

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052325\
 Data File : BF142533.D
 Acq On : 23 May 2025 14:10
 Operator : RC/JU
 Sample : Q2097-03
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RBR200044

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: BF142533.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.116	489	497	506	rBV	157782	240213	9.19%	1.267%
2	5.516	559	565	570	rVB	1509051	2085101	79.80%	11.002%
3	6.516	729	735	753	rVB	1572068	2188532	83.76%	11.548%
4	6.892	794	799	805	rBV	491297	634064	24.27%	3.346%
5	7.457	888	895	900	rBV	1035787	1371814	52.50%	7.238%
6	7.710	934	938	945	rVB	28966	36704	1.40%	0.194%
7	8.180	1012	1018	1023	rBV	647115	829037	31.73%	4.374%
8	9.175	1183	1187	1191	rVV2	20128	29839	1.14%	0.157%
9	9.257	1195	1201	1206	rBV	1964054	2612958	100.00%	13.787%
10	9.333	1210	1214	1218	rBV2	37507	53585	2.05%	0.283%
11	9.645	1263	1267	1271	rBV	119485	156892	6.00%	0.828%
12	9.804	1290	1294	1297	rBV2	71767	108923	4.17%	0.575%
13	9.845	1297	1301	1305	rVB	151195	195538	7.48%	1.032%
14	9.886	1305	1308	1310	rBV3	31422	43440	1.66%	0.229%
15	9.933	1310	1316	1321	rVV	730370	993309	38.01%	5.241%
16	10.192	1358	1360	1366	rBV5	38848	60832	2.33%	0.321%
17	10.345	1382	1386	1390	rVB2	183731	226858	8.68%	1.197%
18	10.651	1434	1438	1442	rBV	384698	483902	18.52%	2.553%
19	10.727	1446	1451	1461	rBV	1222897	1855499	71.01%	9.790%
20	11.427	1566	1570	1574	rBV	628033	784494	30.02%	4.139%
21	11.951	1656	1659	1665	rVB4	229561	313281	11.99%	1.653%
22	13.010	1835	1839	1846	rVB	1544690	2061215	78.88%	10.876%
23	13.904	1988	1991	2007	rVB	82911	202044	7.73%	1.066%
24	14.062	2014	2018	2027	rVB	414491	567693	21.73%	2.995%
25	14.533	2095	2098	2104	rVB2	18166	27778	1.06%	0.147%
26	15.192	2206	2210	2219	rVB	23271	37890	1.45%	0.200%
27	15.315	2227	2231	2236	rVB	26168	37755	1.44%	0.199%
28	15.556	2266	2272	2293	rVB	364816	603526	23.10%	3.184%
29	16.139	2365	2371	2380	rVB	37740	75028	2.87%	0.396%
30	17.233	2553	2557	2565	rVB2	15360	34433	1.32%	0.182%

