

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG032321\
 Data File : BG048480.D
 Acq On : 23 Mar 2021 21:53
 Operator : CG/JU
 Sample : M1779-06
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-1B1-(3.0-3.5)

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-BG031821.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048480.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.177	308	313	321	rVB	35536	53210	1.20%	0.285%
2	5.653	384	394	403	rBV	915091	1458166	32.81%	7.804%
3	7.251	656	666	679	rBV	968677	1676904	37.73%	8.974%
4	8.103	803	811	818	rBV	155578	261228	5.88%	1.398%
5	9.267	1000	1009	1017	rBV	596064	1075810	24.20%	5.757%
6	10.923	1281	1291	1299	rBV	203163	363934	8.19%	1.948%
7	13.368	1699	1707	1715	rBV	1608176	2479915	55.79%	13.272%
8	14.184	1840	1846	1851	rBV	57860	81109	1.82%	0.434%
9	14.742	1933	1941	1948	rBV	370308	563333	12.67%	3.015%
10	16.229	2187	2194	2201	rBV	1649912	2580341	58.05%	13.809%
11	17.492	2403	2409	2415	rBV	485237	748804	16.85%	4.007%
12	18.373	2554	2559	2568	rBV	154148	235698	5.30%	1.261%
13	19.143	2685	2690	2695	rVB2	40493	53500	1.20%	0.286%
14	20.101	2847	2853	2859	rBV	3301245	4444711	100.00%	23.787%
15	21.411	3072	3076	3088	rBV2	153667	339597	7.64%	1.817%
16	21.781	3133	3139	3152	rVB	483417	823344	18.52%	4.406%
17	22.181	3202	3207	3212	rBV6	36227	64981	1.46%	0.348%
18	22.592	3270	3277	3281	rBV6	45609	123281	2.77%	0.660%
19	22.962	3334	3340	3355	rBV3	114929	377505	8.49%	2.020%
20	25.113	3695	3706	3719	rBV	287386	880390	19.81%	4.712%

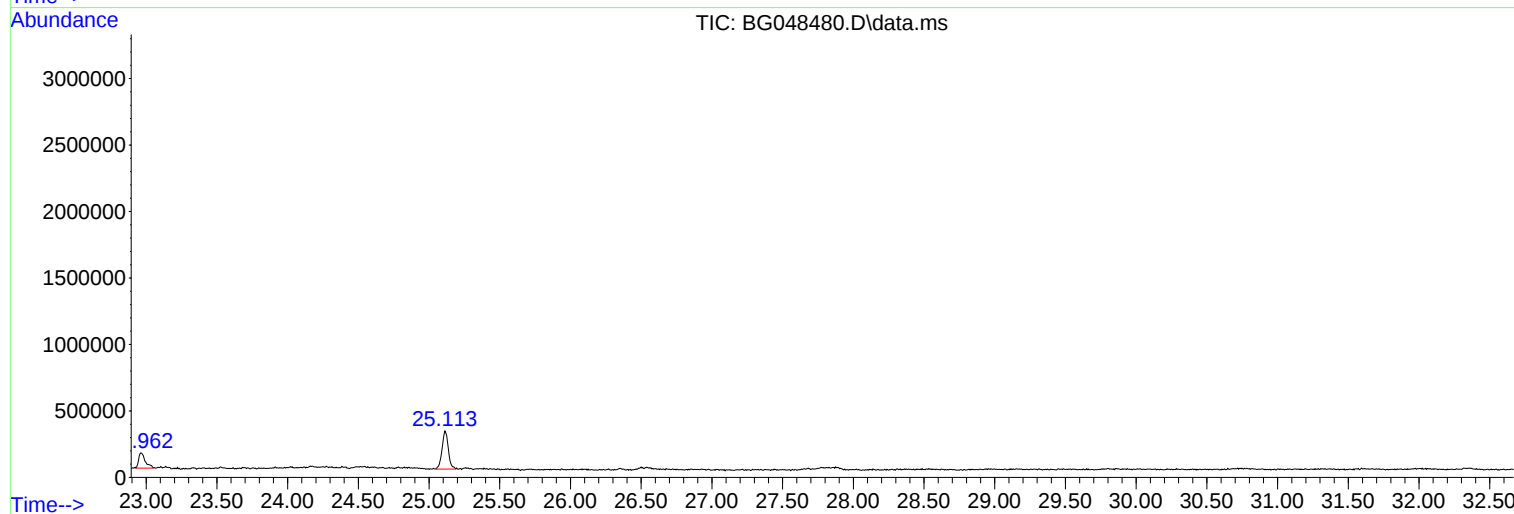
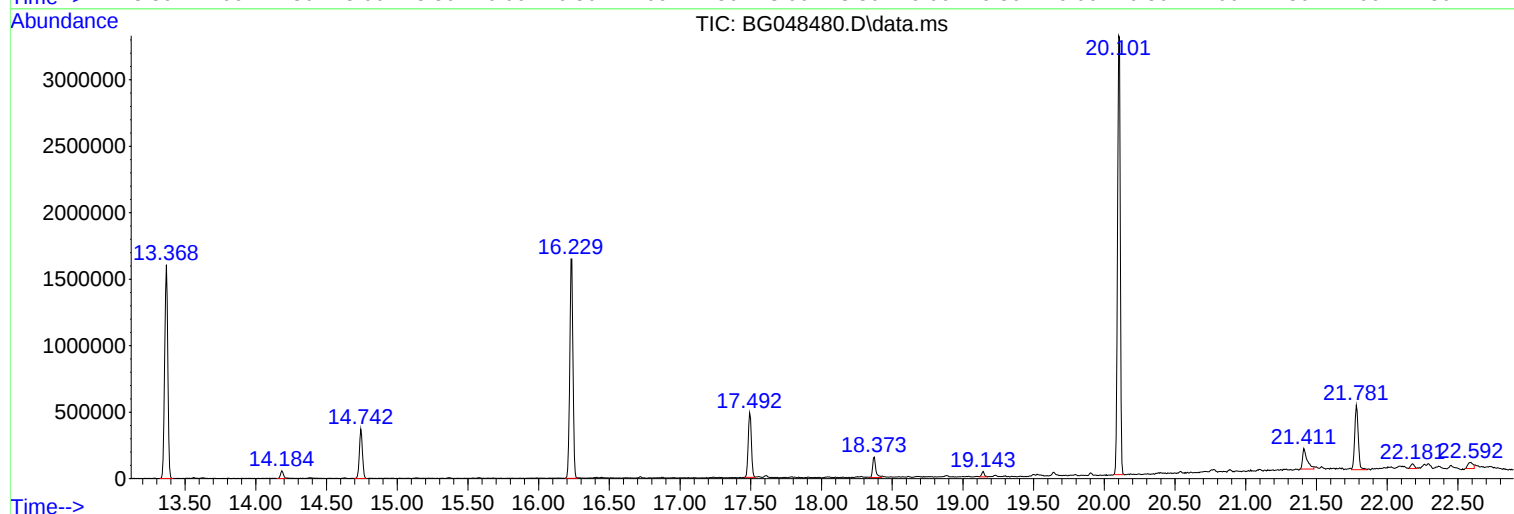
