

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100621\
 Data File : BG050476.D
 Acq On : 6 Oct 2021 20:32
 Operator : CG/JU
 Sample : M4087-09
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 WC-20211005-ROCK

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-BG100621.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG050476.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.261	804	812	824	rVB	182214	324395	41.66%	6.324%
2	10.834	1246	1250	1259	rVB5	7457	15274	1.96%	0.298%
3	11.081	1281	1292	1298	rBV	243588	467753	60.07%	9.119%
4	13.748	1740	1746	1756	rVB	96667	151419	19.44%	2.952%
5	14.876	1930	1938	1945	rVB	380521	611619	78.54%	11.924%
6	15.388	2021	2025	2031	rBV2	19057	27941	3.59%	0.545%
7	17.614	2398	2404	2412	rBV	460176	737143	94.66%	14.371%
8	17.979	2460	2466	2472	rBV8	6580	17508	2.25%	0.341%
9	18.255	2509	2513	2522	rBV	42769	61111	7.85%	1.191%
10	18.472	2546	2550	2554	rBV2	24722	32350	4.15%	0.631%
11	19.330	2692	2696	2702	rBV7	14655	32351	4.15%	0.631%
12	19.389	2702	2706	2707	rVV3	14621	17191	2.21%	0.335%
13	19.418	2707	2711	2715	rVB	140130	170767	21.93%	3.329%
14	19.547	2729	2733	2738	rVB	47158	58631	7.53%	1.143%
15	19.959	2801	2803	2807	rVV5	6884	7929	1.02%	0.155%
16	20.000	2807	2810	2814	rVV6	4485	8093	1.04%	0.158%
17	20.153	2830	2836	2839	rBV7	5348	11538	1.48%	0.225%
18	20.200	2839	2844	2850	rBV8	16276	30913	3.97%	0.603%
19	20.470	2885	2890	2891	rBV4	26537	35336	4.54%	0.689%
20	20.599	2909	2912	2916	rVB6	9943	13404	1.72%	0.261%
21	20.675	2921	2925	2928	rVB6	12127	19267	2.47%	0.376%
22	20.828	2947	2951	2955	rBV	60756	74563	9.57%	1.454%
23	20.946	2968	2971	2974	rVB3	20914	20894	2.68%	0.407%
24	20.993	2976	2979	2982	rVB4	16780	18793	2.41%	0.366%
25	21.480	3058	3062	3064	rBV4	9943	16953	2.18%	0.330%
26	21.522	3064	3069	3081	rVV3	91664	229746	29.50%	4.479%
27	21.616	3081	3085	3090	rVB	33375	52202	6.70%	1.018%
28	21.774	3109	3112	3117	rVB2	31405	40557	5.21%	0.791%
29	21.915	3129	3136	3143	rVB	434955	753069	96.70%	14.681%
30	22.015	3150	3153	3158	rVB5	19629	27024	3.47%	0.527%
31	22.744	3273	3277	3281	rBV8	12471	19538	2.51%	0.381%
32	23.137	3339	3344	3350	rVB6	24184	43075	5.53%	0.840%
33	23.449	3391	3397	3409	rBV5	73693	172676	22.17%	3.366%
34	24.330	3543	3547	3555	rVB7	15222	29763	3.82%	0.580%
35	25.323	3706	3716	3727	rVB2	252037	778734	100.00%	15.181%

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100621\
Data File : BG050476.D
Acq On : 6 Oct 2021 20:32
Operator : CG/JU
Sample : M4087-09
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-20211005-ROCK

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-BG100621.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

