

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM010522\
 Data File : BM033654.D
 Acq On : 05 Jan 2022 21:51
 Operator : CG/JU
 Sample : M5196-03
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 COMPOSITE-SAMPLE-2-SHALLOW

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-BM010522.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM033654.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.525	382	389	397	rBV	2710873	3866782	36.46%	7.658%
2	7.137	655	663	675	rVB	2775612	4338241	40.90%	8.592%
3	7.984	800	807	814	rBV	638644	989858	9.33%	1.960%
4	9.148	997	1005	1014	rBV	1770583	2909609	27.43%	5.763%
5	10.801	1277	1286	1293	rBV	859733	1444320	13.62%	2.861%
6	13.254	1695	1703	1717	rBV	4662457	6628739	62.50%	13.128%
7	14.619	1929	1935	1951	rVB	1313641	1994545	18.81%	3.950%
8	16.101	2180	2187	2195	rBV	3623920	5068126	47.78%	10.038%
9	17.360	2394	2401	2411	rBV	1684884	2494265	23.52%	4.940%
10	18.259	2548	2554	2562	rBV	422702	608877	5.74%	1.206%
11	19.524	2765	2769	2777	rBV	183122	268239	2.53%	0.531%
12	19.971	2839	2845	2851	rBV	8827860	10606157	100.00%	21.006%
13	21.236	3056	3060	3071	rBV	1316379	1606768	15.15%	3.182%
14	21.518	3103	3108	3118	rVB	2356206	2955551	27.87%	5.854%
15	21.689	3134	3137	3142	rVB2	96492	110597	1.04%	0.219%
16	22.165	3214	3218	3225	rVB3	119387	204434	1.93%	0.405%
17	22.647	3296	3300	3308	rBV2	544929	934149	8.81%	1.850%
18	23.947	3514	3521	3533	rVB2	1450766	3085117	29.09%	6.110%
19	24.706	3647	3650	3661	rVB3	178966	377138	3.56%	0.747%

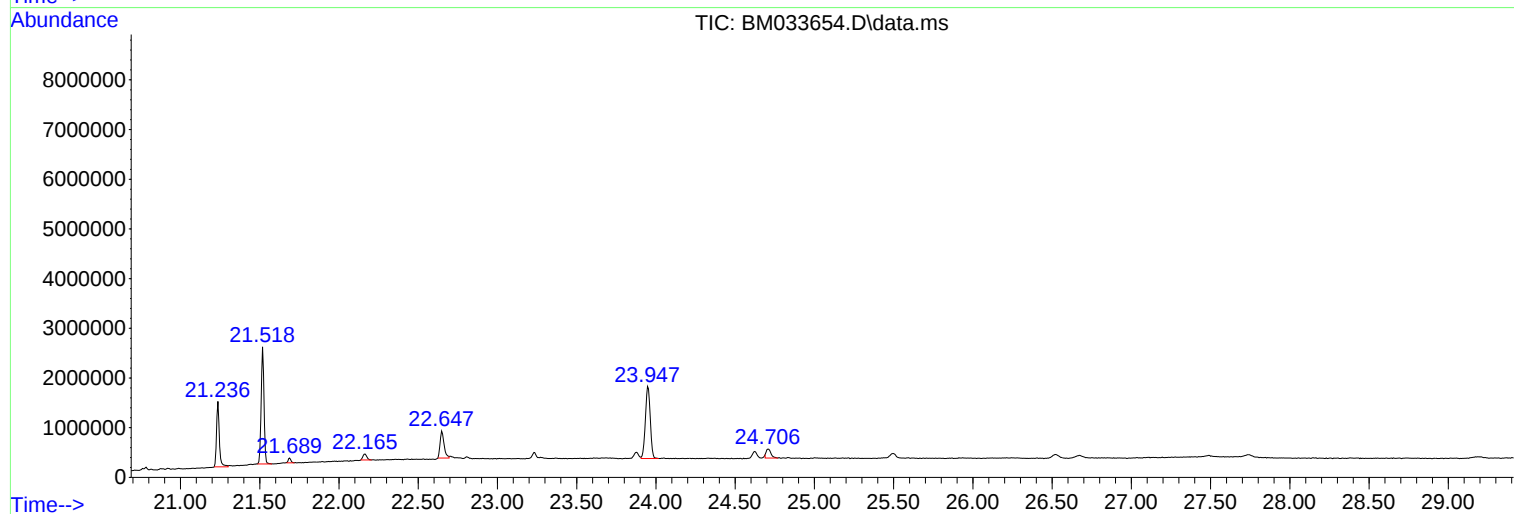
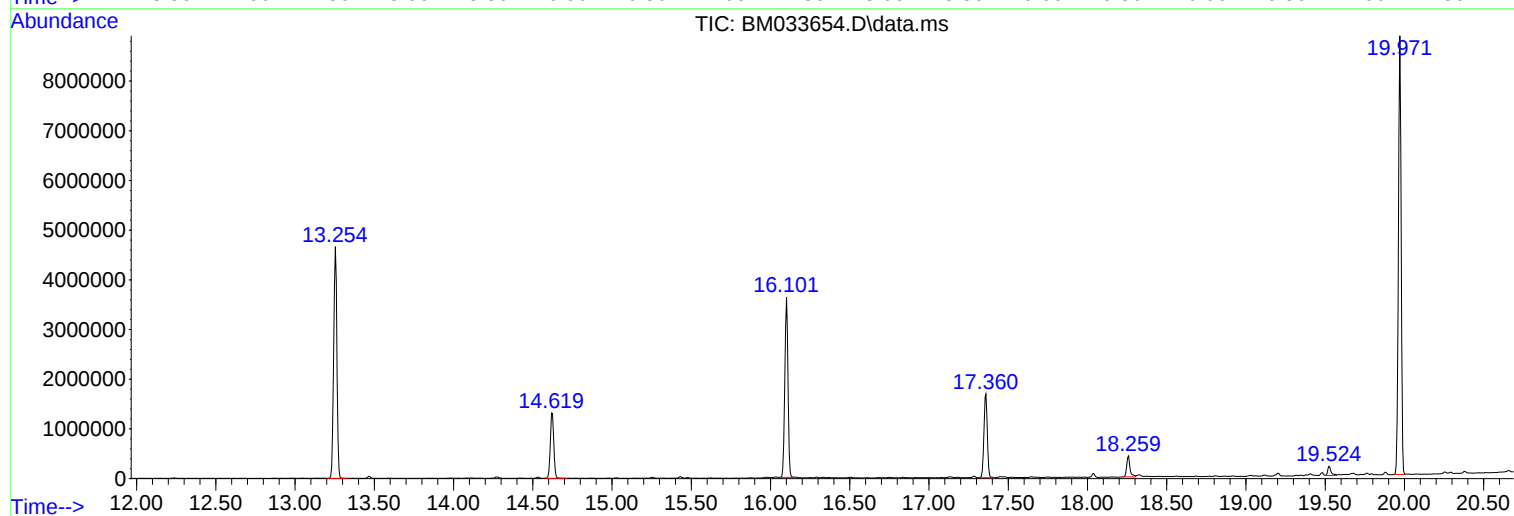
