

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042522\
 Data File : BF127893.D
 Acq On : 25 Apr 2022 21:18
 Operator : CG\JU
 Sample : N2466-05
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 E14ST-EB2-041822-5-10

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-BF042222.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127893.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.193	490	494	502	rVB	40836	50341	1.21%	0.144%
2	5.563	552	557	561	rBV	3525119	3732215	89.58%	10.643%
3	6.563	721	727	730	rBV	3469711	3844750	92.28%	10.964%
4	6.940	787	791	794	rBV	1278897	991617	23.80%	2.828%
5	7.504	881	887	890	rBV	2652553	2661618	63.88%	7.590%
6	7.669	911	915	919	rVB	70661	59363	1.42%	0.169%
7	8.222	1004	1009	1012	rBV	1503358	1293461	31.04%	3.689%
8	9.298	1186	1192	1195	rBV	4569792	4166425	100.00%	11.882%
9	9.369	1200	1204	1206	rVB2	47929	45879	1.10%	0.131%
10	9.981	1301	1308	1311	rBV	1800747	1512805	36.31%	4.314%
11	10.010	1311	1313	1316	rVB	58138	46252	1.11%	0.132%
12	10.528	1397	1401	1406	rVB2	50509	48722	1.17%	0.139%
13	10.769	1438	1442	1446	rBV	2728753	2850678	68.42%	8.130%
14	11.369	1539	1544	1548	rVB2	36093	45035	1.08%	0.128%
15	11.475	1557	1562	1564	rBV	1610361	1609489	38.63%	4.590%
16	11.492	1564	1565	1569	rVV	682546	494769	11.88%	1.411%
17	11.545	1569	1574	1577	rVB	107935	102795	2.47%	0.293%
18	11.698	1594	1600	1606	rBV2	49126	75222	1.81%	0.215%
19	11.851	1623	1626	1629	rBV	128595	95733	2.30%	0.273%
20	11.986	1642	1649	1657	rBV2	443471	665296	15.97%	1.897%
21	12.086	1662	1666	1668	rVV2	138440	171069	4.11%	0.488%
22	12.104	1668	1669	1673	rVB	77483	59525	1.43%	0.170%
23	12.269	1694	1697	1699	rBV	80032	69533	1.67%	0.198%
24	12.292	1699	1701	1705	rVB	69284	57440	1.38%	0.164%
25	12.522	1737	1740	1742	rBV	65474	67692	1.62%	0.193%
26	12.563	1742	1747	1752	rVV4	211043	245093	5.88%	0.699%
27	12.604	1752	1754	1759	rVB2	43877	56831	1.36%	0.162%
28	12.686	1764	1768	1774	rBV	926186	863720	20.73%	2.463%
29	12.774	1781	1783	1788	rBV2	177525	173010	4.15%	0.493%
30	12.916	1801	1807	1810	rBV	846674	867620	20.82%	2.474%
31	13.063	1827	1832	1835	rBV	3632324	3585320	86.05%	10.225%
32	13.127	1840	1843	1848	rBV2	56846	104340	2.50%	0.298%
33	13.222	1856	1859	1861	rBV4	52117	74481	1.79%	0.212%
34	13.245	1861	1863	1865	rVB	102712	78258	1.88%	0.223%
35	13.274	1866	1868	1870	rBV	51107	45570	1.09%	0.130%
36	13.310	1871	1874	1877	rVV2	76059	82581	1.98%	0.236%

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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-BF042222.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.351	1878	1881	1883	rVB2	71473	70055	1.68%	0.200%
38	13.404	1887	1890	1893	rBV2	49130	59666	1.43%	0.170%
39	13.474	1899	1902	1904	rBV	55769	61353	1.47%	0.175%
40	13.621	1924	1927	1929	rBV2	51043	59748	1.43%	0.170%
41	13.916	1975	1977	1981	rBV2	45579	74923	1.80%	0.214%
42	14.116	2007	2011	2014	rBV2	1105855	1118861	26.85%	3.191%
43	14.139	2014	2015	2022	rVB	288161	238171	5.72%	0.679%
44	14.210	2024	2027	2032	rVB2	157565	165305	3.97%	0.471%
45	15.174	2188	2191	2195	rBV	179310	272976	6.55%	0.778%
46	15.245	2200	2203	2208	rVB2	57981	72006	1.73%	0.205%
47	15.498	2242	2246	2252	rVB	135651	189616	4.55%	0.541%
48	15.563	2253	2257	2262	rVB	178443	236850	5.68%	0.675%
49	15.627	2263	2268	2281	rVB	656658	981333	23.55%	2.799%
50	16.104	2345	2349	2357	rVB	65308	112095	2.69%	0.320%
51	17.157	2524	2528	2537	rVB2	86948	186987	4.49%	0.533%
52	17.627	2603	2608	2617	rVB	83657	171297	4.11%	0.489%

