

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062222\
 Data File : BF128935.D
 Acq On : 22 Jun 2022 16:56
 Operator : CG\JU
 Sample : N3384-03
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC-4

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_F\Methods\8270-BF060222.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF128935.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.804	81	88	98	rBV	74697	121756	2.48%	0.502%
2	4.957	451	454	463	rVB	53545	66163	1.35%	0.273%
3	5.387	523	527	542	rBV	1504541	1601797	32.67%	6.599%
4	6.398	696	699	710	rBV	924970	989839	20.19%	4.078%
5	6.745	754	758	762	rBV	758168	632298	12.90%	2.605%
6	7.316	849	855	858	rBV	2029095	2472933	50.43%	10.188%
7	8.028	971	976	983	rVB	918242	841944	17.17%	3.468%
8	8.257	1010	1015	1017	rBV	249917	245848	5.01%	1.013%
9	8.286	1017	1020	1028	rVB	223969	295373	6.02%	1.217%
10	8.910	1117	1126	1130	rBV	95113	90900	1.85%	0.374%
11	9.110	1153	1160	1163	rBV	4934053	4903337	100.00%	20.200%
12	9.780	1269	1274	1278	rVB	978967	934535	19.06%	3.850%
13	10.580	1404	1410	1413	rBV	2739582	2633114	53.70%	10.847%
14	11.251	1520	1524	1525	rBV	400535	353517	7.21%	1.456%
15	11.269	1525	1527	1531	rVB	1137313	979276	19.97%	4.034%
16	11.557	1571	1576	1585	rVB10	18119	49620	1.01%	0.204%
17	11.663	1590	1594	1599	rVB	149962	142542	2.91%	0.587%
18	11.804	1615	1618	1621	rBV	95571	110672	2.26%	0.456%
19	12.369	1708	1714	1723	rVB	211982	195121	3.98%	0.804%
20	12.457	1726	1729	1732	rBV	77907	62388	1.27%	0.257%
21	12.863	1793	1798	1801	rBV	4287464	4638298	94.59%	19.108%
22	13.798	1952	1957	1970	rBV3	106639	267706	5.46%	1.103%
23	13.915	1973	1977	1981	rVB	1012338	863829	17.62%	3.559%
24	14.010	1987	1993	1999	rVB	111195	111189	2.27%	0.458%
25	15.357	2217	2222	2231	rBV	519718	670078	13.67%	2.760%

