LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092221\
Data File : BP007106.D
Acq On : 22 Sep 2021 19:44
Operator : CG/JU
Sample : M3687-19
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : A016015

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: BP007106.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	338	rBV	329234	467046	3.37%	0.637%
2	5.470	398	405	419	rBV	4149816	6068638	43.78%	8.272%
3	7.064	668	676	688	rBV	3843029	6135802	44.26%	8.364%
4	7.899	811	818	825	rBV	970893	1508006	10.88%	2.056%
5	9.058	1006	1015	1026	rBV	2420522	3911685	28.22%	5.332%
6	10.481	1251	1257	1268	rBV	210437	434823	3.14%	0.593%
7	10.699	1284	1294	1306	rBV	1262187	2156523	15.56%	2.940%
8	13.152	1702	1711	1719	rBV	6692152	9592809	69.20%	13.076%
9	14.522	1937	1944	1952	rBV	1939481	2910178	20.99%	3.967%
10	16.010	2191	2197	2215	rBV	5125435	7358124	53.08%	10.030%
11	17.275	2405	2412	2417	rBV	2344947	3423867	24.70%	4.667%
12	18.163	2557	2563	2572	rBV	353652	687133	4.96%	0.937%
13	19.281	2748	2753	2761	rBV	281519	458104	3.30%	0.624%
14	19.392	2767	2772	2789	rBV	1126870	2127449	15.35%	2.900%
15	19.634	2809	2813	2823	rVB	272394	416559	3.00%	0.568%
16	19.828	2841	2846	2852	rBV	10934174	13862758	100.00%	18.897%
17	21.033	3046	3051	3054	rBV	301648	521515	3.76%	0.711%
18	21.075	3054	3058	3064	rVV2	822862	1557179	11.23%	2.123%
19	21.133	3064	3068	3076	rVV	1382485	1691725	12.20%	2.306%
20	21.357	3100	3106	3110	rBV	2977145	3954923	28.53%	5.391%
21	23.763	3509	3515	3532	rVB2	1881255	4116224	29.69%	5.611%