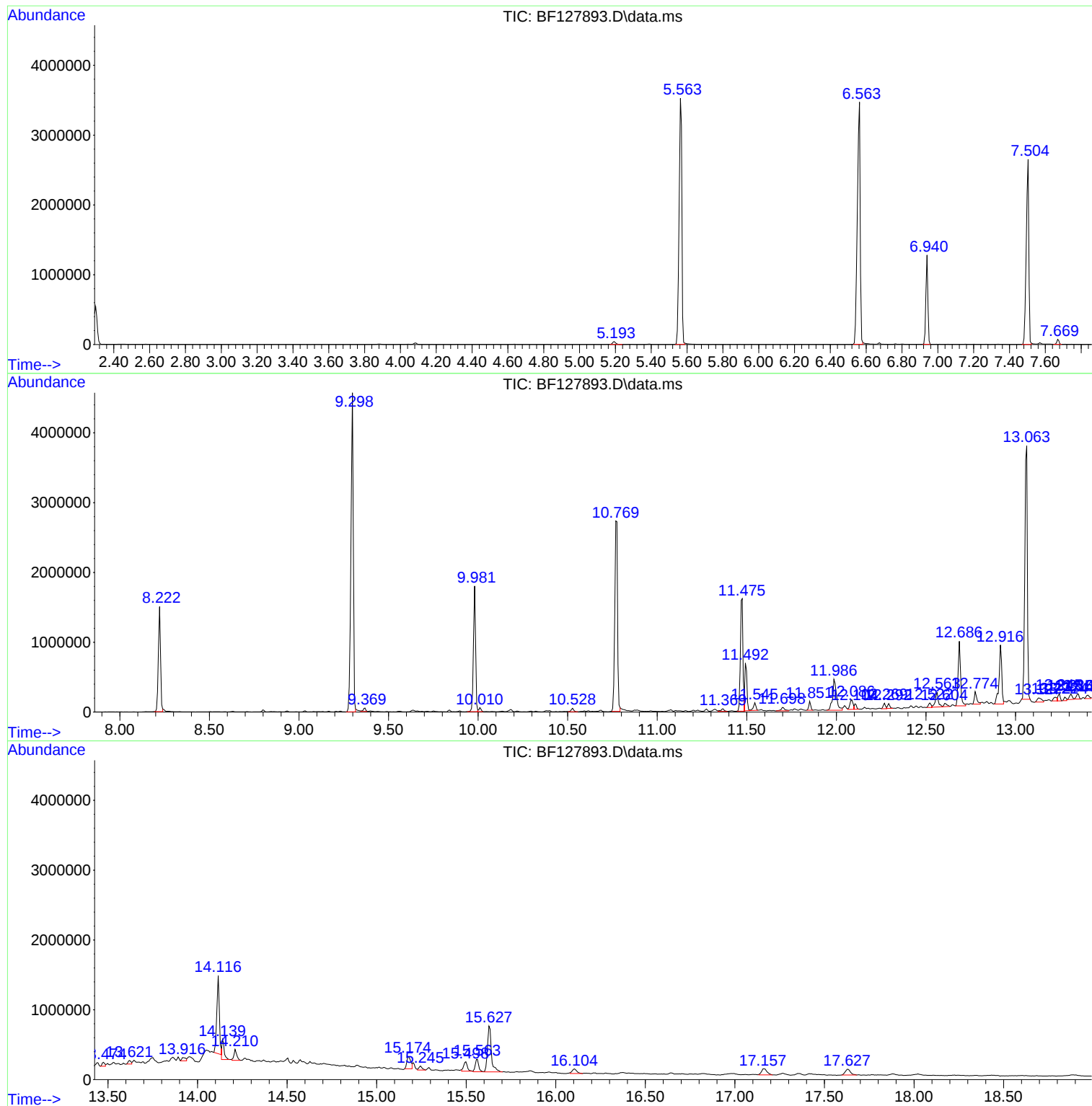
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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BNA_F
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E14ST-EB2-041822-5-10

