

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022221\
 Data File : BF123270.D
 Acq On : 22 Feb 2021 21:26
 Operator : JU/CG
 Sample : M1452-21 5X
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-6

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-BF021921.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123270.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.469	571	575	590	rBV	723645	641691	52.89%	5.687%
2	6.481	744	747	759	rBV	650154	558039	45.99%	4.946%
3	6.857	807	811	814	rBV	926777	761384	62.75%	6.748%
4	7.410	902	905	918	rBV	390002	354429	29.21%	3.141%
5	8.139	1025	1029	1032	rBV	1303510	1002965	82.66%	8.889%
6	9.216	1208	1212	1215	rBV	706748	539057	44.43%	4.777%
7	9.898	1324	1328	1332	rBV	1390379	1133811	93.45%	10.048%
8	10.686	1459	1462	1472	rBV	382746	350133	28.86%	3.103%
9	11.386	1577	1581	1584	rBV	1402633	1213338	100.00%	10.753%
10	11.410	1584	1585	1588	rVV	151009	91861	7.57%	0.814%
11	11.463	1592	1594	1598	rVB	26023	21789	1.80%	0.193%
12	11.892	1664	1667	1669	rBV	23983	22250	1.83%	0.197%
13	11.916	1669	1671	1679	rVV3	91957	129727	10.69%	1.150%
14	12.004	1683	1686	1688	rVV2	31024	37878	3.12%	0.336%
15	12.022	1688	1689	1694	rVB	14428	14983	1.23%	0.133%
16	12.210	1719	1721	1725	rVB5	20424	19573	1.61%	0.173%
17	12.369	1745	1748	1751	rBV	41938	35970	2.96%	0.319%
18	12.445	1756	1761	1763	rBV4	15176	19858	1.64%	0.176%
19	12.527	1772	1775	1778	rBV3	14891	14498	1.19%	0.128%
20	12.604	1784	1788	1793	rBV	276624	242327	19.97%	2.148%
21	12.710	1802	1806	1811	rBV4	37337	66847	5.51%	0.592%
22	12.833	1821	1827	1830	rBV	239208	226509	18.67%	2.007%
23	12.974	1848	1851	1856	rVB	672417	564190	46.50%	5.000%
24	13.045	1861	1863	1872	rBV4	18551	32177	2.65%	0.285%
25	13.139	1875	1879	1881	rVV5	16658	27696	2.28%	0.245%
26	13.163	1881	1883	1887	rVB	44113	38523	3.17%	0.341%
27	13.268	1898	1901	1904	rVB3	23736	22308	1.84%	0.198%
28	13.521	1940	1944	1948	rBV	410783	326168	26.88%	2.891%
29	13.674	1967	1970	1974	rVB	23563	31069	2.56%	0.275%
30	13.810	1991	1993	1996	rBV3	16111	15246	1.26%	0.135%
31	13.880	2003	2005	2008	rVB3	21083	14068	1.16%	0.125%
32	14.039	2027	2032	2034	rBV	1042585	1048263	86.39%	9.290%
33	14.063	2034	2036	2042	rVB	111723	97976	8.07%	0.868%
34	15.080	2205	2209	2218	rBV	96592	195444	16.11%	1.732%
35	15.445	2268	2271	2278	rBV	67668	94650	7.80%	0.839%
36	15.510	2278	2282	2286	rBV	601439	747648	61.62%	6.626%

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ClientSampleId :
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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

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37	16.445	2437	2441	2447	rVB	56225	95189	7.85%	0.844%
38	17.174	2558	2565	2572	rBV3	80373	203745	16.79%	1.806%
39	18.062	2710	2716	2728	rVB3	66026	230180	18.97%	2.040%

