

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041223\
 Data File : BG057074.D
 Acq On : 12 Apr 2023 22:17
 Operator : CG/JU
 Sample : 02283-01
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 20230323-COMP-1

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: BG057074.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	332	rBV	42299	67278	4.72%	1.075%
2	5.917	398	405	414	rBV	380016	617496	43.34%	9.863%
3	7.538	673	681	690	rBV	384074	658163	46.20%	10.512%
4	8.408	819	829	835	rBV	55458	93749	6.58%	1.497%
5	9.583	1020	1029	1036	rBV	220640	389404	27.33%	6.220%
6	11.245	1304	1312	1319	rBV	71610	126822	8.90%	2.026%
7	13.642	1714	1720	1727	rBV	585936	891062	62.54%	14.232%
8	15.016	1948	1954	1961	rBV	118874	182145	12.78%	2.909%
9	16.356	2173	2182	2187	rBV	39193	57665	4.05%	0.921%
10	16.497	2199	2206	2217	rBV	526504	790125	55.46%	12.620%
11	17.754	2413	2420	2426	rBV	159202	236083	16.57%	3.771%
12	18.594	2558	2563	2569	rBV	49618	70438	4.94%	1.125%
13	20.327	2852	2858	2863	rVB	1098026	1424708	100.00%	22.755%
14	21.631	3075	3080	3091	rBV6	31471	61876	4.34%	0.988%
15	22.072	3148	3155	3161	rBV2	149404	257676	18.09%	4.116%
16	23.851	3450	3458	3464	rVB2	44765	88975	6.25%	1.421%
17	25.602	3747	3756	3766	rVB3	82903	247340	17.36%	3.950%

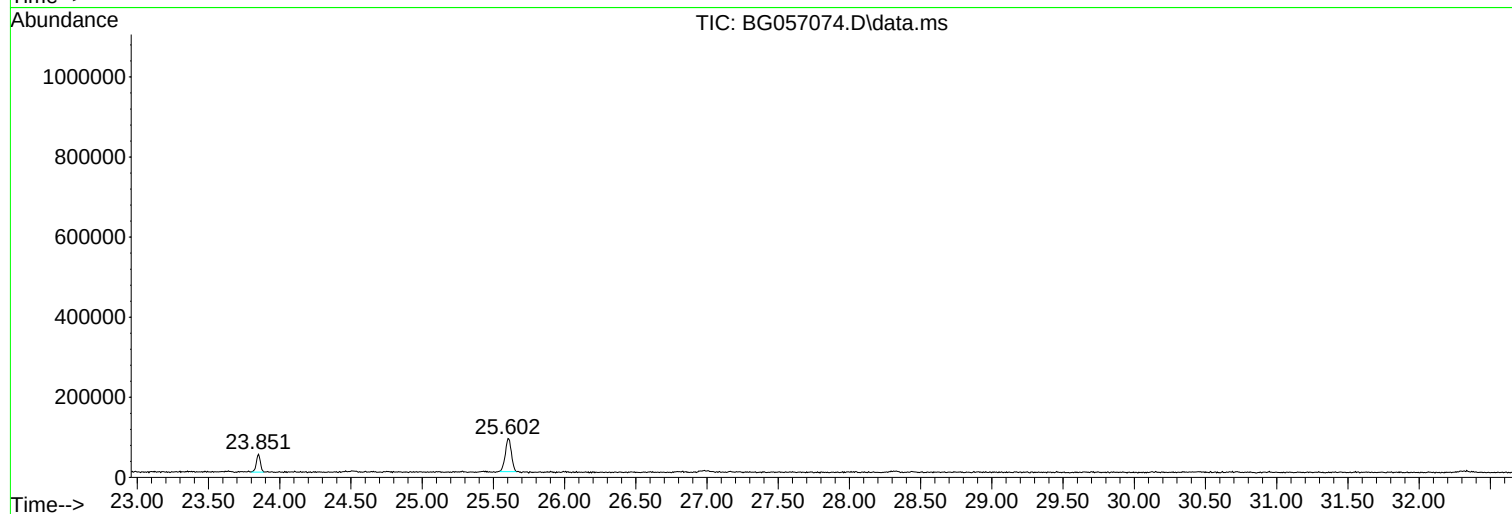
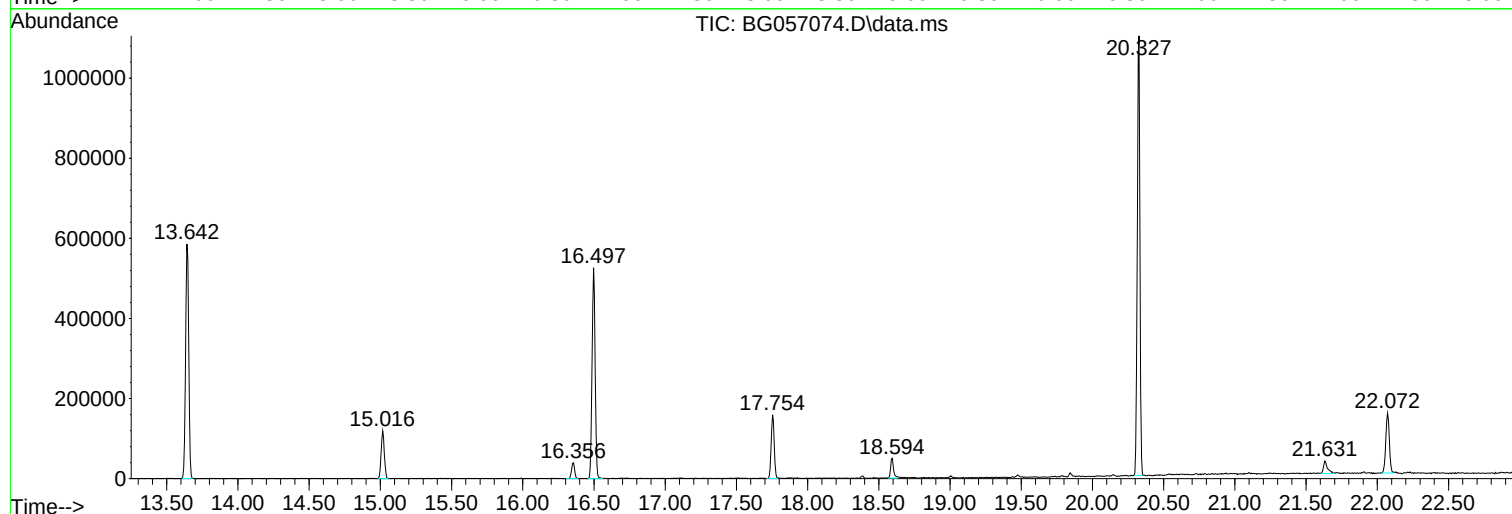
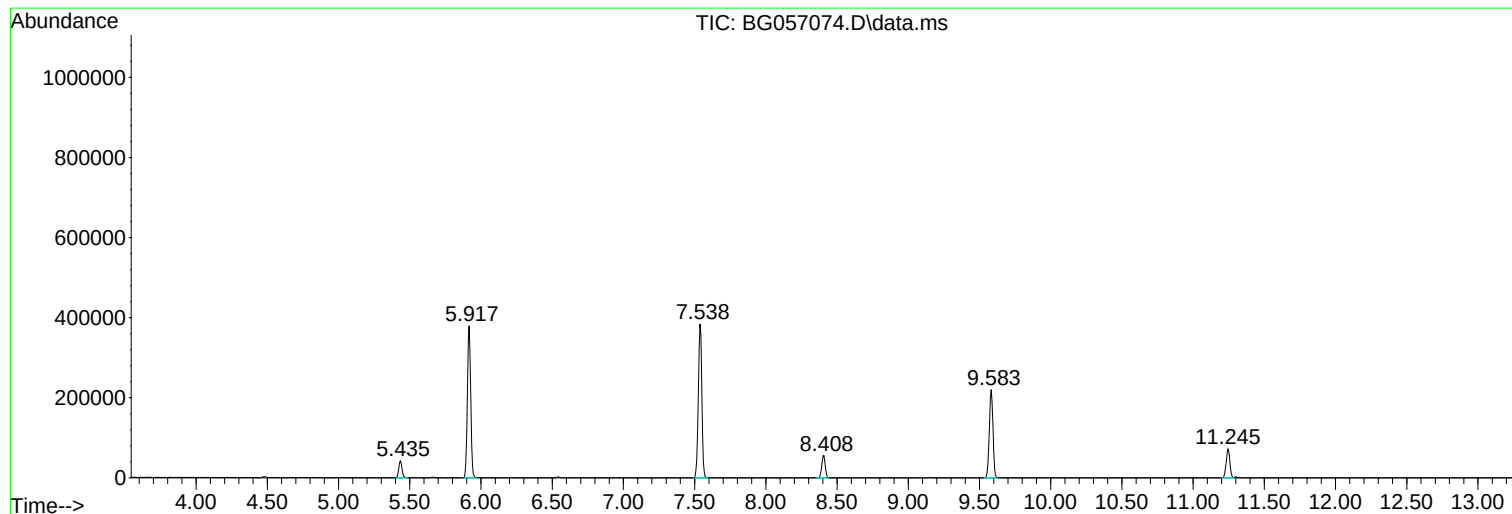
Sum of corrected areas: 6261005

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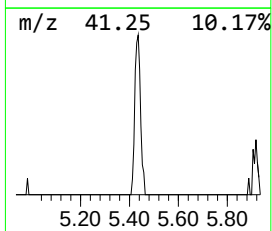
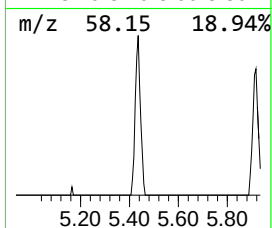
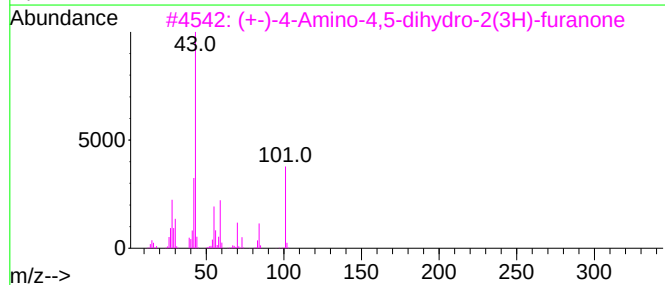
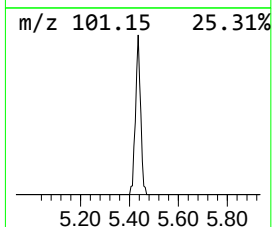
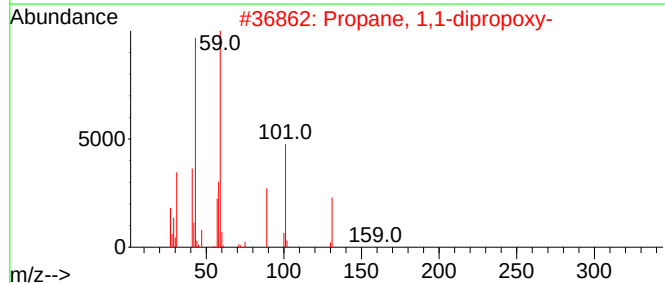
