

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111921\
 Data File : BG051136.D
 Acq On : 20 Nov 2021 00:07
 Operator : CG/JU
 Sample : M4758-05
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TP3

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: BG051136.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.267	298	303	312	rVB2	11153	17295	1.01%	0.220%
2	5.743	378	384	397	rBV	370198	616069	36.08%	7.847%
3	7.359	651	659	672	rBV	375394	691914	40.52%	8.813%
4	8.205	796	803	810	rBV	93505	156978	9.19%	2.000%
5	9.380	995	1003	1013	rBV	236177	435595	25.51%	5.549%
6	10.779	1235	1241	1250	rBV2	11923	24357	1.43%	0.310%
7	11.031	1277	1284	1292	rBV	129255	228217	13.37%	2.907%
8	13.458	1686	1697	1706	rBV	641910	1017547	59.59%	12.961%
9	14.451	1859	1866	1876	rBV2	9302	18690	1.09%	0.238%
10	14.833	1922	1931	1939	rVB	221898	352154	20.62%	4.486%
11	16.325	2178	2185	2195	rBV	540847	859626	50.35%	10.950%
12	17.453	2368	2377	2382	rBV2	19836	26667	1.56%	0.340%
13	17.582	2392	2399	2410	rVB	306670	485772	28.45%	6.188%
14	20.168	2834	2839	2845	rVB	1284819	1707451	100.00%	21.749%
15	21.466	3055	3060	3073	rVB3	70129	140708	8.24%	1.792%
16	21.566	3073	3077	3082	rBV	14907	22665	1.33%	0.289%
17	21.877	3123	3130	3139	rVB2	285909	487708	28.56%	6.212%
18	24.222	3526	3529	3536	rVB5	11543	22427	1.31%	0.286%
19	25.273	3692	3708	3720	rBV2	159827	502045	29.40%	6.395%
20	26.407	3895	3901	3910	rVB5	12947	36759	2.15%	0.468%

