LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP070821\
Data File : BP006141.D
Acq On : 08 Jul 2021 15:53
Operator : CG/JU
Sample : M2963-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : MH-1A-COMP

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: BP006141.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.987	318	323	332	rBV	76870	117817	1.32%	0.234%
2	5.452	396	402	422	rBV	3603659	5515810	62.00%	10.970%
3	7.063	669	676	701	rBV	3086058	5303512	59.62%	10.548%
4	7.875	807	814	825	rBV	673093	1084354	12.19%	2.157%
5	9.046	1005	1013	1035	rBV	1909425	3369301	37.87%	6.701%
6	10.481	1247	1257	1271	rBV	165782	475354	5.34%	0.945%
7	10.681	1283	1291	1304	rBV	756741	1392669	15.65%	2.770%
8	13.140	1701	1709	1729	rBV	4630103	7095946	79.76%	14.113%
9	14.510	1936	1942	1956	rVB	1028731	1616912	18.18%	3.216%
10	15.263	2065	2070	2079	rBV	67223	119835	1.35%	0.238%
11	16.004	2188	2196	2217	rBV	3145068	4902343	55.11%	9.750%
12	17.263	2404	2410	2418	rBV	1115244	1736164	19.52%	3.453%
13	18.145	2556	2560	2565	rBV	135676	210701	2.37%	0.419%
14	19.375	2766	2769	2773	rBV4	59171	93519	1.05%	0.186%
15	19.816	2838	2844	2849	rBV	7558596	8896203	100.00%	17.693%
16	21.010	3043	3047	3050	rBV	184336	305191	3.43%	0.607%
17	21.063	3050	3056	3061	rVV2	382819	828573	9.31%	1.648%
18	21.116	3061	3065	3074	rVB	741808	1027220	11.55%	2.043%
19	21.345	3099	3104	3109	rBV	1403198	1902183	21.38%	3.783%
20	22.427	3283	3288	3299	rVB	1262860	1896787	21.32%	3.772%
21	23.739	3505	3511	3524	rVB2	1140465	2389362	26.86%	4.752%

Sum of corrected areas: 50279756

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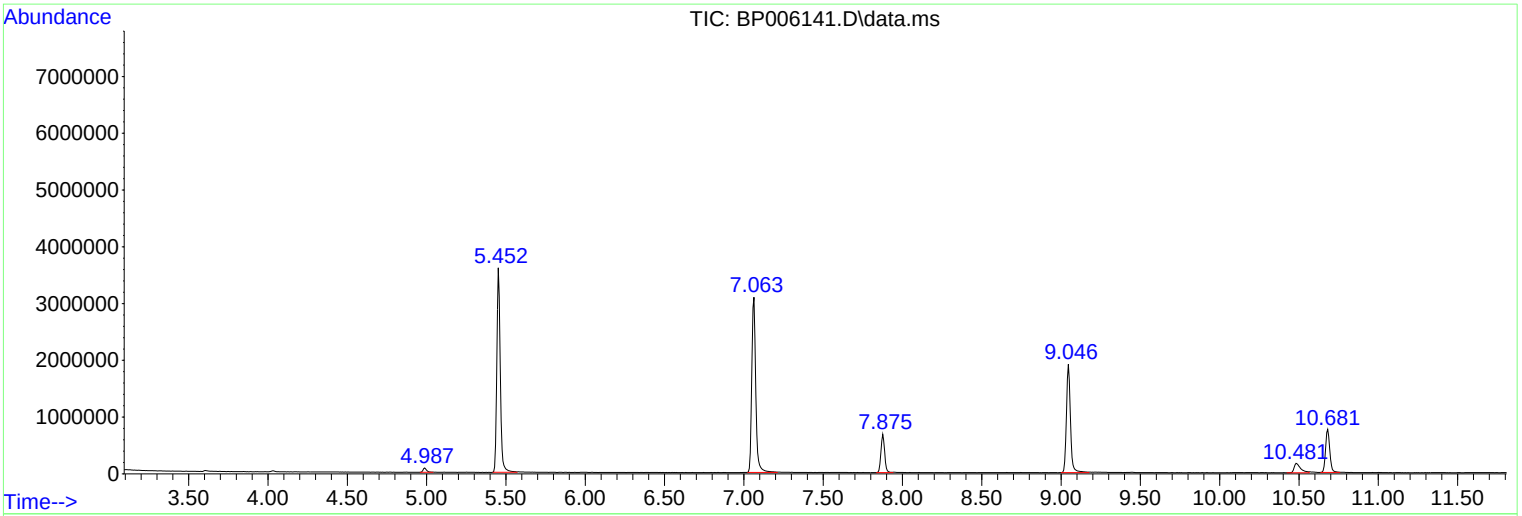
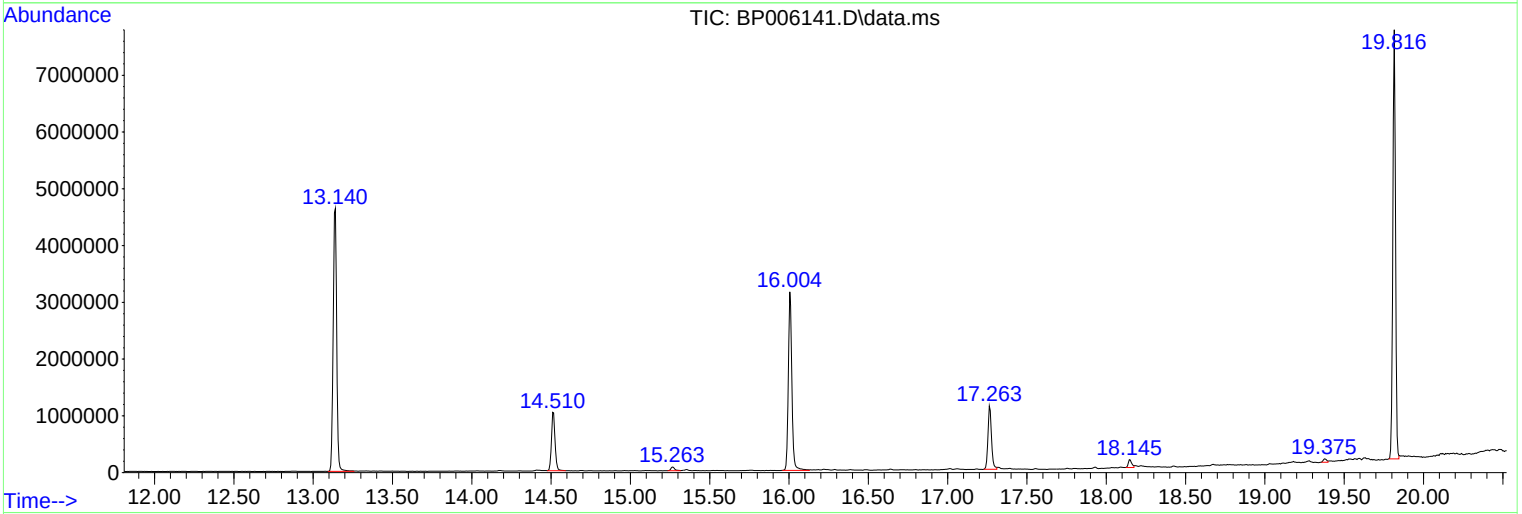
Misc :
ALS Vial : 6 Sample Multiplier: 1

