

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012121\
 Data File : BG047966.D
 Acq On : 21 Jan 2021 23:26
 Operator : CG/JU
 Sample : M1177-03
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PILE-2-(0.5-1.0)

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-BG012121.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG047966.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.700	393	402	415	rVB	801073	1247201	42.12%	7.748%
2	7.293	664	673	685	rBV	806428	1407192	47.52%	8.742%
3	8.145	811	818	825	rBV	182576	309588	10.46%	1.923%
4	9.308	1006	1016	1024	rBV	485534	847624	28.63%	5.266%
5	10.965	1288	1298	1304	rBV	249440	443351	14.97%	2.754%
6	13.397	1703	1712	1719	rBV	1240908	1879558	63.47%	11.677%
7	14.214	1845	1851	1857	rBV	59798	86949	2.94%	0.540%
8	14.772	1939	1946	1952	rVB2	409259	652309	22.03%	4.052%
9	16.253	2189	2198	2210	rBV	1107271	1682538	56.82%	10.453%
10	17.510	2406	2412	2419	rBV	564050	832345	28.11%	5.171%
11	18.391	2557	2562	2570	rBV	226444	319140	10.78%	1.983%
12	19.167	2688	2694	2698	rBV	151043	190400	6.43%	1.183%
13	19.249	2705	2708	2712	rBV	37679	47855	1.62%	0.297%
14	19.661	2773	2778	2787	rBV	135484	202563	6.84%	1.258%
15	19.796	2797	2801	2807	rVB	39830	55373	1.87%	0.344%
16	20.113	2849	2855	2860	rBV	2297211	2961123	100.00%	18.396%
17	20.800	2969	2972	2978	rVB3	28323	39296	1.33%	0.244%
18	21.024	3005	3010	3015	rBV	107767	142967	4.83%	0.888%
19	21.429	3074	3079	3089	rVB	208522	297922	10.06%	1.851%
20	21.793	3134	3141	3147	rBV	571937	953914	32.21%	5.926%
21	22.645	3283	3286	3293	rVB6	26625	48061	1.62%	0.299%
22	23.715	3463	3468	3474	rVB3	58312	100617	3.40%	0.625%
23	24.191	3544	3549	3554	rBV3	27279	59625	2.01%	0.370%
24	24.249	3554	3559	3567	rVB5	66912	152559	5.15%	0.948%
25	25.101	3694	3704	3714	rBV2	331043	931713	31.46%	5.788%
26	26.370	3917	3920	3928	rVB6	29886	61095	2.06%	0.380%
27	26.482	3931	3939	3950	rBV10	45465	143956	4.86%	0.894%