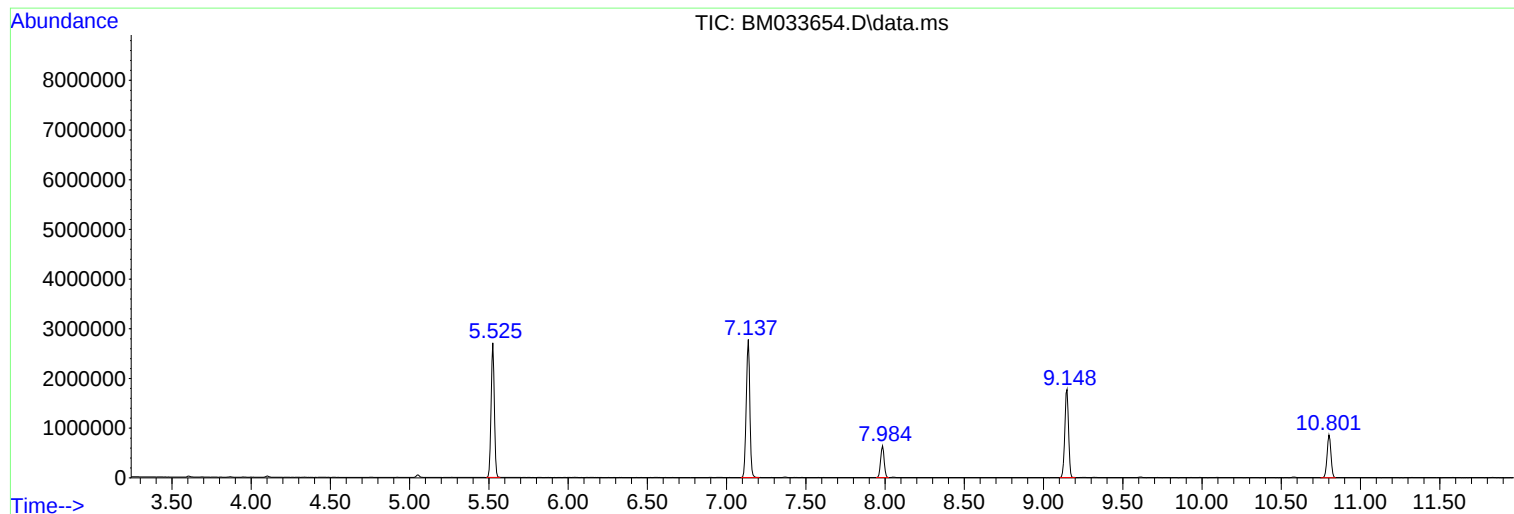
Sum of corrected areas: 50491512

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM010522.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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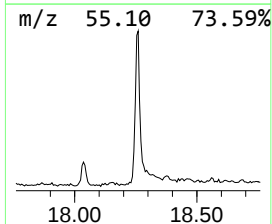
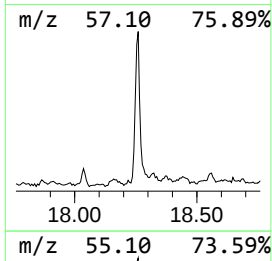
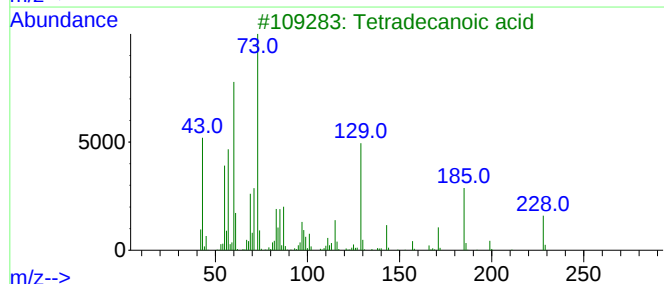
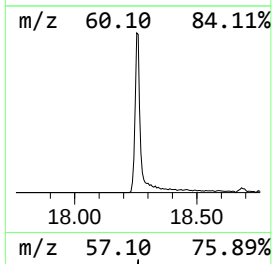
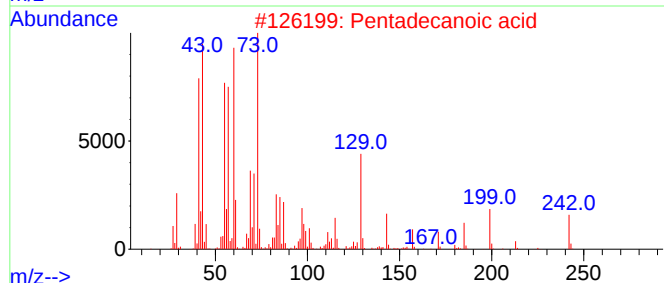
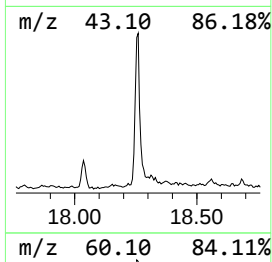
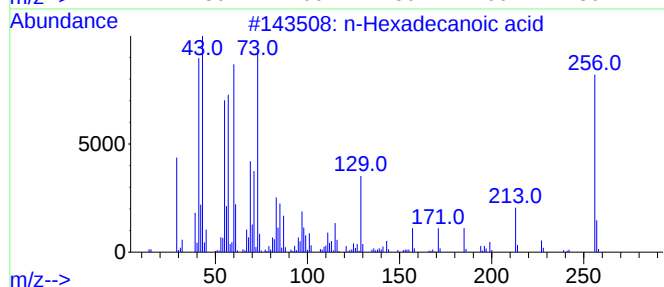
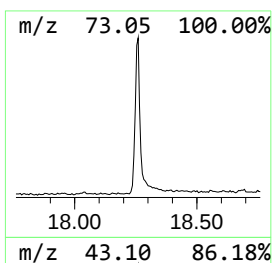
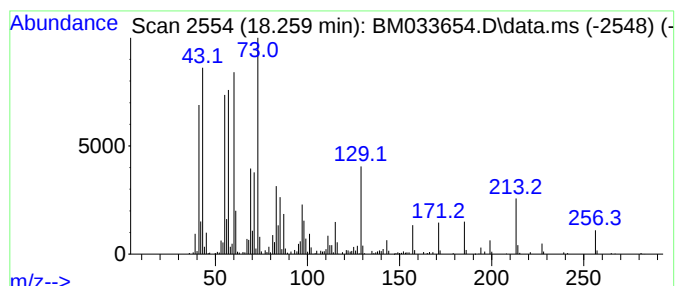
Instrument :
BNA_M
ClientSampleId :
COMPOSITE-SAMPLE-2-SHALLOW

