

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010923\
 Data File : BF131964.D
 Acq On : 09 Jan 2023 15:37
 Operator : CG\JU
 Sample : PB150003BL
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB150003BL

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-BF010923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131964.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.010	492	497	510	rBV	227819	392796	7.20%	1.398%
2	5.410	559	565	568	rBV	2878609	3009581	55.15%	10.712%
3	6.428	732	738	741	rBV	2523202	3101435	56.84%	11.039%
4	6.781	795	798	802	rBV	678879	613222	11.24%	2.183%
5	7.363	890	897	899	rBV	1723506	2067012	37.88%	7.357%
6	8.075	1013	1018	1021	rBV	941246	815448	14.94%	2.902%
7	9.157	1196	1202	1205	rBV	3931417	4243973	77.78%	15.105%
8	9.833	1311	1317	1321	rBV	1156300	1068013	19.57%	3.801%
9	10.633	1447	1453	1456	rBV	3048616	3029697	55.52%	10.783%
10	11.327	1567	1571	1574	rBV	1459359	1208770	22.15%	4.302%
11	12.739	1807	1811	1814	rBV	138013	112813	2.07%	0.402%
12	12.927	1837	1843	1846	rBV	4989966	5456647	100.00%	19.422%
13	13.445	1927	1931	1934	rBV	132006	106288	1.95%	0.378%
14	13.980	2018	2022	2025	rBV	1202796	1062871	19.48%	3.783%
15	14.745	2148	2152	2156	rBV	83843	79724	1.46%	0.284%
16	15.080	2204	2209	2215	rVB	100866	111790	2.05%	0.398%
17	15.445	2265	2271	2280	rBV	736578	951237	17.43%	3.386%
18	15.886	2341	2346	2352	rBV	90204	131314	2.41%	0.467%
19	16.386	2424	2431	2443	rBV2	82290	143746	2.63%	0.512%
20	16.915	2510	2521	2525	rBV4	29617	95714	1.75%	0.341%
21	16.968	2525	2530	2540	rVB	59896	130267	2.39%	0.464%
22	17.656	2640	2647	2659	rVB3	40933	102766	1.88%	0.366%
23	18.480	2779	2787	2795	rVB5	24143	60554	1.11%	0.216%

