

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF033021\
 Data File : BF123532.D
 Acq On : 30 Mar 2021 20:56
 Operator : JU/CG
 Sample : M1832-04
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 IG004

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-BF032321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123532.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.234	15	25	31	rVB	730738	980092	15.98%	2.058%
2	2.340	37	43	51	rVB	134828	172518	2.81%	0.362%
3	5.128	512	517	526	rVB	356204	584059	9.52%	1.227%
4	5.516	577	583	586	rBV	4522328	4893108	79.77%	10.276%
5	6.340	717	723	726	rBV	75896	62459	1.02%	0.131%
6	6.516	746	753	756	rBV	4074064	5299573	86.39%	11.130%
7	6.881	812	815	819	rBV	950295	806623	13.15%	1.694%
8	7.451	905	912	915	rBV	3116493	3440847	56.09%	7.226%
9	8.169	1029	1034	1037	rBV	1246939	1062688	17.32%	2.232%
10	9.251	1211	1218	1221	rBV	6463833	6134286	100.00%	12.882%
11	9.639	1280	1284	1288	rBV	111482	95073	1.55%	0.200%
12	9.928	1326	1333	1337	rBV	1607252	1350650	22.02%	2.836%
13	10.722	1461	1468	1471	rBV	4638114	5051500	82.35%	10.609%
14	11.092	1524	1531	1537	rBV8	25558	67603	1.10%	0.142%
15	11.416	1581	1586	1590	rBV	1486780	1411684	23.01%	2.965%
16	11.633	1620	1623	1627	rVB	93530	71104	1.16%	0.149%
17	11.951	1673	1677	1689	rBV	875371	894316	14.58%	1.878%
18	12.504	1767	1771	1776	rBV2	269346	285849	4.66%	0.600%
19	12.739	1807	1811	1819	rBV	211951	202003	3.29%	0.424%
20	13.016	1852	1858	1861	rBV	5929695	6059390	98.78%	12.725%
21	13.245	1891	1897	1900	rBV2	53063	70044	1.14%	0.147%
22	13.921	2005	2012	2029	rBV2	423927	1123544	18.32%	2.360%
23	14.063	2033	2036	2040	rVB	881825	805458	13.13%	1.692%
24	14.539	2111	2117	2120	rBV	308541	315502	5.14%	0.663%
25	14.580	2120	2124	2128	rVV3	225099	469422	7.65%	0.986%
26	14.621	2128	2131	2142	rVV3	321601	710195	11.58%	1.491%
27	14.710	2142	2146	2153	rVB9	48337	90930	1.48%	0.191%
28	14.857	2168	2171	2177	rVB	67384	78953	1.29%	0.166%
29	15.004	2193	2196	2201	rBV	140764	148467	2.42%	0.312%
30	15.210	2226	2231	2235	rBV	365359	393164	6.41%	0.826%
31	15.268	2235	2241	2247	rBV6	135765	389234	6.35%	0.817%
32	15.410	2262	2265	2271	rVB5	50317	65706	1.07%	0.138%
33	15.557	2285	2290	2294	rBV	489773	629544	10.26%	1.322%
34	15.604	2294	2298	2303	rVB2	43944	64458	1.05%	0.135%
35	15.810	2328	2333	2339	rVB	159984	217094	3.54%	0.456%
36	16.057	2370	2375	2381	rVB	262865	373825	6.09%	0.785%

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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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	16.139	2382	2389	2395	rBV6	131079	418549	6.82%	0.879%
38	16.586	2460	2465	2474	rVB4	27863	62869	1.02%	0.132%
39	16.886	2509	2516	2524	rBV	127859	256299	4.18%	0.538%
40	17.204	2563	2570	2576	rVB	70563	147585	2.41%	0.310%
41	17.351	2588	2595	2596	rBV6	42580	79640	1.30%	0.167%
42	17.739	2654	2661	2678	rVB6	74688	311896	5.08%	0.655%
43	18.280	2744	2753	2763	rVB3	232081	574907	9.37%	1.207%
44	18.568	2791	2802	2819	rBV10	133359	671079	10.94%	1.409%
45	18.745	2827	2832	2846	rVB10	75443	223557	3.64%	0.469%

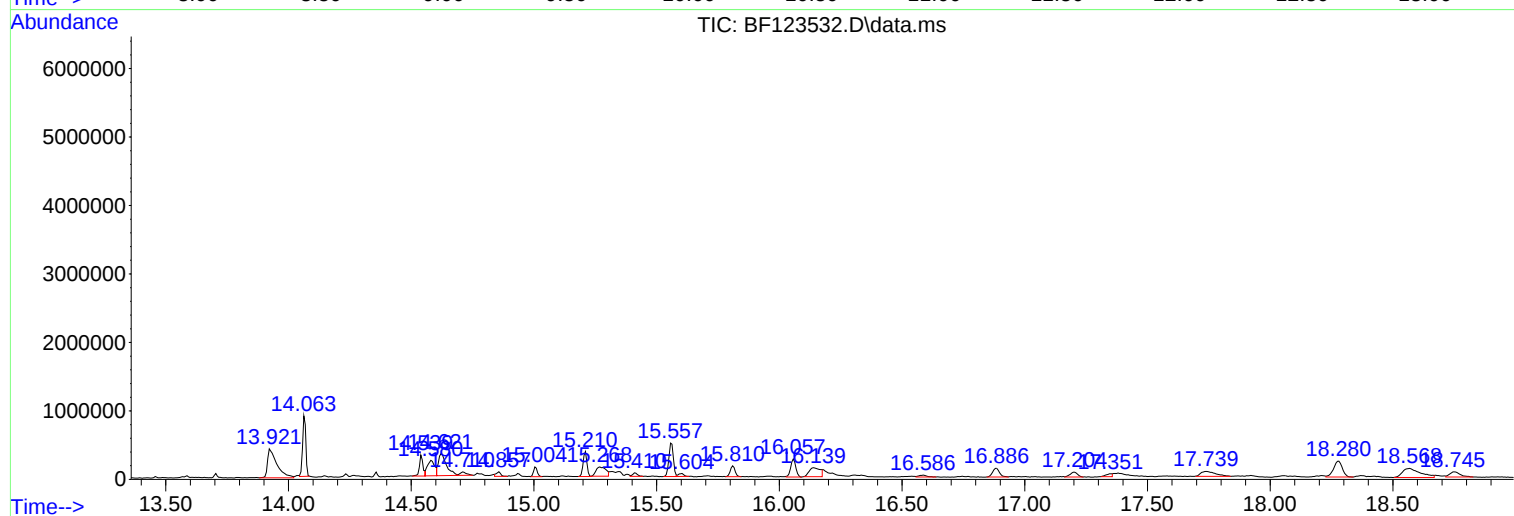
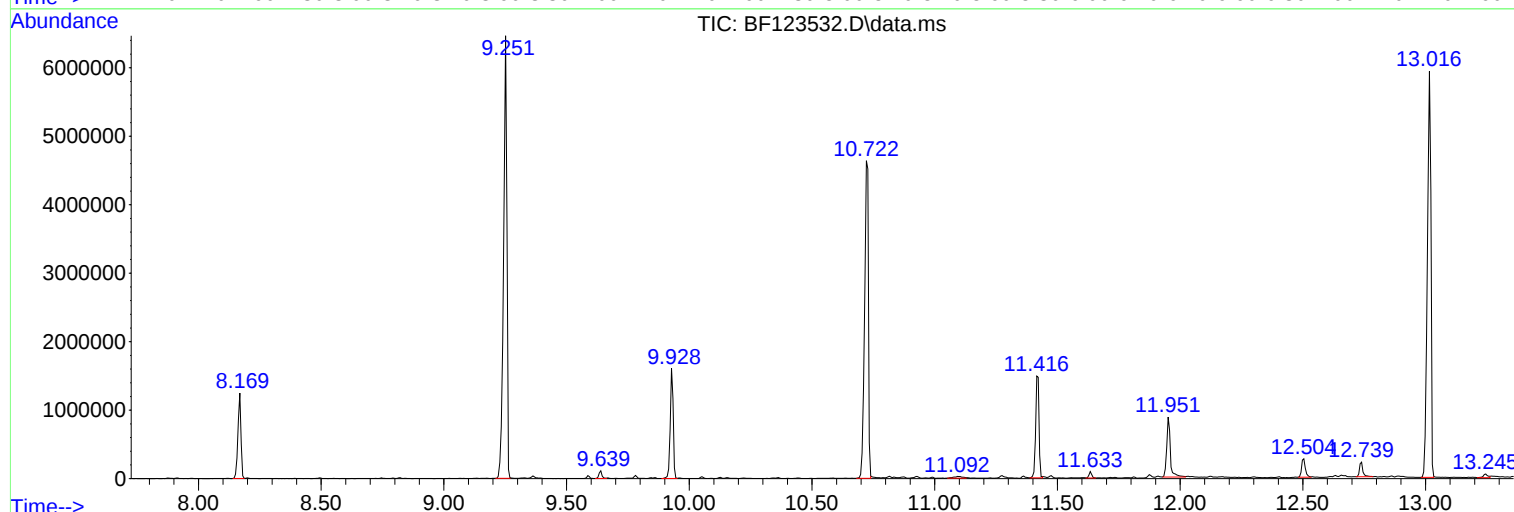
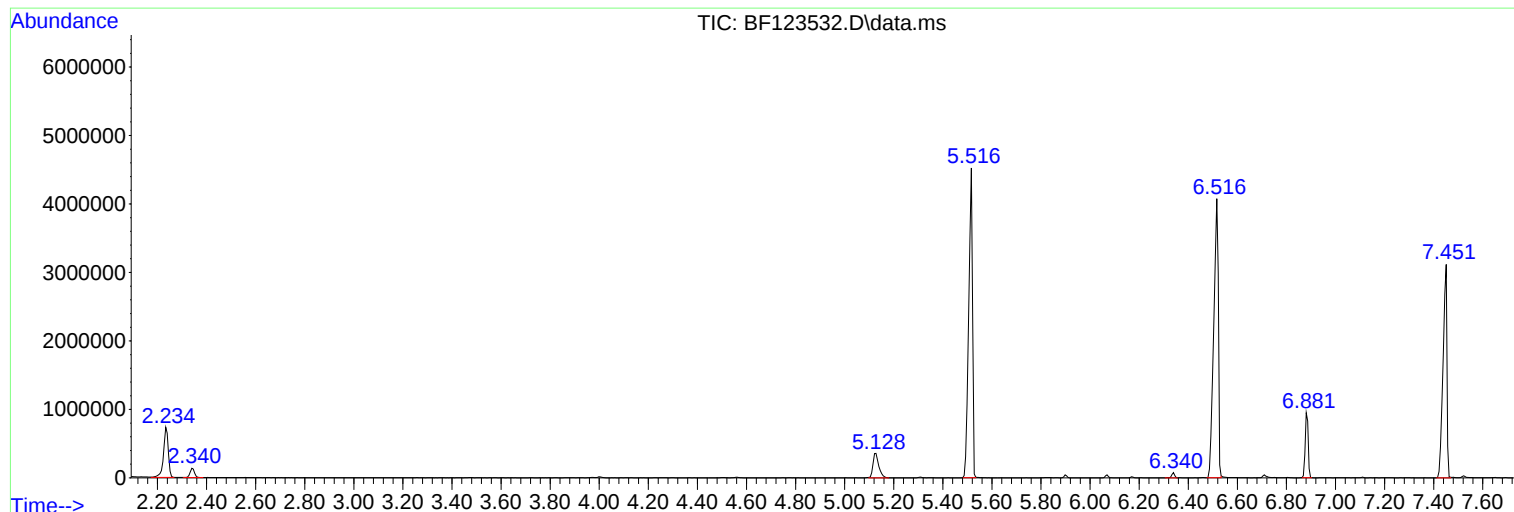
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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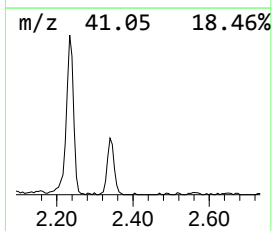
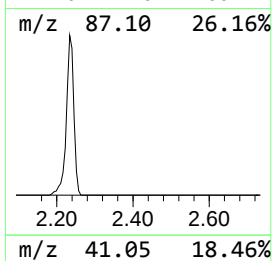
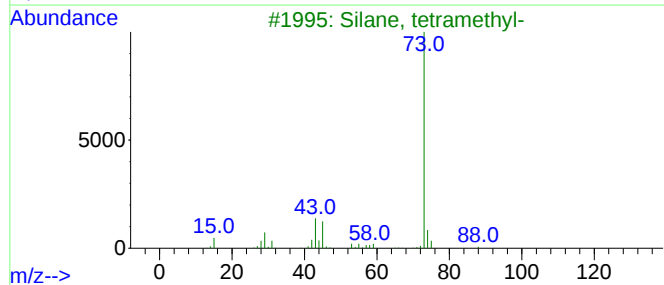
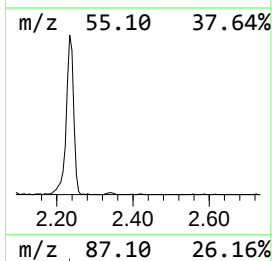
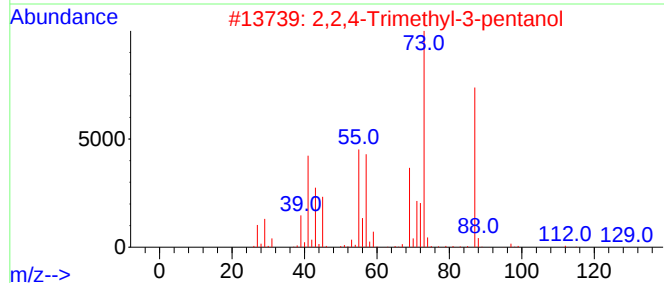
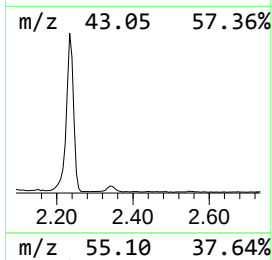
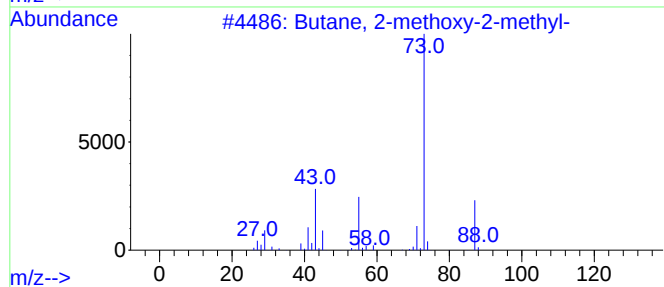
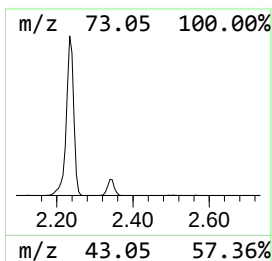
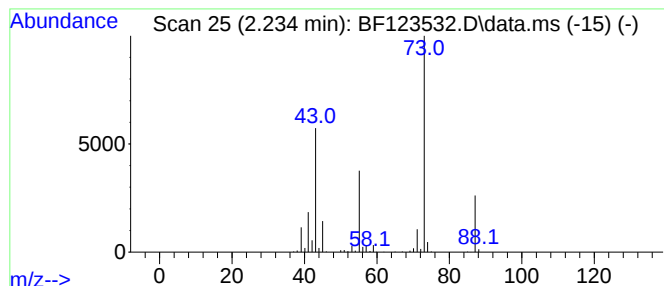
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.234	24.30 ng	980092	1,4-Dichlorobenzene-d4	6.881

