

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051321\
 Data File : BP005529.D
 Acq On : 13 May 2021 20:35
 Operator : CG/JU
 Sample : M2370-02
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 367

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-BP050521.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP005529.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	366	373	384	rBV	253187	360923	40.88%	8.447%
2	6.887	639	646	661	rBV	202519	335987	38.06%	7.864%
3	7.687	774	782	790	rBV	67247	107500	12.18%	2.516%
4	8.857	974	981	987	rBV	137970	231916	26.27%	5.428%
5	8.899	987	988	996	rVB3	6990	9472	1.07%	0.222%
6	10.481	1249	1257	1269	rBV	66532	117873	13.35%	2.759%
7	12.957	1671	1678	1686	rBV	361292	515056	58.34%	12.055%
8	13.240	1720	1726	1735	rVB4	11192	20779	2.35%	0.486%
9	13.810	1816	1823	1833	rBV	33220	53361	6.04%	1.249%
10	14.334	1906	1912	1920	rBV	90040	138500	15.69%	3.242%
11	15.839	2161	2168	2185	rBV	328993	506905	57.42%	11.864%
12	17.092	2375	2381	2386	rBV	117030	171714	19.45%	4.019%
13	17.133	2386	2388	2394	rVB2	8841	11972	1.36%	0.280%
14	17.992	2529	2534	2544	rBV2	32653	52161	5.91%	1.221%
15	19.116	2721	2725	2733	rVB	25236	37368	4.23%	0.875%
16	19.233	2741	2745	2752	rBV10	9892	18768	2.13%	0.439%
17	19.469	2782	2785	2788	rVB	16269	16451	1.86%	0.385%
18	19.669	2813	2819	2825	rBV	767266	882798	100.00%	20.661%
19	20.410	2943	2945	2948	rVB3	14001	13006	1.47%	0.304%
20	20.904	3026	3029	3037	rVB4	47709	75530	8.56%	1.768%
21	20.980	3038	3042	3046	rVB3	22926	32704	3.70%	0.765%
22	21.192	3073	3078	3082	rBV	217868	278344	31.53%	6.514%
23	23.504	3465	3471	3478	rVB2	147607	283604	32.13%	6.638%

