LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092221\
Data File : BP007107.D
Acq On : 22 Sep 2021 20:19
Operator : CG/JU
Sample : M3687-32
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : A013015

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: BP007107.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.469	398	405	420	rBV	3925514	5695393	49.62%	8.674%
2	7.063	668	676	693	rBV	3547561	5702504	49.69%	8.685%
3	7.899	810	818	825	rBV	966720	1538404	13.40%	2.343%
4	9.057	1007	1015	1032	rBV	2175156	3570986	31.11%	5.439%
5	10.481	1251	1257	1274	rBV	187382	425406	3.71%	0.648%
6	10.698	1286	1294	1304	rBV	1198373	2069429	18.03%	3.152%
7	13.151	1703	1711	1726	rBV	5721027	8370975	72.94%	12.749%
8	14.522	1938	1944	1956	rBV	1838473	2678061	23.33%	4.079%
9	16.010	2190	2197	2215	rBV	4599514	6621921	57.70%	10.085%
10	17.275	2405	2412	2425	rBV	2180820	3126341	27.24%	4.761%
11	18.163	2557	2563	2573	rBV	589728	1071027	9.33%	1.631%
12	19.280	2749	2753	2765	rBV5	87849	267203	2.33%	0.407%
13	19.392	2767	2772	2794	rBV	1687380	3128683	27.26%	4.765%
14	19.827	2841	2846	2852	rBV	9190302	11477042	100.00%	17.479%
15	21.027	3046	3050	3054	rBV	272324	456996	3.98%	0.696%
16	21.074	3054	3058	3064	rVV2	650493	1240621	10.81%	1.889%
17	21.133	3064	3068	3075	rVB	1237836	1522707	13.27%	2.319%
18	21.357	3101	3106	3111	rBV	2494517	3238015	28.21%	4.931%
19	23.762	3509	3515	3525	rVB2	1642942	3459487	30.14%	5.269%

