LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081621\
Data File : BG049863.D
Acq On : 16 Aug 2021 23:54
Operator : CG/JU
Sample : M3407-17
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 27S

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-BG080321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG049863.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.140	12	17	22	rBV	97455	163991	10.66%	1.802%
2	5.108	347	352	361	rVB	42049	74452	4.84%	0.818%
3	5.584	426	433	444	rBV	475992	782744	50.86%	8.601%
4	7.194	699	707	720	rBV	501160	888307	57.72%	9.762%
5	8.028	842	849	859	rVB	130871	232777	15.13%	2.558%
6	9.197	1041	1048	1058	rBV	320736	583190	37.89%	6.409%
7	10.613	1283	1289	1297	rBV4	16202	32732	2.13%	0.360%
8	10.848	1322	1329	1342	rVB	171648	316350	20.56%	3.476%
9	13.297	1739	1746	1755	rBV	807662	1251922	81.35%	13.757%
10	14.678	1974	1981	1988	rBV	261607	420824	27.34%	4.624%
11	16.176	2229	2236	2247	rBV	654438	1004858	65.29%	11.042%
12	17.433	2444	2450	2455	rBV	294201	458338	29.78%	5.037%
13	17.474	2455	2457	2465	rVB	15978	24649	1.60%	0.271%
14	19.489	2795	2800	2804	rBV	37509	54842	3.56%	0.603%
15	19.665	2825	2830	2834	rBV6	14419	15904	1.03%	0.175%
16	19.847	2857	2861	2866	rVB	31136	47703	3.10%	0.524%
17	20.047	2888	2895	2900	rBV	1151127	1539001	100.00%	16.912%
18	20.323	2937	2942	2949	rBV	12889	33440	2.17%	0.367%
19	20.681	2999	3003	3007	rBV4	62653	88246	5.73%	0.970%
20	20.723	3007	3010	3017	rVB9	34335	47346	3.08%	0.520%
21	21.345	3111	3116	3124	rBV4	60281	135855	8.83%	1.493%
22	21.715	3173	3179	3185	rVB2	265373	439661	28.57%	4.831%
23	24.993	3729	3737	3747	rVB	161357	446680	29.02%	4.909%
24	27.878	4223	4228	4229	rBV5	10367	16288	1.06%	0.179%

