

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101723\
 Data File : BF135819.D
 Acq On : 17 Oct 2023 18:57
 Operator : CG\JU
 Sample : 04895-02
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 A-2

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-BF101323.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135819.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.957	484	488	503	rBV	405014	547215	27.56%	3.708%
2	5.375	556	559	586	rBV	1506928	1764302	88.85%	11.954%
3	6.392	728	732	759	rBV	1513346	1734548	87.36%	11.752%
4	6.733	787	790	804	rVB	519932	500304	25.20%	3.390%
5	7.304	884	887	908	rBV	1172592	1079267	54.35%	7.312%
6	8.016	1005	1008	1026	rBV	753337	653883	32.93%	4.430%
7	9.092	1188	1191	1202	rBV	2268278	1874293	94.39%	12.699%
8	9.210	1208	1211	1221	rVB	53485	58650	2.95%	0.397%
9	9.774	1303	1307	1322	rVB	855133	735460	37.04%	4.983%
10	10.569	1439	1442	1459	rBV	1258267	1247060	62.81%	8.449%
11	11.268	1558	1561	1571	rBV	942599	821379	41.37%	5.565%
12	11.804	1648	1652	1664	rBV2	244042	291904	14.70%	1.978%
13	12.598	1783	1787	1795	rBV2	32342	55533	2.80%	0.376%
14	12.863	1828	1832	1836	rBV	2074138	1985602	100.00%	13.453%
15	13.827	1988	1996	1998	rBV4	49936	110178	5.55%	0.746%
16	13.939	2011	2015	2027	rVB	558669	609438	30.69%	4.129%
17	14.398	2087	2093	2097	rBV	19578	25966	1.31%	0.176%
18	14.768	2152	2156	2161	rBV	105782	106437	5.36%	0.721%
19	15.409	2261	2265	2278	rBV	353021	533047	26.85%	3.612%
20	15.845	2334	2339	2345	rVB3	14260	24858	1.25%	0.168%

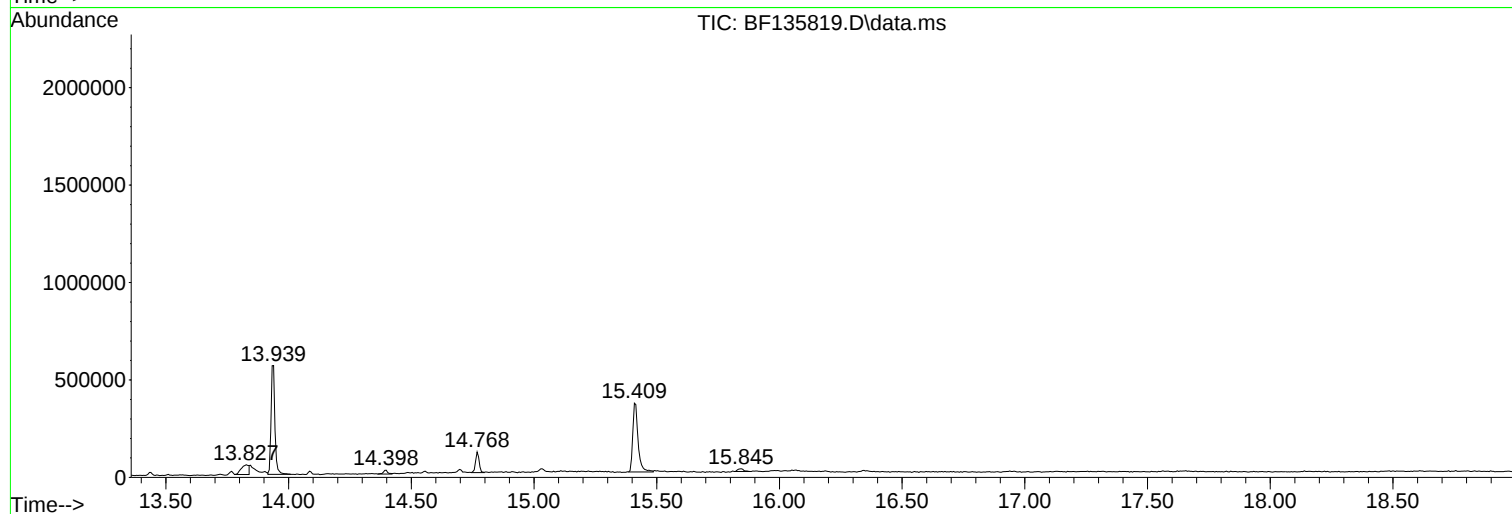
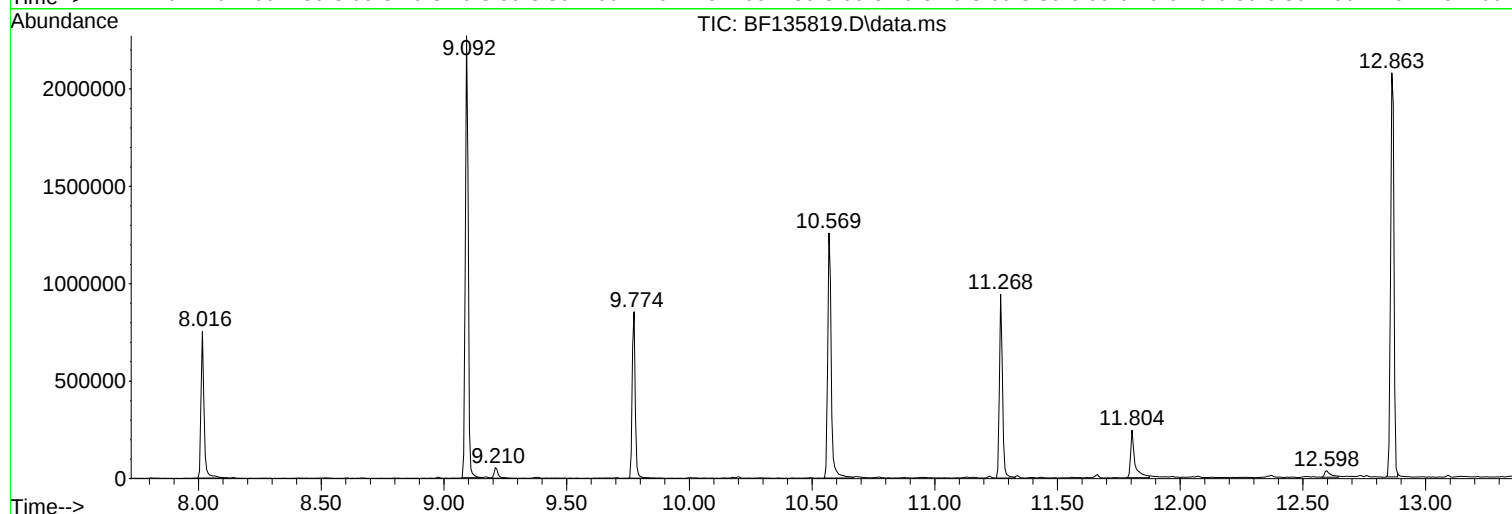
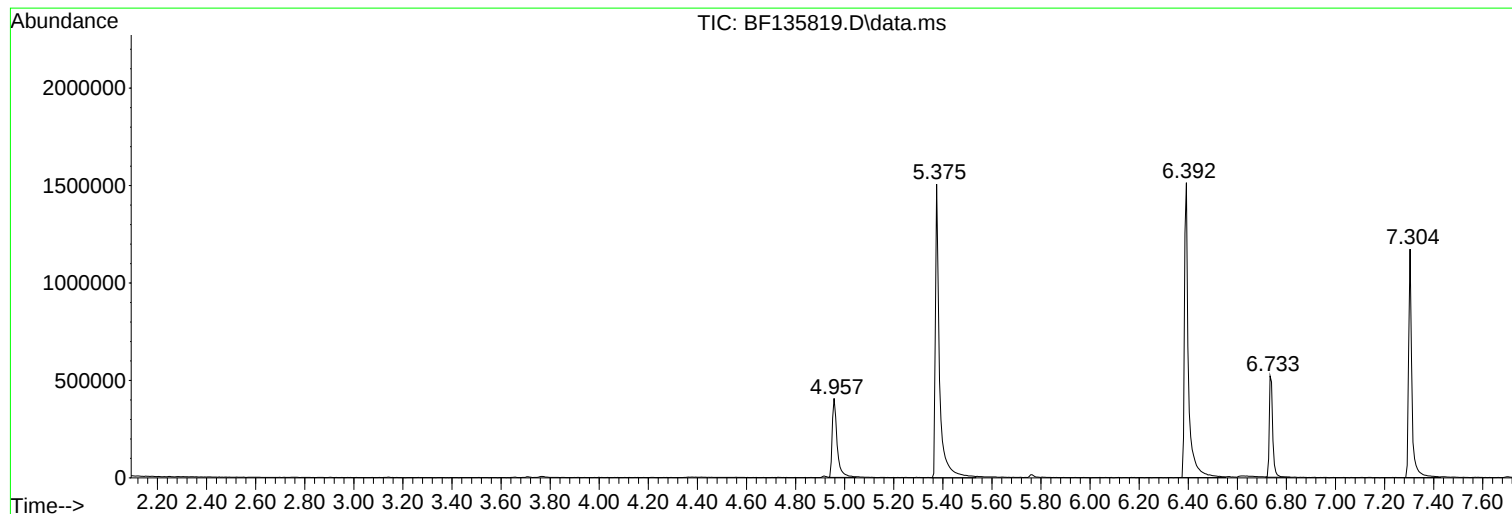
