

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052325\
 Data File : BF142536.D
 Acq On : 23 May 2025 15:37
 Operator : RC/JU
 Sample : Q2100-02
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-22

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-BF052025.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF142536.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.110	485	496	507	rBV	124630	185449	8.83%	1.114%
2	5.510	556	564	569	rBV	1279161	1660588	79.06%	9.975%
3	6.516	728	735	740	rBV	1249880	1692376	80.57%	10.166%
4	6.892	794	799	805	rBV	495263	631154	30.05%	3.791%
5	7.457	888	895	900	rBV	796499	1080004	51.42%	6.488%
6	7.710	933	938	945	rVB	17347	22522	1.07%	0.135%
7	8.181	1012	1018	1027	rBV	648336	860906	40.99%	5.172%
8	9.251	1195	1200	1205	rBV	1634066	2100407	100.00%	12.618%
9	9.933	1311	1316	1321	rBV	774805	967431	46.06%	5.812%
10	10.339	1362	1385	1401	rBV4	20919	172159	8.20%	1.034%
11	10.645	1432	1437	1445	rBV	194860	247997	11.81%	1.490%
12	10.722	1445	1450	1462	rVV	1037363	1309741	62.36%	7.868%
13	11.422	1564	1569	1577	rBV	758771	998712	47.55%	5.999%
14	11.492	1577	1581	1587	rVB3	19359	29868	1.42%	0.179%
15	11.945	1653	1658	1670	rBV	163194	251425	11.97%	1.510%
16	12.039	1671	1674	1682	rVB4	10669	21638	1.03%	0.130%
17	12.198	1698	1701	1708	rVB4	17187	24713	1.18%	0.148%
18	12.639	1772	1776	1780	rBV	32732	42776	2.04%	0.257%
19	12.733	1788	1792	1799	rBV5	21944	41275	1.97%	0.248%
