

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050223\
 Data File : BF133194.D
 Acq On : 02 May 2023 17:52
 Operator : CG\JU
 Sample : 02571-01
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 OE-3-050123

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: BF133194.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.934	479	484	490	rVB	64023	86964	1.77%	0.230%
2	5.346	549	554	557	rBV	4760627	4554206	92.92%	12.069%
3	6.369	723	728	731	rBV	4221600	4717222	96.25%	12.501%
4	6.728	785	789	792	rBV	1660763	1244823	25.40%	3.299%
5	7.292	876	885	888	rBV	3298856	3047423	62.18%	8.076%
6	7.334	890	892	895	rVB	125680	95688	1.95%	0.254%
7	7.539	923	927	930	rVB3	46317	55165	1.13%	0.146%
8	8.010	1003	1007	1010	rBV	1954227	1787654	36.47%	4.737%
9	8.310	1053	1058	1061	rBV6	51172	78310	1.60%	0.208%
10	8.398	1070	1073	1076	rBV2	70720	58731	1.20%	0.156%
11	8.439	1076	1080	1082	rBV2	74206	69820	1.42%	0.185%
12	8.516	1090	1093	1096	rBV2	76657	64964	1.33%	0.172%
13	8.610	1105	1109	1112	rBV	207076	182898	3.73%	0.485%
14	8.710	1123	1126	1132	rVB5	46279	64129	1.31%	0.170%
15	8.834	1141	1147	1150	rBV4	62917	86990	1.77%	0.231%
16	9.039	1180	1182	1186	rVB2	75430	72623	1.48%	0.192%
17	9.092	1186	1191	1194	rBV	5666272	4901102	100.00%	12.988%
18	9.175	1200	1205	1209	rBV	269855	236114	4.82%	0.626%
19	9.498	1254	1260	1262	rBV3	98158	129593	2.64%	0.343%
20	9.551	1266	1269	1272	rVB4	52416	55433	1.13%	0.147%
21	9.704	1293	1295	1299	rVB	252474	194148	3.96%	0.514%
22	9.763	1299	1305	1309	rBV	2135925	1862738	38.01%	4.936%
23	10.204	1377	1380	1383	rVB	227025	173269	3.54%	0.459%
24	10.428	1411	1418	1423	rBV	95337	126436	2.58%	0.335%
25	10.480	1423	1427	1430	rVB	1277808	1044446	21.31%	2.768%
26	10.551	1435	1439	1443	rBV	2907920	2854918	58.25%	7.566%
27	10.675	1457	1460	1465	rBV	206839	246391	5.03%	0.653%
28	11.127	1534	1537	1539	rBV	147710	128481	2.62%	0.340%
29	11.157	1539	1542	1545	rVB	78151	78649	1.60%	0.208%
30	11.245	1553	1557	1560	rBV	2013567	1619837	33.05%	4.293%
31	11.551	1606	1609	1612	rBV	142878	105233	2.15%	0.279%
32	11.786	1645	1649	1657	rBV	515814	535088	10.92%	1.418%
33	11.957	1675	1678	1681	rBV	100923	78416	1.60%	0.208%
34	12.351	1739	1745	1748	rVB2	98753	134375	2.74%	0.356%
35	12.457	1760	1763	1765	rBV	88698	82121	1.68%	0.218%
36	12.486	1766	1768	1777	rVB2	60004	95324	1.94%	0.253%

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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	12.569	1779	1782	1787	rBV3	96714	115051	2.35%	0.305%
38	12.680	1799	1801	1805	rBV	59095	56859	1.16%	0.151%
39	12.833	1823	1827	1830	rBV	4143589	3804810	77.63%	10.083%
40	13.074	1865	1868	1872	rBV2	93914	95309	1.94%	0.253%
41	13.416	1924	1926	1929	rBV	78896	61168	1.25%	0.162%
42	13.751	1980	1983	1992	rBV5	145783	373003	7.61%	0.988%
43	13.880	2001	2005	2008	rBV	1216613	1063888	21.71%	2.819%
44	14.063	2033	2036	2039	rBV	86925	81437	1.66%	0.216%
45	14.368	2085	2088	2090	rBV	96472	90388	1.84%	0.240%
46	14.663	2136	2138	2141	rBV	83698	99976	2.04%	0.265%
47	15.304	2243	2247	2251	rVB	868275	944156	19.26%	2.502%

