

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111621\
 Data File : BG051044.D
 Acq On : 15 Nov 2021 16:40
 Operator : CG/JU
 Sample : M4595-04
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 CMC-OF4-003-004

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-BG111321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG051044.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.300	301	308	315	rVB	68161	108856	3.47%	0.564%
2	5.764	380	387	401	rVB	864555	1404947	44.73%	7.281%
3	7.380	652	662	673	rBV	861965	1556016	49.53%	8.064%
4	8.226	799	806	814	rBV	156418	264981	8.44%	1.373%
5	9.401	998	1006	1017	rBV	523516	962587	30.64%	4.989%
6	10.805	1237	1245	1261	rBV	131767	251978	8.02%	1.306%
7	11.052	1281	1287	1295	rVB	211123	388271	12.36%	2.012%
8	13.479	1692	1700	1707	rVB	1324917	2128806	67.77%	11.033%
9	14.853	1927	1934	1940	rBV	347887	549470	17.49%	2.848%
10	16.340	2180	2187	2196	rBV	1058862	1636050	52.08%	8.479%
11	17.597	2391	2401	2406	rBV	475084	924458	29.43%	4.791%
12	17.873	2427	2448	2461	rVV	231852	1151756	36.66%	5.969%
13	18.056	2463	2479	2497	rVB	586436	2261499	71.99%	11.720%
14	18.232	2504	2509	2511	rBV	43134	67598	2.15%	0.350%
15	18.449	2542	2546	2550	rBV2	59936	88137	2.81%	0.457%
16	19.213	2668	2676	2684	rVB2	53969	145097	4.62%	0.752%
17	19.389	2702	2706	2709	rVB3	48266	59842	1.91%	0.310%
18	20.188	2836	2842	2855	rBV	2183722	3141297	100.00%	16.280%
19	21.046	2983	2988	2994	rVB2	85486	175615	5.59%	0.910%
20	21.487	3060	3063	3075	rVB5	70178	136139	4.33%	0.706%
21	21.593	3078	3081	3086	rVB	49931	65315	2.08%	0.338%
22	21.898	3127	3133	3138	rBV	375809	651047	20.73%	3.374%
23	21.957	3139	3143	3151	rVB2	108224	214845	6.84%	1.113%
24	24.237	3525	3531	3540	rVB5	81525	246383	7.84%	1.277%
25	25.312	3706	3714	3730	rVB2	220843	714779	22.75%	3.704%

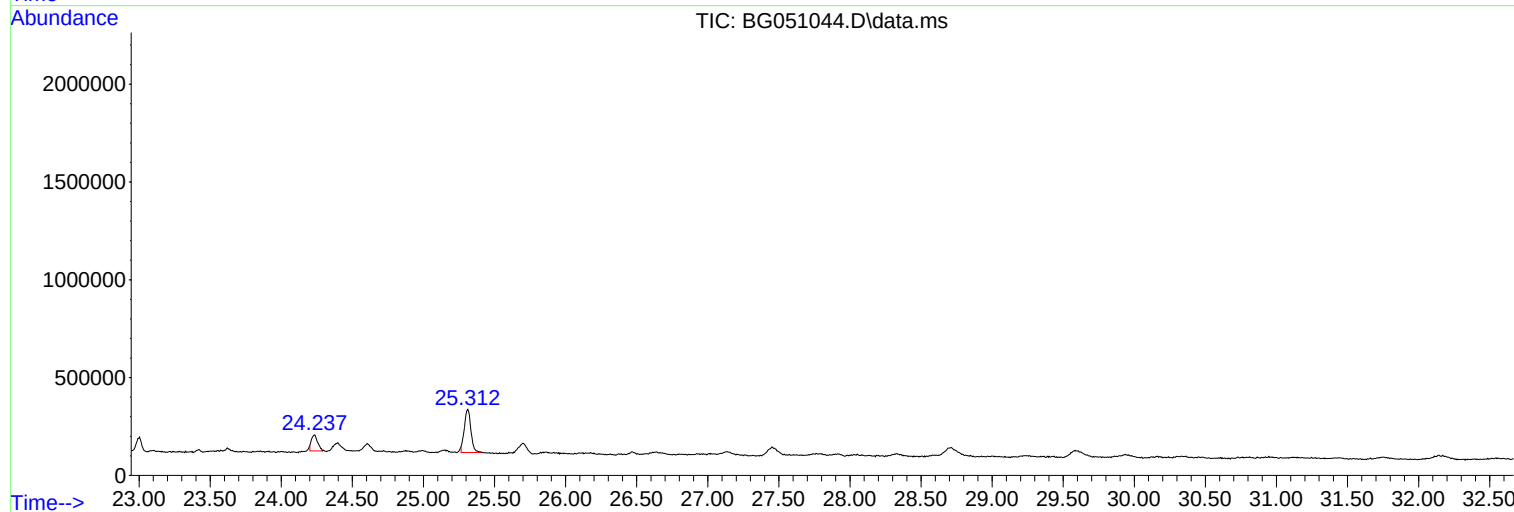
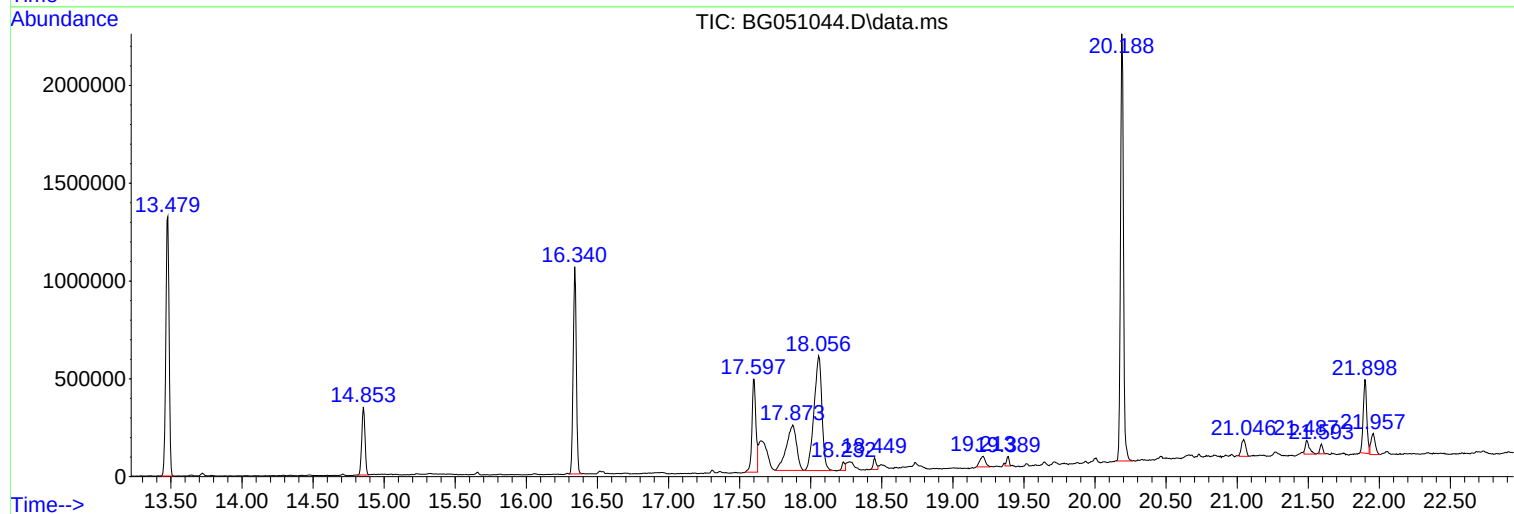
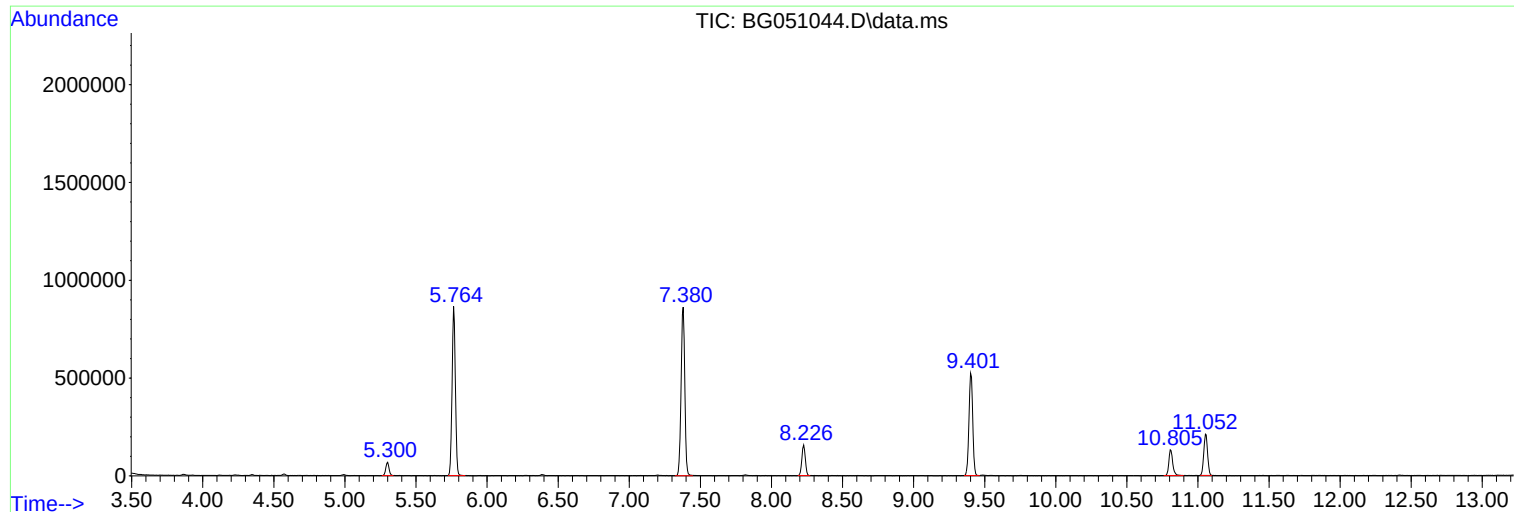
Sum of corrected areas: 19295769