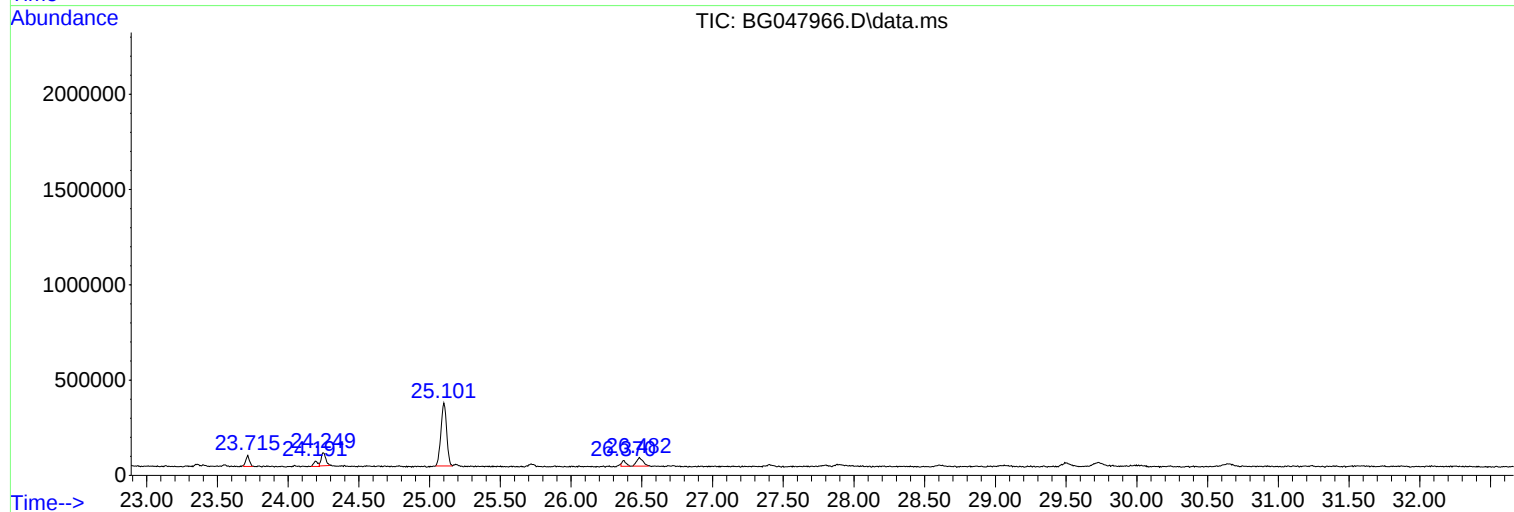
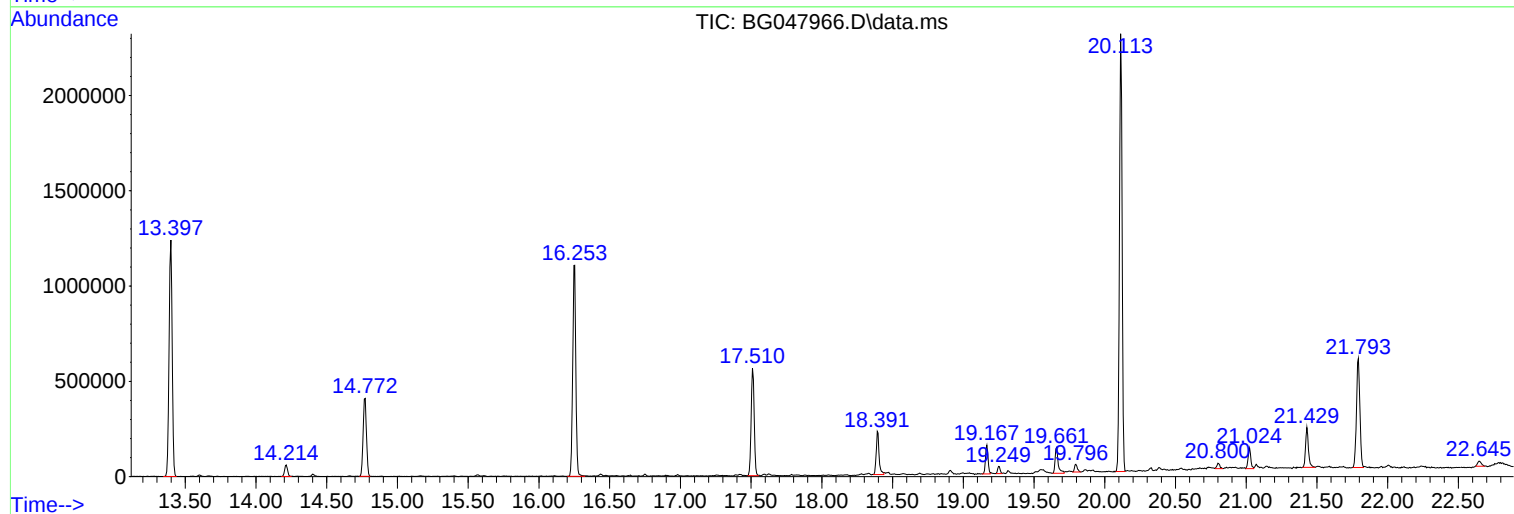
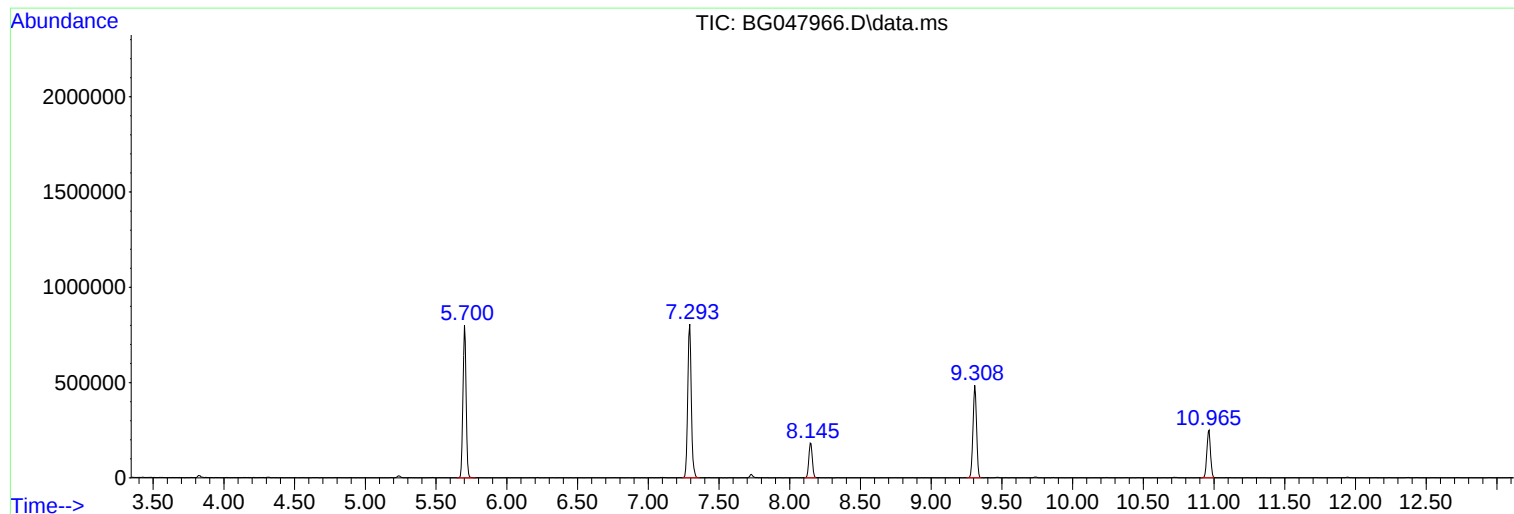
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ClientSampleId :
PILE-2-(0.5-1.0)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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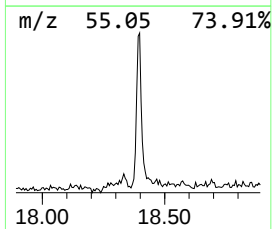
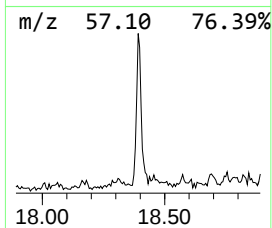
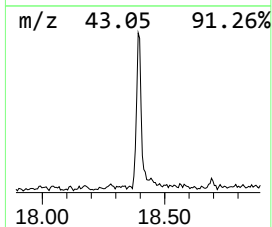
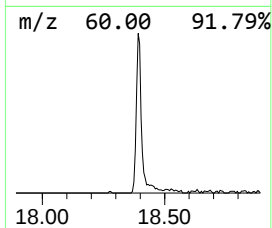
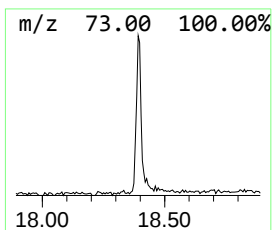
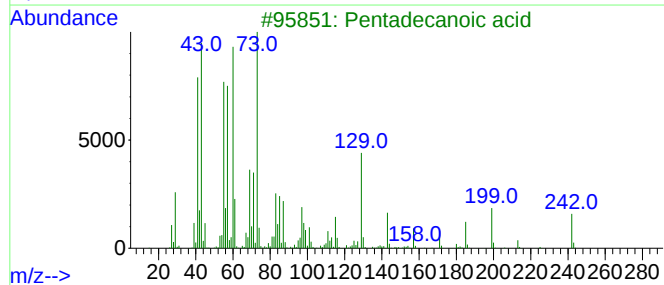
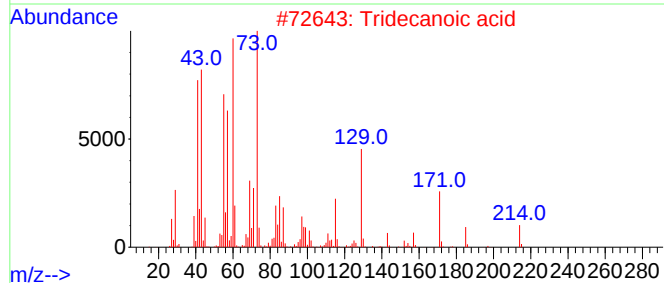
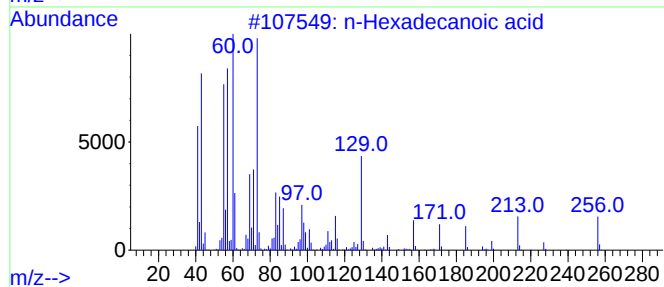
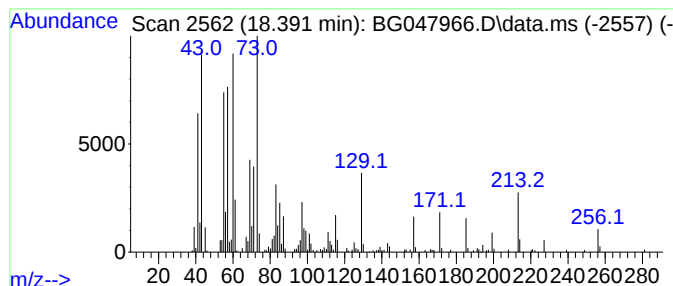
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.391	7.67 ng	319140	Phenanthrene-d10	17.510