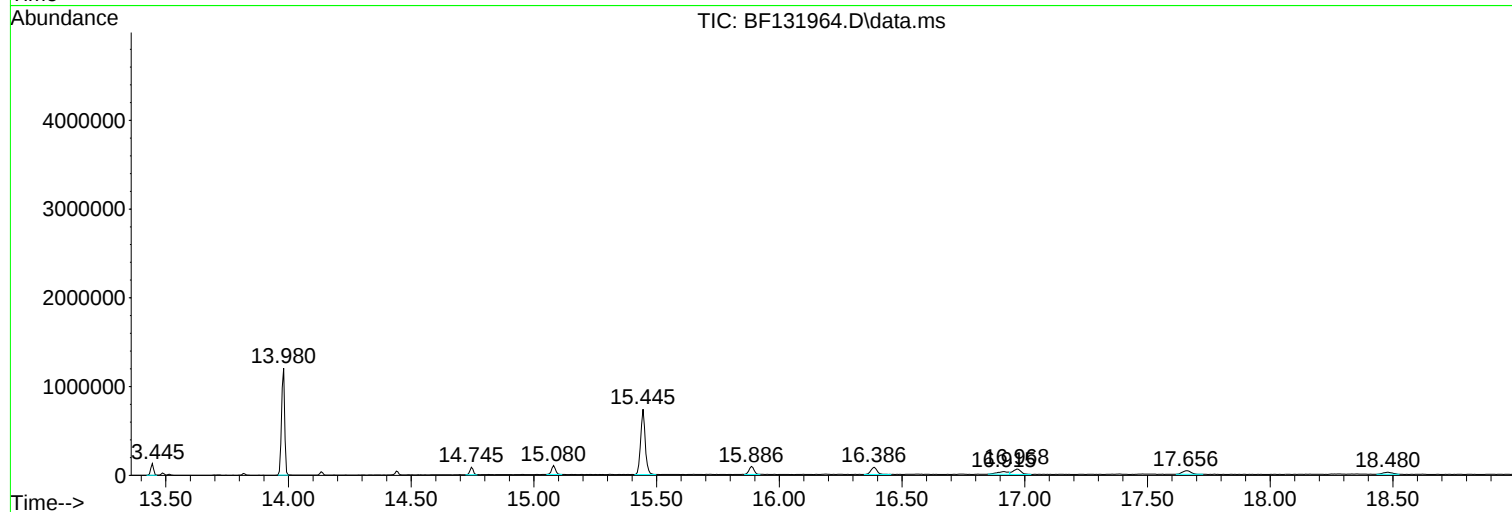
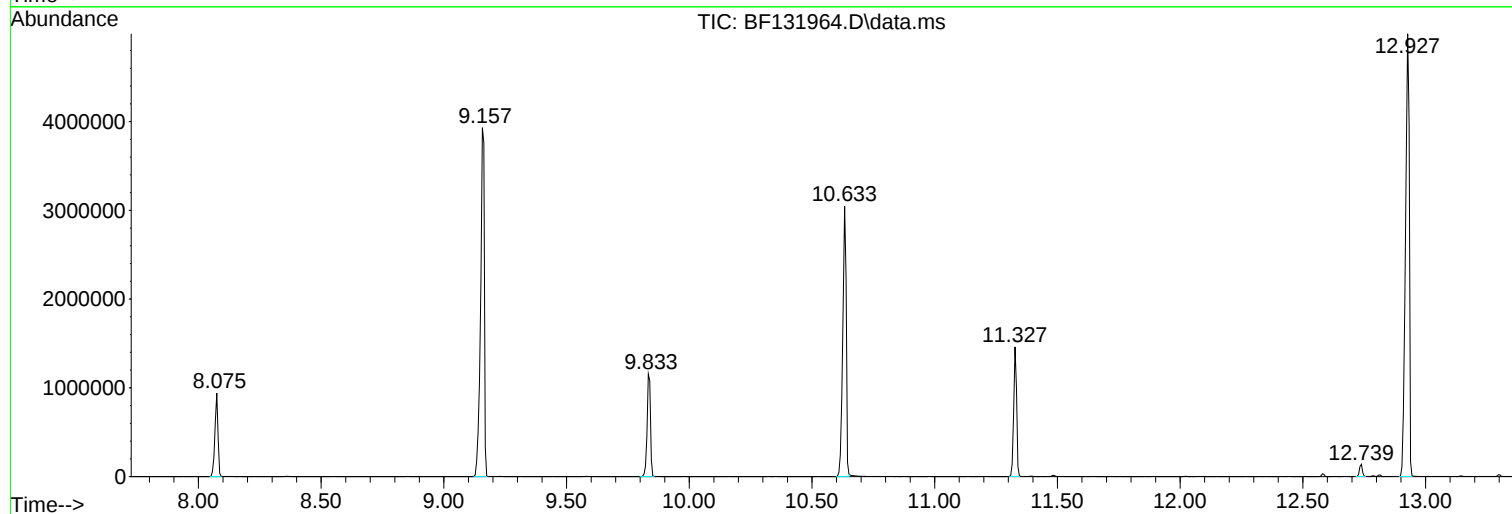
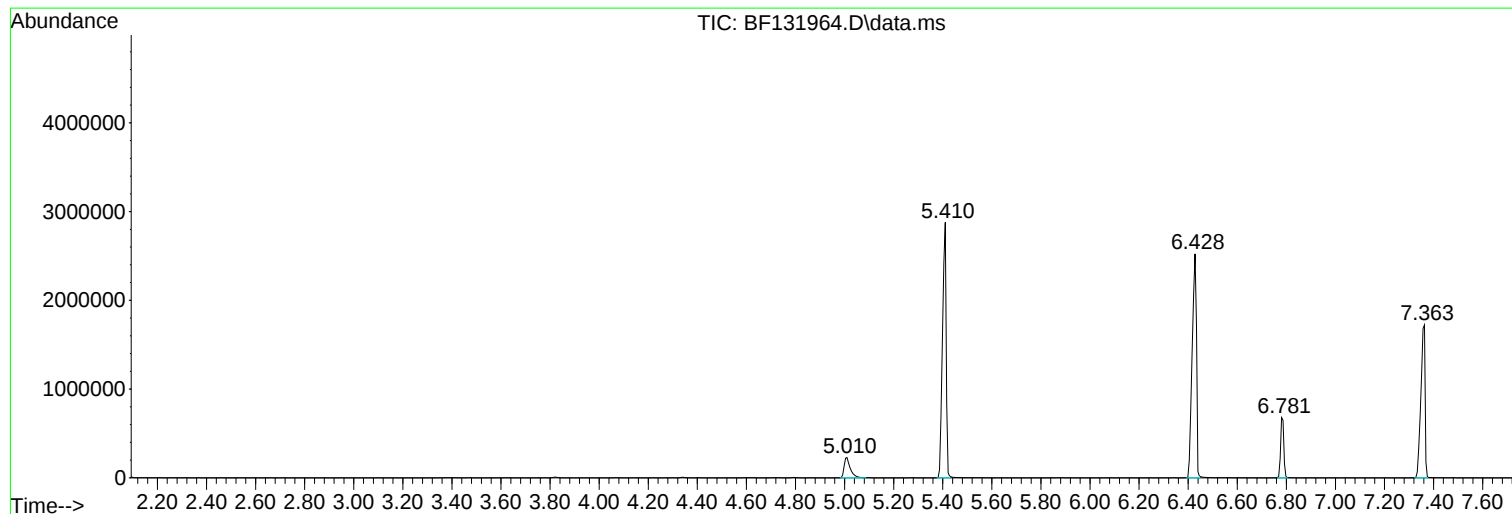
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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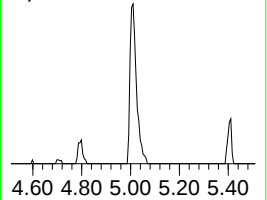
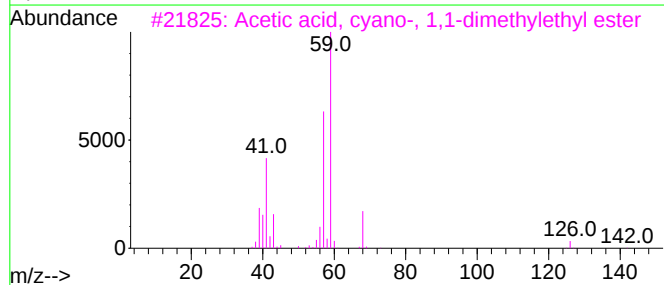
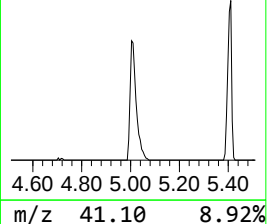
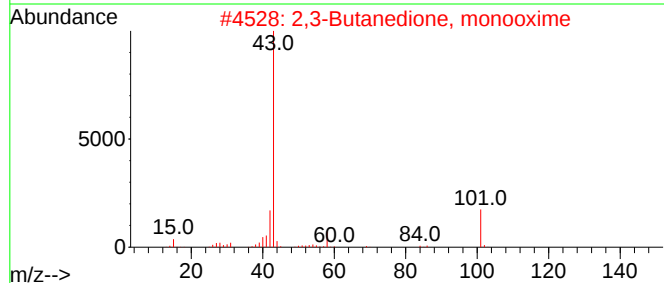
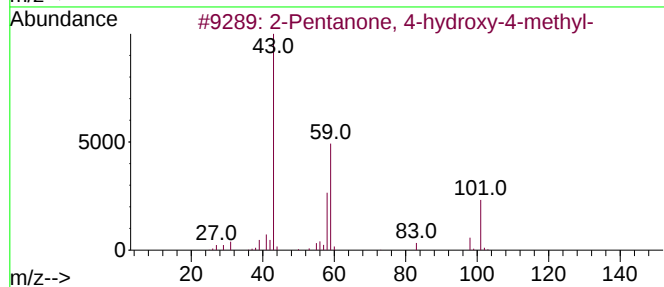
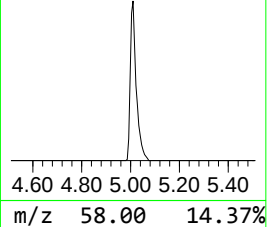
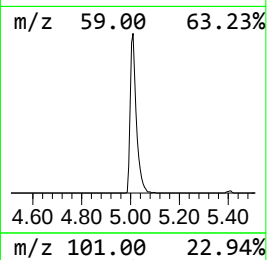
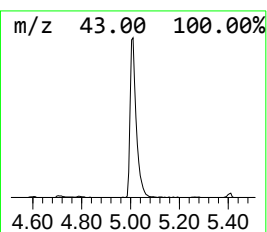
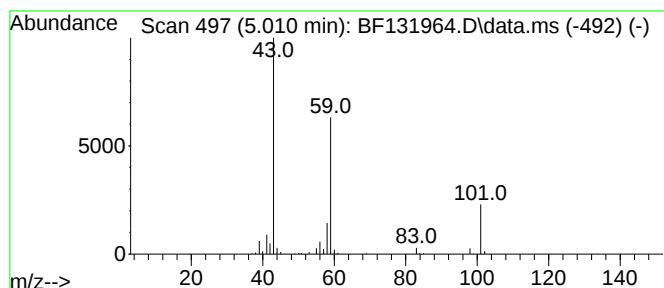
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.010	12.81 ng	392796	1,4-Dichlorobenzene-d4	6.786

