

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020223\
 Data File : BF132297.D
 Acq On : 02 Feb 2023 18:00
 Operator : CG\JU
 Sample : 01363-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-1-WC

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-BF013123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132297.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.307	414	420	427	rVB	1102755	1310975	32.32%	4.600%
2	5.690	480	485	488	rBV	3199314	3099864	76.43%	10.877%
3	6.678	647	653	656	rBV	2978696	3111959	76.73%	10.919%
4	7.066	715	719	722	rBV	1227290	989192	24.39%	3.471%
5	7.625	810	814	817	rBV	2296709	2091517	51.57%	7.339%
6	8.348	934	937	941	rBV	1551849	1333934	32.89%	4.681%
7	9.431	1116	1121	1124	rBV	4499984	4055867	100.00%	14.231%
8	10.113	1234	1237	1241	rVB	1721195	1550711	38.23%	5.441%
9	10.831	1356	1359	1362	rVB	139042	109817	2.71%	0.385%
10	10.907	1368	1372	1375	rBV	3021369	2655662	65.48%	9.318%
11	11.613	1488	1492	1495	rBV	1904381	1562634	38.53%	5.483%
12	12.119	1571	1578	1582	rBV	217543	194152	4.79%	0.681%
13	13.207	1759	1763	1767	rBV	3871607	3617172	89.18%	12.692%
14	13.424	1793	1800	1804	rBV	39030	44802	1.10%	0.157%
15	14.095	1910	1914	1933	rBV2	247637	416650	10.27%	1.462%
16	14.277	1941	1945	1948	rBV	927337	884844	21.82%	3.105%
17	14.419	1965	1969	1974	rBV	42943	44878	1.11%	0.157%
18	14.730	2019	2022	2030	rBV	37343	54014	1.33%	0.190%
19	15.054	2073	2077	2085	rBV3	117356	173111	4.27%	0.607%
20	15.154	2090	2094	2098	rVB	204225	219688	5.42%	0.771%
21	15.860	2209	2214	2221	rVB2	740741	978326	24.12%	3.433%