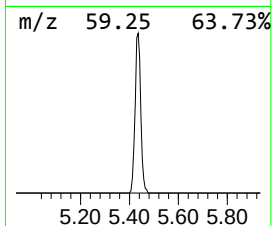
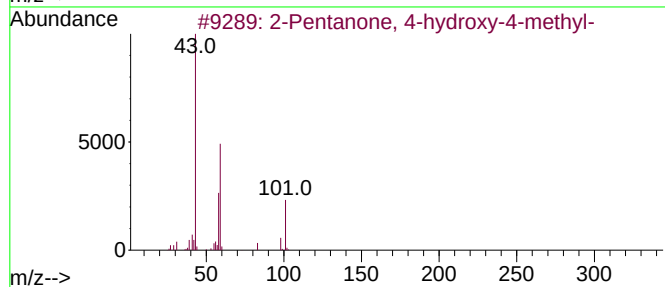
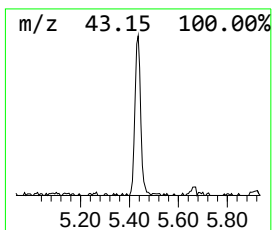
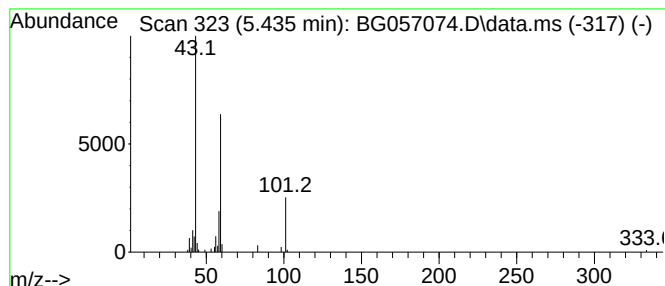
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	14.35 ng	67278	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	50		
2	Propane, 1,1-dipropoxy-	160	C9H20O2	004744-11-0	45		
3	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	38		
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	38		
5	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	28		



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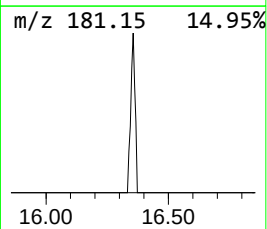
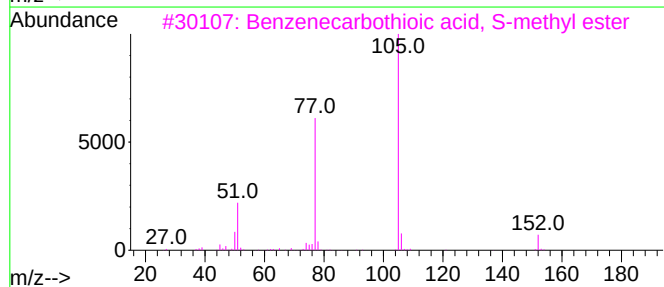
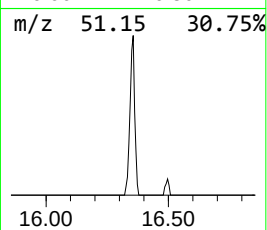
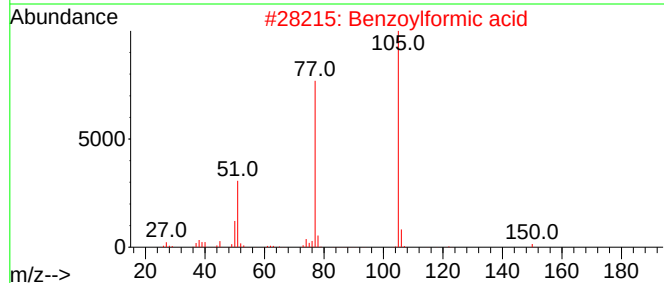
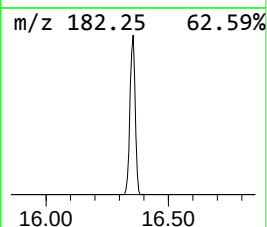
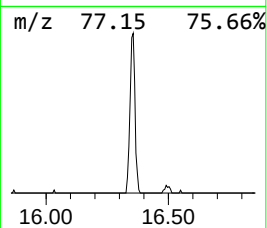
