

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041222\
 Data File : BF127772.D
 Acq On : 12 Apr 2022 21:59
 Operator : CG\JU
 Sample : N2367-01 5X
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 AU-05-041122

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-BF040622.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127772.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.569	554	558	564	rBV	668491	567520	4.94%	1.579%
2	6.569	724	728	731	rBV	726117	565612	4.92%	1.574%
3	6.957	790	794	797	rBV	1034809	809203	7.04%	2.252%
4	7.516	885	889	892	rBV	448492	363914	3.17%	1.013%
5	8.239	1008	1012	1015	rBV	1231930	965235	8.40%	2.686%
6	9.310	1191	1194	1198	rBV	875234	697448	6.07%	1.941%
7	9.998	1307	1311	1314	rVB	1323749	1030679	8.97%	2.868%
8	10.786	1441	1445	1449	rBV	391005	348382	3.03%	0.970%
9	11.492	1561	1565	1567	rBV	955638	919456	8.00%	2.559%
10	11.510	1567	1568	1572	rVB	473583	372764	3.24%	1.037%
11	11.874	1626	1630	1633	rBV	4038865	3271426	28.46%	9.104%
12	12.004	1646	1652	1653	rBV2	79685	125325	1.09%	0.349%
13	12.104	1665	1669	1672	rBV3	145056	163998	1.43%	0.456%
14	12.574	1740	1749	1751	rBV	8667172	11495303	100.00%	31.990%
