

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101323\
 Data File : BF135763.D
 Acq On : 13 Oct 2023 20:42
 Operator : CG\JU
 Sample : 04844-01
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 OR-603-COMP-05

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-BF101323.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135763.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.963	487	489	502	rBV	83847	129012	5.40%	0.752%
2	5.369	555	558	582	rBV	1990136	2388349	100.00%	13.924%
3	6.386	728	731	757	rBV	2255894	2317799	97.05%	13.512%
4	6.734	787	790	801	rBV	702563	641628	26.86%	3.741%
5	7.304	883	887	900	rBV	1617441	1395154	58.41%	8.134%
6	8.016	1005	1008	1022	rVB	891977	756851	31.69%	4.412%
7	9.092	1188	1191	1195	rBV	2691828	2188498	91.63%	12.759%
8	9.210	1208	1211	1215	rVB	36895	37096	1.55%	0.216%
9	9.774	1303	1307	1311	rBV	946149	804641	33.69%	4.691%
10	10.569	1439	1442	1457	rBV	1367426	1254974	52.55%	7.316%
11	11.269	1558	1561	1564	rBV	841410	716625	30.01%	4.178%
12	11.292	1564	1565	1570	rVV	164054	122515	5.13%	0.714%
13	11.351	1570	1575	1580	rVB	29940	38710	1.62%	0.226%
14	11.804	1649	1652	1660	rBV2	221120	234759	9.83%	1.369%
15	12.492	1766	1769	1773	rBV	95891	95048	3.98%	0.554%
16	12.598	1783	1787	1792	rBV4	21518	35612	1.49%	0.208%
17	12.727	1804	1809	1813	rVB	86595	98686	4.13%	0.575%
18	12.863	1828	1832	1836	rBV	1753937	1605985	67.24%	9.363%
19	13.351	1910	1915	1921	rBV	478303	458886	19.21%	2.675%
20	13.439	1926	1930	1933	rBV2	24682	28732	1.20%	0.168%
21	13.857	1993	2001	2009	rBV9	30832	108388	4.54%	0.632%
22	13.933	2010	2014	2018	rVV	578958	586577	24.56%	3.420%
23	13.962	2018	2019	2022	rVB	40044	26212	1.10%	0.153%
24	14.092	2038	2041	2048	rBV2	26697	36929	1.55%	0.215%
25	14.327	2077	2081	2086	rBV4	17254	31457	1.32%	0.183%
26	14.398	2089	2093	2097	rBV	40348	42546	1.78%	0.248%
27	14.704	2141	2145	2151	rVB	35488	41197	1.72%	0.240%
28	14.774	2153	2157	2161	rVB	152141	150715	6.31%	0.879%