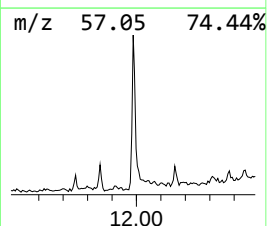
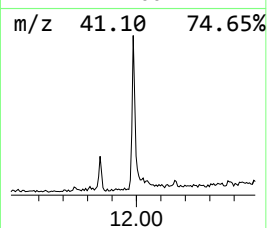
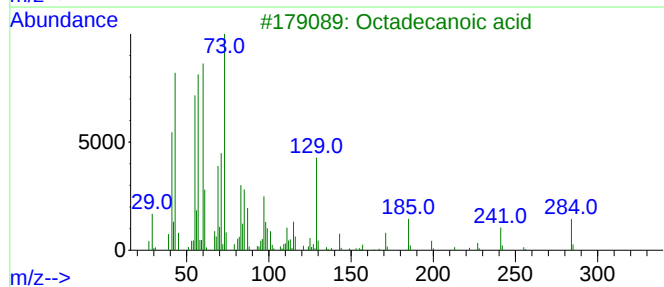
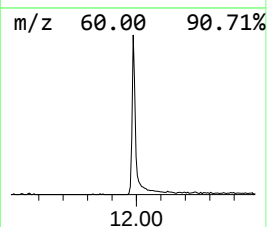
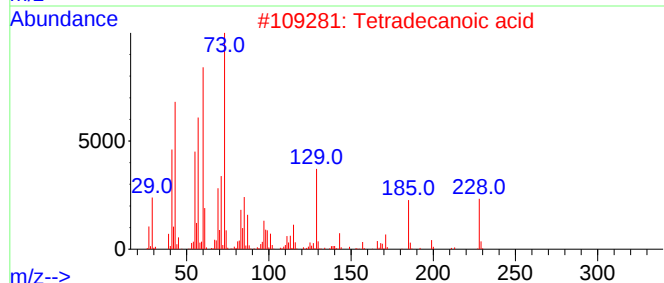
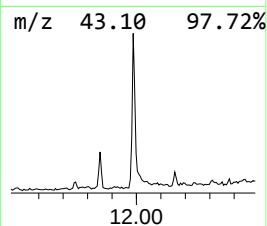
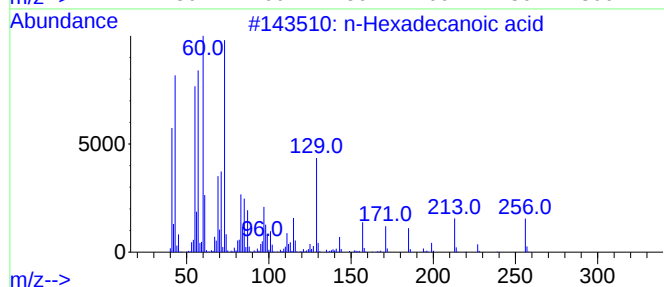
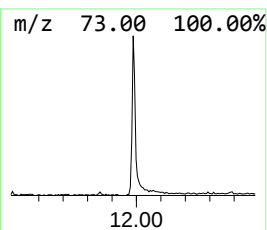
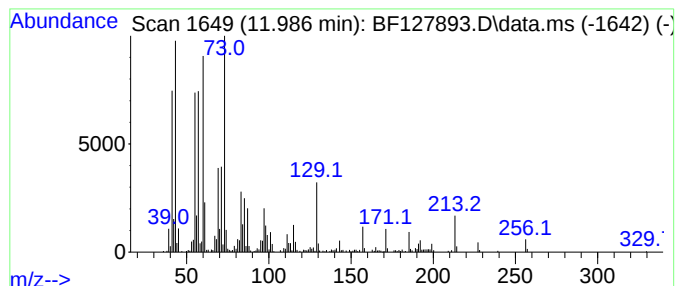
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.986	8.27 ng	665296	Phenanthrene-d10	11.475

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3			Octadecanoic acid	284	C18H36O2	000057-11-4	91
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5			Tridecanoic acid	214	C13H26O2	000638-53-9	90