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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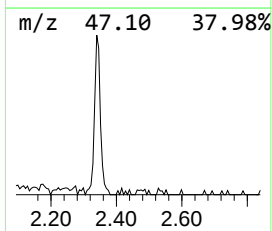
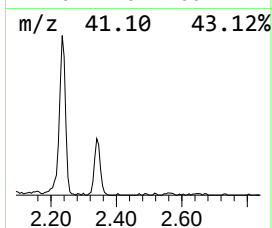
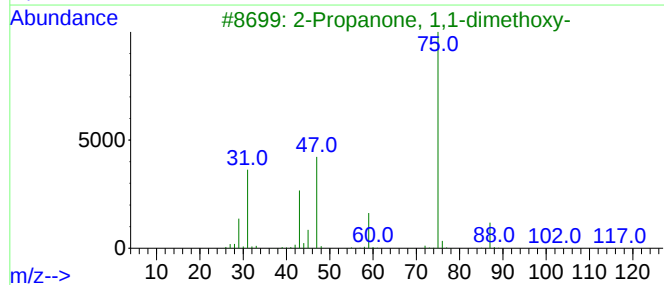
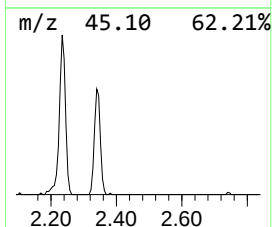
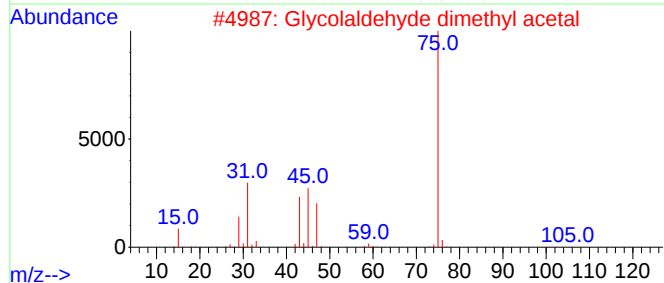
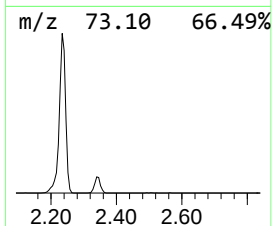
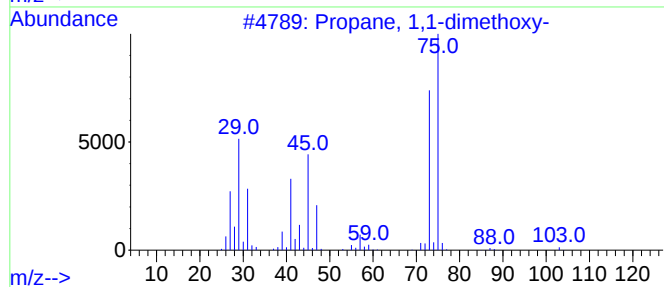
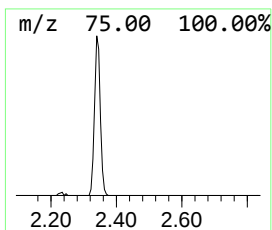
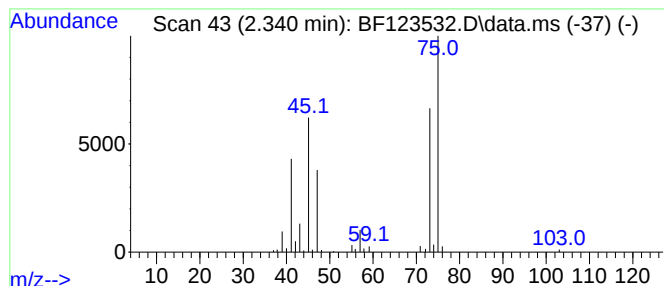
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.340	4.28 ng	172518	1,4-Dichlorobenzene-d4	6.881

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	64
2			Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	45
3			2-Propanone, 1,1-dimethoxy-	118	C5H10O3	006342-56-9	28
4			Methane, trimethoxy-	106	C4H10O3	000149-73-5	28
5			Acetic acid, dimethoxy-, methyl ...	134	C5H10O4	000089-91-8	28



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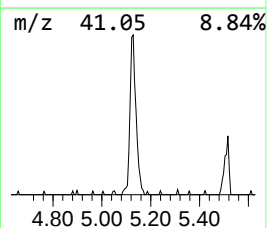
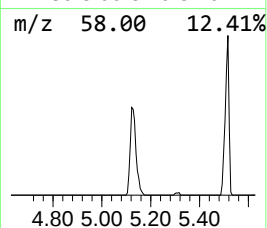
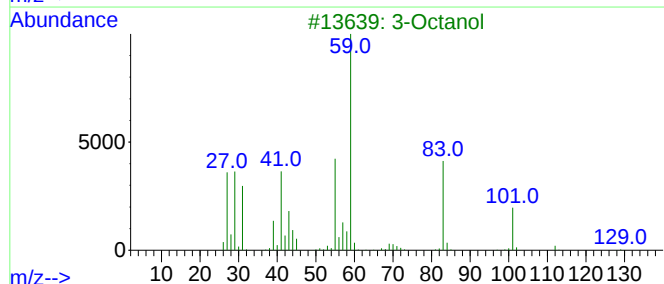
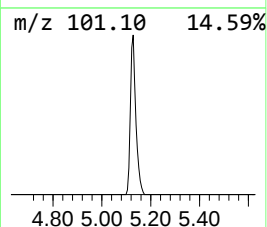
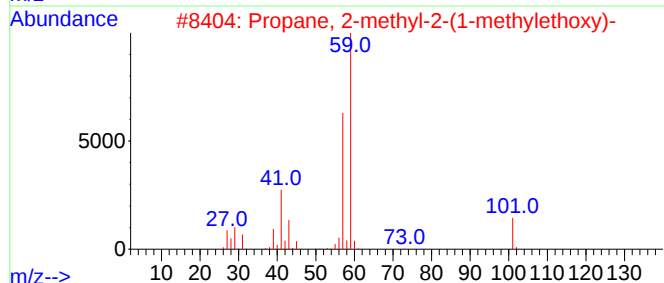
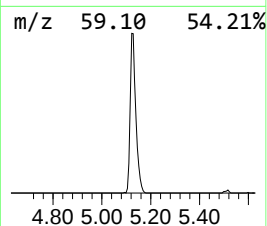
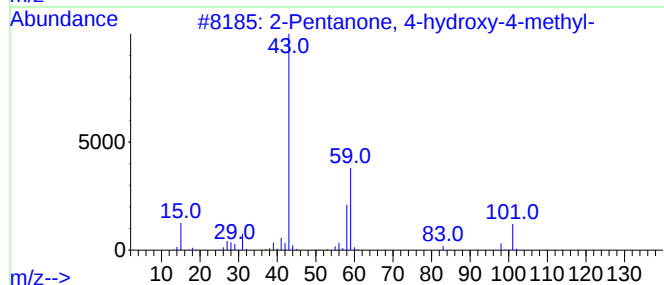
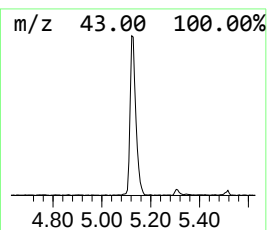
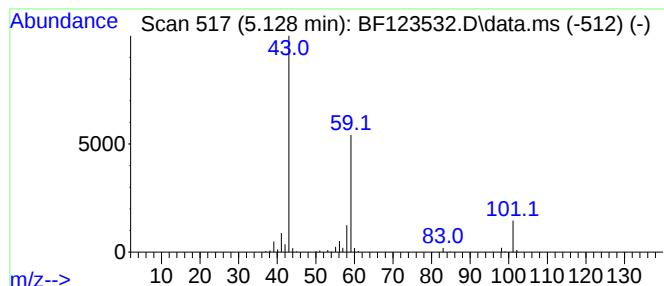
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.128	14.48 ng	584059	1,4-Dichlorobenzene-d4	6.881

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
3			3-Octanol	130	C8H18O	000589-98-0	33
4			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



