

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041423\
 Data File : BG057103.D
 Acq On : 14 Apr 2023 17:05
 Operator : CG/JU
 Sample : 02347-06
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 20230332-COMP-10

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: BG057103.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.430	314	322	331	rBV	93615	152378	12.66%	2.269%
2	5.917	397	405	418	rVB	436525	704738	58.54%	10.492%
3	7.539	673	681	690	rBV	440636	774113	64.30%	11.525%
4	8.402	822	828	834	rBV	74180	121139	10.06%	1.803%
5	9.583	1021	1029	1037	rBV	254869	463223	38.48%	6.896%
6	11.239	1305	1311	1319	rBV	93918	171858	14.28%	2.559%
7	13.642	1713	1720	1728	rBV	631579	944946	78.49%	14.068%
8	15.017	1947	1954	1961	rVB	151205	236879	19.68%	3.527%
9	16.350	2175	2181	2188	rVB	83417	116929	9.71%	1.741%
10	16.497	2199	2206	2216	rBV	553899	844086	70.11%	12.566%
11	17.754	2413	2420	2426	rBV	186392	280658	23.31%	4.178%
12	18.588	2557	2562	2572	rBV2	40984	58028	4.82%	0.864%
13	20.321	2851	2857	2863	rBV	957587	1203883	100.00%	17.923%
14	21.631	3076	3080	3089	rBV4	27497	47765	3.97%	0.711%
15	22.072	3148	3155	3162	rVB2	160975	285307	23.70%	4.247%
16	25.602	3744	3756	3769	rVB	91593	293519	24.38%	4.370%
17	26.801	3954	3960	3966	rVB7	7765	17632	1.46%	0.262%

