LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092221\
Data File : BP007105.D
Acq On : 22 Sep 2021 19:10
Operator : CG/JU
Sample : M3687-17
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : A009015

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_P\Methods\8270E-BP092121.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP007105.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.011	322	327	341	rBV	311089	449048	4.43%	0.775%
2	5.469	398	405	416	rBV	3182084	4600795	45.41%	7.936%
3	7.064	668	676	688	rBV	2770709	4447980	43.90%	7.673%
4	7.899	809	818	826	rBV	861057	1381937	13.64%	2.384%
5	9.058	1007	1015	1024	rBV	1703032	2811253	27.75%	4.849%
6	10.487	1251	1258	1273	rBV2	128992	306076	3.02%	0.528%
7	10.699	1286	1294	1302	rBV	1074371	1815259	17.92%	3.131%
8	13.151	1704	1711	1724	rBV	4608796	6668221	65.81%	11.503%
9	14.522	1936	1944	1953	rBV	1534041	2334376	23.04%	4.027%
10	16.010	2191	2197	2215	rBV	4033606	5803167	57.28%	10.011%
11	17.275	2405	2412	2417	rBV	1949649	2784511	27.48%	4.803%
12	18.163	2557	2563	2572	rBV	350958	685018	6.76%	1.182%
13	19.281	2749	2753	2762	rBV	169776	305277	3.01%	0.527%
14	19.392	2767	2772	2789	rBV	1134810	2242064	22.13%	3.868%
15	19.628	2810	2812	2821	rVB	110566	185812	1.83%	0.321%
16	19.828	2841	2846	2853	rBV	8244873	10132054	100.00%	17.478%
17	21.033	3046	3051	3054	rBV	354024	593386	5.86%	1.024%
18	21.080	3054	3059	3064	rVV2	710899	1318654	13.01%	2.275%
19	21.133	3064	3068	3077	rVV	1482967	1866464	18.42%	3.220%
20	21.357	3101	3106	3111	rBV	2667865	3464209	34.19%	5.976%
21	23.769	3509	3516	3528	rVB2	1892355	3775207	37.26%	6.512%

Sum of corrected areas: 57970768

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092221\
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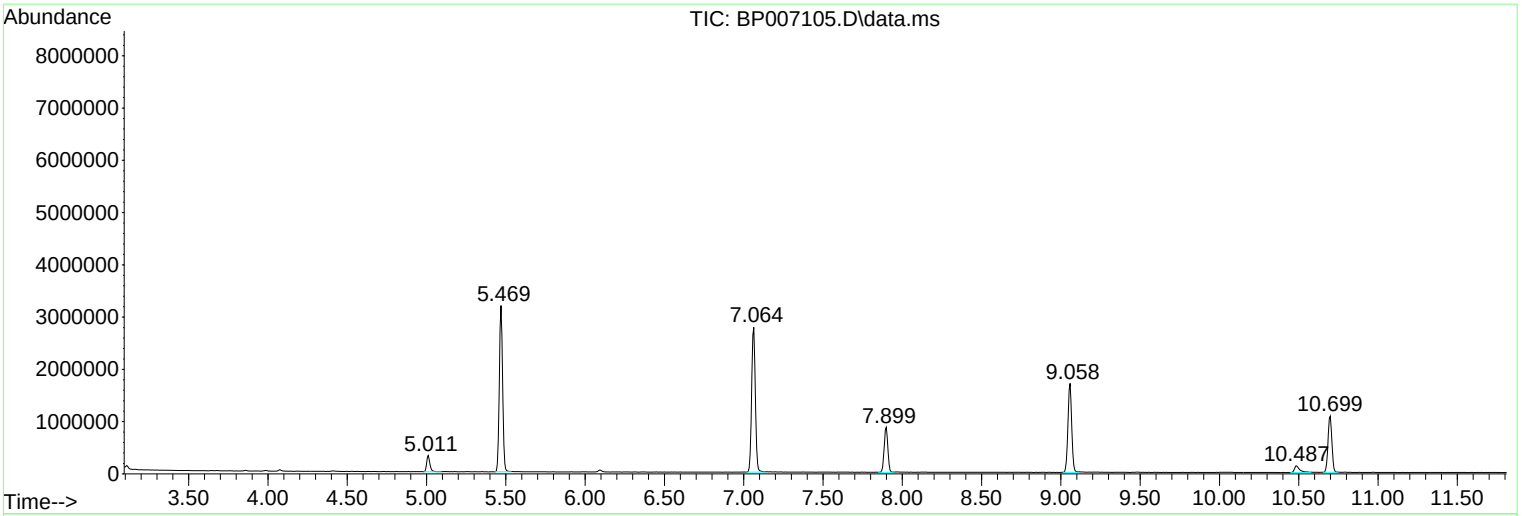
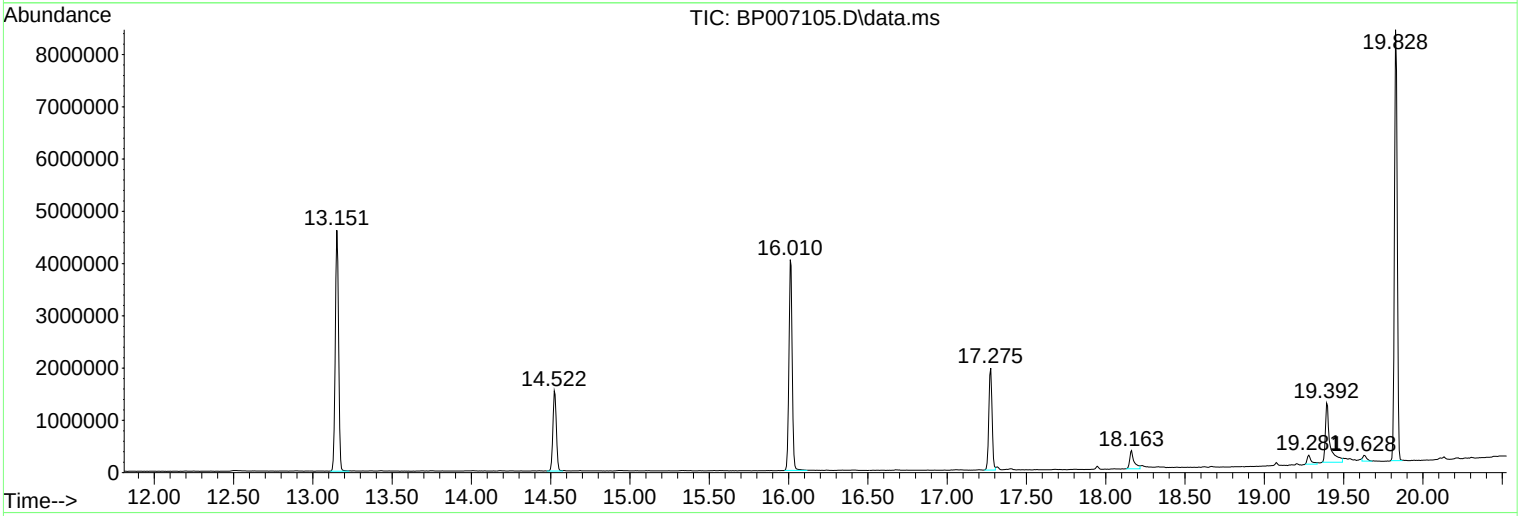
Misc :
ALS Vial : 11 Sample Multiplier: 1

