LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062923\
Data File : BG057911.D
Acq On : 29 Jun 2023 19:32
Operator : CG/JU
Sample : 03429-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-COMP-0627

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-BG062723.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057911.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.015	323	328	335	rBV	61800	96864	2.78%	0.518%
2	5.491	402	409	427	rBV	1120947	1770627	50.85%	9.465%
3	7.083	672	680	694	rBV	1088221	1885340	54.15%	10.078%
4	7.912	814	821	828	rBV	172976	284292	8.16%	1.520%
5	9.075	1010	1019	1028	rBV	634940	1103328	31.69%	5.898%
6	10.714	1291	1298	1309	rVB	231774	415620	11.94%	2.222%
7	13.170	1709	1716	1726	rVB	1512302	2358452	67.73%	12.608%
8	14.545	1944	1950	1959	rVB	378006	600056	17.23%	3.208%
9	15.903	2173	2181	2186	rBV	134355	185141	5.32%	0.990%
10	16.038	2197	2204	2218	rBV	1403504	2195563	63.06%	11.737%
11	16.232	2231	2237	2248	rVB	79265	130853	3.76%	0.700%
12	17.295	2411	2418	2423	rBV	511702	796227	22.87%	4.256%
13	17.336	2423	2425	2429	rVB	34836	37415	1.07%	0.200%
14	18.182	2564	2569	2579	rBV2	148500	298690	8.58%	1.597%
15	19.346	2762	2767	2772	rBV	132822	188496	5.41%	1.008%
16	19.463	2782	2787	2795	rBV	25119	65825	1.89%	0.352%
17	19.710	2820	2829	2834	rBV	108594	202033	5.80%	1.080%
18	19.910	2857	2863	2869	rBV	2680836	3481953	100.00%	18.614%
19	21.196	3077	3082	3091	rVB3	233460	376851	10.82%	2.015%
20	21.543	3134	3141	3146	rBV2	501441	895978	25.73%	4.790%
21	21.737	3170	3174	3181	rVB	109342	148151	4.25%	0.792%
22	22.330	3271	3275	3285	rVB3	103948	211446	6.07%	1.130%
23	23.006	3386	3390	3399	rVB	57994	108679	3.12%	0.581%
24	24.692	3669	3677	3688	rVB	320224	868678	24.95%	4.644%

Sum of corrected areas: 18706558

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062923\
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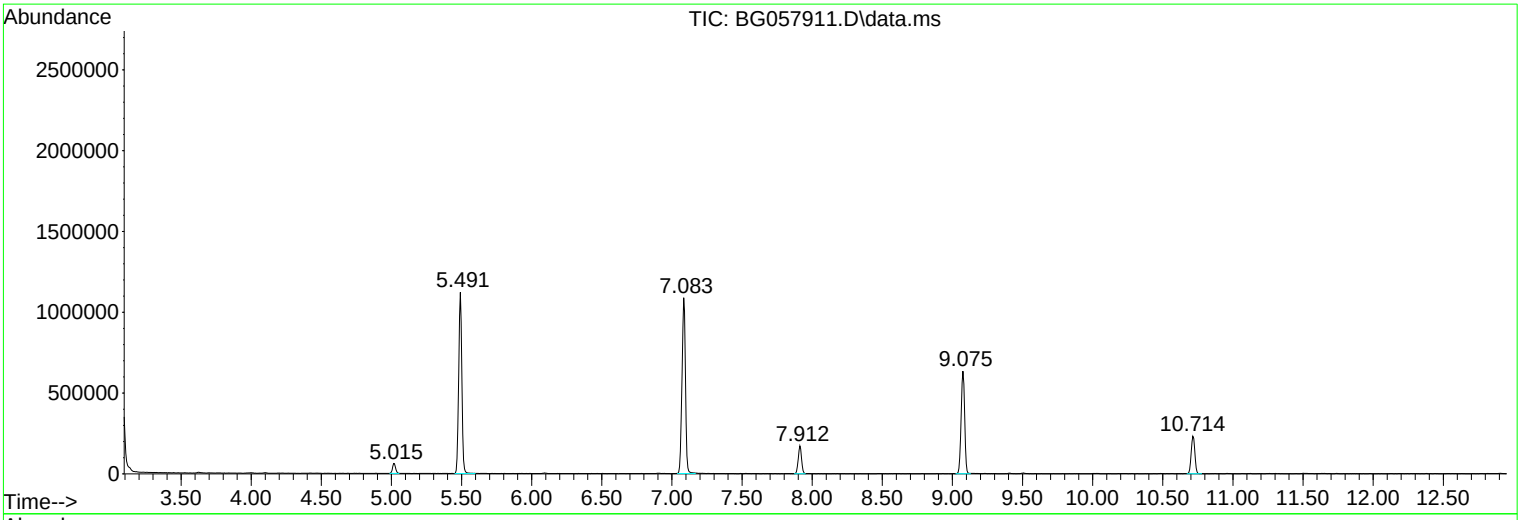
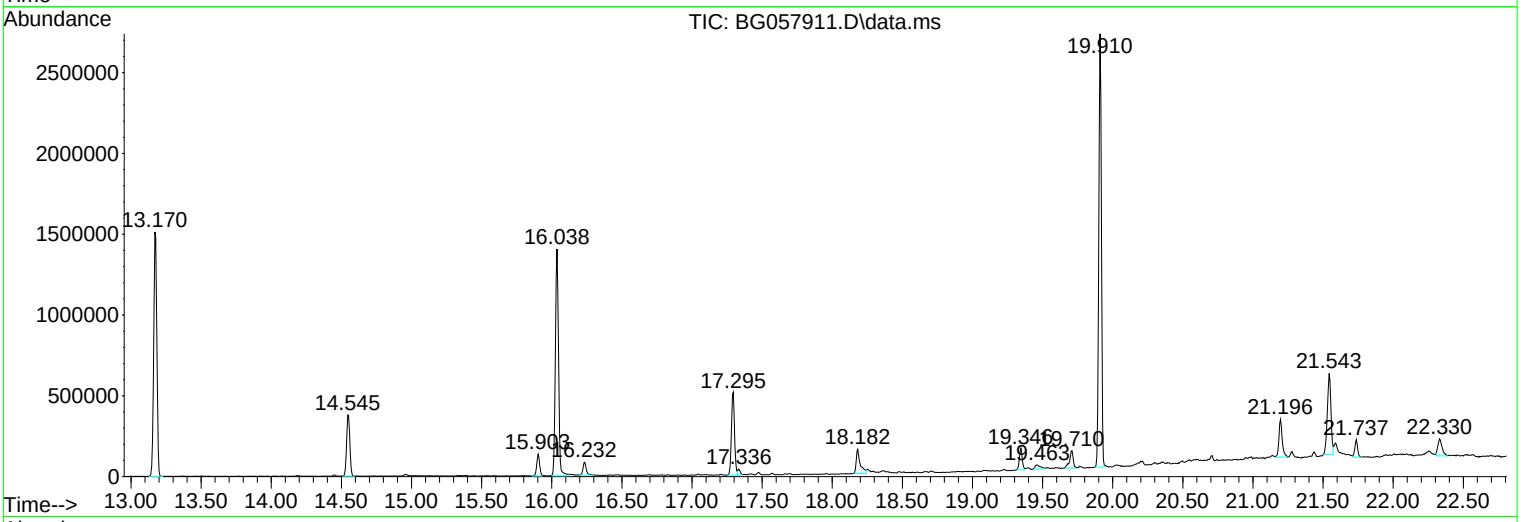
Operator : CG/JU
Sample : 03429-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