Sum of corrected areas: 65661201

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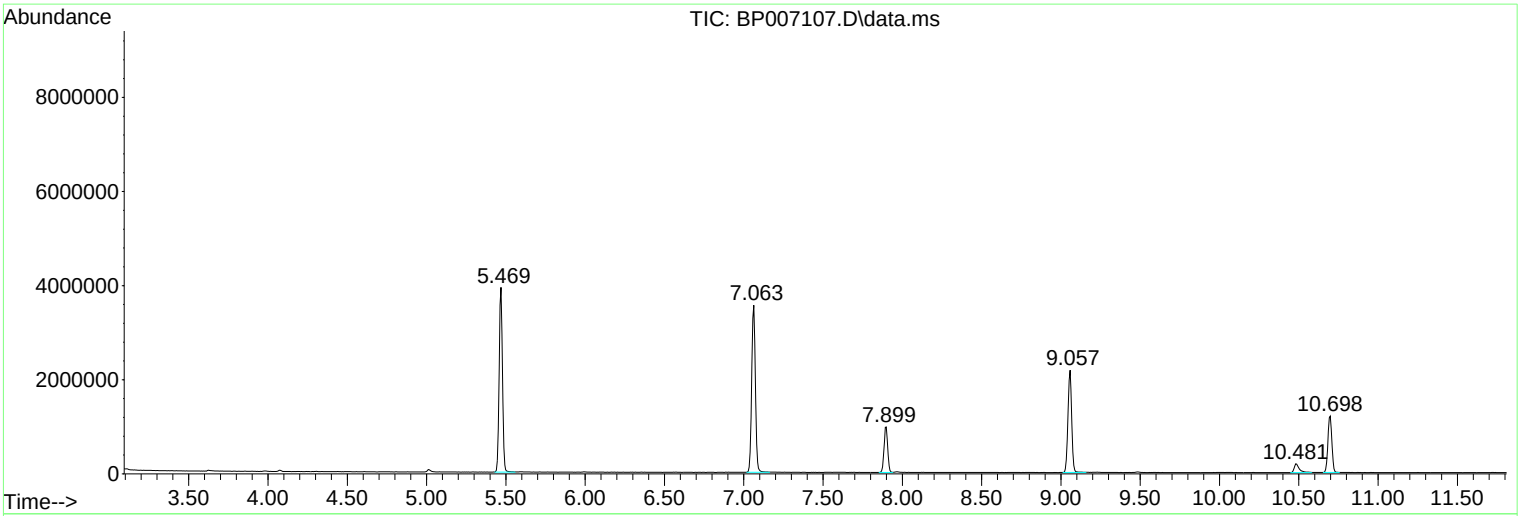
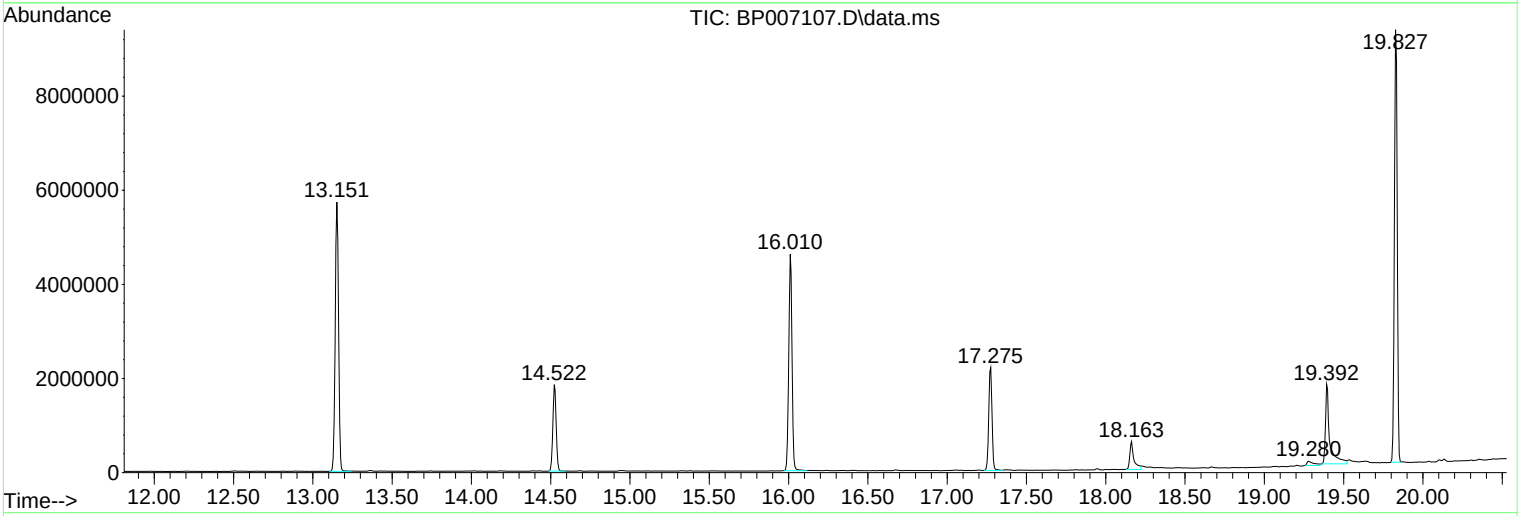
Misc :
ALS Vial : 13 Sample Multiplier: 1

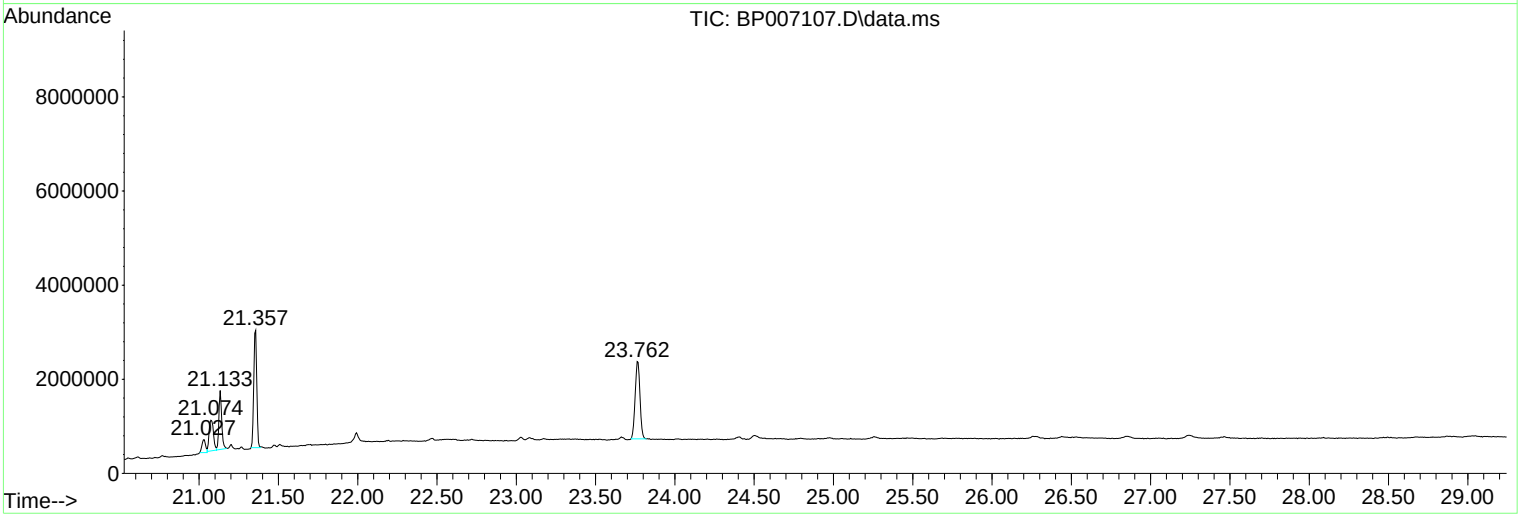
Instrument :
BNA_P
ClientSampleId :
A013015

