LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012423\
Data File : BG056405.D
Acq On : 24 Jan 2023 16:25
Operator : CG/JU
Sample : 01260-22
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-28

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: BG056405.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.330	341	347	356	rBB	104142	157417	5.61%	1.488%
2	5.818	422	430	440	rBV	412743	663262	23.62%	6.271%
3	7.439	698	706	719	rVB	412776	711286	25.33%	6.725%
4	8.291	845	851	859	rBB	103792	177313	6.31%	1.677%
5	9.466	1044	1051	1060	rBV	234240	421055	15.00%	3.981%
6	11.123	1326	1333	1342	rBV	134737	244795	8.72%	2.315%
7	13.532	1736	1743	1755	rBB	959431	1473295	52.47%	13.930%
8	14.907	1970	1977	1985	rBB	267343	428498	15.26%	4.052%
9	16.247	2199	2205	2211	rBB	27077	38104	1.36%	0.360%
10	16.388	2223	2229	2239	rBV	800970	1195988	42.60%	11.308%
11	17.645	2434	2443	2450	rBV	421168	614427	21.88%	5.810%
12	18.491	2582	2587	2595	rBV2	54754	91857	3.27%	0.869%
13	20.218	2875	2881	2887	rBV	2209862	2807810	100.00%	26.548%
14	21.517	3096	3102	3111	rBV4	53558	124921	4.45%	1.181%
15	21.934	3166	3173	3182	rVB	405088	709254	25.26%	6.706%
16	25.359	3747	3756	3767	rVB2	245209	716896	25.53%	6.778%