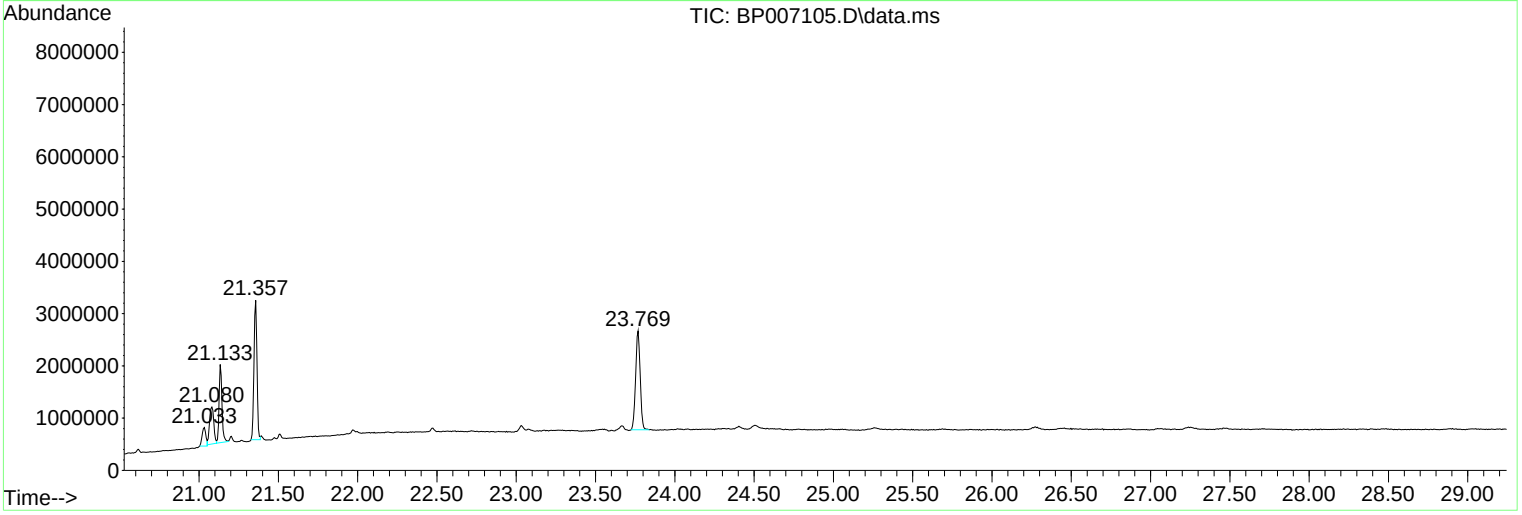
Instrument :
BNA_P
ClientSampleId :
A009015

