

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG063023\
 Data File : BG057925.D
 Acq On : 30 Jun 2023 19:03
 Operator : CG/JU
 Sample : 03358-06
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-4-(22-26)

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-BG062723.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057925.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.015	323	328	340	rVB	30292	46664	1.57%	0.328%
2	5.485	401	408	417	rBV	716959	1109439	37.24%	7.801%
3	7.078	671	679	693	rBV	712186	1186165	39.82%	8.341%
4	7.912	814	821	828	rBV	150861	246458	8.27%	1.733%
5	9.075	1009	1019	1029	rBV	407521	723353	24.28%	5.087%
6	10.715	1290	1298	1308	rBV	207732	362119	12.16%	2.546%
7	13.171	1709	1716	1727	rVB	1123669	1721149	57.78%	12.103%
8	14.551	1944	1951	1960	rVB	373396	591175	19.85%	4.157%
9	15.903	2175	2181	2197	rVB	242131	334724	11.24%	2.354%
10	16.038	2197	2204	2216	rBV	1048676	1640393	55.07%	11.535%
11	16.467	2271	2277	2284	rVB	27223	37977	1.27%	0.267%
12	17.289	2411	2417	2425	rBV	536975	813814	27.32%	5.723%
13	18.176	2563	2568	2586	rBV	110404	232573	7.81%	1.635%
14	19.910	2857	2863	2869	rBV	2245912	2978827	100.00%	20.947%
15	21.196	3078	3082	3090	rBV3	58242	96919	3.25%	0.682%
16	21.279	3092	3096	3106	rVB	21341	40548	1.36%	0.285%
17	21.543	3134	3141	3149	rBV	515371	824217	27.67%	5.796%
18	21.731	3170	3173	3179	rVB	32743	45043	1.51%	0.317%
19	22.330	3271	3275	3280	rVB2	36708	54268	1.82%	0.382%
20	22.988	3381	3387	3399	rVB3	72753	192451	6.46%	1.353%
21	24.686	3666	3676	3691	rVB	338050	942656	31.65%	6.629%

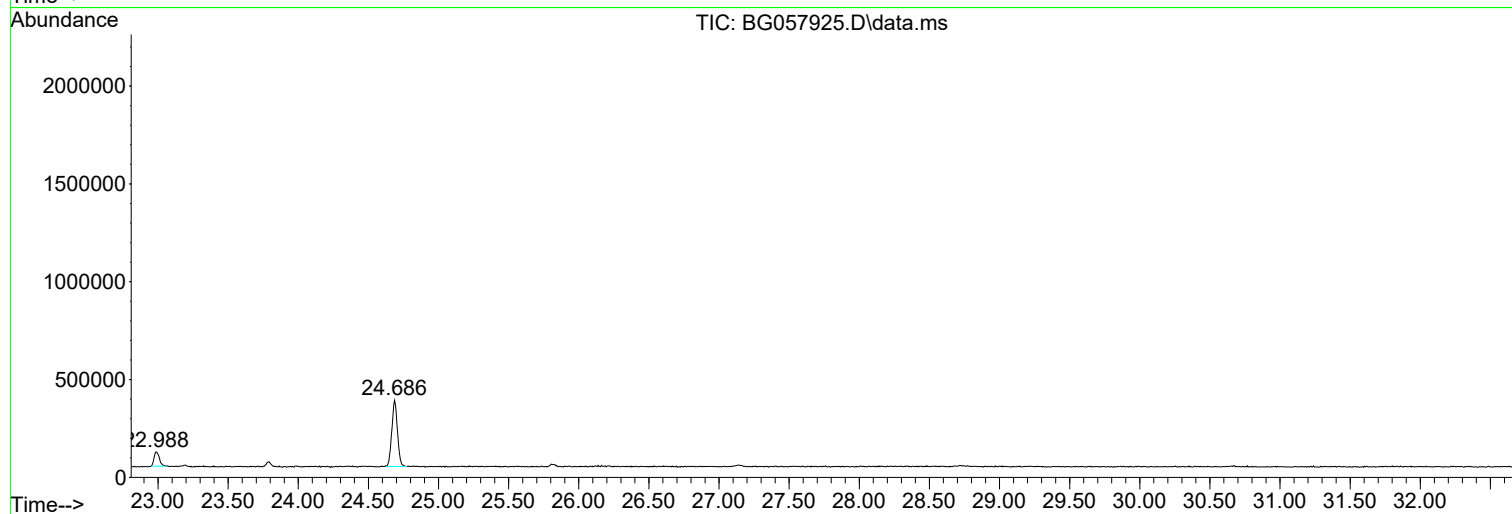
