

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080423\
 Data File : BG058606.D
 Acq On : 4 Aug 2023 11:24
 Operator : MA/JU
 Sample : 03877-07
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 COMP-3

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_G\Methods\8270-BG072823.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG058606.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.908	305	310	318	rVB	32822	50474	1.70%	0.326%
2	5.384	384	391	407	rVB	937554	1481200	49.81%	9.580%
3	6.982	655	663	684	rBV	875872	1551259	52.17%	10.033%
4	7.811	798	804	813	rBV	190770	315116	10.60%	2.038%
5	8.974	994	1002	1019	rBV	512778	949793	31.94%	6.143%
6	10.613	1273	1281	1293	rBV	259914	472425	15.89%	3.056%
7	13.081	1693	1701	1717	rBV	1313482	2067592	69.53%	13.373%
8	14.462	1929	1936	1946	rBV	429457	660411	22.21%	4.271%
9	15.819	2160	2167	2178	rBV	129777	192562	6.48%	1.245%
10	15.954	2183	2190	2211	rBV	1008297	1683292	56.61%	10.887%
11	17.206	2394	2403	2420	rBV	525210	797111	26.80%	5.155%
12	18.099	2549	2555	2572	rBV	136196	257382	8.66%	1.665%
13	19.380	2768	2773	2785	rBV5	20114	51452	1.73%	0.333%
14	19.826	2843	2849	2857	rBV	2305465	2973747	100.00%	19.233%
15	21.136	3062	3072	3074	rBV5	37387	101717	3.42%	0.658%
16	21.448	3119	3125	3139	rBV	507244	832117	27.98%	5.382%
17	23.028	3390	3394	3400	rVB	18930	32704	1.10%	0.212%
18	23.604	3487	3492	3500	rBV5	14303	30360	1.02%	0.196%
19	24.521	3636	3648	3665	rBV	306399	960706	32.31%	6.214%

