LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP070921\
Data File : BP006168.D
Acq On : 09 Jul 2021 19:15
Operator : CG/JU
Sample : M2990-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : TP-K

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-BP070721.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP006168.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.981	317	322	334	rVB	68886	110371	1.47%	0.259%
2	5.446	395	401	426	rBV	2353790	3682184	49.07%	8.653%
3	7.058	668	675	696	rBV	2033309	3648877	48.62%	8.575%
4	7.869	806	813	824	rBV	625758	1014251	13.52%	2.383%
5	9.040	1005	1012	1032	rBV	1238402	2265572	30.19%	5.324%
6	10.475	1249	1256	1274	rBV	193579	544820	7.26%	1.280%
7	10.675	1282	1290	1306	rVB	757648	1355454	18.06%	3.185%
8	13.134	1701	1708	1730	rBV	3478247	5283542	70.40%	12.416%
9	14.510	1936	1942	1962	rVB	1169462	1774692	23.65%	4.170%
10	16.004	2190	2196	2221	rBV	2519106	3841727	51.19%	9.028%
11	17.263	2403	2410	2424	rBV	1285549	2010207	26.79%	4.724%
12	18.145	2556	2560	2568	rBV2	66465	119708	1.60%	0.281%
13	19.816	2838	2844	2851	rBV	6318224	7504503	100.00%	17.635%
14	21.010	3042	3047	3050	rBV	432985	722385	9.63%	1.698%
15	21.063	3050	3056	3061	rVV	687274	1182485	15.76%	2.779%
16	21.116	3061	3065	3073	rVV	2039661	2536201	33.80%	5.960%
17	21.180	3074	3076	3084	rVB2	140404	238652	3.18%	0.561%
18	21.345	3099	3104	3109	rBV	1584932	2198508	29.30%	5.166%
19	23.739	3505	3511	3525	rVB2	1185206	2519947	33.58%	5.922%

