

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF040622\
 Data File : BF127653.D
 Acq On : 06 Apr 2022 17:42
 Operator : CG\JU
 Sample : N2220-09
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 A02145

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-BF040622.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127653.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.193	489	494	498	rVB2	27941	35062	1.11%	0.156%
2	5.575	554	559	562	rBV	2373156	2275199	71.87%	10.106%
3	6.575	723	729	732	rBV	2351773	2337414	73.84%	10.382%
4	6.963	791	795	798	rVB	703699	563641	17.80%	2.504%
5	7.522	885	890	893	rBV	1734679	1559489	49.26%	6.927%
6	8.245	1009	1013	1016	rBV	918909	723855	22.87%	3.215%
7	9.322	1192	1196	1200	rBV	2897583	2807706	88.69%	12.471%
8	9.398	1204	1209	1212	rBV	46957	40205	1.27%	0.179%
9	10.004	1308	1312	1316	rBV	931200	862263	27.24%	3.830%
10	10.798	1442	1447	1450	rBV	2158081	1990534	62.88%	8.841%
11	11.498	1562	1566	1570	rBV	1096455	931623	29.43%	4.138%
12	11.710	1586	1602	1613	rBV6	65076	297150	9.39%	1.320%
13	12.016	1649	1654	1665	rBV	357421	387626	12.24%	1.722%
14	12.192	1682	1684	1693	rVB2	59563	66665	2.11%	0.296%
15	12.727	1769	1775	1781	rBV4	41530	65677	2.07%	0.292%
16	12.804	1783	1788	1795	rBV	114592	125590	3.97%	0.558%
17	12.969	1812	1816	1822	rVB2	38526	52665	1.66%	0.234%
18	13.092	1833	1837	1840	rBV	3636326	3165717	100.00%	14.061%
19	13.439	1890	1896	1905	rBV3	31234	80540	2.54%	0.358%
20	13.980	1985	1988	1993	rBV	737068	695502	21.97%	3.089%
21	14.151	2009	2017	2020	rBV	952555	972705	30.73%	4.320%
22	14.245	2028	2033	2041	rBV	462370	495114	15.64%	2.199%
23	14.621	2093	2097	2105	rBV2	142204	181904	5.75%	0.808%
24	14.704	2107	2111	2114	rBV	32922	50537	1.60%	0.224%
25	15.021	2162	2165	2168	rBV2	41224	45431	1.44%	0.202%
26	15.304	2207	2213	2216	rBV	101701	160566	5.07%	0.713%
27	15.674	2270	2276	2280	rBV	616949	748344	23.64%	3.324%
28	16.186	2358	2363	2367	rBV	75259	115851	3.66%	0.515%
29	16.233	2367	2371	2383	rVB	106192	198059	6.26%	0.880%
30	17.468	2575	2581	2591	rVB6	37219	99762	3.15%	0.443%
31	17.886	2643	2652	2663	rBV9	85032	229468	7.25%	1.019%
32	18.768	2793	2802	2812	rBV9	50126	152228	4.81%	0.676%

