

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060523\
 Data File : BF133572.D
 Acq On : 05 Jun 2023 18:37
 Operator : CG\JU
 Sample : 02986-04
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-14-0A

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_F\Methods\8270-BF052523.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133572.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.204	14	20	27	rBV	47734	65714	1.98%	0.298%
2	5.051	499	504	511	rVB	105692	130898	3.95%	0.594%
3	5.445	566	571	574	rBV	3034454	3139558	94.75%	14.246%
4	6.457	738	743	746	rBV	2872755	3188158	96.22%	14.466%
5	6.833	803	807	810	rBV	990502	805404	24.31%	3.654%
6	7.398	898	903	906	rBV	2138877	1944592	58.69%	8.824%
7	8.116	1021	1025	1028	rBV	1317126	994553	30.02%	4.513%
8	9.192	1204	1208	1211	rBV	4112434	3313365	100.00%	15.034%
9	9.869	1320	1323	1327	rBV	1182712	961096	29.01%	4.361%
10	10.586	1442	1445	1448	rBV	147322	115302	3.48%	0.523%
11	10.657	1453	1457	1461	rBV	2065314	1846172	55.72%	8.377%
12	11.357	1572	1576	1579	rBV	1124284	899939	27.16%	4.083%
13	11.886	1662	1666	1671	rBV	139611	139191	4.20%	0.632%
14	12.951	1842	1847	1850	rBV	3060949	2885209	87.08%	13.092%
15	13.180	1877	1886	1888	rBV3	66733	126247	3.81%	0.573%
16	13.857	1998	2001	2003	rBV	46955	41572	1.25%	0.189%
17	13.904	2003	2009	2014	rBV9	47540	136585	4.12%	0.620%
18	13.998	2022	2025	2029	rVB	762205	663597	20.03%	3.011%
19	14.474	2103	2106	2111	rBV	56952	59321	1.79%	0.269%
20	14.762	2152	2155	2157	rBV	95342	95138	2.87%	0.432%
21	15.456	2269	2273	2277	rBV	403641	487149	14.70%	2.210%

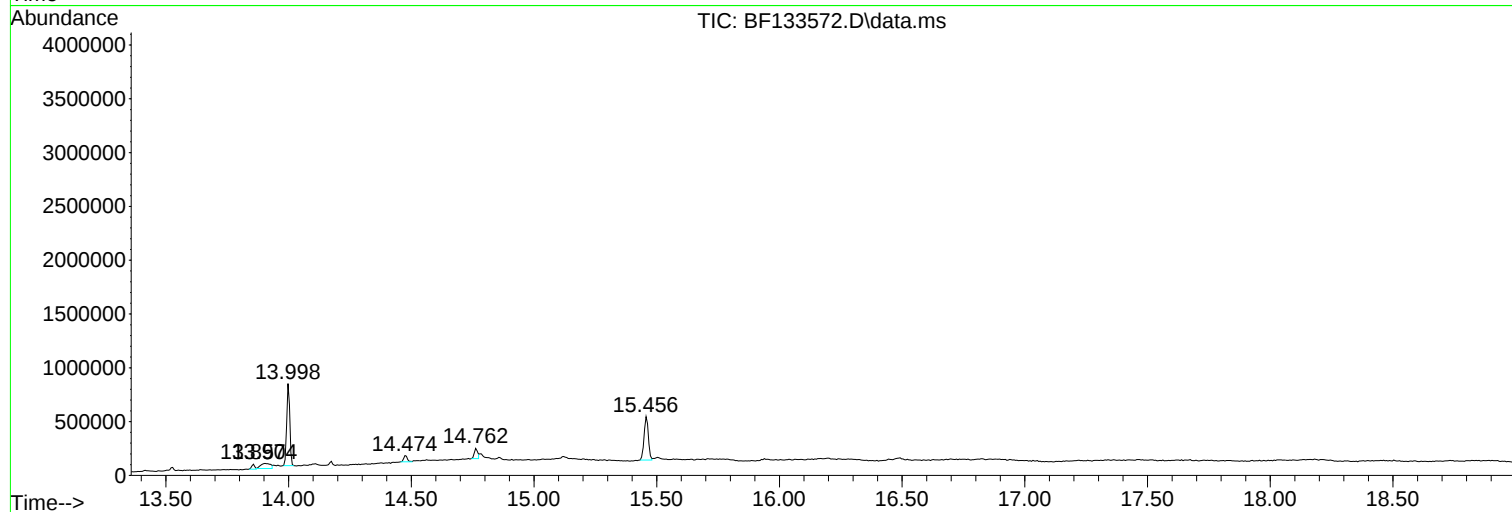
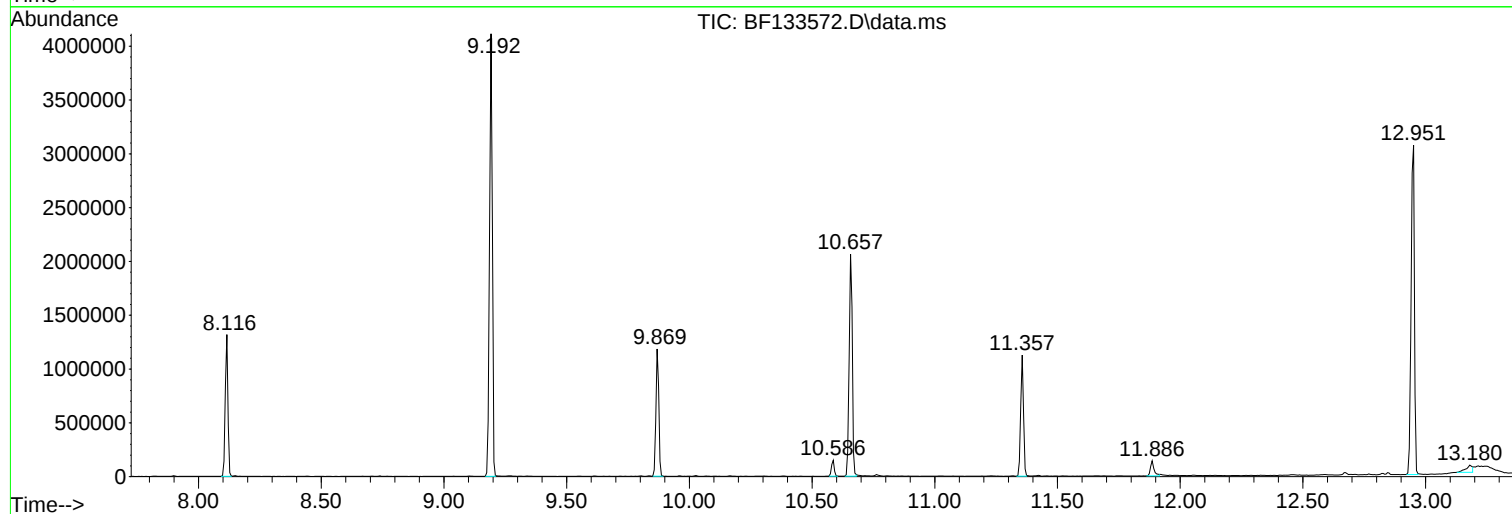
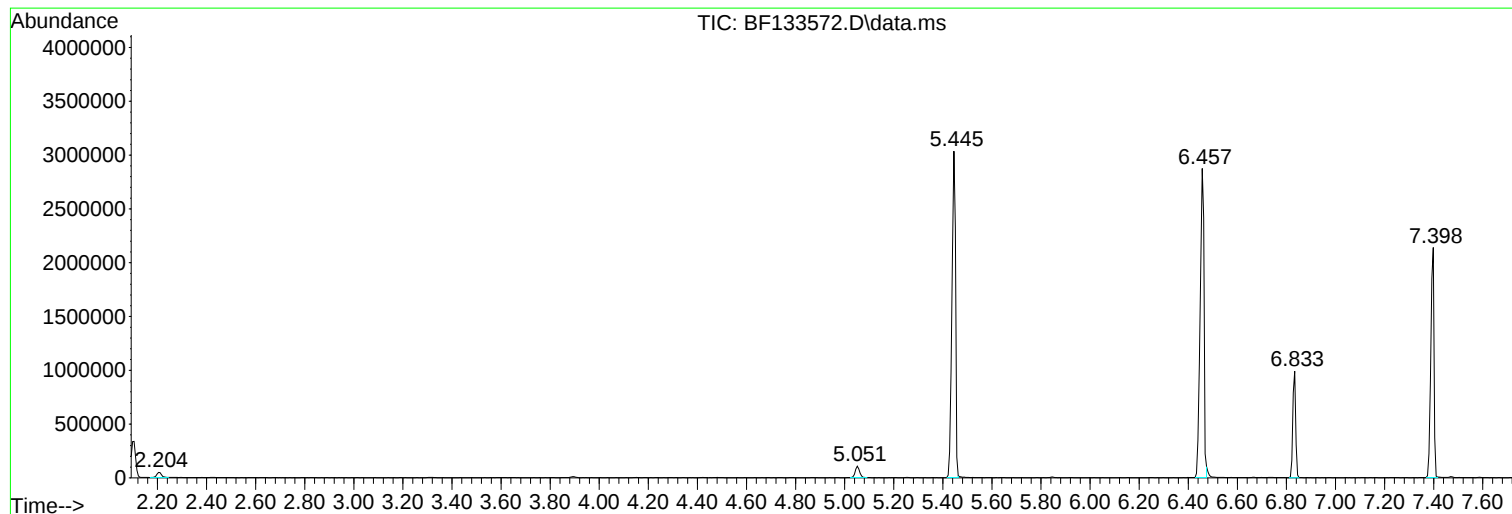
