

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052522\
 Data File : BG053700.D
 Acq On : 25 May 2022 19:10
 Operator : CG/JU
 Sample : N2923-03
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 P024-SS005-0006-01

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-BG050522.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG053700.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.017	3	5	13	rVB2	20169	30136	1.96%	0.409%
2	3.093	13	18	31	rVB	204161	304078	19.75%	4.129%
3	5.555	431	437	452	rVB	272142	457652	29.72%	6.215%
4	7.158	704	710	726	rBV	299801	533694	34.66%	7.247%
5	7.987	843	851	858	rBV	74233	127069	8.25%	1.726%
6	9.150	1041	1049	1061	rBV	184371	338672	22.00%	4.599%
7	10.795	1321	1329	1339	rBV	100695	183042	11.89%	2.486%
8	13.244	1740	1746	1756	rBV	546312	829930	53.90%	11.270%
9	14.625	1974	1981	1989	rBV	187212	291314	18.92%	3.956%
10	16.117	2228	2235	2251	rBV	459200	752540	48.88%	10.219%
11	17.368	2442	2448	2458	rBV	262431	405155	26.31%	5.502%
12	18.267	2596	2601	2608	rBV4	26614	56031	3.64%	0.761%
13	19.976	2886	2892	2899	rVB	1230168	1539655	100.00%	20.908%
14	21.263	3107	3111	3122	rBV3	60151	109067	7.08%	1.481%
15	21.633	3168	3174	3181	rVB2	284884	449336	29.18%	6.102%
16	23.889	3552	3558	3565	rVB3	25667	52703	3.42%	0.716%
17	24.834	3710	3719	3730	rVB2	161582	468126	30.40%	6.357%
18	25.334	3802	3804	3813	rVB9	8940	16896	1.10%	0.229%
19	25.939	3899	3907	3916	rVB4	39572	118958	7.73%	1.615%
20	28.054	4259	4267	4278	rVB7	37220	137563	8.93%	1.868%
21	28.888	4399	4409	4418	rBV2	28671	113070	7.34%	1.535%
22	30.068	4602	4610	4611	rBV7	27108	49216	3.20%	0.668%