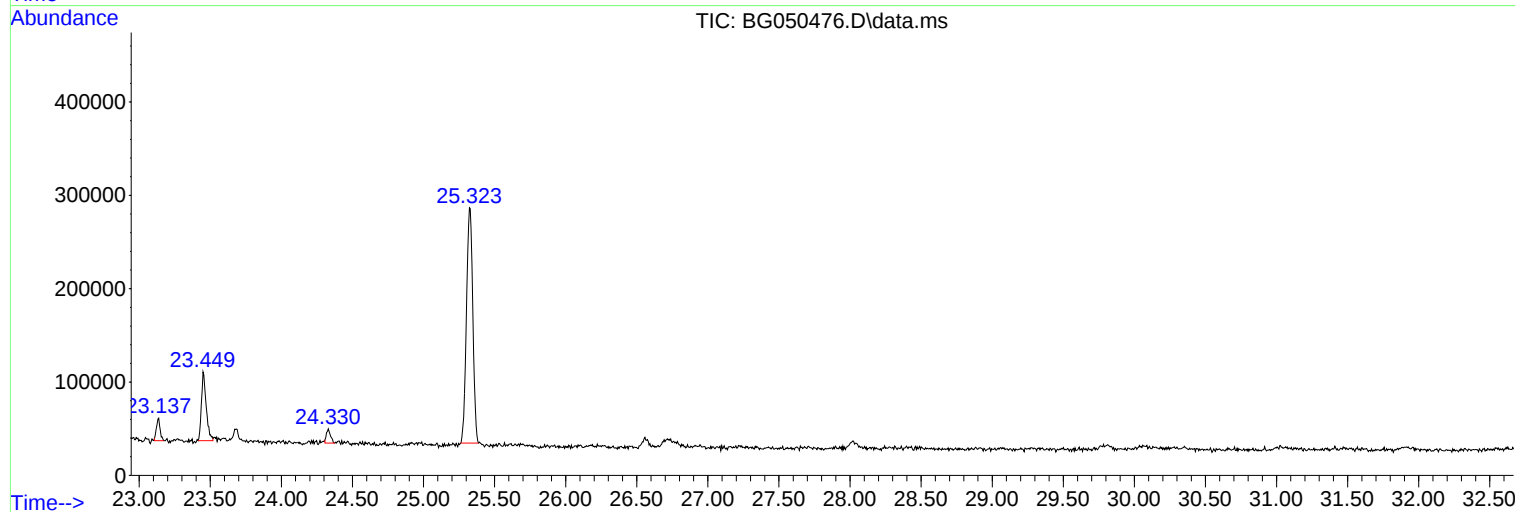
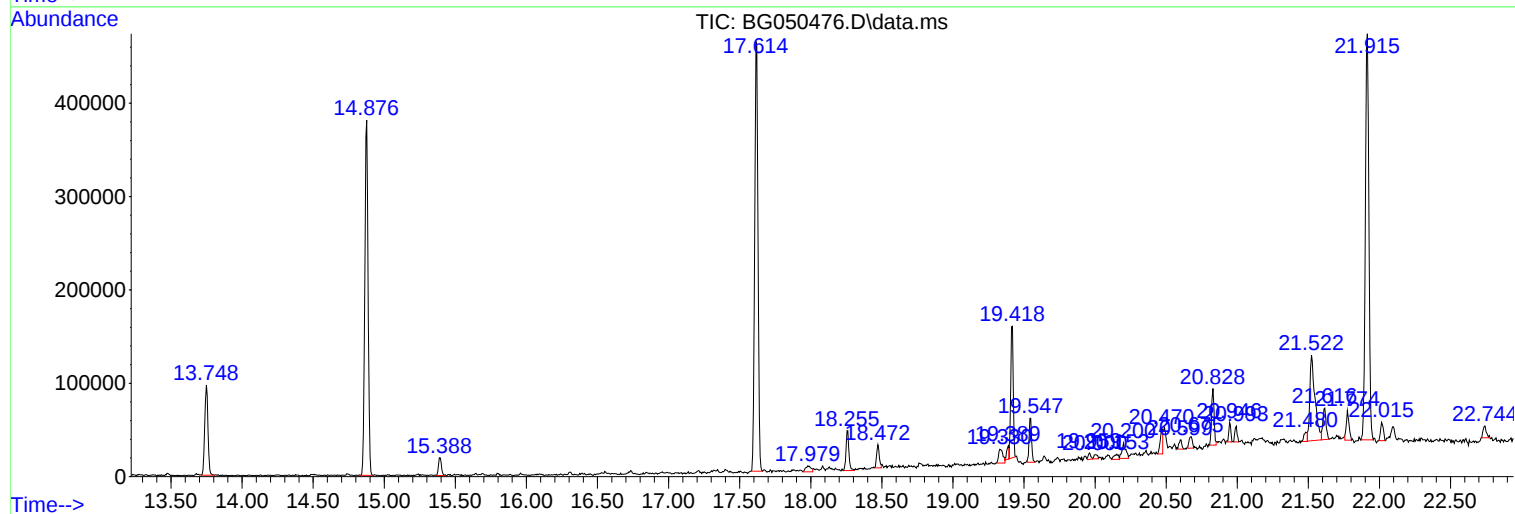
