

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070522\
 Data File : BF129121.D
 Acq On : 05 Jul 2022 13:44
 Operator : CG\JU
 Sample : N3572-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RBR-200033

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-BF062922.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF129121.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.199	492	495	502	rVB	88185	106120	1.57%	0.140%
2	5.581	555	560	563	rBV	6151739	5747258	85.05%	7.572%
3	6.575	724	729	732	rBV	5386857	5506602	81.49%	7.255%
4	6.957	790	794	797	rBV	1943865	1531266	22.66%	2.017%
5	7.516	884	889	892	rBV	4151135	3748557	55.47%	4.939%
6	8.240	1008	1012	1015	rBV	2436985	1935698	28.64%	2.550%
7	9.316	1190	1195	1198	rBV	7225720	6757725	100.00%	8.903%
8	9.857	1281	1287	1291	rBV	214661	184035	2.72%	0.242%
9	9.998	1307	1311	1314	rBV	2467103	1936928	28.66%	2.552%
10	10.028	1314	1316	1321	rVB	71855	70405	1.04%	0.093%
11	10.786	1441	1445	1452	rBV	4172119	3703211	54.80%	4.879%
12	11.492	1561	1565	1567	rBV	1907307	1831430	27.10%	2.413%
13	11.516	1567	1569	1573	rVV	834187	688813	10.19%	0.908%
14	11.563	1574	1577	1580	rVB	195570	162177	2.40%	0.214%
15	11.716	1597	1603	1609	rBV	86635	121399	1.80%	0.160%
16	12.004	1647	1652	1654	rBV	836253	893993	13.23%	1.178%
17	12.104	1666	1669	1671	rBV2	231850	238363	3.53%	0.314%
18	12.128	1671	1673	1676	rVB	112820	90576	1.34%	0.119%
19	12.222	1687	1689	1694	rBV3	94338	101180	1.50%	0.133%
20	12.286	1697	1700	1702	rVV	132776	114670	1.70%	0.151%
21	12.310	1702	1704	1708	rVB2	144338	125064	1.85%	0.165%
22	12.545	1740	1744	1746	rBV	137442	147079	2.18%	0.194%
23	12.627	1756	1758	1762	rBV	121838	109195	1.62%	0.144%
24	12.710	1768	1772	1775	rBV	2420259	2143293	31.72%	2.824%
25	12.792	1780	1786	1790	rBV2	387210	480900	7.12%	0.634%
26	12.939	1808	1811	1816	rVB	2180938	1857544	27.49%	2.447%
27	12.986	1816	1819	1822	rVB2	109552	113324	1.68%	0.149%
28	13.080	1828	1835	1838	rBV	7085396	6570722	97.23%	8.657%
29	13.151	1843	1847	1851	rBV2	169904	269741	3.99%	0.355%
30	13.239	1859	1862	1864	rBV4	155752	198831	2.94%	0.262%
31	13.263	1864	1866	1869	rVB	316787	290669	4.30%	0.383%
32	13.333	1875	1878	1880	rBV2	189728	154172	2.28%	0.203%
33	13.369	1880	1884	1887	rBV2	249685	275620	4.08%	0.363%
34	13.463	1898	1900	1903	rBV	122100	102314	1.51%	0.135%
35	13.492	1903	1905	1907	rBV	112239	126403	1.87%	0.167%
36	13.651	1927	1932	1934	rBV4	90437	152833	2.26%	0.201%

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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-BF062922.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.774	1950	1953	1957	rVB	272188	284315	4.21%	0.375%
38	13.886	1968	1972	1975	rBV2	252685	317638	4.70%	0.418%
39	13.916	1975	1977	1979	rBV	231817	176853	2.62%	0.233%
40	13.939	1979	1981	1985	rBV2	165520	180587	2.67%	0.238%
41	13.980	1985	1988	1991	rBV2	288334	388610	5.75%	0.512%
42	14.110	2006	2010	2012	rBV	3196003	3150428	46.62%	4.151%
43	14.139	2012	2015	2018	rVV2	2695250	3512326	51.97%	4.627%
44	14.169	2018	2020	2025	rVB	1404690	1247710	18.46%	1.644%
45	14.233	2026	2031	2037	rBV	2155786	2466503	36.50%	3.250%
46	14.286	2037	2040	2044	rVB3	145863	163106	2.41%	0.215%
47	14.527	2078	2081	2084	rVB	286799	257034	3.80%	0.339%
48	14.563	2084	2087	2090	rBV2	222136	213559	3.16%	0.281%
49	14.592	2090	2092	2094	rBV2	134124	108780	1.61%	0.143%
50	14.651	2095	2102	2105	rBV3	443124	947550	14.02%	1.248%
51	14.763	2118	2121	2124	rVB	244001	200079	2.96%	0.264%
52	14.998	2158	2161	2163	rBV	107423	113630	1.68%	0.150%
53	15.069	2170	2173	2177	rVB	446968	444035	6.57%	0.585%
54	15.216	2193	2198	2201	rBV	1591859	2660478	39.37%	3.505%
55	15.268	2205	2207	2213	rVB2	279579	335099	4.96%	0.441%
56	15.327	2213	2217	2220	rBV	680411	1176495	17.41%	1.550%
57	15.533	2248	2252	2258	rVB	996461	1267398	18.75%	1.670%
58	15.598	2259	2263	2269	rVB	1271419	1589822	23.53%	2.095%
59	15.668	2270	2275	2278	rVV	1803651	2307380	34.14%	3.040%
60	15.698	2278	2280	2286	rVB2	365686	492331	7.29%	0.649%
61	15.892	2309	2313	2321	rVB3	244261	411761	6.09%	0.542%
62	16.133	2350	2354	2358	rVB2	291860	408473	6.04%	0.538%
63	16.263	2373	2376	2381	rBV3	116440	201402	2.98%	0.265%
64	16.992	2496	2500	2503	rBV3	132280	228907	3.39%	0.302%
65	17.221	2533	2539	2548	rVB2	537340	1204778	17.83%	1.587%
66	17.692	2613	2619	2631	rVB	407403	856668	12.68%	1.129%