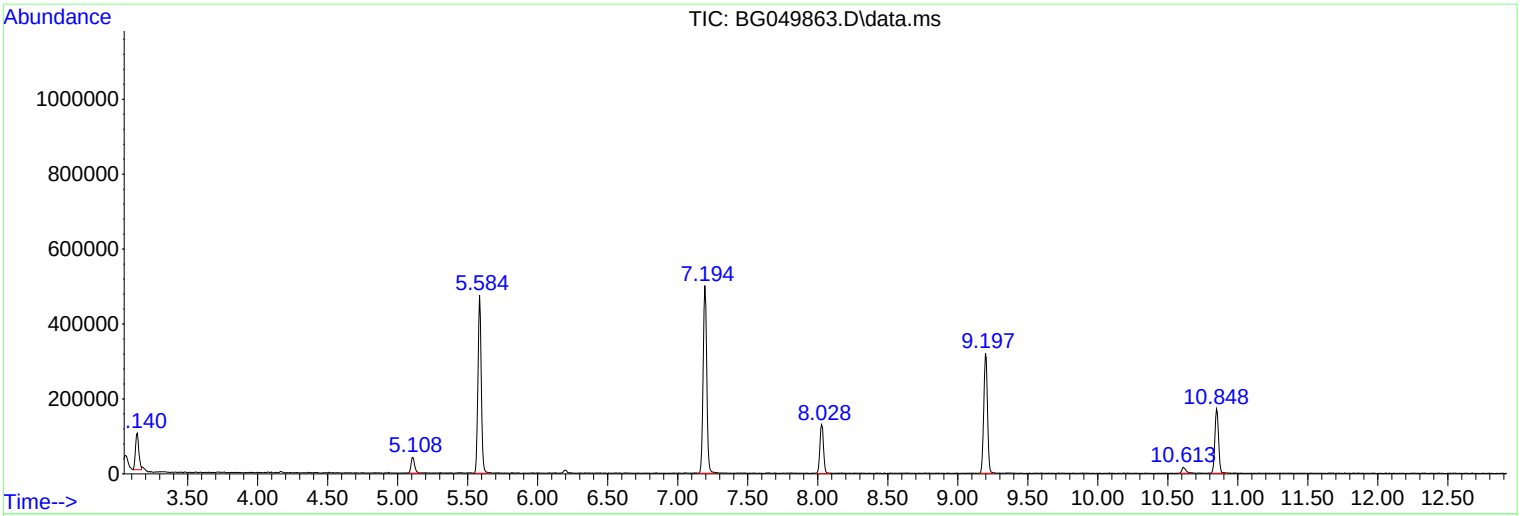
Sum of corrected areas: 9100100

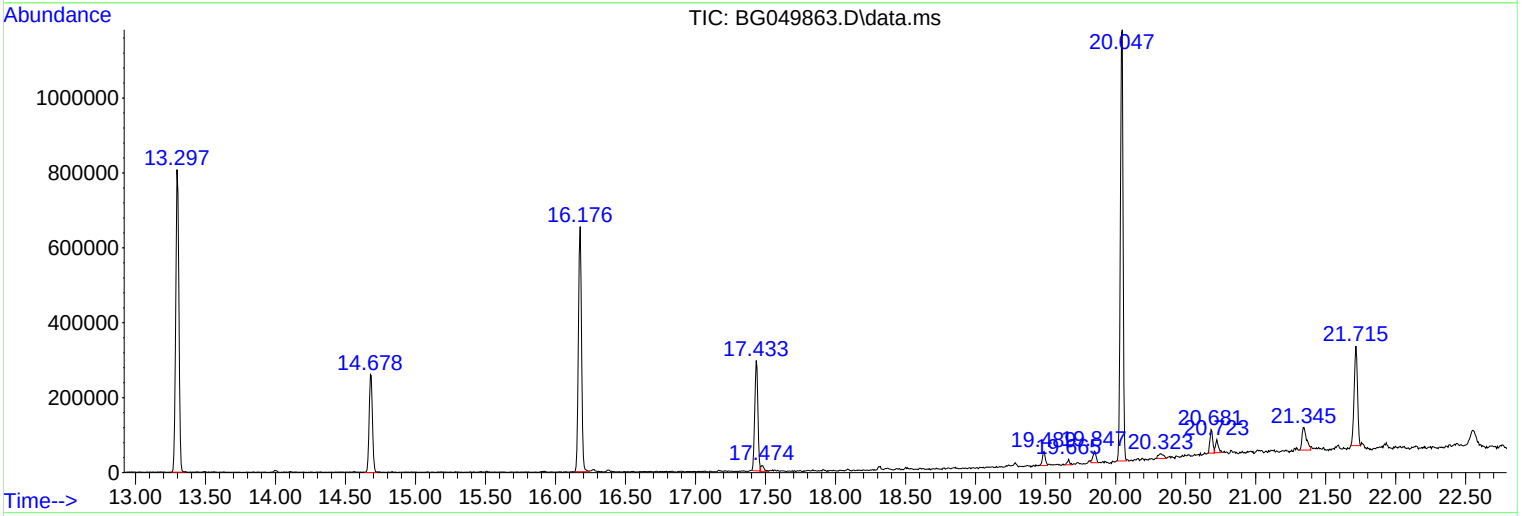
Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081621\
Data File : BG049863.D
Acq On : 16 Aug 2021 23:54
Operator : CG/JU
Sample : M3407-17
Misc :
ALS Vial : 12 Sample Multiplier: 1