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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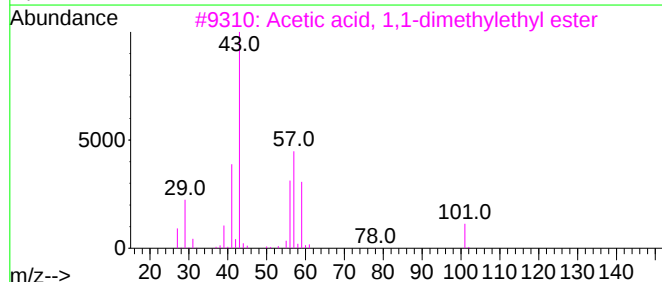
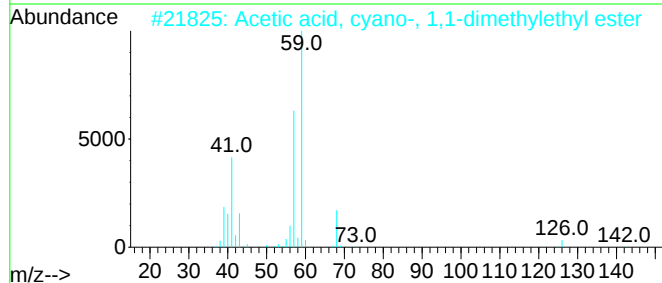
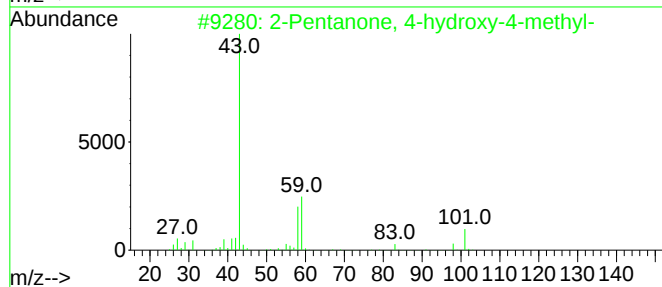
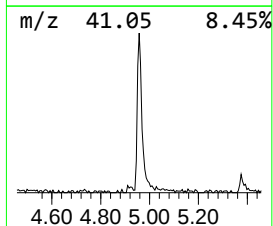
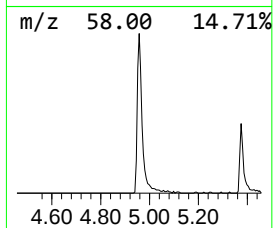
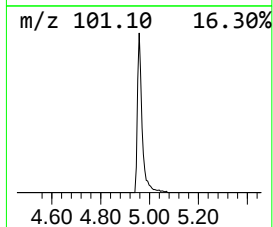
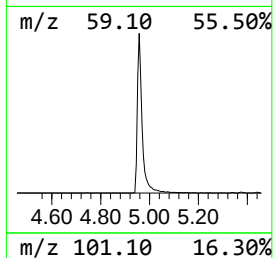
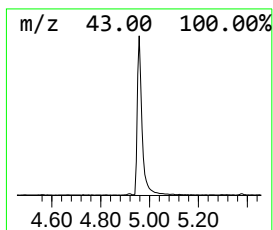
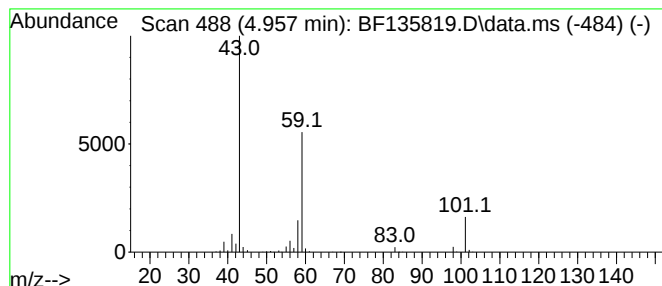
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.957	21.88 ng	547215	1,4-Dichlorobenzene-d4	6.739

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	23		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		
5	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9		



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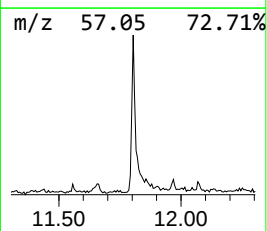