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	38		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9		



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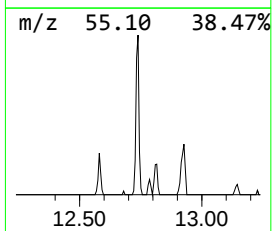
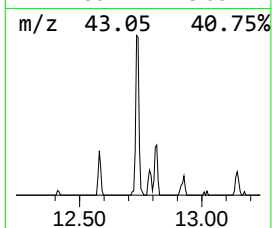
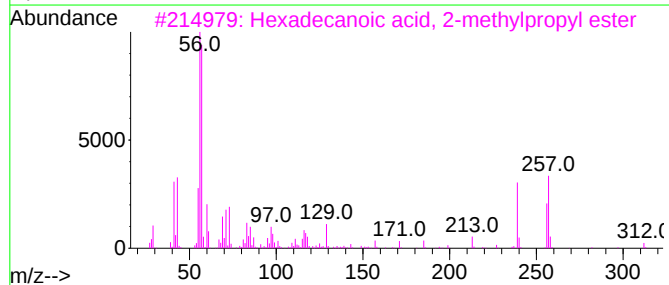
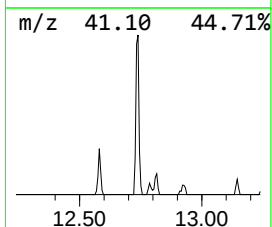
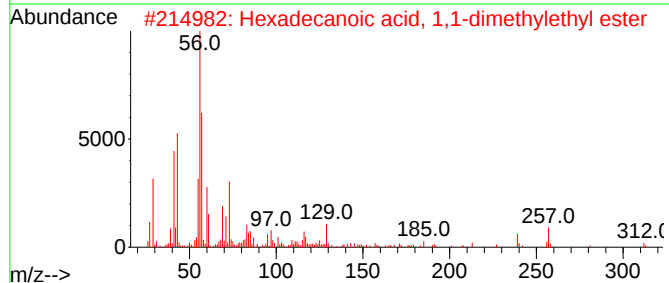
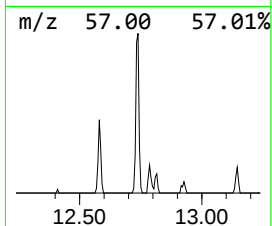
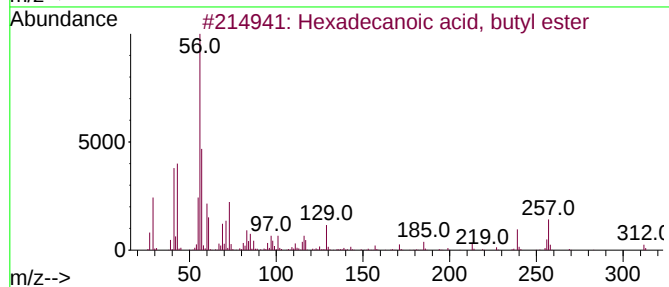
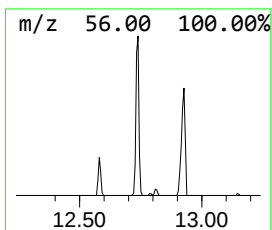
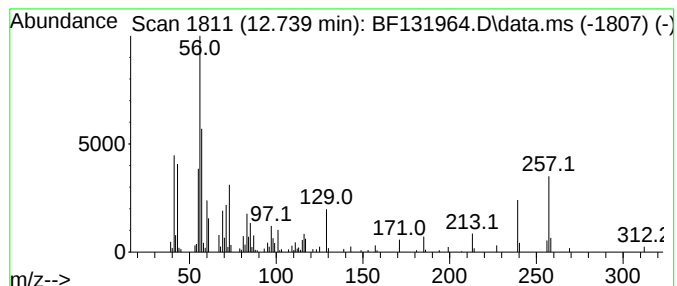
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
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Peak Number 2 Hexadecanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.739	2.12 ng	112813	Chrysene-d12	13.980	
Hit#	of 5	Tentative ID	MW MolForm	CAS#	Qual
1		Hexadecanoic acid, butyl ester	312 C20H40O2	000111-06-8	97
2		Hexadecanoic acid, 1,1-dimethyle...	312 C20H40O2	031158-91-5	70
3		Hexadecanoic acid, 2-methylpropy...	312 C20H40O2	000110-34-9	60
4		Cyclobutane, 1,1-dimethyl-2-octyl-	196 C14H28	062338-30-1	27
5		5-Methyl-2-hexanol, trifluoroace...	212 C9H15F3O2	1000364-20-2	27



