

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042623\
 Data File : BF133068.D
 Acq On : 26 Apr 2023 16:59
 Operator : CG\JU
 Sample : 02448-06
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20230340-COMP-18

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: BF133068.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	490	rVB	42708	57824	1.49%	0.197%
2	5.345	549	554	557	rBV	3167401	3264557	84.02%	11.097%
3	6.369	723	728	731	rBV	3261476	3389261	87.23%	11.521%
4	6.734	786	790	793	rBV	1378366	1030233	26.52%	3.502%
5	7.298	881	886	889	rBV	2304286	2101092	54.08%	7.142%
6	8.016	1004	1008	1011	rBV	1826086	1402089	36.09%	4.766%
7	9.092	1187	1191	1194	rBV	4320139	3676212	94.61%	12.496%
8	9.769	1302	1306	1309	rBV	2054062	1585594	40.81%	5.390%
9	10.480	1423	1427	1430	rVB	287049	219346	5.65%	0.746%
10	10.557	1435	1440	1443	rBV	2724592	2376320	61.16%	8.077%
11	11.251	1554	1558	1561	rBV	1923944	1648158	42.42%	5.602%
12	11.627	1611	1622	1623	rBV3	42452	102097	2.63%	0.347%
13	11.786	1644	1649	1658	rBV	465430	488182	12.56%	1.659%
14	12.569	1777	1782	1793	rBV	193751	259815	6.69%	0.883%
15	12.745	1804	1812	1820	rVB2	93691	224960	5.79%	0.765%
16	12.839	1823	1828	1831	rBV	4358986	3885471	100.00%	13.207%
17	13.486	1932	1938	1945	rBV	116554	231138	5.95%	0.786%
18	13.751	1978	1983	1986	rBV	42538	49627	1.28%	0.169%
19	13.821	1987	1995	2001	rBV7	53744	189641	4.88%	0.645%
20	13.880	2001	2005	2009	rVB	1466748	1270619	32.70%	4.319%
21	14.080	2033	2039	2047	rBV	137979	243971	6.28%	0.829%
22	14.368	2085	2088	2091	rBV	46231	47750	1.23%	0.162%
23	14.586	2121	2125	2132	rBV	124512	180484	4.65%	0.613%
24	14.668	2137	2139	2147	rVB	48544	49187	1.27%	0.167%
25	14.992	2191	2194	2198	rVB3	41764	47132	1.21%	0.160%
26	15.098	2207	2212	2218	rBV	72752	118256	3.04%	0.402%
27	15.298	2242	2246	2252	rBV	810155	967640	24.90%	3.289%
28	15.692	2308	2313	2319	rBV	57863	108193	2.78%	0.368%
29	16.368	2424	2428	2440	rVB3	48149	120764	3.11%	0.410%
30	17.174	2559	2565	2576	rVB5	28920	83501	2.15%	0.284%