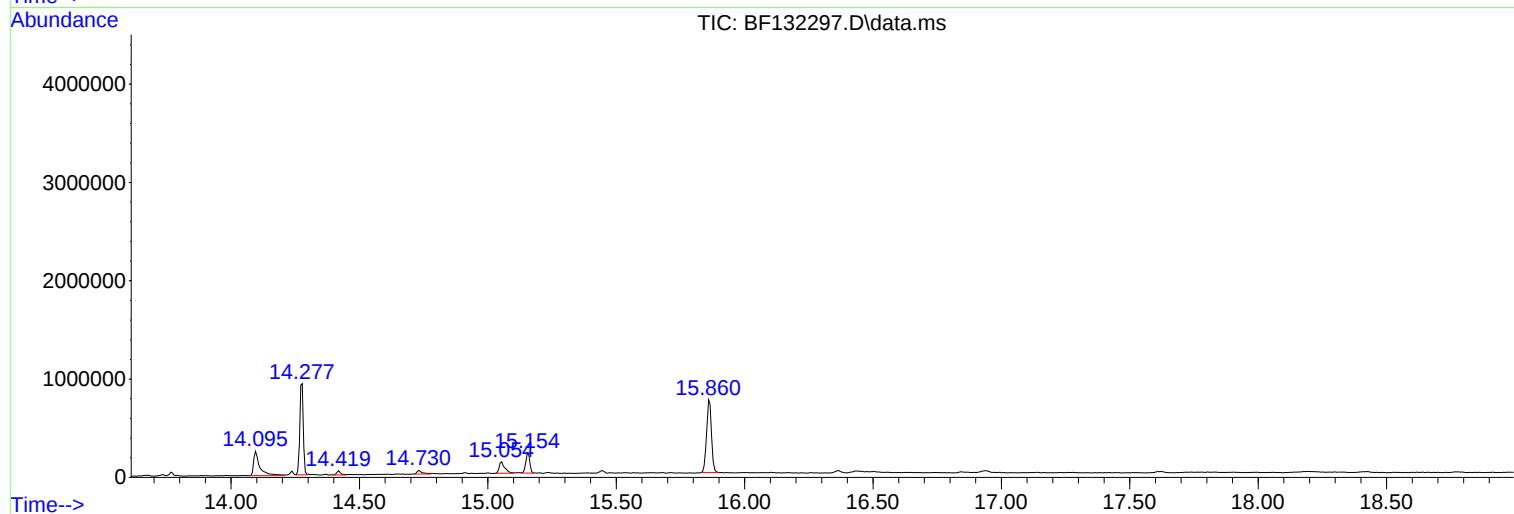
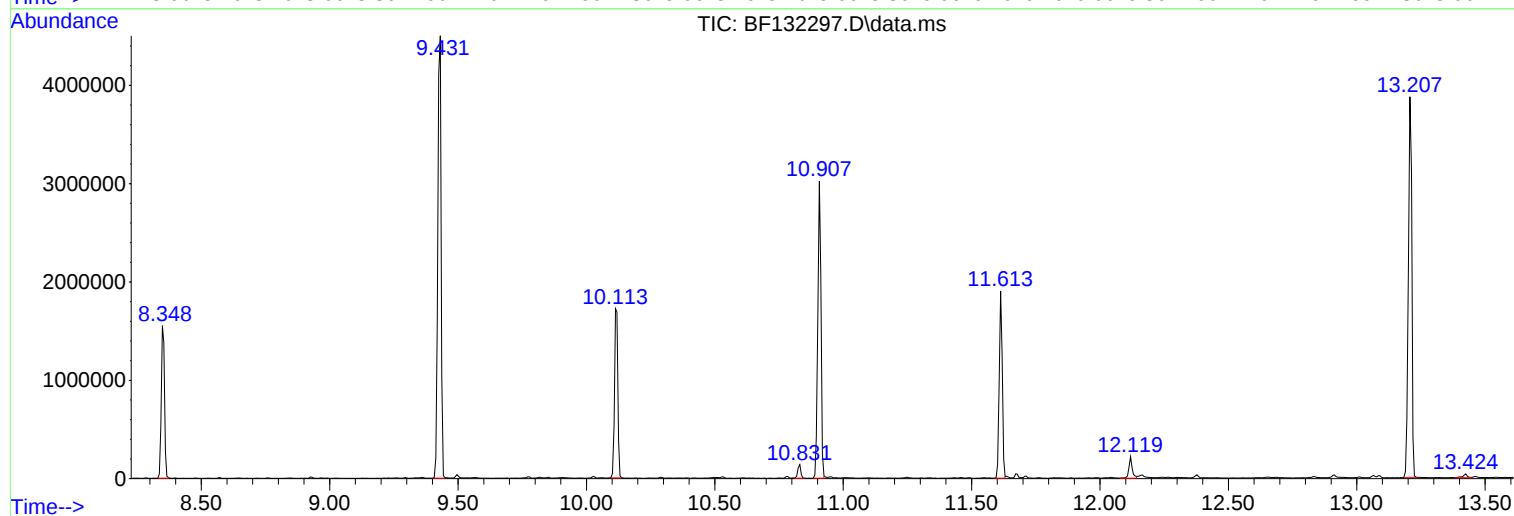
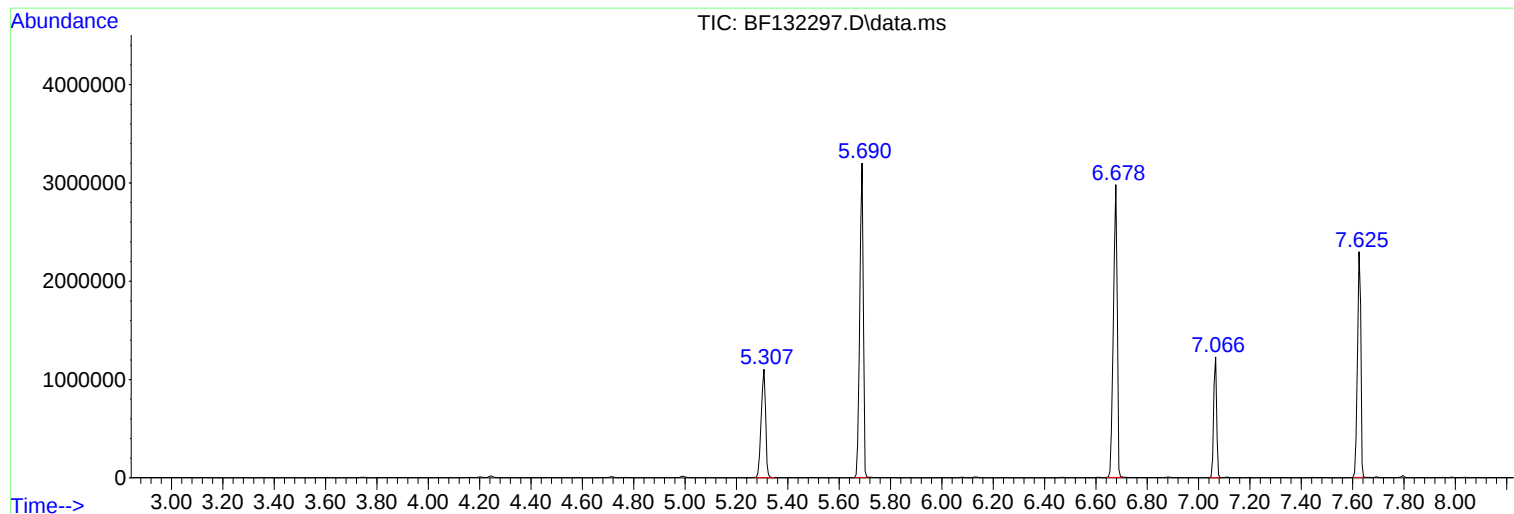
Sum of corrected areas: 28499769

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013123.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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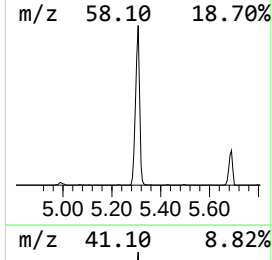
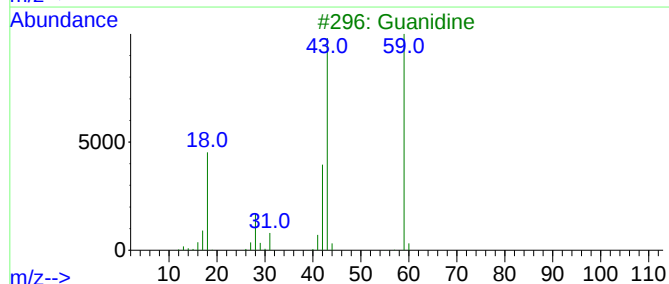
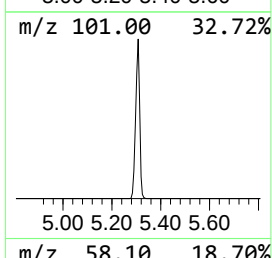
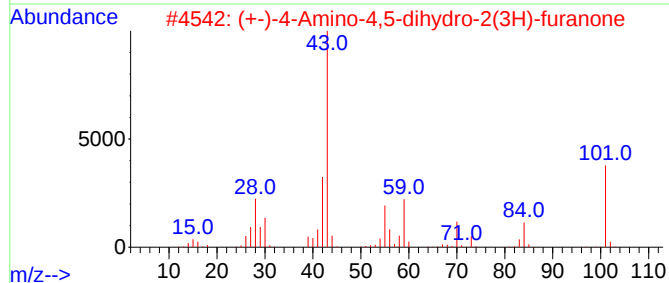
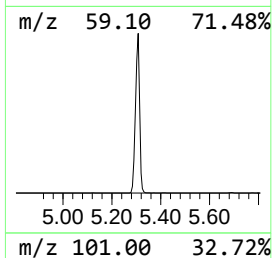
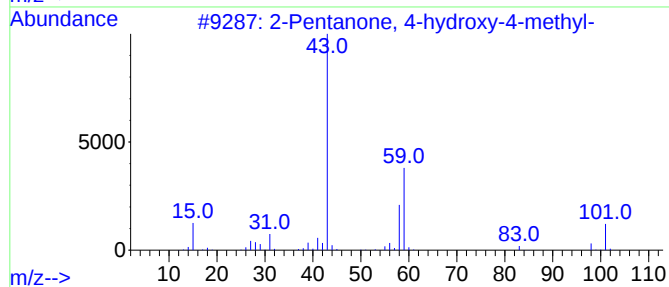
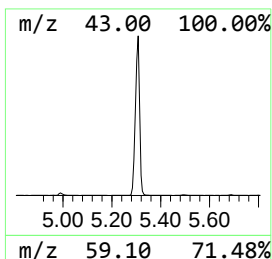
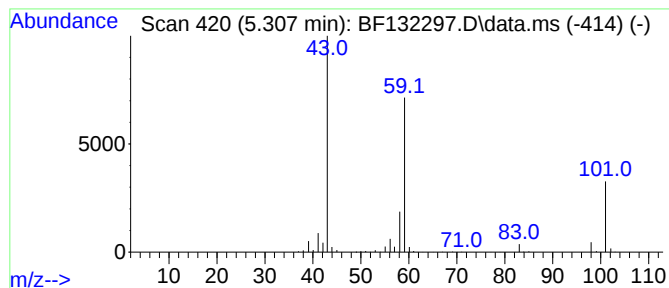
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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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.	