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2			Tridecanoic acid	214	C13H26O2	000638-53-9	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5			Dodecanoic acid	200	C12H24O2	000143-07-7	62



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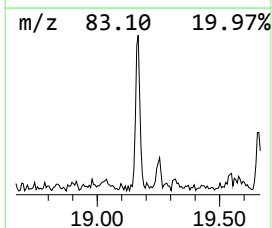
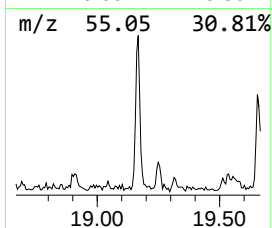
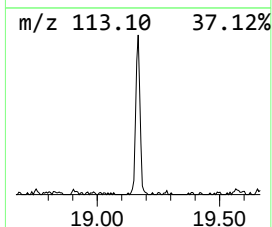
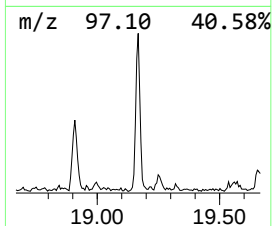
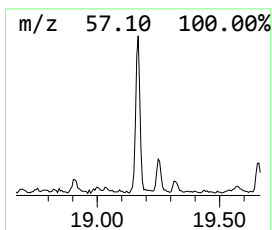
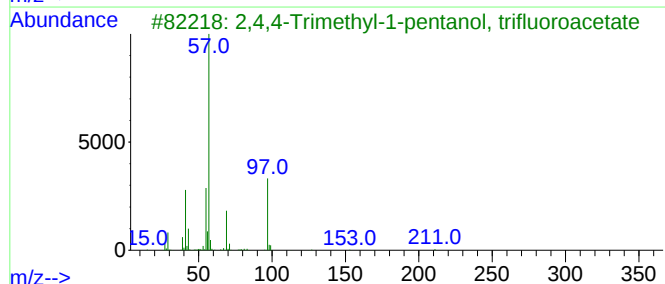
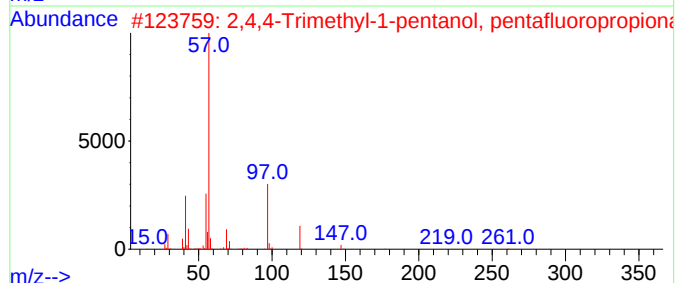
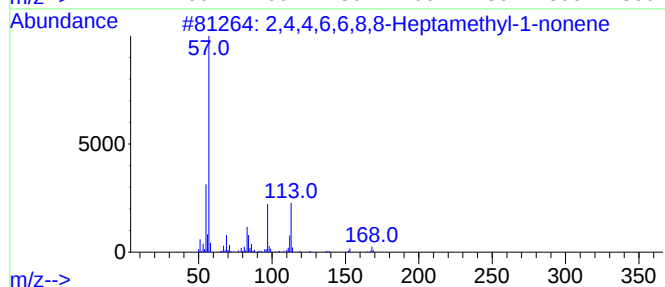
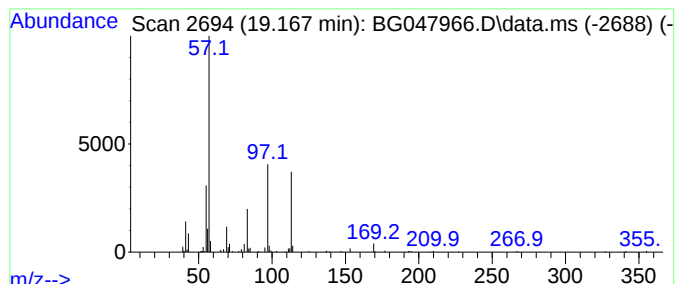
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2,4,4,6,6,8,8-Heptamethyl-1... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.167	4.58 ng	190400	Phenanthrene-d10	17.510