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111621\
Data File : BG051044.D
Acq On : 15 Nov 2021 16:40
Operator : CG/JU
Sample : M4595-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CMC-OF4-003-004

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111321.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\BG111621\
Data File : BG051044.D
Acq On : 15 Nov 2021 16:40
Operator : CG/JU
Sample : M4595-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CMC-OF4-003-004

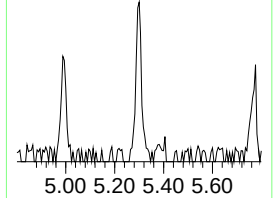
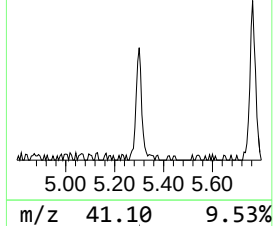
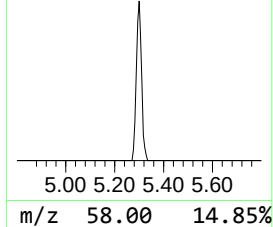
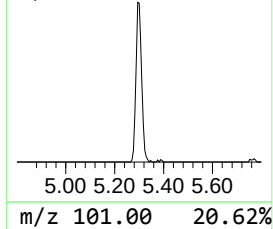
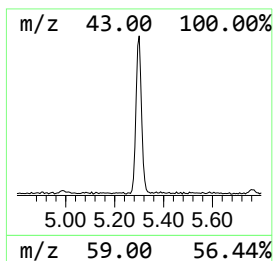
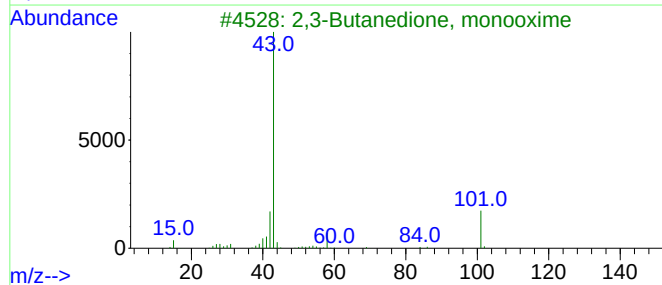
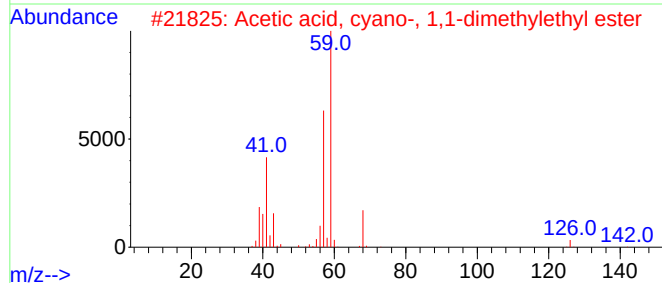
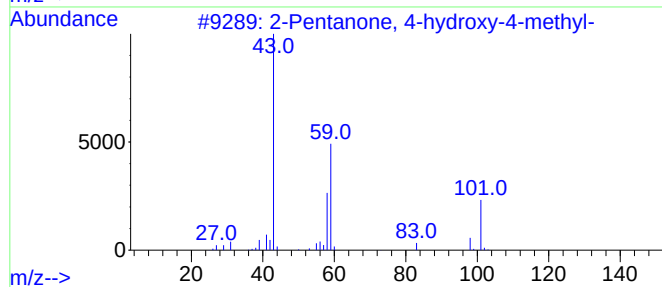
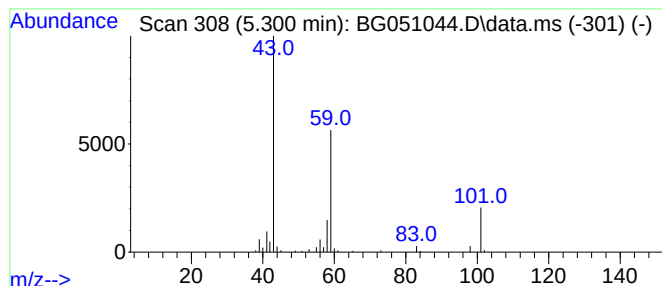
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.300	8.22 ng	108856	1,4-Dichlorobenzene-d4	8.226

