LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP041221\
Data File : BP005265.D
Acq On : 12 Apr 2021 14:34
Operator : CG/JU
Sample : M1967-08
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SB2-C

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-BP040921.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP005265.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.281	368	373	382	rVB	617575	890638	65.57%	10.949%
2	6.863	636	642	655	rVB	478733	784029	57.72%	9.639%
3	7.681	775	781	788	rVB	114284	182918	13.47%	2.249%
4	8.840	971	978	987	rBV	274622	445255	32.78%	5.474%
5	10.469	1248	1255	1261	rBV	120147	201417	14.83%	2.476%
6	12.951	1670	1677	1688	rBV	531063	765824	56.38%	9.415%
7	13.804	1817	1822	1831	rBV3	14465	22753	1.68%	0.280%
8	14.339	1906	1913	1928	rVB2	187179	264737	19.49%	3.255%
9	15.839	2161	2168	2180	rBV	446302	649527	47.82%	7.985%
10	17.104	2377	2383	2388	rBV	238383	321980	23.71%	3.958%
11	17.486	2442	2448	2454	rBV4	8017	18854	1.39%	0.232%
12	18.004	2528	2536	2544	rBV	72245	114045	8.40%	1.402%
13	19.127	2720	2727	2733	rBV	29100	46052	3.39%	0.566%
14	19.245	2742	2747	2757	rBV4	29032	45451	3.35%	0.559%
15	19.480	2780	2787	2789	rBV2	25248	40881	3.01%	0.503%
16	19.504	2789	2791	2796	rVB	29572	38210	2.81%	0.470%
17	19.680	2816	2821	2833	rVB	1212010	1358256	100.00%	16.698%
18	20.886	3020	3026	3029	rBV	85209	149816	11.03%	1.842%
19	20.933	3029	3034	3039	rVV2	178901	356023	26.21%	4.377%
20	20.986	3039	3043	3051	rVV	361044	486266	35.80%	5.978%
21	21.051	3052	3054	3060	rVB	22306	33551	2.47%	0.412%
22	21.204	3075	3080	3084	rBV	366410	464788	34.22%	5.714%
23	23.480	3460	3467	3477	rBV	243373	452938	33.35%	5.568%

