

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052523\
 Data File : BF133493.D
 Acq On : 25 May 2023 18:00
 Operator : CG\JU
 Sample : 02888-04
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FS-SB-20(ELEV-13-11)

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-BF052523.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133493.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.175	11	15	21	rVB2	36218	49506	2.49%	0.298%
2	5.034	497	501	512	rBV	107056	135351	6.80%	0.814%
3	5.439	565	570	573	rBV	2019116	1842686	92.52%	11.075%
4	6.451	737	742	745	rBV	1856701	1831140	91.94%	11.006%
5	6.833	804	807	811	rBV	726659	562270	28.23%	3.379%
6	7.098	849	852	859	rVB3	16655	24347	1.22%	0.146%
7	7.398	898	903	906	rBV	1330569	1143058	57.39%	6.870%
8	8.122	1022	1026	1029	rBV	796508	719849	36.14%	4.327%
9	8.616	1107	1110	1116	rVB	57231	45943	2.31%	0.276%
10	9.198	1205	1209	1212	rBV	2327692	1991614	100.00%	11.970%
11	9.874	1320	1324	1327	rBV	855985	686190	34.45%	4.124%
12	10.586	1441	1445	1448	rBV	147426	112412	5.64%	0.676%
13	10.657	1453	1457	1461	rBV	1276675	1075456	54.00%	6.464%
14	11.357	1573	1576	1580	rBV	755022	653749	32.83%	3.929%
15	11.892	1661	1667	1676	rBV	214517	280374	14.08%	1.685%
16	12.033	1688	1691	1693	rBV2	25164	27011	1.36%	0.162%
17	12.068	1694	1697	1704	rVB5	38341	58567	2.94%	0.352%
18	12.674	1794	1800	1807	rBV	77938	111560	5.60%	0.671%
19	12.951	1843	1847	1850	rVB	1948252	1663003	83.50%	9.995%
20	13.433	1924	1929	1938	rBV	403588	414248	20.80%	2.490%
21	13.510	1939	1942	1944	rBV	26253	25556	1.28%	0.154%
22	13.680	1956	1971	1984	rBV3	128891	501362	25.17%	3.013%
23	13.862	1998	2002	2014	rVB	101079	148936	7.48%	0.895%
24	13.998	2021	2025	2029	rBV	620296	580567	29.15%	3.489%
25	14.180	2053	2056	2058	rBV	22850	22175	1.11%	0.133%
26	14.645	2125	2135	2145	rBV2	151146	410221	20.60%	2.466%
27	14.768	2152	2156	2159	rBV	89785	105916	5.32%	0.637%
28	14.868	2170	2173	2177	rVB	65773	66568	3.34%	0.400%
29	14.998	2189	2195	2205	rVB4	54407	142561	7.16%	0.857%
30	15.133	2214	2218	2221	rBV	29904	41782	2.10%	0.251%
31	15.456	2268	2273	2278	rBV	534810	654462	32.86%	3.934%
32	15.533	2279	2286	2298	rVB3	83733	277436	13.93%	1.667%
33	15.951	2353	2357	2361	rBV3	18303	32757	1.64%	0.197%
34	17.515	2612	2623	2635	rVB3	48453	199365	10.01%	1.198%