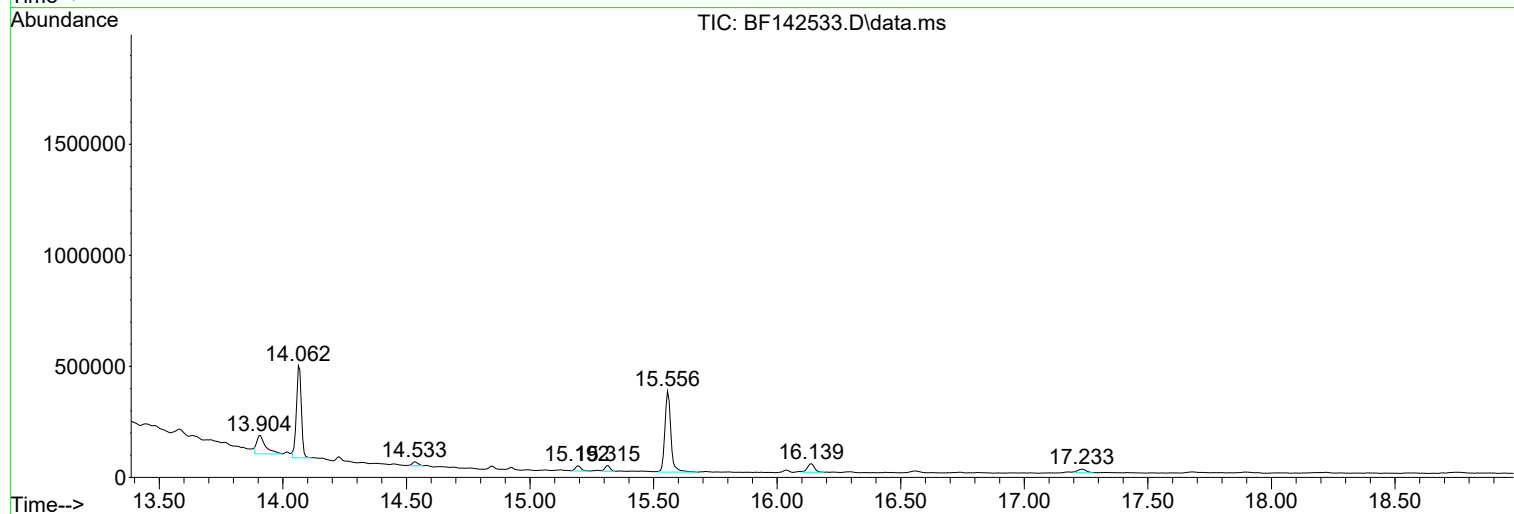
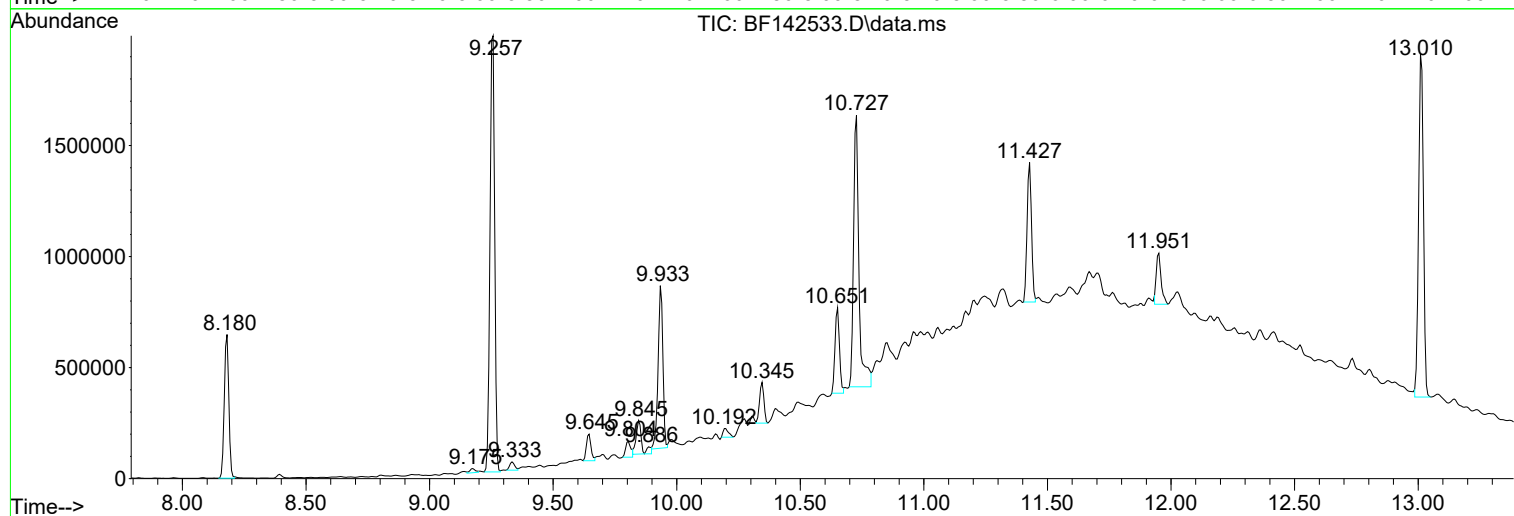
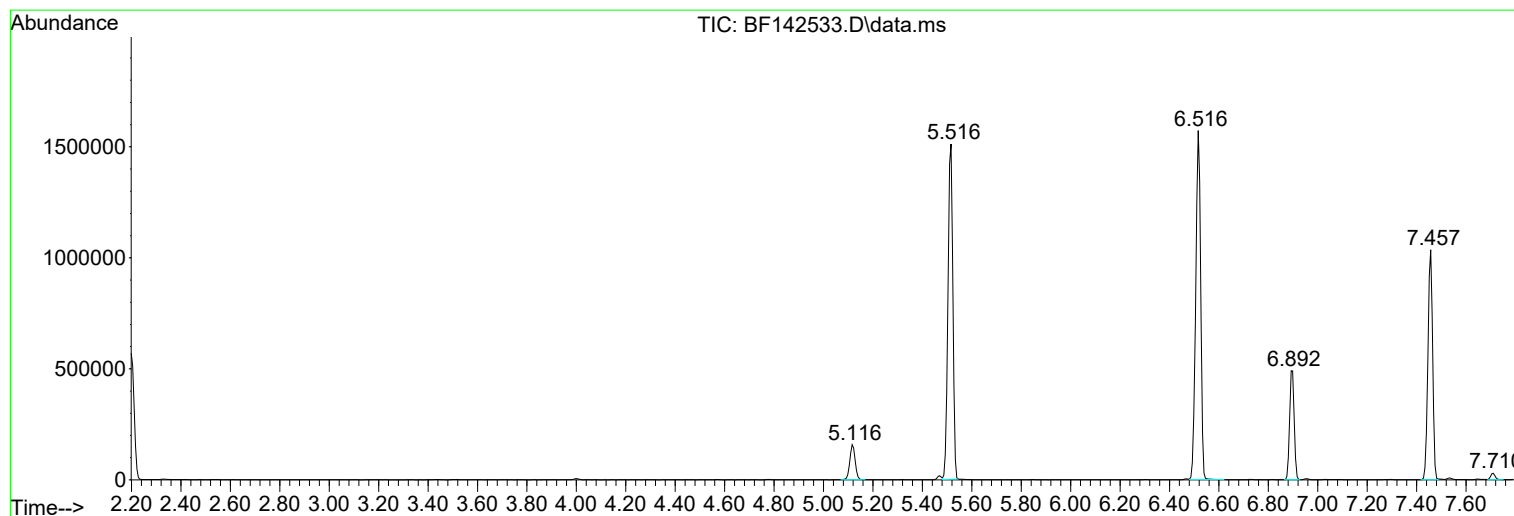
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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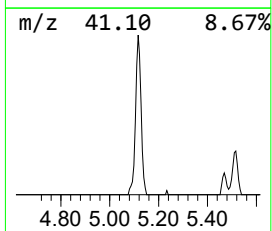
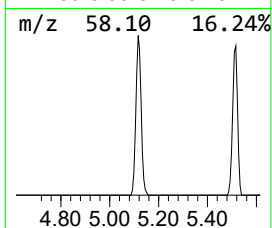
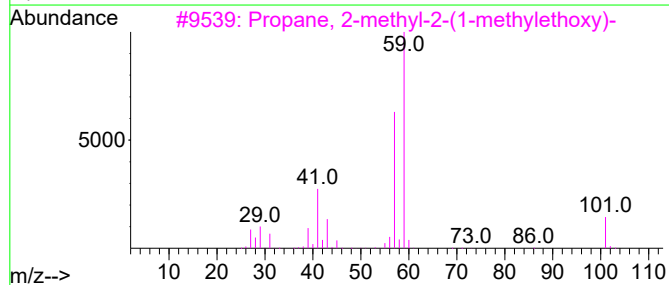
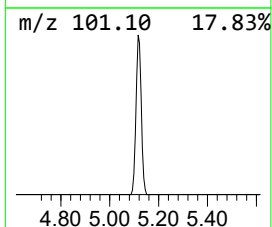
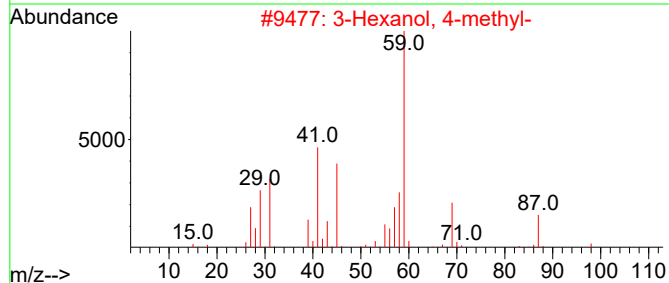
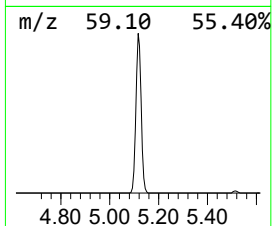
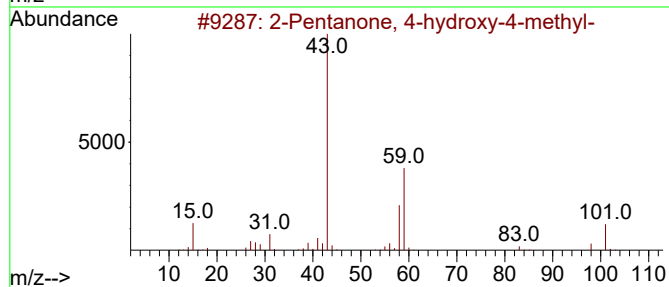
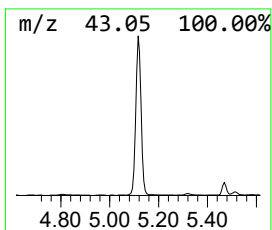
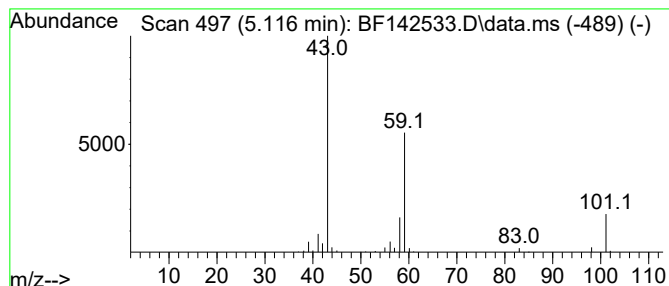
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.116	7.58 ng	240213	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	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		