20	12.869	1811	1815	1829	rVB2	26939	61200	2.91%	0.368%
21	13.010	1833	1839	1844	rBV	1407421	1767652	84.16%	10.619%
22	13.580	1932	1936	1945	rVB3	17617	28476	1.36%	0.171%
23	13.904	1986	1991	2008	rVB	65925	116644	5.55%	0.701%
24	14.063	2013	2018	2031	rVB	462417	630101	30.00%	3.785%
25	14.533	2094	2098	2103	rBV2	20190	32734	1.56%	0.197%
26	15.121	2193	2198	2206	rVB	19174	44719	2.13%	0.269%
27	15.492	2256	2261	2266	rVV	20380	31994	1.52%	0.192%
28	15.557	2266	2272	2288	rVV	387523	629020	29.95%	3.779%
29	17.056	2523	2527	2536	rVB3	10342	23687	1.13%	0.142%
30	17.903	2664	2671	2685	rVB2	51312	132332	6.30%	0.795%
31	18.151	2707	2713	2722	rBV	37093	101247	4.82%	0.608%
32	18.274	2725	2734	2749	rVB4	104754	363772	17.32%	2.185%
33	18.556	2767	2782	2805	rVB7	62856	341990	16.28%	2.054%

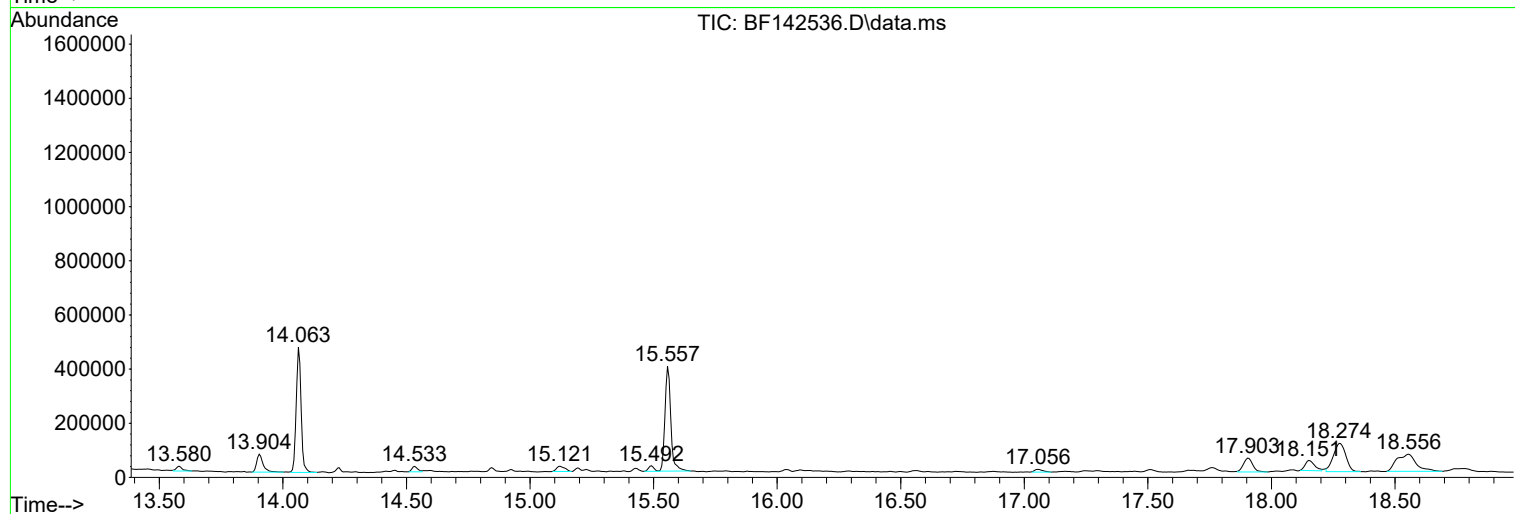
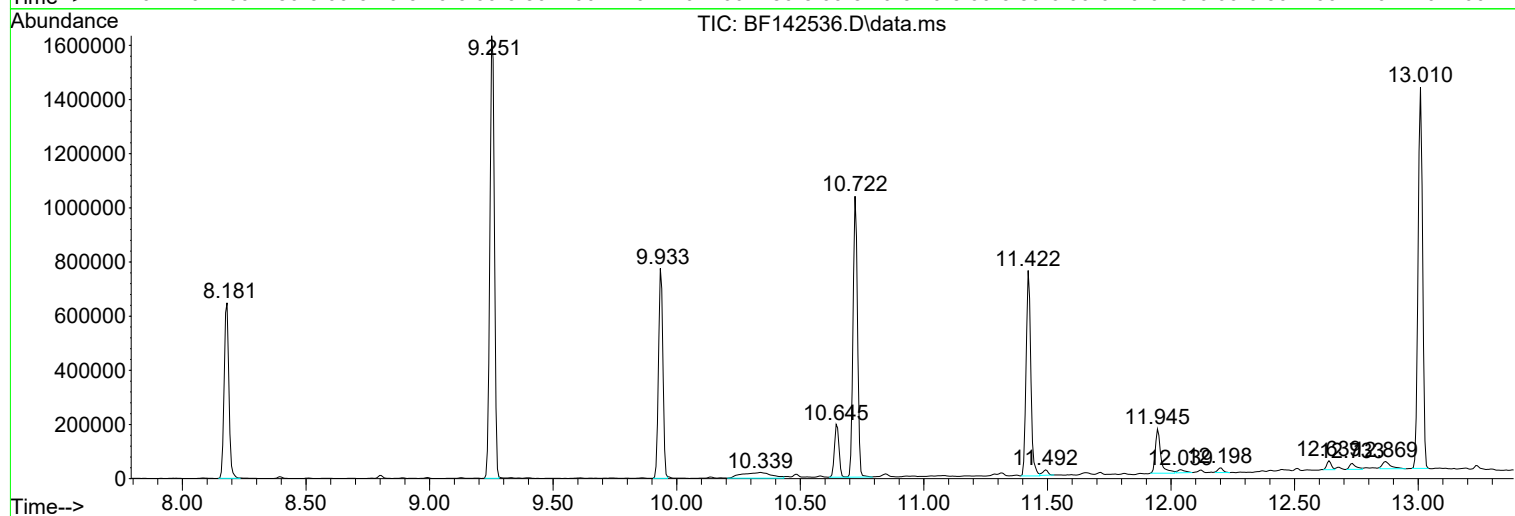
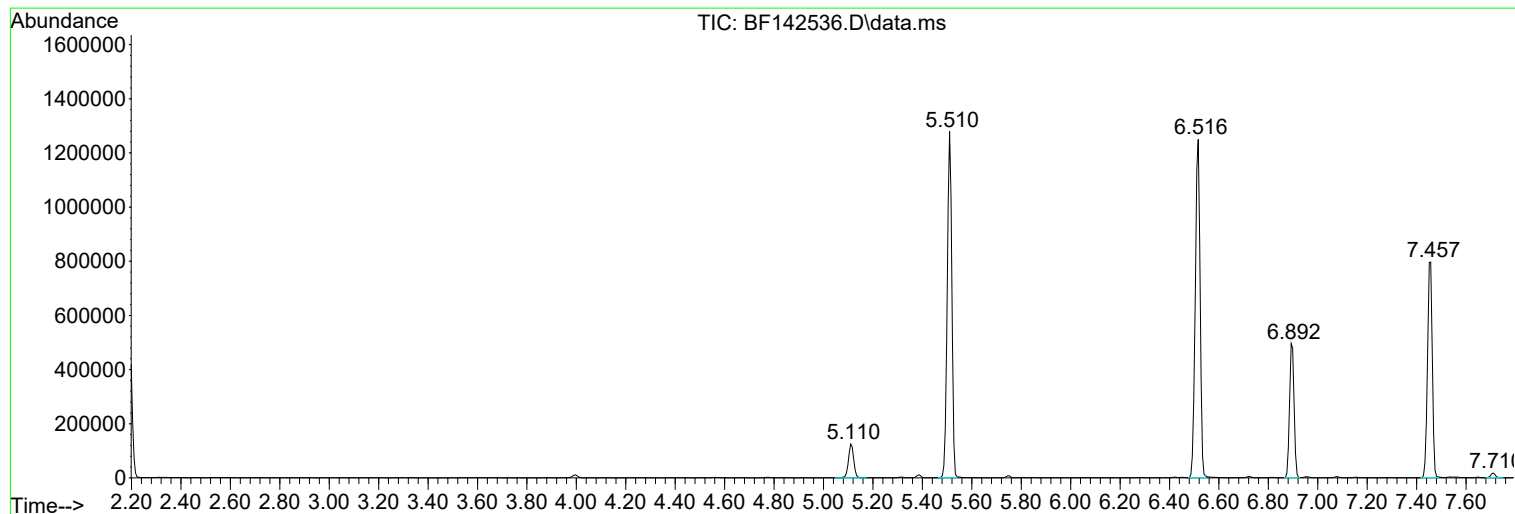
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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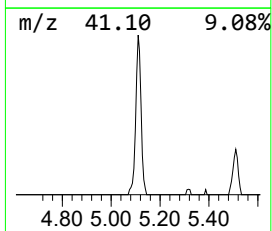
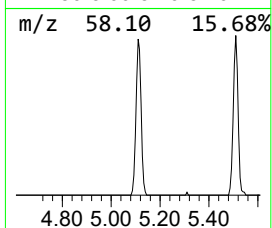
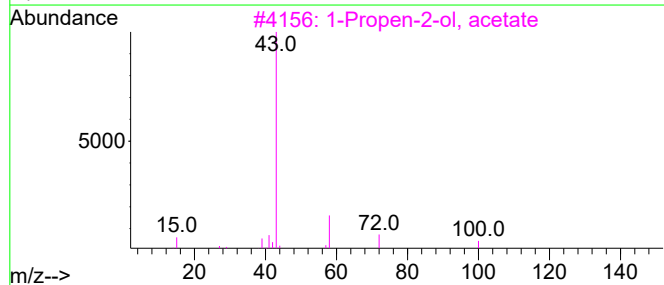
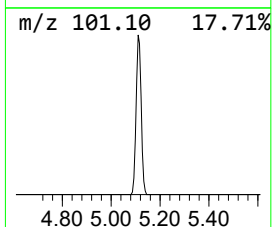
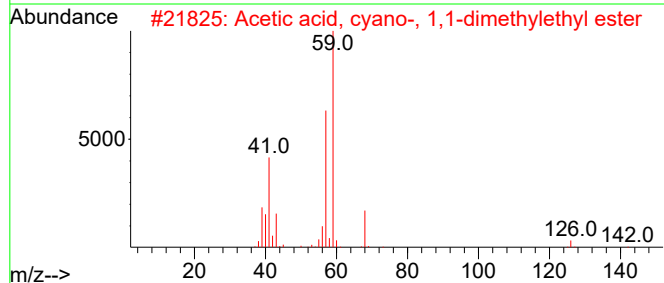
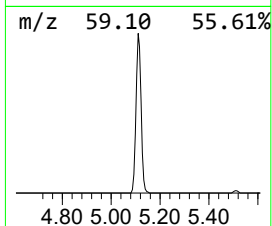
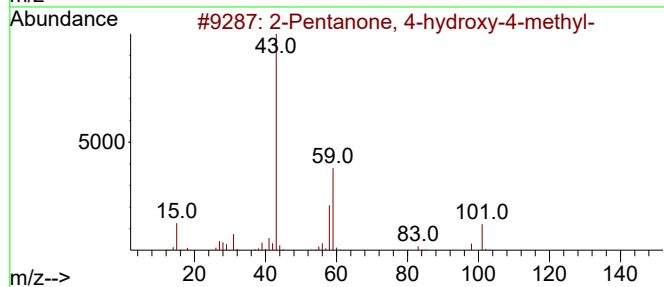
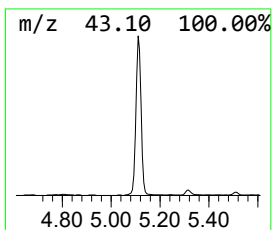
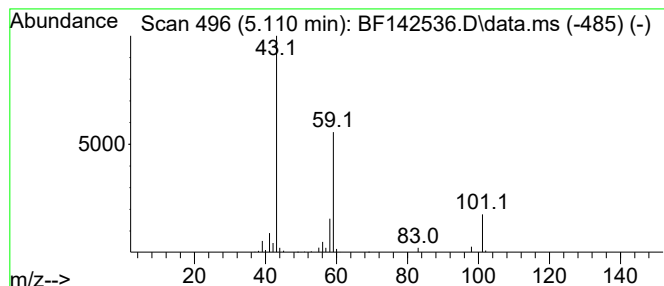
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TIC Library : C:\Database\NIST20.L