Sum of corrected areas: 16637998

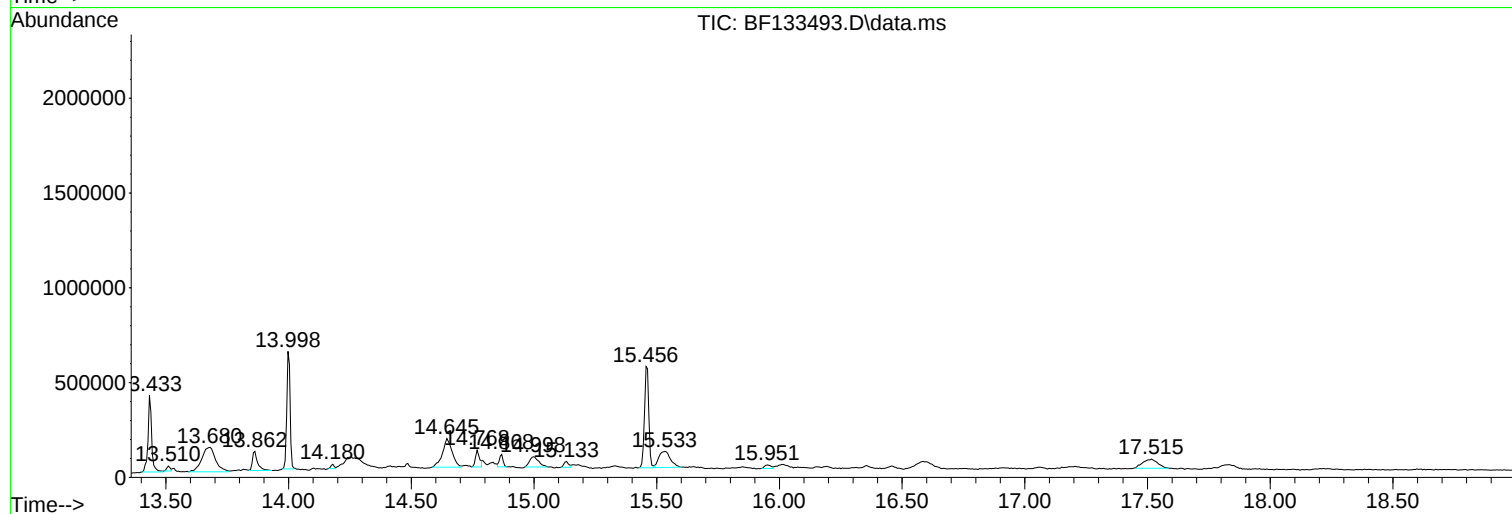
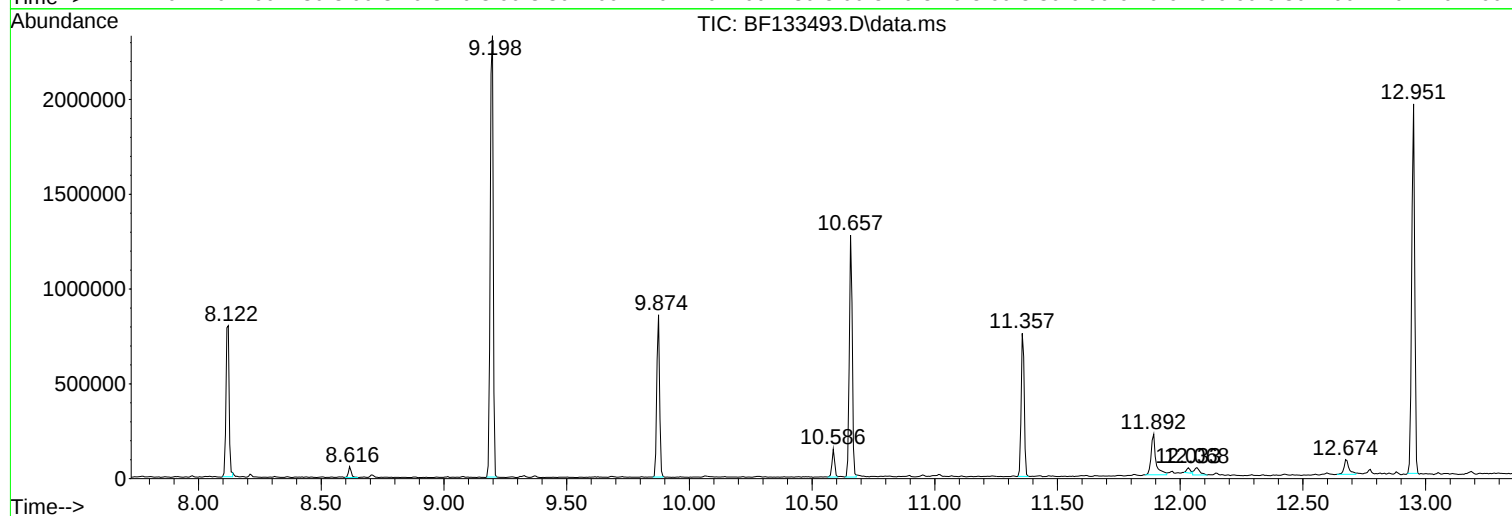
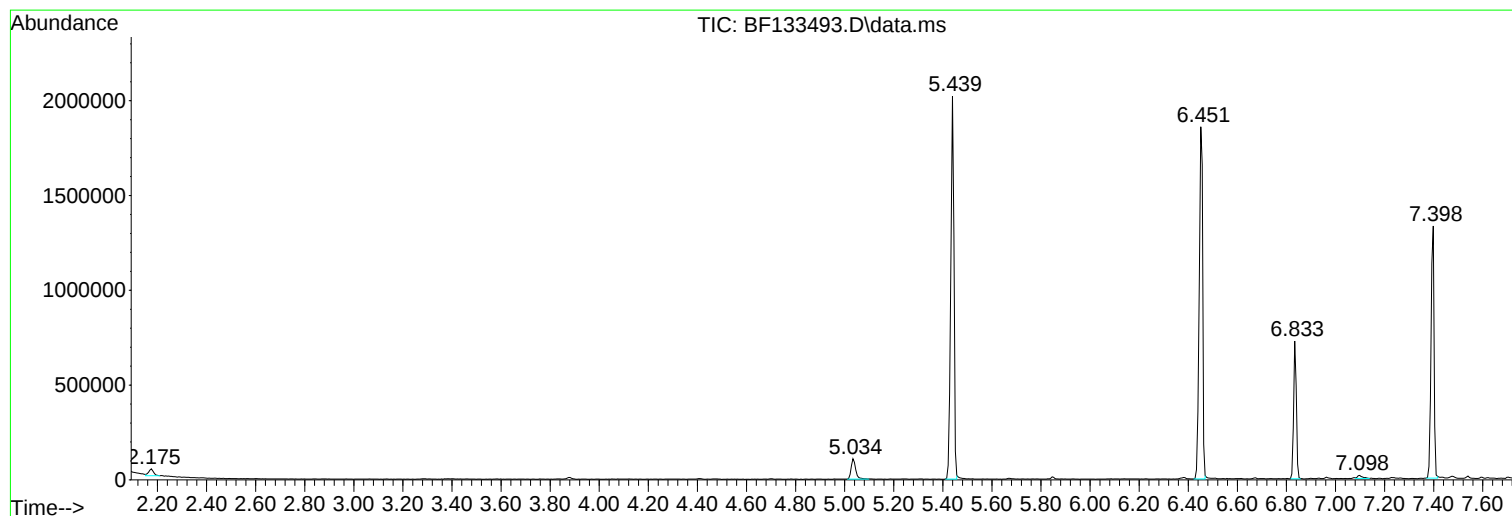
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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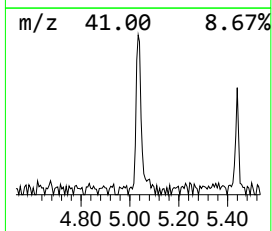
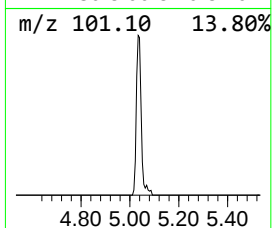
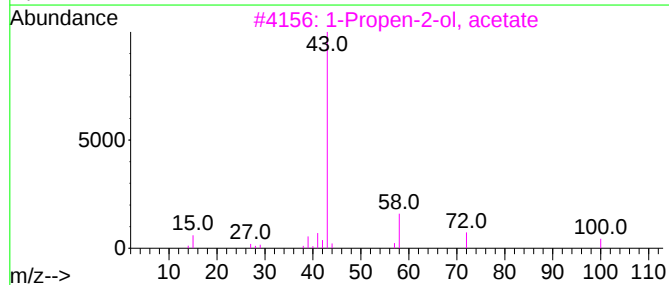
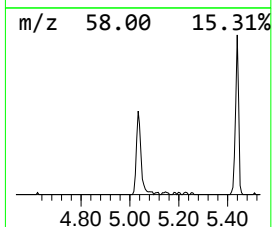
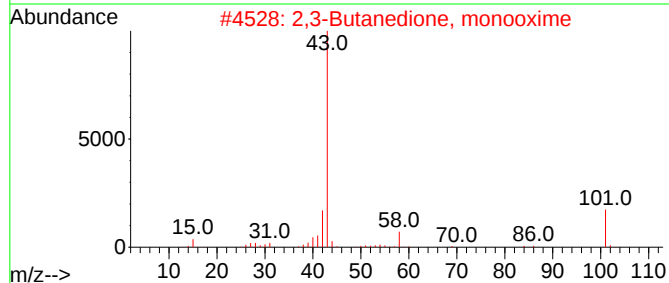
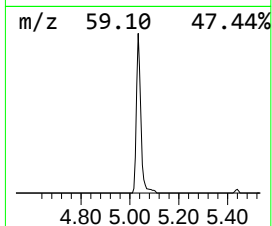
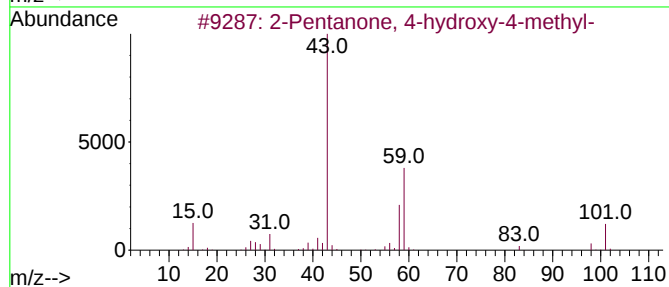
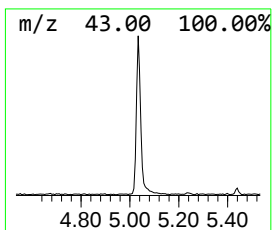
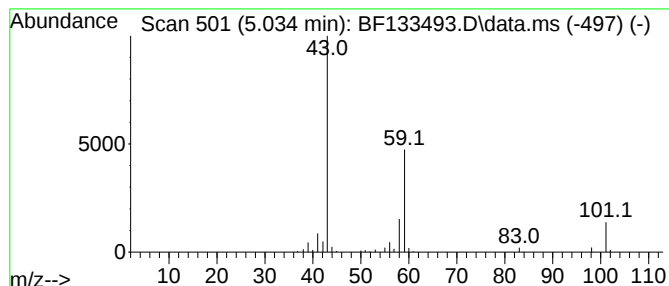
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.034	4.81 ng	135351	1,4-Dichlorobenzene-d4	6.833

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16		
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9		
5	2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9		



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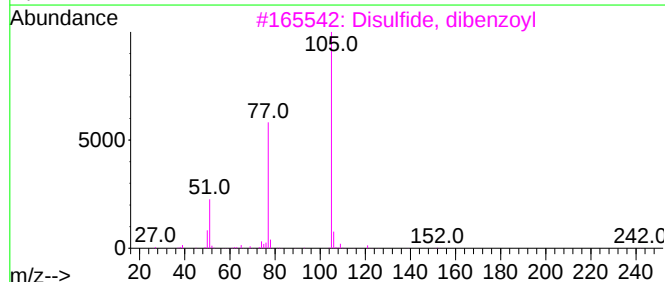
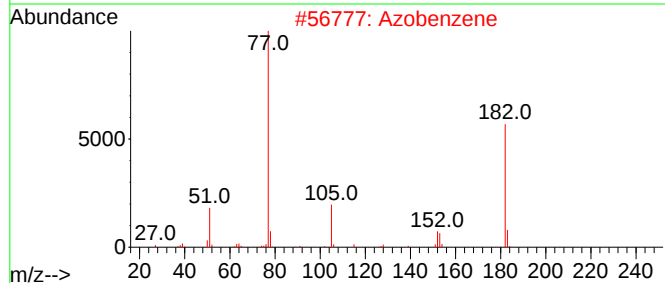
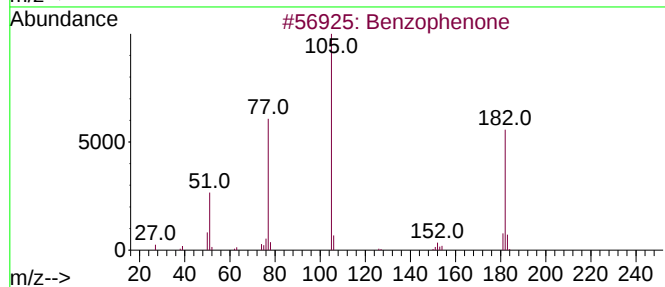
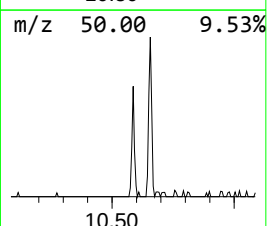
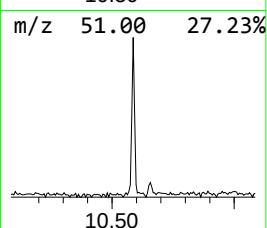
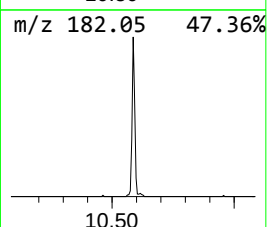
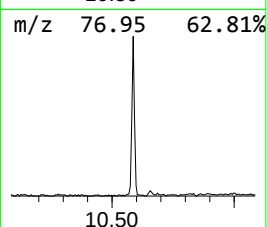
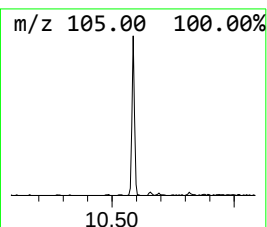
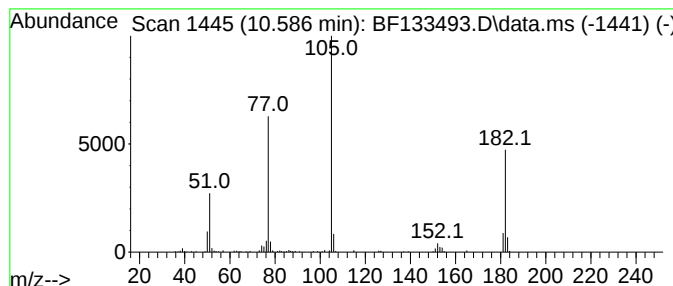
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Peak Number 2 Benzophenone Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.586	3.28 ng	112412	Acenaphthene-d10	9.874

