

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062223\
 Data File : BG057826.D
 Acq On : 23 Jun 2023 3:13
 Operator : CG/JU
 Sample : 03320-10
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 WC-13

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-BG061923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057826.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.430	222	228	233	rBV	18513	26649	1.09%	0.154%
2	5.029	323	330	340	rVB	465848	674278	27.53%	3.907%
3	5.493	402	409	418	rBV	671135	1033583	42.20%	5.989%
4	6.104	508	513	520	rVB	17619	28016	1.14%	0.162%
5	7.080	669	679	693	rBV	668184	1149516	46.93%	6.661%
6	7.920	814	822	831	rBV	162750	271143	11.07%	1.571%
7	9.083	1012	1020	1028	rBV	402293	696907	28.45%	4.038%
8	10.722	1292	1299	1309	rVB	242533	415699	16.97%	2.409%
9	13.178	1708	1717	1725	rBV	968505	1490337	60.85%	8.636%
10	14.553	1944	1951	1958	rBV	378915	580450	23.70%	3.363%
11	15.910	2177	2182	2187	rVB	140320	196938	8.04%	1.141%
12	16.040	2197	2204	2216	rBV	880889	1295349	52.89%	7.506%
13	16.692	2309	2315	2325	rBV	105677	163905	6.69%	0.950%
14	17.109	2381	2386	2396	rVB5	12329	27556	1.13%	0.160%
15	17.256	2406	2411	2413	rBV2	30134	41504	1.69%	0.240%
16	17.297	2413	2418	2424	rVV	482978	708207	28.91%	4.104%
17	17.461	2442	2446	2456	rBV3	89190	145291	5.93%	0.842%
18	17.796	2496	2503	2508	rBV3	12782	26724	1.09%	0.155%
19	18.061	2543	2548	2558	rBV	197712	292305	11.93%	1.694%
20	18.196	2565	2571	2585	rBV	620872	936808	38.25%	5.428%
21	18.554	2625	2632	2638	rVV5	22827	52491	2.14%	0.304%
22	18.736	2658	2663	2672	rBV4	22969	52605	2.15%	0.305%
23	18.860	2680	2684	2690	rBV8	13023	25419	1.04%	0.147%
24	19.342	2759	2766	2774	rBV2	110959	223176	9.11%	1.293%
25	19.459	2783	2786	2798	rBV	82537	125705	5.13%	0.728%
26	19.912	2858	2863	2870	rVB	1551788	2127822	86.87%	12.330%
27	20.288	2923	2927	2930	rBV2	23735	27391	1.12%	0.159%
28	20.716	2997	3000	3004	rVB2	27725	30338	1.24%	0.176%
29	21.204	3079	3083	3092	rVB3	130280	223422	9.12%	1.295%
30	21.286	3092	3097	3103	rBV	53021	77190	3.15%	0.447%
31	21.551	3136	3142	3150	rVB	473217	726342	29.65%	4.209%
32	21.751	3172	3176	3179	rVB2	26943	34460	1.41%	0.200%
33	22.344	3273	3277	3282	rBV5	26873	51025	2.08%	0.296%
34	23.214	3417	3425	3434	rVB	1266863	2449311	100.00%	14.193%
35	24.700	3669	3678	3690	rVB	291484	829623	33.87%	4.807%

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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-BG061923.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