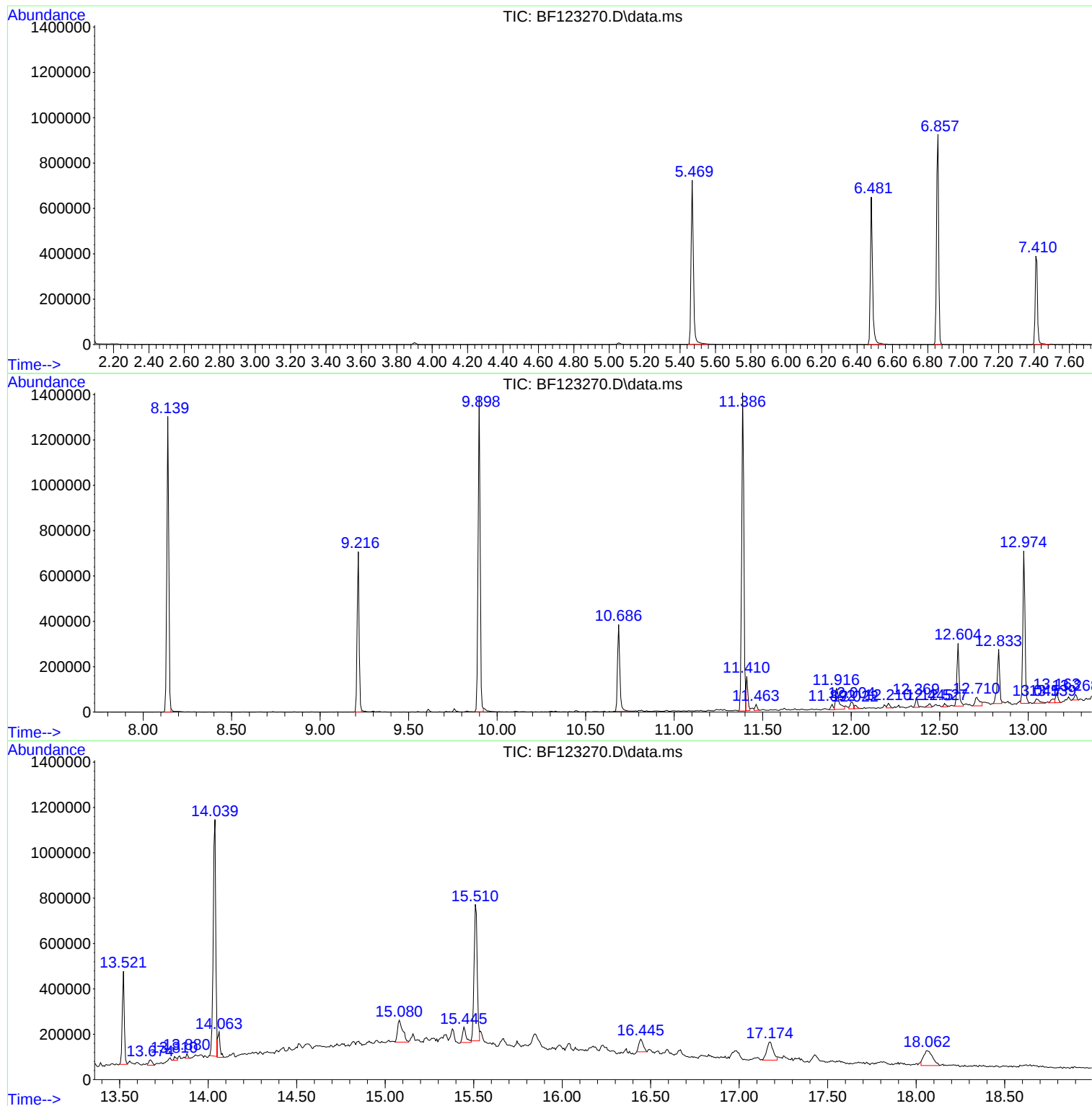
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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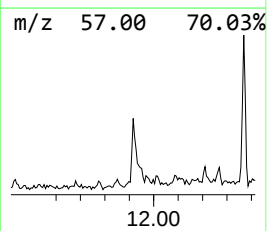
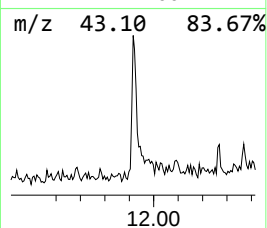
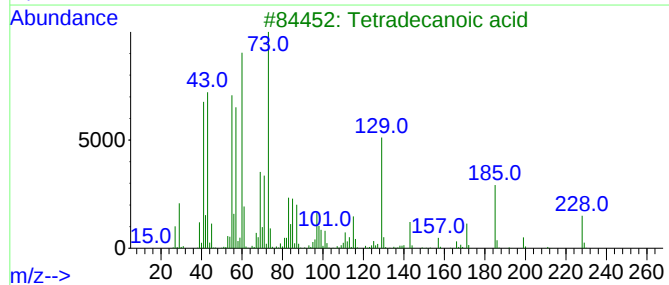
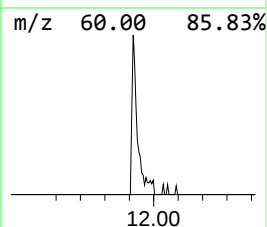
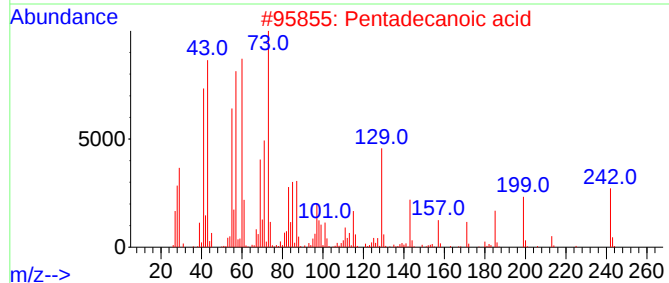
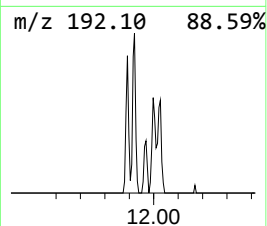
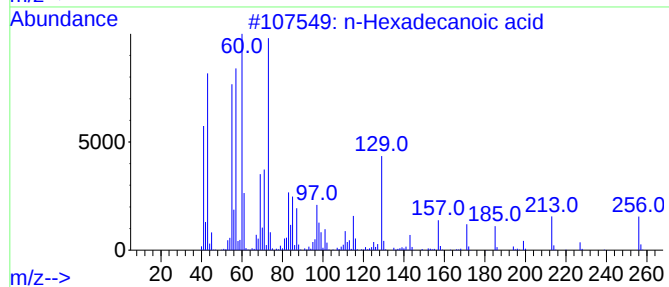
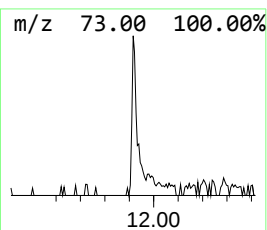
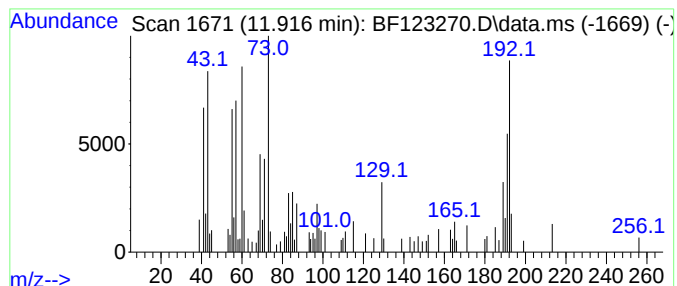
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	2.14 ng	129727	Phenanthrene-d10	11.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	49
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	49
4			Anthracene, 2-methyl-	192	C15H12	000613-12-7	30
5			1a,9b-Dihydro-1H-cyclopropa[a]an...	192	C15H12	006109-24-6	20



