

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101722\
 Data File : BG055198.D
 Acq On : 17 Oct 2022 18:46
 Operator : CG/JU
 Sample : N5145-06
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 MW-9-101322

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-BG101322.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055198.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.323	3	6	36	rVB	636377	1147830	47.57%	10.422%
2	5.344	344	350	360	rBV	43406	68344	2.83%	0.621%
3	5.826	424	432	443	rBV	252225	428371	17.75%	3.890%
4	7.436	699	706	718	rVB	158712	282368	11.70%	2.564%
5	8.299	844	853	860	rBV	115942	198149	8.21%	1.799%
6	9.474	1044	1053	1061	rBV	405887	735605	30.49%	6.679%
7	11.131	1327	1335	1342	rBV	160343	285644	11.84%	2.594%
8	13.540	1735	1745	1752	rBV	1154542	1795793	74.43%	16.306%
9	14.909	1970	1978	1986	rVB	261775	424191	17.58%	3.852%
10	16.078	2172	2177	2182	rBV	18994	26932	1.12%	0.245%
11	16.390	2223	2230	2238	rBV	953170	1463432	60.65%	13.288%
12	17.641	2437	2443	2449	rBV	332950	491035	20.35%	4.459%
13	18.499	2584	2589	2597	rBV2	55896	105547	4.37%	0.958%
14	19.751	2799	2802	2813	rVB3	36743	63365	2.63%	0.575%
15	20.221	2876	2882	2887	rBV	1867912	2412864	100.00%	21.909%
16	21.930	3166	3173	3185	rVB	301390	533420	22.11%	4.843%
17	25.350	3745	3755	3766	rVB2	188164	550378	22.81%	4.997%

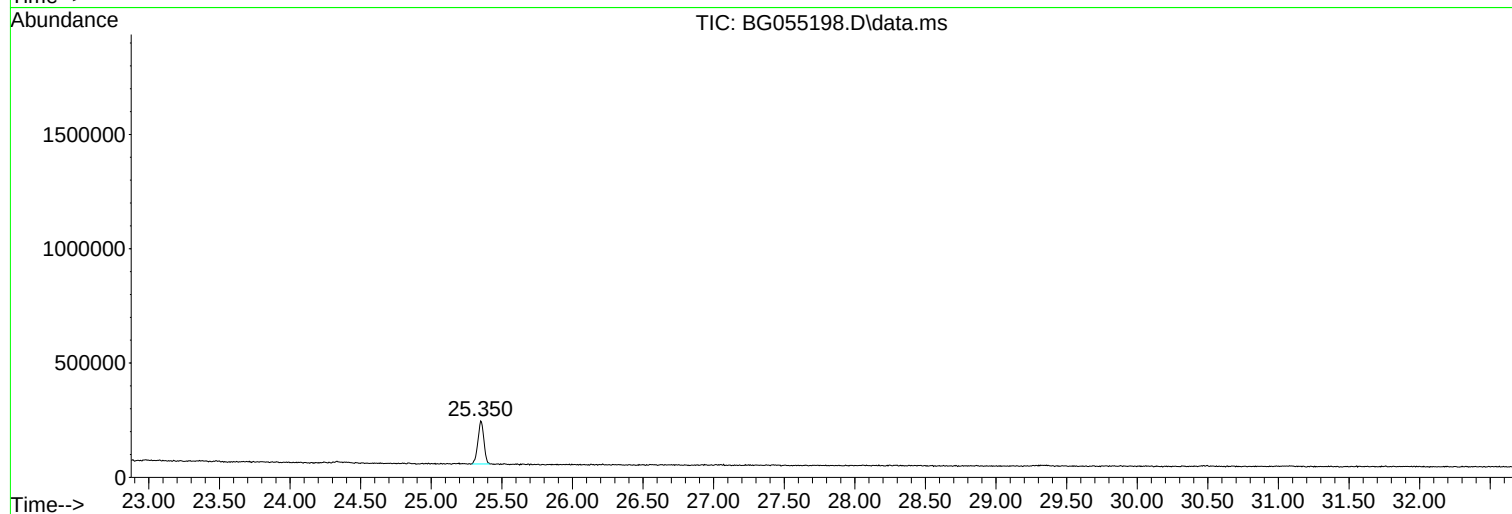
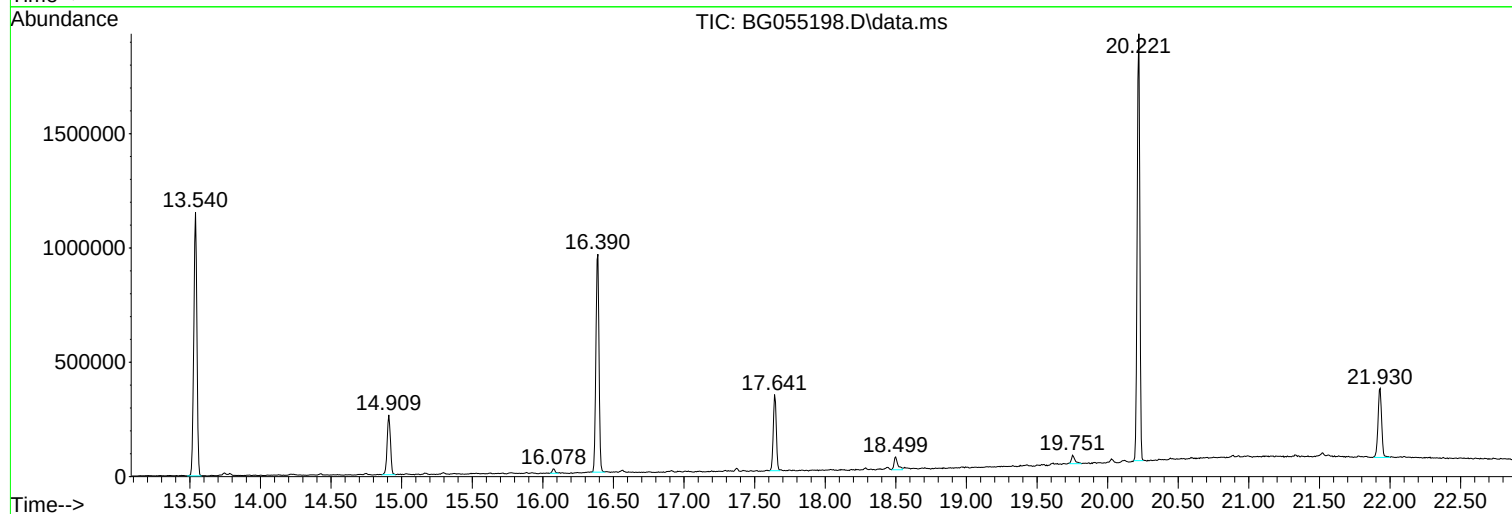
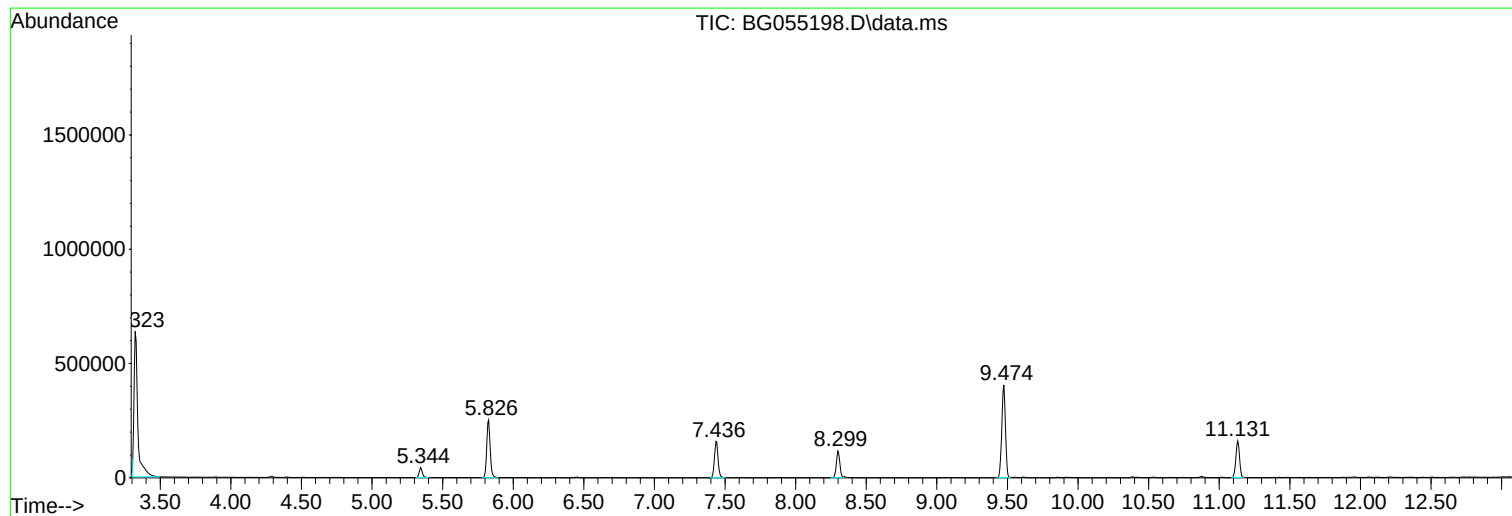
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG101322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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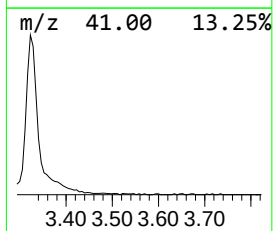
