

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011123\
 Data File : BG056257.D
 Acq On : 11 Jan 2023 19:24
 Operator : CG/JU
 Sample : 01055-05
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 MH-G

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-BG122722.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG056257.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.332	3	7	23	rVB	420825	642256	14.97%	4.418%
2	5.353	345	351	360	rVB	43624	68536	1.60%	0.471%
3	5.829	426	432	441	rBV	287203	473518	11.04%	3.257%
4	7.445	697	707	718	rBV	182927	309065	7.21%	2.126%
5	8.315	848	855	863	rVB2	116962	202066	4.71%	1.390%
6	9.490	1047	1055	1063	rBV	422188	756242	17.63%	5.202%
7	11.147	1329	1337	1344	rBV	161445	281169	6.56%	1.934%
8	13.555	1739	1747	1754	rBV	1675783	2550212	59.46%	17.542%
9	14.924	1972	1980	1988	rBB	315702	498172	11.62%	3.427%
10	16.405	2223	2232	2244	rBV	1309227	1948994	45.44%	13.407%
11	17.662	2440	2446	2453	rBV	448917	693131	16.16%	4.768%
12	18.508	2585	2590	2598	rBV2	70459	98536	2.30%	0.678%
13	18.726	2622	2627	2632	rBV	31438	46737	1.09%	0.321%
14	20.236	2878	2884	2890	rBV	3254525	4289012	100.00%	29.503%
15	21.540	3102	3106	3118	rBV3	44091	91967	2.14%	0.633%
16	21.951	3170	3176	3183	rBV	453172	781175	18.21%	5.374%
17	25.395	3751	3762	3773	rBV2	268889	806637	18.81%	5.549%

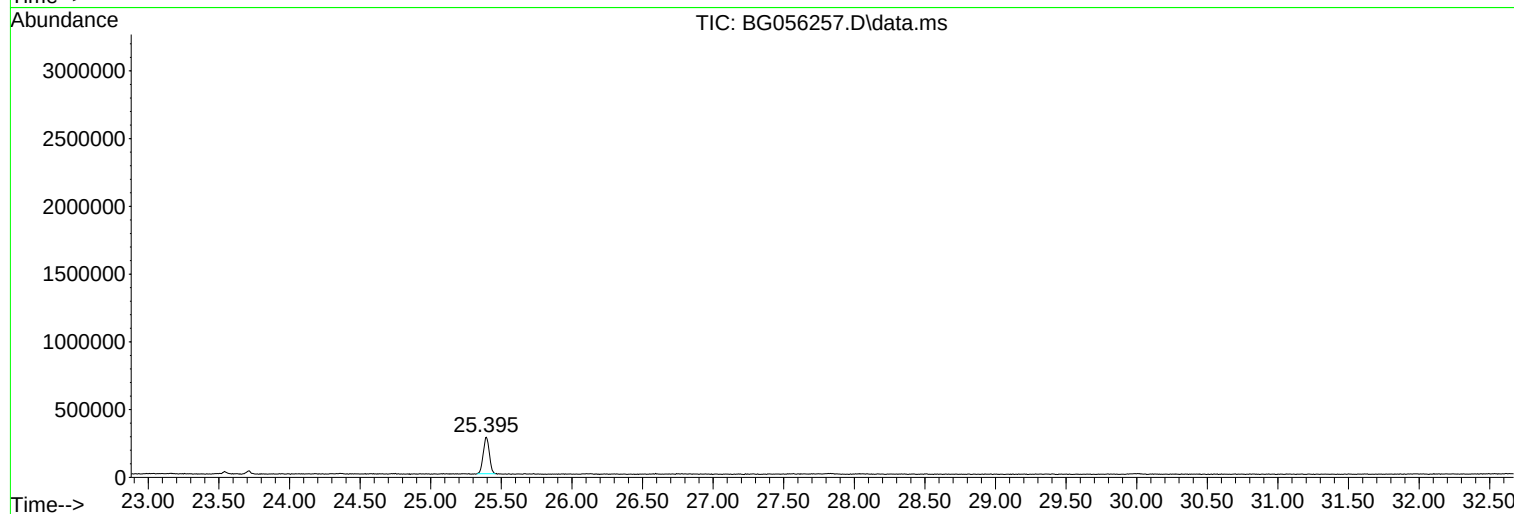
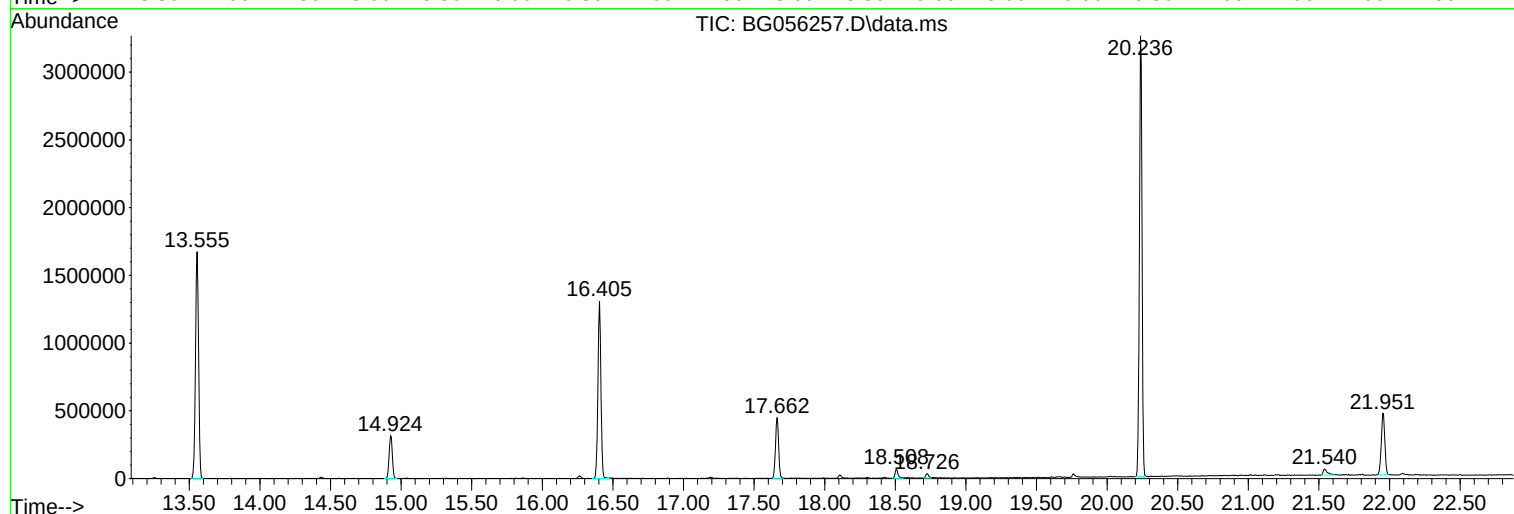
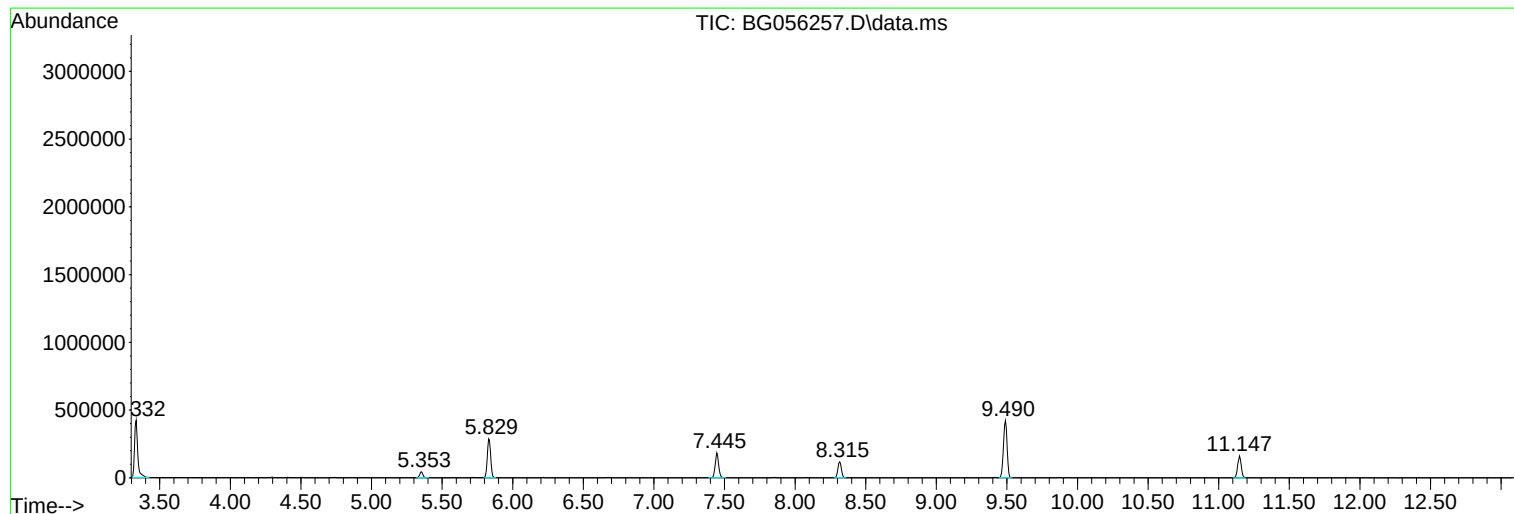
Sum of corrected areas: 14537425

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.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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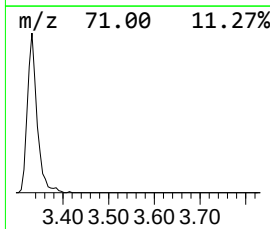
