

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070622\
 Data File : BF129151.D
 Acq On : 06 Jul 2022 19:32
 Operator : CG\JU
 Sample : N3579-01
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 OK-03-070522

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-BF062922.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF129151.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.581	555	560	563	rBV	5749738	5244415	91.35%	10.145%
2	6.575	724	729	732	rBV	5110378	4917295	85.66%	9.512%
3	6.957	790	794	797	rBV	1947452	1511738	26.33%	2.924%
4	7.516	884	889	892	rBV	3688692	3235633	56.36%	6.259%
5	8.239	1008	1012	1015	rBV	2303252	1782783	31.06%	3.449%
6	9.316	1190	1195	1198	rBV	5917090	5413496	94.30%	10.472%
7	9.569	1235	1238	1244	rBV2	72930	70067	1.22%	0.136%
8	9.998	1307	1311	1314	rBV	2079533	1646761	28.69%	3.186%
9	10.786	1441	1445	1449	rBV	3437316	2951630	51.42%	5.710%
10	11.492	1561	1565	1570	rBV	1889010	1779869	31.00%	3.443%
11	11.869	1626	1629	1633	rVB	262025	202693	3.53%	0.392%
12	12.004	1648	1652	1656	rBV	842777	726739	12.66%	1.406%
13	12.186	1679	1683	1687	rBV2	195104	195252	3.40%	0.378%
14	12.580	1745	1750	1755	rVB4	80657	114654	2.00%	0.222%
15	12.698	1767	1770	1783	rBV2	656656	961986	16.76%	1.861%
16	12.792	1783	1786	1791	rVV	234817	227878	3.97%	0.441%
17	12.939	1807	1811	1814	rBV	229219	230477	4.01%	0.446%
18	13.080	1831	1835	1838	rBV	6897986	5740712	100.00%	11.105%
19	13.298	1869	1872	1874	rBV	82447	79852	1.39%	0.154%
20	13.516	1906	1909	1912	rBV	293010	293413	5.11%	0.568%
21	13.969	1983	1986	1988	rBV	235588	182839	3.18%	0.354%
22	14.016	1989	1994	2000	rVV2	242283	543855	9.47%	1.052%
23	14.139	2011	2015	2018	rBV	1985871	1893581	32.99%	3.663%
24	14.233	2028	2031	2035	rVB	484671	468991	8.17%	0.907%
25	14.592	2089	2092	2096	rBV	671589	565299	9.85%	1.094%
26	14.998	2158	2161	2165	rVB	396064	406045	7.07%	0.785%
27	15.274	2203	2208	2215	rVB	2303828	2732485	47.60%	5.286%
28	15.668	2271	2275	2283	rVB2	1156049	1561879	27.21%	3.021%
29	16.139	2350	2355	2361	rVB	1611604	2478144	43.17%	4.794%
30	17.909	2649	2656	2675	rBV2	1215940	3532686	61.54%	6.834%

