

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112021\
 Data File : BG051157.D
 Acq On : 20 Nov 2021 21:20
 Operator : CG/JU
 Sample : M4758-29
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TP15

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-BG111921.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG051157.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.740	376	383	400	rVB	412080	685106	45.57%	8.837%
2	7.356	649	658	674	rBV	410073	734831	48.88%	9.478%
3	8.202	795	802	812	rBV	92629	159249	10.59%	2.054%
4	9.377	994	1002	1016	rBV	258033	463543	30.83%	5.979%
5	10.781	1235	1241	1249	rBV2	9018	18968	1.26%	0.245%
6	11.028	1276	1283	1292	rBV	115987	221568	14.74%	2.858%
7	13.455	1685	1696	1703	rBV	604949	928005	61.73%	11.970%
8	13.702	1729	1738	1745	rVB3	18939	32000	2.13%	0.413%
9	14.836	1921	1931	1939	rVB	190539	307539	20.46%	3.967%
10	16.322	2178	2184	2200	rBV	460892	727686	48.40%	9.386%
11	17.450	2372	2376	2382	rVB2	13748	17637	1.17%	0.227%
12	17.579	2392	2398	2406	rBV	242287	384282	25.56%	4.957%
13	17.685	2412	2416	2420	rVB3	11608	15820	1.05%	0.204%
14	18.208	2501	2505	2511	rVB2	15945	18240	1.21%	0.235%
15	19.277	2683	2687	2694	rBV4	10231	16213	1.08%	0.209%
16	19.371	2700	2703	2707	rVB	40777	45405	3.02%	0.586%
17	19.501	2721	2725	2729	rBV2	14011	15963	1.06%	0.206%
18	20.170	2834	2839	2845	rBV	1120880	1503428	100.00%	19.392%
19	20.447	2883	2886	2890	rVB	20191	22699	1.51%	0.293%
20	20.787	2941	2944	2949	rBV4	12480	15124	1.01%	0.195%
21	20.946	2967	2971	2977	rVB3	21425	25362	1.69%	0.327%
22	21.469	3050	3060	3064	rBV3	80493	167979	11.17%	2.167%
23	21.575	3073	3078	3087	rVB	67920	100112	6.66%	1.291%
24	21.880	3123	3130	3140	rBV	266391	458506	30.50%	5.914%
25	22.033	3152	3156	3163	rVB3	12438	18864	1.25%	0.243%
26	22.662	3260	3263	3268	rBV3	10008	16422	1.09%	0.212%
27	23.390	3382	3387	3394	rVB4	15298	29461	1.96%	0.380%
28	23.584	3417	3420	3430	rVB2	13088	25950	1.73%	0.335%
29	24.230	3525	3530	3537	rVB3	14081	30235	2.01%	0.390%
30	25.282	3695	3709	3721	rVB2	147654	494269	32.88%	6.375%
31	26.422	3895	3903	3914	rVB6	15868	52172	3.47%	0.673%

