

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042121\
 Data File : BG048825.D
 Acq On : 21 Apr 2021 18:44
 Operator : CG/JU
 Sample : M2077-02
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-20-0-2.0

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-BG041421.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048825.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.612	379	387	400	rBV	390595	603108	46.93%	8.647%
2	7.222	654	661	671	rBV	385548	668928	52.06%	9.590%
3	8.062	798	804	810	rBV2	89066	147869	11.51%	2.120%
4	9.237	995	1004	1010	rBV	247442	443301	34.50%	6.355%
5	10.888	1278	1285	1292	rBV	114097	199478	15.52%	2.860%
6	13.338	1695	1702	1709	rBV	591902	879333	68.43%	12.607%
7	14.161	1837	1842	1850	rBV	18543	30358	2.36%	0.435%
8	14.719	1930	1937	1945	rVB	184280	287649	22.39%	4.124%
9	16.217	2185	2192	2200	rBV	496017	766056	59.61%	10.983%
10	17.481	2401	2407	2414	rBV	235939	362586	28.22%	5.198%
11	18.362	2553	2557	2566	rBV6	23057	44646	3.47%	0.640%
12	19.261	2708	2710	2716	rVB5	8755	14571	1.13%	0.209%
13	19.355	2719	2726	2732	rBV2	16063	34091	2.65%	0.489%
14	19.461	2734	2744	2752	rVB	45288	95163	7.41%	1.364%
15	19.531	2752	2756	2763	rBV3	7270	13958	1.09%	0.200%
16	19.890	2814	2817	2825	rVB5	10827	17474	1.36%	0.251%
17	20.089	2845	2851	2857	rVB	1020619	1285006	100.00%	18.423%
18	20.389	2897	2902	2906	rVB5	10020	15024	1.17%	0.215%
19	20.877	2980	2985	2988	rBV4	15267	19602	1.53%	0.281%
20	21.394	3068	3073	3079	rBV2	82633	119482	9.30%	1.713%
21	21.776	3131	3138	3144	rBV2	235892	386258	30.06%	5.538%
22	21.958	3165	3169	3173	rVB5	14295	21504	1.67%	0.308%
23	22.580	3269	3275	3279	rBV5	16475	27194	2.12%	0.390%
24	23.297	3392	3397	3401	rBV5	16182	23165	1.80%	0.332%
25	24.132	3529	3539	3545	rBV9	15805	37777	2.94%	0.542%
26	25.095	3693	3703	3716	rBV3	131007	398399	31.00%	5.712%
27	26.429	3922	3930	3936	rBV3	11242	33103	2.58%	0.475%

