LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062223\
Data File : BG057828.D
Acq On : 23 Jun 2023 4:36
Operator : CG/JU
Sample : 03320-16
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-16

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-BG061923.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057828.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.428	223	228	233	rBV	15176	21670	1.20%	0.177%
2	5.028	324	330	339	rBV	411966	607492	33.72%	4.957%
3	5.498	402	410	420	rVB	588376	941001	52.23%	7.678%
4	6.109	506	514	519	rBV	16501	25767	1.43%	0.210%
5	7.084	672	680	690	rBV	623897	1039753	57.71%	8.483%
6	7.924	816	823	830	rBV	184184	303362	16.84%	2.475%
7	9.082	1012	1020	1032	rBV	359148	630055	34.97%	5.141%
8	10.727	1292	1300	1308	rBV	256564	462482	25.67%	3.773%
9	13.177	1711	1717	1726	rBV	810461	1270962	70.55%	10.370%
10	14.558	1939	1952	1961	rBV	417833	633537	35.17%	5.169%
11	15.909	2176	2182	2188	rBV	139941	193155	10.72%	1.576%
12	16.044	2197	2205	2211	rBV	736292	1137691	63.15%	9.283%
13	17.301	2412	2419	2426	rBV	475901	742473	41.21%	6.058%
14	17.478	2443	2449	2453	rBV6	12616	23186	1.29%	0.189%
15	18.189	2565	2570	2580	rBV	194842	283702	15.75%	2.315%
16	19.464	2783	2787	2793	rBV2	45226	75704	4.20%	0.618%
17	19.916	2858	2864	2871	rVB	1423560	1801561	100.00%	14.699%
18	21.209	3080	3084	3092	rVV2	80664	137575	7.64%	1.122%
19	21.285	3094	3097	3103	rVB	40637	57156	3.17%	0.466%
20	21.549	3137	3142	3151	rVB2	477300	773896	42.96%	6.314%
21	23.212	3419	3425	3432	rVB	142424	265252	14.72%	2.164%
22	24.704	3671	3679	3695	rVB	266289	828807	46.00%	6.762%

