LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062223\
Data File : BG057824.D
Acq On : 23 Jun 2023 1:50
Operator : CG/JU
Sample : 03308-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SP-LEFT

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: BG057824.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.427	224	228	236	rVB2	15960	22953	1.14%	0.191%
2	5.027	324	330	341	rVB	348629	505254	25.10%	4.199%
3	5.491	403	409	418	rBV	503455	778308	38.66%	6.468%
4	7.077	672	679	693	rBV	524424	890062	44.21%	7.396%
5	7.923	816	823	830	rVB	129962	216785	10.77%	1.801%
6	9.081	1012	1020	1028	rBV	310436	529081	26.28%	4.397%
7	10.726	1290	1300	1310	rVB	192382	347968	17.28%	2.892%
8	13.176	1710	1717	1726	rBV	803491	1258257	62.50%	10.456%
9	14.557	1945	1952	1960	rVB	339508	521978	25.93%	4.338%
10	15.908	2177	2182	2192	rVB	223281	309273	15.36%	2.570%
11	16.037	2198	2204	2216	rBV	770587	1131924	56.23%	9.406%
12	16.472	2272	2278	2284	rVB	51277	70273	3.49%	0.584%
13	16.613	2295	2302	2307	rBV	21137	35770	1.78%	0.297%
14	17.136	2386	2391	2397	rVB	18854	26612	1.32%	0.221%
15	17.300	2412	2419	2423	rBV	431629	670841	33.32%	5.575%
16	17.342	2423	2426	2430	rVB	31002	39686	1.97%	0.330%
17	18.188	2563	2570	2580	rBV2	149803	244578	12.15%	2.032%
18	19.351	2759	2768	2772	rBV	91173	141945	7.05%	1.180%
19	19.463	2782	2787	2796	rBV3	48784	93810	4.66%	0.780%
20	19.709	2821	2829	2837	rVB	76233	142330	7.07%	1.183%
21	19.915	2858	2864	2875	rVB	1560730	2013185	100.00%	16.729%
22	21.202	3079	3083	3093	rVB2	136099	244412	12.14%	2.031%
23	21.284	3093	3097	3105	rVB	69731	96979	4.82%	0.806%
24	21.449	3121	3125	3130	rVB	71823	98442	4.89%	0.818%
25	21.548	3135	3142	3147	rBV	441963	771621	38.33%	6.412%
26	24.698	3670	3678	3696	rVB	282815	831638	41.31%	6.911%

Sum of corrected areas: 12033965

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062223\
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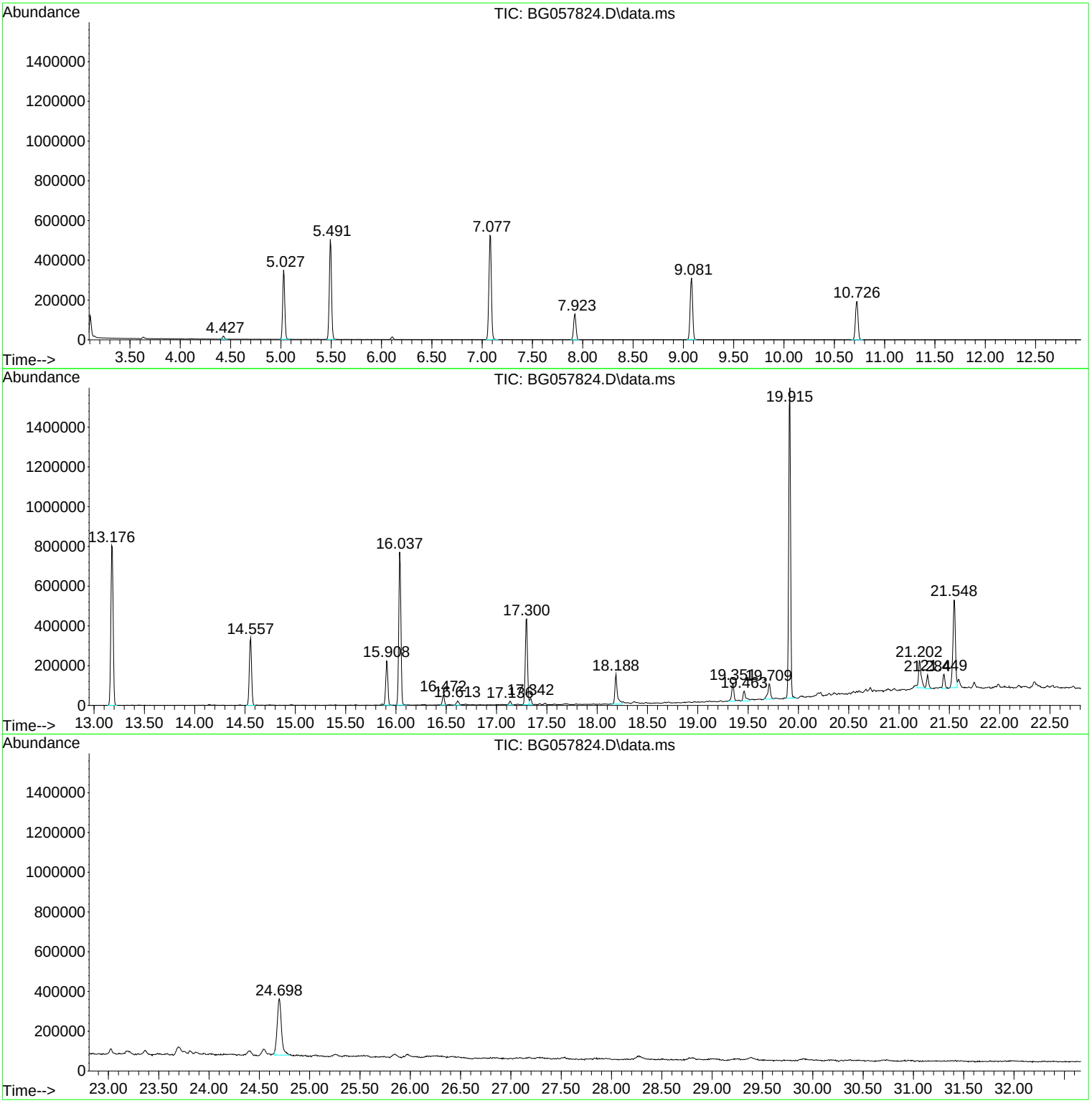
Acq On : 23 Jun 2023 1:50
Operator : CG/JU
Sample : 03308-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SP-LEFT