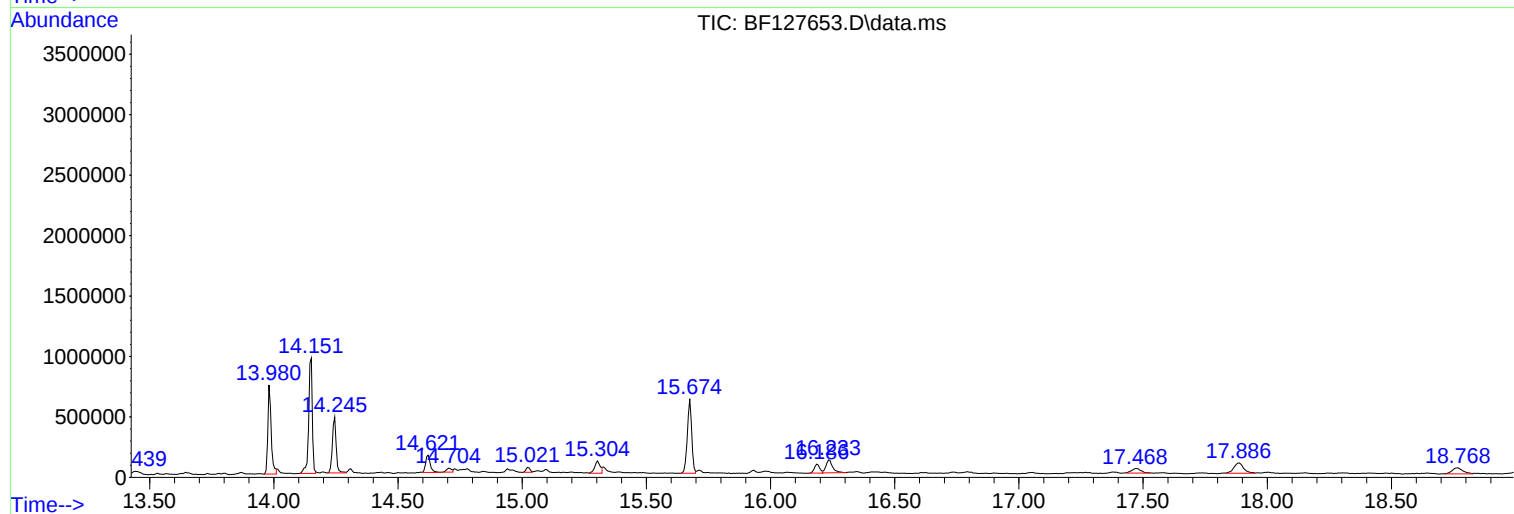
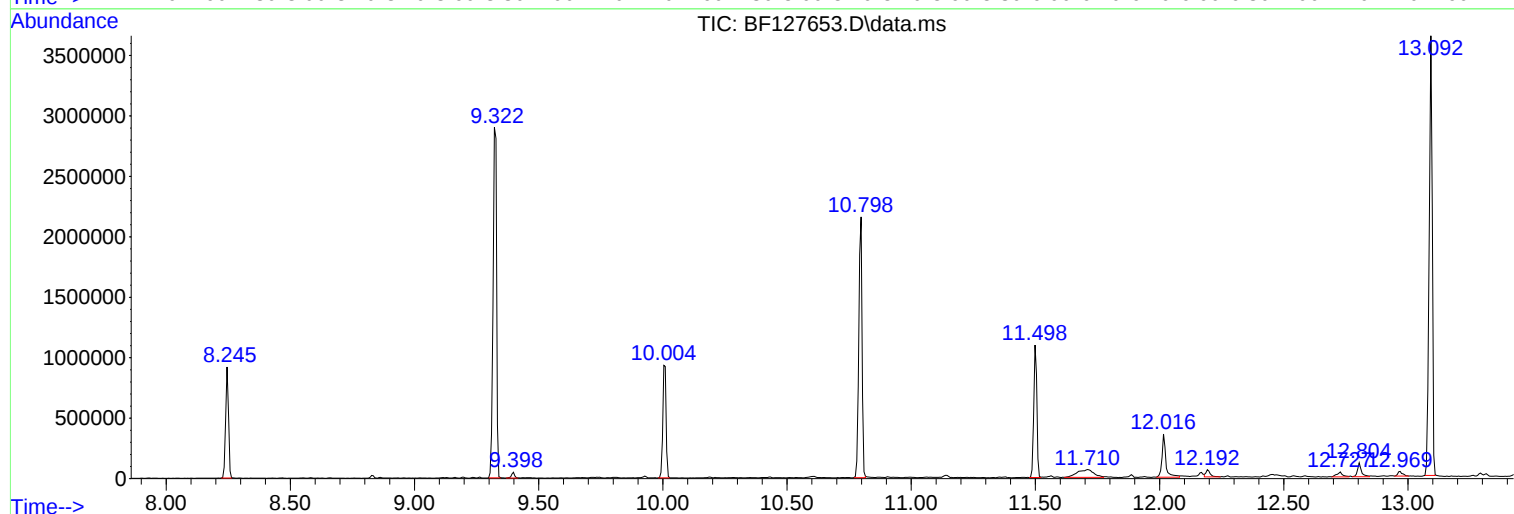
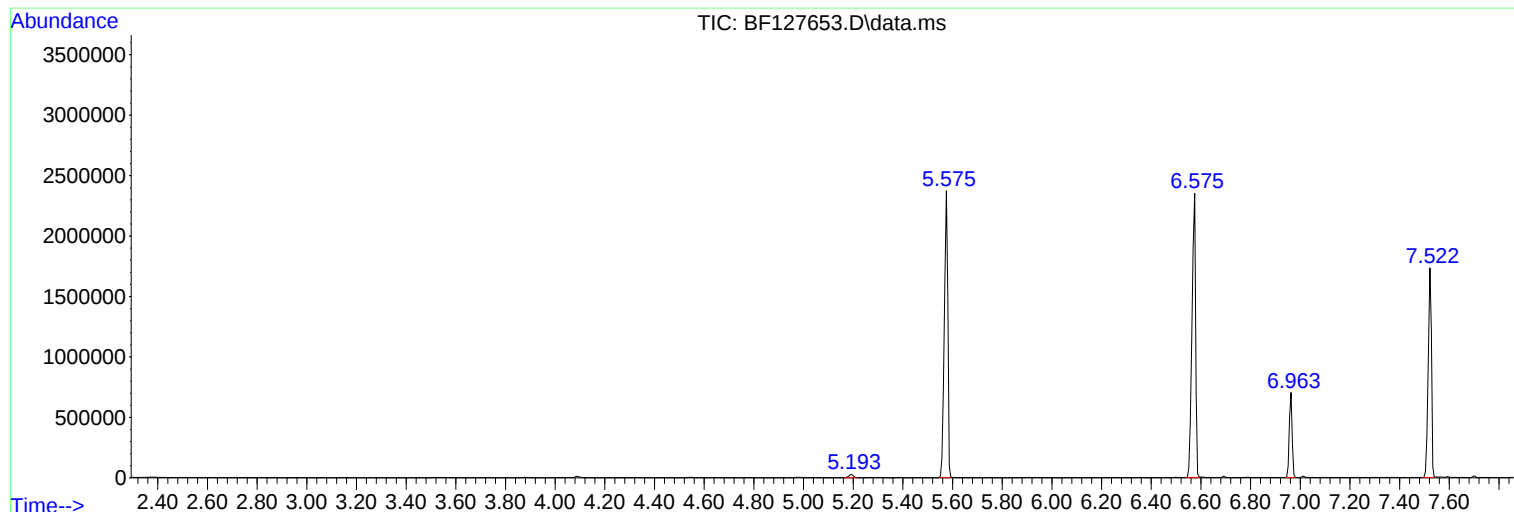
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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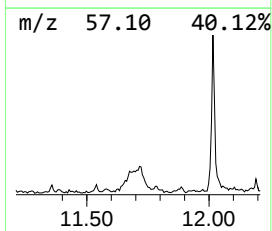
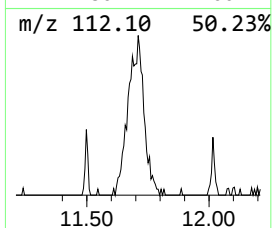
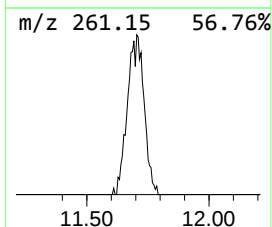
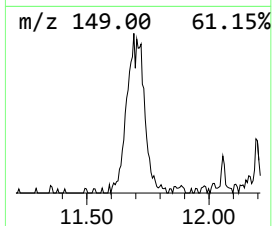
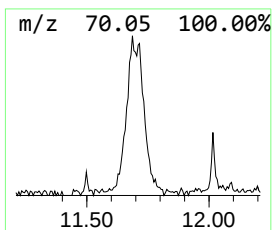
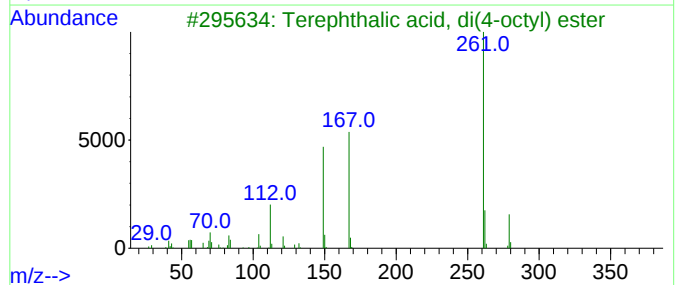
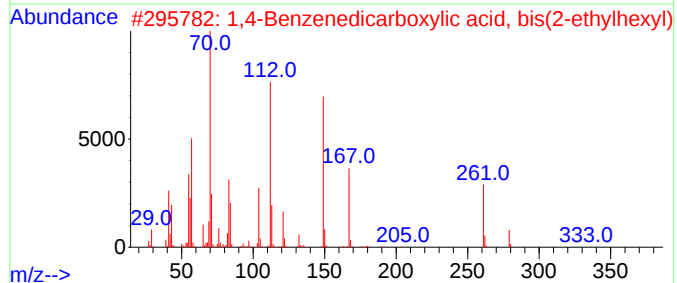
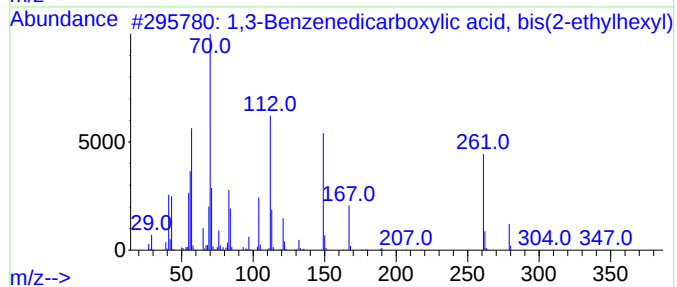
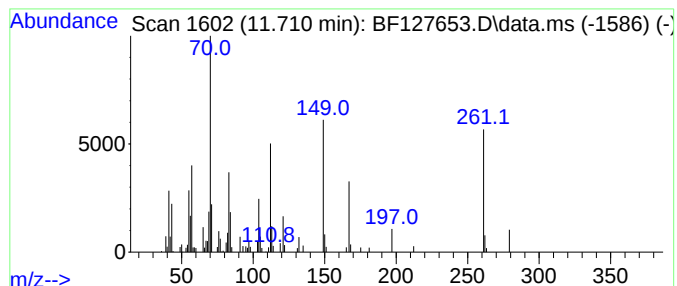
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 1,3-Benzenedicarboxylic aci... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.710	6.38 ng	297150	Phenanthrene-d10	11.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	83		
2	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	70		
3	Terephthalic acid, di(4-octyl) e...	390	C24H38O4	1000323-74-2	38		
4	Terephthalic acid, 4-cyanophenyl...	379	C23H25NO4	1000323-66-6	30		
5	Terephthalic acid, octyl 2,3,4-t...	408	C22H23F3O4	1010415-80-4	27		



