

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG120522\
 Data File : BG055889.D
 Acq On : 5 Dec 2022 17:49
 Operator : CG/JU
 Sample : N5870-02
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 ML-2

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-BG111622.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055889.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.219	321	328	339	rVB	229352	348576	13.57%	3.034%
2	5.706	404	411	426	rVB	556320	901806	35.11%	7.850%
3	7.328	679	687	704	rVB	585688	1002512	39.03%	8.727%
4	8.168	824	830	837	rBV	87141	145239	5.66%	1.264%
5	9.349	1021	1031	1043	rVB	343660	608466	23.69%	5.297%
6	11.000	1304	1312	1321	rBV	129411	227108	8.84%	1.977%
7	13.427	1717	1725	1733	rBV	985238	1460906	56.88%	12.717%
8	14.802	1953	1959	1967	rBV	249615	372526	14.50%	3.243%
9	16.147	2182	2188	2193	rBV	26863	37278	1.45%	0.325%
10	16.288	2205	2212	2228	rBV	940007	1442656	56.17%	12.558%
11	17.545	2419	2426	2432	rBV	367396	533276	20.76%	4.642%
12	18.403	2567	2572	2582	rBV2	56568	99911	3.89%	0.870%
13	18.815	2638	2642	2647	rBV	90995	108399	4.22%	0.944%
14	20.131	2860	2866	2872	rBV	1886288	2568304	100.00%	22.357%
15	21.429	3082	3087	3100	rBV2	74031	199864	7.78%	1.740%
16	21.829	3148	3155	3163	rBV2	362181	610254	23.76%	5.312%
17	23.315	3404	3408	3415	rVB2	19164	40115	1.56%	0.349%
18	23.521	3438	3443	3449	rVB	26122	49210	1.92%	0.428%
19	24.149	3544	3550	3557	rVB3	20767	47688	1.86%	0.415%
20	25.178	3711	3725	3738	rBV2	218424	683626	26.62%	5.951%

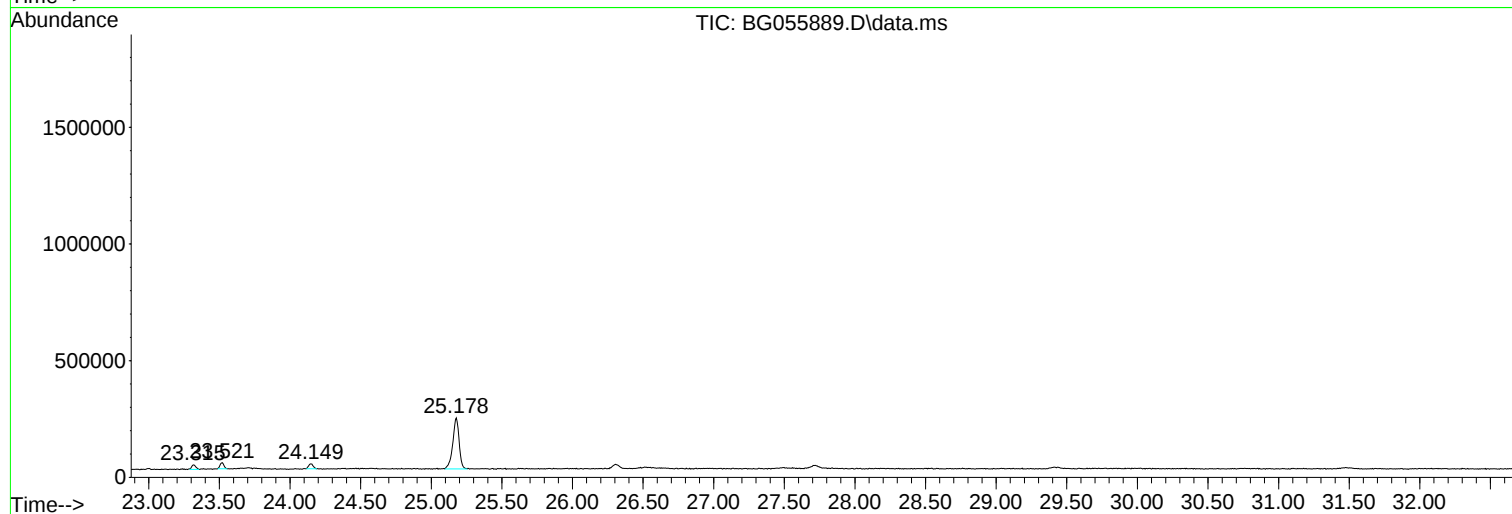
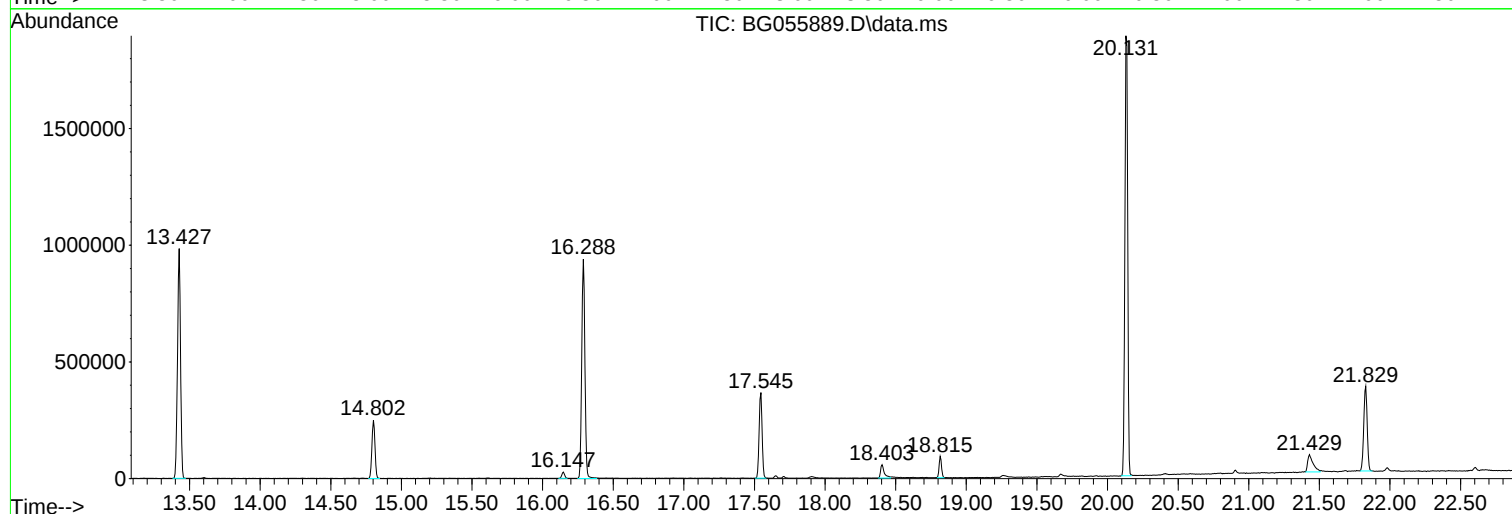
