

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF072822\  
 Data File : BF129404.D  
 Acq On : 28 Jul 2022 12:31  
 Operator : CG\JU  
 Sample : N3893-08  
 Misc :  
 ALS Vial : 7 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 RVE-8

Integration Parameters: rteint.p  
 Integrator: RTE  
 Smoothing : ON  
 Sampling : 1  
 Start Thrs: 0.2  
 Stop Thrs : 0  
 Filtering: 5  
 Min Area: 3 % of largest Peak  
 Max Peaks: 100  
 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-BF072522.M  
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF129404.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.510	205	208	230	rBV	20056	85328	1.51%	0.222%
2	5.128	480	483	492	rVB	43641	56495	1.00%	0.147%
3	5.516	544	549	552	rBV	4752073	4727584	83.83%	12.278%
4	6.522	714	720	723	rBV	4573111	4854039	86.08%	12.607%
5	6.881	778	781	785	rVB	1488554	1159437	20.56%	3.011%
6	7.445	872	877	880	rBV	3058453	3117519	55.28%	8.097%
7	8.163	995	999	1003	rBV	1743326	1540912	27.32%	4.002%
8	9.245	1177	1183	1186	rBV	5772981	5639227	100.00%	14.646%
9	9.922	1294	1298	1302	rBV	1955764	1702425	30.19%	4.421%
10	10.716	1429	1433	1436	rBV	3801238	3382626	59.98%	8.785%
11	11.416	1548	1552	1554	rBV	1853897	1588288	28.16%	4.125%
12	11.433	1554	1555	1561	rVB	127160	109797	1.95%	0.285%
13	11.792	1613	1616	1620	rBV	162064	139302	2.47%	0.362%
14	12.027	1652	1656	1658	rBV2	53213	56659	1.00%	0.147%
15	12.504	1732	1737	1742	rVB2	92415	127042	2.25%	0.330%
16	12.627	1755	1758	1762	rVB	373068	298681	5.30%	0.776%
17	12.857	1791	1797	1804	rBV	383028	412179	7.31%	1.070%
18	13.004	1817	1822	1825	rBV	4851985	4553381	80.74%	11.826%
19	13.274	1865	1868	1874	rVB2	455957	382225	6.78%	0.993%
20	13.574	1914	1919	1923	rBV2	110286	133129	2.36%	0.346%
21	13.810	1954	1959	1961	rBV5	34619	60375	1.07%	0.157%
22	13.904	1970	1975	1984	rVB4	101671	224070	3.97%	0.582%
23	14.057	1996	2001	2004	rBV	1129796	1153703	20.46%	2.996%
24	14.080	2004	2005	2011	rVB	161603	145754	2.58%	0.379%
25	14.510	2075	2078	2081	rBV2	68906	61105	1.08%	0.159%
26	15.110	2176	2180	2187	rBV	177365	313321	5.56%	0.814%
27	15.163	2187	2189	2195	rVB	121718	131359	2.33%	0.341%
28	15.221	2196	2199	2203	rBV2	51428	86454	1.53%	0.225%
29	15.421	2229	2233	2238	rVB	119895	153378	2.72%	0.398%
30	15.486	2240	2244	2249	rVB	158307	207457	3.68%	0.539%
31	15.551	2250	2255	2259	rBV	923744	1109893	19.68%	2.883%
32	15.763	2288	2291	2297	rVB4	52684	74985	1.33%	0.195%
33	15.998	2327	2331	2336	rVB	130291	179274	3.18%	0.466%
34	17.057	2506	2511	2518	rBV2	82435	177080	3.14%	0.460%
35	17.215	2532	2538	2546	rBV8	102837	246067	4.36%	0.639%
36	17.515	2584	2589	2595	rVB	62918	113516	2.01%	0.295%

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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-BF072522.M  
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