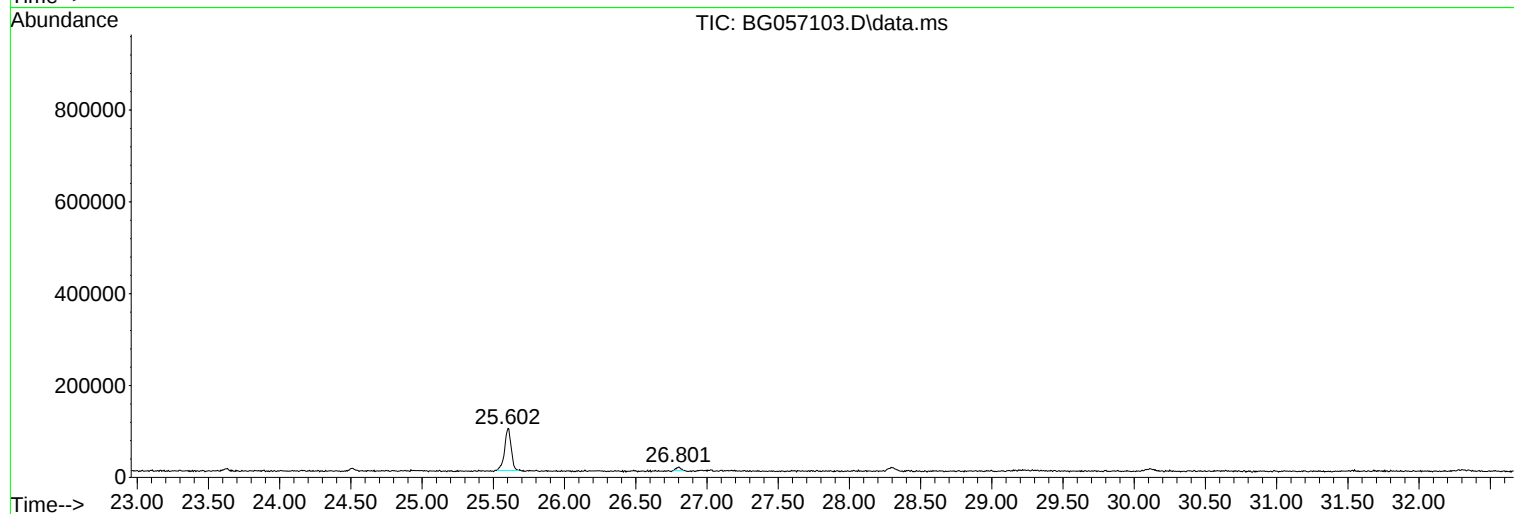
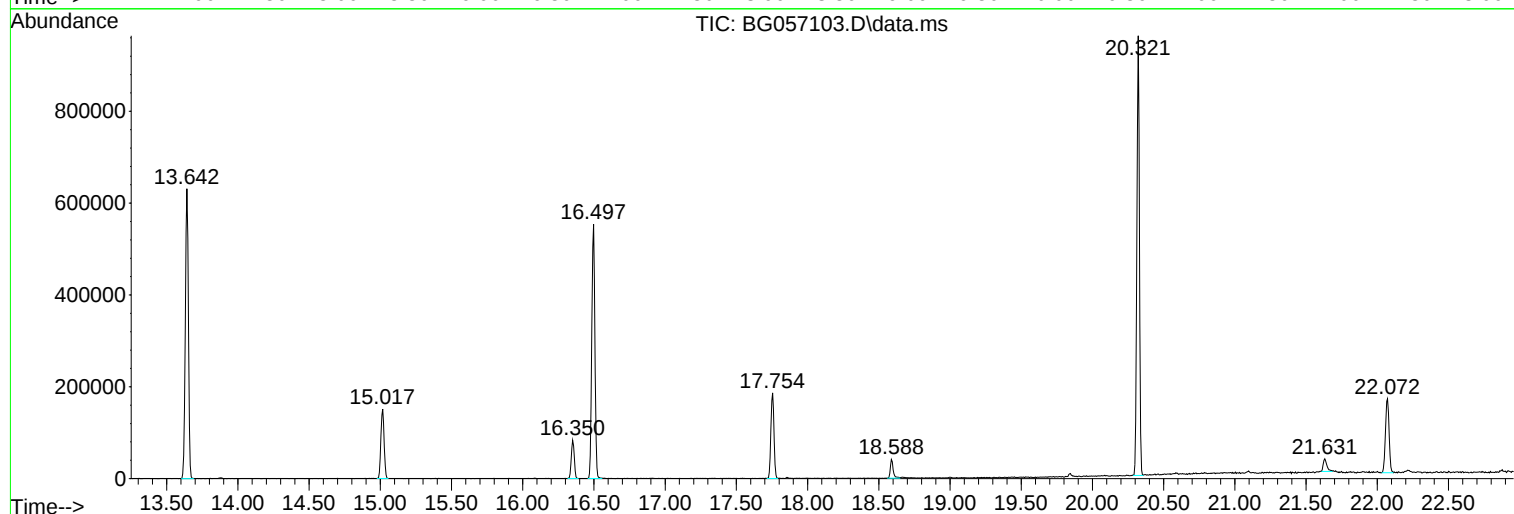