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM010522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.259	4.88 ng	608877	Phenanthrene-d10	17.360	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	Tridecanoic acid	214	C13H26O2	000638-53-9	58
5	n-Decanoic acid	172	C10H20O2	000334-48-5	53



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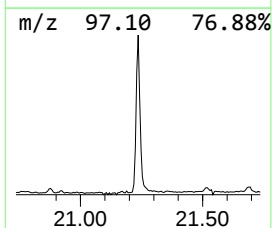
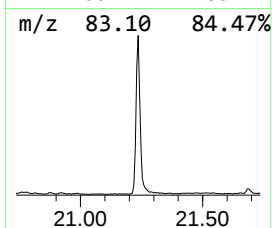
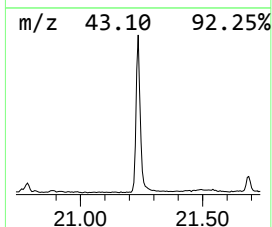
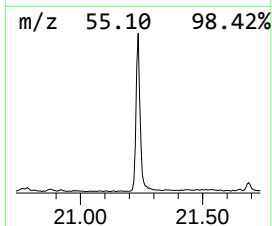
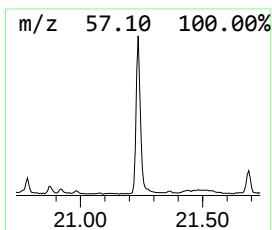
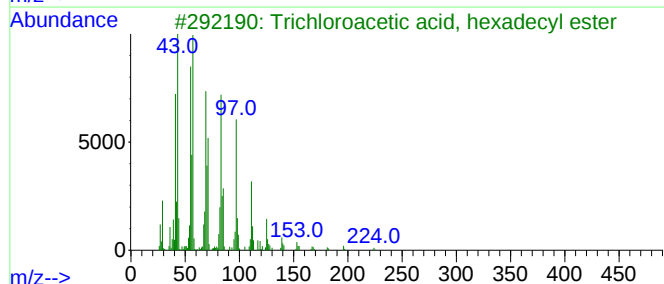
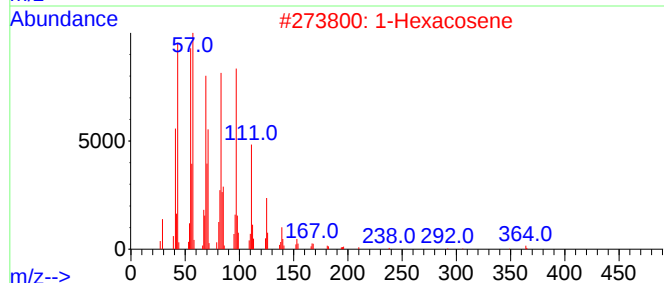
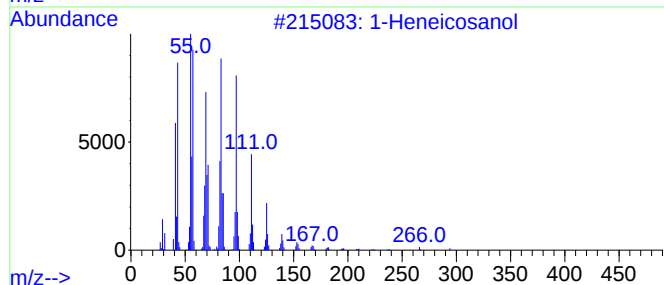
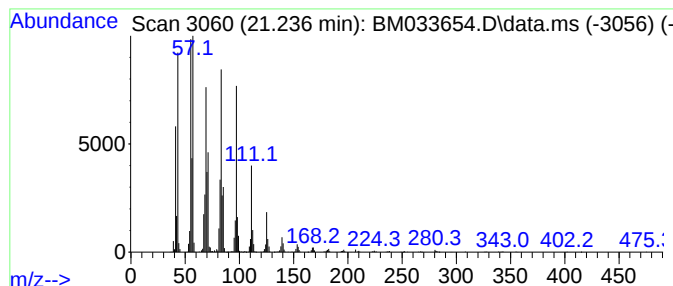
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM010522.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 1-Heneicosanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.236	10.87 ng	1606770	Chrysene-d12	21.518