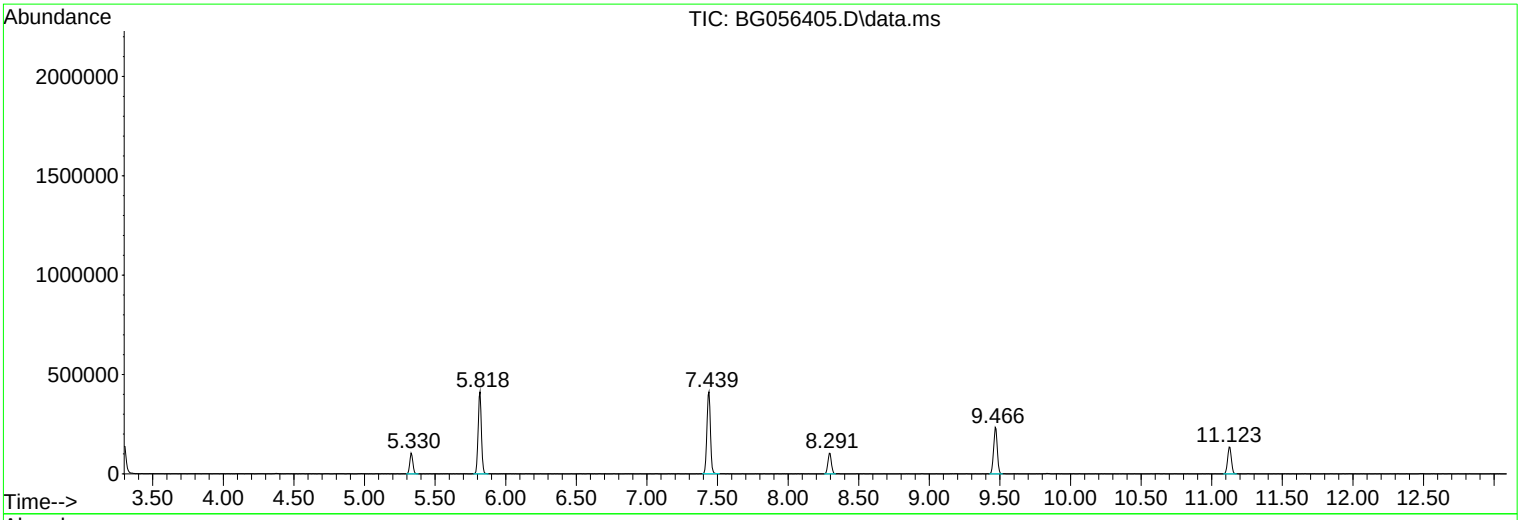
Sum of corrected areas: 10576178

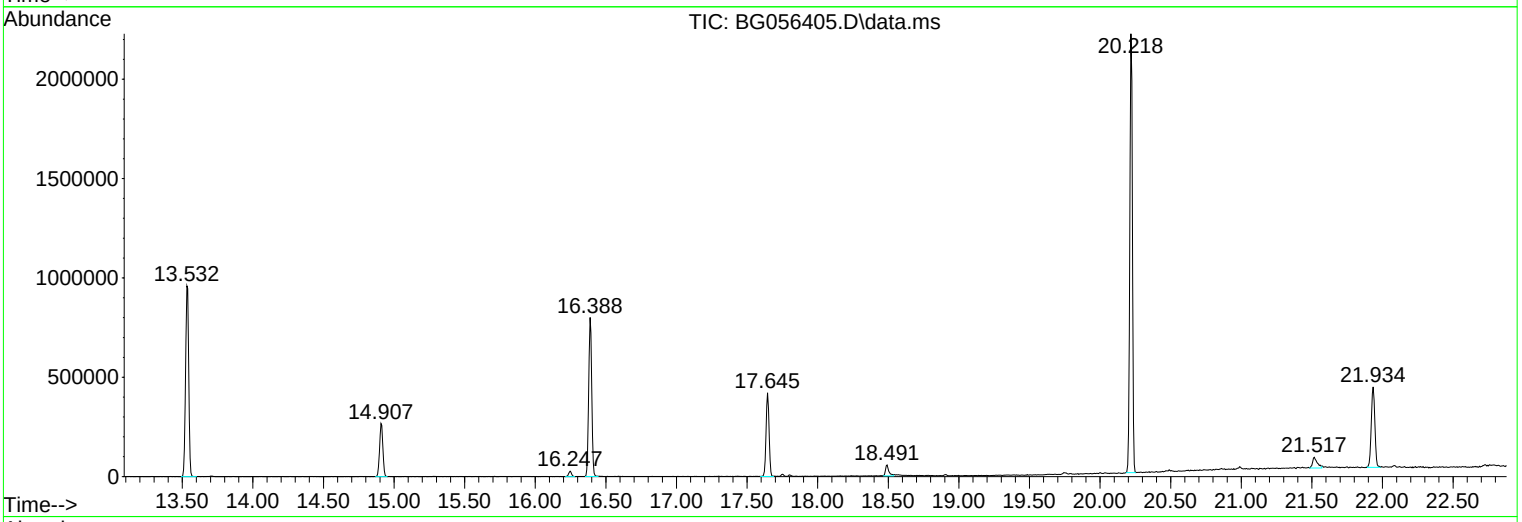
Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012423\
Data File : BG056405.D
Acq On : 24 Jan 2023 16:25
Operator : CG/JU
Sample : 01260-22
Misc :
ALS Vial : 4 Sample Multiplier: 1

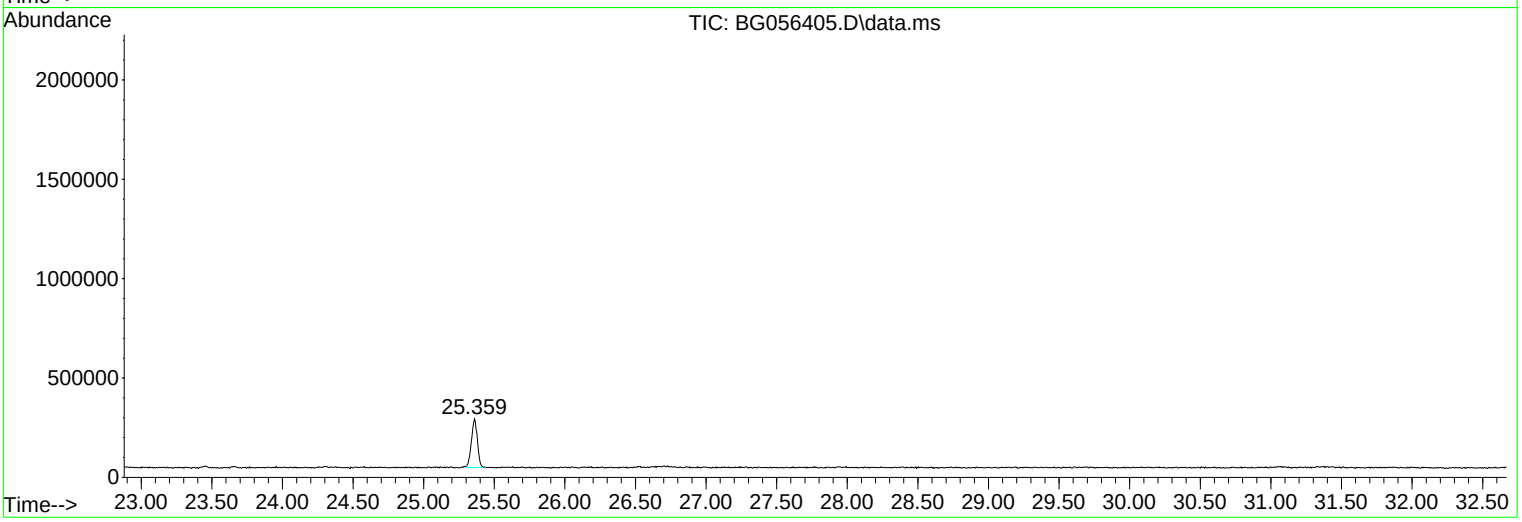
Instrument :
BNA_G
ClientSampleId :
TP-28