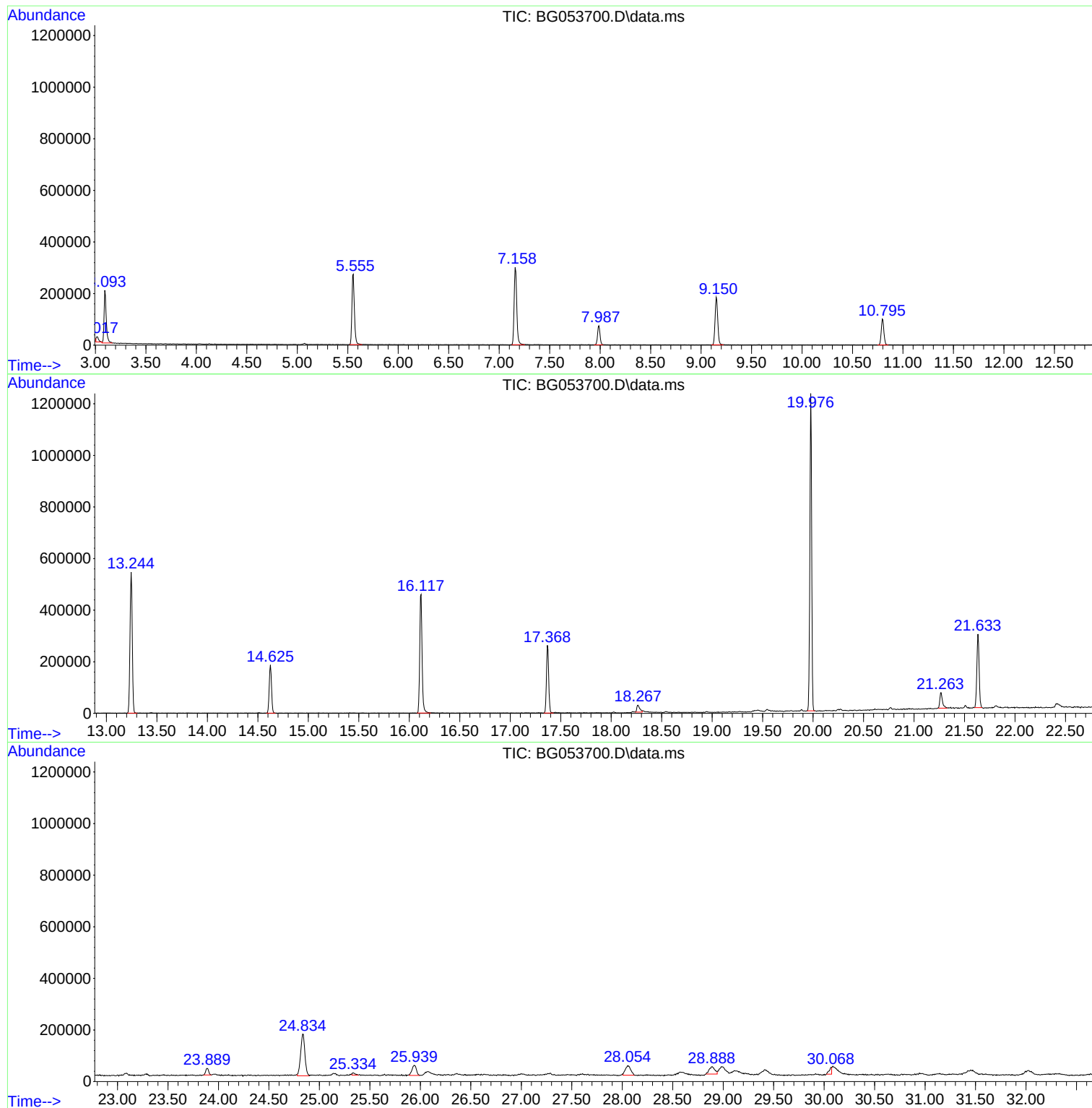
Sum of corrected areas: 7363903

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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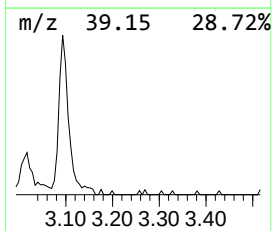
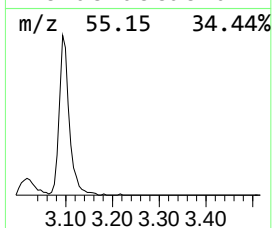
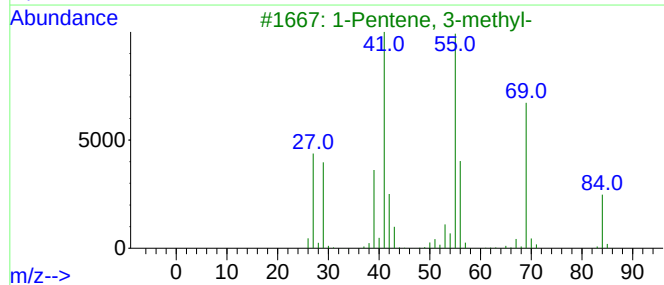
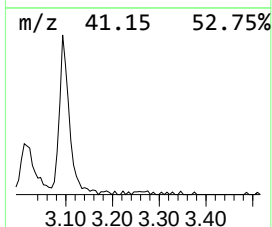
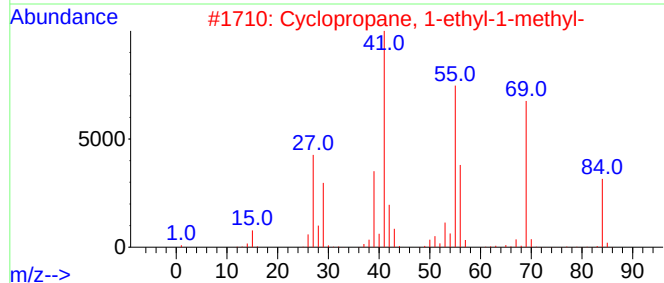
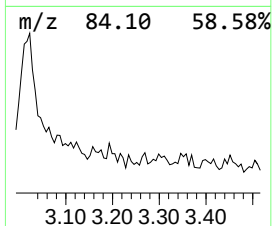
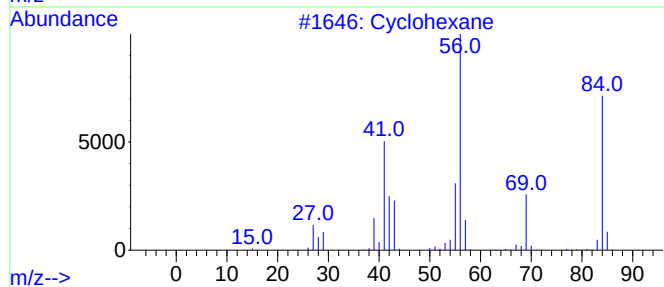
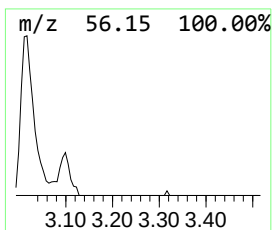
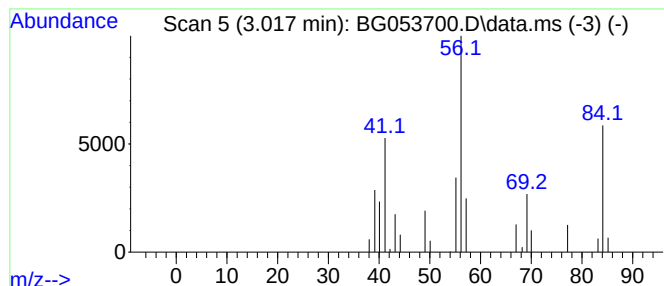
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown3.017 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.017	4.74 ng	30136	1,4-Dichlorobenzene-d4	7.987

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane	84	C6H12	000110-82-7	49
2			Cyclopropane, 1-ethyl-1-methyl-	84	C6H12	053778-43-1	37
3			1-Pentene, 3-methyl-	84	C6H12	000760-20-3	25
4			Allyl isocyanate	83	C4H5NO	001476-23-9	12
5			2-Pentene, 2-methyl-	84	C6H12	000625-27-4	10