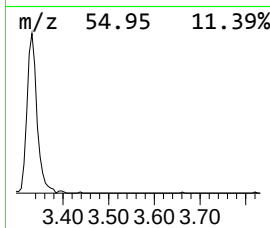
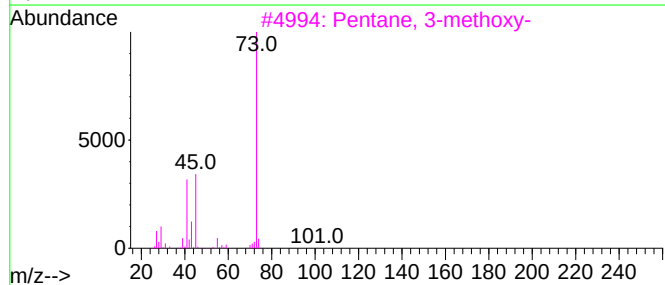
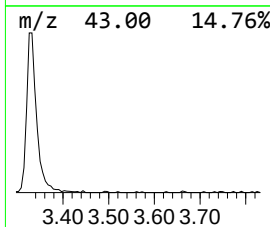
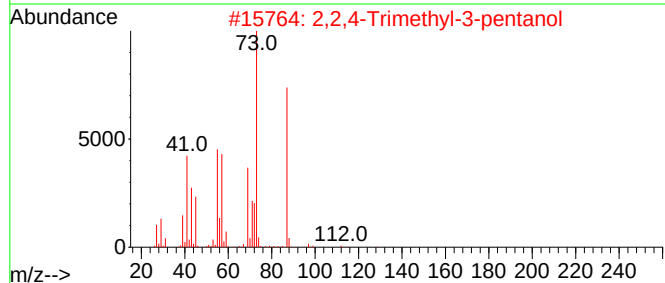
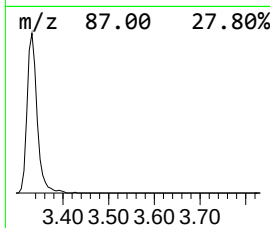
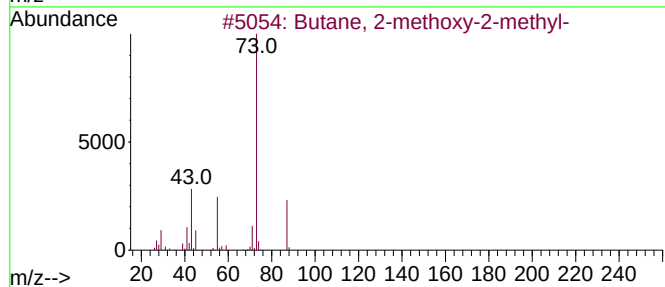
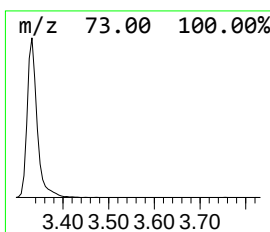
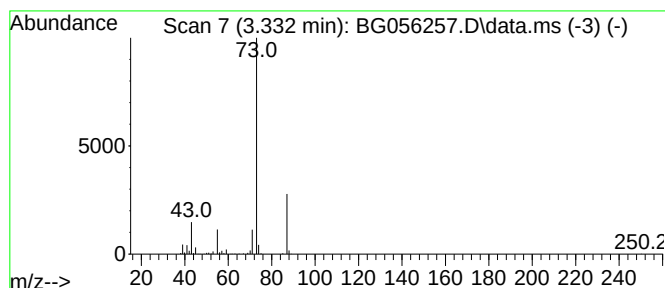
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.332	63.57 ng	642256	1,4-Dichlorobenzene-d4	8.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	43
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
4			N-Ethylformamide	73	C3H7NO	000627-45-2	7
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	7



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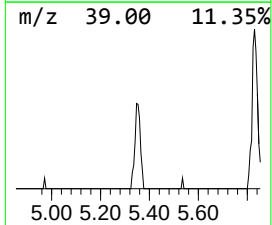
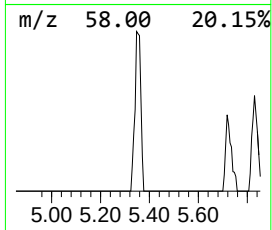
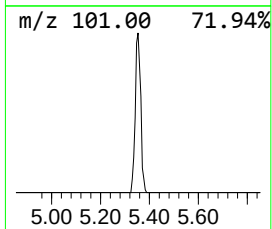