29	14.986	2190	2193	2196	rBV	27396	36895	1.54%	0.215%
30	15.033	2198	2201	2207	rVB2	46279	63295	2.65%	0.369%
31	15.409	2260	2265	2271	rBV	471578	622866	26.08%	3.631%
32	15.845	2336	2339	2346	rVB2	34972	56373	2.36%	0.329%

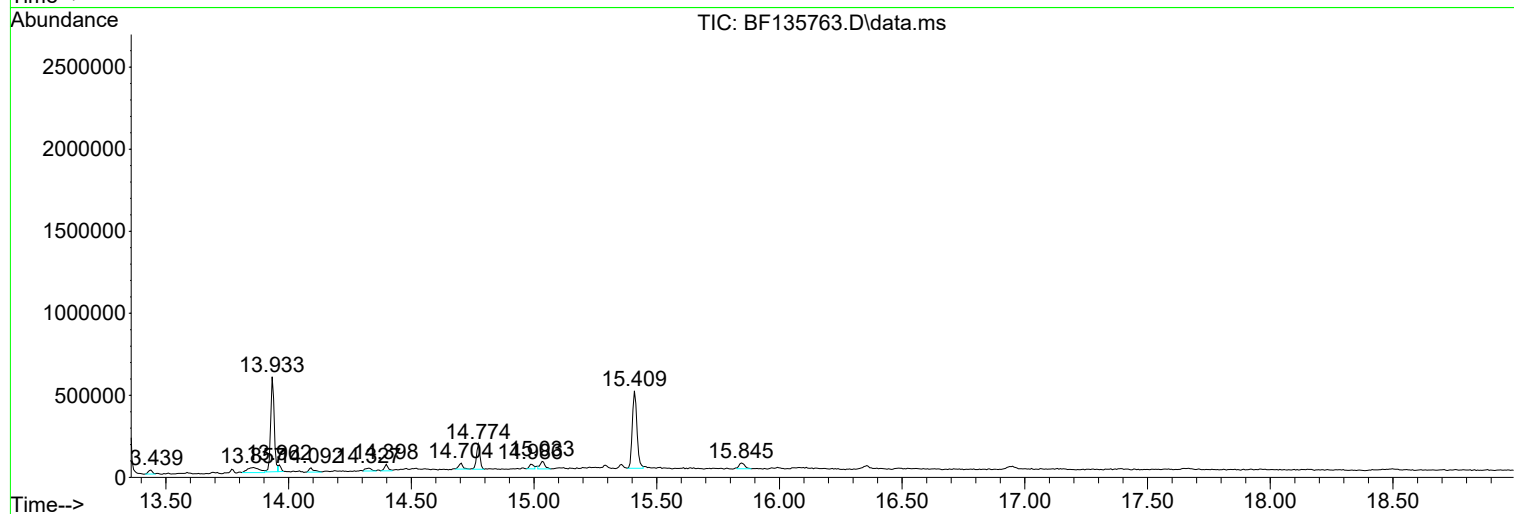
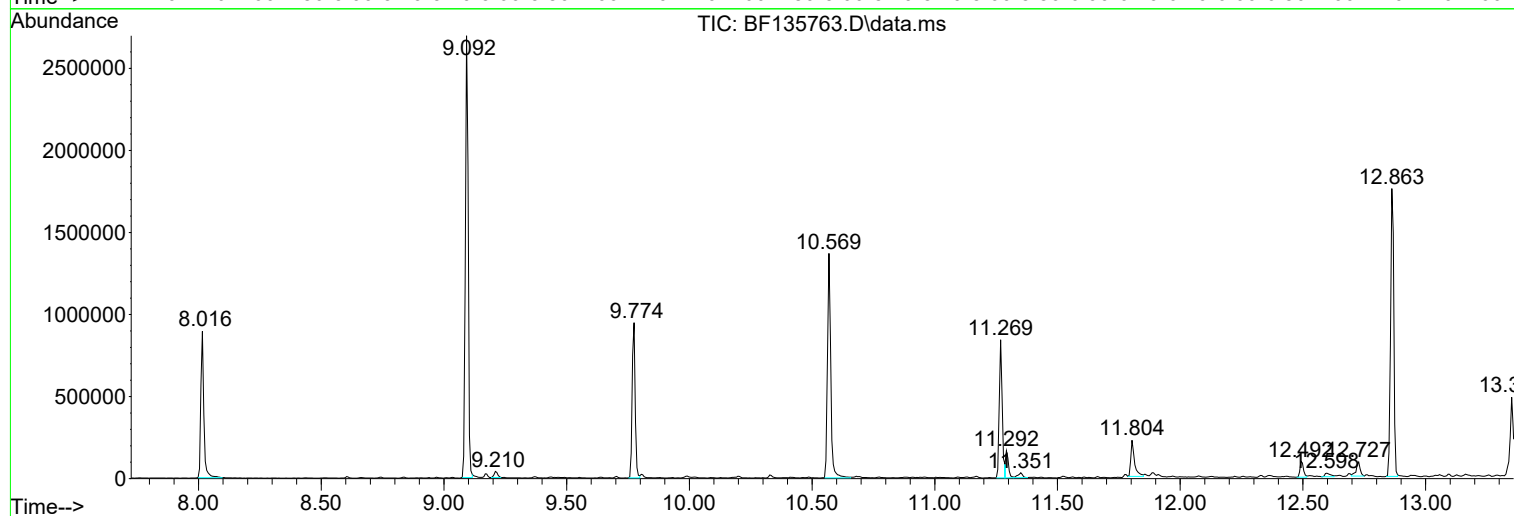
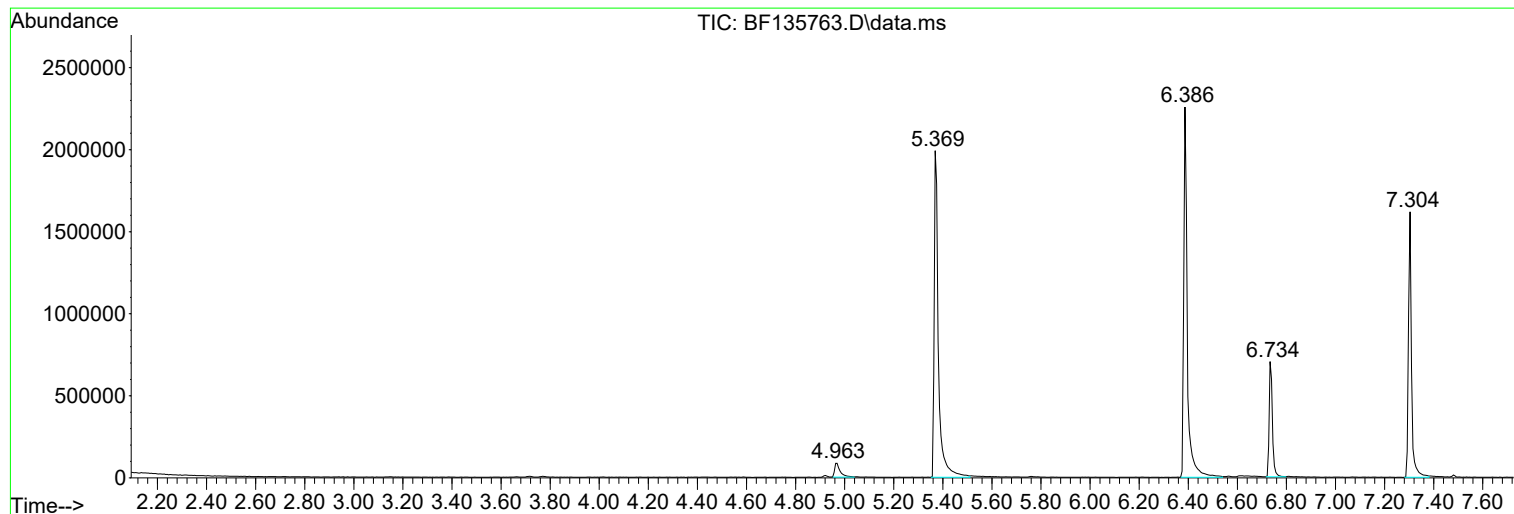
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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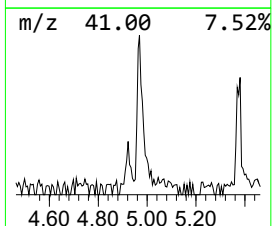
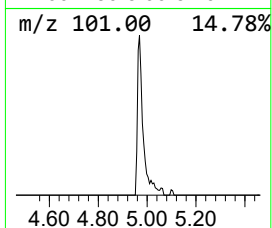
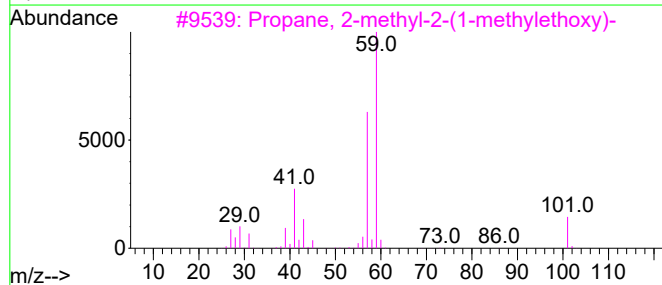
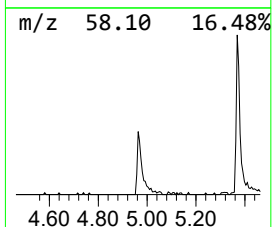
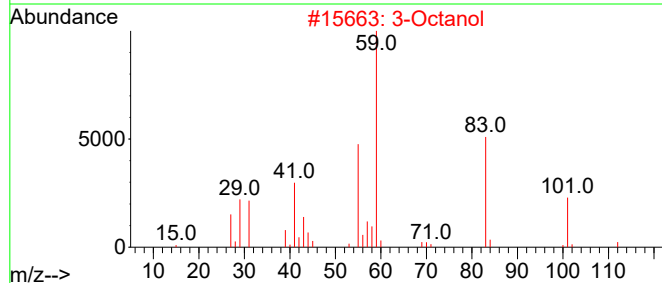
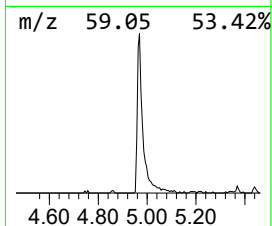
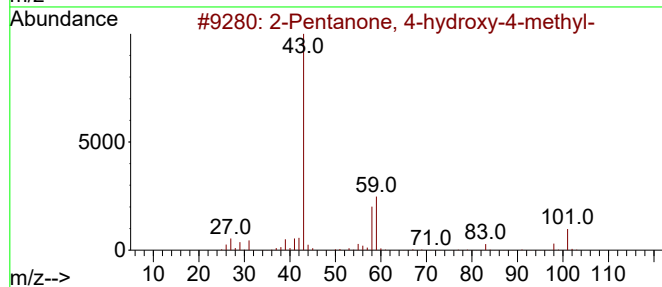
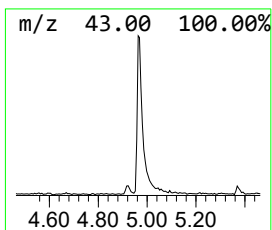
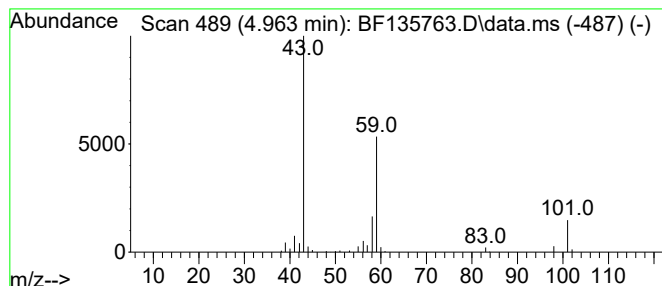
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.963	4.02 ng	129012	1,4-Dichlorobenzene-d4	6.734

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	3-Octanol	130	C8H18O	000589-98-0	36		
