

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101823\
 Data File : BF135845.D
 Acq On : 18 Oct 2023 14:02
 Operator : CG\JU
 Sample : 04724-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 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_F\Methods\8270-BF101323.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135845.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.340	379	383	394	rBV2	20255	43823	1.44%	0.269%
2	4.957	484	488	509	rBV	428889	546331	17.90%	3.358%
3	5.375	556	559	586	rBV	994676	1364081	44.68%	8.385%
4	5.757	620	624	634	rBV	38566	45341	1.49%	0.279%
5	6.392	729	732	759	rBV	531148	826739	27.08%	5.082%
6	6.739	787	791	799	rBV	507245	502829	16.47%	3.091%
7	7.310	884	888	891	rBV	2030008	1807394	59.21%	11.111%
8	8.016	1005	1008	1016	rBV	672463	579078	18.97%	3.560%
9	9.098	1188	1192	1195	rBV	3417701	3052745	100.00%	18.766%
10	9.698	1291	1294	1300	rBV	36833	45890	1.50%	0.282%
11	9.775	1304	1307	1320	rVB	819765	667444	21.86%	4.103%
12	10.575	1439	1443	1459	rBV	1804674	1931218	63.26%	11.872%
13	10.769	1473	1476	1487	rBV3	48603	80117	2.62%	0.493%
14	11.274	1558	1562	1571	rBV	762113	688607	22.56%	4.233%
15	11.810	1649	1653	1665	rBV2	220400	292201	9.57%	1.796%
16	12.521	1768	1774	1781	rBV8	26245	53274	1.75%	0.327%
17	12.598	1784	1787	1797	rVB	98409	121260	3.97%	0.745%
18	12.874	1829	1834	1837	rBV	2847068	2758642	90.37%	16.958%
19	13.839	1993	1998	2004	rVB9	17236	32783	1.07%	0.202%
20	13.939	2011	2015	2025	rBV	436248	419082	13.73%	2.576%
21	15.421	2262	2267	2276	rBV	290382	408267	13.37%	2.510%

