

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092322\
 Data File : BF130391.D
 Acq On : 23 Sep 2022 15:19
 Operator : CG\JU
 Sample : N4780-21
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-3

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-BF091422.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130391.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.828	462	466	480	rVB	188620	247652	11.92%	1.707%
2	5.257	534	539	542	rBV	1755598	1684716	81.07%	11.609%
3	6.293	710	715	730	rBV	1820585	1725965	83.06%	11.894%
4	6.651	772	776	779	rBV	696635	549616	26.45%	3.787%
5	7.216	867	872	875	rBV	1286535	1133870	54.56%	7.814%
6	7.934	990	994	997	rBV	866115	712443	34.28%	4.909%
7	9.010	1173	1177	1180	rBV	2420611	2078084	100.00%	14.320%
8	9.687	1287	1292	1295	rBV	828814	719836	34.64%	4.960%
9	10.469	1421	1425	1429	rBV	1174451	1027520	49.45%	7.081%
10	11.163	1540	1543	1546	rBV	670142	601513	28.95%	4.145%
11	11.704	1632	1635	1645	rBV2	127598	144854	6.97%	0.998%
12	12.375	1744	1749	1752	rBV	30813	28916	1.39%	0.199%
13	12.492	1765	1769	1779	rBV	116053	129637	6.24%	0.893%
14	12.598	1782	1787	1791	rVB	27786	32789	1.58%	0.226%
15	12.751	1809	1813	1817	rBV	1646263	1481526	71.29%	10.209%
16	13.798	1987	1991	1994	rBV	598691	536045	25.80%	3.694%
17	13.904	2004	2009	2013	rBV	116329	130707	6.29%	0.901%
18	14.286	2071	2074	2076	rBV	24122	24405	1.17%	0.168%
19	14.580	2119	2124	2128	rBV3	20311	33111	1.59%	0.228%
20	14.645	2132	2135	2142	rVV2	24961	39813	1.92%	0.274%
21	14.710	2143	2146	2150	rVB4	25825	28659	1.38%	0.197%
22	14.804	2158	2162	2164	rBV	25025	31843	1.53%	0.219%
23	14.886	2173	2176	2182	rVB	82048	93744	4.51%	0.646%
24	15.192	2224	2228	2233	rBV	501988	586526	28.22%	4.042%
25	15.233	2233	2235	2239	rVB2	22362	23151	1.11%	0.160%
26	15.416	2263	2266	2273	rVB4	31603	45462	2.19%	0.313%
27	15.627	2297	2302	2310	rBV	126204	185671	8.93%	1.279%
28	16.086	2376	2380	2384	rVB4	16173	25607	1.23%	0.176%
29	16.345	2420	2424	2431	rVB4	46483	83398	4.01%	0.575%
30	16.615	2466	2470	2475	rBV4	24179	44984	2.16%	0.310%
31	16.668	2475	2479	2485	rVB7	49326	90264	4.34%	0.622%
32	16.774	2494	2497	2501	rBV5	20105	37424	1.80%	0.258%
33	16.821	2502	2505	2513	rVB7	31645	55539	2.67%	0.383%
34	17.968	2694	2700	2711	rVB10	44332	116336	5.60%	0.802%

