

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122922\
 Data File : BG056154.D
 Acq On : 29 Dec 2022 14:49
 Operator : CG/JU
 Sample : N6232-07
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 MW-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-BG122722.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG056154.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.367	6	13	30	rVB	315142	570778	23.18%	3.825%
2	5.382	346	356	362	rBV2	54535	88806	3.61%	0.595%
3	5.858	428	437	447	rBV	262391	442647	17.97%	2.966%
4	7.468	704	711	721	rBV	161894	280302	11.38%	1.878%
5	8.338	852	859	867	rBV	157827	268541	10.90%	1.800%
6	9.507	1049	1058	1067	rBV	406589	720282	29.25%	4.827%
7	11.170	1333	1341	1352	rVB	195250	368752	14.97%	2.471%
8	13.573	1742	1750	1758	rBV	1620710	2462896	100.00%	16.504%
9	14.942	1975	1983	1992	rBV	394367	629120	25.54%	4.216%
10	15.224	2028	2031	2036	rVB2	19378	29161	1.18%	0.195%
11	15.553	2084	2087	2092	rVB2	18783	24886	1.01%	0.167%
12	16.299	2209	2214	2219	rBV3	24542	39165	1.59%	0.262%
13	16.422	2228	2235	2242	rBV	1251523	1912786	77.66%	12.818%
14	16.681	2275	2279	2286	rVB2	33727	51200	2.08%	0.343%
15	17.321	2382	2388	2397	rBV	542088	851174	34.56%	5.704%
16	17.680	2442	2449	2456	rVB	516190	809507	32.87%	5.425%
17	17.926	2488	2491	2496	rVB	21604	25512	1.04%	0.171%
18	18.526	2589	2593	2597	rBV	156055	208967	8.48%	1.400%
19	18.573	2598	2601	2605	rVB4	31785	41694	1.69%	0.279%
20	19.577	2768	2772	2775	rBV	55167	66019	2.68%	0.442%
21	19.783	2802	2807	2823	rBV	542740	783868	31.83%	5.253%
22	20.253	2881	2887	2893	rBV	1860474	2363492	95.96%	15.838%
23	21.975	3173	3180	3186	rVB	528009	915541	37.17%	6.135%
24	25.429	3758	3768	3780	rVB	315938	967642	39.29%	6.484%