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 : BP007107.D
Acq On : 22 Sep 2021 20:19
Operator : CG/JU
Sample : M3687-32
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Instrument : BNA_P
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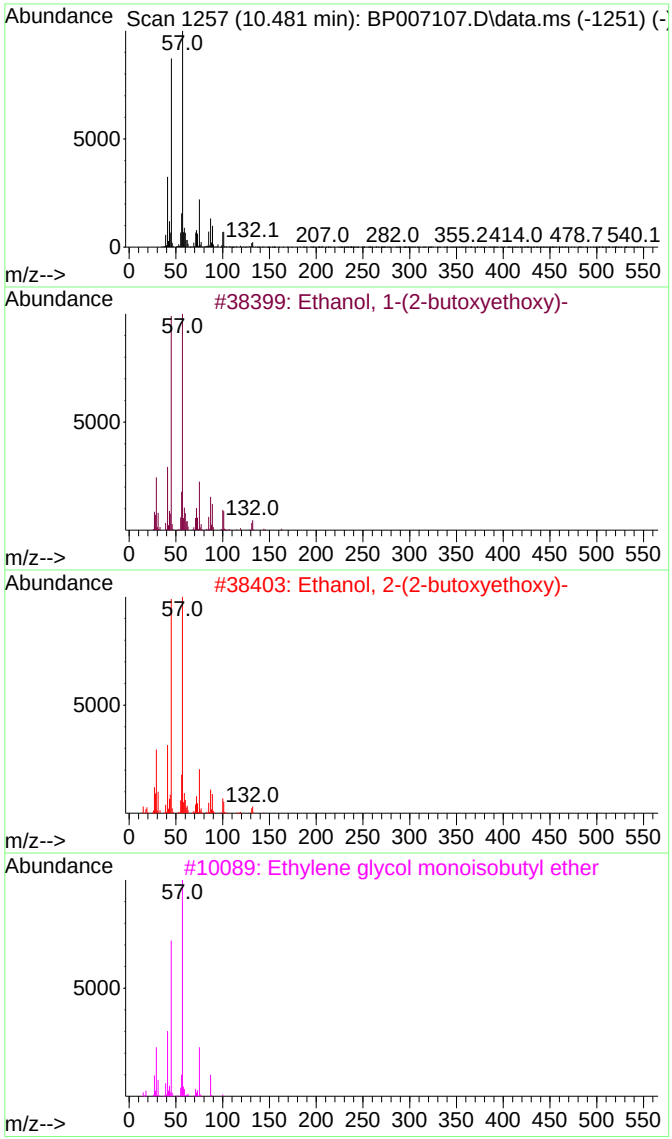
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

