

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072723\
 Data File : BF134512.D
 Acq On : 27 Jul 2023 18:49
 Operator : CG\JU
 Sample : 03706-07
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B-P21A

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-BF072423.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134512.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.069	504	507	515	rBV	38506	50560	3.32%	0.474%
2	5.463	571	574	591	rBV	1537491	1521688	100.00%	14.273%
3	6.469	741	745	771	rBV	1478289	1429655	93.95%	13.409%
4	6.822	802	805	815	rBV	510451	490285	32.22%	4.599%
5	7.386	897	901	912	rBV	835731	814301	53.51%	7.638%
6	8.104	1019	1023	1038	rBV	626219	525409	34.53%	4.928%
7	9.180	1202	1206	1209	rBV	1823451	1493921	98.18%	14.012%
8	9.292	1222	1225	1229	rVB	25724	21945	1.44%	0.206%
9	9.863	1318	1322	1325	rBV	722363	591323	38.86%	5.546%
10	10.239	1383	1386	1392	rBV	69302	53082	3.49%	0.498%
11	10.657	1453	1457	1466	rBV	990731	882531	58.00%	8.278%
12	11.357	1572	1576	1582	rBV	539994	469301	30.84%	4.402%
13	11.851	1657	1660	1663	rBV3	18470	20379	1.34%	0.191%
14	11.886	1663	1666	1678	rVB	189745	221636	14.57%	2.079%
15	12.674	1797	1800	1807	rBV2	37627	48774	3.21%	0.457%
16	12.951	1843	1847	1850	rBV	1234871	1120210	73.62%	10.507%
17	13.857	1997	2001	2013	rBV2	83233	186698	12.27%	1.751%
18	14.015	2025	2028	2032	rBV	437068	379469	24.94%	3.559%
19	14.474	2104	2106	2108	rBV2	22647	18865	1.24%	0.177%
20	15.133	2215	2218	2222	rVB3	25816	32581	2.14%	0.306%
21	15.515	2279	2283	2291	rVB	223049	289027	18.99%	2.711%