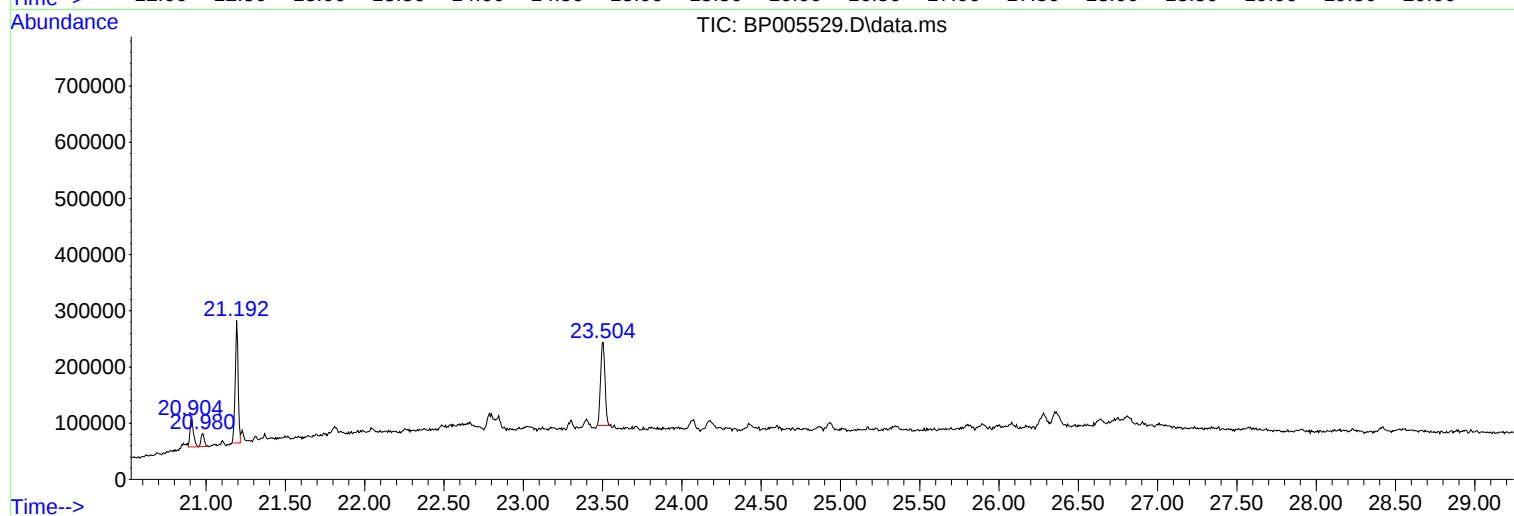
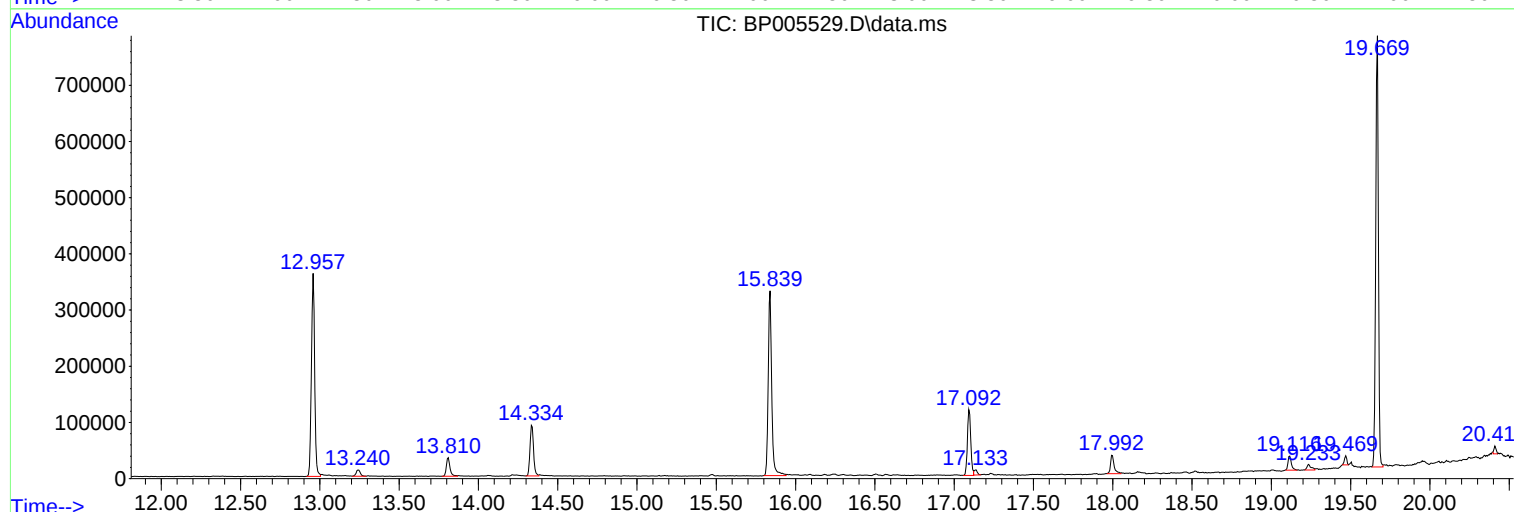