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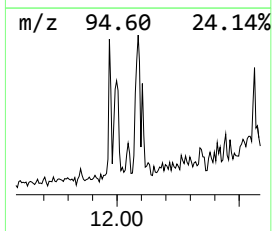
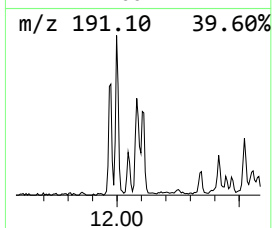
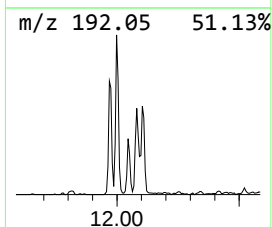
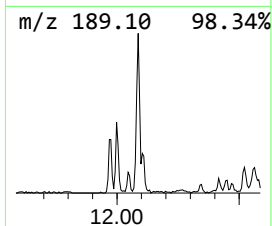
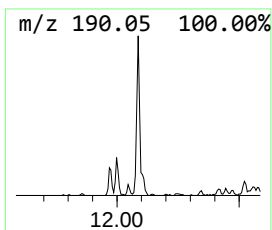
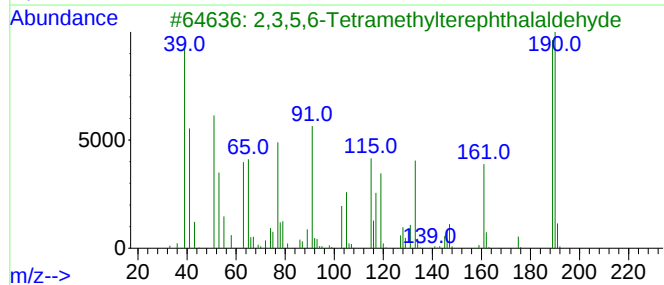
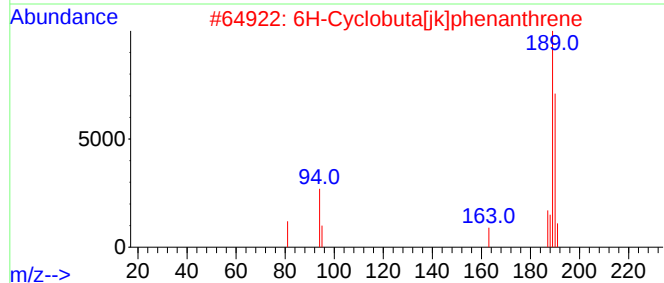
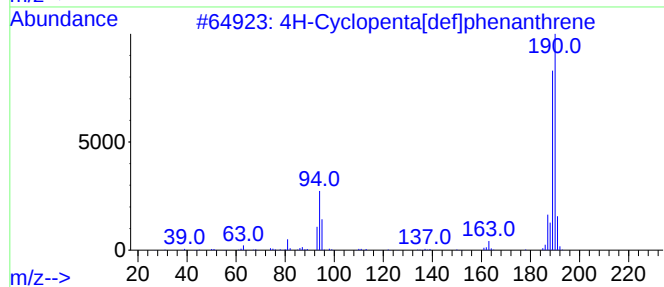
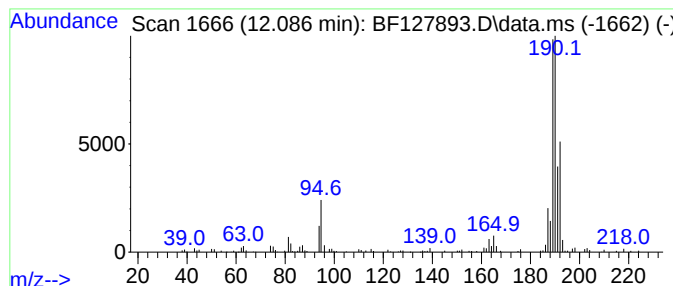
Instrument :
BNA_F
ClientSampleId :
E14ST-EB2-041822-5-10

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.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 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.086	2.13 ng	171069	Phenanthrene-d10	11.475	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	93
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	53
3	2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	43
4	5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	18
5	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	14



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Misc :
ALS Vial : 15 Sample Multiplier: 1

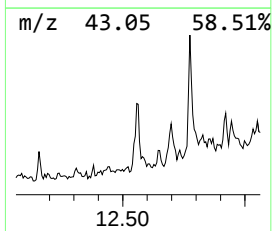
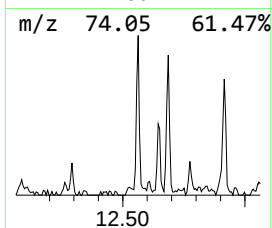
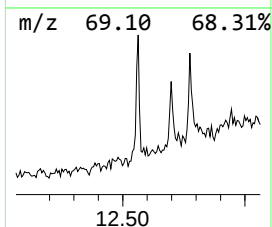
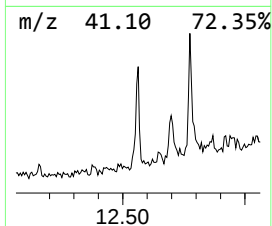
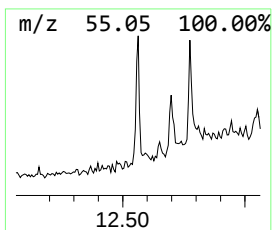
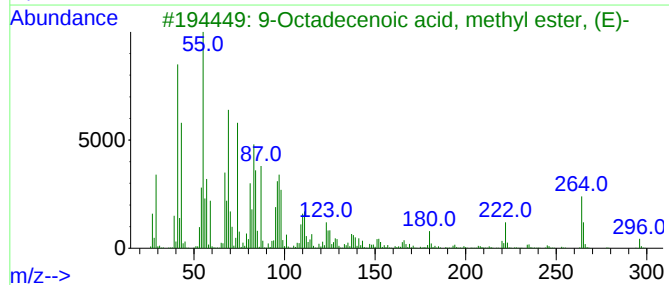
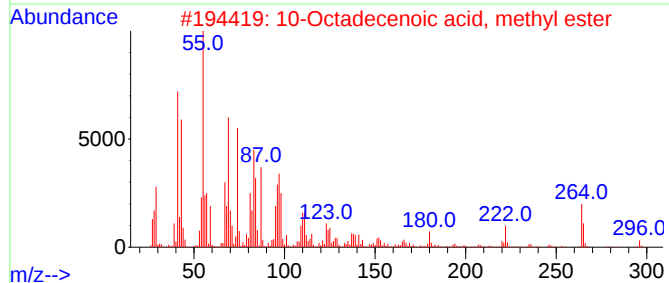
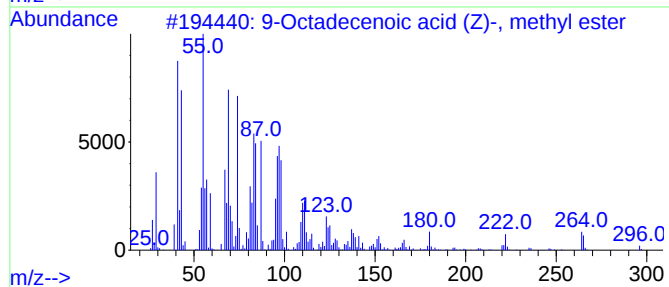
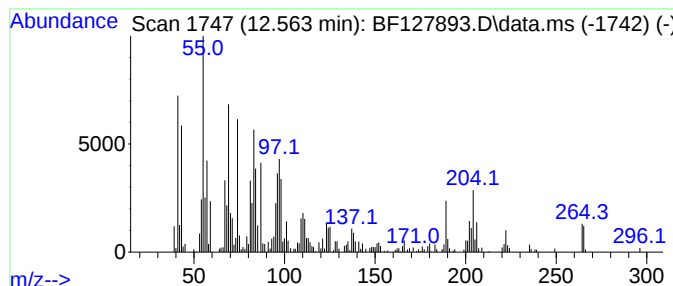
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 9-Octadecenoic acid (Z)-, m... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.563	3.05 ng	245093	Phenanthrene-d10		11.475	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...		296	C19H36O2	000112-62-9	99
2	10-Octadecenoic acid, methyl ester		296	C19H36O2	013481-95-3	99
3	9-Octadecenoic acid, methyl este...		296	C19H36O2	001937-62-8	99
4	8-Octadecenoic acid, methyl ester		296	C19H36O2	002345-29-1	95
5	9-Octadecenoic acid, methyl ester		296	C19H36O2	002462-84-2	95



