

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050123\
 Data File : BF133150.D
 Acq On : 01 May 2023 12:16
 Operator : CG\JU
 Sample : 02495-03
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PZ-02

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: BF133150.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.340	548	553	565	rBV	2062499	2411566	41.01%	5.460%
2	5.422	565	567	575	rVB	55595	77549	1.32%	0.176%
3	6.363	723	727	735	rBV	1668849	1501832	25.54%	3.400%
4	6.728	786	789	793	rVB	1520619	1192116	20.27%	2.699%
5	7.298	880	886	889	rBV	3835790	3554031	60.44%	8.047%
6	7.451	909	912	915	rVB	433822	317728	5.40%	0.719%
7	7.551	925	929	938	rBV2	72916	119541	2.03%	0.271%
8	7.928	988	993	995	rBV4	44309	63540	1.08%	0.144%
9	7.981	999	1002	1004	rVV	112702	92762	1.58%	0.210%
10	8.016	1004	1008	1011	rVV	2088494	1654161	28.13%	3.745%
11	8.339	1060	1063	1066	rBV	97741	97313	1.65%	0.220%
12	9.092	1187	1191	1194	rVB	6297803	5880542	100.00%	13.314%
13	9.769	1302	1306	1309	rVB	2260091	1887134	32.09%	4.273%
14	9.981	1337	1342	1345	rBV4	69654	86566	1.47%	0.196%
15	10.051	1351	1354	1359	rBV	77299	81542	1.39%	0.185%
16	10.480	1424	1427	1430	rVB	930386	713369	12.13%	1.615%
17	10.557	1435	1440	1443	rBV	3608325	3519505	59.85%	7.968%
18	10.839	1485	1488	1492	rBV	141534	121669	2.07%	0.275%
19	11.251	1554	1558	1561	rBV	2123999	1857220	31.58%	4.205%
20	11.798	1641	1651	1662	rVB	2150235	3141170	53.42%	7.112%
21	11.922	1669	1672	1679	rVB	157585	208028	3.54%	0.471%
22	12.433	1756	1759	1762	rBV	150452	178570	3.04%	0.404%
23	12.480	1764	1767	1768	rBV2	131746	143499	2.44%	0.325%
24	12.563	1776	1781	1782	rBV	1820219	1957644	33.29%	4.432%
25	12.586	1782	1785	1790	rVB	3552532	3606850	61.34%	8.166%
26	12.839	1823	1828	1831	rVB	5249074	4973550	84.58%	11.261%
27	13.498	1935	1940	1948	rVB2	150772	304012	5.17%	0.688%
28	13.804	1987	1992	2001	rBV4	111274	279323	4.75%	0.632%
29	13.880	2001	2005	2009	rBV	1292380	1182417	20.11%	2.677%
30	14.092	2034	2041	2046	rBV	216180	370385	6.30%	0.839%
31	14.480	2104	2107	2118	rVB	305940	323220	5.50%	0.732%
32	14.592	2122	2126	2132	rBV	258939	361409	6.15%	0.818%
33	14.739	2148	2151	2156	rVB	105519	100088	1.70%	0.227%
34	14.992	2191	2194	2198	rVB	69343	80384	1.37%	0.182%
35	15.110	2210	2214	2223	rVB	182506	304575	5.18%	0.690%
36	15.304	2242	2247	2252	rBV	981968	1131023	19.23%	2.561%

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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

37	15.704	2310	2315	2322	rVV	117027	210425	3.58%	0.476%
38	15.768	2322	2326	2330	rVB3	58208	81664	1.39%	0.185%

