

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050223\
 Data File : BF133182.D
 Acq On : 02 May 2023 11:39
 Operator : CG\JU
 Sample : 02521-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 GMW-1

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON Filtering: 5
 Sampling : 1 Min Area: 3 % of largest Peak
 Start Thrs: 0.2 Max Peaks: 100
 Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

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

Signal : TIC: BF133182.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.922	478	482	489	rVB	89579	104907	1.57%	0.242%
2	5.339	549	553	557	rBV	3322146	3196486	47.84%	7.374%
3	6.363	723	727	730	rBV	2404659	1993955	29.84%	4.600%
4	6.728	786	789	797	rVB	1606739	1376363	20.60%	3.175%
5	6.910	813	820	824	rVB2	110503	130742	1.96%	0.302%
6	7.298	875	886	889	rBV	4343651	4452008	66.63%	10.270%
7	7.504	918	921	924	rVB2	151290	118637	1.78%	0.274%
8	7.757	960	964	966	rBV2	160110	149234	2.23%	0.344%
9	8.016	1004	1008	1011	rBV	2101665	1741334	26.06%	4.017%
10	8.586	1102	1105	1108	rBV2	67072	72763	1.09%	0.168%
11	9.092	1186	1191	1194	rBV	6672652	6681848	100.00%	15.414%
12	9.769	1302	1306	1309	rVB	2286334	1931133	28.90%	4.455%
13	9.963	1336	1339	1341	rBV4	59011	67776	1.01%	0.156%
14	10.480	1424	1427	1430	rVB	385288	302848	4.53%	0.699%
15	10.557	1435	1440	1443	rBV	4067182	4129539	61.80%	9.526%
16	11.251	1554	1558	1561	rBV	2323685	1937899	29.00%	4.470%
17	11.792	1644	1650	1658	rBV	1681986	1806565	27.04%	4.168%
18	12.574	1780	1783	1794	rVB	1324997	1274113	19.07%	2.939%
19	12.839	1823	1828	1831	rBV	5808287	6322998	94.63%	14.586%
20	13.168	1881	1884	1888	rBV	671739	537518	8.04%	1.240%
21	13.768	1982	1986	1998	rVB2	279962	545737	8.17%	1.259%
22	13.886	2002	2006	2008	rBV	1427268	1370989	20.52%	3.163%
23	14.368	2086	2088	2091	rVB	104568	88860	1.33%	0.205%
24	14.480	2104	2107	2110	rVB	101947	93818	1.40%	0.216%
25	14.662	2133	2138	2145	rVB	176610	256208	3.83%	0.591%
26	14.733	2147	2150	2154	rVB	205461	207057	3.10%	0.478%
27	14.986	2190	2193	2198	rVB	310073	384705	5.76%	0.887%
28	15.304	2243	2247	2251	rBV	899813	1076987	16.12%	2.484%
29	15.351	2251	2255	2263	rVB	321354	431765	6.46%	0.996%
30	15.762	2321	2325	2330	rVB	252775	362704	5.43%	0.837%
31	16.233	2402	2405	2412	rVB	124952	201307	3.01%	0.464%

