

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110520\
 Data File : BG047235.D
 Acq On : 6 Nov 2020 1:44
 Operator : CG/JU
 Sample : L4641-10
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 P0122-CAS001-0002-02

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-BG110420.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG047235.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.305	329	335	343	rBV2	18981	33301	1.10%	0.194%
2	5.564	371	379	388	rBV	734910	1152188	38.02%	6.708%
3	7.162	643	651	663	rBV	787623	1307606	43.15%	7.613%
4	8.008	785	795	802	rBV	215927	371266	12.25%	2.161%
5	9.165	985	992	1000	rBV	484163	833874	27.52%	4.855%
6	10.223	1167	1172	1178	rBV2	43531	72763	2.40%	0.424%
7	10.817	1262	1273	1281	rBV	307641	570721	18.83%	3.323%
8	12.227	1506	1513	1519	rBV2	24913	37005	1.22%	0.215%
9	13.267	1683	1690	1699	rVB	1365600	2081783	68.70%	12.120%
10	13.460	1719	1723	1729	rVB4	22127	34010	1.12%	0.198%
11	13.531	1729	1735	1745	rVB2	97218	155365	5.13%	0.905%
12	14.083	1823	1829	1839	rBV	69800	114748	3.79%	0.668%
13	14.641	1915	1924	1931	rBV	555372	876325	28.92%	5.102%
14	15.752	2108	2113	2122	rBV3	33675	58782	1.94%	0.342%
15	16.128	2170	2177	2190	rBV	1239604	1908869	62.99%	11.113%
16	17.385	2385	2391	2396	rBV	714379	1067420	35.22%	6.214%
17	17.426	2396	2398	2405	rVB	32608	48041	1.59%	0.280%
18	18.267	2537	2541	2550	rBV	230392	379057	12.51%	2.207%
19	18.337	2550	2553	2558	rVB	67284	94934	3.13%	0.553%
20	18.613	2595	2600	2605	rBV3	29075	63279	2.09%	0.368%
21	19.436	2736	2740	2745	rVB	74482	109227	3.60%	0.636%
22	19.542	2754	2758	2762	rBV5	84255	118030	3.89%	0.687%
23	19.994	2830	2835	2844	rBV	2372577	3030389	100.00%	17.643%
24	21.292	3052	3056	3069	rVB2	198499	382541	12.62%	2.227%
25	21.527	3094	3096	3101	rVB2	80797	96935	3.20%	0.564%
26	21.645	3111	3116	3123	rBV2	633827	970453	32.02%	5.650%
27	24.847	3653	3661	3675	rVB4	415222	1207574	39.85%	7.030%