Sum of corrected areas: 42554086

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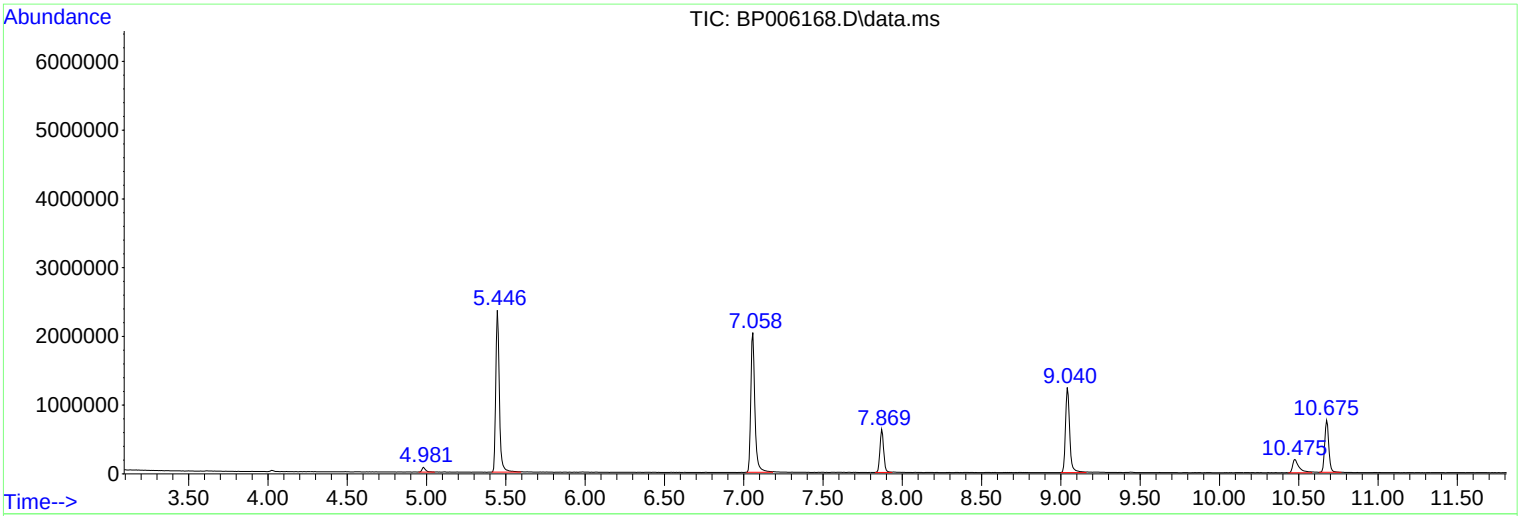
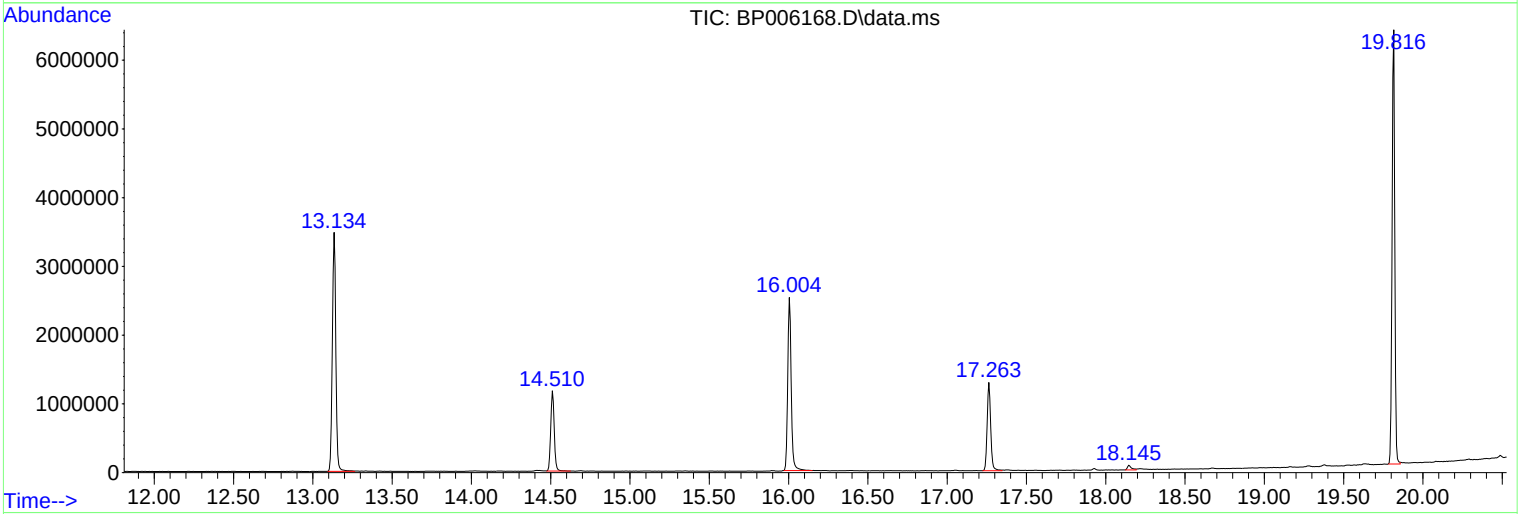
Misc :
ALS Vial : 12 Sample Multiplier: 1

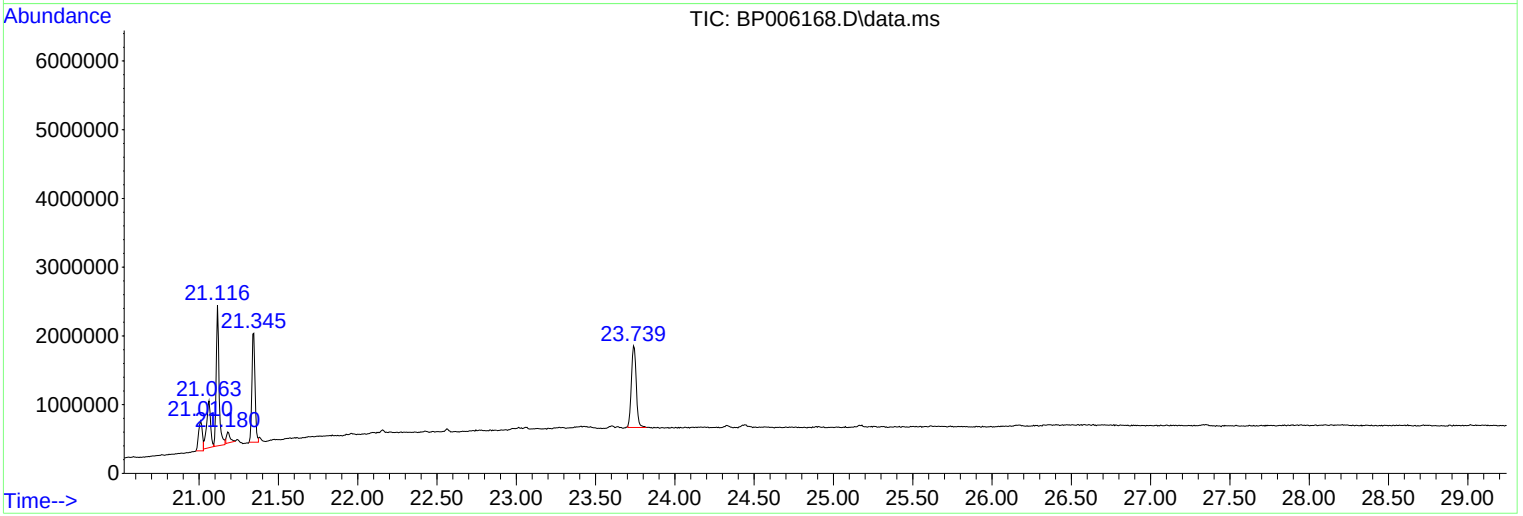
Instrument :
BNA_P
ClientSampleId :
TP-K