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	56		
2	2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F5O2	1000365-51-0	47		
3	2,4,4-Trimethyl-1-pentanol, trif...	226	C10H17F3O2	1000365-19-5	38		
4	1-Pentanol, 3-methyl-2-propyl-	144	C9H20O	054004-40-9	38		
5	Octane, 2-bromo-	192	C8H17Br	000557-35-7	35		



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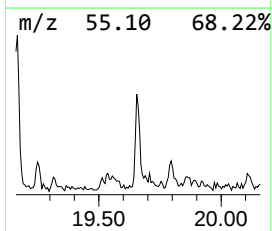
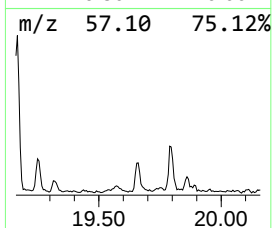
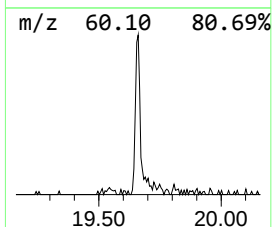
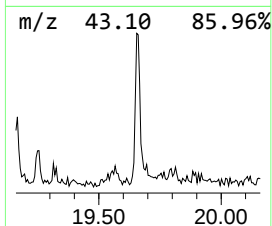
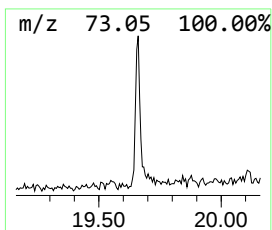
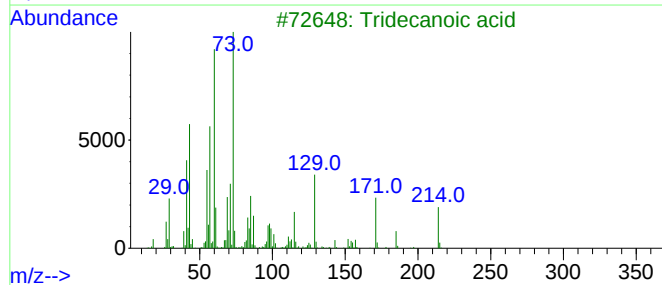
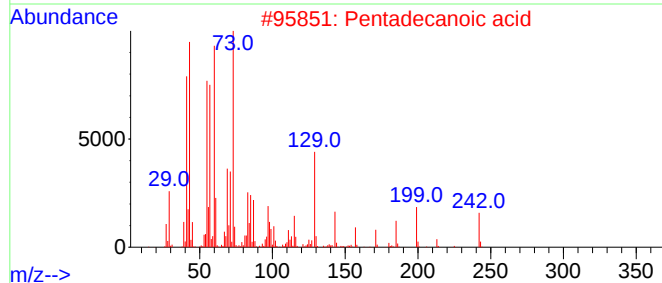
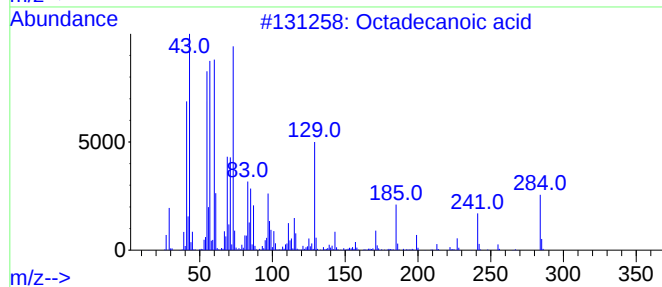
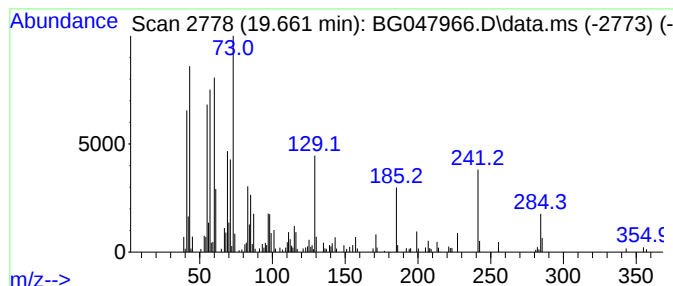
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.660	4.25 ng	202563	Chrysene-d12	21.793