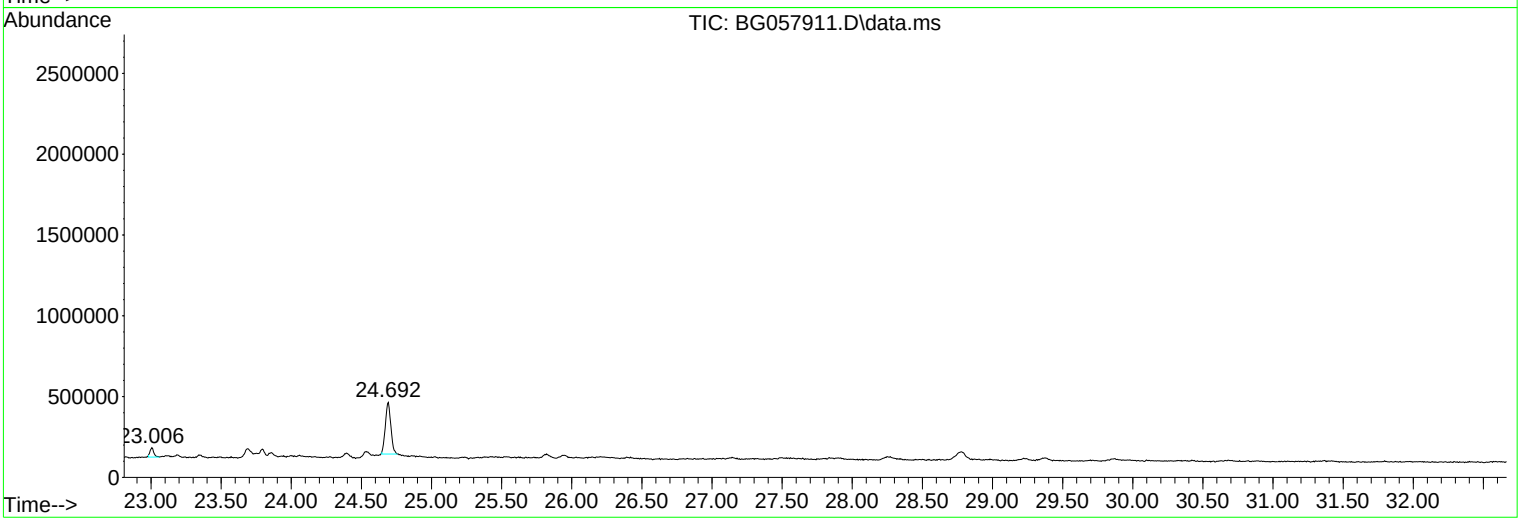
Instrument :
BNA_G
ClientSampleId :
SB-COMP-0627