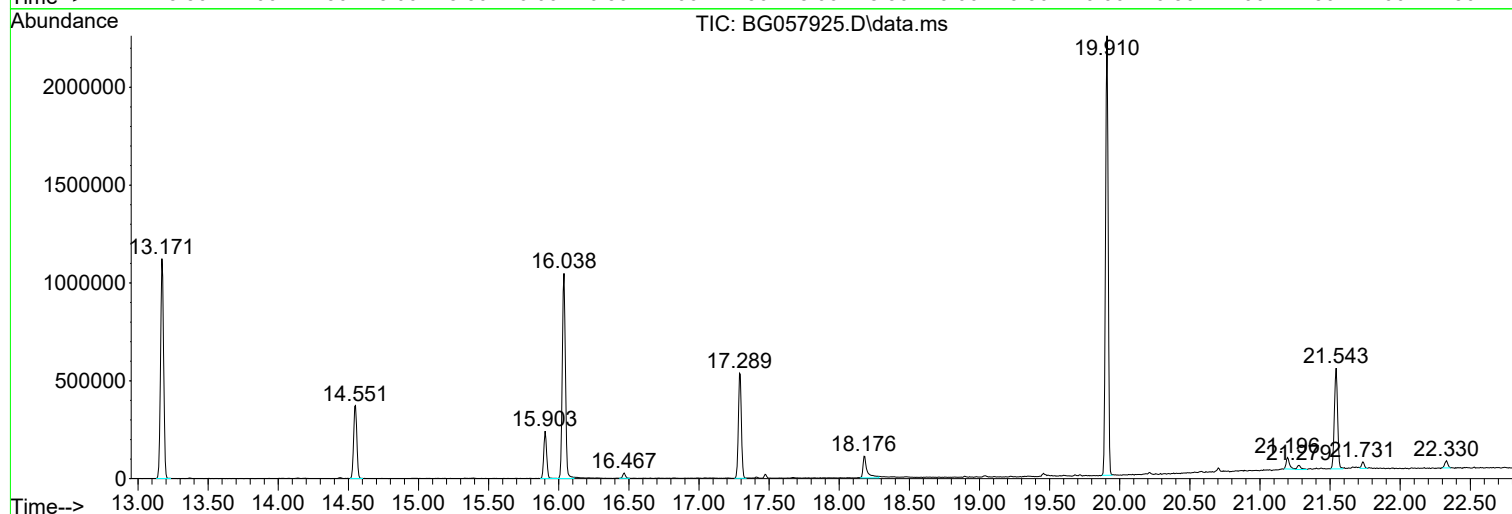
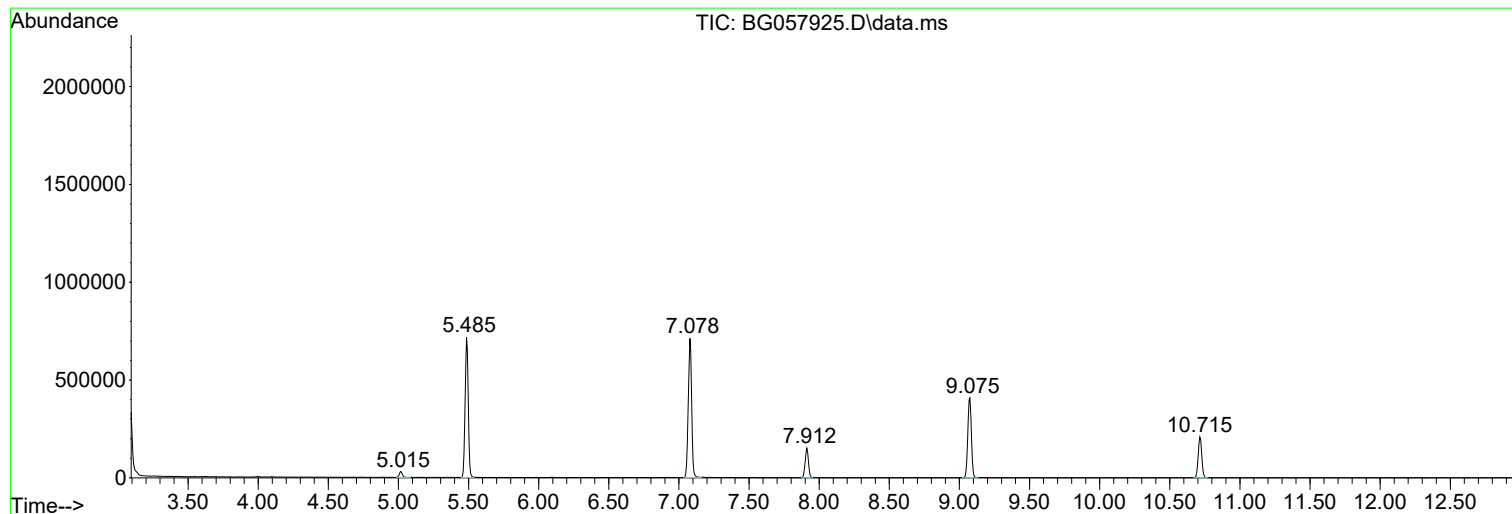
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG062723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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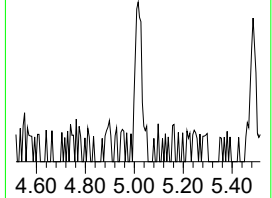
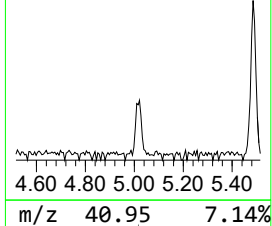
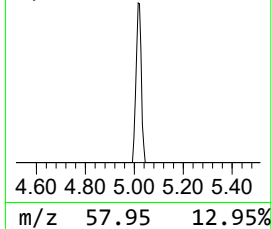
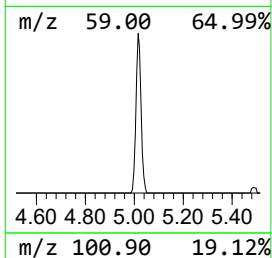
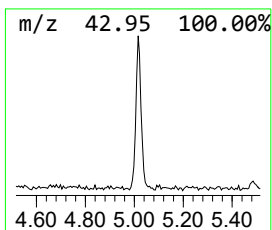
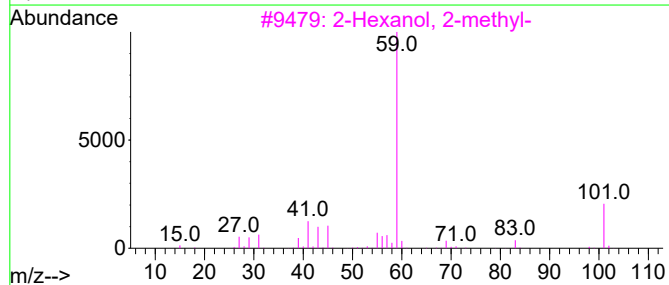
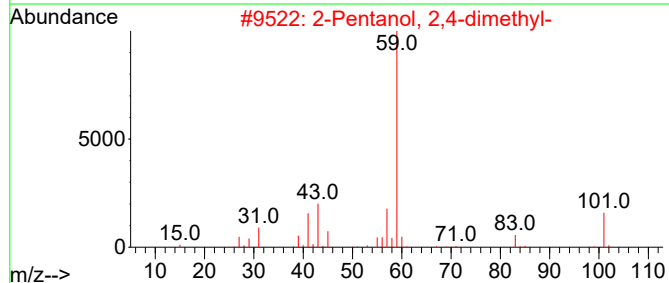
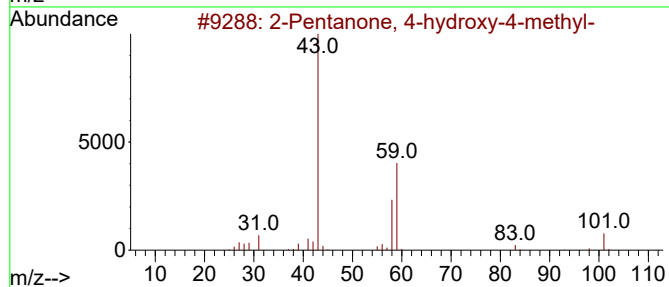
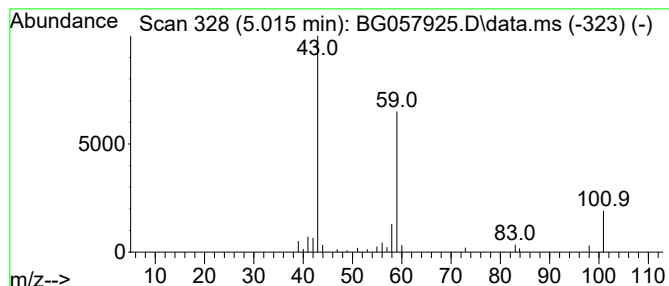
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.015	3.79 ng	46664	1,4-Dichlorobenzene-d4	7.912

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	42		