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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
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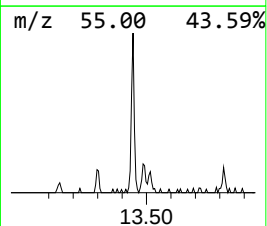
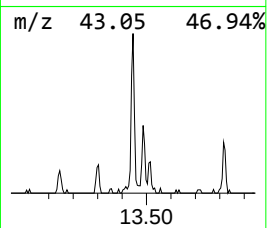
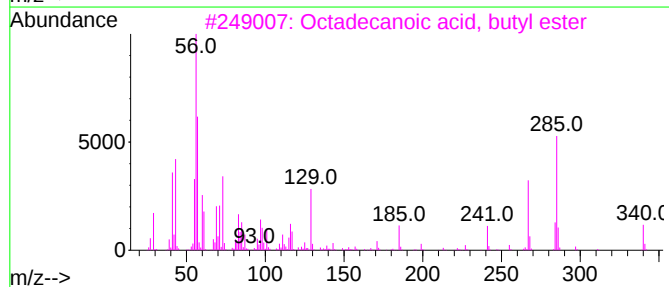
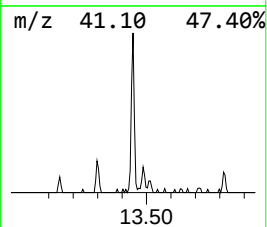
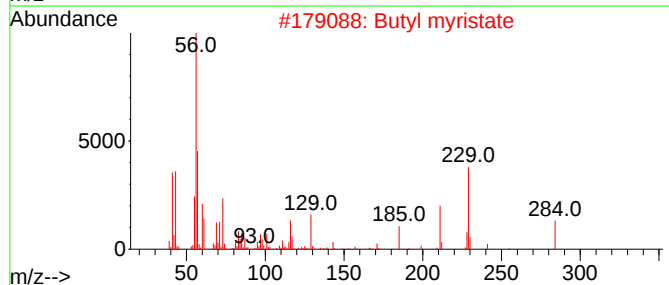
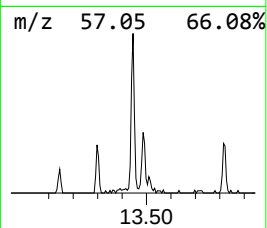
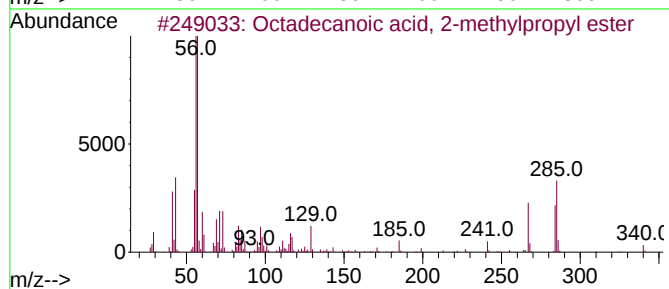
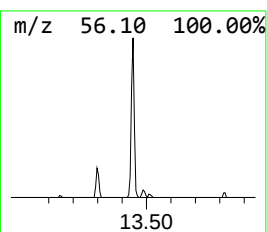
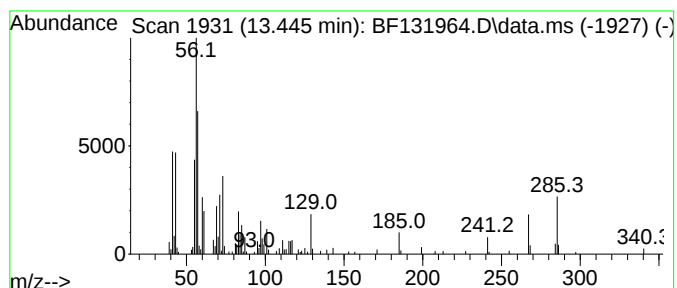
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 3 Octadecanoic acid, 2-methyl... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.445	2.00 ng	106288	Chrysene-d12	13.980

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	64
2			Butyl myristate	284	C18H36O2	000110-36-1	59
3			Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	49
4			Cyclohexanol, 4-amino-, trans-	115	C6H13NO	027489-62-9	30
5			1-Heptene, 2-methyl-	112	C8H16	015870-10-7	30



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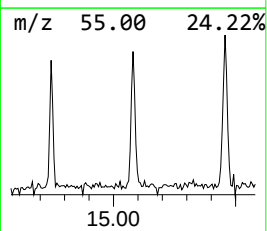
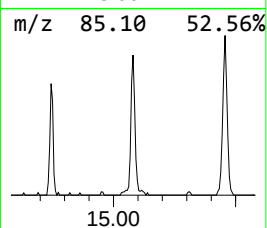
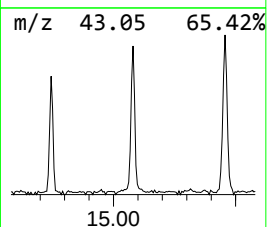
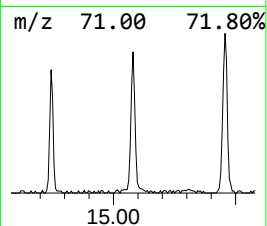
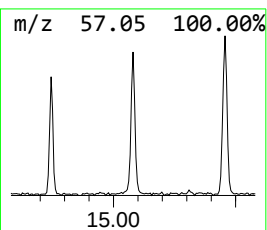
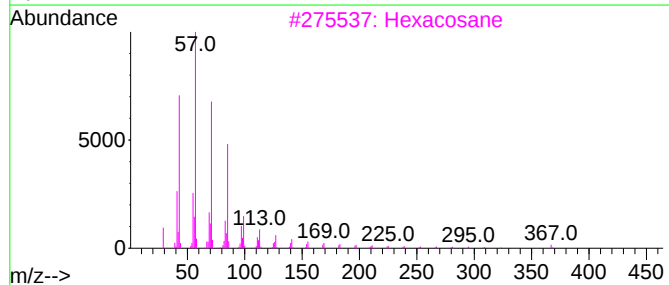
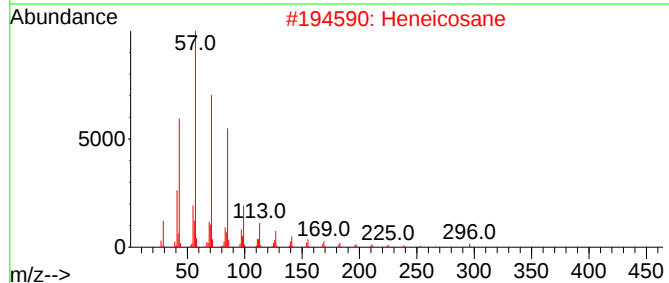
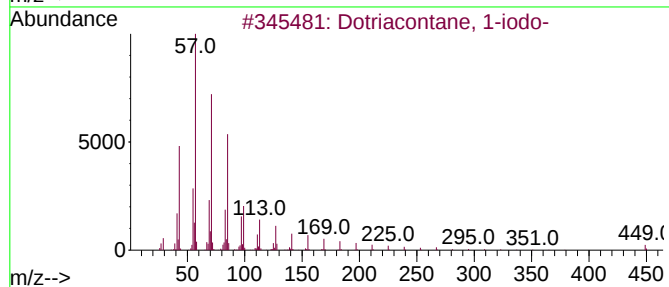
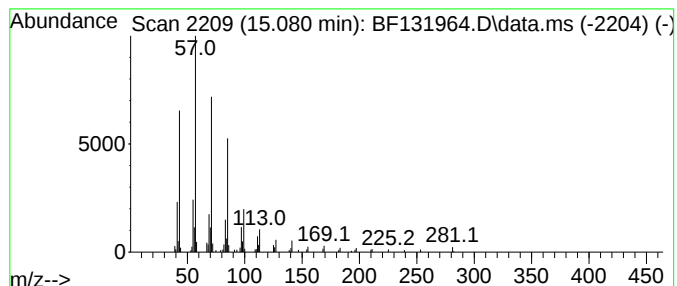
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Peak Number 4 Dotriacontane, 1-iodo- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.080	2.35 ng	111790	Perylene-d12	15.445