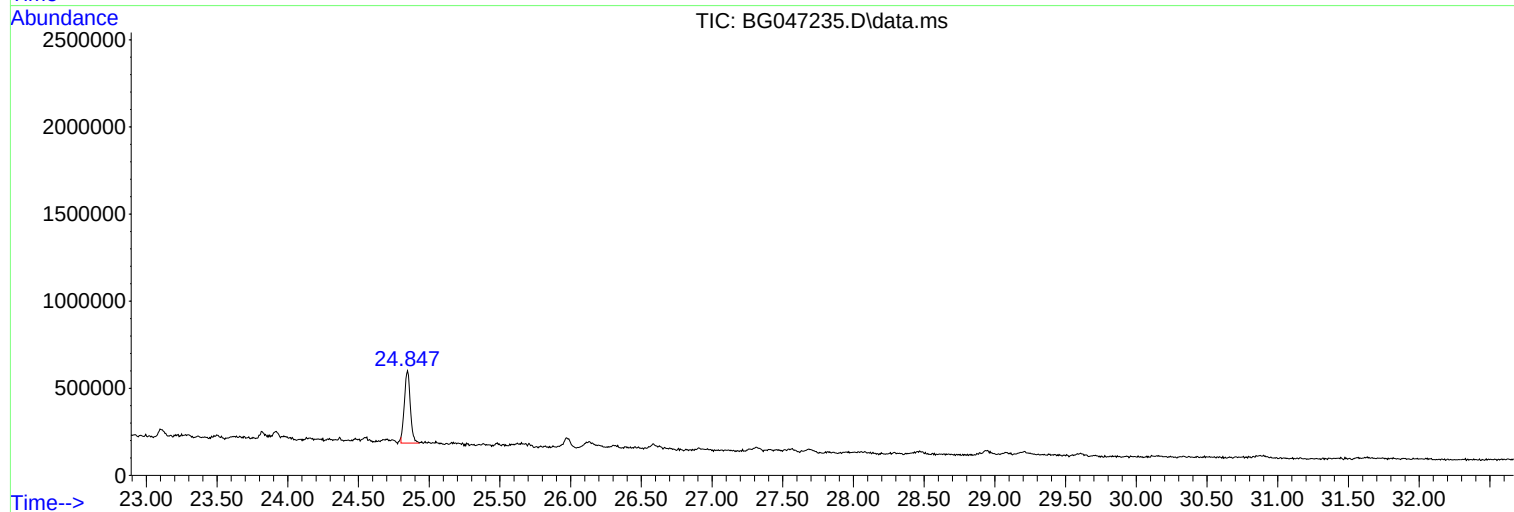
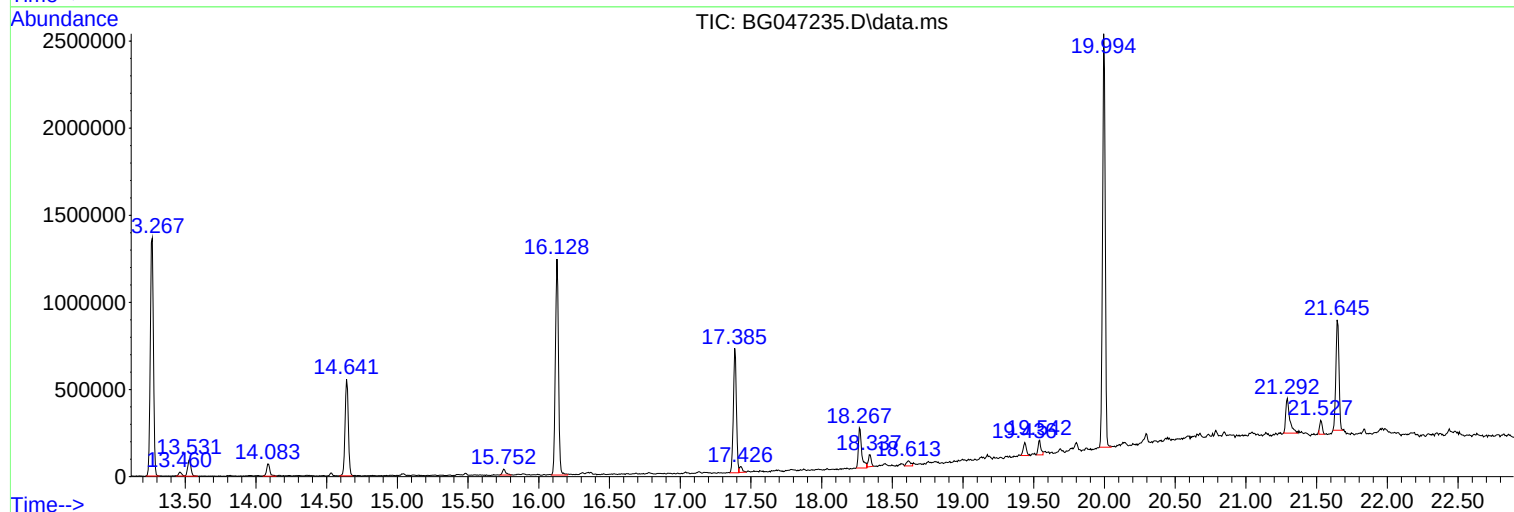
