

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062323\
 Data File : BG057854.D
 Acq On : 23 Jun 2023 23:25
 Operator : CG/JU
 Sample : 03337-10
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 WC-8

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-BG061923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057854.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.028	324	330	337	rVB	33130	49472	2.74%	0.489%
2	5.492	403	409	419	rBV	450909	701937	38.84%	6.936%
3	7.084	672	680	688	rBV	493000	825963	45.71%	8.162%
4	7.918	815	822	830	rBV	131181	221182	12.24%	2.186%
5	9.082	1012	1020	1029	rBV	260995	456358	25.25%	4.510%
6	10.721	1292	1299	1307	rVB	199108	355609	19.68%	3.514%
7	13.177	1710	1717	1725	rBV	733830	1120932	62.03%	11.077%
8	14.552	1945	1951	1959	rVB	353238	551047	30.49%	5.445%
9	15.909	2175	2182	2189	rBV	70413	94073	5.21%	0.930%
10	16.038	2197	2204	2216	rBV	695861	1066177	59.00%	10.536%
11	17.296	2412	2418	2428	rBV	453318	700891	38.79%	6.926%
12	18.183	2564	2569	2580	rBV	116925	189946	10.51%	1.877%
13	19.458	2782	2786	2792	rBV3	30517	48348	2.68%	0.478%
14	19.910	2858	2863	2870	rVB	1327070	1807033	100.00%	17.857%
15	20.709	2996	2999	3003	rVB3	22823	31261	1.73%	0.309%
16	21.203	3078	3083	3089	rBV2	119499	176677	9.78%	1.746%
17	21.550	3136	3142	3149	rVB2	454478	721717	39.94%	7.132%
18	22.995	3384	3388	3397	rVB5	55768	128363	7.10%	1.268%
19	24.699	3670	3678	3692	rVB	299516	872710	48.30%	8.624%

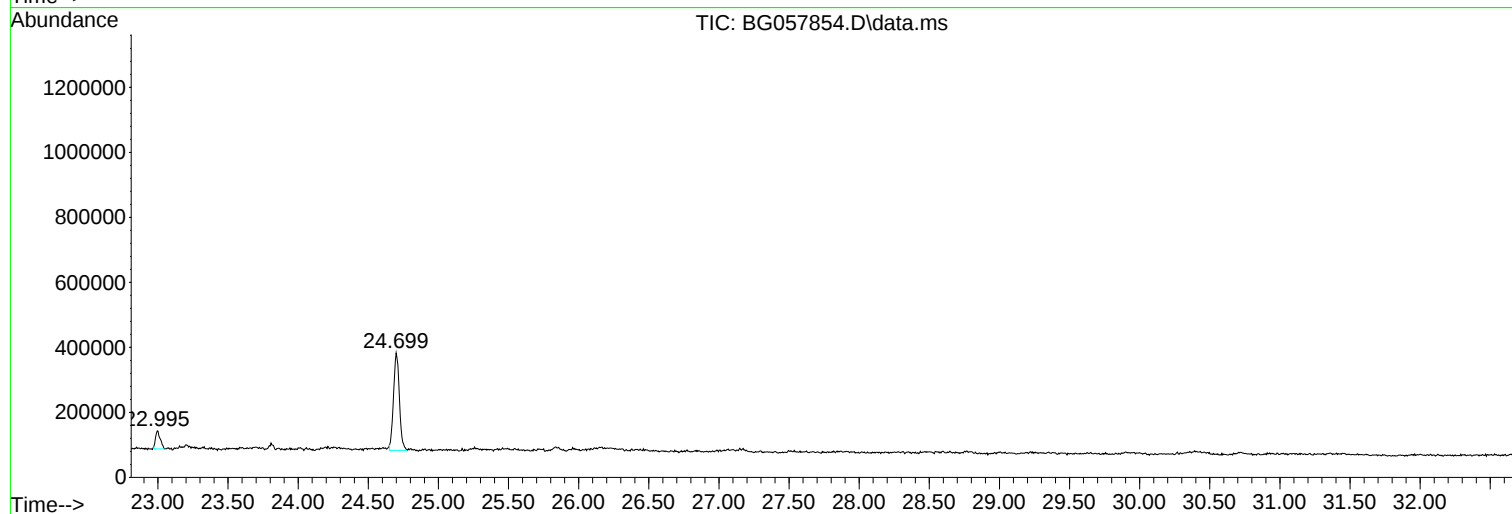