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P







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Operator : CG/JU
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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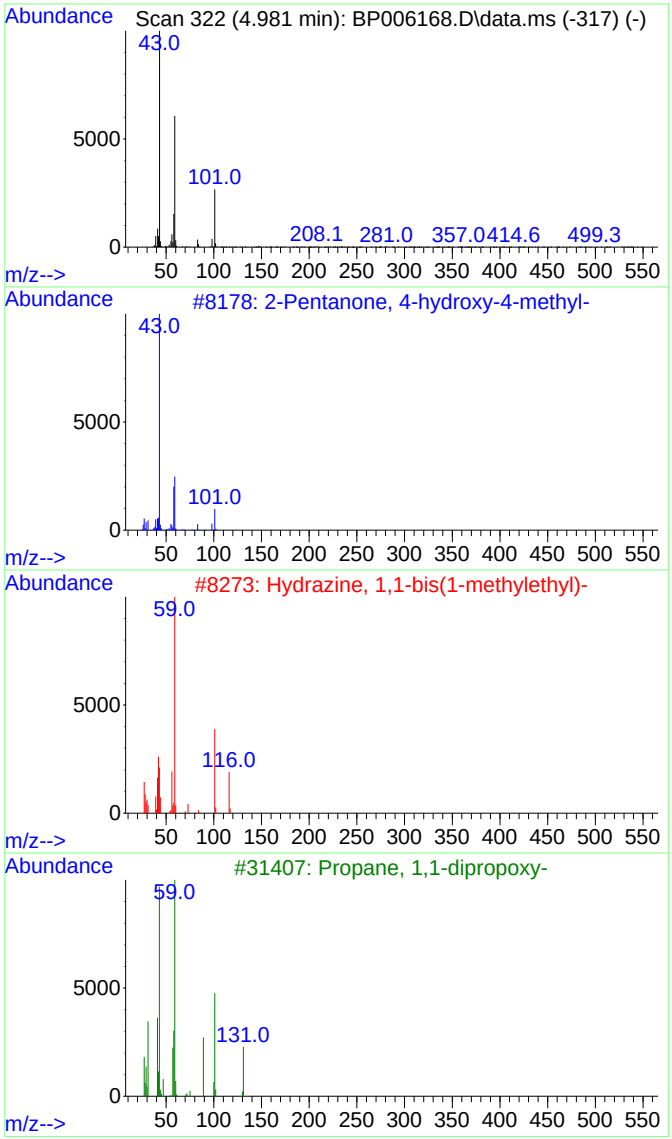
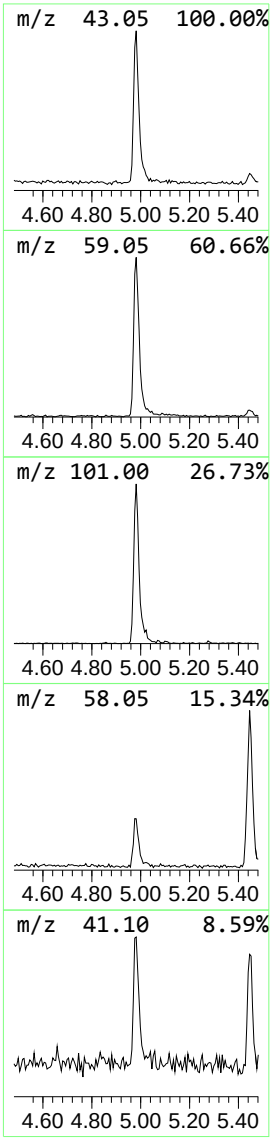
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.981	2.18 ng	110371	1,4-Dichlorobenzene-d4	7.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	38
3	Propane, 1,1-dipropoxy-	160	C9H20O2	004744-11-0	38
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	32
5	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	23





