

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051823\
 Data File : BF133436.D
 Acq On : 18 May 2023 12:28
 Operator : CG\JU
 Sample : 02812-08
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WG-0516-B3-10-20

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-BF042123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133436.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.898	473	478	490	rVB	813149	1098048	20.09%	2.707%
2	5.334	547	552	562	rBV	4782220	4931119	90.22%	12.155%
3	5.722	614	618	622	rBV	79217	78132	1.43%	0.193%
4	6.363	722	727	730	rBV	5058836	4852491	88.78%	11.961%
5	6.710	783	786	790	rBV	1375662	1092397	19.99%	2.693%
6	7.281	878	883	886	rBV	3527679	3132661	57.32%	7.722%
7	7.998	1001	1005	1008	rBV	1756112	1496778	27.39%	3.690%
8	9.075	1184	1188	1191	rBV	6462970	5401158	98.82%	13.314%
9	9.751	1299	1303	1306	rBV	1907500	1692307	30.96%	4.172%
10	10.463	1419	1424	1428	rBV	189765	172438	3.16%	0.425%
11	10.539	1433	1437	1440	rBV	3815326	3387035	61.97%	8.349%
12	11.233	1551	1555	1558	rBV	1991961	1733482	31.72%	4.273%
13	11.769	1641	1646	1666	rBV2	733135	1023564	18.73%	2.523%
14	12.010	1677	1687	1697	rVB4	78918	244220	4.47%	0.602%
15	12.557	1772	1780	1790	rBV	258444	447224	8.18%	1.102%
16	12.821	1820	1825	1828	rBV	5864082	5465474	100.00%	13.472%
17	13.368	1912	1918	1921	rBV3	82296	167093	3.06%	0.412%
18	13.727	1975	1979	1981	rBV	93807	91776	1.68%	0.226%
19	13.757	1981	1984	1995	rVV	134218	331645	6.07%	0.818%
20	13.868	1997	2003	2011	rVB	1544740	1398512	25.59%	3.447%
21	13.986	2016	2023	2029	rVV	80247	173570	3.18%	0.428%
22	14.039	2029	2032	2036	rVB	87775	81823	1.50%	0.202%
23	14.345	2081	2084	2088	rVB	104433	93740	1.72%	0.231%
24	14.498	2106	2110	2118	rBV2	103813	165949	3.04%	0.409%
25	14.639	2131	2134	2138	rVB	93551	100280	1.83%	0.247%
26	14.962	2186	2189	2192	rBV	91551	90482	1.66%	0.223%
27	15.010	2193	2197	2210	rVB2	79461	146100	2.67%	0.360%
28	15.292	2240	2245	2249	rBV	1088359	1334260	24.41%	3.289%
29	15.592	2293	2296	2302	rVB2	42259	68773	1.26%	0.170%
30	15.727	2316	2319	2324	rVB	58142	75479	1.38%	0.186%

