

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051722\
 Data File : BF128301.D
 Acq On : 17 May 2022 20:11
 Operator : CG\JU
 Sample : N2878-06
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P007-SS020-0006-01

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-BF050922.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF128301.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.499	542	546	560	rBV	2107750	1862920	87.29%	12.390%
2	6.510	713	718	721	rBV	2027878	1874144	87.81%	12.464%
3	6.875	776	780	784	rBV	673282	510946	23.94%	3.398%
4	7.440	872	876	879	rBV	1346258	1295583	60.70%	8.617%
5	8.157	994	998	1002	rBV	770686	629497	29.50%	4.187%
6	9.234	1176	1181	1184	rBV	2581512	2134235	100.00%	14.194%
7	9.916	1293	1297	1301	rBV	798433	651933	30.55%	4.336%
8	10.710	1428	1432	1435	rBV	1288169	1113483	52.17%	7.405%
9	11.410	1547	1551	1555	rBV	637382	560132	26.25%	3.725%
10	11.928	1635	1639	1643	rBV	75896	84043	3.94%	0.559%
11	12.998	1816	1821	1824	rVB	1722955	1686415	79.02%	11.216%
12	13.469	1897	1901	1906	rBV2	26507	31369	1.47%	0.209%
13	13.680	1934	1937	1942	rVB6	28207	30478	1.43%	0.203%
14	13.892	1967	1973	1983	rBV3	110572	265759	12.45%	1.767%
15	14.057	1997	2001	2004	rBV	598741	522356	24.48%	3.474%
16	14.504	2075	2077	2079	rBV	37100	26872	1.26%	0.179%
17	15.157	2185	2188	2193	rVB	79170	85021	3.98%	0.565%
18	15.551	2250	2255	2263	rVB	326726	399131	18.70%	2.655%