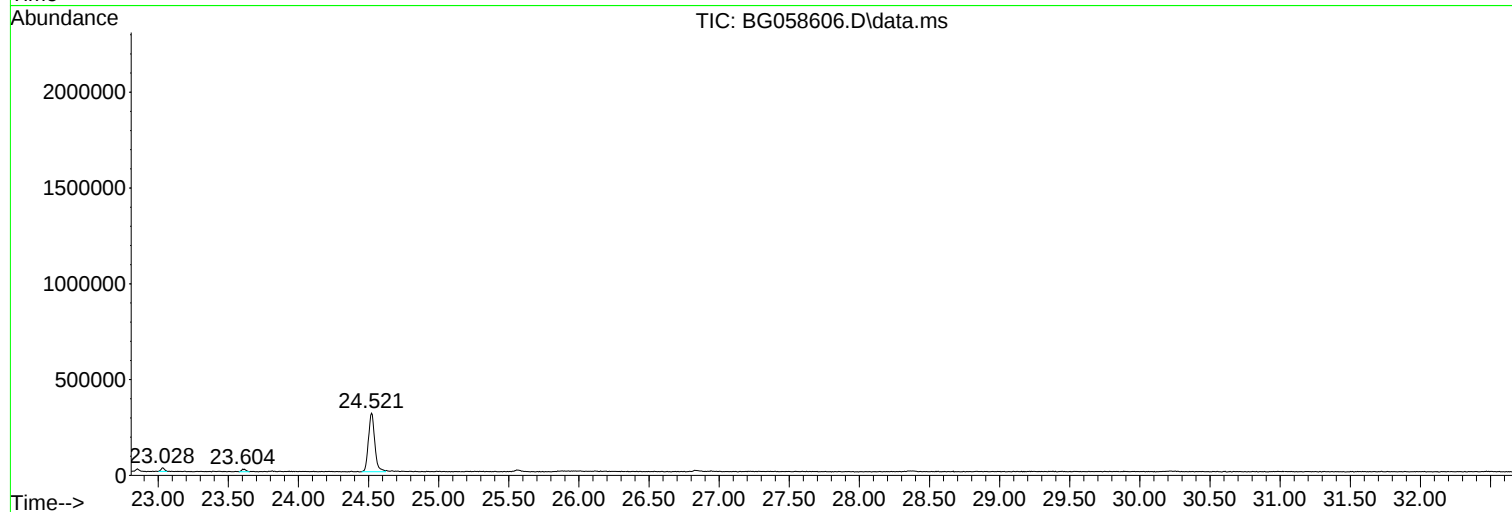
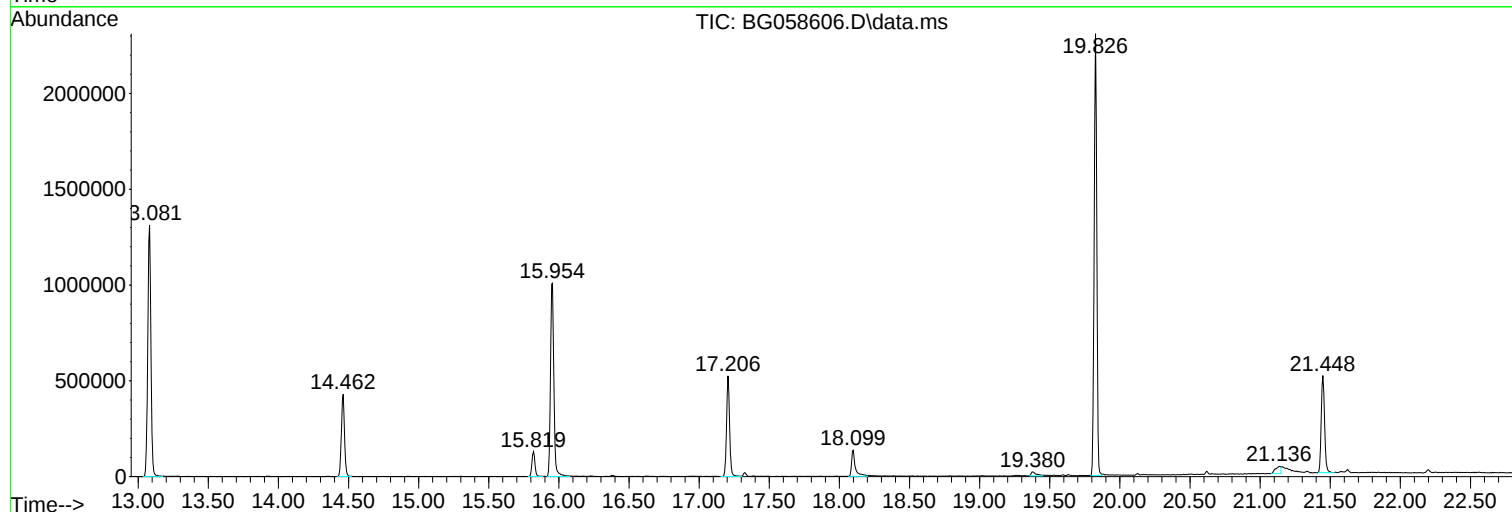
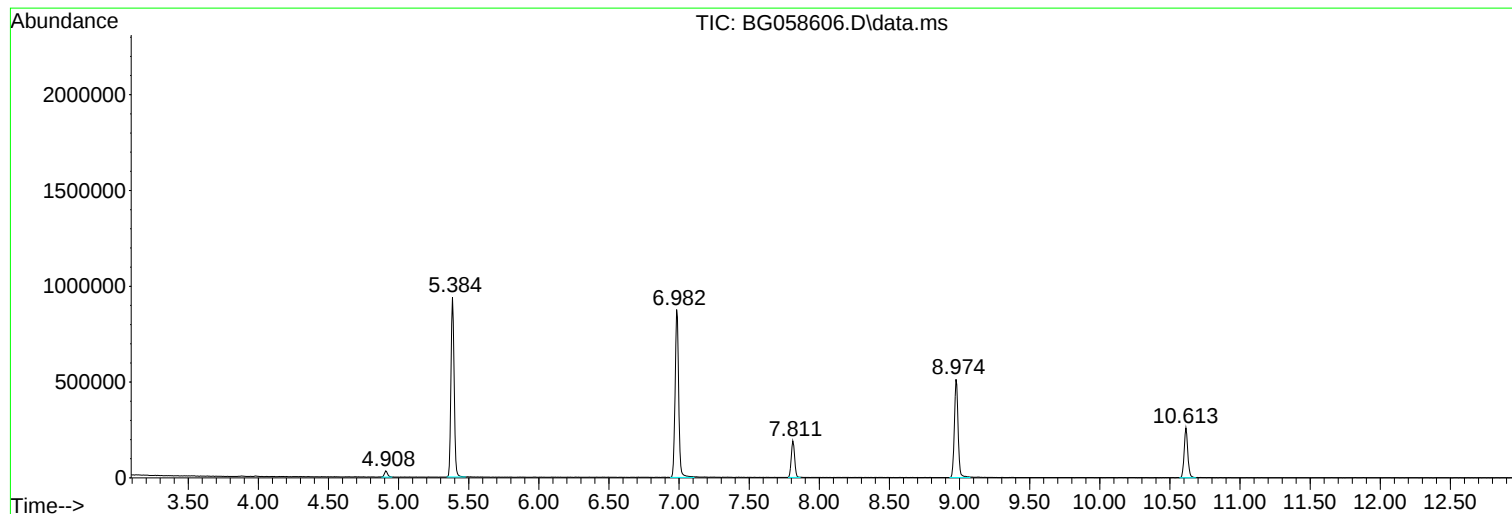
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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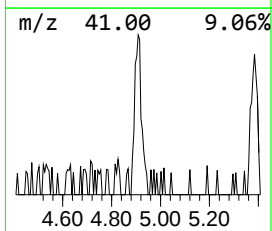
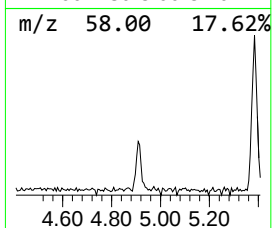
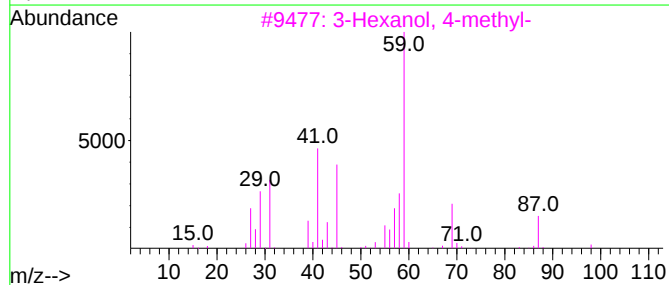
