LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062923\
Data File : BG057909.D
Acq On : 29 Jun 2023 18:08
Operator : CG/JU
Sample : 03358-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-1-(34-36)

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: BG057909.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.022	323	329	335	rVB	26080	40246	1.60%	0.300%
2	5.492	401	409	421	rBV	683520	1093045	43.33%	8.136%
3	7.084	672	680	690	rBV	672889	1172684	46.49%	8.729%
4	7.913	814	821	828	rBV	148131	241079	9.56%	1.795%
5	9.076	1011	1019	1027	rBV	383457	673033	26.68%	5.010%
6	10.715	1291	1298	1307	rVB	197512	345213	13.68%	2.570%
7	13.171	1709	1716	1723	rBV	969845	1476558	58.53%	10.991%
8	14.546	1943	1950	1957	rVB	309523	480789	19.06%	3.579%
9	15.903	2173	2181	2187	rBV	239722	339080	13.44%	2.524%
10	16.038	2197	2204	2217	rBV	829276	1330591	52.75%	9.905%
11	16.467	2272	2277	2285	rVB	43851	64517	2.56%	0.480%
12	17.290	2411	2417	2424	rBV	449486	658998	26.12%	4.905%
13	17.472	2443	2448	2453	rBV2	16383	25966	1.03%	0.193%
14	18.189	2565	2570	2578	rBV5	27991	80954	3.21%	0.603%
15	19.910	2857	2863	2871	rBV	1920905	2522618	100.00%	18.778%
16	20.703	2996	2998	3001	rBV2	30908	37360	1.48%	0.278%
17	21.197	3077	3082	3090	rVB2	294415	434787	17.24%	3.236%
18	21.544	3135	3141	3148	rBV	431904	712111	28.23%	5.301%
19	21.738	3170	3174	3179	rVB	112941	160904	6.38%	1.198%
20	22.331	3271	3275	3286	rVB2	97503	175632	6.96%	1.307%
21	22.989	3381	3387	3401	rVB4	179745	455259	18.05%	3.389%
22	23.788	3520	3523	3530	rVB	36204	67973	2.69%	0.506%
23	24.687	3667	3676	3689	rVB	296539	844523	33.48%	6.286%