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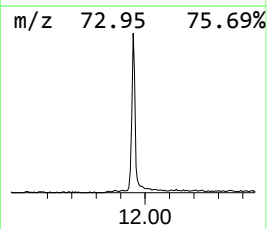
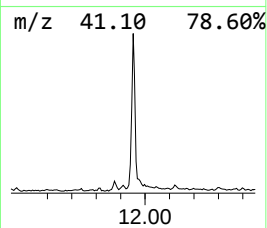
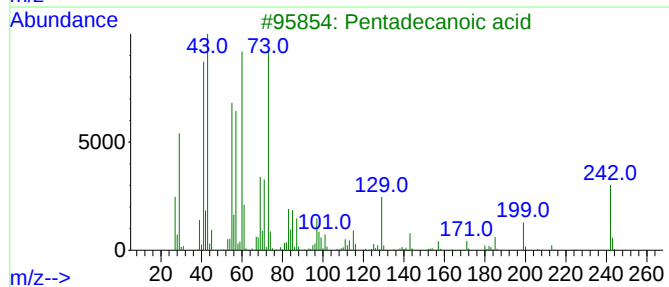
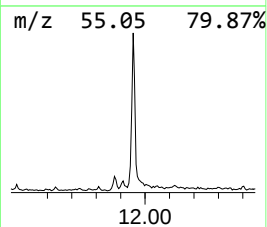
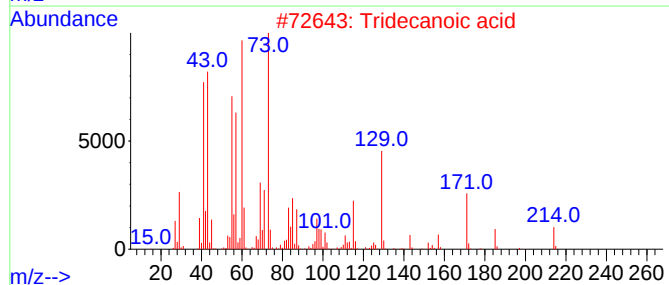
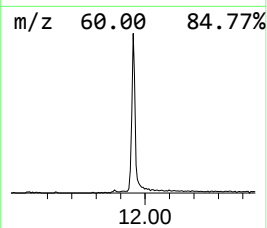
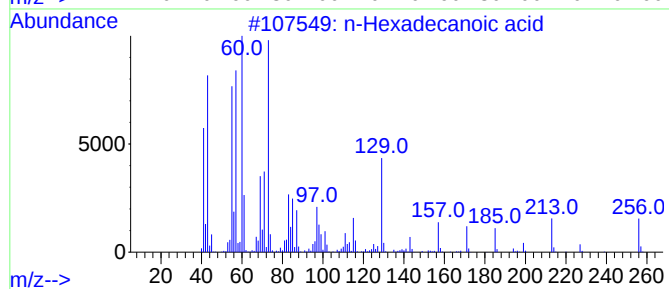
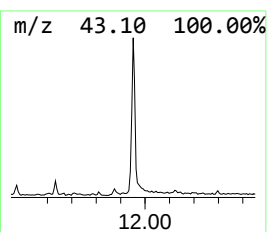
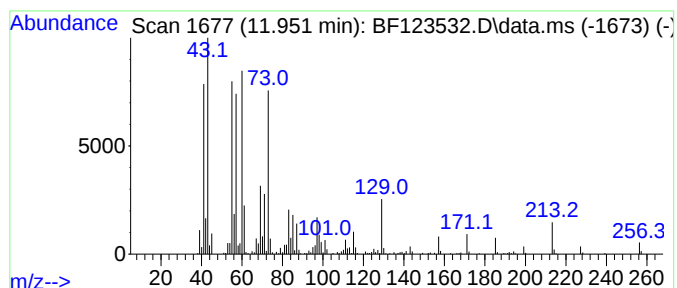
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.951	12.67 ng	894316	Phenanthrene-d10	11.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2			Tridecanoic acid	214	C13H26O2	000638-53-9	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5			n-Decanoic acid	172	C10H20O2	000334-48-5	58



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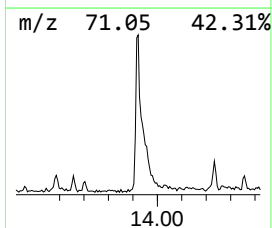
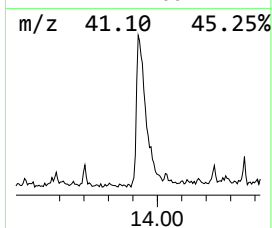
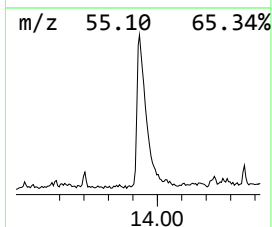
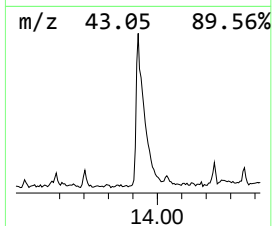
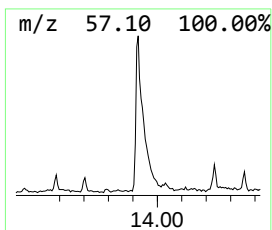
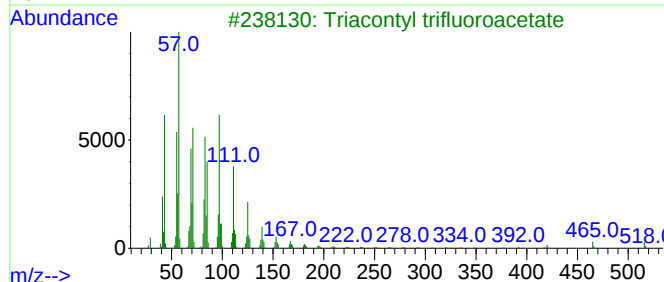
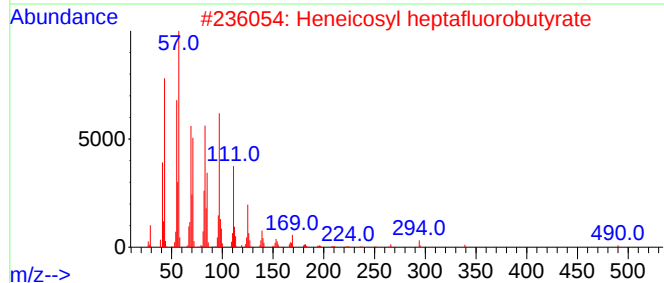
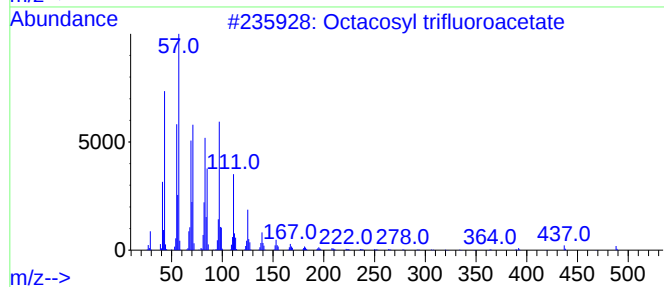
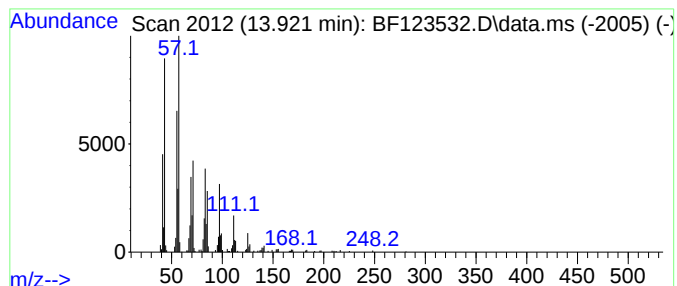
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octacosyl trifluoroacetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.921	27.90 ng	1123540	Chrysene-d12	14.063

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91
2			Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	91
3			Triacontyl trifluoroacetate	534	C32H61F3O2	1000351-75-7	91
4			Hexacosyl trifluoroacetate	478	C28H53F3O2	1000351-75-0	91
5			Hexacosyl pentafluoropropionate	528	C29H53F5O2	1000351-81-2	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF033021\
Data File : BF123532.D
Acq On : 30 Mar 2021 20:56
Operator : JU/CG
Sample : M1832-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
IG004

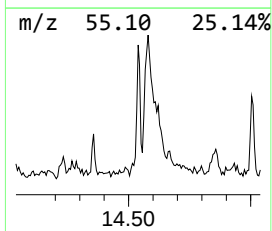
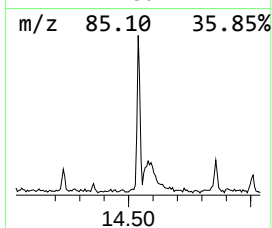
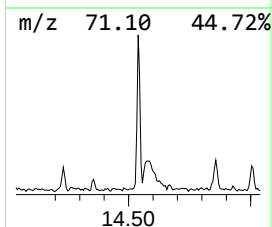
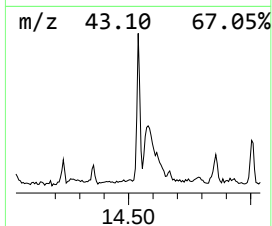
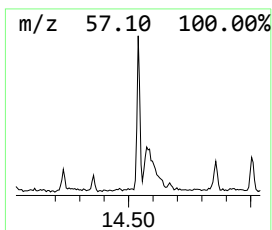
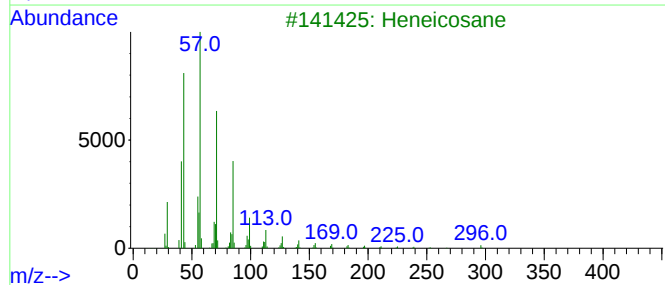
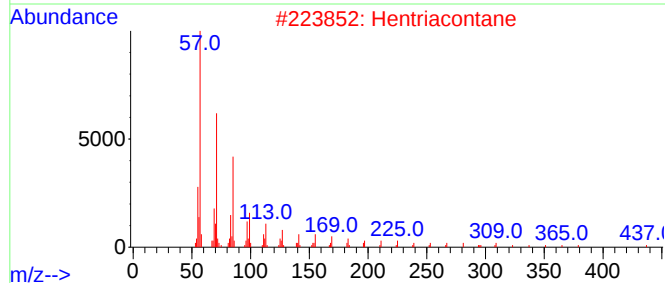
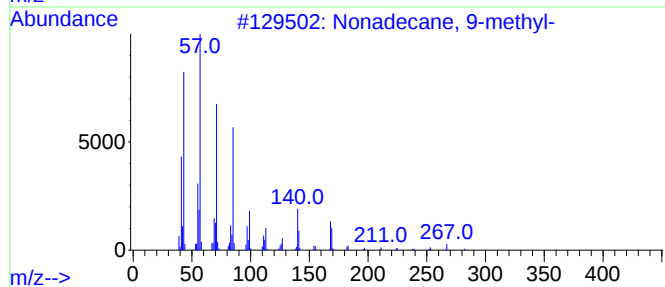
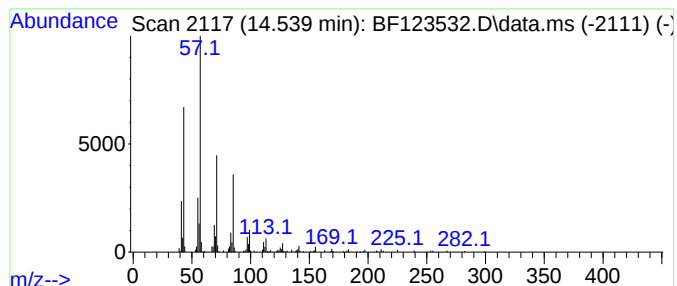
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Nonadecane, 9-methyl- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.539	7.83 ng	315502	Chrysene-d12	14.063

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane, 9-methyl-	282	C20H42	013287-24-6	93
2			Hentriacontane	437	C31H64	000630-04-6	91
3			Heneicosane	296	C21H44	000629-94-7	91
4			Eicosane, 7-hexyl-	366	C26H54	055333-99-8	91
5			Octacosane	394	C28H58	000630-02-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF033021\
Data File : BF123532.D
Acq On : 30 Mar 2021 20:56
Operator : JU/CG
Sample : M1832-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

