

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081123\
 Data File : BM041391.D
 Acq On : 11 Aug 2023 17:30
 Operator : MA/JU
 Sample : 03954-01
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 WC-15

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-BM072823.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM041391.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.893	285	290	295	rBV	145476	207964	3.58%	0.641%
2	5.351	360	368	386	rBV	1417775	2203394	37.91%	6.792%
3	6.957	635	641	660	rBV	1242653	2151415	37.01%	6.632%
4	7.775	773	780	790	rBV	553339	890608	15.32%	2.745%
5	8.951	973	980	1003	rBV	761160	1391927	23.95%	4.291%
6	10.580	1248	1257	1271	rBV	719046	1275938	21.95%	3.933%
7	13.057	1671	1678	1706	rBV	2083661	3233717	55.63%	9.969%
8	13.921	1819	1825	1840	rBV	66082	140668	2.42%	0.434%
9	14.439	1907	1913	1931	rBV	1124617	1823814	31.38%	5.622%
10	15.945	2163	2169	2194	rBV	1748948	2880020	49.55%	8.878%
11	17.204	2377	2383	2397	rBV	1567570	2389641	41.11%	7.367%
12	17.562	2438	2444	2448	rBV	57931	83532	1.44%	0.258%
13	17.721	2467	2471	2477	rVB	60013	81413	1.40%	0.251%
14	18.103	2531	2536	2553	rBV	257427	494538	8.51%	1.525%
15	19.274	2727	2735	2740	rBV5	46507	112050	1.93%	0.345%
16	19.386	2750	2754	2765	rBV	128969	243621	4.19%	0.751%
17	19.845	2826	2832	2845	rVB	4602669	5812653	100.00%	17.919%
18	21.115	3044	3048	3057	rBV2	223860	366690	6.31%	1.130%
19	21.409	3093	3098	3110	rBV	2221488	3072634	52.86%	9.472%
20	21.539	3118	3120	3128	rVB3	86452	124328	2.14%	0.383%