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33		
4	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	27		
5	1,2-Butanediol	90	C4H10O2	000584-03-2	23		



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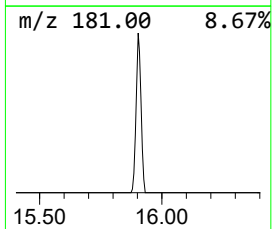
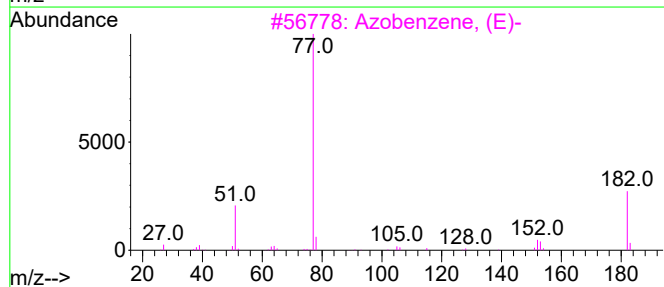
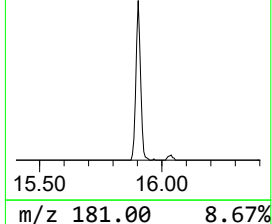
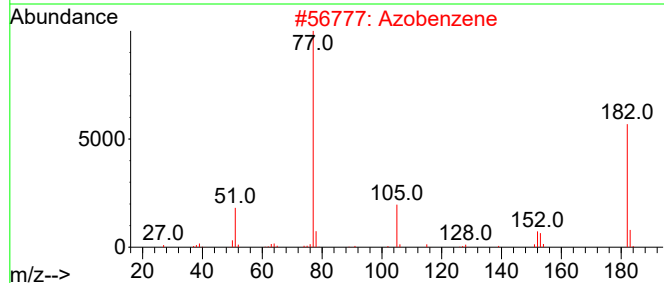
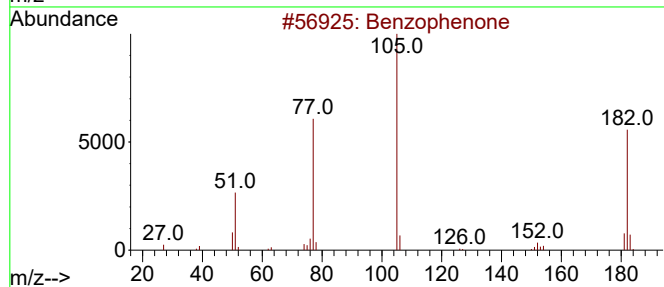
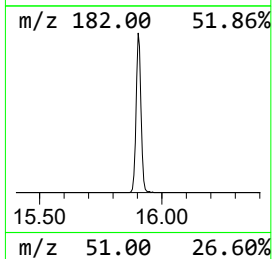
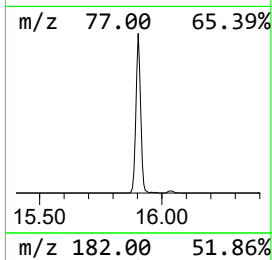
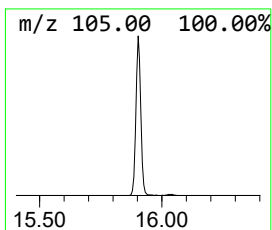
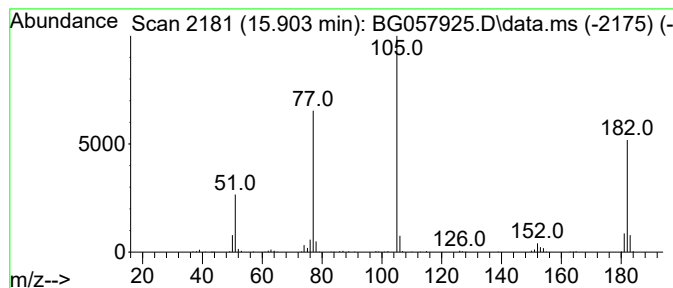
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG062723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Benzophenone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.903	11.32 ng	334724	Acenaphthene-d10	14.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Azobenzene	182	C12H10N2	000103-33-3	59