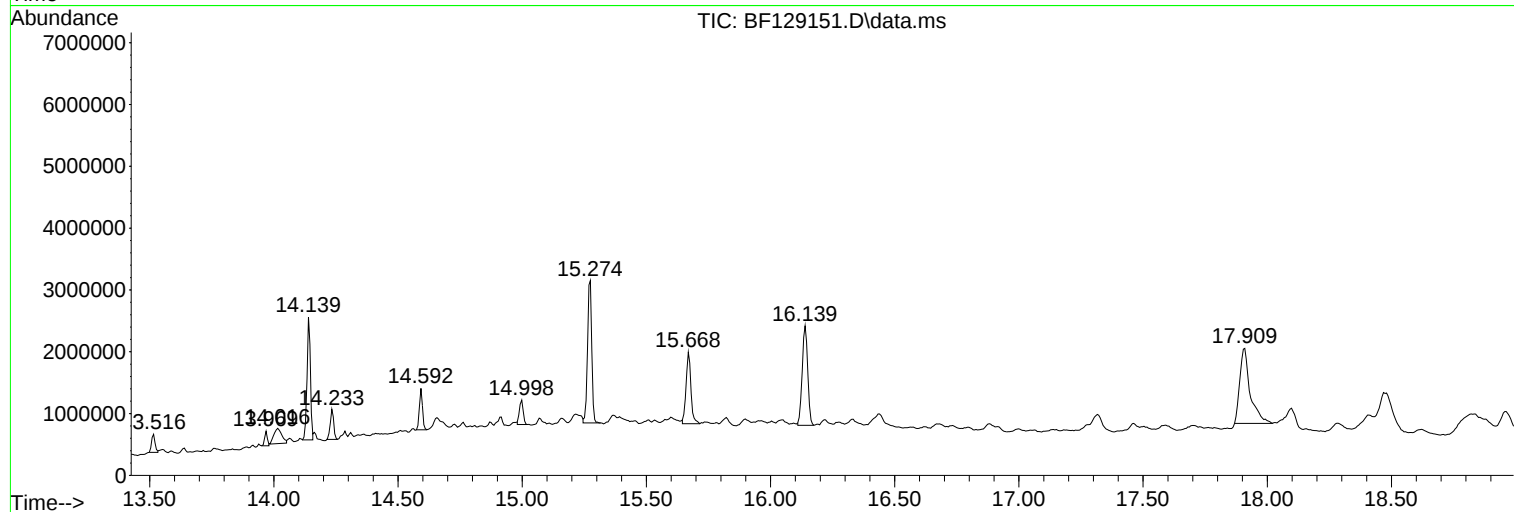
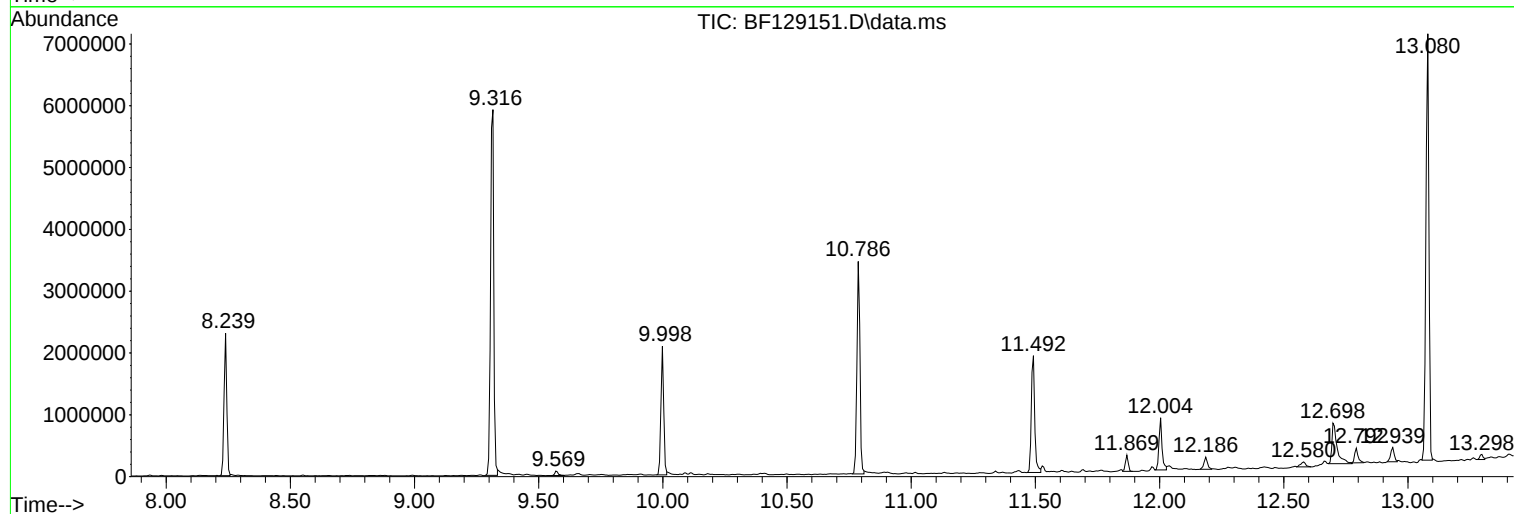
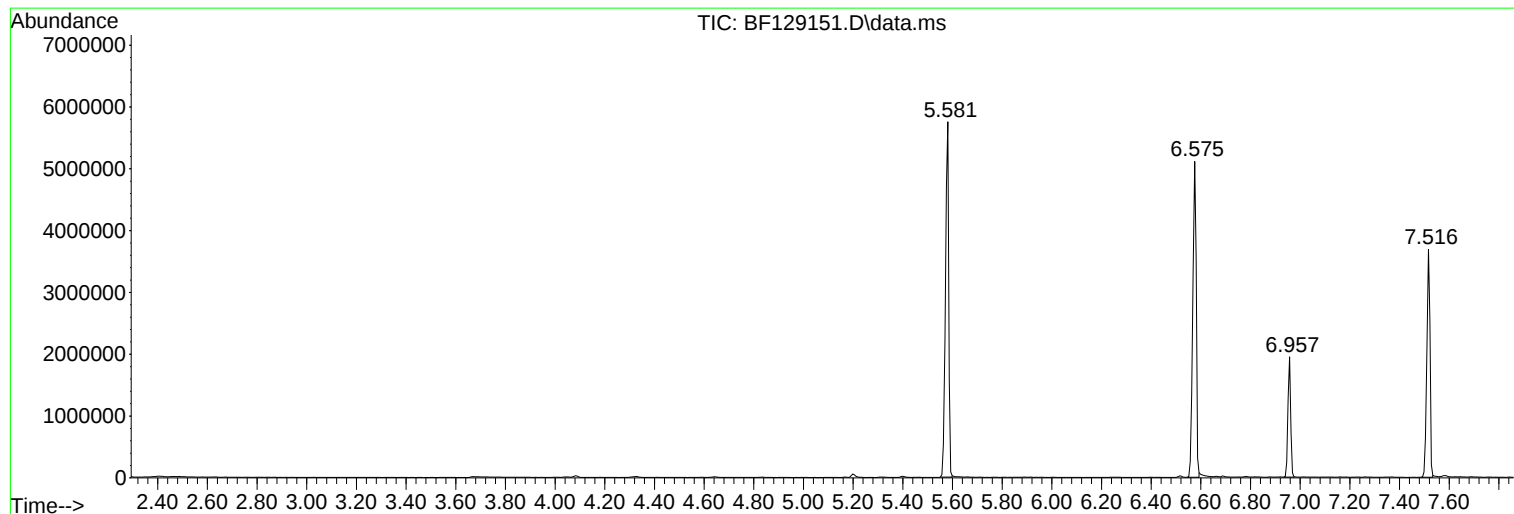
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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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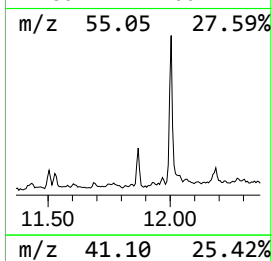
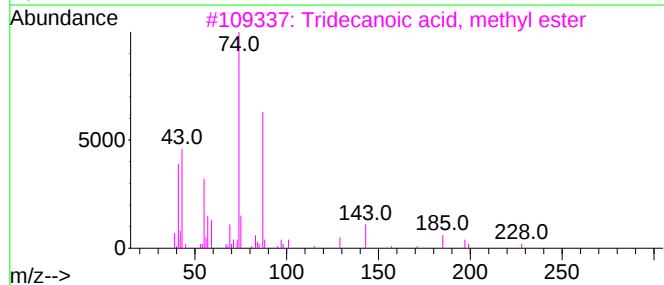
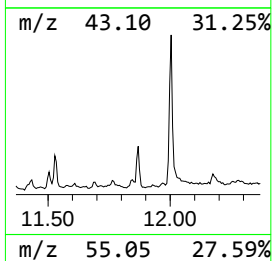
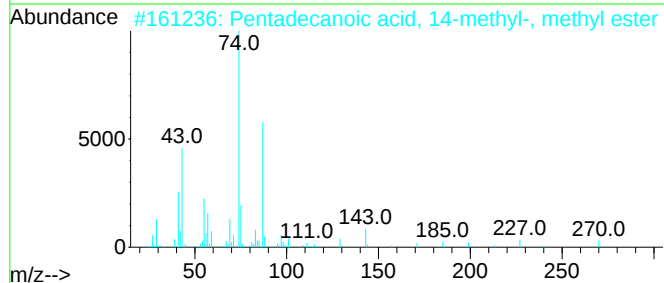
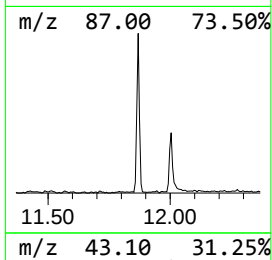
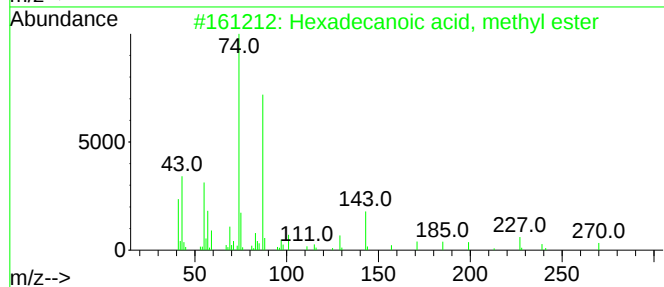
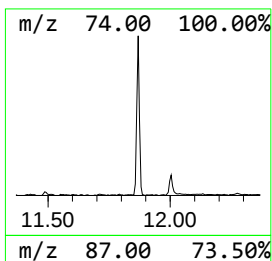
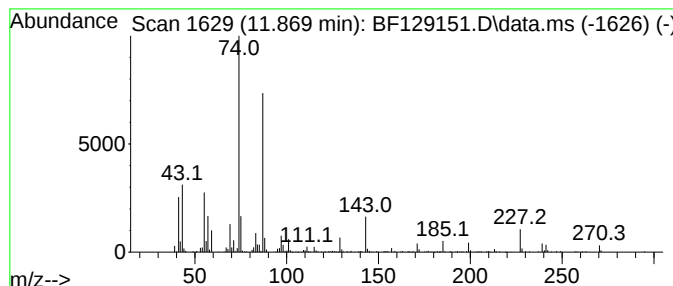
Instrument :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Hexadecanoic acid, methyl e... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.869	2.28 ng	202693	Phenanthrene-d10		11.492	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester		270	C17H34O2	000112-39-0	98
2	Pentadecanoic acid, 14-methyl-, ...		270	C17H34O2	005129-60-2	95
3	Tridecanoic acid, methyl ester		228	C14H28O2	001731-88-0	86
4	Heptadecanoic acid, methyl ester		284	C18H36O2	001731-92-6	86
5	Pentadecanoic acid, methyl ester		256	C16H32O2	007132-64-1	86