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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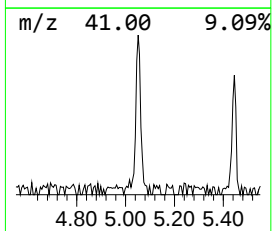
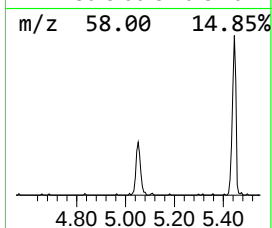
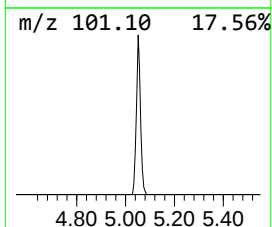
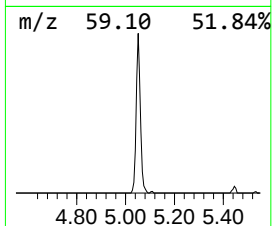
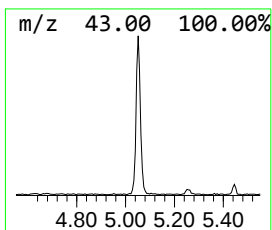
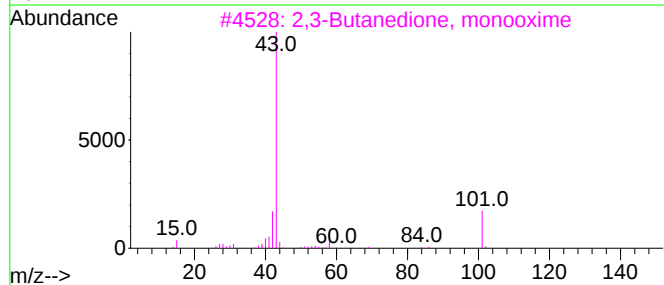
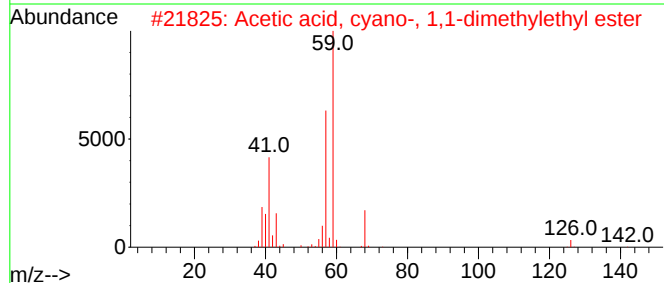
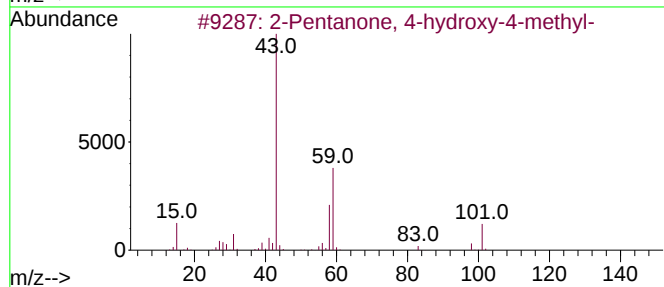
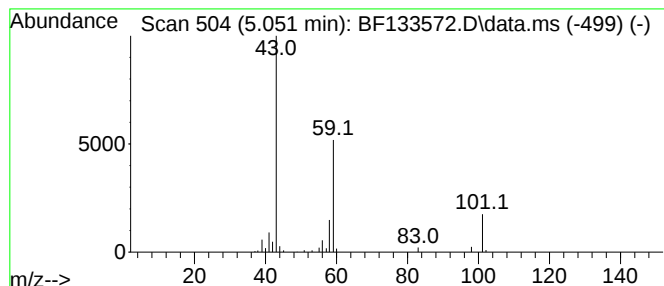
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.051	3.25 ng	130898	1,4-Dichlorobenzene-d4	6.833

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, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
5	Diacetamide	101	C4H7NO2	000625-77-4	9		



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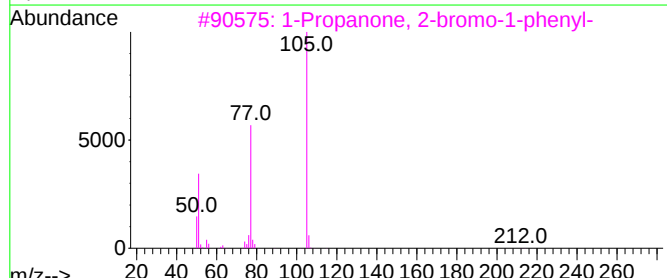
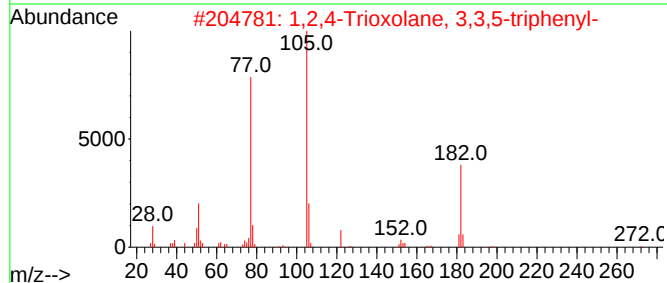
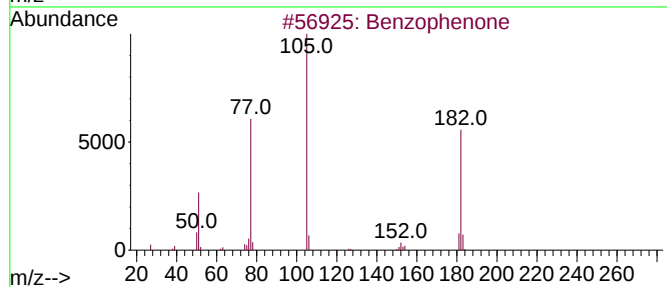
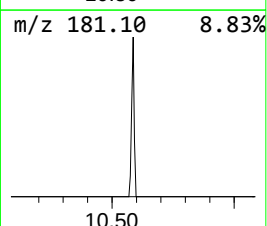