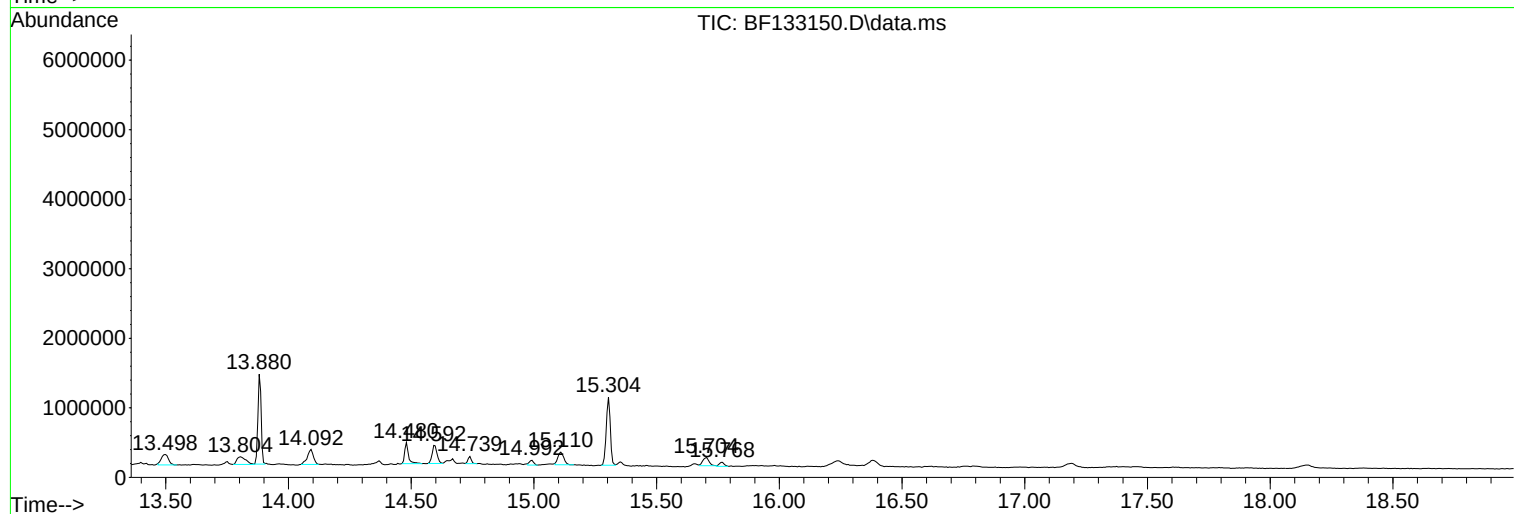
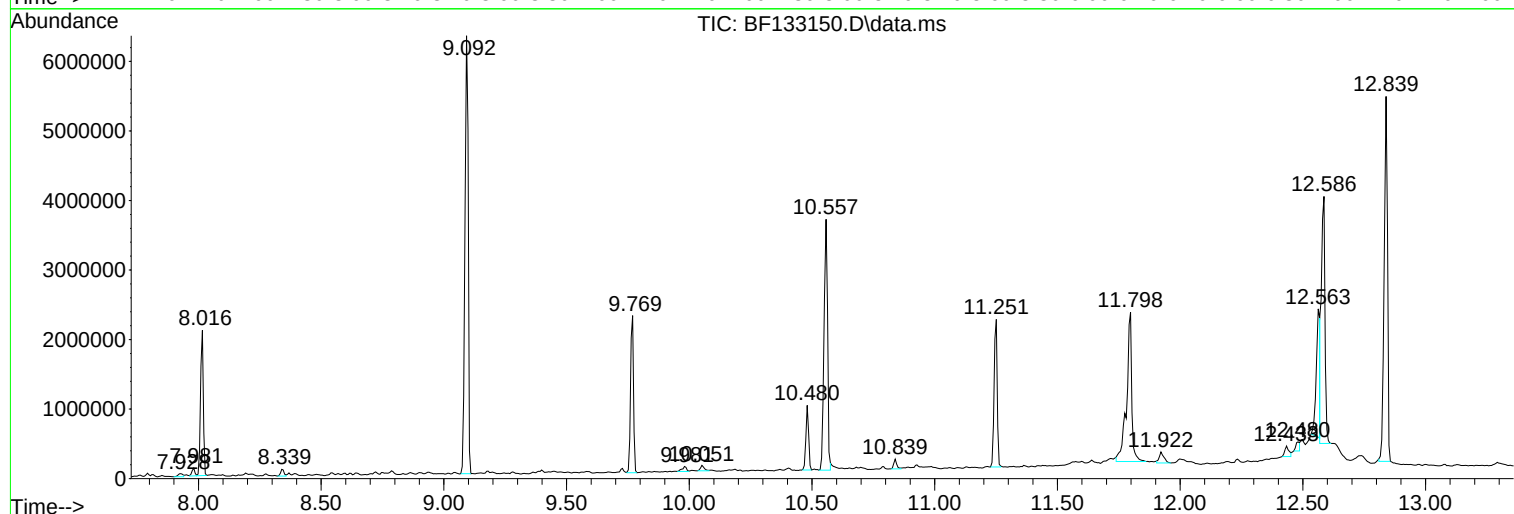
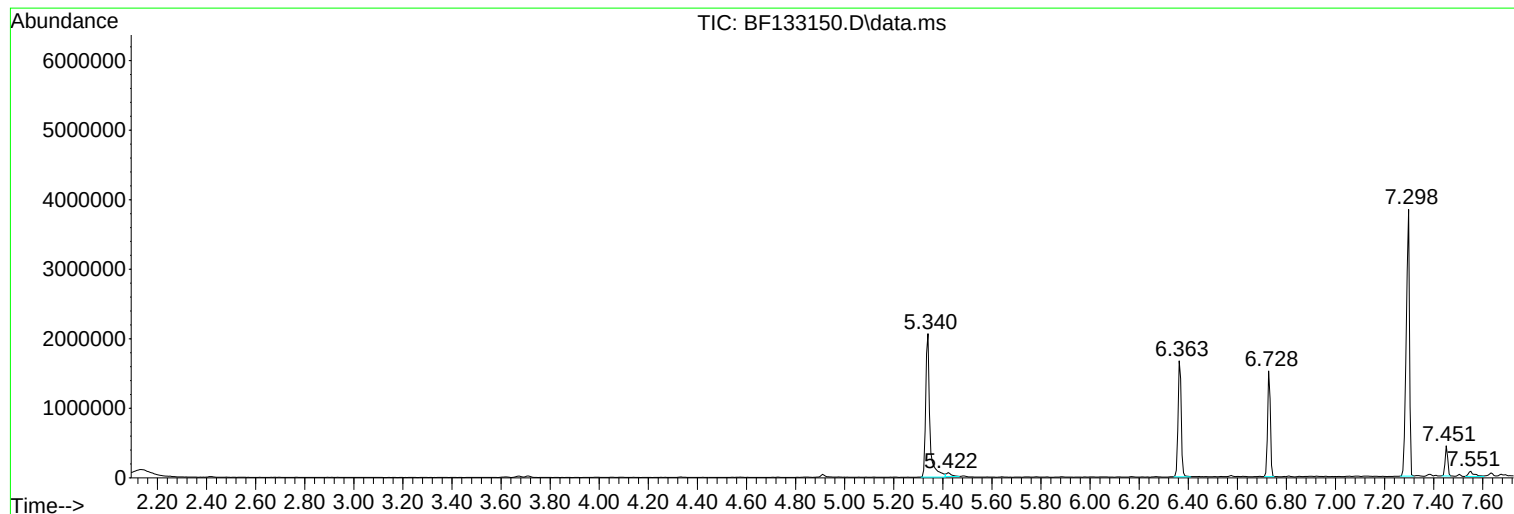
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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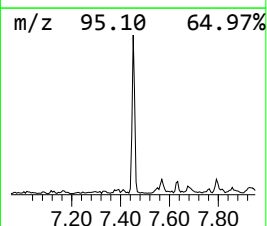
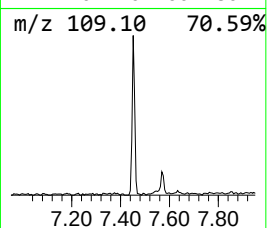
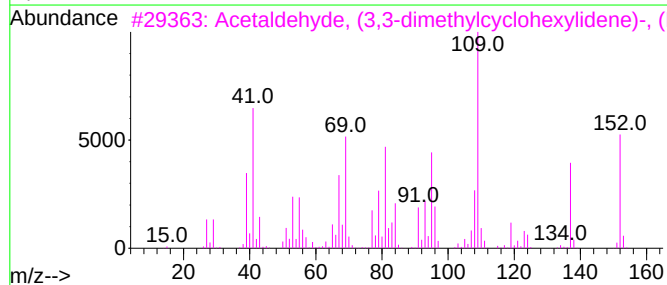
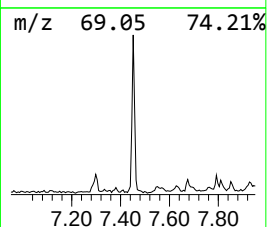
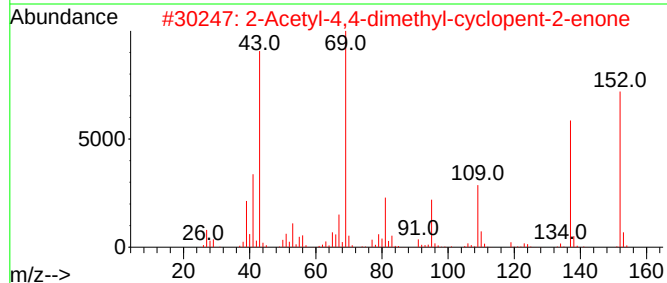
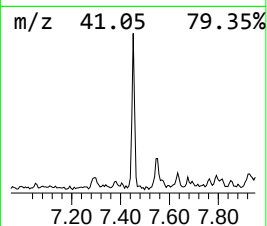
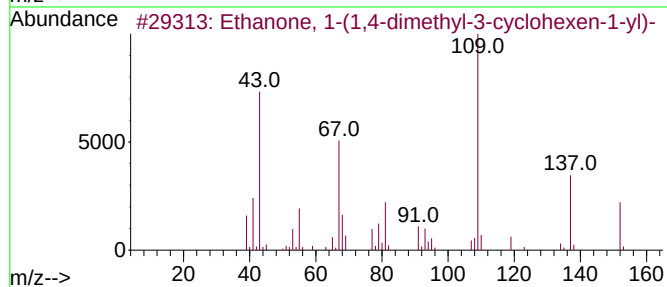
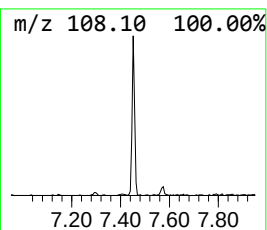
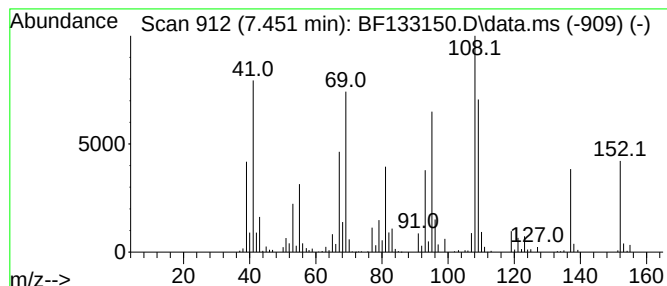
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown7.451 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.451	3.84 ng	317728	Naphthalene-d8	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanone, 1-(1,4-dimethyl-3-cycl...	152	C10H16O	043219-68-7	46
2			2-Acetyl-4,4-dimethyl-cyclopent...	152	C9H12O2	081979-96-6	38
3			Acetaldehyde, (3,3-dimethylcyclo...	152	C10H16O	026532-25-2	38
4			Allyl 2,4-hexadienoate	152	C9H12O2	1000431-58-3	35
5			Ethanol, 2-(3-methylphenoxy)-	152	C9H12O2	013605-19-1	30