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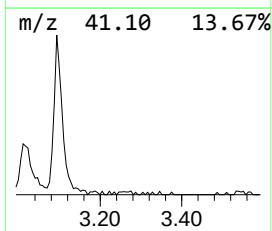
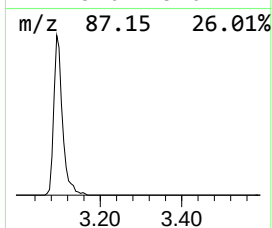
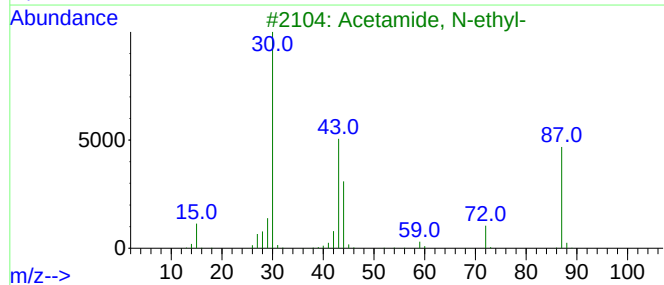
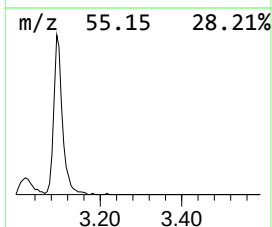
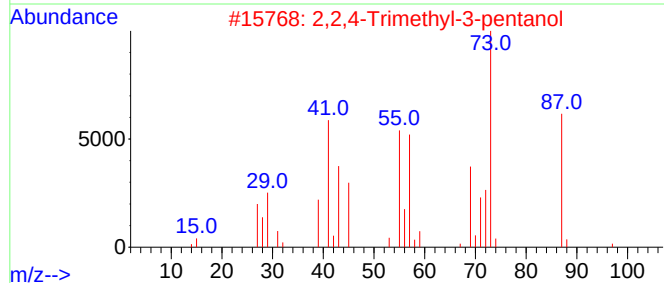
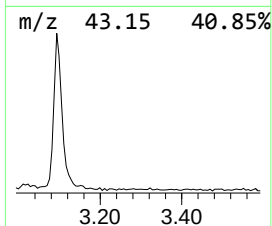
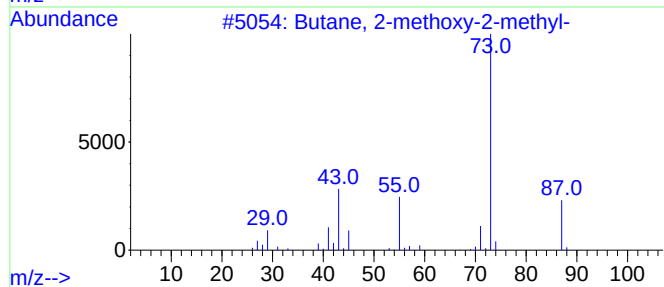
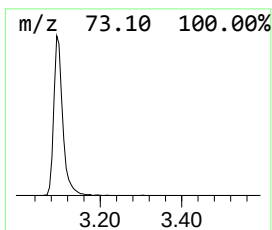
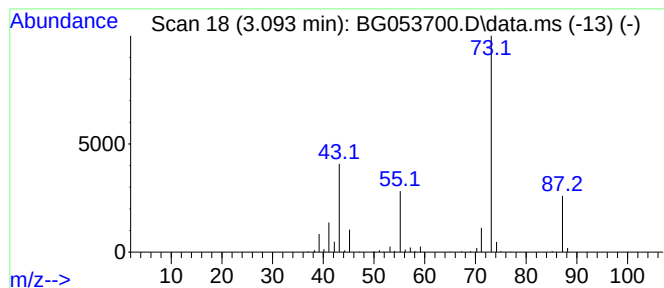
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.093	47.86 ng	304078	1,4-Dichlorobenzene-d4	7.987

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	50
3			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	16
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9



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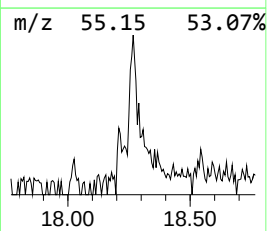
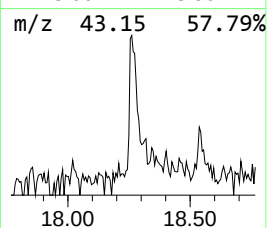
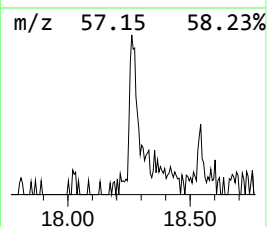
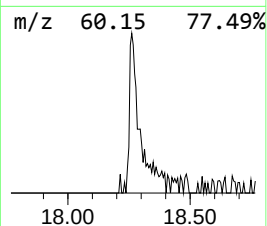
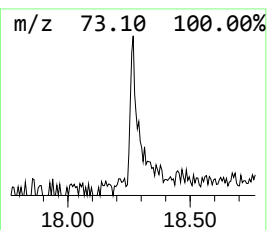
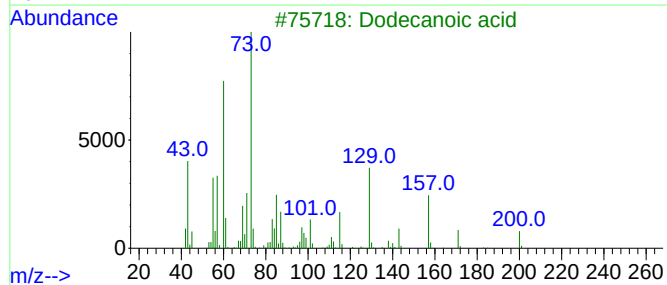
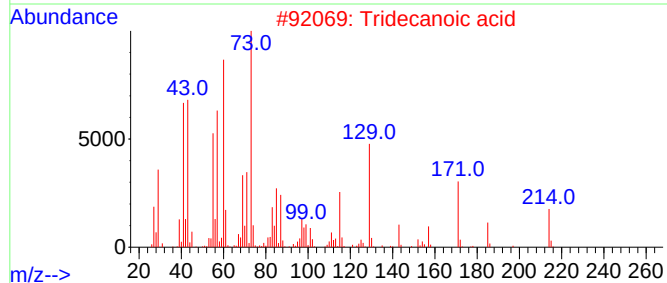
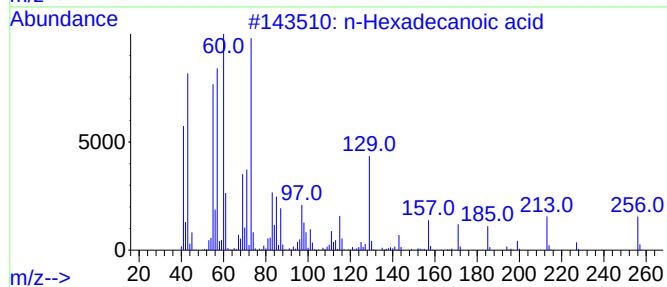
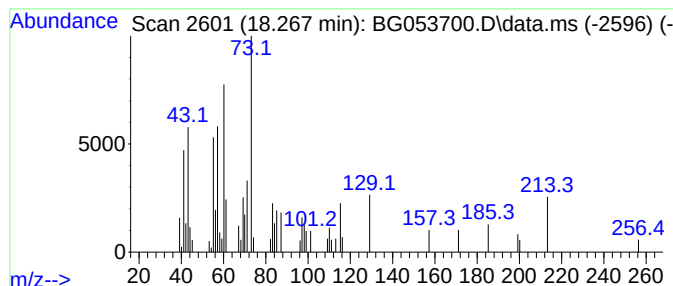
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.267	2.77 ng	56031	Phenanthrene-d10	17.368