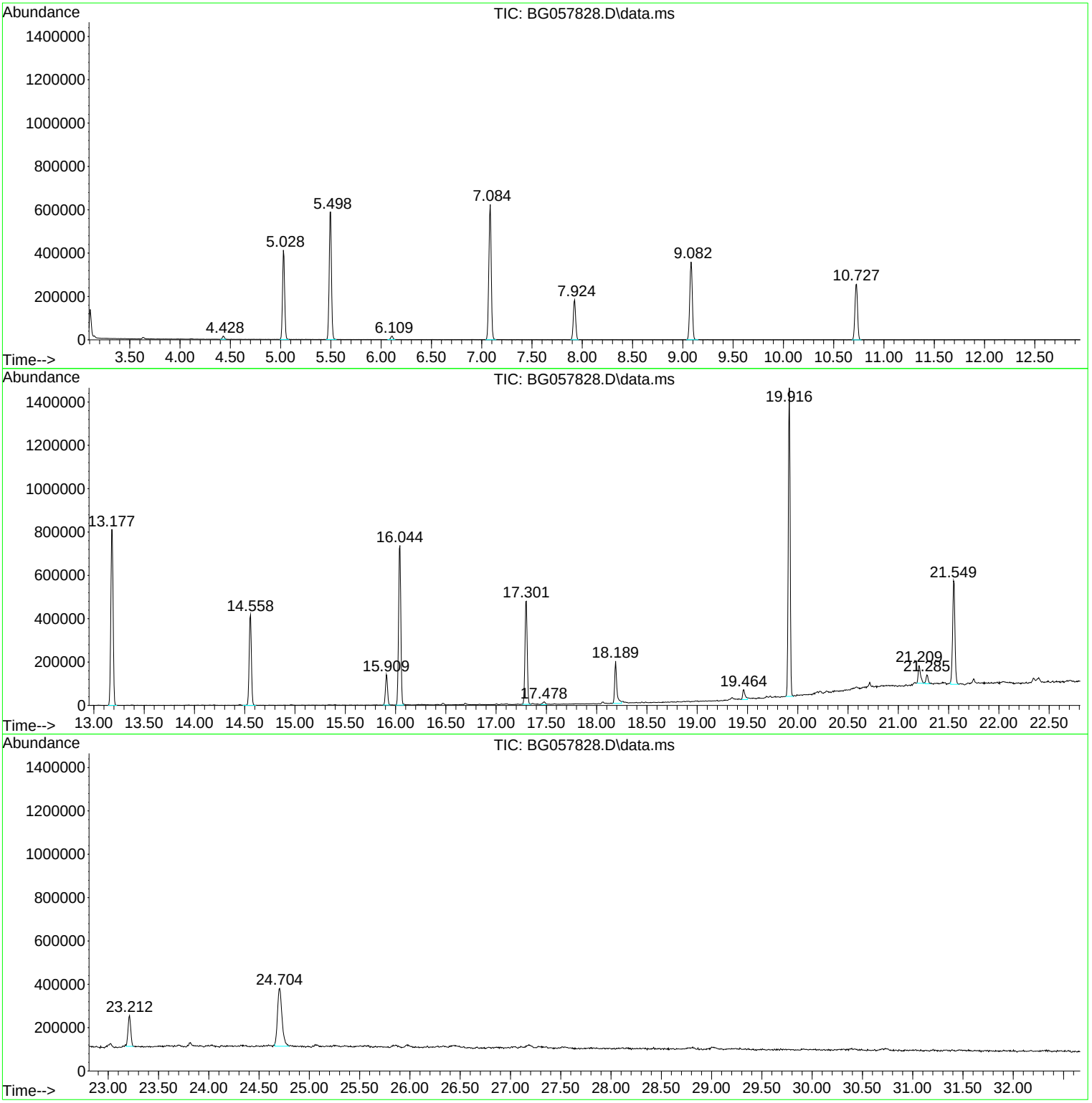
Sum of corrected areas: 12256239

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062223\
Data File : BG057828.D
Acq On : 23 Jun 2023 4:36
Operator : CG/JU
Sample : 03320-16
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-16

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.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\BG062223\
Data File : BG057828.D
Acq On : 23 Jun 2023 4:36
Operator : CG/JU
Sample : 03320-16
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-16

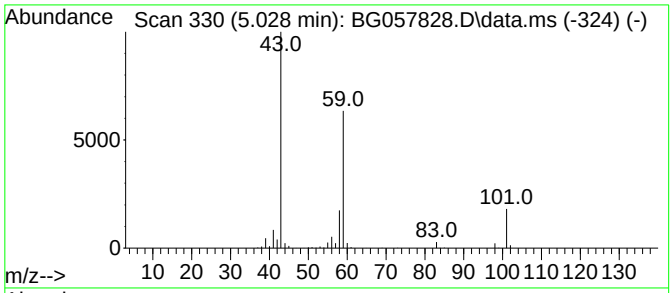
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

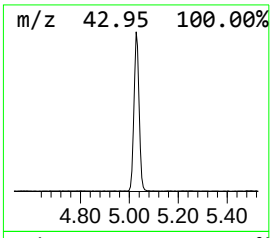
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

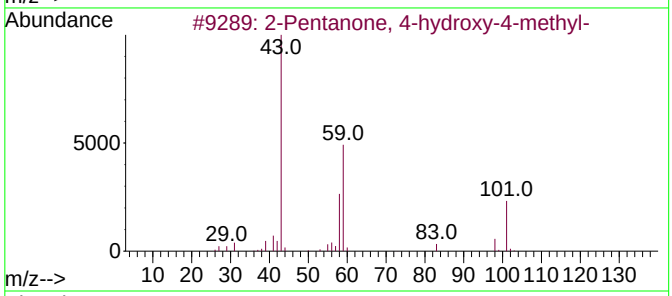
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

