

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011823\
 Data File : BG056341.D
 Acq On : 18 Jan 2023 23:35
 Operator : CG/JU
 Sample : 01159-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TP-E

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-BG122722.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG056341.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.341	342	349	356	rBV	116719	175776	8.14%	1.420%
2	5.823	424	431	443	rVB	475806	768468	35.57%	6.209%
3	7.445	698	707	718	rBV	497492	855151	39.58%	6.909%
4	8.302	846	853	861	rBV	122631	207814	9.62%	1.679%
5	9.478	1043	1053	1063	rBV	289617	519201	24.03%	4.195%
6	11.134	1328	1335	1349	rBB	171802	317423	14.69%	2.565%
7	13.543	1738	1745	1754	rBV	1024878	1518912	70.30%	12.272%
8	14.918	1971	1979	1985	rBV	337928	516948	23.93%	4.177%
9	16.258	2197	2207	2213	rBV	235192	341699	15.81%	2.761%
10	16.399	2224	2231	2238	rBV	811249	1216725	56.31%	9.831%
11	17.656	2437	2445	2449	rBV	445412	662182	30.65%	5.350%
12	17.697	2449	2452	2457	rVB	66653	89893	4.16%	0.726%
13	18.502	2583	2589	2597	rBV2	113343	189781	8.78%	1.533%
14	18.573	2597	2601	2607	rVB3	17044	32748	1.52%	0.265%
15	18.720	2620	2626	2630	rBV6	16963	35727	1.65%	0.289%
16	19.683	2785	2790	2796	rVB	173991	258057	11.94%	2.085%
17	19.754	2796	2802	2805	rBV5	30830	46418	2.15%	0.375%
18	20.012	2842	2846	2848	rBV2	30589	46251	2.14%	0.374%
19	20.048	2848	2852	2859	rVB	163983	235867	10.92%	1.906%
20	20.230	2877	2883	2889	rBV	1700399	2160700	100.00%	17.458%
21	20.365	2901	2906	2913	rBV6	12185	33662	1.56%	0.272%
22	20.529	2932	2934	2938	rVB2	24241	25278	1.17%	0.204%
23	20.905	2995	2998	3003	rVB	19207	22456	1.04%	0.181%
24	21.522	3099	3103	3112	rVB3	105751	204466	9.46%	1.652%
25	21.793	3145	3149	3155	rVB2	34922	47244	2.19%	0.382%
26	21.945	3166	3175	3180	rBV2	440024	871294	40.32%	7.040%
27	21.992	3180	3183	3192	rVB	79581	135228	6.26%	1.093%
28	24.284	3566	3573	3579	rBV2	59458	182803	8.46%	1.477%
29	25.388	3752	3761	3771	rVB2	230557	658408	30.47%	5.320%