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2			Tridecanoic acid	214	C13H26O2	000638-53-9	72
3			Dodecanoic acid	200	C12H24O2	000143-07-7	70
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	53



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ClientSampleId :
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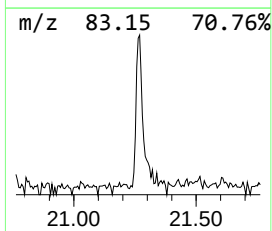
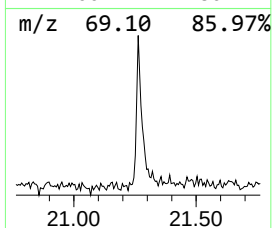
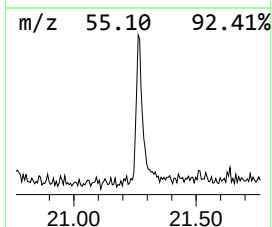
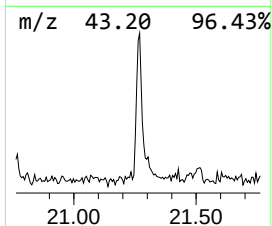
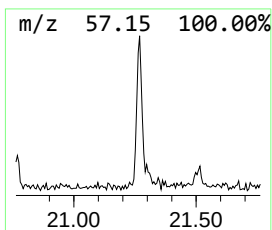
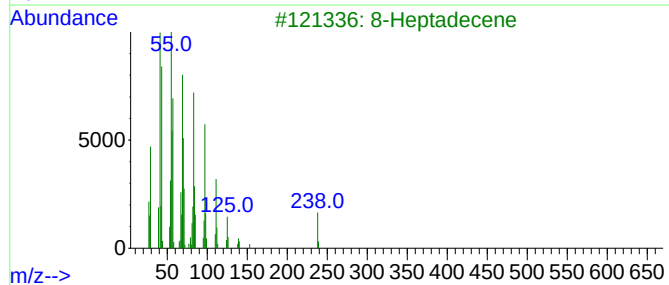
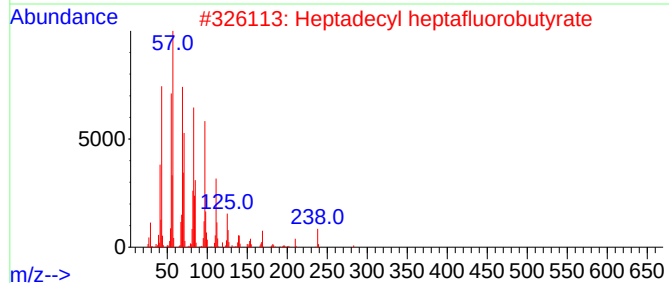
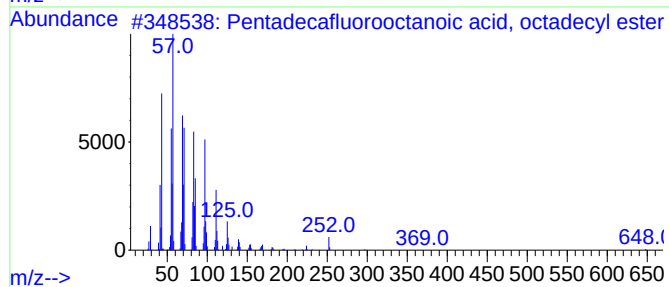
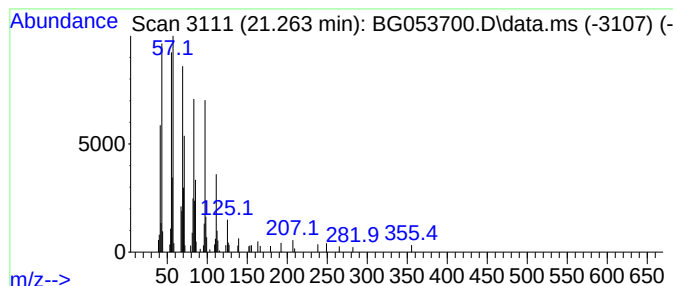
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Peak Number 4 Pentadecafluorooctanoic aci... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.263	4.85 ng	109067	Chrysene-d12	21.633

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
2			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3			8-Heptadecene	238	C17H34	002579-04-6	91
4			1-Hexacosene	364	C26H52	018835-33-1	91
5			1-Heptacosanol	396	C27H56O	002004-39-9	91



