

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050423\
 Data File : BF133244.D
 Acq On : 04 May 2023 22:08
 Operator : CG\JU
 Sample : 02588-02
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 ZONE-B-3-6-05012023

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: BF133244.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.716	272	277	286	rVB	97327	140648	3.12%	0.410%
2	4.922	477	482	490	rVB	86892	119280	2.65%	0.348%
3	5.339	548	553	556	rBV	4356659	4118473	91.36%	12.008%
4	6.363	722	727	730	rBV	3853828	4168004	92.46%	12.153%
5	6.722	785	788	792	rBV	1501663	1228946	27.26%	3.583%
6	7.292	880	885	888	rBV	2842206	2720510	60.35%	7.932%
7	8.010	1003	1007	1010	rBV	2082832	1689699	37.48%	4.927%
8	9.086	1185	1190	1193	rBV	5380020	4508098	100.00%	13.144%
9	9.757	1301	1304	1308	rVB	2104712	1865539	41.38%	5.439%
10	10.469	1422	1425	1429	rBV	365052	333864	7.41%	0.973%
11	10.551	1434	1439	1442	rBV	2758030	2748065	60.96%	8.012%
12	11.239	1552	1556	1559	rBV	2327930	1888197	41.88%	5.505%
13	11.263	1559	1560	1563	rVB	137126	72945	1.62%	0.213%
14	11.780	1643	1648	1656	rBV2	307991	373710	8.29%	1.090%
15	12.451	1758	1762	1766	rBV	242775	222792	4.94%	0.650%
16	12.563	1778	1781	1785	rBV	65949	75138	1.67%	0.219%
17	12.674	1794	1800	1804	rBV	202623	215511	4.78%	0.628%
18	12.827	1822	1826	1829	rBV	4366618	3877257	86.01%	11.305%
19	13.068	1864	1867	1871	rBV2	71396	66045	1.47%	0.193%
20	13.410	1919	1925	1928	rBV3	96096	105612	2.34%	0.308%
21	13.639	1961	1964	1968	rVB2	39171	59418	1.32%	0.173%
22	13.739	1978	1981	1986	rBV	225456	313191	6.95%	0.913%
23	13.786	1986	1989	1993	rVB2	124280	134275	2.98%	0.392%
24	13.874	1999	2004	2007	rBV	1250306	1210030	26.84%	3.528%
25	13.898	2007	2008	2014	rVB	92721	57188	1.27%	0.167%
26	14.051	2031	2034	2037	rBV	62704	60662	1.35%	0.177%
27	14.357	2083	2086	2089	rBV	92032	90438	2.01%	0.264%
