

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080521\
 Data File : BP006519.D
 Acq On : 05 Aug 2021 22:38
 Operator : CG/JU
 Sample : M3279-03
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 20210570-COM-43

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-BP080321.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP006519.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.905	304	309	319	rBV	2093161	2929672	25.85%	4.111%
2	5.358	380	386	401	rVB	5514181	7775864	68.60%	10.910%
3	5.970	484	490	498	rBV	440312	637538	5.62%	0.895%
4	6.940	647	655	664	rBV	5092991	8105478	71.51%	11.373%
5	7.758	787	794	801	rVB	858250	1361216	12.01%	1.910%
6	8.911	982	990	1002	rBV	3134994	5194021	45.82%	7.288%
7	10.328	1225	1231	1241	rBV	478037	769811	6.79%	1.080%
8	10.540	1259	1267	1274	rBV	1175893	1932685	17.05%	2.712%
9	13.010	1679	1687	1697	rBV	6525914	9185990	81.04%	12.889%
10	14.387	1910	1921	1929	rBV	1580069	2384575	21.04%	3.346%
11	15.875	2164	2174	2199	rBV	5247403	7617168	67.20%	10.688%
12	17.134	2382	2388	2401	rBV	1841973	2716800	23.97%	3.812%
13	18.039	2537	2542	2551	rBV	267582	391426	3.45%	0.549%
14	19.281	2749	2753	2763	rBV	175423	258345	2.28%	0.362%
15	19.539	2793	2797	2801	rVB3	111003	137606	1.21%	0.193%
16	19.710	2821	2826	2831	rBV	9879540	11334933	100.00%	15.904%
17	20.022	2876	2879	2883	rVB	118973	123309	1.09%	0.173%
18	20.510	2958	2962	2965	rBV	198068	221151	1.95%	0.310%
19	20.963	3034	3039	3049	rBV	535586	756502	6.67%	1.061%
20	21.233	3079	3085	3096	rVB	2242940	2968826	26.19%	4.166%
21	21.392	3109	3112	3118	rBV	266774	323846	2.86%	0.454%
22	21.845	3186	3189	3199	rVB	267541	377731	3.33%	0.530%
23	22.333	3268	3272	3277	rVB	197132	268566	2.37%	0.377%
24	22.463	3291	3294	3300	rVB	201440	283836	2.50%	0.398%
25	22.869	3360	3363	3369	rVB2	166333	238649	2.11%	0.335%
26	23.557	3473	3480	3489	rVB2	1487479	2975053	26.25%	4.174%

