

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082123\
 Data File : BF134862.D
 Acq On : 21 Aug 2023 12:08
 Operator : CG\JU
 Sample : 04086-18
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 DUP06

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-BF080123.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134862.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.428	563	568	572	rBV	2846730	2848023	25.47%	4.905%
2	6.434	734	739	742	rBV	2654661	2925694	26.17%	5.039%
3	6.792	796	800	803	rBV	1390942	1106043	9.89%	1.905%
4	7.351	890	895	898	rBV	1939947	1907877	17.07%	3.286%
5	8.069	1013	1017	1020	rBV	1816659	1516100	13.56%	2.611%
6	9.151	1195	1201	1204	rBV	3584902	3531605	31.59%	6.082%
7	9.827	1307	1316	1319	rBV	2046958	1809799	16.19%	3.117%
8	10.616	1445	1450	1454	rBV	2491420	2374607	21.24%	4.089%
9	11.316	1565	1569	1571	rBV	2112144	1782787	15.95%	3.070%
10	11.339	1571	1573	1576	rVV	484371	349933	3.13%	0.603%
11	11.386	1578	1581	1584	rVB	140858	125694	1.12%	0.216%
12	11.816	1651	1654	1656	rBV	180903	172778	1.55%	0.298%
13	11.851	1656	1660	1665	rVV2	926195	1310147	11.72%	2.256%
14	11.892	1665	1667	1670	rVV	127469	135307	1.21%	0.233%
15	11.927	1670	1673	1676	rVV	259982	303767	2.72%	0.523%
16	12.368	1745	1748	1751	rBV	151720	164963	1.48%	0.284%
17	12.404	1751	1754	1757	rVV2	91959	125251	1.12%	0.216%
18	12.533	1772	1776	1779	rBV	318780	294949	2.64%	0.508%
19	12.639	1790	1794	1801	rBV	456305	643209	5.75%	1.108%
20	12.763	1810	1815	1817	rBV	410891	409774	3.67%	0.706%
21	12.910	1836	1840	1844	rBV	3289294	3166291	28.32%	5.453%
22	13.768	1973	1986	1989	rBV	2549959	7176359	64.19%	12.359%
23	13.815	1989	1994	1996	rVV2	3784636	7681985	68.71%	13.230%
24	13.857	1996	2001	2003	rVB	6365707	11180042	100.00%	19.254%
25	13.886	2003	2006	2014	rVB	1503511	1355581	12.13%	2.335%
26	13.974	2015	2021	2023	rBV	1296534	1331792	11.91%	2.294%
27	13.998	2023	2025	2030	rVB	212512	189574	1.70%	0.326%
28	14.139	2046	2049	2055	rVB	107126	131580	1.18%	0.227%
29	14.733	2147	2150	2162	rVB2	105312	266876	2.39%	0.460%
30	15.115	2207	2215	2225	rBV7	94196	408006	3.65%	0.703%
31	15.433	2264	2269	2273	rBV	896897	1123624	10.05%	1.935%
32	15.980	2357	2362	2368	rVB2	103084	216330	1.93%	0.373%