Sum of corrected areas: 13433920

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062923\
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Misc :
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Instrument :
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ClientSampleId :
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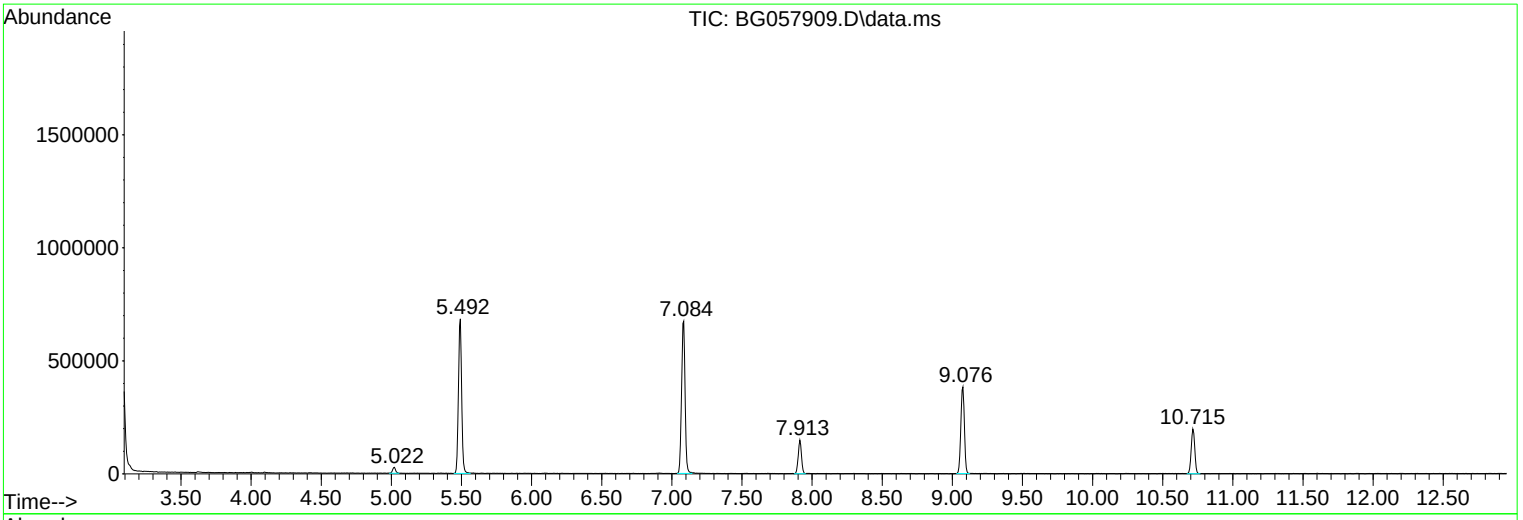
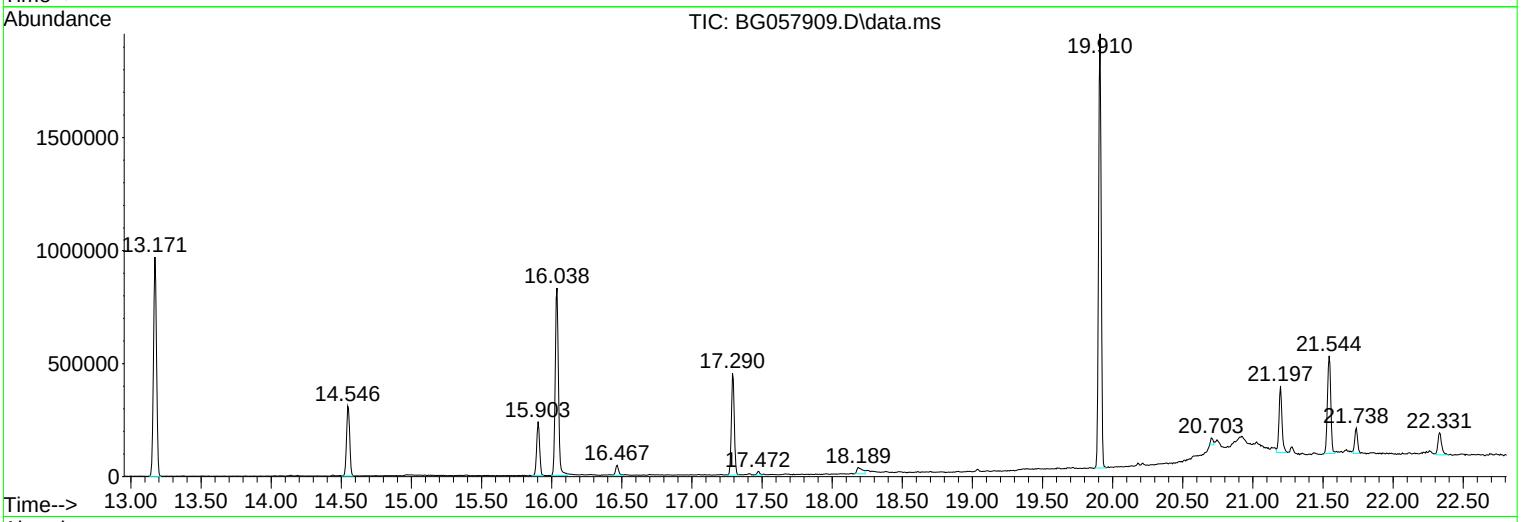
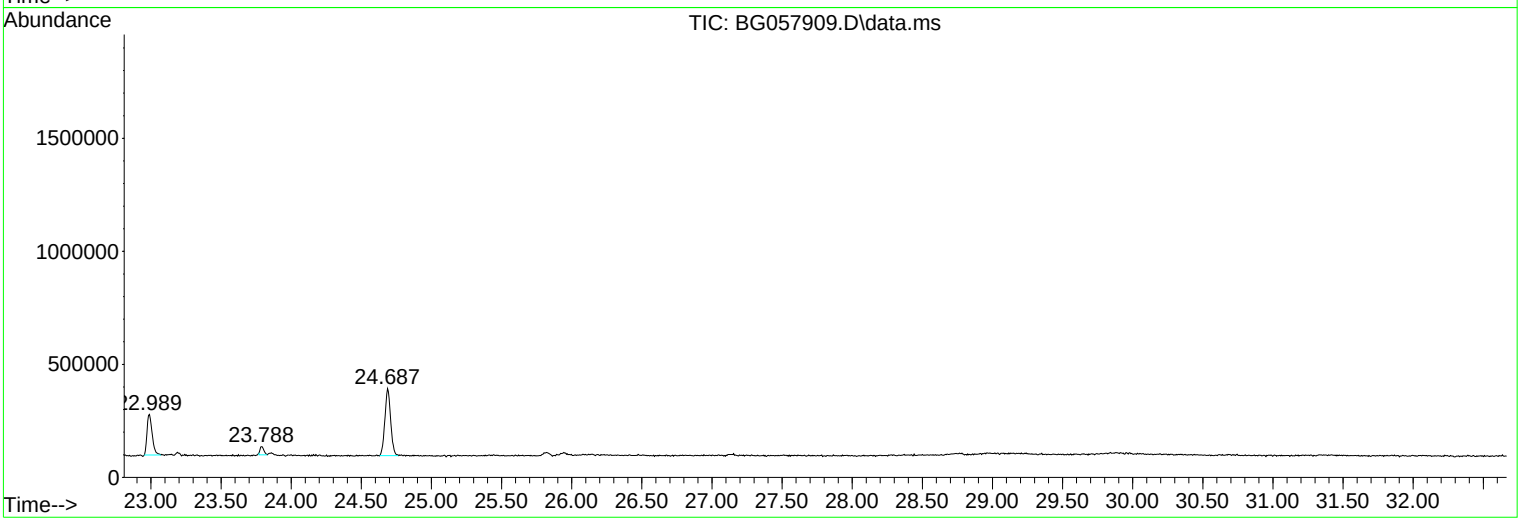
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG062723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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Data File : BG057909.D
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ClientSampleId :
SB-1-(34-36)

