

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042021\
 Data File : BF123653.D
 Acq On : 20 Apr 2021 20:49
 Operator : JU/CG
 Sample : M2076-10
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-16-0-2.0

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-BF041521.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123653.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.063	498	506	512	rBV	82516	110795	1.49%	0.195%
2	5.469	571	575	579	rBV	6374474	5827696	78.26%	10.252%
3	6.486	743	748	760	rVB	6067093	6027665	80.94%	10.604%
4	6.845	806	809	813	rBV	1746671	1506126	20.23%	2.650%
5	7.410	900	905	908	rBV	4507819	3934742	52.84%	6.922%
6	8.133	1024	1028	1031	rBV	2523781	1973170	26.50%	3.471%
7	9.210	1207	1211	1214	rBV	6734735	5902379	79.26%	10.383%
8	9.604	1275	1278	1282	rBV	229502	178550	2.40%	0.314%
9	9.892	1323	1327	1330	rBV	2624550	2091636	28.09%	3.680%
10	10.092	1357	1361	1367	rVB2	74966	75333	1.01%	0.133%
11	10.680	1457	1461	1464	rBV	4915912	4100692	55.07%	7.214%
12	11.380	1576	1580	1582	rBV	2663206	2173690	29.19%	3.824%
13	11.404	1582	1584	1586	rVV	162047	130409	1.75%	0.229%
14	11.451	1586	1592	1596	rVB6	44316	82870	1.11%	0.146%
15	11.916	1667	1671	1675	rBV	1441193	1374356	18.46%	2.418%
16	12.592	1780	1786	1789	rBV	286136	278035	3.73%	0.489%
17	12.704	1801	1805	1811	rBV	634625	634694	8.52%	1.117%
18	12.821	1818	1825	1827	rBV	234280	236281	3.17%	0.416%
19	12.851	1827	1830	1838	rVB3	116446	209272	2.81%	0.368%
20	12.974	1846	1851	1854	rBV	5532840	5247351	70.46%	9.231%
21	13.204	1887	1890	1895	rBV4	75054	110868	1.49%	0.195%
22	13.568	1928	1952	1966	rBV3	1313454	7446825	100.00%	13.100%
23	13.880	2001	2005	2022	rBV	528844	1133394	15.22%	1.994%
24	14.027	2024	2030	2032	rVV	1605751	1647667	22.13%	2.899%
25	14.051	2032	2034	2036	rVB	92149	79475	1.07%	0.140%
26	14.192	2056	2058	2061	rBV	77385	84253	1.13%	0.148%
27	14.498	2108	2110	2112	rBV	117352	109623	1.47%	0.193%
28	14.527	2112	2115	2125	rVB5	151990	346585	4.65%	0.610%
29	14.809	2161	2163	2166	rVB	106856	104504	1.40%	0.184%
30	14.956	2185	2188	2195	rVB3	138921	161569	2.17%	0.284%
31	15.068	2204	2207	2215	rVB	88411	183698	2.47%	0.323%
32	15.156	2218	2222	2225	rBV	252882	270976	3.64%	0.477%
33	15.504	2276	2281	2285	rBV2	1152009	1406273	18.88%	2.474%
34	15.539	2285	2287	2292	rVB2	176512	197955	2.66%	0.348%
35	15.662	2302	2308	2319	rVB8	245895	775894	10.42%	1.365%
36	15.986	2359	2363	2367	rBV	212497	287797	3.86%	0.506%

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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