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	9
5		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111621\
Data File : BG051044.D
Acq On : 15 Nov 2021 16:40
Operator : CG/JU
Sample : M4595-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CMC-OF4-003-004

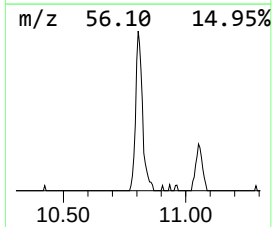
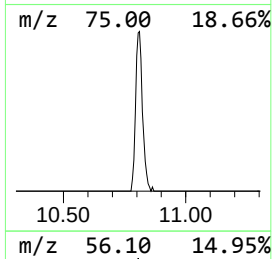
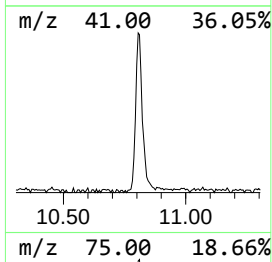
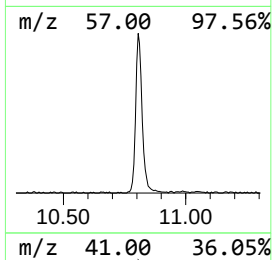
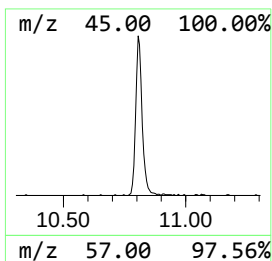
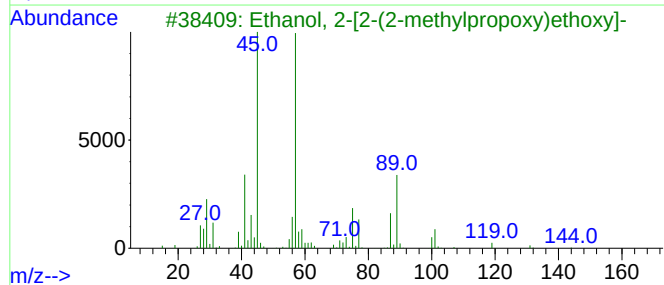
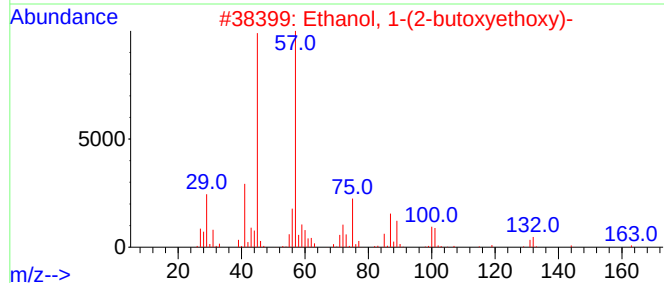
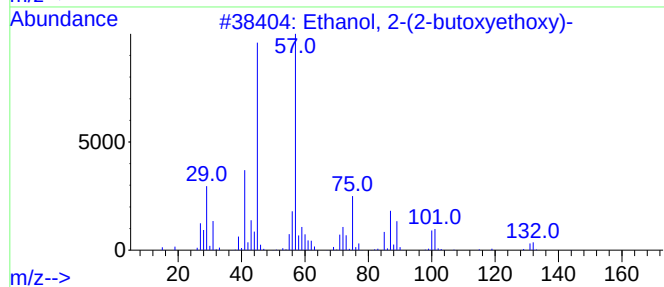
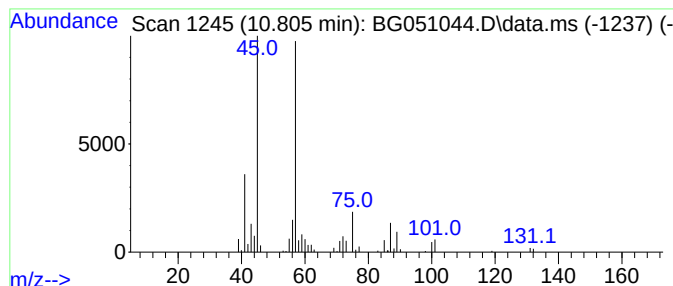
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.805	12.98 ng	251978	Naphthalene-d8	11.052

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	64
4			Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	53
5			Di-sec-Butyl ether	130	C8H18O	006863-58-7	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111621\
Data File : BG051044.D
Acq On : 15 Nov 2021 16:40
Operator : CG/JU
Sample : M4595-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CMC-OF4-003-004

