LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070621\
Data File : BG049193.D
Acq On : 6 Jul 2021 20:15
Operator : CG/JU
Sample : M2933-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 2

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-BG063021.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG049193.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.125	10	15	25	rVV2	56222	126191	7.04%	1.272%
2	3.208	25	29	35	rVB2	18120	29724	1.66%	0.300%
3	5.640	436	443	456	rBV	454070	812965	45.38%	8.194%
4	7.238	707	715	730	rBV	509461	911521	50.88%	9.187%
5	7.373	733	738	745	rVB2	28786	50527	2.82%	0.509%
6	7.679	784	790	798	rBV3	9858	20845	1.16%	0.210%
7	8.084	852	859	867	rBV	132017	233007	13.01%	2.349%
8	9.253	1050	1058	1068	rVB	291514	536200	29.93%	5.404%
9	10.904	1331	1339	1351	rBV	178858	333396	18.61%	3.360%
10	13.349	1747	1755	1764	rBV	832847	1310062	73.13%	13.204%
11	14.171	1888	1895	1904	rBV	106546	161402	9.01%	1.627%
12	14.729	1983	1990	2001	rVB	285213	452235	25.24%	4.558%
13	16.216	2235	2243	2261	rBV	567384	1019751	56.92%	10.278%
14	17.479	2451	2458	2463	rBV	340225	518584	28.95%	5.227%
15	18.355	2602	2607	2612	rBV6	14650	26566	1.48%	0.268%
16	19.524	2800	2806	2811	rBV	28522	43356	2.42%	0.437%
17	19.888	2863	2868	2873	rVB2	21309	30983	1.73%	0.312%
18	20.082	2895	2901	2908	rBV	1410411	1791451	100.00%	18.056%
19	20.370	2946	2950	2956	rVB9	10418	18898	1.05%	0.190%
20	21.392	3119	3124	3135	rVB3	73367	164493	9.18%	1.658%
21	21.762	3179	3187	3192	rBV	338485	591567	33.02%	5.963%
22	21.909	3209	3212	3219	rVB9	17085	24508	1.37%	0.247%
23	23.654	3501	3509	3513	rBV9	13930	36120	2.02%	0.364%
24	24.124	3583	3589	3594	rVB6	16136	33359	1.86%	0.336%
25	25.064	3737	3749	3760	rBV2	192610	598715	33.42%	6.035%
26	26.275	3949	3955	3957	rBV6	24737	44993	2.51%	0.453%

