

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082523\
 Data File : BG058854.D
 Acq On : 25 Aug 2023 18:01
 Operator : MA/JU
 Sample : 04147-03
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-03(48-50)

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-BG081823.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG058854.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.380	384	390	402	rBV	282391	449760	42.38%	8.515%
2	6.978	656	662	673	rBV	268776	458506	43.21%	8.681%
3	7.806	796	803	810	rVB	70799	118837	11.20%	2.250%
4	8.970	993	1001	1008	rBV	150826	272285	25.66%	5.155%
5	10.603	1271	1279	1291	rBV	83311	156113	14.71%	2.956%
6	13.071	1690	1699	1715	rBV	377637	585528	55.18%	11.086%
7	14.451	1927	1934	1946	rVB	131472	215494	20.31%	4.080%
8	15.944	2182	2188	2202	rBV	341780	545735	51.43%	10.332%
9	17.201	2396	2402	2414	rBV	180825	281854	26.56%	5.336%
10	18.088	2548	2553	2563	rBV3	25533	54972	5.18%	1.041%
11	19.816	2841	2847	2855	rBV	831393	1061213	100.00%	20.092%
12	20.609	2977	2982	2986	rBV3	9148	14242	1.34%	0.270%
13	20.738	2992	3004	3010	rBV3	27191	97110	9.15%	1.839%
14	21.055	3051	3058	3060	rBV2	10687	18774	1.77%	0.355%
15	21.091	3060	3064	3074	rVV2	38609	80620	7.60%	1.526%
16	21.179	3074	3079	3085	rVV	32854	53145	5.01%	1.006%
17	21.437	3117	3123	3133	rBV2	217141	358482	33.78%	6.787%
18	21.608	3148	3152	3157	rBV3	9640	13951	1.31%	0.264%
19	22.183	3245	3250	3256	rBV3	8132	13869	1.31%	0.263%
20	22.830	3355	3360	3368	rBV9	10149	20782	1.96%	0.393%
21	24.205	3586	3594	3601	rBV9	8564	30312	2.86%	0.574%
22	24.498	3635	3644	3660	rVB	134089	380233	35.83%	7.199%

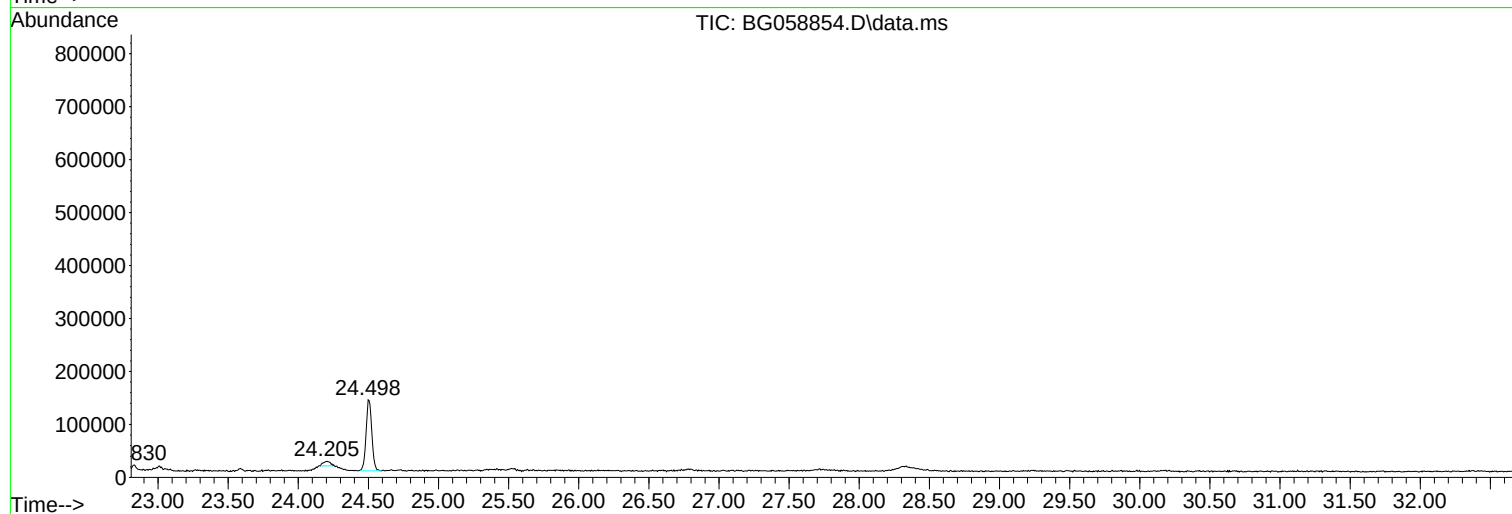
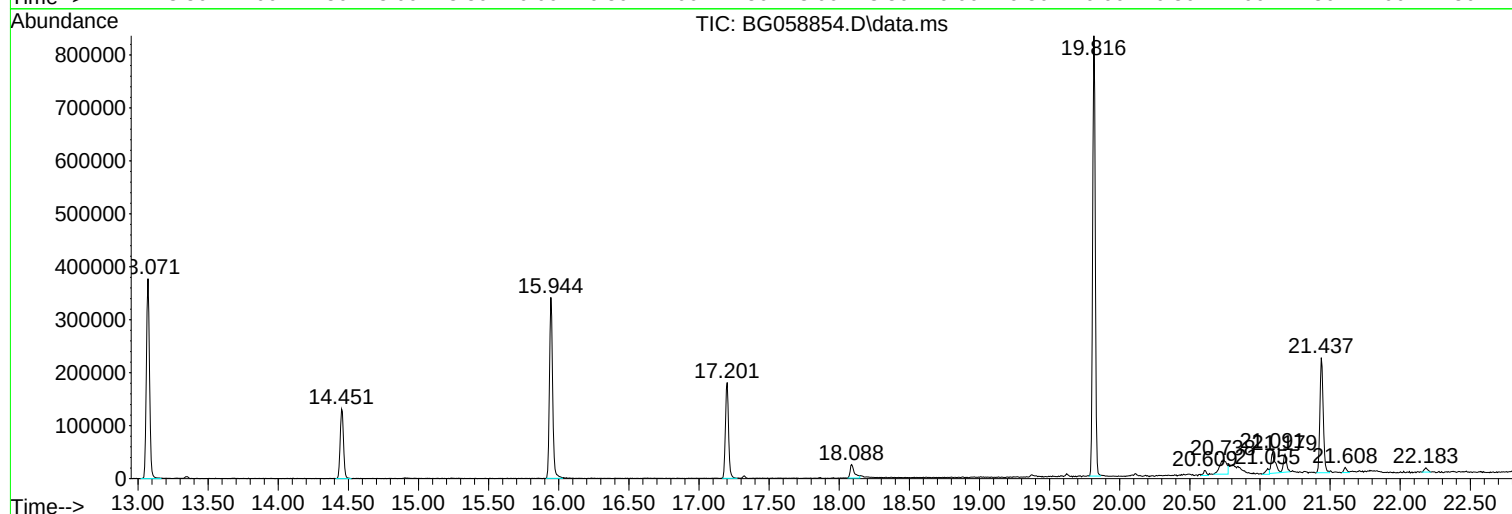
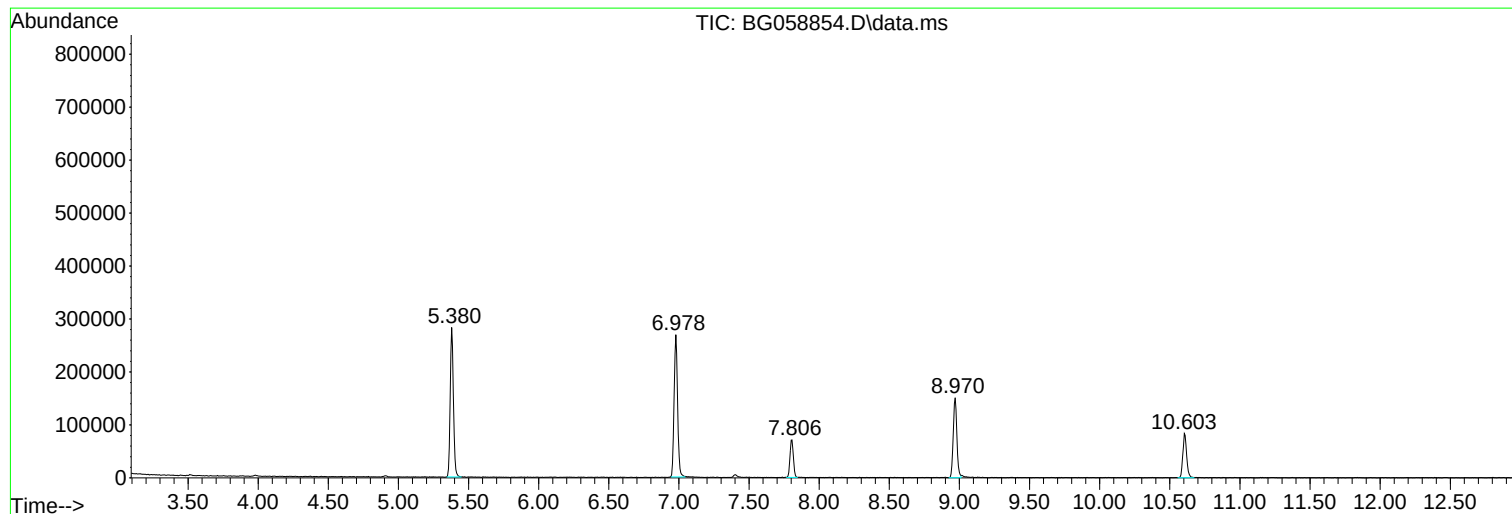
Sum of corrected areas: 5281817

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082523\
Data File : BG058854.D
Acq On : 25 Aug 2023 18:01
Operator : MA/JU