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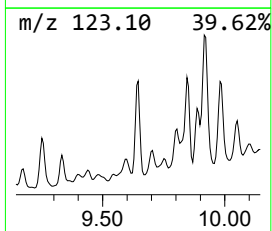
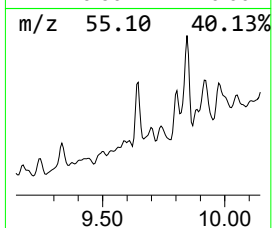
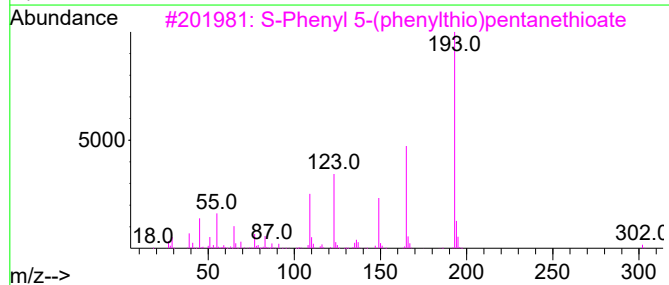
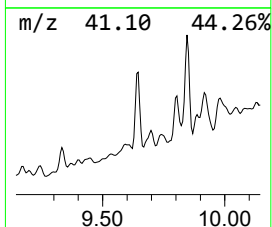
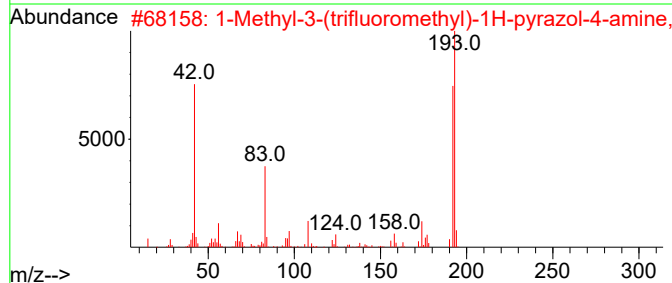
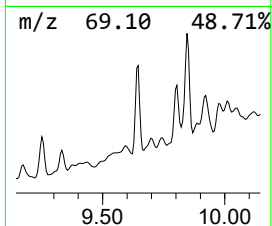
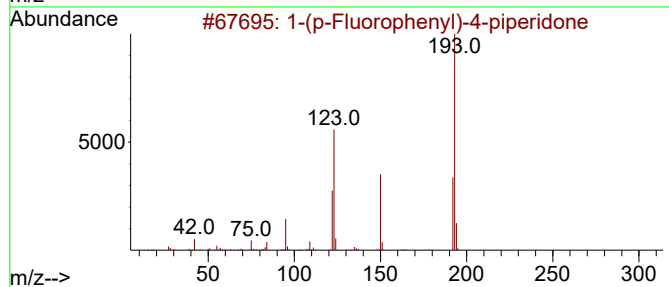
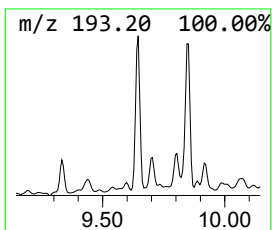
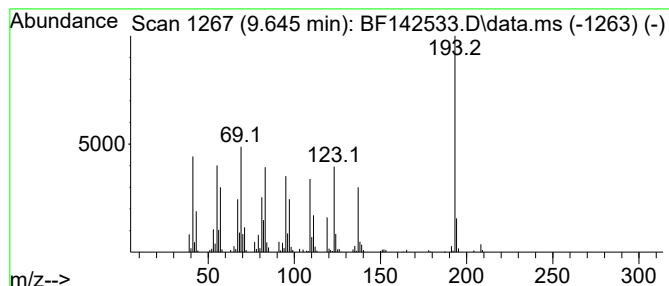
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Peak Number 2 unknown9.645 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.645	3.16 ng	156892	Acenaphthene-d10	9.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	38		
2	1-Methyl-3-(trifluoromethyl)-1H-...	193	C7H10F3N3	1000511-73-1	38		
3	S-Phenyl 5-(phenylthio)pentaneth...	302	C17H18OS2	1000234-40-7	37		
4	1H-Indene, octahydro-2,2,4,7,7...	208	C15H28	054832-83-6	32		
5	Pyrazole, 5-methyl-3-(5-nitro-2-...	193	C8H7N3O3	016239-90-0	27		



