

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051722\
 Data File : BF128296.D
 Acq On : 17 May 2022 17:43
 Operator : CG\JU
 Sample : N2878-11
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P007-SS021-0006-01

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: BF128296.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.498	542	546	559	rBV	2095030	1909020	86.17%	11.775%
2	6.504	713	717	729	rBV	1926435	1951213	88.07%	12.036%
3	6.875	776	780	783	rBV	559910	443548	20.02%	2.736%
4	7.440	871	876	879	rBV	1489910	1312096	59.22%	8.093%
5	8.157	994	998	1001	rBV	703468	563521	25.44%	3.476%
6	9.234	1176	1181	1184	rBV	2617337	2215465	100.00%	13.666%
7	9.563	1233	1237	1240	rBV	33901	27464	1.24%	0.169%
8	9.916	1293	1297	1300	rBV	770831	630430	28.46%	3.889%
9	10.710	1428	1432	1435	rBV	1485241	1332933	60.16%	8.222%
10	10.998	1478	1481	1484	rVB	33244	28342	1.28%	0.175%
11	11.410	1547	1551	1555	rBV	652504	596781	26.94%	3.681%
12	11.922	1635	1638	1642	rBV	83100	84858	3.83%	0.523%
13	12.992	1816	1820	1824	rBV	1876651	1683585	75.99%	10.385%
14	13.127	1839	1843	1848	rBV	51908	52275	2.36%	0.322%
15	13.892	1969	1973	1982	rBV4	125090	271805	12.27%	1.677%
16	14.027	1992	1996	1998	rBV2	89108	85496	3.86%	0.527%
17	14.057	1998	2001	2004	rVV	505207	442668	19.98%	2.730%
18	14.092	2004	2007	2009	rVB	33403	34559	1.56%	0.213%
19	14.245	2031	2033	2038	rVB	27831	25453	1.15%	0.157%
20	14.504	2074	2077	2080	rBV	71562	57026	2.57%	0.352%
21	14.580	2087	2090	2096	rVB	37894	48488	2.19%	0.299%
22	15.157	2185	2188	2193	rVB	123985	129579	5.85%	0.799%
23	15.551	2250	2255	2261	rVB	365953	491792	22.20%	3.034%
24	15.751	2287	2289	2295	rVB	42476	53835	2.43%	0.332%
25	15.986	2326	2329	2337	rVB2	47189	74987	3.38%	0.463%
26	16.080	2339	2345	2355	rBV6	82028	275732	12.45%	1.701%
27	16.810	2463	2469	2479	rVB2	215037	401680	18.13%	2.478%
28	17.251	2538	2544	2559	rBV8	112102	472537	21.33%	2.915%
29	17.374	2561	2565	2573	rVB2	116274	229179	10.34%	1.414%
30	17.668	2608	2615	2632	rBV8	72633	285666	12.89%	1.762%