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	25		



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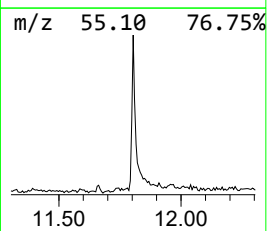
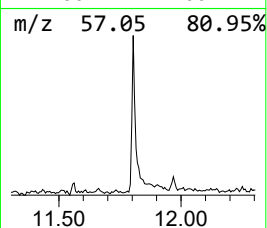
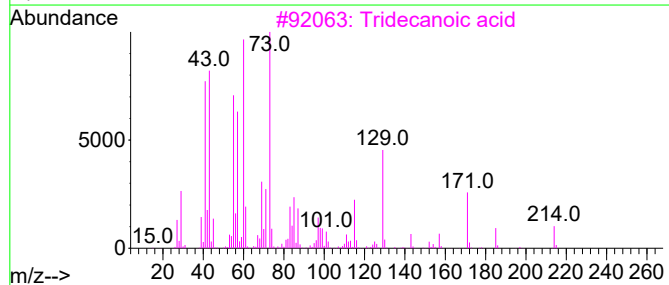
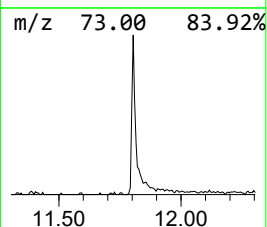
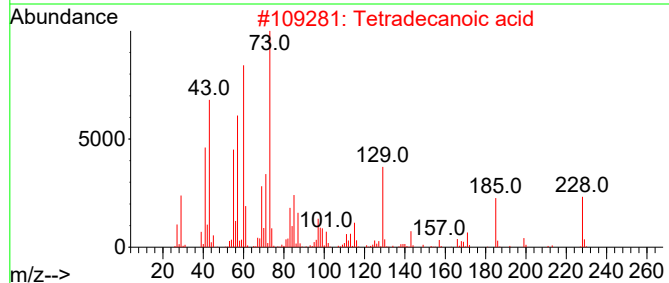
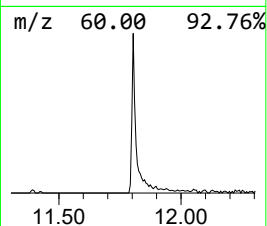
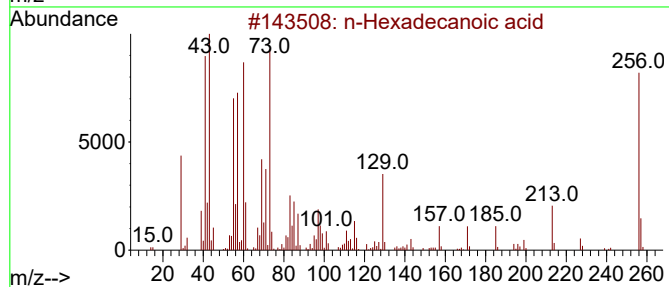
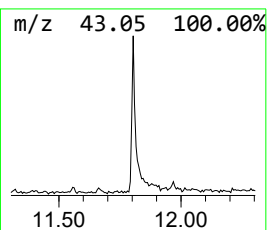
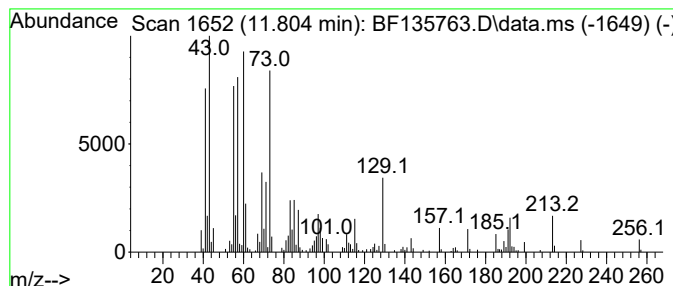
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.804	6.55 ng	234759	Phenanthrene-d10	11.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
3			Tridecanoic acid	214	C13H26O2	000638-53-9	76
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	64
5			Undecanoic acid	186	C11H22O2	000112-37-8	59



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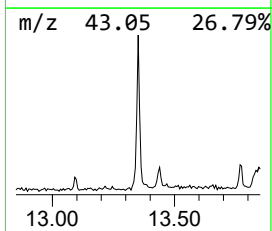
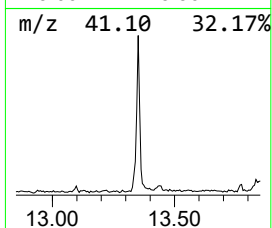