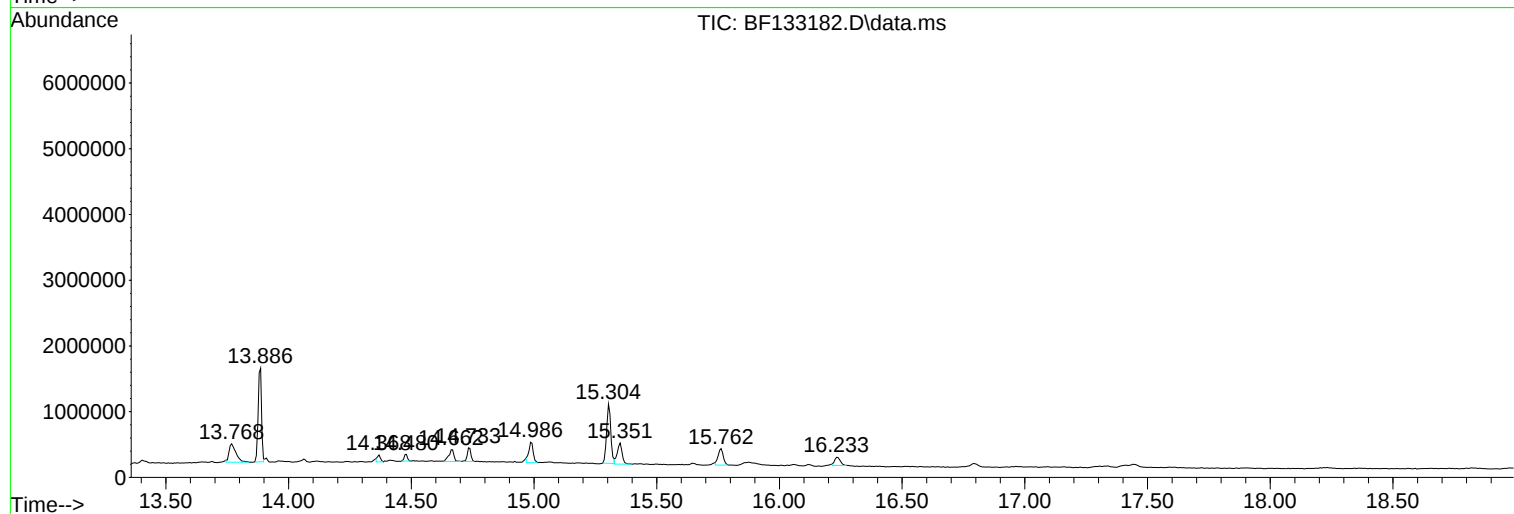
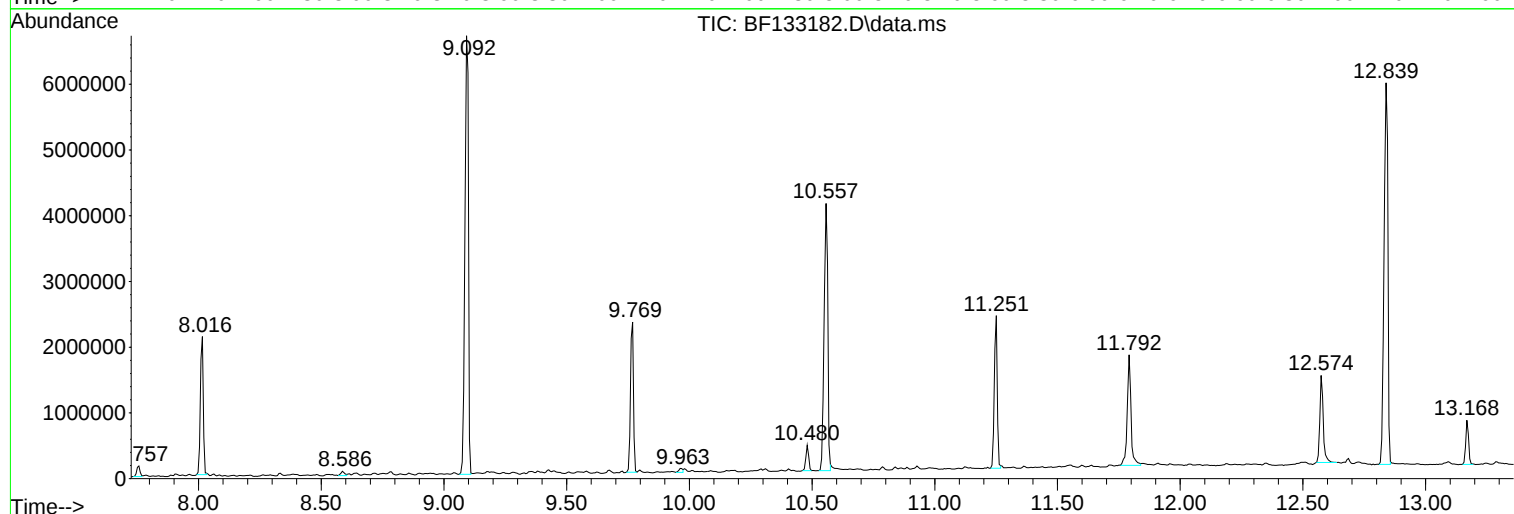
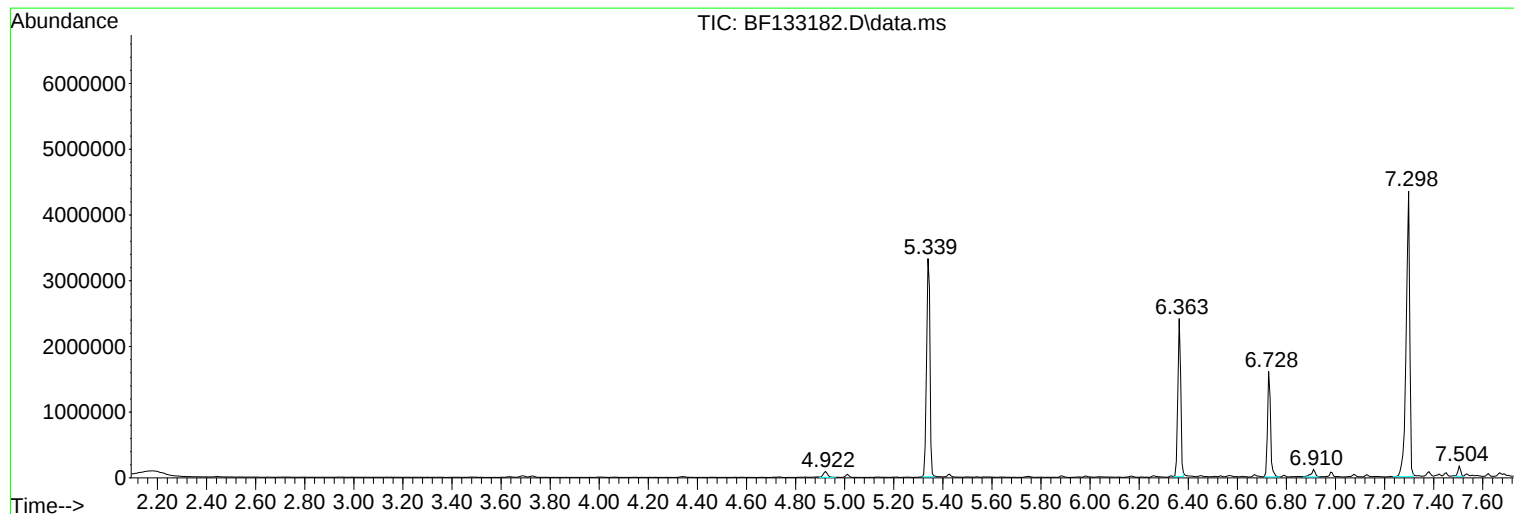
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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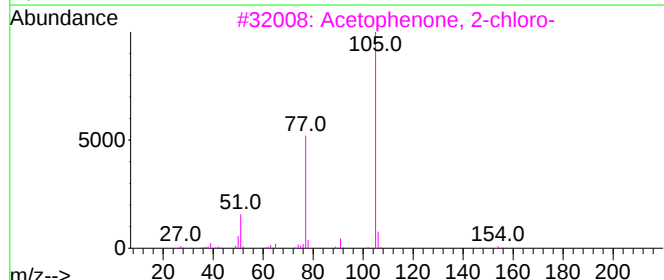
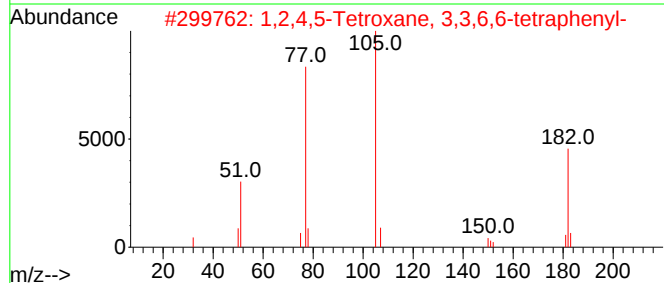
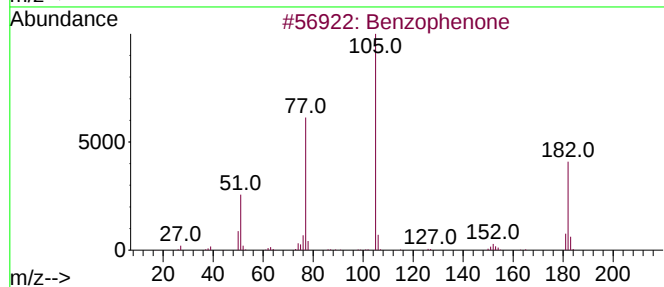
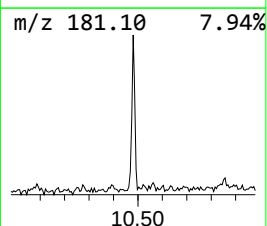
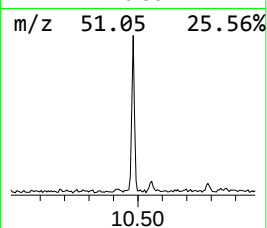
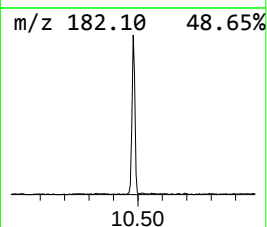
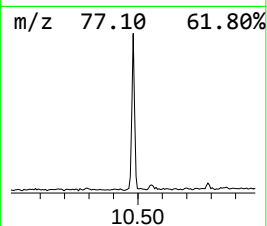
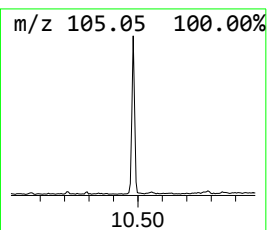
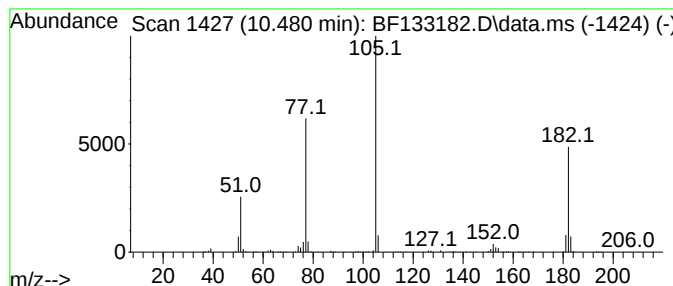
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Benzophenone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.480	3.14 ng	302848	Acenaphthene-d10	9.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			1,2,4,5-Tetroxane, 3,3,6,6-tetra...	396	C26H20O4	016204-36-7	78
3			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	47
4			Pentafluoroethyl phenyl ketone	224	C9H5F5O	000394-52-5	47
5			Methyl 2-benzoyl-4-cyanobutanoate	231	C13H13NO3	1010486-83-8	47



