LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112222\
Data File : BG055743.D
Acq On : 22 Nov 2022 17:12
Operator : CG/JU
Sample : N5749-15
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MH-83.5

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-BG111622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055743.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.298	335	342	348	rBV	103722	163342	8.09%	1.412%
2	5.773	416	423	435	rVB	540373	870086	43.09%	7.522%
3	7.389	690	698	708	rBV	542562	911643	45.15%	7.881%
4	8.241	837	843	850	rBV	128342	216349	10.71%	1.870%
5	9.416	1034	1043	1055	rBV	317270	569835	28.22%	4.926%
6	11.073	1318	1325	1334	rBV	178438	317139	15.71%	2.742%
7	13.494	1730	1737	1746	rBV	839822	1336440	66.18%	11.553%
8	14.869	1965	1971	1978	rVB	292880	475893	23.57%	4.114%
9	15.251	2032	2036	2046	rVB8	13830	30229	1.50%	0.261%
10	16.208	2195	2199	2204	rVB	49593	71179	3.52%	0.615%
11	16.349	2216	2223	2237	rBV	835746	1266968	62.74%	10.953%
12	17.607	2431	2437	2444	rBV	421146	612979	30.36%	5.299%
13	18.464	2578	2583	2599	rVB	215379	376084	18.62%	3.251%
14	18.882	2650	2654	2659	rBV2	31228	48551	2.40%	0.420%
15	19.722	2794	2797	2812	rVB	172845	324513	16.07%	2.805%
16	19.910	2825	2829	2838	rVB4	33745	70870	3.51%	0.613%
17	20.192	2871	2877	2883	rBV	1568205	2019322	100.00%	17.457%
18	21.508	3096	3101	3113	rBV	93877	207180	10.26%	1.791%
19	21.902	3162	3168	3183	rVB2	395591	701400	34.73%	6.064%
20	23.647	3460	3465	3472	rVB	79015	159060	7.88%	1.375%
21	25.309	3739	3748	3759	rVB2	266645	818509	40.53%	7.076%