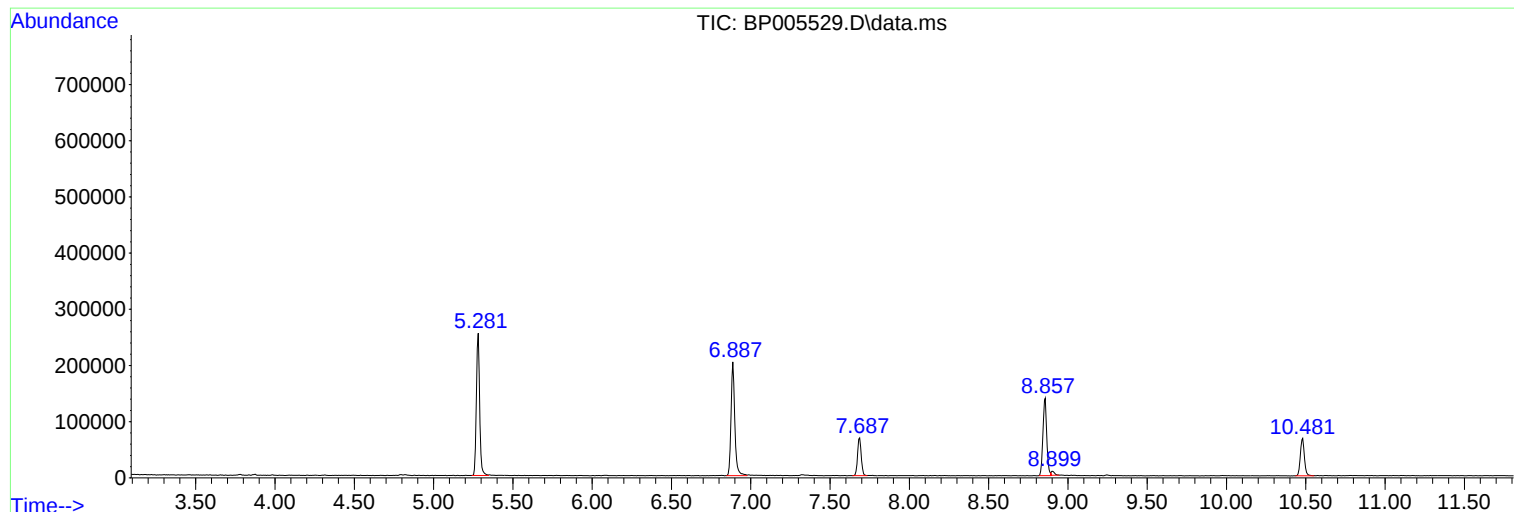
Sum of corrected areas: 4272692