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 : BG057824.D
Acq On : 23 Jun 2023 1:50
Operator : CG/JU
Sample : 03308-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SP-LEFT

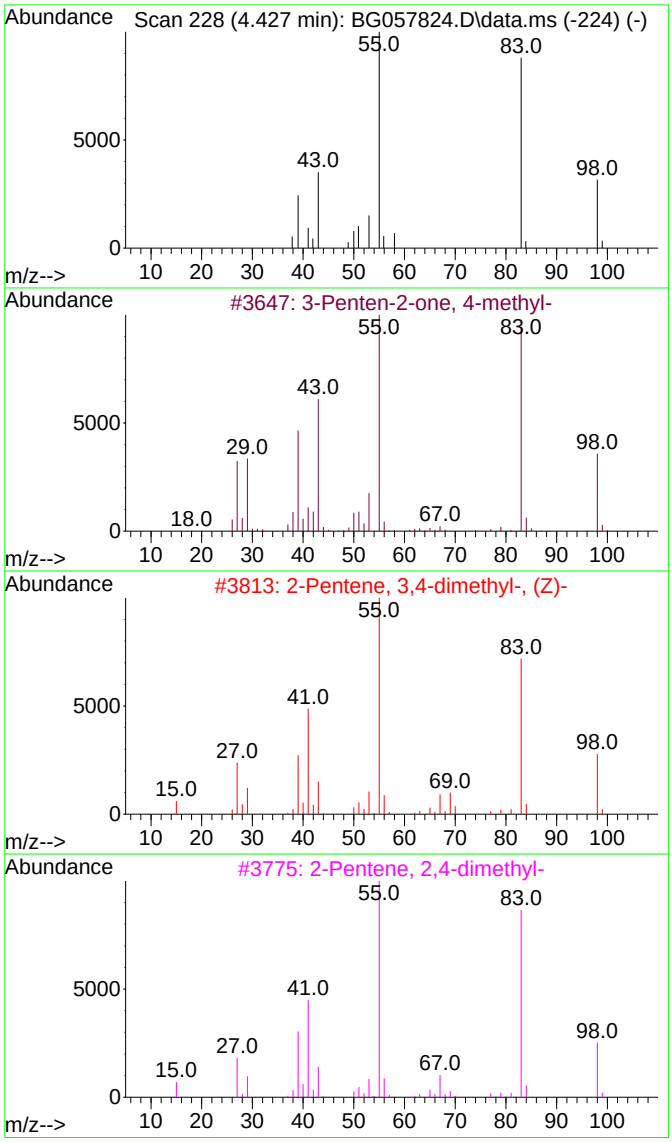
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

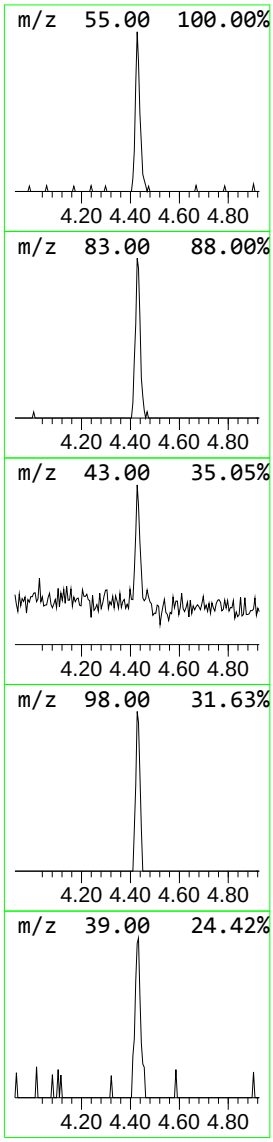
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.427	2.12 ng	22953	1,4-Dichlorobenzene-d4	7.923