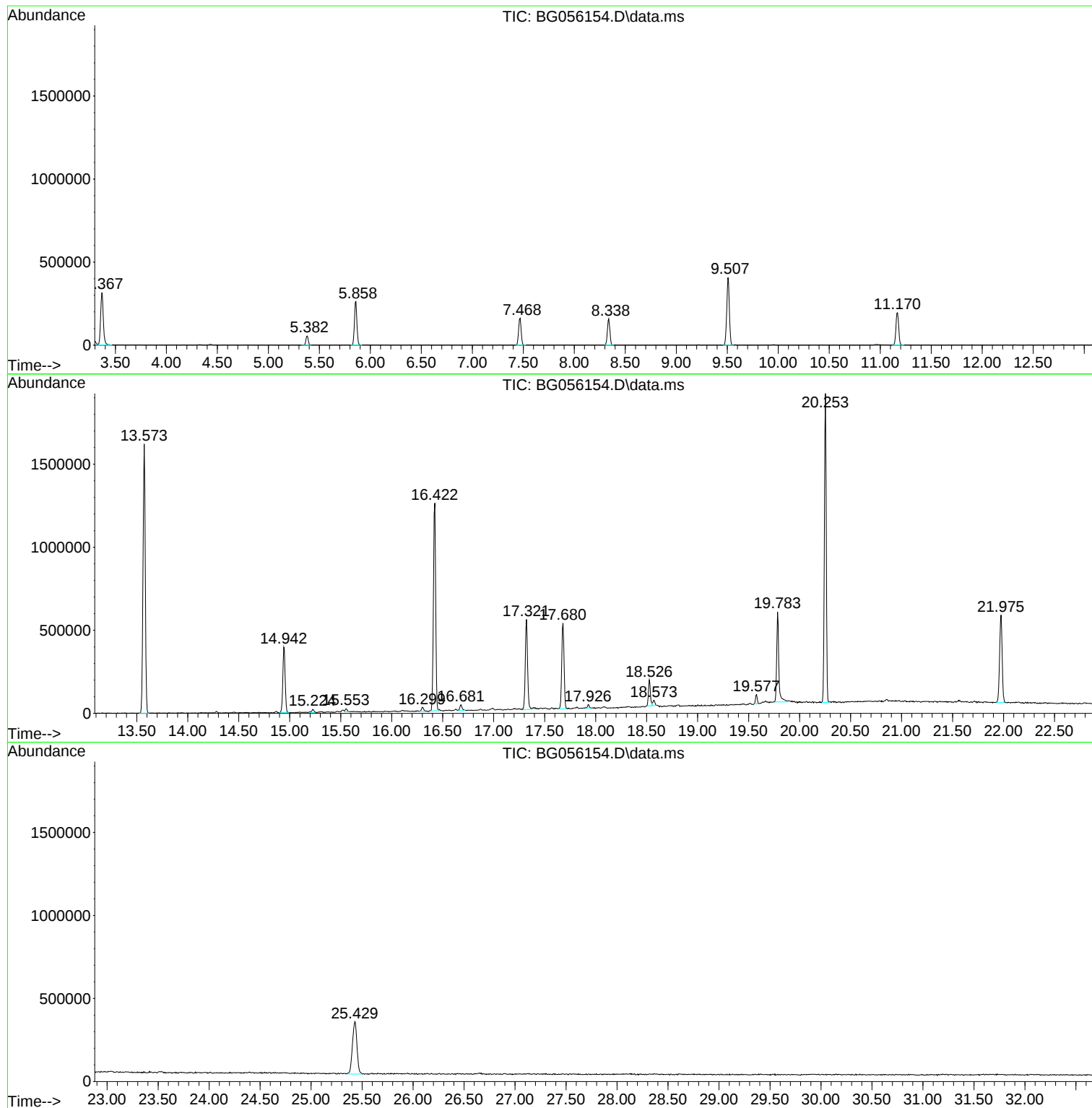
Sum of corrected areas: 14922738

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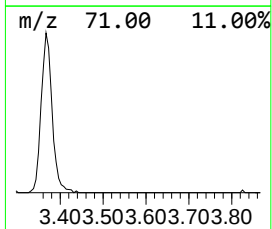
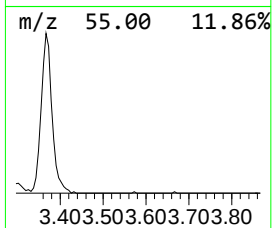
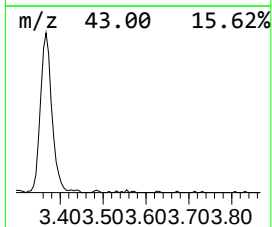
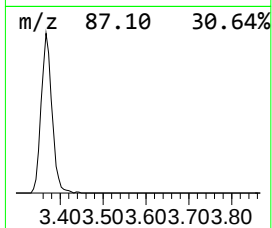
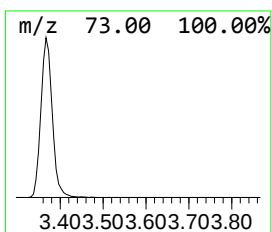
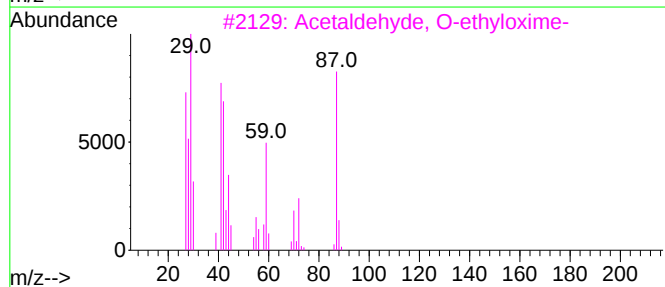
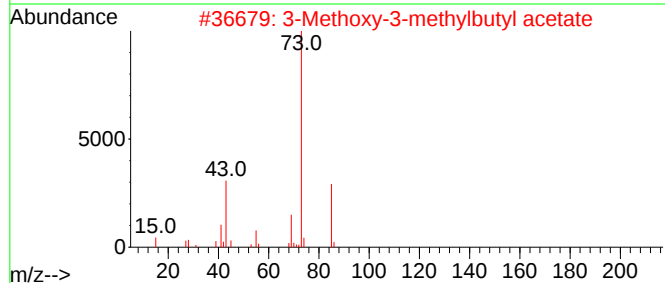
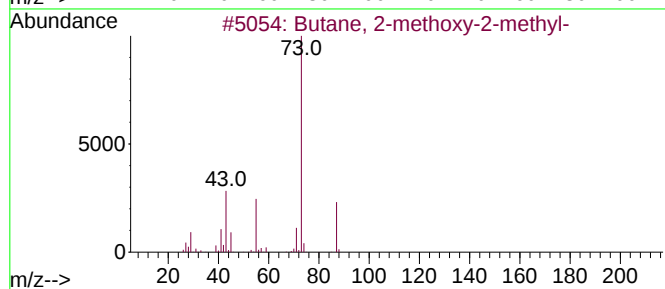
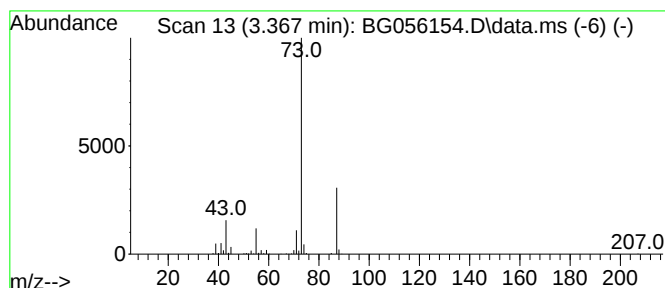
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
3.367	42.51 ng	570778	1,4-Dichlorobenzene-d4	8.338

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	64
2			3-Methoxy-3-methylbutyl acetate	160	C8H16O3	1010430-01-2	17
3			Acetaldehyde, O-ethyloxime-	87	C4H9NO	1000288-34-6	9
4			Azetidine, 1-methyl-	71	C4H9N	004923-79-9	9
5			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	9