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.110	5.88 ng	185449	1,4-Dichlorobenzene-d4	6.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		
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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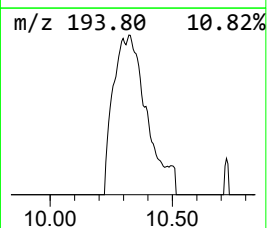
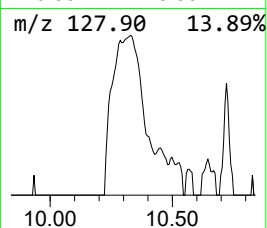
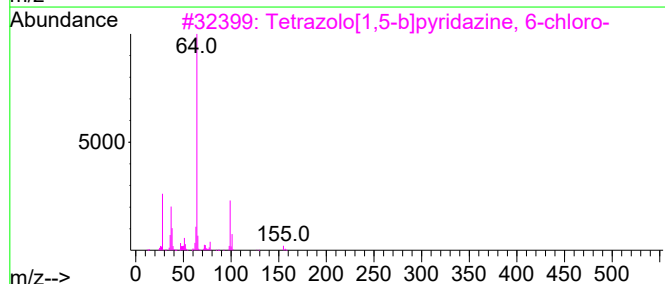
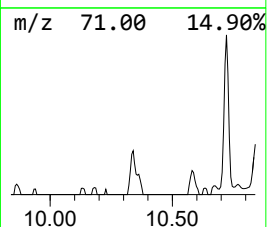
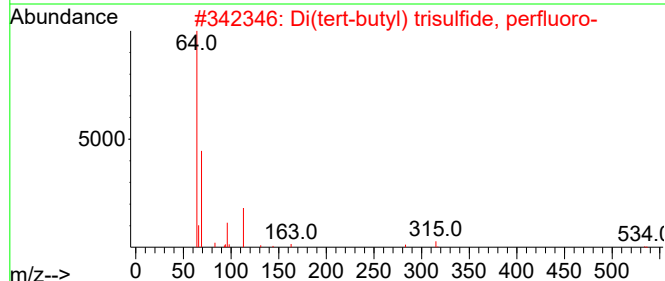
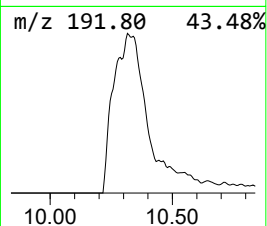
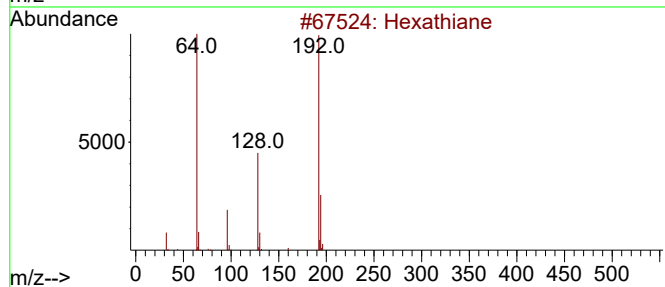
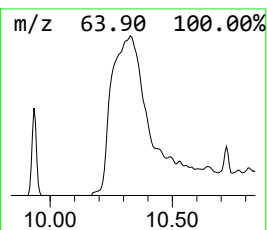
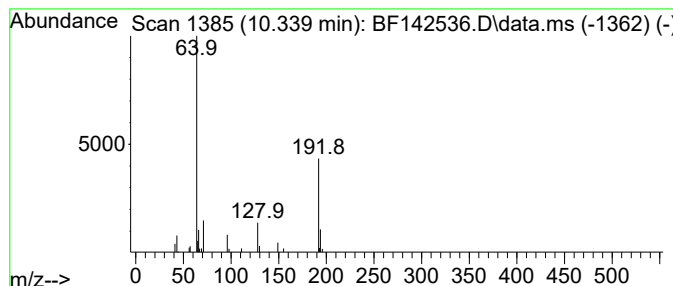
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Peak Number 2 Hexathiane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.339	3.56 ng	172159	Acenaphthene-d10	9.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexathiane	192	S6	013798-23-7	91
2			Di(tert-butyl) trisulfide, perfl...	534	C8F18S3	016005-64-4	9
3			Tetrazolo[1,5-b]pyridazine, 6-ch...	155	C4H2ClN5	021413-15-0	7
4			Sulfur dioxide	64	O2S	007446-09-5	4
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	4



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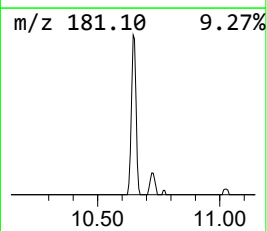
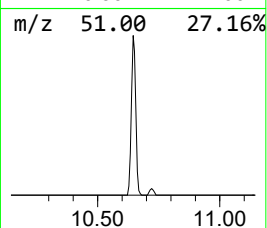
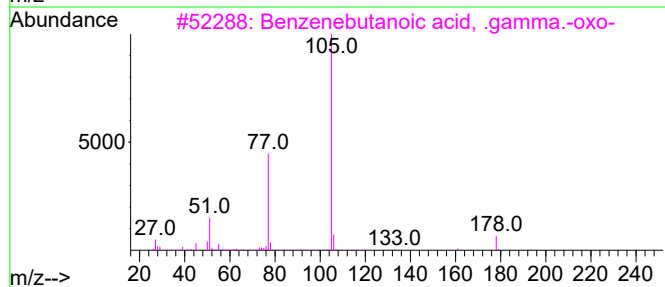
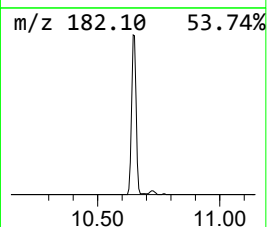
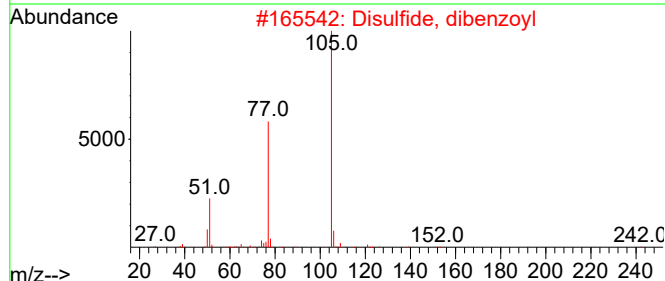
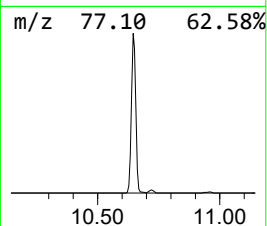
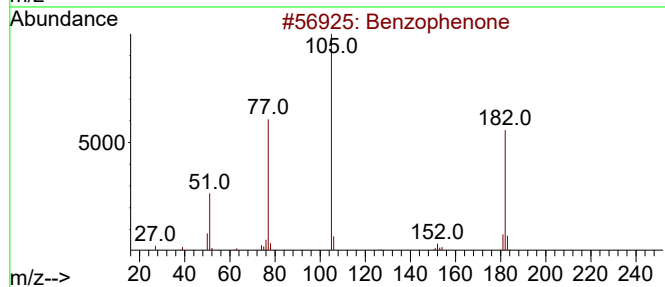