Sum of corrected areas: 73361070

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092221\
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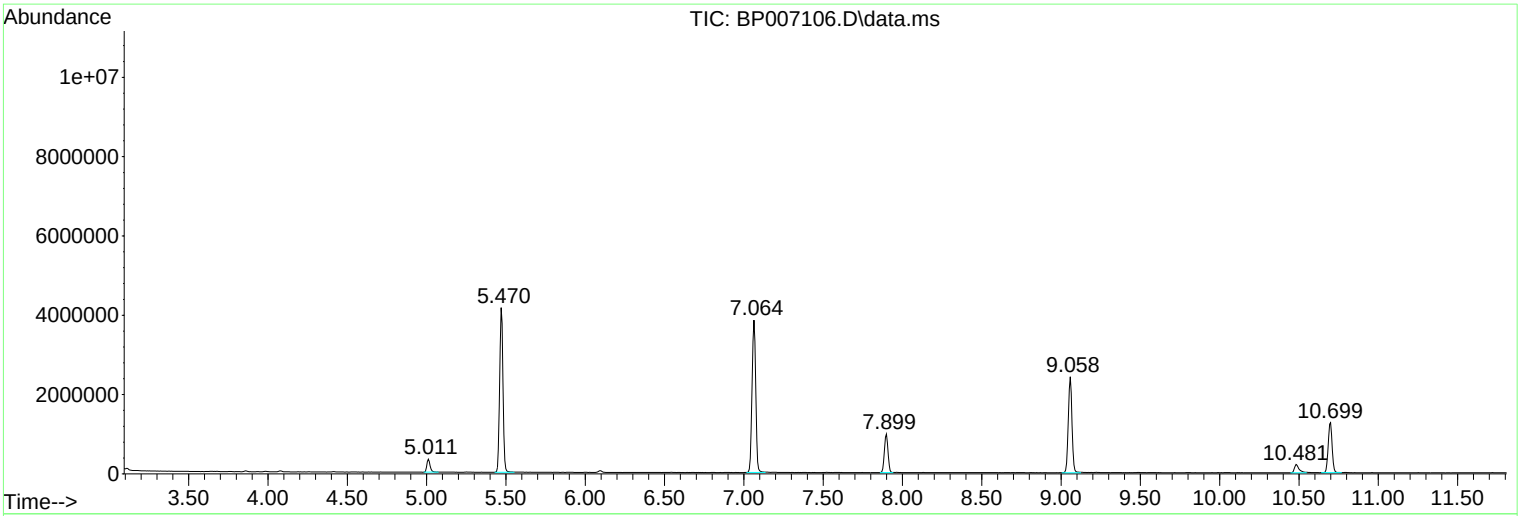
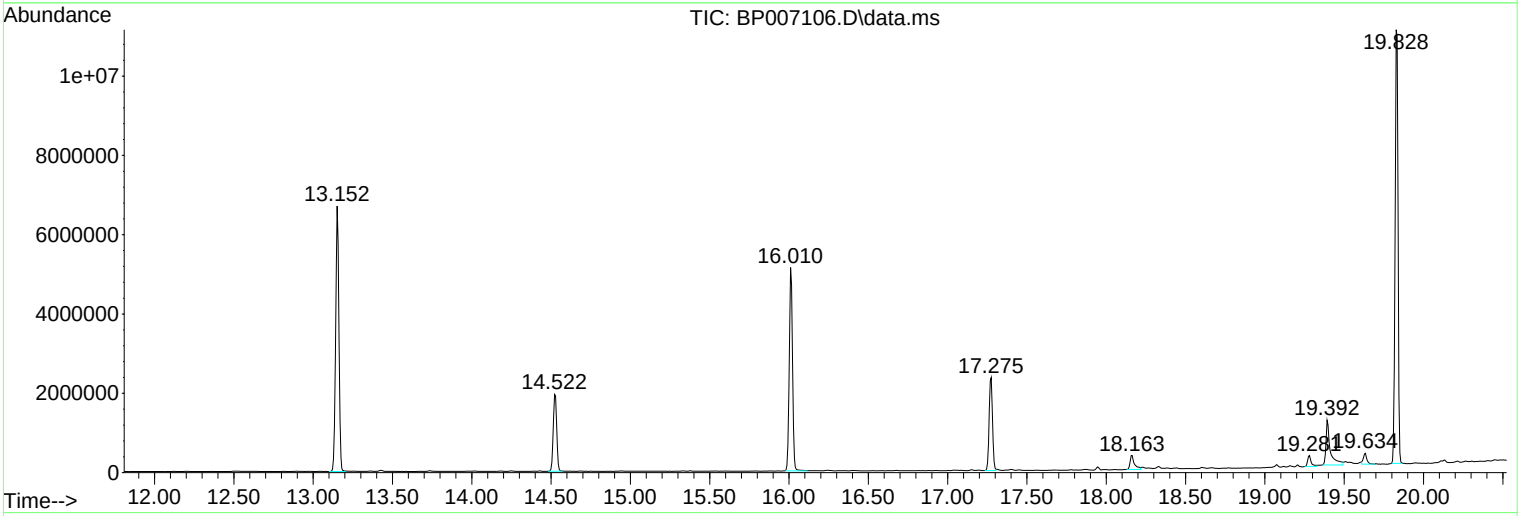
Misc :
ALS Vial : 12 Sample Multiplier: 1

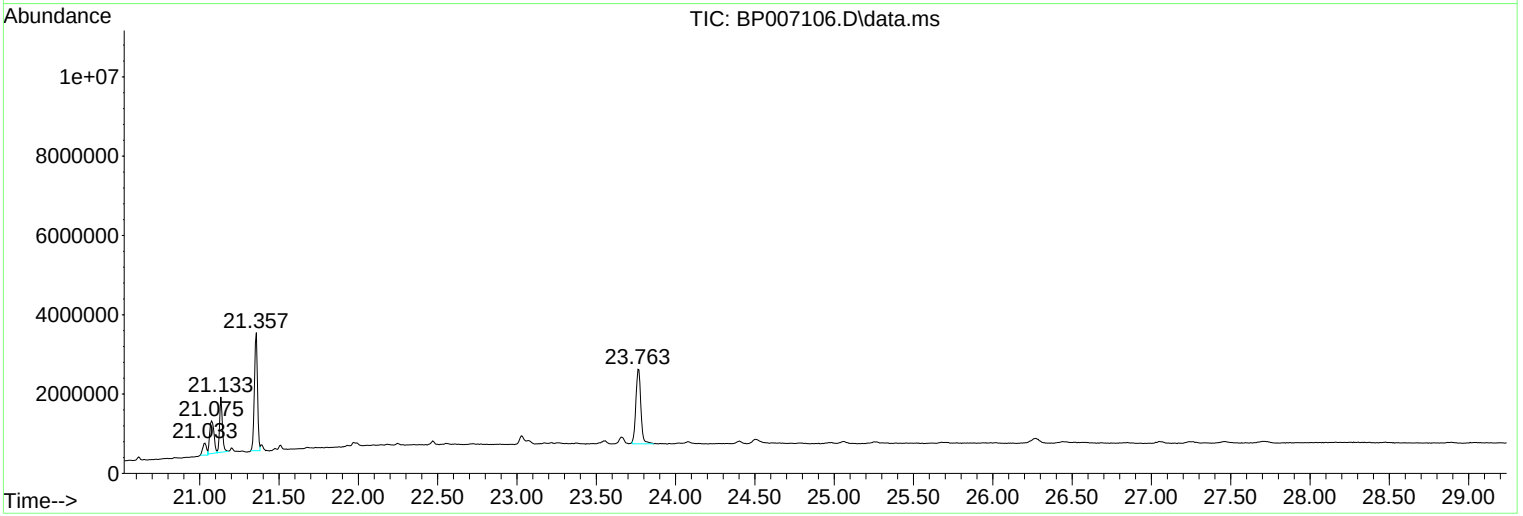
Instrument :
BNA_P
ClientSampleId :
A016015

