

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062221\
 Data File : BP006020.D
 Acq On : 22 Jun 2021 23:38
 Operator : CG/JU
 Sample : M2748-02
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 SB-3B

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-BP060821.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP006020.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.022	325	329	339	rBV	53492	80093	2.26%	0.502%
2	5.493	401	409	425	rBV	773375	1231068	34.72%	7.718%
3	7.093	674	681	695	rBV	694783	1180809	33.30%	7.403%
4	7.916	815	821	829	rBV	220403	368658	10.40%	2.311%
5	9.087	1012	1020	1042	rBV	407286	755190	21.30%	4.735%
6	10.722	1290	1298	1313	rBV	273194	501073	14.13%	3.142%
7	11.987	1505	1513	1523	rBV2	17470	44692	1.26%	0.280%
8	13.175	1708	1715	1730	rBV	1239779	1880182	53.02%	11.788%
9	13.969	1842	1850	1859	rBV2	19805	38283	1.08%	0.240%
10	14.545	1939	1948	1956	rBV	405548	654506	18.46%	4.104%
11	15.345	2078	2084	2091	rBV	85844	121653	3.43%	0.763%
12	16.039	2193	2202	2222	rBV	741148	1298693	36.63%	8.142%
13	17.292	2409	2415	2420	rBV	529199	795595	22.44%	4.988%
14	17.333	2420	2422	2430	rVB	69742	102551	2.89%	0.643%
15	19.298	2751	2756	2763	rBV	106441	147122	4.15%	0.922%
16	19.651	2812	2816	2824	rVB	81012	114974	3.24%	0.721%
17	19.839	2842	2848	2858	rBV	3003889	3545843	100.00%	22.232%
18	21.033	3047	3051	3054	rBV2	45471	68245	1.92%	0.428%
19	21.086	3054	3060	3068	rVB2	107734	229972	6.49%	1.442%
20	21.222	3081	3083	3086	rVB	40189	39433	1.11%	0.247%
21	21.269	3088	3091	3098	rVB	50725	60788	1.71%	0.381%
22	21.363	3102	3107	3112	rBV	858950	1197773	33.78%	7.510%
23	22.239	3252	3256	3260	rVB	186830	231577	6.53%	1.452%
24	23.768	3509	3516	3529	rVB3	574767	1260832	35.56%	7.905%

