

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM071824\
 Data File : BM046711.D
 Acq On : 18 Jul 2024 20:42
 Operator : MA/JU
 Sample : P3246-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 WC-CTW2-BL-01

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_M\Methods\8270-BM071724.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM046711.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.363	60	64	71	rVB	20386	28186	1.15%	0.181%
2	4.687	282	289	297	rVB	57628	86393	3.52%	0.556%
3	5.128	358	364	374	rBV	1048745	1473409	60.09%	9.476%
4	6.687	622	629	637	rBV	1049203	1555025	63.42%	10.001%
5	7.486	758	765	773	rBV	323822	484594	19.76%	3.117%
6	8.628	951	959	967	rBV	693604	1061008	43.27%	6.824%
7	10.245	1223	1234	1241	rBV	368474	583921	23.81%	3.756%
8	10.998	1357	1362	1368	rBV3	29583	55453	2.26%	0.357%
9	12.745	1652	1659	1666	rBV	1583268	2254647	91.95%	14.501%
10	14.133	1888	1895	1901	rBV	507566	731600	29.84%	4.705%
11	15.633	2143	2150	2159	rBV	1276653	1798575	73.35%	11.568%
12	16.886	2357	2363	2370	rVB	583468	790415	32.24%	5.084%
13	17.821	2517	2522	2530	rBV	170751	255893	10.44%	1.646%
14	19.115	2737	2742	2751	rBV2	80364	131491	5.36%	0.846%
15	19.539	2809	2814	2820	rBV	2035123	2451951	100.00%	15.770%
16	20.850	3034	3037	3042	rVB2	90065	109502	4.47%	0.704%
17	21.109	3076	3081	3087	rBV	548615	771093	31.45%	4.959%
18	23.874	3544	3551	3562	rVB	410076	924940	37.72%	5.949%