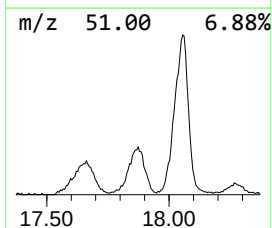
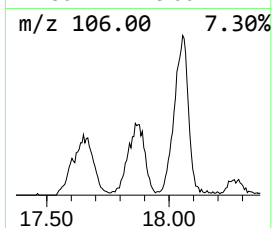
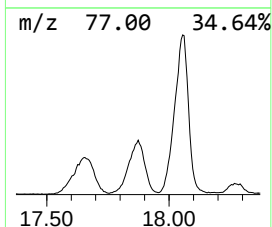
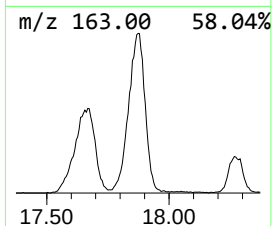
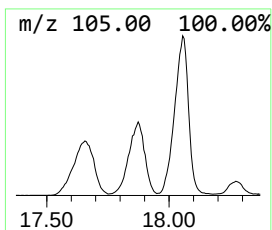
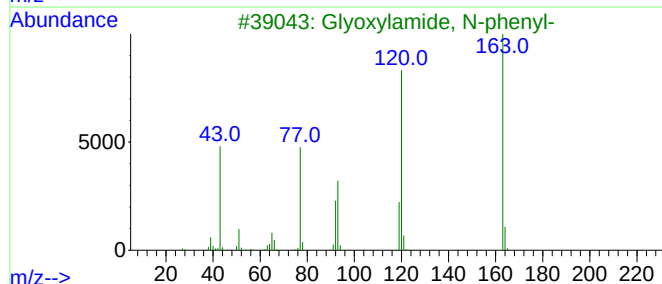
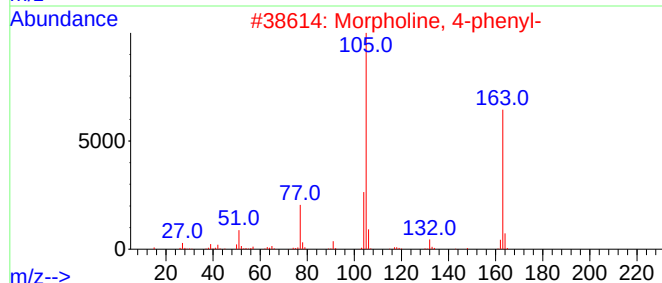
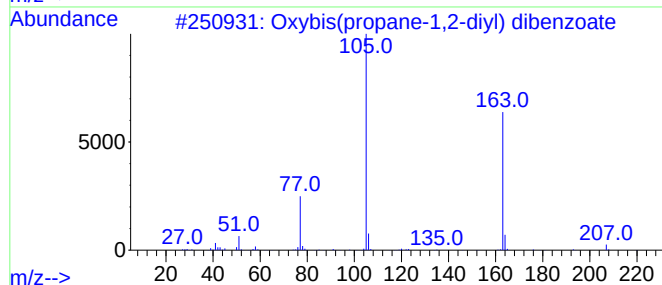
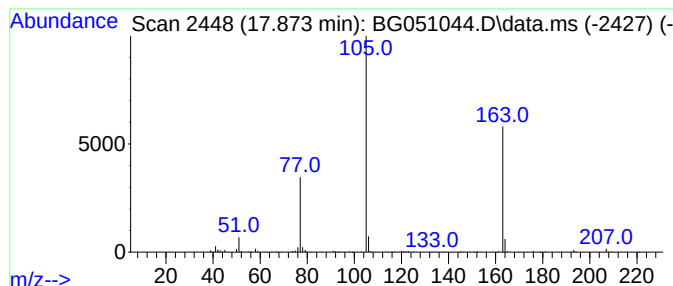
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Oxybis(propene-1,2-diyl) di... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.873	24.92 ng	1151760	Phenanthrene-d10	17.597

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxybis(propene-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	78
2			Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	64
3			Glyoxylamide, N-phenyl-	163	C9H9NO2	032331-52-5	50
4			Phenylglyoxylic acid, butyl ester	206	C12H14O3	1000453-46-6	38
5			Ethanone, 2-bromo-1,2-diphenyl-	274	C14H11BrO	001484-50-0	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111621\
Data File : BG051044.D
Acq On : 15 Nov 2021 16:40
Operator : CG/JU
Sample : M4595-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CMC-OF4-003-004

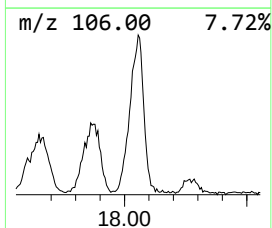
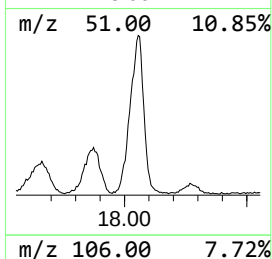
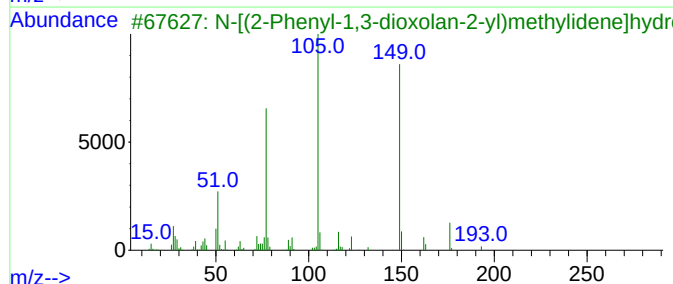
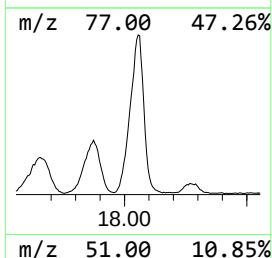
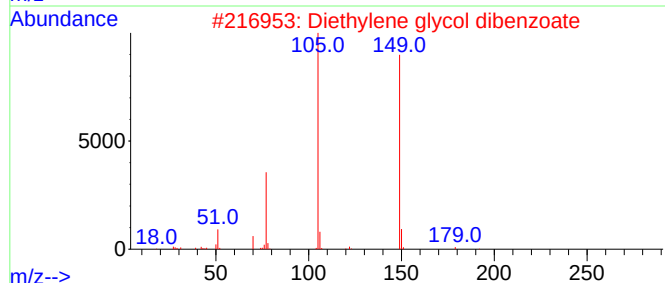
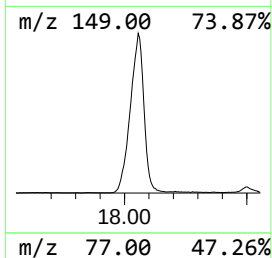
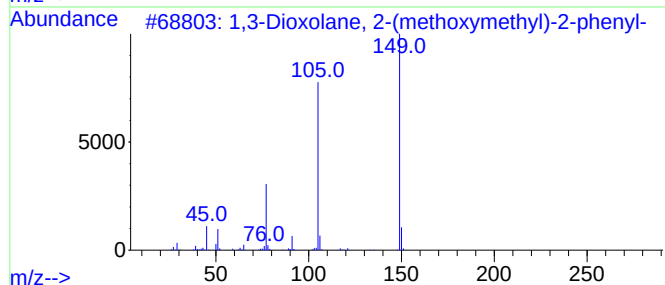
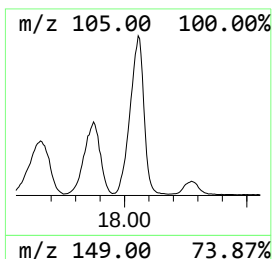
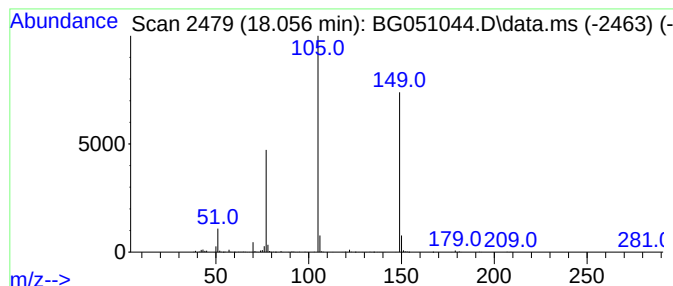
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 1,3-Dioxolane, 2-(methoxyme... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.056	48.93 ng	2261500	Phenanthrene-d10	17.597