15	12.592	1751	1752	1758	rVV2	6485643	5734392	49.88%	15.958%
16	12.668	1762	1765	1768	rVV	1781808	1415190	12.31%	3.938%
17	12.710	1768	1772	1775	rVV	1011013	929421	8.09%	2.587%
18	12.939	1805	1811	1814	rBV	875639	789024	6.86%	2.196%
19	13.074	1831	1834	1837	rBV	575300	466702	4.06%	1.299%
20	13.263	1864	1866	1869	rVB	151912	130745	1.14%	0.364%
21	13.333	1873	1878	1881	rVB2	150704	200088	1.74%	0.557%
22	13.392	1886	1888	1892	rVB	151236	123170	1.07%	0.343%
23	14.062	1999	2002	2006	rVB2	163526	143564	1.25%	0.400%
24	14.133	2010	2014	2017	rVV2	1133562	1493602	12.99%	4.157%
25	14.162	2017	2019	2025	rVB	530839	445231	3.87%	1.239%
26	15.204	2192	2196	2199	rBV	411153	621806	5.41%	1.730%
27	15.527	2247	2251	2257	rVB	229434	311157	2.71%	0.866%
28	15.592	2258	2262	2268	rVB	344922	444289	3.86%	1.236%
29	15.656	2269	2273	2277	rBV	548554	748137	6.51%	2.082%
30	17.203	2532	2536	2545	rVB2	118400	240746	2.09%	0.670%

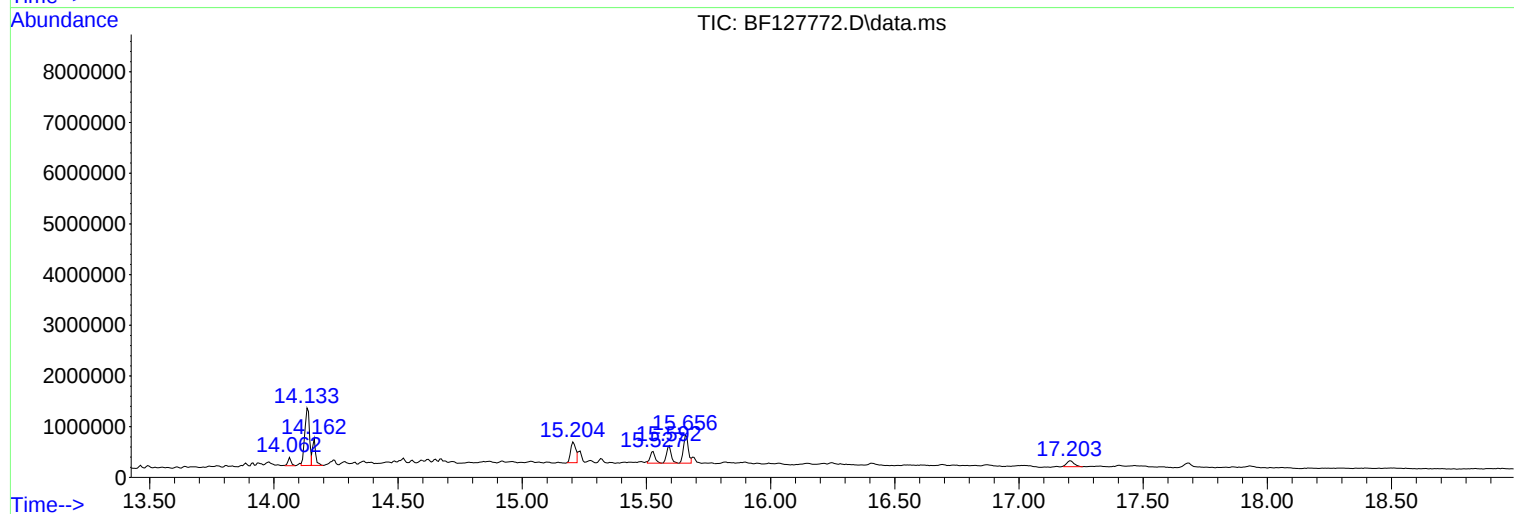
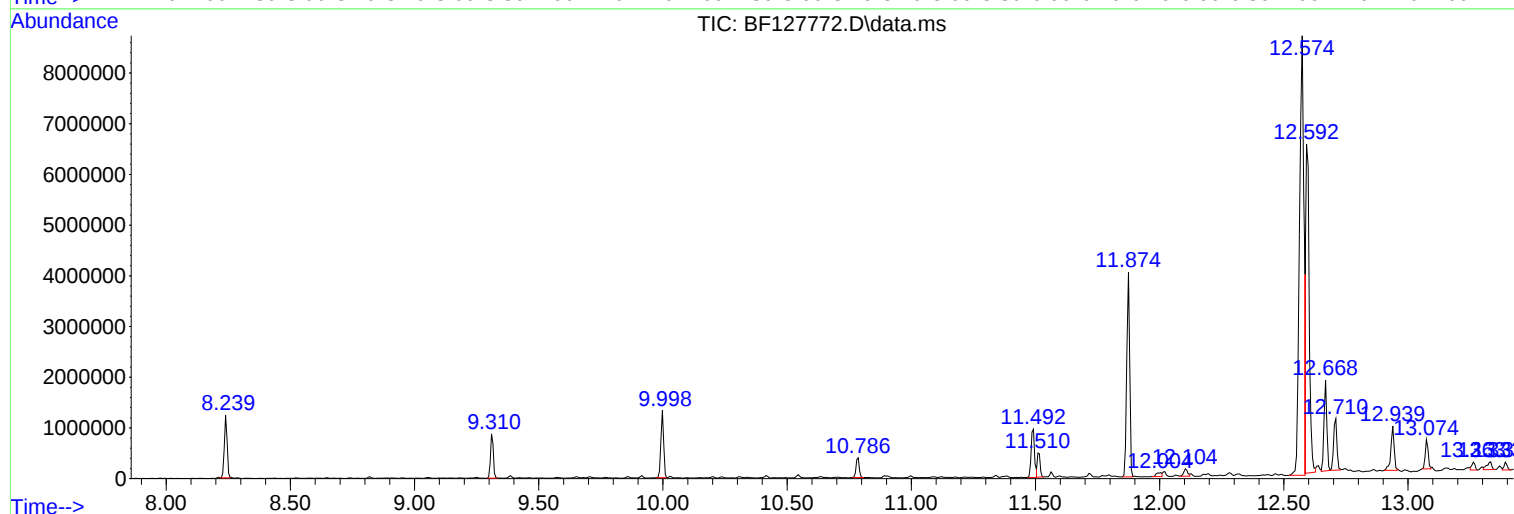
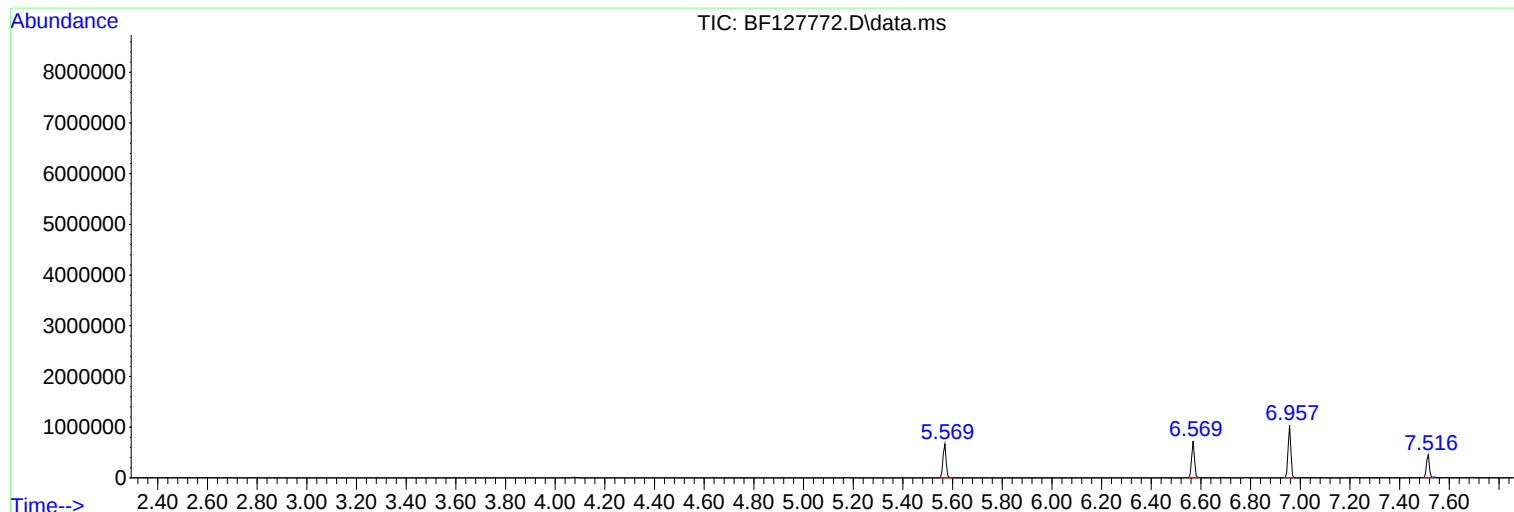
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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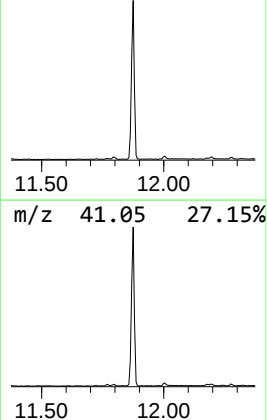