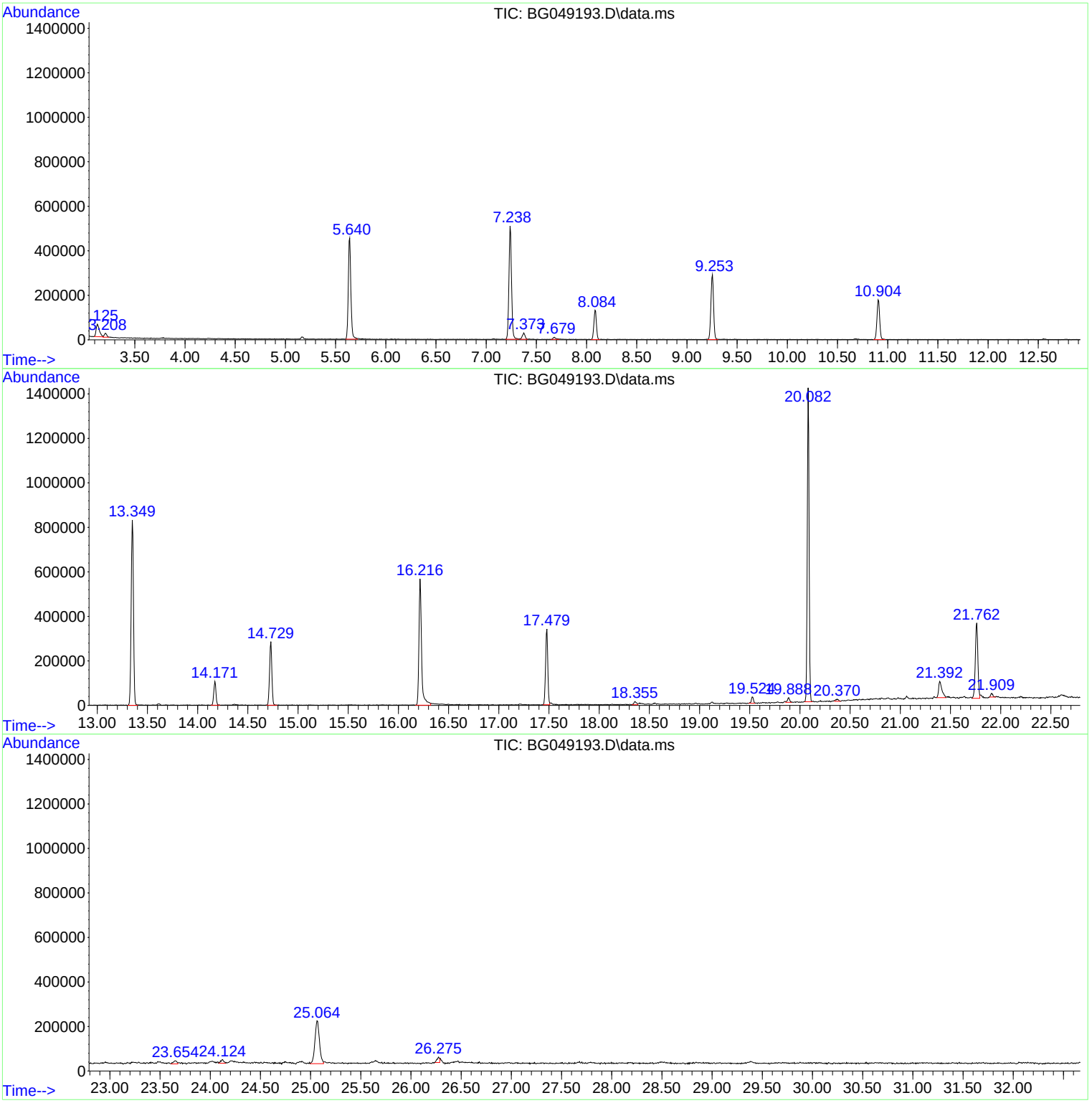
Sum of corrected areas: 9921419

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070621\
Data File : BG049193.D
Acq On : 6 Jul 2021 20:15
Operator : CG/JU
Sample : M2933-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG063021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070621\
Data File : BG049193.D
Acq On : 6 Jul 2021 20:15
Operator : CG/JU
Sample : M2933-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 2

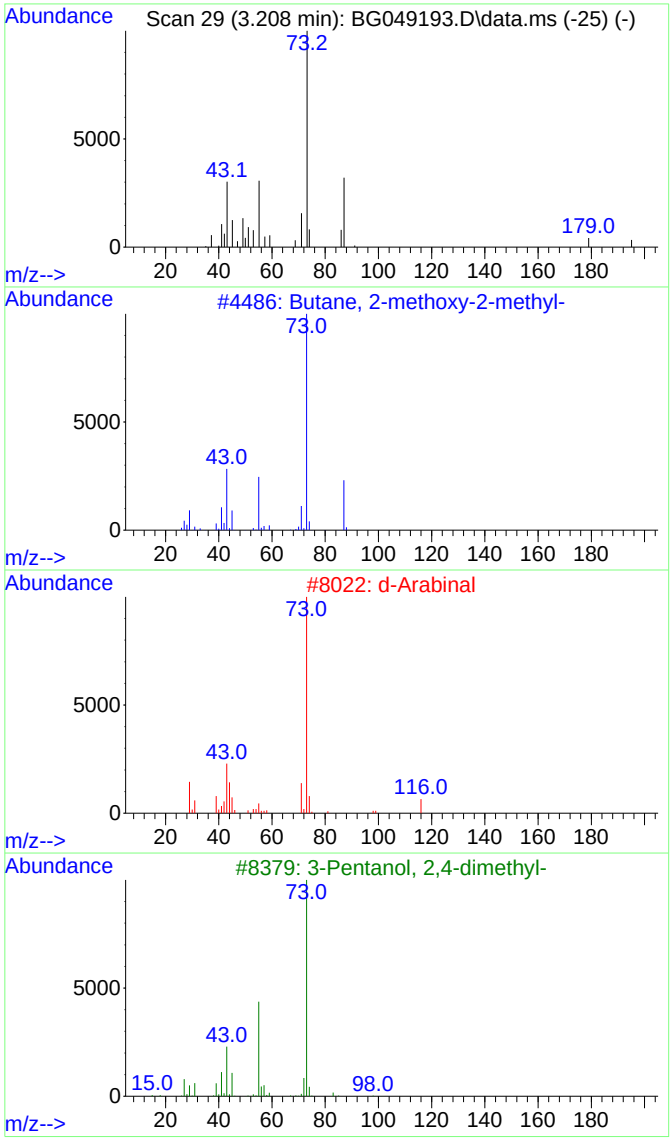
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG063021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