3			Azobenzene, (E)-	182	C12H10N2	017082-12-1	50
4			Benzoic acid, pentafluorophenyl ...	288	C13H5F5O2	1000360-67-9	50
5			Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	47



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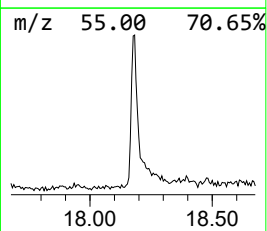
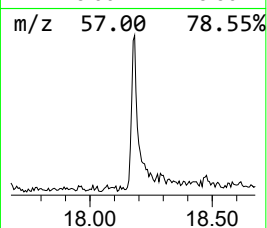
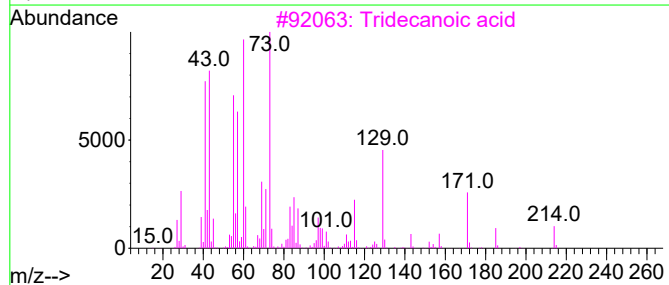
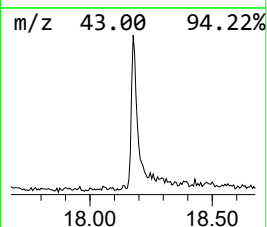
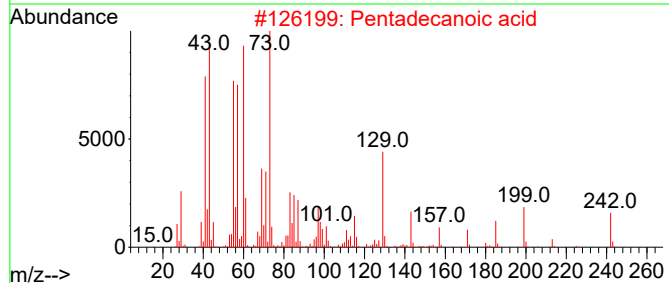
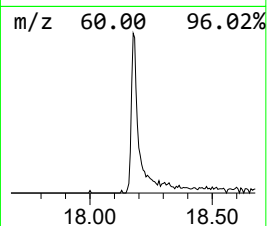
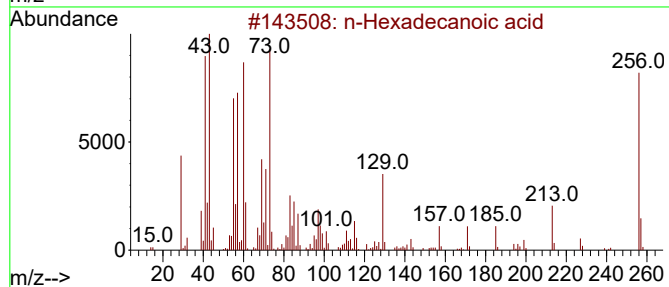
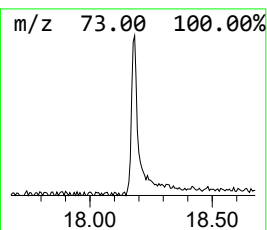
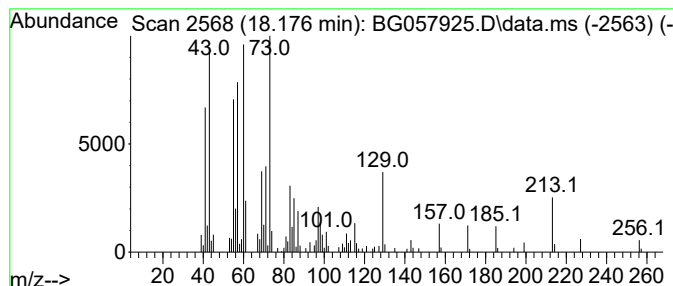
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.176	5.72 ng	232573	Phenanthrene-d10	17.289