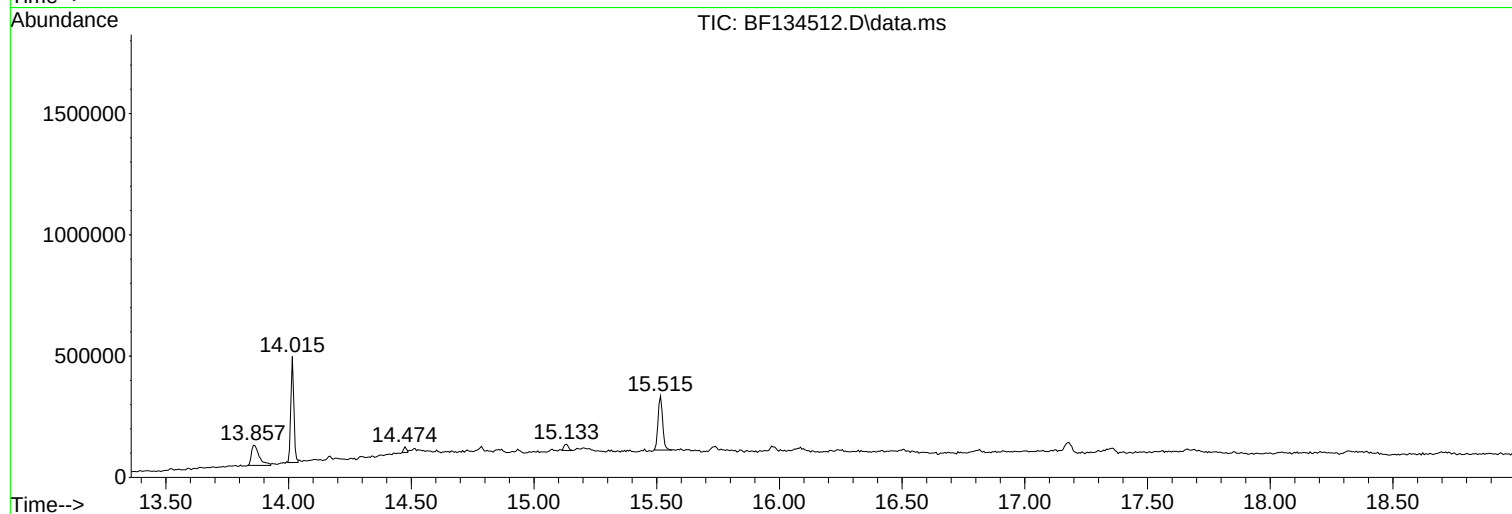
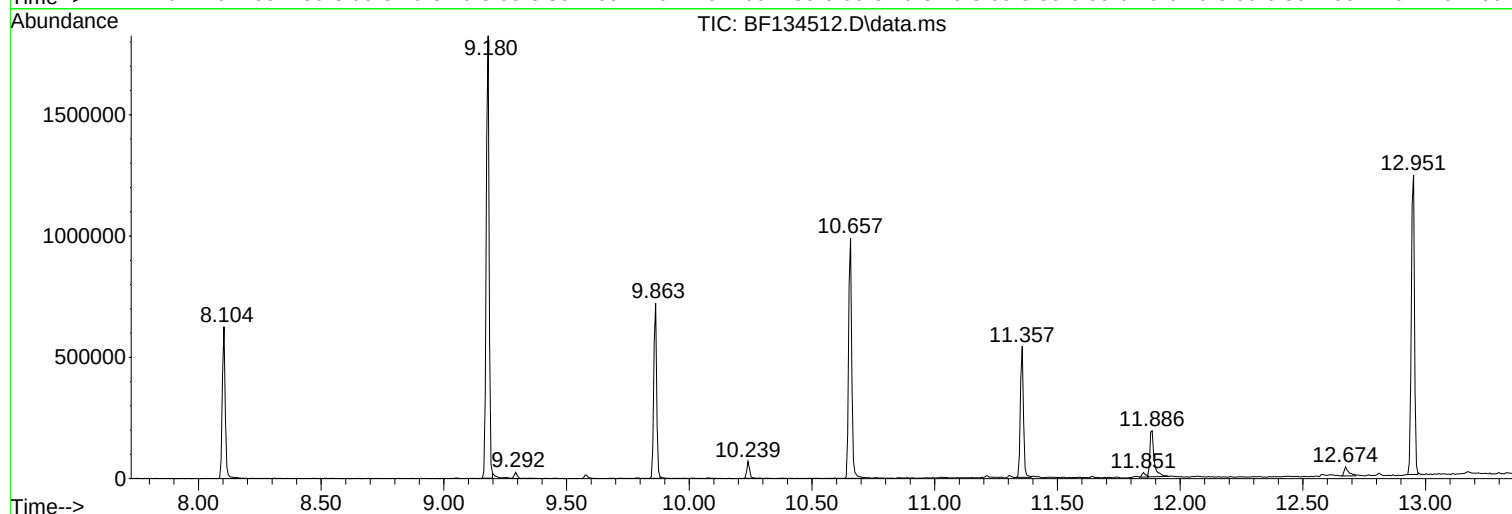
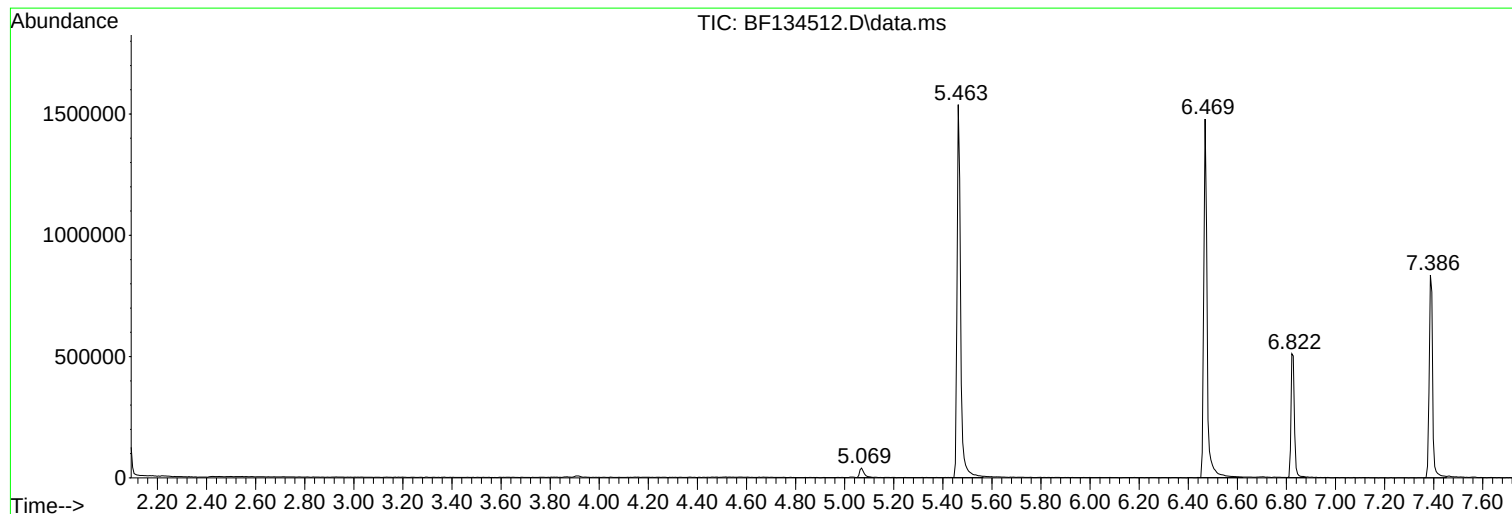
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072423.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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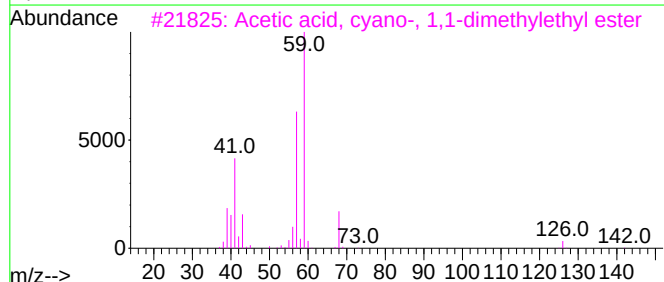
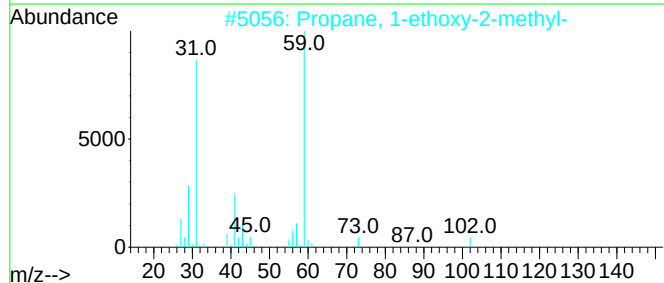
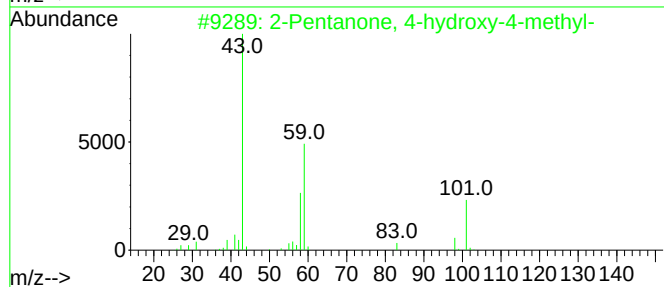
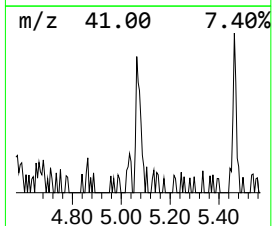
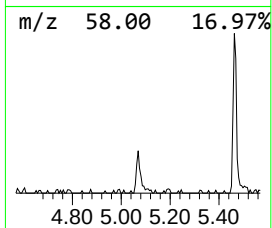
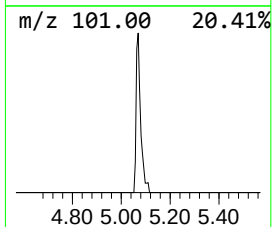
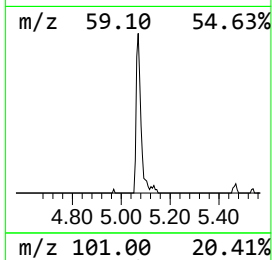
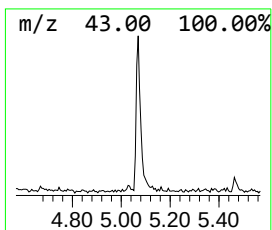
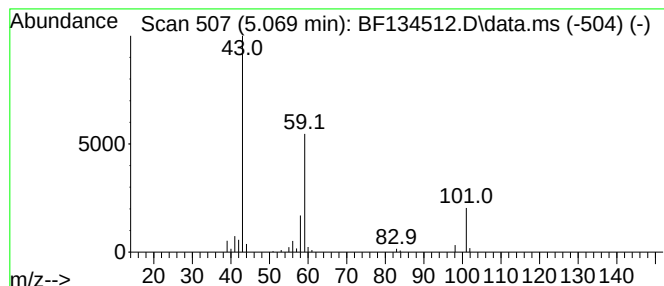
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.069	2.06 ng	50560	1,4-Dichlorobenzene-d4	6.828