Sum of corrected areas: 14511626

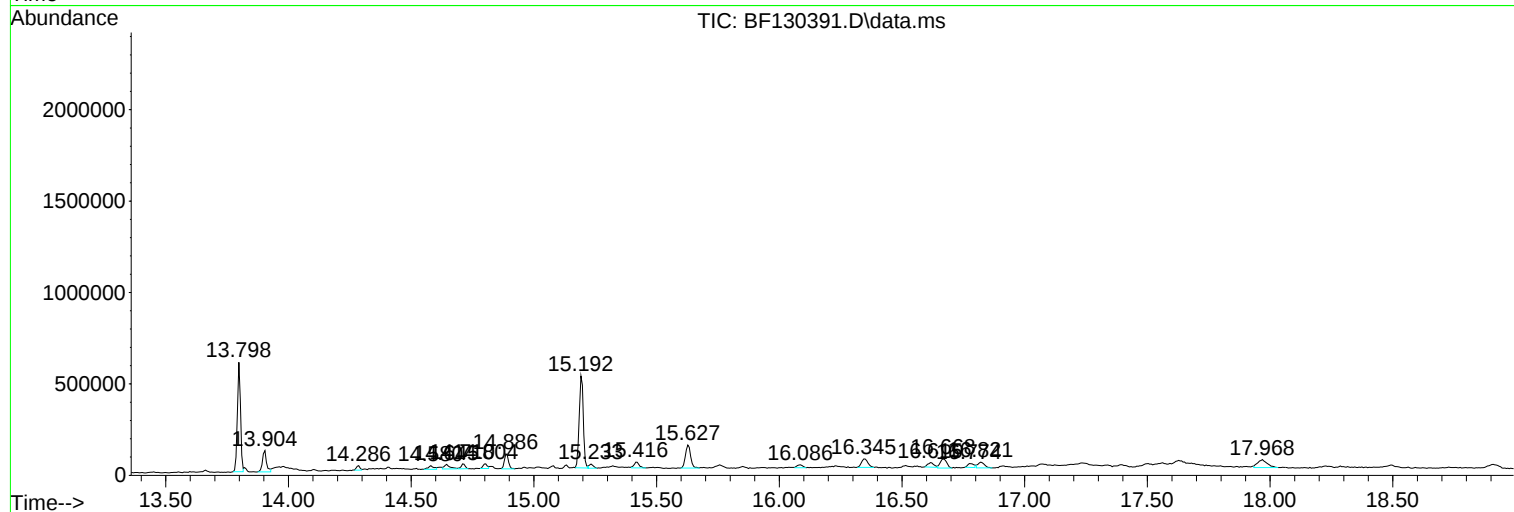
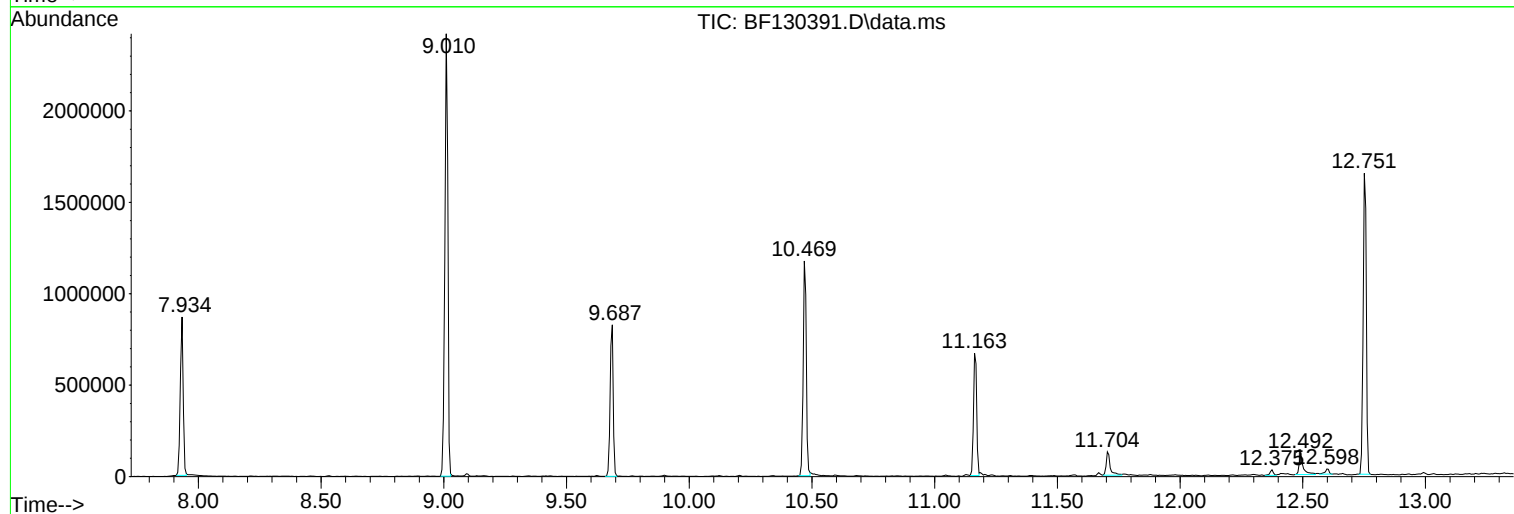
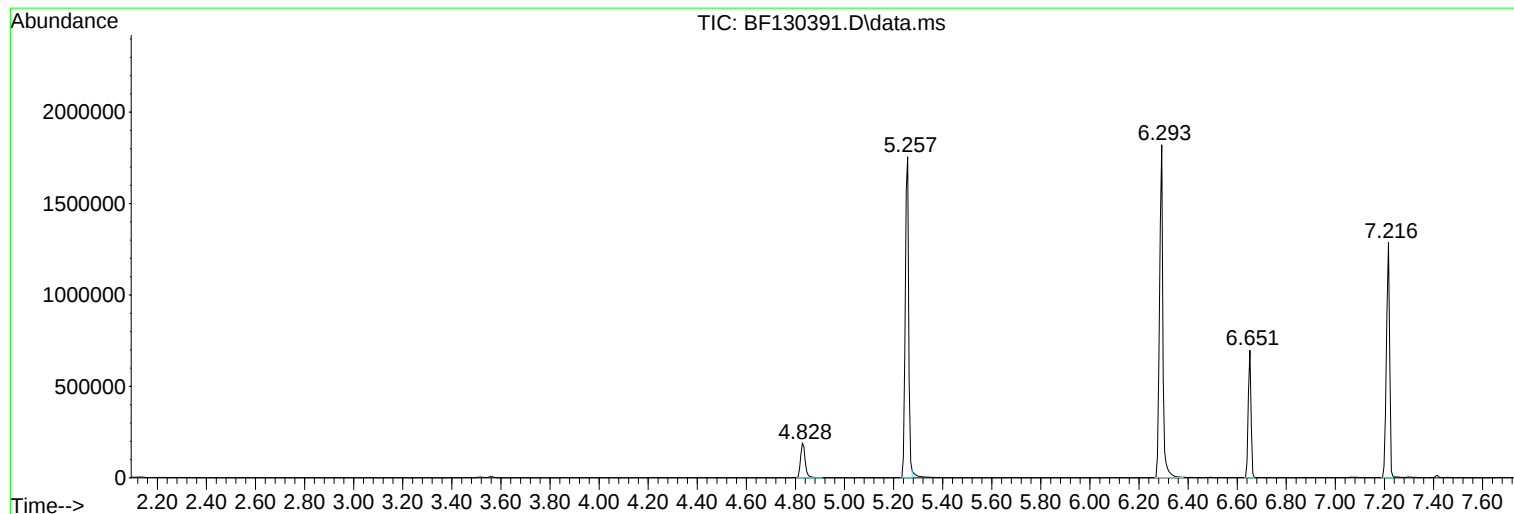
Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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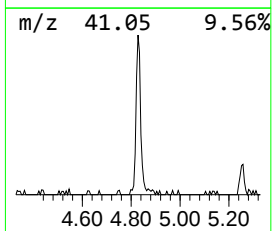
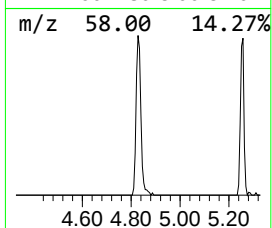
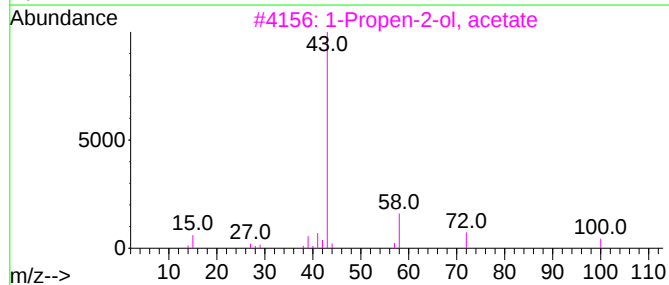
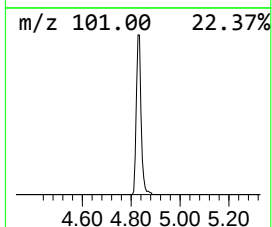
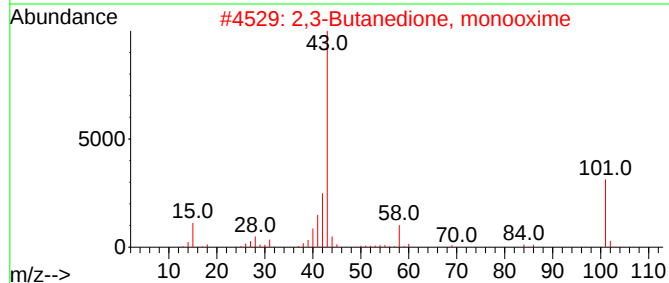
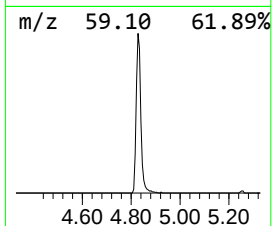
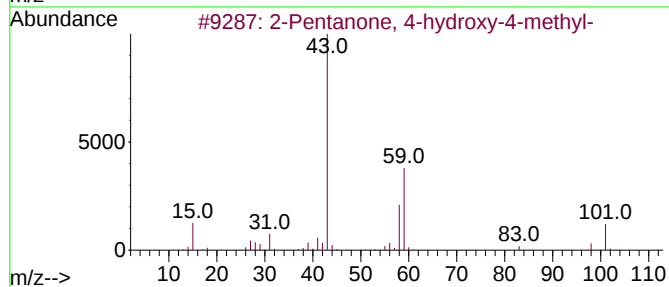
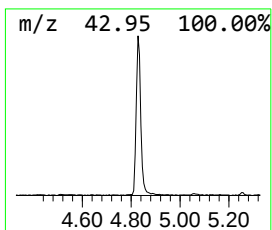
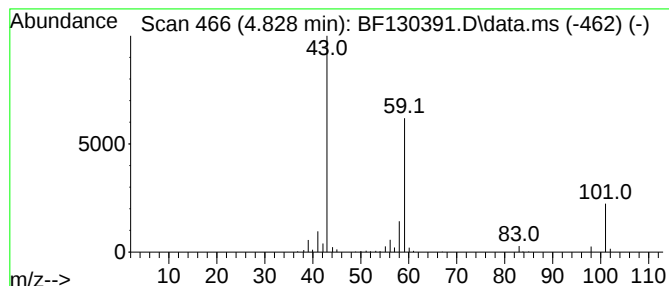
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.828	9.01 ng	247652	1,4-Dichlorobenzene-d4	6.651