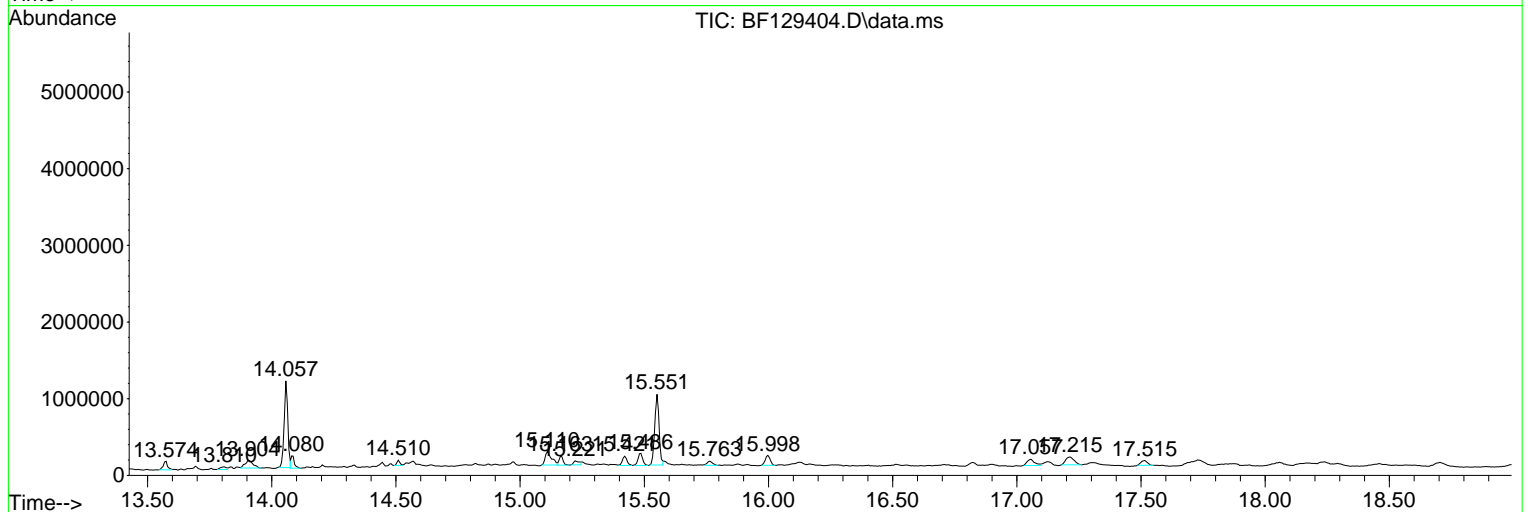
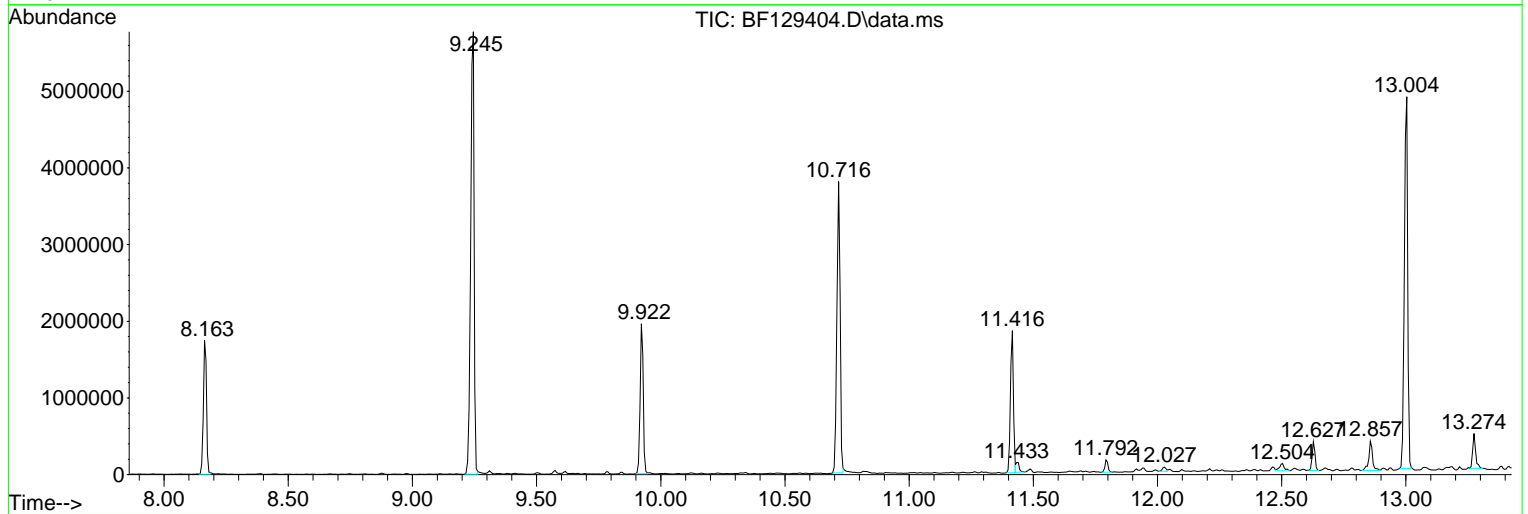
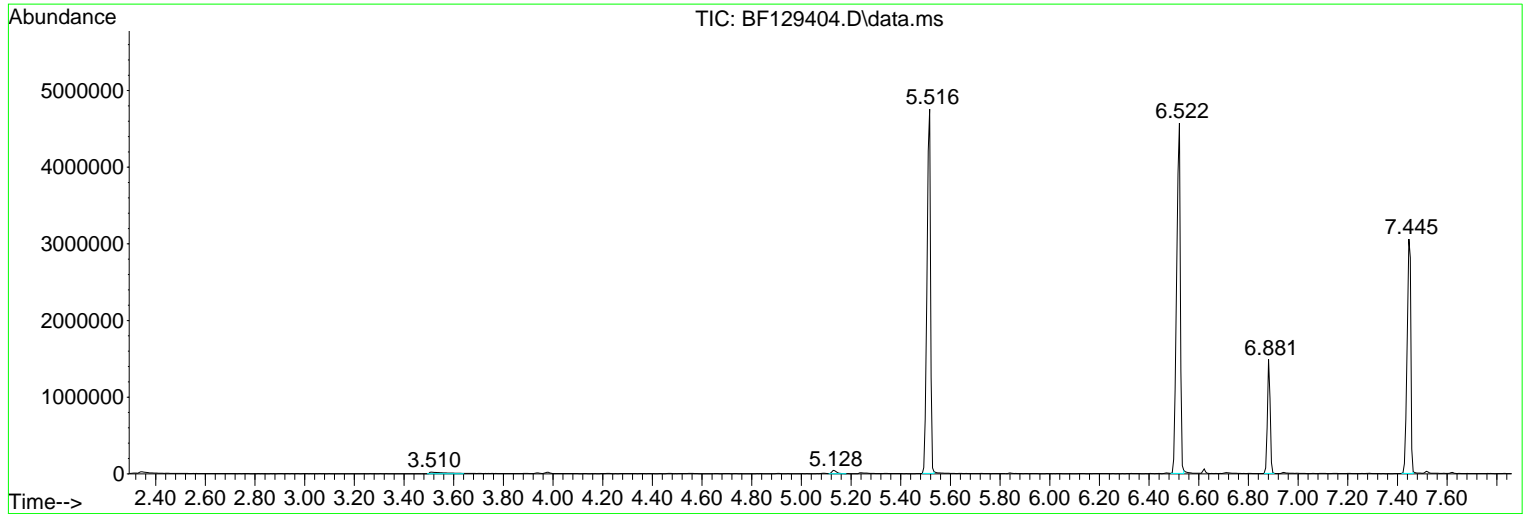
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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF072522.M  
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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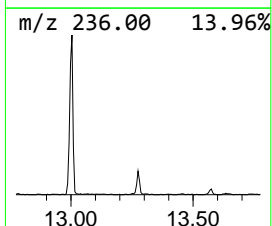
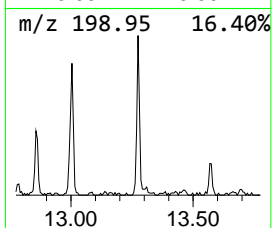
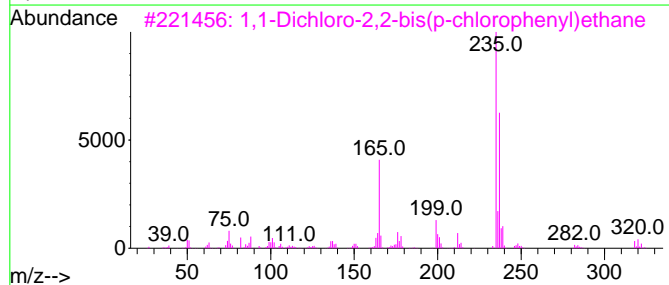
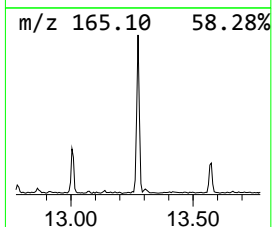