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Azobenzene	182	C12H10N2	000103-33-3	53
3			Disulfide, dibenzoyl	274	C14H10O2S2	000644-32-6	50
4			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	50
5			1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	50



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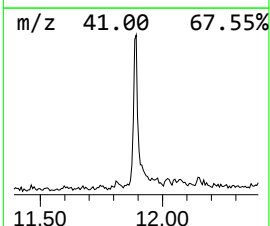
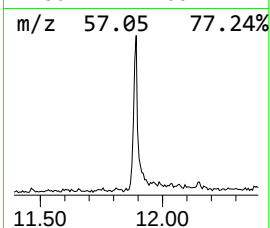
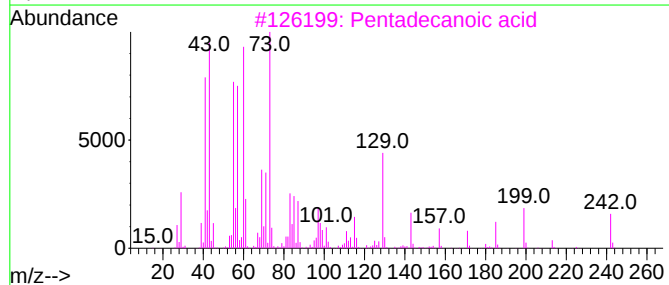
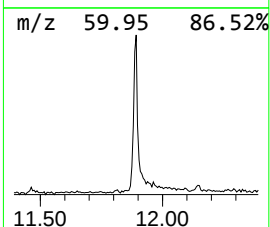
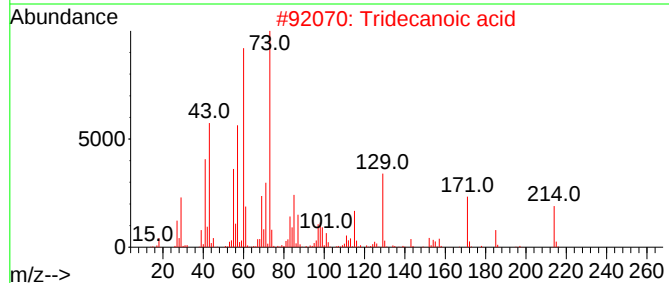
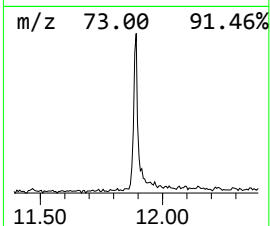
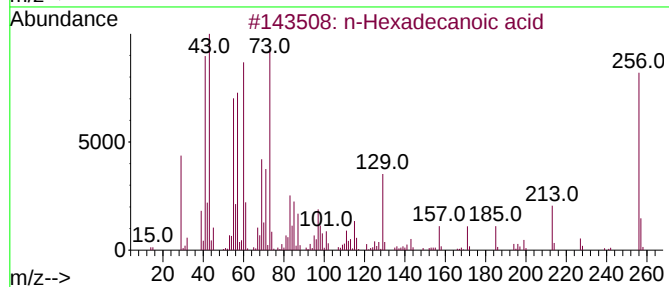
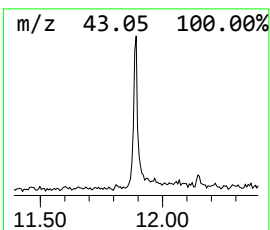
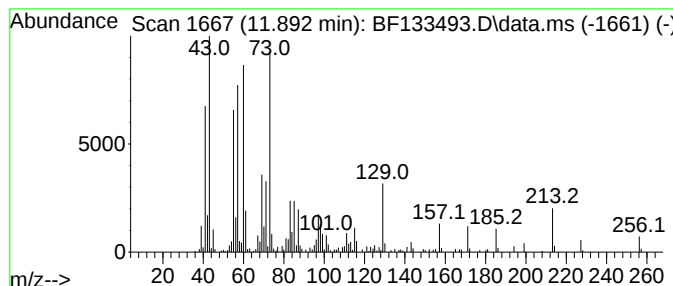
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.892	8.58 ng	280374	Phenanthrene-d10	11.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			Undecanoic acid	186	C11H22O2	000112-37-8	64



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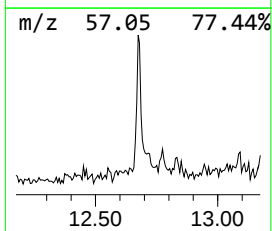
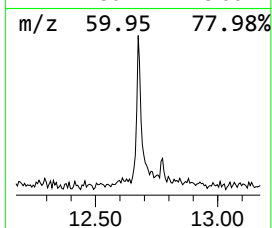
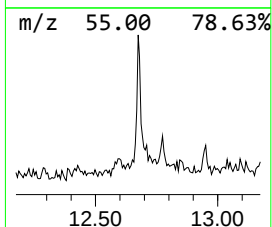
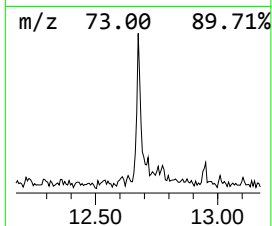
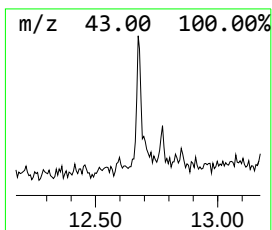
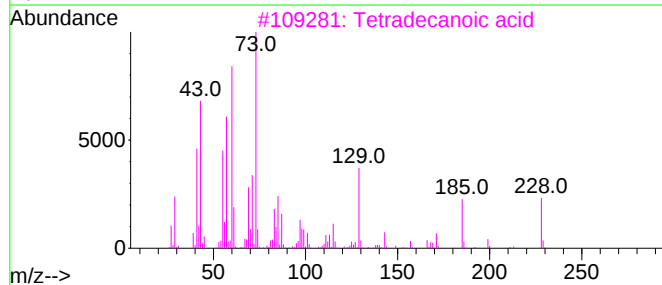
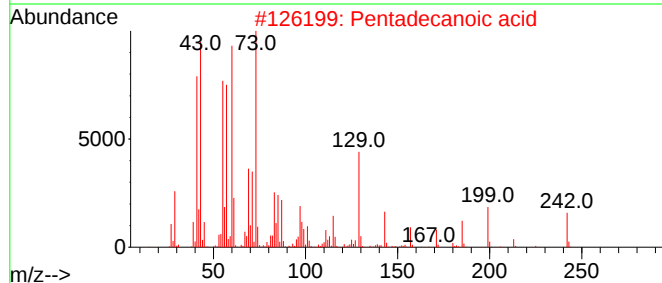
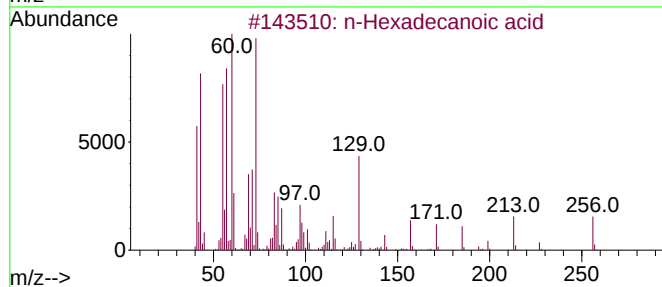
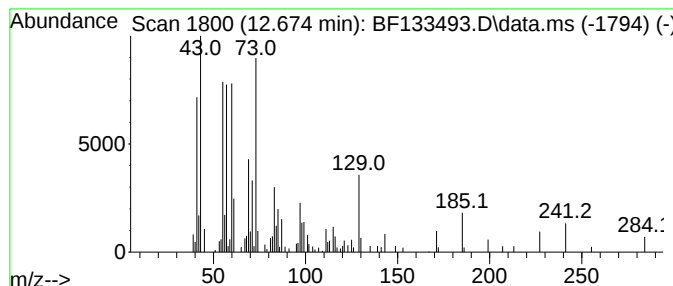
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Peak Number 4 Pentadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.674	3.41 ng	111560	Phenanthrene-d10	11.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4			Tridecanoic acid	214	C13H26O2	000638-53-9	64
5			n-Decanoic acid	172	C10H20O2	000334-48-5	60