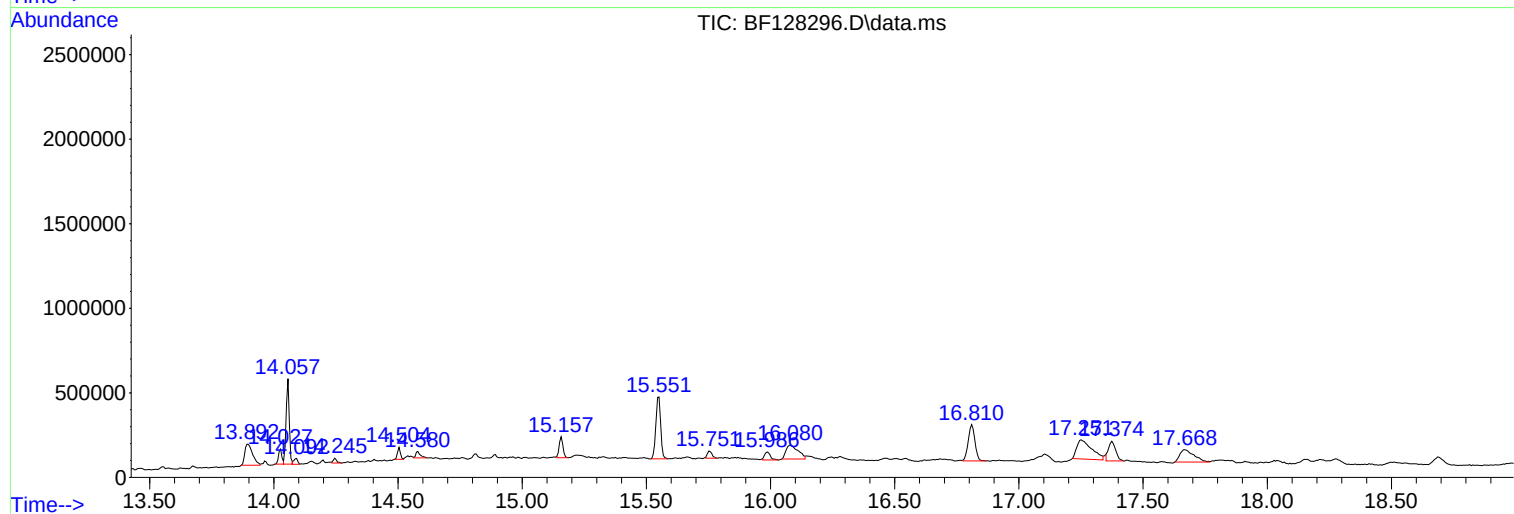
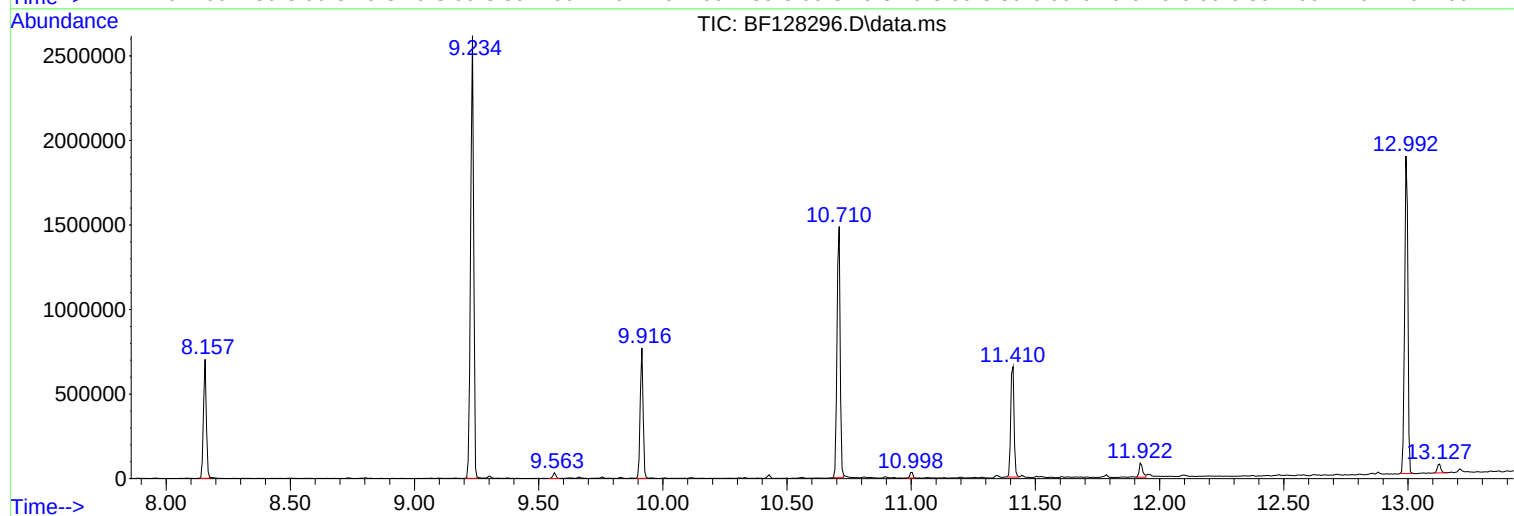
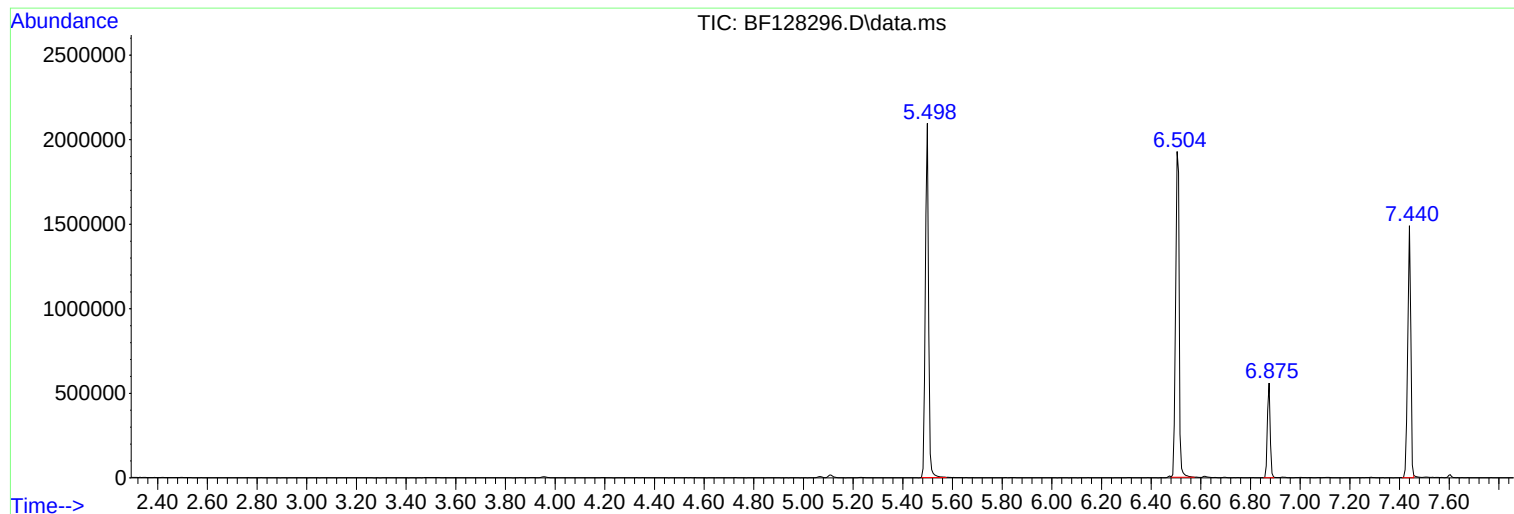
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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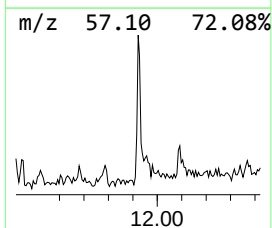
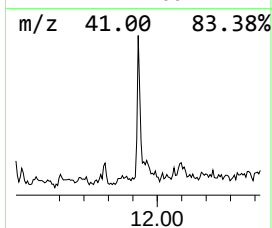
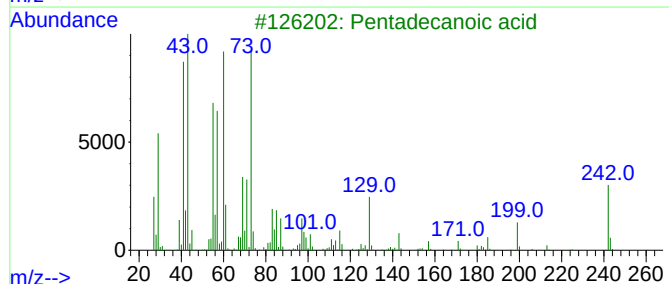
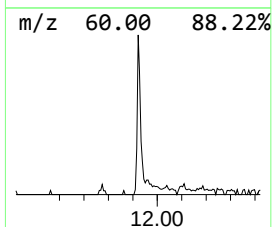
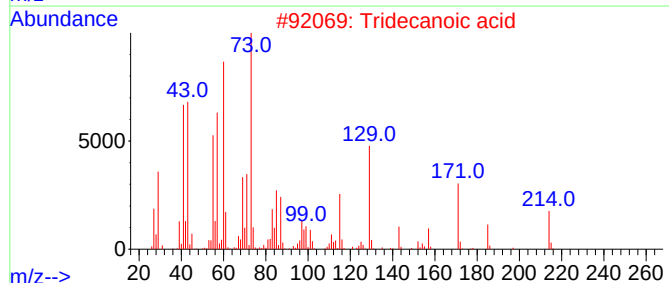
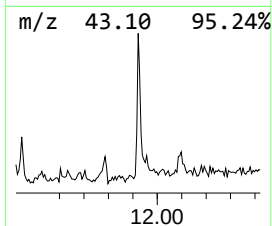
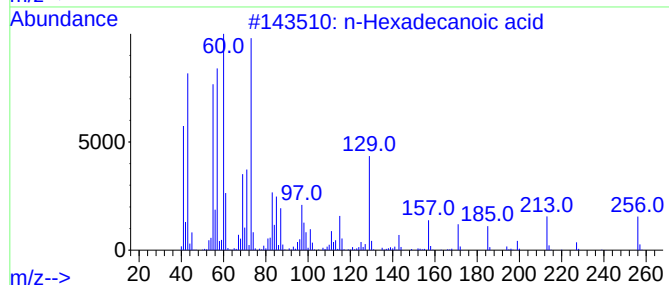
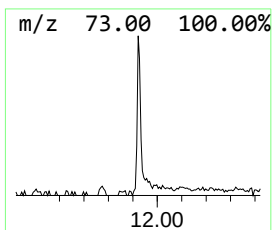
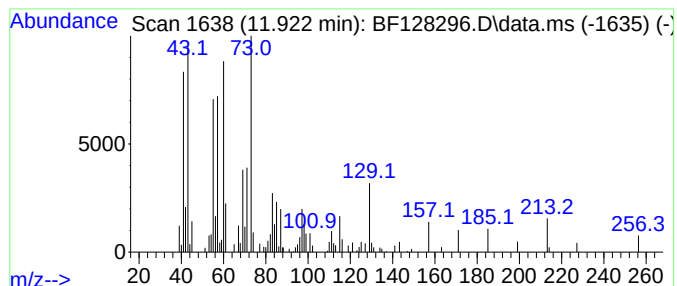
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	2.84 ng	84858	Phenanthrene-d10	11.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	95
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			n-Decanoic acid	172	C10H20O2	000334-48-5	64



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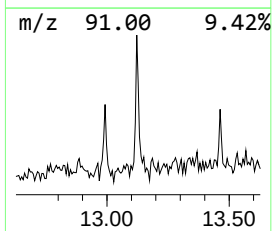
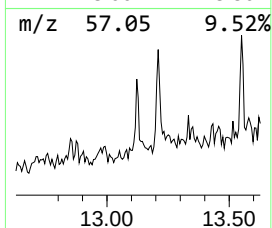
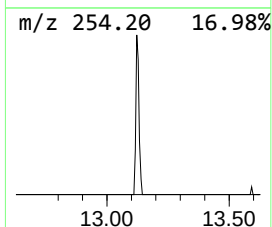
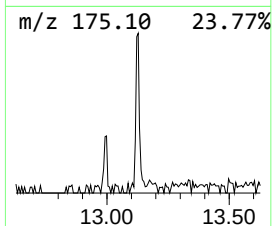
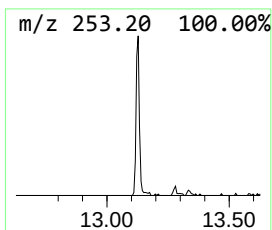
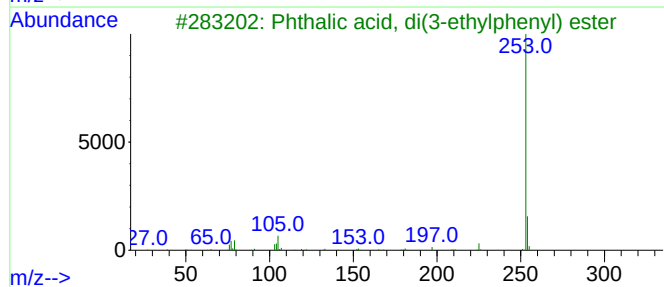
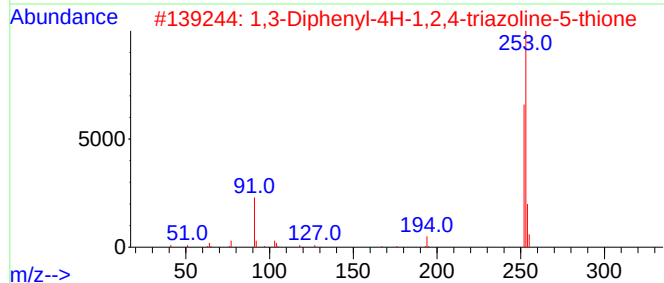
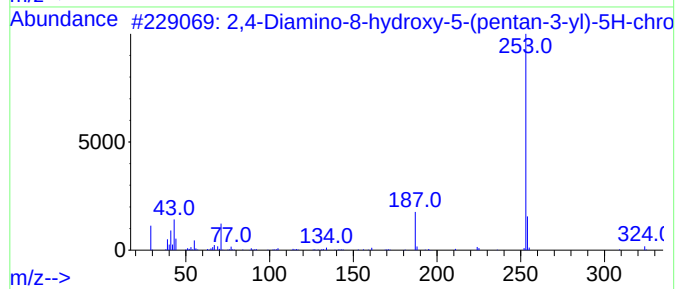
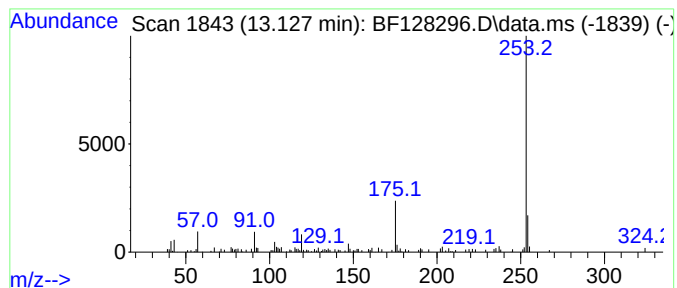
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Peak Number 2 2,4-Diamino-8-hydroxy-5-(pe... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.127	2.36 ng	52275	Chrysene-d12	14.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,4-Diamino-8-hydroxy-5-(pentan-...	324	C18H20N4O2	1000444-37-4	53
2			1,3-Diphenyl-4H-1,2,4-triazoline...	253	C14H11N3S	005055-73-2	53
3			Phthalic acid, di(3-ethylphenyl)...	374	C24H22O4	1000357-08-4	53
4			Phenol, 2-(1,1-dimethylethyl)-4-...	268	C19H24O	056187-92-9	45
5			1H-Inden-5-ol, 2,3-dihydro-3-(4-...	268	C18H20O2	010527-11-4	45