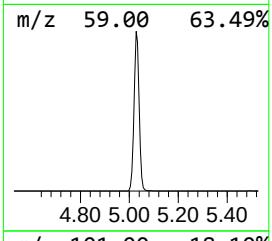
R.T.	EstConc	Area	Relative to ISTD	R.T.
5.028	40.05 ng	607492	1,4-Dichlorobenzene-d4	7.924

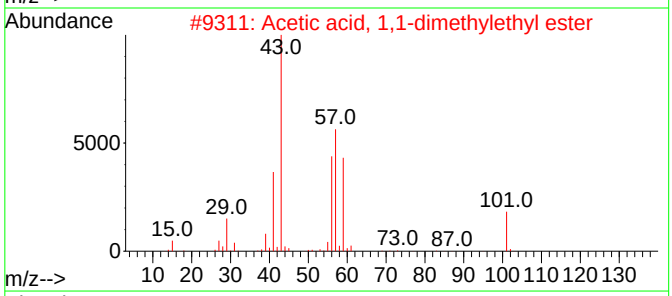
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	3-Octanol	130	C8H18O	000589-98-0	33
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28

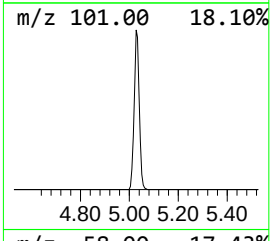


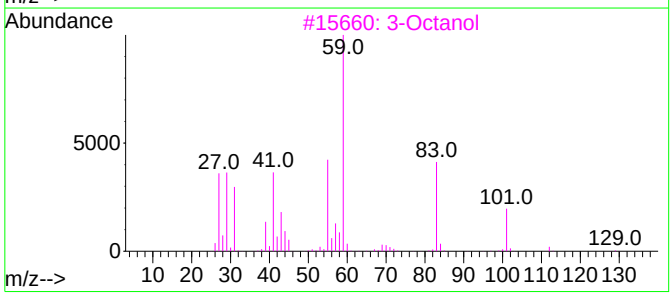


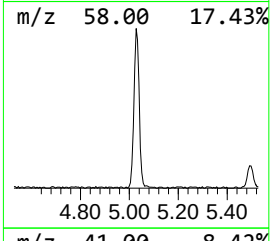


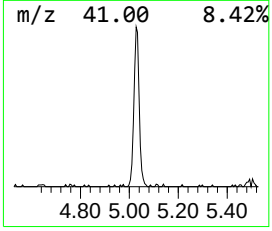












Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062223\
Data File : BG057828.D
Acq On : 23 Jun 2023 4:36
Operator : CG/JU
Sample : 03320-16
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-16