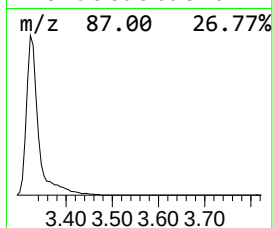
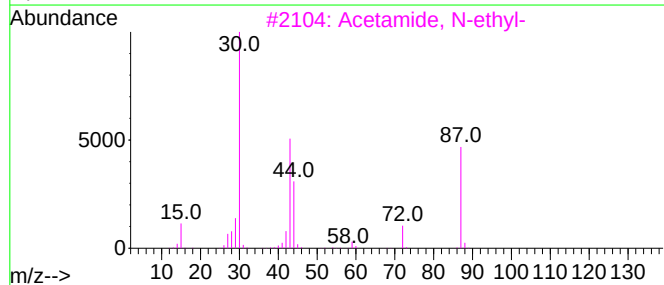
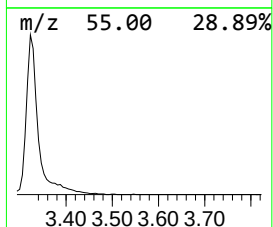
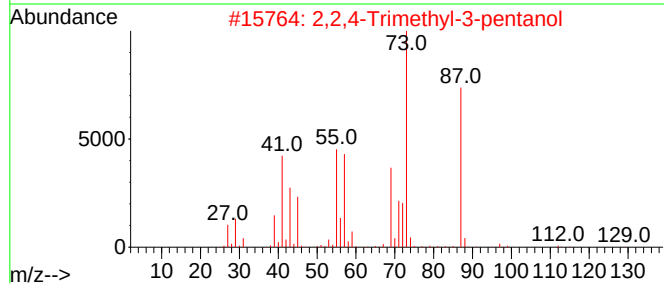
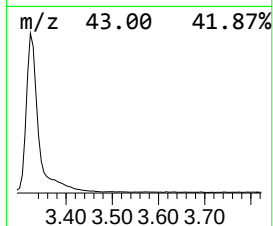
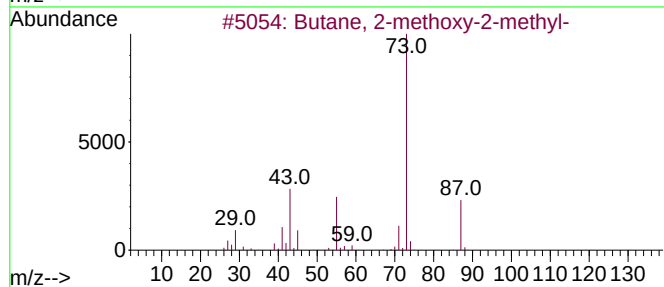
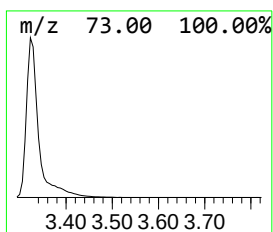
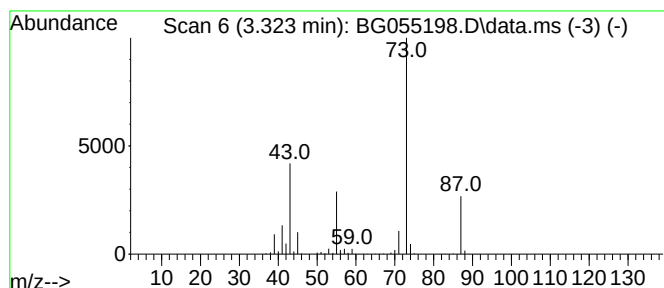
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.323	115.86 ng	1147830	1,4-Dichlorobenzene-d4	8.299

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
3			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	35
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	28
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17



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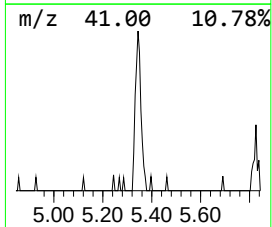