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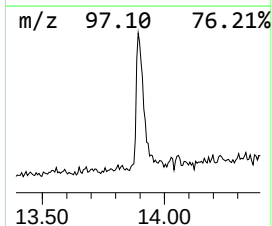
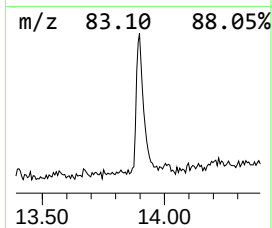
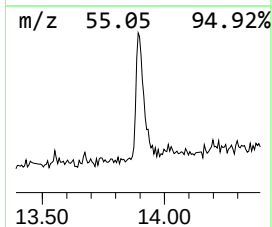
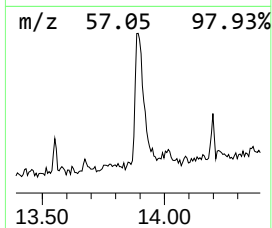
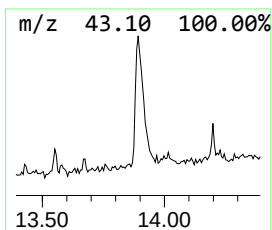
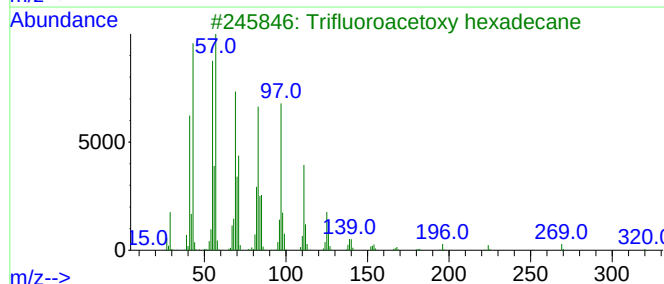
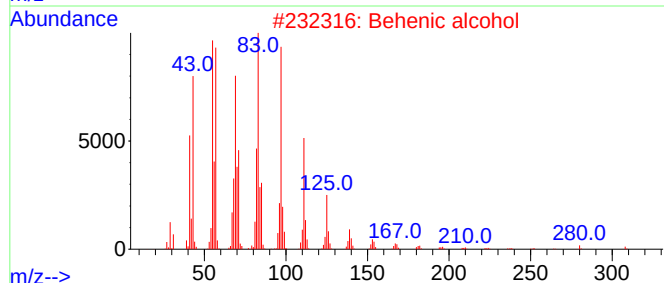
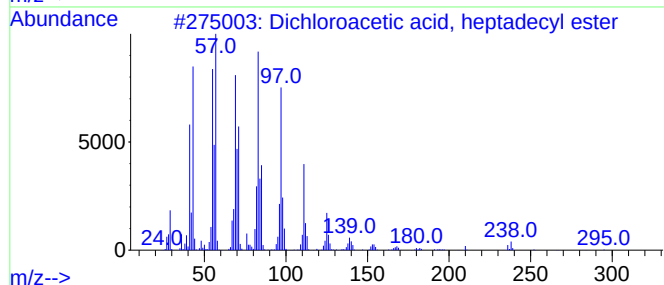
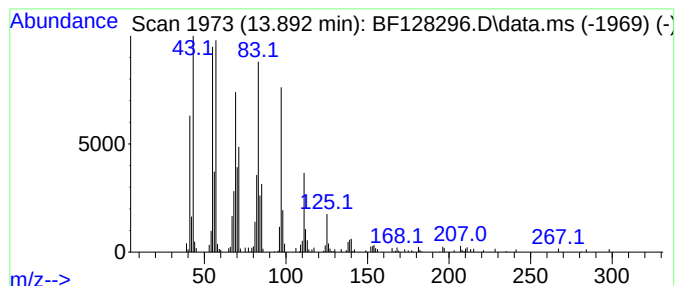
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TIC Integration Parameters: LSCINT.P

Peak Number 3 Dichloroacetic acid, heptad... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	12.28 ng	271805	Chrysene-d12	14.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
2			Behenic alcohol	326	C22H46O	000661-19-8	94
3			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
4			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
5			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93



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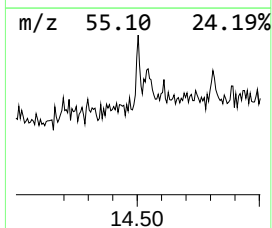
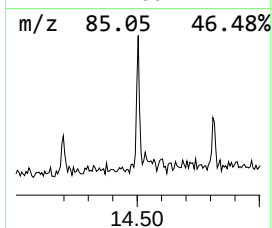
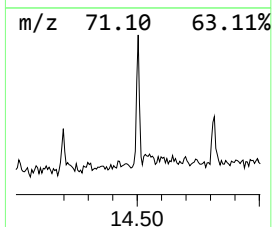
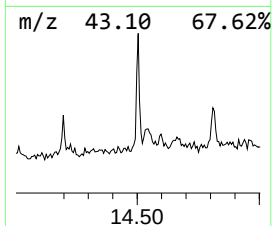
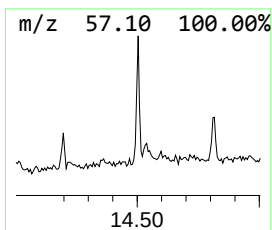
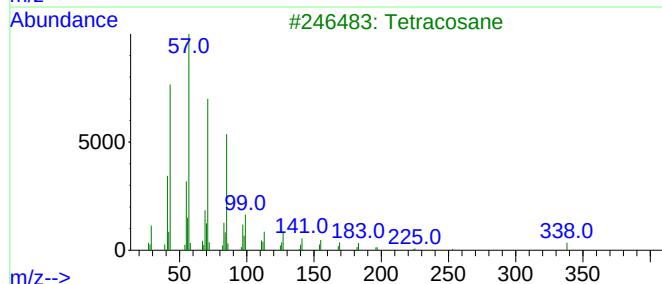
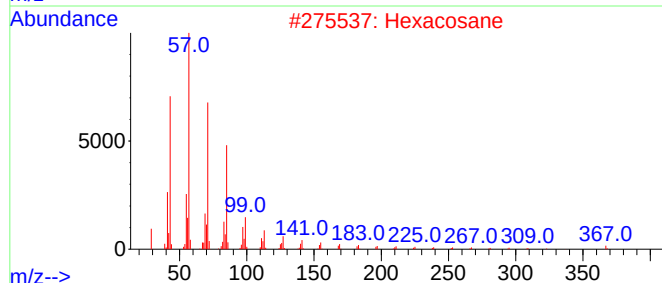
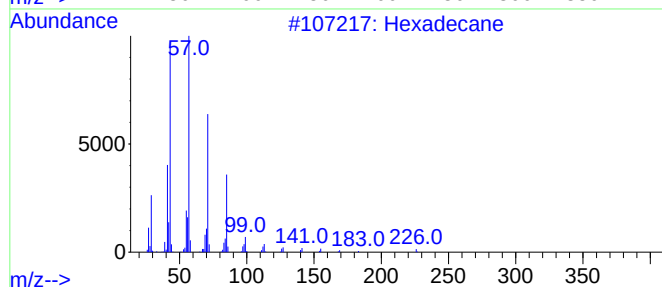
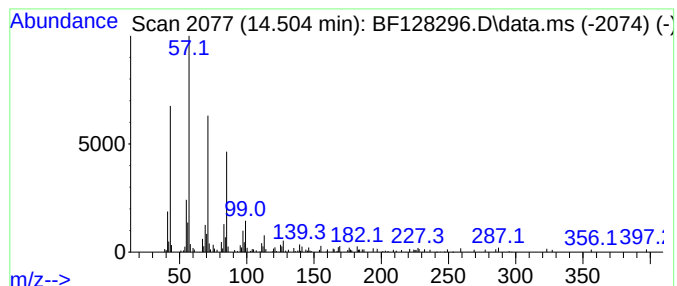
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Peak Number 4 Hexadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.504	2.58 ng	57026	Chrysene-d12	14.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane	226	C16H34	000544-76-3	90
2			Hexacosane	366	C26H54	000630-01-3	90
3			Tetracosane	338	C24H50	000646-31-1	87
4			2-Bromo dodecane	248	C12H25Br	013187-99-0	87
5			Nonadecane	268	C19H40	000629-92-5	87