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

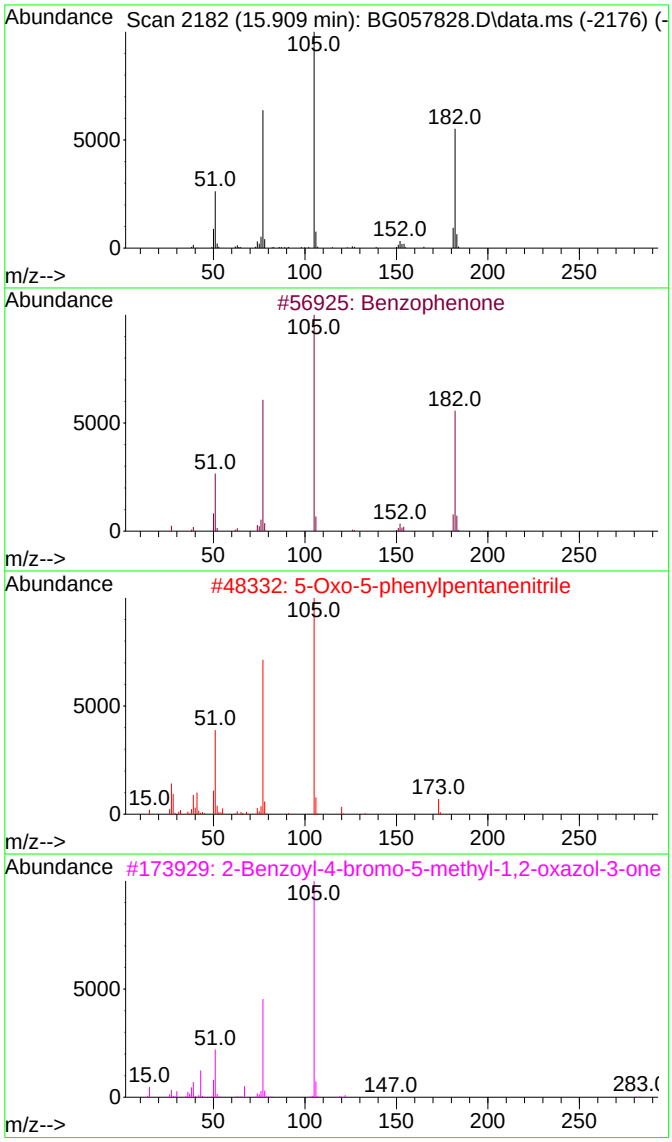
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

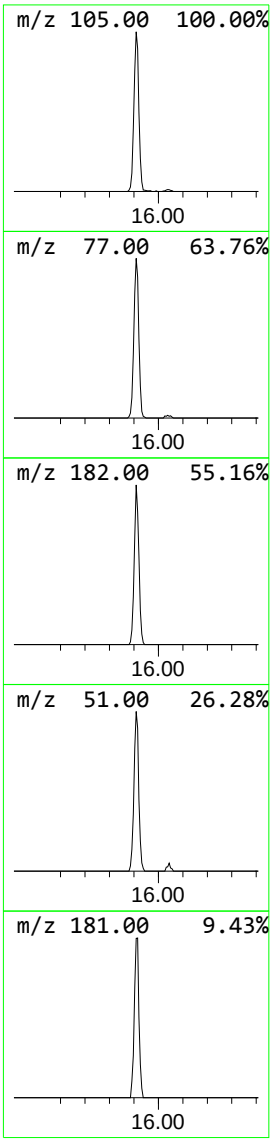
****

Peak Number 2 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.909	6.10 ng	193155	Acenaphthene-d10	14.558

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	5-Oxo-5-phenylpentanenitrile	173	C11H11NO	1000486-83-7	47
3	2-Benzoyl-4-bromo-5-methyl-1,2-o...	281	C11H8BrNO3	1000444-92-3	47
4	1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
5	.alpha.,.alpha.-Dichloroacetophe...	188	C8H6Cl2O	002648-61-5	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062223\
Data File : BG057828.D
Acq On : 23 Jun 2023 4:36
Operator : CG/JU
Sample : 03320-16
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-16