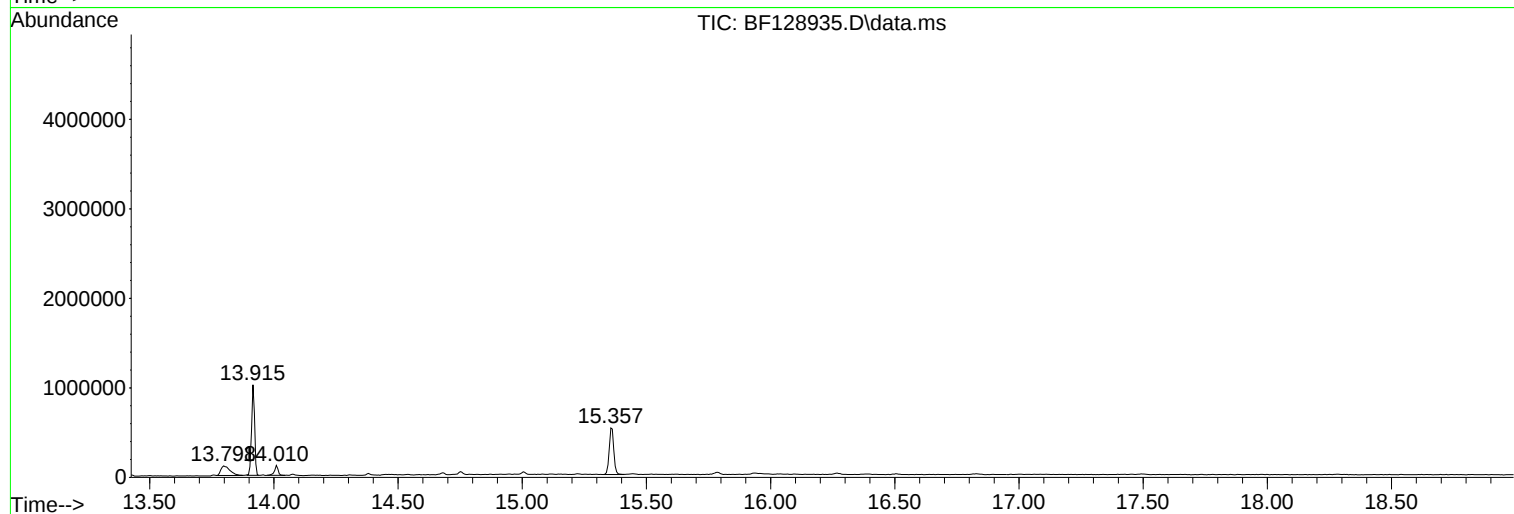
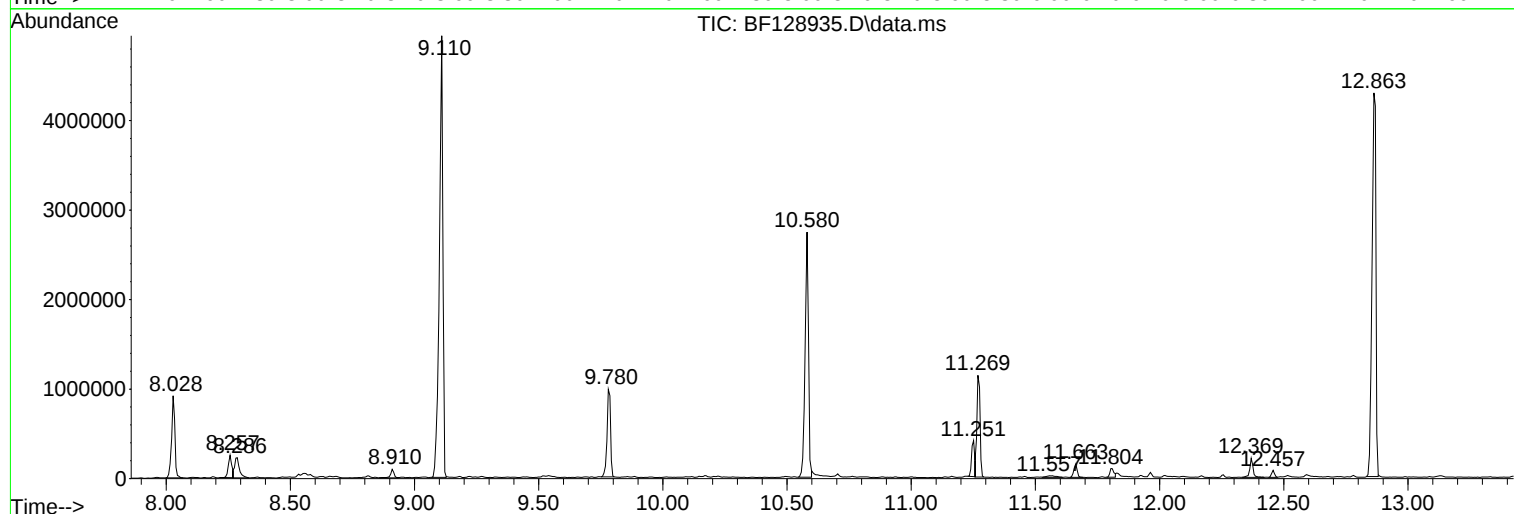
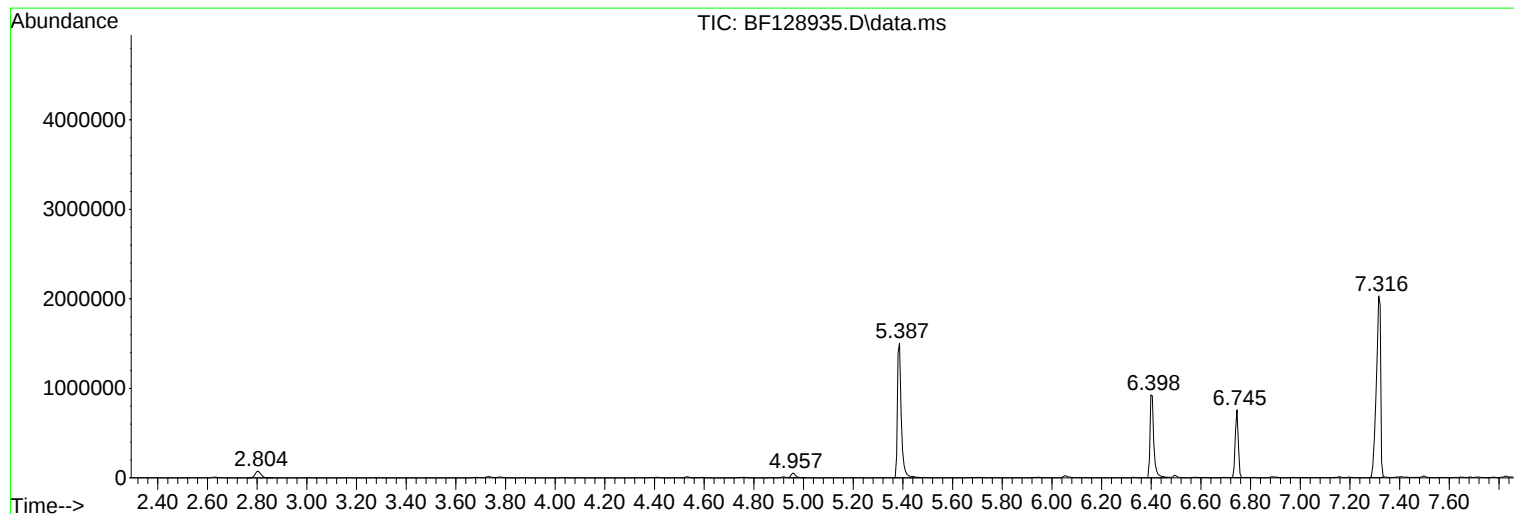
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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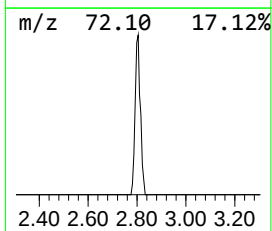
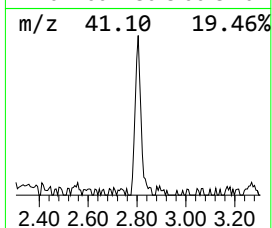
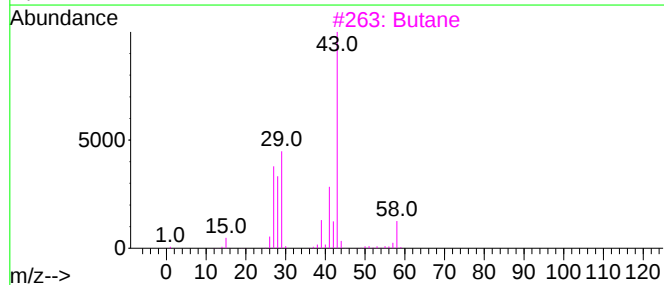
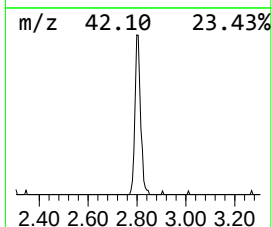
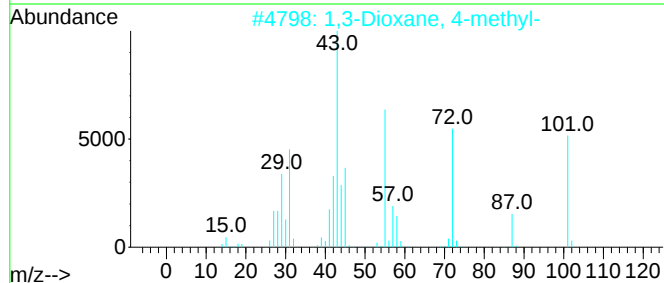
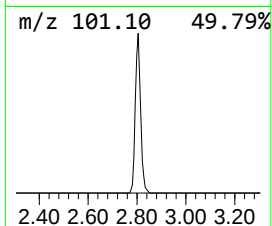
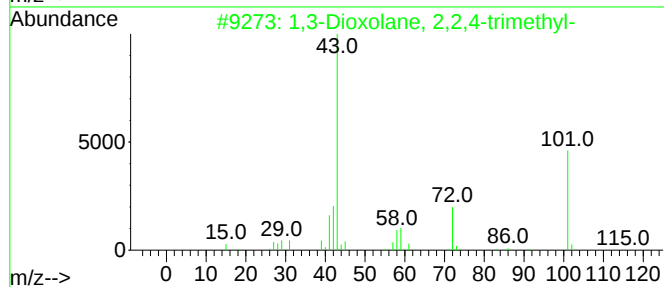
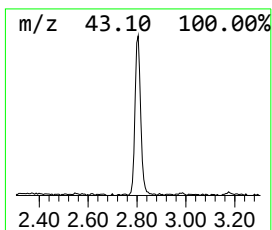
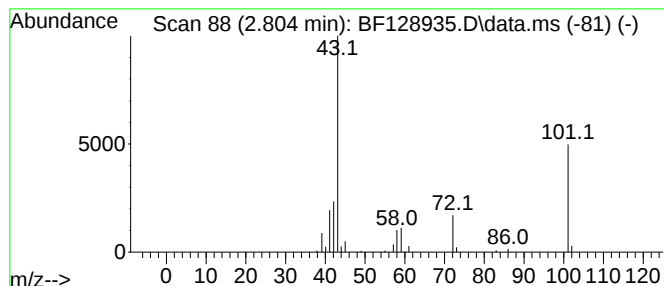
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 1,3-Dioxolane, 2,2,4-trimet... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.804	3.85 ng	121756	1,4-Dichlorobenzene-d4	6.745