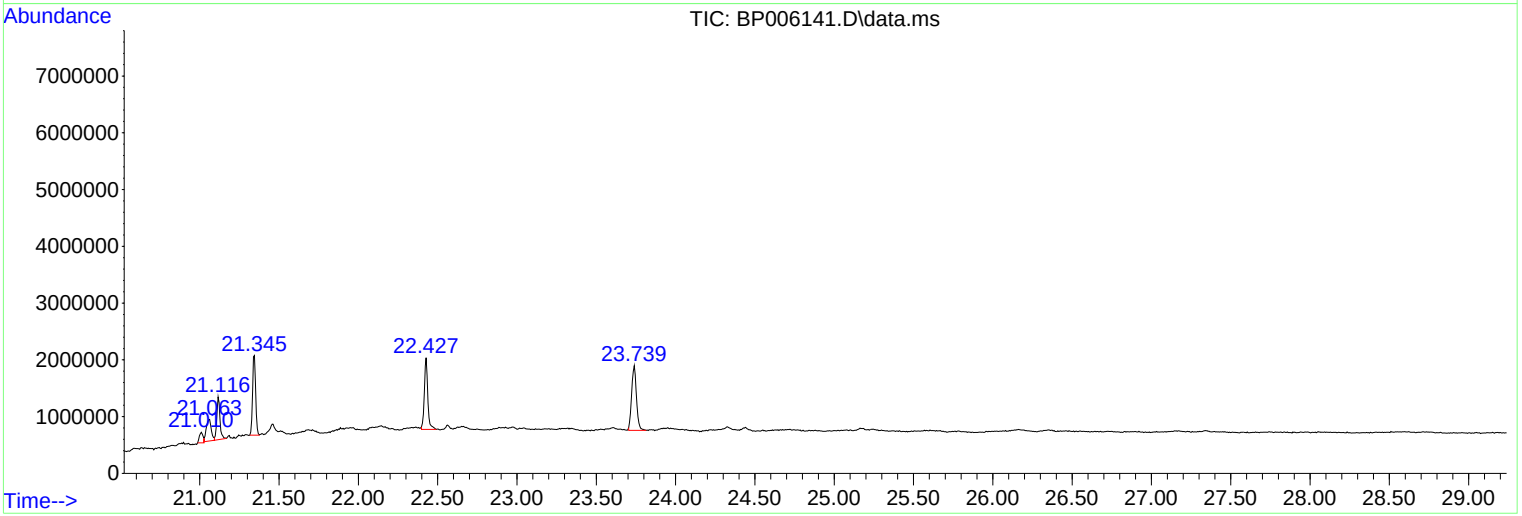
Instrument :
BNA_P
ClientSampleId :
MH-1A-COMP