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3			Tridecanoic acid	214	C13H26O2	000638-53-9	89
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5			n-Decanoic acid	172	C10H20O2	000334-48-5	83



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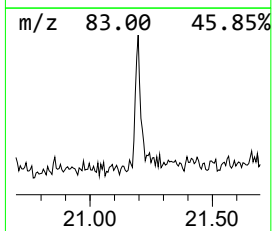
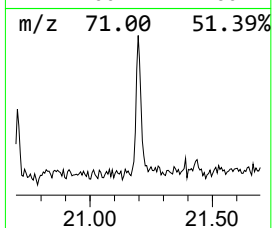
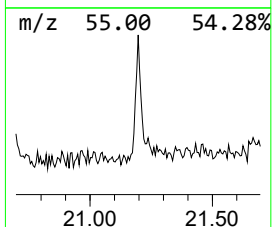
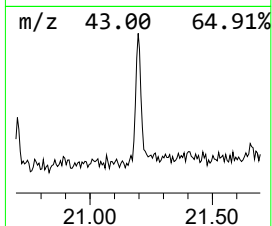
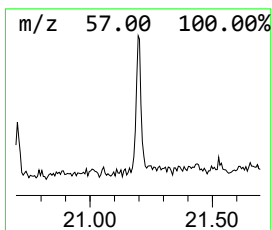
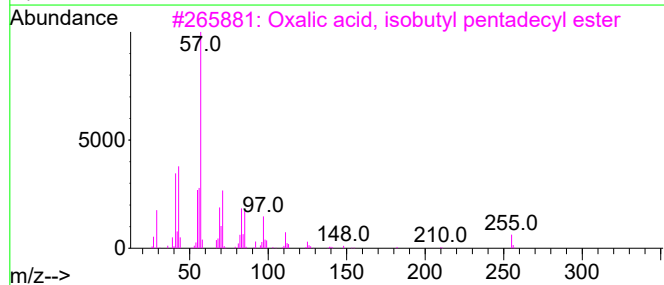
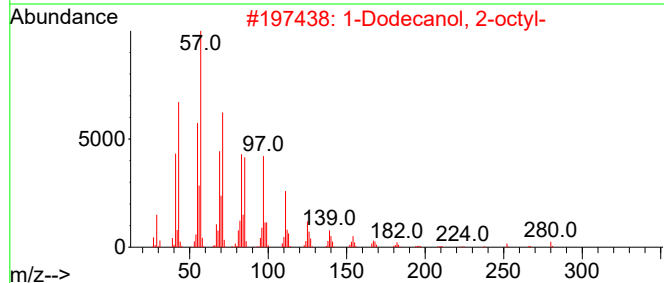
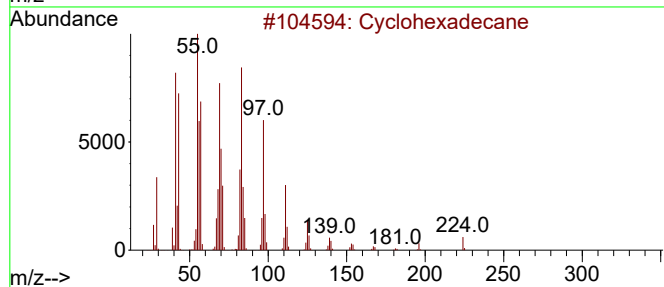
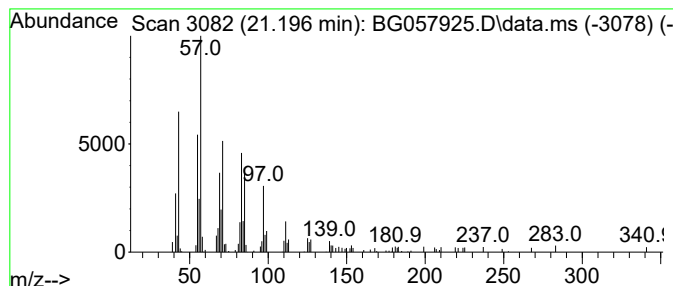
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Peak Number 4 Cyclohexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.196	2.35 ng	96919	Chrysene-d12	21.543