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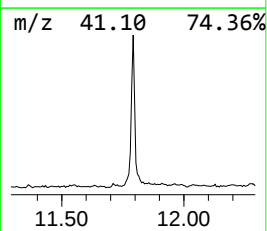
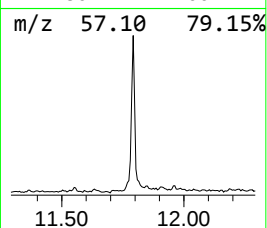
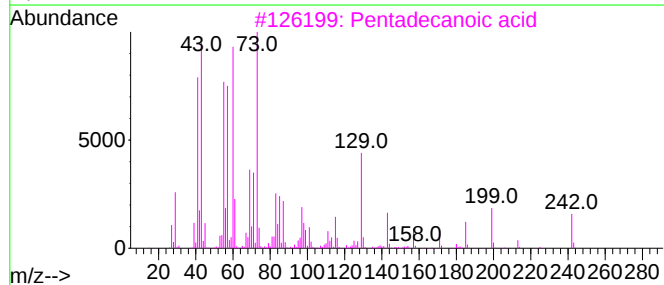
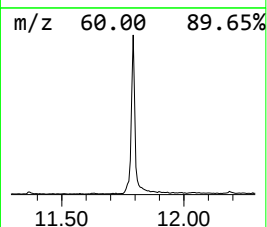
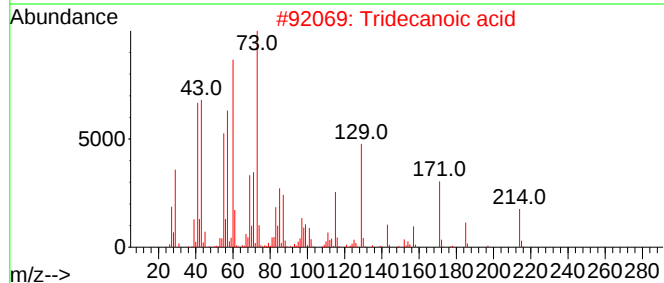
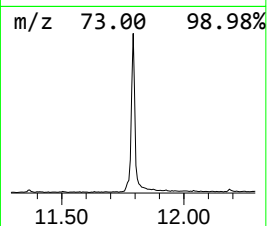
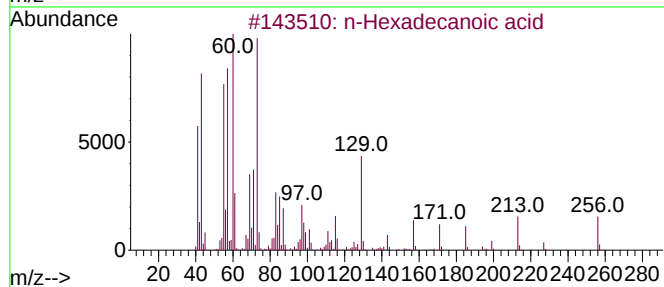
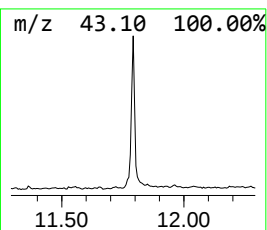
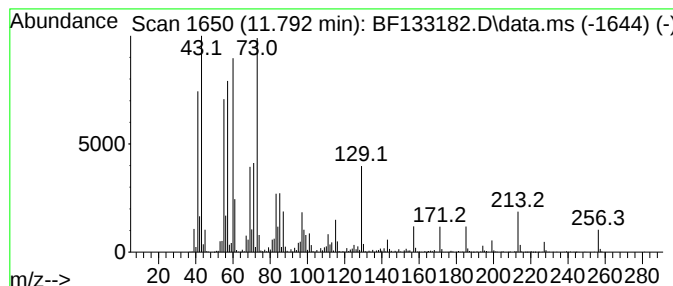
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.792	18.64 ng	1806570	Phenanthrene-d10	11.251

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	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			n-Decanoic acid	172	C10H20O2	000334-48-5	70