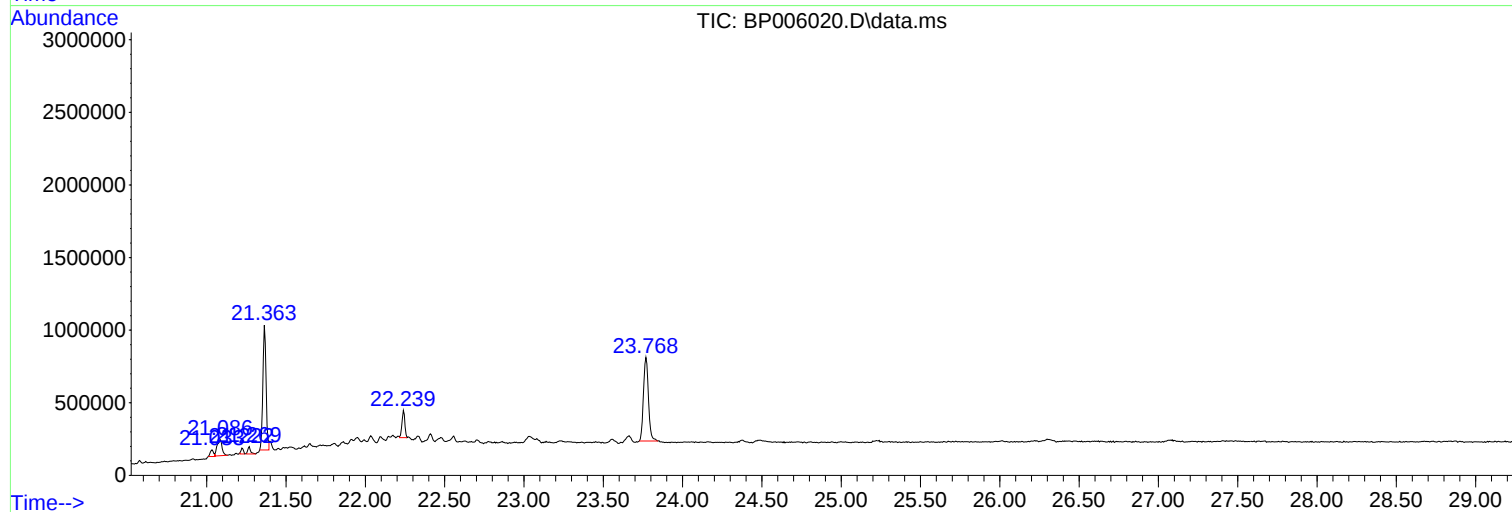
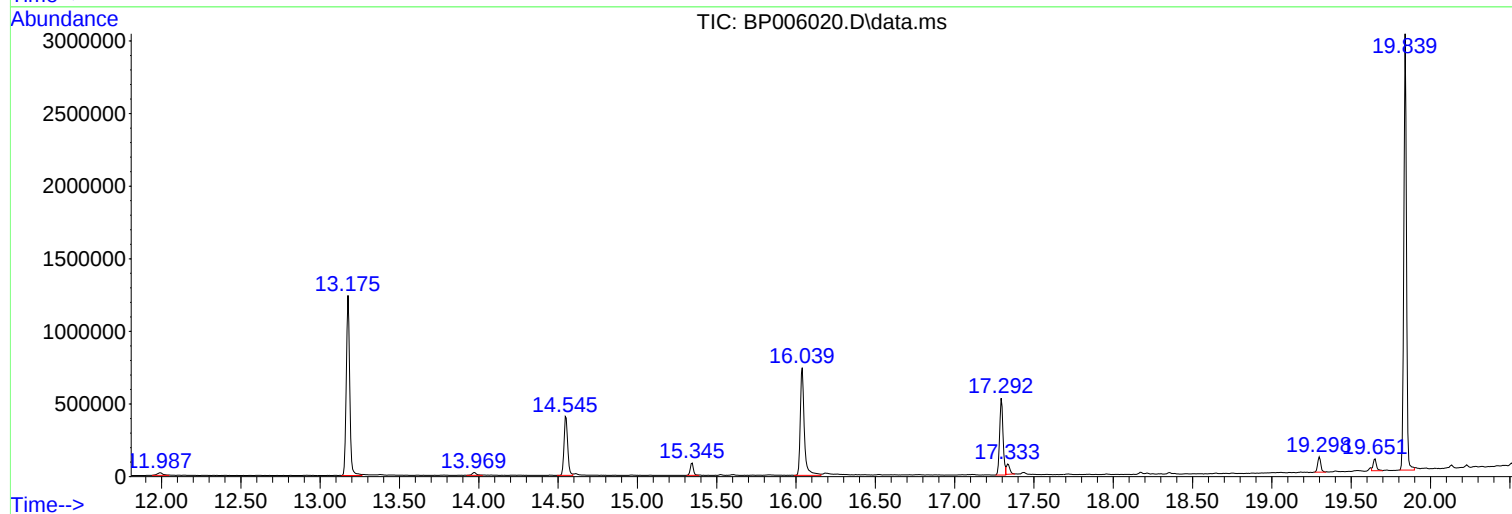