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Hexacosane	366	C26H54	000630-01-3	90
4		Octadecane, 1-iodo-	380	C18H37I	000629-93-6	86
5		Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	83



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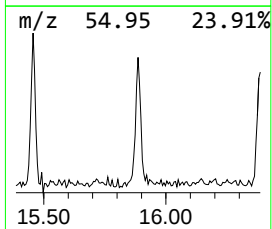
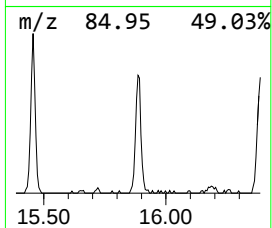
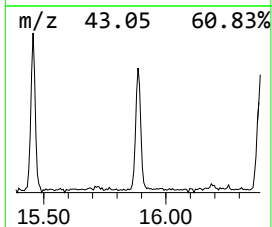
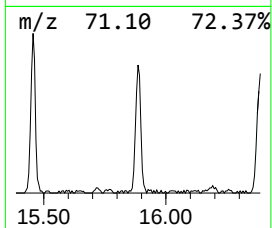
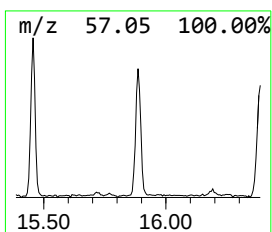
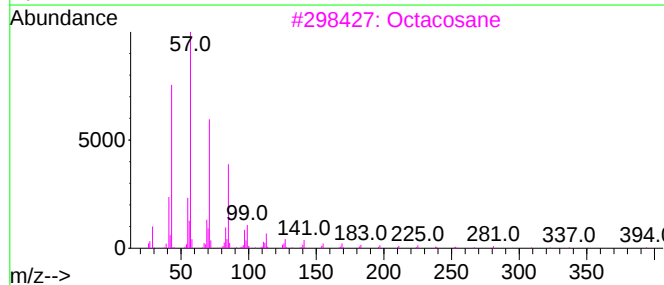
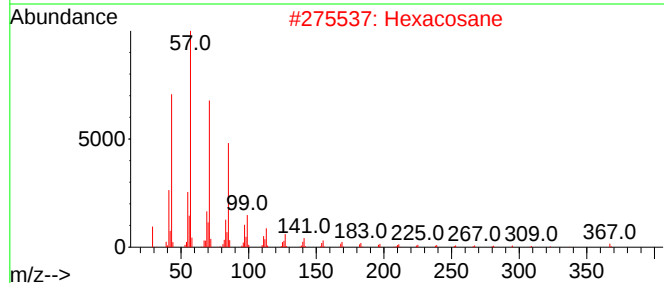
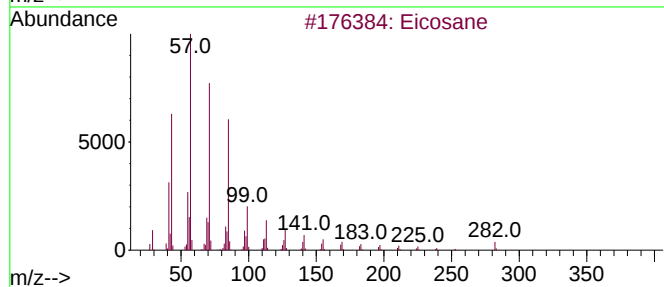
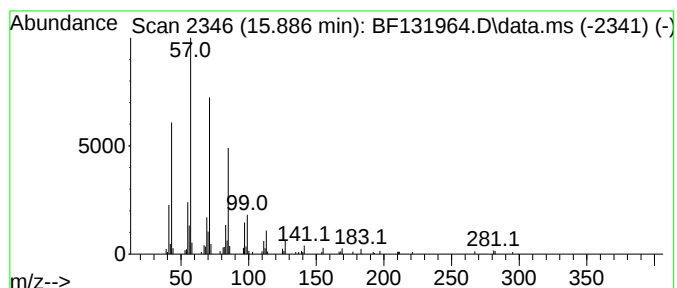
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TIC Integration Parameters: LSCINT.P

Peak Number 5 Eicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.886	2.76 ng	131314	Perylene-d12	15.445

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	91
2			Hexacosane	366	C26H54	000630-01-3	91
3			Octacosane	394	C28H58	000630-02-4	91
4			Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
5			Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	90