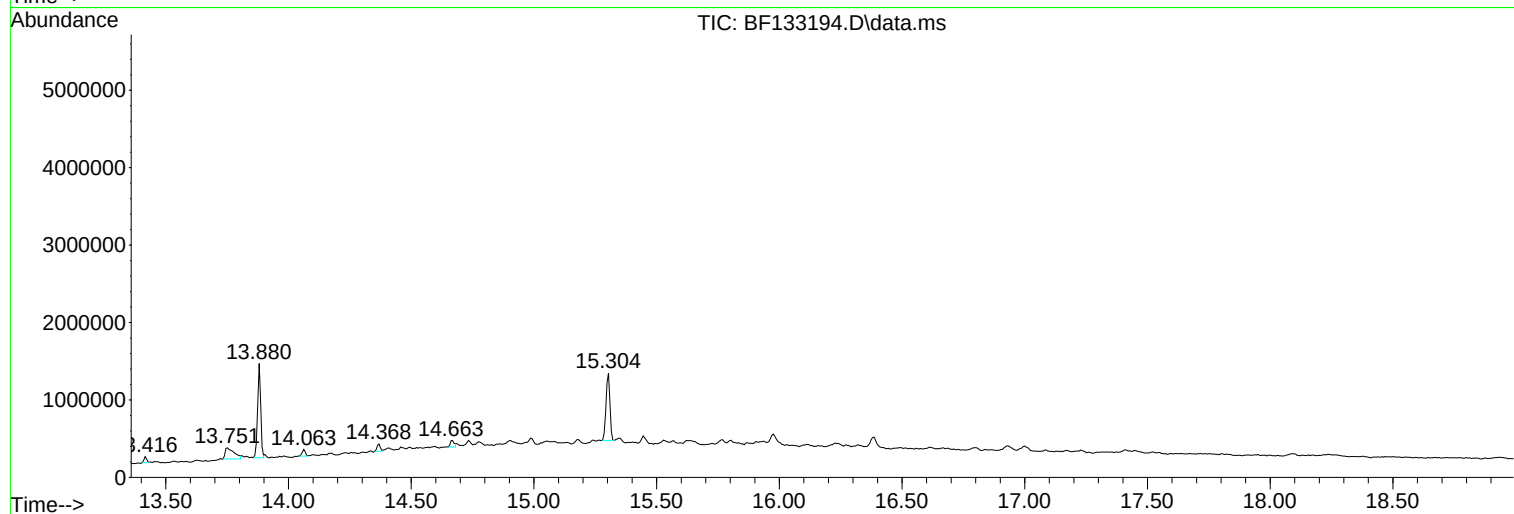
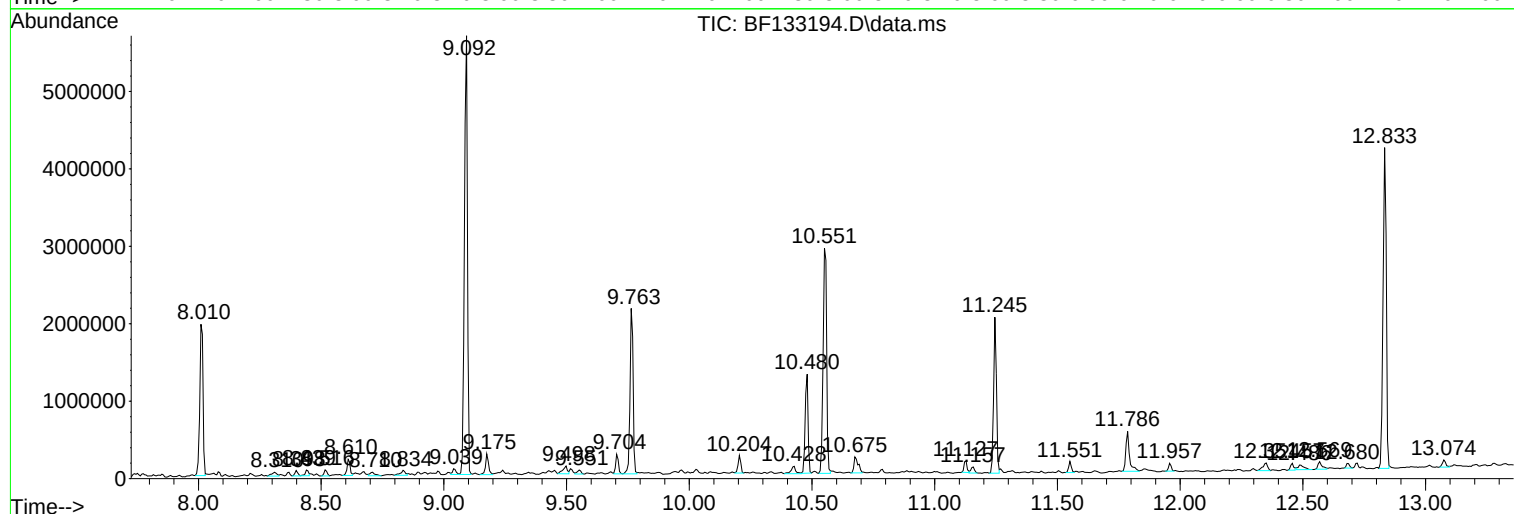
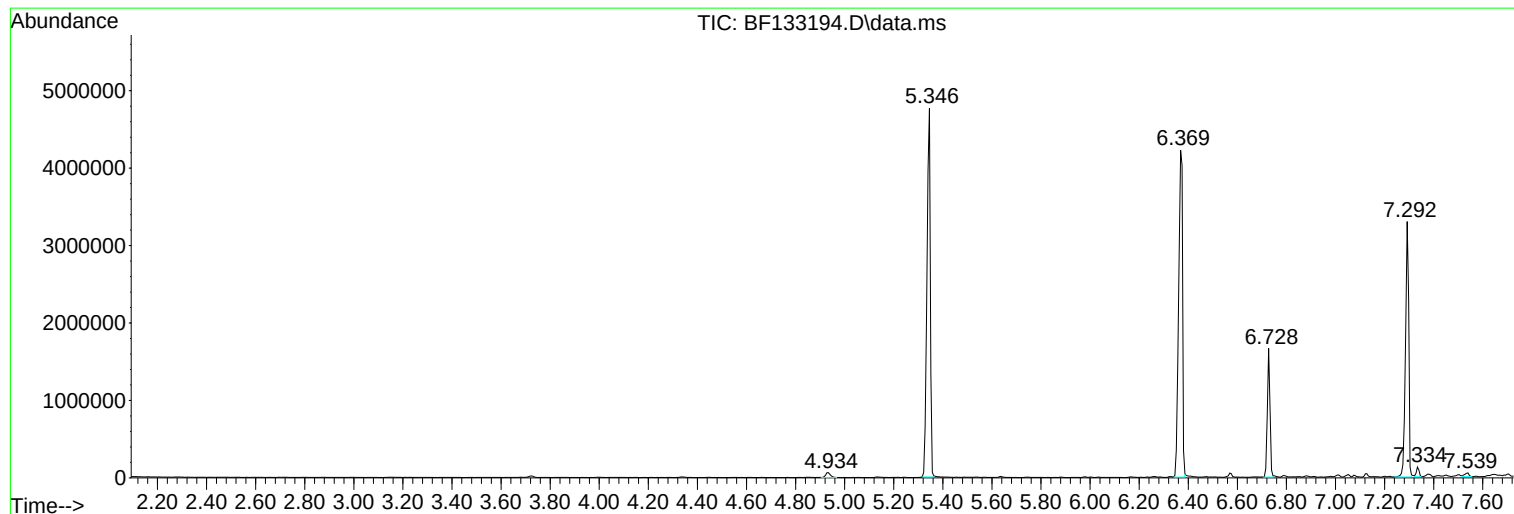
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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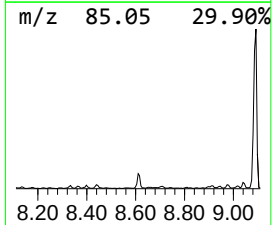
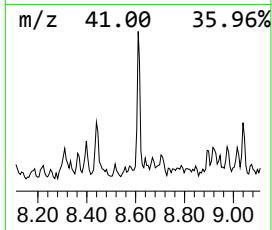
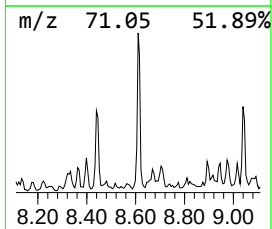
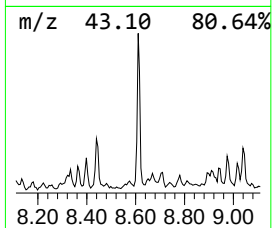
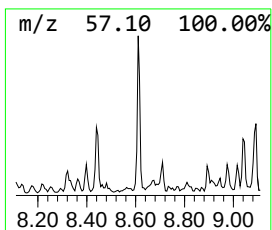
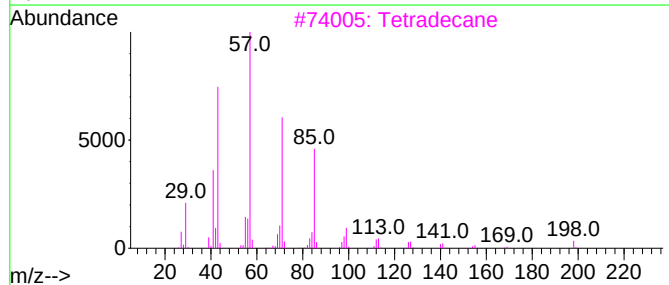
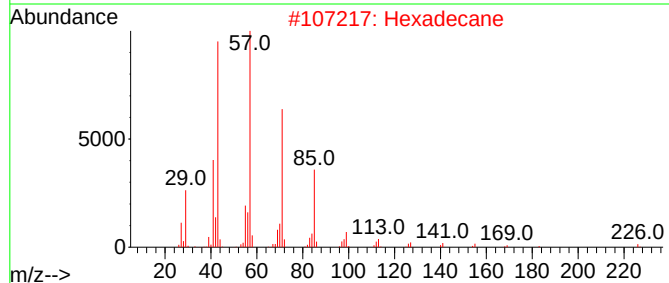
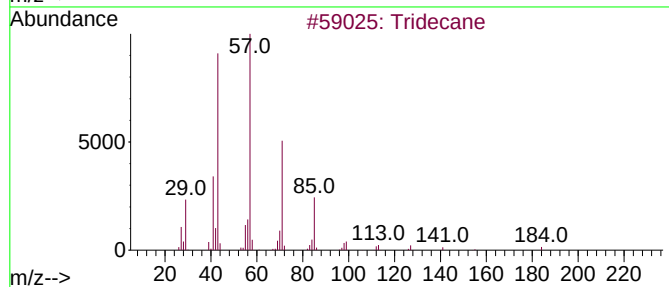
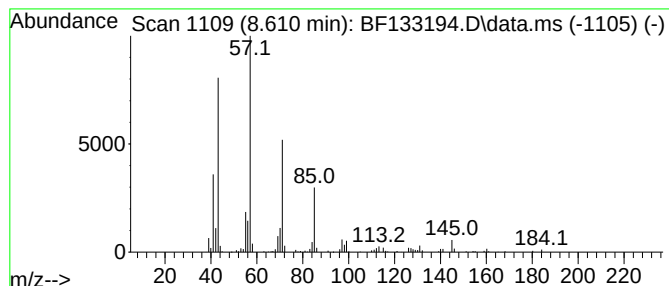
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Tridecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.610	2.05 ng	182898	Naphthalene-d8	8.016