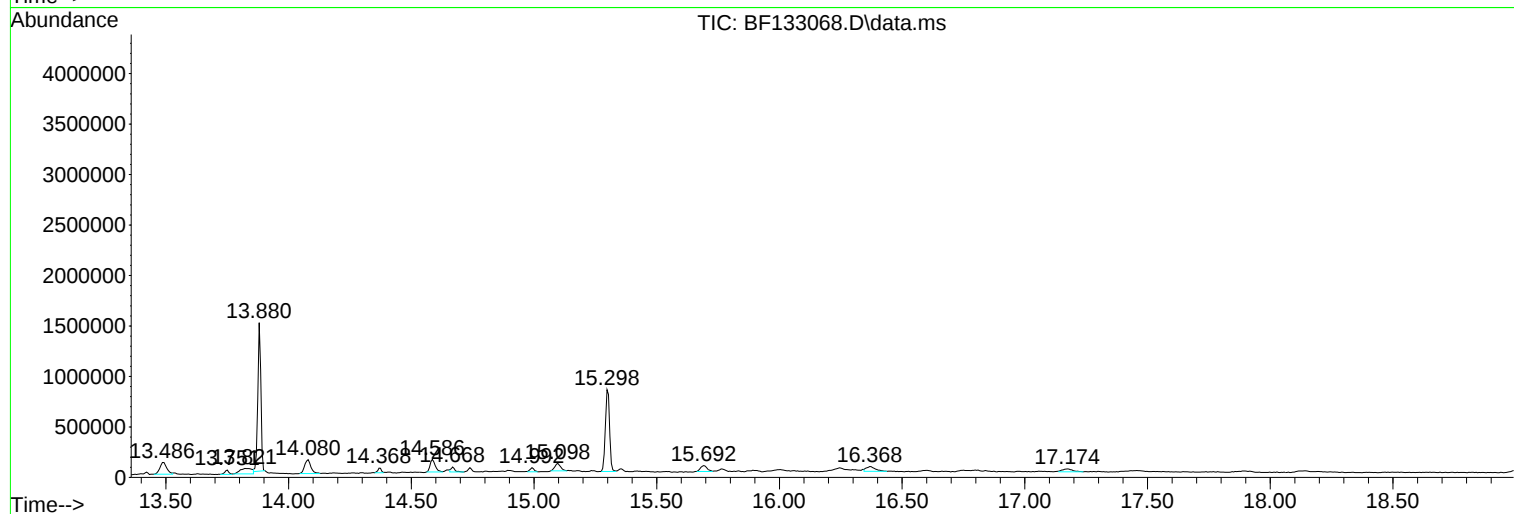
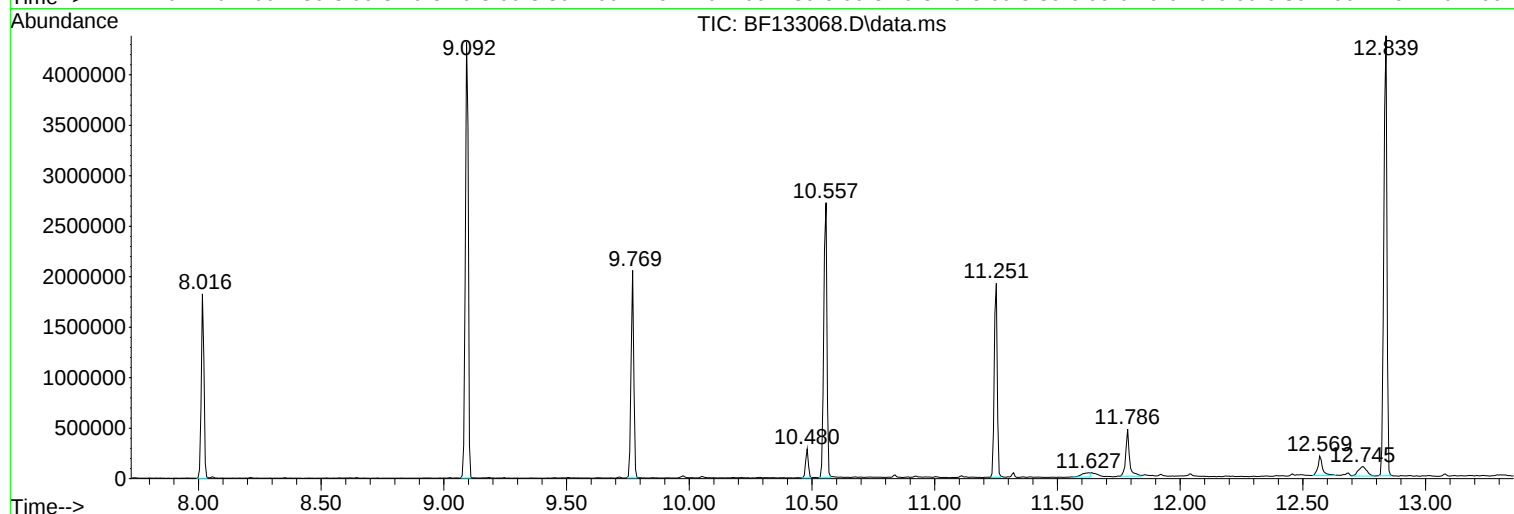
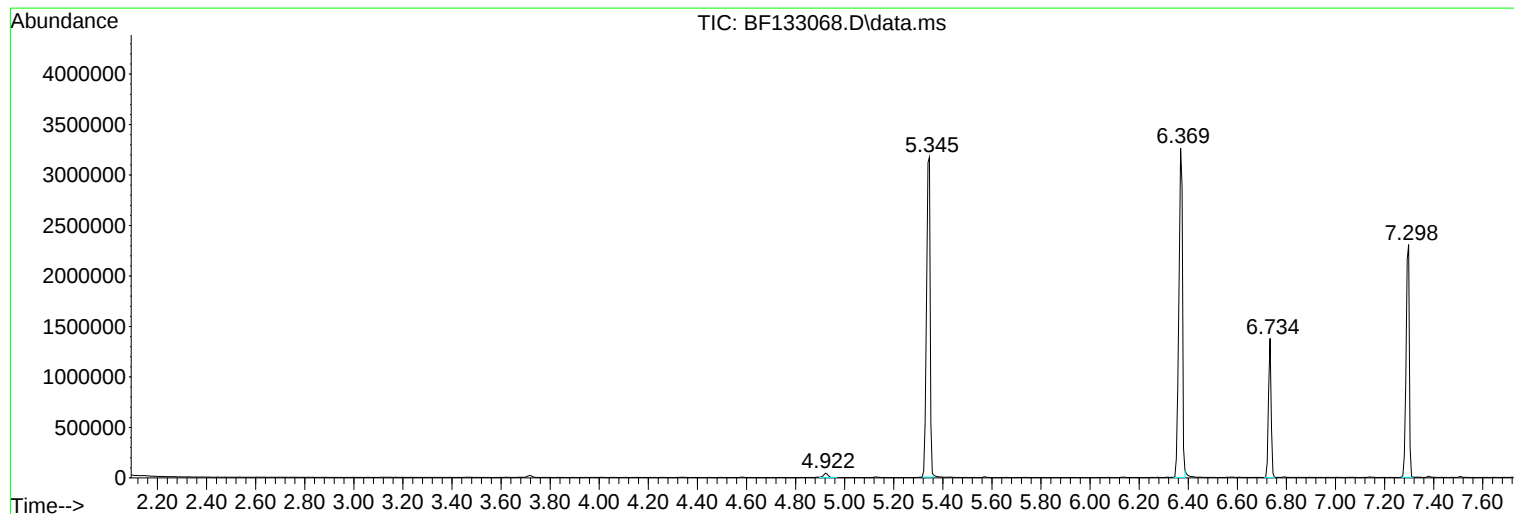
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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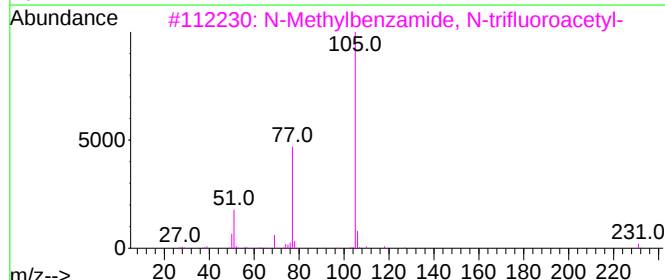
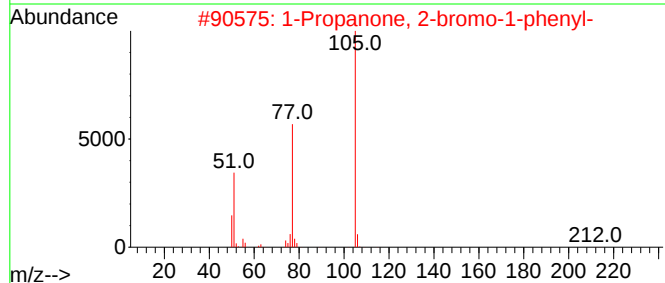
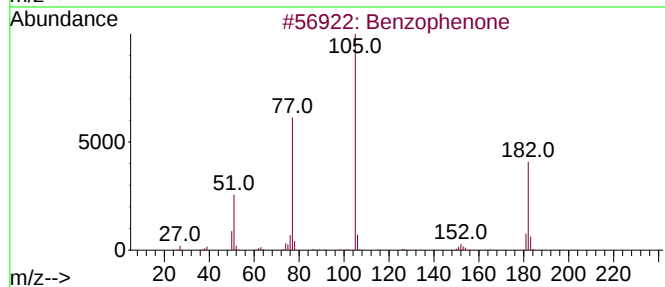
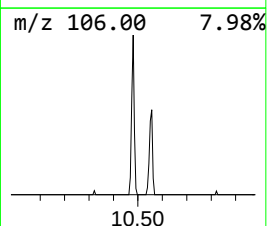
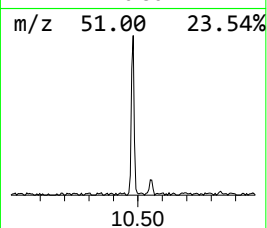
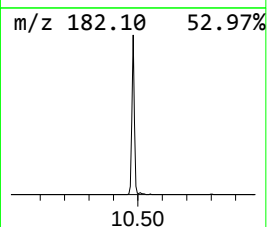
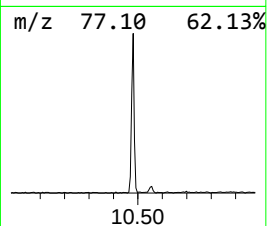
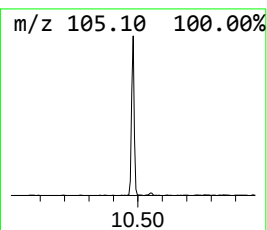
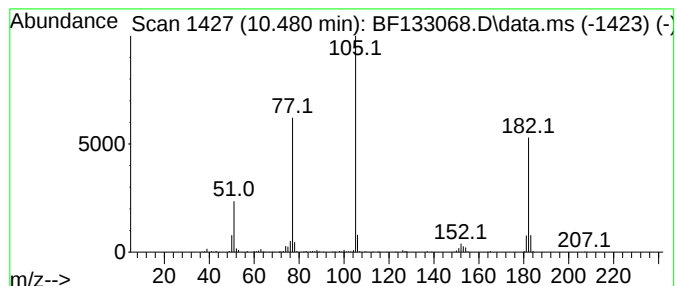
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Benzophenone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.480	2.77 ng	219346	Acenaphthene-d10	9.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
3			N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	47
4			5-Oxo-5-phenylpentanenitrile	173	C11H11NO	1000486-83-7	47
5			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47