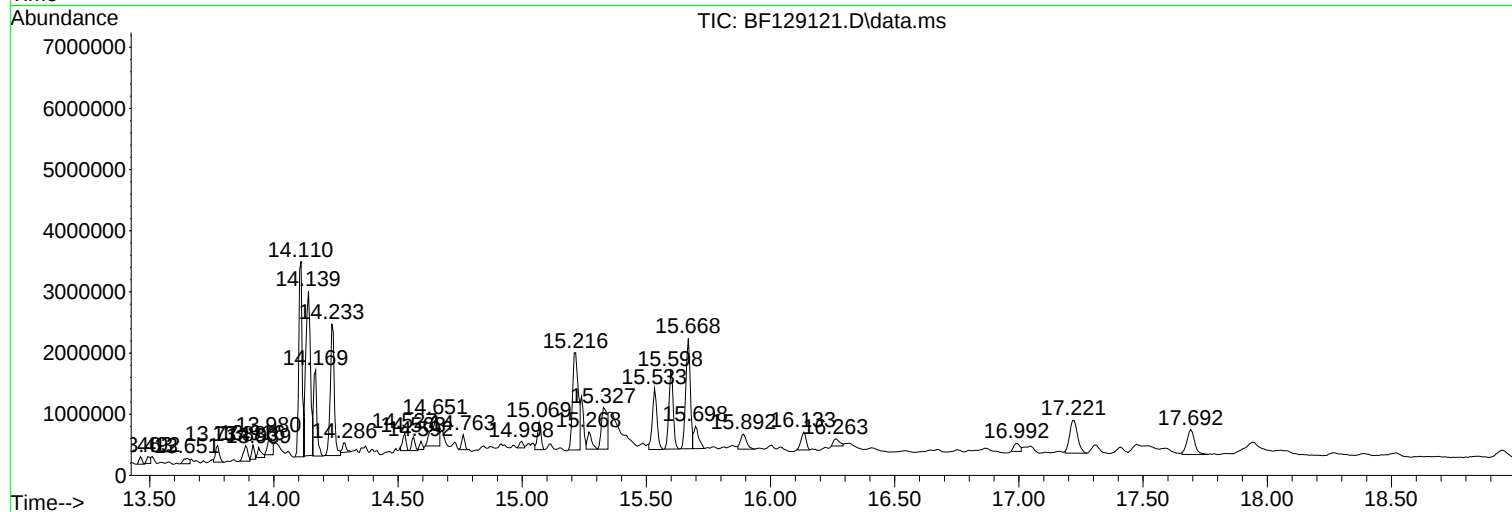
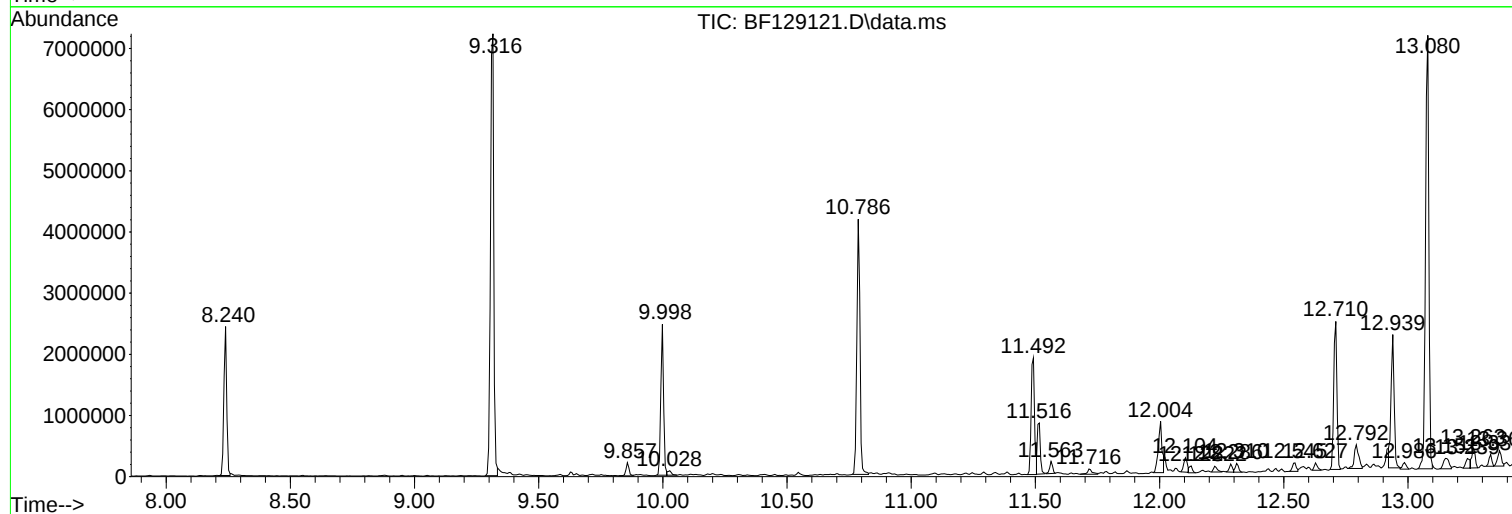
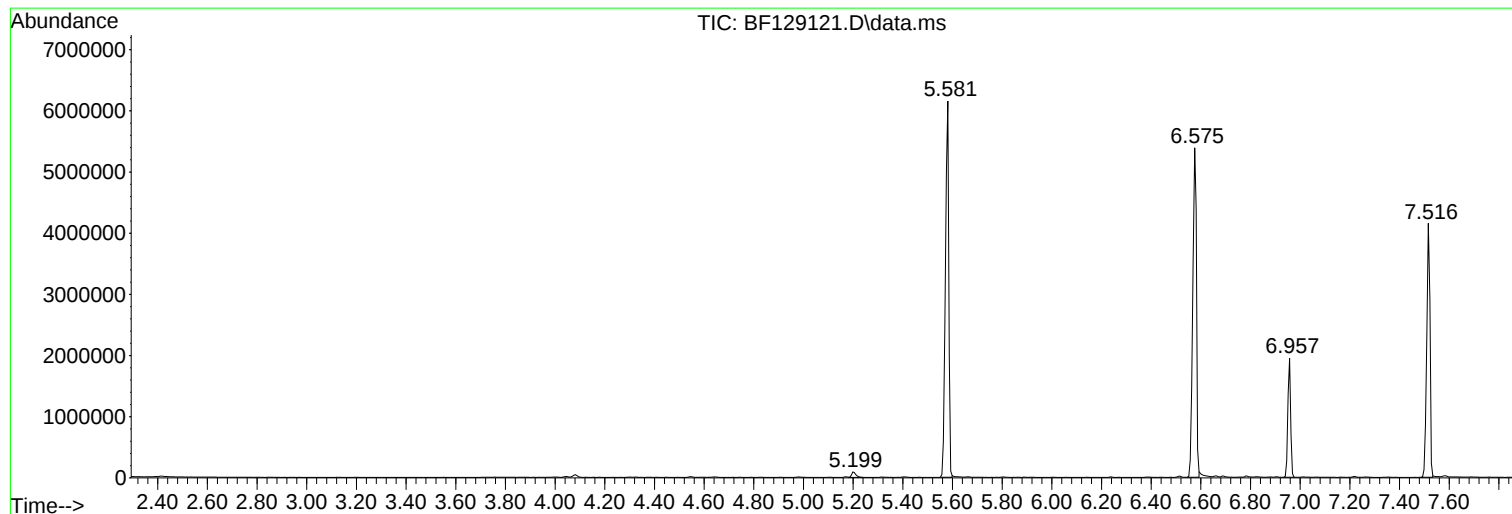
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Sample : N3572-01
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Instrument :
BNA_F
ClientSampleId :
RBR-200033