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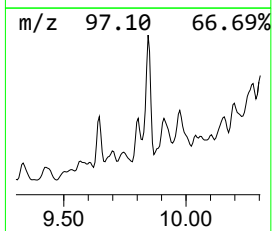
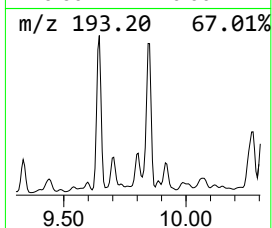
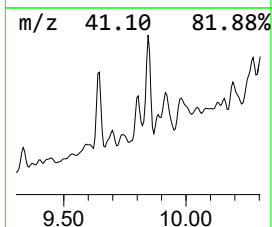
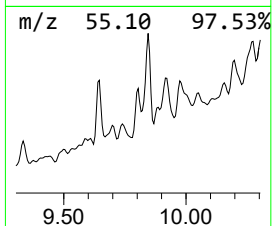
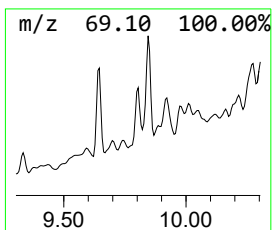
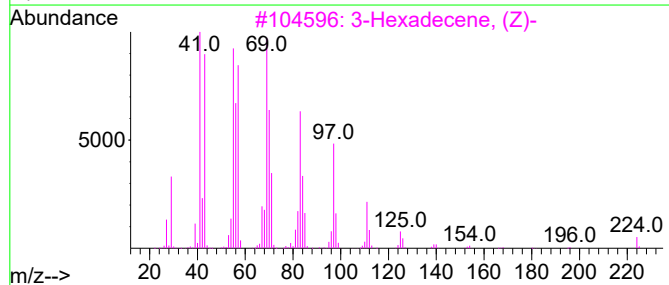
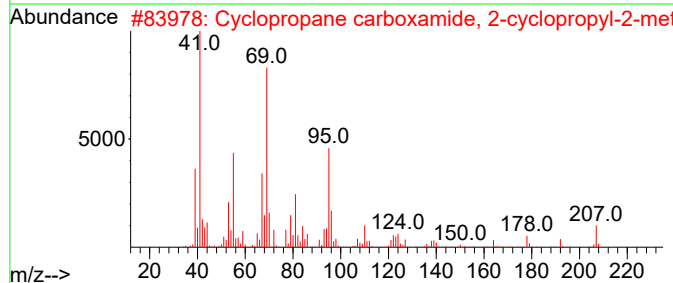
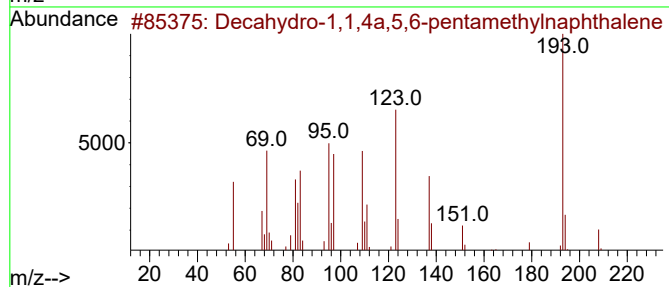
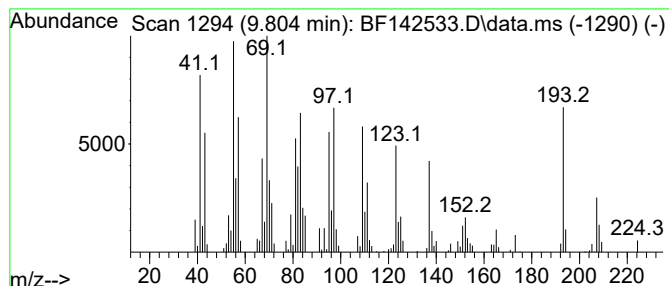
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.804	2.19 ng	108923	Acenaphthene-d10	9.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	98
2			Cyclopropane carboxamide, 2-cycl...	207	C13H21NO	331416-19-4	38
3			3-Hexadecene, (Z)-	224	C16H32	034303-81-6	35
4			2,4,5,5,8a-Pentamethyl-4a,5,6,7,...	208	C14H24O	1010195-30-1	30
5			Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	000547-60-4	30