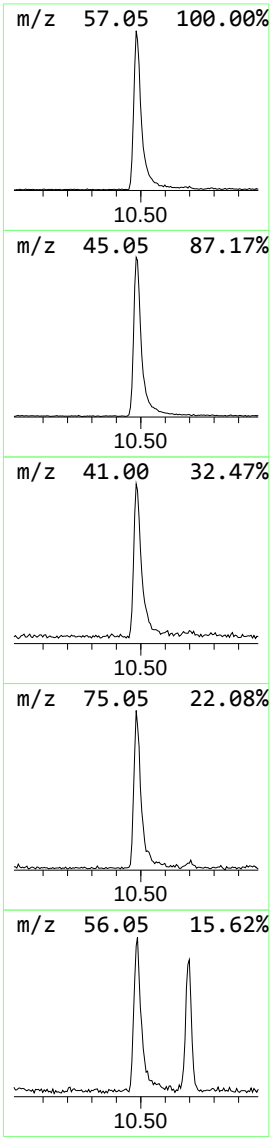
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Ethanol, 1-(2-butoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.481	4.11 ng	425406	Naphthalene-d8	10.698

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
2	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
3	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	64
5	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	50





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Data File : BP007107.D
Acq On : 22 Sep 2021 20:19
Operator : CG/JU
Sample : M3687-32
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : A013015

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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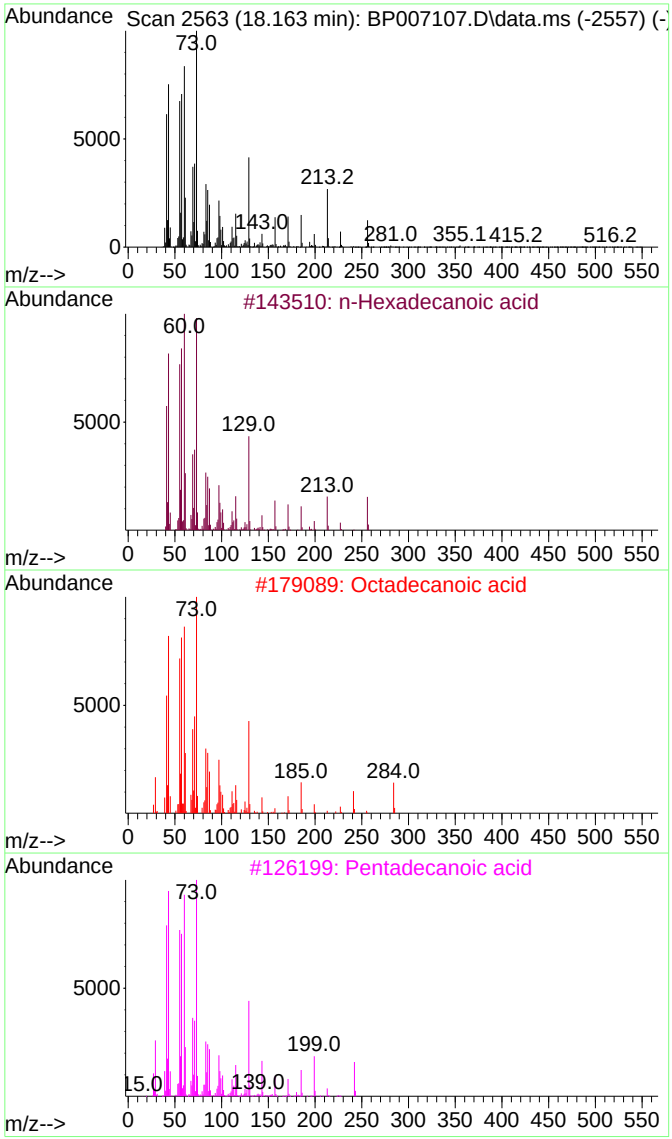
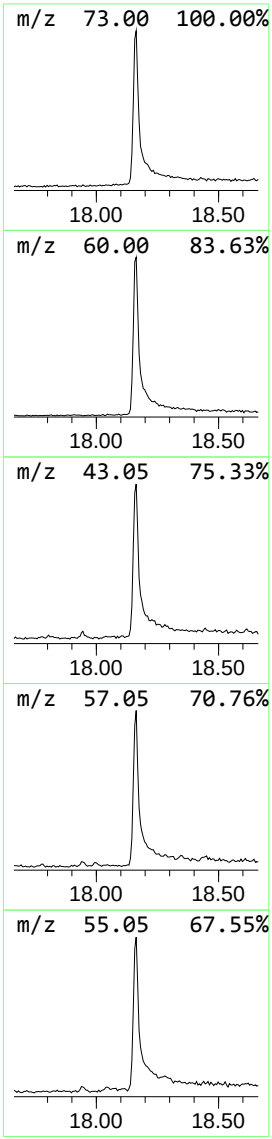
Peak Number 2 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.163	6.85 ng	1071030	Phenanthrene-d10	17.275