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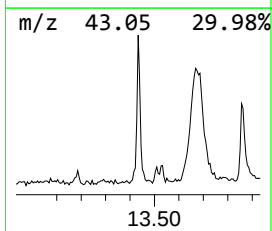
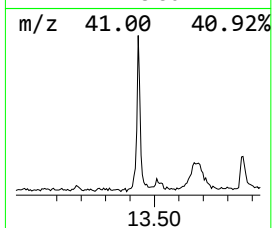
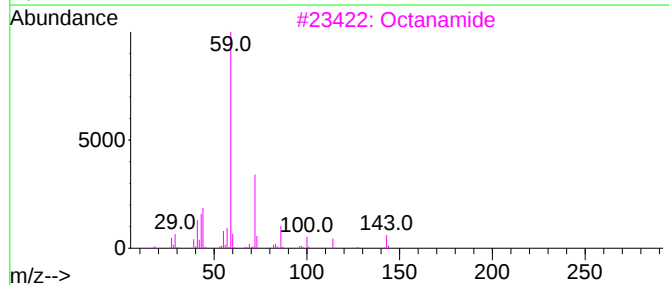
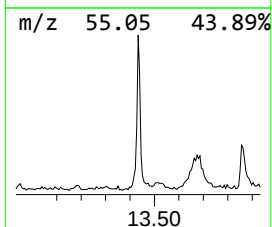
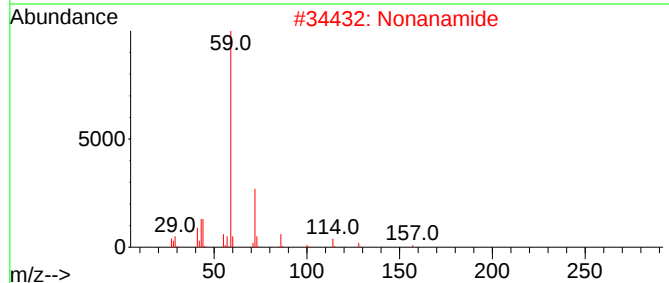
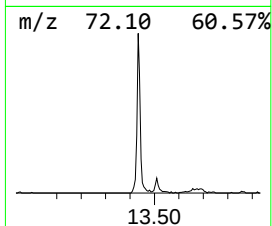
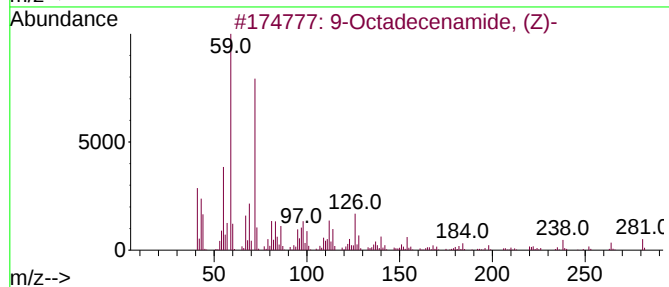
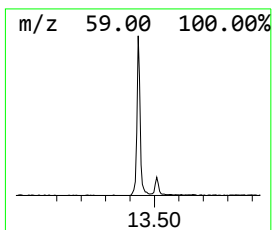
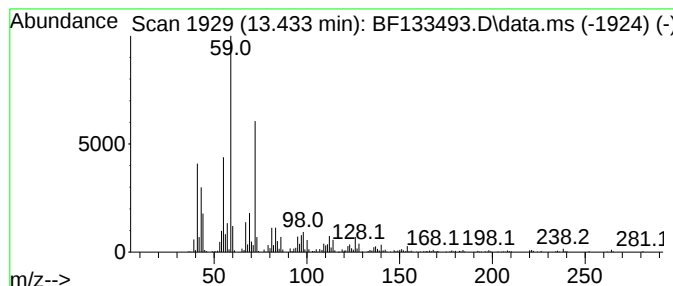
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Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.433	14.27 ng	414248	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	93
2			Nonanamide	157	C9H19NO	001120-07-6	53
3			Octanamide	143	C8H17NO	000629-01-6	50
4			2-Hydroxy-2,4-dimethyl-hept-6-en...	156	C9H16O2	1000192-56-0	43
5			N-Chloroacetyl-dl-erythro-O-meth...	209	C7H12ClNO4	1010214-48-1	43



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BNA_F
ClientSampleId :
FS-SB-20(ELEV-13-11)

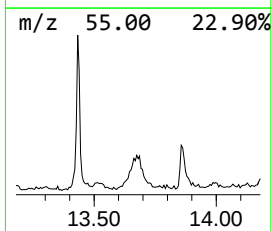
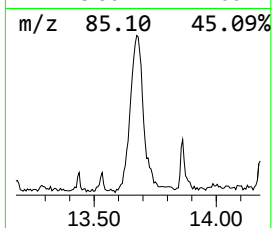
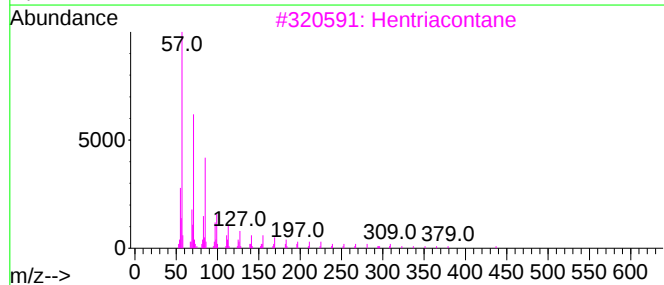
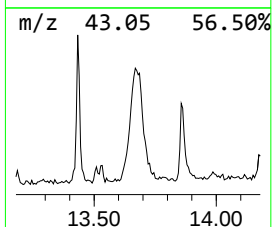
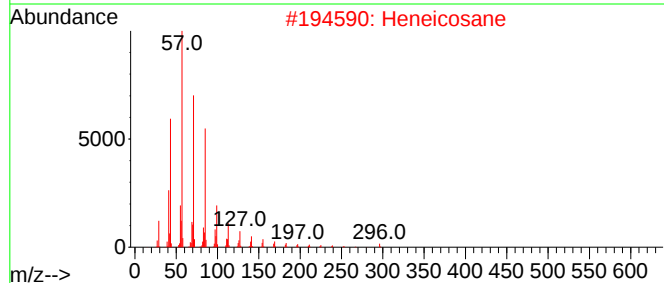
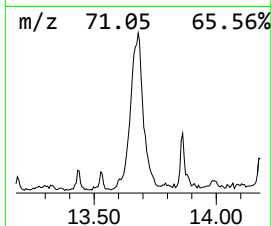
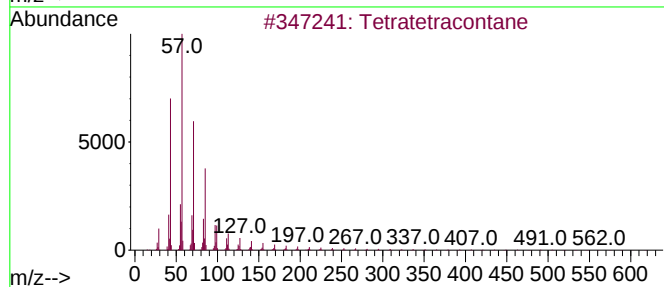
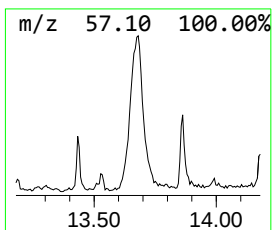
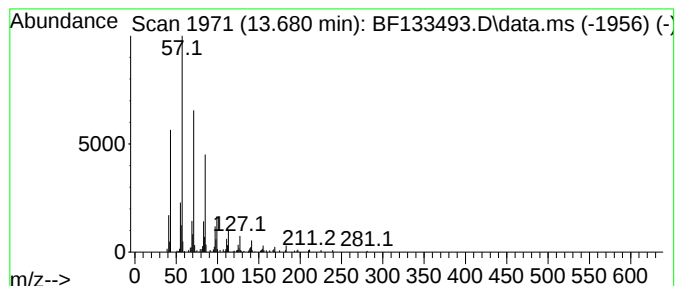
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Tetratetracontane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.680	17.27 ng	501362	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetratetracontane	619	C44H90	007098-22-8	91
2			Heneicosane	296	C21H44	000629-94-7	91
3			Hentriacontane	437	C31H64	000630-04-6	91
4			Hexatriacontane	507	C36H74	000630-06-8	91
5			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052523\
Data File : BF133493.D
Acq On : 25 May 2023 18:00
Operator : CG\JU
Sample : 02888-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

