

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051823\
 Data File : BF133437.D
 Acq On : 18 May 2023 12:59
 Operator : CG\JU
 Sample : 02812-09
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WG-0516-BD

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: BF133437.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.898	473	478	492	rVB	701871	952784	21.61%	3.020%
2	5.328	547	551	562	rBV	4505679	4248001	96.36%	13.465%
3	5.716	614	617	624	rVB	65323	61428	1.39%	0.195%
4	6.357	722	726	743	rBV	4033501	4408663	100.00%	13.974%
5	6.710	783	786	790	rBV	1373464	1060885	24.06%	3.363%
6	7.275	878	882	885	rBV	2767335	2610967	59.22%	8.276%
7	7.998	1001	1005	1011	rBV	1594581	1455528	33.02%	4.614%
8	9.075	1184	1188	1191	rBV	4267712	3610453	81.89%	11.444%
9	9.745	1299	1302	1306	rBV	1438648	1280681	29.05%	4.059%
10	10.463	1419	1424	1427	rBV	130672	114718	2.60%	0.364%
11	10.539	1433	1437	1440	rBV	2859817	2410146	54.67%	7.640%
12	11.233	1551	1555	1558	rBV	1528150	1344750	30.50%	4.263%
13	11.304	1563	1567	1572	rVB4	39068	46290	1.05%	0.147%
14	11.768	1643	1646	1657	rBV3	180915	255670	5.80%	0.810%
15	12.445	1757	1761	1767	rBV	98333	93316	2.12%	0.296%
16	12.557	1775	1780	1790	rBV8	32424	71302	1.62%	0.226%
17	12.668	1793	1799	1802	rVV	101065	101249	2.30%	0.321%
18	12.821	1820	1825	1828	rBV	3829641	3613992	81.97%	11.456%
19	13.057	1859	1865	1870	rBV2	62353	82180	1.86%	0.260%
20	13.727	1975	1979	1981	rBV	117141	138440	3.14%	0.439%
21	13.751	1981	1983	1997	rVB3	110168	255742	5.80%	0.811%
22	13.868	1998	2003	2006	rBV	1305376	1184127	26.86%	3.753%
23	14.039	2029	2032	2035	rBV	76321	73171	1.66%	0.232%
24	14.345	2080	2084	2087	rBV	118991	117869	2.67%	0.374%
25	14.398	2087	2093	2104	rVV4	76209	217750	4.94%	0.690%
26	14.645	2129	2135	2138	rBV	73347	94900	2.15%	0.301%
27	14.886	2173	2176	2184	rVB	42976	74534	1.69%	0.236%
28	14.962	2186	2189	2193	rBV2	89270	88155	2.00%	0.279%
29	15.039	2196	2202	2206	rBV4	55013	98084	2.22%	0.311%