19	15.757	2287	2290	2294	rVB	57514	70592	3.31%	0.469%
20	15.992	2326	2330	2335	rVB	66073	99156	4.65%	0.659%
21	16.080	2339	2345	2357	rBV4	96048	315543	14.78%	2.099%
22	16.815	2464	2470	2477	rVB	208397	381542	17.88%	2.538%
23	17.380	2562	2566	2576	rVB5	70108	135234	6.34%	0.899%
24	17.668	2609	2615	2628	rVB10	79614	269584	12.63%	1.793%

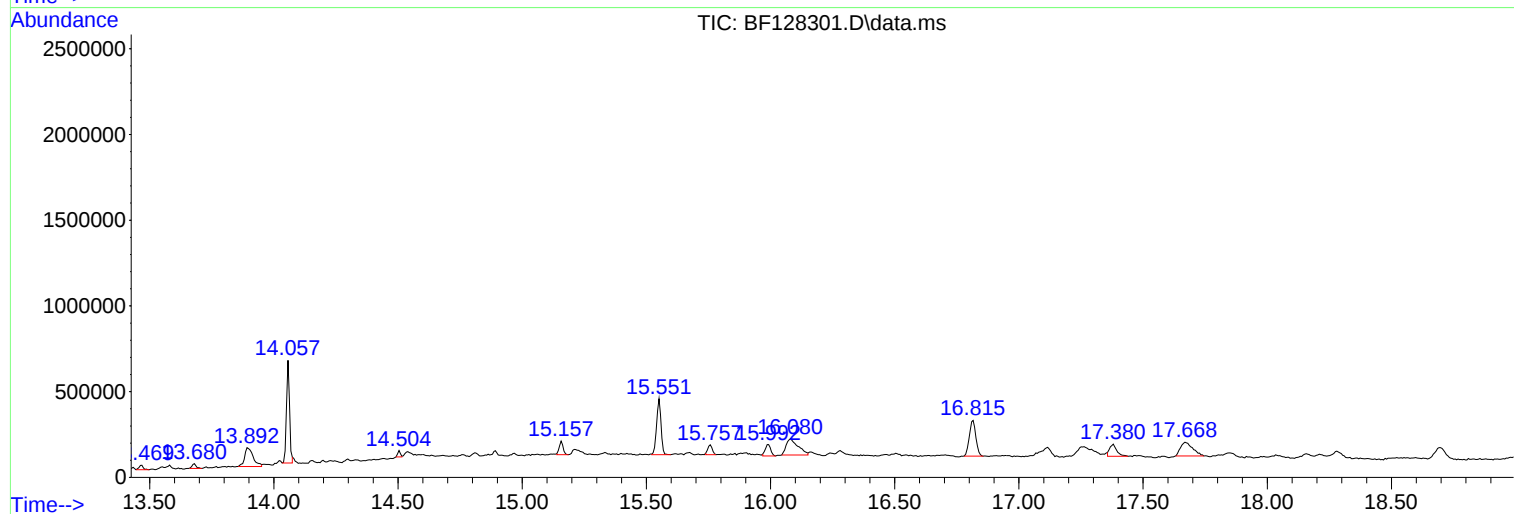
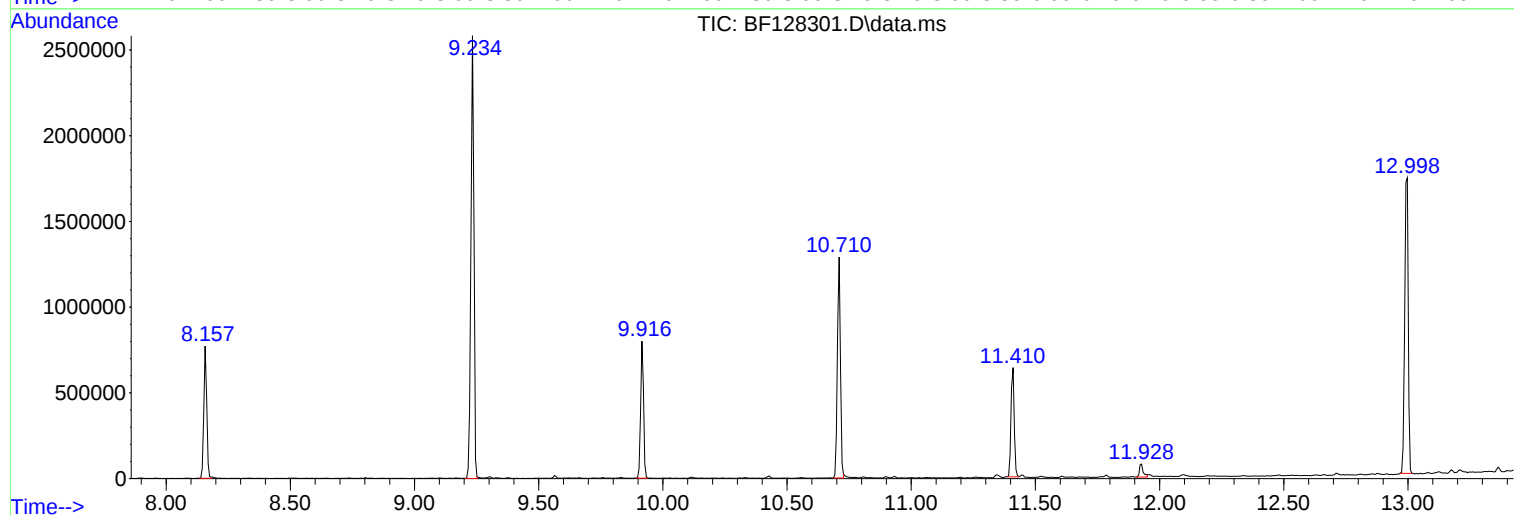
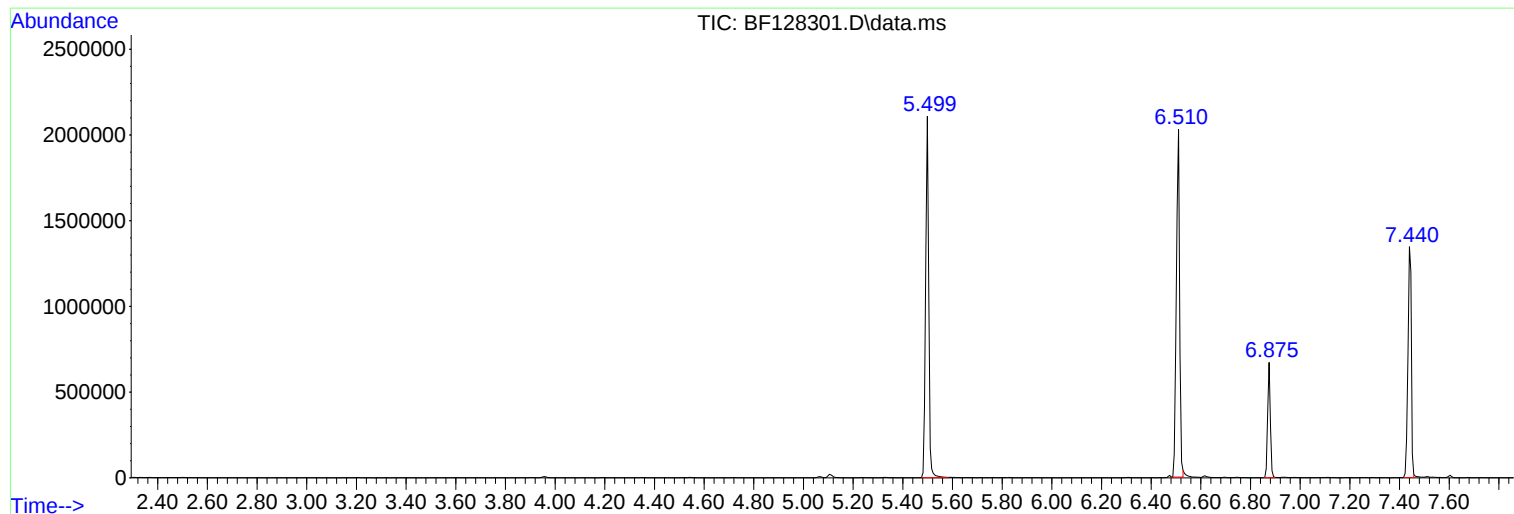
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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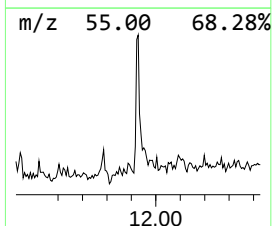
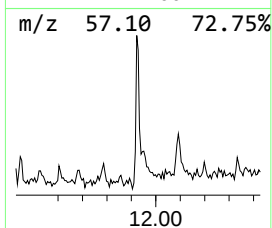
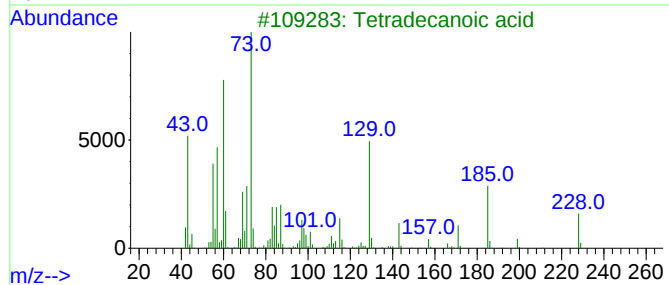
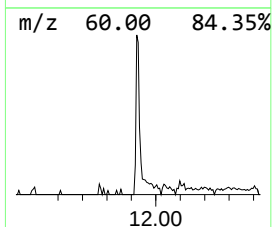
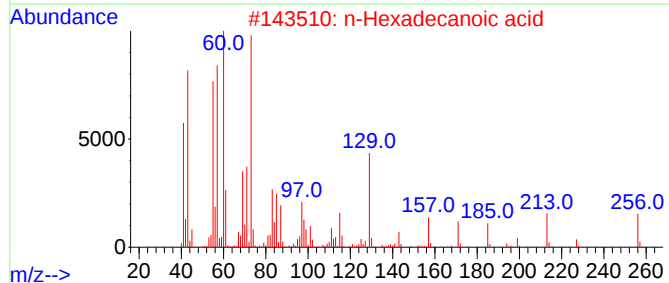
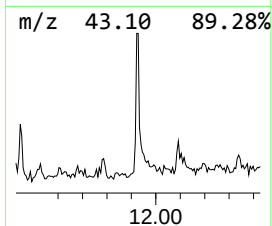
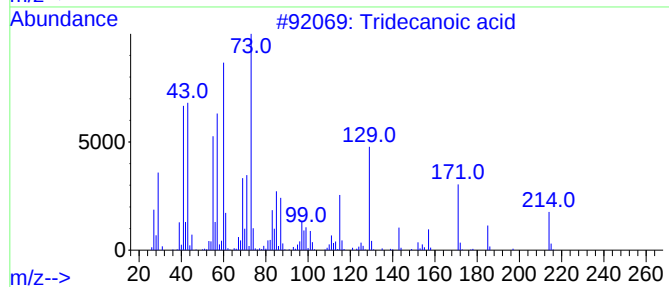
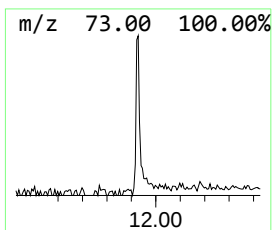
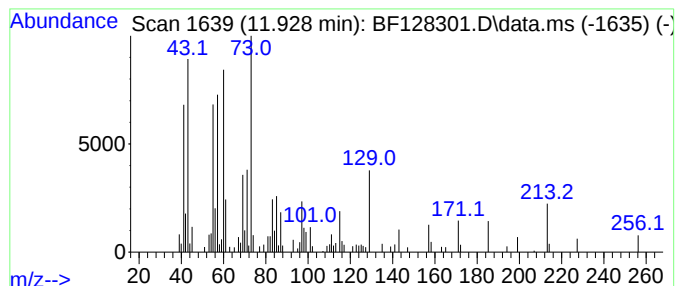
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Tridecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.928	3.00 ng	84043	Phenanthrene-d10	11.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	95
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	80
5			Dodecanoic acid	200	C12H24O2	000143-07-7	64



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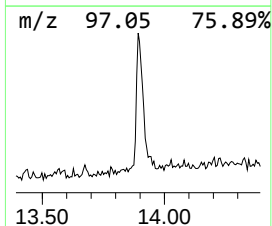
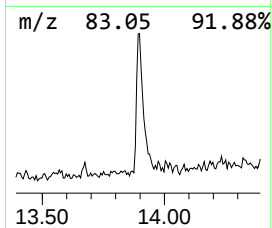