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxolane, 2,2,4-trimethyl-	116	C6H12O2	001193-11-9	90
2			1,3-Dioxane, 4-methyl-	102	C5H10O2	001120-97-4	50
3			Butane	58	C4H10	000106-97-8	10
4			Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	9
5			Thiocyanic acid, propyl ester	101	C4H7NS	004251-16-5	9



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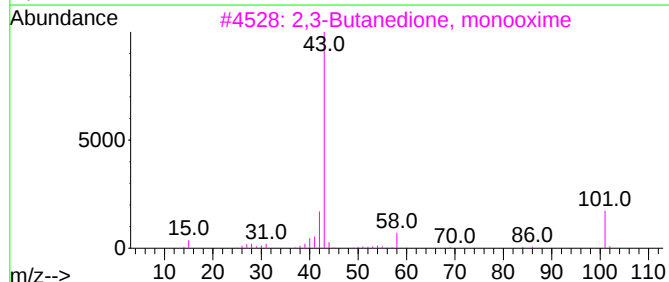
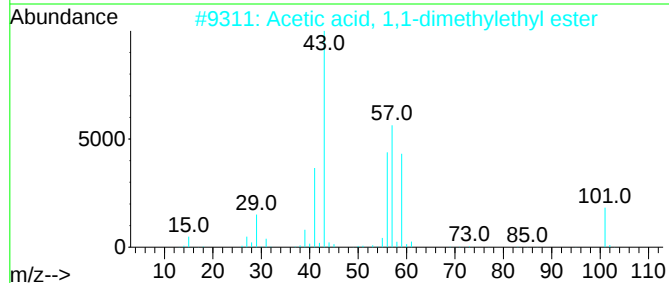
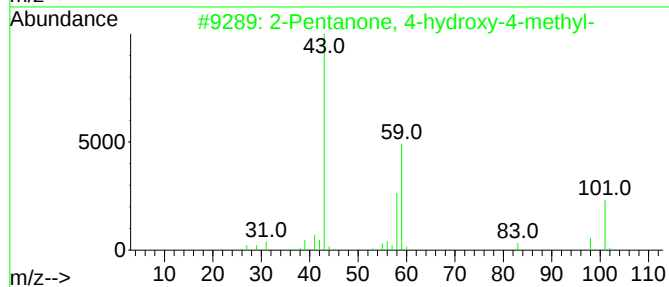
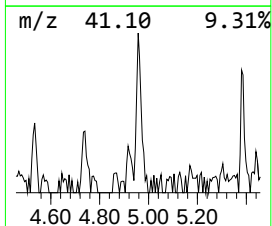
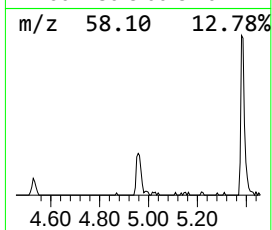
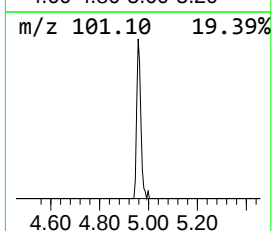
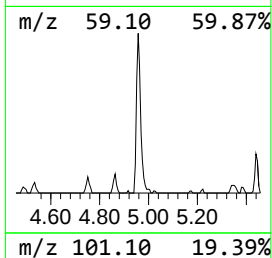
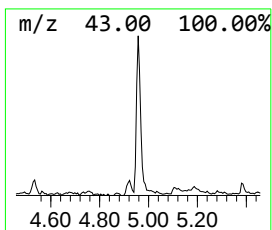
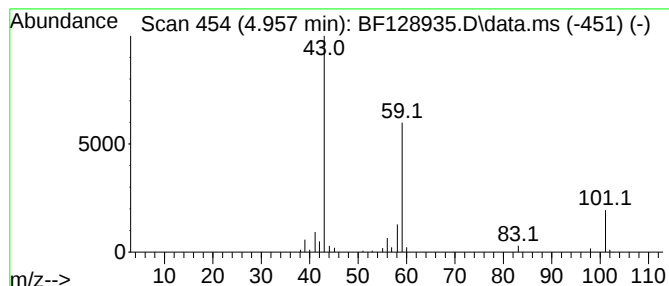
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.957	2.09 ng	66163	1,4-Dichlorobenzene-d4	6.745