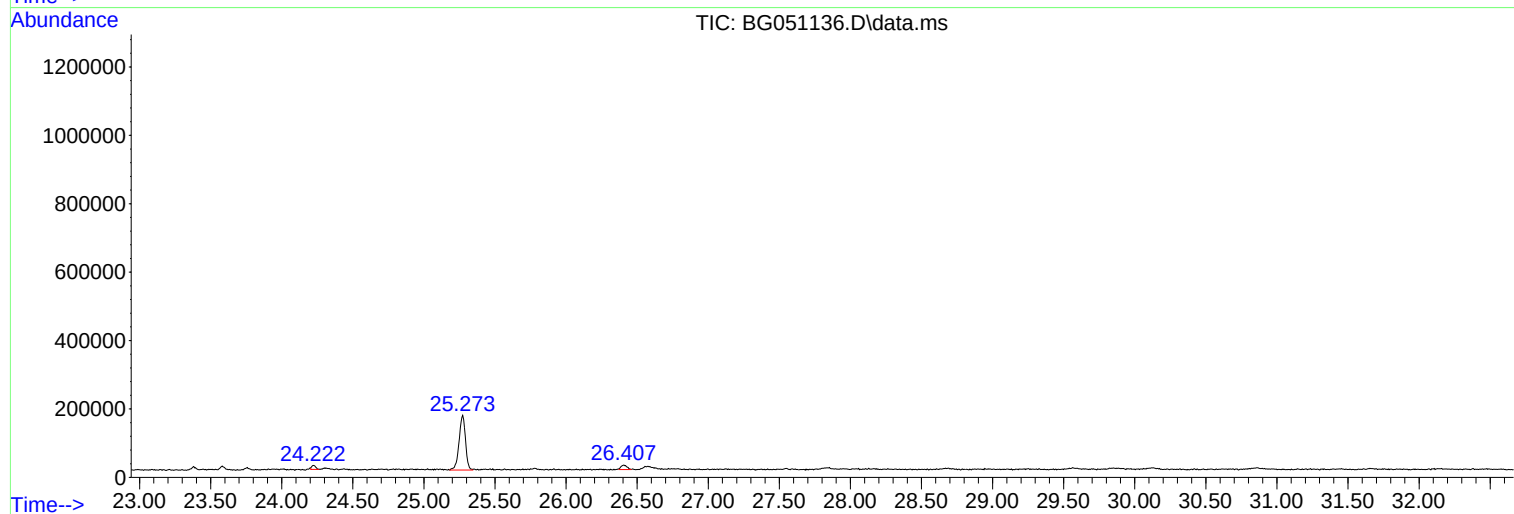
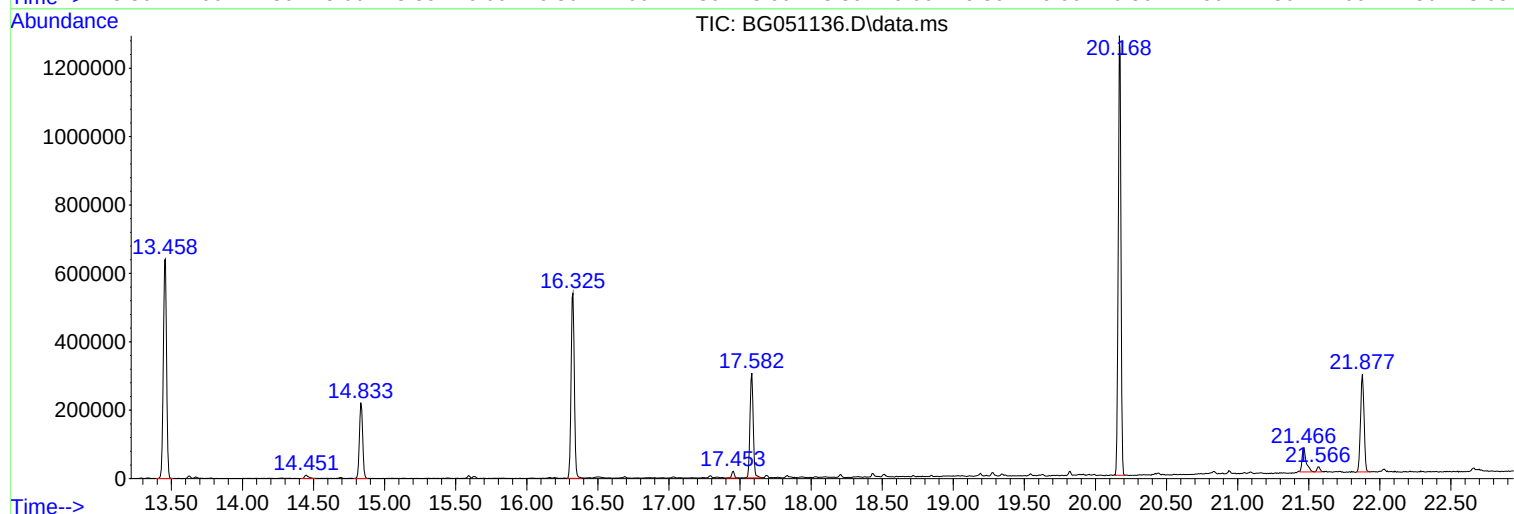
