LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062123\
Data File : BG057791.D
Acq On : 21 Jun 2023 19:25
Operator : CG/JU
Sample : 03289-17
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-06-12.0-14.0-DUP

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: BG057791.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	% max.	% of total
1	5.026	325	330	339	rBV	85008	126778	6.63%	1.316%
2	5.490	402	409	418	rBV	349739	553521	28.93%	5.745%
3	7.083	670	680	686	rBV	364339	611932	31.98%	6.351%
4	7.923	816	823	830	rBV	95518	156594	8.18%	1.625%
5	9.080	1012	1020	1028	rBV	210827	361648	18.90%	3.754%
6	10.726	1291	1300	1307	rBV	141601	245070	12.81%	2.544%
7	13.181	1710	1718	1725	rBV	568034	880571	46.03%	9.140%
8	14.556	1946	1952	1961	rVB	260822	380659	19.90%	3.951%
9	15.914	2177	2183	2189	rVB	61694	86954	4.54%	0.903%
10	16.043	2198	2205	2213	rBV	608579	923487	48.27%	9.585%
11	17.300	2413	2419	2426	rVB	376955	552340	28.87%	5.733%
12	18.187	2565	2570	2589	rBV	172652	281444	14.71%	2.921%
13	19.345	2760	2767	2773	rBV6	15404	36422	1.90%	0.378%
14	19.462	2782	2787	2794	rBV	54355	86588	4.53%	0.899%
15	19.915	2858	2864	2870	rVB	1492907	1913214	100.00%	19.858%
16	21.166	3072	3077	3080	rBV2	56062	102969	5.38%	1.069%
17	21.207	3080	3084	3092	rVV3	111549	281131	14.69%	2.918%
18	21.284	3093	3097	3104	rVB	241332	329958	17.25%	3.425%
19	21.548	3136	3142	3151	rBV2	401582	634540	33.17%	6.586%
20	21.748	3173	3176	3182	rBV	30402	44332	2.32%	0.460%
21	22.341	3274	3277	3286	rBV3	23945	46220	2.42%	0.480%
22	23.029	3391	3394	3399	rVB3	16170	23130	1.21%	0.240%
23	23.217	3419	3426	3432	rBV	145860	272995	14.27%	2.833%
24	24.703	3669	3679	3691	rBV	247119	702074	36.70%	7.287%

Sum of corrected areas: 9634571

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062123\
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Misc :
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Instrument :
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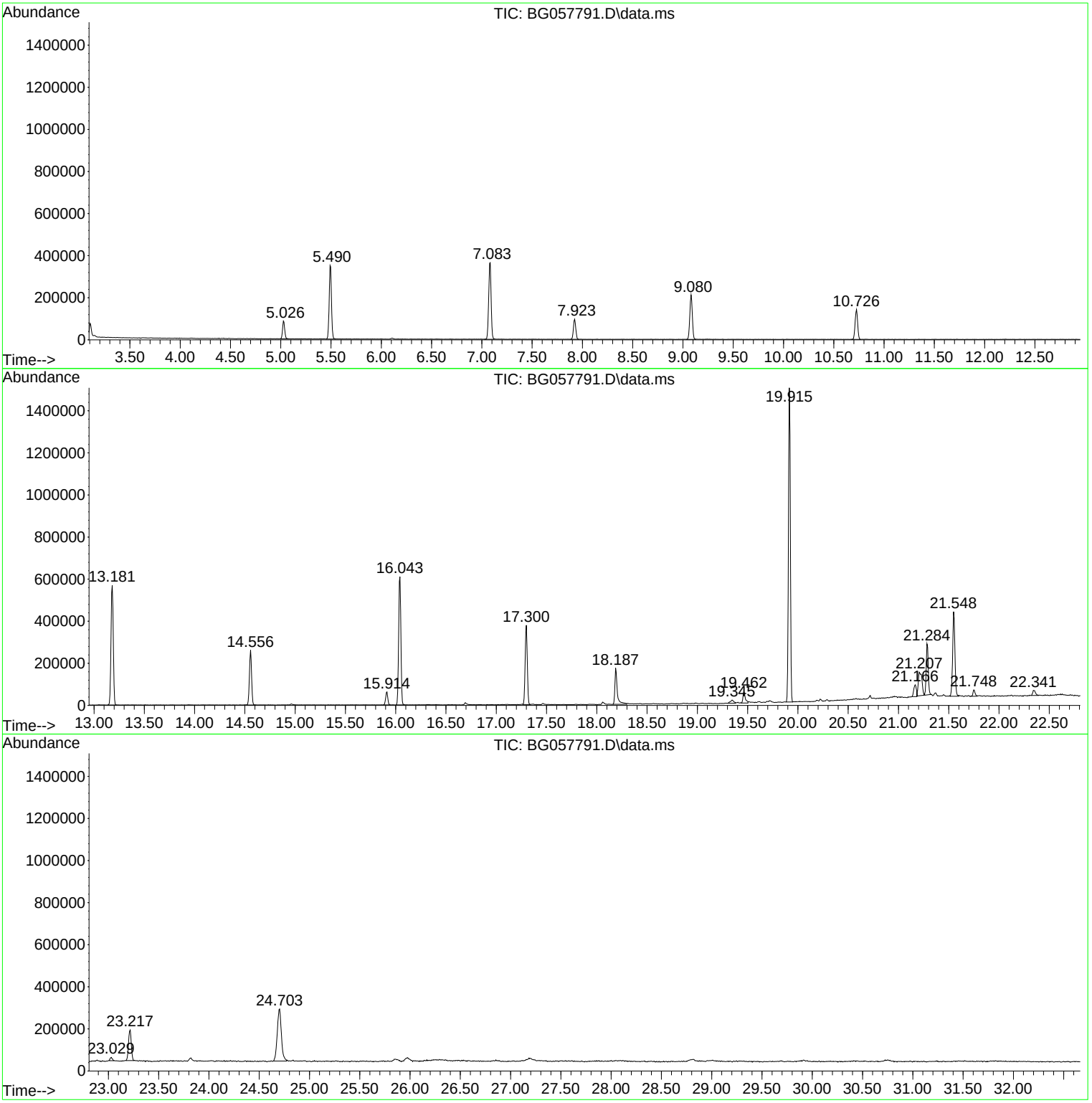
ClientSampleId :
SB-06-12.0-14.0-DUP