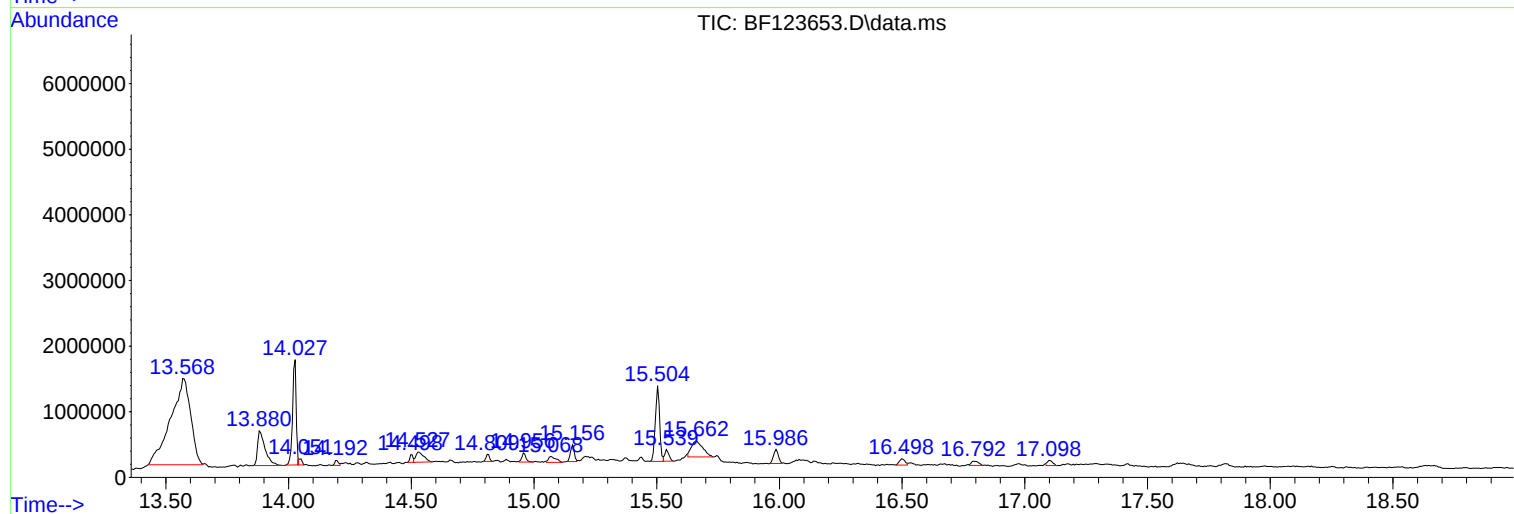
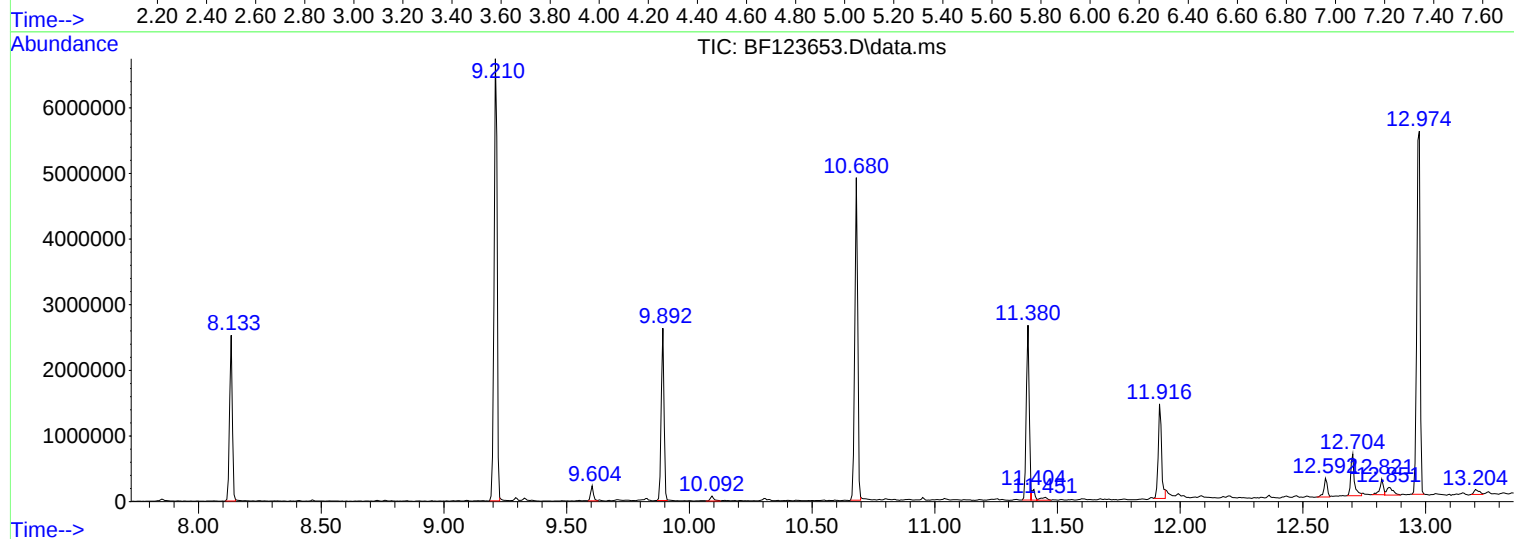
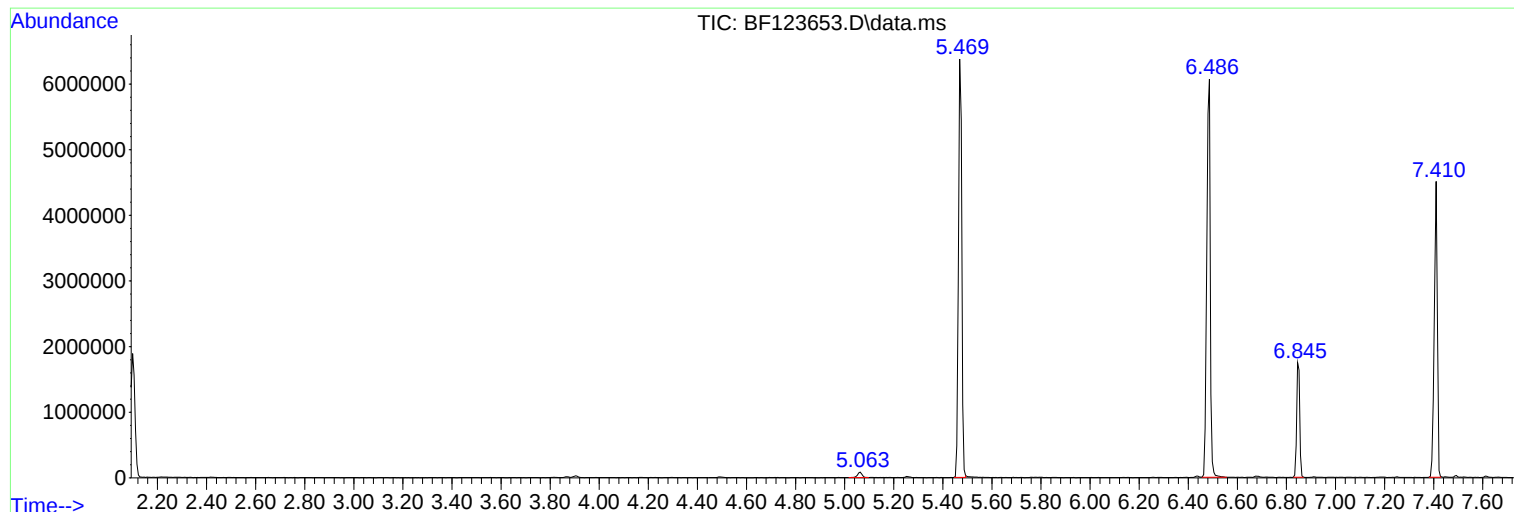
If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	16.498	2446	2450	2454	rBV2	98271	159182	2.14%	0.280%
38	16.792	2497	2500	2506	rVB5	62229	128777	1.73%	0.227%
39	17.098	2550	2552	2558	rVB3	77232	113897	1.53%	0.200%

Sum of corrected areas: 56844954

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



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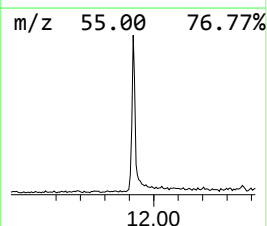
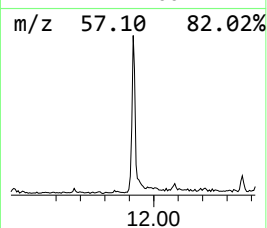
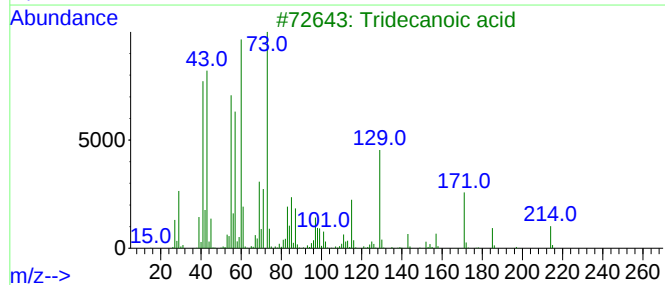
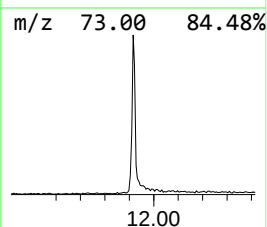
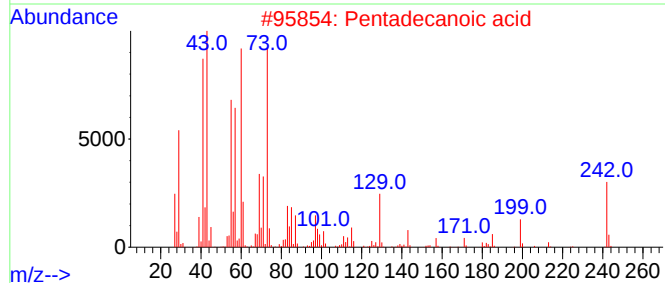
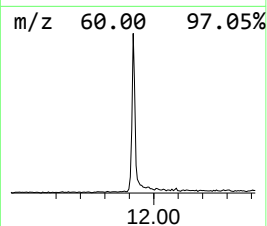
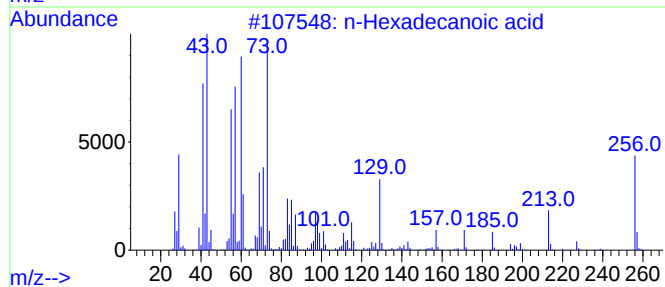
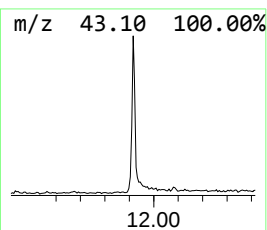
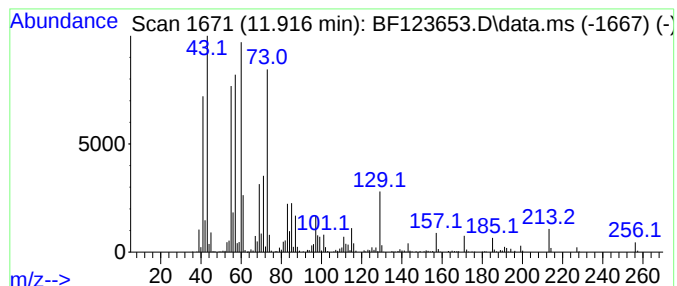
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
11.916	12.65 ng	1374360	Phenanthrene-d10	11.380

