LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061623\
Data File : BG057751.D
Acq On : 17 Jun 2023 2:29
Operator : CG/JU
Sample : 03178-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-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-BG061323.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057751.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.115	3	4	20	rVB	409255	493183	18.38%	4.194%
2	5.036	326	331	336	rBV	27414	40459	1.51%	0.344%
3	5.500	403	410	421	rBV	325036	504163	18.79%	4.287%
4	7.087	673	680	690	rVB	215560	353171	13.16%	3.003%
5	7.933	818	824	831	rVB	119393	196046	7.30%	1.667%
6	9.090	1013	1021	1032	rBV	427073	747090	27.84%	6.353%
7	10.735	1293	1301	1310	rVB	185000	330577	12.32%	2.811%
8	13.191	1712	1719	1730	rVB	1144533	1767571	65.86%	15.032%
9	14.560	1946	1952	1960	rBV	325414	518679	19.33%	4.411%
10	15.917	2178	2183	2190	rVB	34427	47087	1.75%	0.400%
11	16.047	2198	2205	2218	rBV	1002505	1525630	56.84%	12.974%
12	17.304	2413	2419	2426	rBV	466537	686677	25.59%	5.840%
13	18.197	2565	2571	2579	rBV	58429	90538	3.37%	0.770%
14	19.466	2784	2787	2792	rBV2	24364	32842	1.22%	0.279%
15	19.924	2859	2865	2871	rBV	2072104	2683857	100.00%	22.824%
16	21.217	3081	3085	3092	rBV3	50816	88122	3.28%	0.749%
17	21.293	3095	3098	3104	rVB	29233	41992	1.56%	0.357%
18	21.558	3137	3143	3150	rBV	432024	711535	26.51%	6.051%
19	22.363	3278	3280	3288	rVB3	16483	28139	1.05%	0.239%
20	24.719	3670	3681	3698	rVB	277084	823627	30.69%	7.004%
21	25.888	3870	3880	3881	rBV8	24829	48109	1.79%	0.409%

