

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011122\
 Data File : BF126584.D
 Acq On : 11 Jan 2022 10:55
 Operator : JU/CG
 Sample : PB141938BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB141938BL

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-BF122921.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126584.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.004	492	496	503	rBB	21872	30729	1.14%	0.166%
2	5.392	557	562	565	rBV	2347727	2510884	93.52%	13.589%
3	6.410	729	735	738	rBV	2246248	2512577	93.59%	13.598%
4	6.769	792	796	799	rBV	634077	517944	19.29%	2.803%
5	7.334	886	892	895	rBV	1656723	1711362	63.74%	9.262%
6	8.051	1009	1014	1017	rBV	851871	728381	27.13%	3.942%
7	9.133	1192	1198	1201	rBV	2658441	2684799	100.00%	14.530%
8	9.810	1308	1313	1316	rBV	892232	781295	29.10%	4.228%
9	10.604	1443	1448	1451	rBV	1602925	1641798	61.15%	8.885%
10	11.292	1561	1565	1569	rBV	836601	777612	28.96%	4.208%
11	12.710	1803	1806	1809	rBB	63272	49378	1.84%	0.267%
12	12.892	1831	1837	1840	rBV	2568588	2636172	98.19%	14.267%
13	13.415	1923	1926	1930	rBV	40791	38330	1.43%	0.207%