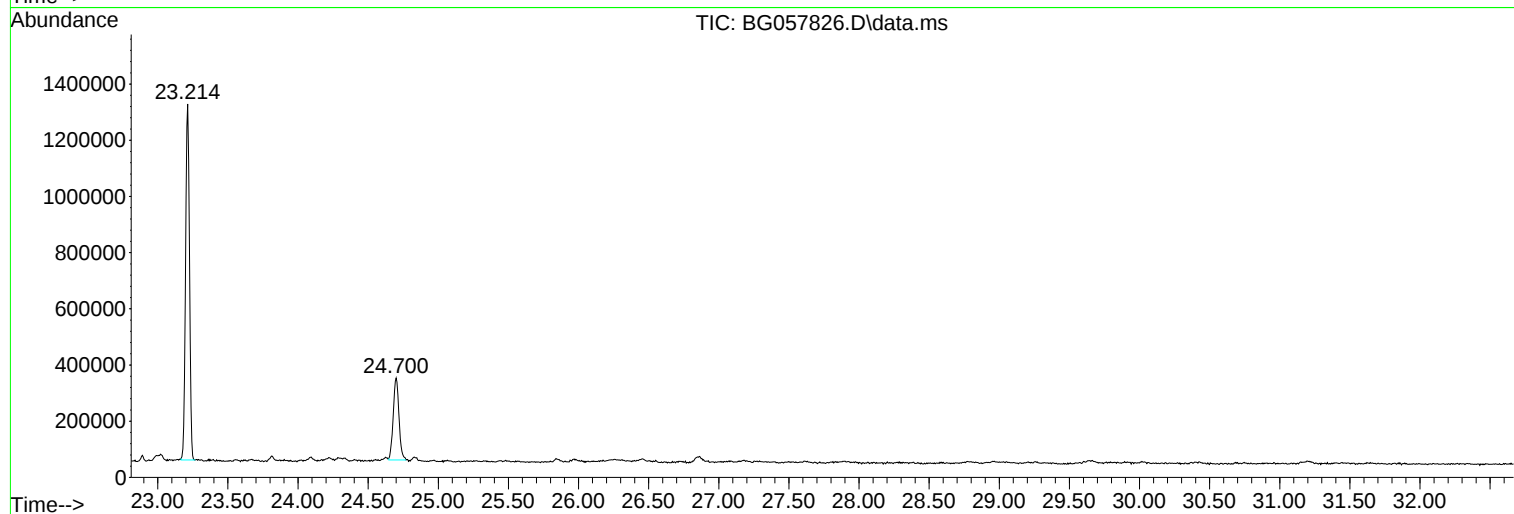
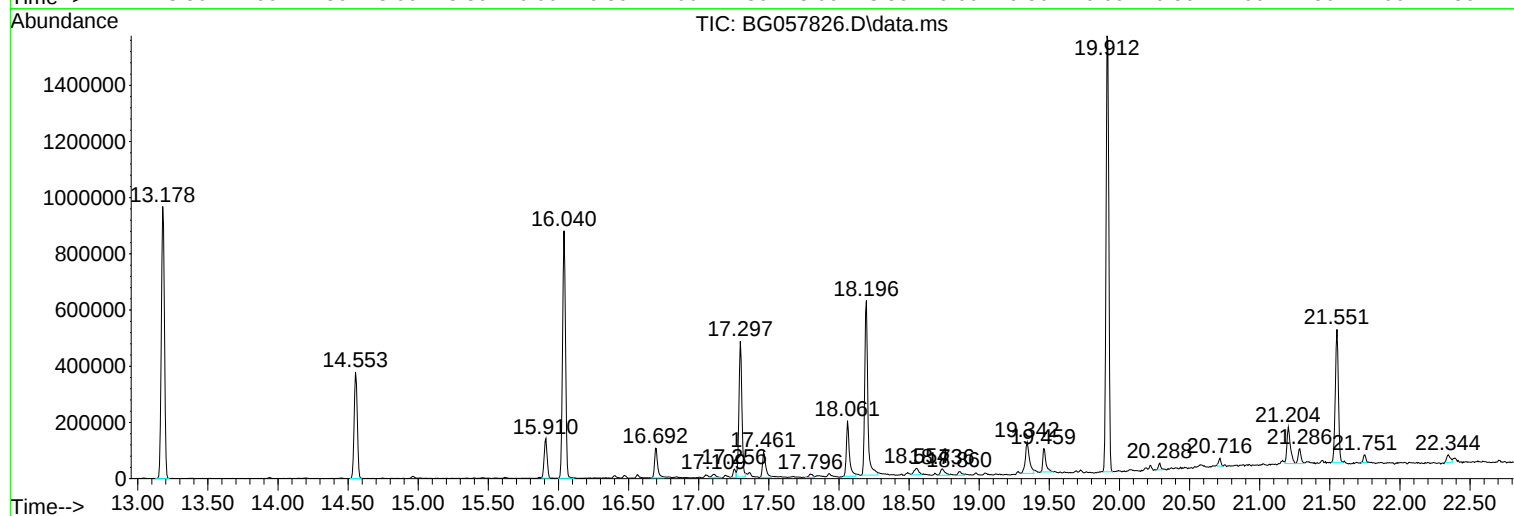
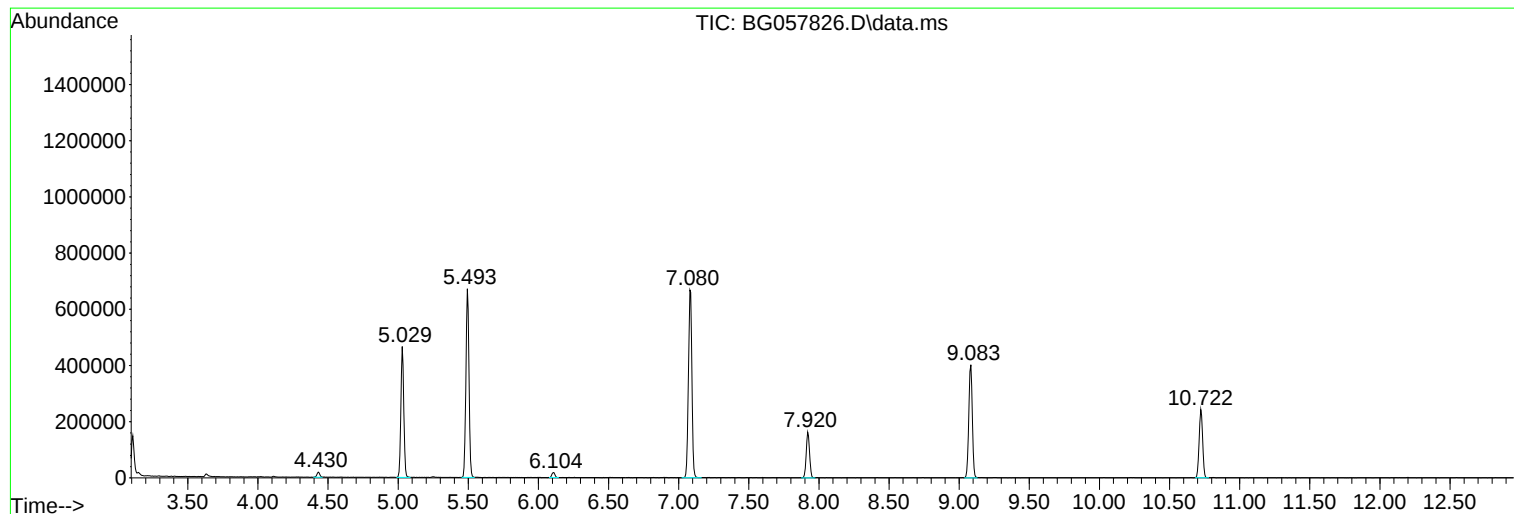
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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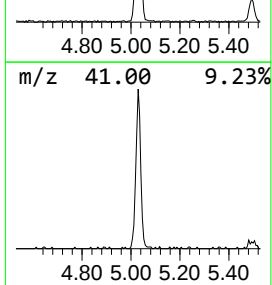
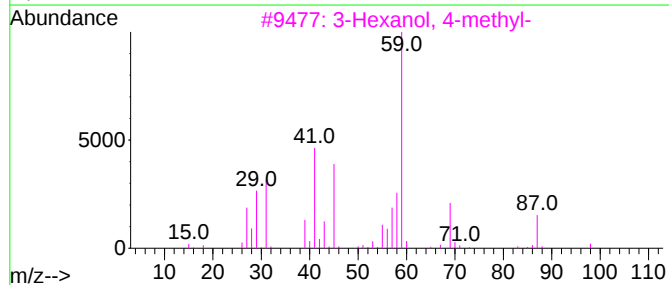
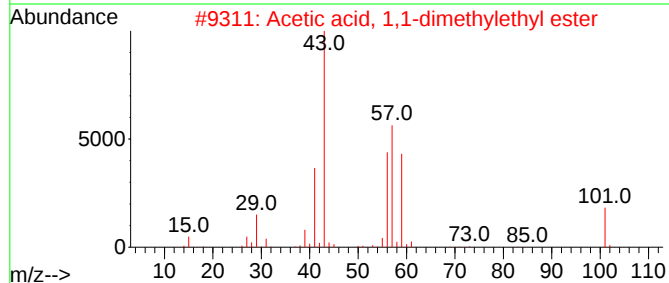
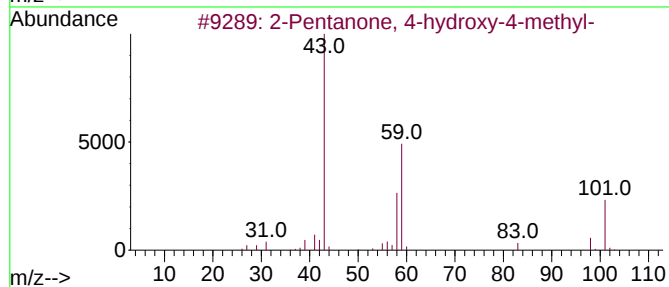
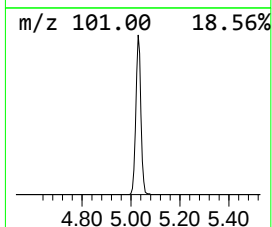
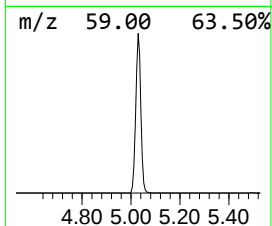
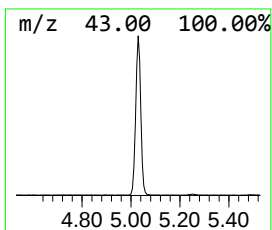
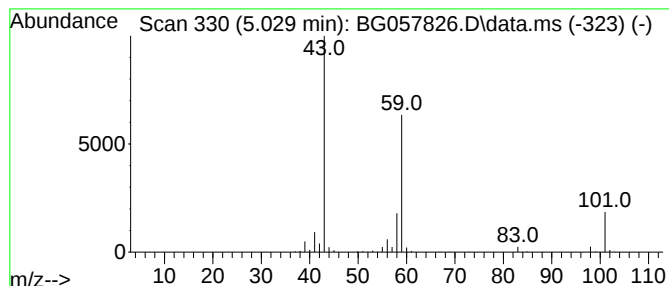
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.029	49.74 ng	674278	1,4-Dichlorobenzene-d4	7.920

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	39		
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		
4	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33		
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32		