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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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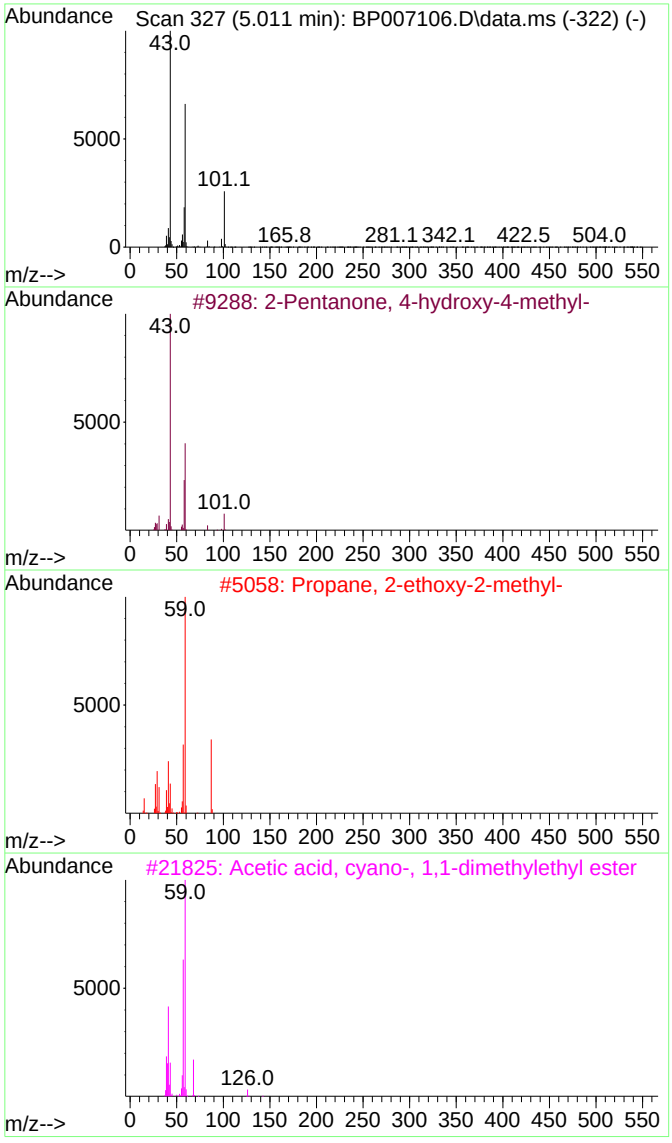
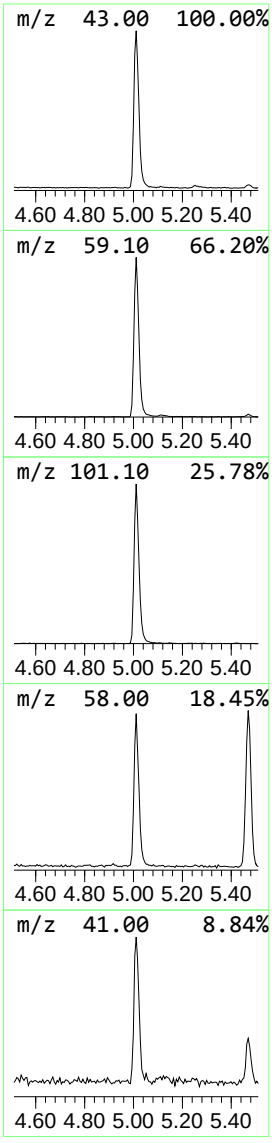
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.011	6.19 ng	467046	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	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	17
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	9





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Operator : CG/JU
Sample : M3687-19
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : A016015

