LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091322\
Data File : BG054933.D
Acq On : 13 Sep 2022 22:32
Operator : CG/JU
Sample : N4578-31
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CHERRY-HILL-COMP-8

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-BG082522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG054933.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.191	319	324	333	rVB	31609	52373	1.88%	0.402%
2	5.679	399	407	419	rBV	660161	1094192	39.36%	8.391%
3	7.295	673	682	696	rBV	654444	1154158	41.52%	8.851%
4	8.135	818	825	835	rVB	130764	225014	8.09%	1.726%
5	9.310	1016	1025	1034	rBV	379613	698077	25.11%	5.353%
6	10.708	1257	1263	1280	rBV	49680	103942	3.74%	0.797%
7	10.961	1299	1306	1318	rBV	181584	326954	11.76%	2.507%
8	13.393	1713	1720	1733	rBV	1144520	1781918	64.10%	13.665%
9	14.774	1947	1955	1962	rBV	303606	504813	18.16%	3.871%
10	16.261	2201	2208	2223	rBV	952760	1583332	56.95%	12.142%
11	16.419	2227	2235	2236	rVV2	16840	37049	1.33%	0.284%
12	16.460	2236	2242	2251	rVB	248157	399941	14.39%	3.067%
13	17.518	2415	2422	2434	rVB	433747	657809	23.66%	5.045%
14	20.121	2858	2865	2876	rBV	2036284	2780032	100.00%	21.320%
15	21.413	3081	3085	3099	rBV3	47036	107356	3.86%	0.823%
16	21.813	3146	3153	3160	rBV	407953	722831	26.00%	5.543%
17	22.600	3284	3287	3292	rVB4	18526	29394	1.06%	0.225%
18	25.185	3716	3727	3742	rVB2	249521	780525	28.08%	5.986%