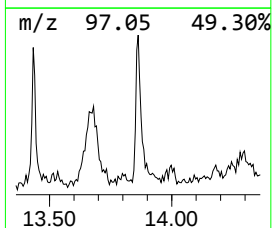
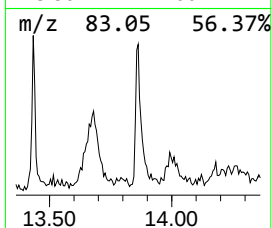
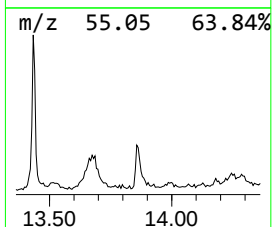
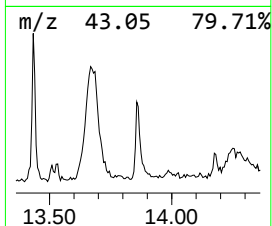
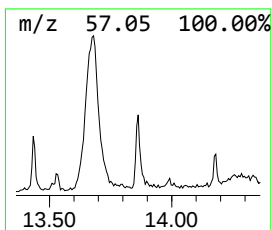
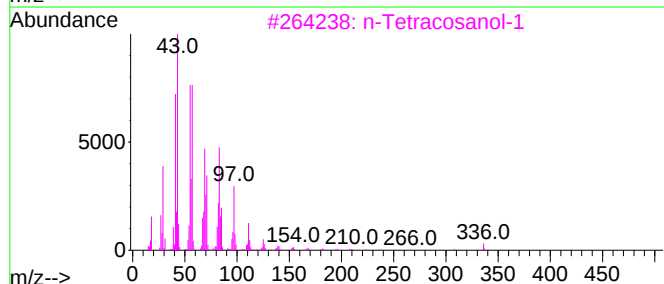
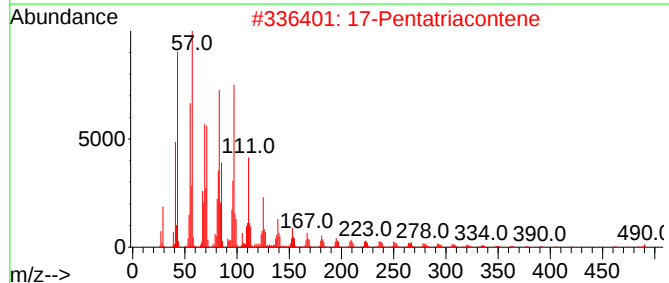
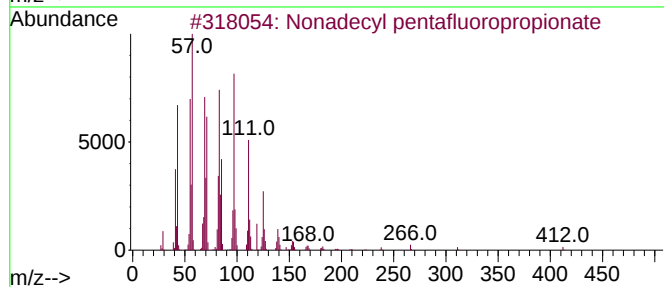
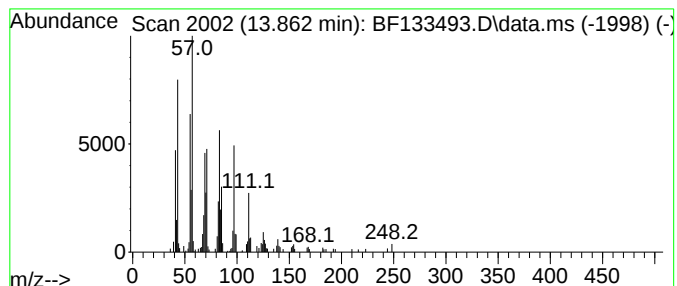
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ClientSampleId :
FS-SB-20(ELEV-13-11)

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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 Nonadecyl pentafluoropropio... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.862	5.13 ng	148936	Chrysene-d12		13.998	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Nonadecyl pentafluoropropionate		430	C22H39F5O2	1000351-88-8	91
2	17-Pentatriacontene		491	C35H70	006971-40-0	87
3	n-Tetracosanol-1		354	C24H50O	000506-51-4	87
4	Tricosyl pentafluoropropionate		486	C26H47F5O2	1000351-81-0	83
5	Octacosyl trifluoroacetate		506	C30H57F3O2	1000351-74-9	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052523\
Data File : BF133493.D
Acq On : 25 May 2023 18:00
Operator : CG\JU
Sample : 02888-04
Misc :
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Instrument :
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ClientSampleId :
FS-SB-20(ELEV-13-11)

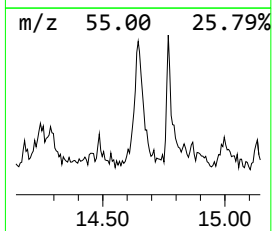
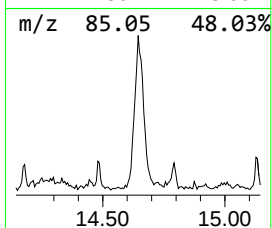
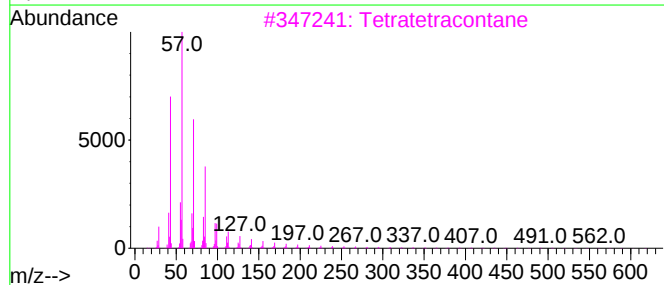
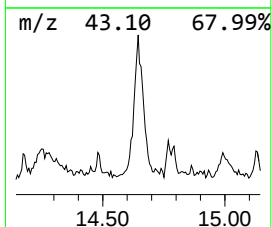
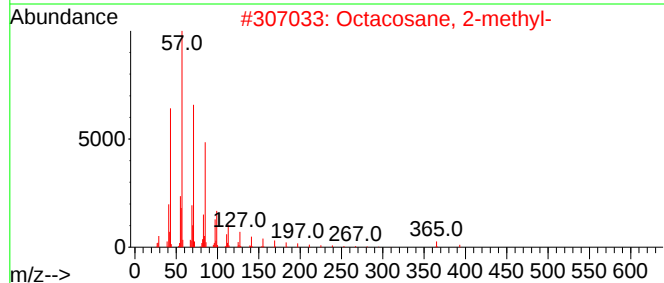
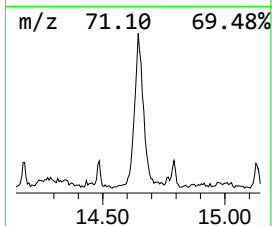
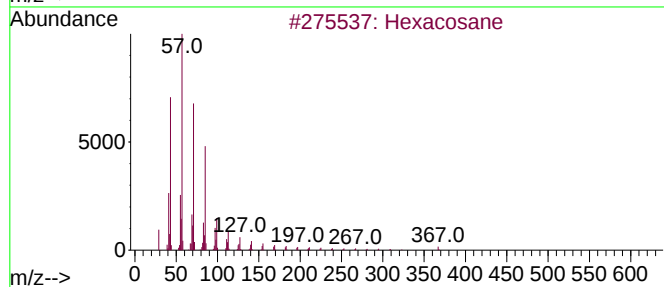
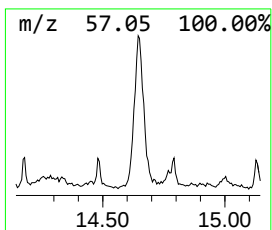
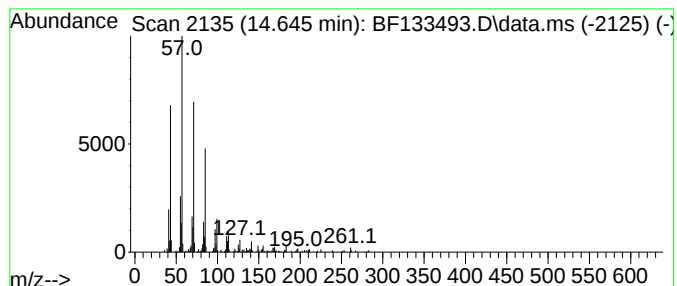
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.645	14.13 ng	410221	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	94
2			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
3			Tetratetracontane	619	C44H90	007098-22-8	91
4			Tetracosane	338	C24H50	000646-31-1	91
5			Octacosane	394	C28H58	000630-02-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052523\
Data File : BF133493.D
Acq On : 25 May 2023 18:00
Operator : CG\JU
Sample : 02888-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
FS-SB-20(ELEV-13-11)