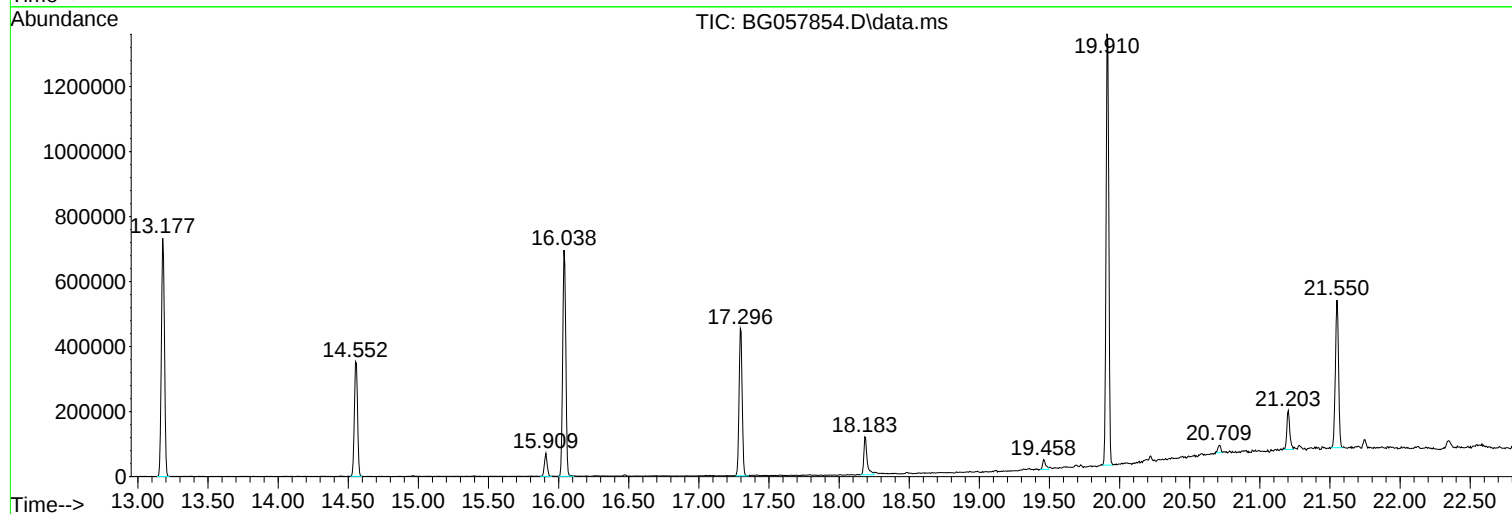
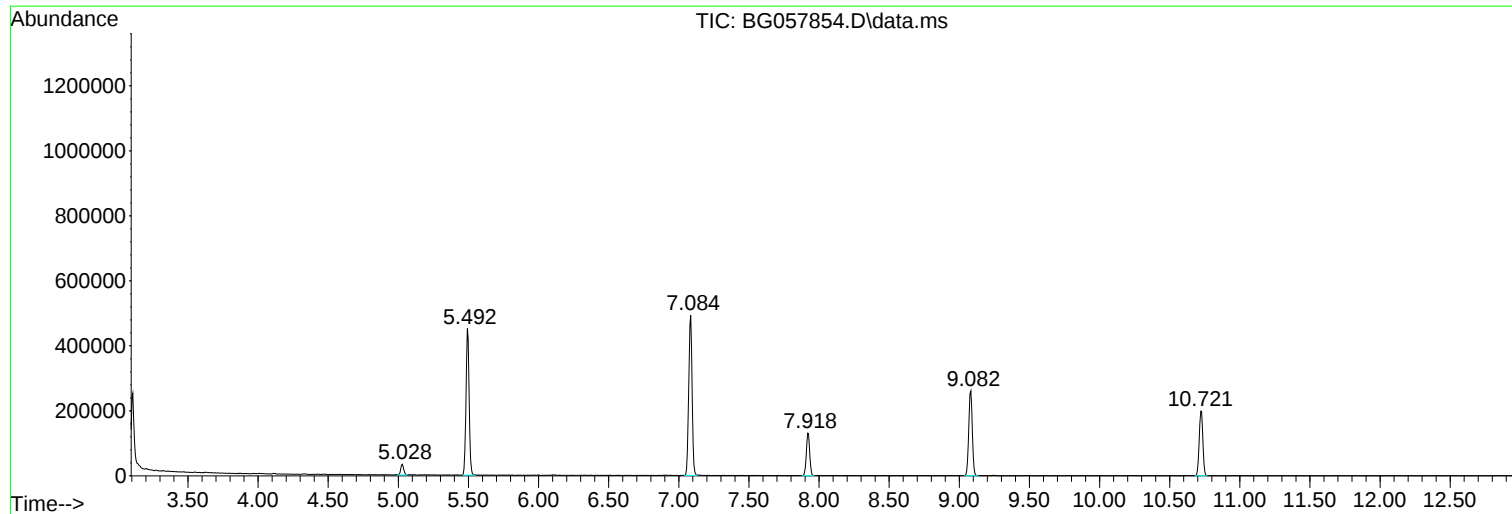
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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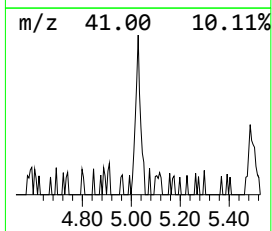
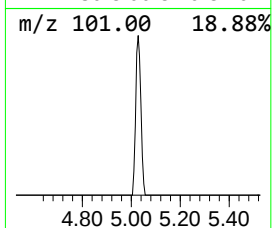
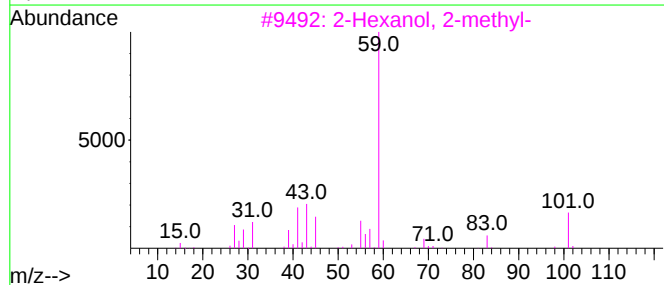
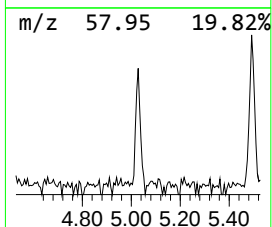
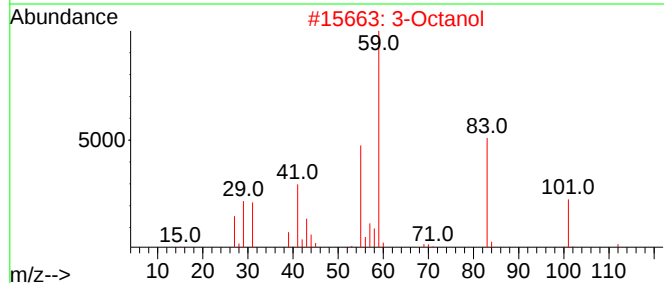
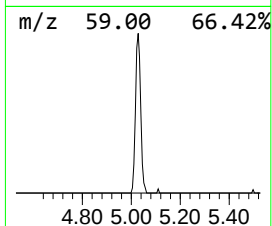
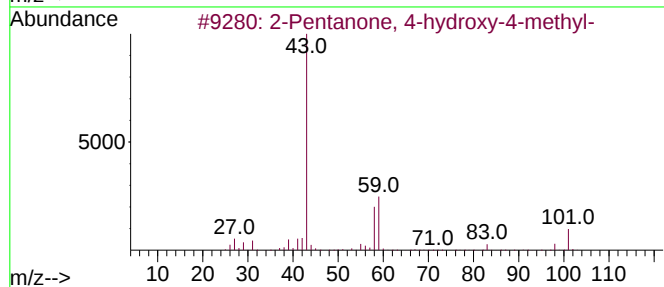
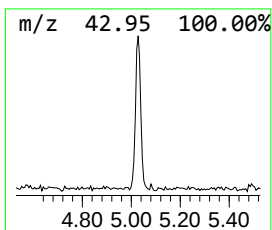
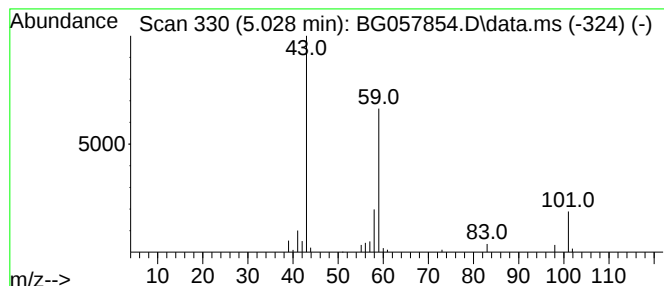
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.028	4.47 ng	49472	1,4-Dichlorobenzene-d4	7.924

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53		
2	3-Octanol	130	C8H18O	000589-98-0	25		