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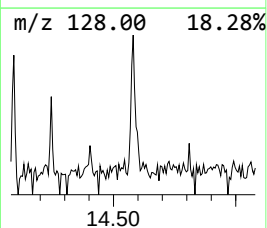
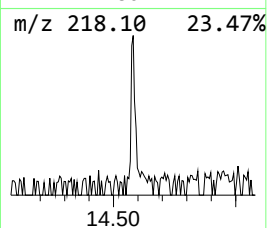
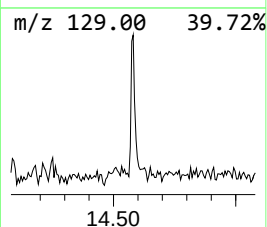
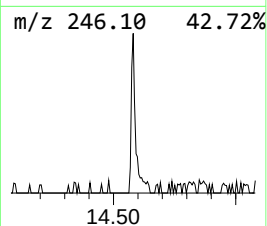
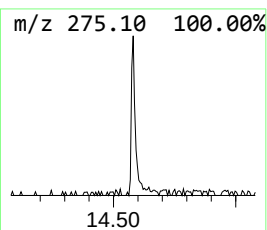
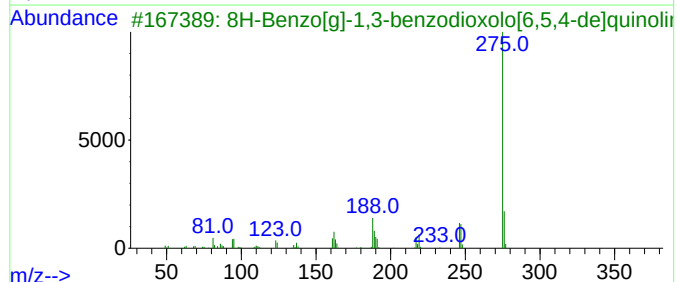
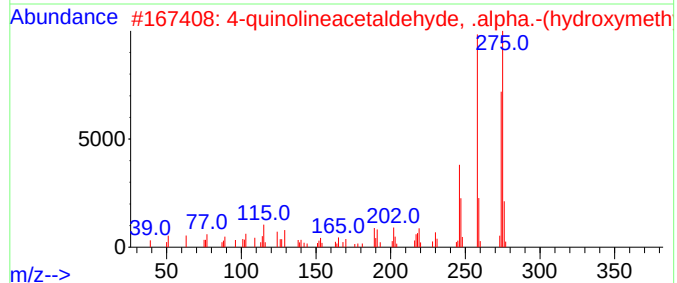
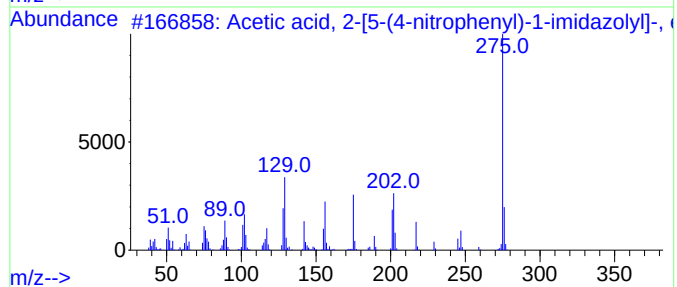
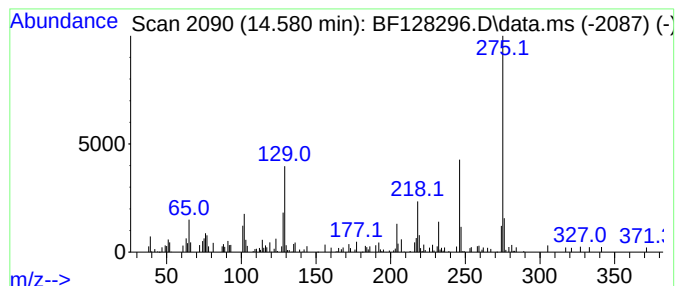
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Peak Number 5 Acetic acid, 2-[5-(4-nitrop... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.580	2.19 ng	48488	Chrysene-d12	14.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, 2-[5-(4-nitrophenyl)...	275	C13H13N3O4	351064-45-4	60
2			4-quinolineacetaldehyde, .alpha....	275	C18H13NO2	1000397-06-0	38
3			8H-Benzo[g]-1,3-benzodioxolo[6,5...	275	C17H9NO3	000475-75-2	35
4			1H-Pyrimido[4,5-b]pyrazolo[4,5-E...	317	C14H15N5O4	349498-69-7	32
5			Benzamide, 3-fluoro-N-(2,4-dimet...	275	C15H14FN03	1000339-95-1	27