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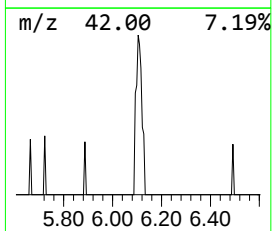
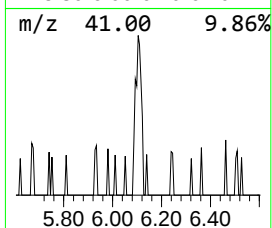
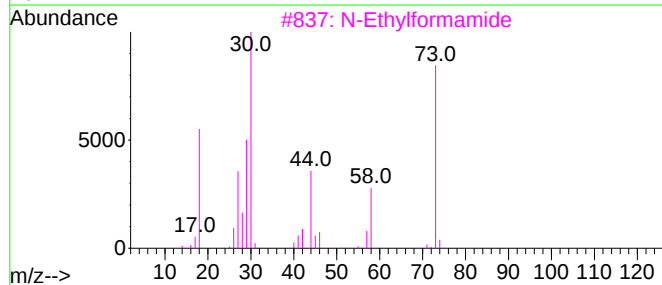
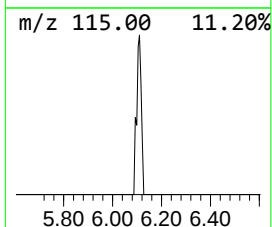
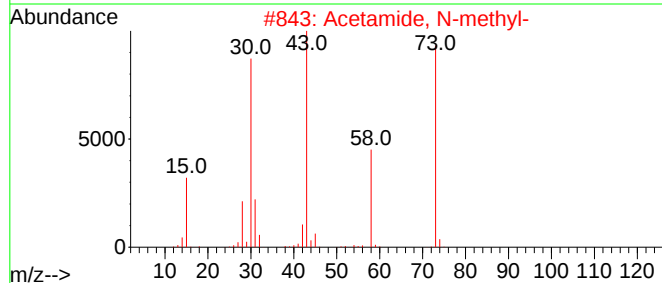
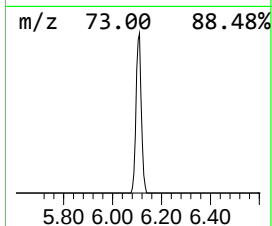
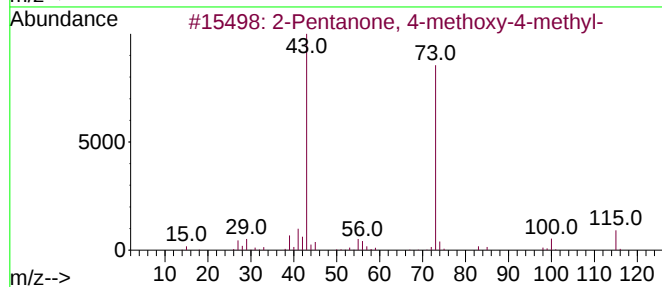
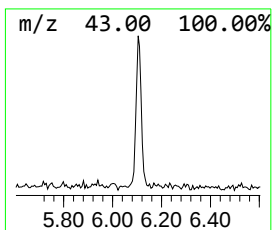
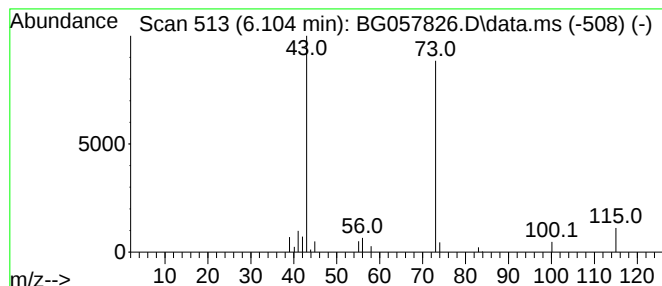
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 2-Pentanone, 4-methoxy-4-me... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.104	2.07 ng	28016	1,4-Dichlorobenzene-d4	7.920

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	40
3		N-Ethylformamide	73	C3H7NO	000627-45-2	9
4		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
5		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9



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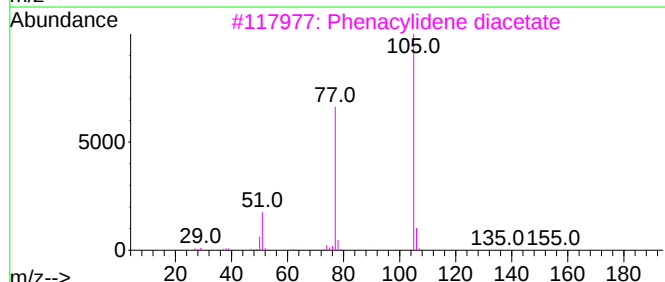
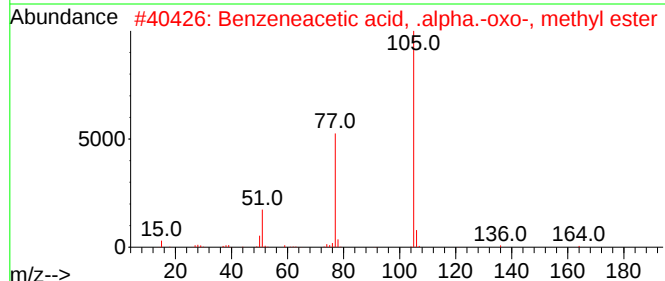
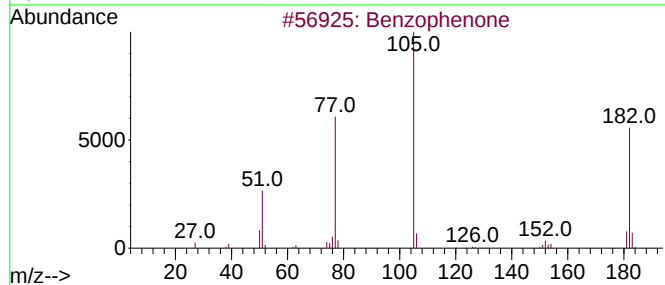
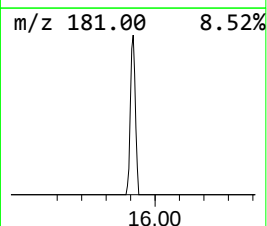
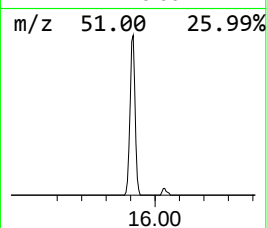
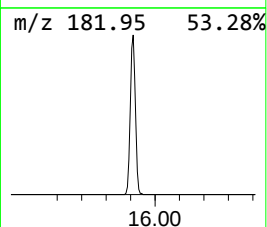
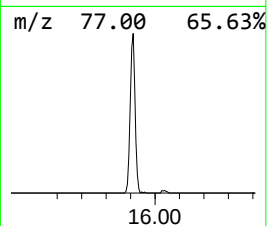
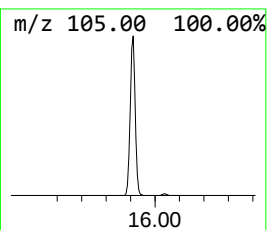
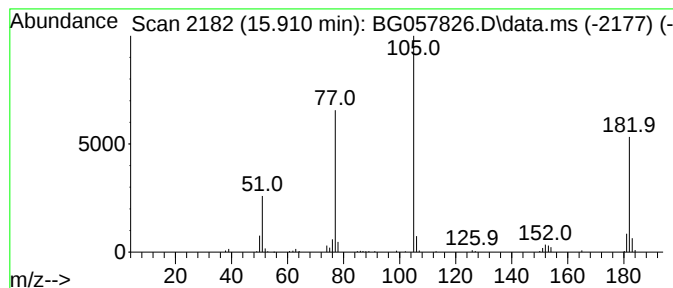
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.910	6.79 ng	196938	Acenaphthene-d10	14.553

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	47
3			Phenacylidene diacetate	236	C12H12O5	005062-30-6	47
4			1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	47
5			1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47