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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Data File : BP007105.D
Acq On : 22 Sep 2021 19:10
Operator : CG/JU
Sample : M3687-17
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : A009015

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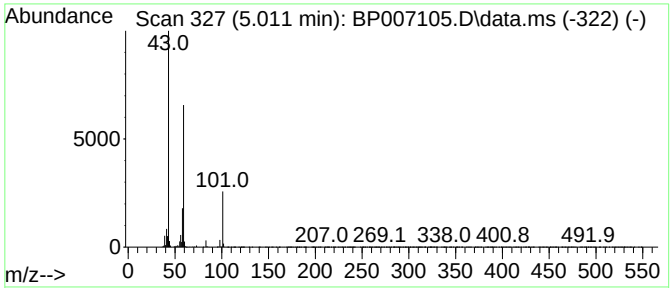
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

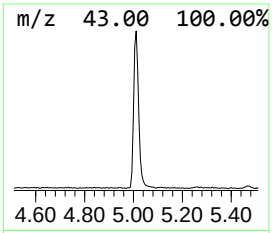
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

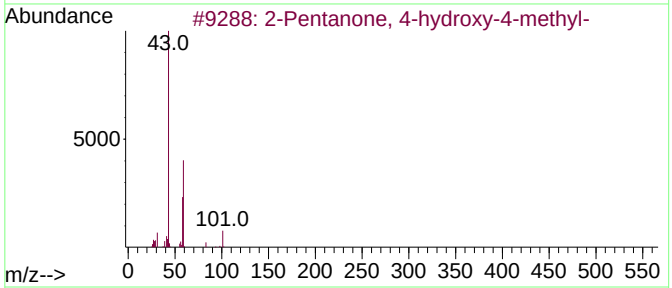
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

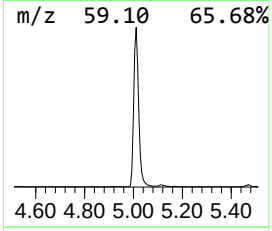
R.T.	EstConc	Area	Relative to ISTD	R.T.
5.011	6.50 ng	449048	1,4-Dichlorobenzene-d4	7.899

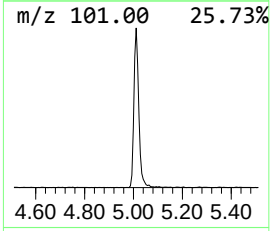
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	1,2-Butanediol	90	C4H10O2	000584-03-2	17
4	Acetone	58	C3H6O	000067-64-1	10
5	Guanidine	59	CH5N3	000113-00-8	9

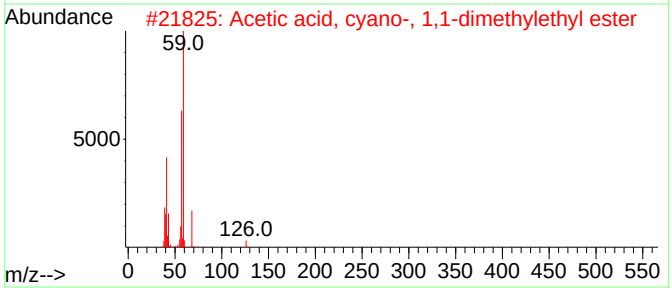


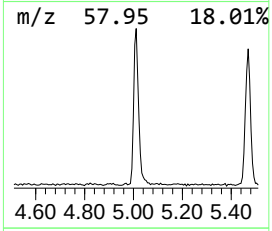


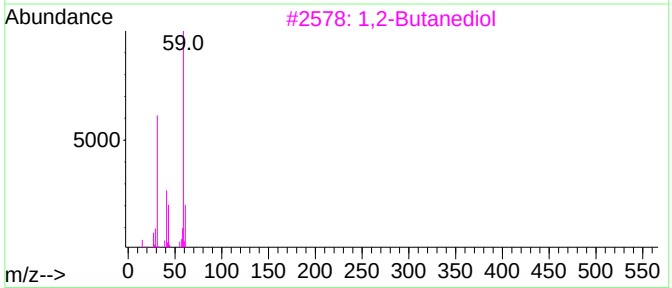


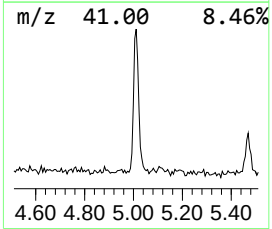












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092221\
Data File : BP007105.D
Acq On : 22 Sep 2021 19:10
Operator : CG/JU
Sample : M3687-17
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A009015