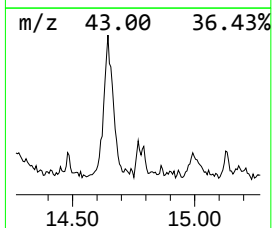
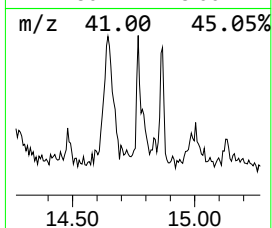
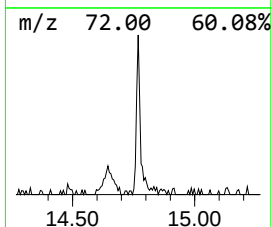
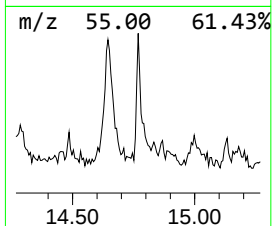
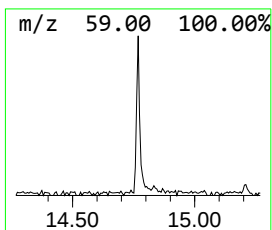
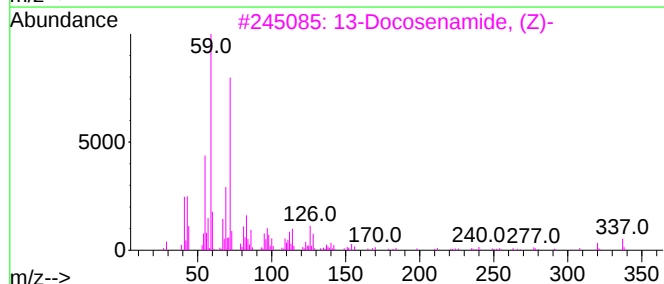
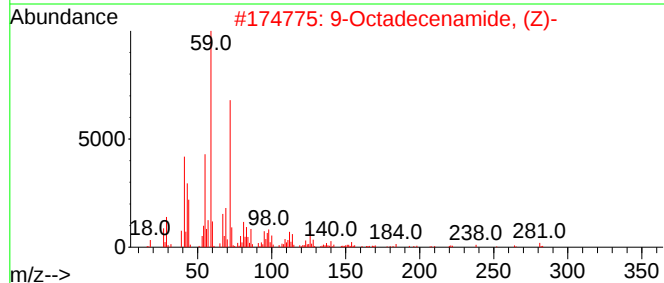
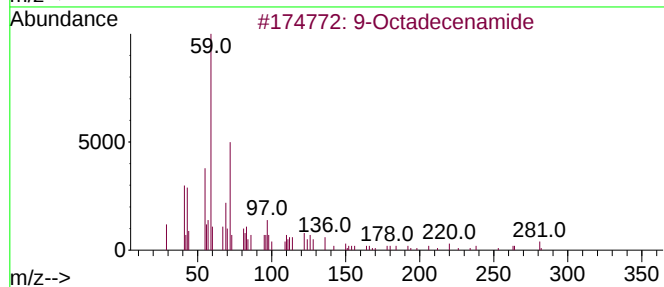
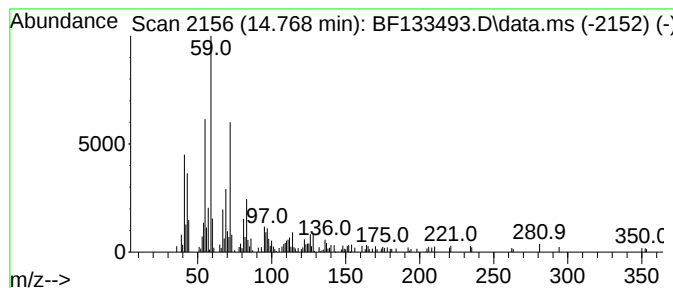
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 9-Octadecenamide Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.768	3.24 ng	105916	Perylene-d12	15.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide			281	C18H35NO	003322-62-1	95
2	9-Octadecenamide, (Z)-			281	C18H35NO	000301-02-0	95
3	13-Docosenamide, (Z)-			337	C22H43NO	000112-84-5	62
4	Tetradecanamide			227	C14H29NO	000638-58-4	59
5	Hexadecanamide			255	C16H33NO	000629-54-9	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052523\
Data File : BF133493.D
Acq On : 25 May 2023 18:00
Operator : CG\JU
Sample : 02888-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
FS-SB-20(ELEV-13-11)

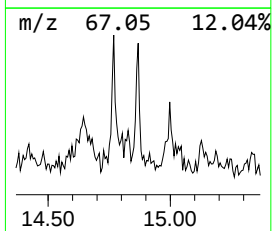
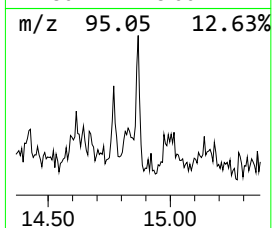
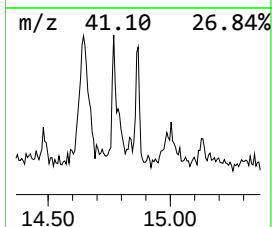
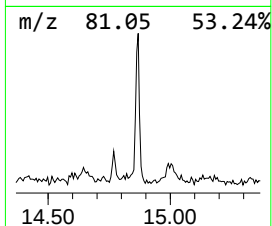
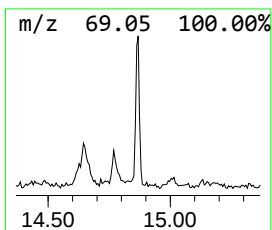
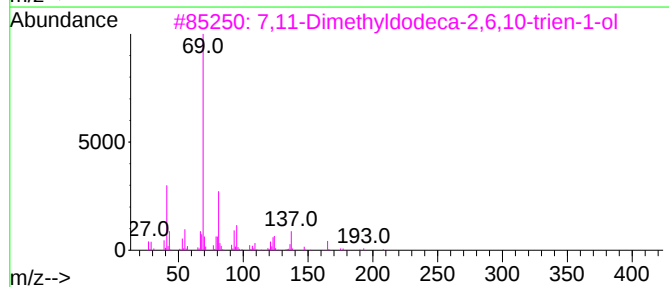
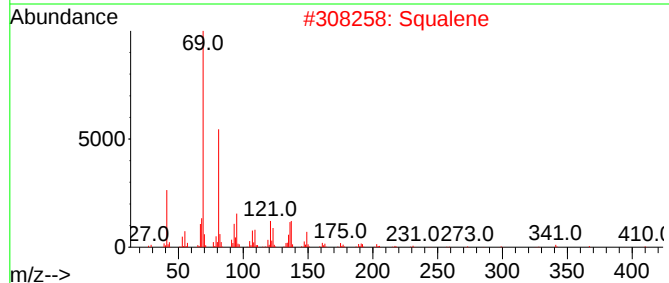
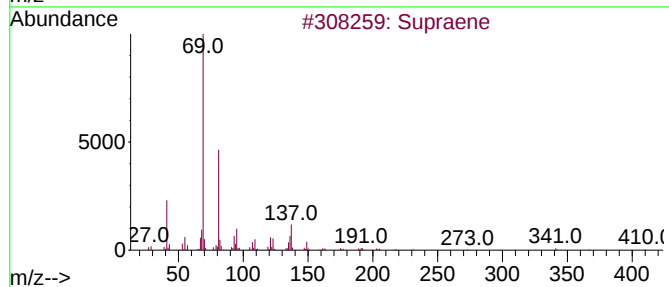
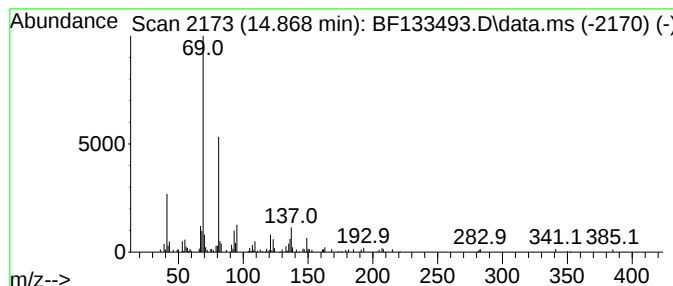
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Supraene Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.868	2.03 ng	66568	Perylene-d12	15.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	87
2			Squalene	410	C30H50	000111-02-4	78
3			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64
4			3,7-Dimethyl-1-phenylsulfonyl-2,...	278	C16H22O2S	1000432-27-5	64
5			4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052523\
Data File : BF133493.D
Acq On : 25 May 2023 18:00
Operator : CG\JU
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Misc :
ALS Vial : 12 Sample Multiplier: 1