14	13.939	2011	2015	2019	rBV	716676	625271	23.29%	3.384%
15	14.039	2025	2032	2040	rBV	29944	39537	1.47%	0.214%
16	14.727	2145	2149	2153	rBV	50231	50428	1.88%	0.273%
17	15.057	2201	2205	2211	rVB	67458	78467	2.92%	0.425%
18	15.392	2256	2262	2265	rBV	400616	480616	17.90%	2.601%
19	15.427	2265	2268	2273	rVB	86466	105005	3.91%	0.568%
20	15.851	2334	2340	2349	rBV	69994	102546	3.82%	0.555%
21	16.339	2417	2423	2431	rBV2	56371	96479	3.59%	0.522%
22	16.686	2472	2482	2501	rVB4	22847	104648	3.90%	0.566%
23	16.909	2513	2520	2527	rBV3	34342	69902	2.60%	0.378%
24	17.592	2626	2636	2643	rBV3	27085	69760	2.60%	0.378%
25	18.392	2766	2772	2779	rVB5	13837	33816	1.26%	0.183%

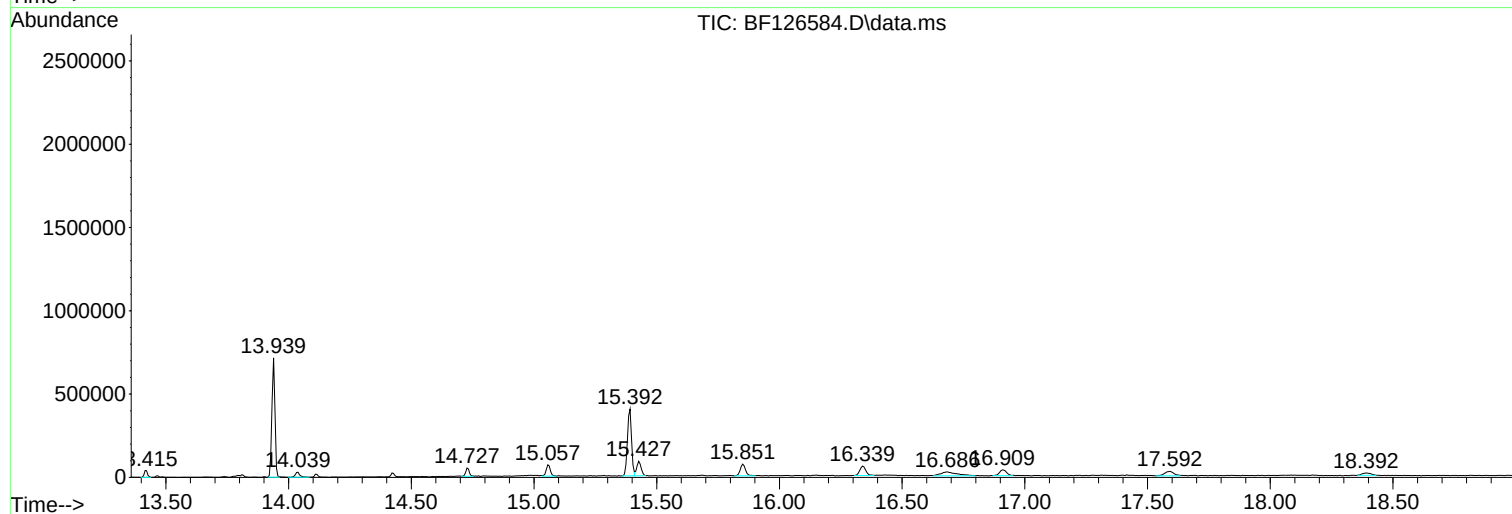
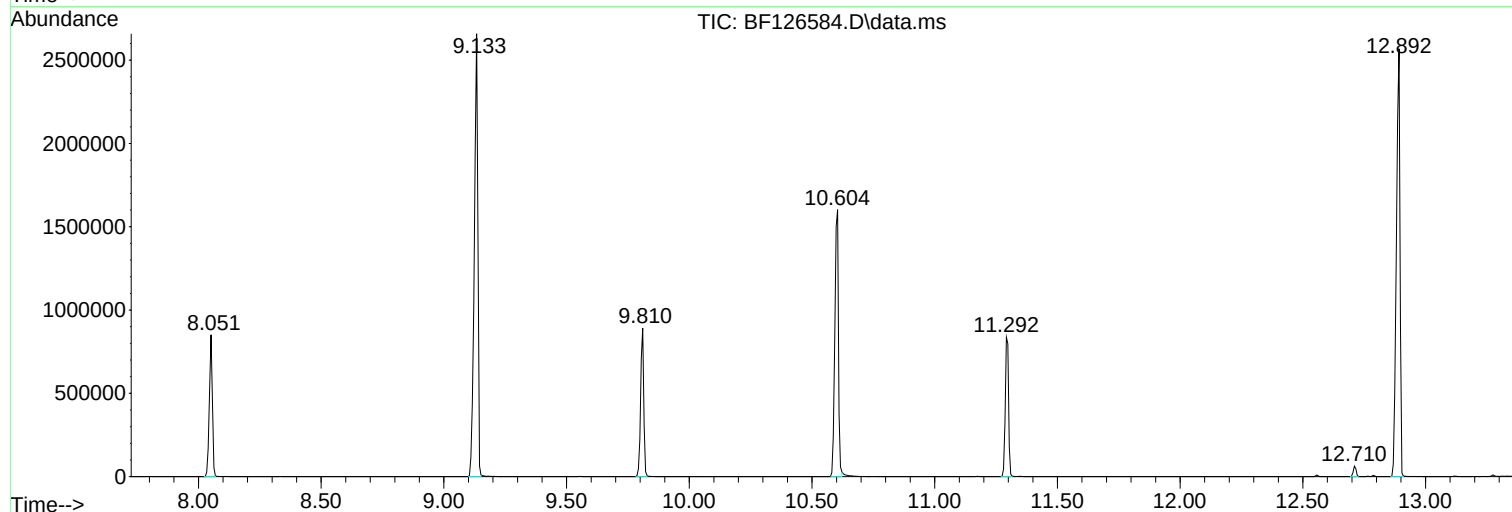
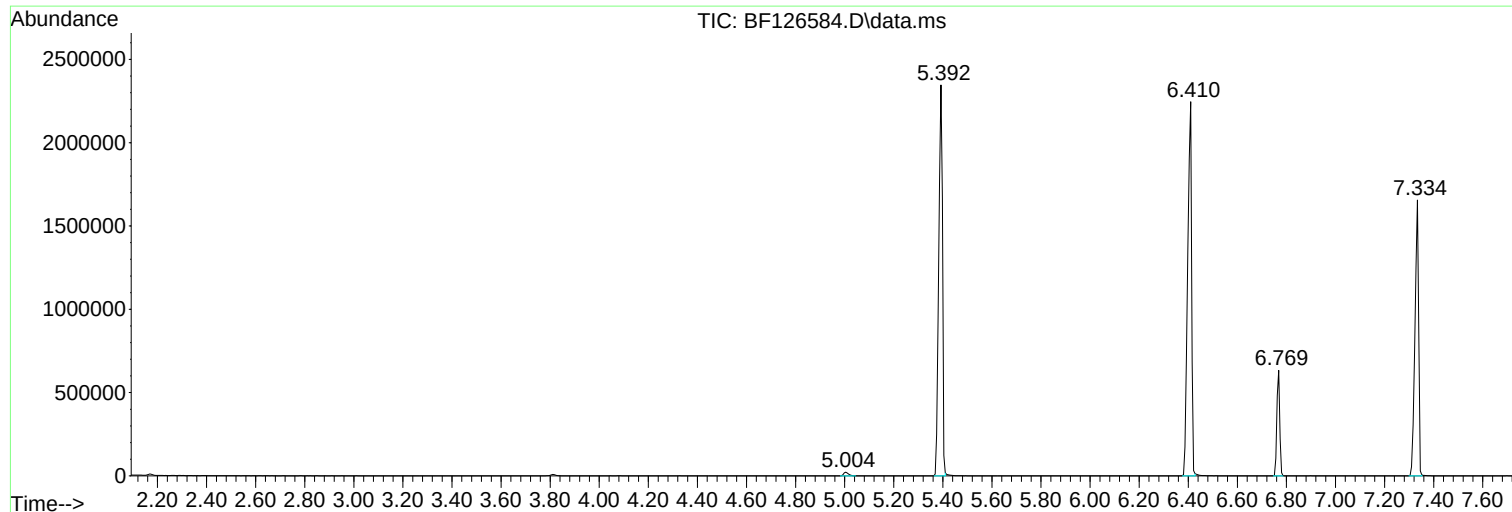
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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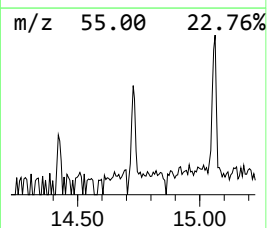
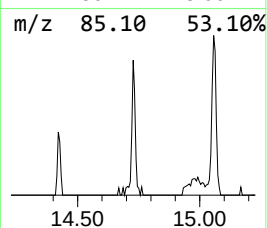
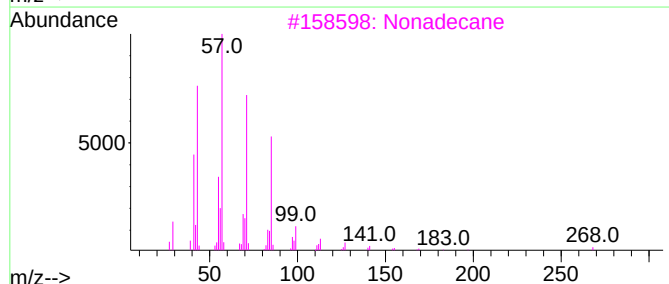
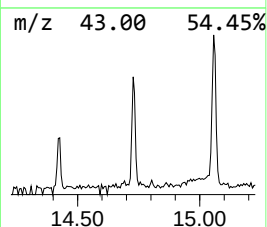
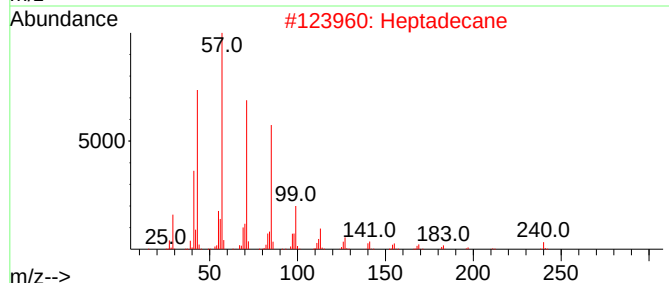
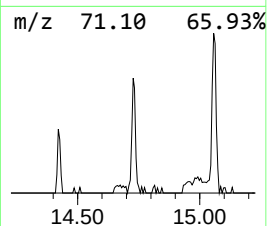