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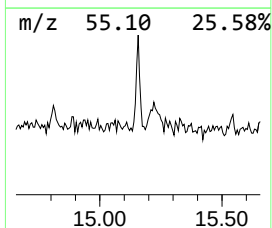
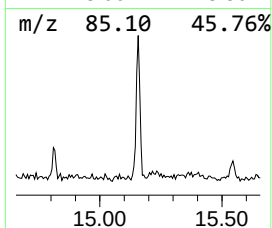
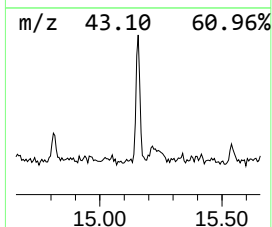
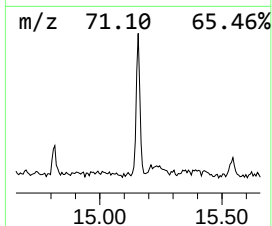
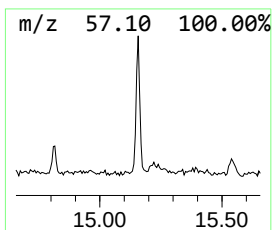
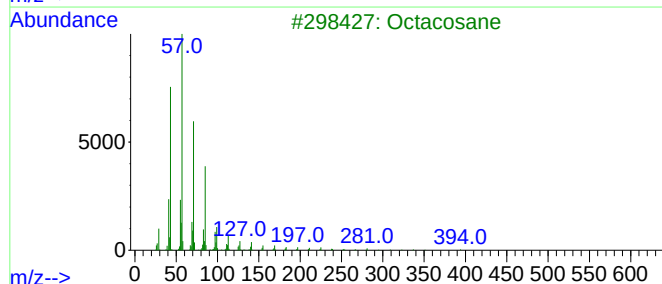
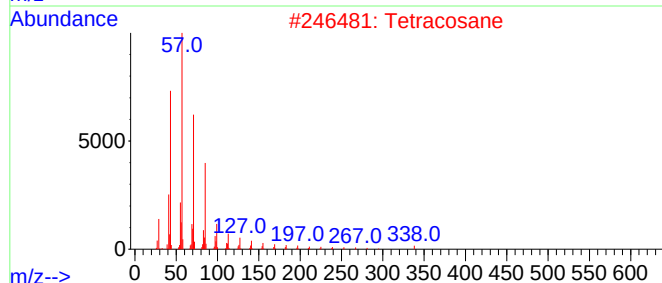
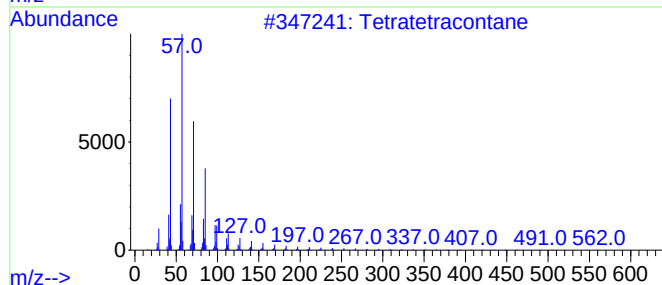
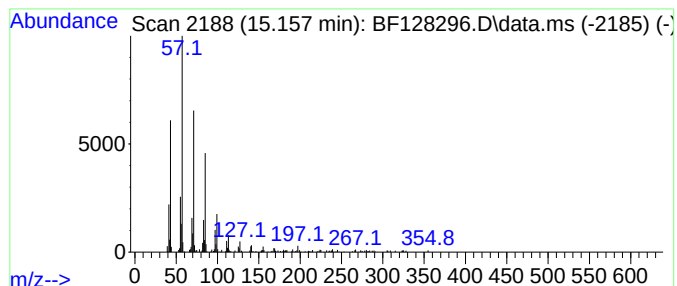
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Tetratetracontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.157	5.27 ng	129579	Perylene-d12	15.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetratetracontane	619	C44H90	007098-22-8	91
2			Tetracosane	338	C24H50	000646-31-1	91
3			Octacosane	394	C28H58	000630-02-4	91
4			Heptacosane	380	C27H56	000593-49-7	87
5			1-Iodoundecane	282	C11H23I	004282-44-4	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051722\
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Acq On : 17 May 2022 17:43
Operator : CG\JU
Sample : N2878-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P007-SS021-0006-01

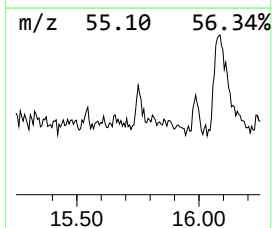
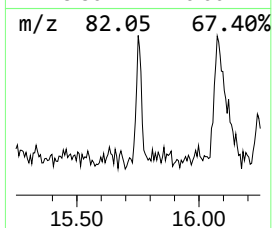
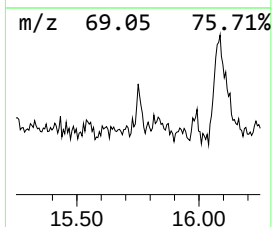
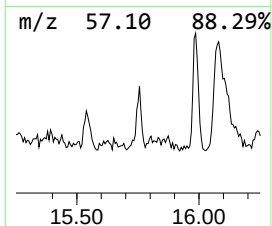
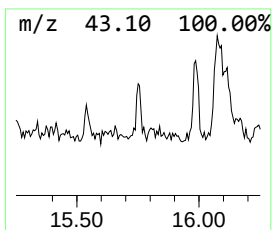
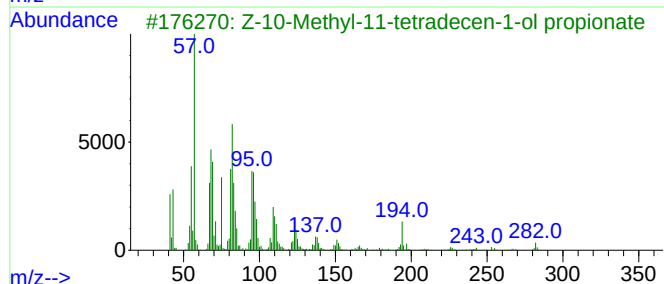
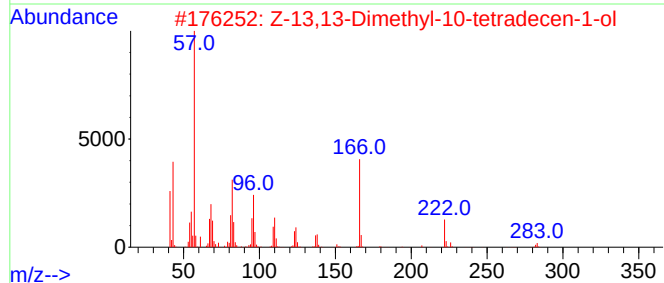
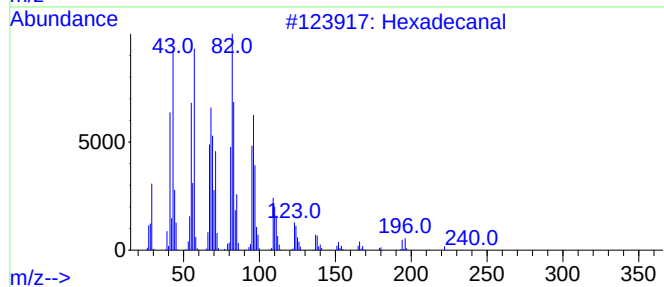
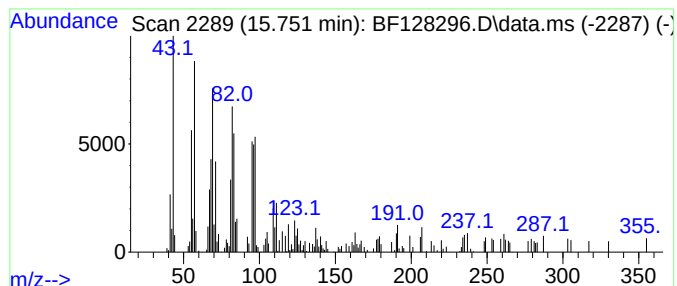
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexadecanal Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.751	2.19 ng	53835	Perylene-d12	15.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanal	240	C16H32O	000629-80-1	53
2			Z-13,13-Dimethyl-10-tetradecen-1-ol	282	C18H34O2	1000130-81-7	50
3			Z-10-Methyl-11-tetradecen-1-ol p...	282	C18H34O2	1000130-77-5	50
4			Octadecanal	268	C18H36O	000638-66-4	49
5			Heptadecanal	254	C17H34O	1000376-70-0	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051722\
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Instrument :
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ClientSampleId :
P007-SS021-0006-01