Sample : 04147-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-03(48-50)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG081823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082523\
Data File : BG058854.D
Acq On : 25 Aug 2023 18:01
Operator : MA/JU
Sample : 04147-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-03(48-50)

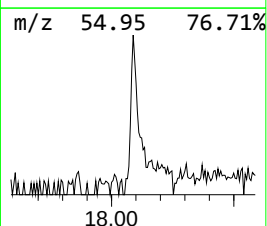
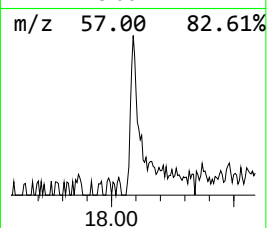
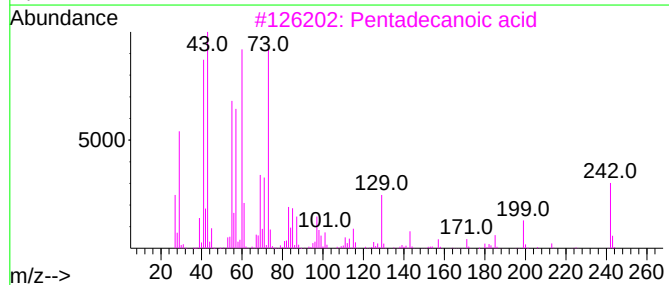
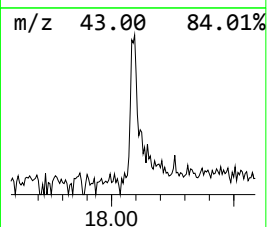
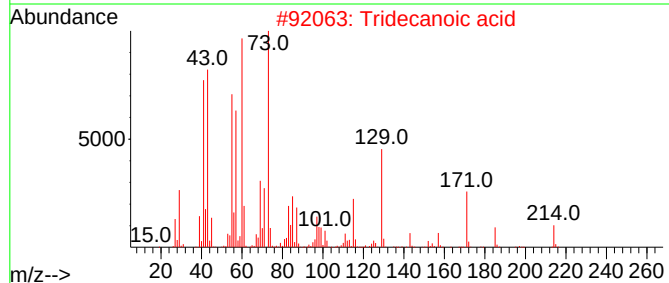
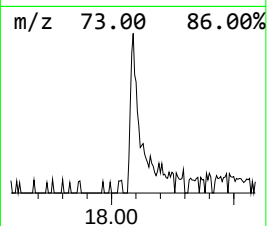
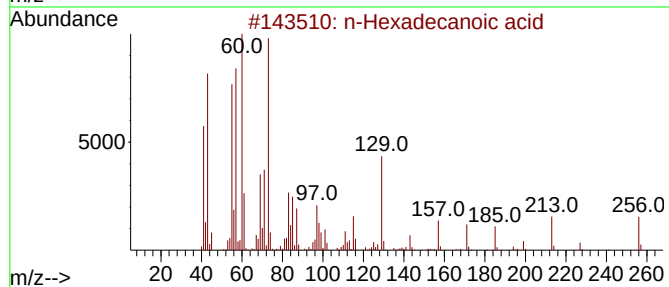
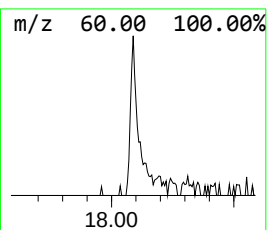
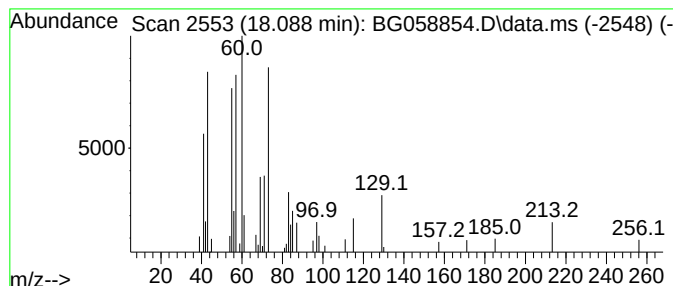
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG081823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.088	3.90 ng	54972	Phenanthrene-d10	17.201

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	72
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	72
4		Undecanoic acid	186	C11H22O2	000112-37-8	64
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082523\