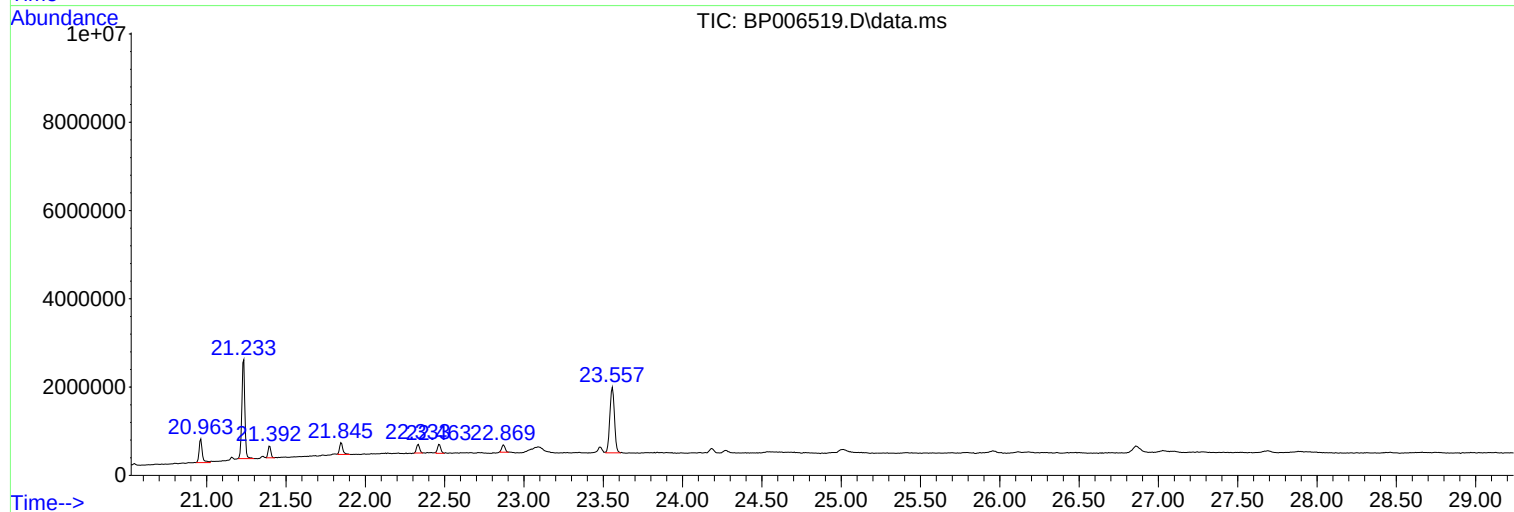
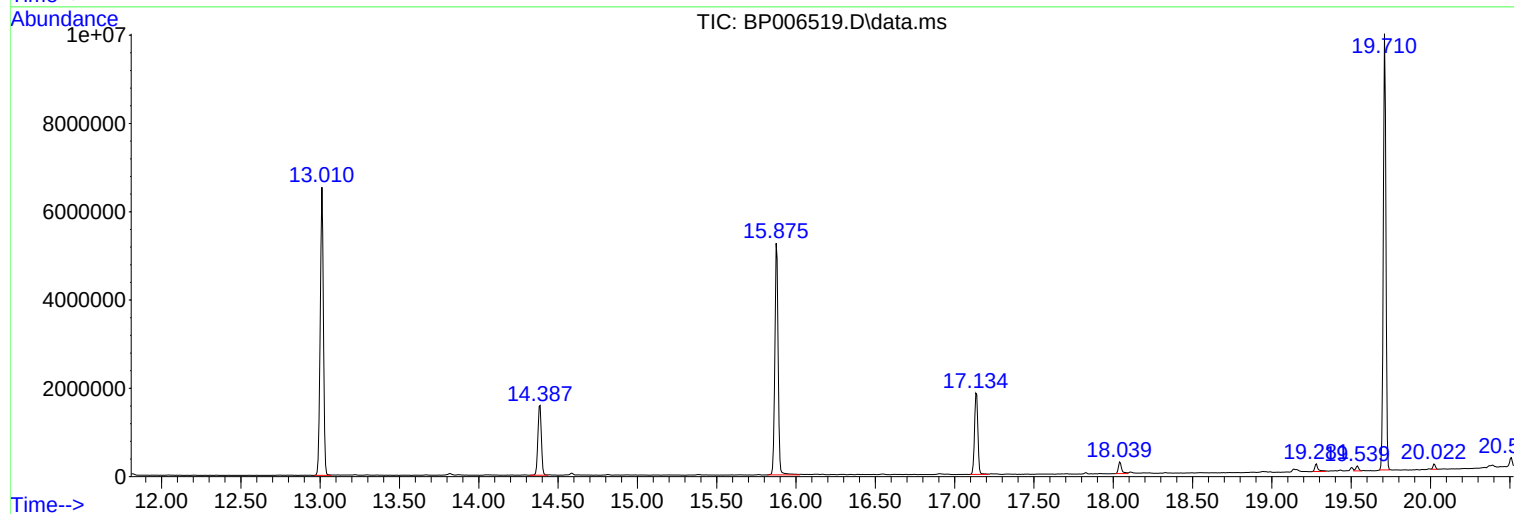
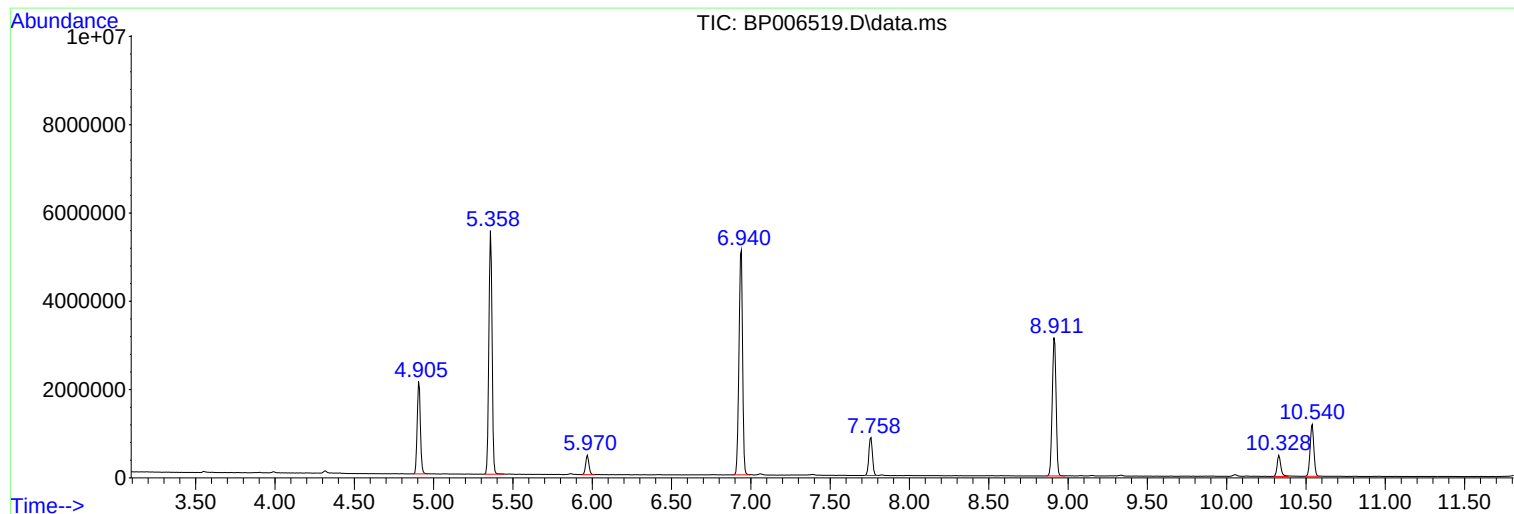
Sum of corrected areas: 71270597