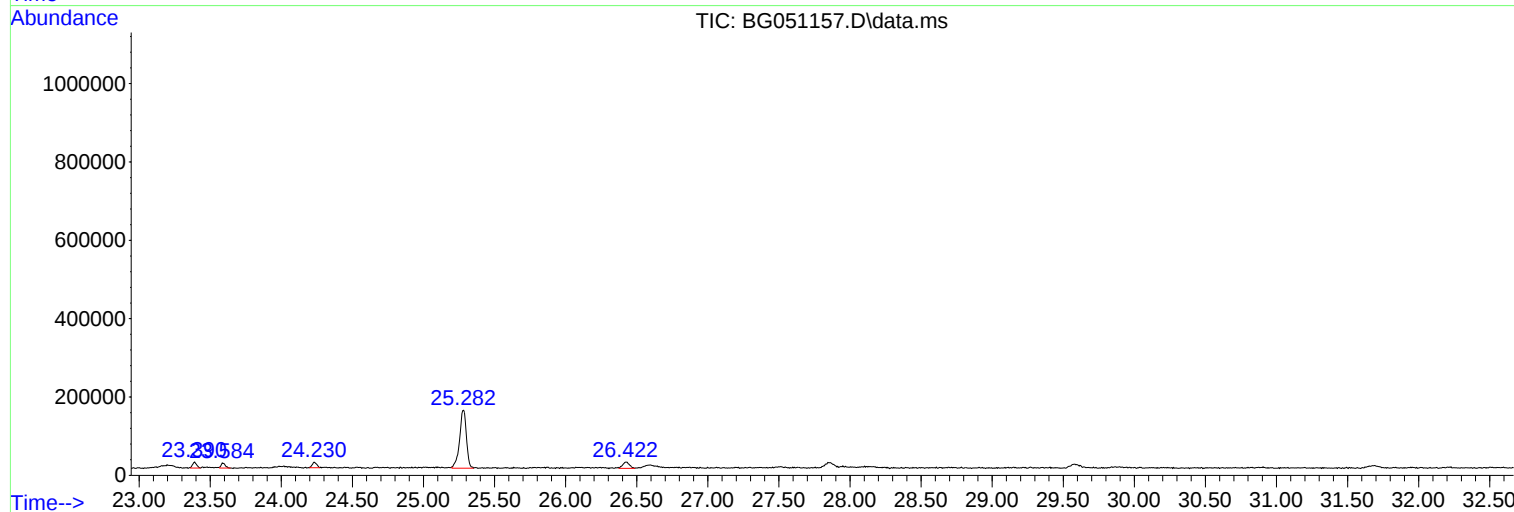
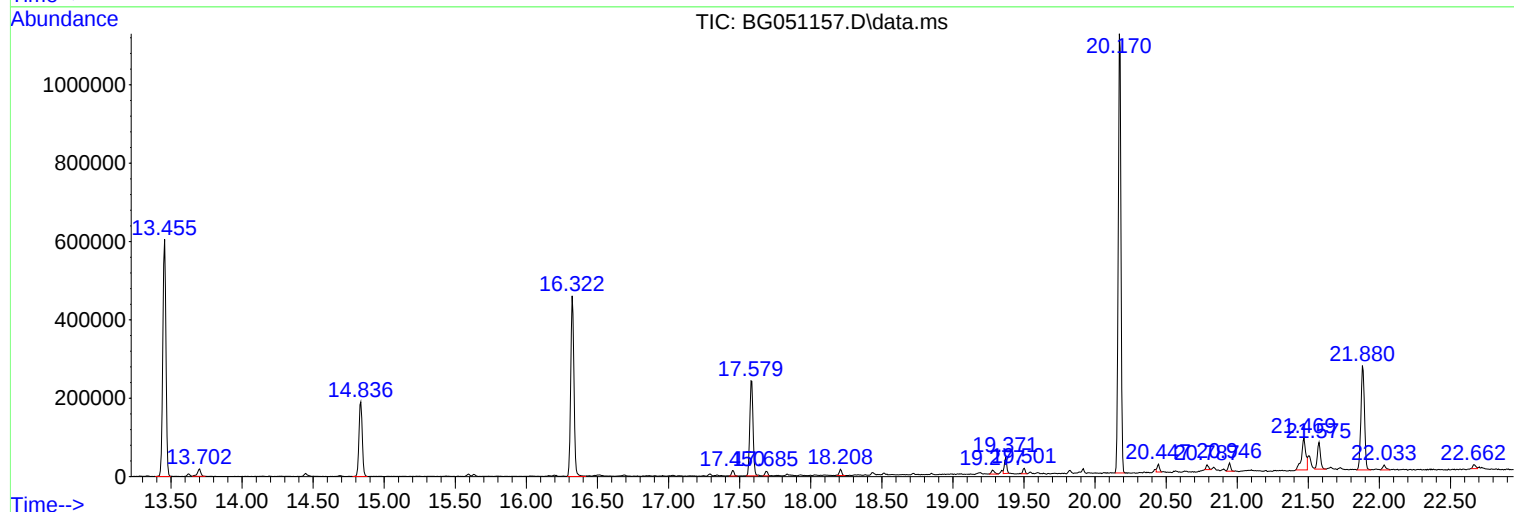