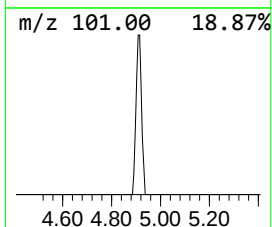
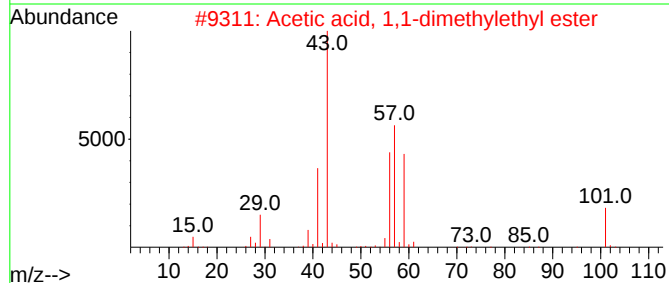
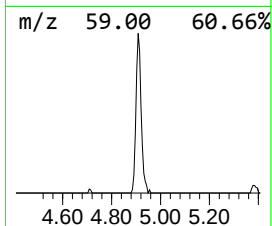
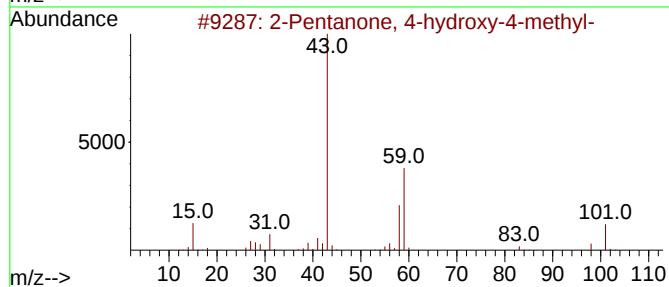
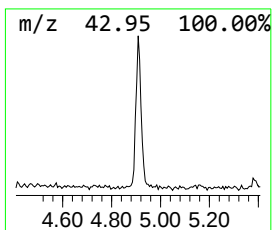
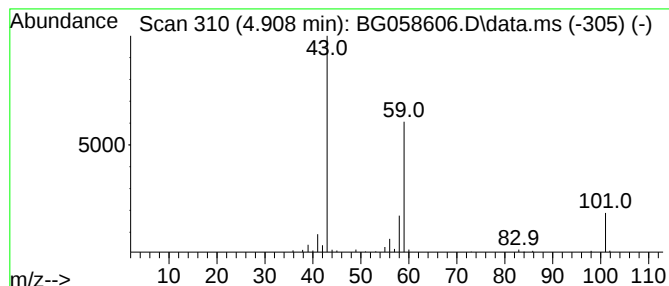
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.908	3.20 ng	50474	1,4-Dichlorobenzene-d4	7.811