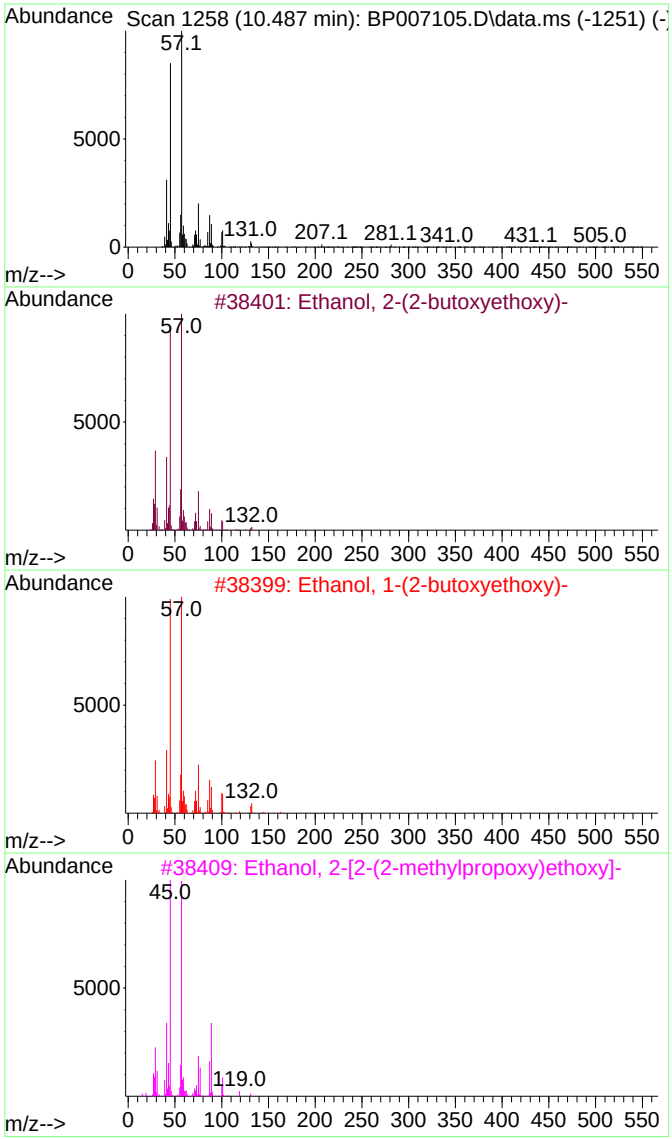
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

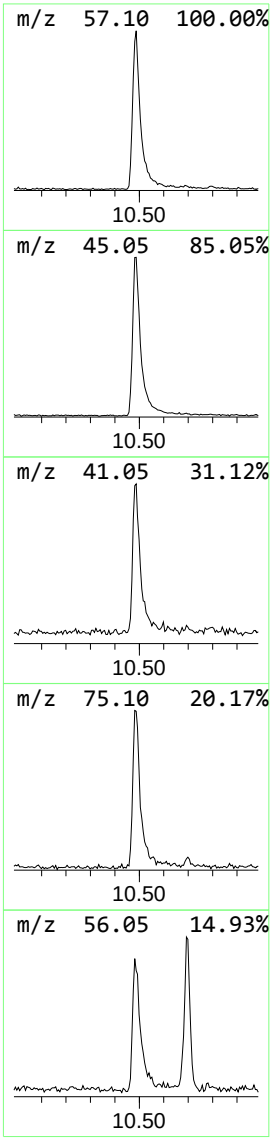
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.487	3.37 ng	306076	Naphthalene-d8	10.699

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	90
3	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	64
4	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
5	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	50





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ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : A009015