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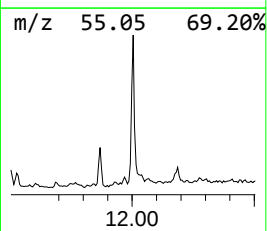
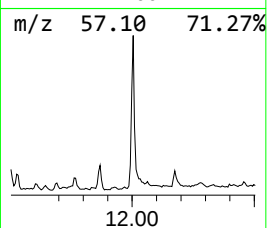
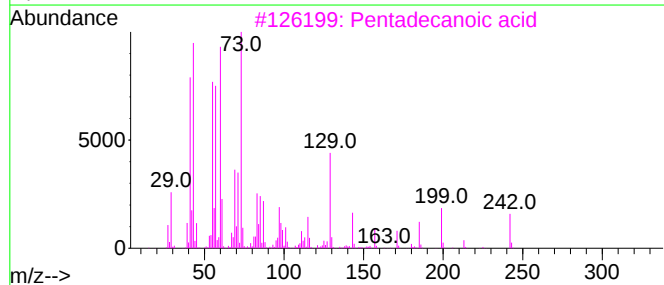
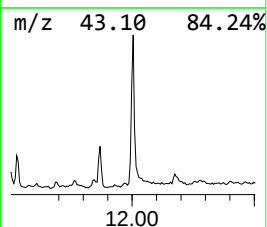
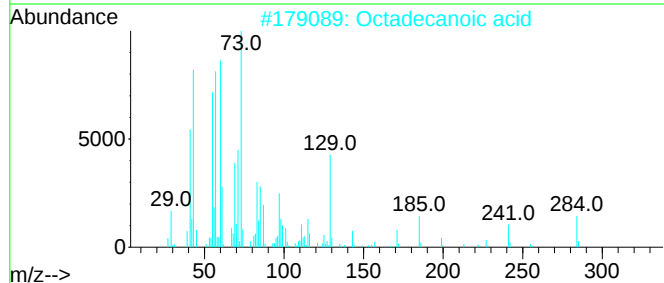
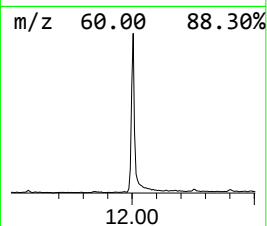
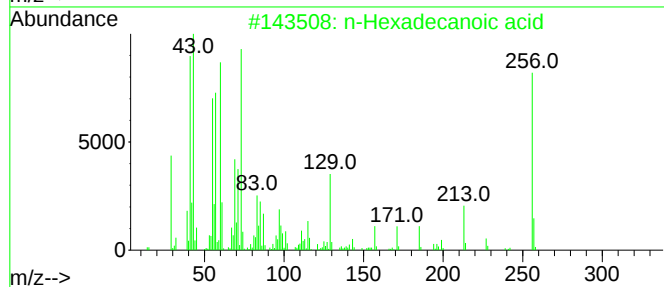
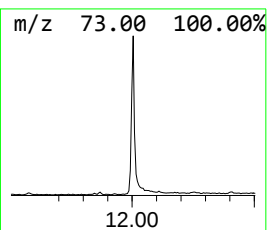
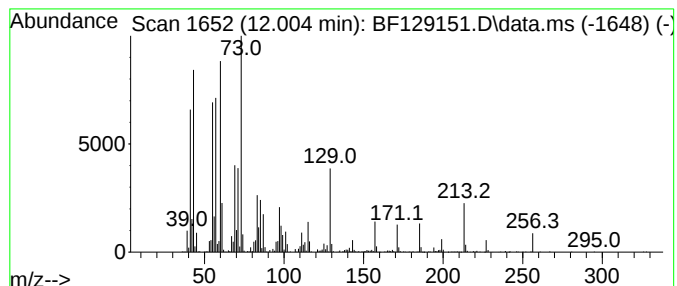
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.004	8.17 ng	726739	Phenanthrene-d10	11.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Octadecanoic acid	284	C18H36O2	000057-11-4	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Tridecanoic acid	214	C13H26O2	000638-53-9	87
5			n-Decanoic acid	172	C10H20O2	000334-48-5	70



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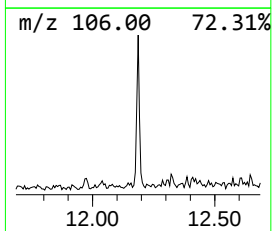
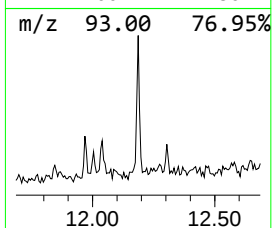
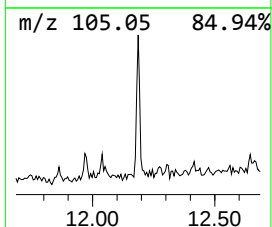
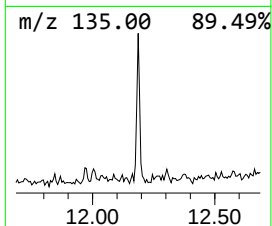
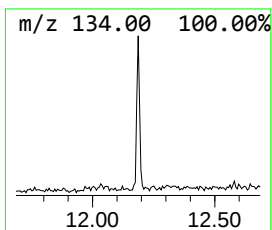
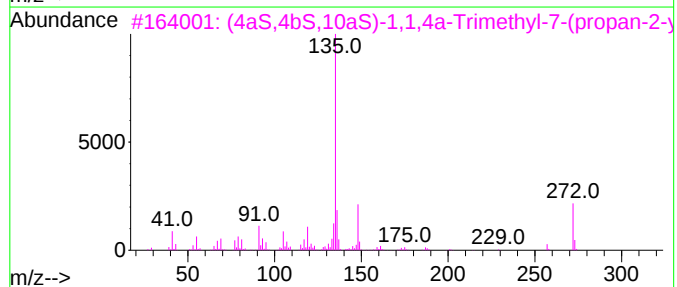
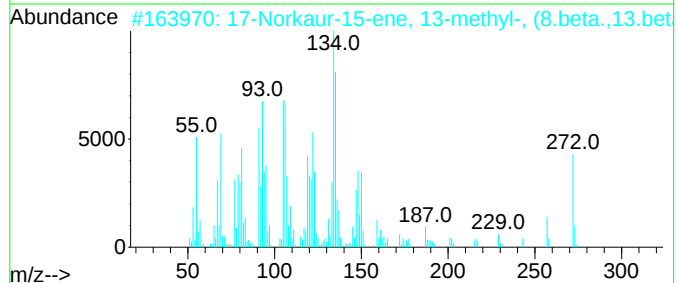
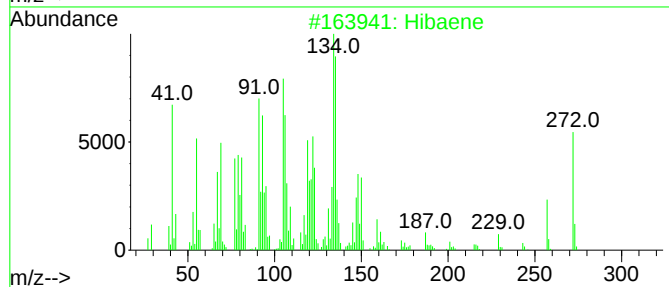
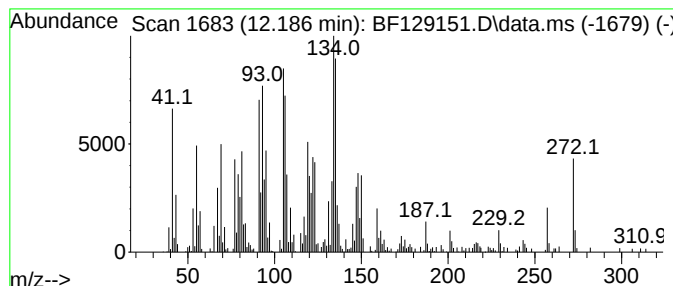
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062922.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Hibaene Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.186	2.19 ng	195252	Phenanthrene-d10	11.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hibaene	272	C20H32	002359-73-1	99
2			17-Norkaur-15-ene, 13-methyl-, (...	272	C20H32	003564-54-3	99
3			(4aS,4bS,10aS)-1,1,4a-Trimethyl-...	272	C20H32	057119-12-7	22
4			2-Methoxybenzamide	151	C8H9NO2	002439-77-2	22
5			2H-1-Benzopyran, 3,4-dihydro-	134	C9H10O	000493-08-3	20