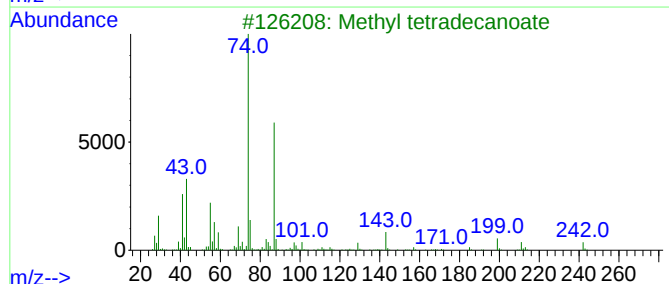
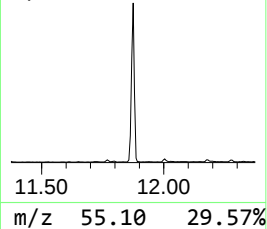
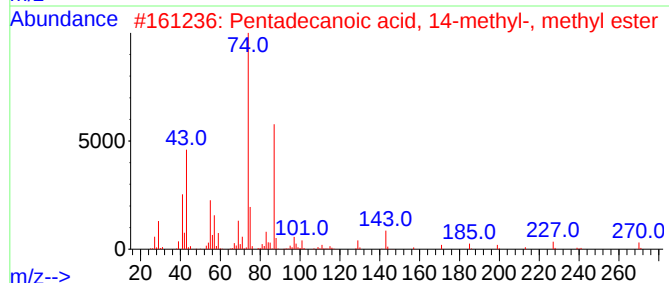
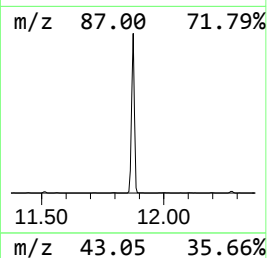
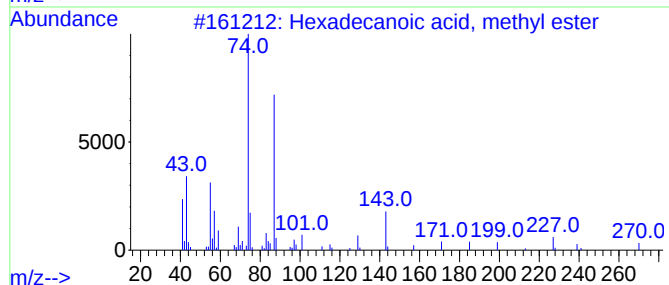
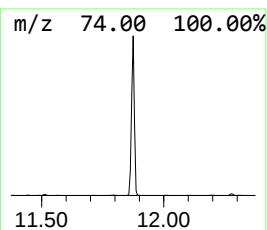
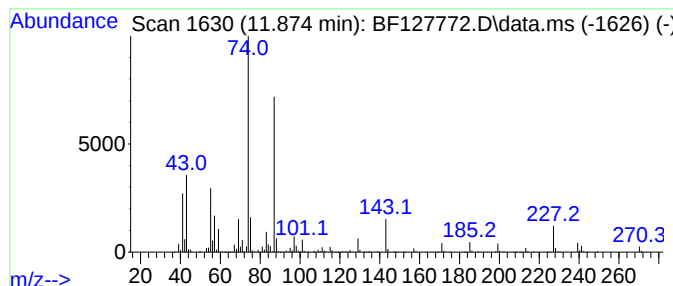
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Peak Number 1 Hexadecanoic acid, methyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.874	71.16 ng	3271430	Phenanthrene-d10	11.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	94
3			Methyl tetradecanoate	242	C15H30O2	000124-10-7	93
4			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	87
5			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86



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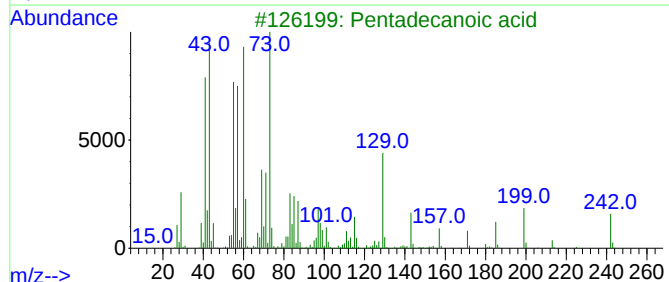
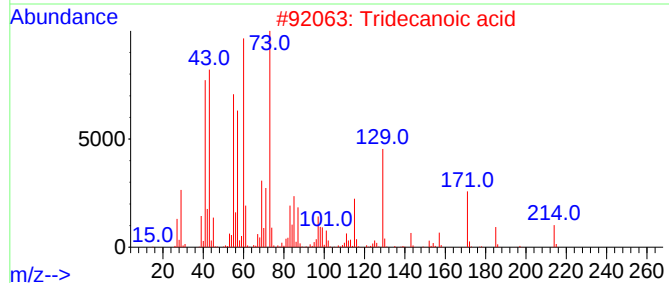
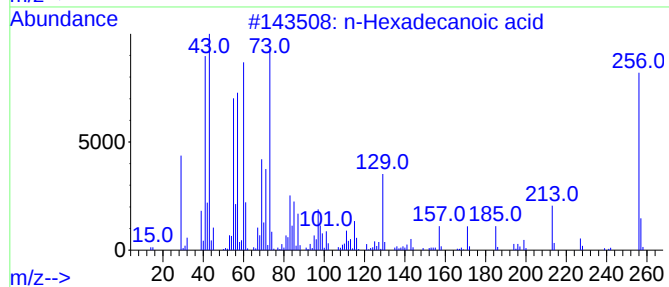
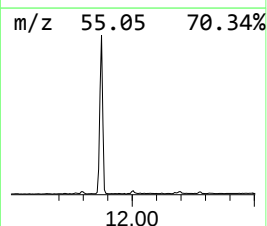
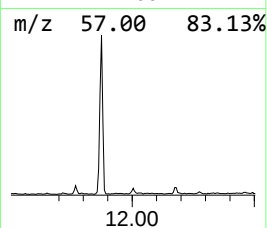
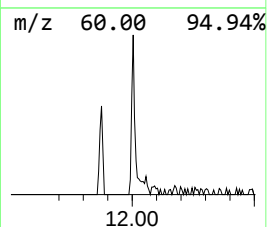
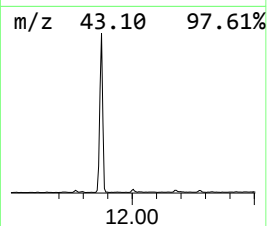
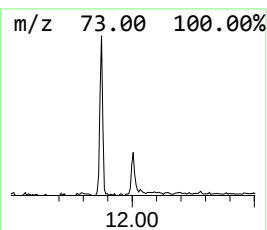