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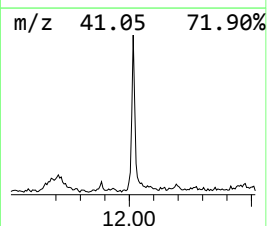
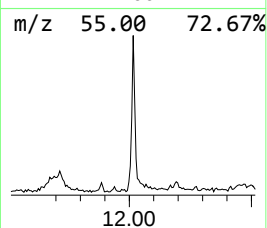
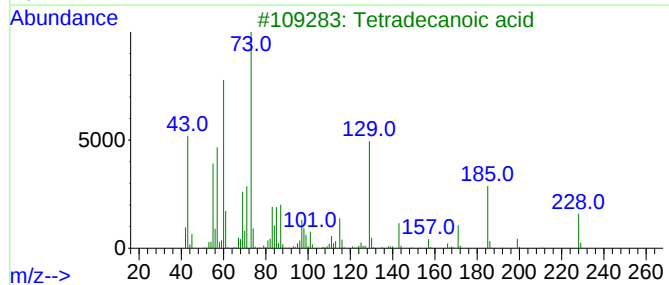
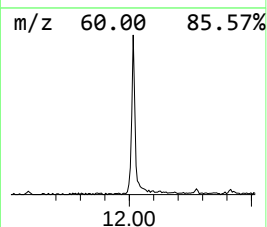
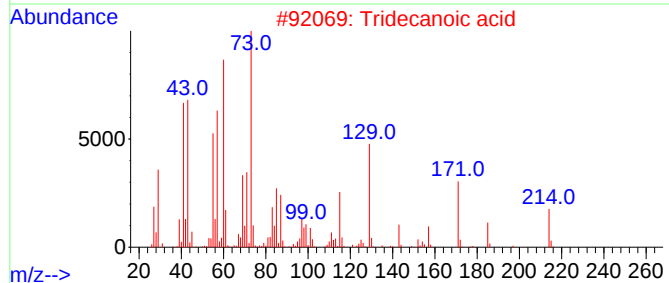
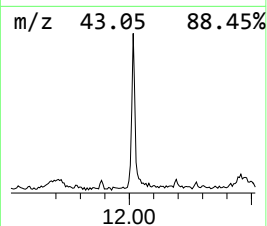
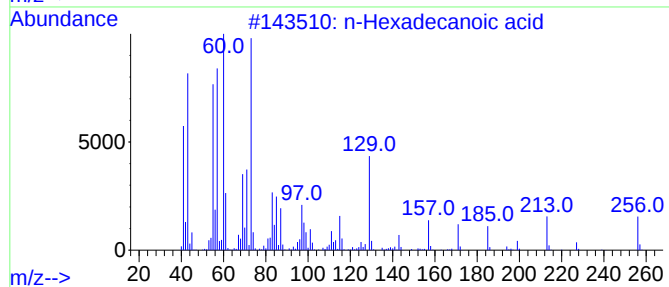
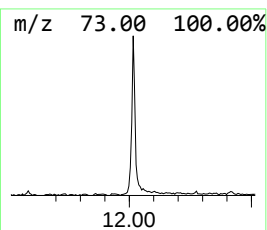
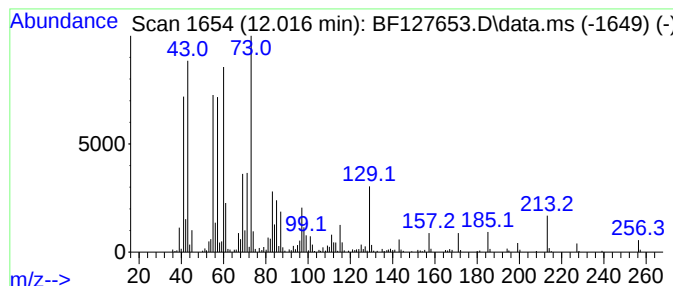
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.016	8.32 ng	387626	Phenanthrene-d10	11.498

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	91
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	91
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5			Isopropyl palmitate	298	C19H38O2	000142-91-6	80



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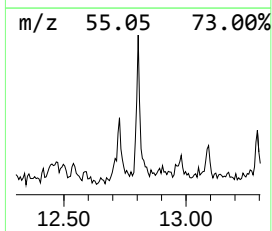
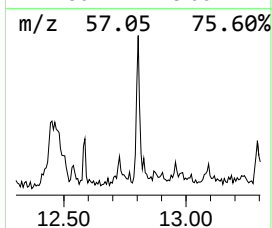
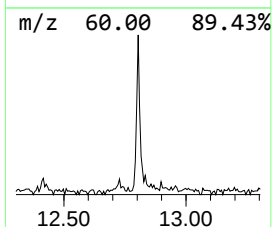
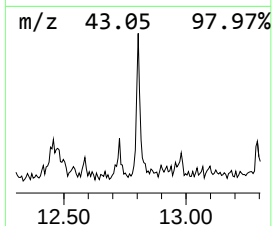
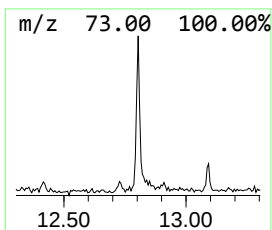
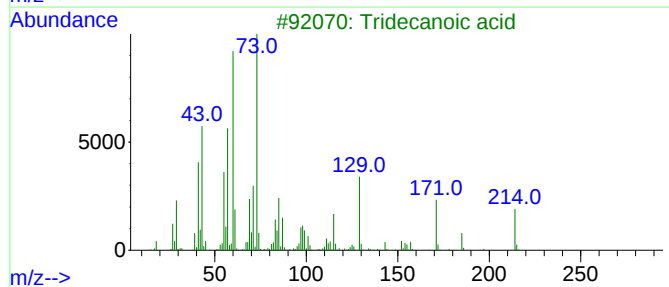
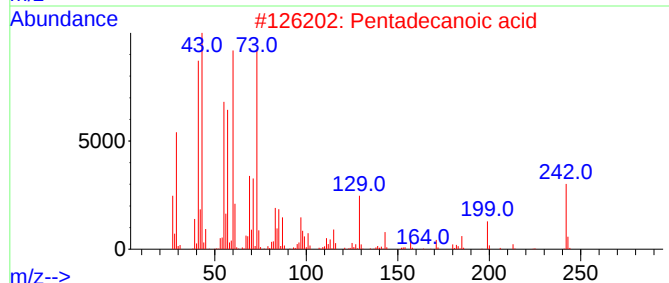
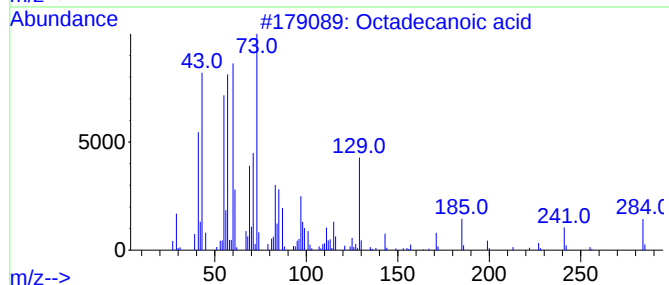
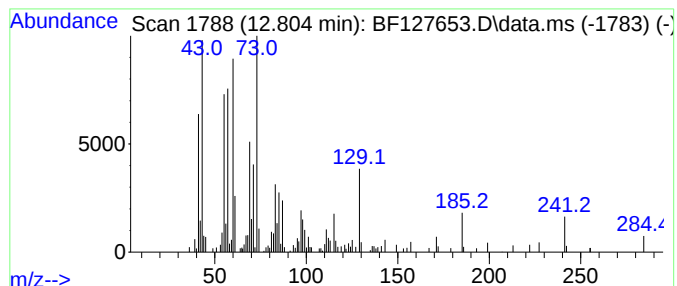
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Octadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.804	2.70 ng	125590	Phenanthrene-d10	11.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	97
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	94
3			Tridecanoic acid	214	C13H26O2	000638-53-9	80
4			n-Decanoic acid	172	C10H20O2	000334-48-5	68
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	64



