

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021721\
 Data File : BF123214.D
 Acq On : 17 Feb 2021 16:09
 Operator : JU/CG
 Sample : M1422-01
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 BU-03-021621

Integration Parameters: rteint.p

Integrator: RTE

Smothing : 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-BF021221.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123214.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.087	501	510	518	rVB	52081	72507	1.69%	0.196%
2	5.487	573	578	581	rBV	3933655	3857116	89.96%	10.447%
3	6.498	744	750	762	rBV	3502629	3936738	91.81%	10.663%
4	6.698	781	784	789	rBV	35561	42994	1.00%	0.116%
5	6.869	809	813	816	rBV	1215789	943638	22.01%	2.556%
6	7.428	903	908	911	rBV	2858540	2587027	60.34%	7.007%
7	8.151	1027	1031	1034	rBV	1608796	1260044	29.39%	3.413%
8	9.228	1210	1214	1218	rBV	4485858	4287693	100.00%	11.613%
9	9.622	1277	1281	1284	rBV	451473	344110	8.03%	0.932%
10	9.839	1310	1318	1326	rBV2	47810	92849	2.17%	0.251%
11	9.910	1326	1330	1334	rVV	1924643	1620169	37.79%	4.388%
12	10.110	1359	1364	1371	rBV4	46699	71951	1.68%	0.195%
13	10.563	1437	1441	1448	rVB	31764	53260	1.24%	0.144%
14	10.704	1460	1465	1468	rBV	3291584	3167954	73.88%	8.580%
15	11.398	1579	1583	1586	rBV	1895479	1669772	38.94%	4.523%
16	11.422	1586	1587	1590	rVV	95847	63149	1.47%	0.171%
17	11.469	1590	1595	1599	rVB3	53834	71982	1.68%	0.195%
18	11.792	1647	1650	1653	rBV	47630	44833	1.05%	0.121%
19	11.933	1670	1674	1686	rBV	763838	992003	23.14%	2.687%
20	12.480	1764	1767	1769	rBV	62630	53495	1.25%	0.145%
21	12.580	1775	1784	1788	rBV5	81862	230121	5.37%	0.623%
22	12.616	1788	1790	1792	rVB	72297	55246	1.29%	0.150%
23	12.721	1805	1808	1821	rBV	345479	472253	11.01%	1.279%
24	12.845	1826	1829	1832	rVB	69666	53145	1.24%	0.144%
25	12.992	1850	1854	1857	rBV	4267194	4064481	94.79%	11.009%
26	13.751	1975	1983	1994	rBV	160750	430250	10.03%	1.165%
27	13.868	1994	2003	2004	rVV4	268435	530278	12.37%	1.436%
28	13.892	2004	2007	2023	rVB3	546660	1049888	24.49%	2.844%
29	14.051	2028	2034	2037	rBV	1353797	1243286	29.00%	3.367%
30	14.216	2059	2062	2064	rBV2	41213	46500	1.08%	0.126%
31	14.274	2065	2072	2081	rVV10	69023	245058	5.72%	0.664%
32	14.516	2107	2113	2126	rBV2	185016	399086	9.31%	1.081%
33	14.827	2164	2166	2171	rVB	53968	55392	1.29%	0.150%
34	15.151	2217	2221	2222	rBV	63104	84425	1.97%	0.229%
35	15.527	2280	2285	2288	rBV	797364	978494	22.82%	2.650%
36	15.580	2288	2294	2309	rVB5	335328	1132490	26.41%	3.067%

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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

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021221.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.998	2361	2365	2371	rVB	89063	125361	2.92%	0.340%
38	16.068	2372	2377	2390	rBV6	61904	188166	4.39%	0.510%
39	16.315	2414	2419	2429	rVB3	123957	303944	7.09%	0.823%

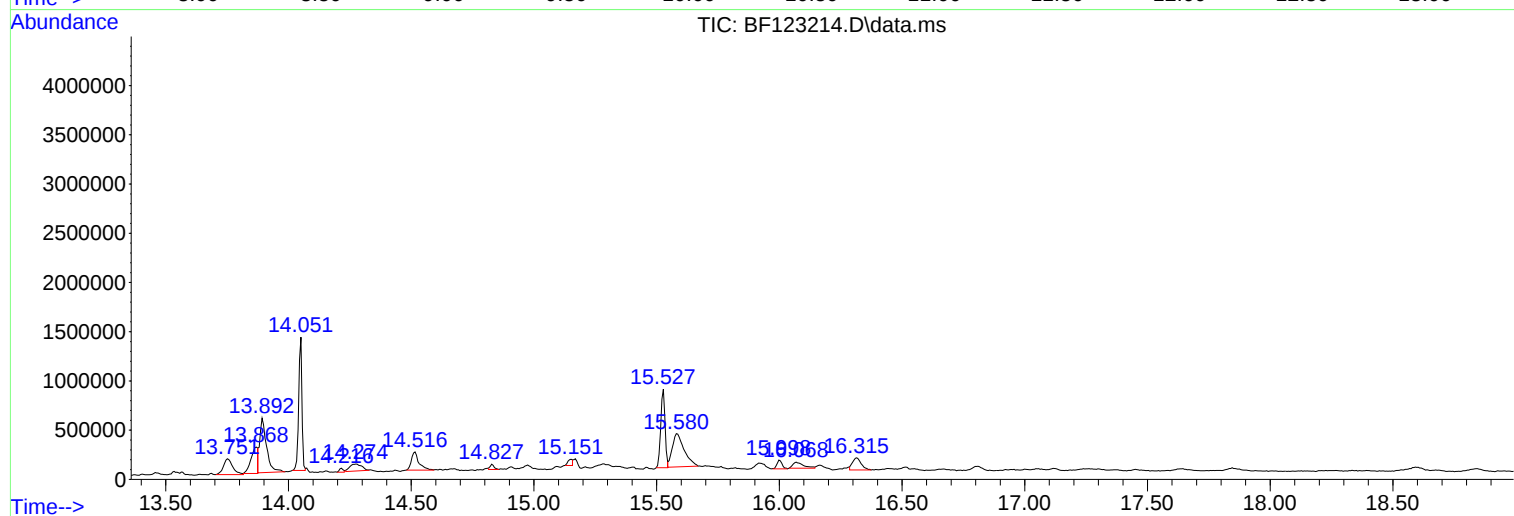
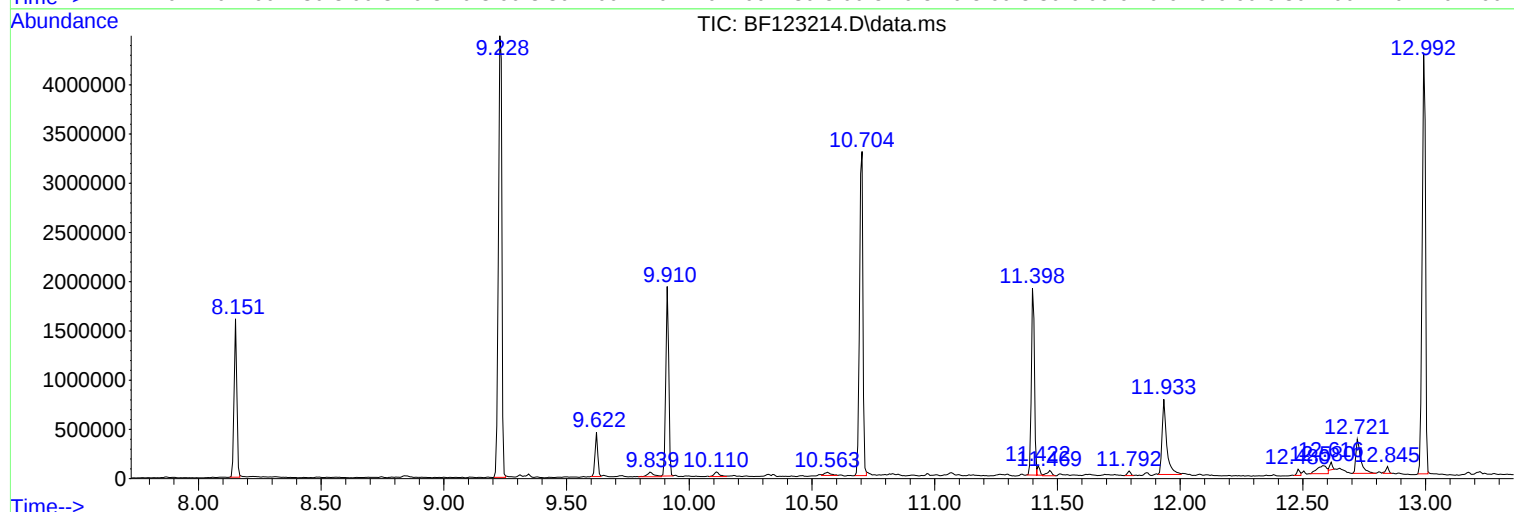
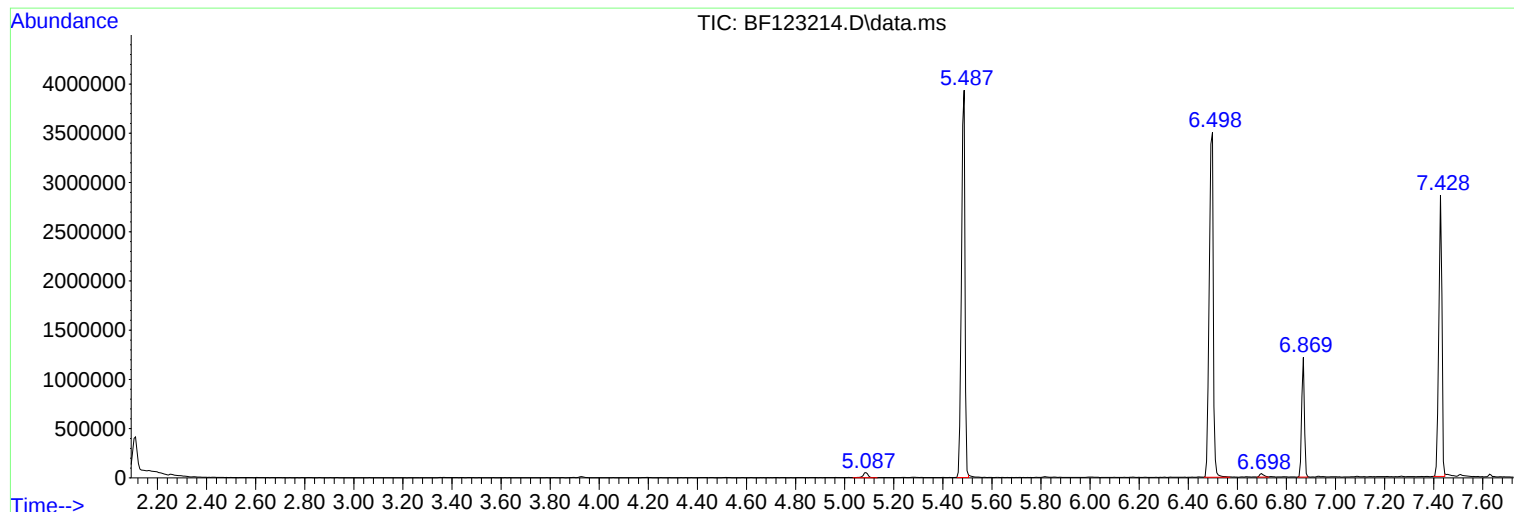
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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ClientSampleId :
BU-03-021621