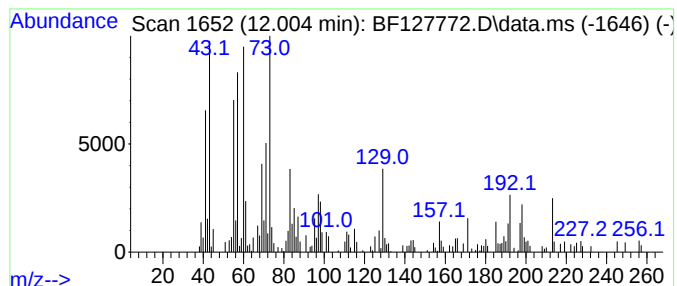
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.004	2.73 ng	125325	Phenanthrene-d10	11.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	62
2			Tridecanoic acid	214	C13H26O2	000638-53-9	60
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	52
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	52
5			Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	46



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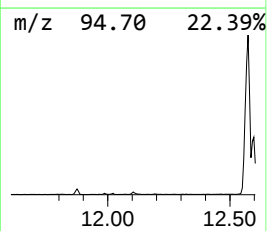
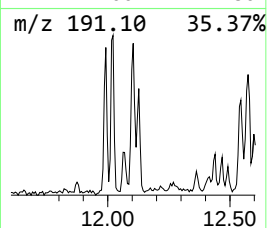
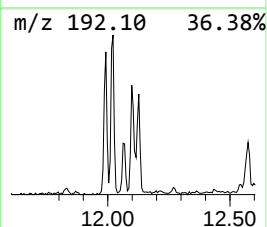
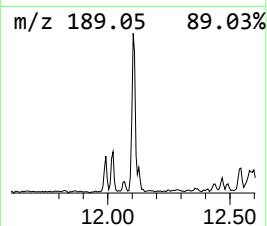
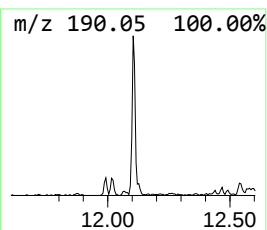
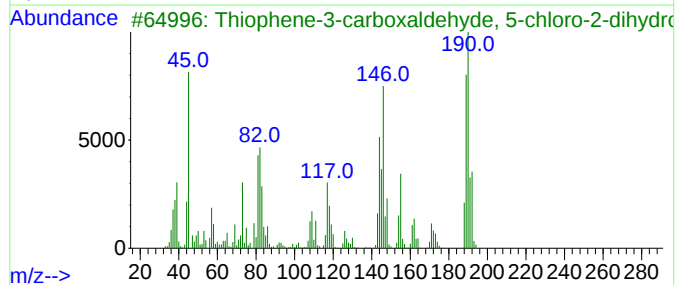
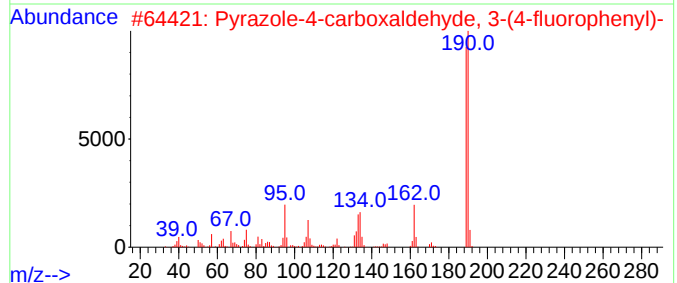
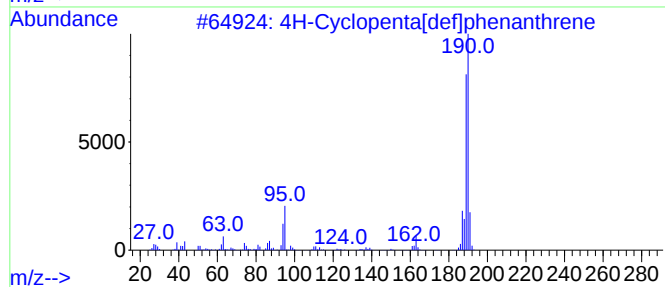
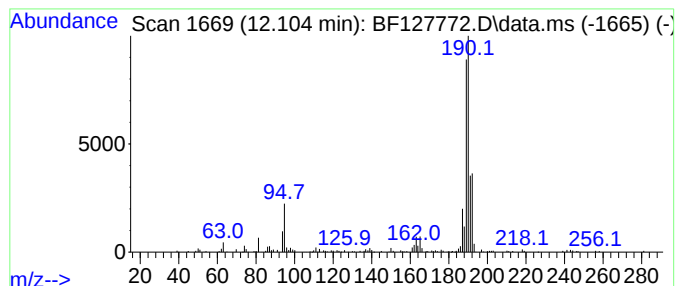
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 4H-Cyclopenta[def]phenanthrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.104	3.57 ng	163998	Phenanthrene-d10	11.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	81
2			Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	58