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	83		
2	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	80		
3	N-[(2-Phenyl-1,3-dioxolan-2-yl)m...	193	C10H11NO3	1000411-48-9	78		
4	2-(2-(2-Methoxyethoxy)ethoxy)eth...	268	C14H20O5	1000366-99-1	74		
5	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	72		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111621\
Data File : BG051044.D
Acq On : 15 Nov 2021 16:40
Operator : CG/JU
Sample : M4595-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CMC-OF4-003-004

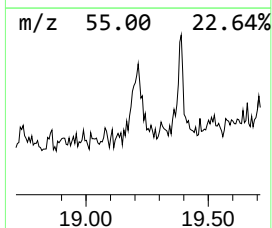
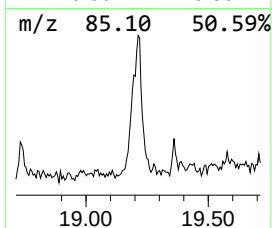
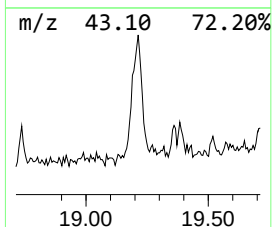
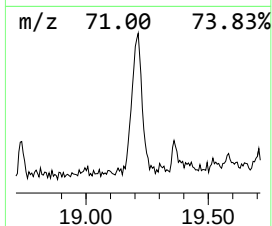
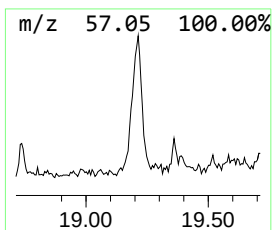
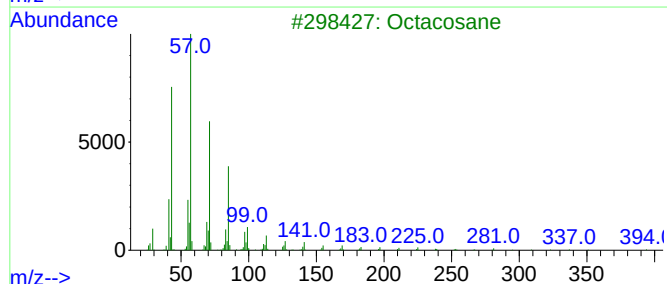
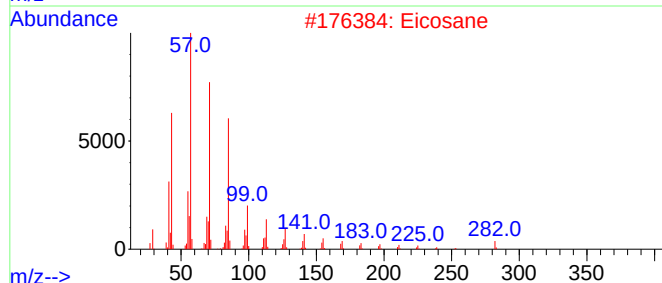
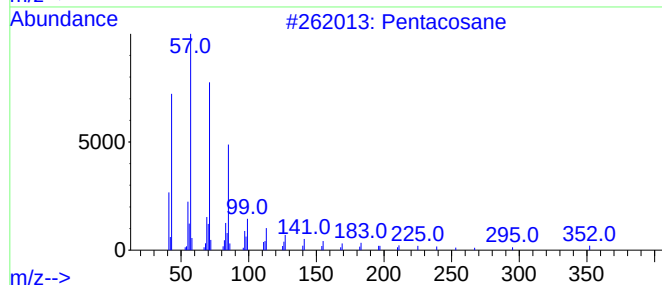
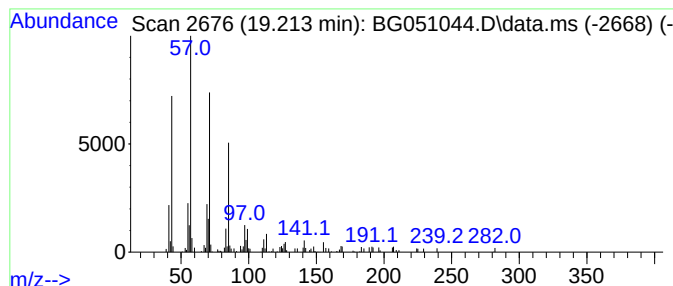
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Pentacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.213	3.14 ng	145097	Phenanthrene-d10	17.597

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentacosane	352	C25H52	000629-99-2	91
2			Eicosane	282	C20H42	000112-95-8	90
3			Octacosane	394	C28H58	000630-02-4	87
4			Tetratetracontane	619	C44H90	007098-22-8	87
5			Decane, 2,3,7-trimethyl-	184	C13H28	062238-13-5	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111621\
Data File : BG051044.D
Acq On : 15 Nov 2021 16:40
Operator : CG/JU
Sample : M4595-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CMC-OF4-003-004