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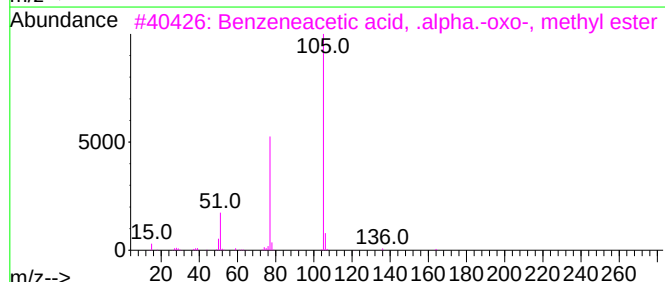
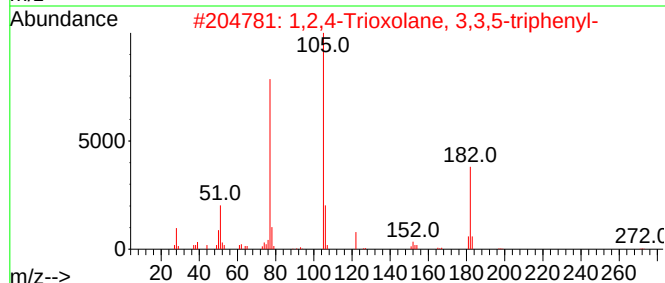
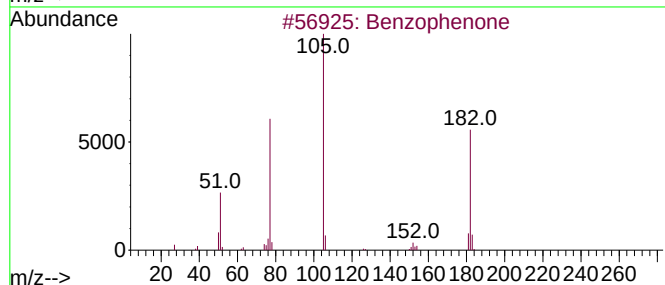
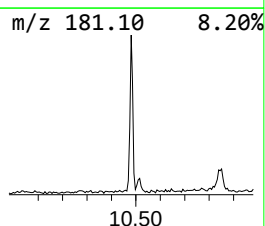
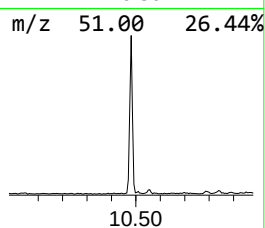
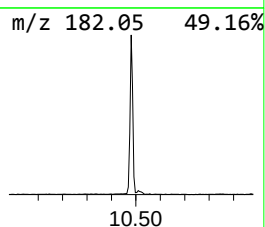
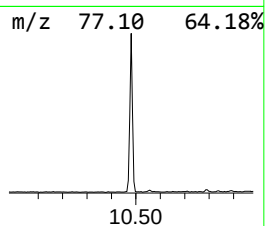
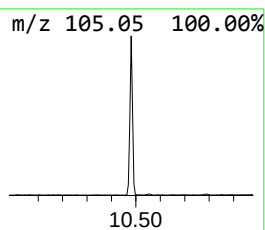
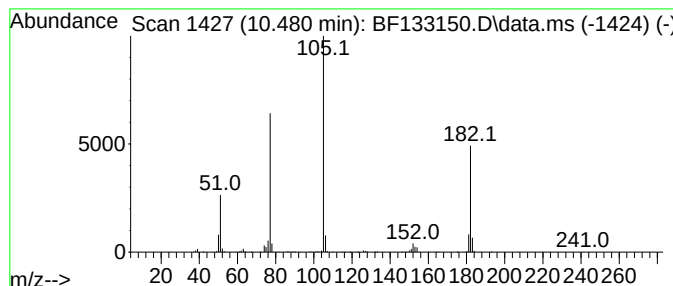
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.480	7.56 ng	713369	Acenaphthene-d10	9.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			1,2,4-Trioxolane, 3,3,5-triphenyl-	304	C20H16O3	023246-12-0	72
3			Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	49
4			1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	47
5			1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47



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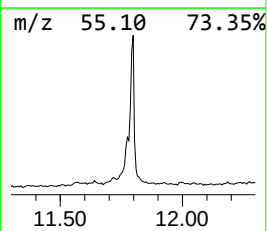
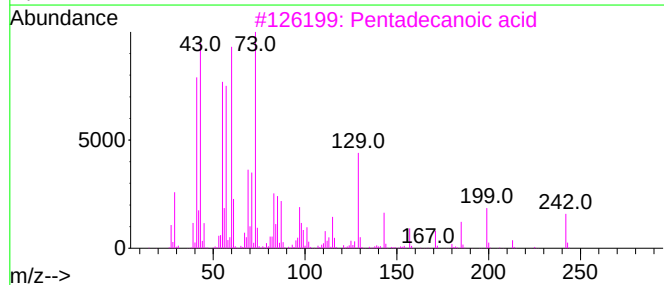
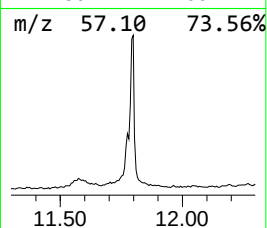
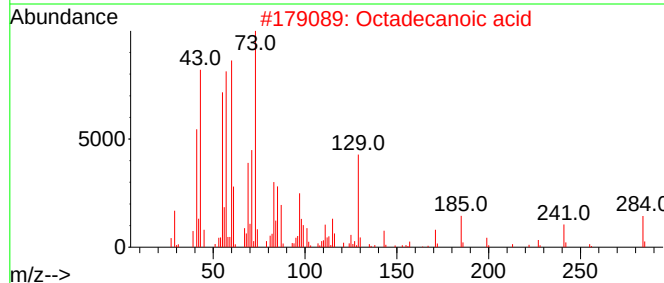
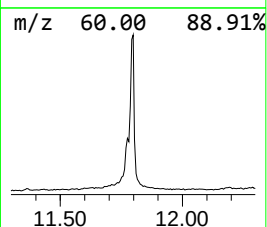
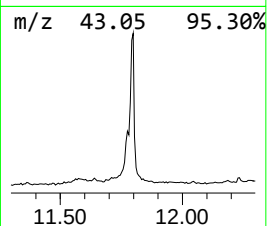
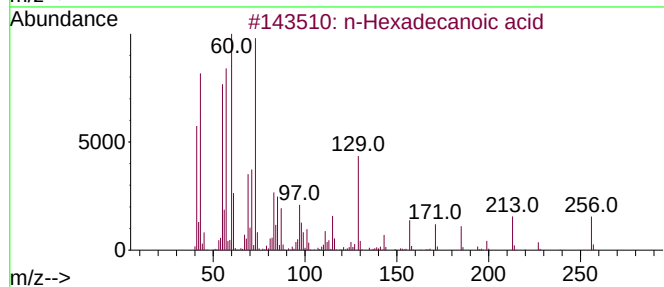
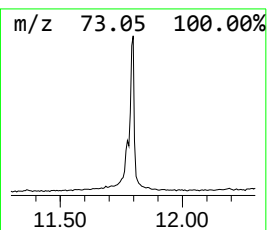
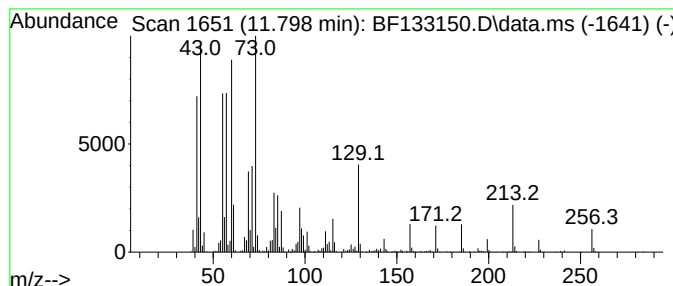
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.798	33.83 ng	3141170	Phenanthrene-d10	11.251

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Octadecanoic acid	284	C18H36O2	000057-11-4	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4			Tridecanoic acid	214	C13H26O2	000638-53-9	92
5			n-Decanoic acid	172	C10H20O2	000334-48-5	70