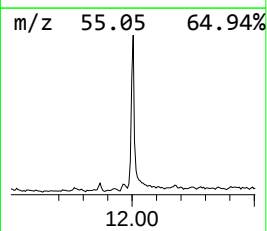
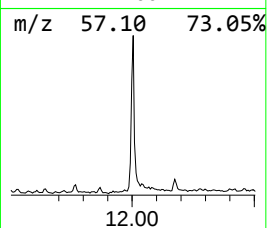
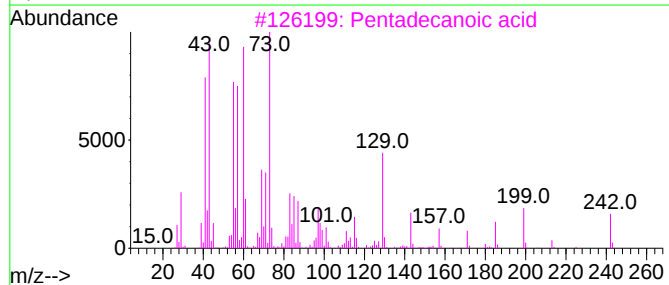
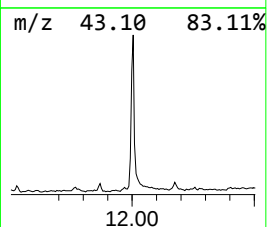
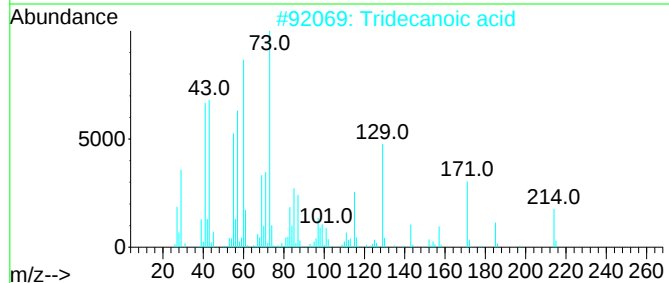
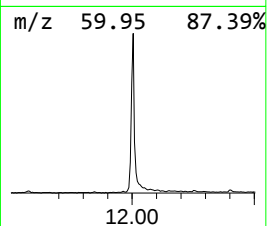
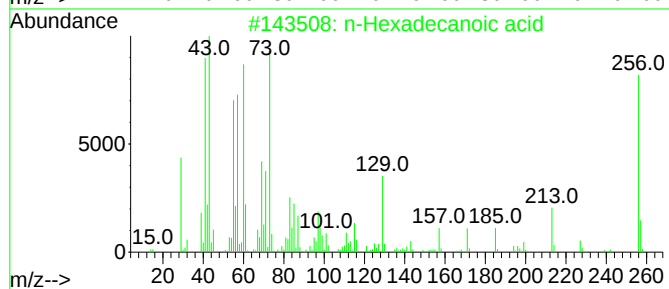
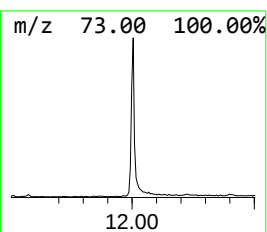
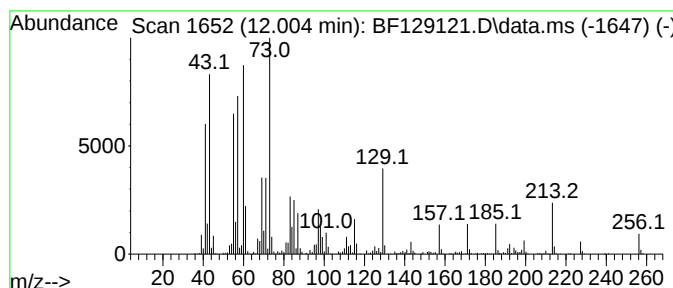
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.004	9.76 ng	893993	Phenanthrene-d10	11.492

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	97
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5			n-Decanoic acid	172	C10H20O2	000334-48-5	64



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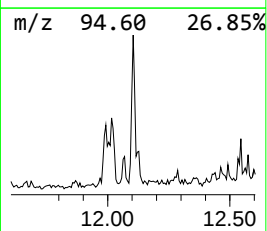
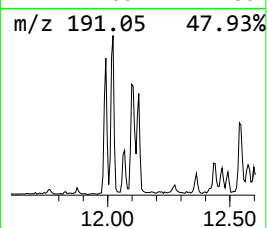
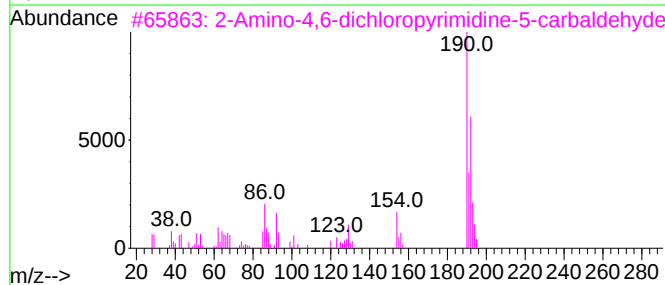
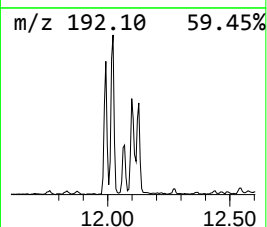
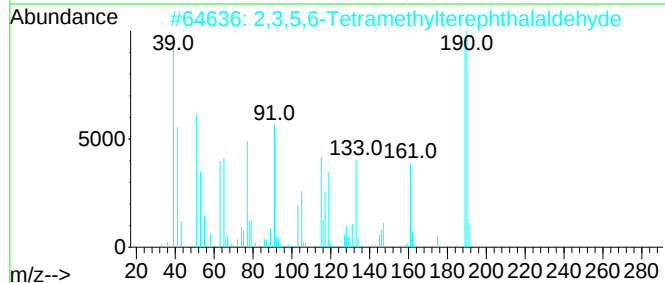
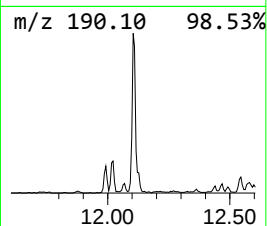
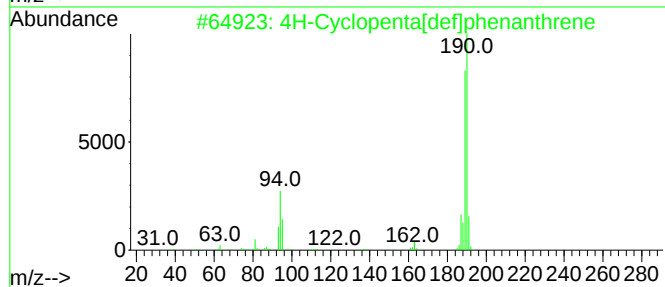
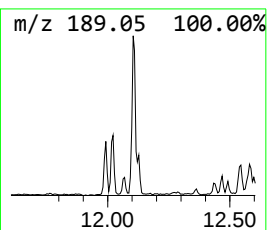
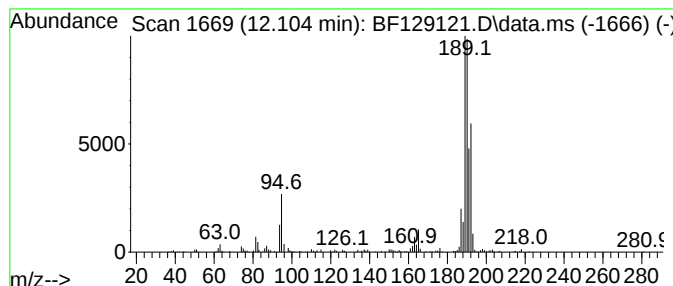
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 4H-Cyclopenta[def]phenanthrene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.104	2.60 ng	238363	Phenanthrene-d10	11.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	93
2			2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	43
3			2-Amino-4,6-dichloropyrimidine-5...	191	C5H3Cl2N3O	005604-46-6	43
4			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	35
5			Anthracene, 2-methyl-	192	C15H12	000613-12-7	25