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080521\
Data File : BP006519.D
Acq On : 05 Aug 2021 22:38
Operator : CG/JU
Sample : M3279-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20210570-COM-43

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080521\
Data File : BP006519.D
Acq On : 05 Aug 2021 22:38
Operator : CG/JU
Sample : M3279-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20210570-COM-43

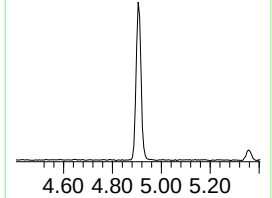
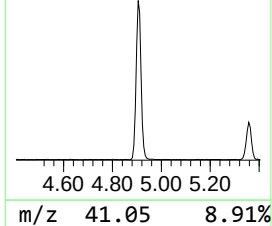
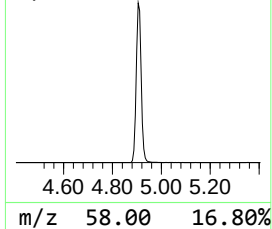
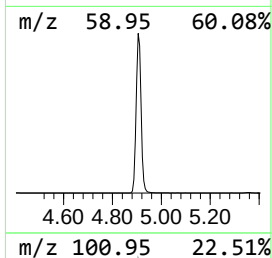
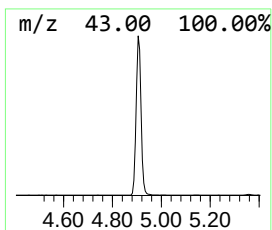
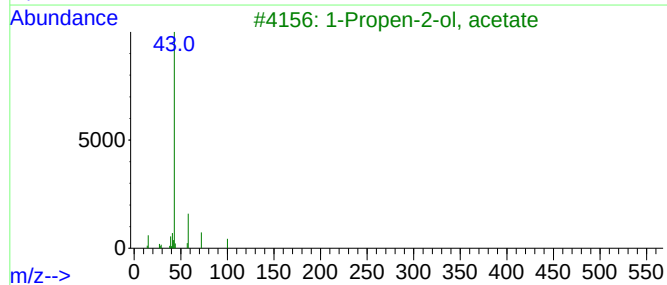
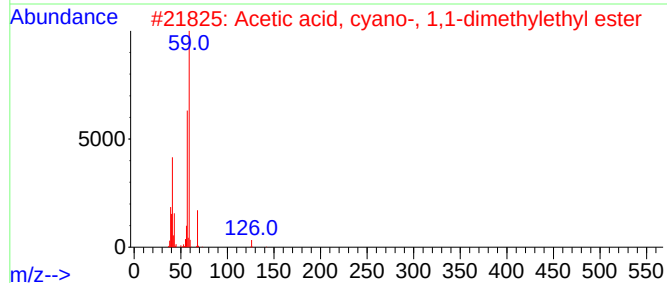
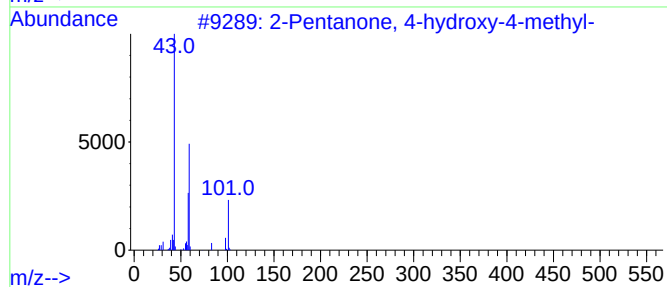
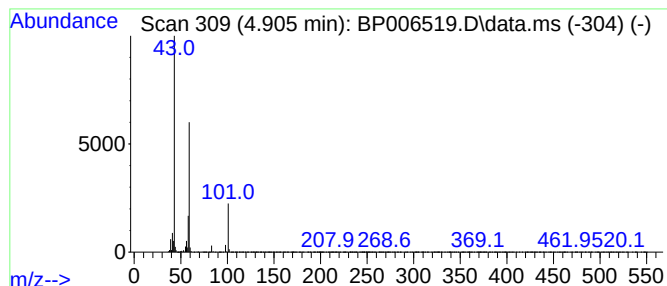
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.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.
4.905	43.04 ng	2929670	1,4-Dichlorobenzene-d4	7.758

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32		
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
4	Acetone	58	C3H6O	000067-64-1	10		
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080521\
Data File : BP006519.D
Acq On : 05 Aug 2021 22:38
Operator : CG/JU
Sample : M3279-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20210570-COM-43