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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Data File : BP006141.D
Acq On : 08 Jul 2021 15:53
Operator : CG/JU
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Misc :
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Instrument :
BNA_P
ClientSampleId :
MH-1A-COMP

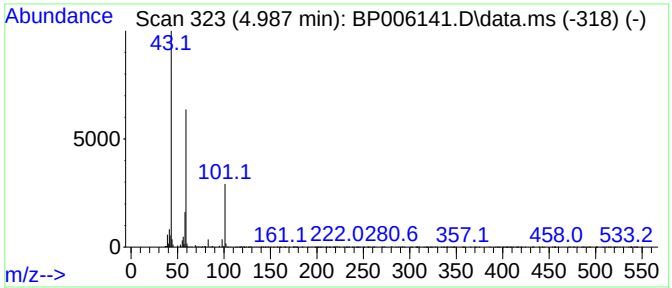
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

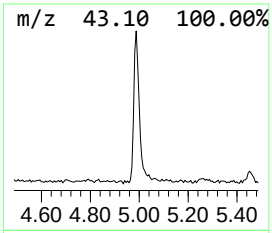
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

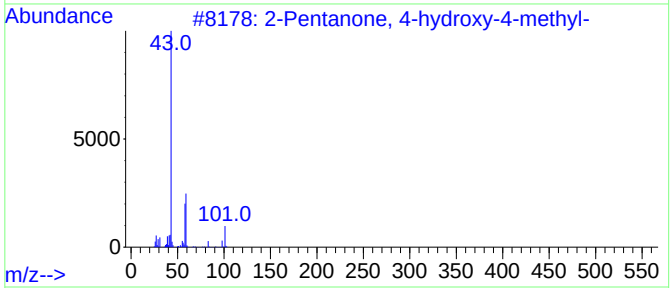
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

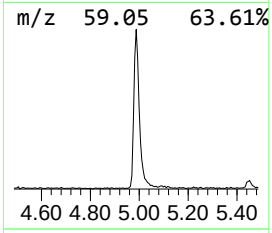
R.T.	EstConc	Area	Relative to ISTD	R.T.
4.987	2.17 ng	117817	1,4-Dichlorobenzene-d4	7.875

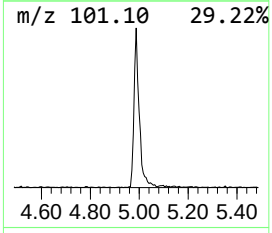
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	12
3	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
4	Guanidine	59	CH5N3	000113-00-8	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9

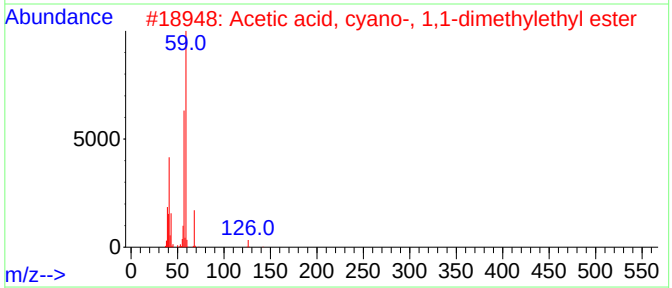


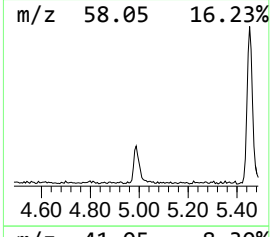


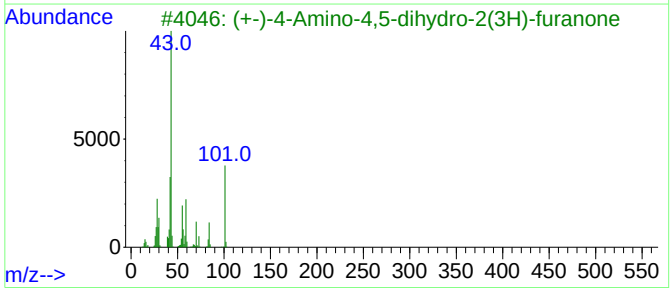


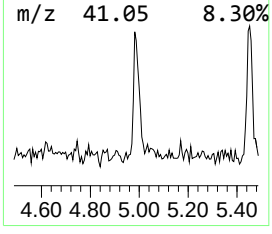












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP070821\
Data File : BP006141.D
Acq On : 08 Jul 2021 15:53
Operator : CG/JU
Sample : M2963-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MH-1A-COMP

