

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010622\
 Data File : BF126526.D
 Acq On : 6 Jan 2022 18:58
 Operator : JU/CG
 Sample : M5196-07
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMPOSITE-SAMPLE-4-SHALLOW

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-BF122921.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126526.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.140	3	9	14	rBV2	29206	42628	2.21%	0.340%
2	4.987	489	493	502	rVB	74238	93690	4.87%	0.747%
3	5.393	558	562	565	rBV	1988056	1855417	96.36%	14.789%
4	6.410	730	735	738	rBV	1838039	1925497	100.00%	15.347%
5	6.775	794	797	801	rVB	518346	467439	24.28%	3.726%
6	7.340	888	893	896	rBV	1383086	1242951	64.55%	9.907%
7	8.063	1012	1016	1019	rBV	690995	625071	32.46%	4.982%
8	9.139	1194	1199	1202	rBV	2165980	1862123	96.71%	14.842%
9	9.222	1210	1213	1218	rVB	30962	28768	1.49%	0.229%
10	9.816	1310	1314	1317	rBV	756182	613120	31.84%	4.887%
11	10.604	1444	1448	1451	rBV	1049658	883965	45.91%	7.046%
12	11.304	1563	1567	1570	rBV	577363	498771	25.90%	3.976%
13	11.839	1655	1658	1661	rBV	23543	23305	1.21%	0.186%
14	12.892	1833	1837	1840	rBV	1379413	1183588	61.47%	9.434%
15	13.798	1987	1991	2004	rBV2	45226	91051	4.73%	0.726%
16	13.945	2012	2016	2021	rBV	407032	363950	18.90%	2.901%
17	14.045	2028	2033	2039	rBV	42256	47909	2.49%	0.382%
18	14.710	2142	2146	2154	rBV	177259	203417	10.56%	1.621%
19	15.392	2257	2262	2266	rBV2	404884	470120	24.42%	3.747%
20	15.857	2337	2341	2346	rBV2	14155	23301	1.21%	0.186%

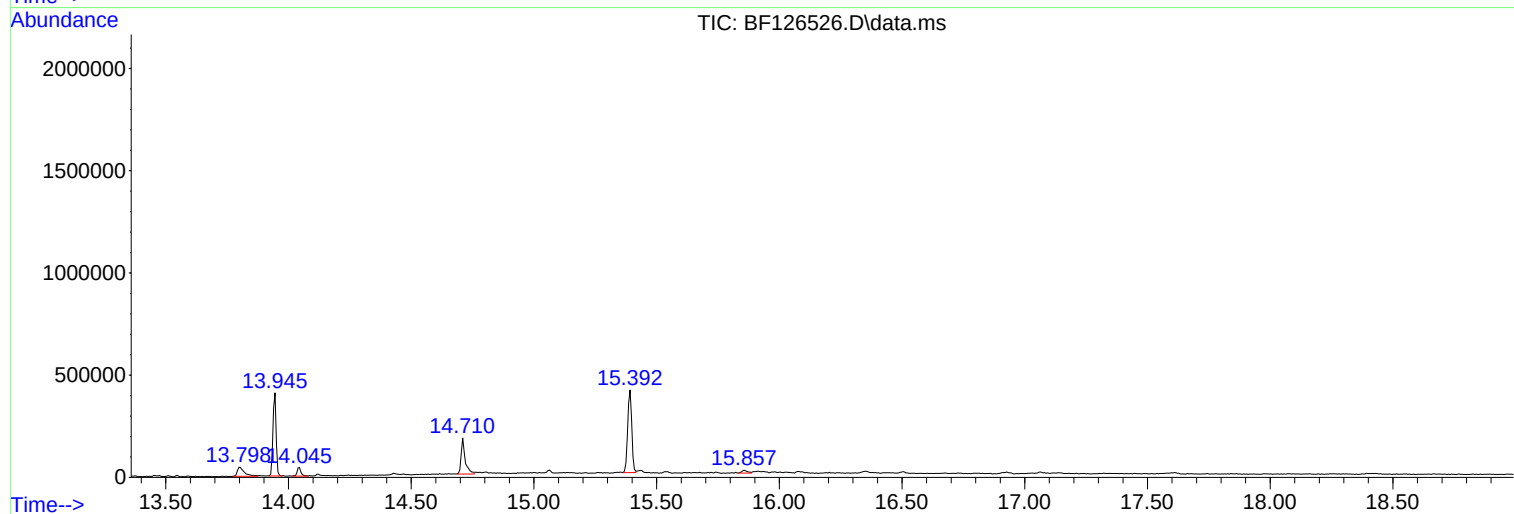
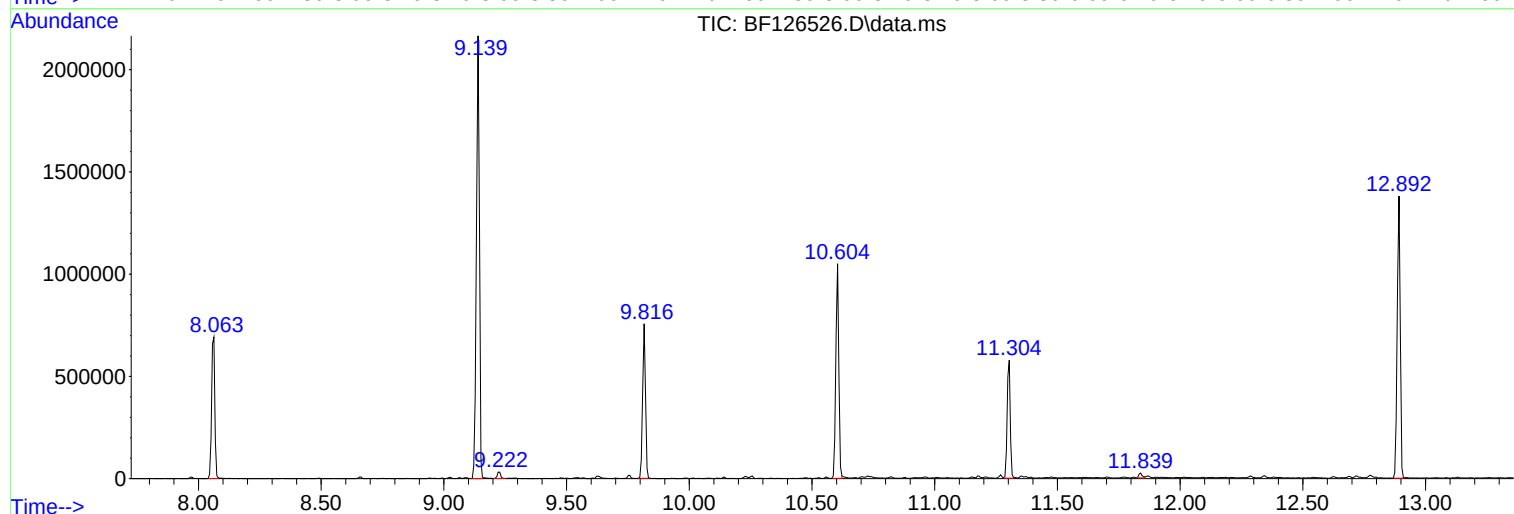
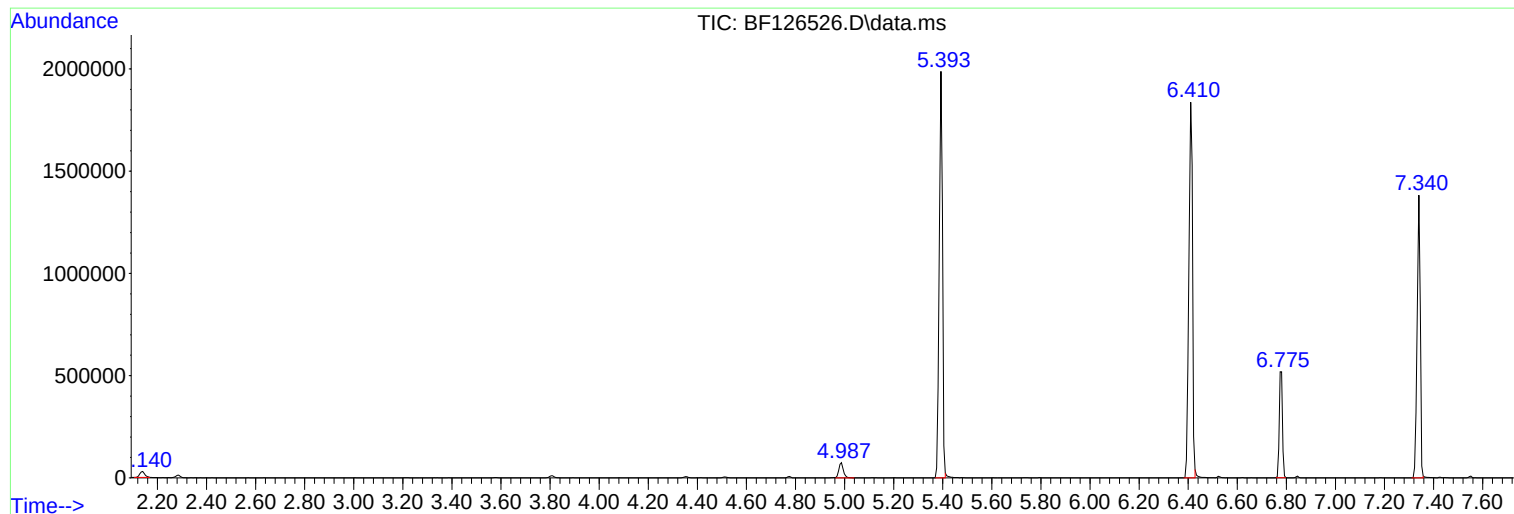
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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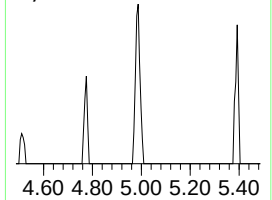
