

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG031721\
 Data File : BG048405.D
 Acq On : 17 Mar 2021 19:49
 Operator : CG/JU
 Sample : M1691-03
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 FK-GF-02-068-B

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-BG031621.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048405.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.420	9	14	26	rVB3	22141	46035	1.25%	0.192%
2	5.194	310	316	321	rVB	39436	66274	1.80%	0.276%
3	5.659	388	395	405	rBV	1072459	1722311	46.80%	7.165%
4	7.257	656	667	683	rVB	1151093	2056358	55.87%	8.555%
5	8.115	805	813	822	rBV2	252287	439244	11.93%	1.827%
6	9.278	1004	1011	1018	rBV	708906	1277355	34.71%	5.314%
7	10.935	1283	1293	1301	rBV	326895	606652	16.48%	2.524%
8	13.379	1701	1709	1715	rBV	1803662	2724562	74.03%	11.335%
9	14.196	1842	1848	1852	rBV	27879	46543	1.26%	0.194%
10	14.754	1933	1943	1949	rBV	550476	864906	23.50%	3.598%
11	16.240	2188	2196	2205	rBV	1555418	2349593	63.84%	9.775%
12	17.504	2405	2411	2415	rBV	669330	975370	26.50%	4.058%
13	17.545	2415	2418	2424	rVB	120474	169897	4.62%	0.707%
14	17.633	2428	2433	2439	rVV	34197	53941	1.47%	0.224%