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Octadecanoic acid	284	C18H36O2	000057-11-4	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4	Tridecanoic acid	214	C13H26O2	000638-53-9	91
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	89





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092221\
Data File : BP007107.D
Acq On : 22 Sep 2021 20:19
Operator : CG/JU
Sample : M3687-32
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : A013015

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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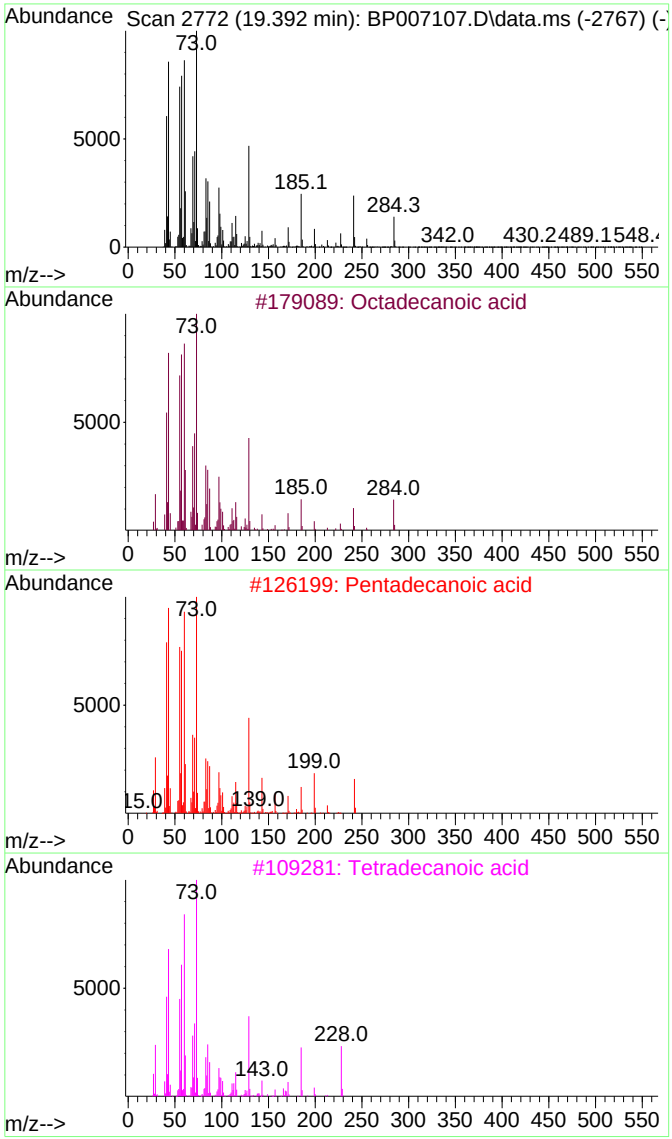
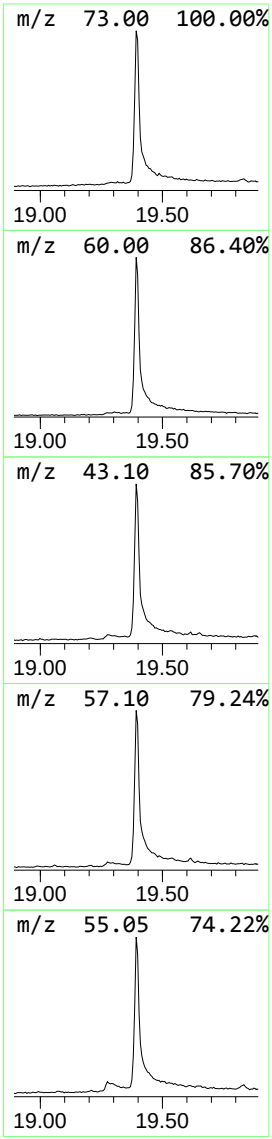
Peak Number 3 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.392	19.32 ng	3128680	Chrysene-d12	21.357

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
5	Tridecanoic acid	214	C13H26O2	000638-53-9	76





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092221\
Data File : BP007107.D
Acq On : 22 Sep 2021 20:19
Operator : CG/JU
Sample : M3687-32
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : A013015