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexadecane	224	C16H32	000295-65-8	87
2			1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	87
3			Oxalic acid, isobutyl pentadecyl...	356	C21H40O4	1000309-38-0	74
4			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	74
5			Oxalic acid, isobutyl tetradecyl...	342	C20H38O4	1000309-37-9	74



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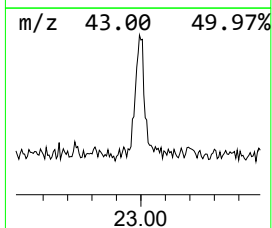
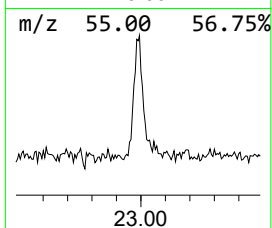
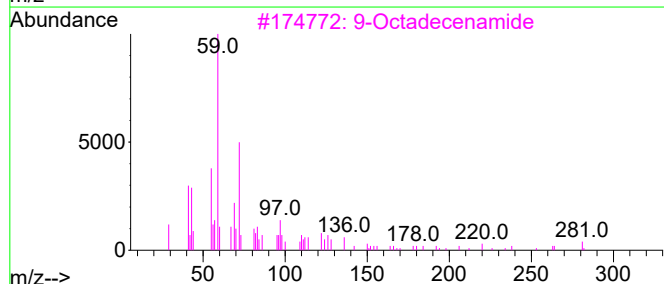
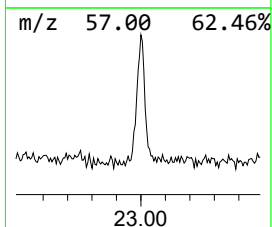
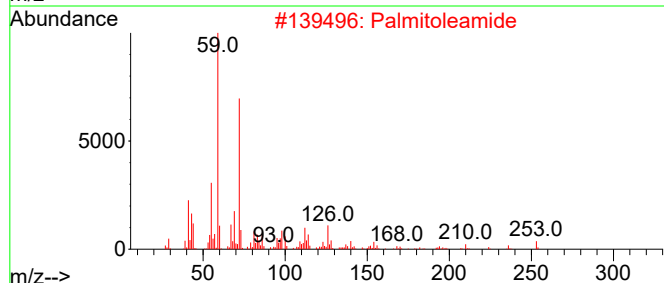
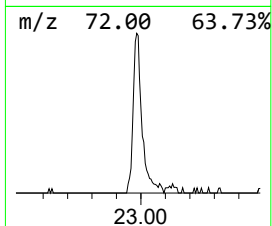
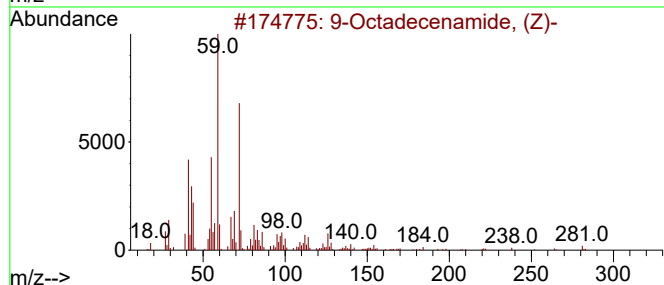
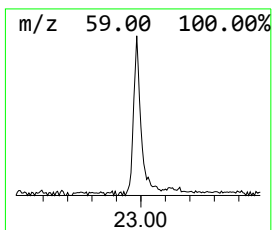