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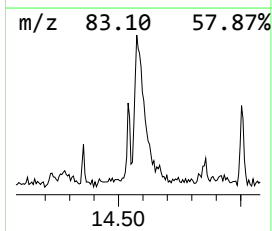
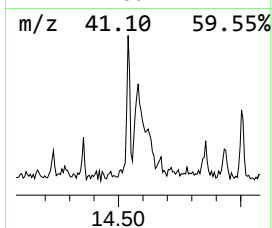
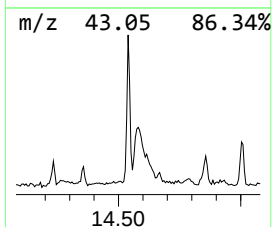
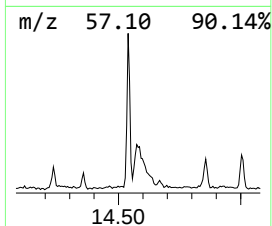
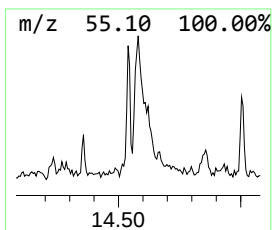
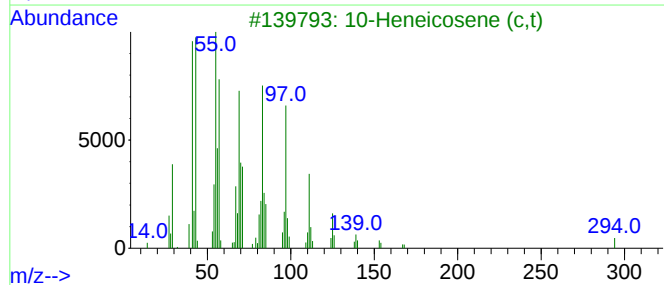
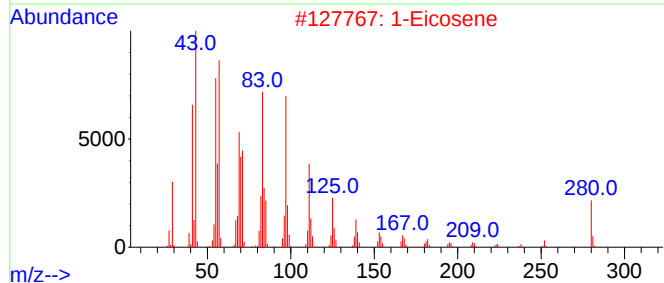
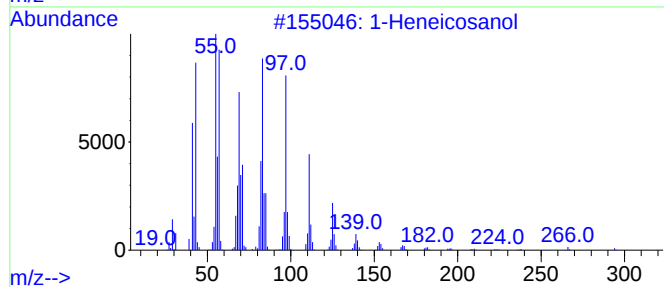
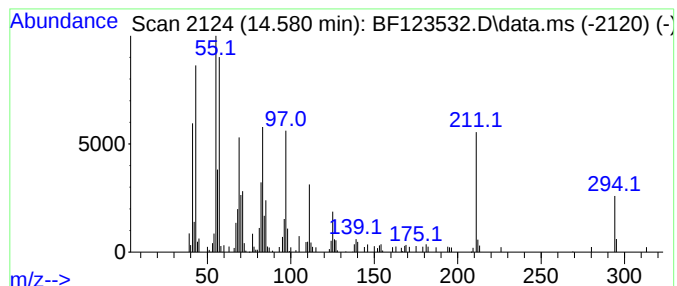
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 1-Heneicosanol Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.580	11.66 ng	469422	Chrysene-d12	14.063

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heneicosanol	312	C21H44O	015594-90-8	86
2		1-Eicosene	280	C20H40	003452-07-1	83
3		10-Heneicosene (c,t)	294	C21H42	095008-11-0	76
4		Cyclohexadecane, 1,2-diethyl-	280	C20H40	1000155-85-3	70
5		1-Hexadecanol	242	C16H34O	036653-82-4	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF033021\
Data File : BF123532.D
Acq On : 30 Mar 2021 20:56
Operator : JU/CG
Sample : M1832-04
Misc :
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Instrument :
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ClientSampleId :
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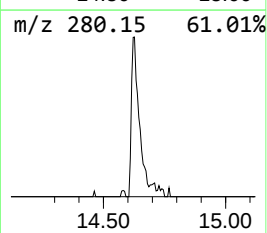
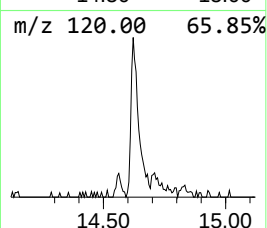
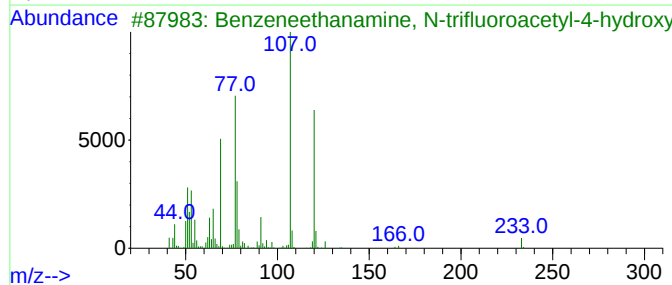
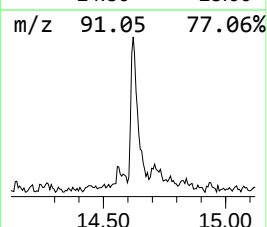
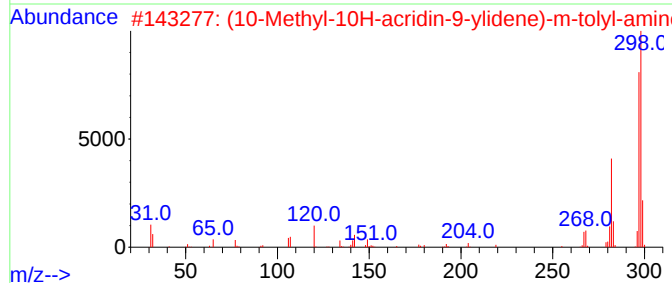
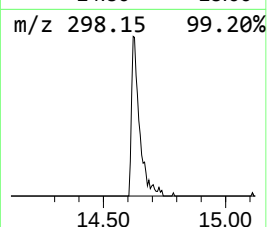
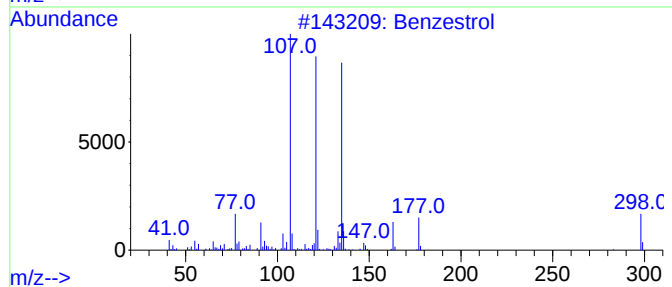
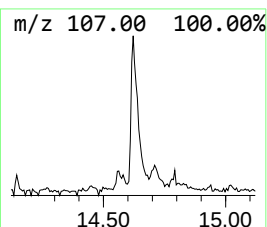
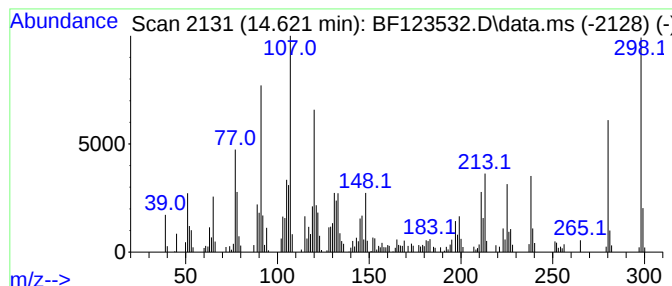
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 unknown14.621 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.621	17.63 ng	710195	Chrysene-d12	14.063

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzestrol	298	C20H26O2	000085-95-0	38
2			(10-Methyl-10H-acridin-9-ylidene...	298	C21H18N2	1000317-84-0	25
3			Benzeneethanamine, N-trifluoroac...	233	C10H10F3NO2	013230-73-4	22
4			2,4-Imidazolidinedithione, 1-met...	298	C16H14N2S2	006826-03-5	20
5			Dibenz[d,f]cycloheptanone, 2,3,9...	298	C18H18O4	145068-61-7	18



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF033021\
Data File : BF123532.D
Acq On : 30 Mar 2021 20:56
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Sample : M1832-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

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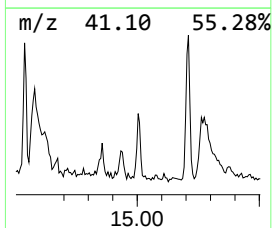
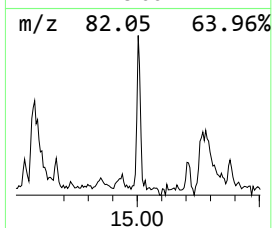
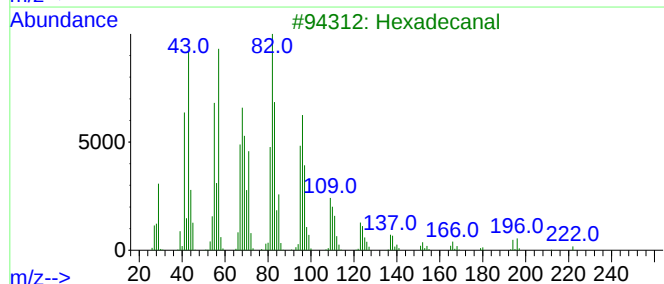
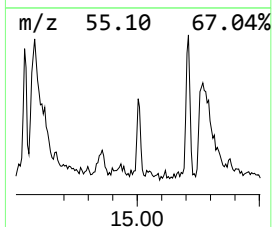
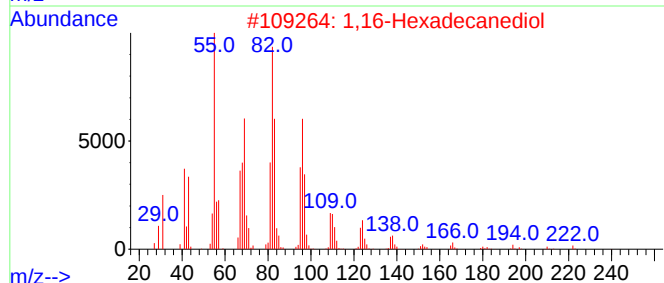
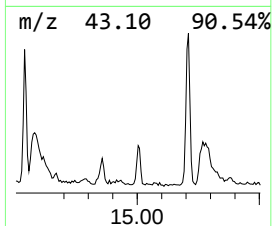
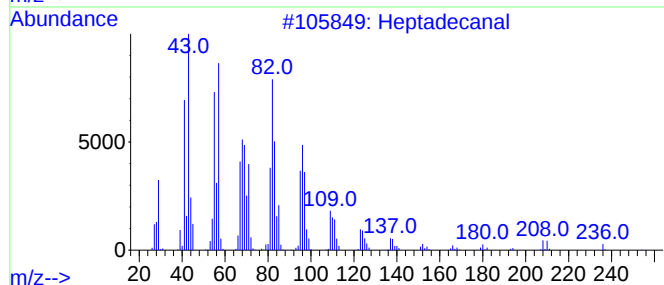
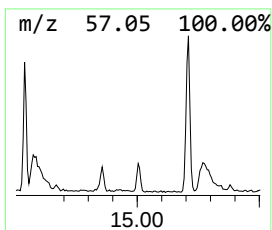
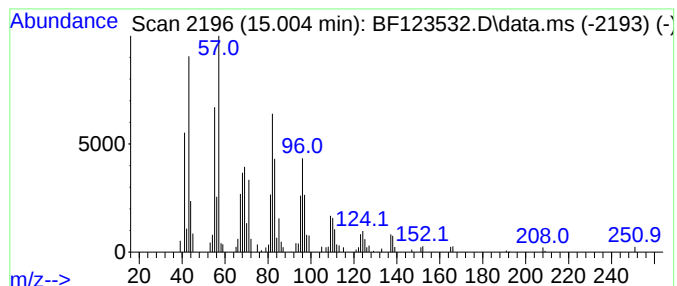
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Heptadecanal Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.004	4.72 ng	148467	Perylene-d12	15.563

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecanal	254	C17H34O	1000376-70-0	91
2			1,16-Hexadecanediol	258	C16H34O2	007735-42-4	91
3			Hexadecanal	240	C16H32O	000629-80-1	91
4			Octadecanal	268	C18H36O	000638-66-4	91
5			Tetradecanal	212	C14H28O	000124-25-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF033021\
Data File : BF123532.D
Acq On : 30 Mar 2021 20:56
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Sample : M1832-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