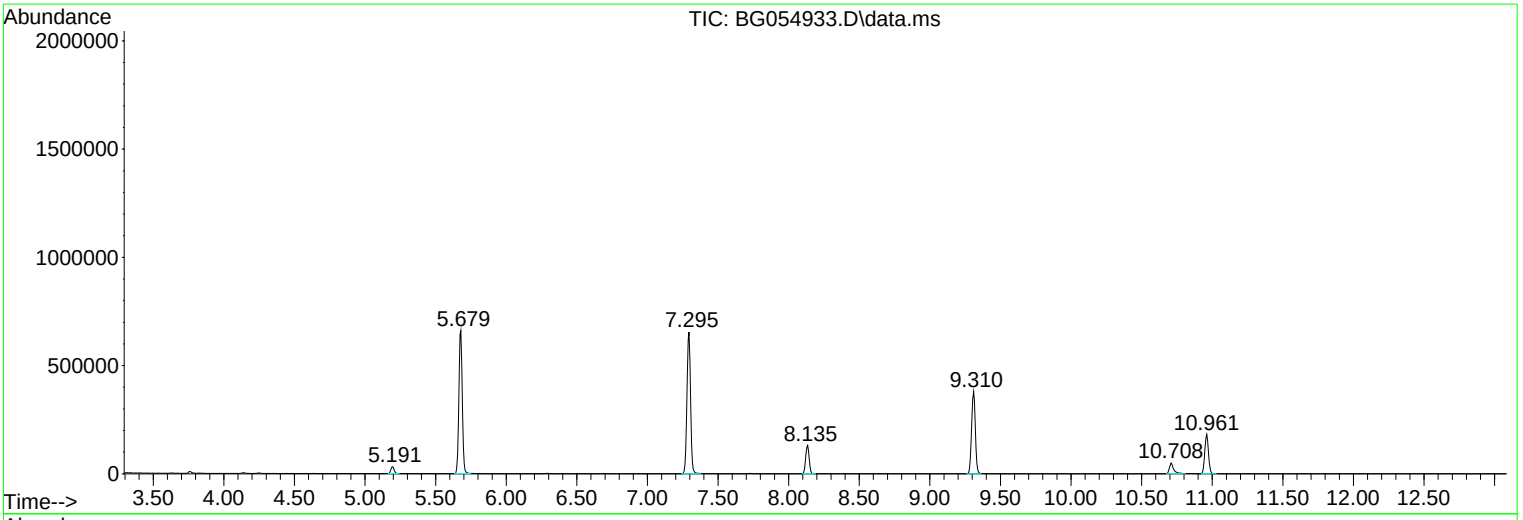
Sum of corrected areas: 13039710

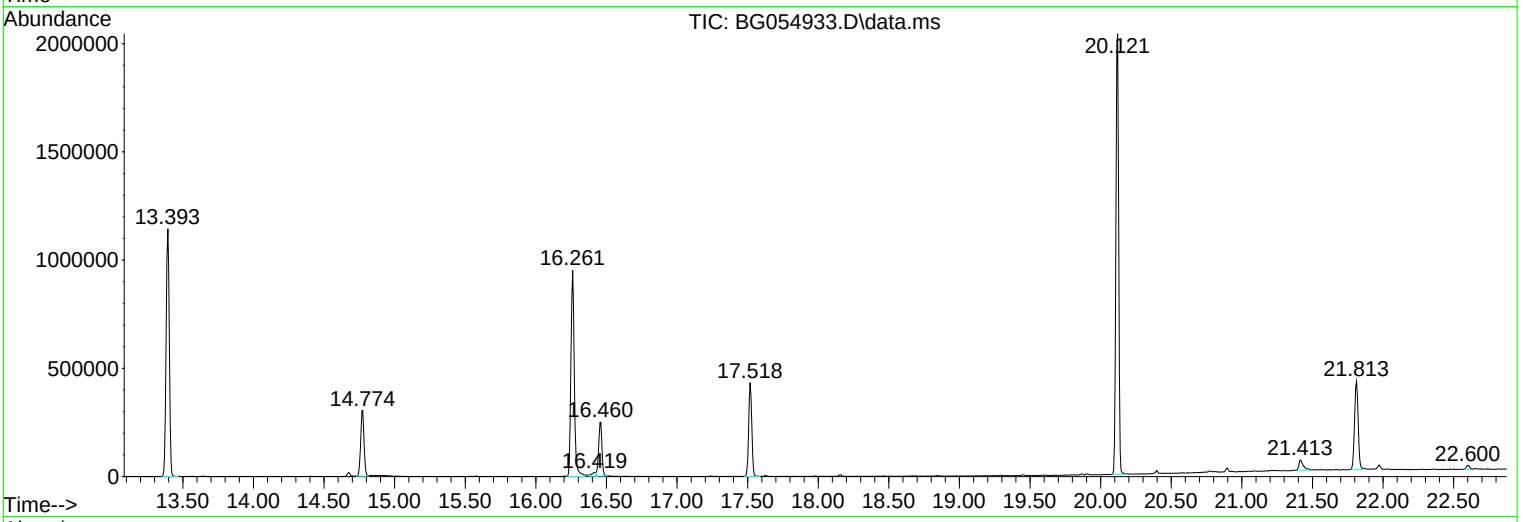
Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091322\
Data File : BG054933.D
Acq On : 13 Sep 2022 22:32
Operator : CG/JU
Sample : N4578-31
Misc :
ALS Vial : 12 Sample Multiplier: 1

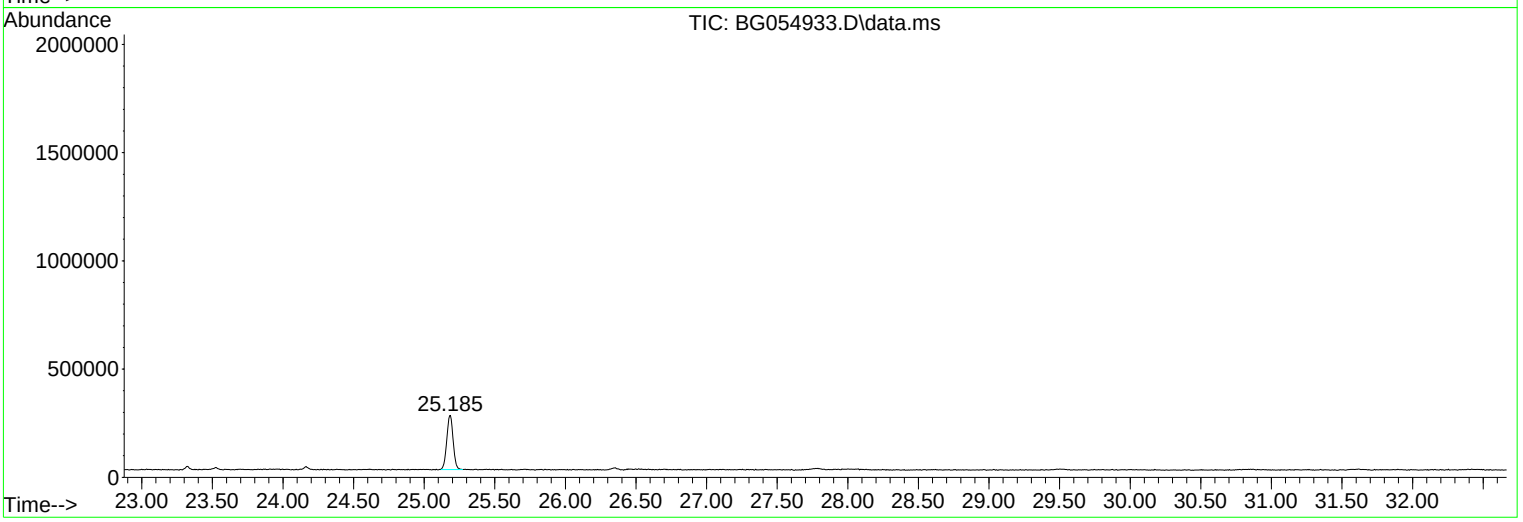
Instrument :
BNA_G
ClientSampleId :
CHERRY-HILL-COMP-8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.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\BG091322\
Data File : BG054933.D
Acq On : 13 Sep 2022 22:32
Operator : CG/JU
Sample : N4578-31
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CHERRY-HILL-COMP-8