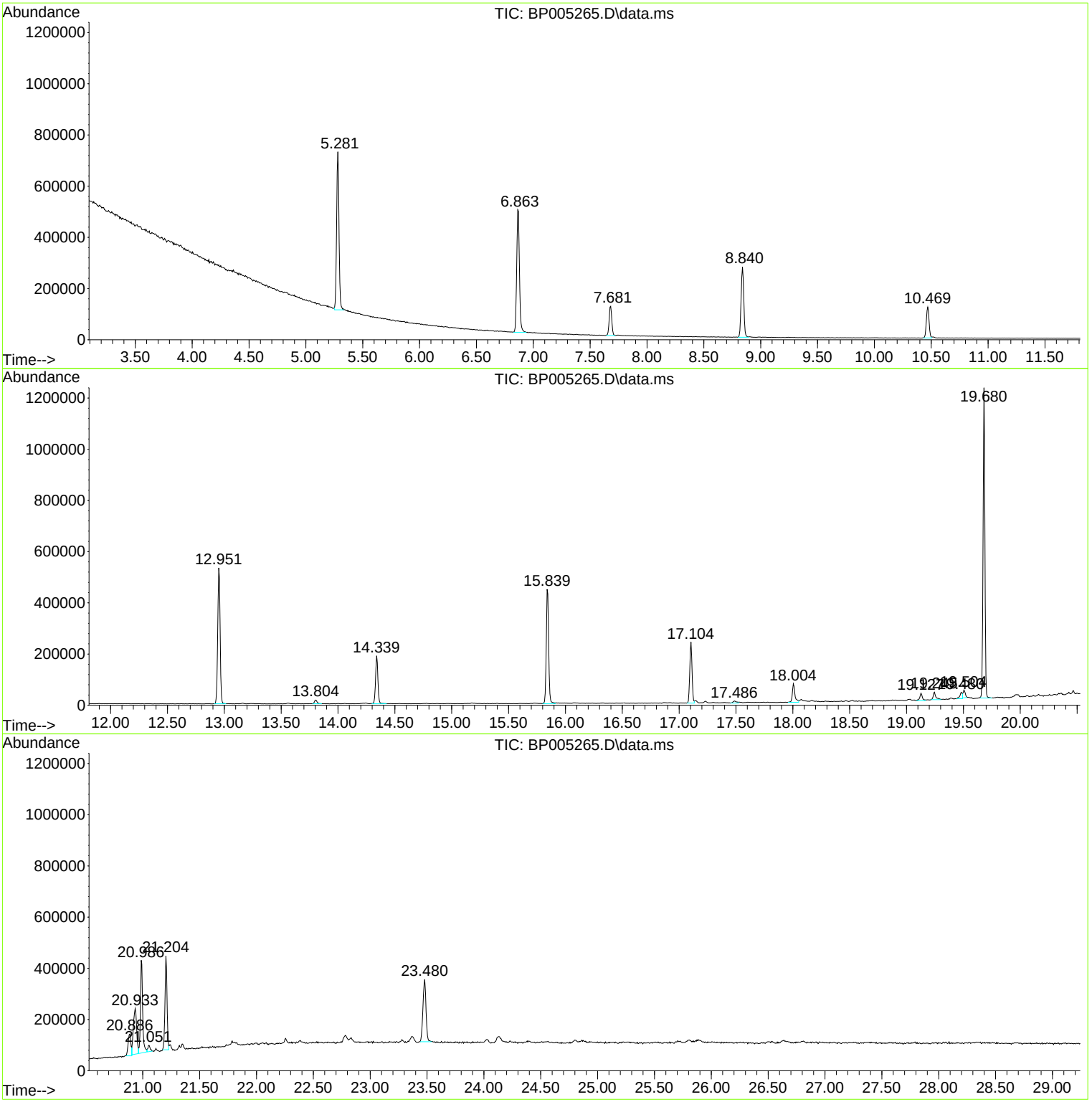
Sum of corrected areas: 8134209

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP041221\
Data File : BP005265.D
Acq On : 12 Apr 2021 14:34
Operator : CG/JU
Sample : M1967-08
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB2-C

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP040921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP041221\
Data File : BP005265.D
Acq On : 12 Apr 2021 14:34
Operator : CG/JU
Sample : M1967-08
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SB2-C

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP040921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

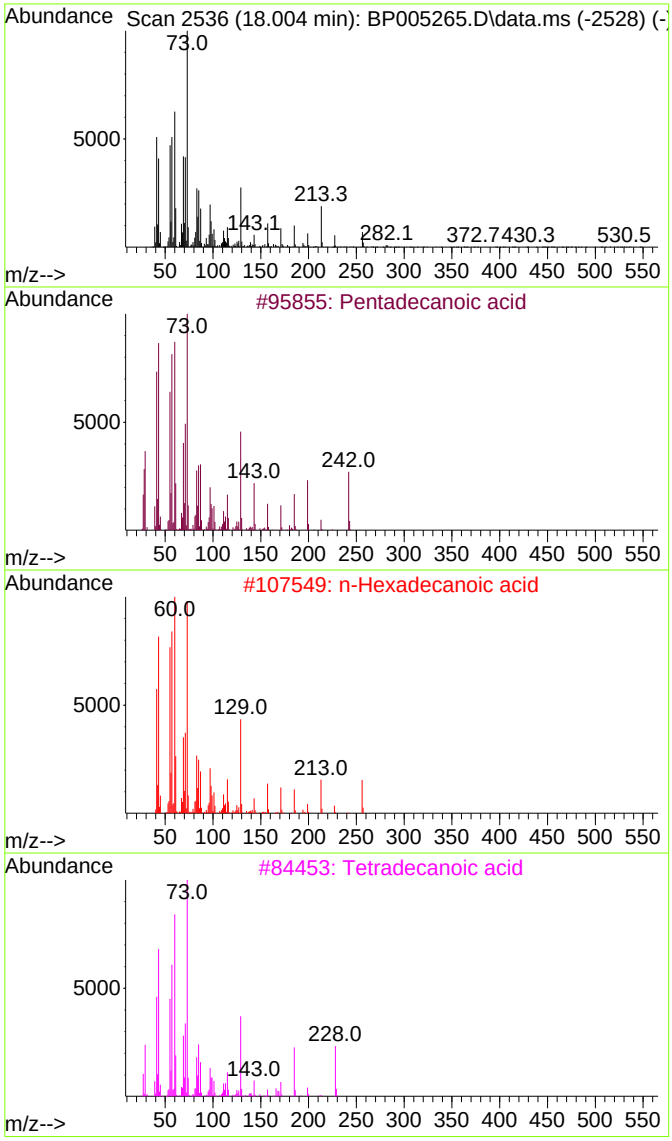
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