30	15.292	2240	2245	2249	rBV	983563	1171269	26.57%	3.713%
31	15.727	2316	2319	2327	rVB2	58862	86674	1.97%	0.275%
32	15.839	2334	2338	2347	rVB4	56882	124337	2.82%	0.394%

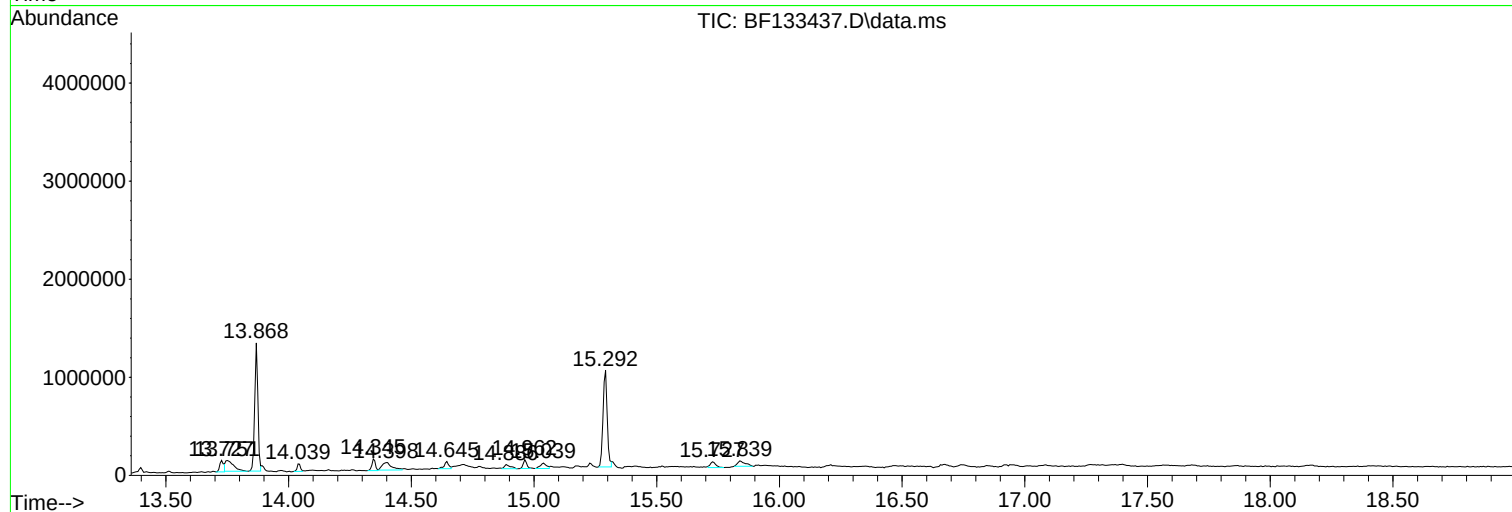
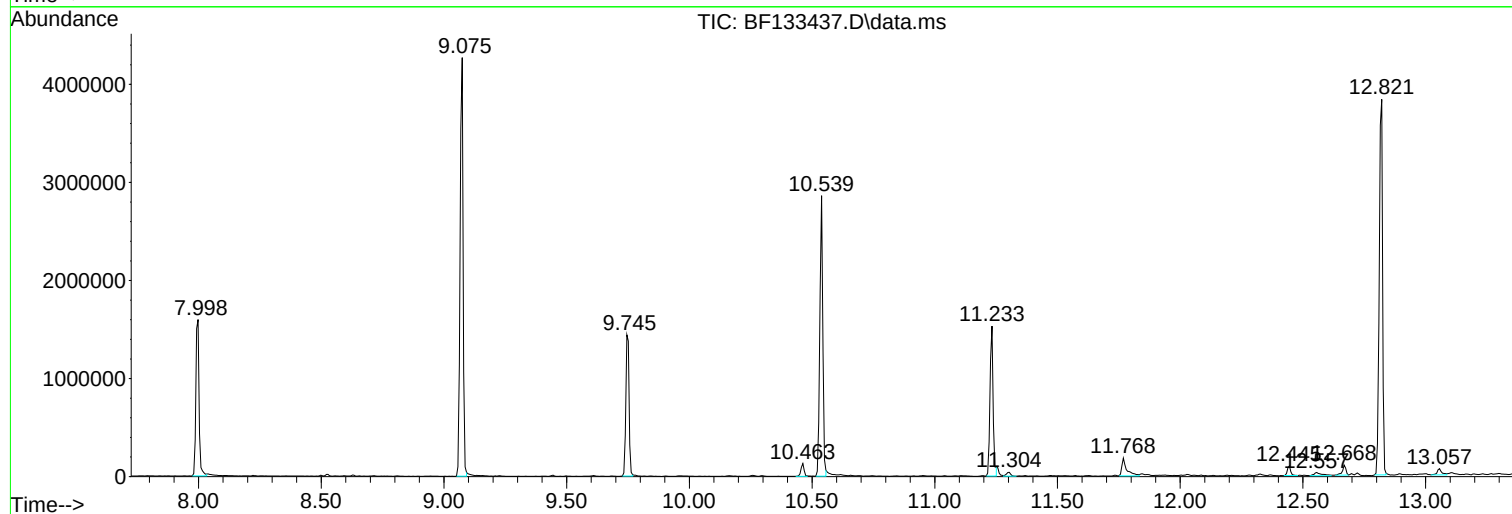
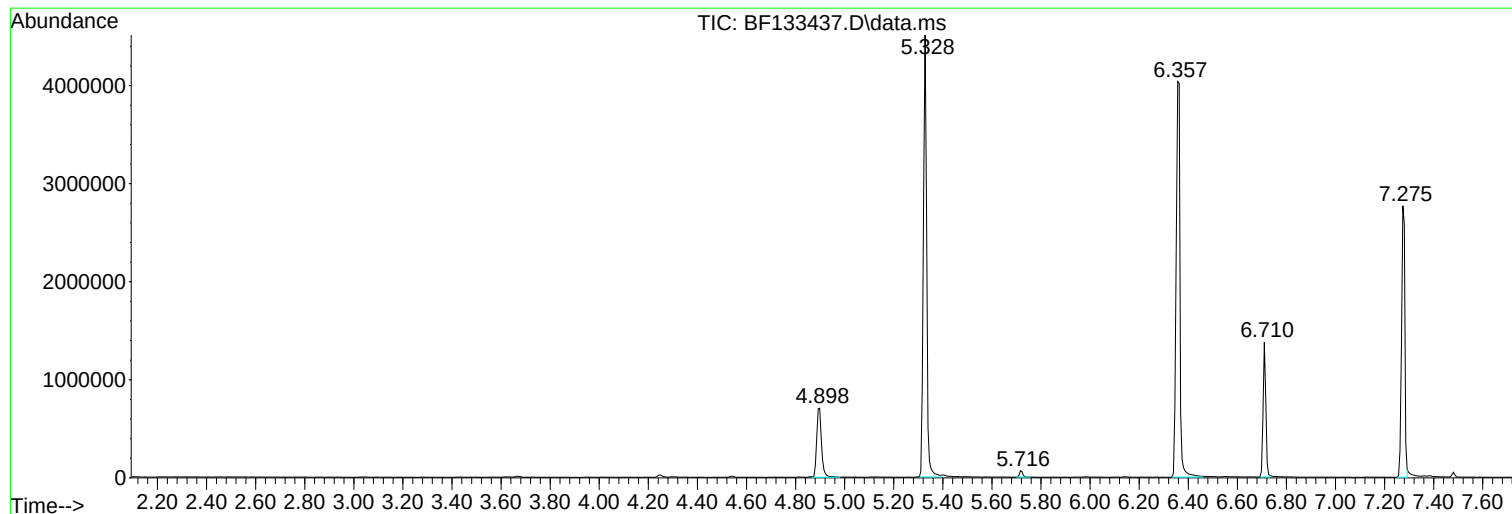
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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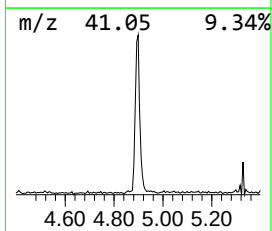
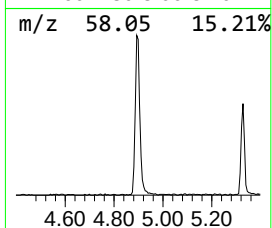
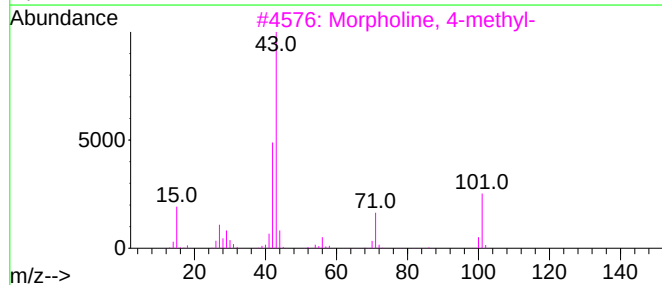
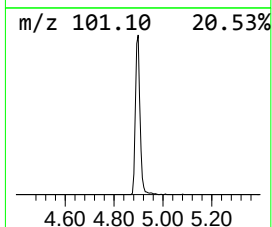
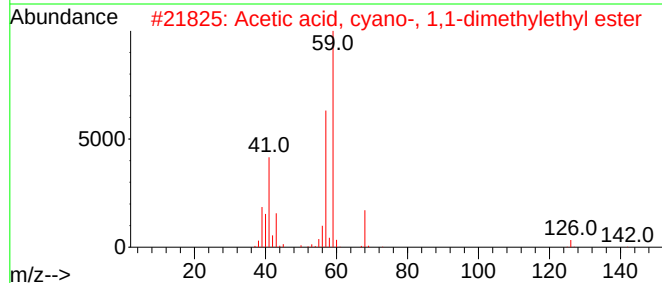
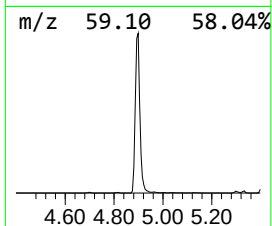
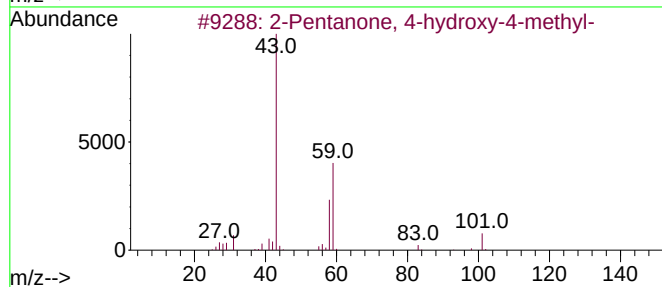
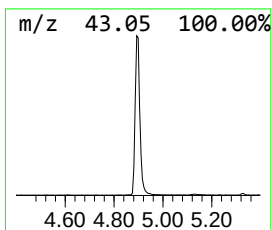
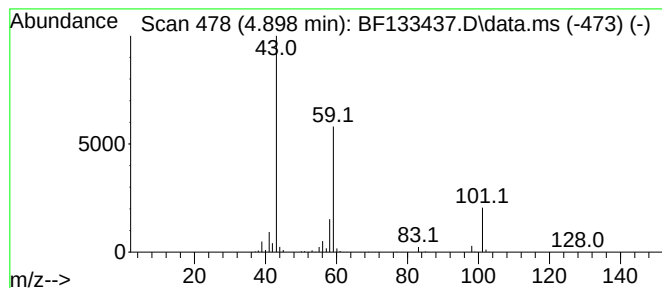
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
4.898	17.96 ng	952784	1,4-Dichlorobenzene-d4	6.710	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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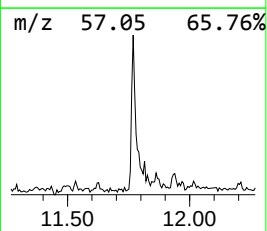