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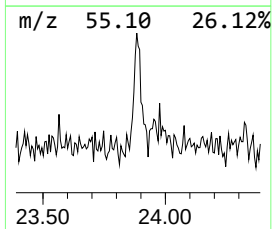
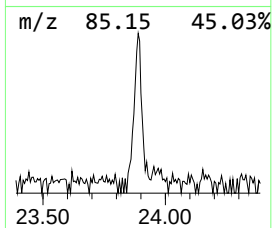
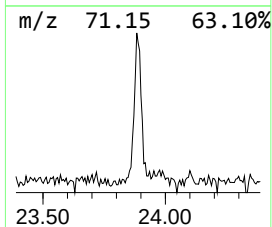
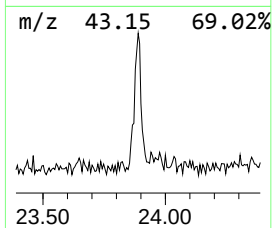
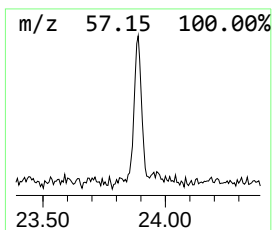
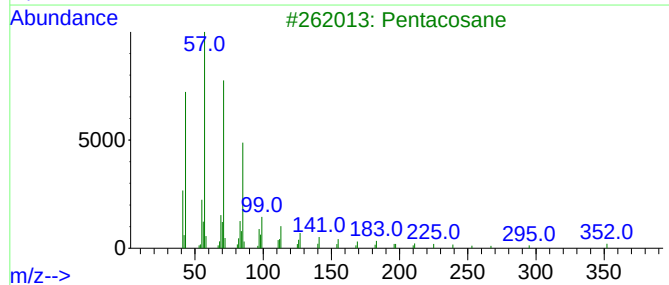
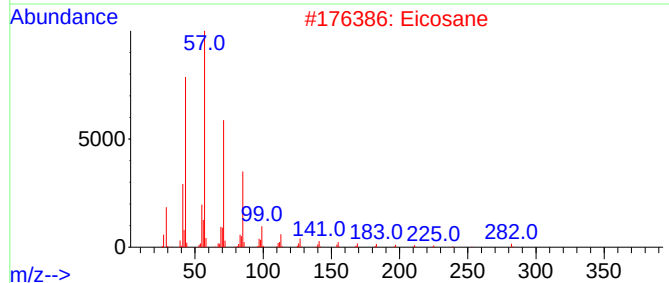
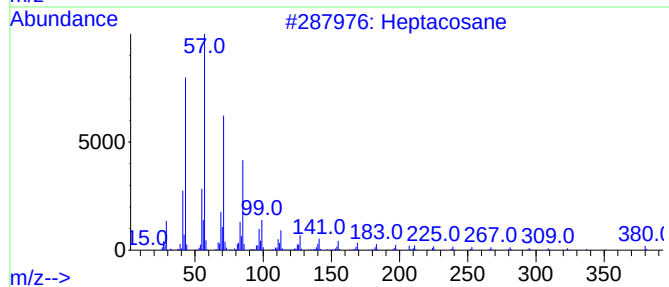
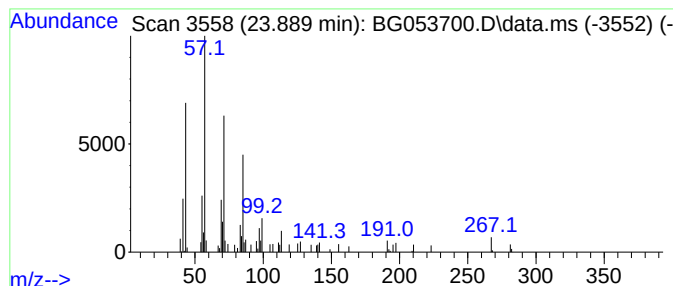
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Heptacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.889	2.25 ng	52703	Perylene-d12	24.840

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	87
2			Eicosane	282	C20H42	000112-95-8	87
3			Pentacosane	352	C25H52	000629-99-2	83
4			Octadecane	254	C18H38	000593-45-3	80
5			Nonadecane	268	C19H40	000629-92-5	80