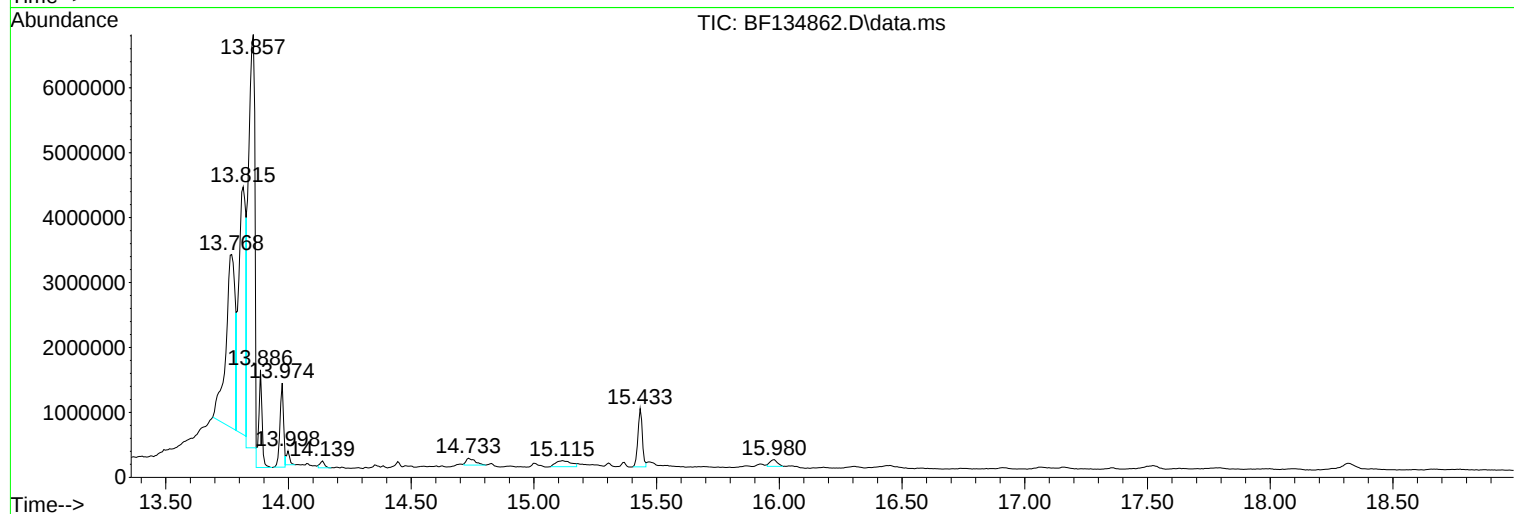
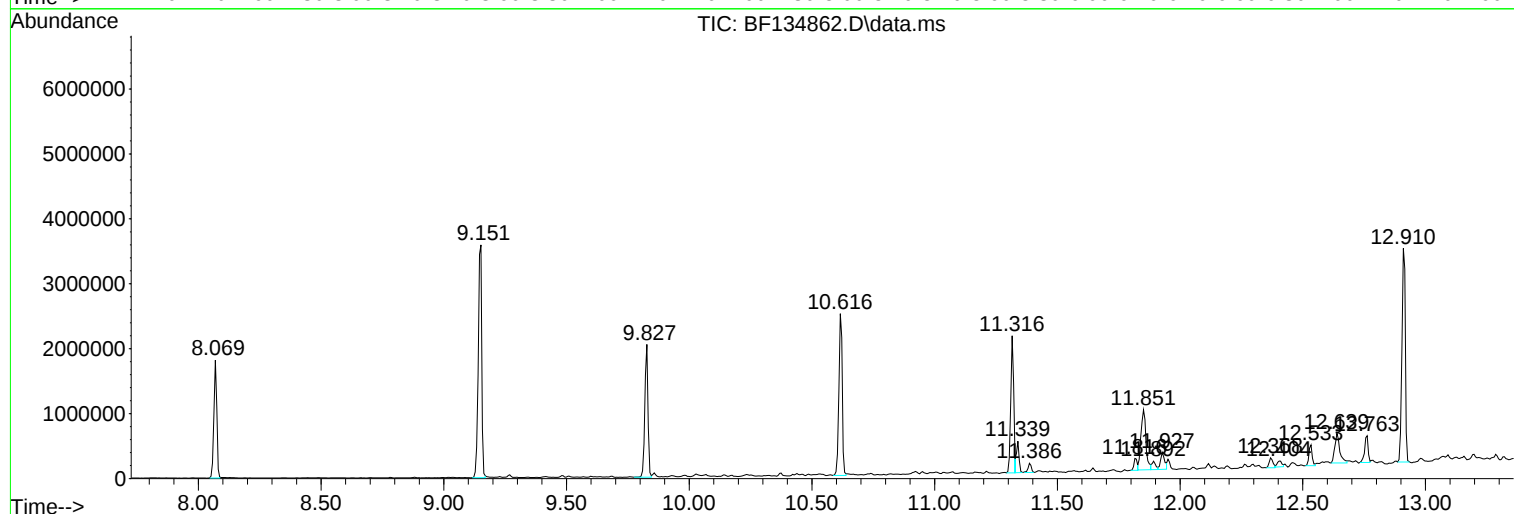
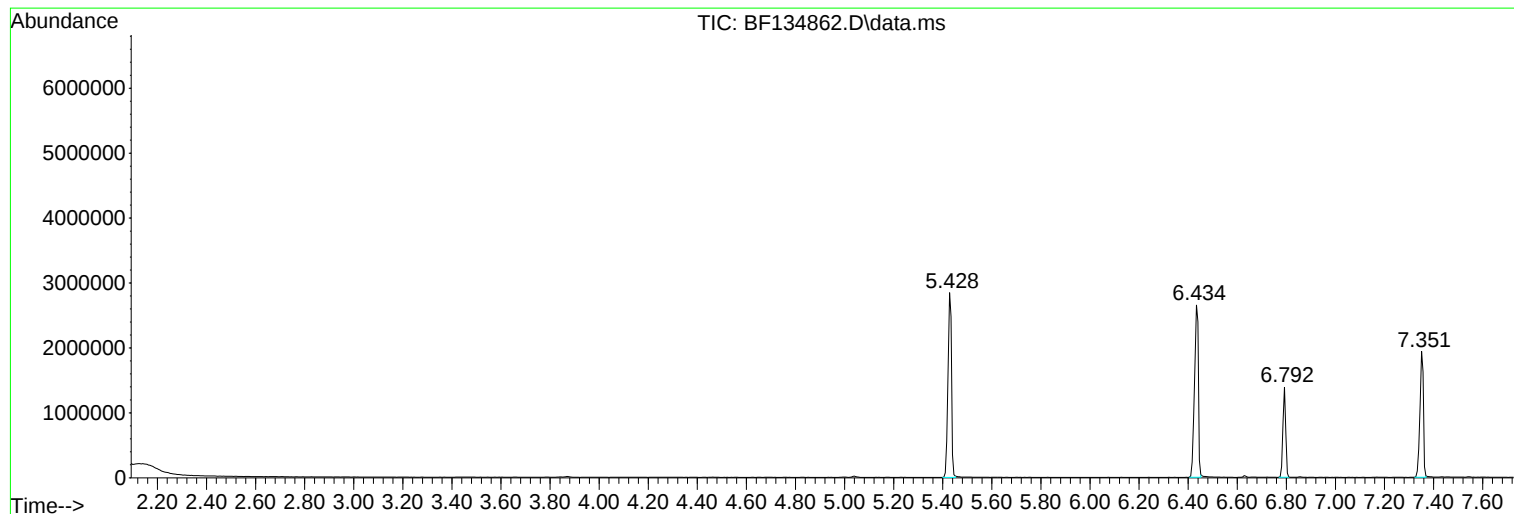
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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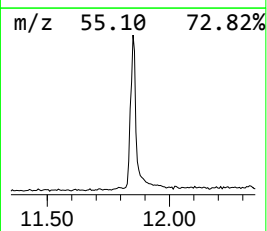
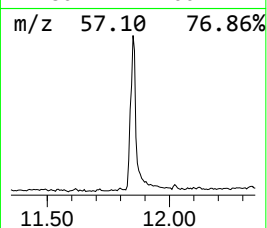
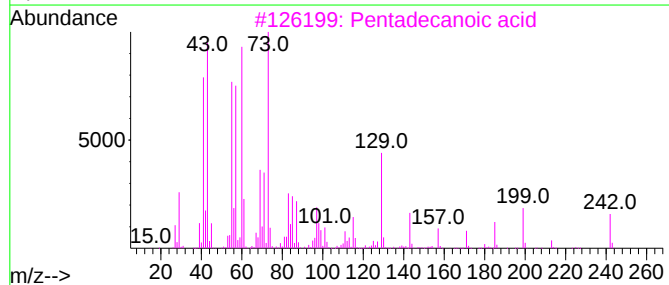
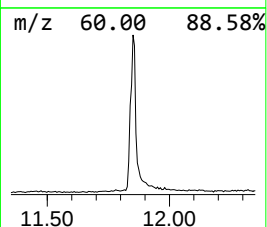
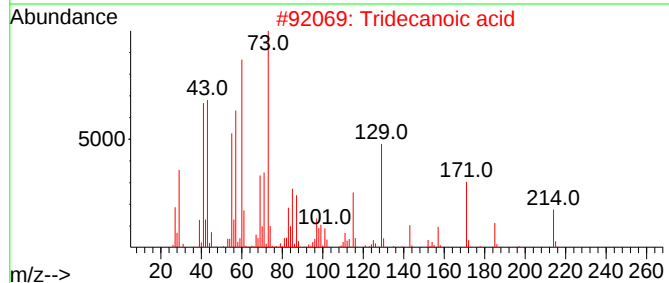
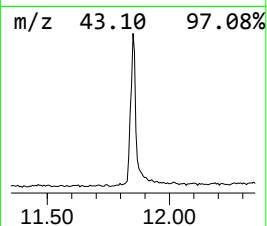
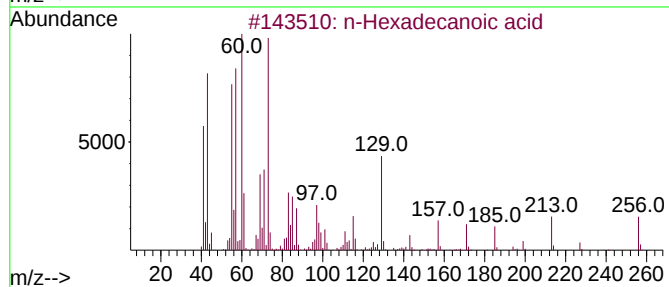
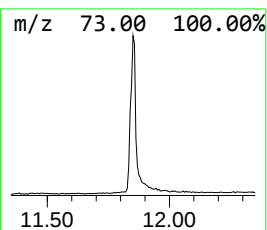
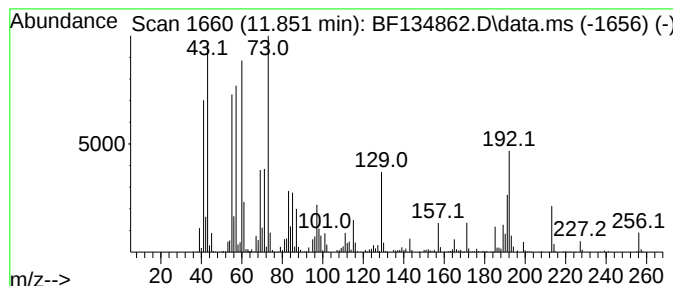
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.851	14.70 ng	1310150	Phenanthrene-d10		11.316	
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	90
3	Pentadecanoic acid		242	C15H30O2	001002-84-2	86
4	Tetradecanoic acid		228	C14H28O2	000544-63-8	64
5	8-Methylnonanoic acid		172	C10H20O2	005963-14-4	55