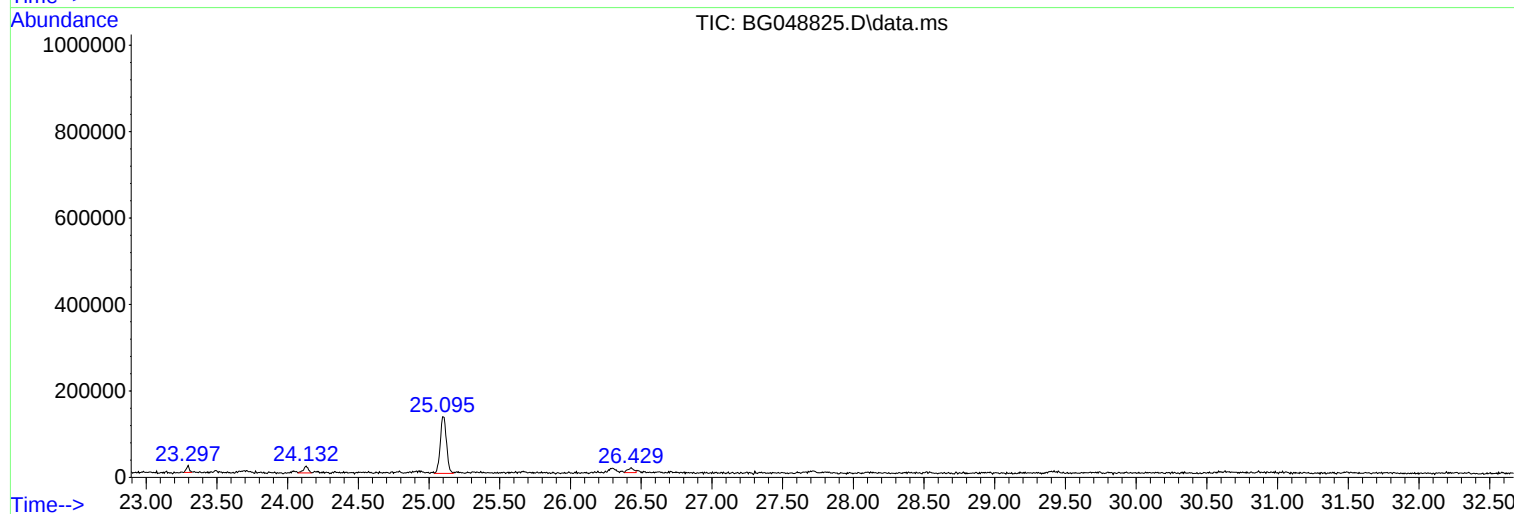
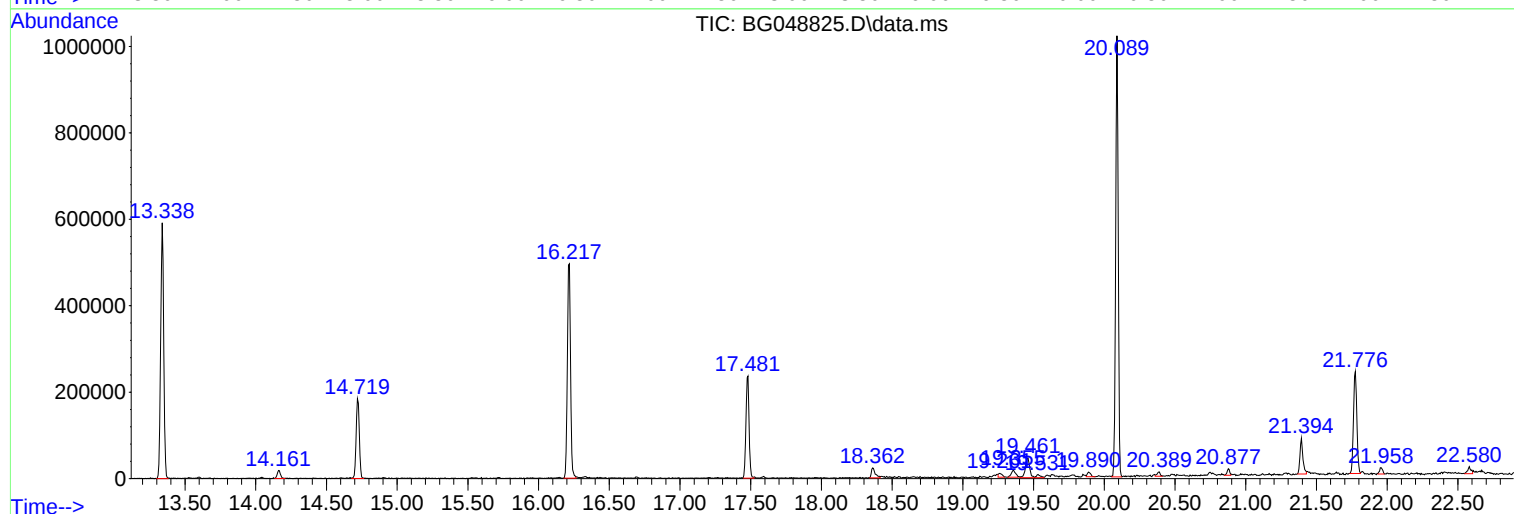