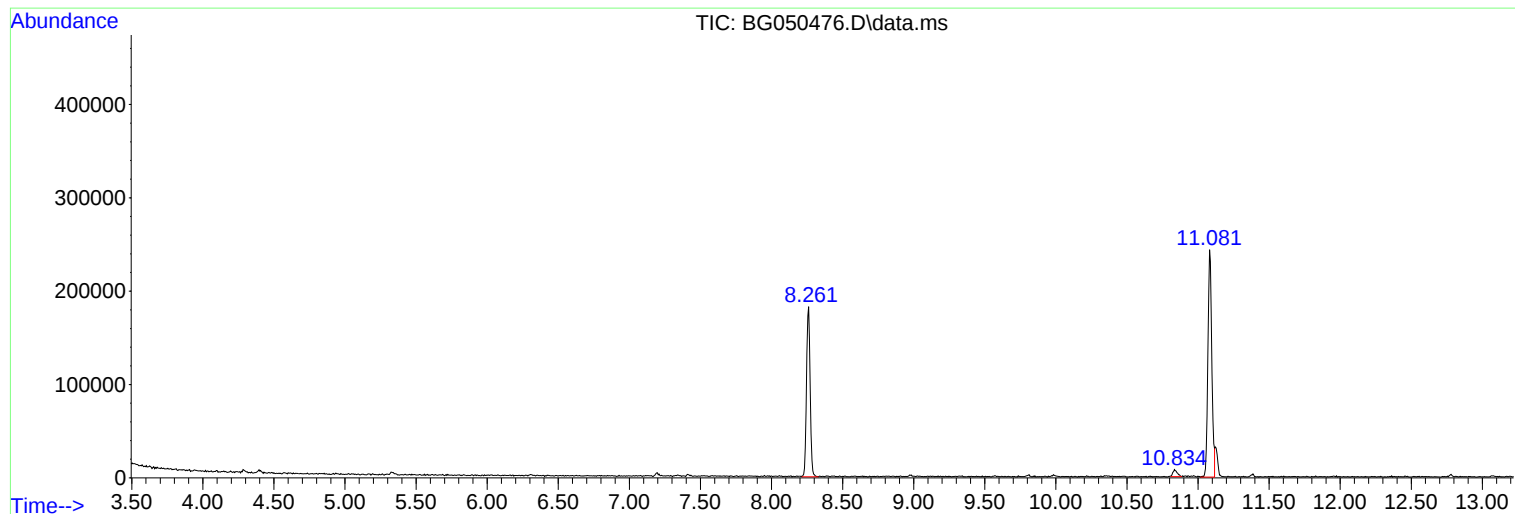
Sum of corrected areas: 5129520

