

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041223\
 Data File : BG057071.D
 Acq On : 12 Apr 2023 20:06
 Operator : CG/JU
 Sample : 02283-04
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 20230328-COMP-6

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: BG057071.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.435	317	323	330	rVB	43684	66708	5.68%	1.363%
2	5.917	398	405	414	rBV	272849	444152	37.80%	9.073%
3	7.538	673	681	697	rBB	279909	475820	40.49%	9.720%
4	8.407	823	829	836	rVB	50513	85581	7.28%	1.748%
5	9.582	1020	1029	1037	rBB	159186	285661	24.31%	5.835%
6	11.245	1305	1312	1320	rBV	64448	111998	9.53%	2.288%
7	13.641	1713	1720	1727	rVB	436643	674877	57.43%	13.786%
8	15.016	1948	1954	1961	rBV	108748	166355	14.16%	3.398%
9	16.349	2177	2181	2187	rBV	25101	35747	3.04%	0.730%
10	16.496	2199	2206	2215	rBV	373734	566875	48.24%	11.580%
11	17.753	2412	2420	2427	rBV2	145915	222421	18.93%	4.544%
12	18.593	2559	2563	2570	rBV2	24769	33491	2.85%	0.684%
13	20.326	2852	2858	2864	rBV	934778	1175088	100.00%	24.005%
14	21.636	3076	3081	3088	rBV5	26799	43725	3.72%	0.893%
15	22.071	3149	3155	3161	rBV	137890	234499	19.96%	4.790%
16	23.851	3454	3458	3465	rVB4	16159	28889	2.46%	0.590%
17	25.607	3747	3757	3771	rVB2	79871	243351	20.71%	4.971%

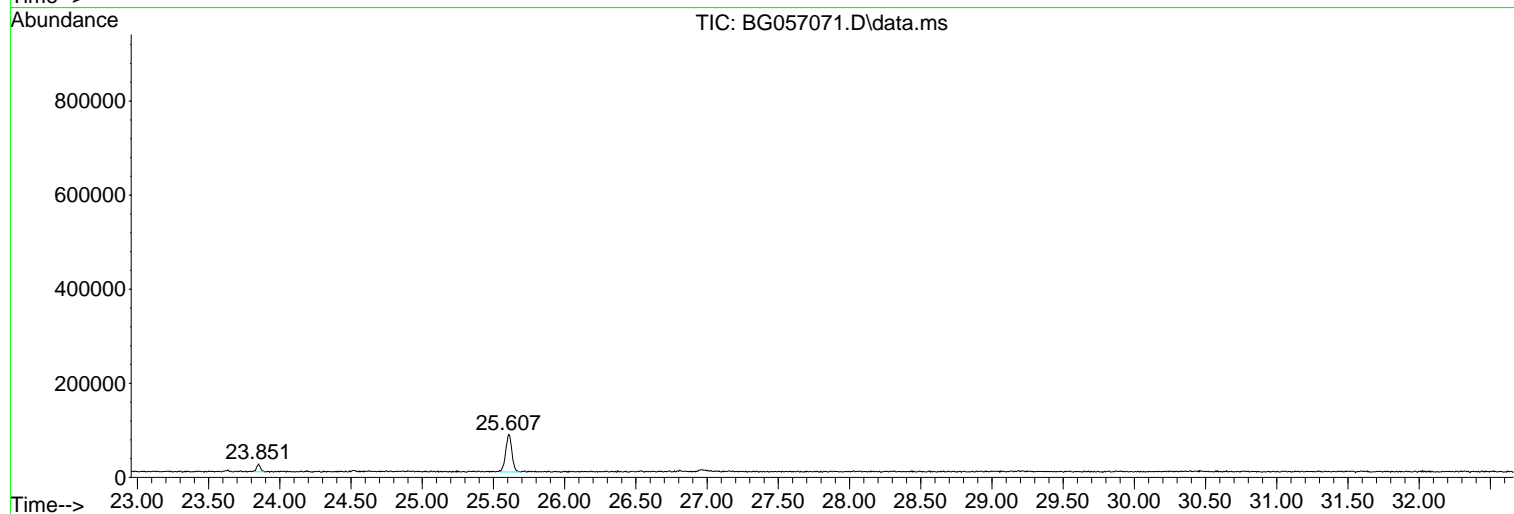
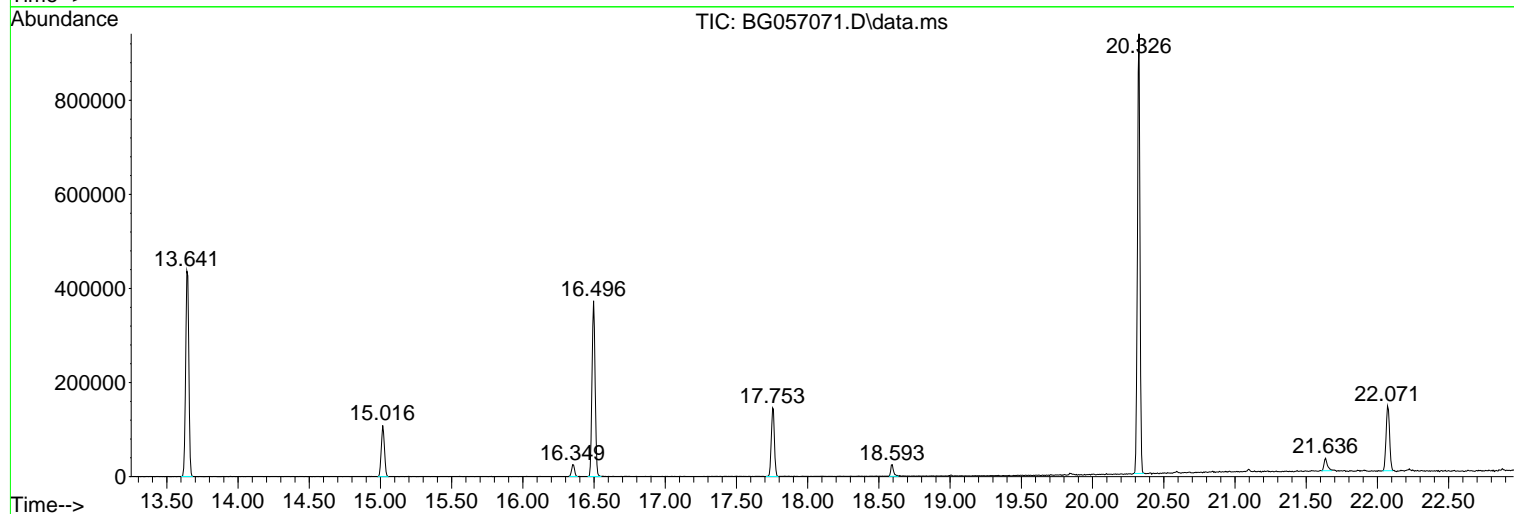
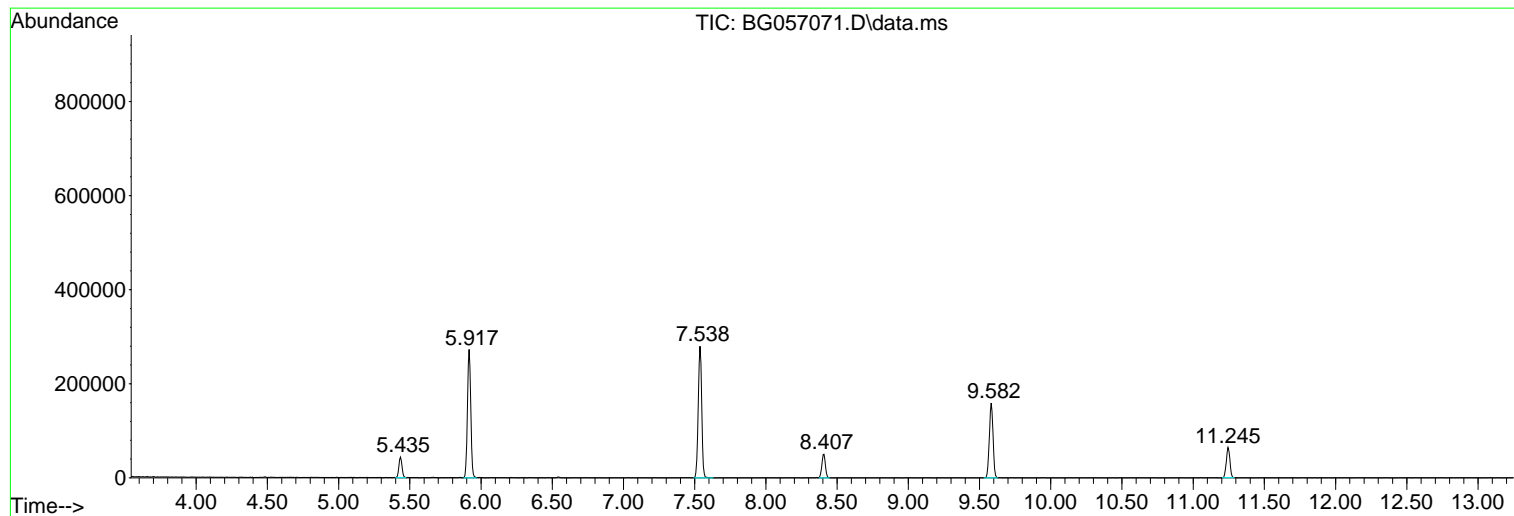
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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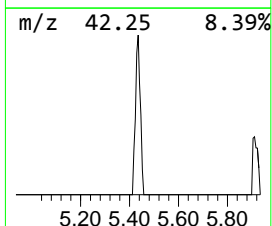