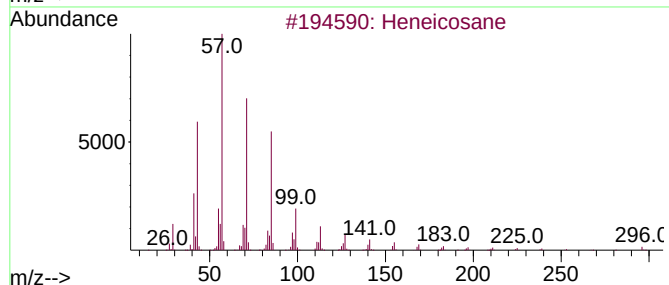
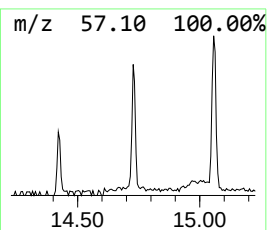
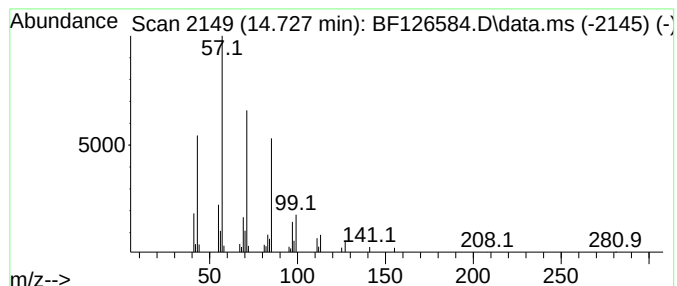
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Nonadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.727	2.10 ng	50428	Perylene-d12	15.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	87
2			Heptadecane	240	C17H36	000629-78-7	86
3			Nonadecane	268	C19H40	000629-92-5	86
4			Hexacosane	366	C26H54	000630-01-3	74
5			Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	72



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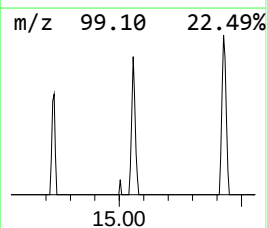
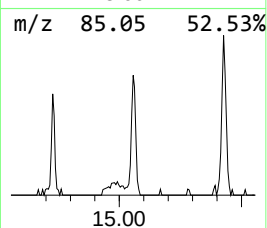
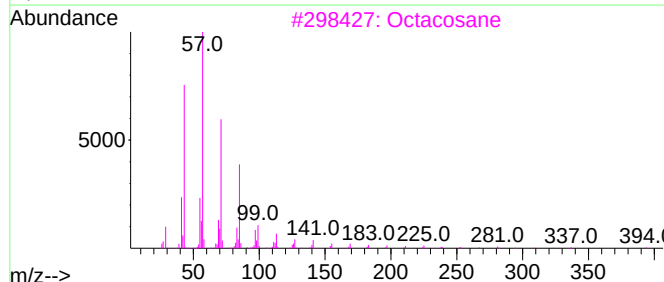
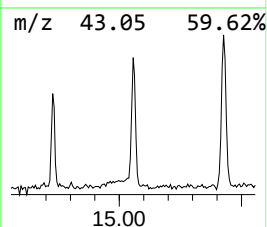
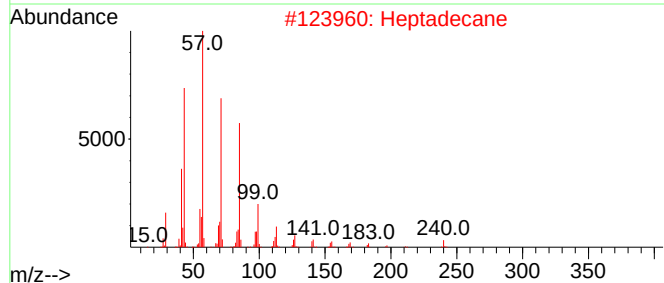
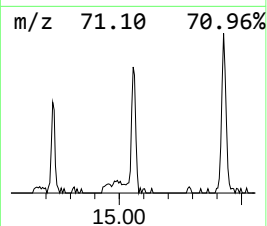
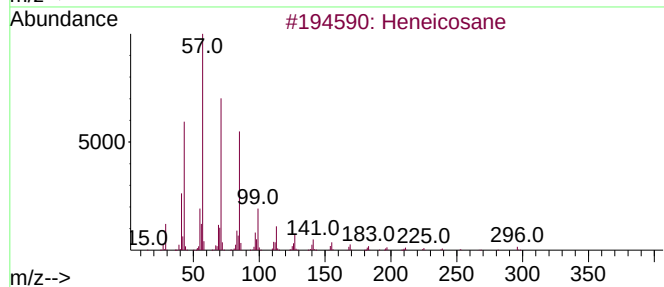
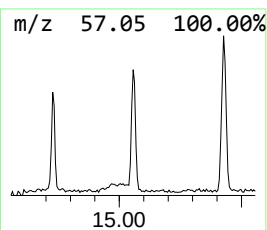
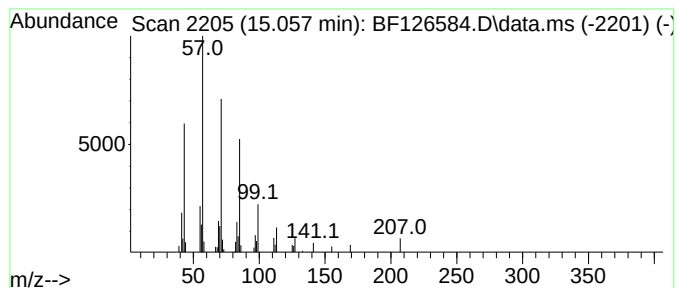
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Heptadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.057	3.27 ng	78467	Perylene-d12	15.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	90