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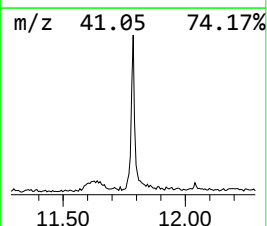
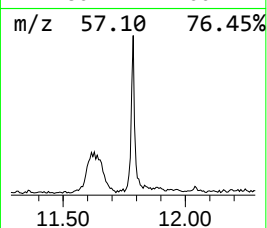
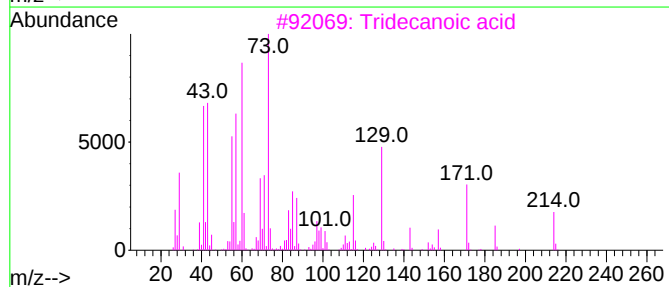
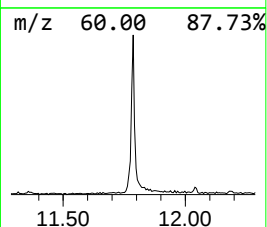
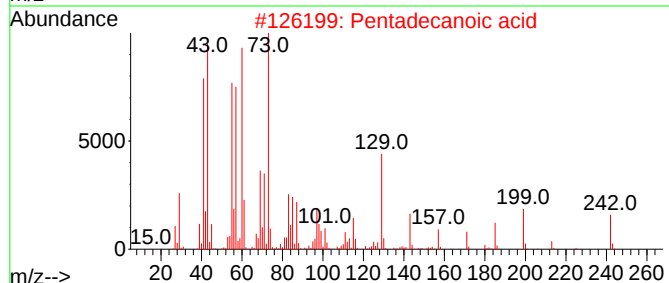
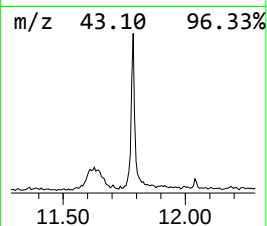
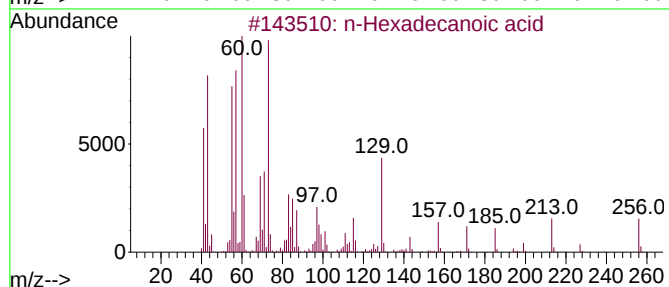
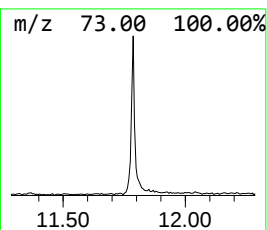
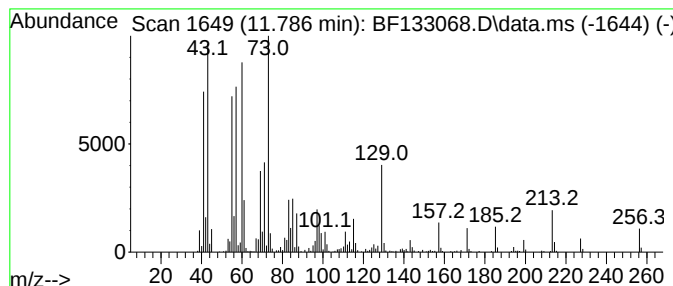
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.786	5.92 ng	488182	Phenanthrene-d10	11.251

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3			Tridecanoic acid	214	C13H26O2	000638-53-9	91
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	81
5			n-Decanoic acid	172	C10H20O2	000334-48-5	70



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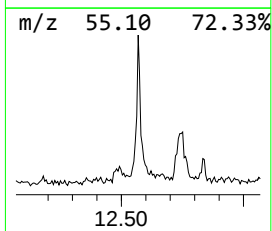
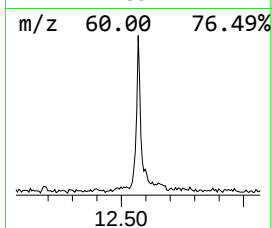
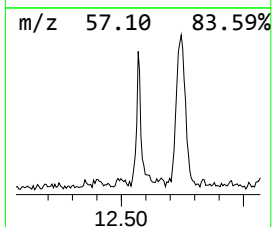
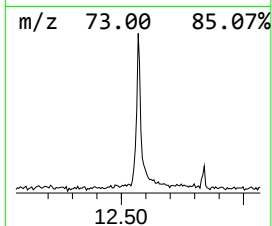
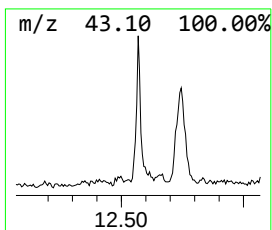
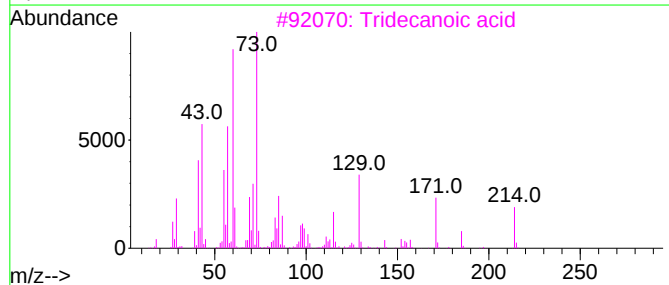
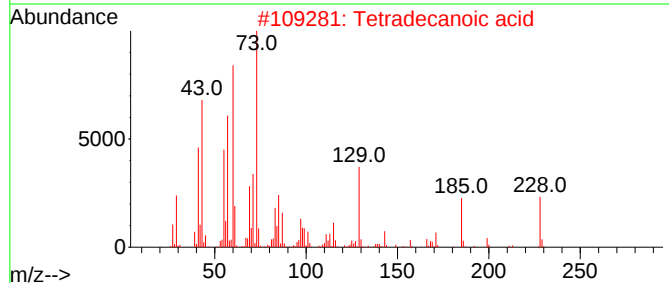
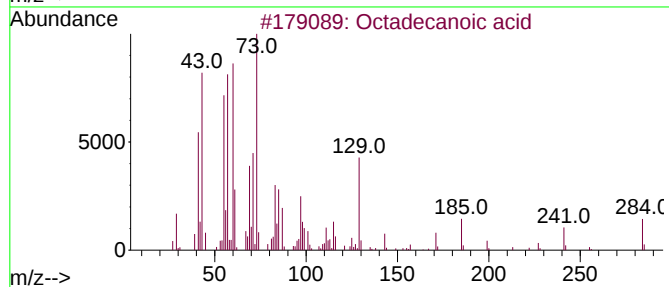
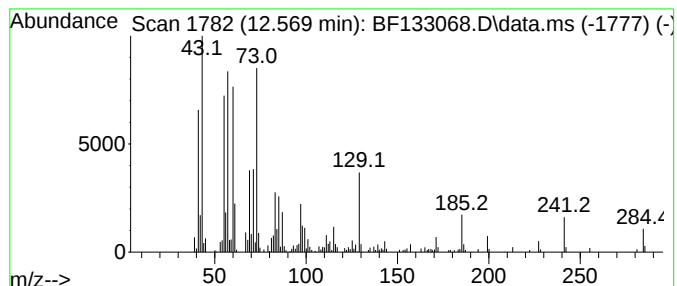
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.569	4.09 ng	259815	Chrysene-d12	13.880