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	90
2	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	78
3	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	78
4	2-Pentene, 4,4-dimethyl-	98	C7H14	026232-98-4	78
5	3-Hexen-2-one	98	C6H10O	000763-93-9	78





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062223\
Data File : BG057824.D
Acq On : 23 Jun 2023 1:50
Operator : CG/JU
Sample : 03308-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SP-LEFT

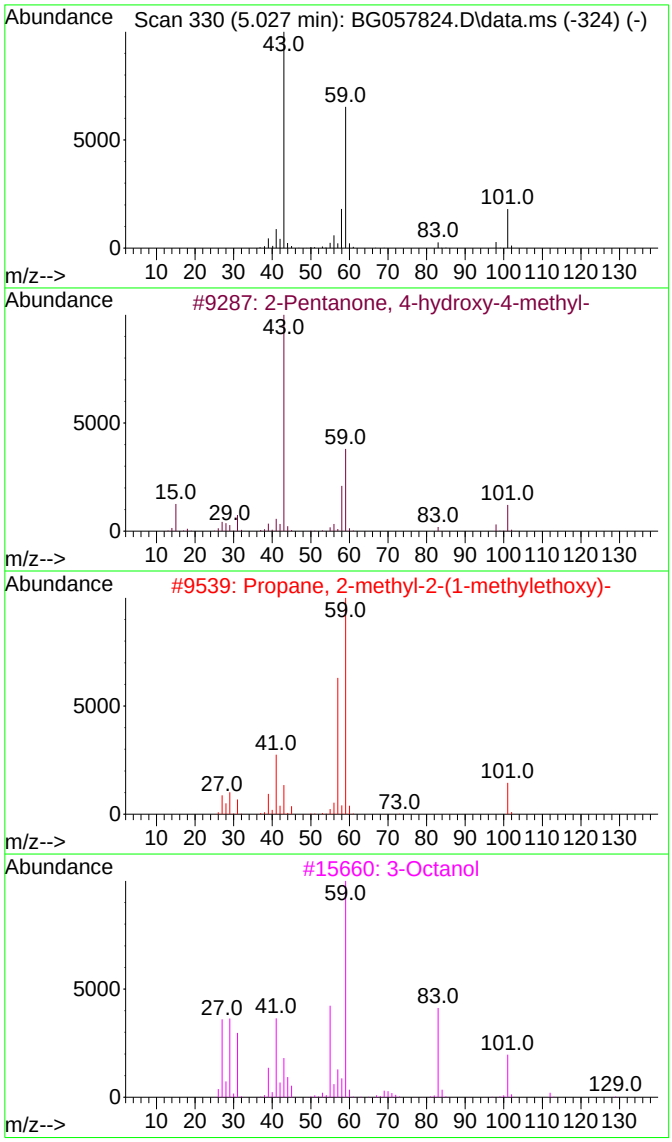
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

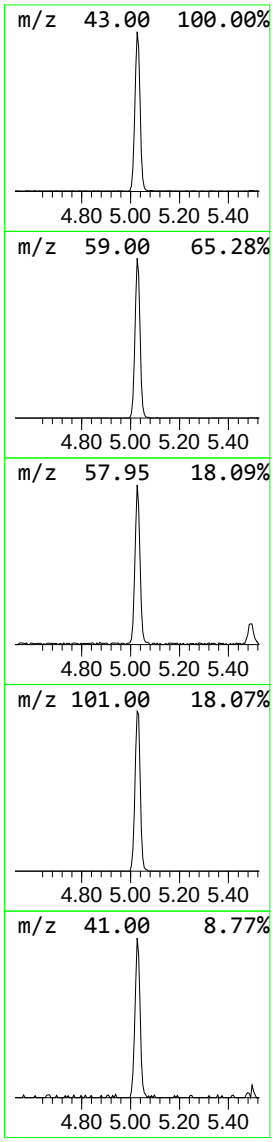
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.027	46.61 ng	505254	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	42
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	33





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062223\
Data File : BG057824.D
Acq On : 23 Jun 2023 1:50
Operator : CG/JU
Sample : 03308-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SP-LEFT