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72		
2	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	17		
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	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9		



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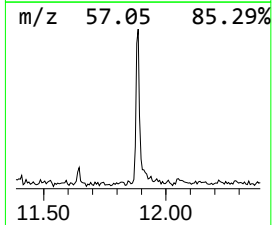
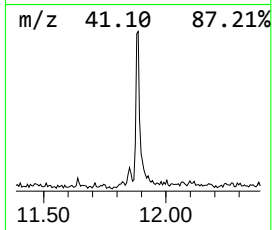
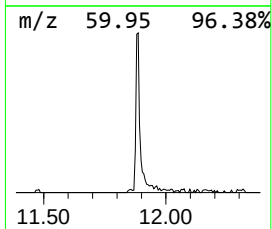
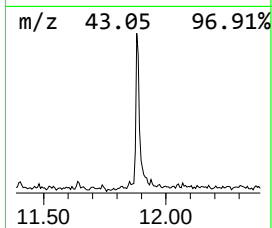
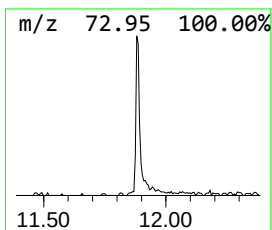
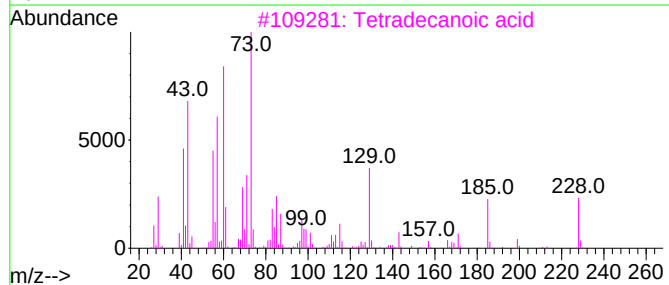
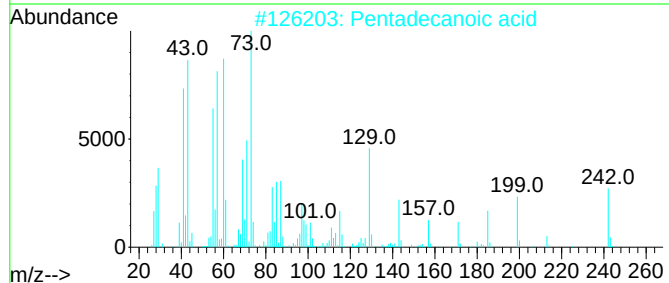
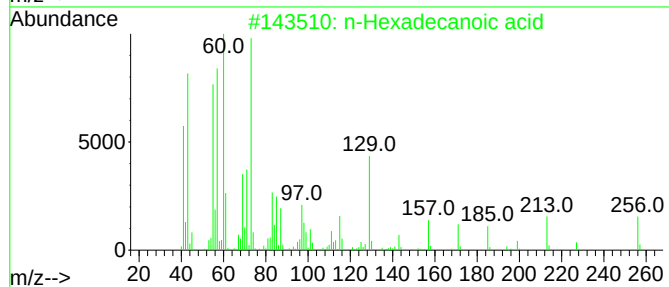
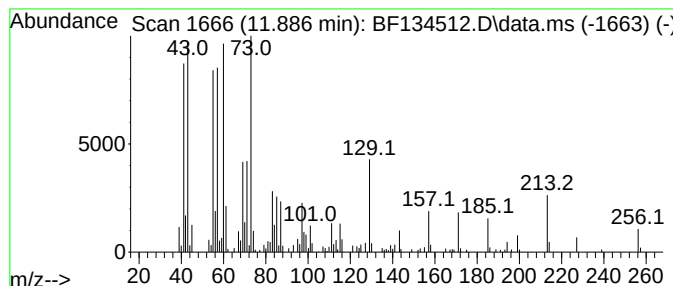
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.886	9.45 ng	221636	Phenanthrene-d10	11.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4			n-Decanoic acid	172	C10H20O2	000334-48-5	76