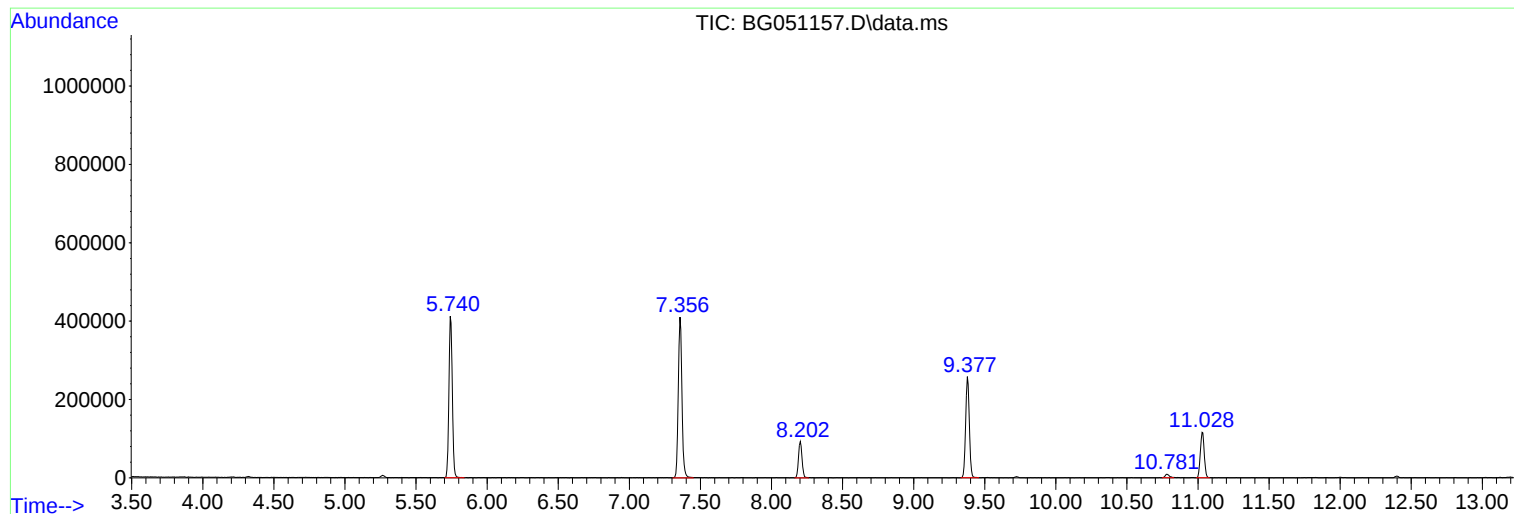
Sum of corrected areas: 7752638

