

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012022\
 Data File : BF126607.D
 Acq On : 20 Jan 2022 12:49
 Operator : CG/JU
 Sample : PB142146BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB142146BL

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-BF011822.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126607.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.369	38	48	53	rBV	118533	163355	3.06%	0.484%
2	5.593	590	596	599	rBV	3925323	4268486	79.94%	12.638%
3	6.581	757	764	767	rBV	3790969	4468482	83.69%	13.230%
4	6.963	825	829	832	rBV	1080995	860825	16.12%	2.549%
5	7.528	919	925	928	rBV	2626303	2964892	55.53%	8.778%
6	8.245	1042	1047	1050	rBV	1231946	1191004	22.31%	3.526%
7	9.322	1224	1230	1233	rBV	4334503	4897613	91.72%	14.500%
8	10.004	1340	1346	1349	rBV	1564044	1410155	26.41%	4.175%
9	10.798	1474	1481	1484	rBV	2882328	3134256	58.70%	9.279%
10	11.498	1594	1600	1603	rBV	1672685	1468563	27.50%	4.348%
11	13.092	1865	1871	1874	rBV	5281811	5339469	100.00%	15.808%
12	14.145	2046	2050	2054	rVB	1363059	1243552	23.29%	3.682%
13	14.951	2183	2187	2193	rVB	97987	94378	1.77%	0.279%
14	15.310	2244	2248	2256	rBV	133873	157024	2.94%	0.465%
15	15.686	2306	2312	2315	rBV	839880	1049370	19.65%	3.107%
16	15.721	2315	2318	2325	rVB	187798	233152	4.37%	0.690%
17	16.192	2392	2398	2409	rVB	149245	235424	4.41%	0.697%
18	16.745	2485	2492	2503	rBV2	115802	224066	4.20%	0.663%
19	17.392	2593	2602	2614	rBV2	65196	149588	2.80%	0.443%
20	17.868	2670	2683	2695	rBV3	28854	106478	1.99%	0.315%
21	18.162	2723	2733	2745	rBV4	41909	116120	2.17%	0.344%