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72		
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	32		
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
4	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9		
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		



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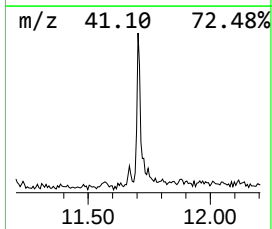
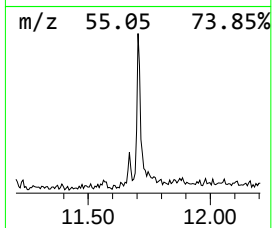
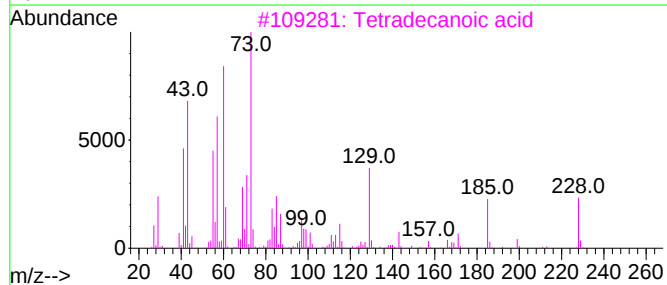
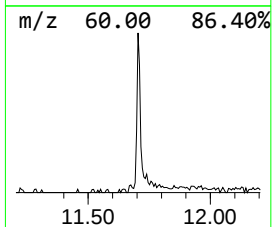
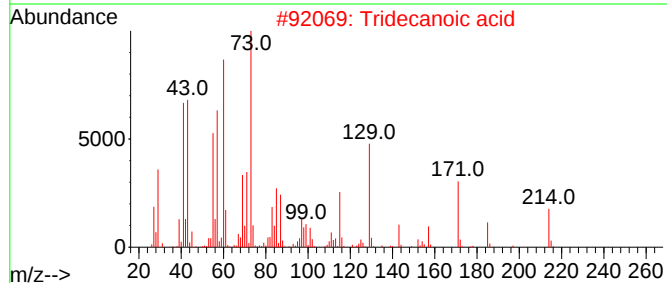
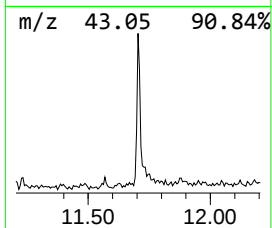
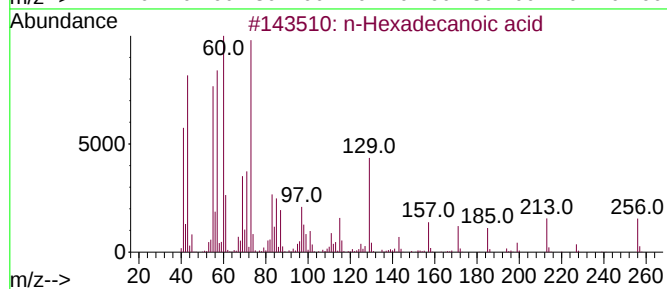
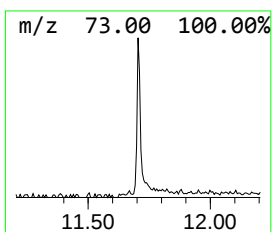
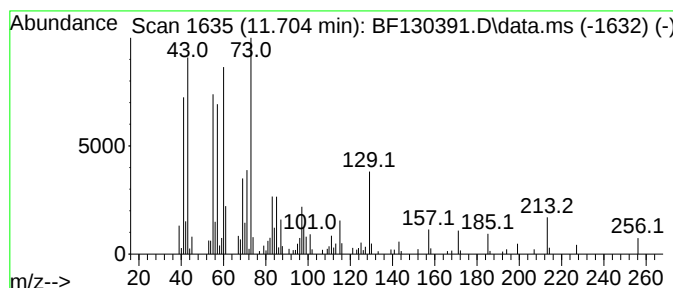
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.704	4.82 ng	144854	Phenanthrene-d10	11.163	
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	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
5	Nonanoic acid	158	C9H18O2	000112-05-0	20