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25		
4	1,2-Butanediol	90	C4H10O2	000584-03-2	17		
5	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	12		



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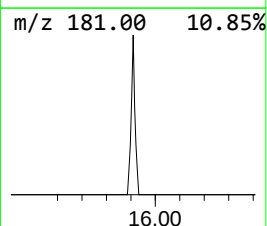
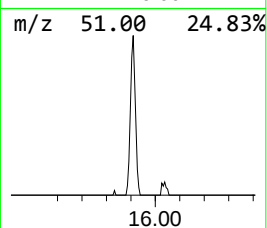
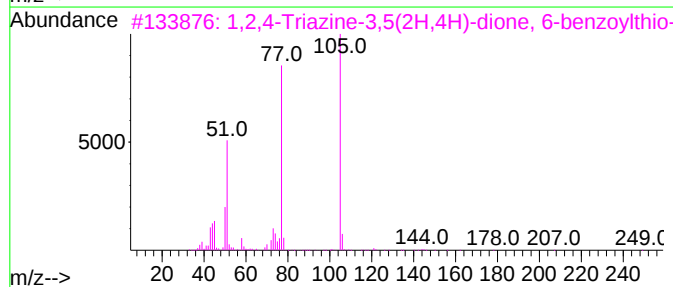
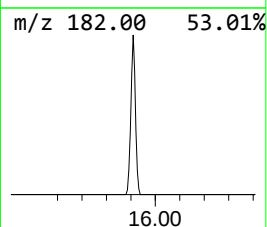
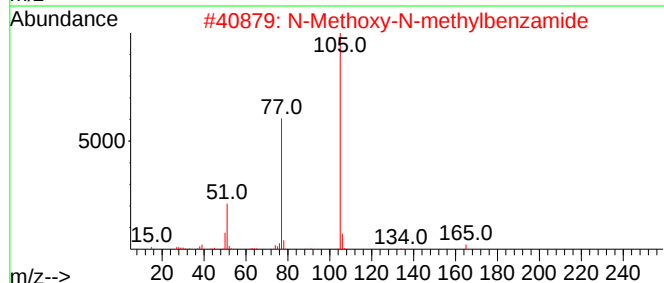
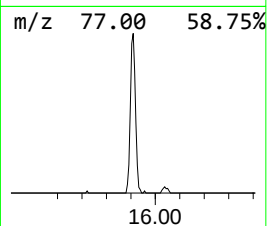
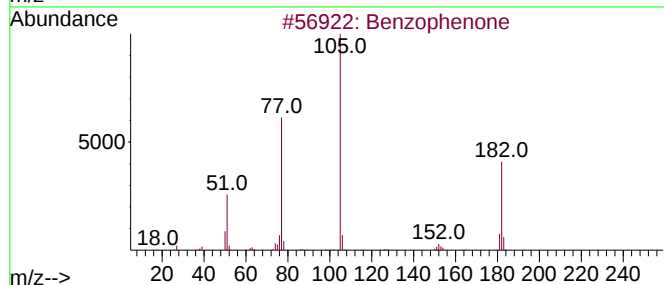
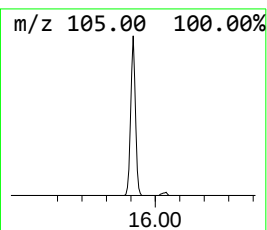
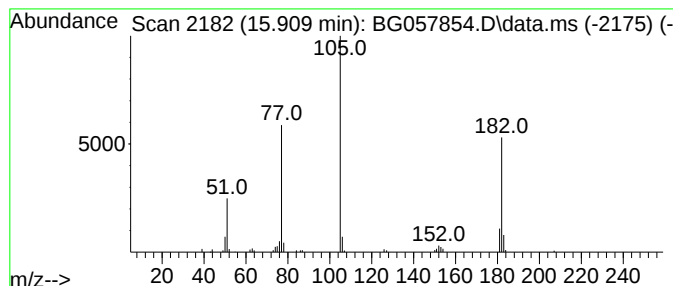
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.909	3.41 ng	94073	Acenaphthene-d10	14.552

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47