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tridecane	184	C13H28	000629-50-5	93
2		Hexadecane	226	C16H34	000544-76-3	87
3		Tetradecane	198	C14H30	000629-59-4	86
4		Decane, 6-ethyl-2-methyl-	184	C13H28	062108-21-8	72
5		Dodecane, 1-iodo-	296	C12H25I	004292-19-7	64



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Misc :
ALS Vial : 17 Sample Multiplier: 1

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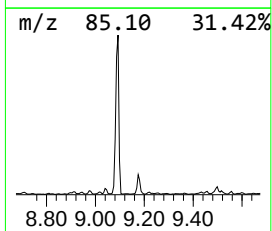
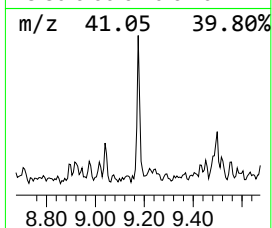
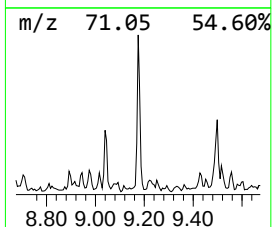
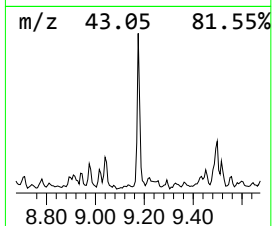
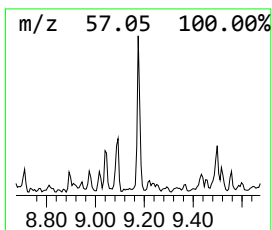
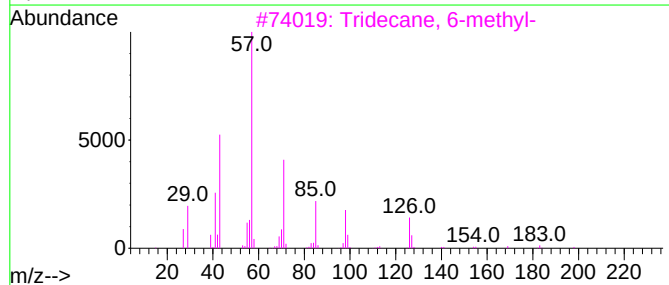
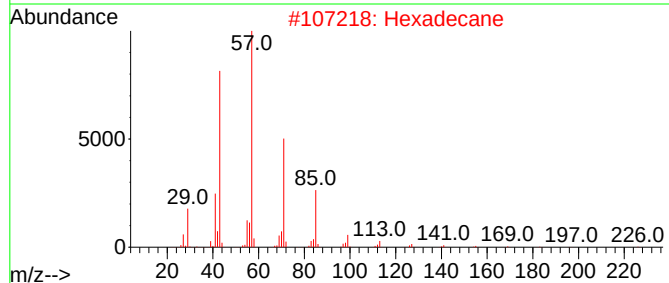
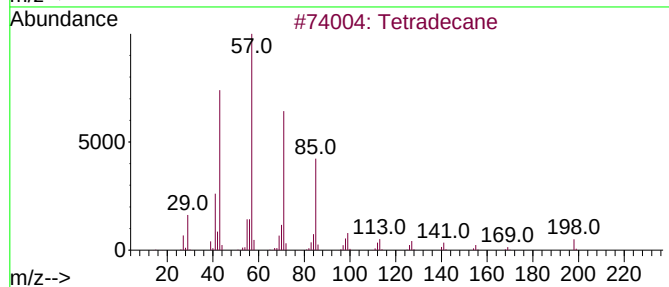
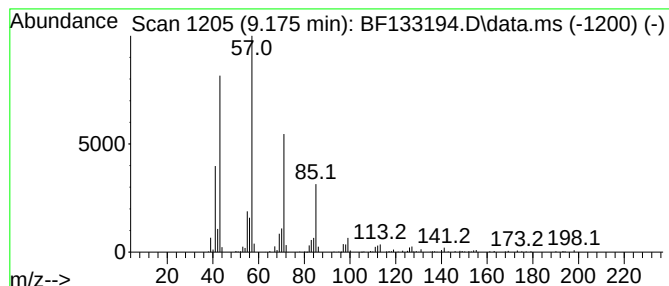
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Tetradecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.175	2.54 ng	236114	Acenaphthene-d10	9.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane	198	C14H30	000629-59-4	95
2			Hexadecane	226	C16H34	000544-76-3	91
3			Tridecane, 6-methyl-	198	C14H30	013287-21-3	90
4			Silane, trichlorooctadecyl-	386	C18H37Cl3Si	000112-04-9	90
5			Nonadecane	268	C19H40	000629-92-5	90