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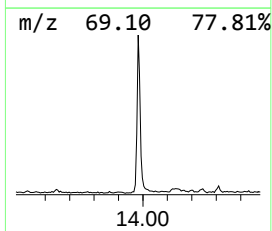
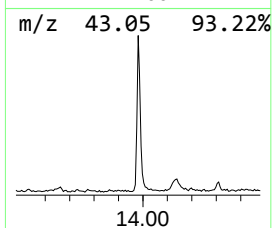
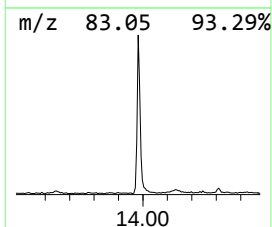
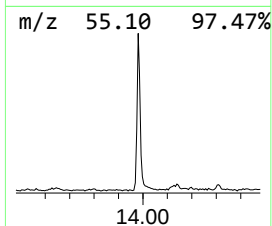
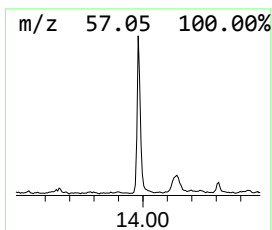
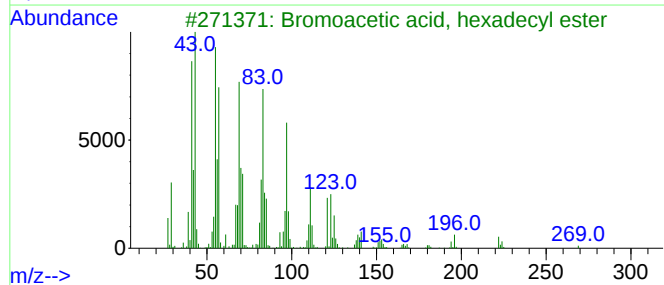
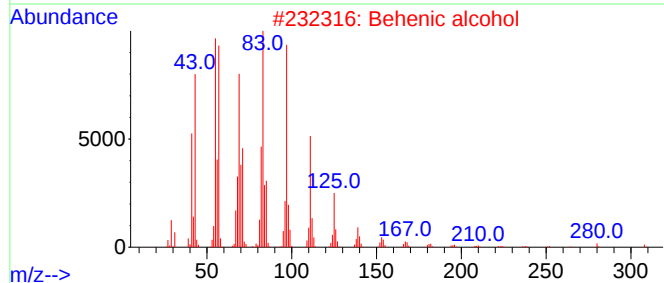
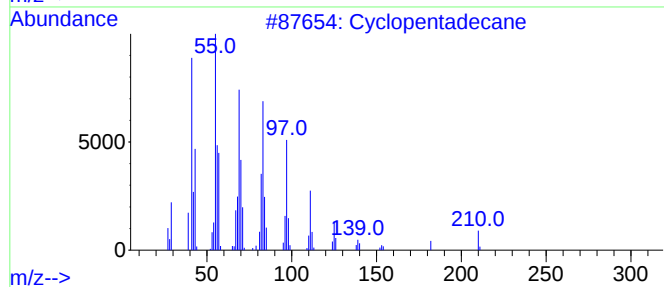
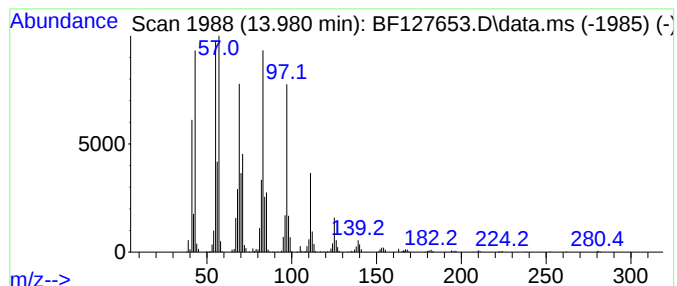
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Peak Number 4 Cyclopentadecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.980	14.30 ng	695502	Chrysene-d12	14.151

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentadecane	210	C15H30	000295-48-7	97
2			Behenic alcohol	326	C22H46O	000661-19-8	94
3			Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	94
4			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
5			1-Hexacosene	364	C26H52	018835-33-1	94