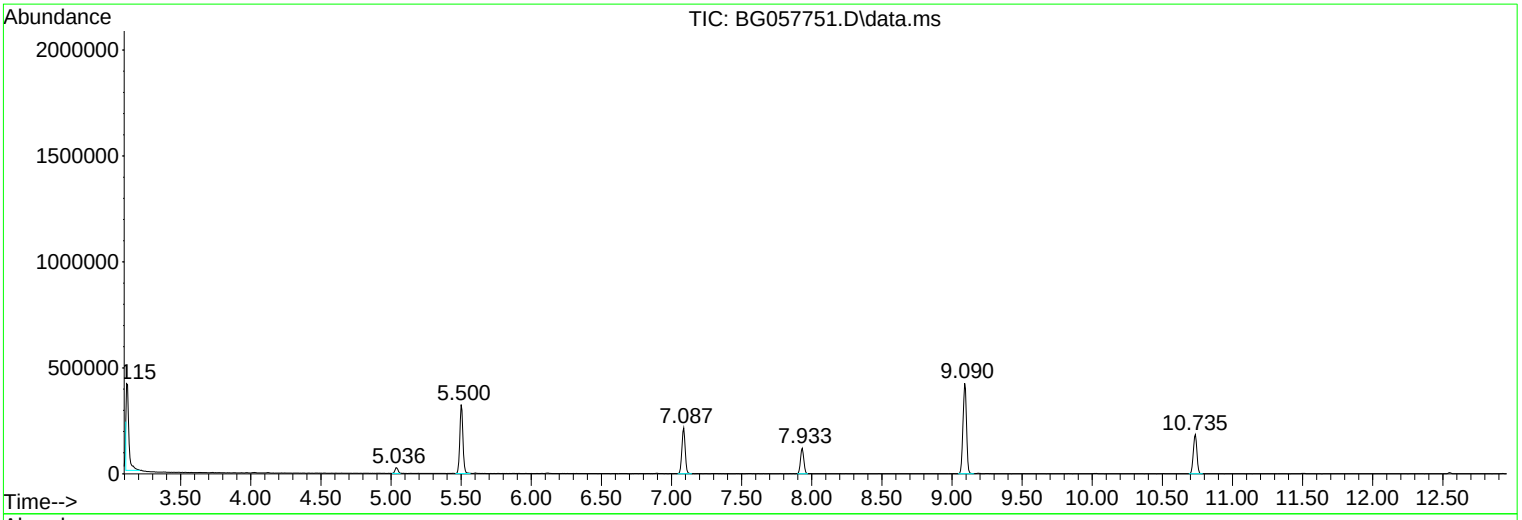
Sum of corrected areas: 11759094

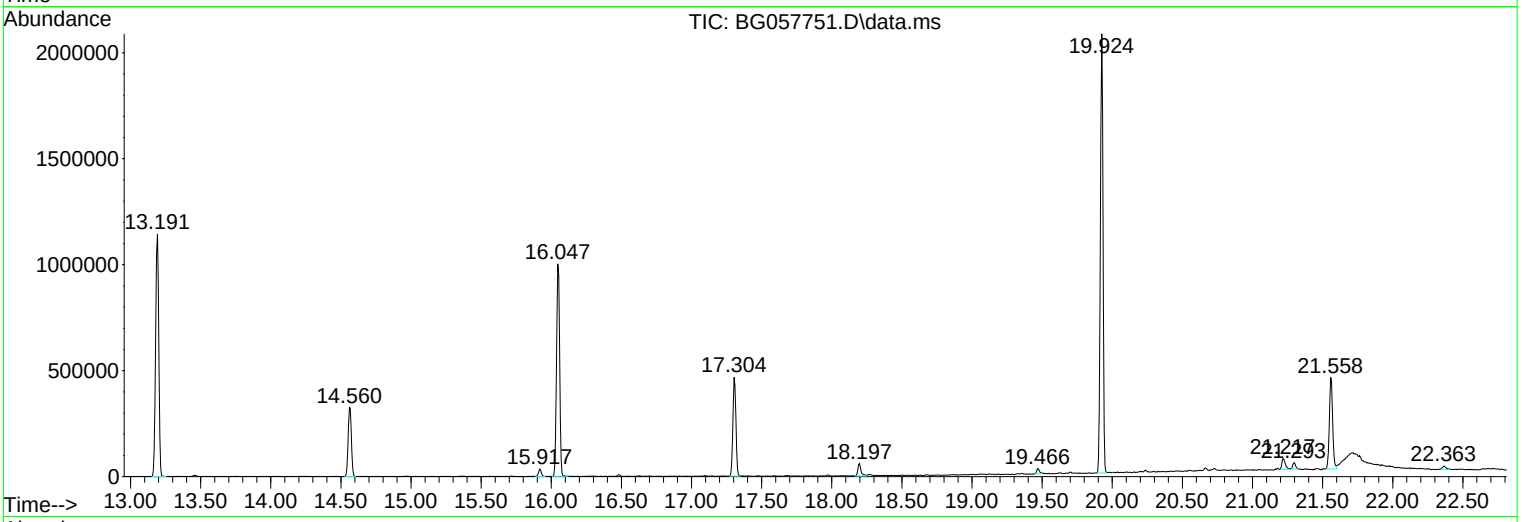
Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061623\
Data File : BG057751.D
Acq On : 17 Jun 2023 2:29
Operator : CG/JU
Sample : 03178-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