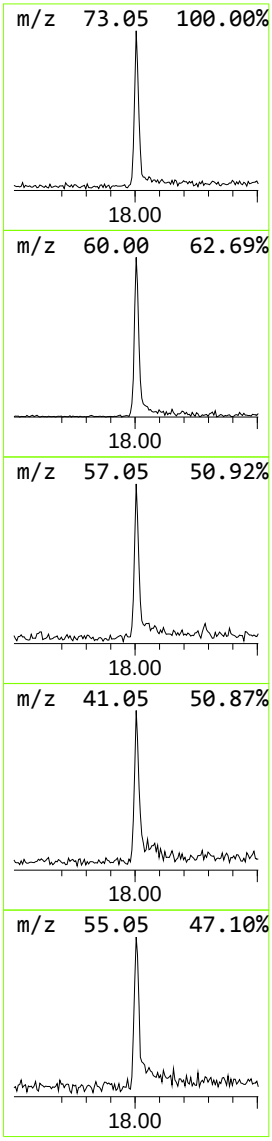
****

Peak Number 1 Pentadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.004	7.08 ng	114045	Phenanthrene-d10	17.104

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	53
4	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	50
5	Trehalose	342	C12H22O11	000099-20-7	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP041221\
Data File : BP005265.D
Acq On : 12 Apr 2021 14:34
Operator : CG/JU
Sample : M1967-08
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SB2-C

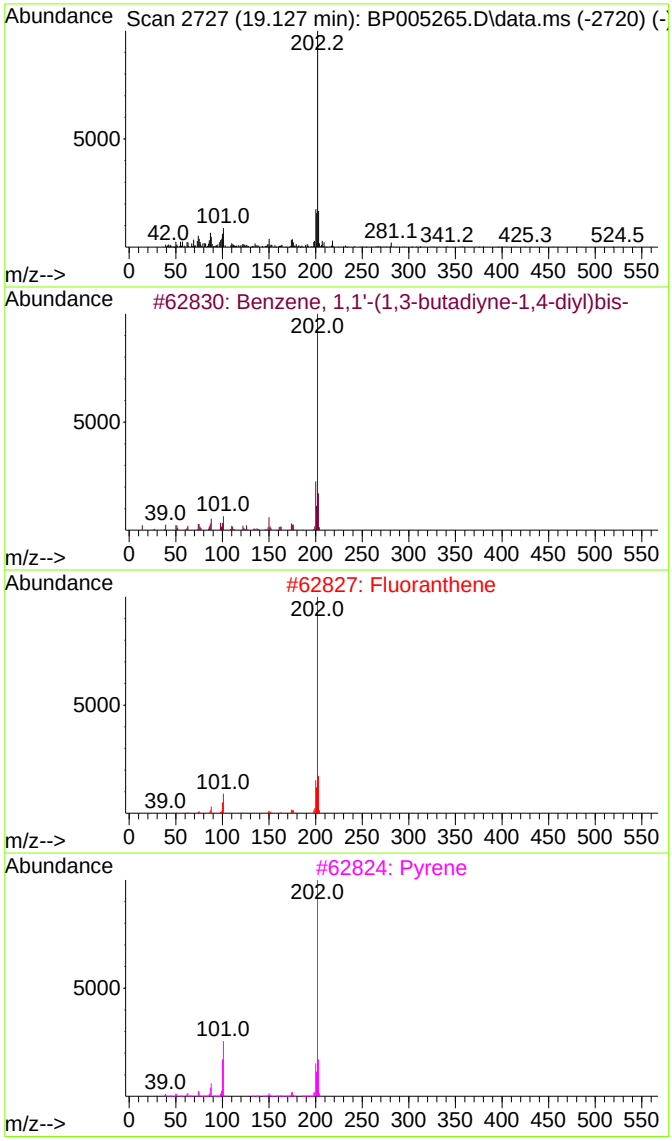
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP040921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