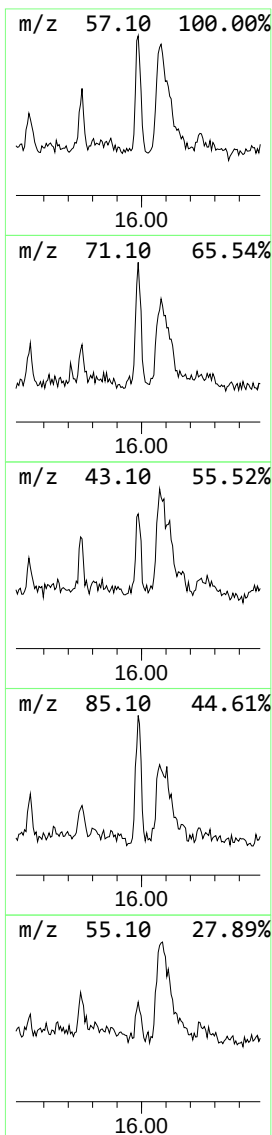
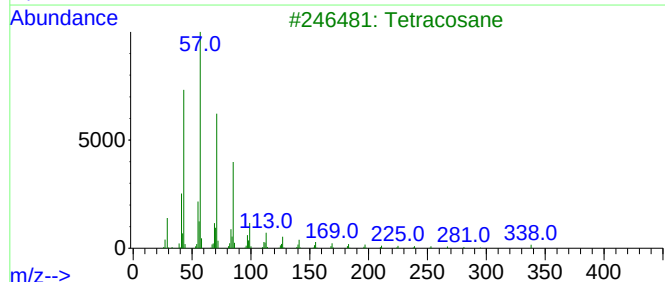
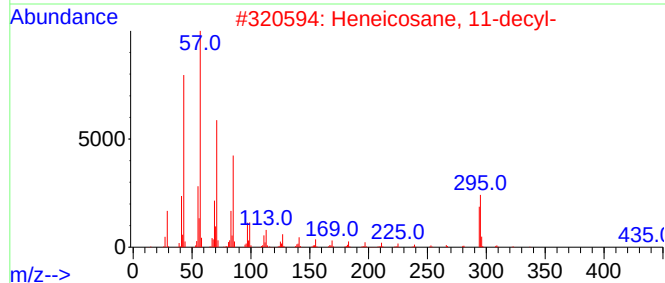
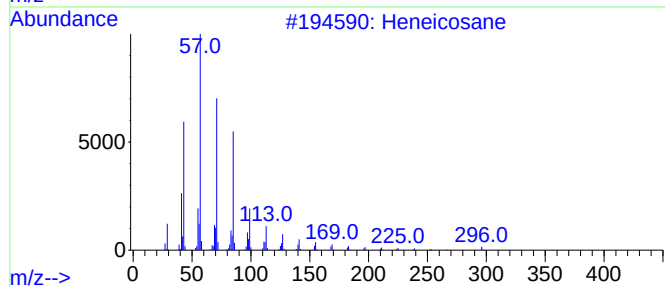
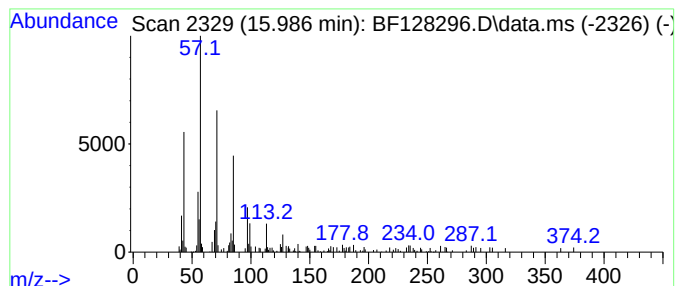
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.986	3.05 ng	74987	Perylene-d12	15.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	74
2			Heneicosane, 11-decyl-	437	C31H64	055320-06-4	72
3			Tetracosane	338	C24H50	000646-31-1	72
4			Docosane	310	C22H46	000629-97-0	72
5			Hexacosane	366	C26H54	000630-01-3	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051722\
Data File : BF128296.D
Acq On : 17 May 2022 17:43
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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
P007-SS021-0006-01

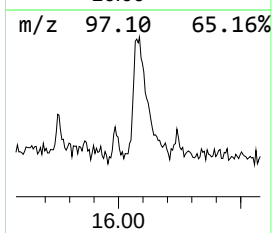
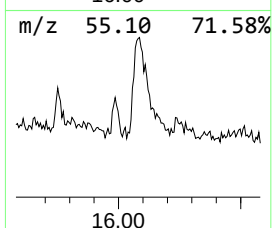
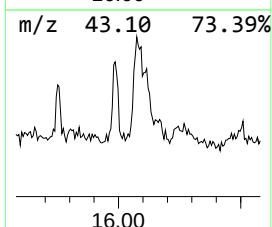
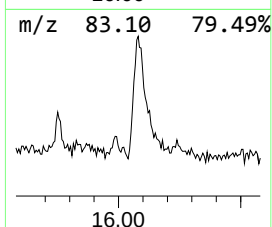
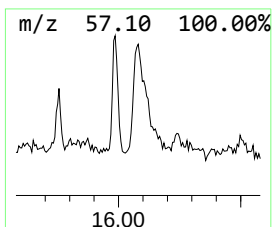
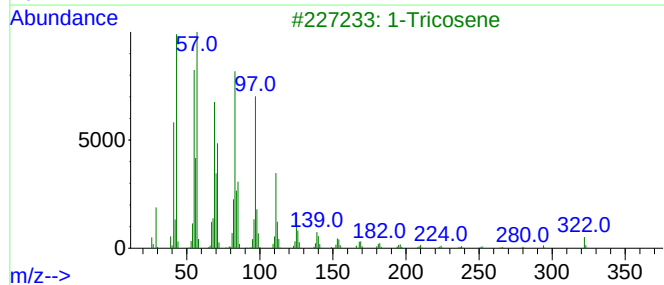
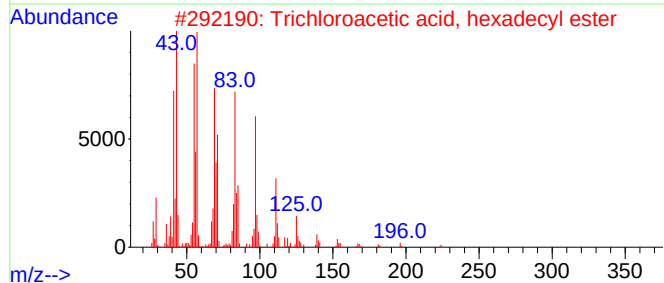
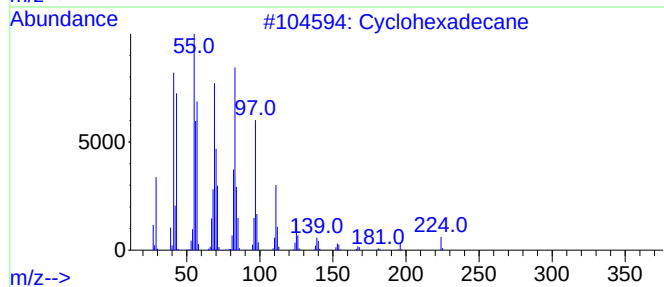
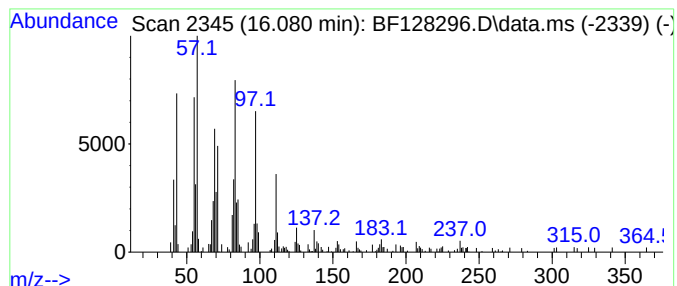
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Cyclohexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.080	11.21 ng	275732	Perylene-d12	15.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexadecane	224	C16H32	000295-65-8	96
2			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3			1-Tricosene	322	C23H46	018835-32-0	91
4			Heptadecafluorononanoic acid, he...	702	C26H35F17O2	1000356-03-3	90
5			1-Heptacosanol	396	C27H56O	002004-39-9	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051722\
Data File : BF128296.D
Acq On : 17 May 2022 17:43
Operator : CG\JU
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Instrument :
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P007-SS021-0006-01

