

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071923\
 Data File : BF134364.D
 Acq On : 19 Jul 2023 18:05
 Operator : CG\JU
 Sample : 03597-15
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RB-49-(0-2)

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-BF062623.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134364.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.134	3	8	14	rVB	385323	486213	27.23%	3.812%
2	5.093	507	511	519	rVB	19674	27132	1.52%	0.213%
3	5.475	572	576	592	rBV	1494899	1554102	87.02%	12.186%
4	6.398	730	733	742	rBV	35114	41708	2.34%	0.327%
5	6.481	742	747	750	rBV	1646343	1538094	86.13%	12.060%
6	6.669	776	779	789	rBV	14188	24500	1.37%	0.192%
7	6.834	804	807	816	rBV	496006	435855	24.41%	3.418%
8	7.404	899	904	914	rBV	1031751	1014982	56.83%	7.959%
9	8.116	1021	1025	1028	rBV	712202	544101	30.47%	4.266%
10	9.192	1204	1208	1211	rBV	2299855	1785881	100.00%	14.003%
11	9.875	1320	1324	1327	rBV	714579	563645	31.56%	4.420%
12	10.669	1455	1459	1472	rBV	1292806	1106502	61.96%	8.676%
13	11.369	1574	1578	1581	rBV	619026	513391	28.75%	4.026%