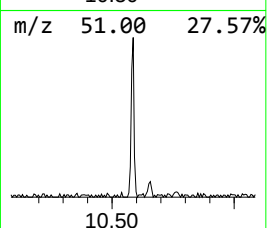
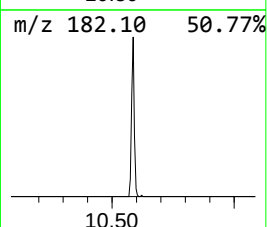
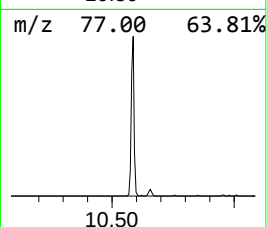
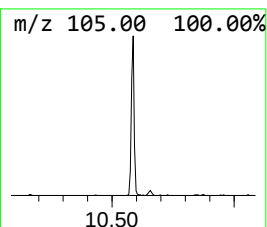
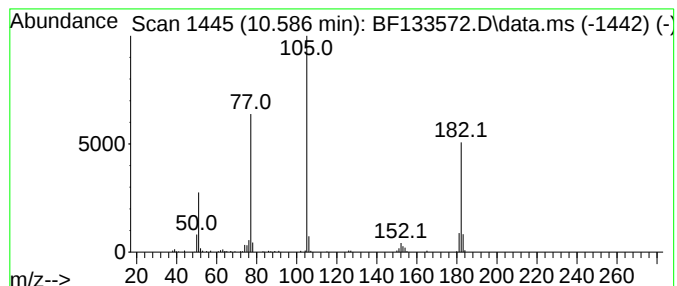
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.586	2.40 ng	115302	Acenaphthene-d10	9.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			1,2,4-Trioxolane, 3,3,5-triphenyl-	304	C20H16O3	023246-12-0	72
3			1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
4			S-Benzoyl(thiohydroxylamine)	153	C7H7NO5	025740-80-1	47
5			Vinyl benzoate	148	C9H8O2	000769-78-8	47



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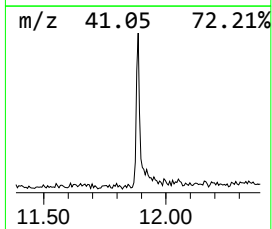
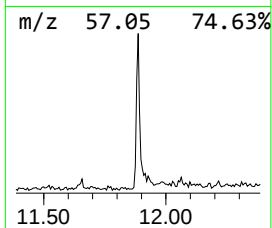
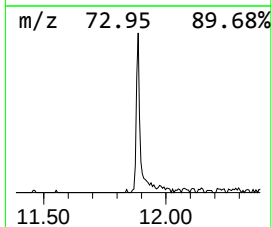
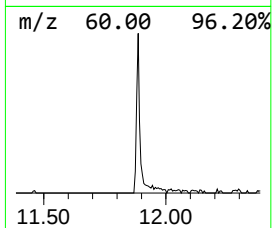
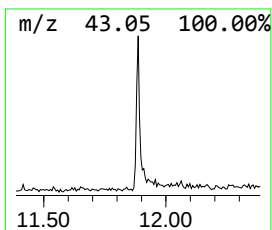
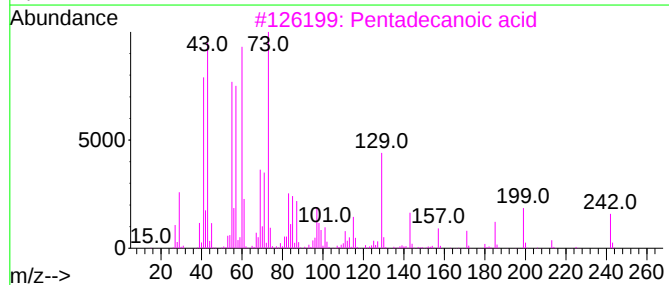