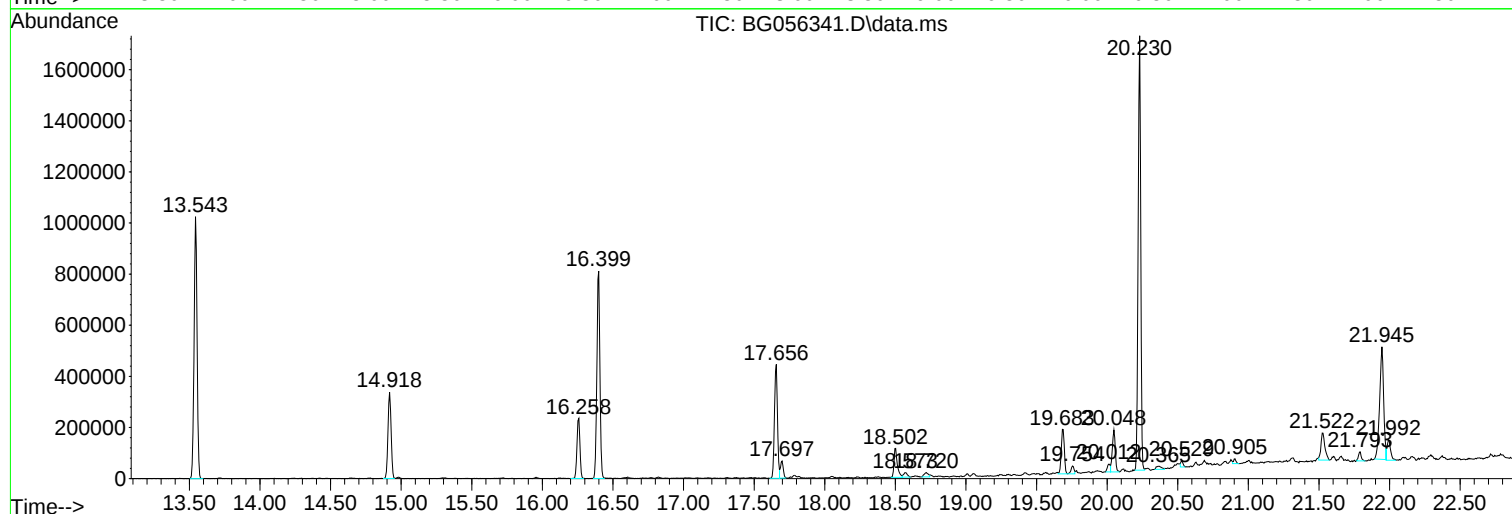
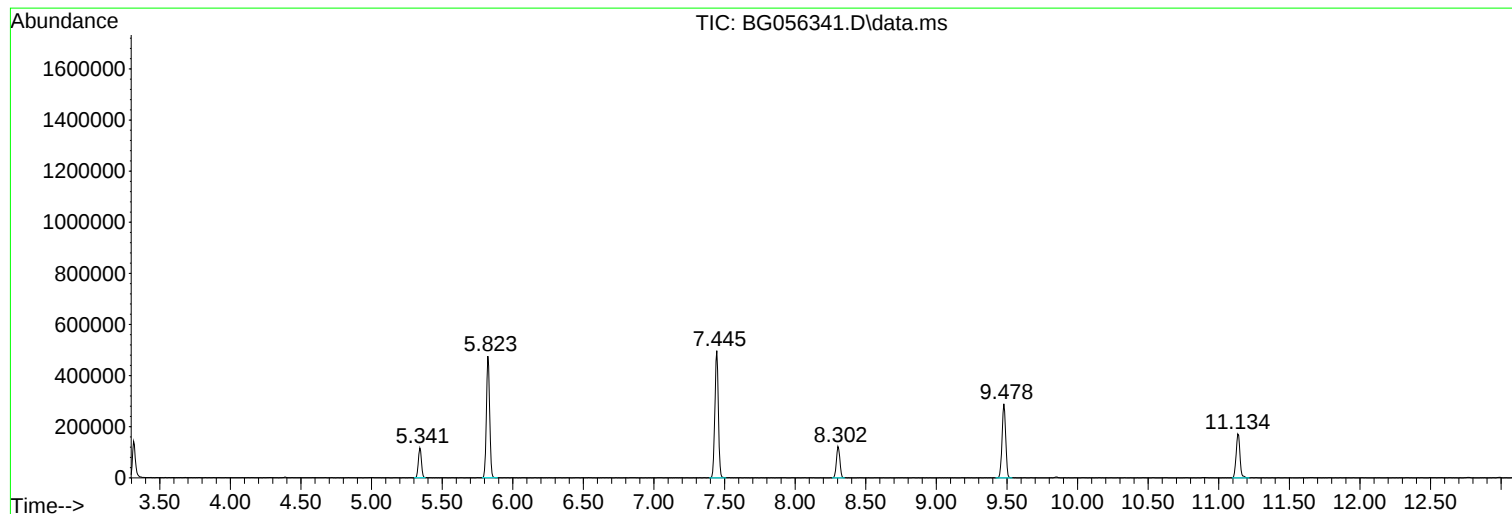
Sum of corrected areas: 12376580

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011823\
Data File : BG056341.D
Acq On : 18 Jan 2023 23:35
Operator : CG/JU
Sample : 01159-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-E

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.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\BG011823\
Data File : BG056341.D
Acq On : 18 Jan 2023 23:35
Operator : CG/JU
Sample : 01159-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-E

