

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032123\
 Data File : BM039072.D
 Acq On : 21 Mar 2023 17:02
 Operator : CG/JU
 Sample : 02020-31
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 SP-4

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_M\Methods\8270-BM030823.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM039072.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.058	295	301	312	rVB	1712894	2369265	31.79%	4.700%
2	5.522	373	380	390	rBV	3923590	5522615	74.09%	10.956%
3	7.128	645	653	665	rBV	3626832	5542639	74.36%	10.996%
4	7.969	789	796	803	rVB	1031463	1592042	21.36%	3.158%
5	9.134	985	994	1004	rBV	2142491	3359389	45.07%	6.664%
6	10.781	1267	1274	1284	rBV	1267040	2062779	27.68%	4.092%
7	13.233	1683	1691	1704	rBV	4303078	6101044	81.85%	12.103%
8	14.610	1914	1925	1933	rBV	1548932	2302769	30.90%	4.568%
9	15.963	2149	2155	2160	rBV	180452	246363	3.31%	0.489%
10	16.092	2170	2177	2194	rBV	3018457	4233114	56.79%	8.398%
11	17.351	2385	2391	2402	rBV	1846327	2527225	33.91%	5.014%
12	18.245	2538	2543	2552	rBV	286335	468011	6.28%	0.928%
13	19.515	2756	2759	2772	rBV2	136063	244278	3.28%	0.485%
14	19.968	2831	2836	2843	rBV	6216075	7453499	100.00%	14.786%
15	21.233	3048	3051	3060	rBV2	388638	534429	7.17%	1.060%
16	21.527	3097	3101	3113	rBV	2191554	2794922	37.50%	5.545%
17	23.962	3509	3515	3524	rVB2	1502626	3053816	40.97%	6.058%

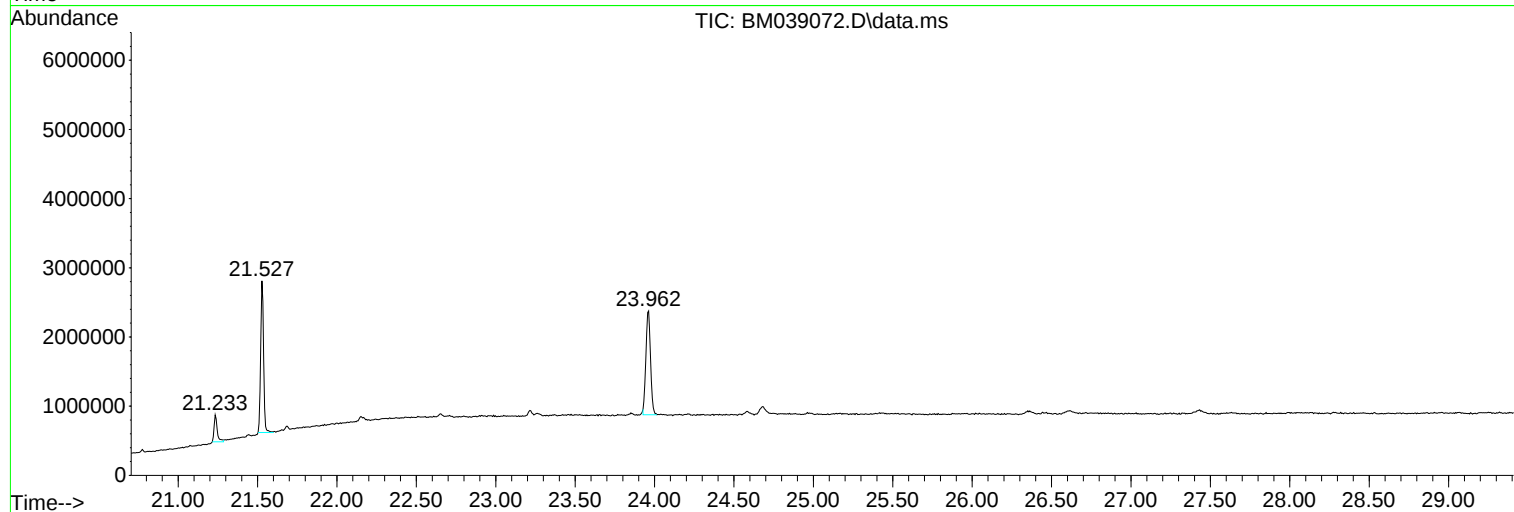
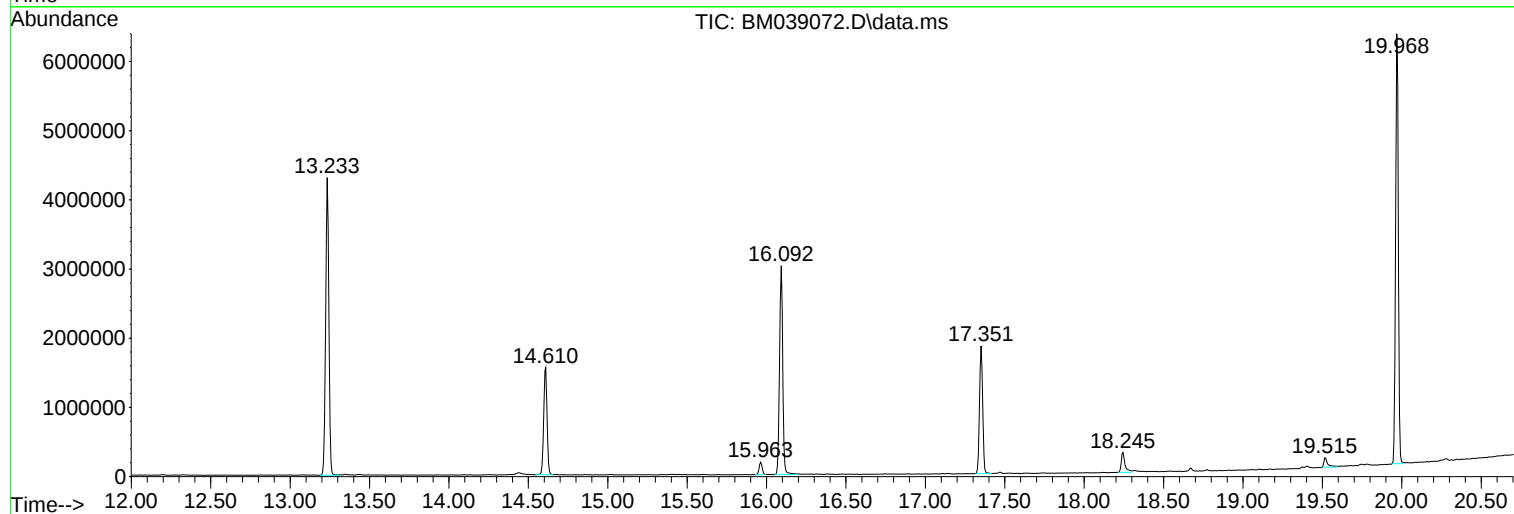
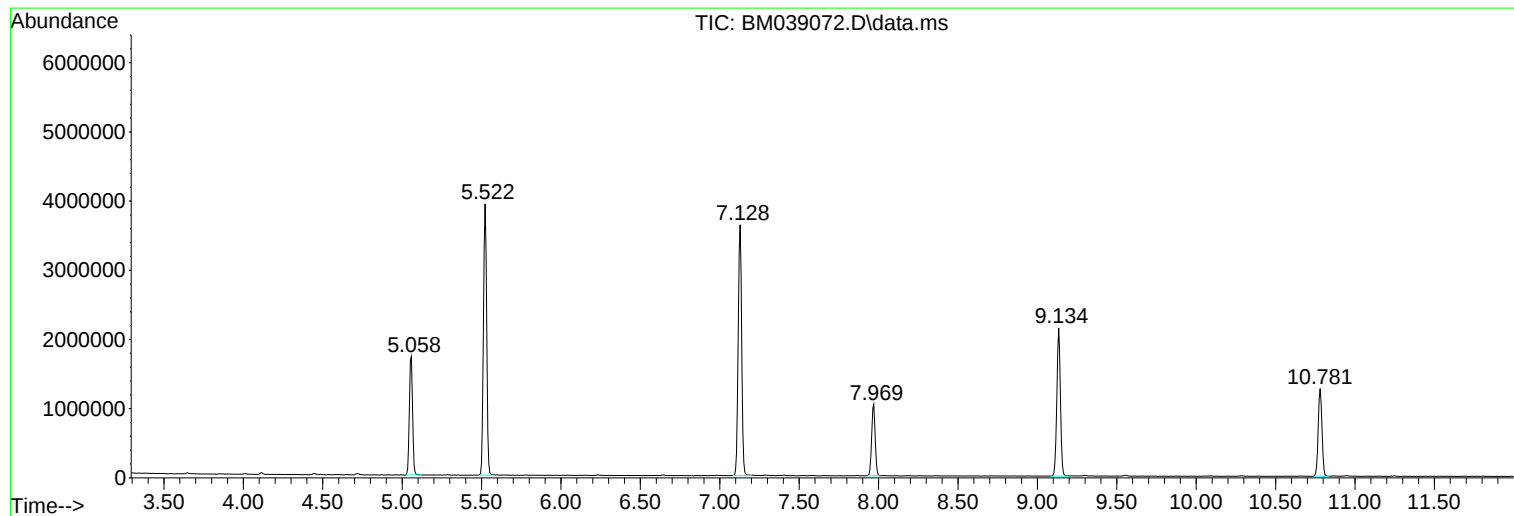