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59	
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38	
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	38	
4	3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	33	
5	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	28	



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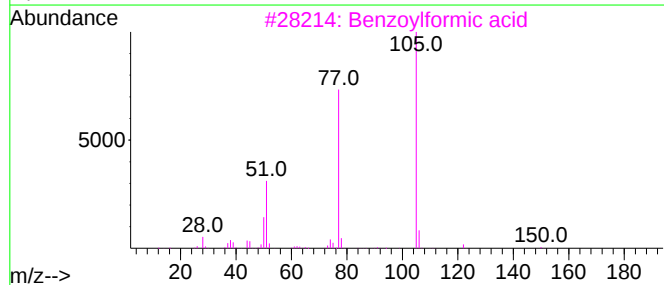
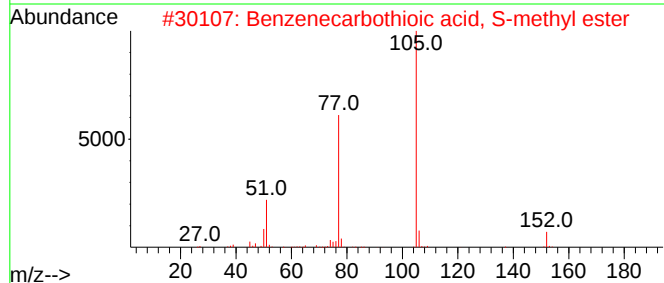
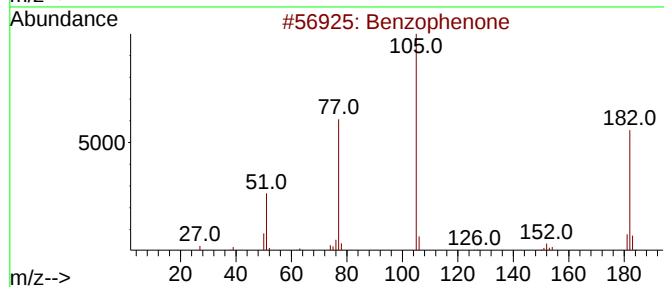
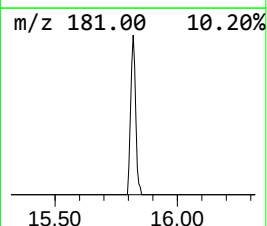
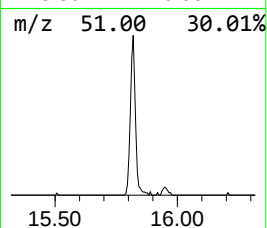
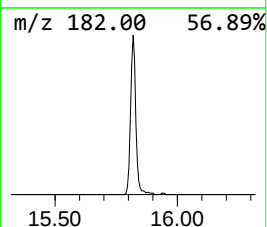
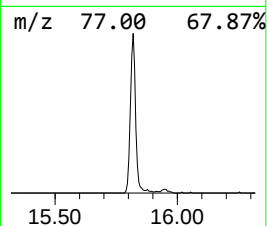
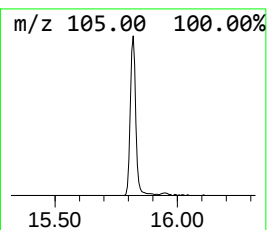
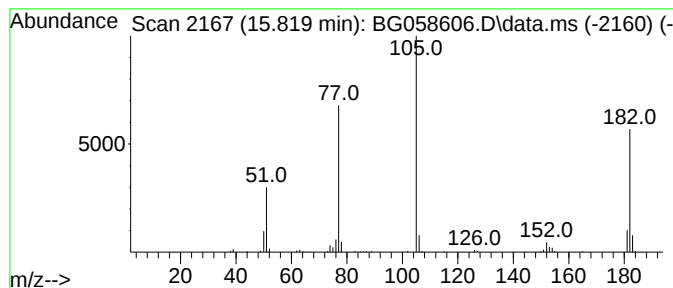
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Peak Number 2 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.819	5.83 ng	192562	Acenaphthene-d10	14.462

