

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080423\
 Data File : BF134623.D
 Acq On : 04 Aug 2023 10:08
 Operator : CG\JU
 Sample : 03686-16
 Misc :
 ALS Vial : 4 Sample Multiplier: 2

Instrument :
 BNA_F
 ClientSampleId :
 SB-28-0-2-20230721

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-BF080123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134623.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.428	563	568	571	rVB	3361949	3293090	81.16%	8.025%
2	6.428	733	738	741	rVB	3442742	3427875	84.48%	8.353%
3	6.628	768	772	778	rBV	183819	176448	4.35%	0.430%
4	6.798	797	801	804	rBV	2607411	2097352	51.69%	5.111%
5	7.357	887	896	899	rBV	2491009	2212123	54.52%	5.390%
6	8.075	1013	1018	1021	rBV	3217622	2832303	69.80%	6.902%
7	8.786	1135	1139	1142	rVB	64504	47279	1.17%	0.115%
8	8.886	1152	1156	1159	rBV	49198	42717	1.05%	0.104%
9	9.151	1196	1201	1204	rBV	4393610	4057608	100.00%	9.888%
10	9.275	1218	1222	1225	rVB	1002552	888403	21.89%	2.165%
11	9.422	1242	1247	1252	rVB3	79884	85182	2.10%	0.208%
12	9.833	1311	1317	1320	rBV	3545146	3107485	76.58%	7.572%
13	10.033	1347	1351	1354	rBV	49364	50335	1.24%	0.123%
14	10.239	1382	1386	1389	rBV4	33219	45694	1.13%	0.111%
15	10.616	1446	1450	1454	rBV	2485187	2376440	58.57%	5.791%
16	10.757	1468	1474	1476	rBV2	44789	66769	1.65%	0.163%
17	11.322	1565	1570	1572	rBV	3225167	2943027	72.53%	7.172%
18	11.339	1572	1573	1576	rVV	228207	145017	3.57%	0.353%
19	11.386	1576	1581	1584	rVB3	60329	70912	1.75%	0.173%
20	11.722	1635	1638	1644	rVB	72369	64629	1.59%	0.157%
21	11.822	1651	1655	1656	rBV	54864	51444	1.27%	0.125%
22	11.857	1656	1661	1665	rVV2	926341	1029819	25.38%	2.509%
23	12.027	1688	1690	1698	rVB	40647	48182	1.19%	0.117%
24	12.433	1752	1759	1761	rBV3	141167	181335	4.47%	0.442%
25	12.533	1771	1776	1779	rBV	274176	271295	6.69%	0.661%
26	12.645	1789	1795	1807	rBV	364512	466054	11.49%	1.136%
27	12.757	1808	1814	1818	rVV	206888	239461	5.90%	0.584%
28	12.916	1836	1841	1844	rBV	3634441	3307222	81.51%	8.059%
29	13.157	1879	1882	1885	rVB	77770	68380	1.69%	0.167%
30	13.386	1916	1921	1930	rBV	21210	50549	1.25%	0.123%
31	13.498	1938	1940	1943	rVB	76631	60809	1.50%	0.148%
32	13.821	1990	1995	2003	rBV3	255672	336646	8.30%	0.820%
33	13.963	2014	2019	2022	rBV	1989780	2068391	50.98%	5.040%
34	13.986	2022	2023	2029	rVB	110620	90794	2.24%	0.221%
35	14.145	2047	2050	2054	rBV2	91787	83497	2.06%	0.203%
36	14.457	2099	2103	2114	rBV2	146450	231747	5.71%	0.565%

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37	14.621	2127	2131	2135	rBV	353904	341856	8.43%	0.833%
38	14.763	2152	2155	2160	rVB2	127507	140317	3.46%	0.342%
39	14.910	2177	2180	2183	rVB2	73575	68292	1.68%	0.166%
40	14.998	2191	2195	2199	rBV	99682	158108	3.90%	0.385%
41	15.110	2210	2214	2216	rBV	189430	219578	5.41%	0.535%
42	15.133	2216	2218	2225	rVB3	81071	110409	2.72%	0.269%
43	15.304	2244	2247	2253	rVB	68745	80494	1.98%	0.196%
44	15.363	2254	2257	2262	rVB	84204	100273	2.47%	0.244%
45	15.439	2264	2270	2274	rVV	1805073	2276509	56.10%	5.547%
46	15.498	2276	2280	2285	rVB	100560	132700	3.27%	0.323%
47	15.704	2312	2315	2321	rVB6	35144	50283	1.24%	0.123%
48	15.945	2351	2356	2361	rBV	272095	406287	10.01%	0.990%
49	15.998	2362	2365	2373	rVB7	41627	66713	1.64%	0.163%
50	16.468	2441	2445	2451	rVB2	64738	108671	2.68%	0.265%
51	17.092	2545	2551	2559	rBV3	60461	160794	3.96%	0.392%