5.307	26.51 ng	1310980	1,4-Dichlorobenzene-d4	7.066	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	47
3	Guanidine	59	CH5N3	000113-00-8	43
4	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17



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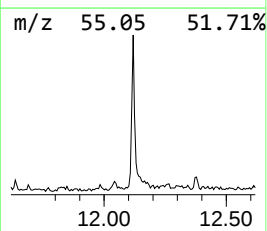
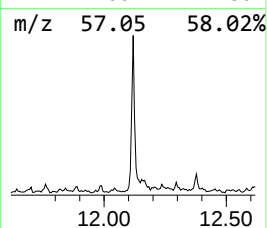
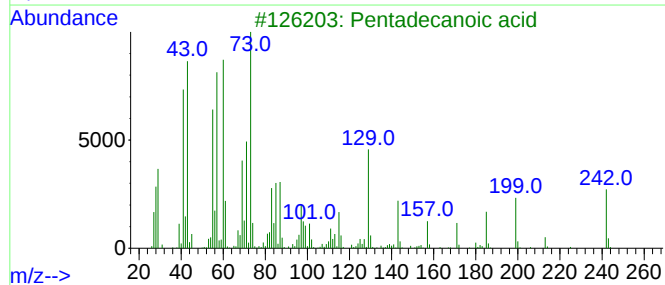
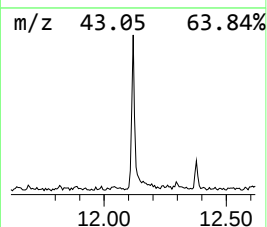
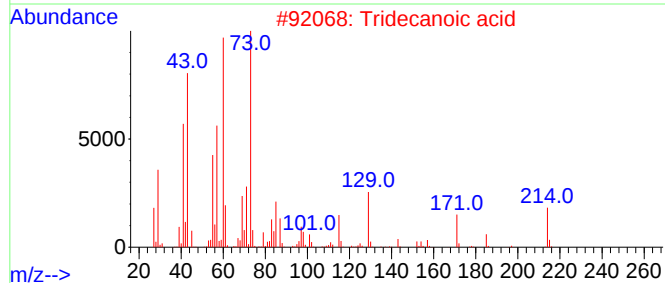
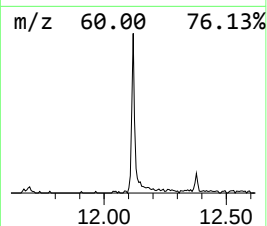
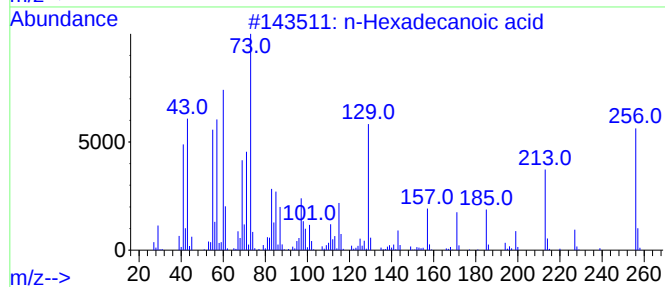
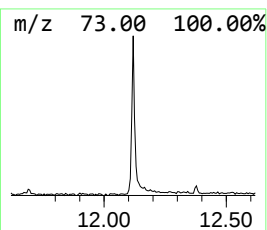
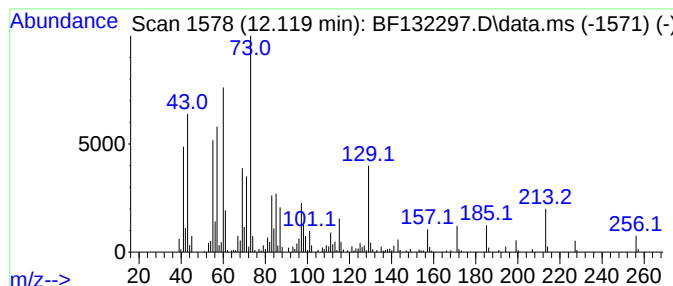
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.119	2.48 ng	194152	Phenanthrene-d10	11.613