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051321\
Data File : BP005529.D
Acq On : 13 May 2021 20:35
Operator : CG/JU
Sample : M2370-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
367

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.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\BP051321\
Data File : BP005529.D
Acq On : 13 May 2021 20:35
Operator : CG/JU
Sample : M2370-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
367

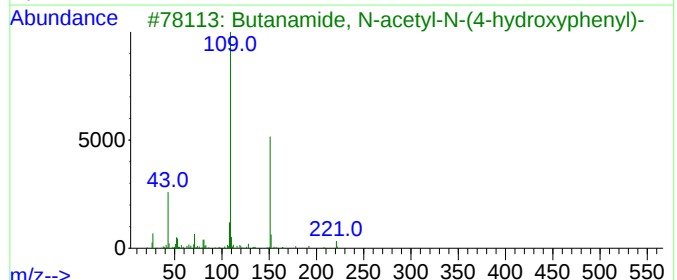
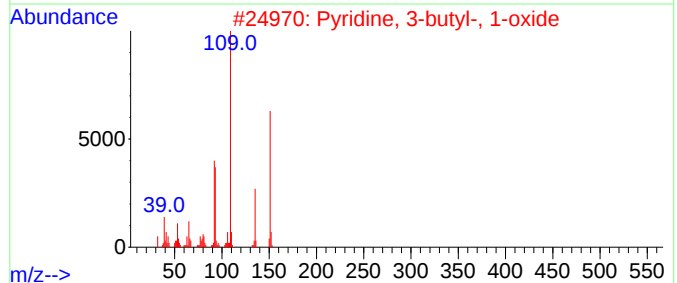
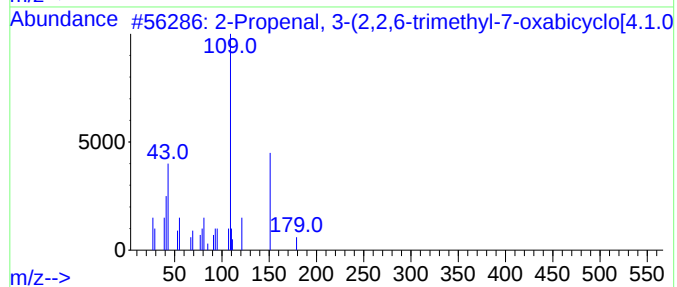
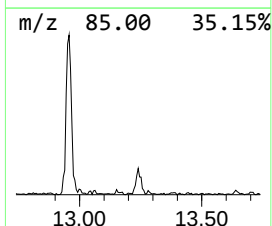
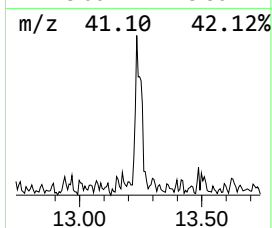
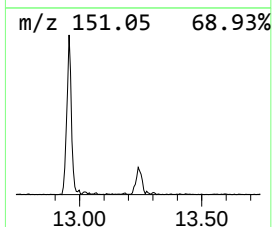
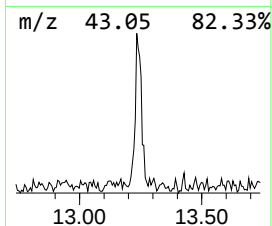
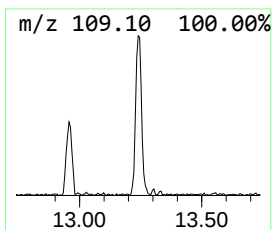
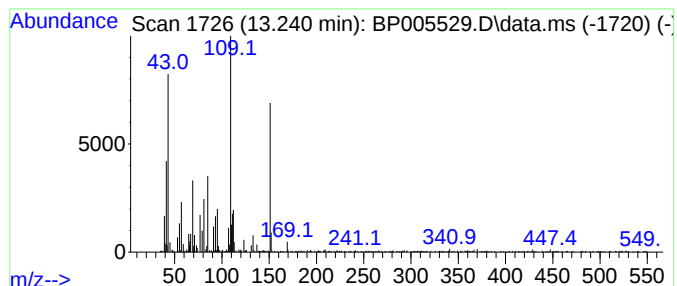
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Propenal, 3-(2,2,6-trimet... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.240	3.00 ng	20779	Acenaphthene-d10	14.334