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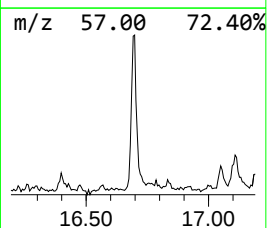
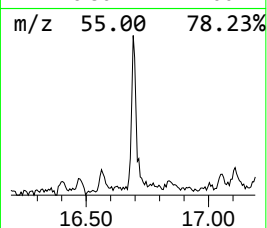
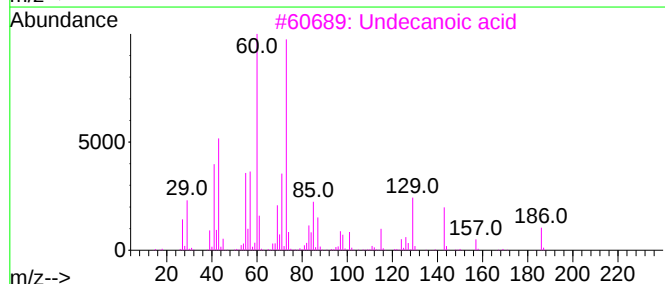
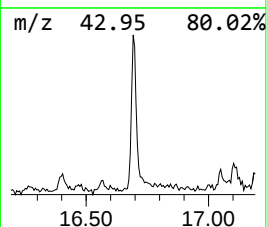
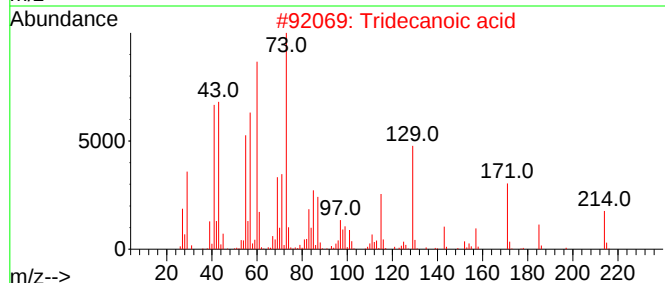
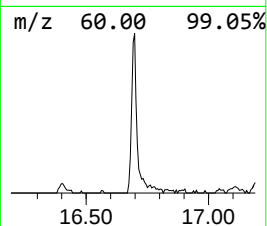
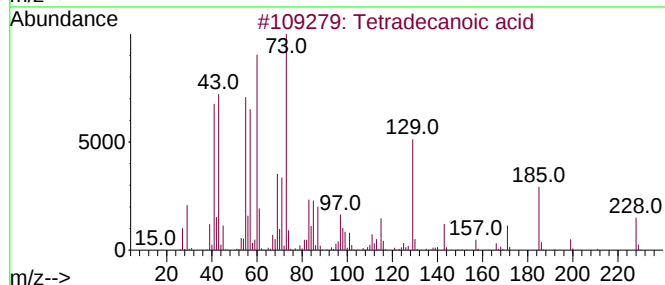
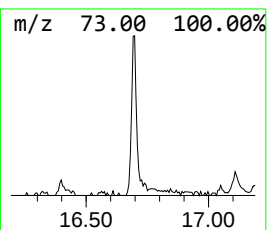
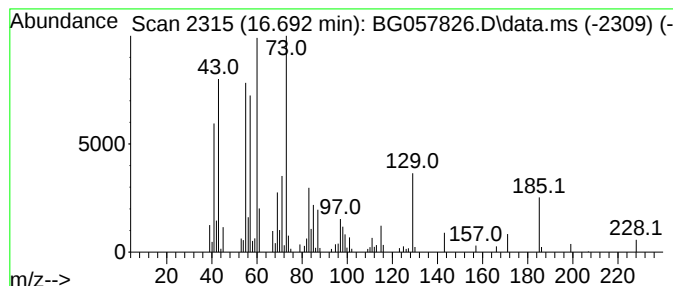
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Tetradecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.692	4.63 ng	163905	Phenanthrene-d10	17.297

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecanoic acid	228	C14H28O2	000544-63-8	91
2			Tridecanoic acid	214	C13H26O2	000638-53-9	86
3			Undecanoic acid	186	C11H22O2	000112-37-8	83
4			Dodecanoic acid	200	C12H24O2	000143-07-7	64
5			n-Decanoic acid	172	C10H20O2	000334-48-5	53



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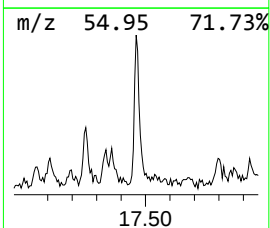
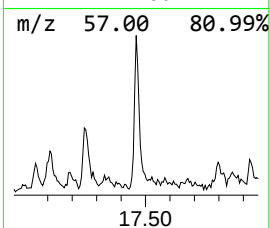
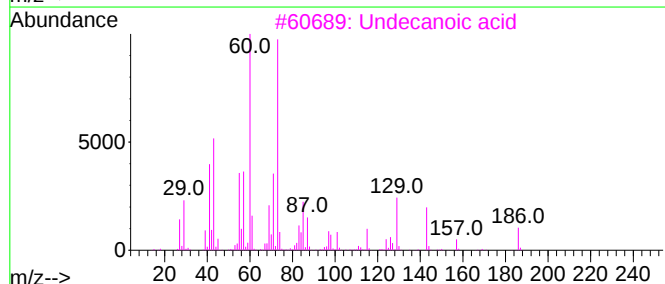
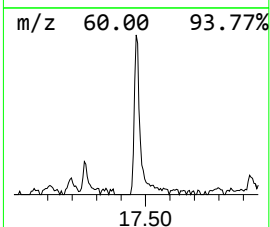
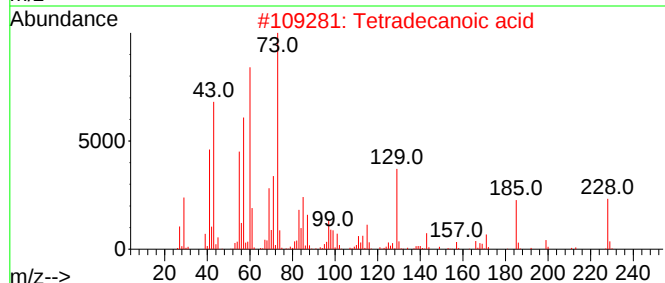
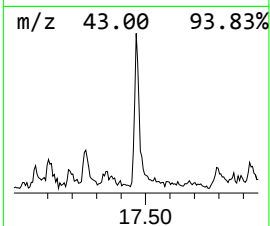
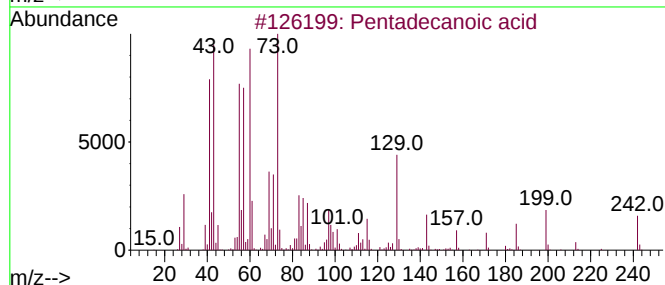
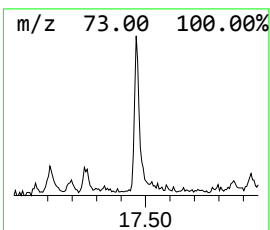
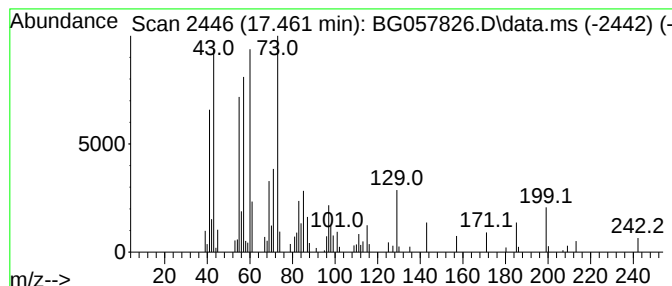
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Pentadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.462	4.10 ng	145291	Phenanthrene-d10	17.297

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
3			Undecanoic acid	186	C11H22O2	000112-37-8	76
4			Dodecanoic acid	200	C12H24O2	000143-07-7	74
5			Tridecanoic acid	214	C13H26O2	000638-53-9	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062223\
Data File : BG057826.D
Acq On : 23 Jun 2023 3:13
Operator : CG/JU
Sample : 03320-10
Misc :
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Instrument :
BNA_G
ClientSampleId :
WC-13