15	18.385	2555	2561	2565	rBV2	293562	413139	11.23%	1.719%
16	18.426	2566	2568	2577	rVB2	47600	77701	2.11%	0.323%
17	18.573	2588	2593	2597	rBV4	49985	95311	2.59%	0.397%
18	18.873	2640	2644	2646	rBV2	31218	41675	1.13%	0.173%
19	19.155	2689	2692	2697	rBV2	46654	61340	1.67%	0.255%
20	19.425	2735	2738	2742	rBV3	26535	38976	1.06%	0.162%
21	19.554	2754	2760	2765	rVB	428882	615832	16.73%	2.562%
22	19.654	2773	2777	2780	rBV3	92482	116150	3.16%	0.483%
23	19.807	2794	2803	2804	rBV7	45200	113127	3.07%	0.471%
24	19.883	2813	2816	2818	rBV2	42023	71062	1.93%	0.296%
25	19.913	2818	2821	2828	rVB	375341	532610	14.47%	2.216%
26	20.112	2848	2855	2860	rBV	2935368	3680511	100.00%	15.312%
27	20.230	2871	2875	2876	rBV4	36655	48943	1.33%	0.204%
28	20.406	2902	2905	2910	rVB2	90241	132570	3.60%	0.552%
29	20.506	2918	2922	2925	rBV2	50264	65065	1.77%	0.271%
30	21.188	3031	3038	3039	rBV4	87575	177489	4.82%	0.738%
31	21.423	3074	3078	3089	rVB5	273677	510928	13.88%	2.126%
32	21.511	3089	3093	3101	rVB	187985	282459	7.67%	1.175%
33	21.793	3133	3141	3146	rBV2	655361	1397811	37.98%	5.815%
34	21.846	3146	3150	3156	rVB	181369	313470	8.52%	1.304%
35	24.072	3523	3529	3537	rBV	138132	435423	11.83%	1.811%