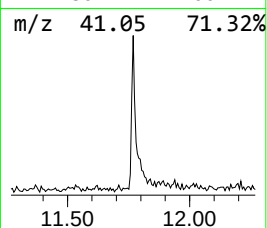
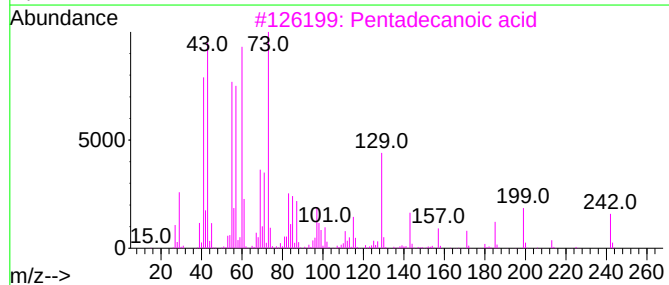
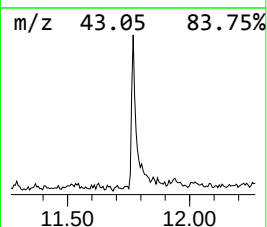
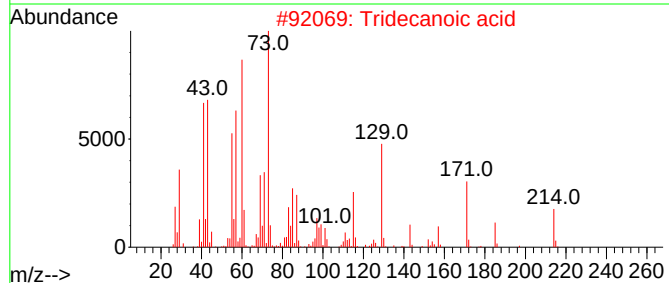
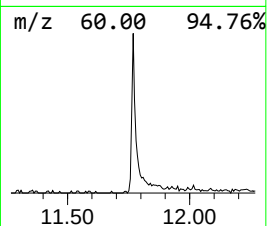
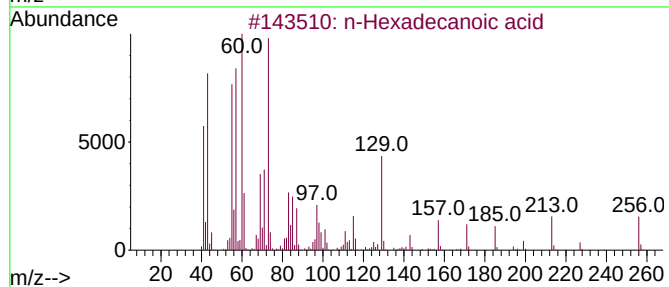
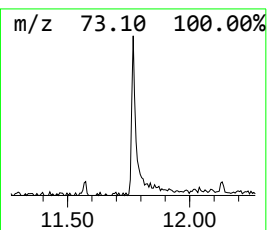
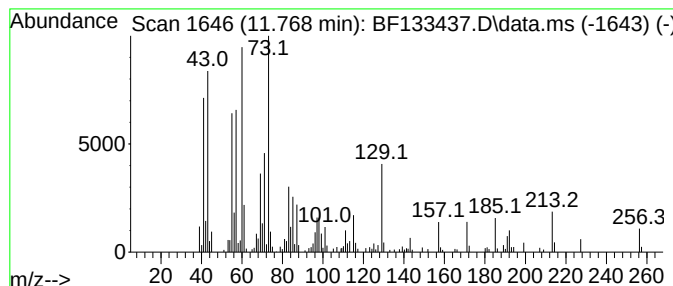
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.769	3.80 ng	255670	Phenanthrene-d10	11.233

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tridecanoic acid	214	C13H26O2	000638-53-9	95
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4		n-Decanoic acid	172	C10H20O2	000334-48-5	81
5		Undecanoic acid	186	C11H22O2	000112-37-8	74



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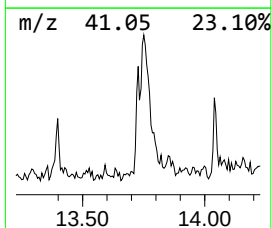
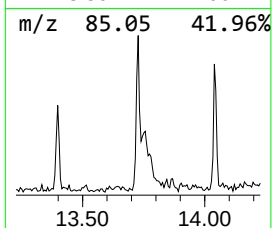
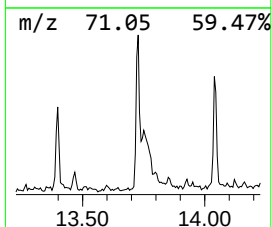
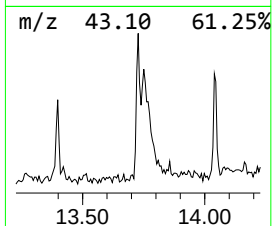
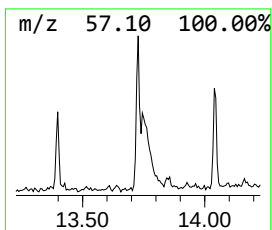