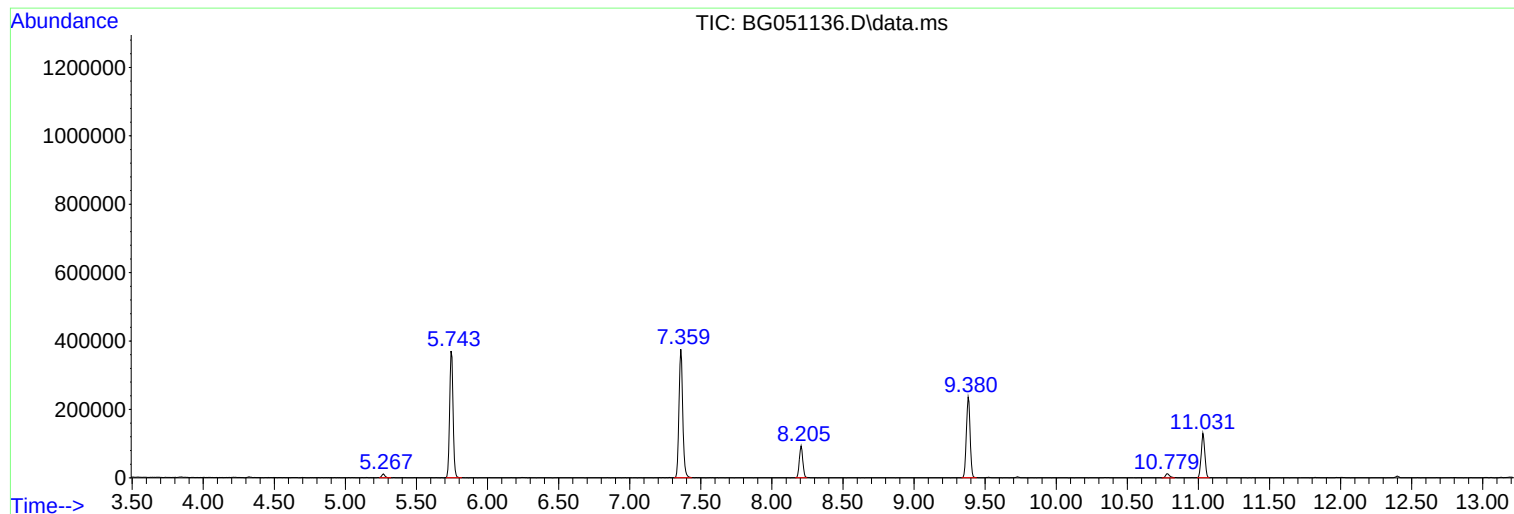
Sum of corrected areas: 7850644