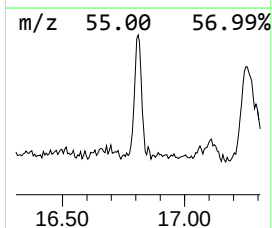
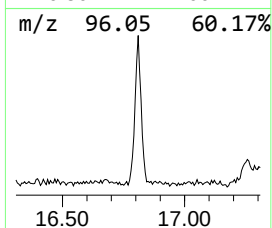
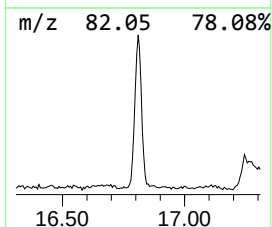
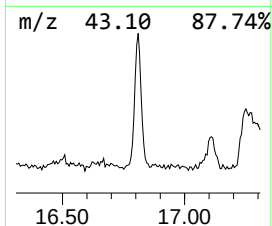
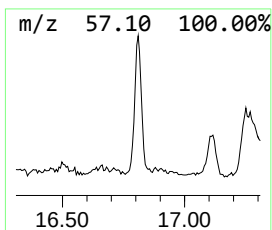
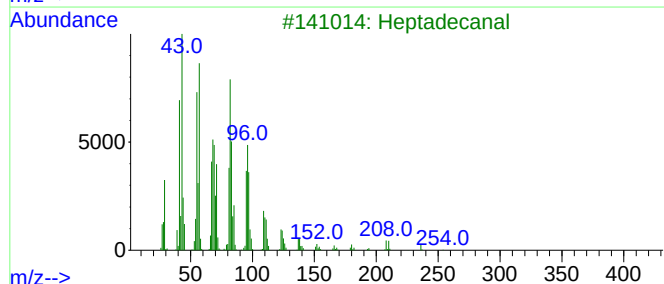
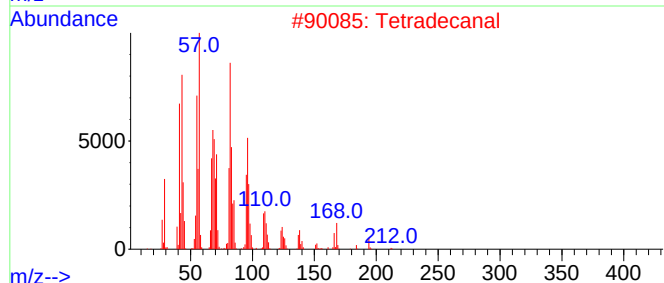
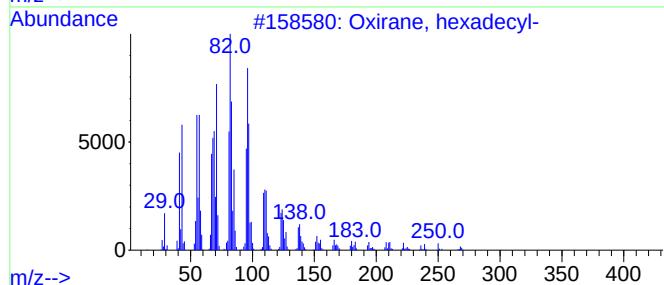
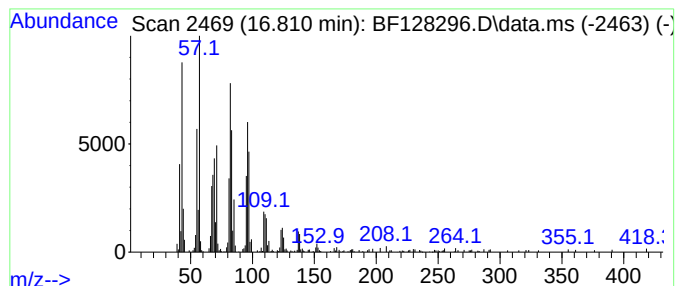
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Oxirane, hexadecyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.810	16.34 ng	401680	Perylene-d12	15.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	94
2			Tetradecanal	212	C14H28O	000124-25-4	93
3			Heptadecanal	254	C17H34O	1000376-70-0	91
4			Octacosanal	408	C28H56O	022725-64-0	90
5			Octadecanal	268	C18H36O	000638-66-4	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051722\
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Acq On : 17 May 2022 17:43
Operator : CG\JU
Sample : N2878-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