Sum of corrected areas: 11567571

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112222\
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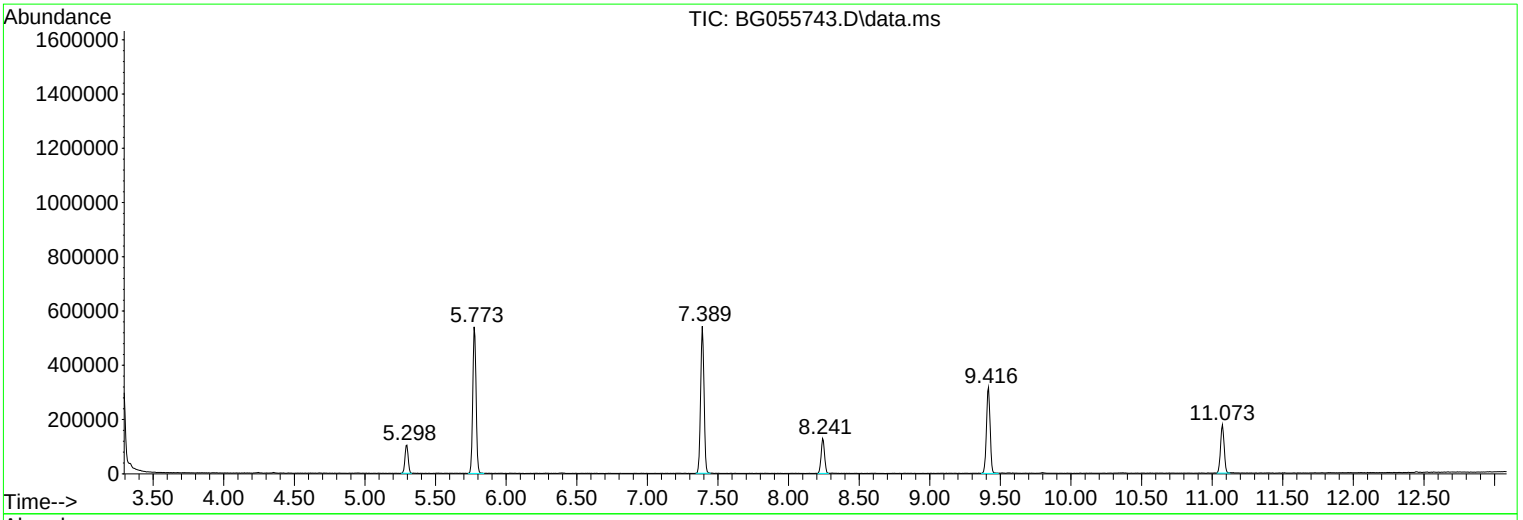
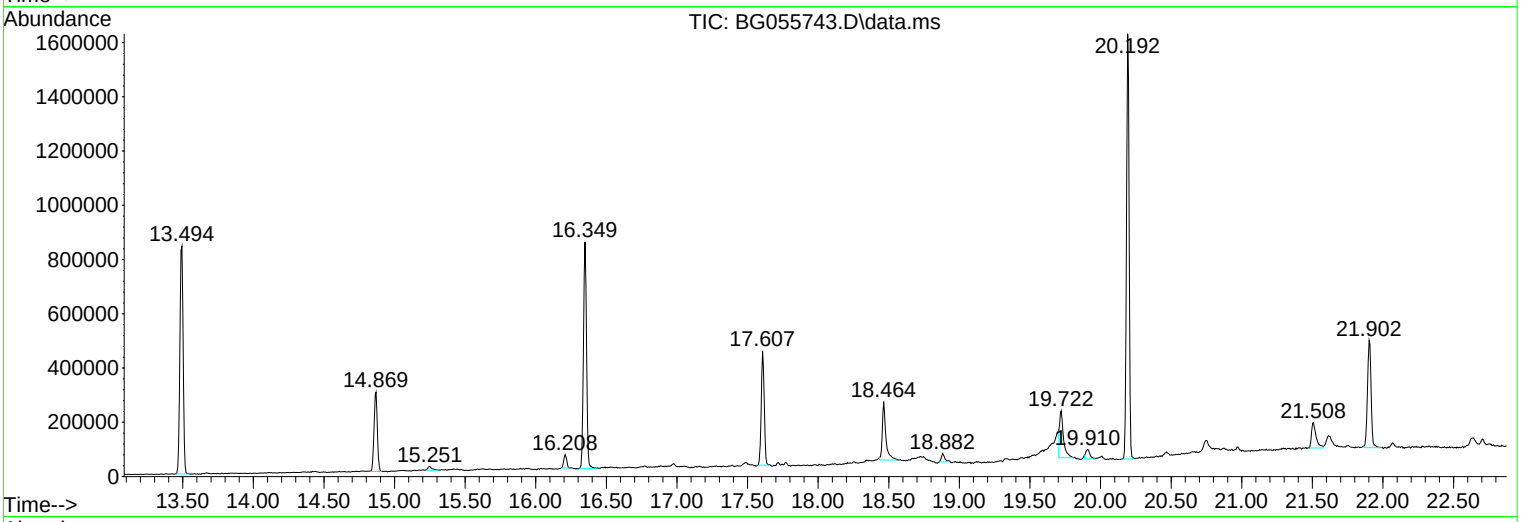
Misc :
ALS Vial : 4 Sample Multiplier: 1