36	24.971	3676	3682	3692	rVB2	138417	376766	10.24%	1.567%

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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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	25.136	3701	3710	3719	rBV2	353248	1039521	28.24%	4.325%
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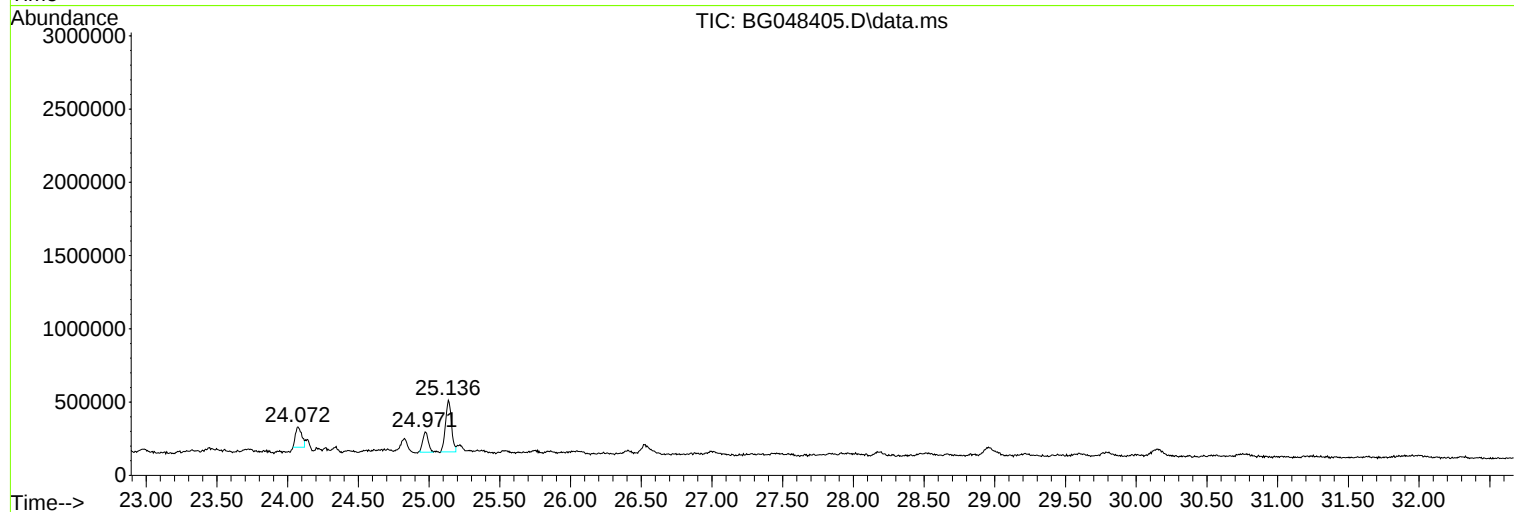
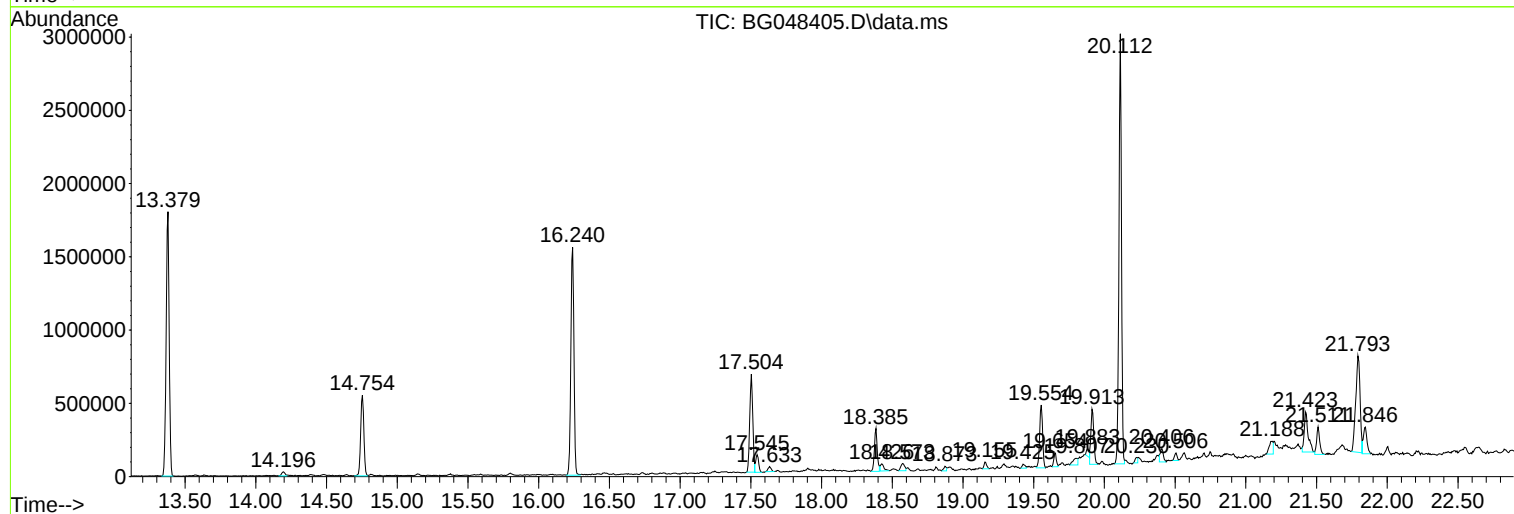
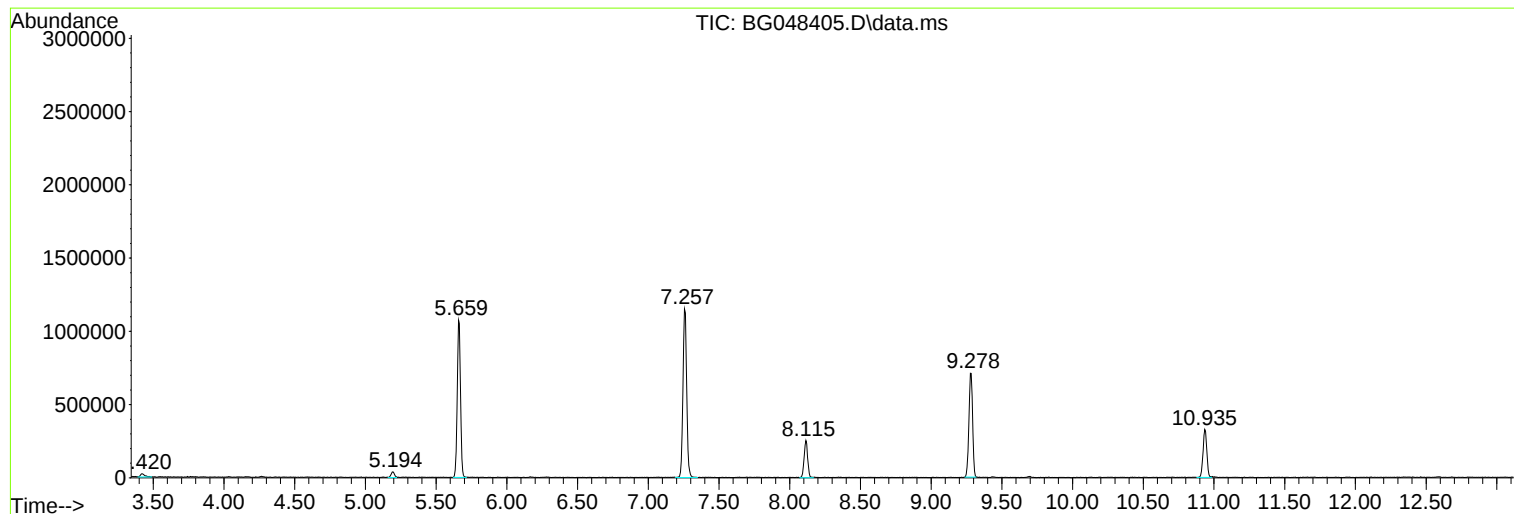
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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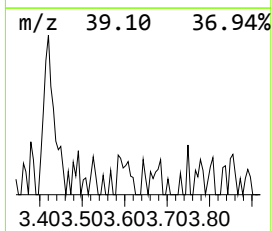
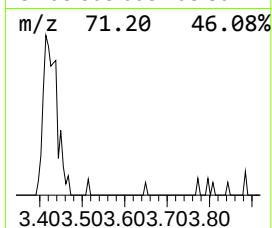
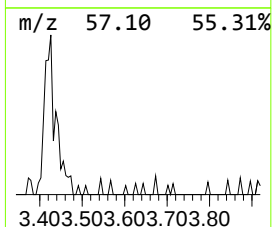
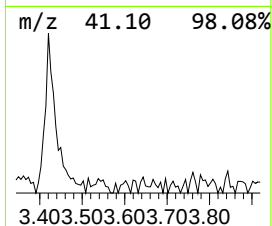
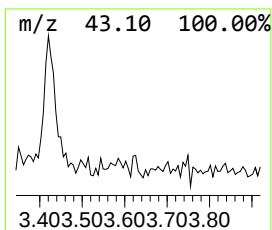
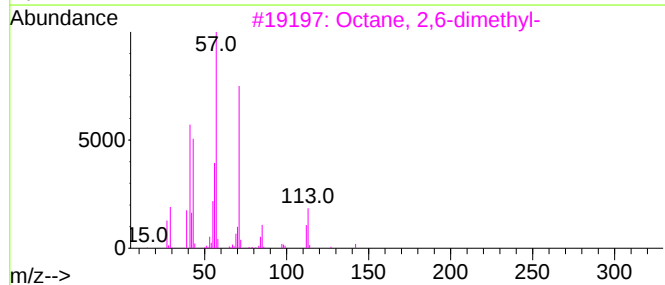
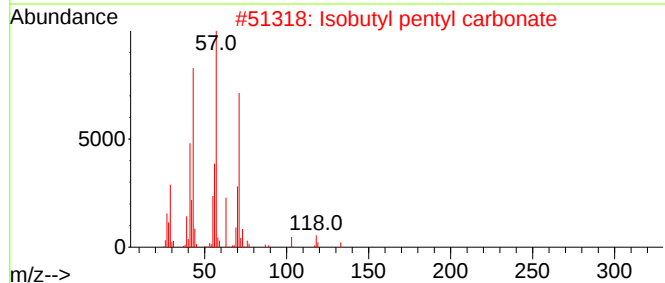
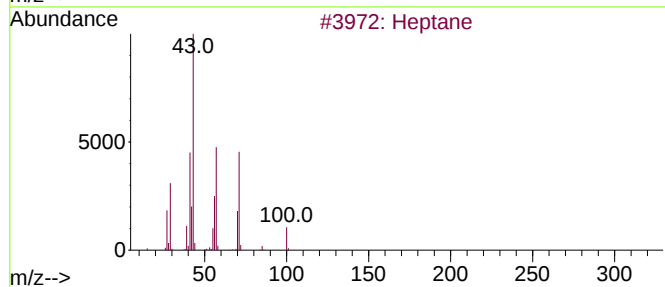
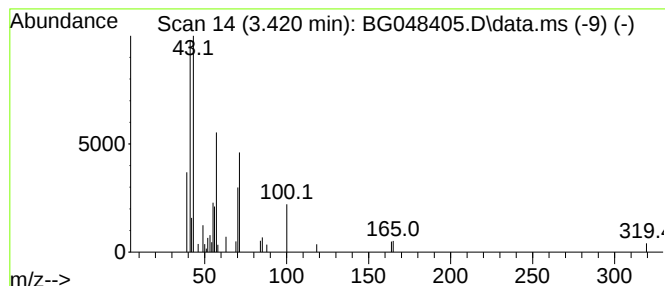
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown3.420 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.420	2.10 ng	46035	1,4-Dichlorobenzene-d4	8.115

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane	100	C7H16	000142-82-5	37