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

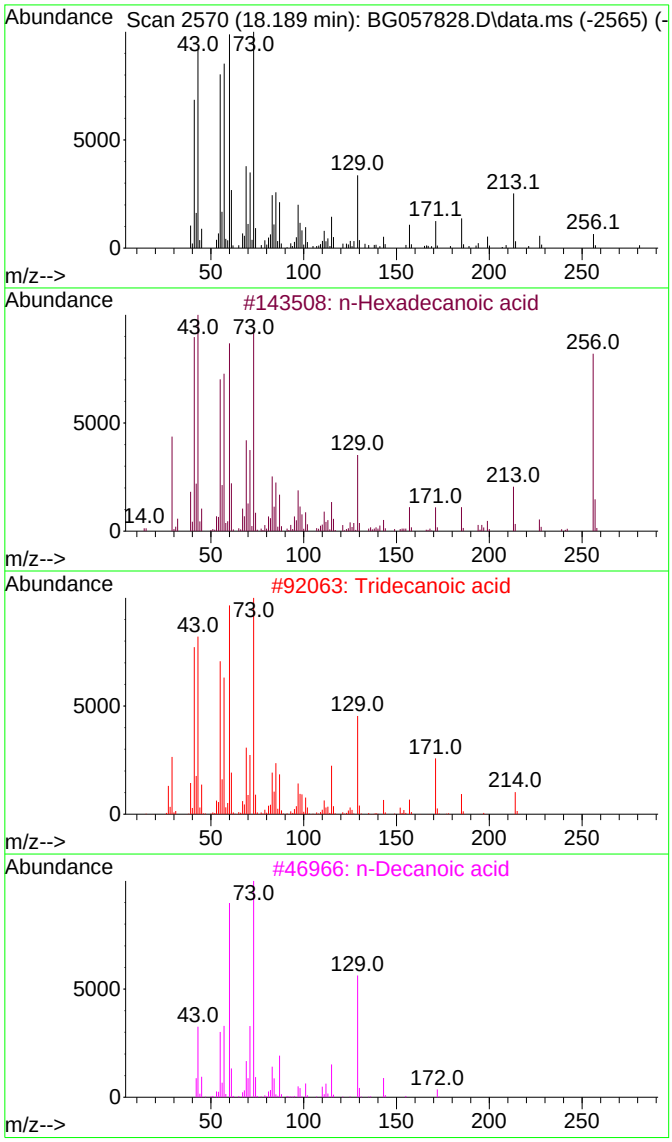
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

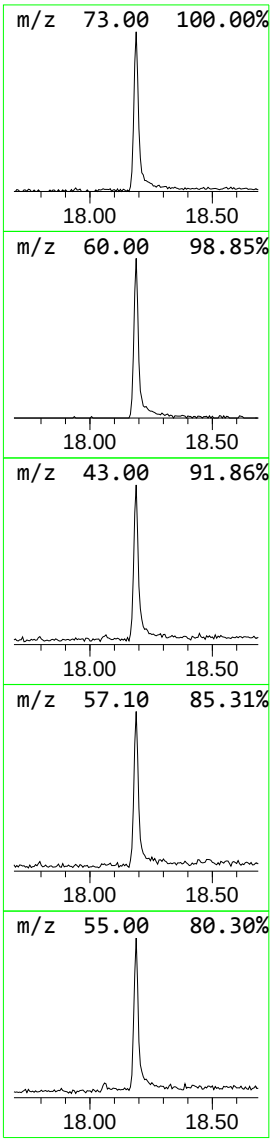
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.189	7.64 ng	283702	Phenanthrene-d10	17.301

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	n-Decanoic acid	172	C10H20O2	000334-48-5	83
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062223\
Data File : BG057828.D
Acq On : 23 Jun 2023 4:36
Operator : CG/JU
Sample : 03320-16
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-16