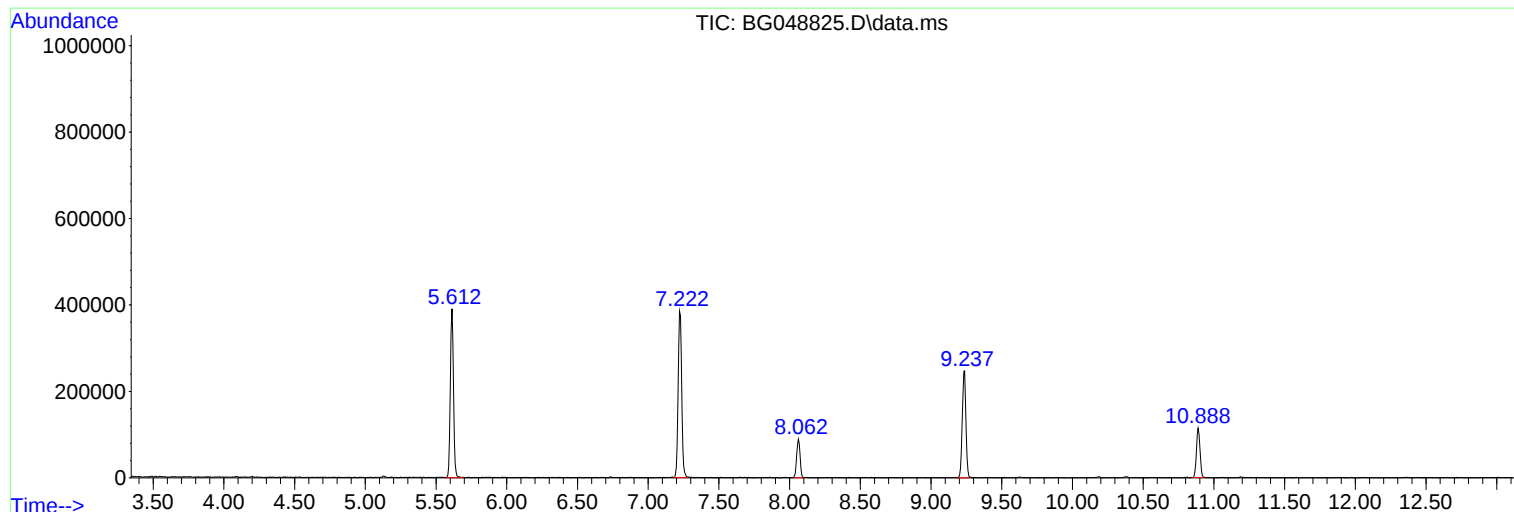
Sum of corrected areas: 6975083