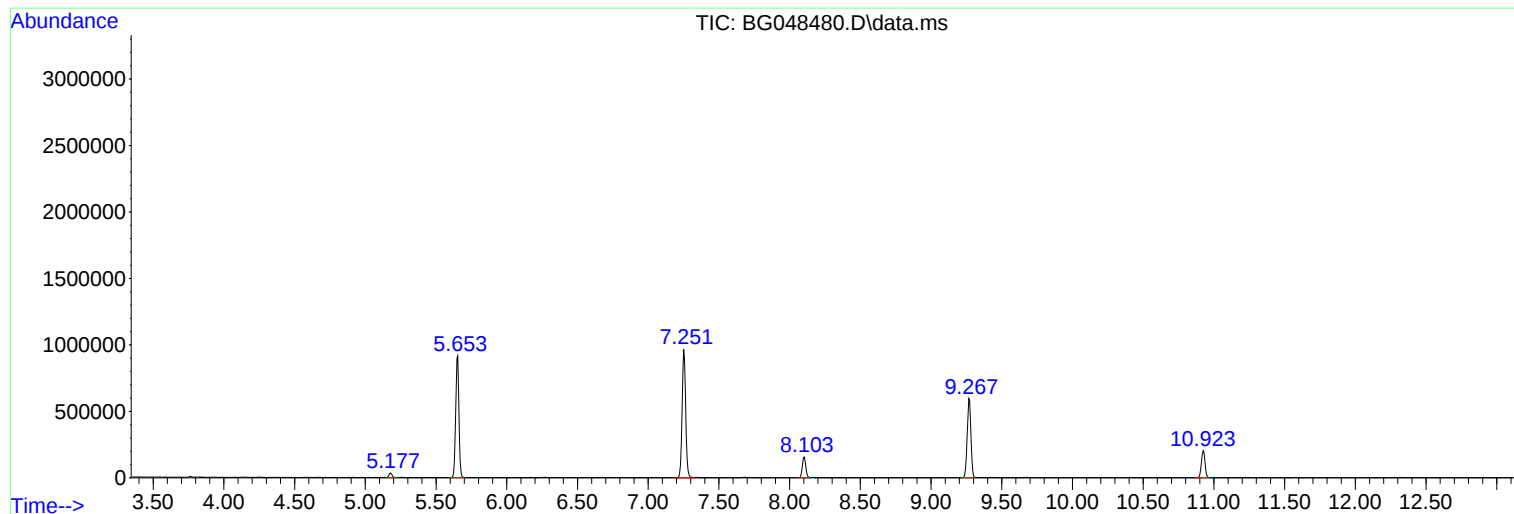
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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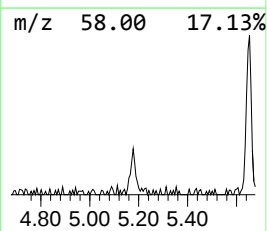
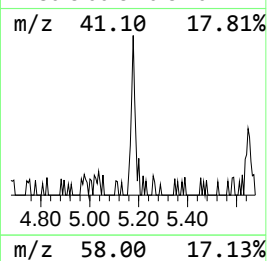
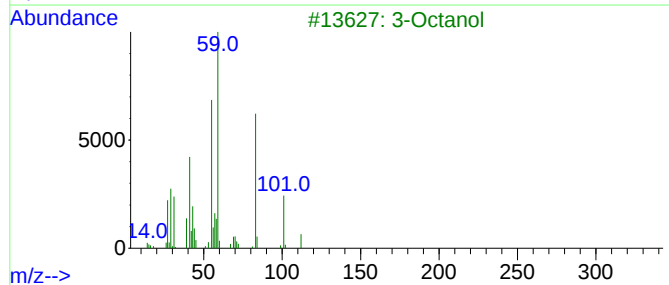
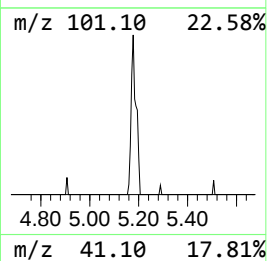
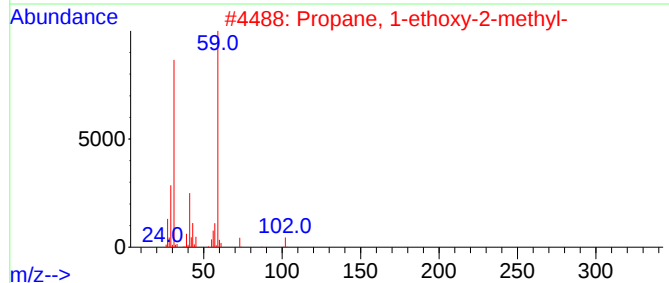
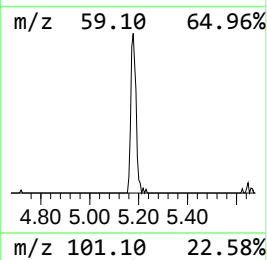
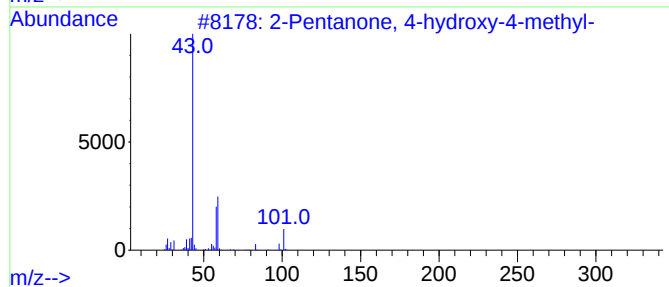
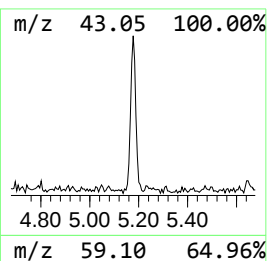
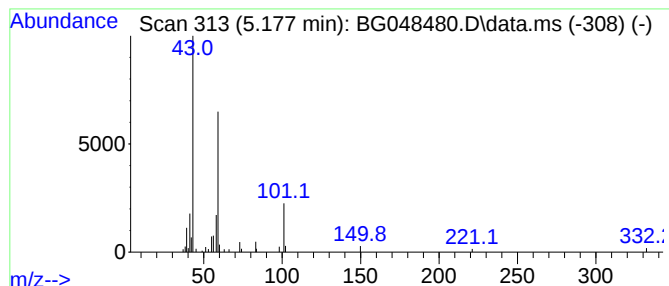
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.177	4.07 ng	53210	1,4-Dichlorobenzene-d4	8.103

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38		
2	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	38		
3	3-Octanol	130	C8H18O	000589-98-0	36		