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

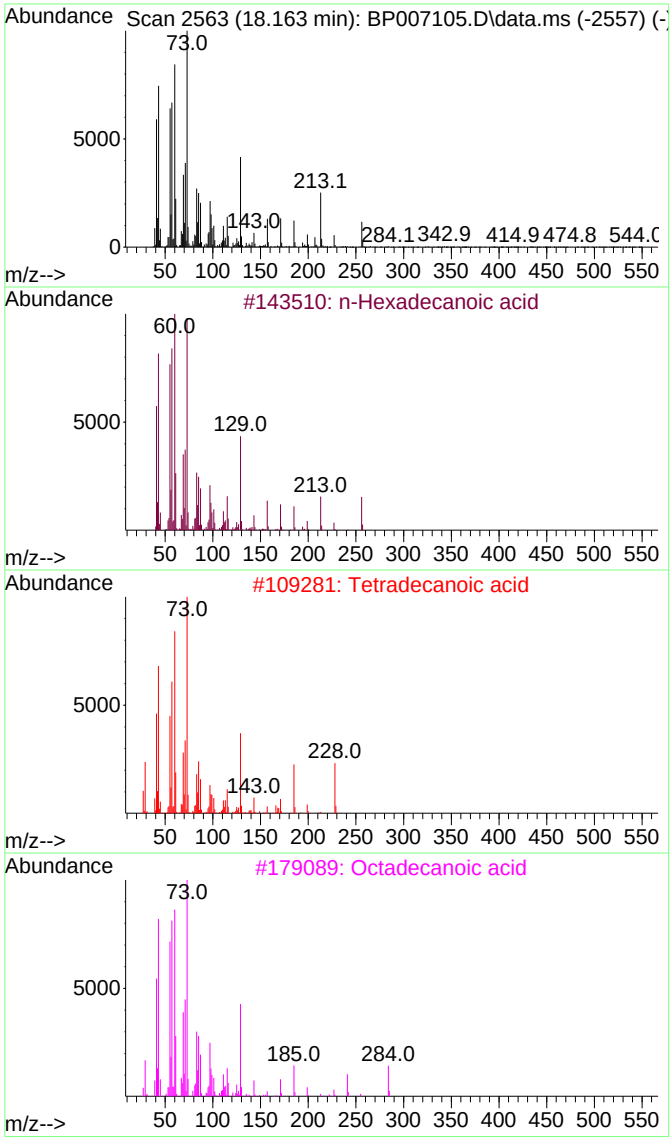
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

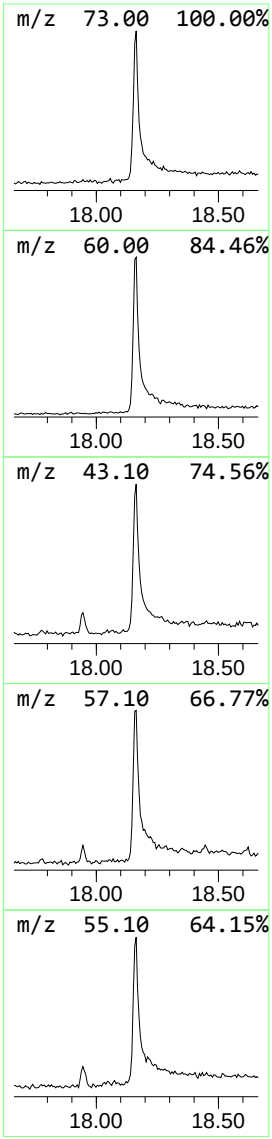
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.163	4.92 ng	685018	Phenanthrene-d10	17.275

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	95
3	Octadecanoic acid	284	C18H36O2	000057-11-4	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5	Tridecanoic acid	214	C13H26O2	000638-53-9	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092221\
Data File : BP007105.D
Acq On : 22 Sep 2021 19:10
Operator : CG/JU
Sample : M3687-17
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A009015

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

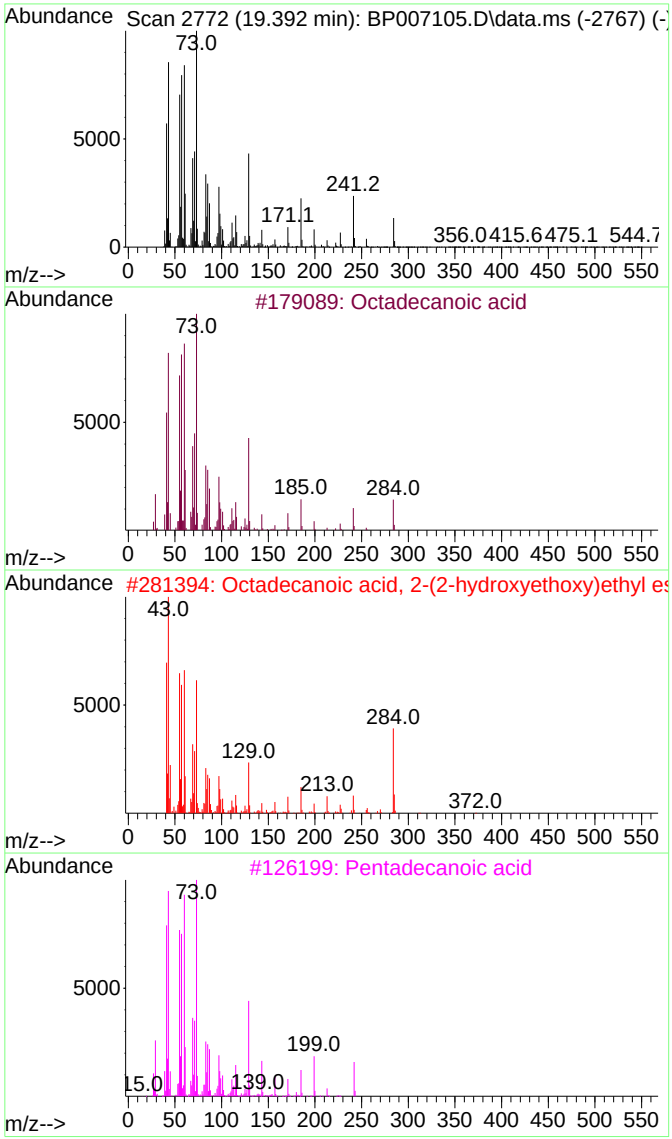
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