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012423\
Data File : BG056405.D
Acq On : 24 Jan 2023 16:25
Operator : CG/JU
Sample : 01260-22
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-28

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

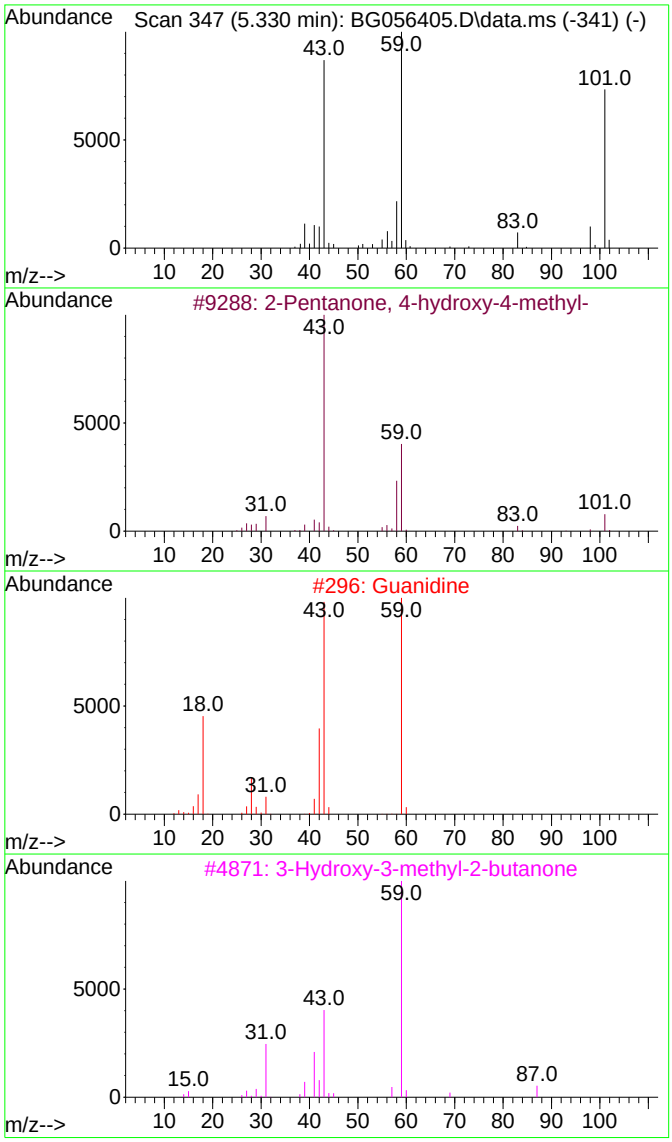
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

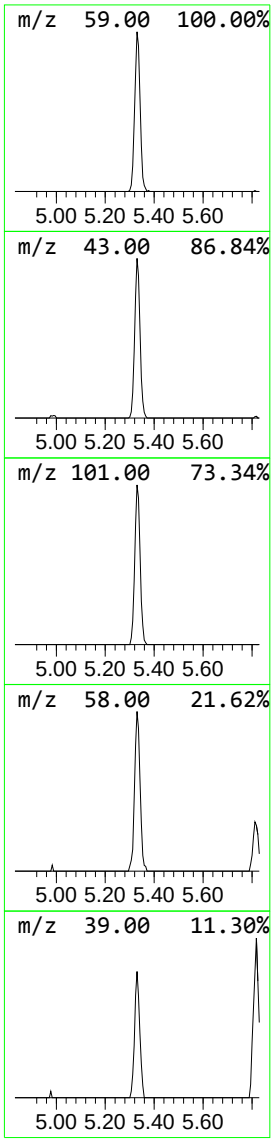
****

Peak Number 1 unknown5.330 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.330	17.76 ng	157417	1,4-Dichlorobenzene-d4	8.297