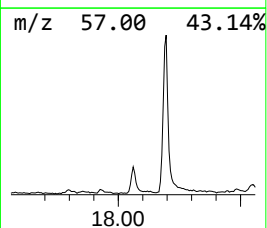
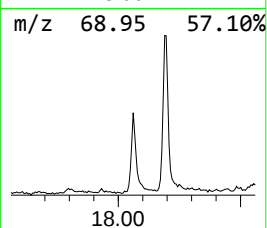
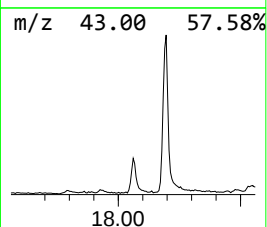
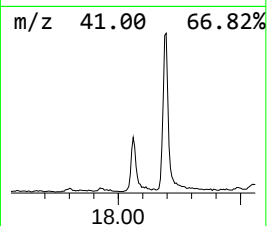
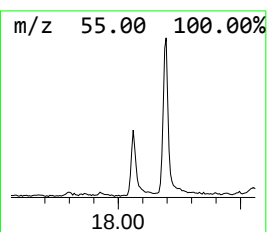
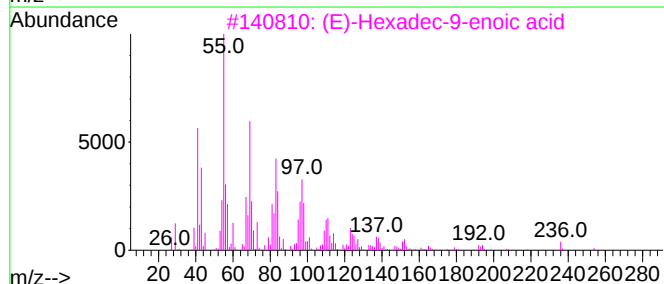
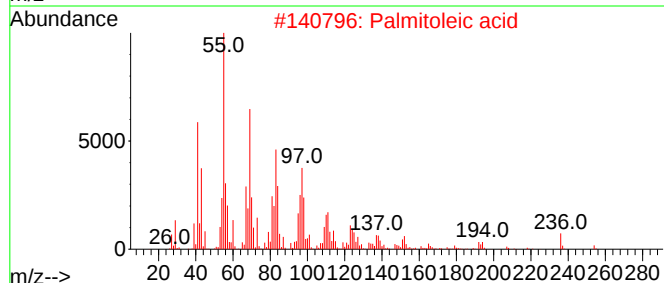
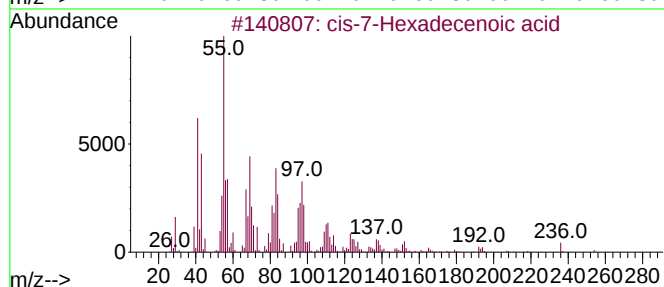
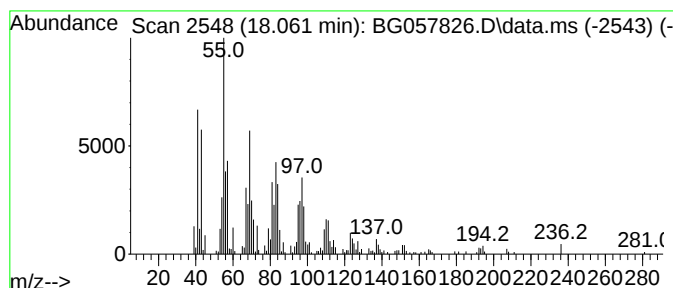
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 cis-7-Hexadecenoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.061	8.25 ng	292305	Phenanthrene-d10	17.297

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis-7-Hexadecenoic acid	254	C16H30O2	002416-19-5	95
2			Palmitoleic acid	254	C16H30O2	000373-49-9	81
3			(E)-Hexadec-9-enoic acid	254	C16H30O2	010030-73-6	81
4			Hexadecenoic acid, Z-11-	254	C16H30O2	002416-20-8	80
5			E-11-Hexadecenoic acid, ethyl ester	282	C18H34O2	1000245-71-9	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062223\
Data File : BG057826.D
Acq On : 23 Jun 2023 3:13
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Sample : 03320-10
Misc :
ALS Vial : 13 Sample Multiplier: 1

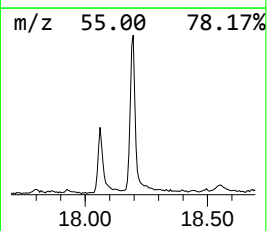
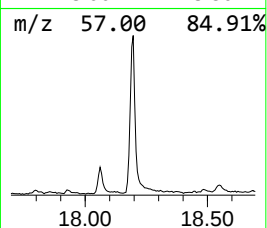
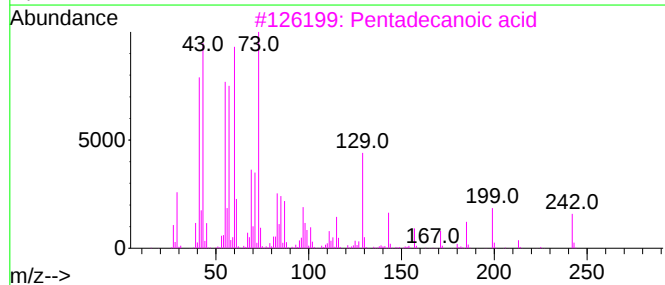
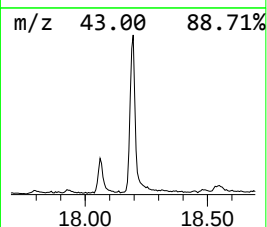
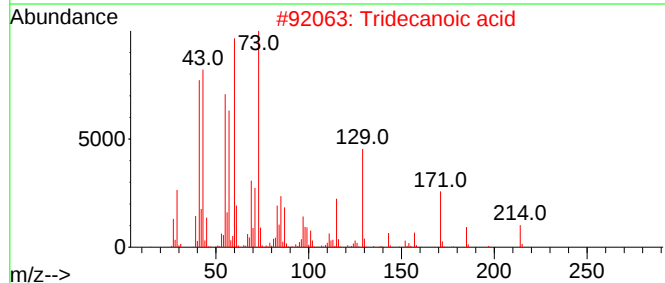
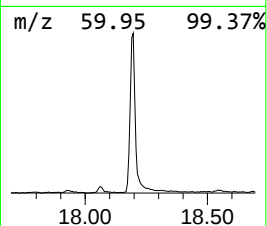
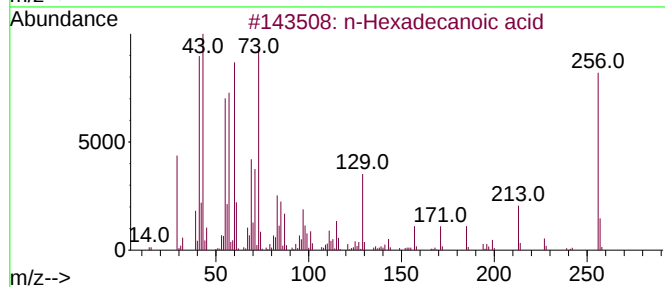
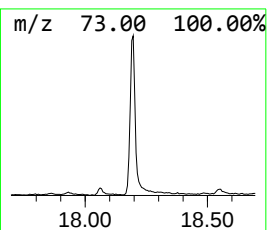
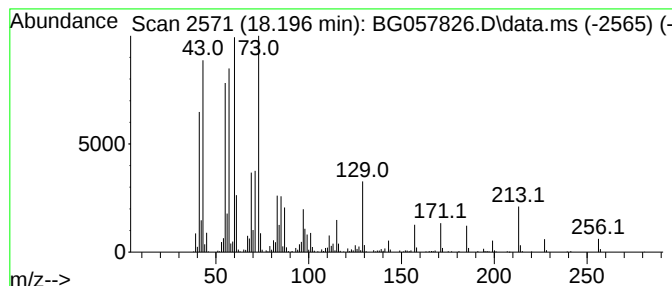
Instrument :
BNA_G
ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.196	26.46 ng	936808	Phenanthrene-d10		17.297	
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	94
3	Pentadecanoic acid		242	C15H30O2	001002-84-2	81
4	Tetradecanoic acid		228	C14H28O2	000544-63-8	80
5	Undecanoic acid		186	C11H22O2	000112-37-8	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062223\
Data File : BG057826.D
Acq On : 23 Jun 2023 3:13
Operator : CG/JU
Sample : 03320-10
Misc :
ALS Vial : 13 Sample Multiplier: 1