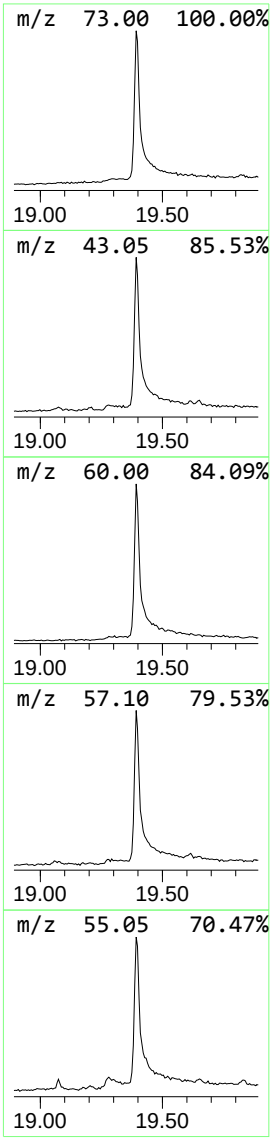
****

Peak Number 5 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.392	12.94 ng	2242060	Chrysene-d12	21.357

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80





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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A009015

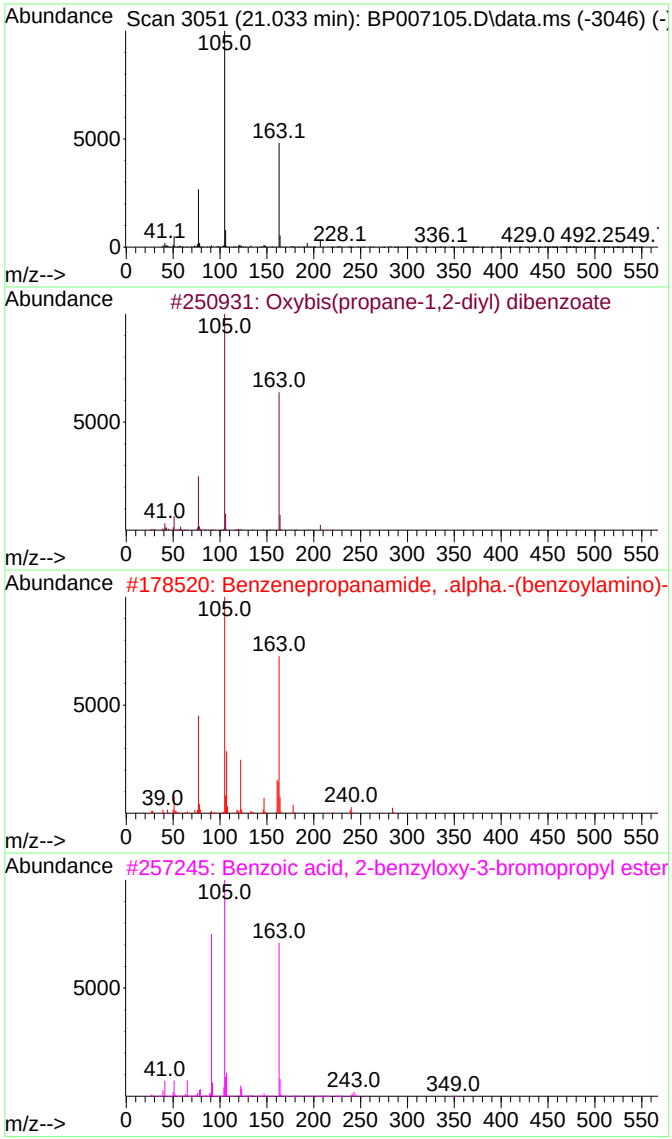
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

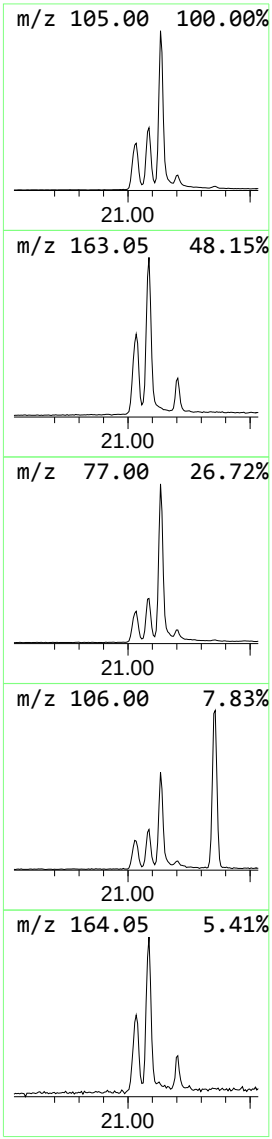
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Oxybis(propane-1,2-diyl) di... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.033	3.43 ng	593386	Chrysene-d12	21.357