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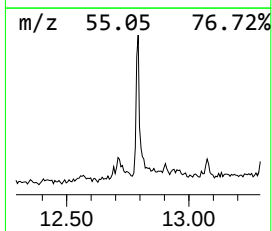
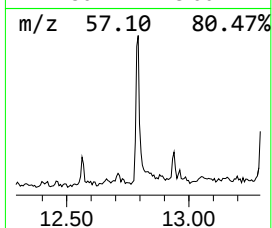
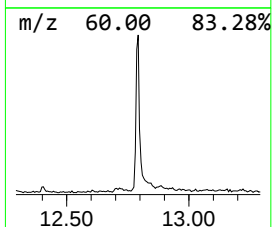
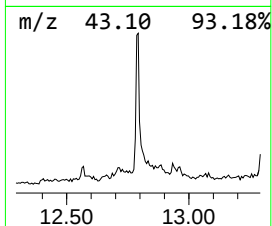
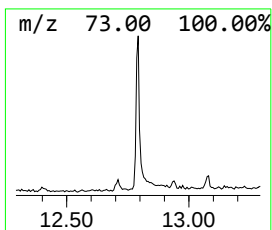
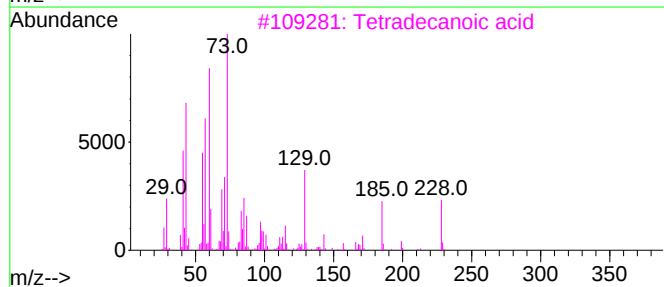
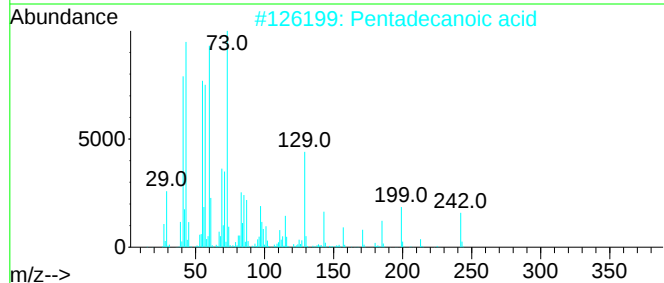
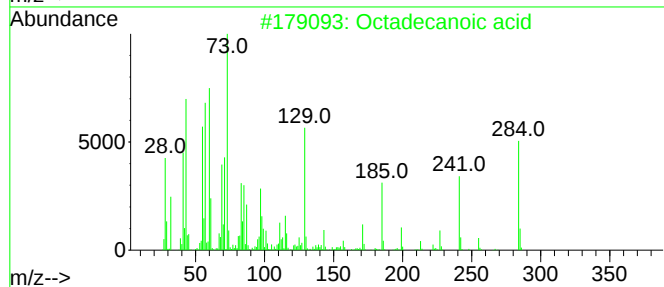
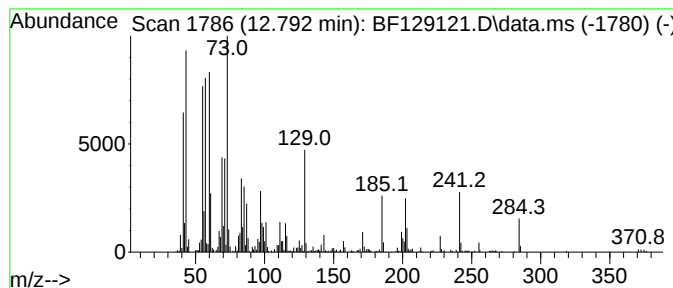
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.792	5.25 ng	480900	Phenanthrene-d10	11.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	89
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	68
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	62
5			n-Decanoic acid	172	C10H20O2	000334-48-5	60



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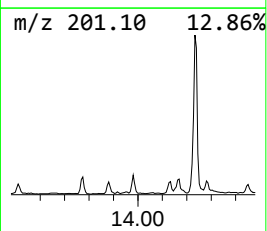
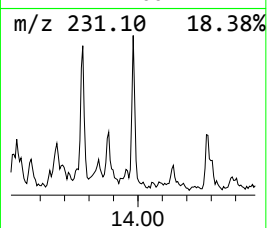
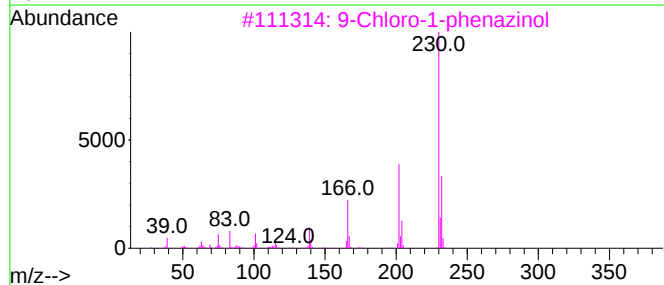
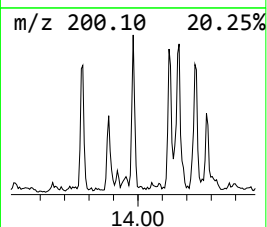
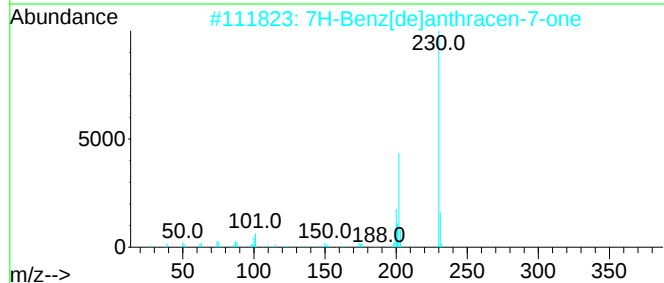
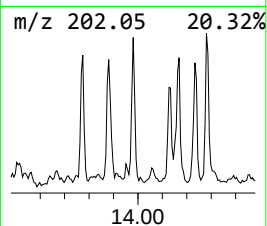
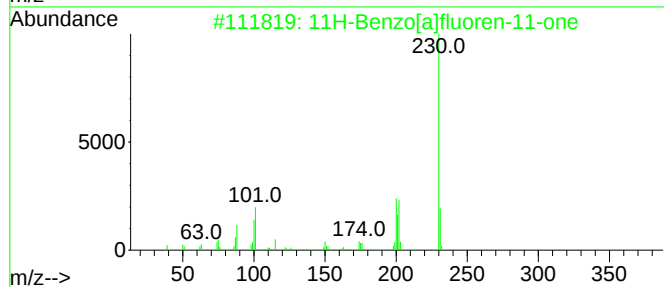
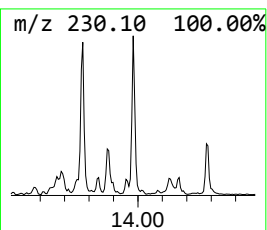
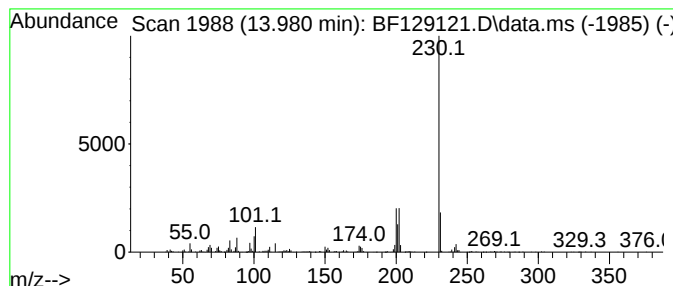
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062922.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 11H-Benzo[a]fluoren-11-one Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.980	2.21 ng	388610	Chrysene-d12	14.139

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	94
2			7H-Benz[de]anthracen-7-one	230	C17H10O	000082-05-3	90
3			9-Chloro-1-phenazinol	230	C12H7ClN2O	091268-03-0	53
4			4-Isothiazolocarboxitrile, 3,5-b...	230	C8H10N2S3	024135-13-5	53
5			Pyrene, 1,3-dimethyl-	230	C18H14	064401-21-4	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070522\
Data File : BF129121.D
Acq On : 05 Jul 2022 13:44
Operator : CG\JU
Sample : N3572-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR-200033