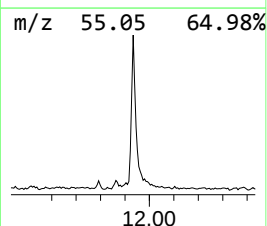
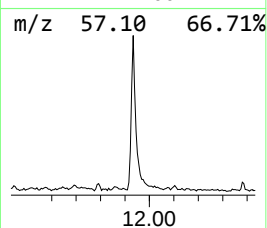
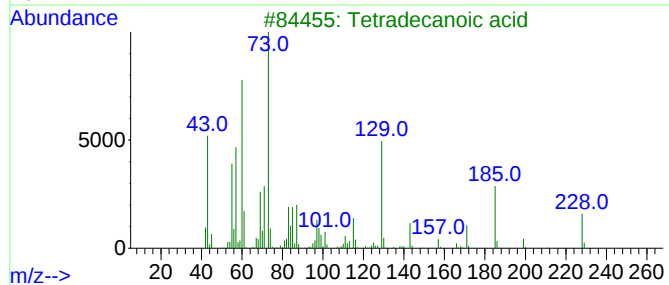
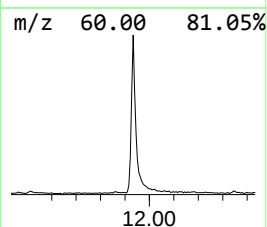
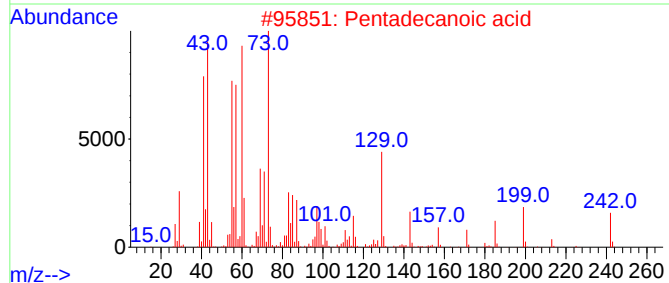
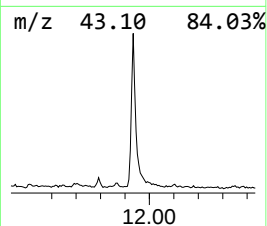
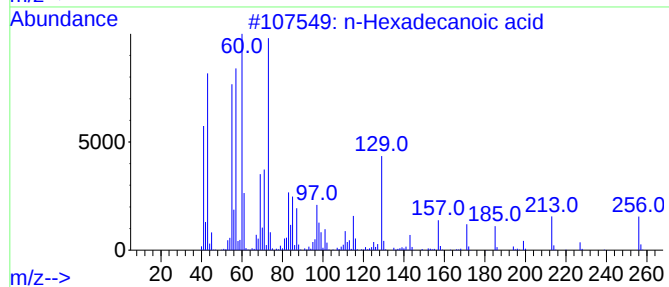
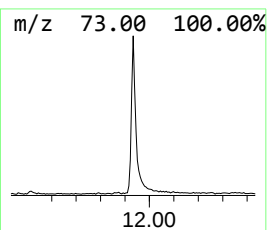
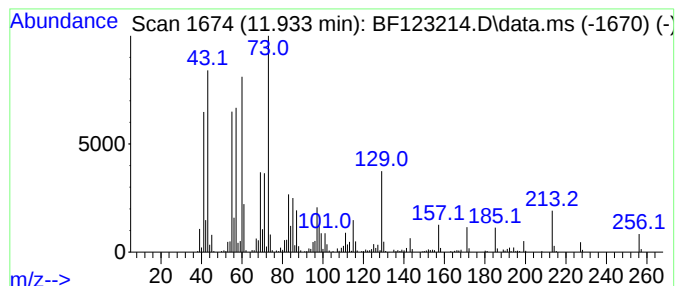
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	11.88 ng	992003	Phenanthrene-d10	11.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4			Tridecanoic acid	214	C13H26O2	000638-53-9	90
5			n-Decanoic acid	172	C10H20O2	000334-48-5	64



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Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
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ClientSampleId :
BU-03-021621