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112021\
Data File : BG051157.D
Acq On : 20 Nov 2021 21:20
Operator : CG/JU
Sample : M4758-29
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP15

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111921.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\BG112021\
Data File : BG051157.D
Acq On : 20 Nov 2021 21:20
Operator : CG/JU
Sample : M4758-29
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP15

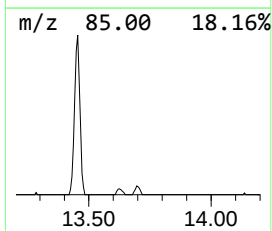
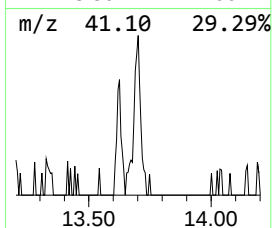
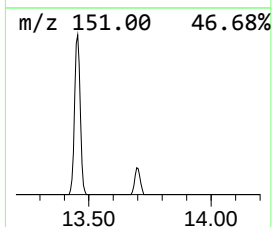
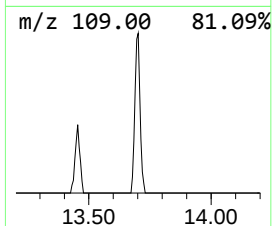
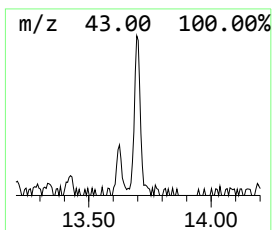
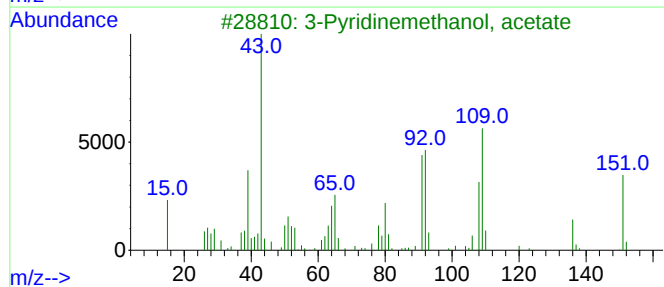
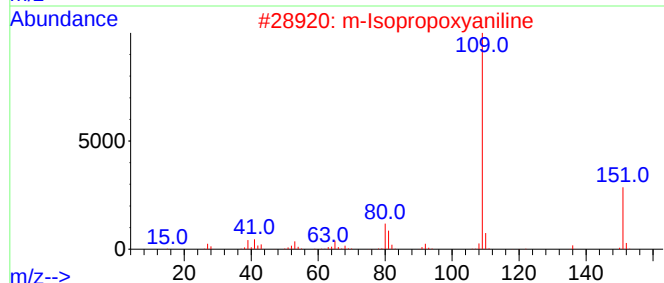
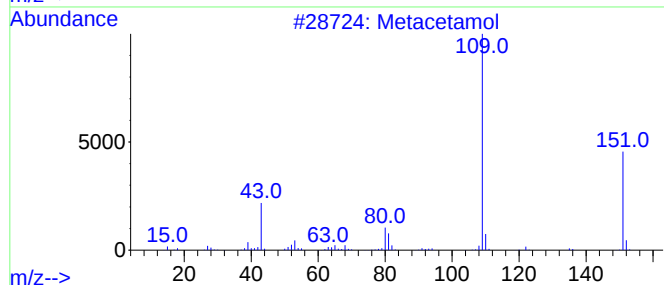
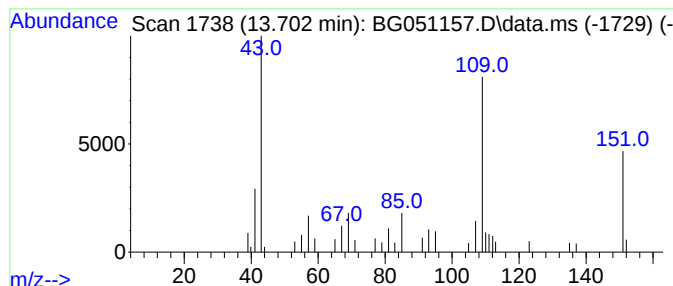
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Metacetamol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.702	2.08 ng	32000	Acenaphthene-d10	14.836

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Metacetamol	151	C8H9NO2	000621-42-1	59
2			m-Isopropoxyaniline	151	C9H13NO	041406-00-2	59
3			3-Pyridinemethanol, acetate	151	C8H9NO2	010072-09-0	59
4			Acetaminophen	151	C8H9NO2	000103-90-2	59
5			(-)-10-Camphorsulfonyl chloride	250	C10H15ClO3S	039262-22-1	56



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112021\
Data File : BG051157.D
Acq On : 20 Nov 2021 21:20
Operator : CG/JU
Sample : M4758-29
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP15