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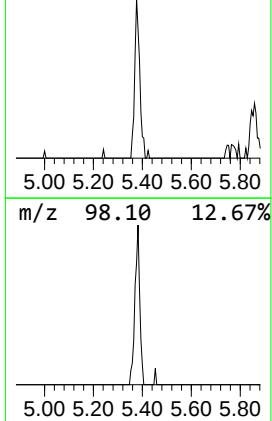
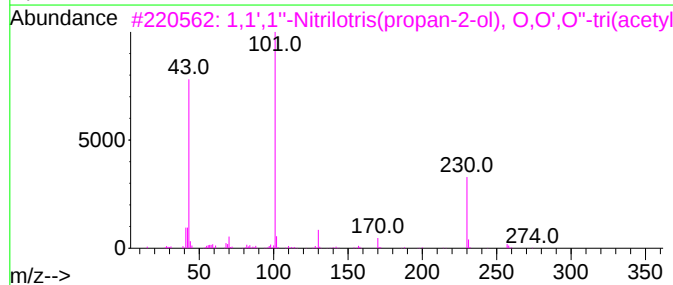
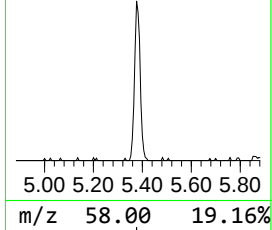
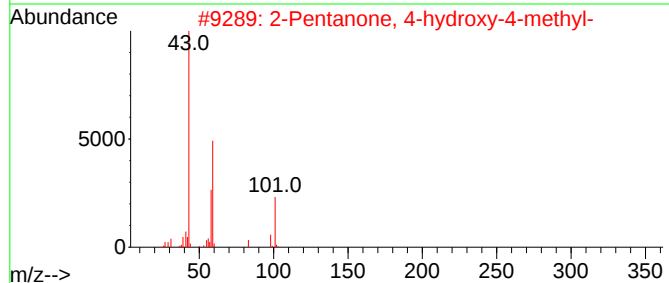
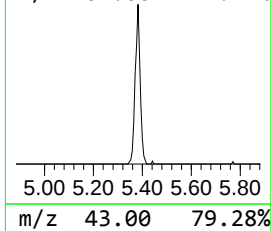
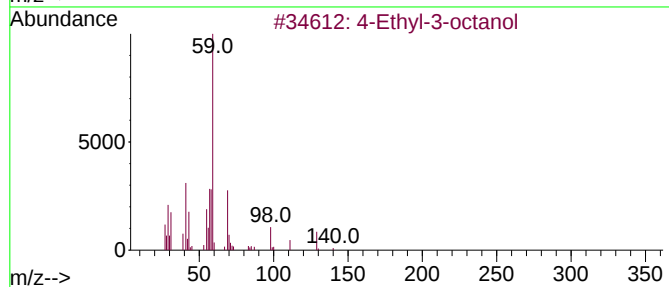
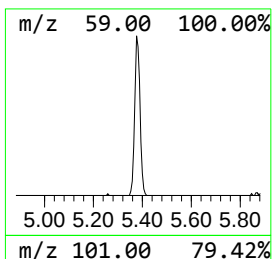
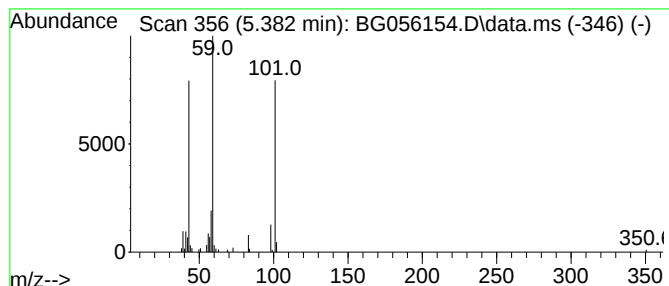
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown5.382 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.382	6.61 ng	88806	1,4-Dichlorobenzene-d4	8.338

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Ethyl-3-octanol	158	C10H22O	019781-26-1	32
2			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	32
3			1,1',1''-Nitrilotris(propan-2-ol...)	317	C15H27NO6	916309-81-4	25
4			Guanidine	59	CH5N3	000113-00-8	25
5			Dipropylene glycol, diacetate	218	C10H18O5	1000506-25-8	23