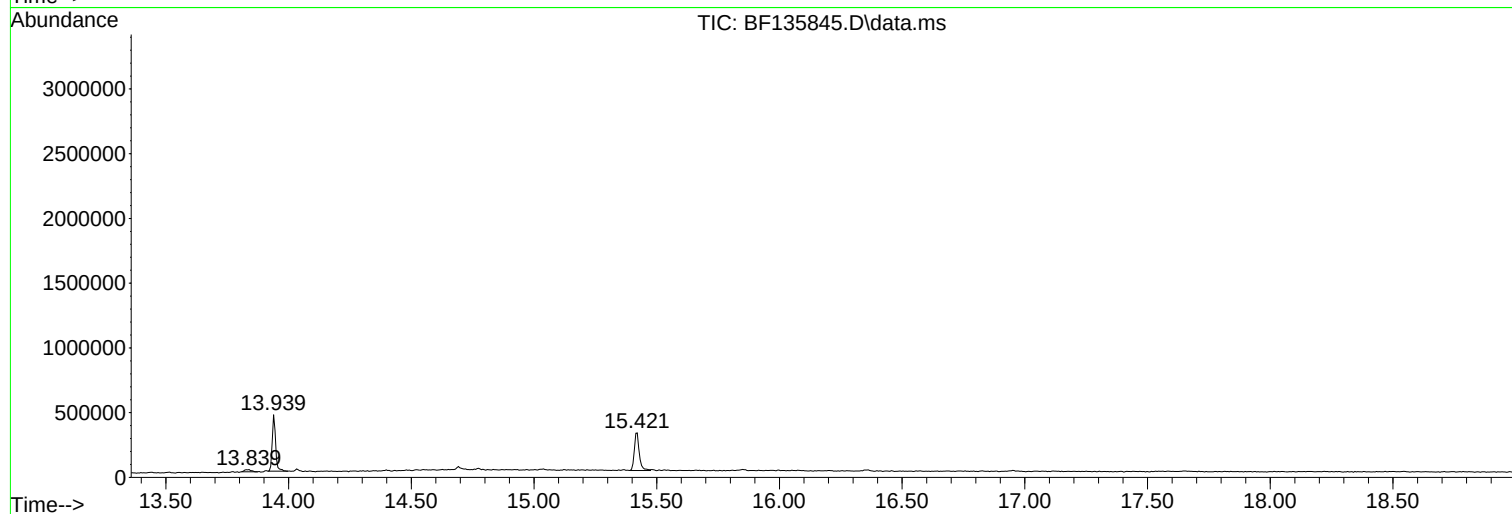
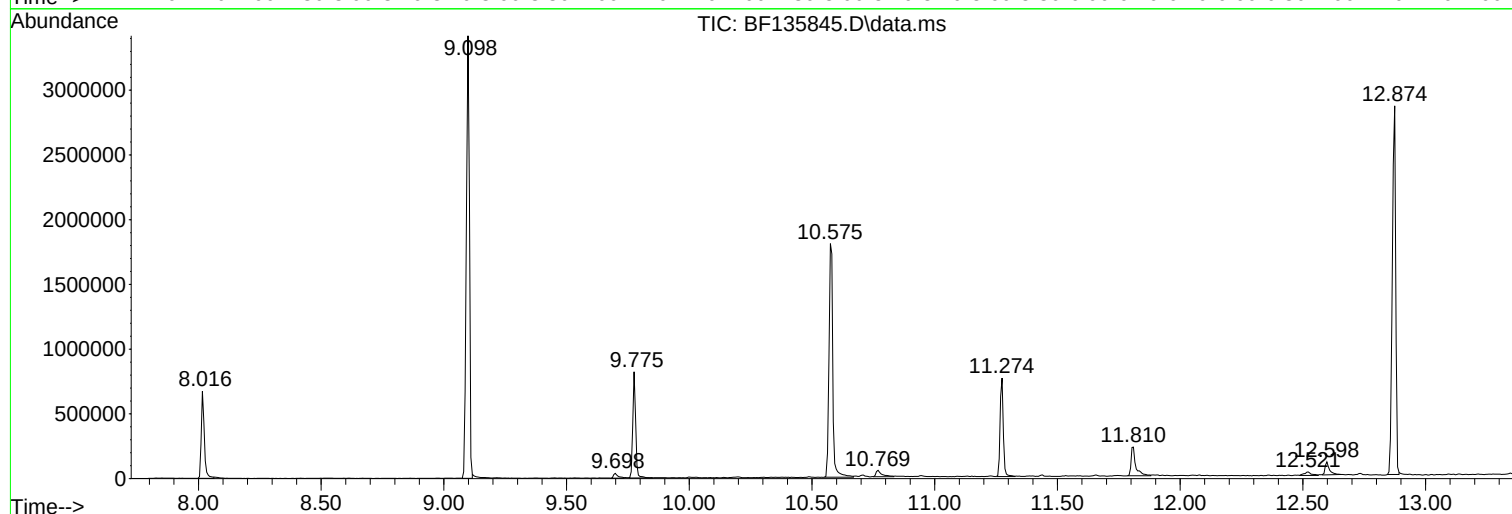
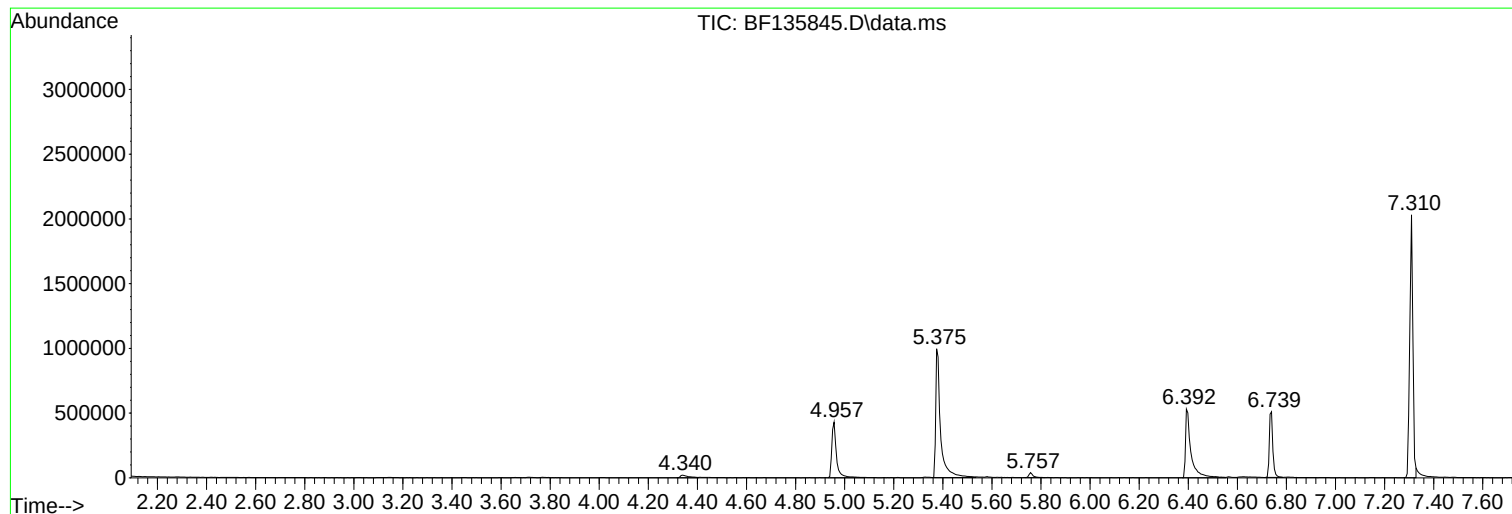
Sum of corrected areas: 16267146