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Instrument :
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ClientSampleId :
E14ST-EB2-041822-5-10

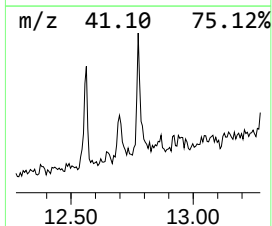
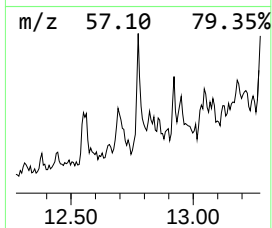
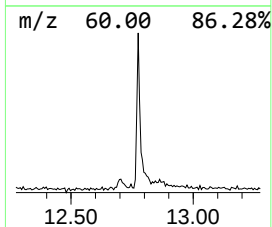
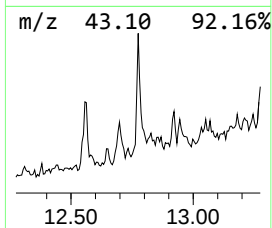
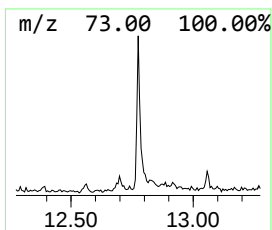
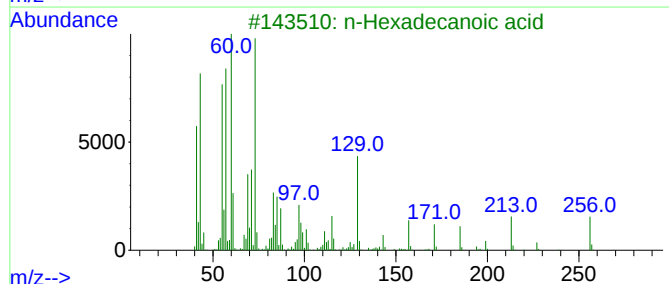
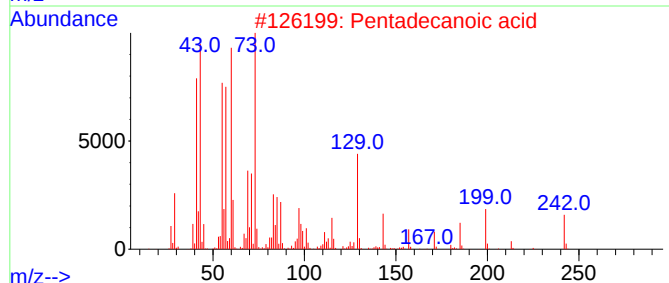
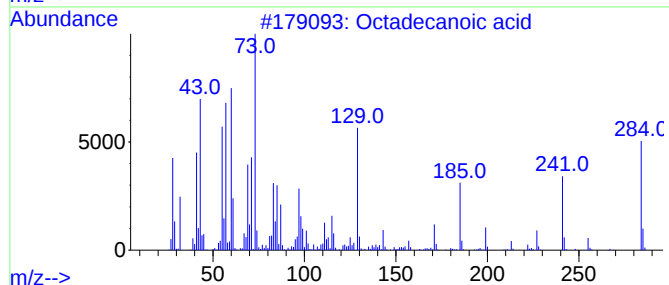
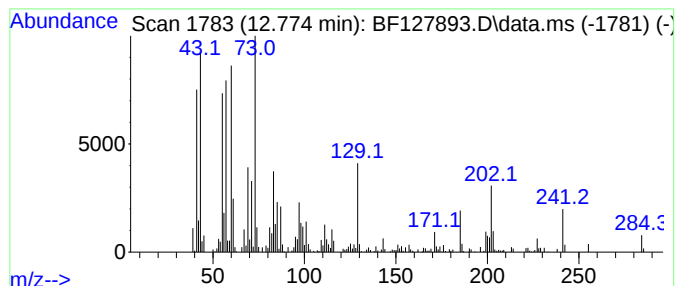
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.775	2.15 ng	173010	Phenanthrene-d10	11.475