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG062723.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\BG062923\
Data File : BG057911.D
Acq On : 29 Jun 2023 19:32
Operator : CG/JU
Sample : 03429-01
Misc :
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Instrument :
BNA_G
ClientSampleId :
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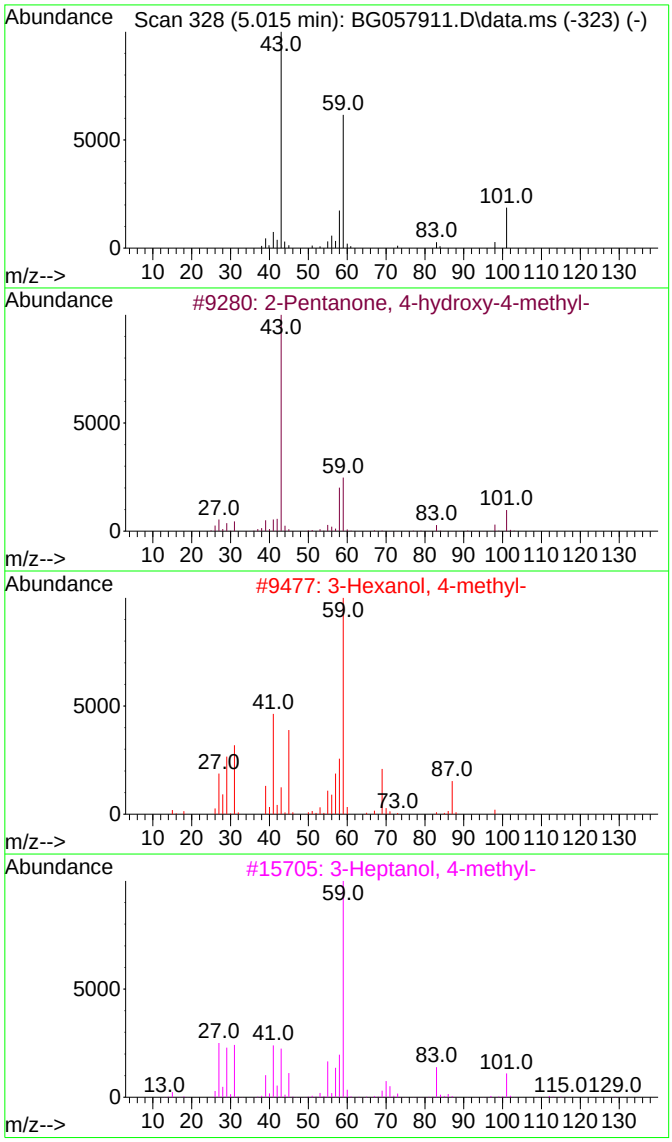
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG062723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

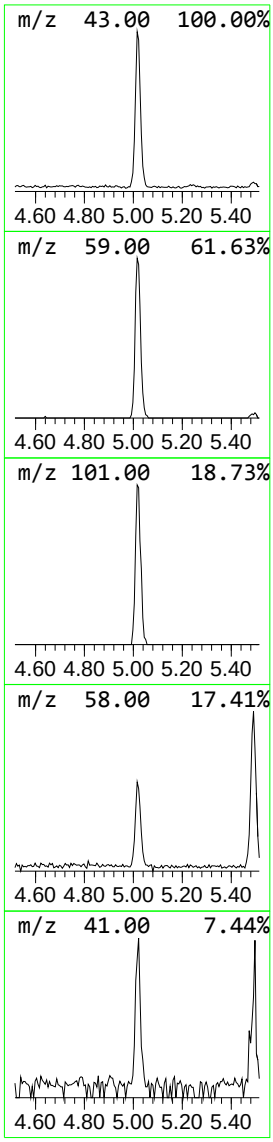
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.015	6.81 ng	96864	1,4-Dichlorobenzene-d4	7.912

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	33
4	3-Hexanol	102	C6H14O	000623-37-0	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062923\
Data File : BG057911.D
Acq On : 29 Jun 2023 19:32
Operator : CG/JU
Sample : 03429-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-COMP-0627

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG062723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

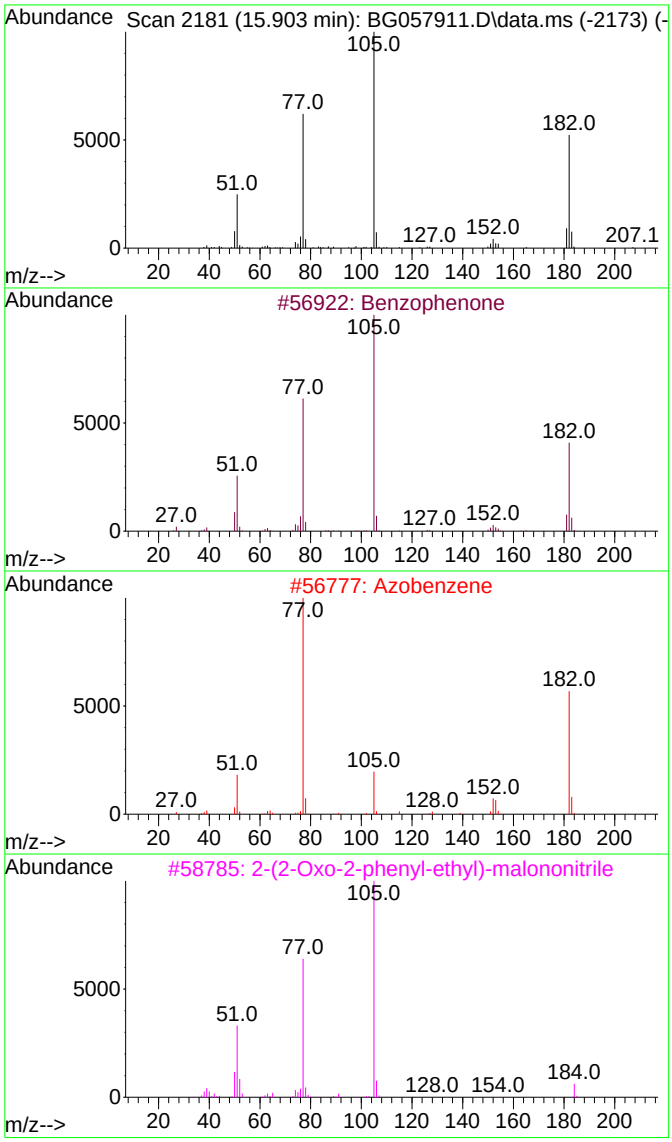
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