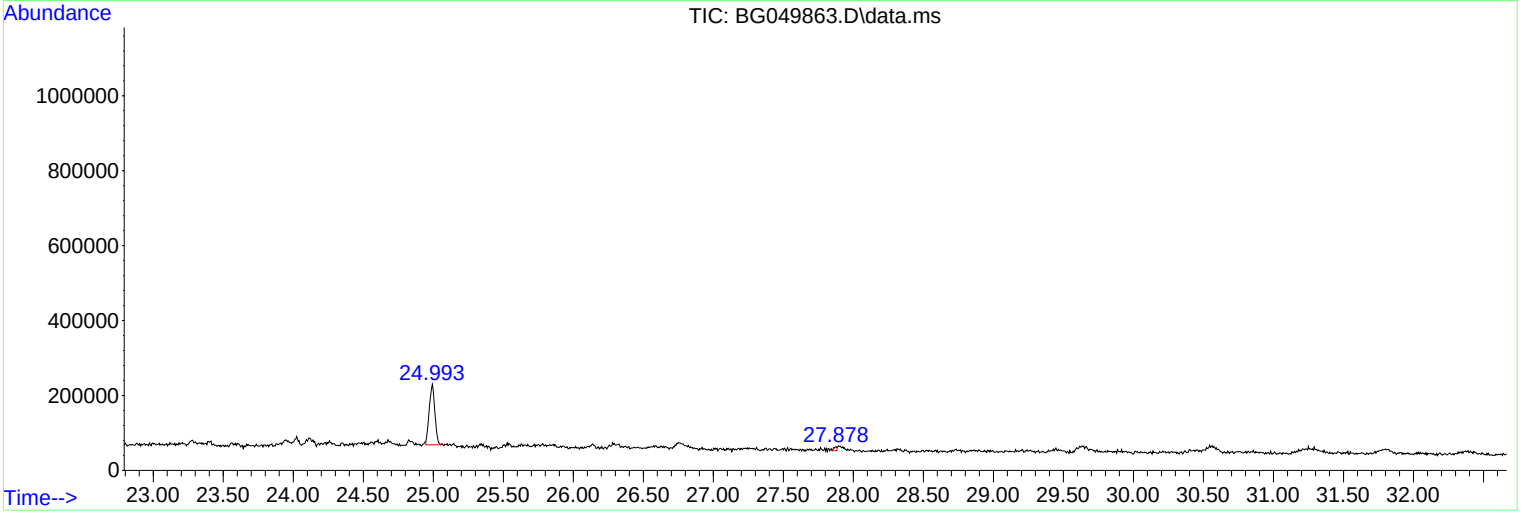
Instrument :
BNA_G
ClientSampleId :
27S

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.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\BG081621\
Data File : BG049863.D
Acq On : 16 Aug 2021 23:54
Operator : CG/JU
Sample : M3407-17
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 27S

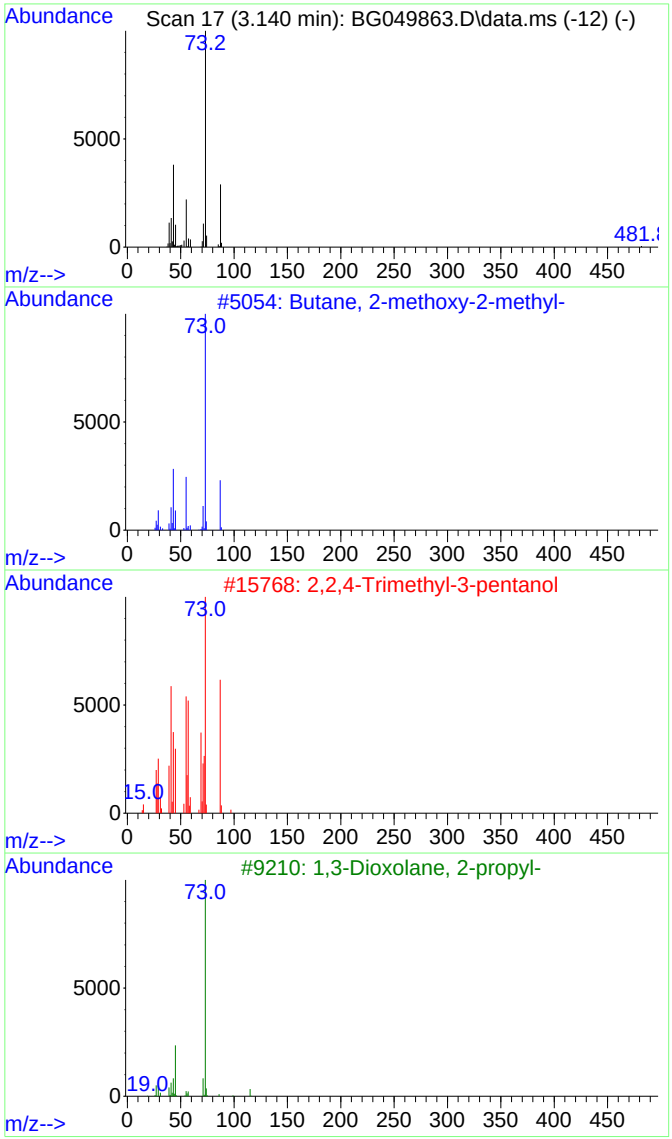
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