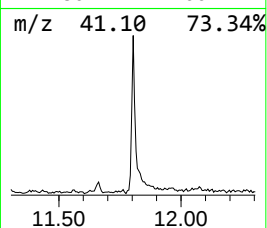
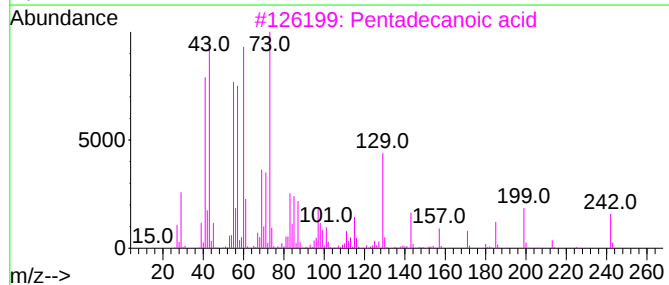
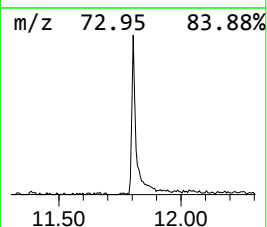
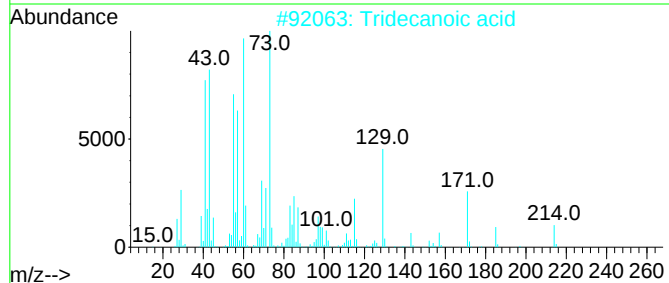
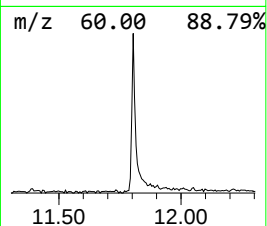
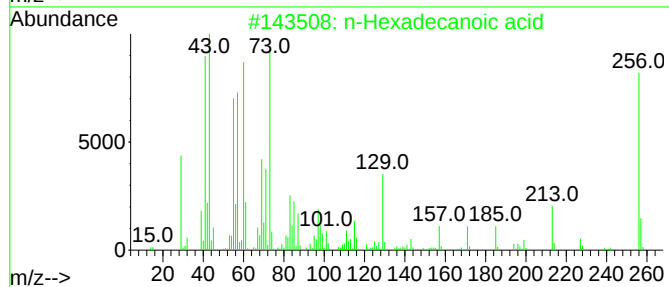
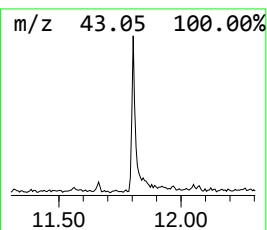
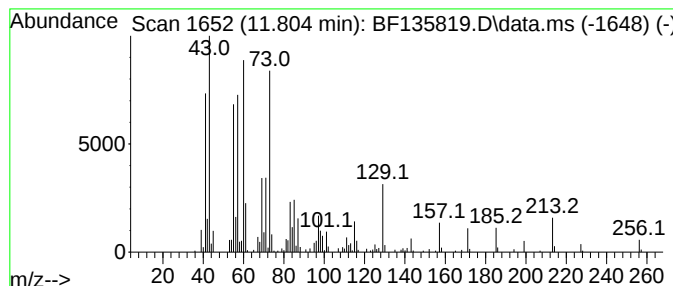
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.804	7.11 ng	291904	Phenanthrene-d10	11.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			n-Decanoic acid	172	C10H20O2	000334-48-5	64



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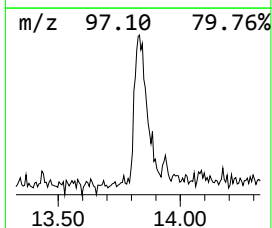
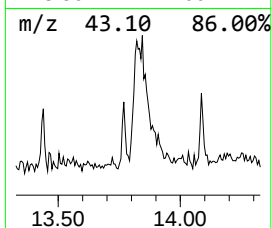
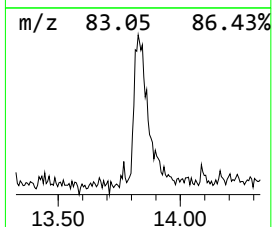
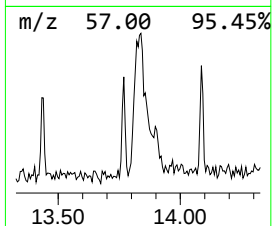
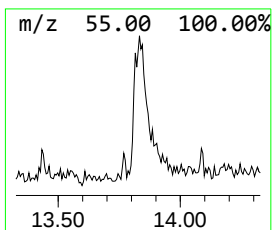
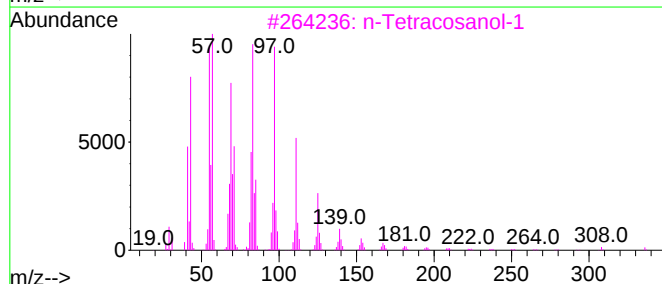