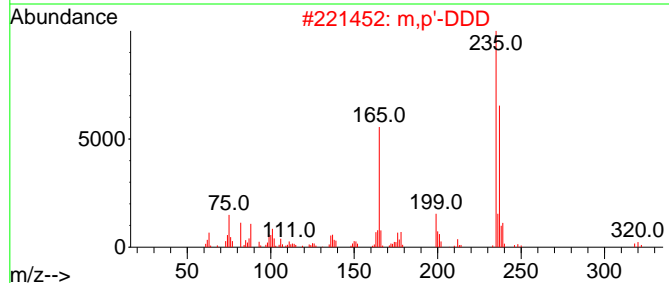
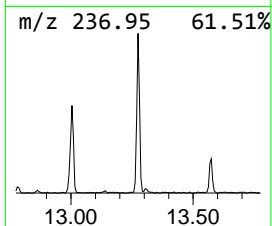
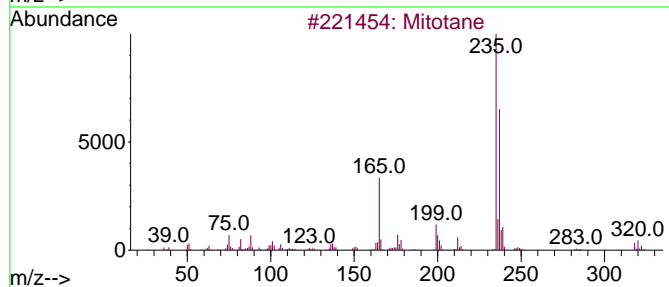
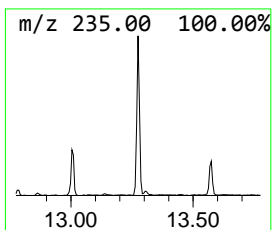
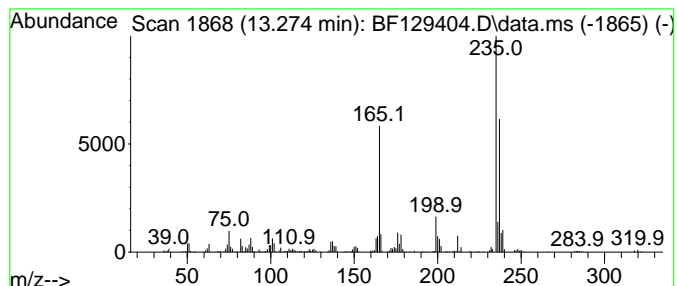
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF072522.M  
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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 Peak Number 1 Mitotane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.275	6.63 ng	382225	Chrysene-d12	14.057