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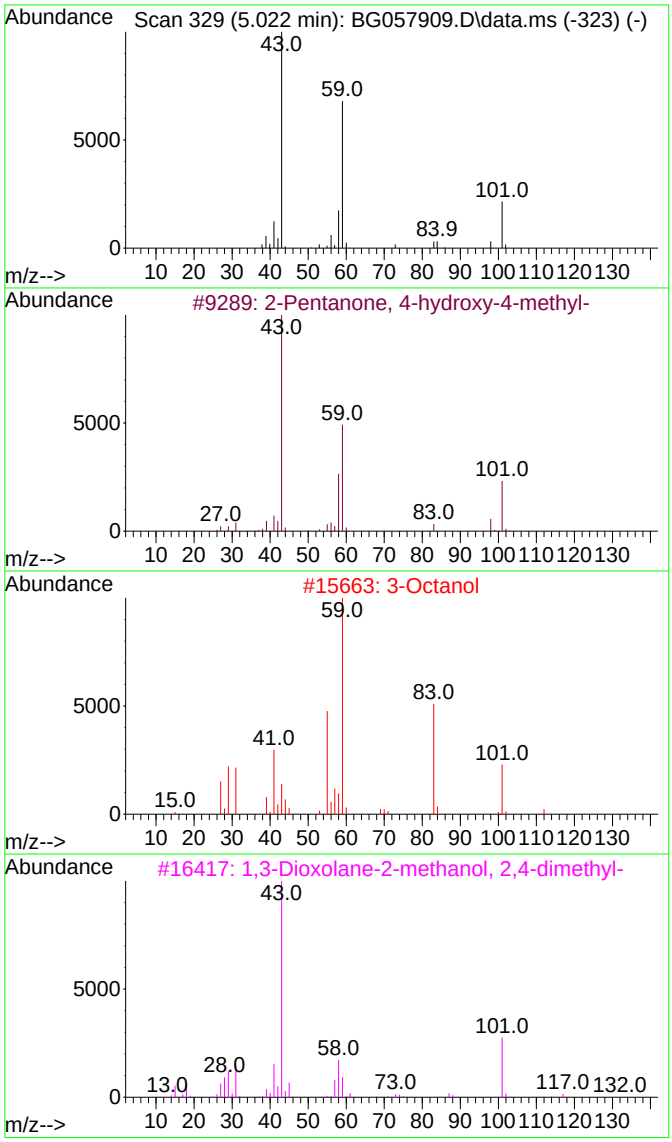
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

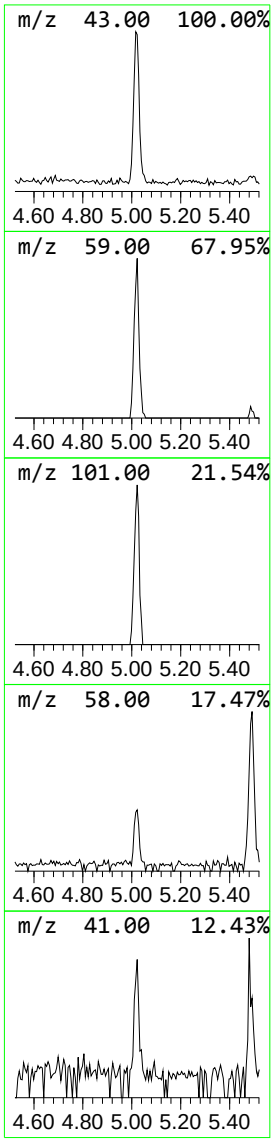
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.022	3.34 ng	40246	1,4-Dichlorobenzene-d4	7.913

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	3-Octanol	130	C8H18O	000589-98-0	42
3	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	25
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





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Operator : CG/JU
Sample : 03358-03
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Instrument :
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ClientSampleId :
SB-1-(34-36)