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxybis(propane-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	78
2	Benzenepropanamide, .alpha.-(ben...	284	C16H16N2O3	058690-81-6	45
3	Benzoic acid, 2-benzyloxy-3-brom...	348	C17H17BrO3	1000191-33-3	42
4	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	40
5	Benzamide, N-acetyl-	163	C9H9NO2	001575-95-7	9





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Data File : BP007105.D
Acq On : 22 Sep 2021 19:10
Operator : CG/JU
Sample : M3687-17
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : A009015

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

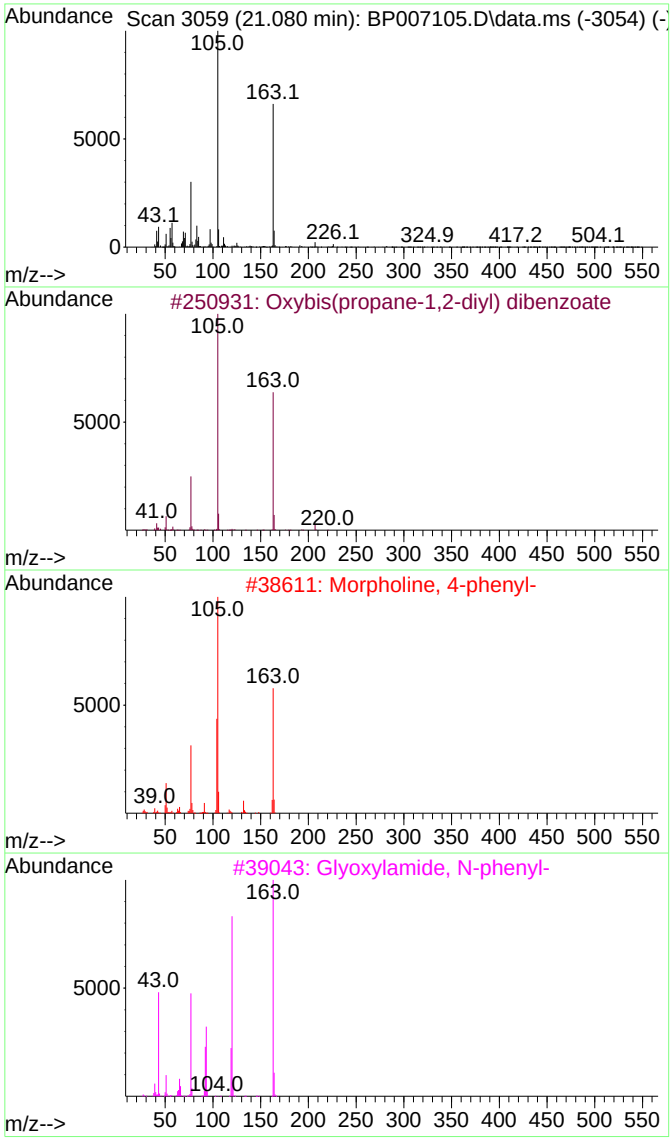
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

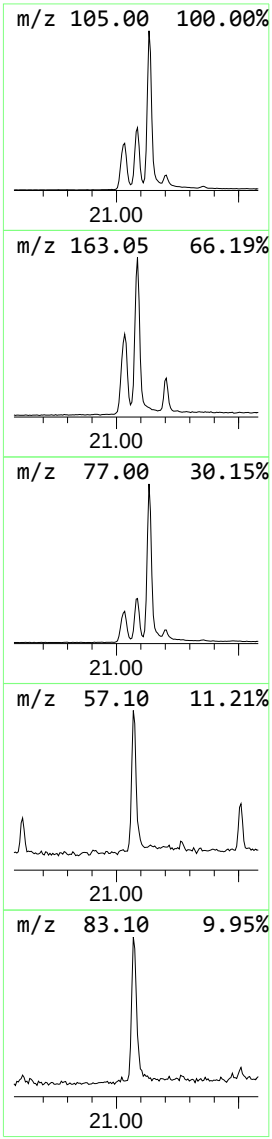
****

Peak Number 7 Morpholine, 4-phenyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.080	7.61 ng	1318650	Chrysene-d12	21.357

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxybis(propane-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	58
2	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	53
3	Glyoxylamide, N-phenyl-	163	C9H9NO2	032331-52-5	38
4	Benzenepropanamide, .alpha.-(ben...	284	C16H16N2O3	058690-81-6	36
5	.delta.2-1,3,4-Oxadiazolin-5-one...	163	C7H5N3O2	002845-82-1	27