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Mitotane	318	C14H10Cl4	000053-19-0	99
2		m,p'-DDD	318	C14H10Cl4	004329-12-8	99
3		1,1-Dichloro-2,2-bis(p-chlorophe...	318	C14H10Cl4	000072-54-8	95
4		2,2-Bis(p-chlorophenyl)ethanol	266	C14H12Cl2O	002642-82-2	91
5		3-Butanone, 1,1-bis(4-chlorophen...	320	C18H18Cl2O	1000158-20-4	80



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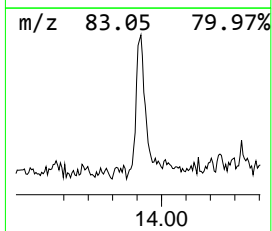
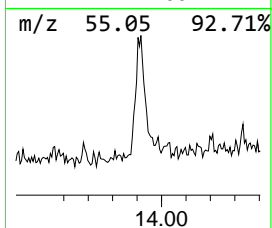
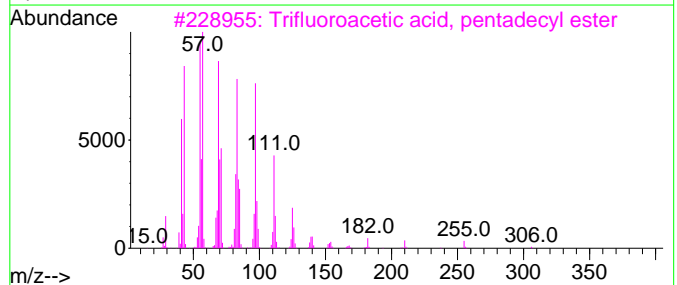
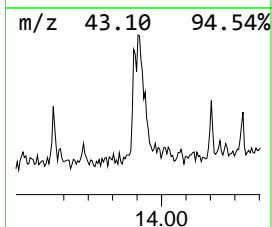
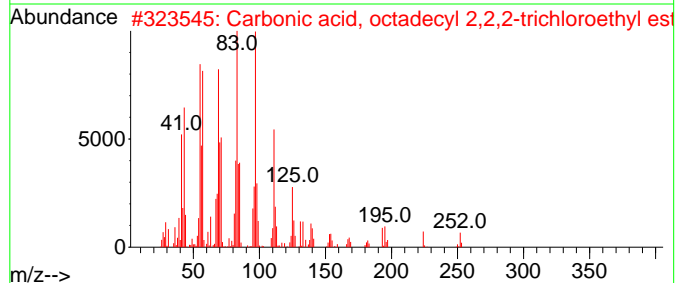
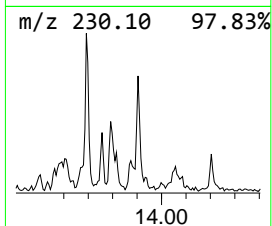
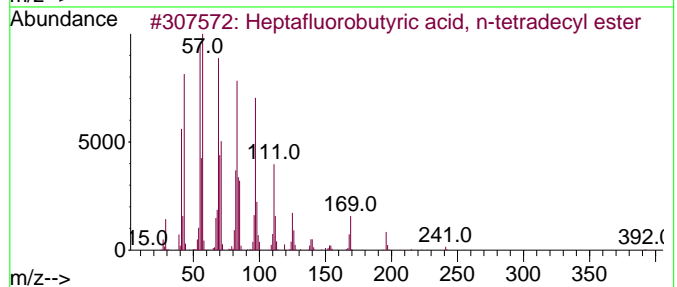
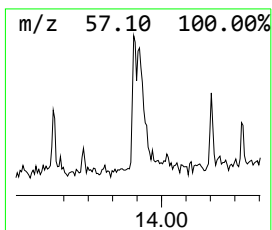
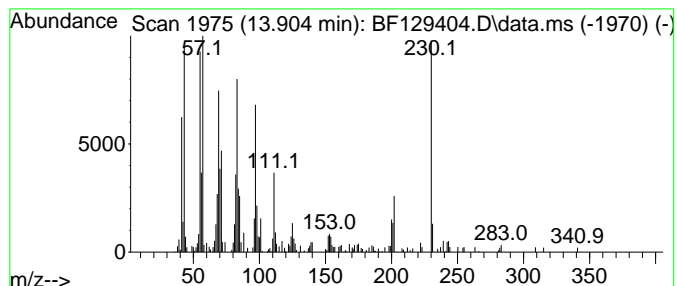
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TIC Library : C:\Database\NIST20.L  
 TIC Integration Parameters: LSCINT.P