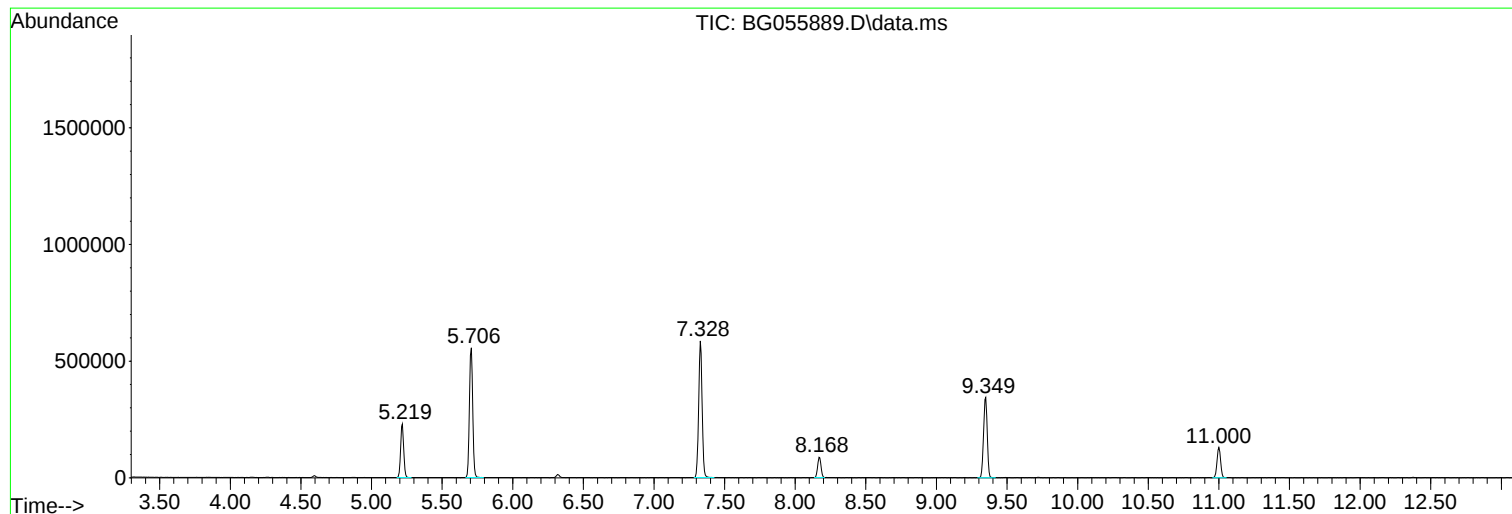
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Data File : BG055889.D
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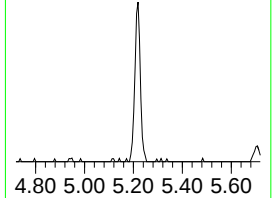
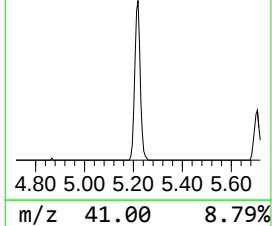
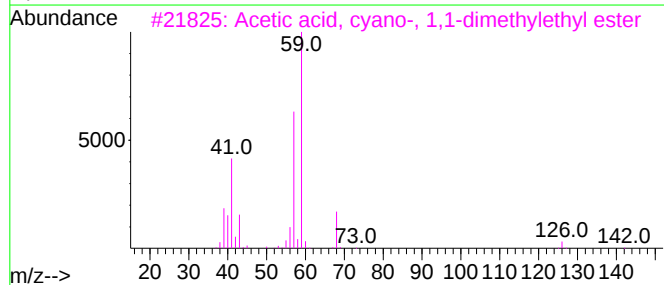
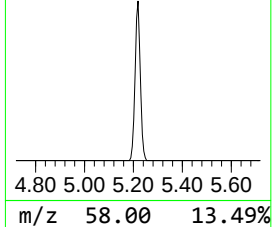
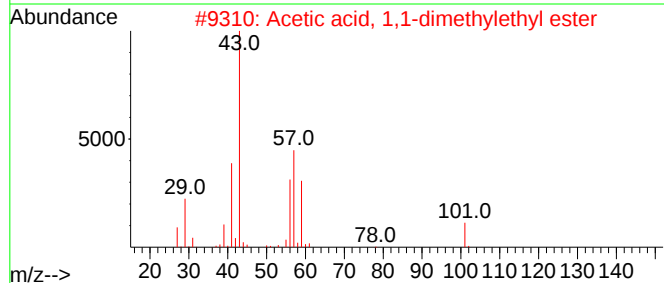
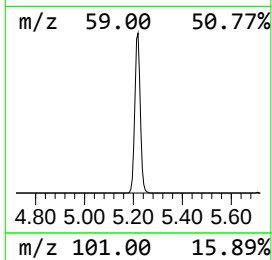
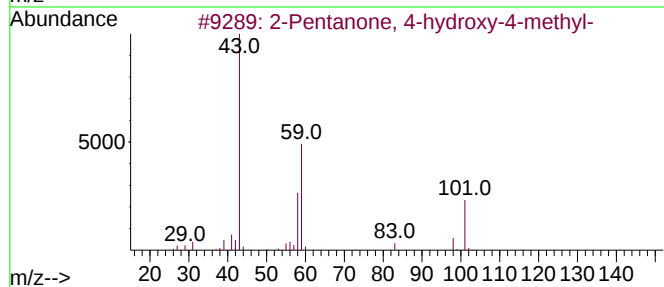
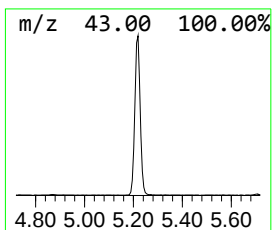
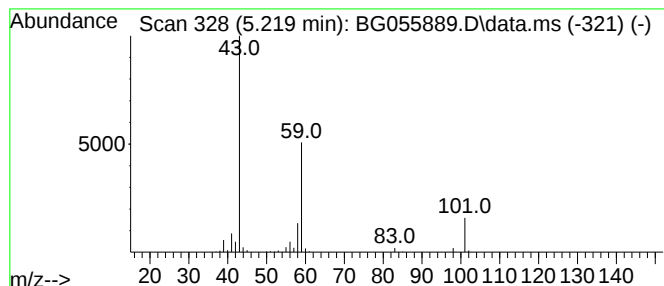
Instrument :
BNA_G
ClientSampleId :
ML-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.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.
5.219	48.00 ng	348576	1,4-Dichlorobenzene-d4			8.168
