

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101723\
 Data File : BF135809.D
 Acq On : 17 Oct 2023 13:35
 Operator : CG\JU
 Sample : 04740-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RW4

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: BF135809.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.328	377	381	394	rBV	18539	40832	1.60%	0.308%
2	4.946	483	486	497	rBV	339454	418038	16.39%	3.149%
3	5.375	555	559	576	rBV	732724	1079188	42.30%	8.130%
4	5.757	619	624	632	rBV	36601	42811	1.68%	0.323%
5	6.393	729	732	755	rBV	398944	610326	23.92%	4.598%
6	6.734	787	790	804	rVB	445960	414537	16.25%	3.123%
7	7.304	883	887	906	rBV	1710994	1563160	61.27%	11.776%
8	8.016	1005	1008	1023	rBV	601812	514814	20.18%	3.878%
9	9.092	1187	1191	1195	rBV	2806275	2551171	100.00%	19.220%
10	9.775	1303	1307	1312	rBV	604958	526002	20.62%	3.963%
11	10.569	1438	1442	1455	rBV	1508087	1518041	59.50%	11.436%
12	11.269	1558	1561	1570	rVB	595807	517797	20.30%	3.901%
13	11.804	1647	1652	1663	rBV2	174082	249067	9.76%	1.876%
14	12.592	1782	1786	1793	rBV	79121	103232	4.05%	0.778%
15	12.869	1828	1833	1836	rBV	2402149	2224768	87.21%	16.761%
16	13.933	2011	2014	2023	rVB	438801	435346	17.06%	3.280%
17	14.027	2024	2030	2035	rBV5	20708	42727	1.67%	0.322%
18	15.033	2198	2201	2206	rVB4	18153	27894	1.09%	0.210%