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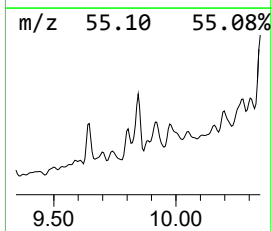
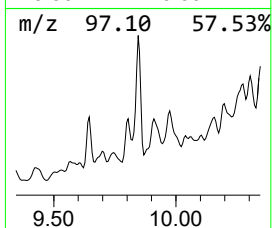
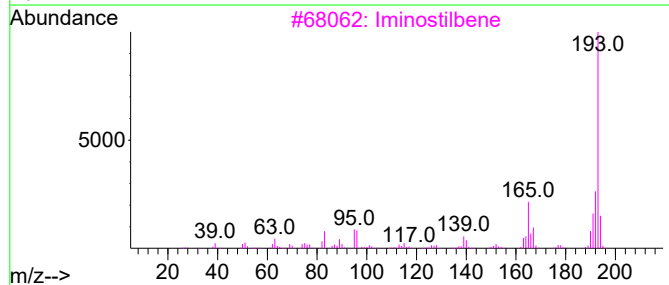
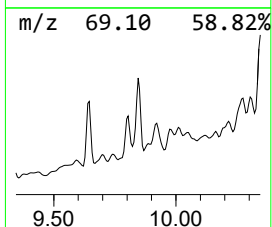
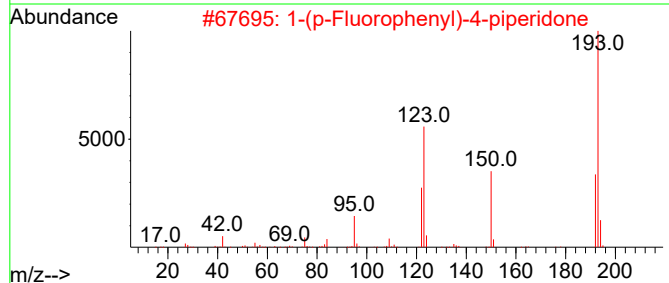
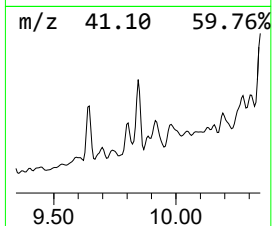
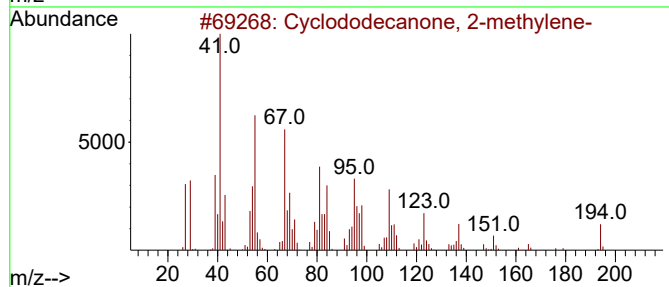
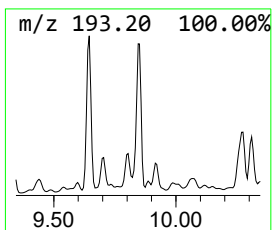
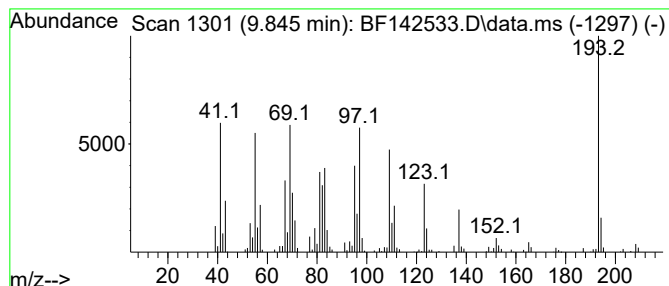
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Peak Number 4 unknown9.845 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.845	3.94 ng	195538	Acenaphthene-d10	9.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclododecanone, 2-methylene-	194	C13H22O	003045-76-9	38
2			1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	35
3			Iminostilbene	193	C14H11N	000256-96-2	25
4			Butan-2-one, 1-[3-(3,3-dimethyl-...	278	C16H26N2O2	1000303-34-2	22
5			2-((Trimethylsilyl)thio)nicotino...	208	C9H12N2SSi	1000474-02-5	18



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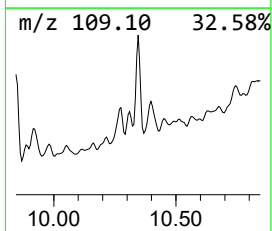
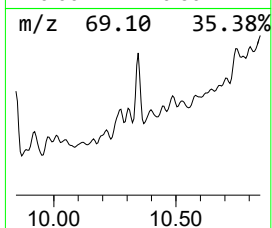
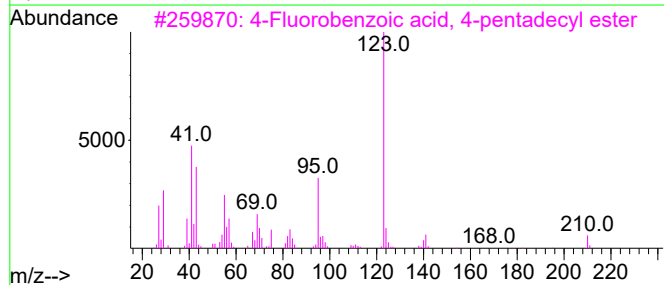
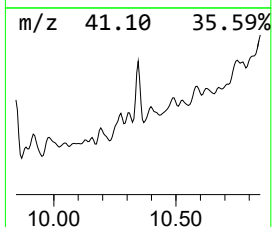
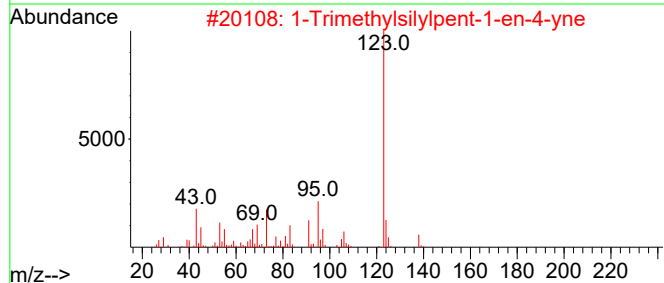
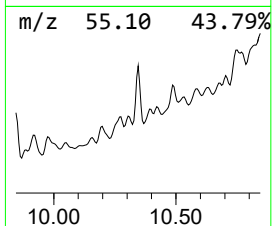
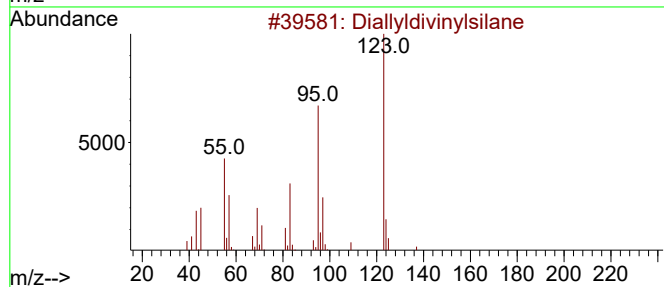
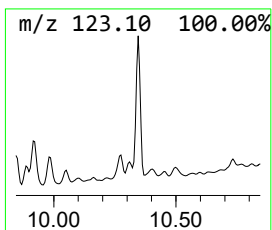
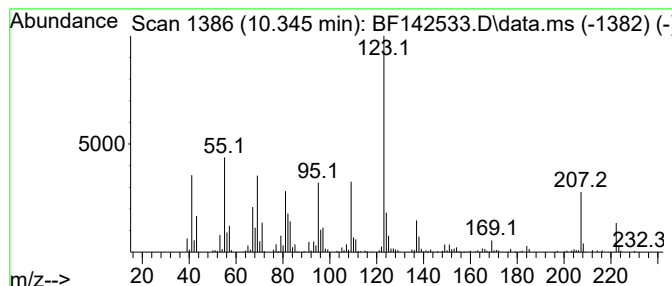
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Peak Number 5 Diallyldivinylsilane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.345	4.57 ng	226858	Acenaphthene-d10	9.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diallyldivinylsilane	164	C10H16Si	119901-88-1	50
2			1-Trimethylsilylpent-1-en-4-yne	138	C8H14Si	079516-25-9	50
3			4-Fluorobenzoic acid, 4-pentadec...	350	C22H35FO2	1000280-68-5	50
4			Benzamide, 3-fluoro-N,N-dipropyl-	223	C13H18FNO	1000438-01-7	50
5			Benzamide, 3-fluoro-N-methyl-N-p...	223	C13H18FNO	1000421-36-9	46