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\BG062123\
Data File : BG057791.D
Acq On : 21 Jun 2023 19:25
Operator : CG/JU
Sample : 03289-17
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-06-12.0-14.0-DUP

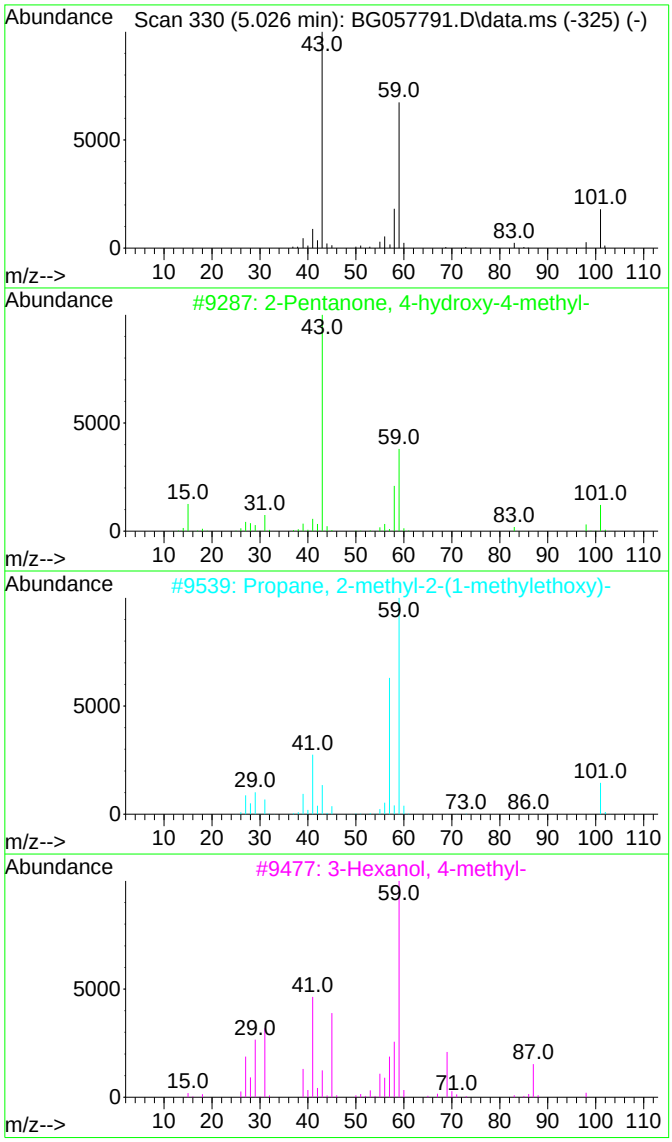
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

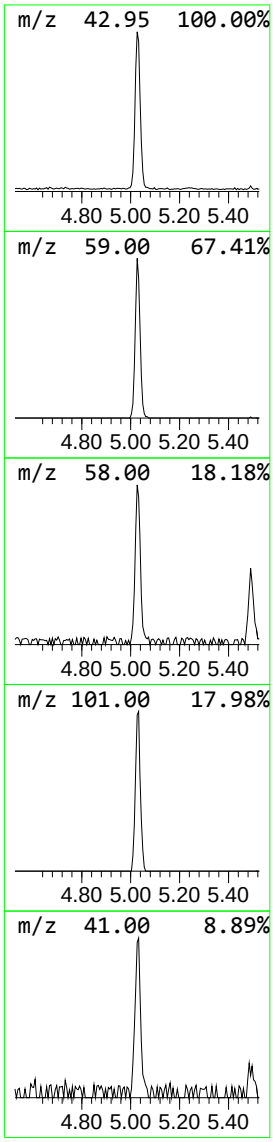
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.026	16.19 ng	126778	1,4-Dichlorobenzene-d4	7.923