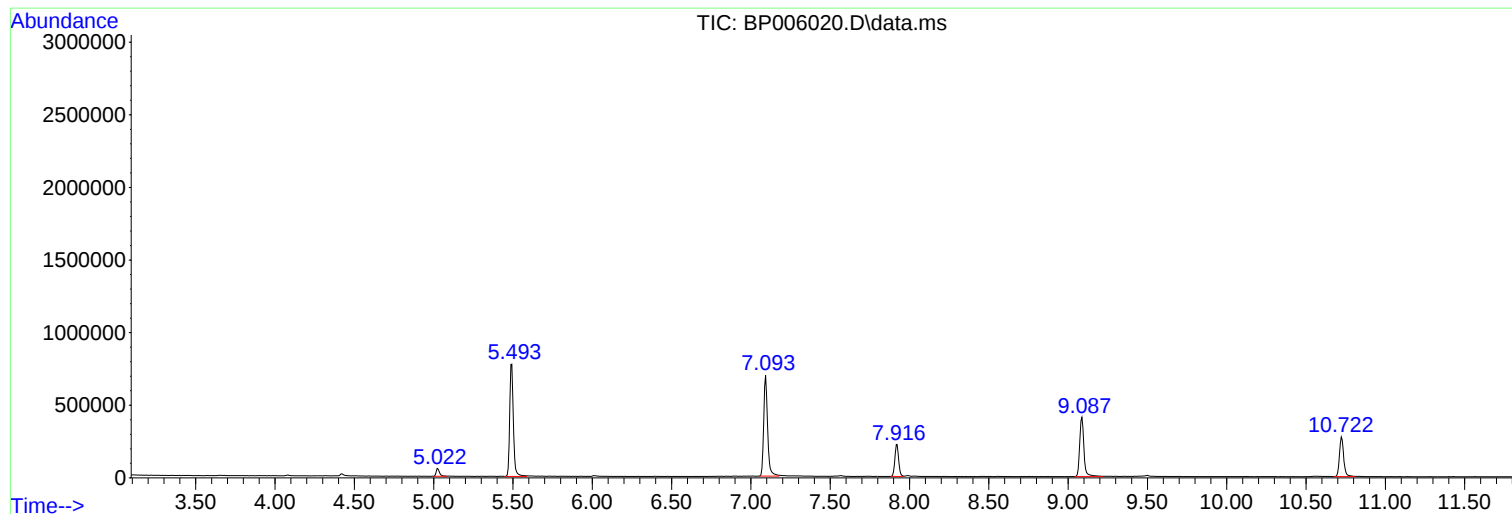
Sum of corrected areas: 15949605