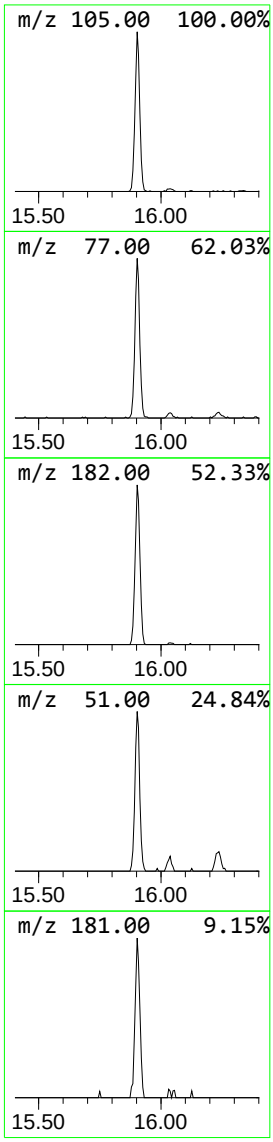
****

Peak Number 2 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.903	6.17 ng	185141	Acenaphthene-d10	14.551

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Azobenzene	182	C12H10N2	000103-33-3	59
3	2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	47
4	N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47
5	1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47





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Data File : BG057911.D
Acq On : 29 Jun 2023 19:32
Operator : CG/JU
Sample : 03429-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-COMP-0627

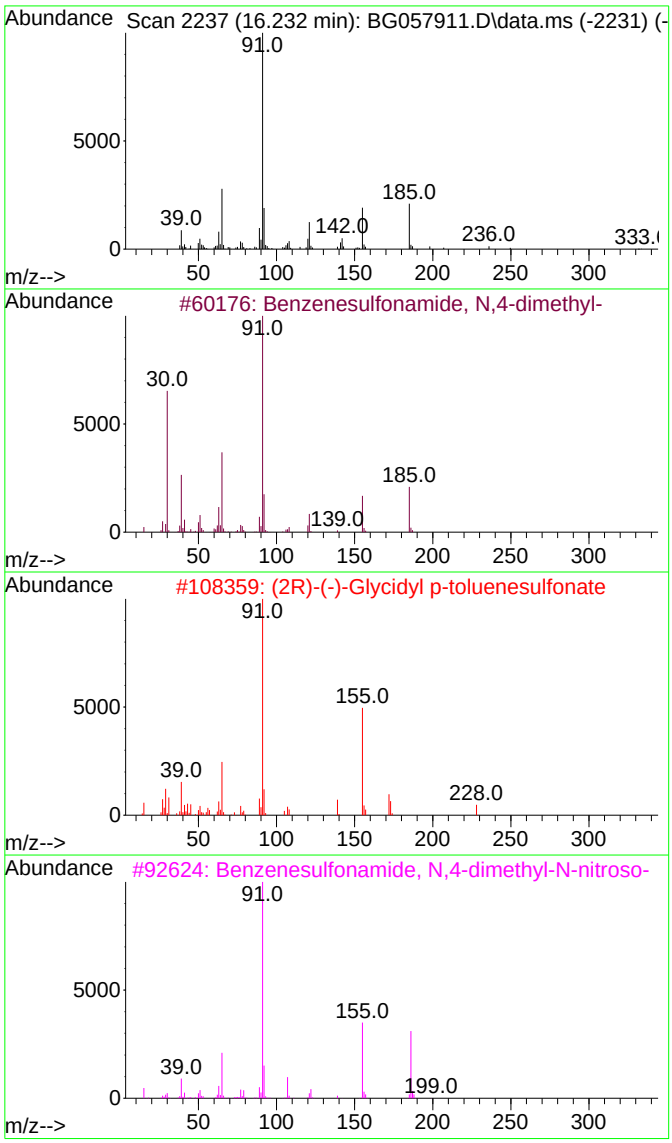
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG062723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

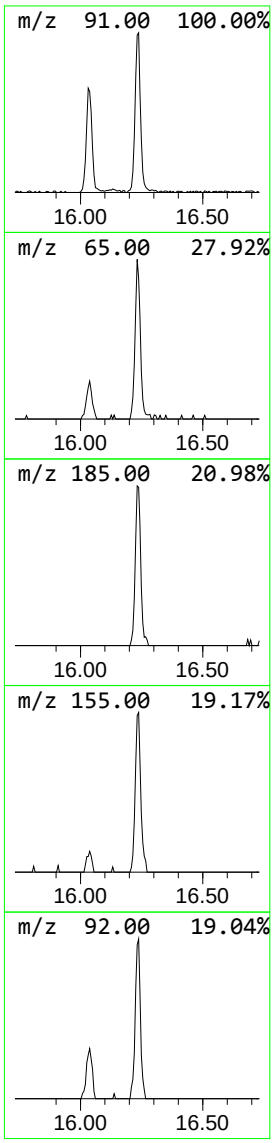
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Benzenesulfonamide, N,4-dim... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.232	3.29 ng	130853	Phenanthrene-d10	17.295