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Acq On : 09 Jul 2021 19:15
Operator : CG/JU
Sample : M2990-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : TP-K

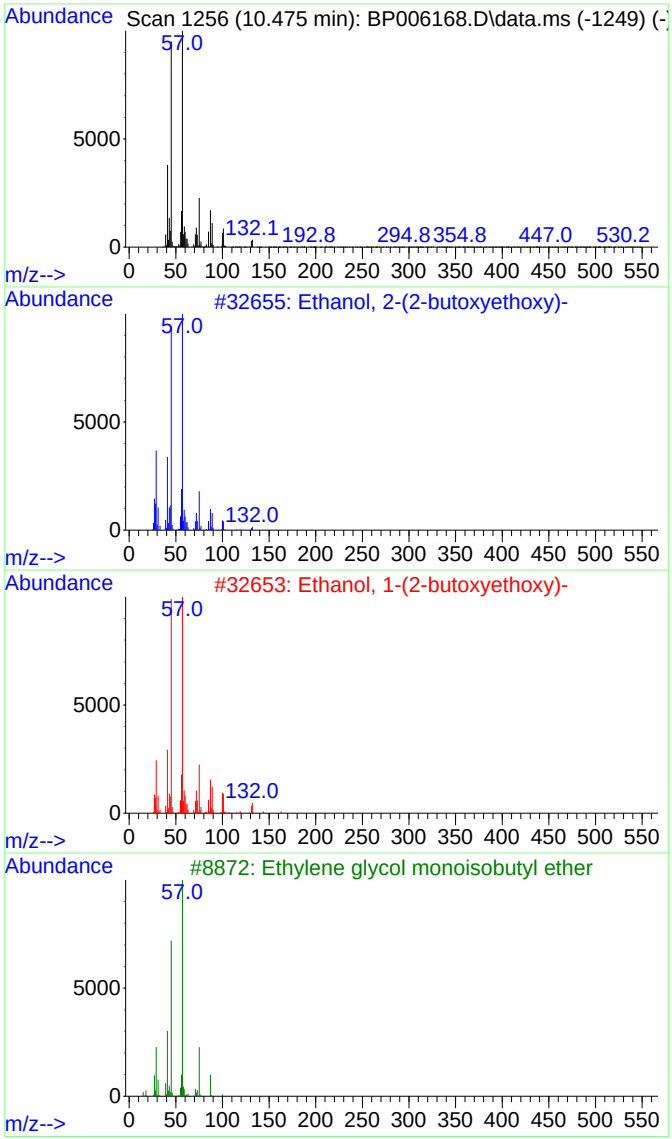
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

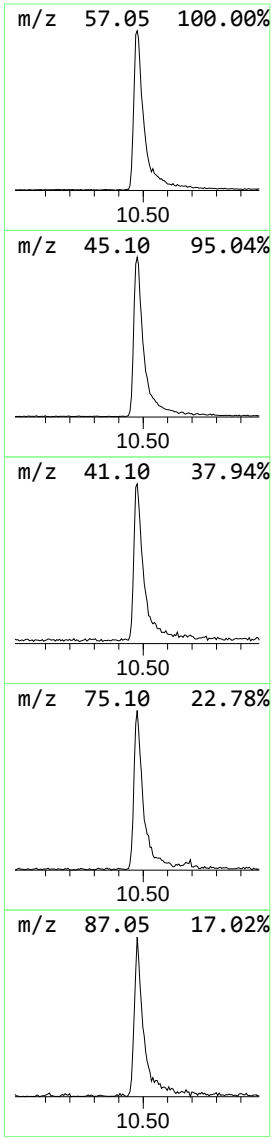
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.475	8.04 ng	544820	Naphthalene-d8	10.675