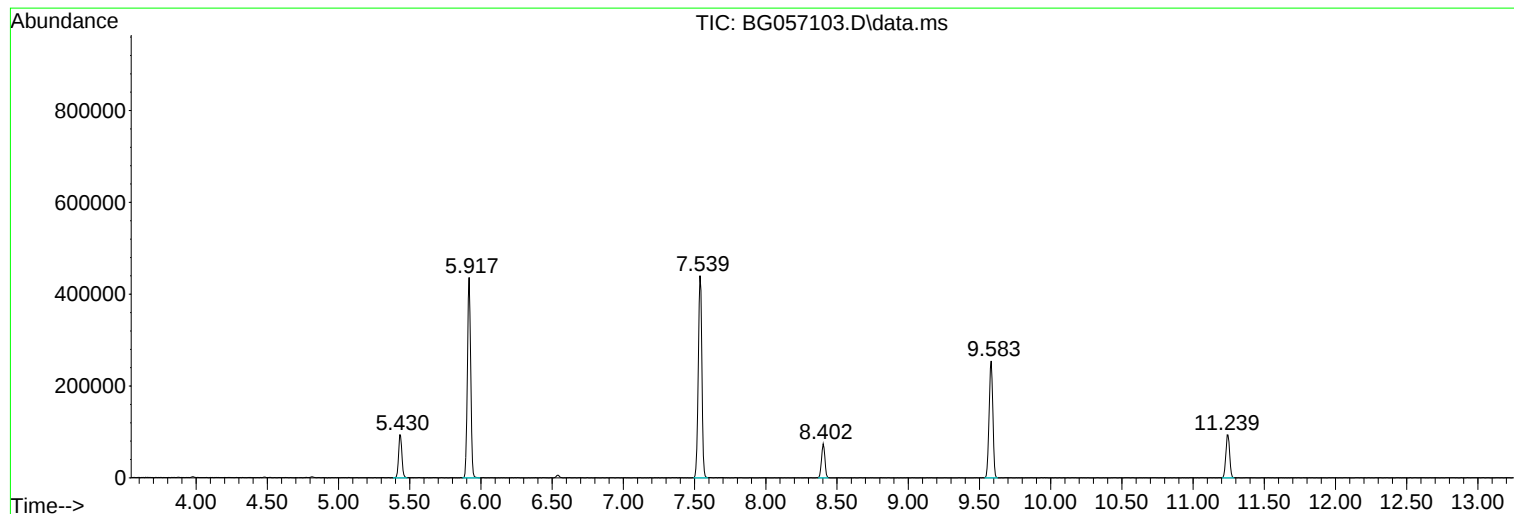
Sum of corrected areas: 6717081