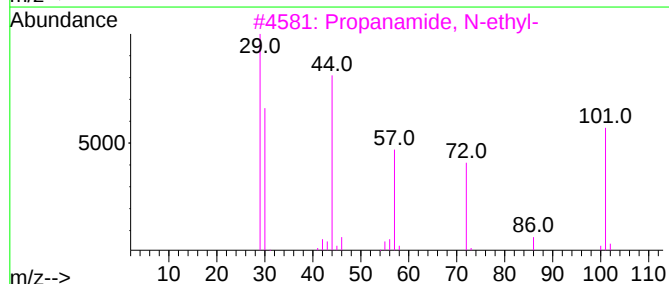
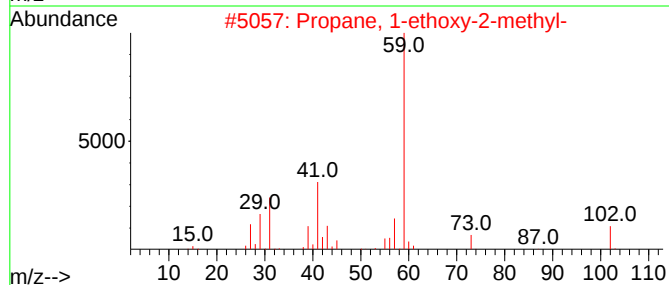
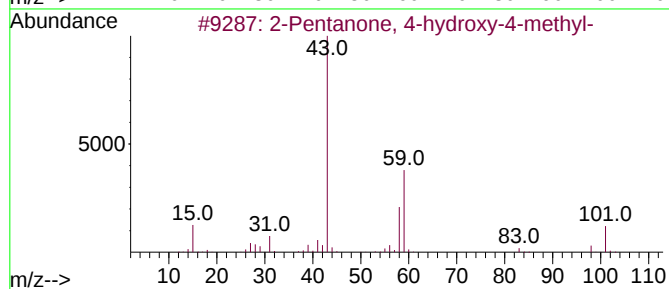
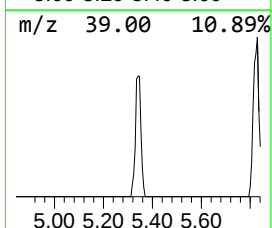
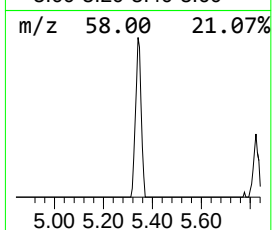
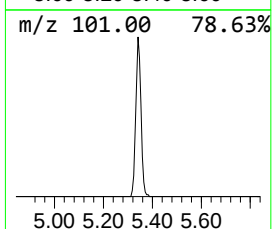
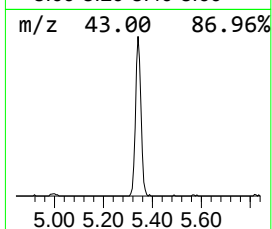
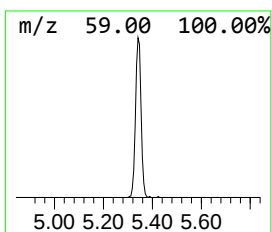
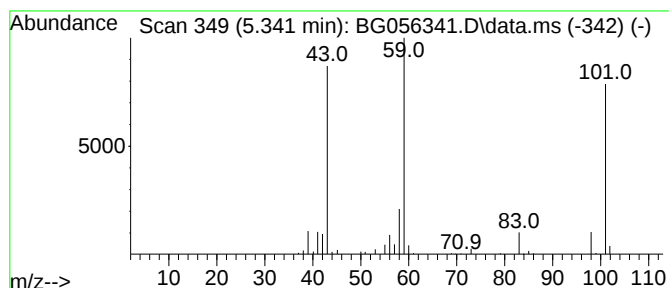
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.341	16.92 ng	175776	1,4-Dichlorobenzene-d4	8.302

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50	
2	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	30	
3	Propanamide, N-ethyl-	101	C5H11NO	005129-72-6	27	
4	Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	12	
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	12	



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011823\
Data File : BG056341.D
Acq On : 18 Jan 2023 23:35
Operator : CG/JU
Sample : 01159-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-E