2			Isobutyl pentyl carbonate	188	C10H20O3	178442-32-5	37
3			Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	35
4			Decane, 4-methyl-	156	C11H24	002847-72-5	32
5			Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	32



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Misc :
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Instrument :
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ClientSampleId :
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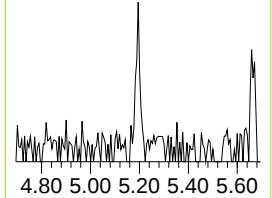
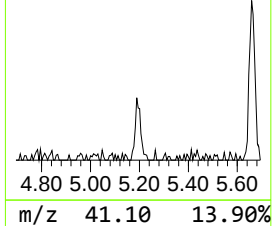
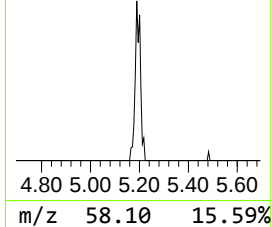
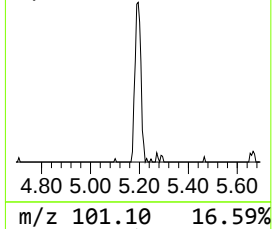
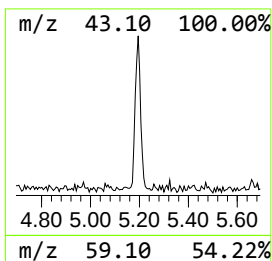
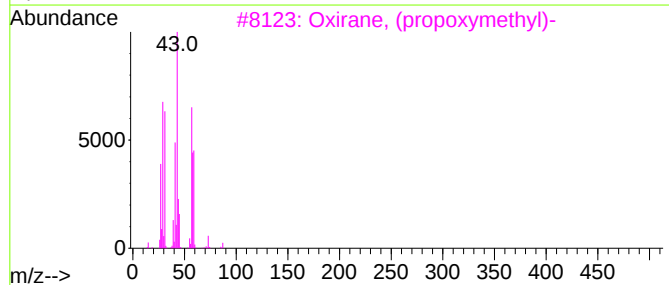
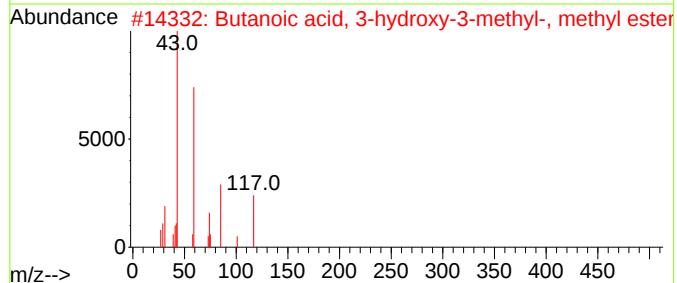
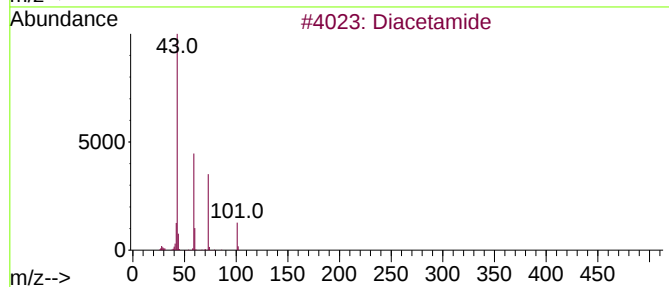
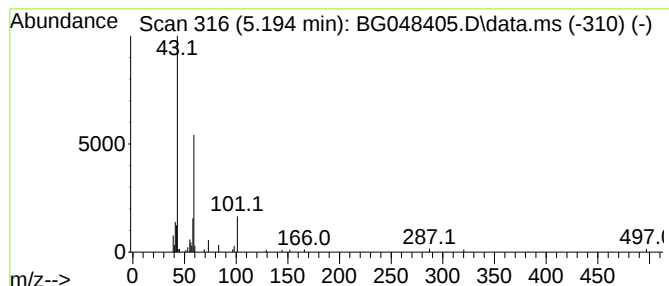
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Peak Number 2 unknown5.194 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.194	3.02 ng	66274	1,4-Dichlorobenzene-d4	8.115

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diacetamide	101	C4H7NO2	000625-77-4	38