Sum of corrected areas: 50408199

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.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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ALS Vial : 9 Sample Multiplier: 1

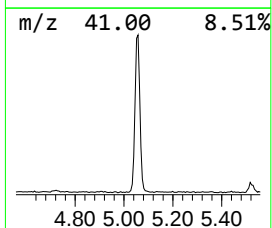
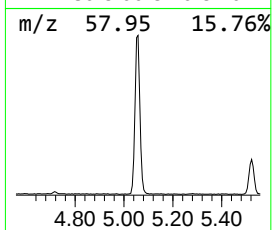
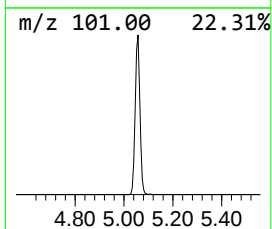
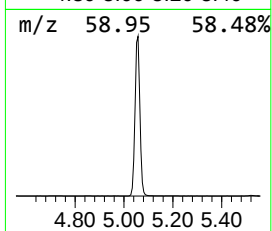
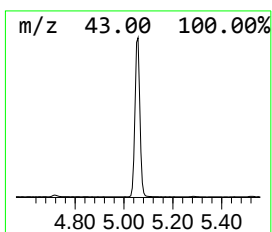
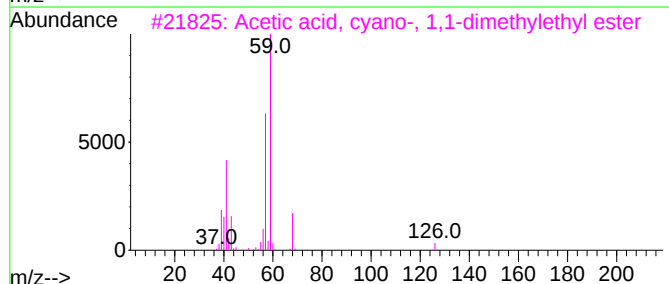
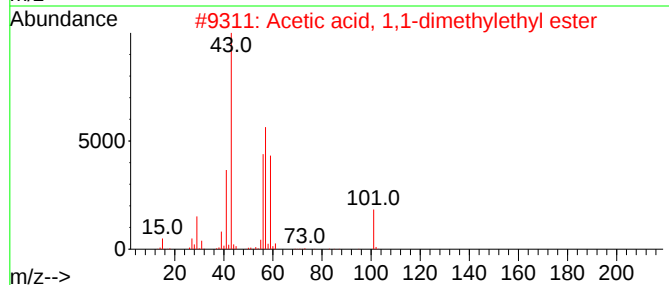
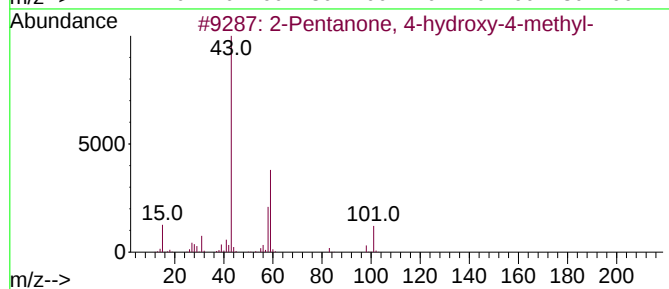
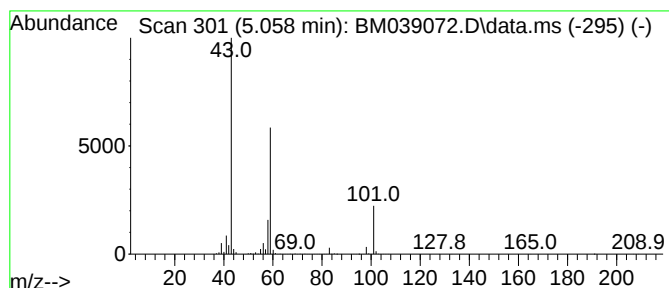
Instrument :
BNA_M
ClientSampleId :
SP-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.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.	