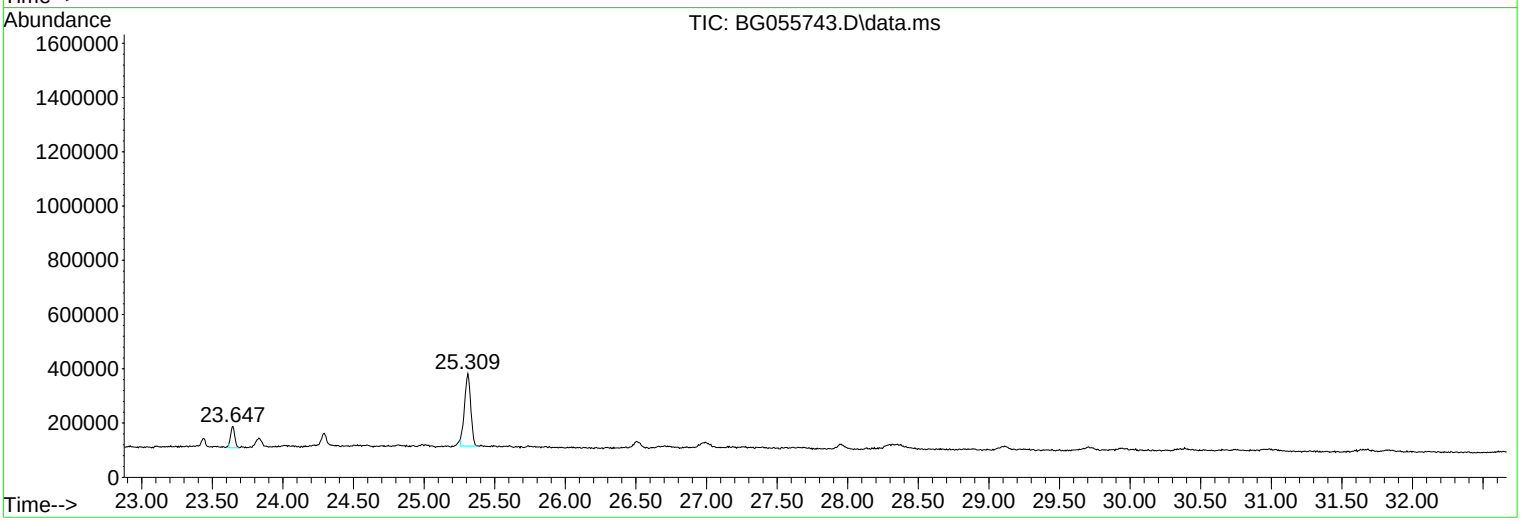
Instrument :
BNA_G
ClientSampleId :
MH-83.5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.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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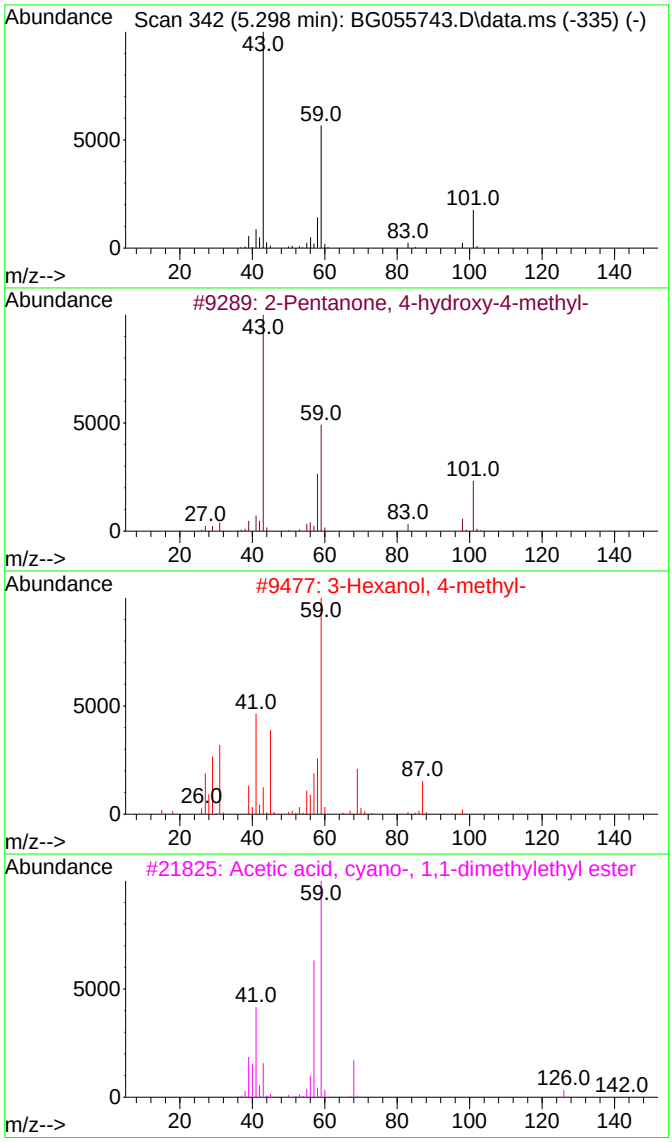
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

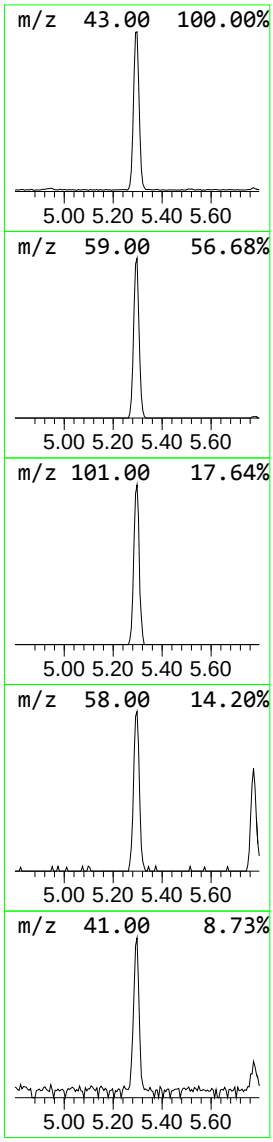
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.298	15.10 ng	163342	1,4-Dichlorobenzene-d4	8.241

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





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Data File : BG055743.D
Acq On : 22 Nov 2022 17:12
Operator : CG/JU
Sample : N5749-15
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MH-83.5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