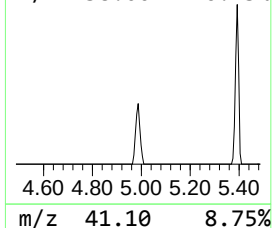
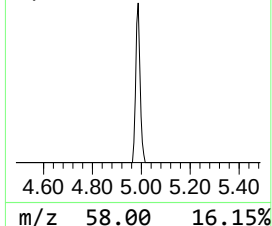
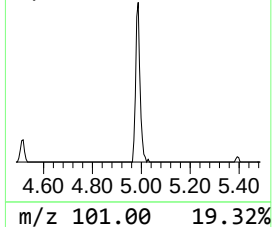
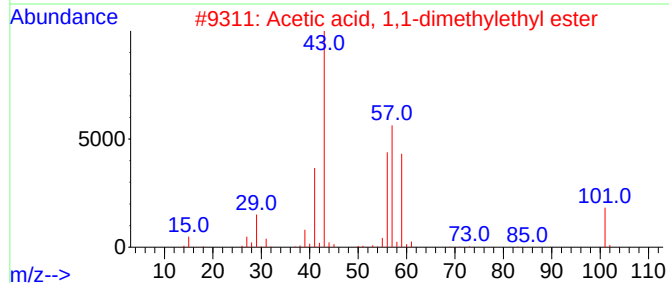
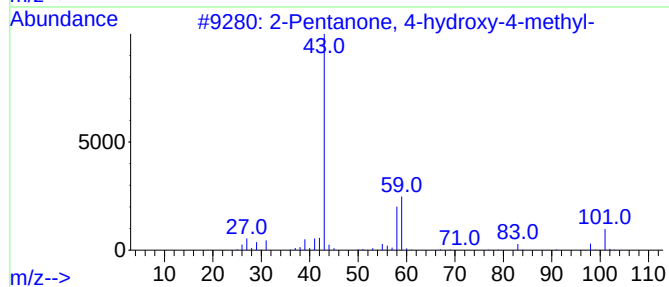
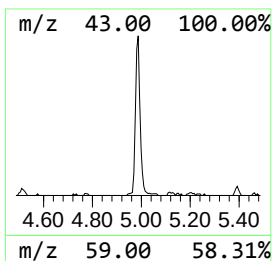
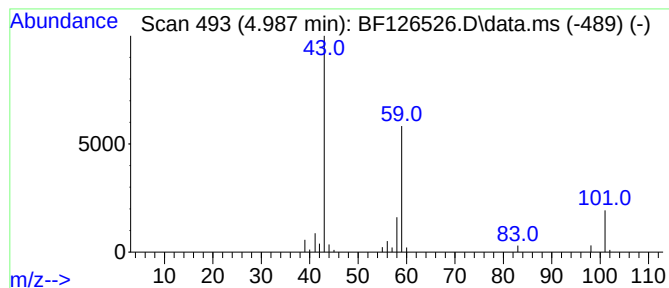
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.987	4.01 ng	93690	1,4-Dichlorobenzene-d4	6.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	40		
3	3-Hexanol	102	C6H14O	000623-37-0	33		
4	3-Octanol	130	C8H18O	000589-98-0	33		
5	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17		



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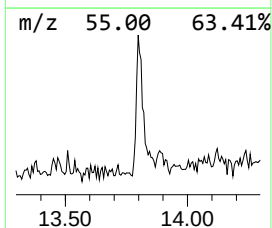
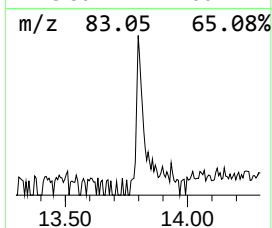
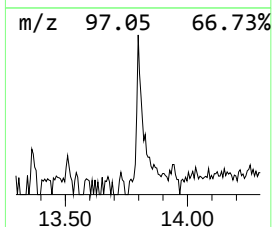
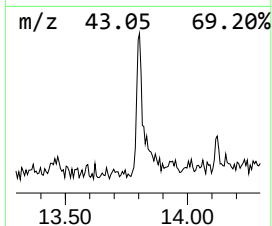
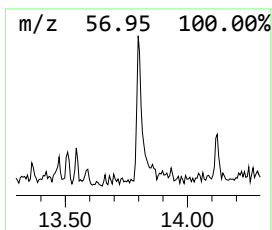
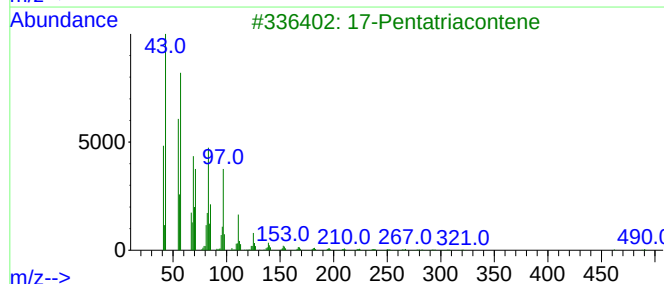