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100621\
Data File : BG050476.D
Acq On : 6 Oct 2021 20:32
Operator : CG/JU
Sample : M4087-09
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-20211005-ROCK

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.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\BG100621\
Data File : BG050476.D
Acq On : 6 Oct 2021 20:32
Operator : CG/JU
Sample : M4087-09
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-20211005-ROCK

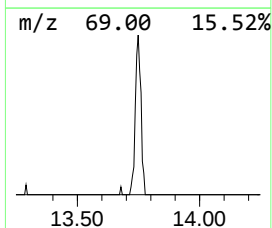
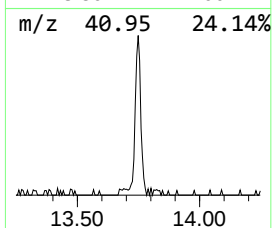
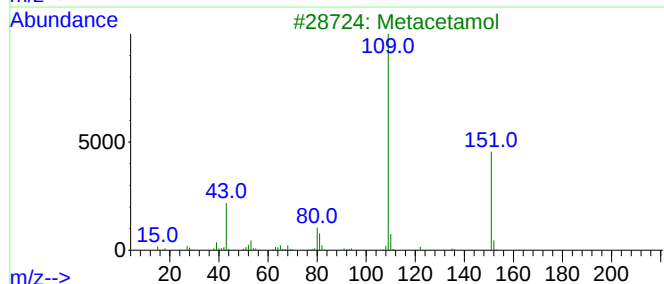
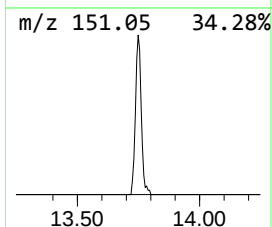
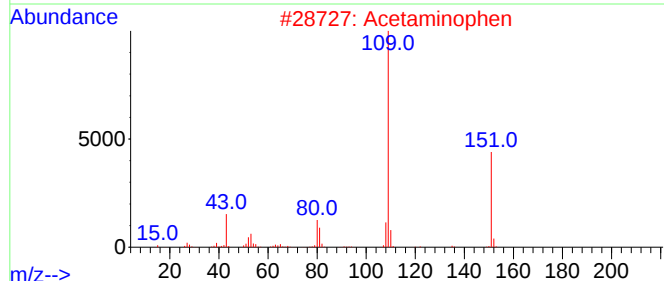
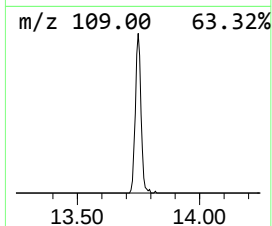
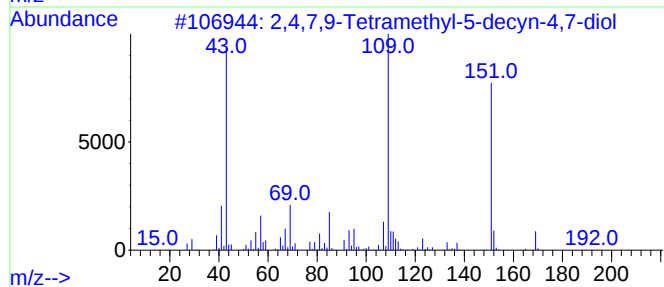
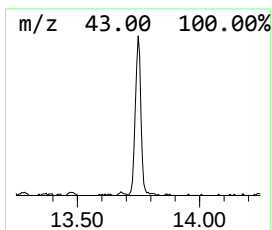
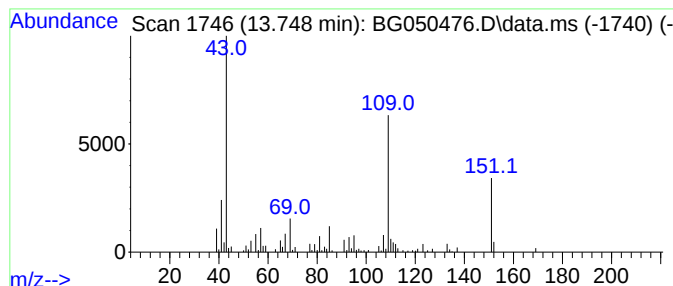
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.748	4.95 ng	151419	Acenaphthene-d10	14.876

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	90		
2	Acetaminophen	151	C8H9NO2	000103-90-2	52		
3	Metacetamol	151	C8H9NO2	000621-42-1	52		
4	Pyridine, 3-butyl-, 1-oxide	151	C9H13NO	031396-33-5	50		
5	1-(1,2,3-Trimethyl-cyclopent-2-e...	152	C10H16O	070987-81-4	43		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100621\
Data File : BG050476.D
Acq On : 6 Oct 2021 20:32
Operator : CG/JU
Sample : M4087-09
Misc :
ALS Vial : 16 Sample Multiplier: 1