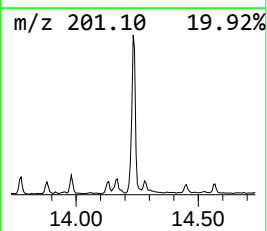
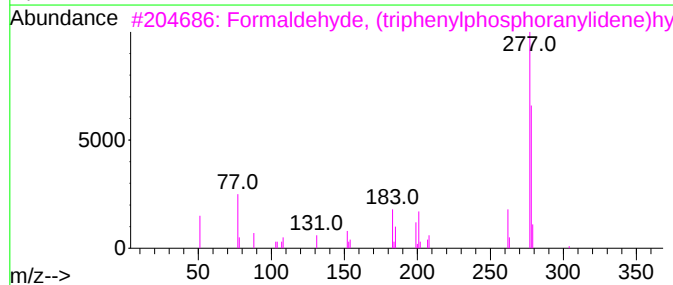
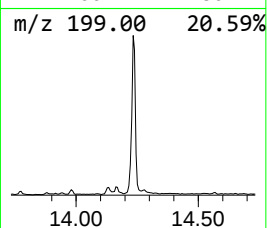
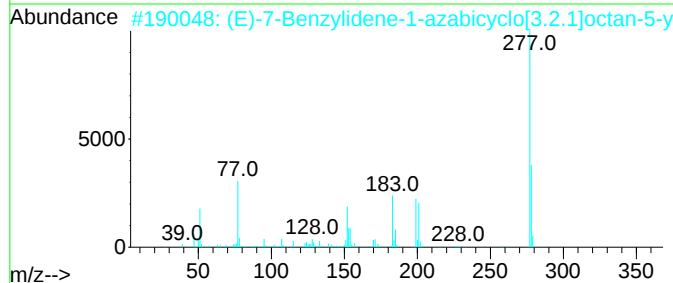
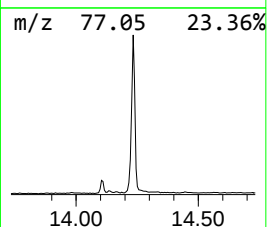
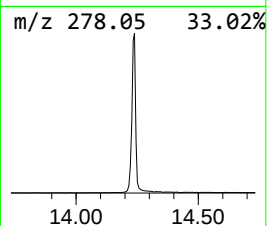
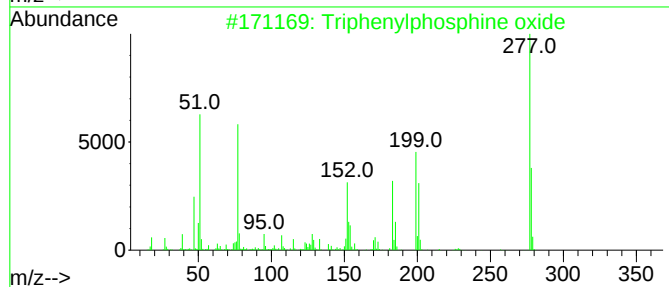
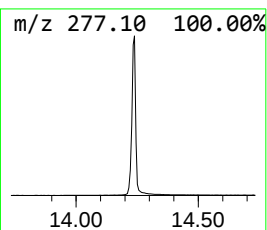
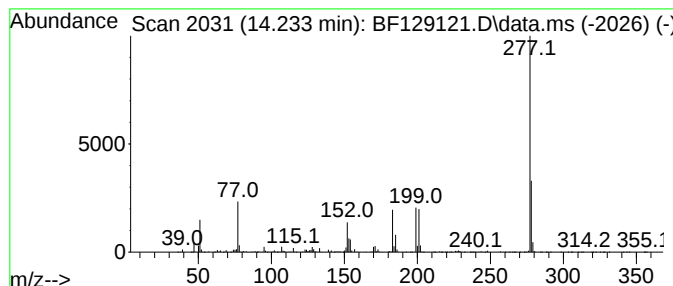
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Triphenylphosphine oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.233	14.04 ng	2466500	Chrysene-d12	14.139

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	93
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	91
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	64
4			Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	25
5			1H-Indole-3-acetic acid, 5-[(tri...	277	C14H19NO3Si	072101-35-0	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070522\
Data File : BF129121.D
Acq On : 05 Jul 2022 13:44
Operator : CG\JU
Sample : N3572-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

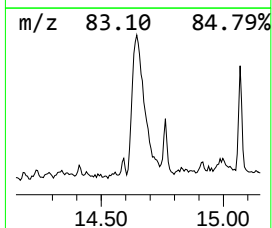
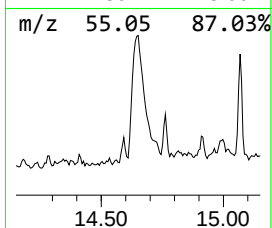
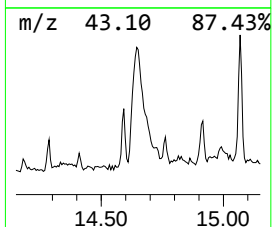
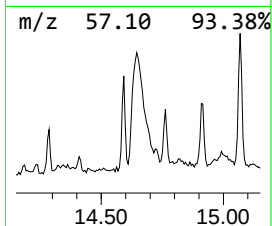
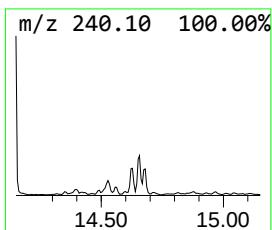
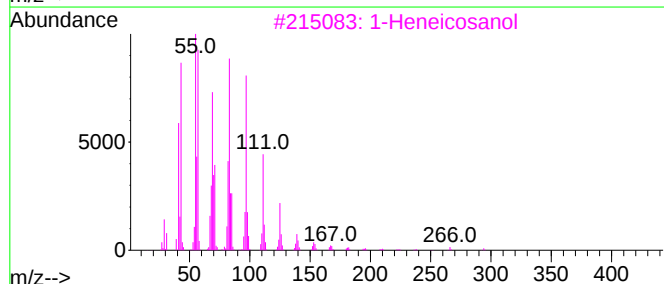
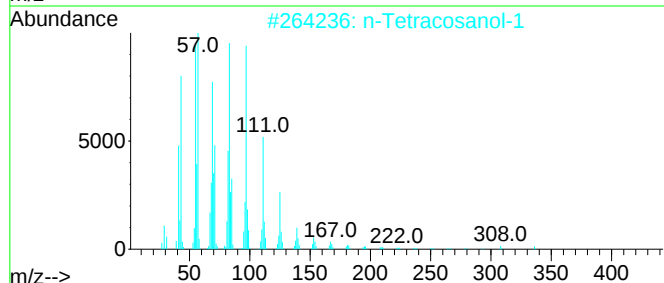
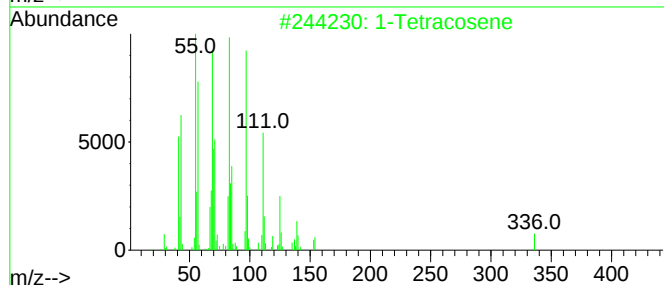
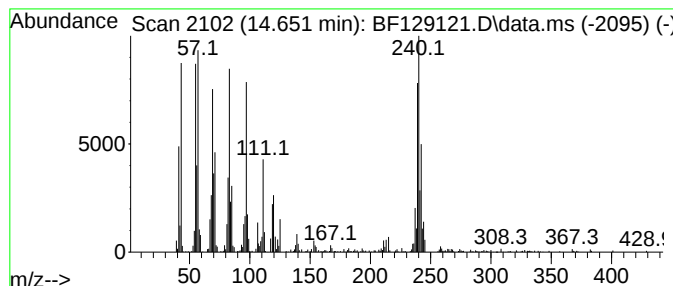
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Tetracosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.651	5.40 ng	947550	Chrysene-d12	14.139	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tetracosene	336	C24H48	010192-32-2	97
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	64
3	1-Heneicosanol	312	C21H44O	015594-90-8	64
4	8-Heptadecene	238	C17H34	002579-04-6	62
5	1-Docosene	308	C22H44	001599-67-3	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070522\
Data File : BF129121.D
Acq On : 05 Jul 2022 13:44
Operator : CG\JU
Sample : N3572-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