28	14.409	2092	2095	2100	rVB3	59617	69208	1.54%	0.202%
29	14.656	2134	2137	2142	rVB	49646	53894	1.20%	0.157%
30	14.886	2172	2176	2184	rVB	94108	174590	3.87%	0.509%
31	14.974	2188	2191	2197	rVB2	75264	93924	2.08%	0.274%
32	15.168	2221	2224	2230	rVB	58947	74058	1.64%	0.216%
33	15.227	2231	2234	2240	rVB	68522	78934	1.75%	0.230%
34	15.292	2240	2245	2249	rBV	980722	1149702	25.50%	3.352%
35	15.745	2318	2322	2327	rBV	58444	83879	1.86%	0.245%
36	16.650	2474	2476	2484	rVB2	36226	55742	1.24%	0.163%

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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

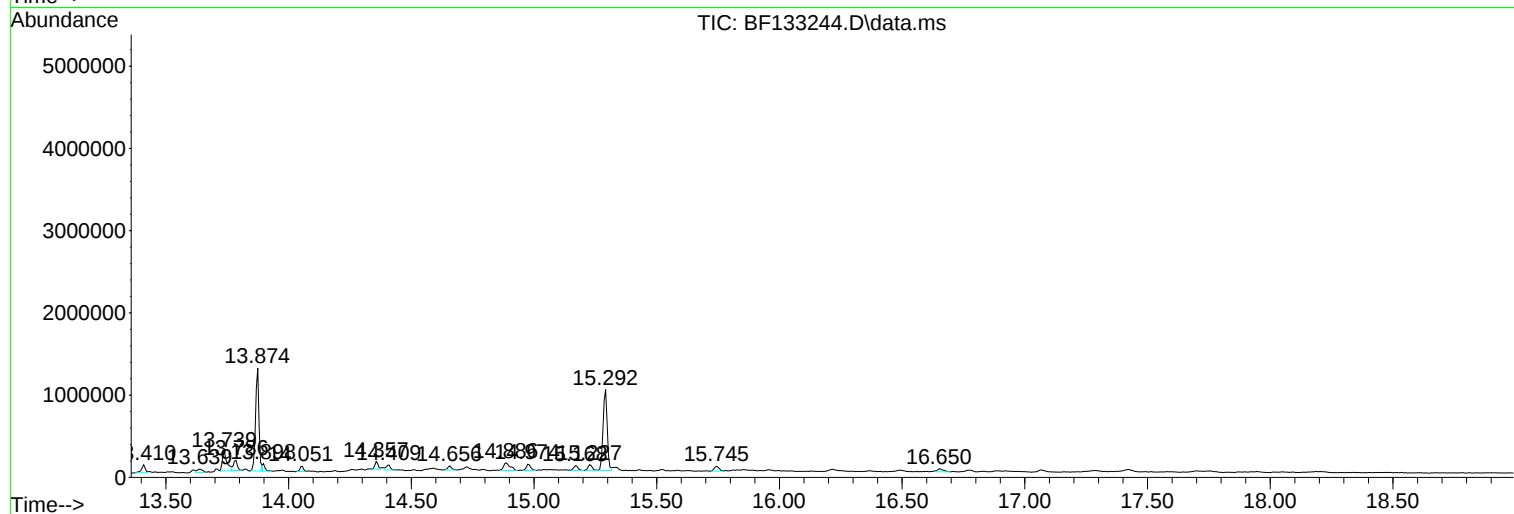
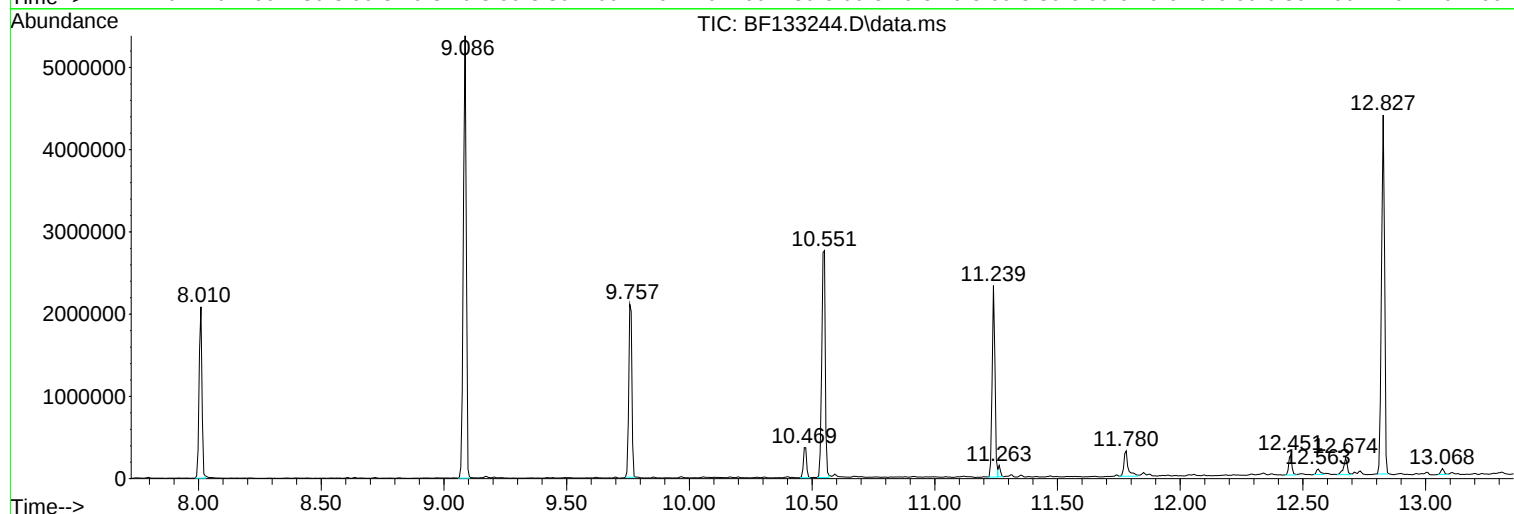
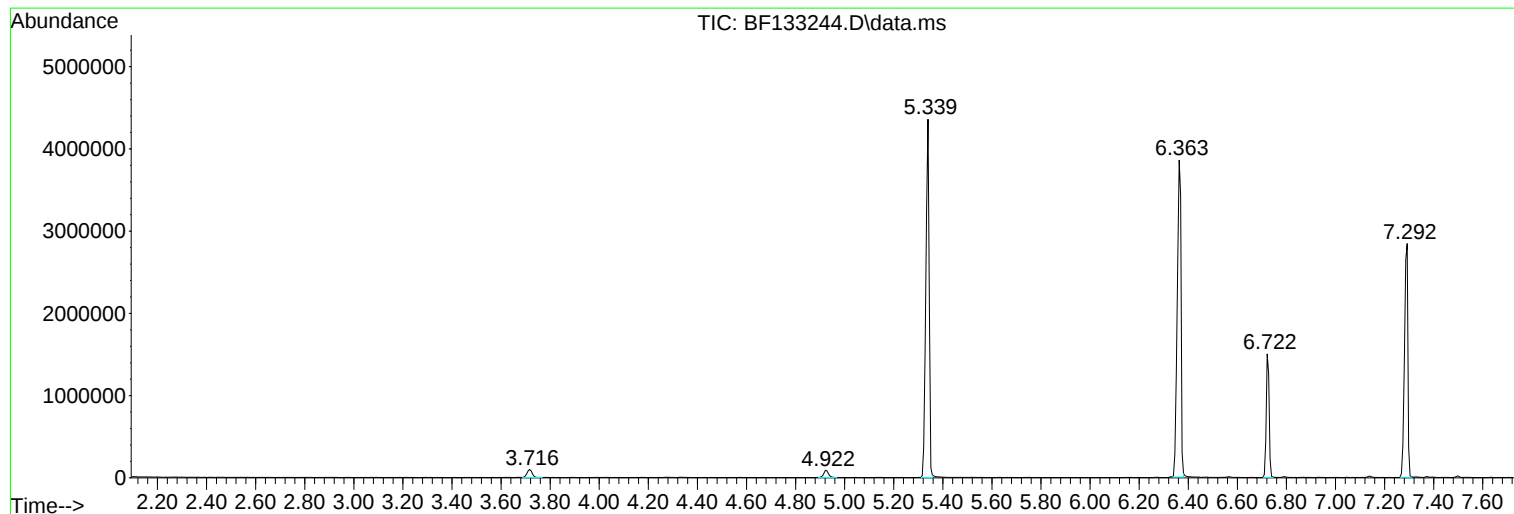
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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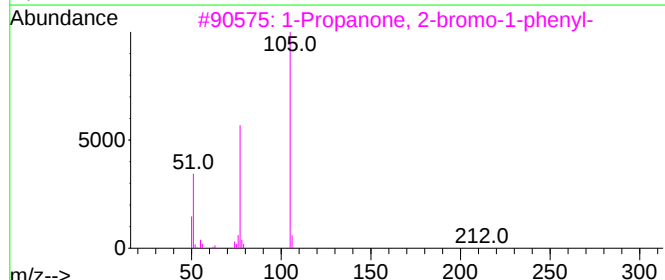
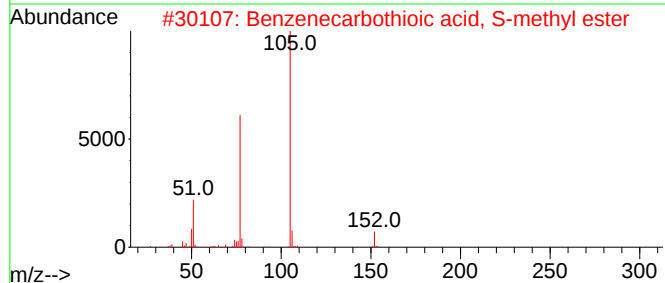