21	22.503	3280	3284	3295	rVB2	312205	479050	8.24%	1.477%
22	23.780	3494	3501	3512	rVB	1395267	2979286	51.26%	9.184%

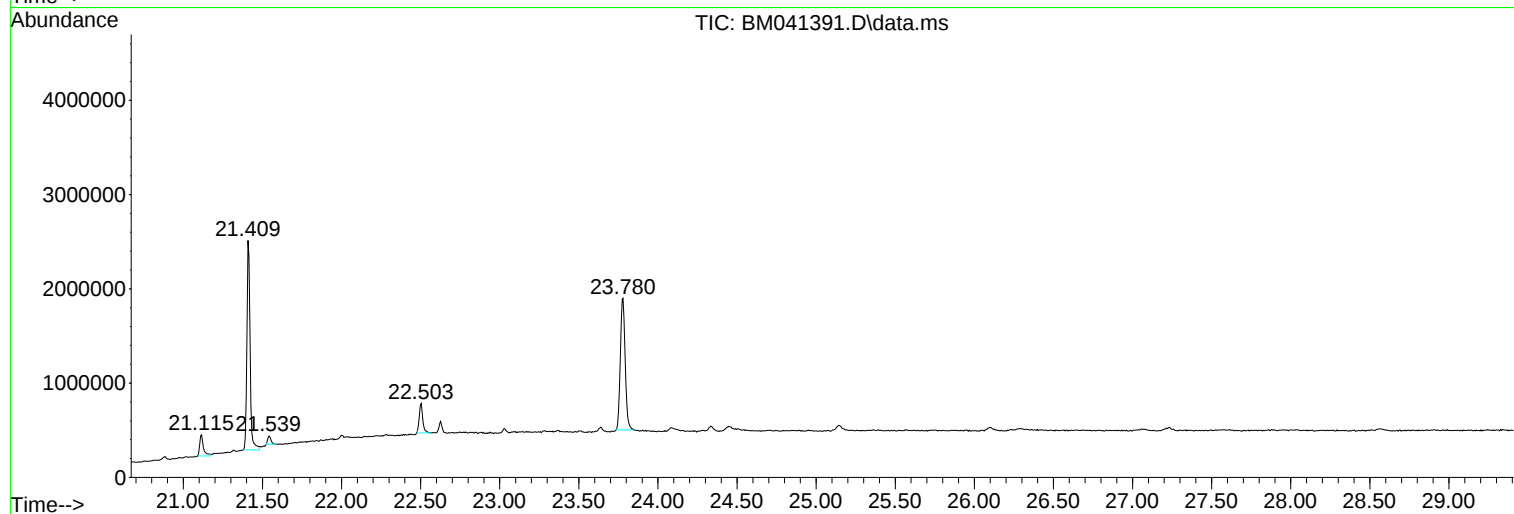
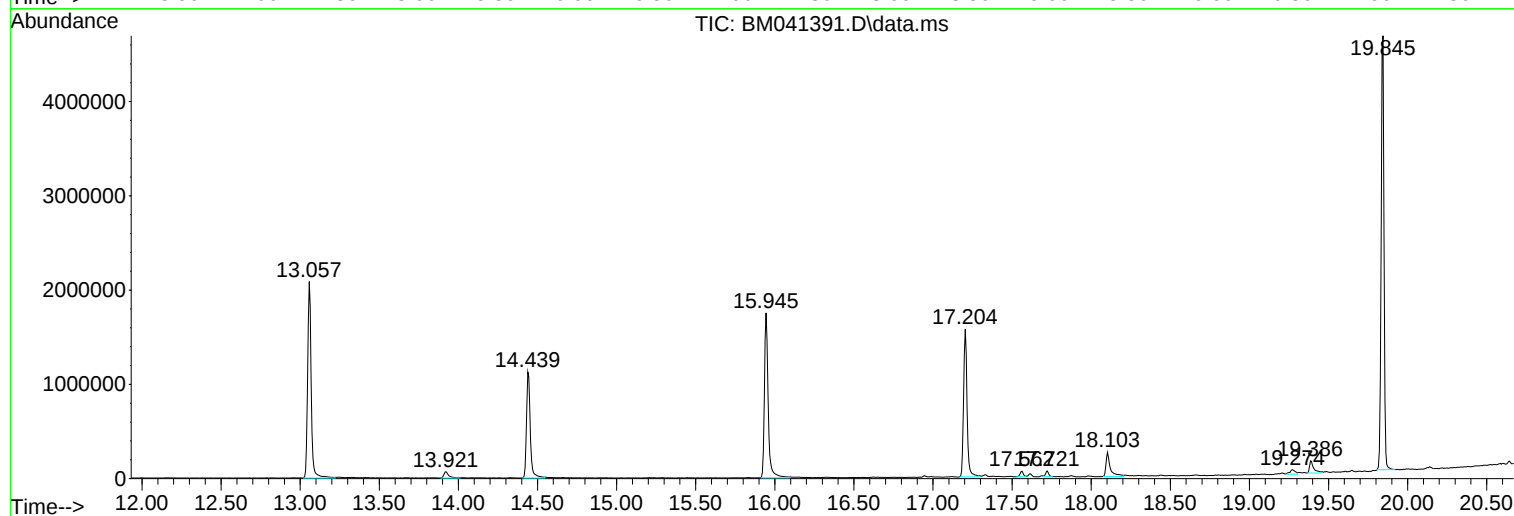
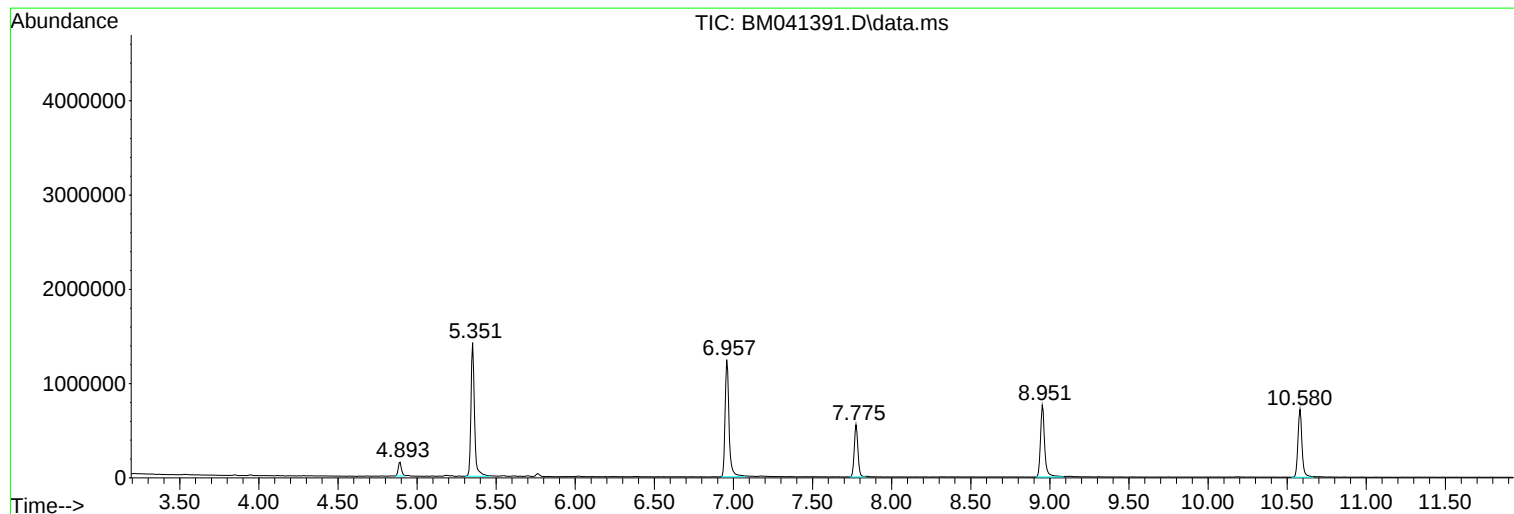
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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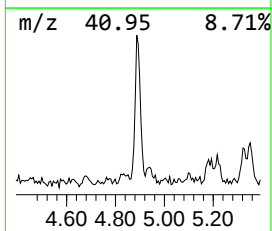
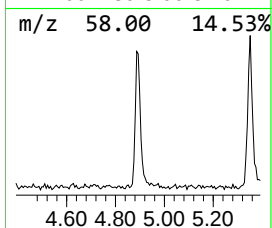
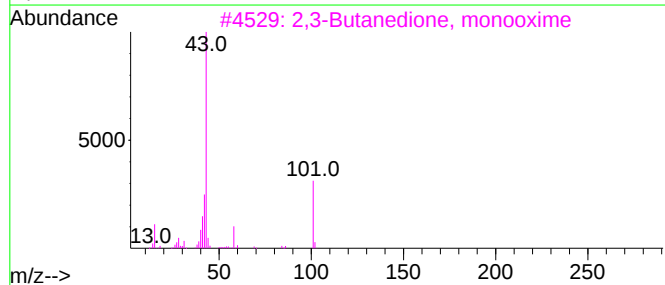
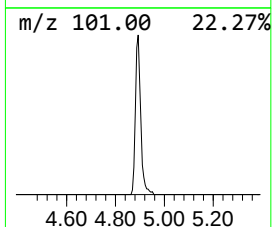
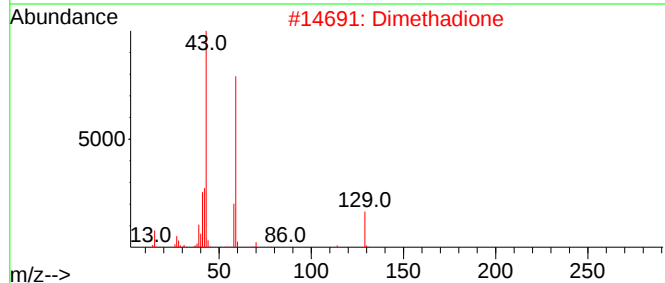
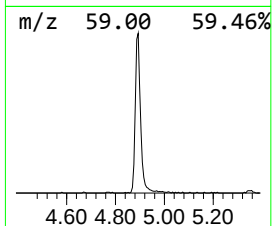
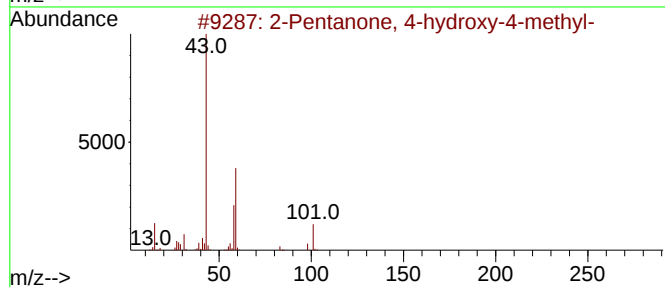
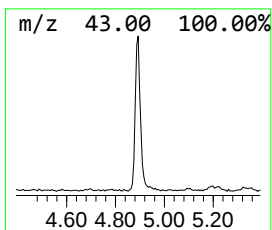
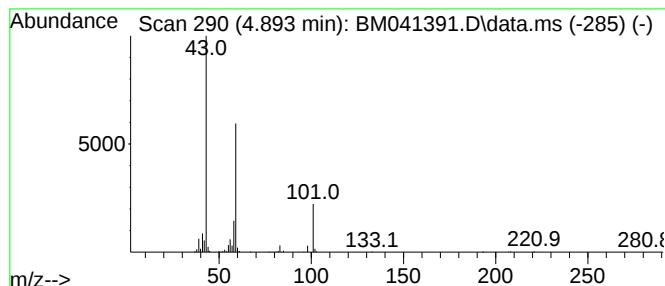