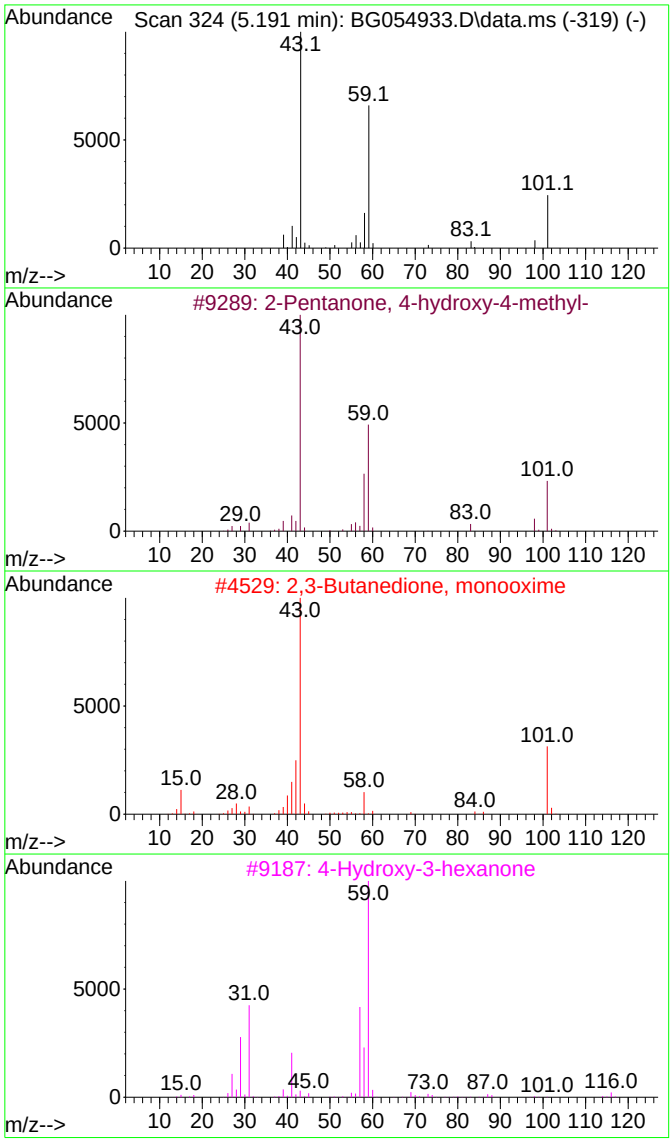
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

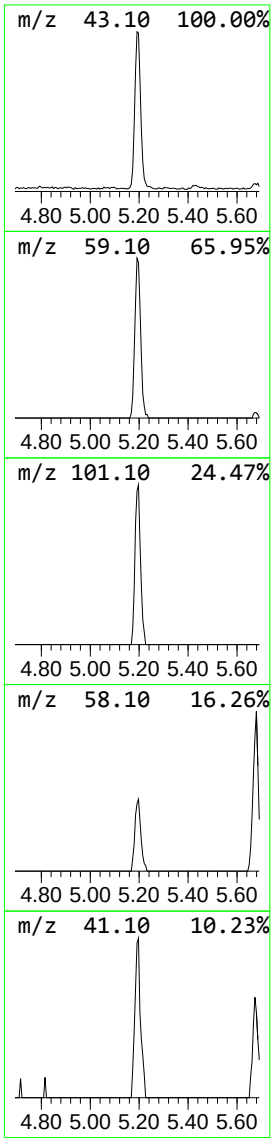
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.191	4.66 ng	52373	1,4-Dichlorobenzene-d4	8.135