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	52
3			Benzoylformic acid	150	C8H6O3	000611-73-4	49
4			2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	47
5			Ethanedione, diphenyl-	210	C14H10O2	000134-81-6	47



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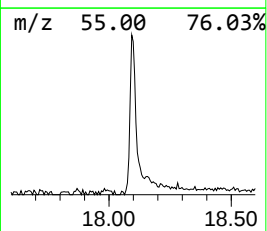
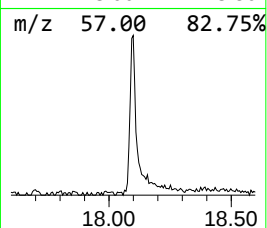
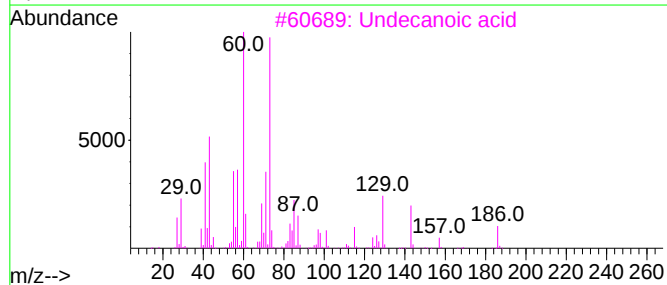
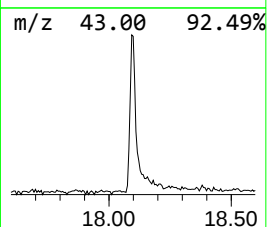
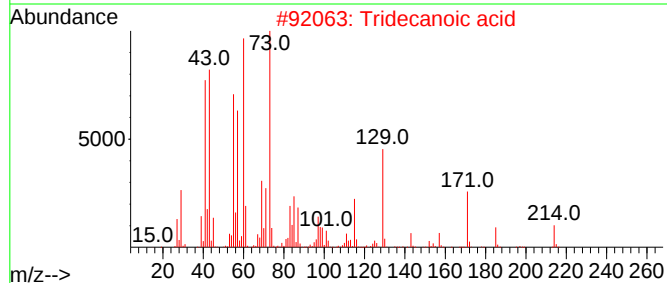
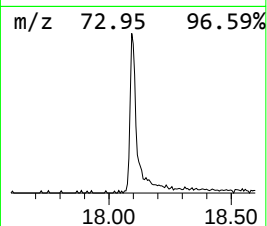
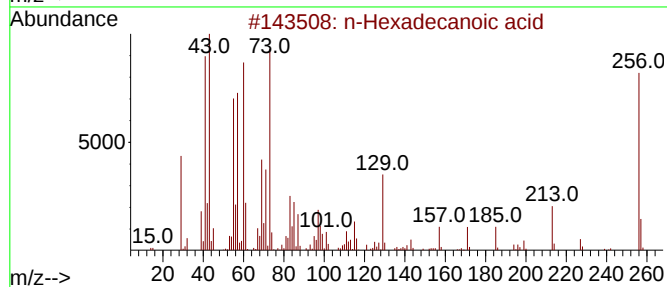
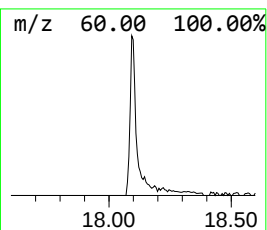
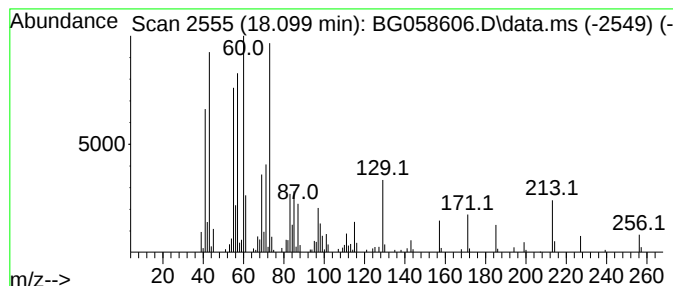
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.099	6.46 ng	257382	Phenanthrene-d10	17.206

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	90
3			Undecanoic acid	186	C11H22O2	000112-37-8	74
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			n-Decanoic acid	172	C10H20O2	000334-48-5	70