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3			Tridecanoic acid	214	C13H26O2	000638-53-9	70
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68



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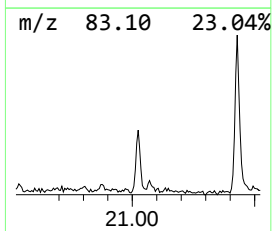
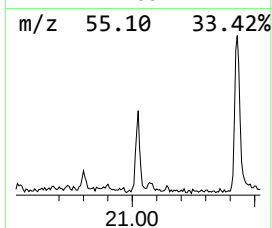
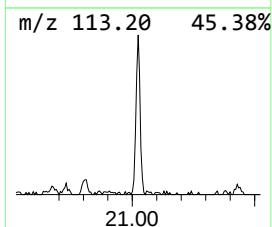
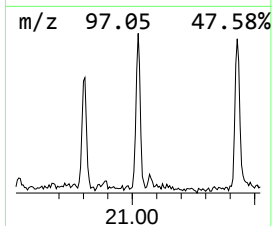
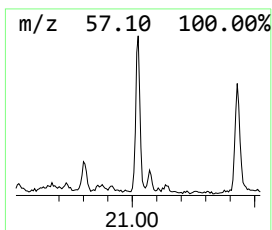
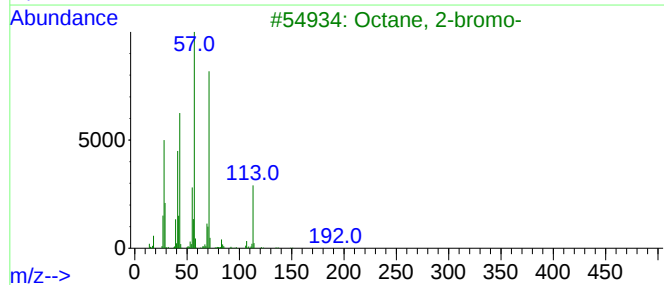
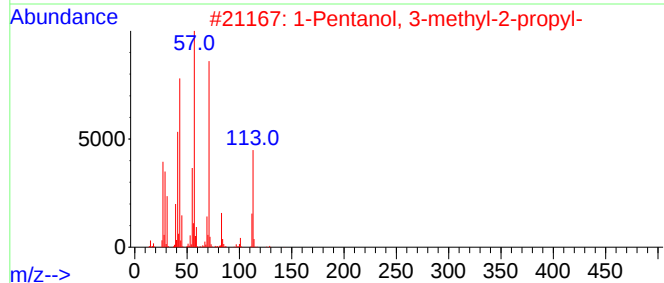
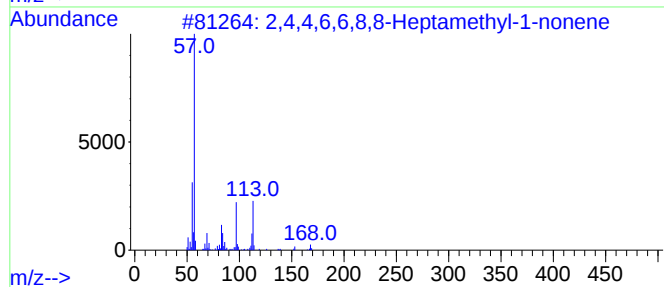
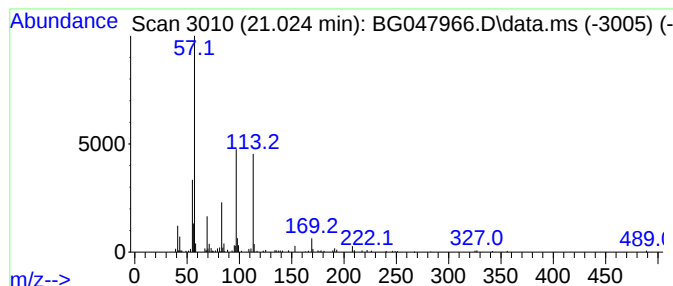
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Peak Number 4 unknown21.024 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.024	3.00 ng	142967	Chrysene-d12	21.793

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	64		
2	1-Pentanol, 3-methyl-2-propyl-	144	C9H20O	054004-40-9	38		
3	Octane, 2-bromo-	192	C8H17Br	000557-35-7	35		
4	Sulfurous acid, di(2-ethylhexyl)...	306	C16H34O3S	1000309-19-1	25		
5	Cyclohexane, 1,1'-[1,2-bis(1,1-d...	306	C22H42	065149-85-1	25		