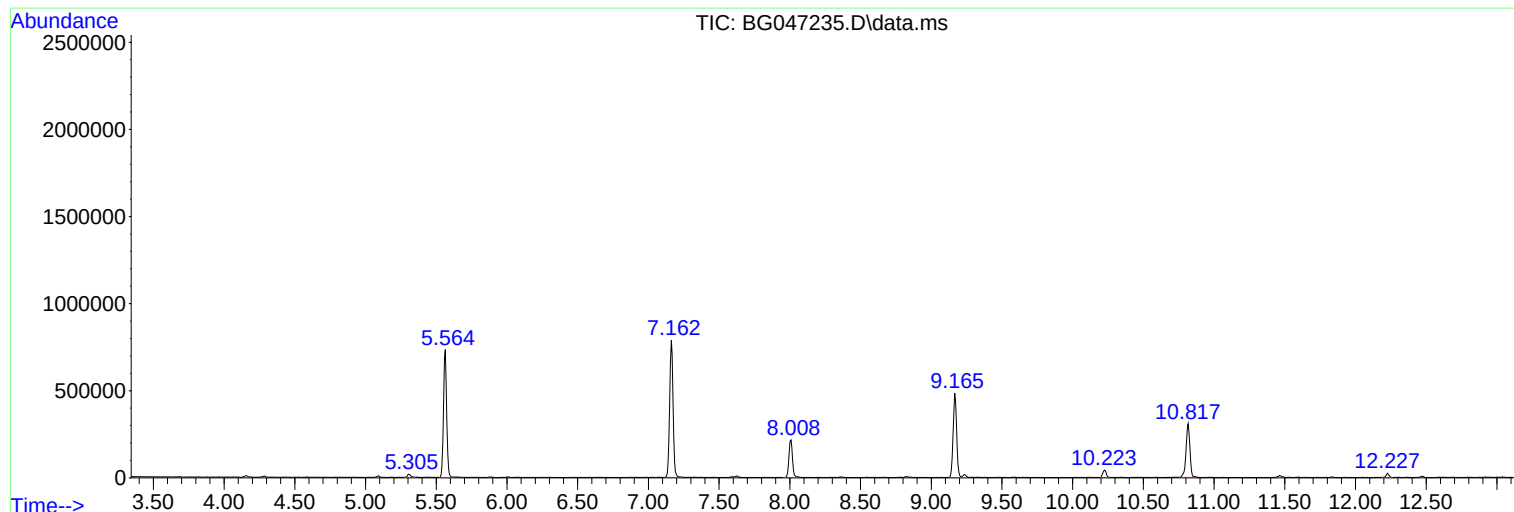
Sum of corrected areas: 17176486