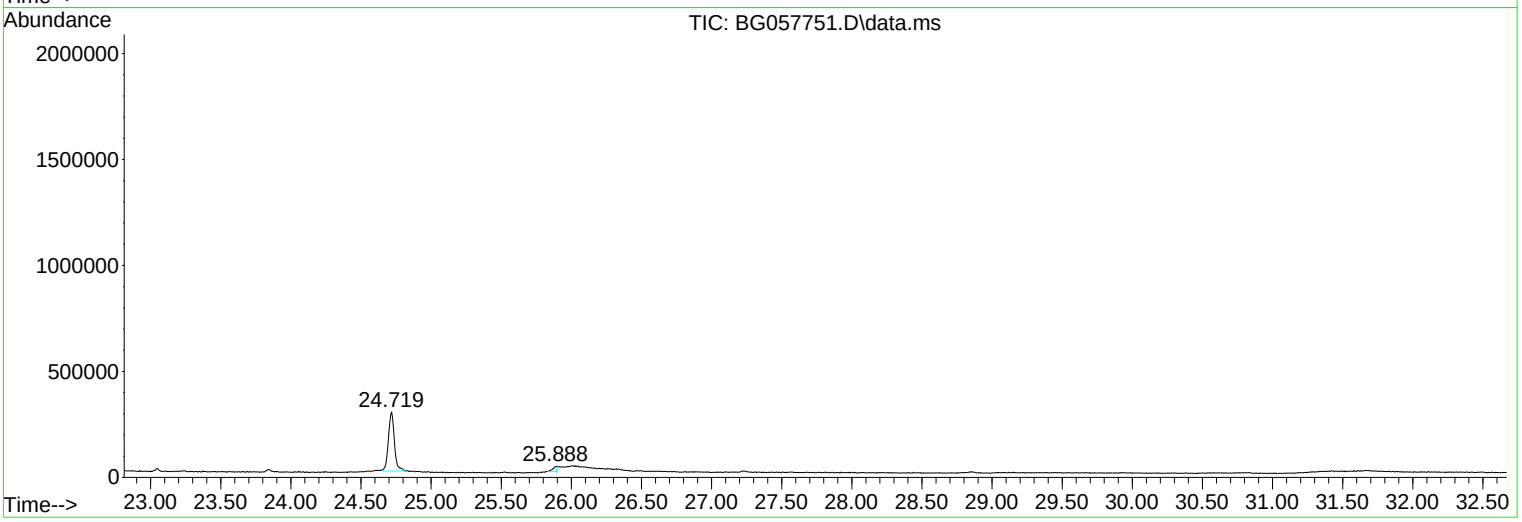
Instrument :
BNA_G
ClientSampleId :
MW-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061323.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\BG061623\
Data File : BG057751.D
Acq On : 17 Jun 2023 2:29
Operator : CG/JU
Sample : 03178-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

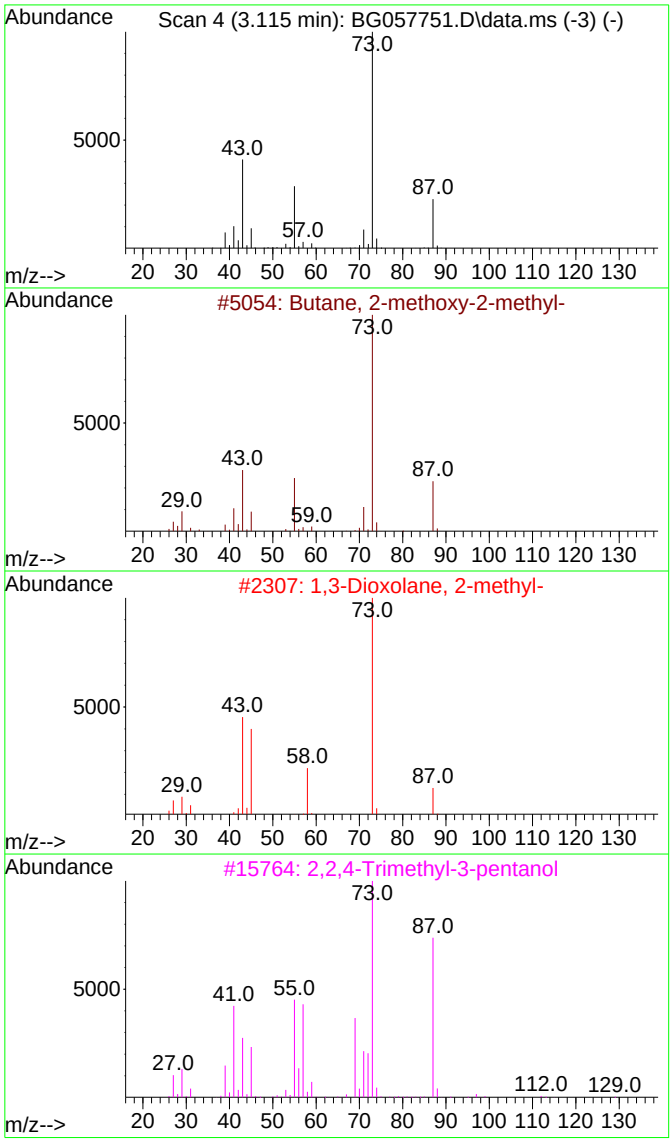
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