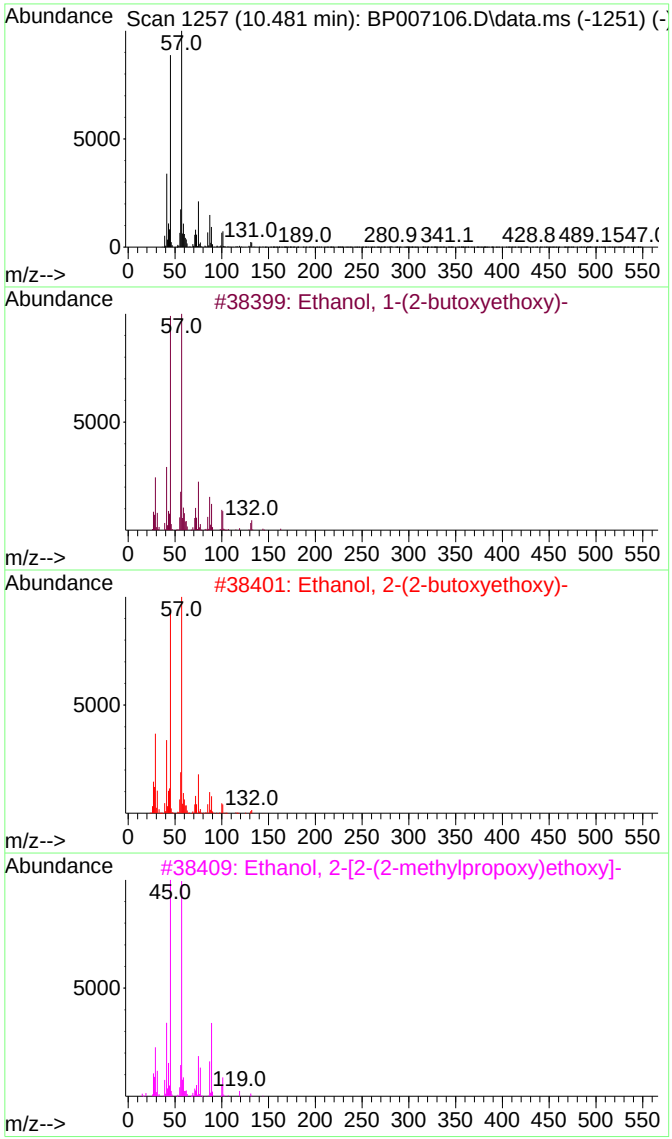
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

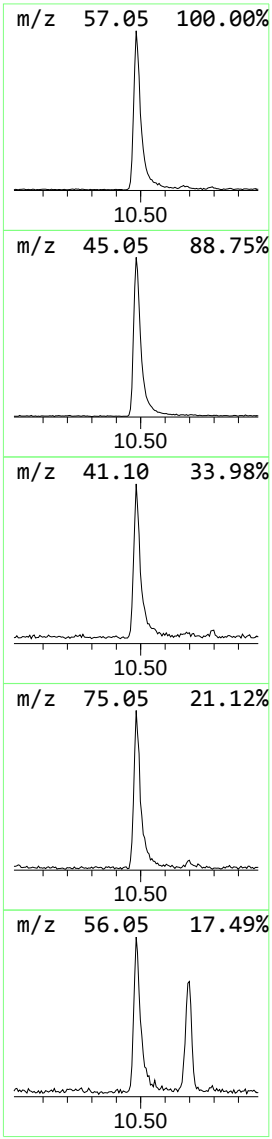
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.481	4.03 ng	434823	Naphthalene-d8	10.699

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	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	78
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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Acq On : 22 Sep 2021 19:44
Operator : CG/JU
Sample : M3687-19
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : A016015

