

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041123\
 Data File : BG057060.D
 Acq On : 11 Apr 2023 19:47
 Operator : CG/JU
 Sample : 02232-03
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 20230325-COMP-3

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_G\Methods\8270-BG033023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057060.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.436	312	323	332	rVB	148146	233291	17.84%	3.939%
2	5.918	398	405	415	rBV	365725	584482	44.69%	9.869%
3	7.539	673	681	689	rVB	365100	630023	48.18%	10.638%
4	8.403	822	828	835	rVB	57486	96069	7.35%	1.622%
5	9.584	1021	1029	1038	rBB	211058	376022	28.75%	6.349%
6	11.246	1302	1312	1318	rBV	73131	128429	9.82%	2.169%
7	13.643	1713	1720	1727	rBV	556292	841804	64.37%	14.215%
8	15.017	1947	1954	1961	rVB2	122291	184282	14.09%	3.112%
9	16.351	2177	2181	2191	rVB	16368	23283	1.78%	0.393%
10	16.498	2200	2206	2215	rBV	452786	680941	52.07%	11.498%
11	17.755	2415	2420	2427	rBV2	150829	225229	17.22%	3.803%
12	18.595	2557	2563	2570	rBV	37621	53218	4.07%	0.899%
13	20.328	2852	2858	2864	rVB	1035812	1307729	100.00%	22.082%
14	21.638	3076	3081	3090	rBV6	19867	39585	3.03%	0.668%
15	22.078	3149	3156	3162	rBV	147885	253278	19.37%	4.277%
16	25.615	3745	3758	3769	rBV2	86726	264451	20.22%	4.465%

