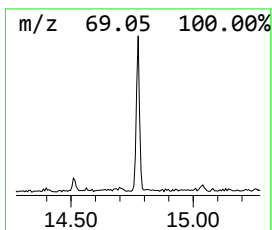
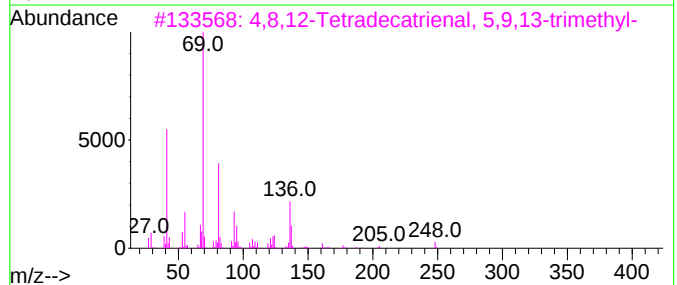
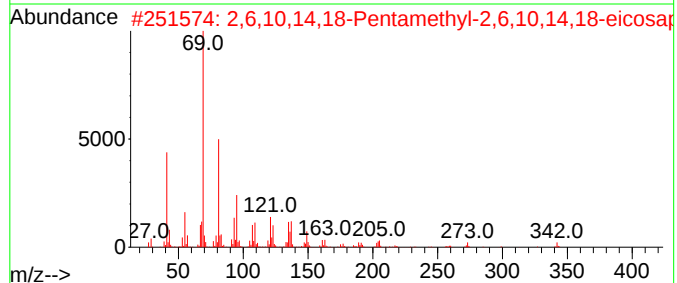
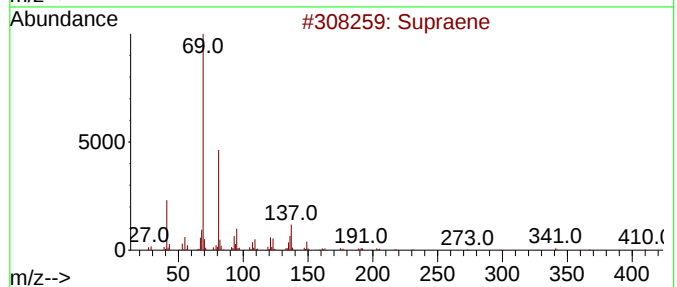
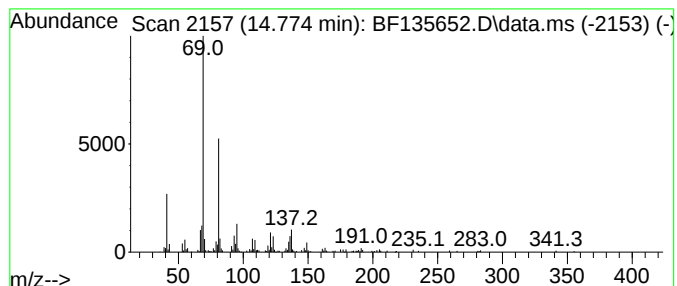
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Peak Number 4 Supraene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.774	2.73 ng	116776	Perylene-d12	15.404

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	87
2			2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	78
3			4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72
4			Umbelliprenin	366	C24H30O3	023838-17-7	72
5			4,8,12-Tetradecatrienenitrile, 5...	245	C17H27N	005981-31-7	59



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2,4,7,9-Tetrame...	9.216	19.6	ng	1250720	3	9.775	1275650	20.0
n-Hexadecanoic ...	11.804	4.0	ng	277752	4	11.269	1395090	20.0
10-Octadecenoic...	12.375	3.4	ng	238409	4	11.269	1395090	20.0
Supraene	14.774	2.7	ng	116776	6	15.404	855465	20.0