2			Butanoic acid, 3-hydroxy-3-methyl-2-butanone	132	C6H12O3	006149-45-7	38
3			Oxirane, (propoxymethyl)-	116	C6H12O2	003126-95-2	36
4			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	28
5			3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	25



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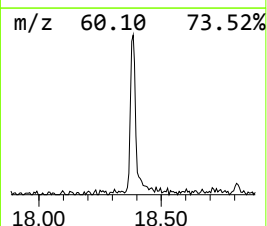
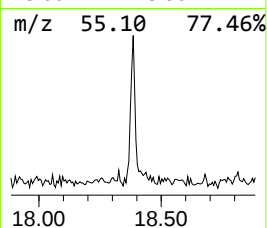
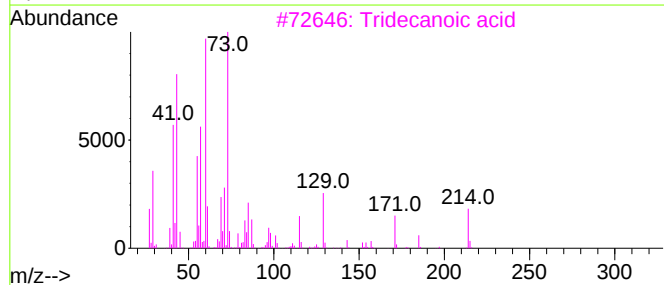
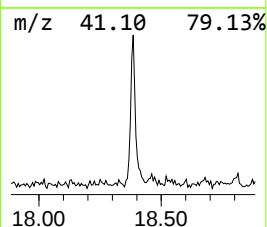
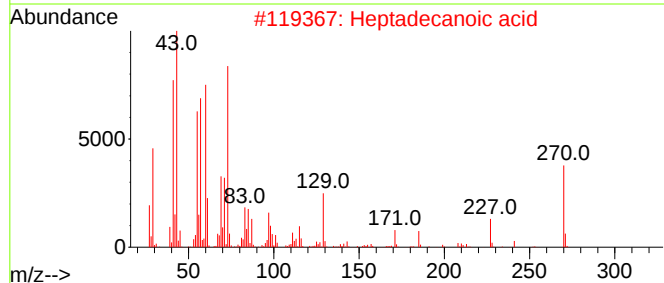
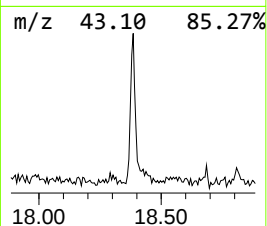
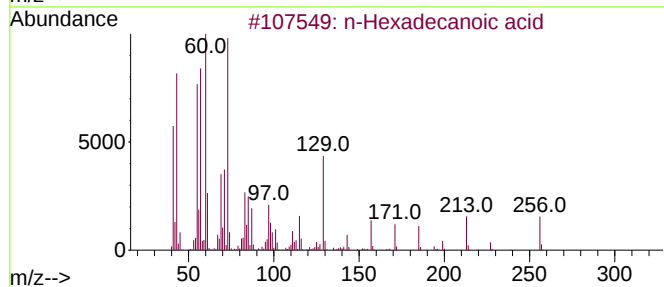
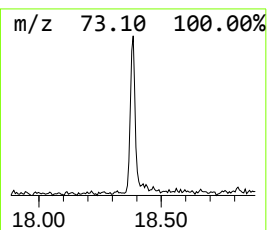
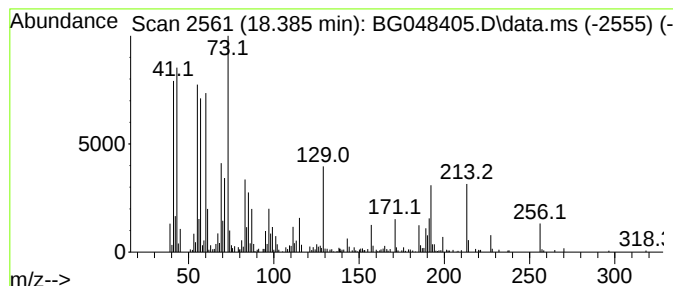
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031621.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.385	8.47 ng	413139	Phenanthrene-d10	17.504

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Heptadecanoic acid	270	C17H34O2	000506-12-7	90
3			Tridecanoic acid	214	C13H26O2	000638-53-9	89
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	68
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	59



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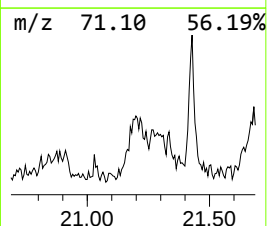