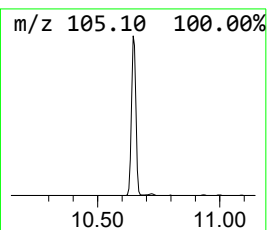
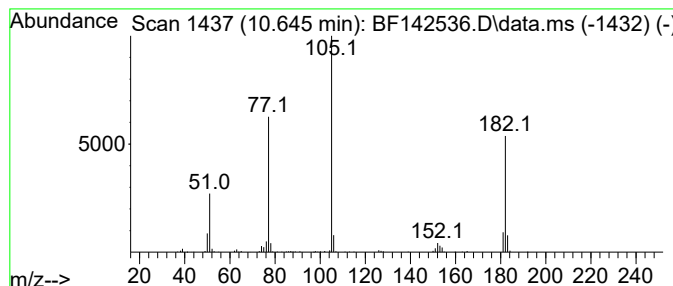
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Peak Number 3 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.645	5.13 ng	247997	Acenaphthene-d10	9.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Disulfide, dibenzoyl	274	C14H10O2S2	000644-32-6	49
3			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47
4			Benzoic acid, phenyl ester	198	C13H10O2	000093-99-2	47
5			Pentafluoroethyl phenyl ketone	224	C9H5F5O	000394-52-5	47



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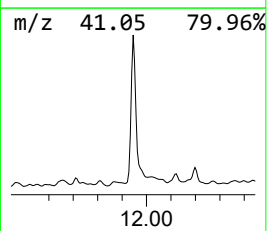
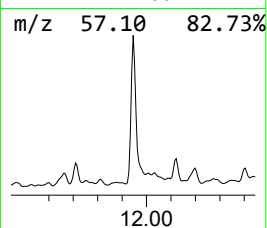
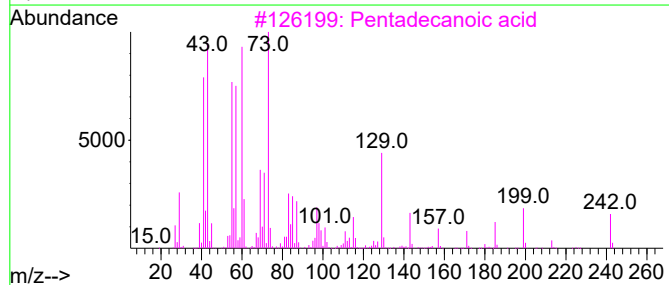
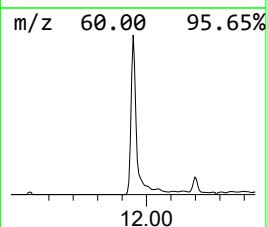
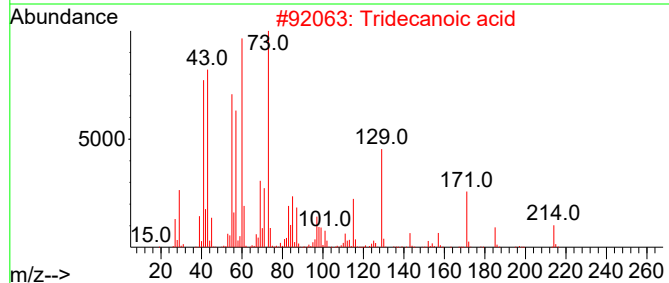
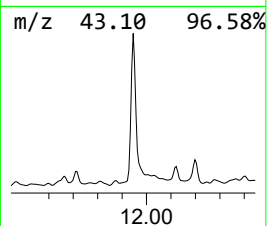
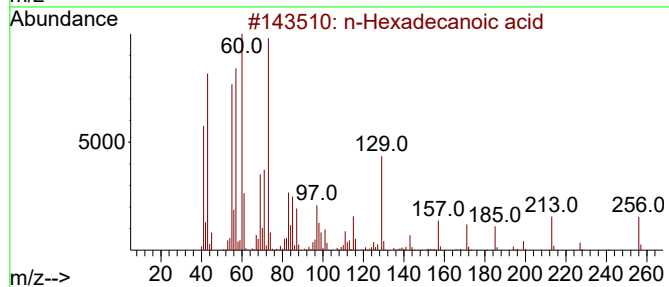
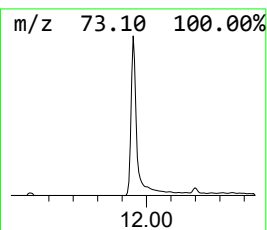
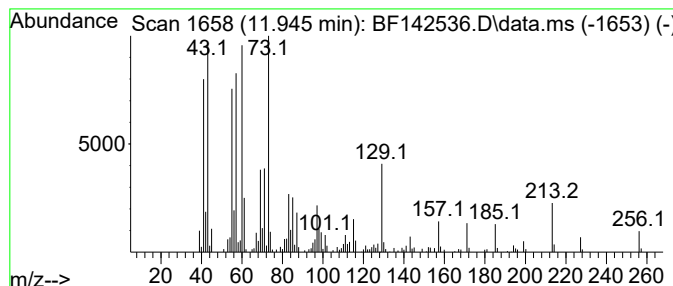
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.945	5.03 ng	251425	Phenanthrene-d10	11.422

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	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	n-Decanoic acid	172	C10H20O2	000334-48-5	86
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	74



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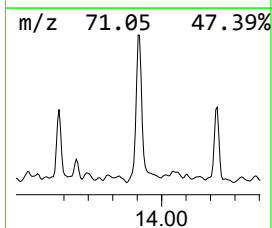
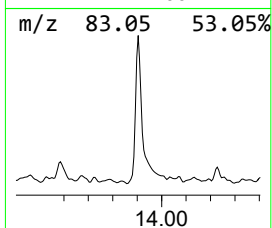
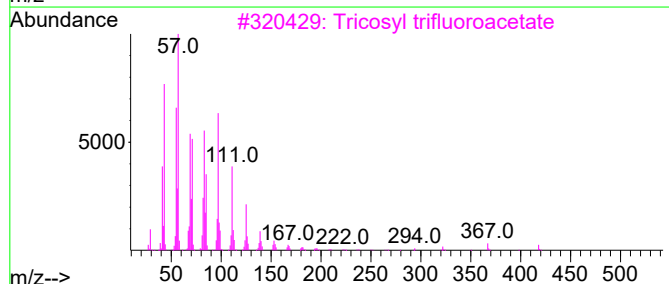
