LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011123\
Data File : BG056258.D
Acq On : 11 Jan 2023 20:05
Operator : CG/JU
Sample : 01069-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-7

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-BG122722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG056258.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.329	3	7	19	rVB	143238	212222	9.47%	1.998%
2	5.350	345	351	358	rBV	102617	162002	7.23%	1.525%
3	5.832	426	433	444	rBV	435714	688587	30.73%	6.484%
4	7.448	697	708	717	rBV	436548	758278	33.84%	7.140%
5	8.312	848	855	863	rBV	113622	195720	8.73%	1.843%
6	9.487	1046	1055	1062	rBV	250931	442459	19.75%	4.166%
7	11.144	1329	1337	1345	rBV	149692	272919	12.18%	2.570%
8	13.553	1740	1747	1755	rBV	895711	1321311	58.97%	12.441%
9	14.927	1974	1981	1989	rVB	302354	476075	21.25%	4.483%
10	16.261	2200	2208	2215	rBV	52013	77678	3.47%	0.731%
11	16.402	2225	2232	2241	rBV	721621	1079587	48.18%	10.165%
12	17.660	2440	2446	2452	rBV	447009	674960	30.12%	6.355%
13	18.506	2585	2590	2598	rBV4	63504	104233	4.65%	0.981%
14	19.692	2787	2792	2798	rVB	19200	28493	1.27%	0.268%
15	19.763	2798	2804	2809	rBV7	15762	30095	1.34%	0.283%
16	20.239	2879	2885	2890	rBV	1696857	2240730	100.00%	21.098%
17	20.903	2991	2998	3007	rBV	116042	170167	7.59%	1.602%
18	21.537	3102	3106	3116	rVB3	47712	86971	3.88%	0.819%
19	21.955	3170	3177	3184	rBV	448439	781530	34.88%	7.359%
20	25.392	3752	3762	3775	rBV2	272998	816515	36.44%	7.688%