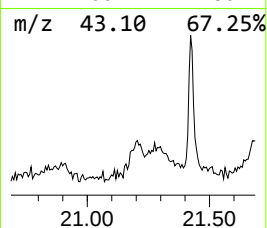
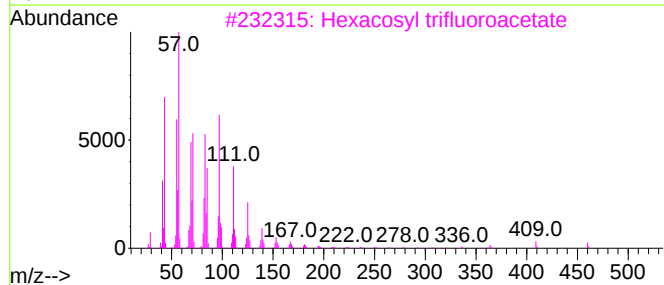
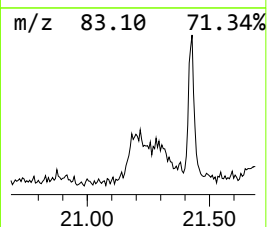
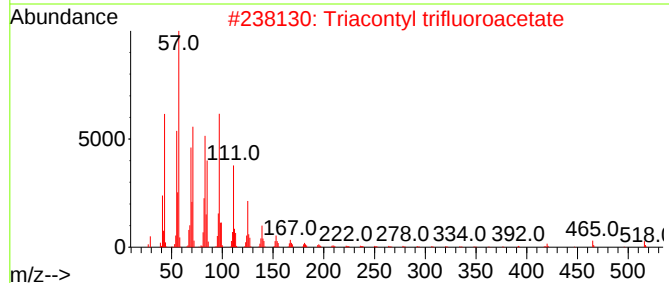
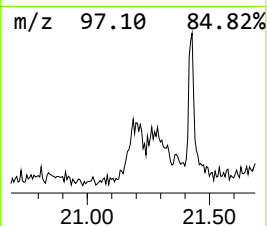
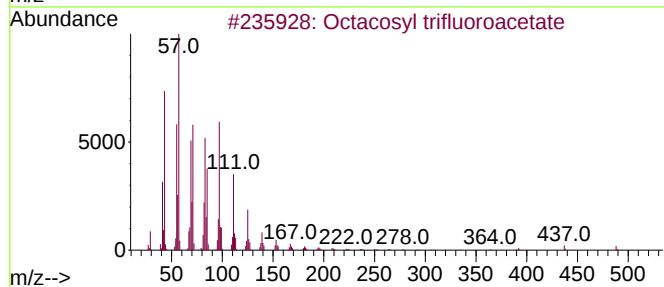
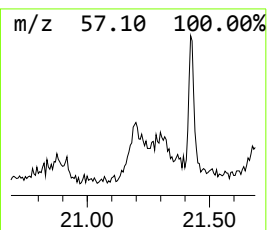
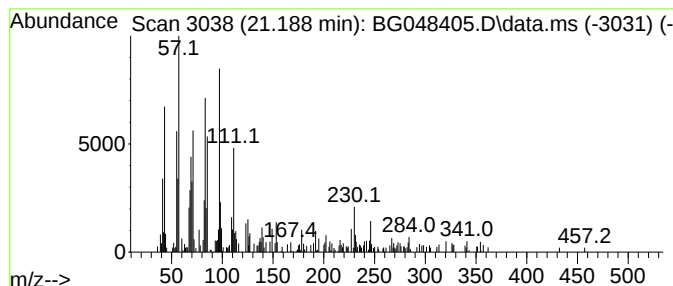
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TIC Library : C:\Database\NIST11.L
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Peak Number 4 Octacosyl trifluoroacetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.188	2.54 ng	177489	Chrysene-d12	21.793	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	87
2	Triacontyl trifluoroacetate	534	C32H61F3O2	1000351-75-7	83
3	Hexacosyl trifluoroacetate	478	C28H53F3O2	1000351-75-0	83
4	Octacosyl heptafluorobutyrate	606	C32H57F7O2	1000351-83-6	83
5	Heptacosyl pentafluoropropionate	542	C30H55F5O2	1000351-81-6	83



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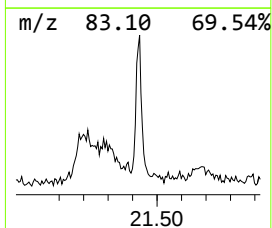
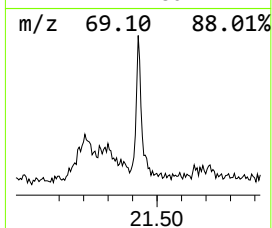
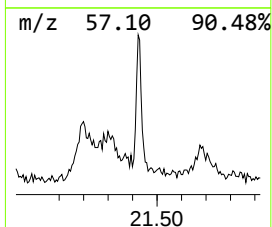
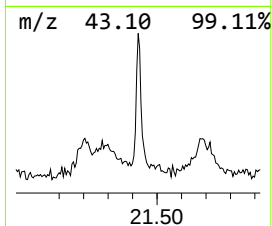