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	89
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4			Dodecanoic acid	200	C12H24O2	000143-07-7	72
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	64



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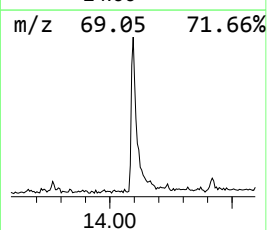
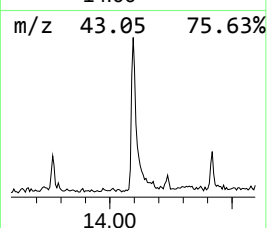
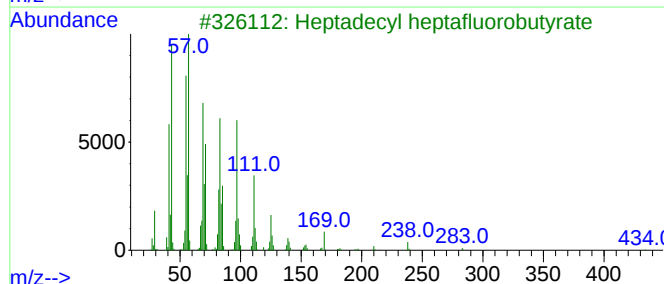
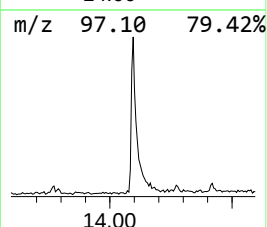
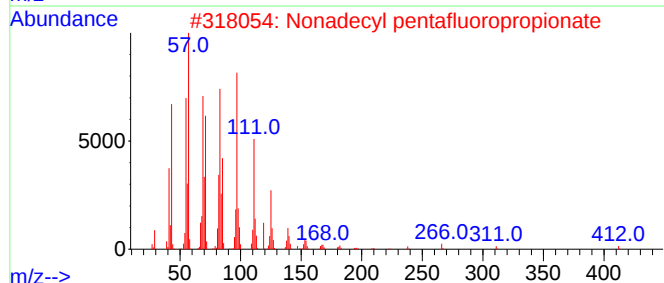
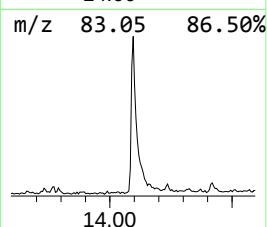
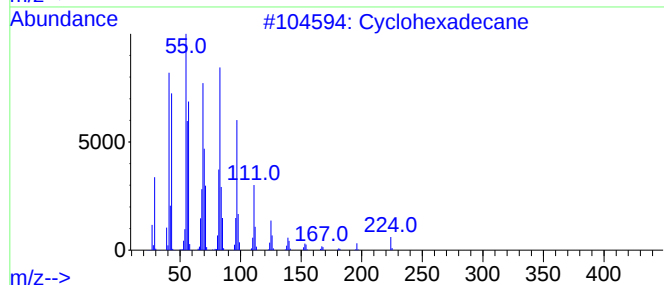
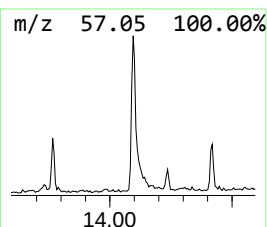
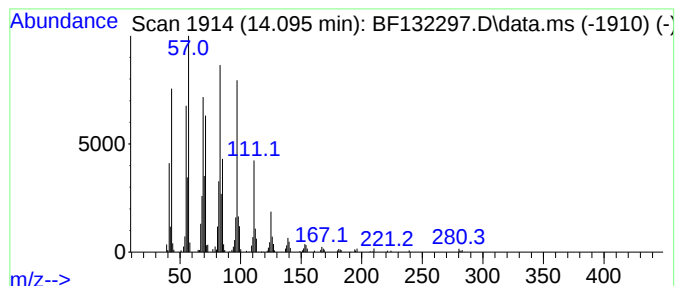
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Cyclohexadecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.095	9.42 ng	416650	Chrysene-d12	14.277