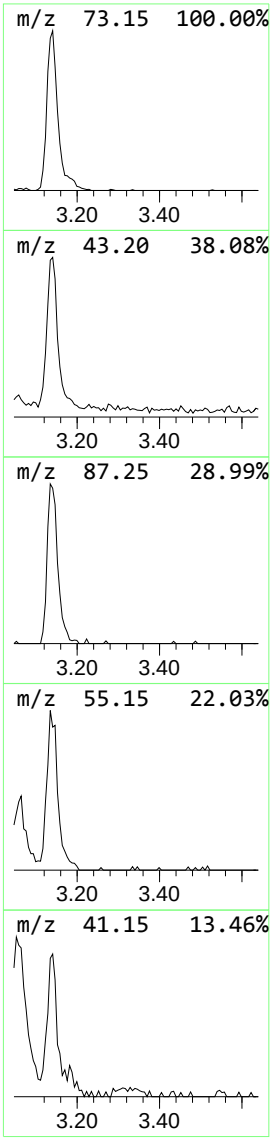
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.140	14.09 ng	163991	1,4-Dichlorobenzene-d4	8.028

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	56
3	1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	12
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	12
5	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081621\
Data File : BG049863.D
Acq On : 16 Aug 2021 23:54
Operator : CG/JU
Sample : M3407-17
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 27S

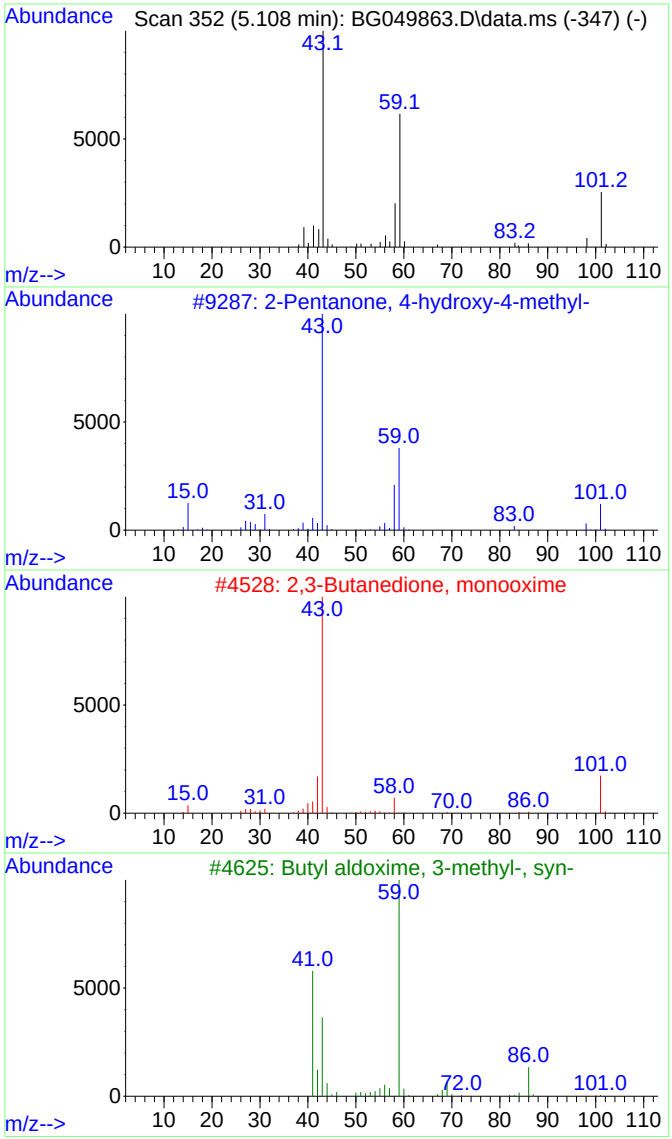
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

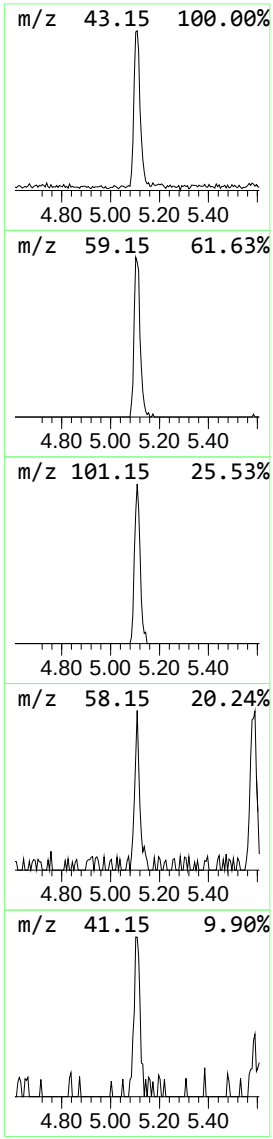
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.108	6.40 ng	74452	1,4-Dichlorobenzene-d4	8.028