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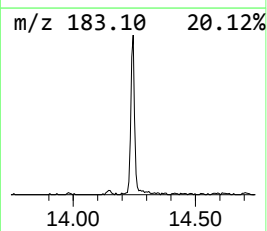
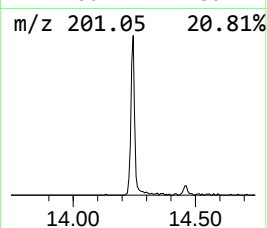
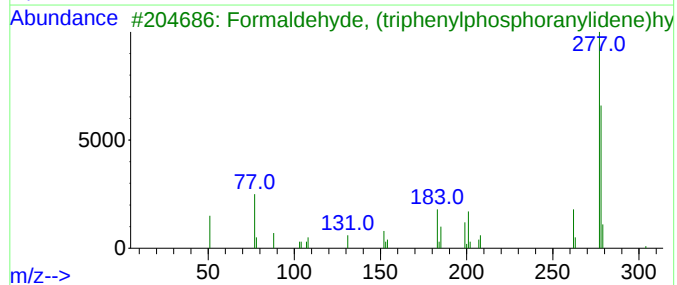
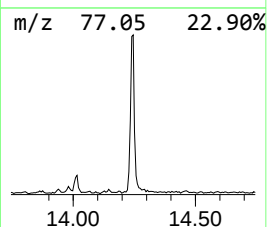
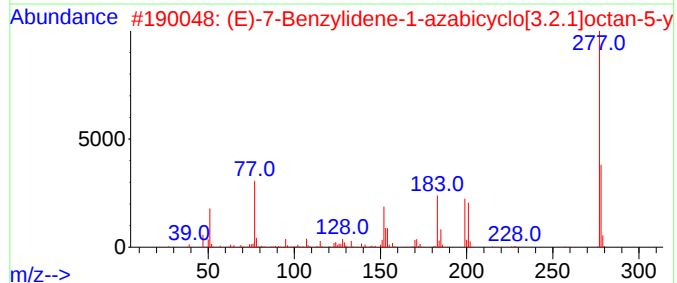
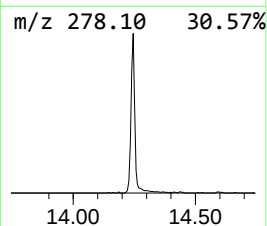
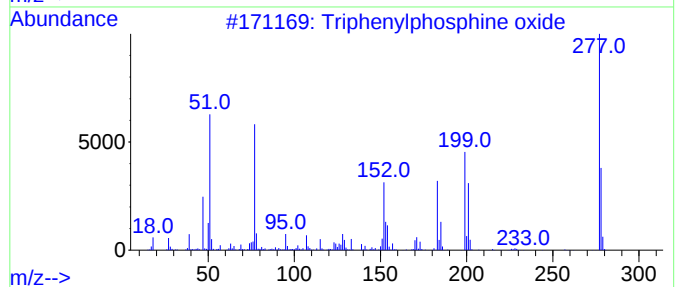
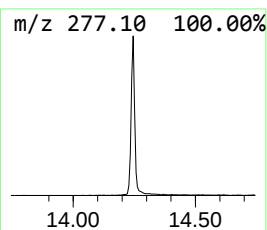
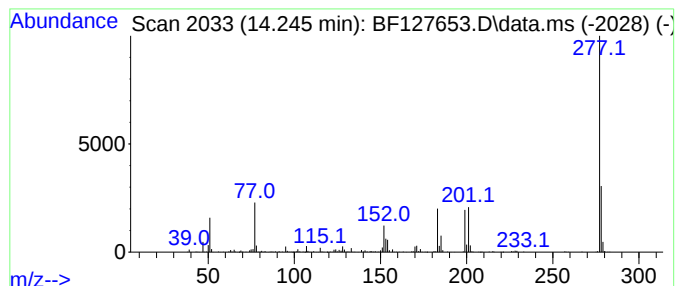
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Peak Number 5 Triphenylphosphine oxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.245	10.18 ng	495114	Chrysene-d12	14.151

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	92
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	91
3			Formaldehyde, (triphenylphosphor...]	304	C19H17N2P	015990-54-2	64
4			Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	32
5			Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	23



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A02145

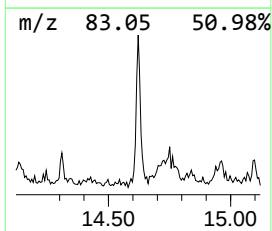
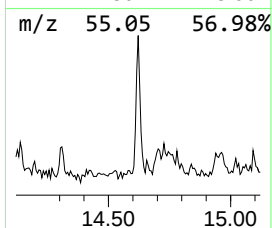
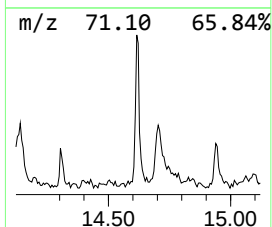
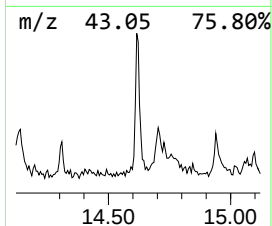
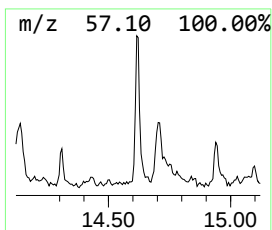
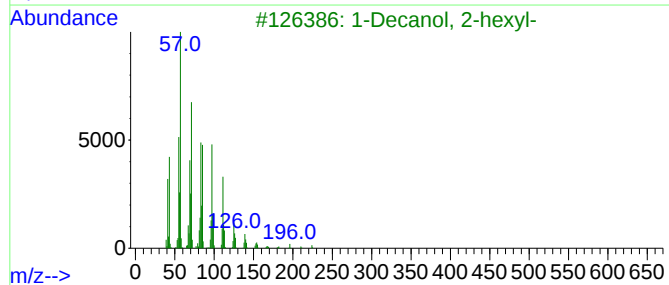
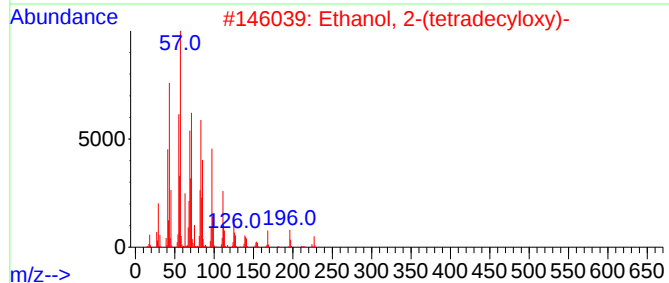
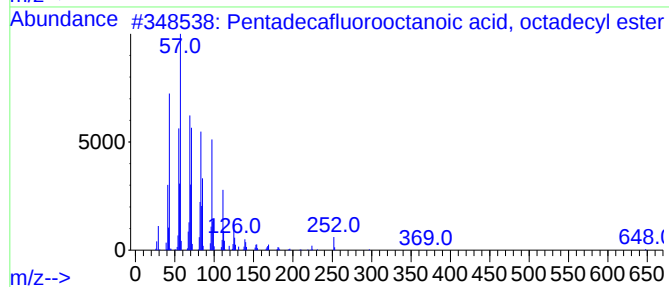
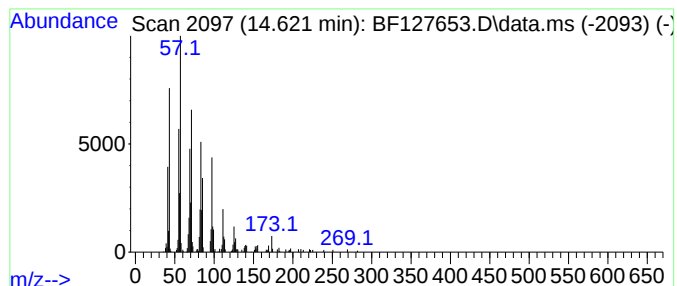
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Pentadecafluorooctanoic aci... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.621	3.74 ng	181904	Chrysene-d12	14.151

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
2			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
3			1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	91
4			Cyclopentadecane	210	C15H30	000295-48-7	91
5			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF040622\
Data File : BF127653.D
Acq On : 06 Apr 2022 17:42
Operator : CG\JU
Sample : N2220-09
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
A02145