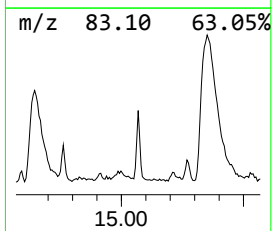
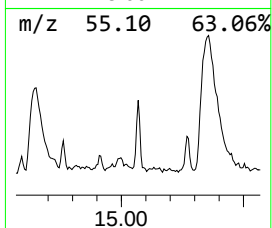
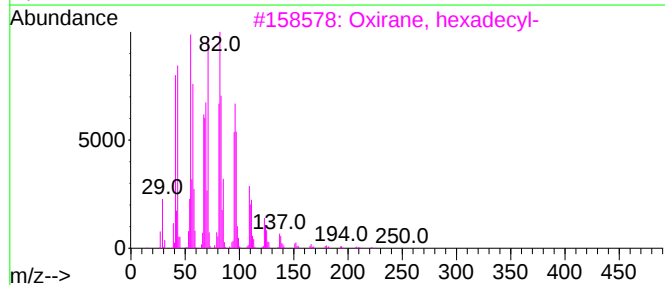
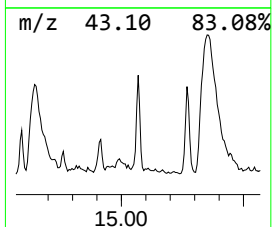
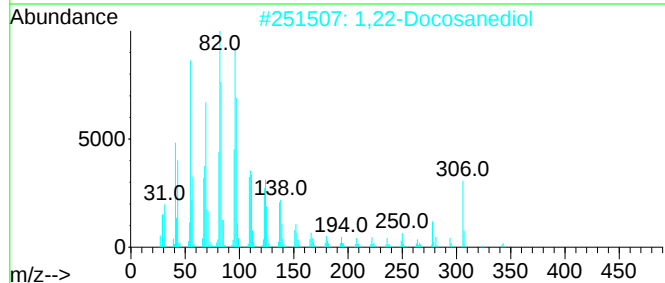
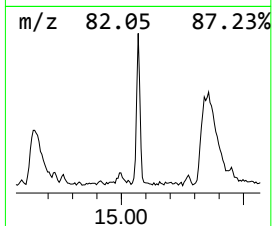
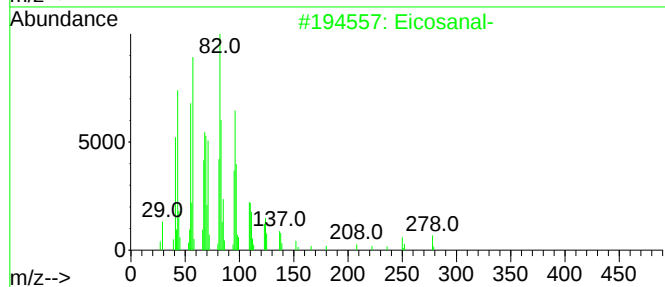
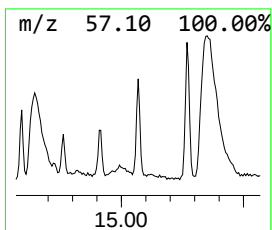
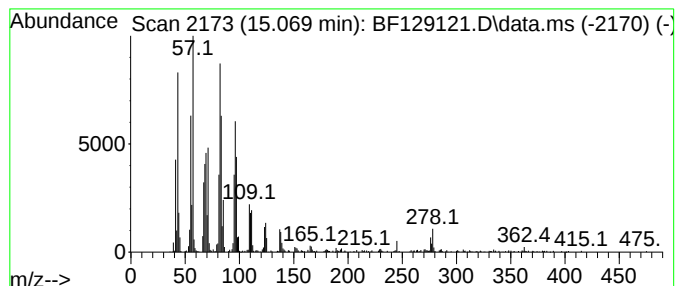
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Eicosanal- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
15.069	3.85 ng	444035	Perylene-d12		15.669	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Eicosanal-		296	C20H40O	002400-66-0	95
2	1,22-Docosanediol		342	C22H46O2	022513-81-1	93
3	Oxirane, hexadecyl-		268	C18H36O	007390-81-0	91
4	Octadecanal		268	C18H36O	000638-66-4	91
5	Hexacosanal		380	C26H52O	026627-85-0	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070522\
Data File : BF129121.D
Acq On : 05 Jul 2022 13:44
Operator : CG\JU
Sample : N3572-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR-200033

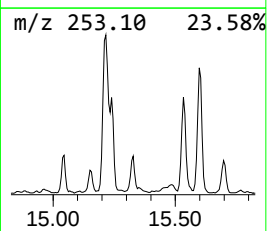
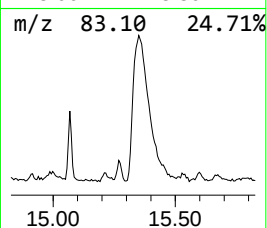
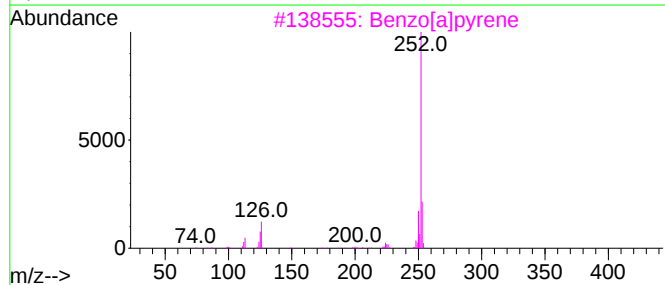
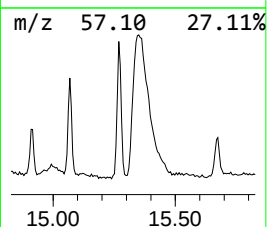
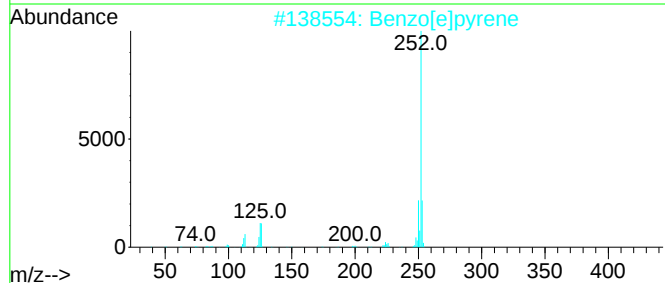
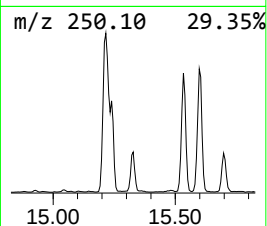
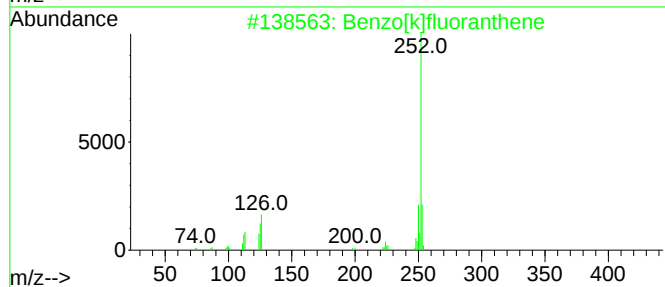
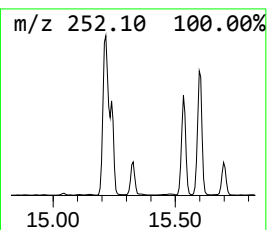
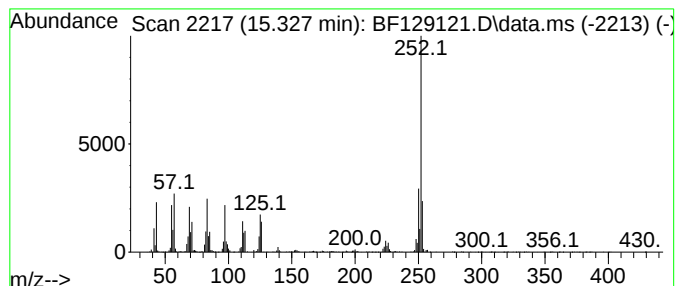
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.327	10.20 ng	1176500	Perylene-d12	15.669