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	12
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081621\
Data File : BG049863.D
Acq On : 16 Aug 2021 23:54
Operator : CG/JU
Sample : M3407-17
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 27S

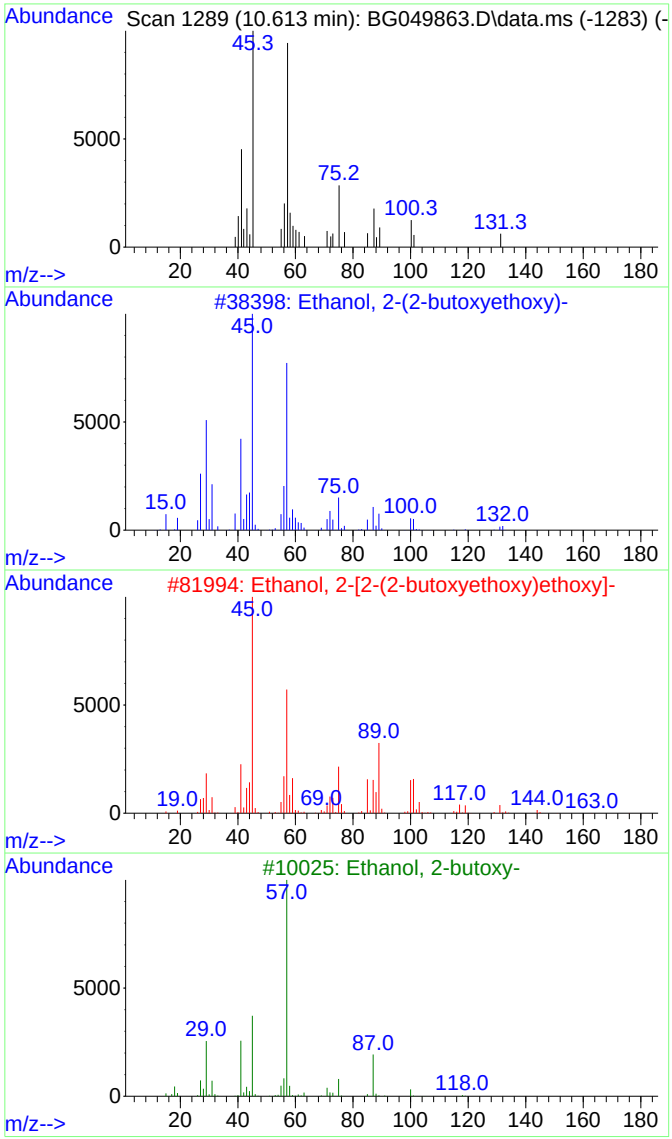
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

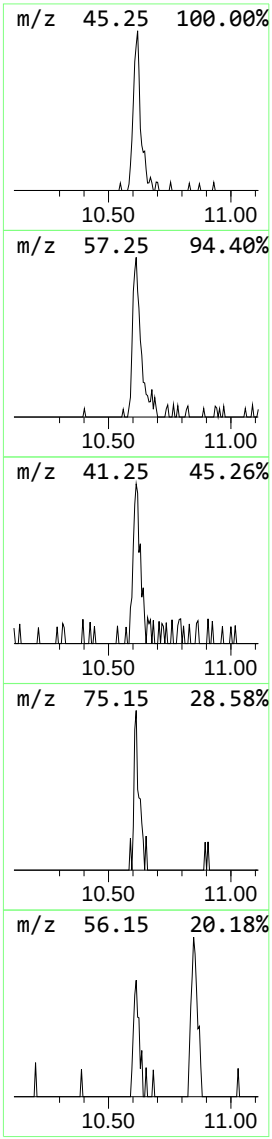
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.613	2.07 ng	32732	Naphthalene-d8	10.848

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	78
2	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	56
3	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	50
4	Propanoic acid, 2-hydroxy-, 2-me...	146	C7H14O3	000585-24-0	45
5	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	40





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081621\
Data File : BG049863.D
Acq On : 16 Aug 2021 23:54
Operator : CG/JU
Sample : M3407-17
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 27S