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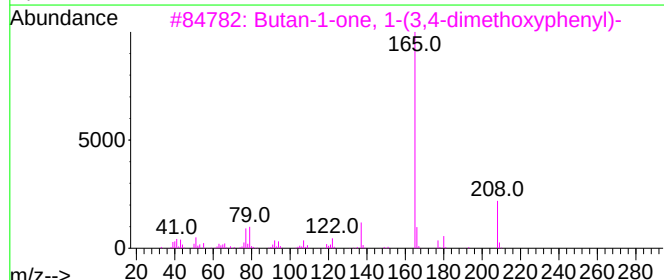
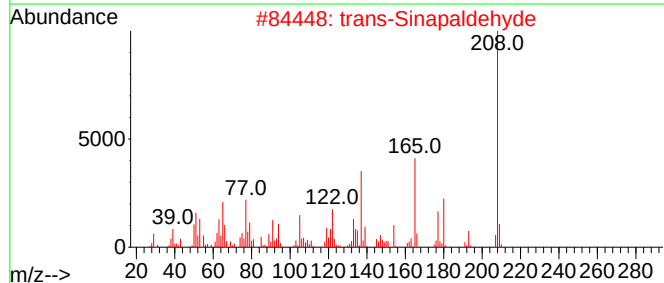
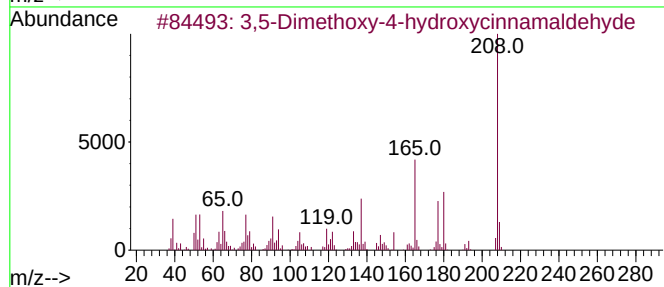
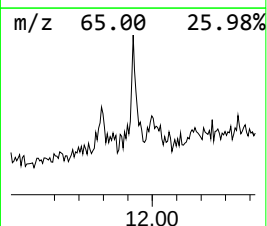
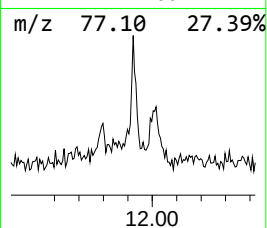
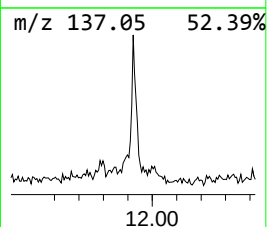
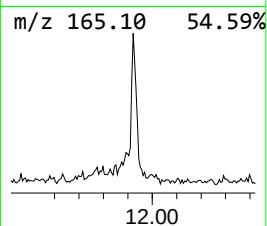
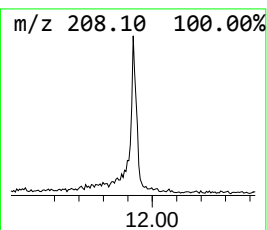
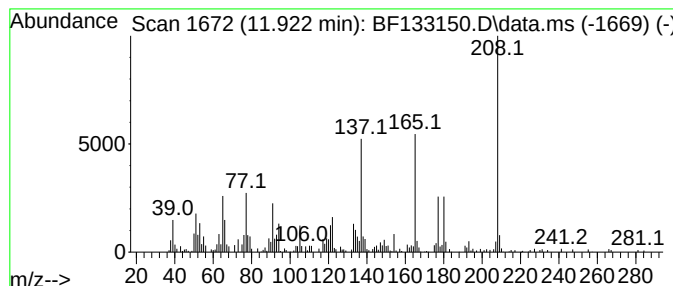
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 3,5-Dimethoxy-4-hydroxycinn... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	2.24 ng	208028	Phenanthrene-d10	11.251

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3,5-Dimethoxy-4-hydroxycinnamal... 208	C11H12O4		087345-53-7	89
2		trans-Sinapaldehyde 208	C11H12O4		004206-58-0	74
3		Butan-1-one, 1-(3,4-dimethoxyphe... 208	C12H16O3		054419-21-5	52
4		2,4,7-Pteridinetriol, 6-ethyl- 208	C8H8N4O3		031053-47-1	41
5		5-(4-Methoxy-phenyl)-[1,3,4]oxad... 208	C9H8N2O2S		023766-26-9	38



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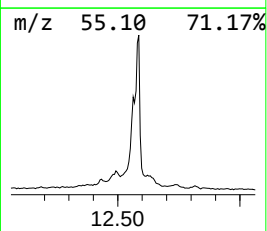
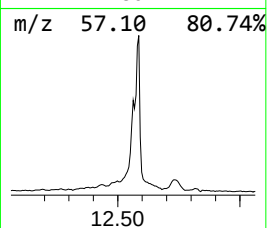
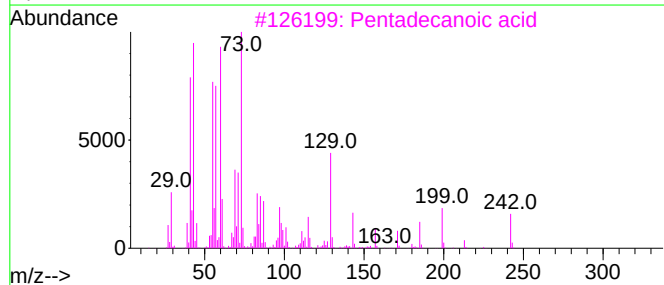
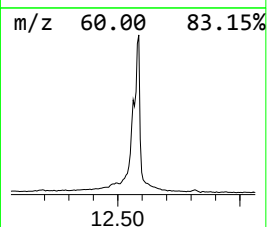
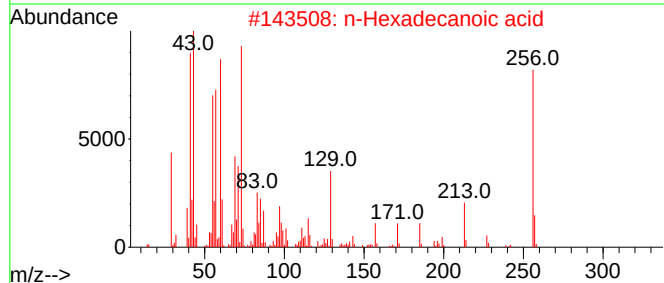
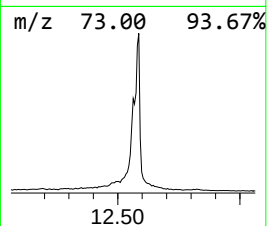
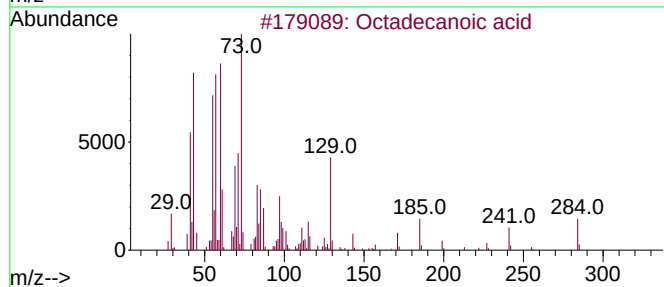
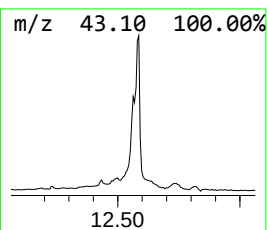
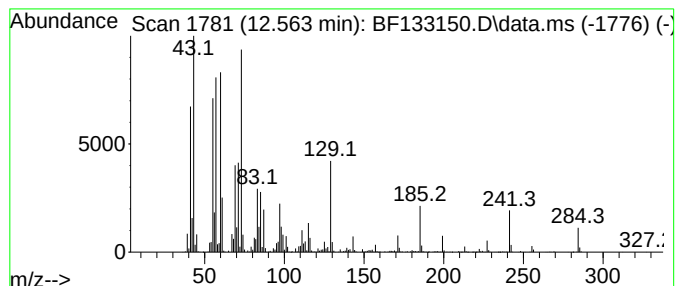
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.563	21.08 ng	1957640	Phenanthrene-d10	11.251

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	91
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5			n-Decanoic acid	172	C10H20O2	000334-48-5	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050123\
Data File : BF133150.D
Acq On : 01 May 2023 12:16
Operator : CG\JU
Sample : 02495-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PZ-02