Sum of corrected areas: 10620532

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Misc :
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Instrument :
BNA_G
ClientSampleId :
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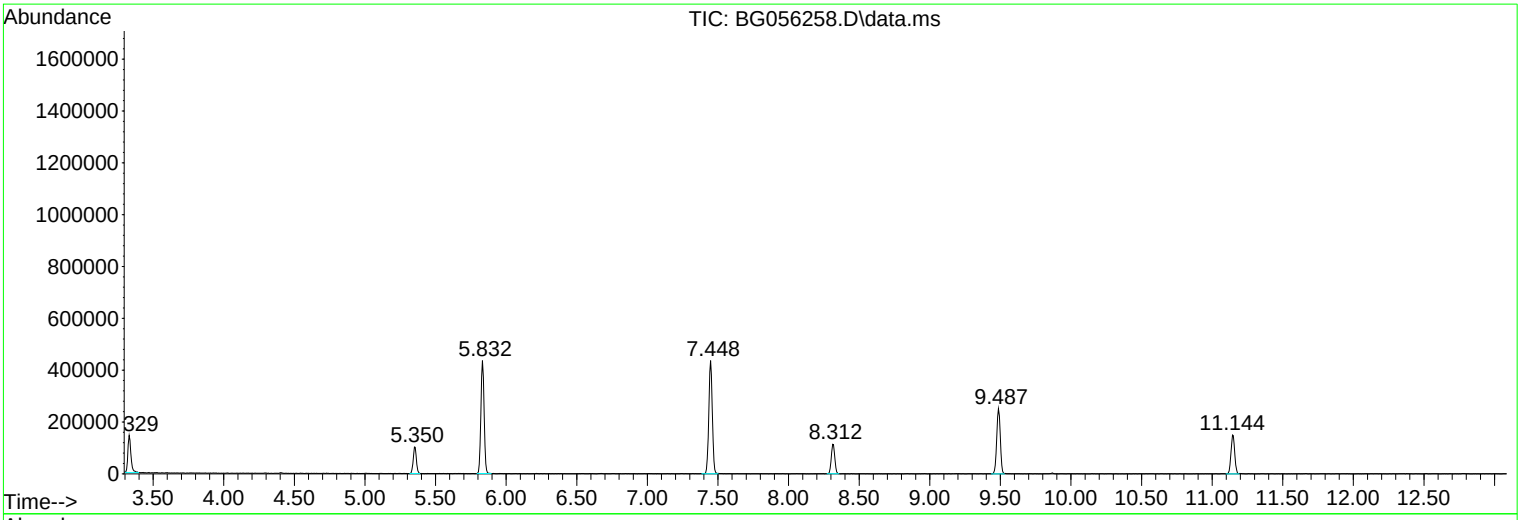
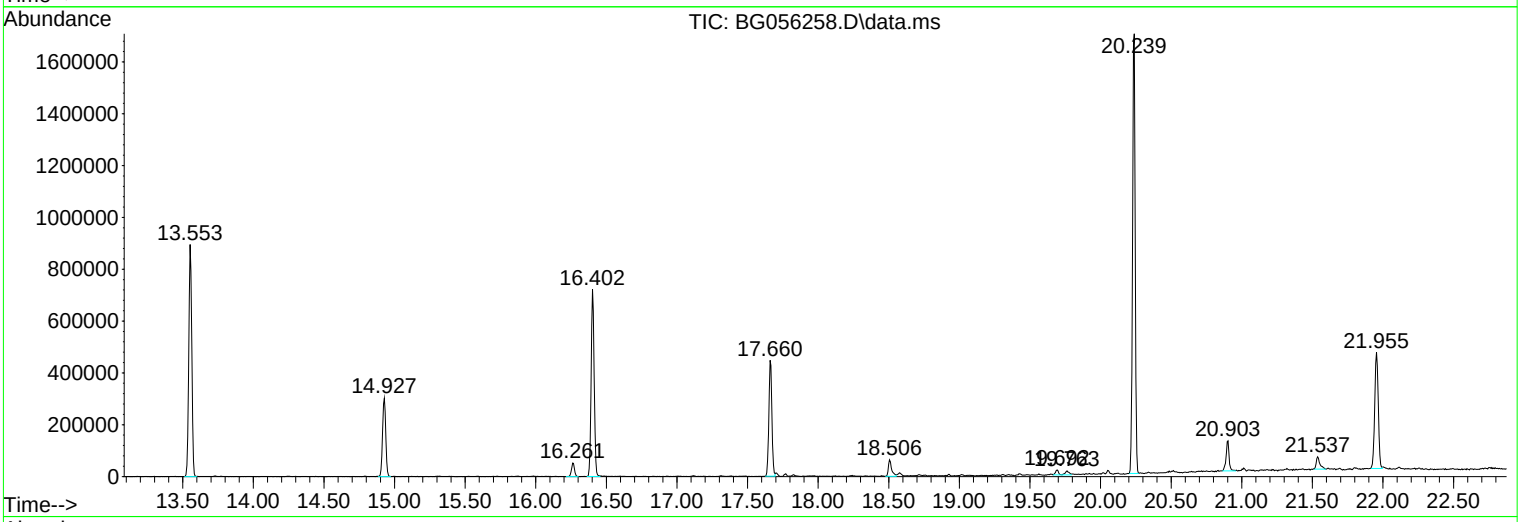