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
3			Tridecanoic acid	214	C13H26O2	000638-53-9	64
4			n-Decanoic acid	172	C10H20O2	000334-48-5	62
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	49



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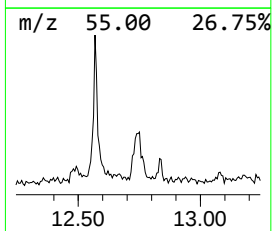
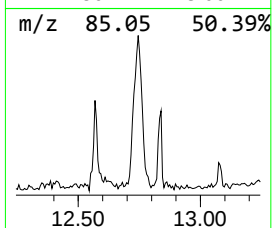
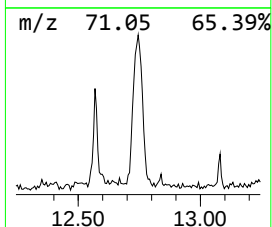
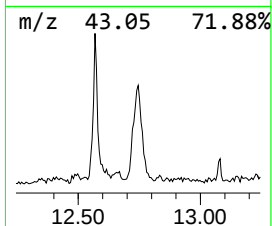
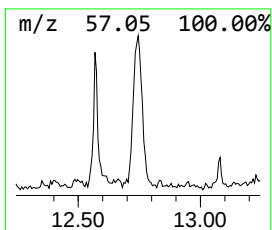
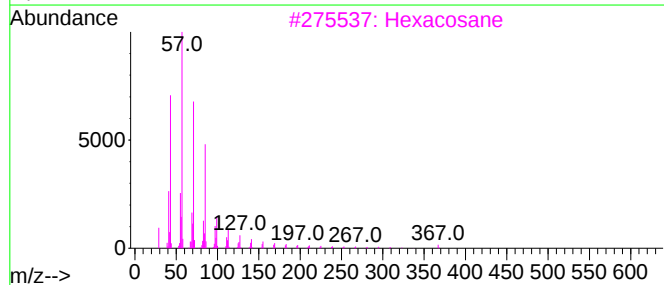
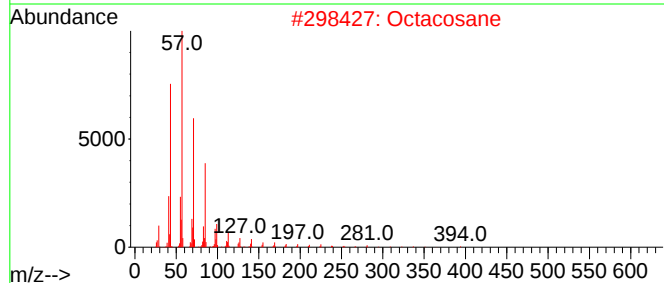
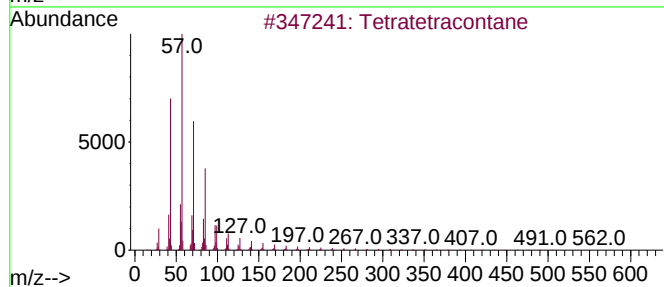
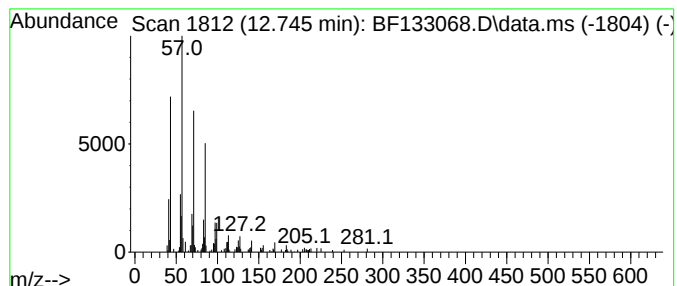
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Peak Number 4 Tetratetracontane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.745	3.54 ng	224960	Chrysene-d12	13.880

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetratetracontane	619	C44H90	007098-22-8	90
2			Octacosane	394	C28H58	000630-02-4	90
3			Hexacosane	366	C26H54	000630-01-3	87
4			Heneicosane	296	C21H44	000629-94-7	87
5			Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	83



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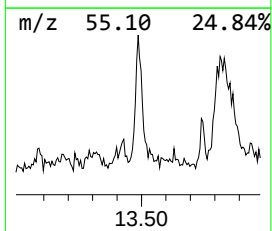
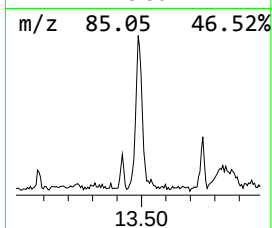
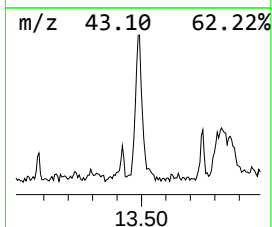
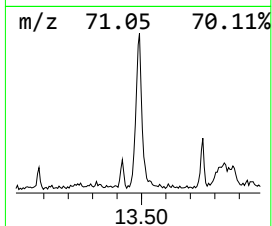
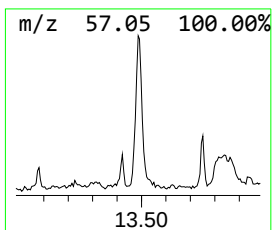
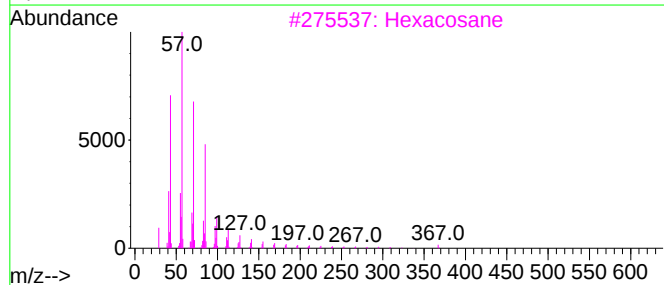
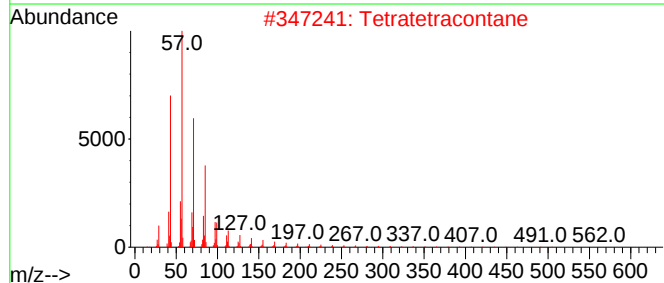
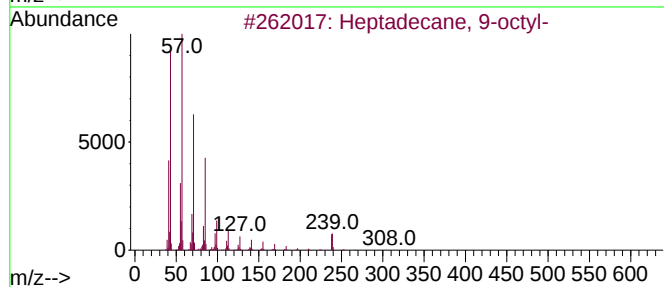
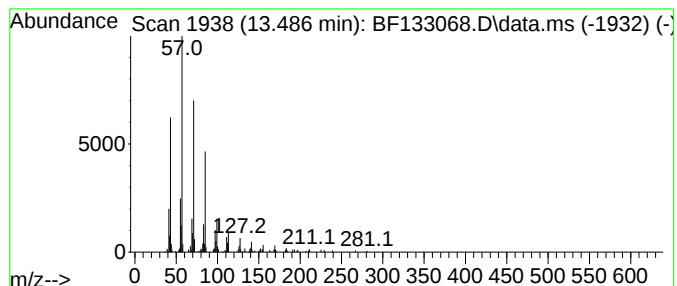
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Heptadecane, 9-octyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.486	3.64 ng	231138	Chrysene-d12	13.880