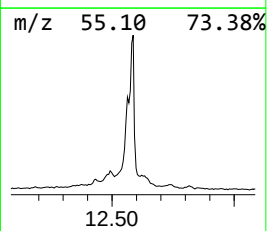
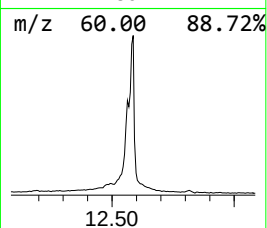
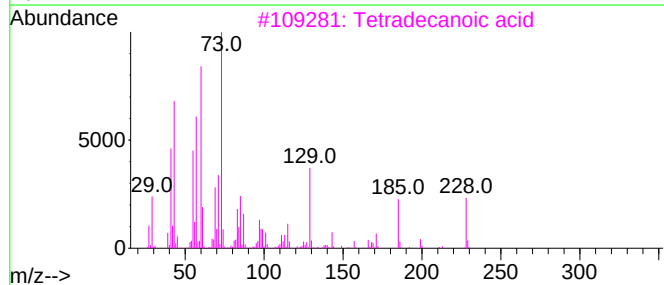
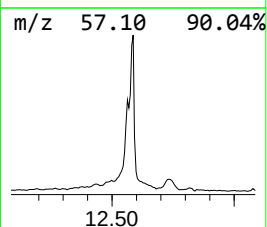
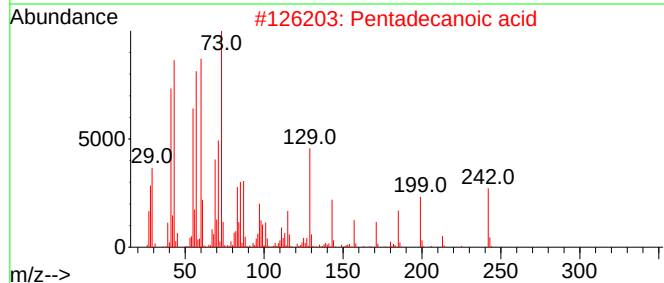
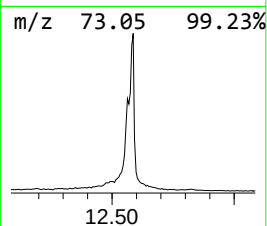
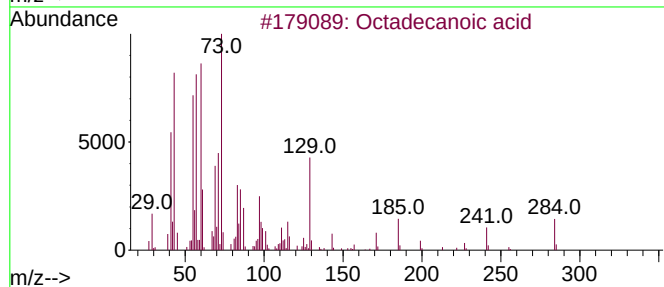
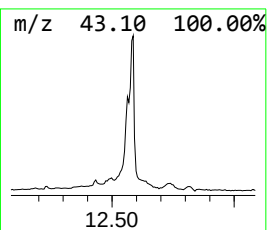
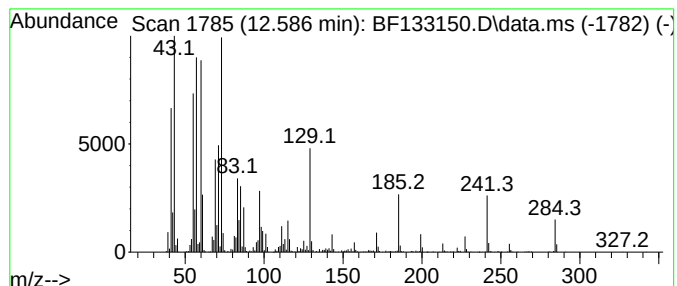
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Pentadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.586	61.01 ng	3606850	Chrysene-d12	13.880

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	93
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4			n-Decanoic acid	172	C10H20O2	000334-48-5	62
5			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050123\
Data File : BF133150.D
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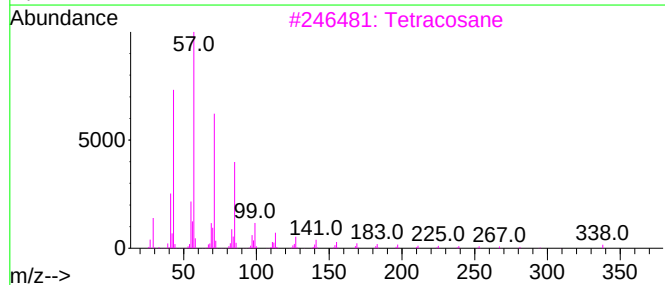
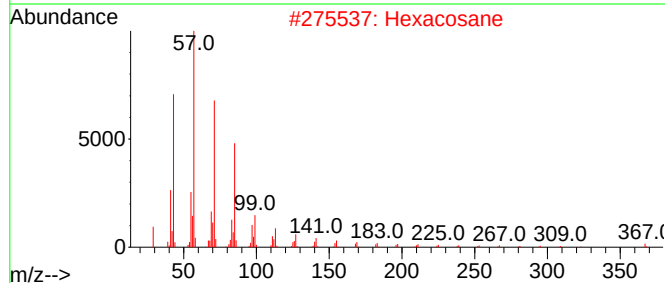
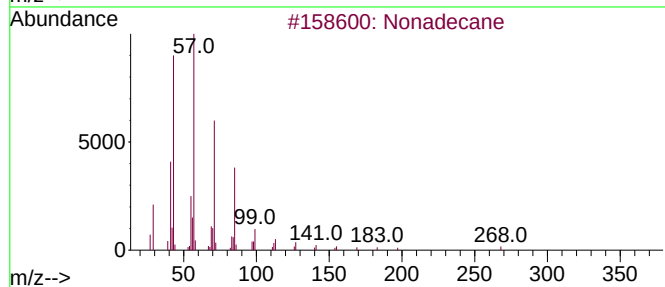
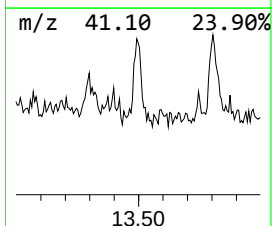
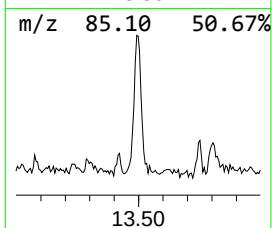
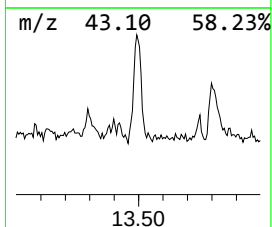
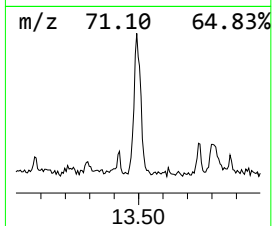
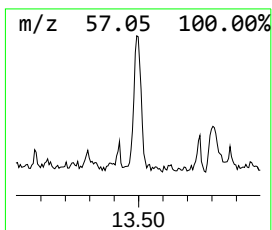
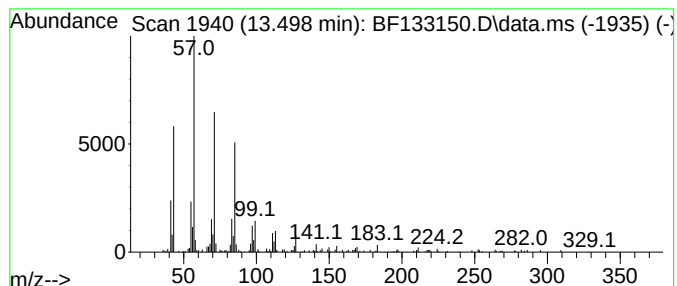
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Nonadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.498	5.14 ng	304012	Chrysene-d12		13.880	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Nonadecane		268	C19H40	000629-92-5	93
2	Hexacosane		366	C26H54	000630-01-3	90
3	Tetracosane		338	C24H50	000646-31-1	87
4	Hentriacontane		437	C31H64	000630-04-6	87
5	Heptadecane		240	C17H36	000629-78-7	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050123\
Data File : BF133150.D
Acq On : 01 May 2023 12:16
Operator : CG\JU
Sample : 02495-03
Misc :
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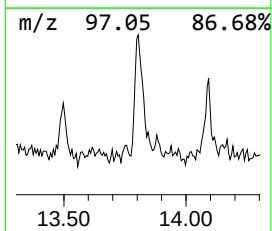
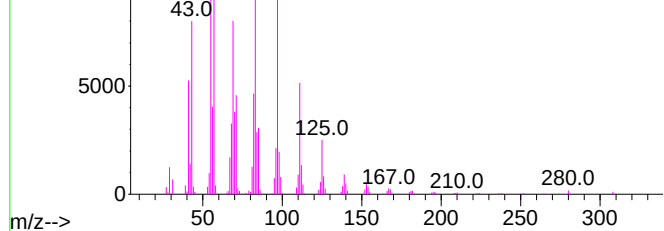
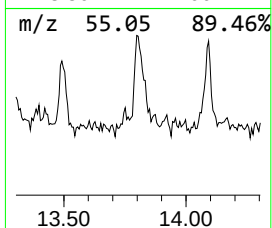
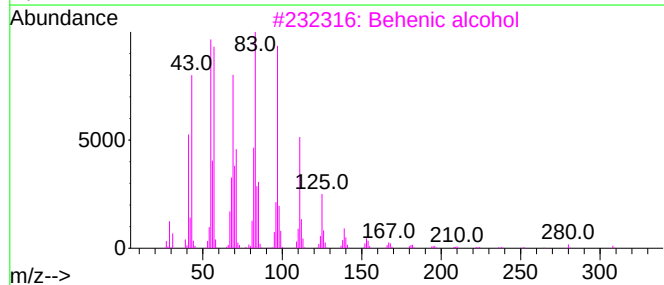
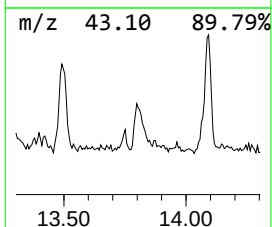
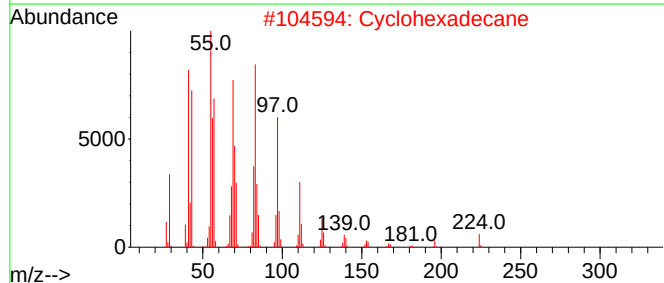
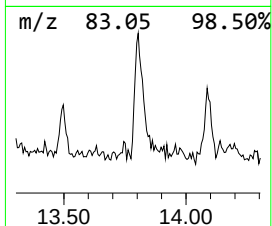
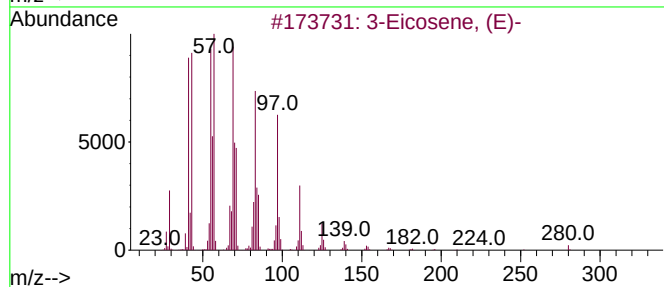
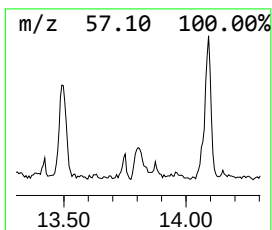
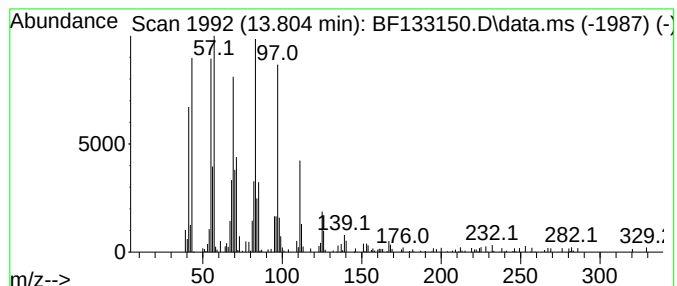
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 3-Eicosene, (E)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.804	4.72 ng	279323	Chrysene-d12		13.880	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-		280	C20H40	074685-33-9	96
2	Cyclohexadecane		224	C16H32	000295-65-8	95
3	Behenic alcohol		326	C22H46O	000661-19-8	95
4	1-Heneicosanol		312	C21H44O	015594-90-8	95
5	5-Eicosene, (E)-		280	C20H40	074685-30-6	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050123\
Data File : BF133150.D
Acq On : 01 May 2023 12:16
Operator : CG\JU
Sample : 02495-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