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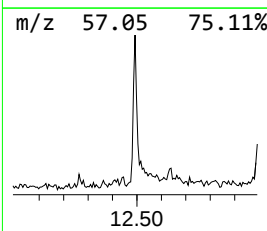
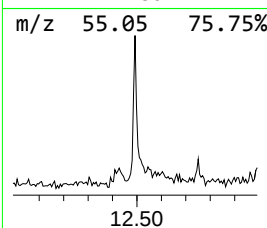
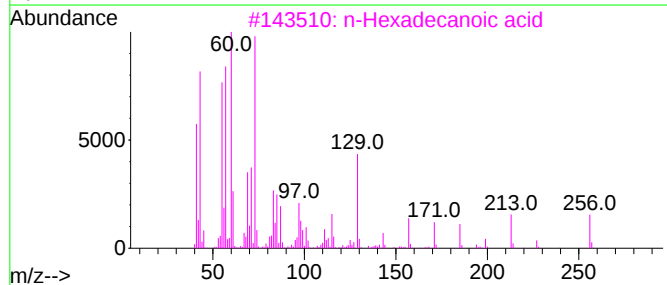
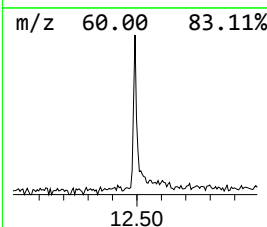
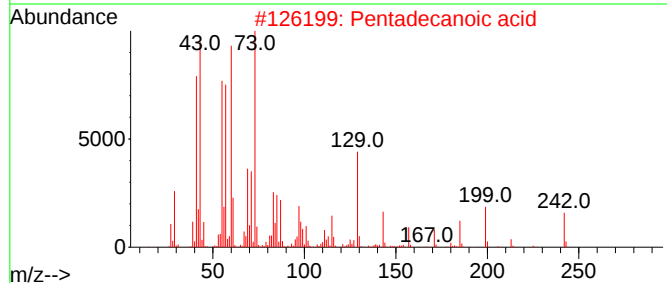
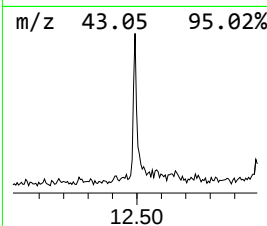
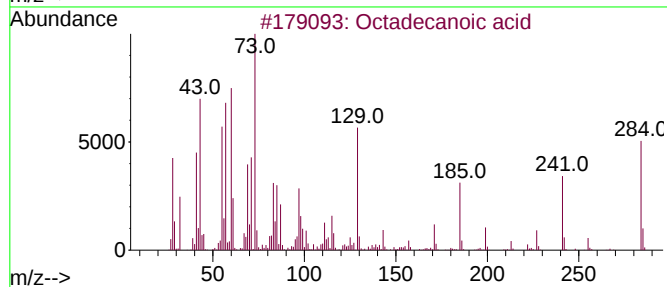
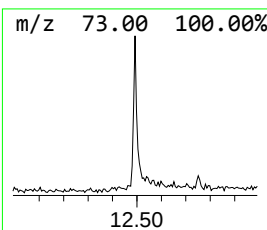
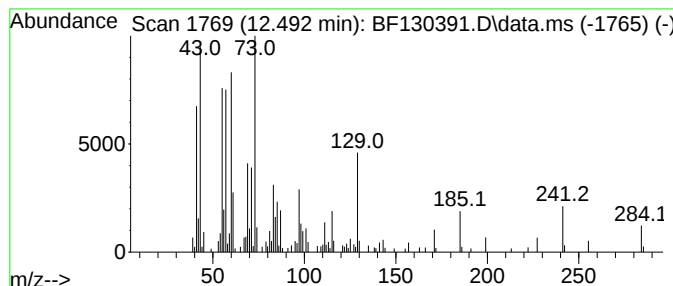
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.492	4.84 ng	129637	Chrysene-d12	13.798

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			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	83
5			n-Decanoic acid	172	C10H20O2	000334-48-5	76



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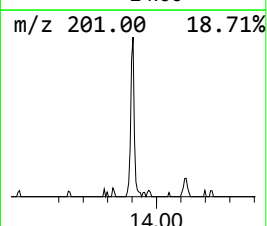
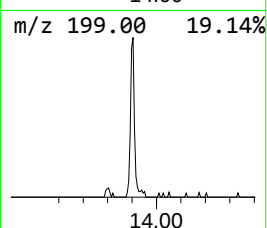
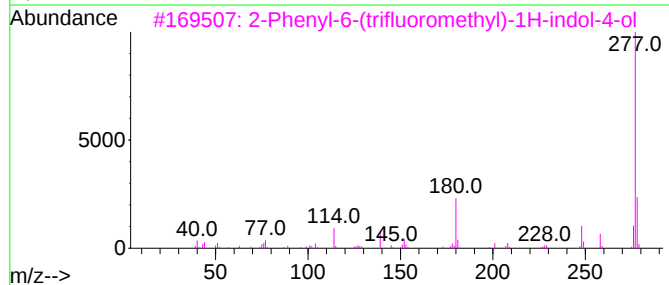
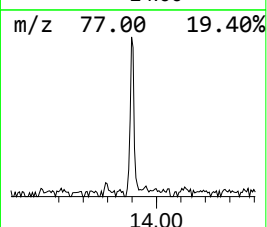
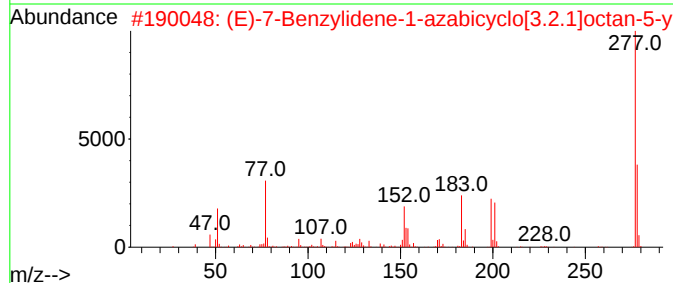
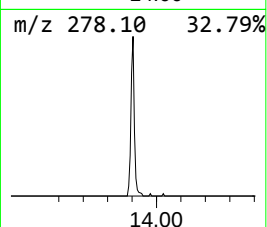
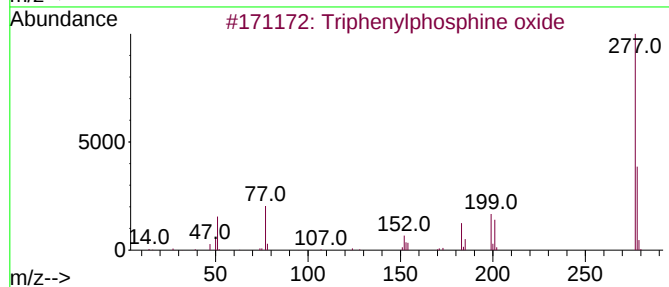
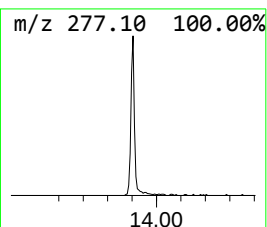
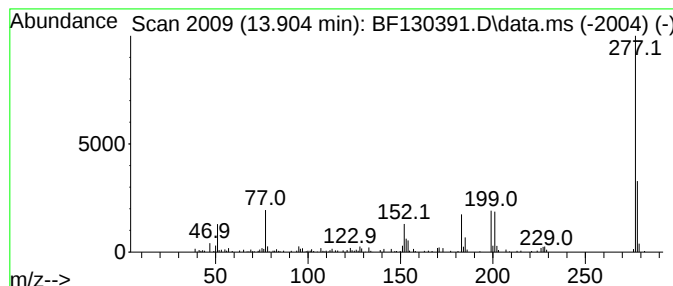
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Triphenylphosphine oxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	4.88 ng	130707	Chrysene-d12	13.798