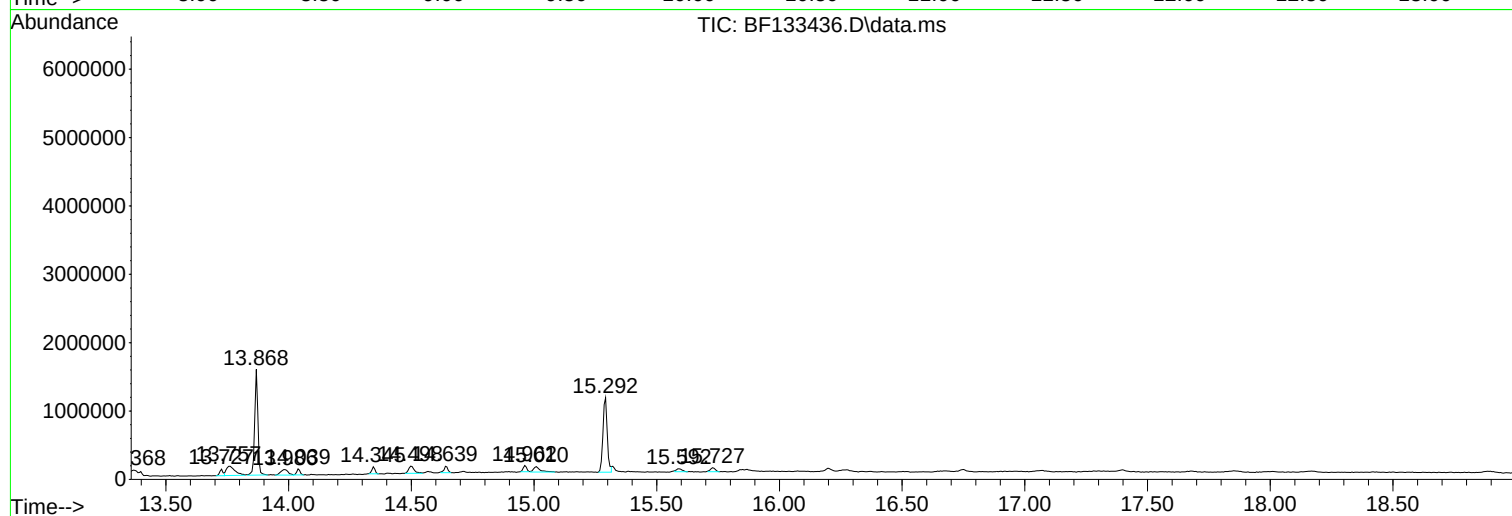
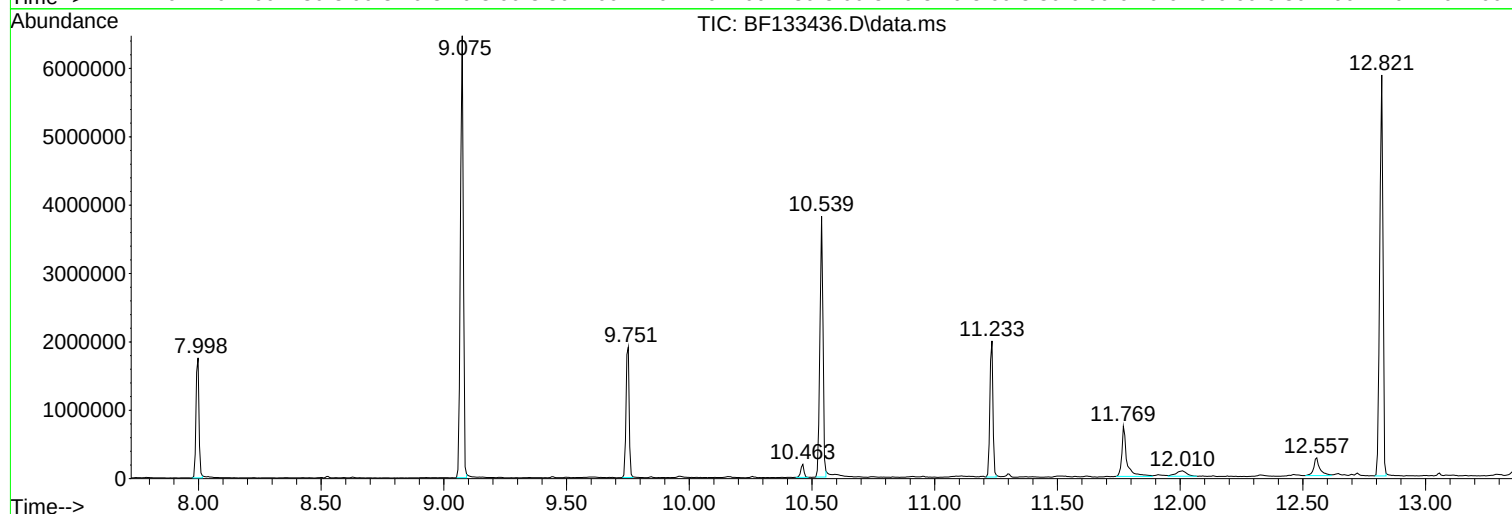
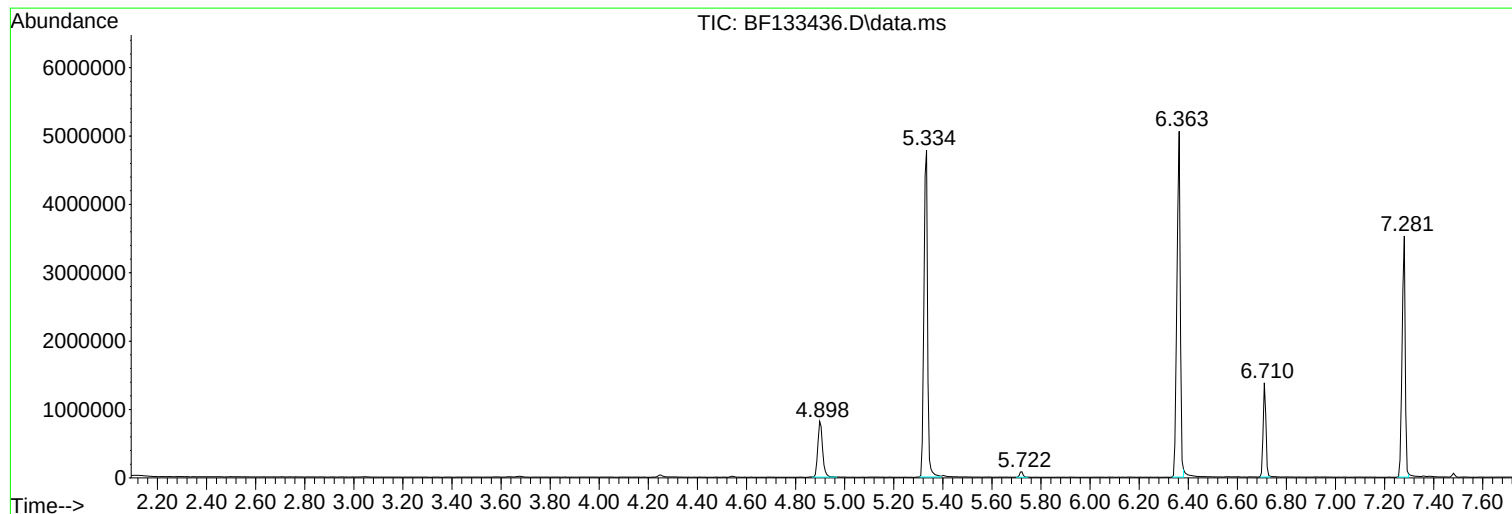
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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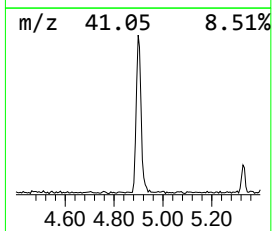
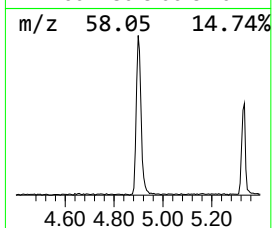
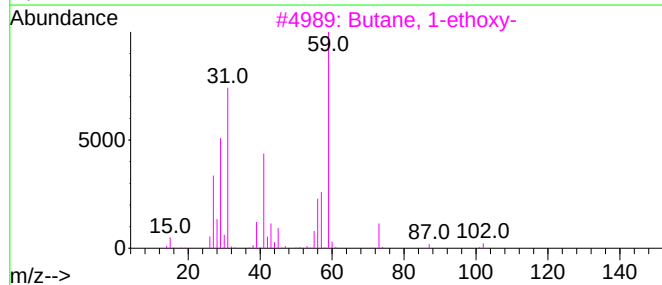
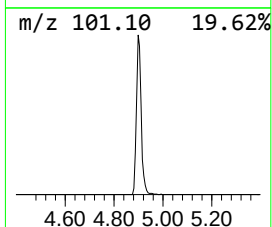
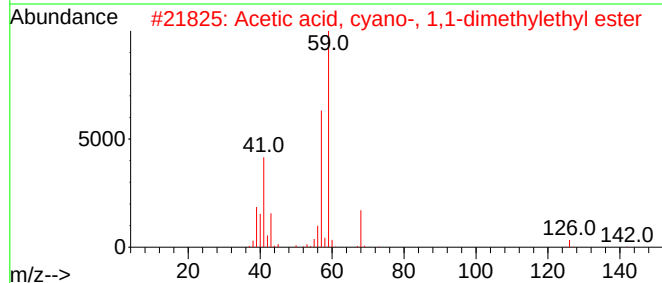
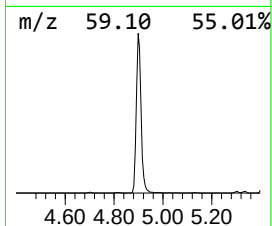
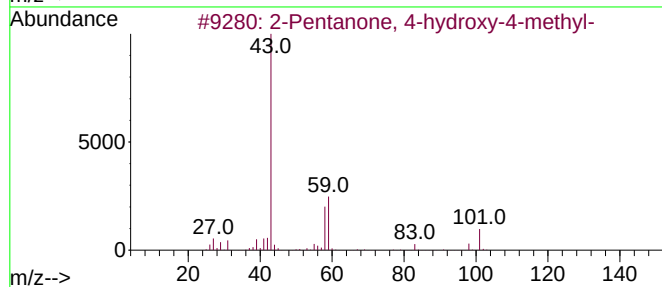
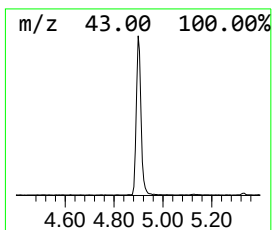
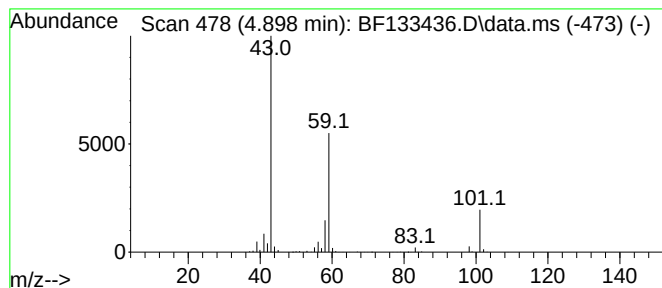
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.898	20.10 ng	1098050	1,4-Dichlorobenzene-d4	6.710