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ClientSampleId :
FS-SB-20(ELEV-13-11)

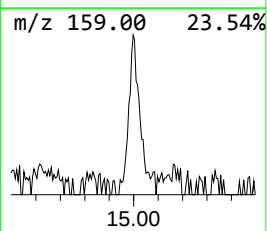
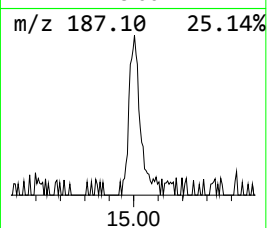
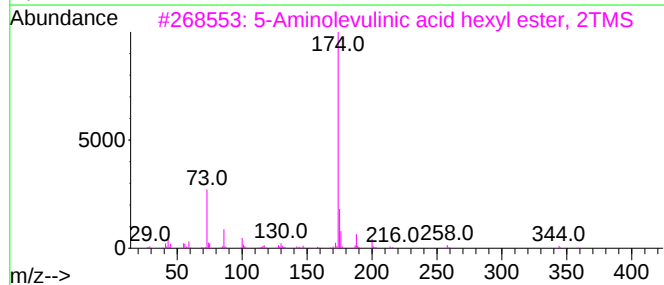
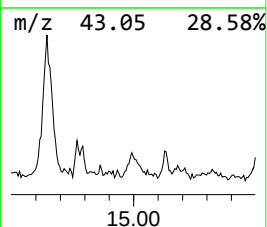
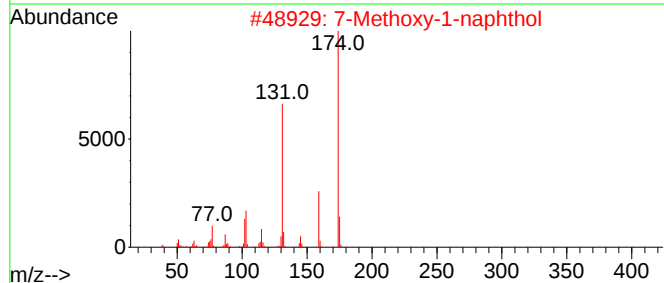
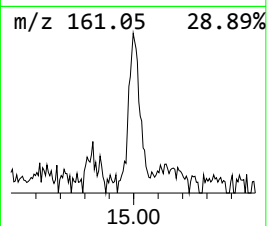
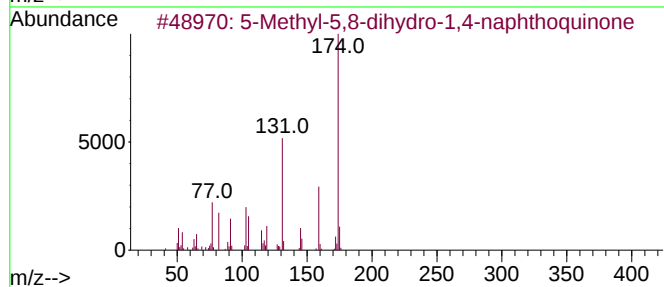
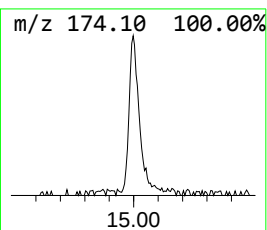
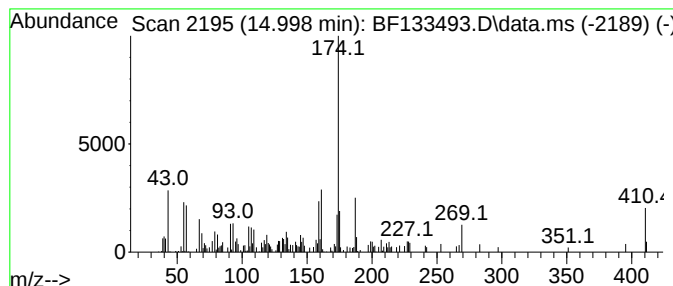
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown14.998 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.998	4.36 ng	142561	Perylene-d12	15.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Methyl-5,8-dihydro-1,4-naphtho...	174	C11H10O2	086759-40-2	43
2			7-Methoxy-1-naphthol	174	C11H10O2	067247-13-6	43
3			5-Aminolevulinic acid hexyl este...	359	C17H37NO3Si2	1000500-32-9	38
4			1H-Isoindole-1,3(2H)-dione, 2-(2...	205	C11H11NO3	211501-36-9	38
5			Thiophene, 2-(4-methylphenyl)-	174	C11H10S	1000380-56-1	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052523\
Data File : BF133493.D
Acq On : 25 May 2023 18:00
Operator : CG\JU
Sample : 02888-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
FS-SB-20(ELEV-13-11)