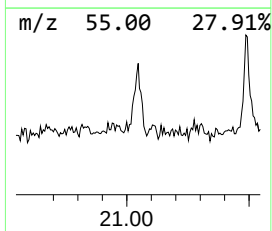
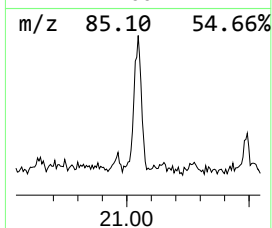
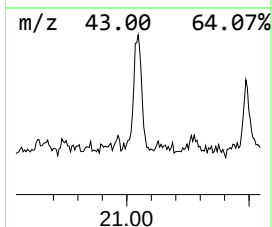
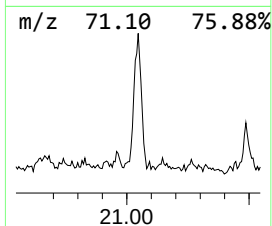
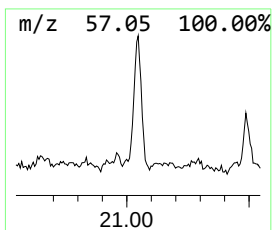
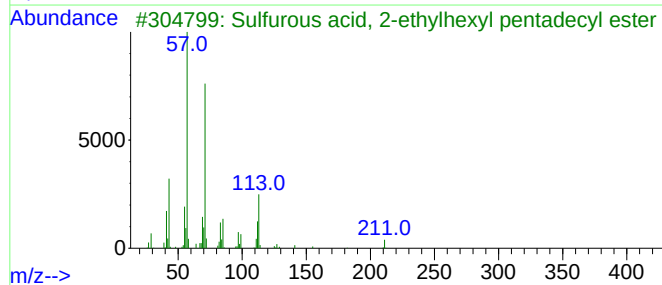
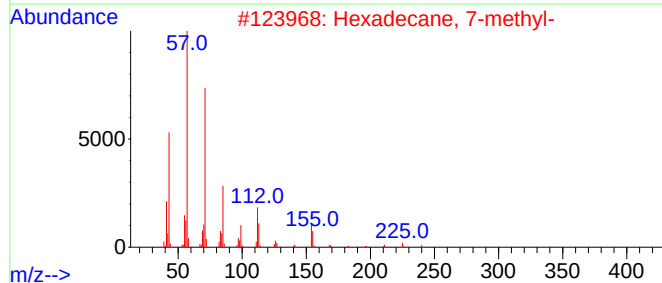
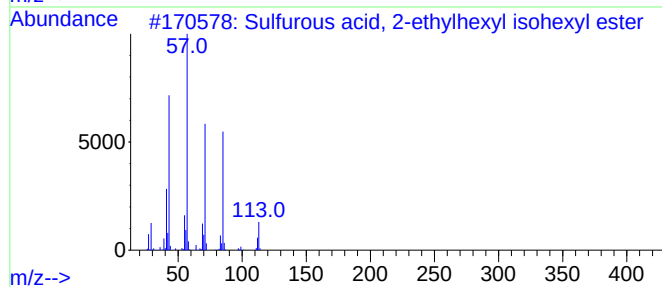
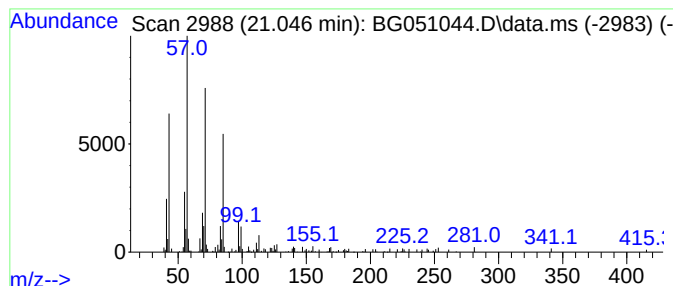
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Sulfurous acid, 2-ethylhexy... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.046	5.39 ng	175615	Chrysene-d12	21.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	72
2			Hexadecane, 7-methyl-	240	C17H36	026730-20-1	68
3			Sulfurous acid, 2-ethylhexyl pen...	404	C23H48O3S	1000309-19-8	68
4			Heptacosane	380	C27H56	000593-49-7	64
5			2,6,10-Trimethyltridecane	226	C16H34	003891-99-4	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111621\
Data File : BG051044.D
Acq On : 15 Nov 2021 16:40
Operator : CG/JU
Sample : M4595-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CMC-OF4-003-004

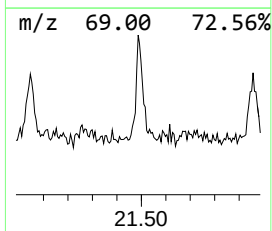
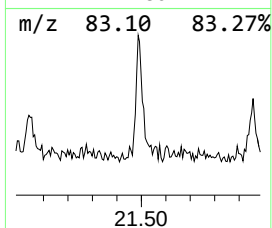
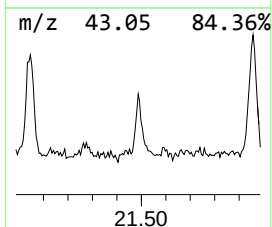
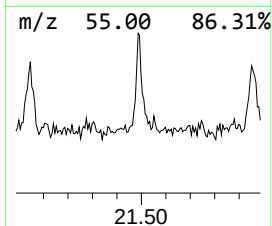
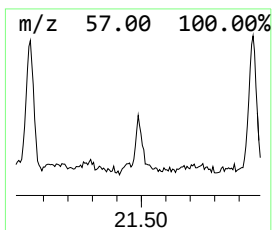
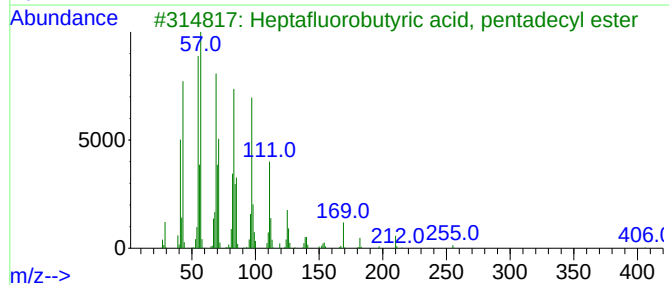
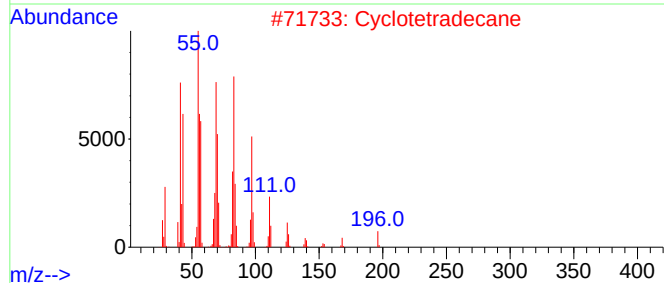
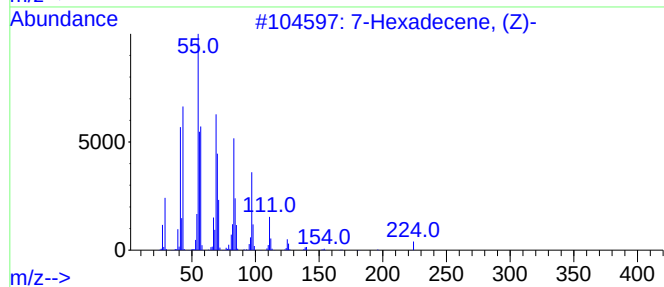
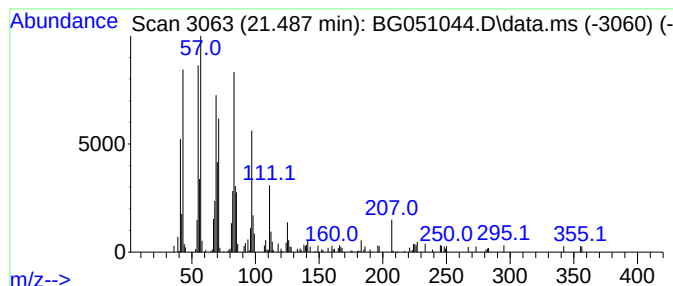
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 7-Hexadecene, (Z)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.487	4.18 ng	136139	Chrysene-d12	21.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			7-Hexadecene, (Z)-	224	C16H32	035507-09-6	97
2			Cyclotetradecane	196	C14H28	000295-17-0	93
3			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
4			2-Tetradecene, (E)-	196	C14H28	035953-54-9	91
5			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111621\
Data File : BG051044.D
Acq On : 15 Nov 2021 16:40
Operator : CG/JU
Sample : M4595-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CMC-OF4-003-004