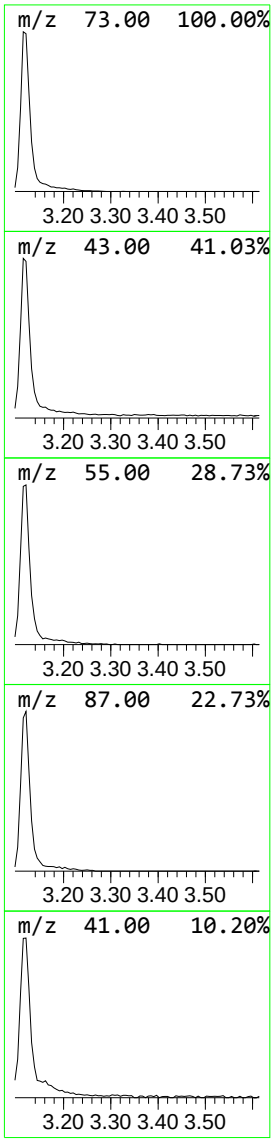
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.115	50.31 ng	493183	1,4-Dichlorobenzene-d4	7.933

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	47
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4	1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	16
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061623\
Data File : BG057751.D
Acq On : 17 Jun 2023 2:29
Operator : CG/JU
Sample : 03178-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-2

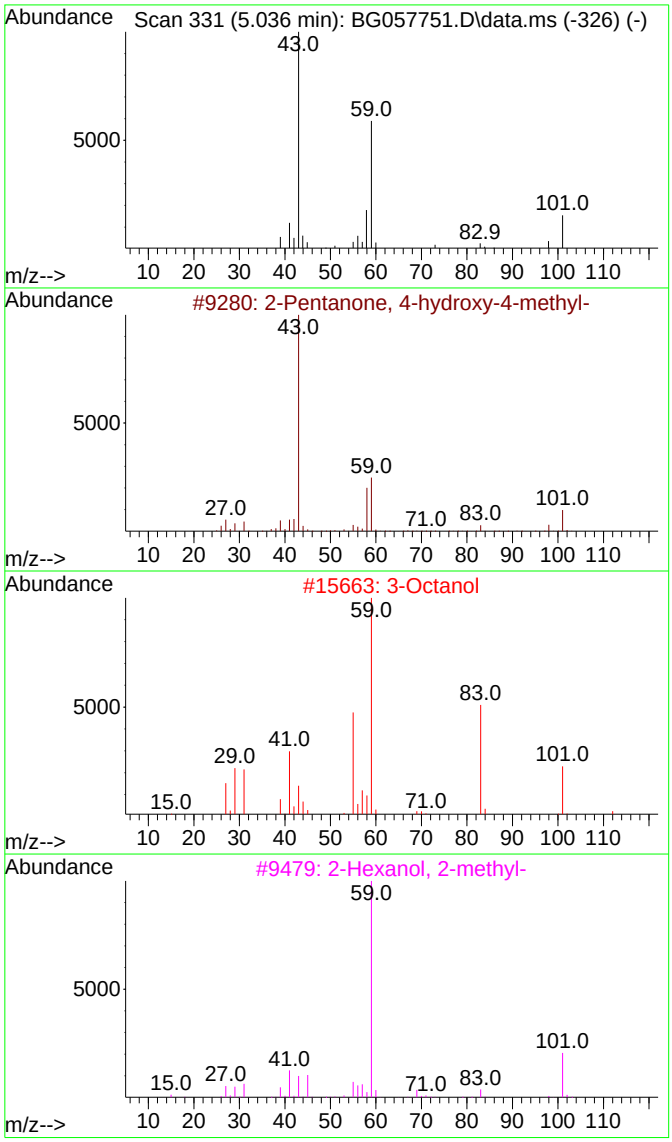
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

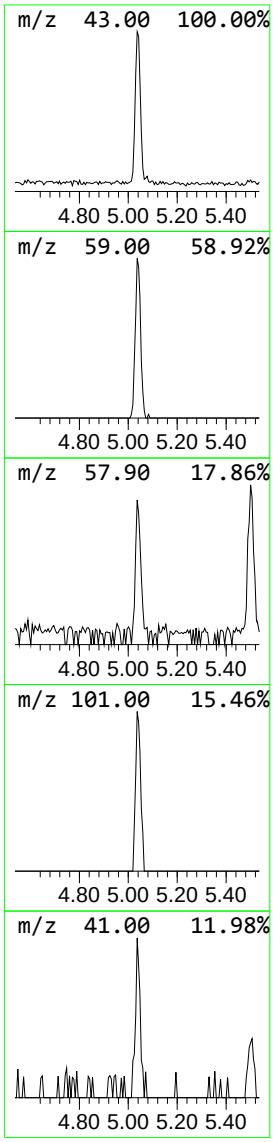
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.036	4.13 ng	40459	1,4-Dichlorobenzene-d4	7.933