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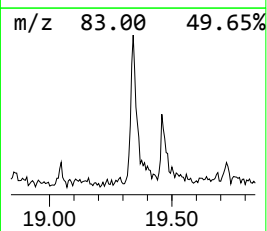
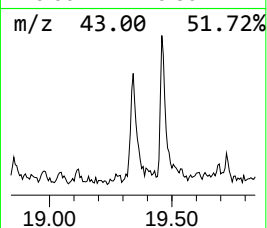
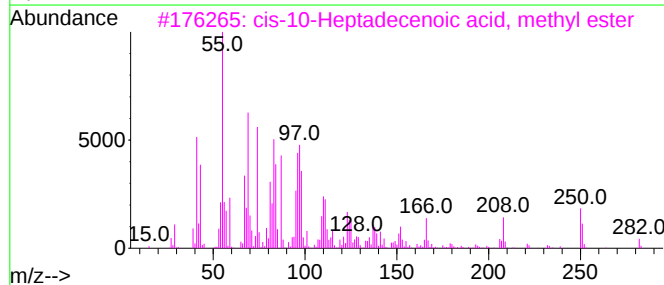
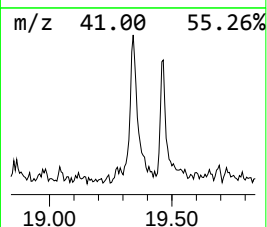
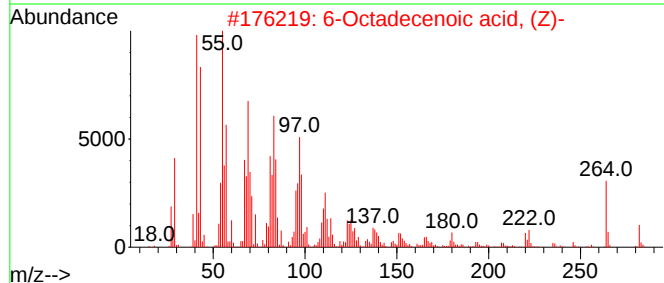
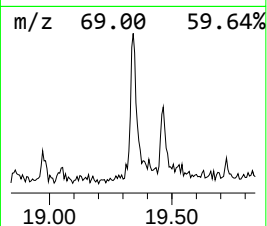
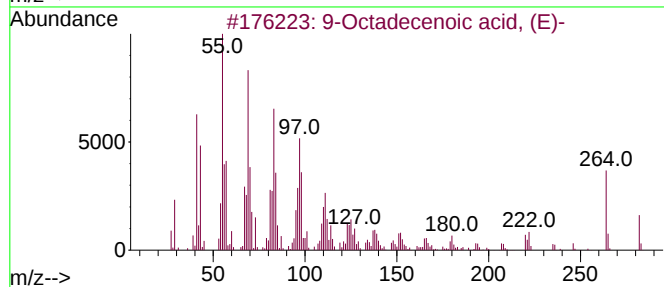
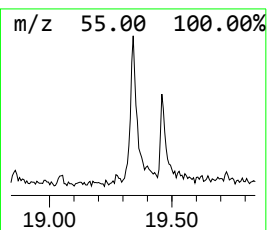
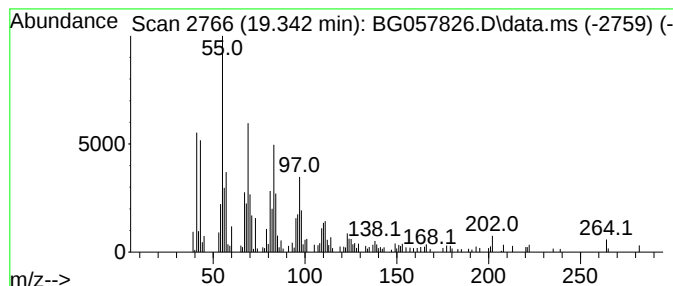
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 9-Octadecenoic acid, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.342	6.30 ng	223176	Phenanthrene-d10	17.297

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	99
2			6-Octadecenoic acid, (Z)-	282	C18H34O2	000593-39-5	98
3			cis-10-Heptadecenoic acid, methyl ester	282	C18H34O2	1000333-62-1	91
4			Oleic Acid	282	C18H34O2	000112-80-1	91
5			trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062223\
Data File : BG057826.D
Acq On : 23 Jun 2023 3:13
Operator : CG/JU
Sample : 03320-10
Misc :
ALS Vial : 13 Sample Multiplier: 1

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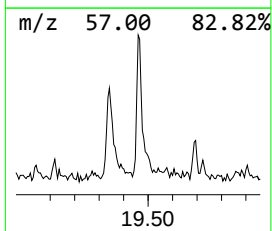
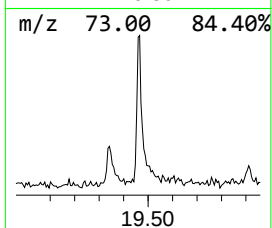
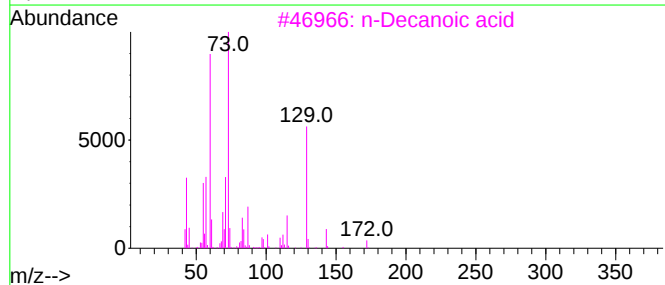
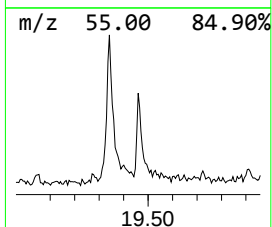
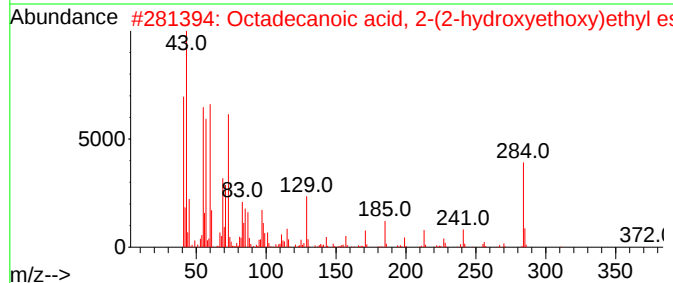
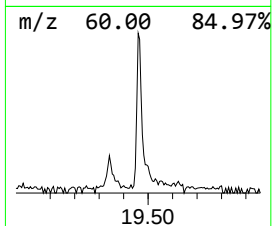
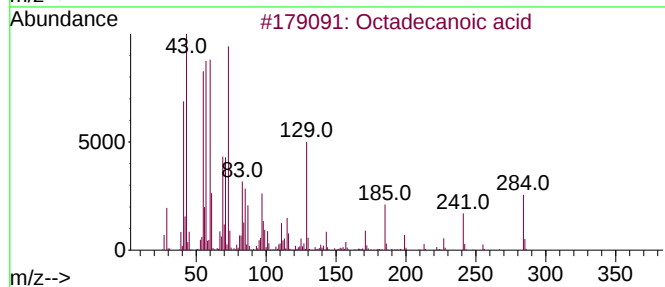
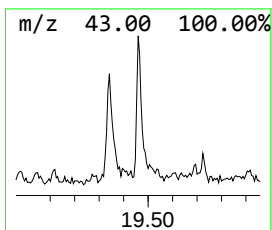
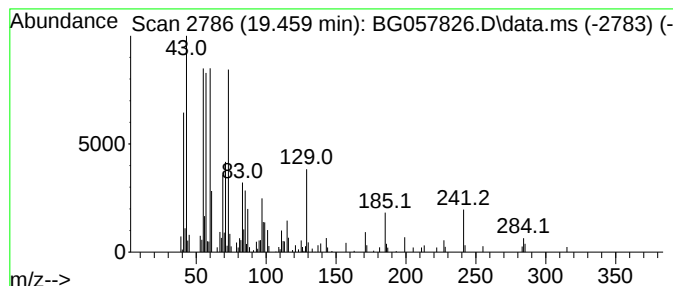
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.459	3.46 ng	125705	Chrysene-d12	21.551