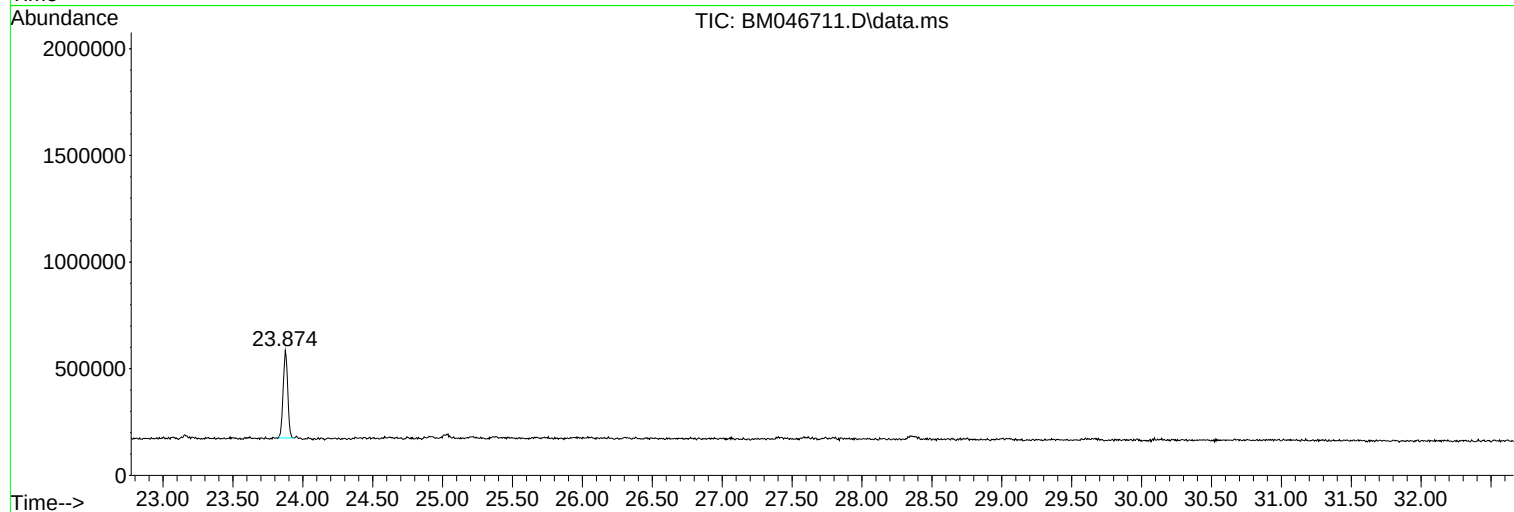
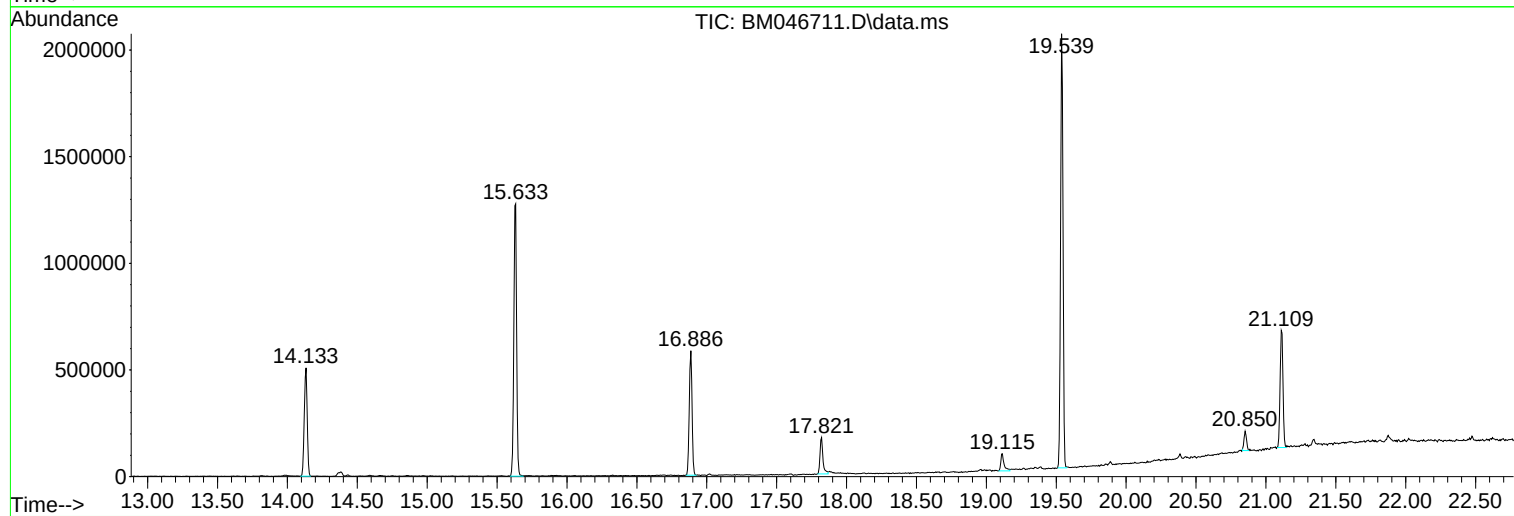
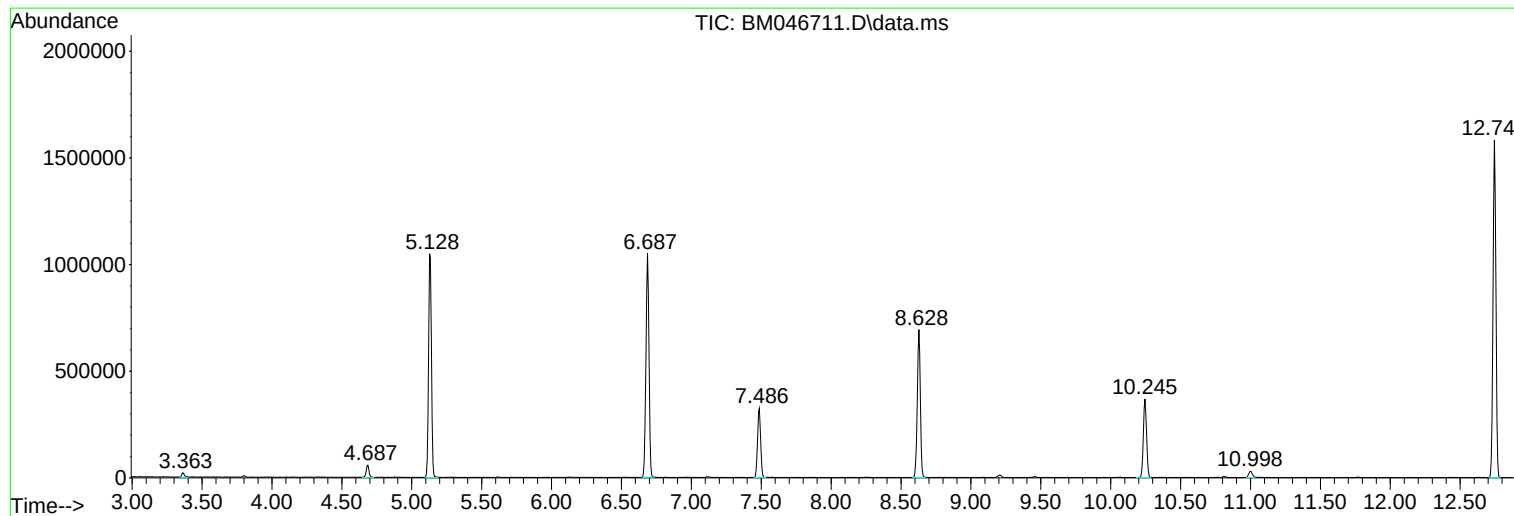
Sum of corrected areas: 15548096