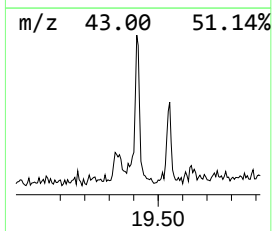
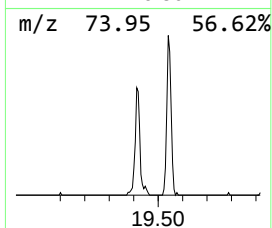
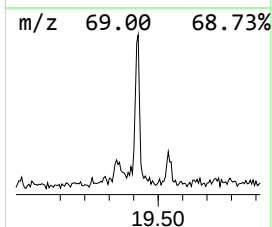
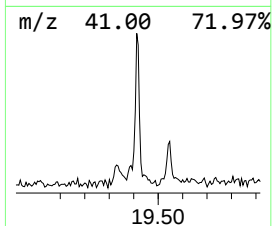
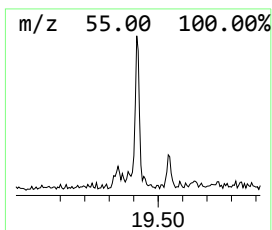
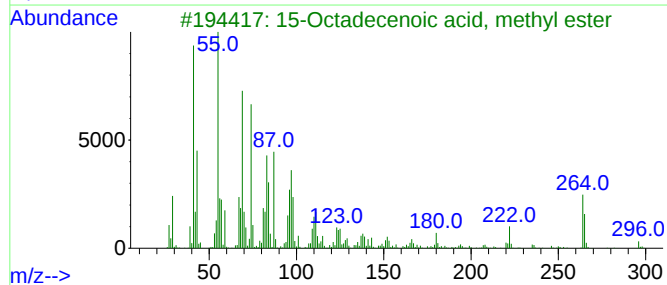
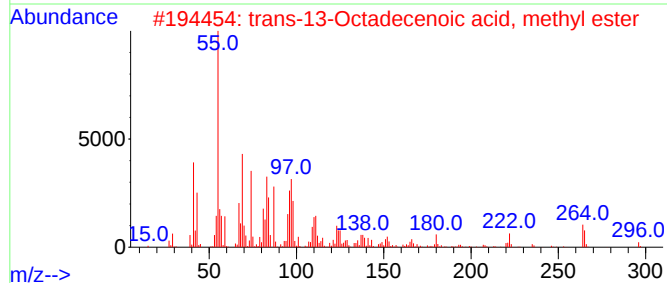
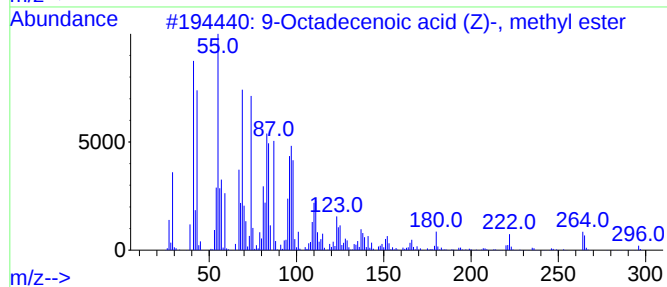
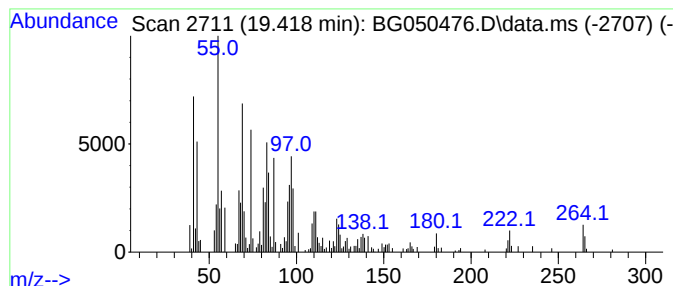
Instrument :
BNA_G
ClientSampleId :
WC-20211005-ROCK

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 9-Octadecenoic acid (Z)-, m... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
19.418	4.63 ng	170767	Phenanthrene-d10		17.620	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...		296	C19H36O2	000112-62-9	95
2	trans-13-Octadecenoic acid, meth...		296	C19H36O2	1000333-61-3	94
3	15-Octadecenoic acid, methyl ester		296	C19H36O2	004764-72-1	91
4	10-Octadecenoic acid, methyl ester		296	C19H36O2	013481-95-3	91
5	13-Octadecenoic acid, methyl ester		296	C19H36O2	056554-47-3	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100621\
Data File : BG050476.D
Acq On : 6 Oct 2021 20:32
Operator : CG/JU
Sample : M4087-09
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-20211005-ROCK