14	11.898	1665	1668	1675	rBV2	141194	149468	8.37%	1.172%
15	12.592	1782	1786	1789	rBV	61924	59234	3.32%	0.464%
16	12.686	1799	1802	1808	rBV2	27052	33361	1.87%	0.262%
17	12.822	1821	1825	1829	rVB	50931	51623	2.89%	0.405%
18	12.963	1845	1849	1853	rBV	1464771	1382991	77.44%	10.844%
19	13.445	1927	1931	1932	rBV	84460	75046	4.20%	0.588%
20	13.463	1932	1934	1938	rVV	103225	91350	5.12%	0.716%
21	13.522	1941	1944	1949	rBV2	18556	25351	1.42%	0.199%
22	13.898	2004	2008	2022	rVB5	48714	117854	6.60%	0.924%
23	14.033	2024	2031	2034	rBV	426084	449803	25.19%	3.527%
24	14.057	2034	2035	2041	rVB	34436	23216	1.30%	0.182%
25	14.121	2041	2046	2050	rBV	35147	43194	2.42%	0.339%
26	14.492	2106	2109	2113	rBV4	18944	22800	1.28%	0.179%
27	14.551	2115	2119	2127	rBV9	15500	38747	2.17%	0.304%
28	14.798	2157	2161	2167	rVB3	56008	96179	5.39%	0.754%
29	15.098	2207	2212	2215	rBV3	23871	40562	2.27%	0.318%
30	15.163	2219	2223	2227	rVV2	21645	23935	1.34%	0.188%
31	15.474	2273	2276	2281	rVB2	18579	23033	1.29%	0.181%
32	15.539	2281	2287	2294	rBV	242050	342865	19.20%	2.688%
33	16.010	2363	2367	2375	rVB4	16620	26584	1.49%	0.208%