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	72
2	Acetic acid, 1,1-dimethylethyl e...		116	C6H12O2	000540-88-5	28
3	Acetic acid, cyano-, 1,1-dimethy...		141	C7H11NO2	001116-98-9	25
4	1-Propen-2-ol, acetate		100	C5H8O2	000108-22-5	12
5	2,3-Butanedione, monooxime		101	C4H7NO2	000057-71-6	9



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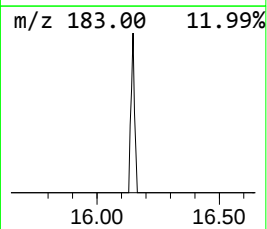
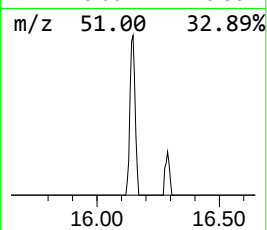
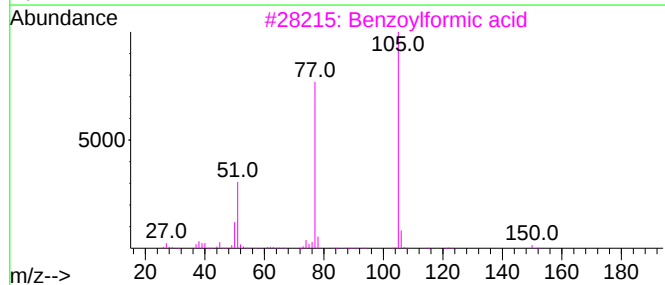
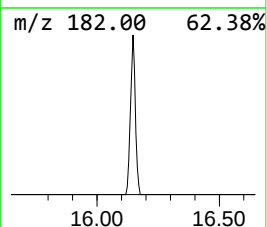
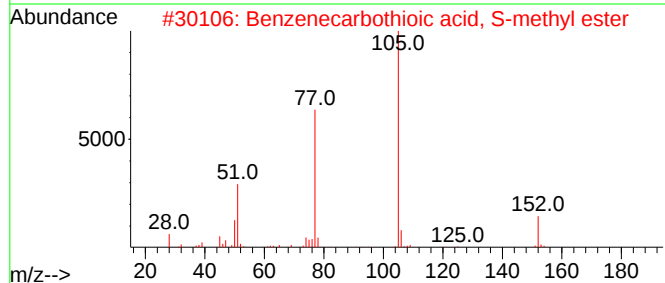
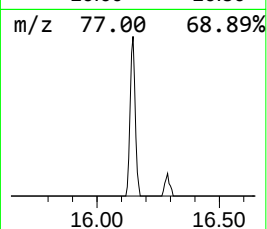
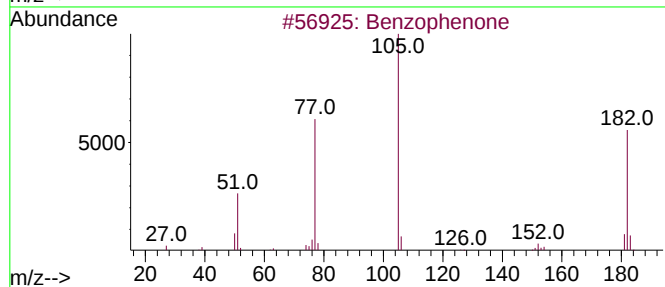
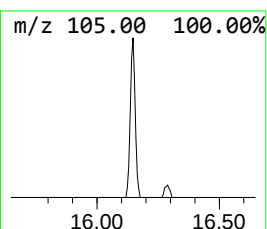
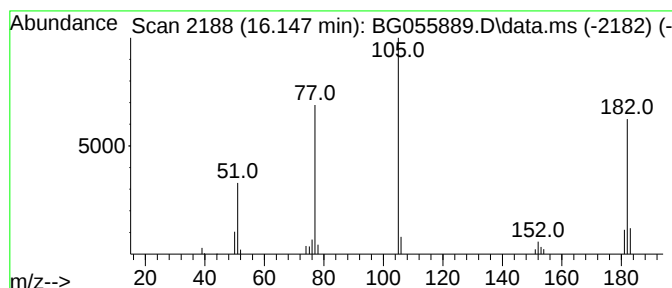
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.147	2.00 ng	37278	Acenaphthene-d10	14.802

