LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG063023\
Data File : BG057929.D
Acq On : 30 Jun 2023 21:52
Operator : CG/JU
Sample : 03358-08
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-6-(8-10)

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-BG062723.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057929.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.617	85	90	98	rBV	22560	34851	1.15%	0.230%
2	5.015	322	328	335	rBV	35056	52916	1.75%	0.350%
3	5.485	401	408	419	rBV	685167	1067850	35.31%	7.055%
4	7.078	671	679	698	rBV	695977	1171269	38.73%	7.738%
5	7.912	814	821	828	rBV	141615	233849	7.73%	1.545%
6	9.069	1009	1018	1032	rBV	408572	717171	23.71%	4.738%
7	10.715	1290	1298	1306	rBV	199546	357751	11.83%	2.364%
8	13.171	1709	1716	1726	rVB	1139728	1765285	58.37%	11.663%
9	14.545	1944	1950	1958	rVB	364623	582843	19.27%	3.851%
10	15.903	2175	2181	2192	rBV	329994	463450	15.32%	3.062%
11	16.032	2197	2203	2215	rBV	1013043	1574457	52.06%	10.402%
12	16.467	2271	2277	2283	rBV	67626	94039	3.11%	0.621%
13	17.289	2411	2417	2423	rBV	530766	790273	26.13%	5.221%
14	17.471	2443	2448	2456	rBV5	24759	40624	1.34%	0.268%
15	18.176	2563	2568	2580	rBV	173255	285210	9.43%	1.884%
16	19.451	2781	2785	2790	rBV2	37029	58004	1.92%	0.383%
17	19.910	2856	2863	2872	rBV	2274640	3024436	100.00%	19.982%
18	21.191	3077	3081	3092	rBV	147496	238576	7.89%	1.576%
19	21.543	3135	3141	3147	rBV2	500730	797447	26.37%	5.269%
20	21.731	3170	3173	3178	rVB2	25635	34577	1.14%	0.228%
21	22.330	3270	3275	3287	rVB3	34314	73794	2.44%	0.488%
22	22.983	3379	3386	3401	rBV2	308330	693547	22.93%	4.582%
23	23.788	3519	3523	3529	rVB2	27311	49146	1.62%	0.325%
24	24.686	3666	3676	3690	rBV	332353	934368	30.89%	6.173%