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ClientSampleId :
RBR200044

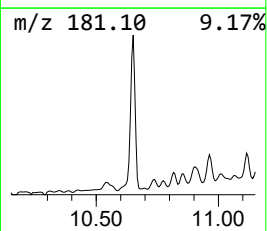
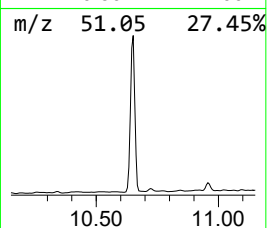
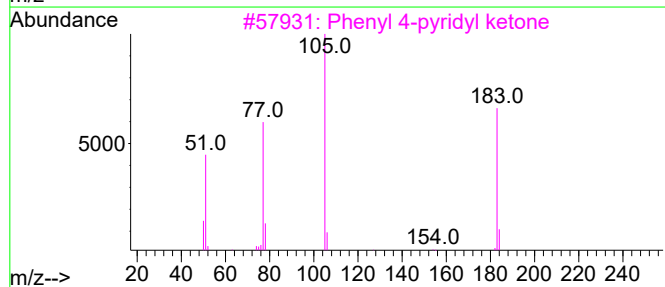
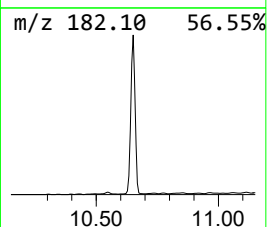
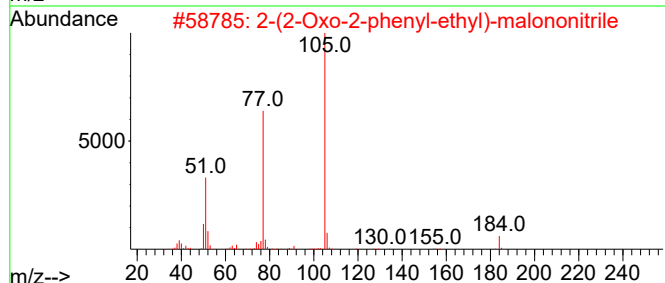
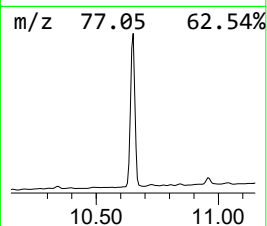
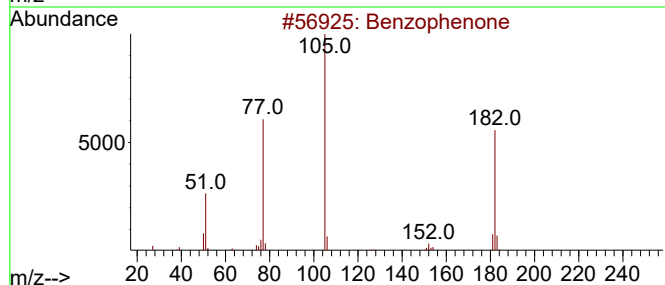
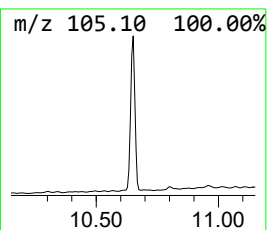
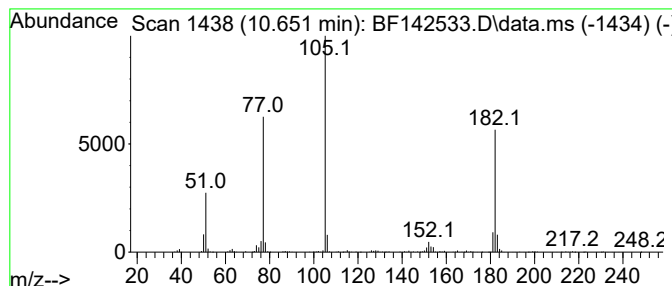
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benzophenone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.651	9.74 ng	483902	Acenaphthene-d10	9.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	53
3			Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	49
4			Vinyl benzoate	148	C9H8O2	000769-78-8	47
5			Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052325\
Data File : BF142533.D
Acq On : 23 May 2025 14:10
Operator : RC/JU
Sample : Q2097-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