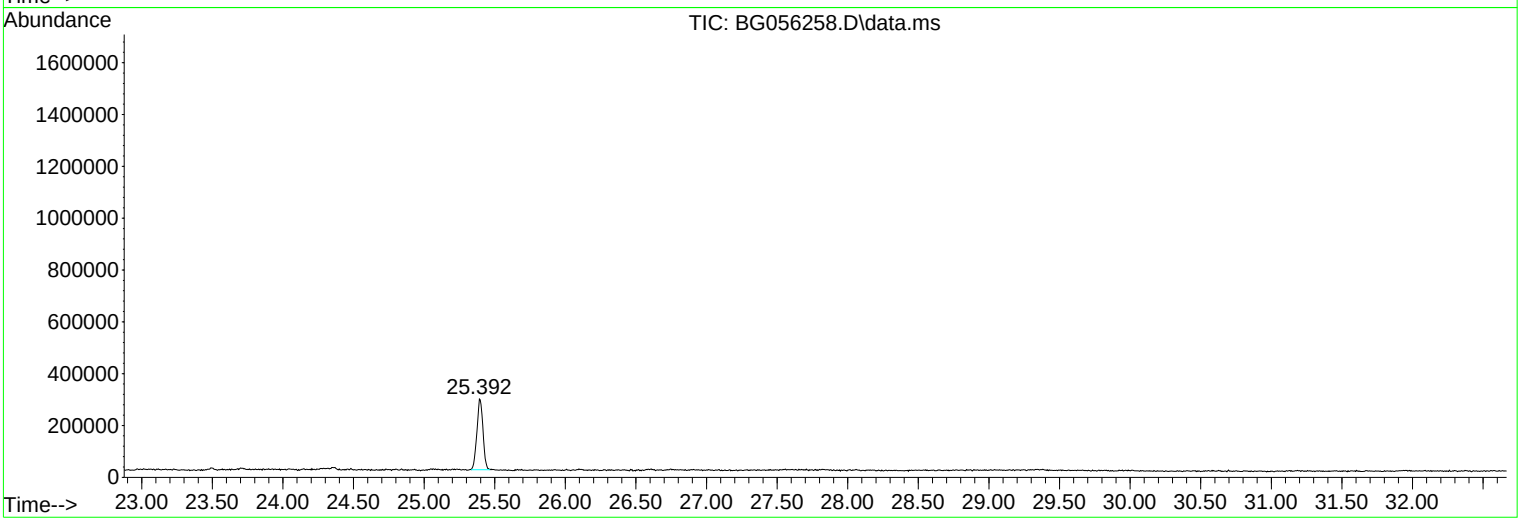
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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ClientSampleId :
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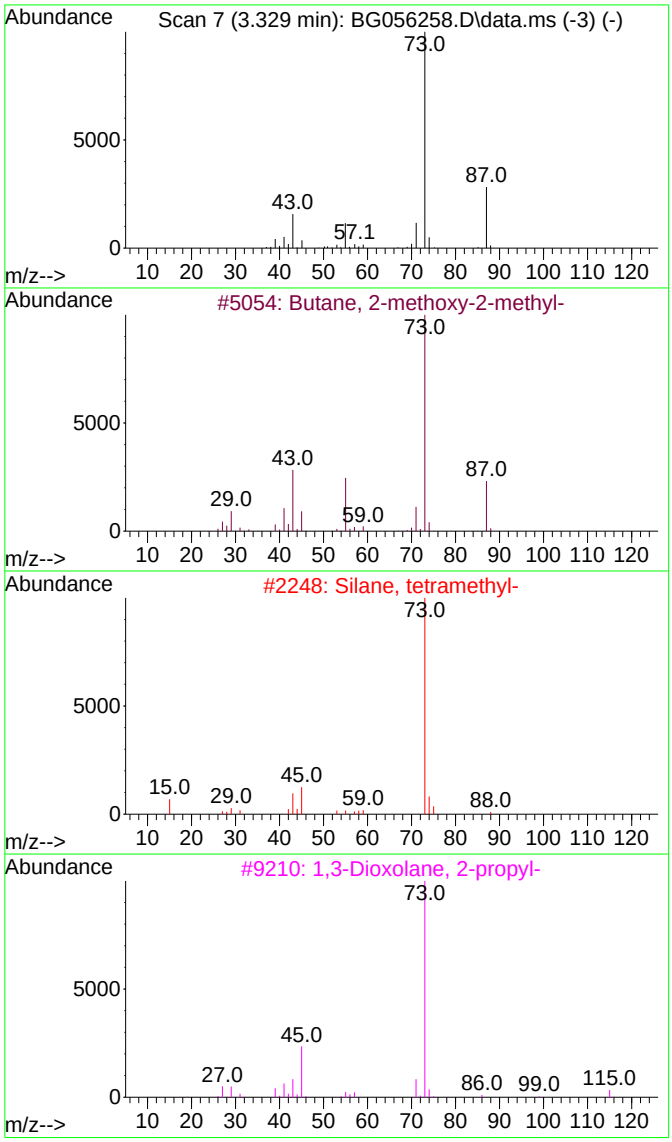
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