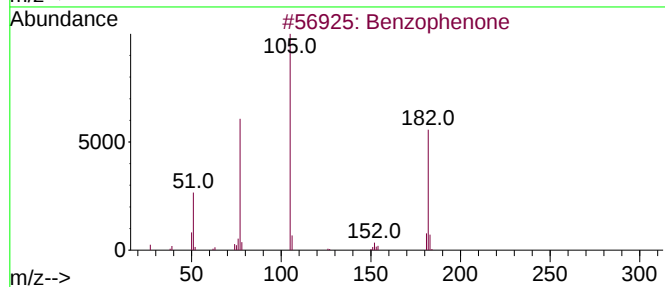
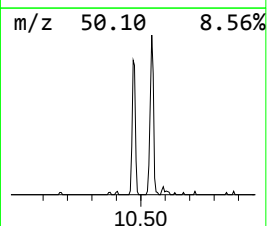
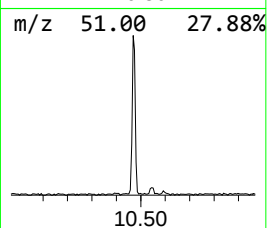
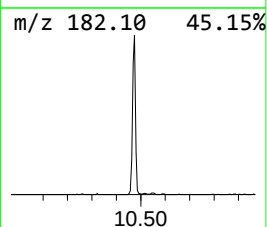
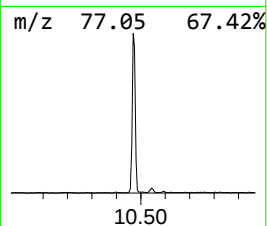
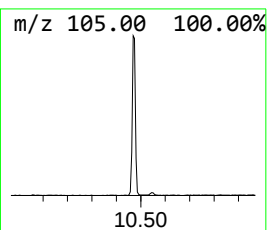
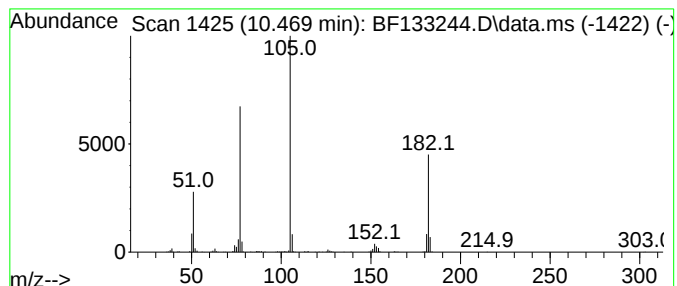
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.469	3.58 ng	333864	Acenaphthene-d10	9.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	49
3			1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
4			acetic acid, 2-bromo-, 2-oxo-2-p...	256	C10H9BrO3	1000401-50-0	47
5			2-(2-Oxo-2-phenyl-ethyl)-malon...	184	C11H8N2O	1000296-76-9	47



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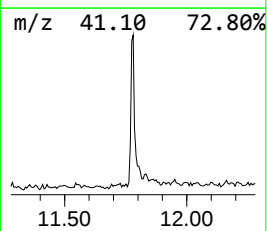
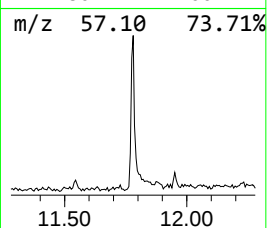
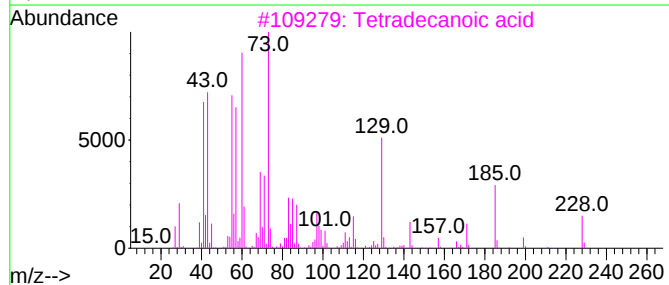
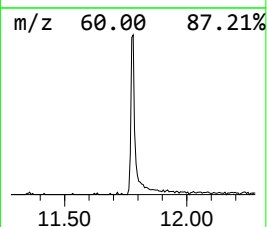
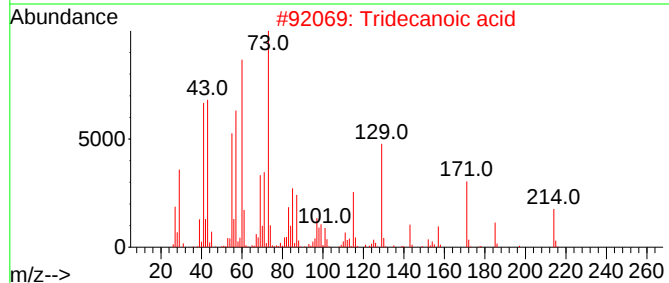
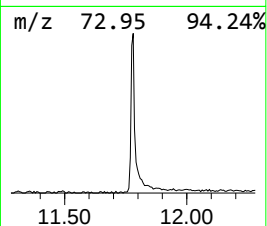