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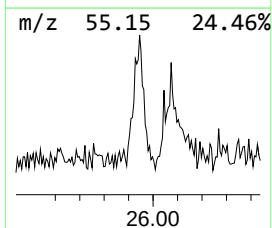
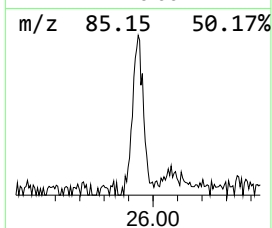
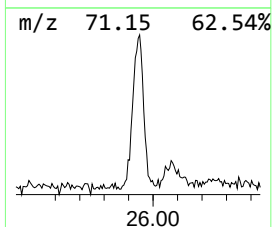
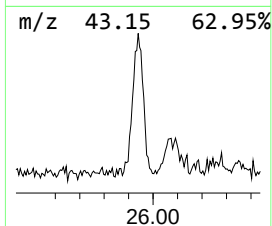
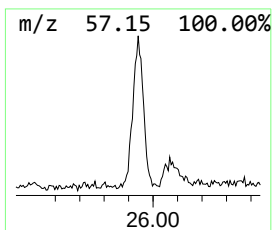
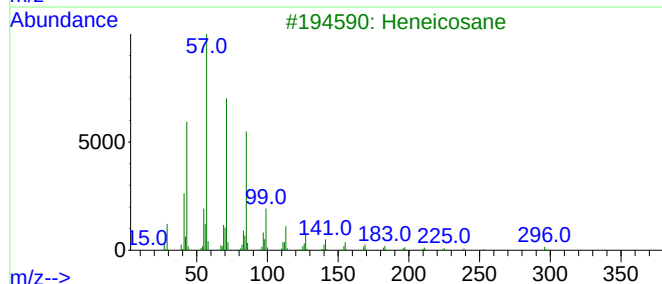
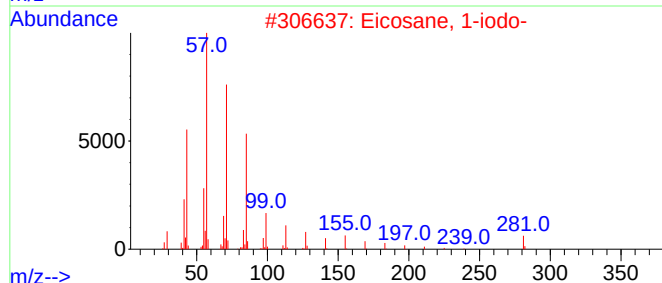
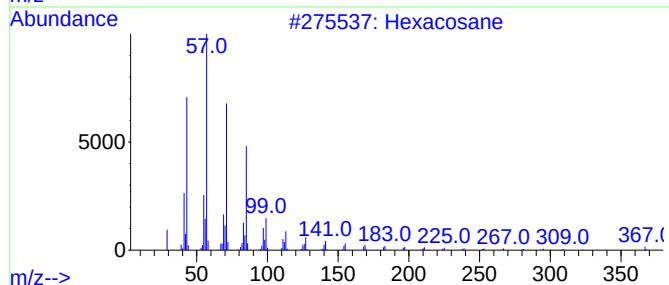
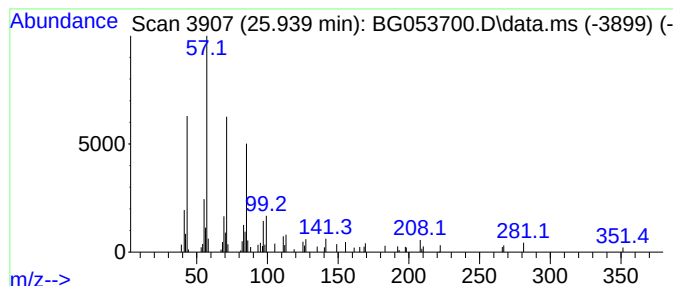
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.939	5.08 ng	118958	Perylene-d12	24.840

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexacosane	366	C26H54	000630-01-3	90
2		Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	83
3		Heneicosane	296	C21H44	000629-94-7	83
4		Tetracosane	338	C24H50	000646-31-1	80
5		Heptadecane	240	C17H36	000629-78-7	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052522\
Data File : BG053700.D
Acq On : 25 May 2022 19:10
Operator : CG/JU
Sample : N2923-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
P024-SS005-0006-01

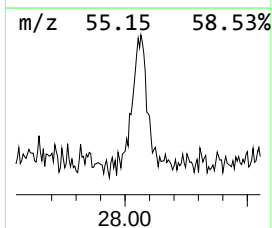
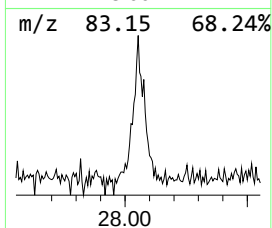
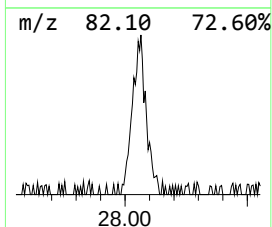
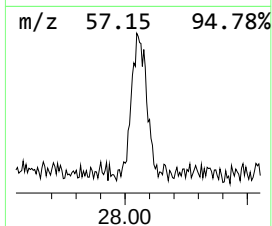
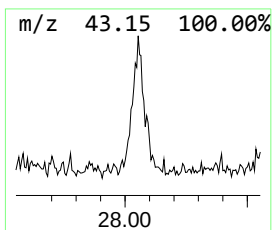
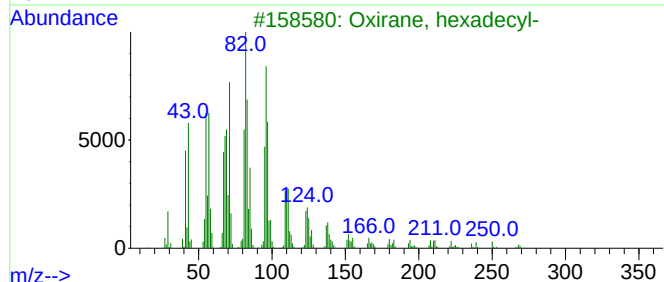
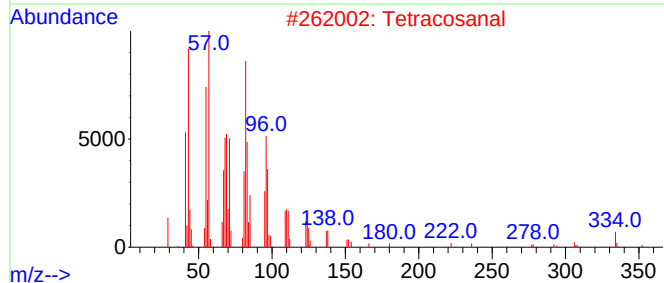
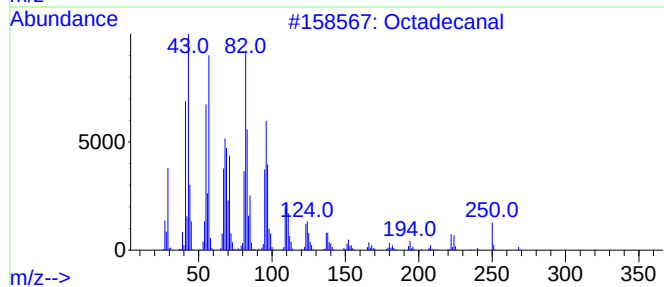
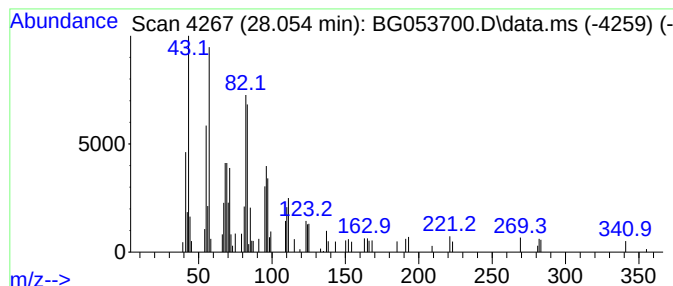
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.054	5.88 ng	137563	Perylene-d12	24.840