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	23
4	1,2-Butanediol	90	C4H10O2	000584-03-2	17
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091322\
Data File : BG054933.D
Acq On : 13 Sep 2022 22:32
Operator : CG/JU
Sample : N4578-31
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CHERRY-HILL-COMP-8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

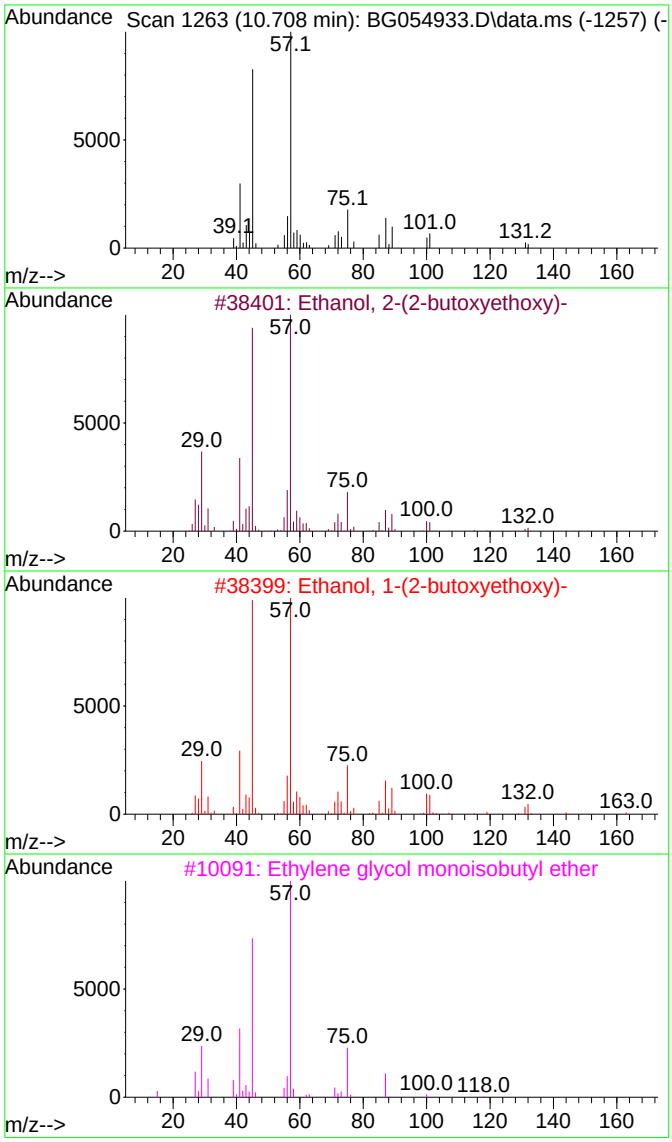
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

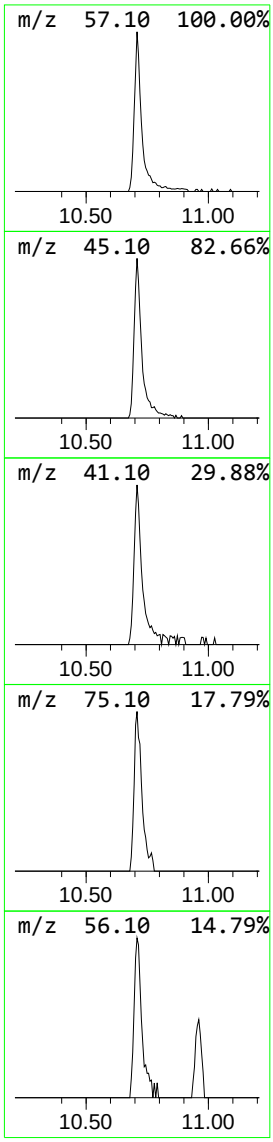
****

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.708	6.36 ng	103942	Naphthalene-d8	10.961