4	Dimethadione	129	C5H7N03	000695-53-4	33		
5	Propane, 1,1-dipropoxy-	160	C9H20O2	004744-11-0	33		



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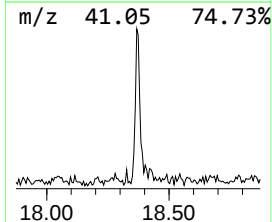
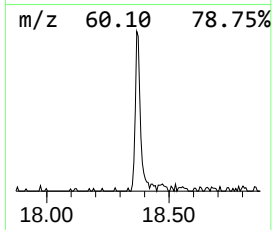
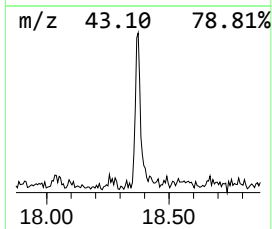
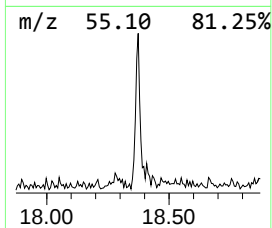
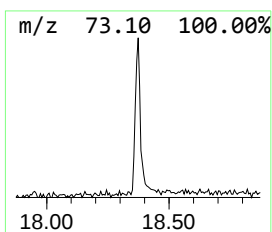
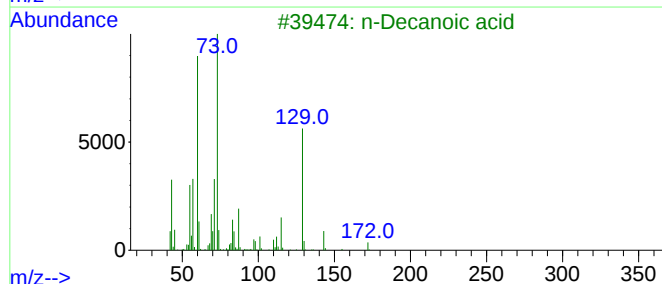
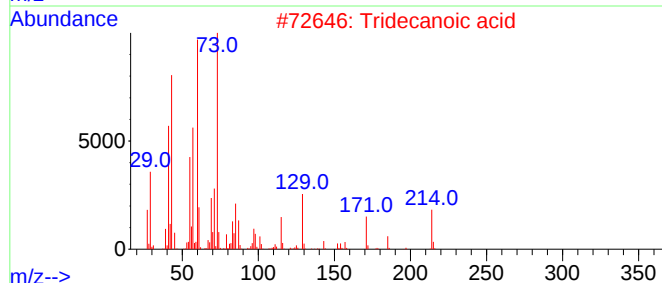
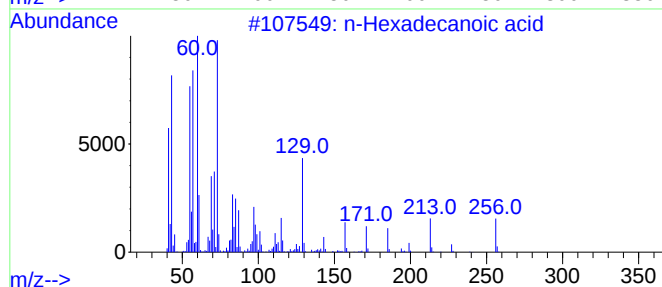
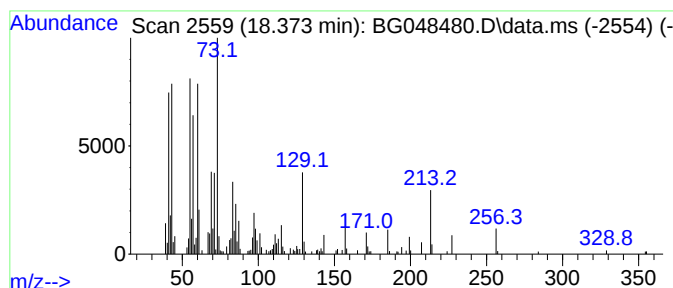
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TIC Library : C:\Database\NIST11.L
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.374	6.30 ng	235698	Phenanthrene-d10	17.492

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	90