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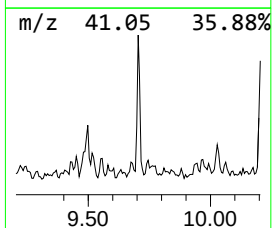
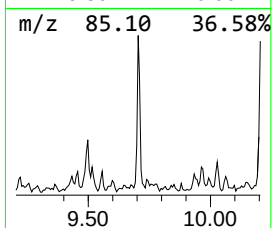
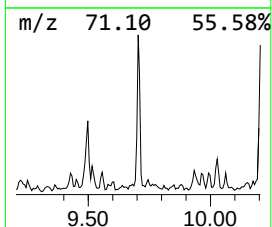
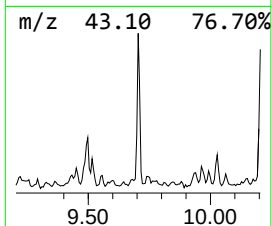
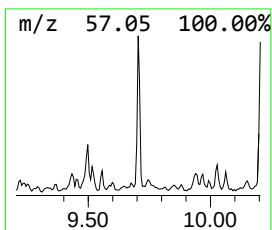
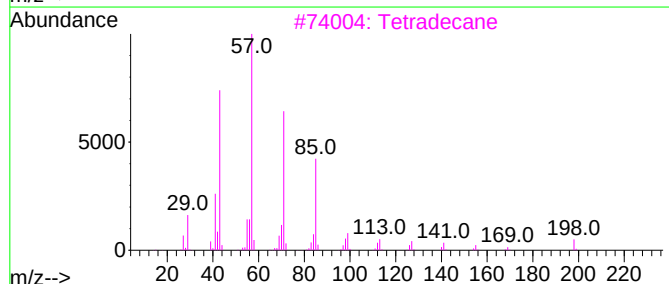
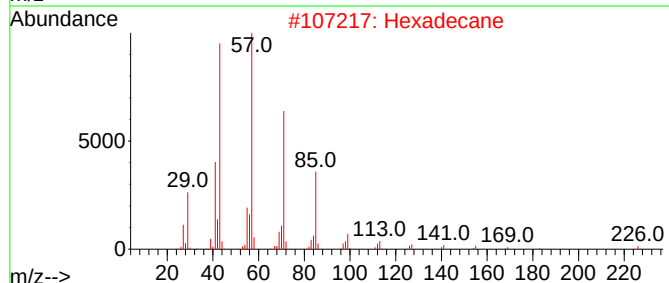
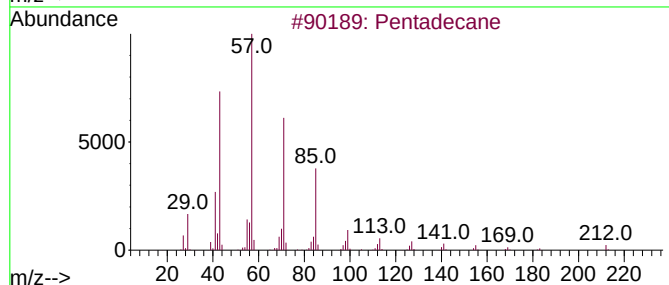
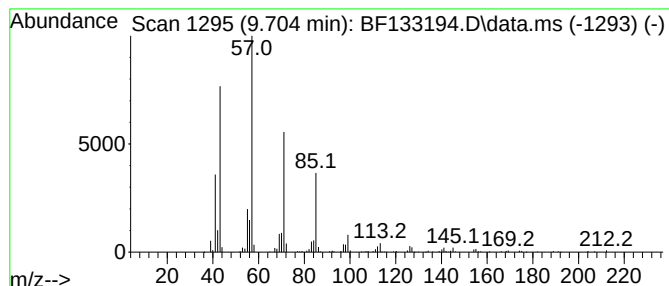
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Pentadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.704	2.08 ng	194148	Acenaphthene-d10	9.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecane	212	C15H32	000629-62-9	95
2			Hexadecane	226	C16H34	000544-76-3	91
3			Tetradecane	198	C14H30	000629-59-4	86
4			Heneicosane	296	C21H44	000629-94-7	86
5			Heptadecane	240	C17H36	000629-78-7	86