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
2			Tetratetracontane	619	C44H90	007098-22-8	91
3			Hexacosane	366	C26H54	000630-01-3	91
4			Octacosane	394	C28H58	000630-02-4	91
5			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91



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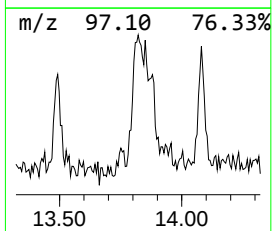
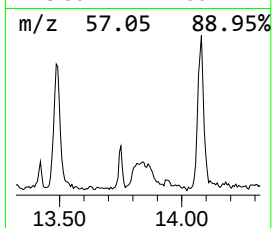
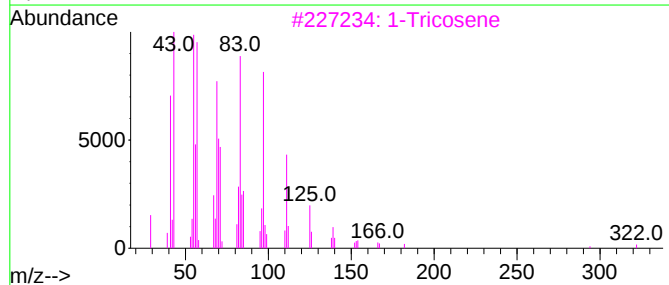
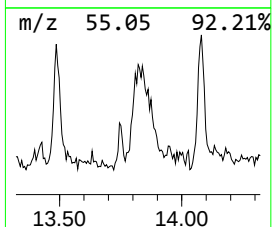
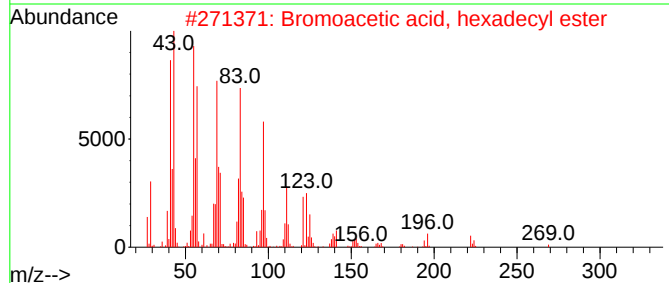
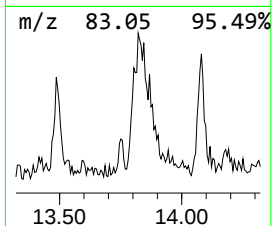
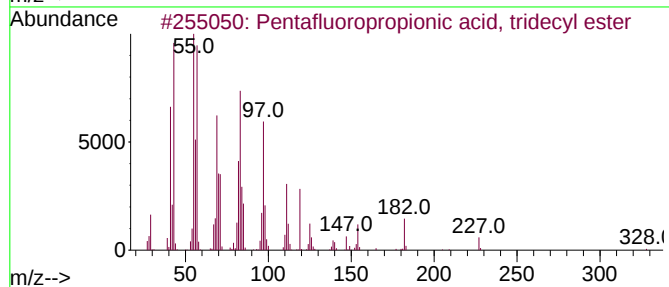
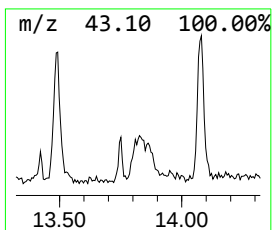
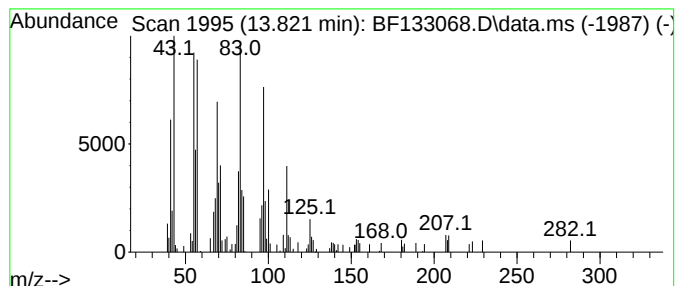
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Pentafluoropropionic acid, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.821	2.99 ng	189641	Chrysene-d12	13.880

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentafluoropropionic acid, tridecyl ester	346	C16H27F5O2	959261-22-4	91
2			Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	87
3			1-Tricosene	322	C23H46	018835-32-0	83
4			Behenic alcohol	326	C22H46O	000661-19-8	81
5			Heptacosyl acetate	438	C29H58O2	1000351-78-2	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042623\
Data File : BF133068.D
Acq On : 26 Apr 2023 16:59
Operator : CG\JU
Sample : 02448-06
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20230340-COMP-18