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	3-Octanol	130	C8H18O	000589-98-0	33
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25
4	3-Hexanol	102	C6H14O	000623-37-0	25
5	1-Butanol, 3-methoxy-	104	C5H12O2	002517-43-3	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061623\
Data File : BG057751.D
Acq On : 17 Jun 2023 2:29
Operator : CG/JU
Sample : 03178-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

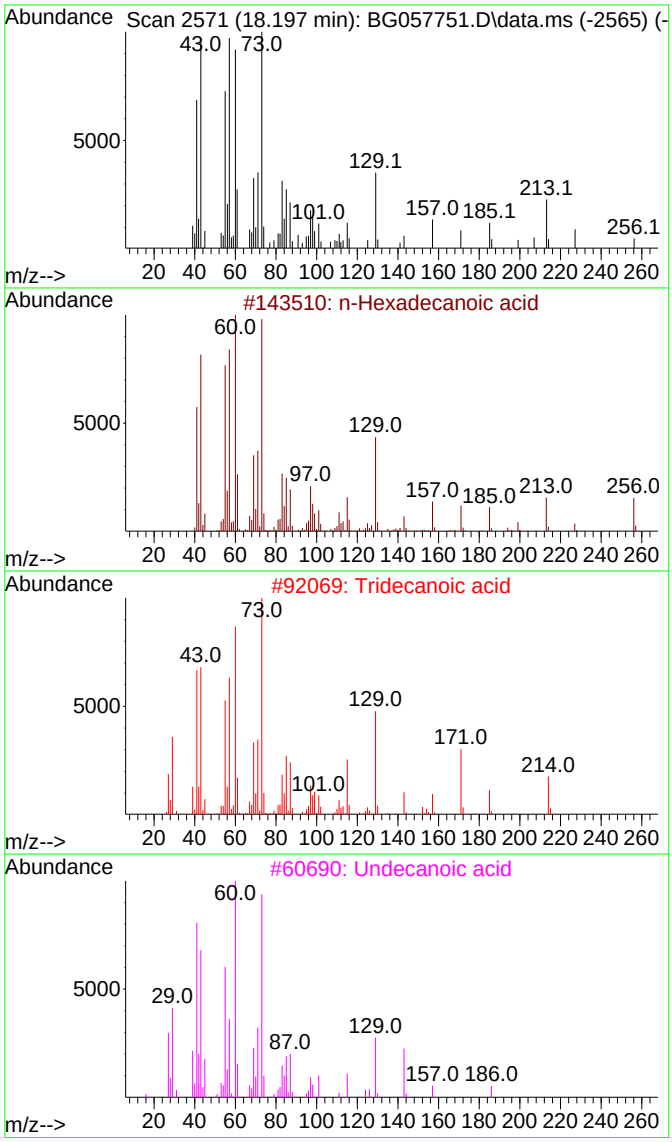
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

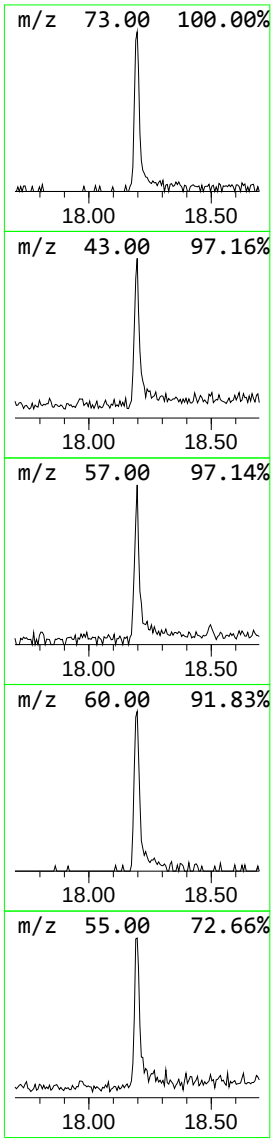
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.197	2.64 ng	90538	Phenanthrene-d10	17.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	90
3	Undecanoic acid	186	C11H22O2	000112-37-8	76
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061623\
Data File : BG057751.D
Acq On : 17 Jun 2023 2:29
Operator : CG/JU
Sample : 03178-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-2