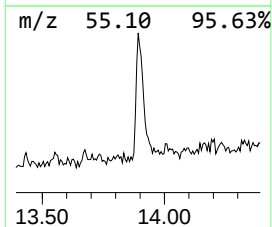
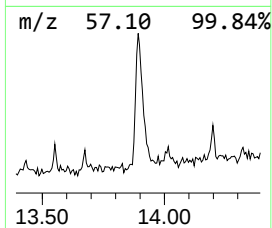
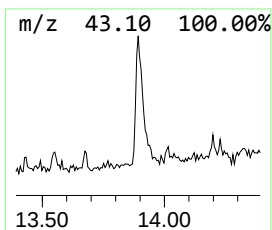
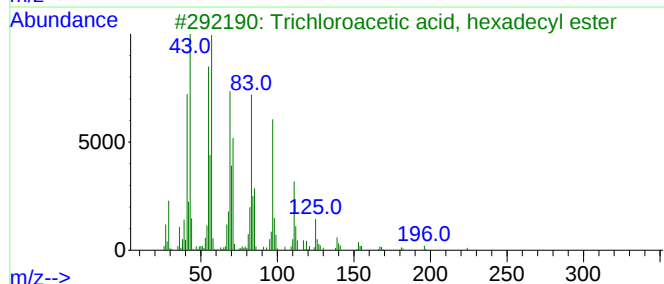
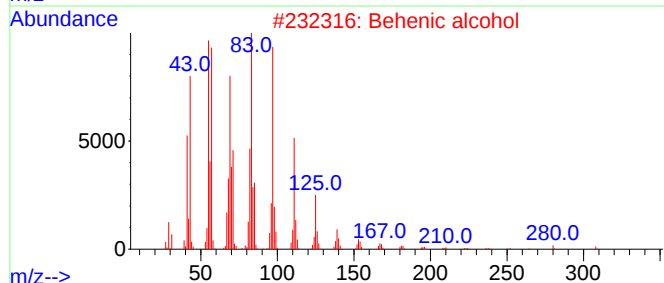
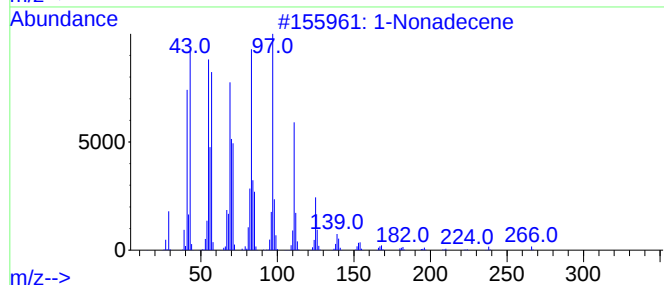
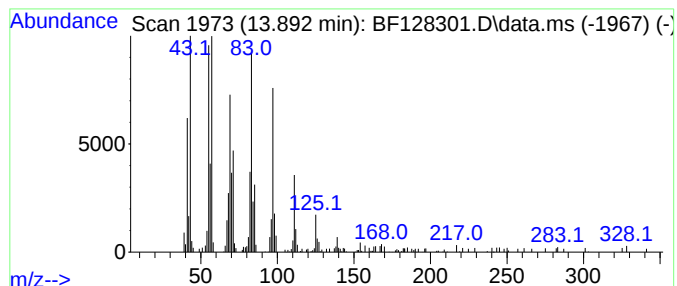
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 1-Nonadecene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	10.18 ng	265759	Chrysene-d12	14.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	96		
2	Behenic alcohol	326	C22H46O	000661-19-8	95		
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94		
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	94		
5	1-Heneicosanol	312	C21H44O	015594-90-8	93		



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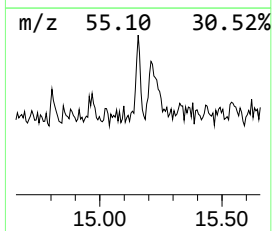
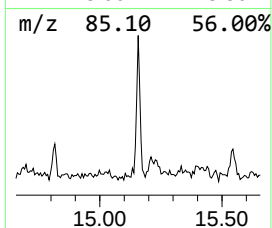
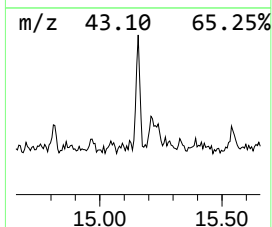
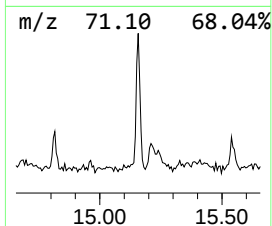
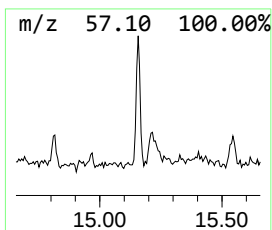
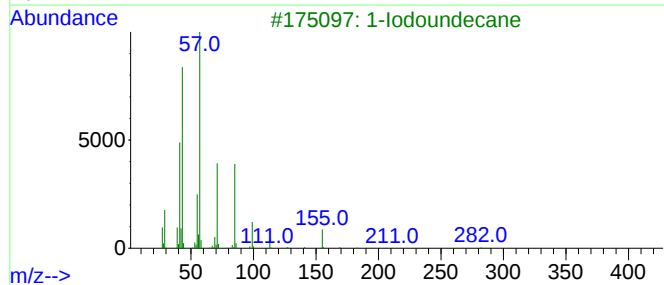
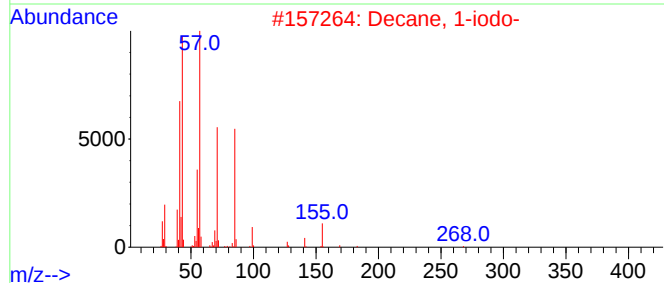
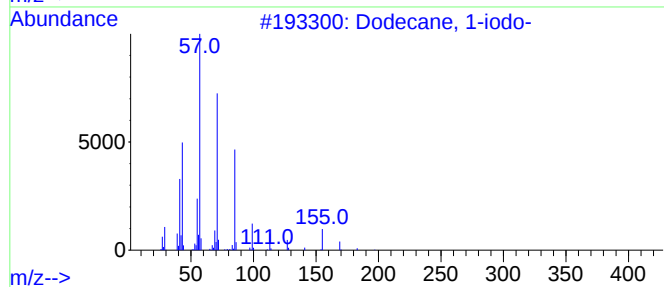
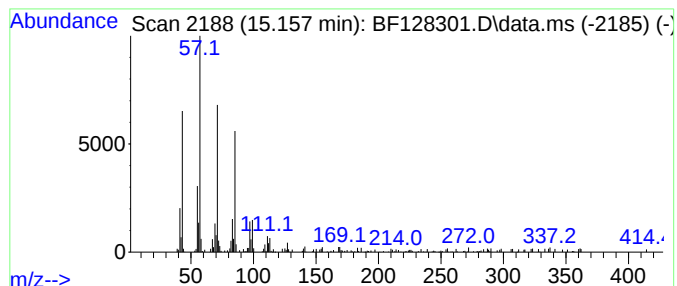
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Dodecane, 1-iodo- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.157	4.26 ng	85021	Perylene-d12	15.551

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Dodecane, 1-iodo-	296	C12H25I	004292-19-7	80