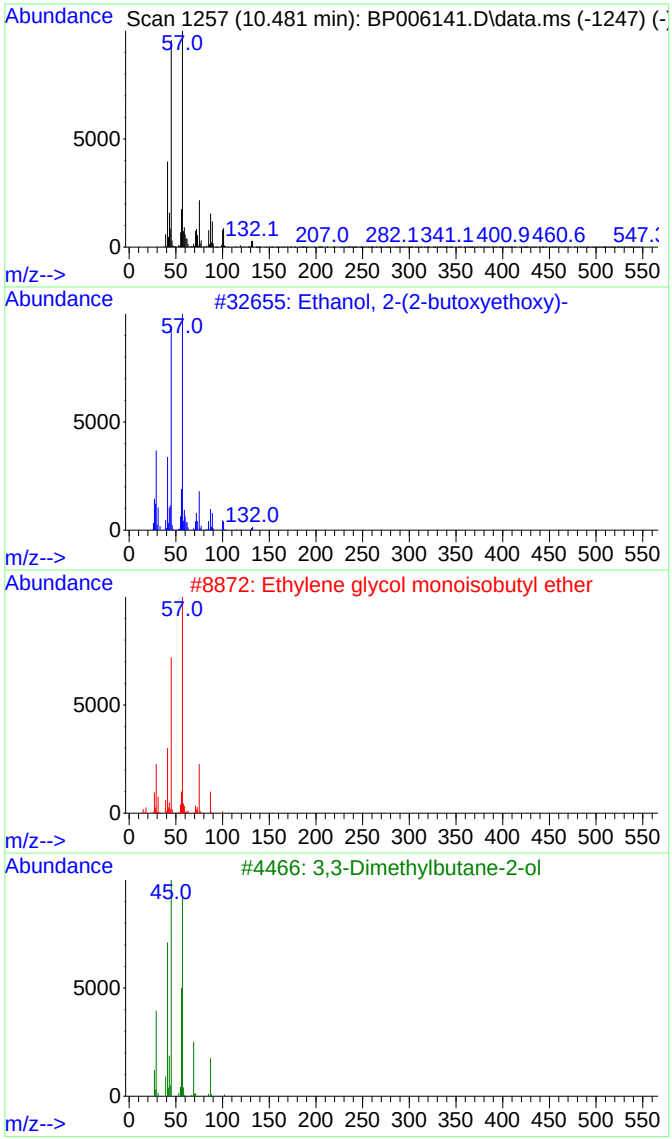
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

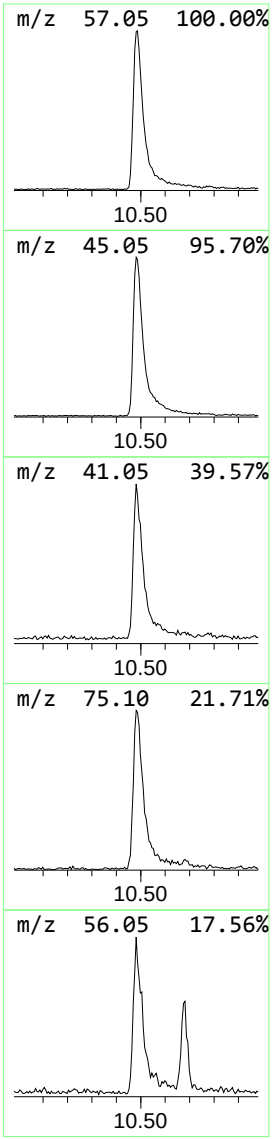
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.481	6.83 ng	475354	Naphthalene-d8	10.681

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
3	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	52
4	Di-sec-butyl ether	130	C8H18O	006863-58-7	50
5	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	50





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Operator : CG/JU
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MH-1A-COMP

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

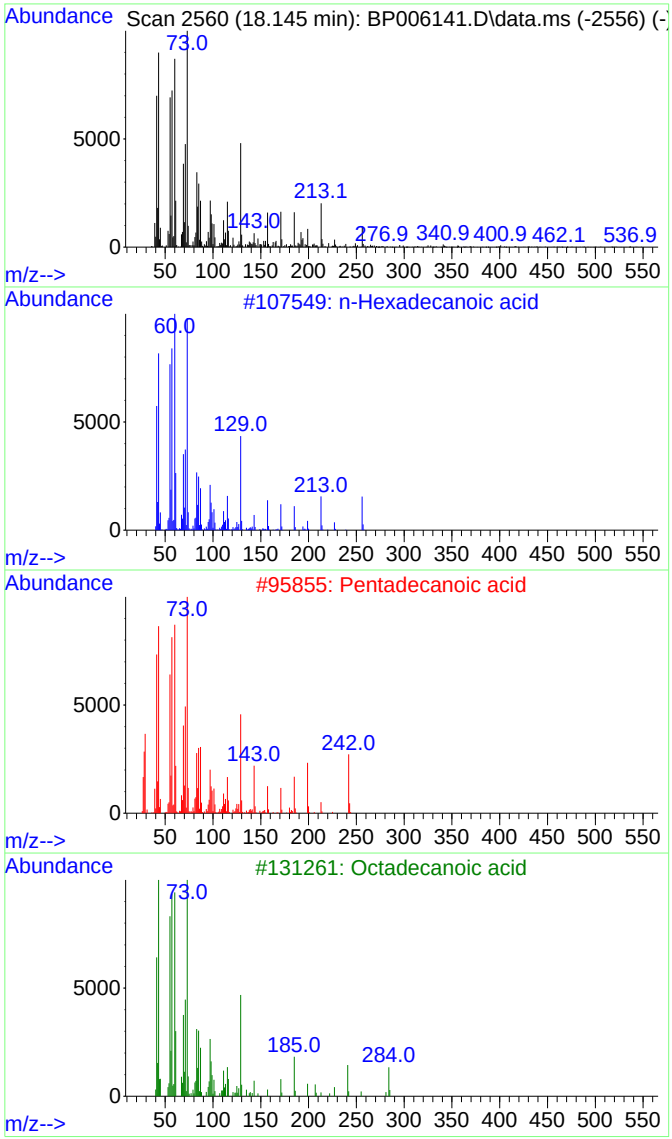
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