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111921\
Data File : BG051136.D
Acq On : 20 Nov 2021 00:07
Operator : CG/JU
Sample : M4758-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP3

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\BG111921\
Data File : BG051136.D
Acq On : 20 Nov 2021 00:07
Operator : CG/JU
Sample : M4758-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP3

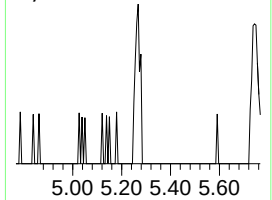
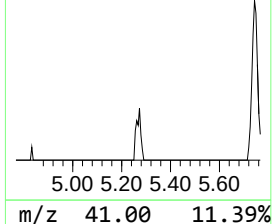
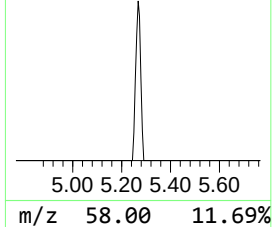
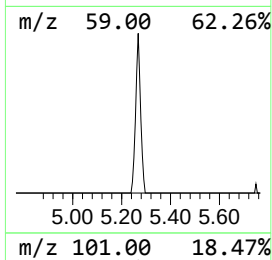
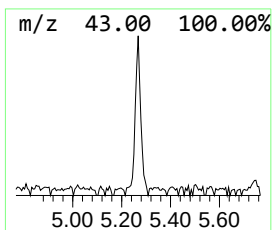
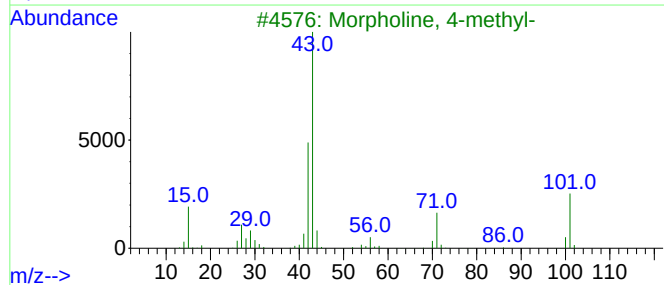
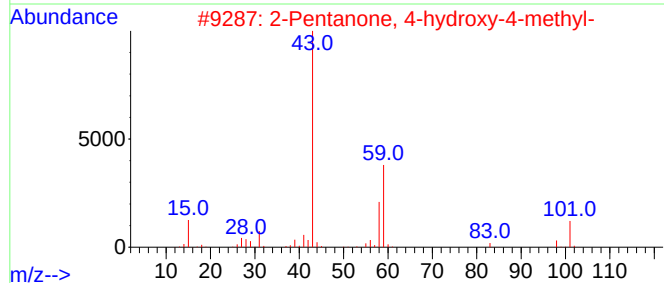
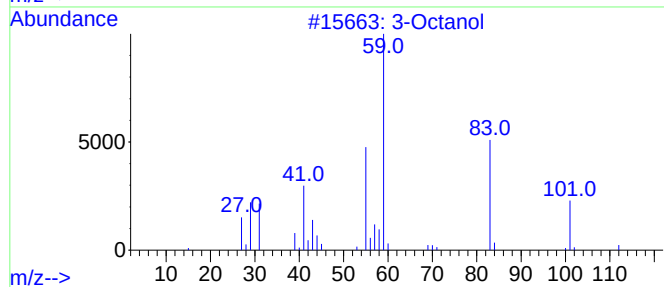
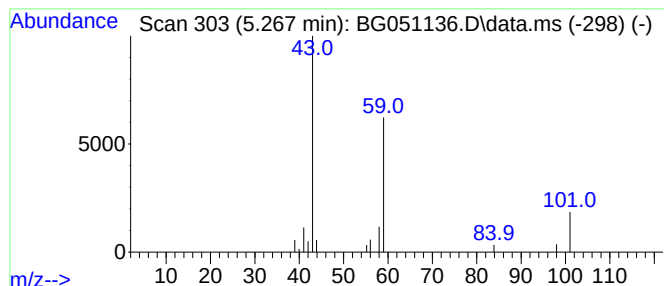
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Octanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.267	2.20 ng	17295	1,4-Dichlorobenzene-d4	8.205

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Octanol	130	C8H18O	000589-98-0	59
2			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
3			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			3-Hexanol	102	C6H14O	000623-37-0	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111921\
Data File : BG051136.D
Acq On : 20 Nov 2021 00:07
Operator : CG/JU
Sample : M4758-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP3