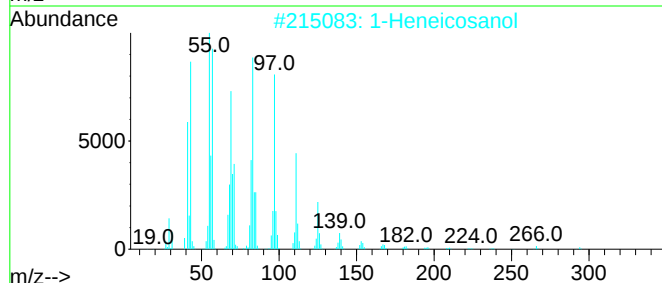
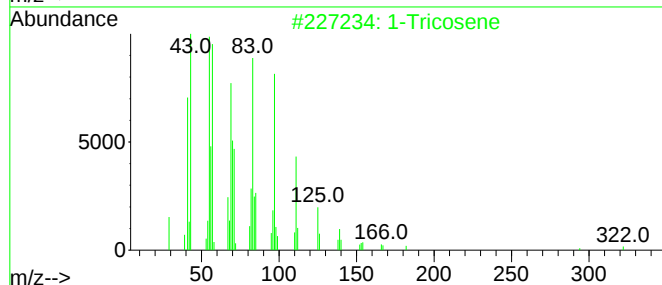
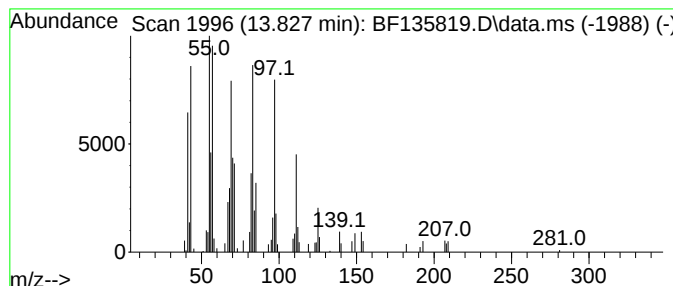
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Peak Number 3 1-Tricosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.827	3.62 ng	110178	Chrysene-d12	13.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tricosene			322	C23H46	018835-32-0	95
2	1-Heneicosanol			312	C21H44O	015594-90-8	94
3	n-Tetracosanol-1			354	C24H50O	000506-51-4	93
4	1-Hexacosene			364	C26H52	018835-33-1	91
5	n-Nonadecanol-1			284	C19H40O	001454-84-8	91



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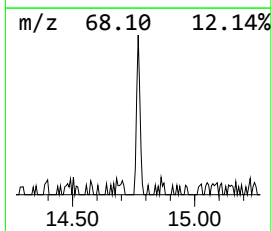
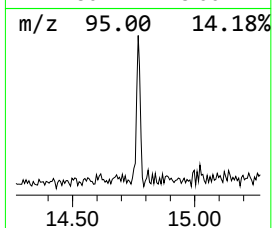
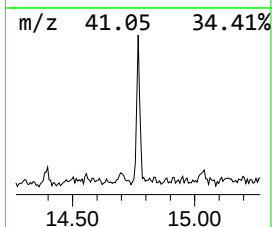
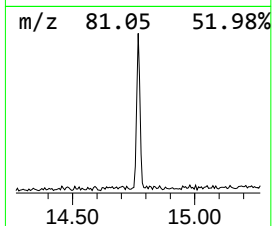
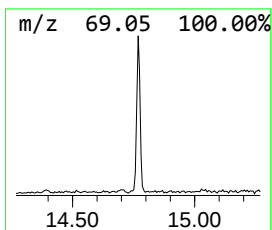