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

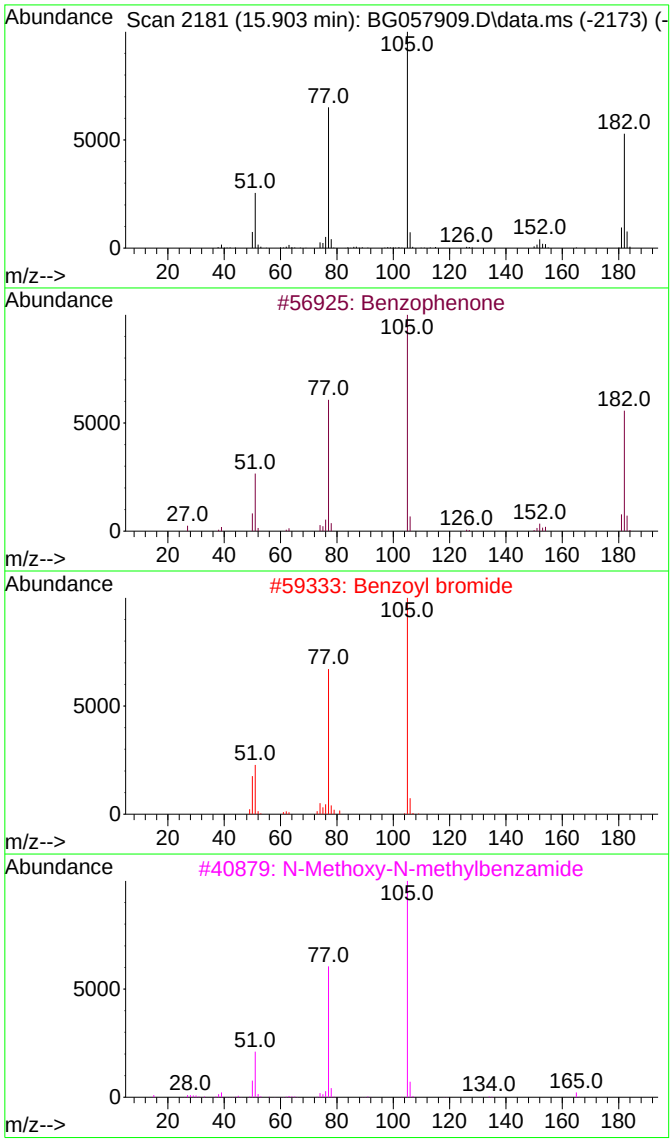
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

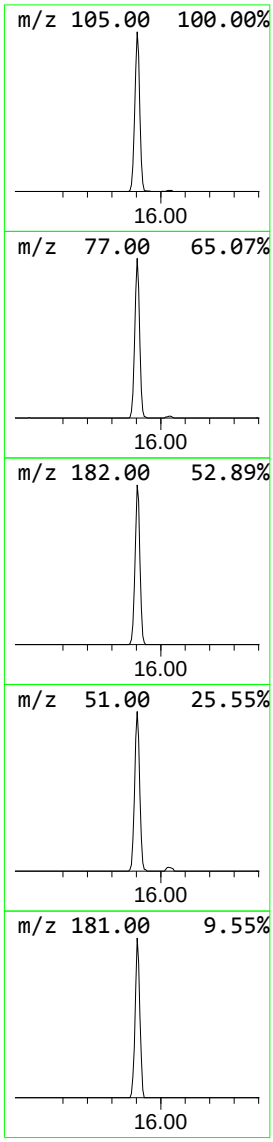
****

Peak Number 2 Benzophenone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.903	14.11 ng	339080	Acenaphthene-d10	14.546

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Benzoyl bromide	184	C7H5BrO	000618-32-6	47
3	N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47
4	Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47
5	Vinyl benzoate	148	C9H8O2	000769-78-8	47





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Sample : 03358-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-1-(34-36)