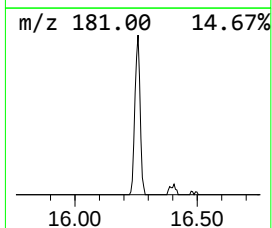
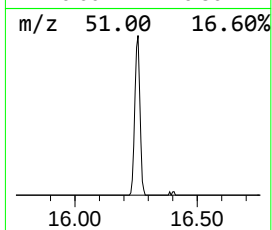
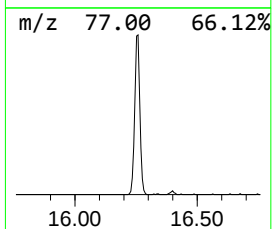
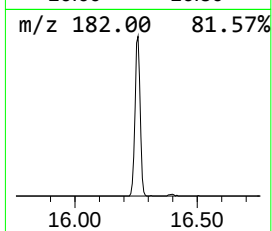
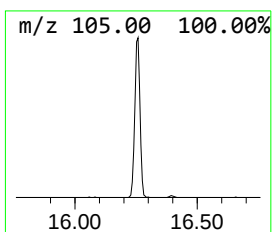
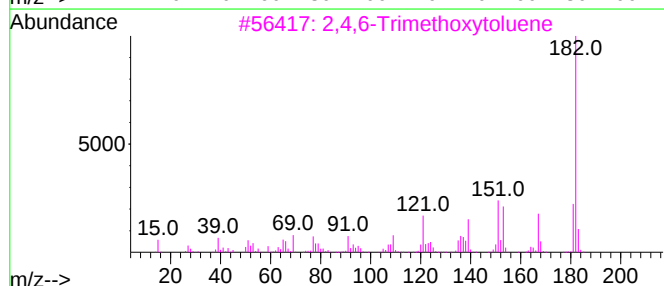
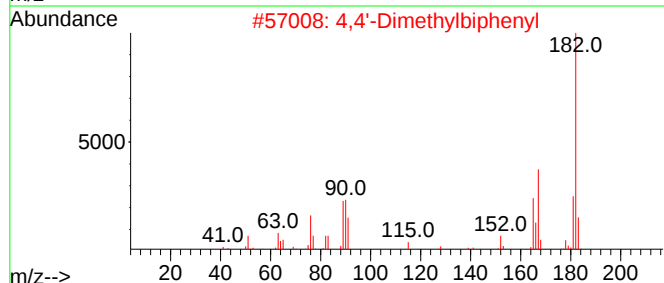
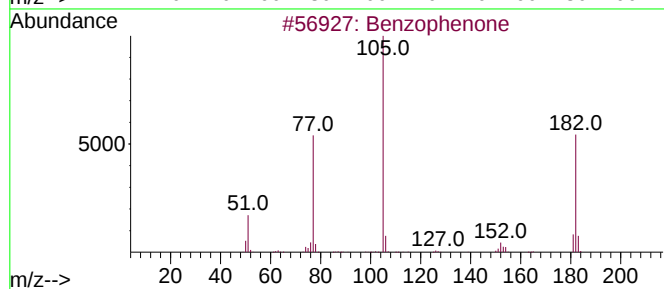
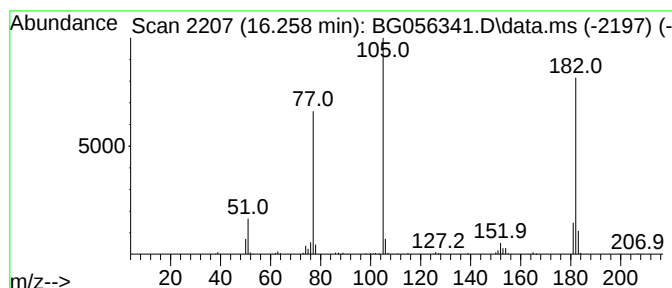
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.258	13.22 ng	341699	Acenaphthene-d10	14.918

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	95
2			4,4'-Dimethylbiphenyl	182	C14H14	000613-33-2	46
3			2,4,6-Trimethoxytoluene	182	C10H14O3	014107-97-2	46
4			2-Methyl-1H-perimidine	182	C12H10N2	005157-10-8	43
5			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011823\
Data File : BG056341.D
Acq On : 18 Jan 2023 23:35
Operator : CG/JU
Sample : 01159-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-E