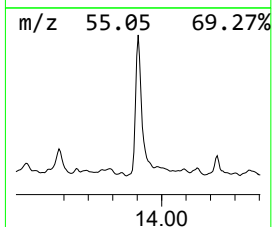
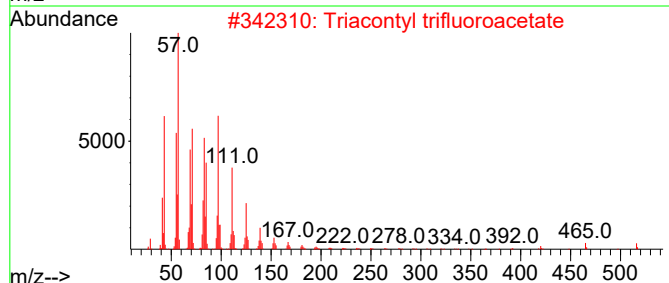
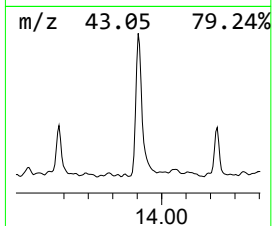
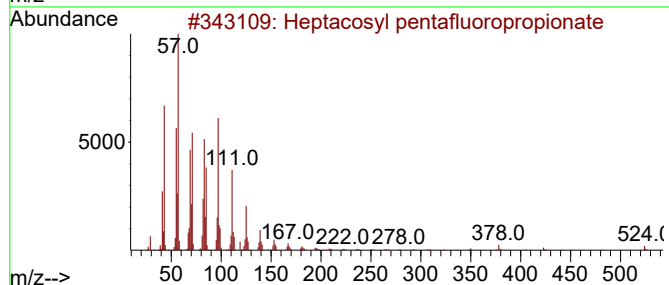
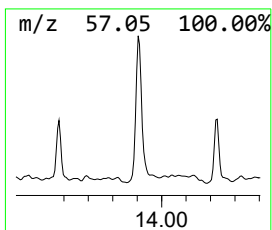
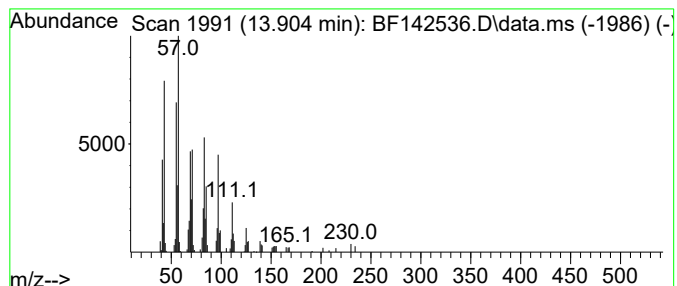
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Peak Number 5 Heptacosyl pentafluoropropi... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	3.70 ng	116644	Chrysene-d12	14.063

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosyl pentafluoropropionate	542	C30H55F5O2	1000351-81-6	91
2			Triacontyl trifluoroacetate	534	C32H61F3O2	1000351-75-7	91
3			Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91
4			Hexacosyl pentafluoropropionate	528	C29H53F5O2	1000351-81-2	91
5			Hexacosyl trifluoroacetate	478	C28H53F3O2	1000351-75-0	91



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ClientSampleId :
TP-22

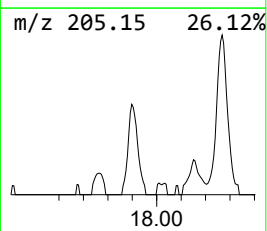
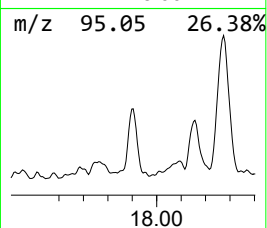
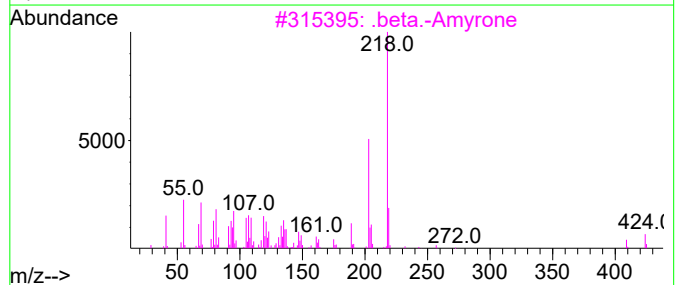
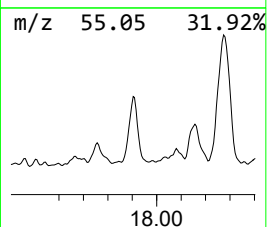
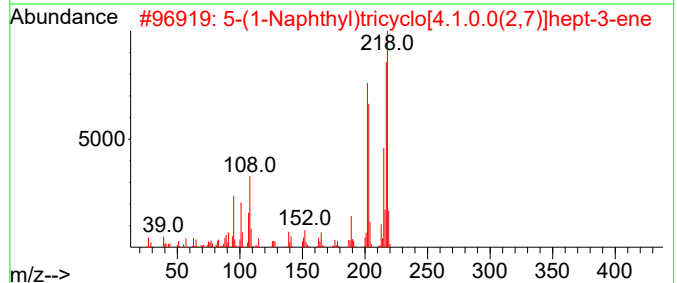
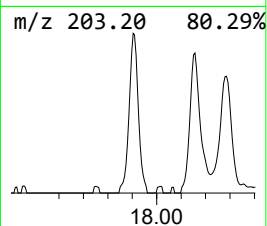
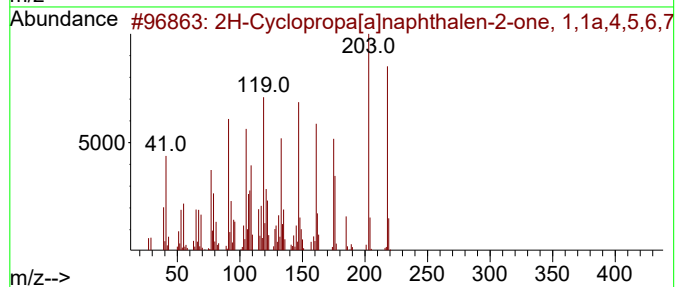
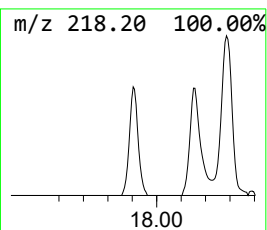
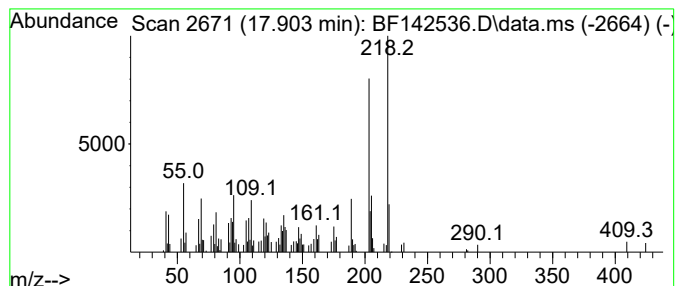
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 2H-Cyclopropa[a]naphthalen-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.904	4.21 ng	132332	Perylene-d12	15.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2H-Cyclopropa[a]naphthalen-2-one...	218	C15H22O	006831-17-0	64