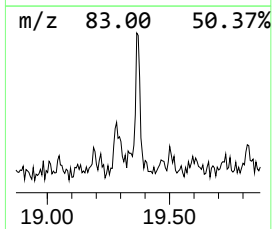
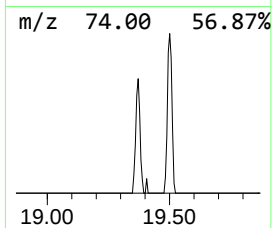
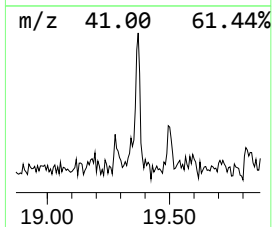
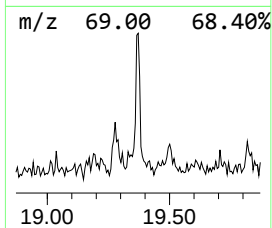
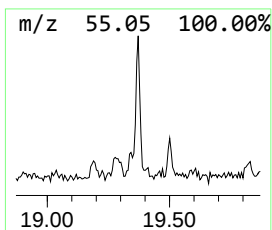
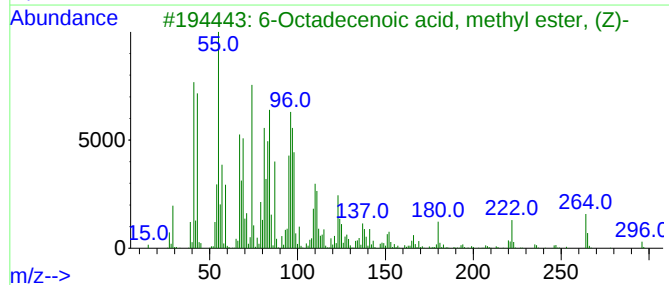
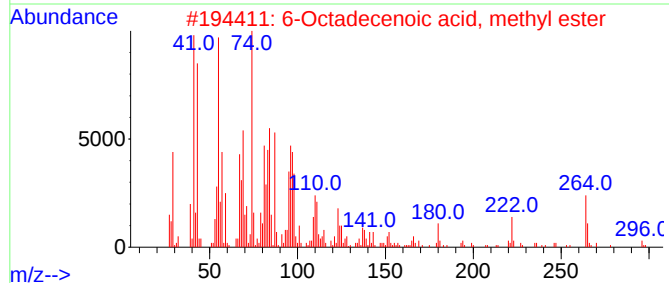
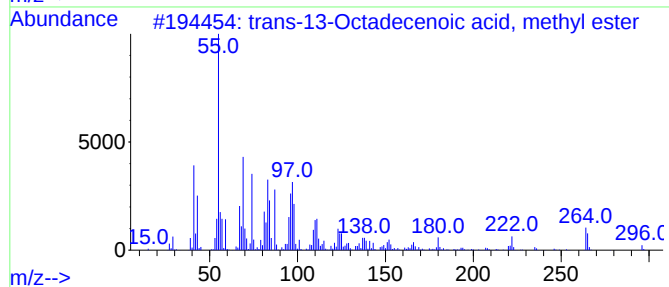
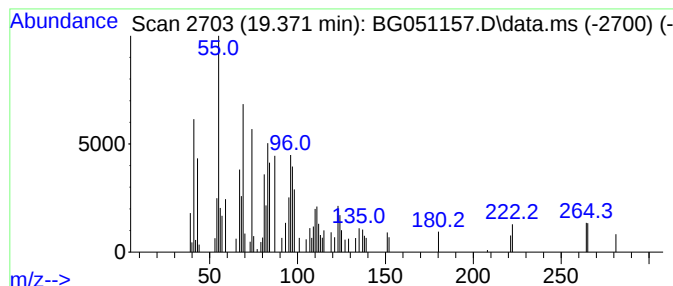
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 trans-13-Octadecenoic acid,... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.371	2.36 ng	45405	Phenanthrene-d10	17.585

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	91
2			6-Octadecenoic acid, methyl ester	296	C19H36O2	052355-31-4	91
3			6-Octadecenoic acid, methyl este...	296	C19H36O2	002777-58-4	90
4			9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	90
5			13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112021\
Data File : BG051157.D
Acq On : 20 Nov 2021 21:20
Operator : CG/JU
Sample : M4758-29
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP15