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110520\
Data File : BG047235.D
Acq On : 6 Nov 2020 1:44
Operator : CG/JU
Sample : L4641-10
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P0122-CAS001-0002-02

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG110420.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110520\
Data File : BG047235.D
Acq On : 6 Nov 2020 1:44
Operator : CG/JU
Sample : L4641-10
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P0122-CAS001-0002-02

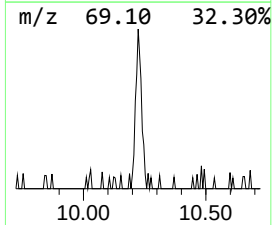
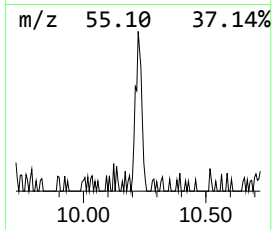
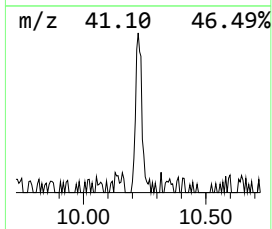
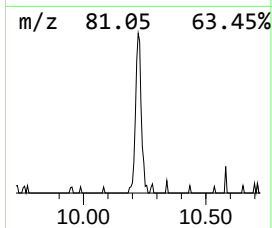
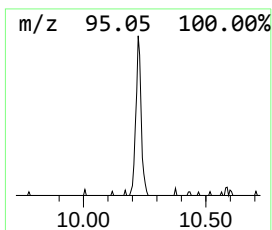
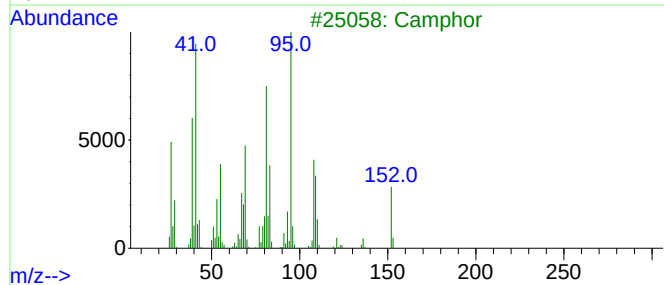
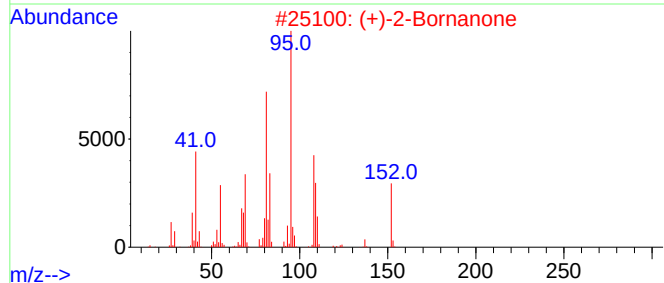
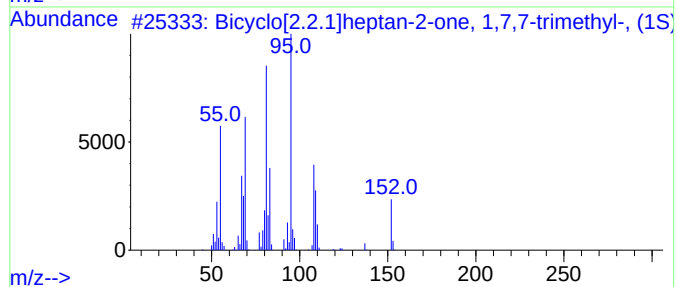
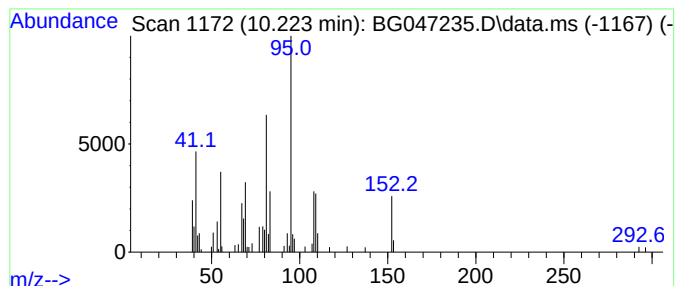
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG110420.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Bicyclo[2.2.1]heptan-2-one,... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.223	2.55 ng	72763	Naphthalene-d8	10.817

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	94
2			(+)-2-Bornanone	152	C10H16O	000464-49-3	93
3			Camphor	152	C10H16O	000076-22-2	93
4			2-Butanone, 4-(5-methyl-2-furanyl)-	152	C9H12O2	013679-56-6	52
5			5,7-Octadien-4-one, 2,6-dimethyl...	152	C10H16O	006752-80-3	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110520\
Data File : BG047235.D
Acq On : 6 Nov 2020 1:44
Operator : CG/JU
Sample : L4641-10
Misc :
ALS Vial : 12 Sample Multiplier: 1