2		Decane, 1-iodo-	268	C10H21I	002050-77-3	74
3		1-Iodoundecane	282	C11H23I	004282-44-4	74
4		Heptadecane	240	C17H36	000629-78-7	74
5		Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	68



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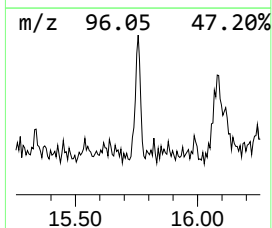
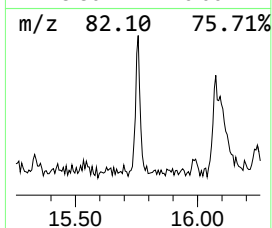
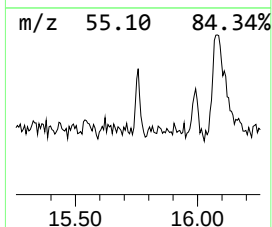
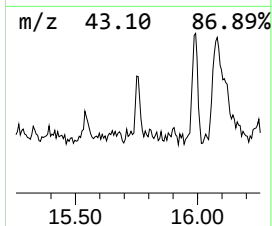
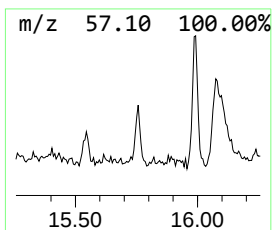
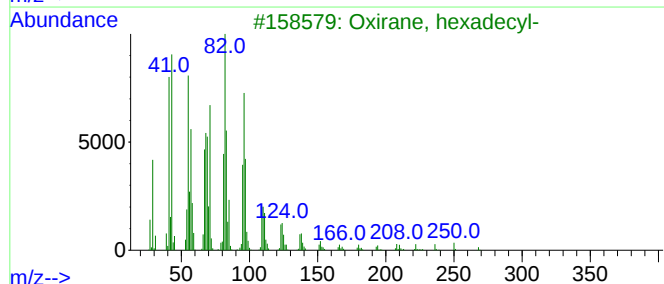
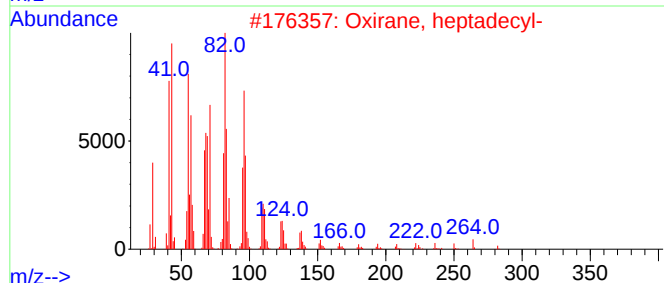
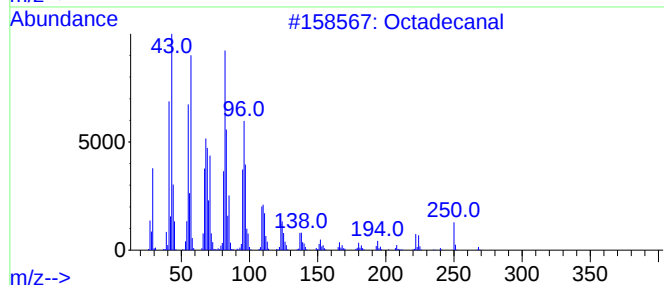
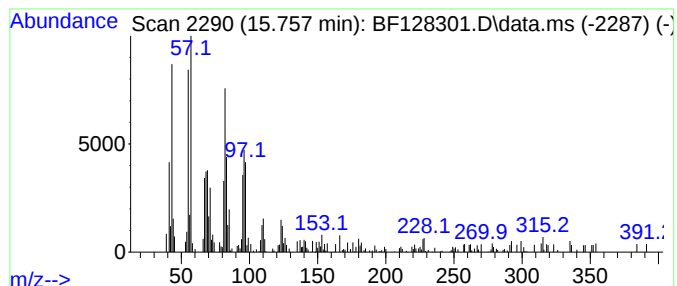
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 4 Octadecanal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.757	3.54 ng	70592	Perylene-d12	15.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanal	268	C18H36O	000638-66-4	93
2			Oxirane, heptadecyl-	282	C19H38O	067860-04-2	91
3			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
4			Eicosanal-	296	C20H40O	002400-66-0	87
5			Hexadecanal	240	C16H32O	000629-80-1	83



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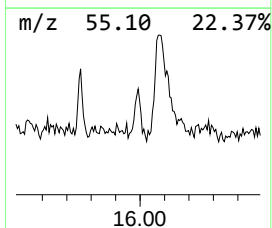
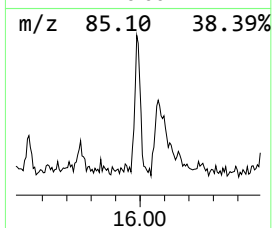
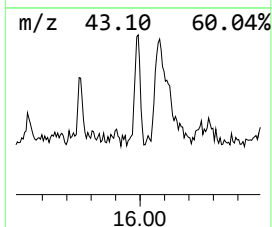
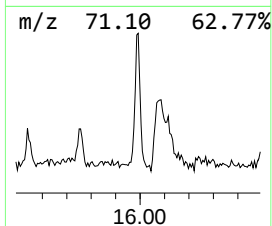
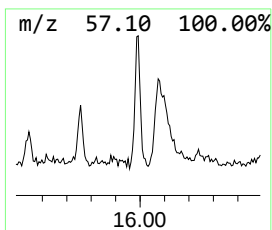
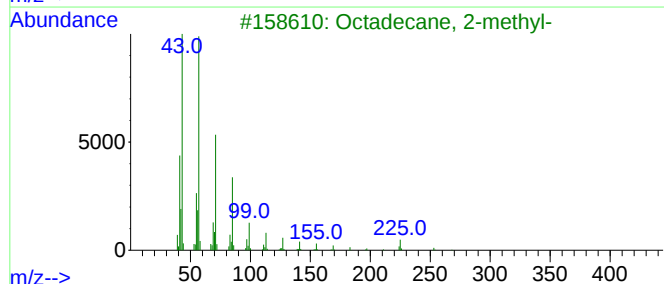