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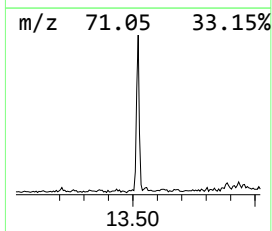
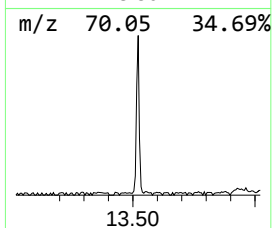
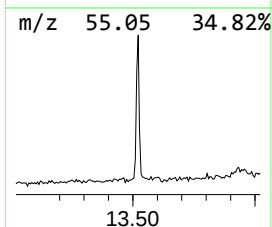
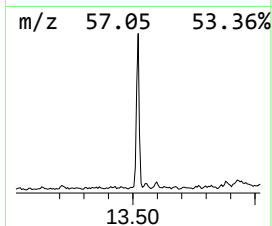
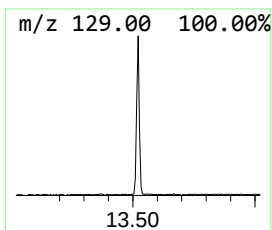
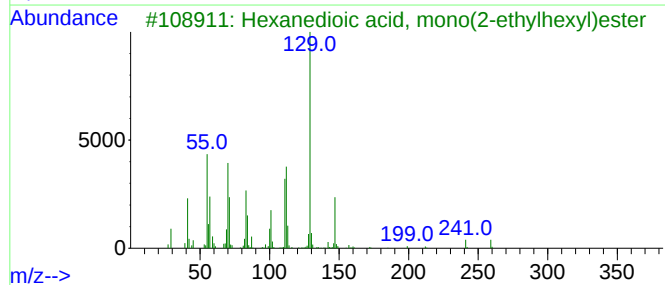
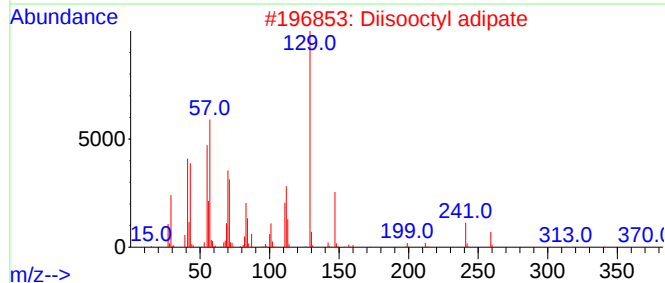
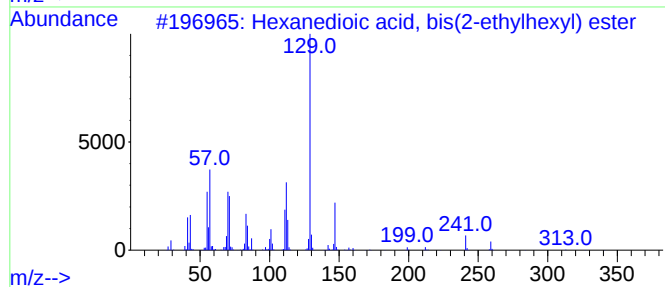
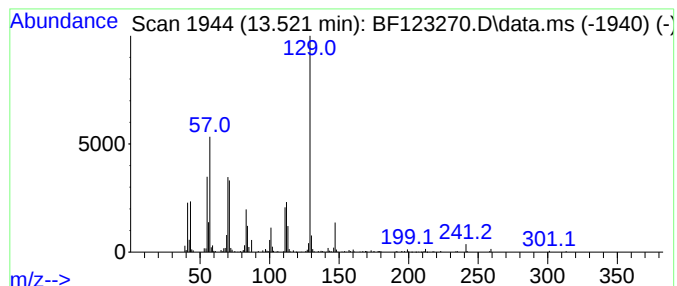
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 Hexanedioic acid, bis(2-eth... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.521	6.22 ng	326168	Chrysene-d12	14.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	91
2			Diisooctyl adipate	370	C22H42O4	001330-86-5	83
3			Hexanedioic acid, mono(2-ethylhe...	258	C14H26O4	004337-65-9	64
4			Hexanedioic acid, dioctyl ester	370	C22H42O4	000123-79-5	58
5			Adipic acid, 2-ethylhexyl pentyl...	328	C19H36O4	1000324-48-2	53