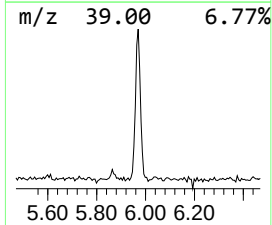
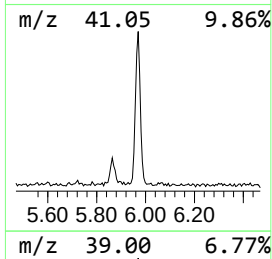
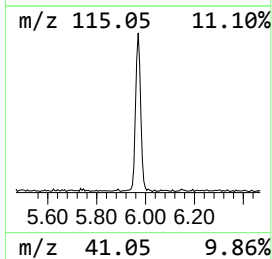
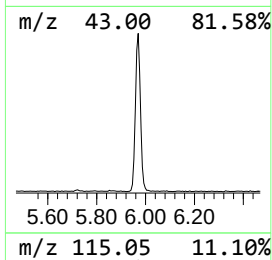
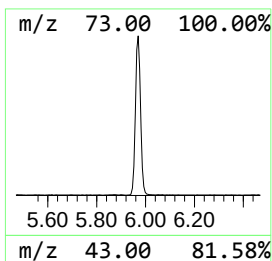
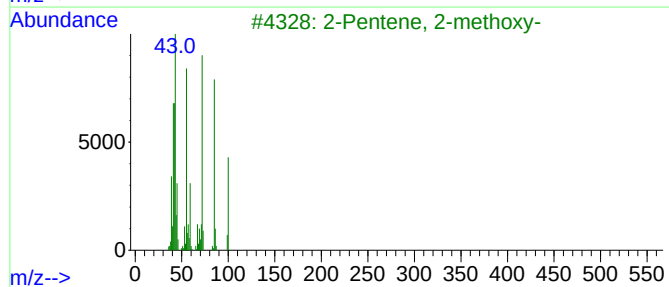
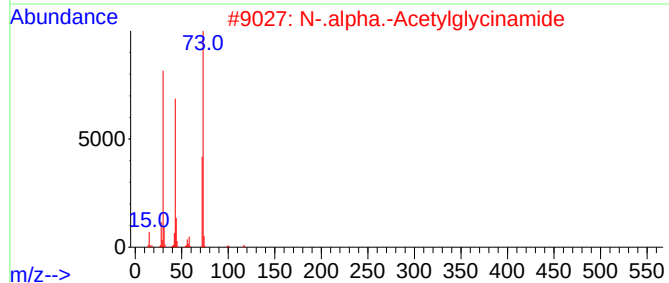
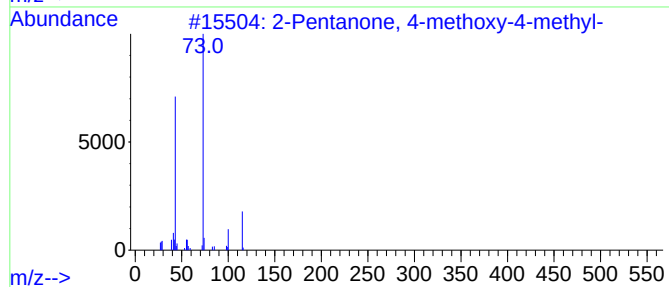
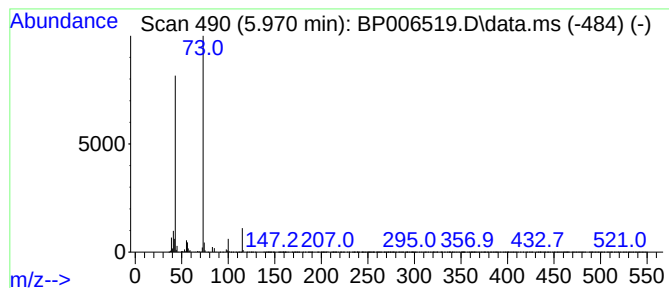
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-methoxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.970	9.37 ng	637538	1,4-Dichlorobenzene-d4	7.758

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2			N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	33
3			2-Pentene, 2-methoxy-	100	C6H12O	061142-47-0	14
4			Acetamide, N-butyl-	115	C6H13NO	001119-49-9	9
5			N-Formylmorpholine	115	C5H9NO2	004394-85-8	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080521\
Data File : BP006519.D
Acq On : 05 Aug 2021 22:38
Operator : CG/JU
Sample : M3279-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20210570-COM-43