3			1,2,4-Triazine-3,5(2H,4H)-dione,...	249	C10H7N3O3S	024168-34-1	47
4			N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	47
5			Vinyl benzoate	148	C9H8O2	000769-78-8	47



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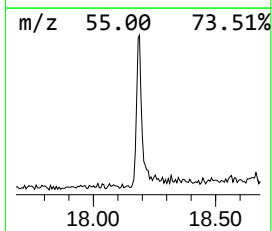
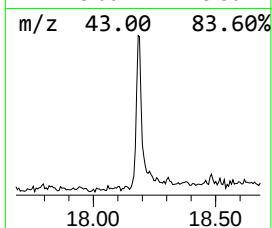
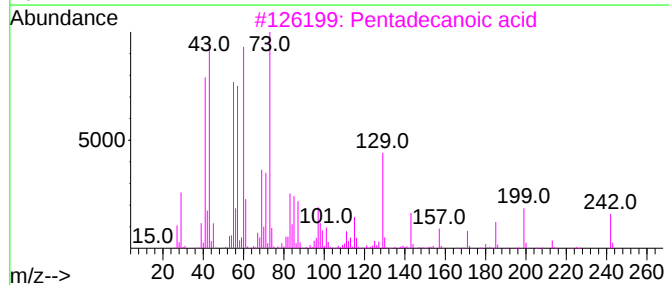
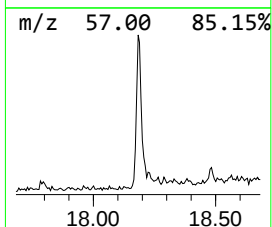
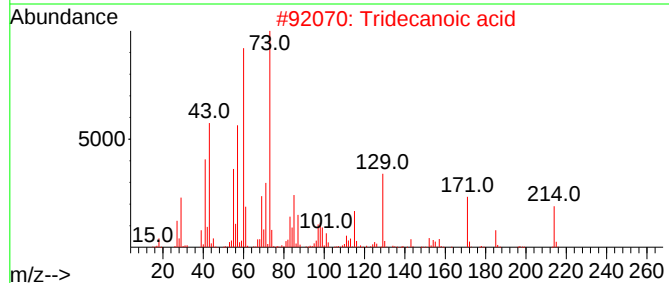
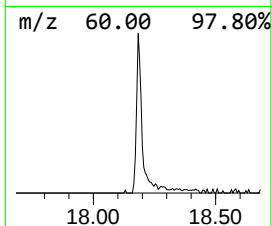
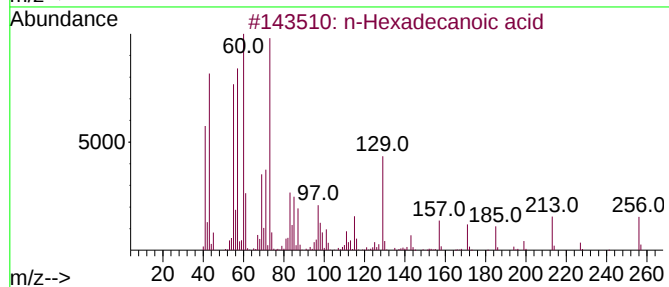
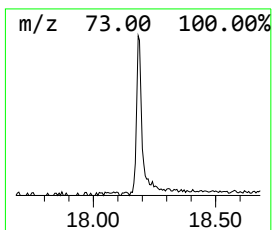
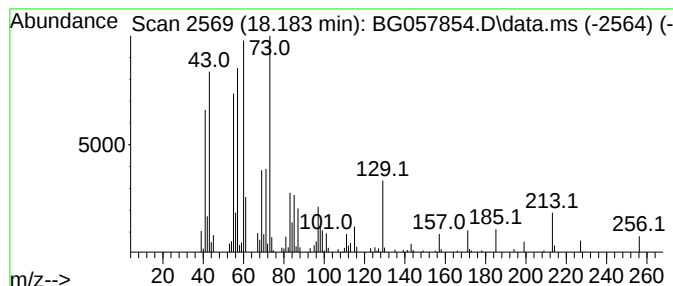
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.183	5.42 ng	189946	Phenanthrene-d10	17.296

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	93