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	49
3			Benzoylformic acid	150	C8H6O3	000611-73-4	47
4			Benzene, (trimethoxymethyl)-	182	C10H14O3	000707-07-3	47
5			1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	47



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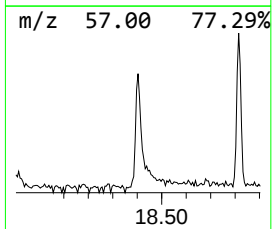
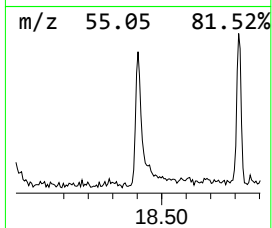
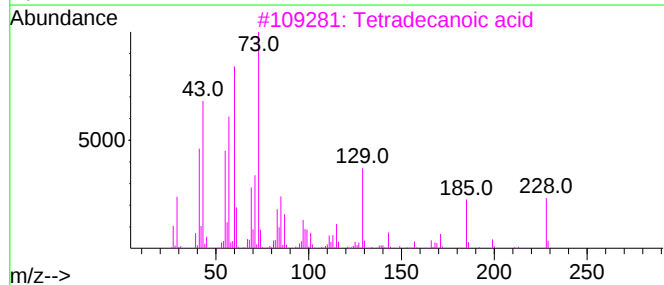
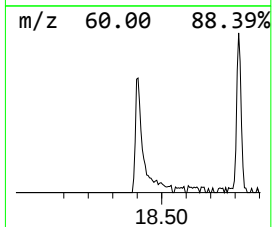
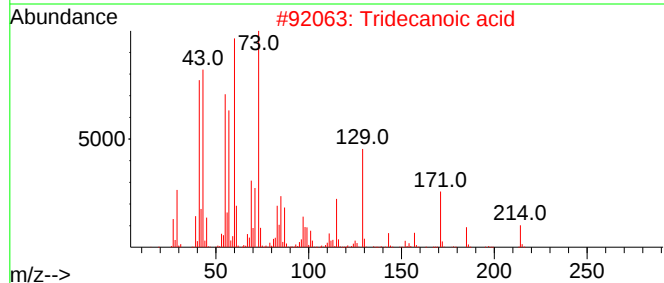
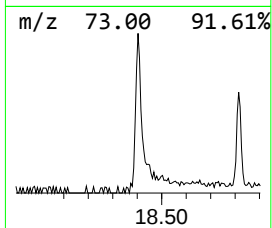
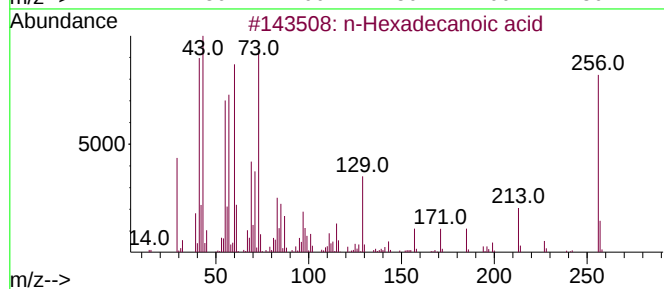
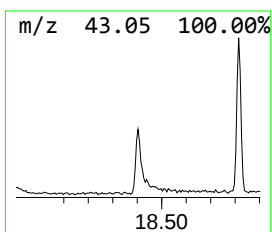
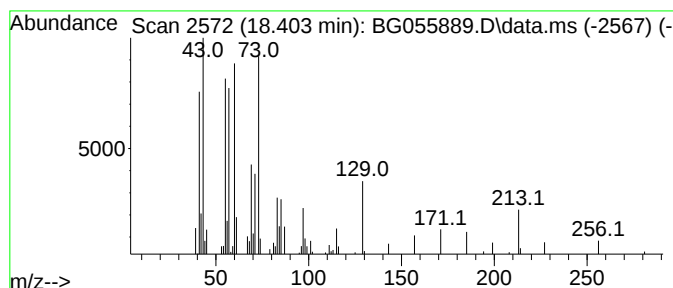
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BNA_G