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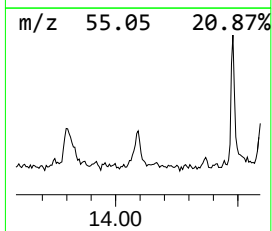
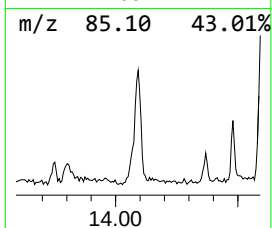
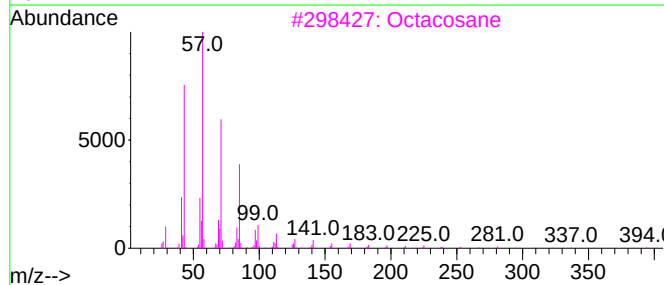
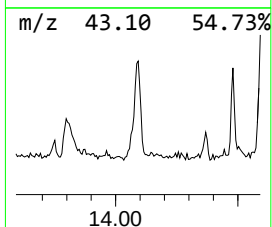
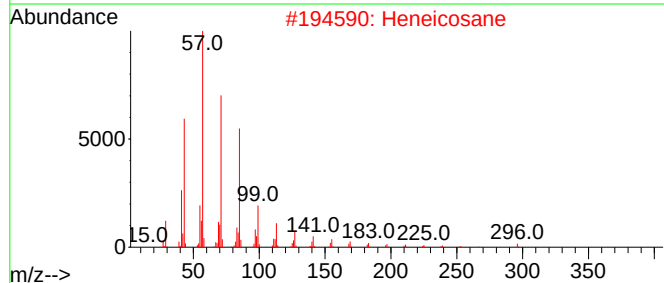
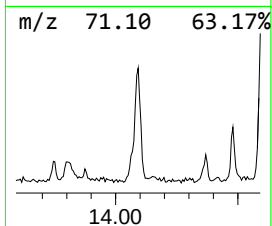
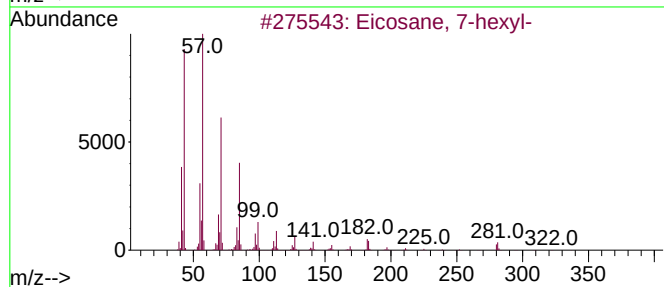
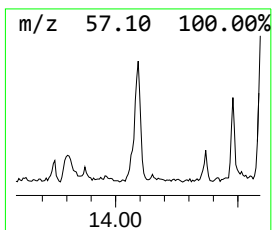
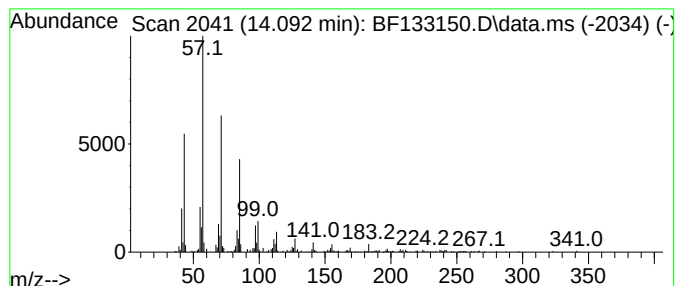
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Eicosane, 7-hexyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.092	6.26 ng	370385	Chrysene-d12	13.880