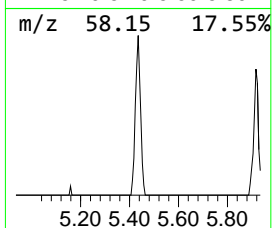
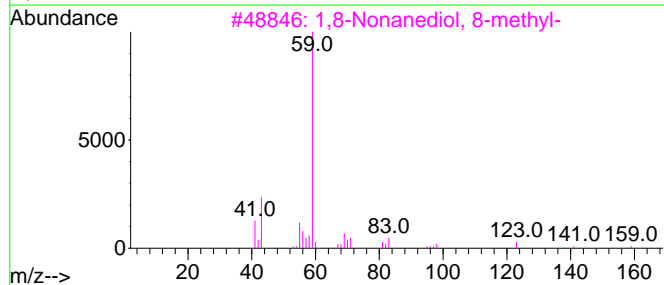
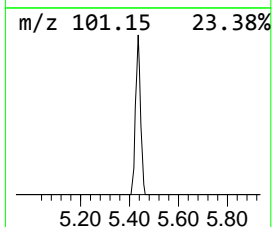
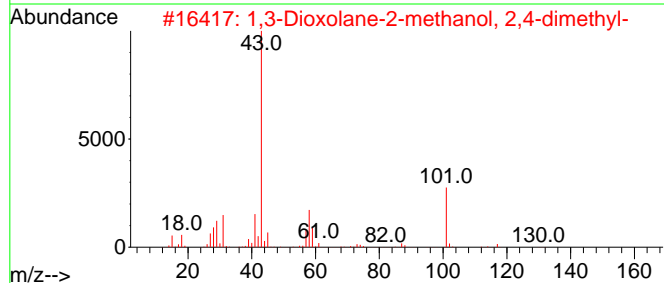
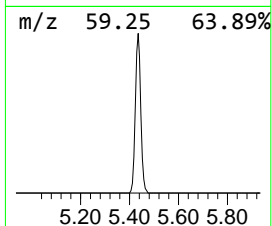
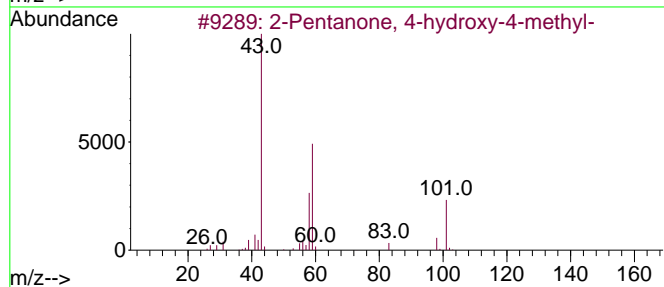
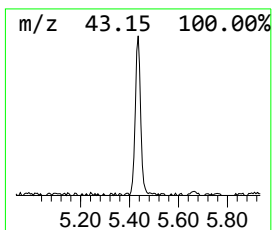
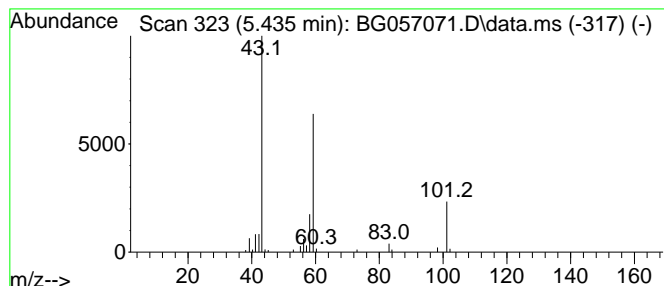
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.435	15.59 ng	66708	1,4-Dichlorobenzene-d4	8.407

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	25
3		1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	17
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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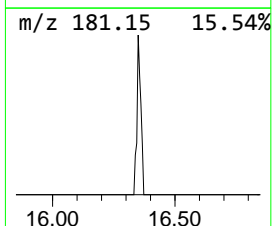
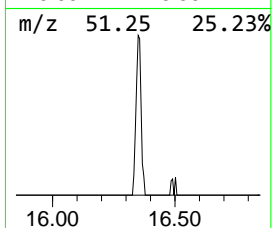