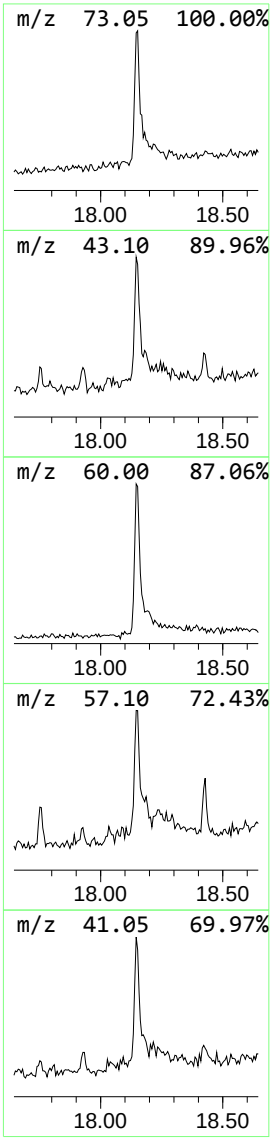
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.145	2.43 ng	210701	Phenanthrene-d10	17.263

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	87
3	Octadecanoic acid	284	C18H36O2	000057-11-4	87
4	Tridecanoic acid	214	C13H26O2	000638-53-9	81
5	n-Decanoic acid	172	C10H20O2	000334-48-5	81





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Instrument :
BNA_P
ClientSampleId :
MH-1A-COMP

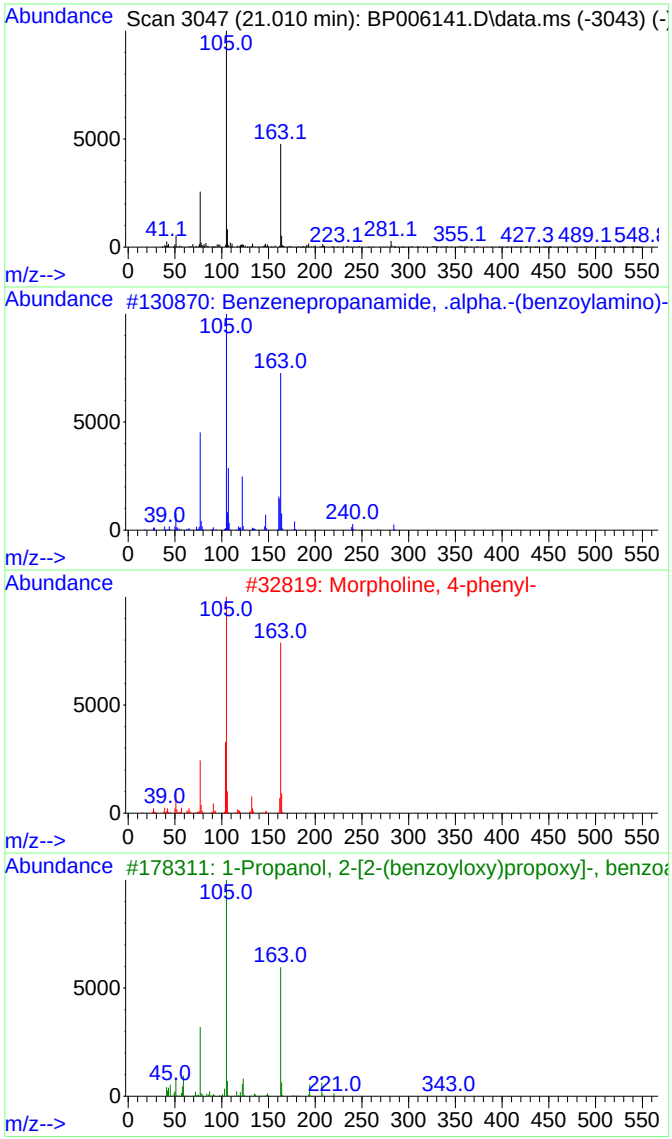
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