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
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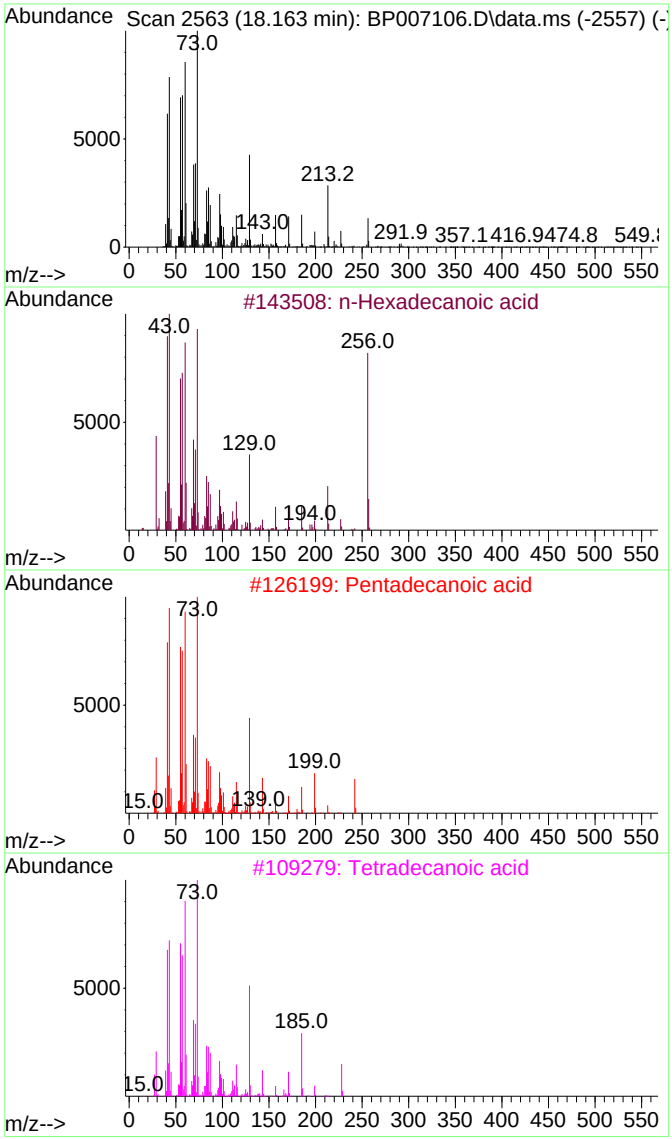
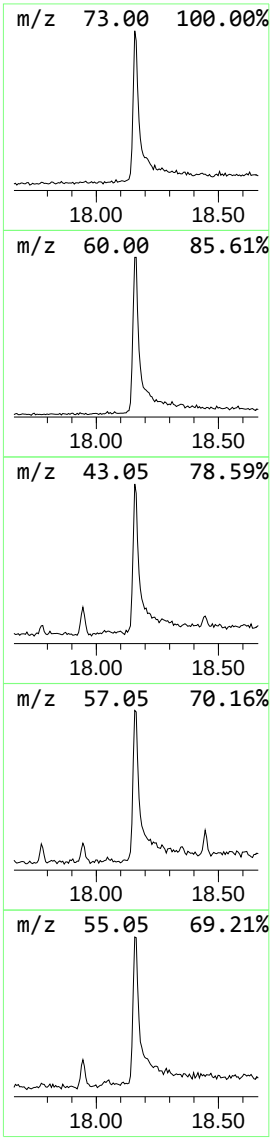
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.163	4.01 ng	687133	Phenanthrene-d10	17.275

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
4	Octadecanoic acid	284	C18H36O2	000057-11-4	90
5	Tridecanoic acid	214	C13H26O2	000638-53-9	87





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Data File : BP007106.D
Acq On : 22 Sep 2021 19:44
Operator : CG/JU
Sample : M3687-19
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A016015

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

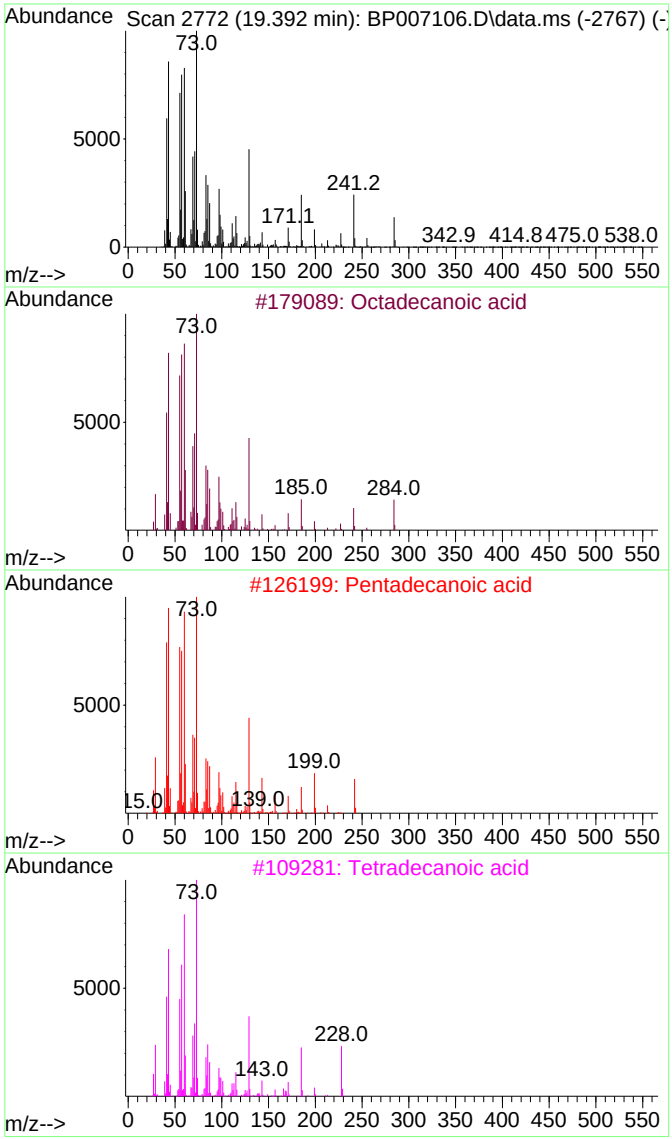
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