3			n-Decanoic acid	172	C10H20O2	000334-48-5	87
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5			Octadecanoic acid	284	C18H36O2	000057-11-4	81



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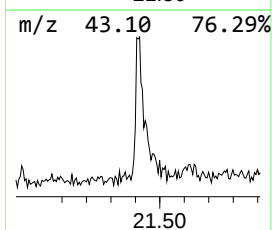
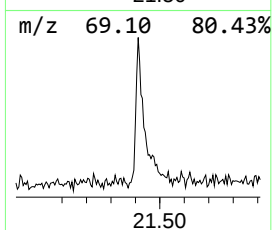
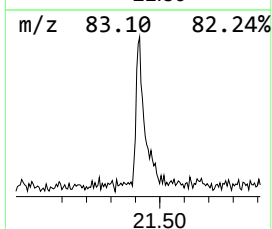
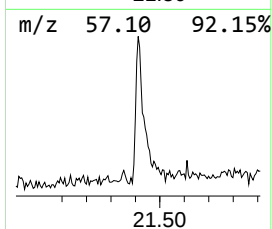
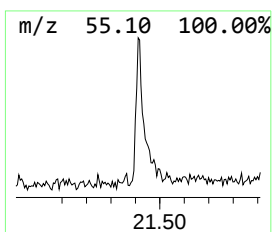
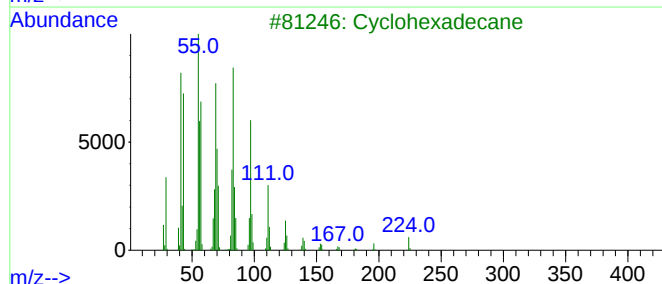
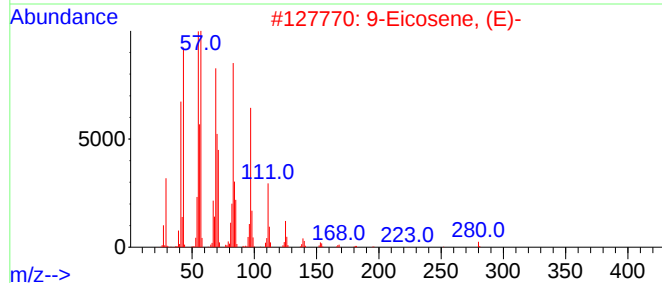
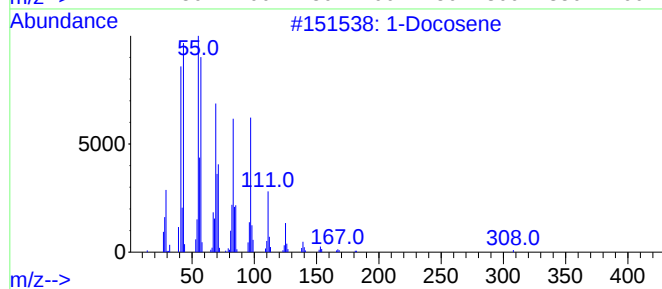
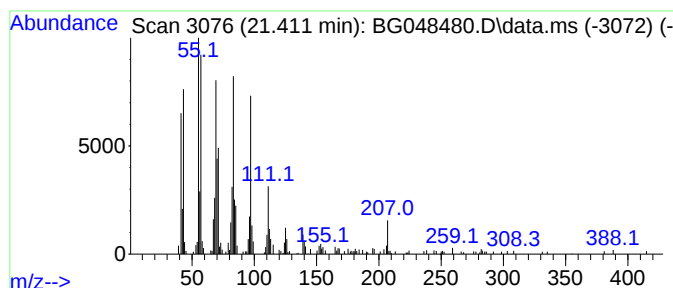
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Peak Number 3 1-Docosene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.411	8.25 ng	339597	Chrysene-d12	21.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Docosene	308	C22H44	001599-67-3	95