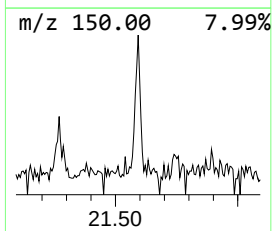
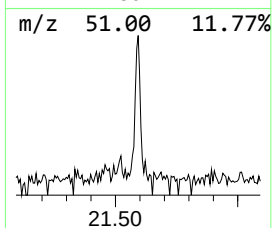
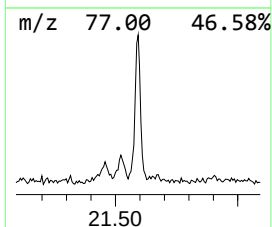
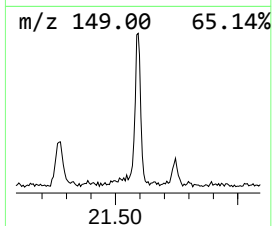
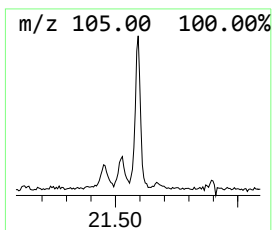
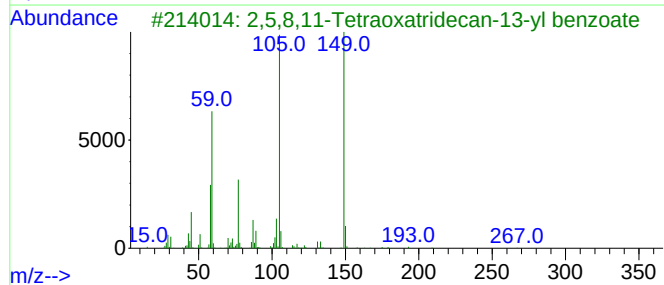
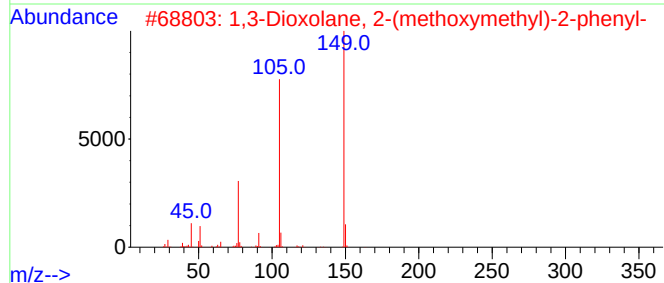
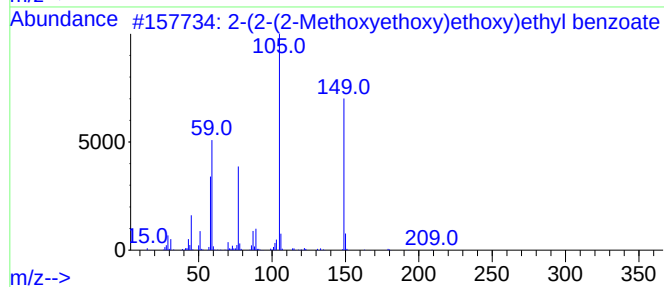
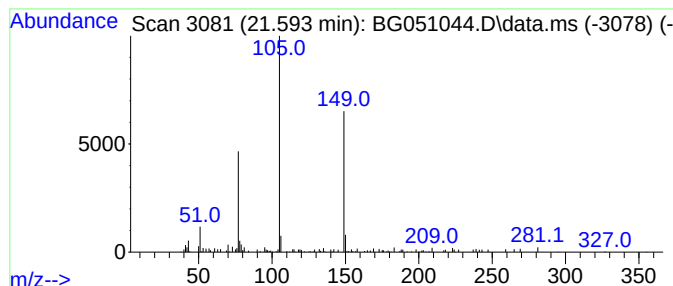
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 2-(2-(2-Methoxyethoxy)ethox... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.593	2.01 ng	65315	Chrysene-d12	21.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(2-(2-Methoxyethoxy)ethoxy)eth...	268	C14H20O5	1000366-99-1	50		
2	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	50		
3	2,5,8,11-Tetraoxatridecan-13-yl ...	312	C16H24O6	1000366-96-7	47		
4	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	47		
5	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	43		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111621\
Data File : BG051044.D
Acq On : 15 Nov 2021 16:40
Operator : CG/JU
Sample : M4595-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CMC-OF4-003-004

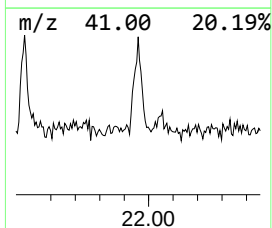
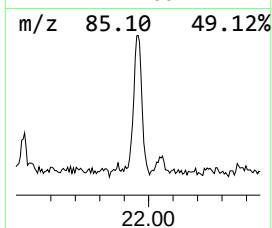
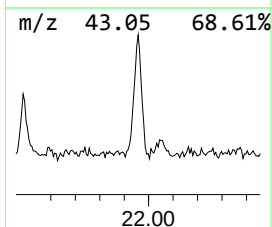
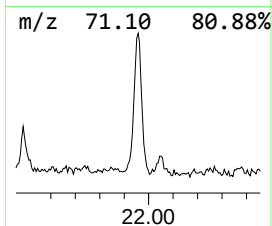
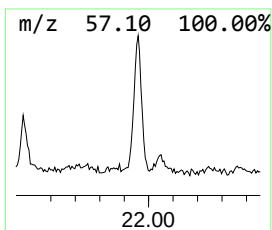
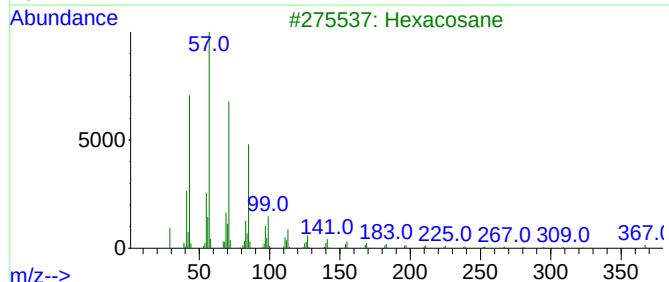
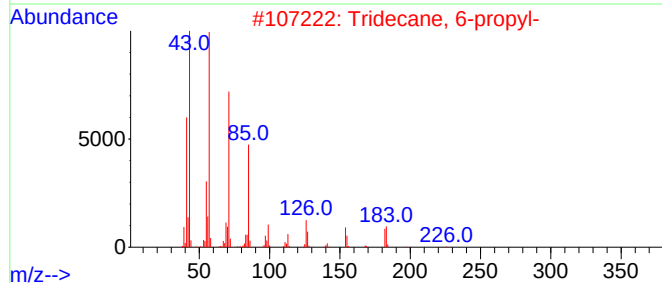
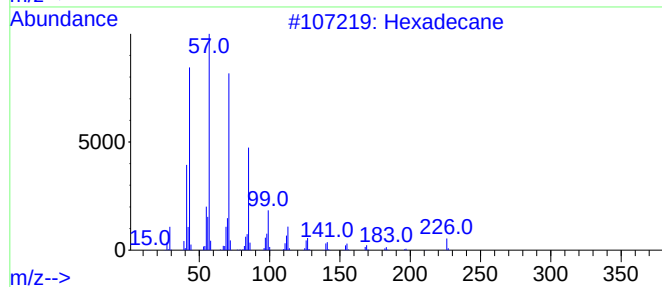
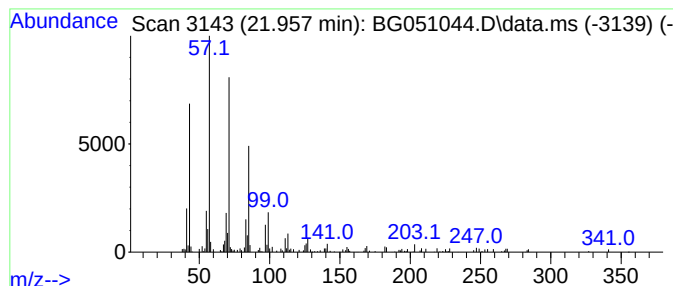
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.957	6.60 ng	214845	Chrysene-d12	21.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane	226	C16H34	000544-76-3	87
2			Tridecane, 6-propyl-	226	C16H34	055045-10-8	87
3			Hexacosane	366	C26H54	000630-01-3	87
4			Docosane	310	C22H46	000629-97-0	86
5			Eicosane, 7-hexyl-	366	C26H54	055333-99-8	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111621\
Data File : BG051044.D
Acq On : 15 Nov 2021 16:40
Operator : CG/JU
Sample : M4595-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CMC-OF4-003-004