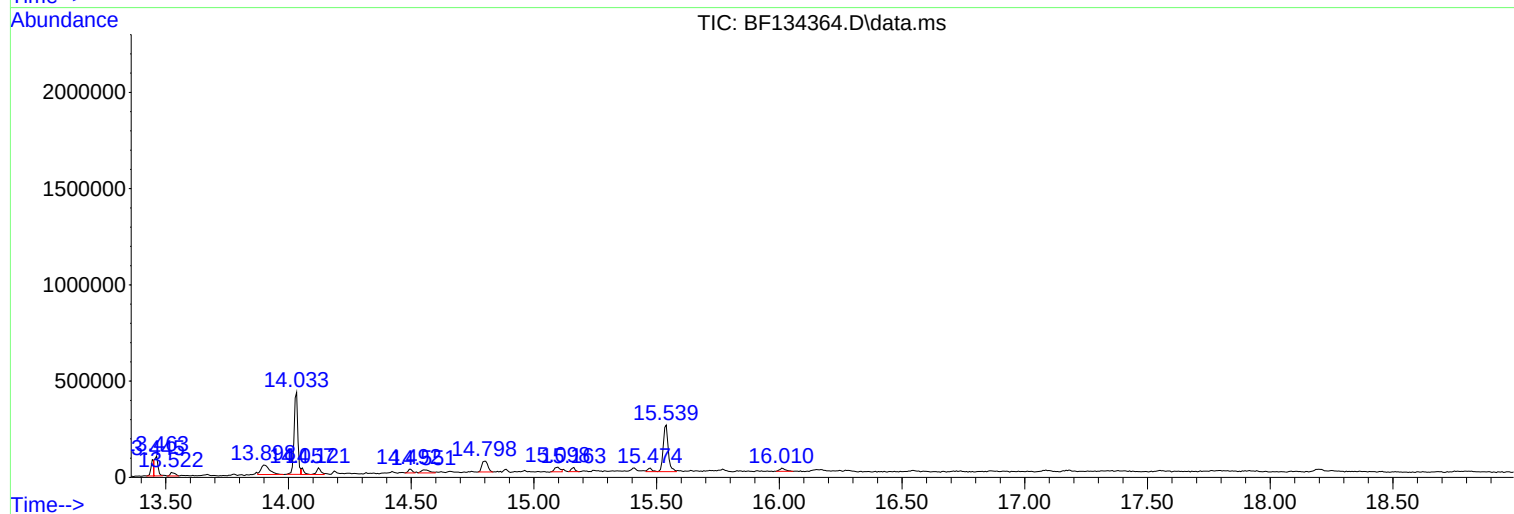
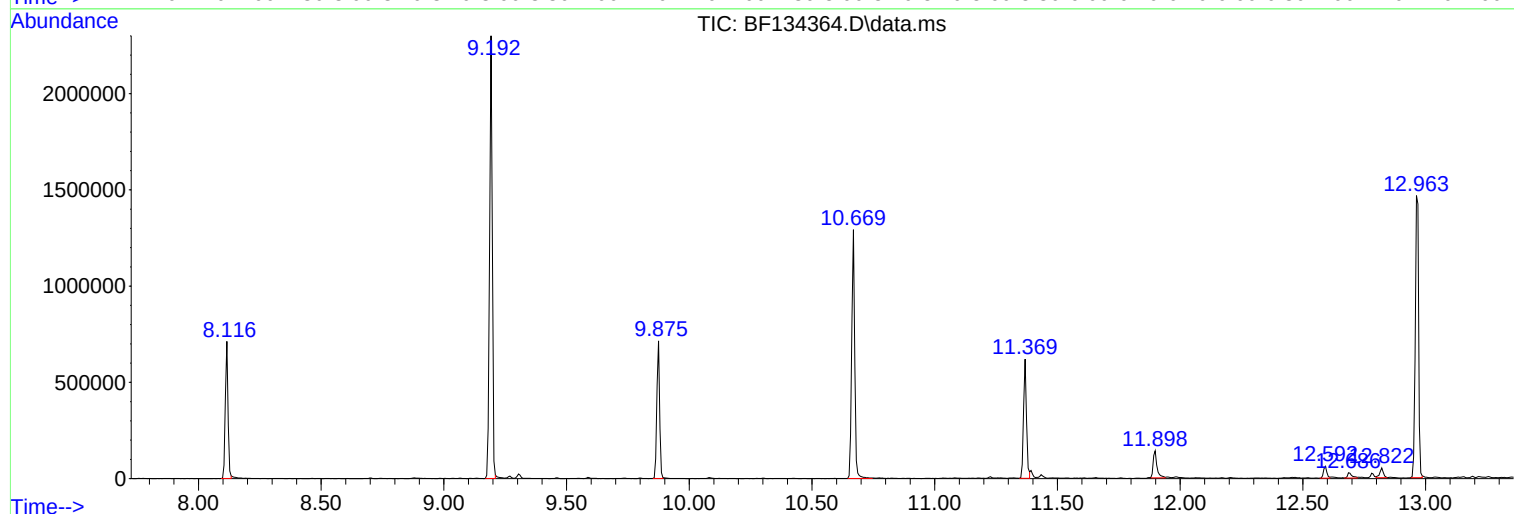
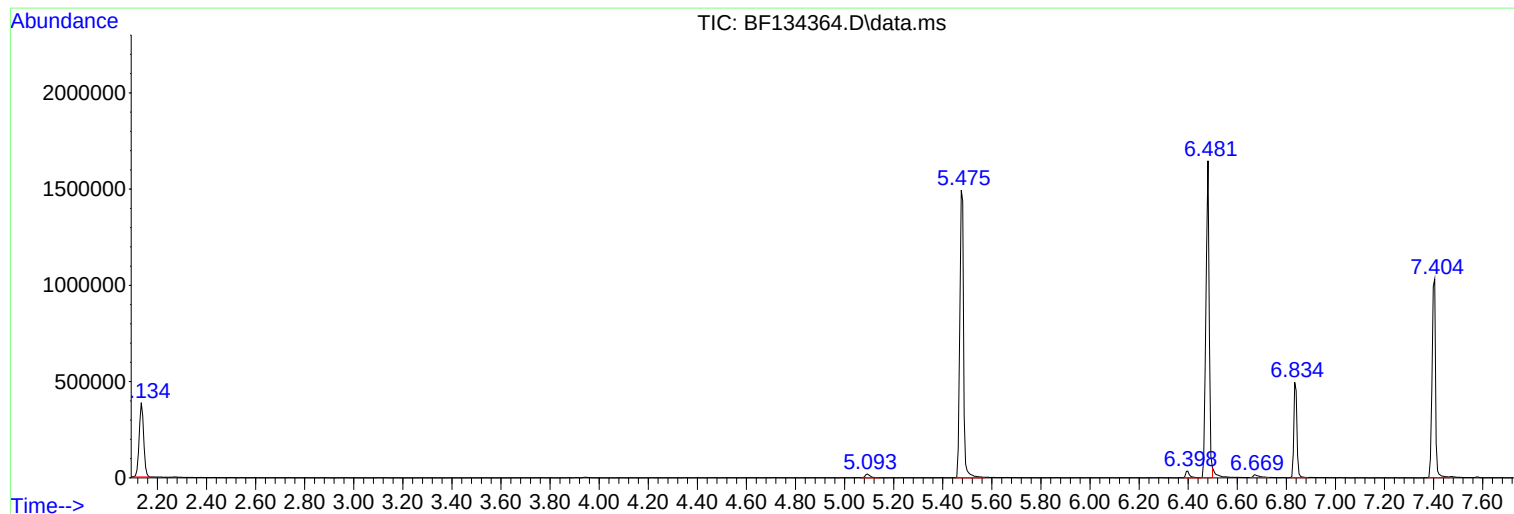
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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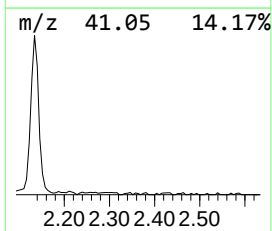
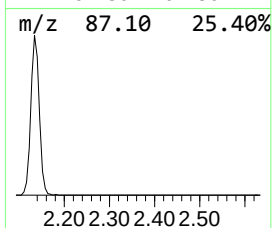
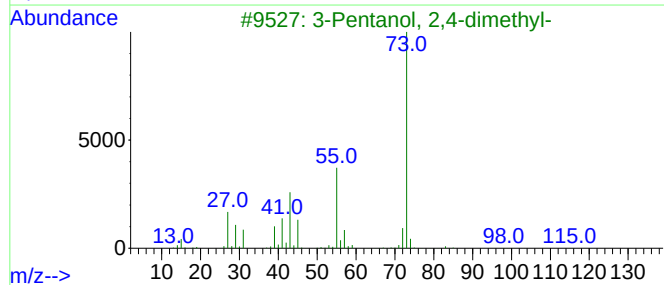
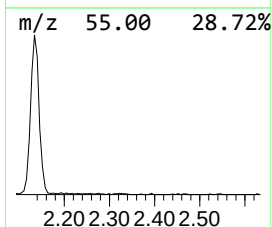
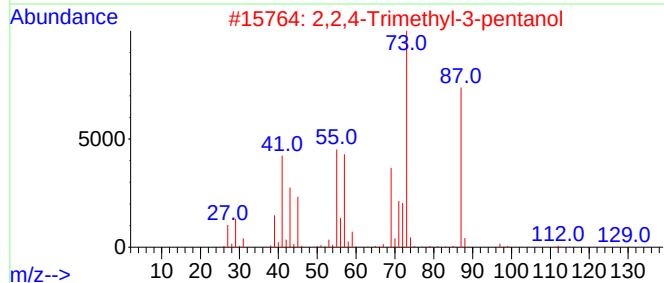
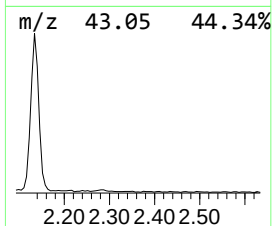
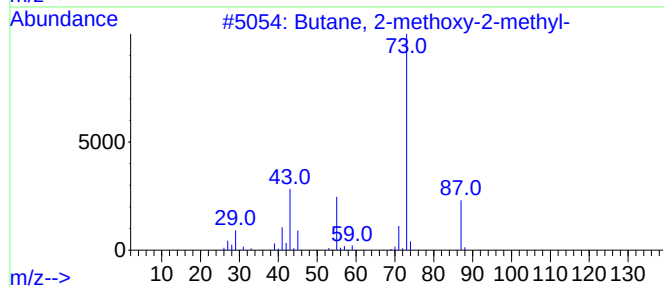
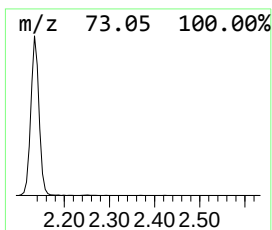
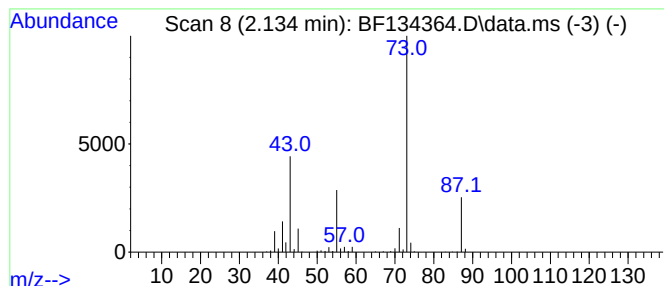
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.134	22.31 ng	486213	1,4-Dichlorobenzene-d4	6.840

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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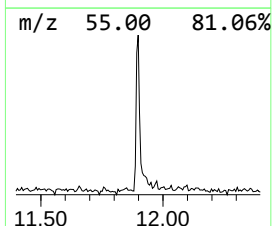
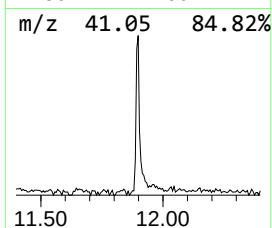
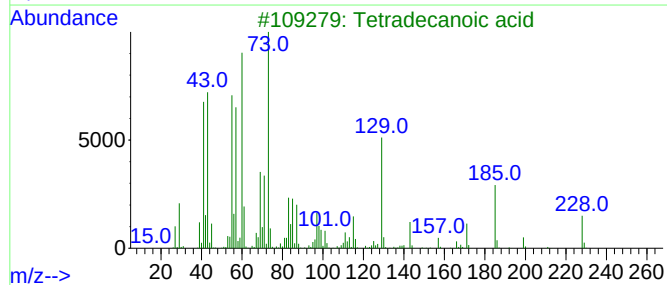
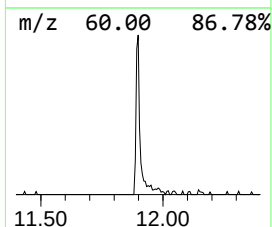
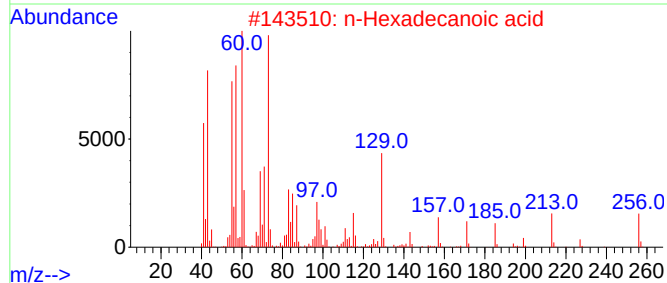
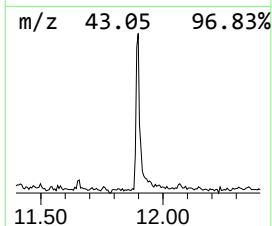
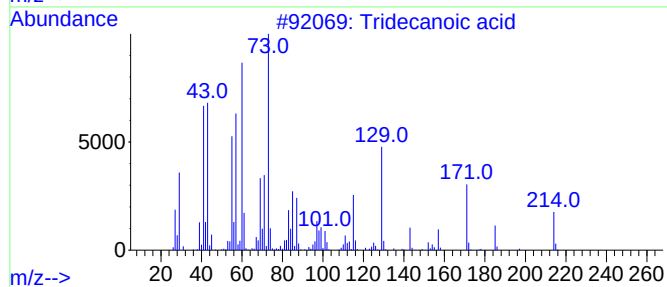