Sum of corrected areas: 15135733

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Instrument :
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ClientSampleId :
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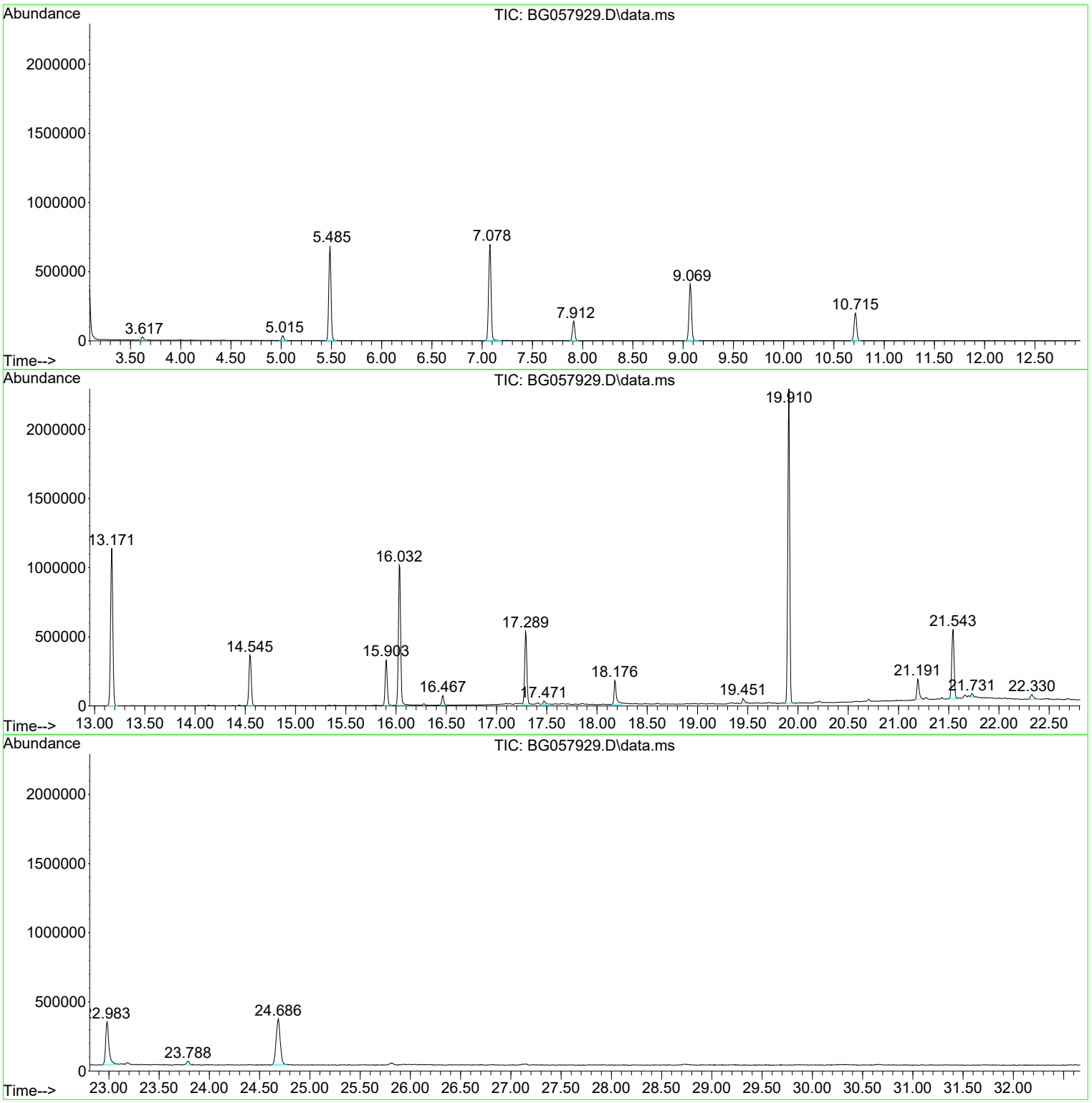
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG062723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG063023\
Data File : BG057929.D
Acq On : 30 Jun 2023 21:52
Operator : CG/JU
Sample : 03358-08
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG062723.M
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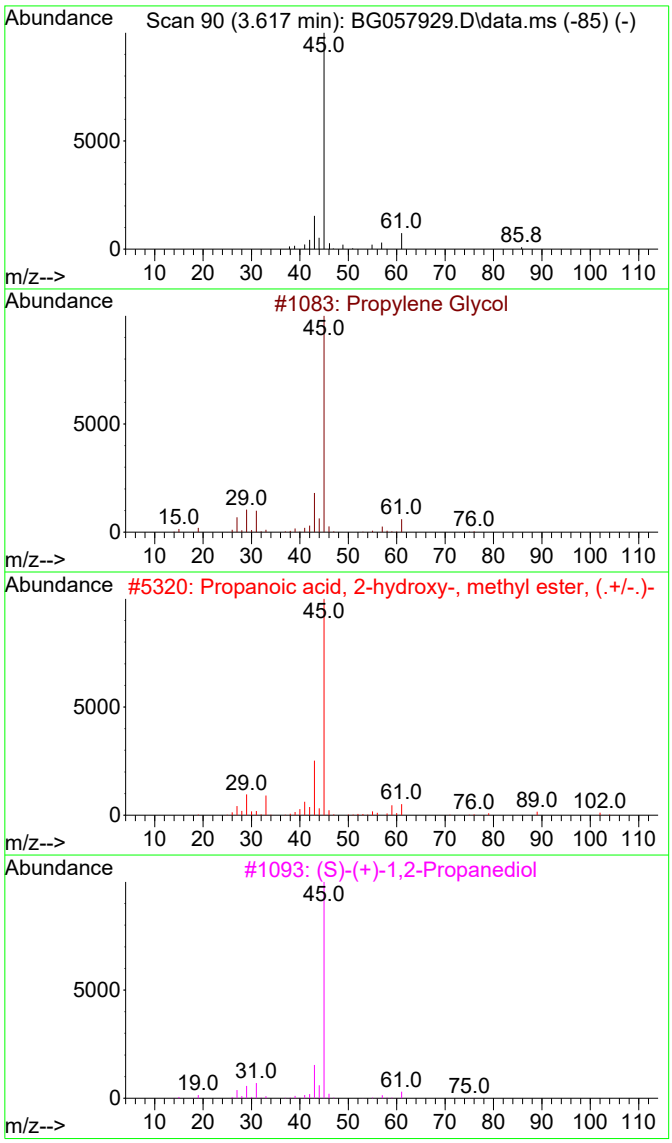
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