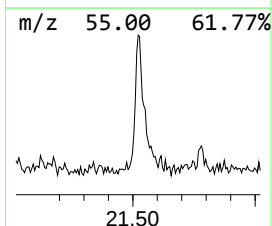
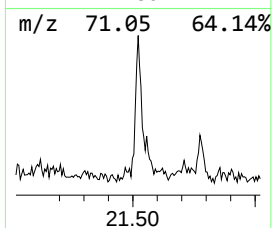
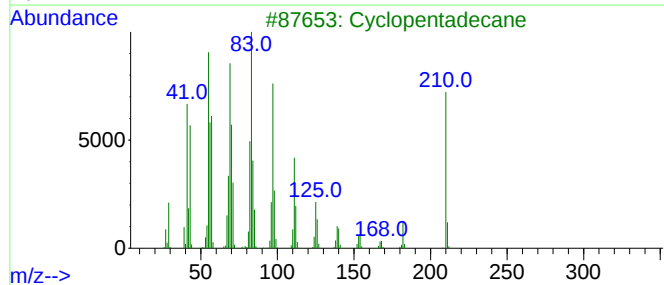
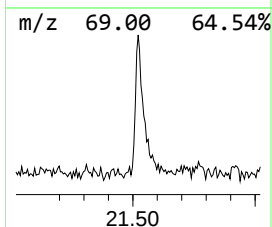
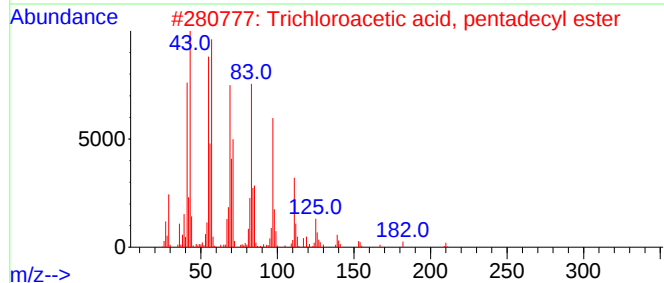
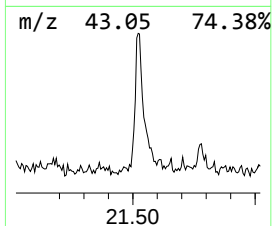
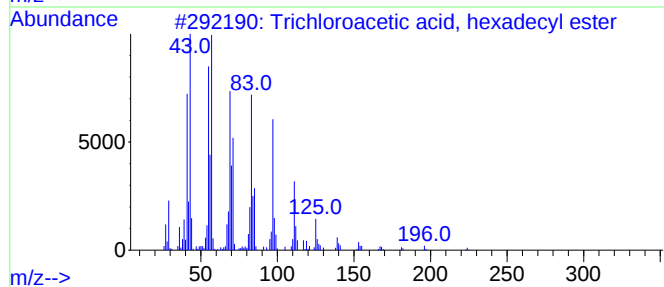
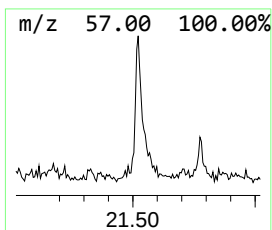
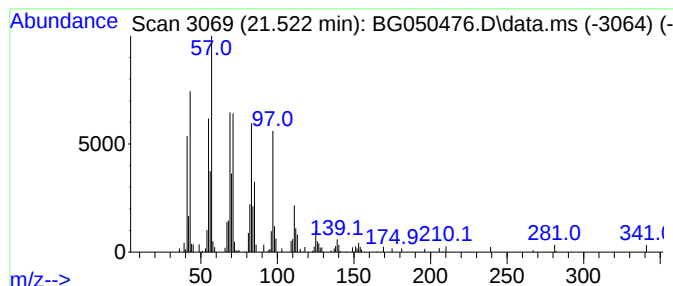
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Trichloroacetic acid, hexad... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.522	6.10 ng	229746	Chrysene-d12	21.915

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93
2			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	93
3			Cyclopentadecane	210	C15H30	000295-48-7	91
4			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
5			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100621\
Data File : BG050476.D
Acq On : 6 Oct 2021 20:32
Operator : CG/JU
Sample : M4087-09
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-20211005-ROCK