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5		Nonanoic acid	158	C9H18O2	000112-05-0	46



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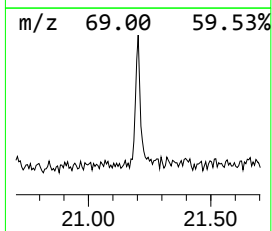
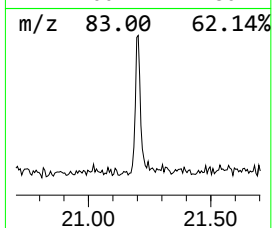
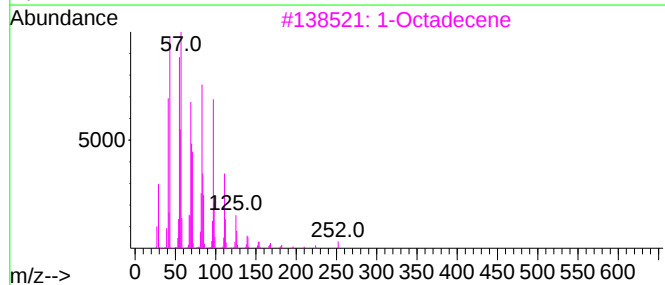
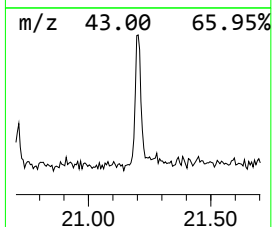
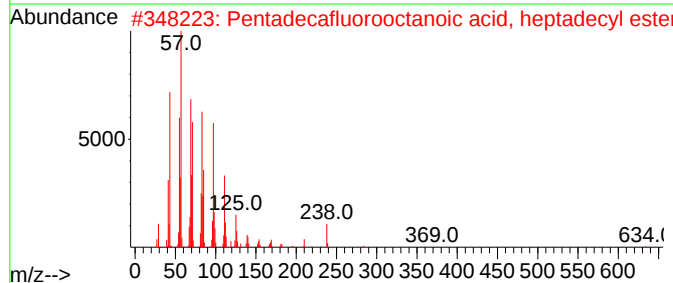
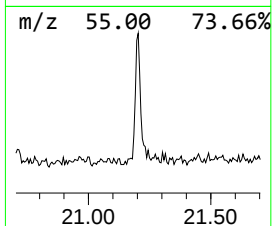
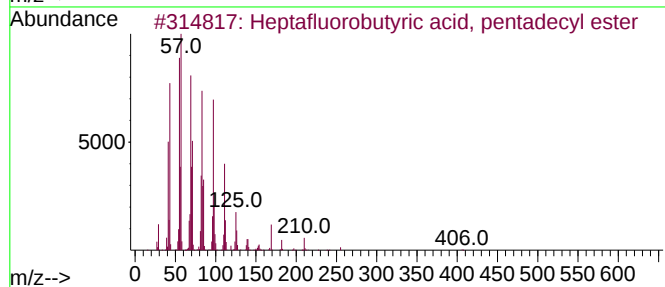
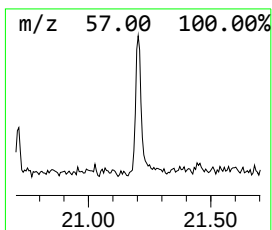
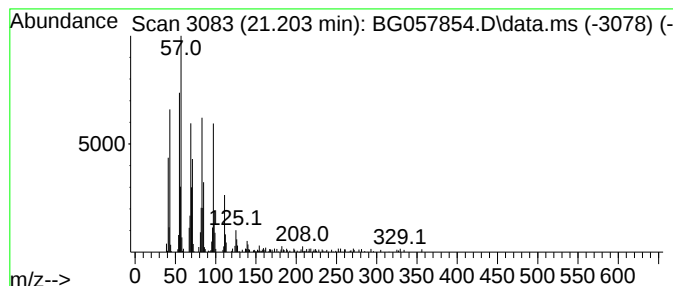
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Peak Number 4 Heptafluorobutyric acid, pe... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.203	4.90 ng	176677	Chrysene-d12	21.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	95