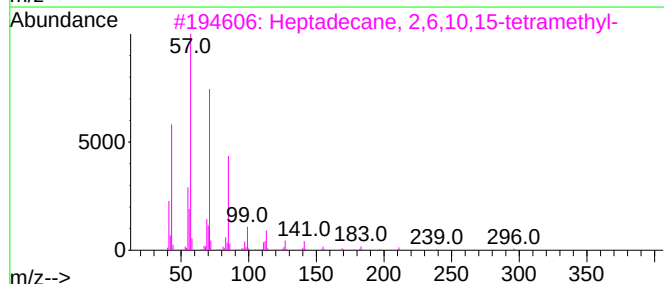
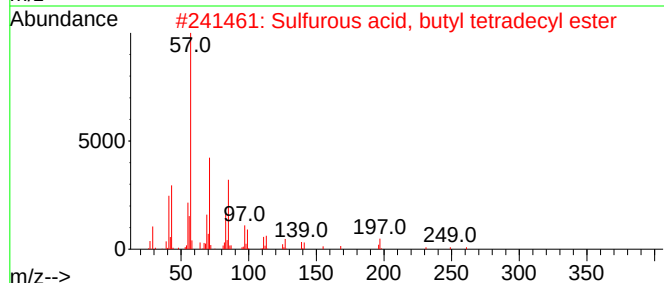
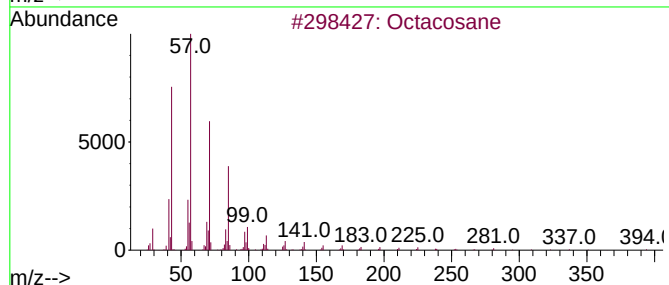
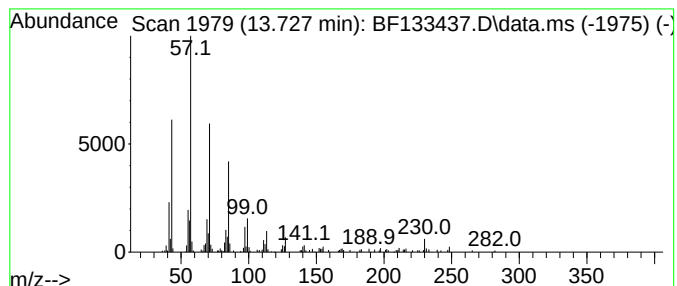
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.727	2.34 ng	138440	Chrysene-d12	13.868

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	90
2			Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1010309-18-1	87
3			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	83
4			Heptadecane	240	C17H36	000629-78-7	83
5			Nonadecane, 2-methyl-	282	C20H42	001560-86-7	83



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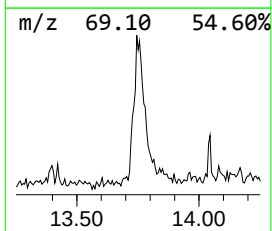
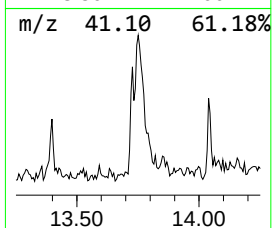
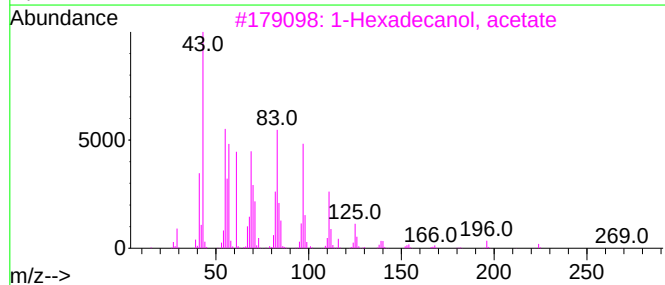
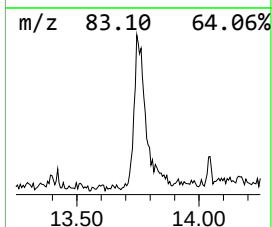
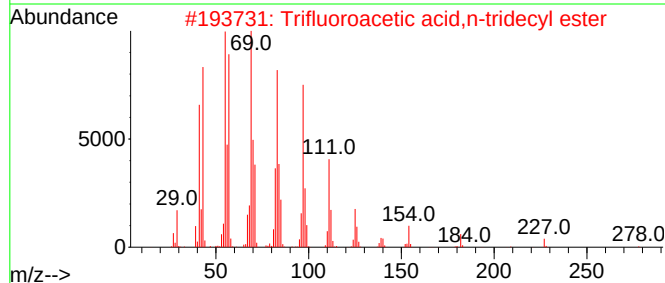
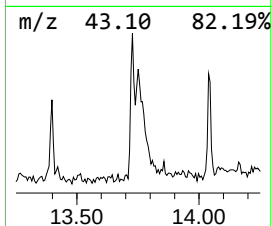
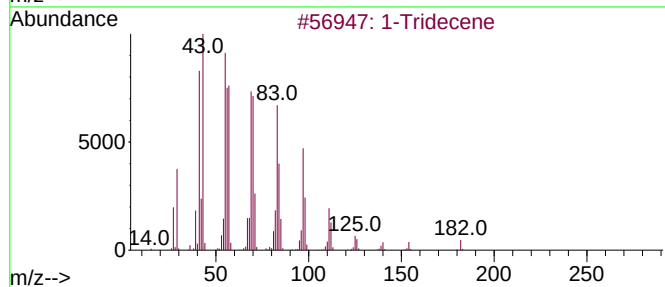
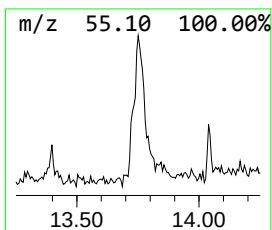
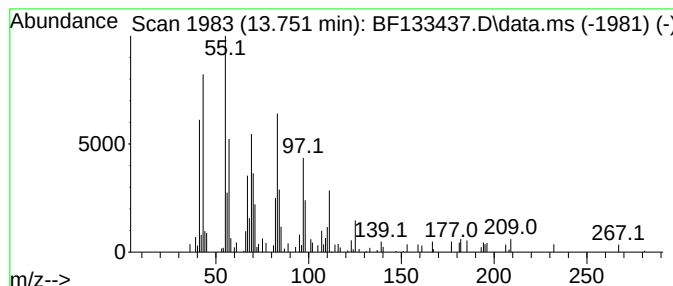