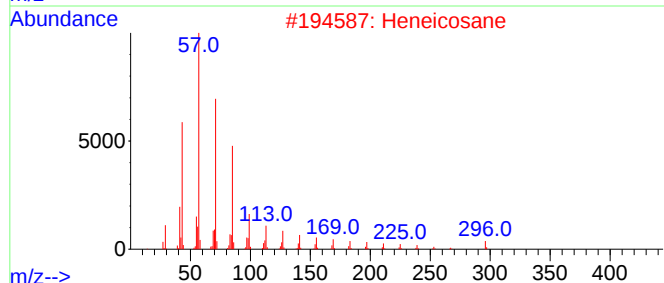
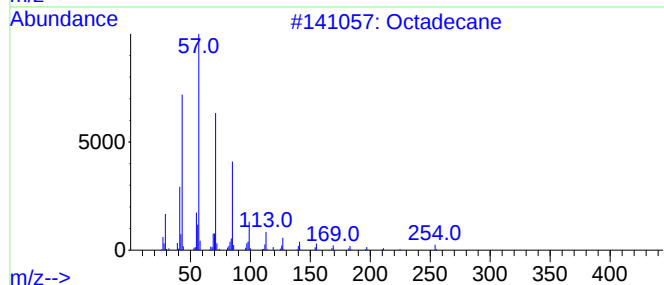
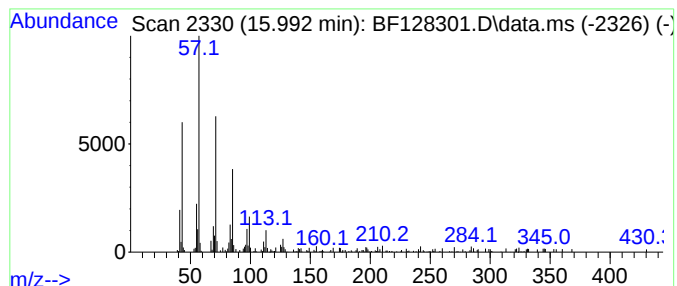
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Octadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.992	4.97 ng	99156	Perylene-d12	15.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane	254	C18H38	000593-45-3	91
2			Heneicosane	296	C21H44	000629-94-7	91
3			Octadecane, 2-methyl-	268	C19H40	001560-88-9	90
4			Octacosane	394	C28H58	000630-02-4	90
5			2-Bromo dodecane	248	C12H25Br	013187-99-0	90



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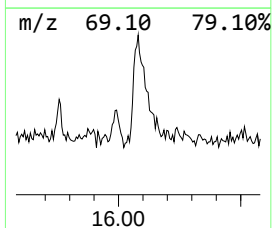
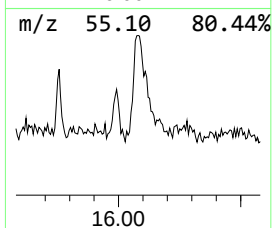
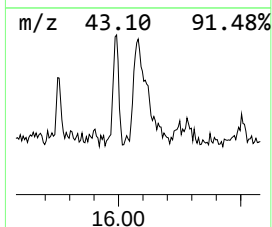
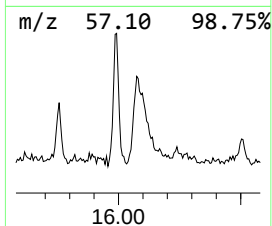
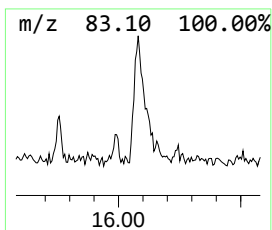
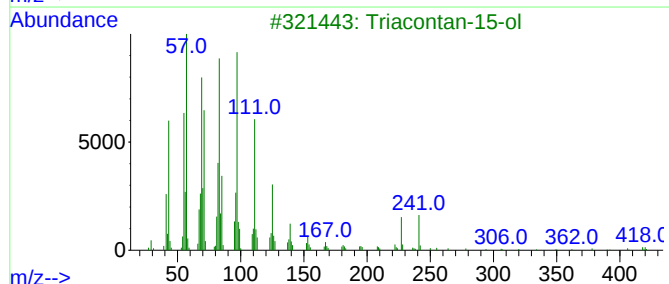
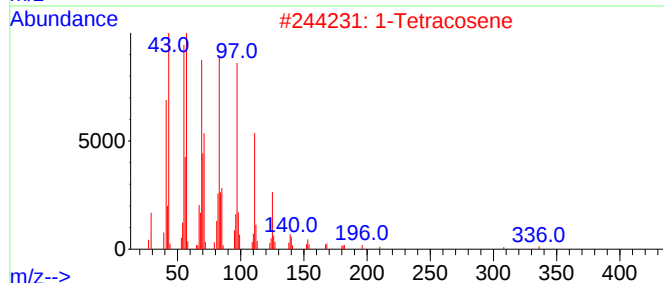
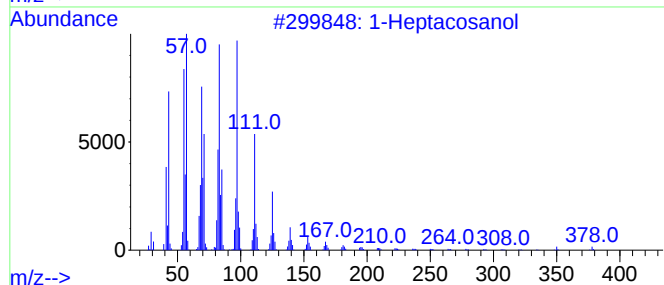
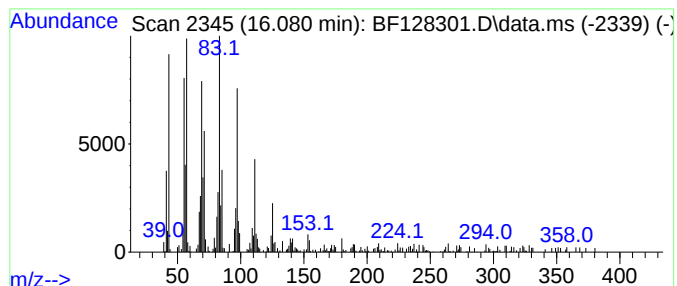
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Heptacosanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.080	15.81 ng	315543	Perylene-d12	15.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heptacosanol	396	C27H56O	002004-39-9	94
2			1-Tetracosene	336	C24H48	010192-32-2	91
3			Triacontan-15-ol	438	C30H62O	031849-26-0	90
4			Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	90