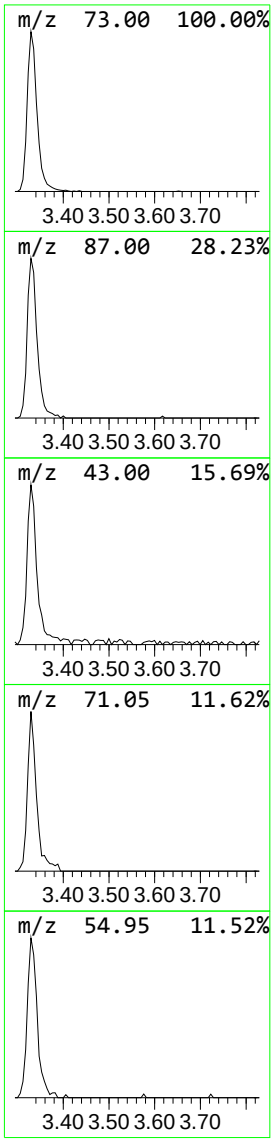
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.329	21.69 ng	212222	1,4-Dichlorobenzene-d4	8.312

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	74
2	Silane, tetramethyl-	88	C4H12Si	000075-76-3	10
3	1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	9
4	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	9
5	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9





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Sample : 01069-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-7

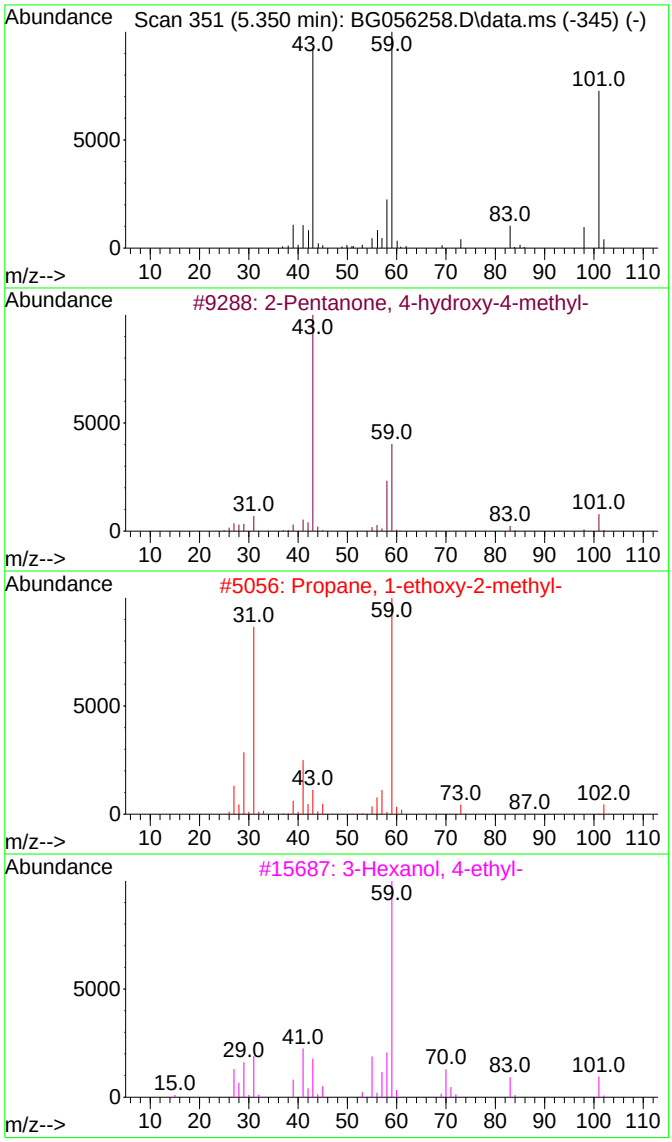
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

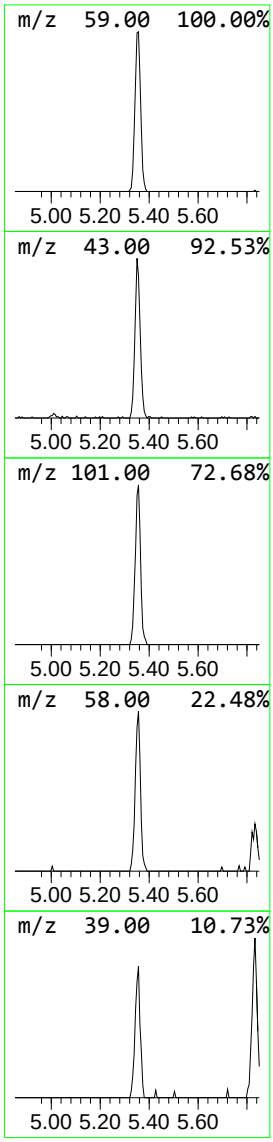
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.350	16.55 ng	162002	1,4-Dichlorobenzene-d4	8.312