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	Acetone	58	C3H6O	000067-64-1	9





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Data File : BG057791.D
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Sample : 03289-17
Misc :
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Instrument :
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SB-06-12.0-14.0-DUP

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
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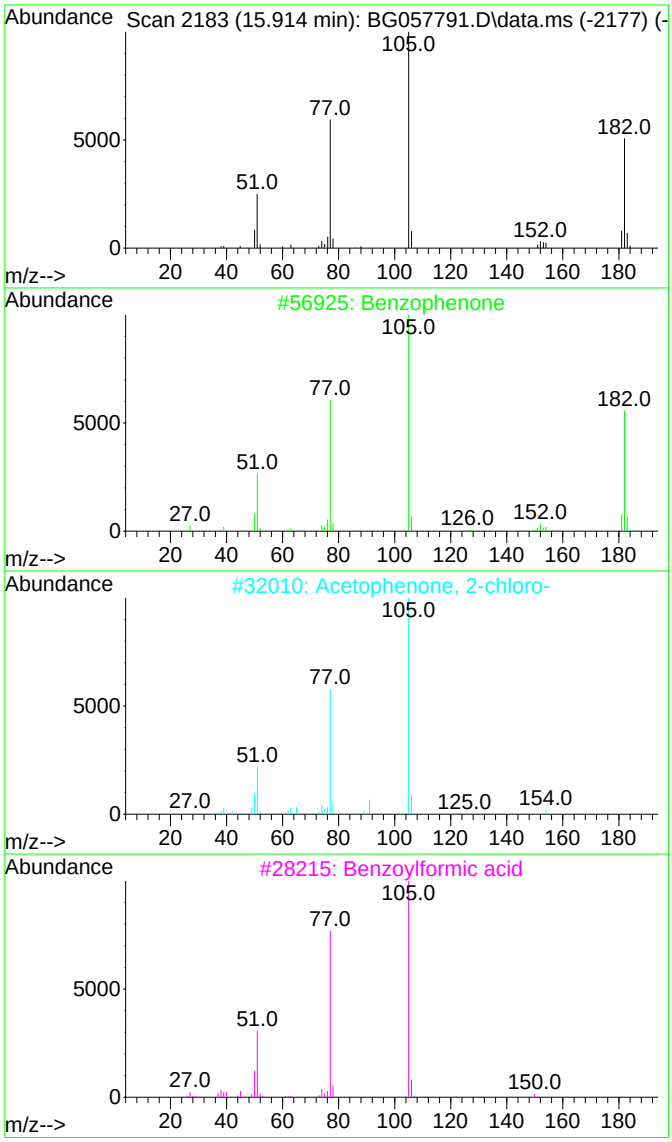
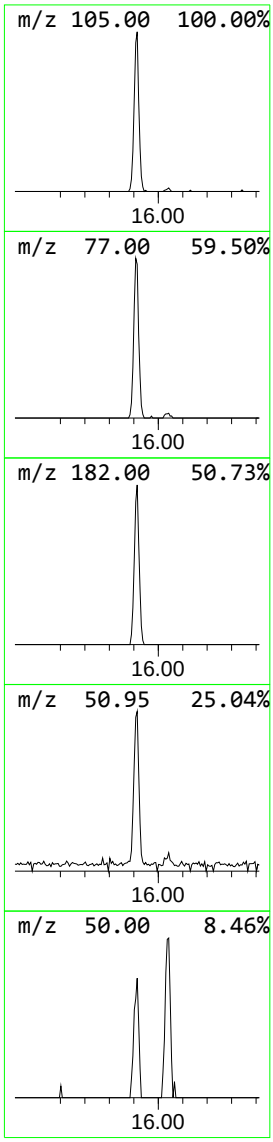
****

Peak Number 2 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.914	4.57 ng	86954	Acenaphthene-d10	14.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
3	Benzoylformic acid	150	C8H6O3	000611-73-4	47
4	Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47
5	Methyl 2-benzoyl-4-cyanobutanoate	231	C13H13NO3	1010486-83-8	47





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Data File : BG057791.D
Acq On : 21 Jun 2023 19:25
Operator : CG/JU
Sample : 03289-17
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-06-12.0-14.0-DUP