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042121\
Data File : BG048825.D
Acq On : 21 Apr 2021 18:44
Operator : CG/JU
Sample : M2077-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-20-0-2.0

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.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\BG042121\
Data File : BG048825.D
Acq On : 21 Apr 2021 18:44
Operator : CG/JU
Sample : M2077-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-20-0-2.0

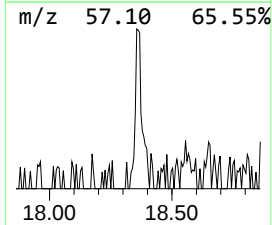
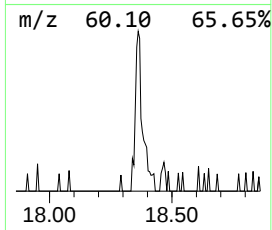
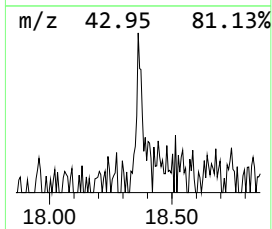
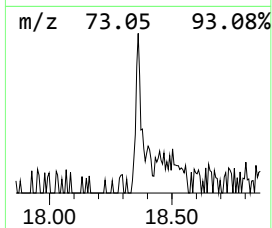
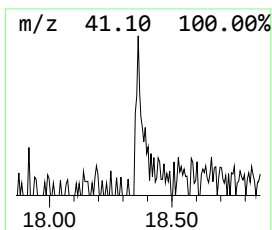
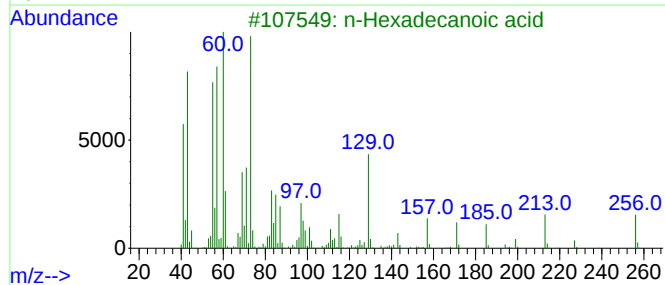
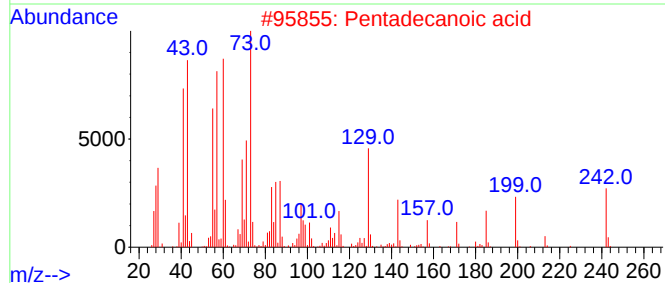
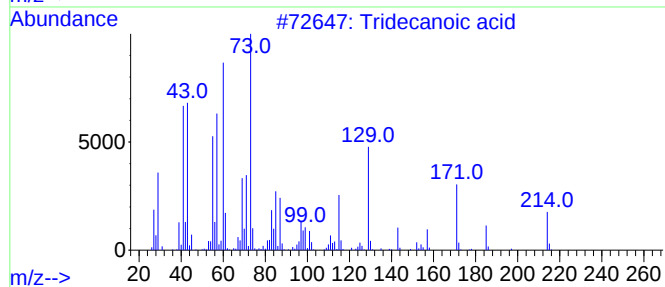
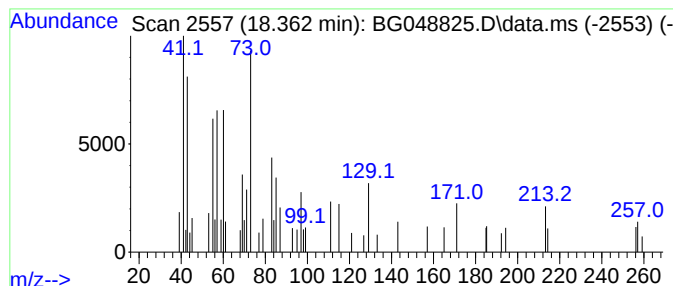
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Tridecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.362	2.46 ng	44646	Phenanthrene-d10	17.475

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	92
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	46
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	46
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	43
5			3,4-Di-O-acetyl-1,5-anhydro-2,6-...	276	C12H20O7	1000357-18-4	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042121\
Data File : BG048825.D
Acq On : 21 Apr 2021 18:44
Operator : CG/JU
Sample : M2077-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-20-0-2.0