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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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ALS Vial : 11 Sample Multiplier: 1

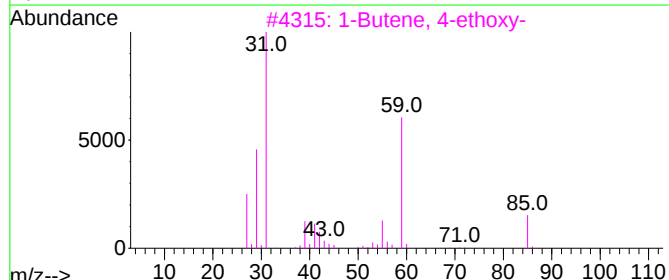
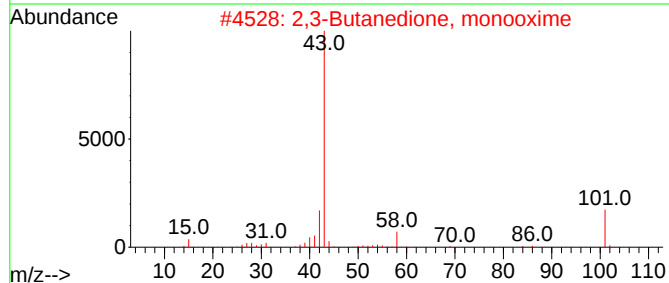
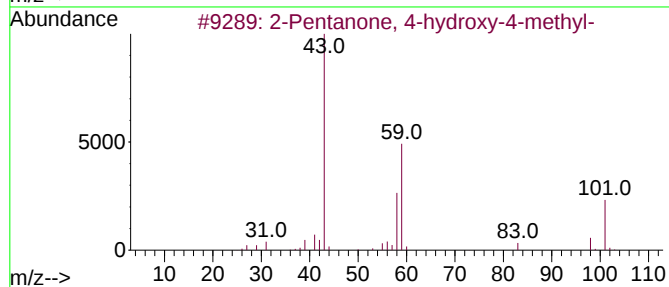
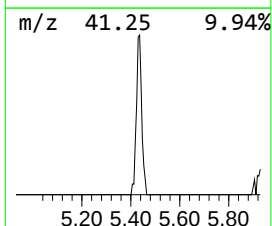
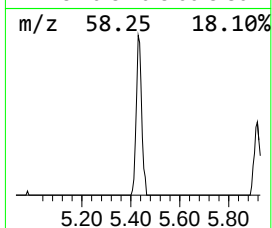
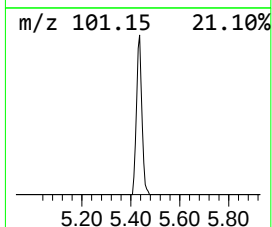
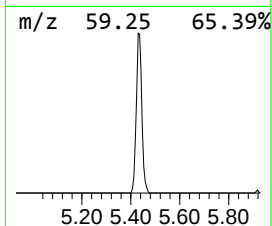
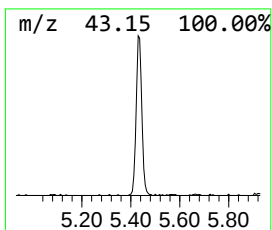
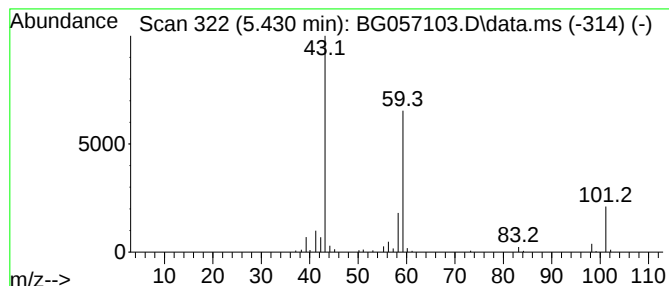
Instrument :
BNA_G
ClientSampleId :
20230332-COMP-10