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062221\
Data File : BP006020.D
Acq On : 22 Jun 2021 23:38
Operator : CG/JU
Sample : M2748-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-3B

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.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\BP062221\
Data File : BP006020.D
Acq On : 22 Jun 2021 23:38
Operator : CG/JU
Sample : M2748-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-3B

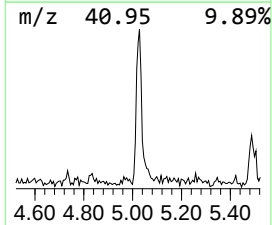
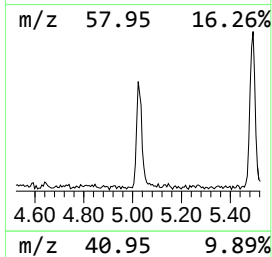
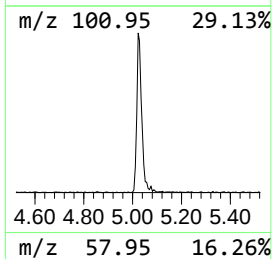
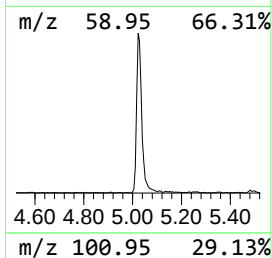
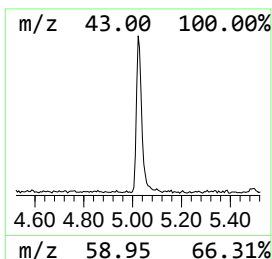
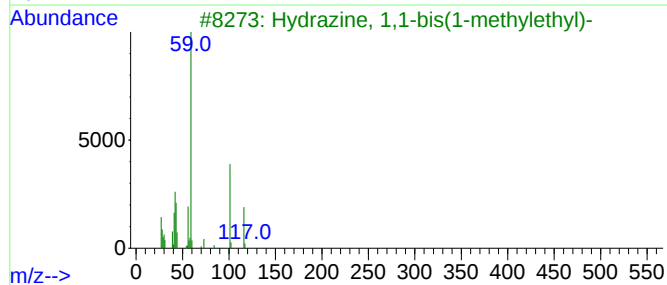
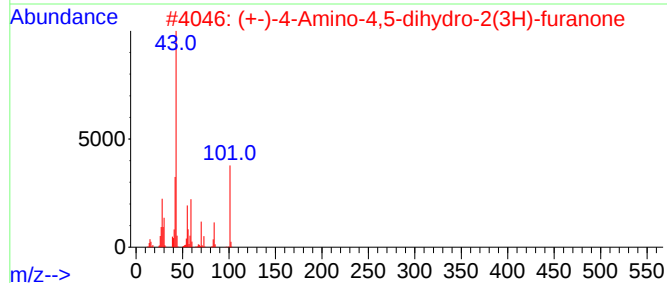
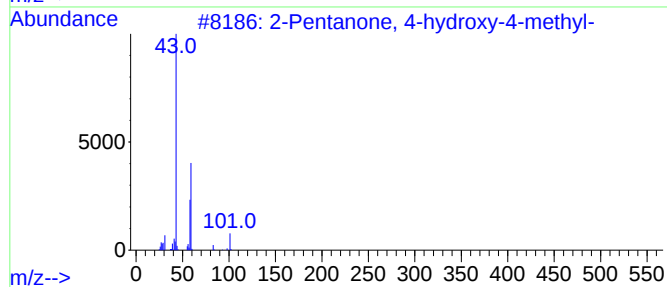
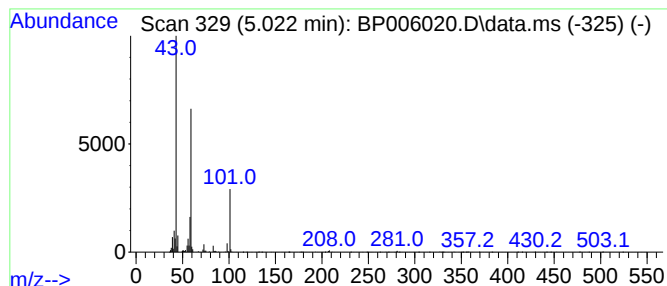
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.022	4.35 ng	80093	1,4-Dichlorobenzene-d4	7.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	43
3			Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	38
4			Tetraglyme	222	C10H22O5	000143-24-8	32
5			Dimethadione	129	C5H7NO3	000695-53-4	28



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062221\
Data File : BP006020.D
Acq On : 22 Jun 2021 23:38
Operator : CG/JU
Sample : M2748-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-3B