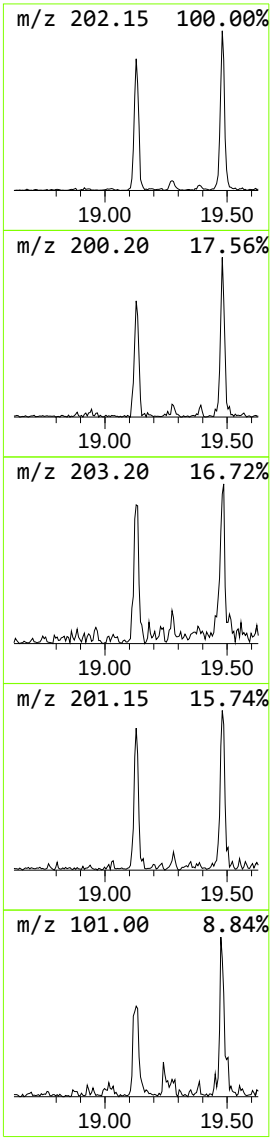
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Benzene, 1,1'-(1,3-butadiyn... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.128	2.86 ng	46052	Phenanthrene-d10	17.104

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	87
2	Fluoranthene	202	C16H10	000206-44-0	87
3	Pyrene	202	C16H10	000129-00-0	81
4	1,4-Pentadiyn-3-one, 1,5-diphenyl-	230	C17H10O	015814-30-9	56
5	l-Leucine, N-methyl-N-(2-methoxy...	471	C27H53NO5	1000328-55-0	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP041221\
Data File : BP005265.D
Acq On : 12 Apr 2021 14:34
Operator : CG/JU
Sample : M1967-08
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SB2-C

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP040921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

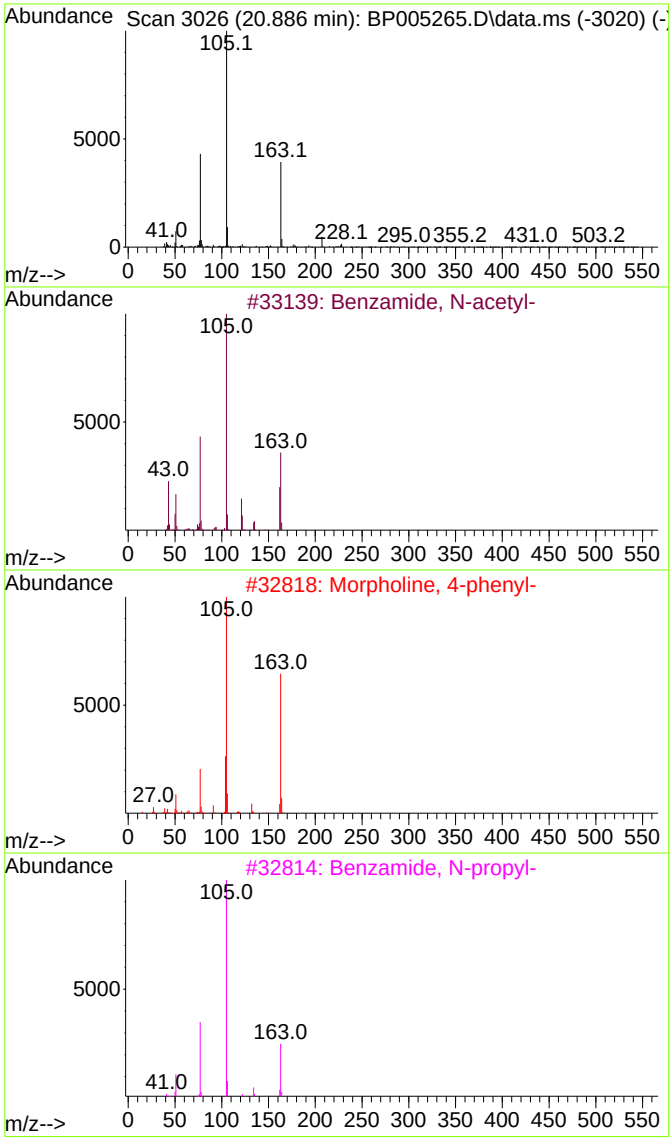
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