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.893	4.67 ng	207964	1,4-Dichlorobenzene-d4	7.775

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	Dimethadione	129	C5H7NO3	000695-53-4	40		
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	32		
4	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	28		
5	Tripropylene glycol, propyl ethe...	348	C18H40O4Si	1000367-07-2	28		



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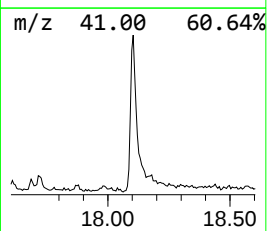
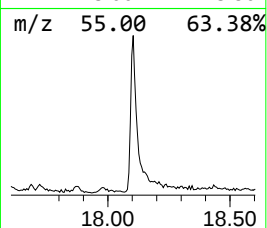
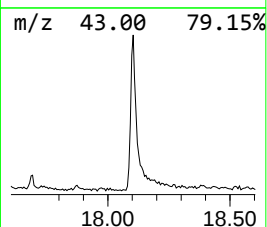
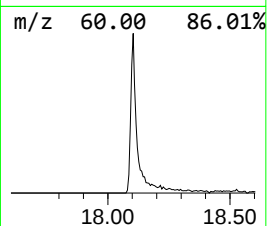
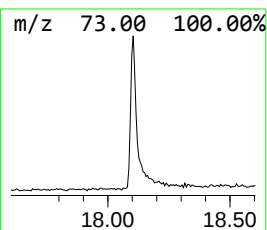
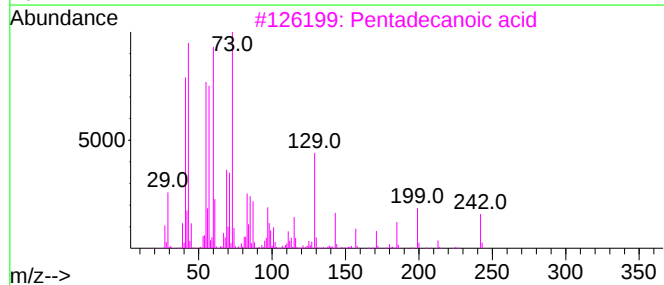
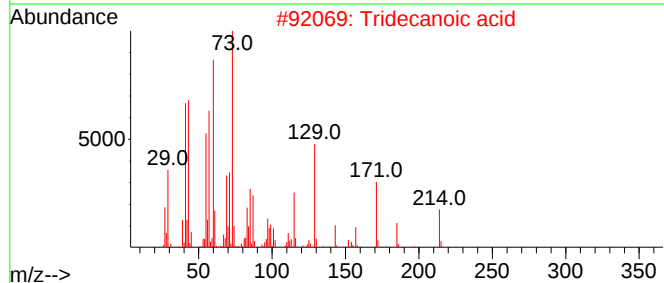
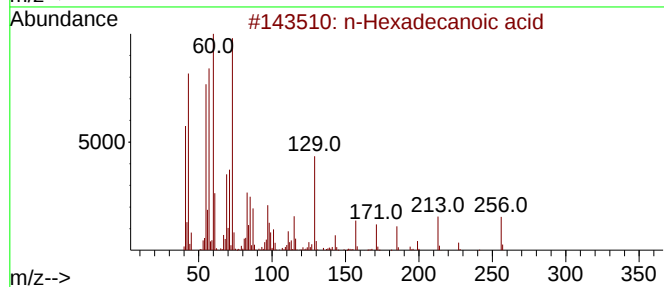