5			Tridecanoic acid	214	C13H26O2	000638-53-9	74



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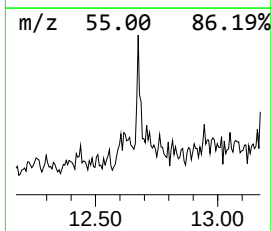
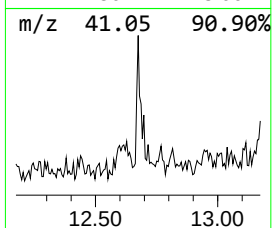
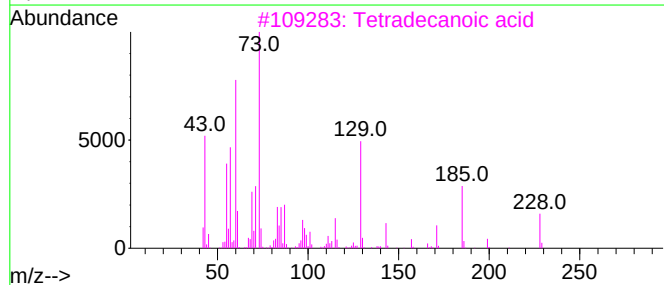
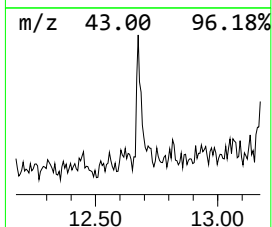
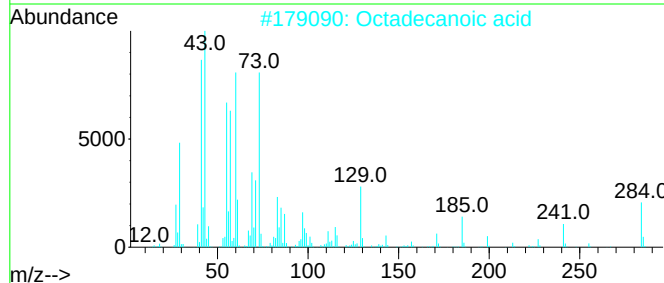
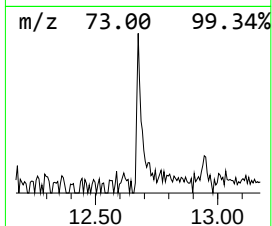
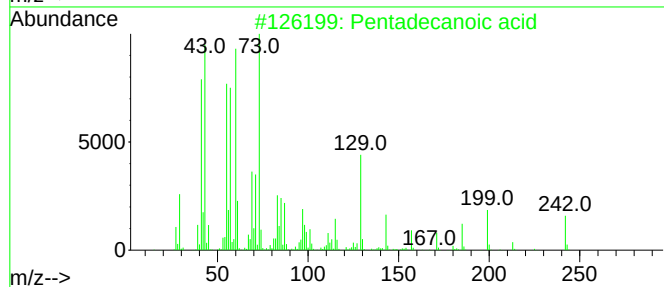
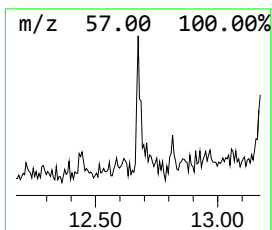
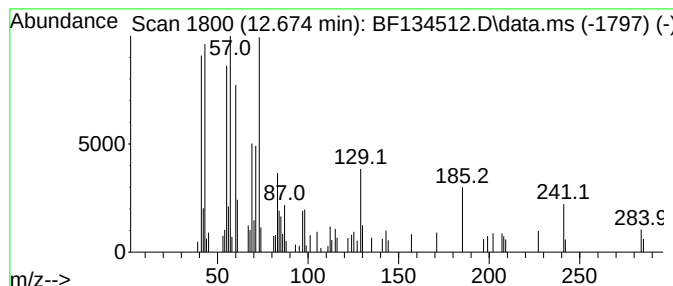
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Peak Number 3 Pentadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.674	2.08 ng	48774	Phenanthrene-d10	11.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