19	15.410	2261	2265	2273	rVB	281908	393977	15.44%	2.968%

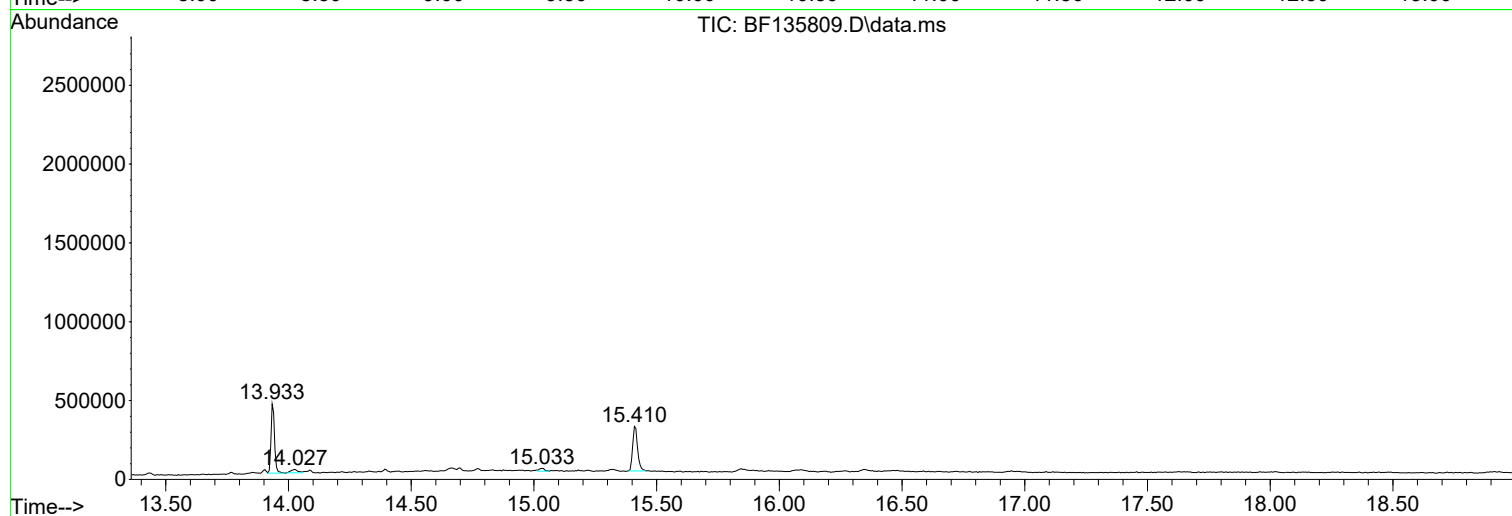
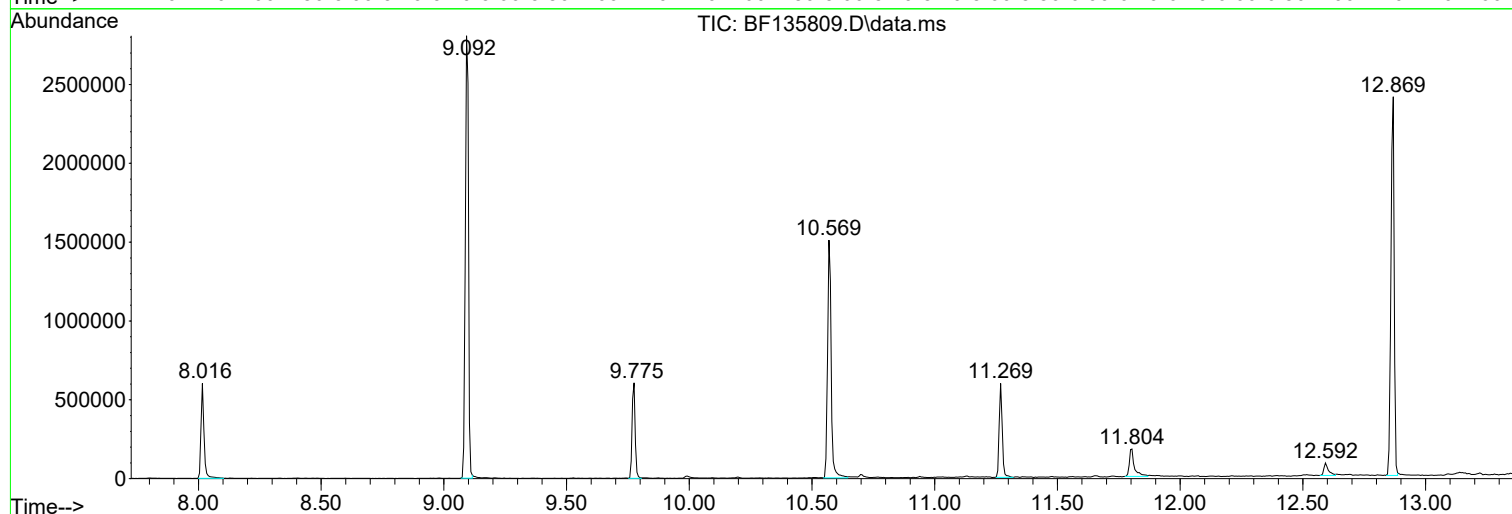
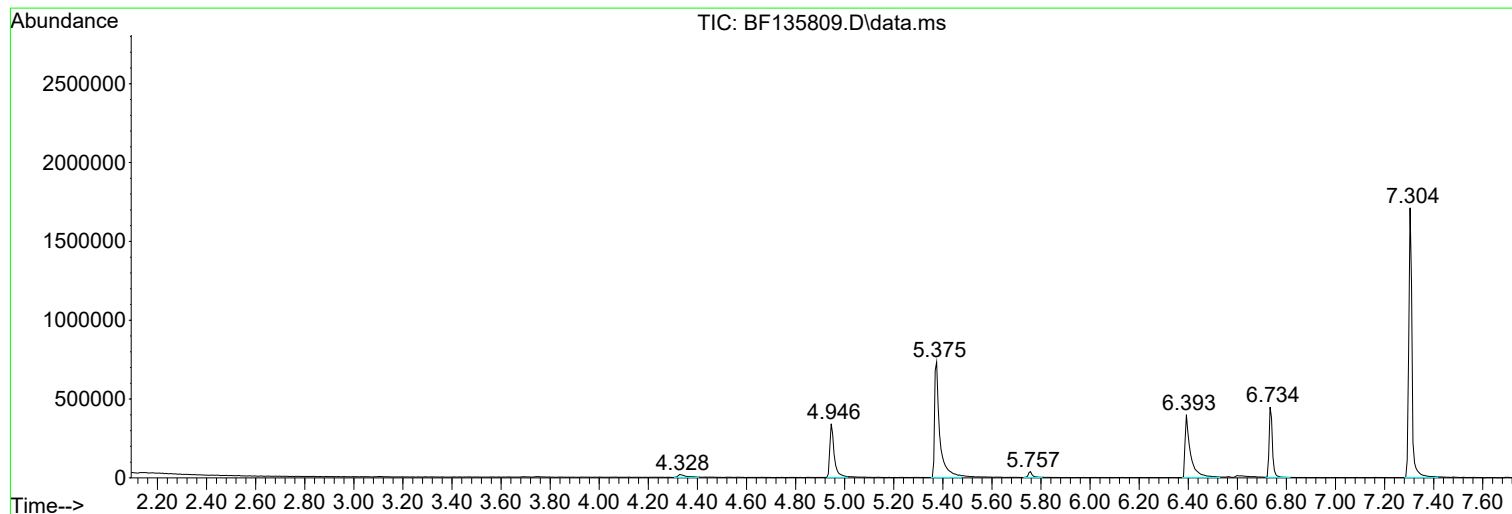
Sum of corrected areas: 13273728

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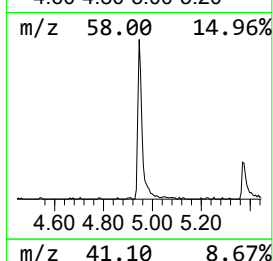
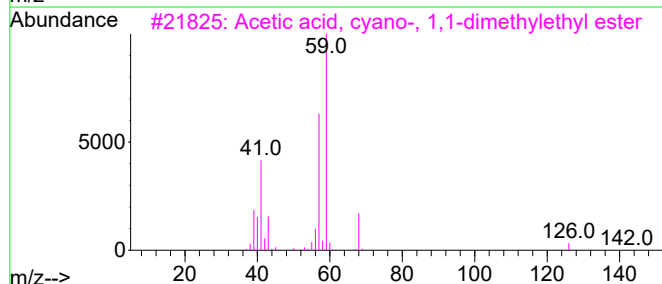
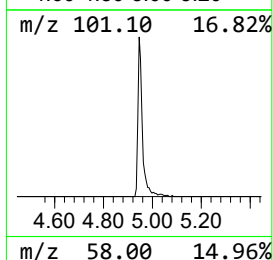
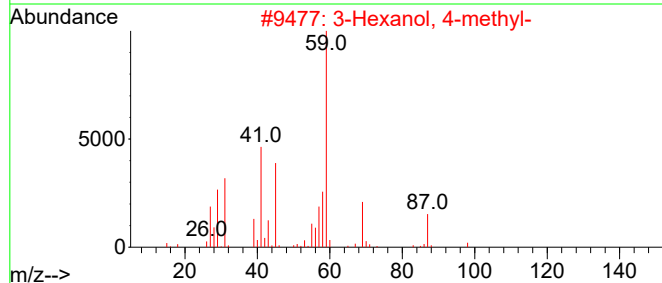
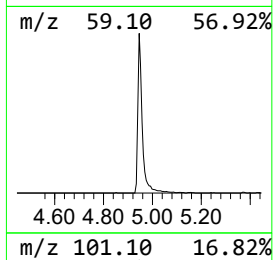
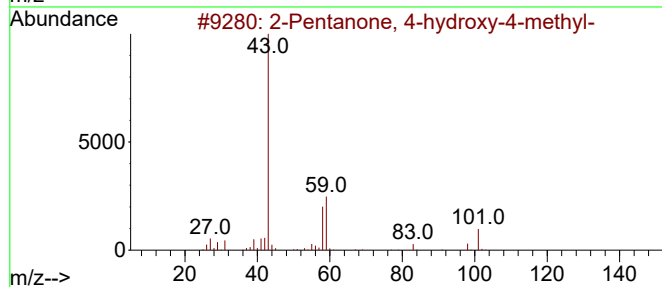
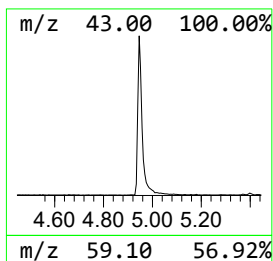
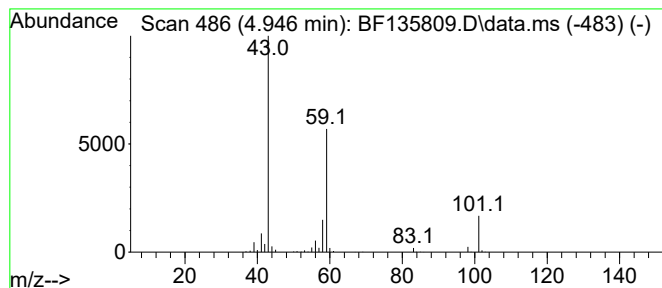
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD			R.T.