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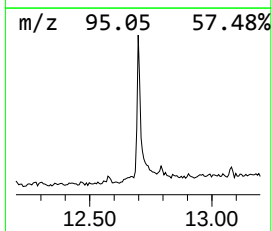
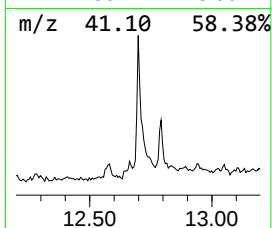
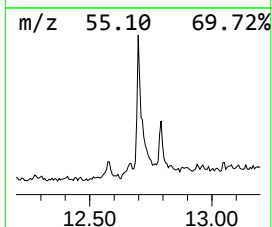
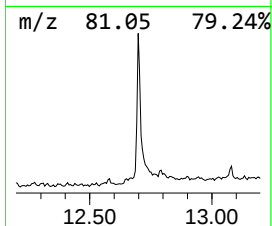
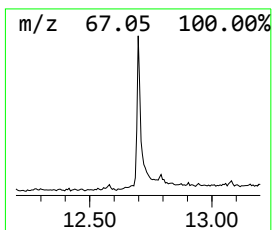
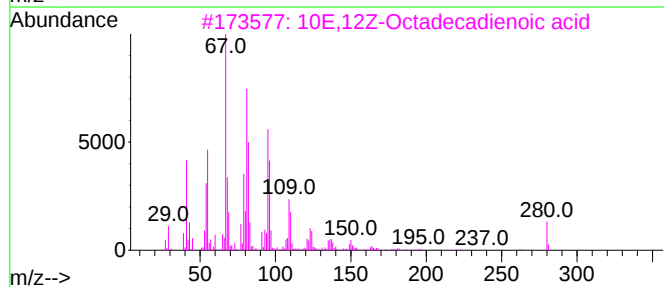
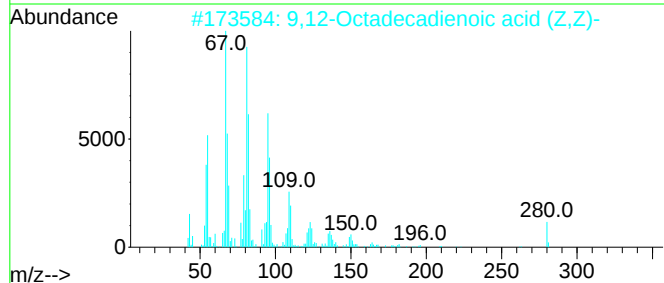
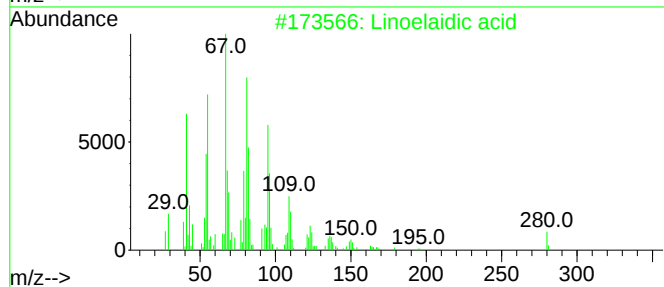
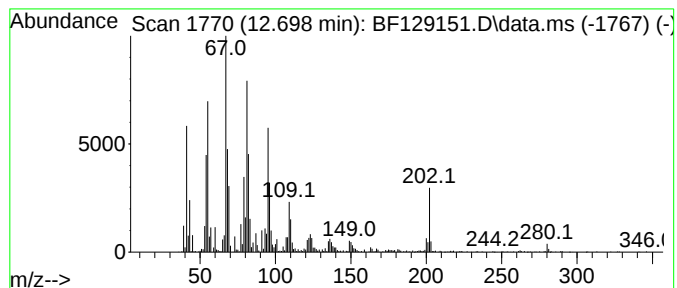
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Peak Number 4 Linoelaidic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.698	10.81 ng	961986	Phenanthrene-d10	11.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Linoelaidic acid	280	C18H32O2	000506-21-8	99
2			9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	99
3			10E,12Z-Octadecadienoic acid	280	C18H32O2	002420-56-6	98
4			(9E,11E)-Octadecadienoic acid	280	C18H32O2	000544-71-8	95
5			11,14-Eicosadienoic acid, methyl...	322	C21H38O2	002463-02-7	92



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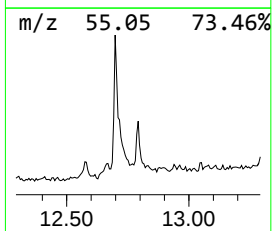
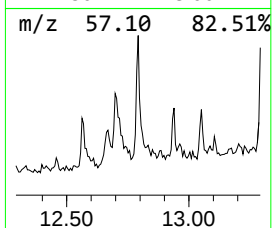
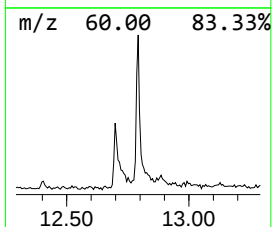
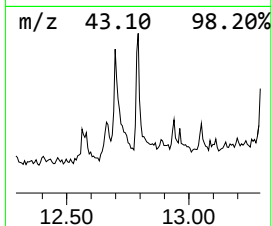
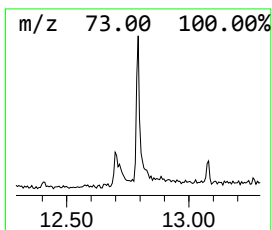
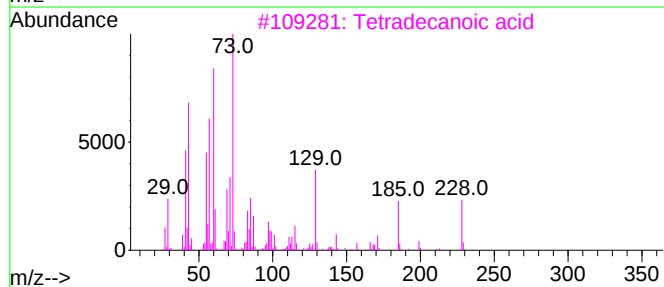
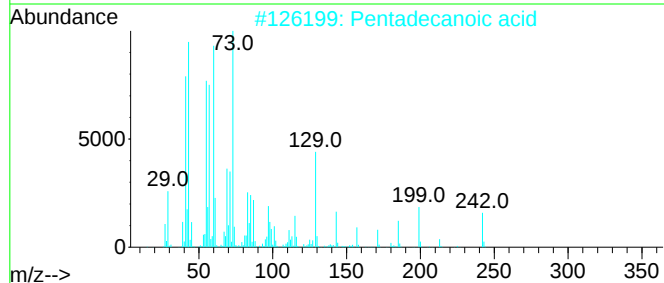
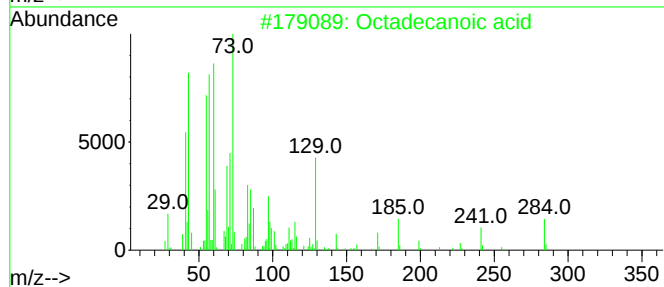
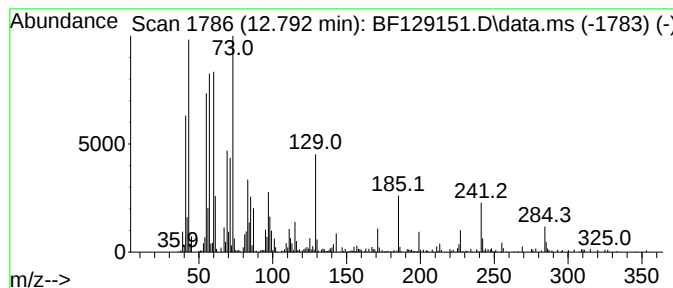
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Octadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.792	2.56 ng	227878	Phenanthrene-d10	11.492	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72
5	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72