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	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
4	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	50
5	Tetraethylene glycol	194	C8H18O5	000112-60-7	47





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Data File : BP006168.D
Acq On : 09 Jul 2021 19:15
Operator : CG/JU
Sample : M2990-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : TP-K

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

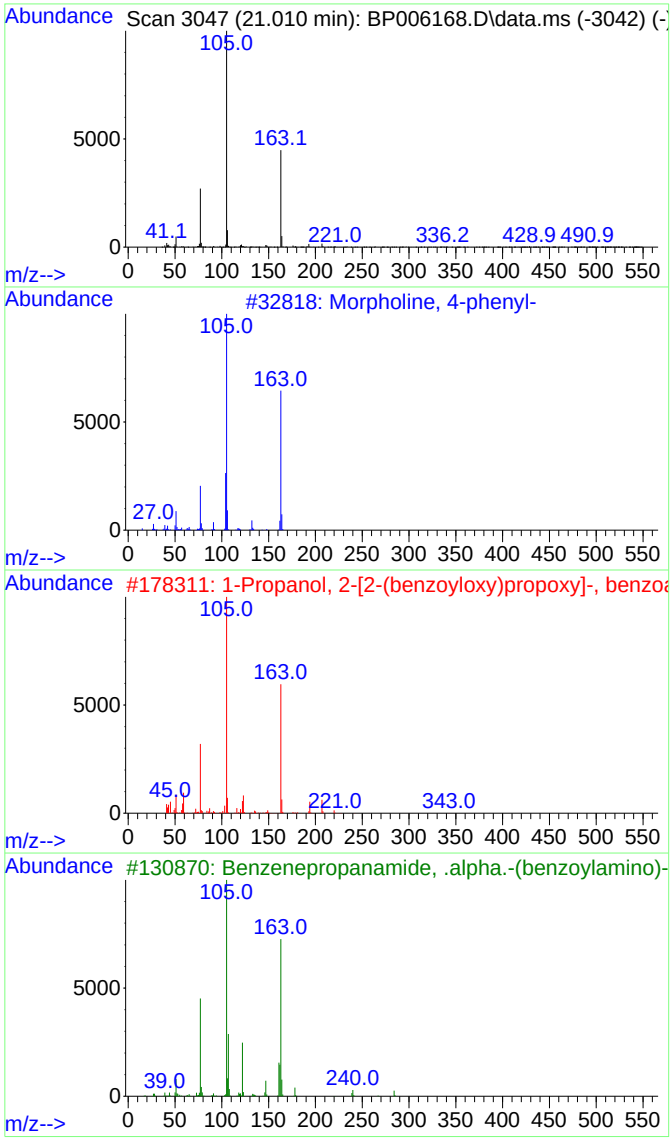
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

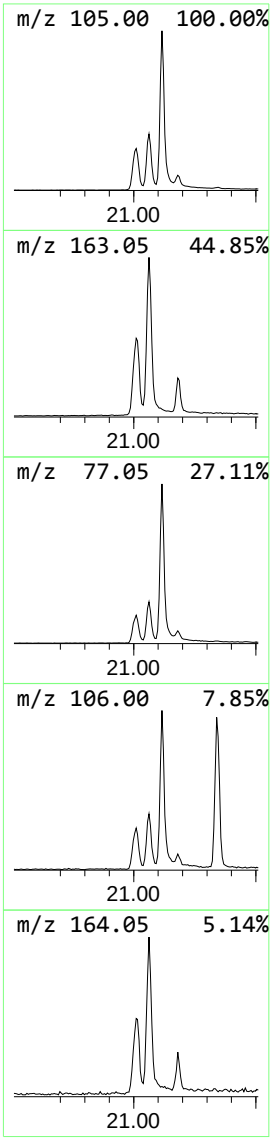
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.010	6.57 ng	722385	Chrysene-d12	21.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	56
2	1-Propanol, 2-[2-(benzoyloxy)pro...	342	C20H22O5	020109-39-1	40
3	Benzenepropanamide, .alpha.-(ben...	284	C16H16N2O3	058690-81-6	38
4	Benzoic acid, 2-benzyloxy-3-brom...	348	C17H17BrO3	1000191-33-3	25
5	1-Benzoyl-2-trichloroacetylhydra...	280	C9H7Cl3N2O2	090273-66-8	17