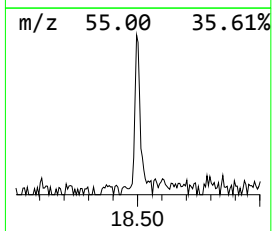
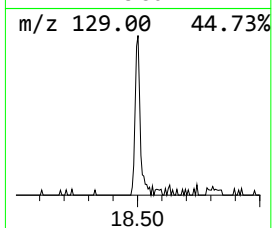
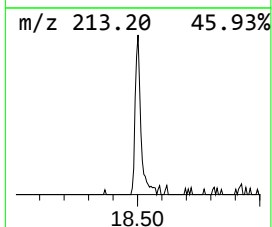
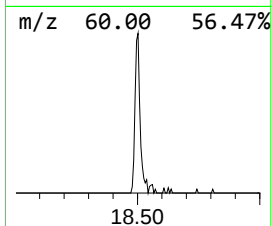
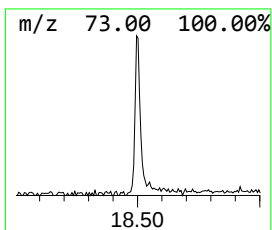
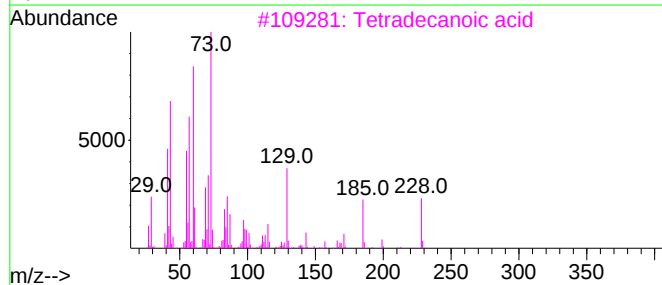
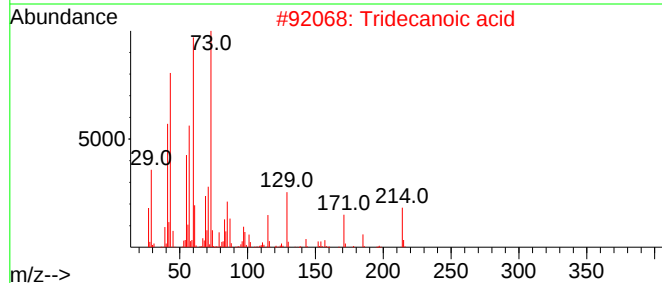
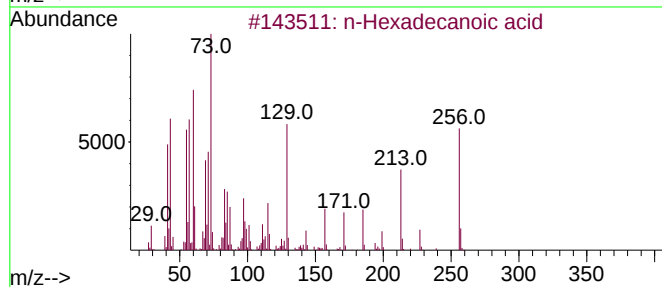
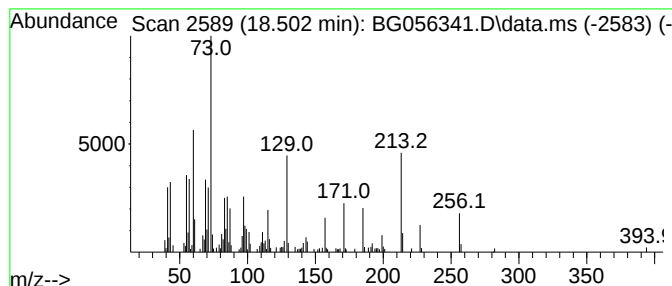
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.502	5.73 ng	189781	Phenanthrene-d10	17.656

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2			Tridecanoic acid	214	C13H26O2	000638-53-9	91
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	60
4			Octadecanoic acid	284	C18H36O2	000057-11-4	49
5			n-Decanoic acid	172	C10H20O2	000334-48-5	42



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011823\
Data File : BG056341.D
Acq On : 18 Jan 2023 23:35
Operator : CG/JU
Sample : 01159-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-E