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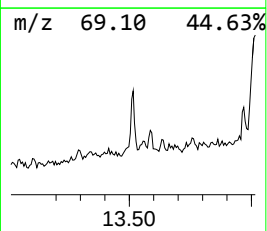
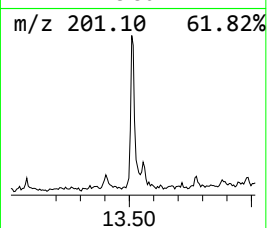
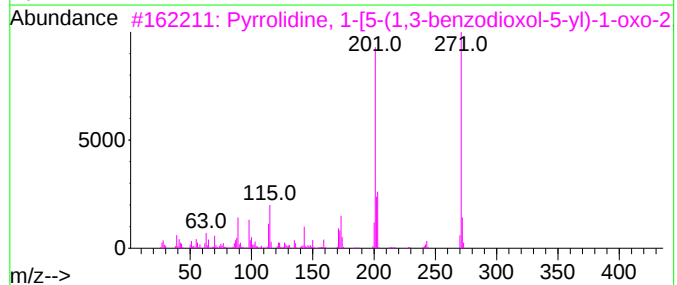
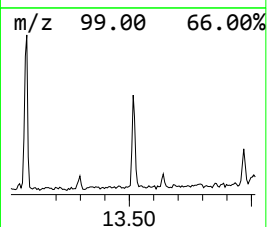
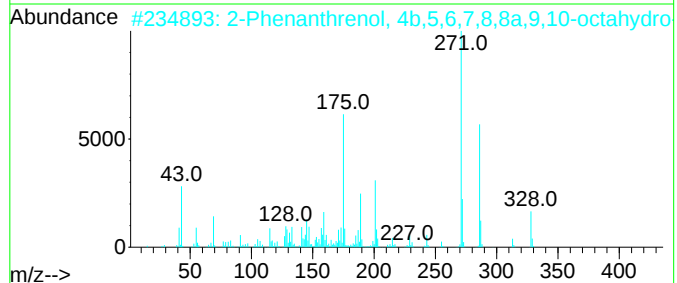
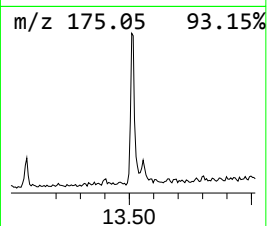
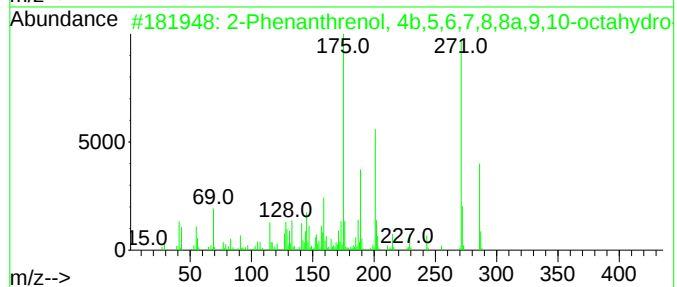
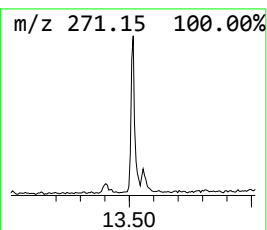
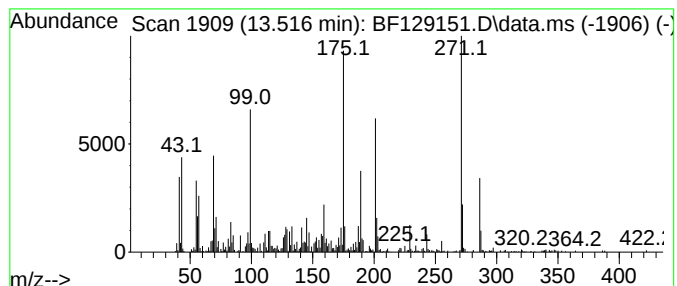
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 2-Phenanthrenol, 4b,5,6,7,8... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.516	3.10 ng	293413	Chrysene-d12	14.139	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	286	C20H300	000511-15-9	99
2	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	328	C22H3202	015340-82-6	81
3	Pyrrolidine, 1-[5-(1,3-benzodiox...	271	C16H17NO3	025924-78-1	42
4	Pisiferol	302	C20H3002	024035-36-7	35
5	13-Isopropylpodocarpin-12-ol-20-al	300	C20H2802	024035-37-8	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070622\
Data File : BF129151.D
Acq On : 06 Jul 2022 19:32
Operator : CG\JU
Sample : N3579-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

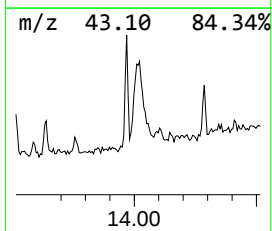
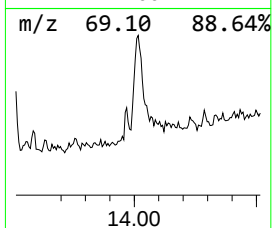
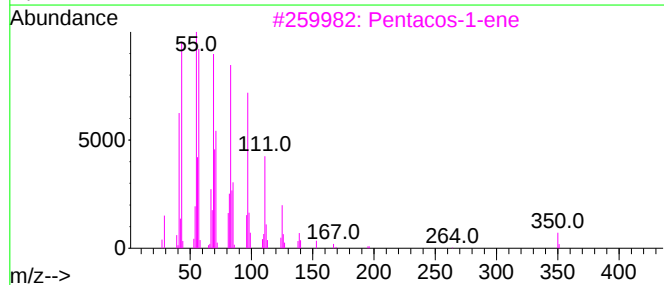
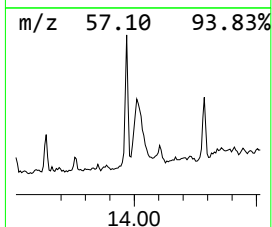
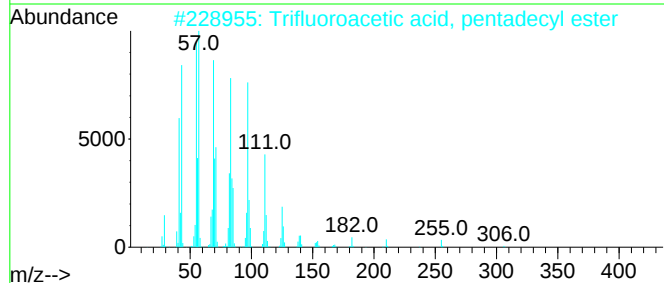
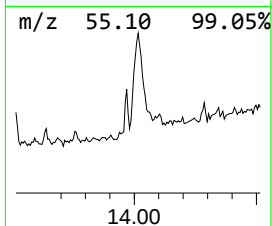
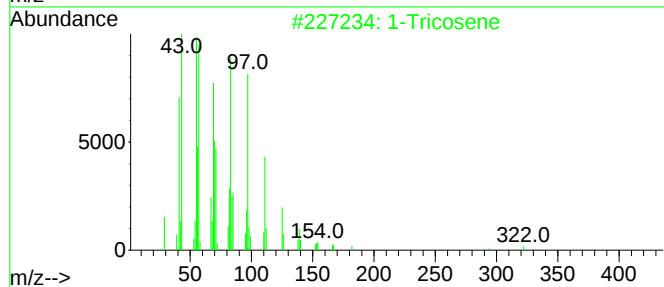
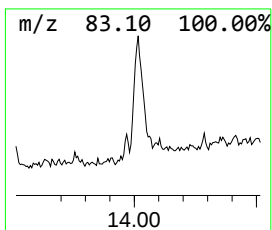
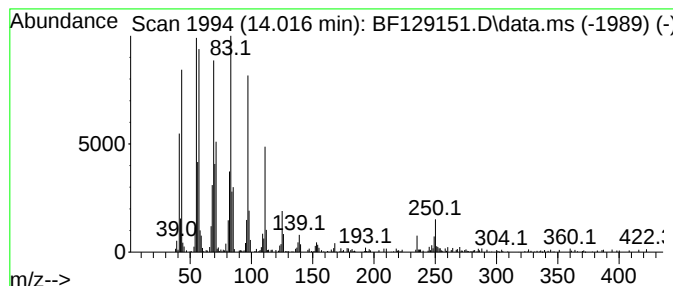
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Tricosene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.016	5.74 ng	543855	Chrysene-d12	14.139	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tricosene	322	C23H46	018835-32-0	94
2	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
3	Pentacos-1-ene	350	C25H50	016980-85-1	94
4	1-Heneicosanol	312	C21H44O	015594-90-8	93
5	Cyclotetracosane	336	C24H48	000297-03-0	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070622\
Data File : BF129151.D
Acq On : 06 Jul 2022 19:32
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Sample : N3579-01
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Instrument :
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ClientSampleId :
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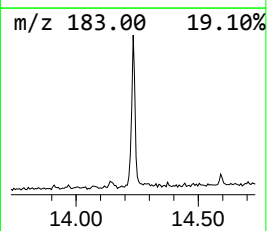
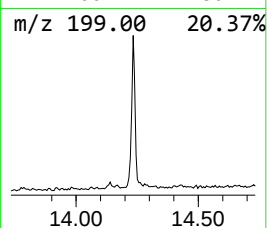
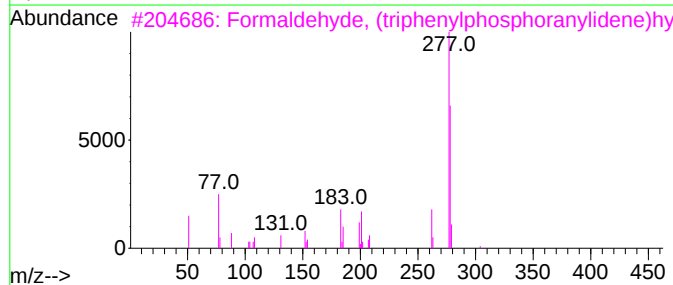
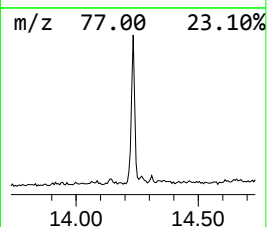
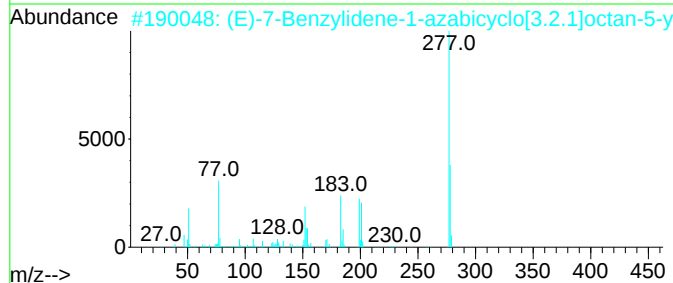
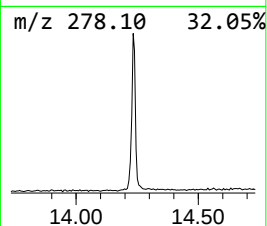
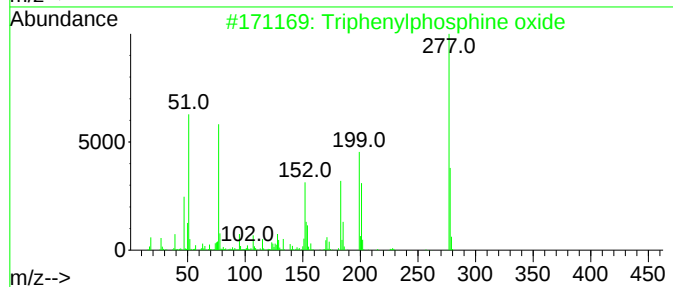
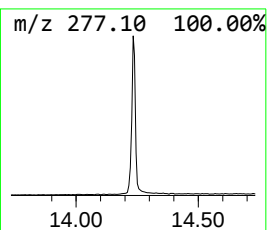
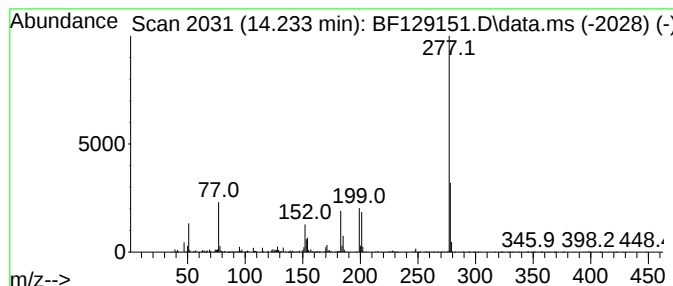
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Triphenylphosphine oxide Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.233	4.95 ng	468991	Chrysene-d12	14.139