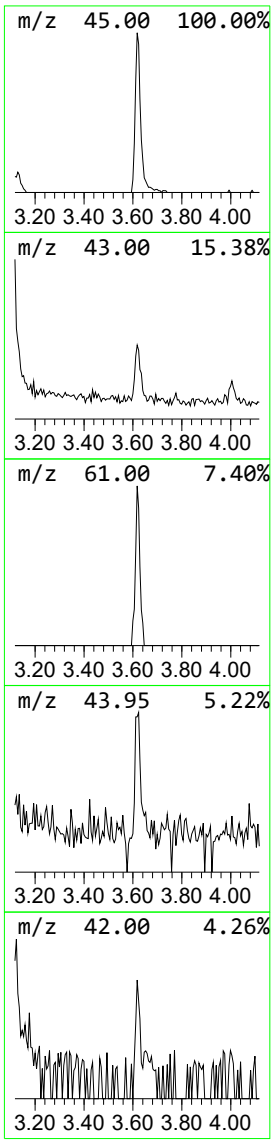
****

Peak Number 1 unknown3.617 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.617	2.98 ng	34851	1,4-Dichlorobenzene-d4	7.912

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	43
2	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
3	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	9
4	2,3-Butanediol	90	C4H10O2	000513-85-9	9
5	Isopropyl Alcohol	60	C3H8O	000067-63-0	9





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Data File : BG057929.D
Acq On : 30 Jun 2023 21:52
Operator : CG/JU
Sample : 03358-08
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-6-(8-10)

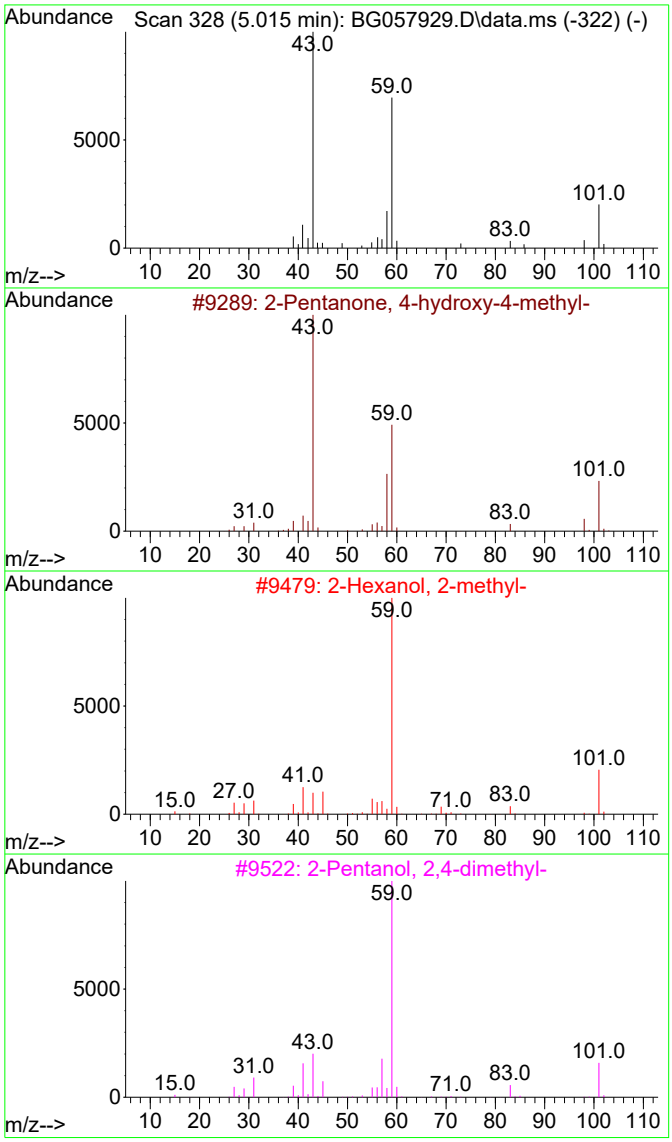
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG062723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