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39		
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35		
4	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	17		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		



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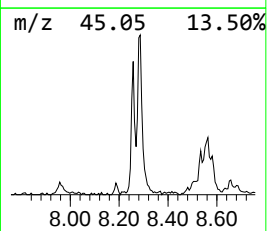
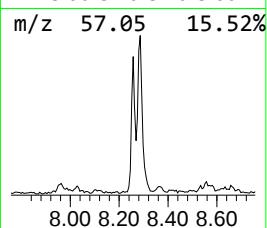
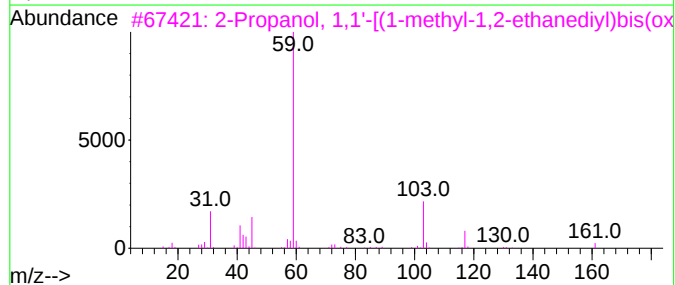
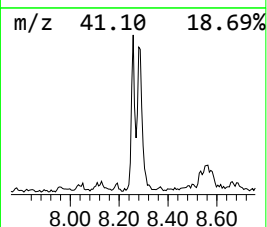
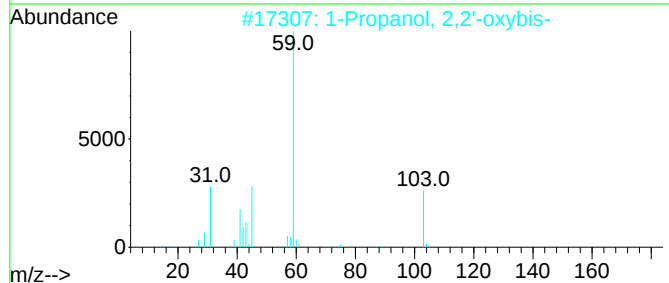
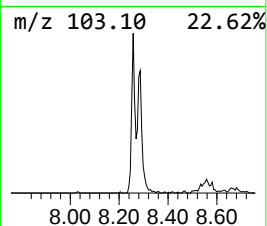
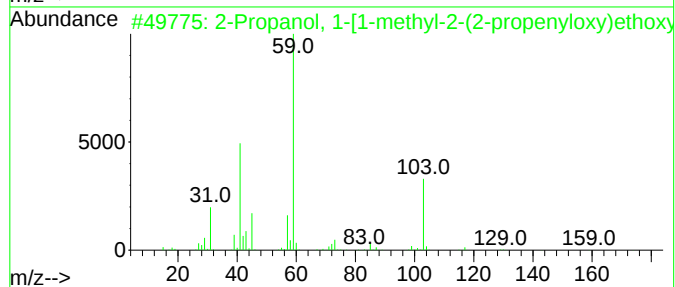
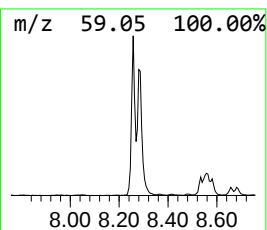
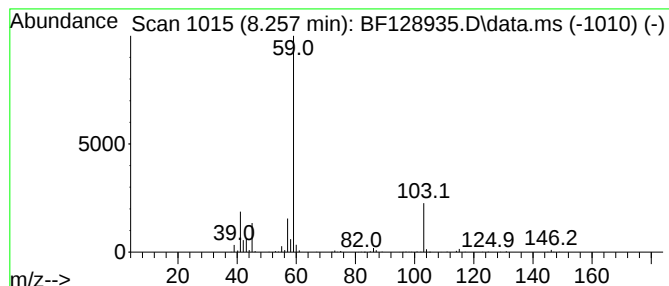
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Propanol, 1-[1-methyl-2-(... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.257	5.84 ng	245848	Naphthalene-d8	8.028

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	83		
2	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	78		
3	2-Propanol, 1,1'-[(1-methyl-1,2-...	192	C9H20O4	001638-16-0	78		
4	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	72		
5	1-(1-tert-Butoxypropan-2-yloxy)p...	190	C10H22O3	132739-31-2	72		