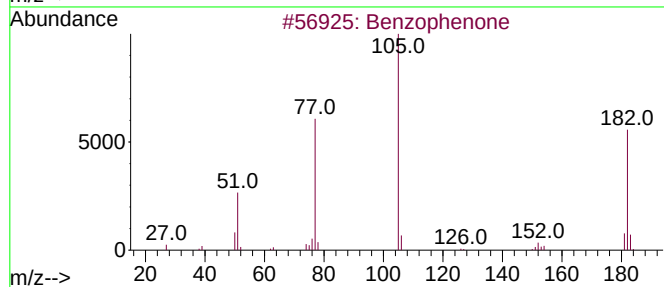
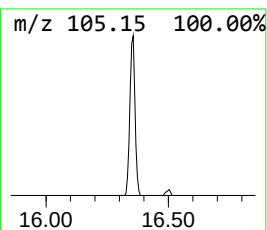
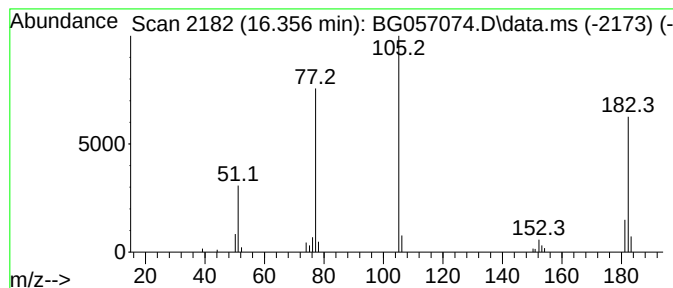
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.356	6.33 ng	57665	Acenaphthene-d10	15.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzoylformic acid	150	C8H6O3	000611-73-4	52
3			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	52
4			1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	50
5			Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	50



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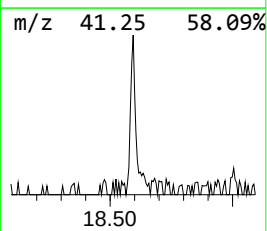
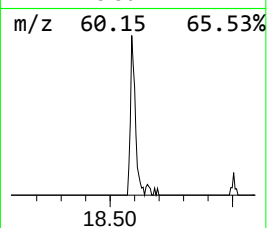
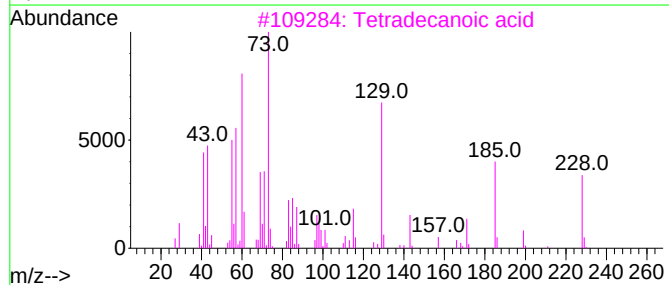
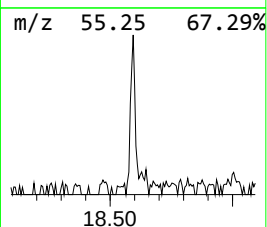
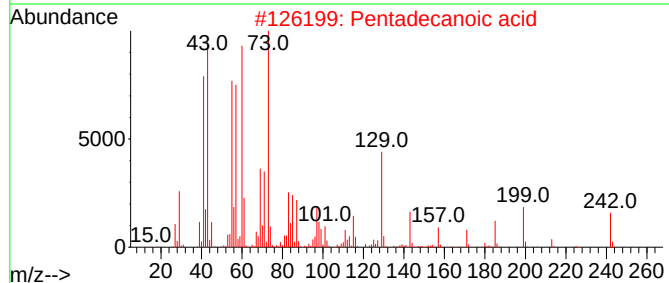
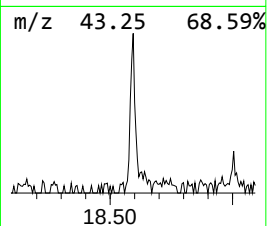
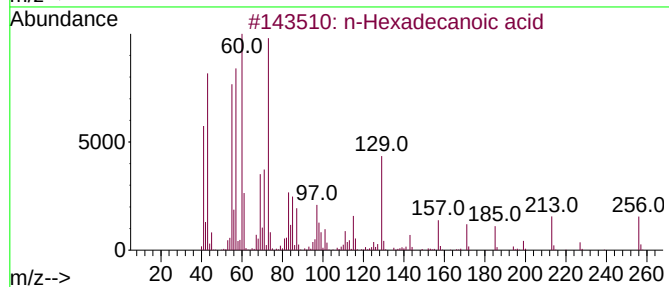