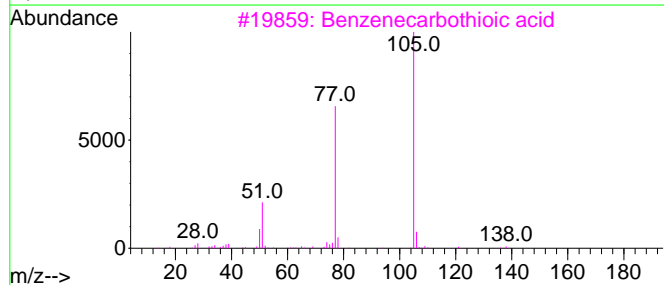
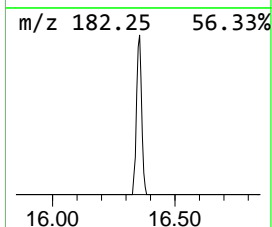
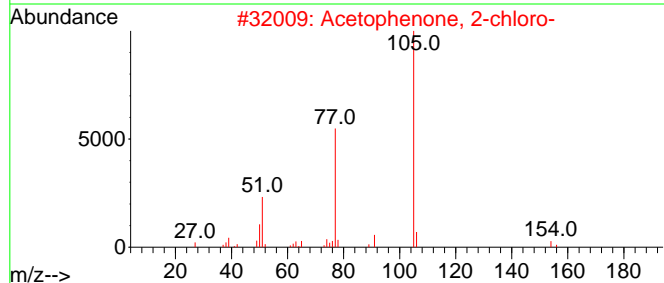
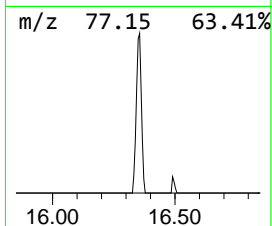
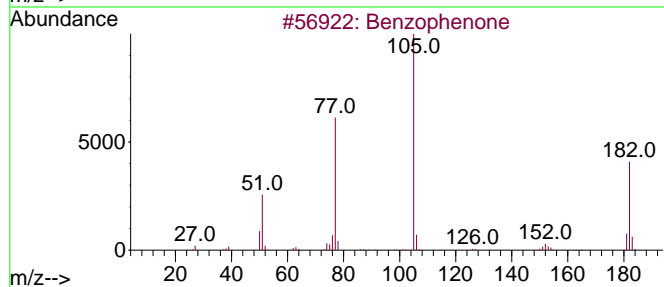
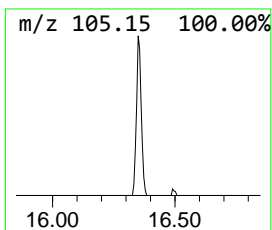
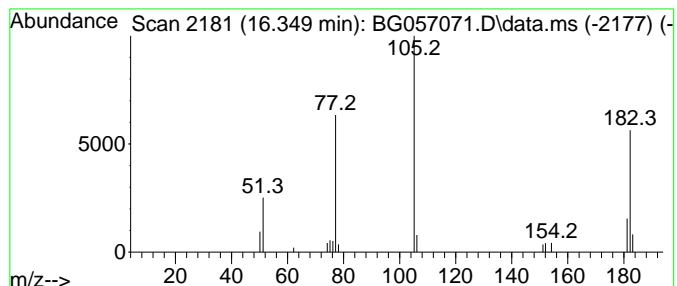
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 2 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.349	4.30 ng	35747	Acenaphthene-d10	15.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	91
2			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
3			Benzenecarbothioic acid	138	C7H6OS	000098-91-9	43
4			Ethanone, 2-bromo-1-phenyl-	198	C8H7BrO	000070-11-1	43
5			Benzoic acid, phenyl ester	198	C13H10O2	000093-99-2	43