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Peak Number 4 1-Tridecene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.751	4.32 ng	255742	Chrysene-d12	13.868

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tridecene			182	C13H26	002437-56-1	76
2	Trifluoroacetic acid,n-tridecyl ...			296	C15H27F3O2	053800-02-5	74
3	1-Hexadecanol, acetate			284	C18H36O2	000629-70-9	72
4	3-Chloropropionic acid, tridecyl...			290	C16H31ClO2	1000281-77-4	72
5	Chloroacetic acid, tridecyl ester			276	C15H29ClO2	018277-85-5	72



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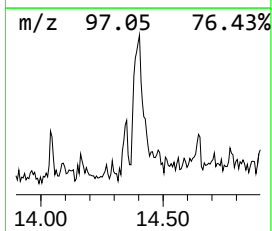
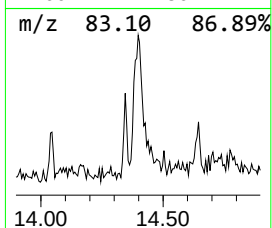
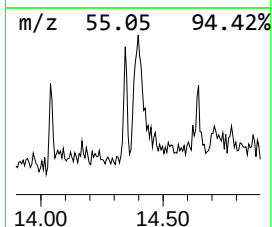
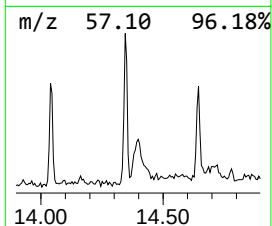
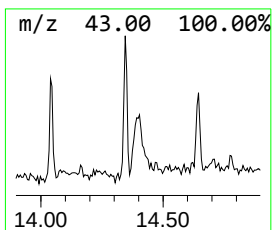
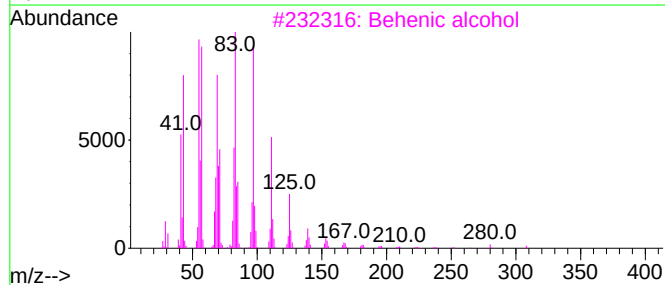
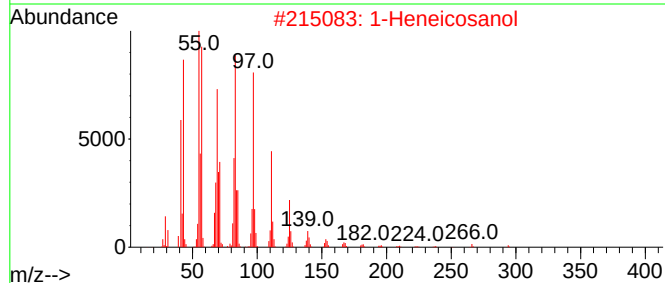
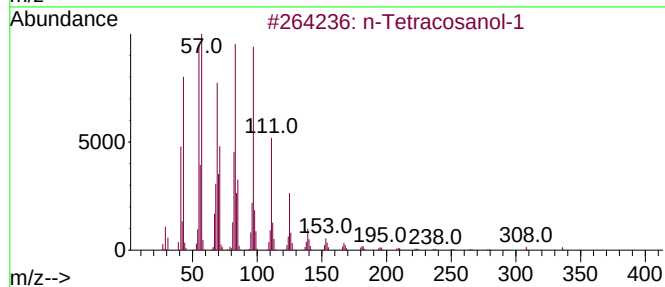
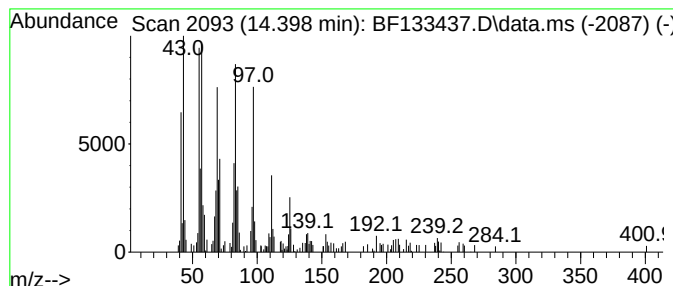