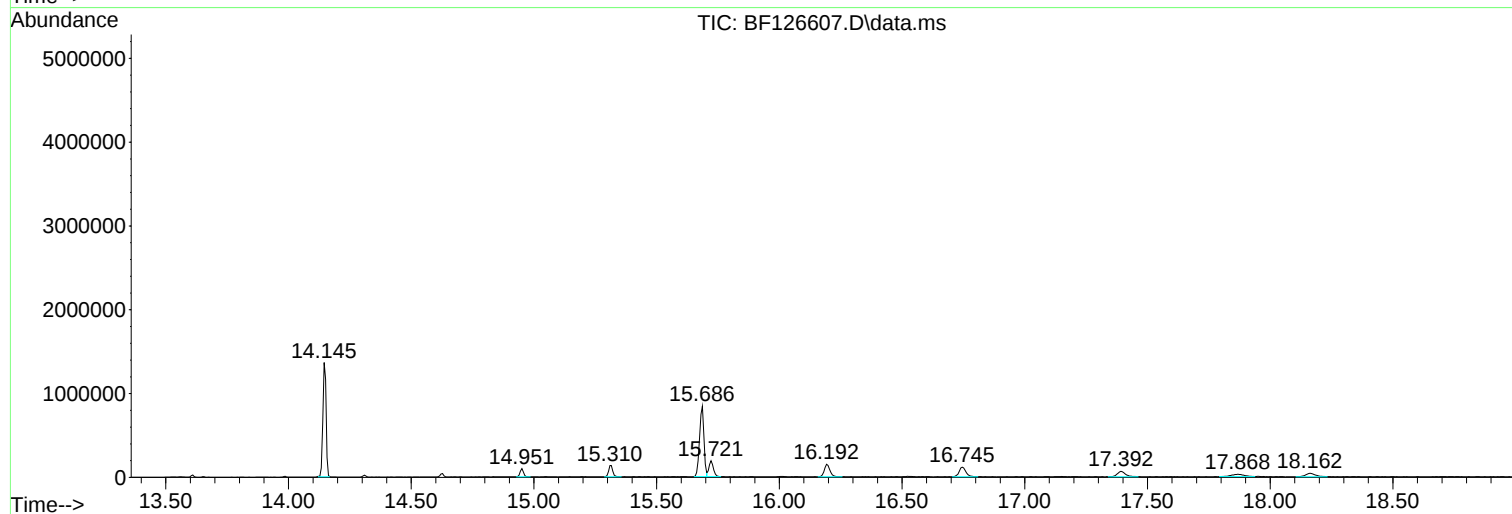
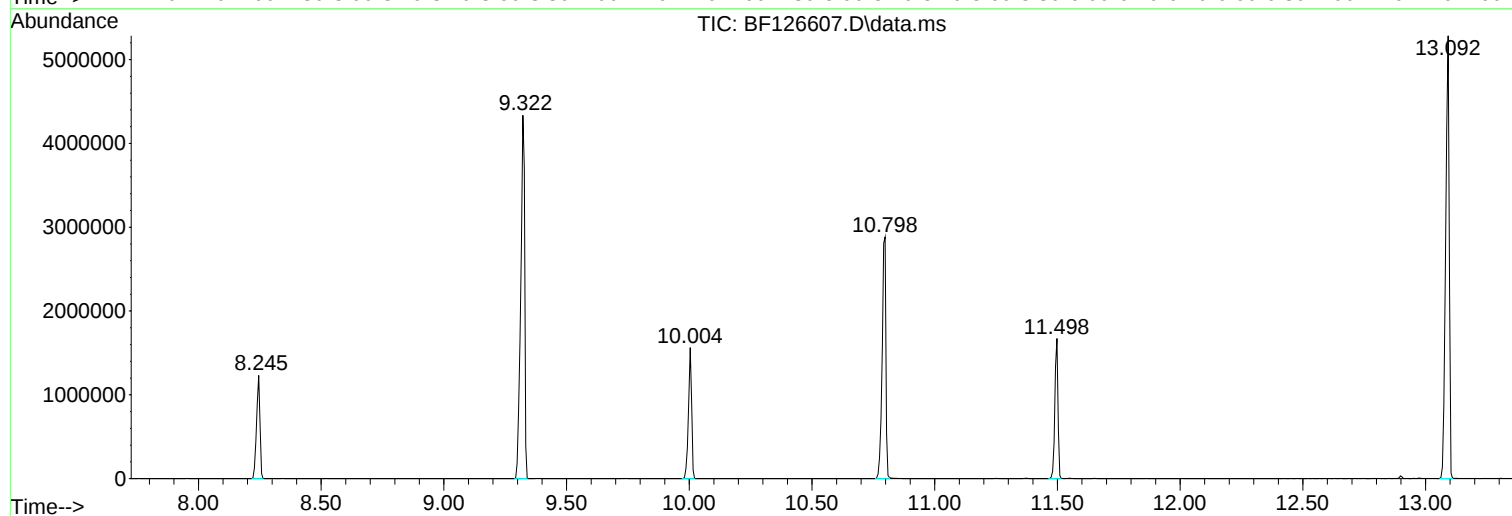
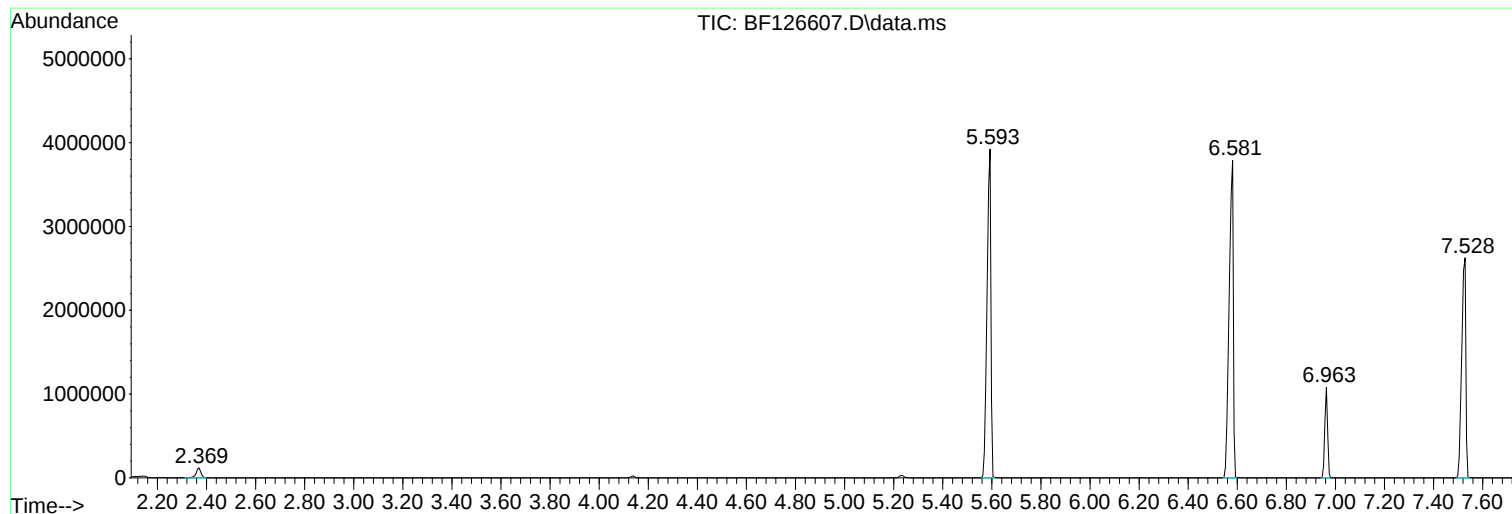
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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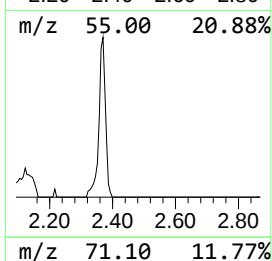
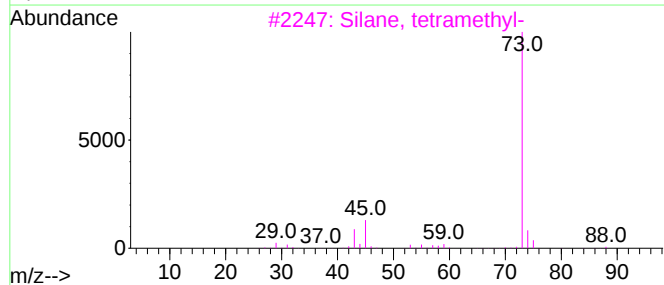
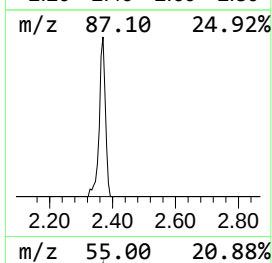
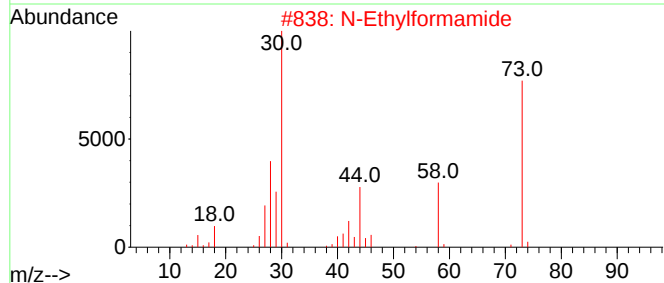
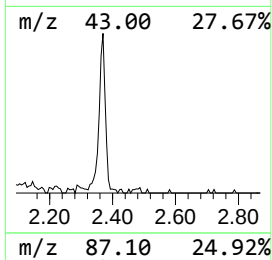
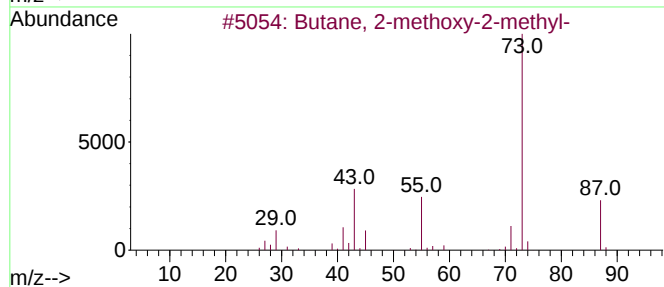
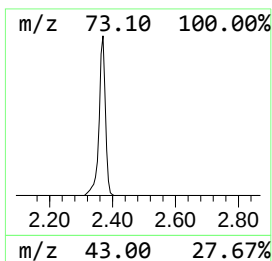
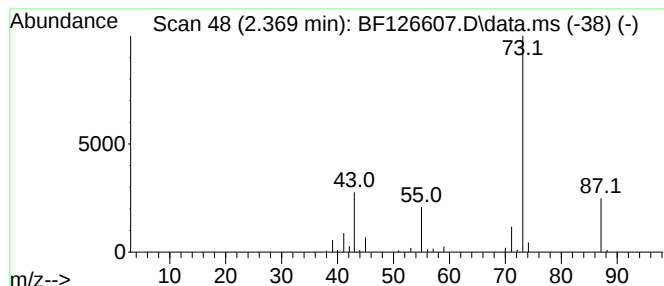
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.369	3.80 ng	163355	1,4-Dichlorobenzene-d4	6.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	90
2			N-Ethylformamide	73	C3H7NO	000627-45-2	9
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
4			Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	9
5			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	9