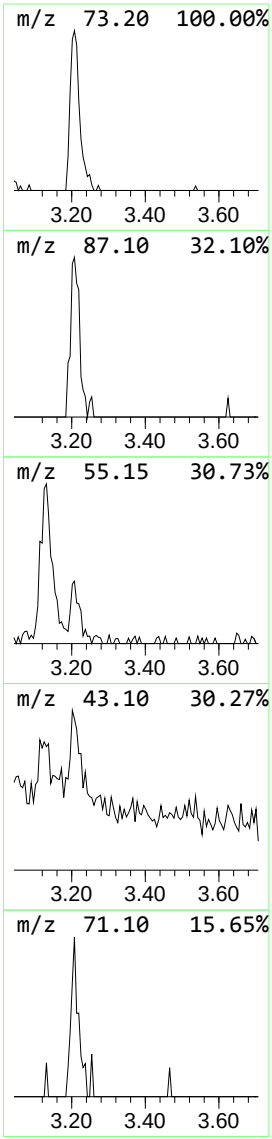
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.208	2.55 ng	29724	1,4-Dichlorobenzene-d4	8.090

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	50
2	d-Arabinal	116	C5H8O3	000496-61-7	9
3	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	9
4	3-Hexanol, 2,4-dimethyl-	130	C8H18O	013432-25-2	9
5	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070621\
Data File : BG049193.D
Acq On : 6 Jul 2021 20:15
Operator : CG/JU
Sample : M2933-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 2

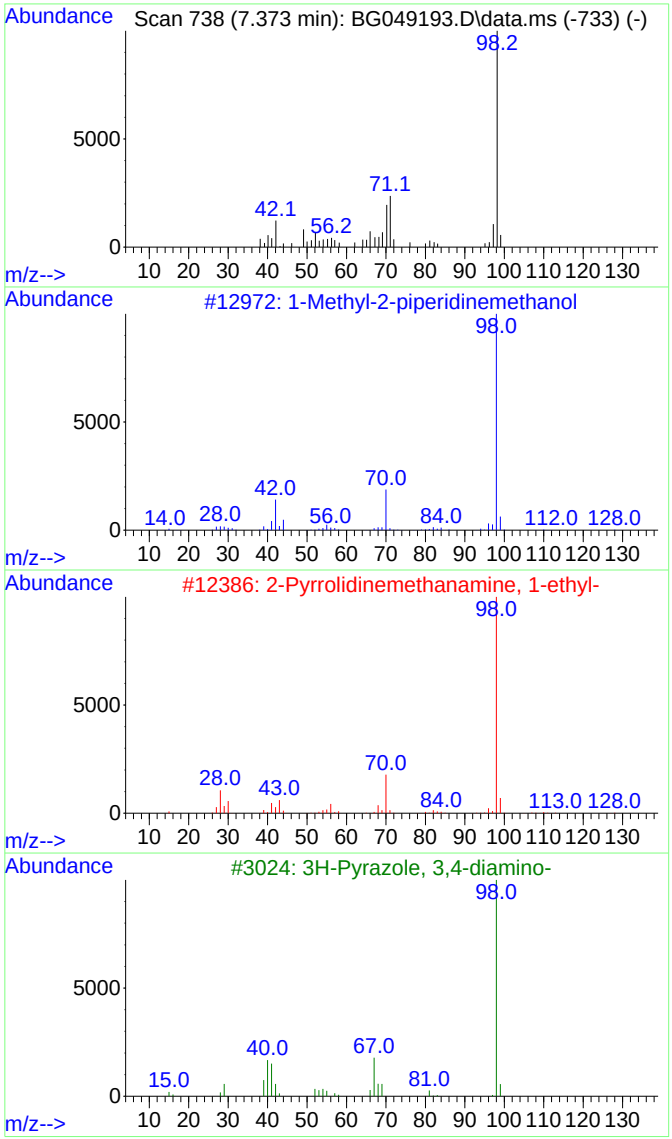
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG063021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

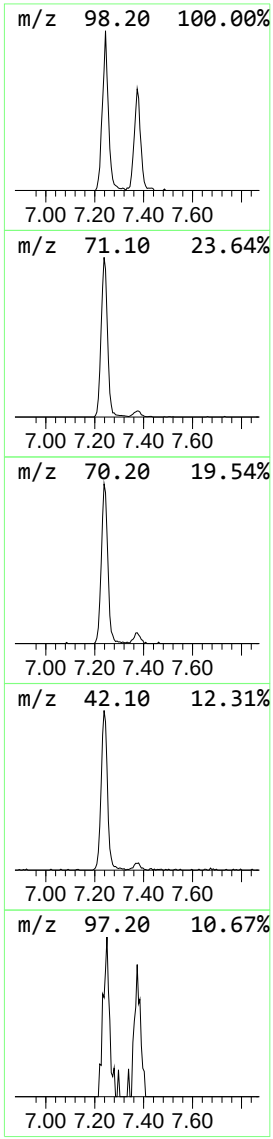
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 1-Methyl-2-piperidinemethanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.373	4.34 ng	50527	1,4-Dichlorobenzene-d4	8.090