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

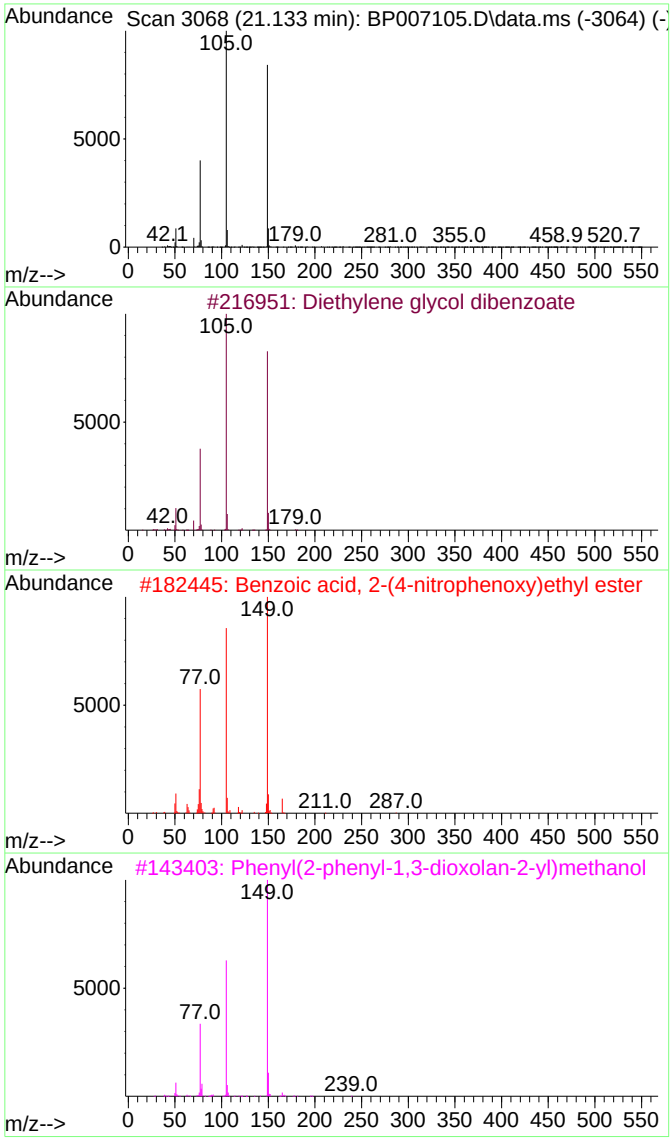
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

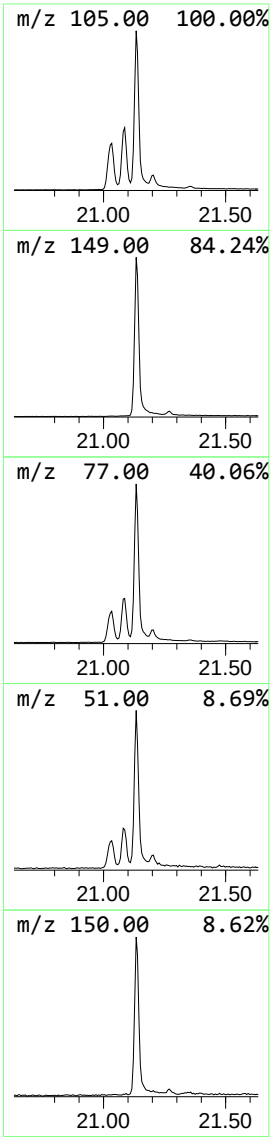
****

Peak Number 8 Diethylene glycol dibenzoate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.133	10.78 ng	1866460	Chrysene-d12	21.357

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	80
2	Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	78
3	Phenyl(2-phenyl-1,3-dioxolan-2-y...	256	C16H16O3	005694-69-9	78
4	2-(2-(2-Methoxyethoxy)ethoxy)eth...	268	C14H20O5	1000366-99-1	74
5	Benzoic acid, 2-(2-chlorophenoxy...	276	C15H13ClO3	1000368-25-9	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092221\
Data File : BP007105.D
Acq On : 22 Sep 2021 19:10
Operator : CG/JU
Sample : M3687-17
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : A009015

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.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-...	5.011	6.5	ng	449048	1	7.899	1381940	20.0
Ethanol, 2-(2-b...	10.487	3.4	ng	306076	2	10.699	1815260	20.0
n-Hexadecanoic ...	18.163	4.9	ng	685018	4	17.275	2784510	20.0
Octadecanoic acid	19.392	12.9	ng	2242060	5	21.357	3464210	20.0
Oxybis(propane-...	21.033	3.4	ng	593386	5	21.357	3464210	20.0
Morpholine, 4-p...	21.080	7.6	ng	1318650	5	21.357	3464210	20.0
Diethylene glyc...	21.133	10.8	ng	1866460	5	21.357	3464210	20.0