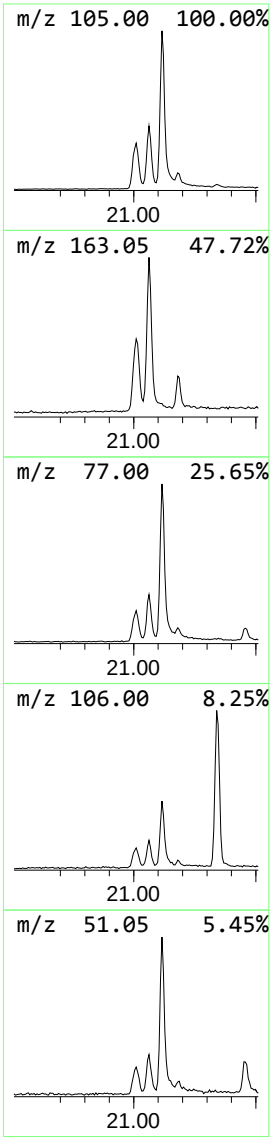
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Benzenepropanamide, .alpha.... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.010	3.21 ng	305191	Chrysene-d12	21.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenepropanamide, .alpha.-(ben...	284	C16H16N2O3	058690-81-6	59
2	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	40
3	1-Propanol, 2-[2-(benzoyloxy)pro...	342	C20H22O5	020109-39-1	38
4	Benzoic acid, 2-benzyloxy-3-brom...	348	C17H17BrO3	1000191-33-3	23
5	3-Amino-1-[2,3,5-tri-O-benzoyl-....	568	C29H24N6O7	1000211-55-2	16





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Sample : M2963-05
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Instrument : BNA_P
ClientSampleId : MH-1A-COMP

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

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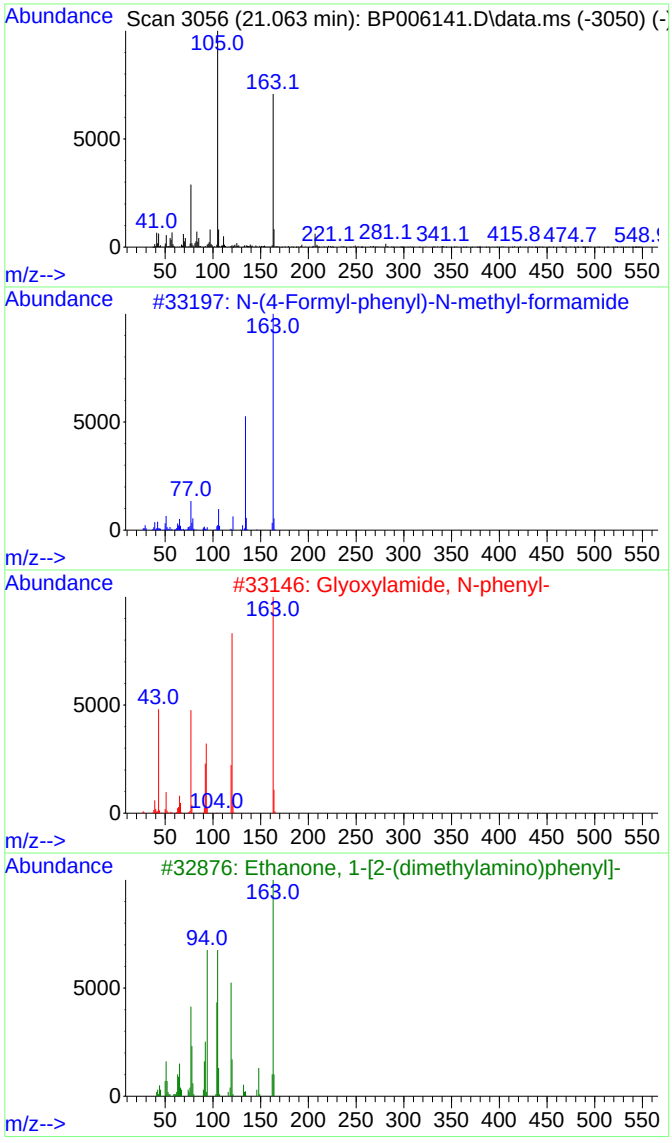
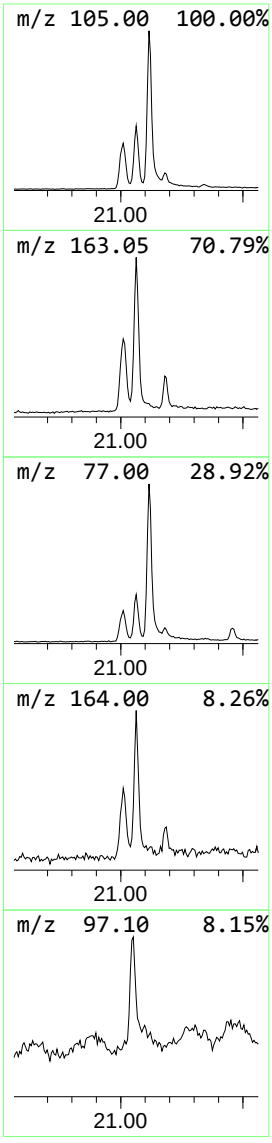
****