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

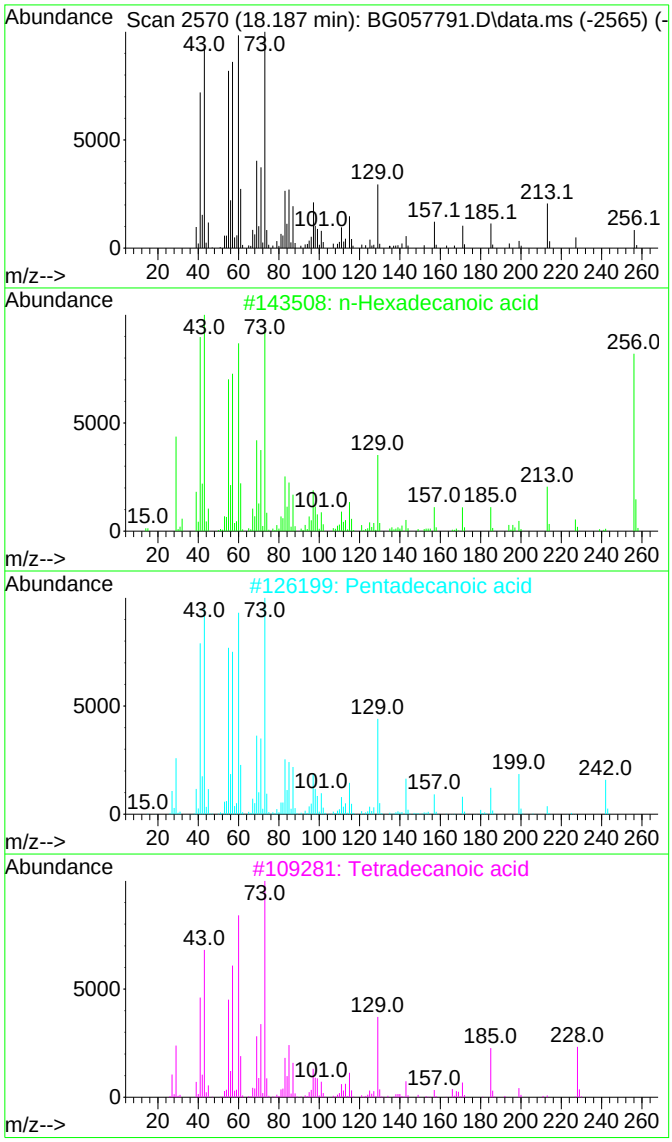
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

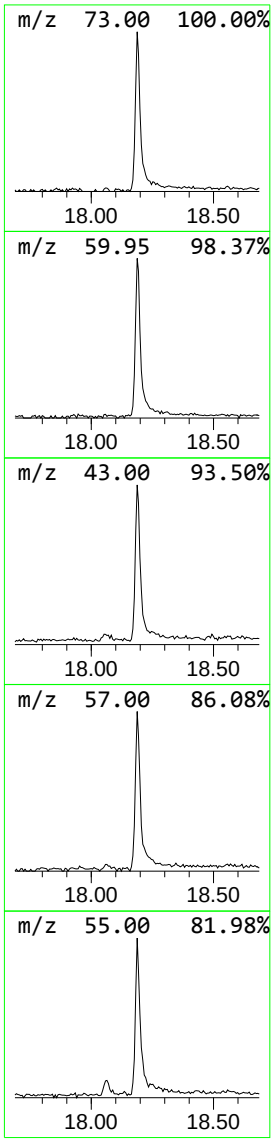
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.187	10.19 ng	281444	Phenanthrene-d10	17.300

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Tridecanoic acid	214	C13H26O2	000638-53-9	76
5	Undecanoic acid	186	C11H22O2	000112-37-8	59





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Data File : BG057791.D
Acq On : 21 Jun 2023 19:25
Operator : CG/JU
Sample : 03289-17
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-06-12.0-14.0-DUP