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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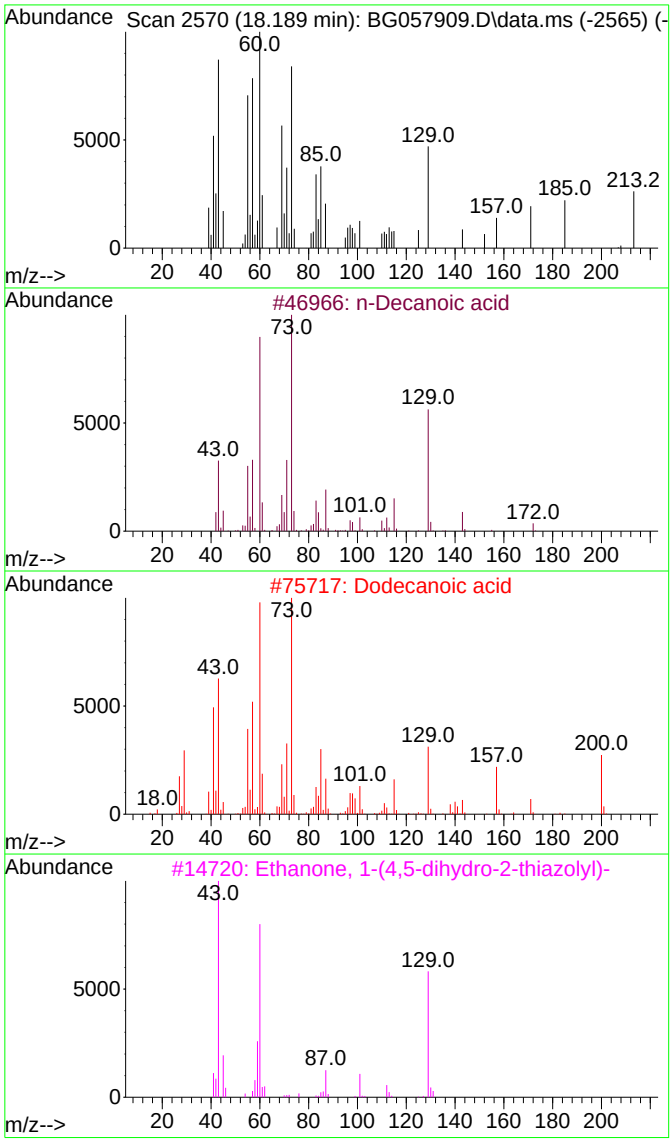
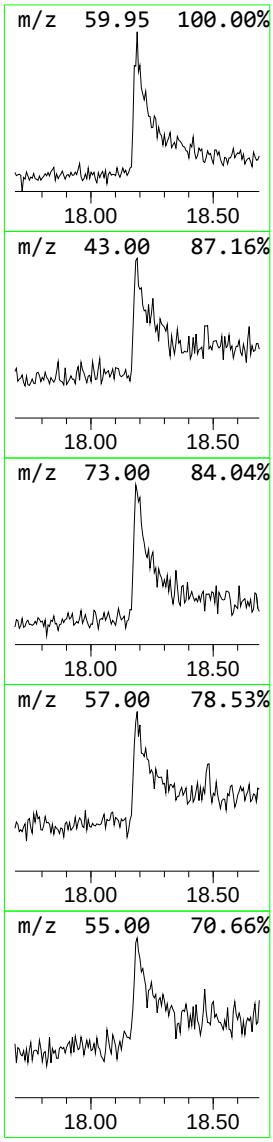
****

Peak Number 3 unknown18.189 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.189	2.46 ng	80954	Phenanthrene-d10	17.290

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Decanoic acid	172	C10H20O2	000334-48-5	47
2	Dodecanoic acid	200	C12H24O2	000143-07-7	47
3	Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	38
4	11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	38
5	Undecanoic acid	186	C11H22O2	000112-37-8	38





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Operator : CG/JU
Sample : 03358-03
Misc :
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Instrument :
BNA_G
ClientSampleId :
SB-1-(34-36)

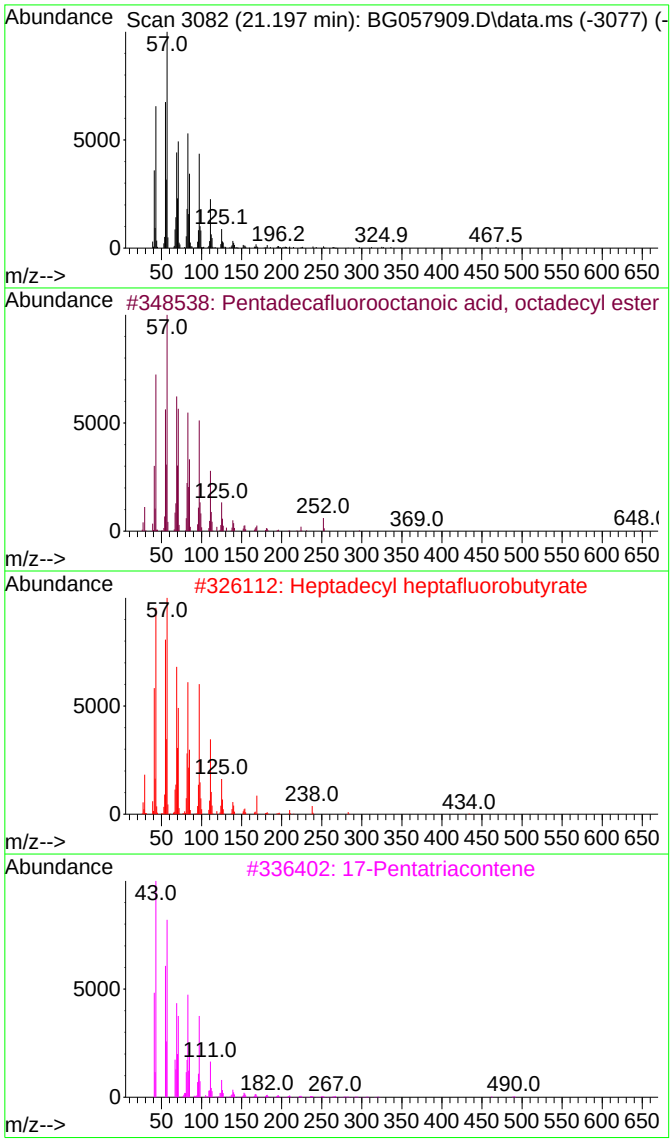
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG062723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