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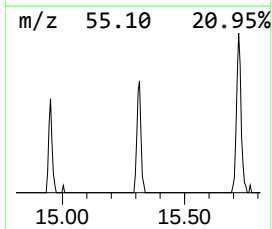
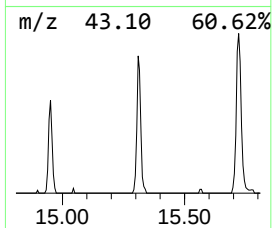
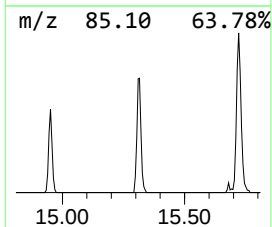
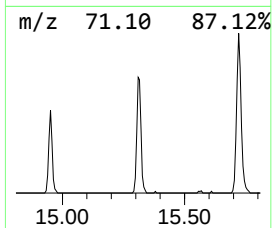
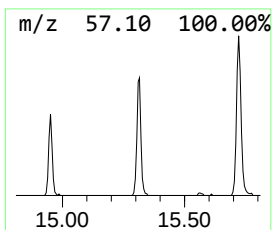
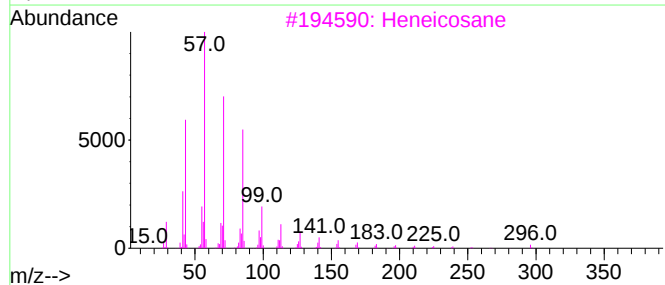
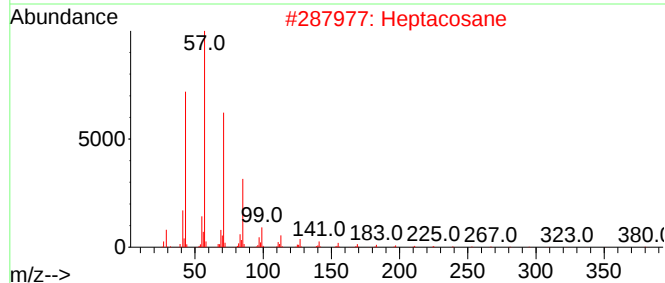
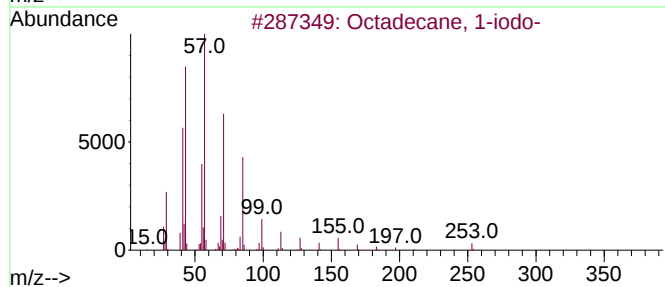
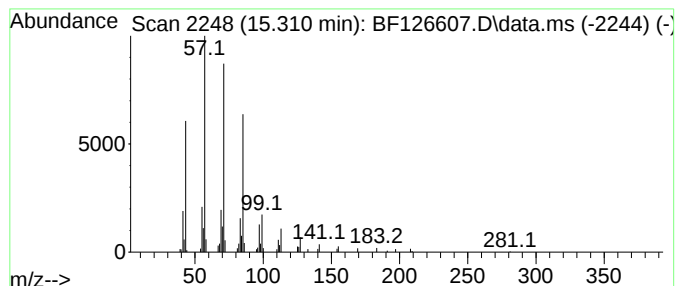
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Peak Number 2 Octadecane, 1-iodo- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.310	2.99 ng	157024	Perylene-d12	15.686