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



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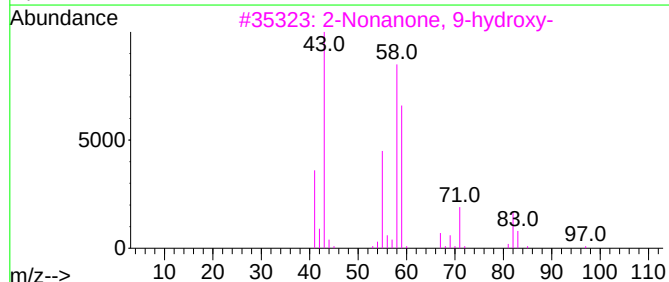
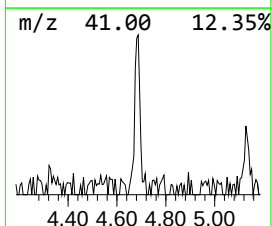
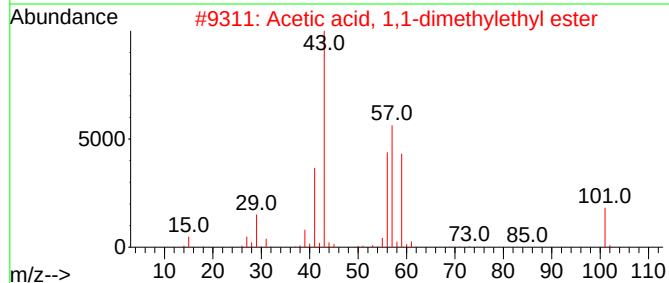
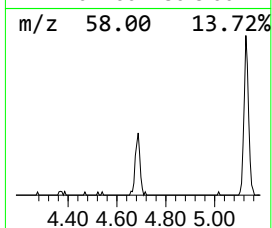
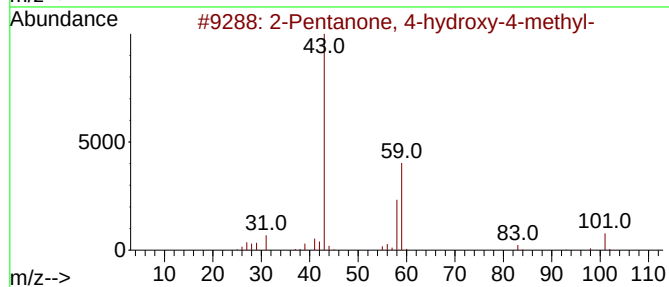
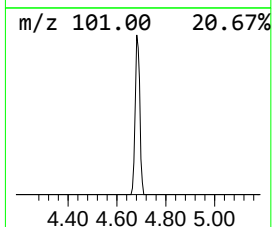
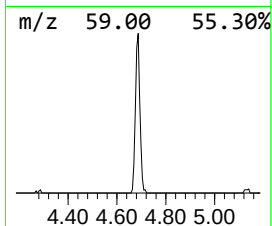
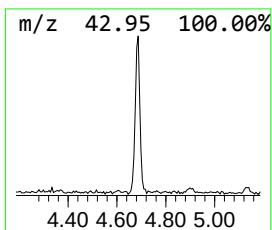
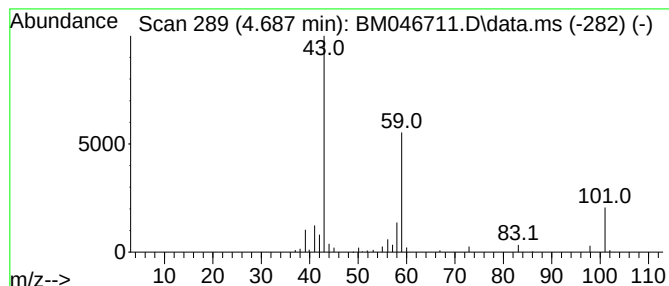
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.687	3.57 ng	86393	1,4-Dichlorobenzene-d4	7.486