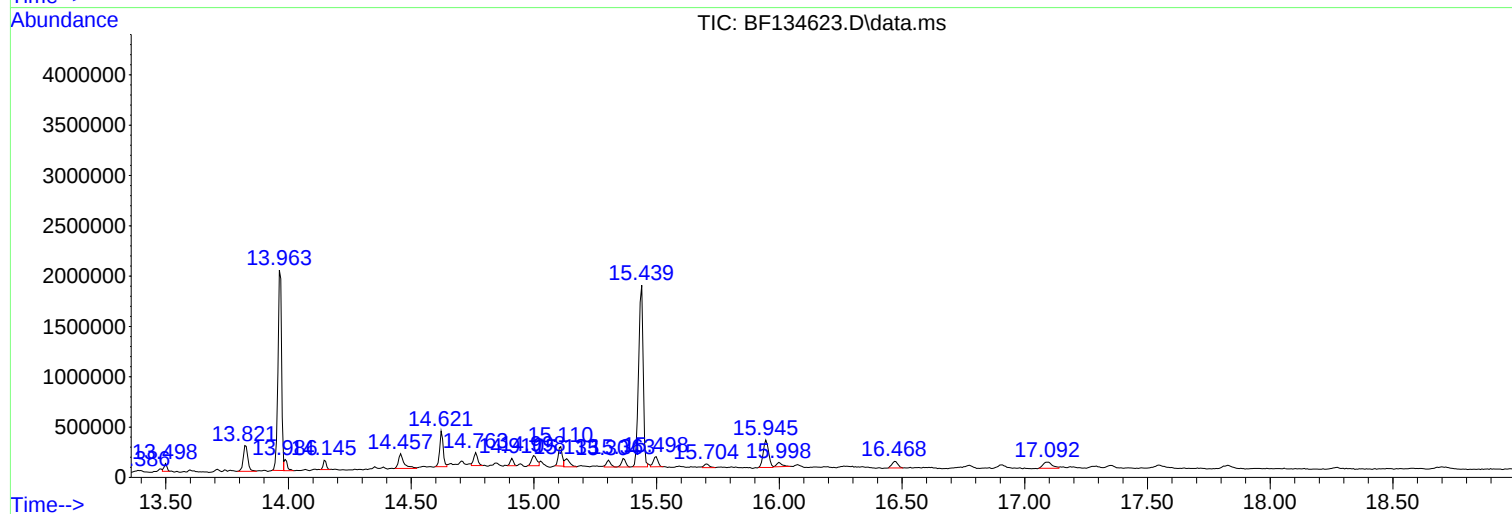
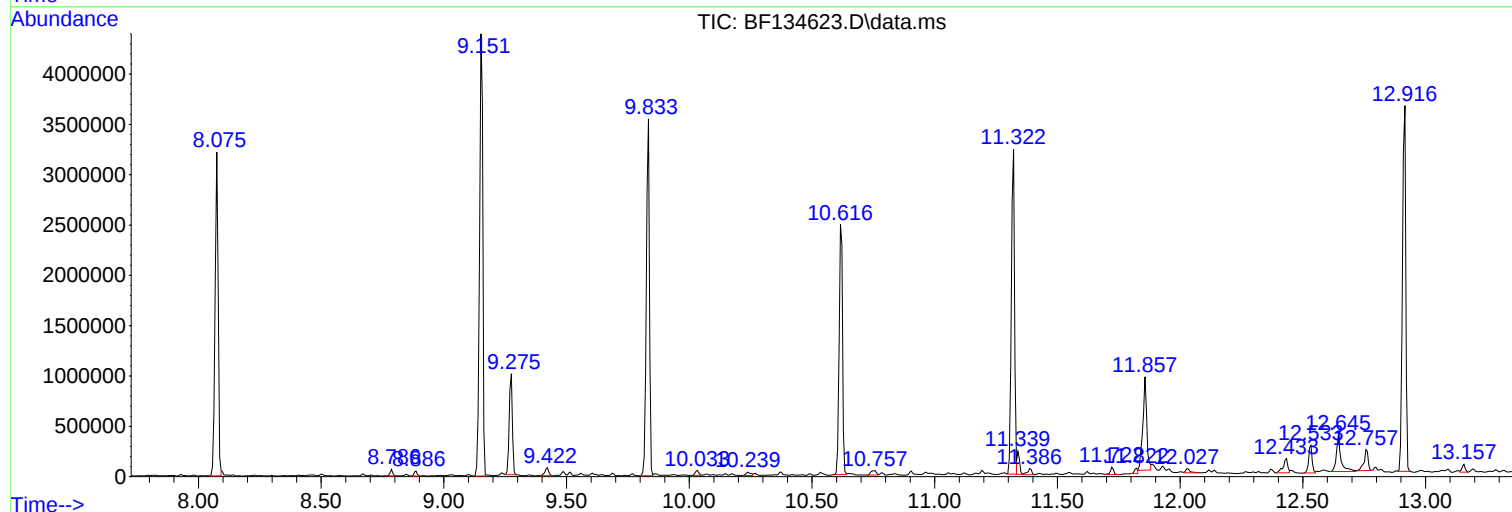
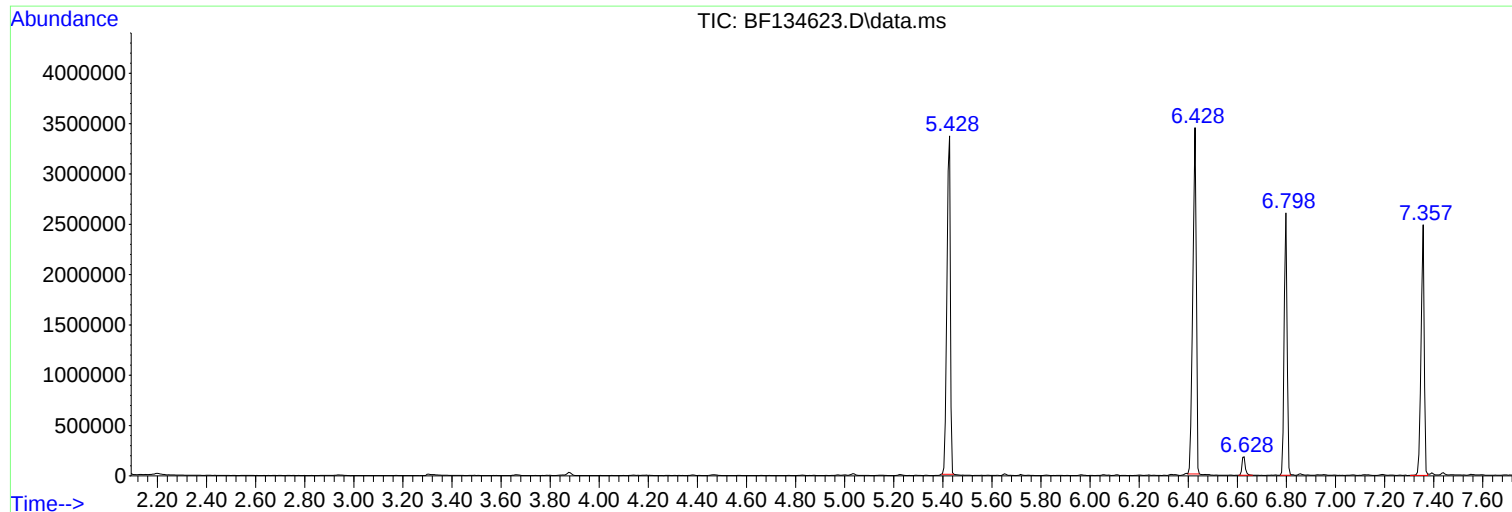
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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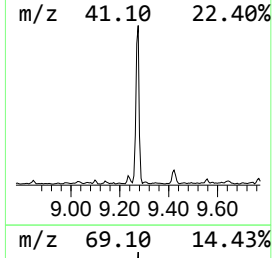
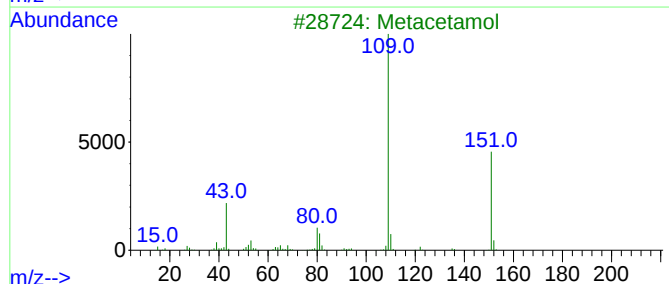