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecane, 1-iodo-	380	C18H37I	000629-93-6	86
2		Heptacosane	380	C27H56	000593-49-7	80
3		Heneicosane	296	C21H44	000629-94-7	64
4		Sulfurous acid, 2-ethylhexyl oct...	446	C26H54O3S	1000309-20-1	62
5		Sulfurous acid, 2-ethylhexyl pen...	404	C23H48O3S	1000309-19-8	58



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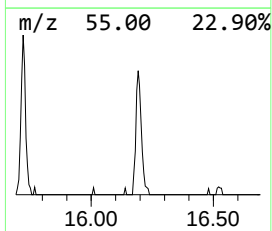
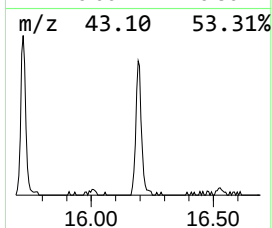
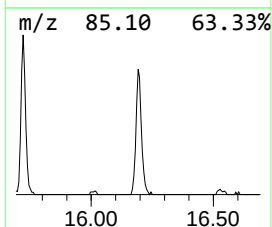
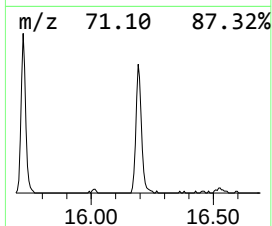
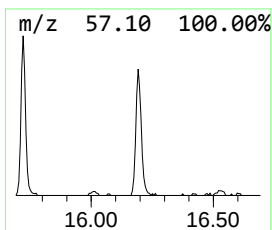
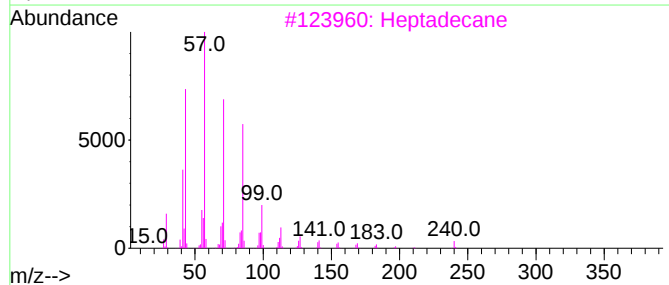
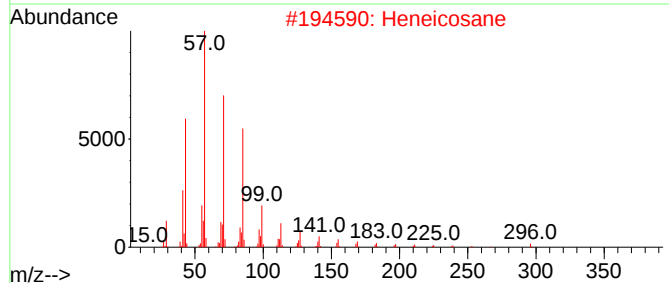
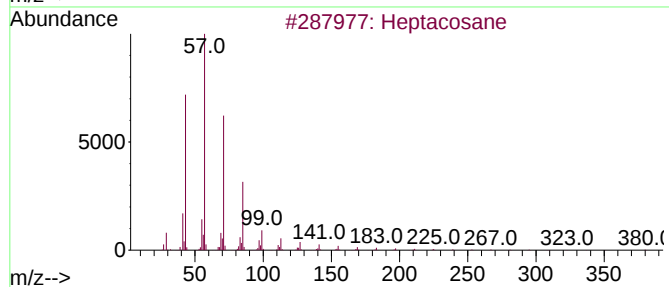
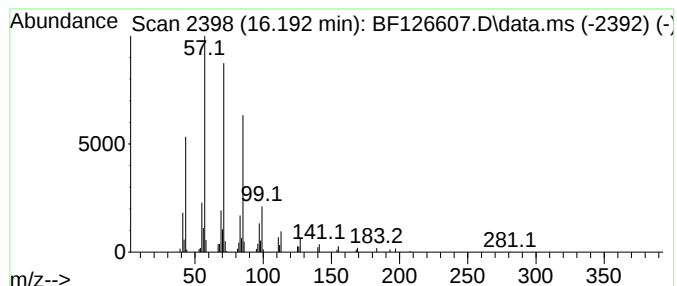
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Peak Number 3 Heptacosane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.192	4.49 ng	235424	Perylene-d12	15.686