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	64
3	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53
5	Methoxyacetic acid, heptyl ester	188	C10H20O3	168920-36-3	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091322\
Data File : BG054933.D
Acq On : 13 Sep 2022 22:32
Operator : CG/JU
Sample : N4578-31
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CHERRY-HILL-COMP-8

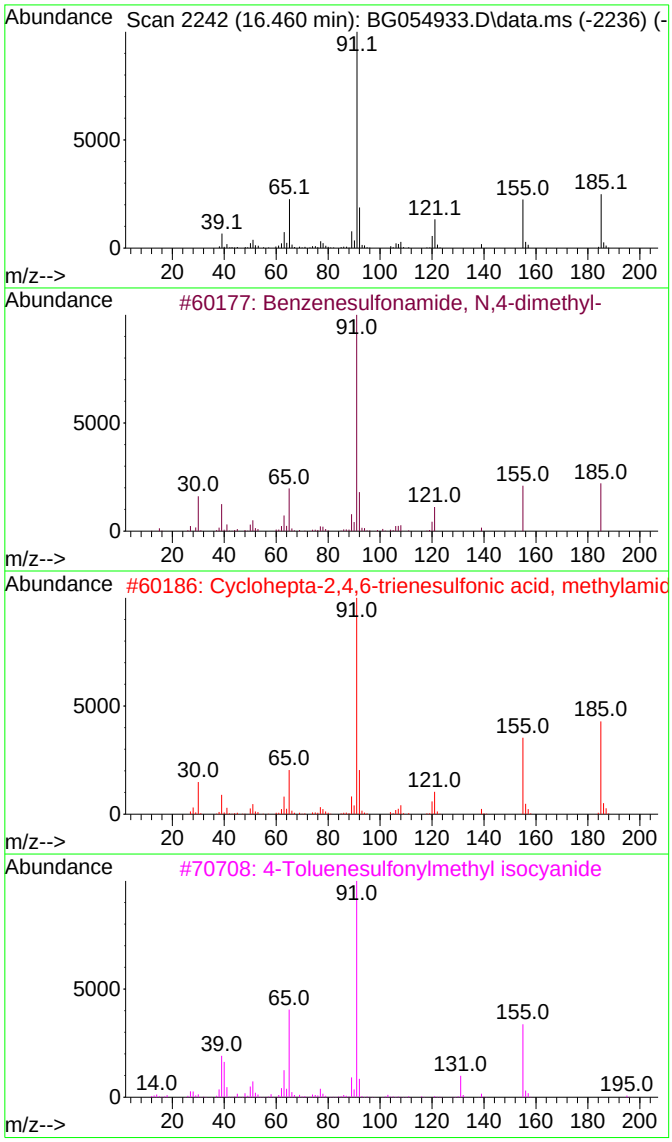
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

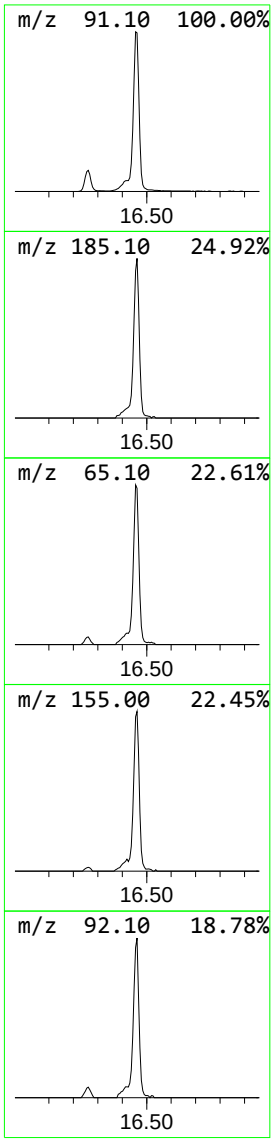
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Benzenesulfonamide, N,4-dim... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.460	12.16 ng	399941	Phenanthrene-d10	17.518

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, N,4-dimethyl-	185	C8H11NO2S	000640-61-9	96
2	Cyclohepta-2,4,6-trienesulfonic ...	185	C8H11NO2S	1000187-28-7	58
3	4-Toluenesulfonylmethyl isocyanide	195	C9H9NO2S	036635-61-7	47
4	(O-p-Tosylisonitroso)malononitrile	249	C10H7N3O3S	020893-01-0	47
5	Benzeneacetaldehyde	120	C8H8O	000122-78-1	45