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

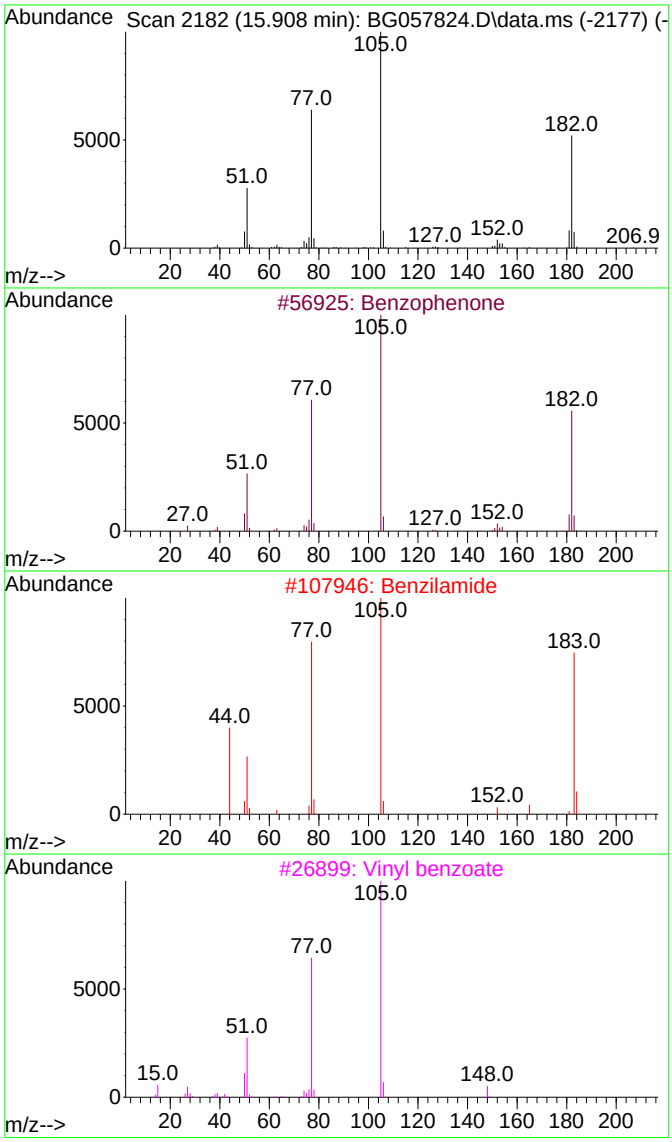
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

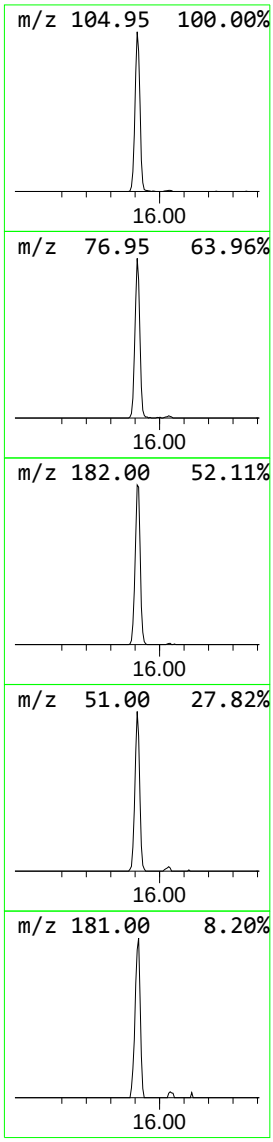
****

Peak Number 3 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.908	11.85 ng	309273	Acenaphthene-d10	14.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Benzilamide	227	C14H13NO2	004746-87-6	47
3	Vinyl benzoate	148	C9H8O2	000769-78-8	47
4	1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
5	Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062223\
Data File : BG057824.D
Acq On : 23 Jun 2023 1:50
Operator : CG/JU
Sample : 03308-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SP-LEFT