2			Heptadecane	240	C17H36	000629-78-7	87
3			Octacosane	394	C28H58	000630-02-4	83
4			Octadecane	254	C18H38	000593-45-3	80
5			Hexadecane	226	C16H34	000544-76-3	80



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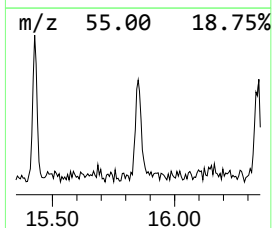
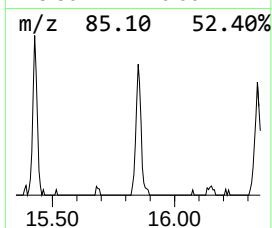
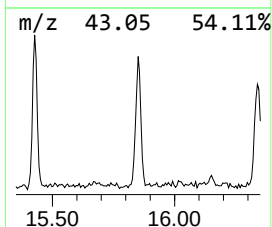
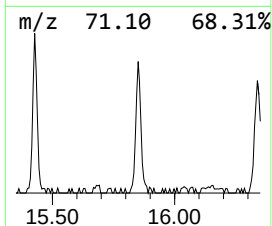
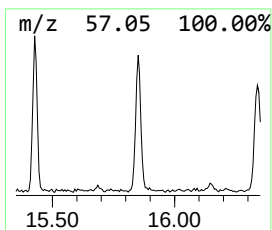
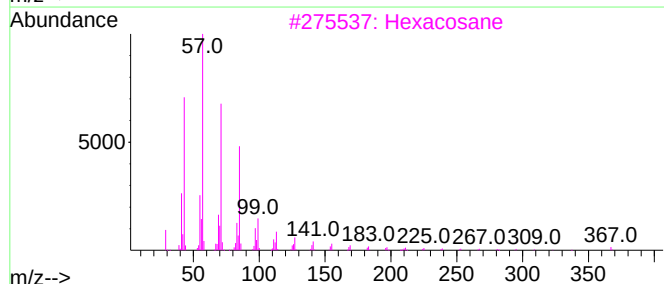
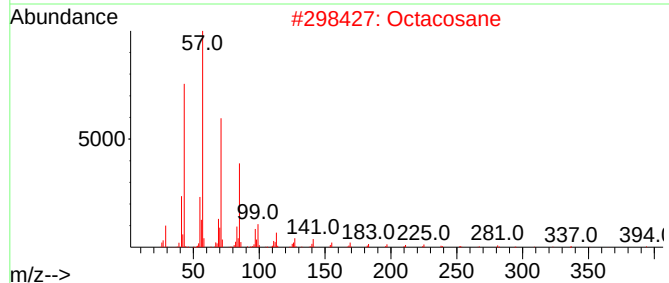
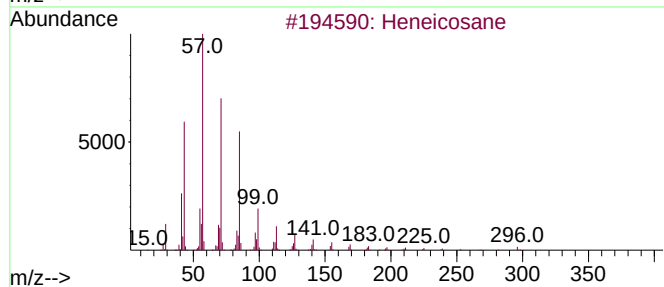
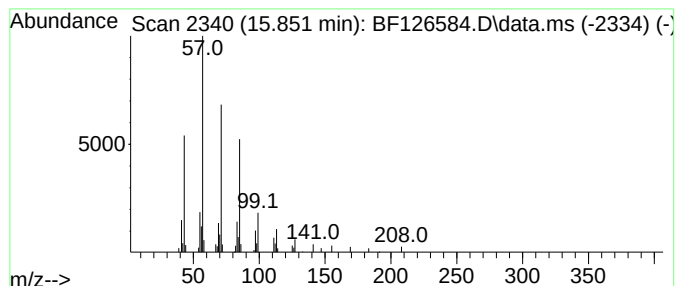
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Heneicosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.851	4.27 ng	102546	Perylene-d12	15.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			Octacosane	394	C28H58	000630-02-4	91
3			Hexacosane	366	C26H54	000630-01-3	91
4			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	90
5			Hexadecane	226	C16H34	000544-76-3	86



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Misc :
ALS Vial : 3 Sample Multiplier: 1