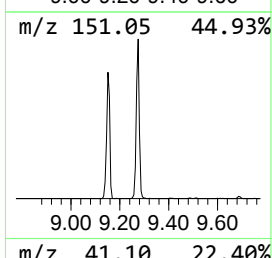
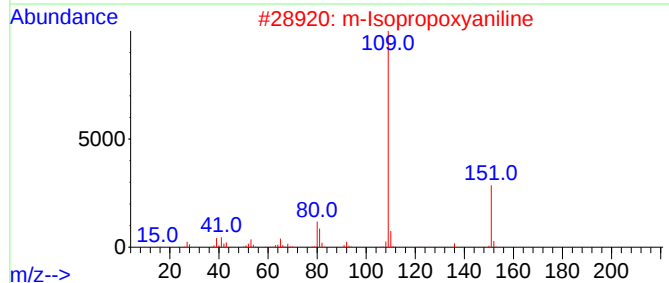
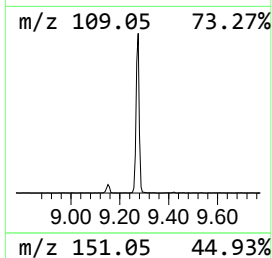
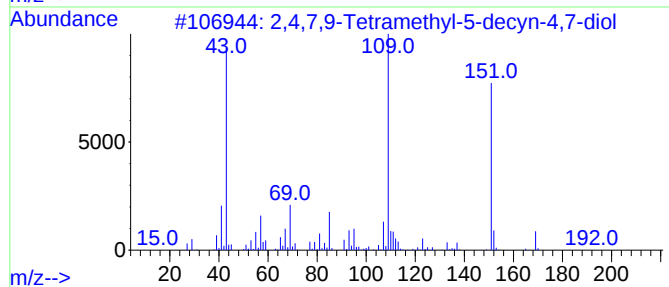
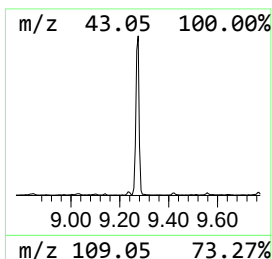
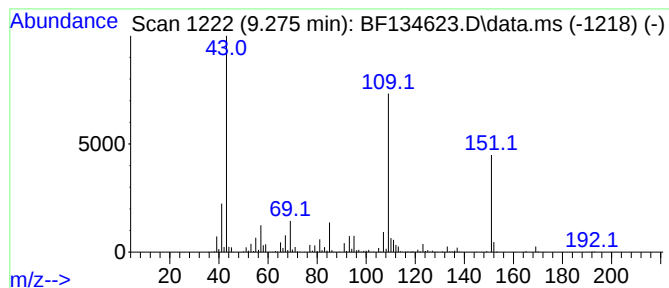
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.275	11.44 ng	888403	Acenaphthene-d10	9.833