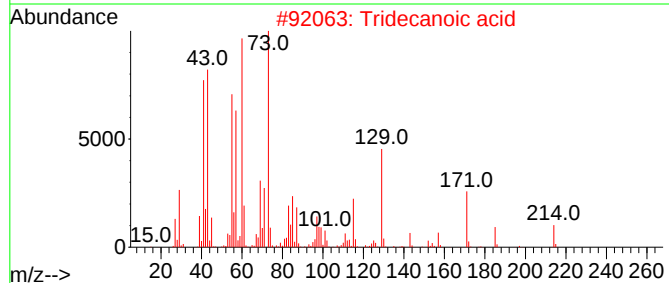
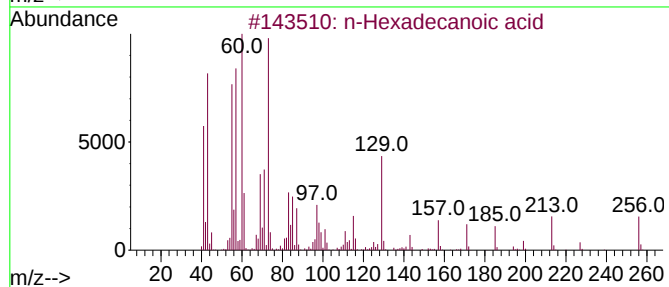
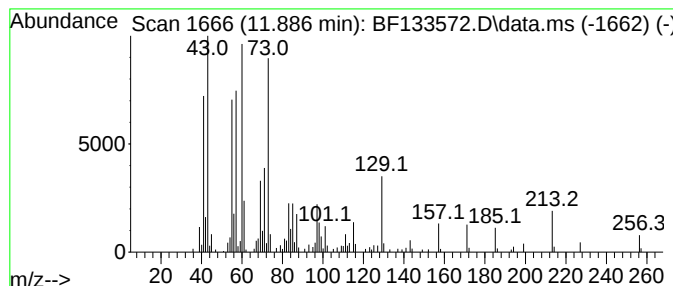
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.886	3.09 ng	139191	Phenanthrene-d10	11.357

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	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	49



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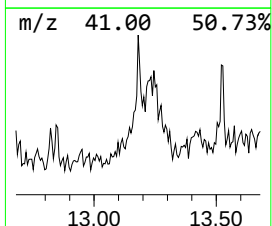
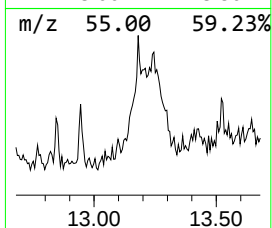
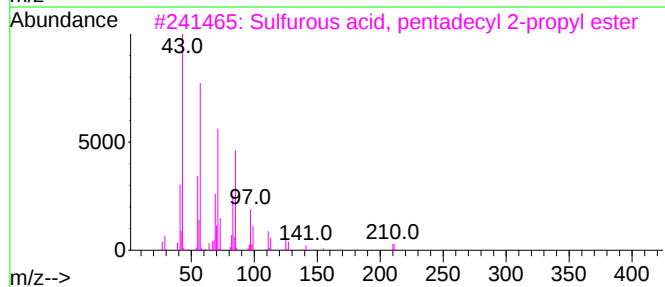
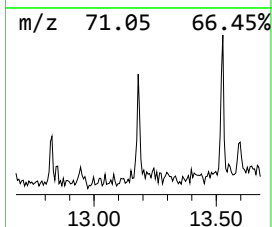
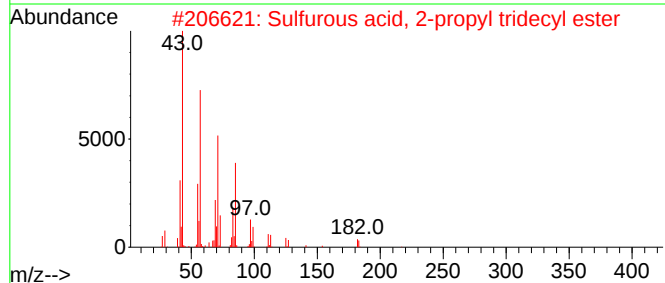
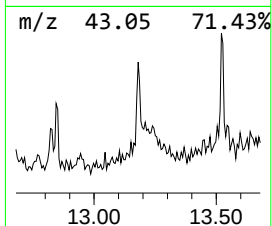
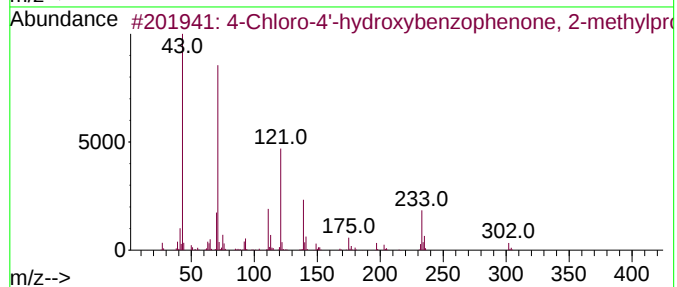
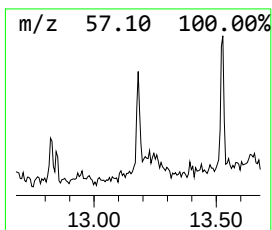
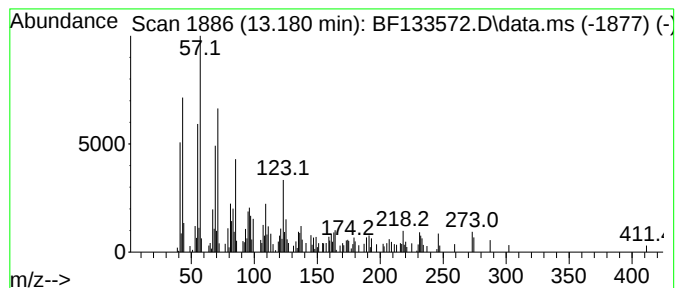