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Peak Number 5 n-Tetracosanol-1 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.398	3.68 ng	217750	Chrysene-d12	13.868

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Tetracosanol-1	354	C24H50O	000506-51-4	95
2			1-Heneicosanol	312	C21H44O	015594-90-8	95
3			Behenic alcohol	326	C22H46O	000661-19-8	95
4			Octacosanol	410	C28H58O	000557-61-9	93
5			1-Hexacosene	364	C26H52	018835-33-1	93



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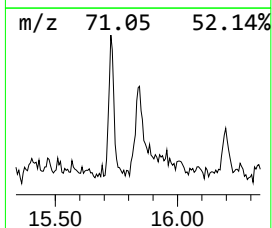
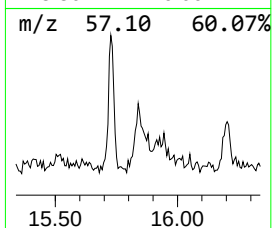
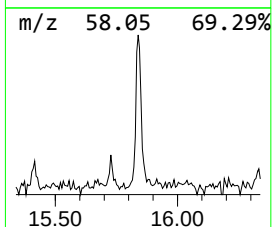
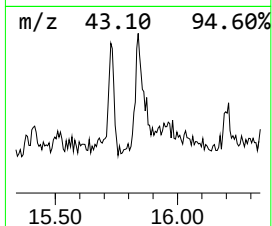
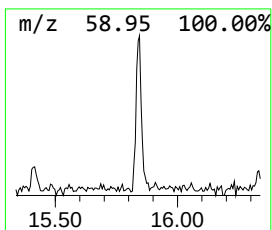
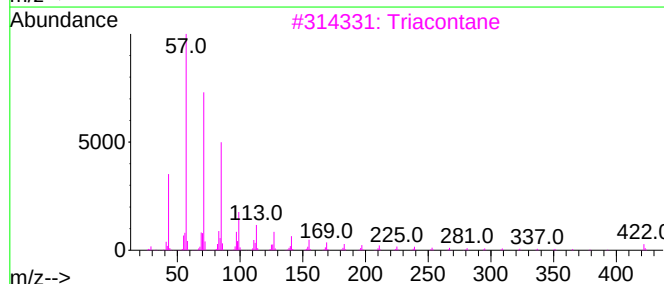
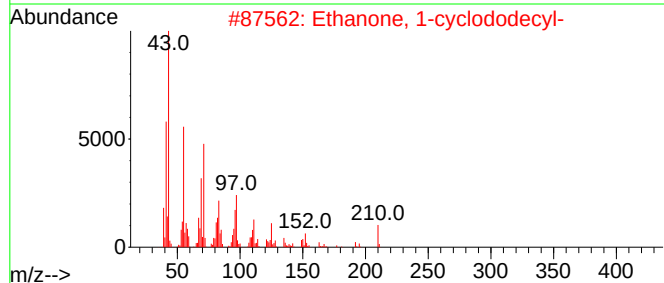
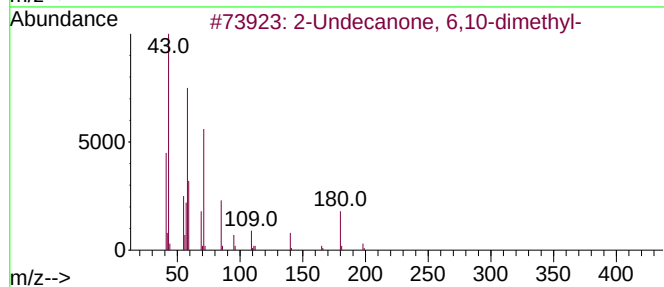
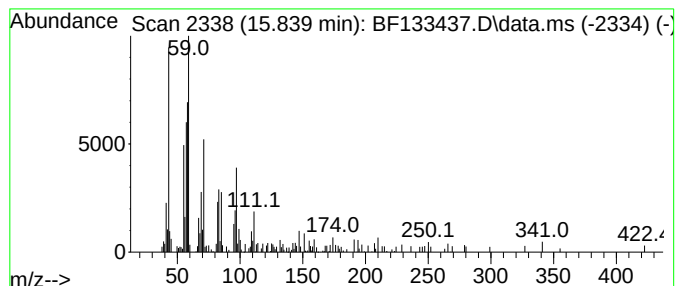
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown15.839 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.839	2.12 ng	124337	Perylene-d12	15.292

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Undecanone, 6,10-dimethyl-	198	C13H26O	001604-34-8	35
2		Ethanone, 1-cyclododecyl-	210	C14H26O	028925-00-0	30
3		Triacontane	422	C30H62	000638-68-6	25
4		6-Undecen-3-one, 5-butyl-2,2-dim...	252	C17H32O	055976-05-1	15
5		Carbonic acid, eicosyl prop-1-en...	382	C24H46O3	1000383-10-8	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051823\
Data File : BF133437.D
Acq On : 18 May 2023 12:59
Operator : CG\JU
Sample : 02812-09
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WG-0516-BD

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.898	18.0	ng	952784	1	6.710	1060890	20.0
n-Hexadecanoic ...	11.769	3.8	ng	255670	4	11.233	1344750	20.0
Octacosane	13.727	2.3	ng	138440	5	13.868	1184130	20.0
1-Tridecene	13.751	4.3	ng	255742	5	13.868	1184130	20.0
n-Tetracosanol-1	14.398	3.7	ng	217750	5	13.868	1184130	20.0
unknown15.839	15.839	2.1	ng	124337	6	15.292	1171270	20.0