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexadecane	224	C16H32	000295-65-8	97
2			Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	94
3			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
4			Behenic alcohol	326	C22H46O	000661-19-8	93
5			Cyclopentadecane	210	C15H30	000295-48-7	91



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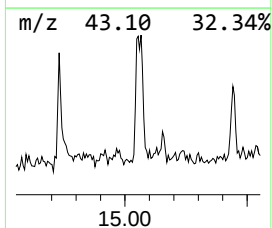
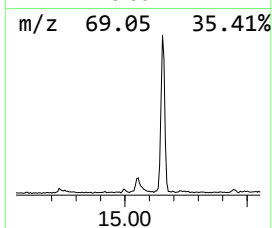
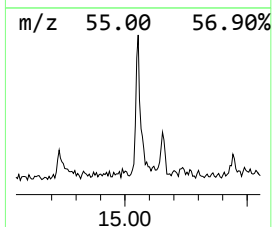
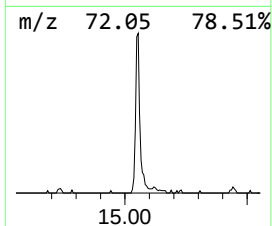
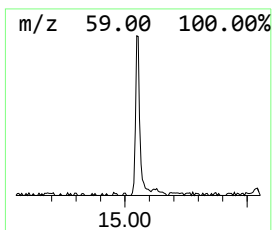
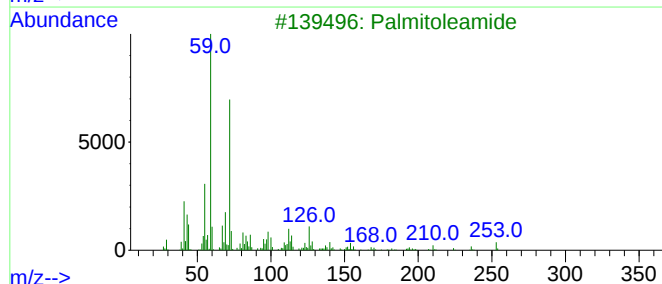
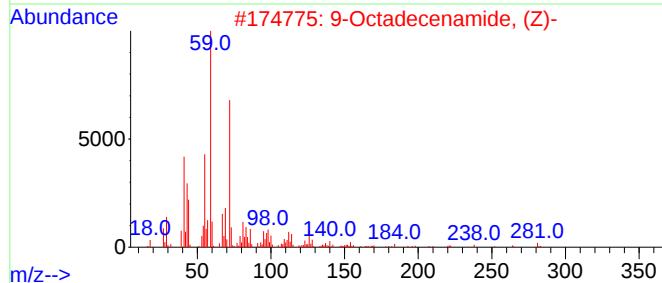
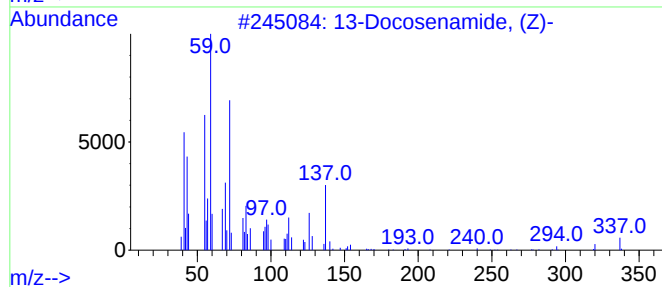
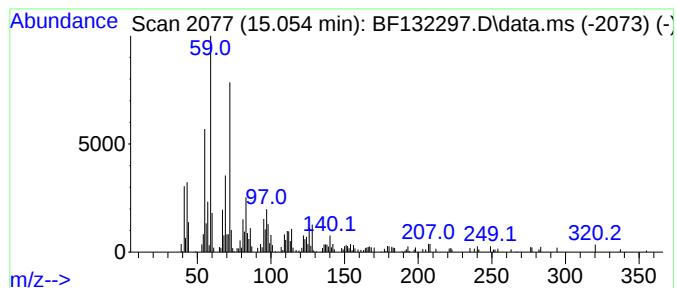