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 Peak Number 3 Heptafluorobutyric acid, n-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	3.88 ng	224070	Chrysene-d12	14.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	89
2			Carbonic acid, octadecyl 2,2,2-t...	444	C21H39Cl3O3	1000314-56-3	76
3			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	76
4			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	76
5			2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	76



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 ClientSampleId :  
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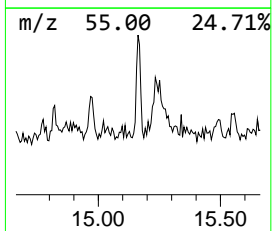
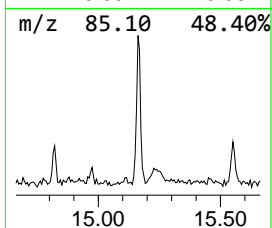
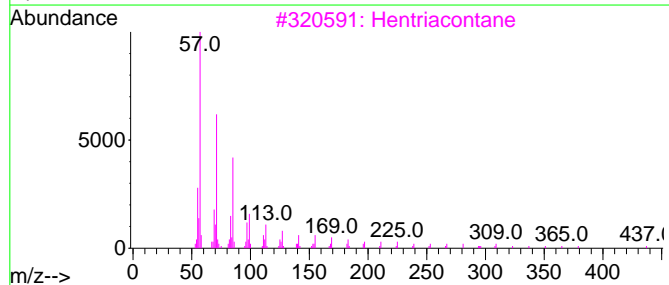
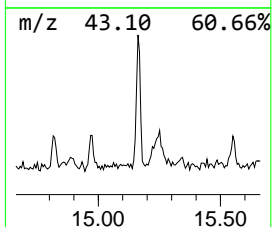
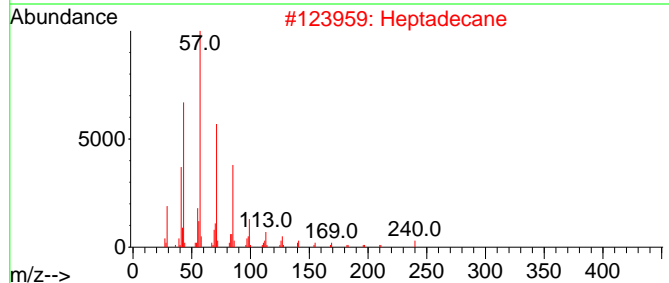
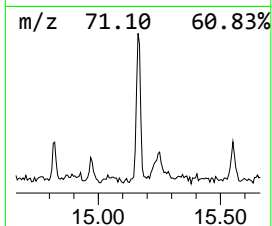
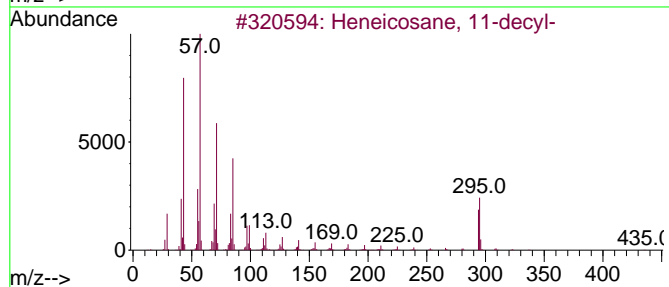
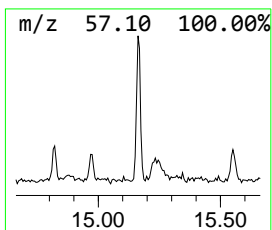
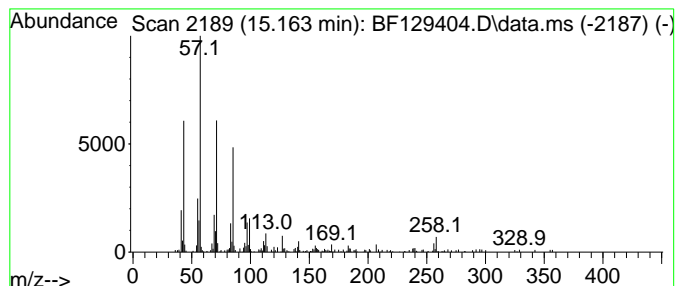
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF072522.M  
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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 Peak Number 4 Heneicosane, 11-decyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.163	2.37 ng	131359	Perylene-d12	15.551