3			Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	53
4			Pyrimidine, 6-oxo-4-(3-fluorophe...	190	C10H7FN2O	085979-55-1	38
5			2,4(1H,3H)-Pyrimidinedione, 5-br...	190	C4H3BrN2O2	000051-20-7	35



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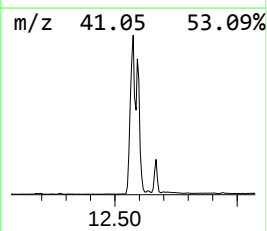
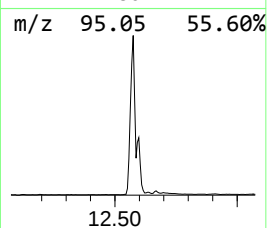
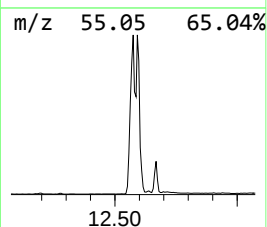
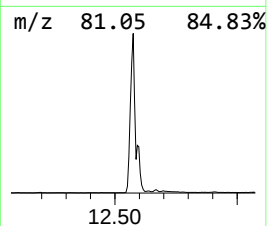
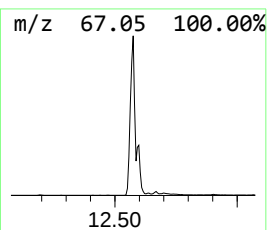
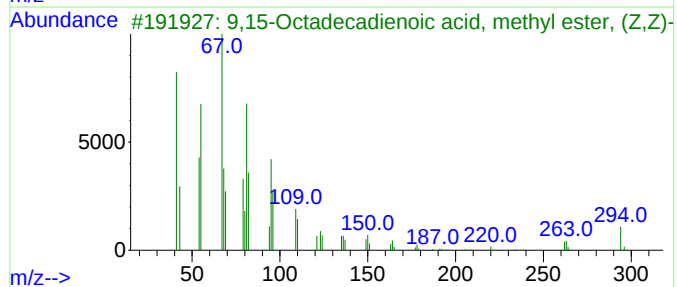
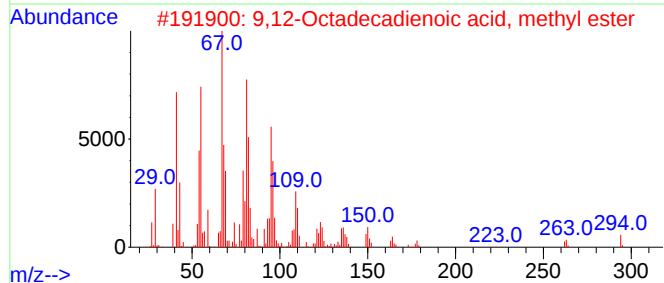
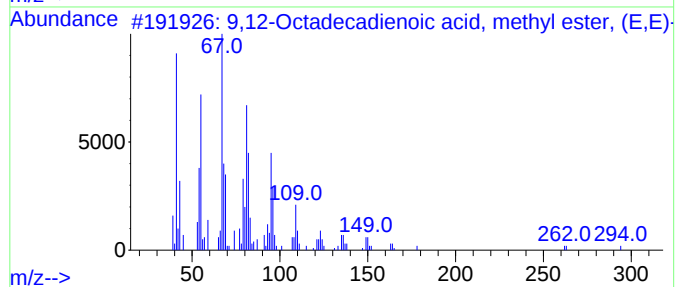
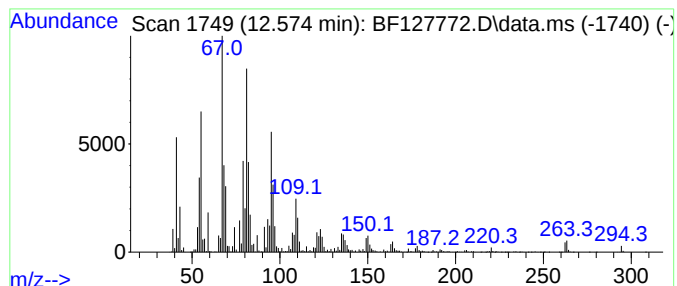
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Peak Number 4 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.574	250.05 ng	11495300	Phenanthrene-d10	11.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99		
2	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99		
3	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	98		
4	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	013058-52-1	98		
5	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	98		