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, N,4-dimethyl-	185	C8H11NO2S	000640-61-9	95
2	(2R)-(-)-Glycidyl p-toluenesulfo...	228	C10H12O4S	113826-06-5	53
3	Benzenesulfonamide, N,4-dimethyl...	214	C8H10N2O3S	000080-11-5	53
4	Benzene, 1-methyl-2-nitroso-	121	C7H7NO	000611-23-4	53
5	Ethyl(E/Z)-.alpha.-cyano-4-nitro...	416	C19H16N2O7S	1000287-26-8	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062923\
Data File : BG057911.D
Acq On : 29 Jun 2023 19:32
Operator : CG/JU
Sample : 03429-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-COMP-0627

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG062723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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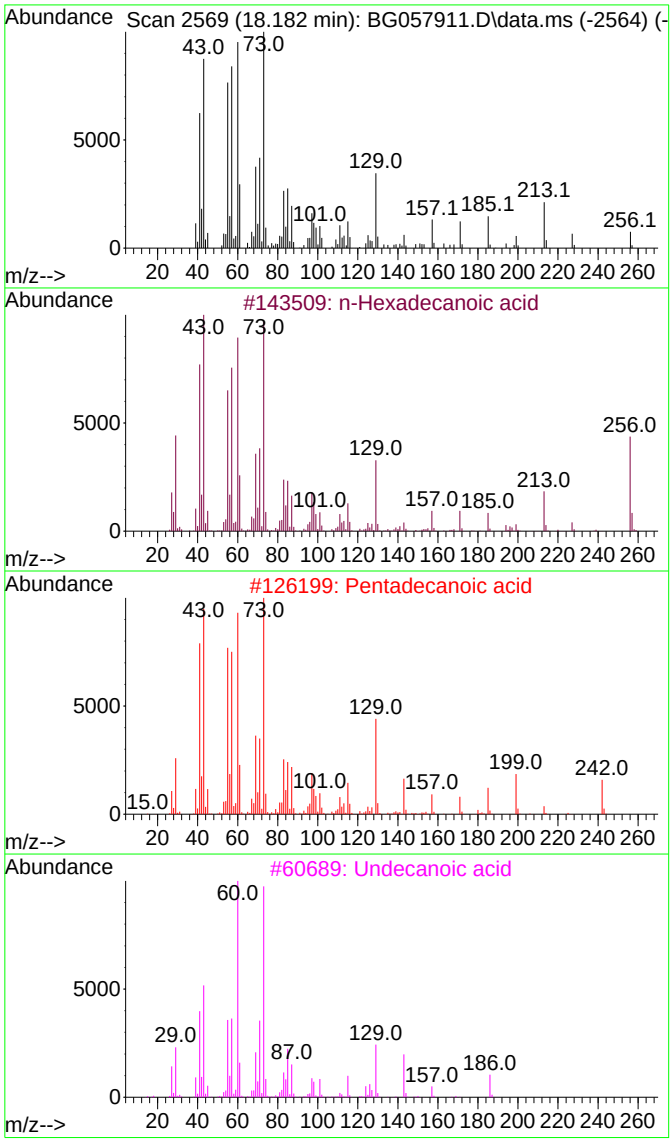
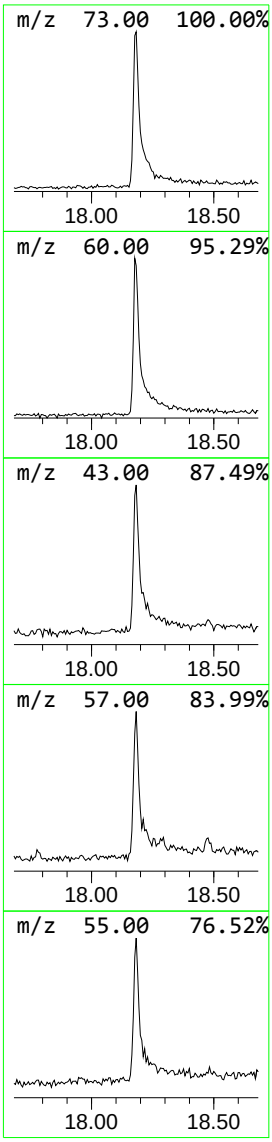
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.182	7.50 ng	298690	Phenanthrene-d10	17.295

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Undecanoic acid	186	C11H22O2	000112-37-8	81
4	Tridecanoic acid	214	C13H26O2	000638-53-9	68
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062923\
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Operator : CG/JU
Sample : 03429-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-COMP-0627