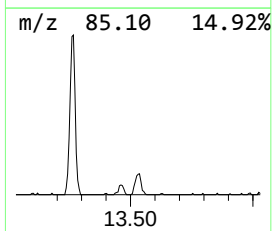
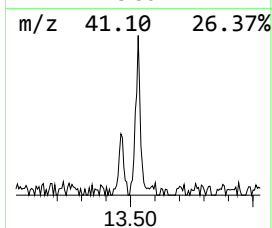
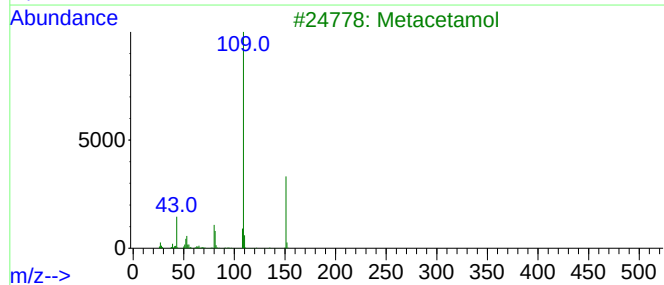
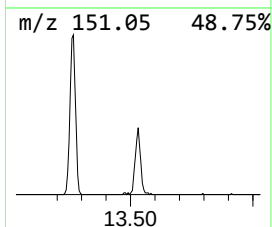
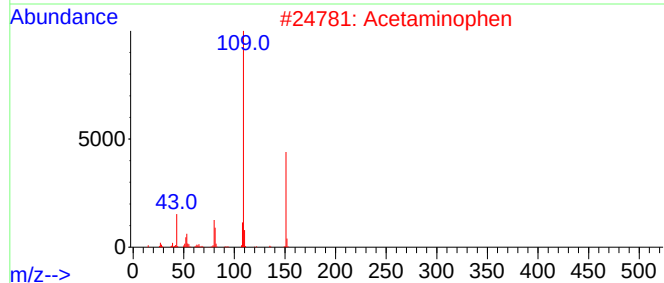
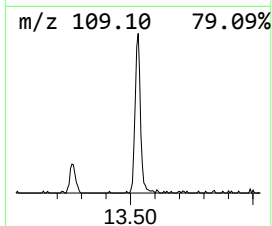
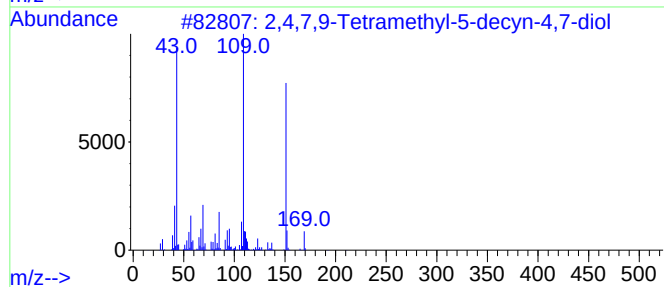
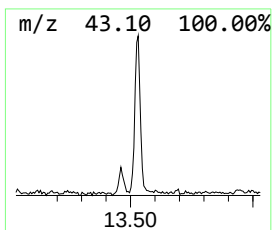
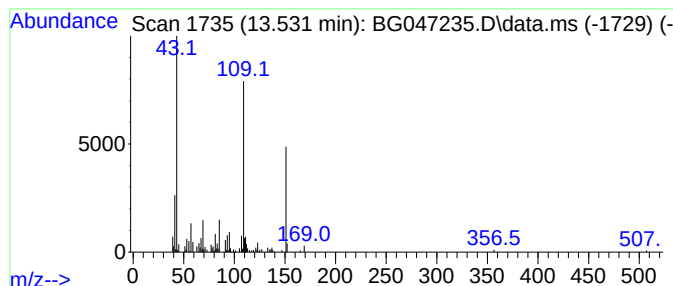
Instrument :
BNA_G
ClientSampleId :
P0122-CAS001-0002-02

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG110420.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.531	3.55 ng	155365	Acenaphthene-d10		14.641	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...		226	C14H26O2	000126-86-3	86
2	Acetaminophen		151	C8H9NO2	000103-90-2	64
3	Metacetamol		151	C8H9NO2	000621-42-1	59
4	3-Pyridinol, 4-methyl-, acetate ...		151	C8H9NO2	001006-96-8	59
5	2-Propenal, 3-(2,2,6-trimethyl-7...		194	C12H18O2	055759-91-6	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110520\
Data File : BG047235.D
Acq On : 6 Nov 2020 1:44
Operator : CG/JU
Sample : L4641-10
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P0122-CAS001-0002-02

