

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042221\
 Data File : BP005376.D
 Acq On : 22 Apr 2021 15:25
 Operator : CG/JU
 Sample : M2112-02
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 M-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_P\Methods\8270E-BP042121.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP005376.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.246	361	367	377	rBV	724015	1030248	43.42%	9.059%
2	6.834	629	637	649	rBV	697702	1096271	46.21%	9.639%
3	7.640	768	774	784	rBV	164626	257848	10.87%	2.267%
4	8.805	965	972	989	rBV	419735	695947	29.33%	6.119%
5	10.428	1239	1248	1256	rBV	184453	320818	13.52%	2.821%
6	12.916	1664	1671	1683	rBV	947563	1363524	57.47%	11.989%
7	13.775	1811	1817	1825	rBV2	18551	32198	1.36%	0.283%
8	14.304	1900	1907	1916	rBV	282278	408616	17.22%	3.593%
9	15.810	2155	2163	2177	rBV	858903	1239912	52.26%	10.902%
10	17.069	2369	2377	2391	rBV	359395	514832	21.70%	4.527%
11	17.969	2525	2530	2539	rBV	92862	136899	5.77%	1.204%
12	19.210	2737	2741	2750	rBV3	35163	55590	2.34%	0.489%
13	19.645	2810	2815	2824	rBV	2104593	2372571	100.00%	20.862%
14	20.886	3021	3026	3036	rBV2	159455	252126	10.63%	2.217%
15	21.169	3070	3074	3083	rBV	511736	632978	26.68%	5.566%
16	22.010	3213	3217	3223	rBV	121934	153458	6.47%	1.349%
17	22.339	3270	3273	3282	rVB2	107288	180882	7.62%	1.590%
18	23.427	3452	3458	3467	rVB	332479	628185	26.48%	5.524%

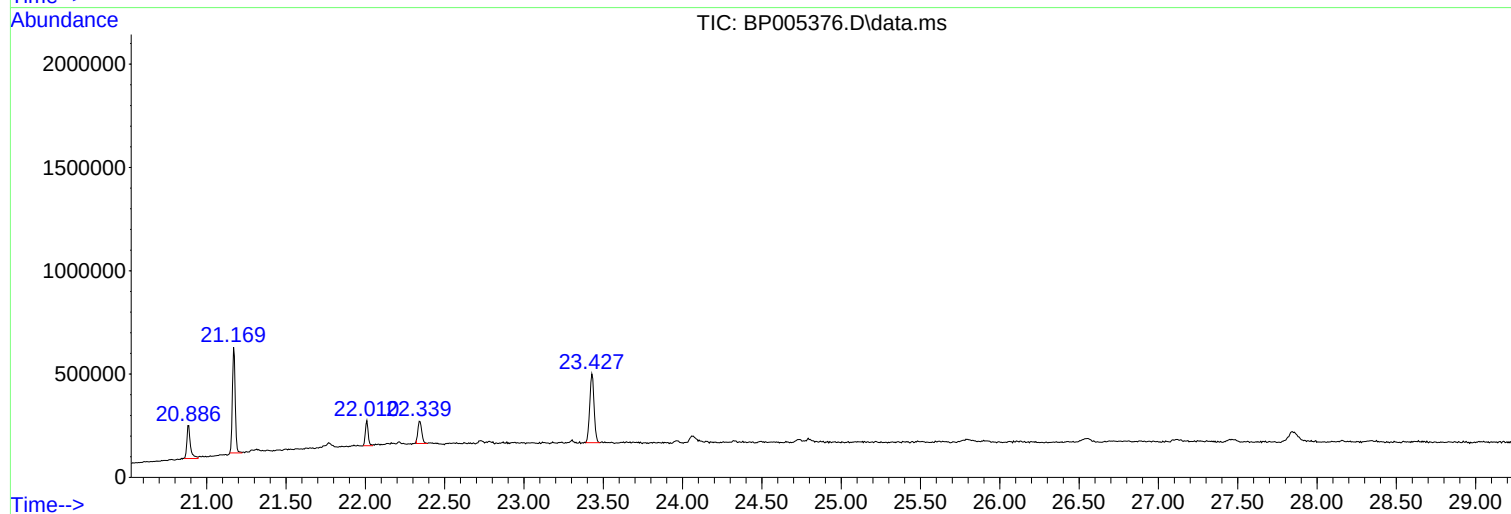
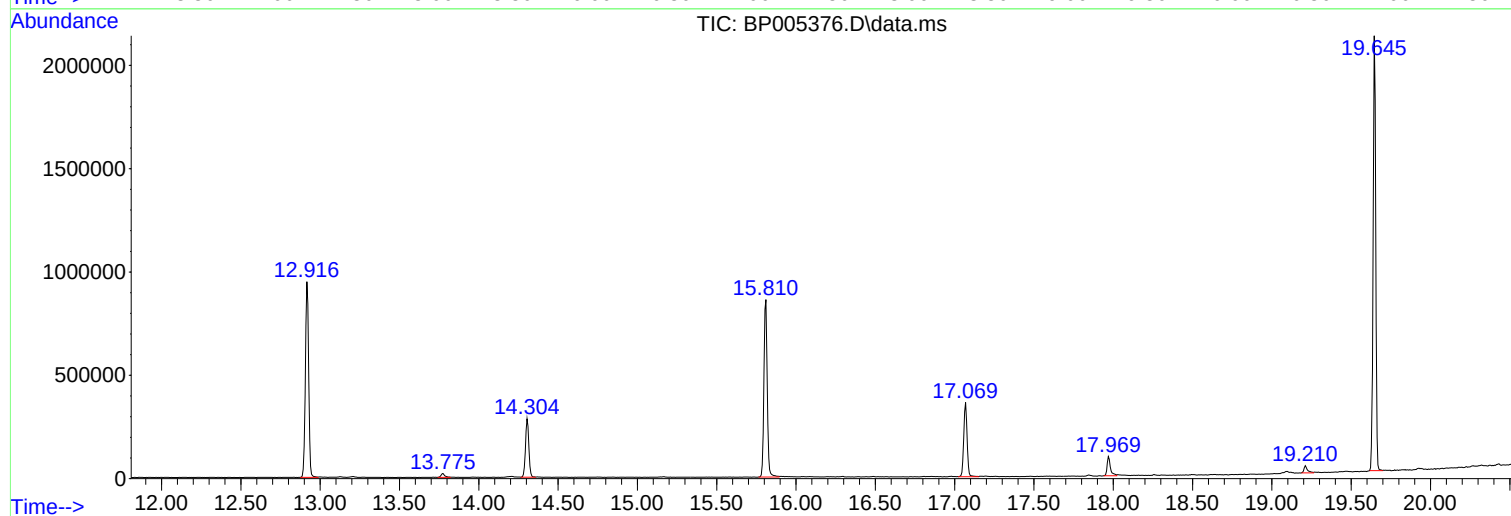
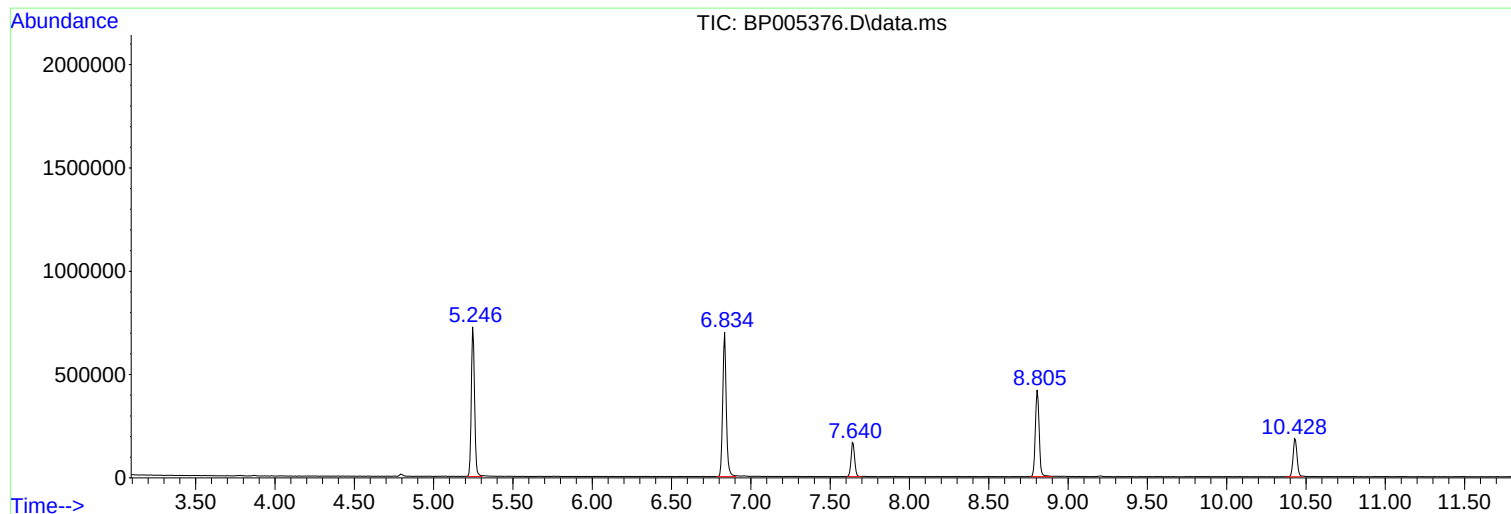