2			9-Eicosene, (E)-	280	C20H40	074685-29-3	91
3			Cyclohexadecane	224	C16H32	000295-65-8	90
4			n-Tetracosanol-1	354	C24H50O	000506-51-4	90
5			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90



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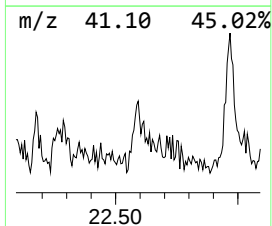
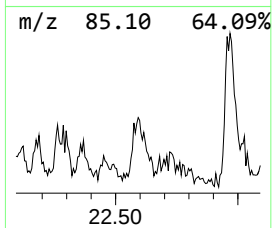
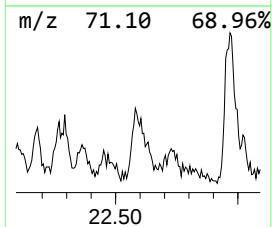
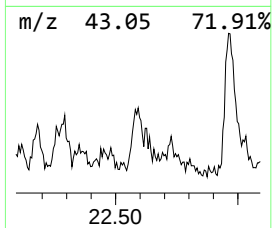
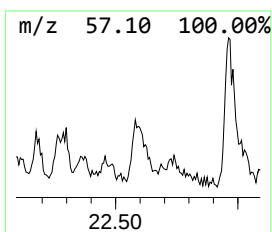
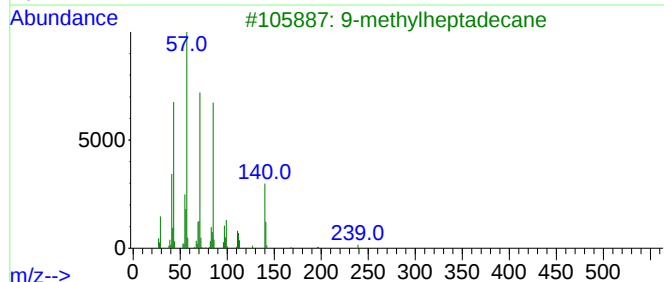
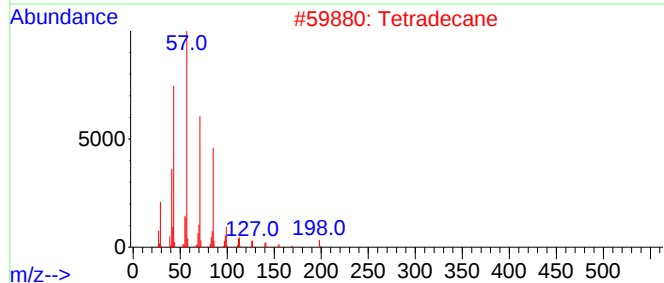
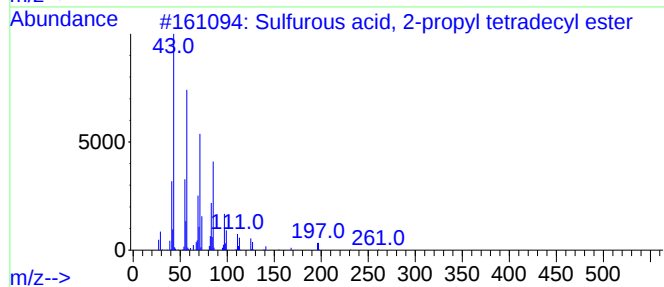
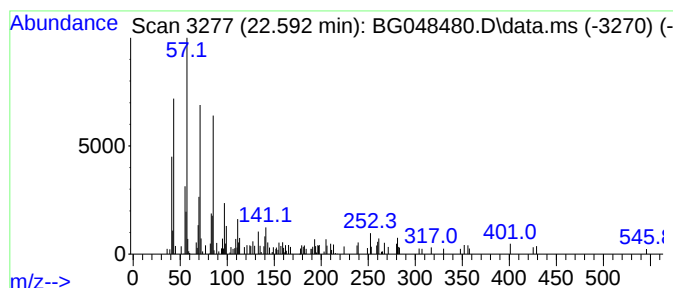
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Peak Number 4 Sulfurous acid, 2-propyl te... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