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3			Tridecanoic acid	214	C13H26O2	000638-53-9	81
4			Dodecanoic acid	200	C12H24O2	000143-07-7	76
5			n-Decanoic acid	172	C10H20O2	000334-48-5	64



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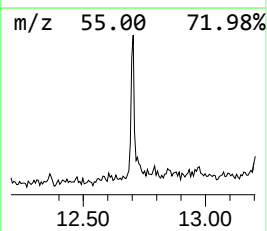
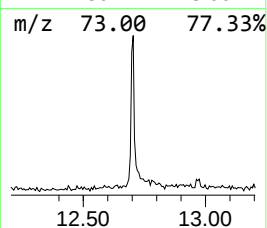
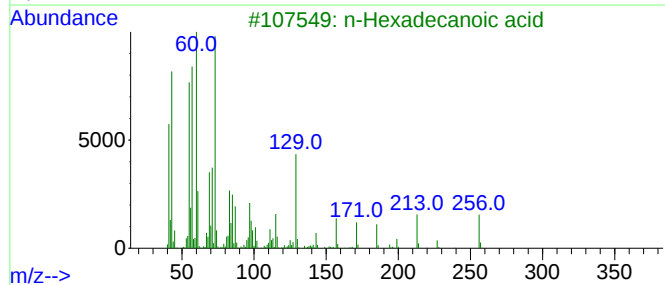
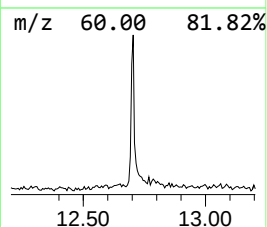
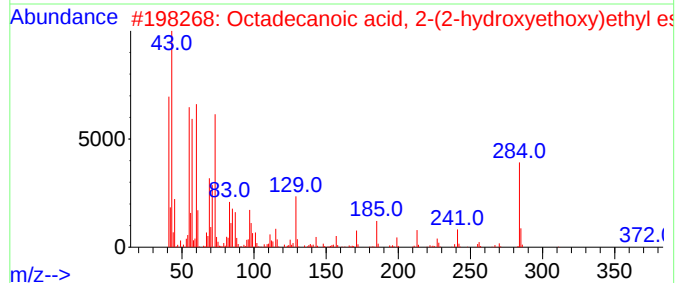
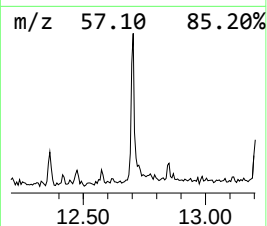
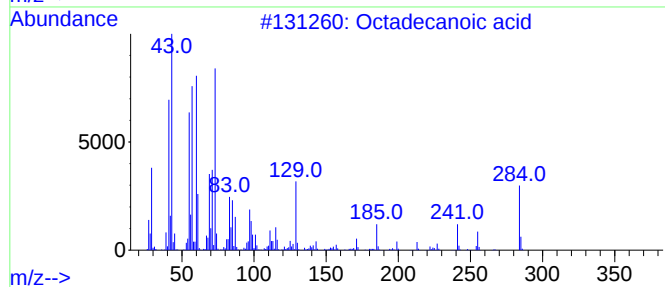
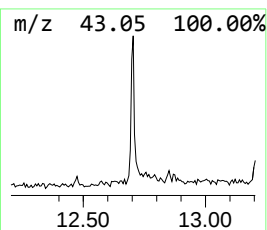
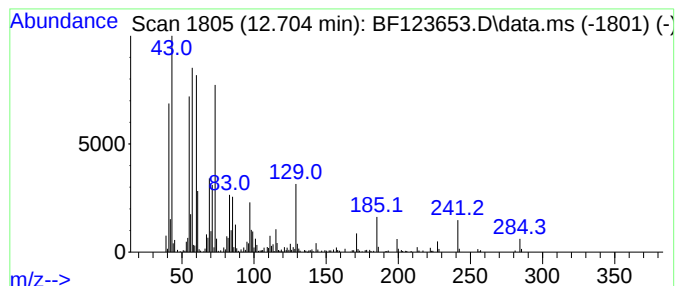
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.704	7.70 ng	634694	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	98
2			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	64
5			n-Decanoic acid	172	C10H20O2	000334-48-5	53



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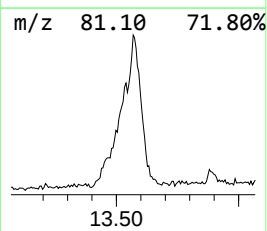
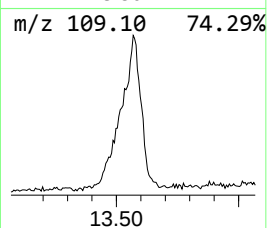
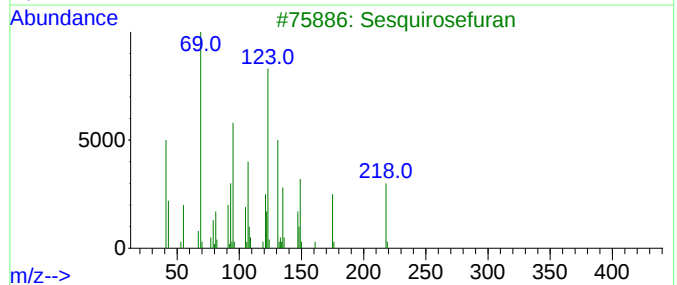
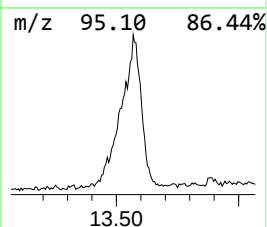
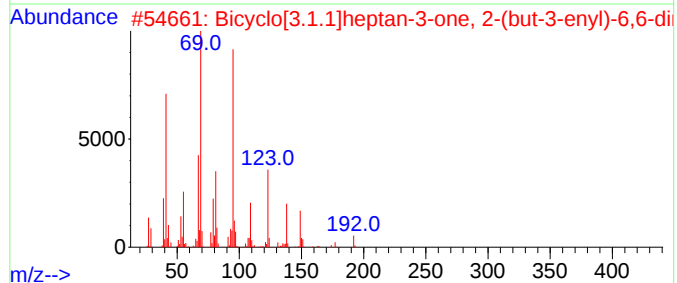
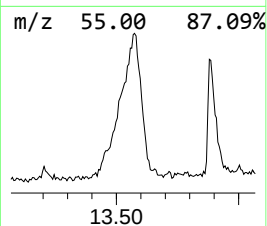
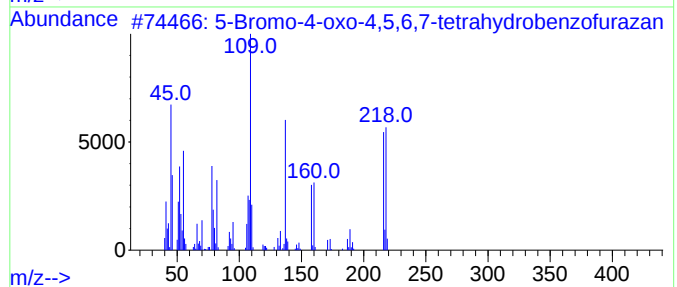
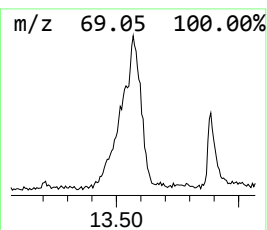
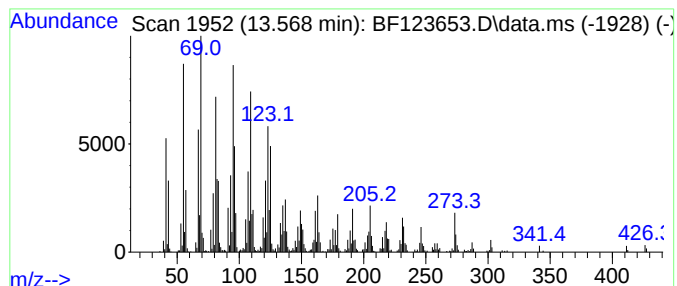
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 5-Bromo-4-oxo-4,5,6,7-tetra... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.568	90.39 ng	7446830	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Bromo-4-oxo-4,5,6,7-tetrahydro...	216	C6H5BrN2O2	300574-36-1	59
2			Bicyclo[3.1.1]heptan-3-one, 2-(b...	192	C13H20O	1000163-96-1	43
3			Sesquirosefuran	218	C15H22O	039007-93-7	42
4			Friedelan-3-one	426	C30H50O	000559-74-0	42
5			1,1,6-trimethyl-3-methylene-2-(3...	452	C33H56	1000373-94-5	30