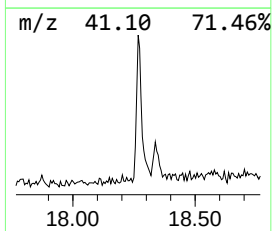
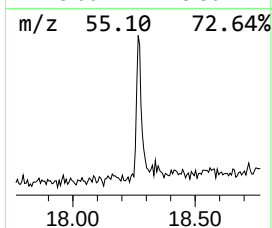
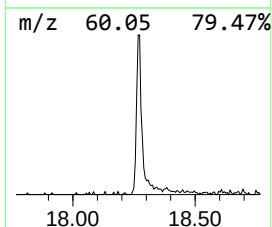
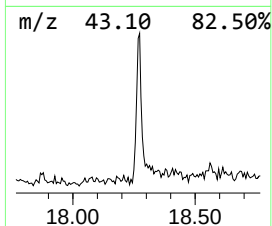
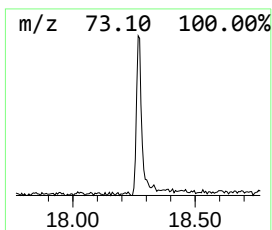
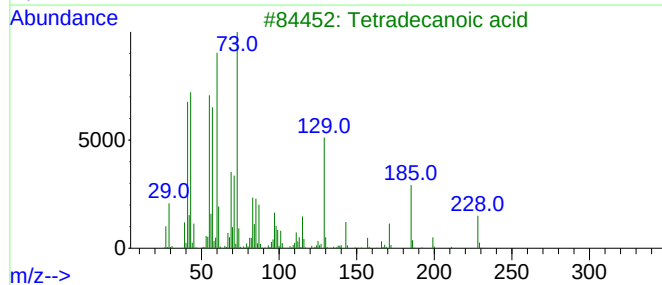
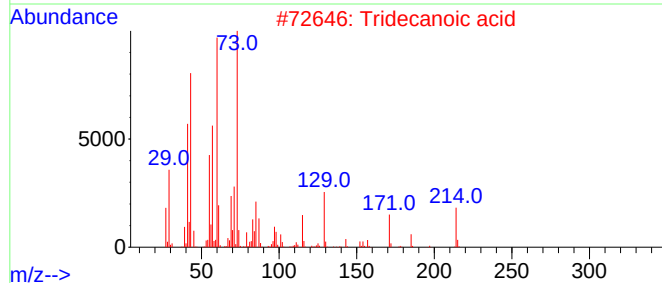
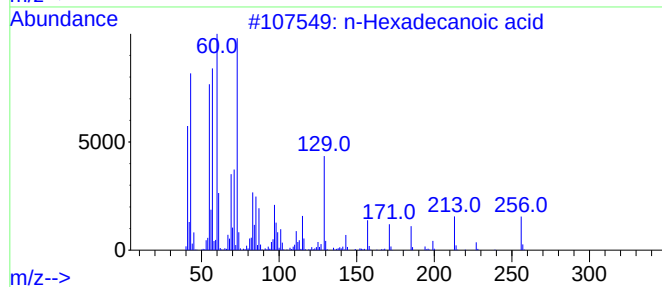
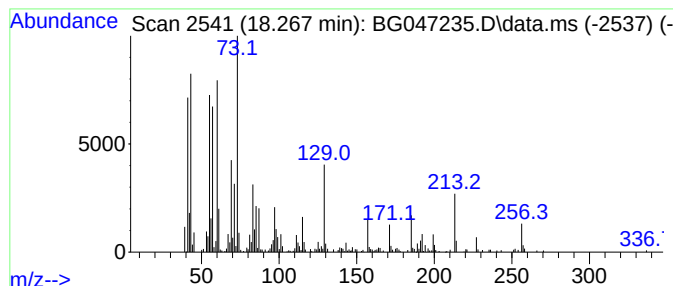
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG110420.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.267	7.10 ng	379057	Phenanthrene-d10	17.385

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	93
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5			Octadecanoic acid	284	C18H36O2	000057-11-4	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110520\
Data File : BG047235.D
Acq On : 6 Nov 2020 1:44
Operator : CG/JU
Sample : L4641-10
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P0122-CAS001-0002-02