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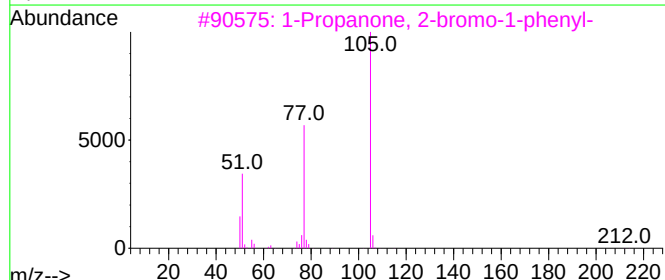
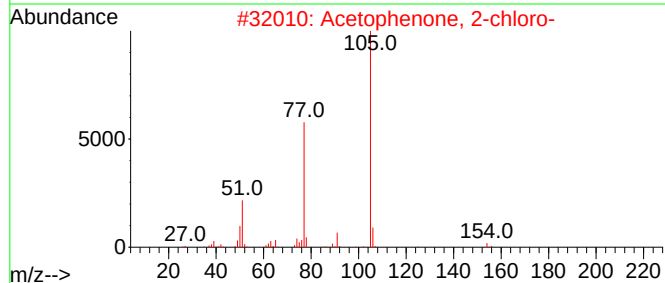
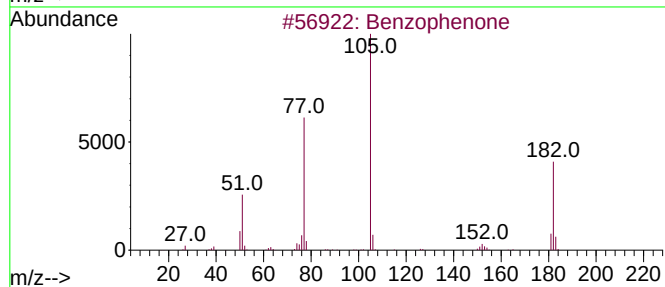
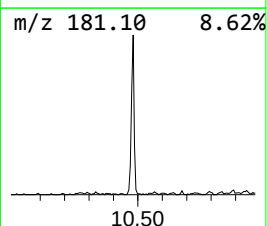
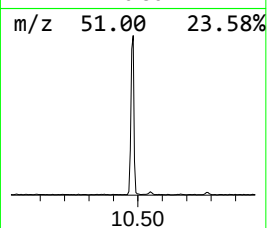
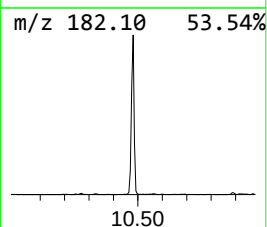
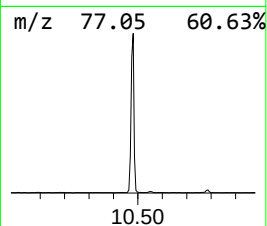
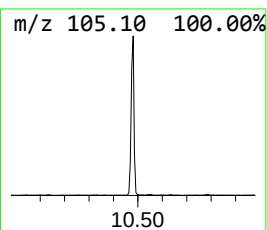
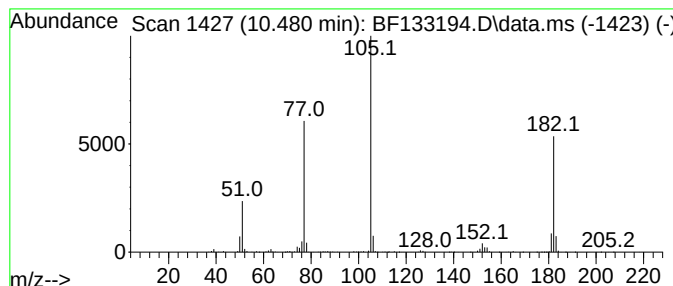
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Benzophenone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.480	11.21 ng	1044450	Acenaphthene-d10	9.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
3			1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
4			acetic acid, 2-bromo-, 2-oxo-2-p...	256	C10H9BrO3	1000401-50-0	47
5			N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	47



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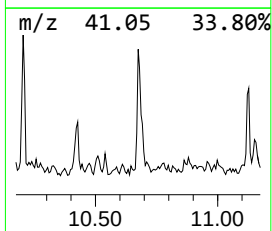
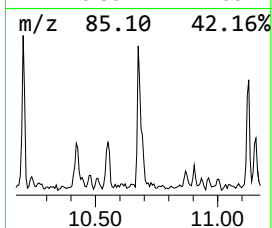
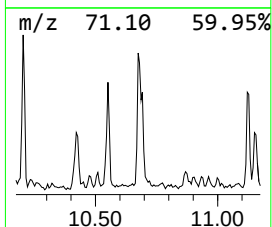
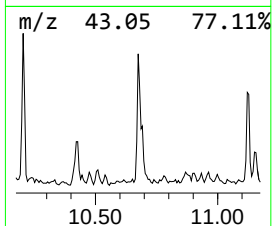
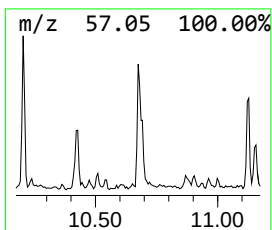
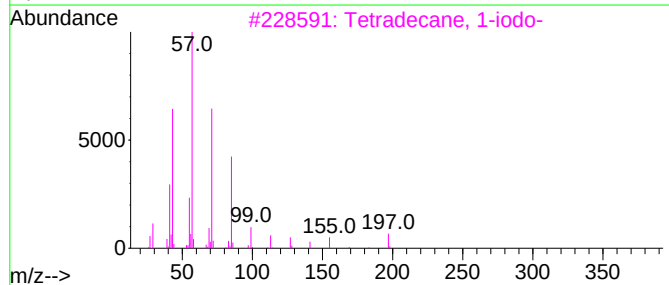
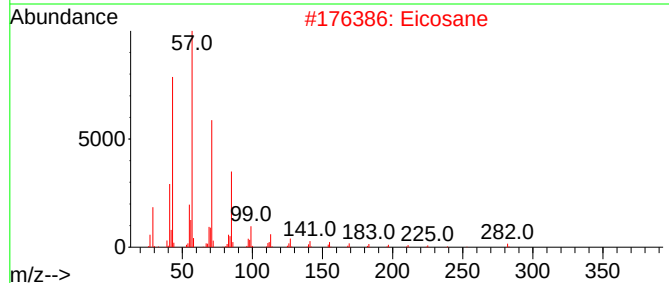
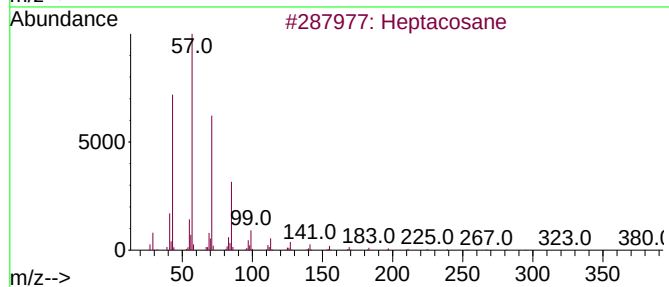
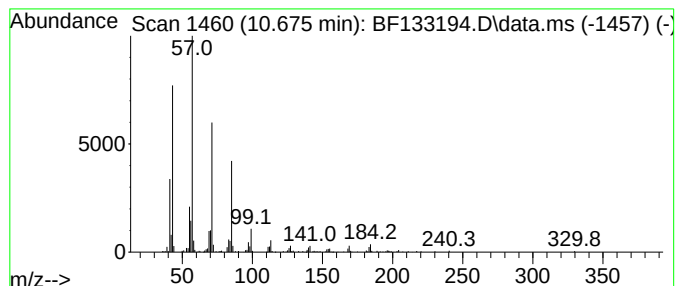
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Heptacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.675	3.04 ng	246391	Phenanthrene-d10	11.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	90
2			Eicosane	282	C20H42	000112-95-8	87
3			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	80
4			Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	80
5			Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050223\
Data File : BF133194.D
Acq On : 02 May 2023 17:52
Operator : CG\JU
Sample : 02571-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OE-3-050123