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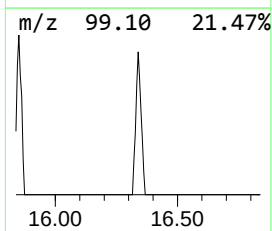
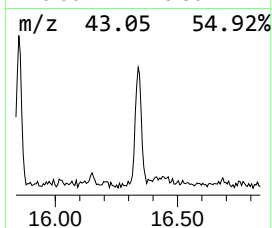
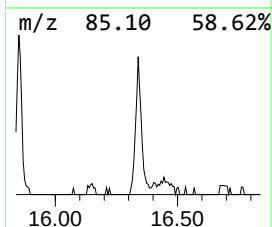
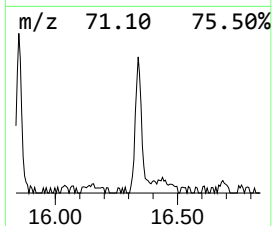
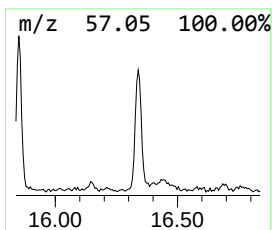
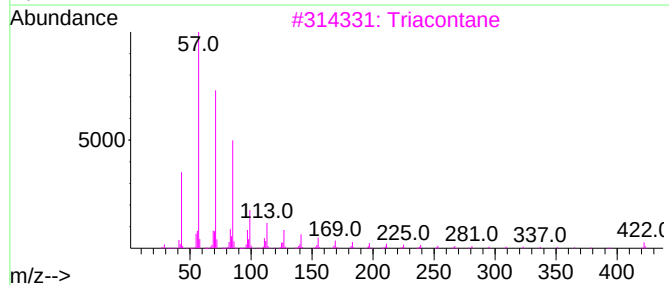
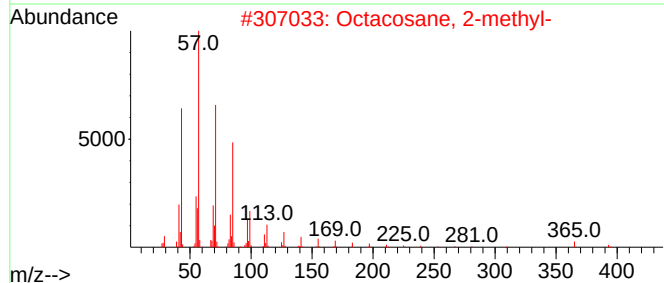
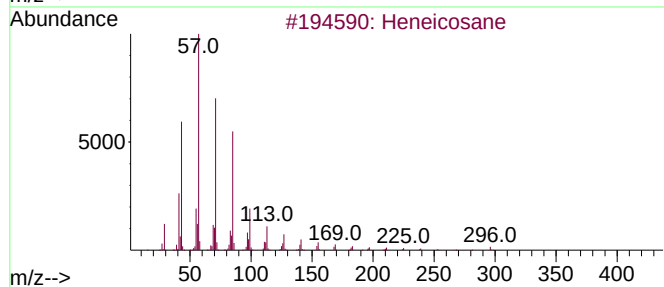
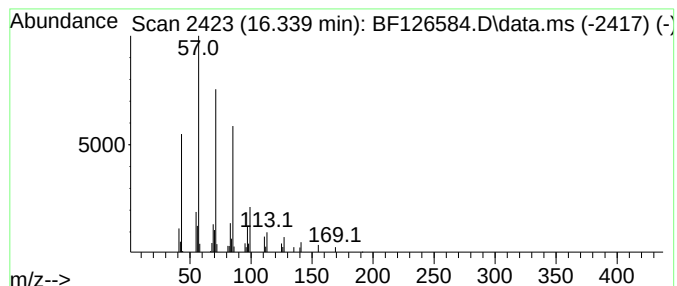
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Peak Number 4 Octacosane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.339	4.01 ng	96479	Perylene-d12	15.392

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heneicosane	296	C21H44	000629-94-7	91
2		Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
3		Triacontane	422	C30H62	000638-68-6	91
4		Hexacosane	366	C26H54	000630-01-3	87
5		Octacosane	394	C28H58	000630-02-4	87



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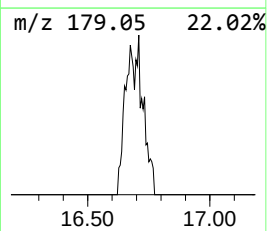
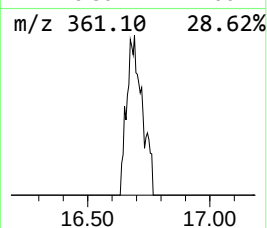
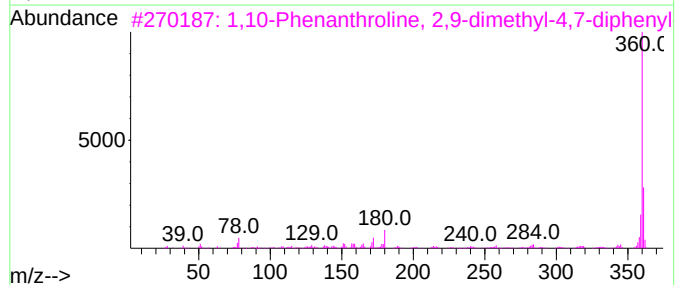
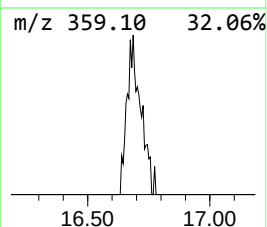
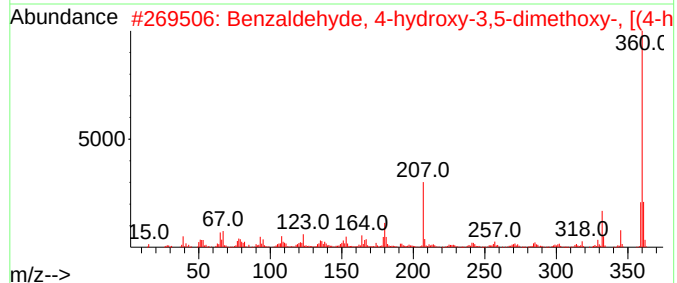