2			Pentadecafluorooctanoic acid, he...	652	C25H35F15O2	1000406-04-7	94
3			1-Octadecene	252	C18H36	000112-88-9	93
4			E-7-Octadecene	252	C18H36	1000130-92-0	92
5			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91



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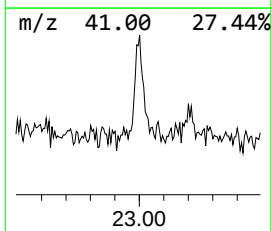
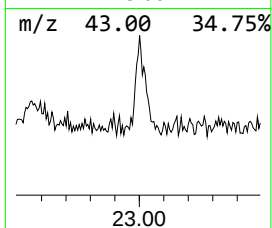
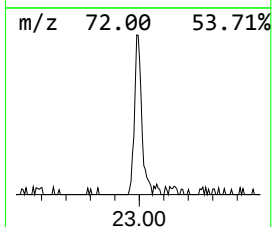
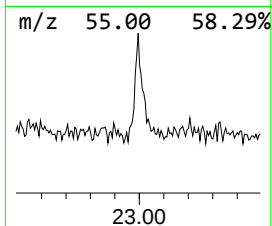
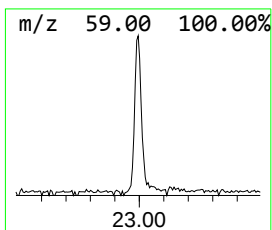
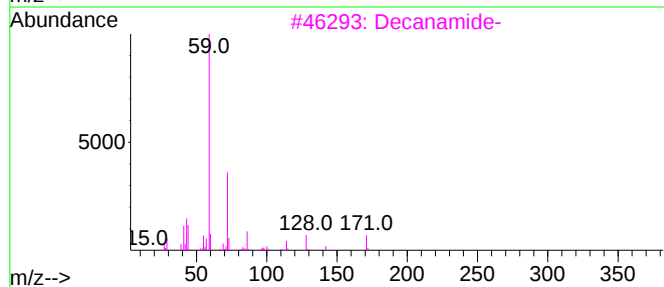
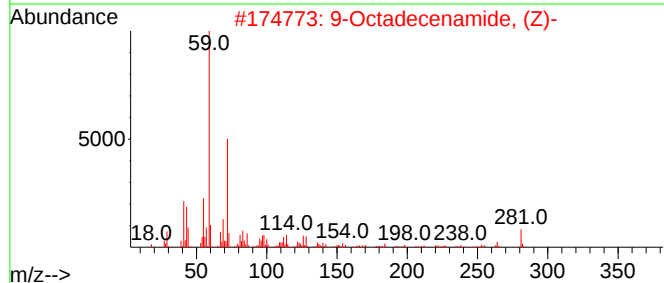
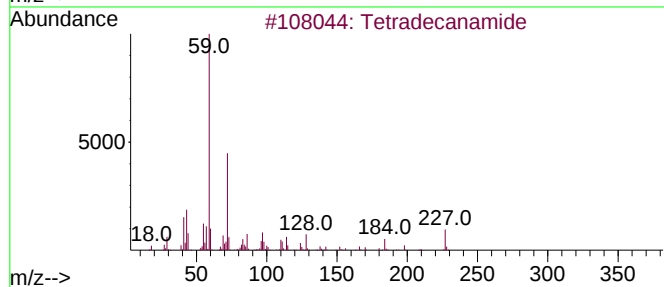
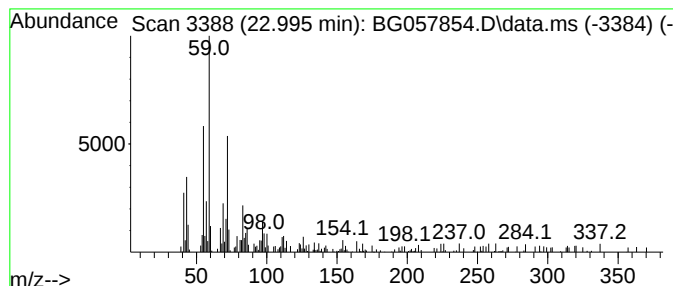
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Peak Number 5 Tetradecanamide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.995	3.56 ng	128363	Chrysene-d12	21.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecanamide	227	C14H29NO	000638-58-4	64
2			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	59
3			Decanamide-	171	C10H21NO	002319-29-1	59
4			Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	58
5			Nonanamide	157	C9H19NO	001120-07-6	49



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.028	4.5	ng	49472	1	7.924	221182	20.0
Benzophenone	15.909	3.4	ng	94073	3	14.552	551047	20.0
n-Hexadecanoic ...	18.183	5.4	ng	189946	4	17.296	700891	20.0
Heptafluorobuty...	21.203	4.9	ng	176677	5	21.550	721717	20.0
Tetradecanamide	22.995	3.6	ng	128363	5	21.550	721717	20.0