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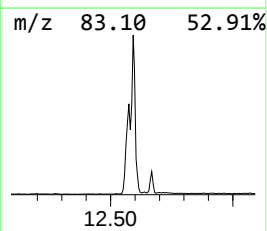
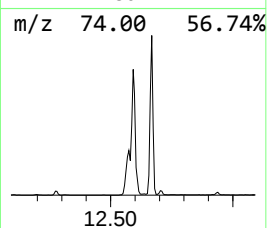
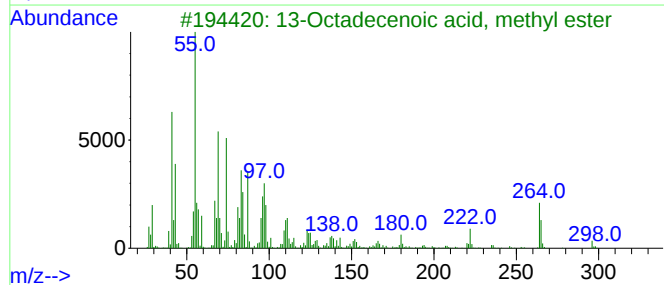
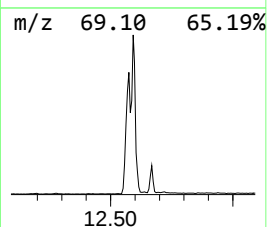
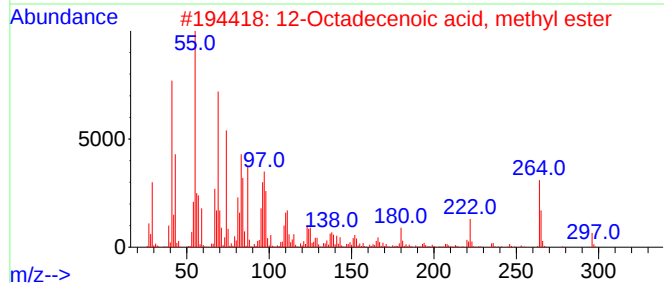
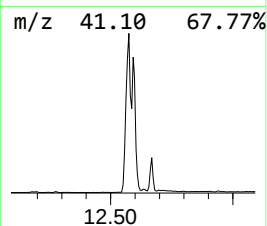
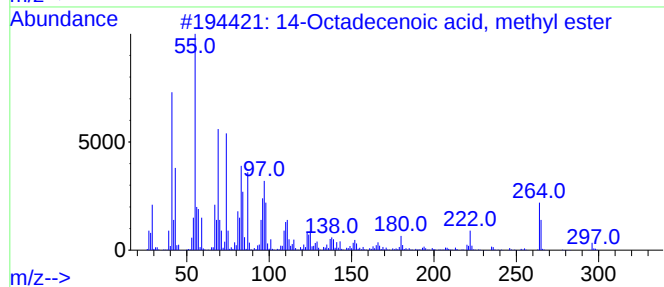
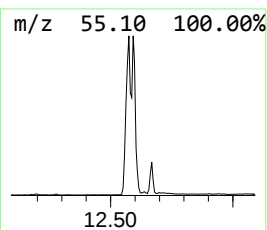
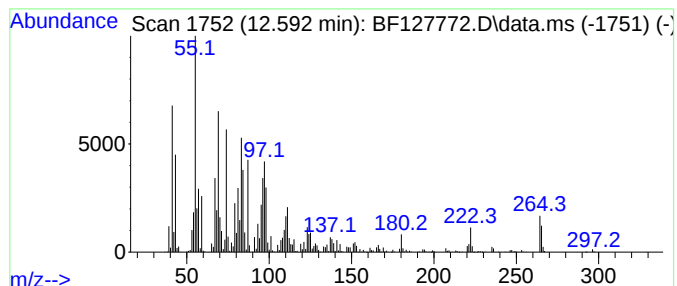
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Peak Number 5 14-Octadecenoic acid, methyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.592	124.73 ng	5734390	Phenanthrene-d10	11.492	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	99
2	12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	99
3	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	99
4	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
5	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	99



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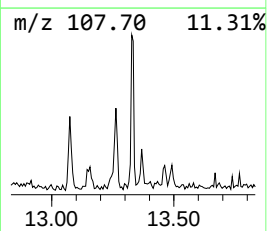
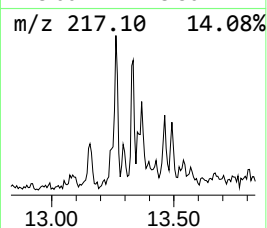
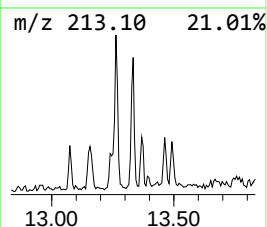
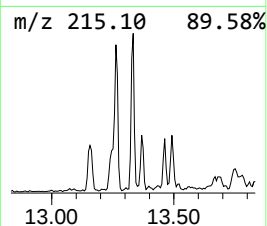
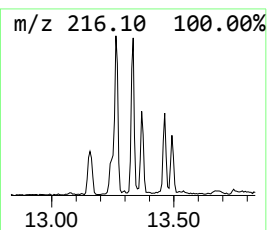