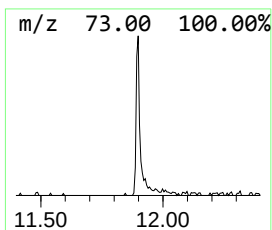
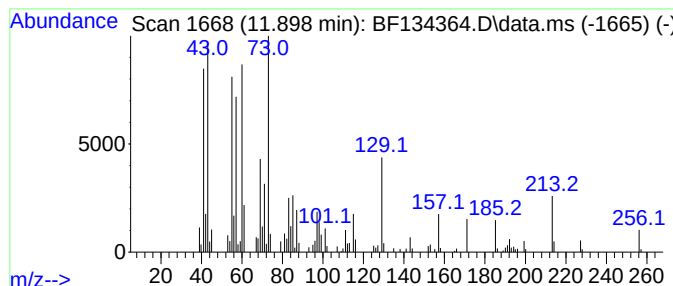
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Tridecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.898	5.82 ng	149468	Phenanthrene-d10	11.369

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	96
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5			Undecanoic acid	186	C11H22O2	000112-37-8	62



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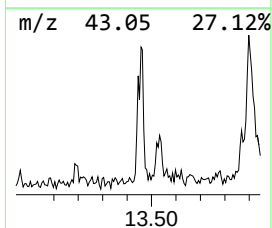
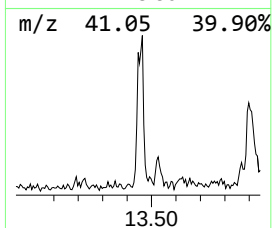
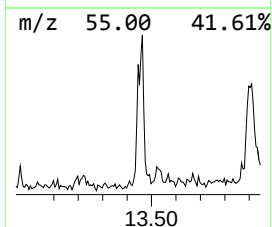
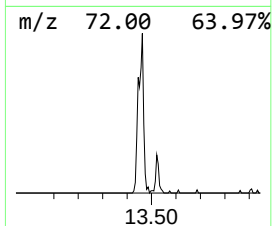
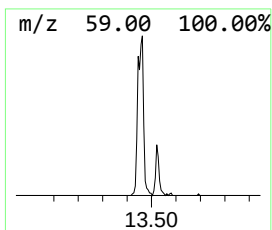
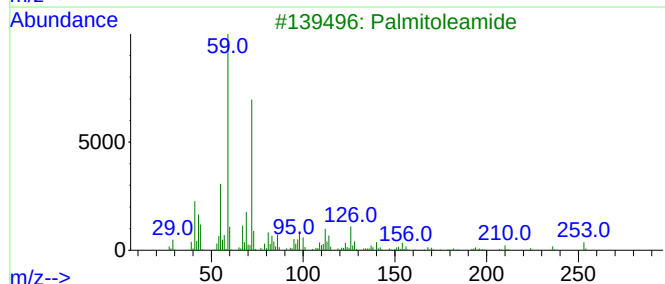
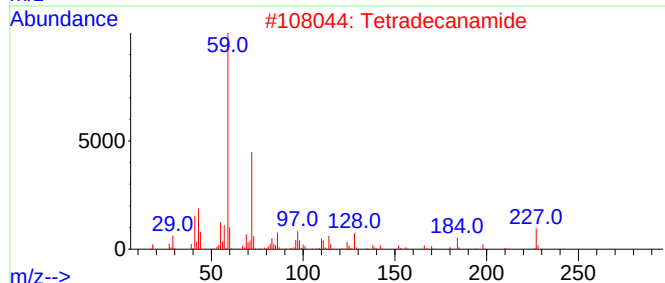
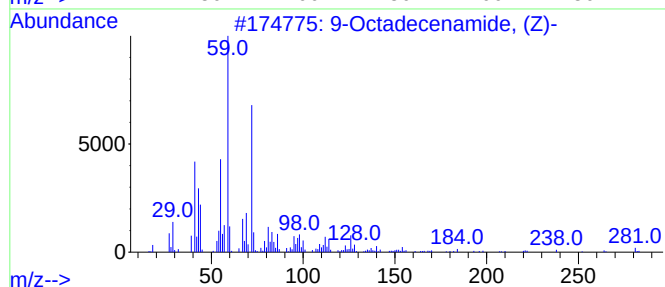
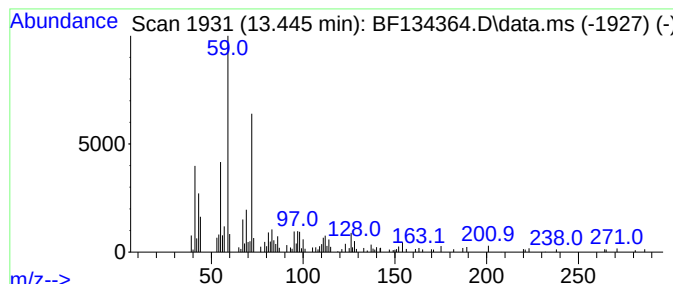
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 9-Octadecenamide, (Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.445	3.34 ng	75046	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	96
2			Tetradecanamide	227	C14H29NO	000638-58-4	53