Peak Number 5 unknown21.063 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.063	8.71 ng	828573	Chrysene-d12	21.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N-(4-Formyl-phenyl)-N-methyl-for...	163	C9H9NO2	079213-80-2	47
2	Glyoxylamide, N-phenyl-	163	C9H9NO2	032331-52-5	47
3	Ethanone, 1-[2-(dimethylamino)ph...	163	C10H13NO	010336-55-7	42
4	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	42
5	1,3-Dioxolane, 2,4-dimethyl-2-ph...	178	C11H14O2	004359-30-2	39





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Misc :
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Instrument : BNA_P
ClientSampleId : MH-1A-COMP

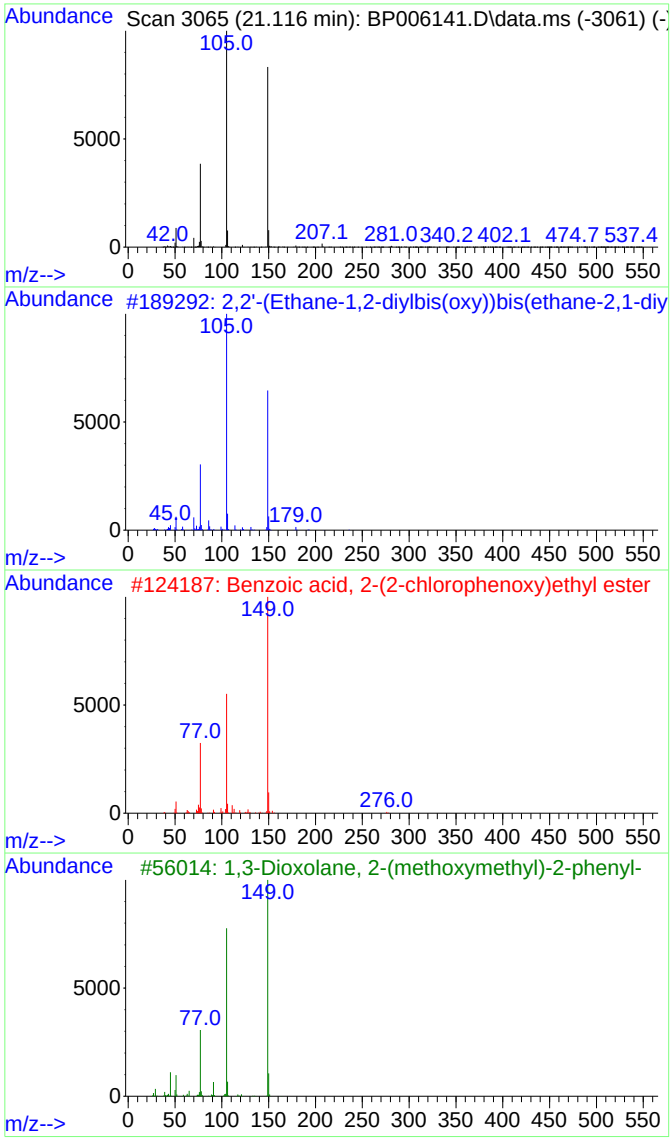
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

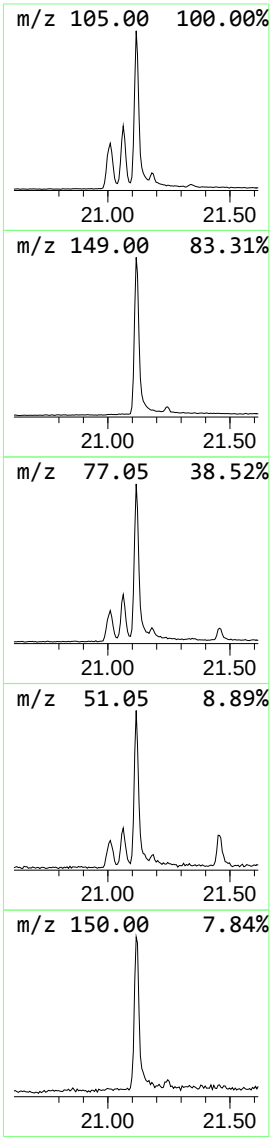
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 2,2'-(Ethane-1,2-diylbis(ox... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.116	10.80 ng	1027220	Chrysene-d12	21.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	78
2	Benzoic acid, 2-(2-chlorophenoxy...	276	C15H13ClO3	1000368-25-9	72
3	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	64
4	2-(2-(2-Methoxyethoxy)ethoxy)eth...	268	C14H20O5	1000366-99-1	64
5	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	59