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.	
5.430	25.16 ng	152378	1,4-Dichlorobenzene-d4	8.402	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	1-Butene, 4-ethoxy-	100	C6H12O	044611-46-3	17
4	Acetone	58	C3H6O	000067-64-1	10
5	Propanenitrile, 3-ethoxy-	99	C5H9NO	002141-62-0	9



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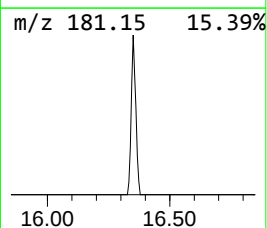
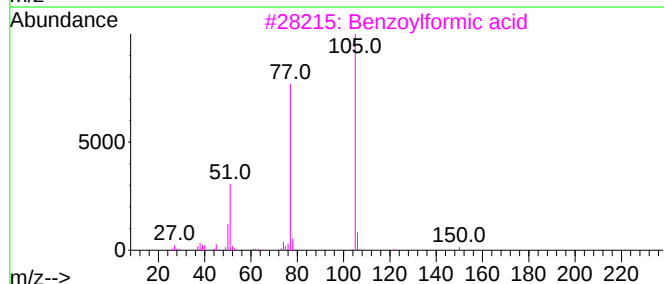
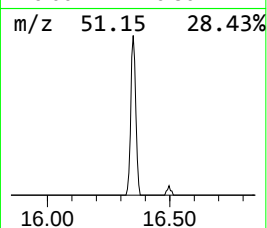
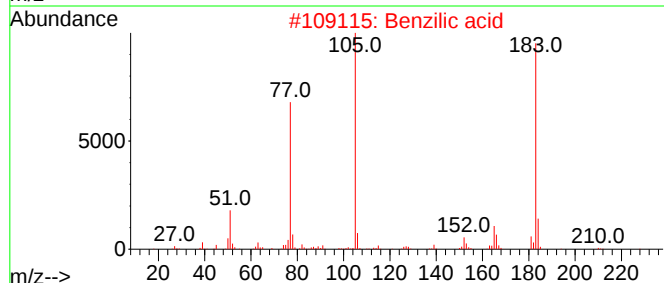
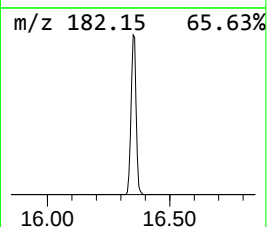
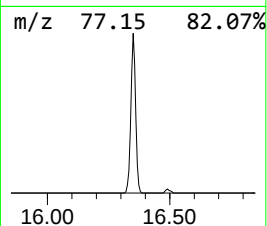
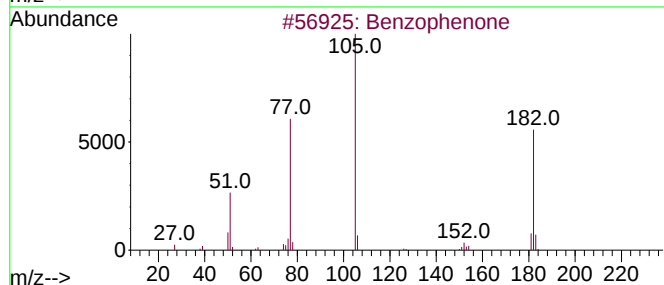
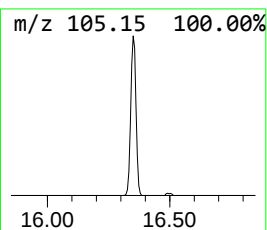
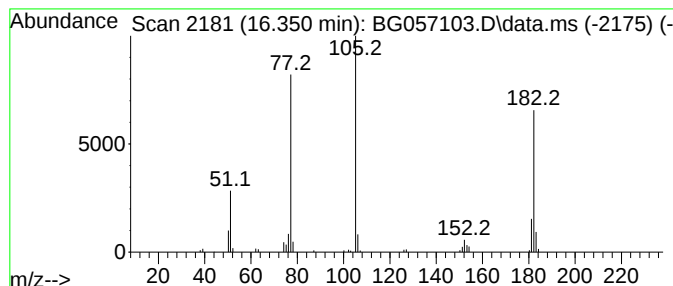
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.350	9.87 ng	116929	Acenaphthene-d10	15.017

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzilic acid	228	C14H12O3	000076-93-7	59
3			Benzoylformic acid	150	C8H6O3	000611-73-4	50
4			N-Methylbenzamide, N-pentafluoro...	281	C11H8F5NO2	1000446-98-1	50
5			N-(1-Cyanovinyl)benzamide	172	C10H8N2O	1000186-19-1	50



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Instrument :
BNA_G
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20230332-COMP-10