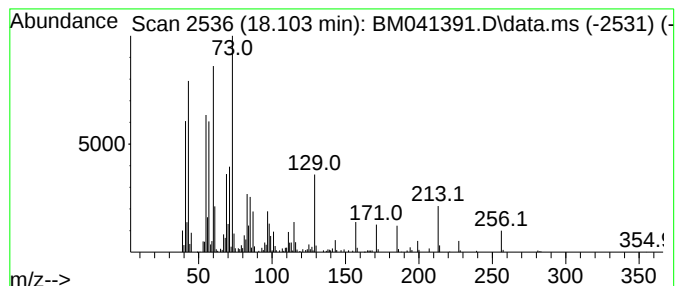
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.104	4.14 ng	494538	Phenanthrene-d10	17.203

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	55



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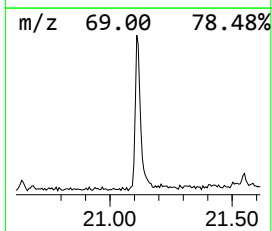
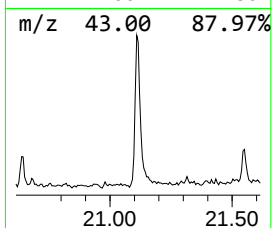
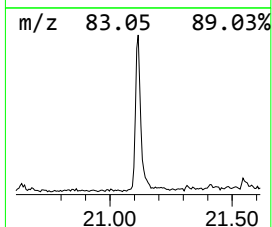
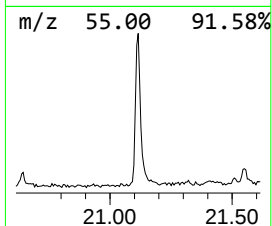
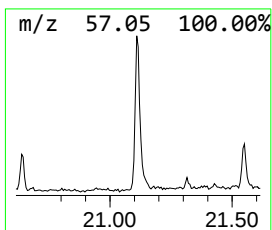
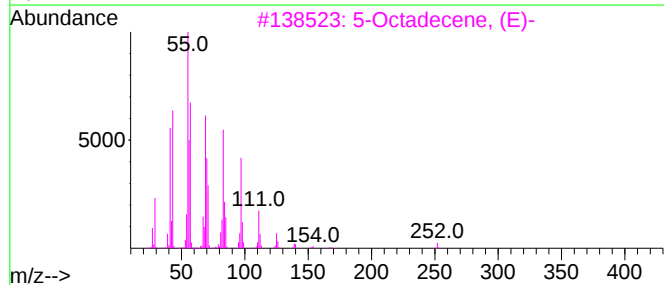
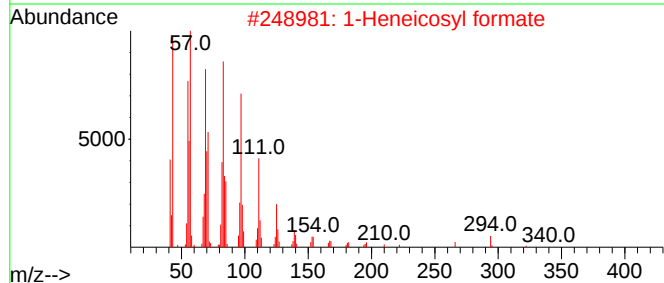
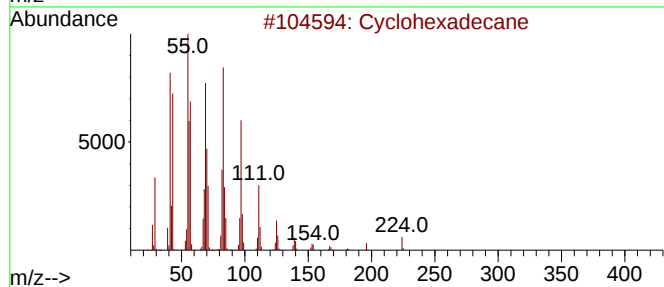
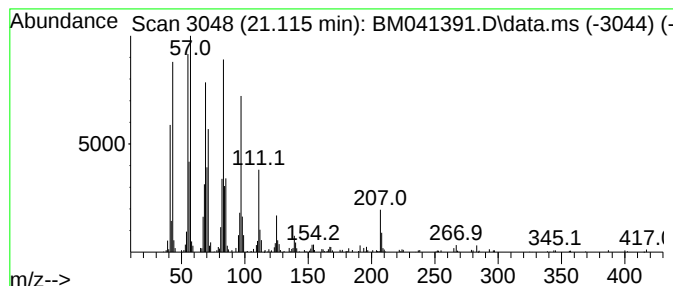
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Peak Number 3 Cyclohexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.115	2.39 ng	366690	Chrysene-d12	21.409