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.403	3.75 ng	99911	Phenanthrene-d10	17.545	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4	Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	30
5	Oxalic acid, allyl octadecyl ester	382	C23H42O4	1000309-24-5	25



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Instrument :
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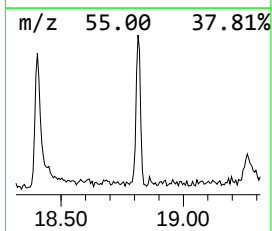
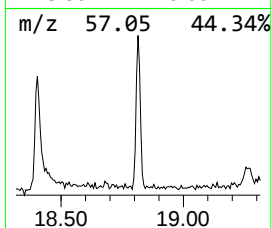
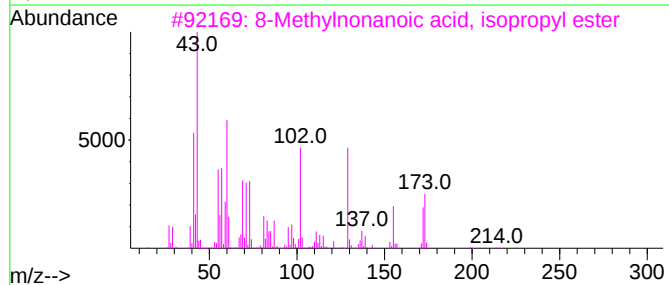
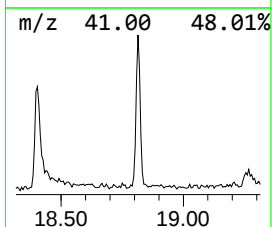
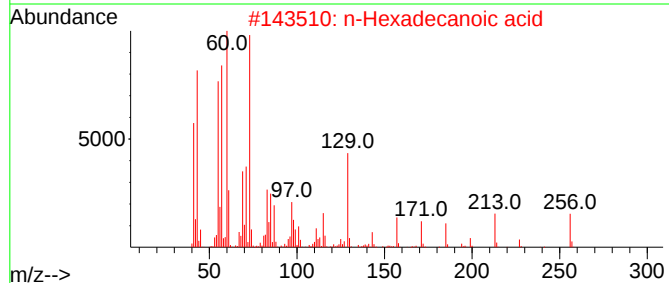
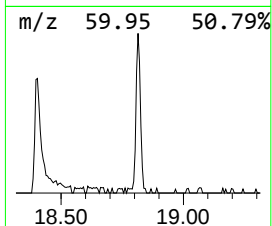
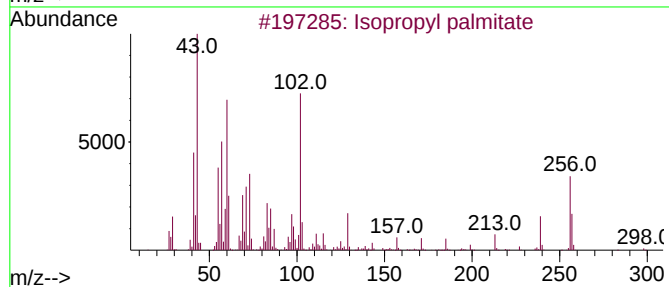
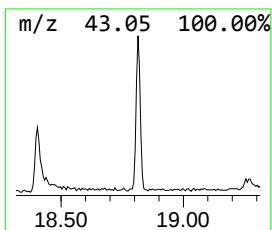
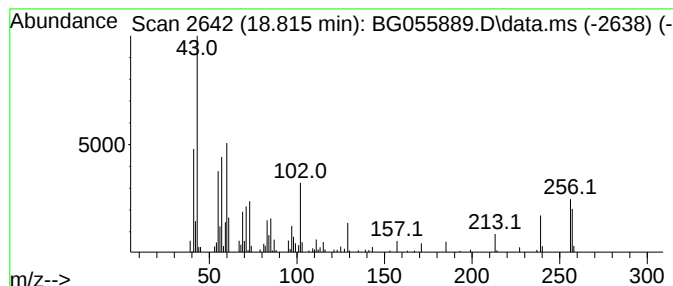