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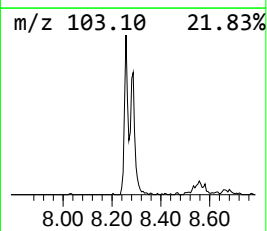
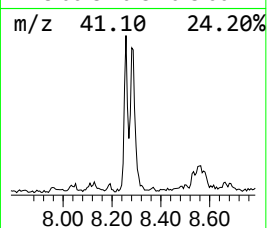
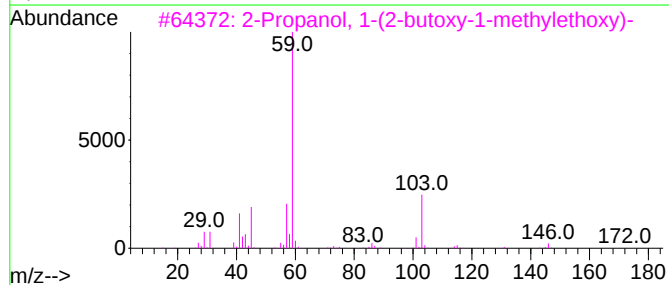
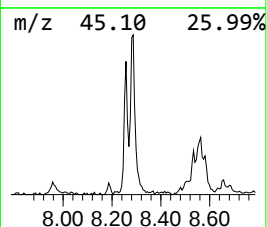
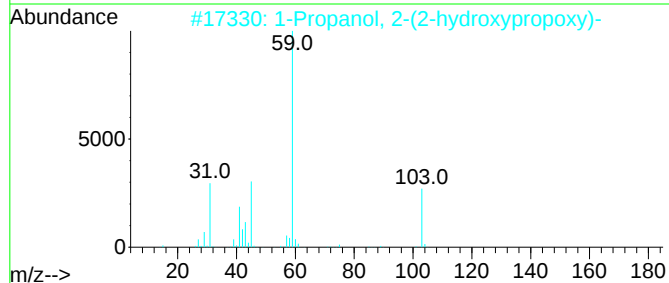
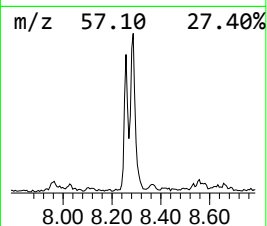
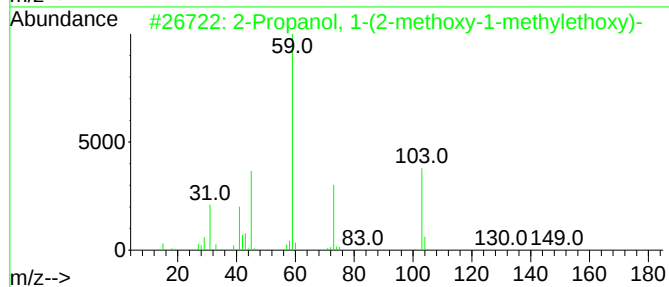
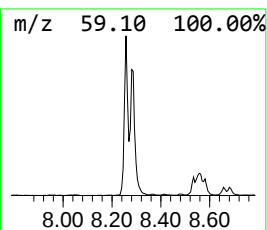
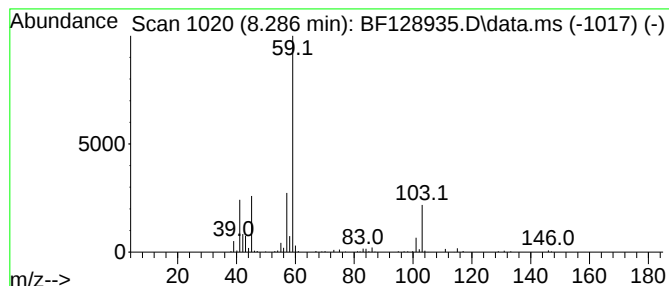
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Peak Number 4 2-Propanol, 1-(2-methoxy-1-... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.286	7.02 ng	295373	Naphthalene-d8	8.028

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	72		
2	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	72		
3	2-Propanol, 1-(2-butoxy-1-methyl...	190	C10H22O3	029911-28-2	56		
4	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	56		
5	Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	56		



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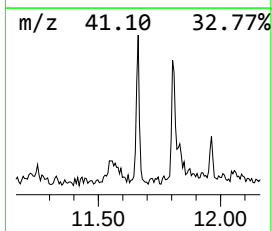
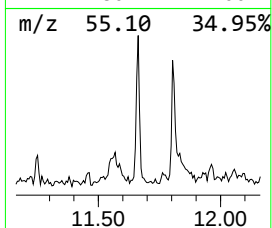
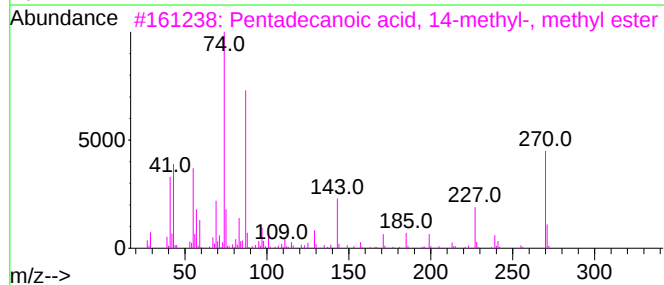
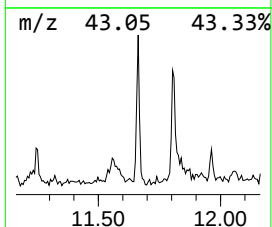
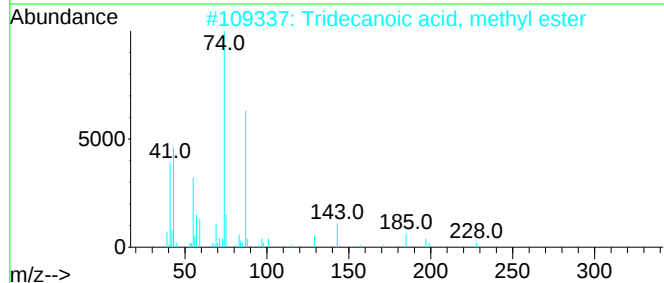
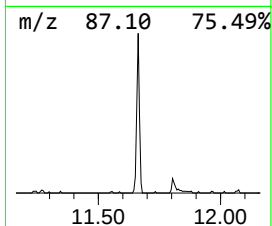
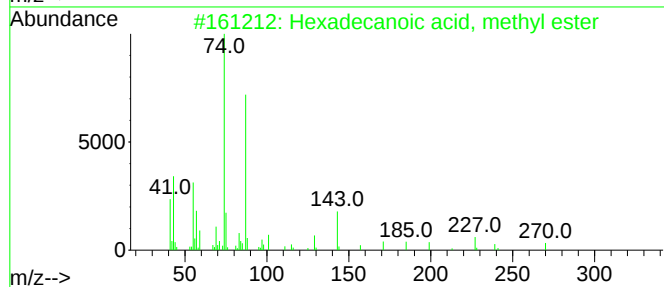
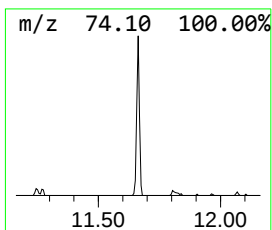
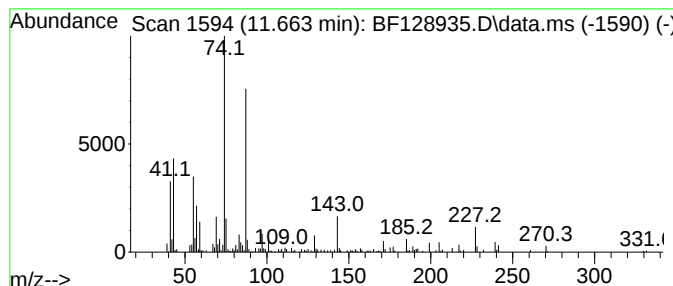
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Peak Number 5 Hexadecanoic acid, methyl e... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.663	2.91 ng	142542	Phenanthrene-d10	11.269	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	96
2	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	93
3	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	93
4	Undecanoic acid, 10-methyl-, met...	214	C13H26O2	005129-56-6	80
5	Hexadecanoic acid, 2-methyl-	270	C17H34O2	027147-71-3	80