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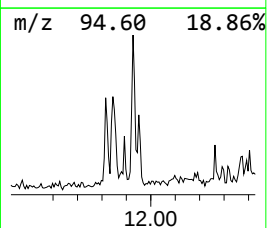
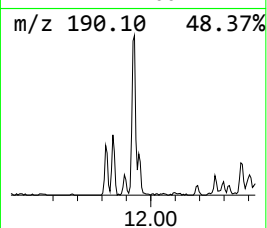
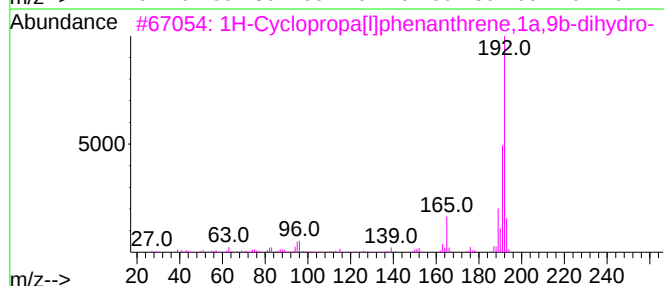
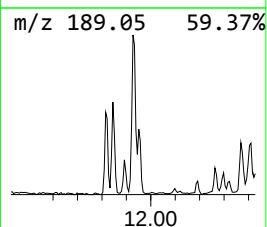
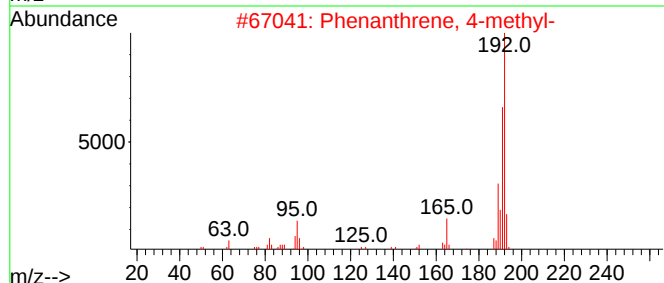
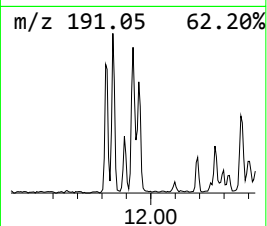
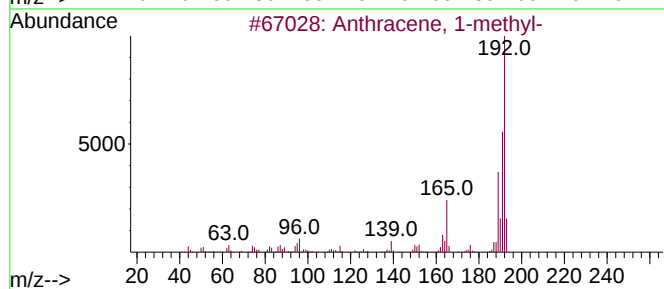
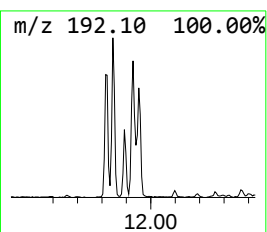
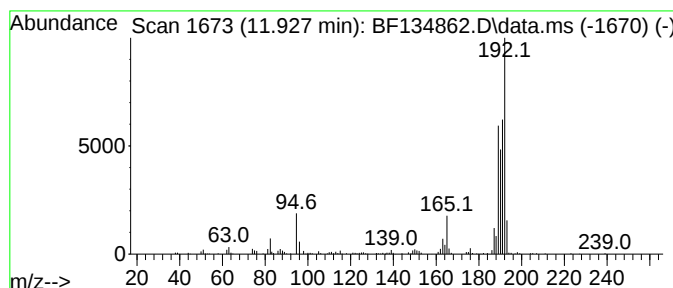
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Anthracene, 1-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.927	3.41 ng	303767	Phenanthrene-d10	11.316

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Anthracene, 1-methyl-	192	C15H12	000610-48-0	78
2			Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	60
3			1H-Cyclopropa[1]phenanthrene,1a,...	192	C15H12	000949-41-7	60
4			Anthracene, 2-methyl-	192	C15H12	000613-12-7	60
5			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	60