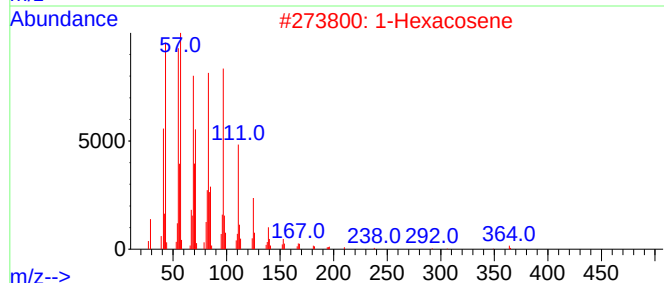
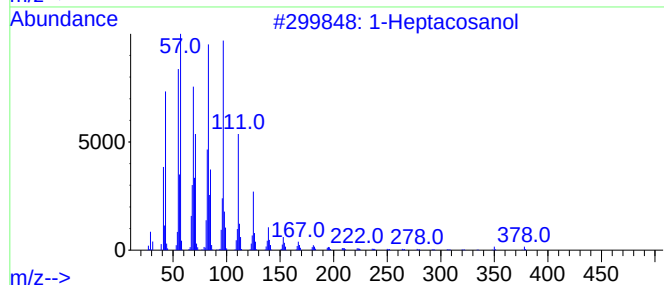
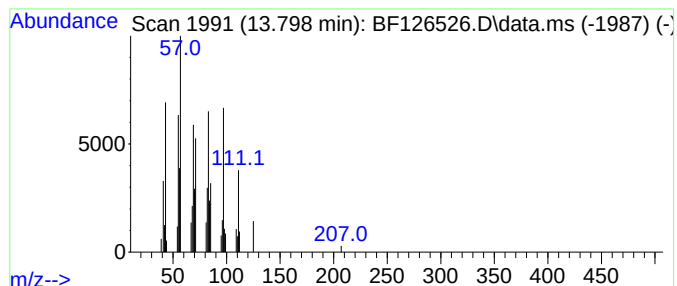
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Peak Number 2 1-Heptacosanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.798	5.00 ng	91051	Chrysene-d12	13.945

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heptacosanol	396	C27H56O	002004-39-9	91
2			1-Hexacosene	364	C26H52	018835-33-1	91
3			17-Pentatriacontene	491	C35H70	006971-40-0	83
4			Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	83
5			1-Heneicosanol	312	C21H44O	015594-90-8	81



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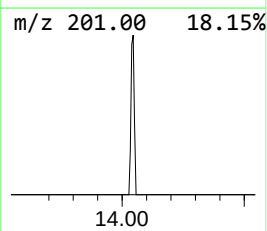
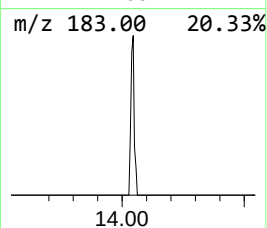
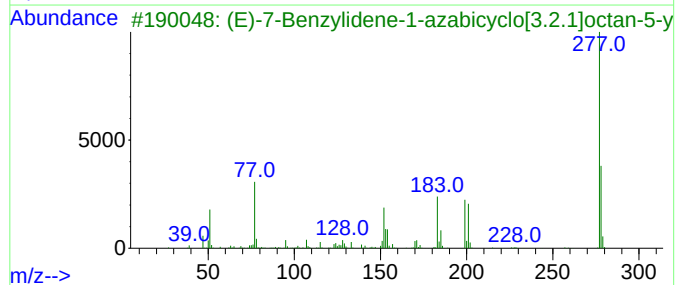
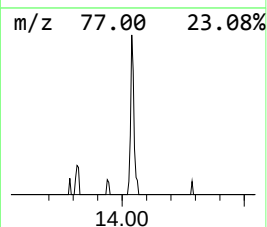
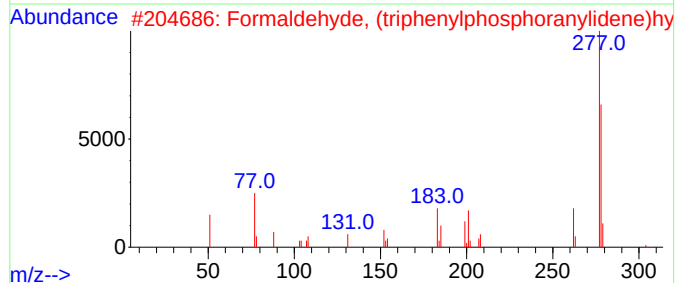
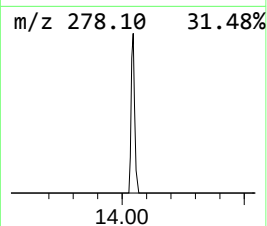