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2		000126-86-3	91
2	m-Isopropoxyaniline	151	C9H13NO		041406-00-2	59
3	Metacetamol	151	C8H9NO2		000621-42-1	59
4	Acetaminophen	151	C8H9NO2		000103-90-2	59
5	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO		031396-32-4	59



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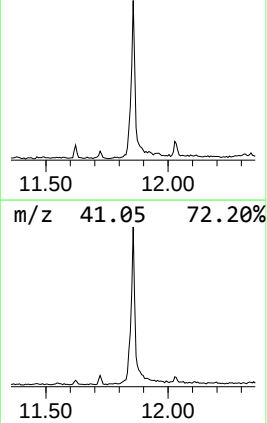
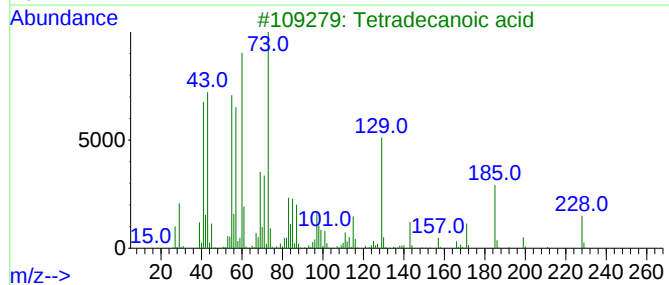
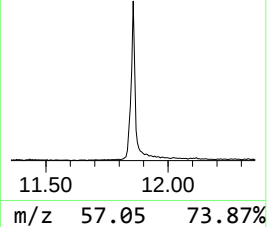
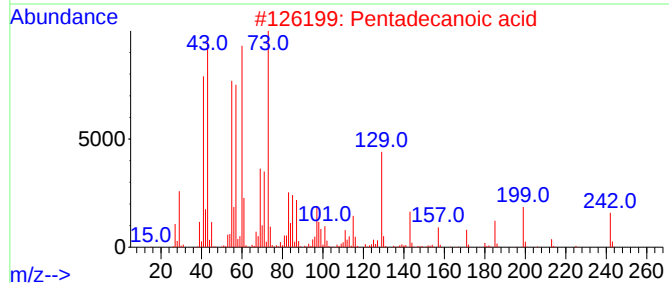
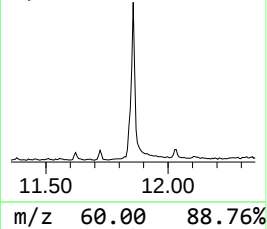
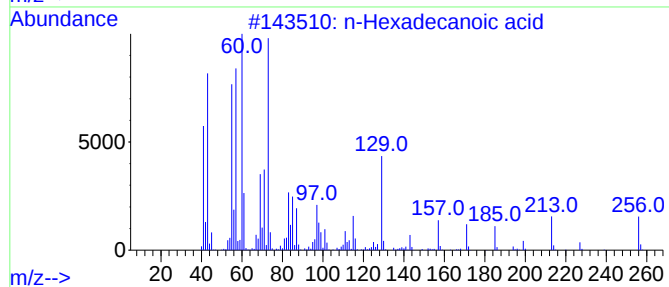
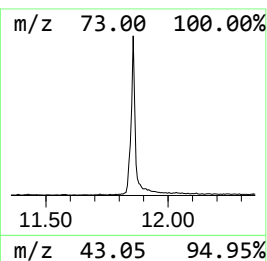
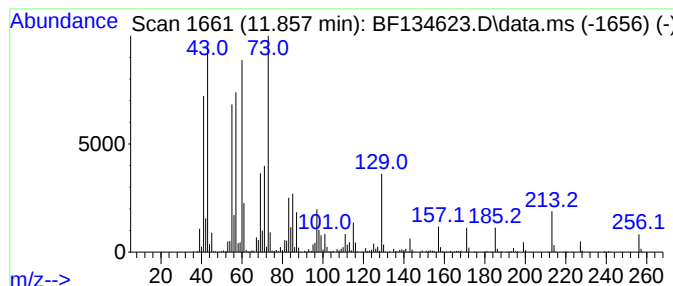
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
11.857	14.00 ng	1029820	Phenanthrene-d10	11.322

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	93
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	91
4		Tridecanoic acid	214	C13H26O2	000638-53-9	76
5		8-Methylnonanoic acid	172	C10H20O2	005963-14-4	49