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heneicosane, 11-decyl-	437	C31H64	055320-06-4	87
2		Heptadecane	240	C17H36	000629-78-7	87
3		Hentriacontane	437	C31H64	000630-04-6	83
4		Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	83
5		Octacosane	394	C28H58	000630-02-4	83



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Instrument :  
 BNA\_F  
 ClientSampleId :  
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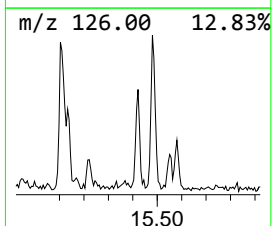
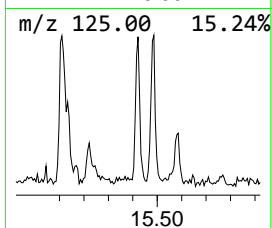
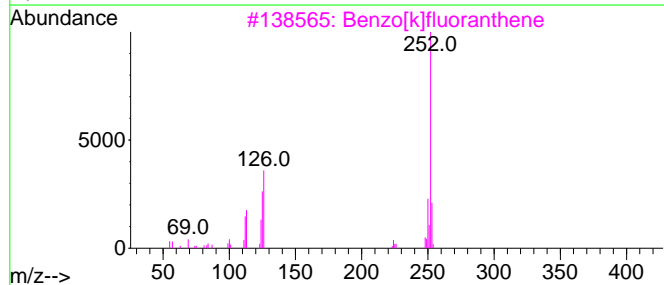
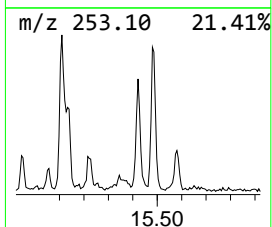
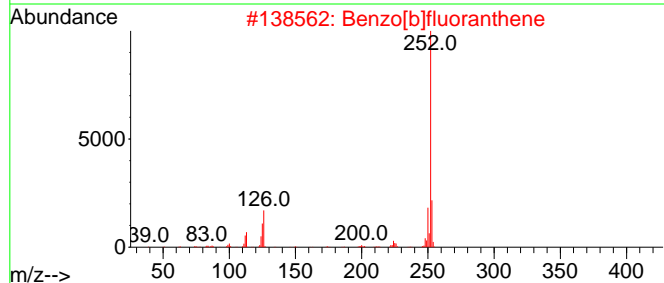
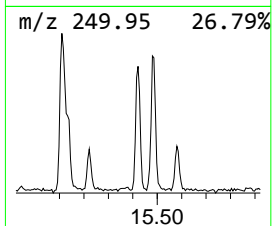
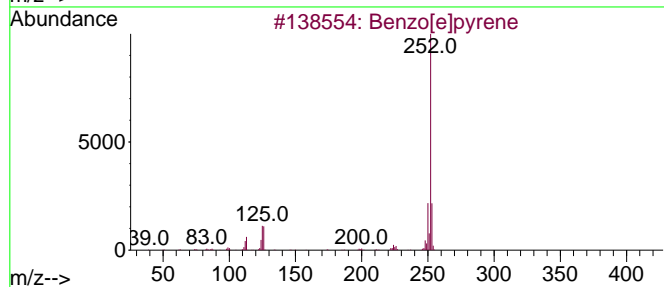
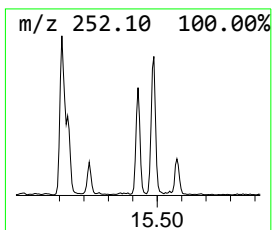
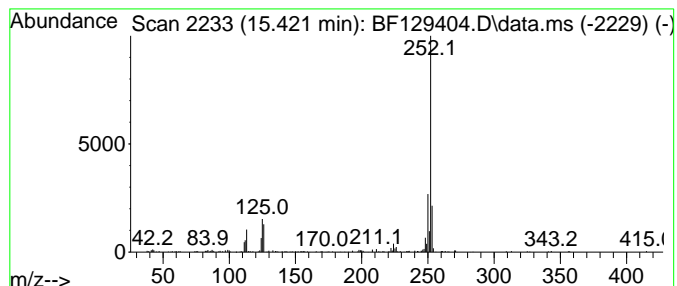
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TIC Library : C:\Database\NIST20.L  
 TIC Integration Parameters: LSCINT.P

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 Peak Number 5 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.421	2.76 ng	153378	Perylene-d12	15.551

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzo[e]pyrene	252	C20H12	000192-97-2	96
2		Benzo[b]fluoranthene	252	C20H12	000205-99-2	95
3		Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
4		Benzo[a]pyrene	252	C20H12	000050-32-8	91
5		Perylene	252	C20H12	000198-55-0	89