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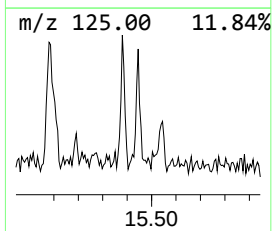
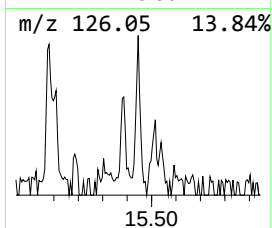
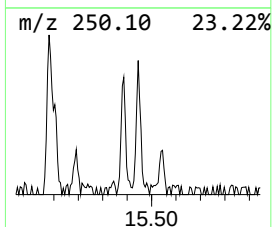
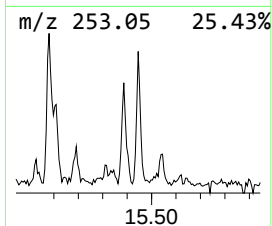
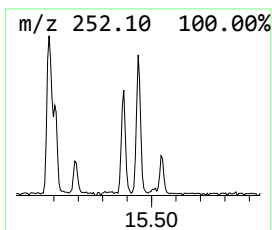
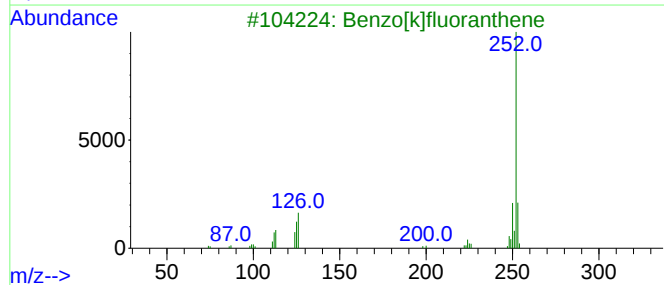
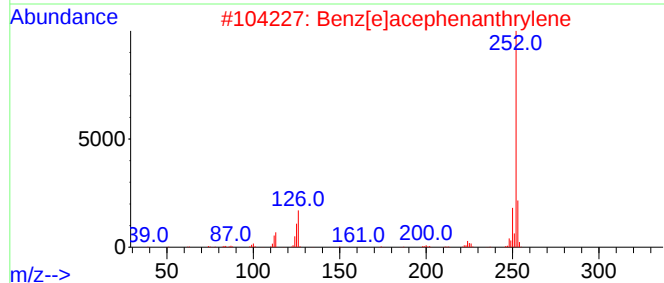
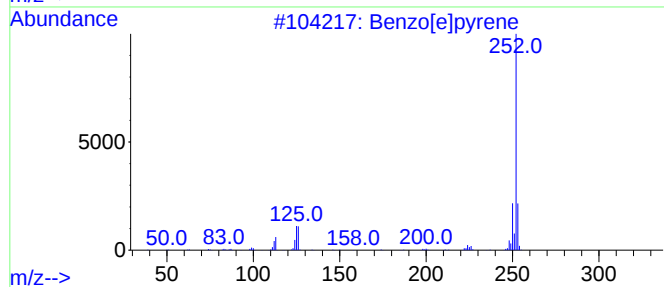
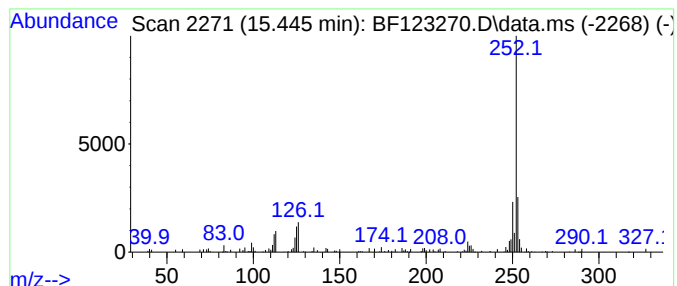
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.445	2.53 ng	94650	Perylene-d12	15.509