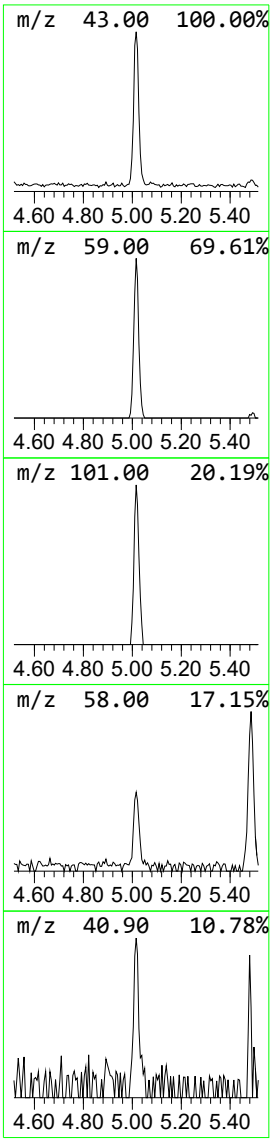
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.015	4.53 ng	52916	1,4-Dichlorobenzene-d4	7.912

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	47
3	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	42
4	3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	36
5	3-Octanol	130	C8H18O	000589-98-0	33





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Data File : BG057929.D
Acq On : 30 Jun 2023 21:52
Operator : CG/JU
Sample : 03358-08
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-6-(8-10)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG062723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

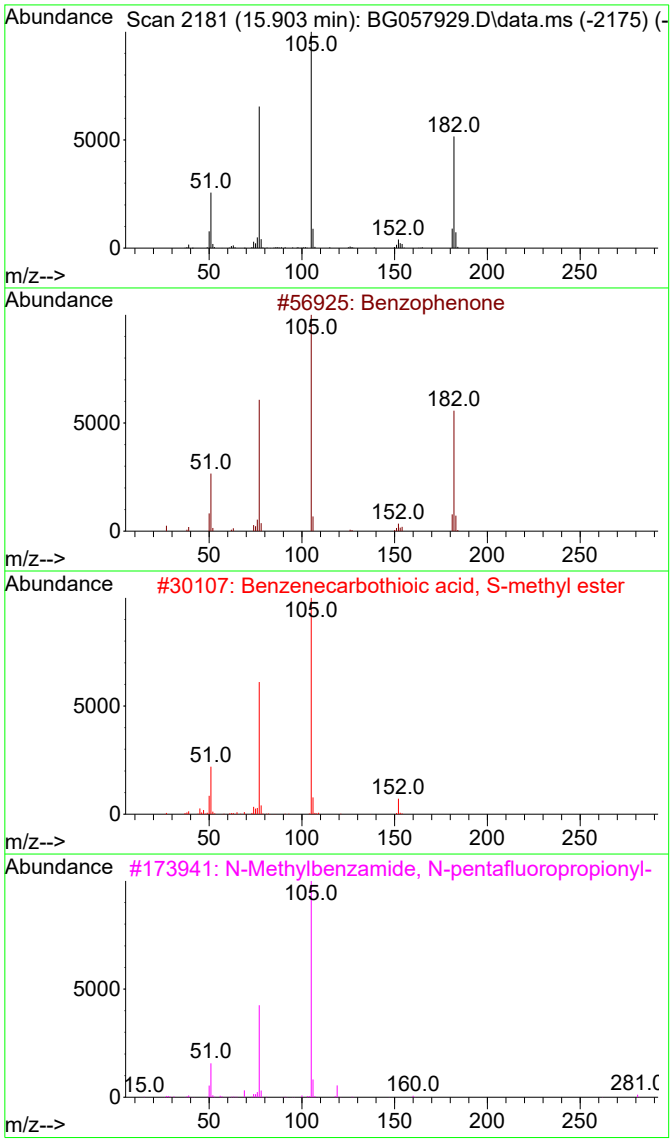
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

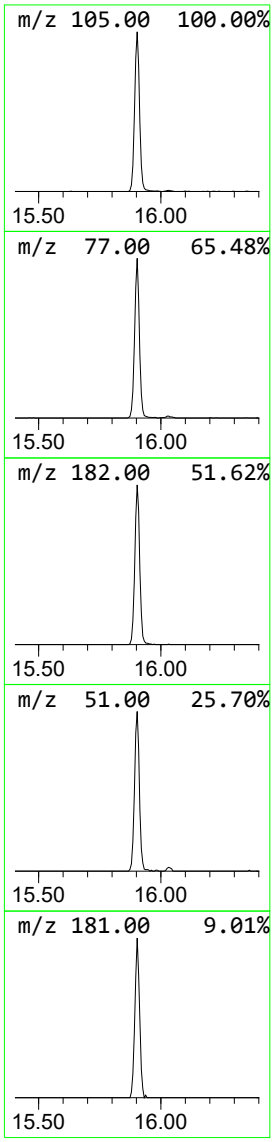
****

Peak Number 3 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.903	15.90 ng	463450	Acenaphthene-d10	14.545