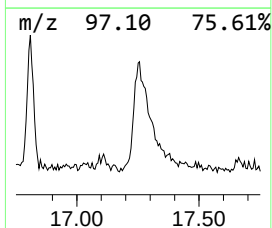
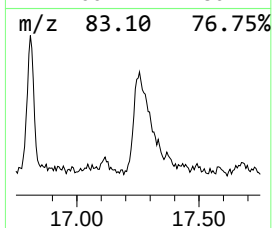
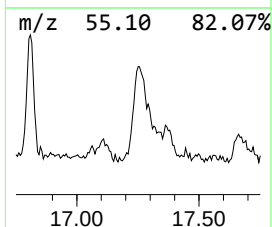
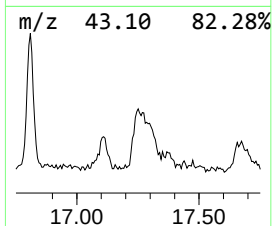
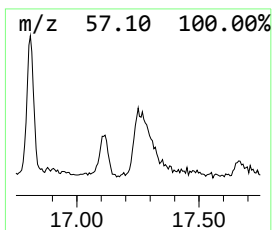
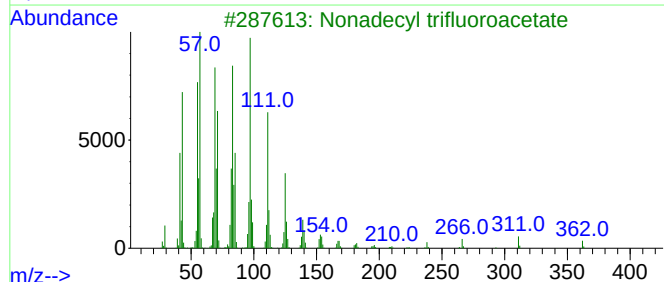
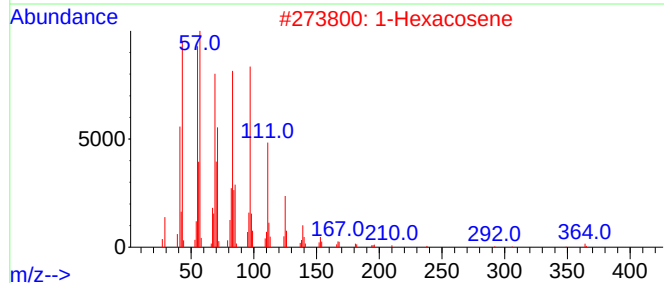
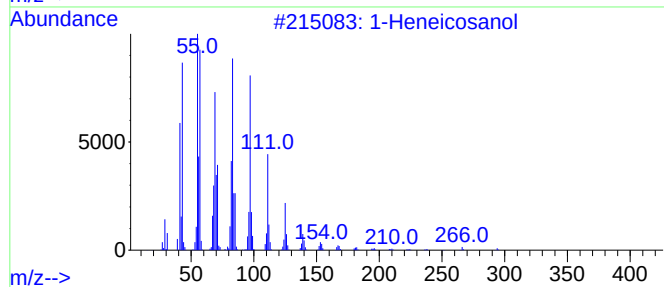
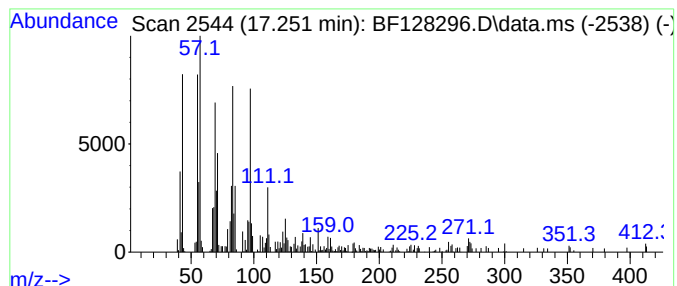
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 1-Heneicosanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.251	19.22 ng	472537	Perylene-d12	15.551	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	93
2	1-Hexacosene	364	C26H52	018835-33-1	93
3	Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	90
4	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	90
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051722\
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Acq On : 17 May 2022 17:43
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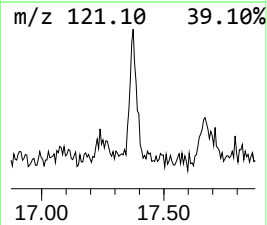
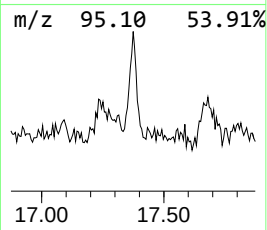
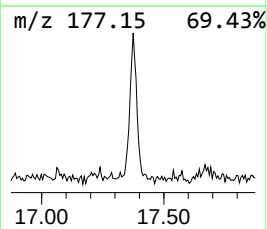
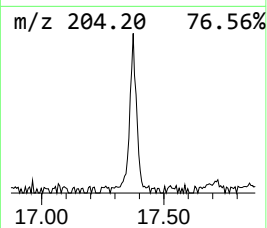
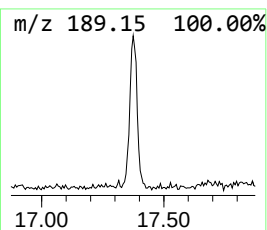
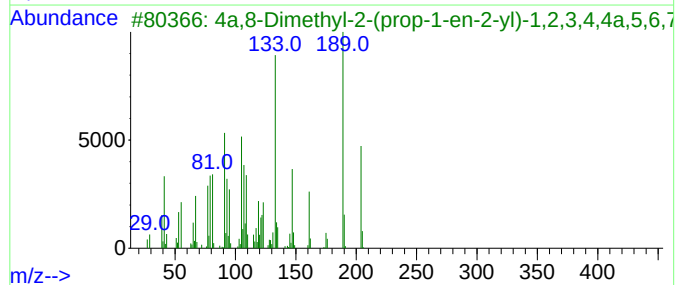
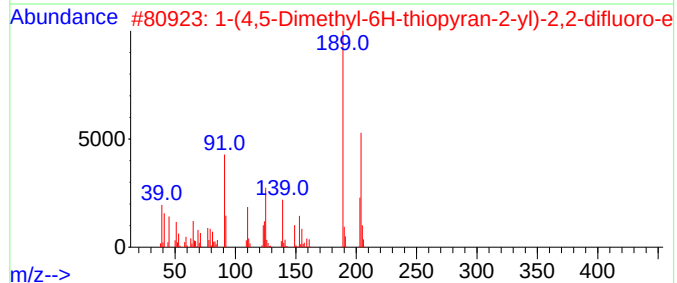
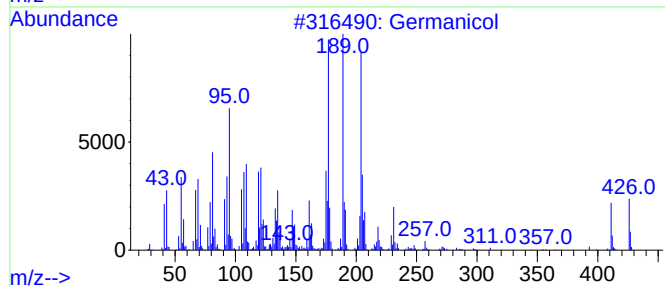
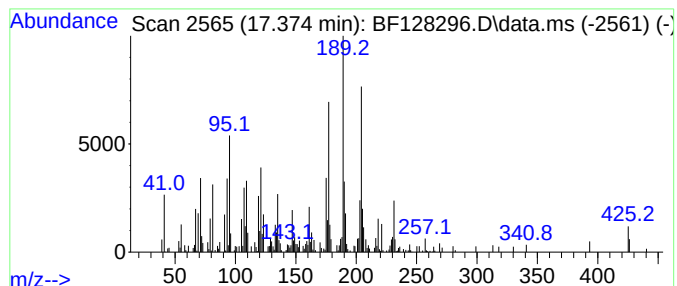
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Germanicol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.374	9.32 ng	229179	Perylene-d12	15.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Germanicol	426	C30H50O	000465-02-1	62
2			1-(4,5-Dimethyl-6H-thiopyran-2-y...	204	C9H10F2OS	1000318-25-0	47
3			4a,8-Dimethyl-2-(prop-1-en-2-yl)...	204	C15H24	103827-22-1	46
4			1H-Indol-6-ylamine, TMS derivative	204	C11H16N2Si	1000484-86-1	43
5			1,3a-Ethano-3aH-indene, 1,2,3,6,...	204	C15H24	004545-68-0	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051722\
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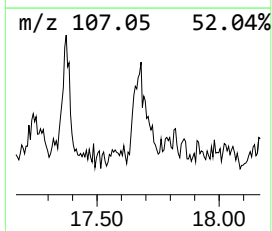
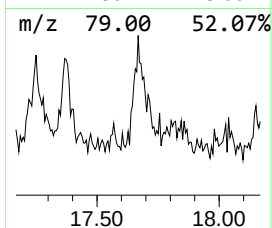
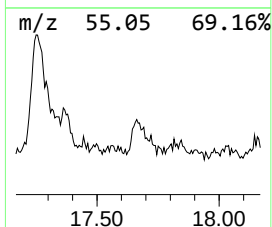
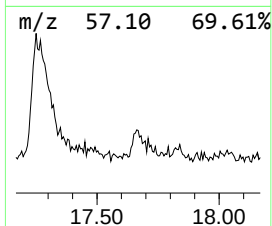
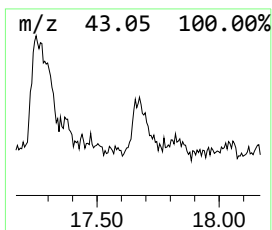
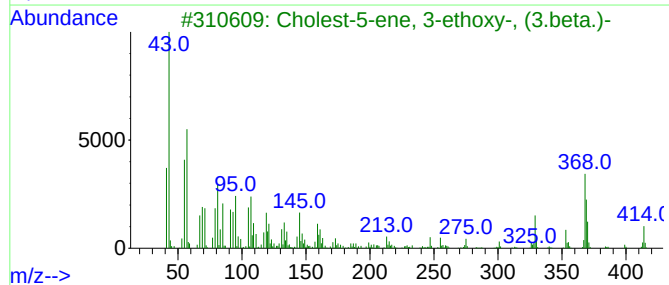
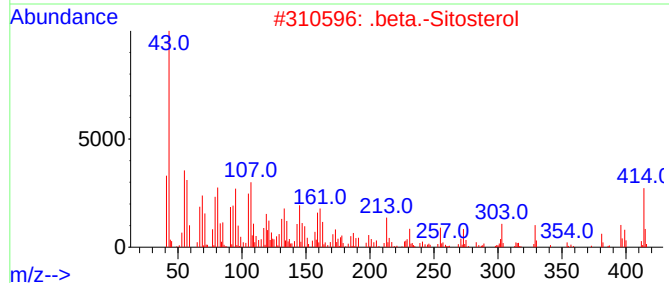
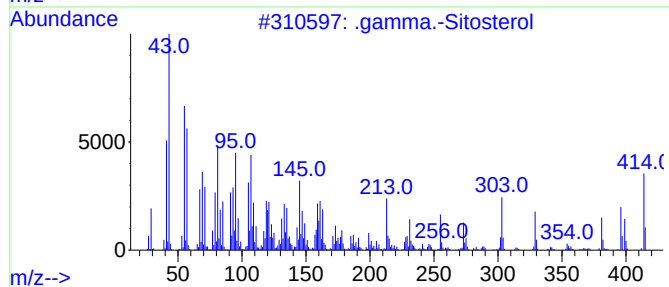
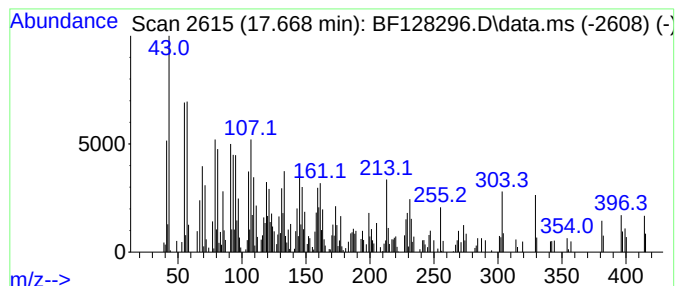
Instrument :
BNA_F
ClientSampleId :
P007-SS021-0006-01

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 13 .gamma.-Sitosterol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.668	11.62 ng	285666	Perylene-d12	15.551	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.gamma.-Sitosterol	414	C29H50O	000083-47-6	93
2	.beta.-Sitosterol	414	C29H50O	000083-46-5	90
3	Cholest-5-ene, 3-ethoxy-, (3.bet...	414	C29H50O	000986-19-6	64
4	Ergost-5-en-3-ol, (3.beta.)-	400	C28H48O	004651-51-8	41
5	Ergost-7-en-3-ol	400	C28H48O	116179-22-7	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051722\
Data File : BF128296.D
Acq On : 17 May 2022 17:43
Operator : CG\JU
Sample : N2878-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P007-SS021-0006-01

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
n-Hexadecanoic ...	11.922	2.8	ng	84858	4	11.410	596781	20.0
2,4-Diamino-8-h...	13.127	2.4	ng	52275	5	14.057	442668	20.0
Dichloroacetic ...	13.892	12.3	ng	271805	5	14.057	442668	20.0
Hexadecane	14.504	2.6	ng	57026	5	14.057	442668	20.0
Acetic acid, 2-...	14.580	2.2	ng	48488	5	14.057	442668	20.0
Tetratetracontane	15.157	5.3	ng	129579	6	15.551	491792	20.0
Hexadecanal	15.751	2.2	ng	53835	6	15.551	491792	20.0
Heneicosane	15.986	3.0	ng	74987	6	15.551	491792	20.0
Cyclohexadecane	16.080	11.2	ng	275732	6	15.551	491792	20.0
Oxirane, hexade...	16.810	16.3	ng	401680	6	15.551	491792	20.0
1-Heneicosanol	17.251	19.2	ng	472537	6	15.551	491792	20.0
Germanicol	17.374	9.3	ng	229179	6	15.551	491792	20.0
.gamma.-Sitosterol	17.668	11.6	ng	285666	6	15.551	491792	20.0