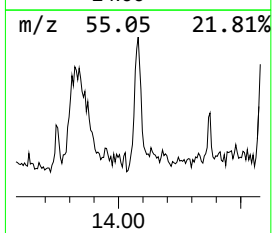
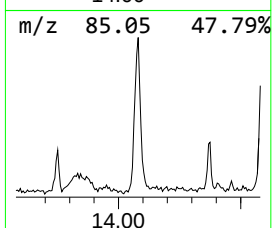
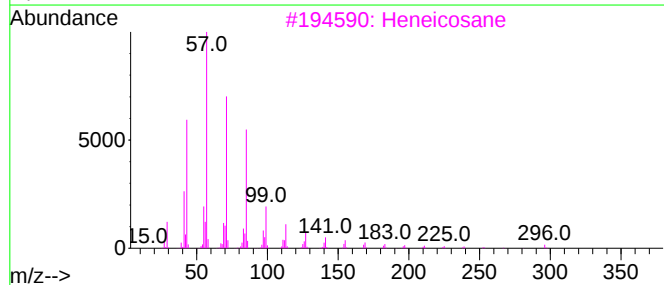
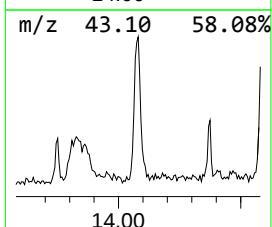
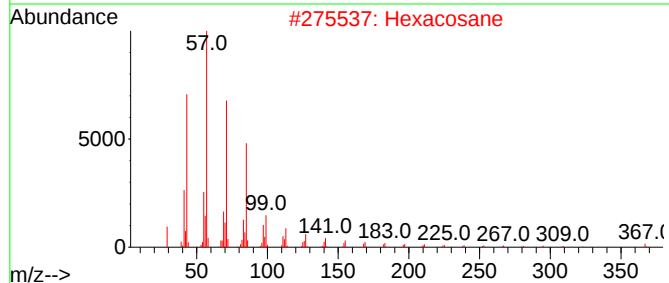
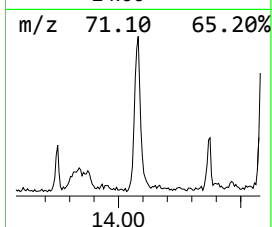
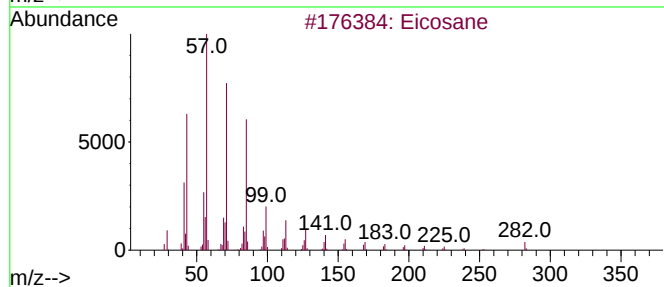
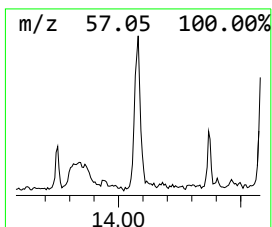
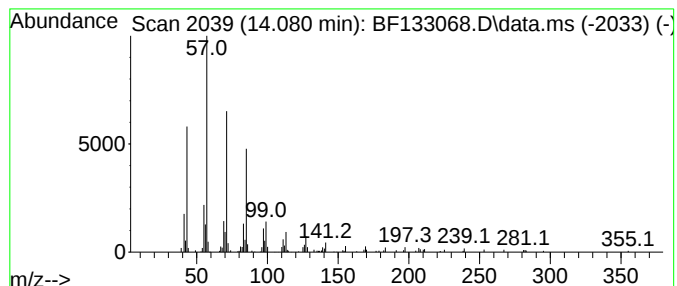
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Eicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.080	3.84 ng	243971	Chrysene-d12	13.880

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane			282	C20H42	000112-95-8	95
2	Hexacosane			366	C26H54	000630-01-3	94
3	Heneicosane			296	C21H44	000629-94-7	91
4	Octacosane			394	C28H58	000630-02-4	91
5	Hexatriacontane			507	C36H74	000630-06-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042623\
Data File : BF133068.D
Acq On : 26 Apr 2023 16:59
Operator : CG\JU
Sample : 02448-06
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20230340-COMP-18

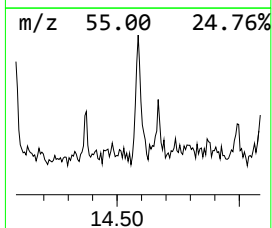
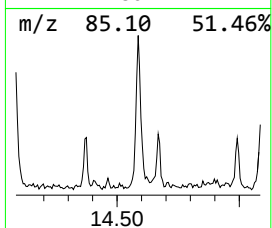
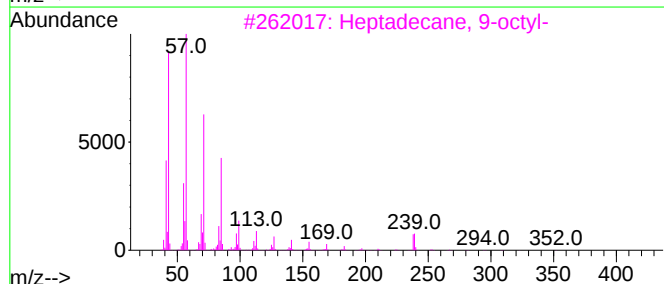
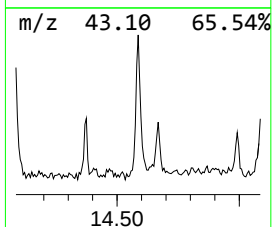
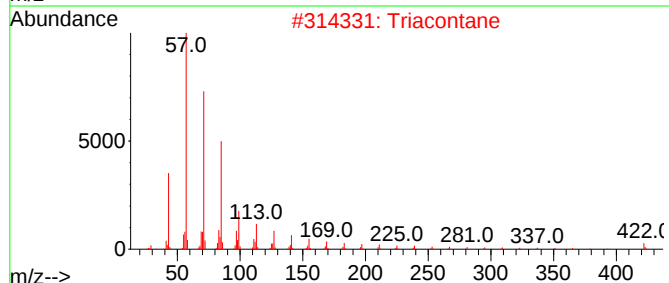
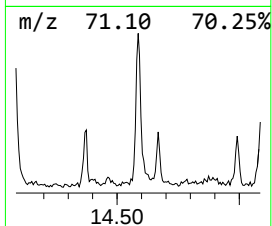
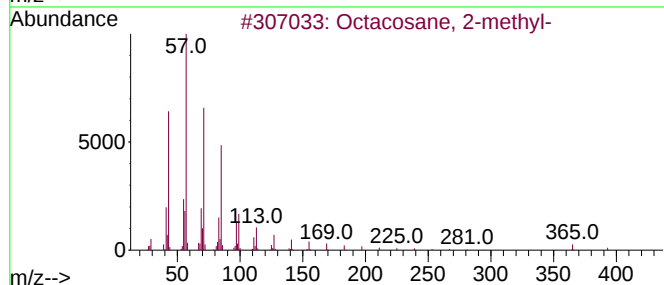
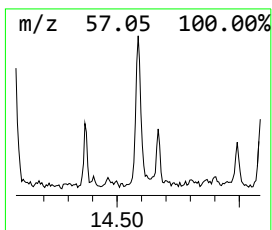
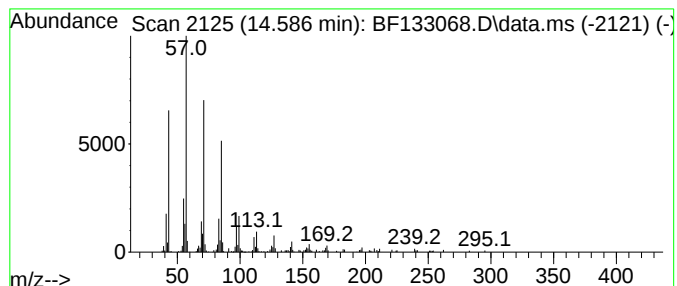
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octacosane, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.586	2.84 ng	180484	Chrysene-d12	13.880