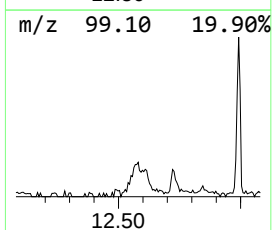
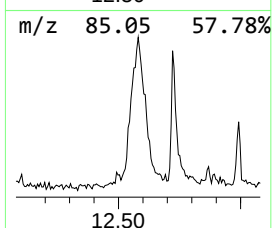
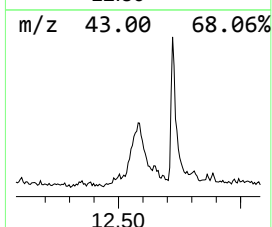
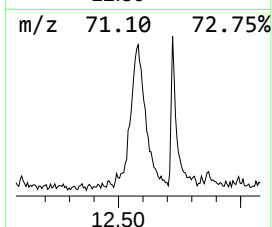
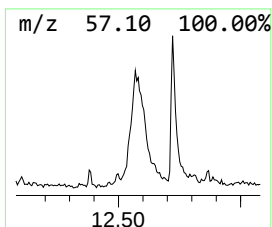
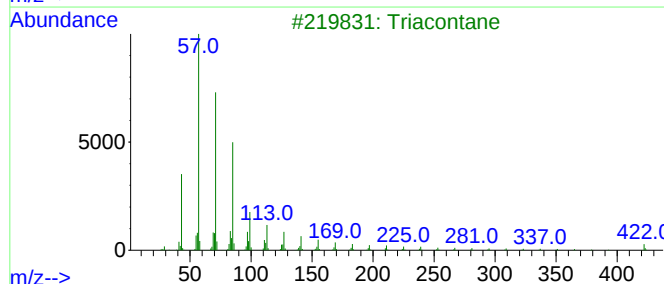
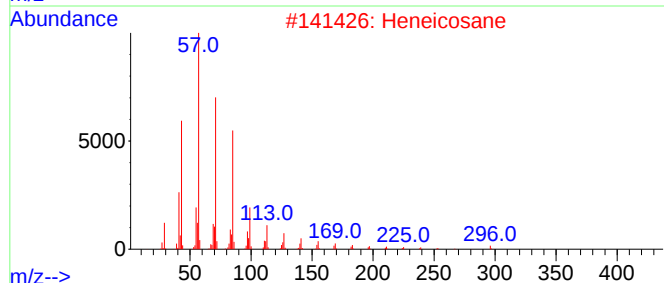
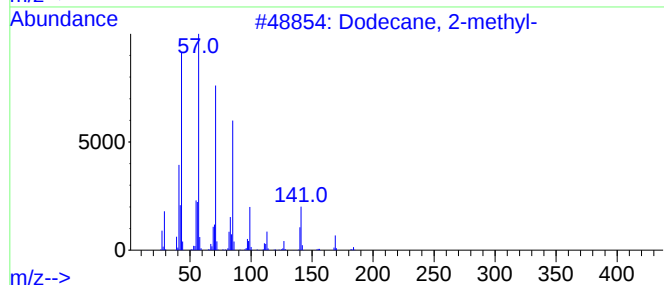
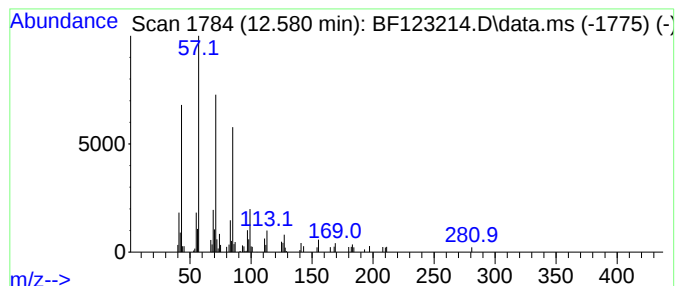
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.580	2.76 ng	230121	Phenanthrene-d10	11.398

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Dodecane, 2-methyl-	184	C13H28	001560-97-0	91
2		Heneicosane	296	C21H44	000629-94-7	90
3		Triacontane	422	C30H62	000638-68-6	87
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86
5		Hexacosane	366	C26H54	000630-01-3	83



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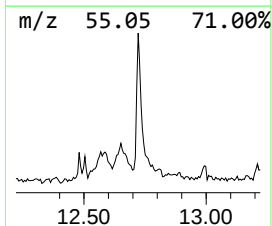
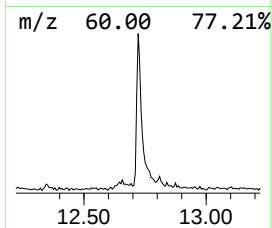
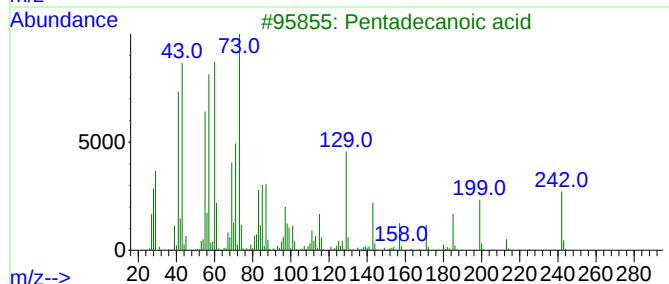
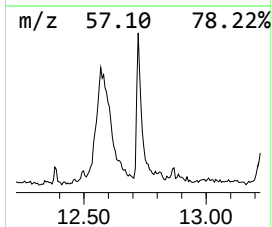
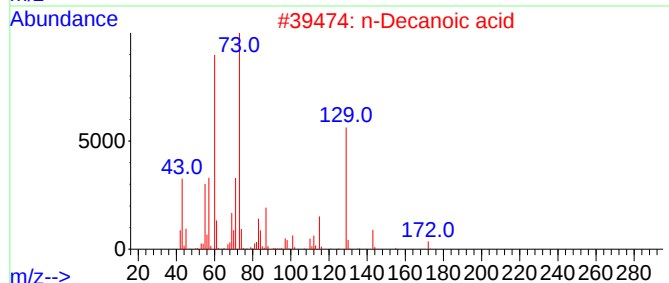
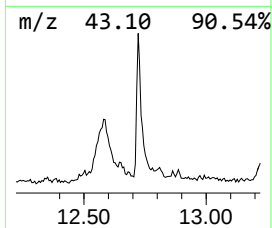
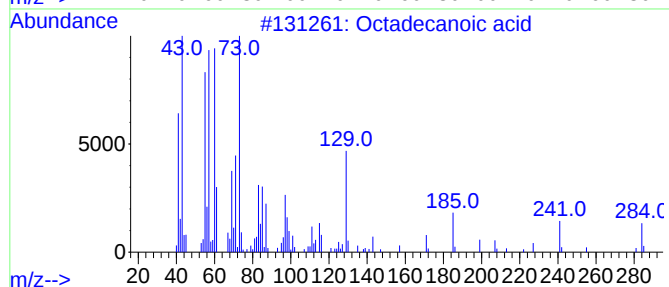
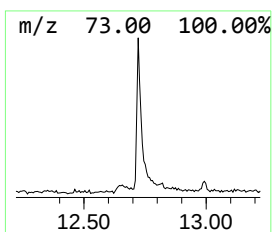
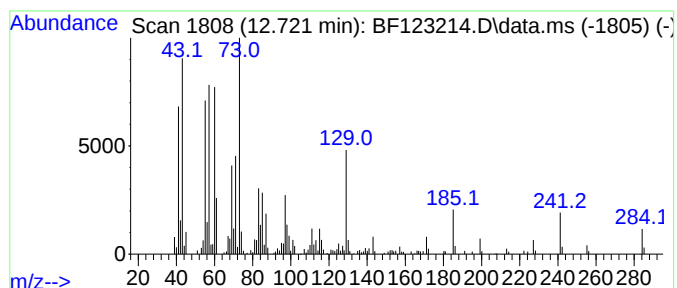
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.722	5.66 ng	472253	Phenanthrene-d10	11.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Decanoic acid	172	C10H20O2	000334-48-5	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	80
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	74