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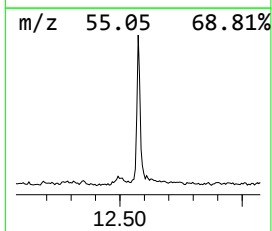
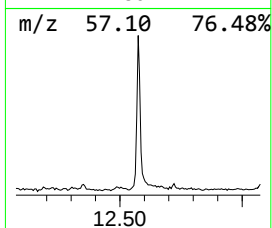
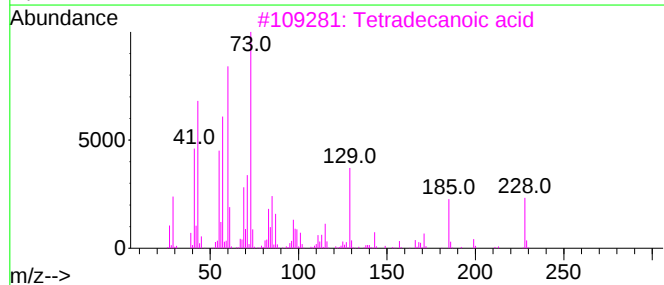
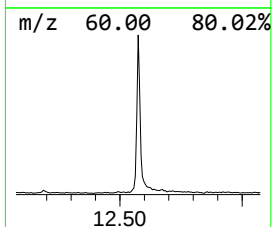
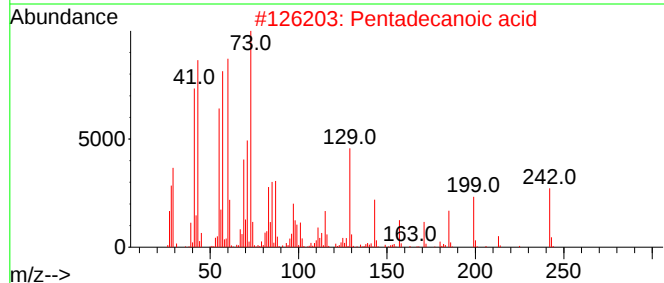
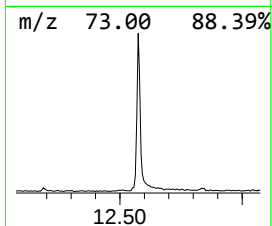
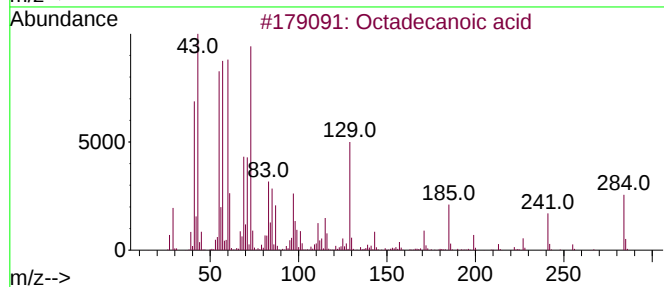
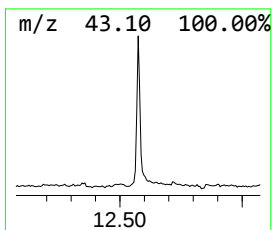
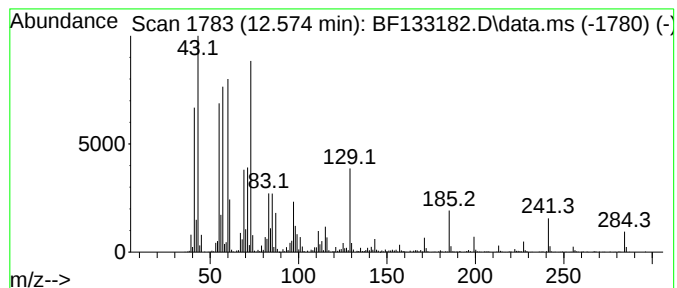
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.574	18.59 ng	1274110	Chrysene-d12	13.886

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	86
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4			n-Decanoic acid	172	C10H20O2	000334-48-5	62
5			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	25



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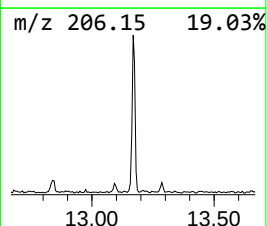
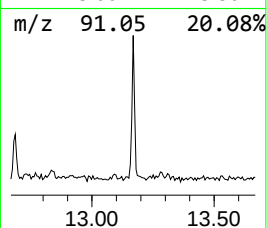
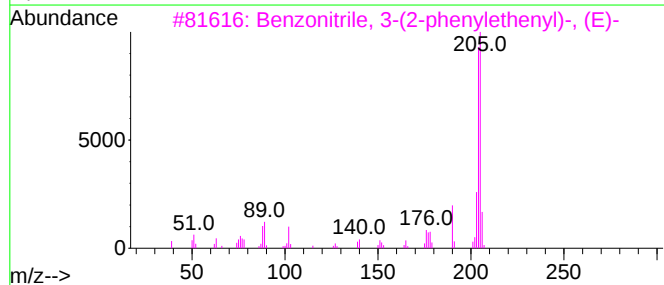
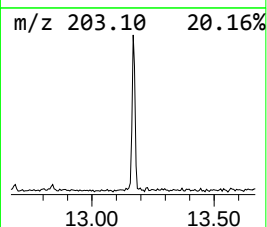
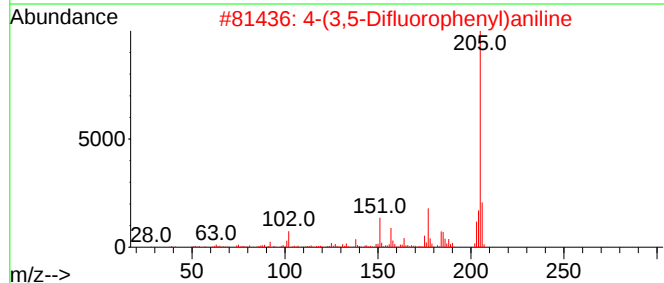
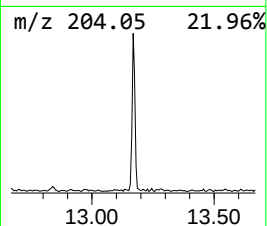
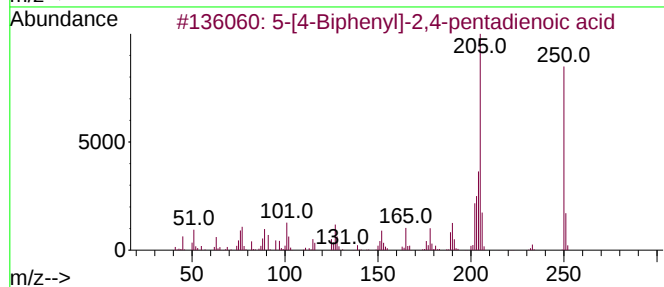
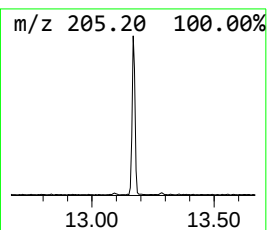
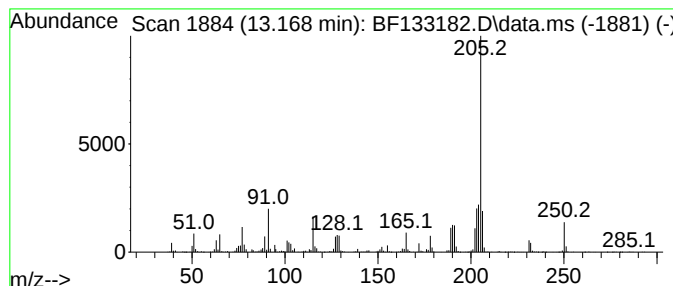
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 unknown13.168 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.168	7.84 ng	537518	Chrysene-d12	13.886