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	95
2			1-Hexacosene	364	C26H52	018835-33-1	94
3			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
4			1-Tetracosene	336	C24H48	010192-32-2	94
5			n-Tetracosanol-1	354	C24H50O	000506-51-4	94



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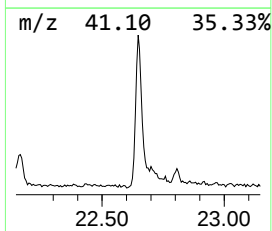
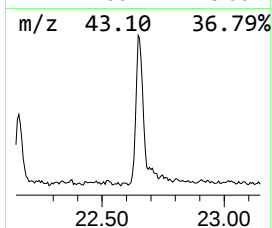
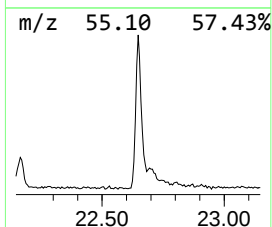
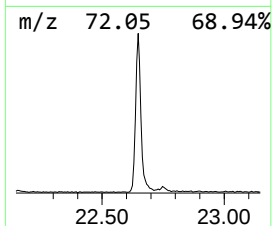
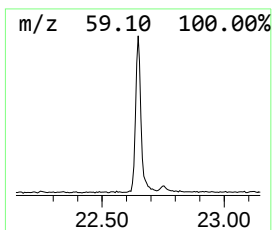
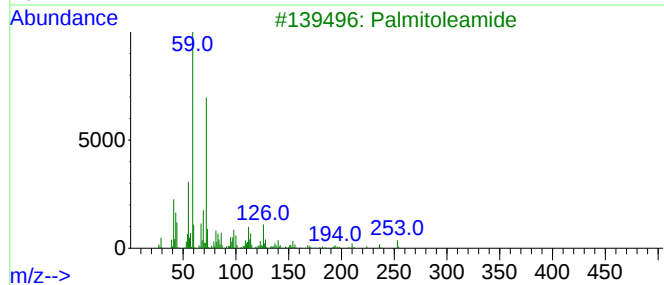
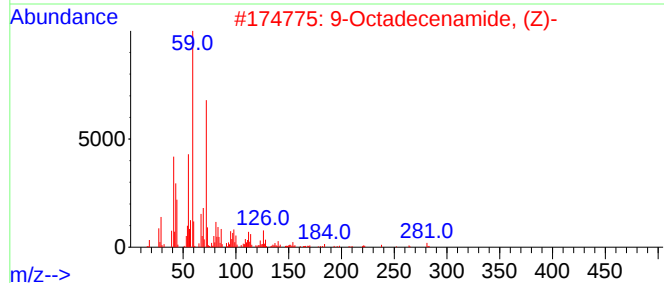
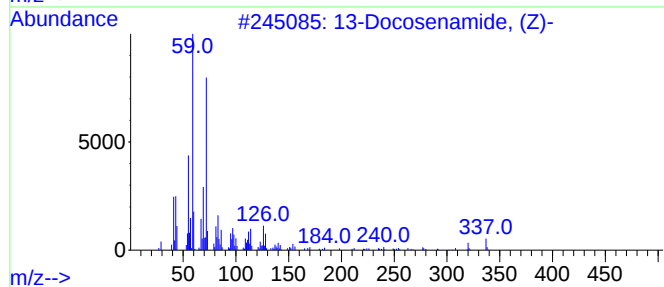
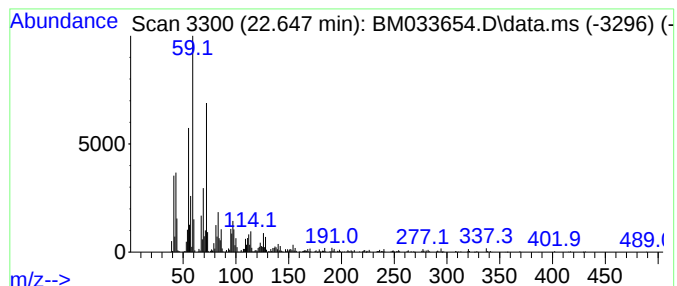