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9		
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		



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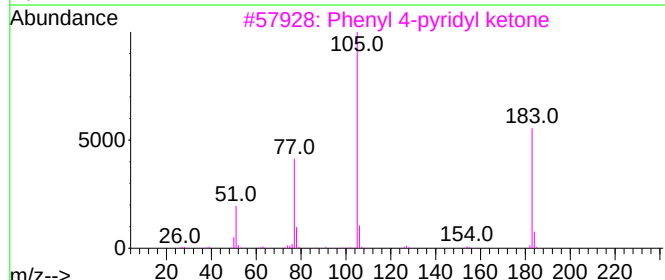
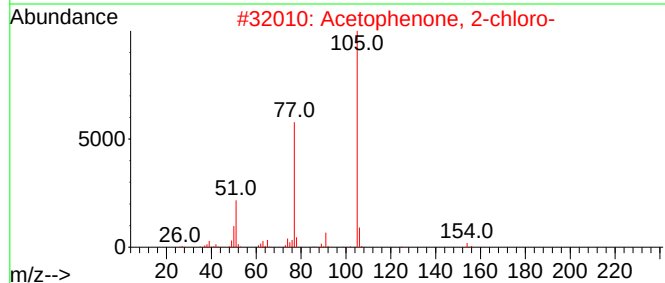
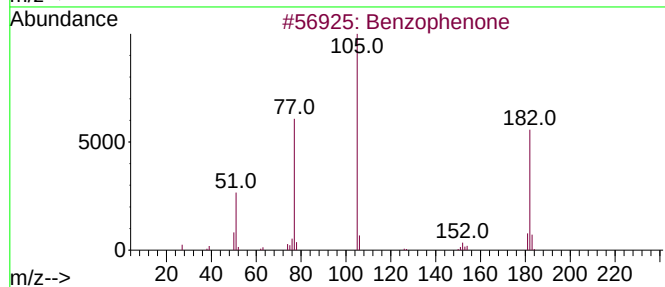
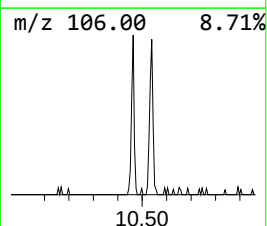
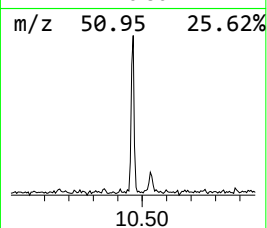
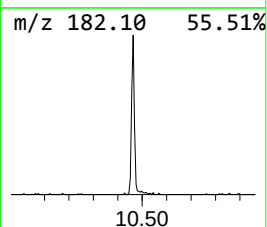
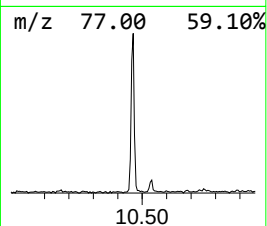
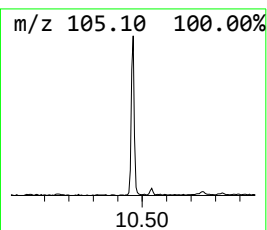
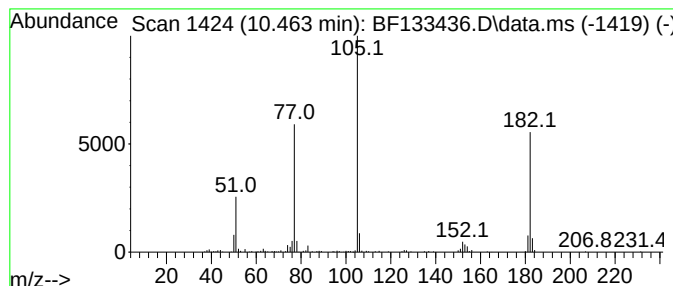
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Benzophenone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.463	2.04 ng	172438	Acenaphthene-d10	9.751

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	53
3			Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	49
4			N-[2,2-Dichloro-1-(toluene-4-sul...	371	C16H15Cl2N03S	136800-77-6	47
5			Disulfide, dibenzoyl	274	C14H10O2S2	000644-32-6	47