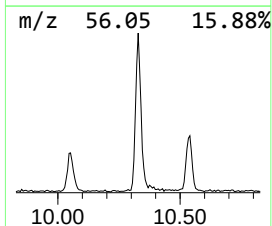
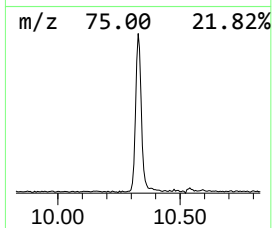
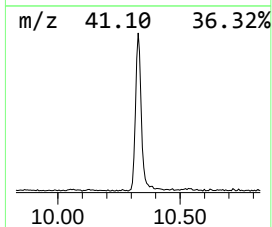
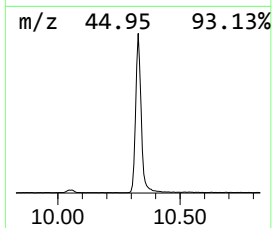
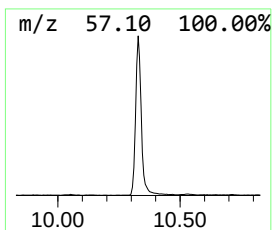
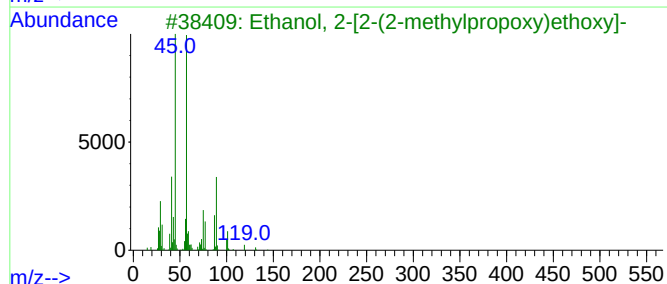
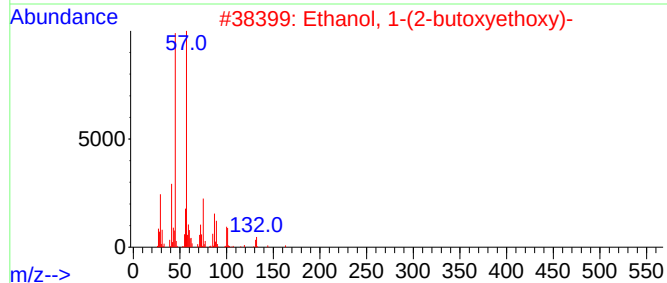
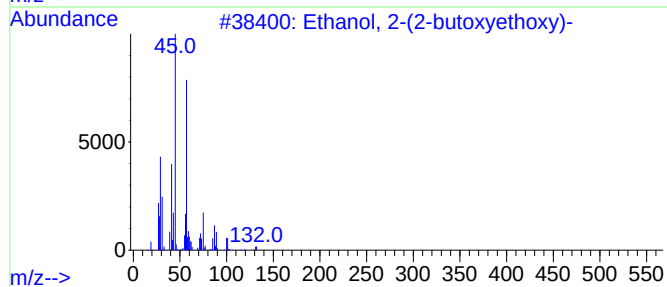
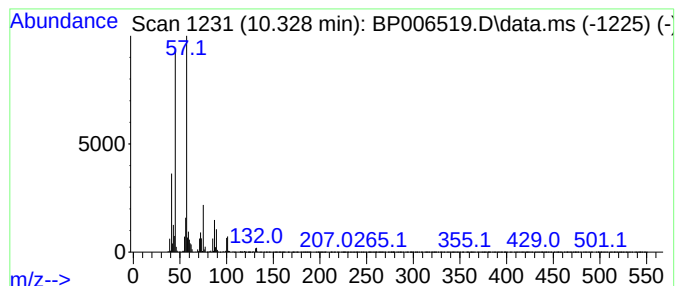
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.328	7.97 ng	769811	Naphthalene-d8	10.540

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			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	64
4			Propanoic acid, 2-(methoxymethoxy)-	134	C5H10O4	081327-29-9	47
5			Heptaethylene glycol	326	C14H30O8	005617-32-3	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080521\
Data File : BP006519.D
Acq On : 05 Aug 2021 22:38
Operator : CG/JU
Sample : M3279-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20210570-COM-43

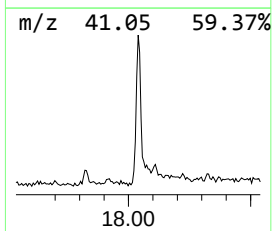
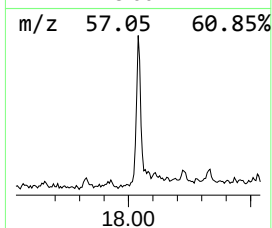
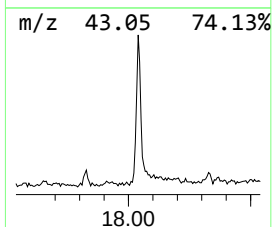
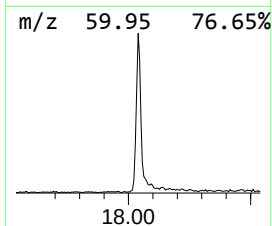
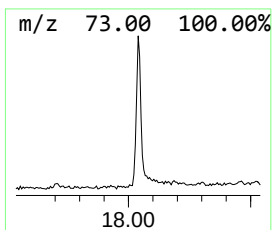
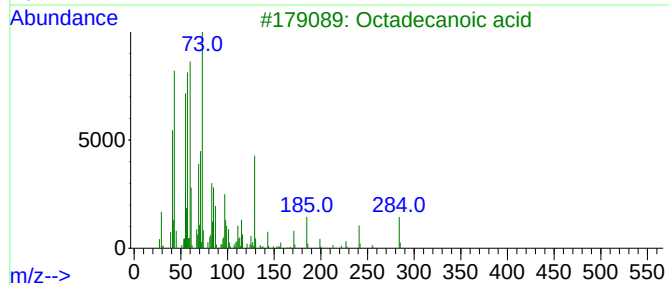
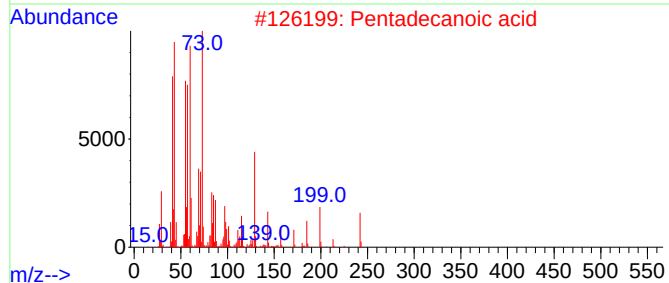
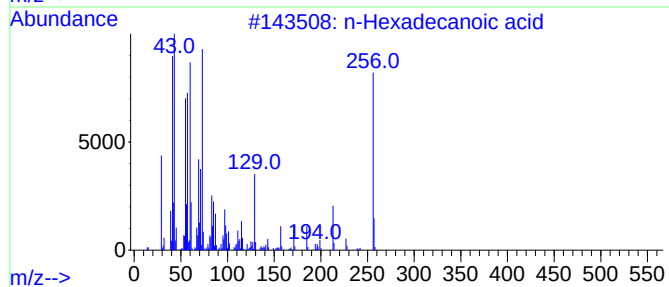
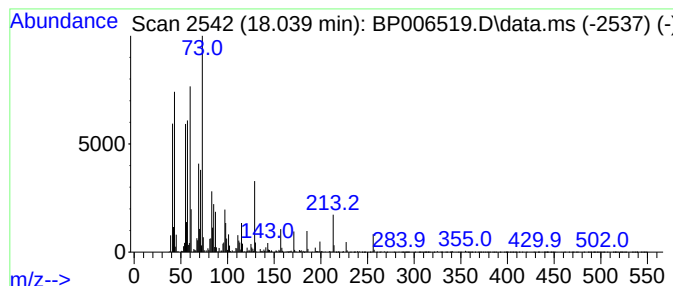
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.040	2.88 ng	391426	Phenanthrene-d10	17.134