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39		
3	2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	33		
4	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	32		
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25		



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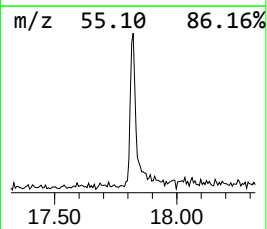
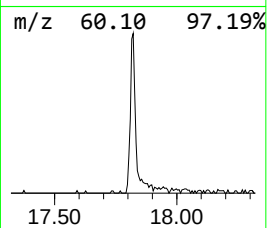
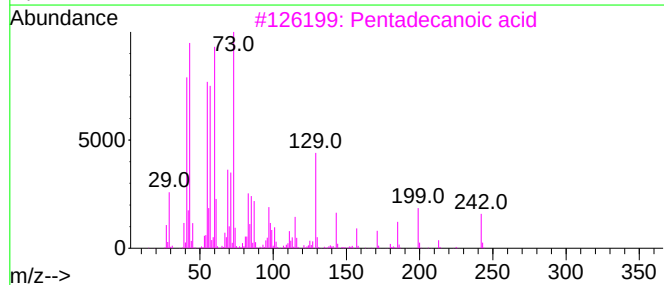
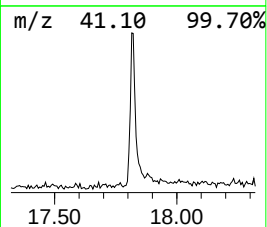
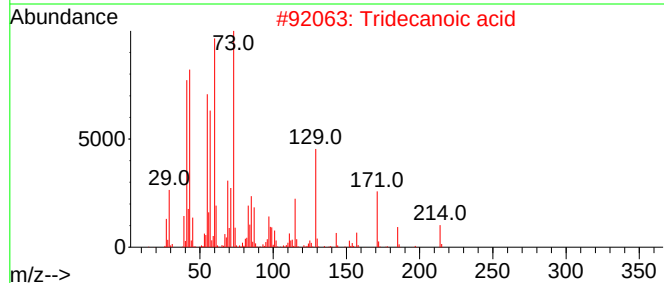
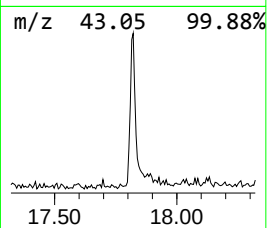
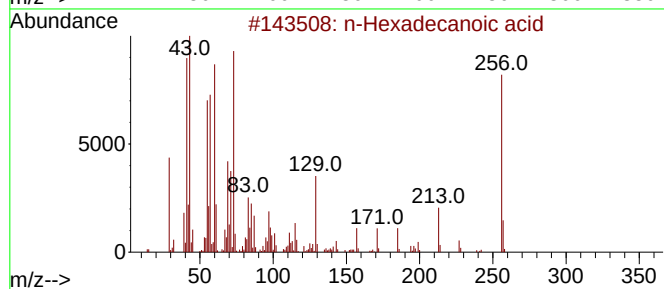
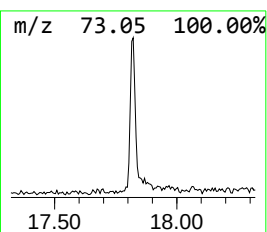
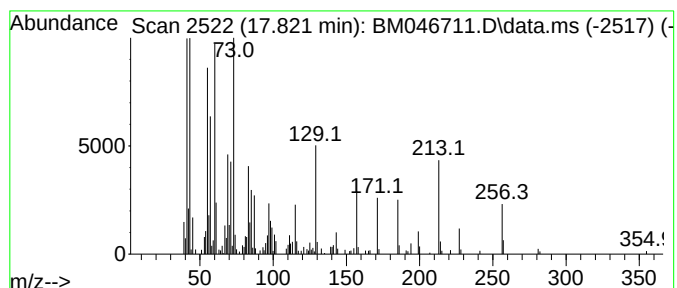
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.821	6.47 ng	255893	Phenanthrene-d10	16.886

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2			Tridecanoic acid	214	C13H26O2	000638-53-9	60
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	52
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	50
5			Dodecanoic acid	200	C12H24O2	000143-07-7	49