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

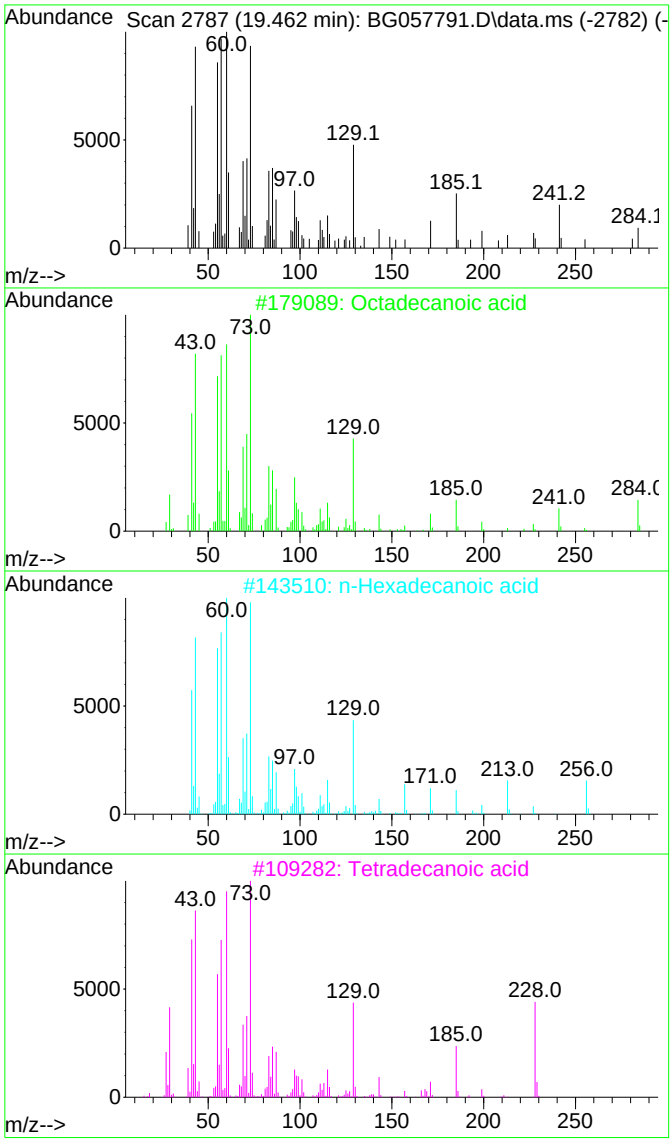
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

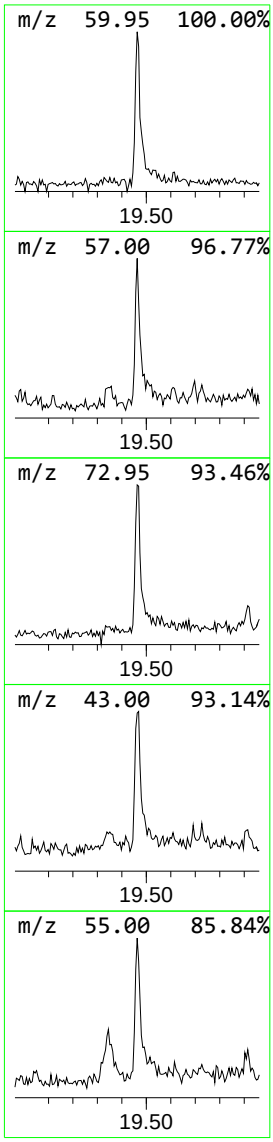
****

Peak Number 4 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.462	2.73 ng	86588	Chrysene-d12	21.548

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	87
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	81
4	n-Decanoic acid	172	C10H20O2	000334-48-5	58
5	Acetamide, N-(4-hydroxycyclohexy...	157	C8H15NO2	027489-61-8	18





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062123\
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Acq On : 21 Jun 2023 19:25
Operator : CG/JU
Sample : 03289-17
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-06-12.0-14.0-DUP

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

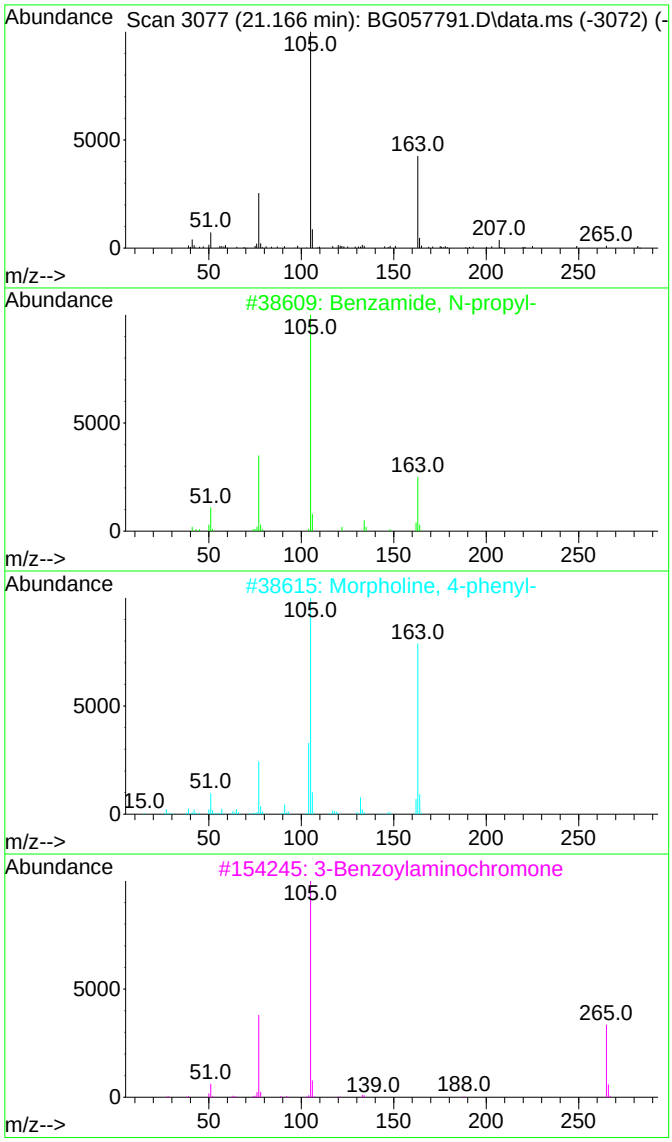
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