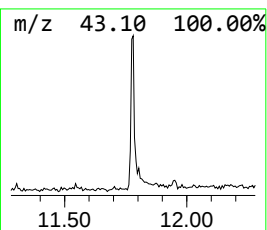
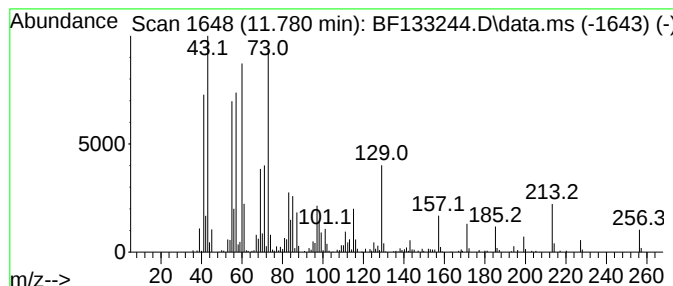
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.780	3.96 ng	373710	Phenanthrene-d10	11.239

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	92
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	91
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5			Undecanoic acid	186	C11H22O2	000112-37-8	58



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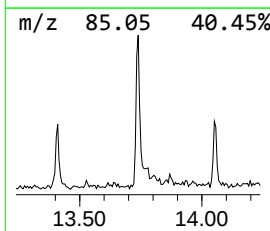
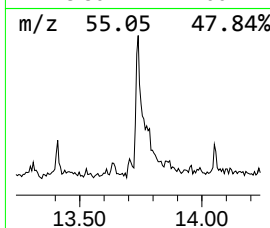
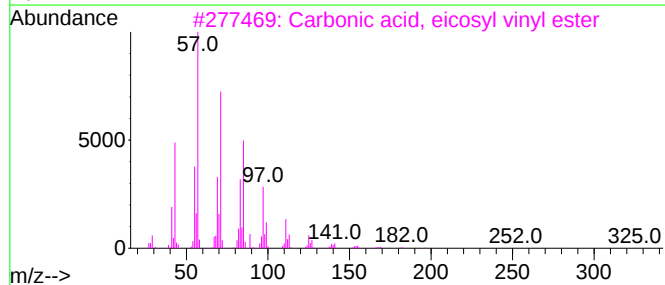
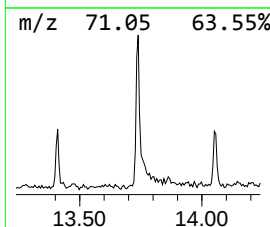
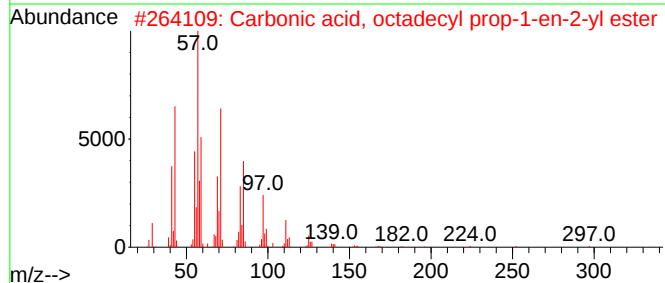
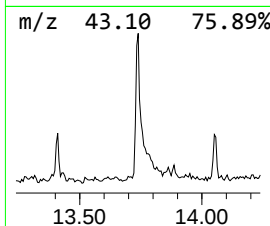
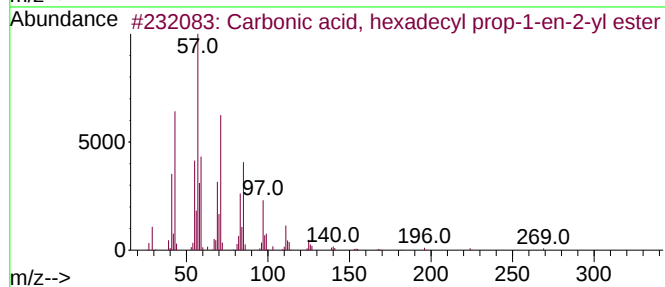
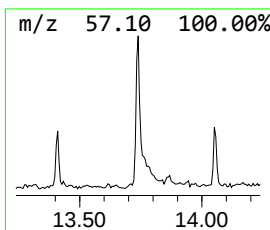
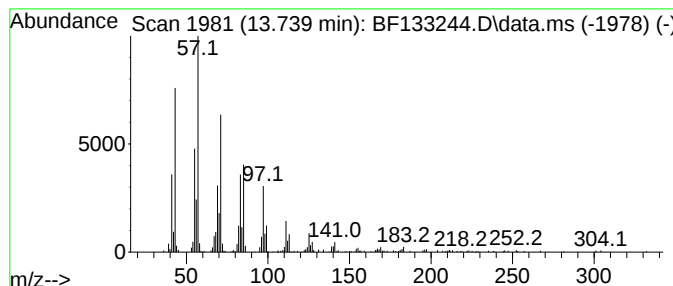
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Carbonic acid, hexadecyl pr... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.739	5.18 ng	313191	Chrysene-d12	13.874