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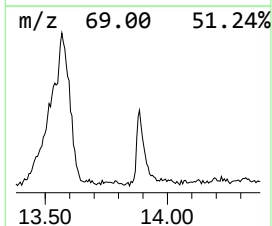
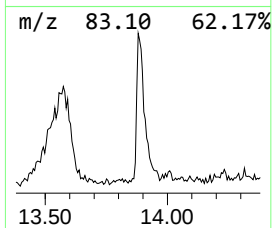
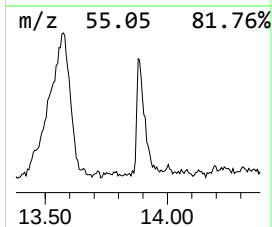
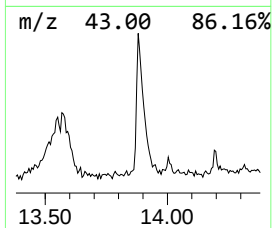
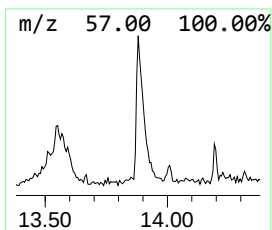
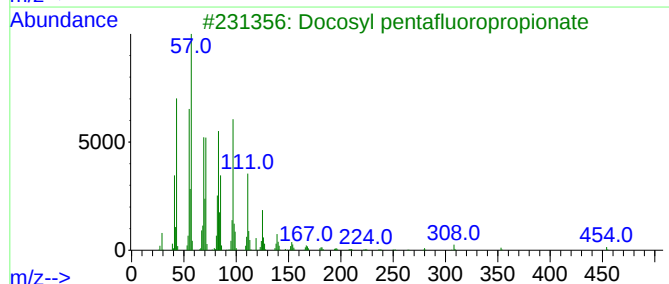
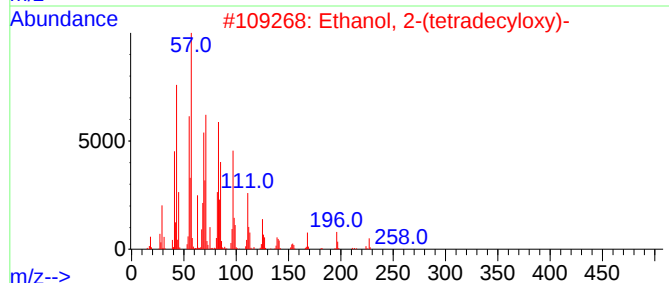
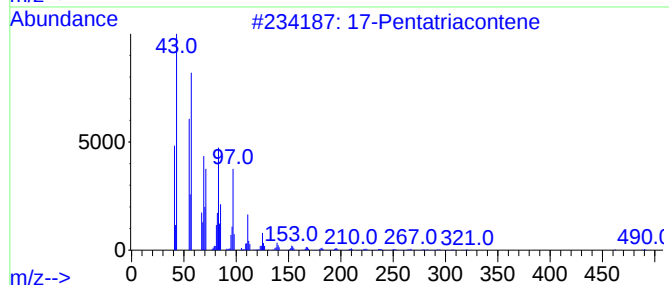
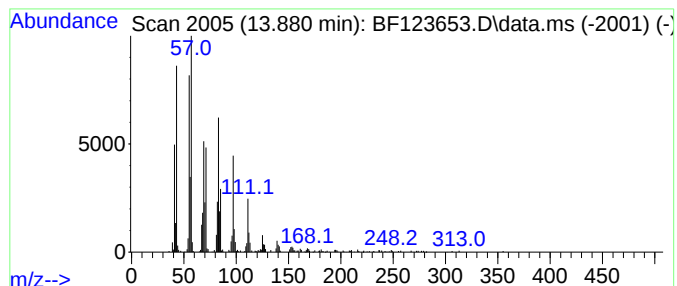
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 17-Pentatriacontene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	13.76 ng	1133390	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			17-Pentatriacontene	491	C35H70	006971-40-0	91
2			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
3			Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	91
4			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91
5			Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	91