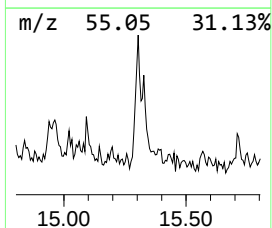
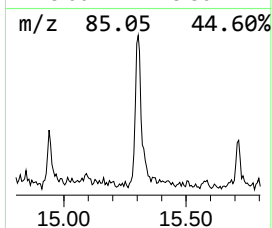
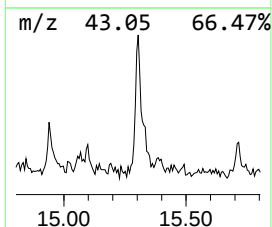
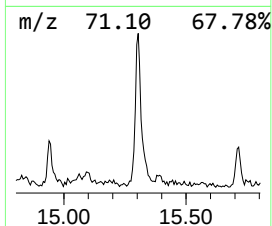
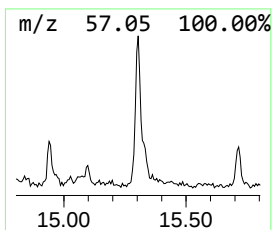
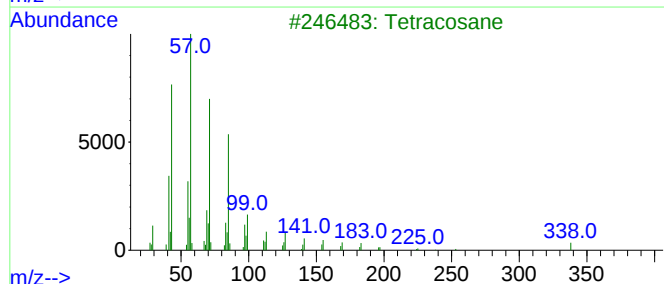
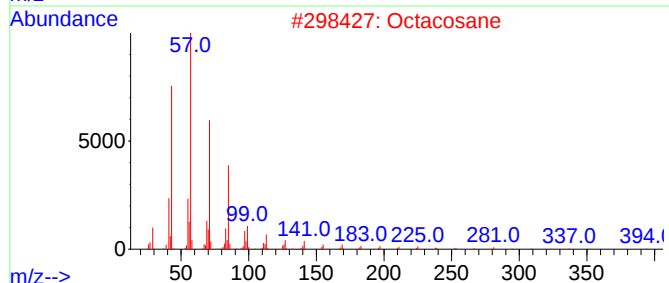
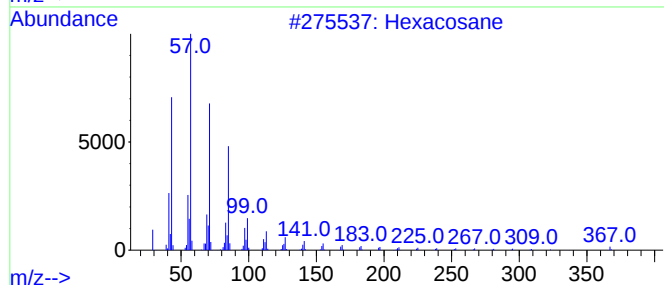
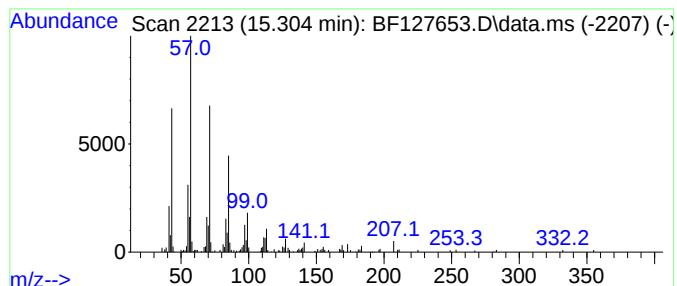
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.304	4.29 ng	160566	Perylene-d12	15.674

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	93
2			Octacosane	394	C28H58	000630-02-4	90
3			Tetracosane	338	C24H50	000646-31-1	90
4			Heneicosane	296	C21H44	000629-94-7	87
5			Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF040622\
Data File : BF127653.D
Acq On : 06 Apr 2022 17:42
Operator : CG\JU
Sample : N2220-09
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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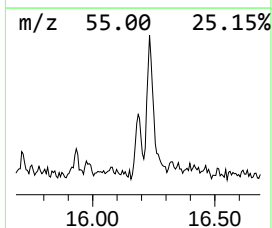
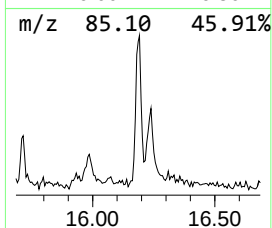
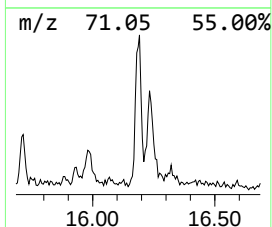
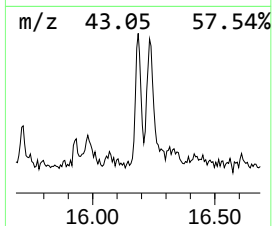
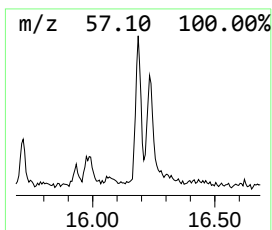
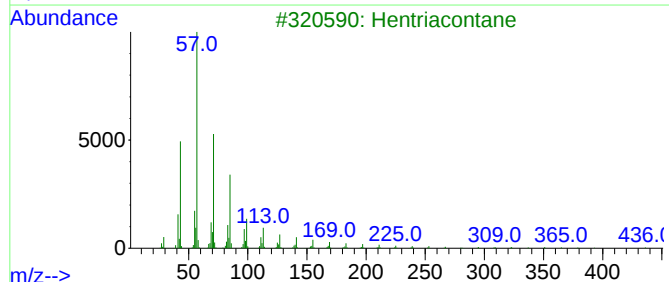
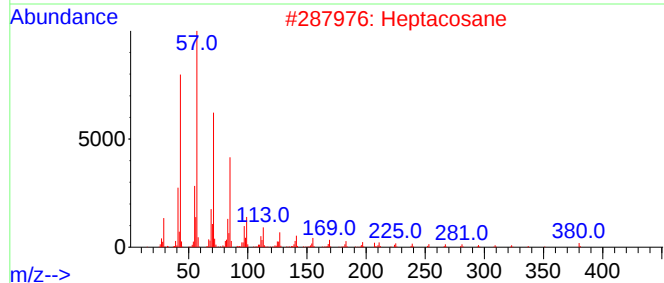
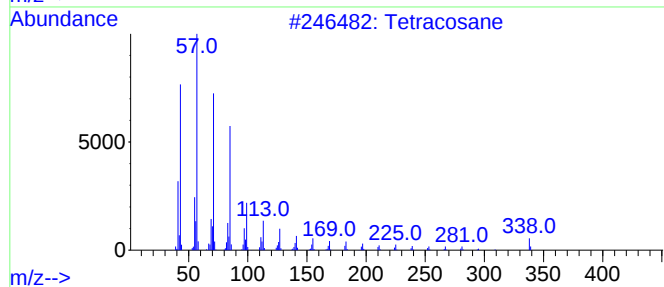
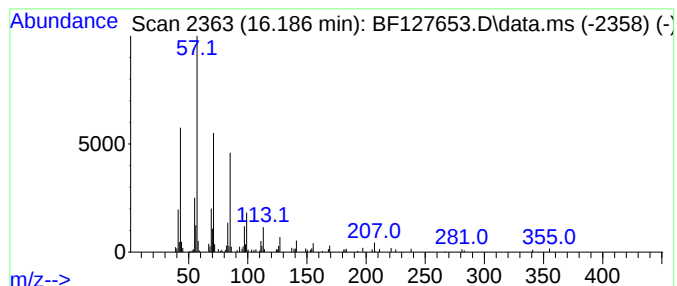
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tetracosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.186	3.10 ng	115851	Perylene-d12	15.674