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	83
2			Heneicosane	296	C21H44	000629-94-7	64
3			Heptadecane	240	C17H36	000629-78-7	58
4			Sulfurous acid, nonyl 2-propyl e...	250	C12H26O3S	1000309-12-0	58
5			Sulfurous acid, 2-ethylhexyl hep...	432	C25H52O3S	1000309-20-0	52



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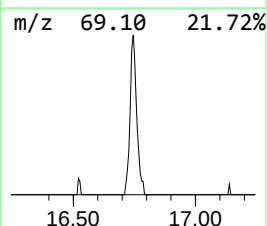
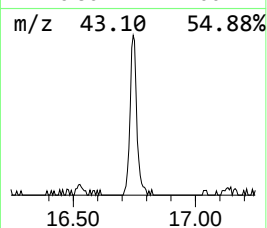
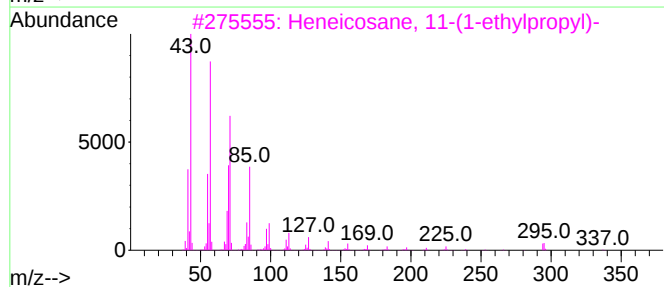
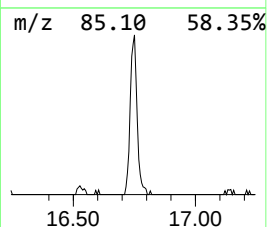
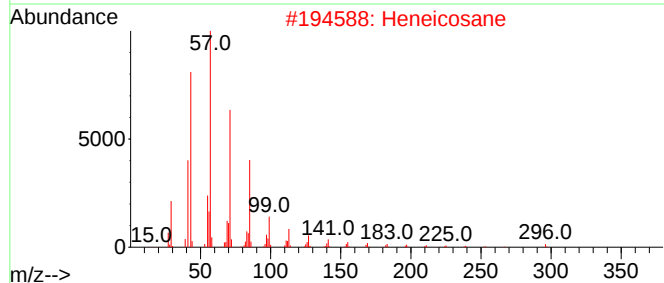
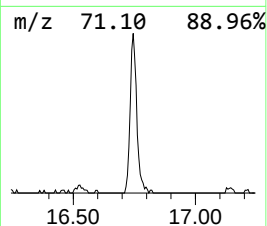
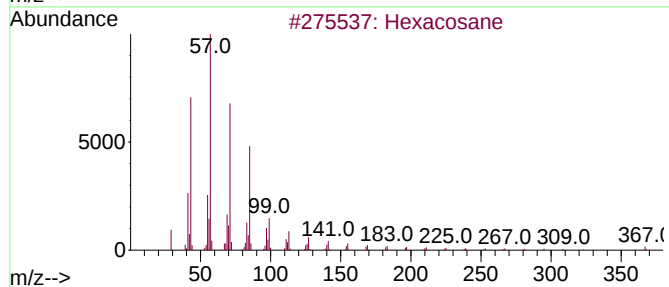
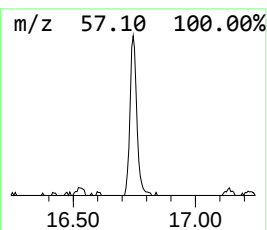
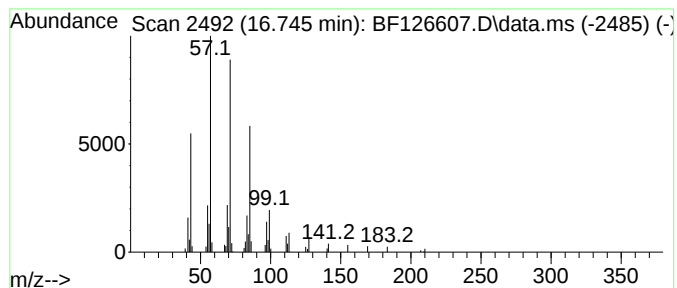
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Peak Number 4 Hexacosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.745	4.27 ng	224066	Perylene-d12	15.686