3			Palmitoleamide	253	C16H31NO	106010-22-4	49
4			Nonanamide	157	C9H19NO	001120-07-6	47
5			2-Methyl-tridecane-2,12-diol	230	C14H30O2	1000187-03-5	47



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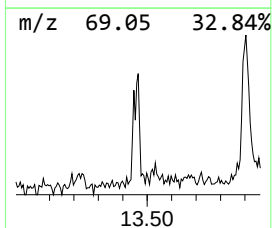
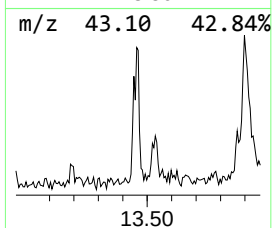
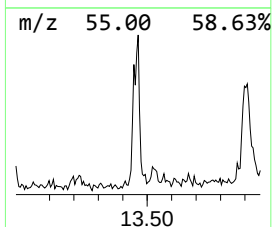
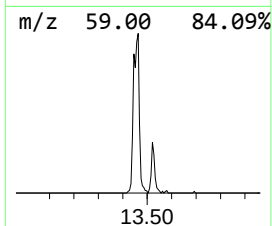
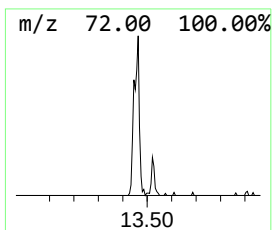
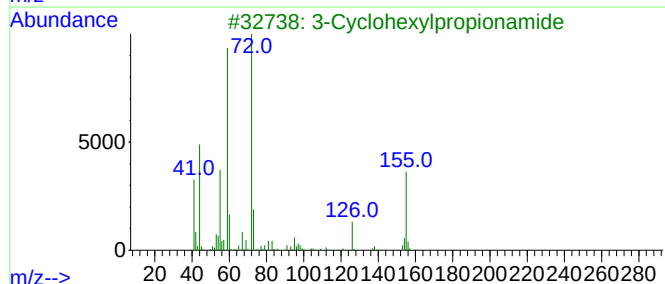
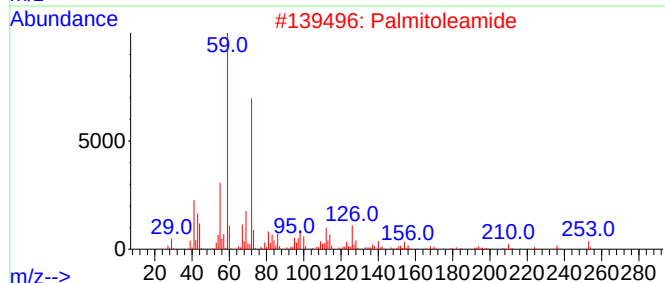
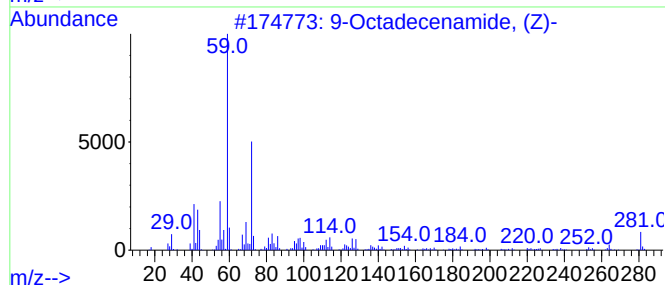
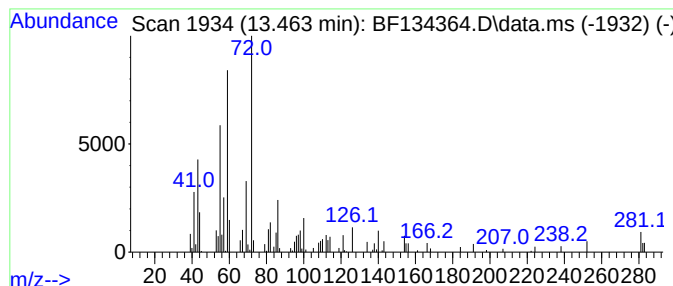
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Peak Number 5 Palmitoleamide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.463	4.06 ng	91350	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-			281	C18H35NO	000301-02-0	64
2	Palmitoleamide			253	C16H31NO	106010-22-4	47
3	3-Cyclohexylpropionamide			155	C9H17NO	004361-29-9	37
4	Octadecanamide			283	C18H37NO	000124-26-5	35
5	Pent-4-enoylamide, 2-methyl-N-pr...			281	C18H35NO	1000438-82-7	35



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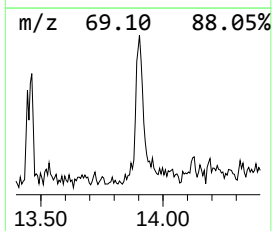