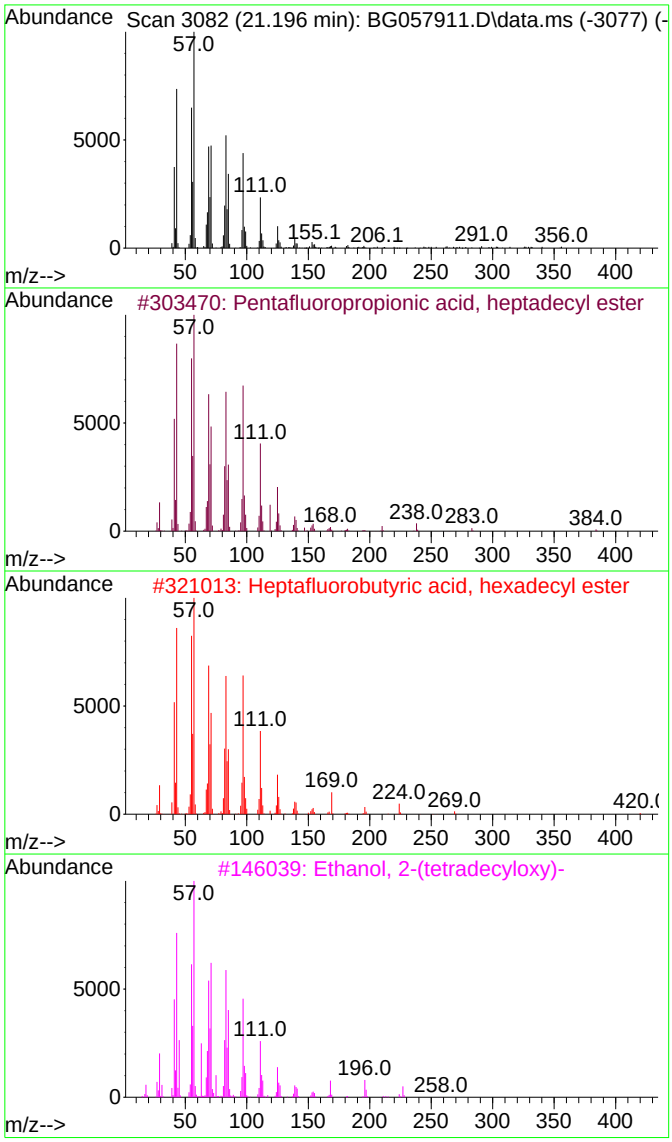
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG062723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

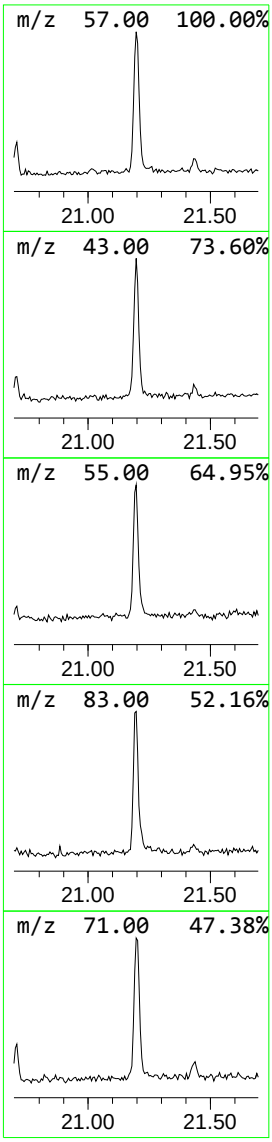
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Pentafluoropropionic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.196	8.41 ng	376851	Chrysene-d12	21.543

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91
2	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91
3	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
4	17-Pentatriacontene	491	C35H70	006971-40-0	91
5	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91





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Data File : BG057911.D
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ClientSampleId :
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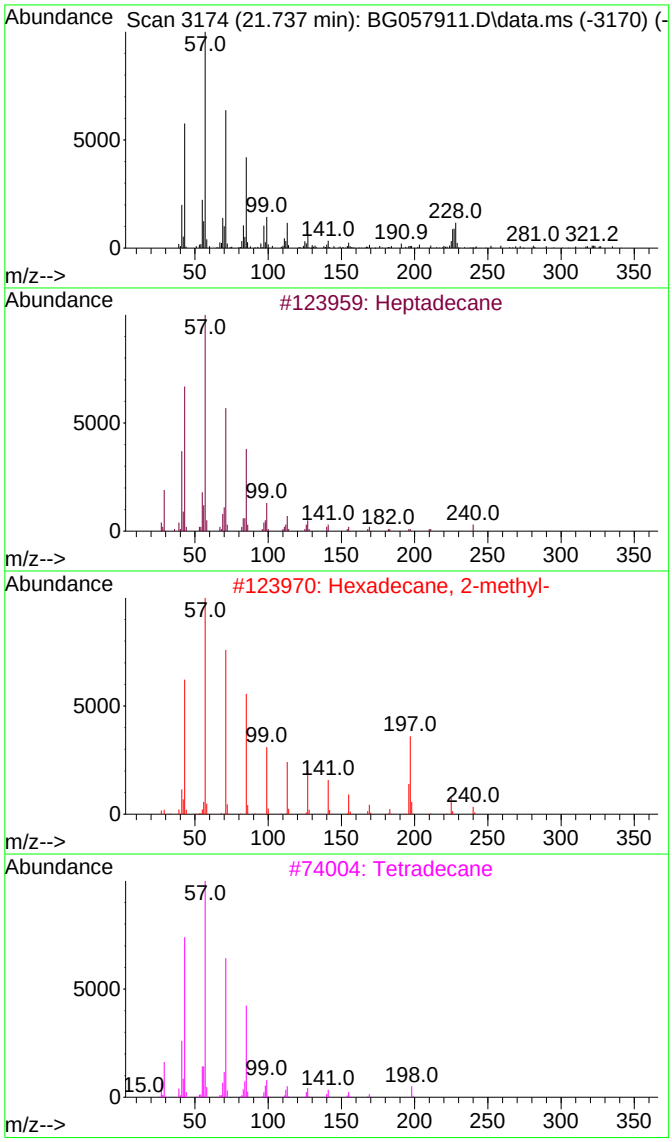
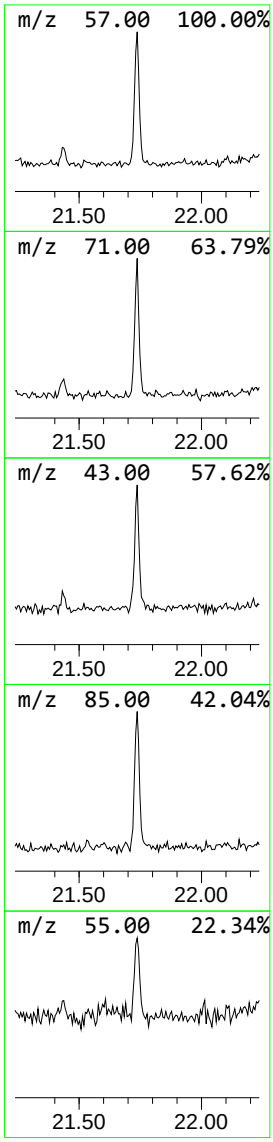
****