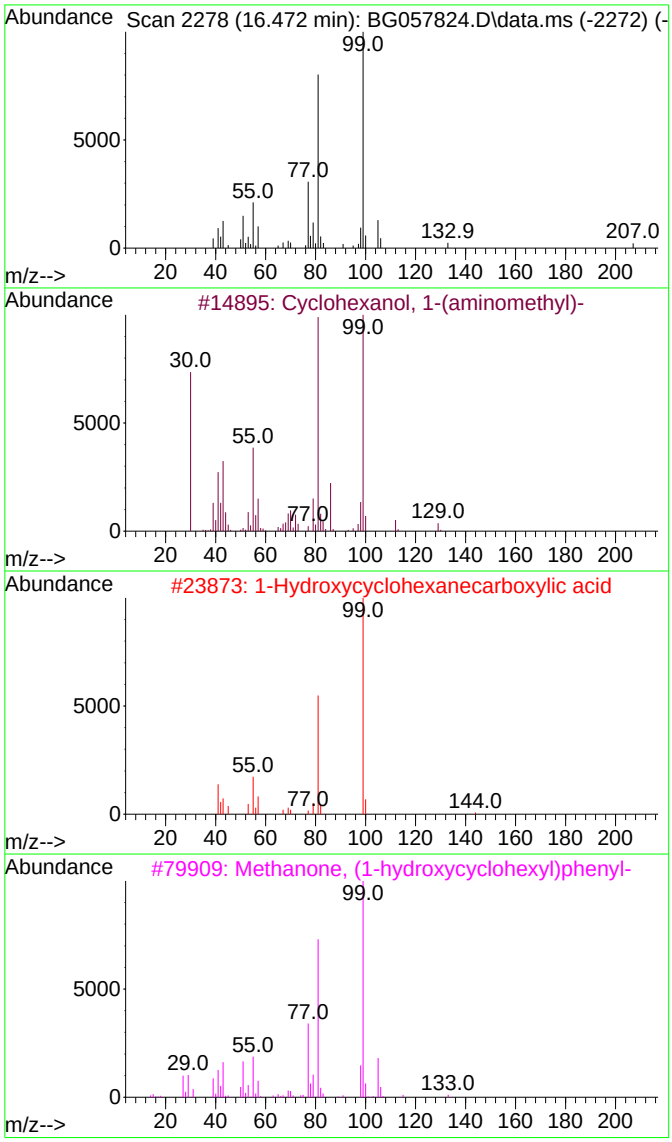
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

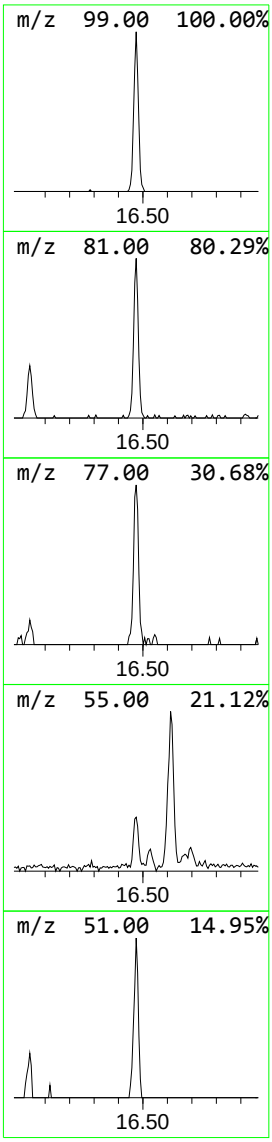
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Cyclohexanol, 1-(aminomethyl)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.472	2.10 ng	70273	Phenanthrene-d10	17.295

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanol, 1-(aminomethyl)-	129	C7H15NO	004000-72-0	64
2	1-Hydroxycyclohexanecarboxylic acid	144	C7H12O3	001123-28-0	59
3	Methanone, (1-hydroxycyclohexyl)...	204	C13H16O2	000947-19-3	46
4	1,1'-Bicyclohexyl-1,1'-diol	198	C12H22O2	002888-11-1	45
5	3-Methylcyclohexyl methylphospho...	194	C8H16FO2P	113548-86-0	42





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Data File : BG057824.D
Acq On : 23 Jun 2023 1:50
Operator : CG/JU
Sample : 03308-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SP-LEFT

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

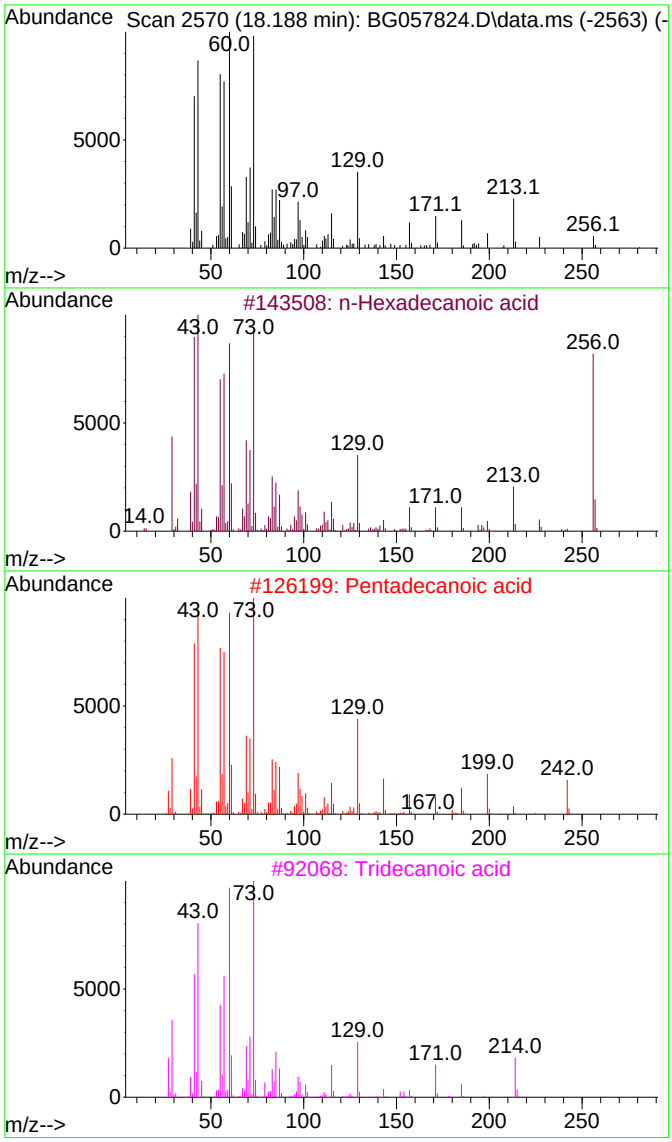
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