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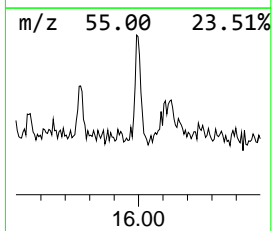
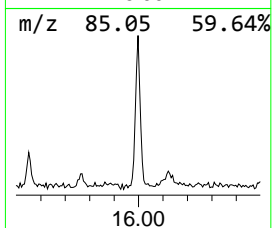
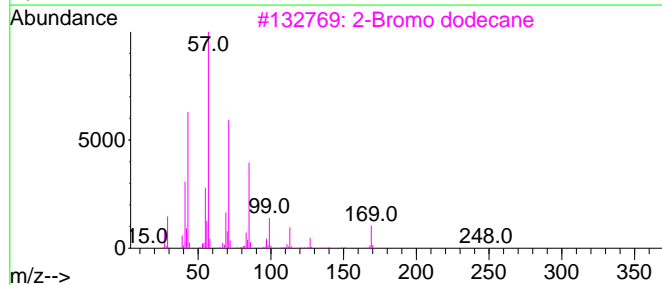
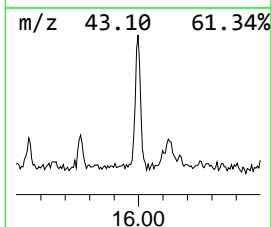
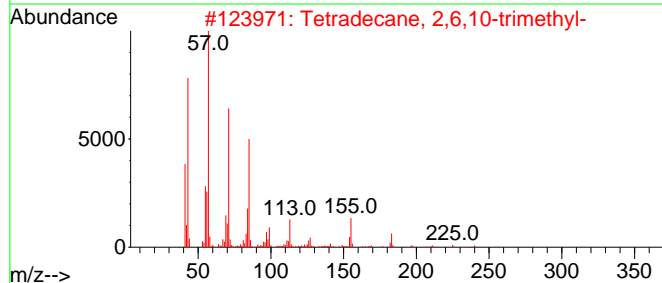
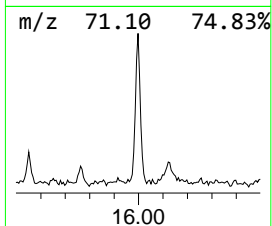
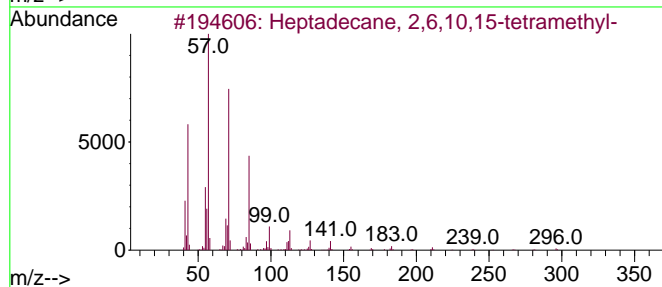
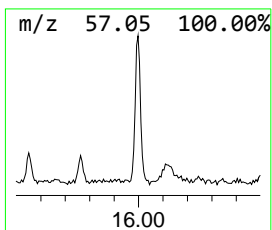
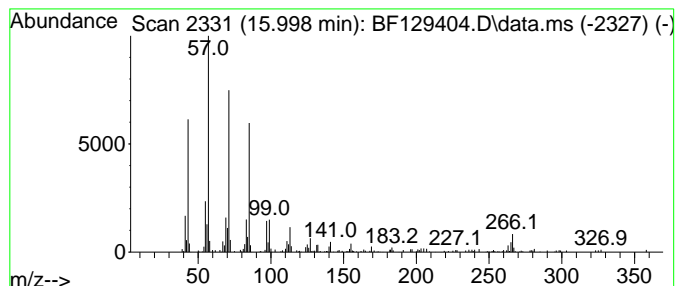
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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 Peak Number 6 Heptadecane, 2,6,10,15-tetr... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.998	3.23 ng	179274	Perylene-d12	15.551

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	94
2		Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	90
3		2-Bromo dodecane	248	C12H25Br	013187-99-0	90
4		Hexacosane	366	C26H54	000630-01-3	90
5		Heneicosane	296	C21H44	000629-94-7	87





Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF072822\  
 Data File : BF129404.D  
 Acq On : 28 Jul 2022 12:31  
 Operator : CG\JU  
 Sample : N3893-08  
 Misc :  
 ALS Vial : 7 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 RVE-8