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091322\
Data File : BG054933.D
Acq On : 13 Sep 2022 22:32
Operator : CG/JU
Sample : N4578-31
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CHERRY-HILL-COMP-8

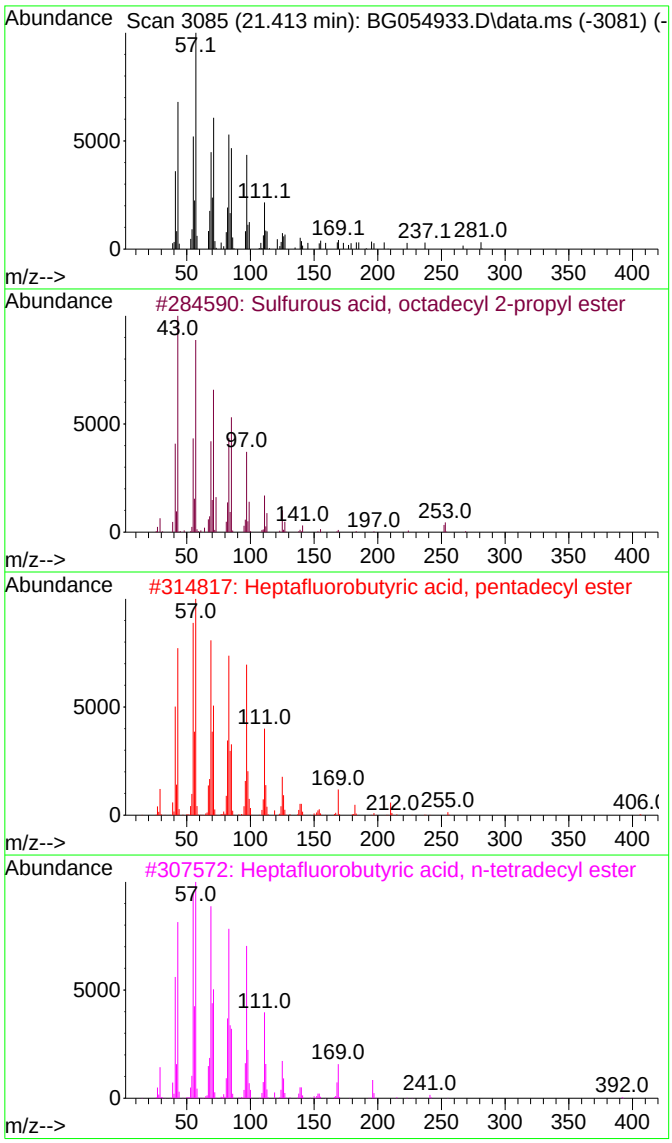
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

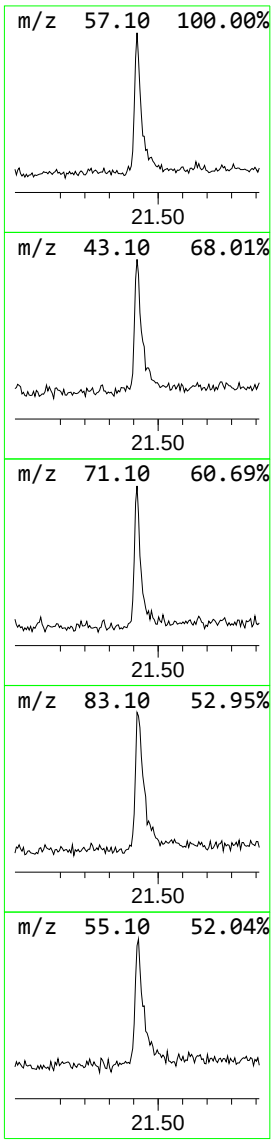
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Sulfurous acid, octadecyl 2... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.413	2.97 ng	107356	Chrysene-d12	21.813

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	87
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	76
3	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	76
4	Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	76
5	Isobutyl octacosyl ether	467	C32H66O	1000406-33-4	74





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091322\
Data File : BG054933.D
Acq On : 13 Sep 2022 22:32
Operator : CG/JU
Sample : N4578-31
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CHERRY-HILL-COMP-8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.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-...	5.191	4.7	ng	52373	1	8.135	225014	20.0
Ethanol, 2-(2-b...	10.708	6.4	ng	103942	2	10.961	326954	20.0
Benzenesulfonam...	16.460	12.2	ng	399941	4	17.518	657809	20.0
Sulfurous acid,...	21.413	3.0	ng	107356	5	21.813	722831	20.0