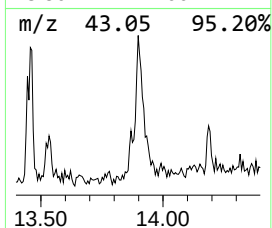
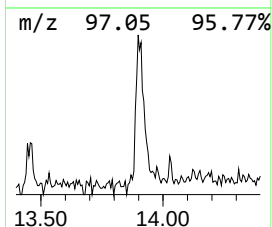
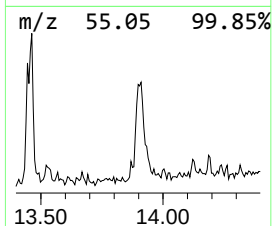
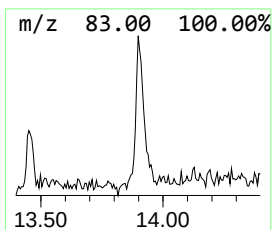
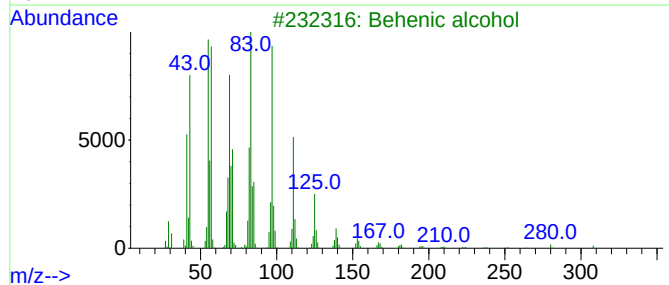
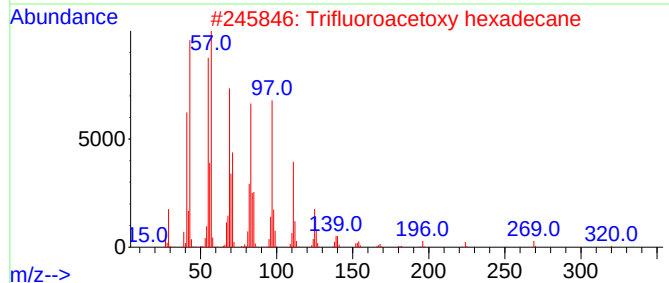
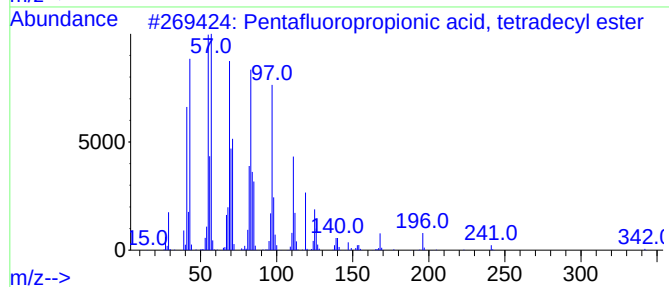
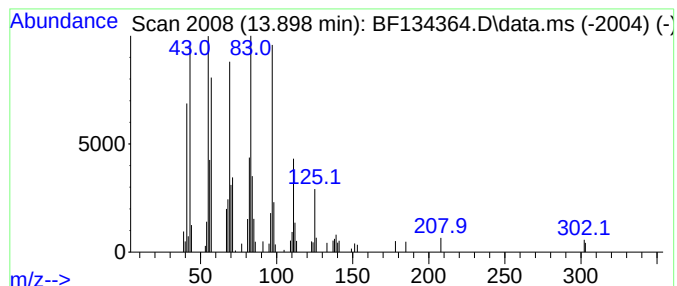
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Peak Number 6 Pentafluoropropionic acid, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	5.24 ng	117854	Chrysene-d12	14.033

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	91
2		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
3		Behenic alcohol	326	C22H46O	000661-19-8	91
4		1-Heneicosanol	312	C21H44O	015594-90-8	91
5		1-Heptacosanol	396	C27H56O	002004-39-9	86



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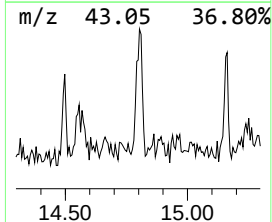
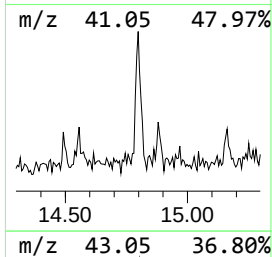
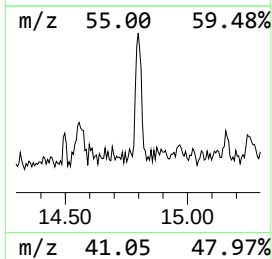
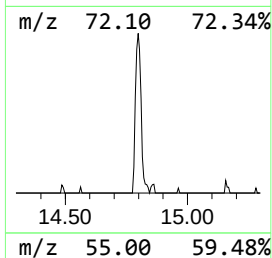
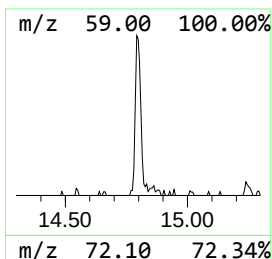
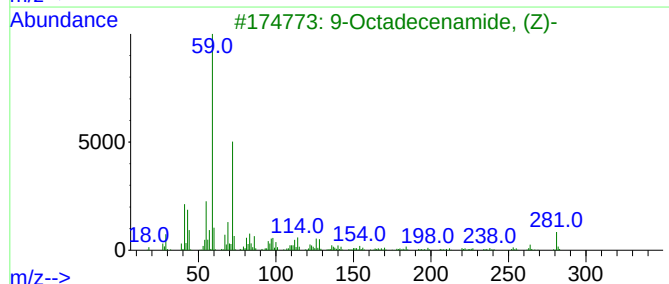