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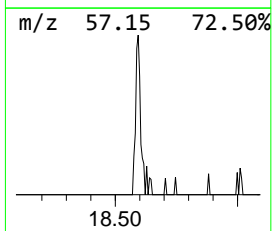
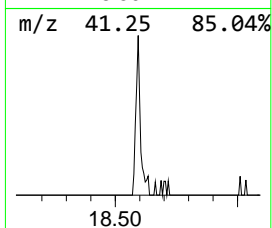
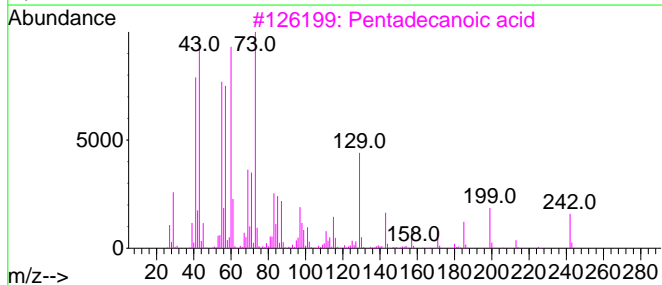
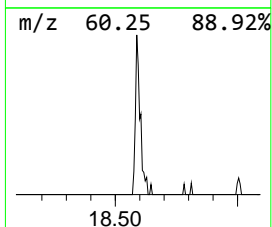
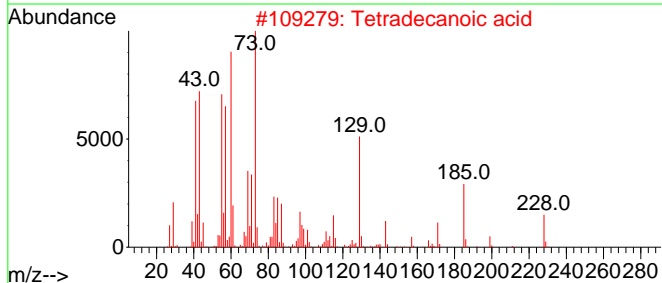
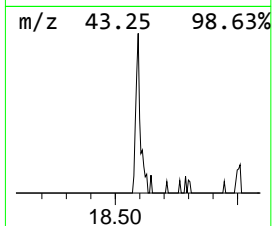
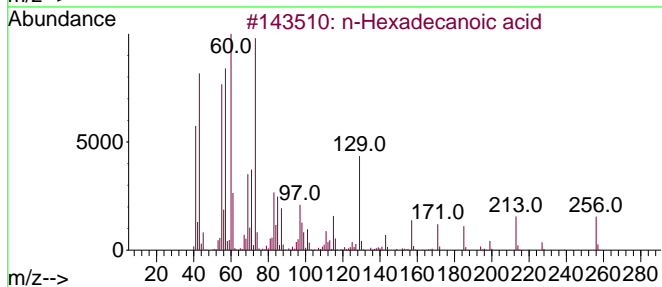
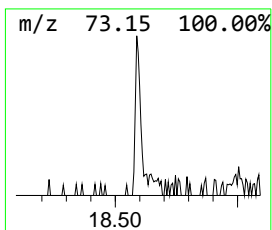
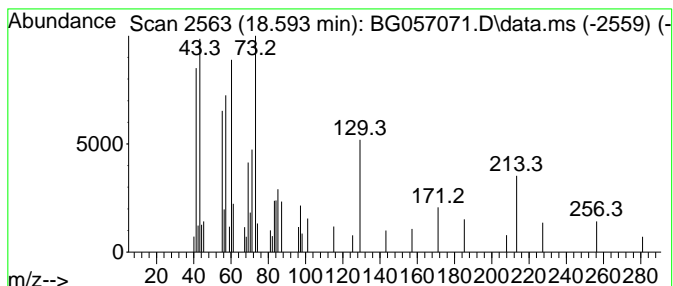
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TIC Library : C:\Database\NIST20.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.593	3.01 ng	33491	Phenanthrene-d10	17.753

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	64
4		1-Phenazincarboxylic acid, 6-[1...	506	C31H42N2O4	120464-92-8	50
5		Estra-1,3,5(10)-trien-17.β. -ol	256	C18H24O	002529-64-8	25