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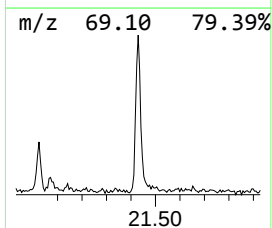
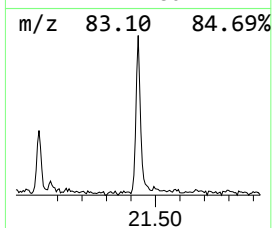
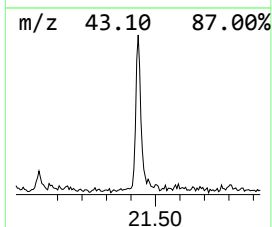
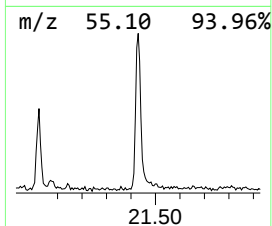
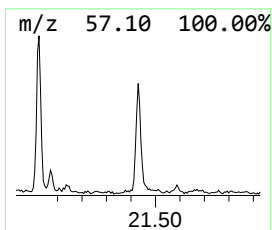
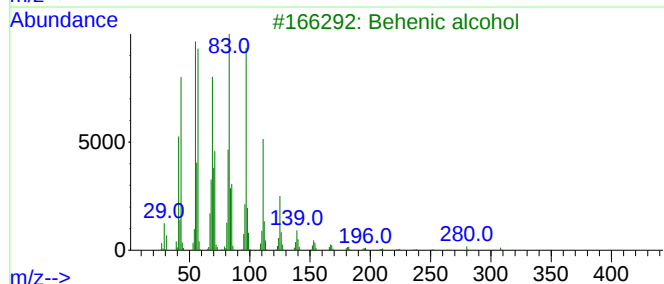
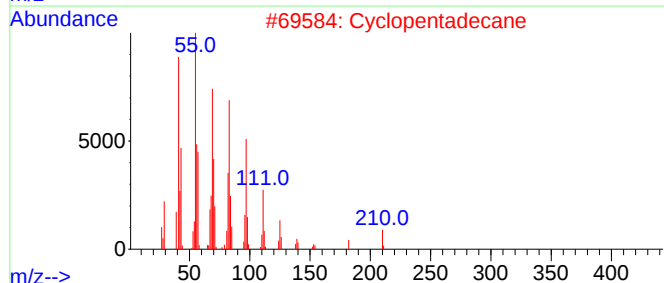
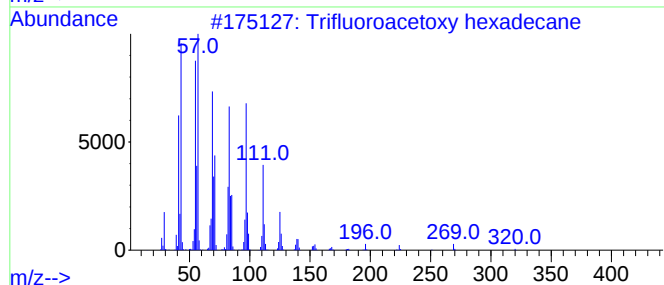
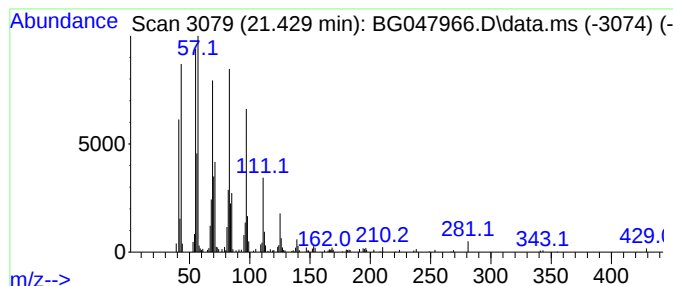
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TIC Library : C:\Database\NIST11.L
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Peak Number 5 Trifluoroacetoxy hexadecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.429	6.25 ng	297922	Chrysene-d12	21.793

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
2			Cyclopentadecane	210	C15H30	000295-48-7	92
3			Behenic alcohol	326	C22H46O	000661-19-8	91
4			1-Heneicosanol	312	C21H44O	015594-90-8	91
5			1-Heneicosyl formate	340	C22H44O2	077899-03-7	91



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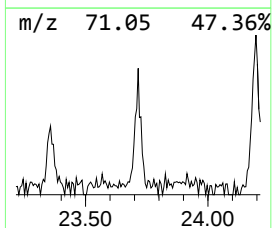
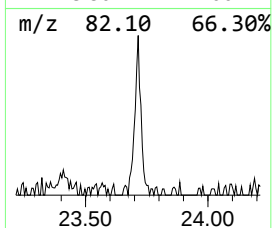
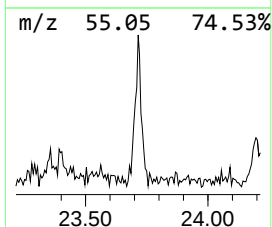
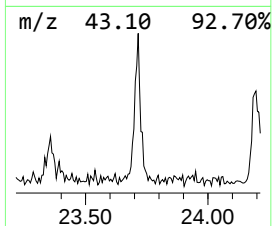
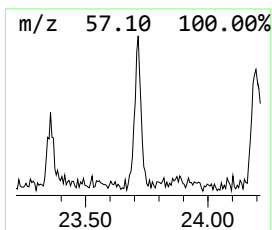
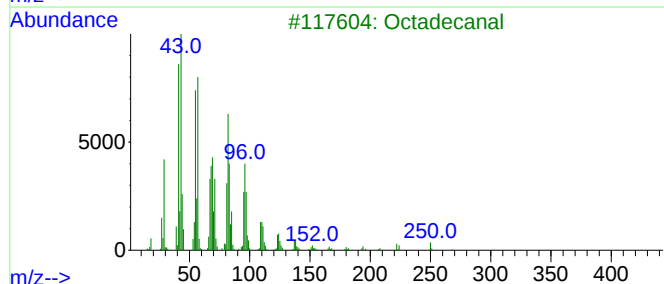
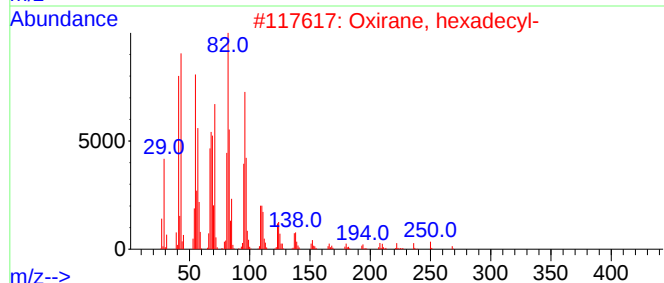
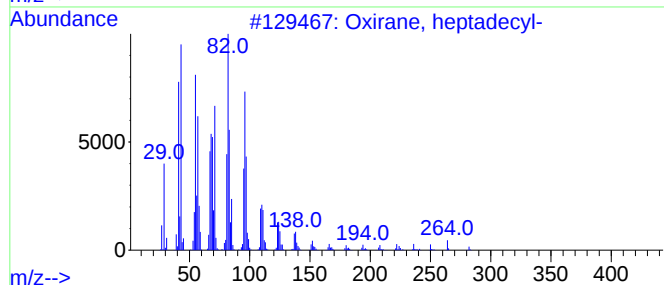
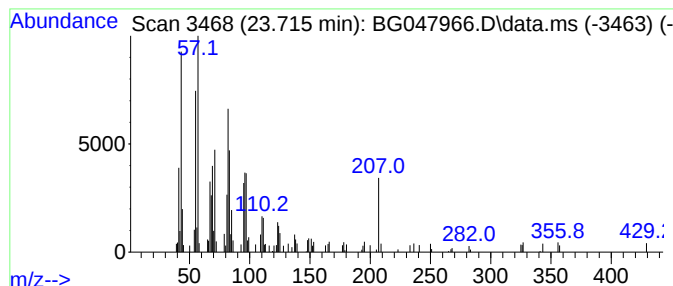
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Oxirane, heptadecyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.715	2.16 ng	100617	Perylene-d12	25.101