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	90
3	Octadecanoic acid	284	C18H36O2	000057-11-4	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Isopropyl palmitate	298	C19H38O2	000142-91-6	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080521\
Data File : BP006519.D
Acq On : 05 Aug 2021 22:38
Operator : CG/JU
Sample : M3279-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20210570-COM-43

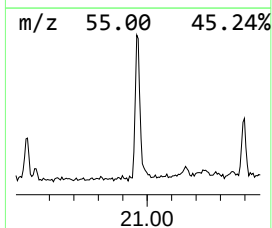
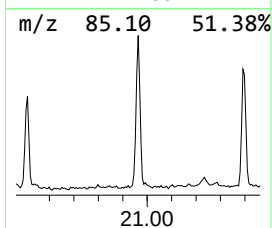
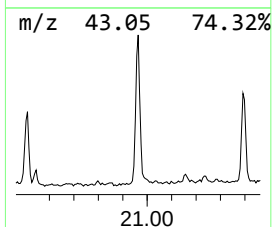
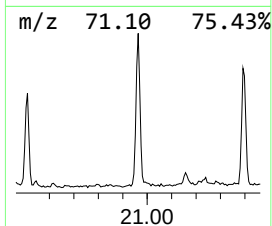
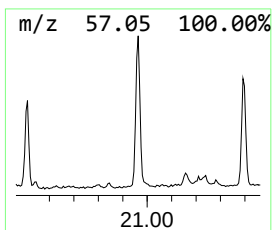
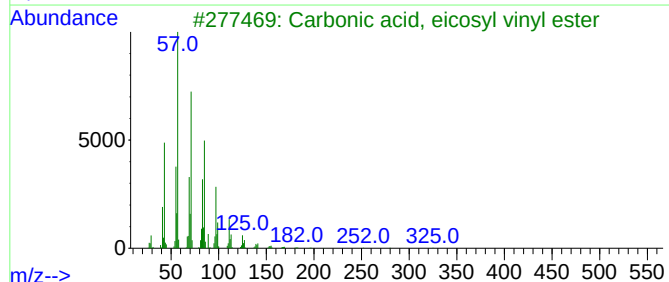
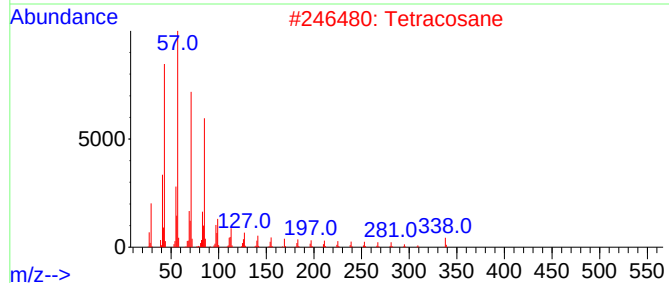
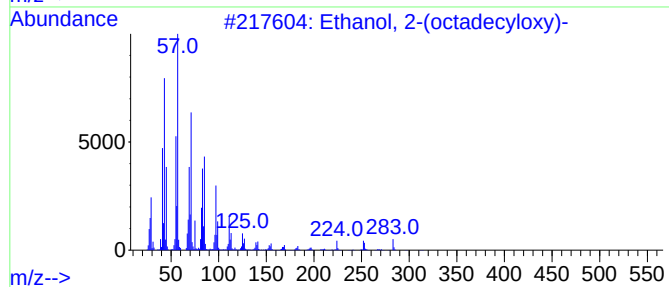
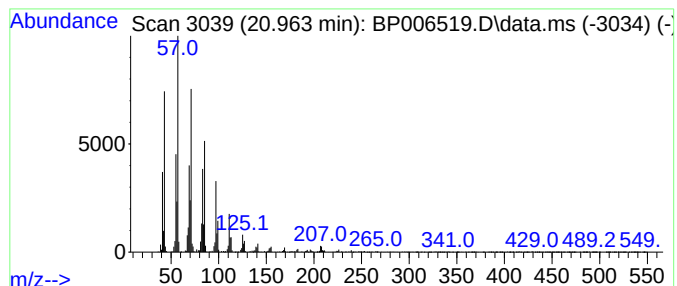
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Ethanol, 2-(octadecyloxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.963	5.10 ng	756502	Chrysene-d12	21.233