5.058	29.76 ng	2369270	1,4-Dichlorobenzene-d4	7.969	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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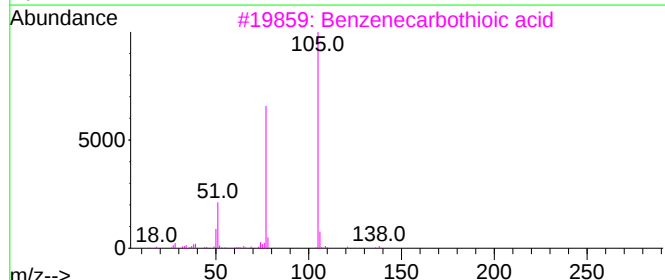
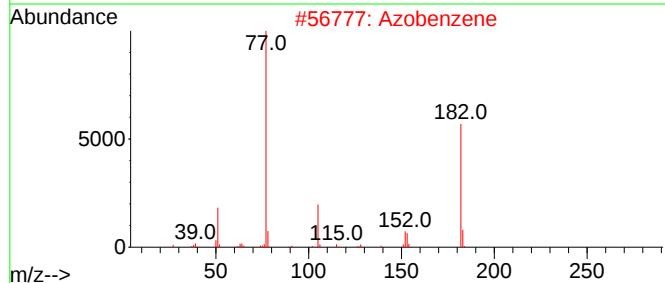
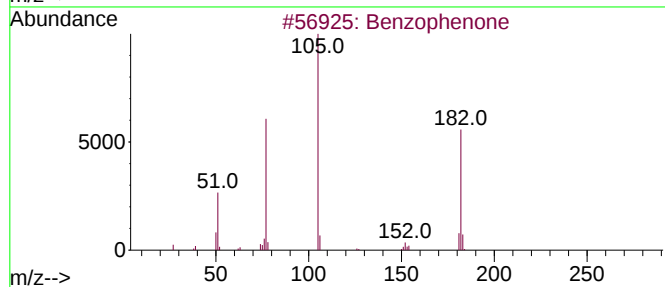
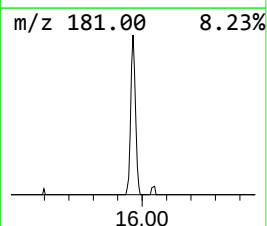
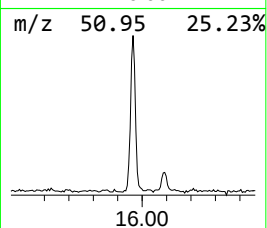
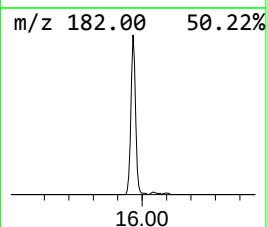
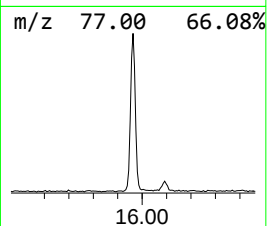
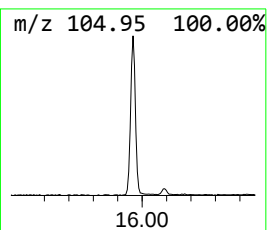
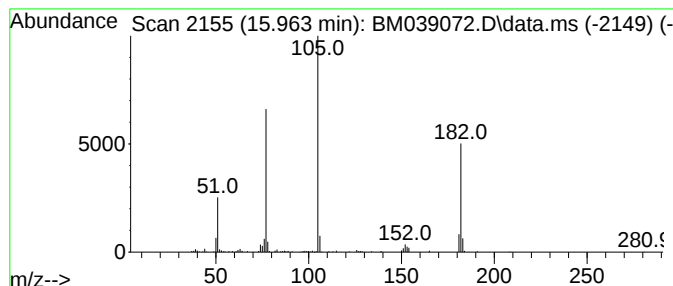
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.963	2.14 ng	246363	Acenaphthene-d10	14.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Azobenzene	182	C12H10N2	000103-33-3	72
3			Benzenecarbothioic acid	138	C7H6OS	000098-91-9	47
4			2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	47
5			Benzopinacol	366	C26H22O2	000464-72-2	47