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	96
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19N03S	1000483-83-4	87
3			2-Phenyl-6-(trifluoromethyl)-1H...	277	C15H10F3NO	1000387-59-3	47
4			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	45
5			5-Methyl-8-phenylfuro[3',2':5,6]...	277	C16H11N3O2	1000460-07-9	33



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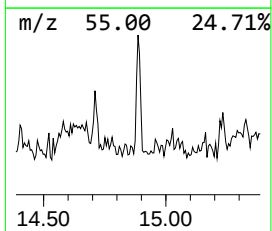
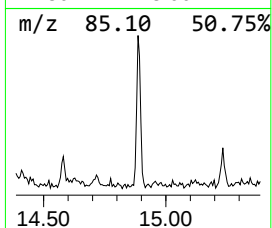
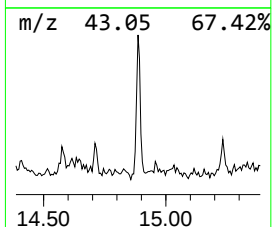
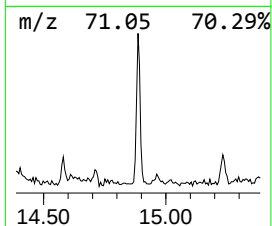
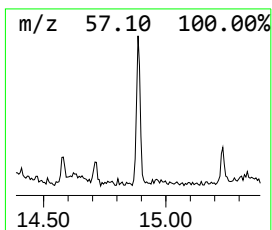
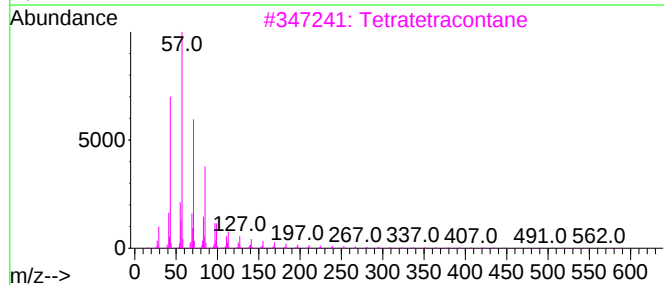
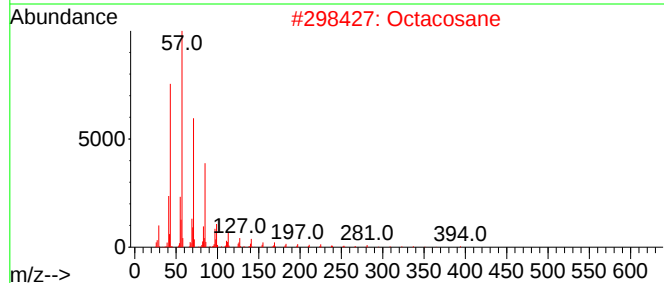
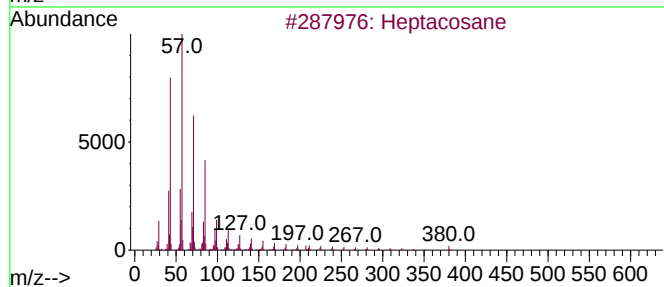
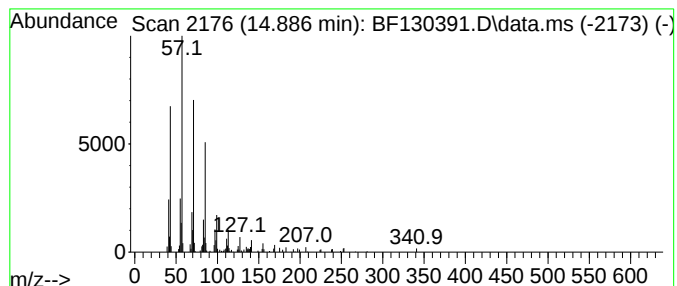
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Peak Number 5 Heptacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.886	3.20 ng	93744	Perylene-d12	15.192

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	91
2			Octacosane	394	C28H58	000630-02-4	90
3			Tetratetracontane	619	C44H90	007098-22-8	90
4			Triacontane	422	C30H62	000638-68-6	90
5			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90