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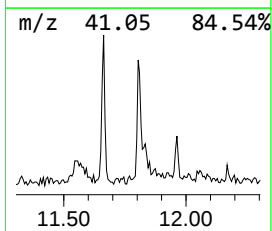
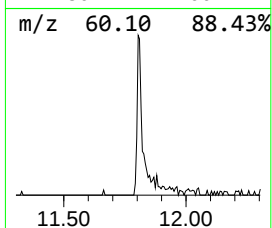
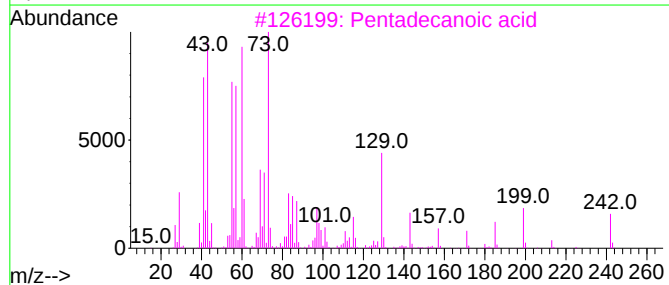
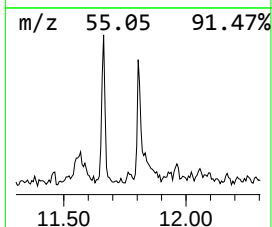
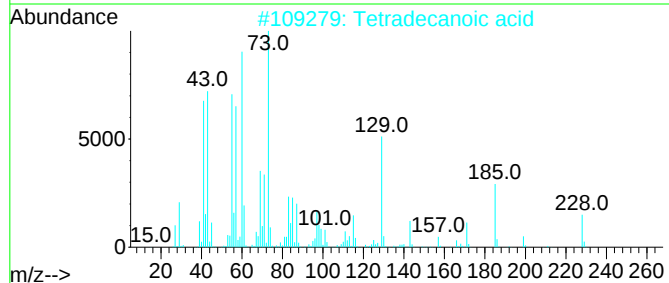
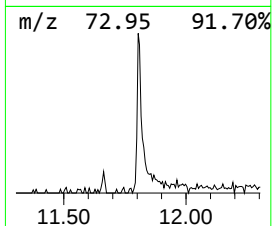
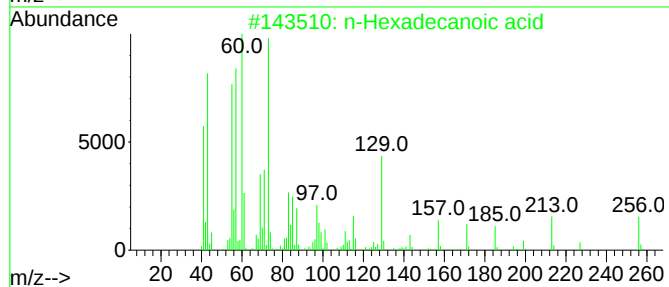
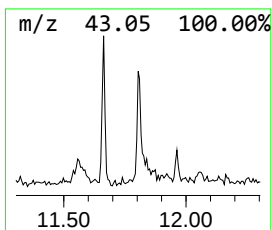
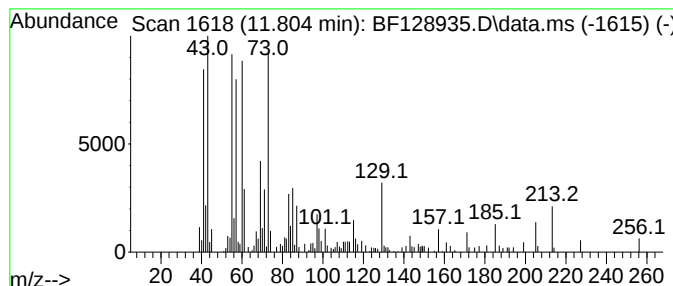
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.804	2.26 ng	110672	Phenanthrene-d10	11.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	62
4			Dodecanoic acid	200	C12H24O2	000143-07-7	58
5			n-Decanoic acid	172	C10H20O2	000334-48-5	55



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062222\
Data File : BF128935.D
Acq On : 22 Jun 2022 16:56
Operator : CG\JU
Sample : N3384-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