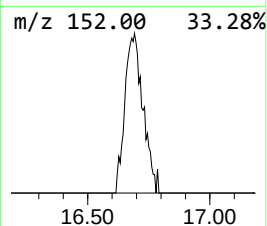
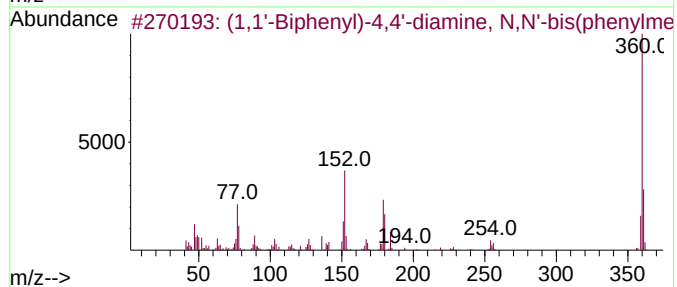
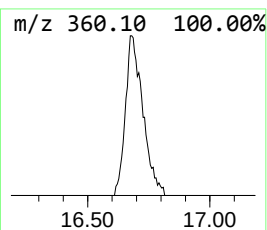
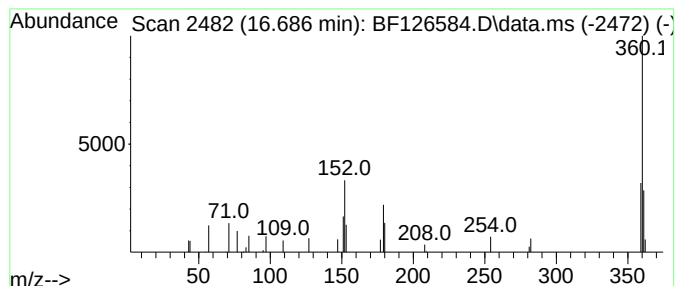
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 (1,1'-Biphenyl)-4,4'-diamin... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.686	4.35 ng	104648	Perylene-d12	15.392	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1,1'-Biphenyl)-4,4'-diamine, N,N'-bis(2,2,2-trifluoroethyl)carbamate	360	C26H20N2	006311-48-4	90
2	Benzaldehyde, 4-hydroxy-3,5-dimethoxyphenylhydrazone	360	C18H20N2O6	014414-32-5	53
3	1,10-Phenanthroline, 2,9-dimethyl-4,7-bis(2,2,2-trifluoroethyl)carbamate	360	C26H20N2	004733-39-5	50
4	Jaceidin	360	C18H16O8	010173-01-0	50
5	1,3,2-Dioxaborolane, bis(spiro[4.5]undec-5-en-2-ylidene)-	360	C20H13B06	1000150-23-7	50



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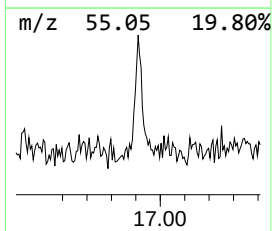
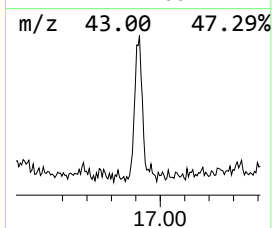
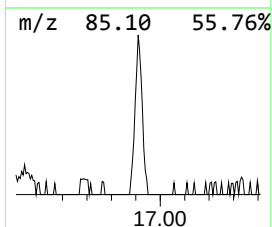
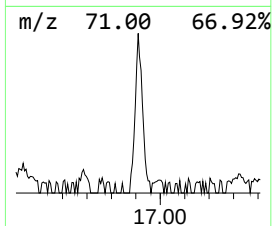
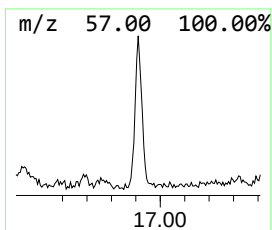
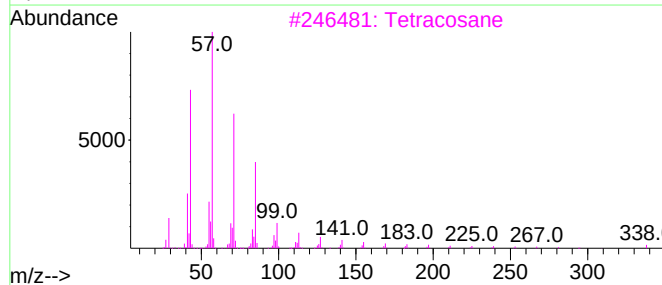