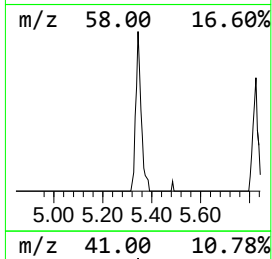
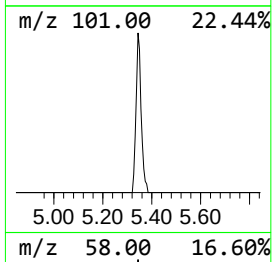
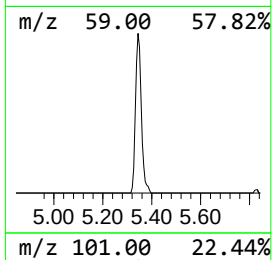
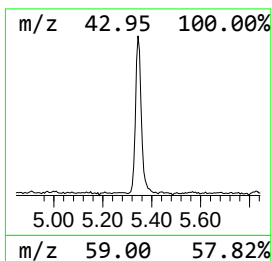
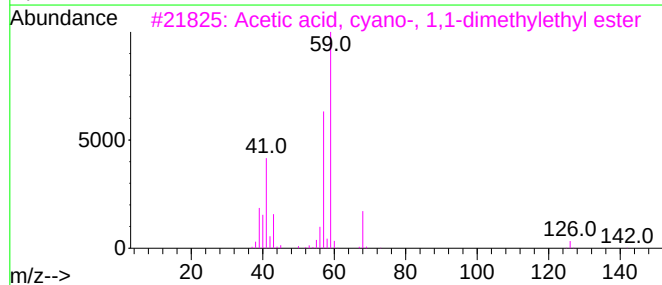
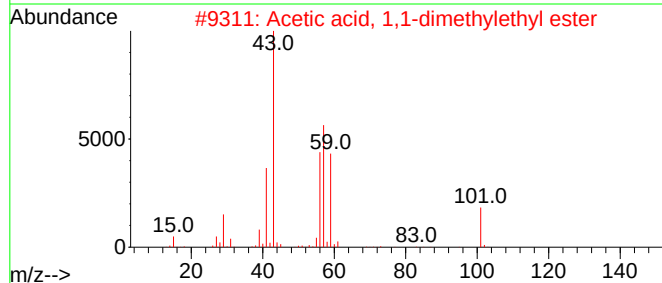
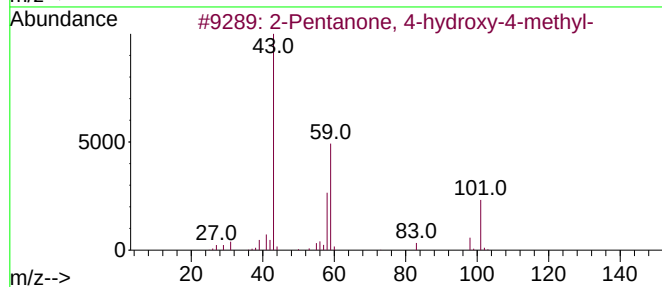
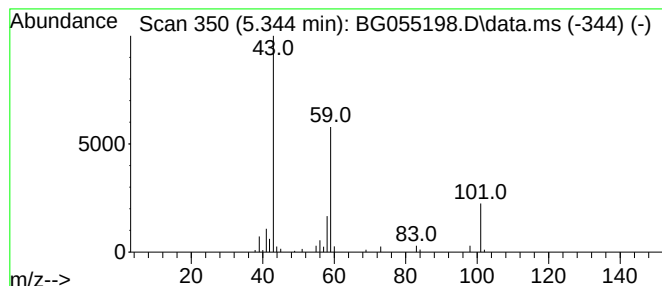
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.344	6.90 ng	68344	1,4-Dichlorobenzene-d4	8.299

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4		Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17
5		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	17



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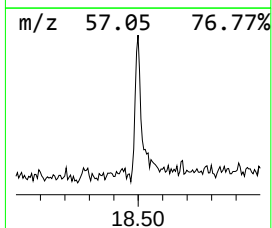
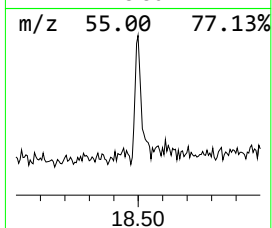
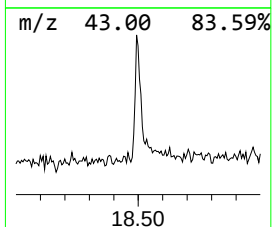
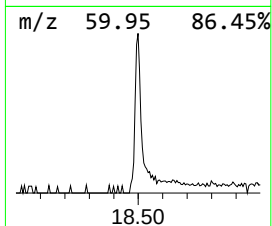