2			5-(1-Naphthyl)tricyclo[4.1.0.0(2...	218	C17H14	107729-05-5	64
3			.beta.-Amyrone	424	C30H48O	000638-97-1	62
4			1H-1,3-Benzodiazole-5-carbaldehy...	218	C11H14N2OSi	1000478-28-4	52
5			Benzo[b]naphtho[2,3-d]furan	218	C16H10O	000243-42-5	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052325\
Data File : BF142536.D
Acq On : 23 May 2025 15:37
Operator : RC/JU
Sample : Q2100-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-22

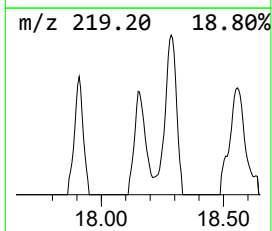
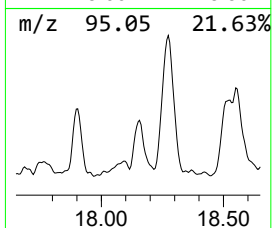
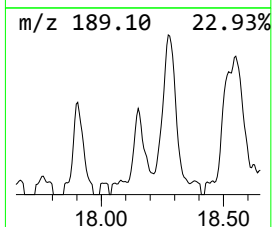
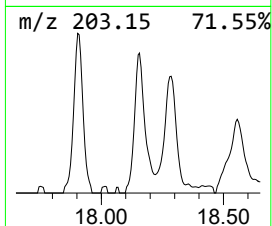
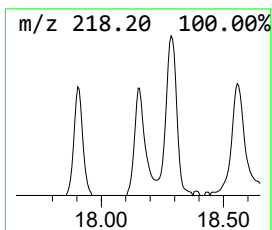
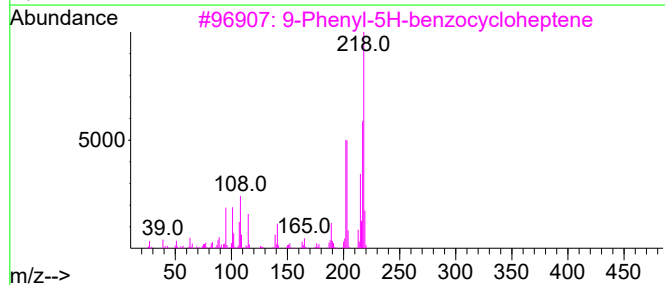
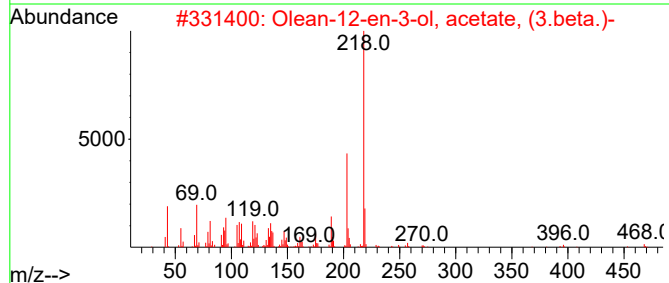
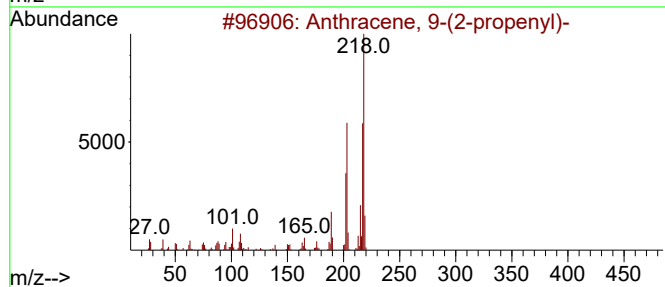
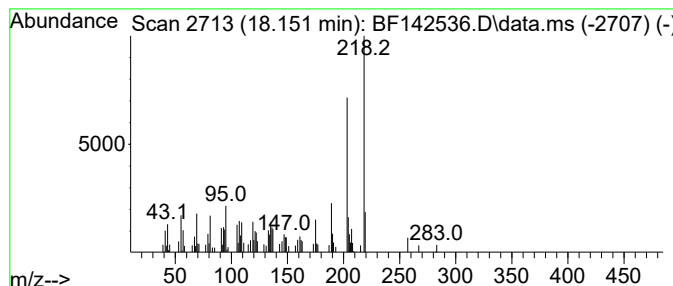
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Anthracene, 9-(2-propenyl)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.151	3.22 ng	101247	Perylene-d12	15.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Anthracene, 9-(2-propenyl)-	218	C17H14	023707-65-5	76
2			Olean-12-en-3-ol, acetate, (3.beta.)	468	C32H52O2	001616-93-9	74
3			9-Phenyl-5H-benzocycloheptene	218	C17H14	138089-71-1	72
4			5-(1-Naphthyl)tricyclo[4.1.0.0(2...	218	C17H14	107729-05-5	72
5			2H-Cyclopropa[a]naphthalen-2-one...	218	C15H22O	006831-17-0	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052325\