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	49
3	N-Methylbenzamide, N-pentafluoro...	281	C11H8F5NO2	1000446-98-1	47
4	N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47
5	Vinyl benzoate	148	C9H8O2	000769-78-8	47





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Acq On : 30 Jun 2023 21:52
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Sample : 03358-08
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Instrument :
BNA_G
ClientSampleId :
SB-6-(8-10)

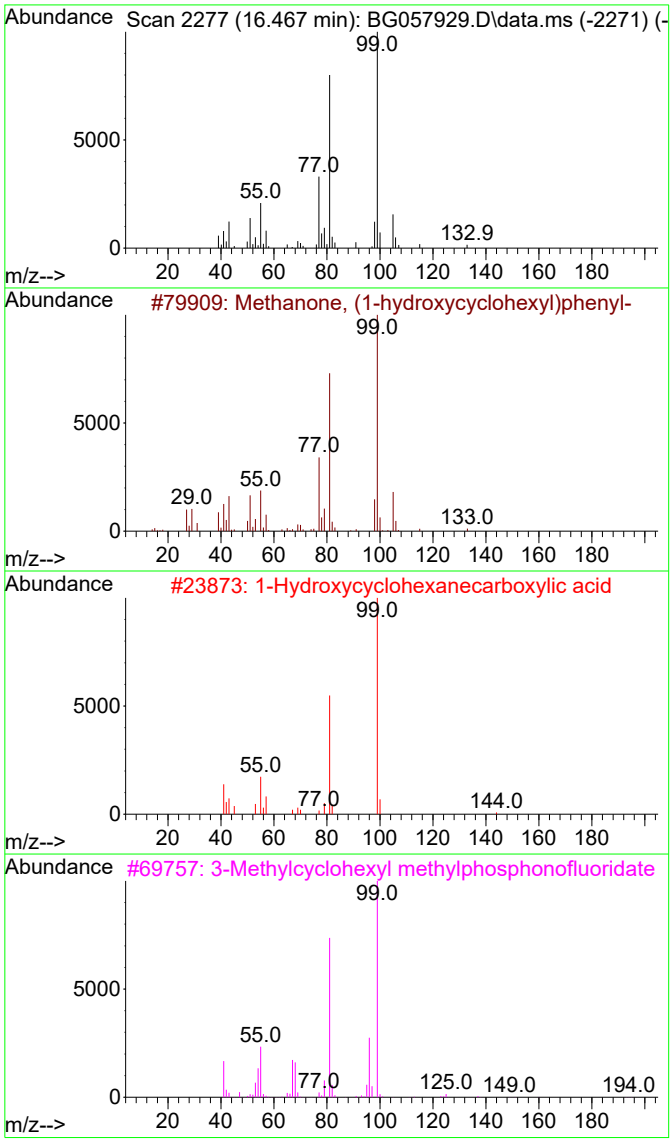
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG062723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

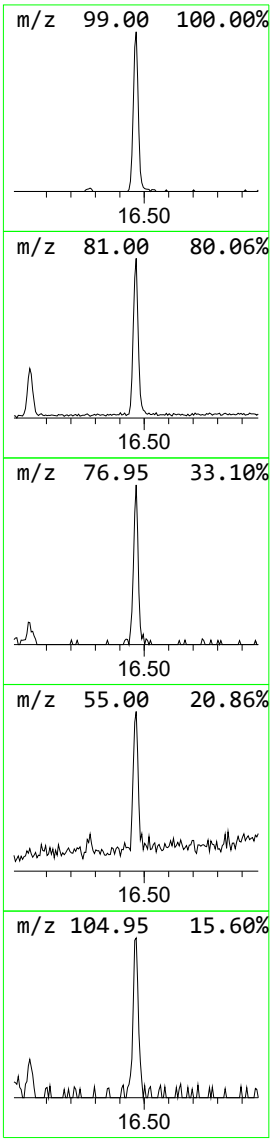
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Methanone, (1-hydroxycycloh... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.467	2.38 ng	94039	Phenanthrene-d10	17.289