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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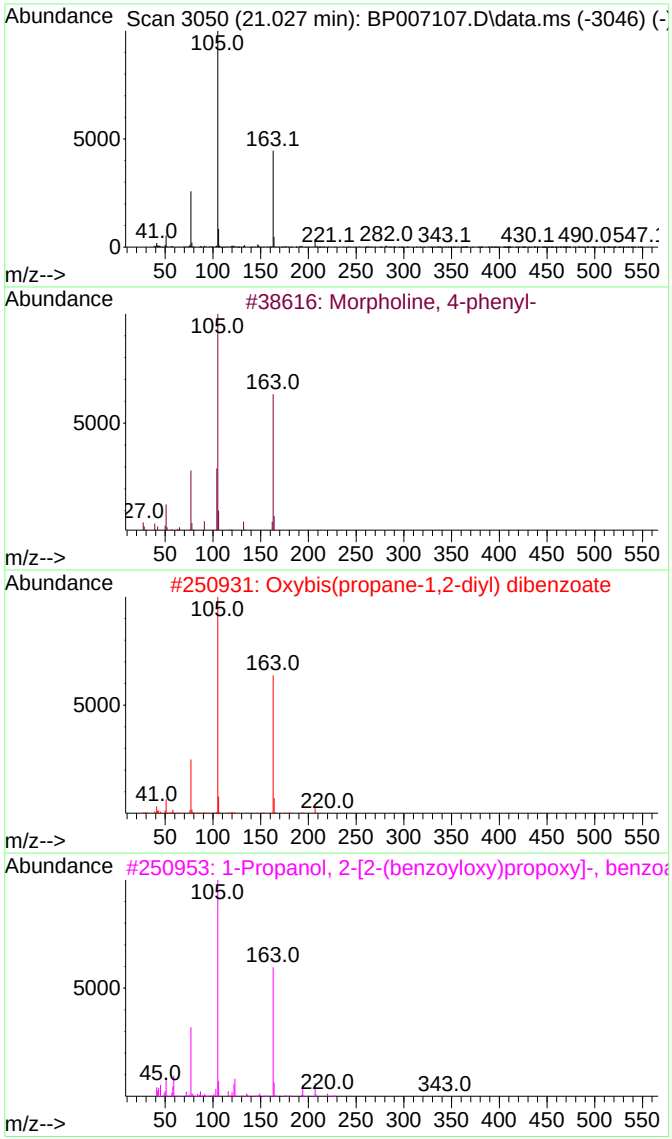
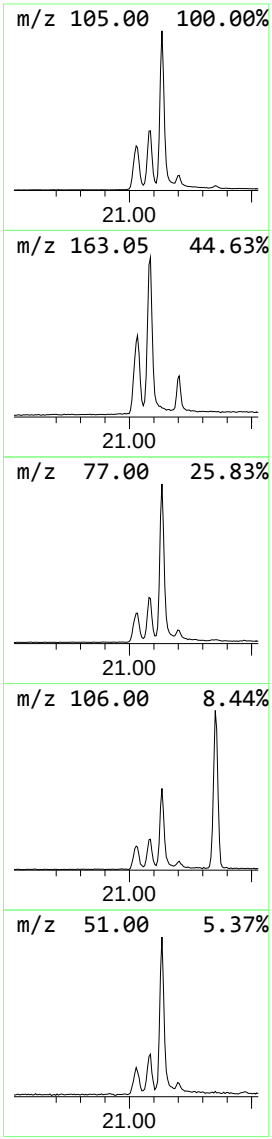
Peak Number 4 Morpholine, 4-phenyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.027	2.82 ng	456996	Chrysene-d12	21.357

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	72
2	Oxybis(propane-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	72
3	1-Propanol, 2-[2-(benzoyloxy)pro...	342	C20H22O5	020109-39-1	50
4	Benzenepropanamide, .alpha.-(ben...	284	C16H16N2O3	058690-81-6	38
5	Benzoic acid, 2-benzyloxy-3-brom...	348	C17H17BrO3	1000191-33-3	37





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092221\
Data File : BP007107.D
Acq On : 22 Sep 2021 20:19
Operator : CG/JU
Sample : M3687-32
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : A013015