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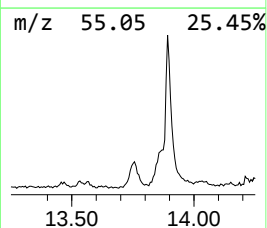
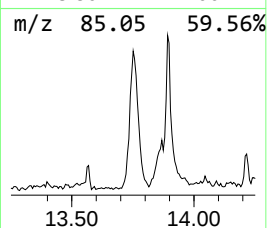
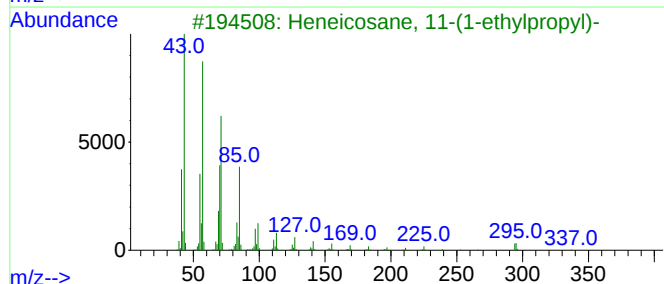
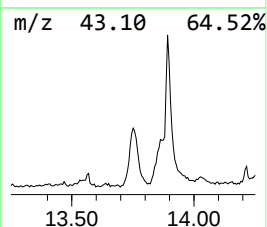
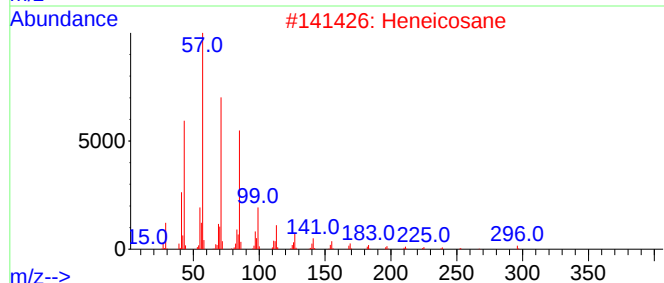
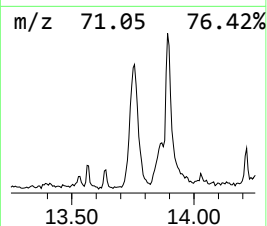
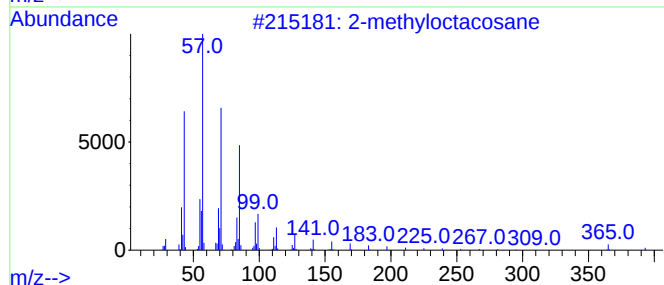
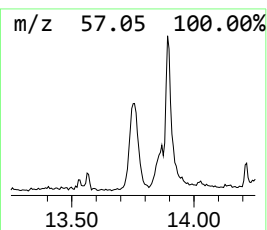
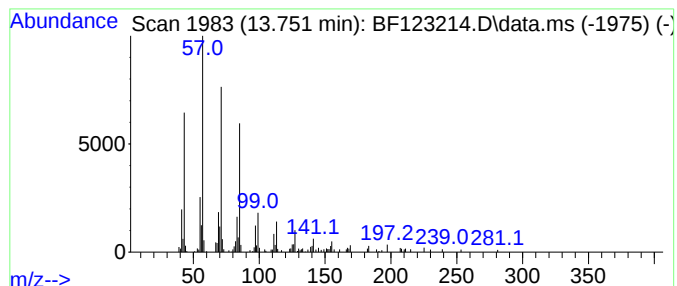
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-methyloctacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.751	6.92 ng	430250	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-methyloctacosane	408	C29H60	1000376-72-8	91
2			Heneicosane	296	C21H44	000629-94-7	91
3			Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5			Hexacosane	366	C26H54	000630-01-3	91



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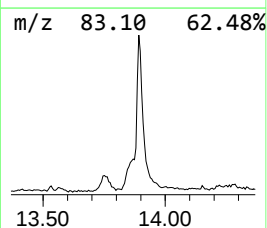
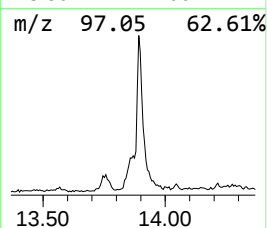
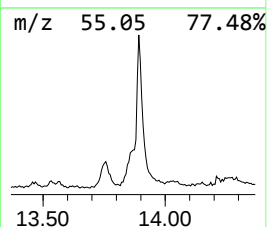
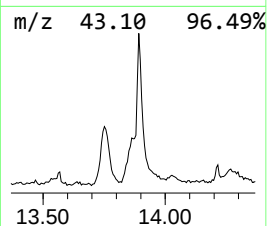
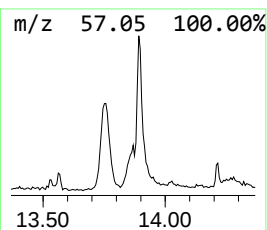
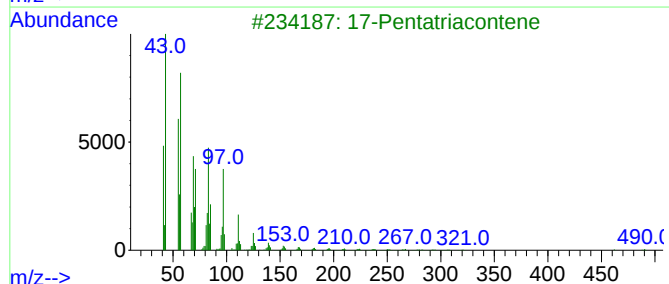
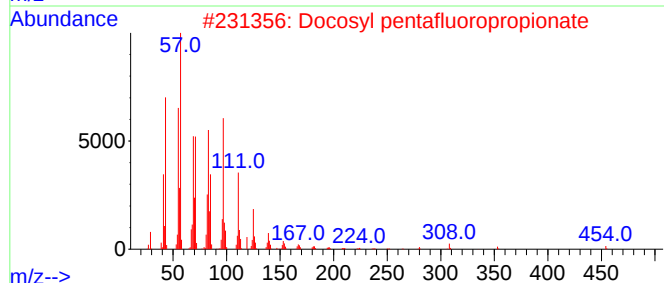
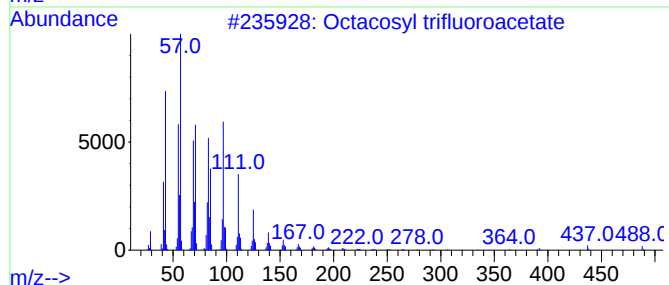
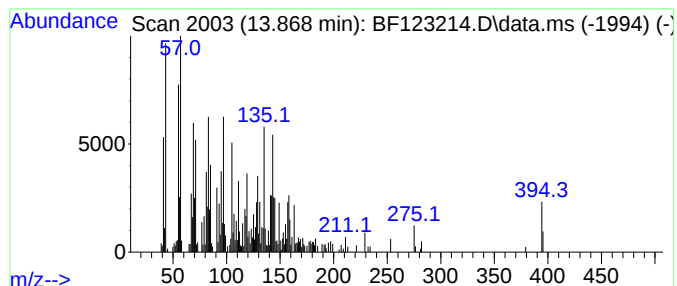
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown13.86 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.868	8.53 ng	530278	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	47
2			Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	35
3			17-Pentatriacontene	491	C35H70	006971-40-0	25
4			Heneicosyl trifluoroacetate	408	C23H43F3O2	1000351-76-5	25
5			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021721\
Data File : BF123214.D
Acq On : 17 Feb 2021 16:09
Operator : JU/CG
Sample : M1422-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BU-03-021621