Data File : BG058854.D
Acq On : 25 Aug 2023 18:01
Operator : MA/JU
Sample : 04147-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-03(48-50)

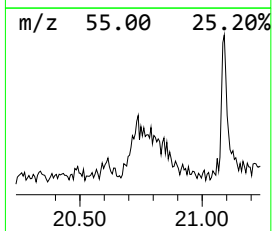
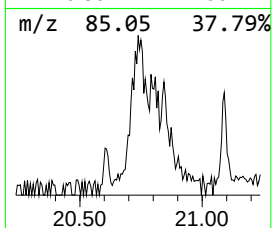
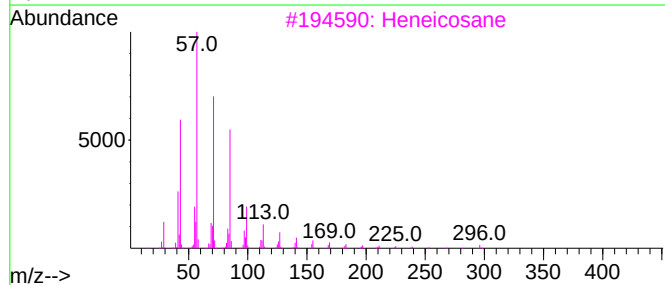
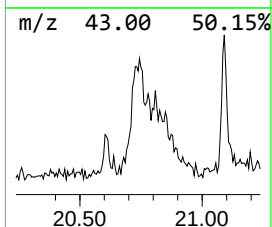
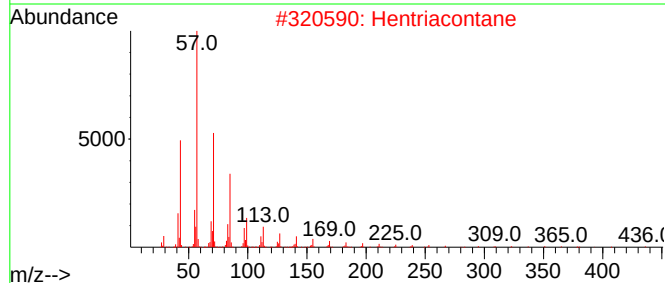
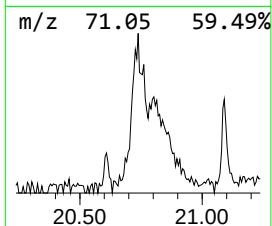
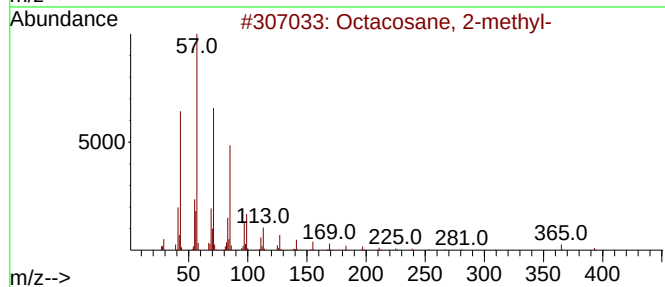
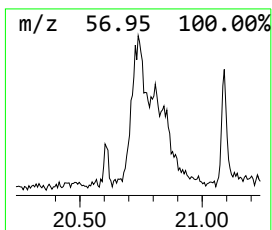
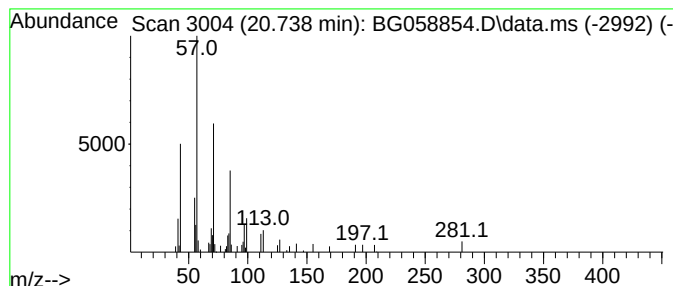
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG081823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Octacosane, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.738	5.42 ng	97110	Chrysene-d12	21.437

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane, 2-methyl-	408	C29H60	001560-98-1	86
2			Hentriacontane	437	C31H64	000630-04-6	86
3			Heneicosane	296	C21H44	000629-94-7	83
4			Heptacosane	380	C27H56	000593-49-7	80