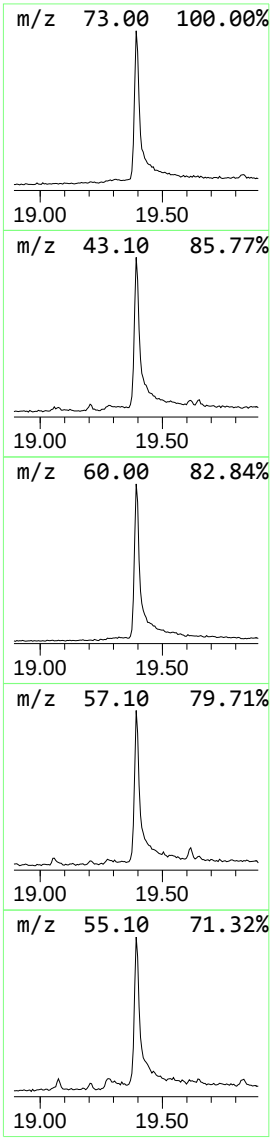
****

Peak Number 5 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.392	10.76 ng	2127450	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	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70





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Data File : BP007106.D
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Operator : CG/JU
Sample : M3687-19
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : A016015

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
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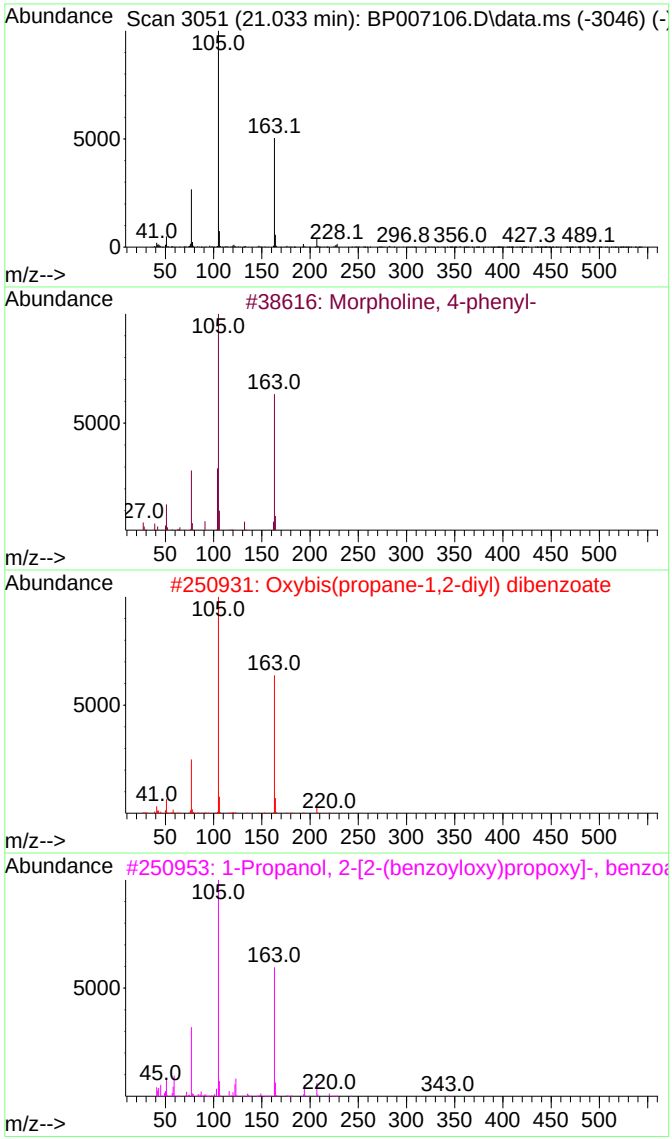
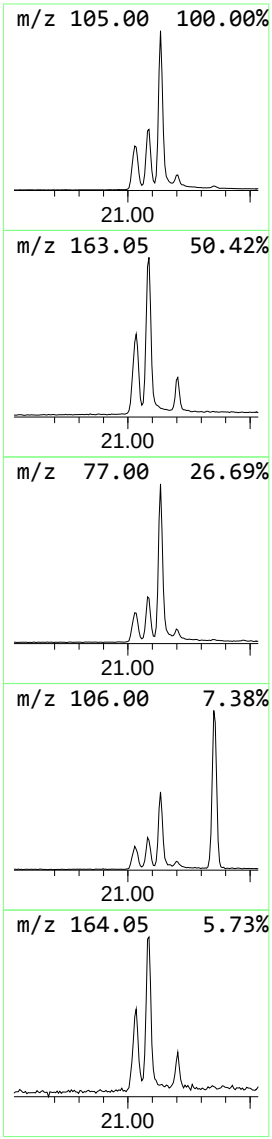
****