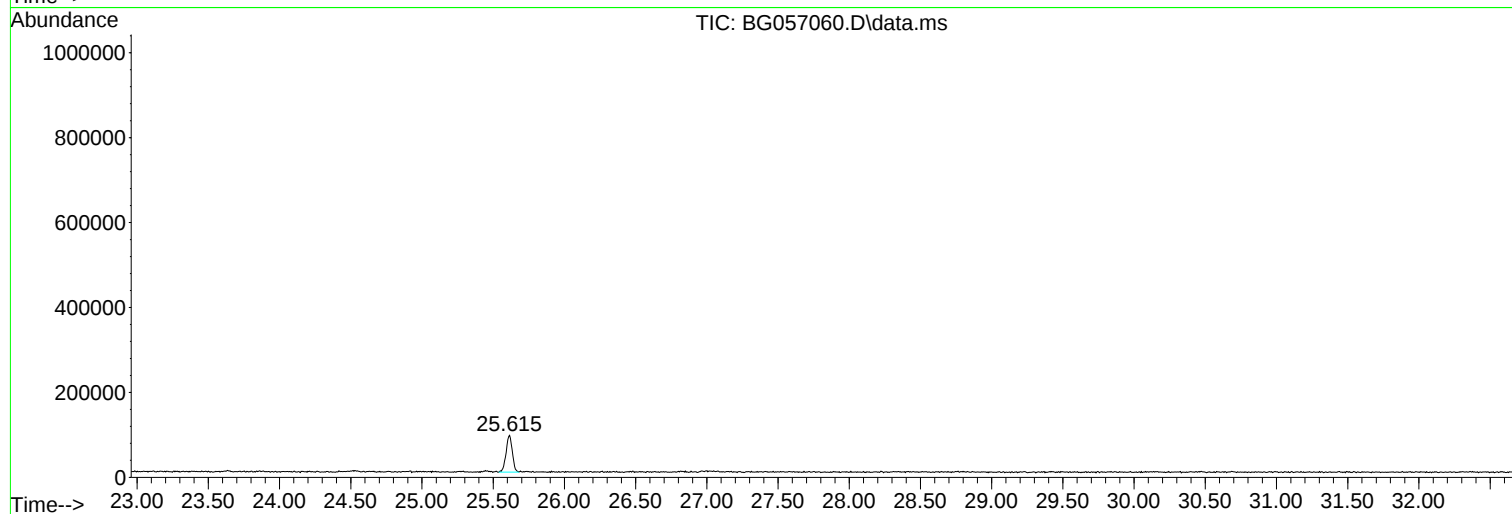
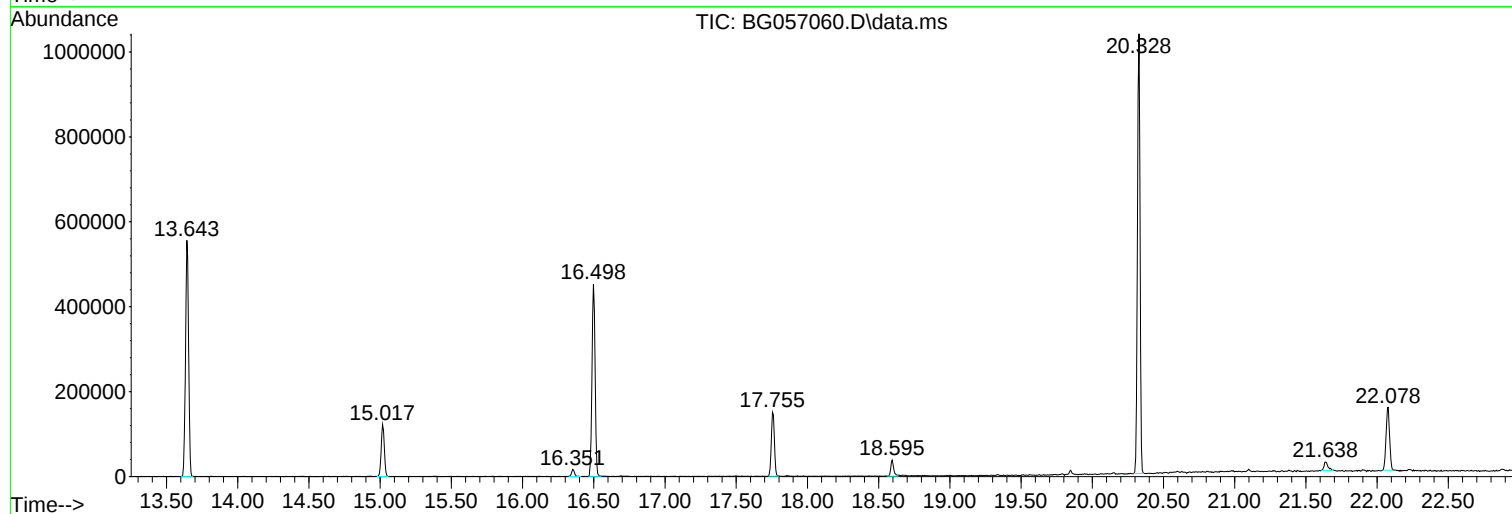
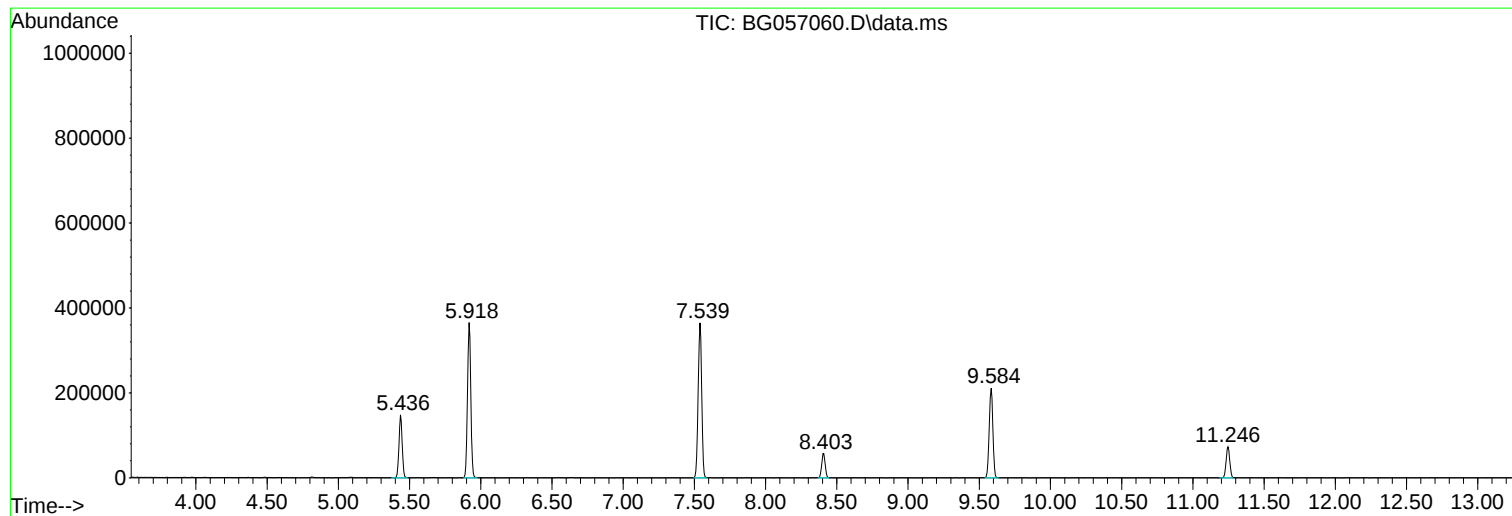
Sum of corrected areas: 5922116