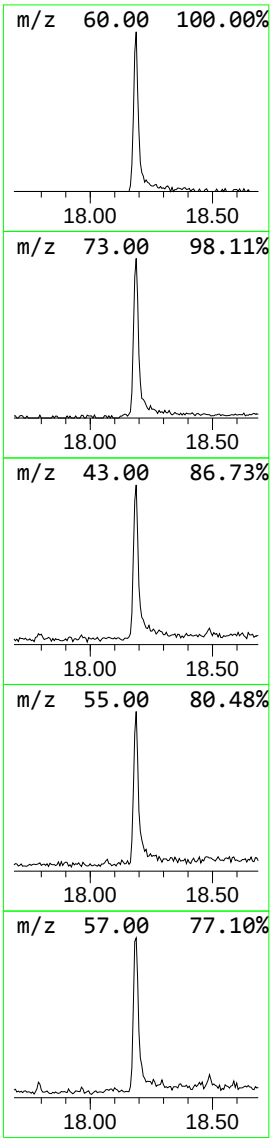
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.188	7.29 ng	244578	Phenanthrene-d10	17.295

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	87
3	Tridecanoic acid	214	C13H26O2	000638-53-9	74
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	58





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Data File : BG057824.D
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ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SP-LEFT

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

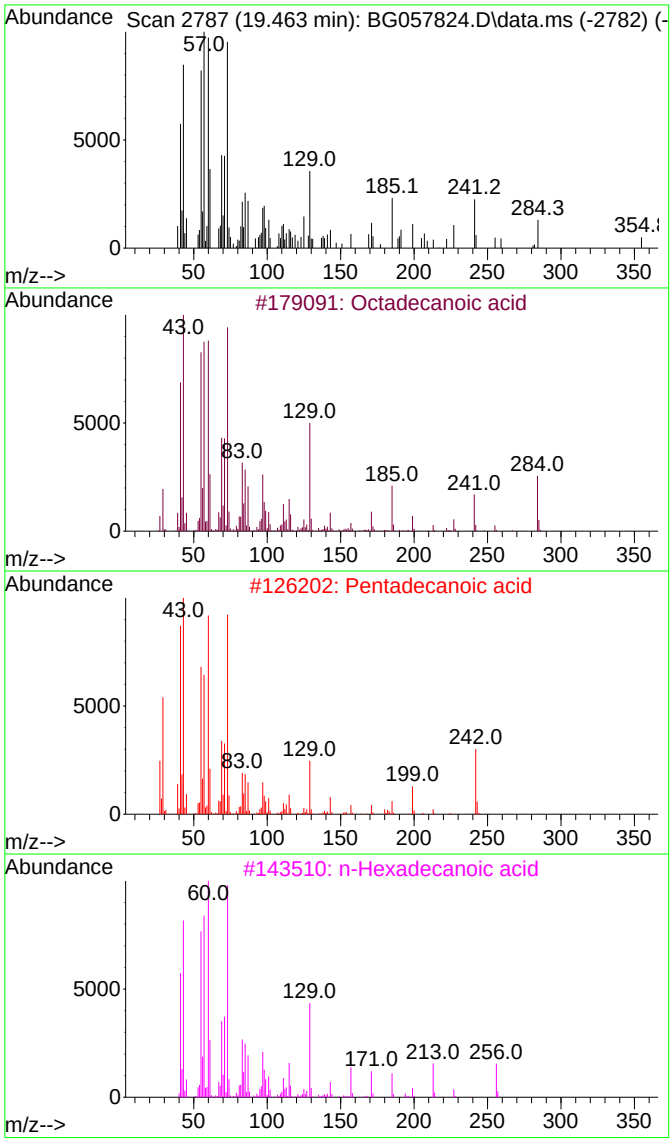
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