4.946	20.17 ng	418038	1,4-Dichlorobenzene-d4			6.734
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59	
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33	
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25	
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10	
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9	



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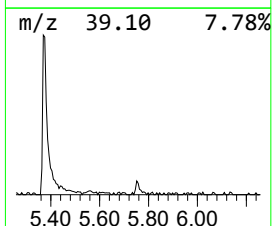
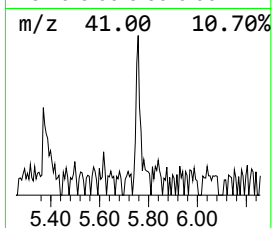
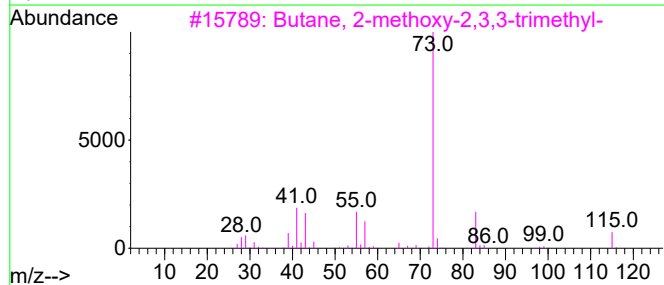
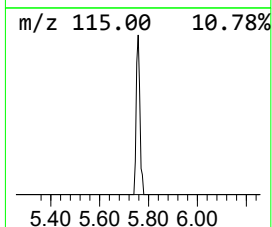
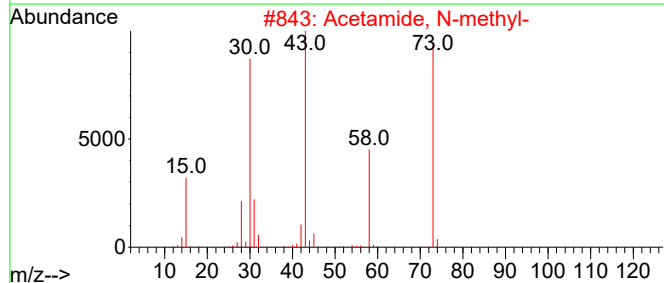
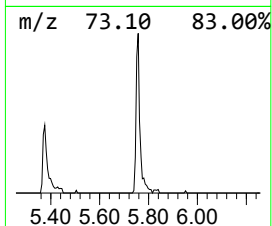
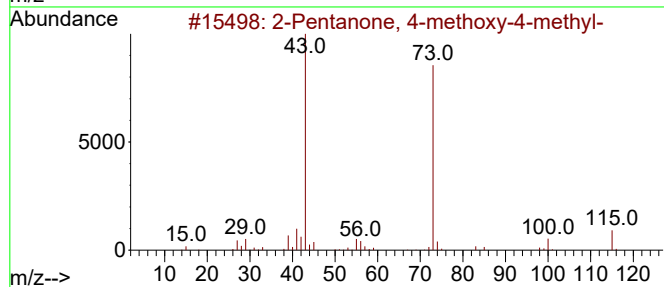
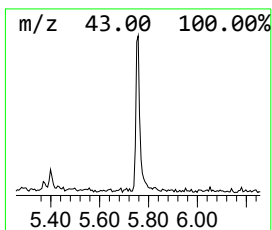
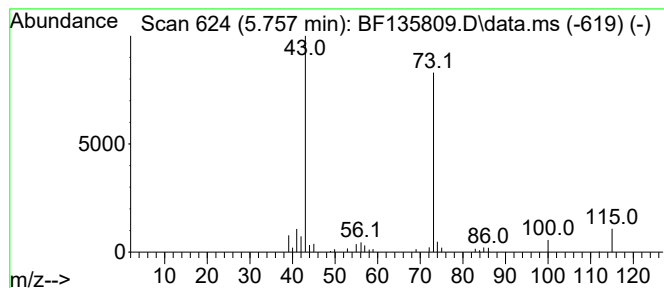
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 2-Pentanone, 4-methoxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.757	2.07 ng	42811	1,4-Dichlorobenzene-d4	6.734

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	90