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexadecane	224	C16H32	000295-65-8	98
2			1-Heneicosyl formate	340	C22H44O2	077899-03-7	95
3			5-Octadecene, (E)-	252	C18H36	007206-21-5	94
4			Pentacos-1-ene	350	C25H50	016980-85-1	94
5			1-Heneicosanol	312	C21H44O	015594-90-8	93



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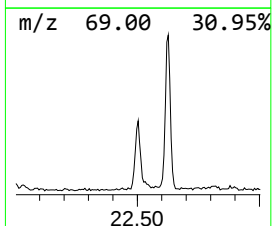
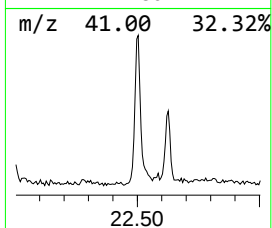
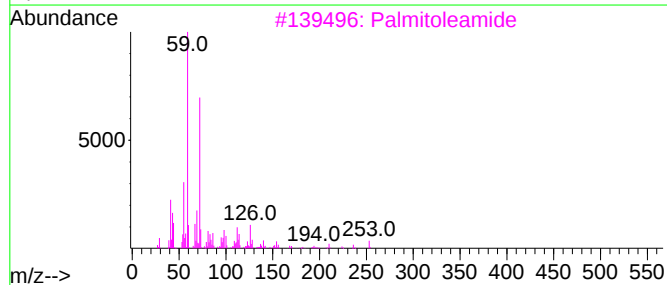
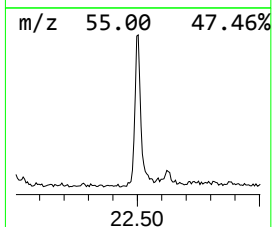
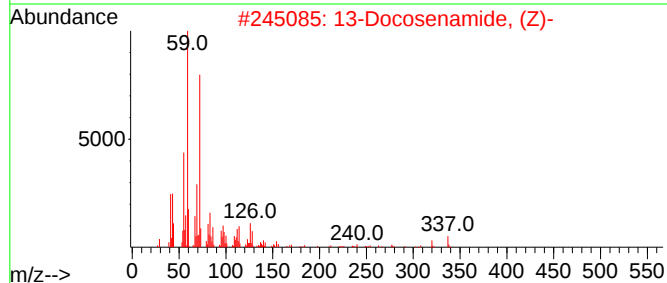
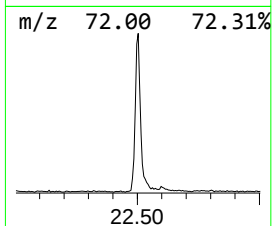
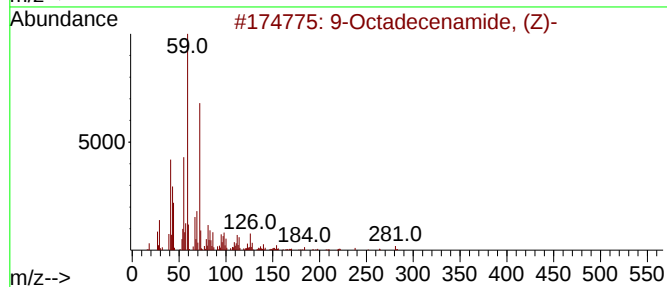
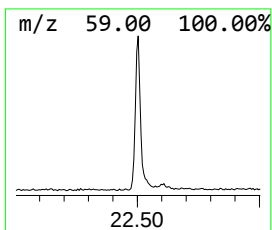