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Peak Number 4 Isopropyl palmitate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.815	4.07 ng	108399	Phenanthrene-d10	17.545

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl palmitate	298	C19H38O2	000142-91-6	74
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	70
3			8-Methylnonanoic acid, isopropyl...	214	C13H26O2	1000452-00-6	43
4			n-Capric acid isopropyl ester	214	C13H26O2	002311-59-3	43
5			Dodecanoic acid, 1-methylethyl e...	242	C15H30O2	010233-13-3	40



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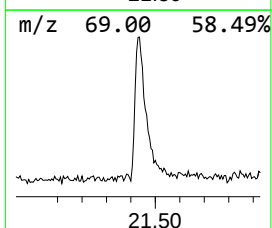
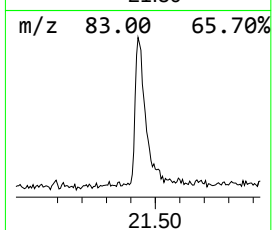
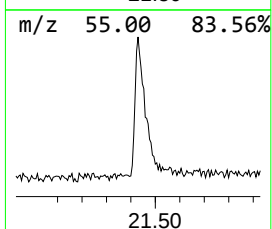
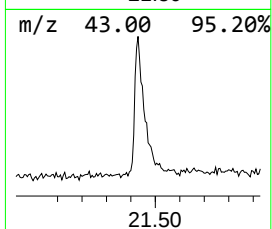
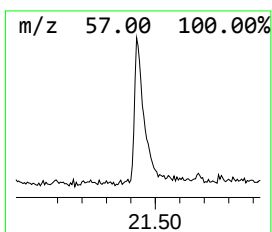
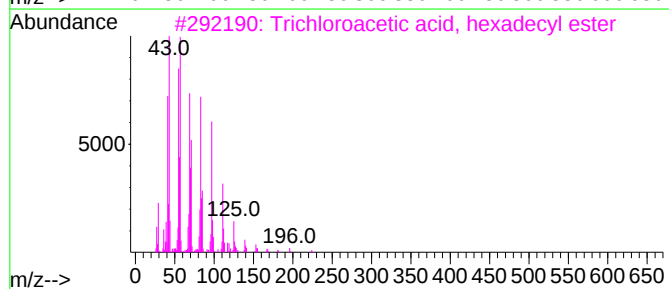