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

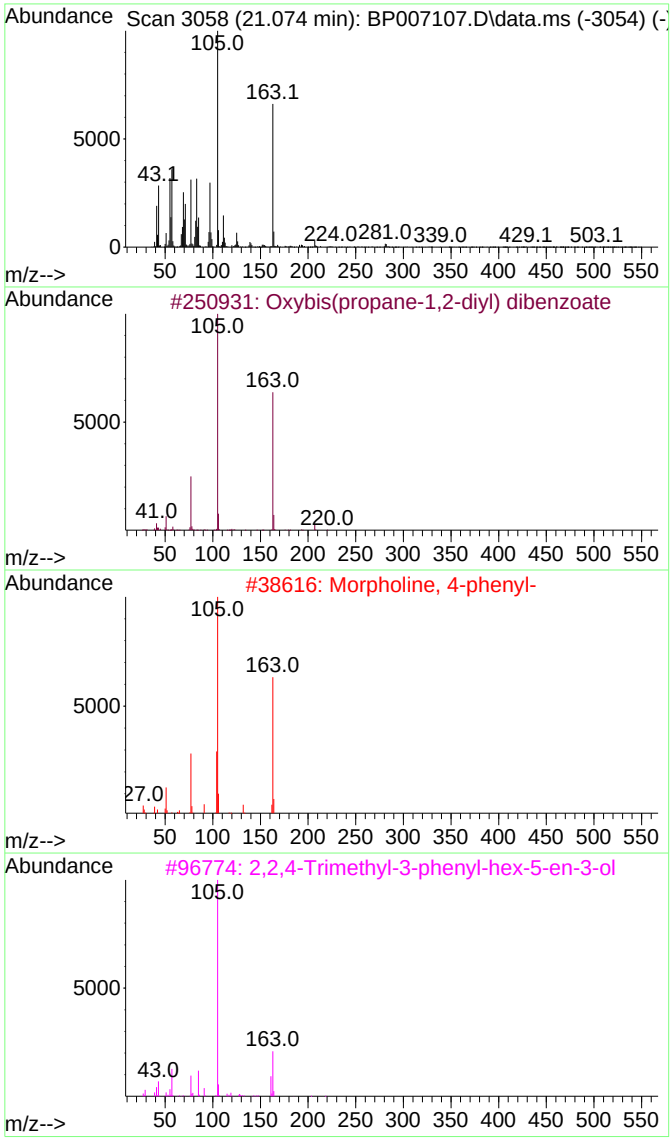
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

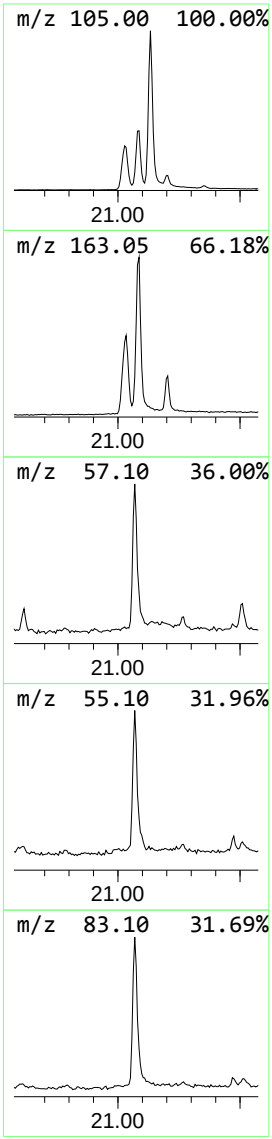
****

Peak Number 5 unknown21.074 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.074	7.66 ng	1240620	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	38
2	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	35
3	2,2,4-Trimethyl-3-phenyl-hex-5-e...	218	C15H22O	066534-36-9	35
4	(3-Phenyloxiran-2-yl)methyl benz...	254	C16H14O3	1000366-96-1	17
5	Succinic acid, nonyl 2,3,4,5-tet...	406	C20H26F4O4	1000381-61-9	16





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Operator : CG/JU
Sample : M3687-32
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A013015