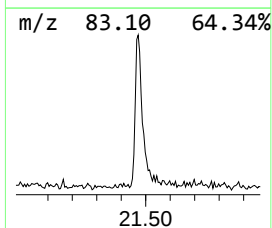
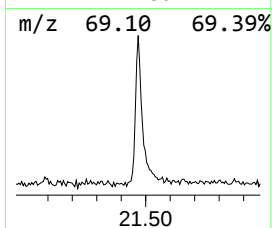
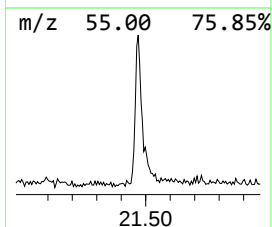
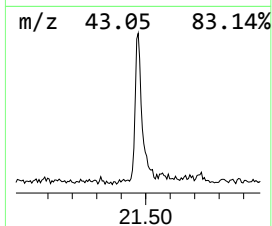
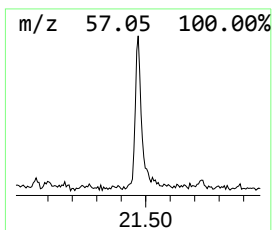
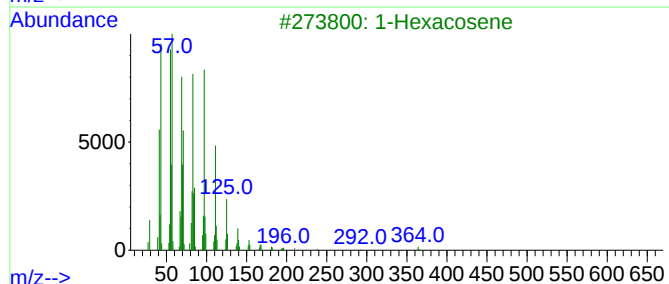
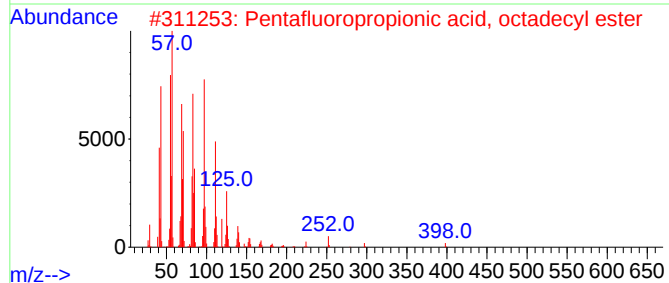
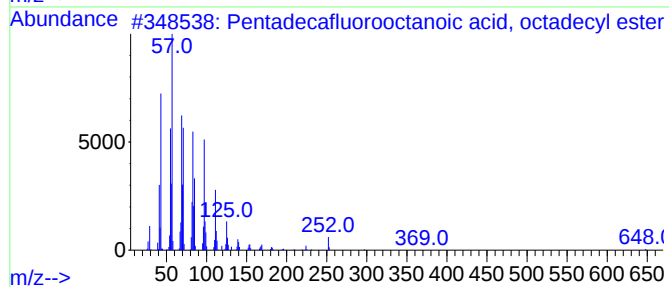
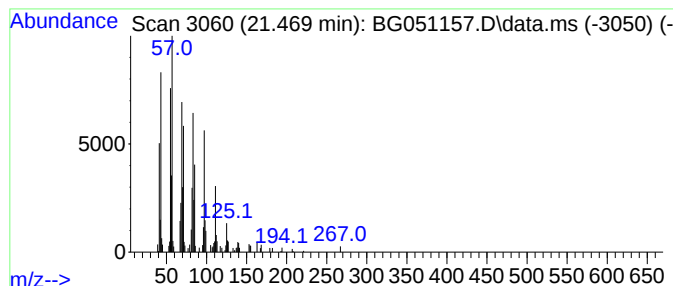
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Pentadecafluorooctanoic aci... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.469	7.33 ng	167979	Chrysene-d12	21.880

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	95
2			Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	90
3			1-Hexacosene	364	C26H52	018835-33-1	87
4			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	87
5			Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112021\
Data File : BG051157.D
Acq On : 20 Nov 2021 21:20
Operator : CG/JU
Sample : M4758-29
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP15