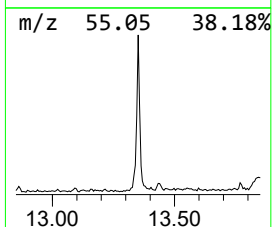
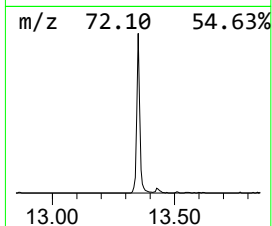
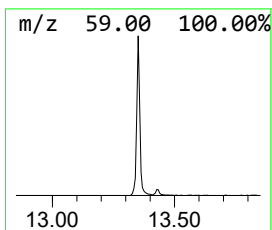
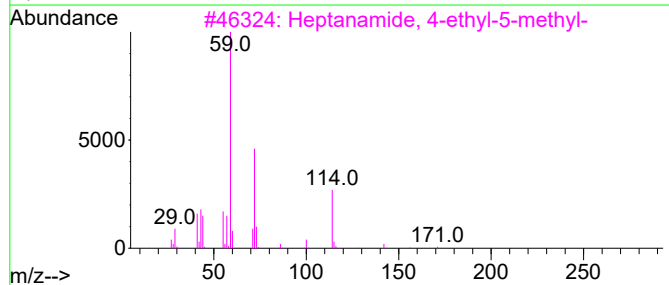
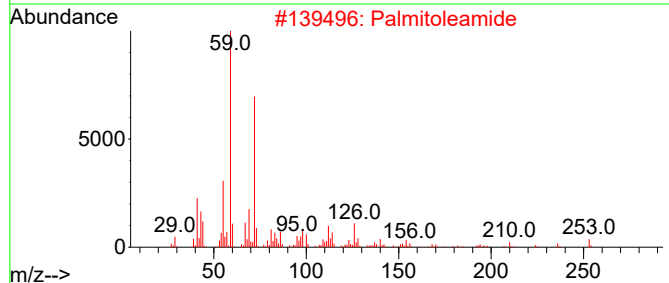
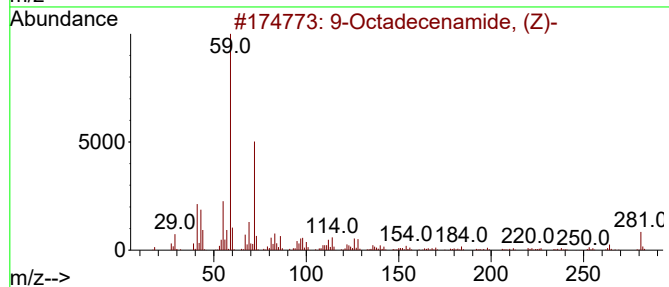
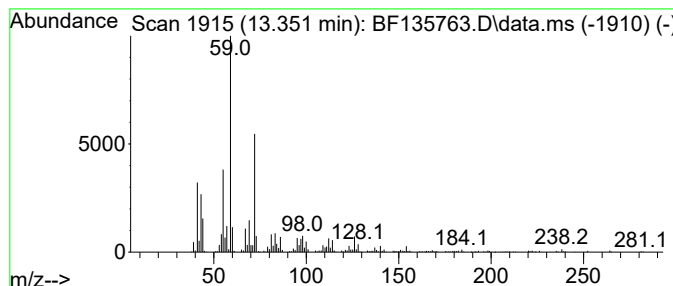
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 9-Octadecenamide, (Z)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.351	15.65 ng	458886	Chrysene-d12	13.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	94
2			Palmitoleamide	253	C16H31NO	106010-22-4	83
3			Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	53
4			Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	50
5			2(5H)-Furanone, 5-(7-hydroxy-6-m...	240	C14H24O3	1000512-93-0	38



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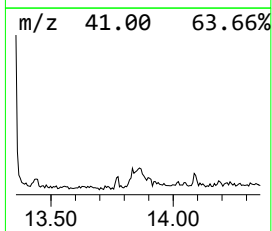
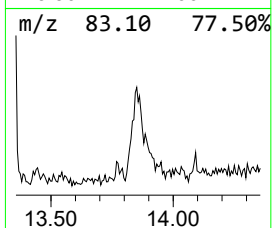
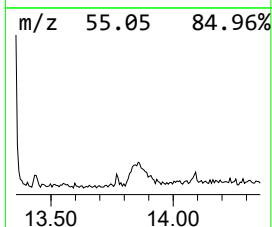
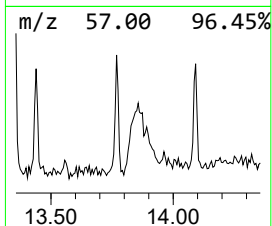