Peak Number 6 Heptadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.737	3.31 ng	148151	Chrysene-d12	21.543

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	81
2	Hexadecane, 2-methyl-	240	C17H36	001560-92-5	76
3	Tetradecane	198	C14H30	000629-59-4	76
4	Hentriacontane	437	C31H64	000630-04-6	74
5	9-Methylheneicosane	310	C22H46	070475-51-3	74





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Data File : BG057911.D
Acq On : 29 Jun 2023 19:32
Operator : CG/JU
Sample : 03429-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-COMP-0627

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG062723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

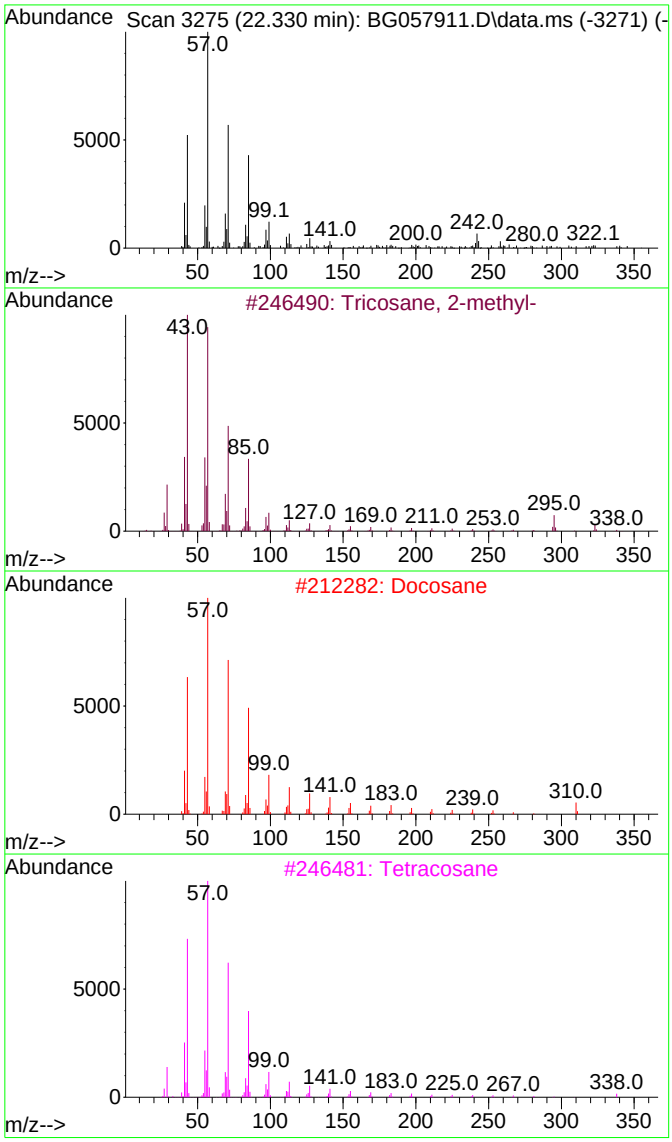
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

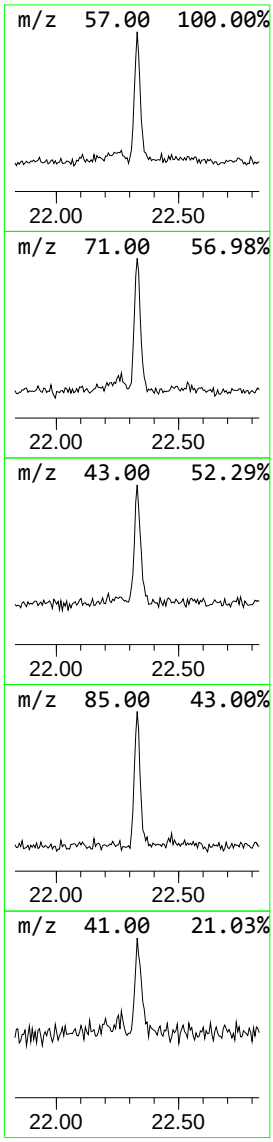
****

Peak Number 7 Tricosane, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.330	4.72 ng	211446	Chrysene-d12	21.543