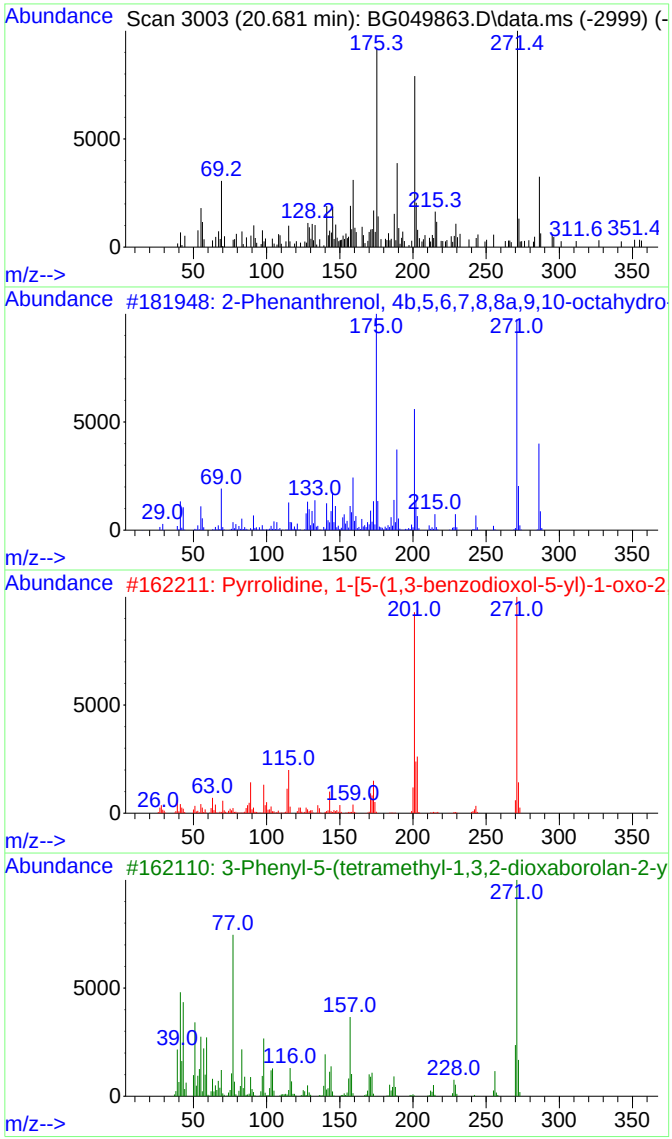
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

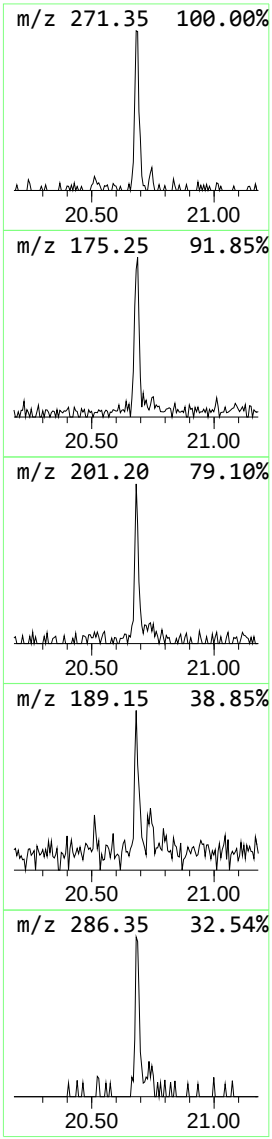
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2-Phenanthrenol, 4b,5,6,7,8... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.681	4.01 ng	88246	Chrysene-d12	21.715

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	286	C20H30O	000511-15-9	87
2	Pyrrolidine, 1-[5-(1,3-benzodiox...	271	C16H17NO3	025924-78-1	64
3	3-Phenyl-5-(tetramethyl-1,3,2-di...	271	C15H18BNO3	1000434-90-0	25
4	Crinan-1-ol, 2,3-didehydro-,(1.a...	271	C16H17NO3	1000111-31-3	25
5	Naphthalene, 1,2,3,4-tetrahydro-...	244	C18H28	029577-17-1	20





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081621\
Data File : BG049863.D
Acq On : 16 Aug 2021 23:54
Operator : CG/JU
Sample : M3407-17
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 27S