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(octadecyloxy)-	314	C20H42O2	002136-72-3	93
2			Tetracosane	338	C24H50	000646-31-1	92
3			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	91
4			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	91
5			Carbonic acid, hexadecyl prop-1-...	326	C20H38O3	1000382-90-3	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080521\
Data File : BP006519.D
Acq On : 05 Aug 2021 22:38
Operator : CG/JU
Sample : M3279-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20210570-COM-43

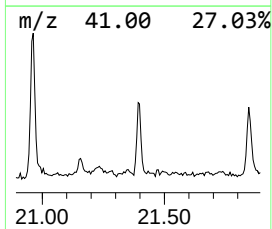
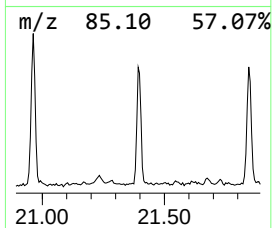
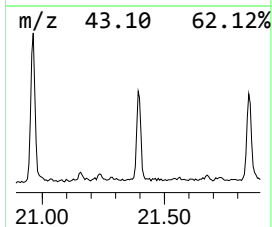
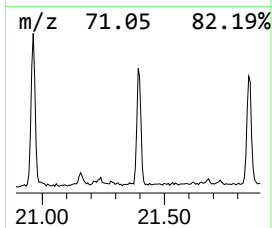
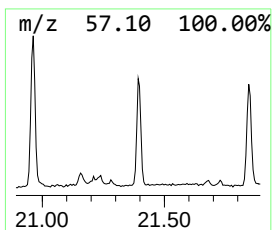
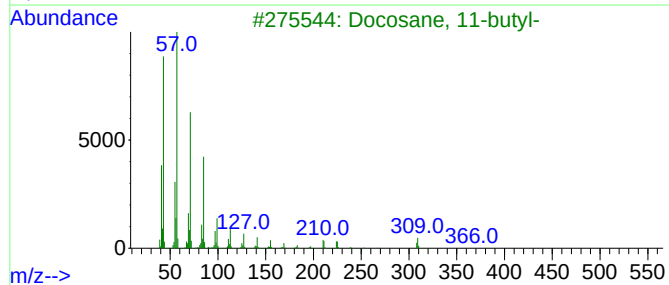
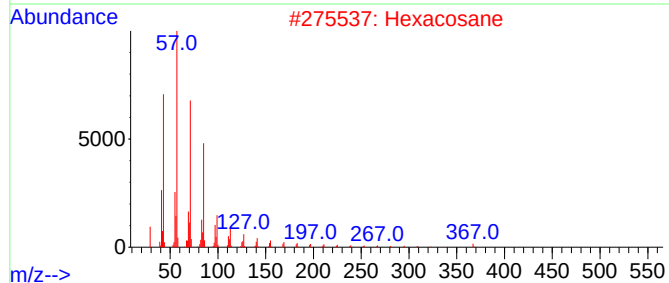
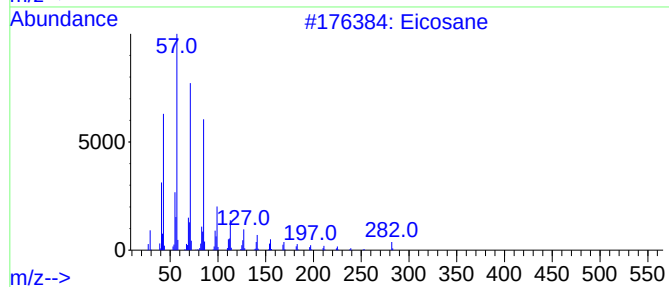
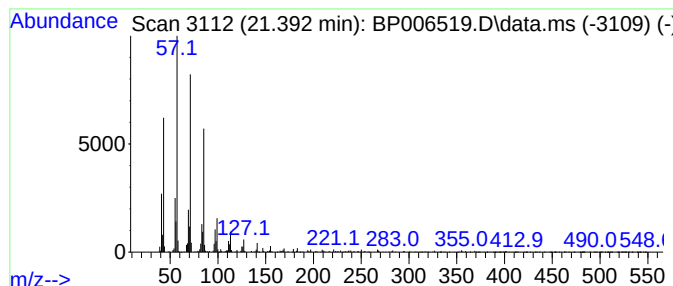
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.392	2.18 ng	323846	Chrysene-d12	21.233

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane			282	C20H42	000112-95-8	97
2	Hexacosane			366	C26H54	000630-01-3	91
3	Docosane, 11-butyl-			366	C26H54	013475-76-8	90
4	Tetracosane			338	C24H50	000646-31-1	90
5	Heptacosane			380	C27H56	000593-49-7	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080521\
Data File : BP006519.D
Acq On : 05 Aug 2021 22:38
Operator : CG/JU
Sample : M3279-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20210570-COM-43