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
2			Triacontane	422	C30H62	000638-68-6	91
3			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91
5			Octacosane	394	C28H58	000630-02-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042623\
Data File : BF133068.D
Acq On : 26 Apr 2023 16:59
Operator : CG\JU
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Misc :
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Instrument :
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ClientSampleId :
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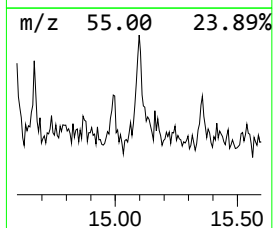
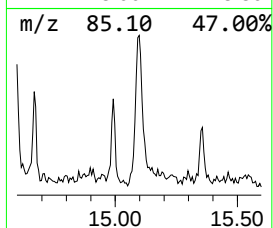
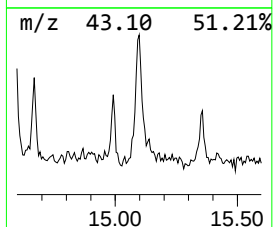
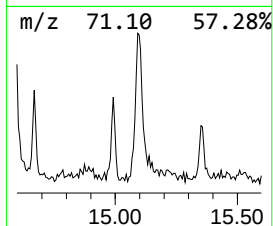
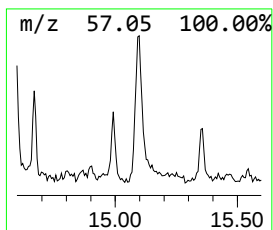
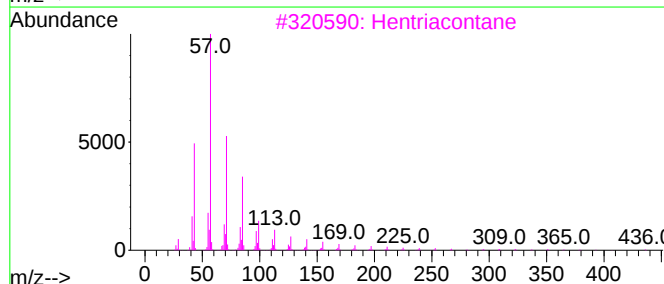
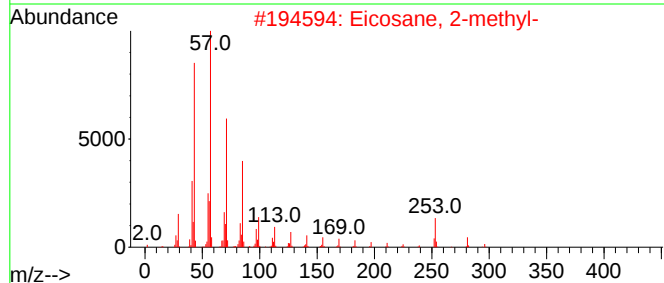
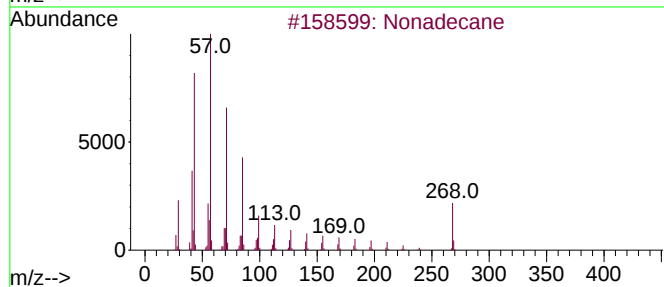
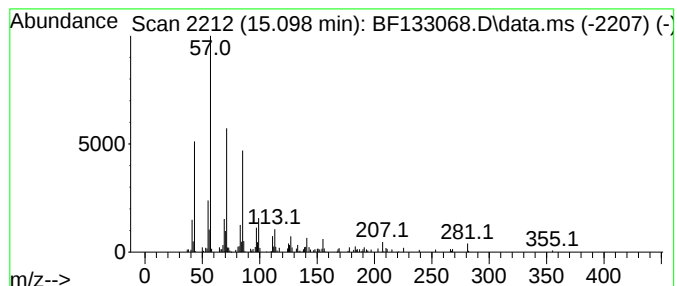
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Nonadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.098	2.44 ng	118256	Perylene-d12	15.298

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Nonadecane	268	C19H40	000629-92-5	91
2		Eicosane, 2-methyl-	296	C21H44	001560-84-5	91
3		Hentriacontane	437	C31H64	000630-04-6	87
4		Hexacosane	366	C26H54	000630-01-3	87
5		Docosane, 11-decyl-	451	C32H66	055401-55-3	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042623\
Data File : BF133068.D
Acq On : 26 Apr 2023 16:59
Operator : CG\JU
Sample : 02448-06
Misc :
ALS Vial : 4 Sample Multiplier: 1

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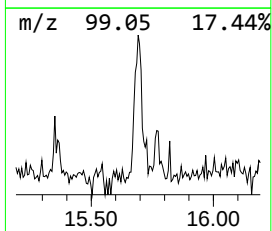
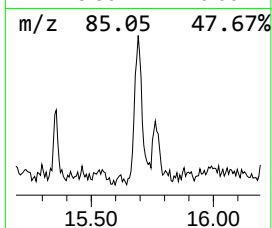
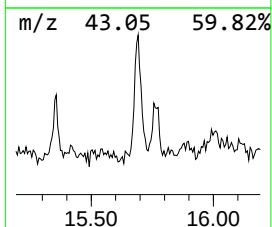
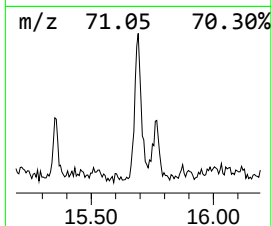
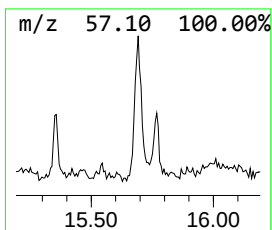
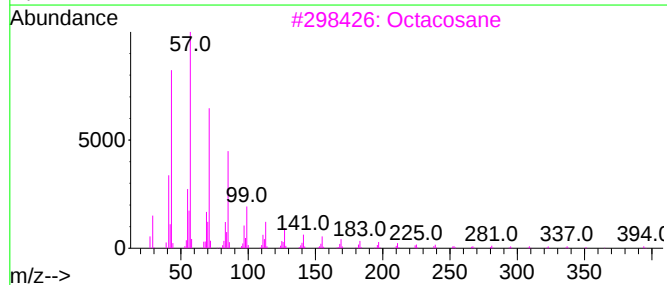
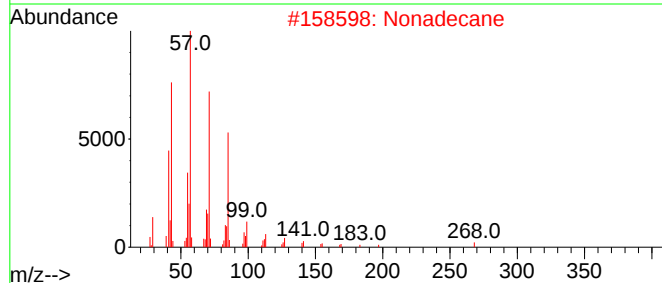
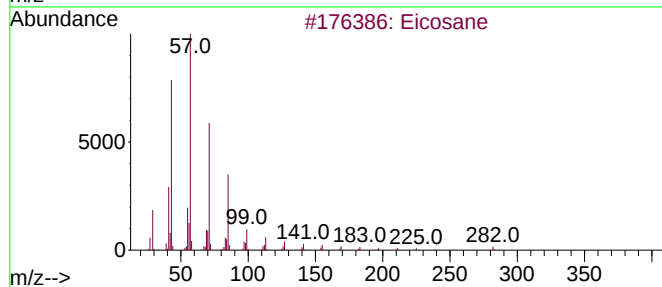
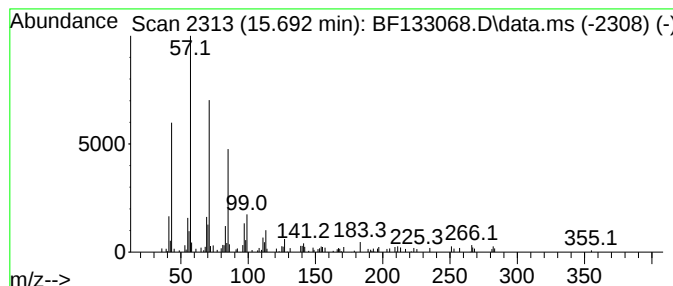
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.692	2.24 ng	108193	Perylene-d12	15.298