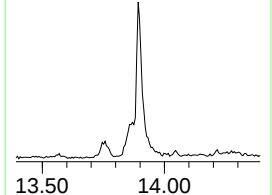
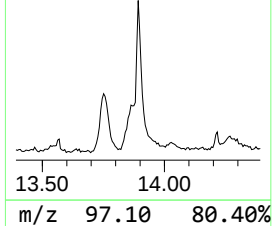
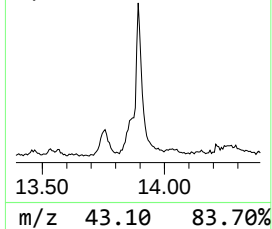
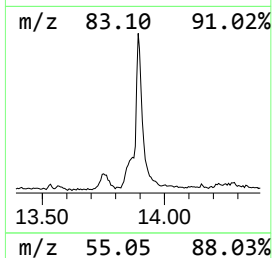
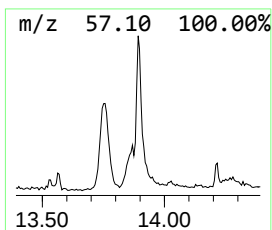
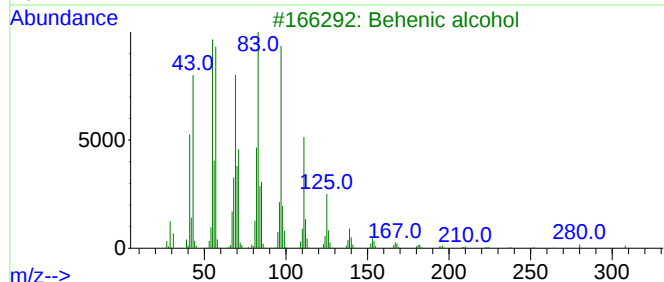
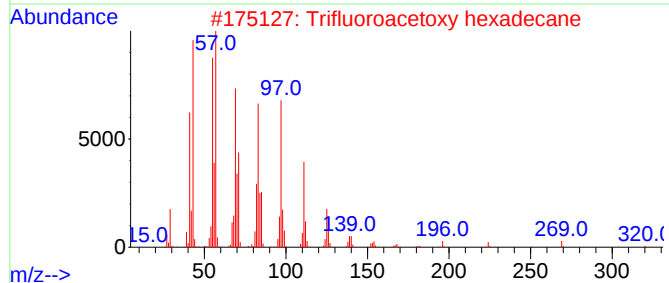
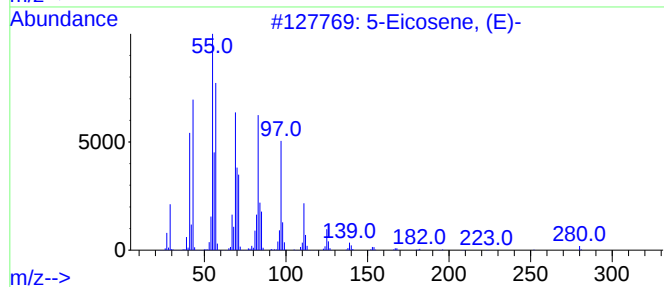
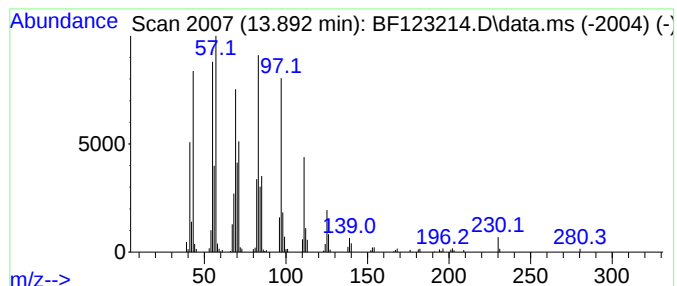
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 5-Eicosene, (E)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	16.89 ng	1049890	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Eicosene, (E)-	280	C20H40	074685-30-6	99
2			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
3			Behenic alcohol	326	C22H46O	000661-19-8	94
4			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
5			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021721\
Data File : BF123214.D
Acq On : 17 Feb 2021 16:09
Operator : JU/CG
Sample : M1422-01
Misc :
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ClientSampleId :
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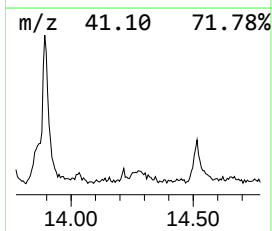
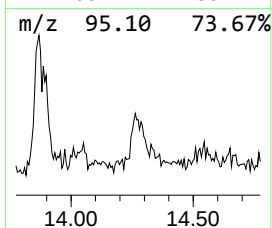
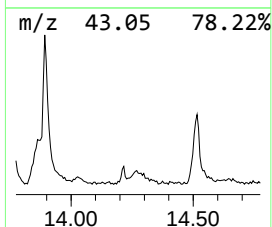
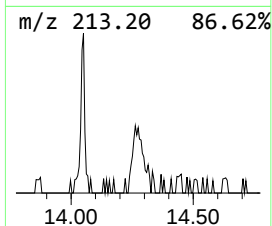
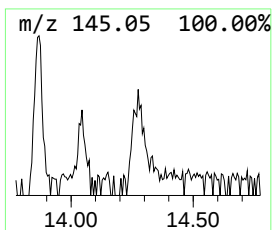
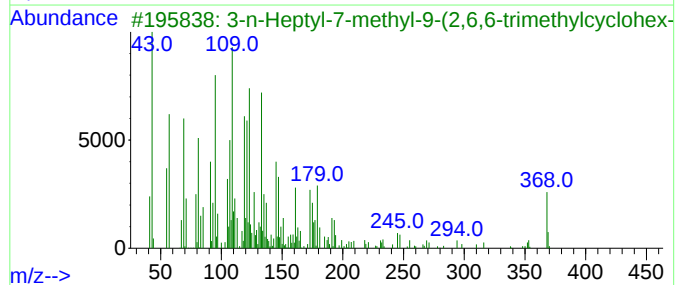
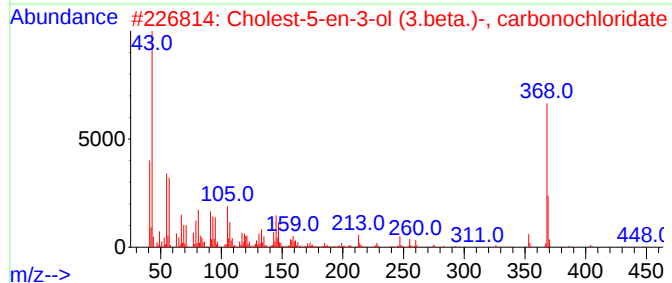
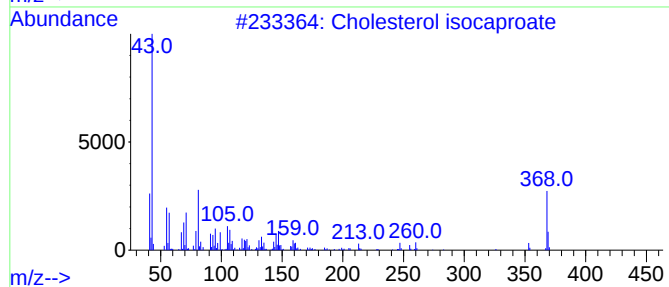
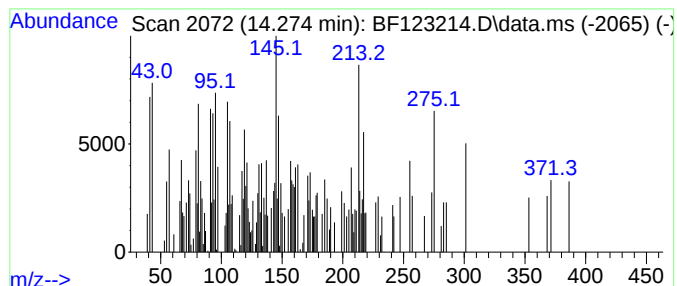
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown14.27 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.274	3.94 ng	245058	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cholesterol isocaproate	484	C33H56O2	1000252-03-0	25
2			Cholest-5-en-3-ol (3.beta.)-, ca...	448	C28H45ClO2	007144-08-3	22
3			3-n-Heptyl-7-methyl-9-(2,6,6-tri...	368	C26H40O	1000216-09-3	15
4			Cyclohexane, 1,5-diethenyl-2,3-d...	164	C12H20	074806-57-8	14
5			1H-Carbazole, 2,3,4,4a-tetrahydr...	275	C20H21N	055255-55-5	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021721\
Data File : BF123214.D
Acq On : 17 Feb 2021 16:09
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Misc :
ALS Vial : 4 Sample Multiplier: 1