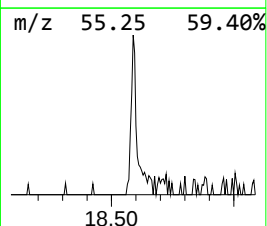
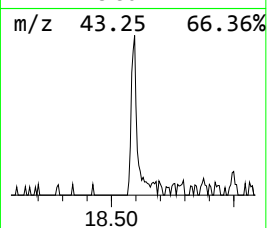
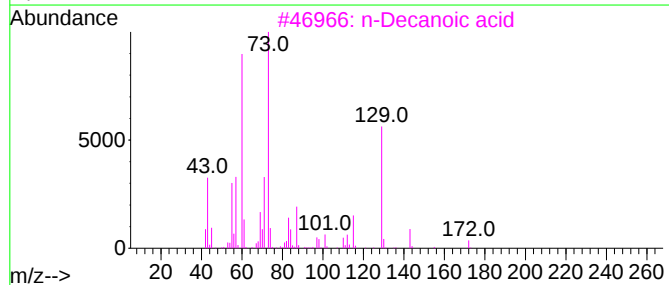
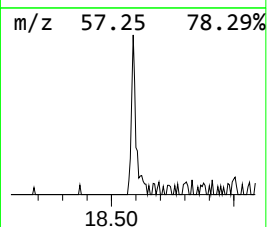
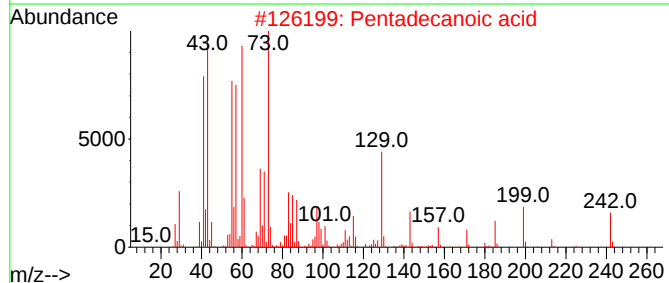
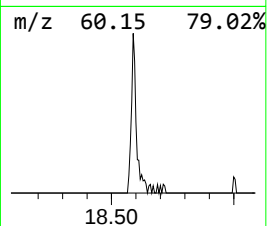
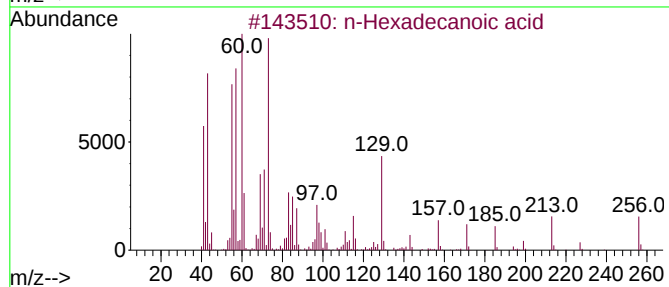
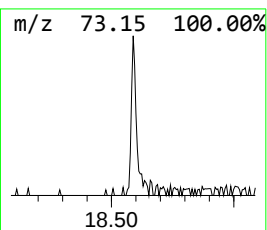
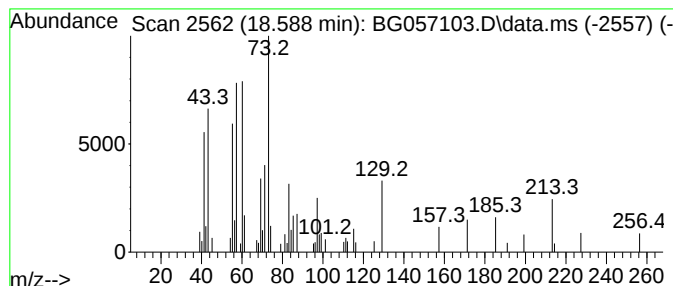
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TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.588	4.14 ng	58028	Phenanthrene-d10	17.754

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	92
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	62
3			n-Decanoic acid	172	C10H20O2	000334-48-5	53
4			Tridecanoic acid	214	C13H26O2	000638-53-9	53
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	53