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal			268	C18H36O	000638-66-4	87
2	Tetracosanal			352	C24H48O	057866-08-7	74
3	Oxirane, hexadecyl-			268	C18H36O	007390-81-0	64
4	Pentadecanal-			226	C15H30O	002765-11-9	64
5	Tetradecanal			212	C14H28O	000124-25-4	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052522\
Data File : BG053700.D
Acq On : 25 May 2022 19:10
Operator : CG/JU
Sample : N2923-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
P024-SS005-0006-01

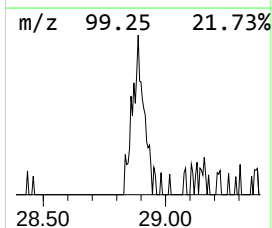
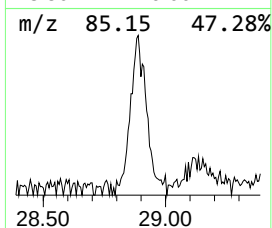
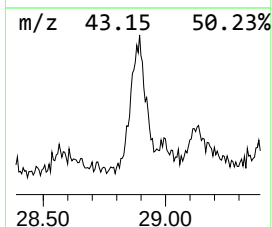
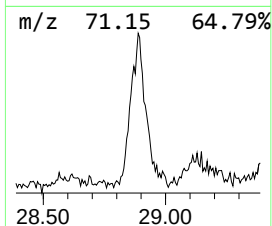
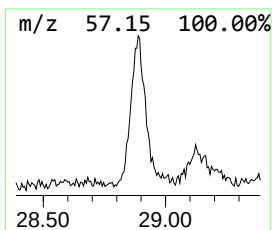
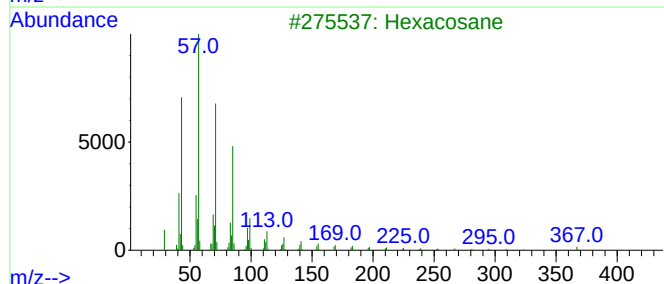
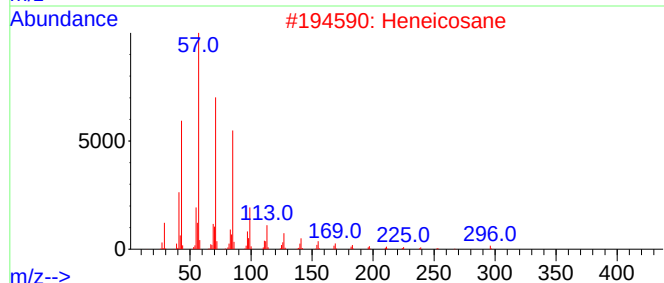
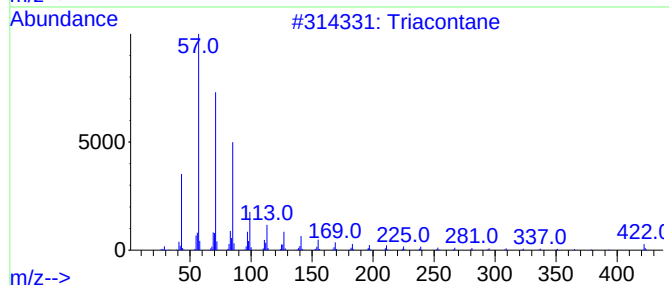
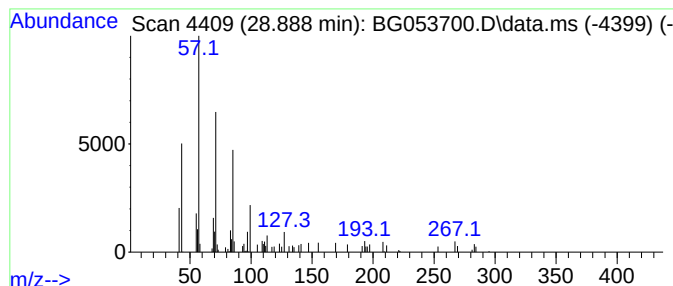
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Triacontane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.888	4.83 ng	113070	Perylene-d12	24.840