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Peak Number 3 13-Docosenamide, (Z)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.648	6.32 ng	934149	Chrysene-d12	21.518

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	95
2			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
3			Palmitoleamide	253	C16H31NO	106010-22-4	81
4			Tetradecanamide	227	C14H29NO	000638-58-4	78
5			Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	59



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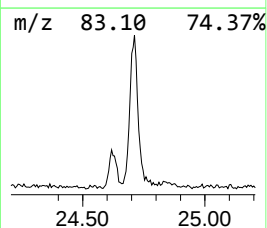
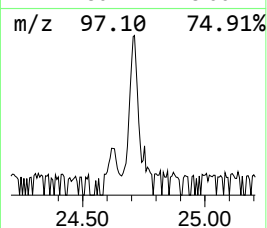
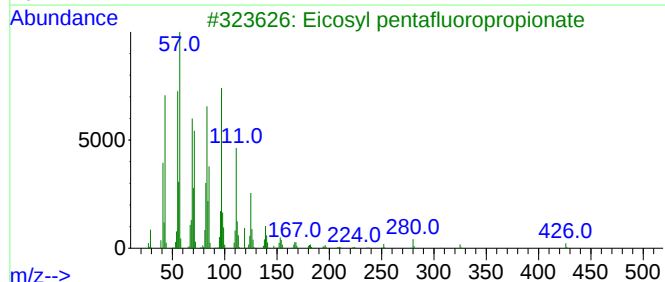
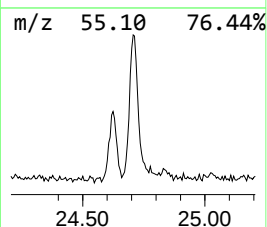
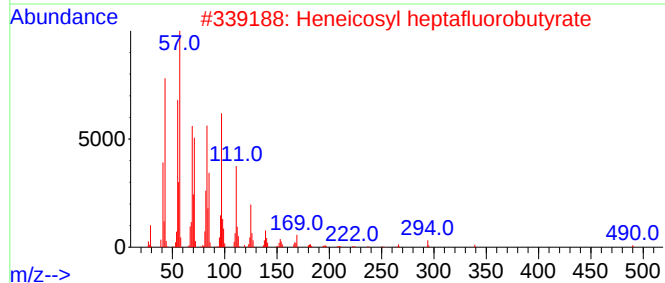
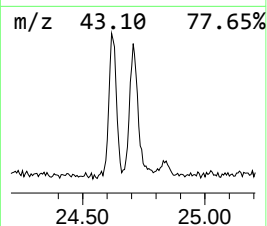
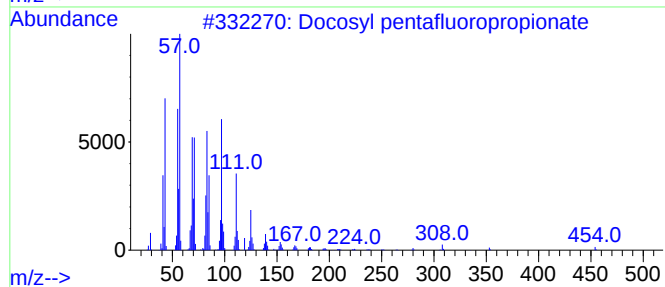
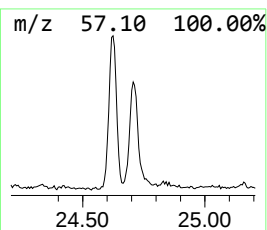