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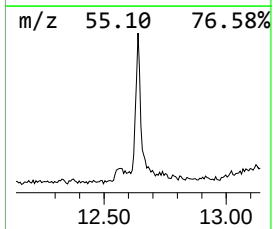
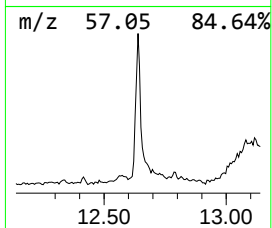
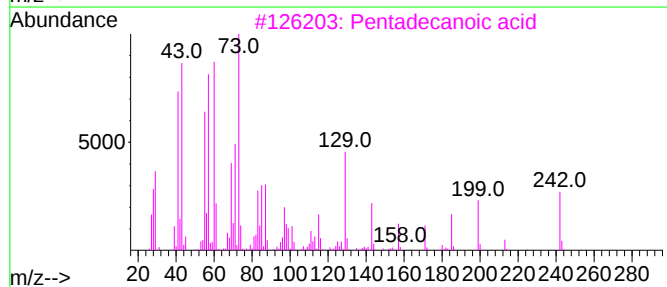
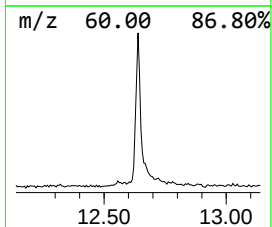
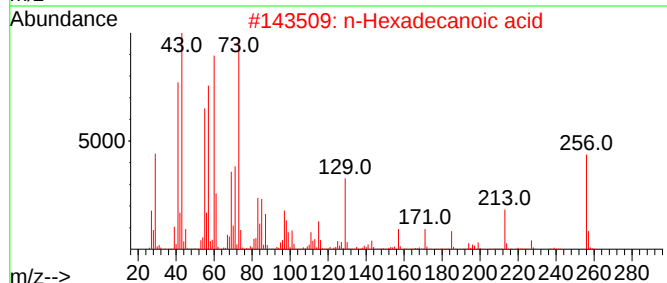
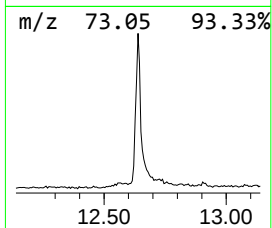
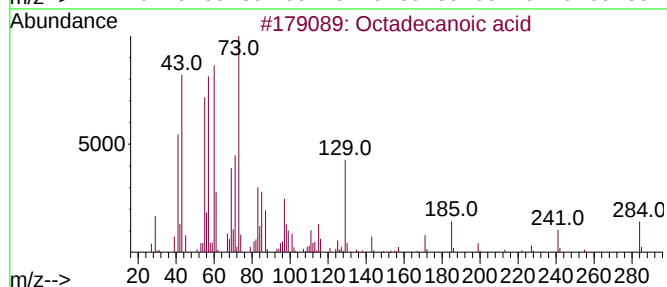
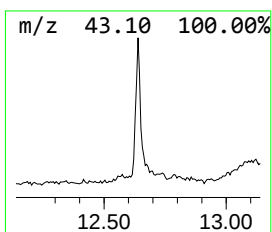
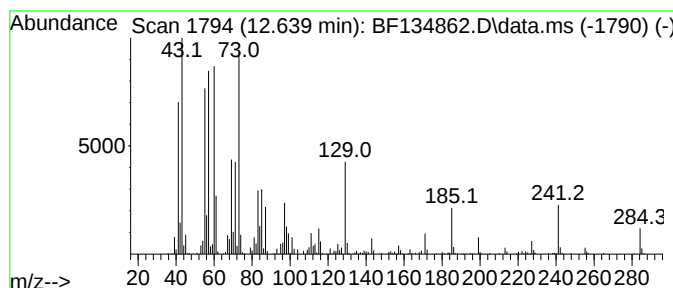
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.639	7.22 ng	643209	Phenanthrene-d10	11.316

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	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	89
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	83



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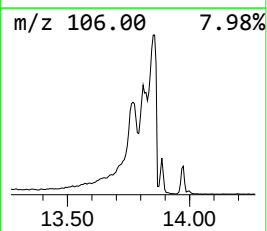
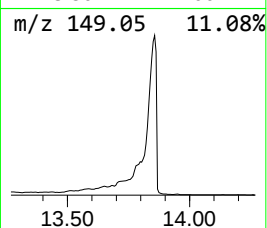
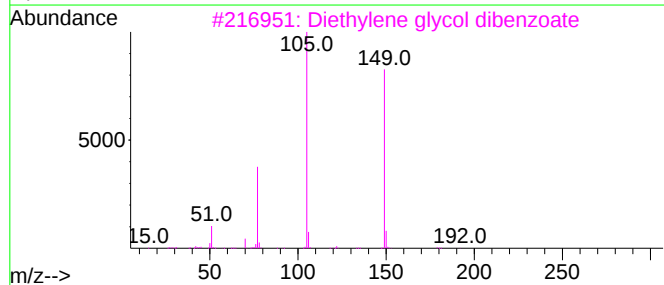
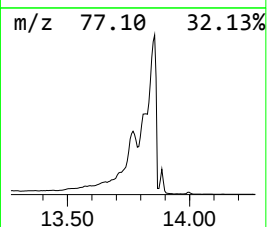
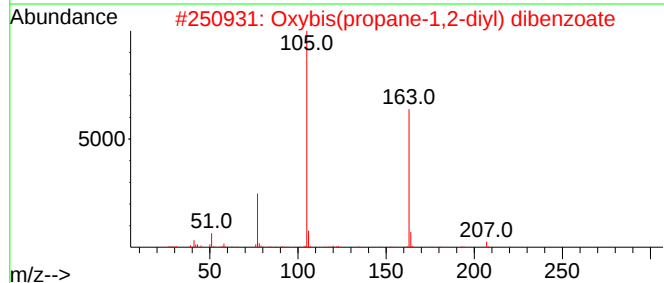
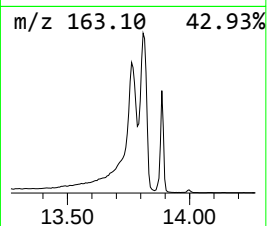
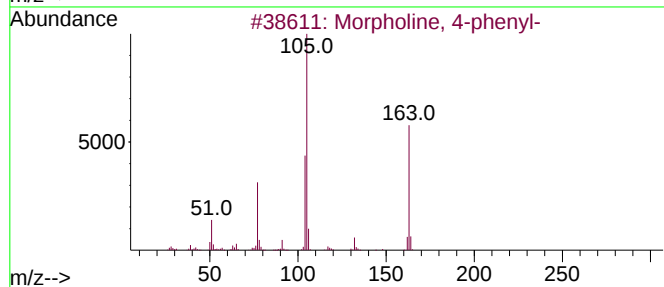
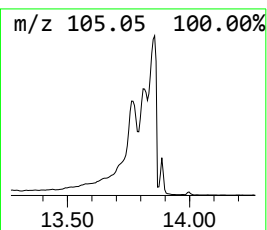
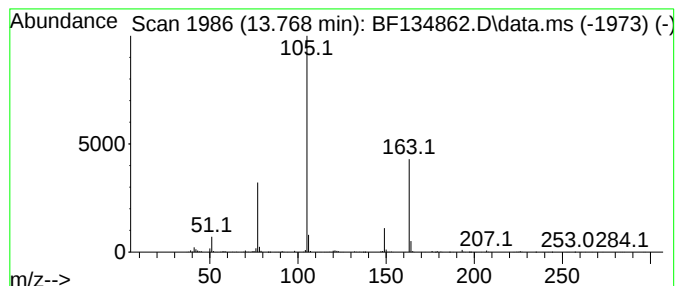
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Peak Number 4 Morpholine, 4-phenyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.768	107.77 ng	7176360	Chrysene-d12	13.974

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	64
2			Oxybis(propane-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	50
3			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	43
4			2-Isopropyl-5-methylphenyl benzoate	254	C17H18O2	1010366-96-0	43
5			2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	43