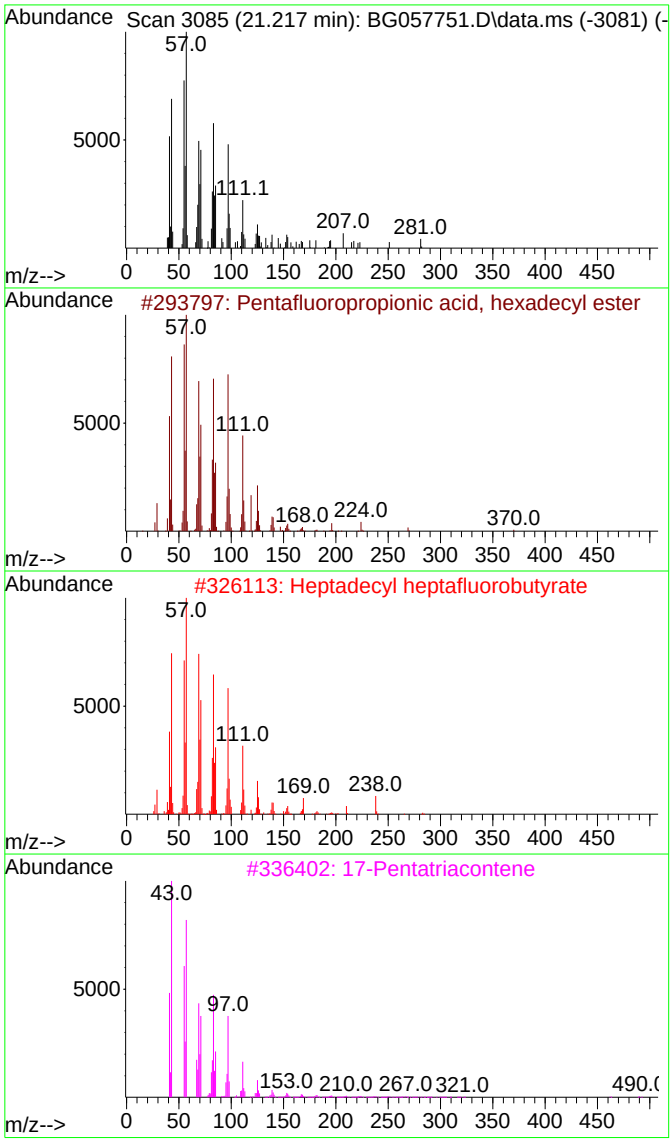
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

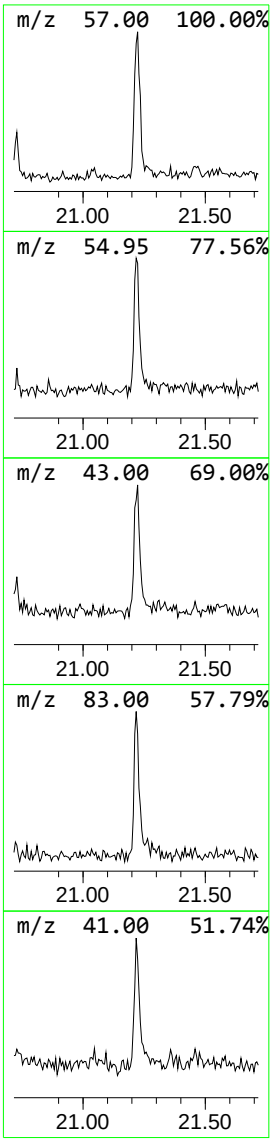
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Pentafluoropropionic acid, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.217	2.48 ng	88122	Chrysene-d12	21.558

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	90
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	90
3	17-Pentatriacontene	491	C35H70	006971-40-0	90
4	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	90
5	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061623\
Data File : BG057751.D
Acq On : 17 Jun 2023 2:29
Operator : CG/JU
Sample : 03178-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061323.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...	3.115	50.3	ng	493183	1	7.933	196046	20.0
2-Pentanone, 4-...	5.036	4.1	ng	40459	1	7.933	196046	20.0
n-Hexadecanoic ...	18.197	2.6	ng	90538	4	17.304	686677	20.0
Pentafluoroprop...	21.217	2.5	ng	88122	5	21.558	711535	20.0