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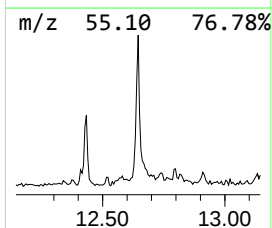
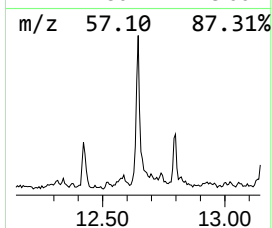
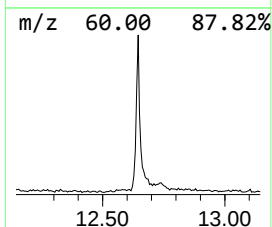
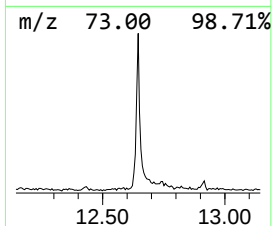
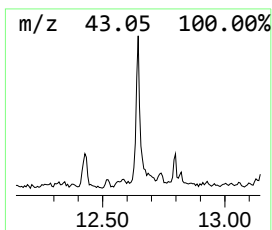
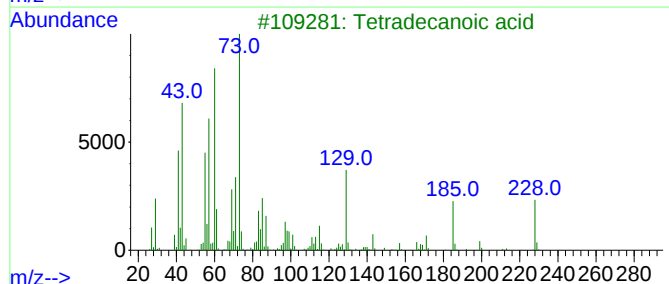
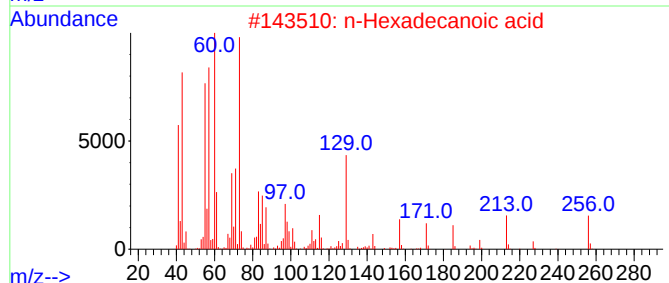
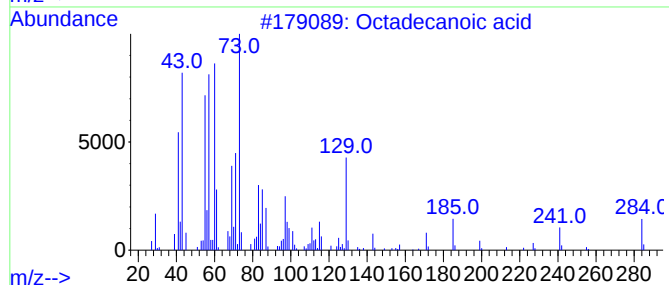
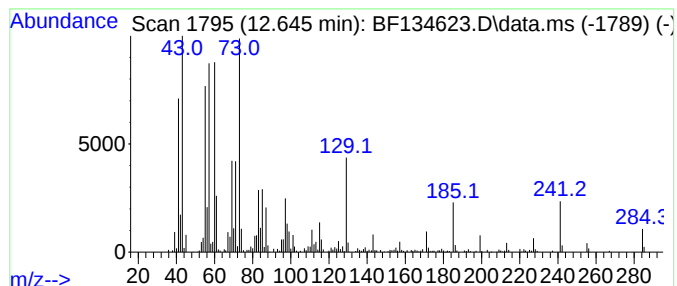
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.645	9.01 ng	466054	Chrysene-d12	13.969

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	94
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4			Tridecanoic acid	214	C13H26O2	000638-53-9	76
5			n-Decanoic acid	172	C10H20O2	000334-48-5	62



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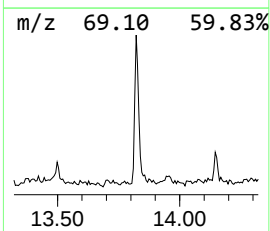
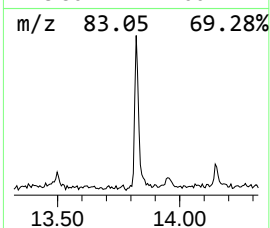
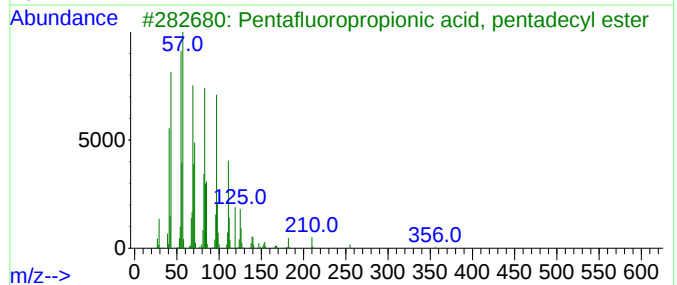
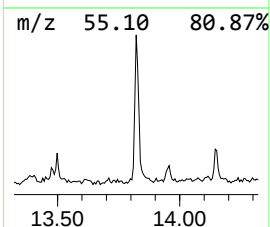
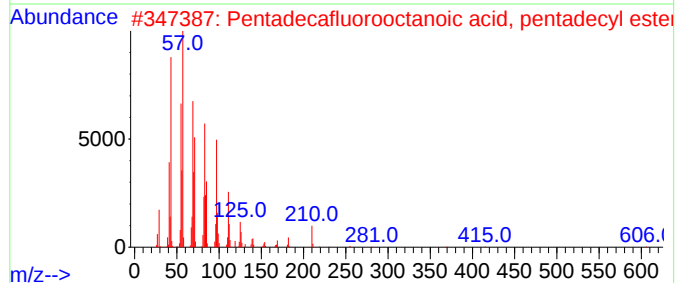
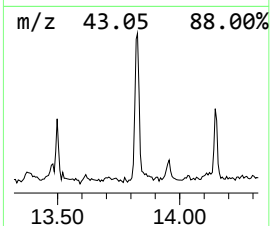
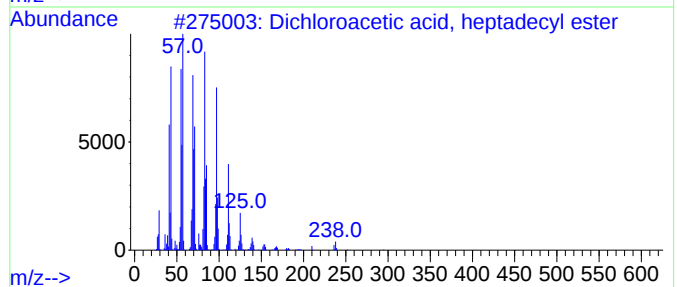
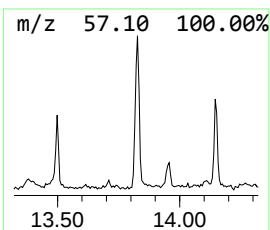
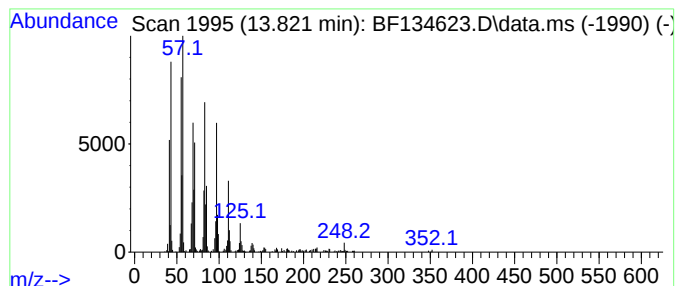
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Dichloroacetic acid, heptad... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.822	6.51 ng	336646	Chrysene-d12	13.969