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Eicosane	282	C20H42	000112-95-8	93
2		Nonadecane	268	C19H40	000629-92-5	91
3		Octacosane	394	C28H58	000630-02-4	90
4		Hexacosane	366	C26H54	000630-01-3	87
5		Hentriacontane	437	C31H64	000630-04-6	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042623\
Data File : BF133068.D
Acq On : 26 Apr 2023 16:59
Operator : CG\JU
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ALS Vial : 4 Sample Multiplier: 1

Instrument :
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ClientSampleId :
20230340-COMP-18

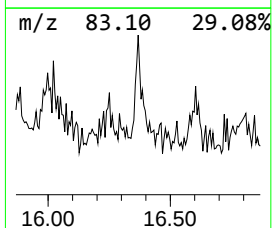
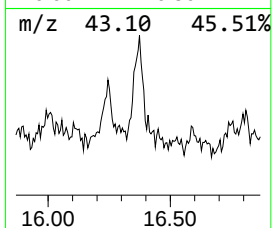
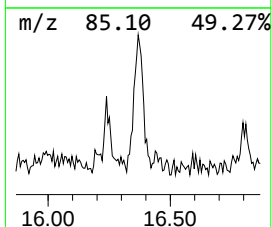
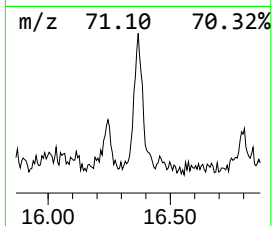
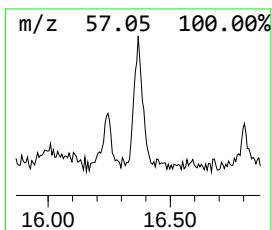
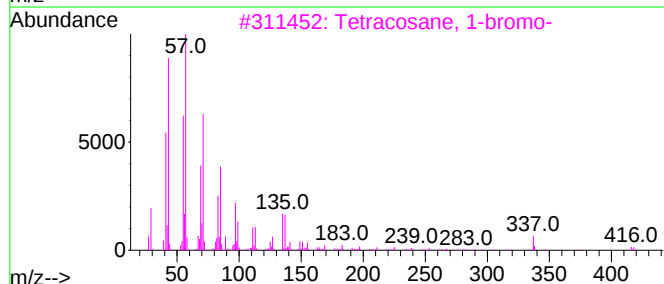
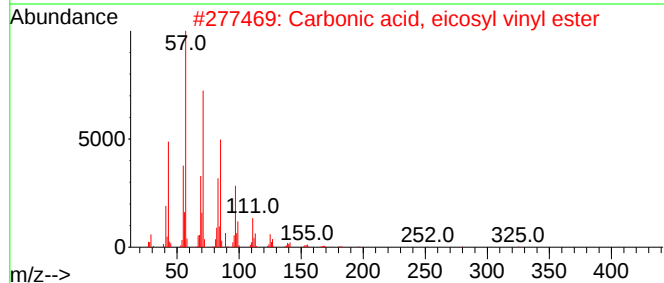
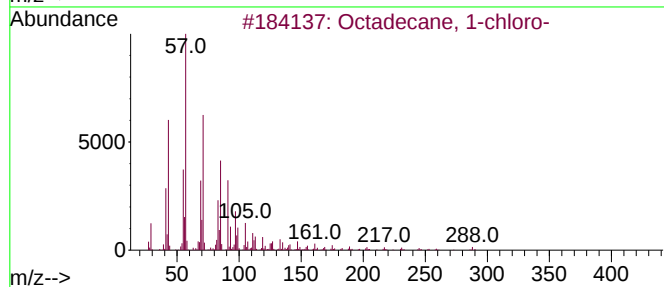
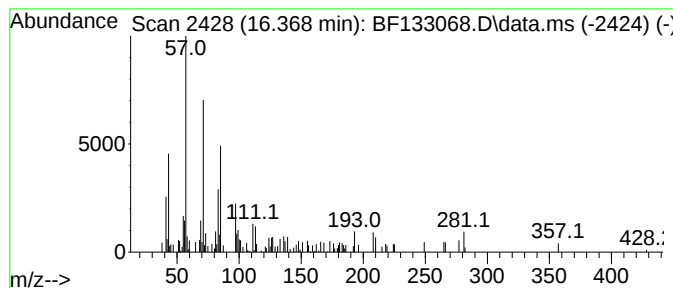
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Octadecane, 1-chloro- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.368	2.50 ng	120764	Perylene-d12	15.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	58
2			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	58
3			Tetracosane, 1-bromo-	416	C24H49Br	006946-24-3	53
4			Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	53
5			Dodecyl nonyl ether	312	C21H44O	1000406-37-5	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042623\
Data File : BF133068.D
Acq On : 26 Apr 2023 16:59
Operator : CG\JU
Sample : 02448-06
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
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
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n-Hexadecanoic ...	11.786	5.9	ng	488182	4	11.251	1648160	20.0
Octadecanoic acid	12.569	4.1	ng	259815	5	13.880	1270620	20.0
Tetratetracontane	12.745	3.5	ng	224960	5	13.880	1270620	20.0
Heptadecane, 9-...	13.486	3.6	ng	231138	5	13.880	1270620	20.0
Pentafluoroprop...	13.821	3.0	ng	189641	5	13.880	1270620	20.0
Eicosane	14.080	3.8	ng	243971	5	13.880	1270620	20.0
Octacosane, 2-m...	14.586	2.8	ng	180484	5	13.880	1270620	20.0
Nonadecane	15.098	2.4	ng	118256	6	15.298	967640	20.0
Octacosane	15.692	2.2	ng	108193	6	15.298	967640	20.0
Octadecane, 1-c...	16.368	2.5	ng	120764	6	15.298	967640	20.0