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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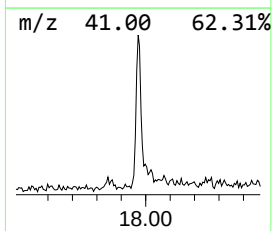
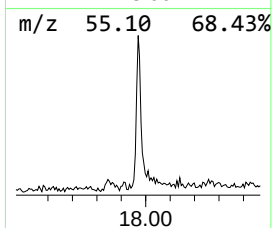
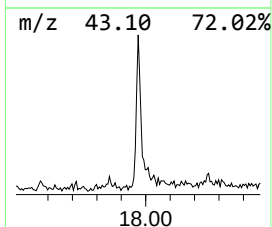
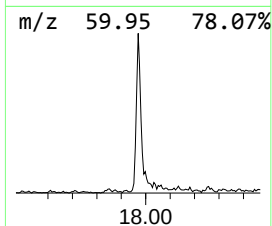
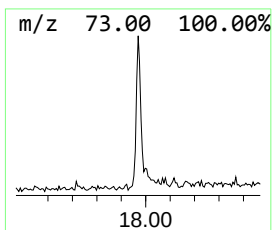
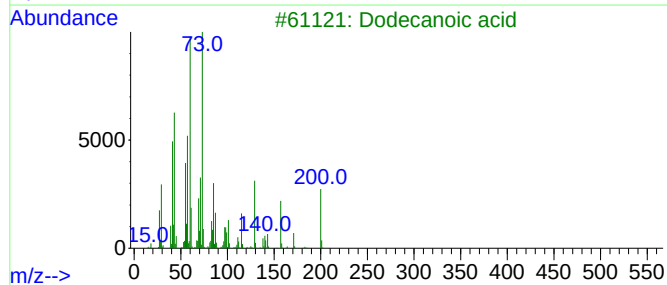
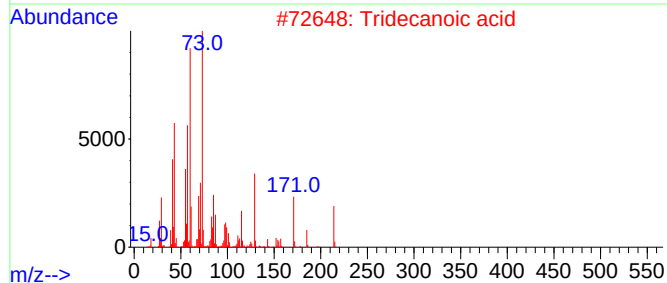
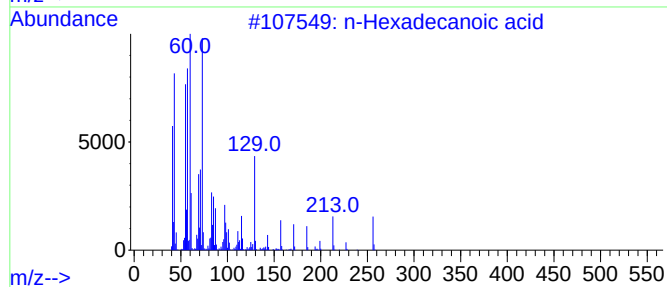
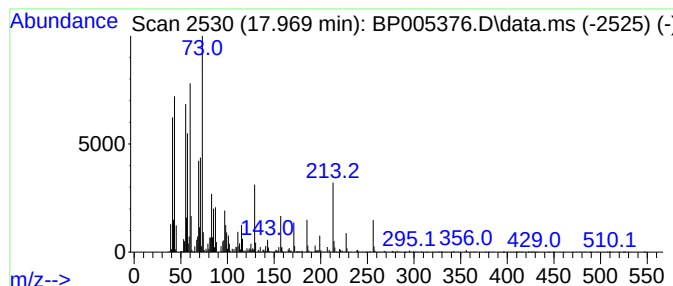
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.969	5.32 ng	136899	Phenanthrene-d10	17.069

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2			Tridecanoic acid	214	C13H26O2	000638-53-9	70
3			Dodecanoic acid	200	C12H24O2	000143-07-7	58
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	50