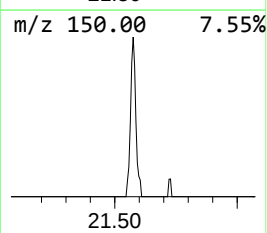
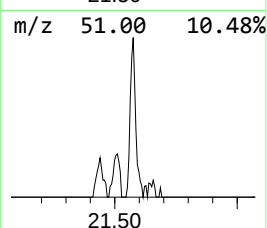
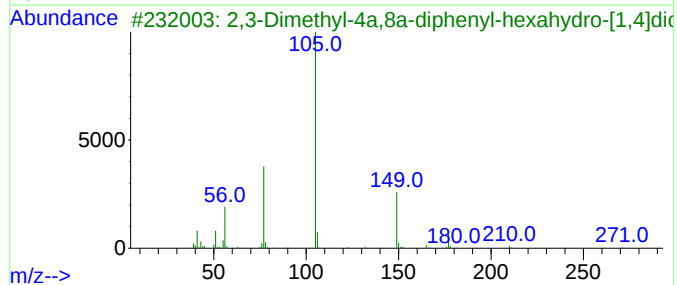
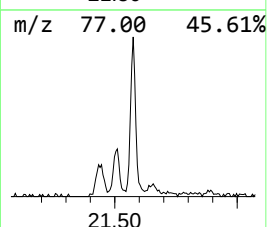
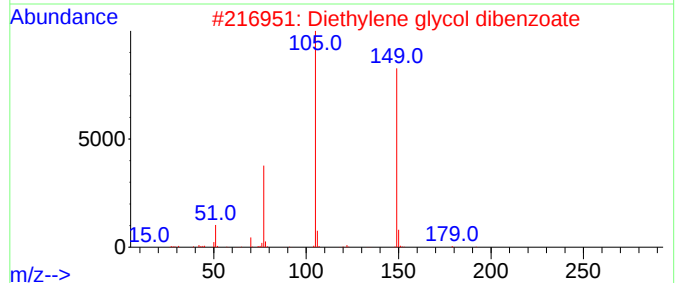
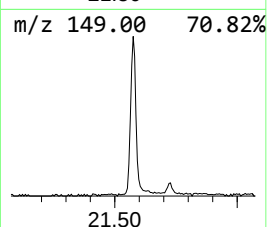
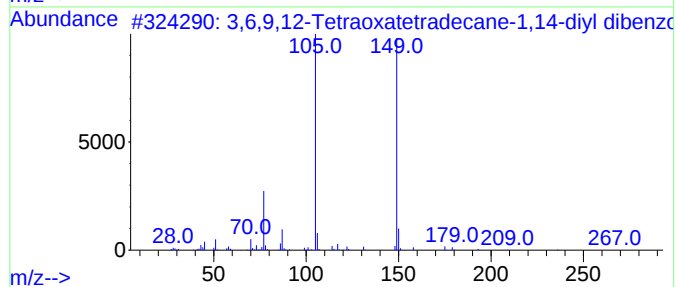
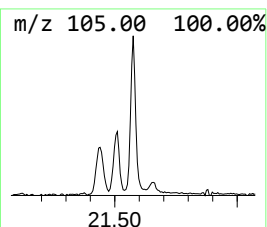
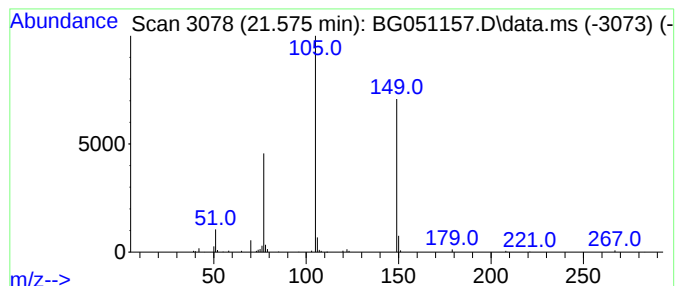
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 3,6,9,12-Tetraoxatetradecan... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.575	4.37 ng	100112	Chrysene-d12	21.880

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,6,9,12-Tetraoxatetradecane-1,1...	446	C24H30O8	1000366-97-0	83		
2	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	83		
3	2,3-Dimethyl-4a,8a-diphenyl-hexa...	326	C20H22O4	1000297-07-0	59		
4	2-Propen-1-one, 1,2-diphenyl-	208	C15H12O	004452-11-3	47		
5	Benzoic acid, (4-nitrophenyl)-me...	269	C14H11N3O3	028123-77-5	47		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112021\
Data File : BG051157.D
Acq On : 20 Nov 2021 21:20
Operator : CG/JU
Sample : M4758-29
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP15