2		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	32
3		Butane, 2-methoxy-2,3,3-trimethyl-	130	C8H18O	027705-21-1	23
4		3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	23
5		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	17



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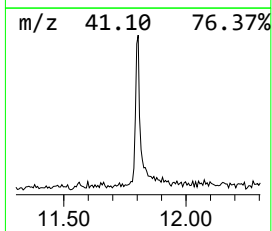
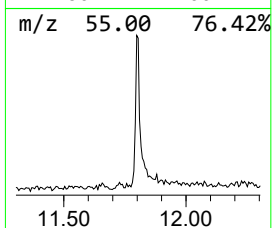
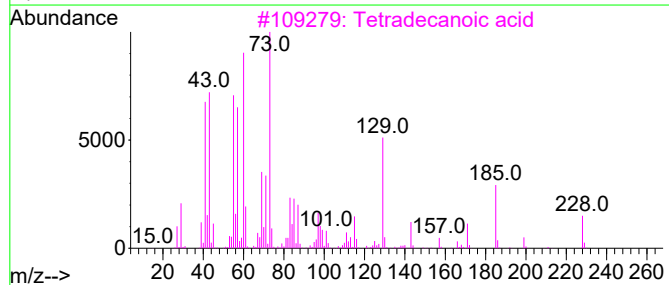
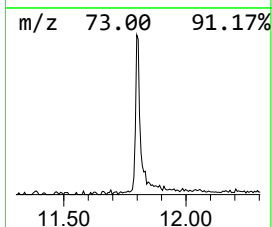
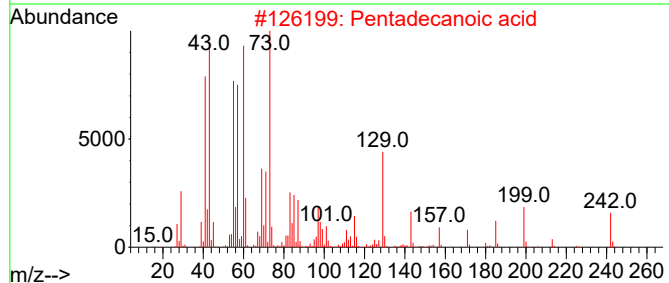
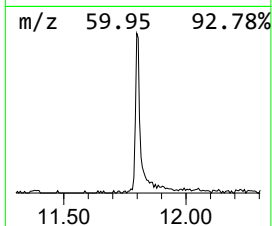
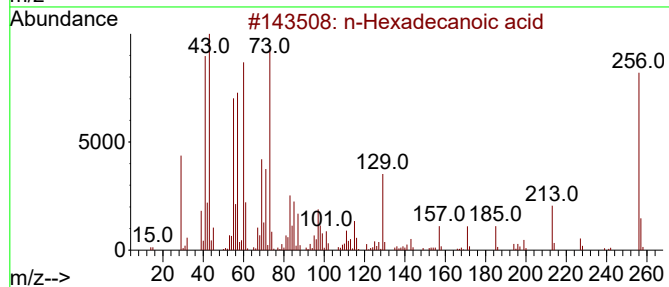
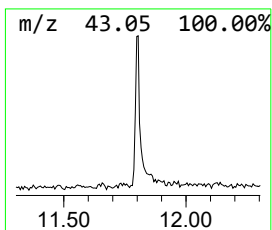
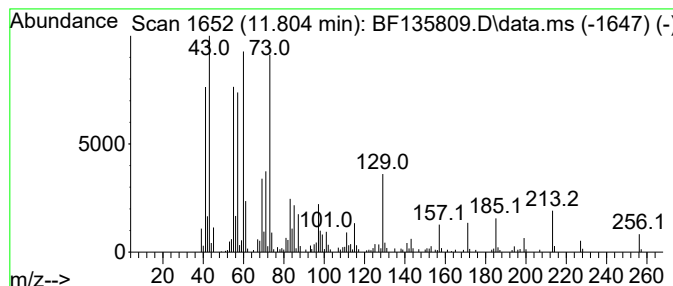
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.804	9.62 ng	249067	Phenanthrene-d10	11.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4			Tridecanoic acid	214	C13H26O2	000638-53-9	62
5			Dodecanoic acid	200	C12H24O2	000143-07-7	58



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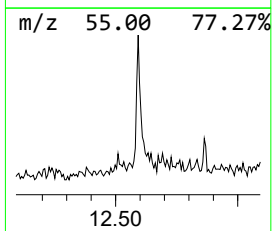