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	96
2			Benz[e]acephenanthrylene	252	C20H12	000205-99-2	95
3			Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
4			Perylene	252	C20H12	000198-55-0	93
5			Benzo[a]pyrene	252	C20H12	000050-32-8	93



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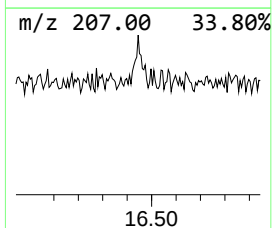
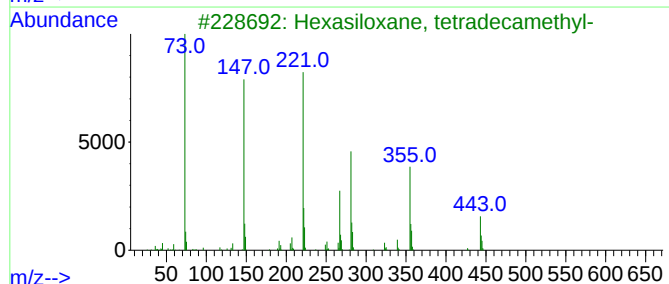
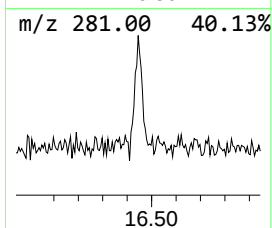
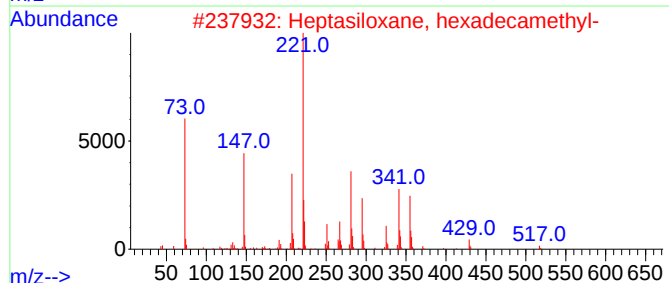
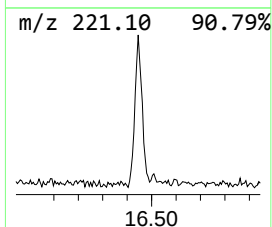
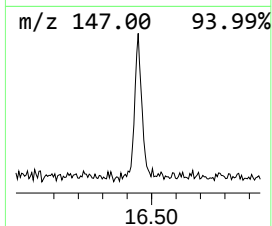
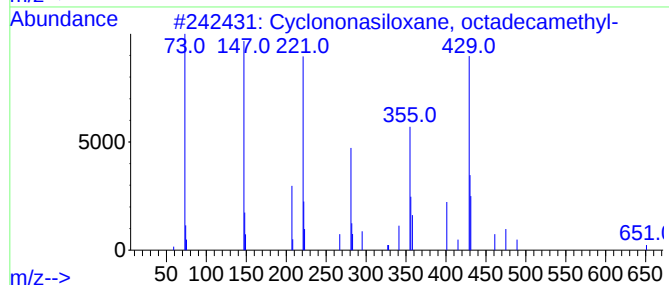
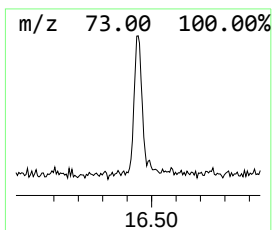
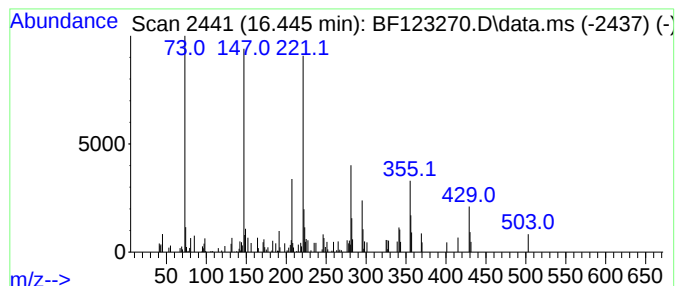
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Cyclononasiloxane, octadeca... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.445	2.55 ng	95189	Perylene-d12	15.509

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	87
2			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	42
3			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	38
4			4-Hydroxybenzyl alcohol, bis(ter...	352	C19H36O2Si2	1000364-43-9	25
5			Tris(trimethylsilyl)borate	278	C9H27B03Si3	004325-85-3	22