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	91
2			Heptacosane	380	C27H56	000593-49-7	91
3			Hentriacontane	437	C31H64	000630-04-6	90
4			Heneicosane	296	C21H44	000629-94-7	90
5			Tetratetracontane	619	C44H90	007098-22-8	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF040622\
Data File : BF127653.D
Acq On : 06 Apr 2022 17:42
Operator : CG\JU
Sample : N2220-09
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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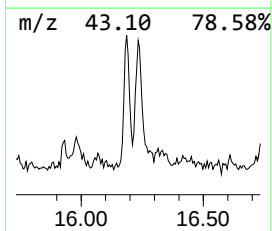
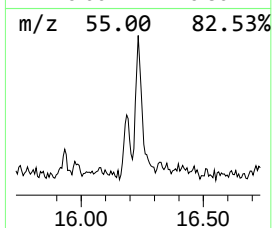
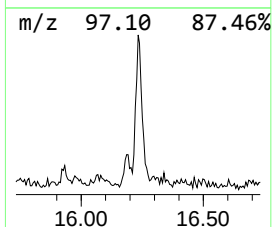
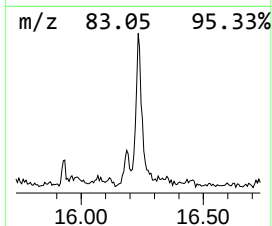
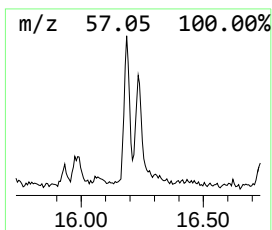
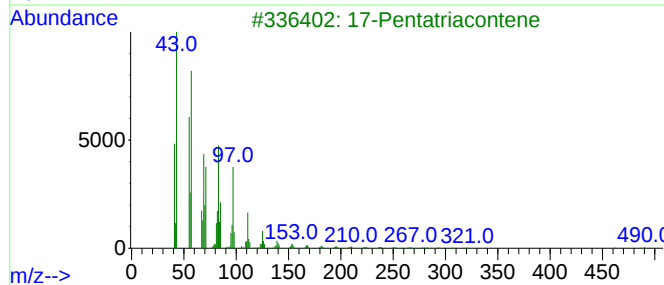
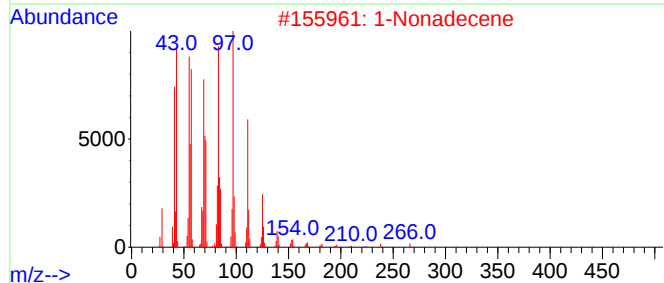
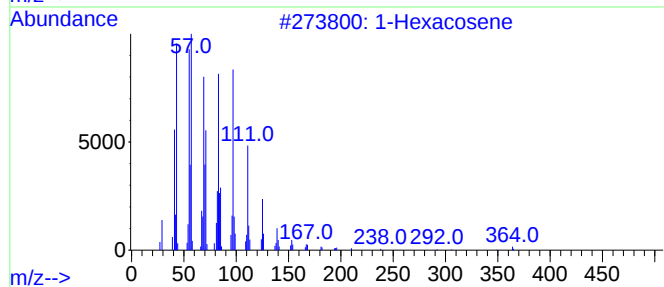
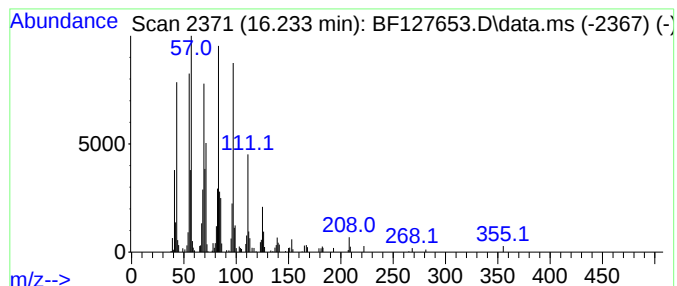
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Hexacosene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.233	5.29 ng	198059	Perylene-d12	15.674

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosene			364	C26H52	018835-33-1	94
2	1-Nonadecene			266	C19H38	018435-45-5	91
3	17-Pentatriacontene			491	C35H70	006971-40-0	91
4	Acetic acid, chloro-, octadecyl ...			346	C20H39ClO2	005348-82-3	87
5	Pentadecafluorooctanoic acid, oc...			666	C26H37F15O2	1000406-04-8	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF040622\
Data File : BF127653.D
Acq On : 06 Apr 2022 17:42
Operator : CG\JU
Sample : N2220-09
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
A02145

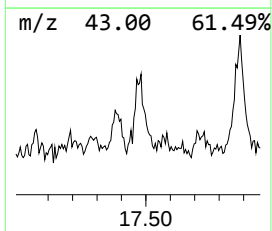
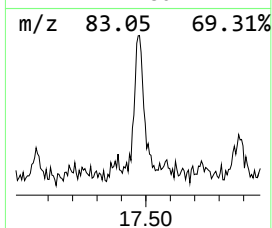
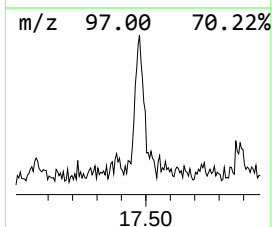
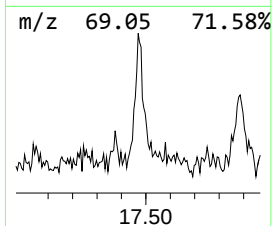
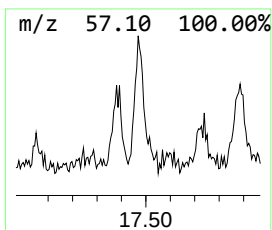
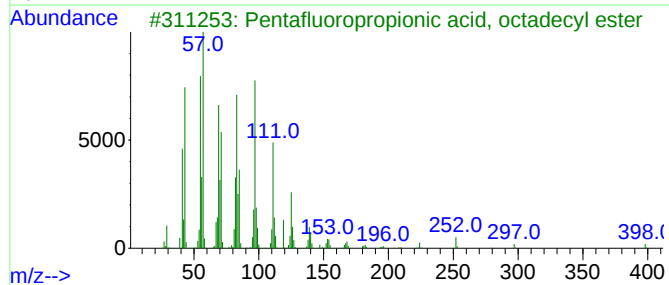
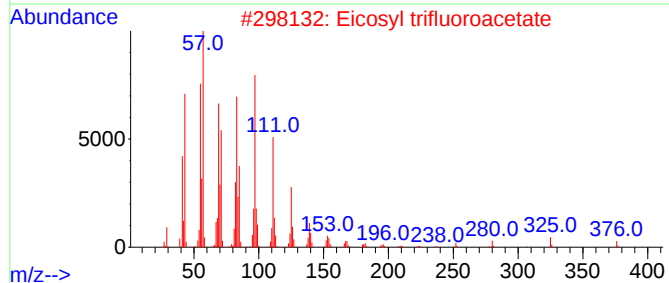
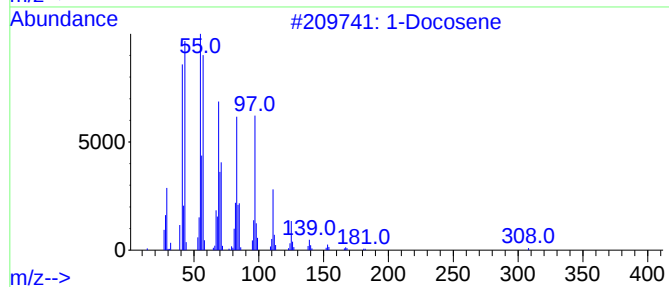
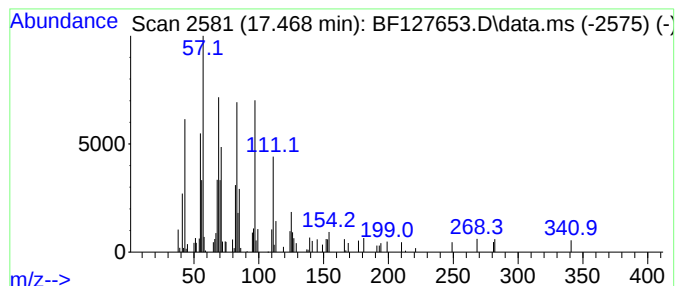
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1-Docosene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.468	2.67 ng	99762	Perylene-d12	15.674