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.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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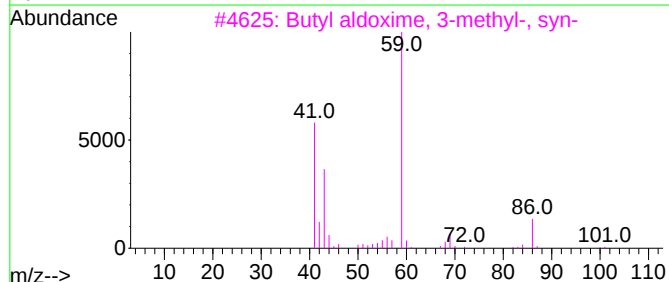
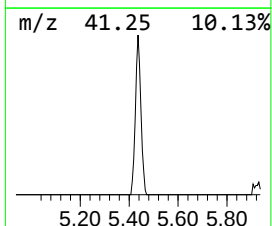
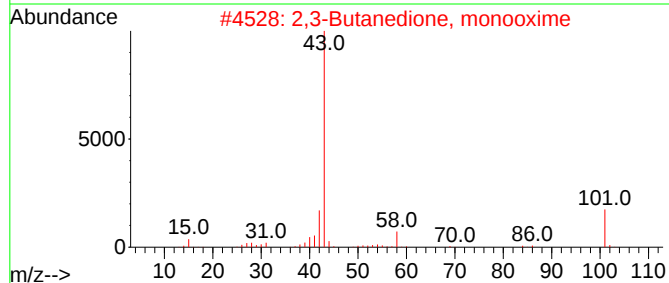
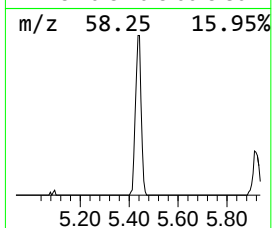
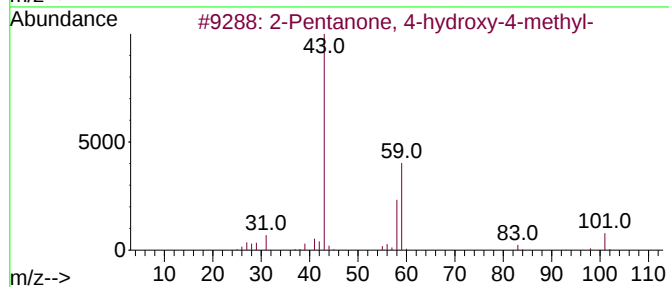
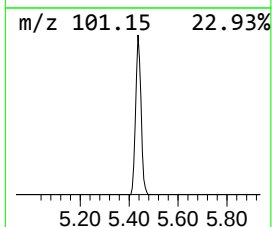
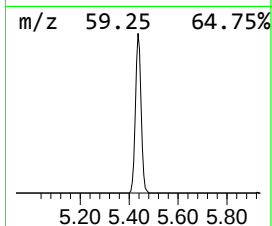
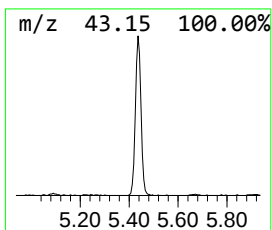
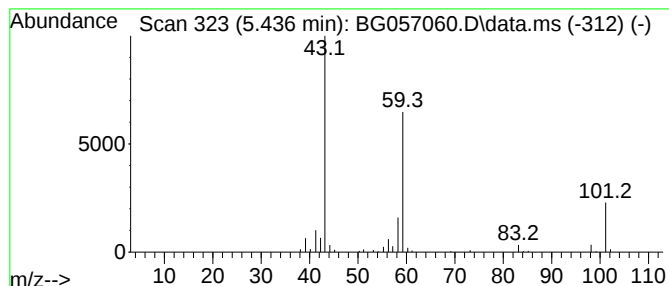
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.436	48.57 ng	233291	1,4-Dichlorobenzene-d4	8.409