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 unknown13.180 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.180	3.80 ng	126247	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Chloro-4'-hydroxybenzophenone,...	302	C17H15ClO3	1000462-37-6	44
2			Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	43
3			Sulfurous acid, pentadecyl 2-pro...	334	C18H38O3S	1000309-12-6	43
4			Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	41
5			1-Bromodocosane	388	C22H45Br	006938-66-5	41



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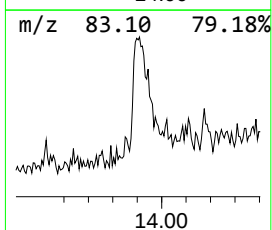
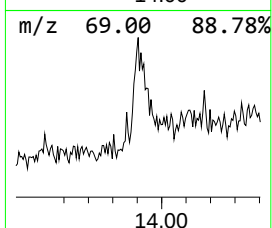
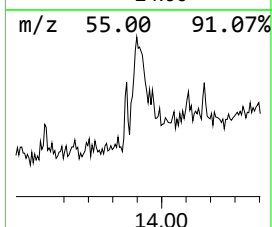
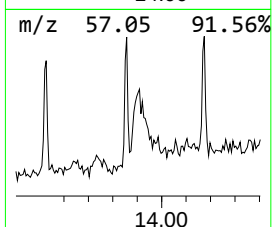
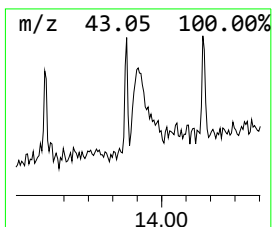
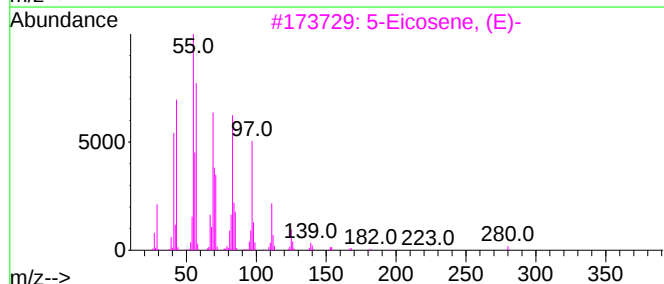
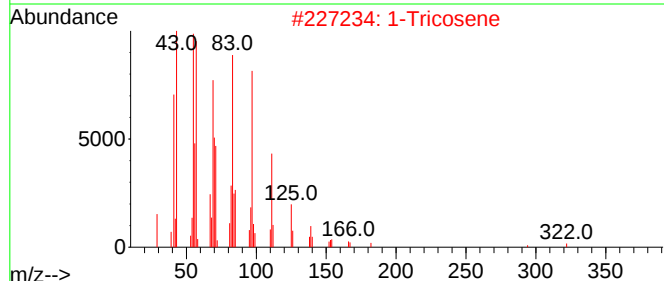
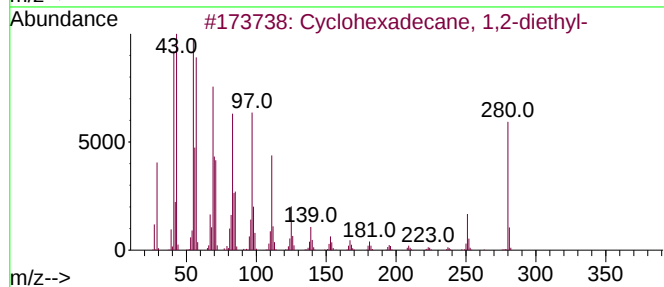
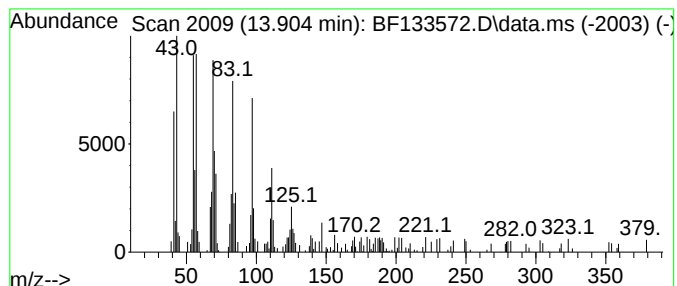