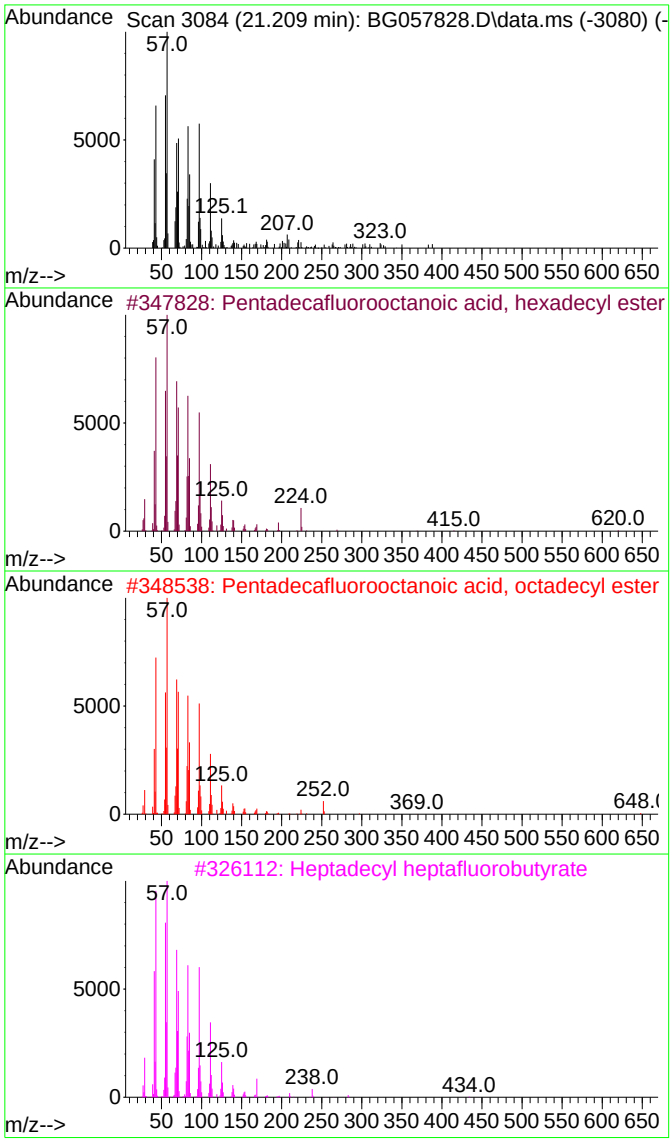
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

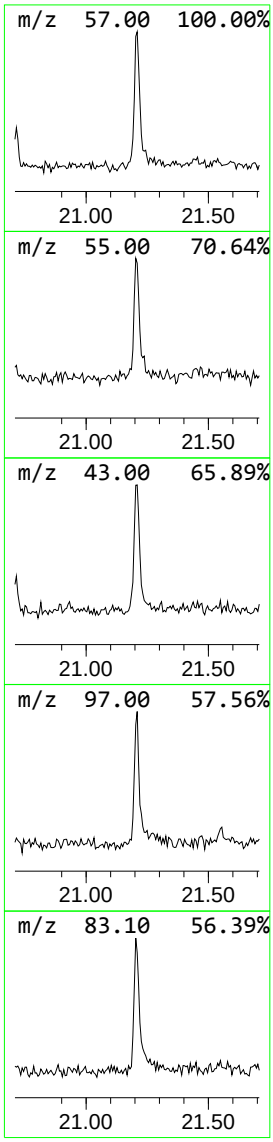
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Pentadecafluorooctanoic aci... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.209	3.56 ng	137575	Chrysene-d12	21.549

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, he...	638	C24H33F15O2	1000406-04-6	94
2	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
4	Cyclohexadecane	224	C16H32	000295-65-8	92
5	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062223\
Data File : BG057828.D
Acq On : 23 Jun 2023 4:36
Operator : CG/JU
Sample : 03320-16
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-16