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

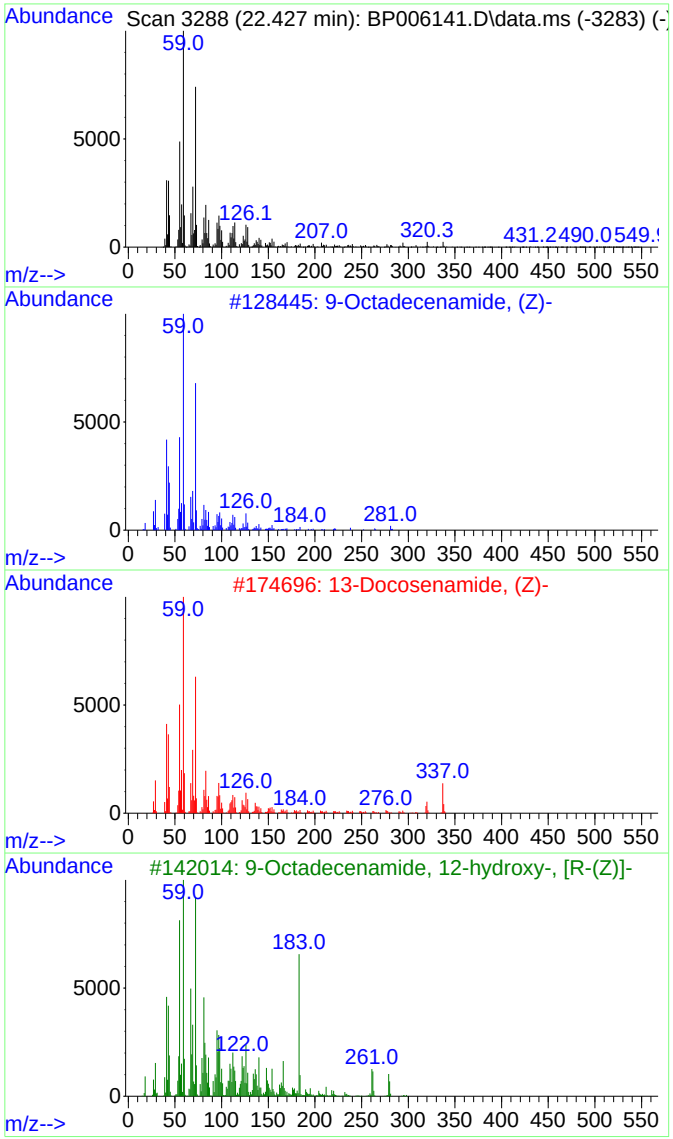
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

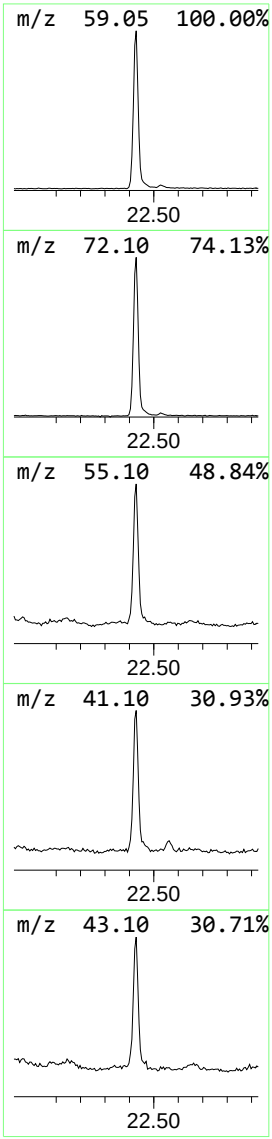
****

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.427	19.94 ng	1896790	Chrysene-d12	21.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	95
2	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	90
3	9-Octadecenamide, 12-hydroxy-, [...	297	C18H35NO2	035732-94-6	30
4	Acetic acid, cyanohydroxyimino-,...	128	C4H4N2O3	061295-92-9	27
5	3-Tridecanone	198	C13H26O	001534-26-5	27





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP070821\
Data File : BP006141.D
Acq On : 08 Jul 2021 15:53
Operator : CG/JU
Sample : M2963-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MH-1A-COMP

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	4.987	2.2	ng	117817	1	7.875	1084350	20.0
Ethanol, 2-(2-b...	10.481	6.8	ng	475354	2	10.681	1392670	20.0
n-Hexadecanoic ...	18.145	2.4	ng	210701	4	17.263	1736160	20.0
Benzenepropanam...	21.010	3.2	ng	305191	5	21.345	1902180	20.0
unknown21.063	21.063	8.7	ng	828573	5	21.345	1902180	20.0
2,2'-(Ethane-1,...	21.116	10.8	ng	1027220	5	21.345	1902180	20.0
9-Octadecenamid...	22.427	19.9	ng	1896790	5	21.345	1902180	20.0