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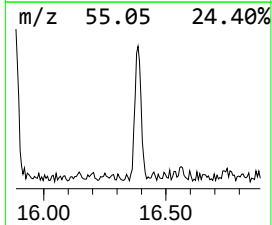
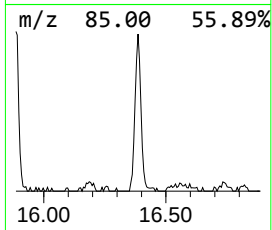
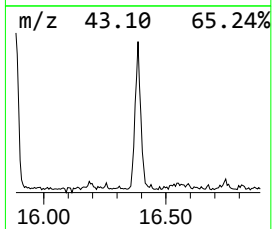
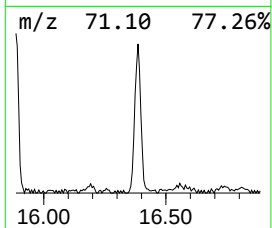
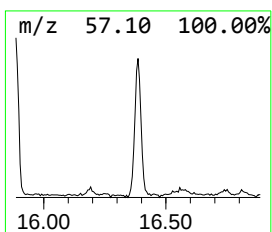
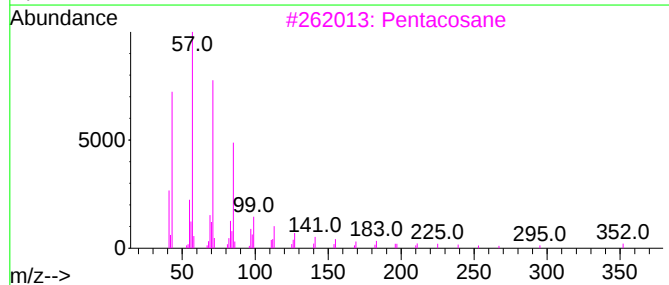
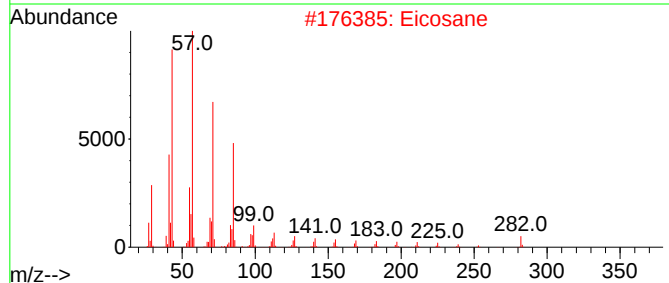
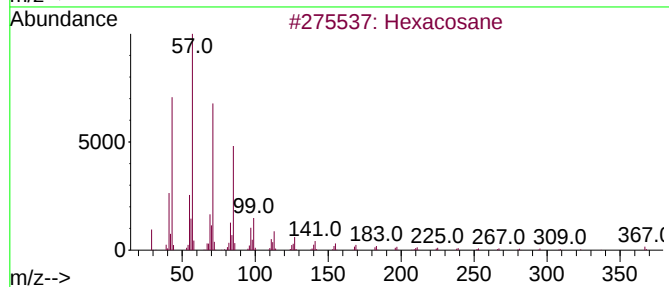
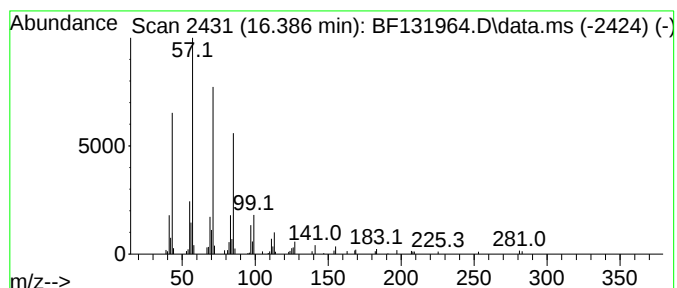
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexacosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.386	3.02 ng	143746	Perylene-d12	15.445

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	91
2			Eicosane	282	C20H42	000112-95-8	91
3			Pentacosane	352	C25H52	000629-99-2	91
4			Heptadecane	240	C17H36	000629-78-7	91
5			Heneicosane	296	C21H44	000629-94-7	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010923\
Data File : BF131964.D
Acq On : 09 Jan 2023 15:37
Operator : CG\JU
Sample : PB150003BL
Misc :
ALS Vial : 11 Sample Multiplier: 1