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.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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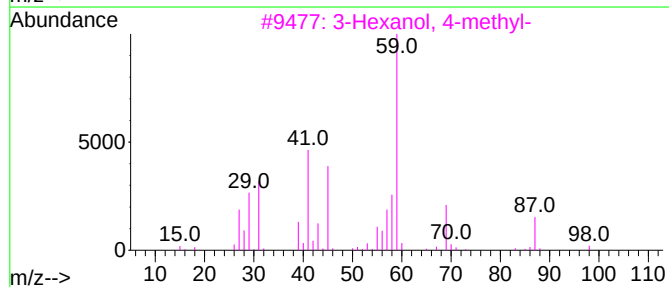
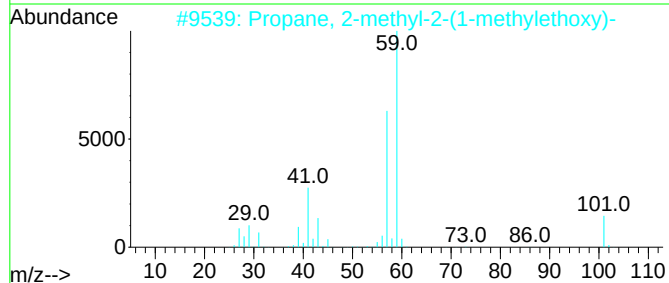
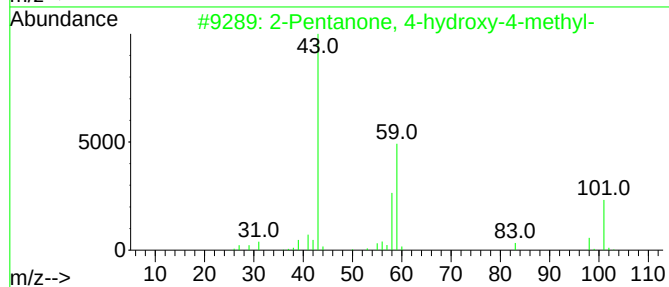
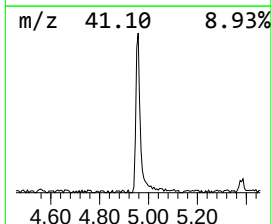
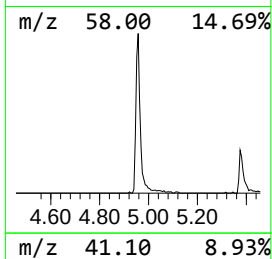
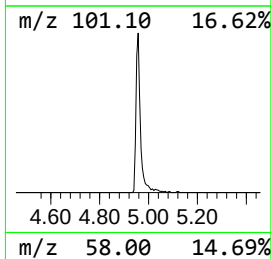
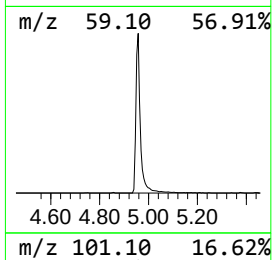
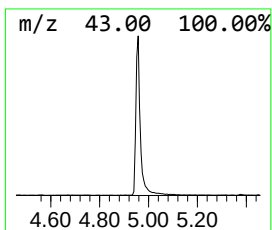
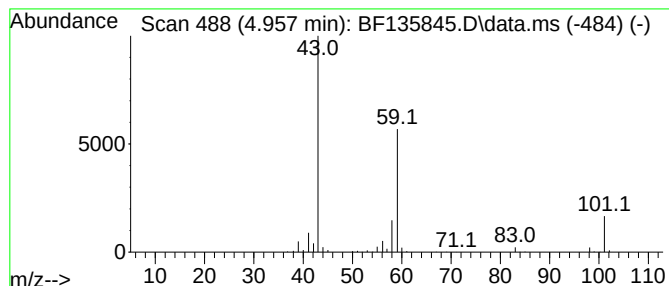
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.957	21.73 ng	546331	1,4-Dichlorobenzene-d4	6.739