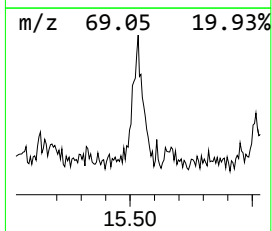
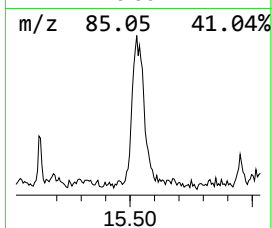
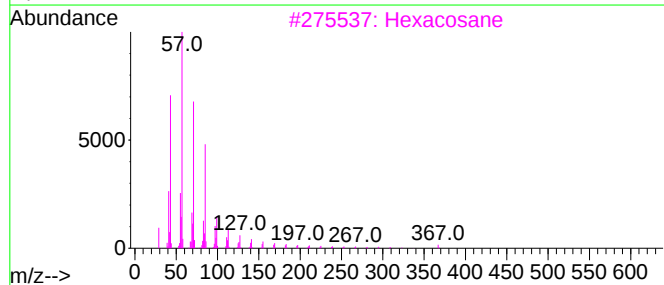
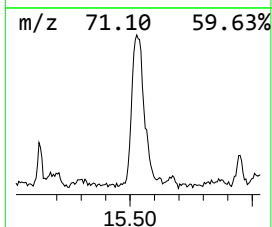
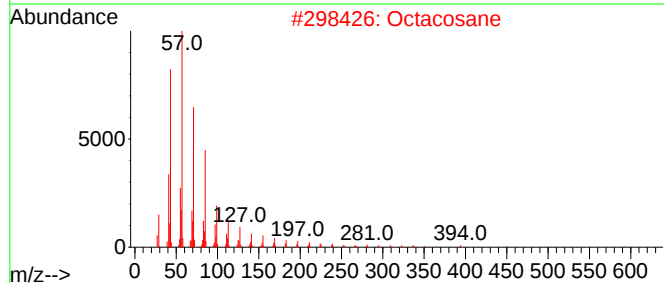
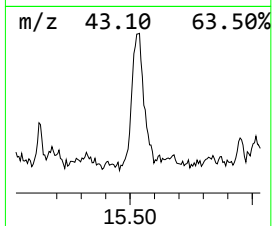
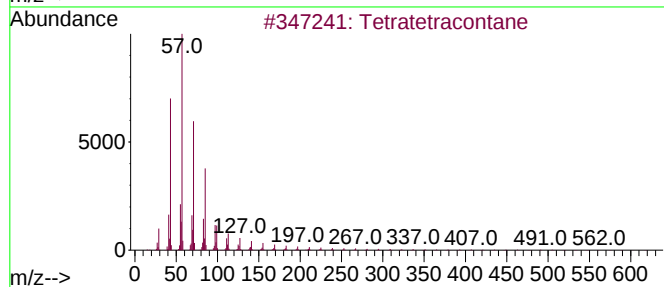
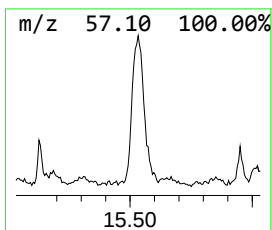
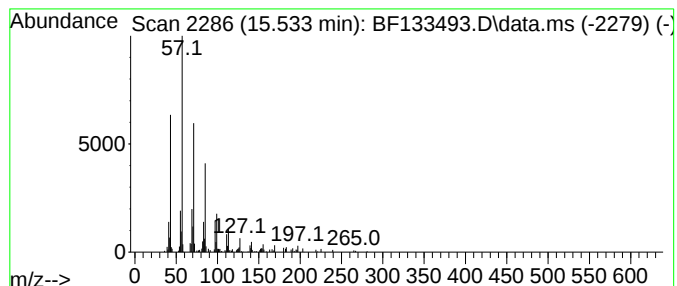
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.533	8.48 ng	277436	Perylene-d12	15.457

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetratetracontane	619	C44H90	007098-22-8	91
2		Octacosane	394	C28H58	000630-02-4	91
3		Hexacosane	366	C26H54	000630-01-3	91
4		Hentriacontane	437	C31H64	000630-04-6	91
5		Pentacosane	352	C25H52	000629-99-2	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052523\
Data File : BF133493.D
Acq On : 25 May 2023 18:00
Operator : CG\JU
Sample : 02888-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FS-SB-20(ELEV-13-11)

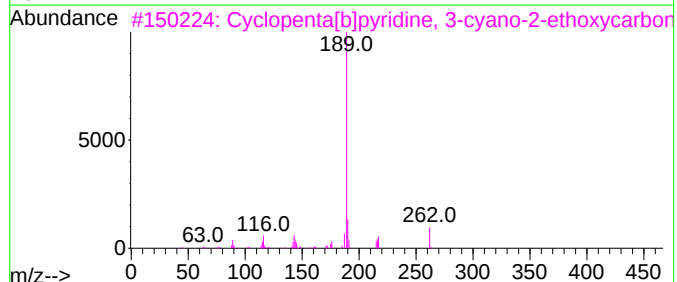
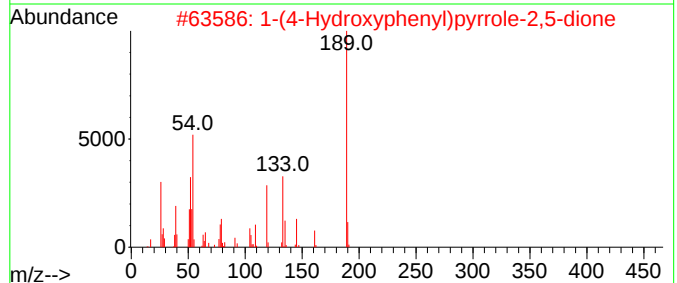
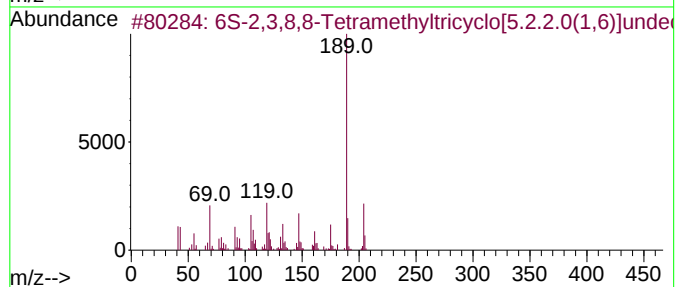
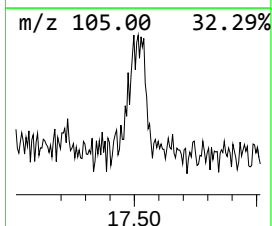
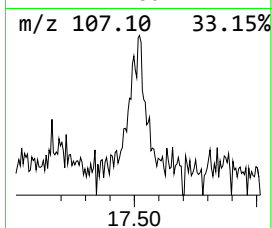
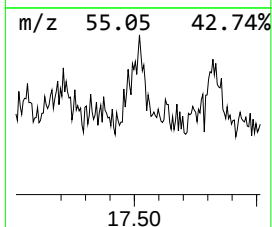
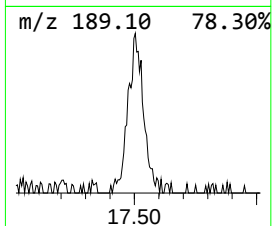
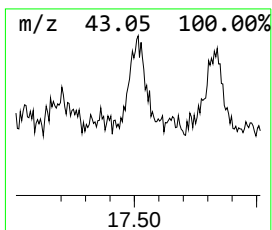
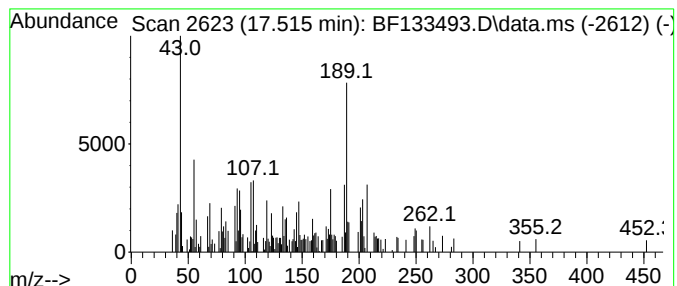
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown17.515 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.515	6.09 ng	199365	Perylene-d12	15.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	6S-2,3,8,8-Tetramethyltricyclo[5...	204	C15H24	137235-48-4	38		
2	1-(4-Hydroxyphenyl)pyrrole-2,5-d...	189	C10H7N03	1010411-37-9	38		
3	Cyclopenta[b]pyridine, 3-cyano-2...	262	C13H14N2O2S	166113-76-4	38		
4	1,5-naphthalenediol, 2-nitroso-	189	C10H7N03	1000395-94-6	30		
5	5,7-Indolinedicarboxaldehyde, 1-...	189	C11H11N02	092287-89-3	30		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052523\
Data File : BF133493.D
Acq On : 25 May 2023 18:00
Operator : CG\JU
Sample : 02888-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FS-SB-20(ELEV-13-11)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.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-...	5.034	4.8	ng	135351	1	6.833	562270	20.0
Benzophenone	10.586	3.3	ng	112412	3	9.874	686190	20.0
n-Hexadecanoic ...	11.892	8.6	ng	280374	4	11.357	653749	20.0
Pentadecanoic acid	12.674	3.4	ng	111560	4	11.357	653749	20.0
9-Octadecenamid...	13.433	14.3	ng	414248	5	13.998	580567	20.0
Tetratetracontane	13.680	17.3	ng	501362	5	13.998	580567	20.0
Nonadecyl penta...	13.862	5.1	ng	148936	5	13.998	580567	20.0
Hexacosane	14.645	14.1	ng	410221	5	13.998	580567	20.0
9-Octadecenamide	14.768	3.2	ng	105916	6	15.457	654462	20.0
Supraene	14.868	2.0	ng	66568	6	15.457	654462	20.0
unknown14.998	14.998	4.4	ng	142561	6	15.457	654462	20.0
Octacosane	15.533	8.5	ng	277436	6	15.457	654462	20.0
unknown17.515	17.515	6.1	ng	199365	6	15.457	654462	20.0