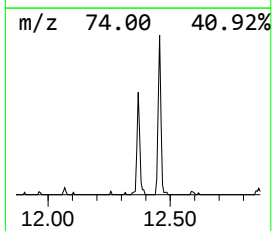
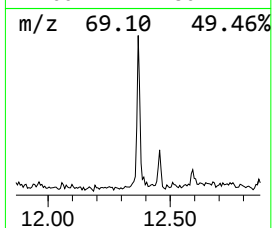
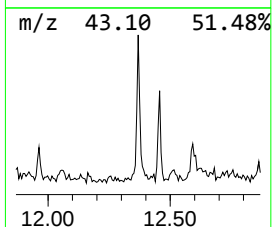
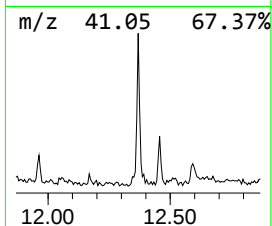
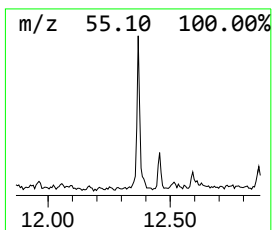
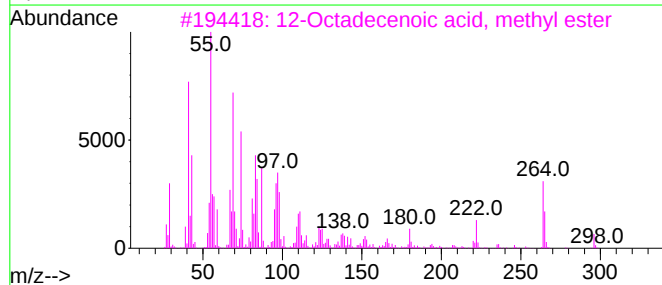
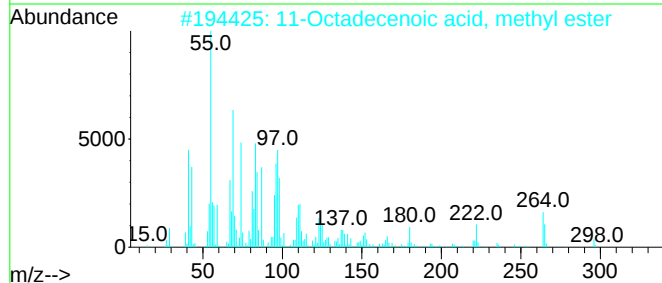
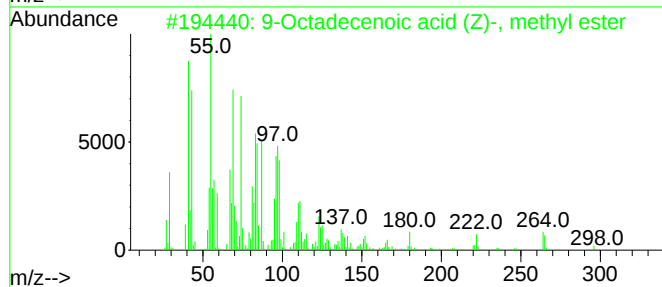
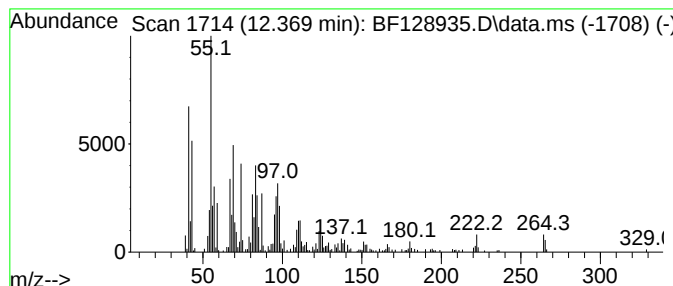
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ClientSampleId :
WC-4

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 9-Octadecenoic acid (Z)-, m... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.368	3.99 ng	195121	Phenanthrene-d10	11.269	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	95
2	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	91
3	12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	91
4	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	91
5	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062222\
Data File : BF128935.D
Acq On : 22 Jun 2022 16:56
Operator : CG\JU
Sample : N3384-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

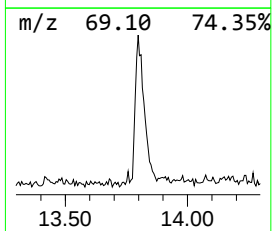
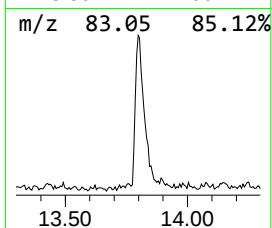
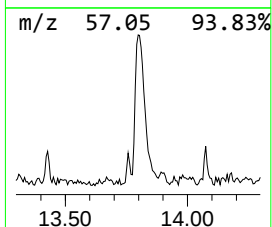
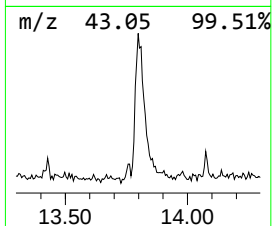
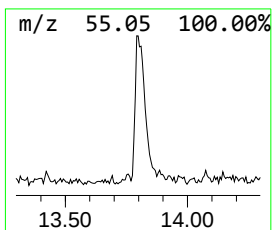
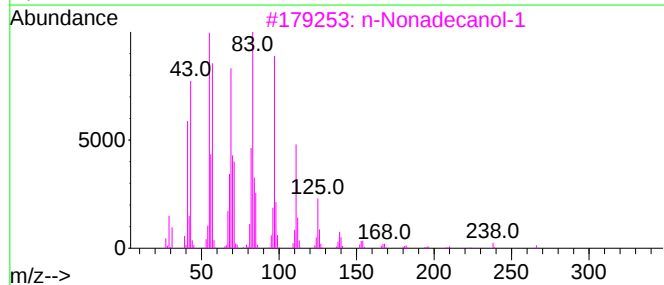
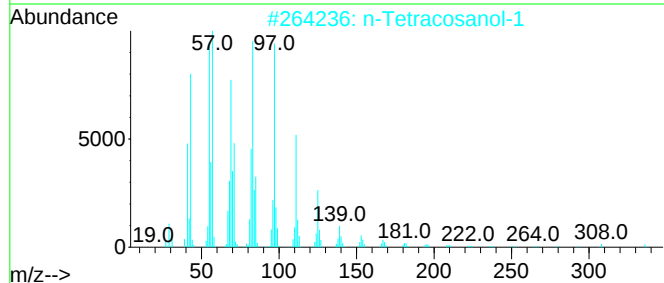
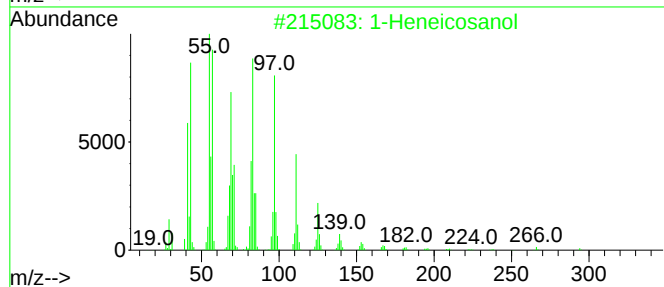
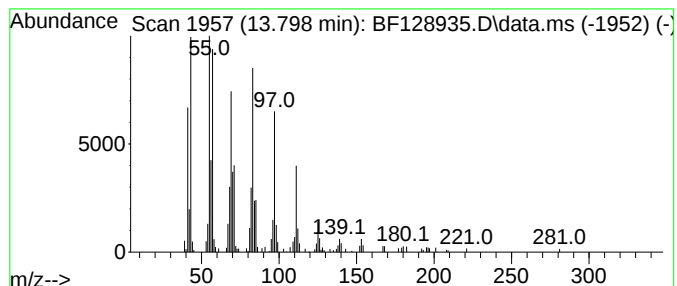
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Heneicosanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.798	6.20 ng	267706	Chrysene-d12	13.916	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	94
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	91
4	Behenic alcohol	326	C22H46O	000661-19-8	91
5	1-Nonadecene	266	C19H38	018435-45-5	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062222\
Data File : BF128935.D
Acq On : 22 Jun 2022 16:56
Operator : CG\JU
Sample : N3384-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