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane, 7-hexyl-	366	C26H54	055333-99-8	91
2			Heneicosane	296	C21H44	000629-94-7	90
3			Octacosane	394	C28H58	000630-02-4	90
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
5			Heptadecane	240	C17H36	000629-78-7	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050123\
Data File : BF133150.D
Acq On : 01 May 2023 12:16
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Instrument :
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ClientSampleId :
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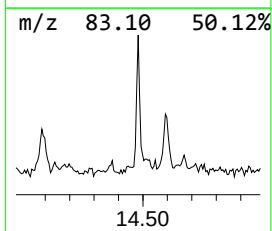
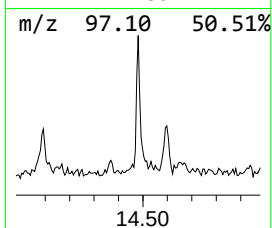
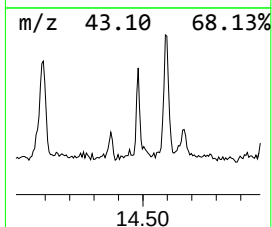
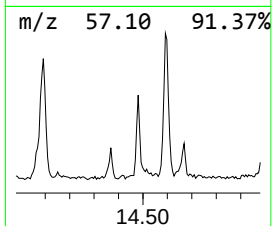
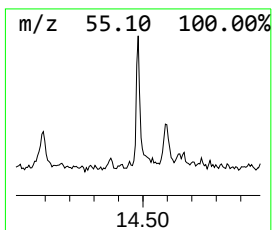
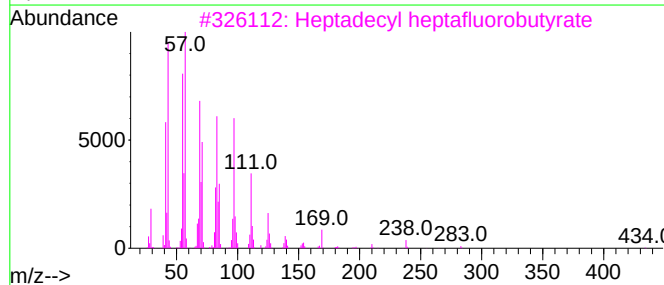
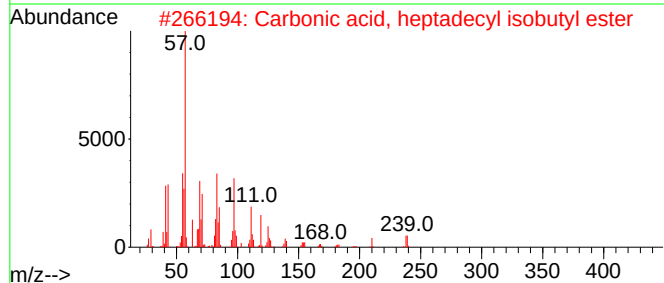
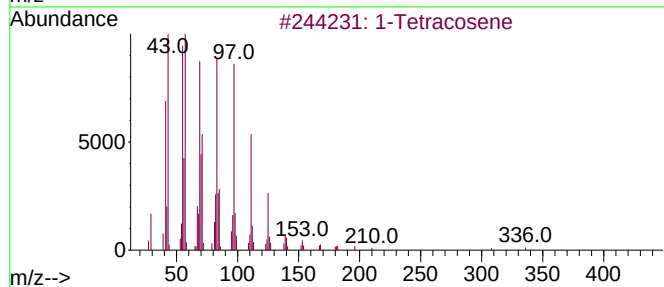
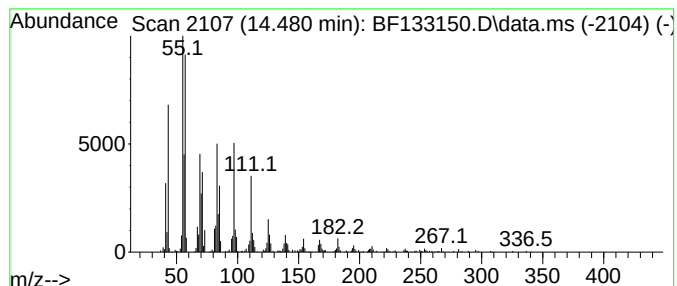
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1-Tetracosene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.480	5.47 ng	323220	Chrysene-d12	13.880

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Tetracosene	336	C24H48	010192-32-2	95
2		Carbonic acid, heptadecyl isobut...	356	C22H44O3	1000314-61-4	91
3		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	87
4		11-Tricosene	322	C23H46	052078-56-5	83
5		Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050123\
Data File : BF133150.D
Acq On : 01 May 2023 12:16
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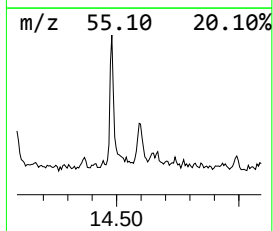
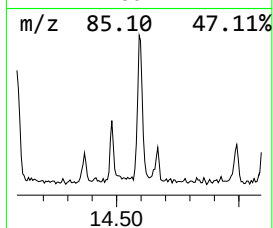
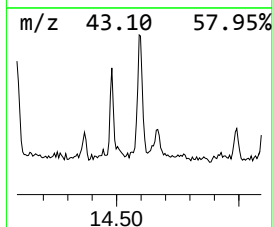
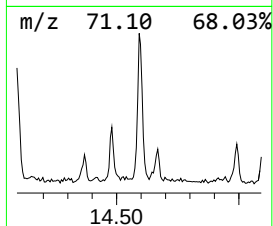
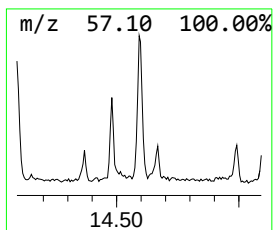
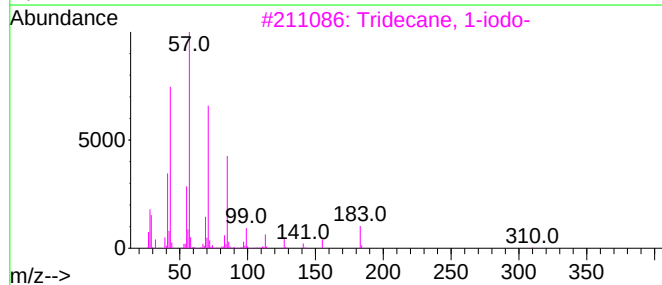
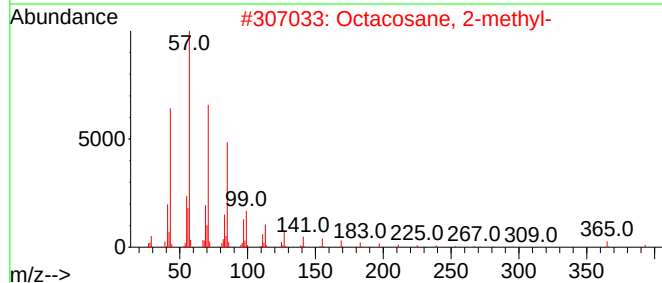
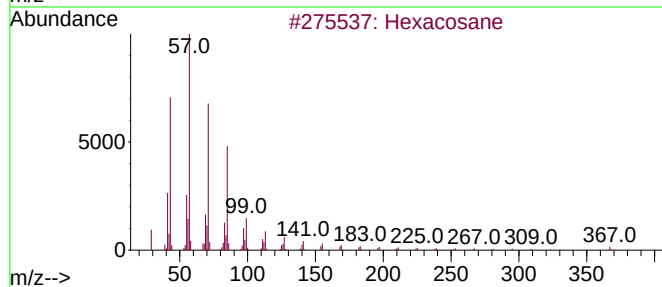
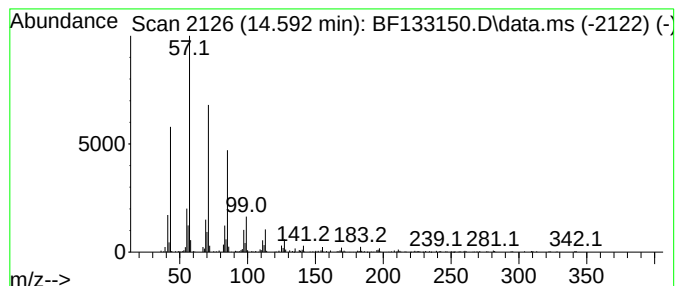
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.592	6.39 ng	361409	Perylene-d12	15.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	91
2			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
3			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	90
4			Nonadecane	268	C19H40	000629-92-5	87
5			Heneicosane	296	C21H44	000629-94-7	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050123\
Data File : BF133150.D
Acq On : 01 May 2023 12:16
Operator : CG\JU
Sample : 02495-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