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	35
3	3-Hexanol, 4-ethyl-	130	C8H18O	019780-44-0	28
4	2-Octanol, 2,6-dimethyl-	158	C10H22O	018479-57-7	23
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	17





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Data File : BG056258.D
Acq On : 11 Jan 2023 20:05
Operator : CG/JU
Sample : 01069-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

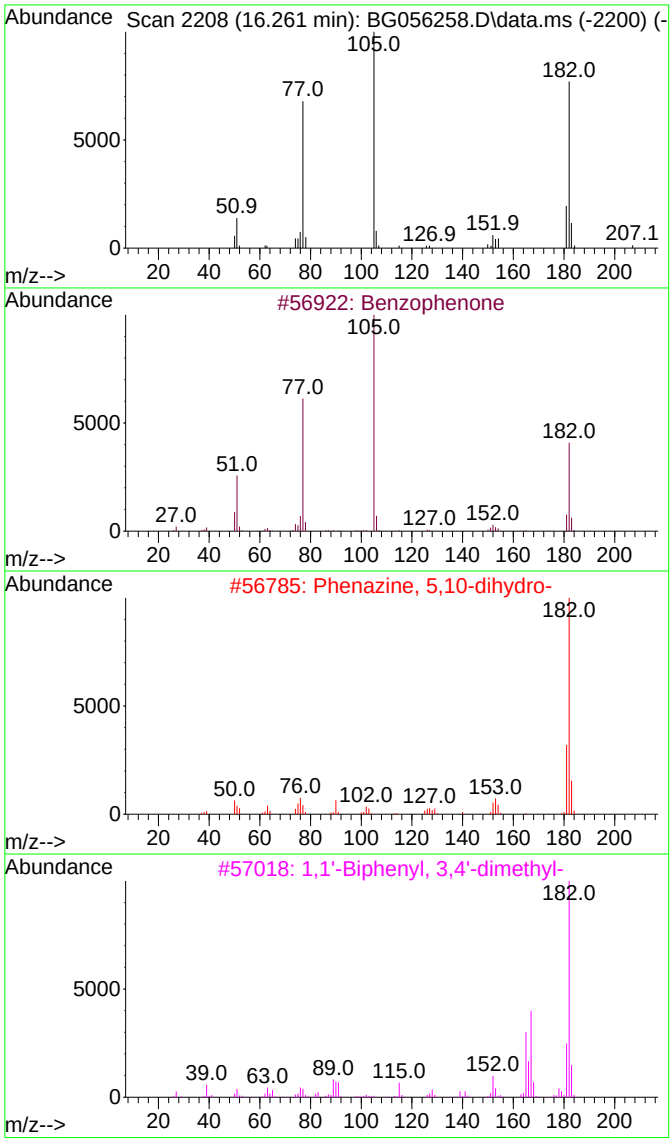
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

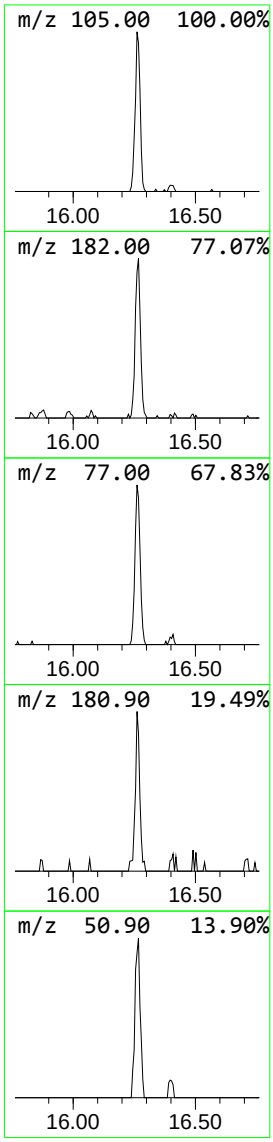
****

Peak Number 3 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.261	3.26 ng	77678	Acenaphthene-d10	14.928