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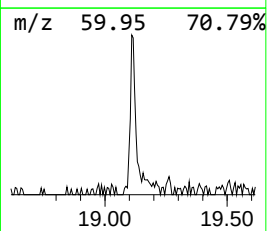
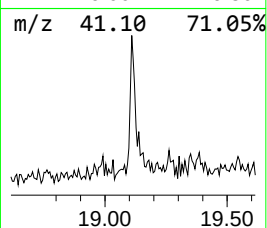
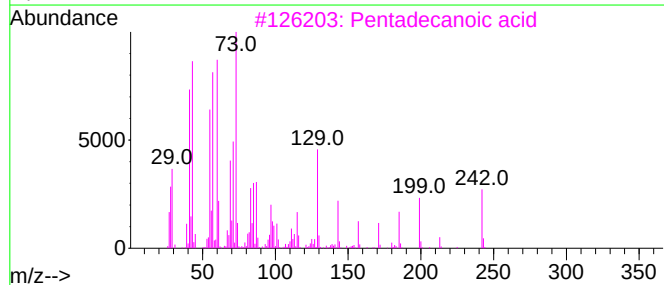
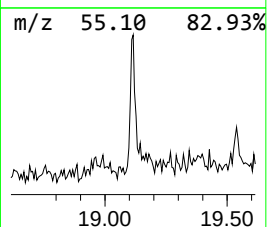
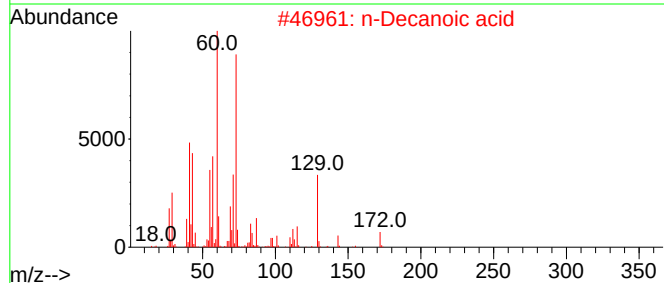
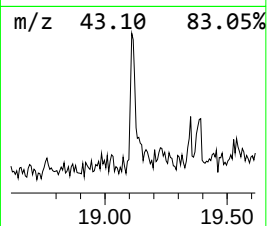
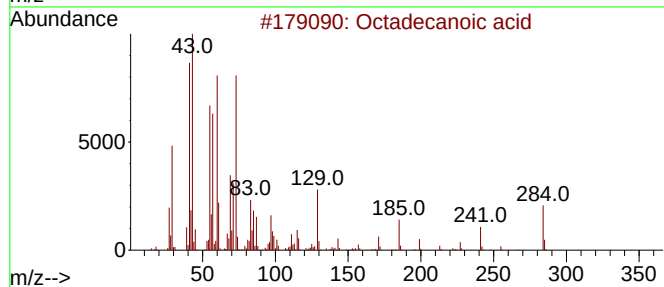
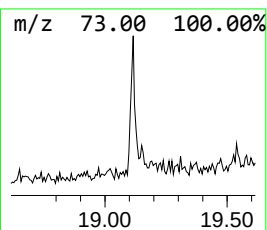
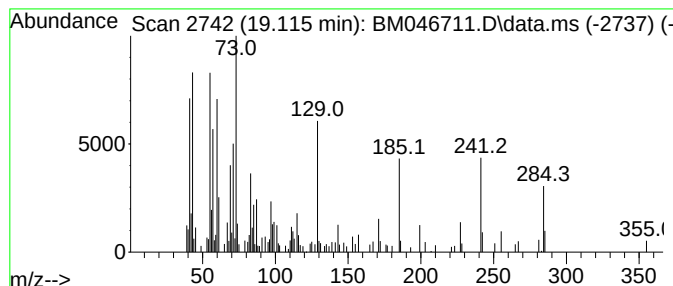
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Peak Number 3 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.115	3.41 ng	131491	Chrysene-d12	21.109

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	97
2			n-Decanoic acid	172	C10H20O2	000334-48-5	70
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	53
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	52
5			Undecanoic acid	186	C11H22O2	000112-37-8	50