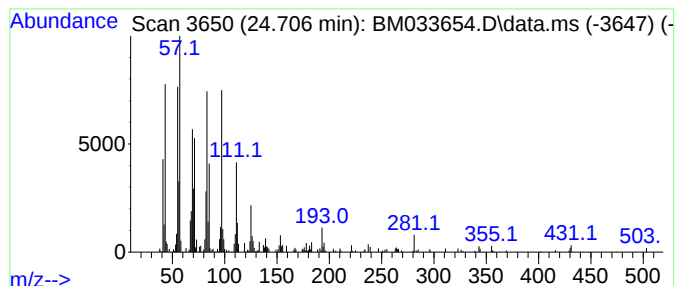
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Peak Number 4 Docosyl pentafluoropropionate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.706	2.44 ng	377138	Perylene-d12	23.947

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	91
2			Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	91
3			Eicosyl pentafluoropropionate	444	C23H41F5O2	1000351-80-8	91
4			1-Nonadecene	266	C19H38	018435-45-5	90
5			Tetratriacontyl trifluoroacetate	591	C36H69F3O2	1000351-75-3	62



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	18.259	4.9	ng	608877	4	17.360	2494270	20.0
1-Heneicosanol	21.236	10.9	ng	1606770	5	21.518	2955550	20.0
13-Docosenamide...	22.648	6.3	ng	934149	5	21.518	2955550	20.0
Docosyl pentafl...	24.706	2.4	ng	377138	6	23.947	3085120	20.0