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	91
2			Heneicosane	296	C21H44	000629-94-7	86
3			Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	86
4			Nonadecane	268	C19H40	000629-92-5	86
5			Octacosane	394	C28H58	000630-02-4	86



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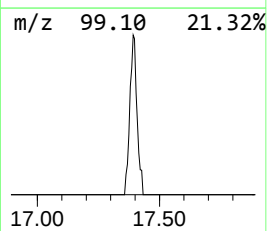
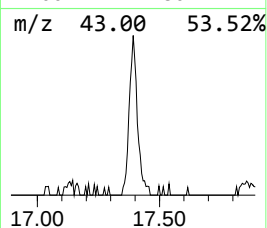
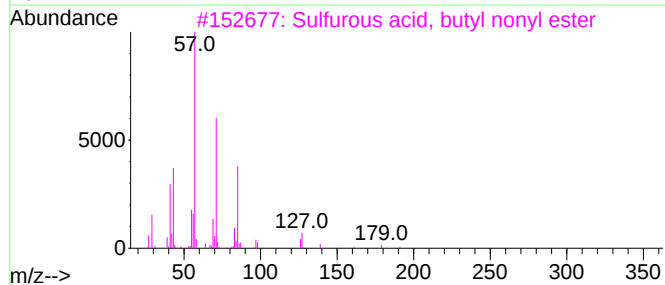
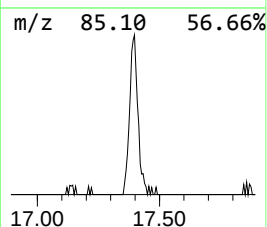
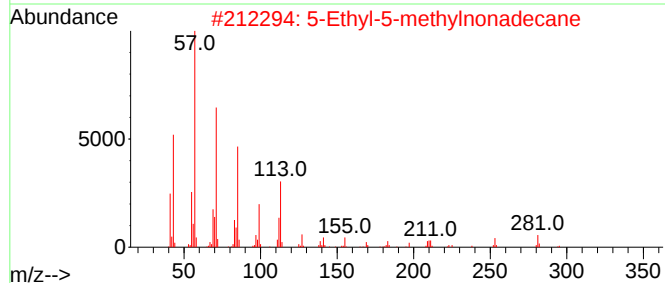
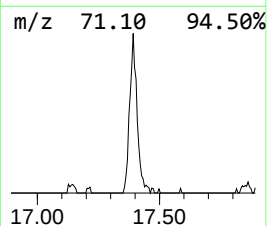
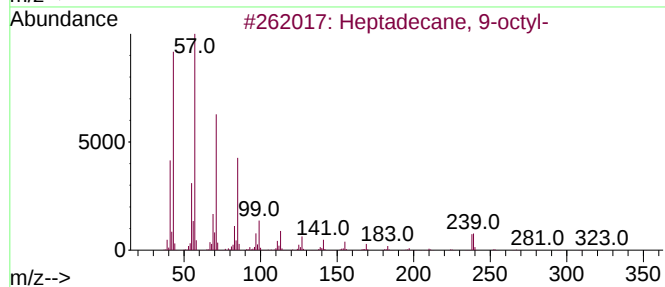
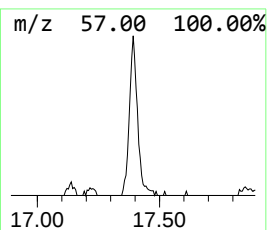
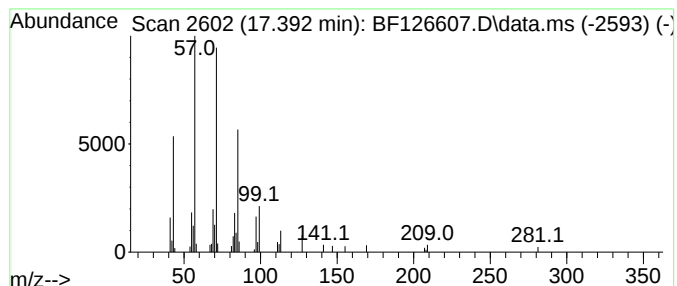
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Heptadecane, 9-octyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.392	2.85 ng	149588	Perylene-d12	15.686