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Methyl-2-piperidinemethanol	129	C7H15NO	020845-34-5	50
2	2-Pyrrolidinemethanamine, 1-ethyl-	128	C7H16N2	026116-12-1	50
3	3H-Pyrazole, 3,4-diamino-	98	C3H6N4	1000288-40-0	46
4	3-Isoxazolamine, 5-methyl-	98	C4H6N2O	001072-67-9	43
5	1,3-Cyclopentanedione	98	C5H6O2	003859-41-4	40





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070621\
Data File : BG049193.D
Acq On : 6 Jul 2021 20:15
Operator : CG/JU
Sample : M2933-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG063021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

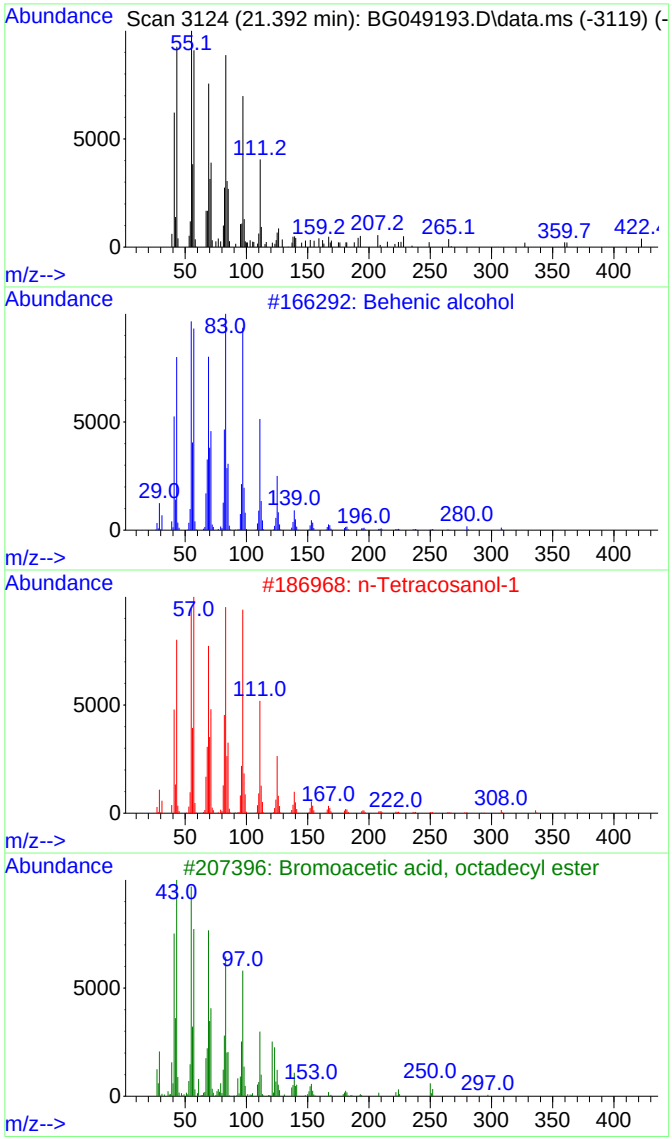
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

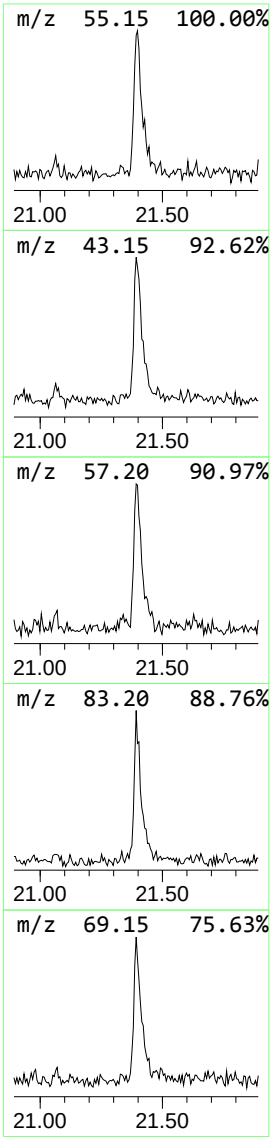
****

Peak Number 4 Behenic alcohol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.392	5.56 ng	164493	Chrysene-d12	21.762

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	91
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
3	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
4	Cyclohexadecane	224	C16H32	000295-65-8	81
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	81





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070621\
Data File : BG049193.D
Acq On : 6 Jul 2021 20:15
Operator : CG/JU
Sample : M2933-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG063021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	3.208	2.5	ng	29724	1	8.090	233007	20.0
1-Methyl-2-pipe...	7.373	4.3	ng	50527	1	8.090	233007	20.0
Behenic alcohol	21.392	5.6	ng	164493	5	21.762	591567	20.0