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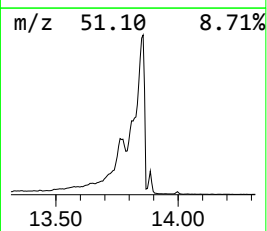
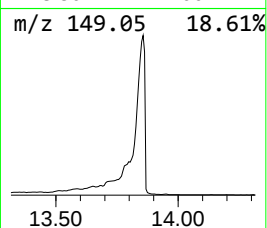
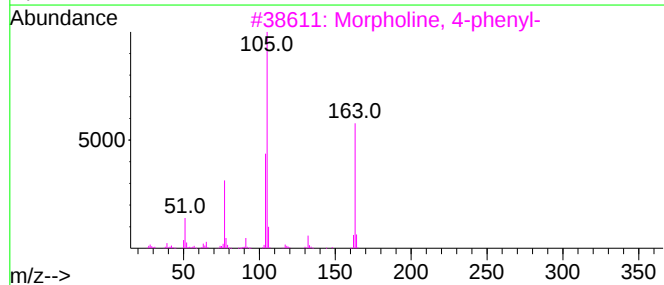
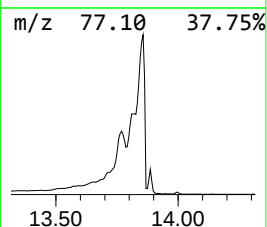
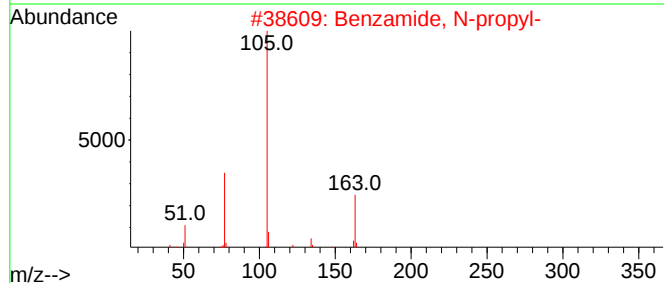
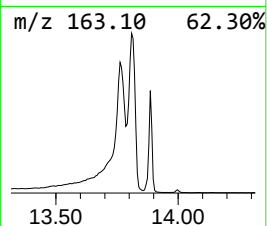
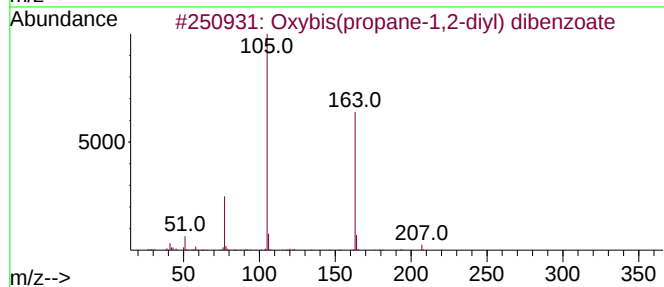
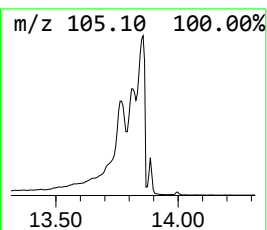
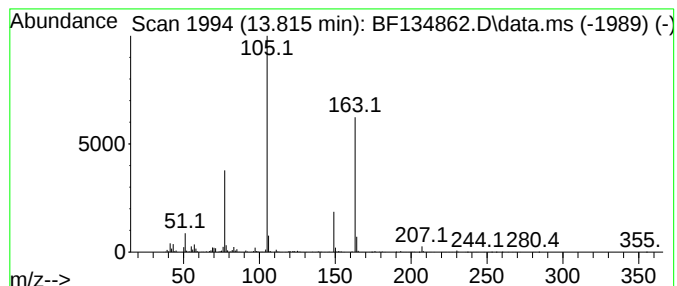
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Peak Number 5 Oxybis(propene-1,2-diyl) di... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.815	115.36 ng	7681990	Chrysene-d12	13.974

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxybis(propene-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	80
2			Benzamide, N-propyl-	163	C10H13NO	010546-70-0	64
3			Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	64
4			Glyoxylamide, N-phenyl-	163	C9H9NO2	032331-52-5	47
5			2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	38



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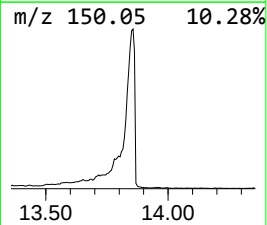
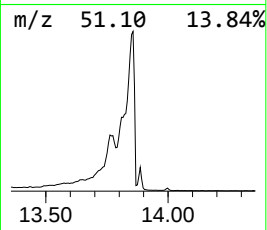
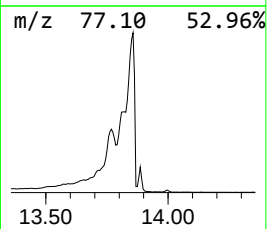
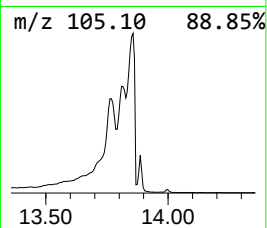
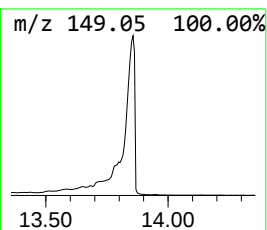
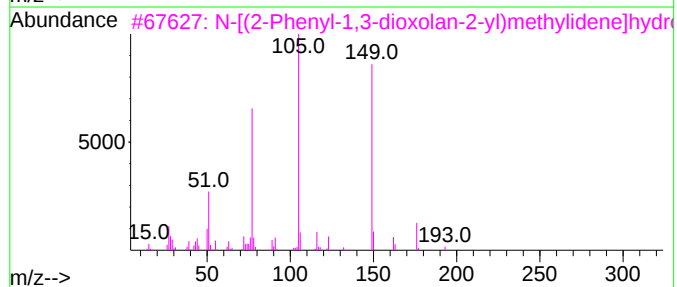
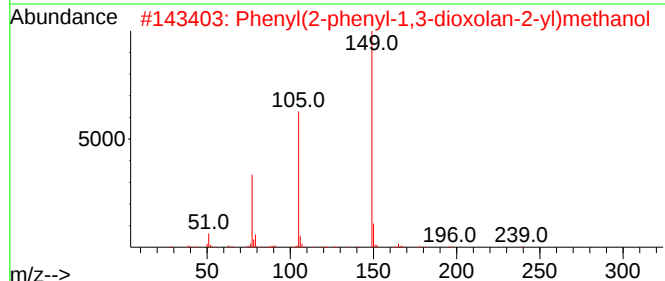
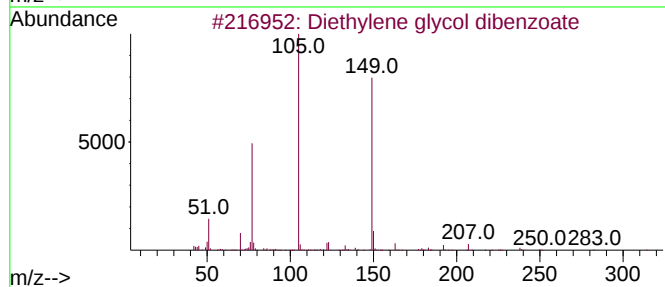
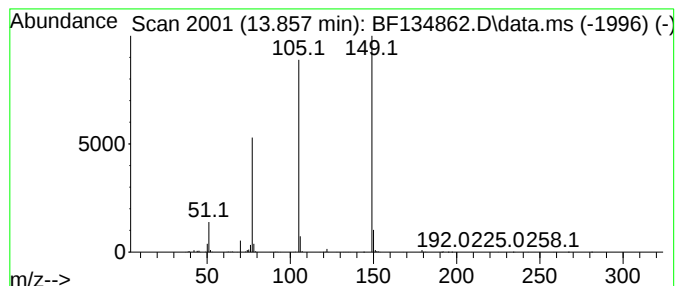
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Diethylene glycol dibenzoate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.857	167.90 ng	11180000	Chrysene-d12	13.974