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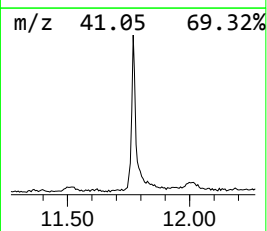
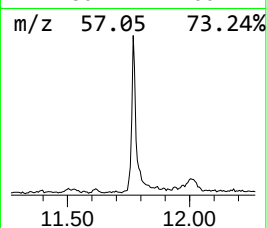
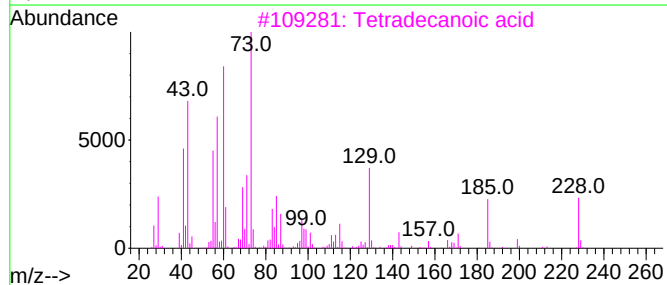
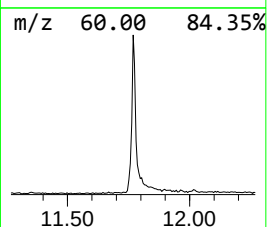
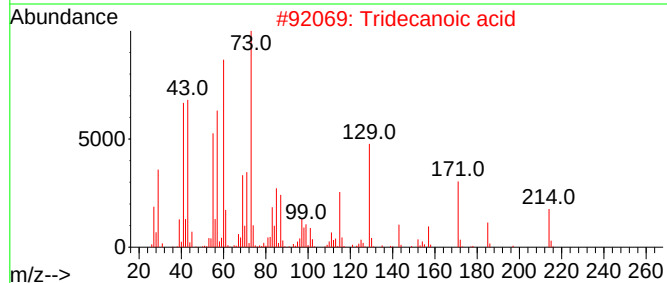
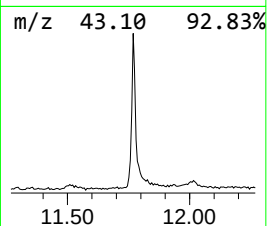
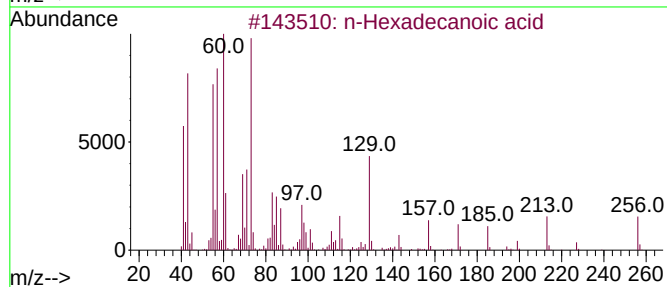
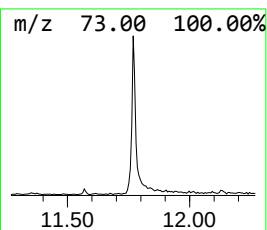
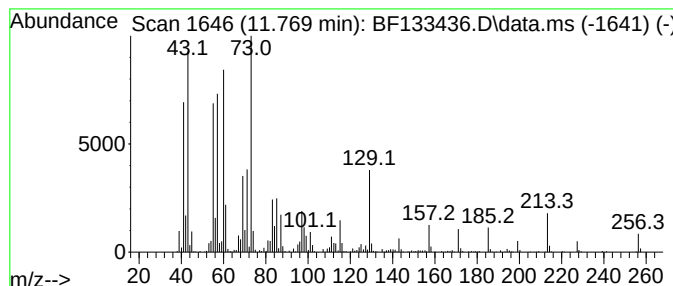
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.769	11.81 ng	1023560	Phenanthrene-d10	11.233

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	95
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5			n-Decanoic acid	172	C10H20O2	000334-48-5	62



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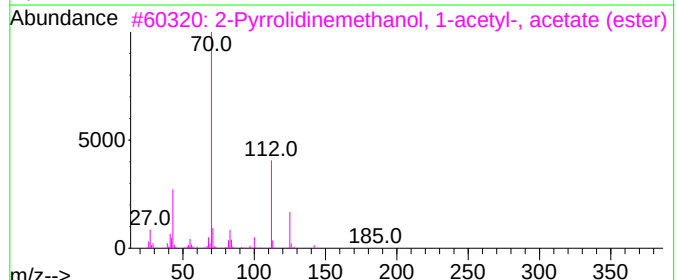
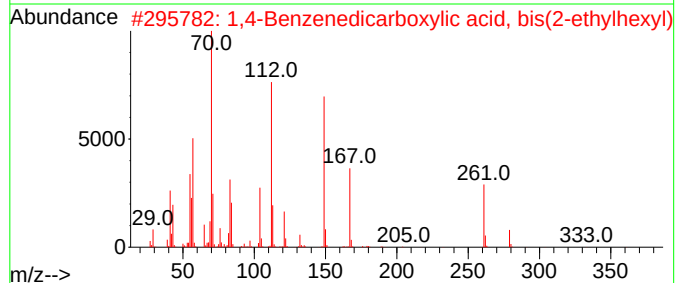
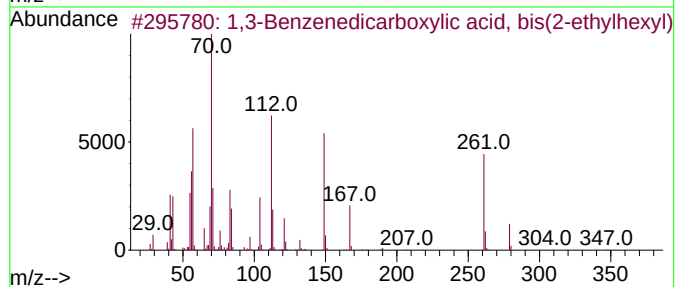
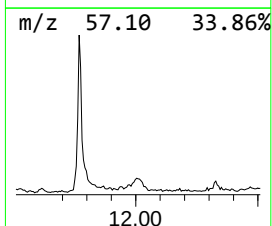
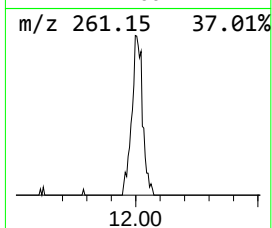
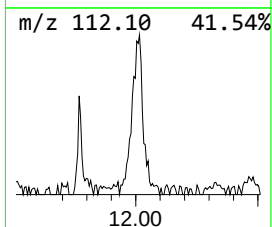
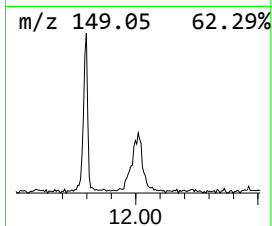
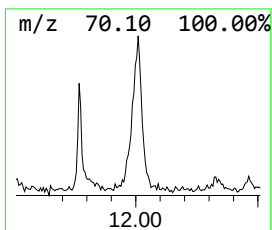
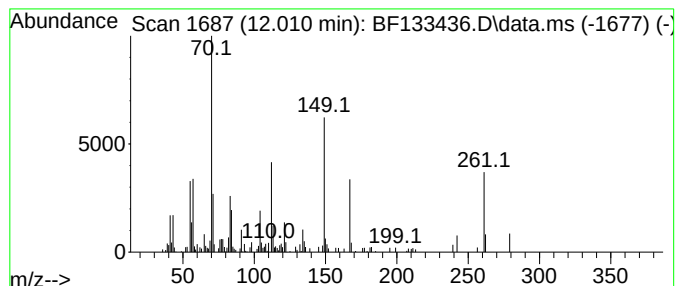
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Peak Number 4 1,3-Benzenedicarboxylic aci... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.010	2.82 ng	244220	Phenanthrene-d10	11.233	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	52
2	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	38
3	2-Pyrrolidinemethanol, 1-acetyl-...	185	C9H15NO3	042366-60-9	35
4	Cyclohexylamine, N-methyl-4,4-di...	141	C9H19N	045815-91-6	27
5	5-Fluoro-2-[(4-methyl-1-piperazi...	261	C14H16FN3O	459168-42-4	16