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	93
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72



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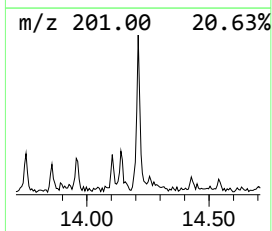
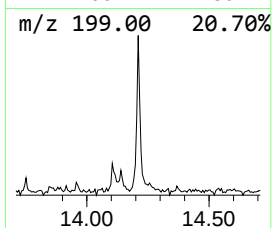
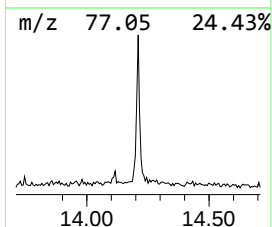
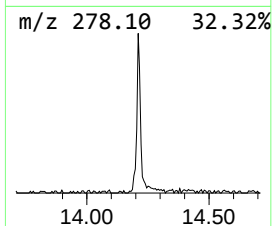
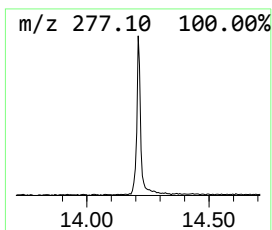
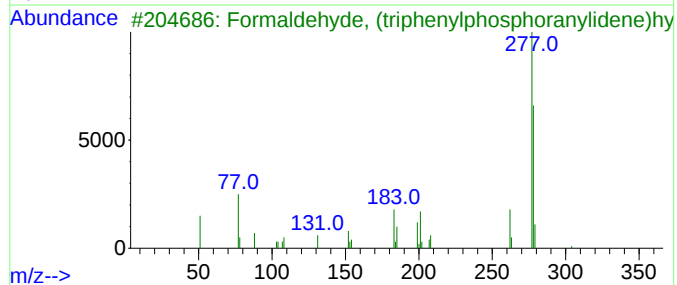
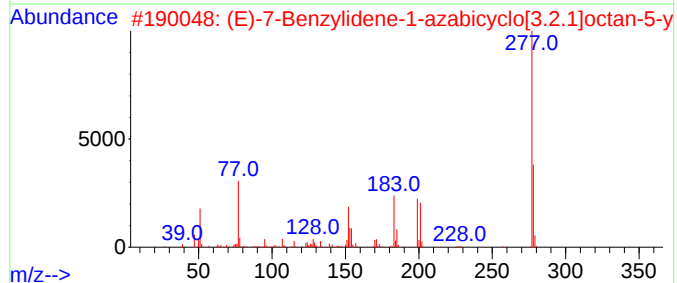
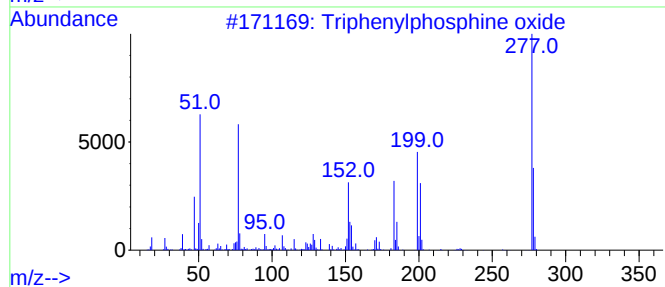
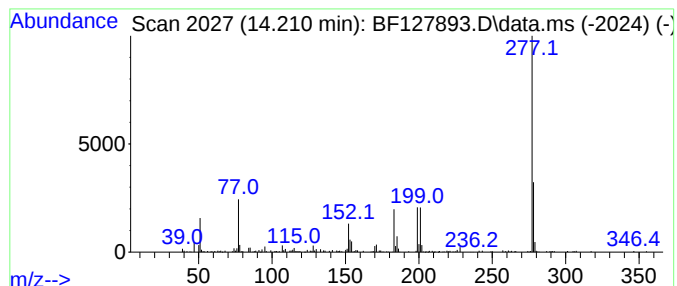
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Triphenylphosphine oxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.210	2.95 ng	165305	Chrysene-d12	14.116