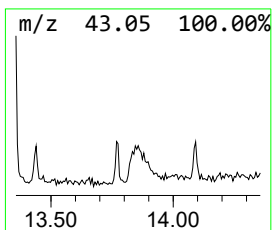
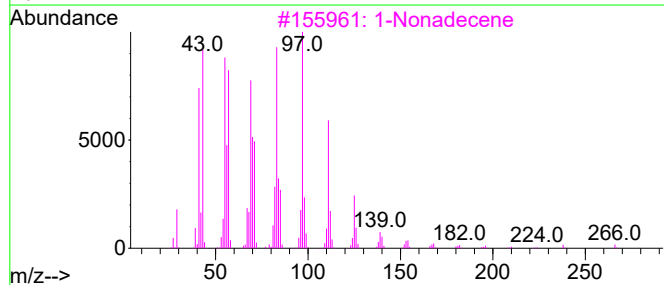
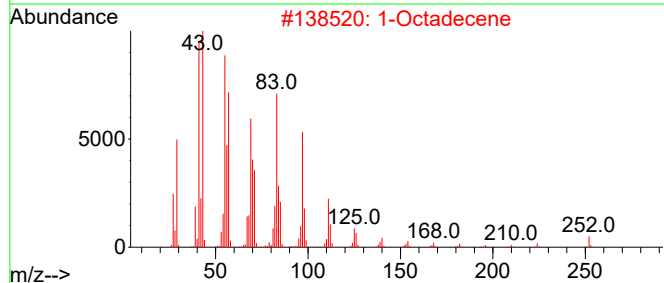
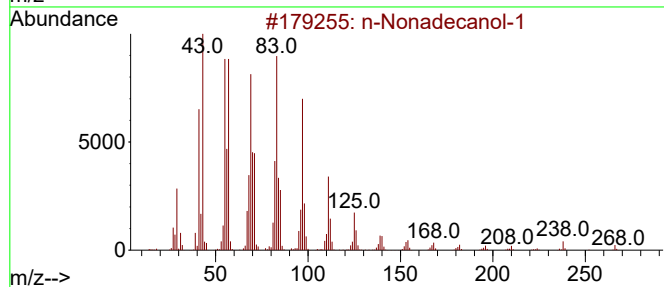
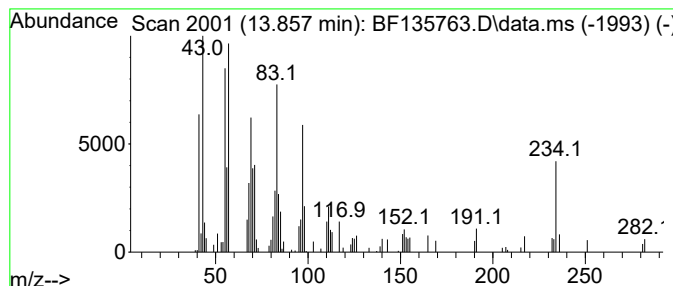
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 n-Nonadecanol-1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.857	3.70 ng	108388	Chrysene-d12	13.933	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	87
2	1-Octadecene	252	C18H36	000112-88-9	87
3	1-Nonadecene	266	C19H38	018435-45-5	83
4	Acetic acid, chloro-, hexadecyl ...	318	C18H35ClO2	052132-58-8	83
5	Dichloroacetic acid, tridecyl ester	310	C15H28Cl2O2	1000280-48-3	81



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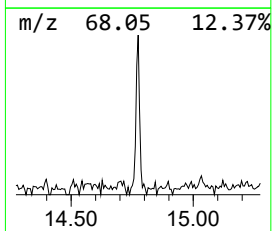
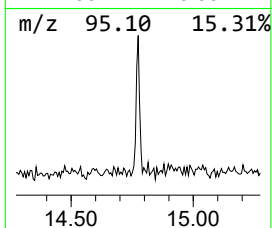
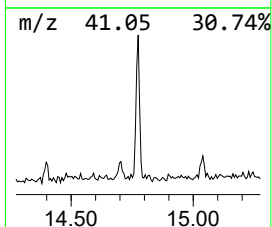
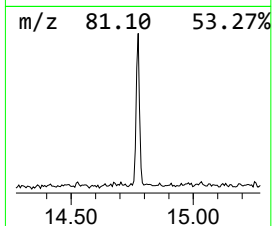
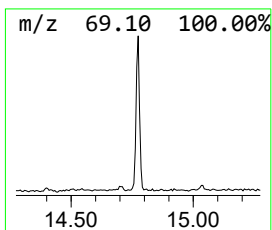
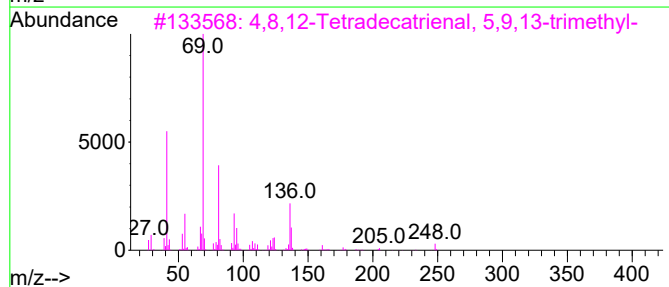
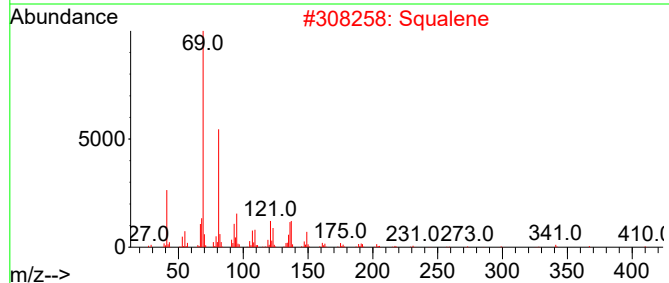