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxirane, heptadecyl-	282	C19H38O	067860-04-2	76
2			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	68
3			Octadecanal	268	C18H36O	000638-66-4	68
4			Dodecane, 6-cyclohexyl-	252	C18H36	013151-86-5	49
5			Dodecane, 5-cyclohexyl-	252	C18H36	013151-85-4	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012121\
Data File : BG047966.D
Acq On : 21 Jan 2021 23:26
Operator : CG/JU
Sample : M1177-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PILE-2-(0.5-1.0)

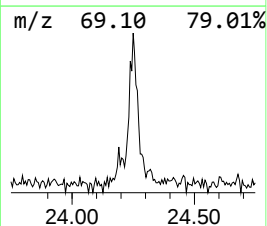
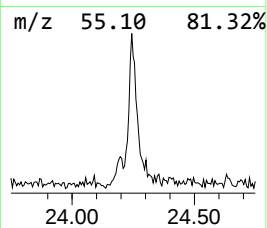
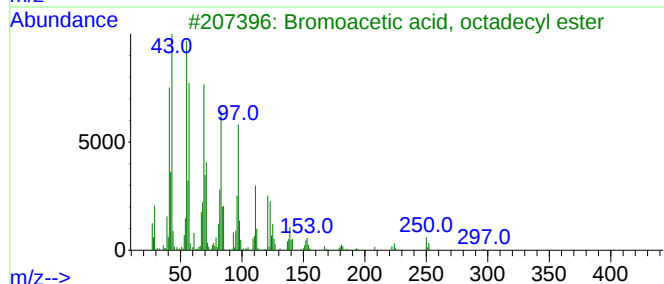
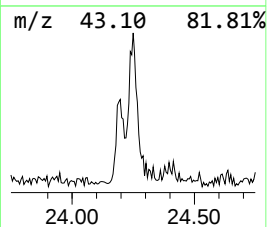
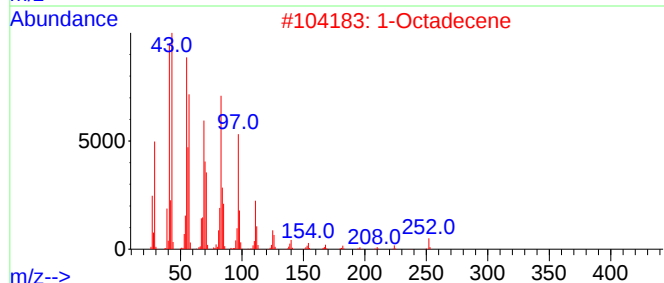
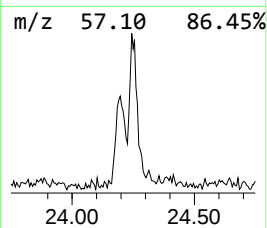
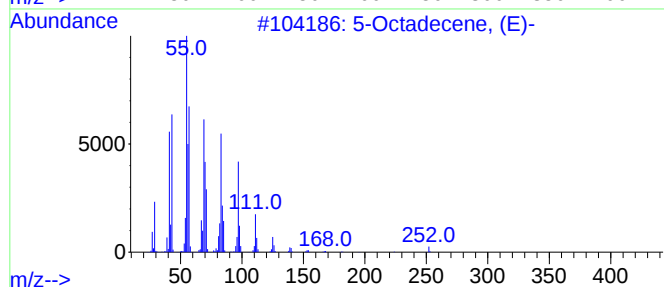
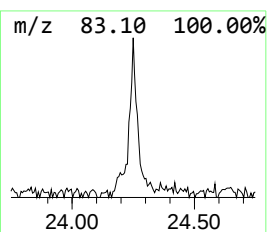
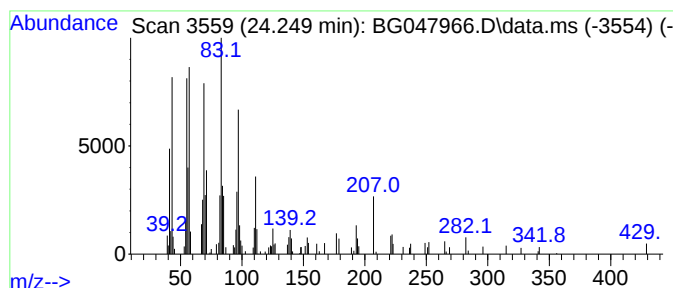
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 5-Octadecene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.249	3.27 ng	152559	Perylene-d12	25.101