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42		
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28		
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	25		



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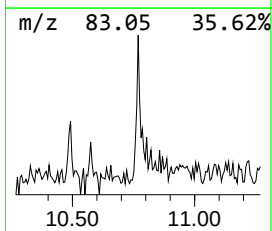
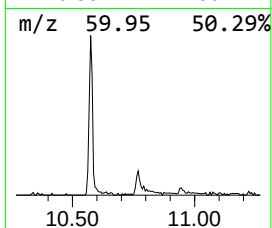
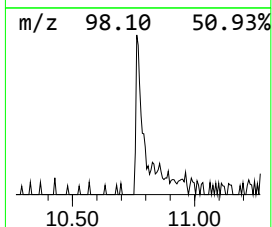
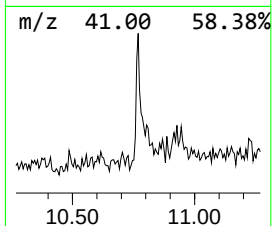
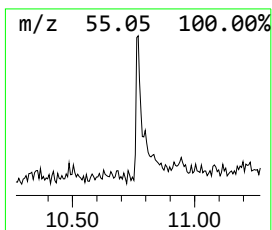
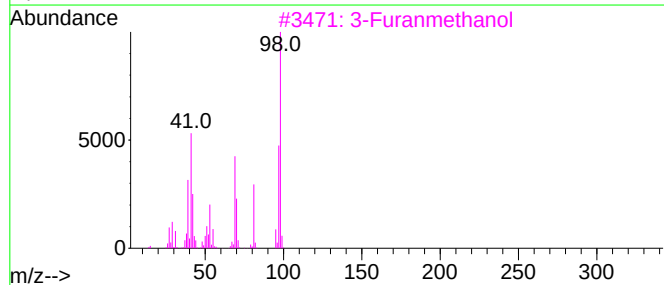
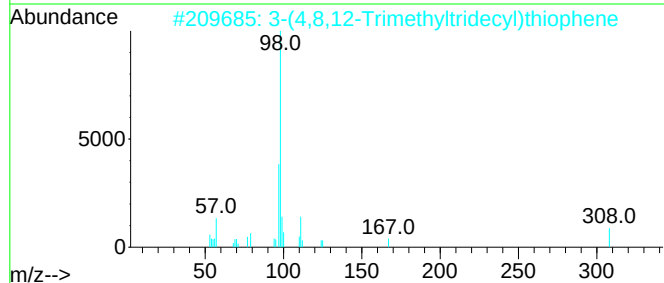
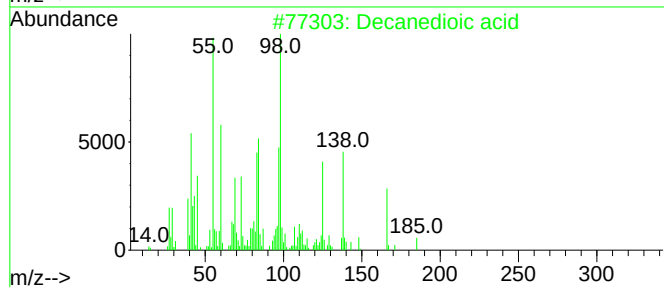
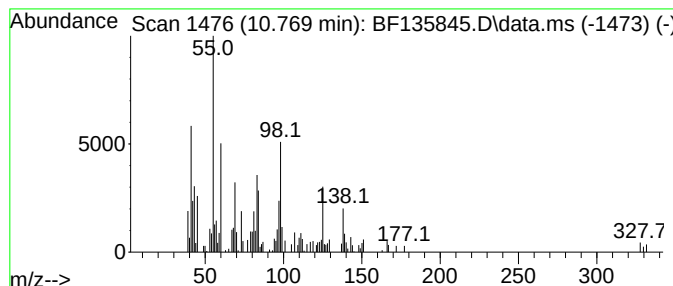
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Decanedioic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.769	2.33 ng	80117	Phenanthrene-d10	11.275