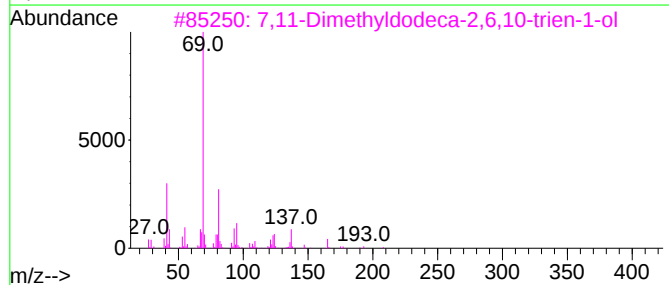
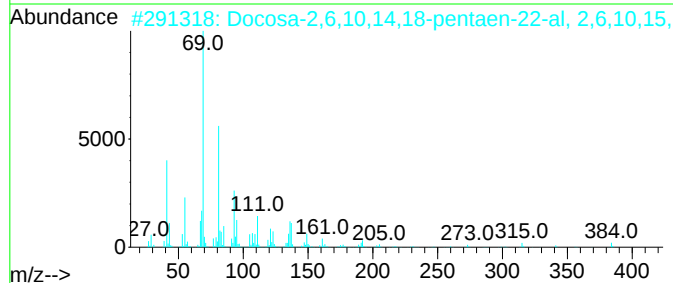
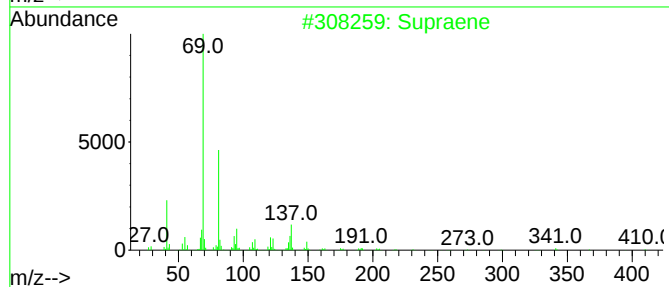
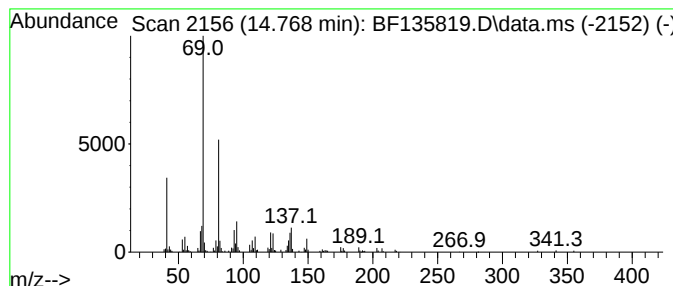
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Peak Number 4 Supraene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.768	3.99 ng	106437	Perylene-d12	15.415

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	90
3			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
4			(.+/-)-Lavandulol, pentafluorop...	300	C13H17F5O2	1000352-63-1	72
5			3,7,11-Trimethyl-2,6,10-dodecatr...	217	C15H23N	029789-67-1	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.957	21.9	ng	547215	1	6.739	500304	20.0
n-Hexadecanoic ...	11.804	7.1	ng	291904	4	11.269	821379	20.0
1-Tricosene	13.827	3.6	ng	110178	5	13.939	609438	20.0
Supraene	14.768	4.0	ng	106437	6	15.415	533047	20.0