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	93
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	91
3			Formaldehyde, (triphenylphosphor...]	304	C19H17N2P	015990-54-2	50
4			(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	50
5			Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070622\
Data File : BF129151.D
Acq On : 06 Jul 2022 19:32
Operator : CG\JU
Sample : N3579-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

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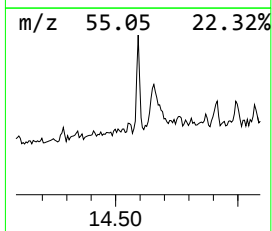
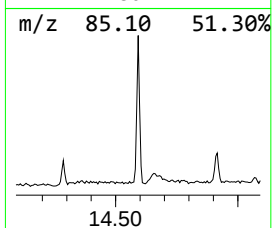
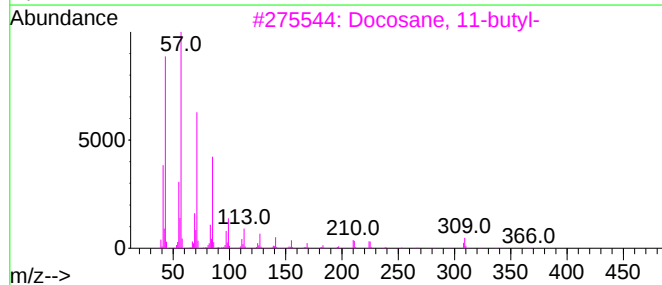
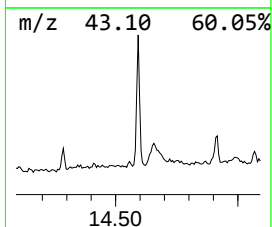
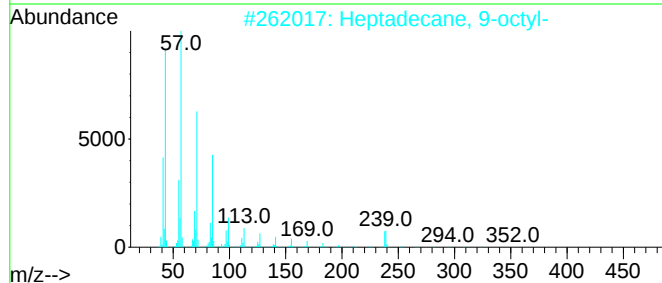
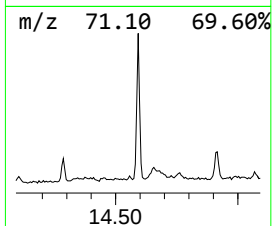
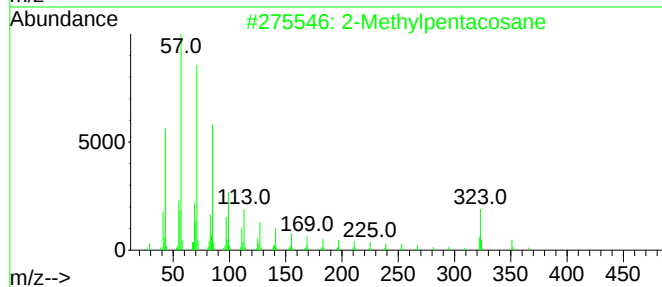
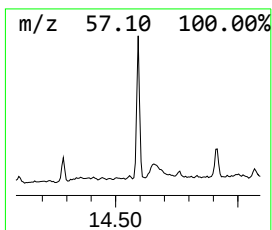
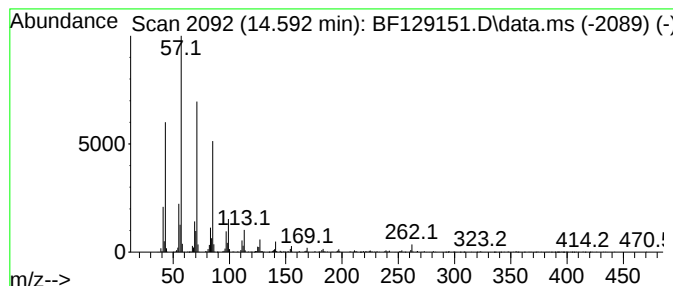
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 2-Methylpentacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.592	5.97 ng	565299	Chrysene-d12	14.139

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Methylpentacosane	366	C26H54	000629-87-8	95
2		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	94
3		Docosane, 11-butyl-	366	C26H54	013475-76-8	94
4		Tetracosane	338	C24H50	000646-31-1	91
5		Heneicosane	296	C21H44	000629-94-7	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070622\
Data File : BF129151.D
Acq On : 06 Jul 2022 19:32
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Misc :
ALS Vial : 16 Sample Multiplier: 1