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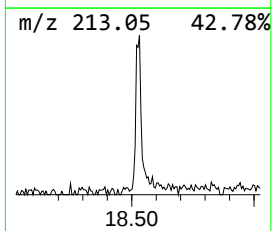
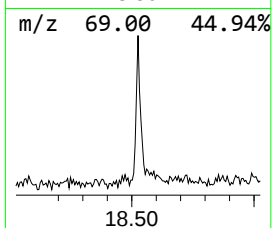
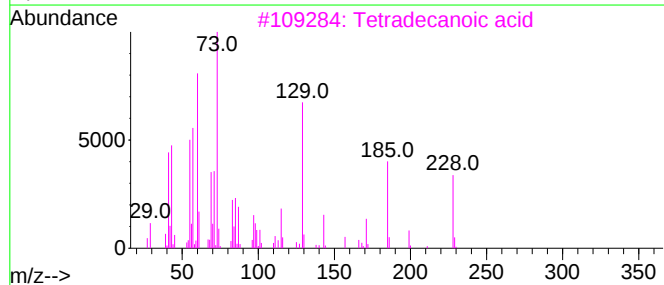
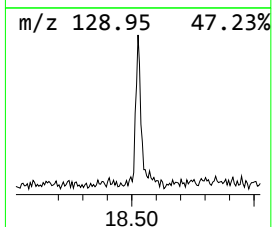
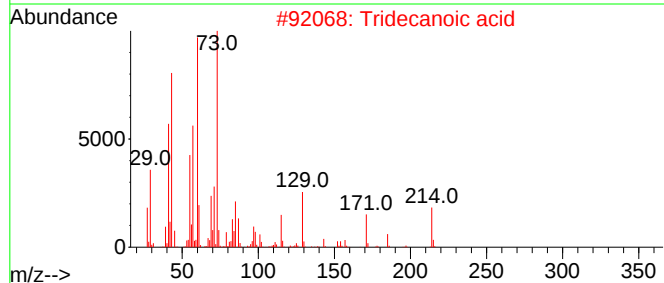
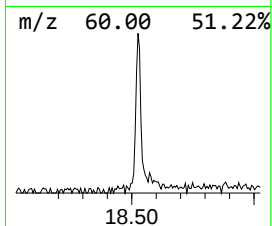
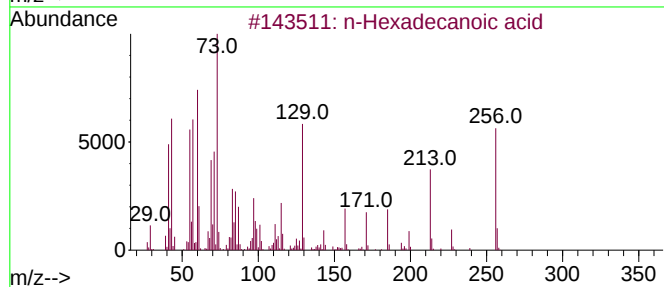
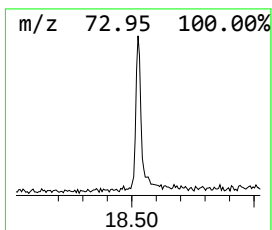
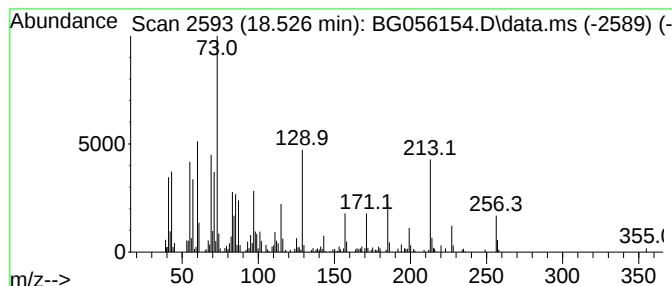
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.526	5.16 ng	208967	Phenanthrene-d10	17.680

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2			Tridecanoic acid	214	C13H26O2	000638-53-9	55
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	43
4			Undecanoic acid	186	C11H22O2	000112-37-8	38
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	27