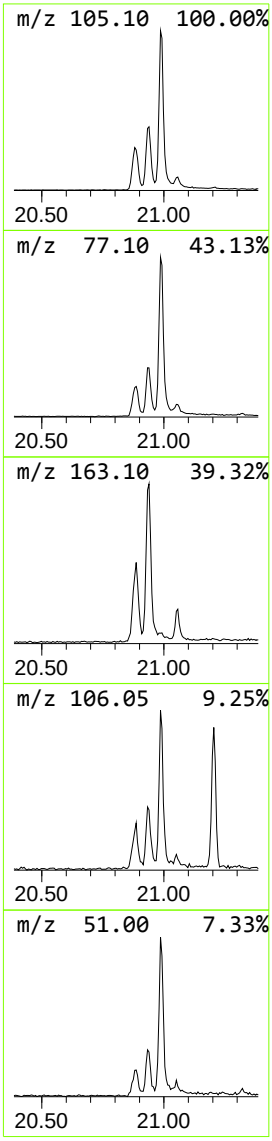
****

Peak Number 3 Benzamide, N-acetyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.886	6.45 ng	149816	Chrysene-d12	21.204

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzamide, N-acetyl-	163	C9H9NO2	001575-95-7	72
2	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	43
3	Benzamide, N-propyl-	163	C10H13NO	010546-70-0	36
4	(3-Phenyloxiran-2-yl)methyl benz...	254	C16H14O3	1000366-96-1	36
5	Anthraquinone, 2-benzamido-	327	C21H13NO3	052869-18-8	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP041221\
Data File : BP005265.D
Acq On : 12 Apr 2021 14:34
Operator : CG/JU
Sample : M1967-08
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SB2-C

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP040921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