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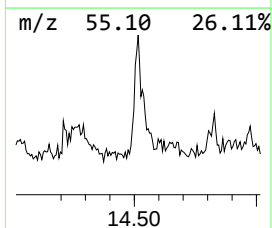
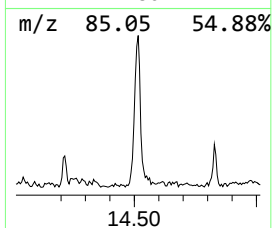
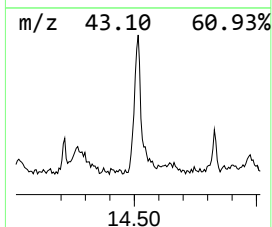
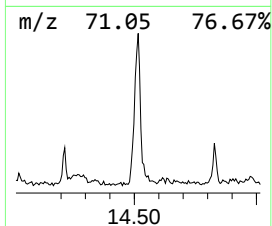
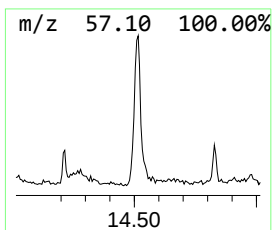
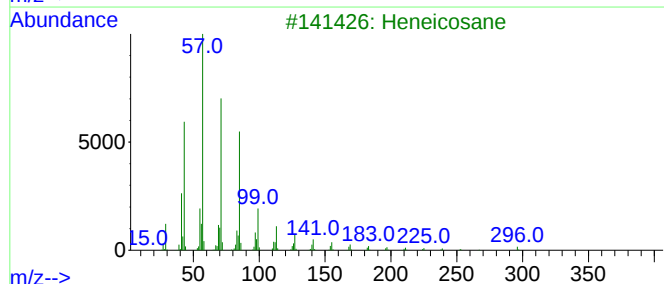
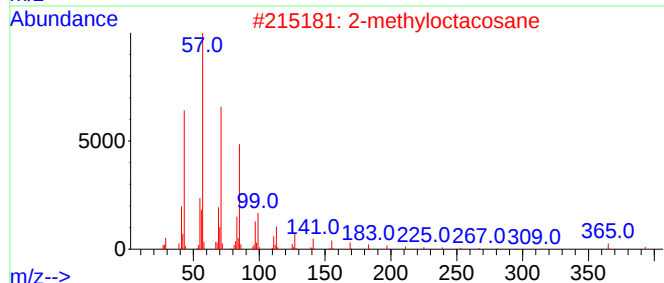
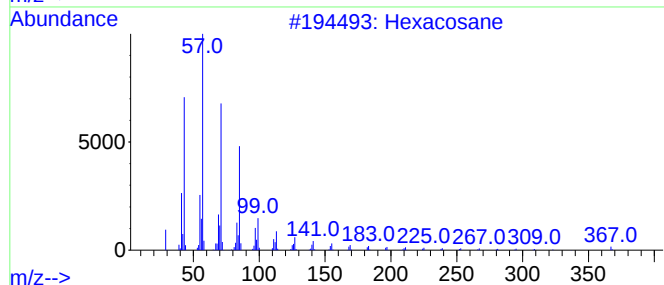
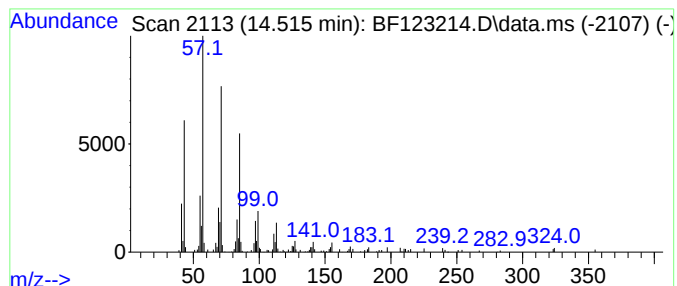
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.515	6.42 ng	399086	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	91
2			2-methyloctacosane	408	C29H60	1000376-72-8	91
3			Heneicosane	296	C21H44	000629-94-7	91
4			10-Methylnonadecane	282	C20H42	056862-62-5	90
5			Nonadecane	268	C19H40	000629-92-5	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021721\
Data File : BF123214.D
Acq On : 17 Feb 2021 16:09
Operator : JU/CG
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Misc :
ALS Vial : 4 Sample Multiplier: 1

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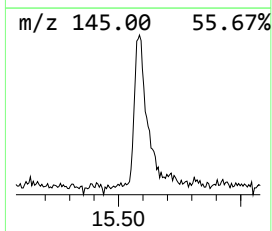
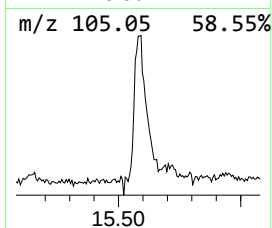
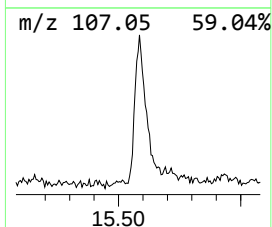
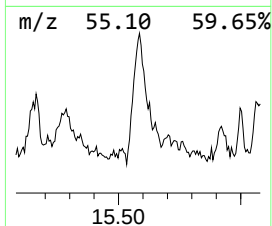
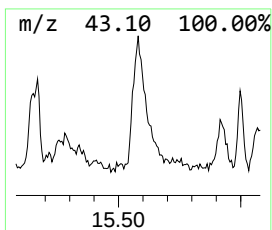
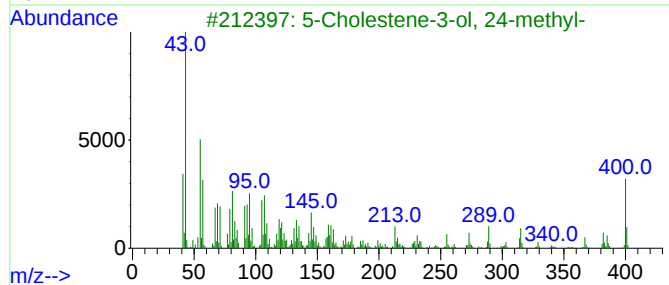
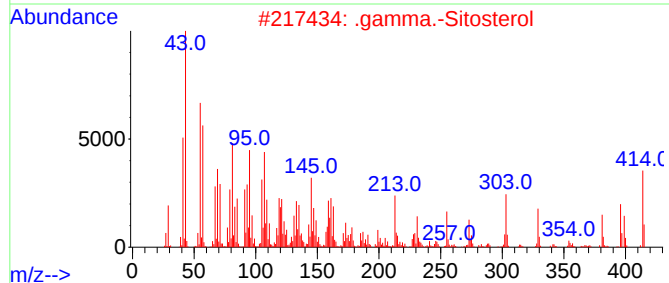
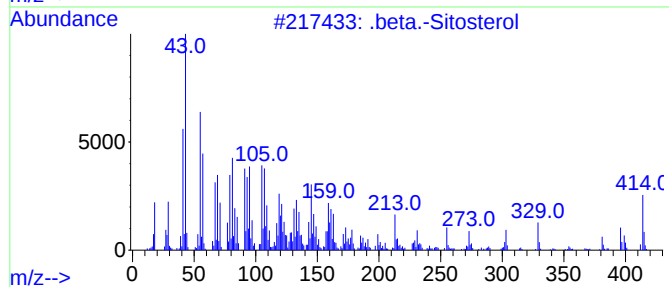
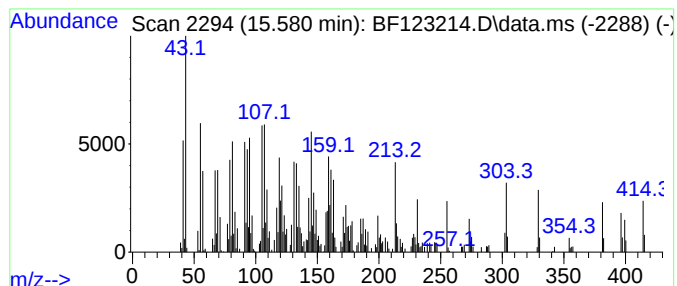
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 .beta.-Sitosterol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.580	23.15 ng	1132490	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			.beta.-Sitosterol	414	C29H50O	000083-46-5	99
2			.gamma.-Sitosterol	414	C29H50O	000083-47-6	93
3			5-Cholestene-3-ol, 24-methyl-	400	C28H48O	1000214-17-4	52
4			Isocholesteryl methyl ether	400	C28H48O	029944-53-4	38
5			Ergost-7-en-3-ol, (3.beta.)-	400	C28H48O	026047-31-4	16