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	91
2	Phenazine, 5,10-dihydro-	182	C12H10N2	000613-32-1	52
3	1,1'-Biphenyl, 3,4'-dimethyl-	182	C14H14	007383-90-6	49
4	9H-Pyrido[3,4-b]indole, 1-methyl-	182	C12H10N2	000486-84-0	49
5	4,4'-Dimethylbiphenyl	182	C14H14	000613-33-2	49





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Instrument :
BNA_G
ClientSampleId :
TP-7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

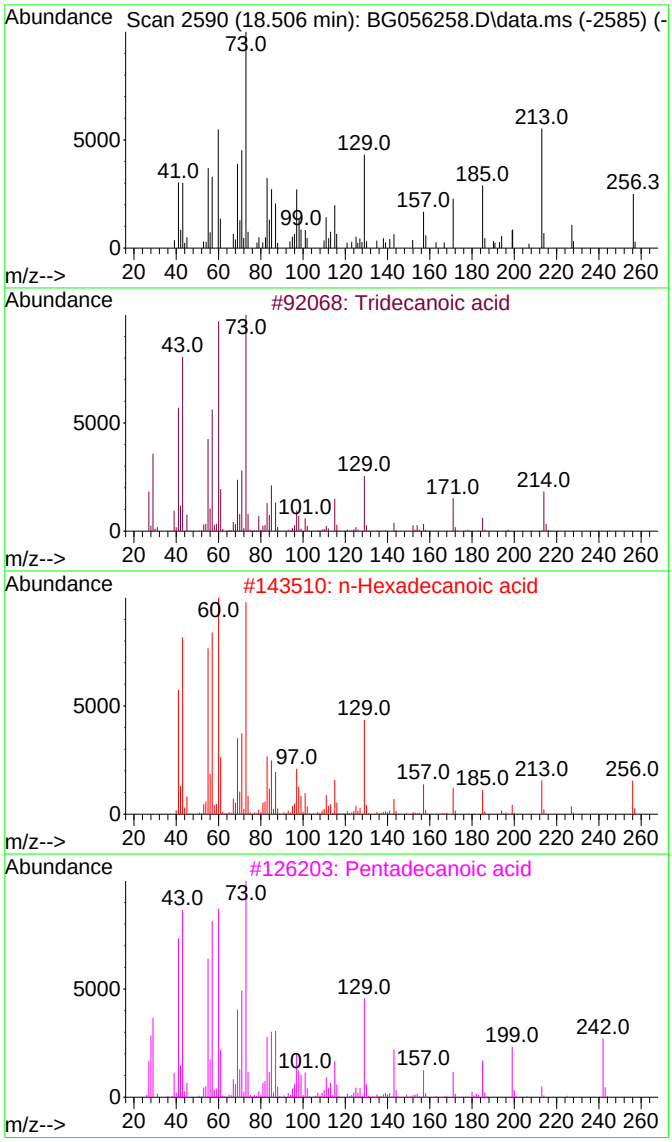
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

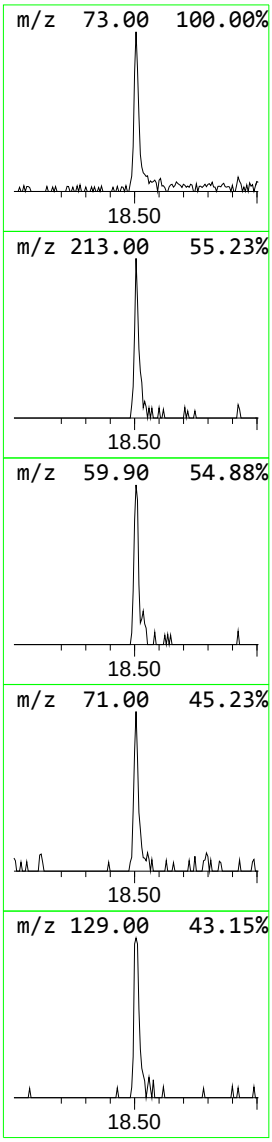
****

Peak Number 4 Tridecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.506	3.09 ng	104233	Phenanthrene-d10	17.660