2			Octadecanoic acid	284	C18H36O2	000057-11-4	68
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4			Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	58
5			n-Decanoic acid	172	C10H20O2	000334-48-5	47



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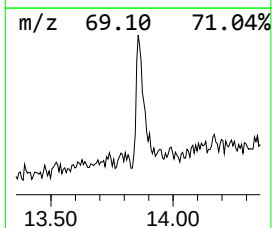
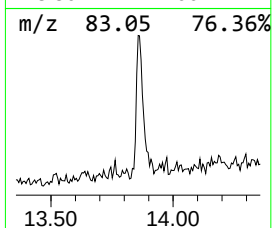
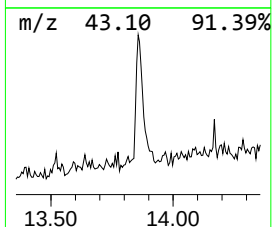
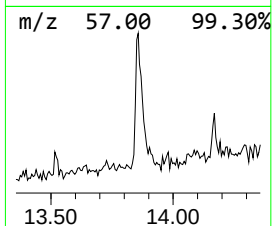
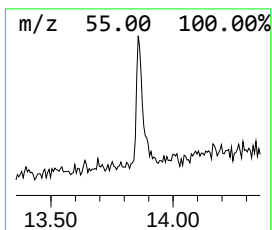
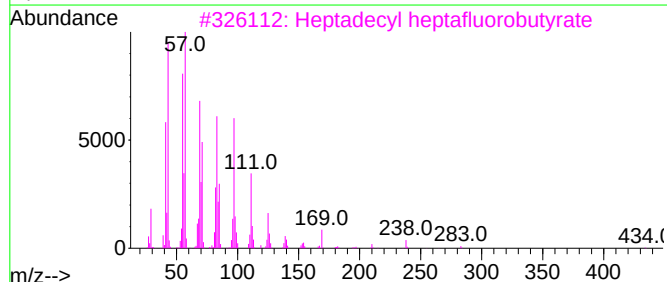
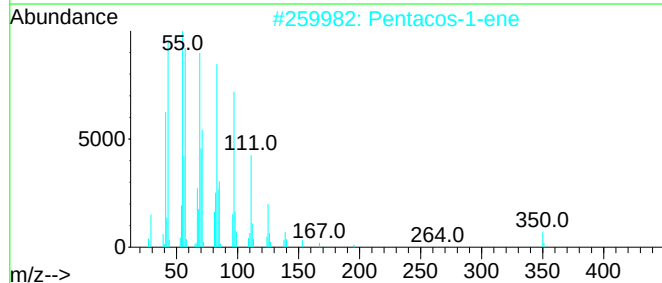
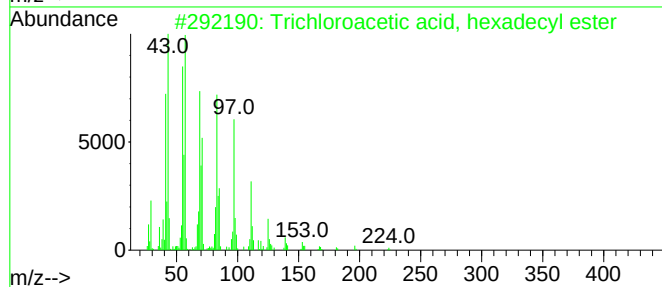
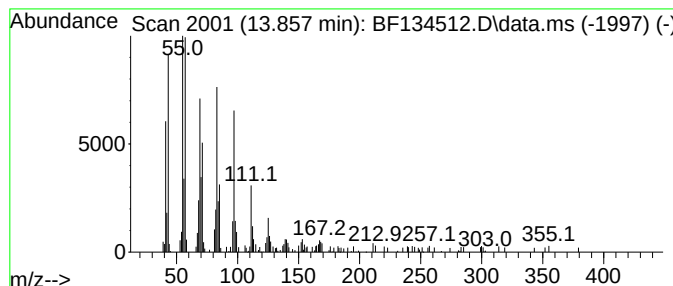