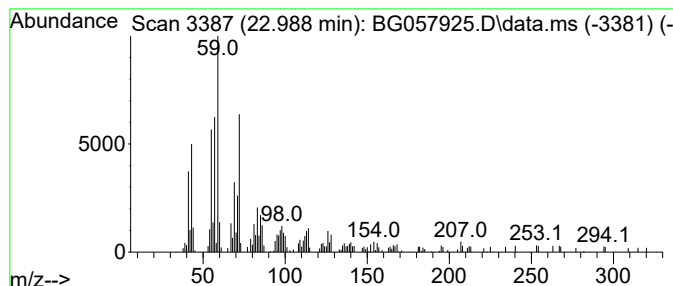
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.988	4.67 ng	192451	Chrysene-d12	21.543

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-			281	C18H35NO	000301-02-0	83
2	Palmitoleamide			253	C16H31NO	106010-22-4	81
3	9-Octadecenamide			281	C18H35NO	003322-62-1	59
4	Dodecanamide			199	C12H25NO	001120-16-7	49
5	2,11-Dimethyl-2,11-dodecanediol			230	C14H30O2	022092-59-7	38



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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.015	3.8	ng	46664	1	7.912	246458	20.0
Benzophenone	15.903	11.3	ng	334724	3	14.551	591175	20.0
n-Hexadecanoic ...	18.176	5.7	ng	232573	4	17.289	813814	20.0
Cyclohexadecane	21.196	2.4	ng	96919	5	21.543	824217	20.0
9-Octadecenamid...	22.988	4.7	ng	192451	5	21.543	824217	20.0