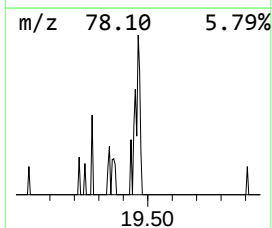
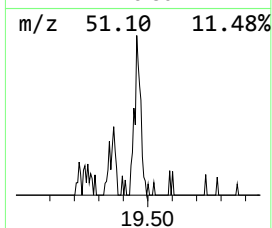
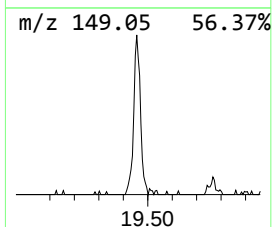
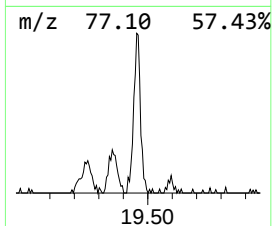
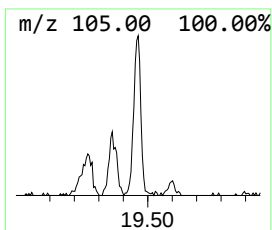
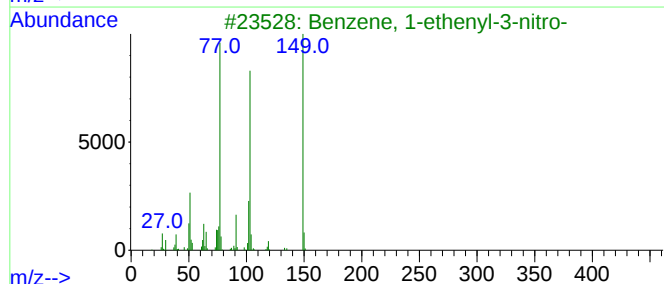
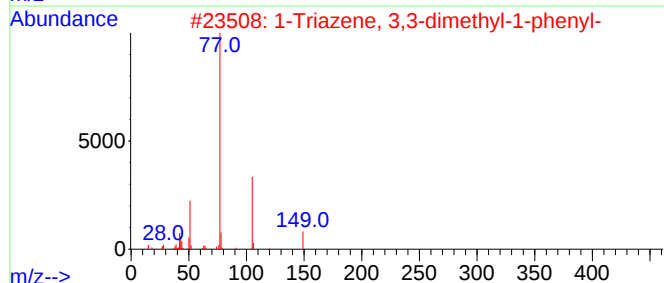
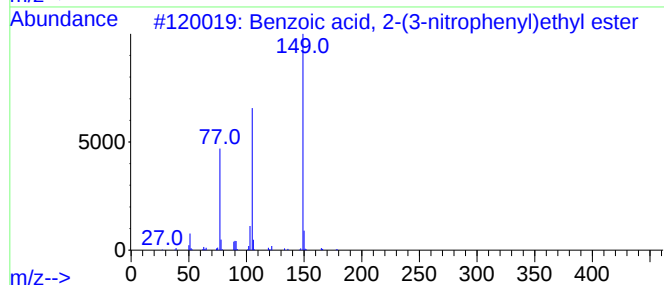
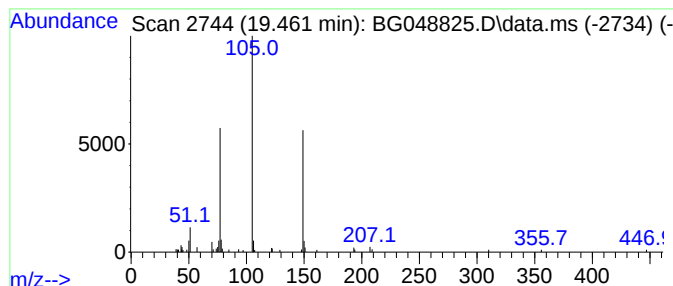
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Benzoic acid, 2-(3-nitrophe... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.461	5.25 ng	95163	Phenanthrene-d10	17.475

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, 2-(3-nitrophenyl)e...	271	C15H13NO4	1000368-22-4	64
2			1-Triazene, 3,3-dimethyl-1-phenyl-	149	C8H11N3	007227-91-0	42
3			Benzene, 1-ethenyl-3-nitro-	149	C8H7NO2	000586-39-0	42
4			S-Benzoyl(thiohydroxylamine)	153	C7H7NO5	025740-80-1	38
5			.alpha.,.alpha.-Dichloroacetophe...	188	C8H6Cl2O	002648-61-5	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042121\
Data File : BG048825.D
Acq On : 21 Apr 2021 18:44
Operator : CG/JU
Sample : M2077-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-20-0-2.0