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methanone, (1-hydroxycyclohexyl)...	204	C13H16O2	000947-19-3	90
2	1-Hydroxycyclohexanecarboxylic acid	144	C7H12O3	001123-28-0	59
3	3-Methylcyclohexyl methylphospho...	194	C8H16FO2P	113548-86-0	45
4	2-Methylcyclosarin	194	C8H16FO2P	085473-32-1	42
5	Cyclohexanol, 1-ethyl-	128	C8H16O	001940-18-7	38





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Data File : BG057929.D
Acq On : 30 Jun 2023 21:52
Operator : CG/JU
Sample : 03358-08
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ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-6-(8-10)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG062723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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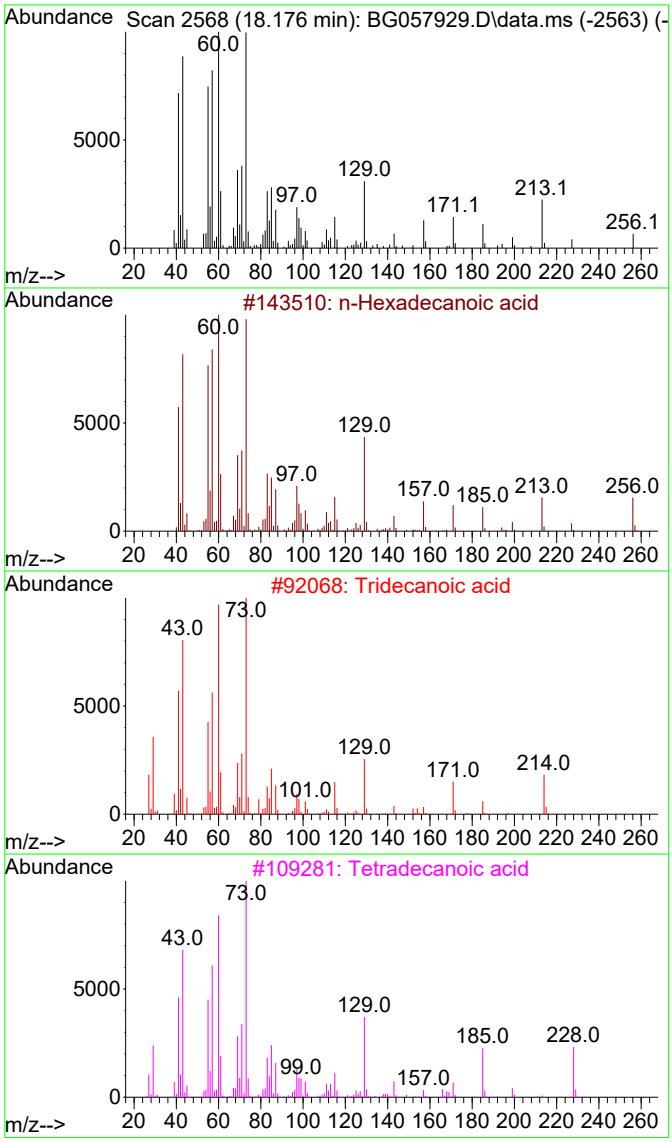
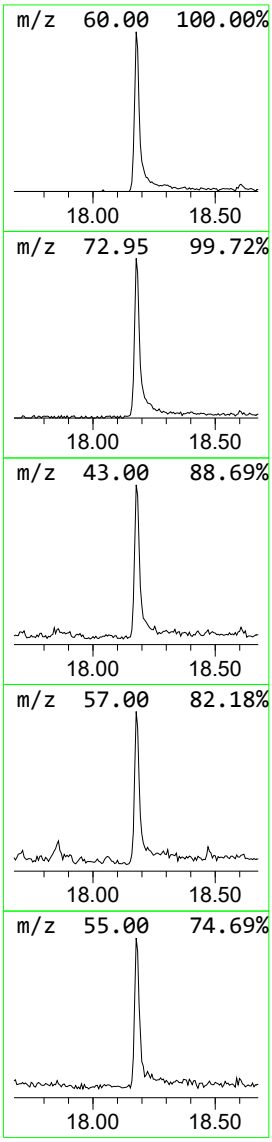
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.177	7.22 ng	285210	Phenanthrene-d10	17.289