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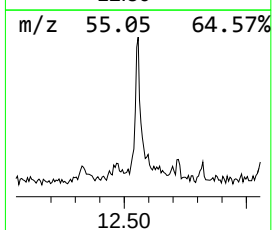
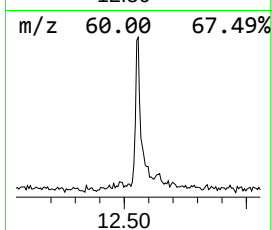
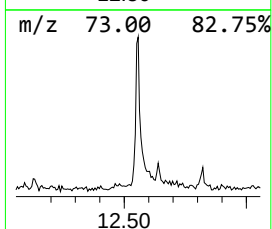
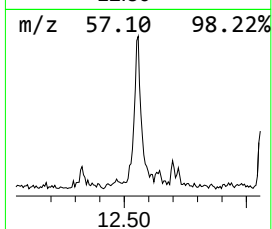
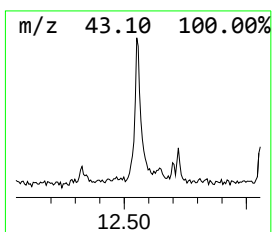
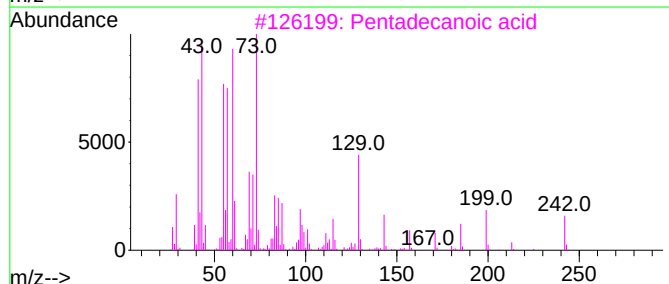
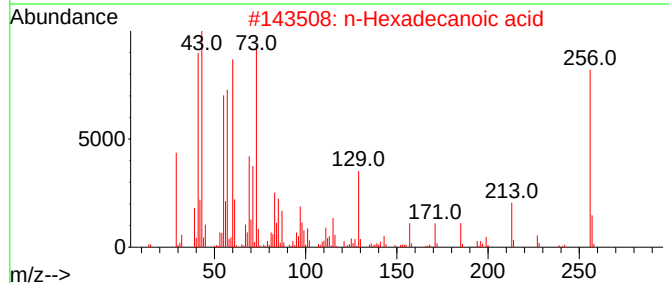
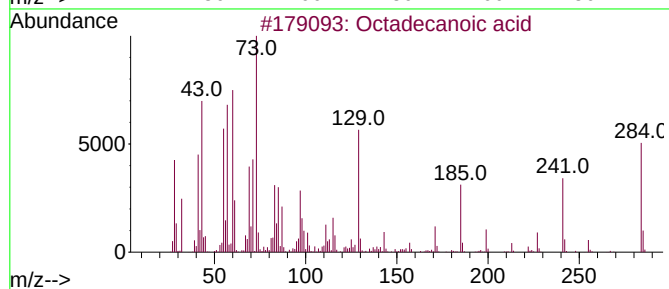
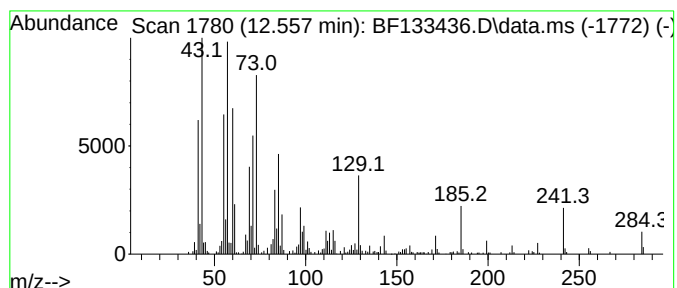
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Peak Number 5 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.557	6.40 ng	447224	Chrysene-d12	13.868

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	78
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	50
4			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	42
5			2-Butenoic acid, 2-methoxy-3-met...	144	C7H12O3	056009-32-6	42



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WG-0516-B3-10-20

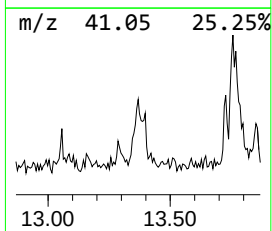
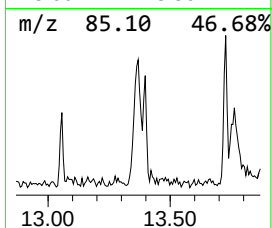
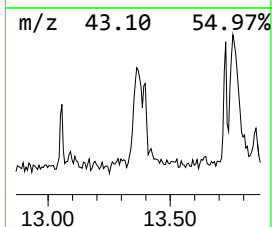
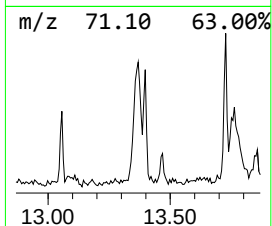
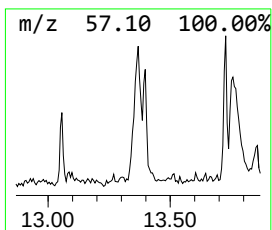
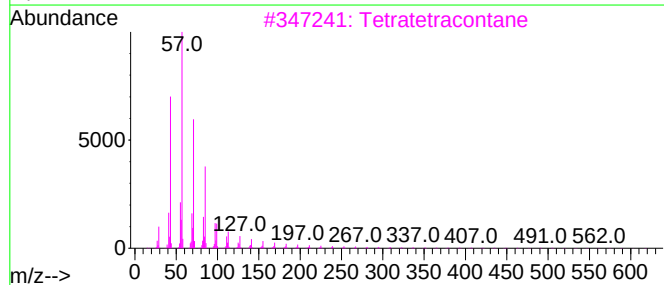
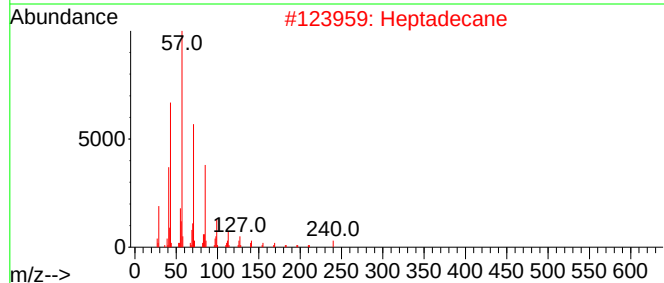
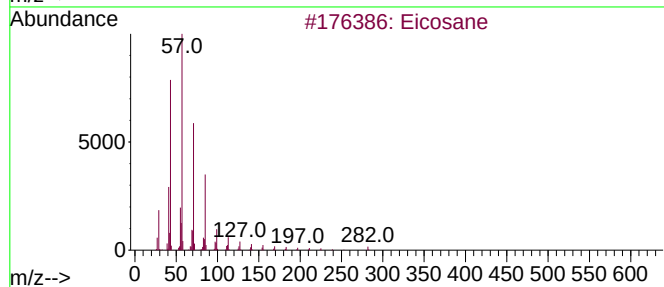
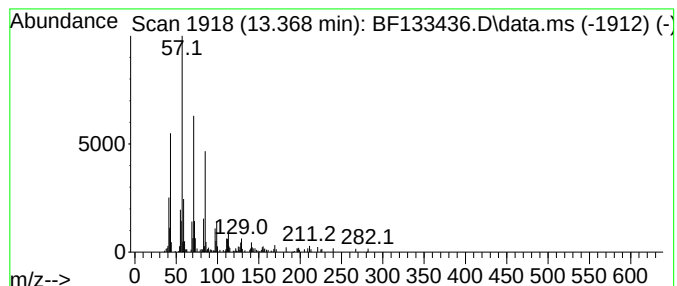
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.368	2.39 ng	167093	Chrysene-d12	13.868