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	83
2			Phenyl(2-phenyl-1,3-dioxolan-2-yl)methanol	256	C16H16O3	005694-69-9	78
3			N-[(2-Phenyl-1,3-dioxolan-2-yl)methyl]benzamide	193	C10H11NO3	1000411-48-9	78
4			Benzoic acid, 2-(3-nitrophenyl)ethyl ester	271	C15H13NO4	1000368-22-4	72
5			3,6,9,12-Tetraoxatetradecane-1,13-diol	446	C24H30O8	1000366-97-0	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082123\
Data File : BF134862.D
Acq On : 21 Aug 2023 12:08
Operator : CG\JU
Sample : 04086-18
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUP06

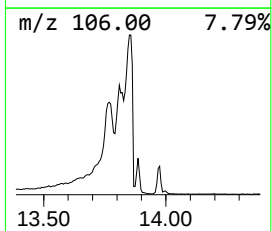
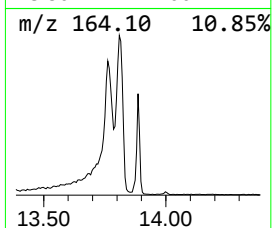
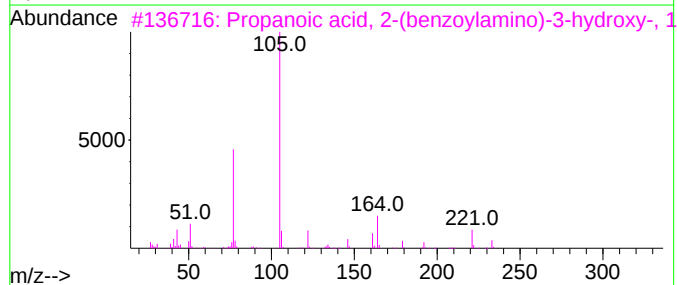
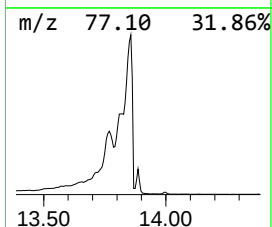
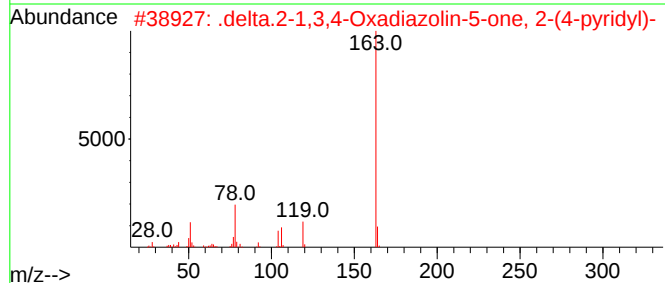
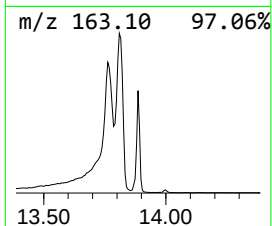
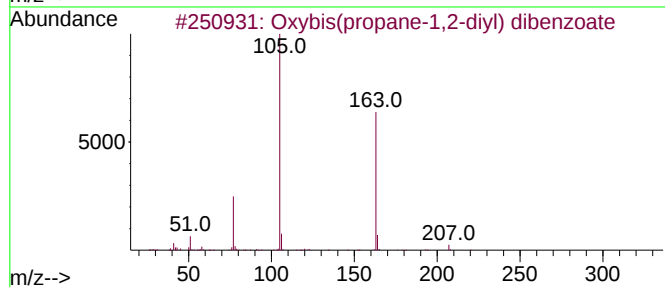
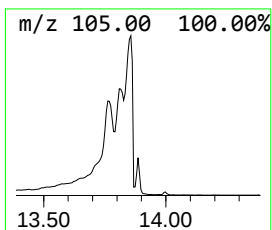
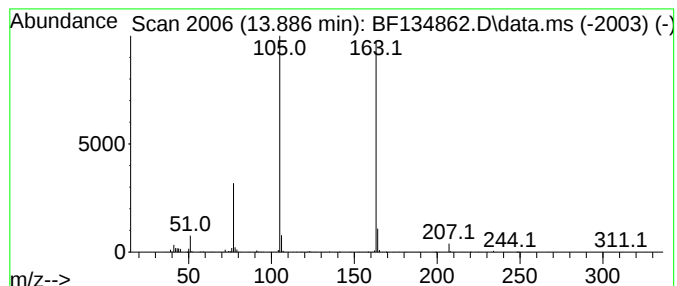
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 .delta.2-1,3,4-Oxadiazolin-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.886	20.36 ng	1355580	Chrysene-d12	13.974

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Oxybis(propene-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	58
2		.delta.2-1,3,4-Oxadiazolin-5-one...	163	C7H5N3O2	002845-82-1	50
3		Propanoic acid, 2-(benzoylamino)...	251	C13H17NO4	141627-52-3	14
4		Phenylglyoxylic Acid, 3-methylbu...	220	C13H16O3	1000453-46-1	14
5		Benzo[b]thiophene-3-carboxylic a...	343	C18H17NO4S	096334-43-9	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082123\
Data File : BF134862.D
Acq On : 21 Aug 2023 12:08
Operator : CG\JU
Sample : 04086-18
Misc :
ALS Vial : 4 Sample Multiplier: 1