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	83
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	58
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	50
4			(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	37
5			2-Phenyl-6-(trifluoromethyl)-1H-...	277	C15H10F3NO	1000387-59-3	32



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042522\
Data File : BF127893.D
Acq On : 25 Apr 2022 21:18
Operator : CG\JU
Sample : N2466-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
E14ST-EB2-041822-5-10

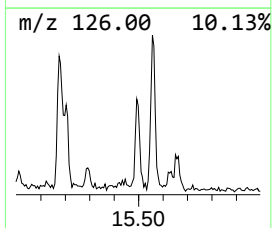
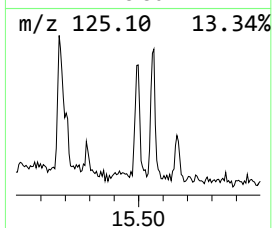
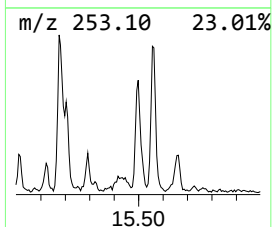
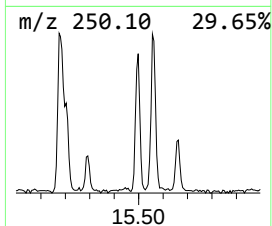
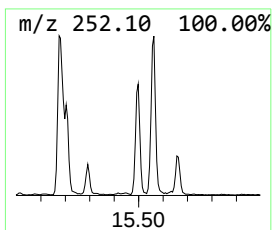
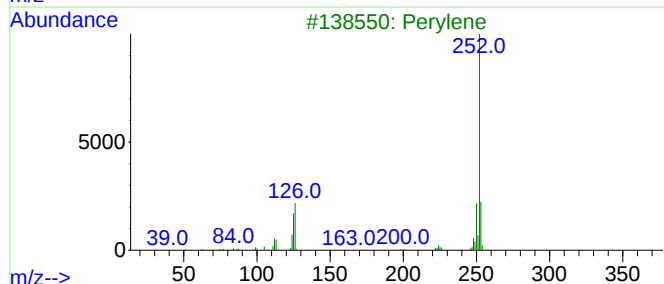
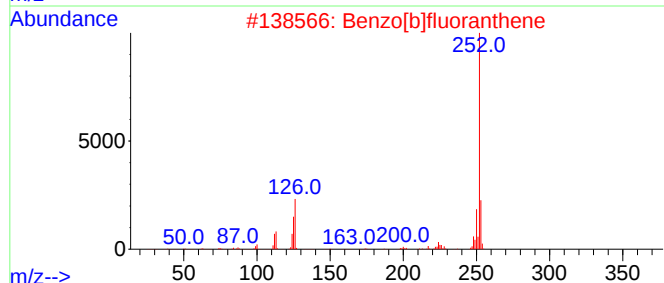
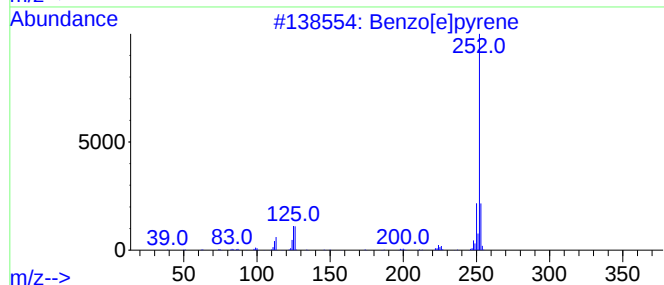
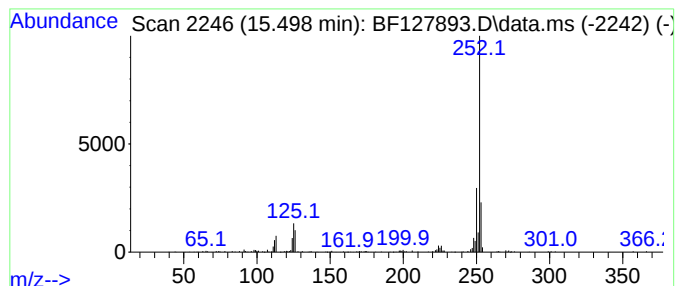
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benzo[e]pyrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.498	3.86 ng	189616	Perylene-d12	15.627

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	97
2			Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
3			Perylene	252	C20H12	000198-55-0	93
4			Benzo[j]fluoranthene	252	C20H12	000205-82-3	93
5			Benzo[k]fluoranthene	252	C20H12	000207-08-9	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042522\
Data File : BF127893.D
Acq On : 25 Apr 2022 21:18
Operator : CG\JU
Sample : N2466-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
E14ST-EB2-041822-5-10