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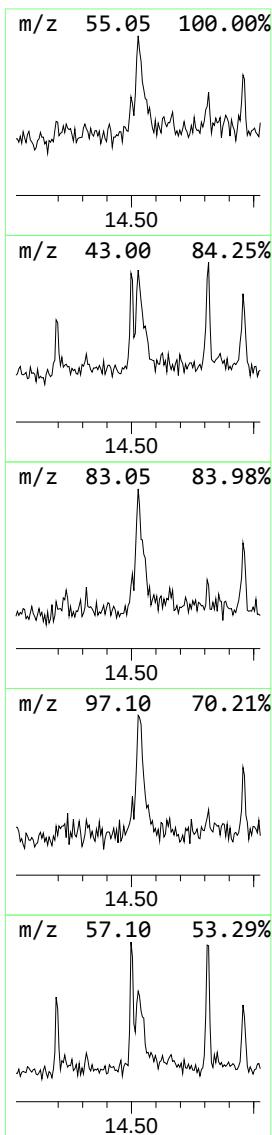
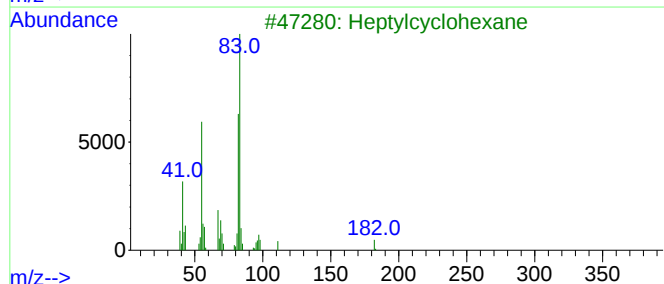
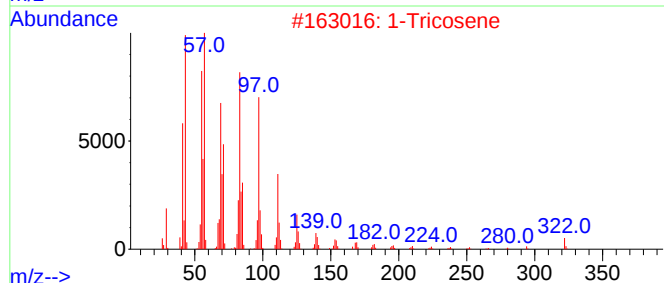
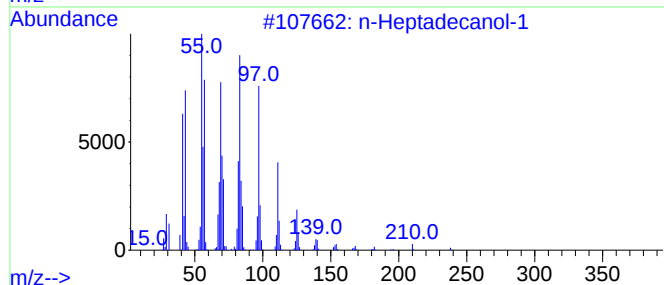
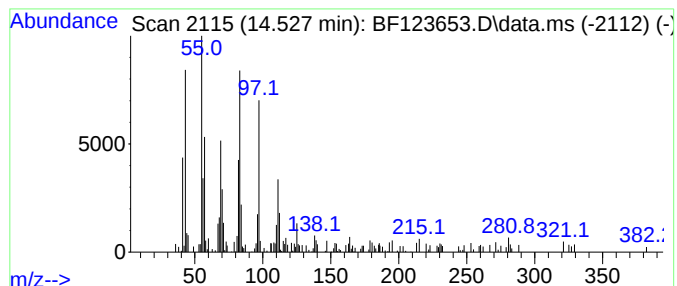
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 n-Heptadecanol-1 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.527	4.21 ng	346585	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Heptadecanol-1	256	C17H36O	001454-85-9	72
2			1-Tricosene	322	C23H46	018835-32-0	59
3			Heptylcyclohexane	182	C13H26	005617-41-4	46
4			Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	46
5			3-Hexene, 2,2-dimethyl-, (E)-	112	C8H16	000690-93-7	46



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Sample : M2076-10
Misc :
ALS Vial : 17 Sample Multiplier: 1

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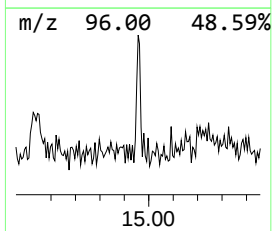
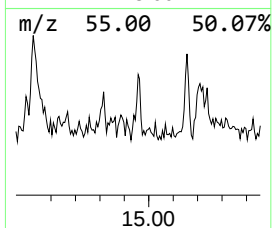
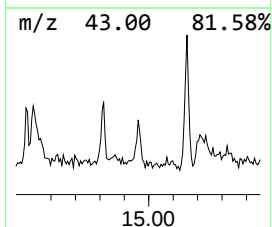
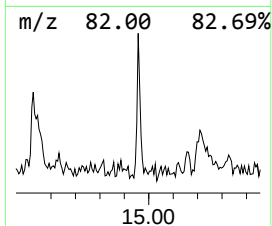
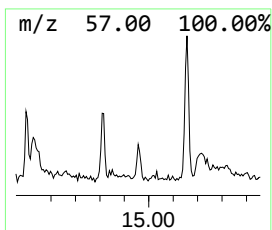
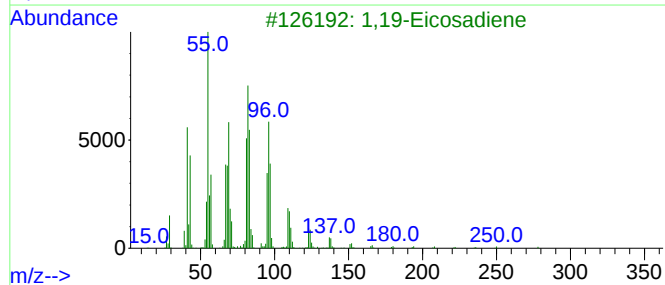
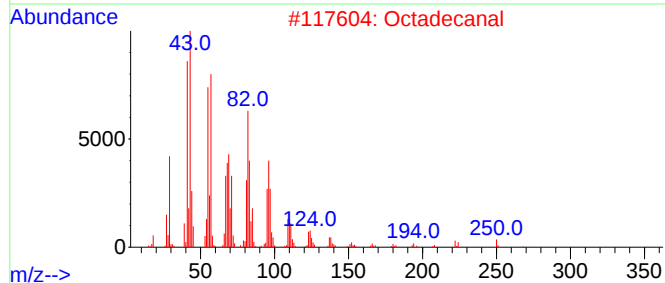
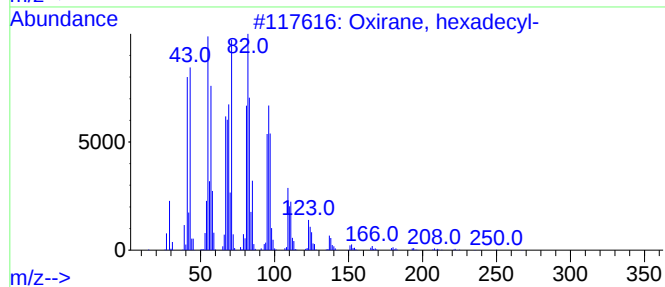
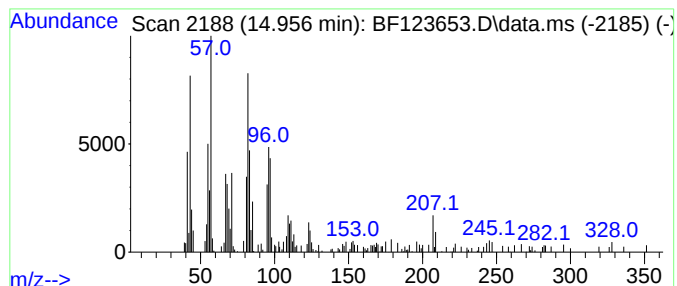
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Oxirane, hexadecyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.957	2.30 ng	161569	Perylene-d12	15.504

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	86
2			Octadecanal	268	C18H36O	000638-66-4	83
3			1,19-Eicosadiene	278	C20H38	014811-95-1	83
4			Tetradecanal	212	C14H28O	000124-25-4	80
5			Oxirane, heptadecyl-	282	C19H38O	067860-04-2	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042021\
Data File : BF123653.D
Acq On : 20 Apr 2021 20:49
Operator : JU/CG
Sample : M2076-10
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-16-0-2.0