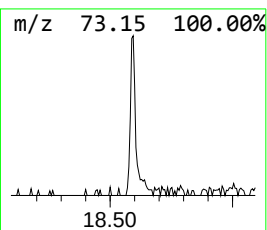
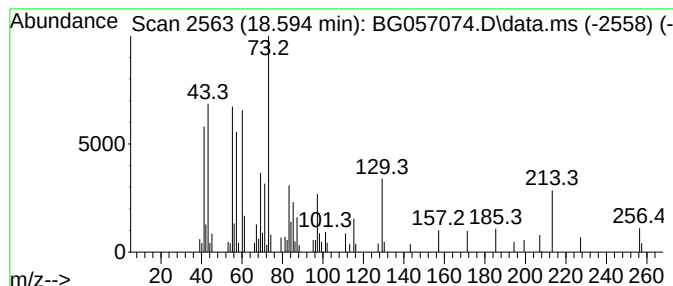
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.594	5.97 ng	70438	Phenanthrene-d10	17.754

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	58
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	53
4			Tridecanoic acid	214	C13H26O2	000638-53-9	38
5			11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	38



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Misc :
ALS Vial : 14 Sample Multiplier: 1

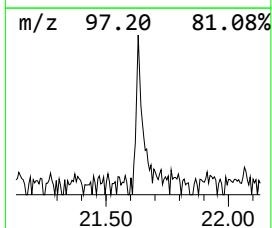
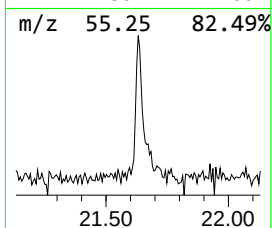
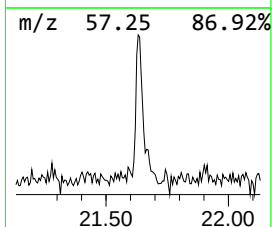
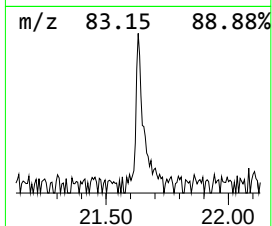
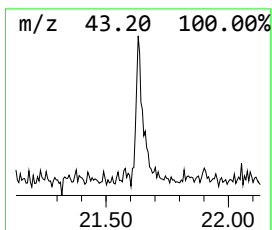
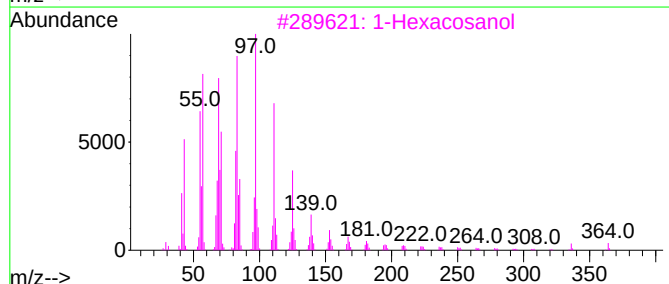
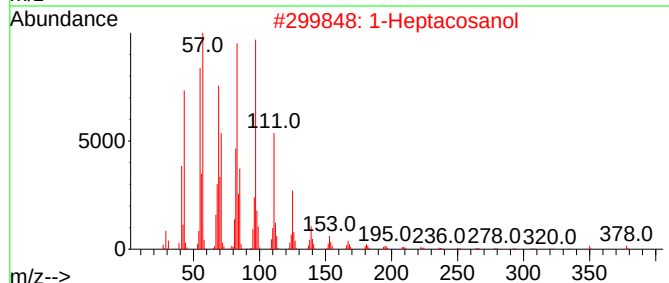
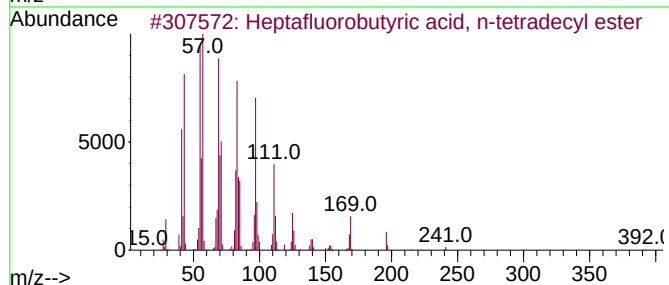