5			17-Pentatriacontene	491	C35H70	006971-40-0	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051722\
Data File : BF128301.D
Acq On : 17 May 2022 20:11
Operator : CG\JU
Sample : N2878-06
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P007-SS020-0006-01

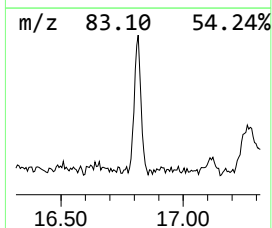
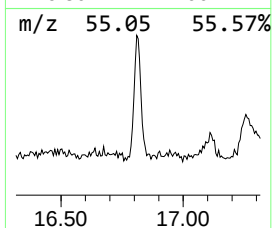
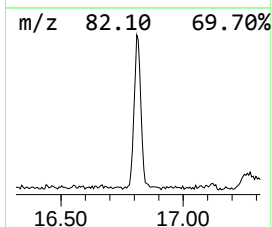
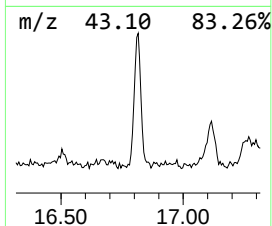
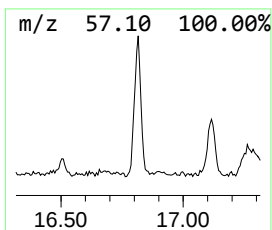
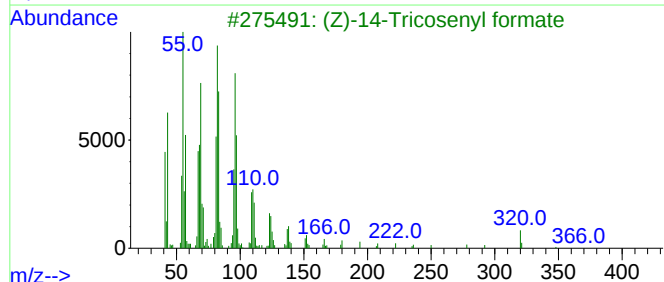
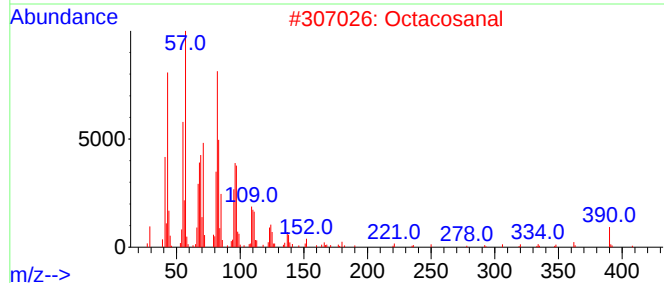
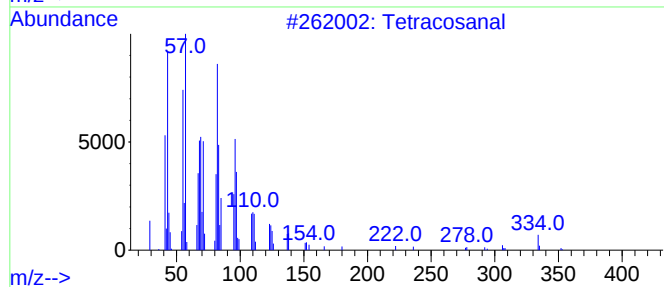
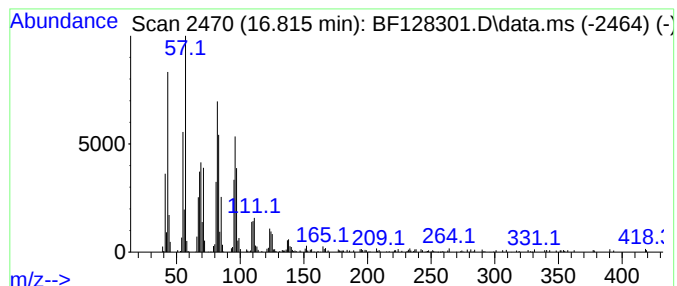
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tetracosanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.816	19.12 ng	381542	Perylene-d12	15.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosanal	352	C24H48O	057866-08-7	91
2			Octacosanal	408	C28H56O	022725-64-0	90
3			(Z)-14-Tricosenyl formate	366	C24H46O2	077899-10-6	89
4			Eicosanal-	296	C20H40O	002400-66-0	87
5			Hexacosanal	380	C26H52O	026627-85-0	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051722\
Data File : BF128301.D
Acq On : 17 May 2022 20:11
Operator : CG\JU
Sample : N2878-06
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P007-SS020-0006-01

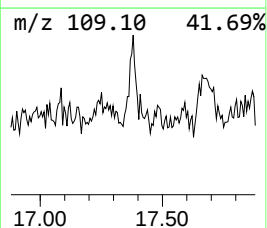
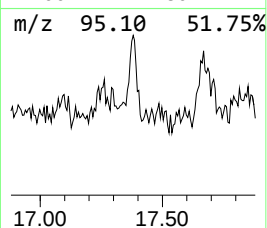
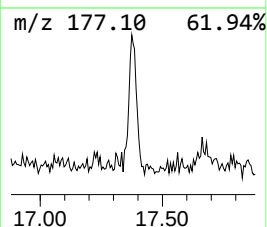