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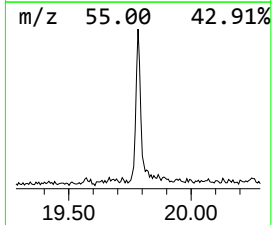
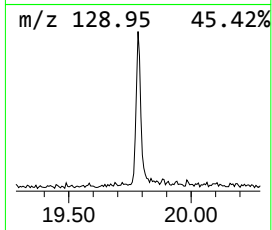
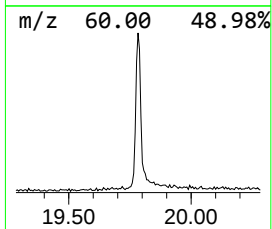
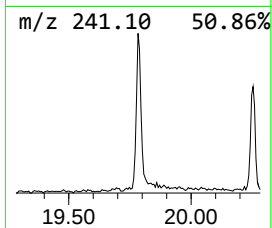
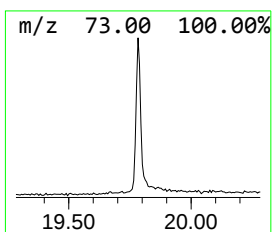
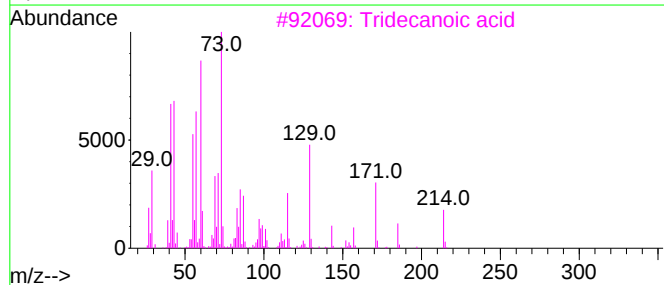
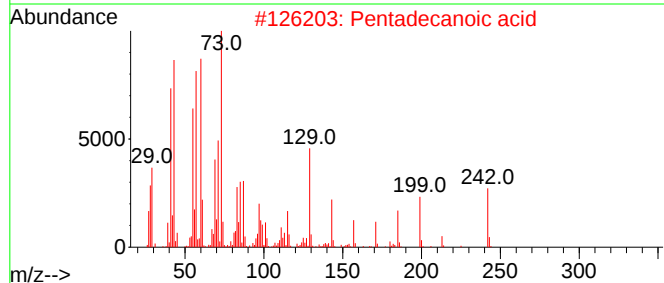
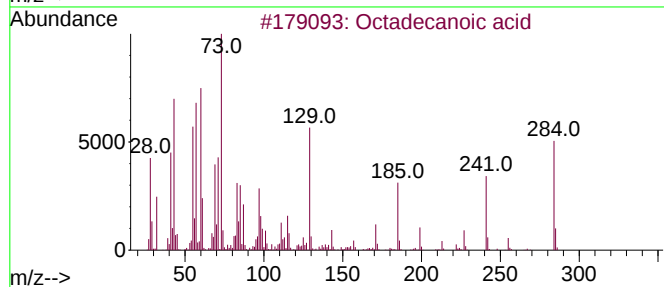
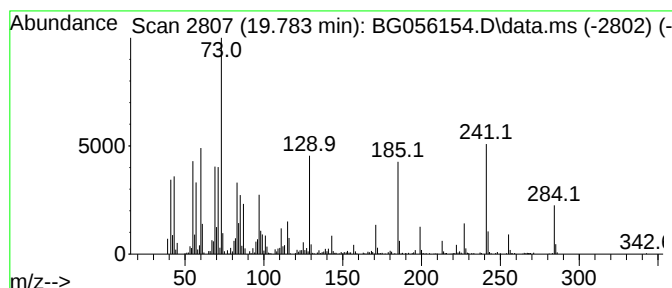
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Peak Number 4 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.783	19.37 ng	783868	Phenanthrene-d10	17.680

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	96
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	78
3			Tridecanoic acid	214	C13H26O2	000638-53-9	46
4			Dodecanoic acid	200	C12H24O2	000143-07-7	43
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	35



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.367	42.5	ng	570778	1	8.338	268541	20.0
unknown5.382	5.382	6.6	ng	88806	1	8.338	268541	20.0
n-Hexadecanoic ...	18.526	5.2	ng	208967	4	17.680	809507	20.0
Octadecanoic acid	19.783	19.4	ng	783868	4	17.680	809507	20.0