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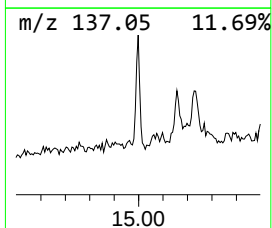
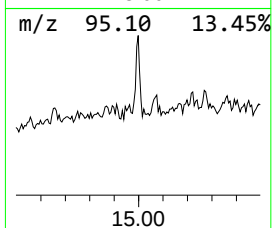
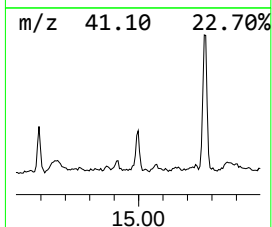
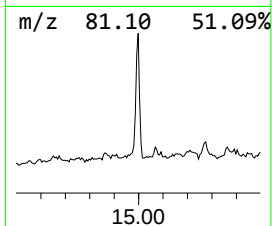
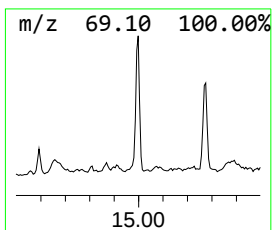
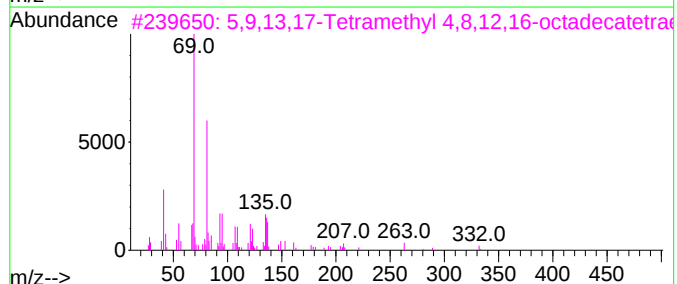
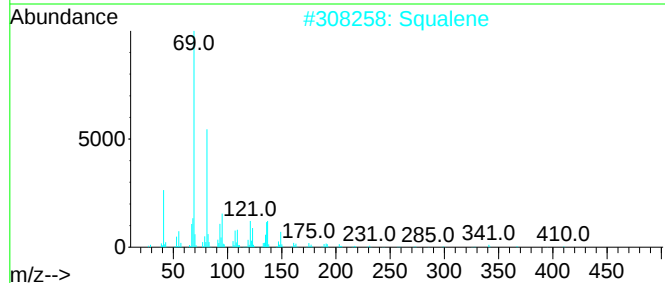
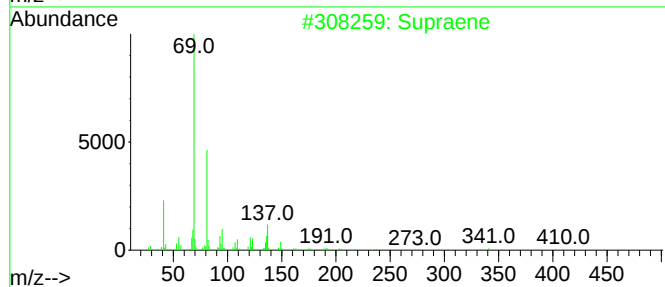
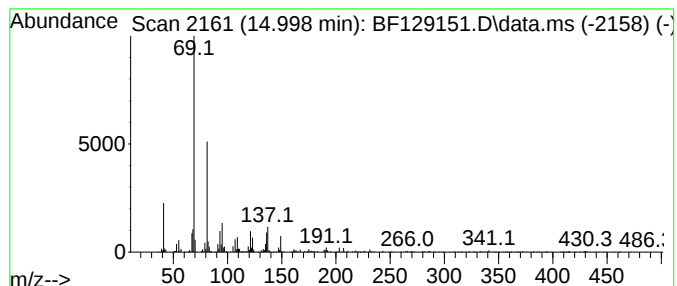
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Supraene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.998	5.20 ng	406045	Perylene-d12	15.668

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	98
2			Squalene	410	C30H50	000111-02-4	93
3			5,9,13,17-Tetramethyl 4,8,12,16-...	332	C22H36O2	1000432-37-9	72
4			3,7,11-Trimethyl-2,6,10-dodecatr...	217	C15H23N	029789-67-1	72
5			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070622\
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ALS Vial : 16 Sample Multiplier: 1

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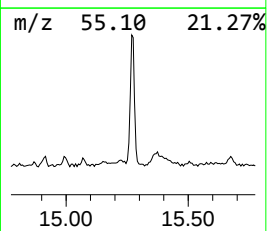
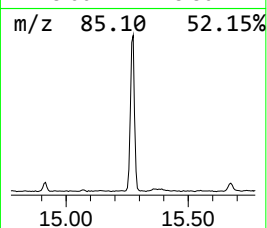
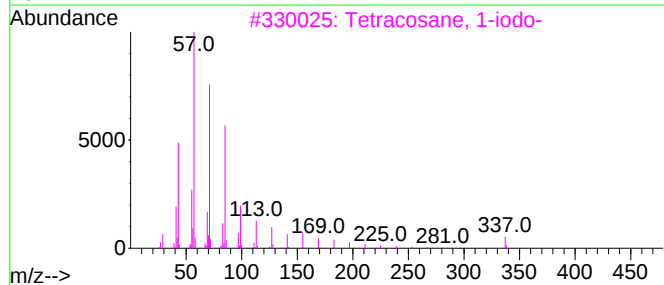
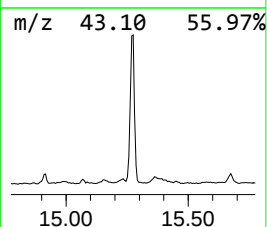
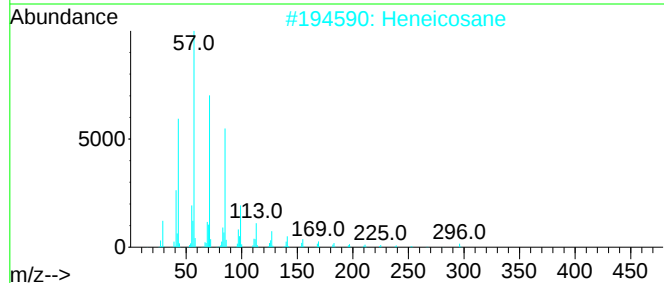
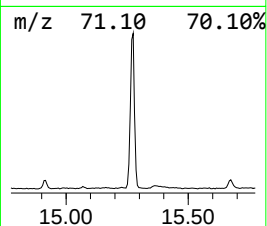
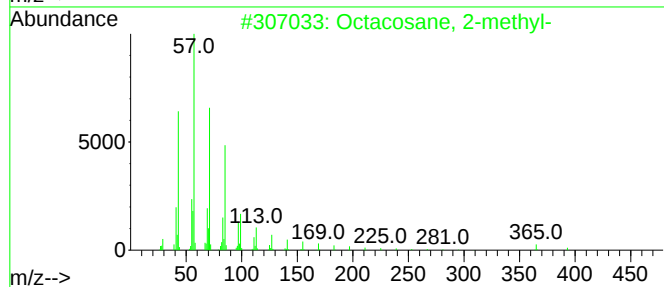
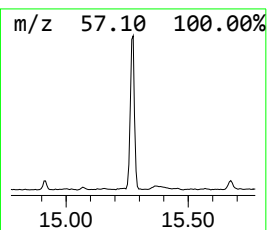
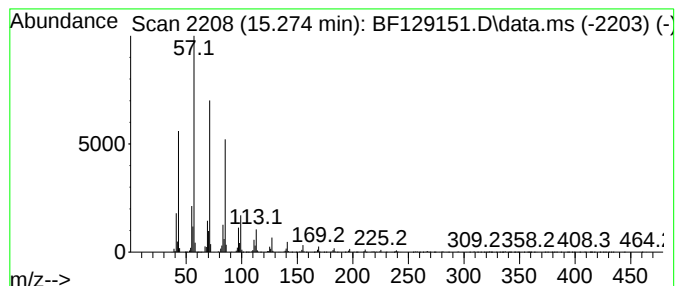
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Octacosane, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.274	34.99 ng	2732490	Perylene-d12	15.668