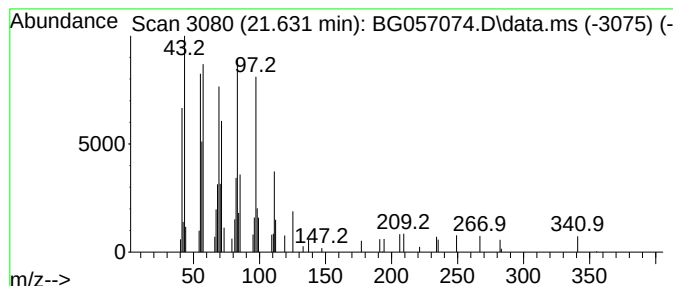
Instrument :
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Heptafluorobutyric acid, n-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.631	4.80 ng	61876	Chrysene-d12	22.072	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	91
2	1-Heptacosanol	396	C27H56O	002004-39-9	90
3	1-Hexacosanol	382	C26H54O	000506-52-5	87
4	1-Tetracosene	336	C24H48	010192-32-2	87
5	1-Hexadecanol	242	C16H34O	036653-82-4	87



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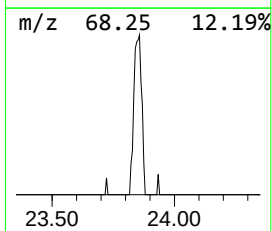
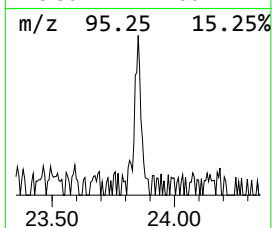
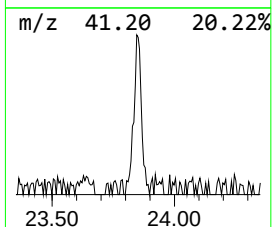
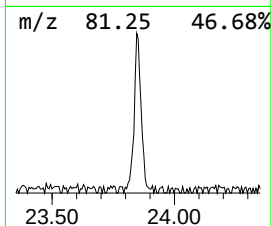
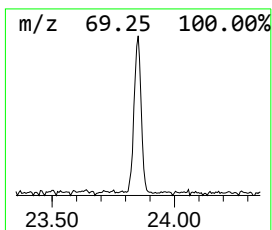
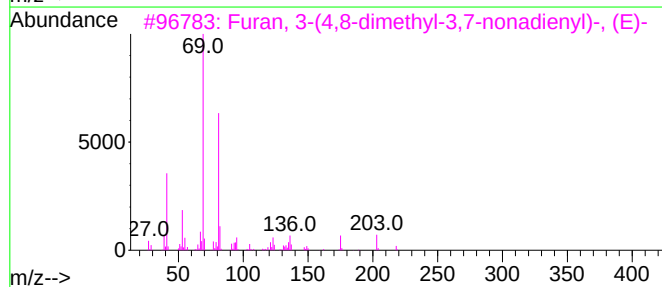
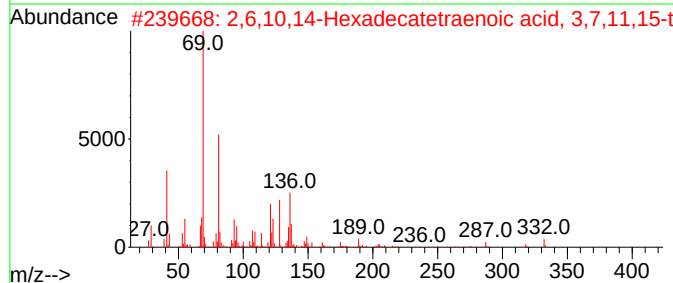