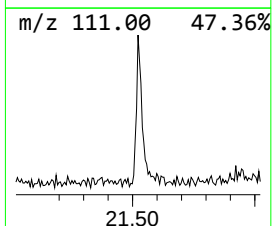
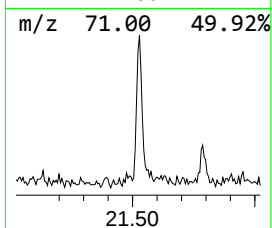
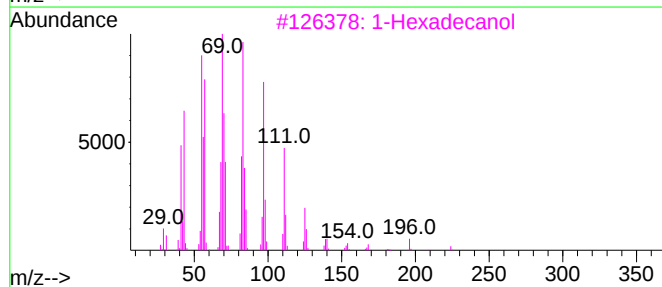
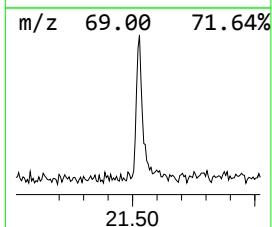
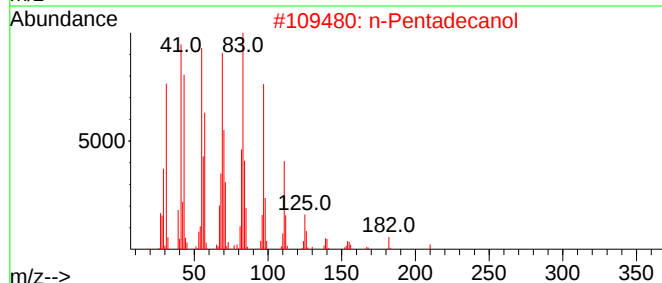
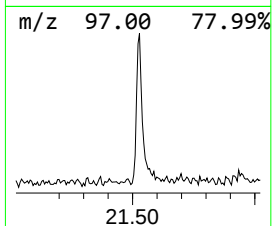
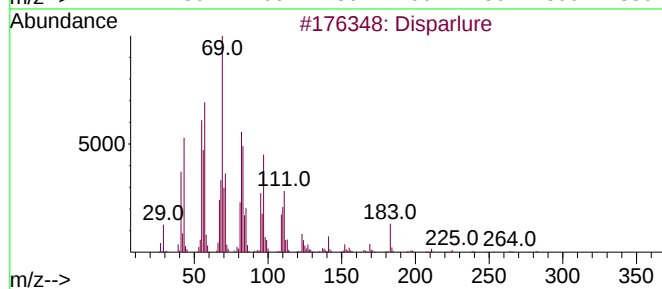
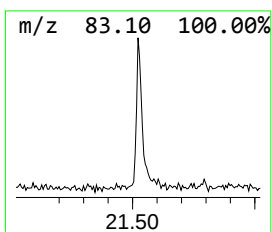
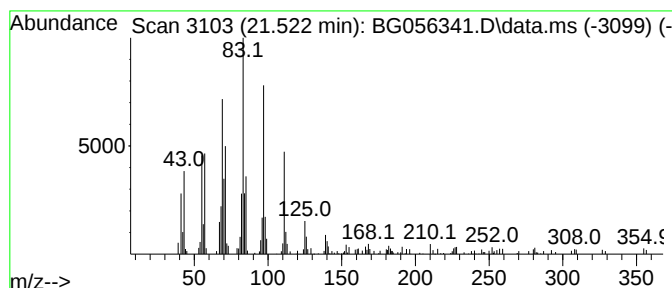
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Disparlure Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.522	4.69 ng	204466	Chrysene-d12	21.945

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Disparlure	282	C19H38O	029804-22-6	64
2			n-Pentadecanol	228	C15H32O	000629-76-5	43
3			1-Hexadecanol	242	C16H34O	036653-82-4	38
4			Acetic acid, chloro-, hexadecyl ...	318	C18H35ClO2	052132-58-8	38
5			Bacteriochlorophyll-c-stearyl	841	C52H72MgN4O4	1010164-49-7	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011823\
Data File : BG056341.D
Acq On : 18 Jan 2023 23:35
Operator : CG/JU
Sample : 01159-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-E

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.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-...	5.341	16.9	ng	175776	1	8.302	207814	20.0
Benzophenone	16.258	13.2	ng	341699	3	14.918	516948	20.0
n-Hexadecanoic ...	18.502	5.7	ng	189781	4	17.656	662182	20.0
Disparlure	21.522	4.7	ng	204466	5	21.945	871294	20.0