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35		
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25		
4	1,2-Butanediol	90	C4H10O2	000584-03-2	17		
5	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	17		



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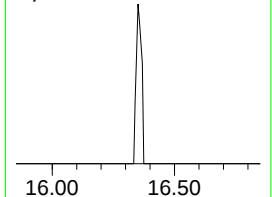
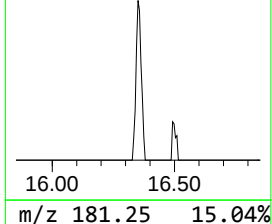
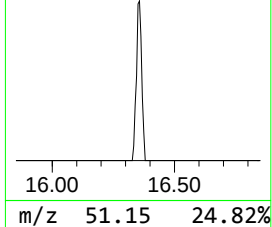
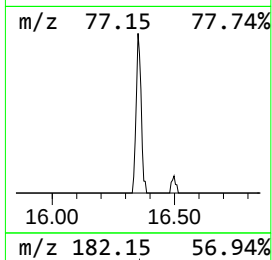
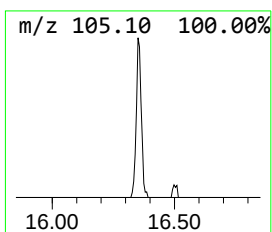
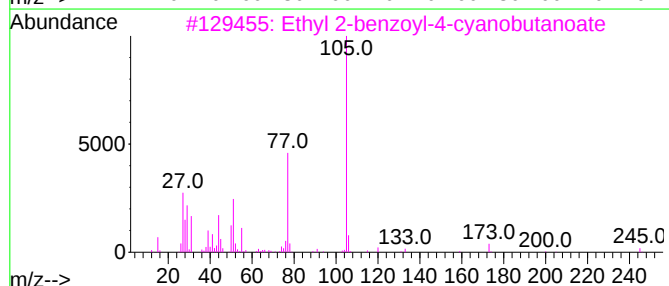
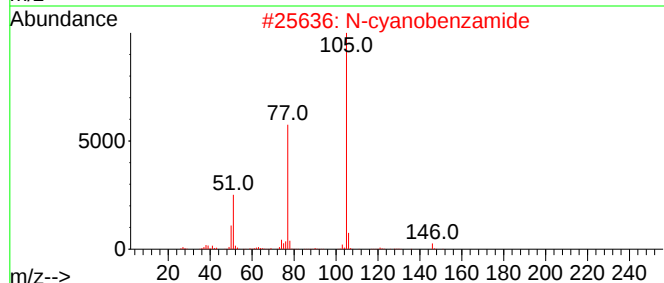
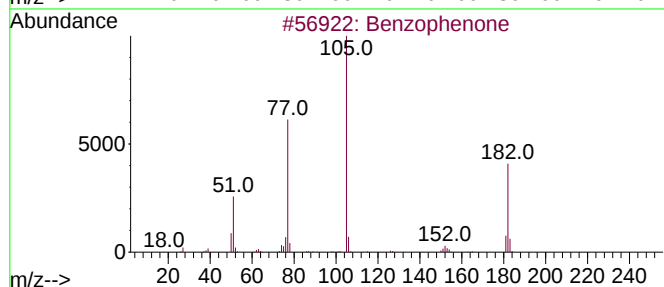
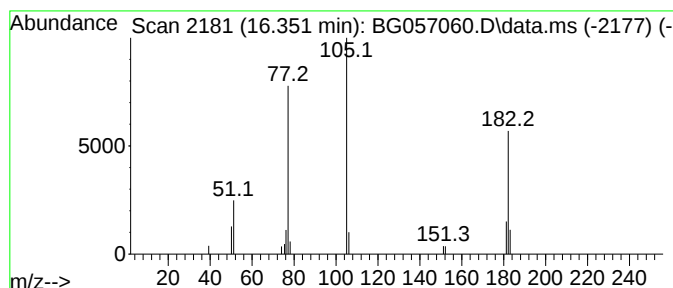
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Peak Number 2 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.351	2.53 ng	23283	Acenaphthene-d10	15.017