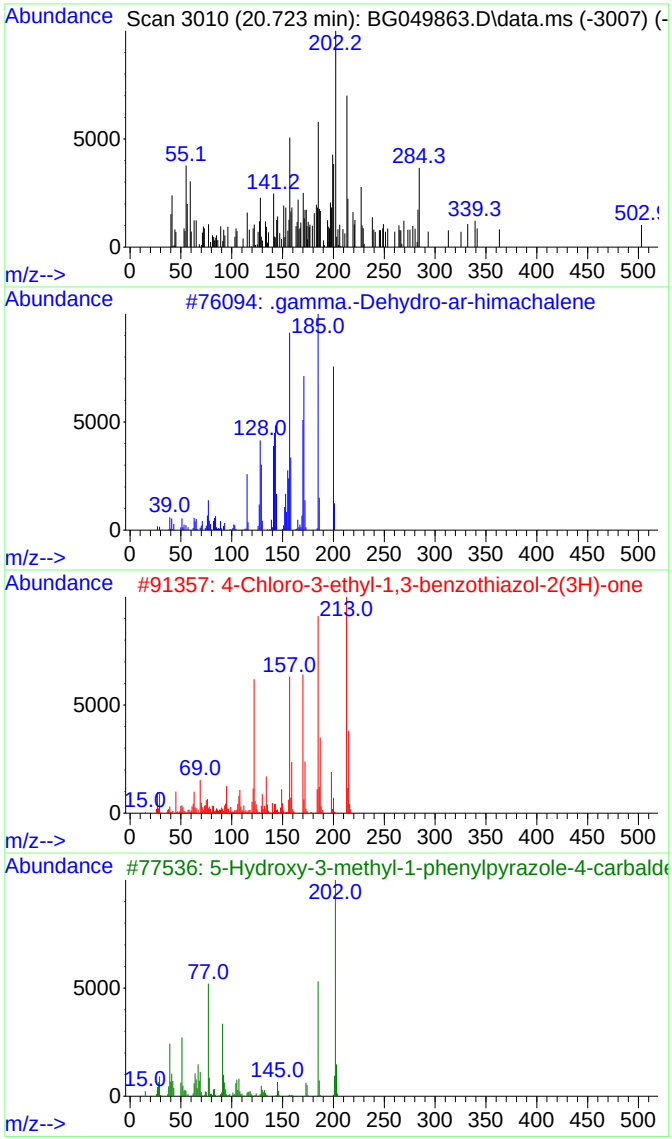
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

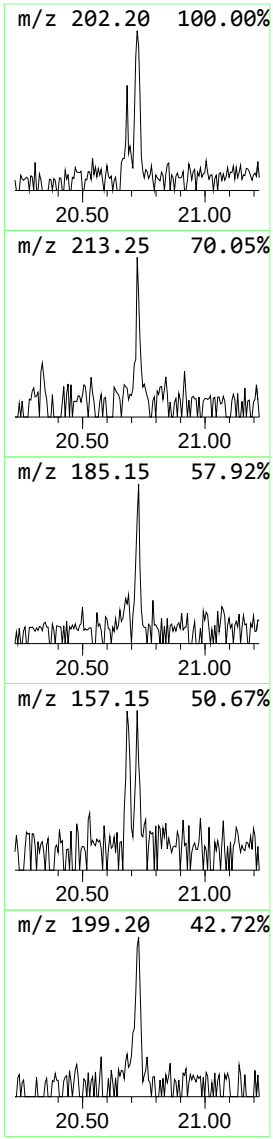
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 .gamma.-Dehydro-ar-himachalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.723	2.15 ng	47346	Chrysene-d12	21.715

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.gamma.-Dehydro-ar-himachalene	200	C15H20	051766-65-5	50
2	4-Chloro-3-ethyl-1,3-benzothiazo...	213	C9H8ClNOS	1000331-84-8	22
3	5-Hydroxy-3-methyl-1-phenylpyraz...	202	C11H10N2O2	060484-29-9	22
4	4-Boc-1-(5-bromo-2-pyridyl)piper...	341	C14H20BrN3O2	153747-97-8	18
5	3,4-Dimethyl(1H)pyrrole, 2-[(3,4...	200	C13H16N2	065539-79-9	14





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081621\
Data File : BG049863.D
Acq On : 16 Aug 2021 23:54
Operator : CG/JU
Sample : M3407-17
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 27S