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ClientSampleId :
SP-3

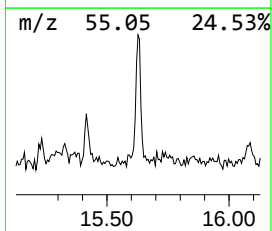
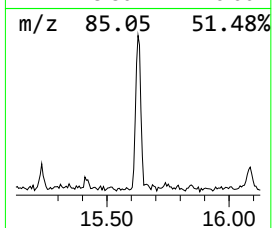
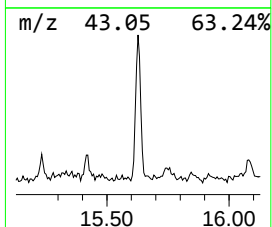
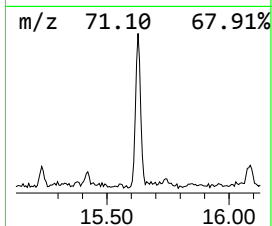
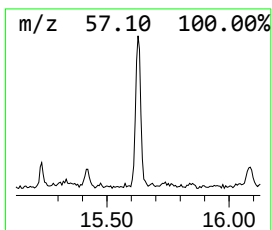
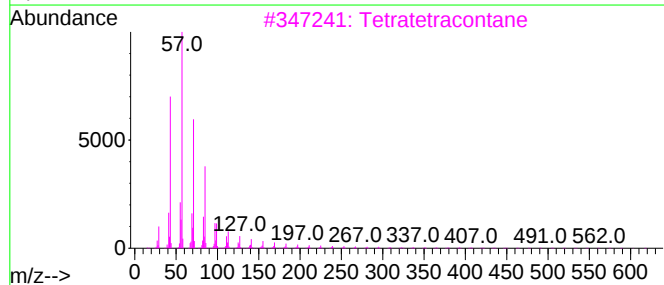
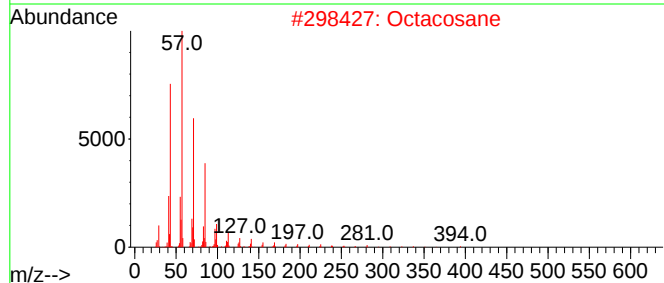
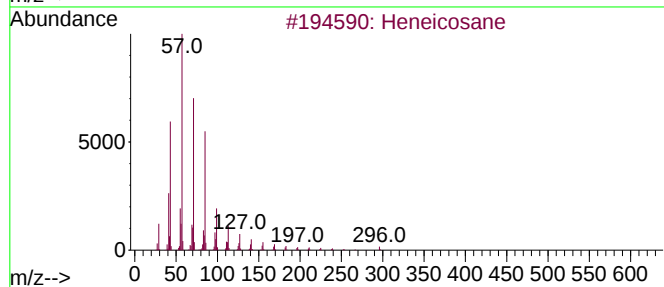
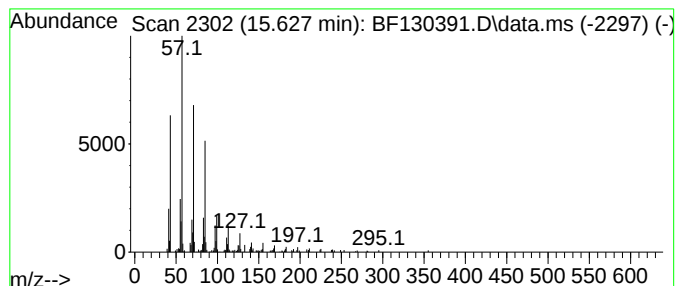
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heneicosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.627	6.33 ng	185671	Perylene-d12	15.192

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			Octacosane	394	C28H58	000630-02-4	91
3			Tetratetracontane	619	C44H90	007098-22-8	91
4			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
5			Tetracosane	338	C24H50	000646-31-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092322\
Data File : BF130391.D
Acq On : 23 Sep 2022 15:19
Operator : CG\JU
Sample : N4780-21
Misc :
ALS Vial : 7 Sample Multiplier: 1