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

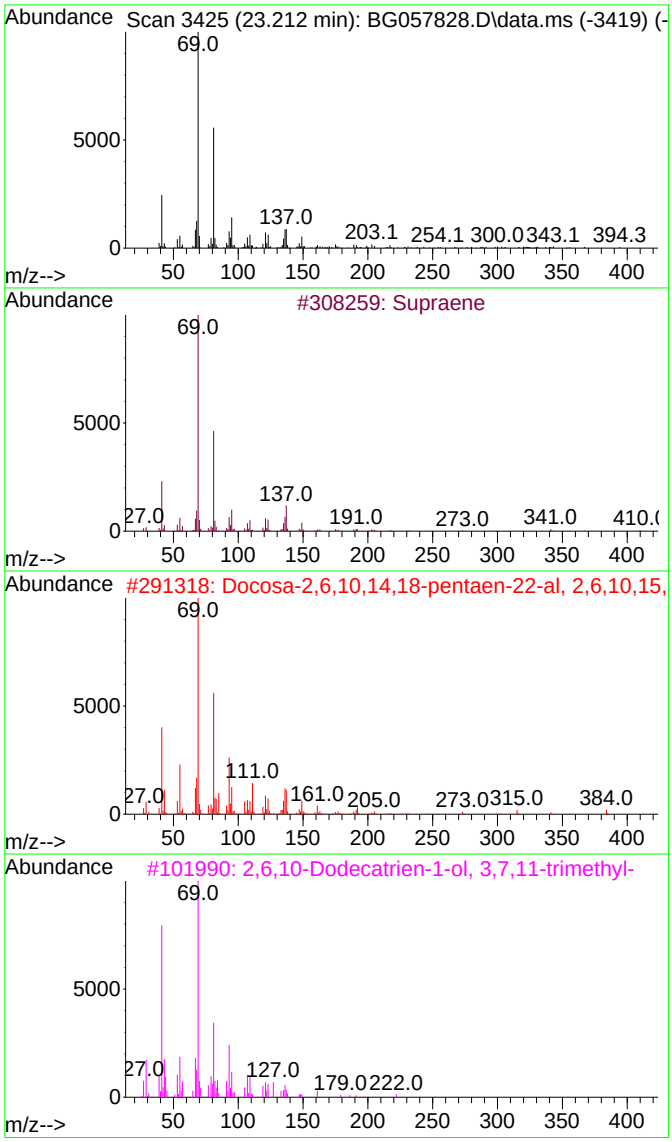
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

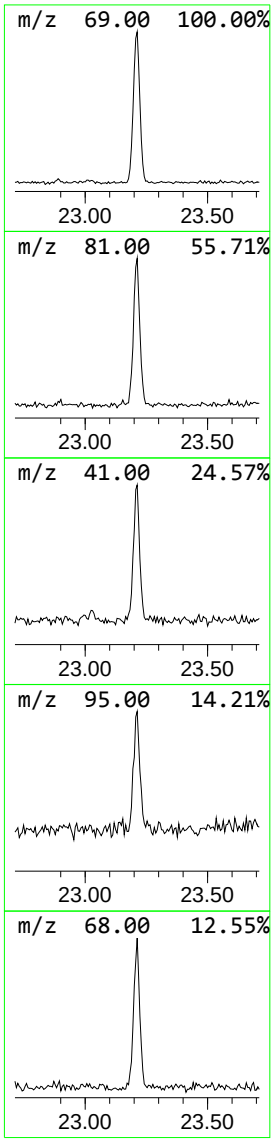
****

Peak Number 5 Supraene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.212	6.40 ng	265252	Perylene-d12	24.704

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	91
2	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	90
3	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	72
4	1,2-Epoxy-3,7,11-trimethyl-(6E,1...	238	C15H26O2	1000432-46-2	72
5	(.+/-.)-Lavandulol, pentafluorop...	300	C13H17F5O2	1000352-63-1	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062223\
Data File : BG057828.D
Acq On : 23 Jun 2023 4:36
Operator : CG/JU
Sample : 03320-16
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-16

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.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
2-Pentanone, 4-...	5.028	40.0	ng	607492	1	7.924	303362	20.0
Benzophenone	15.909	6.1	ng	193155	3	14.558	633537	20.0
n-Hexadecanoic ...	18.189	7.6	ng	283702	4	17.301	742473	20.0
Pentadecafluoro...	21.209	3.6	ng	137575	5	21.549	773896	20.0
Supraene	23.212	6.4	ng	265252	6	24.704	828807	20.0