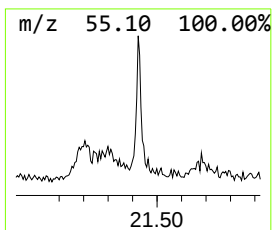
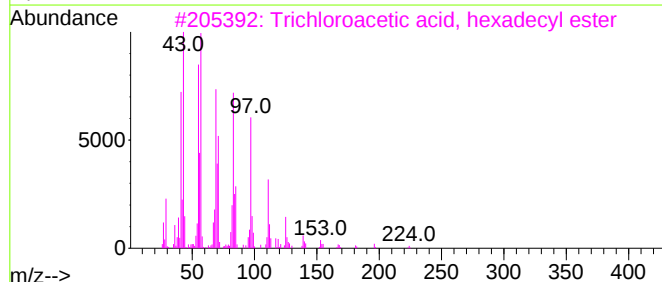
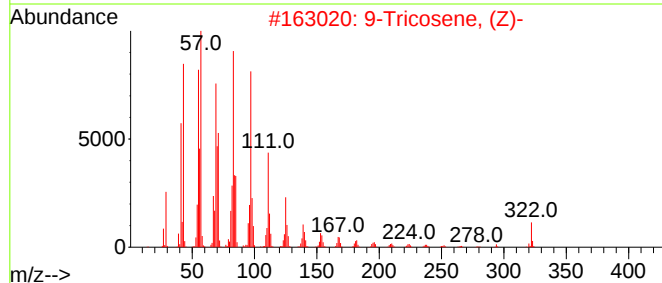
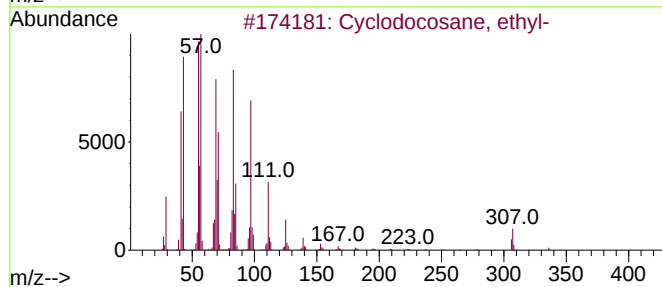
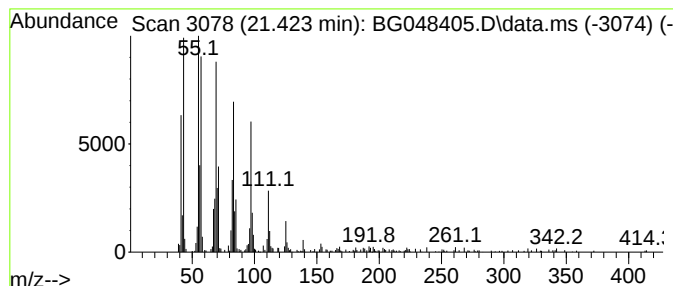
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Cyclodocosane, ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.422	7.31 ng	510928	Chrysene-d12	21.793

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclodocosane, ethyl-	336	C24H48	1000151-22-6	98
2			9-Tricosene, (Z)-	322	C23H46	027519-02-4	95
3			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93
4			1-Docosene	308	C22H44	001599-67-3	93
5			3-Octadecene, (E)-	252	C18H36	007206-19-1	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG031721\
Data File : BG048405.D
Acq On : 17 Mar 2021 19:49
Operator : CG/JU
Sample : M1691-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
FK-GF-02-068-B

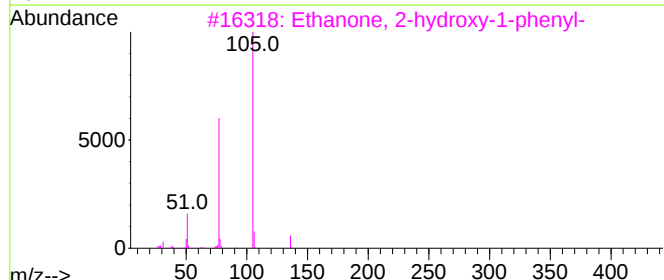
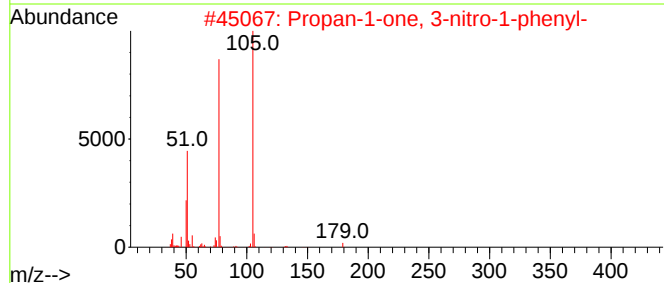
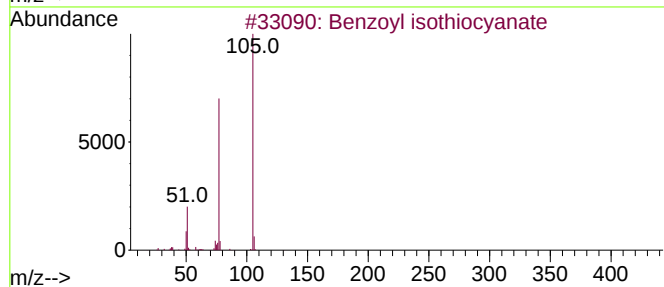
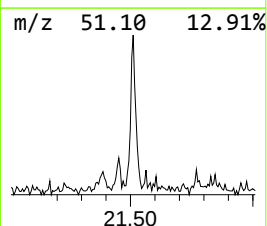
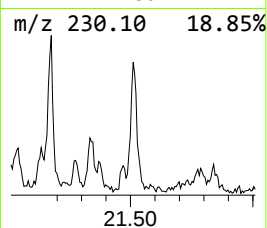
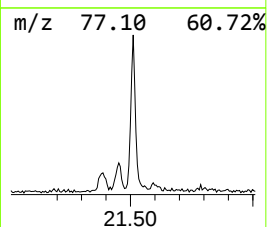
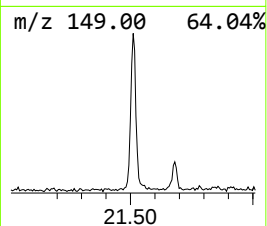