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	5		[4-Biphenyl]-2,4-pentadienoic ...	250	C17H14O2	1000257-33-8	49
2	4		(3,5-Difluorophenyl)aniline	205	C12H9F2N	405058-00-6	47
3	Benzonitrile, 3-(2-phenylethenyl)...	205	C15H11N	014064-35-8	47		
4	2-Amino-4-hydroxy-6,7,8-trimethy...	205	C9H11N5O	013045-86-8	43		
5	6-Phenylisoquinoline	205	C15H11N	070125-61-0	43		



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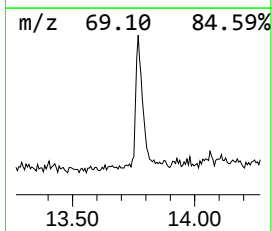
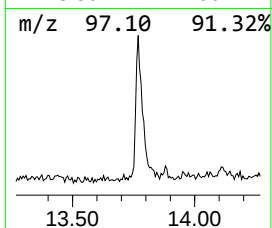
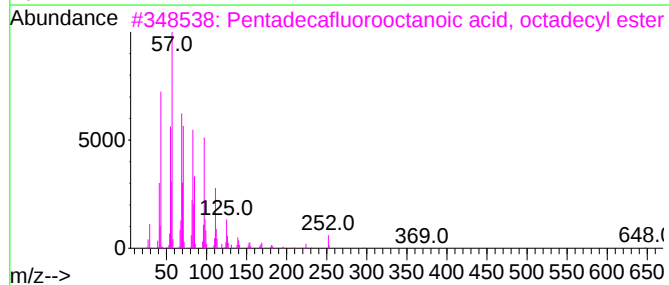
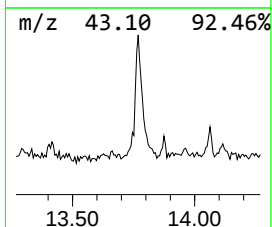
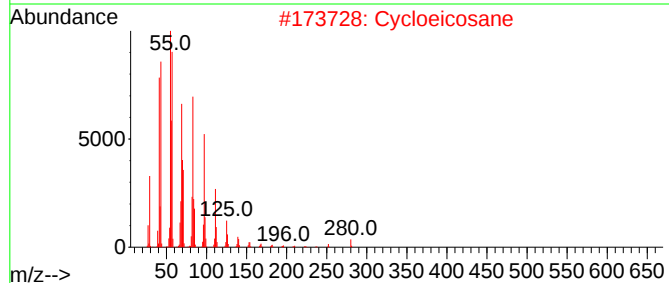
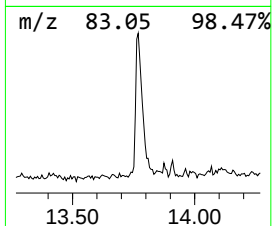
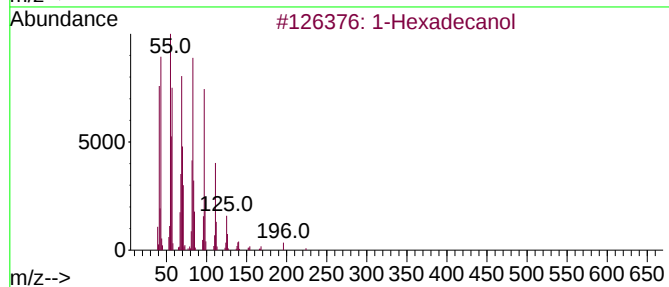
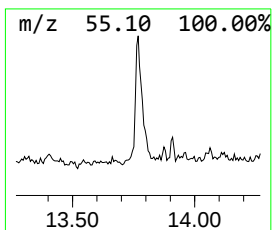
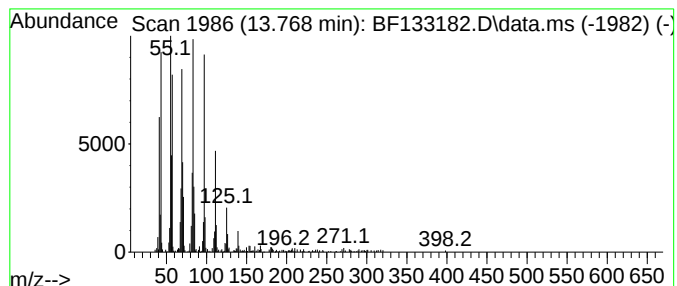
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Peak Number 5 1-Hexadecanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.768	7.96 ng	545737	Chrysene-d12	13.886	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecanol	242	C16H34O	036653-82-4	94
2	Cycloeicosane	280	C20H40	000296-56-0	93
3	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91
4	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	91



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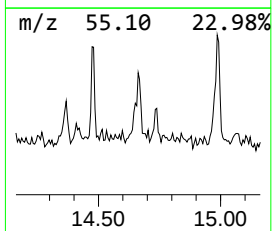
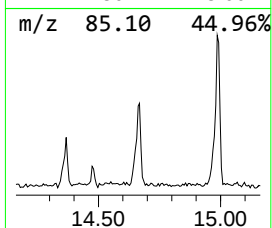
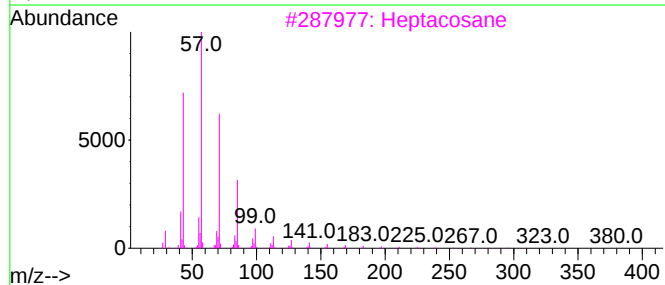
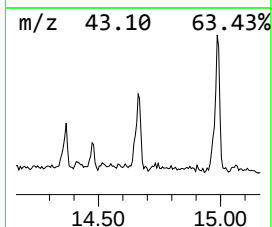
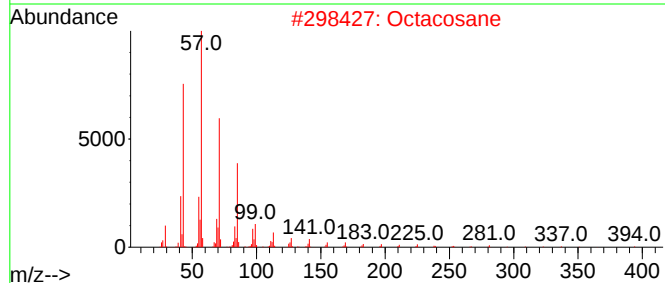
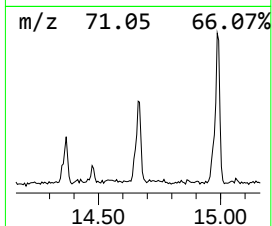
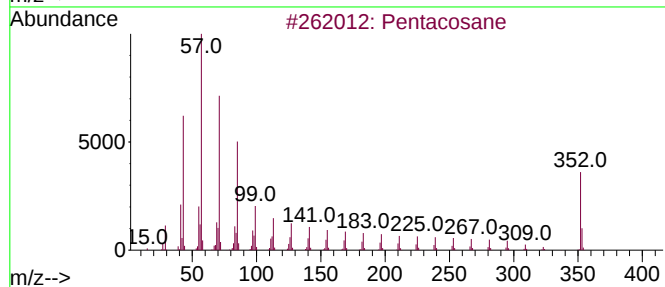
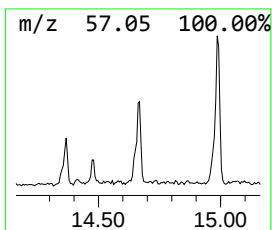
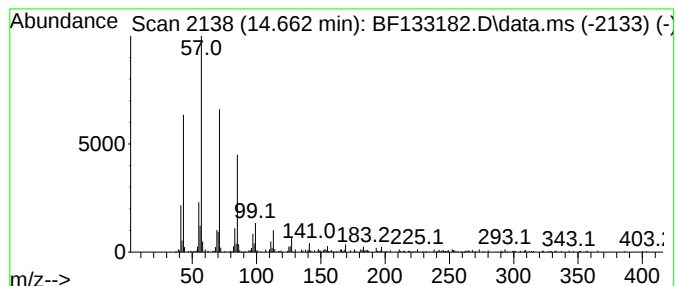
Instrument :
BNA_F
ClientSampleId :
GMW-1