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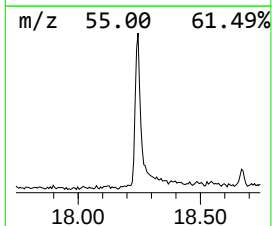
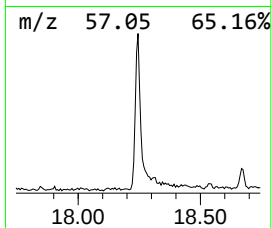
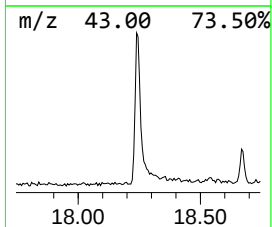
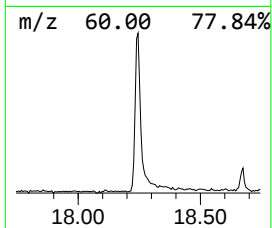
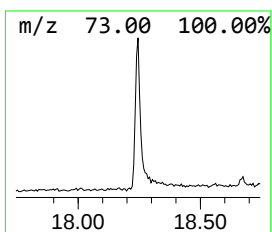
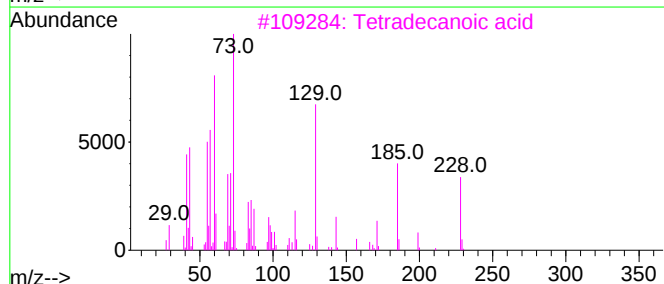
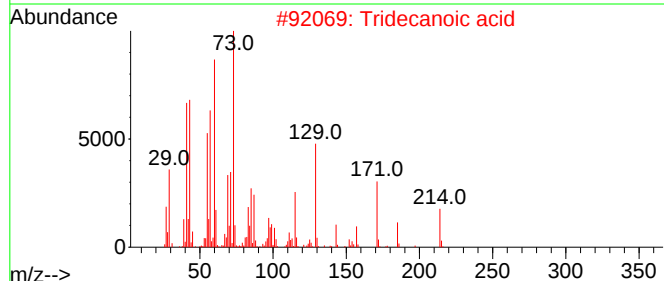
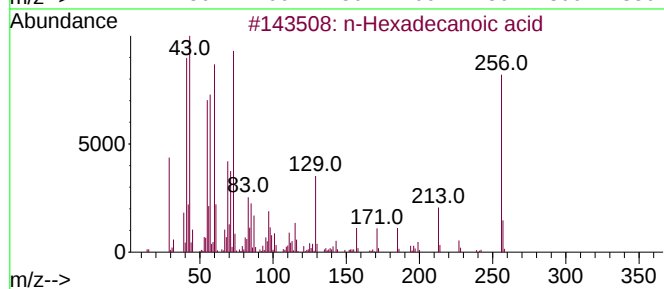
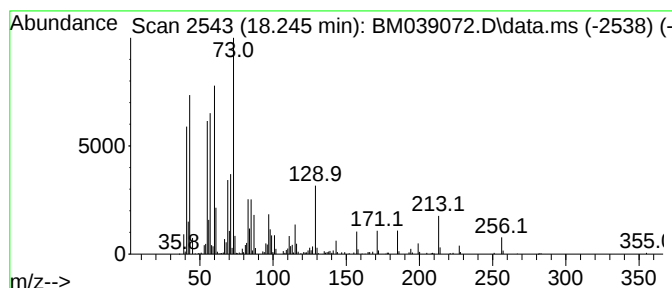
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.245	3.70 ng	468011	Phenanthrene-d10	17.351

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	94
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5			Octadecanoic acid	284	C18H36O2	000057-11-4	83



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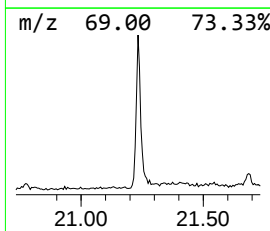
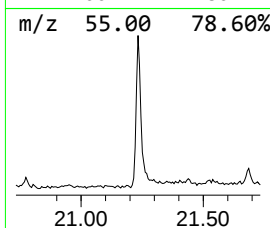
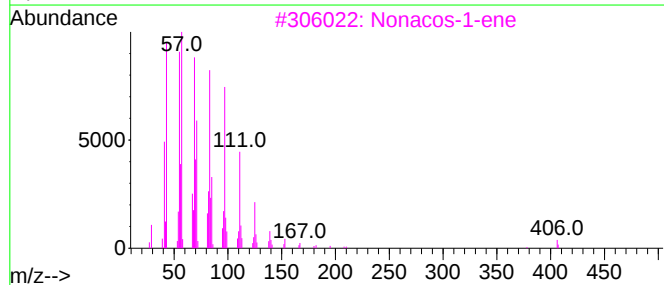
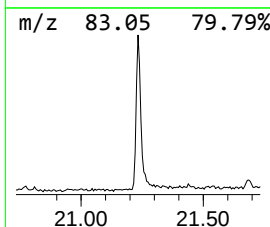