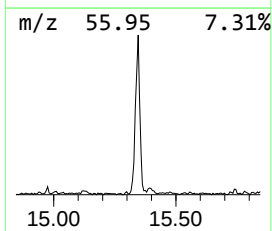
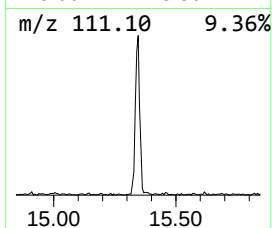
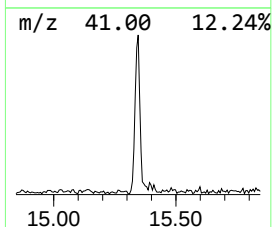
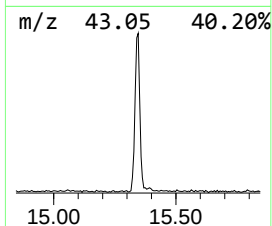
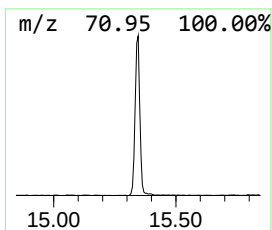
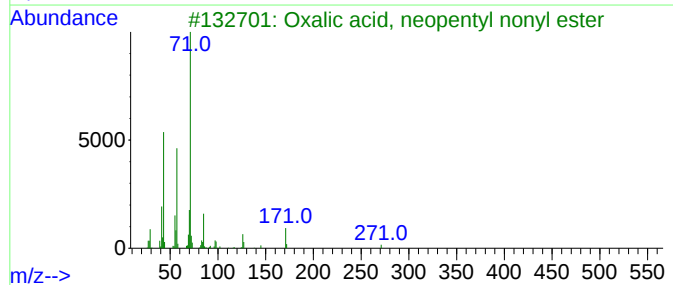
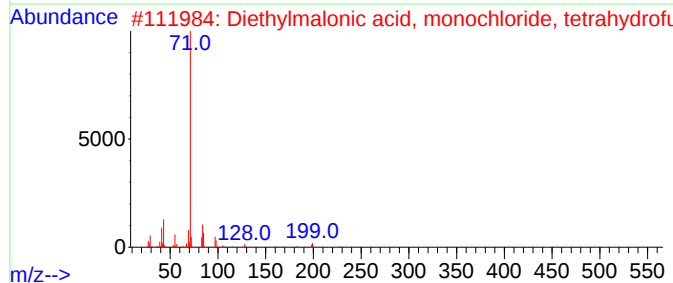
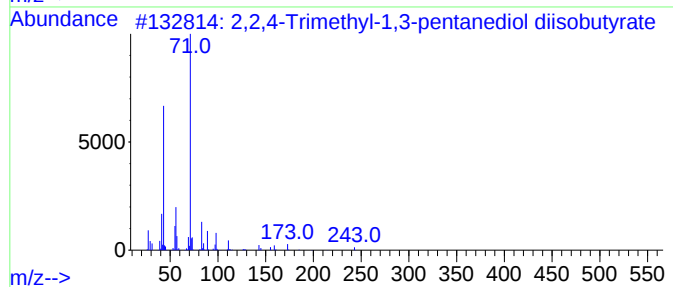
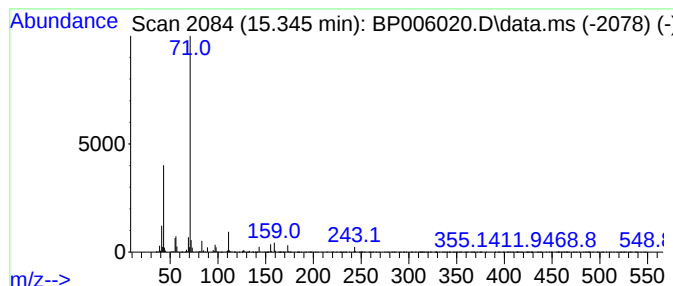
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2,2,4-Trimethyl-1,3-pentane... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.345	3.72 ng	121653	Acenaphthene-d10	14.545

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2,4-Trimethyl-1,3-pentanediol ...	286	C16H30O4	006846-50-0	78		
2	Diethylmalonic acid, monochlorid...	262	C12H19ClO4	1000370-65-0	59		
3	Oxalic acid, neopentyl nonyl ester	286	C16H30O4	1000309-73-3	45		
4	Tetrahydrofuran, 2-propyl-	114	C7H14O	003208-22-8	42		
5	Butanoic acid, 2-butoxy-1-methyl...	216	C11H20O4	007492-70-8	42		



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062221\
Data File : BP006020.D
Acq On : 22 Jun 2021 23:38
Operator : CG/JU
Sample : M2748-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-3B