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, hexadecyl prop-1-...	326	C20H38O3	1000382-90-3	91
2			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	91
3			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	90
4			Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	87
5			1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	87



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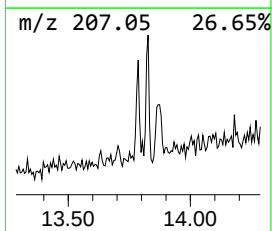
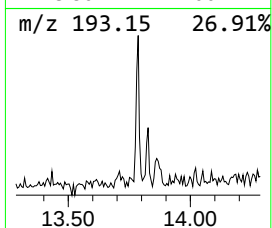
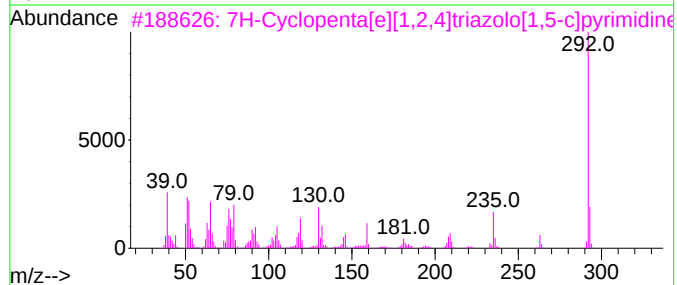
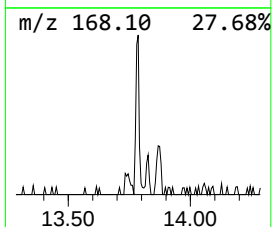
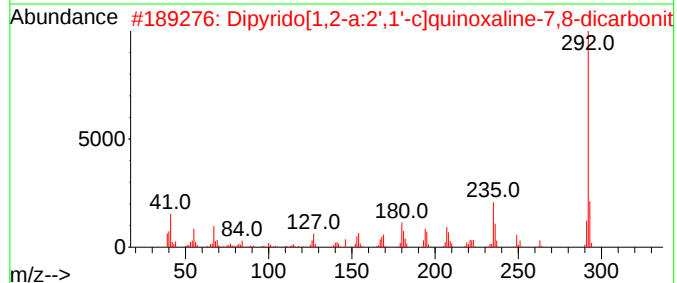
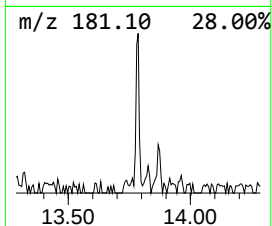
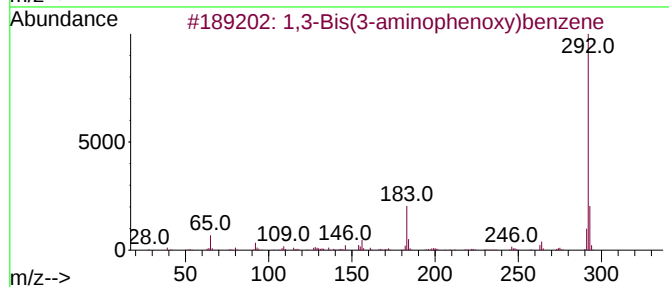
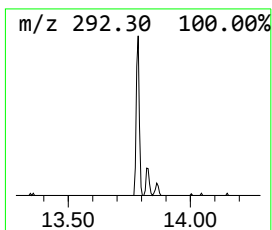
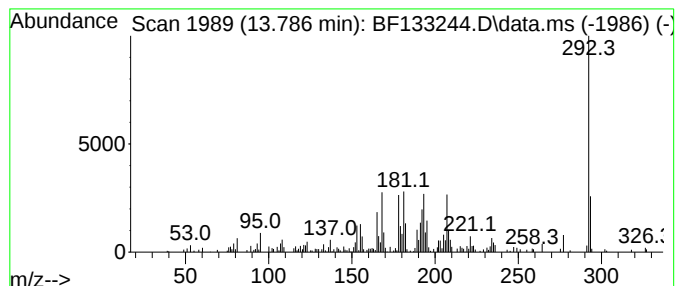