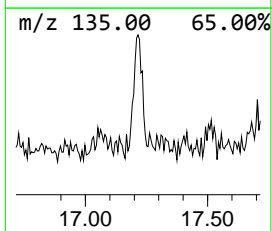
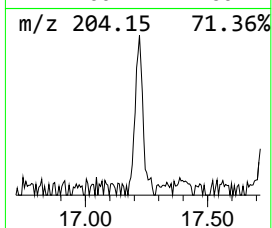
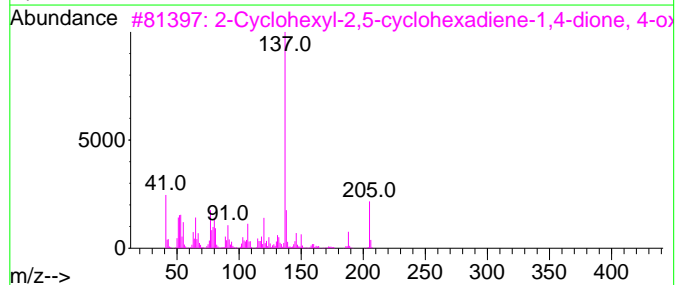
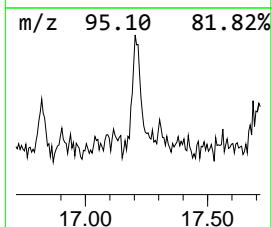
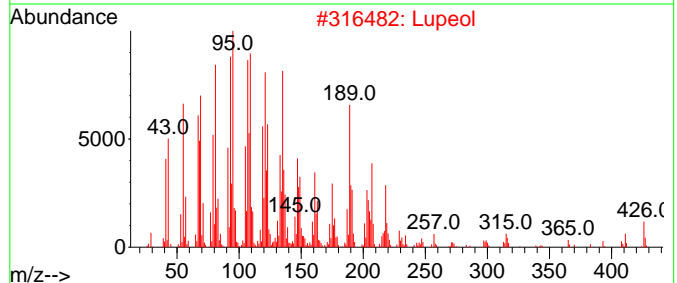
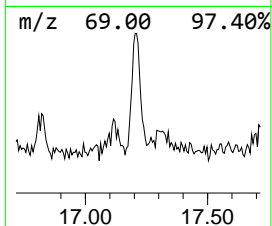
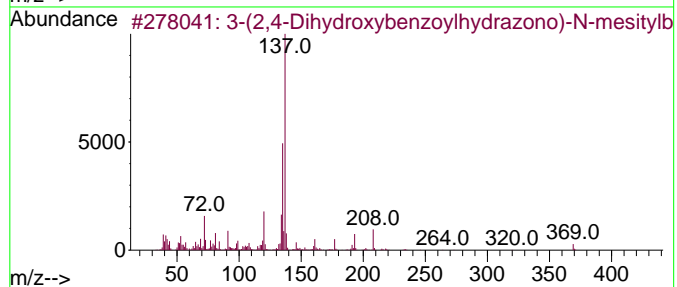
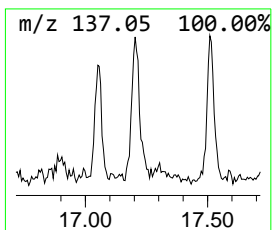
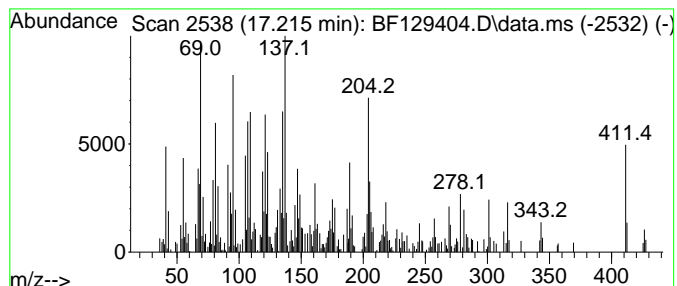
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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 Peak Number 7 unknown17.215 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.215	4.43 ng	246067	Perylene-d12	15.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-(2,4-Dihydroxybenzoylhydrazono...	369	C20H23N3O4	1000225-34-7	44		
2	Lupeol	426	C30H50O	000545-47-1	35		
3	2-Cyclohexyl-2,5-cyclohexadiene-...	205	C12H15NO2	107244-54-2	25		
4	Thieno[2,3-b]pyridine-2-carboxam...	301	C15H15N3O2S	1000350-91-4	20		
5	Bicyclo[3.3.1]nonane-3-carboxami...	301	C18H23NO3	1000319-79-6	20		



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF072822\  
 Data File : BF129404.D  
 Acq On : 28 Jul 2022 12:31  
 Operator : CG\JU  
 Sample : N3893-08  
 Misc :  
 ALS Vial : 7 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 RVE-8

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF072522.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
Mitotane	13.275	6.6	ng	382225	5	14.057	1153700	20.0
Heptafluorobuty...	13.904	3.9	ng	224070	5	14.057	1153700	20.0
Heneicosane, 11...	15.163	2.4	ng	131359	6	15.551	1109890	20.0
Benzo[e]pyrene	15.421	2.8	ng	153378	6	15.551	1109890	20.0
Heptadecane, 2,...	15.998	3.2	ng	179274	6	15.551	1109890	20.0
unknown17.215	17.215	4.4	ng	246067	6	15.551	1109890	20.0