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021721\
Data File : BF123214.D
Acq On : 17 Feb 2021 16:09
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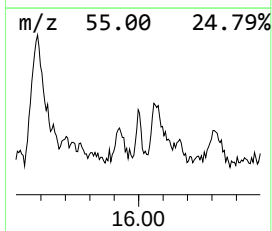
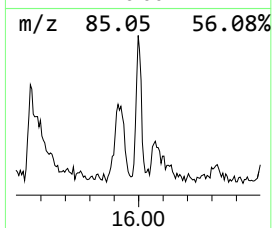
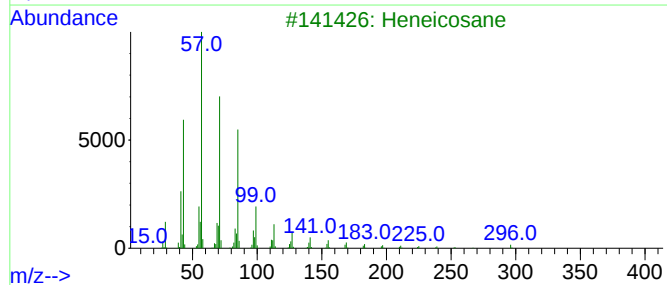
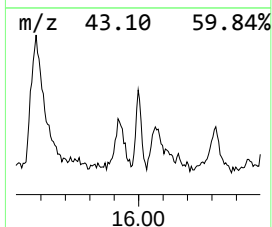
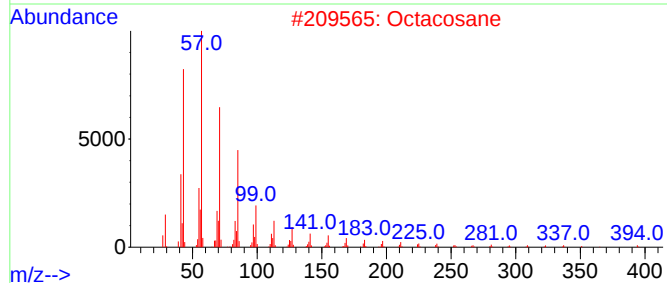
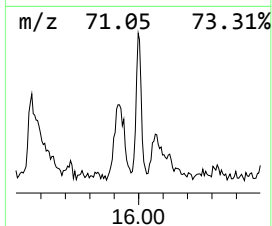
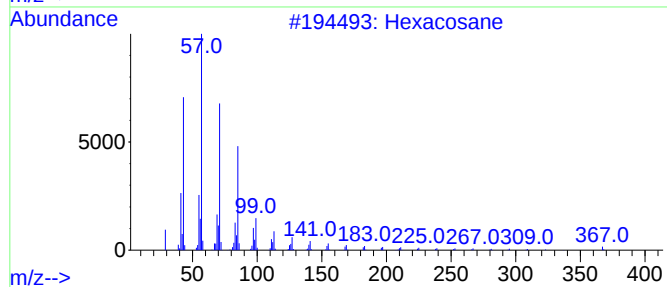
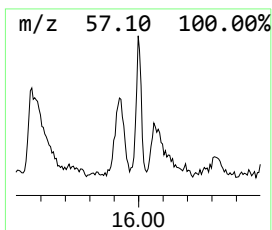
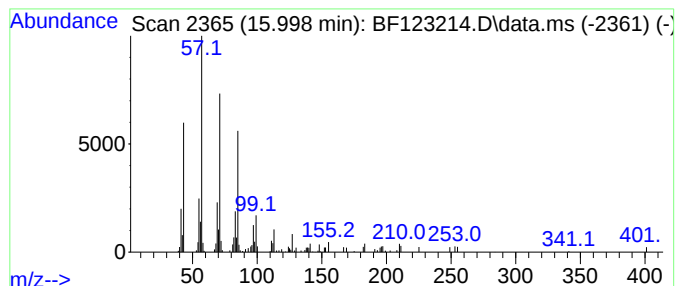
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octacosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.998	2.56 ng	125361	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	91
2			Octacosane	394	C28H58	000630-02-4	91
3			Heneicosane	296	C21H44	000629-94-7	87
4			Tetracosane	338	C24H50	000646-31-1	87
5			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021721\
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ClientSampleId :
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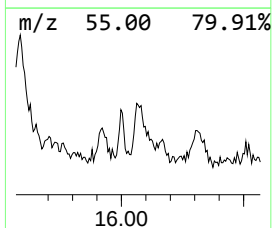
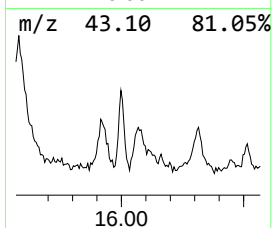
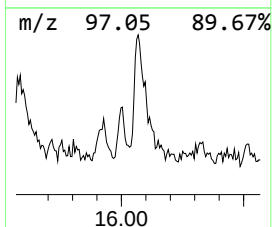
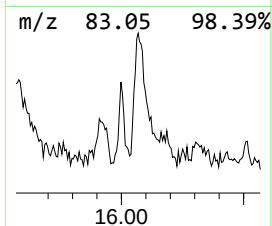
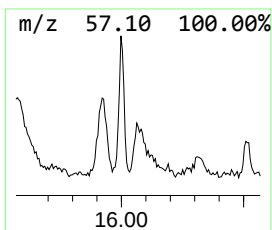
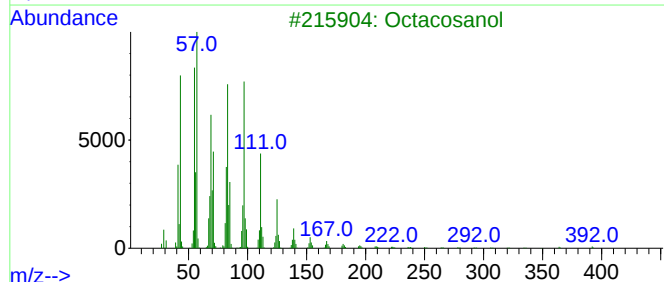
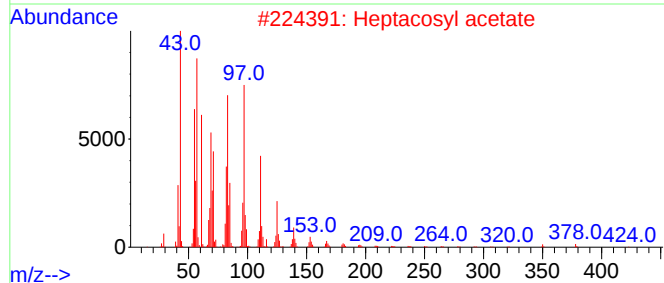
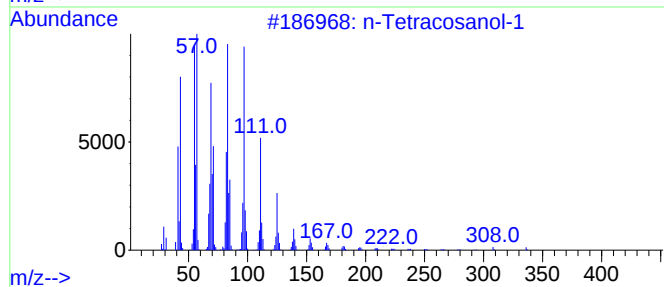
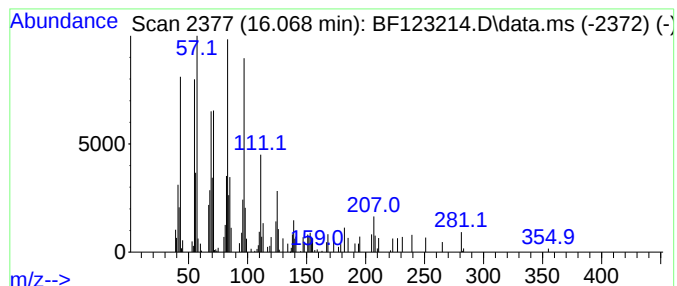
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 n-Tetracosanol-1 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.068	3.85 ng	188166	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
2			Heptacosyl acetate	438	C29H58O2	1000351-78-2	91
3			Octacosanol	410	C28H58O	000557-61-9	91
4			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
5			Carbonic acid, octadecyl 2,2,2-t...	444	C21H39Cl3O3	1000314-56-3	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021721\
Data File : BF123214.D
Acq On : 17 Feb 2021 16:09
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Misc :
ALS Vial : 4 Sample Multiplier: 1