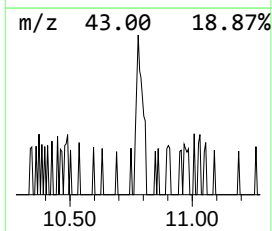
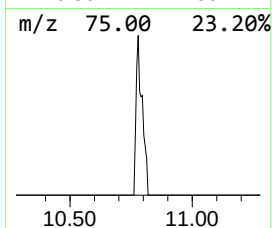
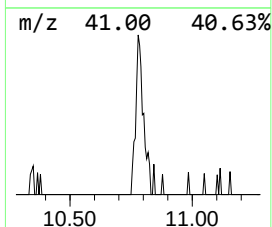
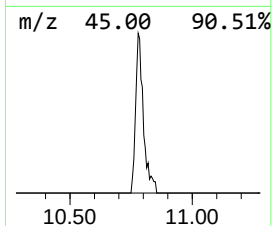
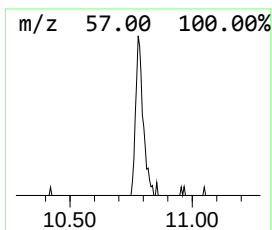
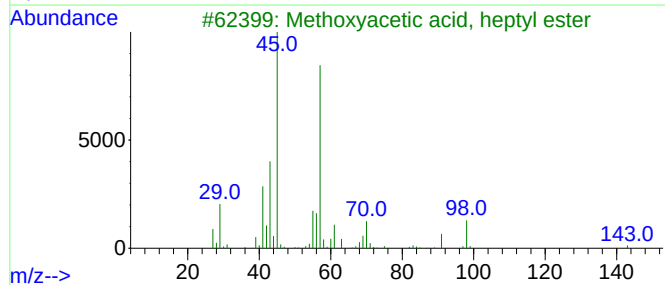
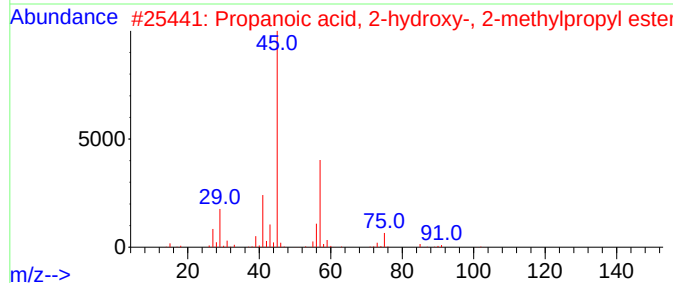
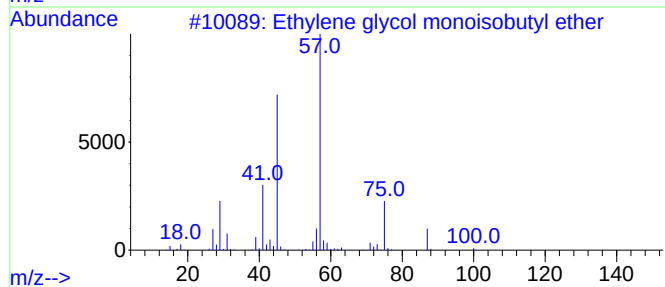
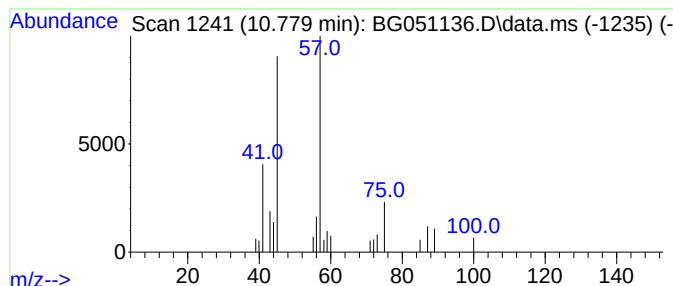
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Ethylene glycol monoisobuty... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.779	2.13 ng	24357	Naphthalene-d8	11.031

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
2			Propanoic acid, 2-hydroxy-, 2-me...	146	C7H14O3	000585-24-0	32
3			Methoxyacetic acid, heptyl ester	188	C10H20O3	168920-36-3	25
4			1,3-Propanediol, 2-(hydroxymethy...	120	C5H12O3	000077-85-0	10
5			1-Methoxy-3-methyl-3-butene	100	C6H12O	034752-58-4	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111921\
Data File : BG051136.D
Acq On : 20 Nov 2021 00:07
Operator : CG/JU
Sample : M4758-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP3