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane			282	C20H42	000112-95-8	89
2	Heptadecane			240	C17H36	000629-78-7	76
3	Tetratetracontane			619	C44H90	007098-22-8	76
4	Pentacosane			352	C25H52	000629-99-2	72
5	Tetradecane			198	C14H30	000629-59-4	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051823\
Data File : BF133436.D
Acq On : 18 May 2023 12:28
Operator : CG\JU
Sample : 02812-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WG-0516-B3-10-20

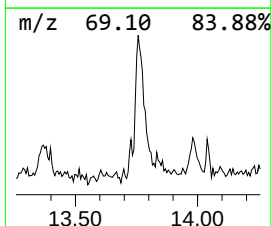
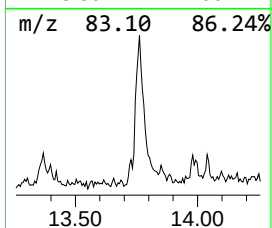
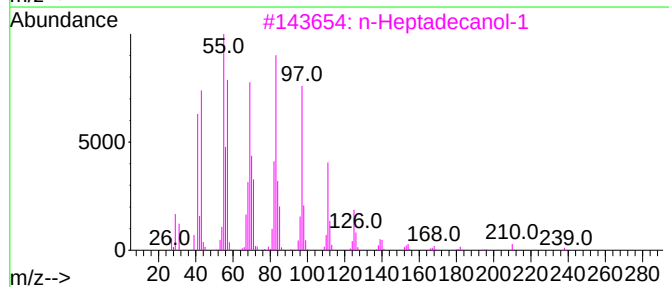
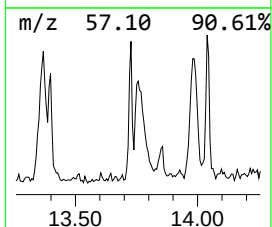
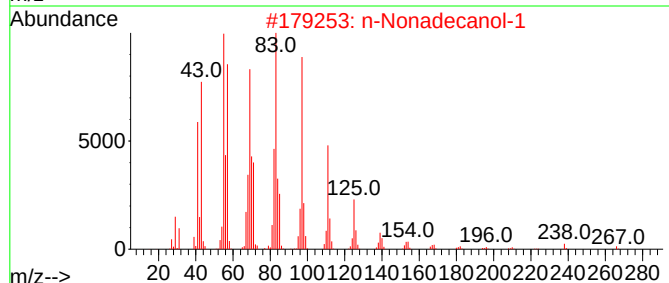
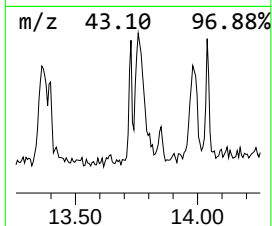
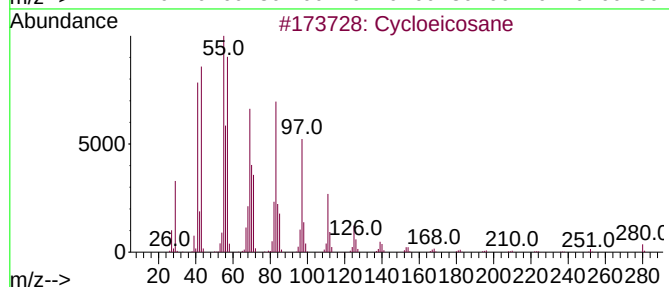
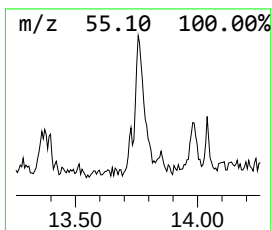
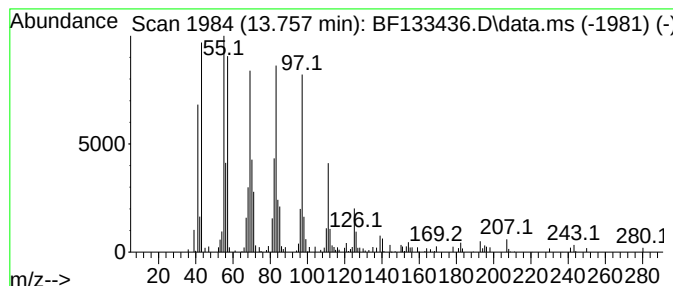
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Cycloeicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.757	4.74 ng	331645	Chrysene-d12	13.868

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cycloeicosane	280	C20H40	000296-56-0	96
2		n-Nonadecanol-1	284	C19H40O	001454-84-8	95
3		n-Heptadecanol-1	256	C17H36O	001454-85-9	94
4		1-Heneicosanol	312	C21H44O	015594-90-8	93
5		Cyclotridecane	182	C13H26	000295-02-3	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051823\
Data File : BF133436.D
Acq On : 18 May 2023 12:28
Operator : CG\JU
Sample : 02812-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
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ClientSampleId :
WG-0516-B3-10-20