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
2			Benzo[e]pyrene	252	C20H12	000192-97-2	93
3			Benzo[a]pyrene	252	C20H12	000050-32-8	89
4			Benzo[b]fluoranthene	252	C20H12	000205-99-2	86
5			Benzo[j]fluoranthene	252	C20H12	000205-82-3	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070522\
Data File : BF129121.D
Acq On : 05 Jul 2022 13:44
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Sample : N3572-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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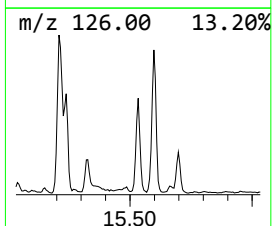
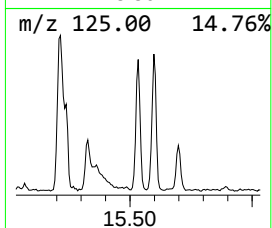
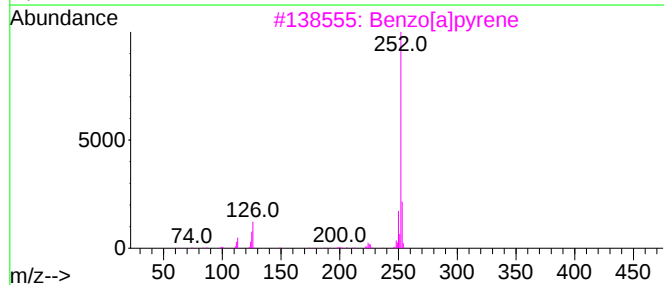
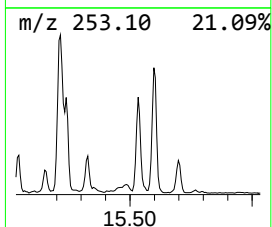
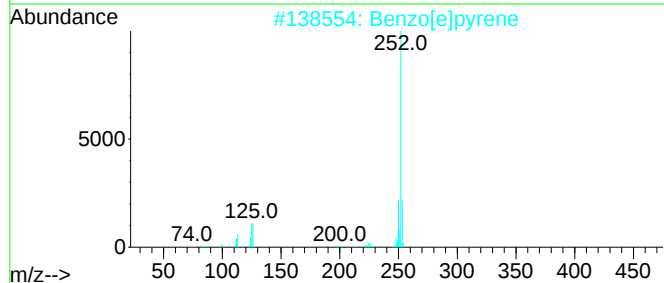
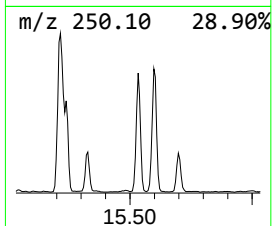
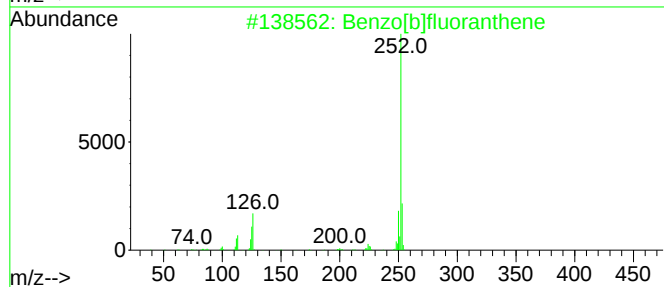
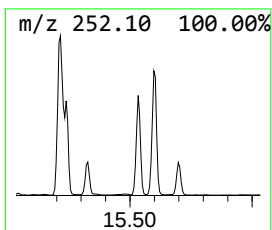
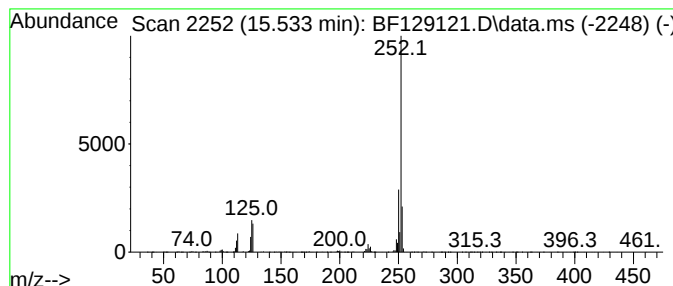
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Perylene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.533	10.99 ng	1267400	Perylene-d12	15.669

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[b]fluoranthene	252	C20H12	000205-99-2	98
2			Benzo[e]pyrene	252	C20H12	000192-97-2	98
3			Benzo[a]pyrene	252	C20H12	000050-32-8	93
4			Benzo[k]fluoranthene	252	C20H12	000207-08-9	91
5			Perylene	252	C20H12	000198-55-0	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070522\
Data File : BF129121.D
Acq On : 05 Jul 2022 13:44
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Misc :
ALS Vial : 8 Sample Multiplier: 1

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ClientSampleId :
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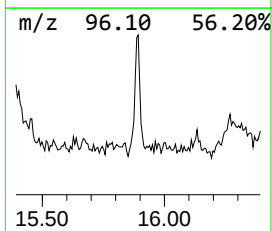
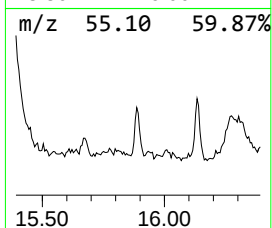
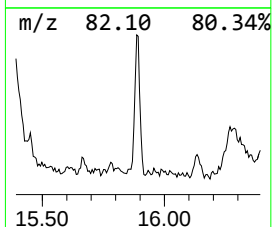
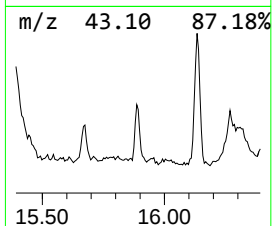
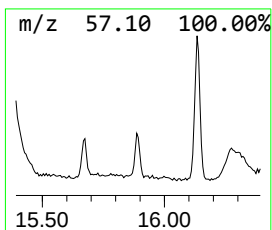
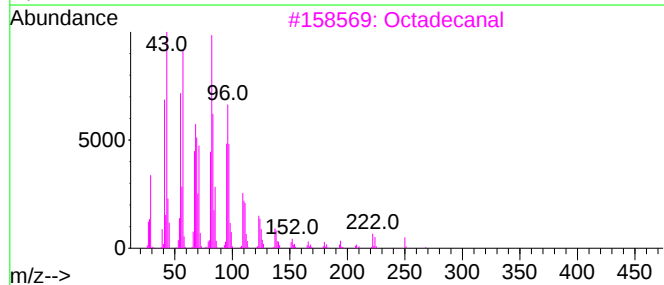
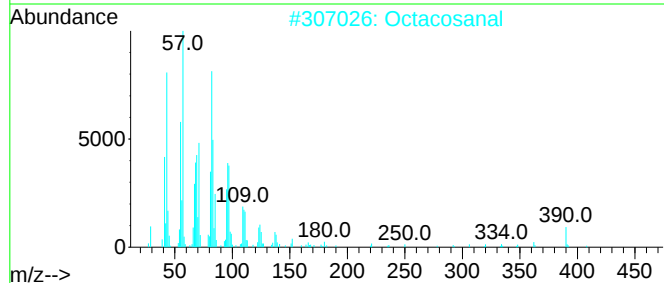
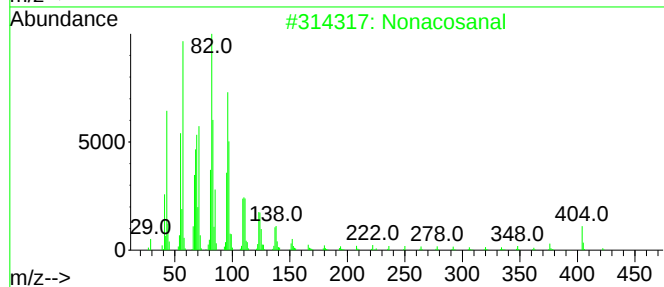
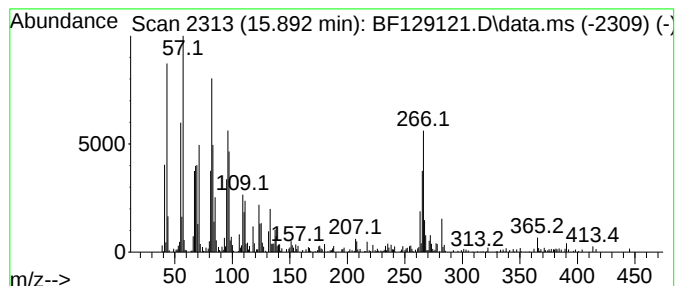
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Nonacosanal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.892	3.57 ng	411761	Perylene-d12	15.669