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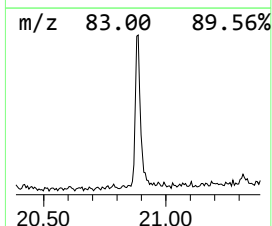
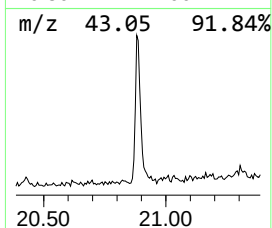
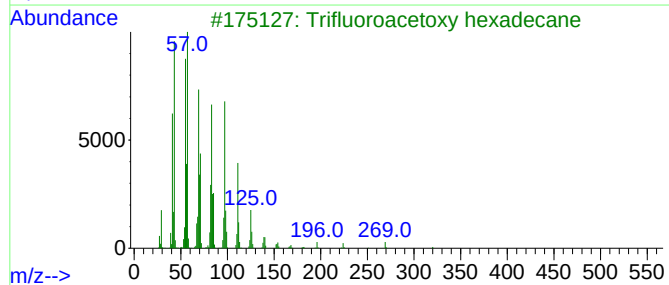
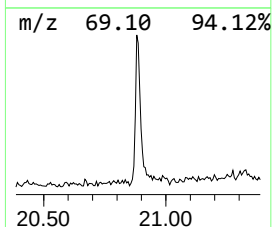
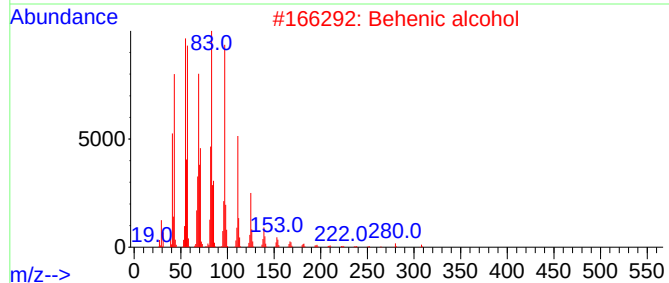
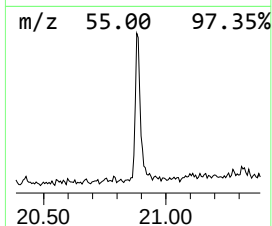
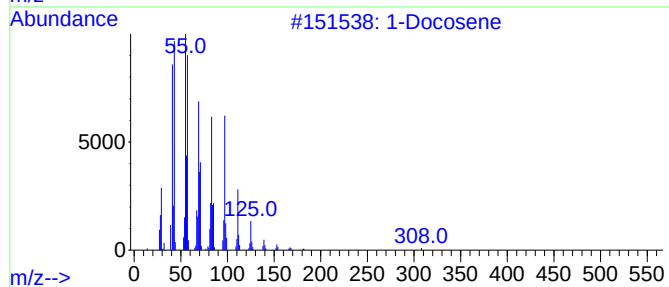
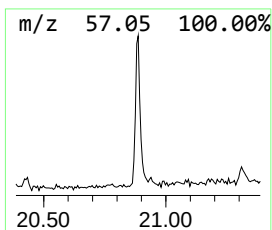
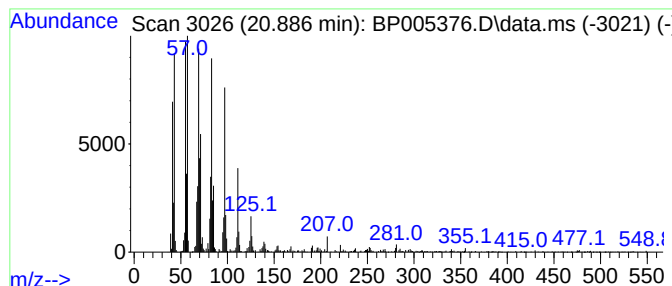
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 1-Docosene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.886	7.97 ng	252126	Chrysene-d12	21.169

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene			308	C22H44	001599-67-3	95
2	Behenic alcohol			326	C22H46O	000661-19-8	94
3	Trifluoroacetoxy hexadecane			338	C18H33F3O2	006222-03-3	94