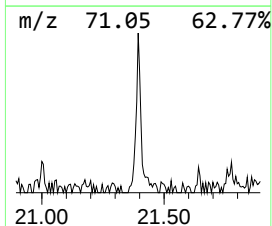
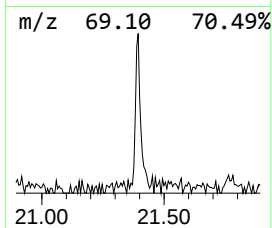
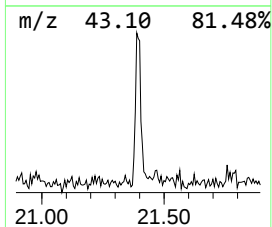
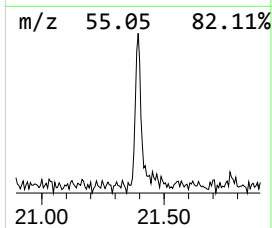
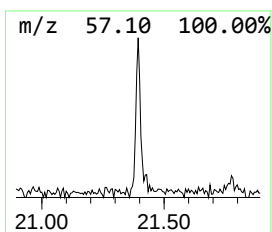
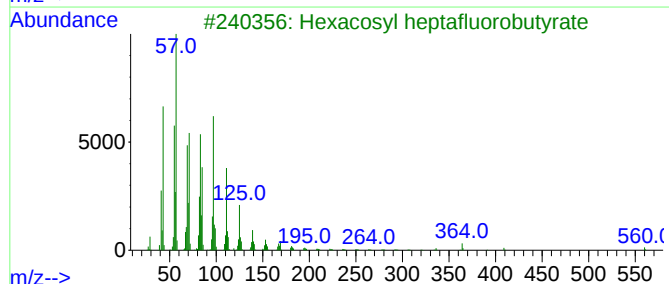
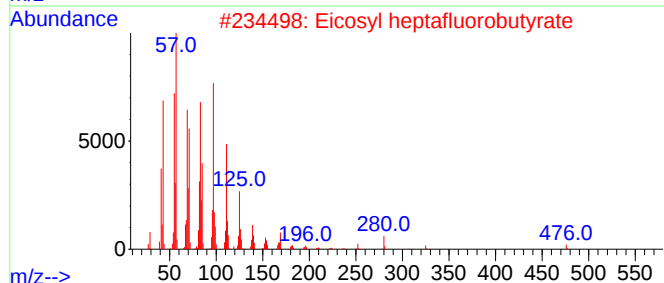
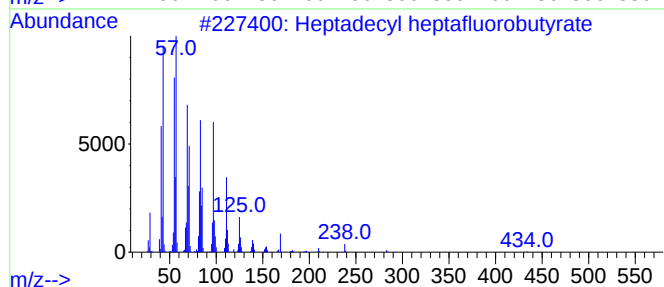
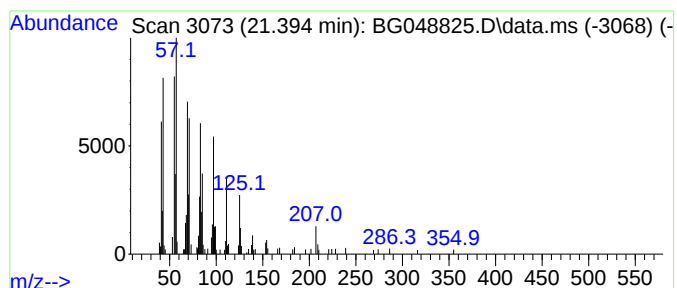
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Heptadecyl heptafluorobutyrate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.394	6.19 ng	119482	Chrysene-d12	21.776

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
2			Eicosyl heptafluorobutyrate	494	C24H41F7O2	1000351-83-5	91
3			Hexacosyl heptafluorobutyrate	578	C30H53F7O2	1000351-83-3	90
4			Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	90
5			Docosyl heptafluorobutyrate	522	C26H45F7O2	1000351-83-1	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042121\
Data File : BG048825.D
Acq On : 21 Apr 2021 18:44
Operator : CG/JU
Sample : M2077-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-20-0-2.0

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.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
Tridecanoic acid	18.362	2.5	ng	44646	4	17.475	362586	20.0
Benzoic acid, 2...	19.461	5.3	ng	95163	4	17.475	362586	20.0
Heptadecyl hept...	21.394	6.2	ng	119482	5	21.776	386258	20.0