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Tetracosane, 1-iodo-	464	C24H49I	1000406-32-0	91
4		Triacontane	422	C30H62	000638-68-6	91
5		Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070622\
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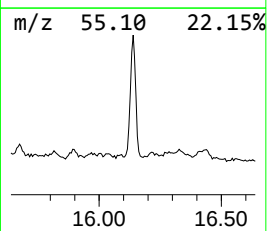
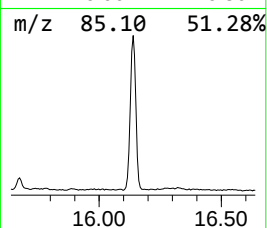
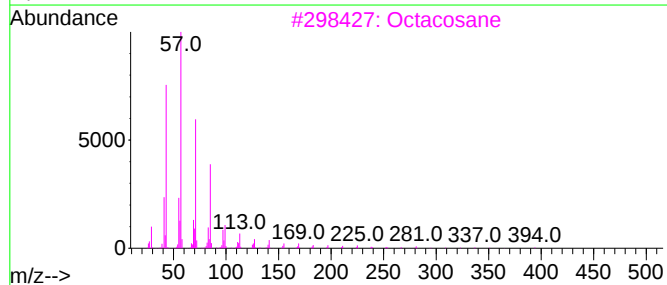
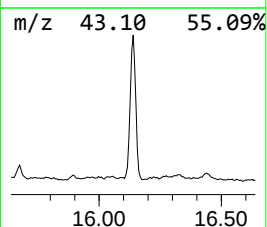
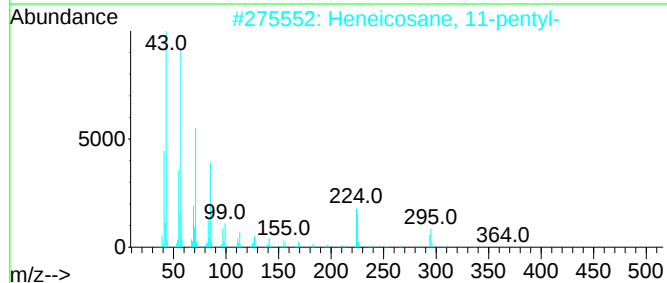
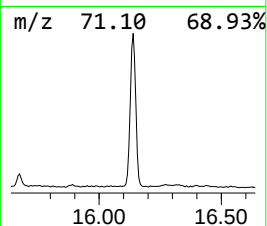
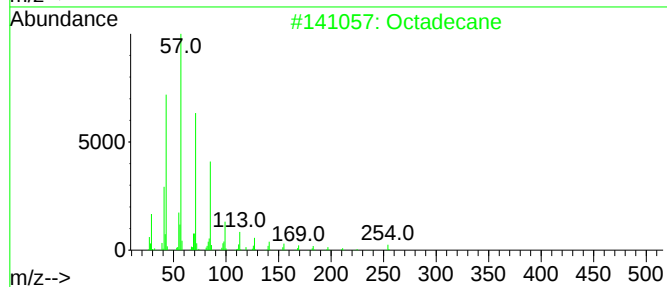
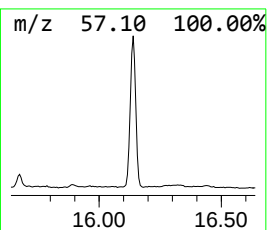
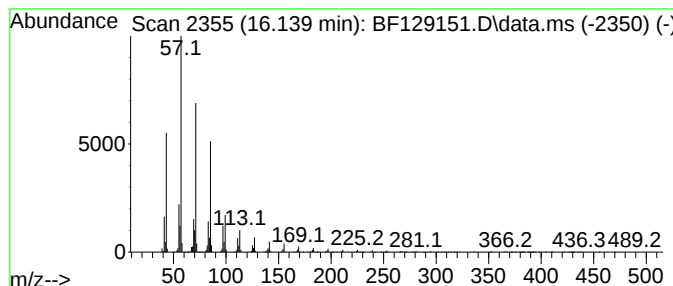
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Octadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.139	31.73 ng	2478140	Perylene-d12	15.668

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane	254	C18H38	000593-45-3	94
2			Heneicosane, 11-pentyl-	366	C26H54	014739-72-1	94
3			Octacosane	394	C28H58	000630-02-4	91
4			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
5			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91



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Data File : BF129151.D
Acq On : 06 Jul 2022 19:32
Operator : CG\JU
Sample : N3579-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OK-03-070522

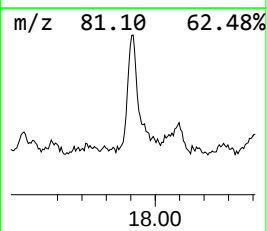
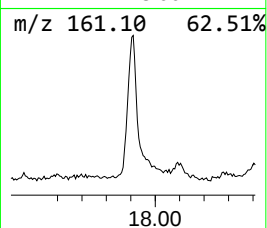
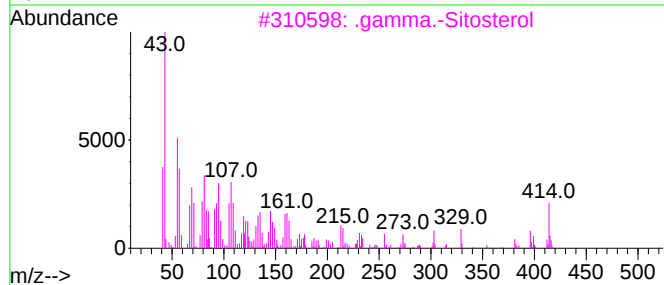
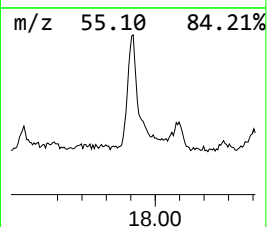
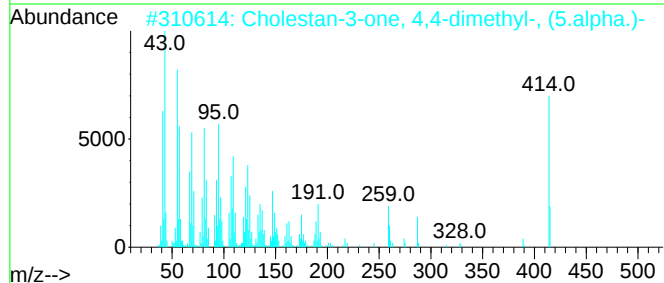
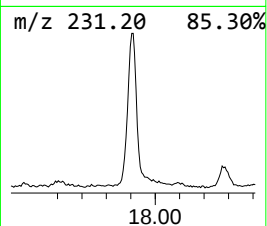
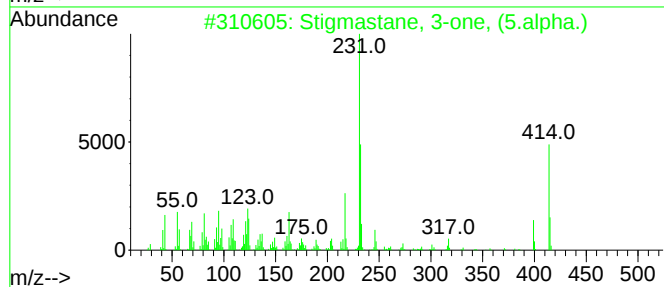
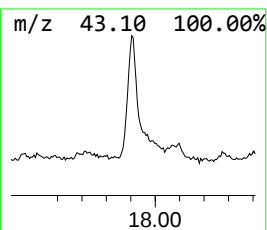
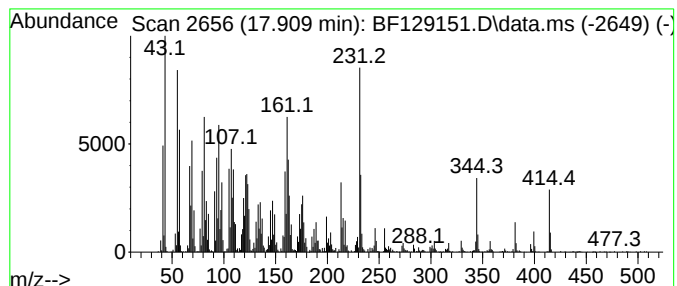
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Stigmastane, 3-one, (5.alpha.) Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.910	45.24 ng	3532690	Perylene-d12	15.668

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Stigmastane, 3-one, (5.alpha.)	414	C29H50O	1000437-00-8	64
2			Cholestan-3-one, 4,4-dimethyl-, ...	414	C29H50O	002097-85-0	55
3			.gamma.-Sitosterol	414	C29H50O	000083-47-6	41
4			Pyrimido[5,4-b]pyrido[3,2-d]thie...	231	C11H9N3OS	201681-22-3	25
5			3-(3,5-Dimethylpyrazol-1-yl)-4-(...	246	C10H10N6O2	1000436-49-9	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070622\
Data File : BF129151.D
Acq On : 06 Jul 2022 19:32
Operator : CG\JU
Sample : N3579-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OK-03-070522

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062922.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
Hexadecanoic ac...	11.869	2.3	ng	202693	4	11.492	1779870	20.0
n-Hexadecanoic ...	12.004	8.2	ng	726739	4	11.492	1779870	20.0
Hibaene	12.186	2.2	ng	195252	4	11.492	1779870	20.0
Linoelaidic acid	12.698	10.8	ng	961986	4	11.492	1779870	20.0
Octadecanoic acid	12.792	2.6	ng	227878	4	11.492	1779870	20.0
2-Phenanthrenol...	13.516	3.1	ng	293413	5	14.139	1893580	20.0
1-Tricosene	14.016	5.7	ng	543855	5	14.139	1893580	20.0
Triphenylphosph...	14.233	5.0	ng	468991	5	14.139	1893580	20.0
2-Methylpentaco...	14.592	6.0	ng	565299	5	14.139	1893580	20.0
Supraene	14.998	5.2	ng	406045	6	15.668	1561880	20.0
Octacosane, 2-m...	15.274	35.0	ng	2732490	6	15.668	1561880	20.0
Octadecane	16.139	31.7	ng	2478140	6	15.668	1561880	20.0
Stigmastane, 3-...	17.910	45.2	ng	3532690	6	15.668	1561880	20.0