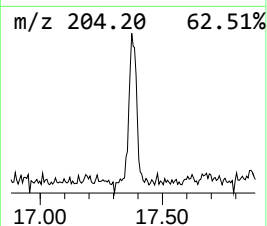
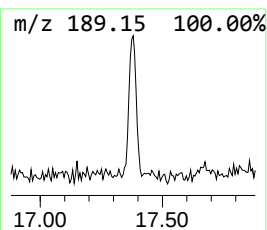
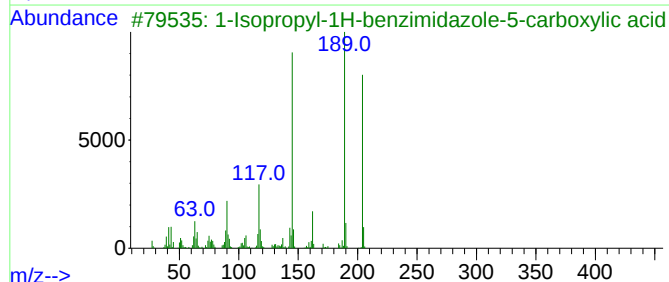
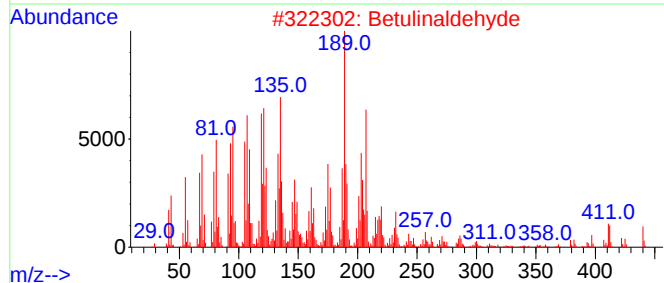
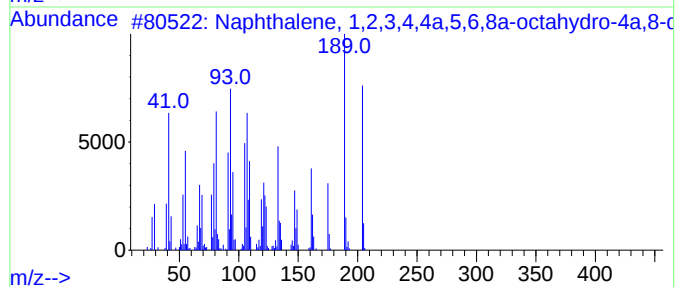
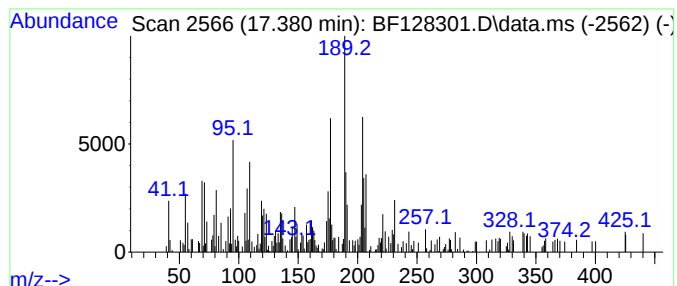
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Naphthalene, 1,2,3,4,4a,5,6... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.380	6.78 ng	135234	Perylene-d12	15.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4,4a,5,6,8a-o...	204	C15H24	000473-13-2	53
2			Betulinaldehyde	440	C30H48O2	013159-28-9	50
3			1-Isopropyl-1H-benzimidazole-5-c...	204	C11H12N2O2	284673-16-1	38
4			Dihydrocoumarin, 4,4,5,7-tetrame...	204	C13H16O2	040662-14-4	38
5			2-Naphthalenemethanol, 1,2,3,4,4...	222	C15H26O	001209-71-8	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051722\
Data File : BF128301.D
Acq On : 17 May 2022 20:11
Operator : CG\JU
Sample : N2878-06
Misc :
ALS Vial : 20 Sample Multiplier: 1

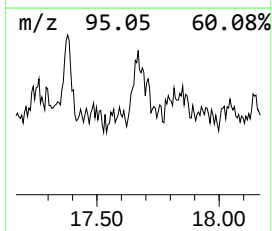
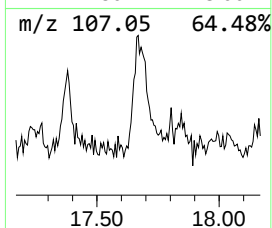
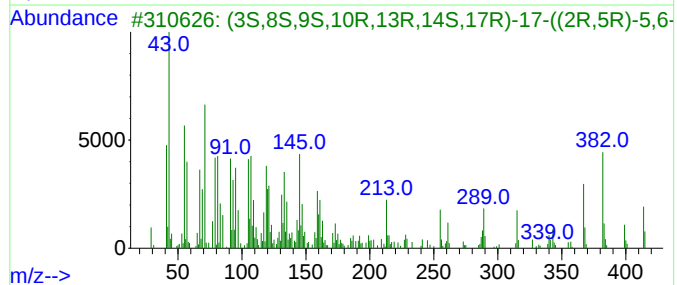
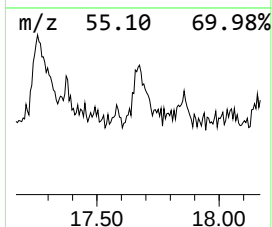
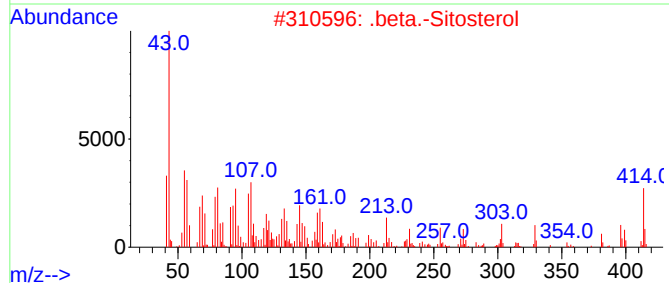
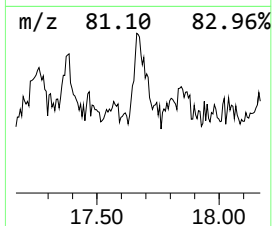
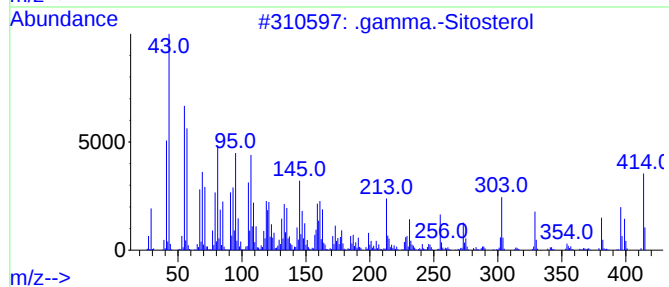
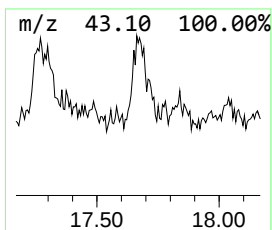
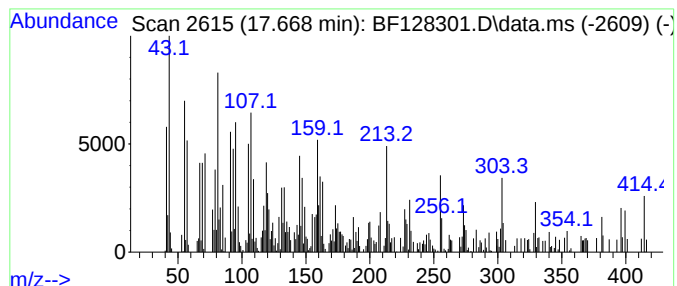
Instrument :
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ClientSampleId :