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	90
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	70
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	43
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	43
5	Undecanoic acid	186	C11H22O2	000112-37-8	27





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Sample : 01069-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

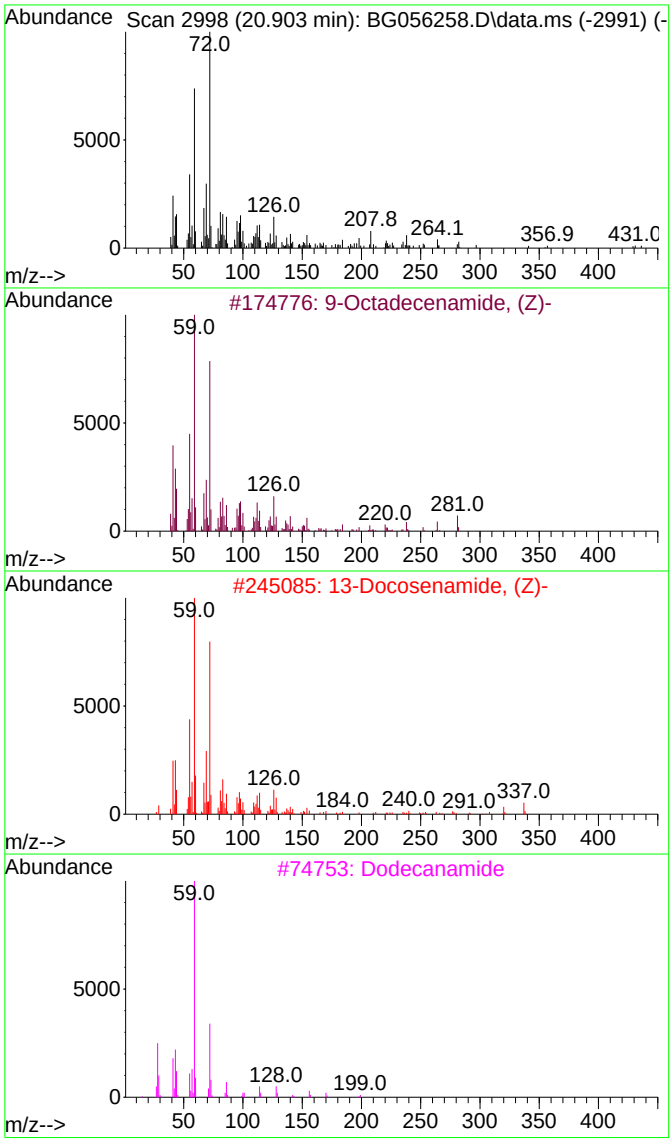
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

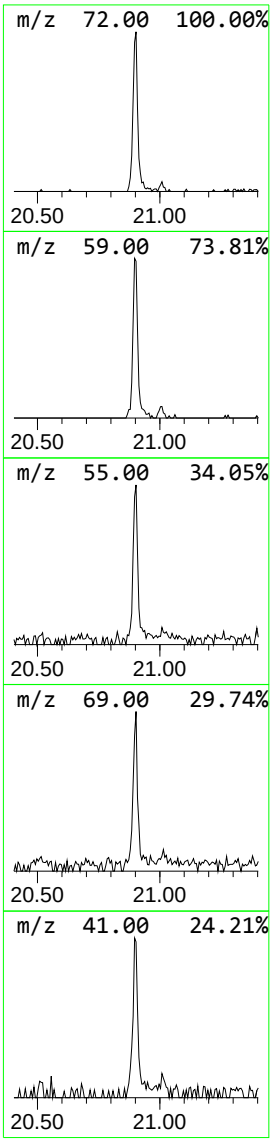
****

Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.903	4.35 ng	170167	Chrysene-d12	21.954

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	70
2	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	52
3	Dodecanamide	199	C12H25NO	001120-16-7	50
4	9-Octadecenamide	281	C18H35NO	003322-62-1	46
5	Tetradecanamide	227	C14H29NO	000638-58-4	46