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propenal, 3-(2,2,6-trimethyl-7...	194	C12H18O2	055759-91-6	50	
2	Pyridine, 3-butyl-, 1-oxide	151	C9H13NO	031396-33-5	47	
3	Butanamide, N-acetyl-N-(4-hydrox...	221	C12H15NO3	1000107-08-7	38	
4	Ethanone, 1-(1,4-dimethyl-3-cycl...	152	C10H16O	043219-68-7	38	
5	2,3-Dehydro-1,8-cineole	152	C10H16O	092760-25-3	35	



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051321\
Data File : BP005529.D
Acq On : 13 May 2021 20:35
Operator : CG/JU
Sample : M2370-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
367

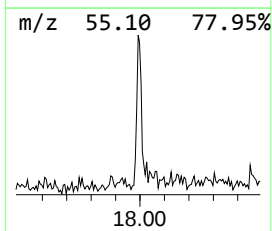
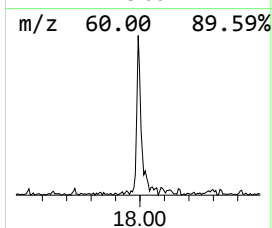
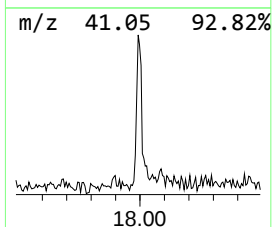
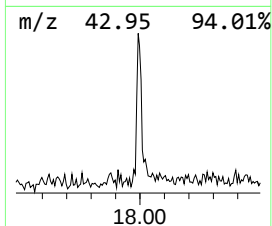
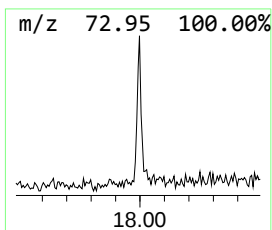
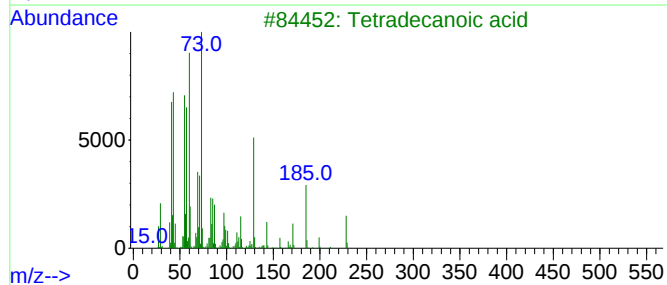
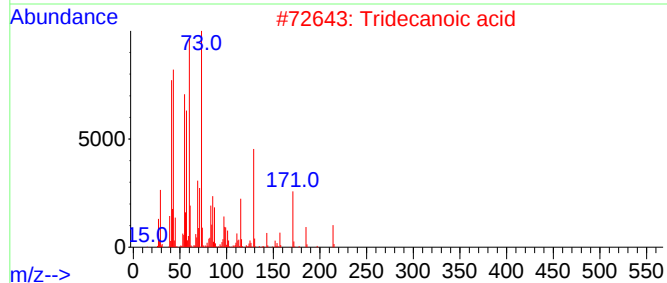
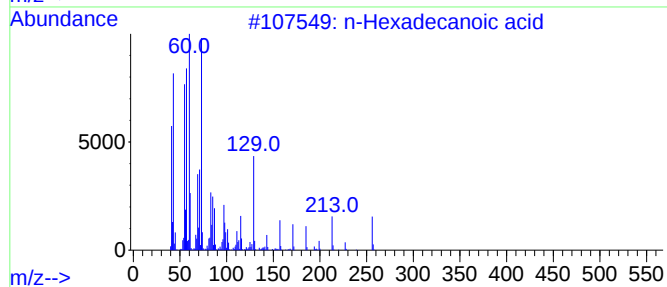
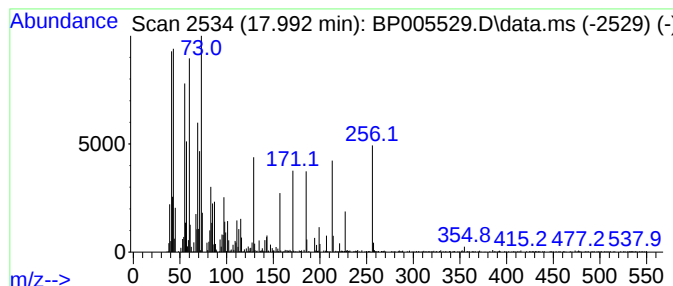
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.992	6.08 ng	52161	Phenanthrene-d10	17.092

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2			Tridecanoic acid	214	C13H26O2	000638-53-9	55
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	52
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	49
5			Dodecanoic acid	200	C12H24O2	000143-07-7	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051321\
Data File : BP005529.D
Acq On : 13 May 2021 20:35
Operator : CG/JU
Sample : M2370-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampled :
367