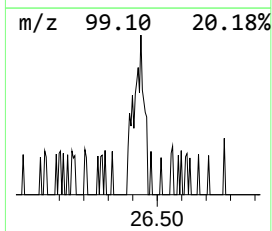
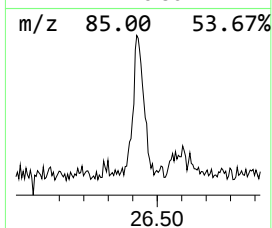
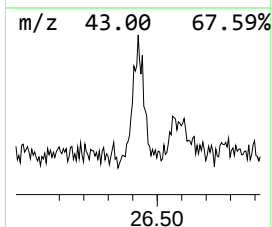
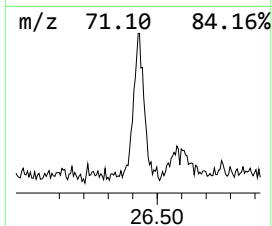
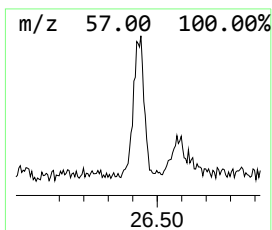
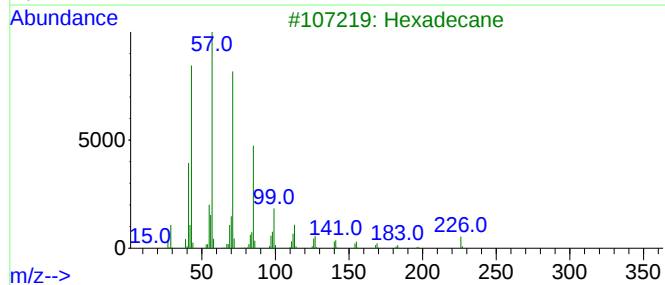
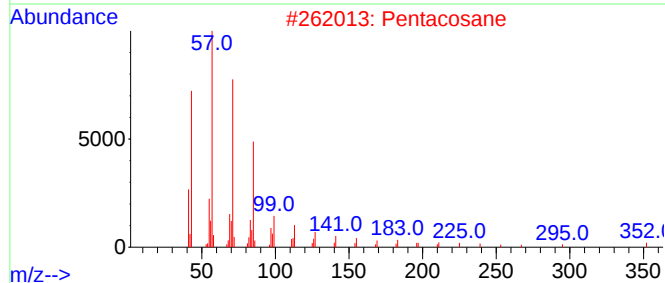
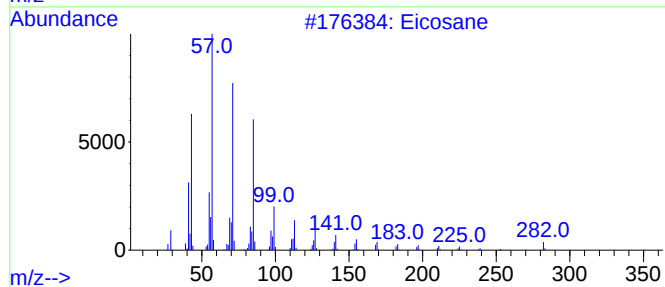
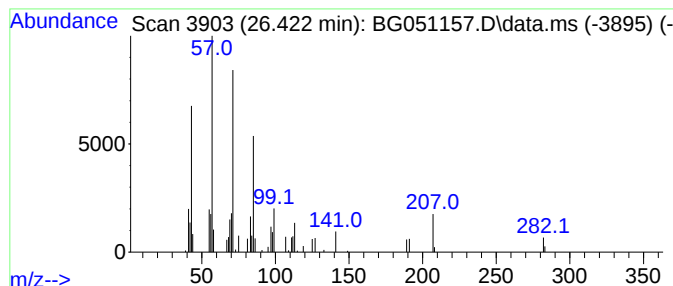
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Eicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.422	2.11 ng	52172	Perylene-d12	25.276

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	94
2			Pentacosane	352	C25H52	000629-99-2	87
3			Hexadecane	226	C16H34	000544-76-3	87
4			Octacosane	394	C28H58	000630-02-4	87
5			Hexacosane	366	C26H54	000630-01-3	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112021\
Data File : BG051157.D
Acq On : 20 Nov 2021 21:20
Operator : CG/JU
Sample : M4758-29
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP15

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111921.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
Metacetamol	13.702	2.1	ng	32000	3	14.836	307539	20.0
trans-13-Octade...	19.371	2.4	ng	45405	4	17.585	384282	20.0
Pentadecafluoro...	21.469	7.3	ng	167979	5	21.880	458506	20.0
3,6,9,12-Tetrao...	21.575	4.4	ng	100112	5	21.880	458506	20.0
Eicosane	26.422	2.1	ng	52172	6	25.276	494269	20.0