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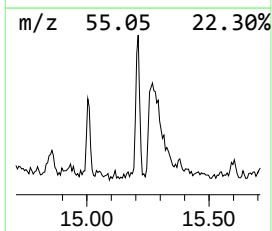
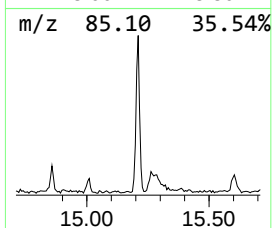
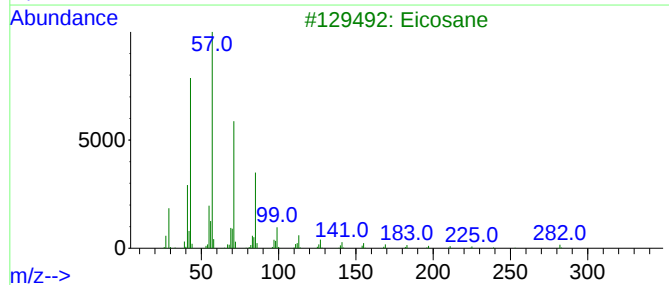
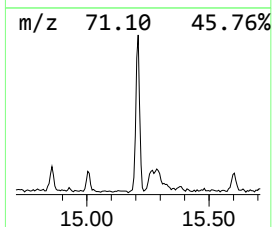
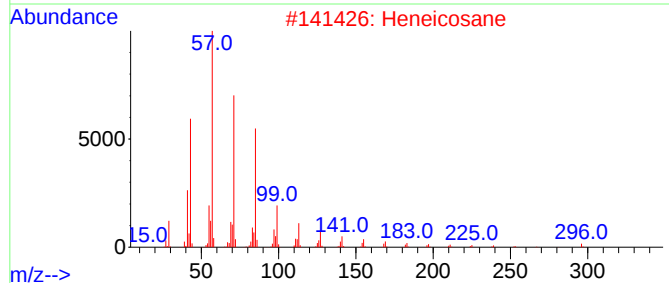
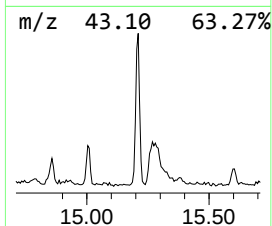
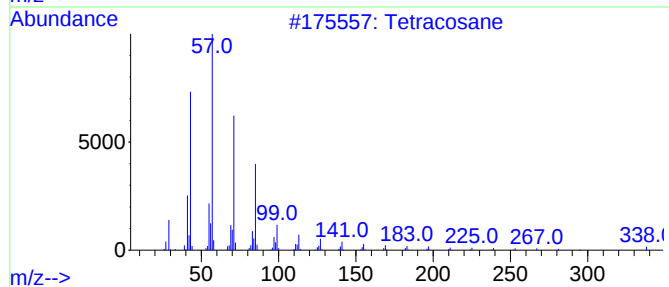
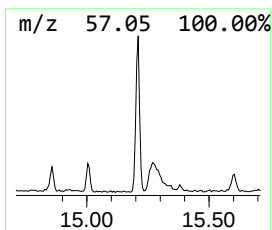
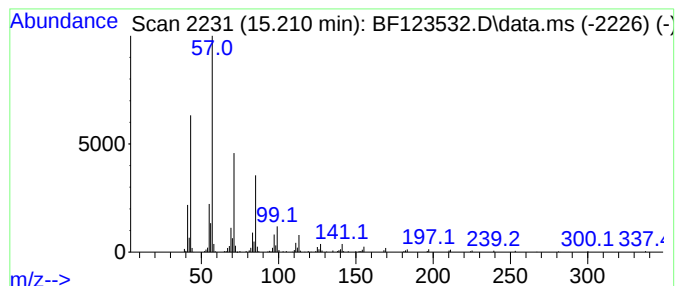
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Tetracosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.210	12.49 ng	393164	Perylene-d12	15.563

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	91
2			Heneicosane	296	C21H44	000629-94-7	90
3			Eicosane	282	C20H42	000112-95-8	90
4			2-methyloctacosane	408	C29H60	1000376-72-8	90
5			Tetratetracontane	619	C44H90	007098-22-8	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF033021\
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Acq On : 30 Mar 2021 20:56
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Sample : M1832-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

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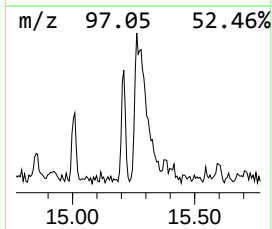
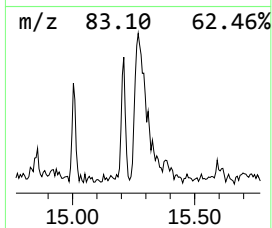
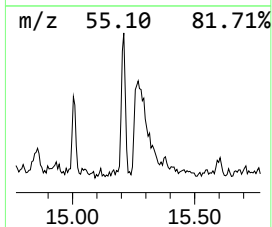
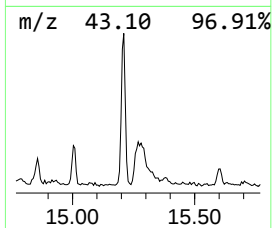
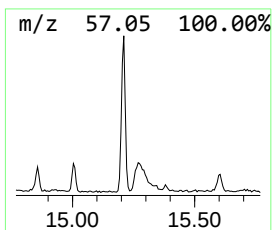
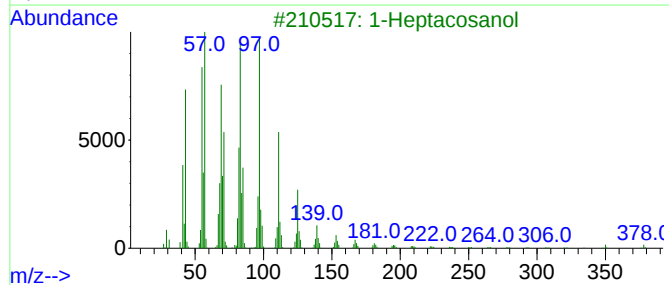
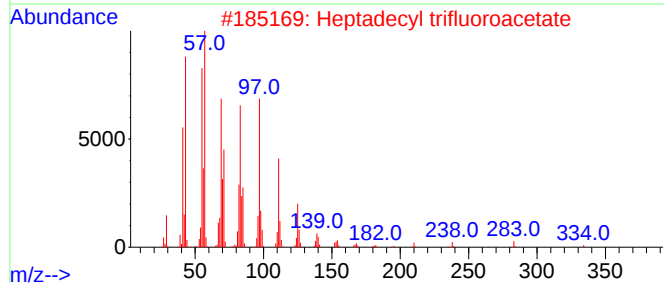
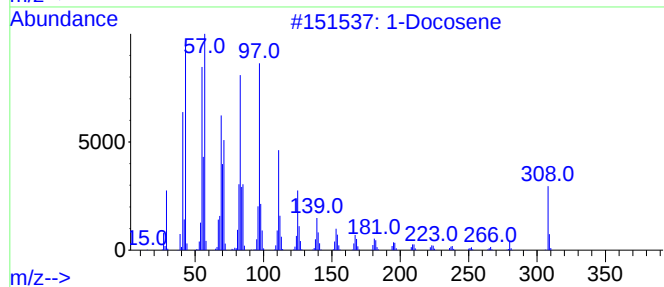
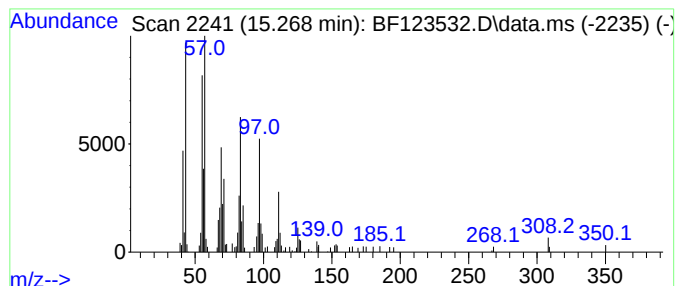
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 1-Docosene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.268	12.37 ng	389234	Perylene-d12	15.563

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene		308	C22H44	001599-67-3	96
2	Heptadecyl trifluoroacetate		352	C19H35F3O2	1000351-87-0	91
3	1-Heptacosanol		396	C27H56O	002004-39-9	91
4	n-Tetracosanol-1		354	C24H50O	000506-51-4	91
5	Octacosanol		410	C28H58O	000557-61-9	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF033021\
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Acq On : 30 Mar 2021 20:56
Operator : JU/CG
Sample : M1832-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

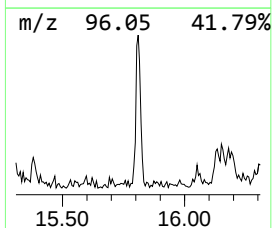
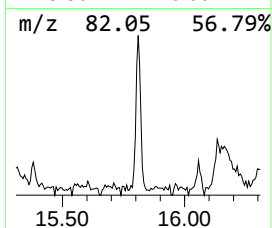
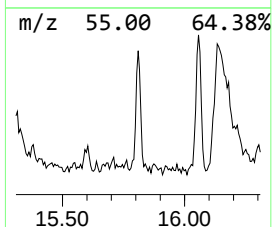
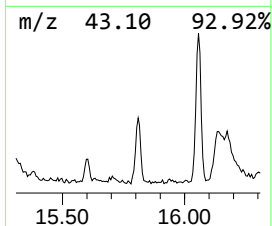
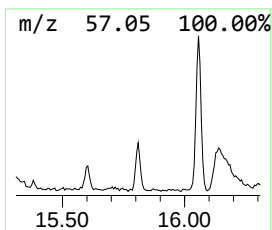
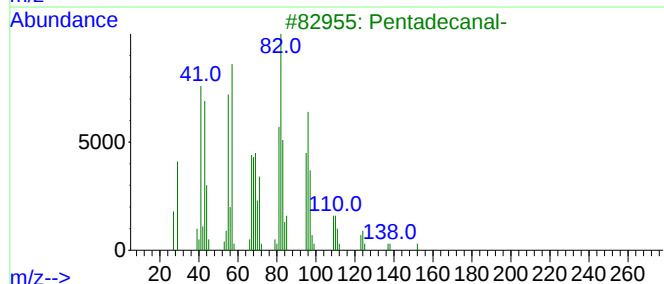
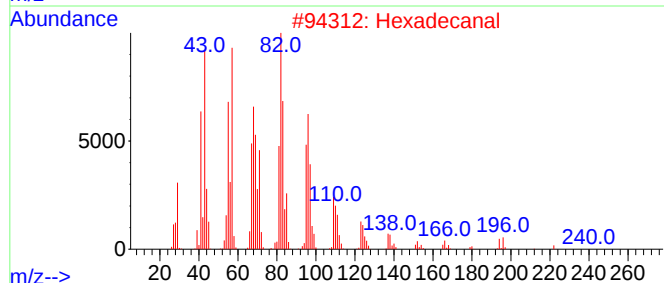
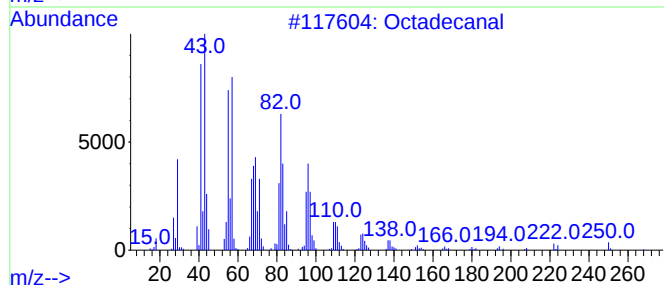
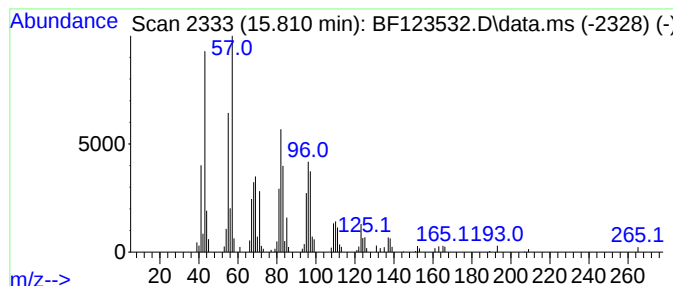
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BNA_F
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Octadecanal Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.810	6.90 ng	217094	Perylene-d12	15.563	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	91
2	Hexadecanal	240	C16H32O	000629-80-1	91
3	Pentadecanal-	226	C15H30O	002765-11-9	91
4	Heptadecanal	254	C17H34O	1000376-70-0	91
5	1,19-Eicosadiene	278	C20H38	014811-95-1	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF033021\
Data File : BF123532.D
Acq On : 30 Mar 2021 20:56
Operator : JU/CG
Sample : M1832-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