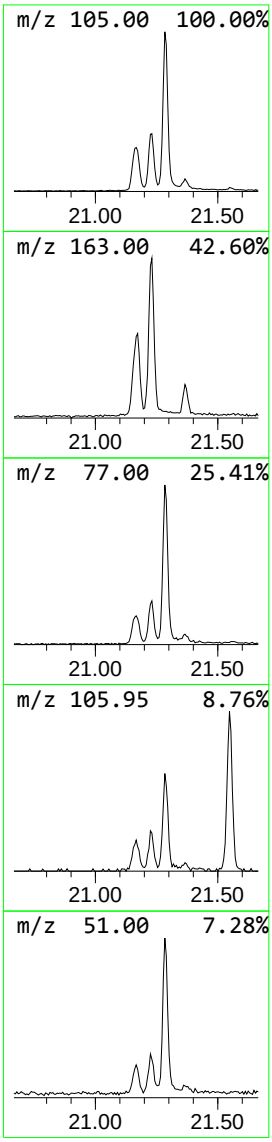
****

Peak Number 5 Benzamide, N-propyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.166	3.25 ng	102969	Chrysene-d12	21.548

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzamide, N-propyl-	163	C10H13NO	010546-70-0	72
2	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	52
3	3-Benzoylaminochromone	265	C16H11NO3	1000243-49-5	35
4	Benzoxiquine	249	C16H11NO2	000086-75-9	35
5	3-Benzoylamino-2-methyl-butyric ...	249	C14H19NO3	1000192-71-7	35





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BNA_G
ClientSampleId :
SB-06-12.0-14.0-DUP

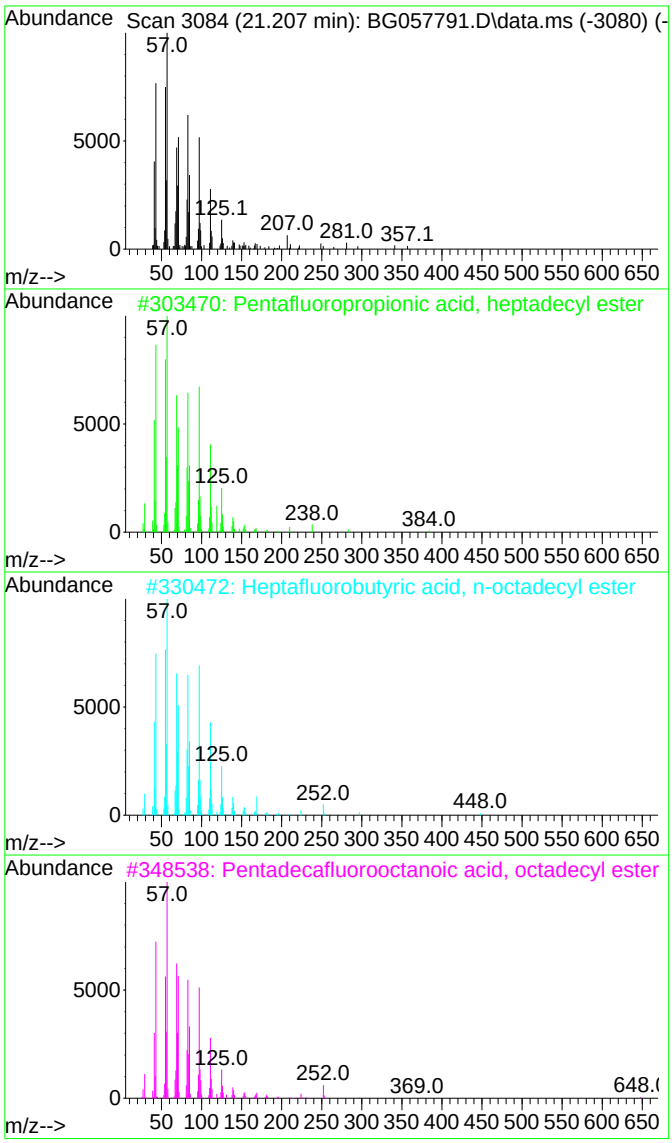
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