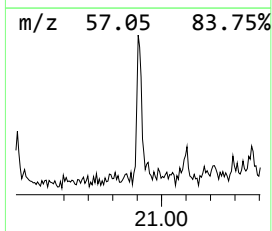
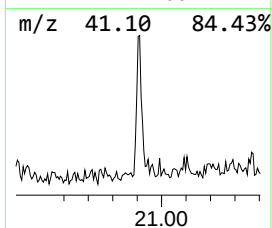
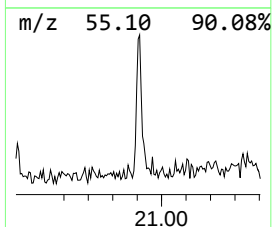
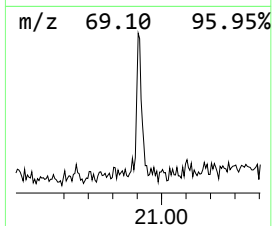
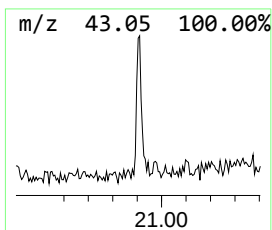
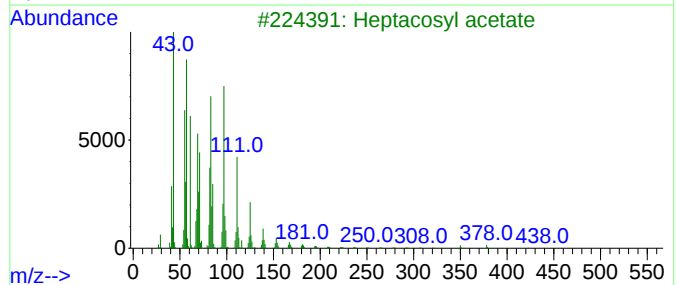
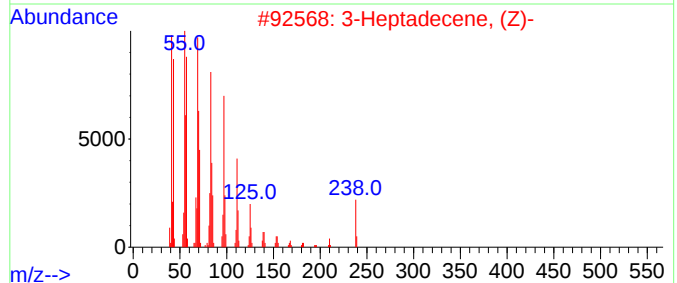
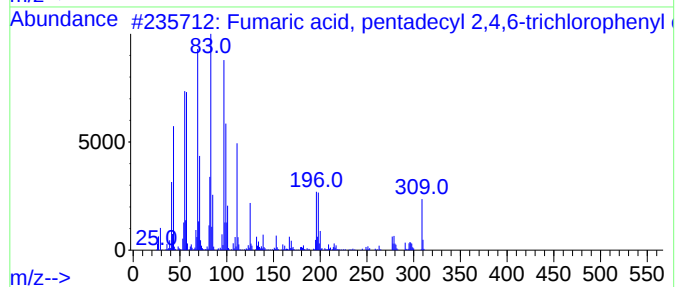
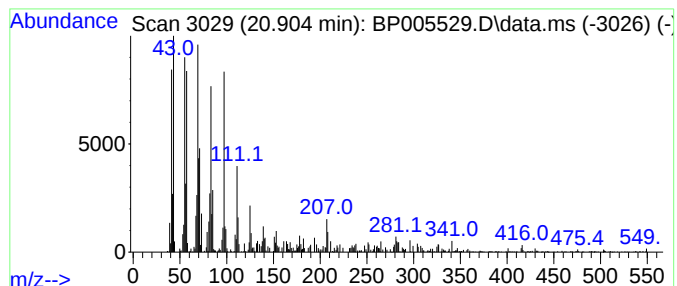
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Fumaric acid, pentadecyl 2,... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.904	5.43 ng	75530	Chrysene-d12	21.192

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Fumaric acid, pentadecyl 2,4,6-t...	504	C25H35Cl3O4	1000348-27-8	91
2			3-Heptadecene, (Z)-	238	C17H34	1000141-67-3	91
3			Heptacosyl acetate	438	C29H58O2	1000351-78-2	89
4			1-Octadecene	252	C18H36	000112-88-9	86
5			E-14-Hexadecenal	238	C16H30O	330207-53-9	78



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051321\
Data File : BP005529.D
Acq On : 13 May 2021 20:35
Operator : CG/JU
Sample : M2370-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
367