4	1-Heneicosanol			312	C21H44O	015594-90-8	93
5	n-Tetracosanol-1			354	C24H50O	000506-51-4	93



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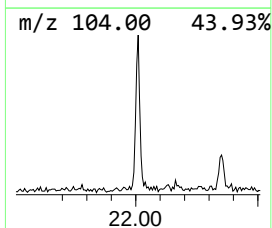
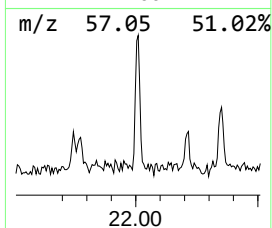
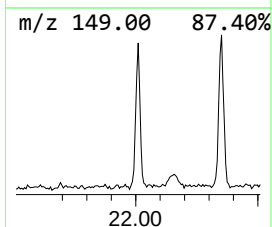
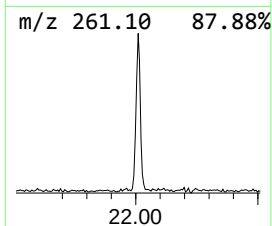
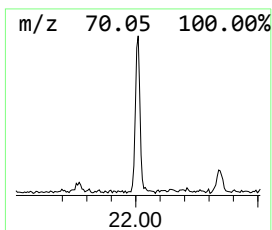
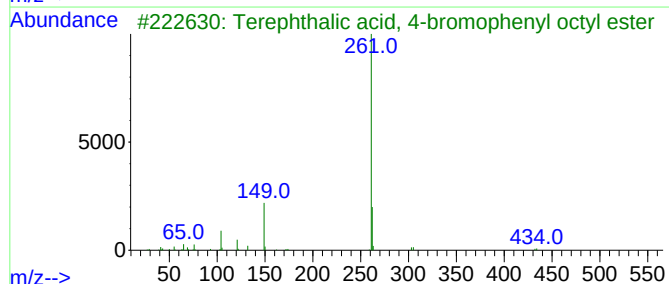
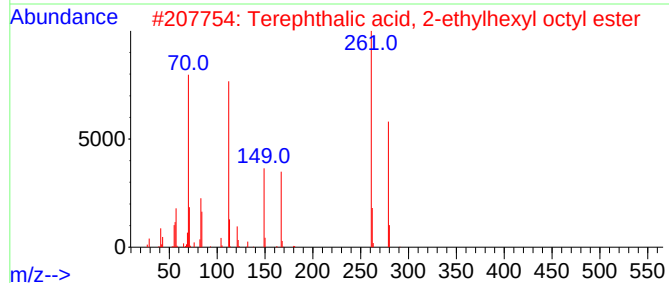
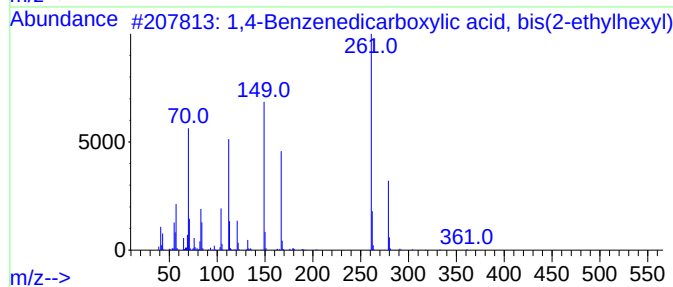
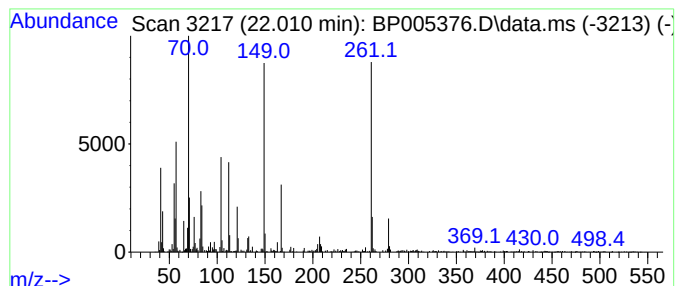
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Peak Number 3 1,4-Benzenedicarboxylic aci... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.010	4.85 ng	153458	Chrysene-d12	21.169

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	64