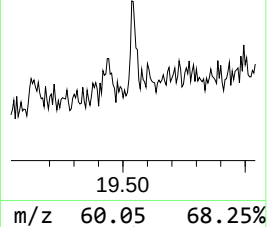
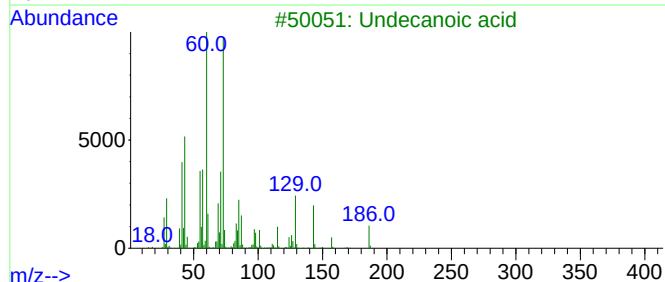
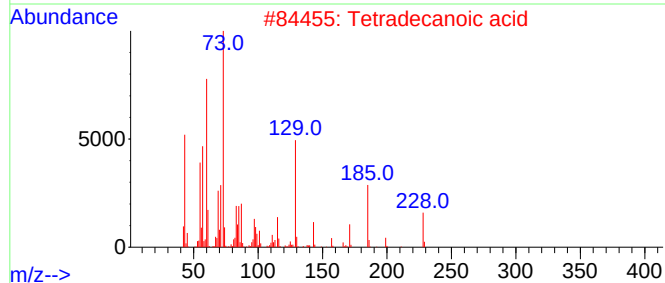
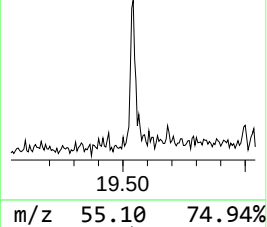
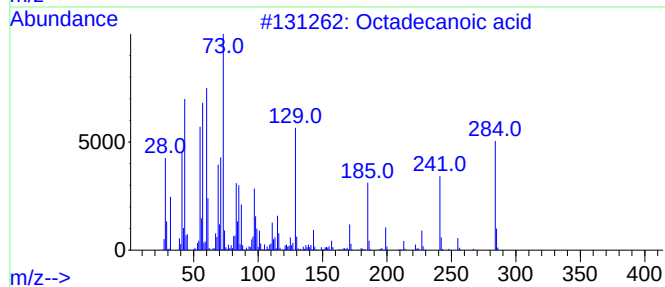
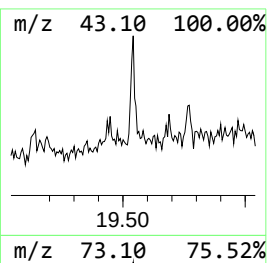
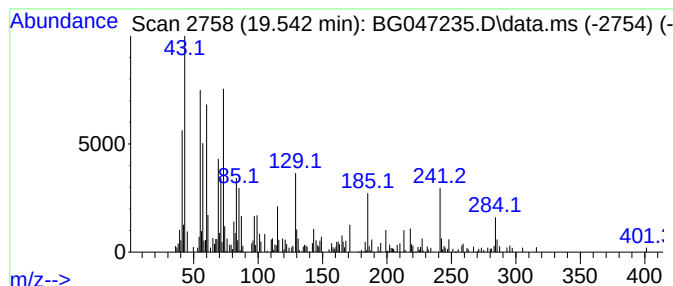
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG110420.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.542	2.43 ng	118030	Chrysene-d12	21.645

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	70
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	50
3			Undecanoic acid	186	C11H22O2	000112-37-8	47
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	43
5			Nonanoic acid	158	C9H18O2	000112-05-0	42



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110520\
Data File : BG047235.D
Acq On : 6 Nov 2020 1:44
Operator : CG/JU
Sample : L4641-10
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P0122-CAS001-0002-02