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	39
2	Guanidine	59	CH5N3	000113-00-8	25
3	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	12
4	1-Butene, 4-ethoxy-	100	C6H12O	044611-46-3	12
5	HEX-5-EN-3-OL	100	C6H12O	000688-99-3	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012423\
Data File : BG056405.D
Acq On : 24 Jan 2023 16:25
Operator : CG/JU
Sample : 01260-22
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-28

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

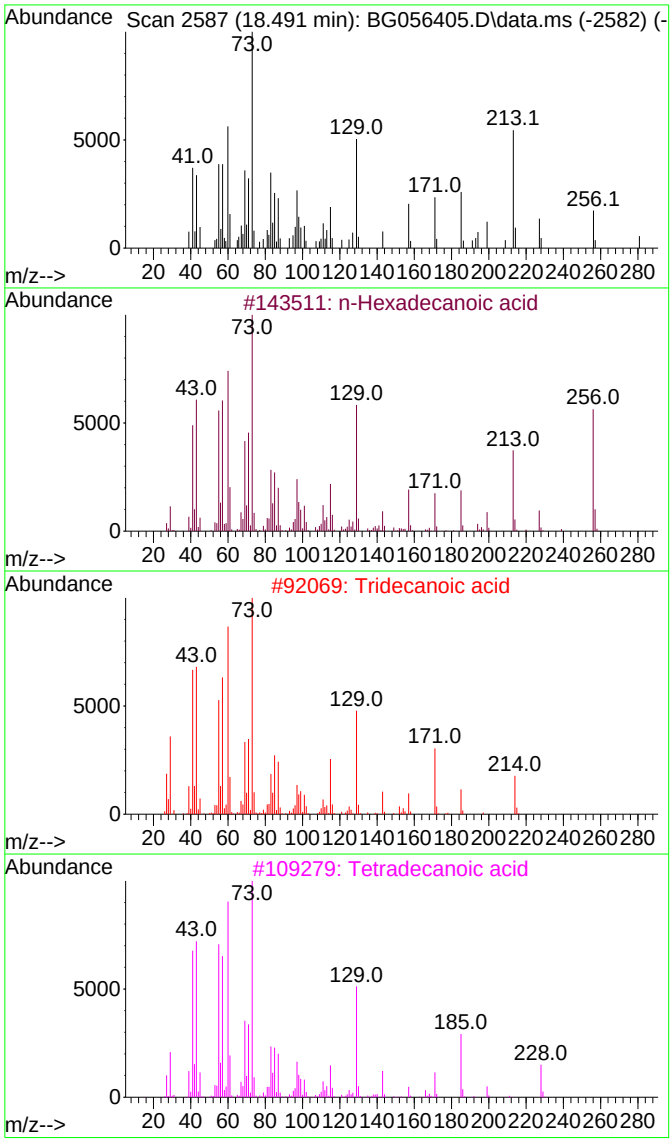
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

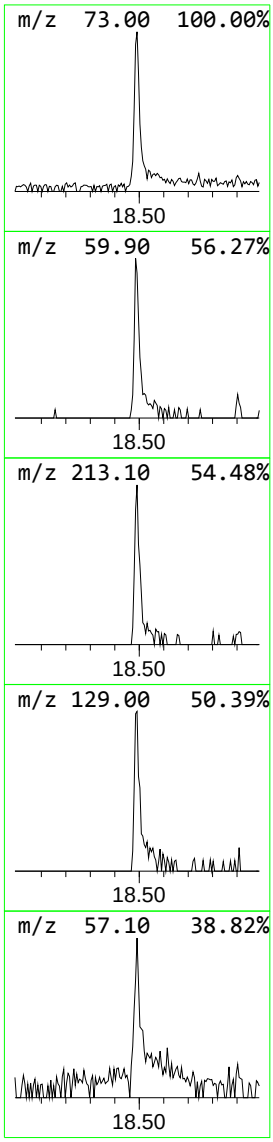
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.491	2.99 ng	91857	Phenanthrene-d10	17.645