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
2			Pentadecafluorooctanoic acid, pe...	624	C23H31F15O2	1000406-04-5	94
3			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
4			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	94
5			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94



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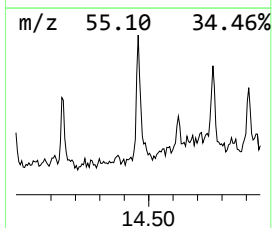
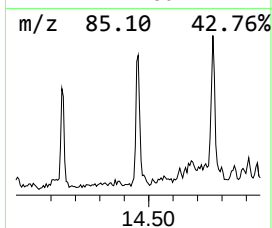
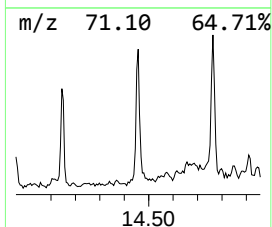
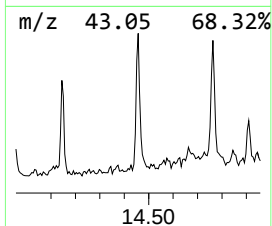
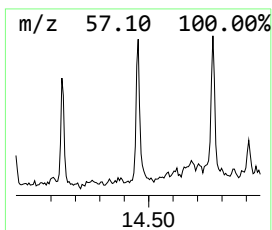
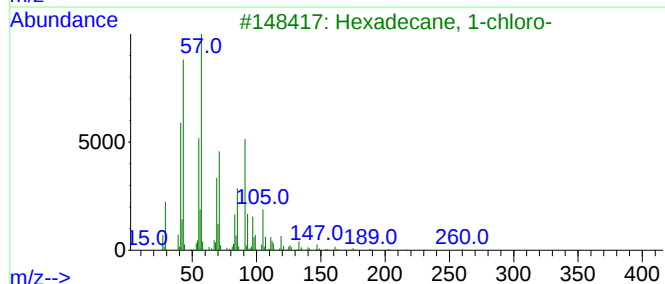
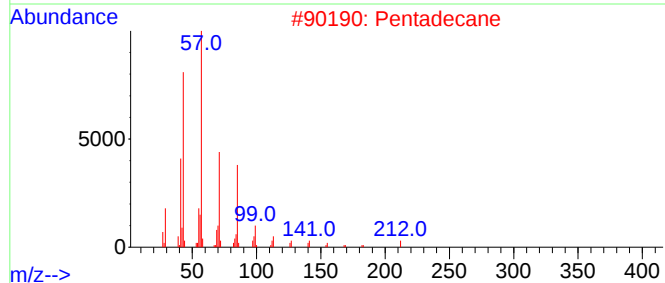
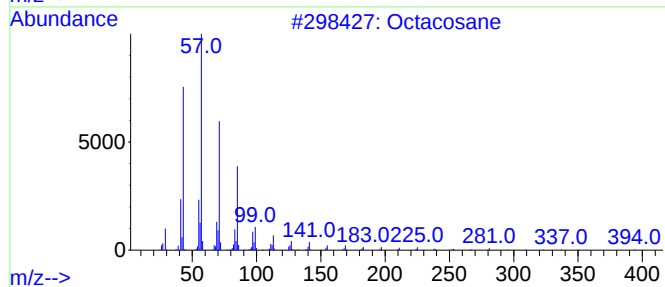
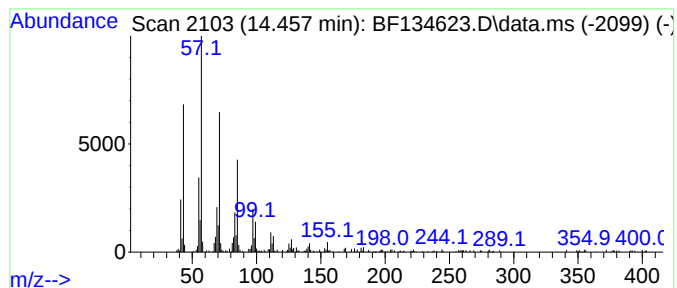
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.457	4.48 ng	231747	Chrysene-d12	13.969