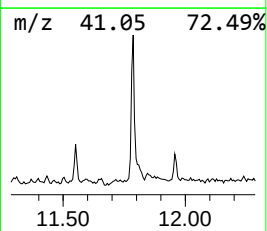
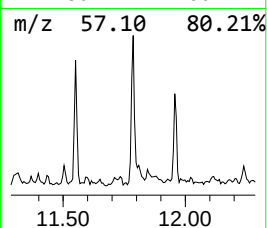
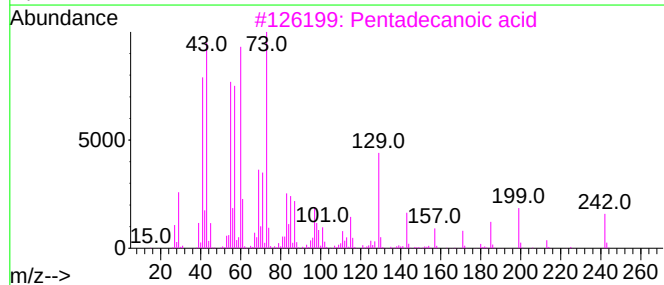
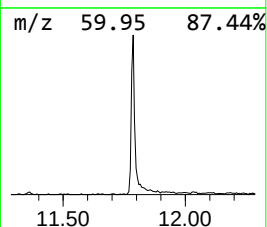
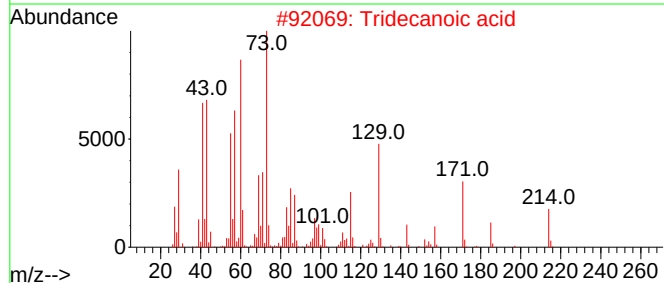
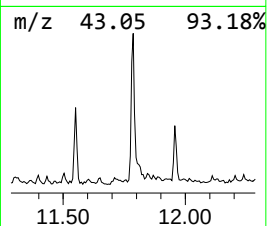
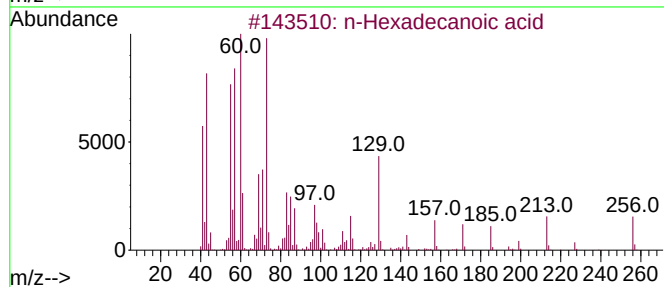
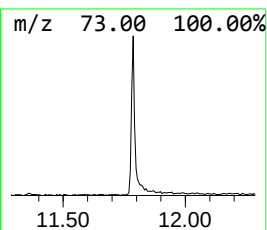
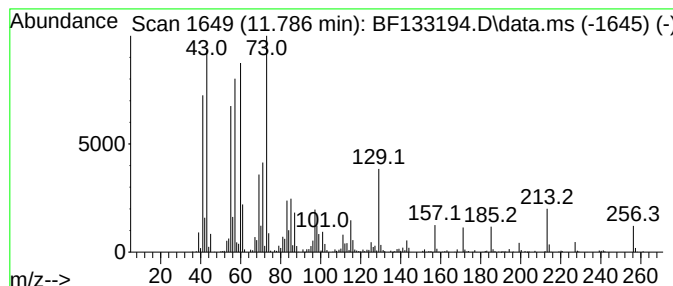
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.786	6.61 ng	535088	Phenanthrene-d10	11.245

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	81
4			n-Decanoic acid	172	C10H20O2	000334-48-5	76
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050223\
Data File : BF133194.D
Acq On : 02 May 2023 17:52
Operator : CG\JU
Sample : 02571-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