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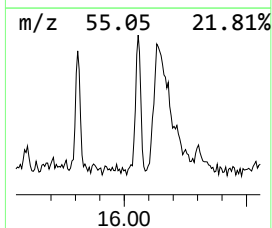
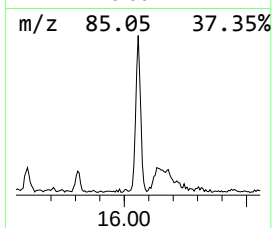
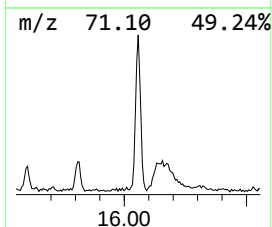
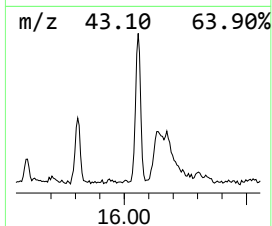
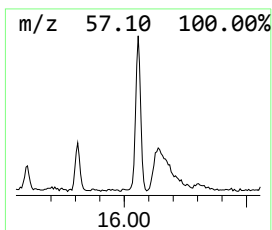
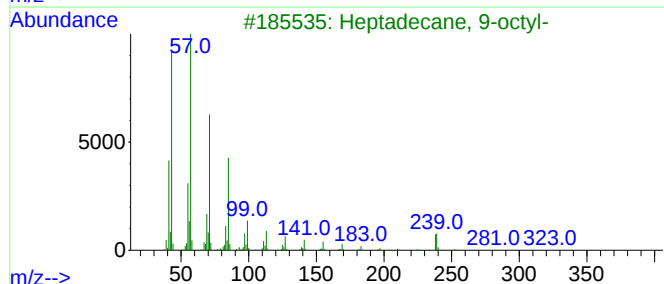
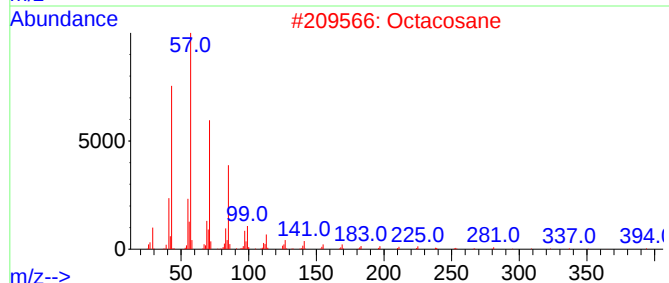
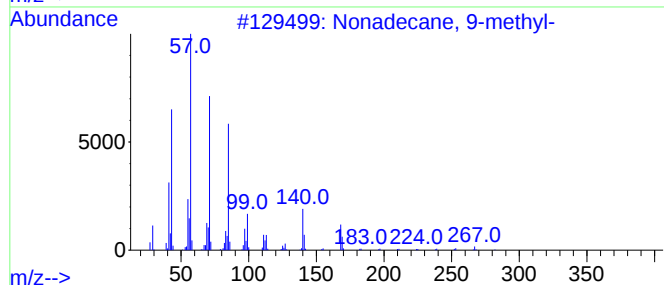
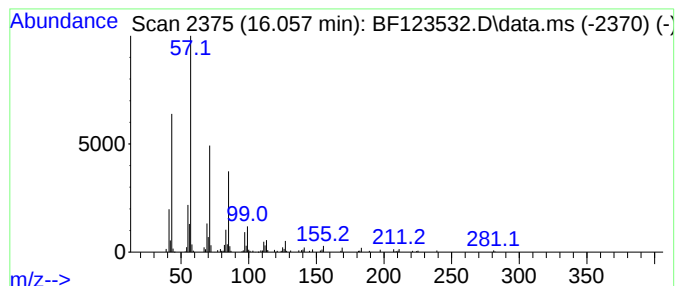
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Octacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.057	11.88 ng	373825	Perylene-d12	15.563

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane, 9-methyl-	282	C20H42	013287-24-6	93
2			Octacosane	394	C28H58	000630-02-4	91
3			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4			Hentriacontane	437	C31H64	000630-04-6	91
5			Hexacosane	366	C26H54	000630-01-3	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF033021\
Data File : BF123532.D
Acq On : 30 Mar 2021 20:56
Operator : JU/CG
Sample : M1832-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

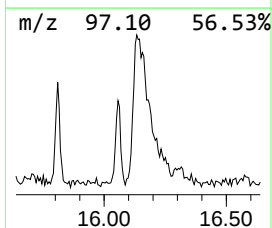
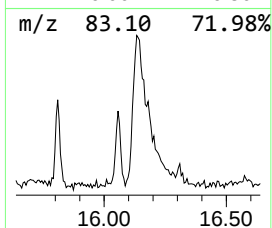
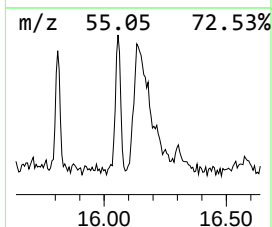
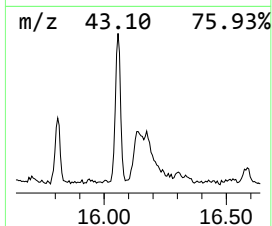
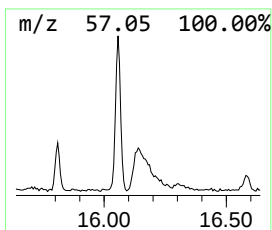
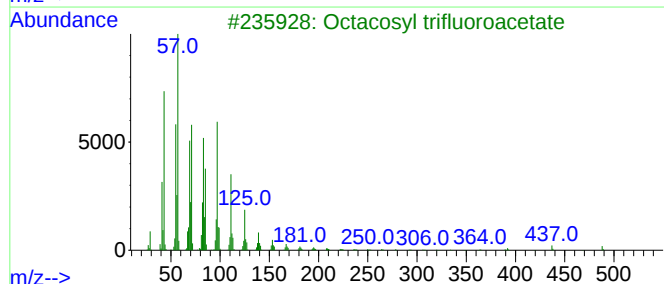
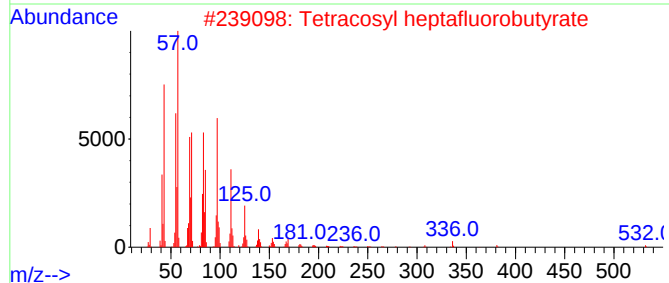
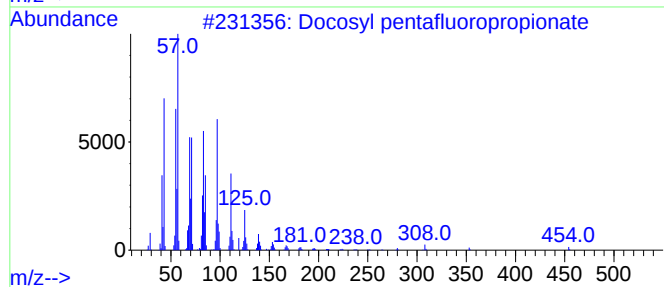
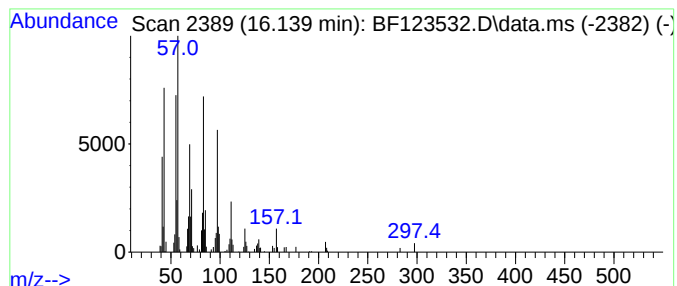
Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 Docosyl pentafluoropropionate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.139	13.30 ng	418549	Perylene-d12	15.563	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	70
2	Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	70
3	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	64
4	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	62
5	Octacosyl heptafluorobutyrate	606	C32H57F7O2	1000351-83-6	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF033021\
Data File : BF123532.D
Acq On : 30 Mar 2021 20:56
Operator : JU/CG
Sample : M1832-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

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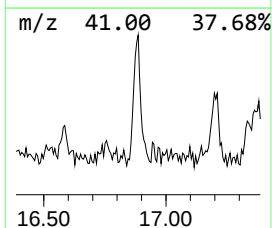
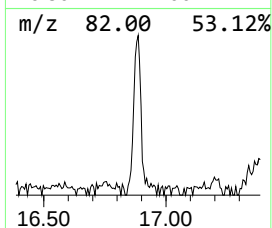
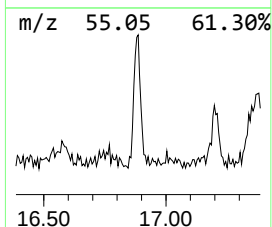
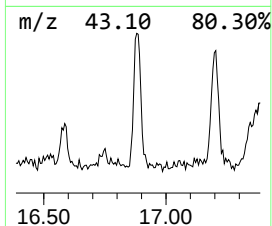
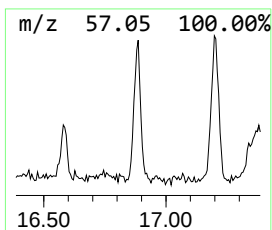
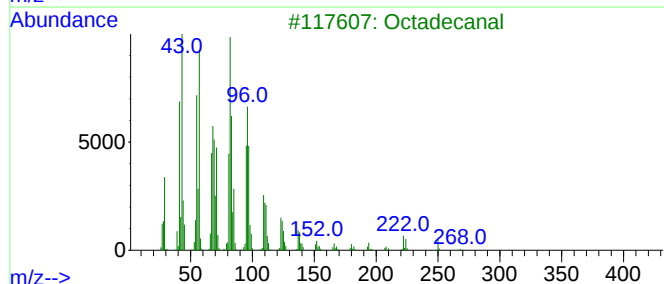
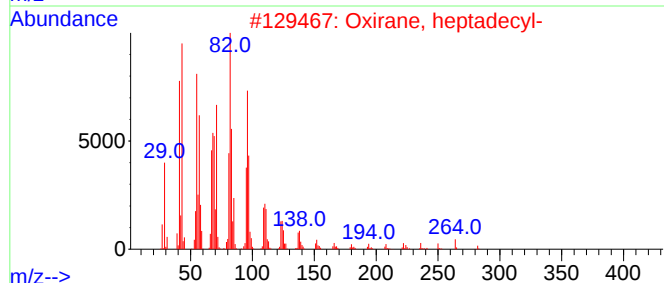
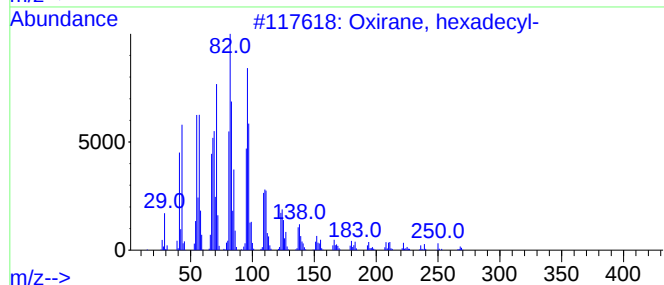
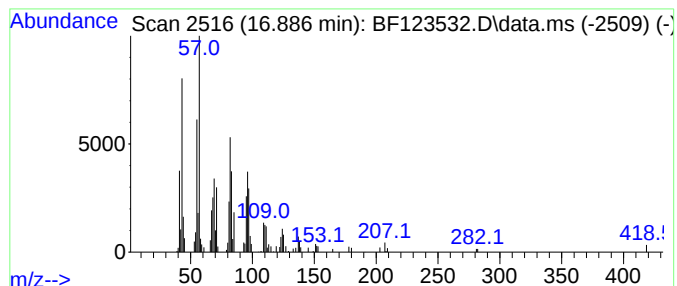
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 15 Oxirane, hexadecyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.886	8.14 ng	256299	Perylene-d12	15.563