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	47
5	n-Decanoic acid	172	C10H20O2	000334-48-5	30





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012423\
Data File : BG056405.D
Acq On : 24 Jan 2023 16:25
Operator : CG/JU
Sample : 01260-22
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-28

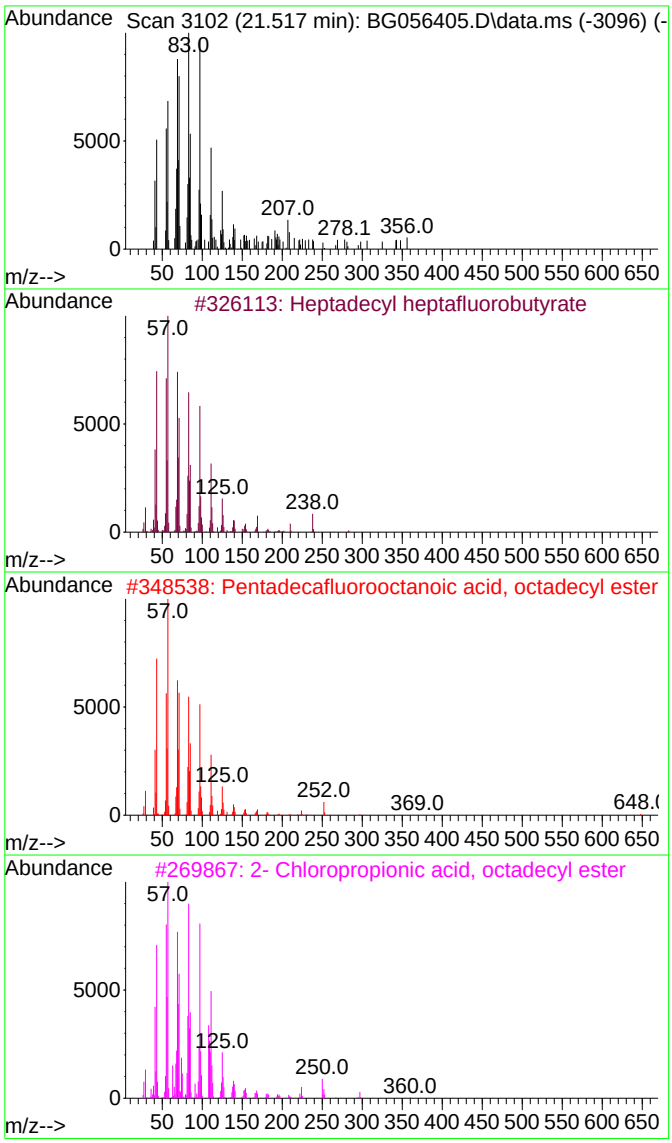
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

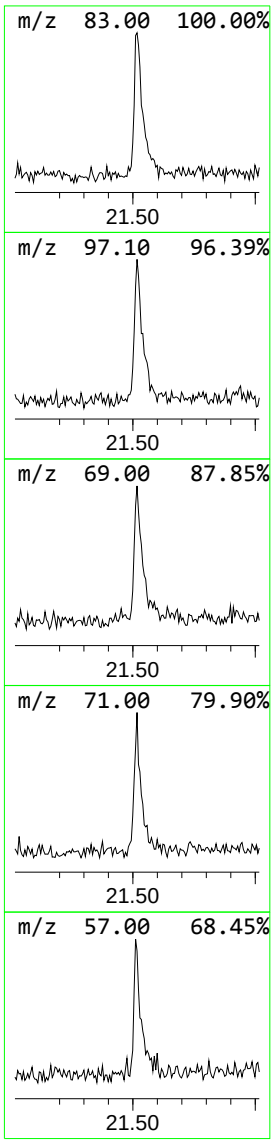
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Heptadecyl heptafluorobutyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.517	3.52 ng	124921	Chrysene-d12	21.934

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
2	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91
3	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	90
4	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	87
5	1-Docosanol, methyl ether	340	C23H48O	1000333-91-9	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012423\
Data File : BG056405.D
Acq On : 24 Jan 2023 16:25
Operator : CG/JU
Sample : 01260-22
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-28

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown5.330	5.330	17.8	ng	157417	1	8.297	177313	20.0
n-Hexadecanoic ...	18.491	3.0	ng	91857	4	17.645	614427	20.0
Heptadecyl hept...	21.517	3.5	ng	124921	5	21.934	709254	20.0