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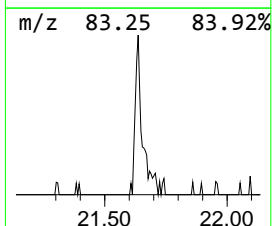
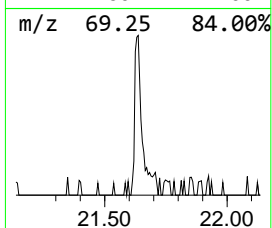
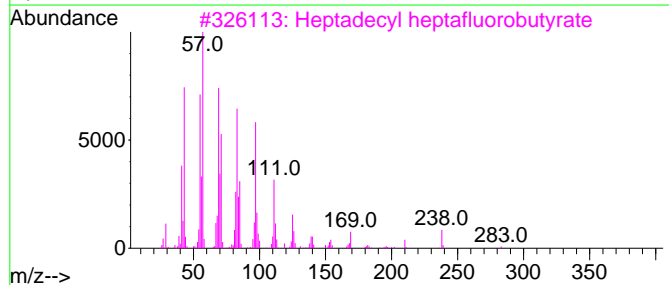
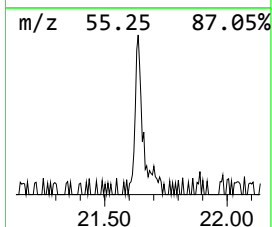
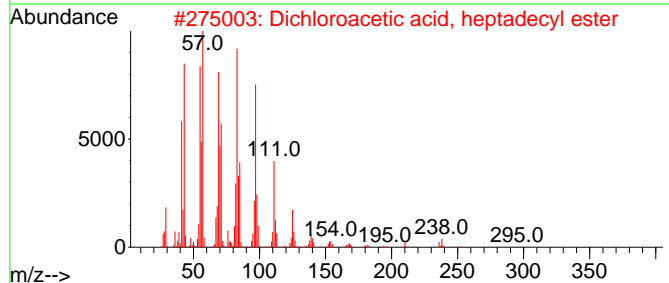
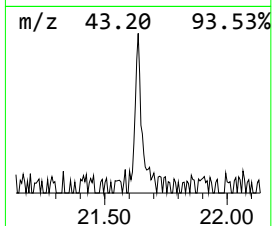
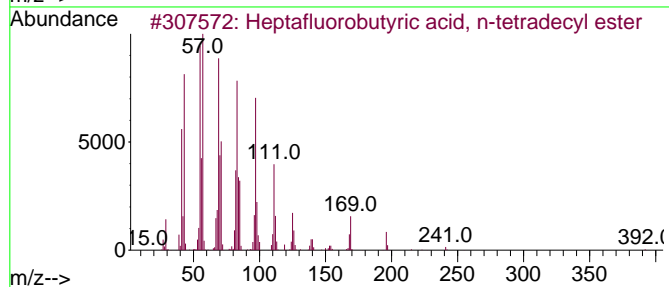
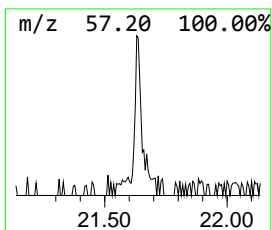
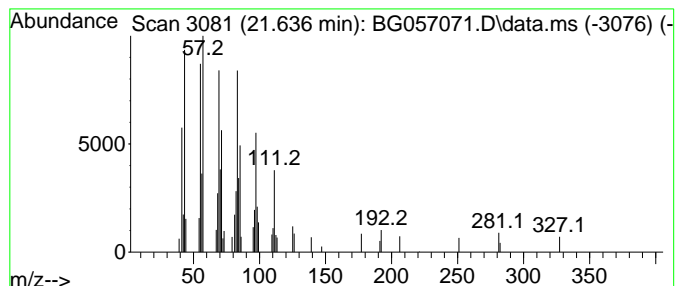
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TIC Library : C:\Database\NIST0.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 4 Heptafluorobutyric acid, n-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.636	3.73 ng	43725	Chrysene-d12	22.071

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	90