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
2	Tridecanoic acid	214	C13H26O2	000638-53-9	87
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
5	Dodecanoic acid	200	C12H24O2	000143-07-7	64





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Instrument :
BNA_G
ClientSampleId :
SB-6-(8-10)

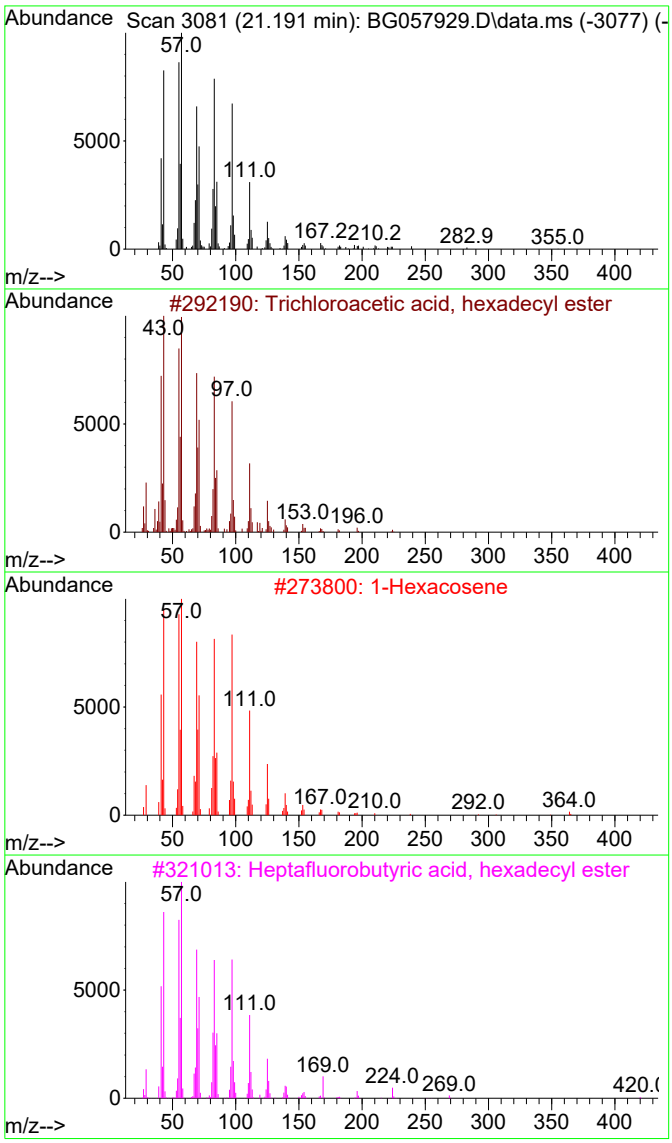
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG062723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

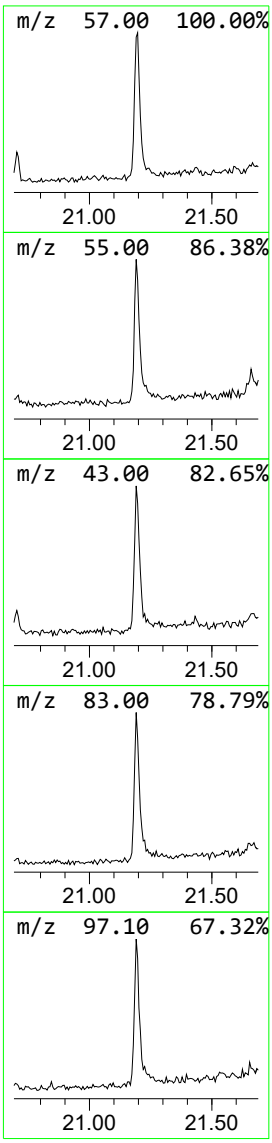
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Trichloroacetic acid, hexad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.191	5.98 ng	238576	Chrysene-d12	21.543

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2	1-Hexacosene	364	C26H52	018835-33-1	91
3	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91
4	1-Heneicosanol	312	C21H44O	015594-90-8	90
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	90





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SB-6-(8-10)