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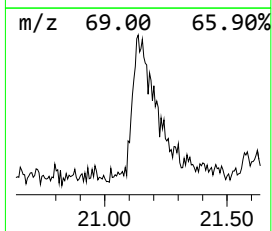
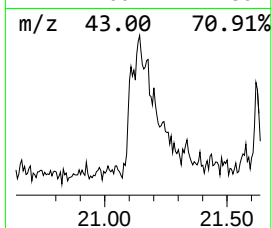
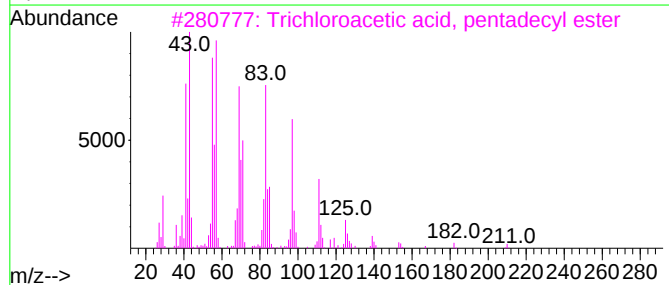
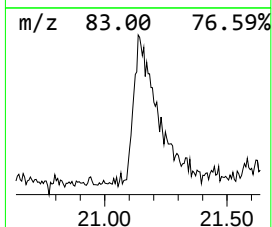
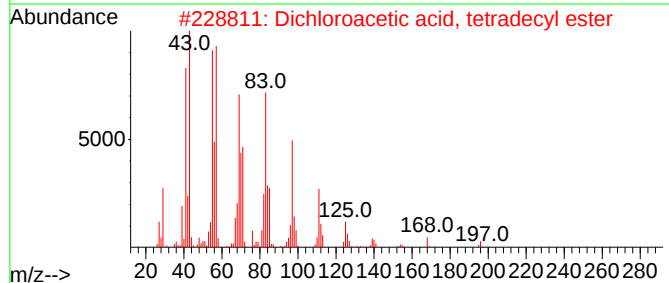
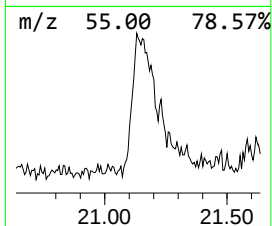
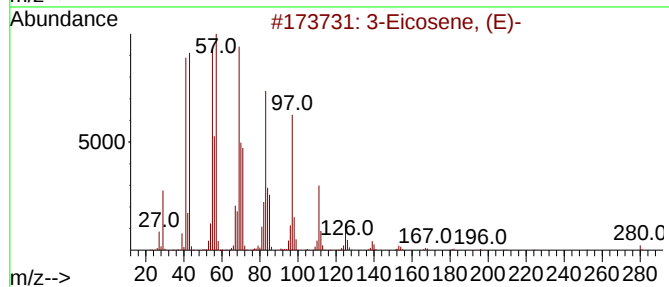
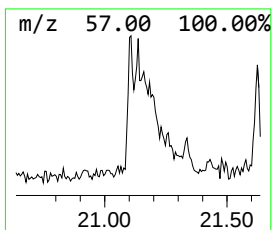
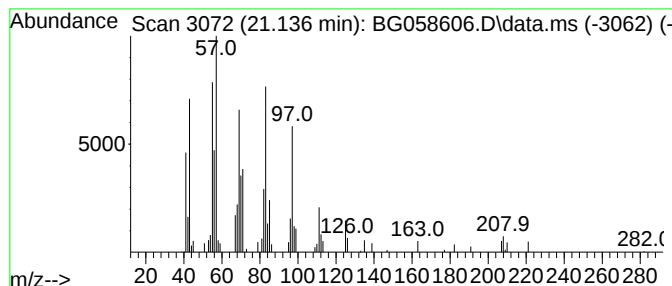
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Peak Number 4 3-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.136	2.44 ng	101717	Chrysene-d12	21.448

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Eicosene, (E)-	280	C20H40	074685-33-9	90
2			Dichloroacetic acid, tetradecyl ...	324	C16H30Cl2O2	083005-02-1	90
3			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	87
4			Acetic acid, chloro-, octadecyl ...	346	C20H39ClO2	005348-82-3	87
5			1-Pentadecene	210	C15H30	013360-61-7	83



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.908	3.2	ng	50474	1	7.811	315116	20.0
Benzophenone	15.819	5.8	ng	192562	3	14.462	660411	20.0
n-Hexadecanoic ...	18.099	6.5	ng	257382	4	17.206	797111	20.0
3-Eicosene, (E)-	21.136	2.4	ng	101717	5	21.448	832117	20.0