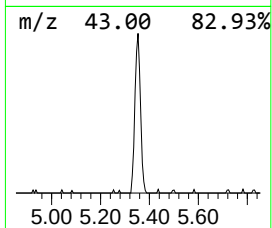
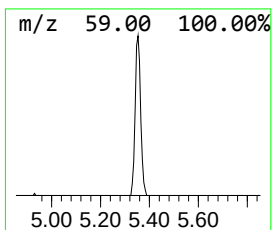
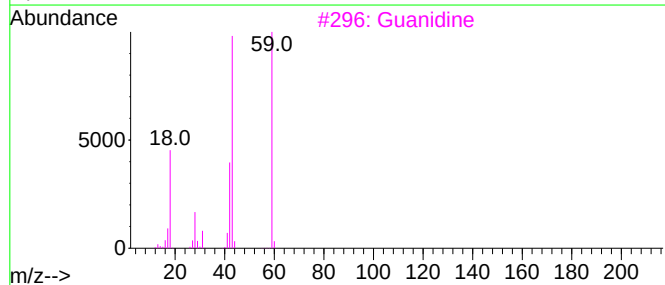
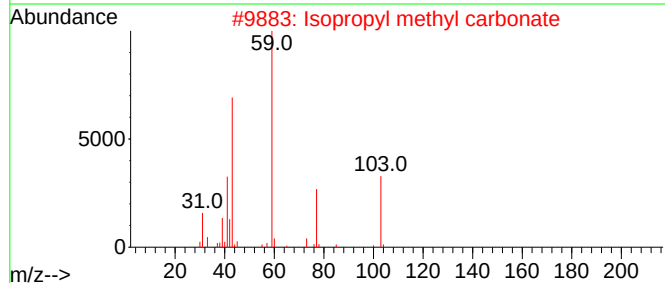
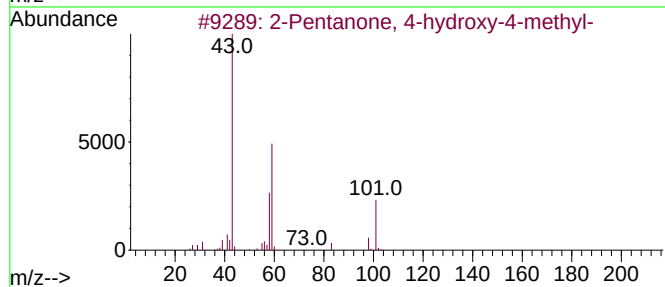
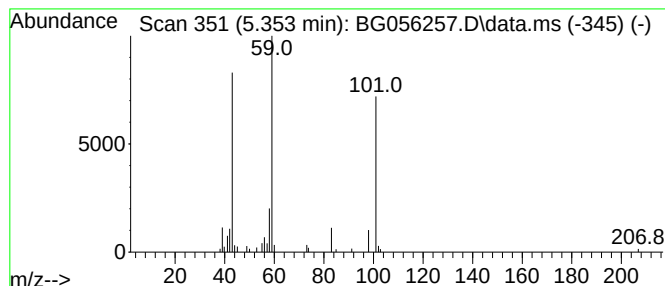
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.353	6.78 ng	68536	1,4-Dichlorobenzene-d4	8.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Isopropyl methyl carbonate	118	C5H10O3	051729-83-0	37
3			Guanidine	59	CH5N3	000113-00-8	32
4			Oxetane, 2,2,4-trimethyl-	100	C6H12O	023120-44-7	25
5			3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	25



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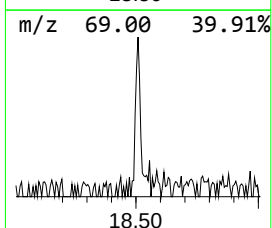
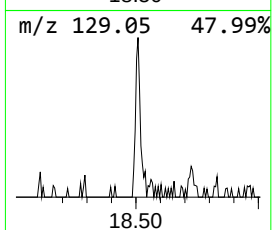
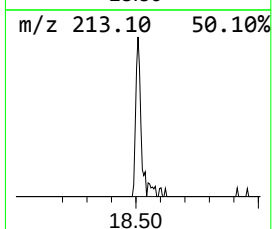
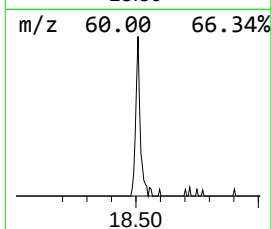