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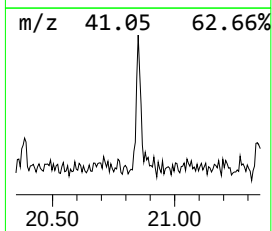
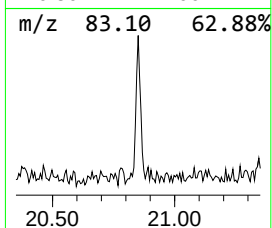
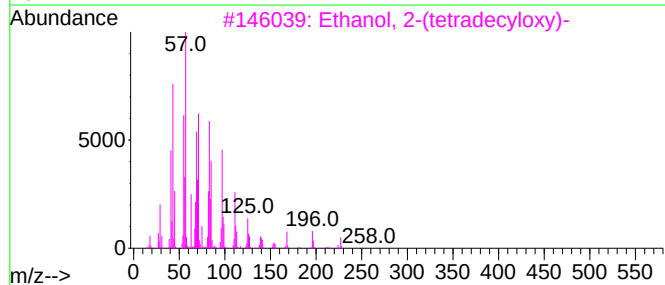
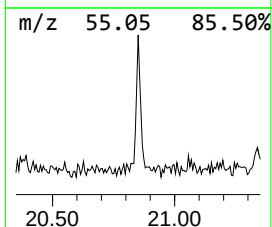
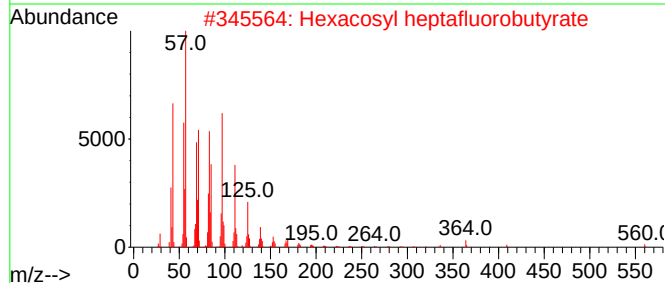
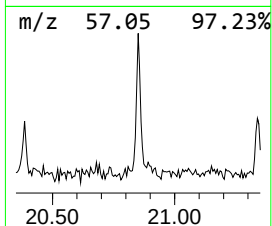
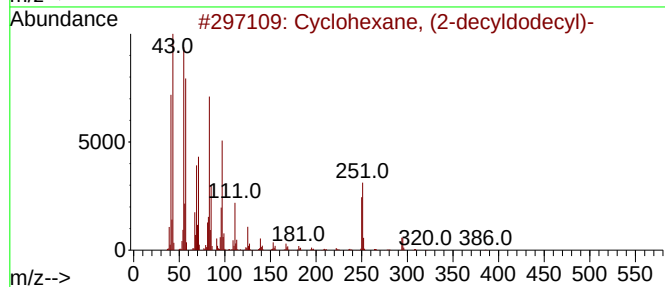
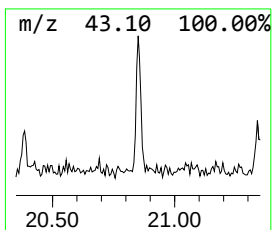
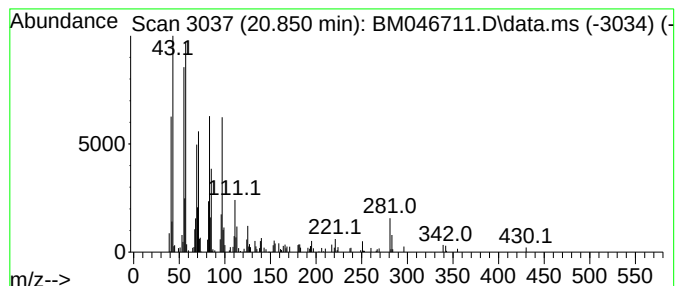
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Peak Number 4 Cyclohexane, (2-decyldodecyl)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.850	2.84 ng	109502	Chrysene-d12	21.109

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, (2-decyldodecyl)-	392	C28H56	006704-00-3	90
2			Hexacosyl heptafluorobutyrate	578	C30H53F7O2	1000351-83-3	70
3			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	68
4			Hexacosyl pentafluoropropionate	528	C29H53F5O2	1000351-81-2	62
5			1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	62



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.687	3.6	ng	86393	1	7.486	484594	20.0
n-Hexadecanoic ...	17.821	6.5	ng	255893	4	16.886	790415	20.0
Octadecanoic acid	19.115	3.4	ng	131491	5	21.109	771093	20.0
Cyclohexane, (2...	20.850	2.8	ng	109502	5	21.109	771093	20.0