5			Octadecane	254	C18H38	000593-45-3	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082523\
Data File : BG058854.D
Acq On : 25 Aug 2023 18:01
Operator : MA/JU
Sample : 04147-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

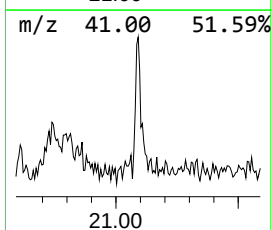
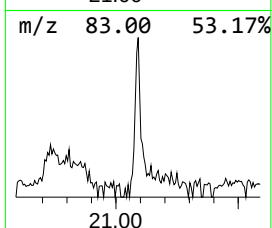
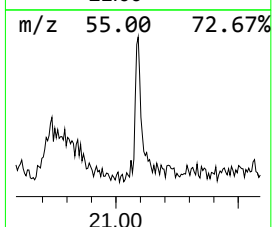
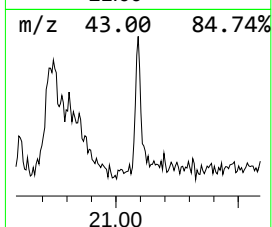
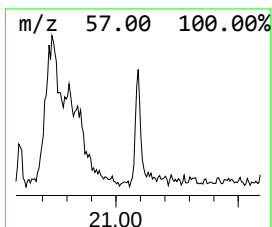
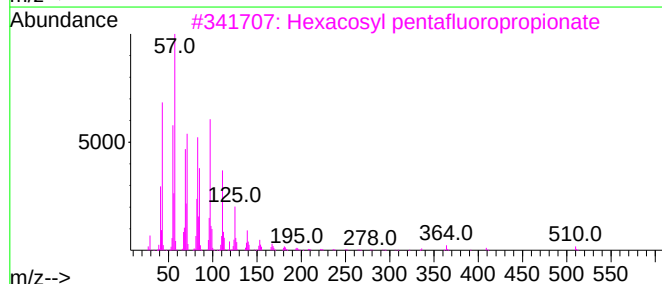
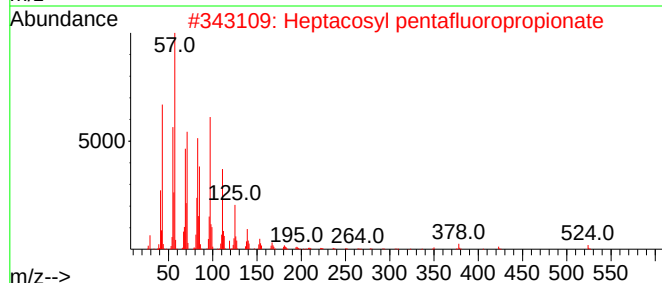
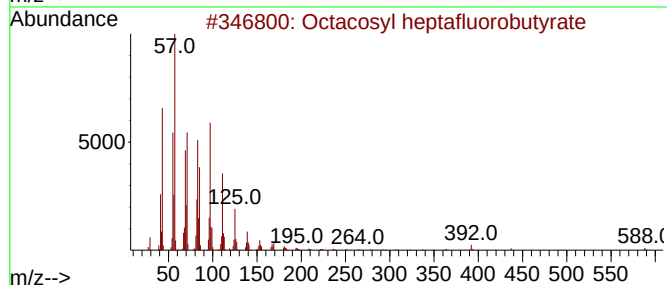
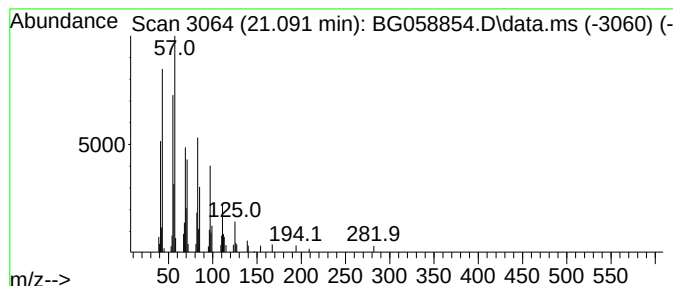
Instrument :
BNA_G
ClientSampleId :
SB-03(48-50)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG081823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Octacosyl heptafluorobutyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.091	4.50 ng	80620	Chrysene-d12	21.437	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosyl heptafluorobutyrate	606	C32H57F7O2	1010351-83-6	91