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	96
2			Pentadecane	212	C15H32	000629-62-9	93
3			Hexadecane, 1-chloro-	260	C16H33Cl	004860-03-1	90
4			Heptadecane	240	C17H36	000629-78-7	89
5			Tetratetracontane	619	C44H90	007098-22-8	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080423\
Data File : BF134623.D
Acq On : 04 Aug 2023 10:08
Operator : CG\JU
Sample : 03686-16
Misc :
ALS Vial : 4 Sample Multiplier: 2

Instrument :
BNA_F
ClientSampleId :
SB-28-0-2-20230721

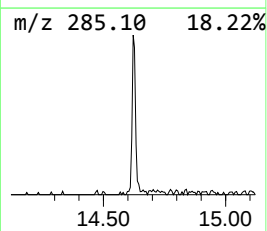
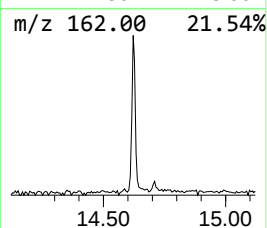
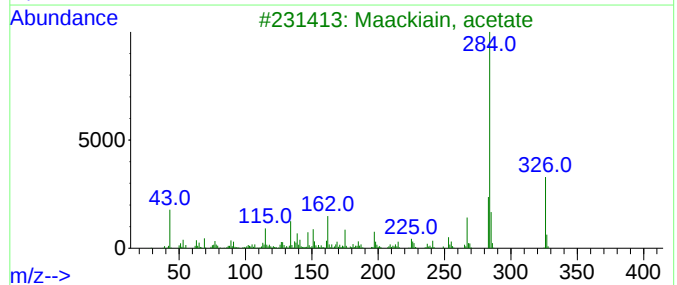
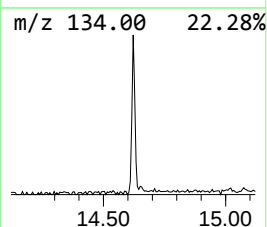
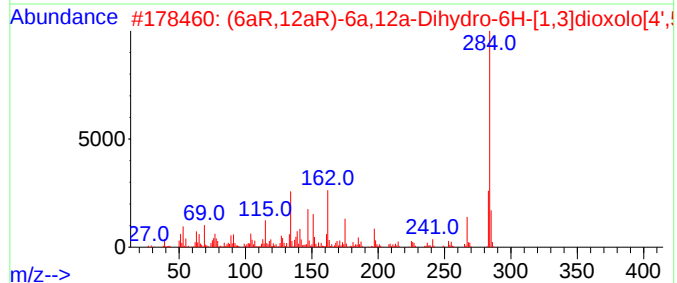
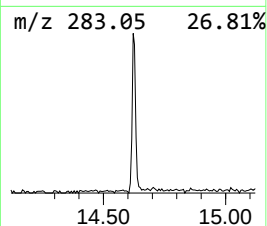
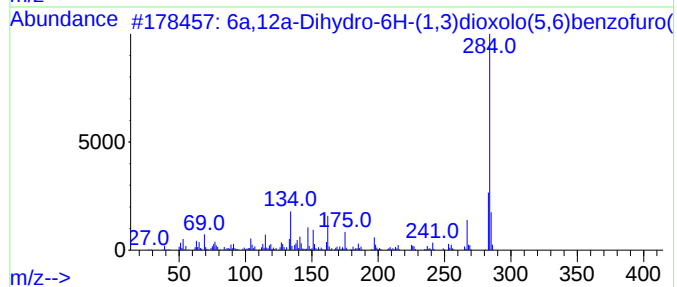
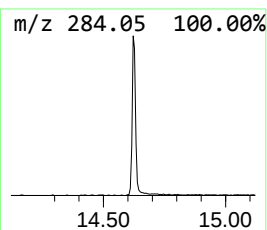
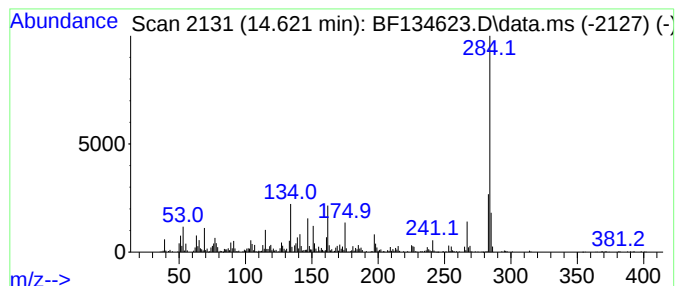
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 6a,12a-Dihydro-6H-(1,3)diox... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.621	6.61 ng	341856	Chrysene-d12	13.969

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			6a,12a-Dihydro-6H-(1,3)dioxolo(5...	284	C16H12O5	076496-57-6	96
2			(6aR,12aR)-6a,12a-Dihydro-6H-[1...	284	C16H12O5	002035-15-6	96
3			Maackiain, acetate	326	C18H14O6	002035-16-7	74
4			4-Amino-5-(4-nitrophenylazo)benz...	284	C12H8N6O3	166766-07-0	50
5			trans-4-Methoxy-4'-(methylthio)c...	284	C17H16O2S	126443-13-8	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080423\
Data File : BF134623.D
Acq On : 04 Aug 2023 10:08
Operator : CG\JU
Sample : 03686-16
Misc :
ALS Vial : 4 Sample Multiplier: 2