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 unknown13.786 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.786	2.22 ng	134275	Chrysene-d12	13.874

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Bis(3-aminophenoxy)benzene	292	C18H16N2O2	010526-07-5	42
2			Dipyrido[1,2-a:2',1'-c]quinoxali...	292	C18H20N4	1000303-96-3	38
3			7H-Cyclopenta[e][1,2,4]triazolo[...	292	C15H12N6O	1000350-92-3	35
4			1-(m-Chlorophenyl)piperazine, 4-...	292	C12H12ClF3N2O	003798-91-2	30
5			2-Methylamino-3-(N-methyl-N-phen...	292	C18H16N2O2	134614-15-6	30



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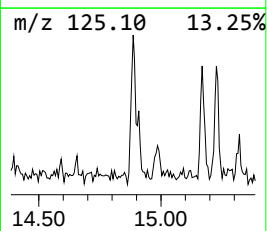
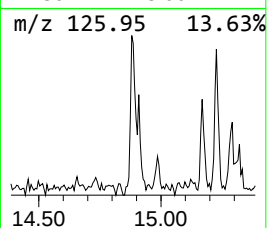
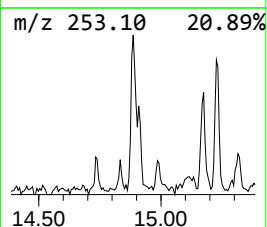
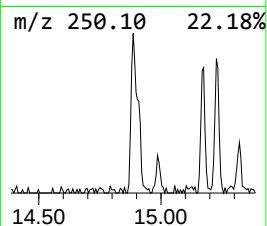
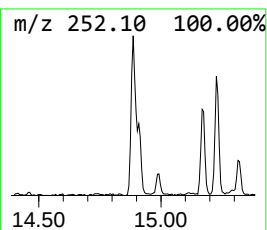
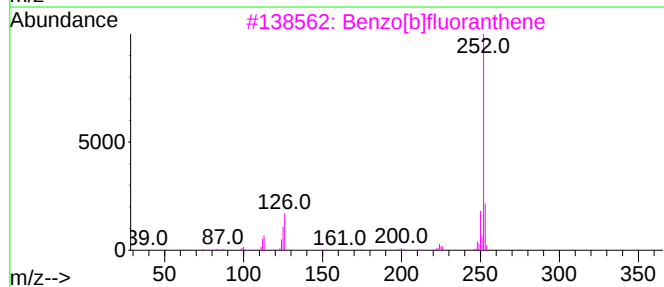
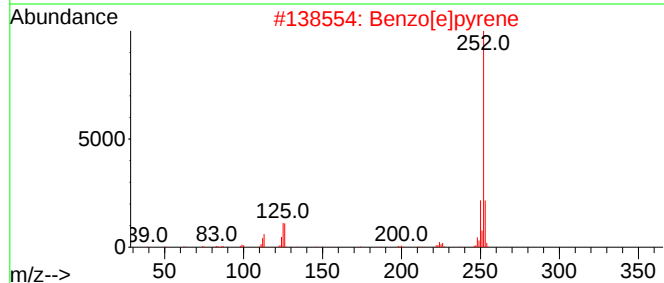
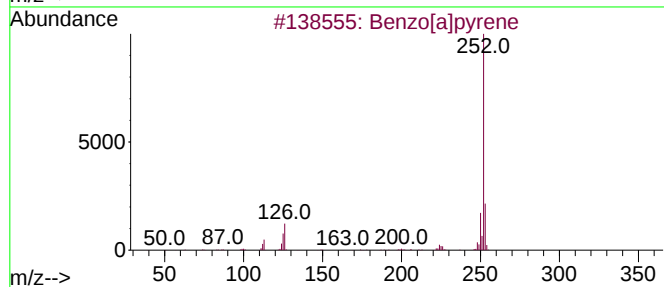
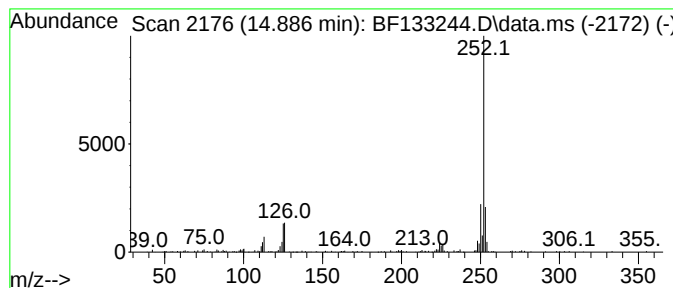
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.886	3.04 ng	174590	Perylene-d12	15.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[a]pyrene	252	C20H12	000050-32-8	98
2			Benzo[e]pyrene	252	C20H12	000192-97-2	98
3			Benzo[b]fluoranthene	252	C20H12	000205-99-2	96
4			Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
5			Perylene	252	C20H12	000198-55-0	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050423\
Data File : BF133244.D
Acq On : 04 May 2023 22:08
Operator : CG\JU
Sample : 02588-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ZONE-B-3-6-05012023

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
Benzophenone	10.469	3.6	ng	333864	3	9.757	1865540	20.0
n-Hexadecanoic ...	11.780	4.0	ng	373710	4	11.239	1888200	20.0
Carbonic acid, ...	13.739	5.2	ng	313191	5	13.874	1210030	20.0
unknown13.786	13.786	2.2	ng	134275	5	13.874	1210030	20.0
Benzo[e]pyrene	14.886	3.0	ng	174590	6	15.292	1149700	20.0