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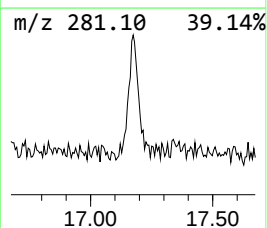
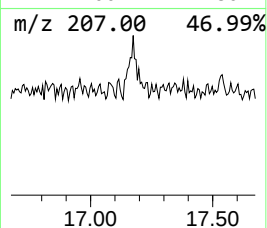
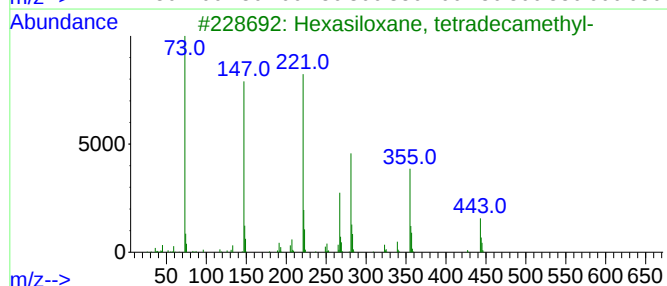
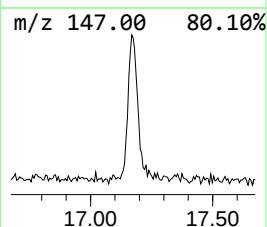
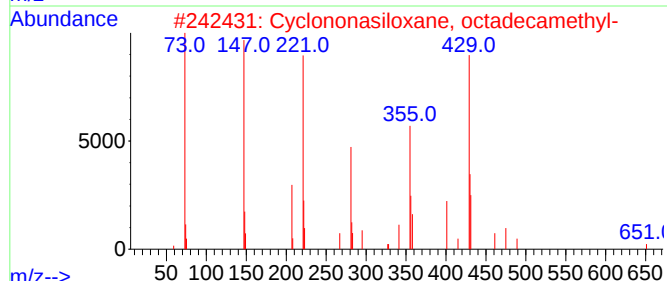
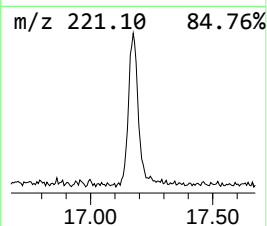
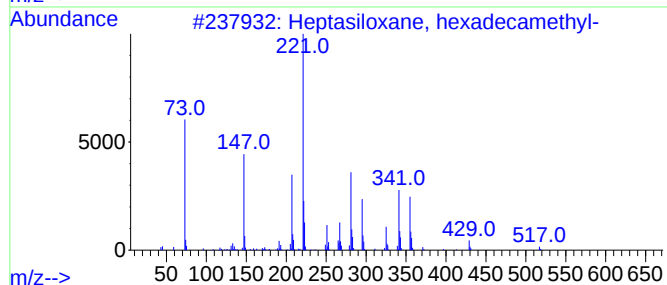
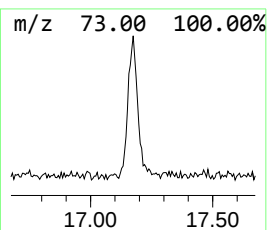
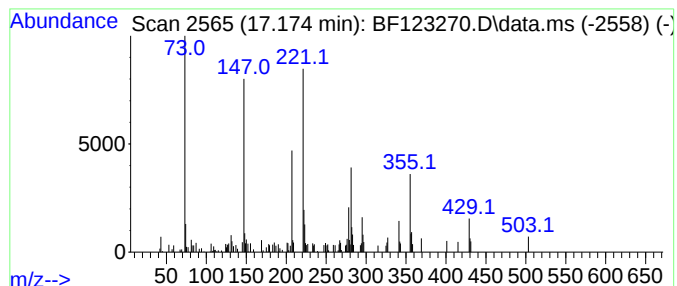
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Heptasiloxane, hexadecamethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.174	5.45 ng	203745	Perylene-d12	15.509

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	72
2			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	59
3			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	37
4			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	30
5			3-Isopropoxy-1,1,1,7,7,7-hexamet...	576	C18H52O7Si7	071579-69-6	16



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022221\
Data File : BF123270.D
Acq On : 22 Feb 2021 21:26
Operator : JU/CG
Sample : M1452-21 5X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-6