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Triacontane	422	C30H62	000638-68-6	86
2		Heneicosane	296	C21H44	000629-94-7	74
3		Hexacosane	366	C26H54	000630-01-3	74
4		Pentacosane	352	C25H52	000629-99-2	74
5		Nonadecane	268	C19H40	000629-92-5	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052522\
Data File : BG053700.D
Acq On : 25 May 2022 19:10
Operator : CG/JU
Sample : N2923-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P024-SS005-0006-01

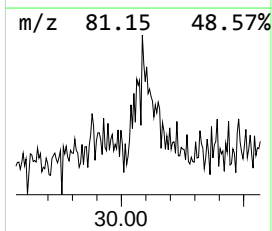
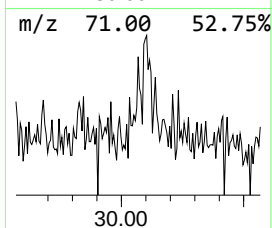
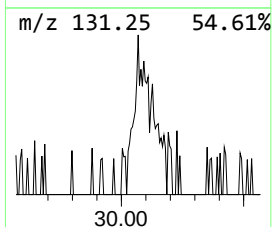
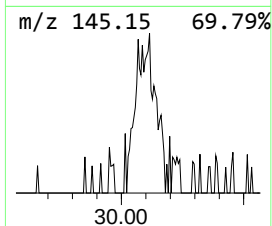
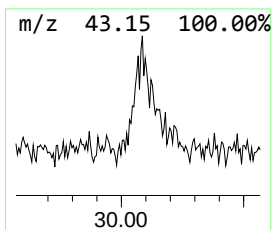
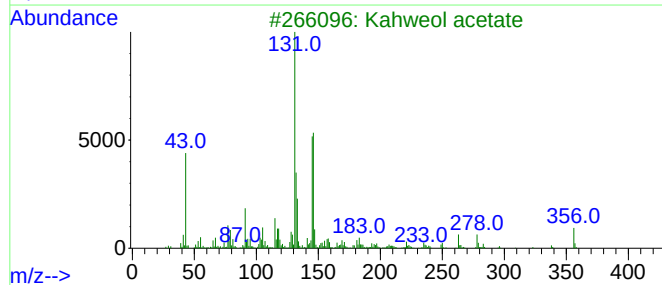
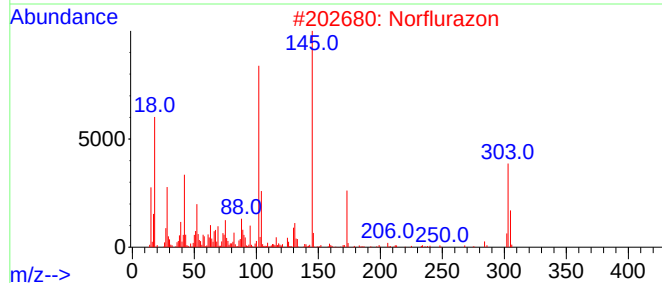
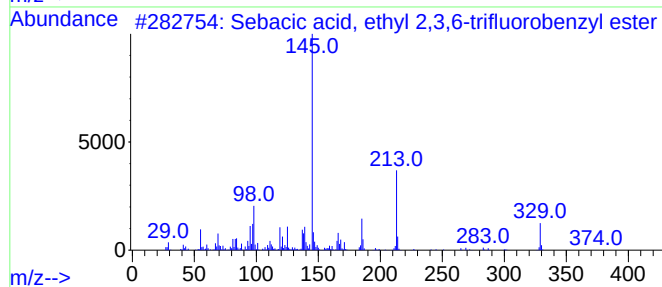
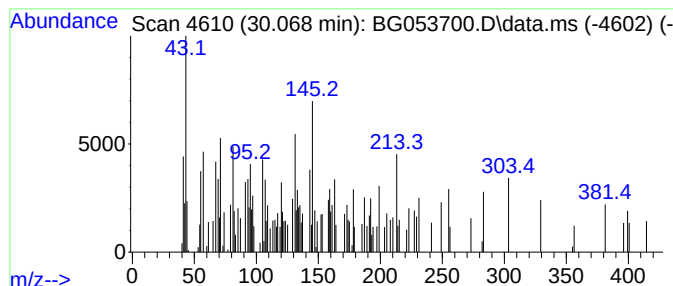
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown30.068 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
30.068	2.10 ng	49216	Perylene-d12	24.840

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sebacic acid, ethyl 2,3,6-triflu...	374	C19H25F3O4	1000380-79-0	10
2			Norflurazon	303	C12H9ClF3N3O	027314-13-2	10
3			Kahweol acetate	356	C22H28O4	081760-47-6	9
4			Sebacic acid, pentyl 2,3,6-trifl...	416	C22H31F3O4	1000380-79-4	9
5			Sebacic acid, propyl 2,3,6-trifl...	388	C20H27F3O4	1000380-79-1	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052522\
Data File : BG053700.D
Acq On : 25 May 2022 19:10
Operator : CG/JU
Sample : N2923-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P024-SS005-0006-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Butane, 2-metho...	3.093	47.9	ng	304078	1	7.987	127069	20.0
n-Hexadecanoic ...	18.267	2.8	ng	56031	4	17.368	405155	20.0
Pentadecafluoro...	21.263	4.8	ng	109067	5	21.633	449336	20.0
Heptacosane	23.889	2.3	ng	52703	6	24.840	468126	20.0
Hexacosane	25.939	5.1	ng	118958	6	24.840	468126	20.0
Octadecanal	28.054	5.9	ng	137563	6	24.840	468126	20.0
triacontane	28.888	4.8	ng	113070	6	24.840	468126	20.0
unknown30.068	30.068	2.1	ng	49216	6	24.840	468126	20.0