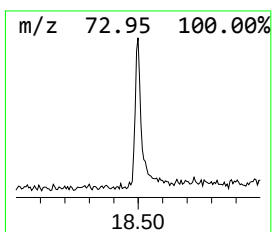
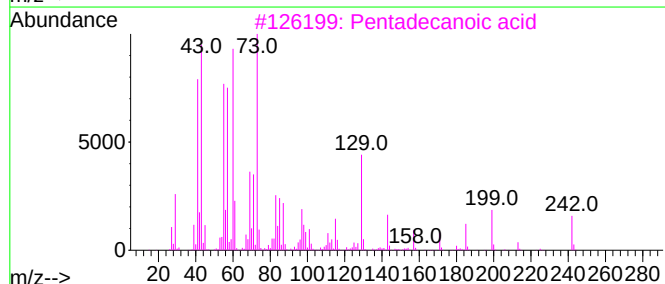
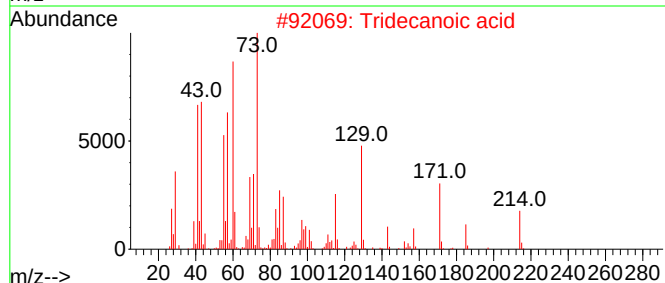
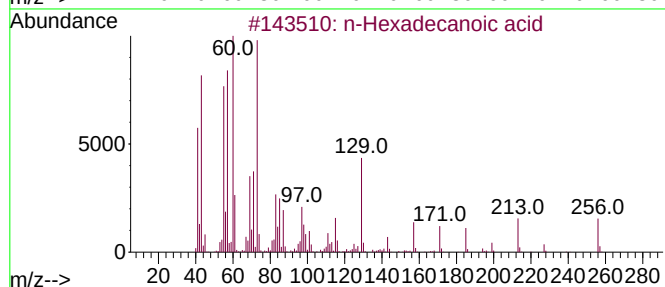
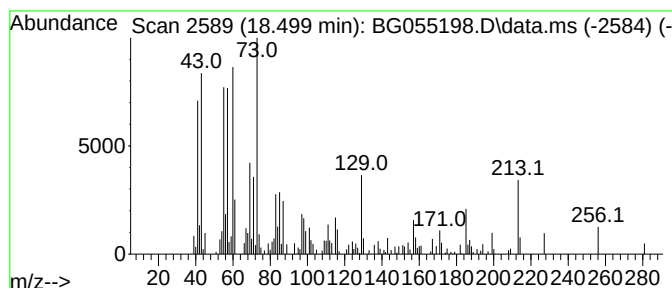
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.499	4.30 ng	105547	Phenanthrene-d10	17.641	
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	89
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Undecanoic acid	186	C11H22O2	000112-37-8	64



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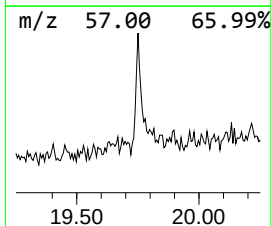
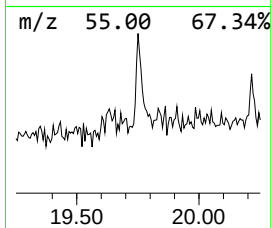
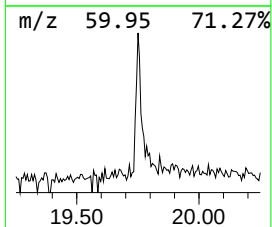
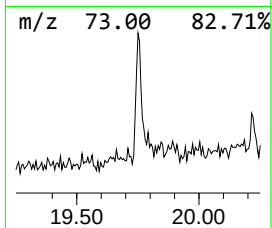
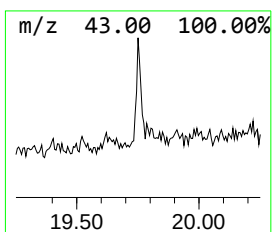
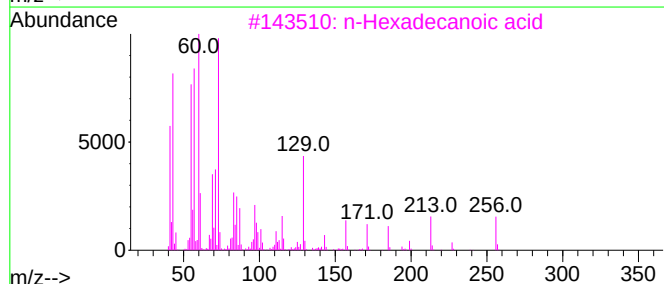
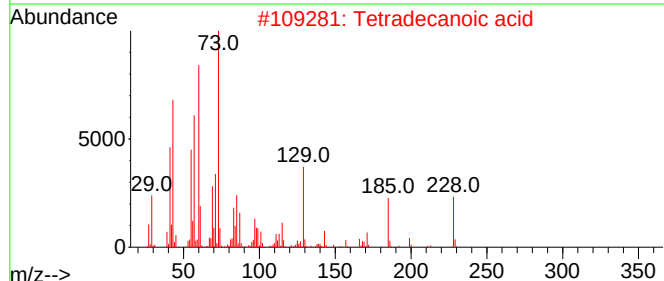