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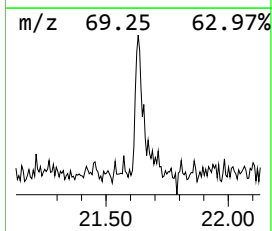
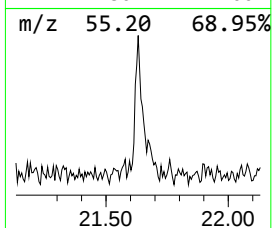
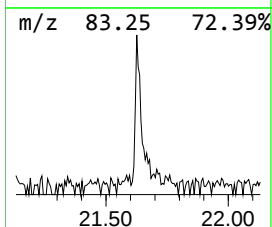
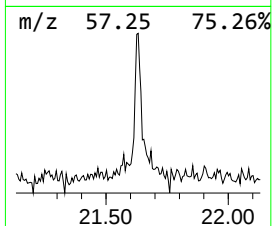
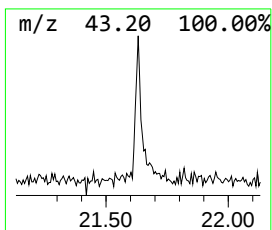
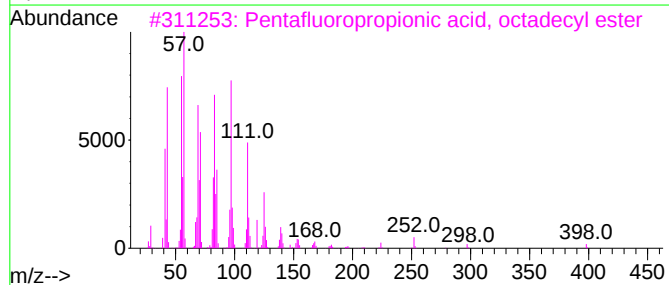
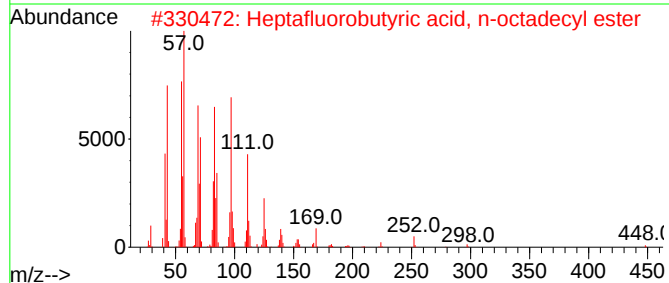
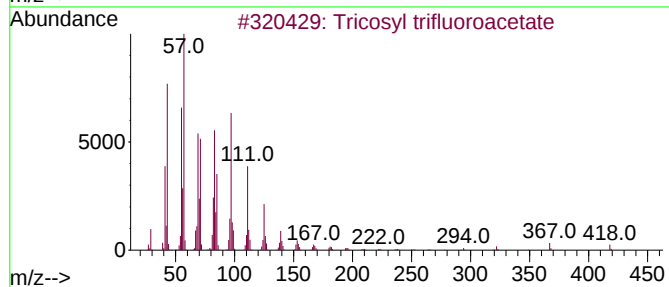
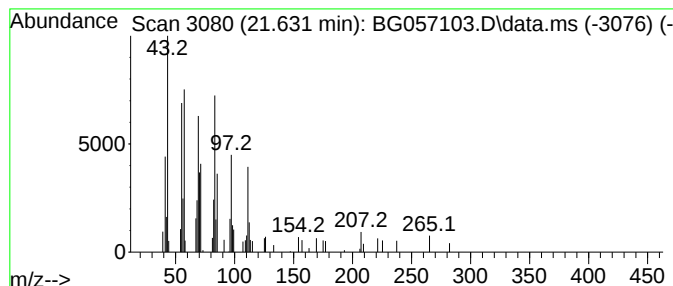
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Tricosyl trifluoroacetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.631	3.35 ng	47765	Chrysene-d12	22.072

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	87
2			Heptafluorobutyric acid, n-octadecyl ester	466	C22H37F7O2	000400-57-7	83
3			Pentafluoropropionic acid, octadecyl ester	416	C21H37F5O2	959261-25-7	83
4			Eicosyl heptafluorobutyrate	494	C24H41F7O2	1000351-83-5	83
5			Tricosyl pentafluoropropionate	486	C26H47F5O2	1000351-81-0	83



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.430	25.2	ng	152378	1	8.402	121139	20.0
Benzophenone	16.350	9.9	ng	116929	3	15.017	236879	20.0
n-Hexadecanoic ...	18.588	4.1	ng	58028	4	17.754	280658	20.0
Tricosyl triflu...	21.631	3.4	ng	47765	5	22.072	285307	20.0