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	72
2			5-Ethyl-5-methylnonadecane	310	C22H46	1000360-42-7	72
3			Sulfurous acid, butyl nonyl ester	264	C13H28O3S	1000309-17-6	64
4			Tetratetracontane	619	C44H90	007098-22-8	64
5			Sulfurous acid, butyl undecyl ester	292	C15H32O3S	1000309-17-8	58



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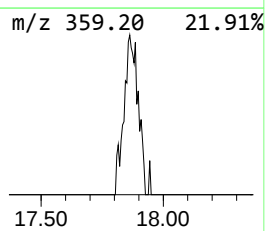
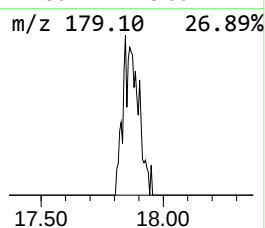
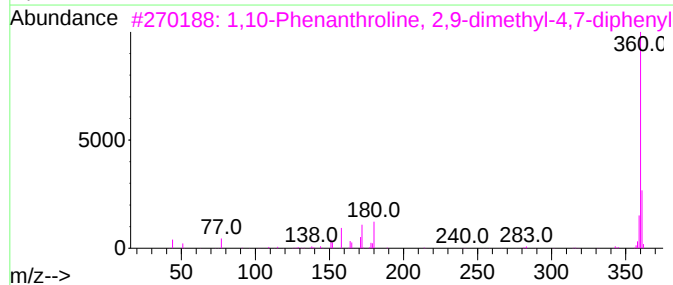
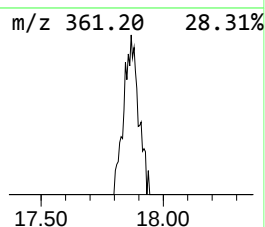
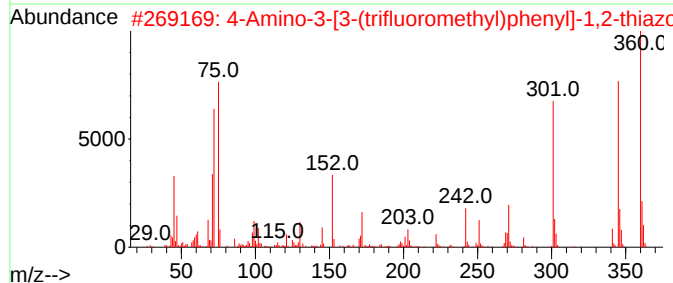
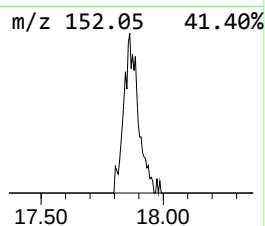
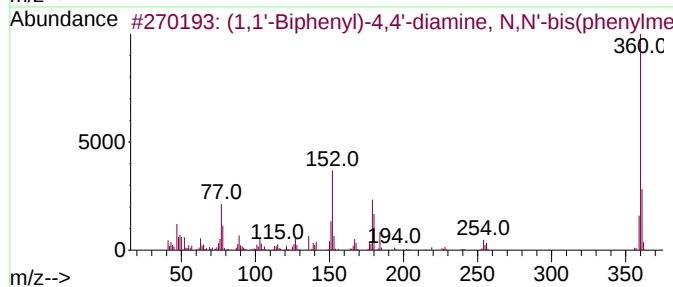
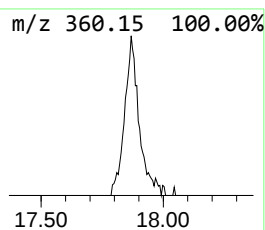
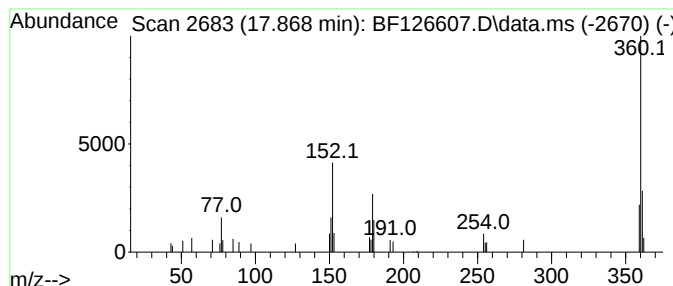
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 (1,1'-Biphenyl)-4,4'-diamin... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.868	2.03 ng	106478	Perylene-d12	15.686

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(1,1'-Biphenyl)-4,4'-diamine, N,...	360	C26H20N2	006311-48-4	93
2			4-Amino-3-[3-(trifluoromethyl)ph...	360	C14H15F3N2O2SSi	1010500-98-0	58
3			1,10-Phenanthroline, 2,9-dimethy...	360	C26H20N2	004733-39-5	50
4			Benzaldehyde, 4-hydroxy-3,5-dime...	360	C18H20N2O6	014414-32-5	49
5			Androst-4-ene-3,17-dione, 12-hyd...	360	C21H32N2O3	069688-31-9	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012022\
Data File : BF126607.D
Acq On : 20 Jan 2022 12:49
Operator : CG/JU
Sample : PB142146BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB142146BL