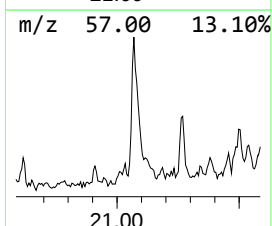
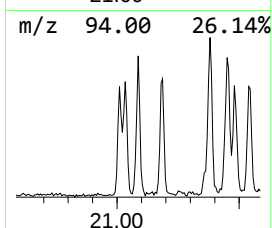
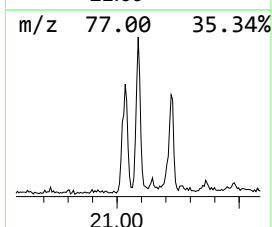
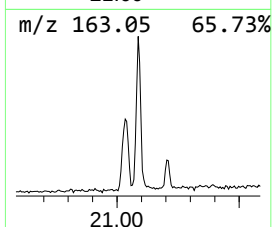
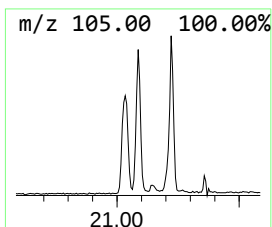
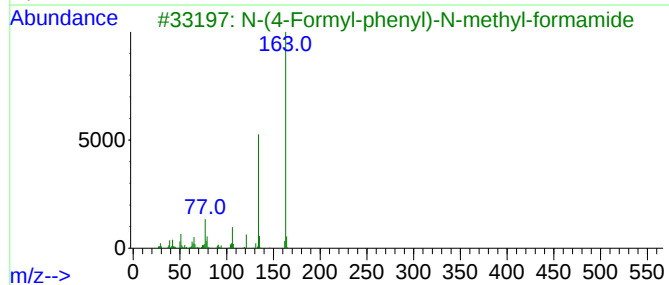
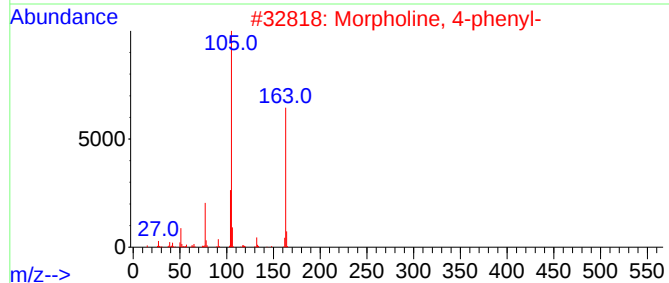
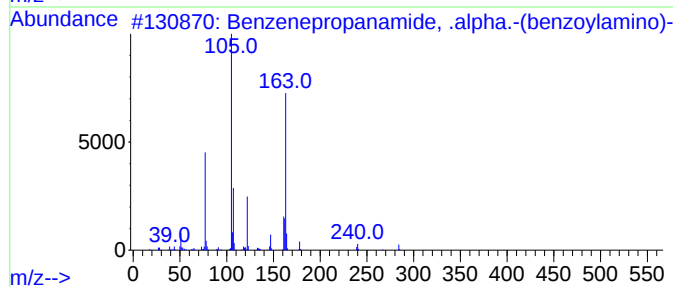
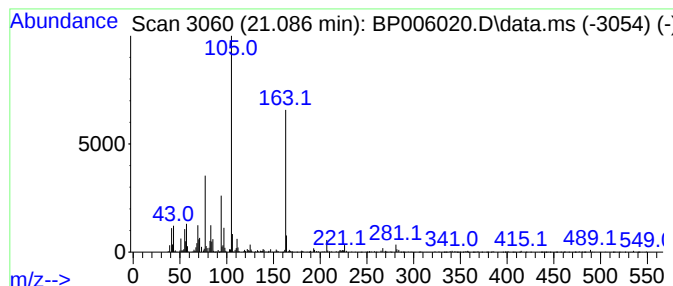
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown21.086 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.086	3.84 ng	229972	Chrysene-d12	21.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzenepropanamide, .alpha.-(ben...	284	C16H16N2O3	058690-81-6	47
2			Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	47
3			N-(4-Formyl-phenyl)-N-methyl-for...	163	C9H9NO2	079213-80-2	43
4			2-Pyrimidinamine, 4-(trifluorome...	163	C5H4F3N3	016075-42-6	35
5			Glyoxylamide, N-phenyl-	163	C9H9NO2	032331-52-5	32



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062221\
Data File : BP006020.D
Acq On : 22 Jun 2021 23:38
Operator : CG/JU
Sample : M2748-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