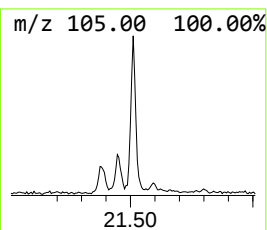
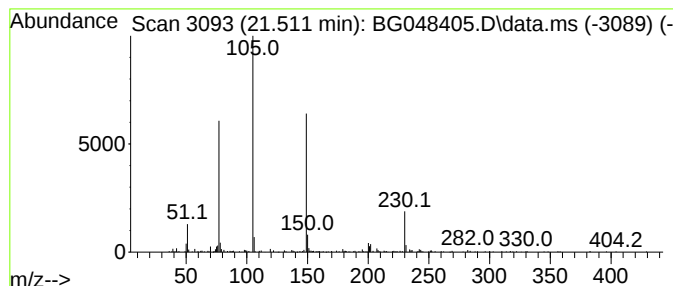
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown21.511 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.511	4.04 ng	282459	Chrysene-d12	21.793

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	35
2			Propan-1-one, 3-nitro-1-phenyl-	179	C9H9NO3	062847-52-3	35
3			Ethanone, 2-hydroxy-1-phenyl-	136	C8H8O2	000582-24-1	35
4			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	35
5			1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG031721\
Data File : BG048405.D
Acq On : 17 Mar 2021 19:49
Operator : CG/JU
Sample : M1691-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
FK-GF-02-068-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031621.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
unknown3.420	3.420	2.1	ng	46035	1	8.115	439244	20.0
unknown5.194	5.194	3.0	ng	66274	1	8.115	439244	20.0
n-Hexadecanoic ...	18.385	8.5	ng	413139	4	17.504	975370	20.0
Octacosyl trifl...	21.188	2.5	ng	177489	5	21.793	1397810	20.0
Cyclodocosane, ...	21.422	7.3	ng	510928	5	21.793	1397810	20.0
unknown21.511	21.511	4.0	ng	282459	5	21.793	1397810	20.0