Peak Number 7 Morpholine, 4-phenyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.034	2.64 ng	521515	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	59
3	1-Propanol, 2-[2-(benzoyloxy)pro...	342	C20H22O5	020109-39-1	50
4	Glyoxylamide, N-phenyl-	163	C9H9NO2	032331-52-5	47
5	Benzenepropanamide, .alpha.-(ben...	284	C16H16N2O3	058690-81-6	38





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Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : A016015

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

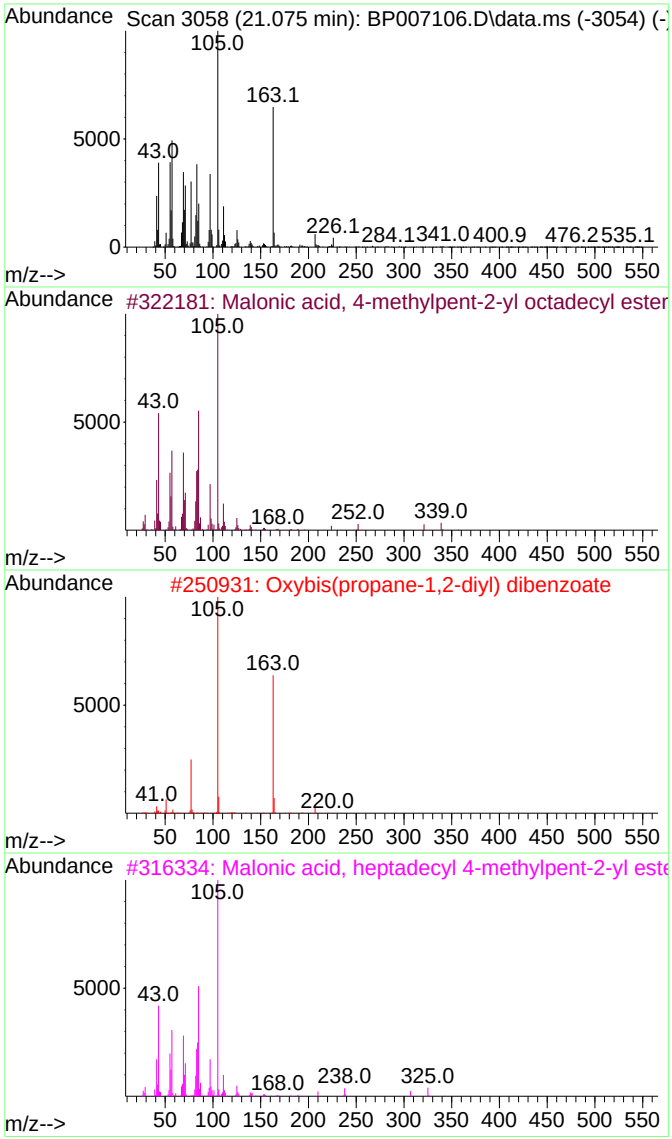
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

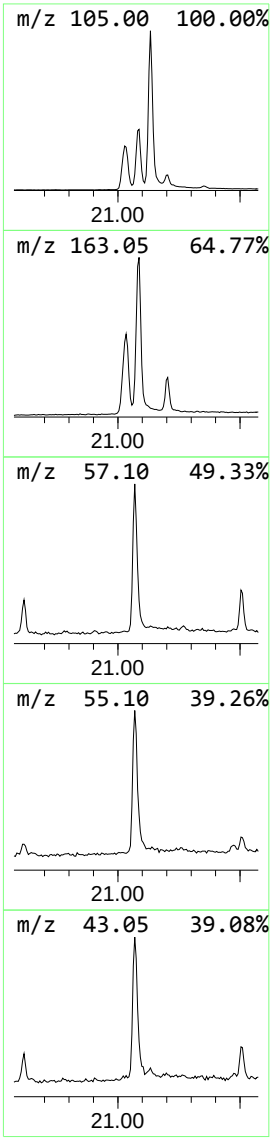
****

Peak Number 8 unknown21.075 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.075	7.87 ng	1557180	Chrysene-d12	21.357

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Malonic acid, 4-methylpent-2-yl ...	440	C27H52O4	1000349-34-5	38
2	Oxybis(propane-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	30
3	Malonic acid, heptadecyl 4-methy...	426	C26H50O4	1000349-34-4	30
4	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	27
5	Malonic acid, 3,3-dimethylbut-2-...	440	C27H52O4	1000348-66-8	27