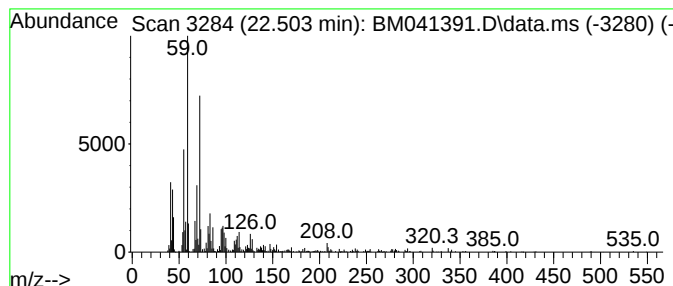
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Peak Number 4 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.503	3.12 ng	479050	Chrysene-d12	21.409

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	98
2		13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	96
3		Palmitoleamide	253	C16H31NO	106010-22-4	59
4		Acetic acid, cyanohydroxyimino-,...	128	C4H4N2O3	061295-92-9	43
5		2-Propanone, 1-cyclohexyl-	140	C9H16O	000103-78-6	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.893	4.7	ng	207964	1	7.775	890608	20.0
n-Hexadecanoic ...	18.104	4.1	ng	494538	4	17.203	2389640	20.0
Cyclohexadecane	21.115	2.4	ng	366690	5	21.409	3072630	20.0
9-Octadecenamid...	22.503	3.1	ng	479050	5	21.409	3072630	20.0