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene			308	C22H44	001599-67-3	83
2	Eicosyl trifluoroacetate			394	C22H41F3O2	1000351-75-2	80
3	Pentafluoropropionic acid, octadecyl ester			416	C21H37F5O2	959261-25-7	80
4	Heptafluorobutyric acid, n-octadecyl ester			466	C22H37F7O2	000400-57-7	80
5	Heptadecyl heptafluorobutyrate			452	C21H35F7O2	959085-66-6	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF040622\
Data File : BF127653.D
Acq On : 06 Apr 2022 17:42
Operator : CG\JU
Sample : N2220-09
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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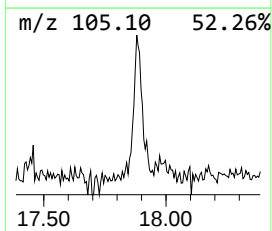
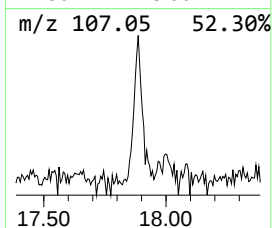
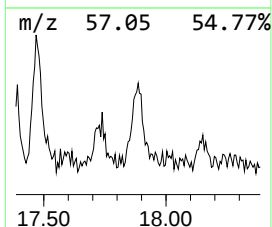
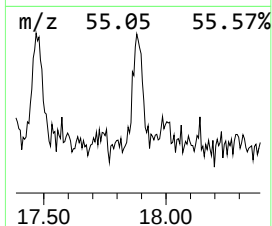
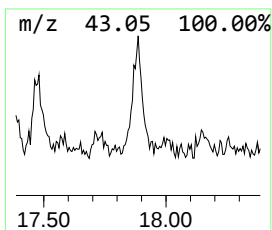
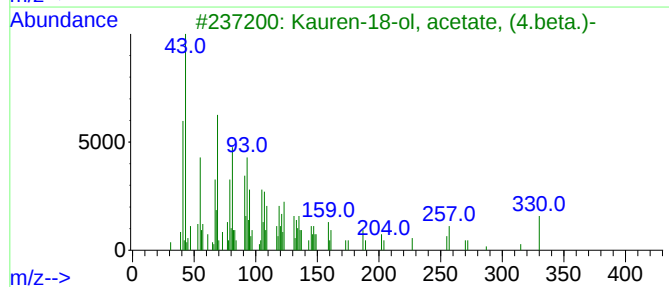
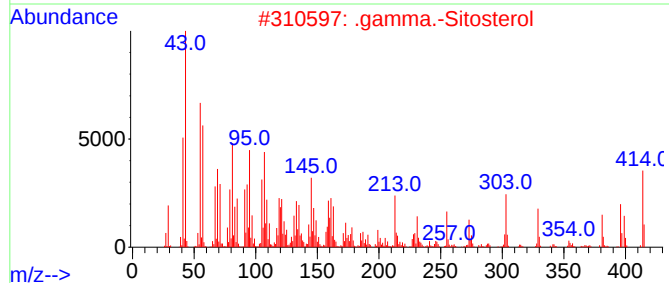
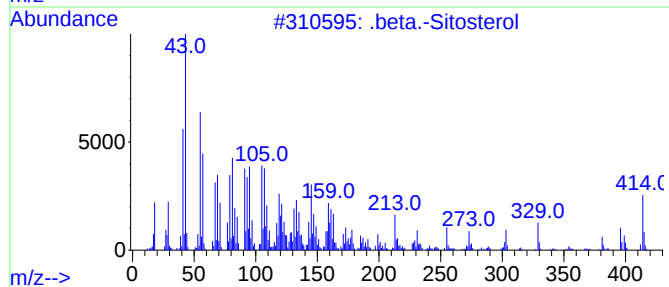
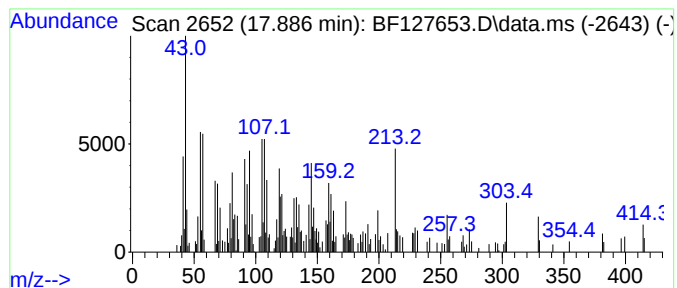
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 .beta.-Sitosterol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.886	6.13 ng	229468	Perylene-d12	15.674

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		.beta.-Sitosterol	414	C29H50O	000083-46-5	99
2		.gamma.-Sitosterol	414	C29H50O	000083-47-6	95
3		Kauren-18-ol, acetate, (4.beta.)-	330	C22H34O2	072150-74-4	49
4		(3S,8S,9S,10R,13R,14S,17R)-17-((...)	414	C29H50O	029365-29-5	30
5		.beta.-Sitosterol acetate	456	C31H52O2	000915-05-9	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF040622\
Data File : BF127653.D
Acq On : 06 Apr 2022 17:42
Operator : CG\JU
Sample : N2220-09
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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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
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n-Hexadecanoic ...	12.016	8.3	ng	387626	4	11.498	931623	20.0
Octadecanoic acid	12.804	2.7	ng	125590	4	11.498	931623	20.0
Cyclopentadecane	13.980	14.3	ng	695502	5	14.151	972705	20.0
Triphenylphosph...	14.245	10.2	ng	495114	5	14.151	972705	20.0
Pentadecafluoro...	14.621	3.7	ng	181904	5	14.151	972705	20.0
Hexacosane	15.304	4.3	ng	160566	6	15.674	748344	20.0
Tetracosane	16.186	3.1	ng	115851	6	15.674	748344	20.0
1-Hexacosene	16.233	5.3	ng	198059	6	15.674	748344	20.0
1-Docosene	17.468	2.7	ng	99762	6	15.674	748344	20.0
.beta.-Sitosterol	17.886	6.1	ng	229468	6	15.674	748344	20.0
(-)-Isolongifol...	18.768	4.1	ng	152228	6	15.674	748344	20.0