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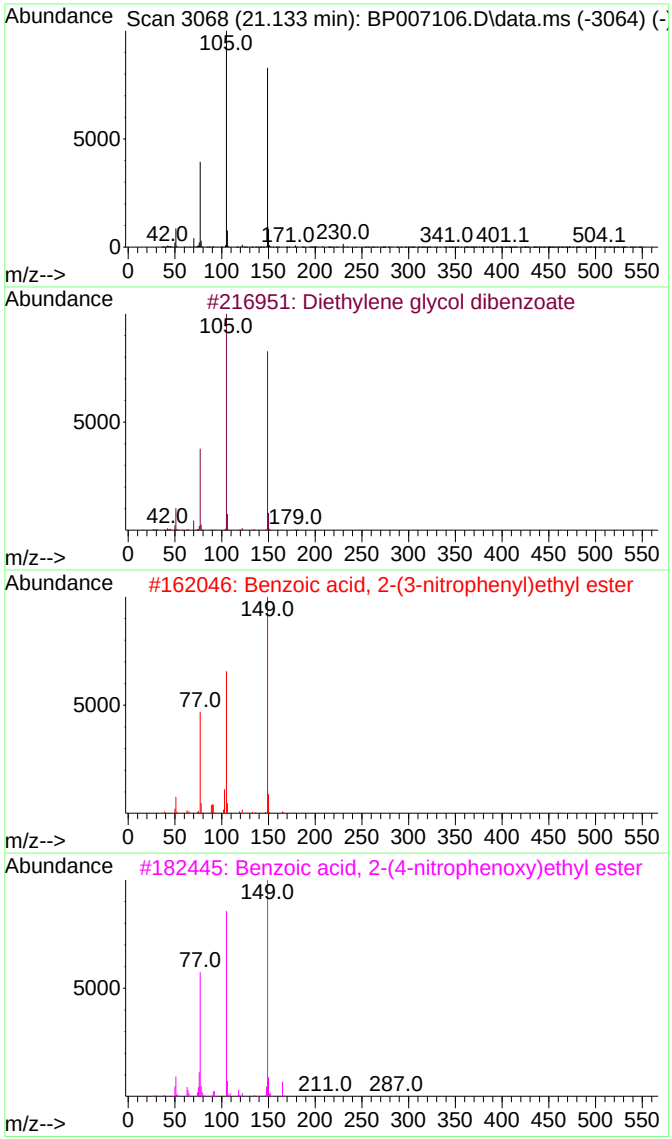
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

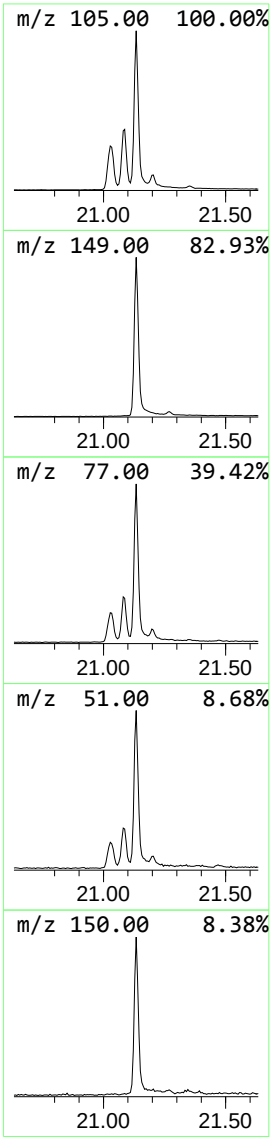
****

Peak Number 9 Diethylene glycol dibenzoate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.134	8.56 ng	1691730	Chrysene-d12	21.357

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	91
2	Benzoic acid, 2-(3-nitrophenyl)e...	271	C15H13NO4	1000368-22-4	78
3	Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	64
4	Phenyl(2-phenyl-1,3-dioxolan-2-y...	298	C18H18O4	006963-16-2	64
5	3,6,9,12-Tetraoxatetradecane-1,1...	446	C24H30O8	1000366-97-0	64





Tentatively Identified Compound (LSC) summary

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					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	5.011	6.2	ng	467046	1	7.899	1508010	20.0
Ethanol, 1-(2-b...	10.481	4.0	ng	434823	2	10.699	2156520	20.0
n-Hexadecanoic ...	18.163	4.0	ng	687133	4	17.275	3423870	20.0
Octadecanoic acid	19.392	10.8	ng	2127450	5	21.357	3954920	20.0
Morpholine, 4-p...	21.034	2.6	ng	521515	5	21.357	3954920	20.0
unknown21.075	21.075	7.9	ng	1557180	5	21.357	3954920	20.0
Diethylene glyc...	21.134	8.6	ng	1691730	5	21.357	3954920	20.0