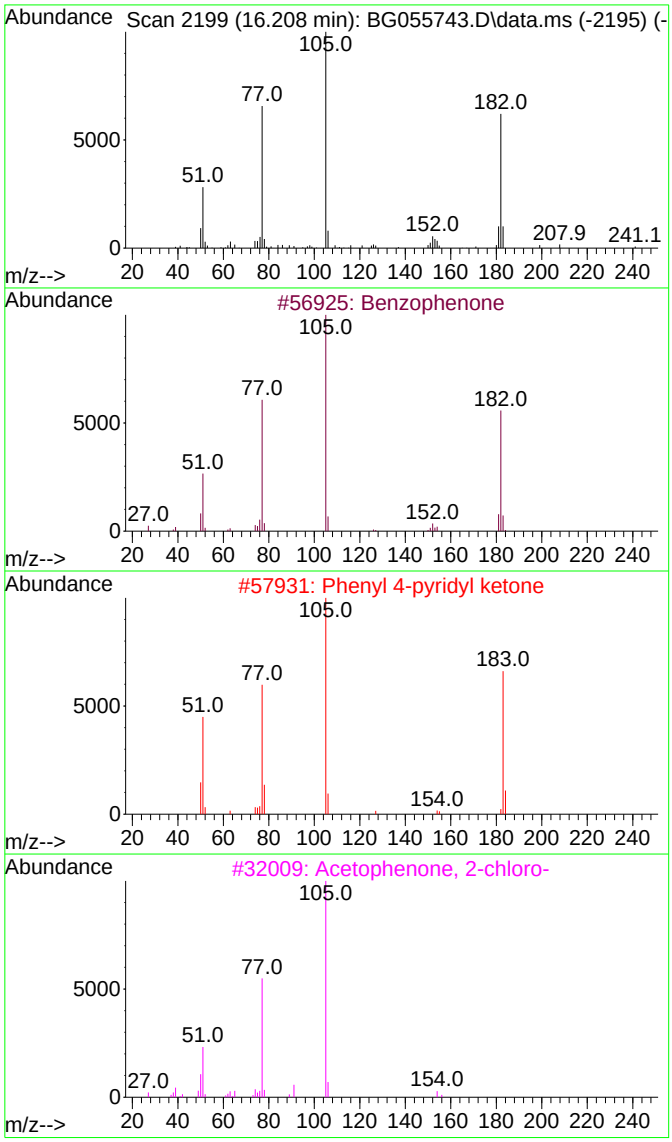
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

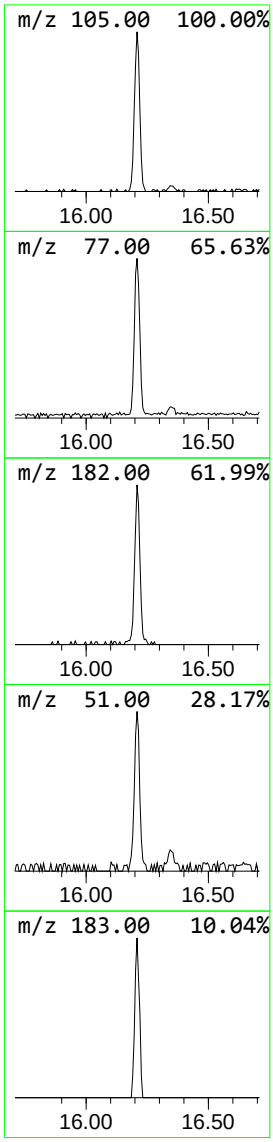
****

Peak Number 2 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.208	2.99 ng	71179	Acenaphthene-d10	14.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	53
3	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	50
4	Benzoylformic acid	150	C8H6O3	000611-73-4	45
5	Glyoxylohydroximoyl chloride, 2-...	183	C8H6ClNO2	004937-87-5	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112222\
Data File : BG055743.D
Acq On : 22 Nov 2022 17:12
Operator : CG/JU
Sample : N5749-15
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MH-83.5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