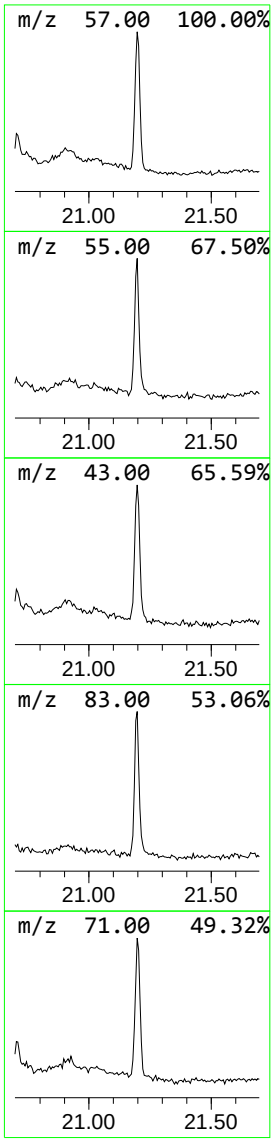
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Pentadecafluorooctanoic aci... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.197	12.21 ng	434787	Chrysene-d12	21.544

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
3	17-Pentatriacontene	491	C35H70	006971-40-0	91
4	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	91
5	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062923\
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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-1-(34-36)

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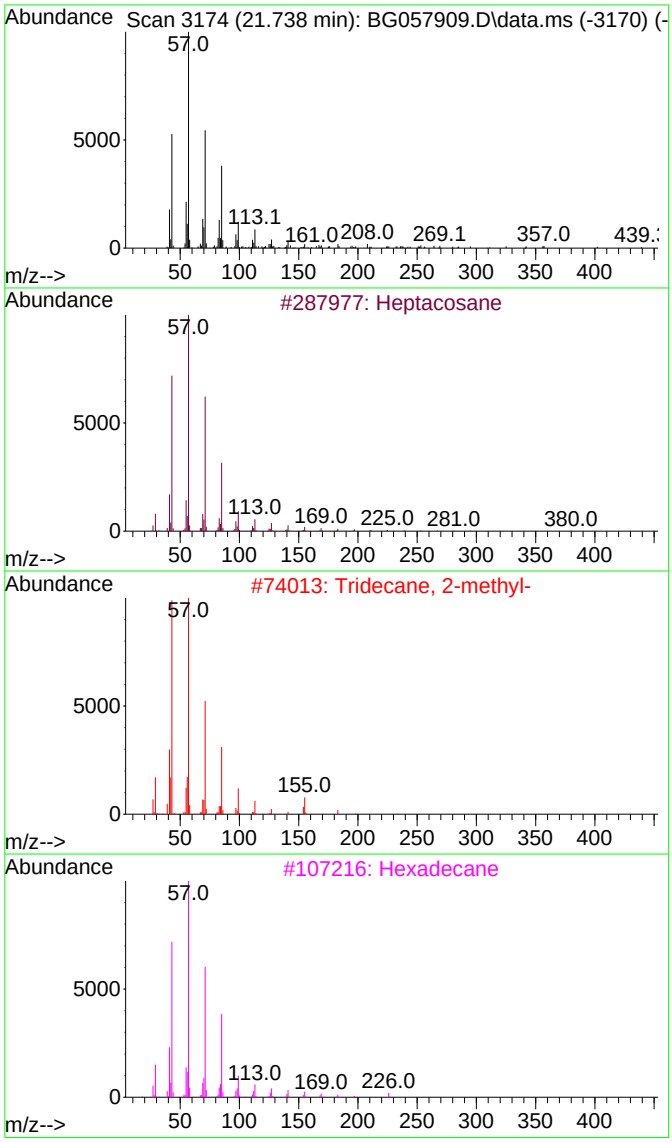
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