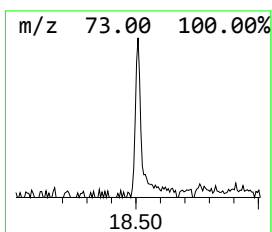
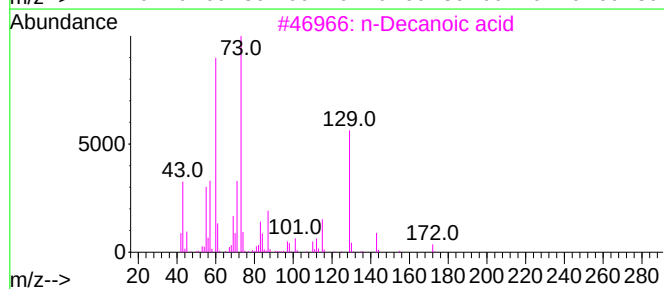
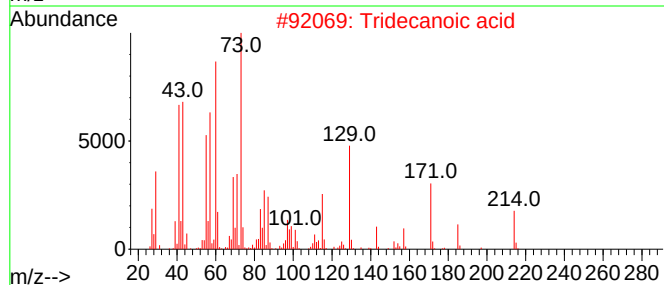
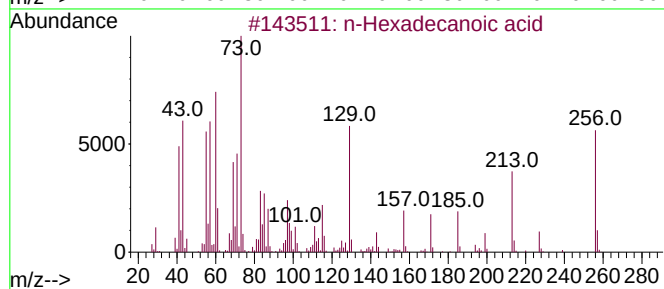
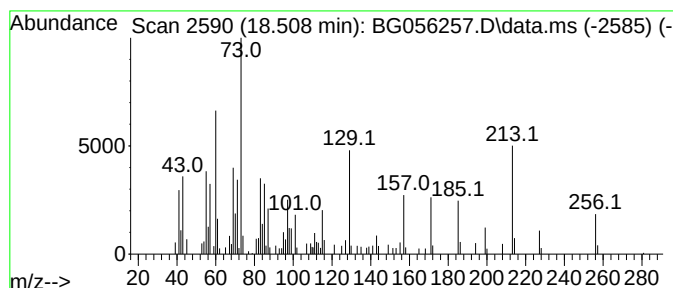
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.509	2.84 ng	98536	Phenanthrene-d10	17.662

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2			Tridecanoic acid	214	C13H26O2	000638-53-9	94
3			n-Decanoic acid	172	C10H20O2	000334-48-5	83
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	52
5			Undecanoic acid	186	C11H22O2	000112-37-8	47



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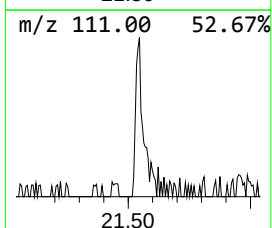
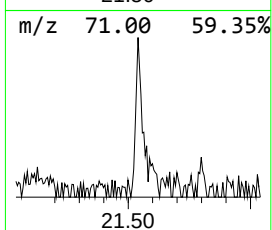
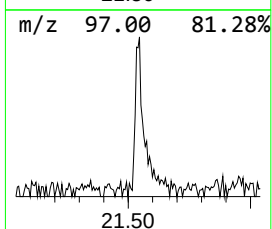
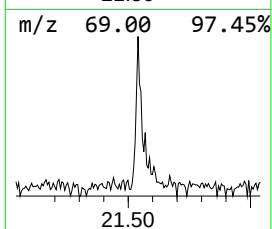
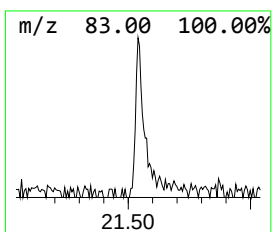