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Peak Number 4 Trichloroacetic acid, hexad... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.857	9.84 ng	186698	Chrysene-d12	14.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	95
2			Pentacos-1-ene	350	C25H50	016980-85-1	94
3			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
4			Cyclotetracosane	336	C24H48	000297-03-0	94
5			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	91



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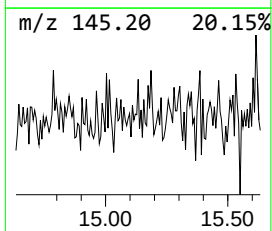
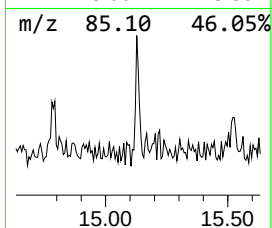
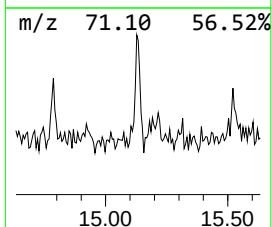
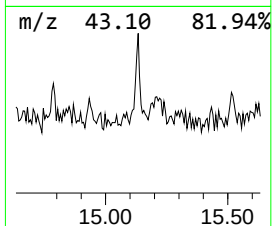
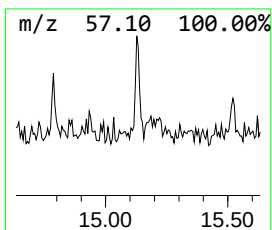
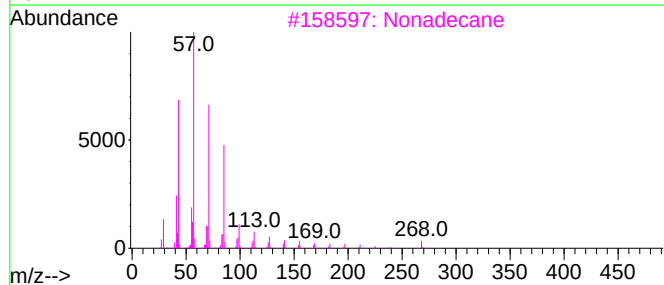
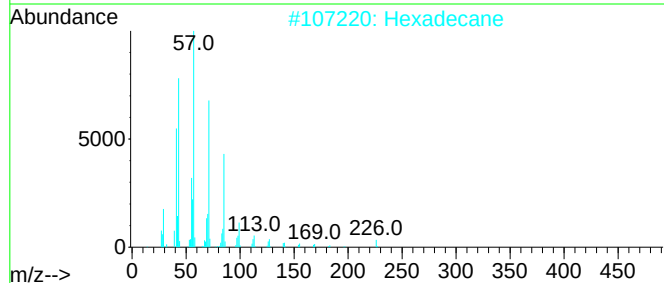
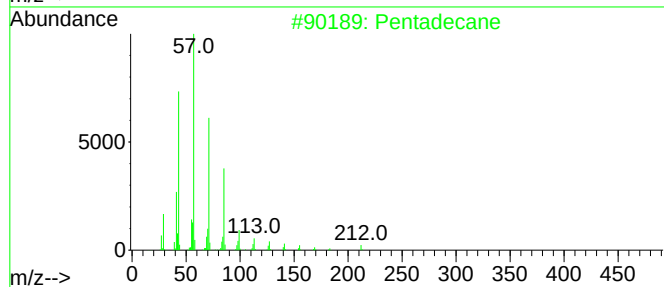
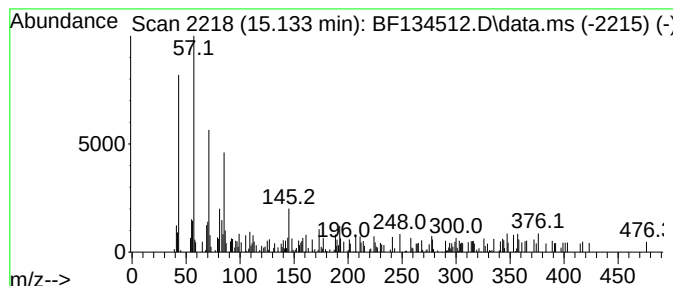
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Peak Number 5 Pentadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.133	2.25 ng	32581	Perylene-d12	15.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecane	212	C15H32	000629-62-9	62
2			Hexadecane	226	C16H34	000544-76-3	56
3			Nonadecane	268	C19H40	000629-92-5	41
4			Pentadecane, 5-methyl-	226	C16H34	025117-33-3	41
5			Heptadecane, 3-methyl-	254	C18H38	006418-44-6	41



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.069	2.1	ng	50560	1	6.828	490285	20.0
n-Hexadecanoic ...	11.886	9.4	ng	221636	4	11.357	469301	20.0
Pentadecanoic acid	12.674	2.1	ng	48774	4	11.357	469301	20.0
Trichloroacetic...	13.857	9.8	ng	186698	5	14.015	379469	20.0
Pentadecane	15.133	2.3	ng	32581	6	15.515	289027	20.0