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

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

Peak Number 6 Pentacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.662	4.76 ng	256208	Perylene-d12	15.304	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	87
2	Octacosane	394	C28H58	000630-02-4	87
3	Heptacosane	380	C27H56	000593-49-7	87
4	Docosane	310	C22H46	000629-97-0	87
5	Tridecane, 3-ethyl-	212	C15H32	013286-73-2	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050223\
Data File : BF133182.D
Acq On : 02 May 2023 11:39
Operator : CG\JU
Sample : 02521-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GMW-1

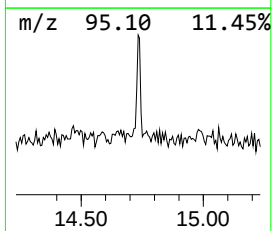
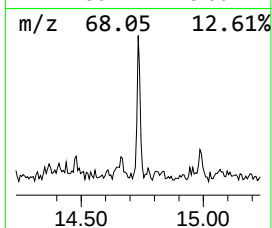
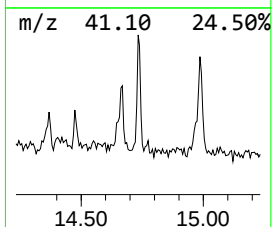
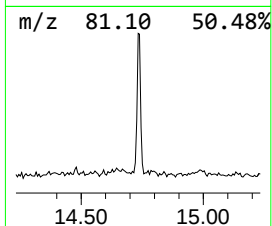
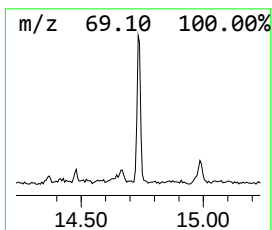
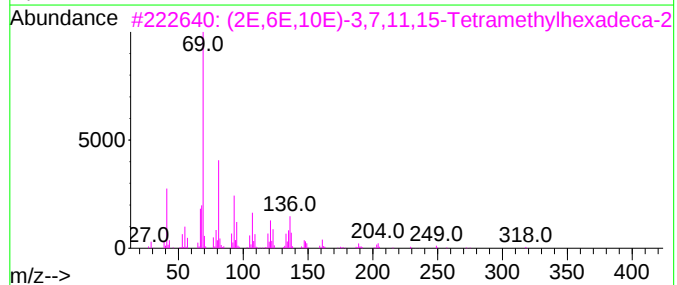
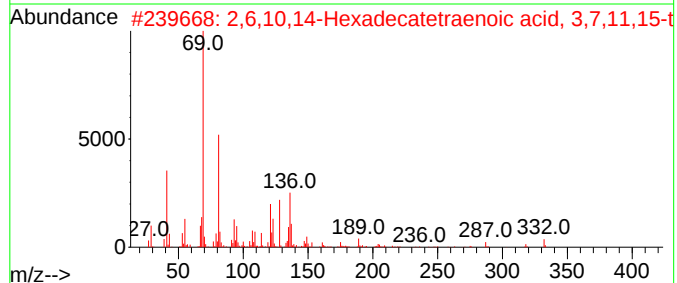
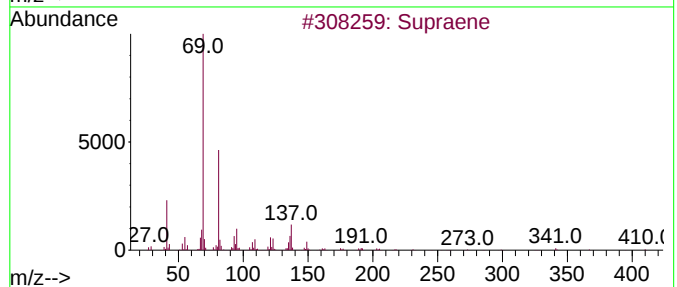
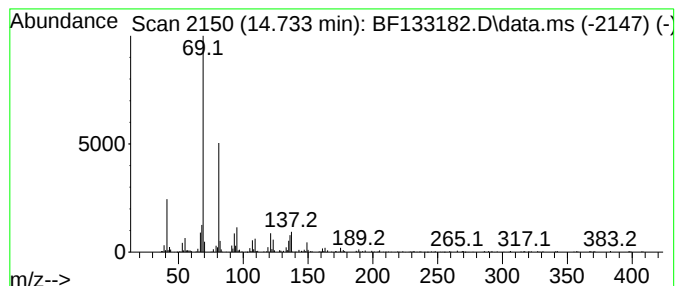
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Supraene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.733	3.85 ng	207057	Perylene-d12	15.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	72
3			(2E,6E,10E)-3,7,11,15-Tetramethy...	318	C21H34O2	125456-63-5	72
4			2,6-Octadiene, 4-methyl-	124	C9H16	074498-94-5	50
5			2-Furancarboxylic acid, 3,4-dime...	172	C7H8O5	1000338-00-3	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050223\
Data File : BF133182.D
Acq On : 02 May 2023 11:39
Operator : CG\JU
Sample : 02521-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