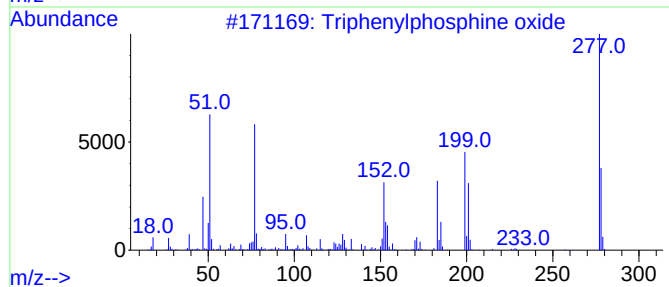
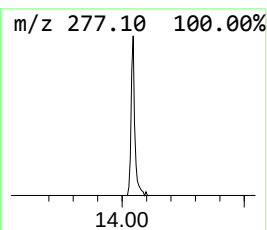
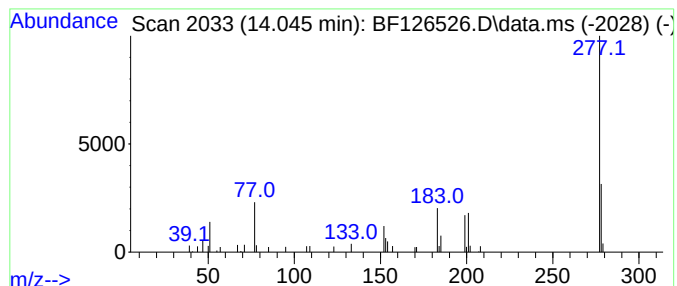
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Peak Number 3 Triphenylphosphine oxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.045	2.63 ng	47909	Chrysene-d12	13.945

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	83
2			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	72
3			(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19N03S	1000483-83-4	68
4			2-Phenyl-6-(trifluoromethyl)-1H...	277	C15H10F3NO	1000387-59-3	38
5			Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	25



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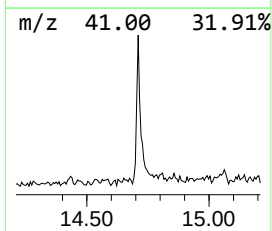
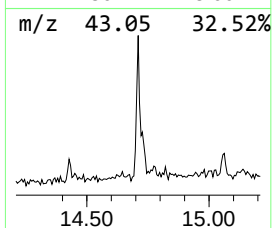
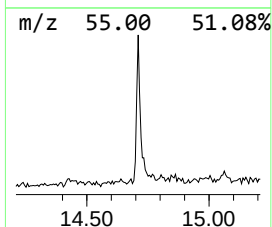
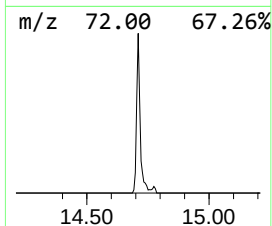