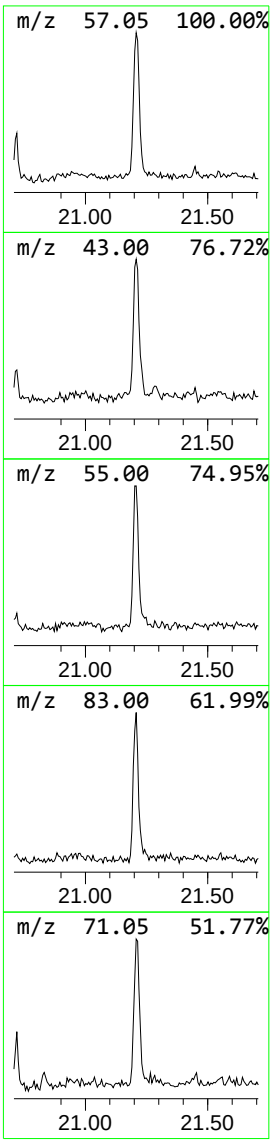
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Pentafluoropropionic acid, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.207	8.86 ng	281131	Chrysene-d12	21.548

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91
2	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
3	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91
4	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	91
5	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91





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ClientSampleId :
SB-06-12.0-14.0-DUP

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

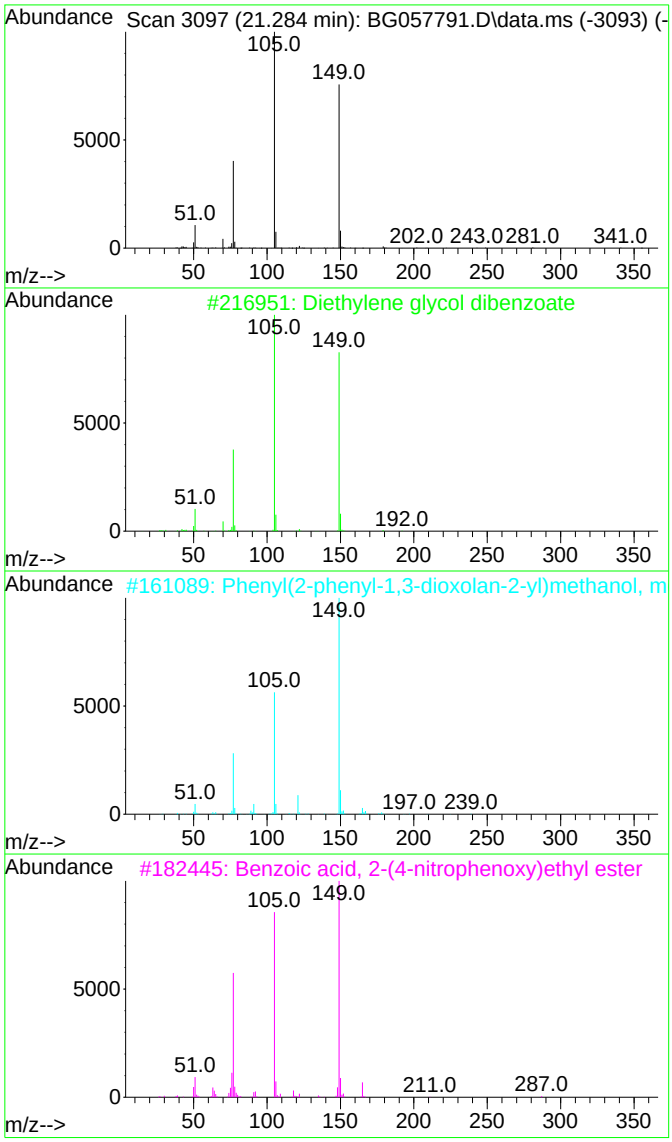
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

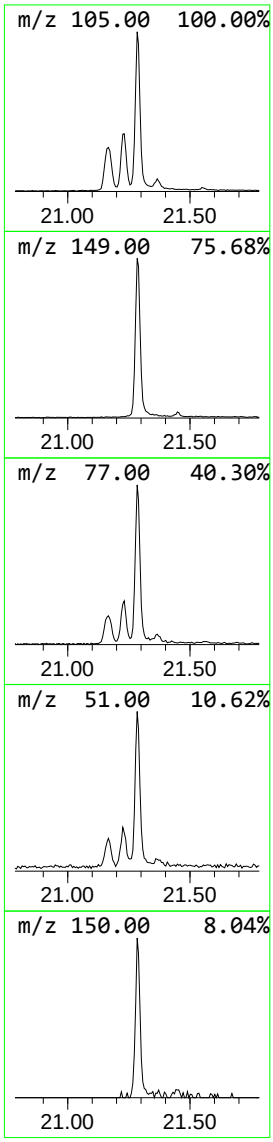
****

Peak Number 7 Diethylene glycol dibenzoate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.284	10.40 ng	329958	Chrysene-d12	21.548