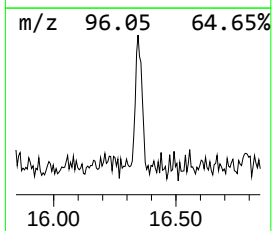
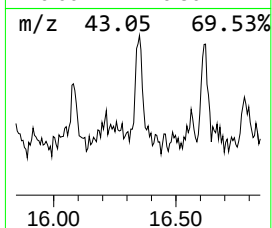
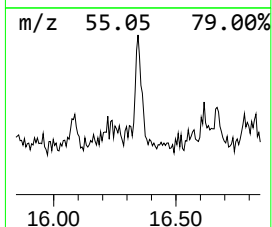
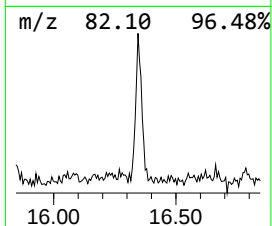
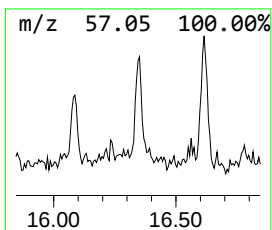
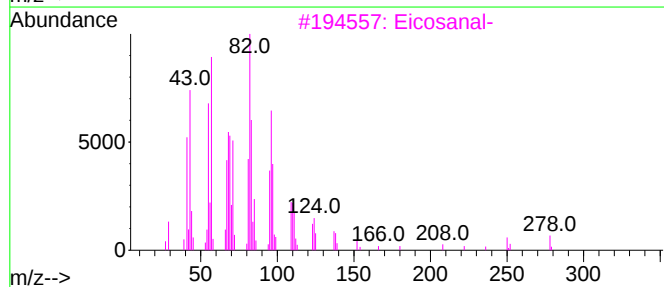
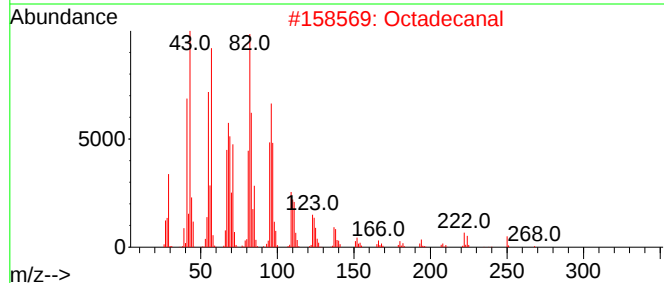
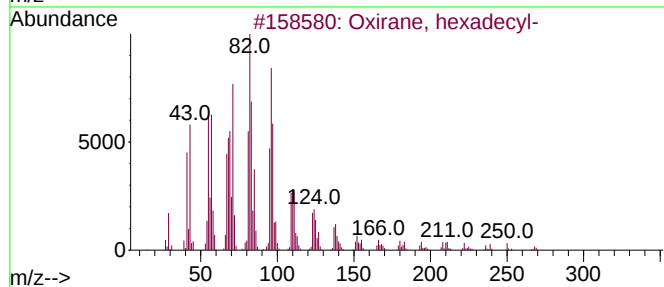
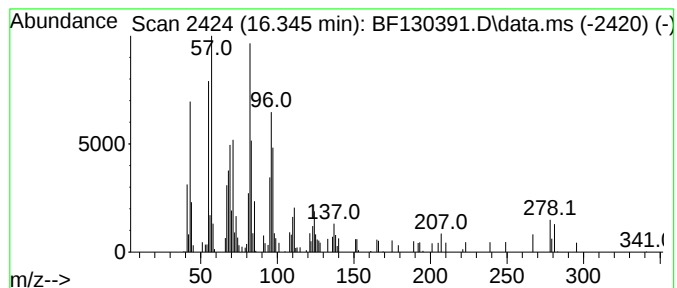
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Oxirane, hexadecyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.	
16.345	2.84 ng	83398	Perylene-d12		15.192	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Oxirane, hexadecyl-		268	C18H36O	007390-81-0	81
2	Octadecanal		268	C18H36O	000638-66-4	74
3	Eicosanal-		296	C20H40O	002400-66-0	64
4	1,16-Hexadecanediol		258	C16H34O2	007735-42-4	58
5	Oxirane, heptadecyl-		282	C19H38O	067860-04-2	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092322\
Data File : BF130391.D
Acq On : 23 Sep 2022 15:19
Operator : CG\JU
Sample : N4780-21
Misc :
ALS Vial : 7 Sample Multiplier: 1

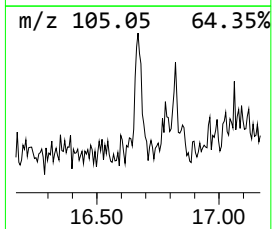
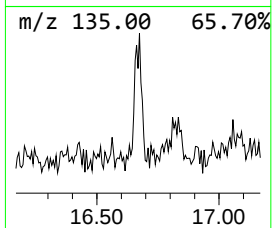
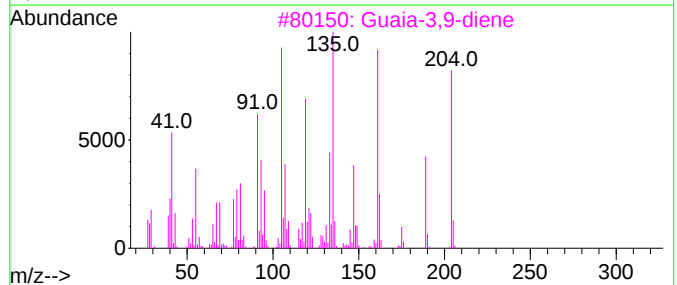
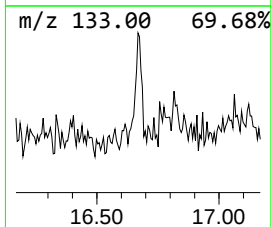
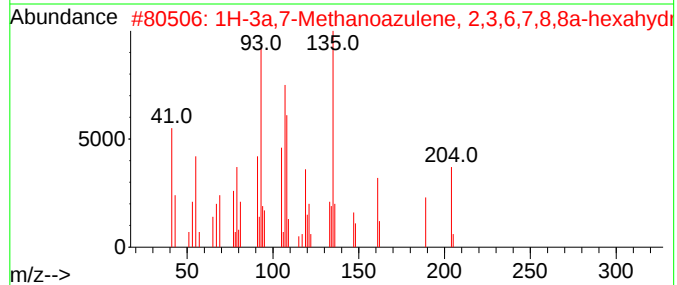
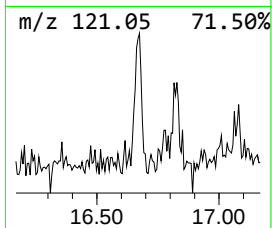
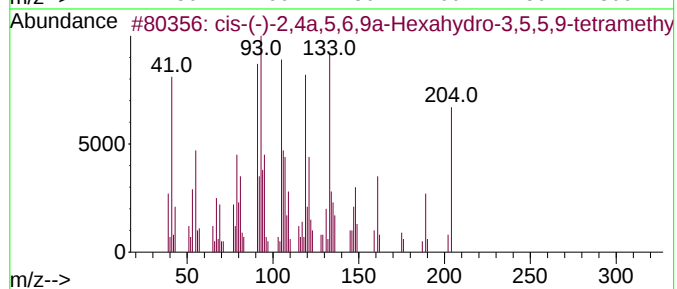
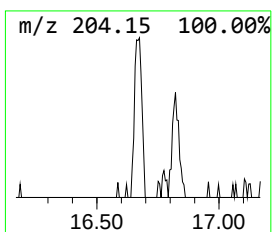
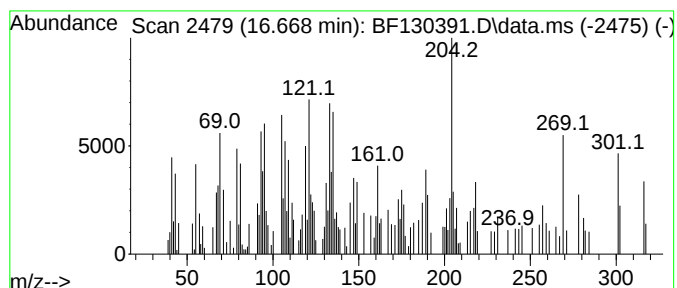
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 cis-(-)-2,4a,5,6,9a-Hexahyd... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.		
16.668	3.08 ng	90264	Perylene-d12	15.192		
Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-(-)-2,4a,5,6,9a-Hexahydro-3,...	204	C15H24	1000104-20-1	60	
2	1H-3a,7-Methanoazulene, 2,3,6,7,...	204	C15H24	000560-32-7	55	
3	Guaia-3,9-diene	204	C15H24	000489-83-8	46	
4	Azulene, 1,2,3,5,6,7,8,8a-octahy...	204	C15H24	003691-11-0	45	
5	Naphthalene, 1,2,3,4,4a,5,6,8a-o...	204	C15H24	000473-13-2	44	