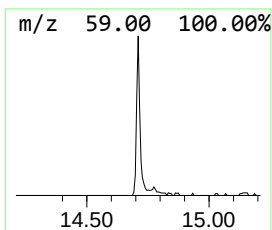
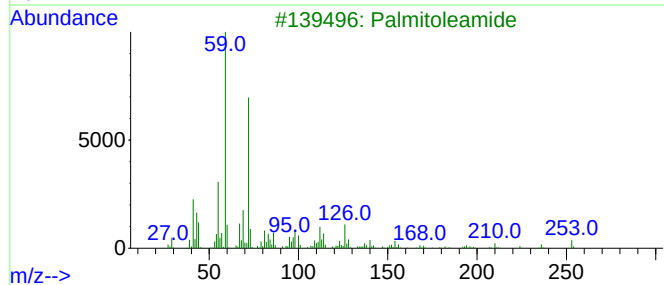
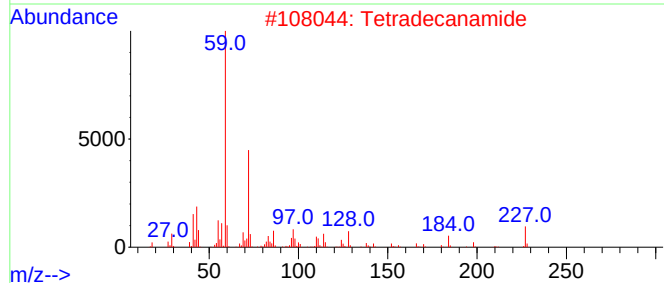
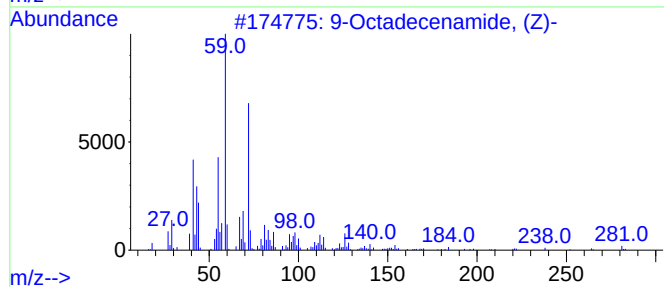
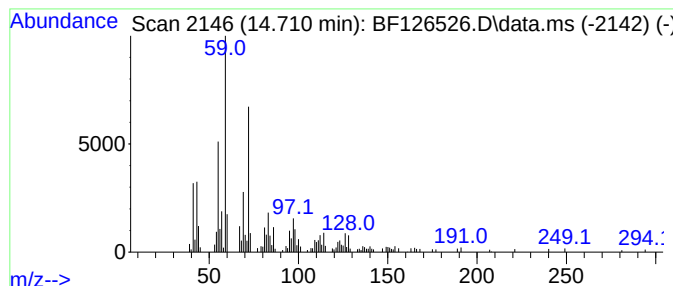
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Peak Number 4 9-Octadecenamide, (Z)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.710	8.65 ng	203417	Perylene-d12	15.392

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	90	
2	Tetradecanamide	227	C14H29NO	000638-58-4	72	
3	Palmitoleamide	253	C16H31NO	106010-22-4	64	
4	Hexadecanamide	255	C16H33NO	000629-54-9	64	
5	Octadecanamide	283	C18H37NO	000124-26-5	50	



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.987	4.0	ng	93690	1	6.781	467439	20.0
1-Heptacosanol	13.798	5.0	ng	91051	5	13.945	363950	20.0
Triphenylphosph...	14.045	2.6	ng	47909	5	13.945	363950	20.0
9-Octadecenamid...	14.710	8.7	ng	203417	6	15.392	470120	20.0