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Octadecene, (E)-	252	C18H36	007206-21-5	87
2			1-Octadecene	252	C18H36	000112-88-9	78
3			Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	70
4			E-15-Heptadecenal	252	C17H32O	1000130-97-9	66
5			n-Tetracosanol-1	354	C24H50O	000506-51-4	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012121\
Data File : BG047966.D
Acq On : 21 Jan 2021 23:26
Operator : CG/JU
Sample : M1177-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PILE-2-(0.5-1.0)

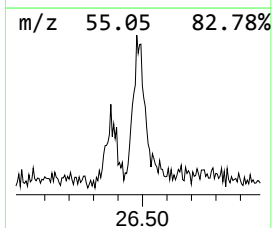
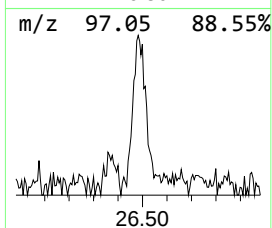
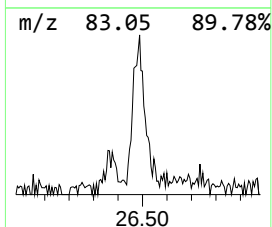
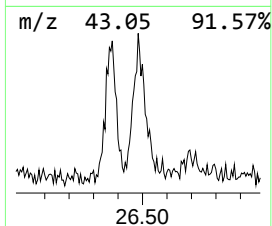
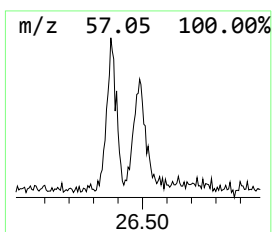
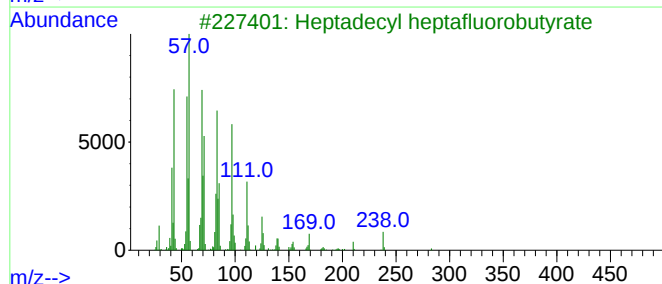
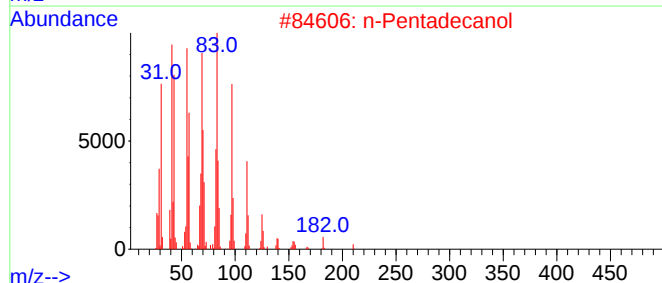
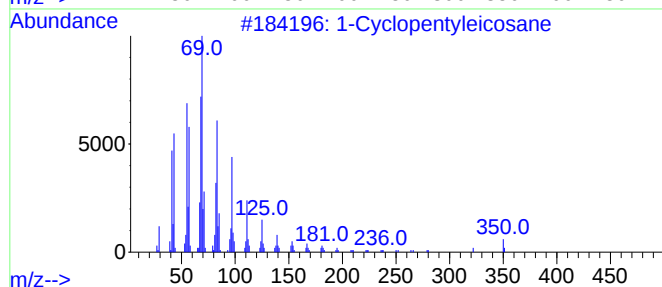
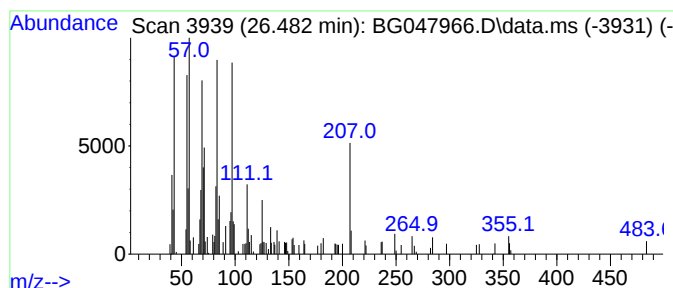
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Cyclopentyleicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.482	3.09 ng	143956	Perylene-d12	25.101

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Cyclopentyleicosane	350	C25H50	1000357-25-6	53
2			n-Pentadecanol	228	C15H32O	000629-76-5	52
3			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	46
4			1-Tridecene	182	C13H26	002437-56-1	45
5			Octacosanol	410	C28H58O	000557-61-9	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012121\
Data File : BG047966.D
Acq On : 21 Jan 2021 23:26
Operator : CG/JU
Sample : M1177-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PILE-2-(0.5-1.0)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012121.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
n-Hexadecanoic ...	18.391	7.7	ng	319140	4	17.510	832345	20.0
2,4,4,6,6,8,8-H...	19.167	4.6	ng	190400	4	17.510	832345	20.0
Octadecanoic acid	19.660	4.3	ng	202563	5	21.793	953914	20.0
unknown21.024	21.024	3.0	ng	142967	5	21.793	953914	20.0
Trifluoroacetox...	21.429	6.3	ng	297922	5	21.793	953914	20.0
Oxirane, heptad...	23.715	2.2	ng	100617	6	25.101	931713	20.0
5-Octadecene, (E)-	24.249	3.3	ng	152559	6	25.101	931713	20.0
1-Cyclopentylei...	26.482	3.1	ng	143956	6	25.101	931713	20.0