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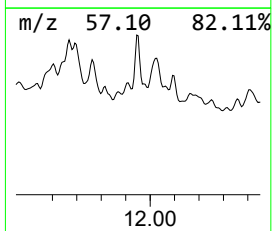
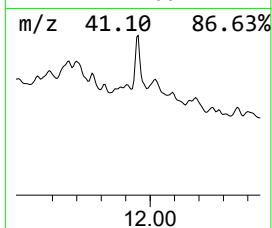
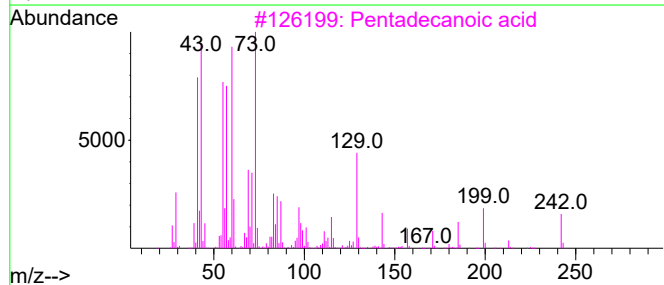
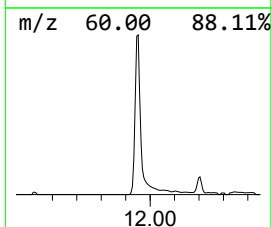
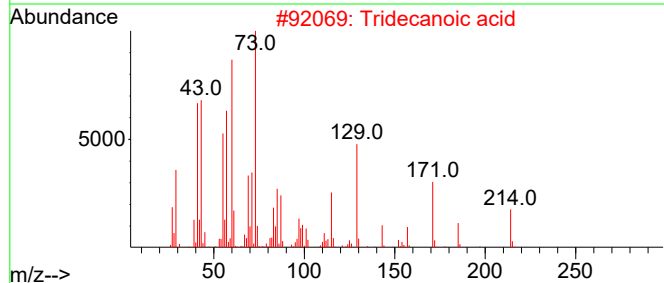
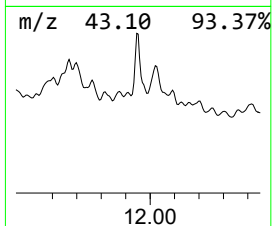
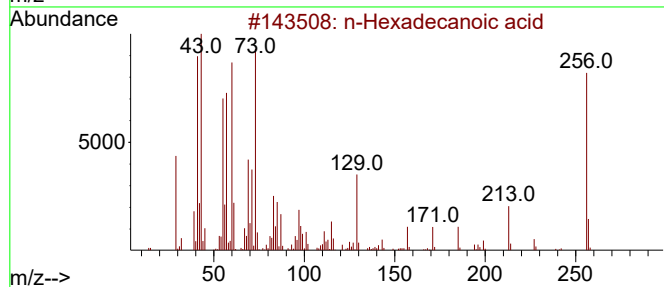
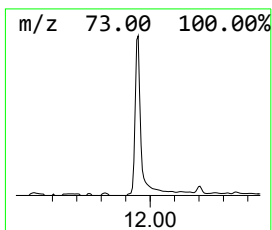
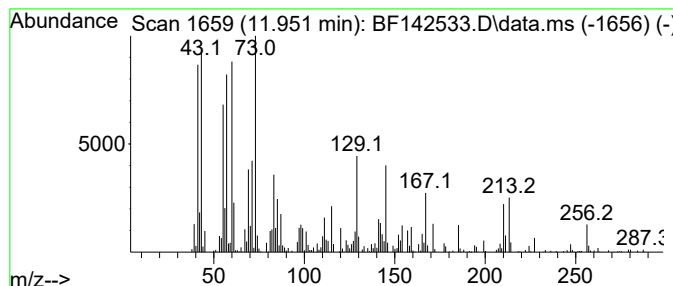
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.951	7.99 ng	313281	Phenanthrene-d10	11.427

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2		Tridecanoic acid	214	C13H26O2	000638-53-9	87
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	64
4		Octadecanoic acid	284	C18H36O2	000057-11-4	64
5		n-Decanoic acid	172	C10H20O2	000334-48-5	60



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052325\
Data File : BF142533.D
Acq On : 23 May 2025 14:10
Operator : RC/JU
Sample : Q2097-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR200044

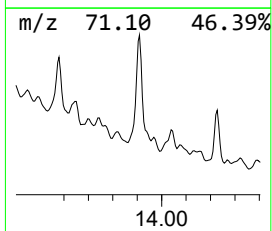
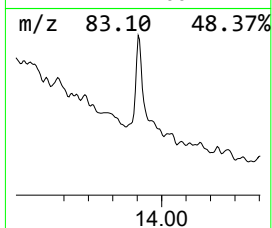
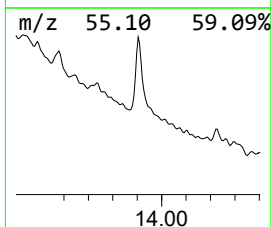
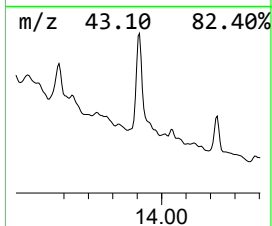
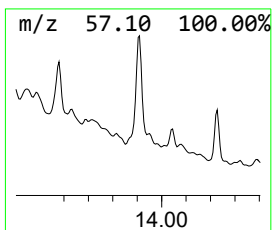
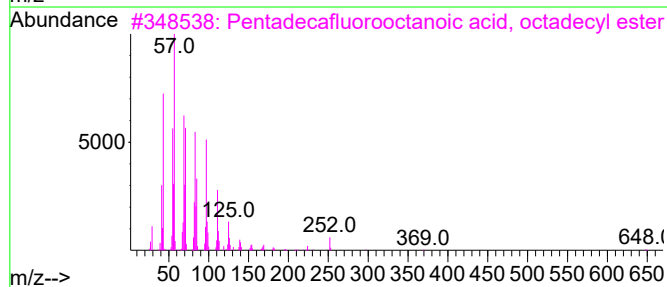
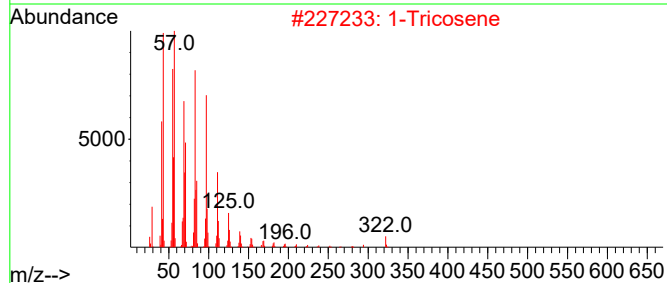
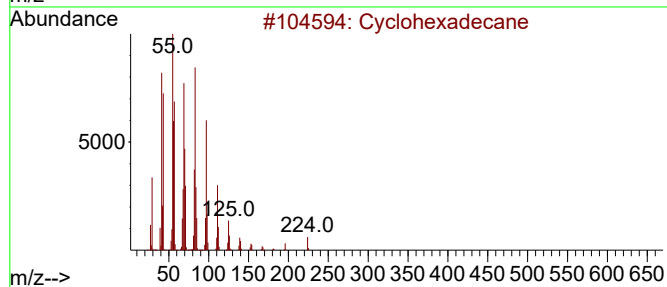
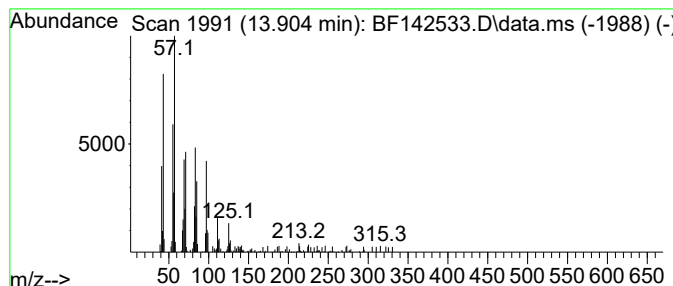
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Cyclohexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	7.12 ng	202044	Chrysene-d12	14.063