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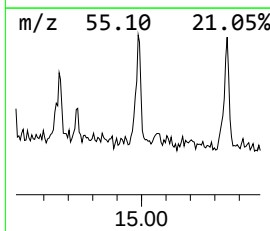
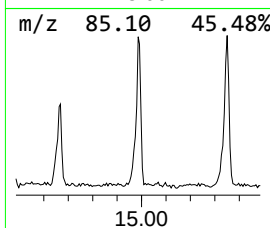
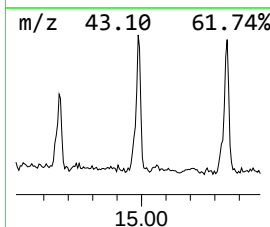
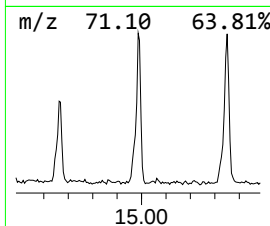
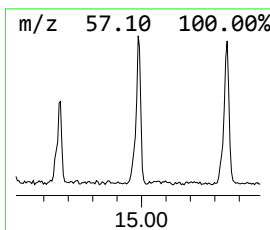
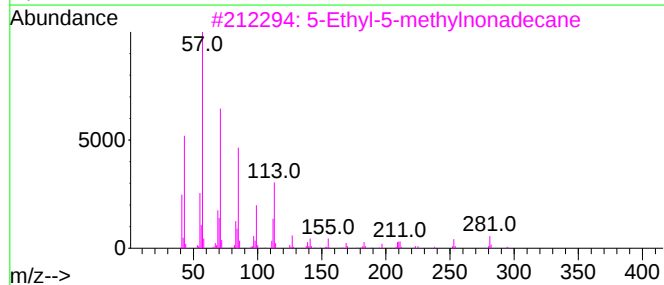
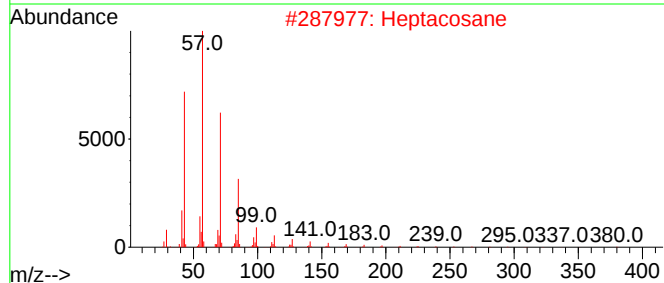
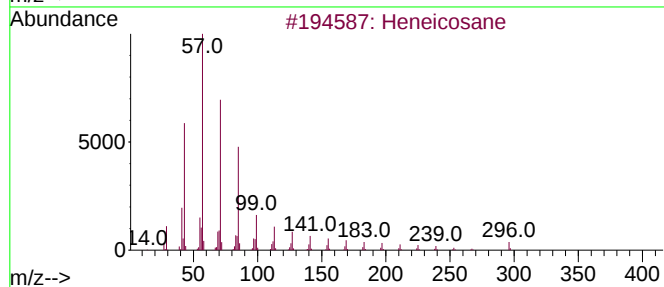
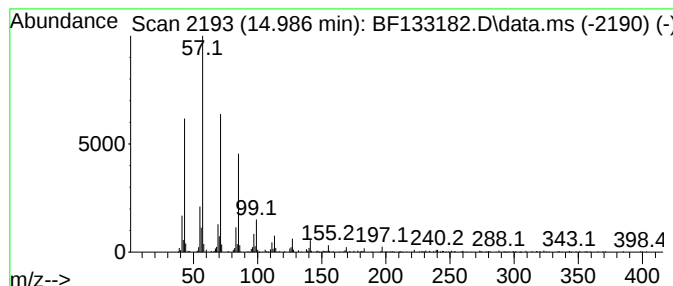
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.986	7.14 ng	384705	Perylene-d12	15.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	93
2			Heptacosane	380	C27H56	000593-49-7	90
3			5-Ethyl-5-methylnonadecane	310	C22H46	1000360-42-7	90
4			Heptadecane	240	C17H36	000629-78-7	90
5			Tetracosane, 1-iodo-	464	C24H49I	1000406-32-0	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050223\
Data File : BF133182.D
Acq On : 02 May 2023 11:39
Operator : CG\JU
Sample : 02521-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

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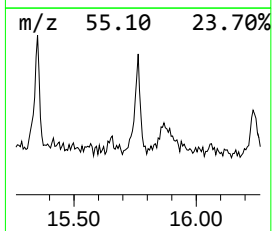
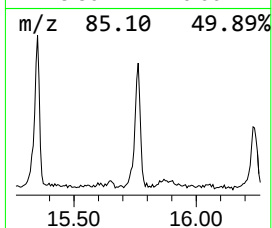
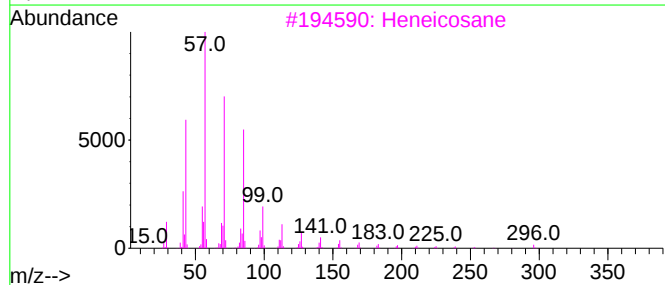
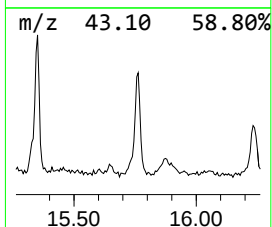
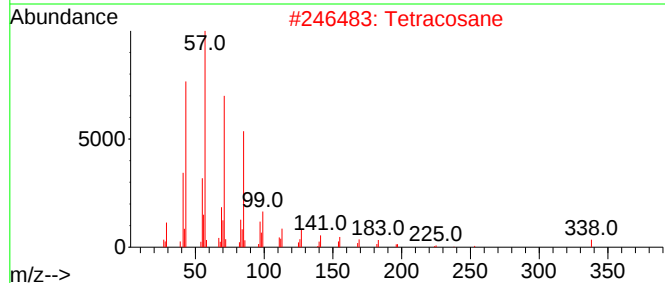
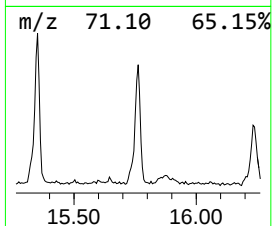
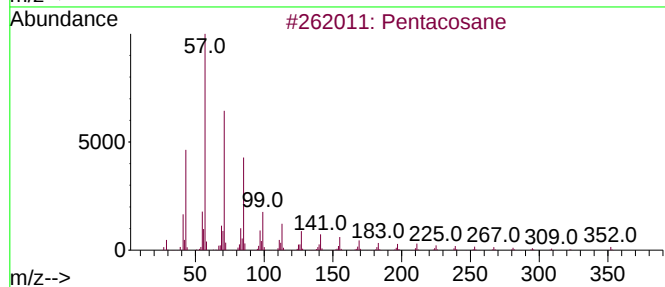
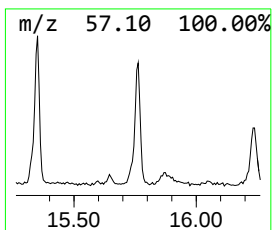
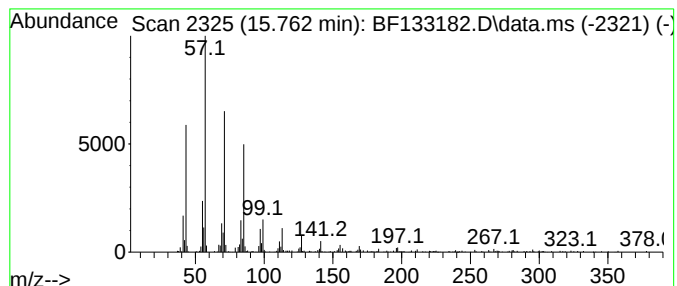
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tetracosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.762	6.74 ng	362704	Perylene-d12	15.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentacosane	352	C25H52	000629-99-2	91
2			Tetracosane	338	C24H50	000646-31-1	90
3			Heneicosane	296	C21H44	000629-94-7	90
4			Octacosane	394	C28H58	000630-02-4	90
5			Eicosane	282	C20H42	000112-95-8	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050223\
Data File : BF133182.D
Acq On : 02 May 2023 11:39
Operator : CG\JU
Sample : 02521-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