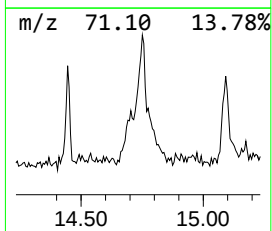
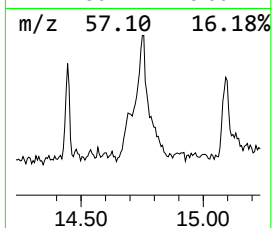
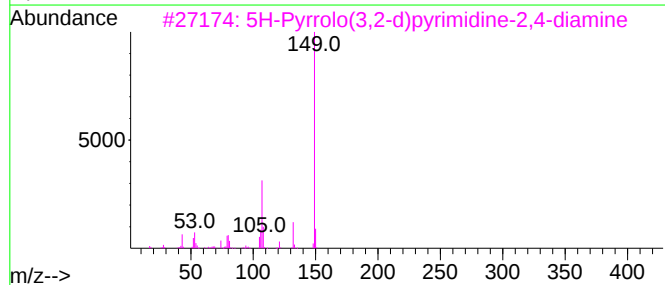
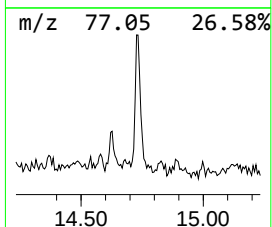
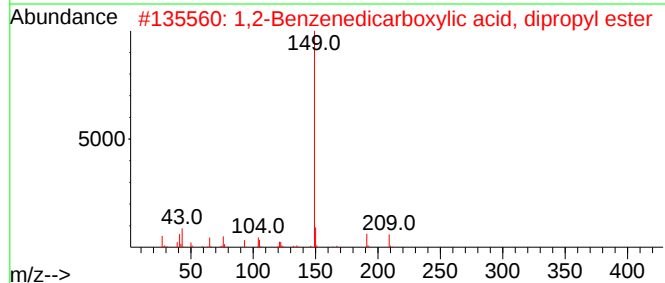
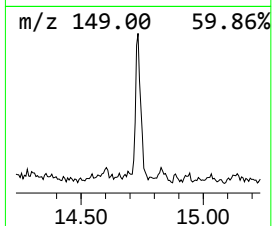
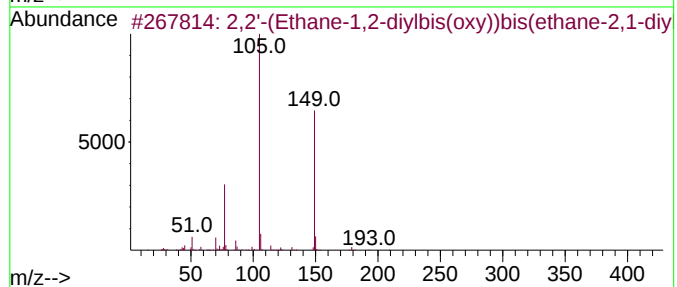
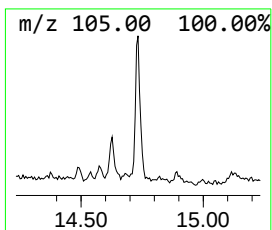
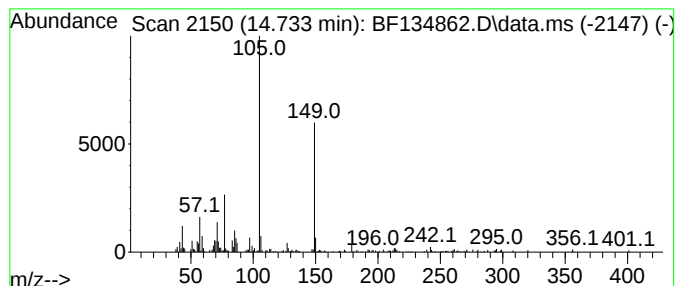
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 2,2'-(Ethane-1,2-diylbis(ox... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.733	4.75 ng	266876	Perylene-d12	15.433	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	59
2	1,2-Benzenedicarboxylic acid, di...	250	C14H18O4	000131-16-8	27
3	5H-Pyrrolo(3,2-d)pyrimidine-2,4-...	149	C6H7N5	1000244-21-4	27
4	Benzoic acid 3,5-dichloro-2,6-di...	295	C14H11Cl2NO2	037169-06-5	27
5	Phthalic acid, 3,5-difluoropheny...	390	C22H24F2O4	1000315-51-3	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082123\
Data File : BF134862.D
Acq On : 21 Aug 2023 12:08
Operator : CG\JU
Sample : 04086-18
Misc :
ALS Vial : 4 Sample Multiplier: 1

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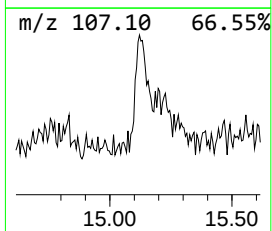
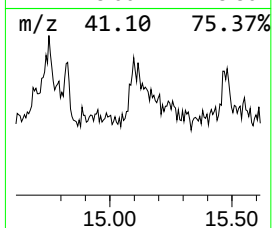
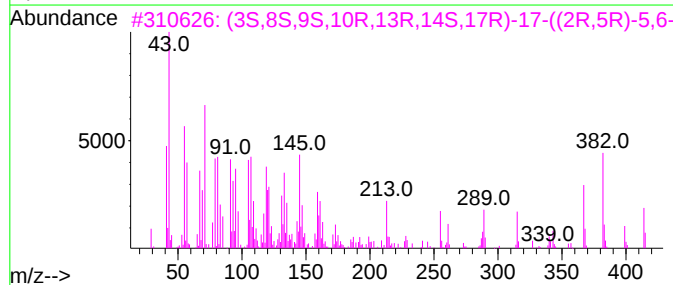
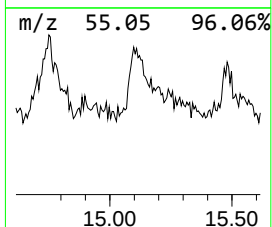
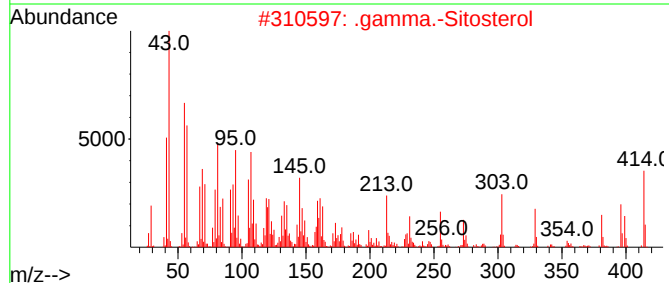
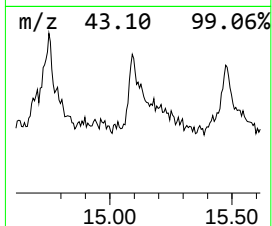
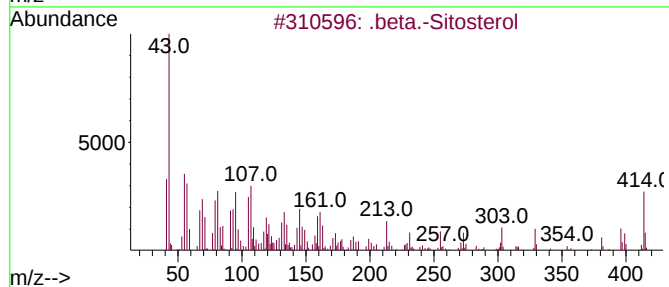
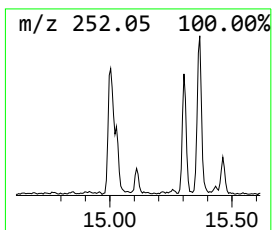
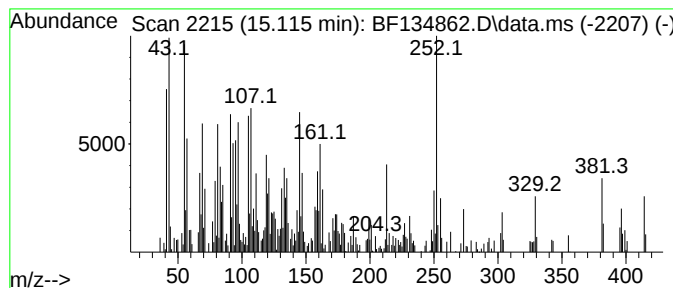
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 .beta.-Sitosterol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.115	7.26 ng	408006	Perylene-d12	15.433