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decanedioic acid	202	C10H18O4	000111-20-6	64
2			3-(4,8,12-Trimethyltridecyl)thio...	308	C20H36S	102037-89-8	22
3			3-Furanmethanol	98	C5H6O2	004412-91-3	14
4			6-Methoxy-2,6-dihydropyran-3-one	128	C6H8O3	1000411-44-4	14
5			2-Furanmethanol	98	C5H6O2	000098-00-0	14



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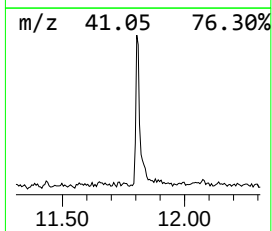
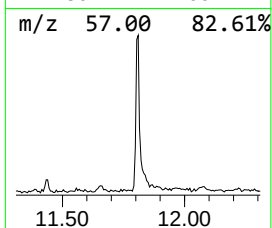
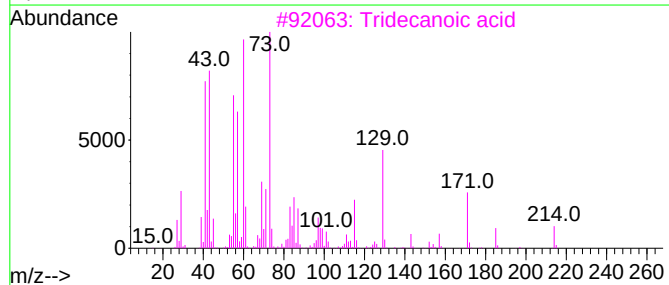
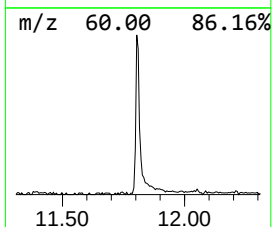
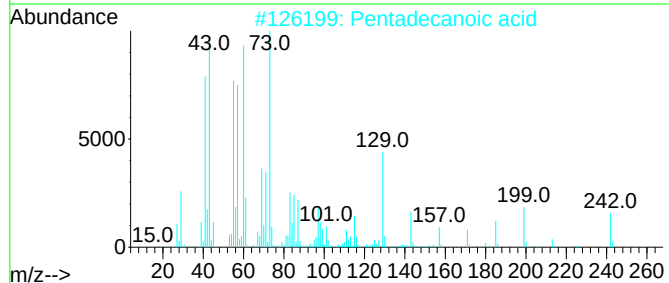
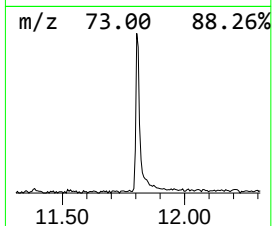
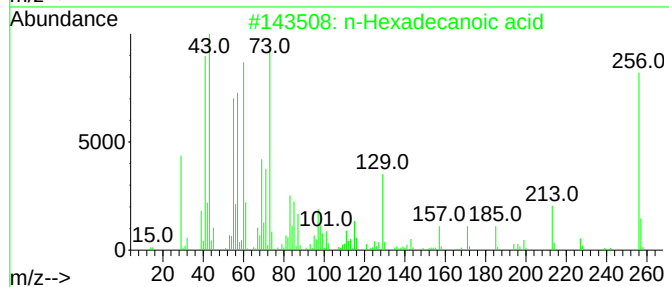
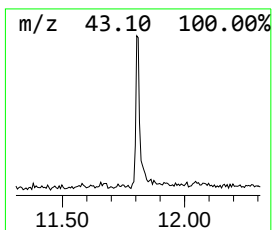
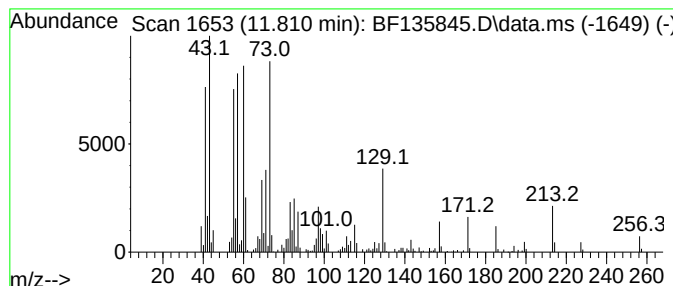
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.810	8.49 ng	292201	Phenanthrene-d10	11.275

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3			Tridecanoic acid	214	C13H26O2	000638-53-9	90
4			n-Decanoic acid	172	C10H20O2	000334-48-5	60
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	53