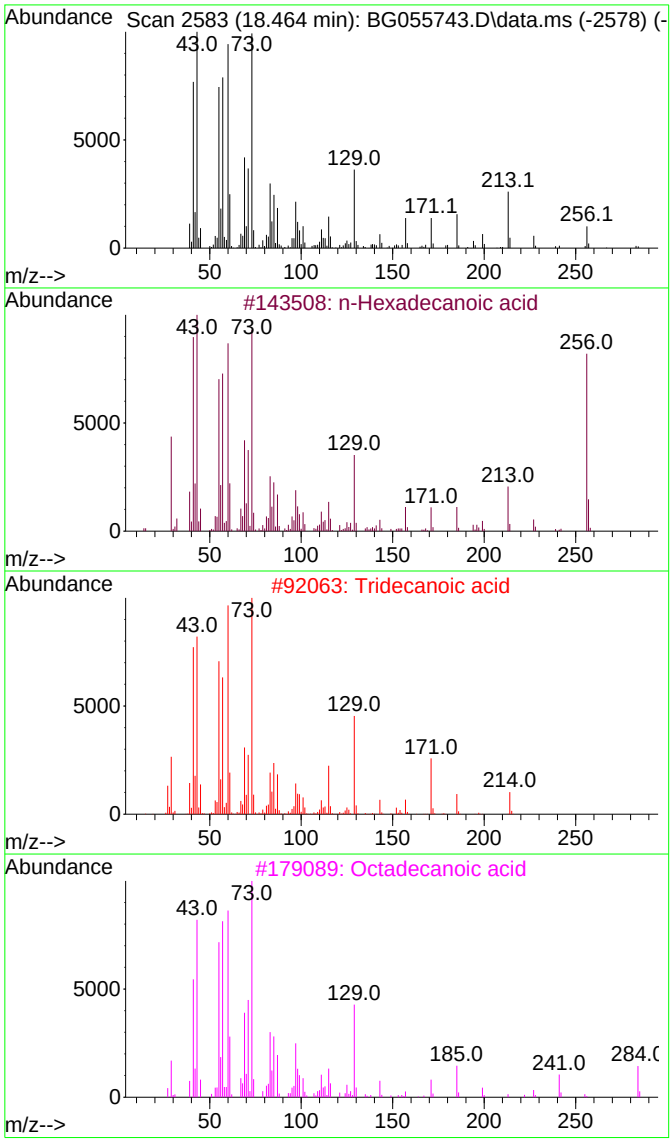
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

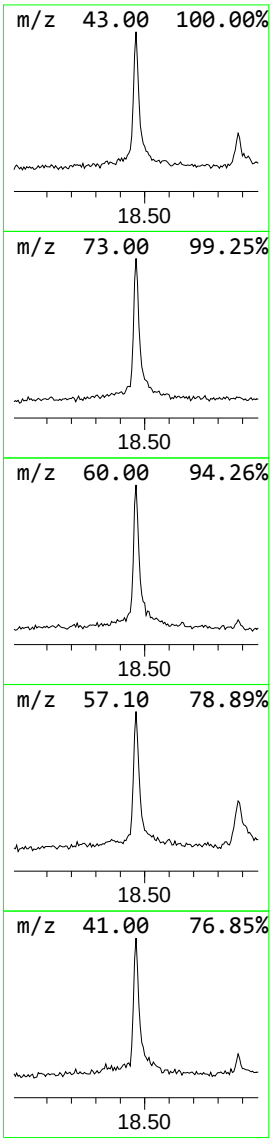
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.464	12.27 ng	376084	Phenanthrene-d10	17.607

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	90
3	Octadecanoic acid	284	C18H36O2	000057-11-4	87
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	58





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Data File : BG055743.D
Acq On : 22 Nov 2022 17:12
Operator : CG/JU
Sample : N5749-15
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MH-83.5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

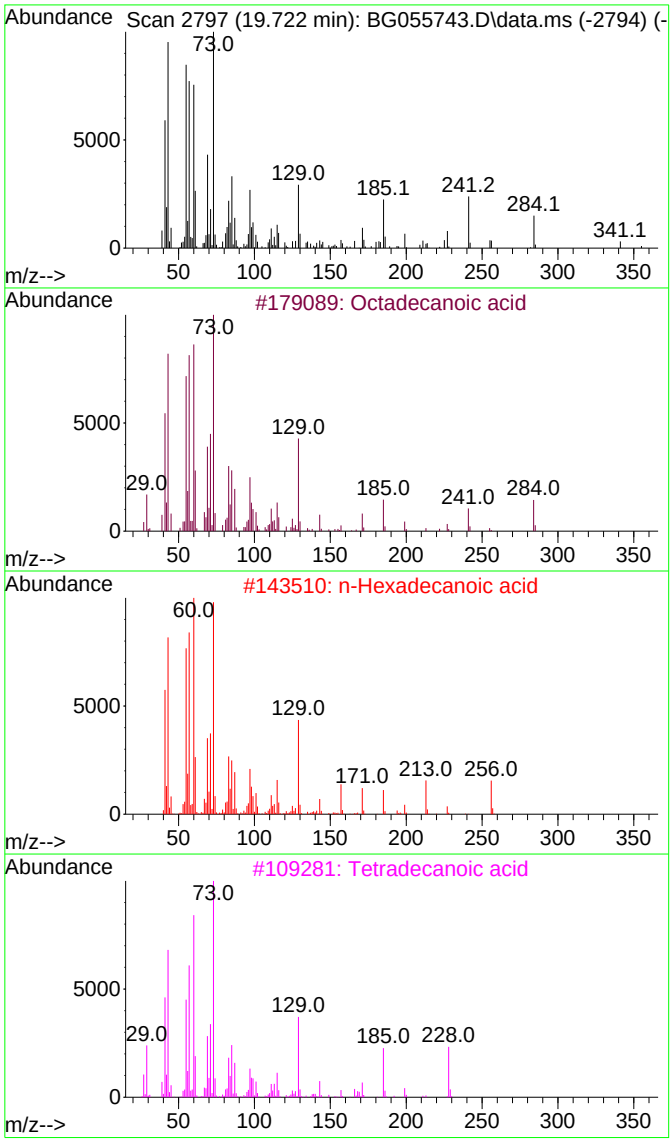
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