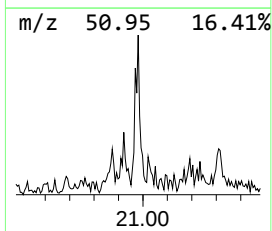
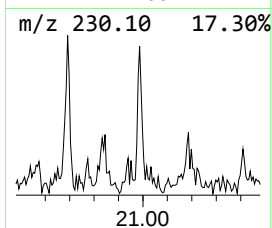
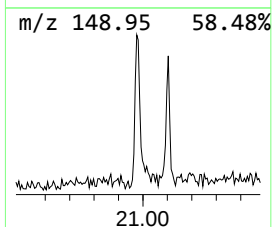
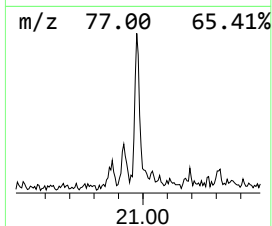
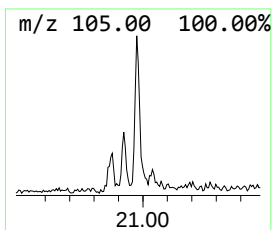
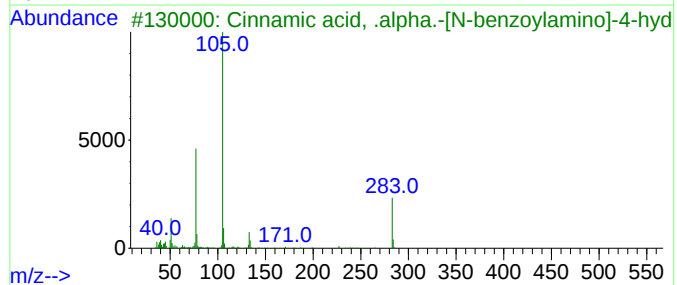
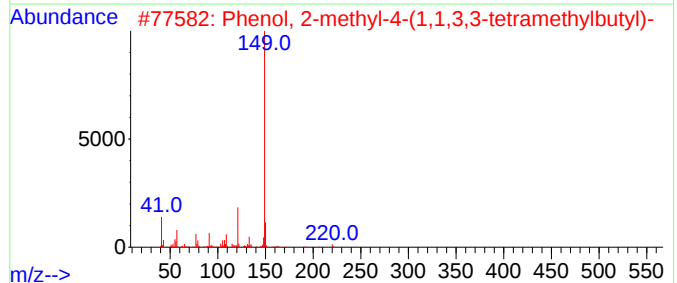
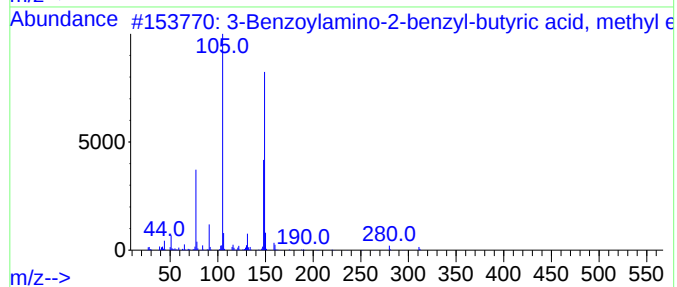
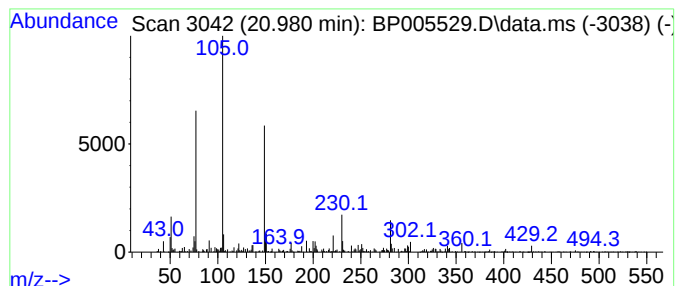
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 3-Benzoylamino-2-benzyl-but... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.980	2.35 ng	32704	Chrysene-d12	21.192

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Benzoylamino-2-benzyl-butyric ...	311	C19H21NO3	1000193-12-7	53
2			Phenol, 2-methyl-4-(1,1,3,3-tetr...	220	C15H24O	002219-84-3	27
3			Cinnamic acid, .alpha.-[N-benzoy...	283	C16H13NO4	1000301-68-3	25
4			Acethydrazide, 2-(2-methoxypheno...	300	C16H16N2O4	1000294-06-0	25
5			1,2-Benzenedicarboxylic acid, mo...	222	C12H14O4	000131-70-4	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051321\
Data File : BP005529.D
Acq On : 13 May 2021 20:35
Operator : CG/JU
Sample : M2370-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
367

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.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-Propenal, 3-(...	13.240	3.0	ng	20779	3	14.334	138500	20.0
n-Hexadecanoic ...	17.992	6.1	ng	52161	4	17.092	171714	20.0
Fumaric acid, p...	20.904	5.4	ng	75530	5	21.192	278344	20.0
3-Benzoylamino-...	20.980	2.4	ng	32704	5	21.192	278344	20.0