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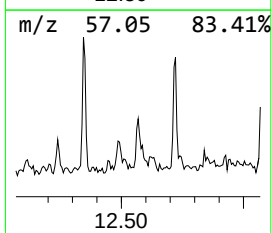
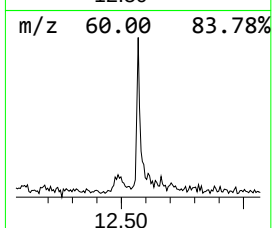
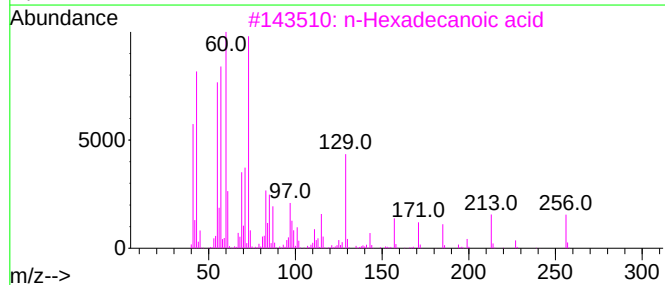
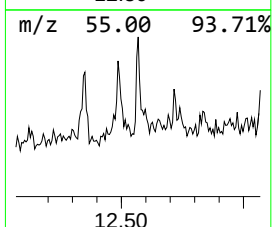
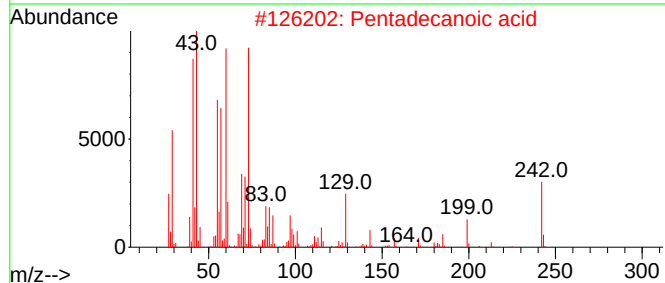
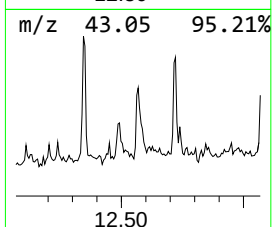
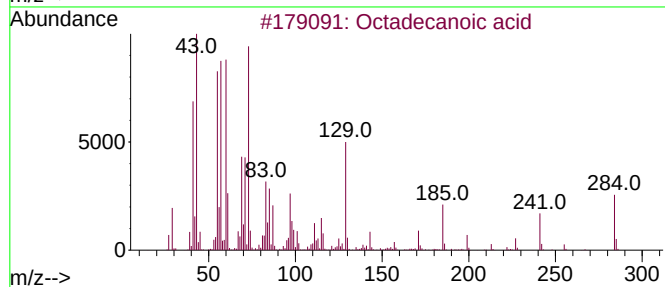
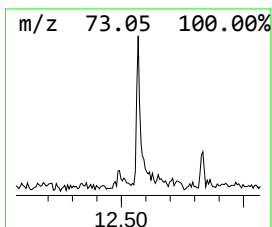
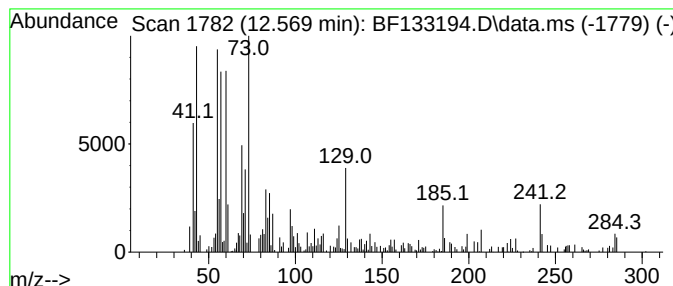
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.569	2.16 ng	115051	Chrysene-d12	13.880

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			Undecanoic acid	186	C11H22O2	000112-37-8	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050223\
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Acq On : 02 May 2023 17:52
Operator : CG\JU
Sample : 02571-01
Misc :
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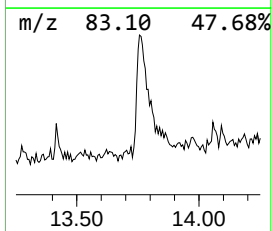
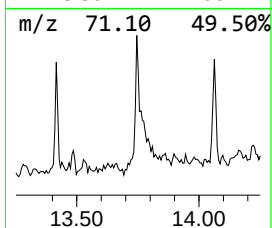
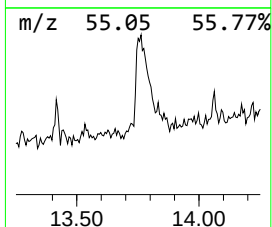
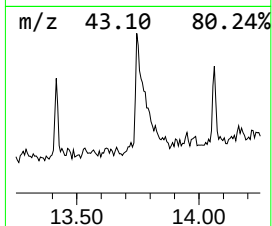
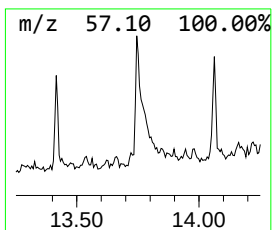
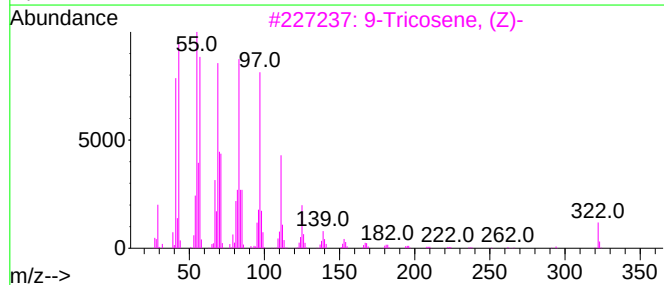
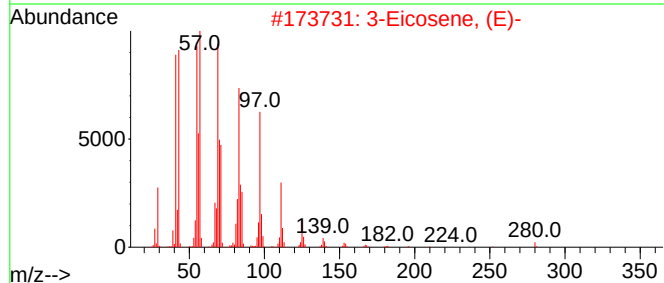
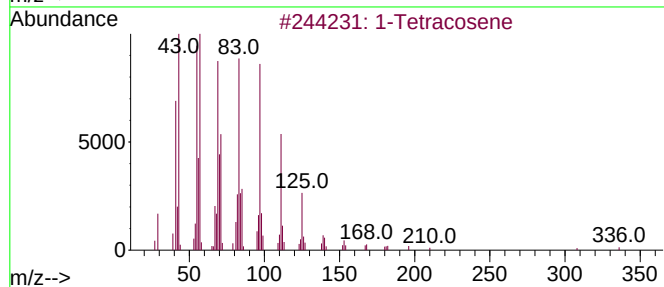
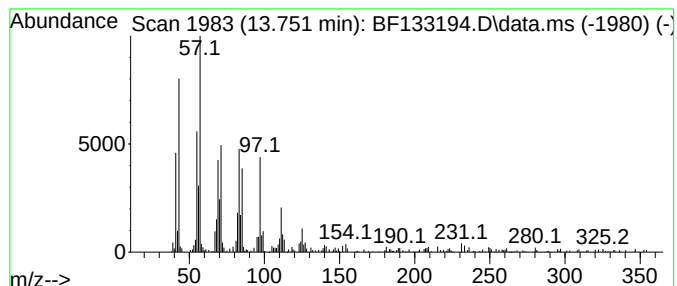
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Tetracosene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.751	7.01 ng	373003	Chrysene-d12	13.880	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tetracosene	336	C24H48	010192-32-2	96
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	92
3	9-Tricosene, (Z)-	322	C23H46	027519-02-4	92
4	5-Eicosene, (E)-	280	C20H40	074685-30-6	87
5	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050223\
Data File : BF133194.D
Acq On : 02 May 2023 17:52
Operator : CG\JU
Sample : 02571-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