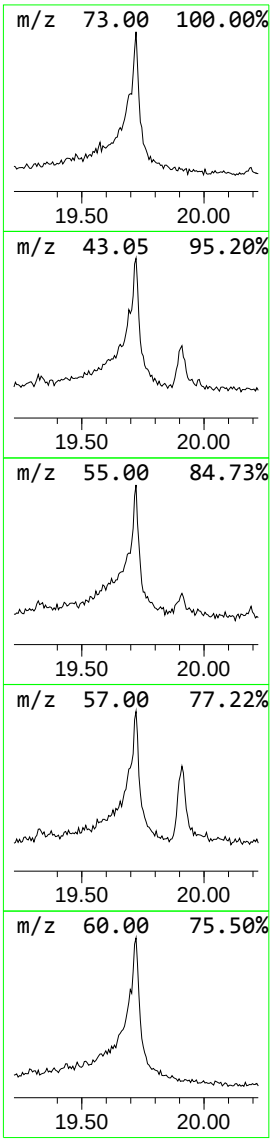
****

Peak Number 4 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.722	10.59 ng	324513	Phenanthrene-d10	17.607

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	91
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	86
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	53
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	47
5	Undecanoic acid	186	C11H22O2	000112-37-8	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112222\
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Operator : CG/JU
Sample : N5749-15
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MH-83.5

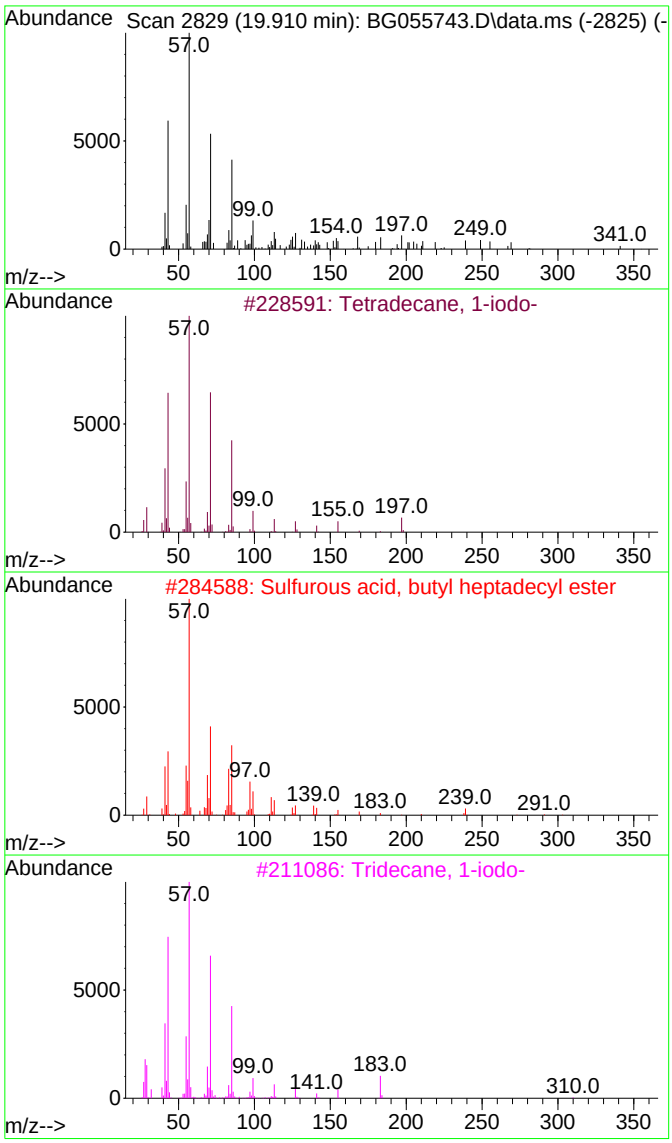
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