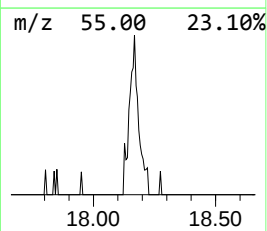
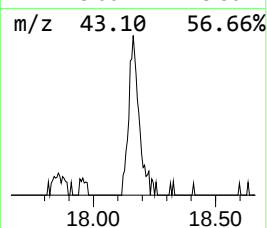
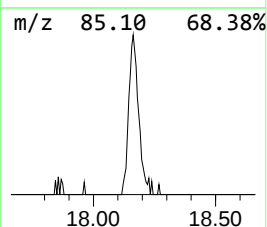
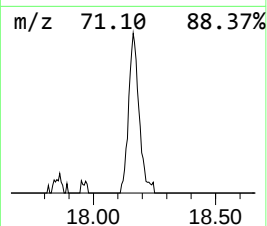
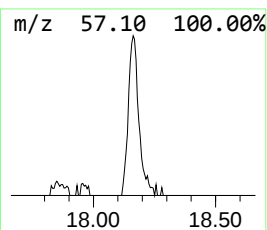
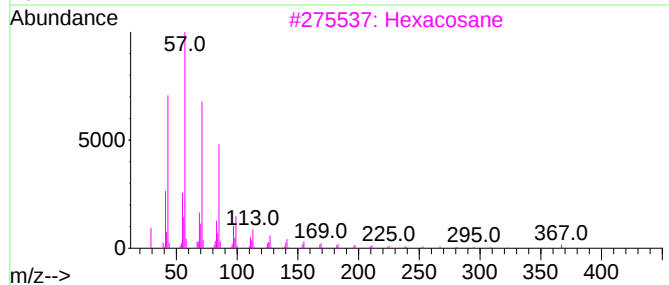
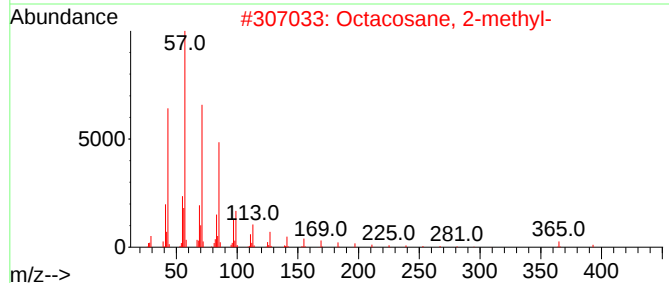
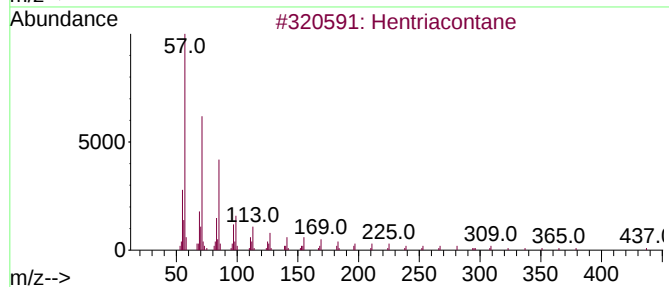
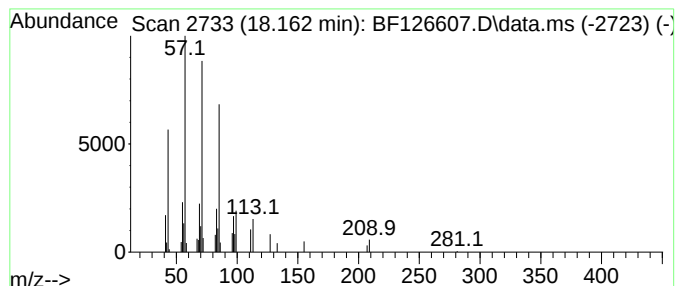
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hentriacontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.162	2.21 ng	116120	Perylene-d12	15.686

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hentriacontane	437	C31H64	000630-04-6	90
2			Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
3			Hexacosane	366	C26H54	000630-01-3	90
4			Octacosane	394	C28H58	000630-02-4	86
5			Pentacosane	352	C25H52	000629-99-2	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012022\
Data File : BF126607.D
Acq On : 20 Jan 2022 12:49
Operator : CG/JU
Sample : PB142146BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB142146BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.369	3.8	ng	163355	1	6.963	860825	20.0
Octadecane, 1-i...	15.310	3.0	ng	157024	6	15.686	1049370	20.0
Heptacosane	16.192	4.5	ng	235424	6	15.686	1049370	20.0
Hexacosane	16.745	4.3	ng	224066	6	15.686	1049370	20.0
Heptadecane, 9-...	17.392	2.9	ng	149588	6	15.686	1049370	20.0
(1,1'-Biphenyl)...	17.868	2.0	ng	106478	6	15.686	1049370	20.0
Hentriacontane	18.162	2.2	ng	116120	6	15.686	1049370	20.0