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexadecane	224	C16H32	000295-65-8	97
2			1-Tricosene	322	C23H46	018835-32-0	93
3			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91
4			17-Pentatriacontene	491	C35H70	006971-40-0	91
5			Butyl hexadecyl ether	298	C20H42O	1010406-40-5	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052325\
Data File : BF142533.D
Acq On : 23 May 2025 14:10
Operator : RC/JU
Sample : Q2097-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR200044

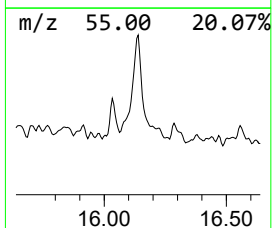
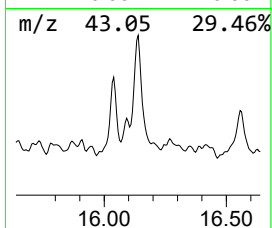
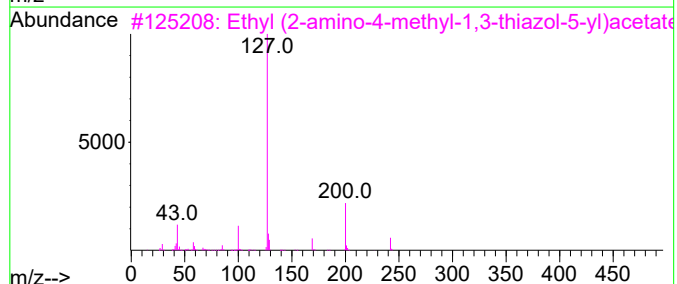
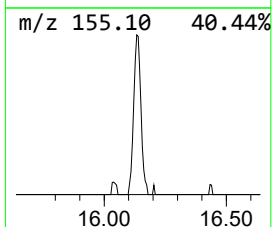
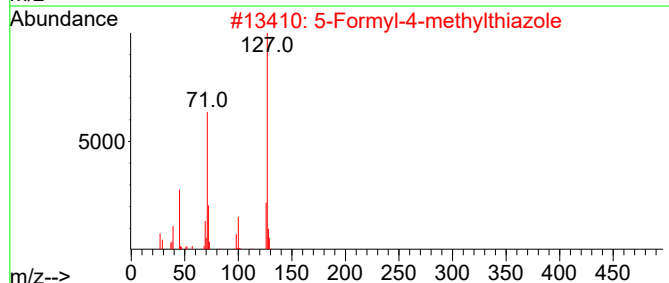
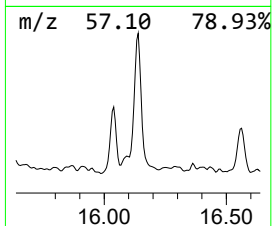
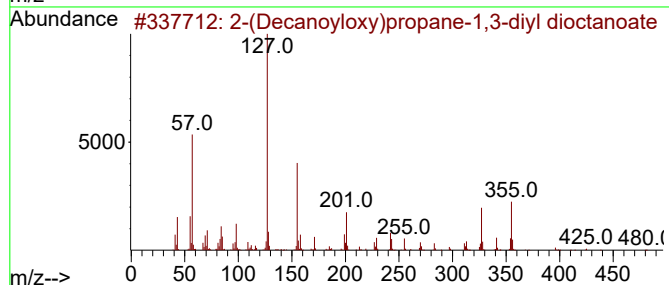
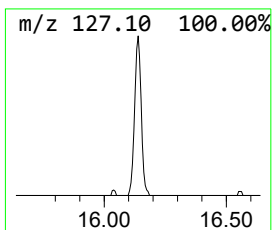
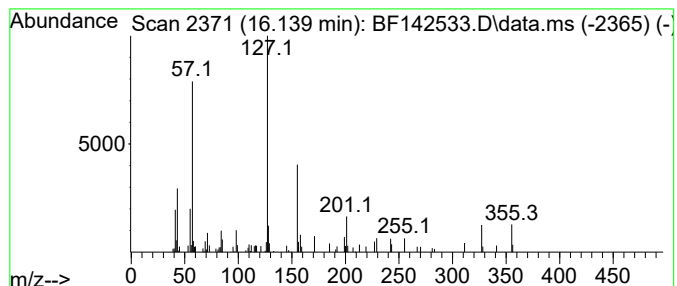
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 2-(Decanoyloxy)propane-1,3-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.139	2.49 ng	75028	Perylene-d12	15.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(Decanoyloxy)propane-1,3-diyl ...	498	C29H54O6	033368-87-5	78		
2	5-Formyl-4-methylthiazole	127	C5H5NOS	082294-70-0	43		
3	Ethyl (2-amino-4-methyl-1,3-thia...	242	C10H14N2O3S	1000475-13-3	43		
4	Caprylic anhydride	270	C16H30O3	000623-66-5	43		
5	4-Dimethylamino-2(5H)-furanone	127	C6H9NO2	1000427-45-6	43		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052325\
Data File : BF142533.D
Acq On : 23 May 2025 14:10
Operator : RC/JU
Sample : Q2097-03
Misc :
ALS Vial : 8 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
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unknown9.645	9.645	3.2	ng	156892	3	9.933	993309	20.0
Decahydro-1,1,4...	9.804	2.2	ng	108923	3	9.933	993309	20.0
unknown9.845	9.845	3.9	ng	195538	3	9.933	993309	20.0
Diallyldivinyls...	10.345	4.6	ng	226858	3	9.933	993309	20.0
Benzophenone	10.651	9.7	ng	483902	3	9.933	993309	20.0
n-Hexadecanoic ...	11.951	8.0	ng	313281	4	11.427	784494	20.0
Cyclohexadecane	13.904	7.1	ng	202044	5	14.063	567693	20.0
2-(Decanoyloxy)...	16.139	2.5	ng	75028	6	15.557	603526	20.0