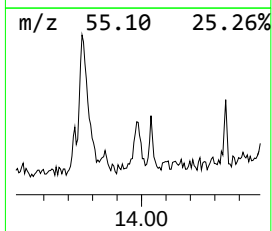
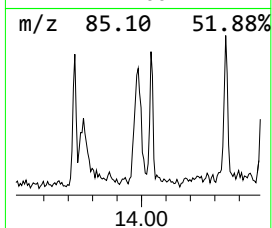
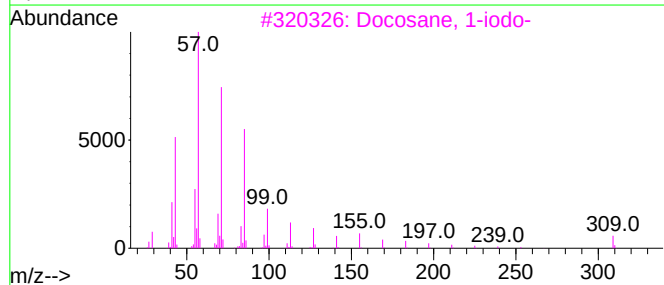
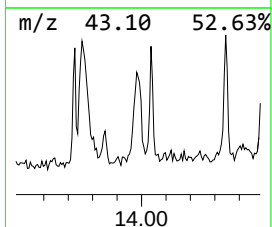
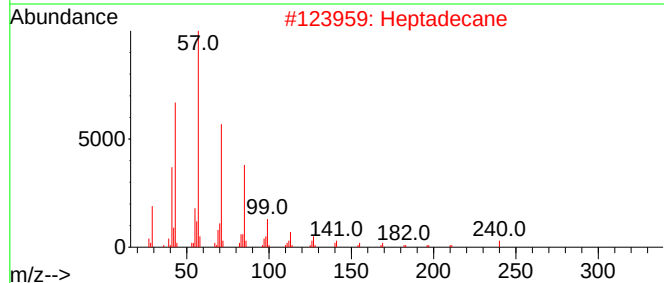
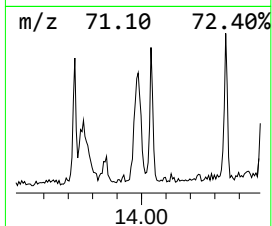
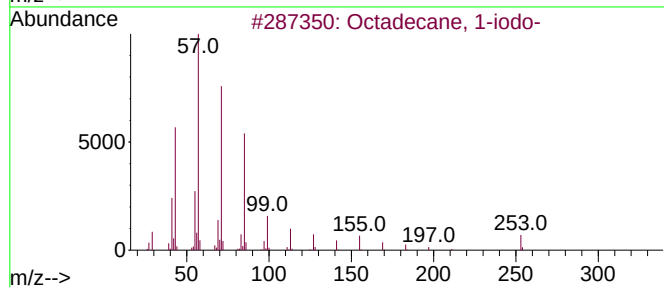
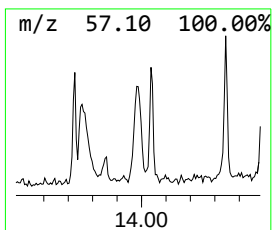
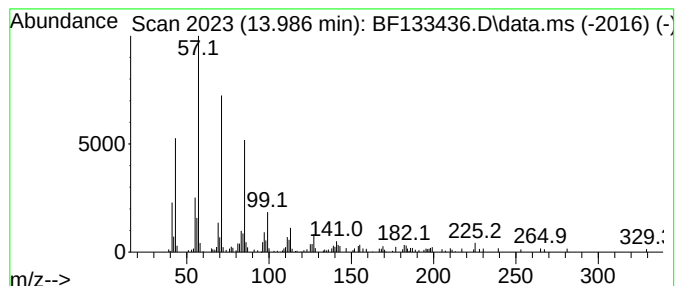
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecane, 1-iodo- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.986	2.48 ng	173570	Chrysene-d12	13.868

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane, 1-iodo-	380	C18H37I	000629-93-6	87
2			Heptadecane	240	C17H36	000629-78-7	87
3			Docosane, 1-iodo-	436	C22H45I	1000406-31-9	87
4			Octadecane	254	C18H38	000593-45-3	87
5			Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051823\
Data File : BF133436.D
Acq On : 18 May 2023 12:28
Operator : CG\JU
Sample : 02812-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
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ClientSampleId :
WG-0516-B3-10-20

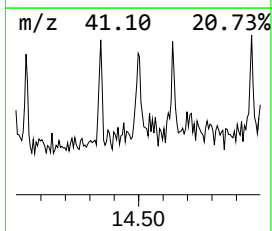
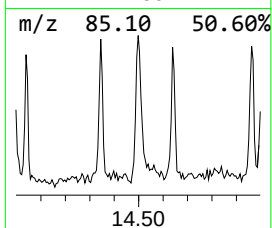
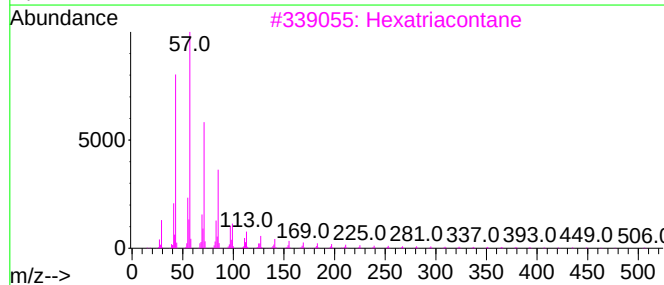
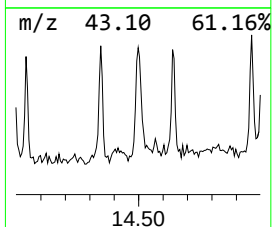
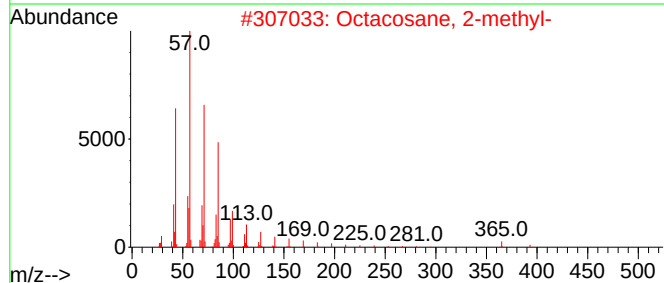
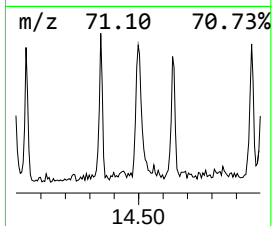
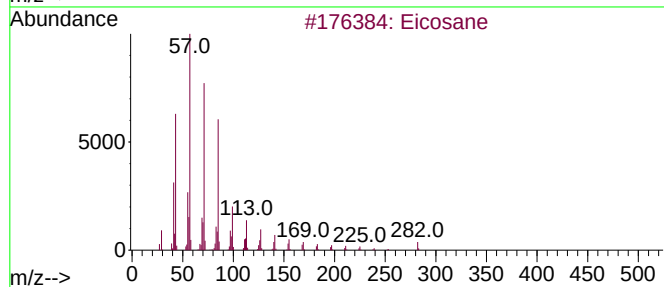
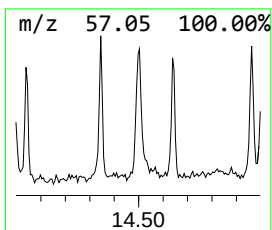
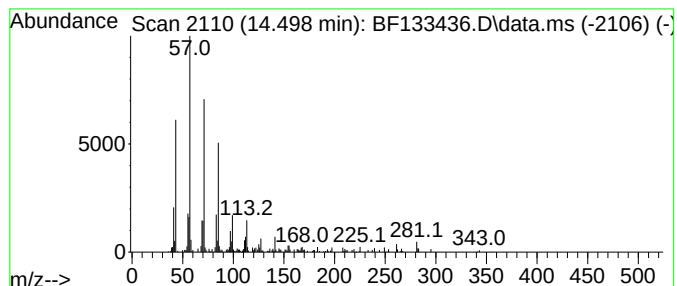
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octacosane, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.498	2.37 ng	165949	Chrysene-d12	13.868