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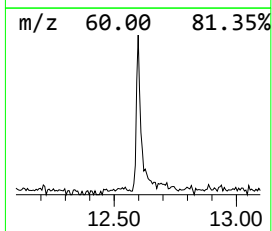
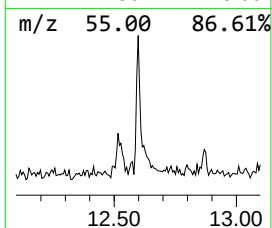
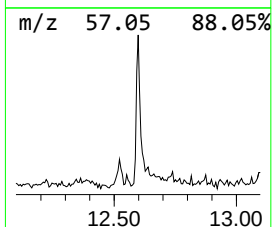
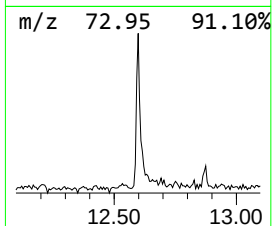
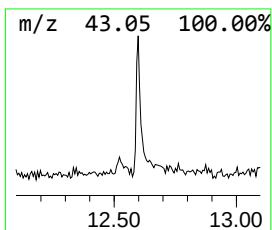
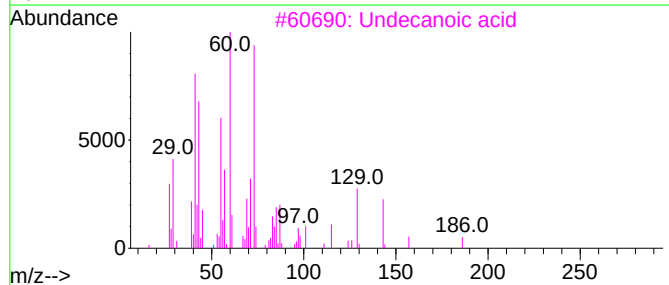
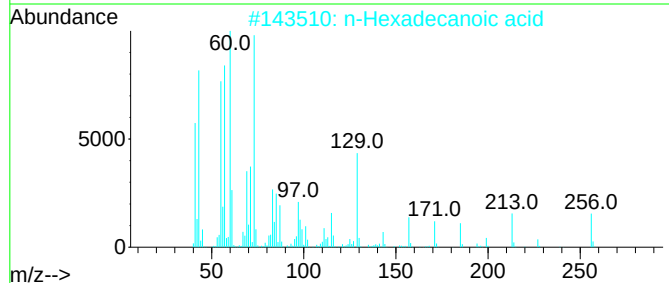
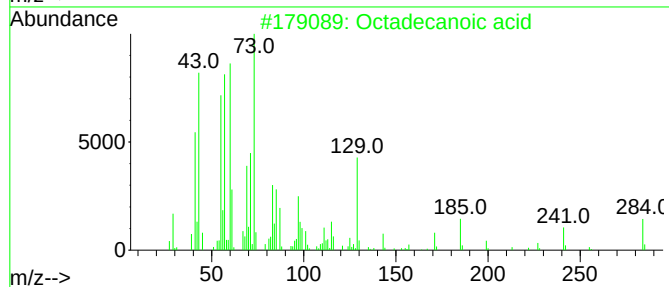
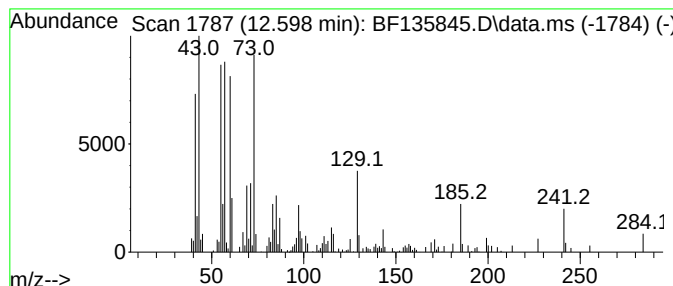
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Peak Number 4 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.598	3.52 ng	121260	Phenanthrene-d10	11.275

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	87
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81
3			Undecanoic acid	186	C11H22O2	000112-37-8	64
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	59
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	58



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.957	21.7	ng	546331	1	6.739	502829	20.0
Decanedioic acid	10.769	2.3	ng	80117	4	11.275	688607	20.0
n-Hexadecanoic ...	11.810	8.5	ng	292201	4	11.275	688607	20.0
Octadecanoic acid	12.598	3.5	ng	121260	4	11.275	688607	20.0