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ClientSampleId :
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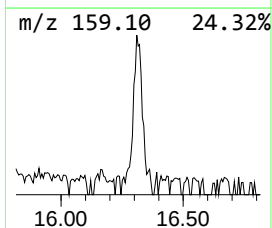
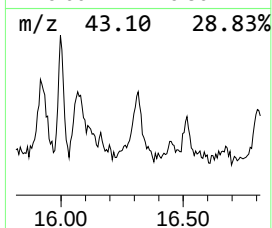
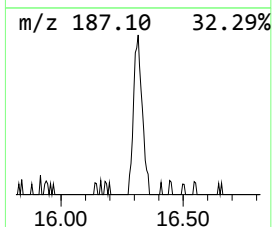
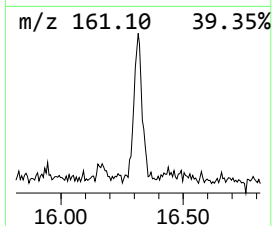
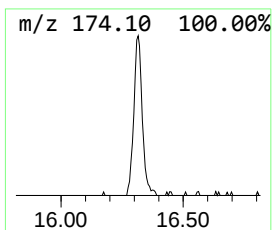
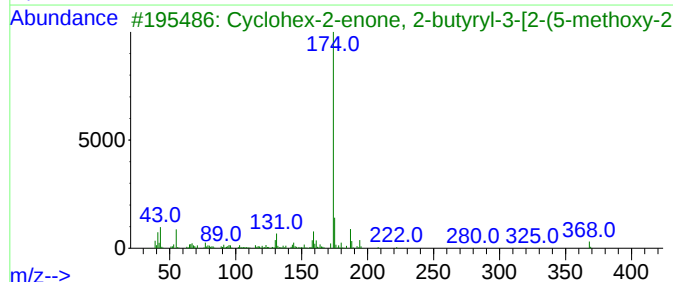
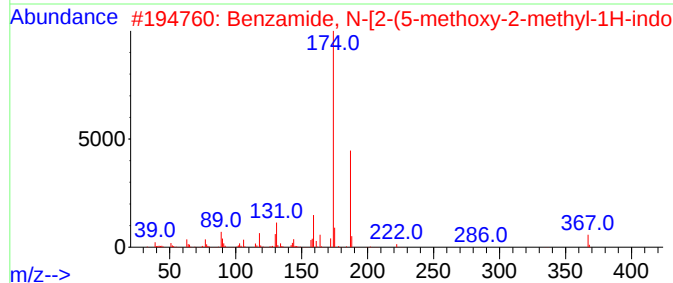
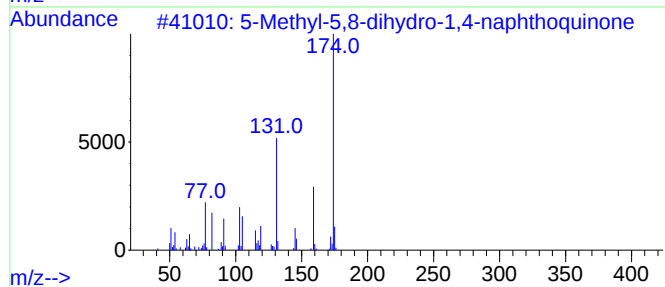
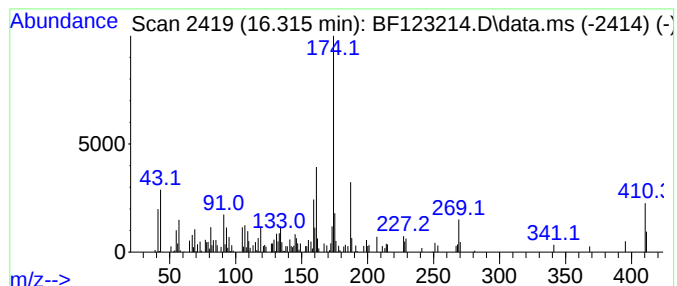
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown16.31 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.315	6.21 ng	303944	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Methyl-5,8-dihydro-1,4-naphtho...	174	C11H10O2	086759-40-2	38
2			Benzamide, N-[2-(5-methoxy-2-met...	367	C20H21N3O4	1000310-70-6	32
3			Cyclohex-2-enone, 2-butyryl-3-[2...	368	C22H28N2O3	1000302-14-0	27
4			2,2,4-Trimethyl-1,2-dihydro-quin...	189	C12H15NO	117330-56-0	27
5			2,8,9-Trioxa-5-aza-1-silabicyclo...	251	C12H17N3Si	002097-19-0	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021721\
 Data File : BF123214.D
 Acq On : 17 Feb 2021 16:09
 Operator : JU/CG
 Sample : M1422-01
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 BU-03-021621

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021221.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
n-Hexadecanoic ...	11.933	11.9	ng	992003	4	11.398	1669770	20.0
Dodecane, 2-met...	12.580	2.8	ng	230121	4	11.398	1669770	20.0
Octadecanoic acid	12.722	5.7	ng	472253	4	11.398	1669770	20.0
2-methyloctacosane	13.751	6.9	ng	430250	5	14.051	1243290	20.0
unknown13.86	13.868	8.5	ng	530278	5	14.051	1243290	20.0
5-Eicosene, (E)-	13.892	16.9	ng	1049890	5	14.051	1243290	20.0
unknown14.27	14.274	3.9	ng	245058	5	14.051	1243290	20.0
Hexacosane	14.515	6.4	ng	399086	5	14.051	1243290	20.0
.beta.-Sitosterol	15.580	23.1	ng	1132490	6	15.527	978494	20.0
Octacosane	15.998	2.6	ng	125361	6	15.527	978494	20.0
n-Tetracosanol-1	16.068	3.9	ng	188166	6	15.527	978494	20.0
unknown16.31	16.315	6.2	ng	303944	6	15.527	978494	20.0