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	.		.beta.-Sitosterol	414	C29H50O	000083-46-5	78
2	.		.gamma.-Sitosterol	414	C29H50O	000083-47-6	78
3	(3S,8S,9S,10R,13R,14S,17R)-17-((...			414	C29H50O	029365-29-5	35
4	1-Amino-4-(phenylthio)isoquinoline			252	C15H12N2S	019653-19-1	25
5	3-Amino-6-(3-pyridinyl)thieno[2,...			252	C13H8N4S	118947-66-3	15



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082123\
Data File : BF134862.D
Acq On : 21 Aug 2023 12:08
Operator : CG\JU
Sample : 04086-18
Misc :
ALS Vial : 4 Sample Multiplier: 1

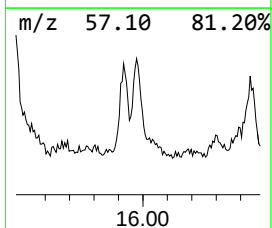
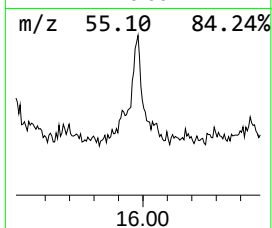
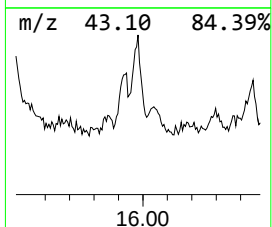
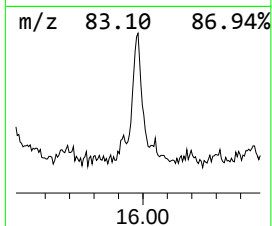
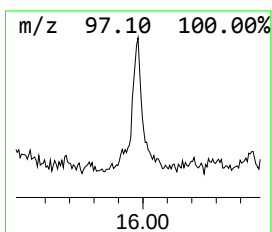
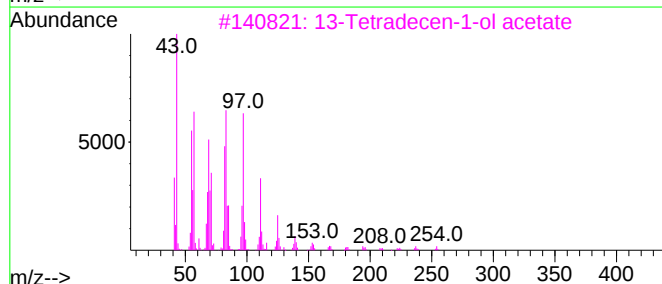
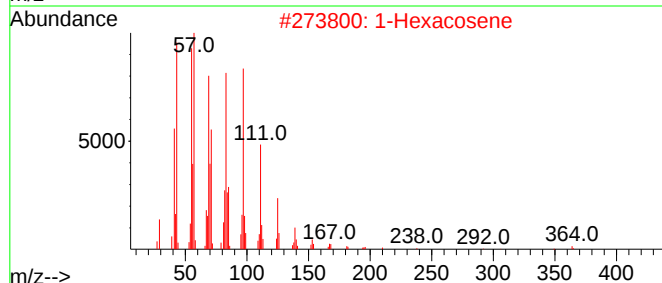
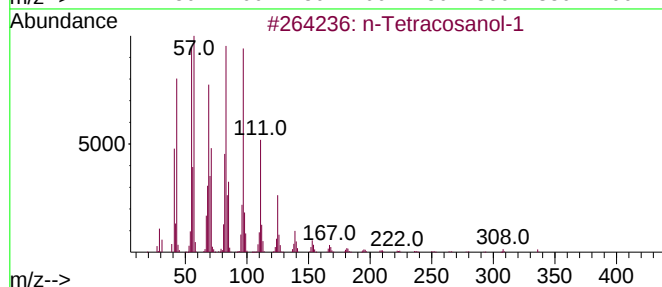
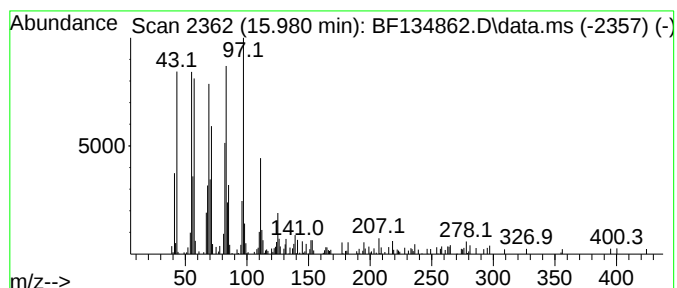
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 n-Tetracosanol-1 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.980	3.85 ng	216330	Perylene-d12	15.433	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
2	1-Hexacosene	364	C26H52	018835-33-1	93
3	13-Tetradecen-1-ol acetate	254	C16H30O2	056221-91-1	91
4	1-Heptacosanol	396	C27H56O	002004-39-9	90
5	Cyclopentane, 1-pentyl-2-propyl-	182	C13H26	062199-51-3	89



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082123\
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Sample : 04086-18
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	11.851	14.7	ng	1310150	4	11.316	1782790	20.0
Anthracene, 1-m...	11.927	3.4	ng	303767	4	11.316	1782790	20.0
Octadecanoic acid	12.639	7.2	ng	643209	4	11.316	1782790	20.0
Morpholine, 4-p...	13.768	107.8	ng	7176360	5	13.974	1331790	20.0
Oxybis(propane-...	13.815	115.4	ng	7681990	5	13.974	1331790	20.0
Diethylene glyc...	13.857	167.9	ng	11180000	5	13.974	1331790	20.0
.delta.2-1,3,4-...	13.886	20.4	ng	1355580	5	13.974	1331790	20.0
2,2'-(Ethane-1,...	14.733	4.8	ng	266876	6	15.433	1123620	20.0
.beta.-Sitosterol	15.115	7.3	ng	408006	6	15.433	1123620	20.0
n-Tetracosanol-1	15.980	3.9	ng	216330	6	15.433	1123620	20.0