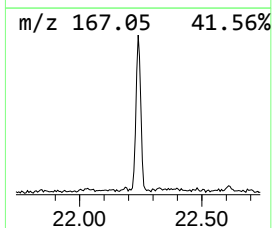
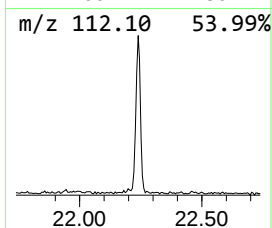
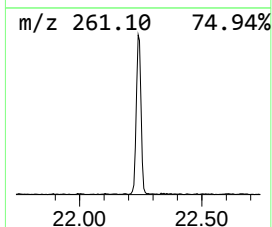
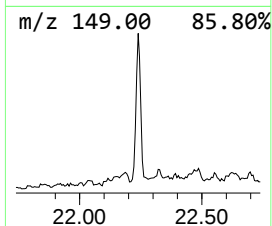
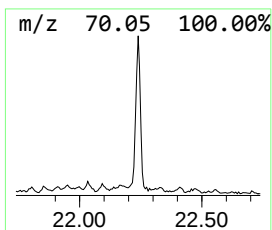
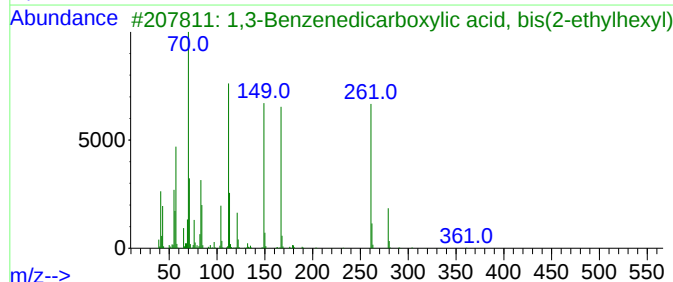
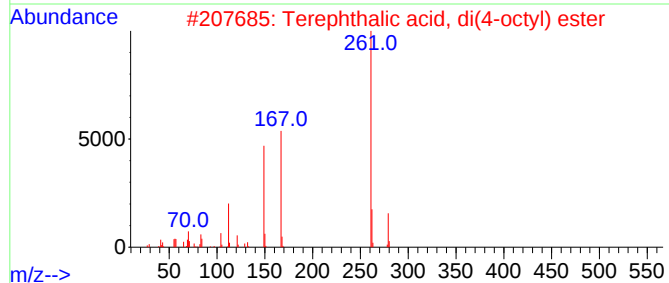
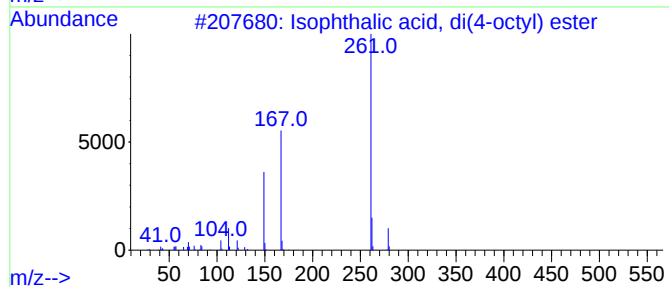
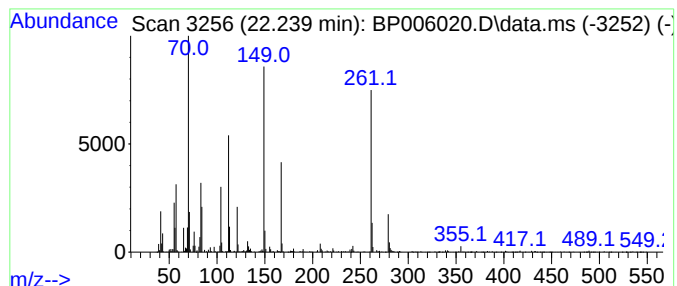
Instrument :
BNA_P
ClientSampleId :
SB-3B

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Isophthalic acid, di(4-octyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
22.239	3.87 ng	231577	Chrysene-d12	21.363	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isophthalic acid, di(4-octyl) ester	390	C24H38O4	1000344-04-3	87
2	Terephthalic acid, di(4-octyl) e...	390	C24H38O4	1000323-74-2	74
3	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	59
4	Isophthalic acid, 2-chlorophenyl...	388	C22H25ClO4	1000344-50-0	38
5	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062221\
Data File : BP006020.D
Acq On : 22 Jun 2021 23:38
Operator : CG/JU
Sample : M2748-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-3B

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.022	4.3	ng	80093	1	7.916	368658	20.0
2,2,4-Trimethyl...	15.345	3.7	ng	121653	3	14.545	654506	20.0
unknown21.086	21.086	3.8	ng	229972	5	21.363	1197770	20.0
Isophthalic aci...	22.239	3.9	ng	231577	5	21.363	1197770	20.0