2			Terephthalic acid, 2-ethylhexyl ...	390	C24H38O4	1000324-00-5	49
3			Terephthalic acid, 4-bromophenyl...	432	C22H25BrO4	1000323-68-4	43
4			Isophthalic acid, 4-nitrophenyl ...	399	C22H25NO6	1000344-68-5	38
5			Isophthalic acid, 2-chlorophenyl...	388	C22H25ClO4	1000344-50-0	38



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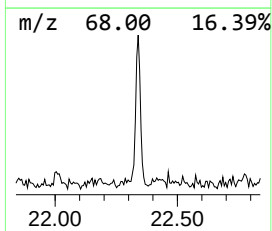
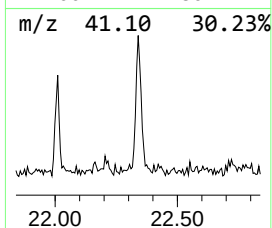
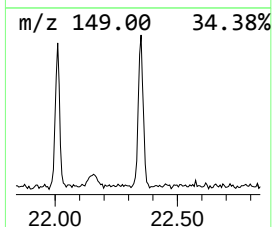
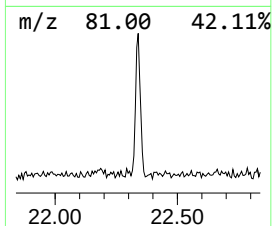
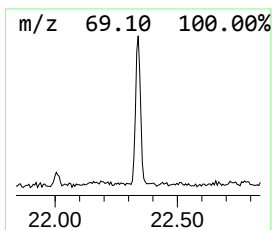
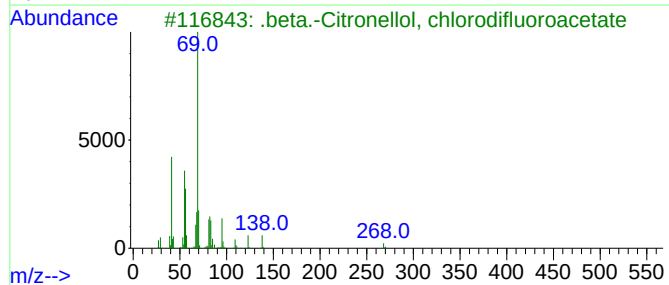
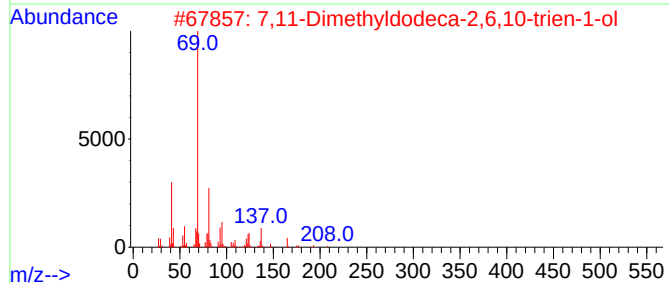
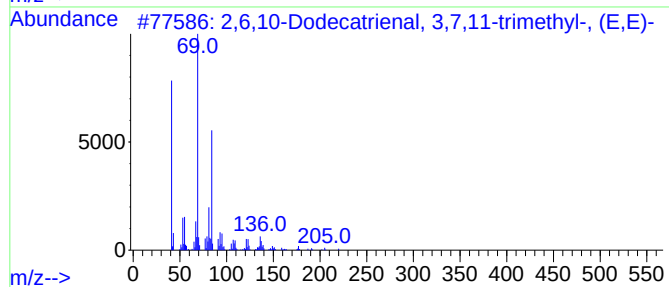
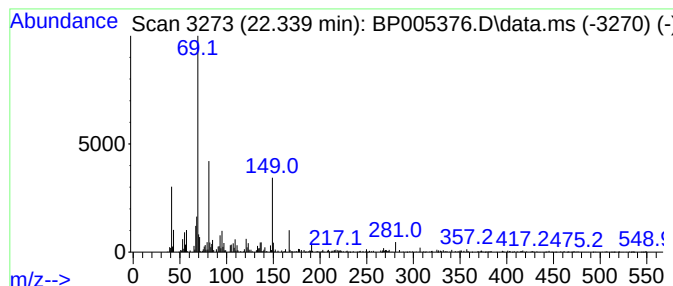
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Peak Number 4 2,6,10-Dodecatrienal, 3,7,11... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.339	5.76 ng	180882	Perylene-d12	23.427

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6,10-Dodecatrienal, 3,7,11-tri...	220	C15H24O	000502-67-0	64		
2	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	52		
3	.beta.-Citronellol, chlorodifluo...	268	C12H19ClF2O2	1000376-20-8	52		
4	4-Methyl-1,5-Heptadiene	110	C8H14	000998-94-7	52		
5	Farnesol isomer a	222	C15H26O	1000108-92-4	50		



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	17.969	5.3	ng	136899	4	17.069	514832	20.0
1-Docosene	20.886	8.0	ng	252126	5	21.169	632978	20.0
1,4-Benzenedica...	22.010	4.8	ng	153458	5	21.169	632978	20.0
2,6,10-Dodecatr...	22.339	5.8	ng	180882	6	23.427	628185	20.0