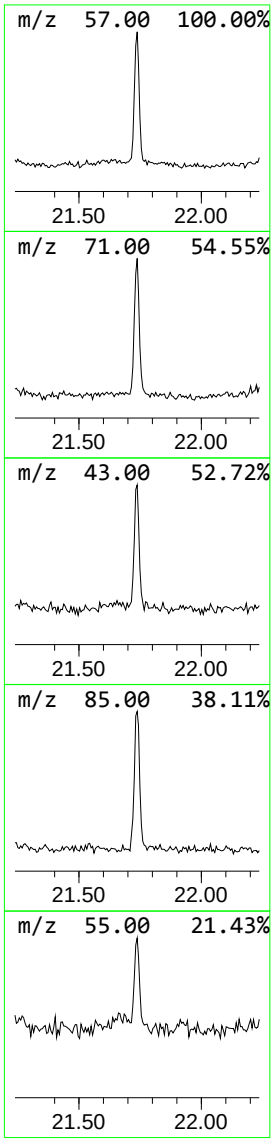
****

Peak Number 5 Heptacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.738	4.52 ng	160904	Chrysene-d12	21.544

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	90
2	Tridecane, 2-methyl-	198	C14H30	001560-96-9	87
3	Hexadecane	226	C16H34	000544-76-3	87
4	Heneicosane	296	C21H44	000629-94-7	86
5	Tricosane, 2-methyl-	338	C24H50	001928-30-9	86





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Sample : 03358-03
Misc :
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BNA_G
ClientSampleId :
SB-1-(34-36)

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

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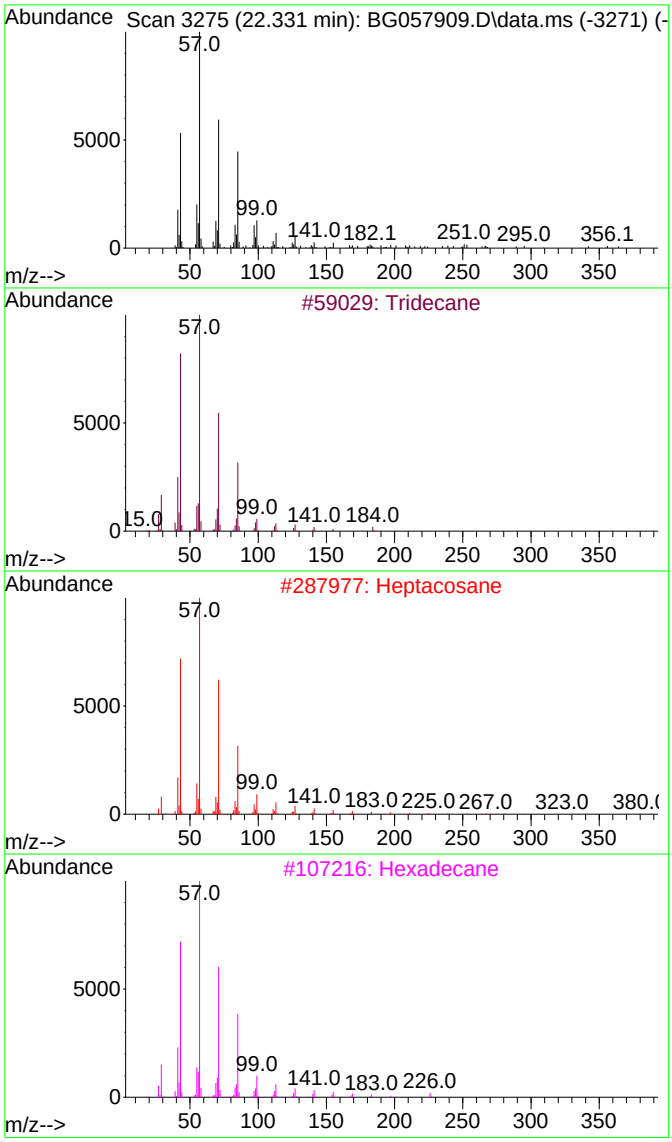
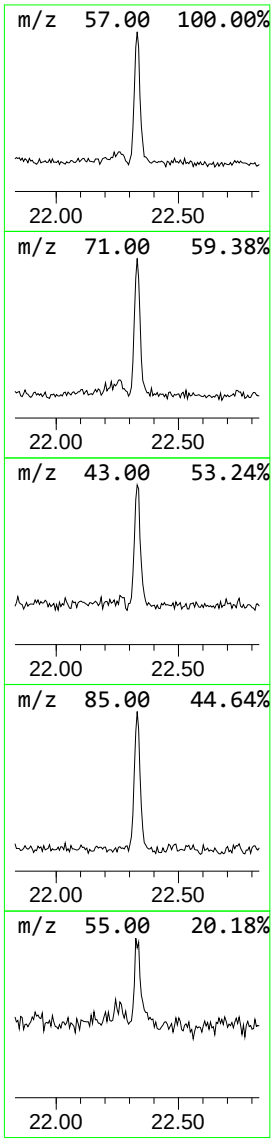
Peak Number 6 Tridecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.331	4.93 ng	175632	Chrysene-d12	21.544