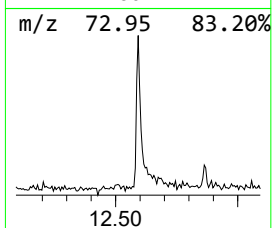
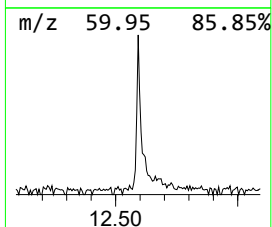
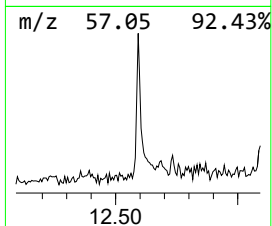
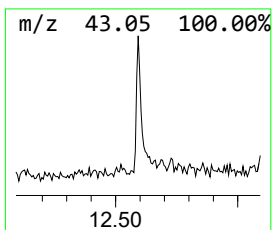
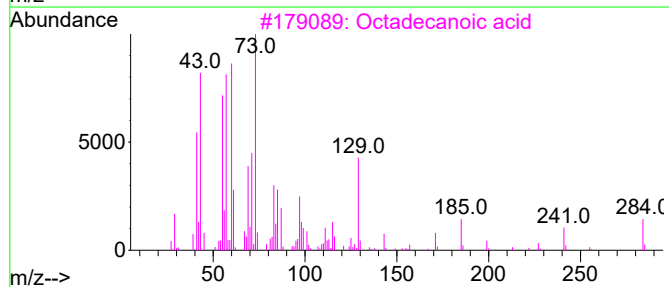
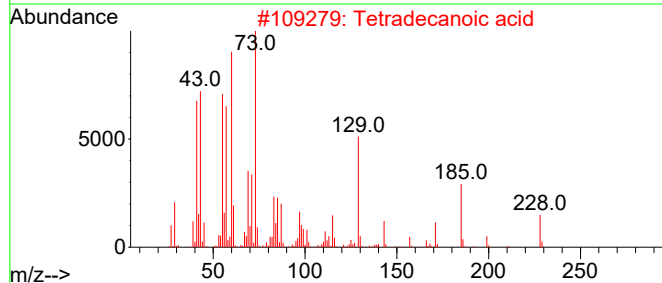
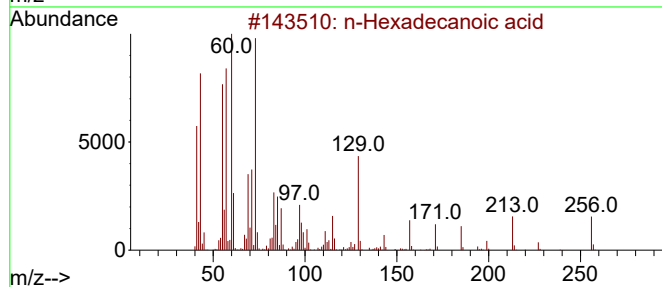
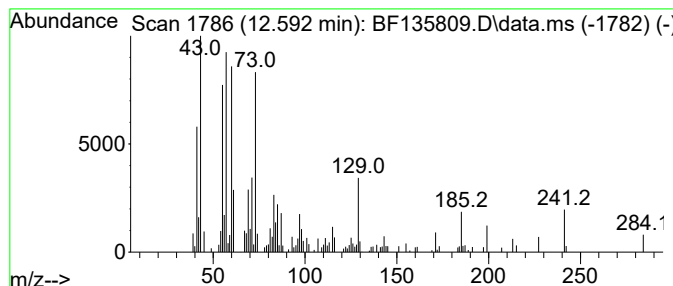
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Peak Number 4 Tetradecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.592	3.99 ng	103232	Phenanthrene-d10	11.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
3			Octadecanoic acid	284	C18H36O2	000057-11-4	72
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	64
5			Dodecanoic acid	200	C12H24O2	000143-07-7	59



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.946	20.2	ng	418038	1	6.734	414537	20.0
2-Pentanone, 4-...	5.757	2.1	ng	42811	1	6.734	414537	20.0
n-Hexadecanoic ...	11.804	9.6	ng	249067	4	11.269	517797	20.0
Tetradecanoic acid	12.592	4.0	ng	103232	4	11.269	517797	20.0