Instrument :
BNA_F
ClientSampleId :
SB-28-0-2-20230721

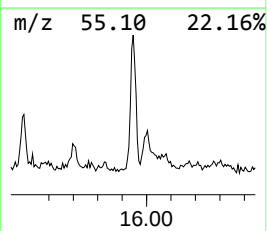
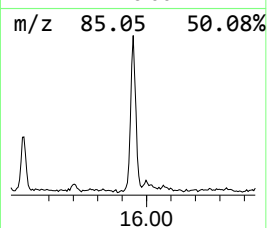
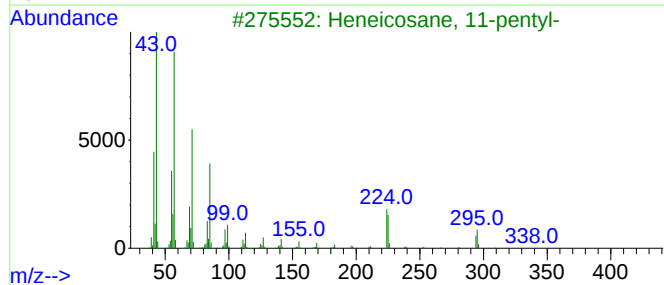
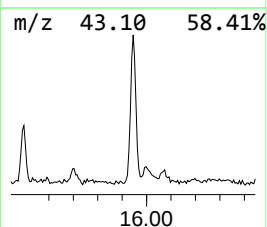
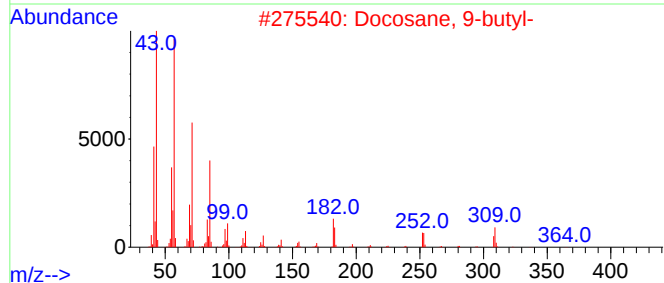
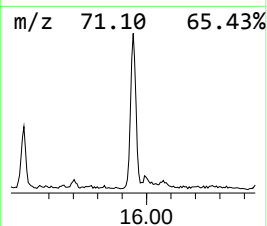
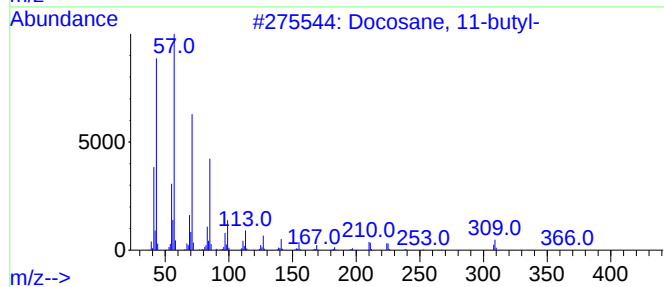
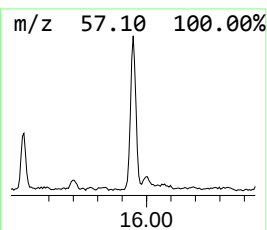
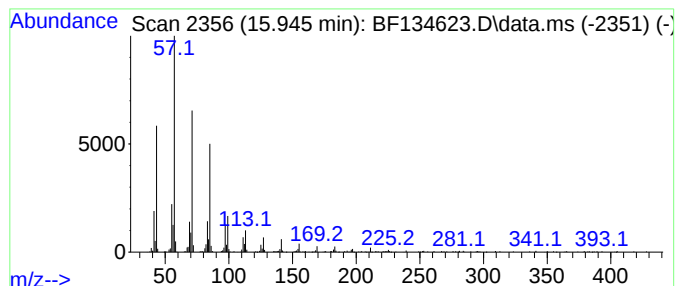
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Docosane, 11-butyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.945	7.14 ng	406287	Perylene-d12	15.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Docosane, 11-butyl-	366	C26H54	013475-76-8	93
2			Docosane, 9-butyl-	366	C26H54	055282-14-9	93
3			Heneicosane, 11-pentyl-	366	C26H54	014739-72-1	93
4			Hexacosane	366	C26H54	000630-01-3	90
5			2-Methylpentacosane	366	C26H54	000629-87-8	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080423\
Data File : BF134623.D
Acq On : 04 Aug 2023 10:08
Operator : CG\JU
Sample : 03686-16
Misc :
ALS Vial : 4 Sample Multiplier: 2

Instrument :
BNA_F
ClientSampleId :
SB-28-0-2-20230721

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.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
2,4,7,9-Tetrame...	9.275	11.4	ng	888403	3	9.833	3107490	20.0
n-Hexadecanoic ...	11.857	14.0	ng	1029820	4	11.322	2943030	20.0
Octadecanoic acid	12.645	9.0	ng	466054	5	13.969	2068390	20.0
Dichloroacetic ...	13.822	6.5	ng	336646	5	13.969	2068390	20.0
Octacosane	14.457	4.5	ng	231747	5	13.969	2068390	20.0
6a,12a-Dihydro-...	14.621	6.6	ng	341856	5	13.969	2068390	20.0
Docosane, 11-bu...	15.945	7.1	ng	406287	6	15.439	2276510	20.0