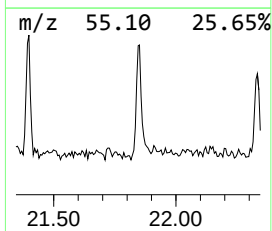
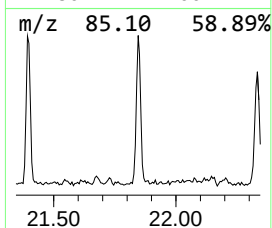
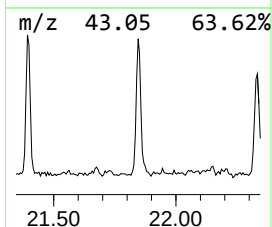
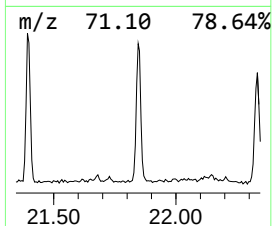
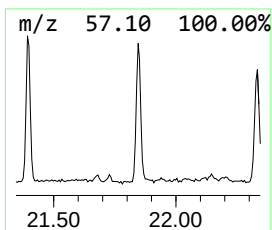
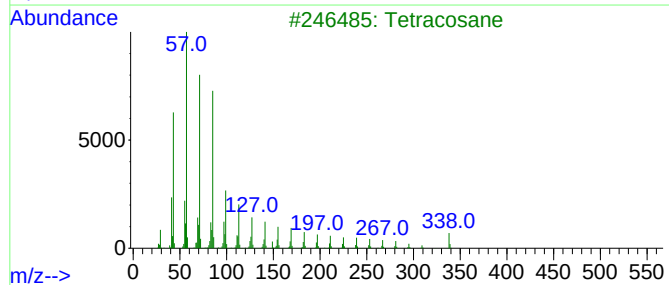
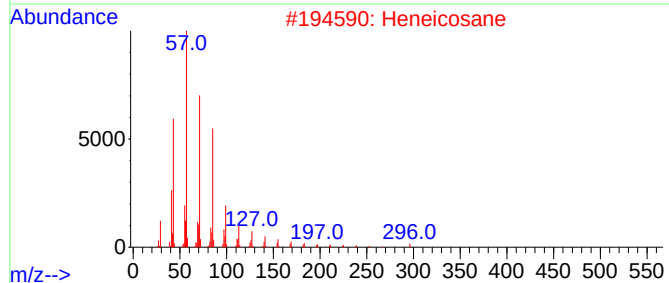
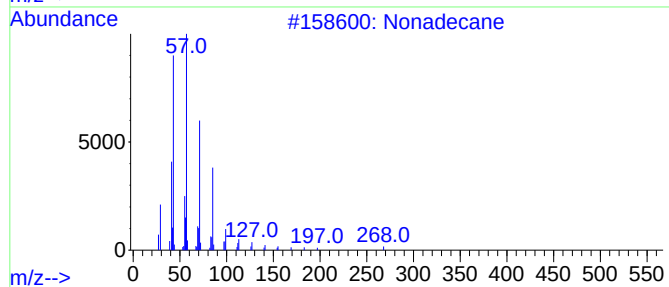
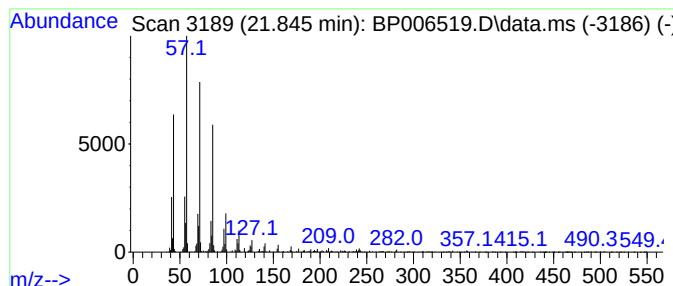
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Nonadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.845	2.54 ng	377731	Chrysene-d12	21.233

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	94
2			Heneicosane	296	C21H44	000629-94-7	91
3			Tetracosane	338	C24H50	000646-31-1	91
4			Heptadecane	240	C17H36	000629-78-7	91
5			Hexacosane	366	C26H54	000630-01-3	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080521\
Data File : BP006519.D
Acq On : 05 Aug 2021 22:38
Operator : CG/JU
Sample : M3279-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20210570-COM-43

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.905	43.0	ng	2929670	1	7.758	1361220	20.0
2-Pentanone, 4-...	5.970	9.4	ng	637538	1	7.758	1361220	20.0
Ethanol, 2-(2-b...	10.328	8.0	ng	769811	2	10.540	1932690	20.0
n-Hexadecanoic ...	18.040	2.9	ng	391426	4	17.134	2716800	20.0
Ethanol, 2-(oct...	20.963	5.1	ng	756502	5	21.233	2968830	20.0
Eicosane	21.392	2.2	ng	323846	5	21.233	2968830	20.0
Nonadecane	21.845	2.5	ng	377731	5	21.233	2968830	20.0