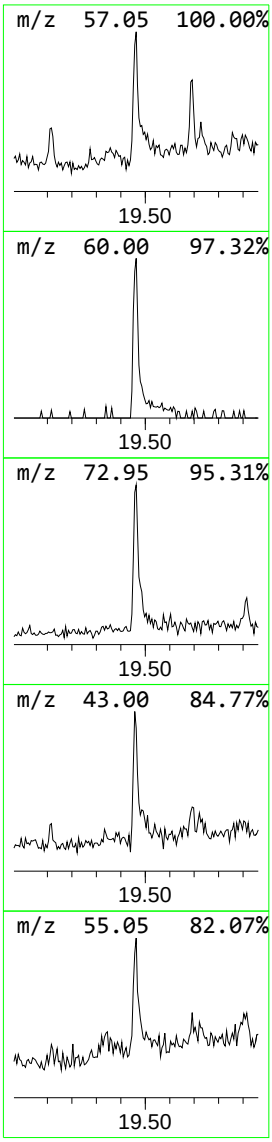
****

Peak Number 6 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.463	2.43 ng	93810	Chrysene-d12	21.548

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	96
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	95
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	n-Decanoic acid	172	C10H20O2	000334-48-5	64





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Data File : BG057824.D
Acq On : 23 Jun 2023 1:50
Operator : CG/JU
Sample : 03308-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SP-LEFT

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

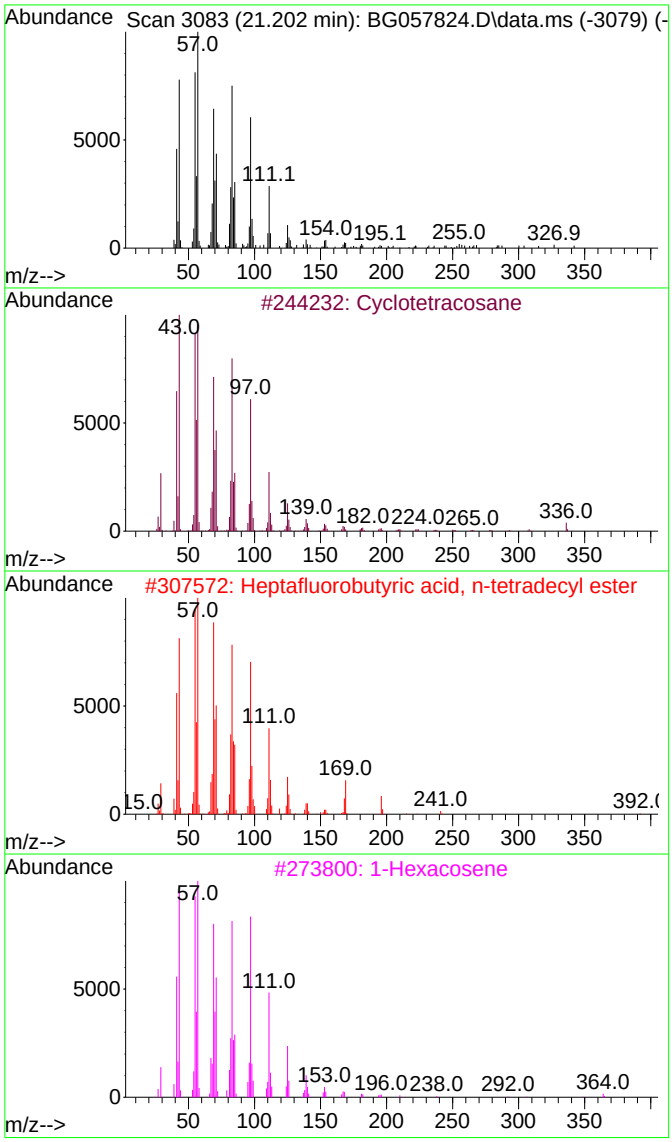
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

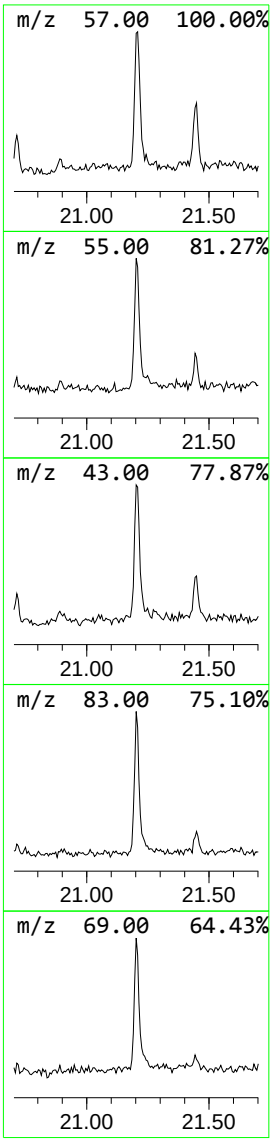
****

Peak Number 7 Cyclotetracosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.202	6.34 ng	244412	Chrysene-d12	21.548

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetracosane	336	C24H48	000297-03-0	91
2	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	91
3	1-Hexacosene	364	C26H52	018835-33-1	90
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	87
5	1-Heneicosanol	312	C21H44O	015594-90-8	87