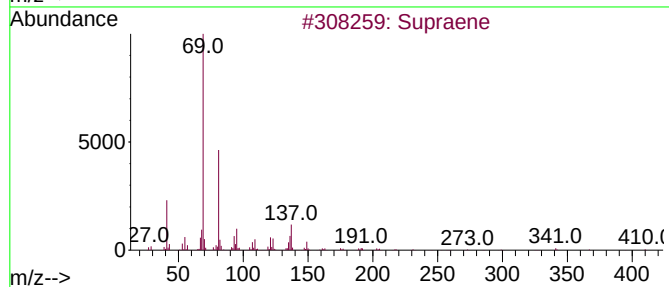
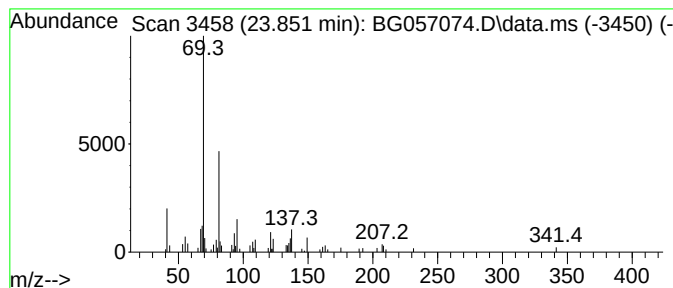
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Supraene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.852	7.19 ng	88975	Perylene-d12	25.602

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	74
2			2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	59
3			Furan, 3-(4,8-dimethyl-3,7-nonad...	218	C15H22O	023262-34-2	53
4			trans-Farnesol	222	C15H26O	000106-28-5	53
5			Bis(3-methylbut-3-enyl) phthalate	302	C18H22O4	022711-53-1	53



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.435	14.4	ng	67278	1	8.402	93749	20.0
Benzophenone	16.356	6.3	ng	57665	3	15.016	182145	20.0
n-Hexadecanoic ...	18.594	6.0	ng	70438	4	17.754	236083	20.0
Heptafluorobuty...	21.631	4.8	ng	61876	5	22.072	257676	20.0
Supraene	23.852	7.2	ng	88975	6	25.602	247340	20.0