Data File : BF142536.D
Acq On : 23 May 2025 15:37
Operator : RC/JU
Sample : Q2100-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-22

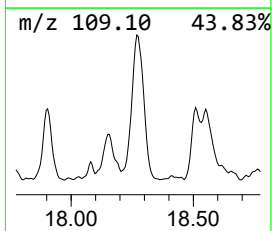
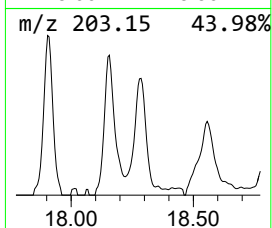
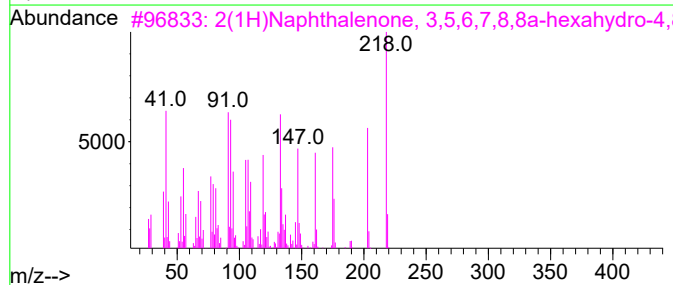
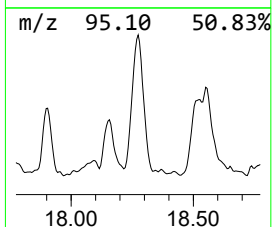
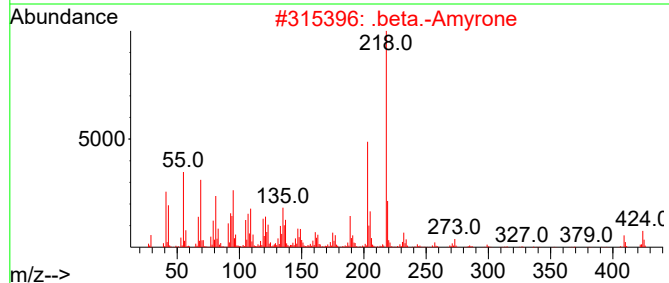
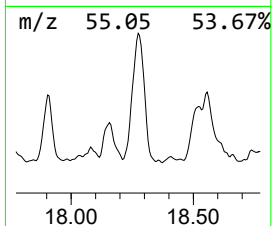
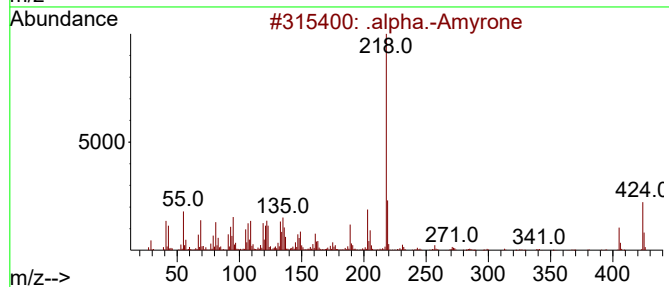
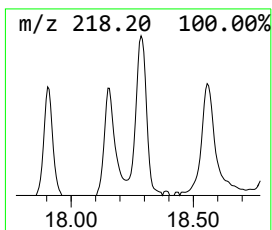
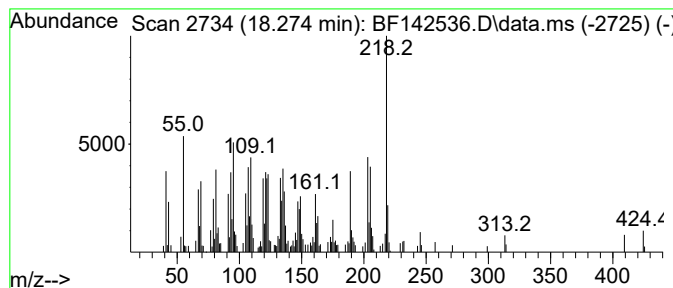
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 .alpha.-Amyrone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.274	11.57 ng	363772	Perylene-d12	15.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	.	alpha.-Amyrone	424	C30H48O	000638-96-0	98	
2	.	beta.-Amyrone	424	C30H48O	000638-97-1	50	
3	2(1H)	Naphthalenone, 3,5,6,7,8,8a...	218	C15H22O	1000188-66-5	49	
4	24-	Noroleana-3,12-diene	394	C29H46	201358-24-9	46	
5	.	alpha.-Boswellic acid, 0,0-bis-...	484	C32H52O3	1010507-05-0	43	



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052325\
Data File : BF142536.D
Acq On : 23 May 2025 15:37
Operator : RC/JU
Sample : Q2100-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-22

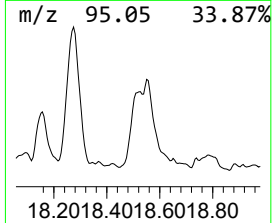
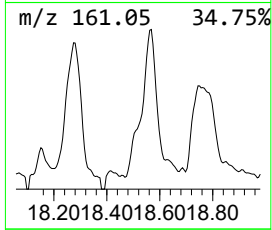
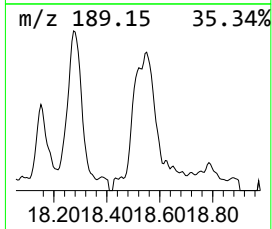
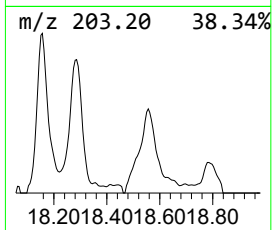
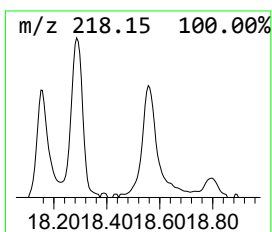