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

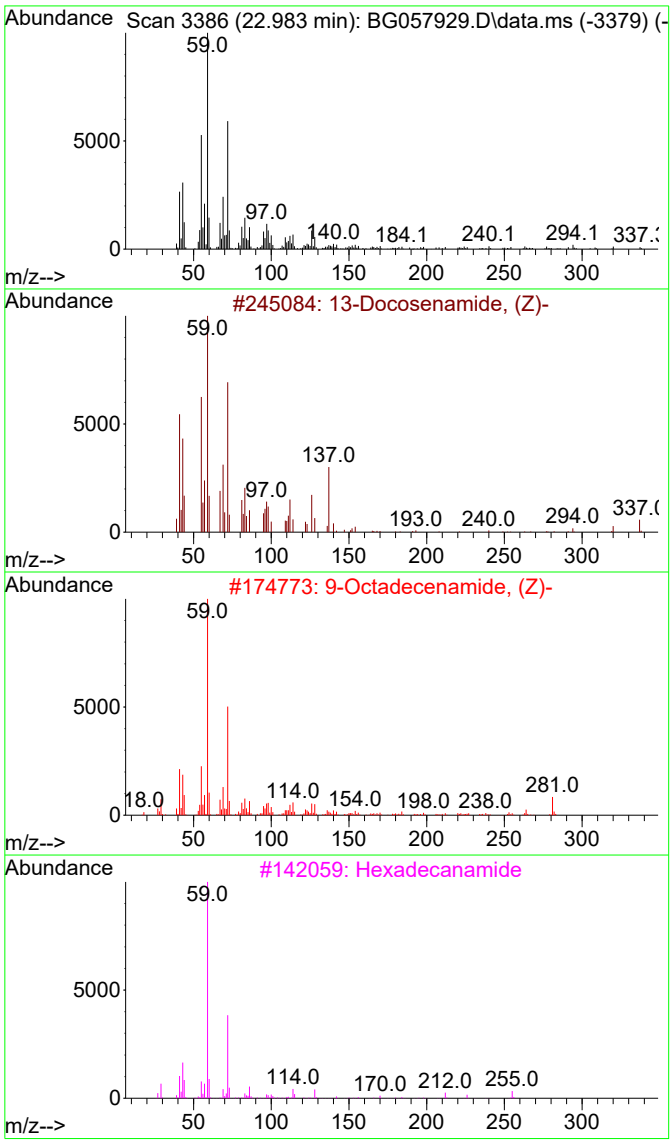
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

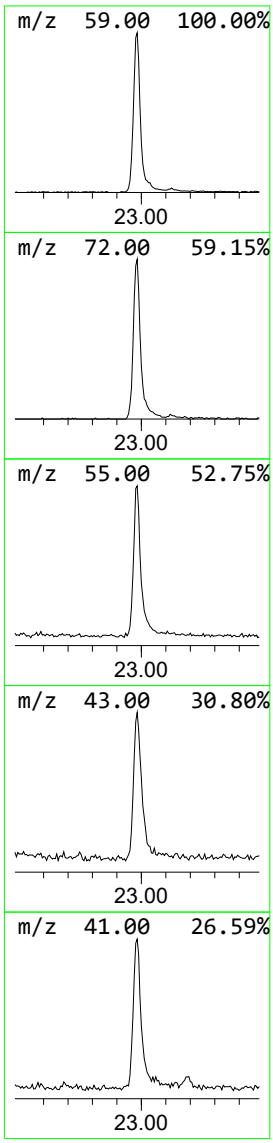
****

Peak Number 7 13-Docosenamide, (Z)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.983	17.39 ng	693547	Chrysene-d12	21.543

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	93
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	87
3	Hexadecanamide	255	C16H33NO	000629-54-9	78
4	Tetradecanamide	227	C14H29NO	000638-58-4	78
5	Palmitoleamide	253	C16H31NO	106010-22-4	64





Tentatively Identified Compound (LSC) summary

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown3.617	3.617	3.0	ng	34851	1	7.912	233849	20.0
2-Pentanone, 4-...	5.015	4.5	ng	52916	1	7.912	233849	20.0
Benzophenone	15.903	15.9	ng	463450	3	14.545	582843	20.0
Methanone, (1-h...	16.467	2.4	ng	94039	4	17.289	790273	20.0
n-Hexadecanoic ...	18.177	7.2	ng	285210	4	17.289	790273	20.0
Trichloroacetic...	21.191	6.0	ng	238576	5	21.543	797447	20.0
13-Docosenamide...	22.983	17.4	ng	693547	5	21.543	797447	20.0