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
2		Oxirane, heptadecyl-	282	C19H38O	067860-04-2	91
3		Octadecanal	268	C18H36O	000638-66-4	91
4		Hexadecanal	240	C16H32O	000629-80-1	90
5		Heptadecanal	254	C17H34O	1000376-70-0	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF033021\
Data File : BF123532.D
Acq On : 30 Mar 2021 20:56
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Sample : M1832-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

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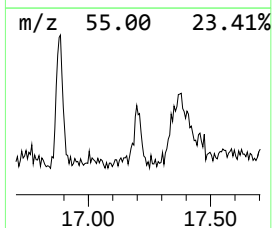
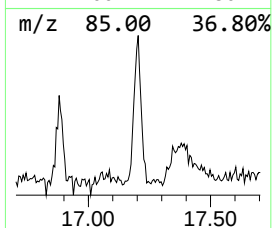
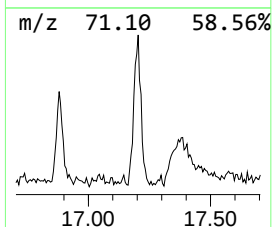
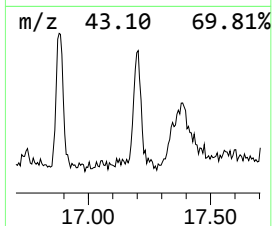
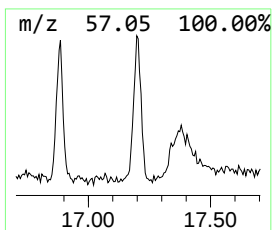
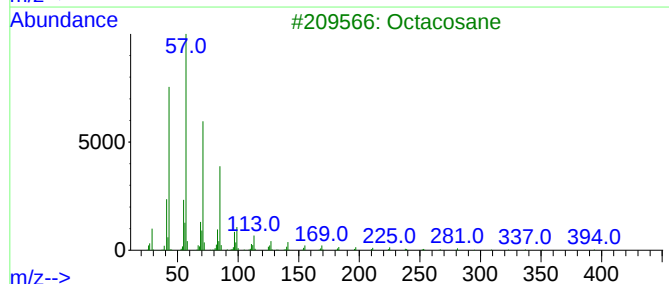
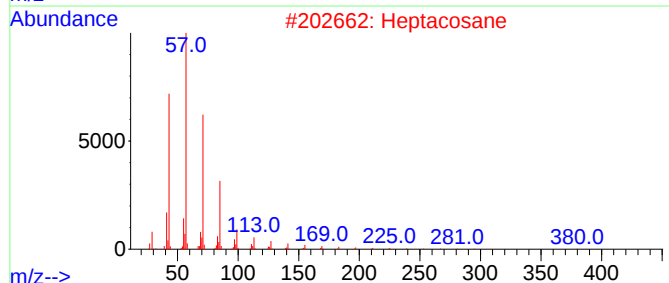
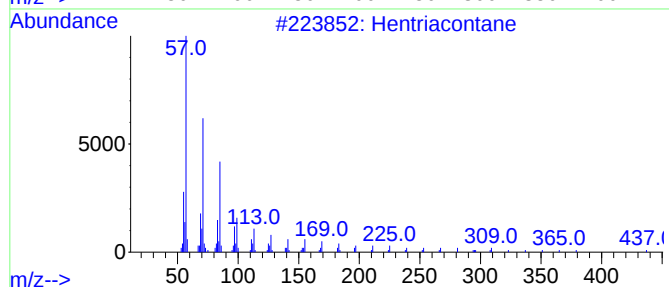
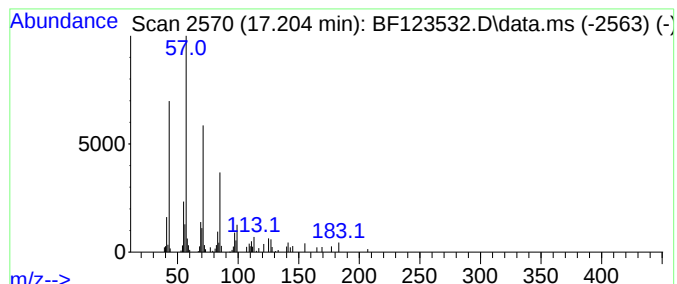
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 16 Hentriacontane Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.204	4.69 ng	147585	Perylene-d12	15.563

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hentriacontane	437	C31H64	000630-04-6	91
2		Heptacosane	380	C27H56	000593-49-7	91
3		Octacosane	394	C28H58	000630-02-4	90
4		Tetracosane	338	C24H50	000646-31-1	87
5		Hexacosane	366	C26H54	000630-01-3	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF033021\
Data File : BF123532.D
Acq On : 30 Mar 2021 20:56
Operator : JU/CG
Sample : M1832-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

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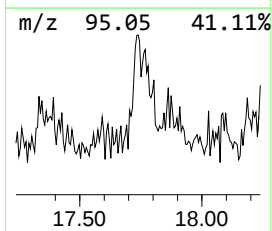
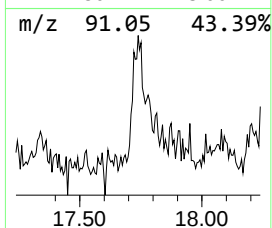
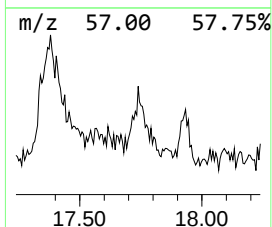
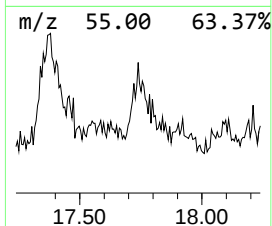
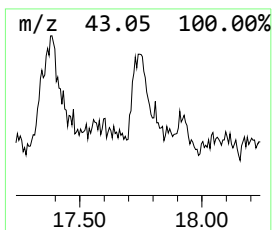
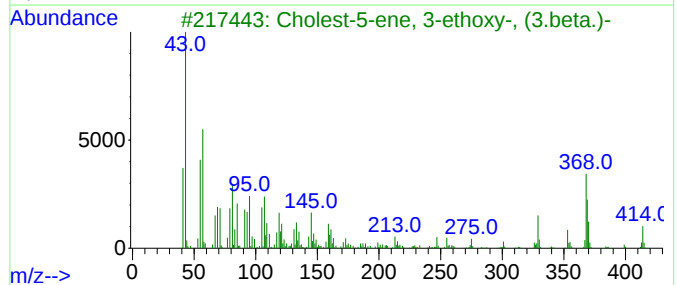
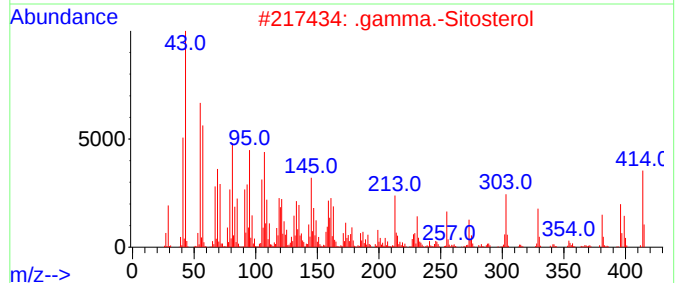
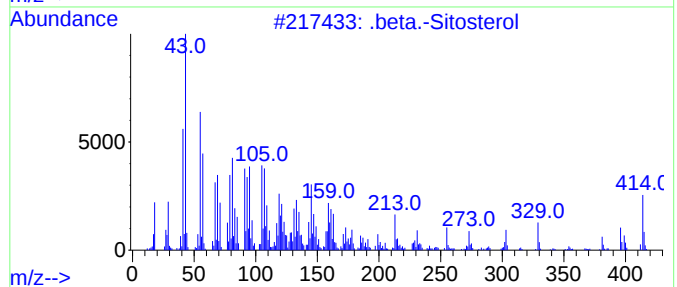
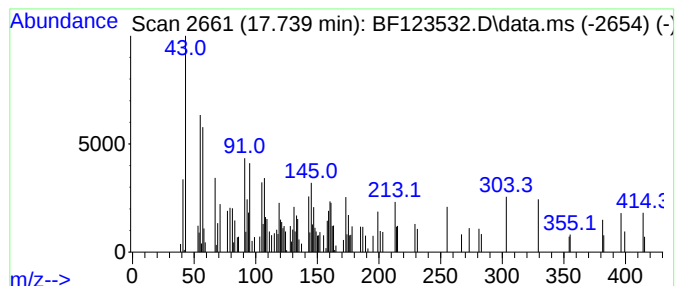
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 17 .beta.-Sitosterol Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.739	9.91 ng	311896	Perylene-d12	15.563

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			.beta.-Sitosterol	414	C29H50O	000083-46-5	96
2			.gamma.-Sitosterol	414	C29H50O	000083-47-6	90
3			Cholest-5-ene, 3-ethoxy-, (3.beta...	414	C29H50O	000986-19-6	50
4			Stigmastan-3-en-6-ol	414	C29H50O	1000214-19-7	32
5			N-Nitrosotomatidine	444	C27H44N2O3	004847-05-6	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF033021\
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Acq On : 30 Mar 2021 20:56
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Sample : M1832-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

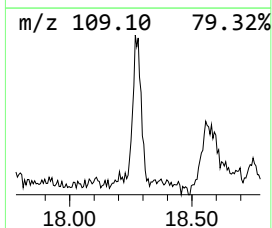
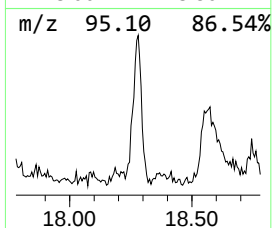
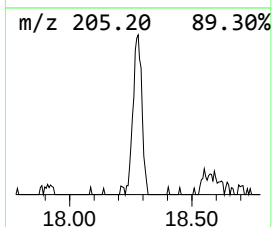
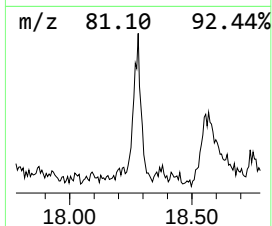
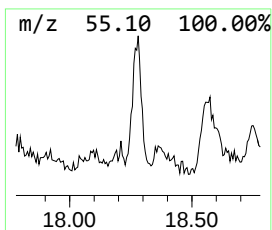
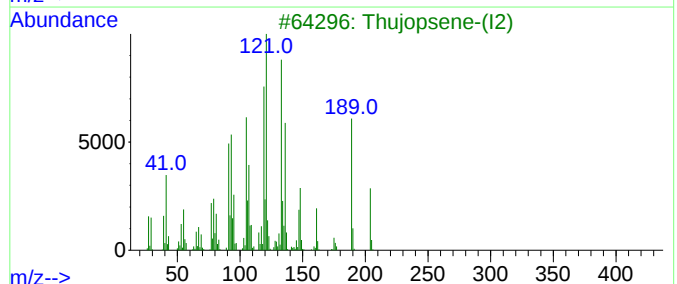
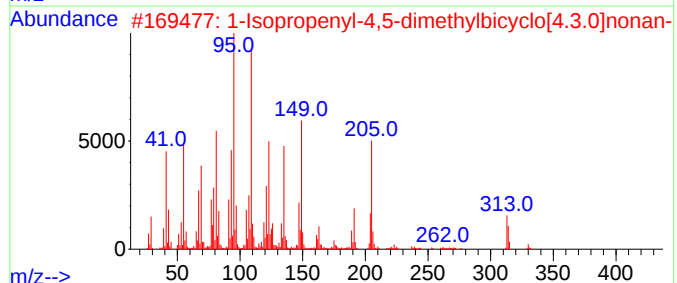
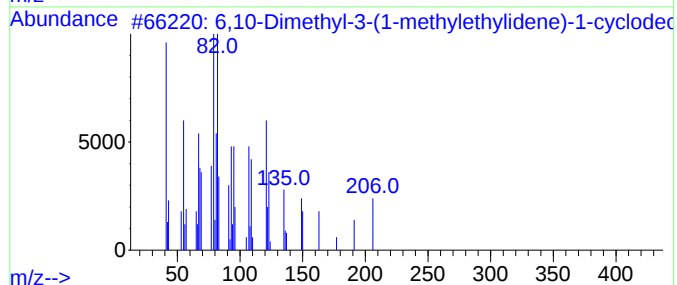
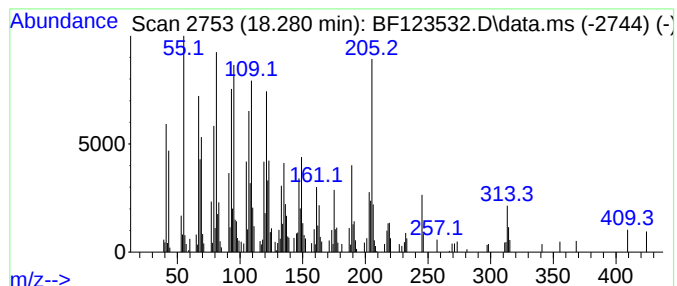
Instrument :
BNA_F
ClientSampled :
IG004