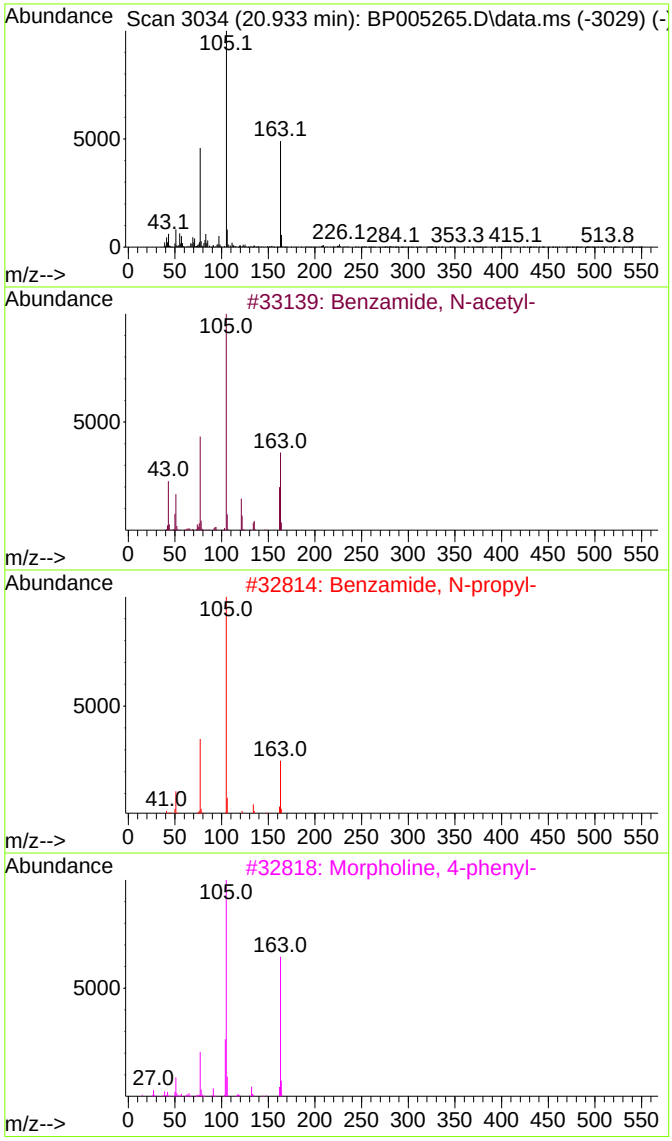
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

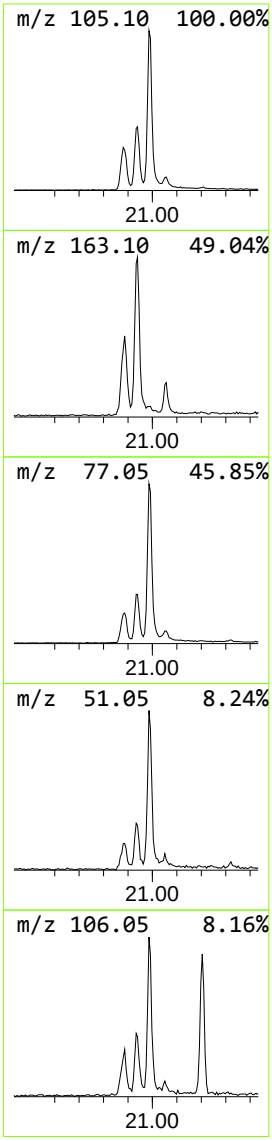
****

Peak Number 4 Benzamide, N-propyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.933	15.32 ng	356023	Chrysene-d12	21.204

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzamide, N-acetyl-	163	C9H9NO2	001575-95-7	56
2	Benzamide, N-propyl-	163	C10H13NO	010546-70-0	56
3	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	47
4	1-Propanol, 2-[2-(benzoyloxy)pro...	342	C20H22O5	020109-39-1	42
5	2-Pyrrolidinone, 3-hydroxy-4-met...	191	C11H13NO2	104194-17-4	40





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP041221\
Data File : BP005265.D
Acq On : 12 Apr 2021 14:34
Operator : CG/JU
Sample : M1967-08
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SB2-C

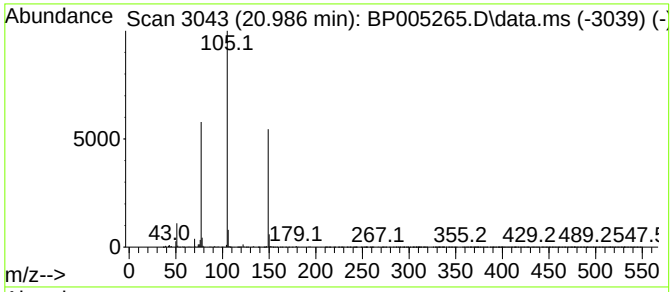
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP040921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

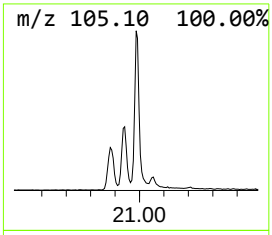
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