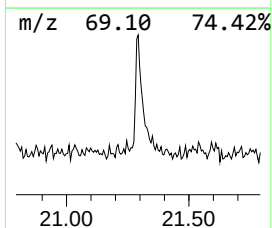
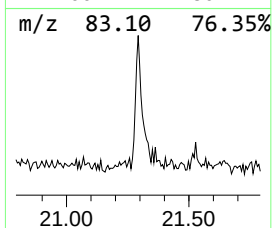
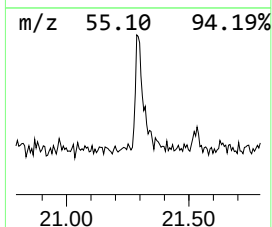
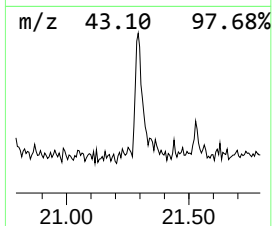
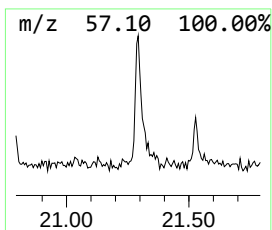
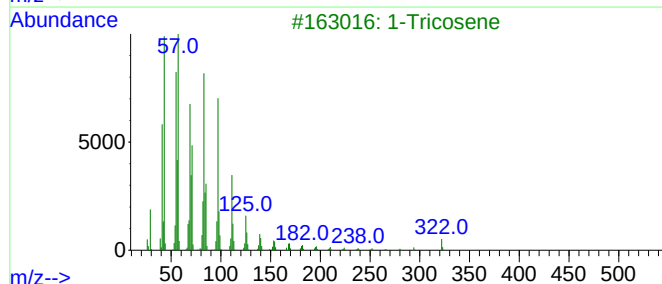
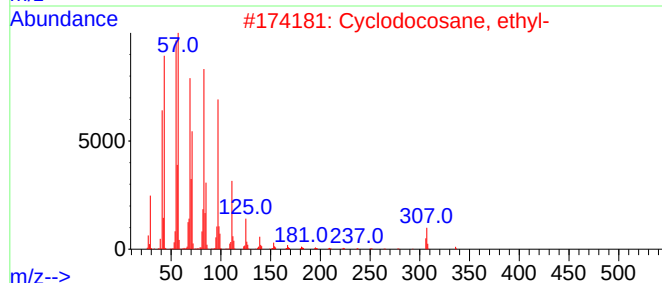
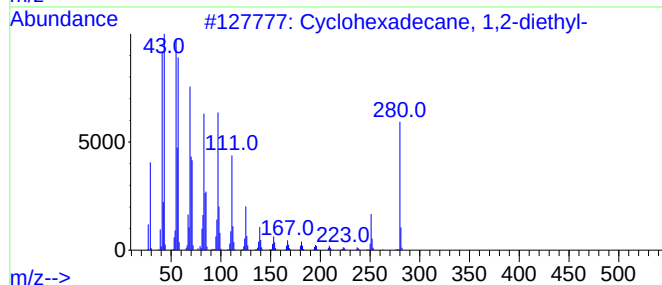
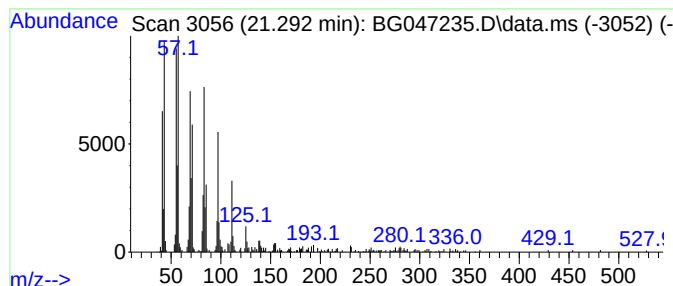
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG110420.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Cyclohexadecane, 1,2-diethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.293	7.88 ng	382541	Chrysene-d12	21.645

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexadecane, 1,2-diethyl-	280	C20H40	1000155-85-3	97
2			Cyclodocosane, ethyl-	336	C24H48	1000151-22-6	96
3			1-Tricosene	322	C23H46	018835-32-0	95
4			3-Eicosene, (E)-	280	C20H40	074685-33-9	94
5			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110520\
Data File : BG047235.D
Acq On : 6 Nov 2020 1:44
Operator : CG/JU
Sample : L4641-10
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P0122-CAS001-0002-02

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG110420.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Bicyclo[2.2.1]h...	10.223	2.5	ng	72763	2	10.817	570721	20.0
2,4,7,9-Tetrame...	13.531	3.5	ng	155365	3	14.641	876325	20.0
n-Hexadecanoic ...	18.267	7.1	ng	379057	4	17.385	1067420	20.0
Octadecanoic acid	19.542	2.4	ng	118030	5	21.645	970453	20.0
Cyclohexadecane...	21.293	7.9	ng	382541	5	21.645	970453	20.0