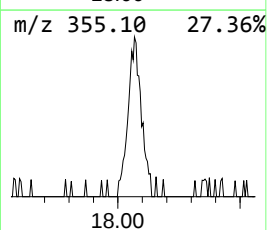
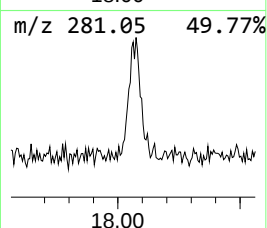
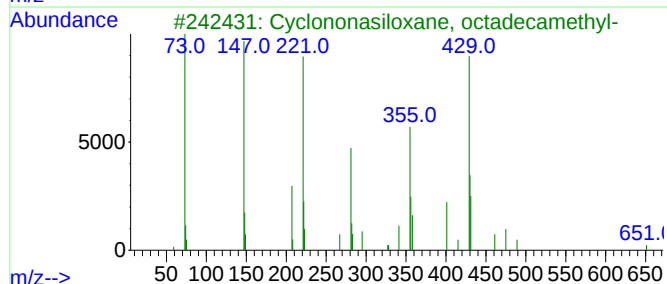
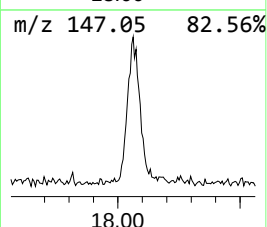
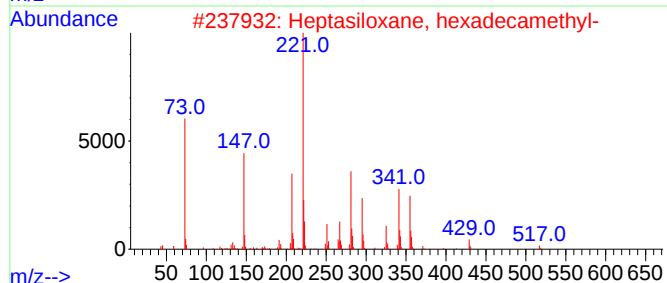
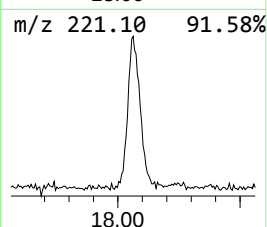
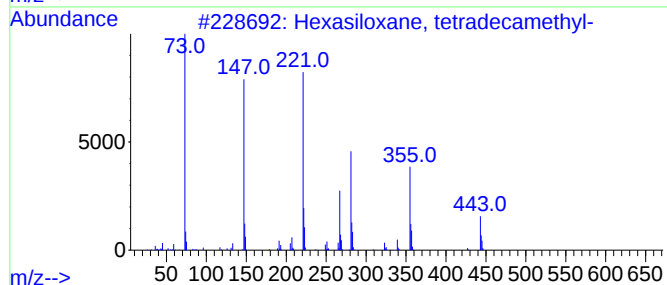
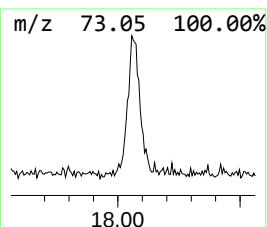
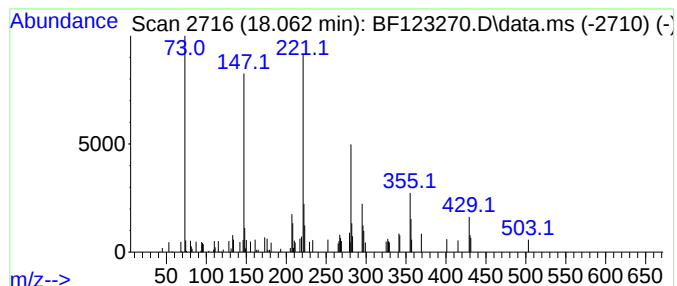
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Hexasiloxane, tetradecamethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.062	6.16 ng	230180	Perylene-d12	15.509

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	72
2		Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	58
3		Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	50
4		3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	40
5		Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022221\
Data File : BF123270.D
Acq On : 22 Feb 2021 21:26
Operator : JU/CG
Sample : M1452-21 5X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	11.916	2.1	ng	129727	4	11.386	1213340	20.0
Hexanedioic aci...	13.521	6.2	ng	326168	5	14.039	1048260	20.0
Benzo[e]pyrene	15.445	2.5	ng	94650	6	15.509	747648	20.0
Cyclononasiloxa...	16.445	2.5	ng	95189	6	15.509	747648	20.0
Heptasiloxane, ...	17.174	5.5	ng	203745	6	15.509	747648	20.0
Hexasiloxane, t...	18.062	6.2	ng	230180	6	15.509	747648	20.0