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	87
2	Heptacosane	380	C27H56	000593-49-7	83
3	Hexadecane	226	C16H34	000544-76-3	80
4	Nonadecane	268	C19H40	000629-92-5	80
5	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	80





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ClientSampleId :
SB-1-(34-36)

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

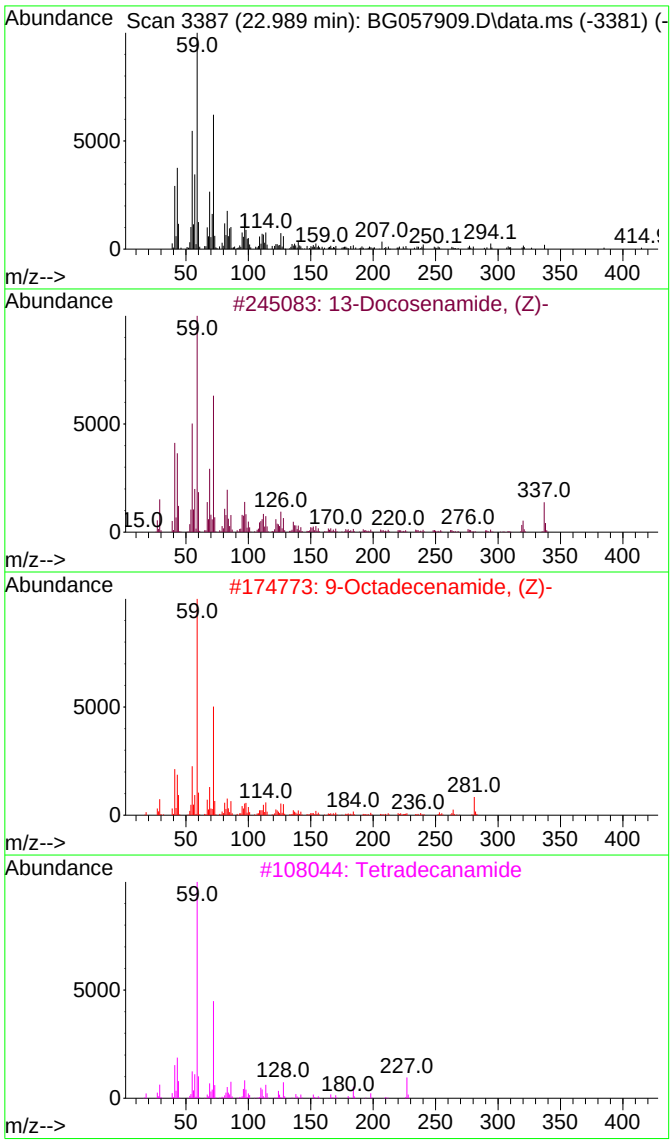
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

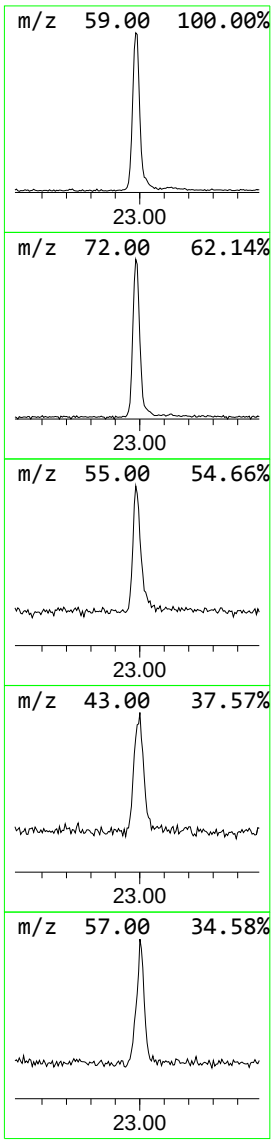
****

Peak Number 7 13-Docosenamide, (Z)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.989	12.79 ng	455259	Chrysene-d12	21.544

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	90
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	83
3	Tetradecanamide	227	C14H29NO	000638-58-4	59
4	Palmitoleamide	253	C16H31NO	106010-22-4	43
5	2-Hydroxy-2-methylundec-5-en-3-one	198	C12H22O2	1000191-46-2	38





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
2-Pentanone, 4-...	5.022	3.3	ng	40246	1	7.913	241079	20.0
Benzophenone	15.903	14.1	ng	339080	3	14.546	480789	20.0
unknown18.189	18.189	2.5	ng	80954	4	17.290	658998	20.0
Pentadecafluoro...	21.197	12.2	ng	434787	5	21.544	712111	20.0
Heptacosane	21.738	4.5	ng	160904	5	21.544	712111	20.0
Tridecane	22.331	4.9	ng	175632	5	21.544	712111	20.0
13-Docosenamide...	22.989	12.8	ng	455259	5	21.544	712111	20.0