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Data File : BP006168.D
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Operator : CG/JU
Sample : M2990-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : TP-K

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

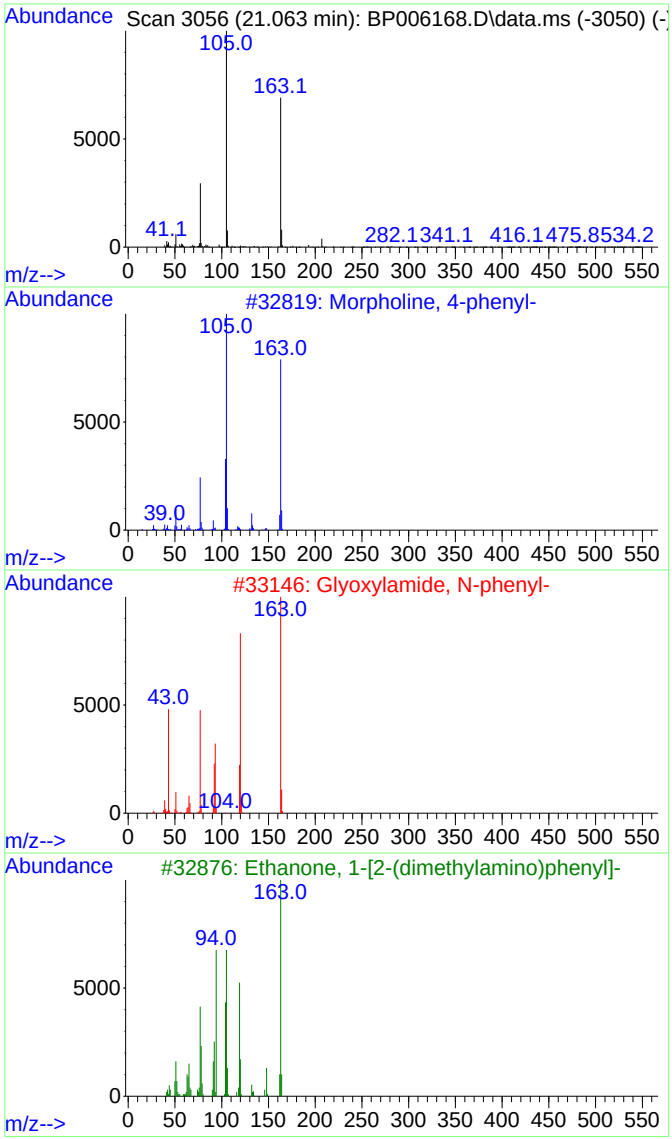
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

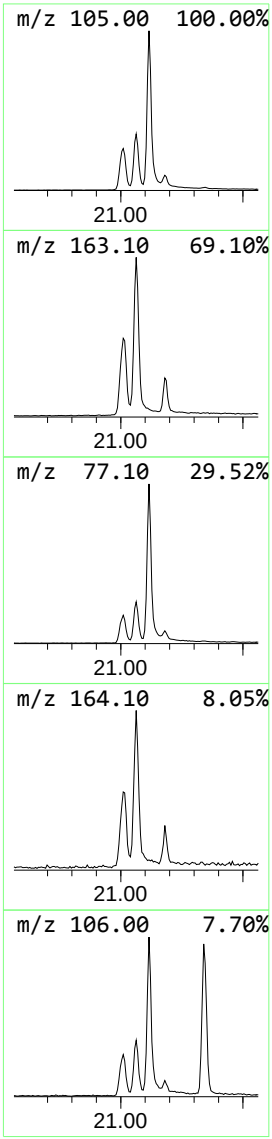
****

Peak Number 4 unknown21.063 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.063	10.76 ng	1182490	Chrysene-d12	21.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	56
2	Glyoxylamide, N-phenyl-	163	C9H9NO2	032331-52-5	47
3	Ethanone, 1-[2-(dimethylamino)ph...	163	C10H13NO	010336-55-7	45
4	.delta.2-1,3,4-Oxadiazolin-5-one...	163	C7H5N3O2	002845-82-1	38
5	Phthalic acid, 4-fluoro-2-nitrop...	319	C15H10FNO6	1000315-63-4	17





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Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-K