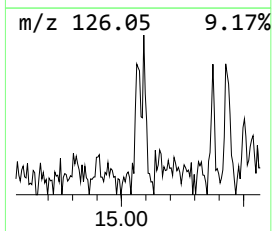
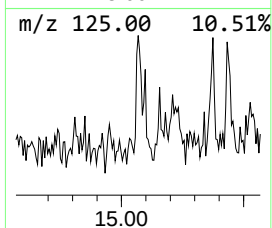
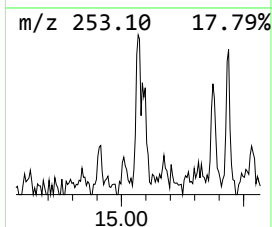
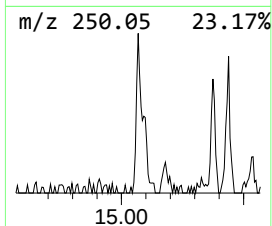
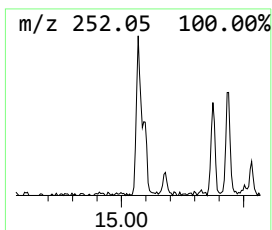
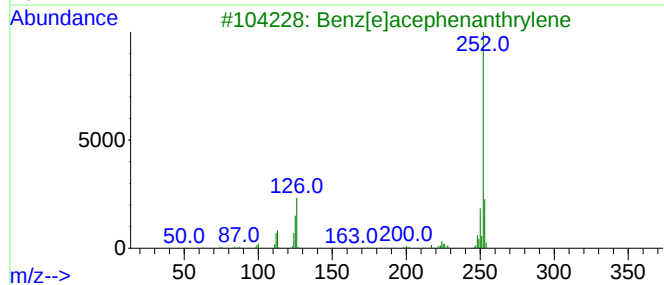
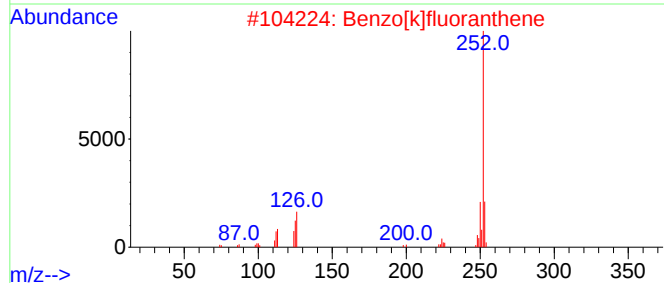
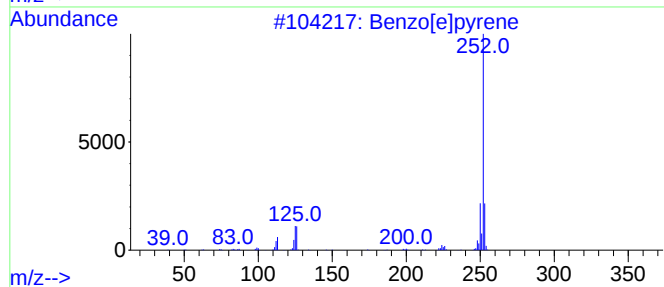
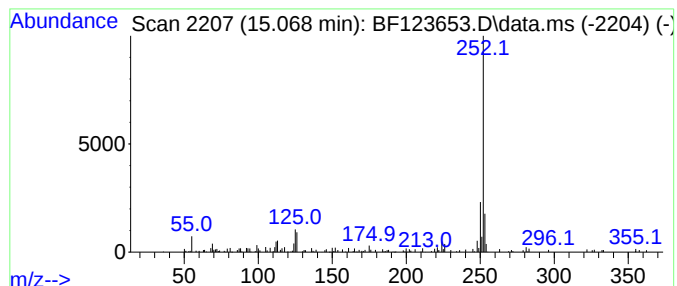
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzo[e]pyrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.068	2.61 ng	183698	Perylene-d12	15.504

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	90
2			Benzo[k]fluoranthene	252	C20H12	000207-08-9	90
3			Benz[e]acephenanthrylene	252	C20H12	000205-99-2	81
4			Benzo[a]pyrene	252	C20H12	000050-32-8	81
5			Benzo[j]fluoranthene	252	C20H12	000205-82-3	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042021\
Data File : BF123653.D
Acq On : 20 Apr 2021 20:49
Operator : JU/CG
Sample : M2076-10
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Instrument :
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ClientSampleId :
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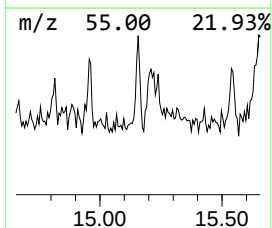
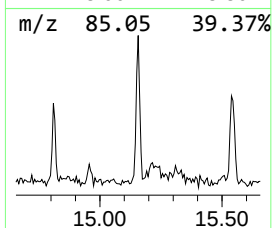
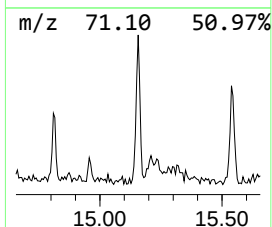
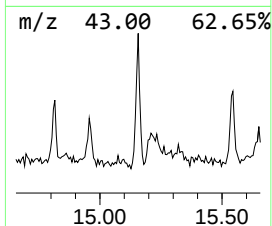
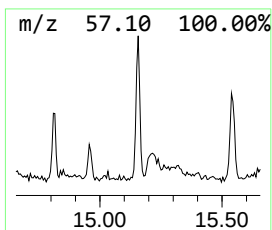
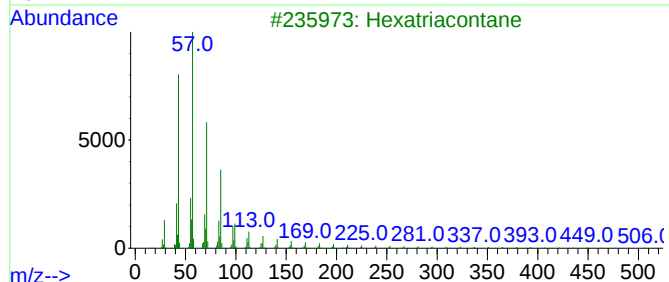
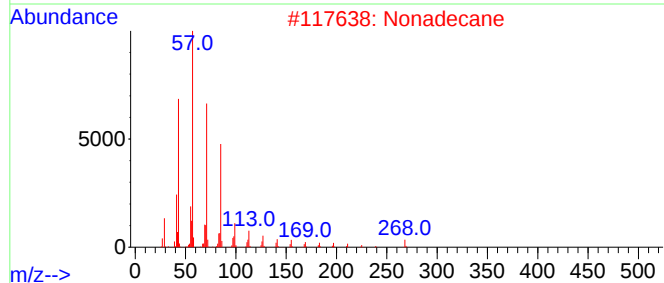
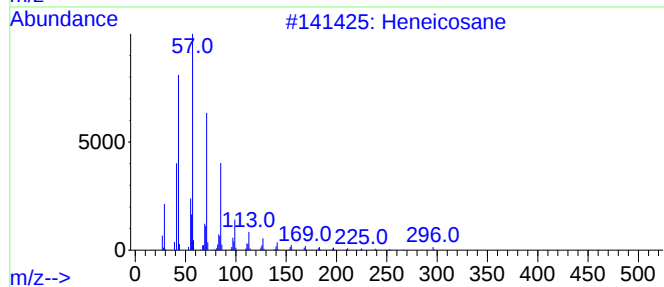
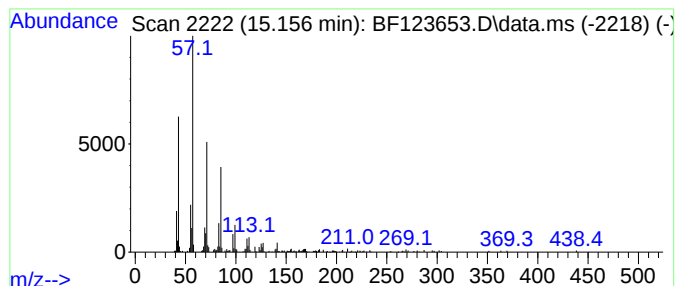
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.156	3.85 ng	270976	Perylene-d12	15.504