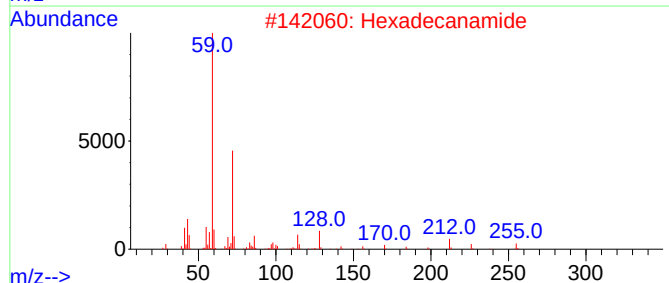
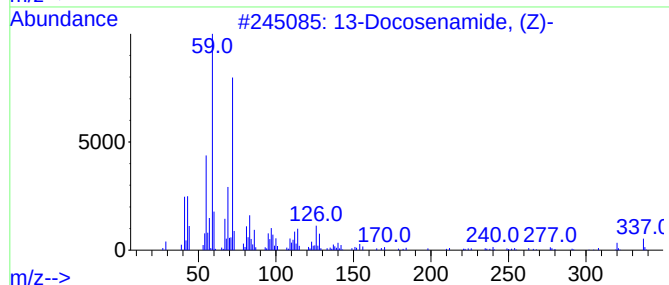
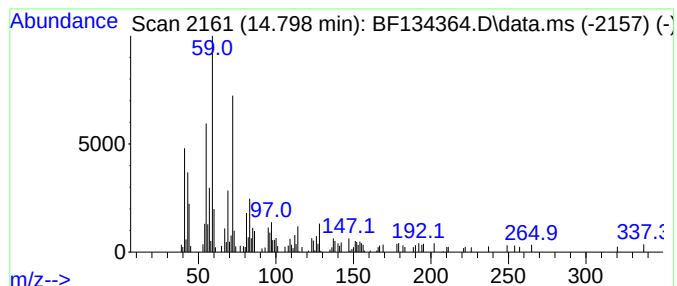
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 13-Docosenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.798	5.61 ng	96179	Perylene-d12	15.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	93
2			Hexadecanamide	255	C16H33NO	000629-54-9	64
3			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	64
4			Tetradecanamide	227	C14H29NO	000638-58-4	59
5			Cyclohexane, (ethoxymethoxy)-	158	C9H18O2	054699-29-5	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071923\
Data File : BF134364.D
Acq On : 19 Jul 2023 18:05
Operator : CG\JU
Sample : 03597-15
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-49-(0-2)

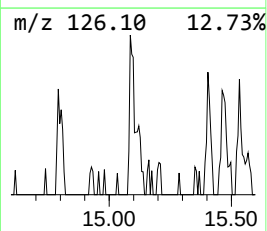
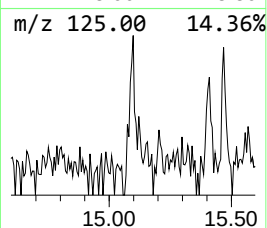
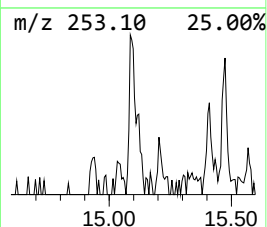
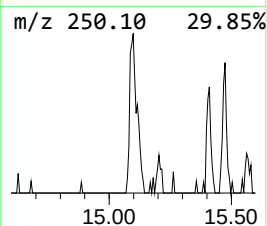
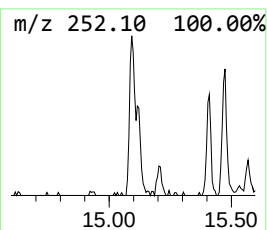
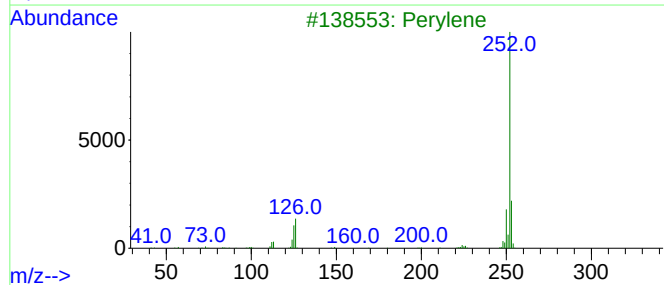
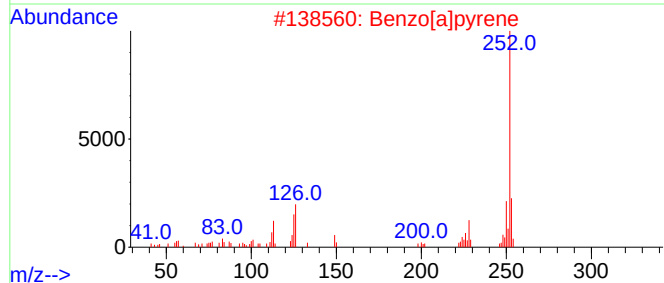
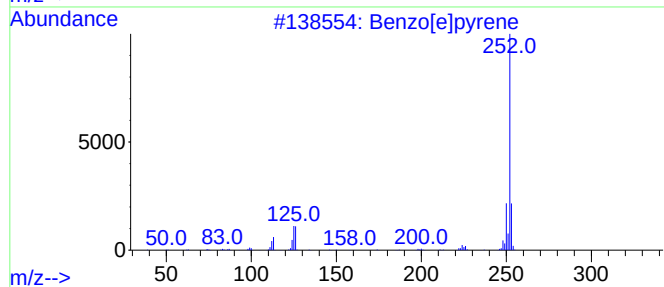