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	94
2			N-cyanobenzamide	146	C8H6N2O	015150-25-1	50
3			Ethyl 2-benzoyl-4-cyanobutanoate	245	C14H15N03	1000486-83-9	50
4			Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	50
5			Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	50



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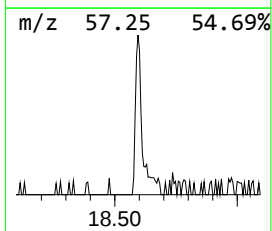
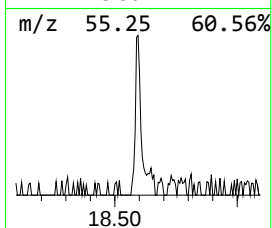
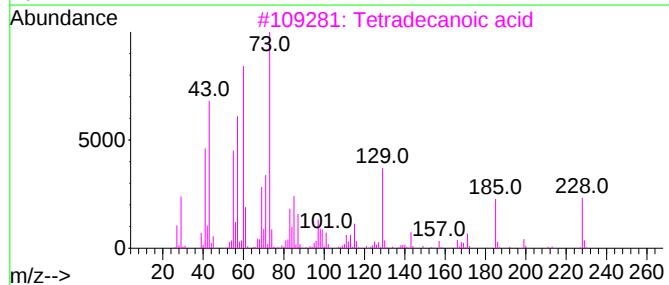
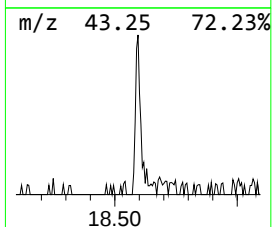
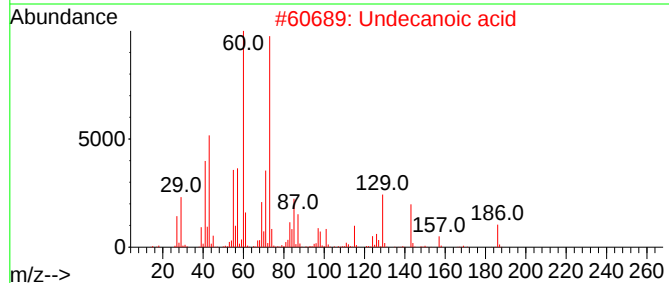
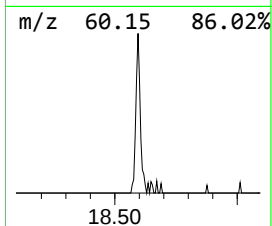
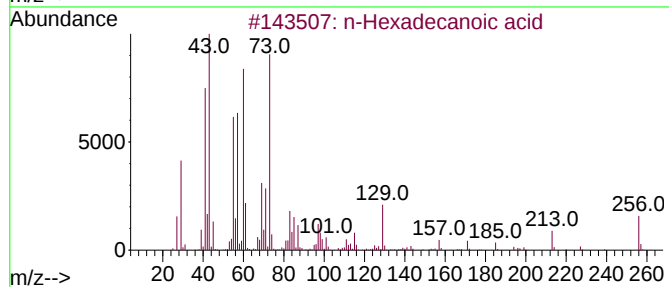
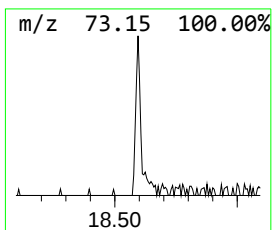
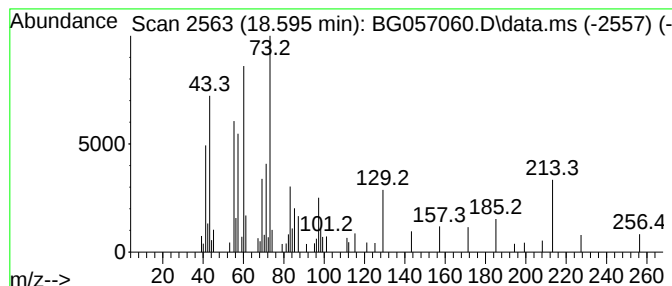
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.595	4.73 ng	53218	Phenanthrene-d10	17.755

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
2			Undecanoic acid	186	C11H22O2	000112-37-8	64
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4			n-Decanoic acid	172	C10H20O2	000334-48-5	50
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	46