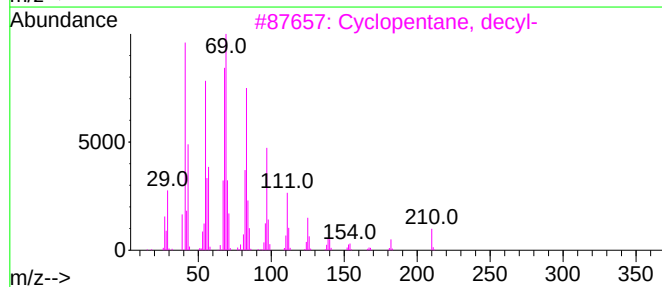
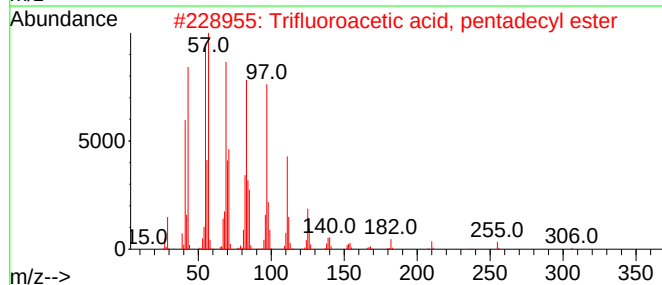
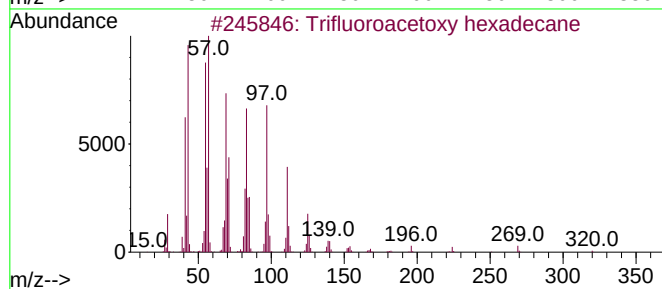
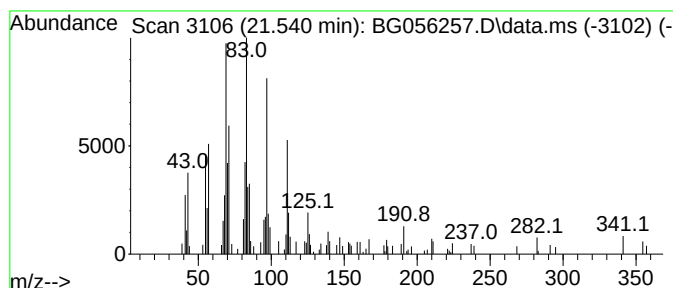
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Trifluoroacetoxy hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.540	2.35 ng	91967	Chrysene-d12	21.951

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
2			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	91
3			Cyclopentane, decyl-	210	C15H30	001795-21-7	91
4			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
5			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.332	63.6	ng	642256	1	8.315	202066	20.0
2-Pentanone, 4-...	5.353	6.8	ng	68536	1	8.315	202066	20.0
n-Hexadecanoic ...	18.509	2.8	ng	98536	4	17.662	693131	20.0
Trifluoroacetox...	21.540	2.4	ng	91967	5	21.951	781175	20.0