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092322\
Data File : BF130391.D
Acq On : 23 Sep 2022 15:19
Operator : CG\JU
Sample : N4780-21
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-3

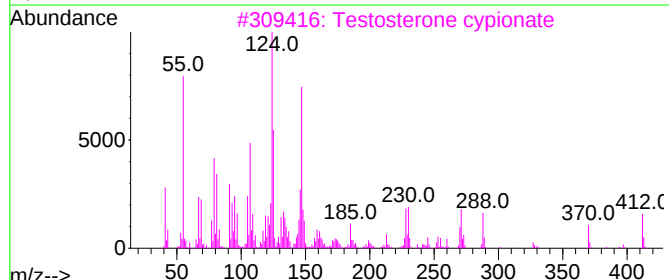
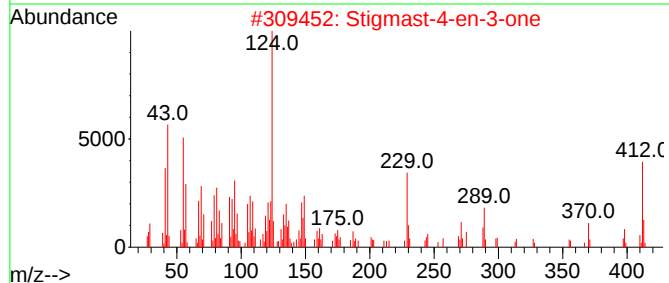
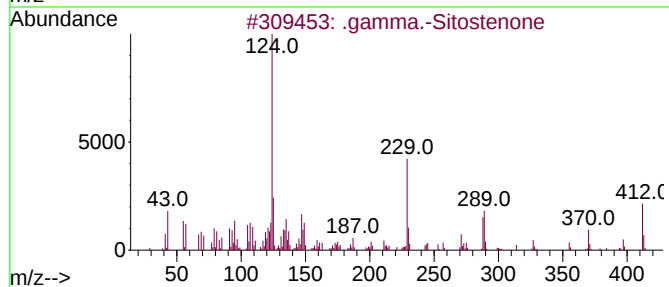
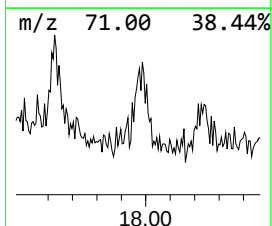
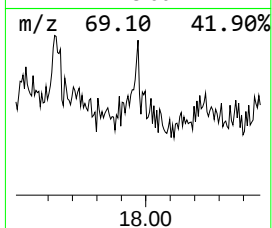
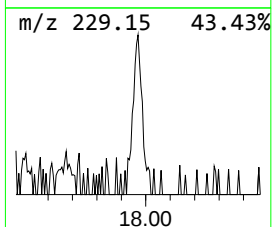
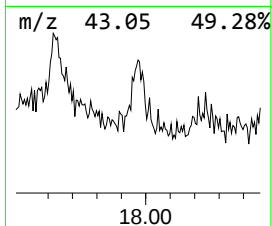
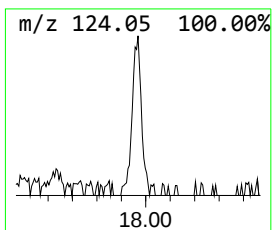
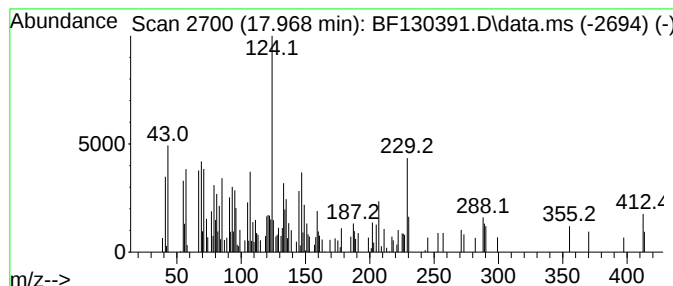
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 .gamma.-Sitostenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.968	3.97 ng	116336	Perylene-d12	15.192

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			.gamma.-Sitostenone	412	C29H48O	084924-96-9	83
2			Stigmast-4-en-3-one	412	C29H48O	001058-61-3	76
3			Testosterone cypionate	412	C27H40O3	000058-20-8	42
4			(Z)-1-(3-(2-chloro-3'-methoxy-[1...	355	C22H26ClNO	318276-19-6	35
5			3-(3-Fluoroanilino)-1-(3-nitroph...	288	C15H13FN2O3	300726-64-1	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092322\
Data File : BF130391.D
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Operator : CG\JU
Sample : N4780-21
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.828	9.0	ng	247652	1	6.651	549616	20.0
n-Hexadecanoic ...	11.704	4.8	ng	144854	4	11.163	601513	20.0
Octadecanoic acid	12.492	4.8	ng	129637	5	13.798	536045	20.0
Triphenylphosph...	13.904	4.9	ng	130707	5	13.798	536045	20.0
Heptacosane	14.886	3.2	ng	93744	6	15.192	586526	20.0
Heneicosane	15.627	6.3	ng	185671	6	15.192	586526	20.0
Oxirane, hexade...	16.345	2.8	ng	83398	6	15.192	586526	20.0
cis-(-)-2,4a,5,...	16.668	3.1	ng	90264	6	15.192	586526	20.0
.gamma.-Sitoste...	17.968	4.0	ng	116336	6	15.192	586526	20.0