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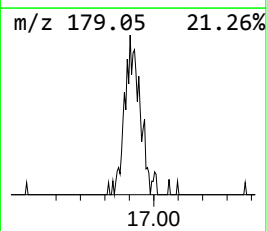
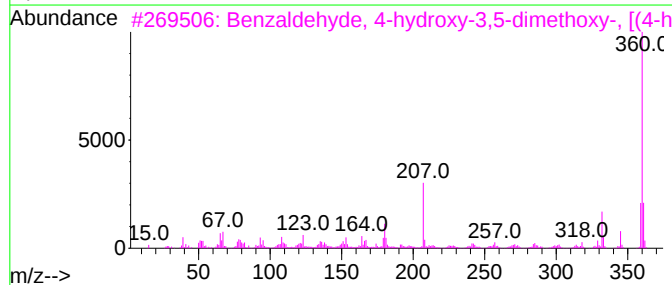
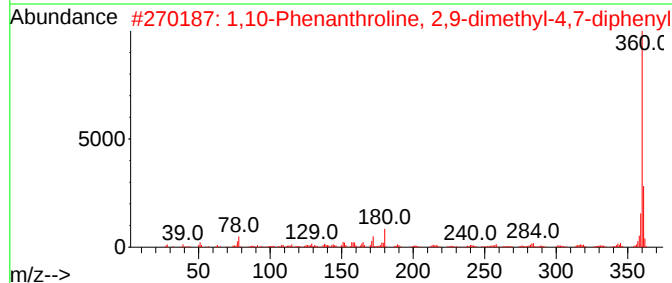
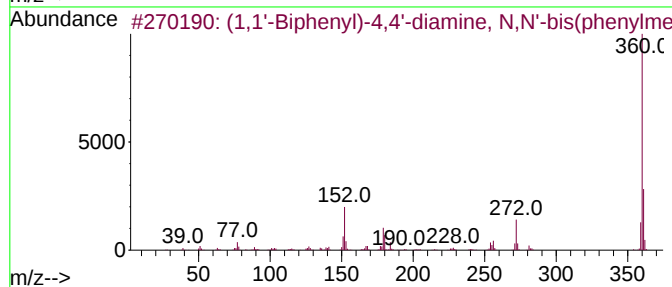
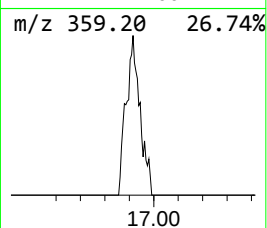
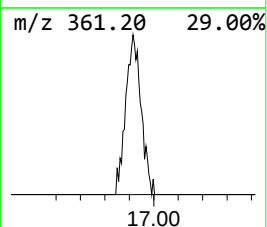
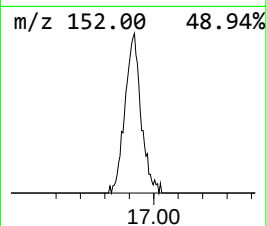
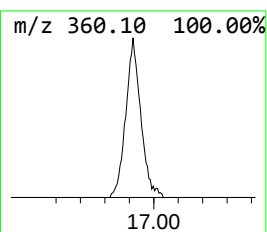
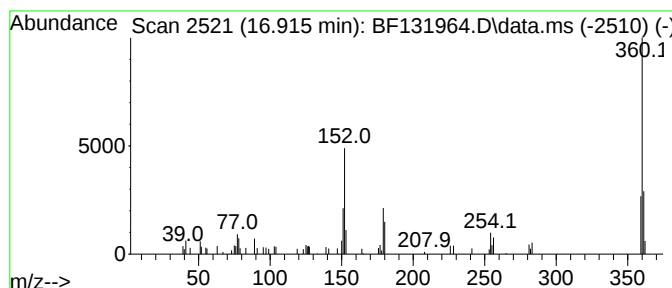
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 (1,1'-Biphenyl)-4,4'-diamin... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.915	2.01 ng	95714	Perylene-d12	15.445

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(1,1'-Biphenyl)-4,4'-diamine, N,...	360	C26H20N2	006311-48-4	90
2			1,10-Phenanthroline, 2,9-dimethy...	360	C26H20N2	004733-39-5	43
3			Benzaldehyde, 4-hydroxy-3,5-dime...	360	C18H20N2O6	014414-32-5	43
4			1,3,2-Dioxaborolane, bis(spiro[4...	360	C20H13B06	1000150-23-7	43
5			Ethene, 1-(anthracen-9-yl)-2-(4-...	360	C27H20O	1000163-55-1	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010923\
Data File : BF131964.D
Acq On : 09 Jan 2023 15:37
Operator : CG\JU
Sample : PB150003BL
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB150003BL

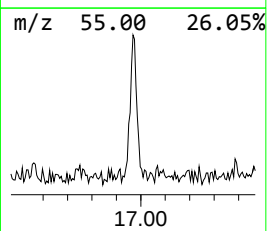
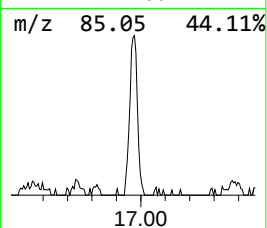
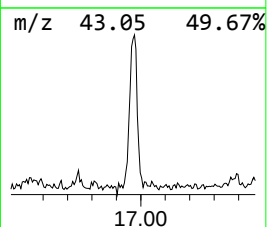
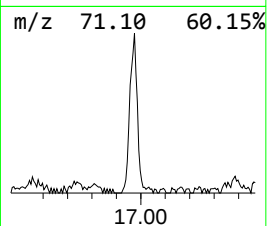
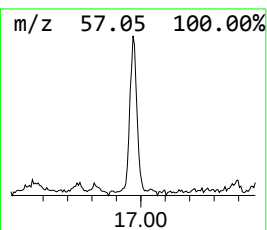
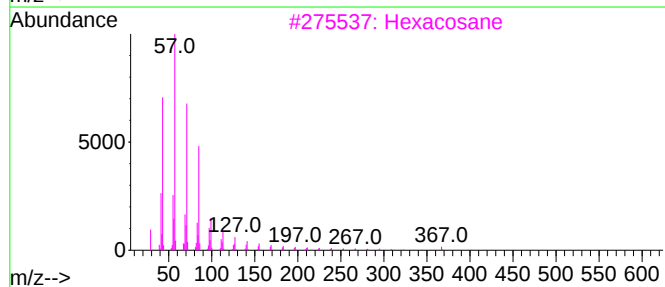
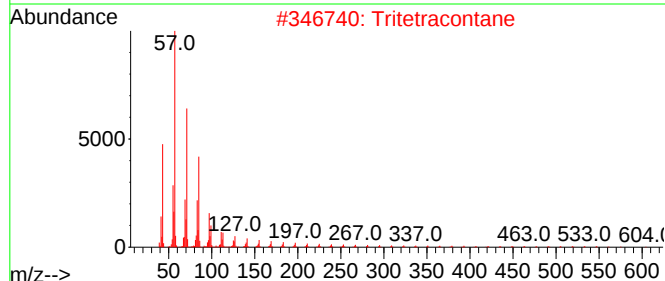
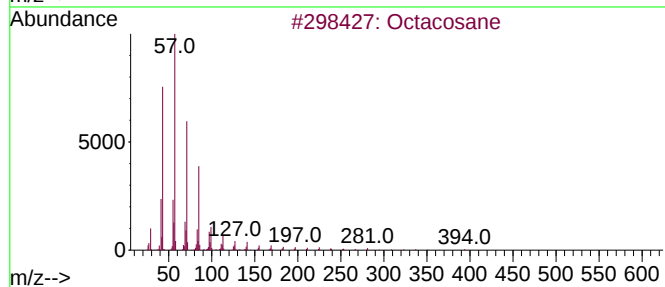
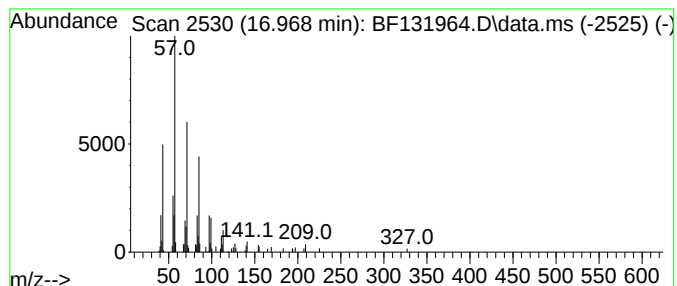
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.968	2.74 ng	130267	Perylene-d12	15.445