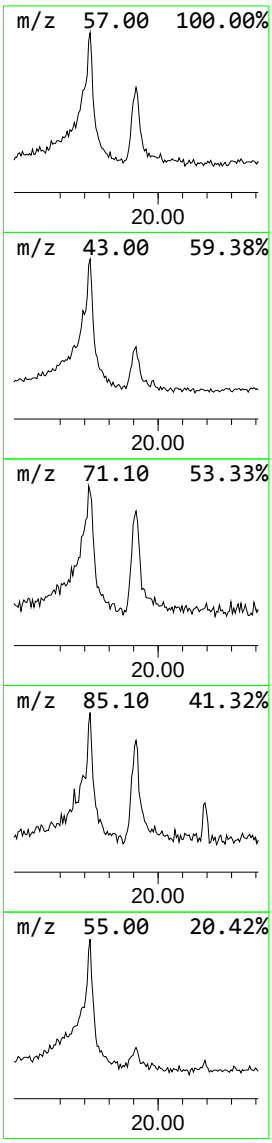
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Tetradecane, 1-iodo- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.910	2.02 ng	70870	Chrysene-d12	21.902

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	72
2	Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	72
3	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	64
4	Pentadecane	212	C15H32	000629-62-9	64
5	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	64





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ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MH-83.5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

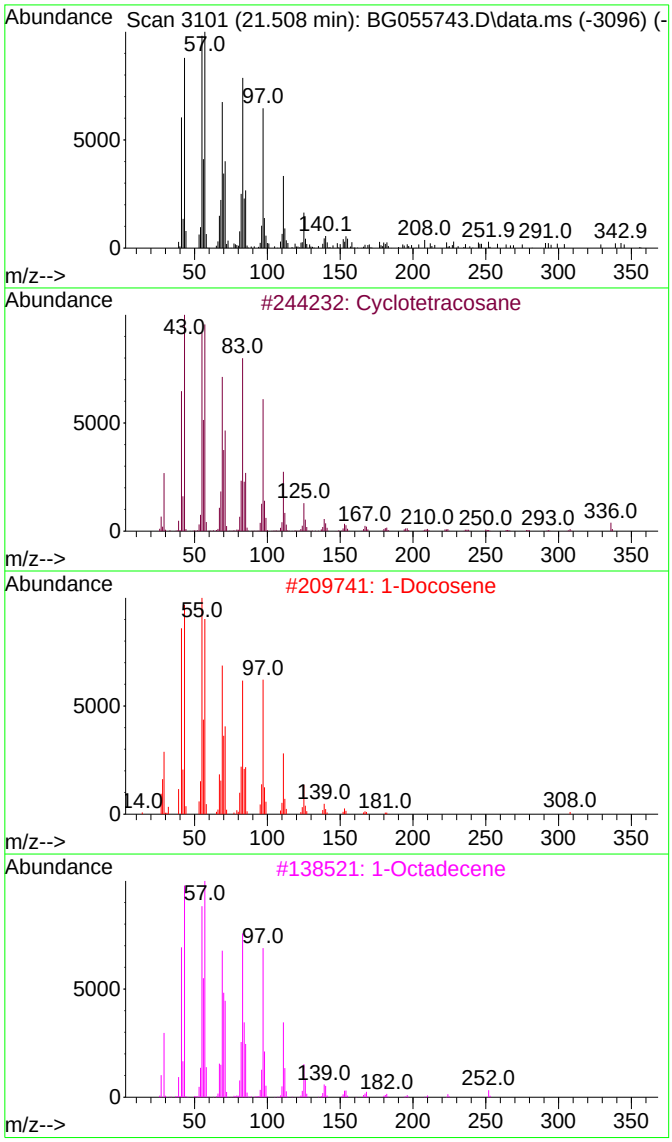
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

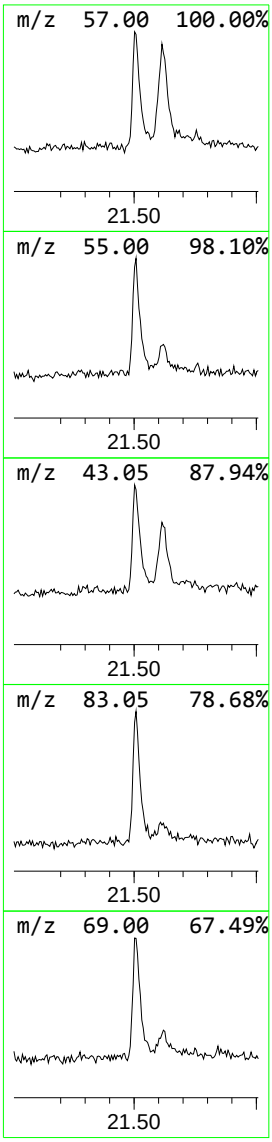
****

Peak Number 6 Cyclotetracosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.508	5.91 ng	207180	Chrysene-d12	21.902

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetracosane	336	C24H48	000297-03-0	94
2	1-Docosene	308	C22H44	001599-67-3	94
3	1-Octadecene	252	C18H36	000112-88-9	93
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
5	5-Eicosene, (E)-	280	C20H40	074685-30-6	91