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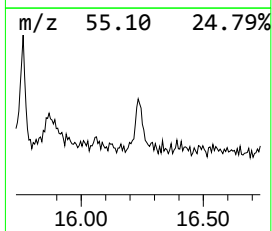
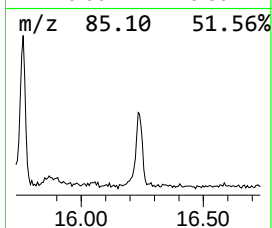
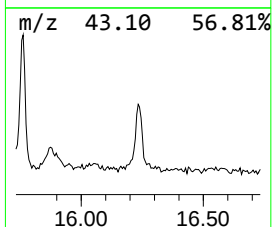
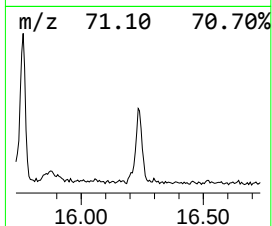
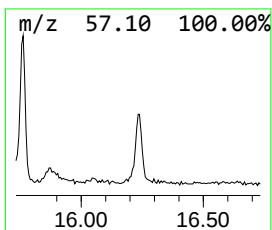
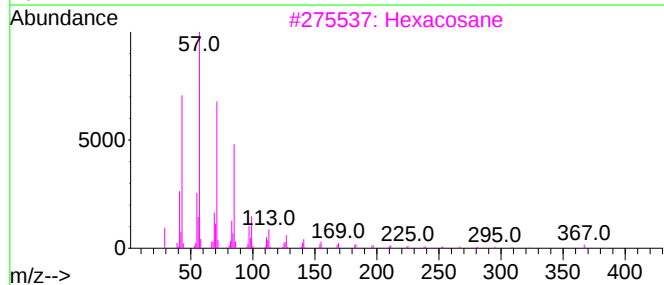
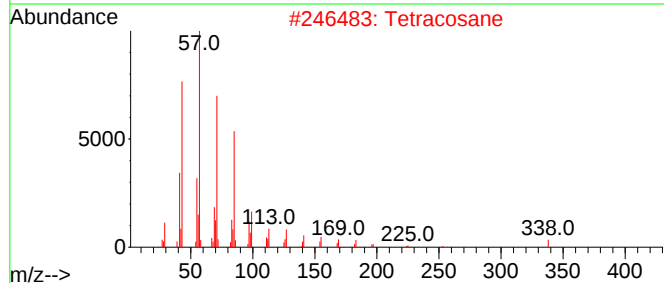
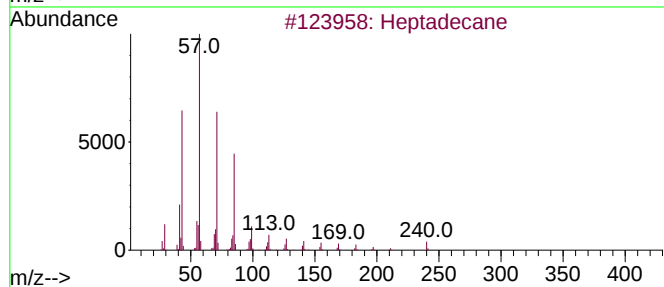
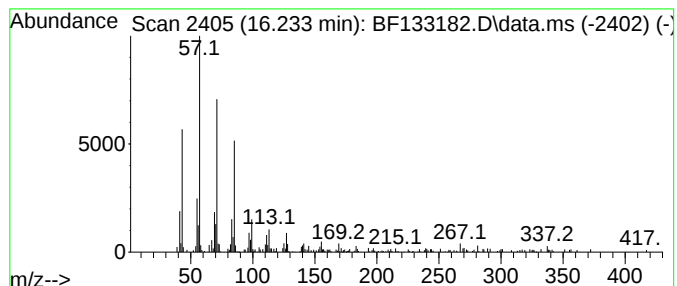
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heptadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.233	3.74 ng	201307	Perylene-d12	15.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane	240	C17H36	000629-78-7	94
2			Tetracosane	338	C24H50	000646-31-1	94
3			Hexacosane	366	C26H54	000630-01-3	93
4			Tricosane, 2-methyl-	338	C24H50	001928-30-9	93
5			Tetratetracontane	619	C44H90	007098-22-8	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050223\
Data File : BF133182.D
Acq On : 02 May 2023 11:39
Operator : CG\JU
Sample : 02521-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GMW-1

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

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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n-Hexadecanoic ...	11.792	18.6	ng	1806570	4	11.251	1937900	20.0
Octadecanoic acid	12.574	18.6	ng	1274110	5	13.886	1370990	20.0
unknown13.168	13.168	7.8	ng	537518	5	13.886	1370990	20.0
1-Hexadecanol	13.768	8.0	ng	545737	5	13.886	1370990	20.0
Pentacosane	14.662	4.8	ng	256208	6	15.304	1076990	20.0
Supraene	14.733	3.9	ng	207057	6	15.304	1076990	20.0
Heneicosane	14.986	7.1	ng	384705	6	15.304	1076990	20.0
Tetracosane	15.762	6.7	ng	362704	6	15.304	1076990	20.0
Heptadecane	16.233	3.7	ng	201307	6	15.304	1076990	20.0