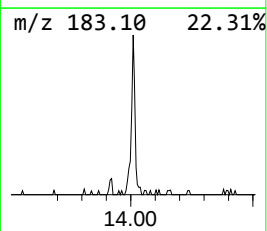
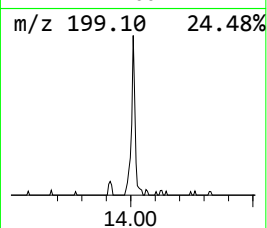
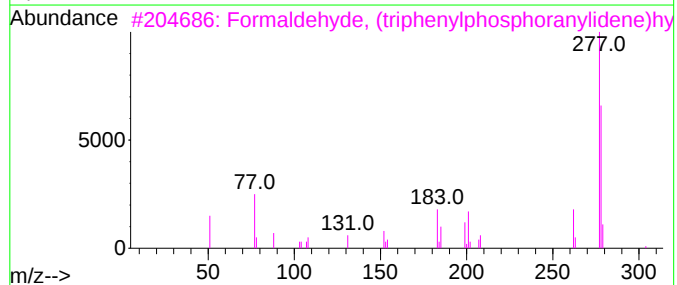
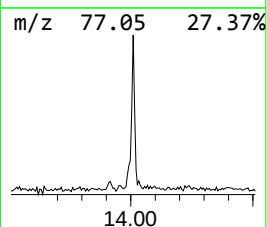
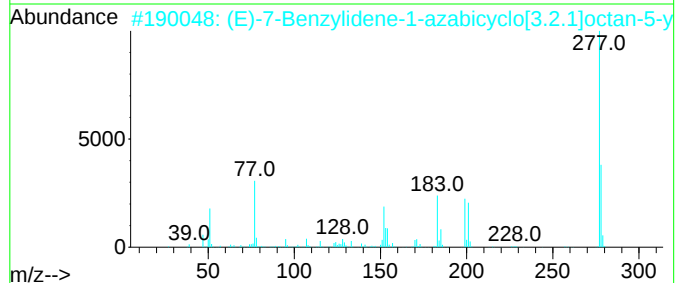
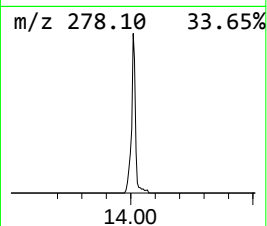
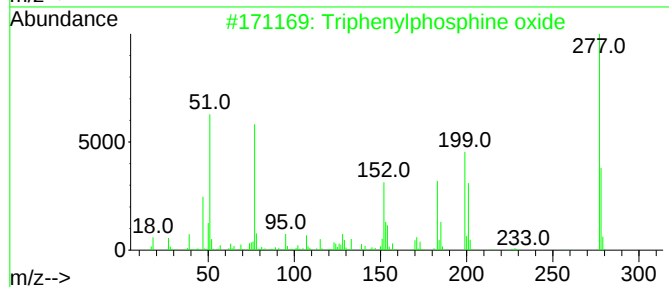
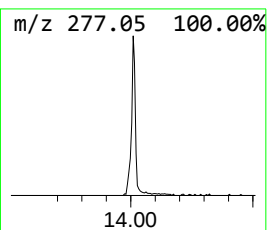
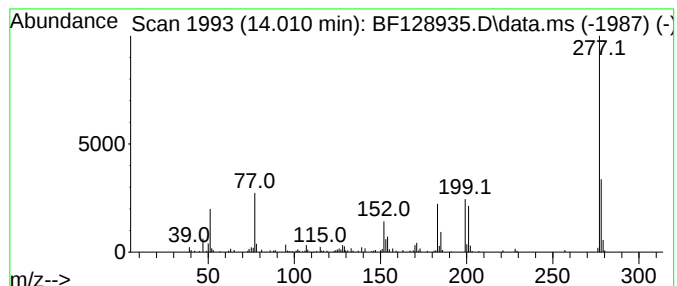
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Triphenylphosphine oxide Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.010	2.57 ng	111189	Chrysene-d12	13.916	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	97
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	81
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	72
4	1H-Indole-3-acetic acid, 5-[(tri...	277	C14H19NO3Si	072101-35-0	12
5	6H-Pyrazolo[3,4-H]quinazoline, 2...	278	C15H14N6	1000302-25-8	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062222\
Data File : BF128935.D
Acq On : 22 Jun 2022 16:56
Operator : CG\JU
Sample : N3384-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.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
1,3-Dioxolane, ...	2.804	3.9	ng	121756	1	6.745	632298	20.0
2-Pentanone, 4-...	4.957	2.1	ng	66163	1	6.745	632298	20.0
2-Propanol, 1-[...	8.257	5.8	ng	245848	2	8.028	841944	20.0
2-Propanol, 1-(...	8.286	7.0	ng	295373	2	8.028	841944	20.0
Hexadecanoic ac...	11.663	2.9	ng	142542	4	11.269	979276	20.0
n-Hexadecanoic ...	11.804	2.3	ng	110672	4	11.269	979276	20.0
9-Octadecenoic ...	12.368	4.0	ng	195121	4	11.269	979276	20.0
1-Heneicosanol	13.798	6.2	ng	267706	5	13.916	863829	20.0
Triphenylphosph...	14.010	2.6	ng	111189	5	13.916	863829	20.0