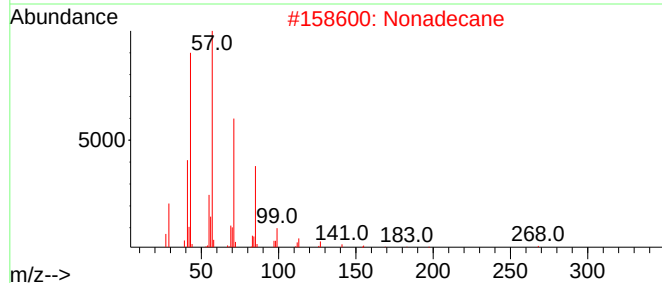
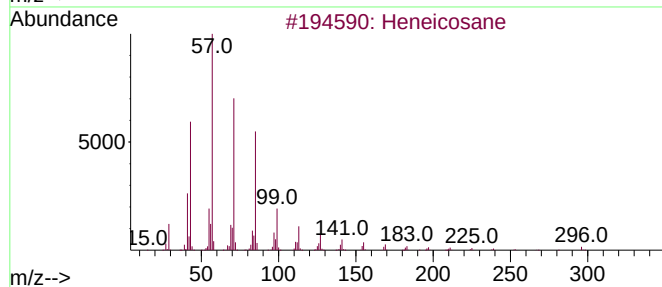
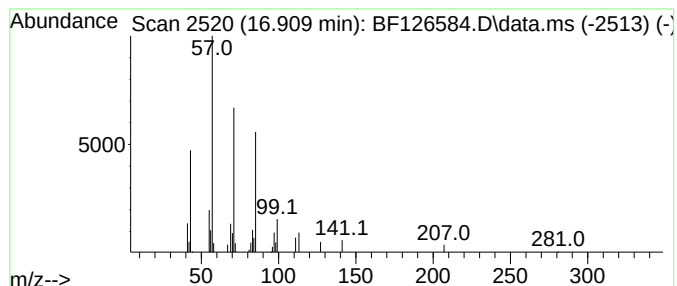
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Tetracosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.909	2.91 ng	69902	Perylene-d12	15.392

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heneicosane	296	C21H44	000629-94-7	91
2		Nonadecane	268	C19H40	000629-92-5	86
3		Tetracosane	338	C24H50	000646-31-1	86
4		Heptadecane	240	C17H36	000629-78-7	86
5		Octacosane	394	C28H58	000630-02-4	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011122\
Data File : BF126584.D
Acq On : 11 Jan 2022 10:55
Operator : JU/CG
Sample : PB141938BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB141938BL

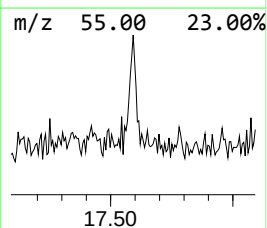
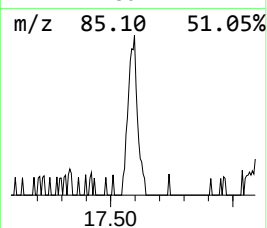
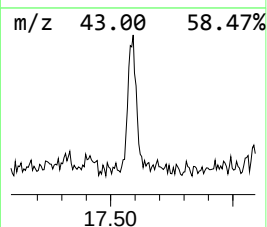
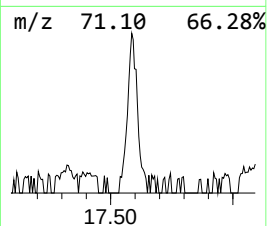
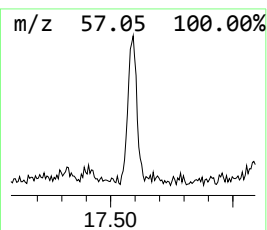
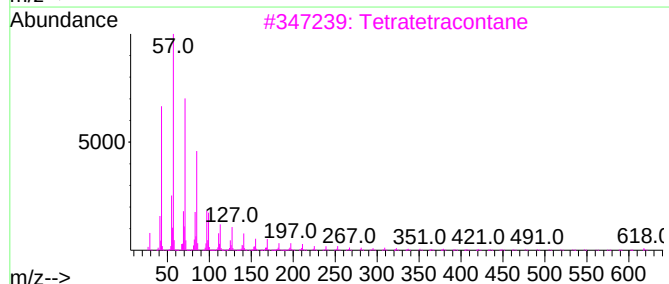
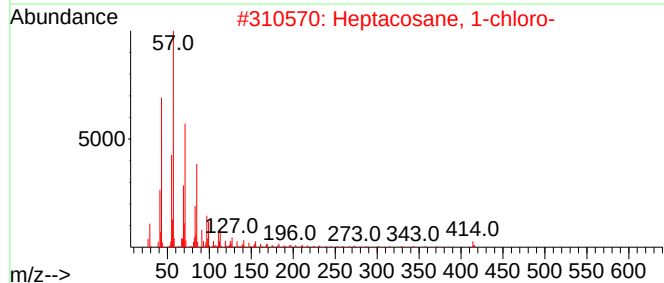
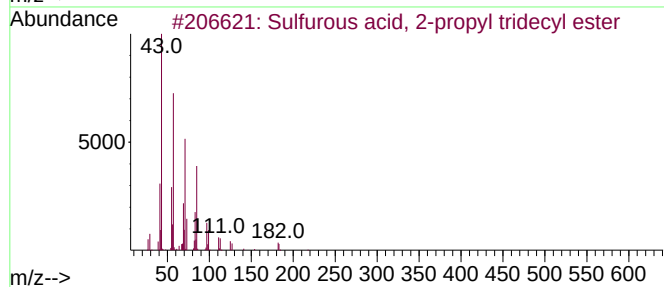
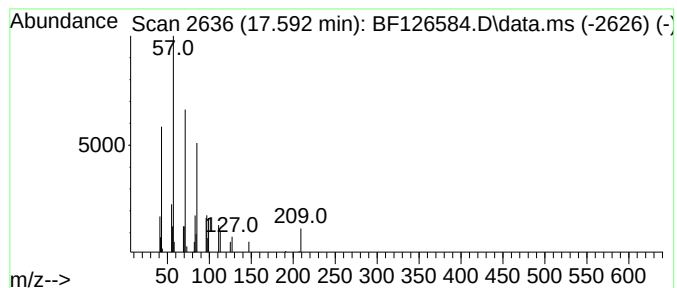
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Sulfurous acid, 2-propyl tr... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.592	2.90 ng	69760	Perylene-d12	15.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	86
2			Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	80
3			Tetratetracontane	619	C44H90	007098-22-8	80
4			Hentriacontane	437	C31H64	000630-04-6	80
5			Hexacosane	366	C26H54	000630-01-3	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011122\
Data File : BF126584.D
Acq On : 11 Jan 2022 10:55
Operator : JU/CG
Sample : PB141938BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB141938BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.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
Nonadecane	14.727	2.1	ng	50428	6	15.392	480616	20.0
Heptadecane	15.057	3.3	ng	78467	6	15.392	480616	20.0
Heneicosane	15.851	4.3	ng	102546	6	15.392	480616	20.0
Octacosane, 2-m...	16.339	4.0	ng	96479	6	15.392	480616	20.0
(1,1'-Biphenyl)...	16.686	4.3	ng	104648	6	15.392	480616	20.0
Tetracosane	16.909	2.9	ng	69902	6	15.392	480616	20.0
Sulfurous acid,...	17.592	2.9	ng	69760	6	15.392	480616	20.0