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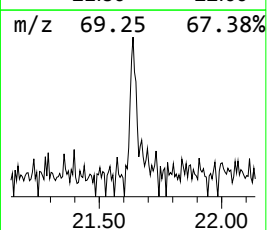
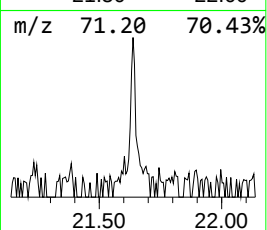
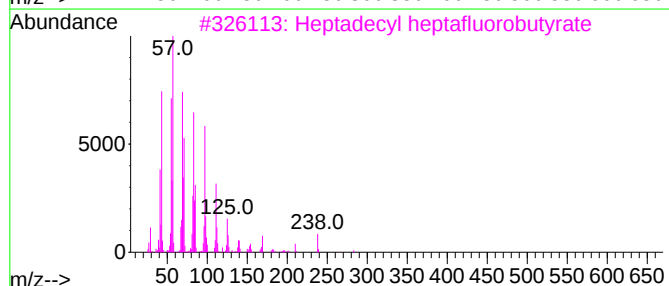
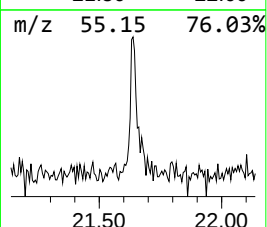
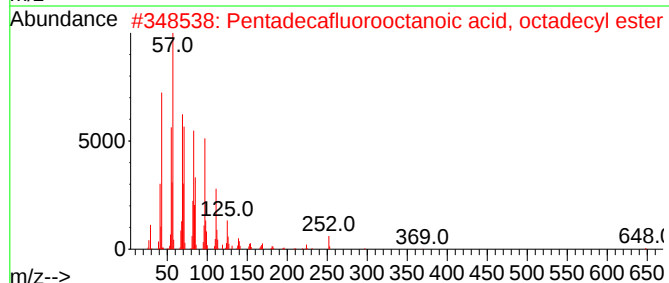
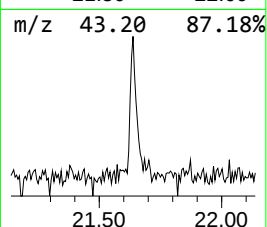
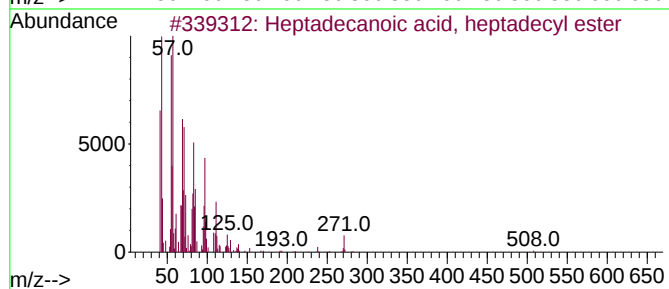
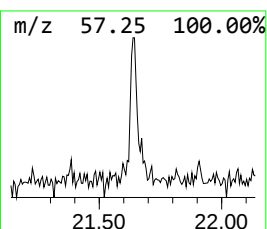
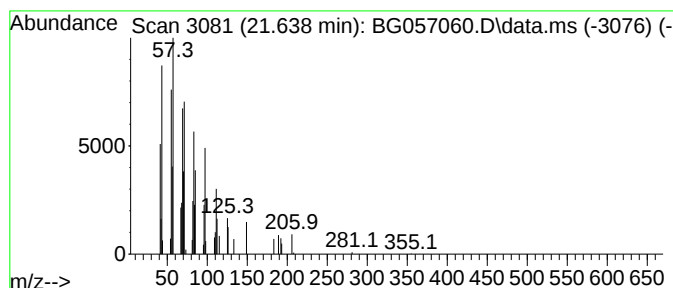
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Peak Number 4 Heptadecanoic acid, heptade... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.638	3.13 ng	39585	Chrysene-d12	22.078

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecanoic acid, heptadecyl e...	509	C34H68O2	036617-50-2	91
2			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	90
3			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	87
4			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	87
5			Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	76



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.436	48.6	ng	233291	1	8.409	96069	20.0
Benzophenone	16.351	2.5	ng	23283	3	15.017	184282	20.0
n-Hexadecanoic ...	18.595	4.7	ng	53218	4	17.755	225229	20.0
Heptadecanoic a...	21.638	3.1	ng	39585	5	22.078	253278	20.0