22.592	2.99 ng	123281	Chrysene-d12	21.781	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, 2-propyl tetradec...	320	C17H36O3S	1000309-12-5	64
2	Tetradecane	198	C14H30	000629-59-4	60
3	9-methylheptadecane	254	C18H38	026741-18-4	52
4	Ethanol, 2-(dodecyloxy)-	230	C14H30O2	004536-30-5	49
5	Nonadecane	268	C19H40	000629-92-5	49



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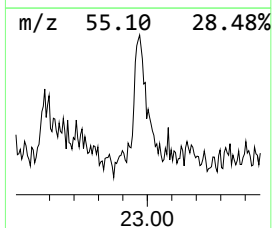
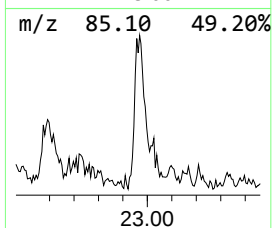
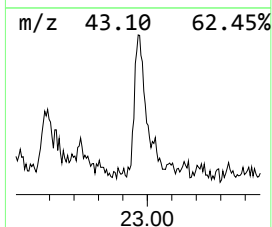
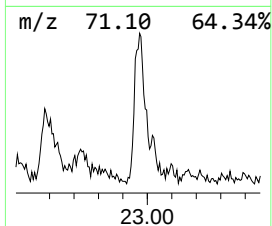
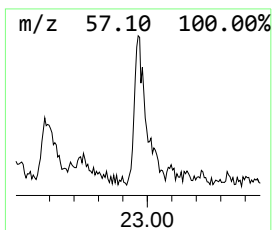
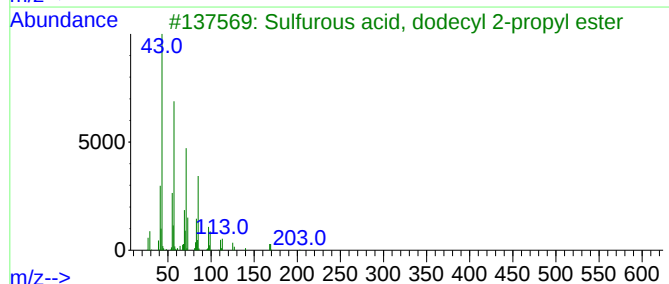
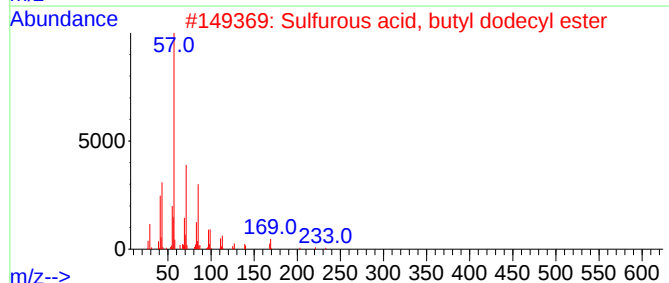
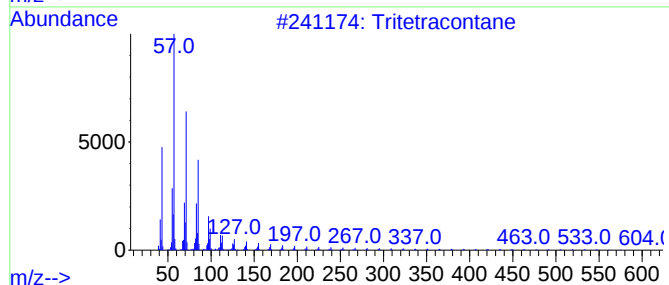
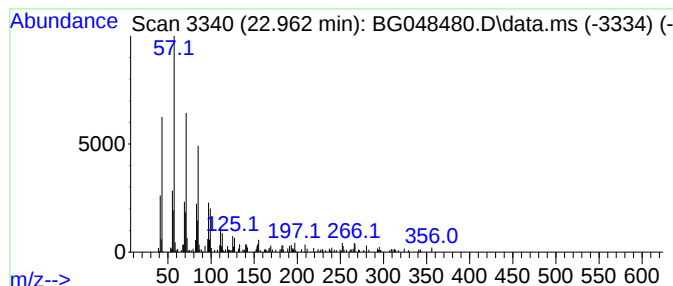
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Tritetracontane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.962	9.17 ng	377505	Chrysene-d12	21.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tritetracontane	605	C43H88	007098-21-7	86
2			Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	86
3			Sulfurous acid, dodecyl 2-propyl...	292	C15H32O3S	1000309-12-3	86
4			Heneicosane	296	C21H44	000629-94-7	83
5			10-Methylnonadecane	282	C20H42	056862-62-5	83



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.177	4.1	ng	53210	1	8.103	261228	20.0
n-Hexadecanoic ...	18.374	6.3	ng	235698	4	17.492	748804	20.0
1-Docosene	21.411	8.3	ng	339597	5	21.781	823344	20.0
Sulfurous acid,...	22.592	3.0	ng	123281	5	21.781	823344	20.0
Tritetracontane	22.962	9.2	ng	377505	5	21.781	823344	20.0