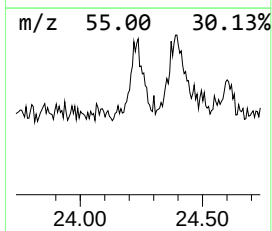
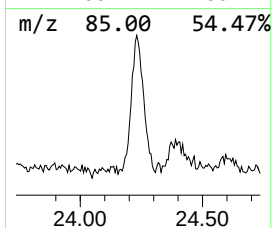
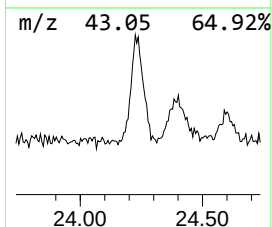
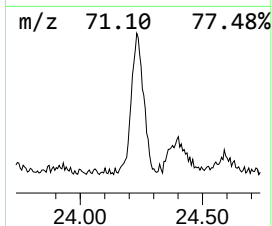
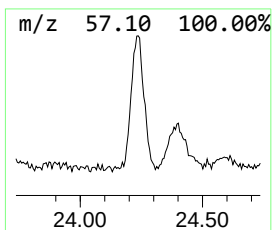
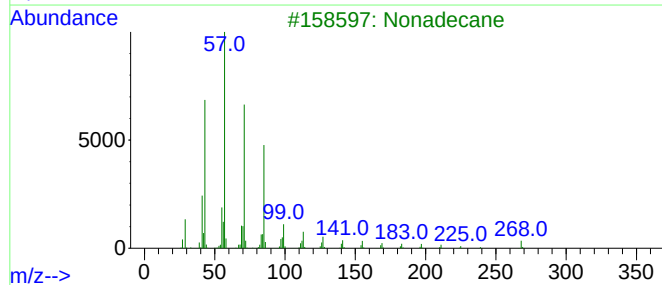
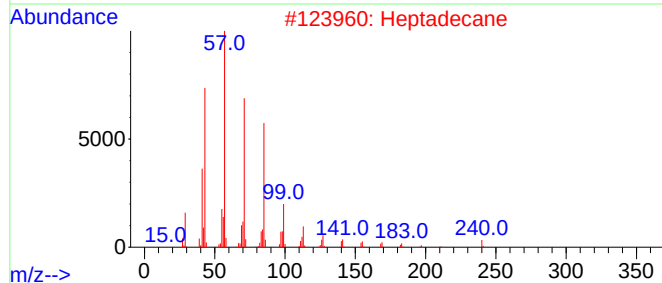
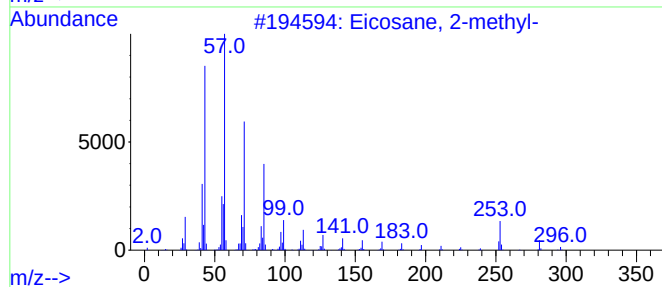
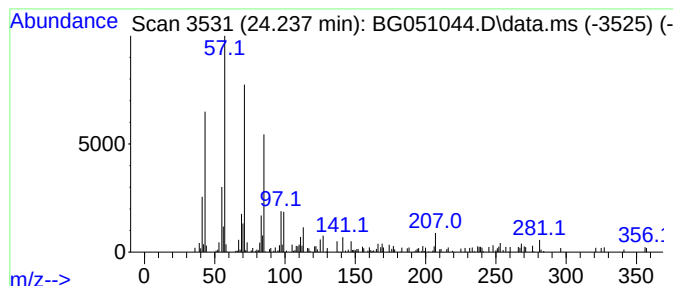
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Eicosane, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.237	6.89 ng	246383	Perylene-d12	25.306

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Eicosane, 2-methyl-	296	C21H44	001560-84-5	93
2		Heptadecane	240	C17H36	000629-78-7	90
3		Nonadecane	268	C19H40	000629-92-5	90
4		Heneicosane	296	C21H44	000629-94-7	89
5		Eicosane	282	C20H42	000112-95-8	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111621\
Data File : BG051044.D
Acq On : 15 Nov 2021 16:40
Operator : CG/JU
Sample : M4595-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CMC-OF4-003-004

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111321.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-...	5.300	8.2	ng	108856	1	8.226	264981	20.0
Ethanol, 2-(2-b...	10.805	13.0	ng	251978	2	11.052	388271	20.0
Oxybis(propane-...	17.873	24.9	ng	1151760	4	17.597	924458	20.0
1,3-Dioxolane, ...	18.056	48.9	ng	2261500	4	17.597	924458	20.0
Pentacosane	19.213	3.1	ng	145097	4	17.597	924458	20.0
Sulfurous acid,...	21.046	5.4	ng	175615	5	21.898	651047	20.0
7-Hexadecene, (Z)-	21.487	4.2	ng	136139	5	21.898	651047	20.0
2-(2-(2-Methoxy...	21.593	2.0	ng	65315	5	21.898	651047	20.0
Hexadecane	21.957	6.6	ng	214845	5	21.898	651047	20.0
Eicosane, 2-met...	24.237	6.9	ng	246383	6	25.306	714779	20.0