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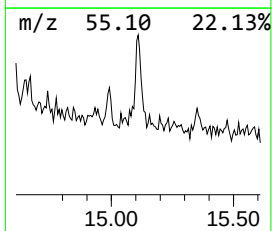
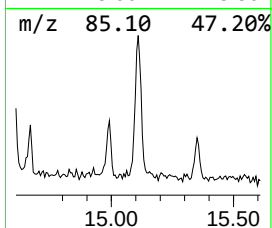
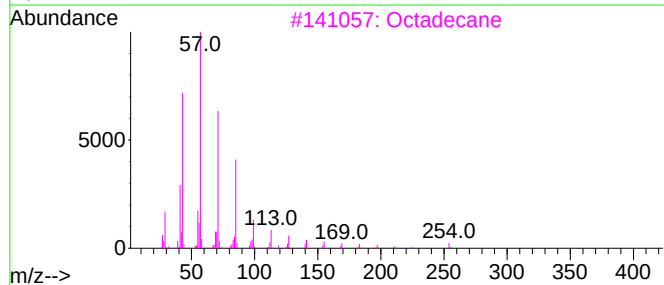
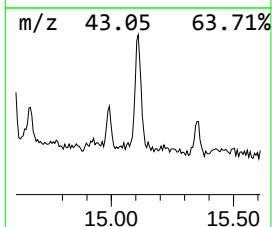
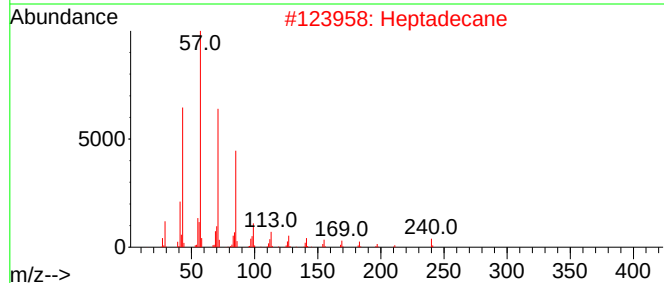
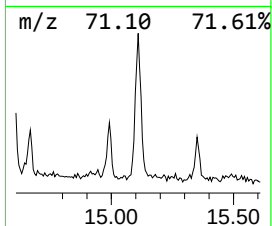
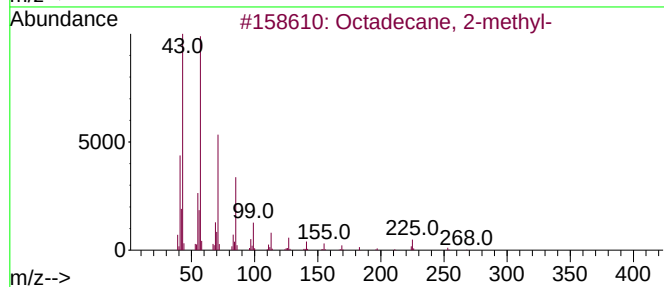
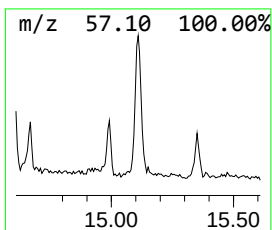
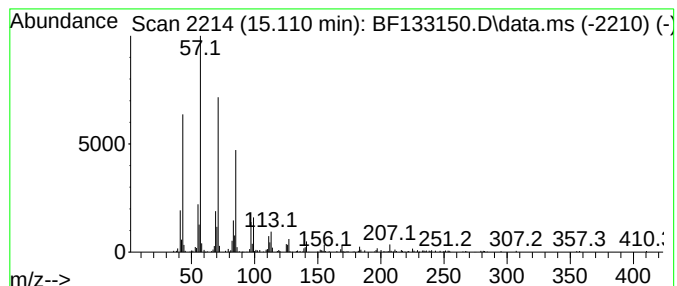
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Octadecane, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.110	5.39 ng	304575	Perylene-d12	15.304

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecane, 2-methyl-	268	C19H40	001560-88-9	93
2		Heptadecane	240	C17H36	000629-78-7	93
3		Octadecane	254	C18H38	000593-45-3	91
4		Hexacosane	366	C26H54	000630-01-3	90
5		Heneicosane	296	C21H44	000629-94-7	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050123\
Data File : BF133150.D
Acq On : 01 May 2023 12:16
Operator : CG\JU
Sample : 02495-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PZ-02

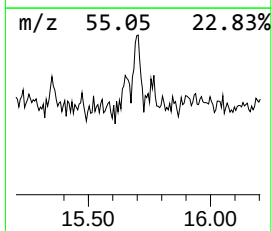
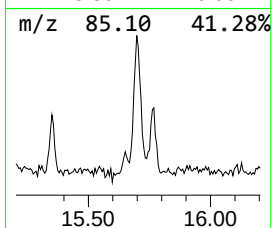
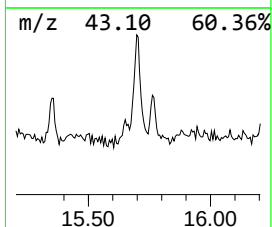
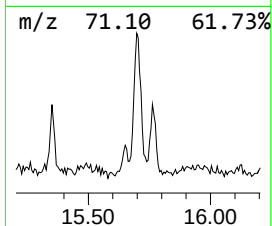
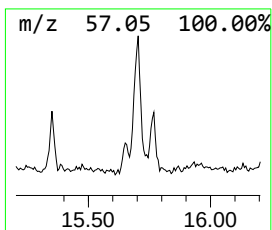
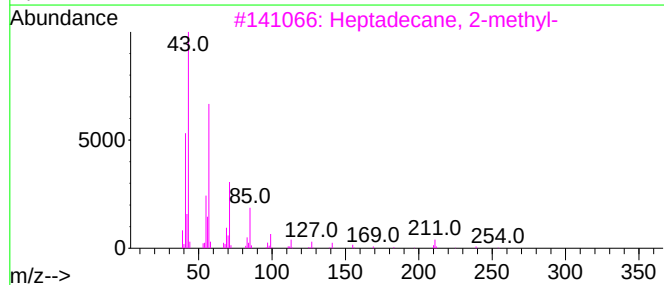
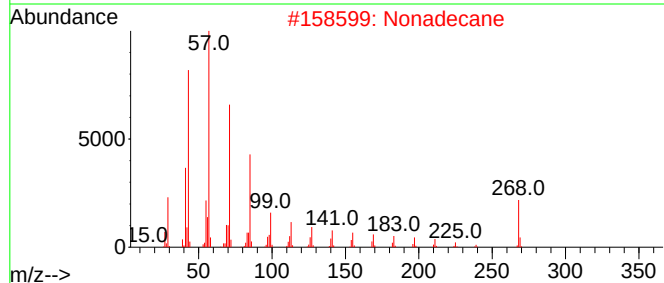
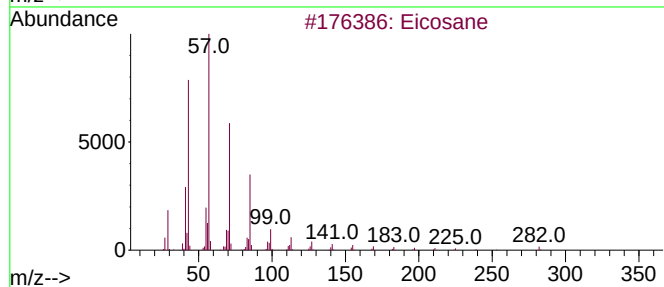
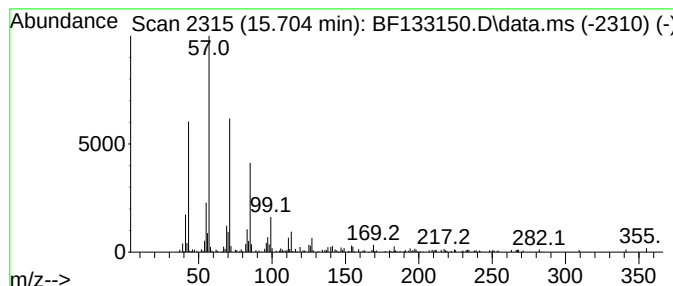
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Eicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.704	3.72 ng	210425	Perylene-d12	15.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	94
2			Nonadecane	268	C19H40	000629-92-5	93
3			Heptadecane, 2-methyl-	254	C18H38	001560-89-0	90
4			Tetracosane	338	C24H50	000646-31-1	90
5			Heptacosane	380	C27H56	000593-49-7	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050123\
Data File : BF133150.D
Acq On : 01 May 2023 12:16
Operator : CG\JU
Sample : 02495-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PZ-02

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
unknown7.451	7.451	3.8	ng	317728	2	8.016	1654160	20.0
Benzophenone	10.480	7.6	ng	713369	3	9.769	1887130	20.0
n-Hexadecanoic ...	11.798	33.8	ng	3141170	4	11.251	1857220	20.0
3,5-Dimethoxy-4...	11.922	2.2	ng	208028	4	11.251	1857220	20.0
Octadecanoic acid	12.563	21.1	ng	1957640	4	11.251	1857220	20.0
Pentadecanoic acid	12.586	61.0	ng	3606850	5	13.880	1182420	20.0
Nonadecane	13.498	5.1	ng	304012	5	13.880	1182420	20.0
3-Eicosene, (E)-	13.804	4.7	ng	279323	5	13.880	1182420	20.0
Eicosane, 7-hexyl-	14.092	6.3	ng	370385	5	13.880	1182420	20.0
1-Tetracosene	14.480	5.5	ng	323220	5	13.880	1182420	20.0
Hexacosane	14.592	6.4	ng	361409	6	15.304	1131020	20.0
Octadecane, 2-m...	15.110	5.4	ng	304575	6	15.304	1131020	20.0
Eicosane	15.704	3.7	ng	210425	6	15.304	1131020	20.0