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

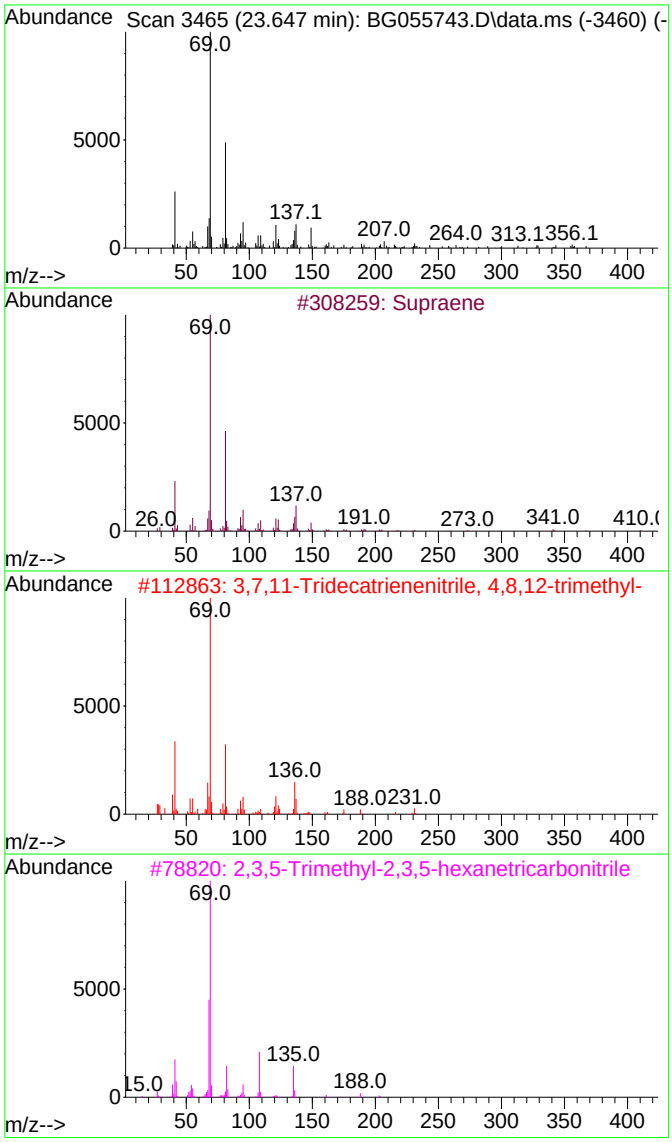
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

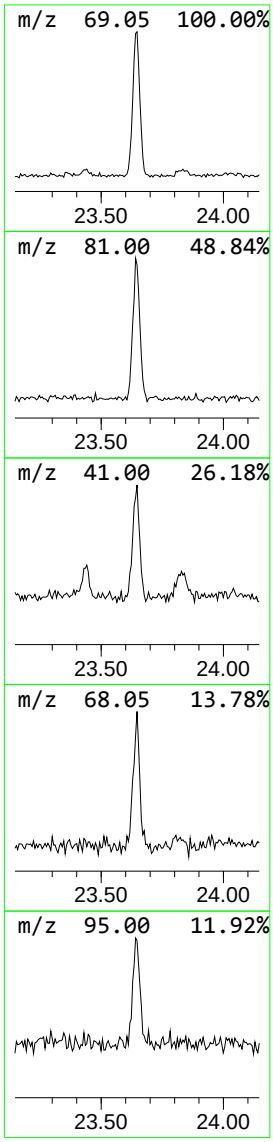
****

Peak Number 7 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.647	3.89 ng	159060	Perylene-d12	25.309

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	83
2	3,7,11-Tridecatrienenitrile, 4,8...	231	C16H25N	006006-01-5	72
3	2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	50
4	(.+/-.)-Lavandulol, pentafluorop...	300	C13H17F5O2	1000352-63-1	50
5	2,6-Octadiene, 4-methyl-	124	C9H16	074498-94-5	50





Tentatively Identified Compound (LSC) summary

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	5.298	15.1	ng	163342	1	8.241	216349	20.0
Benzophenone	16.208	3.0	ng	71179	3	14.869	475893	20.0
n-Hexadecanoic ...	18.464	12.3	ng	376084	4	17.607	612979	20.0
Octadecanoic acid	19.722	10.6	ng	324513	4	17.607	612979	20.0
Tetradecane, 1-...	19.910	2.0	ng	70870	5	21.902	701400	20.0
Cyclotetracosane	21.508	5.9	ng	207180	5	21.902	701400	20.0
Supraene	23.647	3.9	ng	159060	6	25.309	818509	20.0