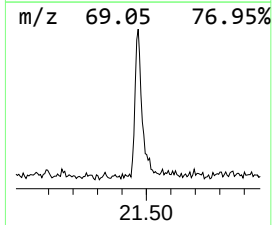
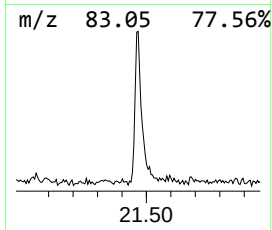
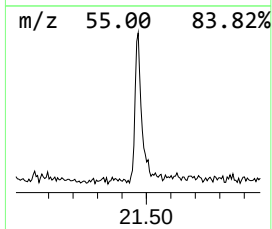
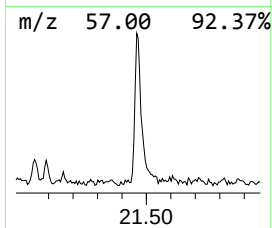
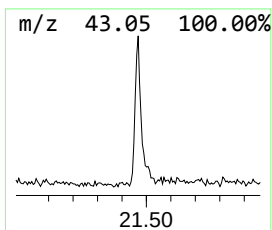
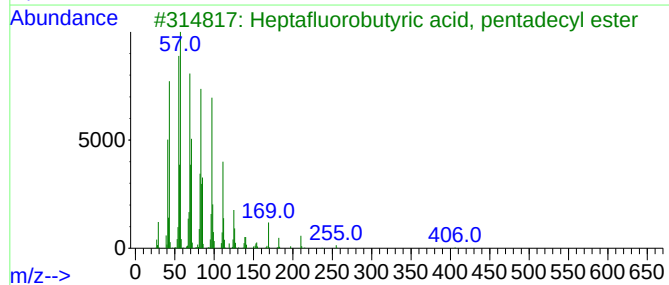
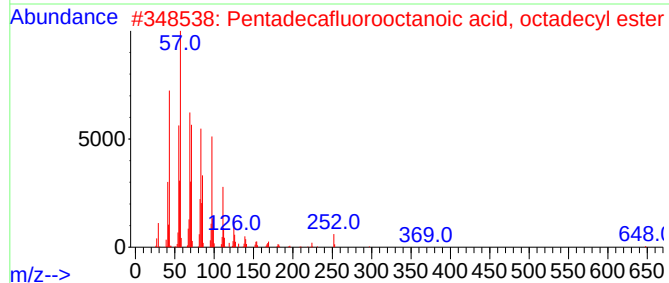
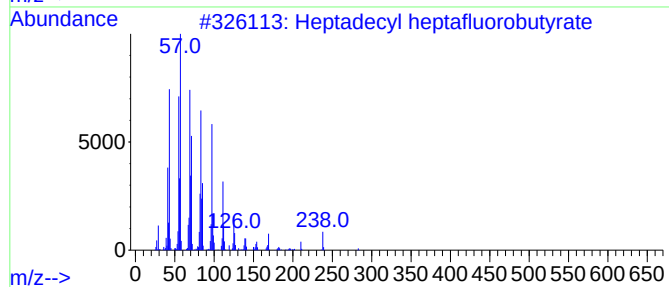
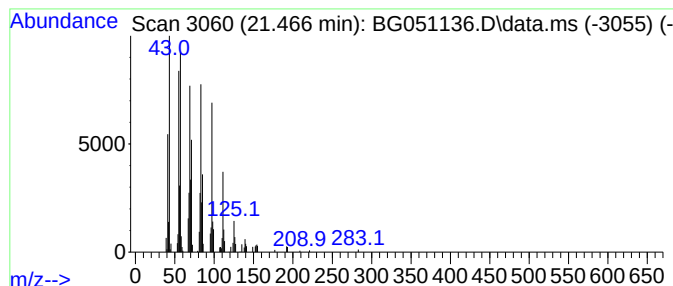
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Heptadecyl heptafluorobutyrate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.466	5.77 ng	140708	Chrysene-d12	21.877

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	93
3			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
4			1-Tetracosene	336	C24H48	010192-32-2	91
5			1-Hexacosene	364	C26H52	018835-33-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111921\
Data File : BG051136.D
Acq On : 20 Nov 2021 00:07
Operator : CG/JU
Sample : M4758-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP3

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
3-Octanol	5.267	2.2	ng	17295	1	8.205	156978	20.0
Ethylene glycol...	10.779	2.1	ng	24357	2	11.031	228217	20.0
Heptadecyl hept...	21.466	5.8	ng	140708	5	21.877	487708	20.0