2			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	90
3			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	87
4			n-Tetracosanol-1	354	C24H50O	000506-51-4	87
5			1-Heneicosyl formate	340	C22H44O2	077899-03-7	86



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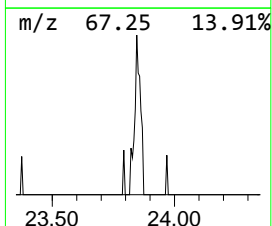
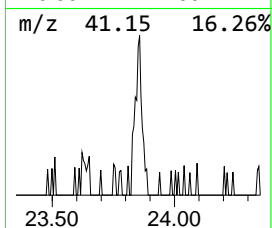
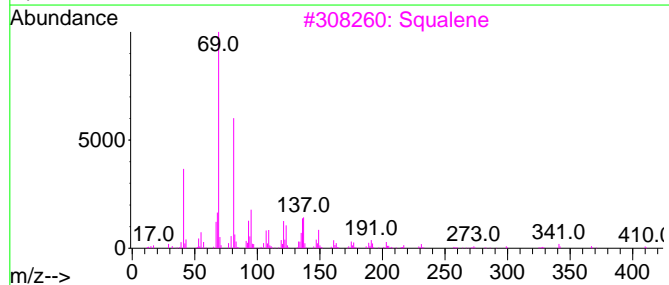
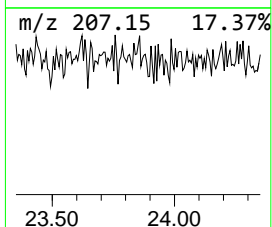
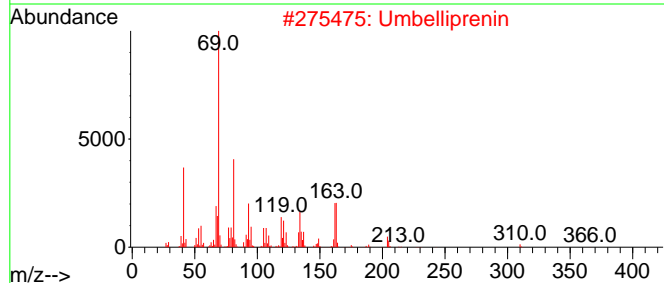
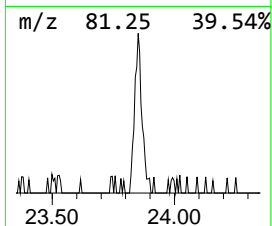
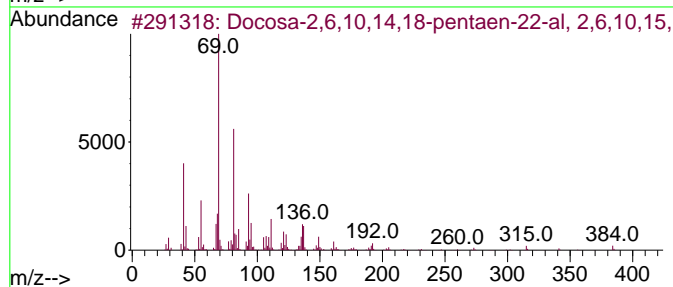
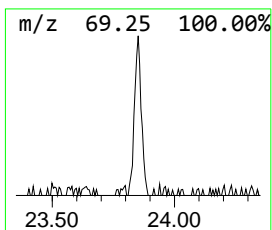
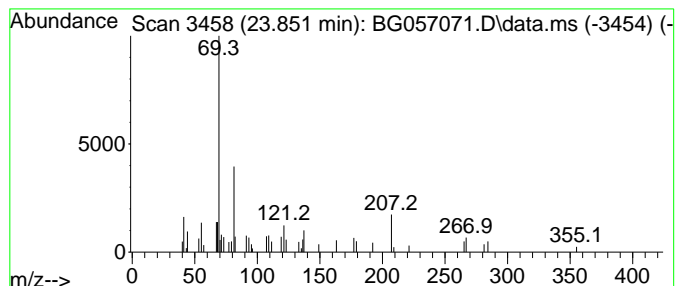
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TIC Library : C:\Database\NIST20.L
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 Peak Number 5 unknown23.851 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.851	2.37 ng	28889	Perylene-d12	25.608

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	45
2			Umbelliprenin	366	C24H30O3	023838-17-7	42
3			Squalene	410	C30H50	000111-02-4	42
4			2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	42
5			Supraene	410	C30H50	007683-64-9	42



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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-...	5.435	15.6	ng	66708	1	8.407	85581	20.0
Benzophenone	16.349	4.3	ng	35747	3	15.016	166355	20.0
n-Hexadecanoic ...	18.593	3.0	ng	33491	4	17.753	222421	20.0
Heptafluorobuty...	21.636	3.7	ng	43725	5	22.071	234499	20.0
unknown23.851	23.851	2.4	ng	28889	6	25.608	243351	20.0