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonacosanal	422	C29H58O	072934-04-4	60
2			Octacosanal	408	C28H56O	022725-64-0	55
3			Octadecanal	268	C18H36O	000638-66-4	49
4			Heptadecanal	254	C17H34O	1000376-70-0	46
5			1,19-Eicosadiene	278	C20H38	014811-95-1	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070522\
Data File : BF129121.D
Acq On : 05 Jul 2022 13:44
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ALS Vial : 8 Sample Multiplier: 1

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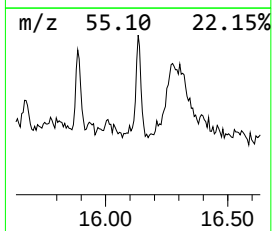
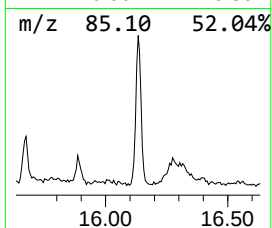
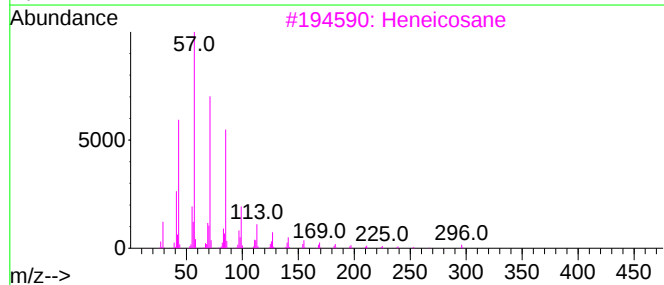
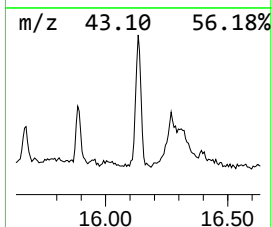
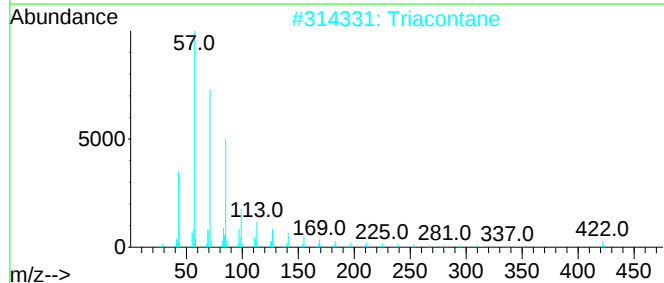
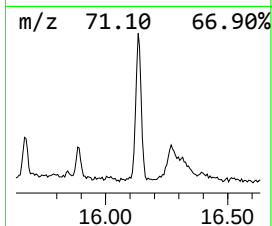
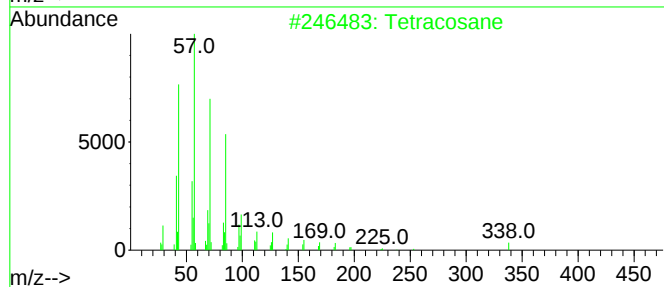
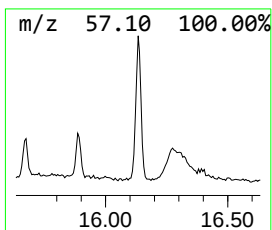
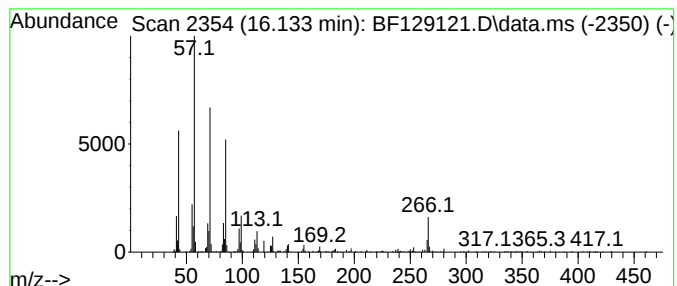
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Tetracosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.133	3.54 ng	408473	Perylene-d12	15.669

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	98
2			Triacotane	422	C30H62	000638-68-6	91
3			Heneicosane	296	C21H44	000629-94-7	87
4			Dotriacotane, 1-iodo-	576	C32H65I	1000406-32-4	83
5			Docosane, 1-iodo-	436	C22H45I	1000406-31-9	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070522\
Data File : BF129121.D
Acq On : 05 Jul 2022 13:44
Operator : CG\JU
Sample : N3572-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR-200033

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	12.004	9.8	ng	893993	4	11.492	1831430	20.0
4H-Cyclopenta[d]...	12.104	2.6	ng	238363	4	11.492	1831430	20.0
Octadecanoic acid	12.792	5.3	ng	480900	4	11.492	1831430	20.0
11H-Benzo[a]flu...	13.980	2.2	ng	388610	5	14.139	3512330	20.0
Triphenylphosph...	14.233	14.0	ng	2466500	5	14.139	3512330	20.0
1-Tetracosene	14.651	5.4	ng	947550	5	14.139	3512330	20.0
Eicosanal-	15.069	3.9	ng	444035	6	15.669	2307380	20.0
Benzo[e]pyrene	15.327	10.2	ng	1176500	6	15.669	2307380	20.0
Perylene	15.533	11.0	ng	1267400	6	15.669	2307380	20.0
Nonacosanal	15.892	3.6	ng	411761	6	15.669	2307380	20.0
Tetracosane	16.133	3.5	ng	408473	6	15.669	2307380	20.0