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	87
2			Nonadecane	268	C19H40	000629-92-5	86
3			Hexatriacontane	507	C36H74	000630-06-8	86
4			Heptadecane	240	C17H36	000629-78-7	86
5			Tetracosane	338	C24H50	000646-31-1	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042021\
Data File : BF123653.D
Acq On : 20 Apr 2021 20:49
Operator : JU/CG
Sample : M2076-10
Misc :
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Instrument :
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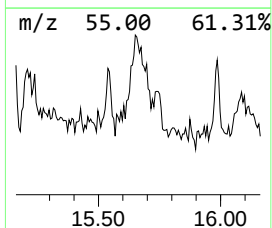
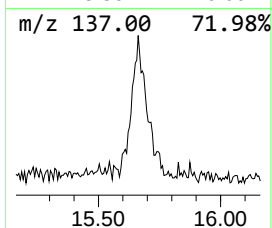
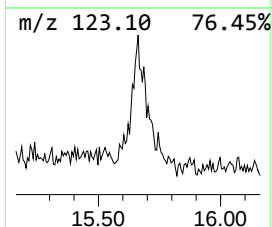
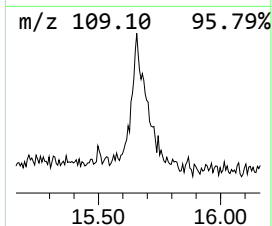
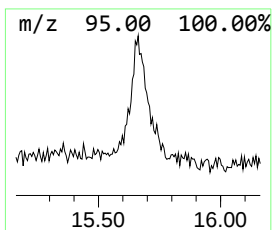
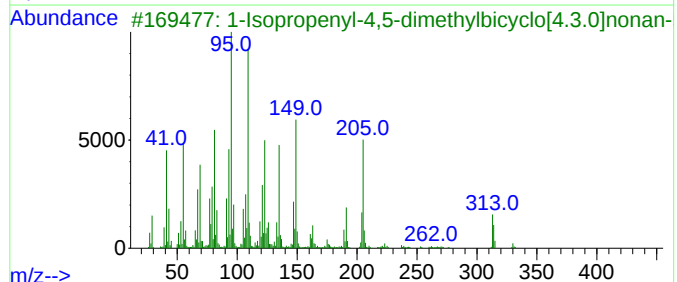
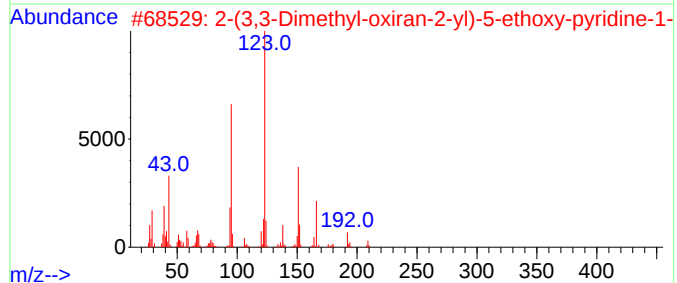
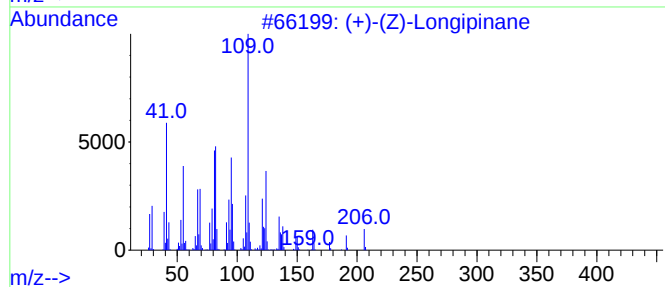
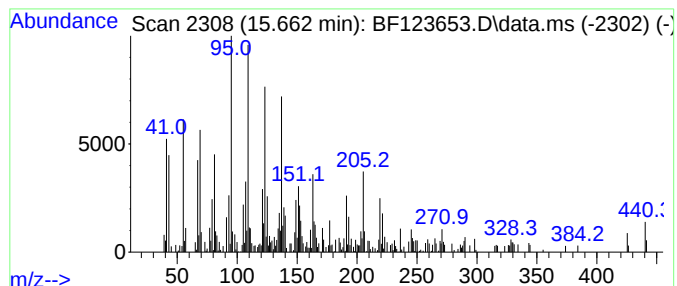
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown15.662 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.662	11.03 ng	775894	Perylene-d12	15.504

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(+)-(Z)-Longipinane	206	C15H26	1000156-12-3	47		
2	2-(3,3-Dimethyl-oxiran-2-yl)-5-e...	209	C11H15NO3	1000194-95-4	46		
3	1-Isopropenyl-4,5-dimethylbicycl...	330	C21H30O5	1000195-85-4	46		
4	4,4-Dimethoxy-2,5-cyclohexadien...	154	C8H10O3	000935-50-2	41		
5	2-Cyclohexen-1-one, 5-bromo-4,4...	202	C8H11BrO	1000327-26-6	38		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042021\
Data File : BF123653.D
Acq On : 20 Apr 2021 20:49
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Sample : M2076-10
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Instrument :
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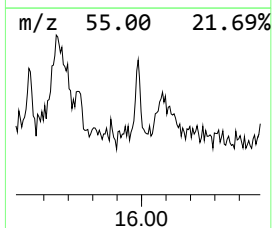
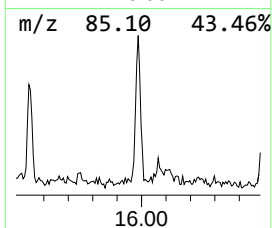
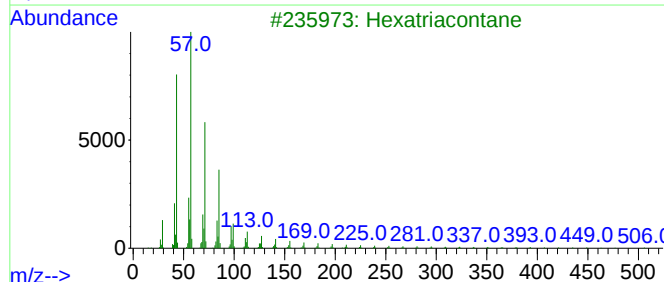
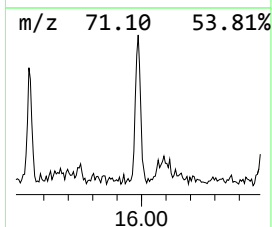
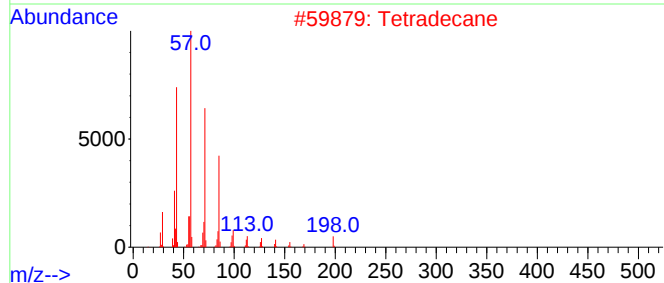
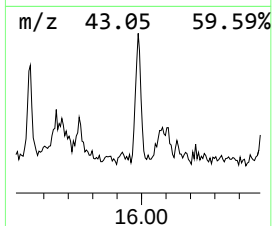
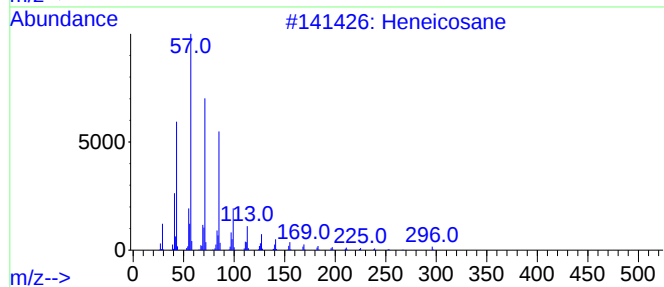
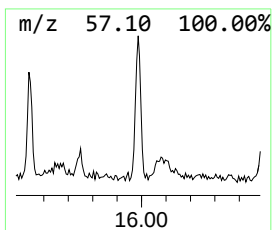
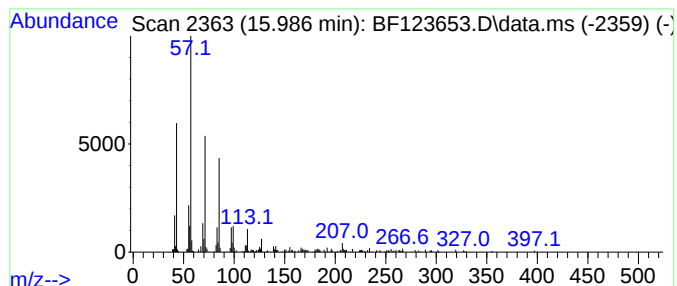
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Tetradecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.986	4.09 ng	287797	Perylene-d12	15.504