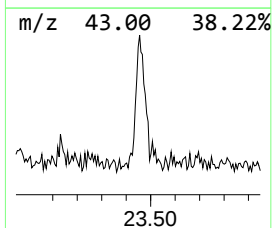
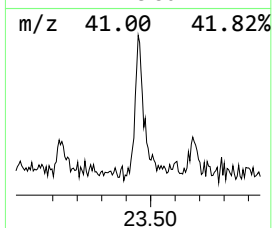
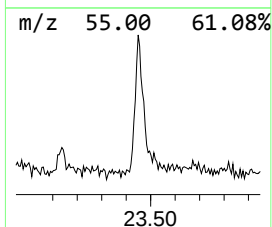
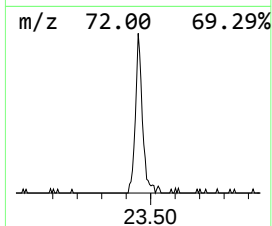
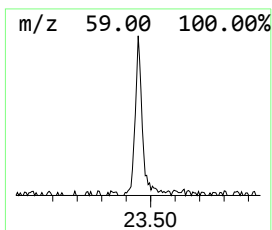
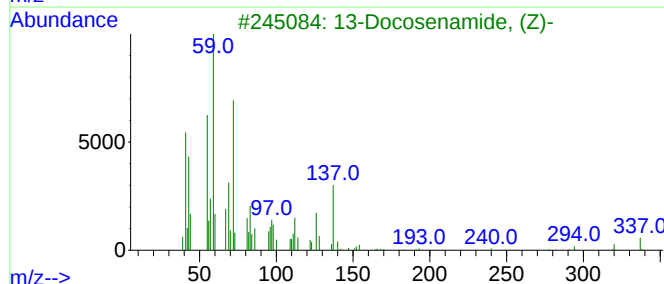
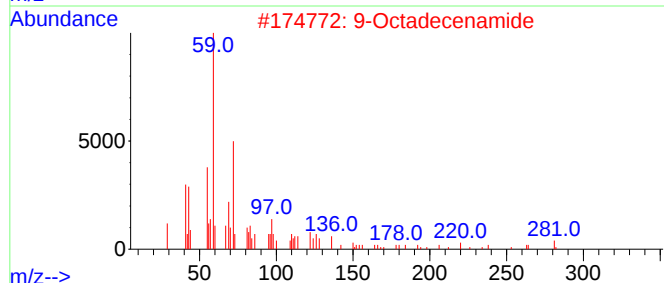
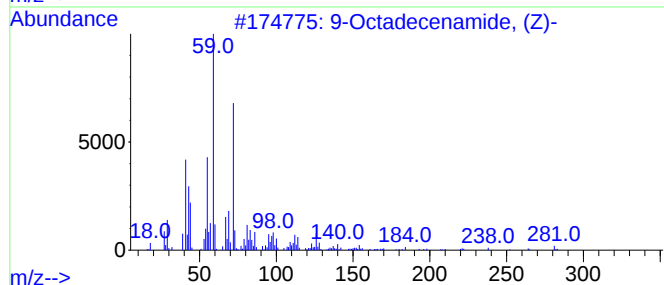
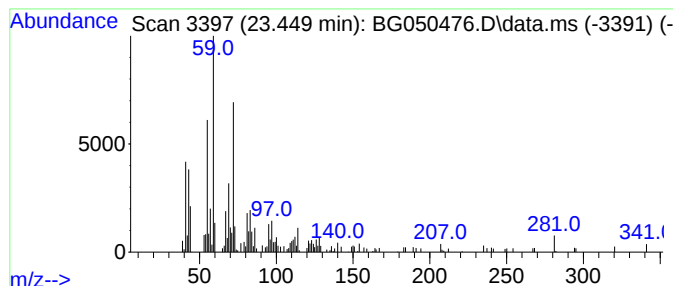
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.449	4.59 ng	172676	Chrysene-d12	21.915

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	93
2			9-Octadecenamide	281	C18H35NO	003322-62-1	70
3			13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	64
4			Dodecanamide	199	C12H25NO	001120-16-7	47
5			7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100621\
Data File : BG050476.D
Acq On : 6 Oct 2021 20:32
Operator : CG/JU
Sample : M4087-09
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-20211005-ROCK

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.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
2,4,7,9-Tetrame...	13.748	5.0	ng	151419	3	14.876	611619	20.0
9-Octadecenoic ...	19.418	4.6	ng	170767	4	17.620	737143	20.0
Trichloroacetic...	21.522	6.1	ng	229746	5	21.915	753069	20.0
9-Octadecenamid...	23.449	4.6	ng	172676	5	21.915	753069	20.0