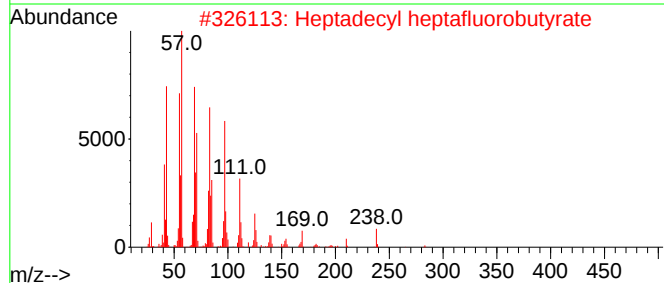
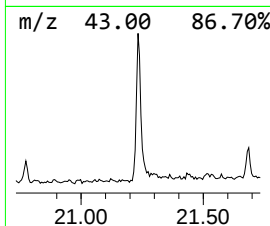
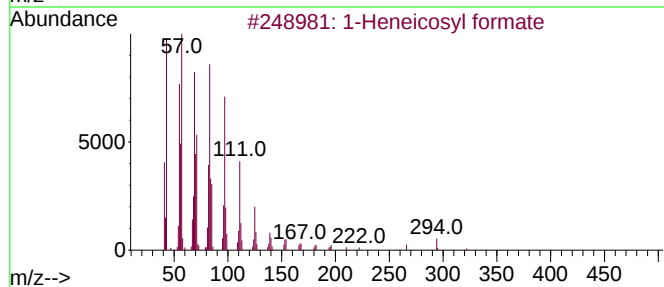
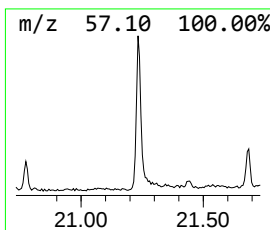
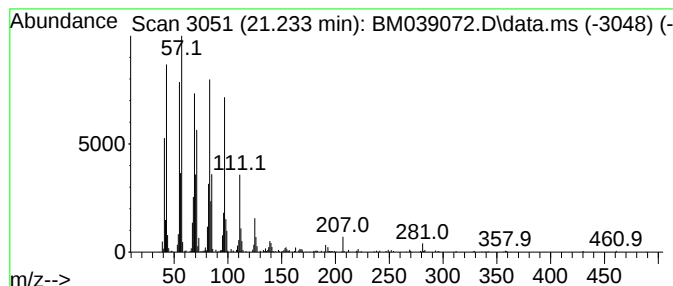
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Peak Number 4 1-Heneicosyl formate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.233	3.82 ng	534429	Chrysene-d12	21.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
2			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3			Nonacos-1-ene	406	C29H58	018835-35-3	94
4			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
5			2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.058	29.8	ng	2369270	1	7.969	1592040	20.0
Benzophenone	15.963	2.1	ng	246363	3	14.610	2302770	20.0
n-Hexadecanoic ...	18.245	3.7	ng	468011	4	17.351	2527230	20.0
1-Heneicosyl fo...	21.233	3.8	ng	534429	5	21.527	2794920	20.0