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 18 6,10-Dimethyl-3-(1-methylet... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.280	18.26 ng	574907	Perylene-d12	15.563	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6,10-Dimethyl-3-(1-methylethylid...	206	C15H26	069239-71-0	56
2	1-Isopropenyl-4,5-dimethylbicycl...	330	C21H30OS	1000195-85-4	38
3	Thujopsene-(I2)	204	C15H24	1000152-20-4	35
4	6-(3-Isopropenylcycloprop-1-enyl...	204	C14H20O	1000195-43-0	25
5	9-Borabicyclo[3.3.1]nonan-9-amin...	205	C13H24BN	143122-94-5	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF033021\
Data File : BF123532.D
Acq On : 30 Mar 2021 20:56
Operator : JU/CG
Sample : M1832-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

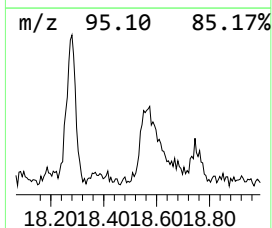
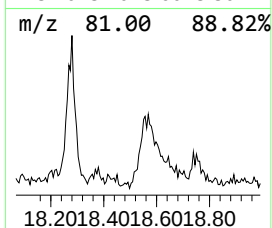
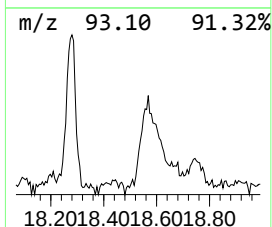
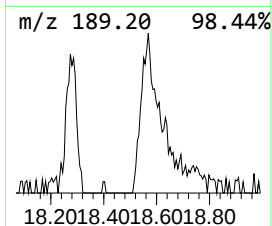
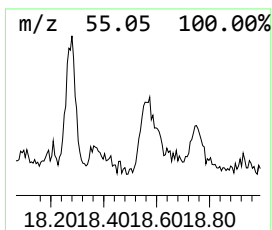
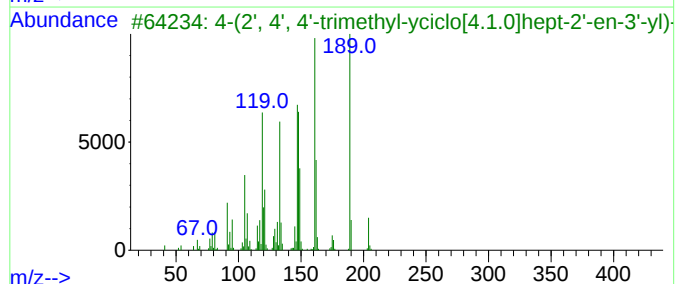
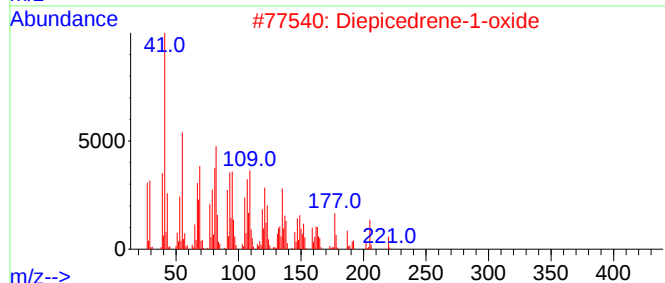
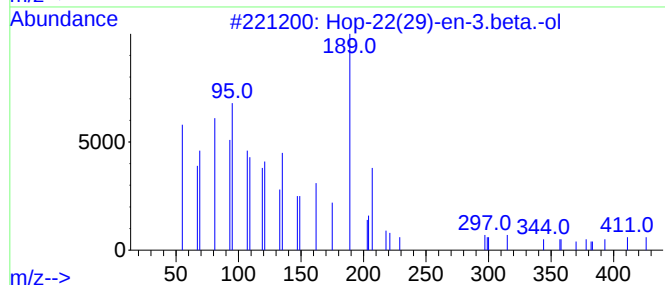
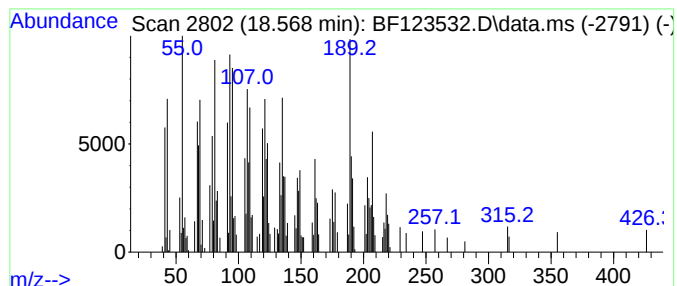
Instrument :
BNA_F
ClientSampleId :
IG004

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 19 Hop-22(29)-en-3.beta.-ol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.568	21.32 ng	671079	Perylene-d12	15.563	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hop-22(29)-en-3.beta.-ol	426	C30H50O	058801-23-3	91
2	Diepicedrene-1-oxide	220	C15H24O	1000156-11-0	59
3	4-(2', 4', 4'-trimethyl-yciclo[4...	204	C14H20O	1000373-94-4	59
4	Guaia-1(10),11-diene	204	C15H24	1000374-19-7	50
5	Isoaromadendrene epoxide	220	C15H24O	1000159-36-6	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF033021\
Data File : BF123532.D
Acq On : 30 Mar 2021 20:56
Operator : JU/CG
Sample : M1832-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
IG004

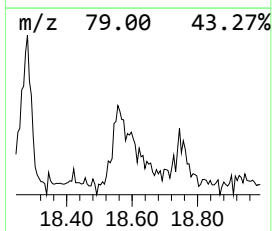
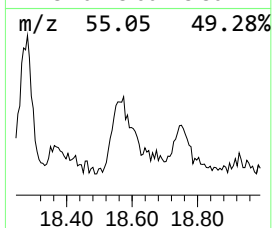
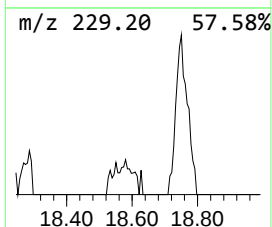
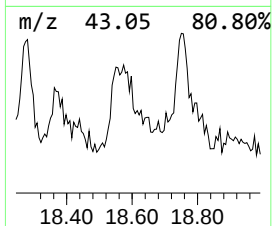
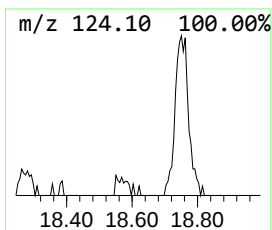
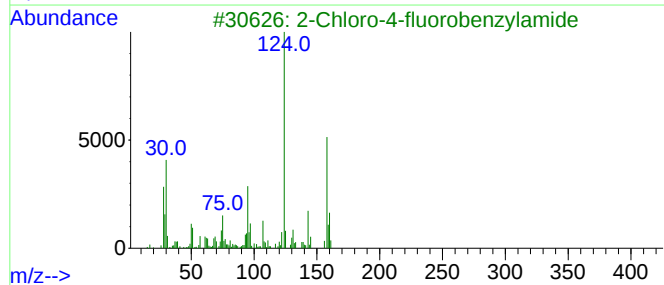
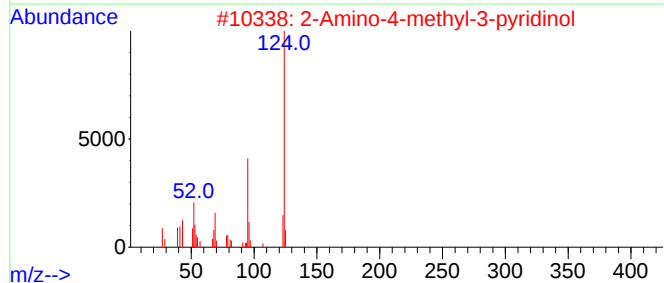
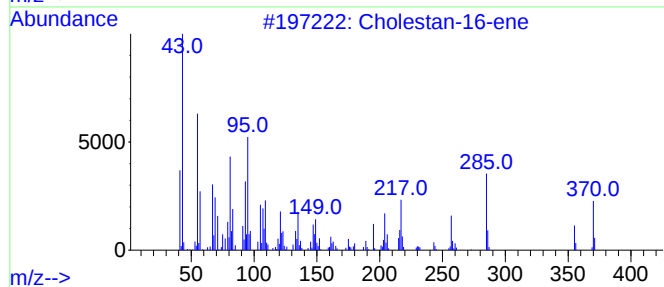
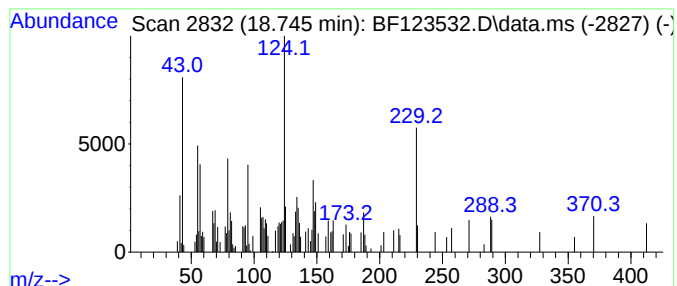
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 20 unknown18.745 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.745	7.10 ng	223557	Perylene-d12	15.563

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cholestan-16-ene	370	C27H46	1000252-60-8	44
2			2-Amino-4-methyl-3-pyridinol	124	C6H8N2O	020348-18-9	43
3			2-Chloro-4-fluorobenzylamide	159	C7H7ClFN	1000343-00-9	38
4			Pyrazine, 2-methoxy-6-methyl-	124	C6H8N2O	002882-21-5	38
5			cis-4-Octylcyclohexylmethyl nico...	331	C21H33NO2	104519-18-8	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF033021\
 Data File : BF123532.D
 Acq On : 30 Mar 2021 20:56
 Operator : JU/CG
 Sample : M1832-04
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 IG004

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.234	24.3	ng	980092	1	6.881	806623	20.0
Propane, 1,1-di...	2.340	4.3	ng	172518	1	6.881	806623	20.0
2-Pentanone, 4-...	5.128	14.5	ng	584059	1	6.881	806623	20.0
n-Hexadecanoic ...	11.951	12.7	ng	894316	4	11.422	1411680	20.0
Octacosyl trifl...	13.921	27.9	ng	1123540	5	14.063	805458	20.0
Nonadecane, 9-m...	14.539	7.8	ng	315502	5	14.063	805458	20.0
1-Heneicosanol	14.580	11.7	ng	469422	5	14.063	805458	20.0
unknown14.621	14.621	17.6	ng	710195	5	14.063	805458	20.0
Heptadecanal	15.004	4.7	ng	148467	6	15.563	629544	20.0
Tetracosane	15.210	12.5	ng	393164	6	15.563	629544	20.0
1-Docosene	15.268	12.4	ng	389234	6	15.563	629544	20.0
Octadecanal	15.810	6.9	ng	217094	6	15.563	629544	20.0
Octacosane	16.057	11.9	ng	373825	6	15.563	629544	20.0
Docosyl pentafl...	16.139	13.3	ng	418549	6	15.563	629544	20.0
Oxirane, hexade...	16.886	8.1	ng	256299	6	15.563	629544	20.0
Hentriacontane	17.204	4.7	ng	147585	6	15.563	629544	20.0
.beta.-Sitosterol	17.739	9.9	ng	311896	6	15.563	629544	20.0
6,10-Dimethyl-3...	18.280	18.3	ng	574907	6	15.563	629544	20.0
Hop-22(29)-en-3...	18.568	21.3	ng	671079	6	15.563	629544	20.0
unknown18.745	18.745	7.1	ng	223557	6	15.563	629544	20.0