P007-SS020-0006-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 .gamma.-Sitosterol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.668	13.51 ng	269584	Perylene-d12	15.551	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.gamma.-Sitosterol	414	C29H50O	000083-47-6	95
2	.beta.-Sitosterol	414	C29H50O	000083-46-5	78
3	(3S,8S,9S,10R,13R,14S,17R)-17-((...	414	C29H50O	029365-29-5	17
4	22,26-Oxido-4,17-cholestadien-3...	414	C27H42O3	1000252-80-4	10
5	Cholestan-26-oic acid, 3,7-bis(a...	532	C32H52O6	060354-52-1	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051722\
Data File : BF128301.D
Acq On : 17 May 2022 20:11
Operator : CG\JU
Sample : N2878-06
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P007-SS020-0006-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050922.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
Tridecanoic acid	11.928	3.0	ng	84043	4	11.410	560132	20.0
1-Nonadecene	13.892	10.2	ng	265759	5	14.057	522356	20.0
Dodecane, 1-iodo-	15.157	4.3	ng	85021	6	15.551	399131	20.0
Octadecanal	15.757	3.5	ng	70592	6	15.551	399131	20.0
Octadecane	15.992	5.0	ng	99156	6	15.551	399131	20.0
1-Heptacosanol	16.080	15.8	ng	315543	6	15.551	399131	20.0
Tetracosanal	16.816	19.1	ng	381542	6	15.551	399131	20.0
Naphthalene, 1,...	17.380	6.8	ng	135234	6	15.551	399131	20.0
.gamma.-Sitosterol	17.668	13.5	ng	269584	6	15.551	399131	20.0