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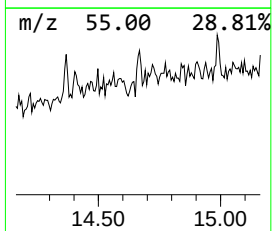
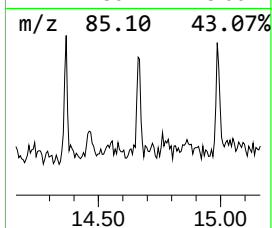
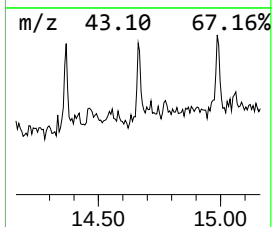
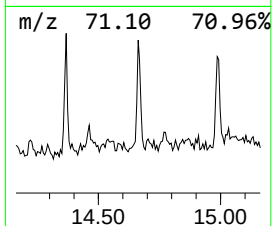
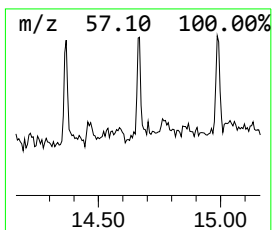
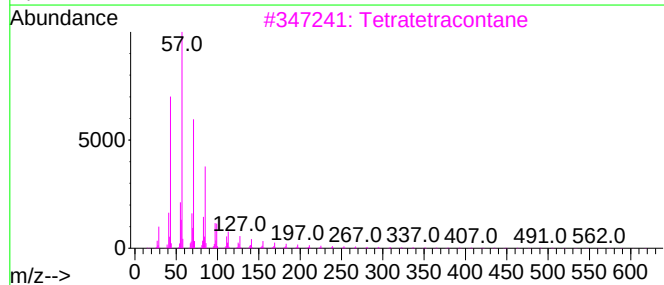
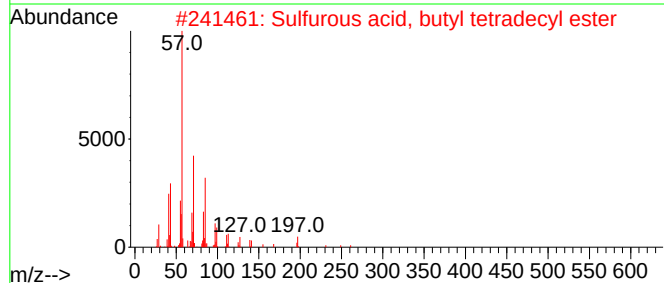
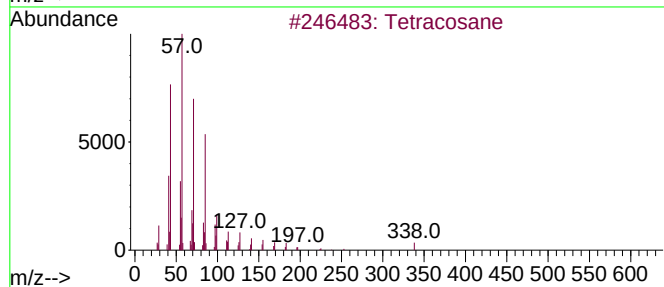
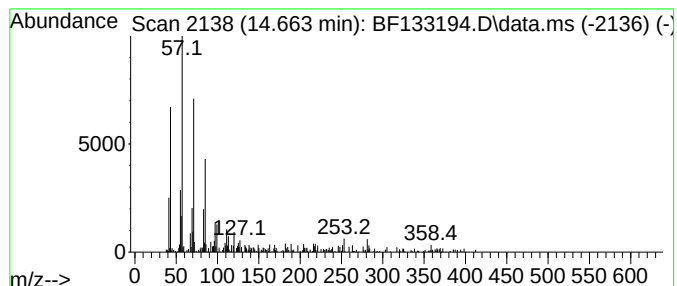
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tetracosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.663	2.12 ng	99976	Perylene-d12	15.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	86
2			Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1010309-18-1	83
3			Tetratetracontane	619	C44H90	007098-22-8	83
4			Sulfurous acid, butyl tridecyl e...	320	C17H36O3S	1000309-18-0	83
5			Sulfurous acid, dodecyl 2-propyl...	292	C15H32O3S	1000309-12-3	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050223\
Data File : BF133194.D
Acq On : 02 May 2023 17:52
Operator : CG\JU
Sample : 02571-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
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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\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Tridecane	8.610	2.0	ng	182898	2	8.016	1787650	20.0
Tetradecane	9.175	2.5	ng	236114	3	9.763	1862740	20.0
Pentadecane	9.704	2.1	ng	194148	3	9.763	1862740	20.0
Benzophenone	10.480	11.2	ng	1044450	3	9.763	1862740	20.0
Heptacosane	10.675	3.0	ng	246391	4	11.245	1619840	20.0
n-Hexadecanoic ...	11.786	6.6	ng	535088	4	11.245	1619840	20.0
Octadecanoic acid	12.569	2.2	ng	115051	5	13.880	1063890	20.0
1-Tetracosene	13.751	7.0	ng	373003	5	13.880	1063890	20.0
Tetracosane	14.663	2.1	ng	99976	6	15.304	944156	20.0