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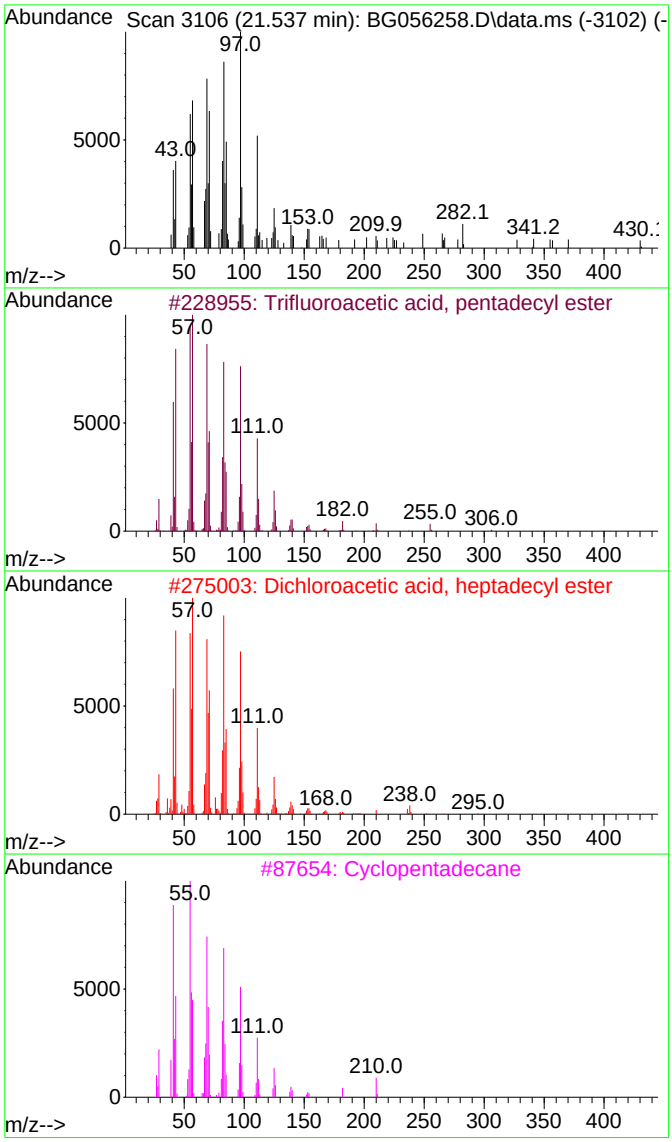
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

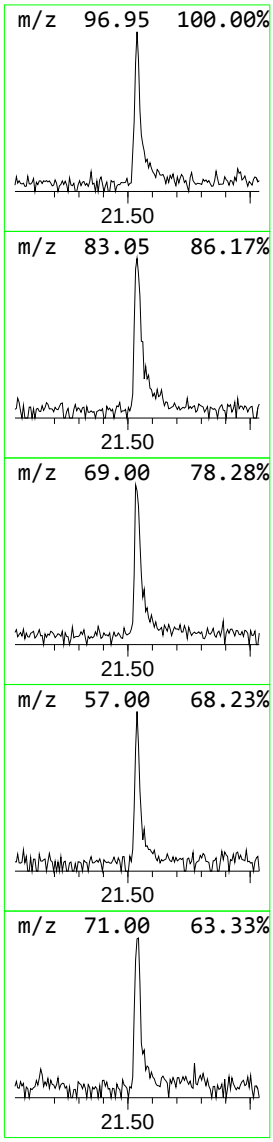
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Trifluoroacetic acid, penta... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.537	2.23 ng	86971	Chrysene-d12	21.954

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	87
2	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	87
3	Cyclopentadecane	210	C15H30	000295-48-7	86
4	Pentadecafluorooctanoic acid, he...	638	C24H33F15O2	1000406-04-6	74
5	Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	72





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	3.329	21.7	ng	212222	1	8.312	195720	20.0
2-Pentanone, 4-...	5.350	16.6	ng	162002	1	8.312	195720	20.0
Benzophenone	16.261	3.3	ng	77678	3	14.928	476075	20.0
Tridecanoic acid	18.506	3.1	ng	104233	4	17.660	674960	20.0
9-Octadecenamid...	20.903	4.3	ng	170167	5	21.954	781530	20.0
Trifluoroacetic...	21.537	2.2	ng	86971	5	21.954	781530	20.0