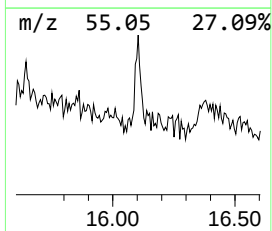
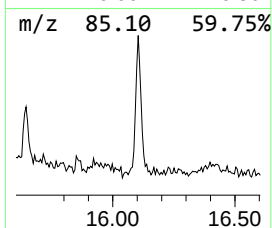
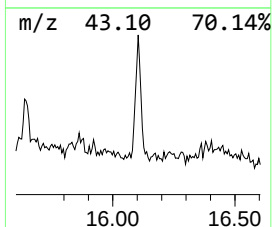
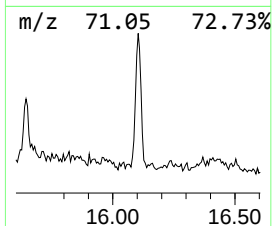
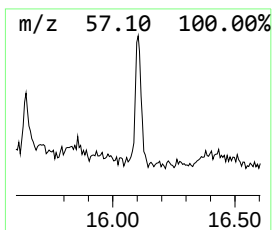
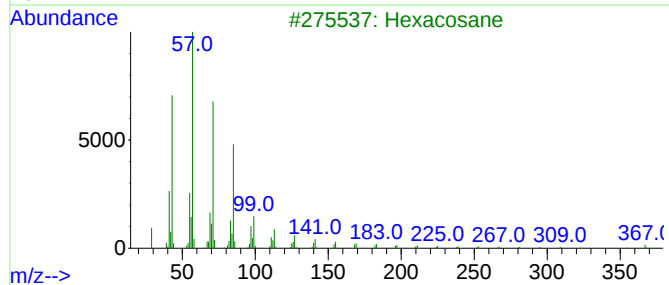
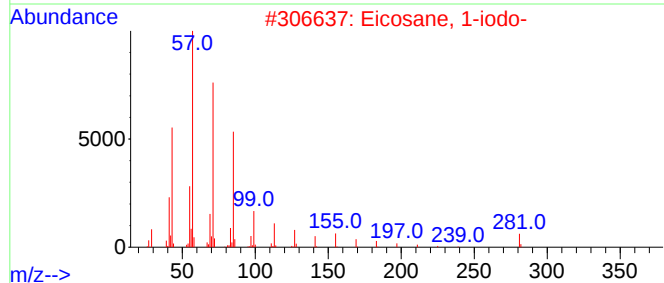
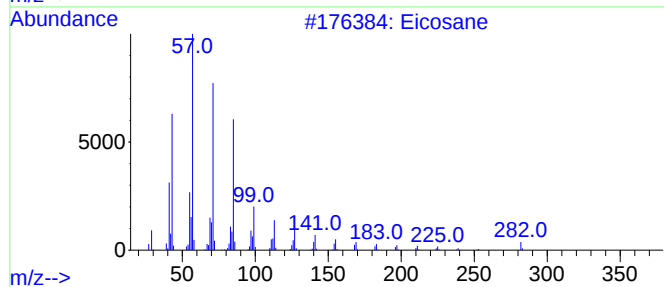
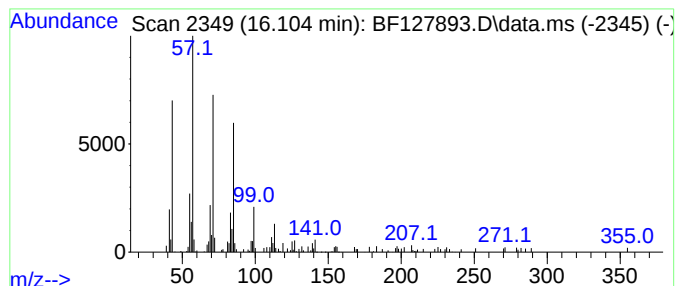
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.104	2.28 ng	112095	Perylene-d12	15.627

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane			282	C20H42	000112-95-8	91
2	Eicosane, 1-iodo-			408	C20H41I	1000406-31-8	87
3	Hexacosane			366	C26H54	000630-01-3	83
4	Docosane, 1-iodo-			436	C22H45I	1000406-31-9	80
5	1,3-Propanediol, ethyl tetradecy...			300	C19H40O2	1000406-35-2	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042522\
Data File : BF127893.D
Acq On : 25 Apr 2022 21:18
Operator : CG\JU
Sample : N2466-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
E14ST-EB2-041822-5-10

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.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
n-Hexadecanoic ...	11.986	8.3	ng	665296	4	11.475	1609490	20.0
4H-Cyclopenta[d]...	12.086	2.1	ng	171069	4	11.475	1609490	20.0
9-Octadecenoic ...	12.563	3.0	ng	245093	4	11.475	1609490	20.0
Octadecanoic acid	12.775	2.1	ng	173010	4	11.475	1609490	20.0
Triphenylphosph...	14.210	3.0	ng	165305	5	14.116	1118860	20.0
Benzo[e]pyrene	15.498	3.9	ng	189616	6	15.627	981333	20.0
Eicosane	16.104	2.3	ng	112095	6	15.627	981333	20.0