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	90
2	Phenyl(2-phenyl-1,3-dioxolan-2-y...	270	C17H18O3	1000507-07-6	78
3	Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	72
4	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	59
5	2-(2-Carboxyvinyl)pyridine, trans	149	C8H7NO2	007340-22-9	49





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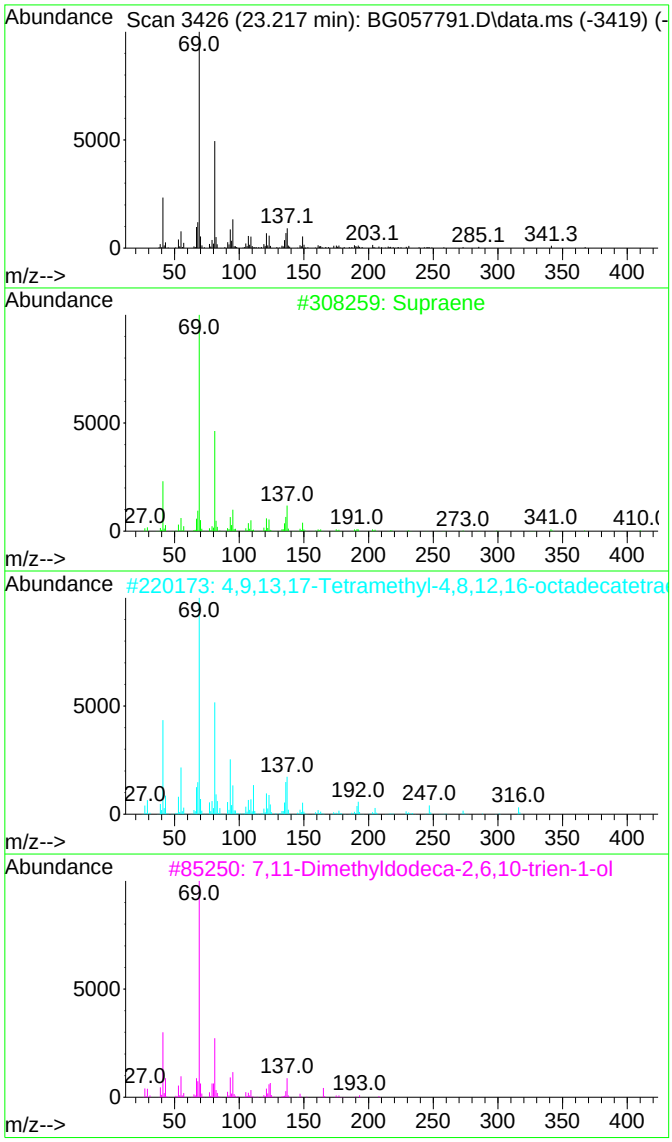
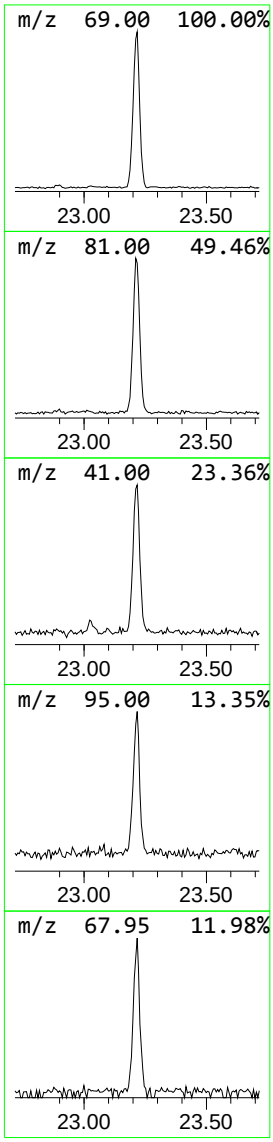
****

Peak Number 8 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.217	7.78 ng	272995	Perylene-d12	24.697

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	91
2	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	83
3	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	80
4	5,9,13-Pentadecatrien-2-one, 6,1...	262	C18H30O	001117-52-8	64
5	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	64





Tentatively Identified Compound (LSC) summary

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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-...	5.026	16.2	ng	126778	1	7.923	156594	20.0
Benzophenone	15.914	4.6	ng	86954	3	14.556	380659	20.0
n-Hexadecanoic ...	18.187	10.2	ng	281444	4	17.300	552340	20.0
Octadecanoic acid	19.462	2.7	ng	86588	5	21.548	634540	20.0
Benzamide, N-pr...	21.166	3.3	ng	102969	5	21.548	634540	20.0
Pentafluoroprop...	21.207	8.9	ng	281131	5	21.548	634540	20.0
Diethylene glyc...	21.284	10.4	ng	329958	5	21.548	634540	20.0
Supraene	23.217	7.8	ng	272995	6	24.697	702074	20.0