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricosane, 2-methyl-	338	C24H50	001928-30-9	94
2	Docosane	310	C22H46	000629-97-0	91
3	Tetracosane	338	C24H50	000646-31-1	83
4	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	83
5	Tridecane, 2-methyl-	198	C14H30	001560-96-9	83





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Instrument :
BNA_G
ClientSampleId :
SB-COMP-0627

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG062723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

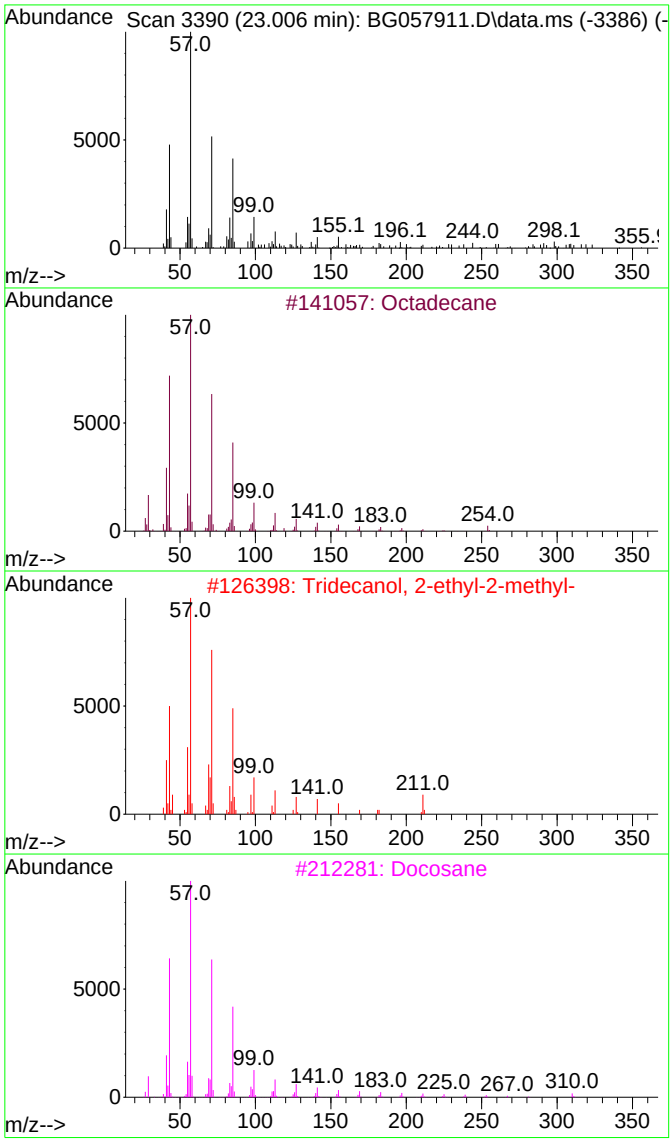
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

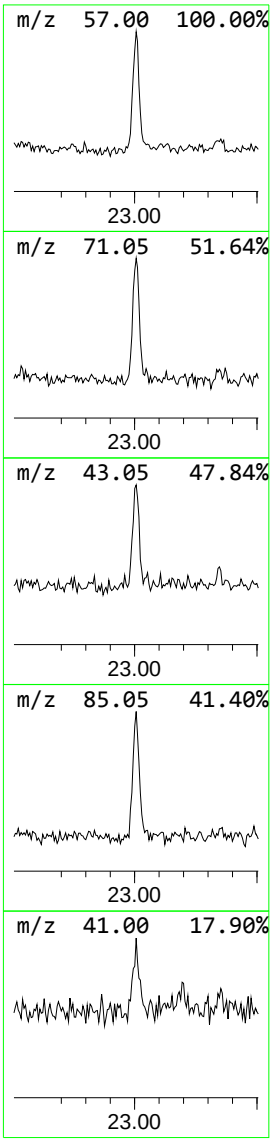
****

Peak Number 8 Octadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.006	2.43 ng	108679	Chrysene-d12	21.543

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	80
2	Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1010115-66-1	80
3	Docosane	310	C22H46	000629-97-0	80
4	Pentadecane, 7-(bromomethyl)-	304	C16H33Br	052997-43-0	74
5	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062923\
Data File : BG057911.D
Acq On : 29 Jun 2023 19:32
Operator : CG/JU
Sample : 03429-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-COMP-0627

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG062723.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-...	5.015	6.8	ng	96864	1	7.912	284292	20.0
Benzophenone	15.903	6.2	ng	185141	3	14.551	600056	20.0
Benzenesulfonam...	16.232	3.3	ng	130853	4	17.295	796227	20.0
n-Hexadecanoic ...	18.182	7.5	ng	298690	4	17.295	796227	20.0
Pentafluoroprop...	21.196	8.4	ng	376851	5	21.543	895978	20.0
Heptadecane	21.737	3.3	ng	148151	5	21.543	895978	20.0
Tricosane, 2-me...	22.330	4.7	ng	211446	5	21.543	895978	20.0
Octadecane	23.006	2.4	ng	108679	5	21.543	895978	20.0