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	90
2			Tritetracontane	605	C43H88	007098-21-7	90
3			Hexacosane	366	C26H54	000630-01-3	90
4			10-Methylnonadecane	282	C20H42	056862-62-5	87
5			Pentacosane	352	C25H52	000629-99-2	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010923\
Data File : BF131964.D
Acq On : 09 Jan 2023 15:37
Operator : CG\JU
Sample : PB150003BL
Misc :
ALS Vial : 11 Sample Multiplier: 1

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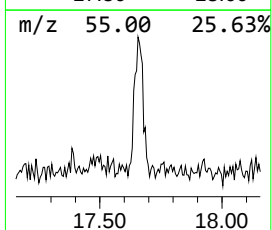
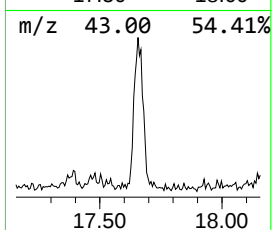
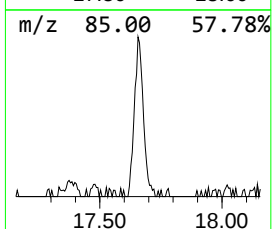
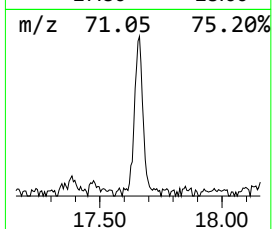
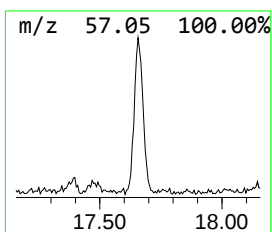
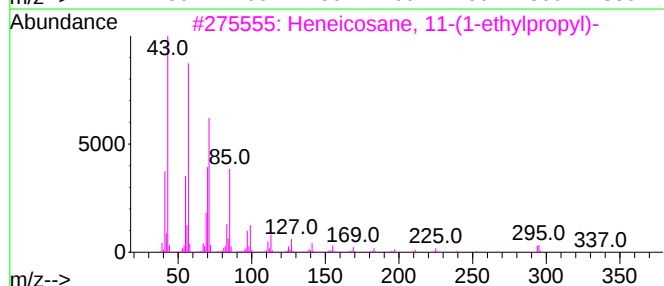
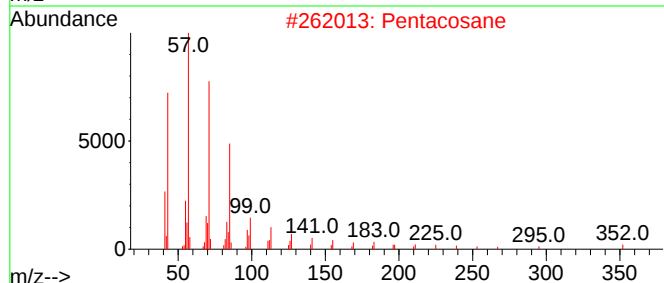
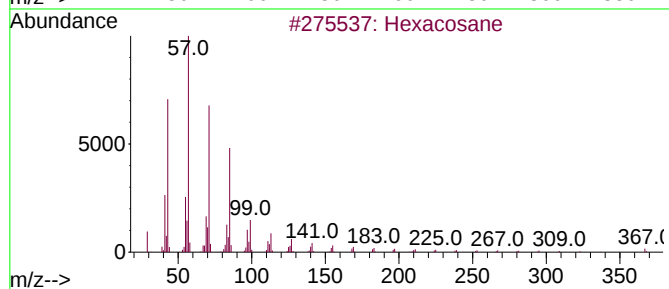
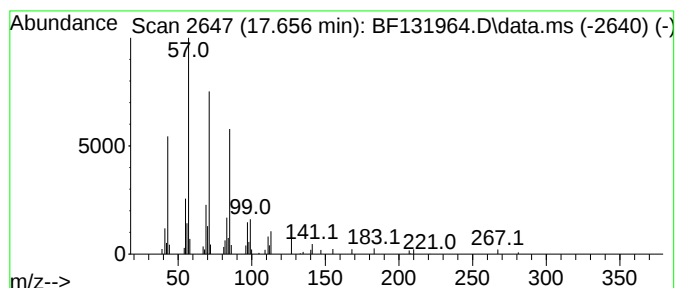
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Pentacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.656	2.16 ng	102766	Perylene-d12	15.445

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane			366	C26H54	000630-01-3	91
2	Pentacosane			352	C25H52	000629-99-2	91
3	Heneicosane, 11-(1-ethylpropyl)-			366	C26H54	055282-11-6	91
4	Heptadecane			240	C17H36	000629-78-7	91
5	Nonadecane			268	C19H40	000629-92-5	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010923\
Data File : BF131964.D
Acq On : 09 Jan 2023 15:37
Operator : CG\JU
Sample : PB150003BL
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB150003BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.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
2-Pentanone, 4-...	5.010	12.8	ng	392796	1	6.786	613222	20.0
Hexadecanoic ac...	12.739	2.1	ng	112813	5	13.980	1062870	20.0
Octadecanoic ac...	13.445	2.0	ng	106288	5	13.980	1062870	20.0
Dotriacontane, ...	15.080	2.4	ng	111790	6	15.445	951237	20.0
Eicosane	15.886	2.8	ng	131314	6	15.445	951237	20.0
Hexacosane	16.386	3.0	ng	143746	6	15.445	951237	20.0
(1,1'-Biphenyl)...	16.915	2.0	ng	95714	6	15.445	951237	20.0
Octacosane	16.968	2.7	ng	130267	6	15.445	951237	20.0
Pentacosane	17.656	2.2	ng	102766	6	15.445	951237	20.0