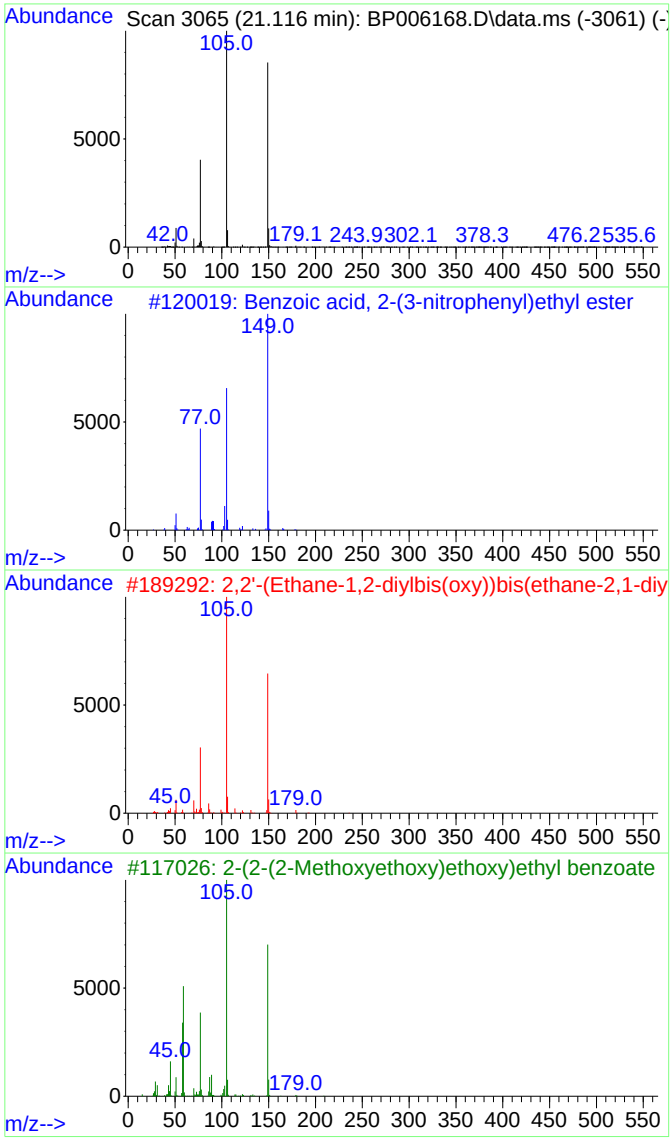
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

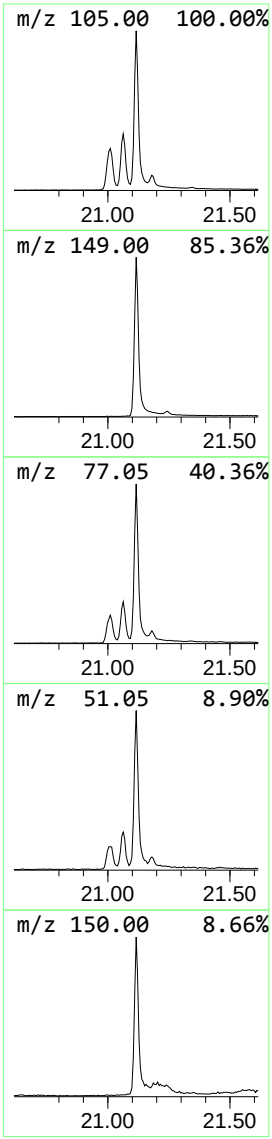
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzoic acid, 2-(3-nitrophe... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.116	23.07 ng	2536200	Chrysene-d12	21.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 2-(3-nitrophenyl)e...	271	C15H13NO4	1000368-22-4	78
2	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	74
3	2-(2-(2-Methoxyethoxy)ethoxy)eth...	268	C14H20O5	1000366-99-1	74
4	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	74
5	Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	64