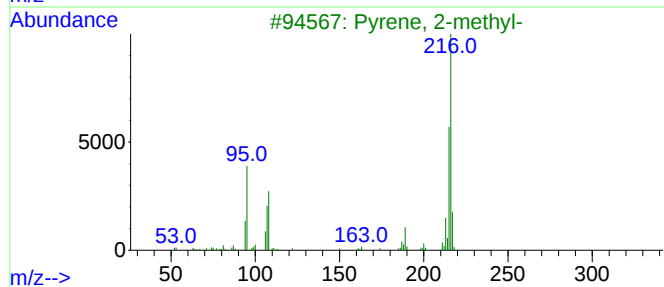
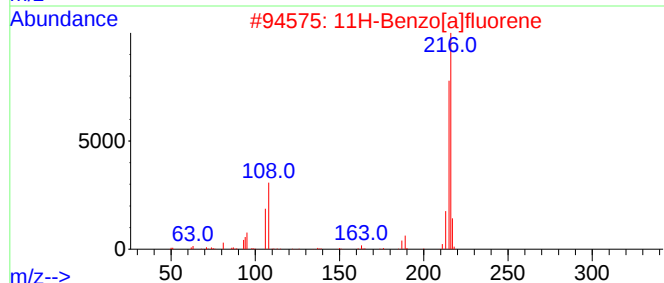
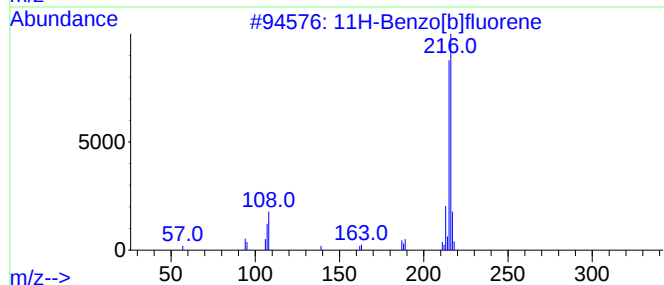
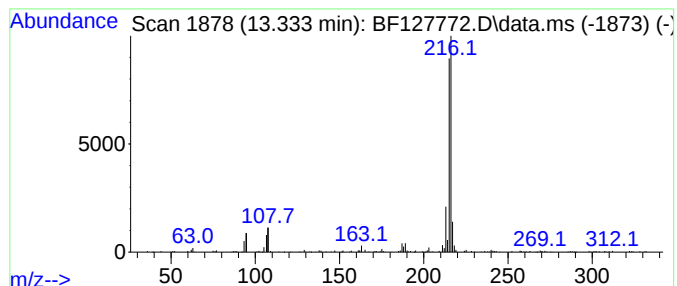
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 11H-Benzo[b]fluorene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.333	2.68 ng	200088	Chrysene-d12	14.139

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			11H-Benzo[b]fluorene	216	C17H12	000243-17-4	93
2			11H-Benzo[a]fluorene	216	C17H12	000238-84-6	91
3			Pyrene, 2-methyl-	216	C17H12	003442-78-2	76
4			Pyrene, 1-methyl-	216	C17H12	002381-21-7	72
5			Benzoic acid, 3-(3,5-dimethyl-1-...	216	C12H12N2O2	312531-88-7	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041222\
Data File : BF127772.D
Acq On : 12 Apr 2022 21:59
Operator : CG\JU
Sample : N2367-01 5X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
AU-05-041122

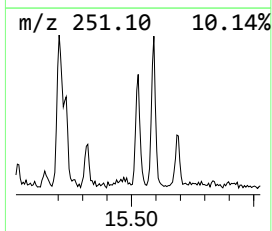
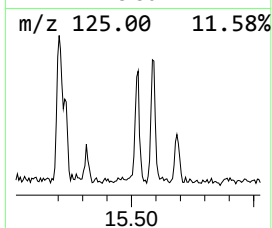
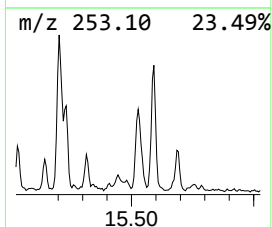
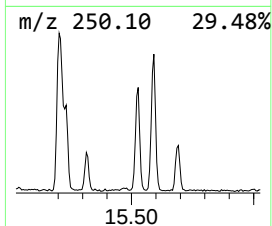
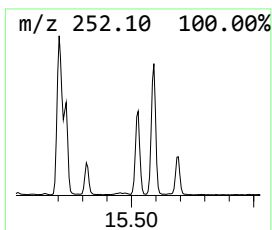
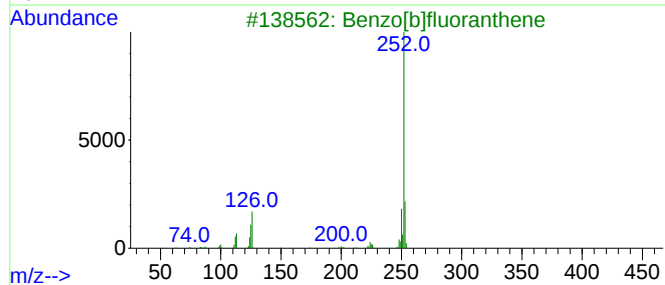
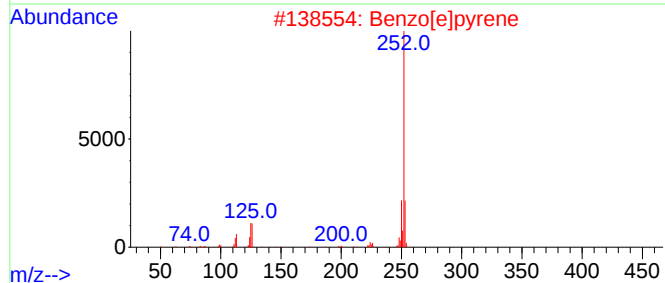