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heneicosane	296	C21H44	000629-94-7	74
2		Tetradecane	198	C14H30	000629-59-4	72
3		Hexatriacontane	507	C36H74	000630-06-8	62
4		Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	60
5		Eicosane	282	C20H42	000112-95-8	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042021\
Data File : BF123653.D
Acq On : 20 Apr 2021 20:49
Operator : JU/CG
Sample : M2076-10
Misc :
ALS Vial : 17 Sample Multiplier: 1

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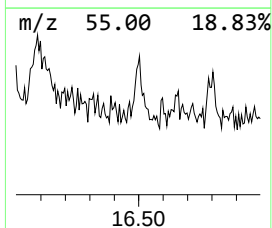
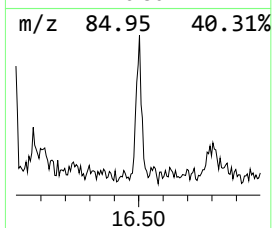
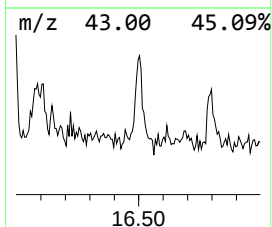
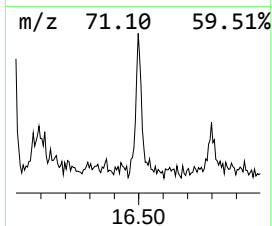
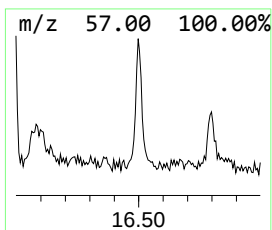
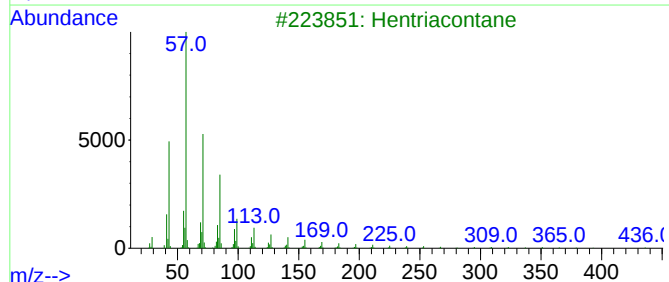
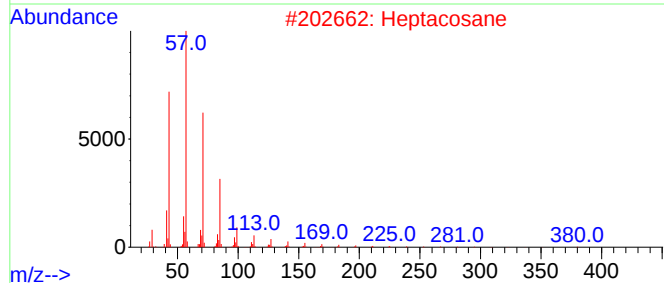
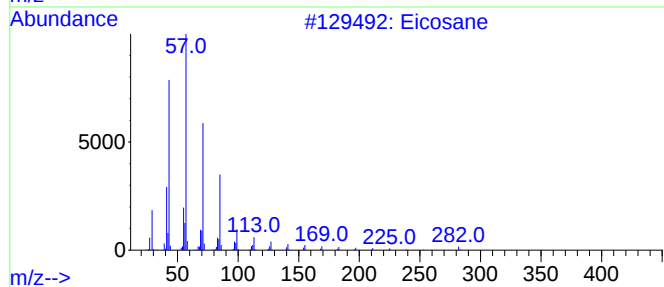
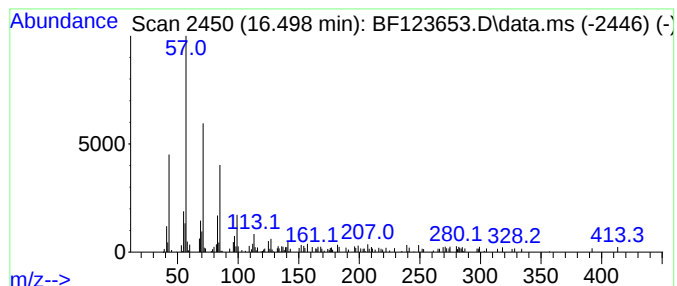
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Eicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.498	2.26 ng	159182	Perylene-d12	15.504

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	91
2			Heptacosane	380	C27H56	000593-49-7	83
3			Hentriacontane	437	C31H64	000630-04-6	80
4			Nonadecane, 2-methyl-	282	C20H42	001560-86-7	80
5			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042021\
Data File : BF123653.D
Acq On : 20 Apr 2021 20:49
Operator : JU/CG
Sample : M2076-10
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-16-0-2.0

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.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 ...	11.916	12.7	ng	1374360	4	11.380	2173690	20.0
Octadecanoic acid	12.704	7.7	ng	634694	5	14.027	1647670	20.0
5-Bromo-4-oxo-4...	13.568	90.4	ng	7446830	5	14.027	1647670	20.0
17-Pentatriacon...	13.880	13.8	ng	1133390	5	14.027	1647670	20.0
n-Heptadecanol-1	14.527	4.2	ng	346585	5	14.027	1647670	20.0
Oxirane, hexade...	14.957	2.3	ng	161569	6	15.504	1406270	20.0
Benzo[e]pyrene	15.068	2.6	ng	183698	6	15.504	1406270	20.0
Heneicosane	15.156	3.9	ng	270976	6	15.504	1406270	20.0
unknown15.662	15.662	11.0	ng	775894	6	15.504	1406270	20.0
Tetradecane	15.986	4.1	ng	287797	6	15.504	1406270	20.0
Eicosane	16.498	2.3	ng	159182	6	15.504	1406270	20.0