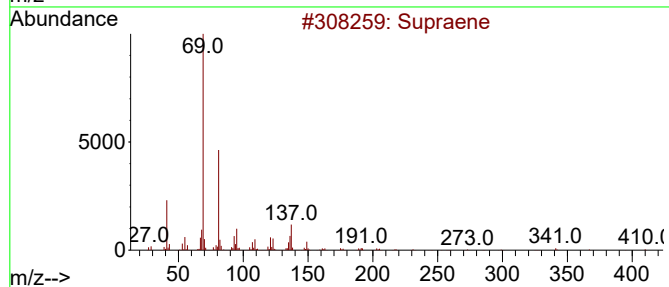
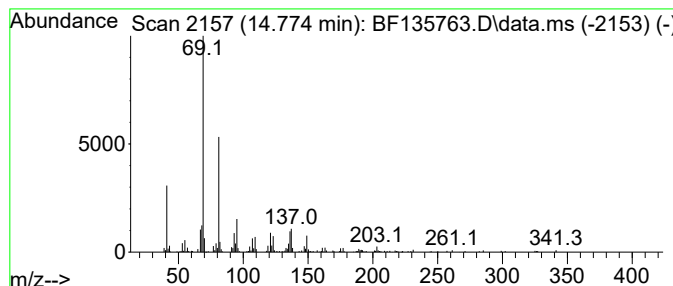
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TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Supraene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.774	4.84 ng	150715	Perylene-d12	15.409

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			Squalene	410	C30H50	000111-02-4	91
3			4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72
4			trans-Farnesol	222	C15H26O	000106-28-5	72
5			(3E,7E)-4,8,12-Trimethyltrideca-...	218	C16H26	062235-06-7	72



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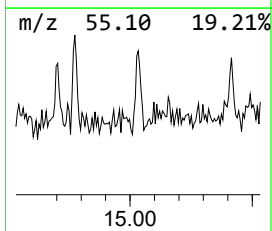
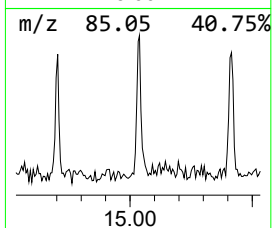
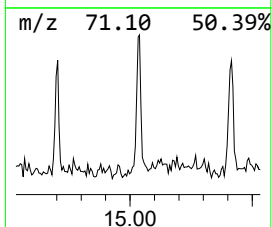
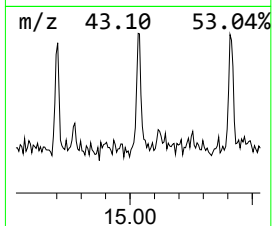
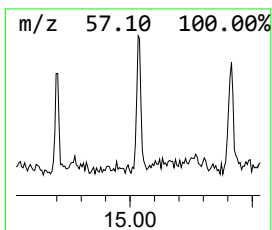
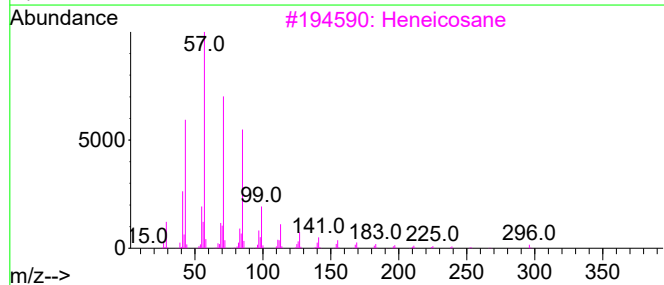
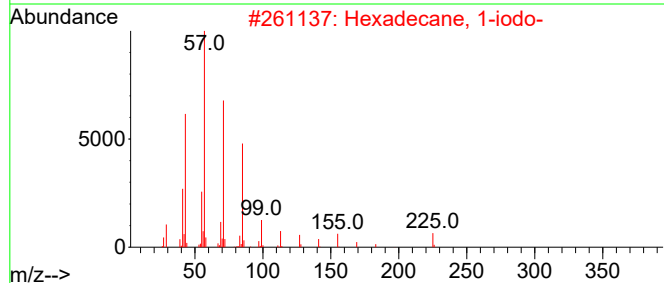
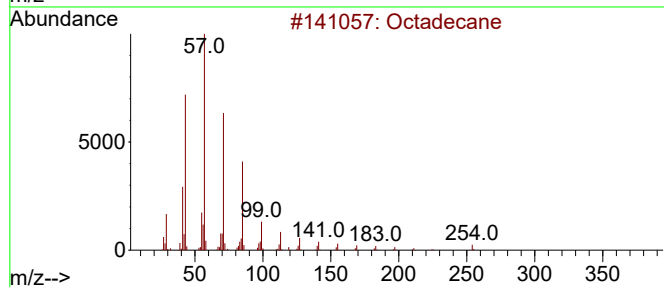