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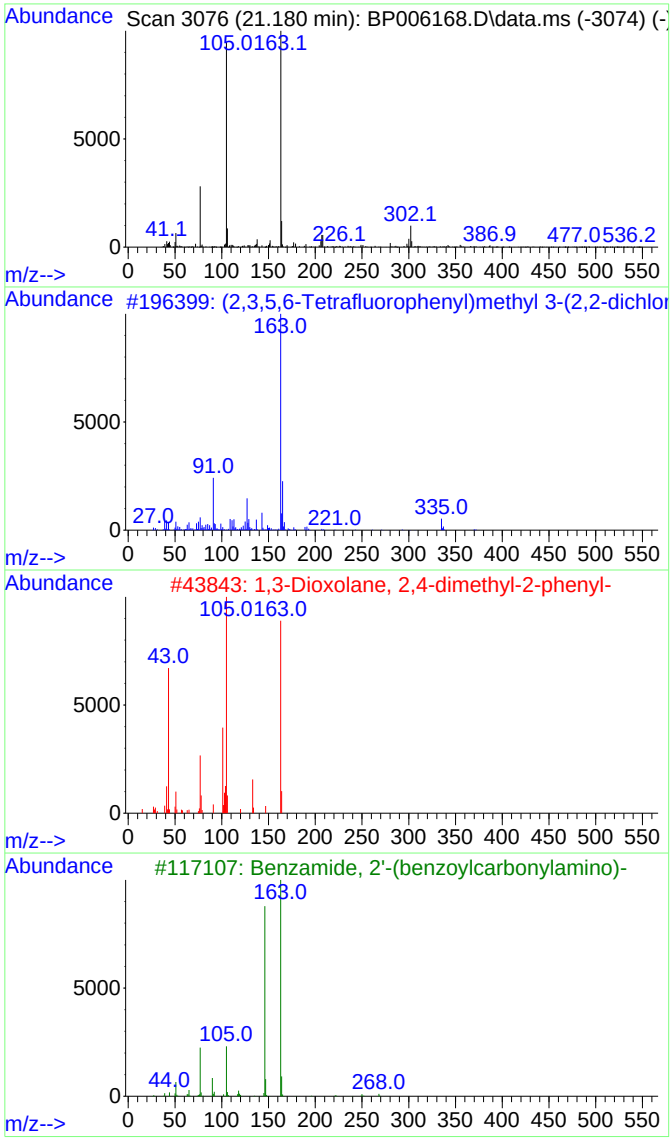
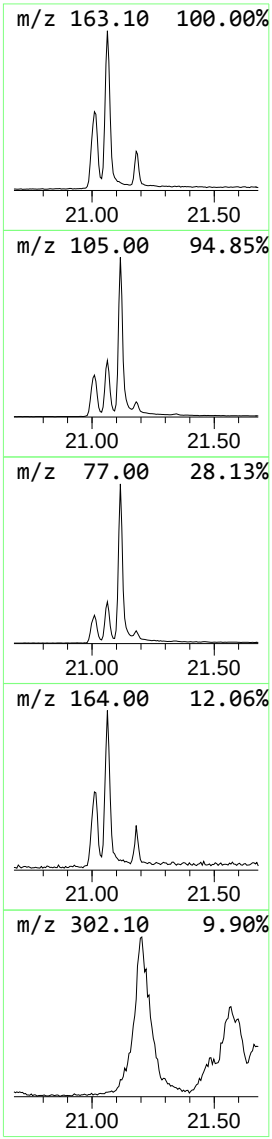
****

Peak Number 6 unknown21.180 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.180	2.17 ng	238652	Chrysene-d12	21.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(2,3,5,6-Tetrafluorophenyl)methy...	370	C15H12Cl2F4O2	118712-89-3	43
2	1,3-Dioxolane, 2,4-dimethyl-2-ph...	178	C11H14O2	004359-30-2	39
3	Benzamide, 2'-(benzoylcarbonylam...	268	C15H12N2O3	129768-51-0	39
4	Phthalic acid, 2,6-dimethoxyphen...	316	C17H16O6	1000315-74-1	38
5	Phthalic acid, 3,5-dimethylpheny...	284	C17H16O4	1000315-70-8	28





Tentatively Identified Compound (LSC) summary

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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	4.981	2.2	ng	110371	1	7.869	1014250	20.0
Ethanol, 2-(2-b...	10.475	8.0	ng	544820	2	10.675	1355450	20.0
Morpholine, 4-p...	21.010	6.6	ng	722385	5	21.345	2198510	20.0
unknown21.063	21.063	10.8	ng	1182490	5	21.345	2198510	20.0
Benzoic acid, 2...	21.116	23.1	ng	2536200	5	21.345	2198510	20.0
unknown21.180	21.180	2.2	ng	238652	5	21.345	2198510	20.0