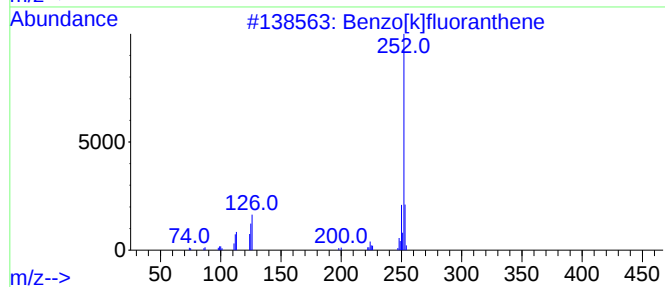
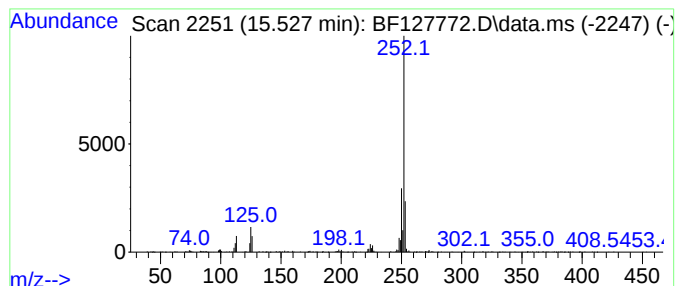
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.527	8.32 ng	311157	Perylene-d12	15.656

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[b]fluoranthene	252	C20H12	000205-99-2	93
4			Benzo[a]pyrene	252	C20H12	000050-32-8	91
5			Benzo[j]fluoranthene	252	C20H12	000205-82-3	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041222\
Data File : BF127772.D
Acq On : 12 Apr 2022 21:59
Operator : CG\JU
Sample : N2367-01 5X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
AU-05-041122

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.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
Hexadecanoic ac...	11.874	71.2	ng	3271430	4	11.492	919456	20.0
n-Hexadecanoic ...	12.004	2.7	ng	125325	4	11.492	919456	20.0
4H-Cyclopenta[d...]	12.104	3.6	ng	163998	4	11.492	919456	20.0
9,12-Octadecadi...	12.574	250.1	ng	11495300	4	11.492	919456	20.0
14-Octadecenoic...	12.592	124.7	ng	5734390	4	11.492	919456	20.0
11H-Benzo[b]flu...	13.333	2.7	ng	200088	5	14.139	1493600	20.0
Benzo[e]pyrene	15.527	8.3	ng	311157	6	15.656	748137	20.0