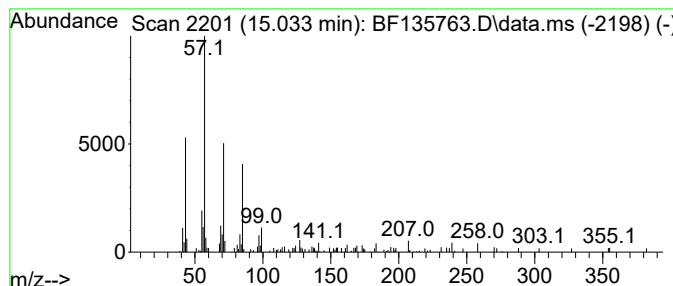
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.033	2.03 ng	63295	Perylene-d12	15.409

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane	254	C18H38	000593-45-3	80
2			Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	80
3			Heneicosane	296	C21H44	000629-94-7	64
4			Octacosane	394	C28H58	000630-02-4	62
5			Heptacosane	380	C27H56	000593-49-7	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101323\
Data File : BF135763.D
Acq On : 13 Oct 2023 20:42
Operator : CG\JU
Sample : 04844-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OR-603-COMP-05

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.963	4.0	ng	129012	1	6.734	641628	20.0
n-Hexadecanoic ...	11.804	6.5	ng	234759	4	11.269	716625	20.0
9-Octadecenamid...	13.351	15.7	ng	458886	5	13.933	586577	20.0
n-Nonadecanol-1	13.857	3.7	ng	108388	5	13.933	586577	20.0
Supraene	14.774	4.8	ng	150715	6	15.409	622866	20.0
Octadecane	15.033	2.0	ng	63295	6	15.409	622866	20.0