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Eicosane	282	C20H42	000112-95-8	93
2		Octacosane, 2-methyl-	408	C29H60	001560-98-1	87
3		Hexatriacontane	507	C36H74	000630-06-8	87
4		Heneicosane	296	C21H44	000629-94-7	87
5		Octacosane	394	C28H58	000630-02-4	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051823\
Data File : BF133436.D
Acq On : 18 May 2023 12:28
Operator : CG\JU
Sample : 02812-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
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ClientSampleId :
WG-0516-B3-10-20

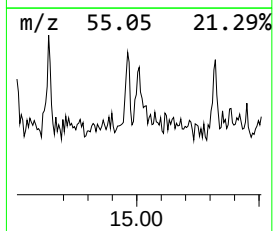
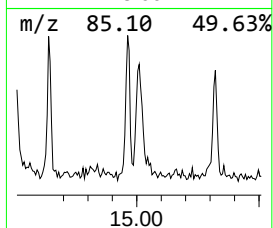
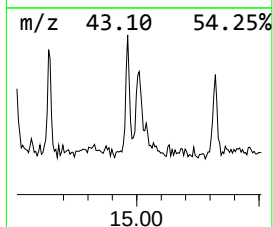
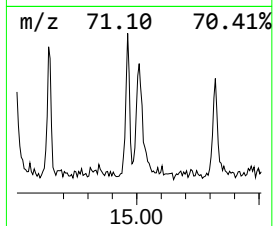
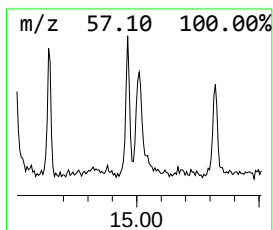
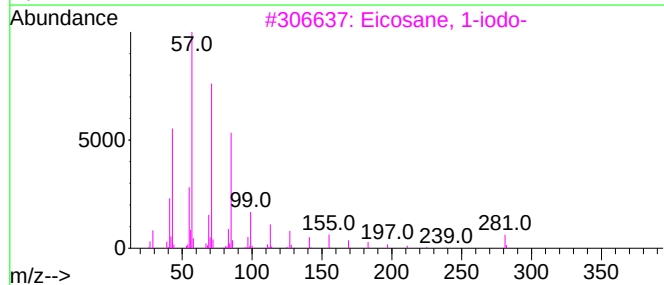
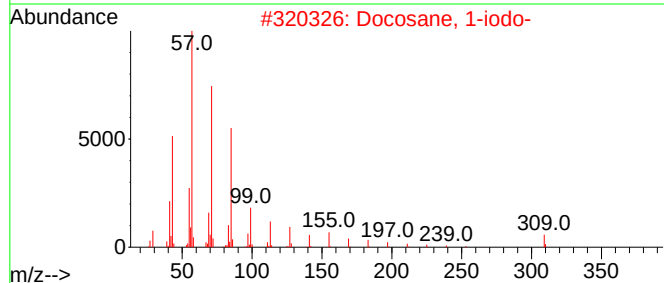
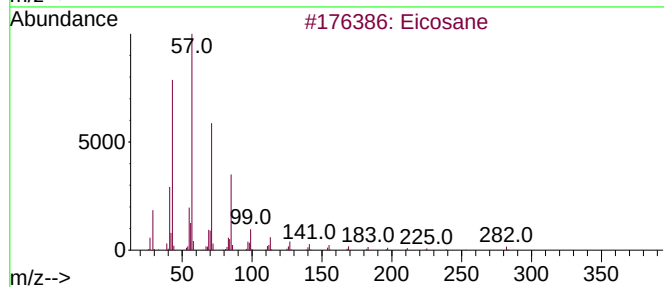
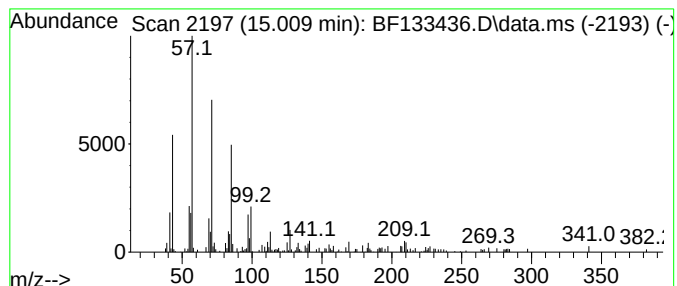
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Docosane, 1-iodo- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.009	2.19 ng	146100	Perylene-d12	15.292

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Eicosane	282	C20H42	000112-95-8	91
2		Docosane, 1-iodo-	436	C22H45I	1000406-31-9	87
3		Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	87
4		Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	86
5		Tetracosane, 1-iodo-	464	C24H49I	1000406-32-0	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051823\
Data File : BF133436.D
Acq On : 18 May 2023 12:28
Operator : CG\JU
Sample : 02812-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WG-0516-B3-10-20

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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
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Benzophenone	10.463	2.0	ng	172438	3	9.751	1692310	20.0
n-Hexadecanoic ...	11.769	11.8	ng	1023560	4	11.233	1733480	20.0
1,3-Benzenedica...	12.010	2.8	ng	244220	4	11.233	1733480	20.0
Octadecanoic acid	12.557	6.4	ng	447224	5	13.868	1398510	20.0
Eicosane	13.368	2.4	ng	167093	5	13.868	1398510	20.0
Cycloeicosane	13.757	4.7	ng	331645	5	13.868	1398510	20.0
Octadecane, 1-i...	13.986	2.5	ng	173570	5	13.868	1398510	20.0
Octacosane, 2-m...	14.498	2.4	ng	165949	5	13.868	1398510	20.0
Docosane, 1-iodo-	15.009	2.2	ng	146100	6	15.292	1334260	20.0