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	94
2		Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	90
3		n-Decanoic acid	172	C10H20O2	000334-48-5	89
4		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
5		Undecanoic acid	186	C11H22O2	000112-37-8	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062223\
Data File : BG057826.D
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Misc :
ALS Vial : 13 Sample Multiplier: 1

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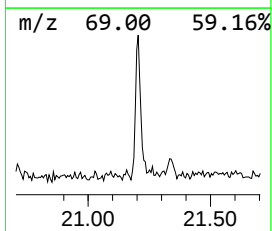
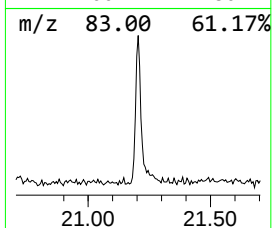
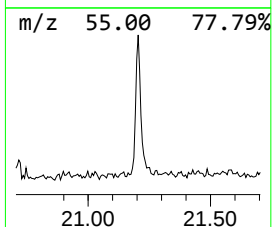
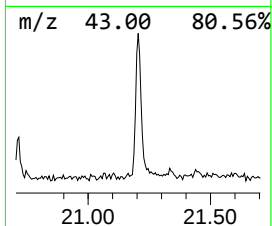
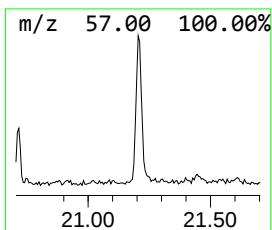
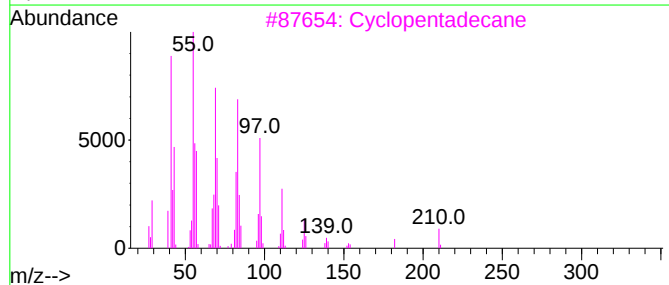
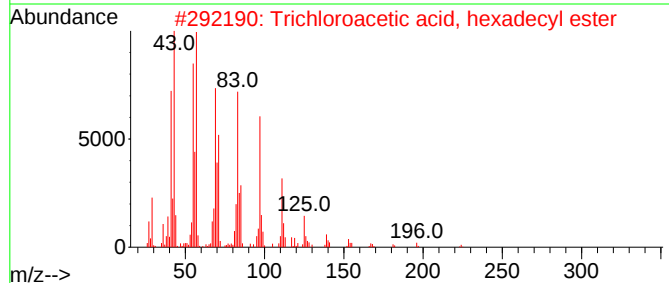
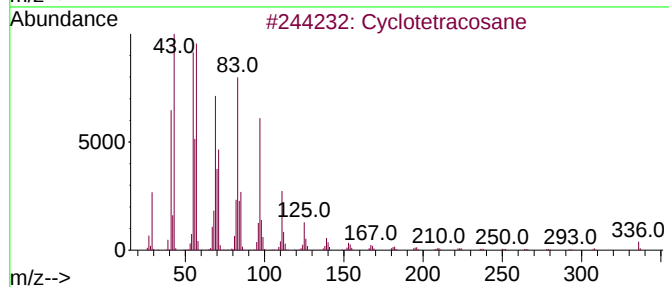
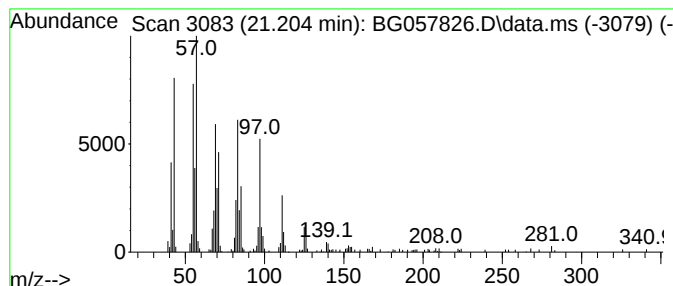
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Cyclotetracosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.204	6.15 ng	223422	Chrysene-d12	21.551