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Peak Number 4 13-Docosenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.054	3.91 ng	173111	Chrysene-d12	14.277

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	90
2			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	74
3			Palmitoleamide	253	C16H31NO	106010-22-4	64
4			Octadecanamide	283	C18H37NO	000124-26-5	38
5			1,1,2-Trimethyl-1-silacyclobutane	114	C6H14Si	030681-90-4	38



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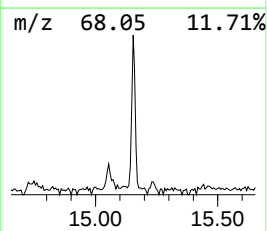
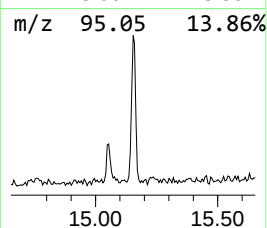
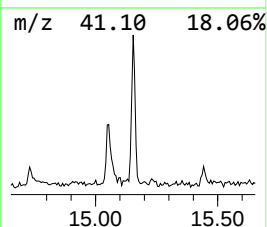
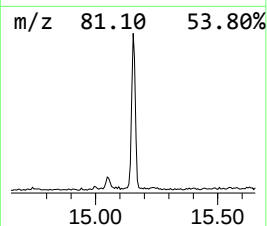
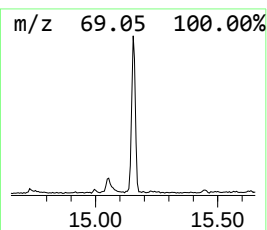
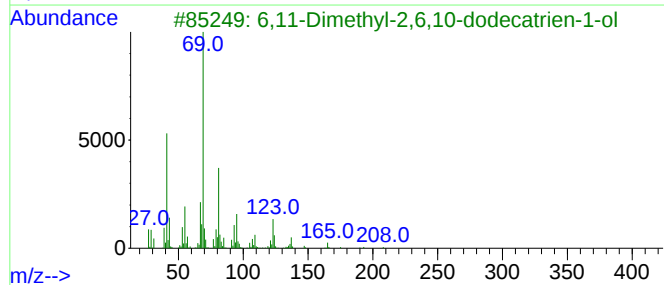
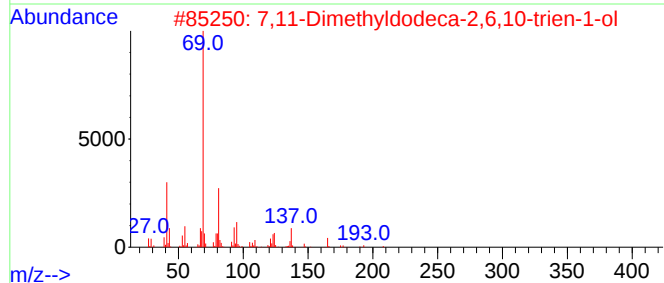
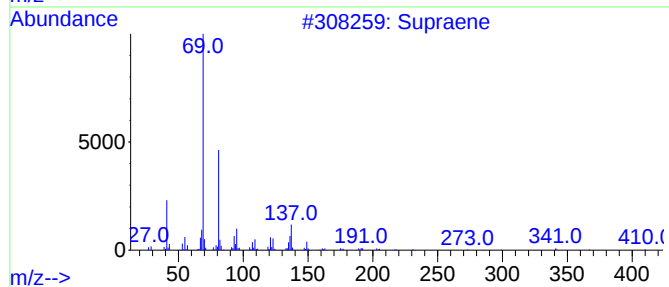