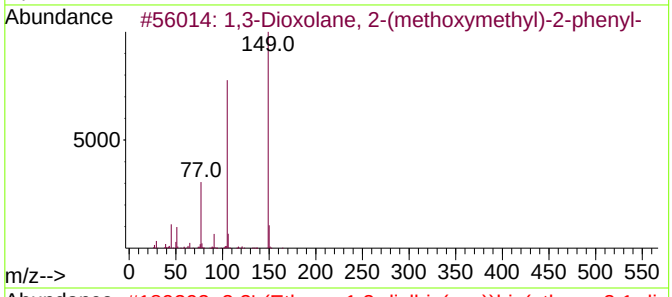
****
Peak Number 5 1,3-Dioxolane, 2-(methoxyme... Concentration Rank 1

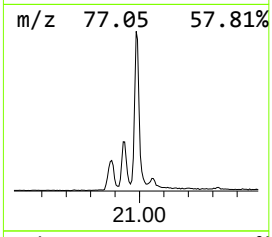
R.T.	EstConc	Area	Relative to ISTD	R.T.
20.986	20.92 ng	486266	Chrysene-d12	21.204

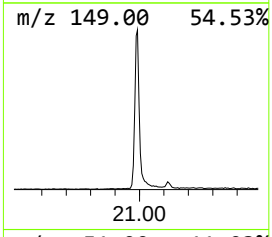
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	64
2	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	50
3	Vinyl benzoate	148	C9H8O2	000769-78-8	47
4	2-Phenyl-4-ethylidene-2-oxazolin...	187	C11H9NO2	037791-41-6	47
5	1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	47

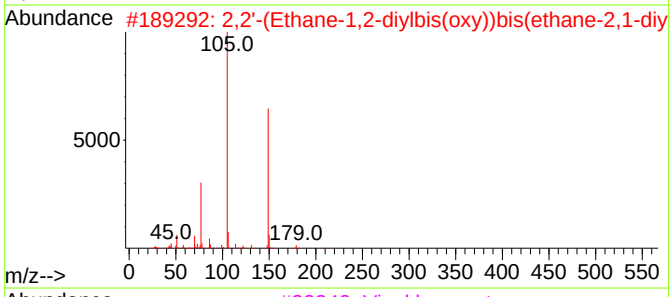


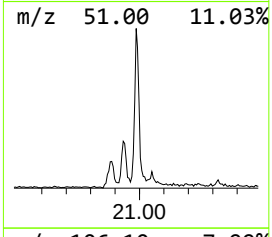


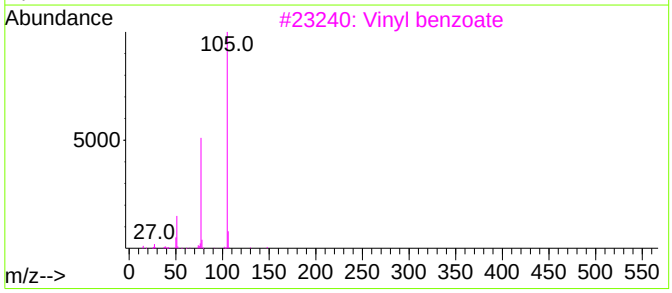


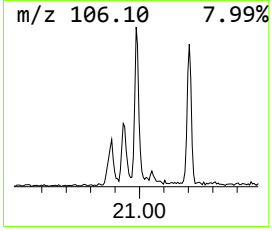












Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP041221\
Data File : BP005265.D
Acq On : 12 Apr 2021 14:34
Operator : CG/JU
Sample : M1967-08
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SB2-C

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP040921.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
Pentadecanoic acid	18.004	7.1	ng	114045	4	17.104	321980	20.0
Benzene, 1,1'-(...	19.128	2.9	ng	46052	4	17.104	321980	20.0
Benzamide, N-ac...	20.886	6.5	ng	149816	5	21.204	464788	20.0
Benzamide, N-pr...	20.933	15.3	ng	356023	5	21.204	464788	20.0
1,3-Dioxolane, ...	20.986	20.9	ng	486266	5	21.204	464788	20.0