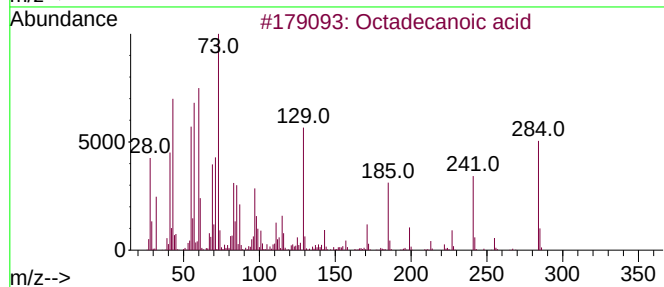
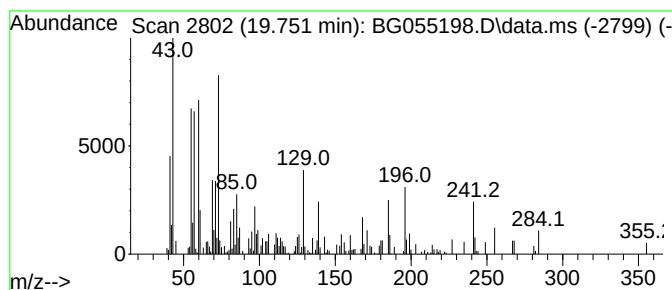
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Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.751	2.58 ng	63365	Phenanthrene-d10	17.641

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	97
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	52
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	46
4			i-Propyl 16-methyl-heptadecanoate	326	C21H42O2	1000336-66-3	43
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	35



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.323	115.9	ng	1147830	1	8.299	198149	20.0
2-Pentanone, 4-...	5.344	6.9	ng	68344	1	8.299	198149	20.0
n-Hexadecanoic ...	18.499	4.3	ng	105547	4	17.641	491035	20.0
Octadecanoic acid	19.751	2.6	ng	63365	4	17.641	491035	20.0