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclotetracosane	336	C24H48	000297-03-0	95
2		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3		Cyclopentadecane	210	C15H30	000295-48-7	93
4		Pentadecafluorooctanoic acid, pe...	624	C23H31F15O2	1000406-04-5	93
5		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062223\
Data File : BG057826.D
Acq On : 23 Jun 2023 3:13
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ClientSampleId :
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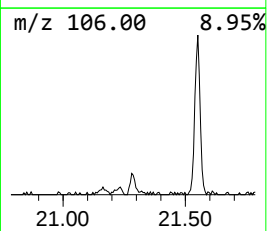
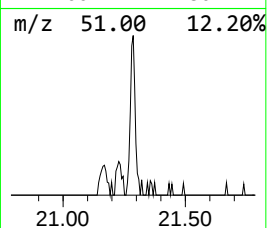
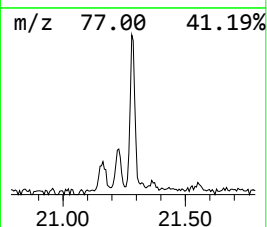
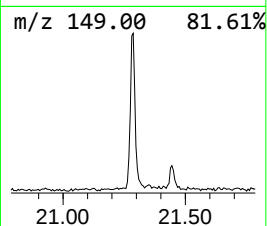
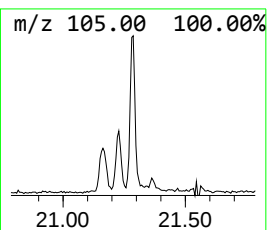
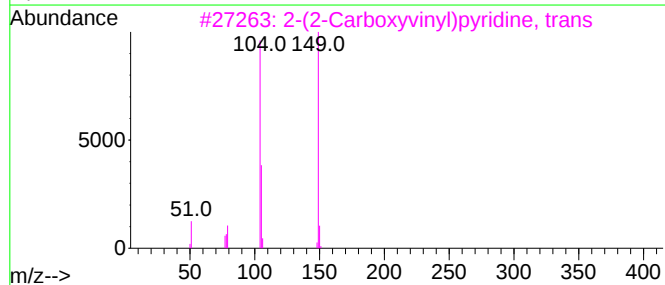
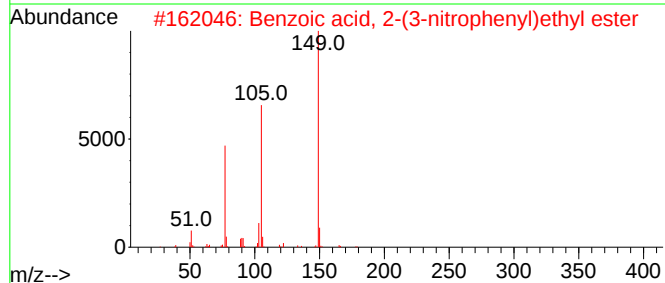
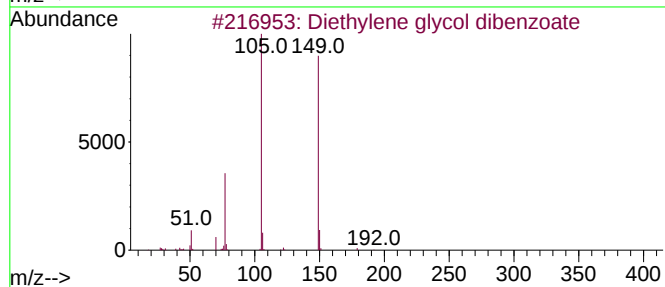
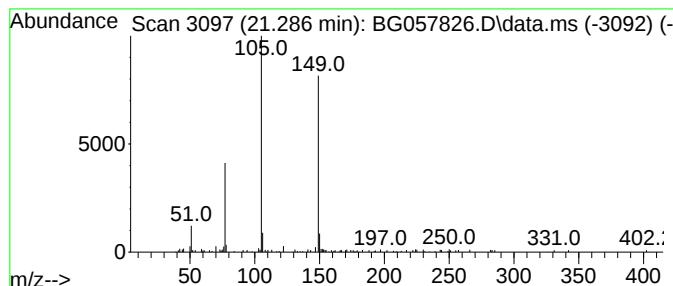
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Diethylene glycol dibenzoate Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.286	2.13 ng	77190	Chrysene-d12	21.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	86
2			Benzoic acid, 2-(3-nitrophenyl)e...	271	C15H13NO4	1000368-22-4	72
3			2-(2-Carboxyvinyl)pyridine, trans	149	C8H7NO2	007340-22-9	49
4			Benzoic acid, 2-(1-oxopropyl)-	178	C10H10O3	002360-45-4	47
5			3-(Benzoylthio)-2-methylpropanoi...	224	C11H12O3S	067714-34-5	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062223\
Data File : BG057826.D
Acq On : 23 Jun 2023 3:13
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ALS Vial : 13 Sample Multiplier: 1

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ClientSampleId :
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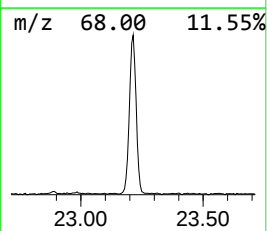
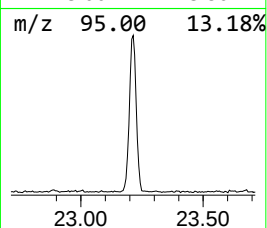
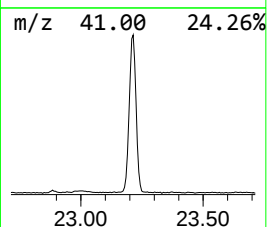
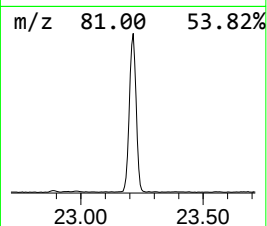
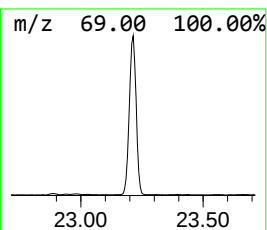
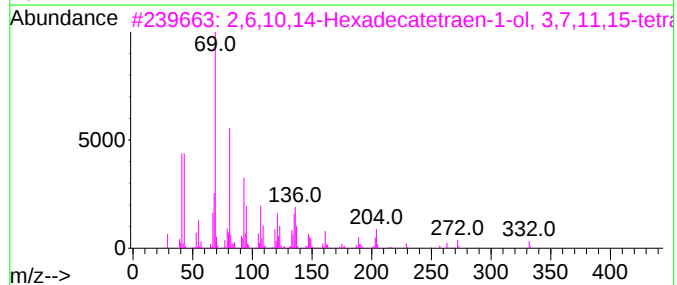
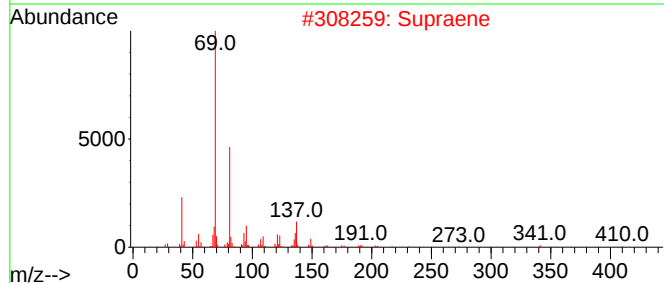
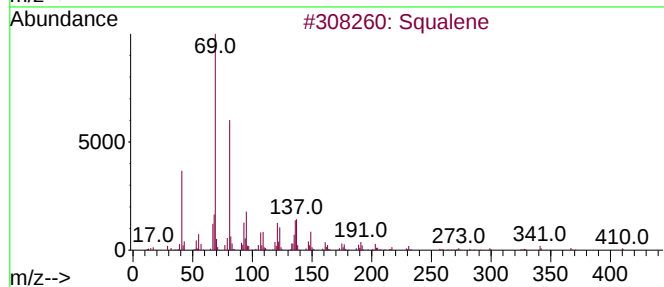
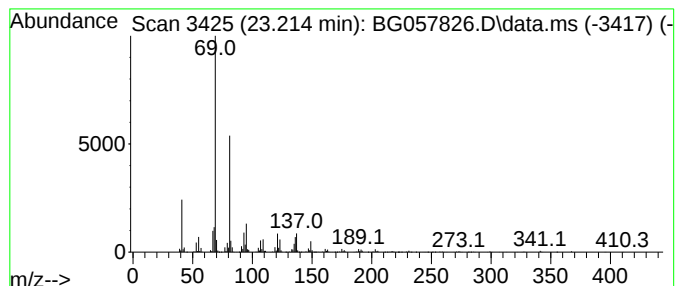
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Squalene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.214	59.05 ng	2449310	Perylene-d12	24.700

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	97
2			Supraene	410	C30H50	007683-64-9	91
3			2,6,10,14-Hexadecatetraen-1-ol, ...	332	C22H36O2	061691-98-3	78
4			2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	72
5			Farnesol isomer a	222	C15H26O	1000108-92-4	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062223\
Data File : BG057826.D
Acq On : 23 Jun 2023 3:13
Operator : CG/JU
Sample : 03320-10
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-13

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.029	49.7	ng	674278	1	7.920	271143	20.0
2-Pentanone, 4-...	6.104	2.1	ng	28016	1	7.920	271143	20.0
Benzophenone	15.910	6.8	ng	196938	3	14.553	580450	20.0
Tetradecanoic acid	16.692	4.6	ng	163905	4	17.297	708207	20.0
Pentadecanoic acid	17.462	4.1	ng	145291	4	17.297	708207	20.0
cis-7-Hexadecen...	18.061	8.3	ng	292305	4	17.297	708207	20.0
n-Hexadecanoic ...	18.196	26.5	ng	936808	4	17.297	708207	20.0
9-Octadecenoic ...	19.342	6.3	ng	223176	4	17.297	708207	20.0
Octadecanoic acid	19.459	3.5	ng	125705	5	21.551	726342	20.0
Cyclotetracosane	21.204	6.2	ng	223422	5	21.551	726342	20.0
Diethylene glyc...	21.286	2.1	ng	77190	5	21.551	726342	20.0
Squalene	23.214	59.0	ng	2449310	6	24.700	829623	20.0