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Cyclohexadecane, 1,2-diethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.904	4.12 ng	136585	Chrysene-d12	13.998	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane, 1,2-diethyl-	280	C20H40	1000155-85-3	96
2	1-Tricosene	322	C23H46	018835-32-0	95
3	5-Eicosene, (E)-	280	C20H40	074685-30-6	93
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
5	1-Eicosene	280	C20H40	003452-07-1	93



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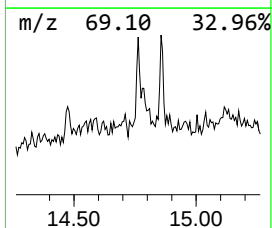
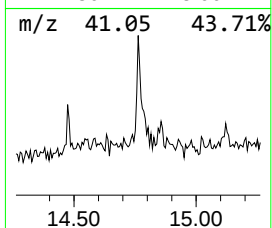
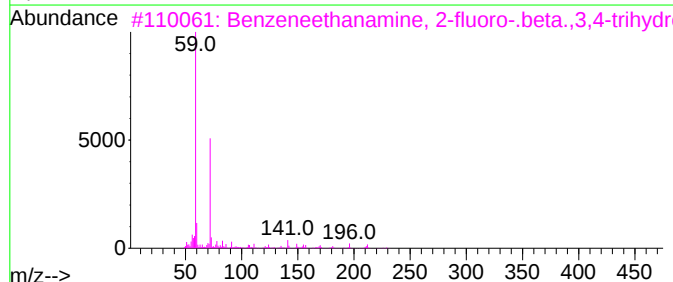
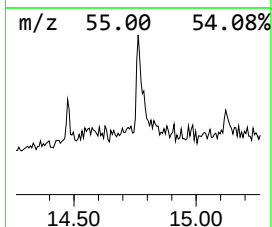
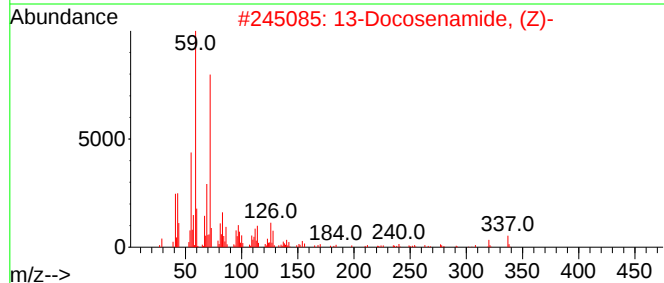
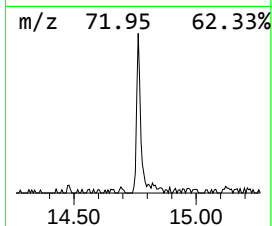
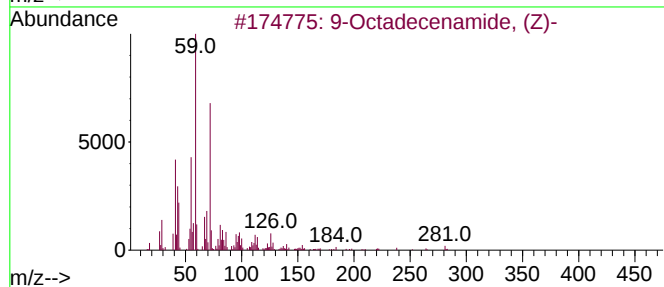
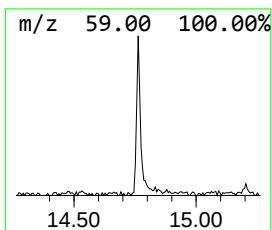
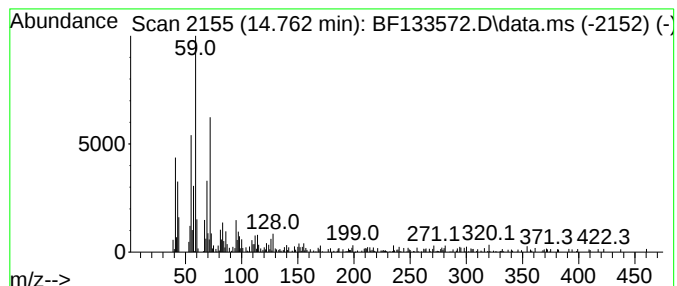
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.762	3.91 ng	95138	Perylene-d12	15.457

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	87
3			Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	81
4			9-Octadecenamide	281	C18H35NO	003322-62-1	62
5			Octadecanamide	283	C18H37NO	000124-26-5	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060523\
Data File : BF133572.D
Acq On : 05 Jun 2023 18:37
Operator : CG\JU
Sample : 02986-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-14-0A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.M
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-...	5.051	3.3	ng	130898	1	6.833	805404	20.0
Benzophenone	10.586	2.4	ng	115302	3	9.869	961096	20.0
n-Hexadecanoic ...	11.886	3.1	ng	139191	4	11.357	899939	20.0
unknown13.180	13.180	3.8	ng	126247	5	13.998	663597	20.0
Cyclohexadecane...	13.904	4.1	ng	136585	5	13.998	663597	20.0
9-Octadecenamid...	14.762	3.9	ng	95138	6	15.457	487149	20.0