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

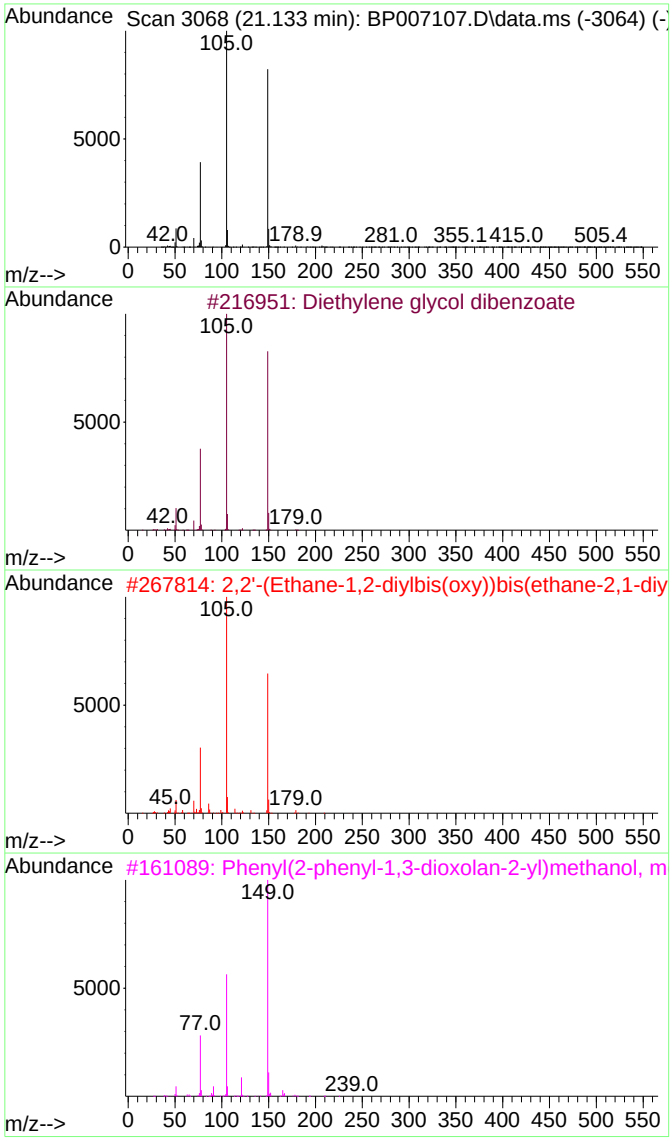
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

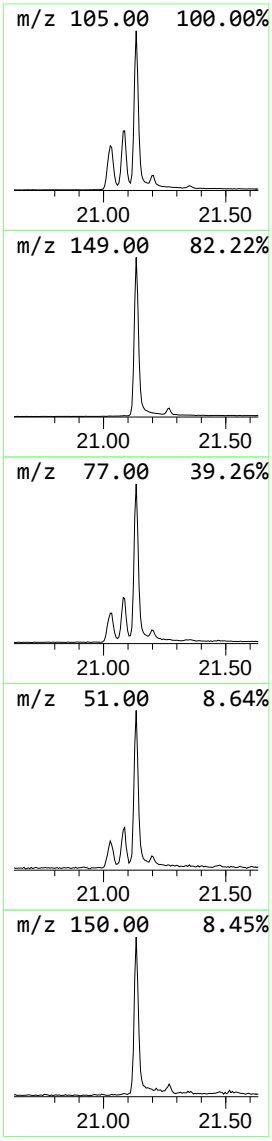
****

Peak Number 6 Diethylene glycol dibenzoate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.133	9.41 ng	1522710	Chrysene-d12	21.357

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	91
2	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	83
3	Phenyl(2-phenyl-1,3-dioxolan-2-y...	270	C17H18O3	1000507-07-6	78
4	Phenyl(2-phenyl-1,3-dioxolan-2-y...	256	C16H16O3	005694-69-9	78
5	2-(2-(2-Methoxyethoxy)ethoxy)eth...	268	C14H20O5	1000366-99-1	74





Tentatively Identified Compound (LSC) summary

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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
Ethanol, 1-(2-b...	10.481	4.1	ng	425406	2	10.698	2069430	20.0
n-Hexadecanoic ...	18.163	6.8	ng	1071030	4	17.275	3126340	20.0
Octadecanoic acid	19.392	19.3	ng	3128680	5	21.357	3238020	20.0
Morpholine, 4-p...	21.027	2.8	ng	456996	5	21.357	3238020	20.0
unknown21.074	21.074	7.7	ng	1240620	5	21.357	3238020	20.0
Diethylene glyc...	21.133	9.4	ng	1522710	5	21.357	3238020	20.0