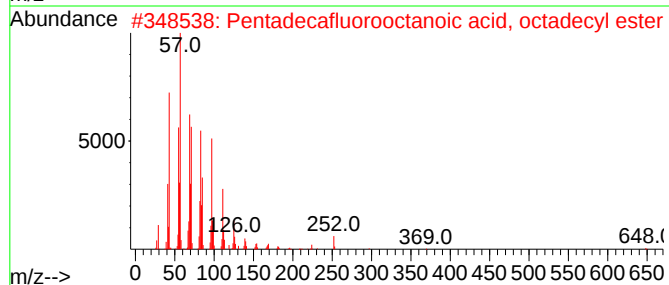
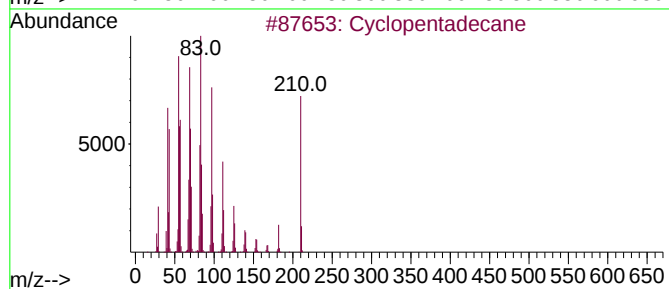
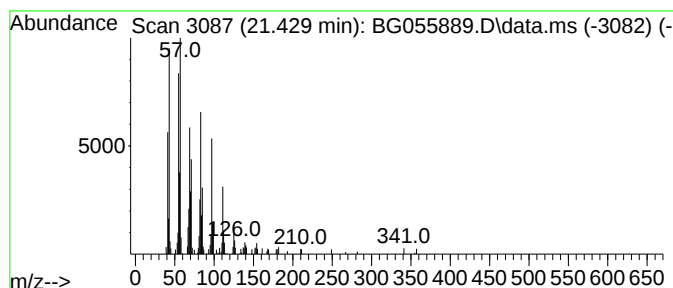
Instrument :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Cyclopentadecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.429	6.55 ng	199864	Chrysene-d12	21.829	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	95
2	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93
4	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	93
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.219	48.0	ng	348576	1	8.168	145239	20.0
Benzophenone	16.147	2.0	ng	37278	3	14.802	372526	20.0
n-Hexadecanoic ...	18.403	3.8	ng	99911	4	17.545	533276	20.0
Isopropyl palmi...	18.815	4.1	ng	108399	4	17.545	533276	20.0
Cyclopentadecane	21.429	6.5	ng	199864	5	21.829	610254	20.0