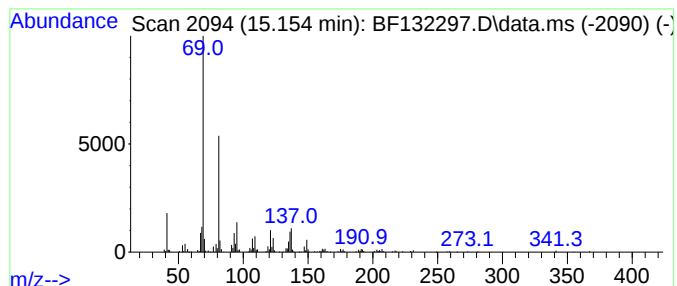
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Peak Number 5 Supraene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.154	4.49 ng	219688	Perylene-d12	15.860

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
3			6,11-Dimethyl-2,6,10-dodecatrien...	208	C14H24O	1000196-53-3	53
4			Squalene	410	C30H50	000111-02-4	50
5			2-propenoic acid, 2-methyl-, 4-f...	190	C11H10O3	1000400-21-0	47



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.307	26.5	ng	1310980	1	7.066	989192	20.0
n-Hexadecanoic ...	12.119	2.5	ng	194152	4	11.613	1562630	20.0
Cyclohexadecane	14.095	9.4	ng	416650	5	14.277	884844	20.0
13-Docosenamide...	15.054	3.9	ng	173111	5	14.277	884844	20.0
Supraene	15.154	4.5	ng	219688	6	15.860	978326	20.0