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Sample : 03308-01
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ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SP-LEFT

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

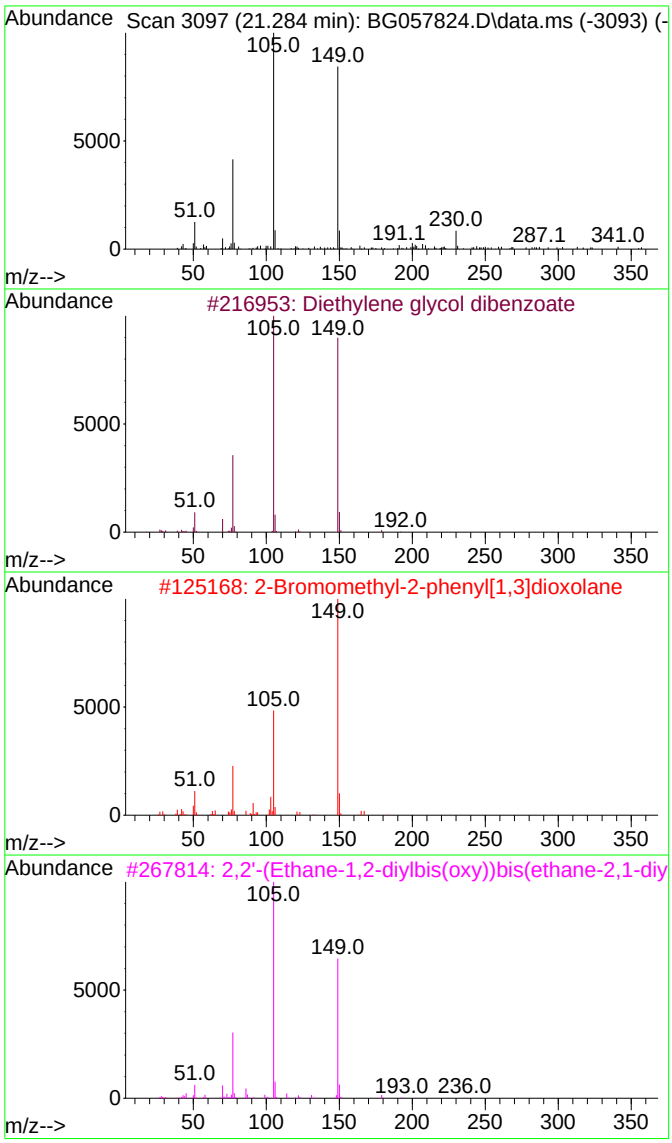
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

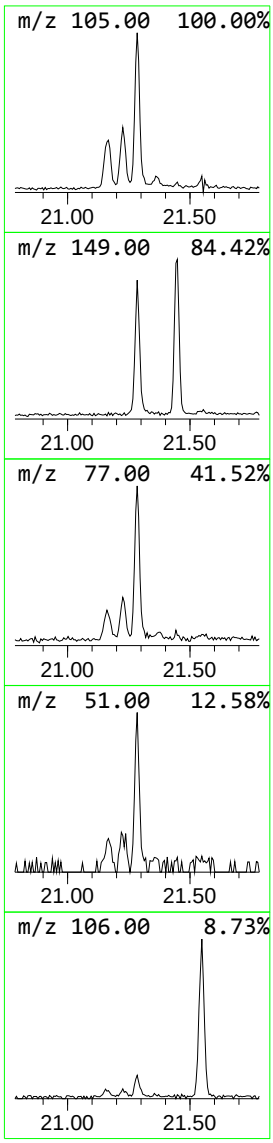
****

Peak Number 8 Diethylene glycol dibenzoate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.284	2.51 ng	96979	Chrysene-d12	21.548

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	80
2	2-Bromomethyl-2-phenyl[1,3]dioxo...	242	C10H11BrO2	003418-21-1	72
3	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	72
4	Phenyl(2-phenyl-1,3-dioxolan-2-y...	256	C16H16O3	005694-69-9	64
5	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	50





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062223\
Data File : BG057824.D
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Operator : CG/JU
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Instrument :
BNA_G
ClientSampleId :
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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
3-Penten-2-one,...	4.427	2.1	ng	22953	1	7.923	216785	20.0
2-Pentanone, 4-...	5.027	46.6	ng	505254	1	7.923	216785	20.0
Benzophenone	15.908	11.9	ng	309273	3	14.557	521978	20.0
Cyclohexanol, 1...	16.472	2.1	ng	70273	4	17.295	670841	20.0
n-Hexadecanoic ...	18.188	7.3	ng	244578	4	17.295	670841	20.0
Octadecanoic acid	19.463	2.4	ng	93810	5	21.548	771621	20.0
Cyclotetracosane	21.202	6.3	ng	244412	5	21.548	771621	20.0
Diethylene glyc...	21.284	2.5	ng	96979	5	21.548	771621	20.0