2	Heptacosyl pentafluoropropionate	542	C30H55F5O2	1000351-81-6	91
3	Hexacosyl pentafluoropropionate	528	C29H53F5O2	1000351-81-2	91
4	Butyl hexacosyl ether	438	C30H62O	1000406-41-0	91
5	Propyl triacontyl ether	481	C33H68O	1000406-28-6	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082523\
Data File : BG058854.D
Acq On : 25 Aug 2023 18:01
Operator : MA/JU
Sample : 04147-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-03(48-50)

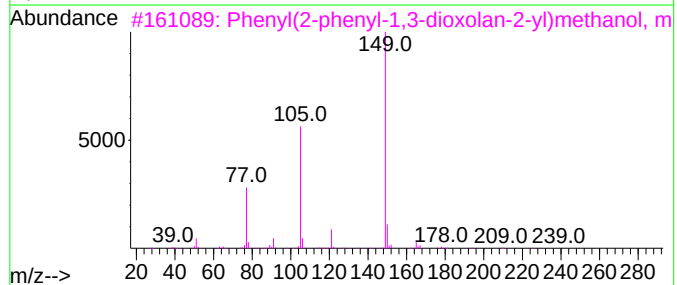
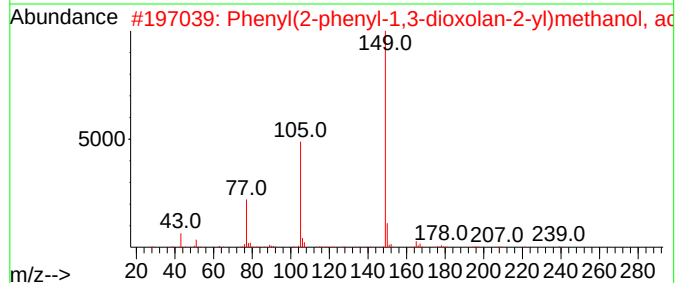
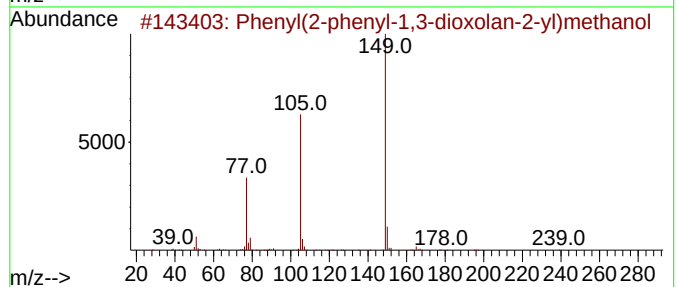
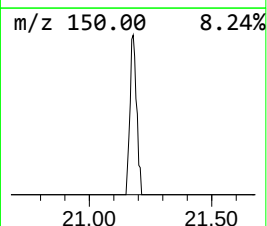
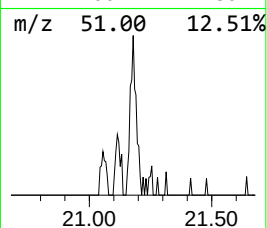
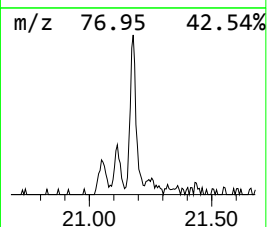
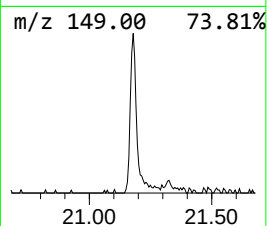
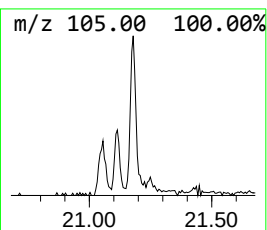
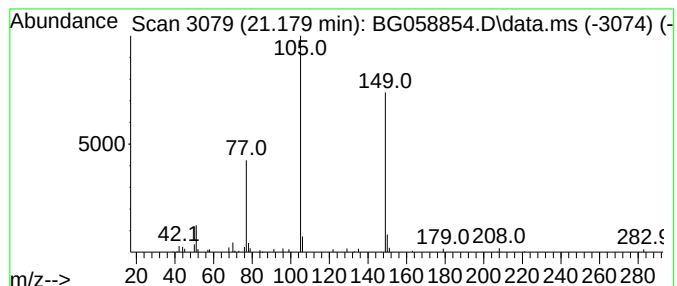
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG081823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Phenyl(2-phenyl-1,3-dioxola... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.179	2.96 ng	53145	Chrysene-d12	21.437

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenyl(2-phenyl-1,3-dioxolan-2-y...	256	C16H16O3	005694-69-9	78
2			Phenyl(2-phenyl-1,3-dioxolan-2-y...	298	C18H18O4	006963-16-2	78
3			Phenyl(2-phenyl-1,3-dioxolan-2-y...	270	C17H18O3	1000507-07-6	78
4			3,6,9,12-Tetraoxatetradecane-1,1...	446	C24H30O8	1000366-97-0	64
5			5-Formyl-2-methoxyphenyl benzoate	256	C15H12O4	1000411-55-4	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082523\
Data File : BG058854.D
Acq On : 25 Aug 2023 18:01
Operator : MA/JU
Sample : 04147-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-03(48-50)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG081823.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
n-Hexadecanoic ...	18.088	3.9	ng	54972	4	17.201	281854	20.0
Octacosane, 2-m...	20.738	5.4	ng	97110	5	21.437	358482	20.0
Octacosyl hepta...	21.091	4.5	ng	80620	5	21.437	358482	20.0
Phenyl(2-phenyl...	21.179	3.0	ng	53145	5	21.437	358482	20.0