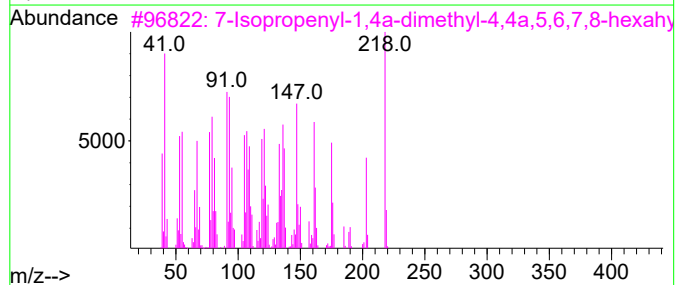
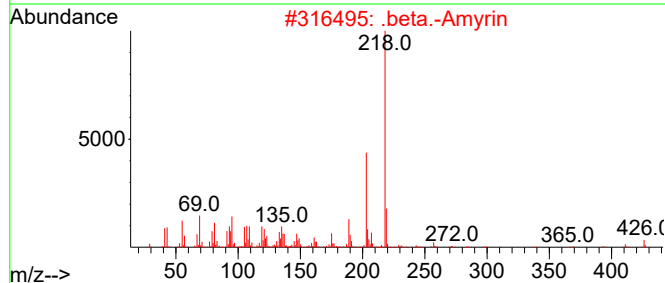
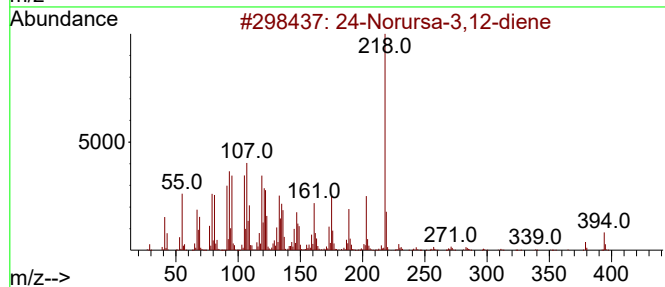
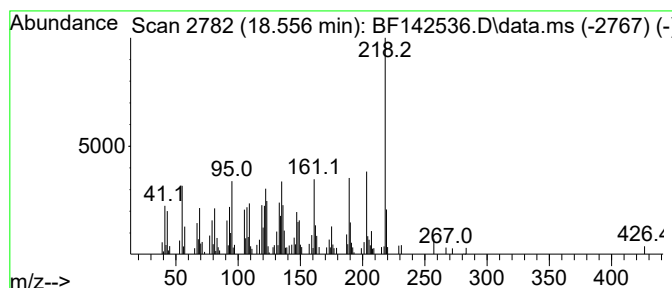
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 24-Norursa-3,12-diene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.556	10.87 ng	341990	Perylene-d12	15.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			24-Norursa-3,12-diene	394	C29H46	201358-25-0	64
2			.beta.-Amyrin	426	C30H50O	000559-70-6	58
3			7-Isopropenyl-1,4a-dimethyl-4,4a...	218	C15H22O	000473-08-5	58
4			Urs-12-en-3-ol, acetate, (3.beta.)-	468	C32H52O2	000863-76-3	58
5			5(1H)-Azulenone, 2,4,6,7,8,8a-he...	218	C15H22O	006754-66-1	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052325\
Data File : BF142536.D
Acq On : 23 May 2025 15:37
Operator : RC/JU
Sample : Q2100-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052025.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-...	5.110	5.9	ng	185449	1	6.898	631154	20.0
Hexathiane	10.339	3.6	ng	172159	3	9.933	967431	20.0
Benzophenone	10.645	5.1	ng	247997	3	9.933	967431	20.0
n-Hexadecanoic ...	11.945	5.0	ng	251425	4	11.422	998712	20.0
Heptacosyl pent...	13.904	3.7	ng	116644	5	14.063	630101	20.0
2H-Cyclopropa[a]...	17.904	4.2	ng	132332	6	15.557	629020	20.0
Anthracene, 9-(...	18.151	3.2	ng	101247	6	15.557	629020	20.0
.alpha.-Amyrone	18.274	11.6	ng	363772	6	15.557	629020	20.0
24-Norursa-3,12...	18.556	10.9	ng	341990	6	15.557	629020	20.0