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

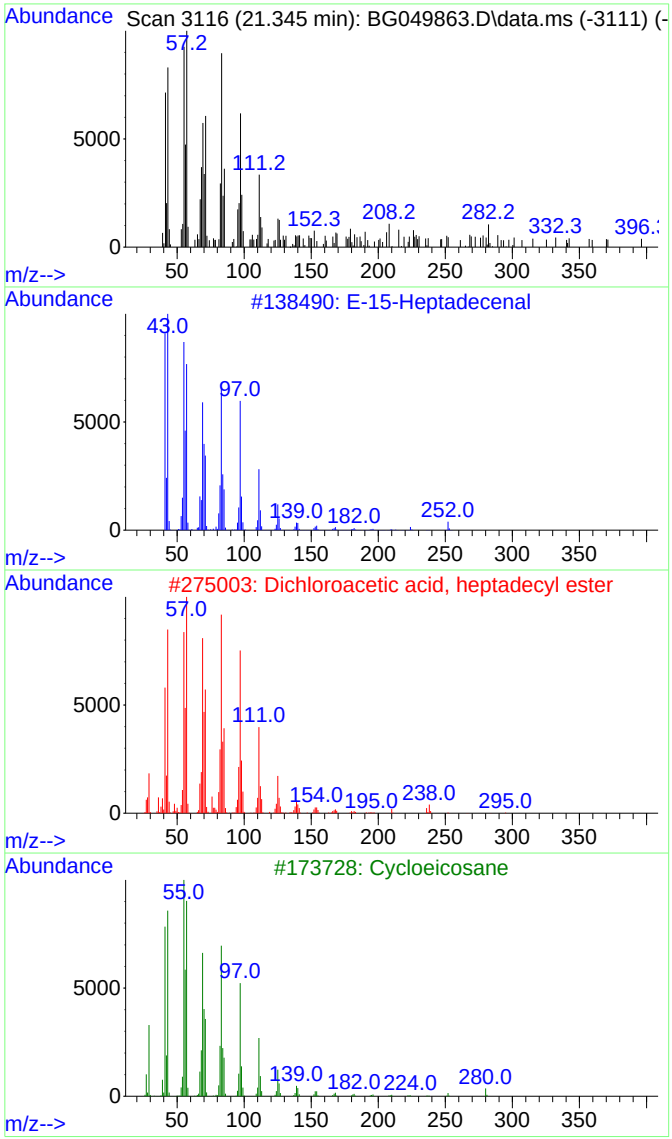
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

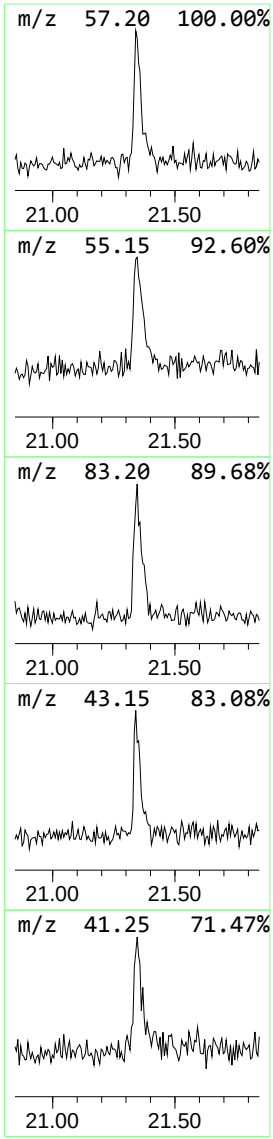
****

Peak Number 7 E-15-Heptadecenal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.345	6.18 ng	135855	Chrysene-d12	21.715

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-15-Heptadecenal	252	C17H32O	1000130-97-9	95
2	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	93
3	Cycloeicosane	280	C20H40	000296-56-0	90
4	1-Octadecene	252	C18H36	000112-88-9	89
5	5-Eicosene, (E)-	280	C20H40	074685-30-6	89





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081621\
Data File : BG049863.D
Acq On : 16 Aug 2021 23:54
Operator : CG/JU
Sample : M3407-17
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 27S

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
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...	3.140	14.1	ng	163991	1	8.028	232777	20.0
2-Pentanone, 4-...	5.108	6.4	ng	74452	1	8.028	232777	20.0
Ethanol, 2-(2-b...	10.613	2.1	ng	32732	2	10.848	316350	20.0
2-Phenanthrenol...	20.681	4.0	ng	88246	5	21.715	439661	20.0
.gamma.-Dehydro...	20.723	2.1	ng	47346	5	21.715	439661	20.0
E-15-Heptadecenal	21.345	6.2	ng	135855	5	21.715	439661	20.0