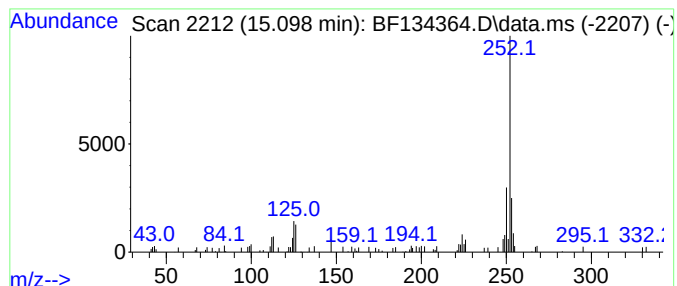
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.098	2.37 ng	40562	Perylene-d12	15.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	81
2			Benzo[a]pyrene	252	C20H12	000050-32-8	74
3			Perylene	252	C20H12	000198-55-0	72
4			Benzo[b]fluoranthene	252	C20H12	000205-99-2	70
5			Benzo[k]fluoranthene	252	C20H12	000207-08-9	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071923\
Data File : BF134364.D
Acq On : 19 Jul 2023 18:05
Operator : CG\JU
Sample : 03597-15
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-49-(0-2)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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
Butane, 2-metho...	2.134	22.3	ng	486213	1	6.840	435855	20.0
Tridecanoic acid	11.898	5.8	ng	149468	4	11.369	513391	20.0
9-Octadecenamid...	13.445	3.3	ng	75046	5	14.033	449803	20.0
Palmitoleamide	13.463	4.1	ng	91350	5	14.033	449803	20.0
Pentafluoroprop...	13.898	5.2	ng	117854	5	14.033	449803	20.0
13-Docosenamide...	14.798	5.6	ng	96179	6	15.539	342865	20.0
Benzo[e]pyrene	15.098	2.4	ng	40562	6	15.539	342865	20.0